



# wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 01:49 AM JST

PDB ID : 8WMW  
EMDB ID : EMD-37660  
Title : The structure of PSI-11CAC at the stationary growth phase  
Authors : Zhang, S.M.; Si, L.; Li, M.  
Deposited on : 2023-10-04  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
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) : 2.39

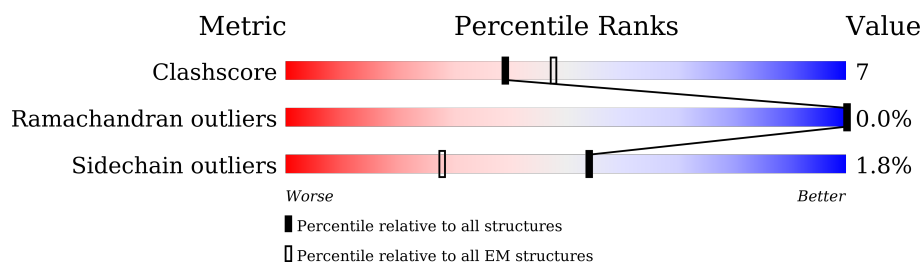
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	752	 88% 11% .
2	B	734	 87% 12%
3	C	81	 85% 14% .
4	D	141	 85% 13% .
5	E	64	 77% 16% . 6%
6	F	188	 79% 7% 14%
7	I	36	 81% 14% 6%
8	J	42	 88% 12%

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Mol	Chain	Length	Quality of chain
9	L	153	
10	M	30	
11	O	146	
12	K	87	
13	c	216	
14	a	216	
15	b	223	
16	h	225	
17	e	203	
18	k	241	
19	f	212	
19	j	212	
20	i	218	
21	d	213	
22	g	255	
23	R	129	

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
24	CLA	A	801	X	-	-	-
24	CLA	A	802	X	-	-	-
24	CLA	A	803	X	-	-	-
24	CLA	A	804	X	-	-	-
24	CLA	A	805	X	-	-	-
24	CLA	A	807	X	-	-	-
24	CLA	A	808	X	-	-	-
24	CLA	A	809	X	-	-	-
24	CLA	A	810	X	-	-	-
24	CLA	A	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	812	X	-	-	-
24	CLA	A	813	X	-	-	-
24	CLA	A	815	X	-	-	-
24	CLA	A	816	X	-	-	-
24	CLA	A	817	X	-	-	-
24	CLA	A	819	X	-	-	-
24	CLA	A	820	X	-	-	-
24	CLA	A	821	X	-	-	-
24	CLA	A	822	X	-	-	-
24	CLA	A	823	X	-	-	-
24	CLA	A	824	X	-	-	-
24	CLA	A	825	X	-	-	-
24	CLA	A	826	X	-	-	-
24	CLA	A	827	X	-	-	-
24	CLA	A	828	X	-	-	-
24	CLA	A	829	X	-	-	-
24	CLA	A	830	X	-	-	-
24	CLA	A	831	X	-	-	-
24	CLA	A	833	X	-	-	-
24	CLA	A	834	X	-	-	-
24	CLA	A	835	X	-	-	-
24	CLA	A	836	X	-	-	-
24	CLA	A	837	X	-	-	-
24	CLA	A	838	X	-	-	-
24	CLA	A	839	X	-	-	-
24	CLA	A	840	X	-	-	-
24	CLA	A	841	X	-	-	-
24	CLA	A	842	X	-	-	-
24	CLA	A	852	X	-	-	-
24	CLA	A	853	X	-	-	-
24	CLA	A	855	X	-	-	-
24	CLA	A	856	X	-	-	-
24	CLA	B	801	X	-	-	-
24	CLA	B	803	X	-	-	-
24	CLA	B	804	X	-	-	-
24	CLA	B	805	X	-	-	-
24	CLA	B	806	X	-	-	-
24	CLA	B	807	X	-	-	-
24	CLA	B	808	X	-	-	-
24	CLA	B	809	X	-	-	-
24	CLA	B	810	X	-	-	-
24	CLA	B	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	812	X	-	-	-
24	CLA	B	813	X	-	-	-
24	CLA	B	814	X	-	-	-
24	CLA	B	815	X	-	-	-
24	CLA	B	816	X	-	-	-
24	CLA	B	818	X	-	-	-
24	CLA	B	821	X	-	-	-
24	CLA	B	822	X	-	-	-
24	CLA	B	823	X	-	-	-
24	CLA	B	824	X	-	-	-
24	CLA	B	825	X	-	-	-
24	CLA	B	826	X	-	-	-
24	CLA	B	827	X	-	-	-
24	CLA	B	829	X	-	-	-
24	CLA	B	830	X	-	-	-
24	CLA	B	831	X	-	-	-
24	CLA	B	832	X	-	-	-
24	CLA	B	833	X	-	-	-
24	CLA	B	834	X	-	-	-
24	CLA	B	835	X	-	-	-
24	CLA	B	836	X	-	-	-
24	CLA	B	837	X	-	-	-
24	CLA	B	838	X	-	-	-
24	CLA	B	839	X	-	-	-
24	CLA	F	201	X	-	-	-
24	CLA	F	202	X	-	-	-
24	CLA	I	102	X	-	-	-
24	CLA	J	103	X	-	-	-
24	CLA	J	105	X	-	-	-
24	CLA	K	101	X	-	-	-
24	CLA	K	102	X	-	-	-
24	CLA	L	202	X	-	-	-
24	CLA	L	203	X	-	-	-
24	CLA	L	204	X	-	-	-
24	CLA	L	207	X	-	-	-
24	CLA	O	201	X	-	-	-
24	CLA	O	205	X	-	-	-
24	CLA	R	203	X	-	-	-
24	CLA	a	302	X	-	-	-
24	CLA	a	303	X	-	-	-
24	CLA	a	304	X	-	-	-
24	CLA	a	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	a	306	X	-	-	-
24	CLA	a	307	X	-	-	-
24	CLA	a	308	X	-	-	-
24	CLA	a	309	X	-	-	-
24	CLA	a	310	X	-	-	-
24	CLA	a	311	X	-	-	-
24	CLA	a	312	X	-	-	-
24	CLA	b	303	X	-	-	-
24	CLA	b	304	X	-	-	-
24	CLA	b	305	X	-	-	-
24	CLA	b	307	X	-	-	-
24	CLA	b	308	X	-	-	-
24	CLA	b	309	X	-	-	-
24	CLA	b	310	X	-	-	-
24	CLA	b	311	X	-	-	-
24	CLA	b	312	X	-	-	-
24	CLA	b	313	X	-	-	-
24	CLA	c	601	X	-	-	-
24	CLA	c	602	X	-	-	-
24	CLA	c	603	X	-	-	-
24	CLA	c	604	X	-	-	-
24	CLA	c	605	X	-	-	-
24	CLA	c	607	X	-	-	-
24	CLA	c	608	X	-	-	-
24	CLA	c	609	X	-	-	-
24	CLA	c	611	X	-	-	-
24	CLA	c	612	X	-	-	-
24	CLA	d	301	X	-	-	-
24	CLA	d	302	X	-	-	-
24	CLA	d	303	X	-	-	-
24	CLA	d	304	X	-	-	-
24	CLA	d	306	X	-	-	-
24	CLA	d	307	X	-	-	-
24	CLA	d	308	X	-	-	-
24	CLA	d	309	X	-	-	-
24	CLA	e	601	X	-	-	-
24	CLA	e	602	X	-	-	-
24	CLA	e	603	X	-	-	-
24	CLA	e	604	X	-	-	-
24	CLA	e	605	X	-	-	-
24	CLA	e	606	X	-	-	-
24	CLA	e	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	e	608	X	-	-	-
24	CLA	e	611	X	-	-	-
24	CLA	f	601	X	-	-	-
24	CLA	f	602	X	-	-	-
24	CLA	f	603	X	-	-	-
24	CLA	f	607	X	-	-	-
24	CLA	f	608	X	-	-	-
24	CLA	f	609	X	-	-	-
24	CLA	f	610	X	-	-	-
24	CLA	f	612	X	-	-	-
24	CLA	f	613	X	-	-	-
24	CLA	g	302	X	-	-	-
24	CLA	g	303	X	-	-	-
24	CLA	g	304	X	-	-	-
24	CLA	g	305	X	-	-	-
24	CLA	g	306	X	-	-	-
24	CLA	g	307	X	-	-	-
24	CLA	g	308	X	-	-	-
24	CLA	g	309	X	-	-	-
24	CLA	g	310	X	-	-	-
24	CLA	g	311	X	-	-	-
24	CLA	g	315	X	-	-	-
24	CLA	g	322	X	-	-	-
24	CLA	h	301	X	-	-	-
24	CLA	h	302	X	-	-	-
24	CLA	h	303	X	-	-	-
24	CLA	h	304	X	-	-	-
24	CLA	h	305	X	-	-	-
24	CLA	h	306	X	-	-	-
24	CLA	h	307	X	-	-	-
24	CLA	h	312	X	-	-	-
24	CLA	i	601	X	-	-	-
24	CLA	i	602	X	-	-	-
24	CLA	i	603	X	-	-	-
24	CLA	i	604	X	-	-	-
24	CLA	i	605	X	-	-	-
24	CLA	i	606	X	-	-	-
24	CLA	i	607	X	-	-	-
24	CLA	i	608	X	-	-	-
24	CLA	i	610	X	-	-	-
24	CLA	i	611	X	-	-	-
24	CLA	j	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	j	303	X	-	-	-
24	CLA	j	304	X	-	-	-
24	CLA	j	306	X	-	-	-
24	CLA	j	307	X	-	-	-
24	CLA	j	308	X	-	-	-
24	CLA	j	309	X	-	-	-
24	CLA	j	310	X	-	-	-
24	CLA	j	311	X	-	-	-
24	CLA	j	313	X	-	-	-
24	CLA	j	314	X	-	-	-
24	CLA	k	601	X	-	-	-
24	CLA	k	602	X	-	-	-
24	CLA	k	603	X	-	-	-
24	CLA	k	604	X	-	-	-
24	CLA	k	605	X	-	-	-
24	CLA	k	607	X	-	-	-
24	CLA	k	608	X	-	-	-
24	CLA	k	609	X	-	-	-
24	CLA	k	610	X	-	-	-
29	SF4	A	854	-	-	X	-
29	SF4	C	101	-	-	X	-
29	SF4	C	102	-	-	X	-

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 51054 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	742	Total	C	N	O	S	0	0
			5825	3802	994	1001	28		

- 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	1	0
			5826	3844	982	985	15		

- 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
			592	361	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1084	692	186	203	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	60	Total	C	N	O	0	0
			485	309	84	92		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1254	814	212	226	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			264	182	35	45	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	S	0	0
			351	240	49	59	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	151	Total	C	N	O	S	0	0
			1146	753	182	208	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			232	155	38	38	1		

- Molecule 11 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	104	Total	C	N	O	S	0	0
			773	515	117	138	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	69	Total	C	N	O	S	0	0
			488	319	80	87	2		

- Molecule 13 is a protein called CAC-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	170	Total	C	N	O	S	0	0
			1357	897	221	236	3		

- Molecule 14 is a protein called CAC-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	175	Total	C	N	O	S	0	0
			1361	889	217	245	10		

- Molecule 15 is a protein called CAC-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	b	194	Total	C	N	O	S	0	0
			1439	916	251	258	14		

- Molecule 16 is a protein called CAC-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	162	Total	C	N	O	S	0	0
			1200	778	202	214	6		

- Molecule 17 is a protein called CAC-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	169	Total	C	N	O	S	0	0
			1286	843	207	228	8		

- Molecule 18 is a protein called CAC-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	180	Total	C	N	O	S	0	0
			1346	872	223	239	12		

- Molecule 19 is a protein called CAC-f.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	174	Total	C	N	O	S	0	0
			1302	842	212	240	8		
19	j	172	Total	C	N	O	S	0	0
			1293	834	212	239	8		

- Molecule 20 is a protein called CAC-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	175	Total	C	N	O	S	0	0
			1324	849	227	237	11		

- Molecule 21 is a protein called CAC-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	126	Total	C	N	O	S	0	0
			950	609	165	167	9		

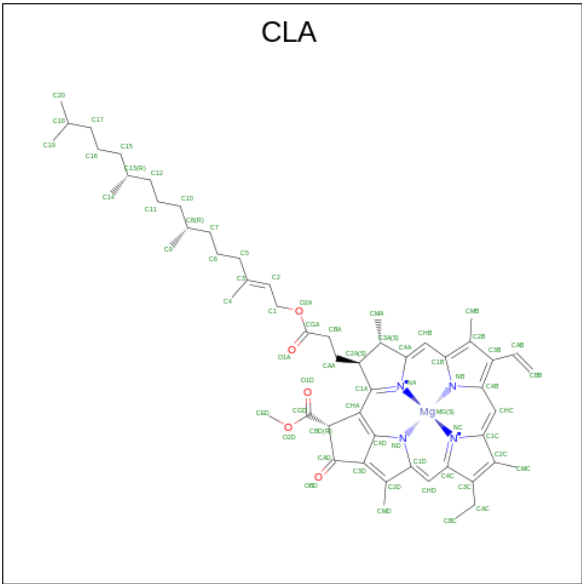
- Molecule 22 is a protein called CAC-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	219	Total	C	N	O	S	0	0
			1630	1060	267	292	11		

- Molecule 23 is a protein called PsarR.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	90	Total	C	N	O	S	0	0
			664	434	105	124	1		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	J	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	L	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	K	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	K	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	c	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	c	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	c	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	a	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	e	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	k	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	k	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	f	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	f	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	i	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 61	C 51	Mg 1	N 4	O 5	0

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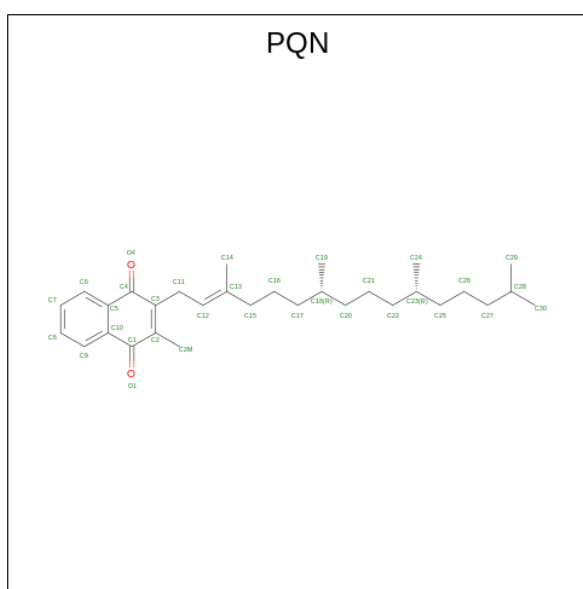
Mol	Chain	Residues	Atoms					AltConf
24	j	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	d	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	d	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	d	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	g	1	Total 51	C 41	Mg 1	N 4	O 5	0

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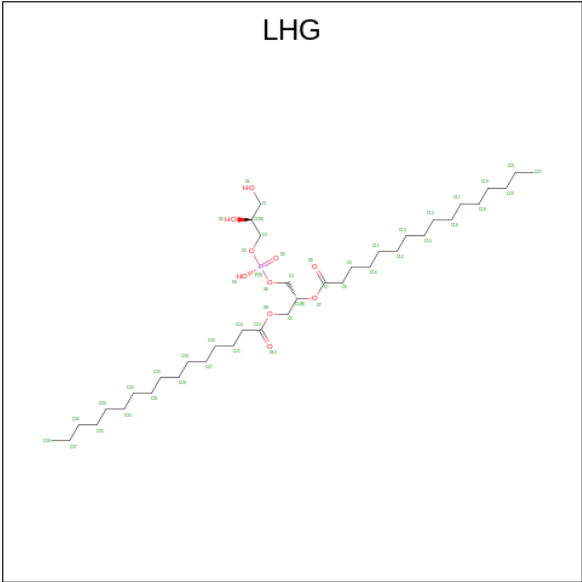
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	R	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

- Molecule 25 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



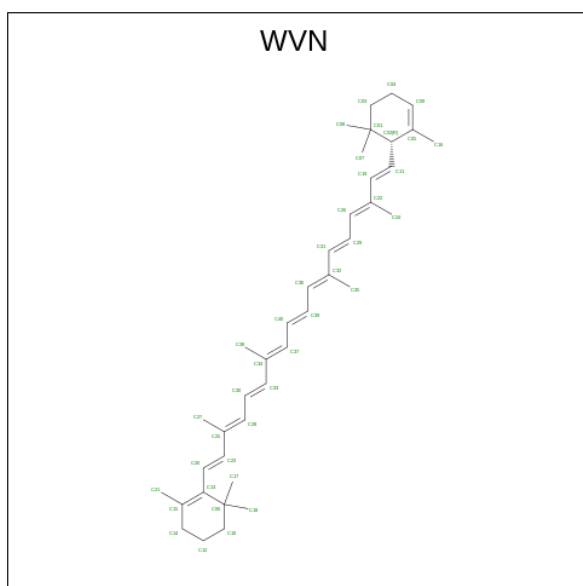
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			48	37	10	1	
26	A	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			38	27	10	1	
26	J	1	Total	C	O	P	0
			49	38	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	c	1	Total	C	O	P	0
			37	26	10	1	
26	a	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	b	1	Total	C	O	P	0
			49	38	10	1	
26	e	1	Total	C	O	P	0
			37	26	10	1	
26	k	1	Total	C	O	P	0
			37	26	10	1	
26	f	1	Total	C	O	P	0
			37	26	10	1	
26	f	1	Total	C	O	P	0
			49	38	10	1	
26	i	1	Total	C	O	P	0
			37	26	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	j	1	Total	C	O	P	0
			30	19	10	1	
26	d	1	Total	C	O	P	0
			37	26	10	1	
26	g	1	Total	C	O	P	0
			49	38	10	1	
26	g	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 27 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (three-letter code: WVN) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	A	1	Total	C	0
			40	40	
27	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	F	1	Total C 40 40	0
27	I	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	J	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	L	1	Total C 40 40	0
27	M	1	Total C 40 40	0
27	K	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	e	1	Total C 40 40	0
27	j	1	Total C 40 40	0
27	R	1	Total C 40 40	0
27	R	1	Total C 40 40	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



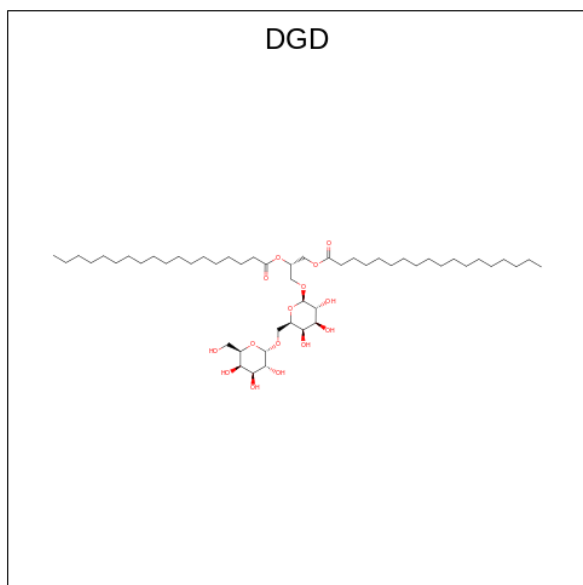
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total 35	C 24	O 11	0
28	F	1	Total 24	C 18	O 6	0
28	a	1	Total 35	C 24	O 11	0
28	b	1	Total 24	C 18	O 6	0

- Molecule 29 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

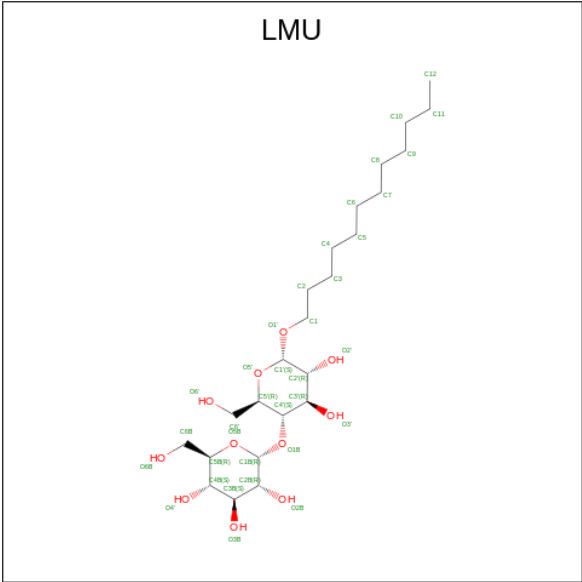
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			60	45	15	

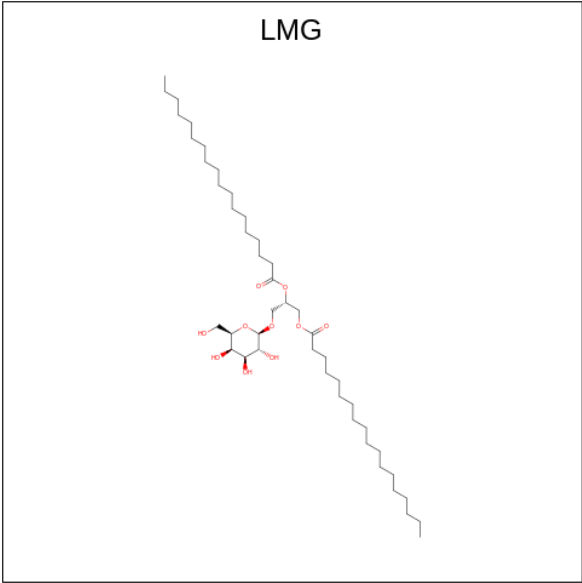
- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).





Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			35	24	11	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



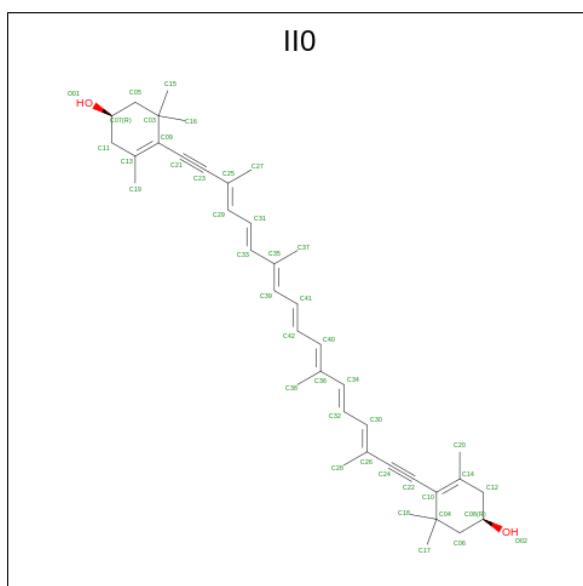
Mol	Chain	Residues	Atoms			AltConf
32	F	1	Total	C	O	0
			48	38	10	
32	J	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
32	L	1	Total	C	O	0
			55	45	10	
32	O	1	Total	C	O	0
			26	16	10	
32	b	1	Total	C	O	0
			55	45	10	

- Molecule 33 is (1 {R})-3,5,5-trimethyl-4-[(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-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (three-letter code: II0) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
33	J	1	Total	C	O	0
			42	40	2	
33	O	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	c	1	Total	C	O	0
			42	40	2	
33	a	1	Total	C	O	0
			42	40	2	
33	a	1	Total	C	O	0
			42	40	2	

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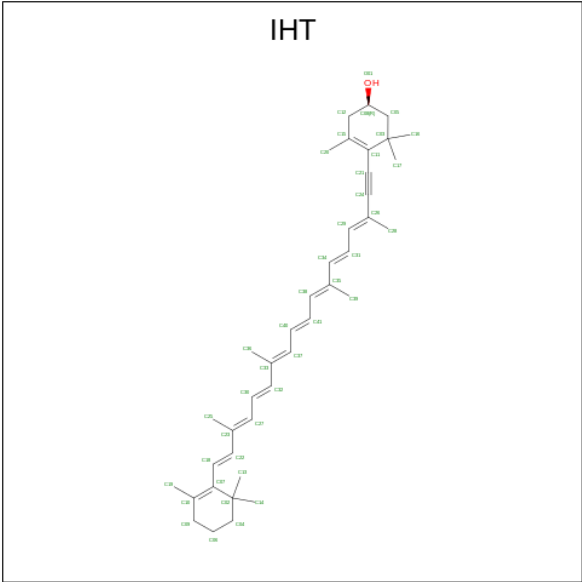
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total 42	C 40	O 2	0
33	a	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	b	1	Total 42	C 40	O 2	0
33	h	1	Total 28	C 27	O 1	0
33	h	1	Total 42	C 40	O 2	0
33	h	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	e	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	k	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0
33	f	1	Total 42	C 40	O 2	0

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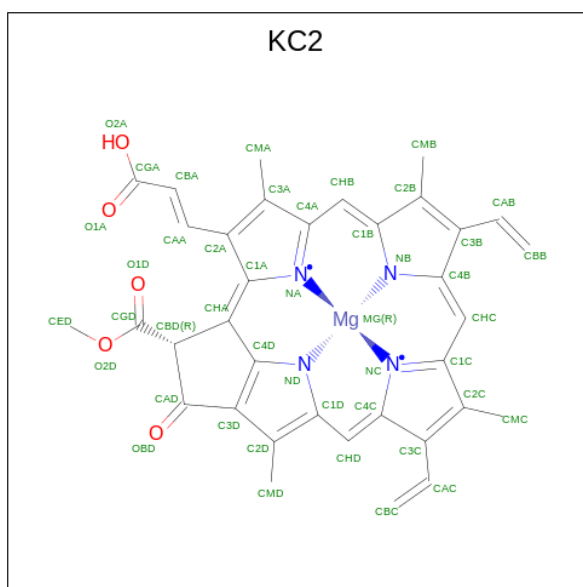
Mol	Chain	Residues	Atoms			AltConf
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	i	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	j	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	d	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	
33	g	1	Total	C	O	0
			42	40	2	

- Molecule 34 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: IHT) (formula: C<sub>40</sub>H<sub>54</sub>O).



Mol	Chain	Residues	Atoms			AltConf
34	O	1	Total	C	O	0
			41	40	1	
34	c	1	Total	C	O	0
			41	40	1	
34	a	1	Total	C	O	0
			41	40	1	
34	b	1	Total	C	O	0
			41	40	1	
34	b	1	Total	C	O	0
			41	40	1	
34	k	1	Total	C	O	0
			41	40	1	
34	f	1	Total	C	O	0
			41	40	1	
34	j	1	Total	C	O	0
			41	40	1	
34	g	1	Total	C	O	0
			41	40	1	
34	R	1	Total	C	O	0
			41	40	1	

- Molecule 35 is Chlorophyll c2 (three-letter code: KC2) (formula: C<sub>35</sub>H<sub>28</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0

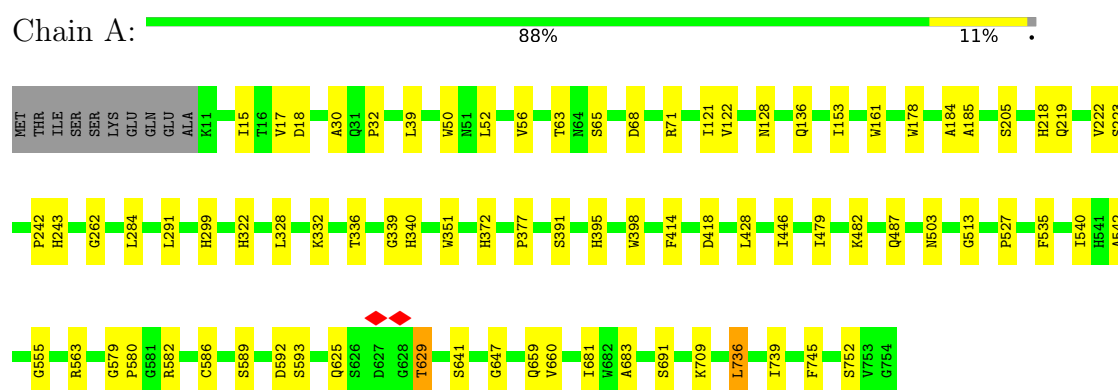
- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	50	Total 50	O 50	0
36	B	59	Total 59	O 59	0
36	C	7	Total 7	O 7	0
36	D	1	Total 1	O 1	0
36	F	3	Total 3	O 3	0
36	I	1	Total 1	O 1	0
36	J	1	Total 1	O 1	0
36	L	1	Total 1	O 1	0
36	O	1	Total 1	O 1	0
36	K	1	Total 1	O 1	0
36	a	1	Total 1	O 1	0
36	b	1	Total 1	O 1	0
36	h	1	Total 1	O 1	0
36	e	4	Total 4	O 4	0

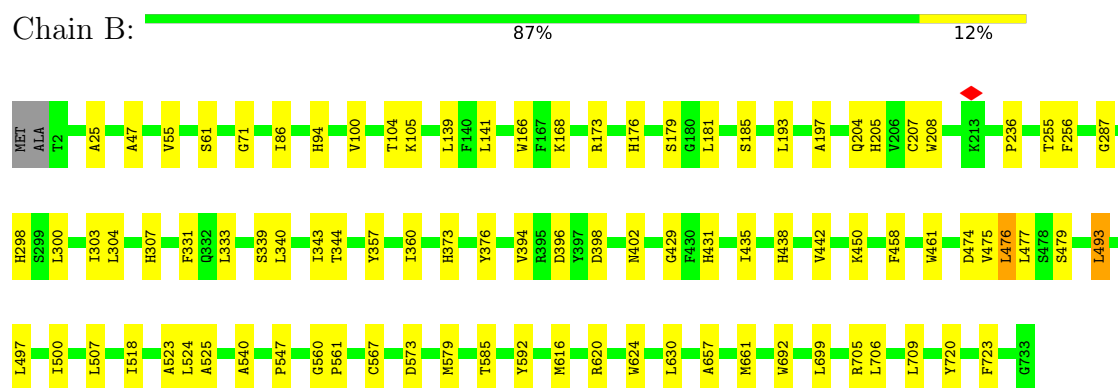
### 3 Residue-property plots

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

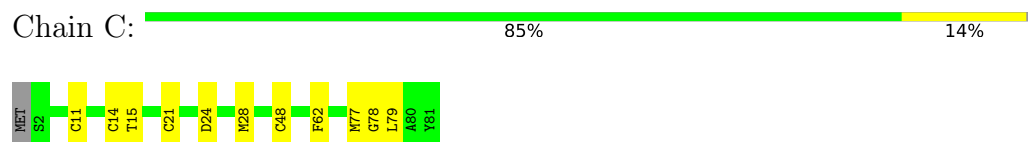
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2




- Molecule 3: Photosystem I iron-sulfur center




- Molecule 4: Photosystem I reaction center subunit II

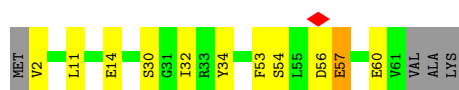


Chain D:  85% 13%




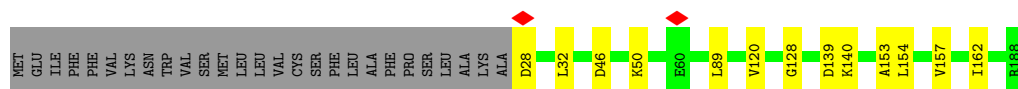
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  77% 16% 6%




- Molecule 6: Photosystem I reaction center subunit III

Chain F:  79% 7% 14%




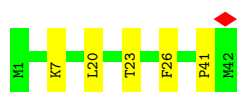
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  81% 14% 6%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  88% 12%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L:  92% 6% ..

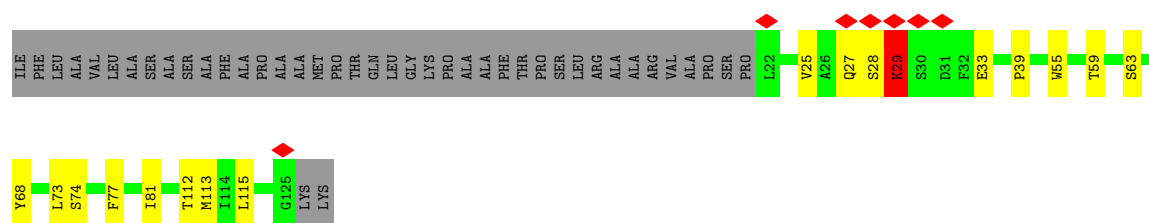


- Molecule 10: Photosystem I reaction center subunit XII

Chain M:  90% 10%



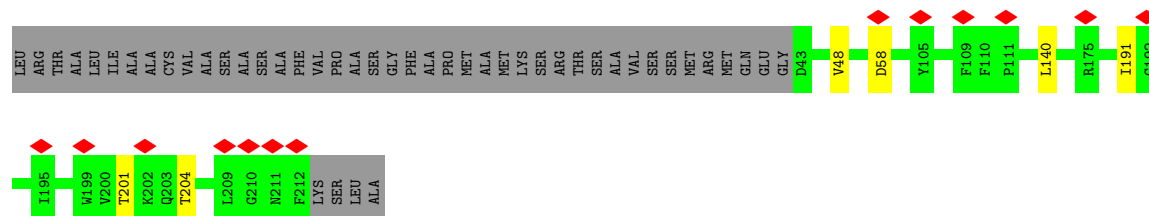
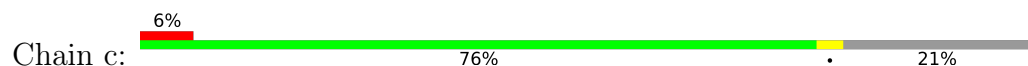
- Molecule 11: PsaO



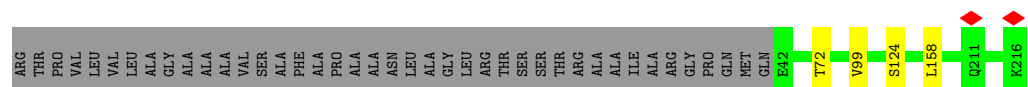
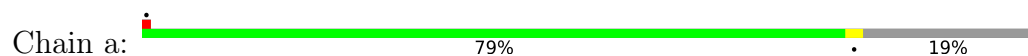
• Molecule 12: Photosystem I reaction center subunit PsaK



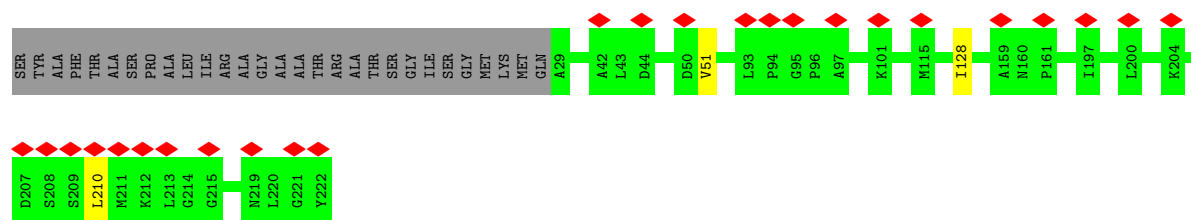
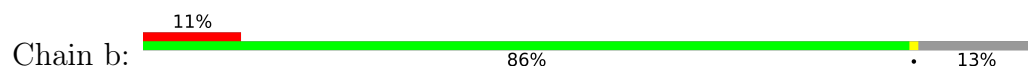
• Molecule 13: CAC-c



• Molecule 14: CAC-a



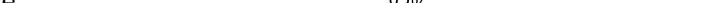
• Molecule 15: CAC-b

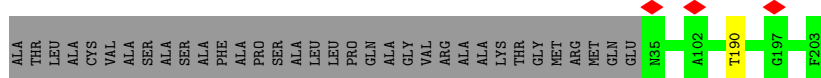


• Molecule 16: CAC-h

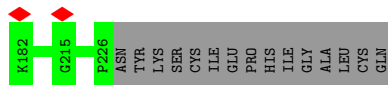
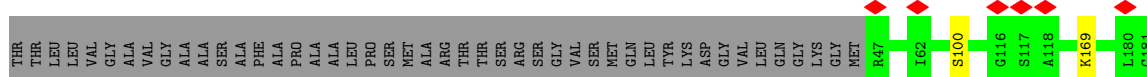




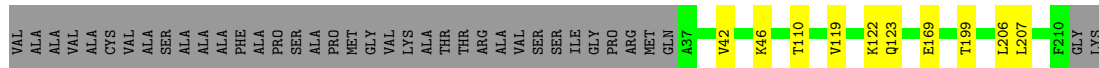
Chain e:  83% 17%

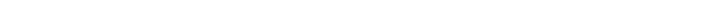


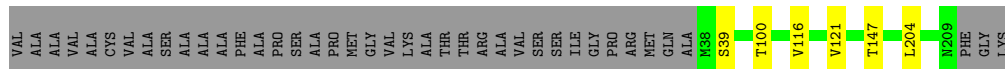
Chain k:  74% 25%

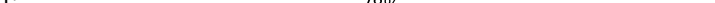


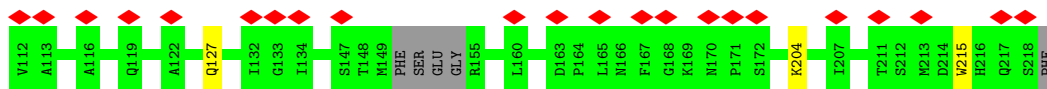
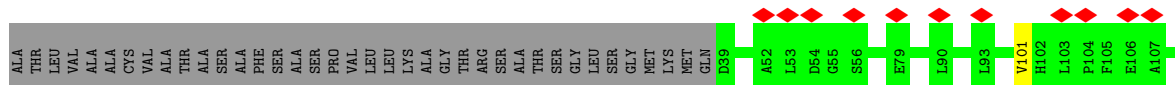
Chain f:  77% 5% 18%

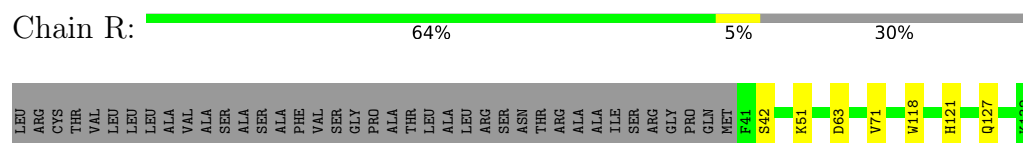


Chain j:  78% 19%



Chain i:  15% 78% 20%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31215	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	332.8131, 332.8131, 332.8131	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.040041, 1.040041, 1.040041	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WVN, SF4, DGD, IHT, LMU, PQN, CLA, LMG, LHG, LMT, KC2, II0

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	0.52	0/6019	0.57	0/8204
2	B	0.52	0/6045	0.59	0/8254
3	C	0.49	0/601	0.59	0/813
4	D	0.48	0/1109	0.57	0/1500
5	E	0.50	0/493	0.54	0/667
6	F	0.48	0/1287	0.58	0/1747
7	I	0.49	0/271	0.60	0/370
8	J	0.52	0/364	0.62	0/495
9	L	0.48	0/1175	0.56	0/1599
10	M	0.40	0/233	0.54	0/315
11	O	0.54	0/799	0.61	0/1094
12	K	0.41	0/495	0.59	0/672
13	c	0.39	0/1396	0.52	0/1889
14	a	0.39	0/1406	0.49	0/1903
15	b	0.38	0/1469	0.58	0/1983
16	h	0.41	0/1226	0.54	0/1667
17	e	0.40	0/1324	0.55	0/1795
18	k	0.43	0/1380	0.56	0/1869
19	f	0.45	0/1328	0.55	0/1790
19	j	0.41	0/1318	0.56	0/1775
20	i	0.36	0/1359	0.60	0/1835
21	d	0.47	0/969	0.54	0/1304
22	g	0.41	0/1673	0.56	0/2264
23	R	0.44	0/686	0.52	0/940
All	All	0.47	0/34425	0.57	0/46744

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5678	64	0
2	B	5826	0	5642	70	0
3	C	592	0	574	12	0
4	D	1084	0	1080	11	0
5	E	485	0	489	7	0
6	F	1254	0	1264	10	0
7	I	264	0	276	4	0
8	J	351	0	344	4	0
9	L	1146	0	1160	8	0
10	M	232	0	265	3	0
11	O	773	0	763	15	0
12	K	488	0	516	3	0
13	c	1357	0	1337	0	0
14	a	1361	0	1305	0	0
15	b	1439	0	1456	0	0
16	h	1200	0	1228	0	0
17	e	1286	0	1262	0	0
18	k	1346	0	1349	0	0
19	f	1302	0	1320	0	0
19	j	1293	0	1321	0	0
20	i	1324	0	1298	0	0
21	d	950	0	949	0	0
22	g	1630	0	1644	0	0
23	R	664	0	647	5	0
24	A	2758	0	2820	103	0
24	B	2403	0	2442	88	0
24	F	117	0	115	5	0
24	I	65	0	72	2	0
24	J	93	0	72	4	0
24	K	93	0	72	2	0
24	L	215	0	191	8	0
24	O	130	0	144	9	0
24	R	51	0	41	1	0
24	a	601	0	551	0	0
24	b	673	0	696	0	0
24	c	586	0	520	0	0
24	d	498	0	407	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	e	582	0	578	0	0
24	f	700	0	695	0	0
24	g	661	0	611	0	0
24	h	440	0	398	0	0
24	i	528	0	451	0	0
24	j	637	0	556	0	0
24	k	596	0	534	0	0
25	A	33	0	46	2	0
25	B	33	0	46	5	0
26	A	75	0	93	3	0
26	B	38	0	49	3	0
26	J	49	0	74	5	0
26	a	49	0	74	0	0
26	b	98	0	148	0	0
26	c	74	0	88	0	0
26	d	37	0	44	0	0
26	e	37	0	44	0	0
26	f	86	0	118	0	0
26	g	86	0	118	0	0
26	i	37	0	44	0	0
26	j	30	0	30	0	0
26	k	37	0	44	0	0
27	A	200	0	0	0	0
27	B	200	0	0	0	0
27	F	80	0	0	0	0
27	I	40	0	0	0	0
27	J	80	0	0	0	0
27	K	40	0	0	0	0
27	L	120	0	0	0	0
27	M	40	0	0	0	0
27	R	80	0	0	0	0
27	e	40	0	0	0	0
27	h	40	0	0	0	0
27	j	40	0	0	0	0
28	A	35	0	42	1	0
28	F	24	0	33	0	0
28	a	35	0	45	0	0
28	b	24	0	34	0	0
29	A	8	0	0	4	0
29	C	16	0	0	7	0
30	B	60	0	81	3	0
31	B	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	F	48	0	69	2	0
32	J	55	0	86	3	0
32	L	55	0	86	2	0
32	O	26	0	22	0	0
32	b	55	0	86	0	0
33	J	42	0	0	0	0
33	O	42	0	0	0	0
33	a	168	0	0	0	0
33	b	126	0	0	0	0
33	c	126	0	0	0	0
33	d	126	0	0	0	0
33	e	168	0	0	0	0
33	f	168	0	0	0	0
33	g	168	0	0	0	0
33	h	112	0	0	0	0
33	i	126	0	0	0	0
33	j	126	0	0	0	0
33	k	210	0	0	0	0
34	O	41	0	0	0	0
34	R	41	0	0	0	0
34	a	41	0	0	0	0
34	b	82	0	0	0	0
34	c	41	0	0	0	0
34	f	41	0	0	0	0
34	g	41	0	0	0	0
34	j	41	0	0	0	0
34	k	41	0	0	0	0
35	c	45	0	0	0	0
35	d	90	0	0	0	0
35	e	45	0	0	0	0
35	f	45	0	0	0	0
35	g	135	0	0	0	0
35	i	90	0	0	0	0
35	j	45	0	0	0	0
35	k	135	0	0	0	0
36	A	50	0	0	0	0
36	B	59	0	0	1	0
36	C	7	0	0	0	0
36	D	1	0	0	0	0
36	F	3	0	0	0	0
36	I	1	0	0	0	0
36	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	O	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	0	0
36	e	4	0	0	0	0
36	h	1	0	0	0	0
All	All	51054	0	46823	364	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 7.

The worst 5 of 364 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)
1:A:586:CYS:HG	29:A:854:SF4:FE2	0.77	0.96
3:C:48:CYS:HG	29:C:101:SF4:FE4	0.73	0.96
3:C:14:CYS:HG	29:C:102:SF4:FE3	0.74	0.95
3:C:11:CYS:HG	29:C:102:SF4:FE4	0.66	0.94
2:B:438:HIS:HE1	24:B:829:CLA:NA	1.62	0.92

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	740/752 (98%)	723 (98%)	17 (2%)	0	100	100
2	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	137/141 (97%)	135 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	58/64 (91%)	55 (95%)	3 (5%)	0	100	100
6	F	159/188 (85%)	155 (98%)	4 (2%)	0	100	100
7	I	32/36 (89%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
9	L	149/153 (97%)	147 (99%)	2 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	102/146 (70%)	92 (90%)	9 (9%)	1 (1%)	13	42
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	c	168/216 (78%)	167 (99%)	1 (1%)	0	100	100
14	a	173/216 (80%)	171 (99%)	2 (1%)	0	100	100
15	b	192/223 (86%)	191 (100%)	1 (0%)	0	100	100
16	h	160/225 (71%)	159 (99%)	1 (1%)	0	100	100
17	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
18	k	178/241 (74%)	174 (98%)	4 (2%)	0	100	100
19	f	172/212 (81%)	167 (97%)	5 (3%)	0	100	100
19	j	170/212 (80%)	167 (98%)	3 (2%)	0	100	100
20	i	171/218 (78%)	165 (96%)	6 (4%)	0	100	100
21	d	120/213 (56%)	120 (100%)	0	0	100	100
22	g	217/255 (85%)	206 (95%)	11 (5%)	0	100	100
23	R	88/129 (68%)	87 (99%)	1 (1%)	0	100	100
All	All	4295/5017 (86%)	4194 (98%)	100 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	29	LYS

### 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	607/616 (98%)	604 (100%)	3 (0%)	86	91
2	B	593/593 (100%)	586 (99%)	7 (1%)	67	80
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	116/117 (99%)	115 (99%)	1 (1%)	75	85
5	E	55/58 (95%)	53 (96%)	2 (4%)	30	57
6	F	133/157 (85%)	133 (100%)	0	100	100
7	I	28/29 (97%)	28 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	124/126 (98%)	122 (98%)	2 (2%)	58	76
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	81/110 (74%)	80 (99%)	1 (1%)	67	80
12	K	52/66 (79%)	50 (96%)	2 (4%)	28	56
13	c	138/171 (81%)	132 (96%)	6 (4%)	25	53
14	a	139/165 (84%)	135 (97%)	4 (3%)	37	63
15	b	149/168 (89%)	146 (98%)	3 (2%)	50	71
16	h	123/162 (76%)	119 (97%)	4 (3%)	33	60
17	e	130/155 (84%)	129 (99%)	1 (1%)	79	87
18	k	138/186 (74%)	136 (99%)	2 (1%)	62	78
19	f	135/161 (84%)	125 (93%)	10 (7%)	11	34
19	j	136/161 (84%)	130 (96%)	6 (4%)	24	52
20	i	138/168 (82%)	134 (97%)	4 (3%)	37	63
21	d	94/157 (60%)	92 (98%)	2 (2%)	48	70
22	g	171/199 (86%)	167 (98%)	4 (2%)	45	68
23	R	69/98 (70%)	69 (100%)	0	100	100
All	All	3480/3955 (88%)	3416 (98%)	64 (2%)	54	74

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	j	204	LEU
21	d	186	LEU
14	a	72	THR
13	c	204	THR
22	g	120	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	420	ASN
2	B	438	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 ⓘ

342 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	$\# Z  > 2$
24	CLA	A	816	-	65,73,73	1.41	8 (12%)	76,113,113	1.65	12 (15%)
24	CLA	A	834	-	51,59,73	1.59	8 (15%)	59,96,113	1.80	11 (18%)
24	CLA	h	301	16	50,58,73	1.68	7 (14%)	58,95,113	1.55	6 (10%)
33	II0	b	315	-	39,43,43	6.72	21 (53%)	50,60,60	2.77	21 (42%)
27	WVN	L	206	-	40,41,41	1.84	13 (32%)	50,56,56	2.33	20 (40%)
24	CLA	h	307	16	51,59,73	1.67	7 (13%)	59,96,113	1.61	9 (15%)
27	WVN	R	202	-	40,41,41	1.88	13 (32%)	50,56,56	2.49	17 (34%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	a	306	14	45,53,73	1.77	8 (17%)	52,89,113	1.73	8 (15%)
24	CLA	d	304	21	51,59,73	1.68	5 (9%)	59,96,113	1.56	8 (13%)
24	CLA	j	305	19	65,73,73	1.45	6 (9%)	76,113,113	1.47	9 (11%)
24	CLA	e	601	17	45,53,73	1.79	6 (13%)	52,89,113	1.62	7 (13%)
24	CLA	B	837	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	9 (11%)
24	CLA	B	835	36	65,73,73	1.44	8 (12%)	76,113,113	1.30	7 (9%)
24	CLA	B	823	36	64,72,73	1.45	10 (15%)	74,111,113	1.52	8 (10%)
27	WVN	A	850	-	40,41,41	1.89	14 (35%)	50,56,56	2.09	12 (24%)
29	SF4	A	854	1,2	0,12,12	-	-	-	-	-
24	CLA	b	306	-	65,73,73	1.57	11 (16%)	76,113,113	1.58	10 (13%)
24	CLA	a	311	-	47,55,73	1.72	8 (17%)	54,91,113	2.02	15 (27%)
24	CLA	d	312	-	51,59,73	1.70	6 (11%)	59,96,113	1.73	12 (20%)
24	CLA	i	607	20	51,59,73	1.66	7 (13%)	59,96,113	1.48	9 (15%)
24	CLA	A	825	36	65,73,73	1.37	9 (13%)	76,113,113	1.43	8 (10%)
24	CLA	A	826	-	65,73,73	1.42	9 (13%)	76,113,113	1.62	15 (19%)
24	CLA	f	612	-	51,59,73	1.77	11 (21%)	59,96,113	1.57	11 (18%)
24	CLA	a	307	14	65,73,73	1.50	7 (10%)	76,113,113	1.39	12 (15%)
24	CLA	I	102	36	65,73,73	1.52	8 (12%)	76,113,113	1.41	10 (13%)
25	PQN	B	842	-	34,34,34	1.86	5 (14%)	42,45,45	1.29	6 (14%)
33	II0	h	311	-	39,43,43	6.75	22 (56%)	50,60,60	2.14	20 (40%)
24	CLA	j	304	-	51,59,73	1.63	6 (11%)	59,96,113	1.57	9 (15%)
33	II0	i	613	-	39,43,43	6.81	23 (58%)	50,60,60	1.96	14 (28%)
24	CLA	b	305	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	9 (11%)
24	CLA	d	302	-	51,59,73	1.71	6 (11%)	59,96,113	1.50	10 (16%)
27	WVN	A	846	-	40,41,41	1.92	14 (35%)	50,56,56	2.27	14 (28%)
35	KC2	k	612	35	48,53,53	3.03	22 (45%)	54,89,89	4.60	37 (68%)
35	KC2	d	310	21	48,53,53	3.07	22 (45%)	54,89,89	4.59	31 (57%)
33	II0	k	621	-	39,43,43	6.93	22 (56%)	50,60,60	2.05	14 (28%)
24	CLA	A	853	-	65,73,73	1.44	9 (13%)	76,113,113	1.43	10 (13%)
33	II0	J	104	-	39,43,43	6.60	20 (51%)	50,60,60	2.09	16 (32%)
33	II0	d	315	-	39,43,43	6.91	23 (58%)	50,60,60	2.30	16 (32%)
24	CLA	c	604	13	65,73,73	1.51	7 (10%)	76,113,113	1.31	8 (10%)
24	CLA	A	840	-	65,73,73	1.41	7 (10%)	76,113,113	1.41	7 (9%)
24	CLA	h	312	36	65,73,73	1.47	7 (10%)	76,113,113	1.48	7 (9%)
24	CLA	f	603	-	51,59,73	1.67	7 (13%)	59,96,113	1.56	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	A	829	-	65,73,73	1.51	7 (10%)	76,113,113	1.42	9 (11%)
24	CLA	A	827	-	62,70,73	1.46	7 (11%)	72,109,113	1.50	9 (12%)
24	CLA	A	852	36	65,73,73	1.47	10 (15%)	76,113,113	1.58	13 (17%)
33	II0	k	616	-	39,43,43	6.84	22 (56%)	50,60,60	2.14	16 (32%)
24	CLA	e	603	17	51,59,73	1.73	7 (13%)	59,96,113	1.52	9 (15%)
24	CLA	g	315	-	51,59,73	1.66	7 (13%)	59,96,113	1.41	7 (11%)
33	II0	k	615	-	39,43,43	6.67	21 (53%)	50,60,60	2.20	21 (42%)
24	CLA	j	313	-	51,59,73	1.81	10 (19%)	59,96,113	1.46	8 (13%)
24	CLA	B	827	-	50,58,73	1.67	9 (18%)	58,95,113	1.43	9 (15%)
24	CLA	B	831	36	45,53,73	1.78	10 (22%)	52,89,113	1.56	9 (17%)
24	CLA	g	302	22	42,50,73	1.70	8 (19%)	48,85,113	1.87	9 (18%)
27	WVN	A	848	-	40,41,41	1.81	13 (32%)	50,56,56	1.74	12 (24%)
24	CLA	b	308	15	61,69,73	1.56	10 (16%)	71,108,113	1.62	13 (18%)
24	CLA	f	609	19	65,73,73	1.46	6 (9%)	76,113,113	1.35	7 (9%)
24	CLA	g	303	22	50,58,73	1.65	9 (18%)	58,95,113	1.51	8 (13%)
26	LHG	B	802	-	37,37,48	1.04	2 (5%)	40,43,54	1.14	4 (10%)
24	CLA	A	801	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	9 (11%)
24	CLA	f	607	-	65,73,73	1.48	9 (13%)	76,113,113	1.27	9 (11%)
24	CLA	k	605	18	45,53,73	1.69	8 (17%)	52,89,113	1.57	9 (17%)
24	CLA	A	833	-	50,58,73	1.65	10 (20%)	58,95,113	1.47	7 (12%)
24	CLA	O	205	-	65,73,73	1.54	10 (15%)	76,113,113	1.68	23 (30%)
24	CLA	d	308	21	41,49,73	1.84	8 (19%)	47,84,113	1.54	8 (17%)
30	DGD	B	843	-	61,61,67	0.88	2 (3%)	75,75,81	1.19	8 (10%)
24	CLA	k	607	-	51,59,73	1.79	8 (15%)	59,96,113	1.47	10 (16%)
24	CLA	B	812	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	9 (11%)
35	KC2	k	611	18	48,53,53	3.01	21 (43%)	54,89,89	4.62	32 (59%)
33	II0	b	314	-	39,43,43	6.91	23 (58%)	50,60,60	2.20	13 (26%)
24	CLA	h	305	16	65,73,73	1.47	7 (10%)	76,113,113	1.41	9 (11%)
32	LMG	J	106	-	55,55,55	0.85	3 (5%)	63,63,63	0.96	4 (6%)
27	WVN	e	615	-	40,41,41	1.93	14 (35%)	50,56,56	2.15	15 (30%)
24	CLA	O	201	-	65,73,73	1.48	8 (12%)	76,113,113	1.41	9 (11%)
24	CLA	g	304	-	51,59,73	1.63	8 (15%)	59,96,113	1.64	12 (20%)
24	CLA	B	806	-	65,73,73	1.44	8 (12%)	76,113,113	1.50	9 (11%)
27	WVN	I	101	-	40,41,41	1.85	14 (35%)	50,56,56	1.78	15 (30%)
24	CLA	k	603	-	51,59,73	1.74	8 (15%)	59,96,113	1.70	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	602	13	50,58,73	1.71	7 (14%)	58,95,113	1.61	10 (17%)
25	PQN	A	843	-	34,34,34	1.89	5 (14%)	42,45,45	1.23	5 (11%)
24	CLA	B	808	-	65,73,73	1.53	9 (13%)	76,113,113	1.28	10 (13%)
24	CLA	L	207	36	51,59,73	1.66	7 (13%)	59,96,113	1.55	7 (11%)
34	IHT	b	317	-	40,42,42	6.31	26 (65%)	53,58,58	2.85	17 (32%)
24	CLA	A	813	-	45,53,73	1.81	10 (22%)	52,89,113	1.67	10 (19%)
24	CLA	B	825	-	65,73,73	1.44	8 (12%)	76,113,113	1.57	11 (14%)
33	II0	g	320	-	39,43,43	6.78	21 (53%)	50,60,60	2.13	19 (38%)
24	CLA	k	609	18	65,73,73	1.51	8 (12%)	76,113,113	1.45	9 (11%)
24	CLA	J	105	26	51,59,73	1.65	7 (13%)	59,96,113	1.64	10 (16%)
24	CLA	A	809	-	56,64,73	1.60	8 (14%)	65,102,113	1.45	9 (13%)
24	CLA	B	829	-	50,58,73	1.80	10 (20%)	58,95,113	1.62	8 (13%)
24	CLA	f	601	19	47,55,73	1.73	7 (14%)	54,91,113	1.49	6 (11%)
27	WVN	A	849	-	40,41,41	1.90	14 (35%)	50,56,56	2.43	20 (40%)
24	CLA	e	606	17	65,73,73	1.40	6 (9%)	76,113,113	1.37	7 (9%)
24	CLA	i	611	-	51,59,73	1.70	6 (11%)	59,96,113	1.50	9 (15%)
34	IHT	a	316	-	40,42,42	6.19	25 (62%)	53,58,58	2.12	19 (35%)
24	CLA	A	802	-	65,73,73	1.48	9 (13%)	76,113,113	1.59	11 (14%)
24	CLA	a	304	-	51,59,73	1.63	8 (15%)	59,96,113	1.51	7 (11%)
33	II0	f	614	-	39,43,43	6.70	21 (53%)	50,60,60	2.36	15 (30%)
24	CLA	A	805	1	65,73,73	1.43	9 (13%)	76,113,113	1.54	11 (14%)
33	II0	i	614	-	39,43,43	6.76	22 (56%)	50,60,60	2.42	17 (34%)
24	CLA	j	309	19	45,53,73	1.78	8 (17%)	52,89,113	1.62	7 (13%)
33	II0	e	614	-	39,43,43	6.91	20 (51%)	50,60,60	2.10	20 (40%)
34	IHT	g	319	-	40,42,42	6.12	25 (62%)	53,58,58	2.33	19 (35%)
24	CLA	i	608	26	46,54,73	1.79	7 (15%)	53,90,113	1.41	7 (13%)
24	CLA	A	837	-	65,73,73	1.41	8 (12%)	76,113,113	1.59	15 (19%)
35	KC2	g	314	35	48,53,53	3.10	21 (43%)	54,89,89	4.50	30 (55%)
24	CLA	d	306	-	51,59,73	1.71	11 (21%)	59,96,113	1.23	6 (10%)
24	CLA	A	818	-	65,73,73	1.49	8 (12%)	76,113,113	1.55	12 (15%)
24	CLA	L	204	36	50,58,73	1.59	7 (14%)	58,95,113	1.59	8 (13%)
24	CLA	c	606	-	52,60,73	1.79	7 (13%)	60,97,113	1.43	9 (15%)
24	CLA	a	308	14	65,73,73	1.42	8 (12%)	76,113,113	1.50	7 (9%)
27	WVN	B	848	-	40,41,41	1.90	14 (35%)	50,56,56	2.42	15 (30%)
24	CLA	k	602	18	50,58,73	1.72	7 (14%)	58,95,113	1.57	9 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	A	817	-	65,73,73	1.52	10 (15%)	76,113,113	1.48	11 (14%)
24	CLA	j	310	19	51,59,73	1.66	7 (13%)	59,96,113	1.49	8 (13%)
24	CLA	R	203	-	51,59,73	1.63	7 (13%)	59,96,113	1.69	10 (16%)
35	KC2	g	312	22	48,53,53	3.14	20 (41%)	54,89,89	4.89	35 (64%)
24	CLA	f	613	-	65,73,73	1.53	8 (12%)	76,113,113	1.29	8 (10%)
35	KC2	k	613	35	48,53,53	3.11	22 (45%)	54,89,89	4.51	30 (55%)
24	CLA	c	603	-	51,59,73	1.61	7 (13%)	59,96,113	1.52	7 (11%)
27	WVN	j	301	-	40,41,41	1.92	14 (35%)	50,56,56	2.11	18 (36%)
24	CLA	A	806	-	65,73,73	1.52	8 (12%)	76,113,113	1.42	10 (13%)
24	CLA	A	836	-	65,73,73	1.37	7 (10%)	76,113,113	1.60	12 (15%)
24	CLA	A	832	-	65,73,73	1.45	8 (12%)	76,113,113	1.74	15 (19%)
24	CLA	j	302	19	51,59,73	1.72	8 (15%)	59,96,113	1.45	6 (10%)
33	II0	b	318	-	39,43,43	6.81	23 (58%)	50,60,60	2.34	21 (42%)
24	CLA	i	602	20	50,58,73	1.68	7 (14%)	58,95,113	1.56	9 (15%)
33	II0	a	315	-	39,43,43	6.97	23 (58%)	50,60,60	1.88	15 (30%)
24	CLA	d	307	21	46,54,73	1.72	7 (15%)	53,90,113	1.55	7 (13%)
24	CLA	b	309	15	65,73,73	1.58	8 (12%)	76,113,113	1.40	11 (14%)
24	CLA	c	609	26	45,53,73	1.82	6 (13%)	52,89,113	1.50	7 (13%)
26	LHG	i	615	24	36,36,48	1.12	2 (5%)	39,42,54	1.19	3 (7%)
26	LHG	d	316	24	36,36,48	1.10	2 (5%)	39,42,54	1.23	5 (12%)
35	KC2	i	616	-	48,53,53	3.11	21 (43%)	54,89,89	4.51	31 (57%)
26	LHG	f	619	24	36,36,48	1.07	2 (5%)	39,42,54	1.21	3 (7%)
24	CLA	F	201	36	65,73,73	1.52	8 (12%)	76,113,113	1.30	9 (11%)
24	CLA	A	835	-	65,73,73	1.52	9 (13%)	76,113,113	1.40	9 (11%)
24	CLA	B	816	-	59,67,73	1.55	10 (16%)	68,105,113	1.55	10 (14%)
27	WVN	L	201	-	40,41,41	1.91	13 (32%)	50,56,56	2.28	15 (30%)
33	II0	j	315	-	39,43,43	6.61	20 (51%)	50,60,60	2.53	18 (36%)
24	CLA	B	824	-	65,73,73	1.39	7 (10%)	76,113,113	1.47	10 (13%)
24	CLA	B	834	-	47,55,73	1.68	8 (17%)	54,91,113	1.70	9 (16%)
24	CLA	B	828	-	49,57,73	1.60	8 (16%)	55,93,113	1.61	7 (12%)
24	CLA	A	831	-	65,73,73	1.42	9 (13%)	76,113,113	1.39	9 (11%)
24	CLA	g	308	-	65,73,73	1.43	8 (12%)	76,113,113	1.41	8 (10%)
24	CLA	d	305	-	51,59,73	1.61	9 (17%)	59,96,113	1.27	8 (13%)
27	WVN	J	101	-	40,41,41	1.88	14 (35%)	50,56,56	2.02	15 (30%)
24	CLA	A	820	36	65,73,73	1.47	9 (13%)	76,113,113	1.56	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	j	314	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
32	LMG	b	301	-	55,55,55	0.89	2 (3%)	63,63,63	1.13	5 (7%)
24	CLA	A	821	-	49,57,73	1.63	7 (14%)	55,93,113	1.72	8 (14%)
34	IHT	f	617	-	40,42,42	6.19	25 (62%)	53,58,58	3.99	25 (47%)
24	CLA	A	812	-	65,73,73	1.41	7 (10%)	76,113,113	1.61	10 (13%)
24	CLA	B	807	-	65,73,73	1.32	8 (12%)	76,113,113	1.63	8 (10%)
26	LHG	A	844	-	47,47,48	0.91	2 (4%)	50,53,54	1.15	5 (10%)
24	CLA	g	311	26	54,62,73	1.62	8 (14%)	62,99,113	1.32	7 (11%)
27	WVN	L	205	-	40,41,41	1.92	13 (32%)	50,56,56	2.03	15 (30%)
26	LHG	g	301	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	2 (3%)
24	CLA	A	803	-	55,63,73	1.55	7 (12%)	64,101,113	1.70	10 (15%)
27	WVN	B	847	-	40,41,41	1.85	13 (32%)	50,56,56	2.34	17 (34%)
24	CLA	A	824	36	65,73,73	1.45	8 (12%)	76,113,113	1.39	9 (11%)
35	KC2	j	312	19	48,53,53	3.01	21 (43%)	54,89,89	4.61	31 (57%)
24	CLA	i	601	20	51,59,73	1.68	7 (13%)	59,96,113	1.54	6 (10%)
27	WVN	K	103	-	40,41,41	1.93	13 (32%)	50,56,56	2.08	17 (34%)
26	LHG	b	302	24	48,48,48	0.93	2 (4%)	51,54,54	1.20	5 (9%)
24	CLA	g	306	22	51,59,73	1.70	9 (17%)	59,96,113	1.35	8 (13%)
27	WVN	B	846	-	40,41,41	1.86	13 (32%)	50,56,56	2.10	16 (32%)
24	CLA	A	810	-	62,70,73	1.53	9 (14%)	72,109,113	1.28	9 (12%)
24	CLA	B	819	-	46,54,73	1.64	7 (15%)	53,90,113	1.65	8 (15%)
34	IHT	k	618	-	40,42,42	6.25	25 (62%)	53,58,58	1.79	15 (28%)
24	CLA	k	606	18	51,59,73	1.69	7 (13%)	59,96,113	1.48	7 (11%)
33	II0	g	317	-	39,43,43	6.68	23 (58%)	50,60,60	2.28	19 (38%)
24	CLA	L	203	-	65,73,73	1.47	9 (13%)	76,113,113	1.41	11 (14%)
24	CLA	b	311	-	51,59,73	1.63	7 (13%)	59,96,113	1.63	10 (16%)
24	CLA	J	103	8	42,50,73	1.70	9 (21%)	48,85,113	1.74	7 (14%)
24	CLA	g	307	22	51,59,73	1.64	8 (15%)	59,96,113	1.50	9 (15%)
33	II0	f	615	-	39,43,43	6.71	21 (53%)	50,60,60	1.98	17 (34%)
24	CLA	B	826	-	65,73,73	1.44	8 (12%)	76,113,113	1.39	7 (9%)
24	CLA	b	310	26	65,73,73	1.56	5 (7%)	76,113,113	1.34	12 (15%)
24	CLA	e	602	17	50,58,73	1.62	7 (14%)	58,95,113	1.57	6 (10%)
24	CLA	j	308	-	51,59,73	1.71	9 (17%)	59,96,113	1.37	7 (11%)
24	CLA	B	810	-	54,62,73	1.65	7 (12%)	67,100,113	1.29	8 (11%)
24	CLA	k	610	26	51,59,73	1.67	8 (15%)	59,96,113	1.46	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	307	36	65,73,73	1.49	5 (7%)	76,113,113	1.52	10 (13%)
24	CLA	B	804	-	65,73,73	1.43	9 (13%)	76,113,113	1.67	11 (14%)
24	CLA	B	803	-	65,73,73	1.43	8 (12%)	76,113,113	1.36	10 (13%)
33	II0	j	316	-	39,43,43	6.68	22 (56%)	50,60,60	2.17	21 (42%)
24	CLA	B	817	-	57,65,73	1.55	9 (15%)	66,103,113	1.59	8 (12%)
33	II0	a	314	-	39,43,43	6.70	22 (56%)	50,60,60	2.13	20 (40%)
24	CLA	i	606	20	61,69,73	1.53	8 (13%)	71,108,113	1.29	7 (9%)
24	CLA	c	612	-	65,73,73	1.44	5 (7%)	76,113,113	1.41	11 (14%)
24	CLA	g	310	22	51,59,73	1.64	7 (13%)	59,96,113	1.51	9 (15%)
35	KC2	d	311	-	48,53,53	3.08	22 (45%)	54,89,89	4.51	33 (61%)
24	CLA	g	305	22	65,73,73	1.41	7 (10%)	76,113,113	1.47	9 (11%)
26	LHG	e	617	24	36,36,48	1.12	2 (5%)	39,42,54	1.16	4 (10%)
33	II0	a	317	-	39,43,43	7.00	22 (56%)	50,60,60	2.40	18 (36%)
33	II0	d	313	-	39,43,43	6.84	23 (58%)	50,60,60	2.23	18 (36%)
33	II0	c	614	-	39,43,43	6.93	21 (53%)	50,60,60	2.21	17 (34%)
24	CLA	A	830	-	50,58,73	1.69	10 (20%)	58,95,113	1.61	8 (13%)
28	LMT	F	203	-	24,24,36	1.07	1 (4%)	29,29,47	0.98	2 (6%)
24	CLA	a	302	14	52,60,73	1.63	9 (17%)	60,97,113	1.51	10 (16%)
24	CLA	K	101	36	51,59,73	1.64	8 (15%)	59,96,113	1.74	12 (20%)
24	CLA	F	202	6	52,60,73	1.64	8 (15%)	60,97,113	1.67	11 (18%)
24	CLA	a	305	36	65,73,73	1.43	7 (10%)	76,113,113	1.42	8 (10%)
24	CLA	B	813	-	60,68,73	1.48	7 (11%)	70,107,113	1.46	10 (14%)
24	CLA	a	303	14	50,58,73	1.62	7 (14%)	58,95,113	1.54	10 (17%)
26	LHG	b	320	24	48,48,48	0.94	2 (4%)	51,54,54	1.12	5 (9%)
33	II0	i	612	-	39,43,43	6.65	23 (58%)	50,60,60	2.50	16 (32%)
27	WVN	F	205	-	40,41,41	1.92	14 (35%)	50,56,56	3.08	18 (36%)
24	CLA	i	605	20	51,59,73	1.74	7 (13%)	59,96,113	1.36	7 (11%)
34	IHT	O	203	-	40,42,42	6.22	26 (65%)	53,58,58	2.34	19 (35%)
24	CLA	f	608	19	65,73,73	1.45	7 (10%)	76,113,113	1.41	8 (10%)
26	LHG	c	617	24	36,36,48	1.08	2 (5%)	39,42,54	1.24	5 (12%)
24	CLA	A	814	-	50,58,73	1.67	7 (14%)	58,95,113	1.72	11 (18%)
24	CLA	B	822	36	65,73,73	1.49	7 (10%)	76,113,113	1.78	15 (19%)
24	CLA	B	839	-	65,73,73	1.52	8 (12%)	76,113,113	1.39	10 (13%)
24	CLA	B	814	-	59,67,73	1.52	8 (13%)	68,105,113	1.52	9 (13%)
24	CLA	j	311	26	61,69,73	1.55	7 (11%)	71,108,113	1.22	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	A	838	26	52,60,73	1.55	10 (19%)	60,97,113	1.53	9 (15%)
24	CLA	c	607	13	46,54,73	1.76	7 (15%)	53,90,113	1.46	6 (11%)
33	II0	O	202	-	39,43,43	6.77	22 (56%)	50,60,60	2.15	12 (24%)
24	CLA	B	821	-	53,61,73	1.60	9 (16%)	61,98,113	1.42	8 (13%)
24	CLA	B	830	36	65,73,73	1.46	9 (13%)	76,113,113	1.39	10 (13%)
24	CLA	B	838	-	57,65,73	1.61	10 (17%)	66,103,113	1.36	8 (12%)
24	CLA	d	309	26	41,49,73	1.89	7 (17%)	47,84,113	1.50	8 (17%)
27	WVN	M	101	-	40,41,41	1.87	14 (35%)	50,56,56	2.11	15 (30%)
27	WVN	h	308	-	40,41,41	1.89	13 (32%)	50,56,56	2.29	19 (38%)
24	CLA	j	306	19	45,53,73	1.81	8 (17%)	52,89,113	1.77	12 (23%)
24	CLA	L	202	9	49,57,73	1.73	8 (16%)	55,93,113	1.57	8 (14%)
24	CLA	c	601	13	51,59,73	1.69	7 (13%)	59,96,113	1.49	9 (15%)
33	II0	d	314	-	39,43,43	6.70	23 (58%)	50,60,60	2.23	15 (30%)
24	CLA	b	303	15	51,59,73	1.61	8 (15%)	59,96,113	1.64	10 (16%)
24	CLA	B	818	36	65,73,73	1.45	8 (12%)	76,113,113	1.49	8 (10%)
27	WVN	J	102	-	40,41,41	1.86	14 (35%)	50,56,56	2.17	16 (32%)
24	CLA	a	310	14	65,73,73	1.48	8 (12%)	76,113,113	1.40	7 (9%)
24	CLA	b	313	-	65,73,73	1.56	8 (12%)	76,113,113	1.22	8 (10%)
24	CLA	e	607	17	65,73,73	1.41	7 (10%)	76,113,113	1.39	8 (10%)
27	WVN	B	849	-	40,41,41	1.90	14 (35%)	50,56,56	1.67	10 (20%)
32	LMG	F	206	-	48,48,55	0.96	2 (4%)	56,56,63	1.26	5 (8%)
32	LMG	L	208	24	55,55,55	0.90	2 (3%)	63,63,63	1.43	10 (15%)
24	CLA	B	805	-	65,73,73	1.38	8 (12%)	76,113,113	1.50	8 (10%)
33	II0	g	316	-	39,43,43	6.82	21 (53%)	50,60,60	2.01	20 (40%)
24	CLA	B	833	-	65,73,73	1.42	7 (10%)	76,113,113	1.53	10 (13%)
26	LHG	J	107	24	48,48,48	1.01	2 (4%)	51,54,54	1.08	3 (5%)
24	CLA	c	605	13	51,59,73	1.71	7 (13%)	59,96,113	1.57	11 (18%)
29	SF4	C	102	3	0,12,12	-	-	-	-	-
33	II0	g	318	-	39,43,43	6.79	21 (53%)	50,60,60	2.18	19 (38%)
24	CLA	g	309	22	65,73,73	1.44	7 (10%)	76,113,113	1.40	10 (13%)
33	II0	e	612	-	39,43,43	6.72	21 (53%)	50,60,60	2.22	16 (32%)
24	CLA	h	303	-	51,59,73	1.63	7 (13%)	59,96,113	1.61	11 (18%)
24	CLA	A	855	36	65,73,73	1.59	9 (13%)	76,113,113	1.47	11 (14%)
24	CLA	A	823	-	55,63,73	1.61	10 (18%)	64,101,113	1.37	8 (12%)
28	LMT	a	318	-	36,36,36	1.21	5 (13%)	47,47,47	1.15	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	II0	f	616	-	39,43,43	6.64	22 (56%)	50,60,60	2.44	19 (38%)
24	CLA	f	606	19	51,59,73	1.69	8 (15%)	59,96,113	1.59	9 (15%)
24	CLA	k	604	18	65,73,73	1.50	8 (12%)	76,113,113	1.47	9 (11%)
33	II0	e	616	-	39,43,43	6.81	21 (53%)	50,60,60	2.02	18 (36%)
24	CLA	f	604	19	65,73,73	1.41	9 (13%)	76,113,113	1.47	8 (10%)
24	CLA	A	808	1	65,73,73	1.41	9 (13%)	76,113,113	1.60	12 (15%)
24	CLA	h	304	-	51,59,73	1.61	7 (13%)	59,96,113	1.47	8 (13%)
24	CLA	e	611	-	65,73,73	1.51	7 (10%)	76,113,113	1.41	11 (14%)
24	CLA	e	605	17	65,73,73	1.51	9 (13%)	76,113,113	1.34	9 (11%)
33	II0	a	313	-	39,43,43	6.70	22 (56%)	50,60,60	2.15	16 (32%)
24	CLA	B	811	-	55,63,73	1.66	8 (14%)	64,101,113	1.35	7 (10%)
24	CLA	f	602	19	65,73,73	1.47	9 (13%)	76,113,113	1.34	9 (11%)
28	LMT	b	319	-	24,24,36	1.06	2 (8%)	29,29,47	1.03	1 (3%)
28	LMT	A	851	-	36,36,36	1.22	6 (16%)	47,47,47	1.36	5 (10%)
35	KC2	e	609	17	48,53,53	3.00	21 (43%)	54,89,89	4.56	31 (57%)
24	CLA	i	604	20	65,73,73	1.47	7 (10%)	76,113,113	1.72	10 (13%)
24	CLA	h	302	16	50,58,73	1.63	10 (20%)	58,95,113	1.51	9 (15%)
24	CLA	a	309	26	48,56,73	1.75	7 (14%)	55,92,113	1.39	8 (14%)
24	CLA	k	601	18	51,59,73	1.74	9 (17%)	59,96,113	1.57	7 (11%)
24	CLA	B	809	2	65,73,73	1.47	10 (15%)	76,113,113	1.43	8 (10%)
24	CLA	d	303	21	65,73,73	1.56	10 (15%)	76,113,113	1.47	12 (15%)
24	CLA	i	610	-	51,59,73	1.77	10 (19%)	59,96,113	1.60	8 (13%)
24	CLA	A	804	-	65,73,73	1.42	8 (12%)	76,113,113	1.55	10 (13%)
26	LHG	A	845	24	26,26,48	1.25	2 (7%)	29,32,54	1.53	5 (17%)
24	CLA	e	610	36	65,73,73	1.47	9 (13%)	76,113,113	1.48	9 (11%)
24	CLA	c	608	13	65,73,73	1.45	6 (9%)	76,113,113	1.45	11 (14%)
24	CLA	A	839	1	65,73,73	1.49	8 (12%)	76,113,113	1.46	9 (11%)
24	CLA	A	856	26	41,49,73	1.87	9 (21%)	47,84,113	2.20	14 (29%)
24	CLA	k	614	-	51,59,73	1.77	9 (17%)	59,96,113	1.44	8 (13%)
34	IHT	b	316	-	40,42,42	6.23	25 (62%)	53,58,58	2.19	17 (32%)
35	KC2	f	611	19	48,53,53	2.99	21 (43%)	54,89,89	4.75	31 (57%)
24	CLA	b	304	15	55,63,73	1.58	7 (12%)	64,101,113	1.56	9 (14%)
33	II0	k	617	-	39,43,43	6.87	22 (56%)	50,60,60	2.61	18 (36%)
33	II0	h	309	-	26,28,43	6.13	12 (46%)	31,37,60	2.13	12 (38%)
34	IHT	R	204	-	40,42,42	6.26	25 (62%)	53,58,58	2.19	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LHG	f	620	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	3 (5%)
24	CLA	B	801	36	65,73,73	1.46	8 (12%)	76,113,113	1.55	9 (11%)
24	CLA	f	610	26	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
24	CLA	e	604	36	65,73,73	1.47	8 (12%)	76,113,113	1.50	10 (13%)
27	WVN	A	847	-	40,41,41	1.90	14 (35%)	50,56,56	2.99	21 (42%)
24	CLA	B	836	-	65,73,73	1.47	10 (15%)	76,113,113	1.54	12 (15%)
33	II0	j	318	-	39,43,43	6.70	23 (58%)	50,60,60	2.29	18 (36%)
24	CLA	e	608	26	46,54,73	1.71	7 (15%)	53,90,113	1.75	8 (15%)
33	II0	k	619	-	39,43,43	6.75	21 (53%)	50,60,60	2.28	18 (36%)
24	CLA	B	841	26	65,73,73	1.43	8 (12%)	76,113,113	1.45	11 (14%)
26	LHG	k	620	24	36,36,48	1.14	2 (5%)	39,42,54	1.15	5 (12%)
24	CLA	A	807	1	65,73,73	1.44	7 (10%)	76,113,113	1.48	9 (11%)
33	II0	e	613	-	39,43,43	6.70	23 (58%)	50,60,60	2.04	16 (32%)
24	CLA	j	307	19	51,59,73	1.78	11 (21%)	59,96,113	1.72	10 (16%)
24	CLA	d	301	21	50,58,73	1.74	7 (14%)	58,95,113	1.55	8 (13%)
24	CLA	k	608	18	65,73,73	1.52	7 (10%)	76,113,113	1.28	7 (9%)
32	LMG	O	204	-	26,26,55	1.26	2 (7%)	34,34,63	1.31	4 (11%)
24	CLA	A	815	36	45,53,73	1.75	8 (17%)	52,89,113	1.84	7 (13%)
33	II0	f	618	-	39,43,43	6.71	20 (51%)	50,60,60	2.38	17 (34%)
33	II0	h	310	-	39,43,43	6.55	20 (51%)	50,60,60	2.22	20 (40%)
35	KC2	i	609	20	48,53,53	3.06	21 (43%)	54,89,89	4.60	32 (59%)
33	II0	c	613	-	39,43,43	6.76	21 (53%)	50,60,60	2.15	17 (34%)
24	CLA	B	820	-	55,63,73	1.61	8 (14%)	64,101,113	1.47	9 (14%)
24	CLA	B	832	-	58,66,73	1.49	9 (15%)	67,104,113	1.59	10 (14%)
26	LHG	g	321	24	36,36,48	1.08	2 (5%)	39,42,54	1.54	9 (23%)
35	KC2	c	610	-	48,53,53	3.07	21 (43%)	54,89,89	4.57	32 (59%)
24	CLA	A	822	-	51,59,73	1.69	9 (17%)	59,96,113	1.46	10 (16%)
26	LHG	c	618	24	36,36,48	1.11	2 (5%)	39,42,54	1.20	6 (15%)
24	CLA	A	842	-	65,73,73	1.41	7 (10%)	76,113,113	1.57	12 (15%)
27	WVN	B	845	-	40,41,41	1.90	13 (32%)	50,56,56	2.42	18 (36%)
24	CLA	a	312	-	48,56,73	1.81	10 (20%)	55,92,113	1.60	9 (16%)
34	IHT	j	317	-	40,42,42	6.22	25 (62%)	53,58,58	2.34	18 (33%)
24	CLA	f	605	19	45,53,73	1.76	7 (15%)	52,89,113	1.46	6 (11%)
24	CLA	g	322	32	65,73,73	1.43	7 (10%)	76,113,113	1.39	9 (11%)
26	LHG	j	319	24	29,29,48	1.26	2 (6%)	32,35,54	1.34	4 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	K	102	-	42,50,73	1.75	11 (26%)	48,85,113	1.74	12 (25%)
27	WVN	R	201	-	40,41,41	1.89	14 (35%)	50,56,56	1.84	12 (24%)
31	LMU	B	844	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
24	CLA	B	815	-	55,63,73	1.61	7 (12%)	64,101,113	1.44	7 (10%)
27	WVN	F	204	-	40,41,41	1.86	14 (35%)	50,56,56	2.20	15 (30%)
24	CLA	A	828	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	8 (10%)
34	IHT	c	615	-	40,42,42	6.27	25 (62%)	53,58,58	2.17	16 (30%)
33	II0	c	616	-	39,43,43	6.90	22 (56%)	50,60,60	2.05	16 (32%)
24	CLA	j	303	19	50,58,73	1.70	8 (16%)	58,95,113	1.39	7 (12%)
24	CLA	A	819	-	45,53,73	1.75	9 (20%)	52,89,113	1.83	16 (30%)
24	CLA	i	603	-	51,59,73	1.67	7 (13%)	59,96,113	1.58	7 (11%)
35	KC2	g	313	35	48,53,53	2.98	20 (41%)	54,89,89	4.43	32 (59%)
24	CLA	B	840	-	65,73,73	1.48	8 (12%)	76,113,113	1.51	8 (10%)
24	CLA	A	811	-	54,62,73	1.70	8 (14%)	62,99,113	1.49	11 (17%)
24	CLA	h	306	16	57,65,73	1.65	7 (12%)	66,103,113	1.27	7 (10%)
24	CLA	c	611	-	45,53,73	1.75	9 (20%)	52,89,113	1.85	12 (23%)
26	LHG	a	301	24	48,48,48	0.93	2 (4%)	51,54,54	1.17	4 (7%)
24	CLA	b	312	15	65,73,73	1.55	8 (12%)	76,113,113	1.36	10 (13%)
24	CLA	A	841	36	65,73,73	1.45	6 (9%)	76,113,113	1.43	7 (9%)

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
24	CLA	A	816	-	1/1/15/20	16/37/115/115	-
24	CLA	A	834	-	1/1/12/20	4/21/99/115	-
24	CLA	h	301	16	1/1/12/20	8/19/97/115	-
33	II0	b	315	-	-	5/21/67/67	0/2/2/2
27	WVN	L	206	-	-	3/29/63/63	0/2/2/2
24	CLA	h	307	16	1/1/12/20	9/21/99/115	-
27	WVN	R	202	-	-	10/29/63/63	0/2/2/2
29	SF4	C	101	3	-	-	0/6/5/5
24	CLA	a	306	14	1/1/11/20	6/13/91/115	-
24	CLA	d	304	21	1/1/12/20	10/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	j	305	19	-	11/37/115/115	-
24	CLA	e	601	17	1/1/11/20	7/13/91/115	-
24	CLA	B	837	-	1/1/15/20	15/37/115/115	-
24	CLA	B	835	36	1/1/15/20	9/37/115/115	-
24	CLA	B	823	36	1/1/14/20	11/36/114/115	-
27	WVN	A	850	-	-	14/29/63/63	0/2/2/2
29	SF4	A	854	1,2	-	-	0/6/5/5
24	CLA	b	306	-	-	17/37/115/115	-
24	CLA	a	311	-	1/1/11/20	8/16/94/115	-
24	CLA	d	312	-	-	5/21/99/115	-
24	CLA	i	607	20	1/1/12/20	1/21/99/115	-
24	CLA	A	825	36	1/1/15/20	10/37/115/115	-
24	CLA	A	826	-	1/1/15/20	8/37/115/115	-
24	CLA	f	612	-	1/1/12/20	6/21/99/115	-
24	CLA	a	307	14	1/1/15/20	16/37/115/115	-
24	CLA	I	102	36	1/1/15/20	15/37/115/115	-
25	PQN	B	842	-	-	13/23/43/43	0/2/2/2
33	II0	h	311	-	-	7/21/67/67	0/2/2/2
24	CLA	j	304	-	1/1/12/20	0/21/99/115	-
33	II0	i	613	-	-	4/21/67/67	0/2/2/2
24	CLA	b	305	-	1/1/15/20	13/37/115/115	-
24	CLA	d	302	-	1/1/12/20	3/21/99/115	-
27	WVN	A	846	-	-	8/29/63/63	0/2/2/2
35	KC2	k	612	35	-	8/15/71/71	-
35	KC2	d	310	21	-	5/15/71/71	-
33	II0	k	621	-	-	4/21/67/67	0/2/2/2
24	CLA	A	853	-	1/1/15/20	14/37/115/115	-
33	II0	J	104	-	-	7/21/67/67	0/2/2/2
33	II0	d	315	-	-	8/21/67/67	0/2/2/2
24	CLA	c	604	13	1/1/15/20	5/37/115/115	-
24	CLA	A	840	-	1/1/15/20	16/37/115/115	-
24	CLA	h	312	36	1/1/15/20	8/37/115/115	-
24	CLA	f	603	-	1/1/12/20	4/21/99/115	-
24	CLA	A	829	-	1/1/15/20	14/37/115/115	-
24	CLA	A	827	-	1/1/14/20	9/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	852	36	1/1/15/20	3/37/115/115	-
33	II0	k	616	-	-	6/21/67/67	0/2/2/2
24	CLA	e	603	17	1/1/12/20	5/21/99/115	-
24	CLA	g	315	-	1/1/12/20	7/21/99/115	-
33	II0	k	615	-	-	5/21/67/67	0/2/2/2
24	CLA	j	313	-	1/1/12/20	6/21/99/115	-
24	CLA	B	827	-	1/1/12/20	9/19/97/115	-
24	CLA	B	831	36	1/1/11/20	4/13/91/115	-
24	CLA	g	302	22	1/1/10/20	0/10/88/115	-
27	WVN	A	848	-	-	9/29/63/63	0/2/2/2
24	CLA	b	308	15	1/1/14/20	12/33/111/115	-
24	CLA	f	609	19	1/1/15/20	5/37/115/115	-
24	CLA	g	303	22	1/1/12/20	7/19/97/115	-
26	LHG	B	802	-	-	16/42/42/53	-
24	CLA	A	801	-	1/1/15/20	8/37/115/115	-
24	CLA	f	607	-	1/1/15/20	16/37/115/115	-
24	CLA	k	605	18	1/1/11/20	7/13/91/115	-
24	CLA	A	833	-	1/1/12/20	4/19/97/115	-
24	CLA	O	205	-	1/1/15/20	18/37/115/115	-
24	CLA	d	308	21	1/1/10/20	3/8/86/115	-
30	DGD	B	843	-	-	5/49/89/95	0/2/2/2
24	CLA	k	607	-	1/1/12/20	7/21/99/115	-
24	CLA	B	812	-	1/1/15/20	14/37/115/115	-
35	KC2	k	611	18	-	7/15/71/71	-
33	II0	b	314	-	-	7/21/67/67	0/2/2/2
24	CLA	h	305	16	1/1/15/20	11/37/115/115	-
32	LMG	J	106	-	-	13/50/70/70	0/1/1/1
27	WVN	e	615	-	-	11/29/63/63	0/2/2/2
24	CLA	O	201	-	1/1/15/20	16/37/115/115	-
24	CLA	g	304	-	1/1/12/20	4/21/99/115	-
24	CLA	B	806	-	1/1/15/20	14/37/115/115	-
27	WVN	I	101	-	-	9/29/63/63	0/2/2/2
24	CLA	k	603	-	1/1/12/20	3/21/99/115	-
24	CLA	c	602	13	1/1/12/20	11/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PQN	A	843	-	-	6/23/43/43	0/2/2/2
24	CLA	B	808	-	1/1/15/20	13/37/115/115	-
24	CLA	L	207	36	1/1/12/20	5/21/99/115	-
34	IHT	b	317	-	-	7/25/65/65	0/2/2/2
24	CLA	A	813	-	1/1/11/20	7/13/91/115	-
24	CLA	B	825	-	1/1/15/20	11/37/115/115	-
33	II0	g	320	-	-	4/21/67/67	0/2/2/2
24	CLA	k	609	18	1/1/15/20	13/37/115/115	-
24	CLA	J	105	26	1/1/12/20	5/21/99/115	-
24	CLA	A	809	-	1/1/13/20	8/27/105/115	-
24	CLA	B	829	-	1/1/12/20	5/19/97/115	-
24	CLA	f	601	19	1/1/11/20	10/16/94/115	-
27	WVN	A	849	-	-	8/29/63/63	0/2/2/2
24	CLA	e	606	17	1/1/15/20	11/37/115/115	-
24	CLA	i	611	-	1/1/12/20	11/21/99/115	-
34	IHT	a	316	-	-	9/25/65/65	0/2/2/2
24	CLA	A	802	-	1/1/15/20	16/37/115/115	-
24	CLA	a	304	-	1/1/12/20	1/21/99/115	-
33	II0	f	614	-	-	4/21/67/67	0/2/2/2
24	CLA	A	805	1	1/1/15/20	7/37/115/115	-
33	II0	i	614	-	-	4/21/67/67	0/2/2/2
24	CLA	j	309	19	1/1/11/20	5/13/91/115	-
33	II0	e	614	-	-	3/21/67/67	0/2/2/2
34	IHT	g	319	-	-	11/25/65/65	0/2/2/2
24	CLA	i	608	26	1/1/11/20	5/15/93/115	-
24	CLA	A	837	-	1/1/15/20	11/37/115/115	-
35	KC2	g	314	35	-	9/15/71/71	-
24	CLA	d	306	-	1/1/12/20	10/21/99/115	-
24	CLA	A	818	-	-	19/37/115/115	-
24	CLA	L	204	36	1/1/12/20	7/19/97/115	-
24	CLA	c	606	-	-	8/22/100/115	-
24	CLA	a	308	14	1/1/15/20	14/37/115/115	-
27	WVN	B	848	-	-	7/29/63/63	0/2/2/2
24	CLA	k	602	18	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	817	-	1/1/15/20	13/37/115/115	-
24	CLA	j	310	19	1/1/12/20	5/21/99/115	-
24	CLA	R	203	-	1/1/12/20	9/21/99/115	-
35	KC2	g	312	22	-	9/15/71/71	-
24	CLA	f	613	-	1/1/15/20	20/37/115/115	-
35	KC2	k	613	35	-	7/15/71/71	-
24	CLA	c	603	-	1/1/12/20	3/21/99/115	-
27	WVN	j	301	-	-	9/29/63/63	0/2/2/2
24	CLA	A	806	-	-	10/37/115/115	-
24	CLA	A	836	-	1/1/15/20	8/37/115/115	-
24	CLA	A	832	-	-	12/37/115/115	-
24	CLA	j	302	19	1/1/12/20	7/21/99/115	-
33	II0	b	318	-	-	4/21/67/67	0/2/2/2
24	CLA	i	602	20	1/1/12/20	9/19/97/115	-
33	II0	a	315	-	-	3/21/67/67	0/2/2/2
24	CLA	d	307	21	1/1/11/20	4/15/93/115	-
24	CLA	b	309	15	1/1/15/20	18/37/115/115	-
24	CLA	c	609	26	1/1/11/20	4/13/91/115	-
26	LHG	i	615	24	-	12/41/41/53	-
26	LHG	d	316	24	-	11/41/41/53	-
35	KC2	i	616	-	-	10/15/71/71	-
26	LHG	f	619	24	-	22/41/41/53	-
24	CLA	F	201	36	1/1/15/20	14/37/115/115	-
24	CLA	A	835	-	1/1/15/20	12/37/115/115	-
24	CLA	B	816	-	1/1/13/20	7/30/108/115	-
27	WVN	L	201	-	-	10/29/63/63	0/2/2/2
33	II0	j	315	-	-	5/21/67/67	0/2/2/2
24	CLA	B	824	-	1/1/15/20	3/37/115/115	-
24	CLA	B	834	-	1/1/11/20	2/16/94/115	-
24	CLA	B	828	-	-	4/18/96/115	-
24	CLA	A	831	-	1/1/15/20	9/37/115/115	-
24	CLA	g	308	-	1/1/15/20	18/37/115/115	-
24	CLA	d	305	-	-	5/21/99/115	-
27	WVN	J	101	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	820	36	1/1/15/20	5/37/115/115	-
24	CLA	j	314	-	1/1/15/20	14/37/115/115	-
32	LMG	b	301	-	-	17/50/70/70	0/1/1/1
24	CLA	A	821	-	1/1/11/20	7/18/96/115	-
34	IHT	f	617	-	-	4/25/65/65	0/2/2/2
24	CLA	A	812	-	1/1/15/20	22/37/115/115	-
24	CLA	B	807	-	1/1/15/20	10/37/115/115	-
26	LHG	A	844	-	-	7/52/52/53	-
24	CLA	g	311	26	1/1/12/20	10/24/102/115	-
27	WVN	L	205	-	-	6/29/63/63	0/2/2/2
26	LHG	g	301	-	-	14/53/53/53	-
24	CLA	A	803	-	1/1/13/20	6/25/103/115	-
27	WVN	B	847	-	-	12/29/63/63	0/2/2/2
24	CLA	A	824	36	1/1/15/20	11/37/115/115	-
35	KC2	j	312	19	-	5/15/71/71	-
24	CLA	i	601	20	1/1/12/20	9/21/99/115	-
27	WVN	K	103	-	-	6/29/63/63	0/2/2/2
26	LHG	b	302	24	-	13/53/53/53	-
24	CLA	g	306	22	1/1/12/20	7/21/99/115	-
27	WVN	B	846	-	-	0/29/63/63	0/2/2/2
24	CLA	A	810	-	1/1/14/20	8/34/112/115	-
24	CLA	B	819	-	-	3/15/93/115	-
34	IHT	k	618	-	-	7/25/65/65	0/2/2/2
24	CLA	k	606	18	-	6/21/99/115	-
33	II0	g	317	-	-	5/21/67/67	0/2/2/2
24	CLA	L	203	-	1/1/15/20	11/37/115/115	-
24	CLA	b	311	-	1/1/12/20	6/21/99/115	-
24	CLA	J	103	8	1/1/10/20	5/10/88/115	-
24	CLA	g	307	22	1/1/12/20	7/21/99/115	-
33	II0	f	615	-	-	4/21/67/67	0/2/2/2
24	CLA	B	826	-	1/1/15/20	9/37/115/115	-
24	CLA	b	310	26	1/1/15/20	11/37/115/115	-
24	CLA	e	602	17	1/1/12/20	6/19/97/115	-
24	CLA	j	308	-	1/1/12/20	8/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	810	-	1/1/13/20	5/25/101/115	-
24	CLA	k	610	26	1/1/12/20	11/21/99/115	-
24	CLA	b	307	36	1/1/15/20	10/37/115/115	-
24	CLA	B	804	-	1/1/15/20	9/37/115/115	-
24	CLA	B	803	-	1/1/15/20	19/37/115/115	-
33	II0	j	316	-	-	2/21/67/67	0/2/2/2
24	CLA	B	817	-	-	7/28/106/115	-
33	II0	a	314	-	-	7/21/67/67	0/2/2/2
24	CLA	i	606	20	1/1/14/20	11/33/111/115	-
24	CLA	c	612	-	1/1/15/20	11/37/115/115	-
24	CLA	g	310	22	1/1/12/20	6/21/99/115	-
35	KC2	d	311	-	-	7/15/71/71	-
24	CLA	g	305	22	1/1/15/20	16/37/115/115	-
26	LHG	e	617	24	-	11/41/41/53	-
33	II0	a	317	-	-	7/21/67/67	0/2/2/2
33	II0	d	313	-	-	6/21/67/67	0/2/2/2
33	II0	c	614	-	-	1/21/67/67	0/2/2/2
24	CLA	A	830	-	1/1/12/20	4/19/97/115	-
28	LMT	F	203	-	-	4/15/35/61	0/1/1/2
24	CLA	a	302	14	1/1/12/20	9/22/100/115	-
24	CLA	K	101	36	1/1/12/20	3/21/99/115	-
24	CLA	F	202	6	1/1/12/20	11/22/100/115	-
24	CLA	a	305	36	1/1/15/20	9/37/115/115	-
24	CLA	B	813	-	1/1/14/20	14/31/109/115	-
24	CLA	a	303	14	1/1/12/20	6/19/97/115	-
26	LHG	b	320	24	-	17/53/53/53	-
33	II0	i	612	-	-	7/21/67/67	0/2/2/2
27	WVN	F	205	-	-	12/29/63/63	0/2/2/2
24	CLA	i	605	20	1/1/12/20	6/21/99/115	-
34	IHT	O	203	-	-	5/25/65/65	0/2/2/2
24	CLA	f	608	19	1/1/15/20	9/37/115/115	-
26	LHG	c	617	24	-	14/41/41/53	-
24	CLA	A	814	-	-	9/19/97/115	-
24	CLA	B	822	36	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	839	-	1/1/15/20	10/37/115/115	-
24	CLA	B	814	-	1/1/13/20	13/30/108/115	-
24	CLA	j	311	26	1/1/14/20	13/33/111/115	-
24	CLA	A	838	26	1/1/12/20	5/22/100/115	-
24	CLA	c	607	13	1/1/11/20	2/15/93/115	-
33	II0	O	202	-	-	3/21/67/67	0/2/2/2
24	CLA	B	821	-	1/1/12/20	7/23/101/115	-
24	CLA	B	830	36	1/1/15/20	13/37/115/115	-
24	CLA	B	838	-	1/1/13/20	9/28/106/115	-
24	CLA	d	309	26	1/1/10/20	0/8/86/115	-
27	WVN	M	101	-	-	9/29/63/63	0/2/2/2
27	WVN	h	308	-	-	5/29/63/63	0/2/2/2
24	CLA	j	306	19	1/1/11/20	5/13/91/115	-
24	CLA	L	202	9	1/1/11/20	9/18/96/115	-
24	CLA	c	601	13	1/1/12/20	10/21/99/115	-
33	II0	d	314	-	-	5/21/67/67	0/2/2/2
24	CLA	b	303	15	1/1/12/20	7/21/99/115	-
24	CLA	B	818	36	1/1/15/20	7/37/115/115	-
27	WVN	J	102	-	-	8/29/63/63	0/2/2/2
24	CLA	a	310	14	1/1/15/20	13/37/115/115	-
24	CLA	b	313	-	1/1/15/20	23/37/115/115	-
24	CLA	e	607	17	1/1/15/20	10/37/115/115	-
27	WVN	B	849	-	-	13/29/63/63	0/2/2/2
32	LMG	F	206	-	-	11/43/63/70	0/1/1/1
32	LMG	L	208	24	-	19/50/70/70	0/1/1/1
24	CLA	B	805	-	1/1/15/20	17/37/115/115	-
33	II0	g	316	-	-	7/21/67/67	0/2/2/2
24	CLA	B	833	-	1/1/15/20	9/37/115/115	-
26	LHG	J	107	24	-	19/53/53/53	-
24	CLA	c	605	13	1/1/12/20	7/21/99/115	-
33	II0	g	318	-	-	2/21/67/67	0/2/2/2
29	SF4	C	102	3	-	-	0/6/5/5
24	CLA	g	309	22	1/1/15/20	6/37/115/115	-
33	II0	e	612	-	-	4/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	h	303	-	1/1/12/20	5/21/99/115	-
24	CLA	A	855	36	1/1/15/20	16/37/115/115	-
24	CLA	A	823	-	1/1/13/20	6/25/103/115	-
28	LMT	a	318	-	-	3/21/61/61	0/2/2/2
33	II0	f	616	-	-	5/21/67/67	0/2/2/2
24	CLA	f	606	19	-	2/21/99/115	-
24	CLA	k	604	18	1/1/15/20	11/37/115/115	-
33	II0	e	616	-	-	5/21/67/67	0/2/2/2
24	CLA	f	604	19	-	8/37/115/115	-
24	CLA	A	808	1	1/1/15/20	11/37/115/115	-
24	CLA	h	304	-	1/1/12/20	6/21/99/115	-
24	CLA	e	611	-	1/1/15/20	14/37/115/115	-
24	CLA	e	605	17	1/1/15/20	15/37/115/115	-
33	II0	a	313	-	-	1/21/67/67	0/2/2/2
24	CLA	B	811	-	1/1/13/20	6/25/103/115	-
24	CLA	f	602	19	1/1/15/20	17/37/115/115	-
28	LMT	b	319	-	-	9/15/35/61	0/1/1/2
28	LMT	A	851	-	-	9/21/61/61	0/2/2/2
35	KC2	e	609	17	-	5/15/71/71	-
24	CLA	i	604	20	1/1/15/20	12/37/115/115	-
24	CLA	h	302	16	1/1/12/20	9/19/97/115	-
24	CLA	a	309	26	1/1/11/20	6/17/95/115	-
24	CLA	k	601	18	1/1/12/20	10/21/99/115	-
24	CLA	B	809	2	1/1/15/20	11/37/115/115	-
24	CLA	d	303	21	1/1/15/20	17/37/115/115	-
24	CLA	i	610	-	1/1/12/20	7/21/99/115	-
24	CLA	A	804	-	1/1/15/20	7/37/115/115	-
26	LHG	A	845	24	-	6/31/31/53	-
24	CLA	e	610	36	-	14/37/115/115	-
24	CLA	c	608	13	1/1/15/20	17/37/115/115	-
24	CLA	A	839	1	1/1/15/20	15/37/115/115	-
24	CLA	A	856	26	1/1/10/20	4/8/86/115	-
24	CLA	k	614	-	-	7/21/99/115	-
34	IHT	b	316	-	-	3/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	KC2	f	611	19	-	7/15/71/71	-
24	CLA	b	304	15	1/1/13/20	8/25/103/115	-
33	II0	k	617	-	-	3/21/67/67	0/2/2/2
33	II0	h	309	-	-	3/17/40/67	0/1/1/2
34	IHT	R	204	-	-	4/25/65/65	0/2/2/2
26	LHG	f	620	-	-	17/53/53/53	-
24	CLA	B	801	36	1/1/15/20	13/37/115/115	-
24	CLA	f	610	26	1/1/15/20	15/37/115/115	-
24	CLA	e	604	36	1/1/15/20	9/37/115/115	-
27	WVN	A	847	-	-	10/29/63/63	0/2/2/2
24	CLA	B	836	-	1/1/15/20	25/37/115/115	-
33	II0	j	318	-	-	5/21/67/67	0/2/2/2
24	CLA	e	608	26	1/1/11/20	10/15/93/115	-
33	II0	k	619	-	-	5/21/67/67	0/2/2/2
24	CLA	B	841	26	-	3/37/115/115	-
26	LHG	k	620	24	-	14/41/41/53	-
24	CLA	A	807	1	1/1/15/20	9/37/115/115	-
33	II0	e	613	-	-	6/21/67/67	0/2/2/2
24	CLA	j	307	19	1/1/12/20	9/21/99/115	-
24	CLA	d	301	21	1/1/12/20	7/19/97/115	-
24	CLA	k	608	18	1/1/15/20	14/37/115/115	-
32	LMG	O	204	-	-	7/21/41/70	0/1/1/1
24	CLA	A	815	36	1/1/11/20	7/13/91/115	-
33	II0	f	618	-	-	7/21/67/67	0/2/2/2
33	II0	h	310	-	-	8/21/67/67	0/2/2/2
35	KC2	i	609	20	-	9/15/71/71	-
33	II0	c	613	-	-	3/21/67/67	0/2/2/2
24	CLA	B	820	-	-	8/25/103/115	-
24	CLA	B	832	-	1/1/13/20	8/29/107/115	-
26	LHG	g	321	24	-	12/41/41/53	-
35	KC2	c	610	-	-	10/15/71/71	-
24	CLA	A	822	-	1/1/12/20	6/21/99/115	-
26	LHG	c	618	24	-	11/41/41/53	-
24	CLA	A	842	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	WVN	B	845	-	-	6/29/63/63	0/2/2/2
24	CLA	a	312	-	1/1/11/20	6/17/95/115	-
34	IHT	j	317	-	-	7/25/65/65	0/2/2/2
24	CLA	f	605	19	-	7/13/91/115	-
24	CLA	g	322	32	1/1/15/20	13/37/115/115	-
26	LHG	j	319	24	-	5/34/34/53	-
24	CLA	K	102	-	1/1/10/20	5/10/88/115	-
27	WVN	R	201	-	-	6/29/63/63	0/2/2/2
31	LMU	B	844	-	-	8/21/61/61	0/2/2/2
24	CLA	B	815	-	1/1/13/20	7/25/103/115	-
27	WVN	F	204	-	-	10/29/63/63	0/2/2/2
24	CLA	A	828	-	1/1/15/20	8/37/115/115	-
34	IHT	c	615	-	-	10/25/65/65	0/2/2/2
33	II0	c	616	-	-	3/21/67/67	0/2/2/2
24	CLA	j	303	19	1/1/12/20	2/19/97/115	-
24	CLA	A	819	-	1/1/11/20	5/13/91/115	-
24	CLA	i	603	-	1/1/12/20	4/21/99/115	-
35	KC2	g	313	35	-	2/15/71/71	-
24	CLA	B	840	-	-	11/37/115/115	-
24	CLA	A	811	-	1/1/12/20	7/24/102/115	-
24	CLA	h	306	16	1/1/13/20	7/28/106/115	-
24	CLA	c	611	-	1/1/11/20	5/13/91/115	-
26	LHG	a	301	24	-	15/53/53/53	-
24	CLA	b	312	15	1/1/15/20	20/37/115/115	-
24	CLA	A	841	36	1/1/15/20	22/37/115/115	-

The worst 5 of 3566 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	317	IHT	C15-C11	25.48	1.63	1.34
34	R	204	IHT	C15-C11	25.36	1.63	1.34
34	c	615	IHT	C15-C11	25.20	1.63	1.34
34	k	618	IHT	C15-C11	25.15	1.63	1.34
34	j	317	IHT	C15-C11	25.06	1.62	1.34

The worst 5 of 3883 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	617	IHT	C40-C37-C33	-13.58	107.93	127.31
35	f	611	KC2	C1A-NA-C4A	-12.51	101.08	106.71
34	b	317	IHT	C40-C37-C33	-12.44	109.55	127.31
35	k	613	KC2	C1A-NA-C4A	-11.85	101.38	106.71
34	f	617	IHT	C30-C27-C23	-11.73	110.57	127.31

5 of 197 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	801	CLA	ND
24	A	802	CLA	ND
24	A	803	CLA	ND
24	A	804	CLA	ND
24	A	805	CLA	ND

5 of 2931 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	801	CLA	CBD-CGD-O2D-CED
24	A	802	CLA	C1A-C2A-CAA-CBA
24	A	802	CLA	CBA-CGA-O2A-C1
24	A	802	CLA	O1A-CGA-O2A-C1
24	A	802	CLA	C11-C10-C8-C9

There are no ring outliers.

107 monomers are involved in 243 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	834	CLA	1	0
29	C	101	SF4	4	0
24	B	837	CLA	4	0
24	B	835	CLA	4	0
24	B	823	CLA	6	0
29	A	854	SF4	4	0
24	I	102	CLA	2	0
25	B	842	PQN	5	0
24	A	853	CLA	2	0
24	A	840	CLA	5	0
24	A	829	CLA	3	0
24	A	827	CLA	6	0
24	A	852	CLA	2	0
24	B	827	CLA	4	0
24	B	831	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	802	LHG	3	0
24	A	801	CLA	4	0
24	O	205	CLA	6	0
30	B	843	DGD	3	0
24	B	812	CLA	4	0
32	J	106	LMG	3	0
24	O	201	CLA	3	0
24	B	806	CLA	3	0
25	A	843	PQN	2	0
24	B	808	CLA	1	0
24	L	207	CLA	1	0
24	A	813	CLA	2	0
24	B	825	CLA	3	0
24	J	105	CLA	3	0
24	A	809	CLA	3	0
24	B	829	CLA	2	0
24	A	802	CLA	6	0
24	A	805	CLA	1	0
24	A	837	CLA	2	0
24	A	818	CLA	2	0
24	L	204	CLA	1	0
24	A	817	CLA	4	0
24	R	203	CLA	1	0
24	A	806	CLA	6	0
24	A	836	CLA	3	0
24	F	201	CLA	3	0
24	A	835	CLA	3	0
24	B	816	CLA	2	0
24	B	824	CLA	3	0
24	B	834	CLA	3	0
24	B	828	CLA	2	0
24	A	831	CLA	1	0
24	A	820	CLA	4	0
24	A	821	CLA	2	0
24	A	812	CLA	2	0
24	B	807	CLA	2	0
26	A	844	LHG	2	0
24	A	803	CLA	3	0
24	A	824	CLA	2	0
24	A	810	CLA	1	0
24	B	819	CLA	1	0
24	L	203	CLA	4	0

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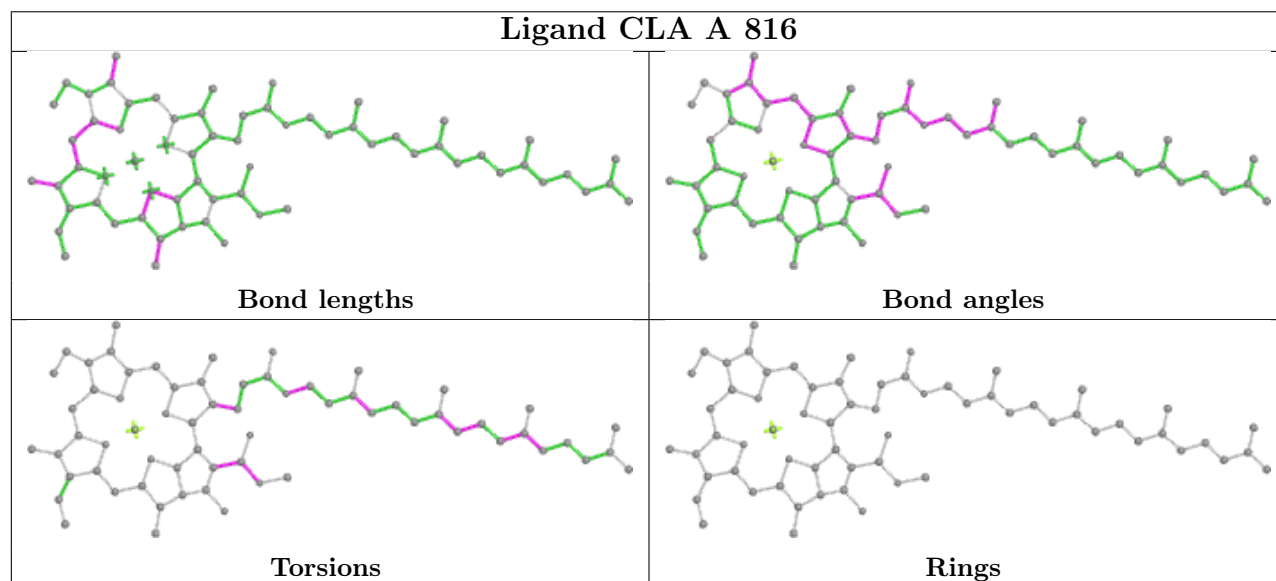
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	J	103	CLA	1	0
24	B	826	CLA	1	0
24	B	810	CLA	2	0
24	B	804	CLA	3	0
24	B	803	CLA	4	0
24	B	817	CLA	2	0
24	A	830	CLA	1	0
24	K	101	CLA	2	0
24	F	202	CLA	2	0
24	A	814	CLA	2	0
24	B	822	CLA	6	0
24	B	839	CLA	2	0
24	B	814	CLA	1	0
24	A	838	CLA	2	0
24	B	821	CLA	1	0
24	B	830	CLA	3	0
24	L	202	CLA	2	0
24	B	818	CLA	1	0
32	F	206	LMG	2	0
32	L	208	LMG	2	0
24	B	805	CLA	1	0
24	B	833	CLA	3	0
26	J	107	LHG	5	0
29	C	102	SF4	3	0
24	A	855	CLA	6	0
24	A	823	CLA	3	0
24	A	808	CLA	1	0
24	B	811	CLA	1	0
28	A	851	LMT	1	0
24	B	809	CLA	1	0
24	A	804	CLA	3	0
26	A	845	LHG	1	0
24	A	839	CLA	5	0
24	A	856	CLA	1	0
24	B	801	CLA	7	0
24	B	836	CLA	5	0
24	B	841	CLA	5	0
24	A	807	CLA	4	0
24	A	815	CLA	2	0
24	B	820	CLA	4	0
24	B	832	CLA	4	0
24	A	822	CLA	2	0

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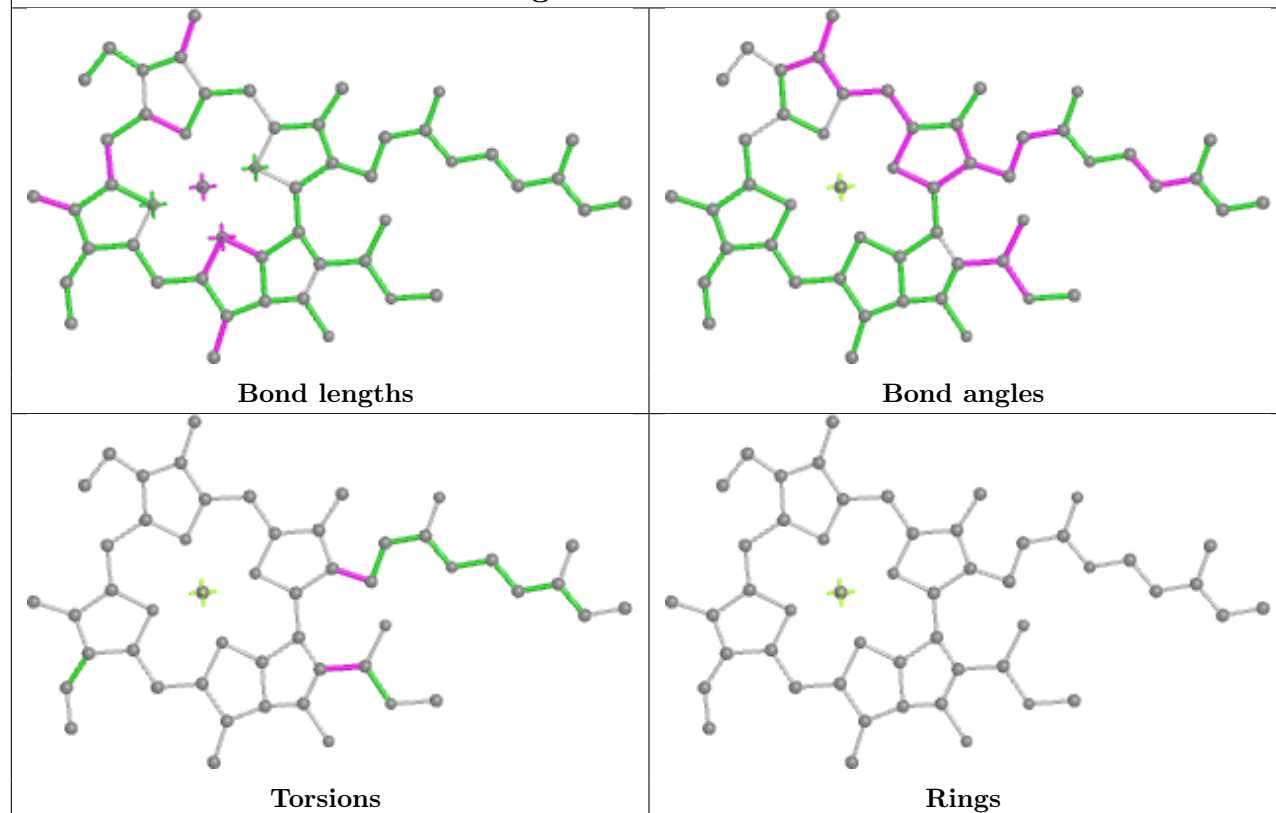
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	842	CLA	8	0
31	B	844	LMU	1	0
24	B	815	CLA	1	0
24	A	828	CLA	2	0
24	A	819	CLA	1	0
24	B	840	CLA	2	0
24	A	811	CLA	2	0
24	A	841	CLA	3	0

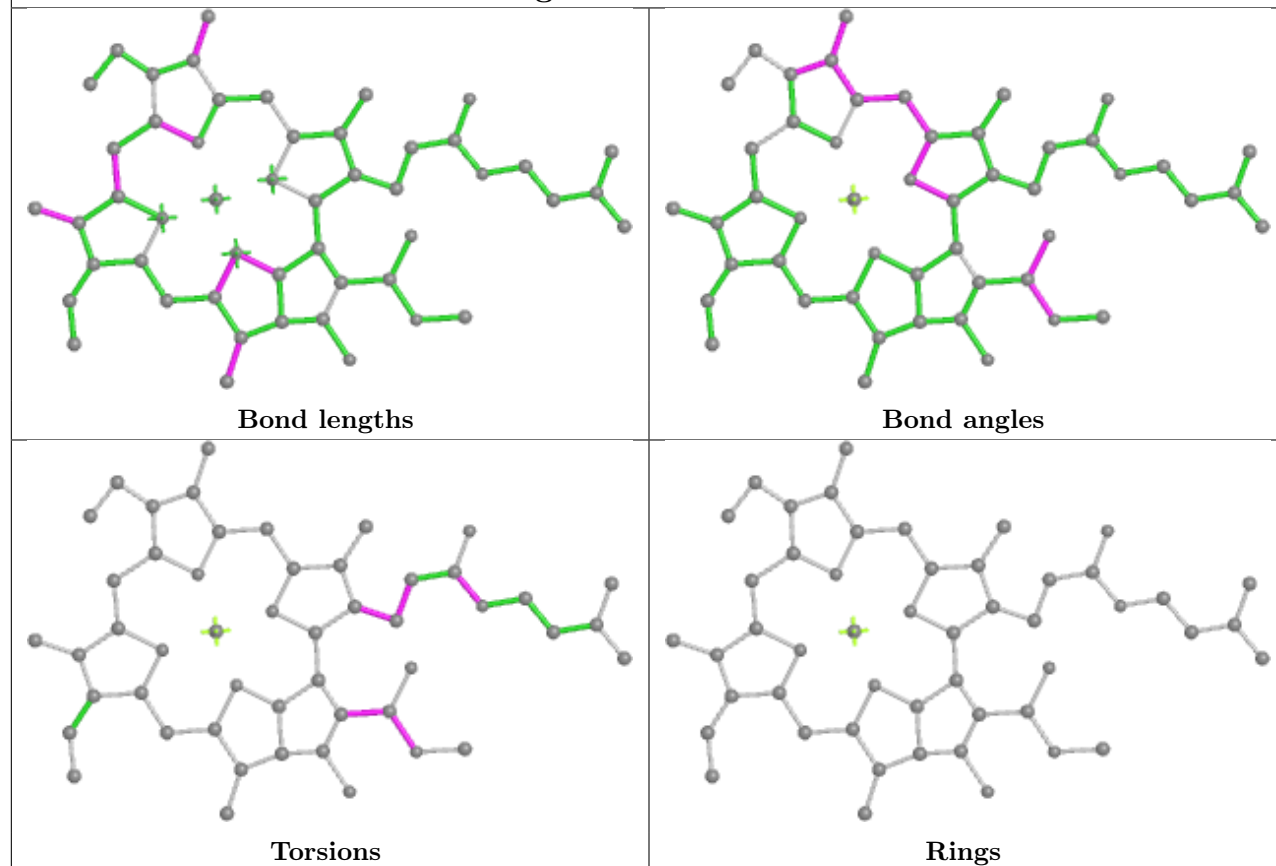
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



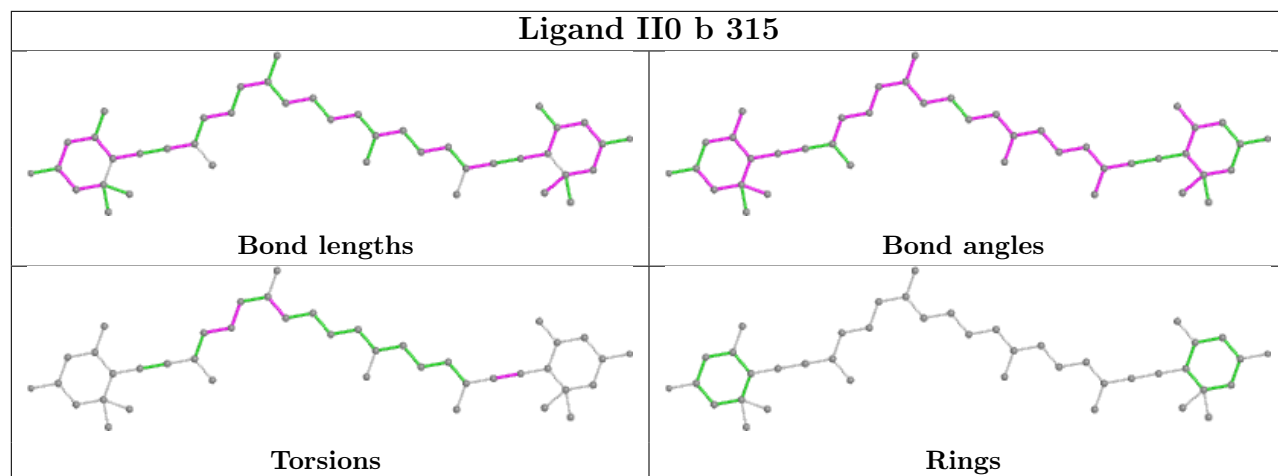
## Ligand CLA A 834



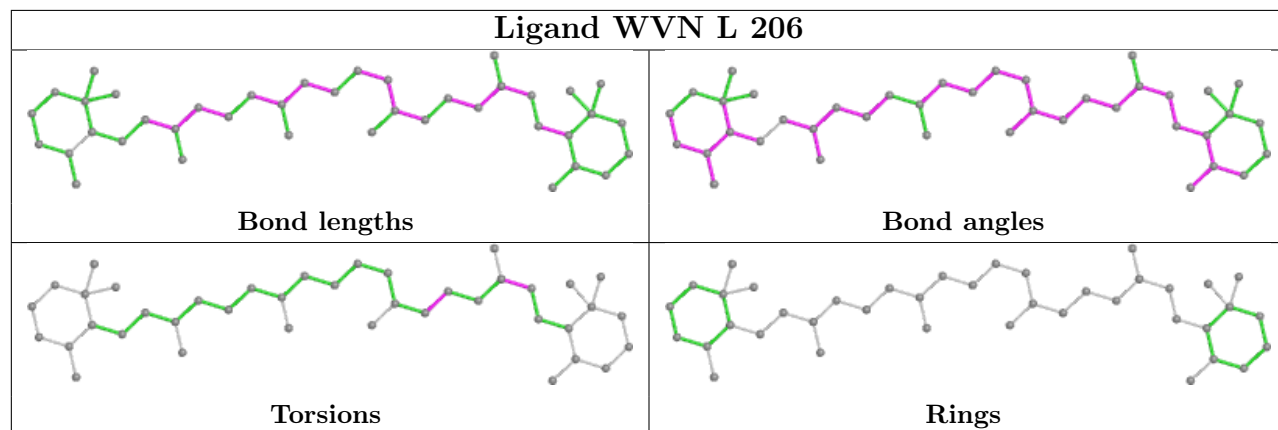
## Ligand CLA h 301



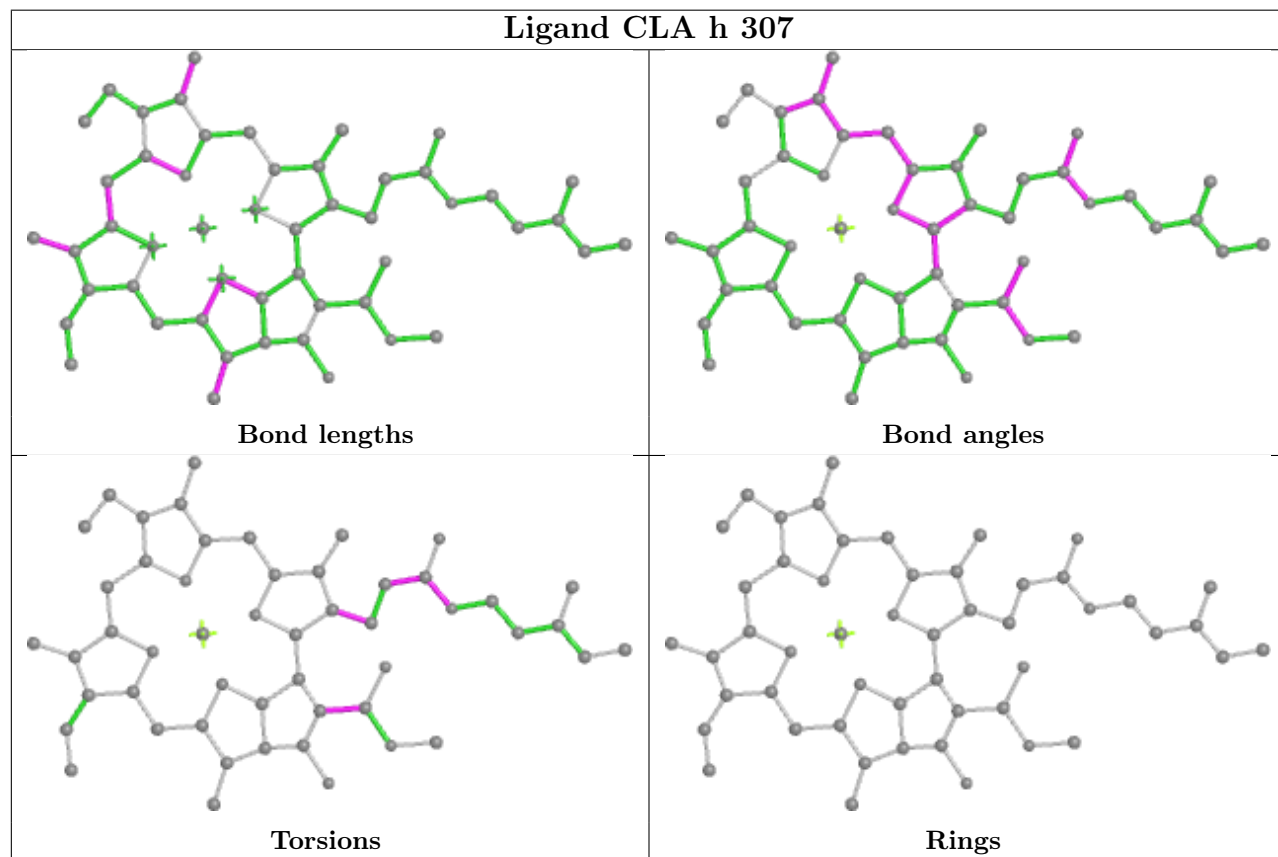
## Ligand II0 b 315

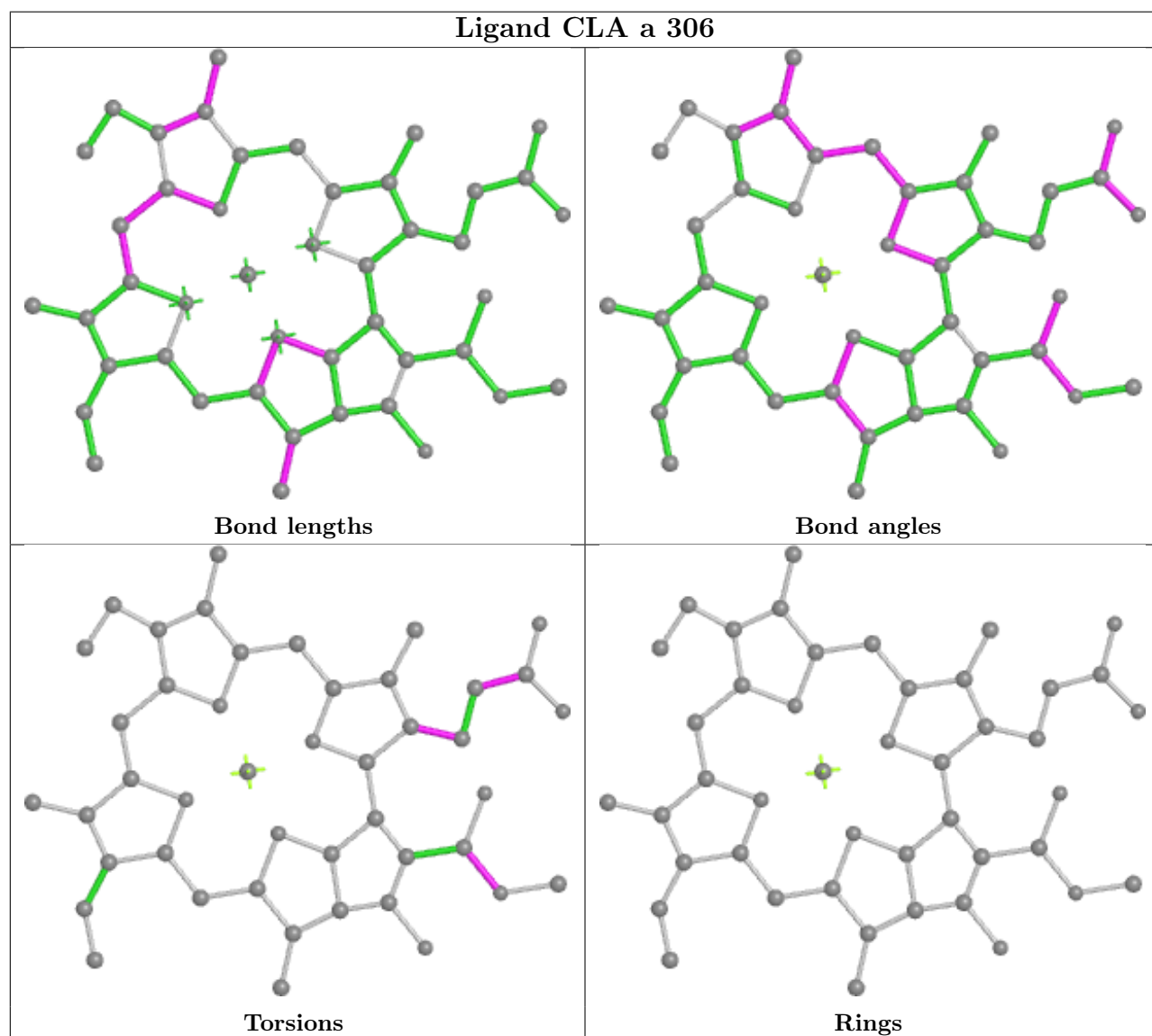
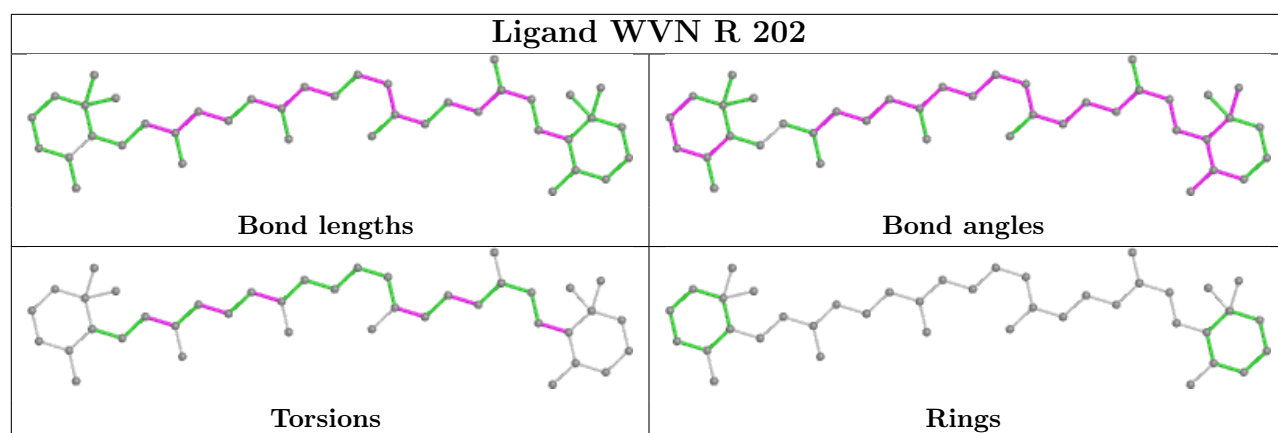


## Ligand WVN L 206



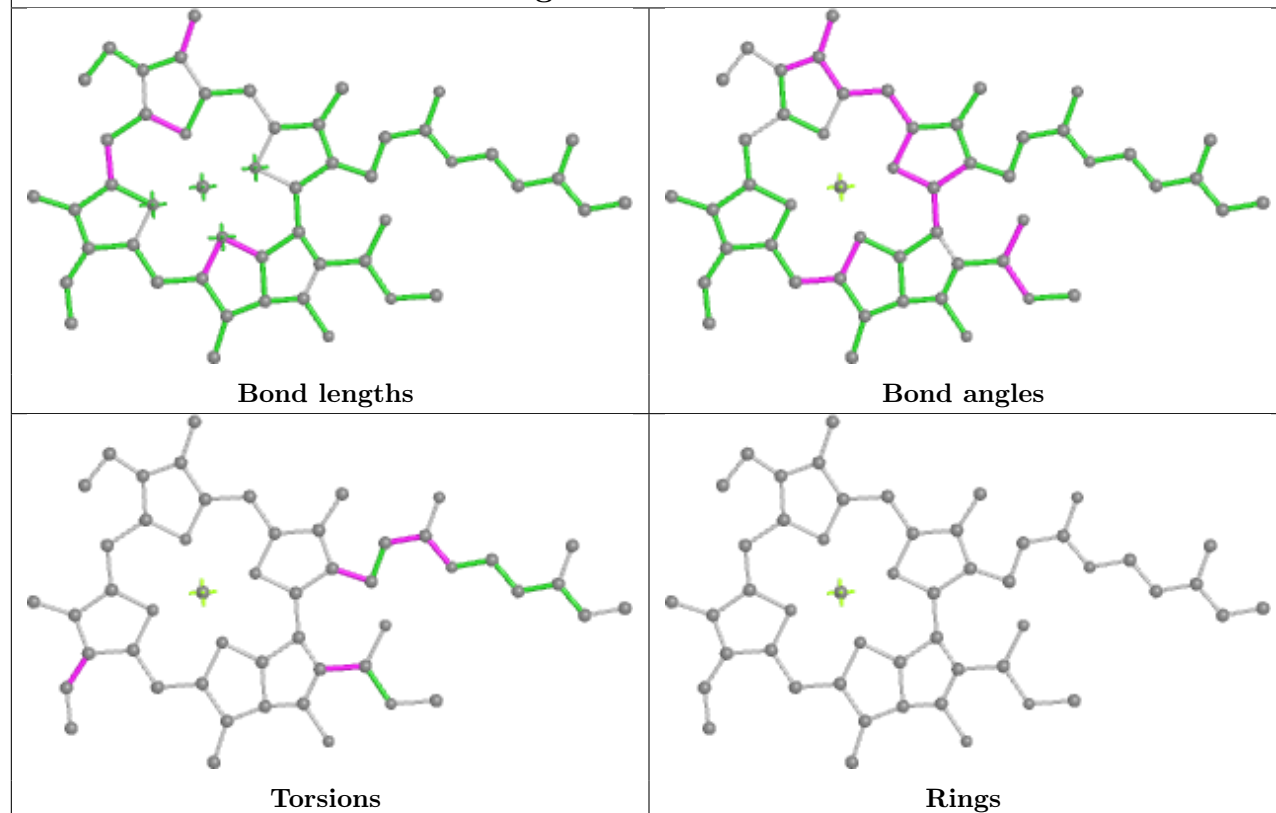
## Ligand CLA h 307



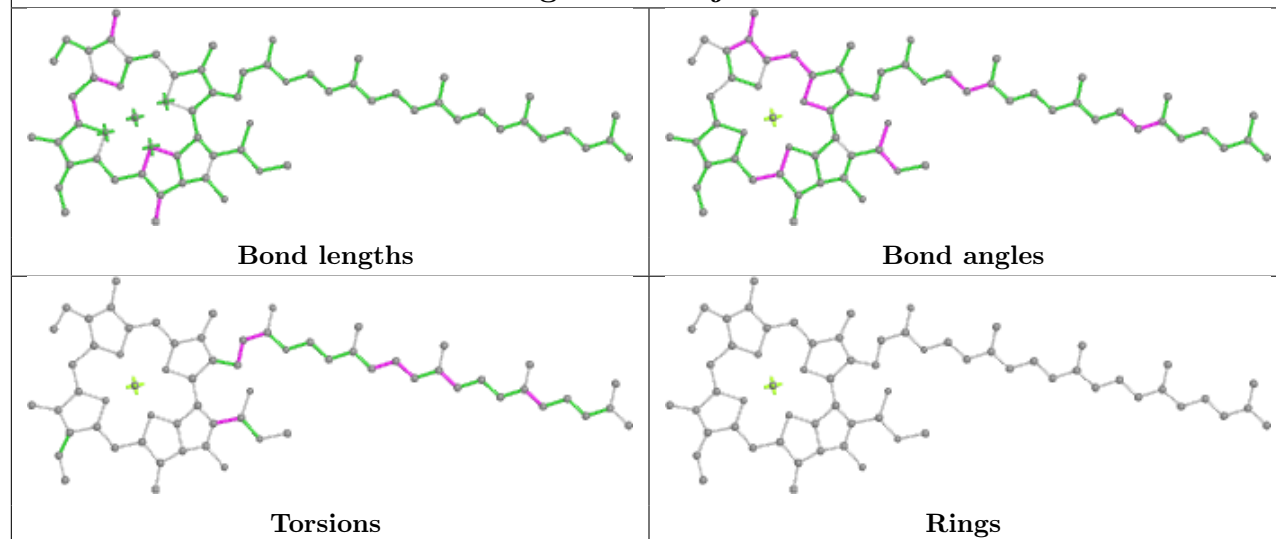




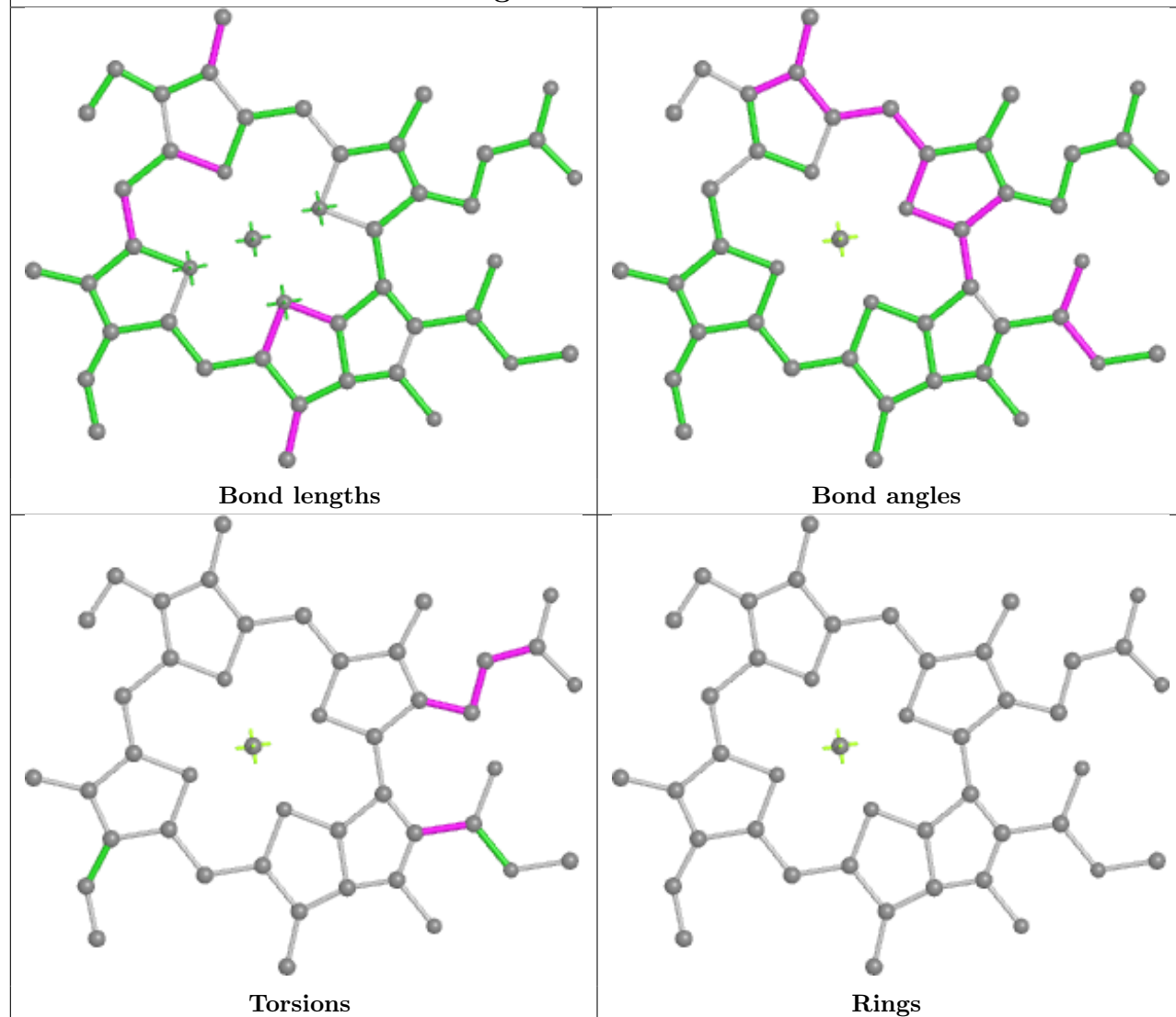
## Ligand CLA d 304



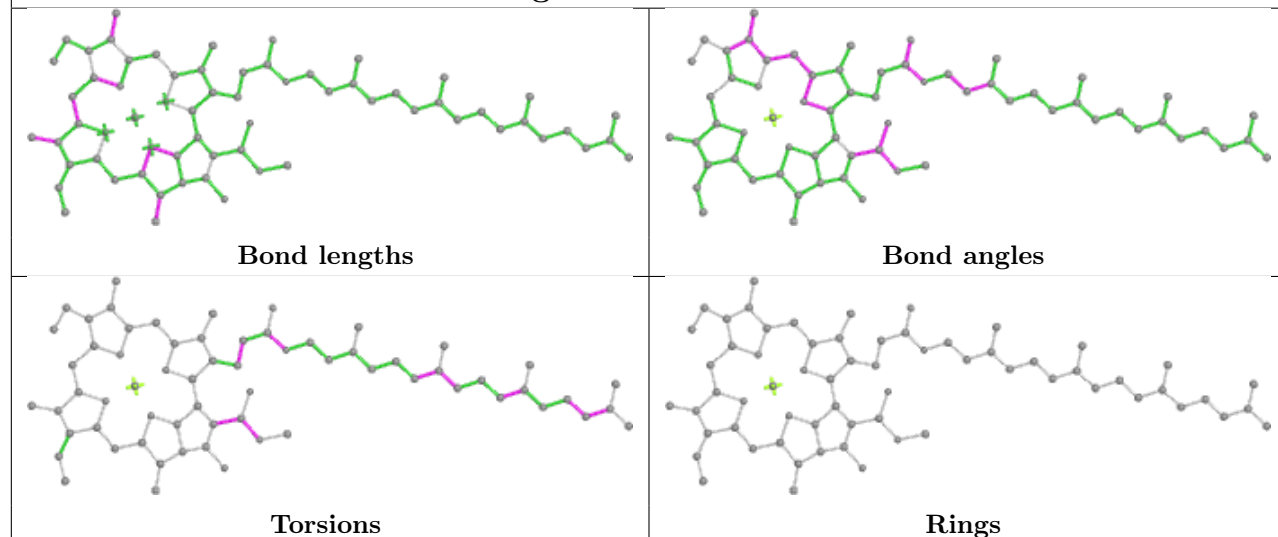
## Ligand CLA j 305

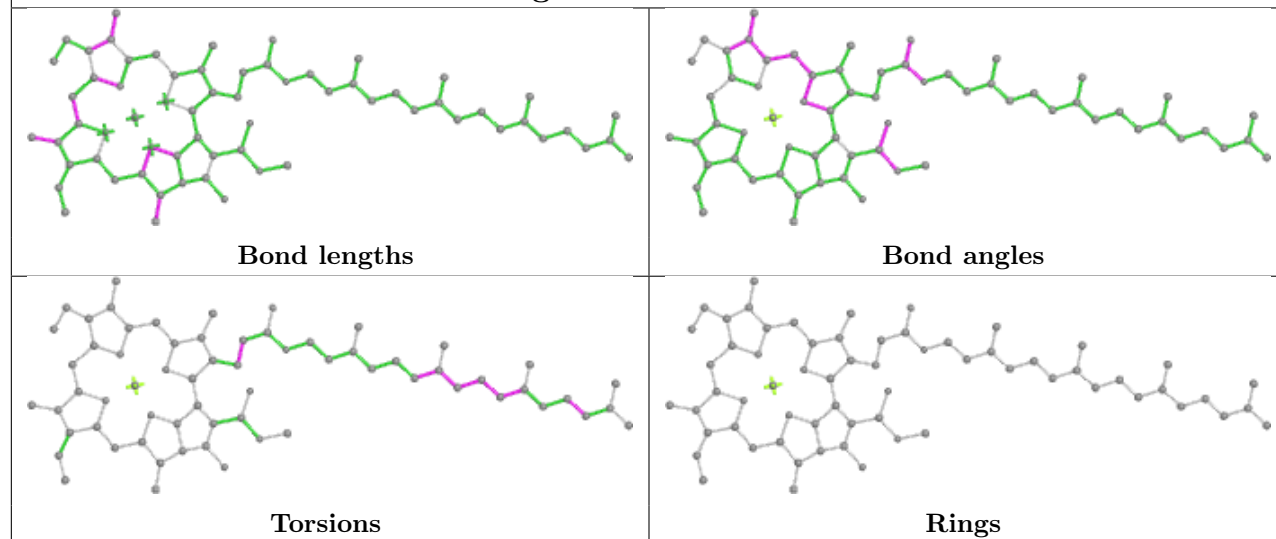
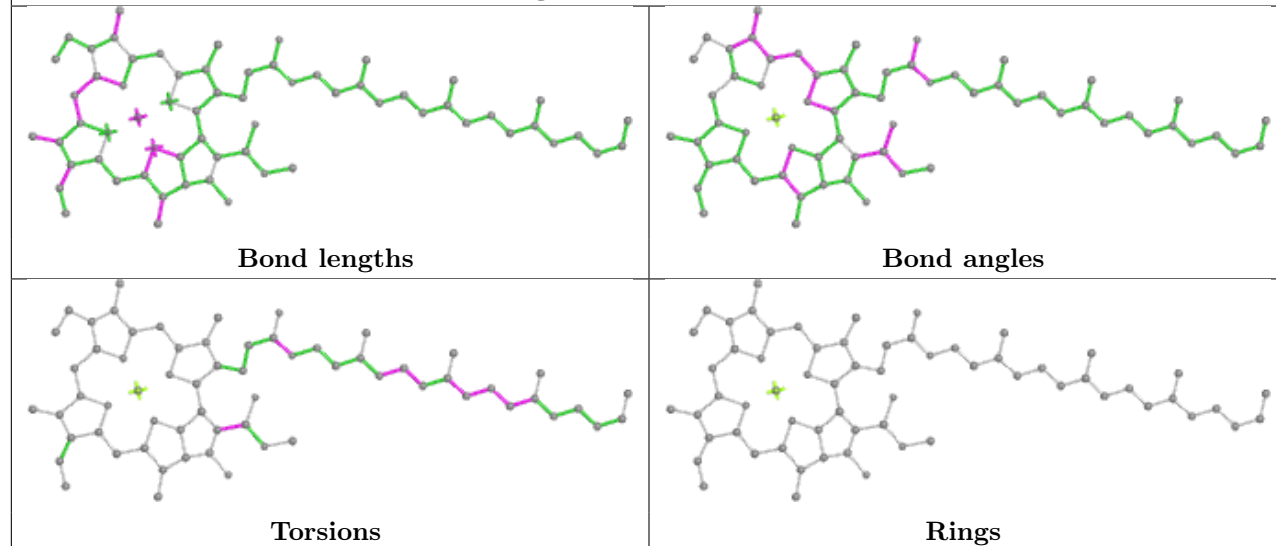
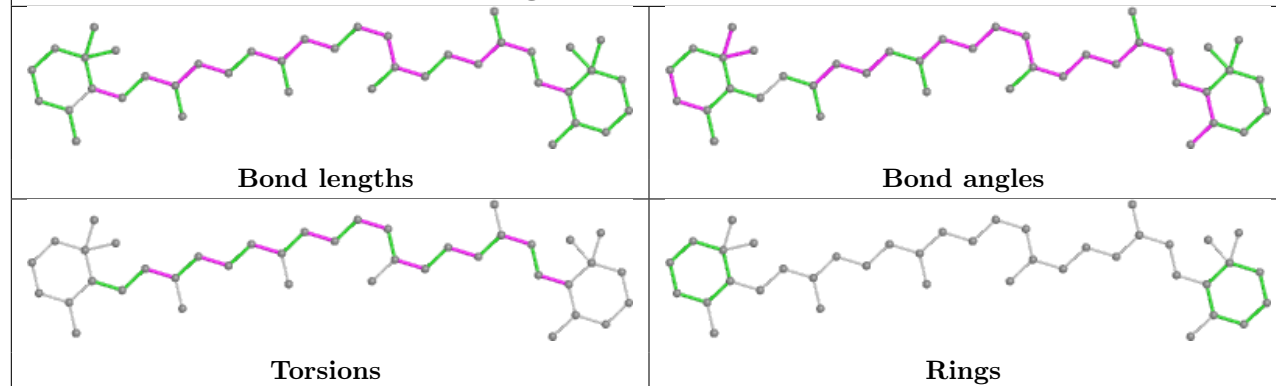


## Ligand CLA e 601

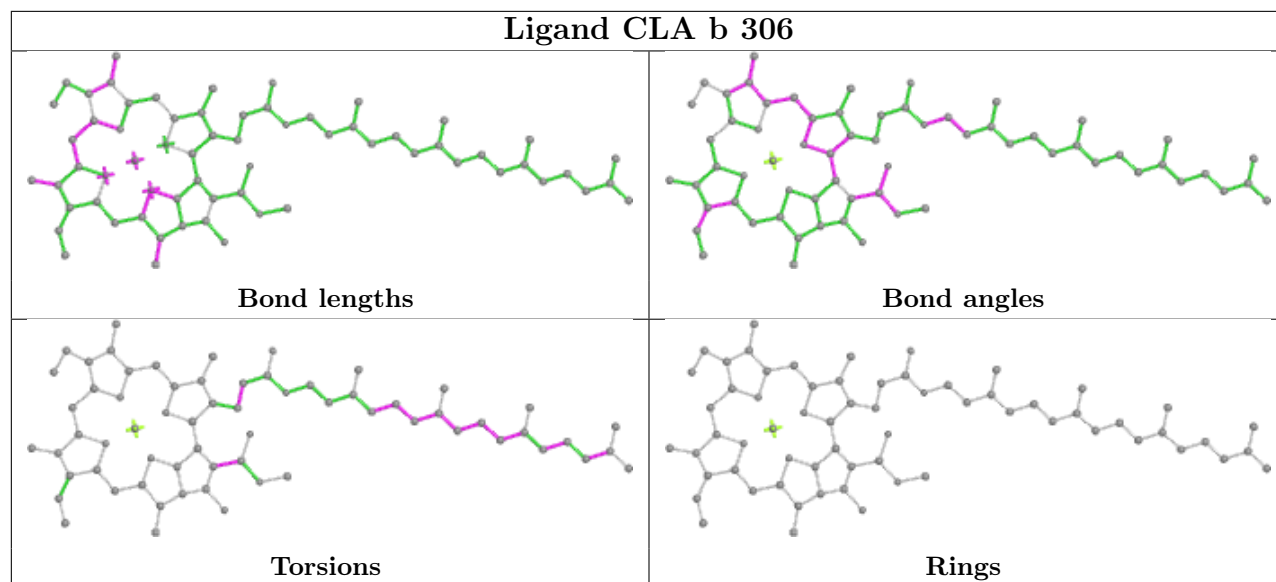


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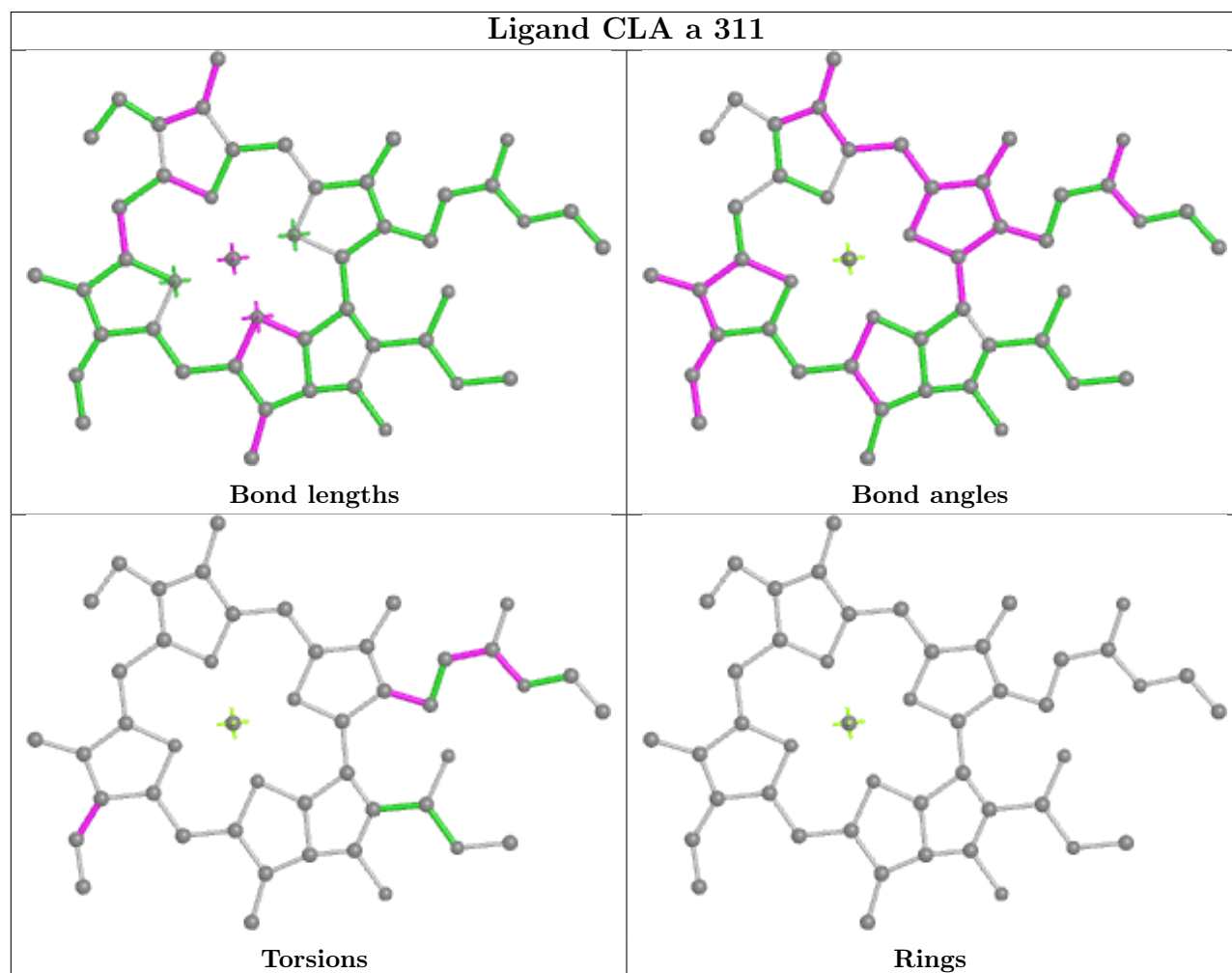


**Ligand CLA B 835****Ligand CLA B 823****Ligand WVN A 850**

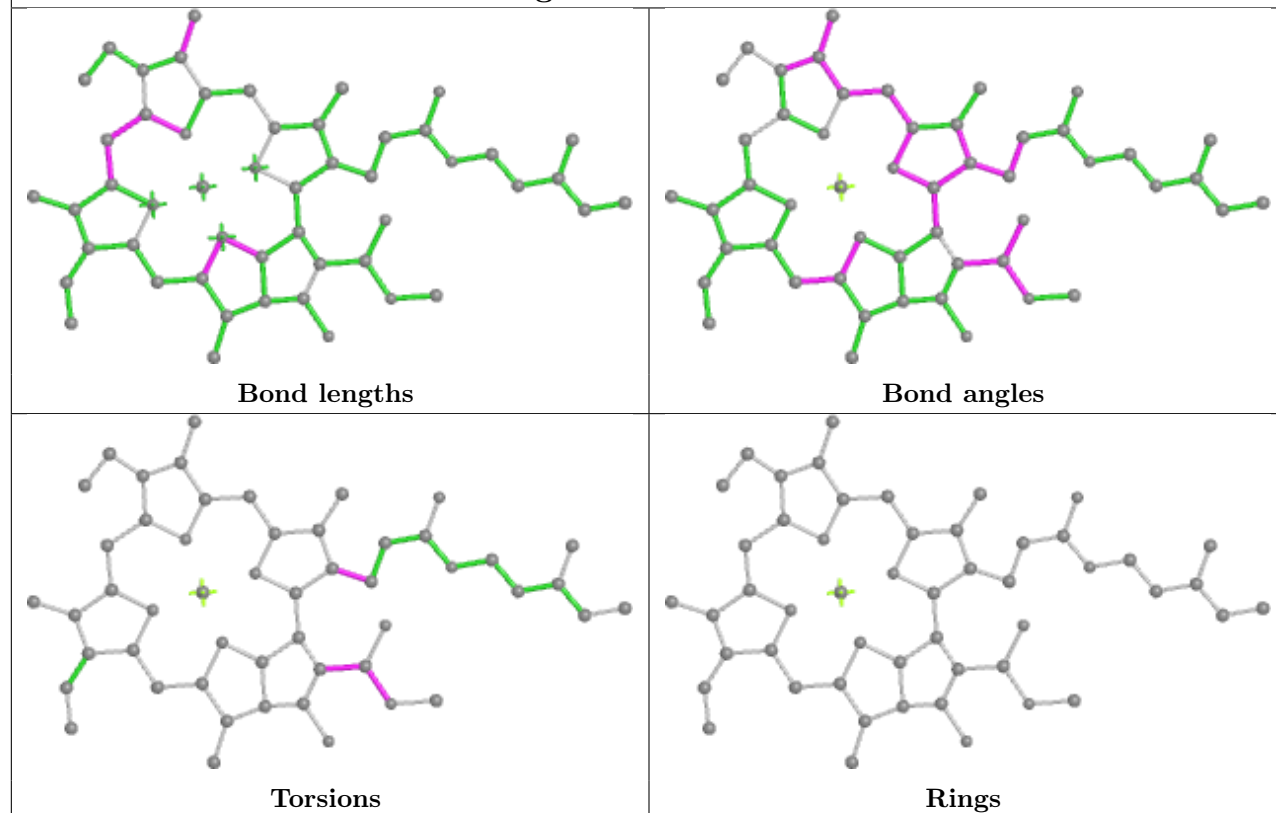
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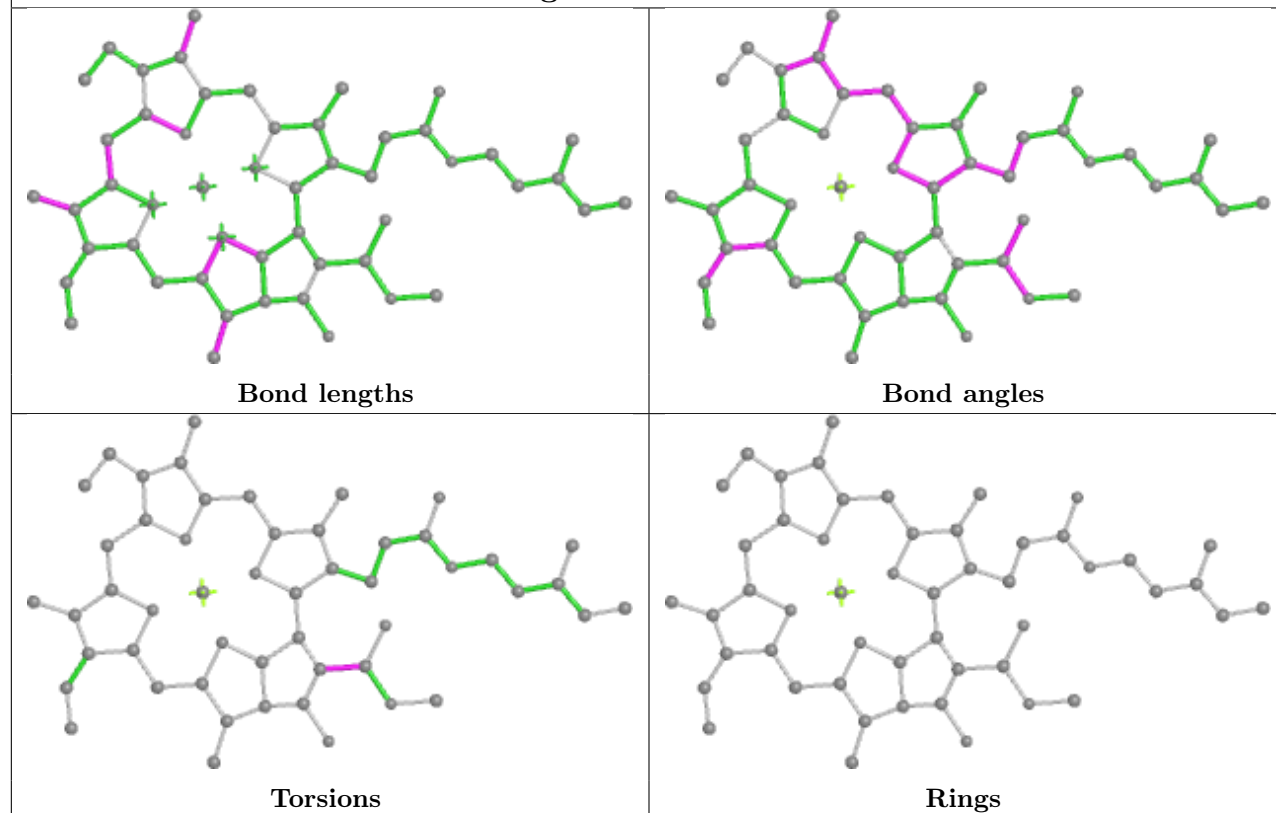
## Ligand CLA a 311



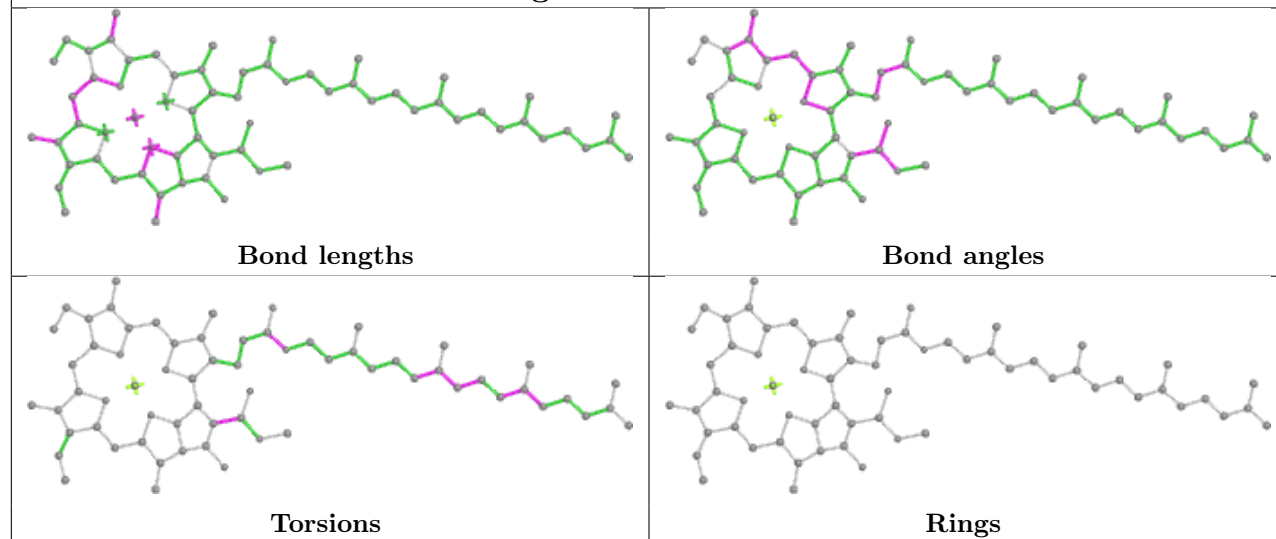
## Ligand CLA d 312



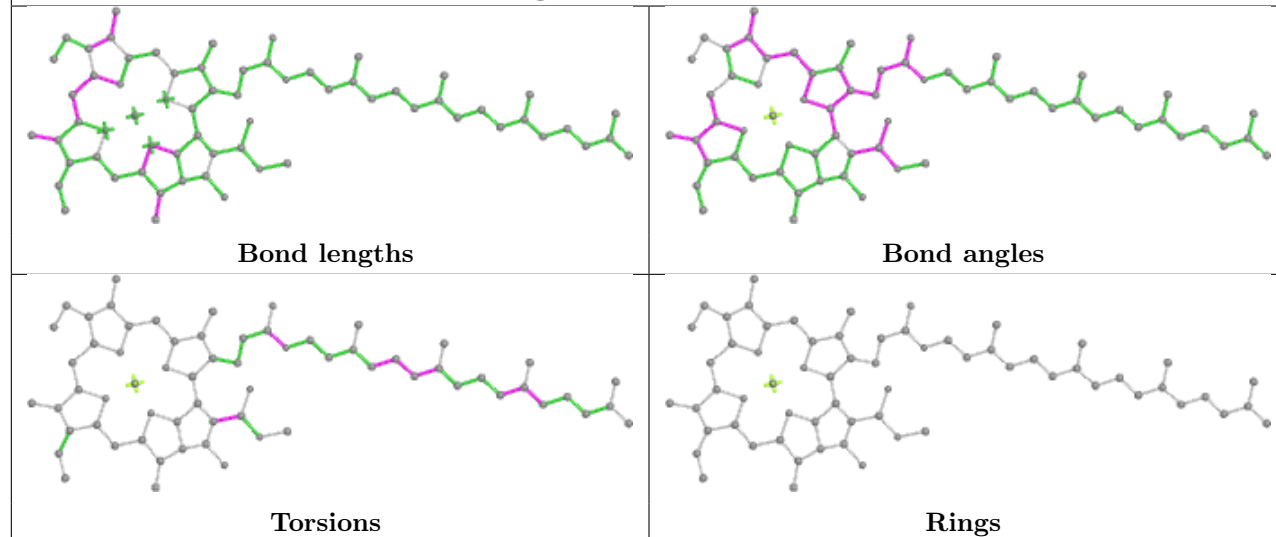
## Ligand CLA i 607

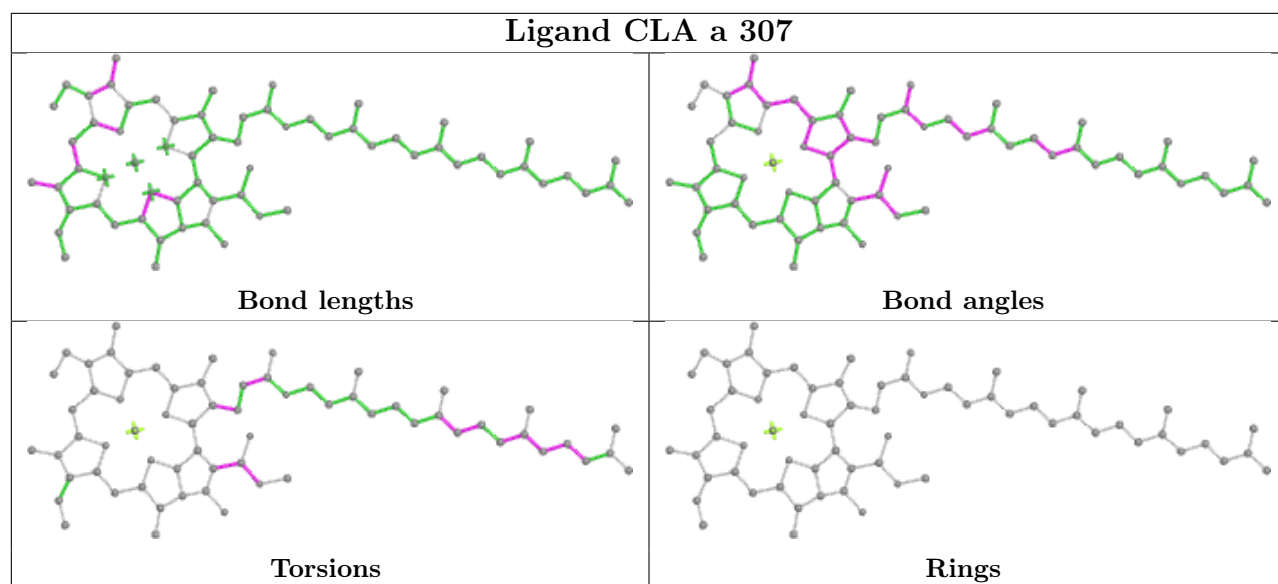
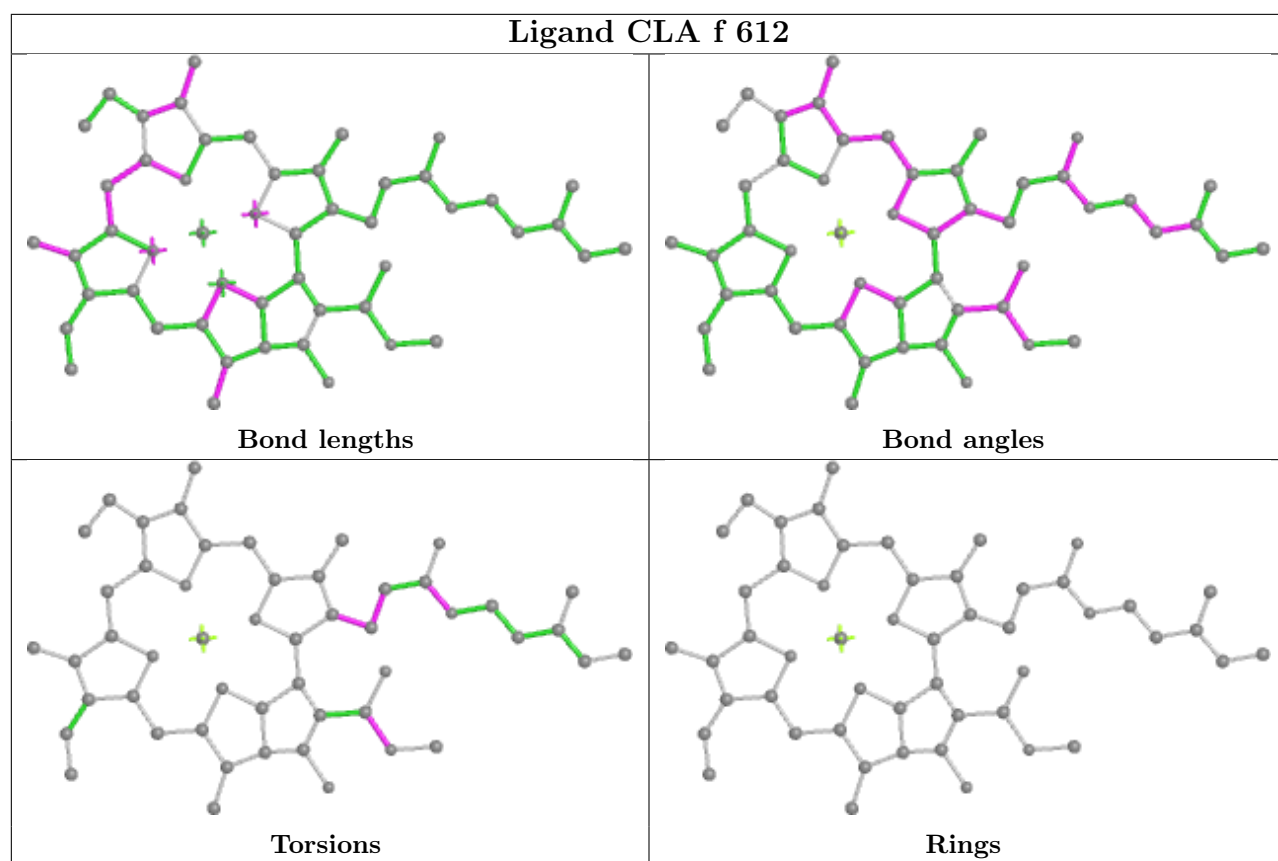


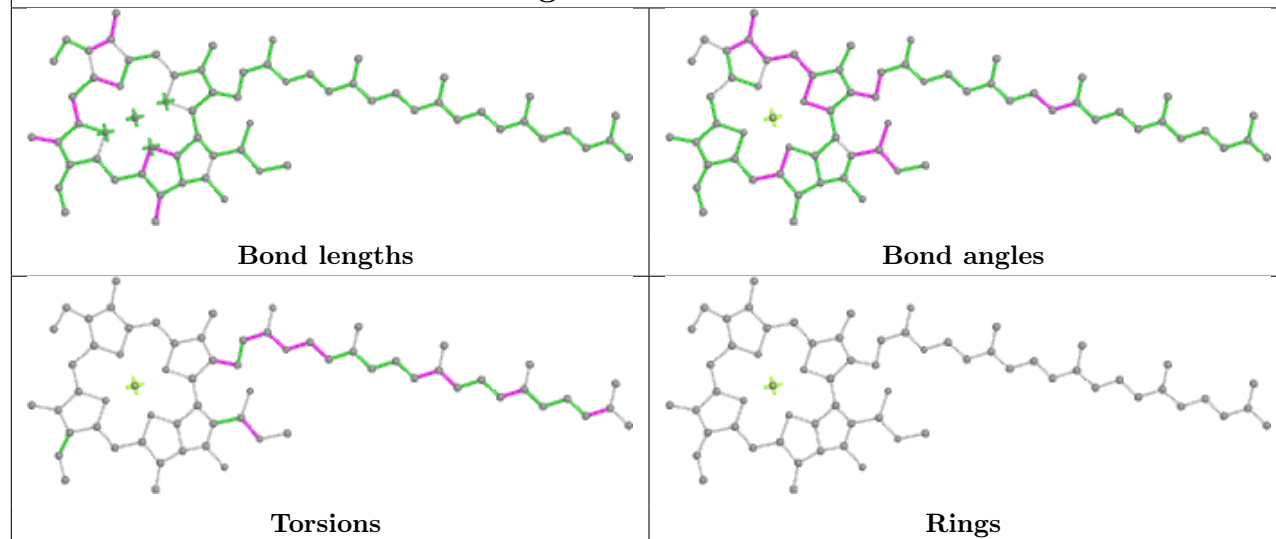
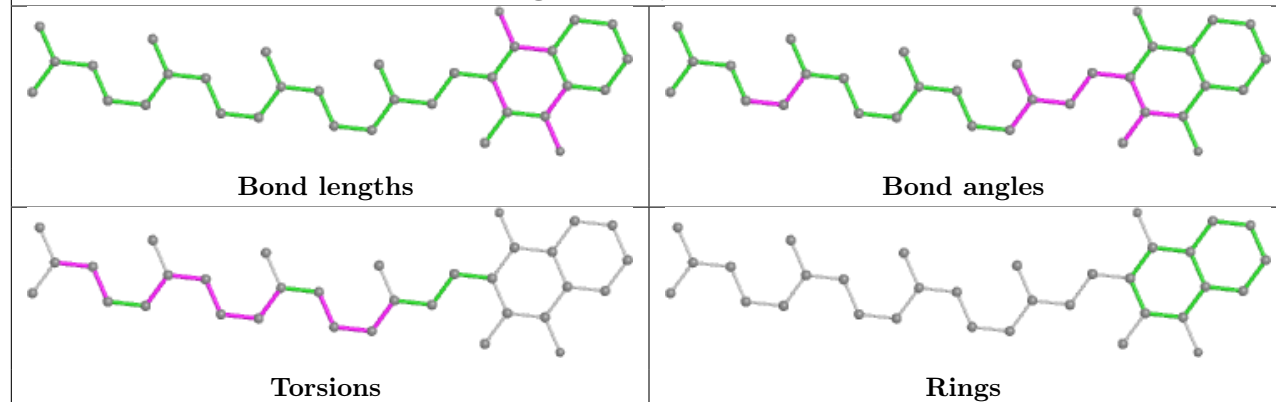
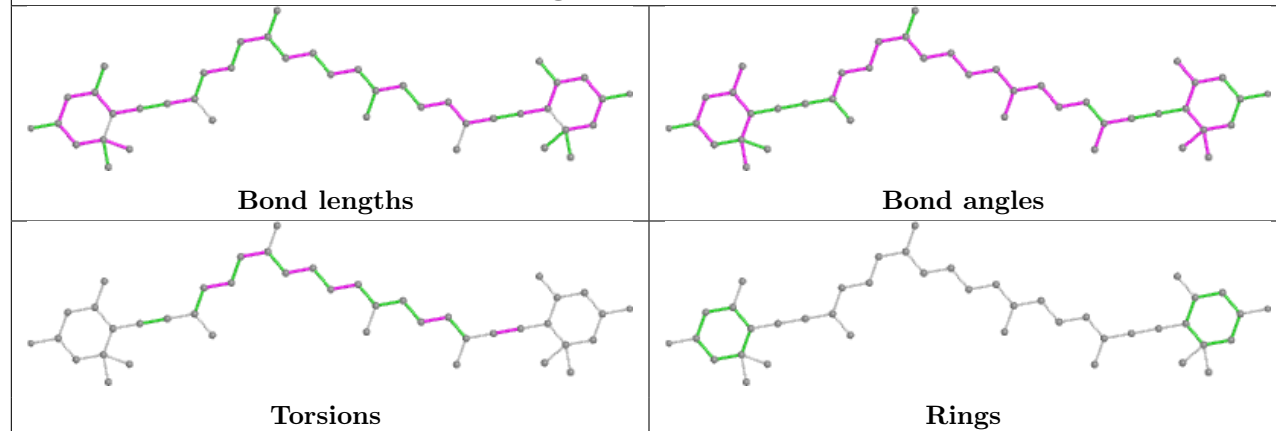
## Ligand CLA A 825



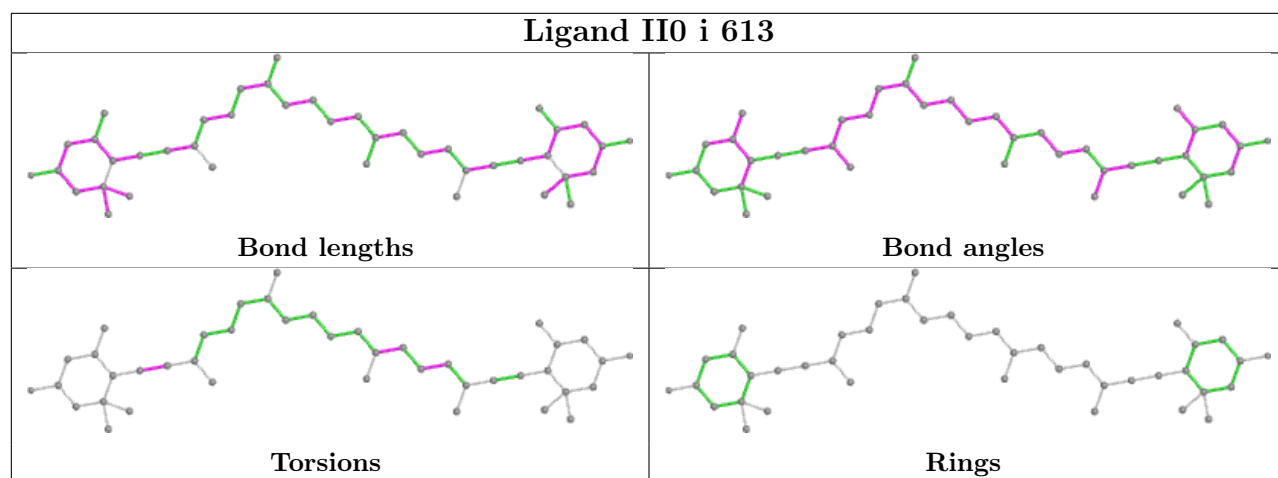
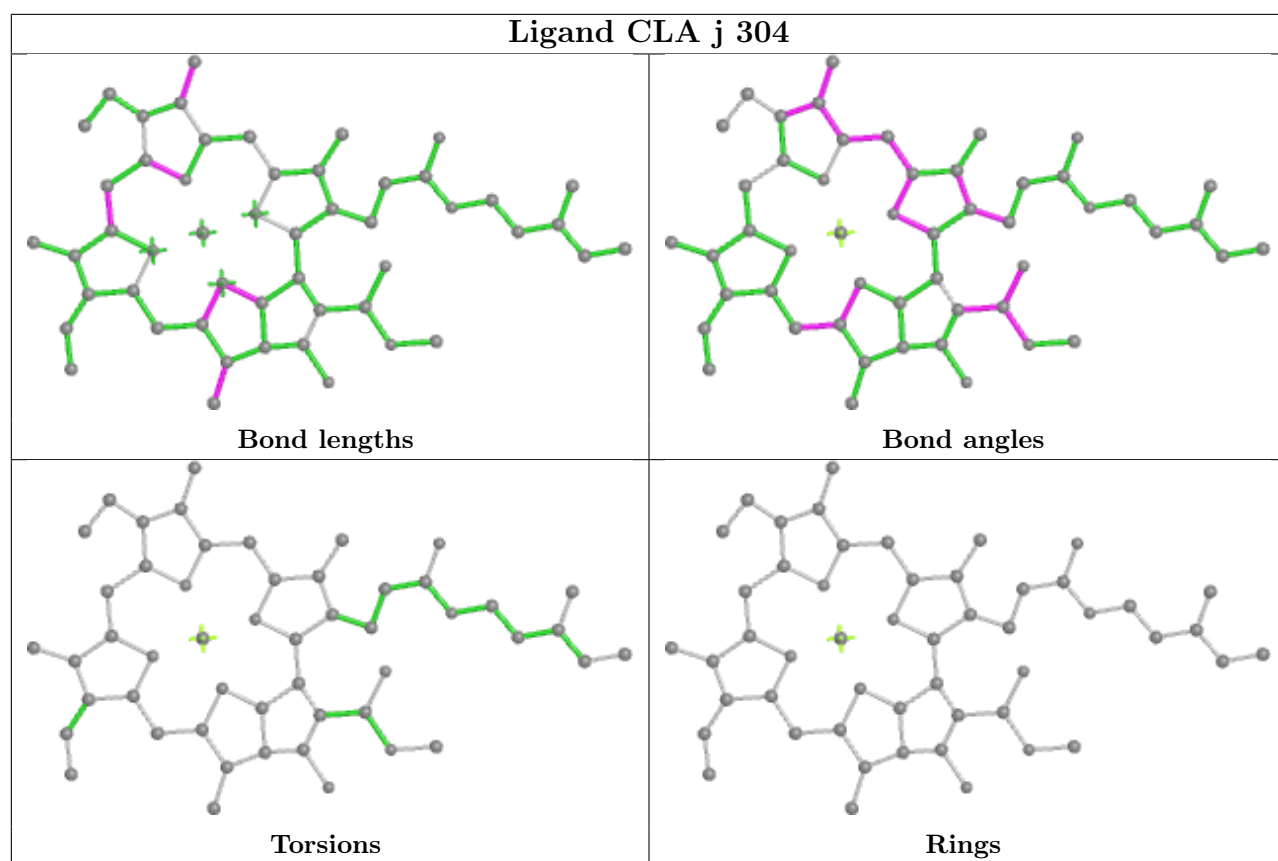
## Ligand CLA A 826



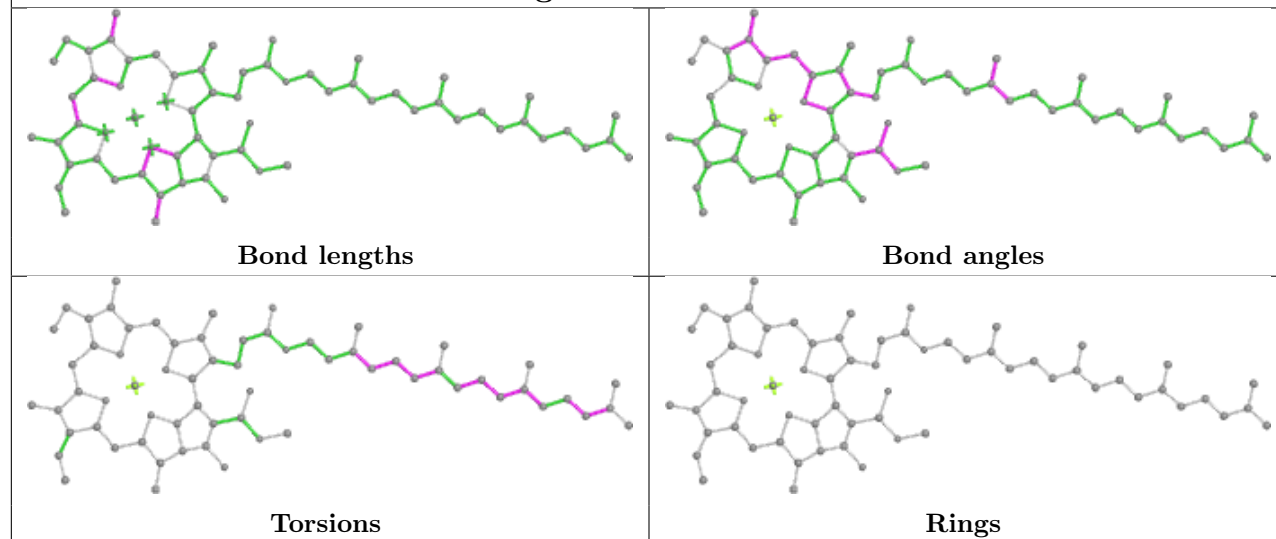


**Ligand CLA I 102****Ligand PQN B 842****Ligand II0 h 311**

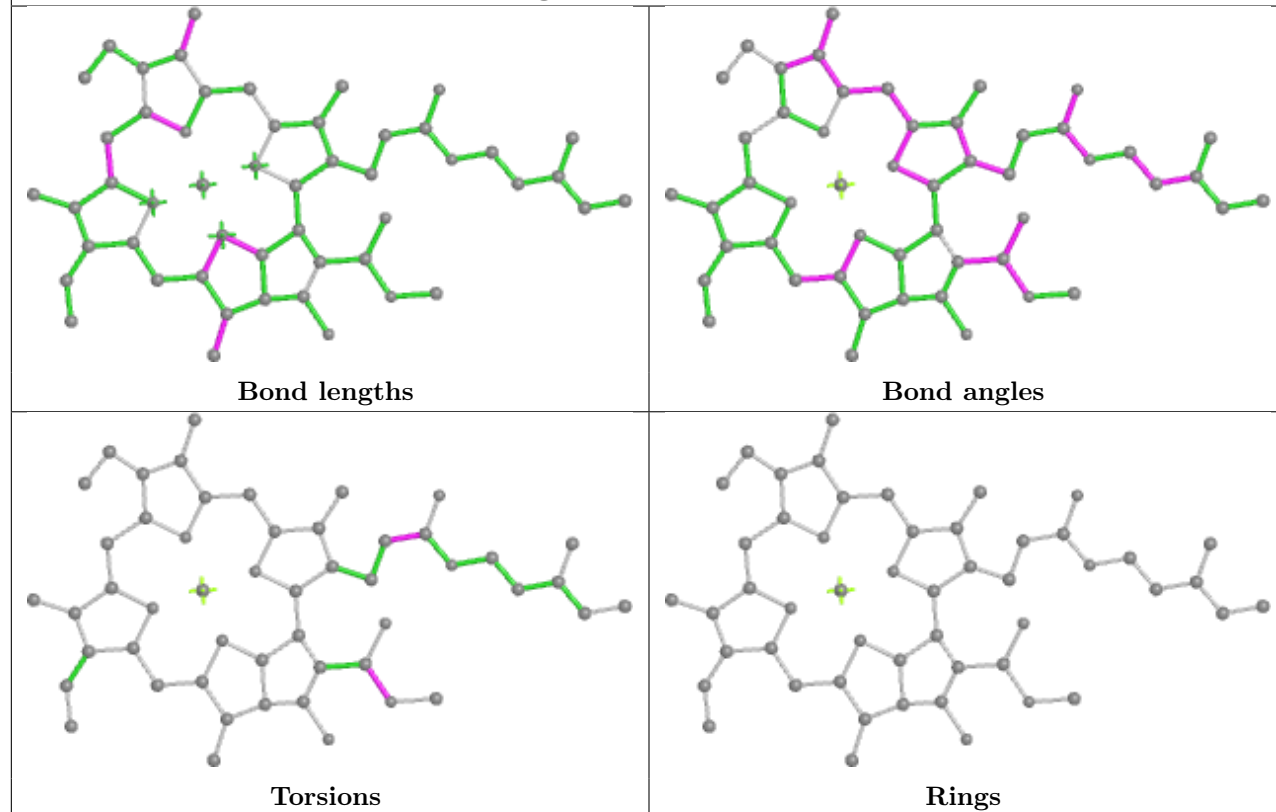


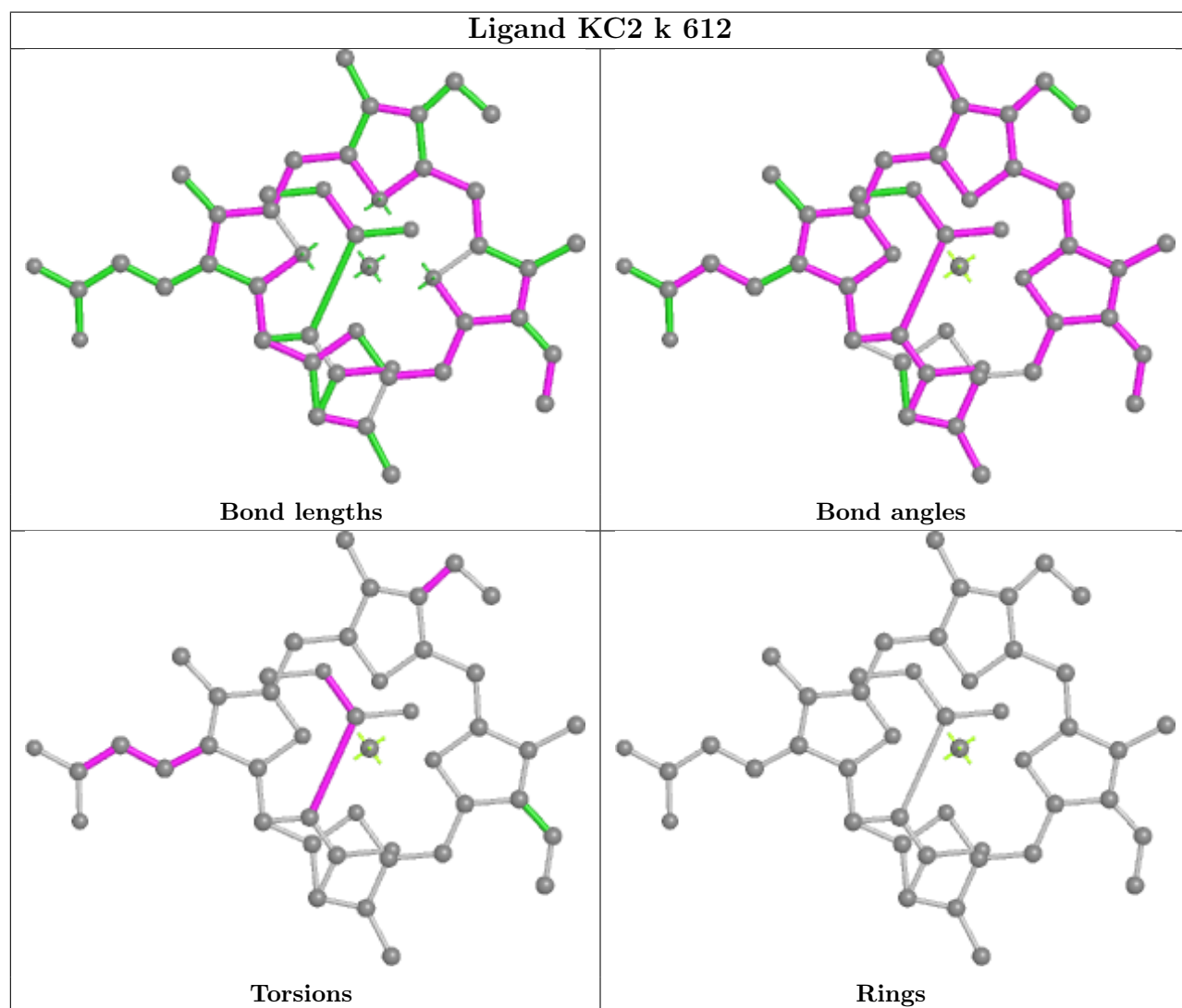
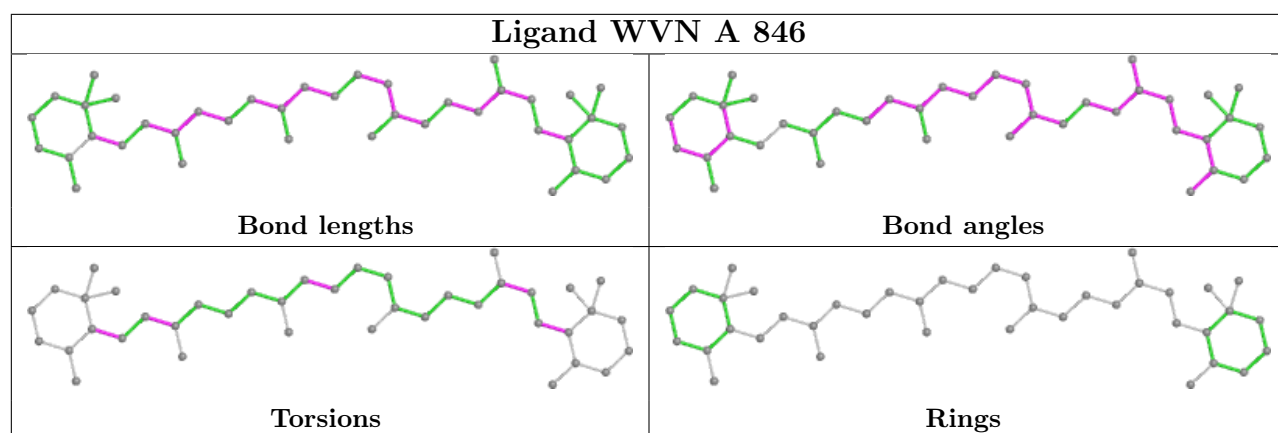


## Ligand CLA b 305

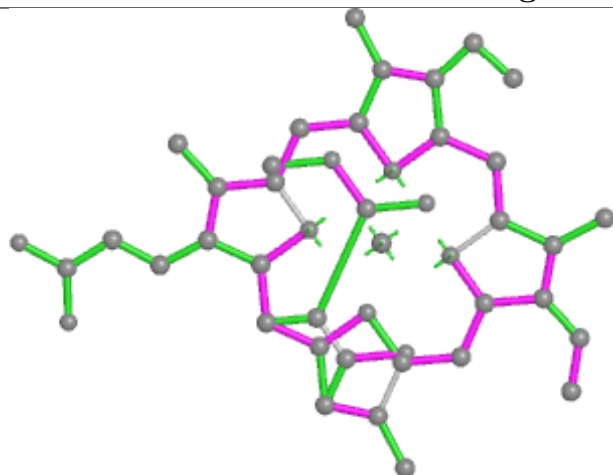


## Ligand CLA d 302

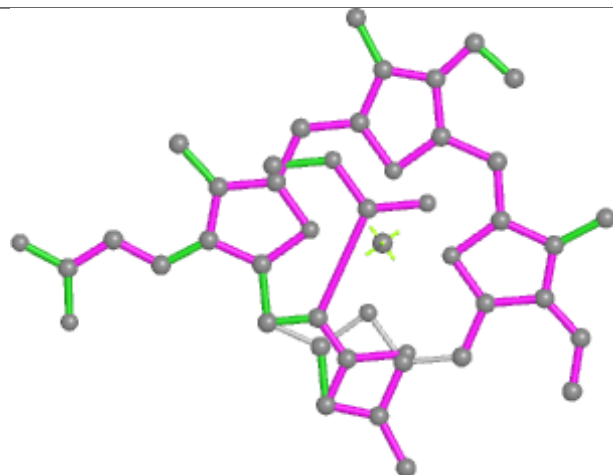




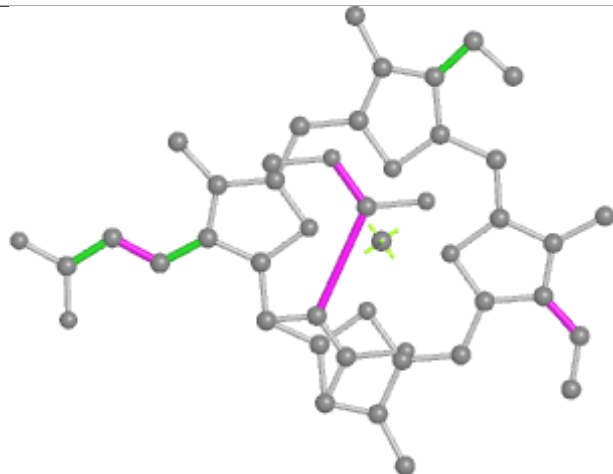
## Ligand KC2 d 310



Bond lengths



Bond angles

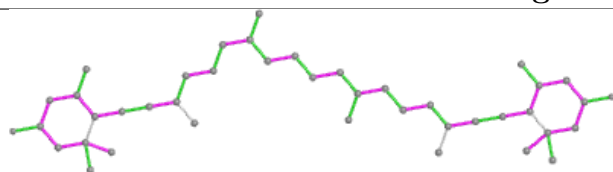


Torsions

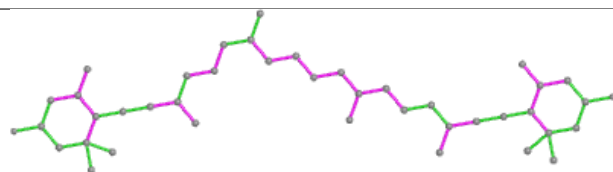


Rings

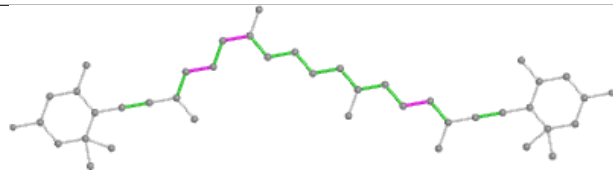
## Ligand II0 k 621



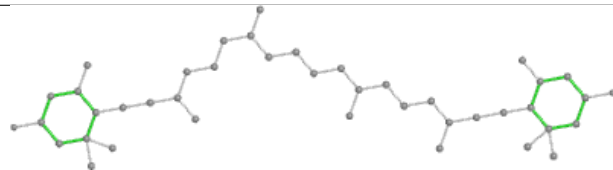
Bond lengths



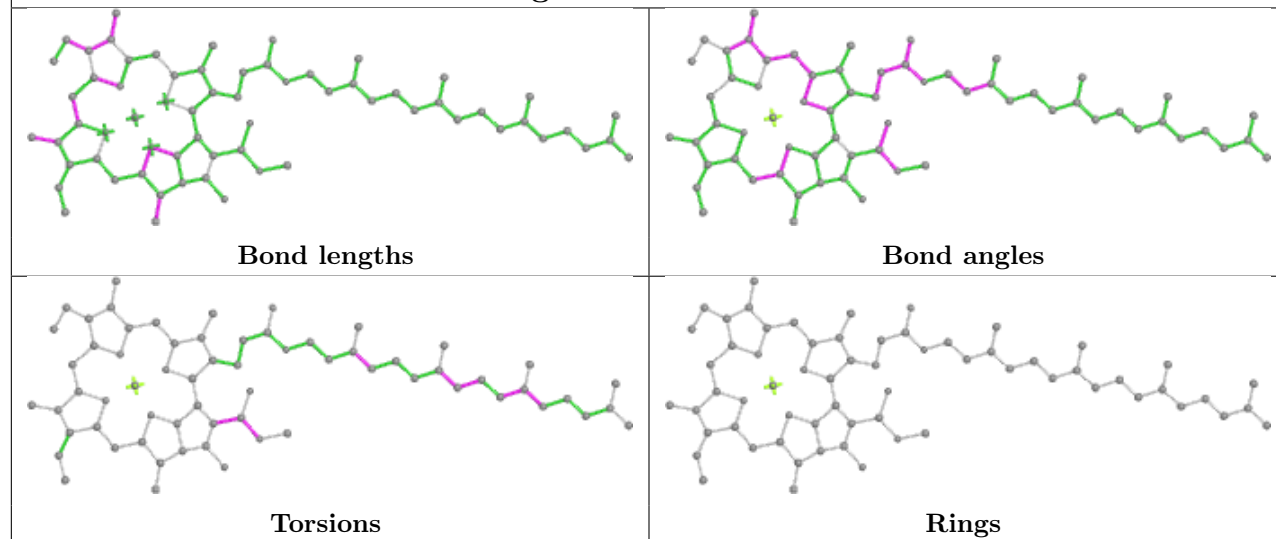
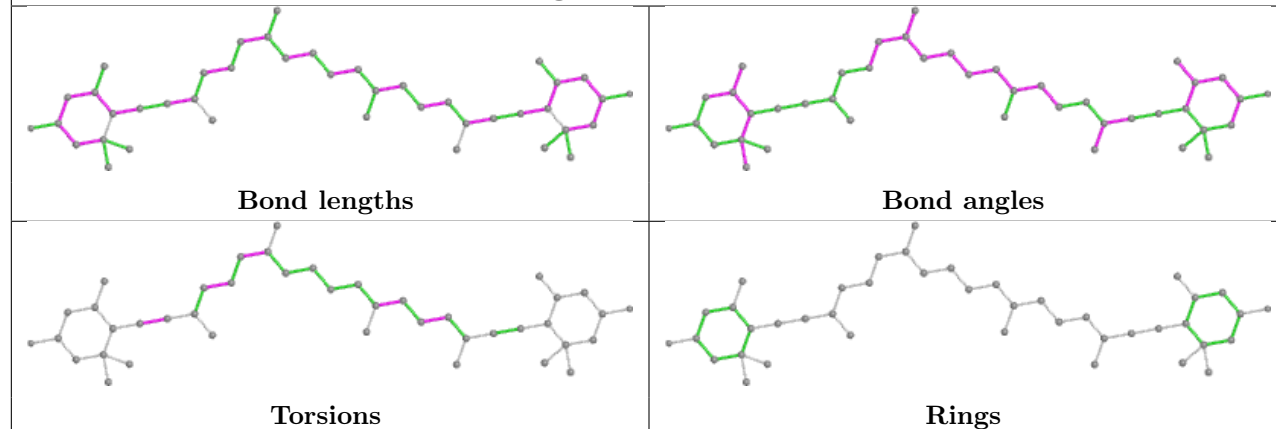
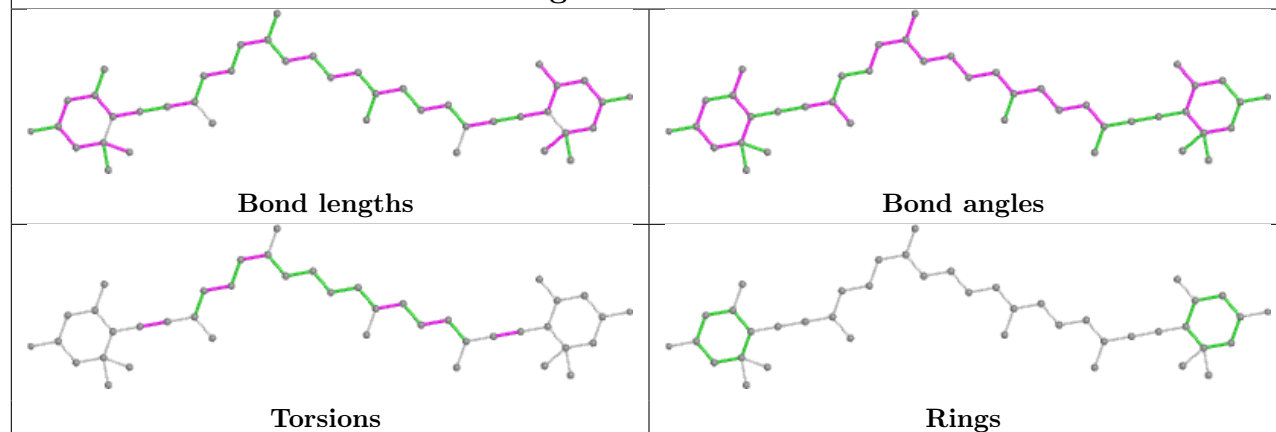
Bond angles



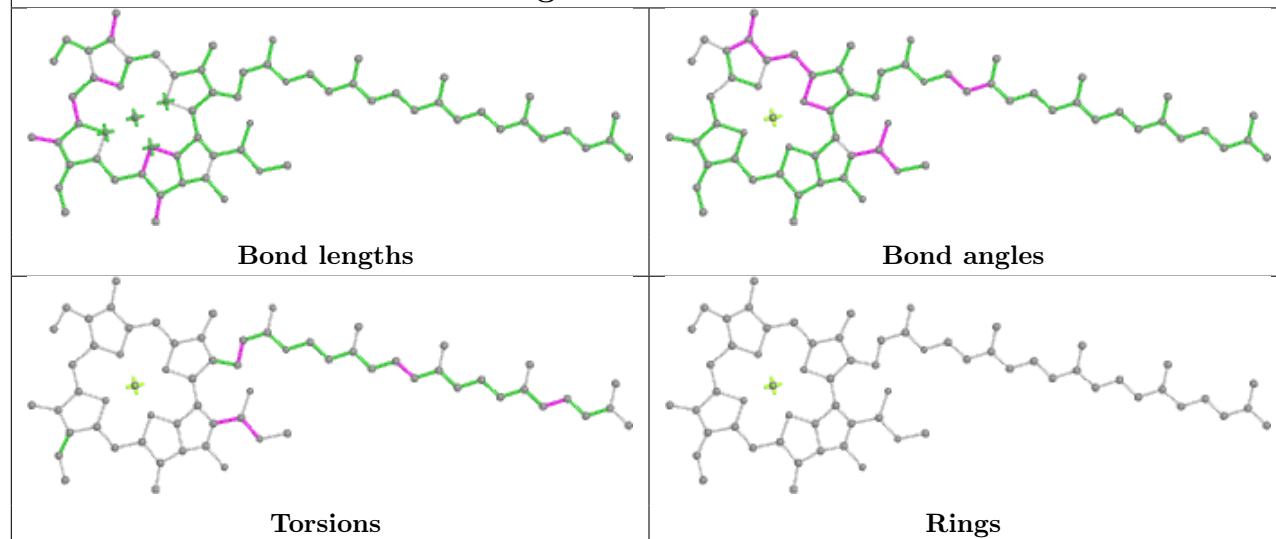
Torsions



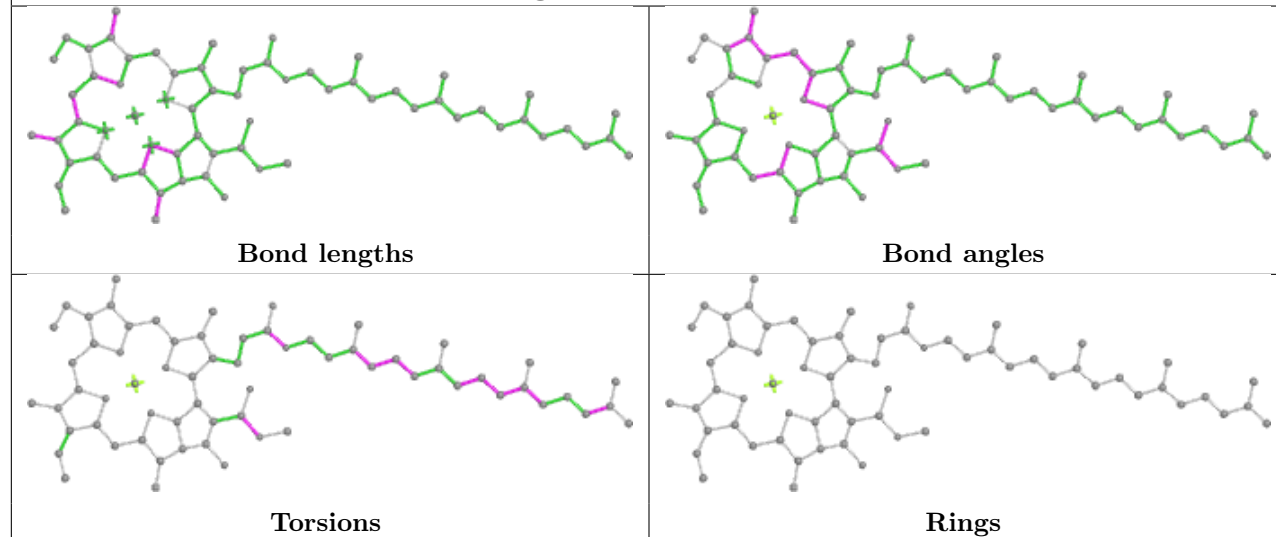
Rings

**Ligand CLA A 853****Ligand II0 J 104****Ligand II0 d 315**

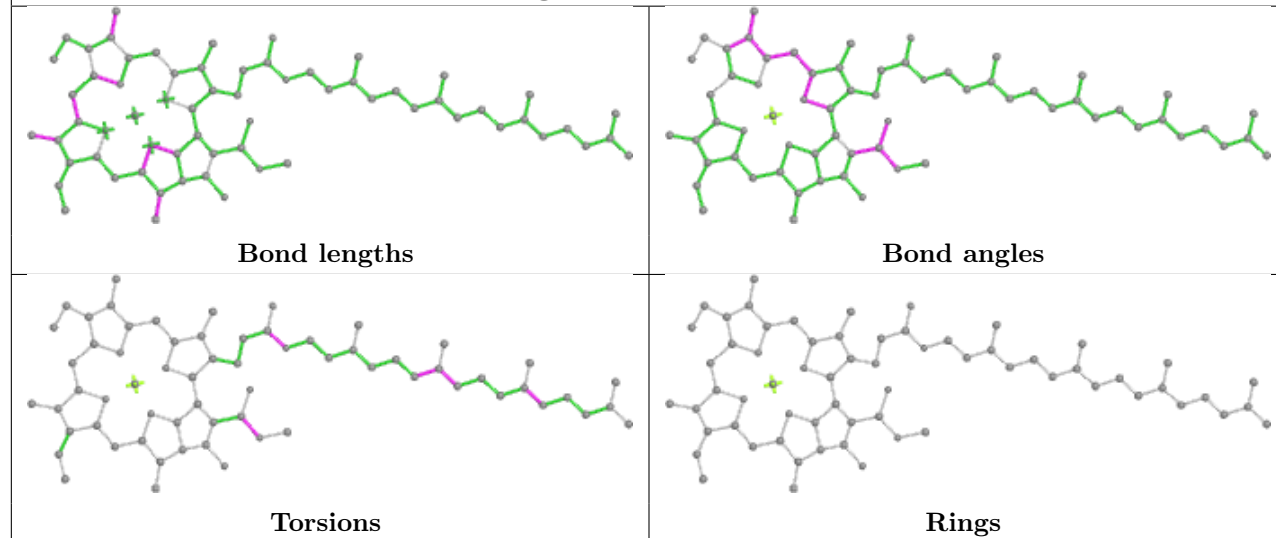
## Ligand CLA c 604



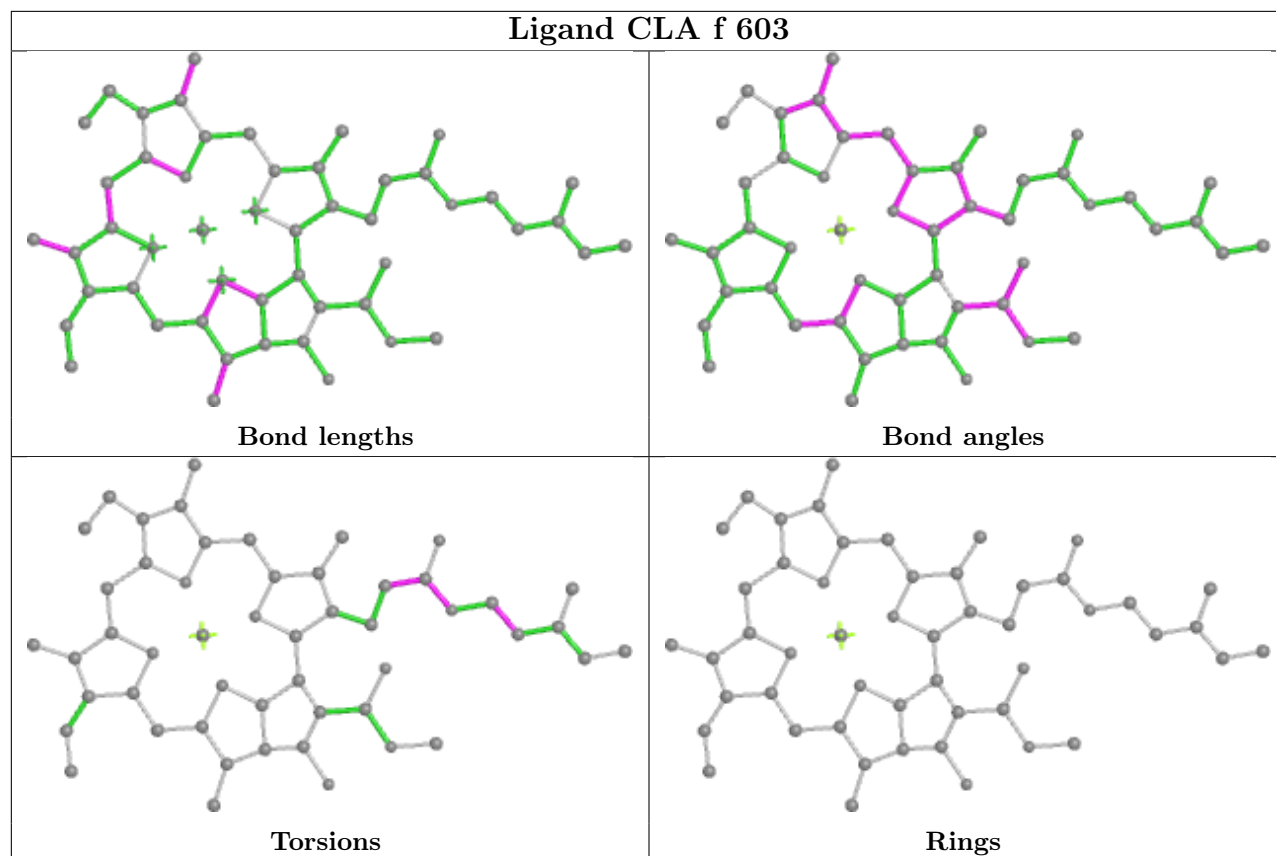
## Ligand CLA A 840



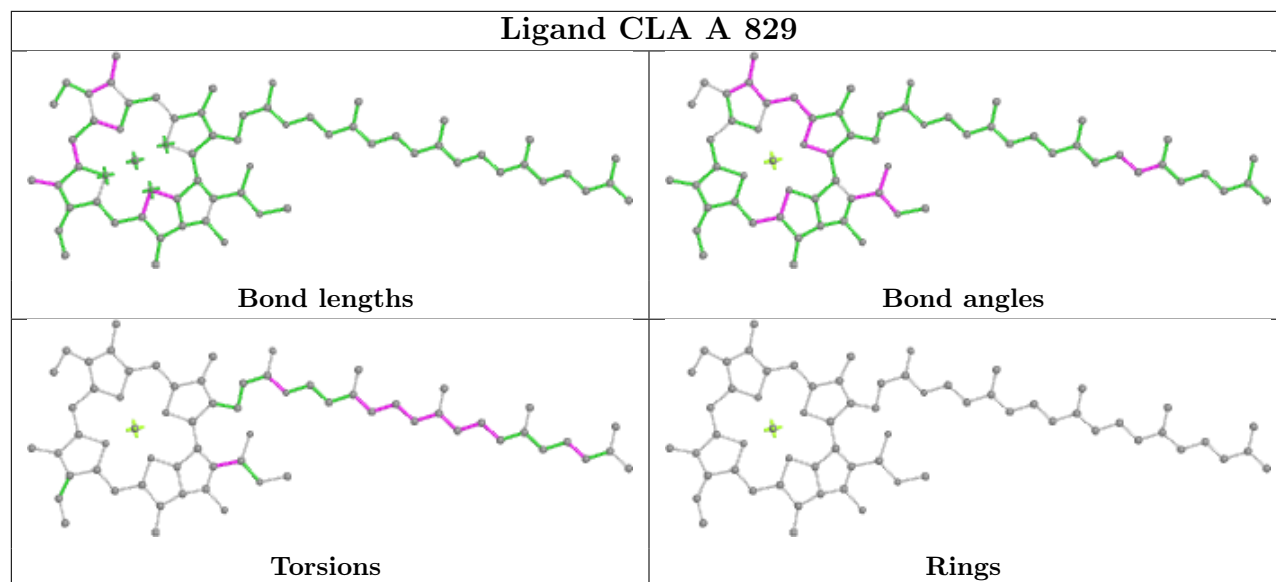
## Ligand CLA h 312

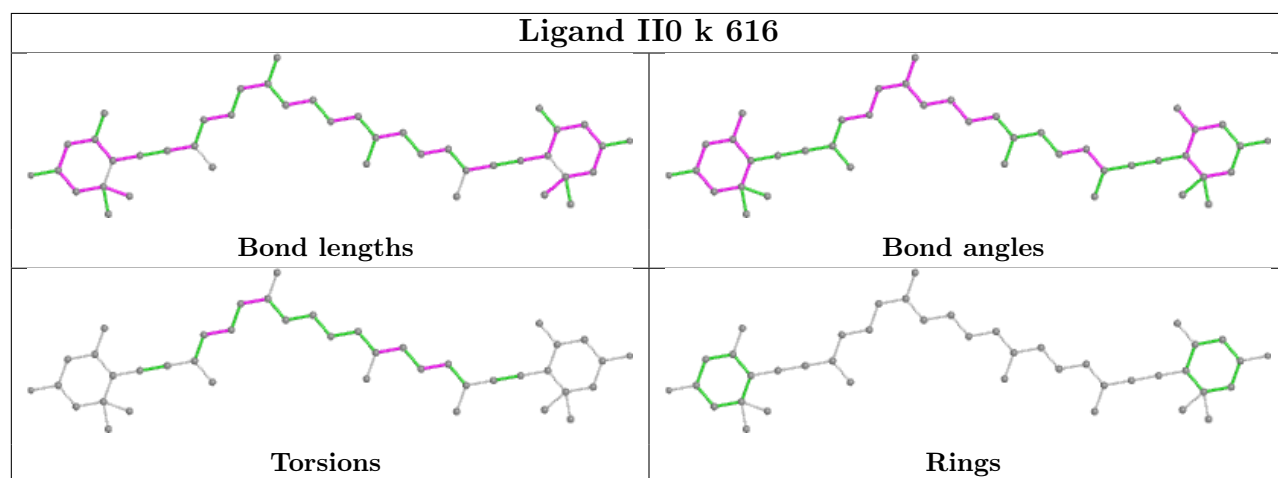
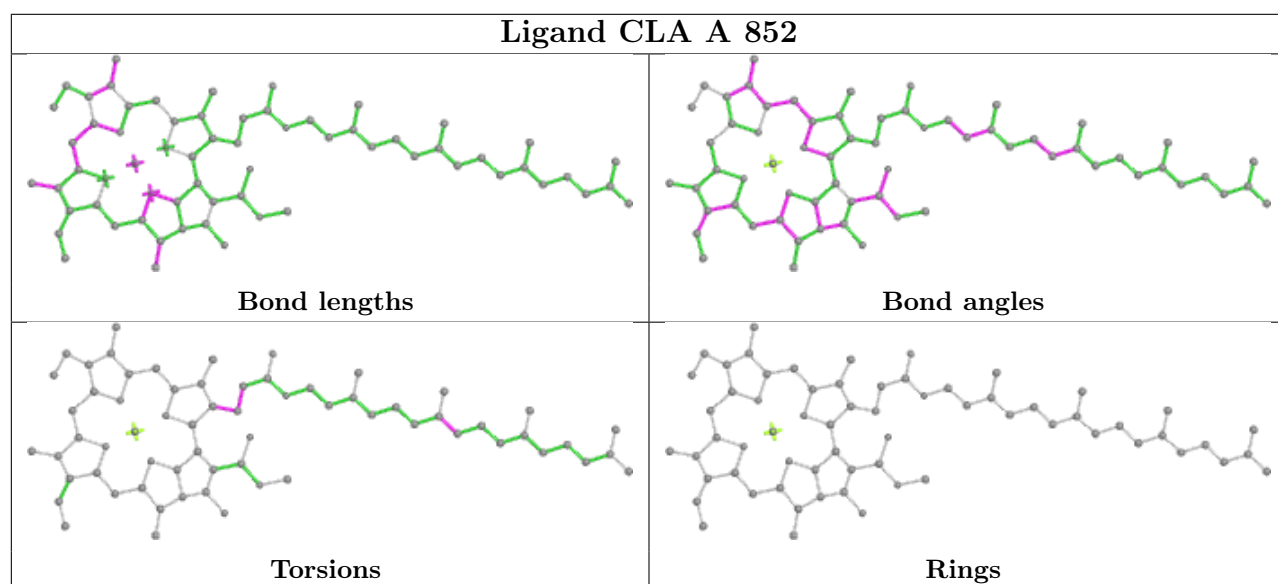
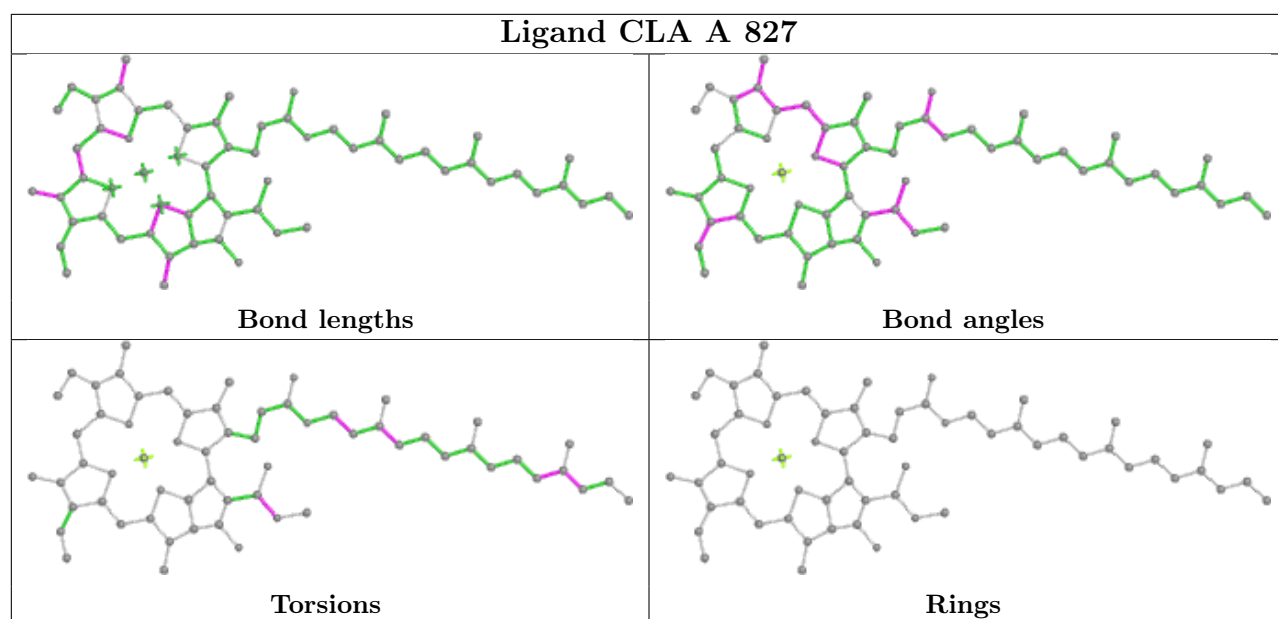


## Ligand CLA f 603



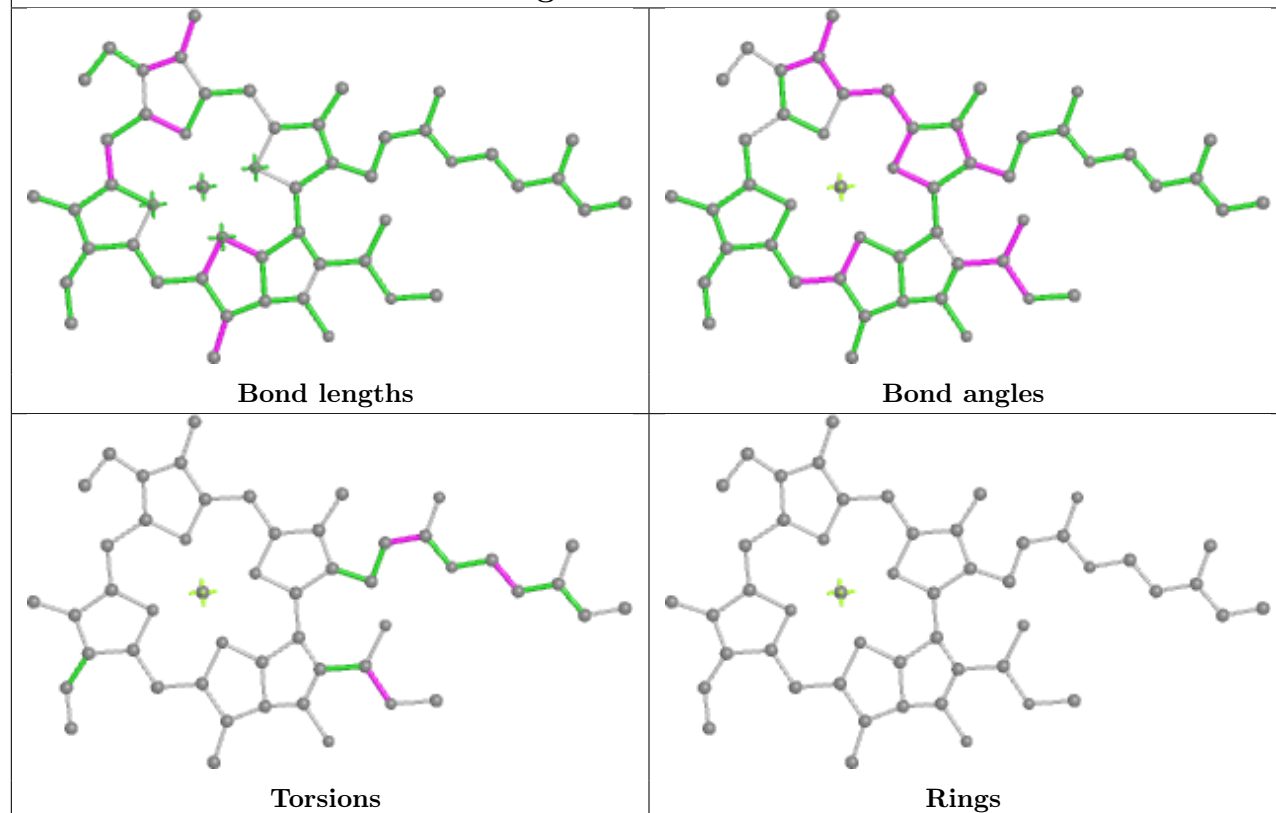
## Ligand CLA A 829



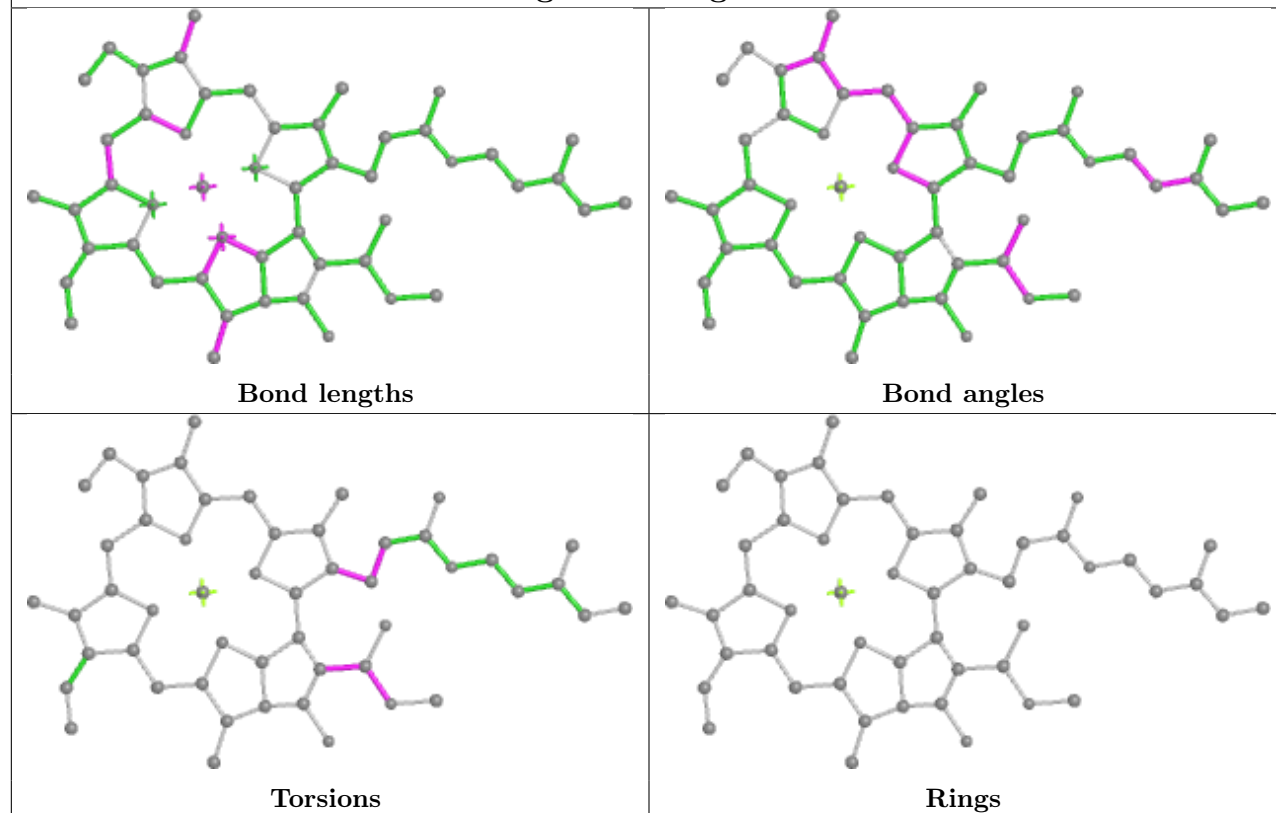


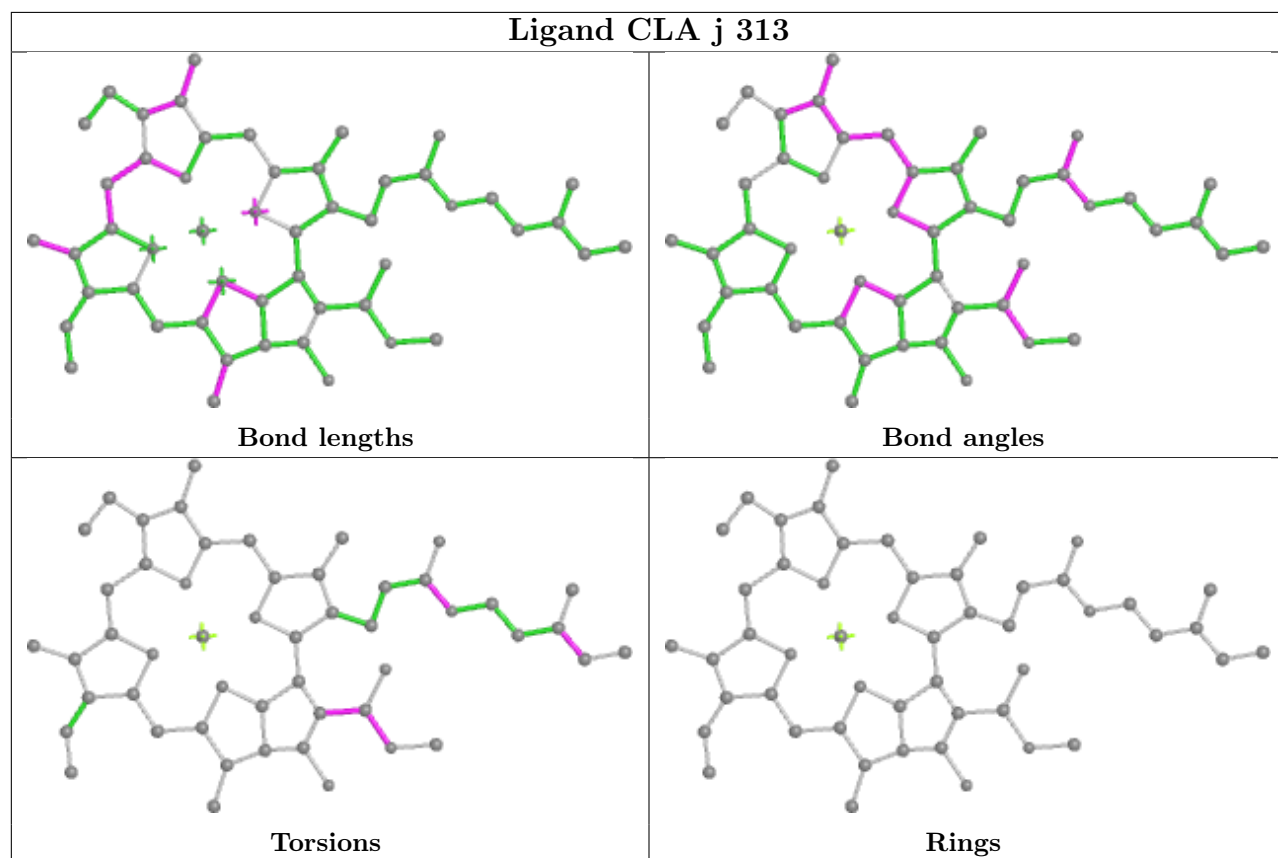
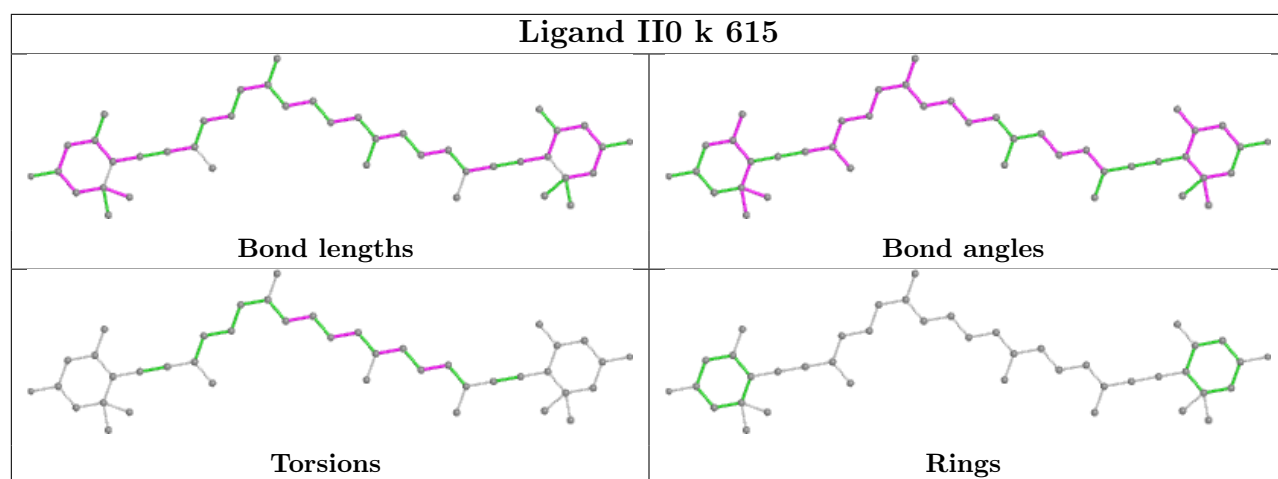


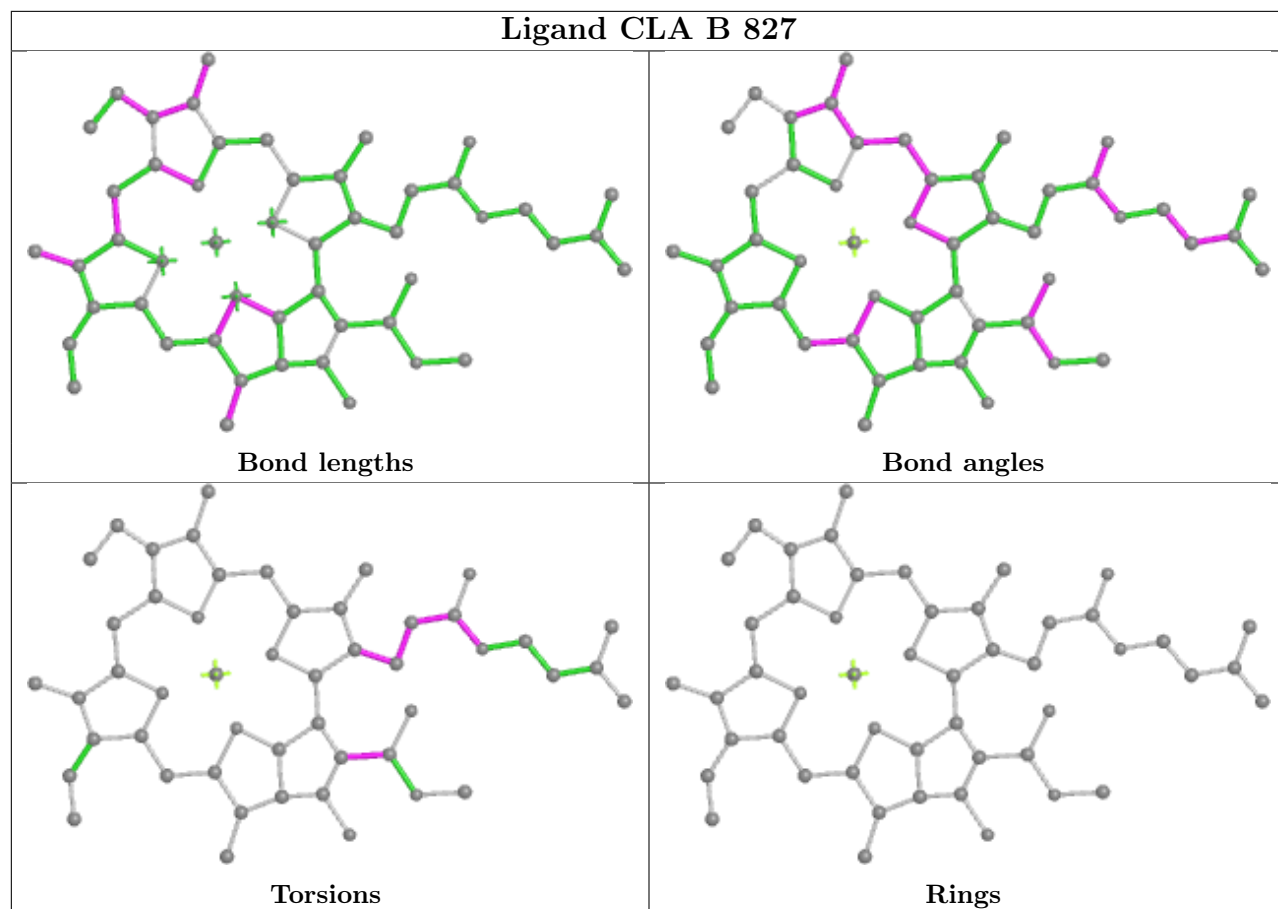
## Ligand CLA e 603



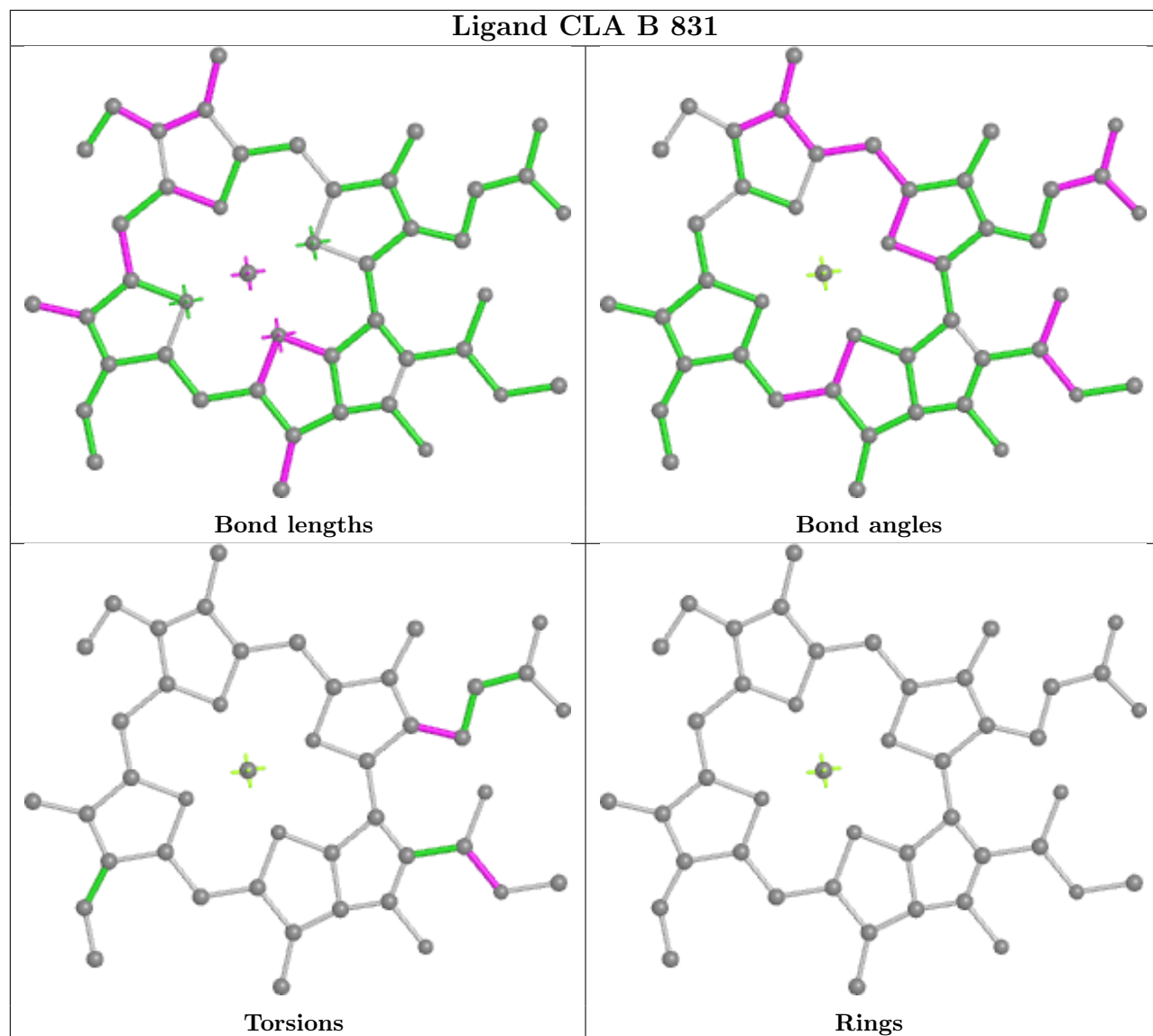
## Ligand CLA g 315



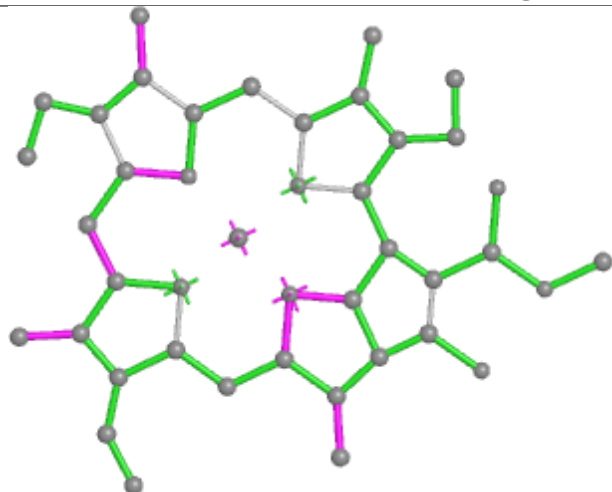




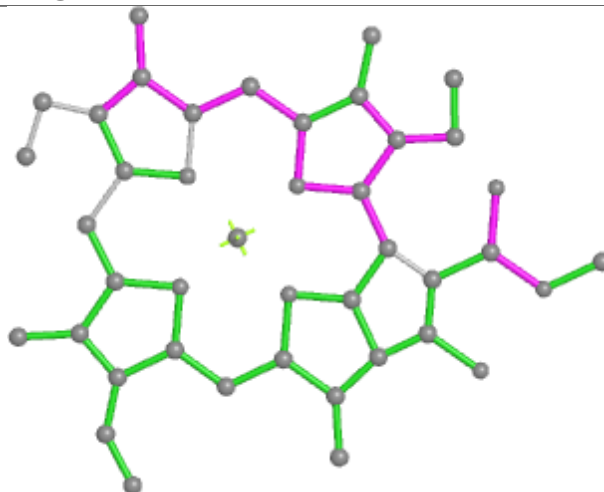
## Ligand CLA B 831



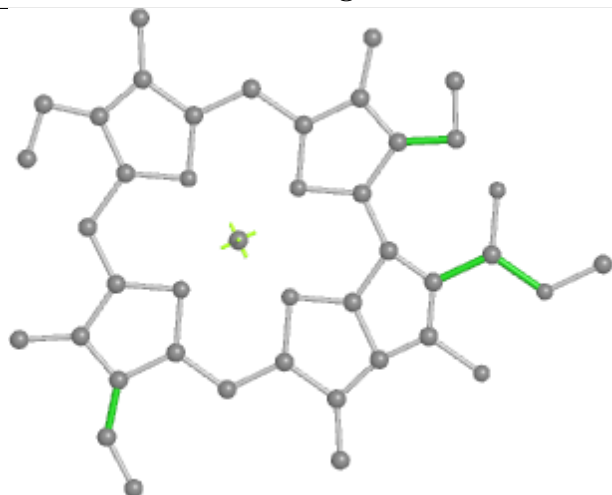
## Ligand CLA g 302



Bond lengths



Bond angles

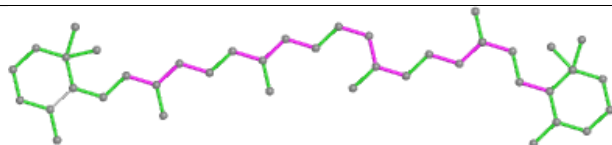


Torsions

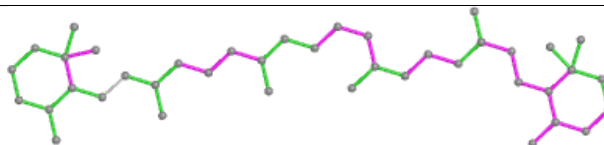


Rings

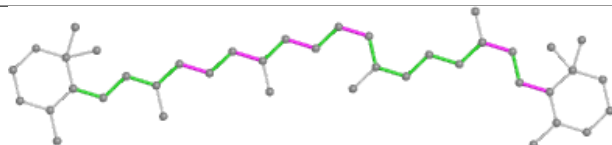
## Ligand WVN A 848



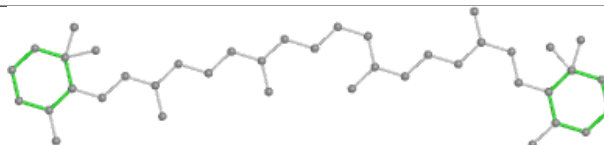
Bond lengths



Bond angles

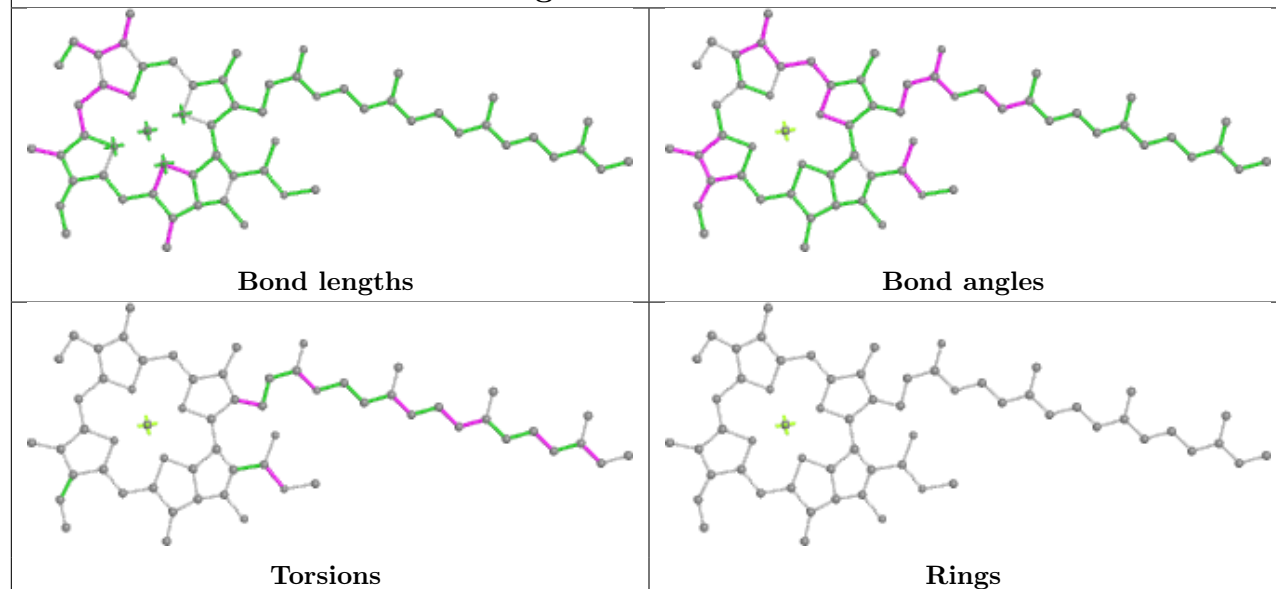


Torsions

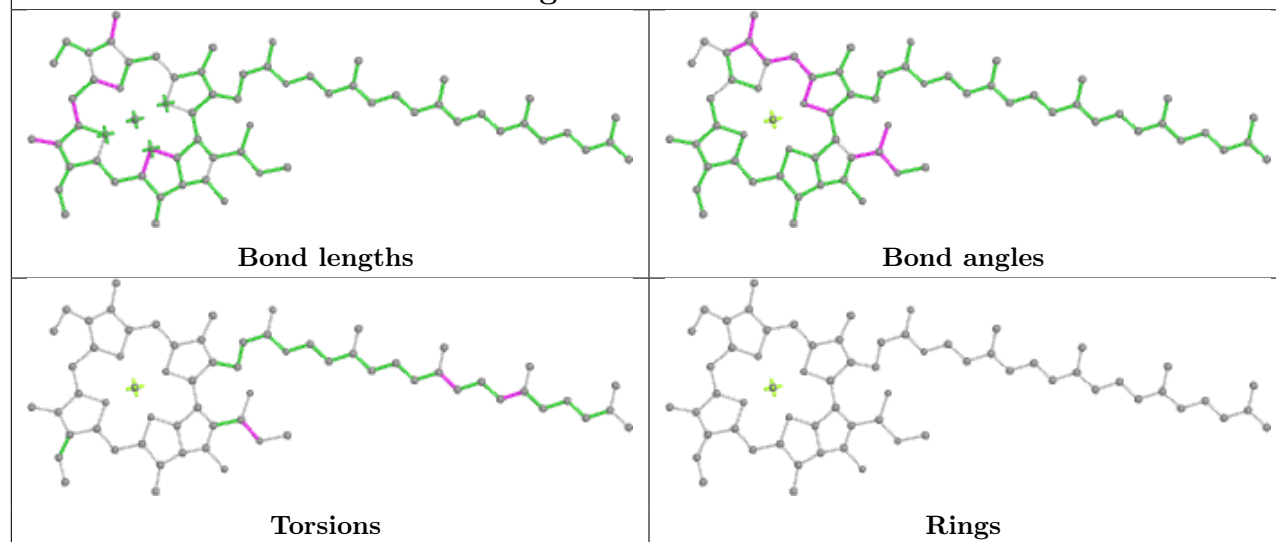


Rings

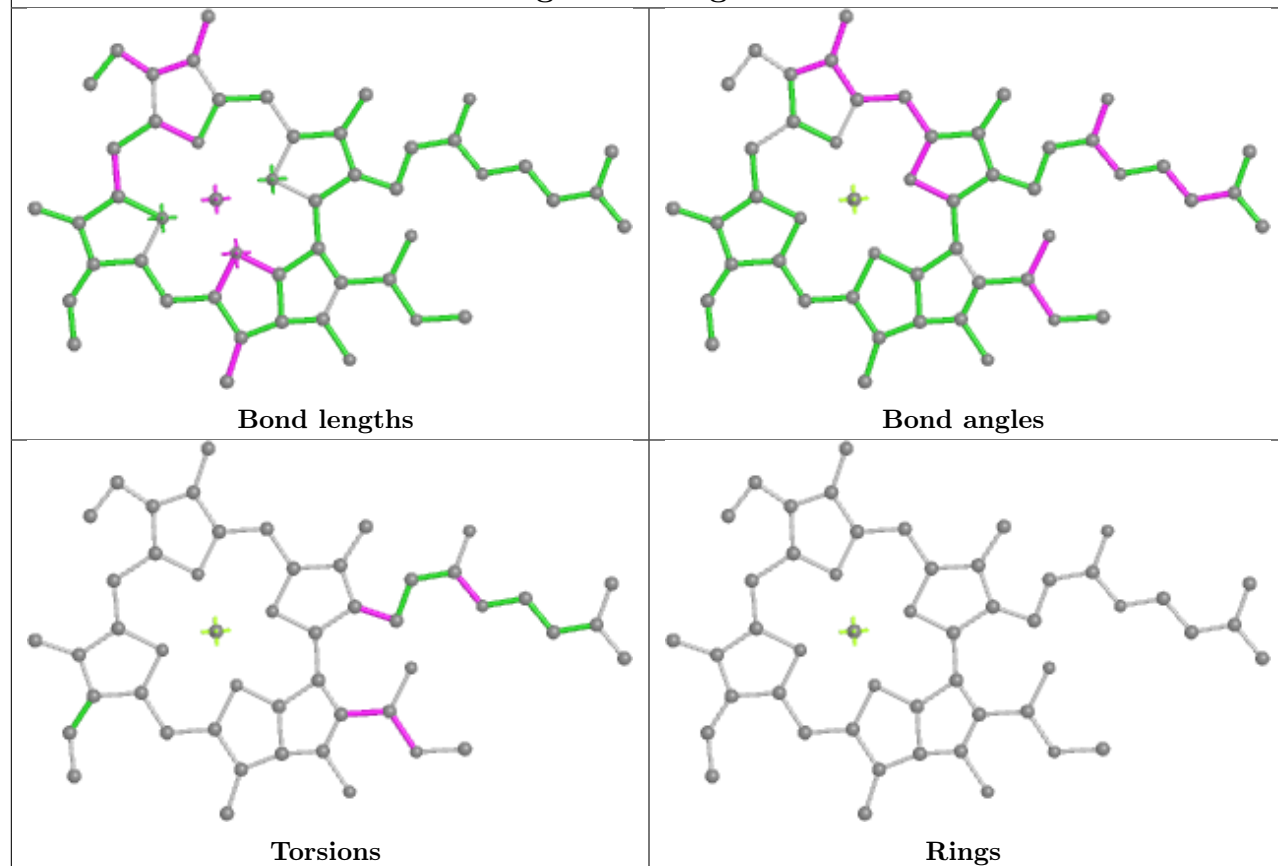
## Ligand CLA b 308



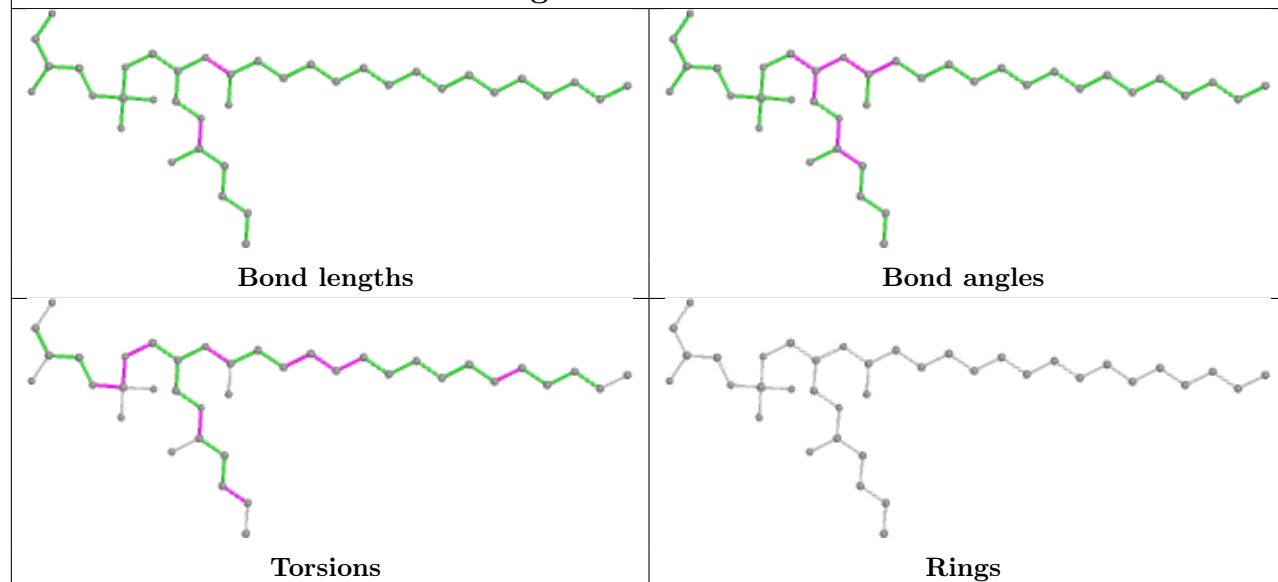
## Ligand CLA f 609

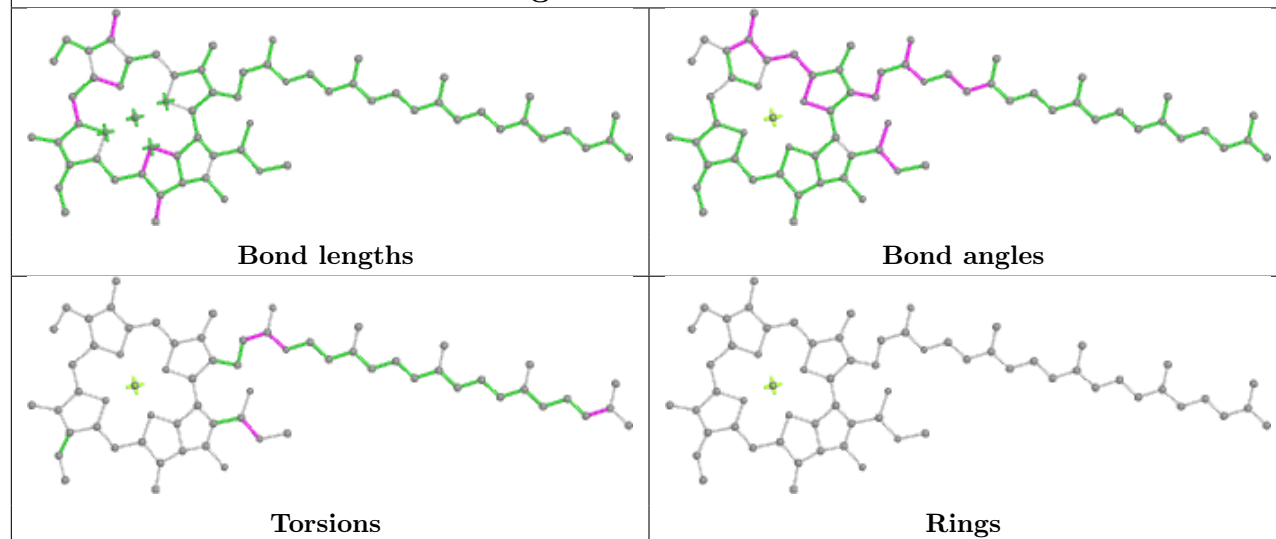
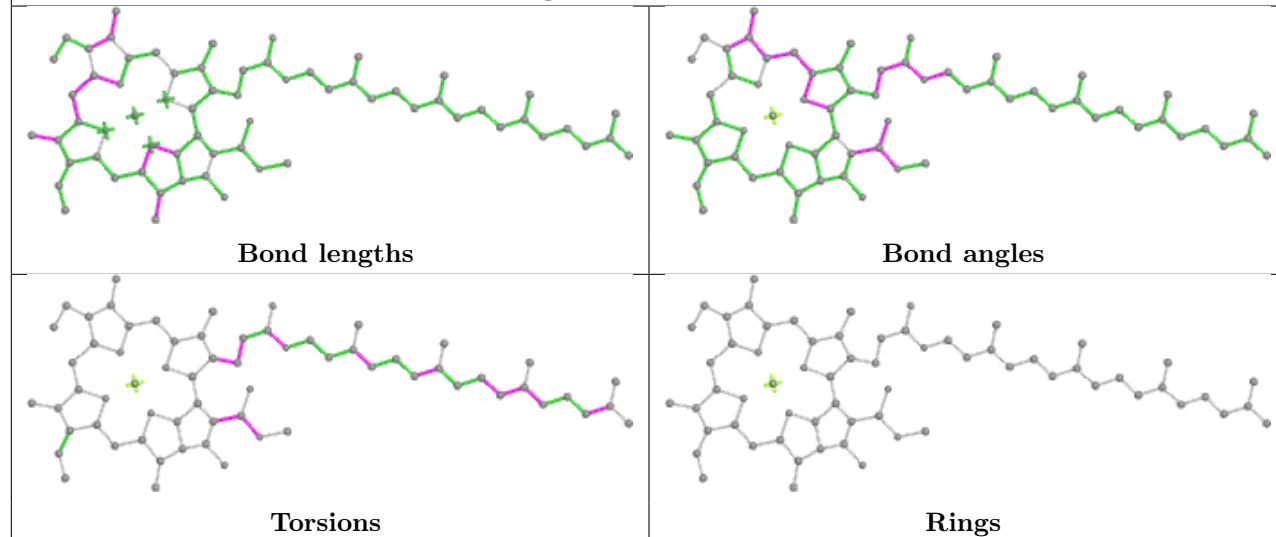


## Ligand CLA g 303



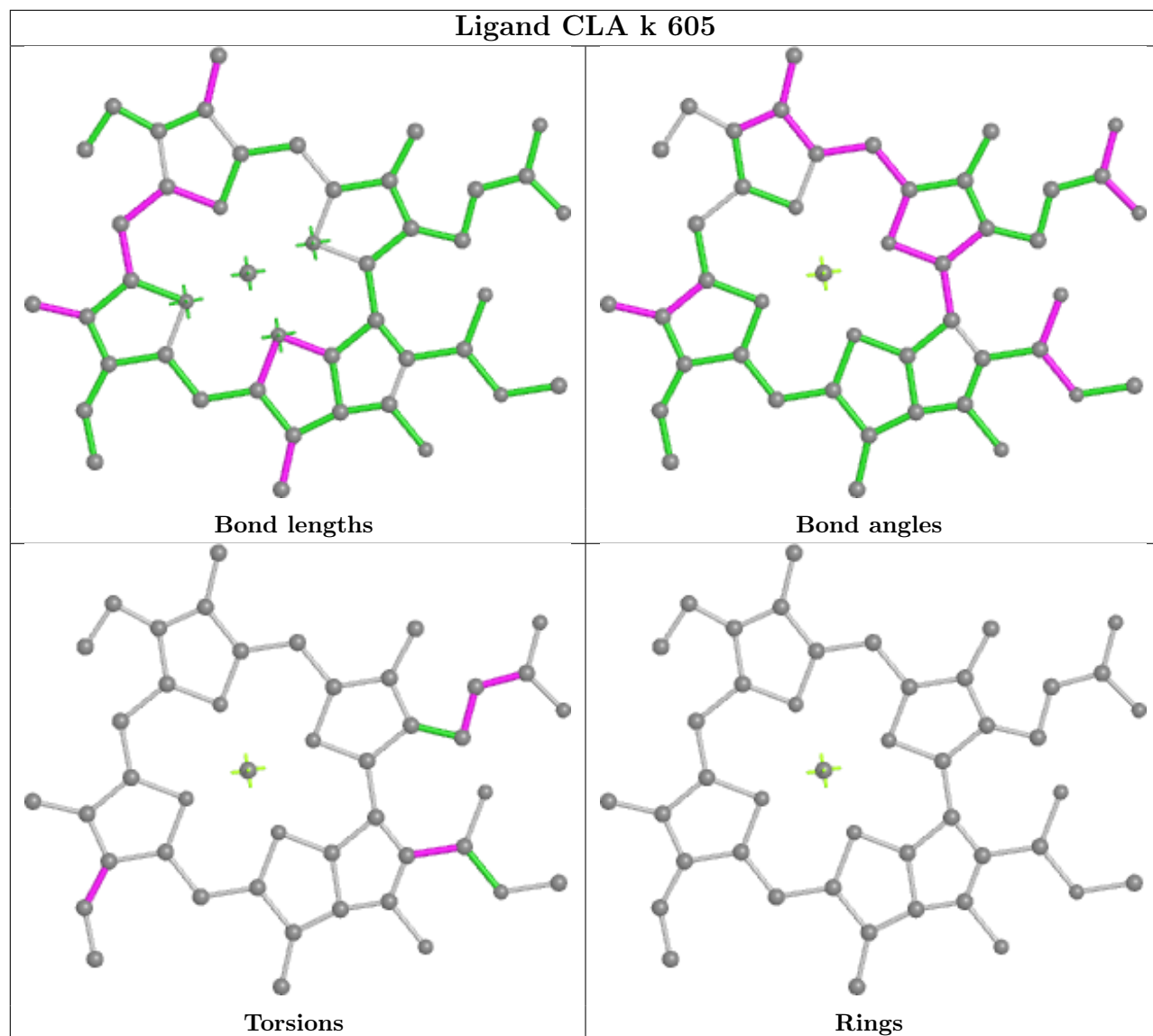
## Ligand LHG B 802



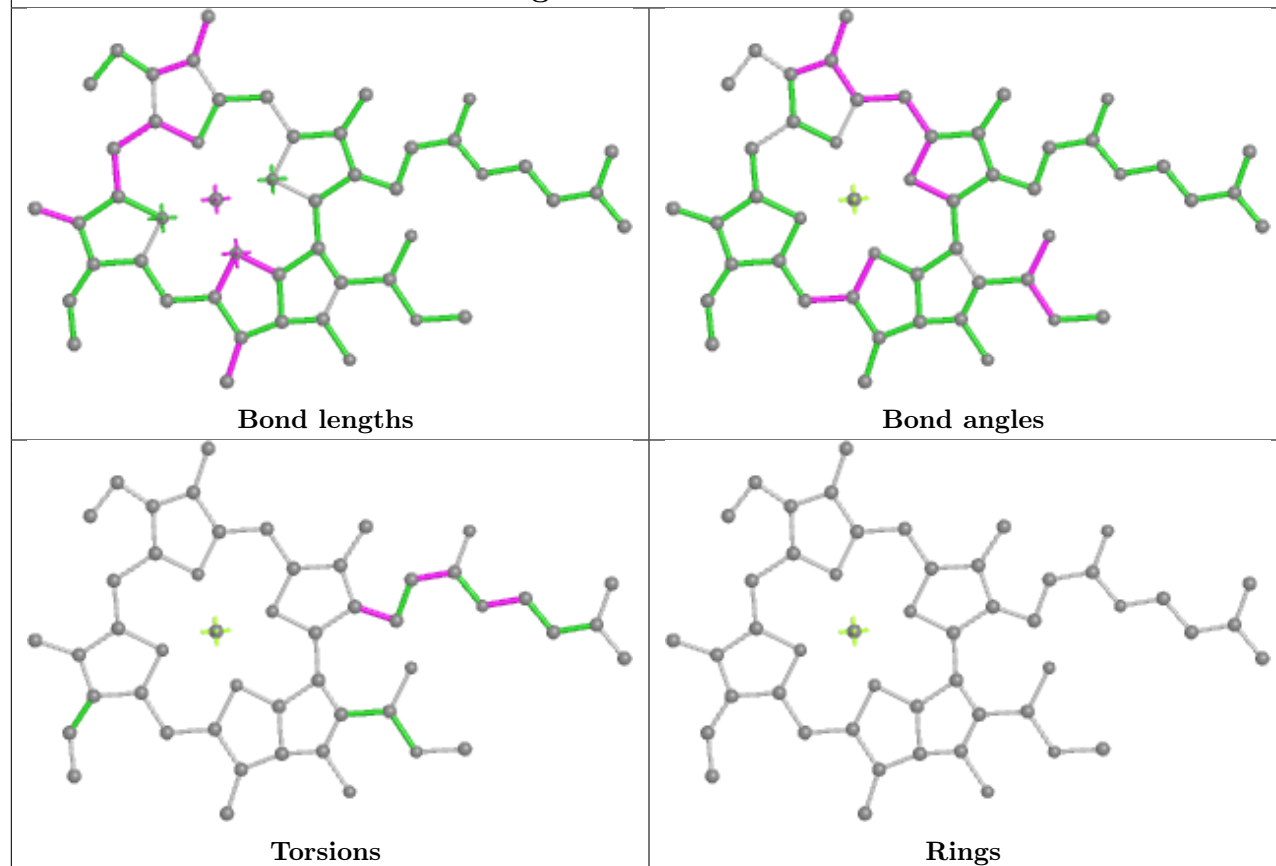
**Ligand CLA A 801****Ligand CLA f 607**



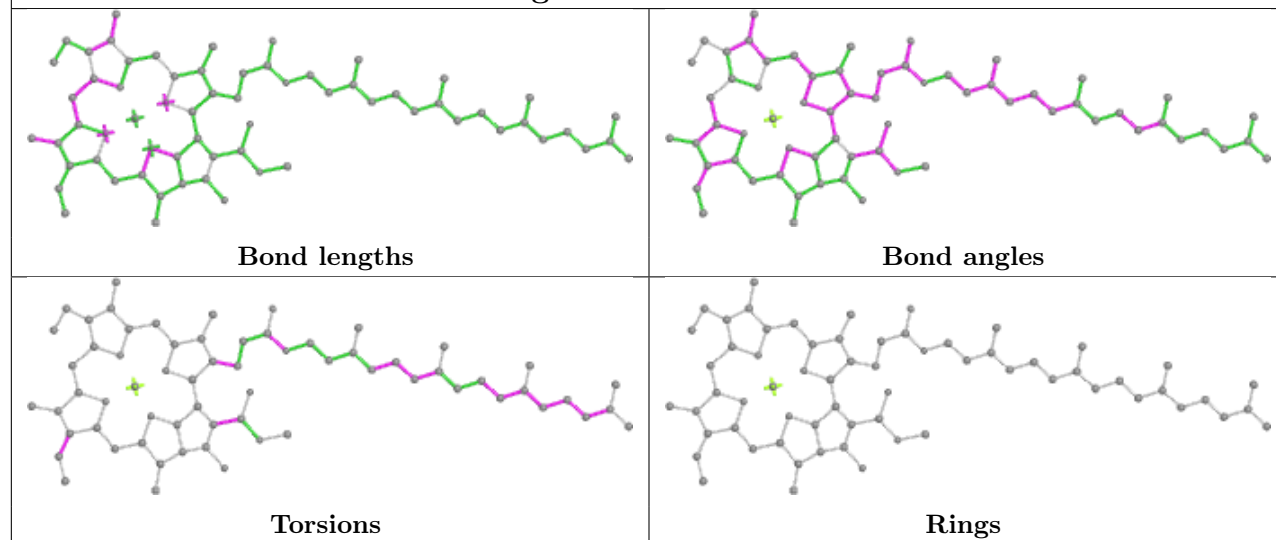
## Ligand CLA k 605



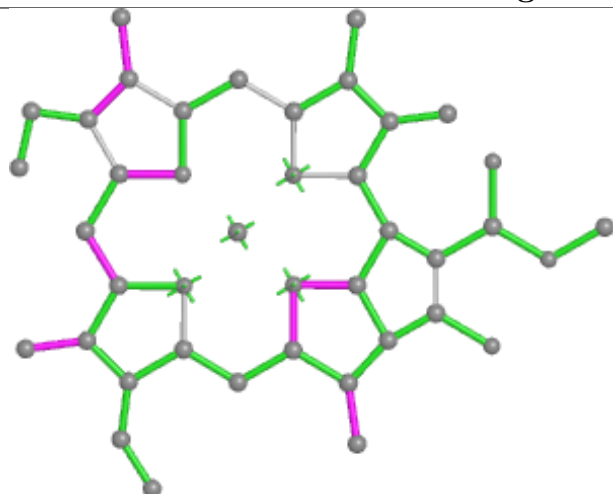
## Ligand CLA A 833



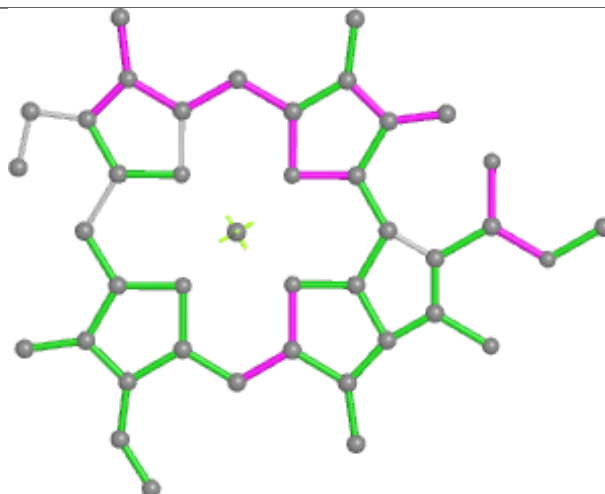
## Ligand CLA O 205



## Ligand CLA d 308



Bond lengths



Bond angles

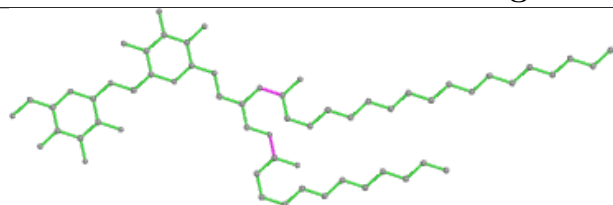


Torsions

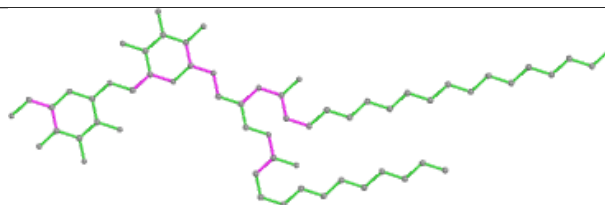


Rings

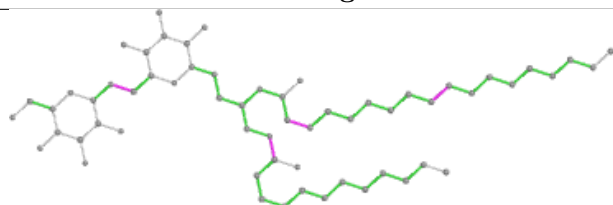
## Ligand DGD B 843



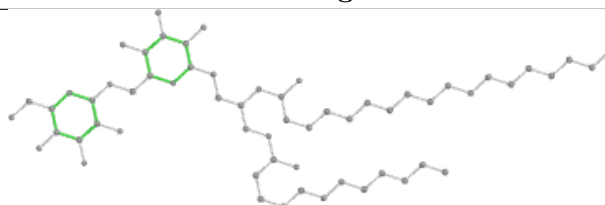
Bond lengths



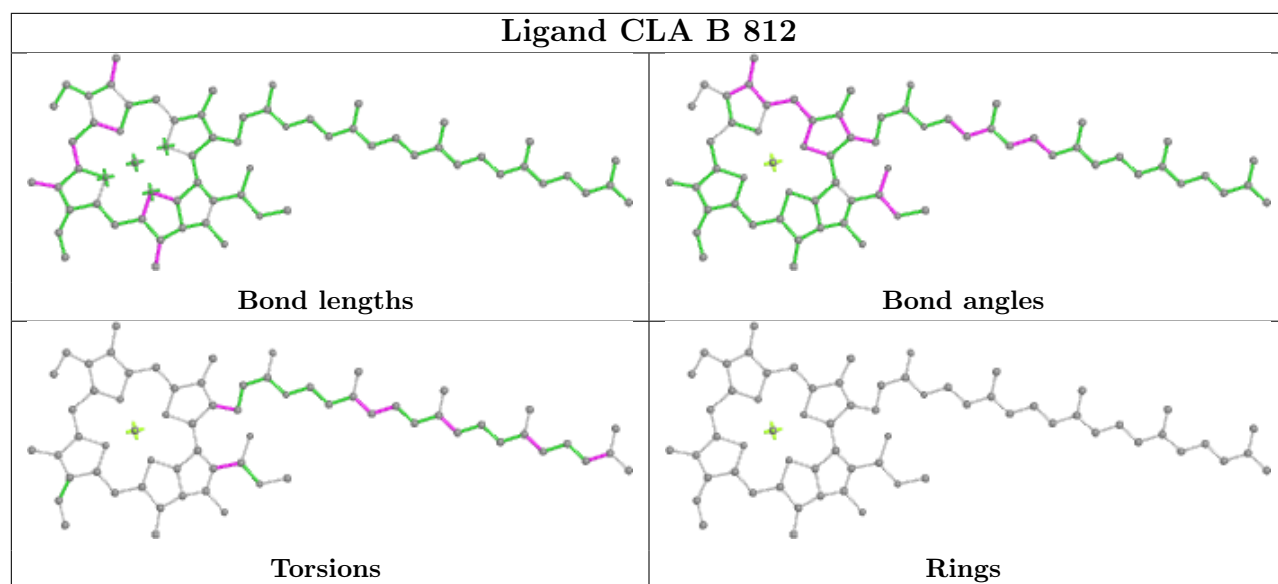
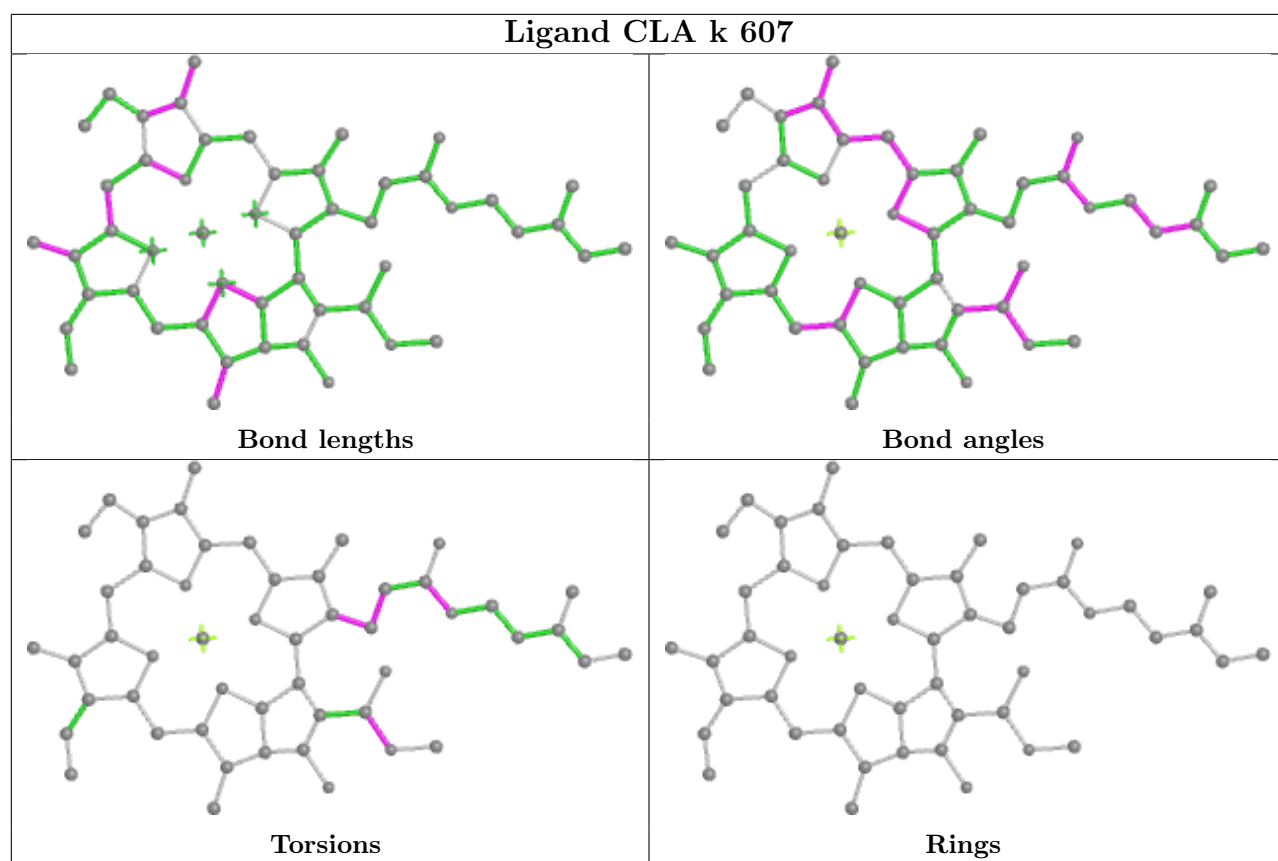
Bond angles



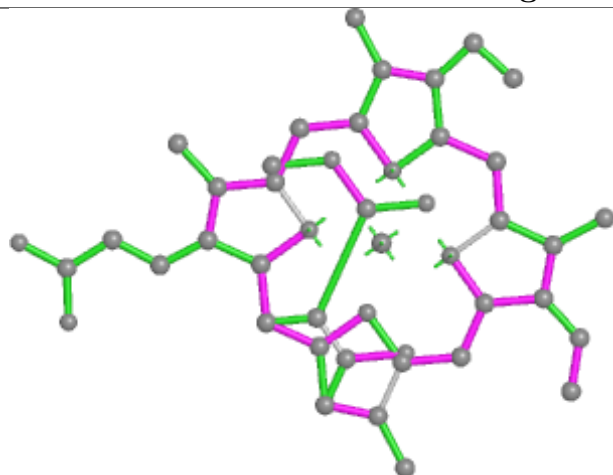
Torsions



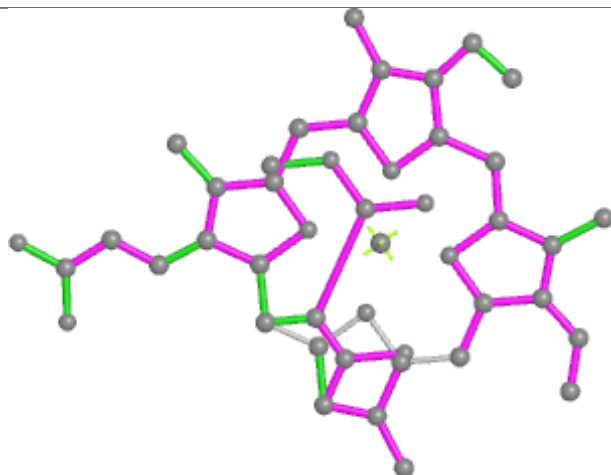
Rings



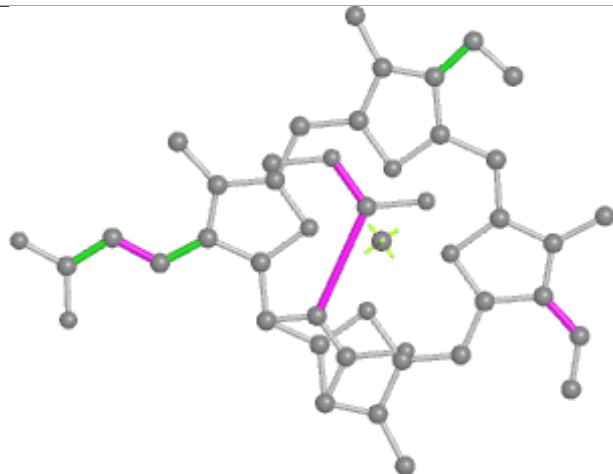
## Ligand KC2 k 611



Bond lengths



Bond angles

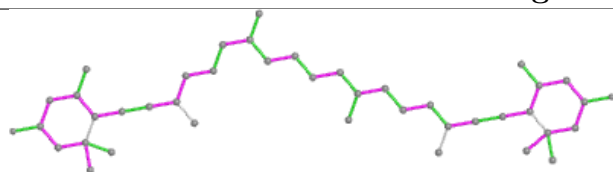


Torsions

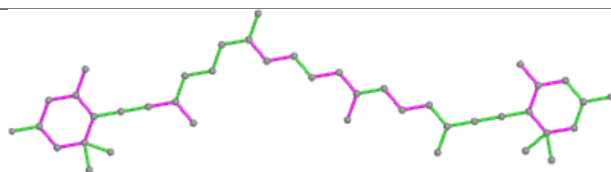


Rings

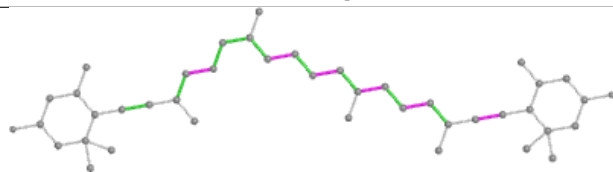
## Ligand II0 b 314



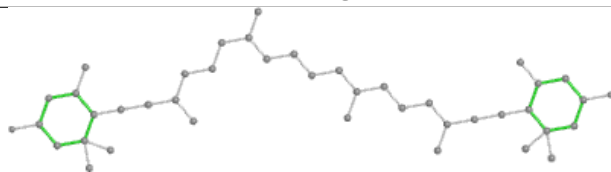
Bond lengths



Bond angles

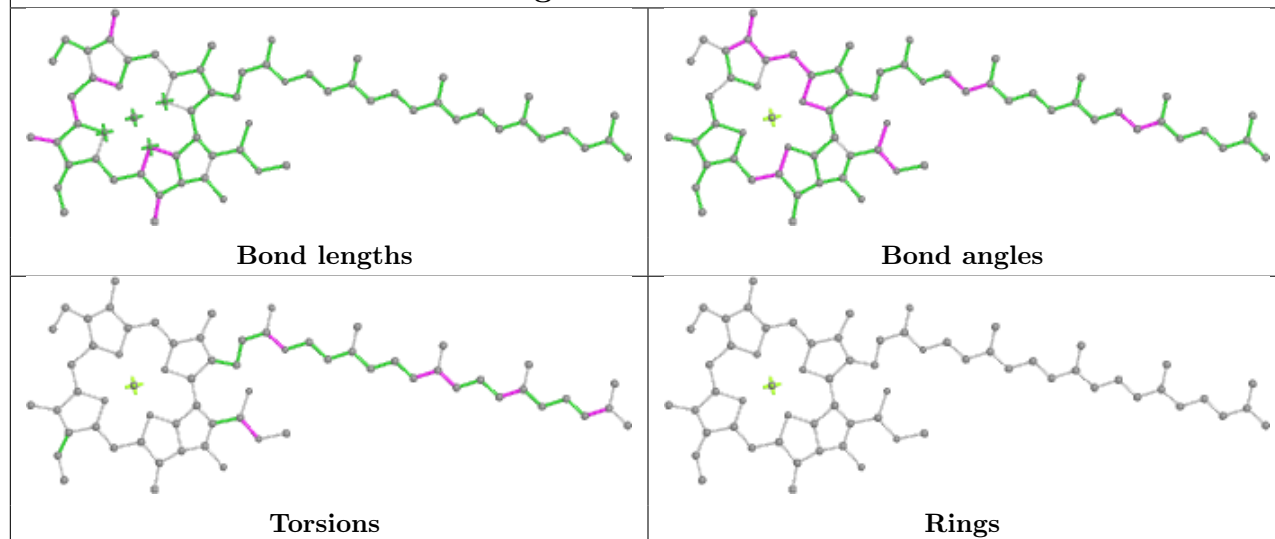


Torsions

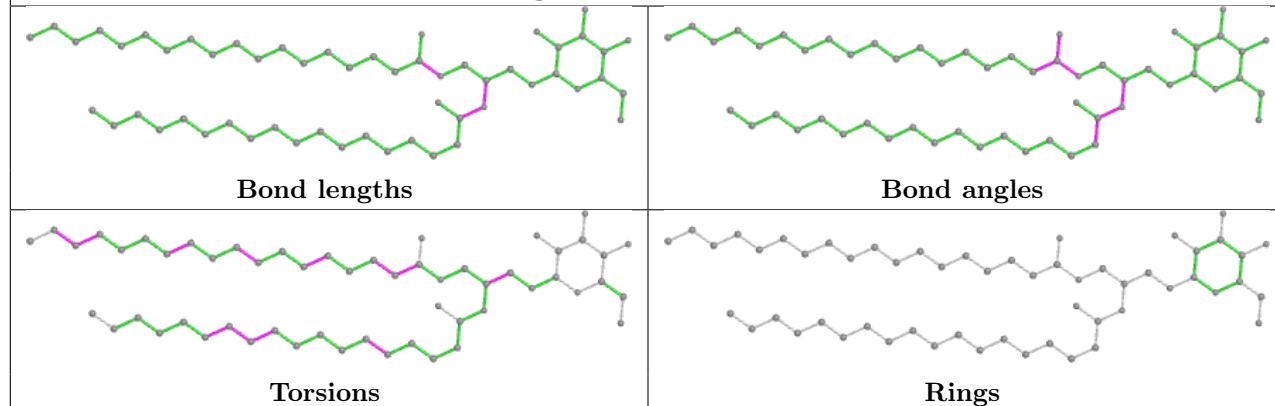


Rings

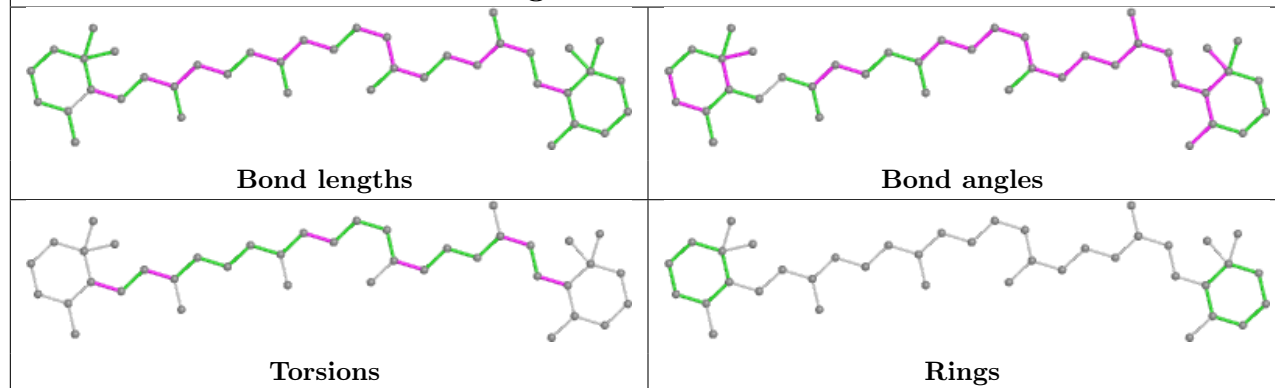
## Ligand CLA h 305



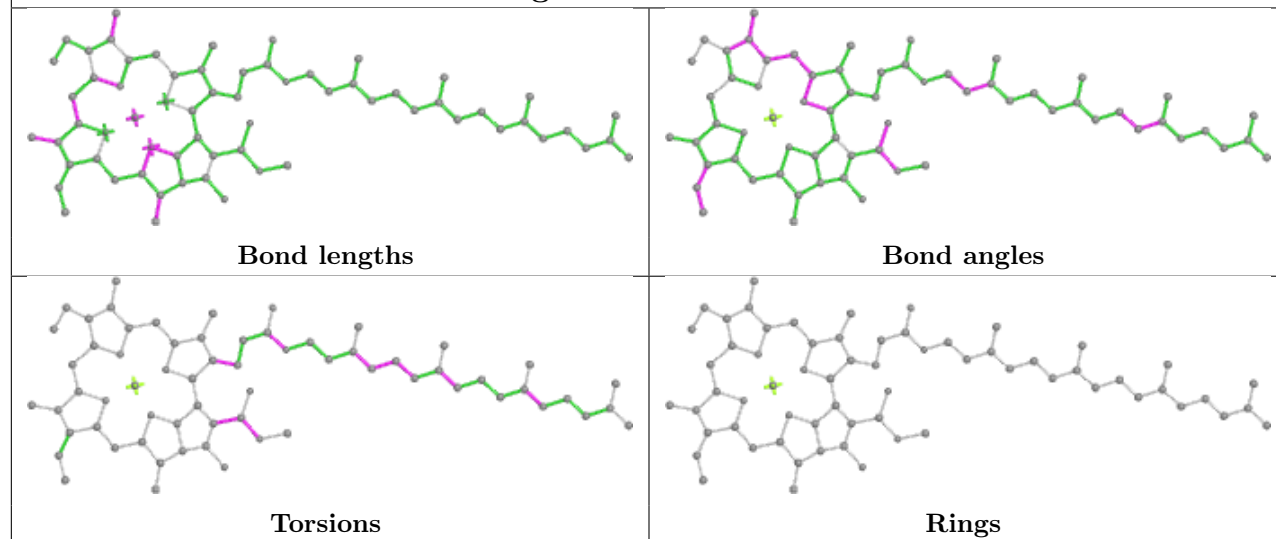
## Ligand LMG J 106



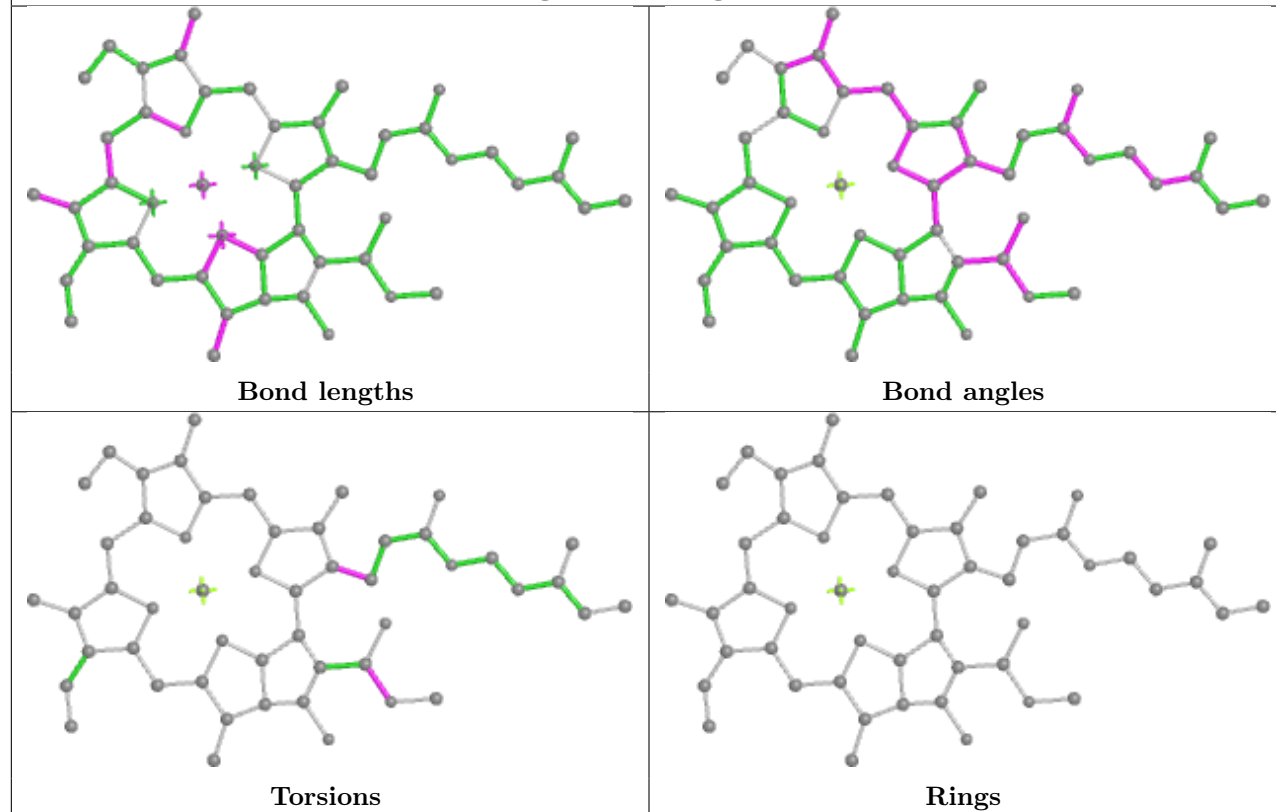
## Ligand WVN e 615

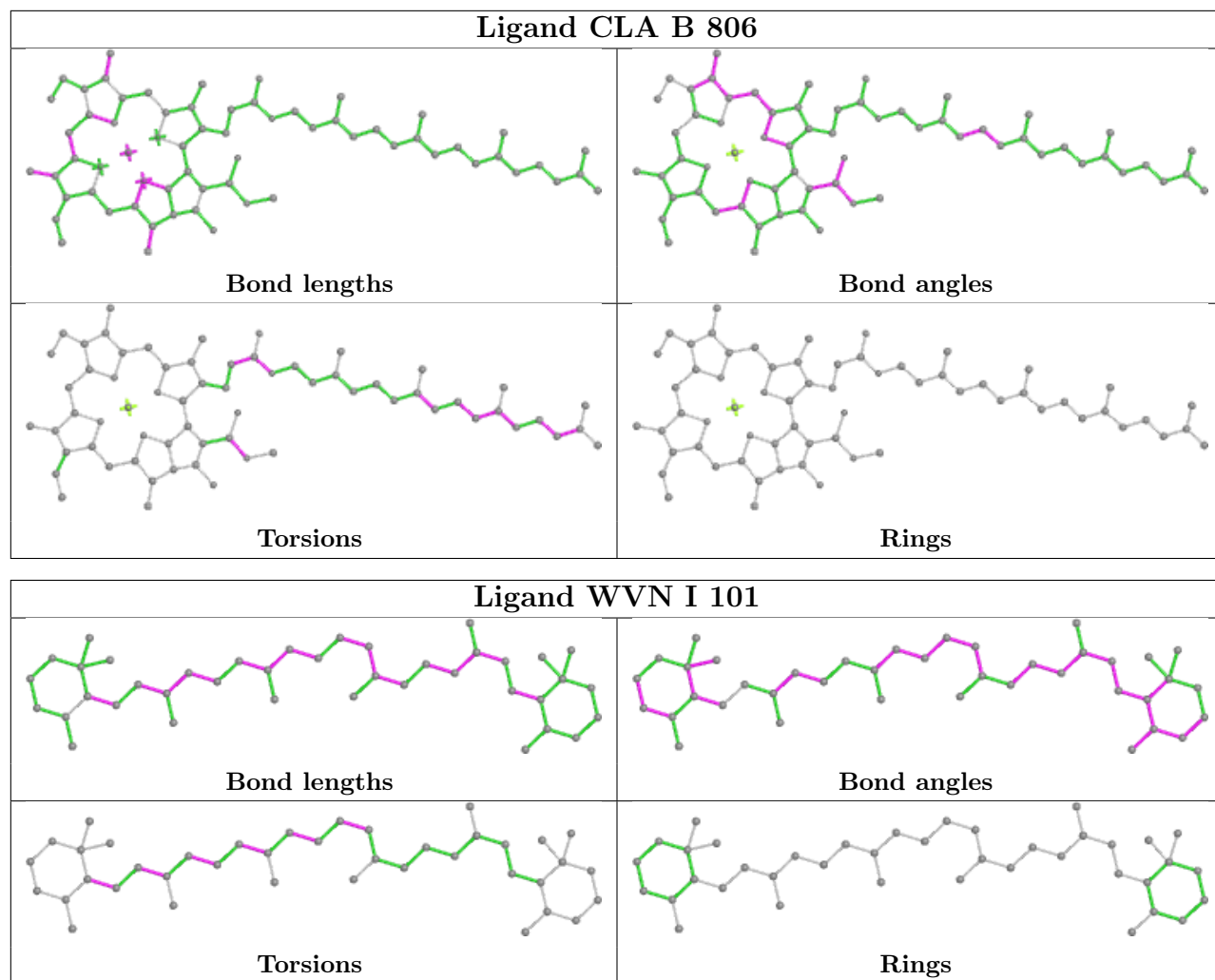


## Ligand CLA O 201



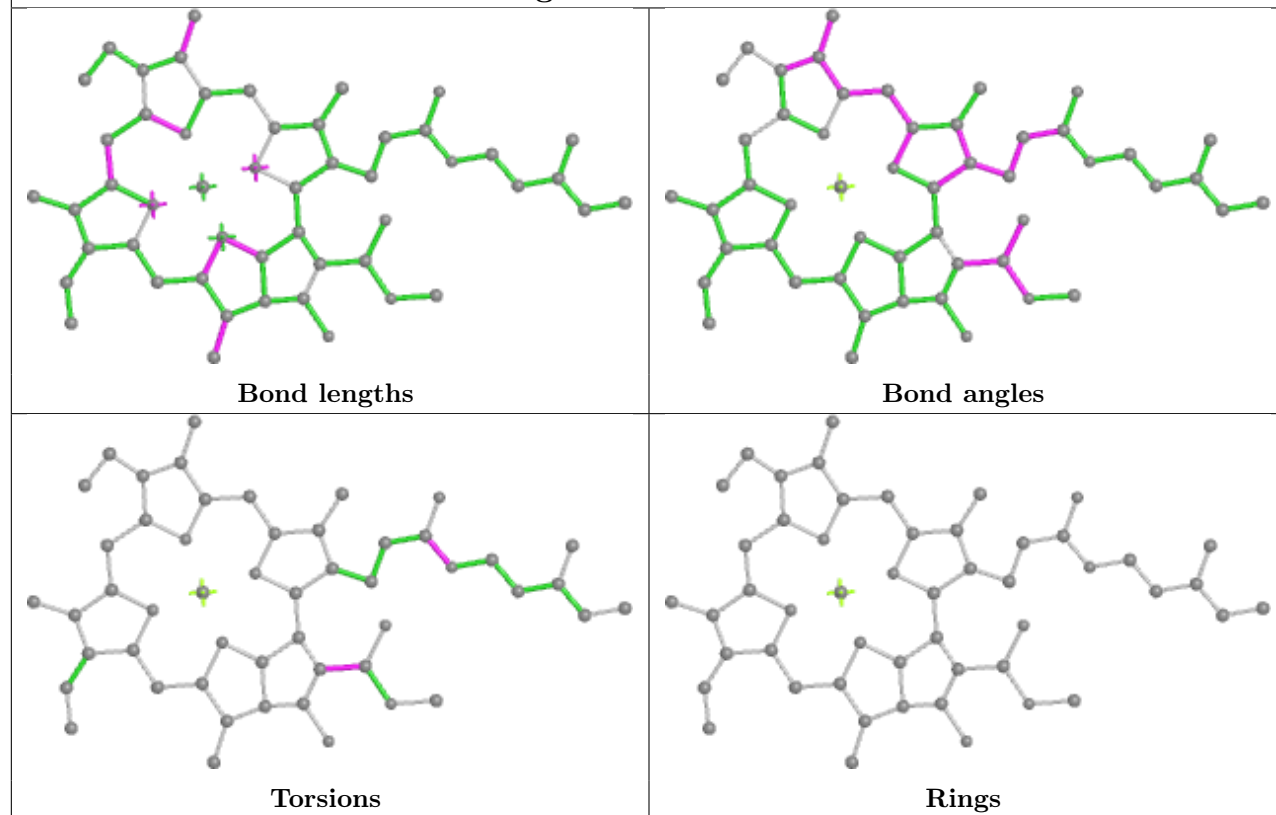
## Ligand CLA g 304



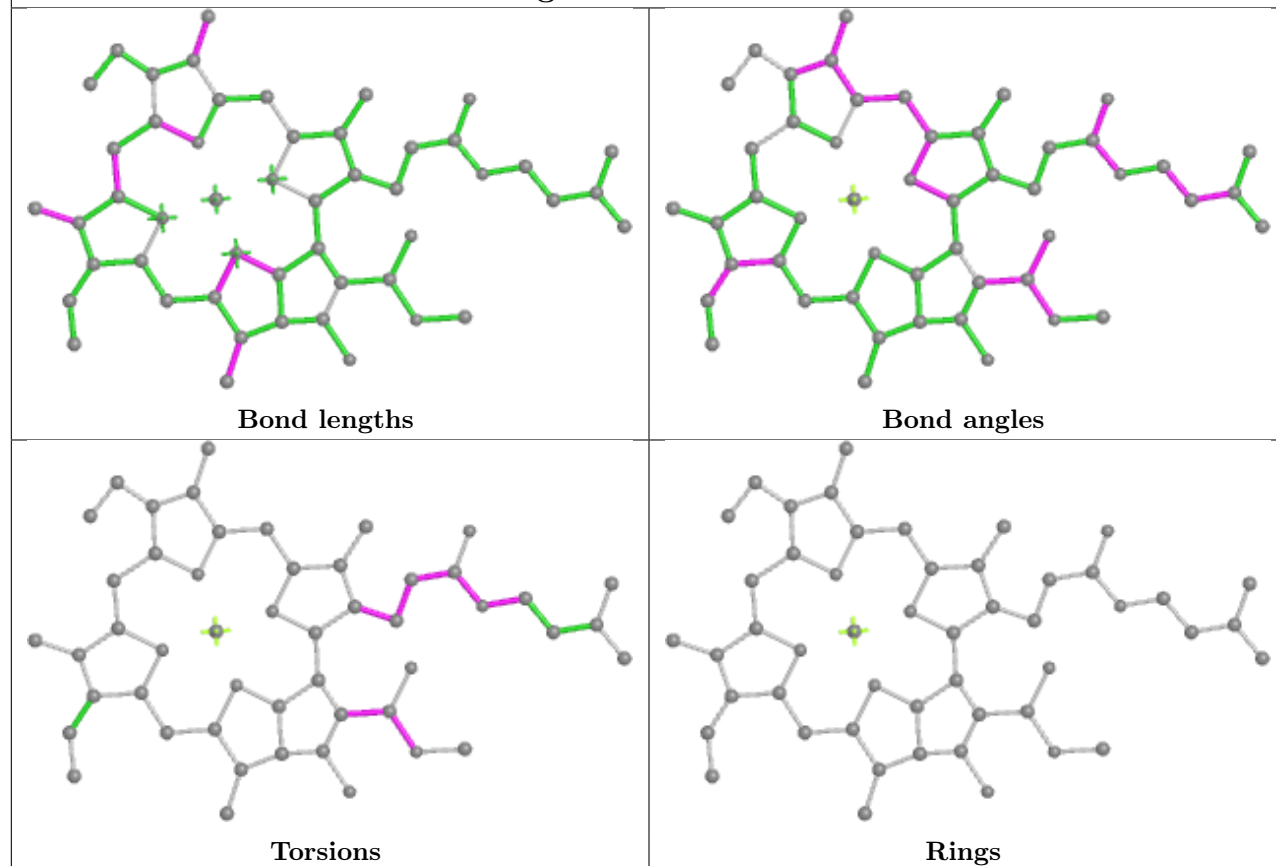


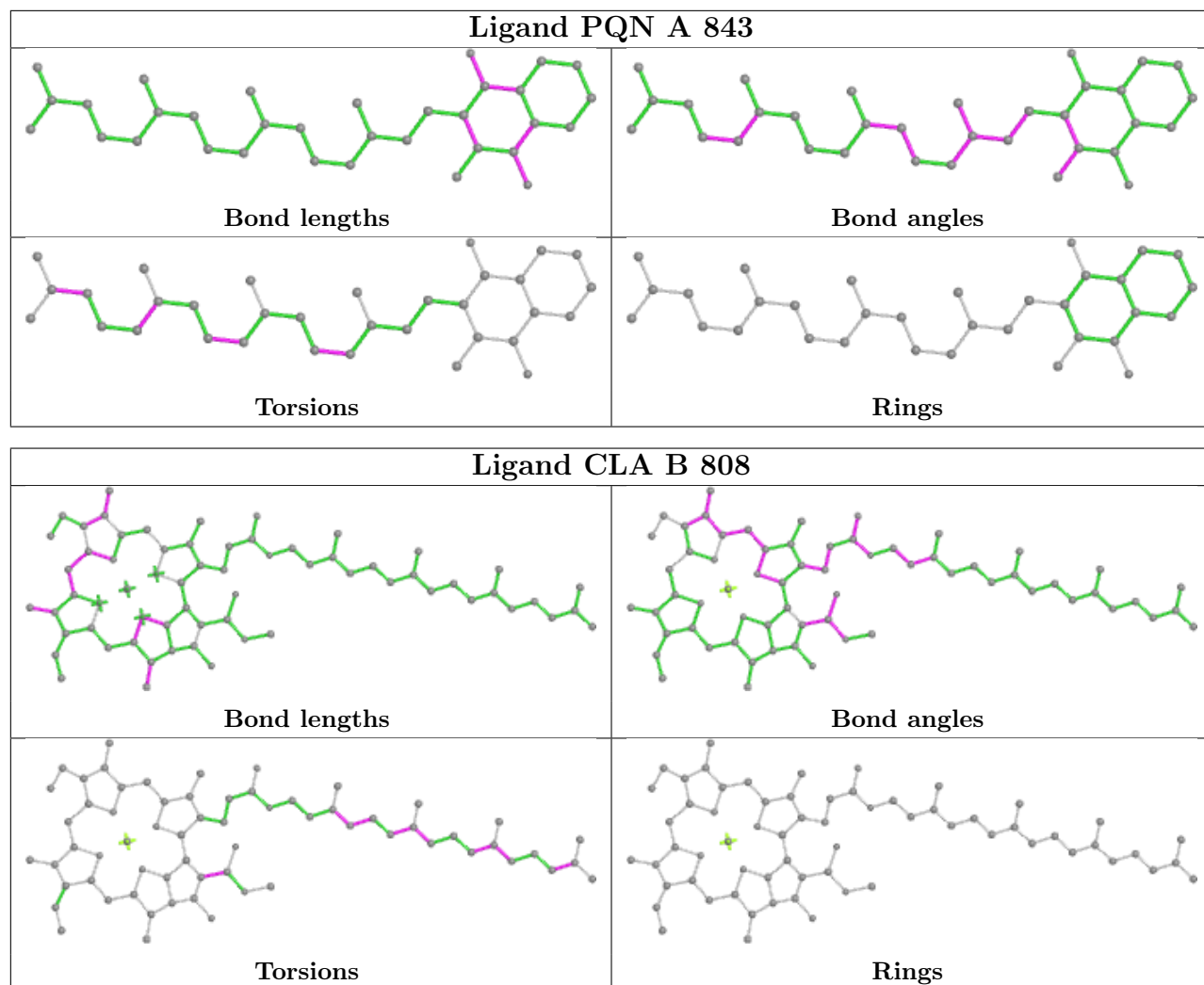


## Ligand CLA k 603

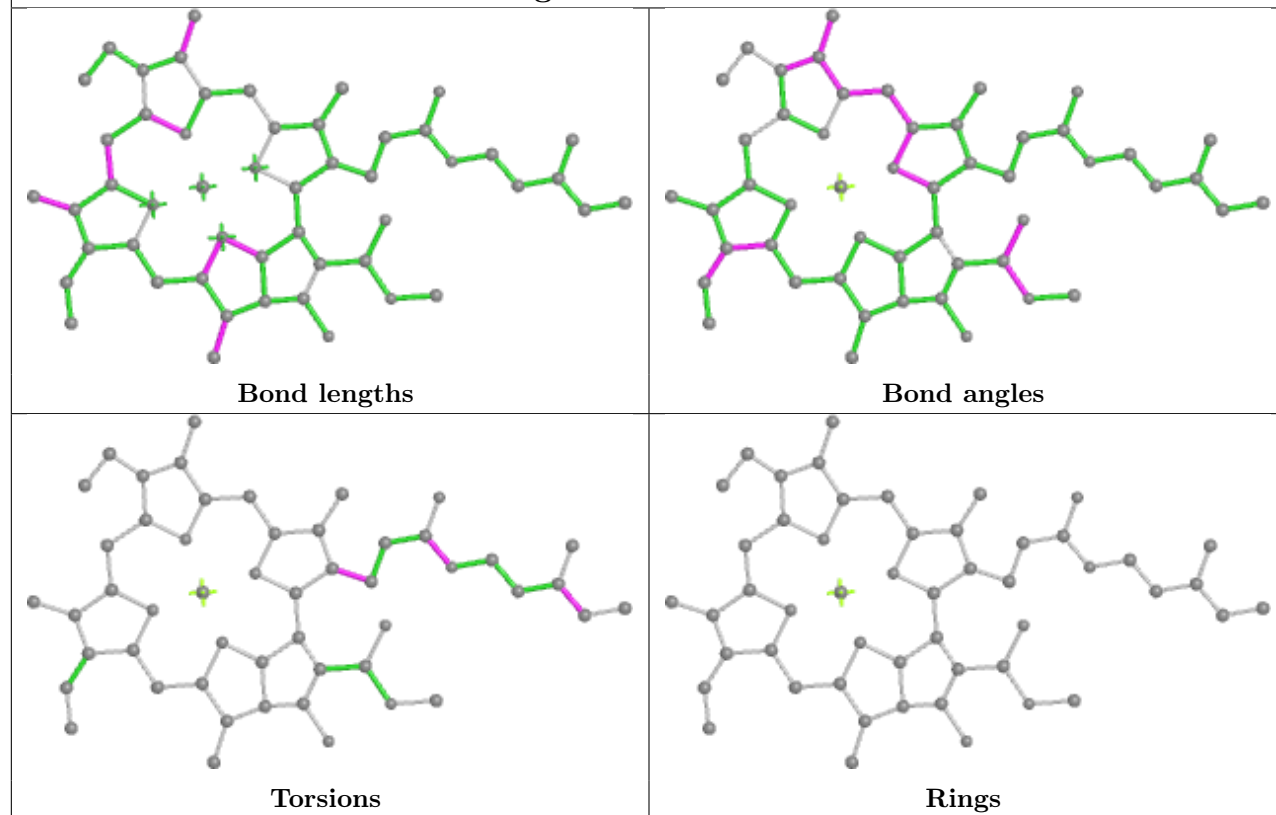


## Ligand CLA c 602

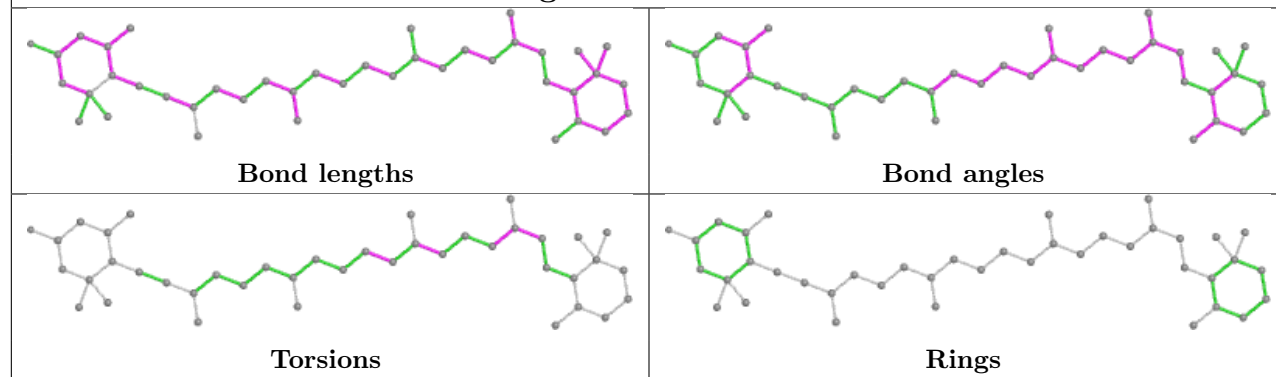




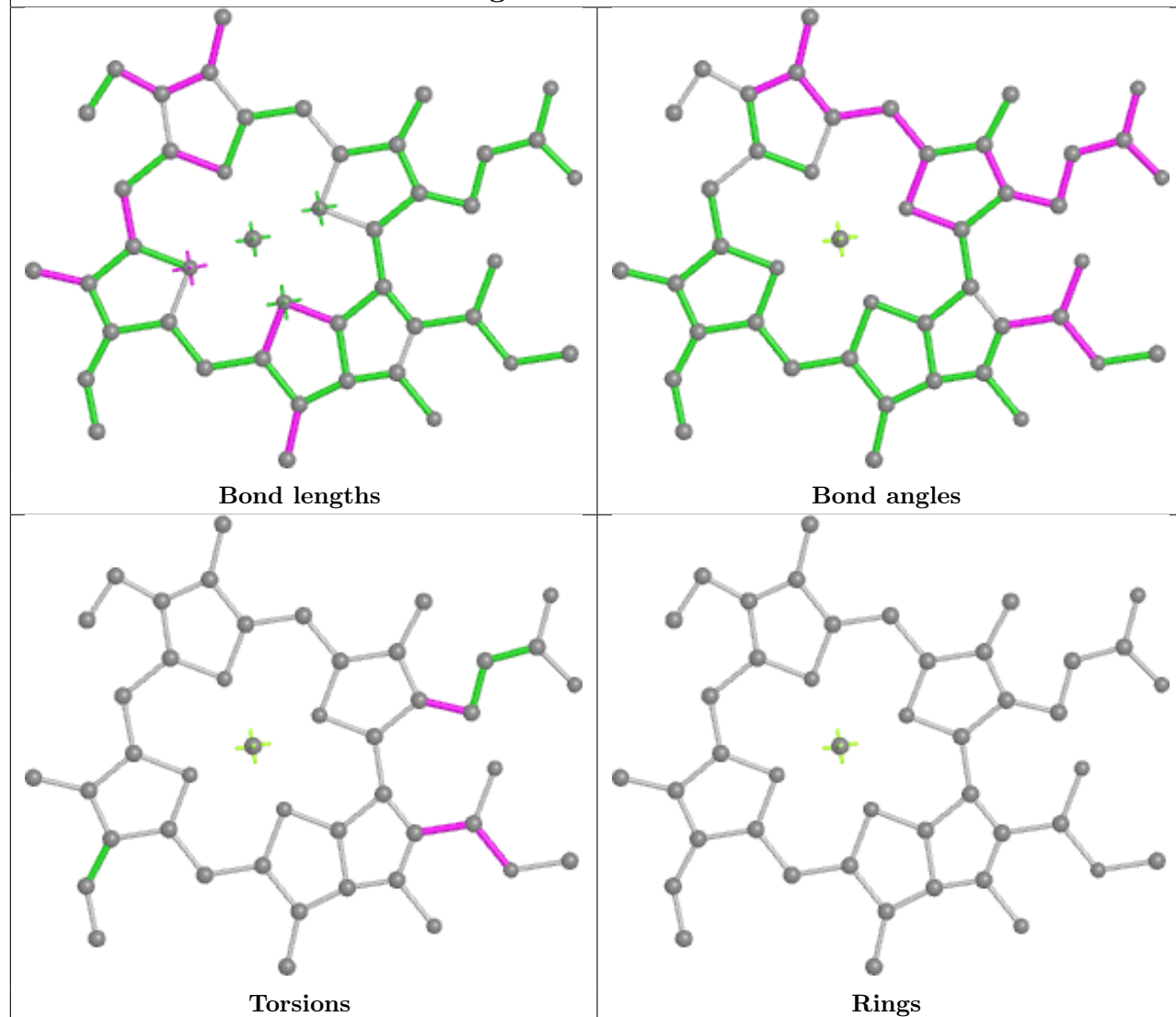
## Ligand CLA L 207



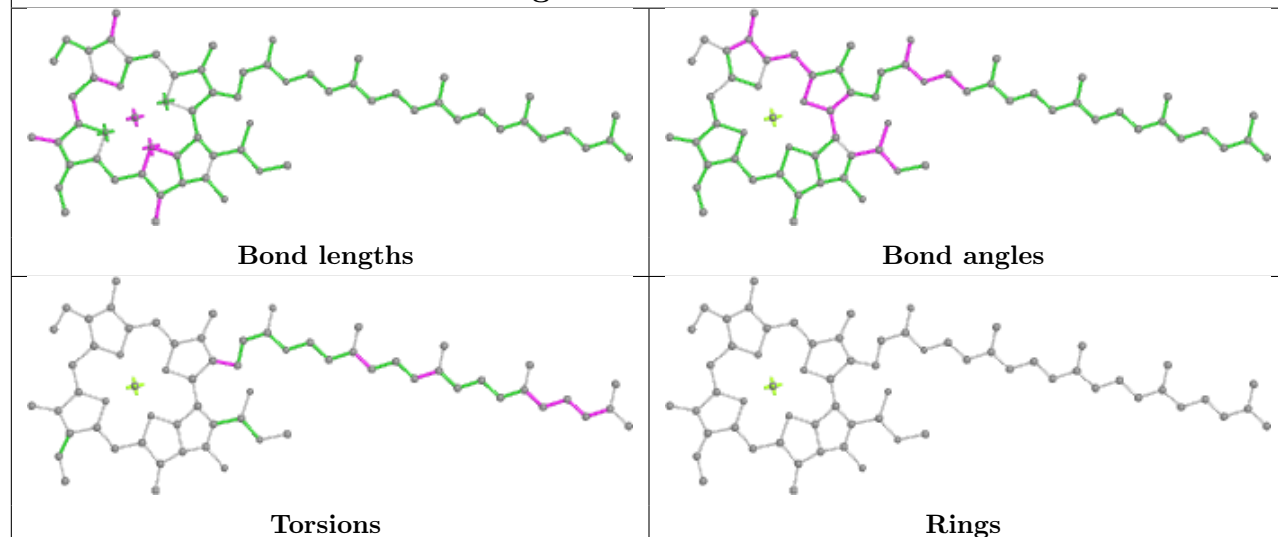
## Ligand IHT b 317

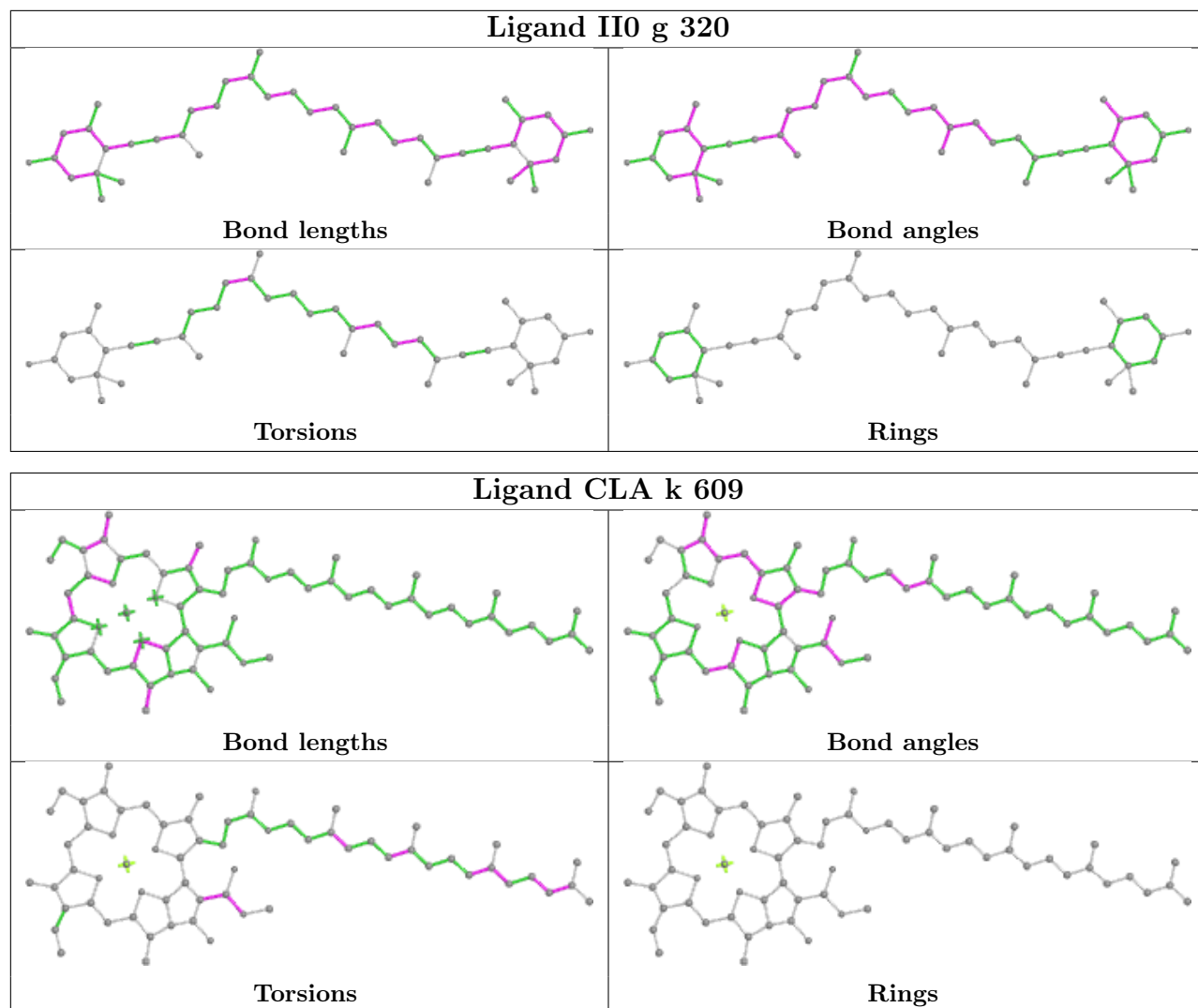


## Ligand CLA A 813

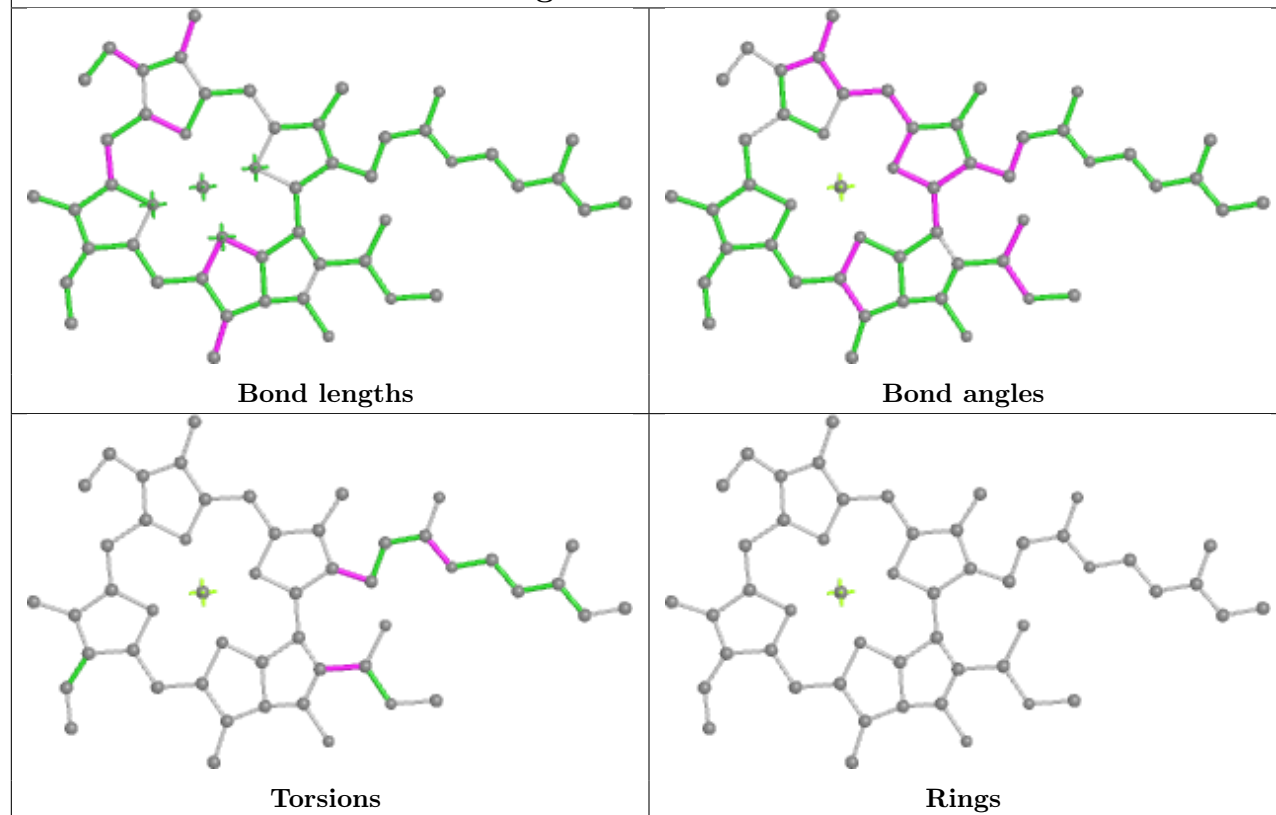


## Ligand CLA B 825

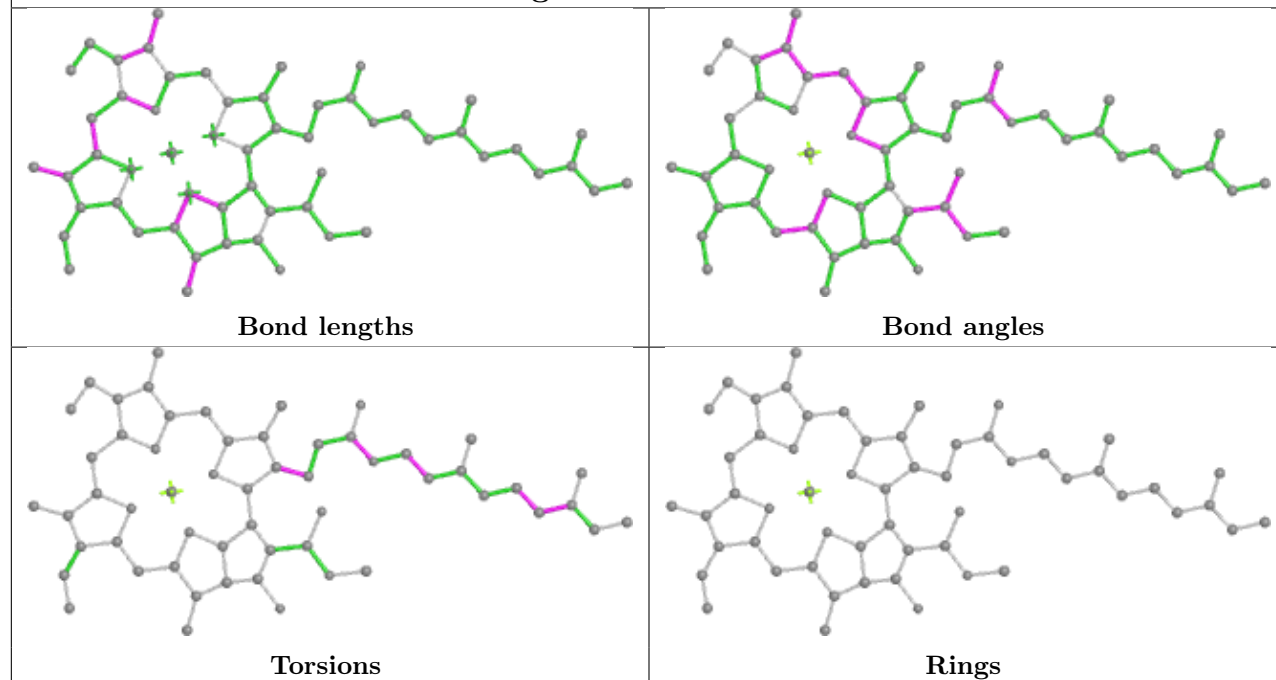




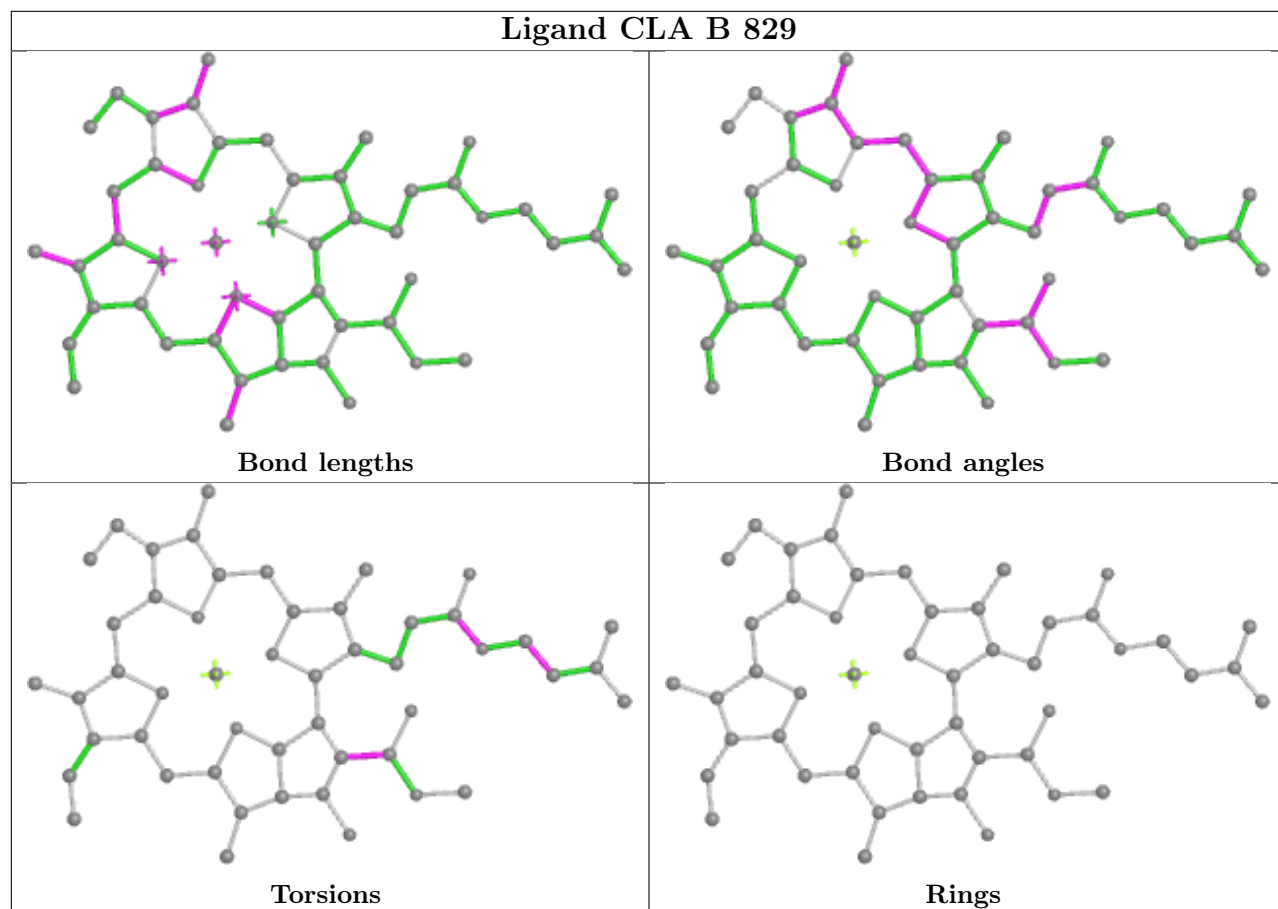
## Ligand CLA J 105



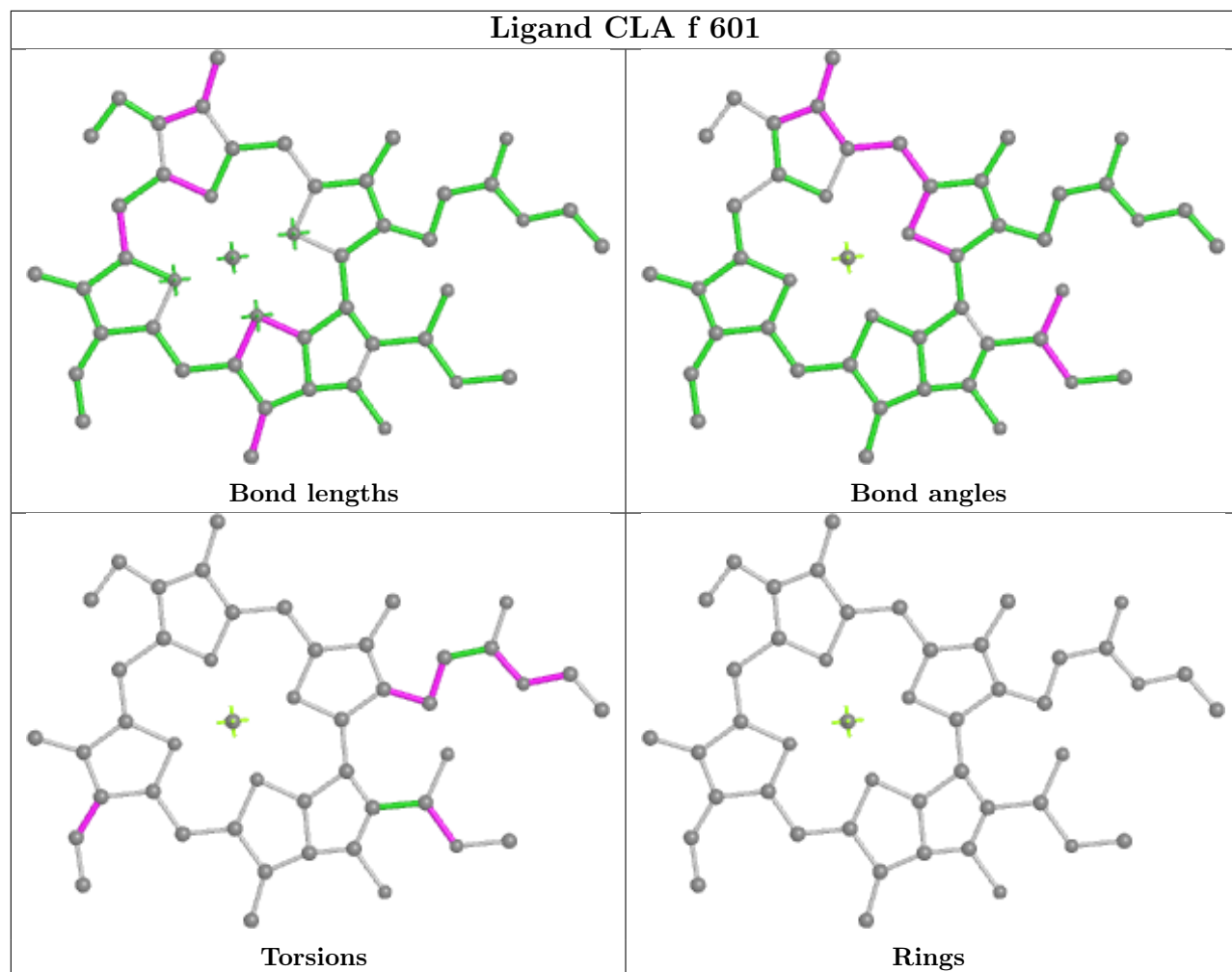
## Ligand CLA A 809



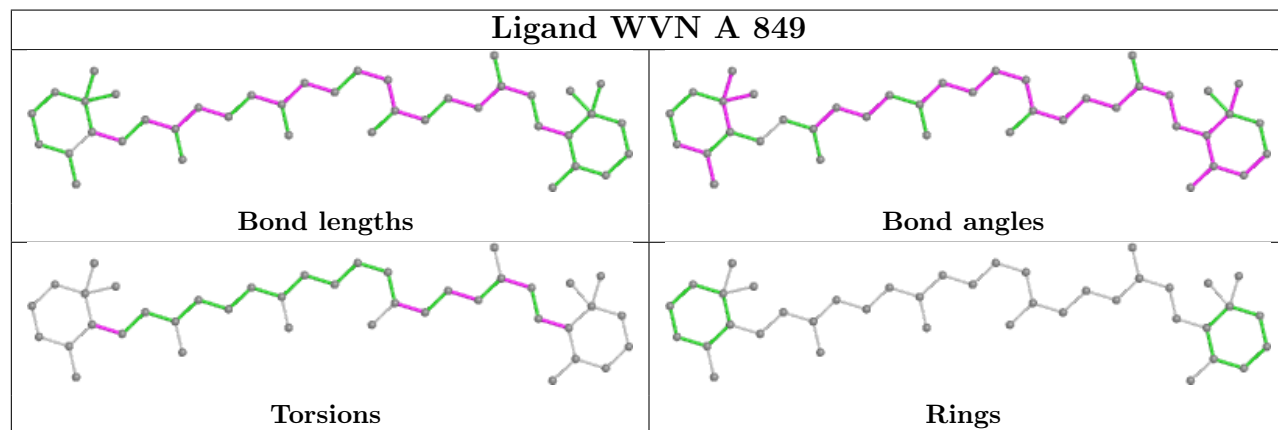
## Ligand CLA B 829



## Ligand CLA f 601

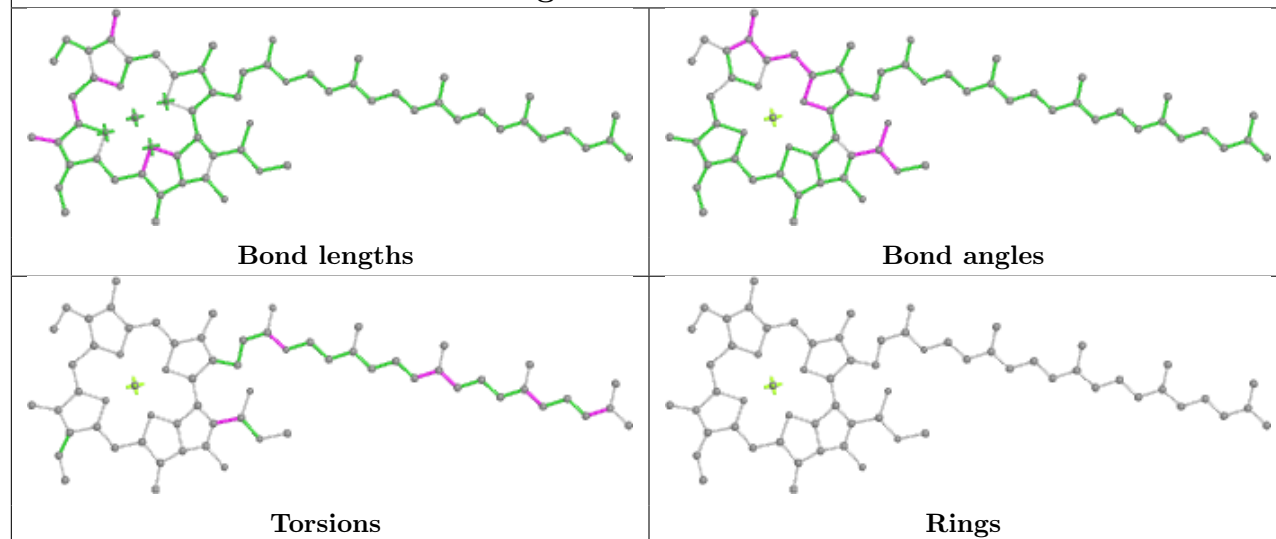


## Ligand WVN A 849

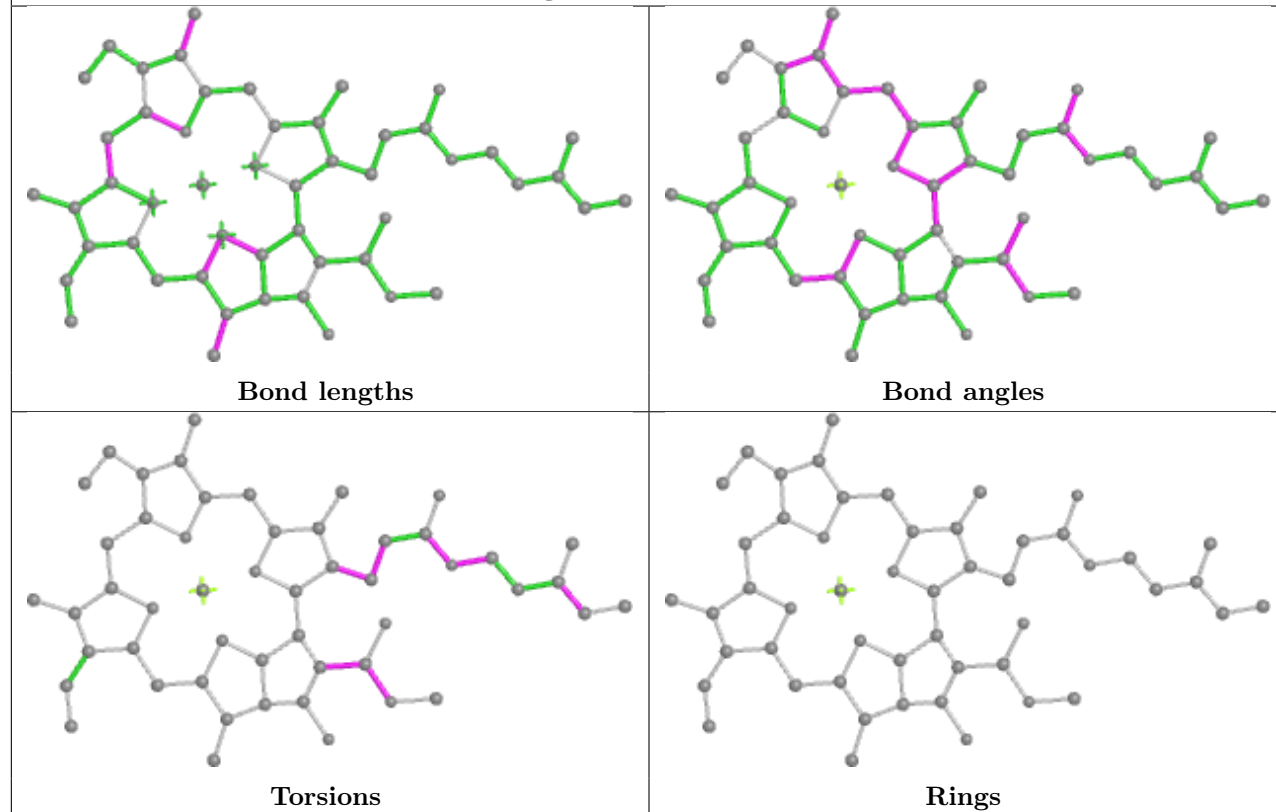


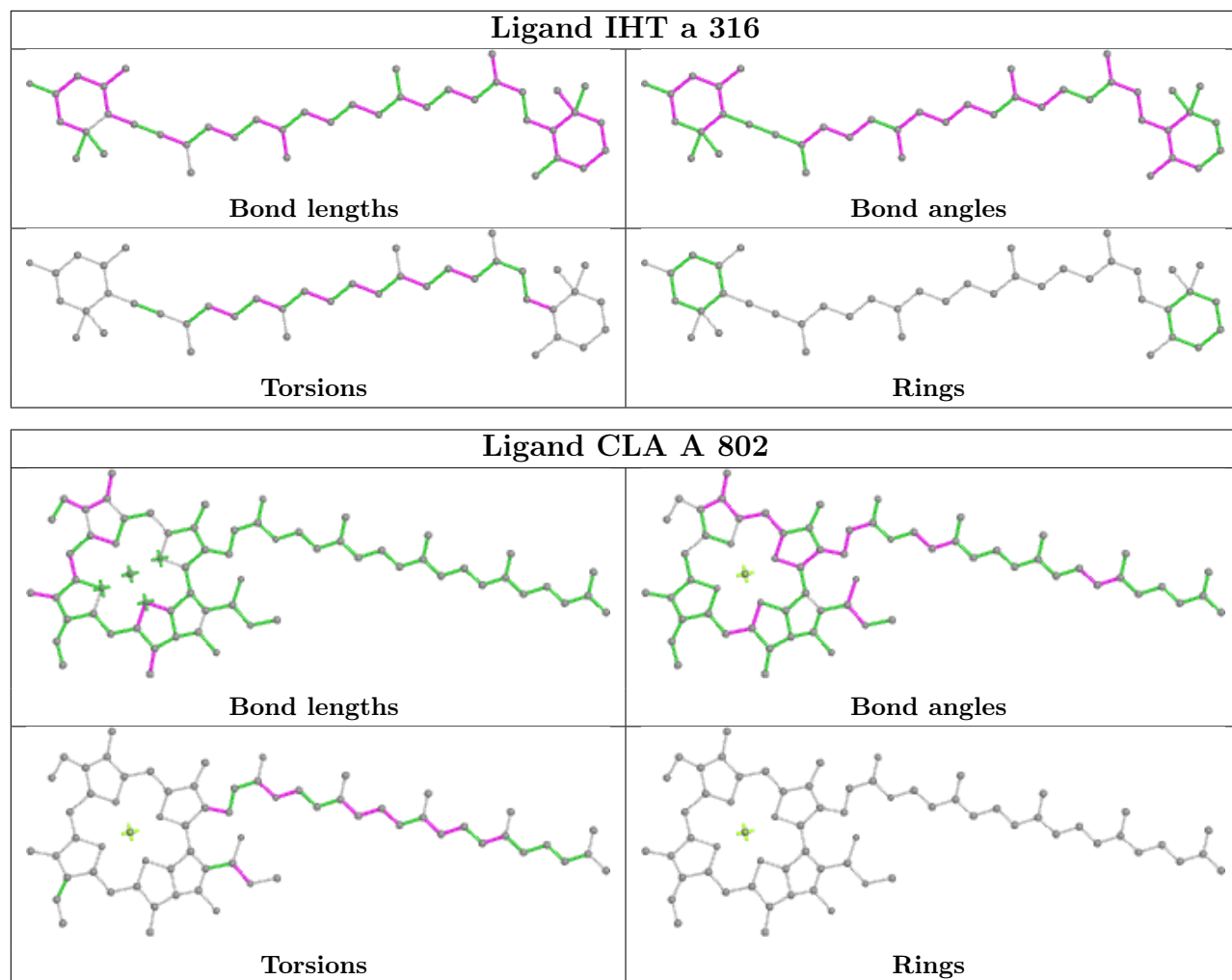


## Ligand CLA e 606

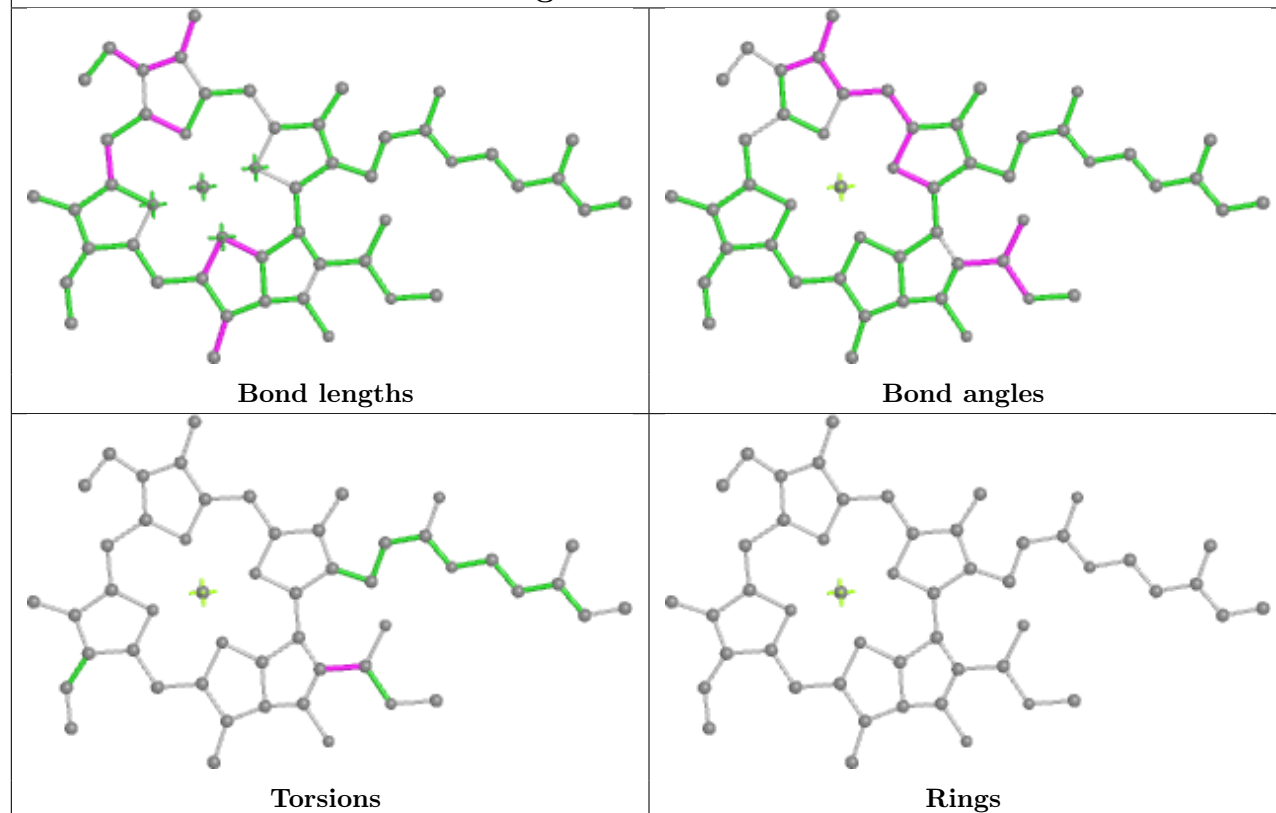


## Ligand CLA i 611

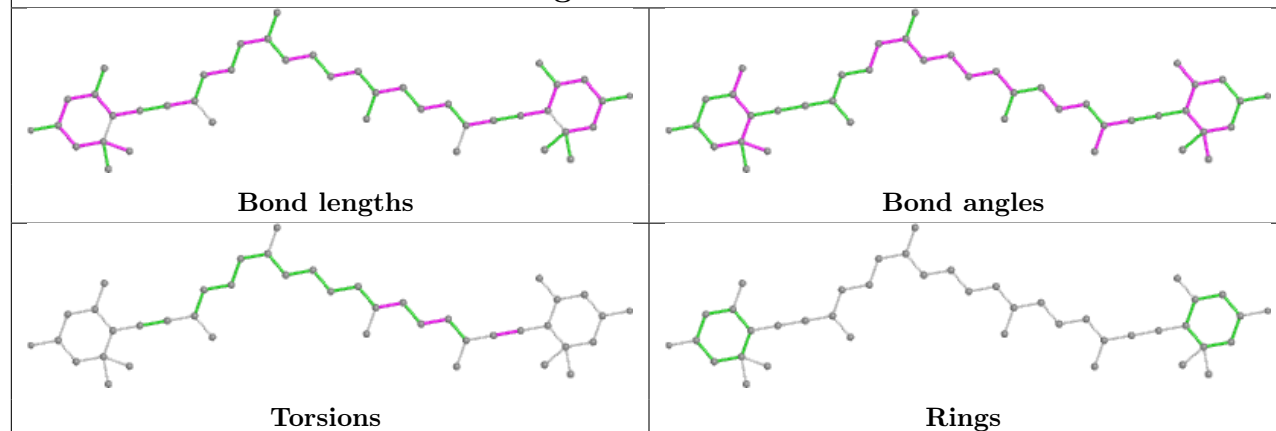


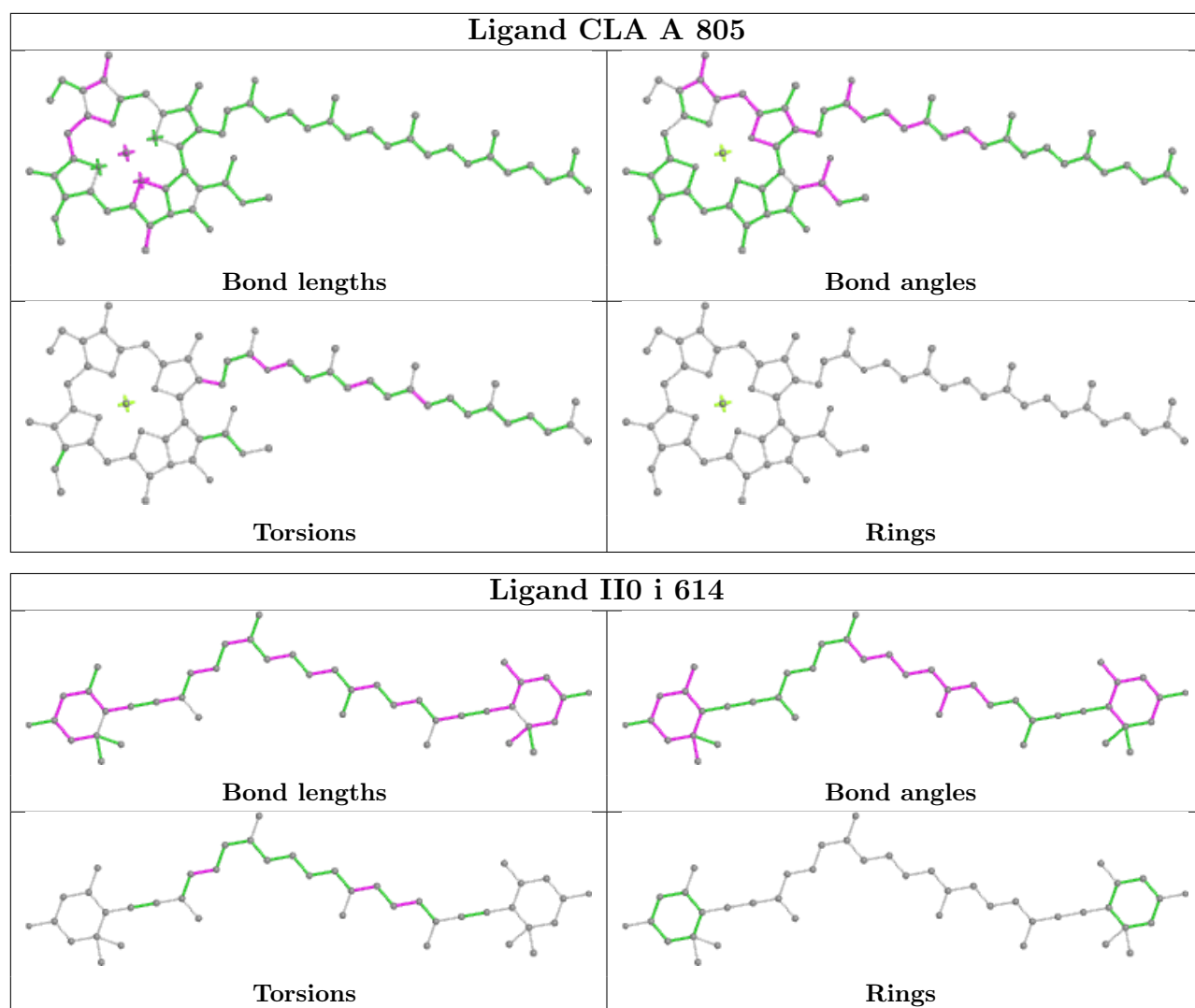


## Ligand CLA a 304

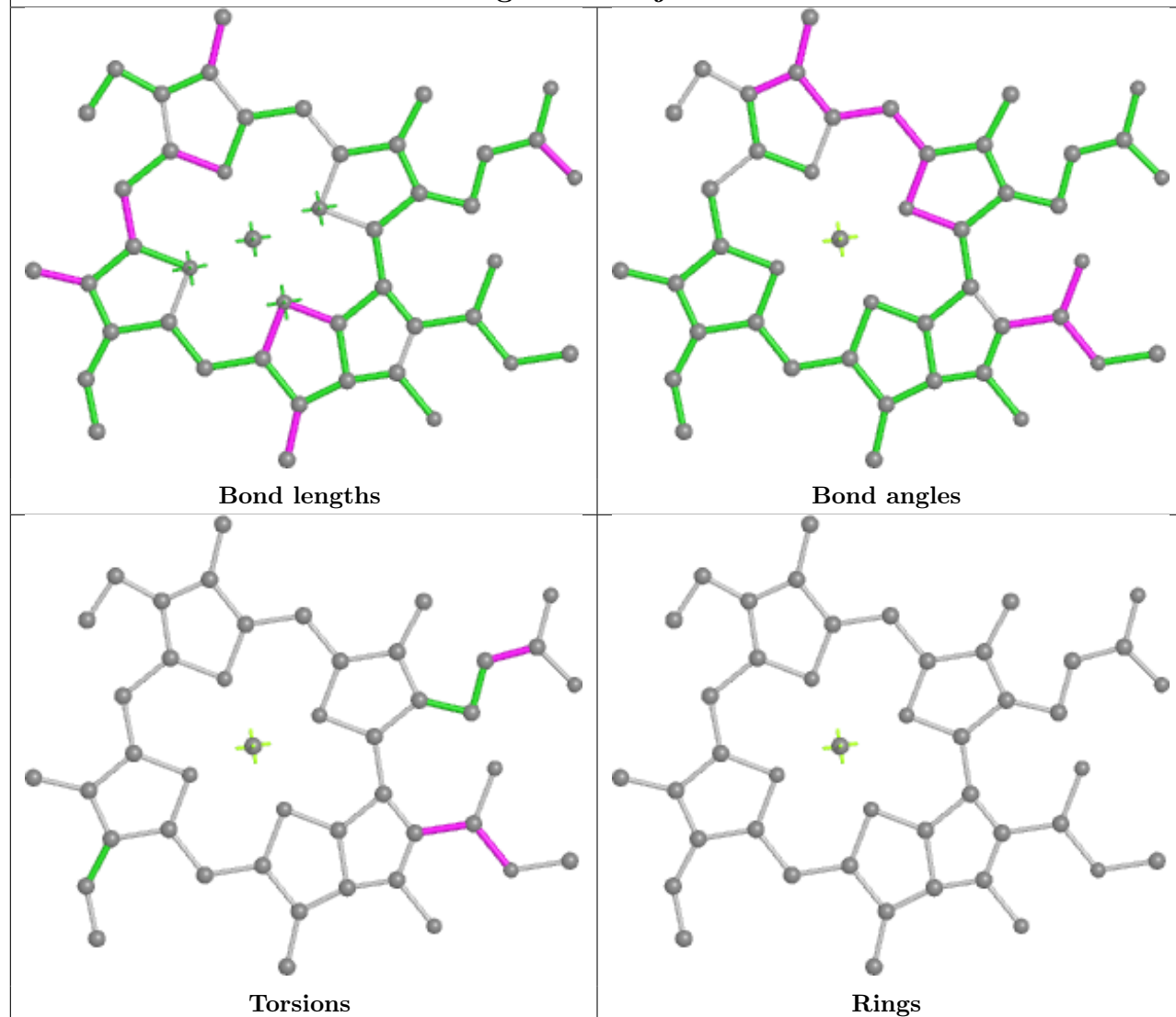


## Ligand II0 f 614

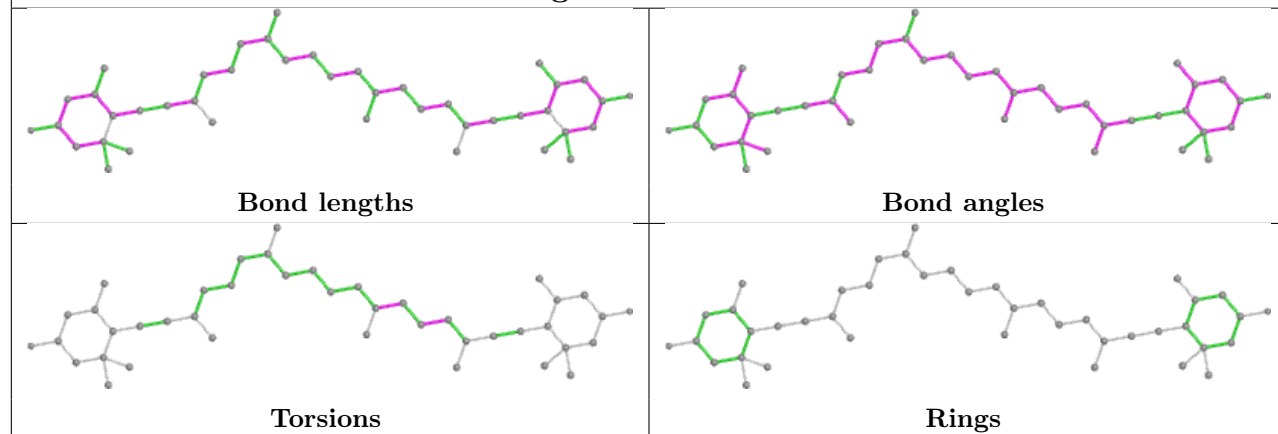


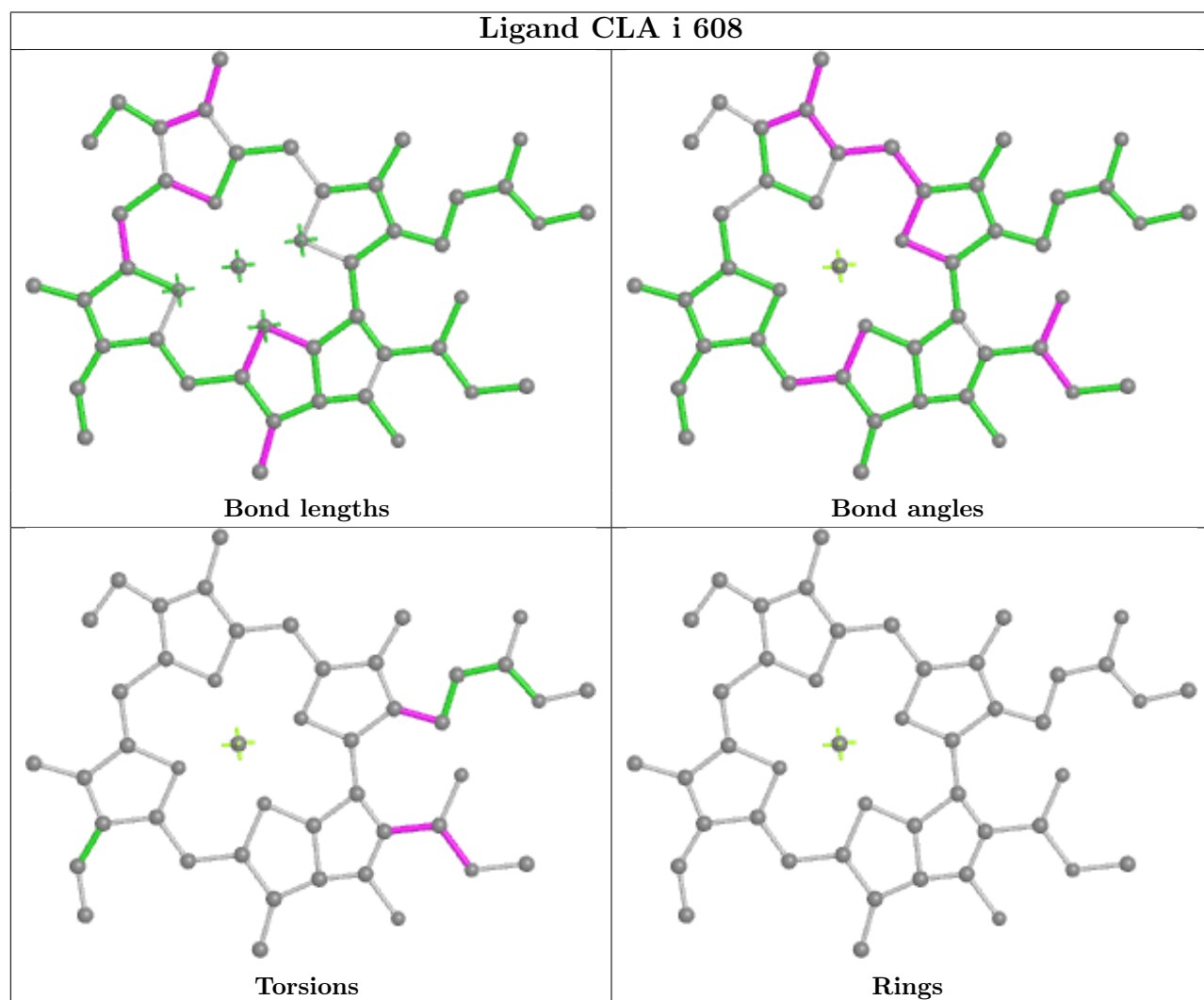
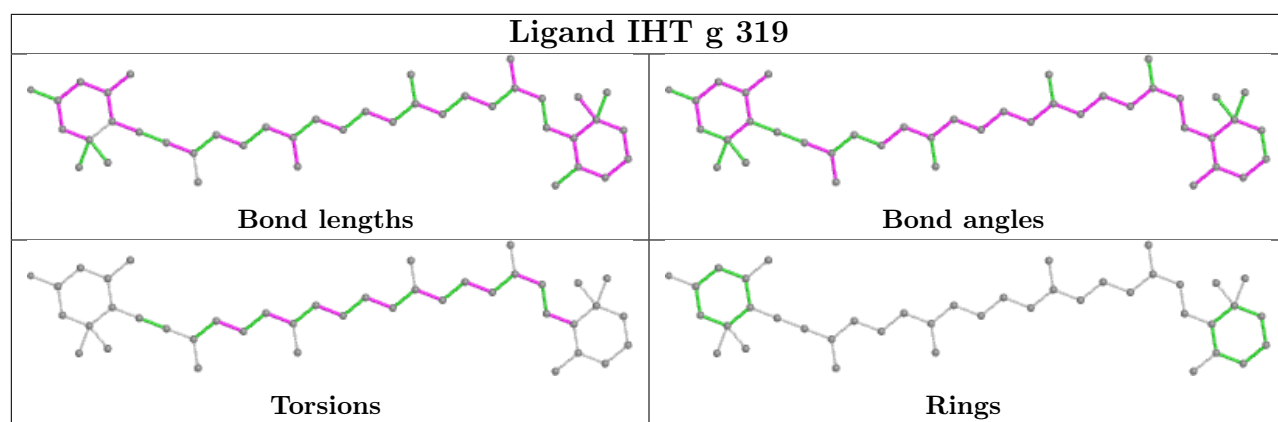


## Ligand CLA j 309

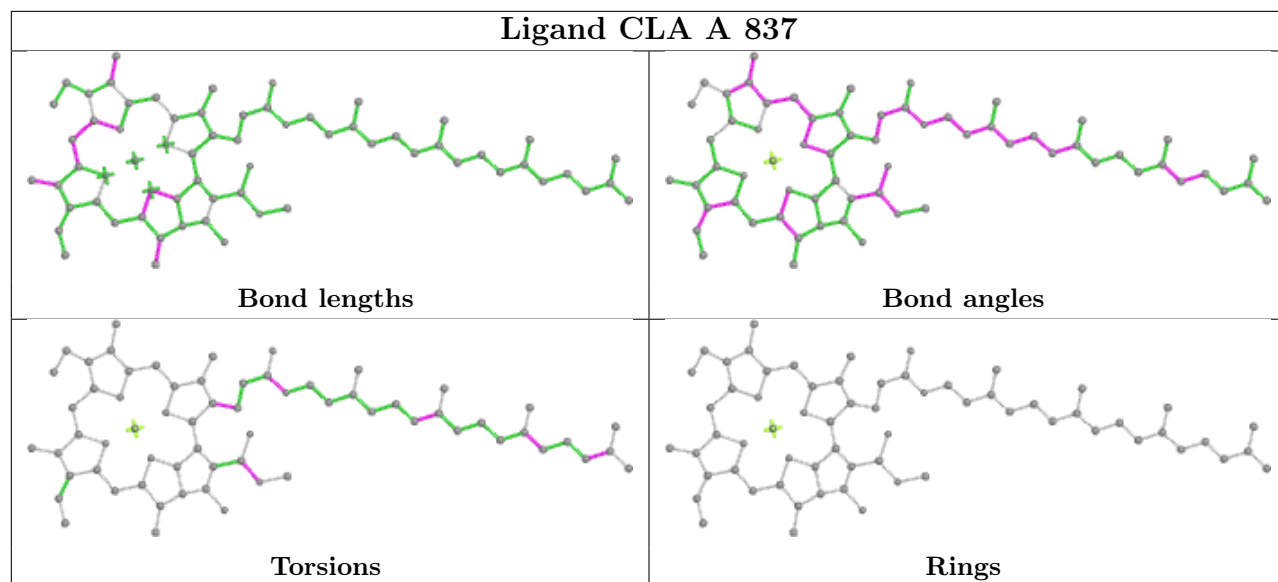


## Ligand II0 e 614

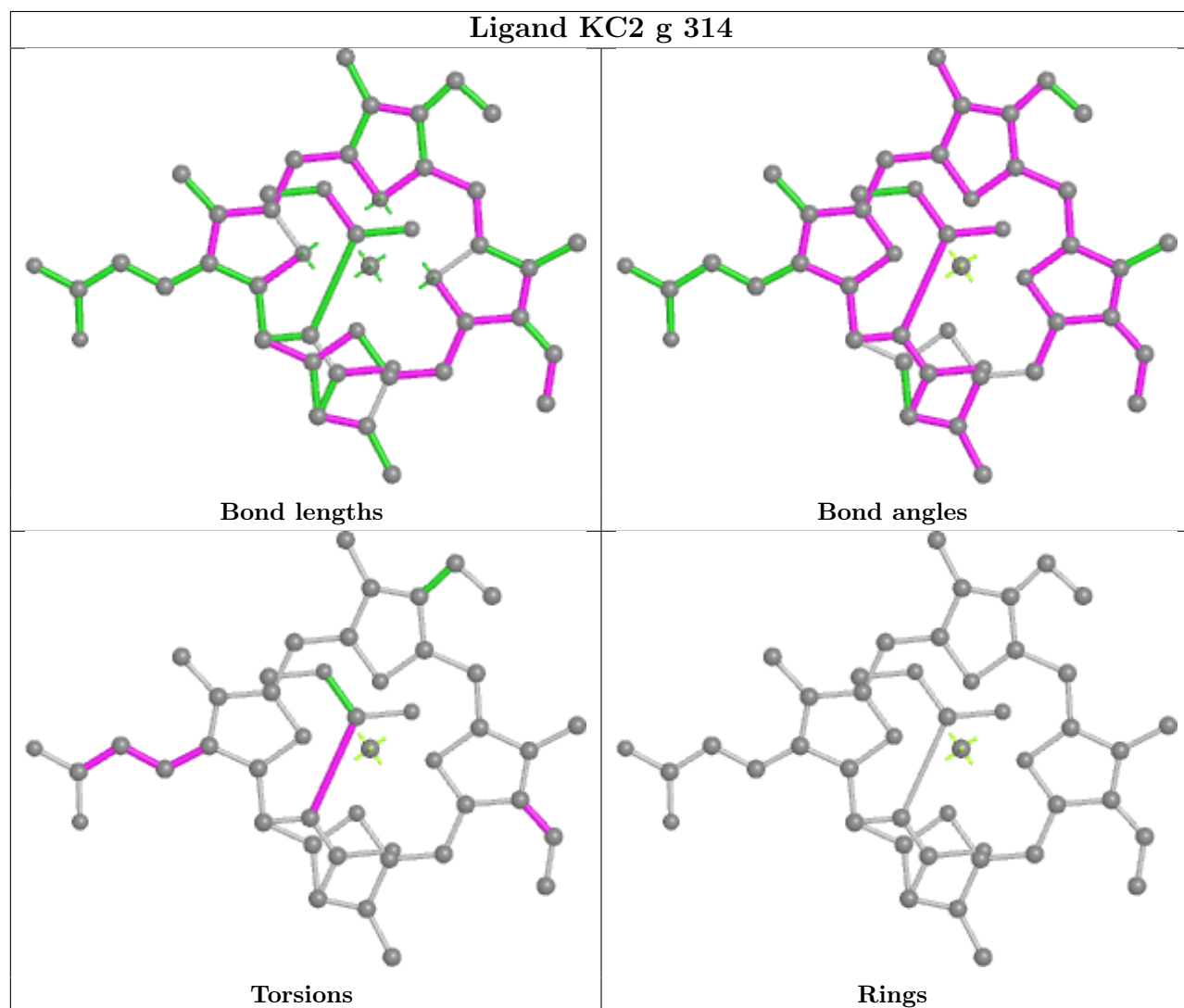




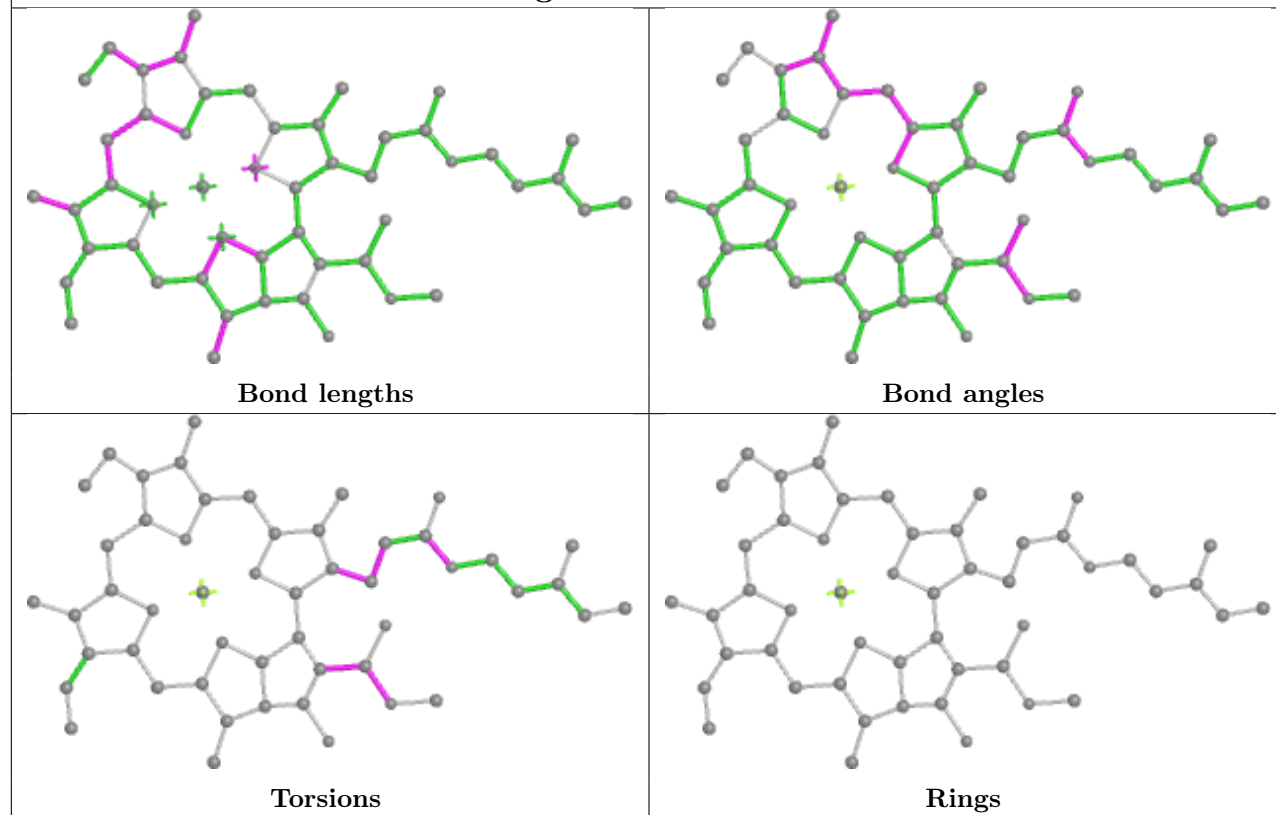
## Ligand CLA A 837



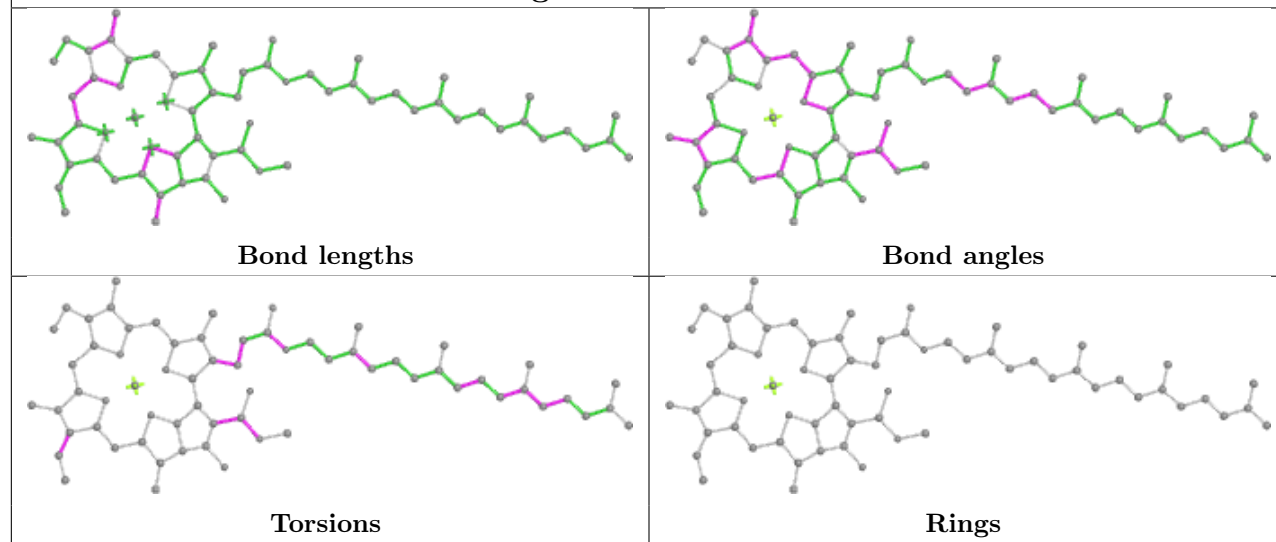
## Ligand KC2 g 314



## Ligand CLA d 306

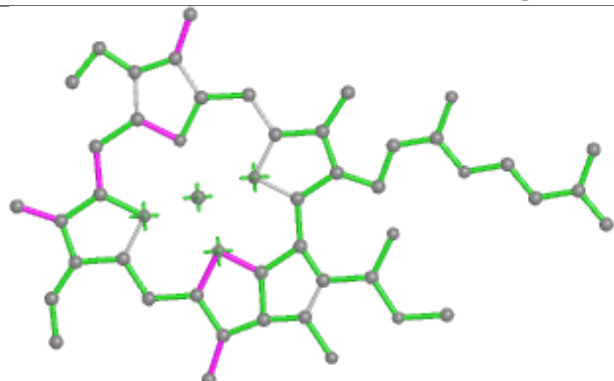


## Ligand CLA A 818

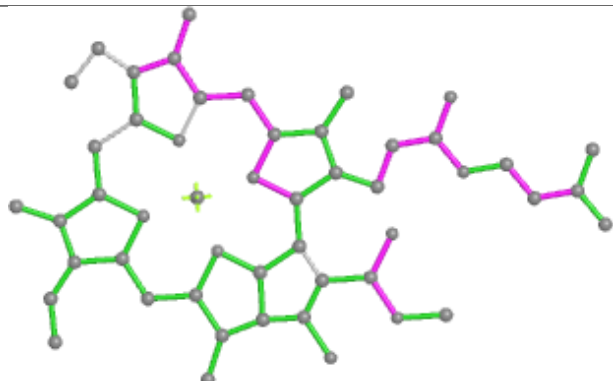




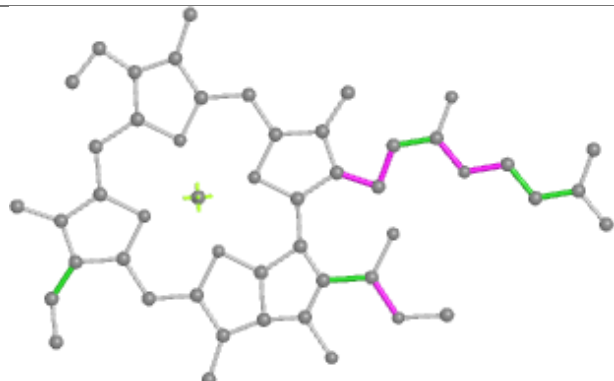
## Ligand CLA L 204



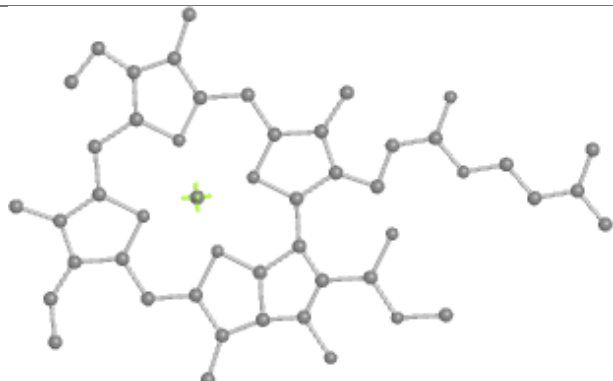
Bond lengths



Bond angles

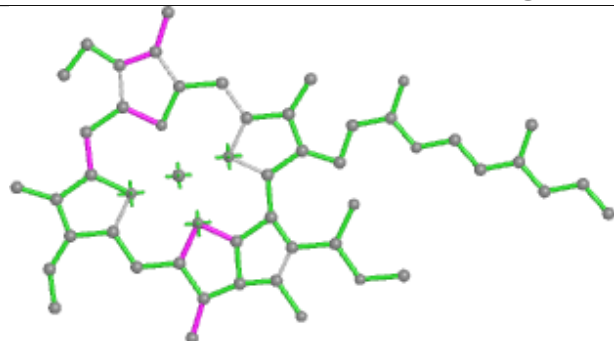


Torsions

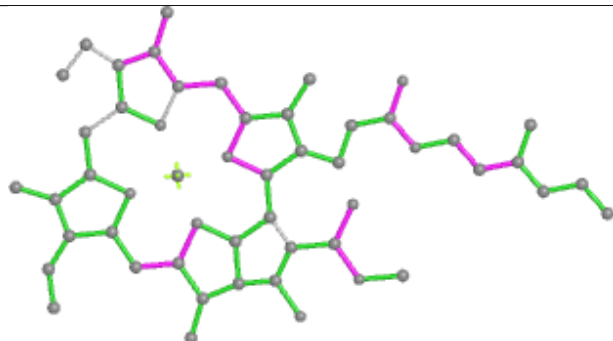


Rings

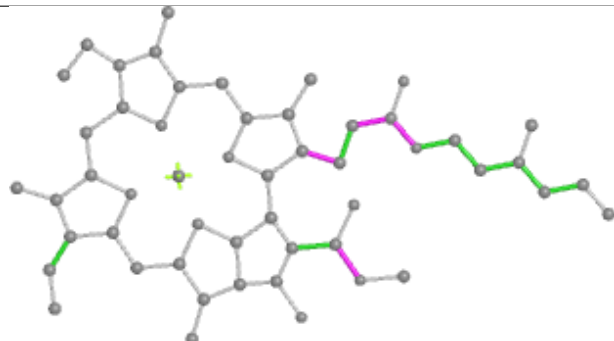
## Ligand CLA c 606



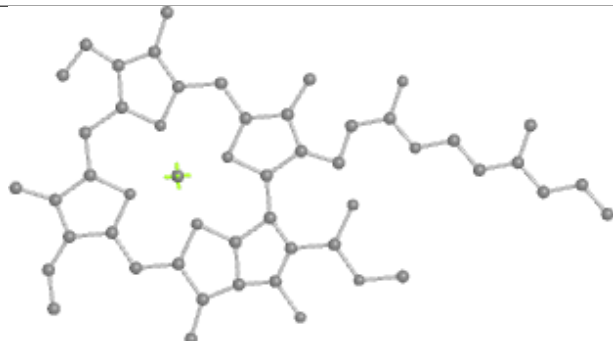
Bond lengths



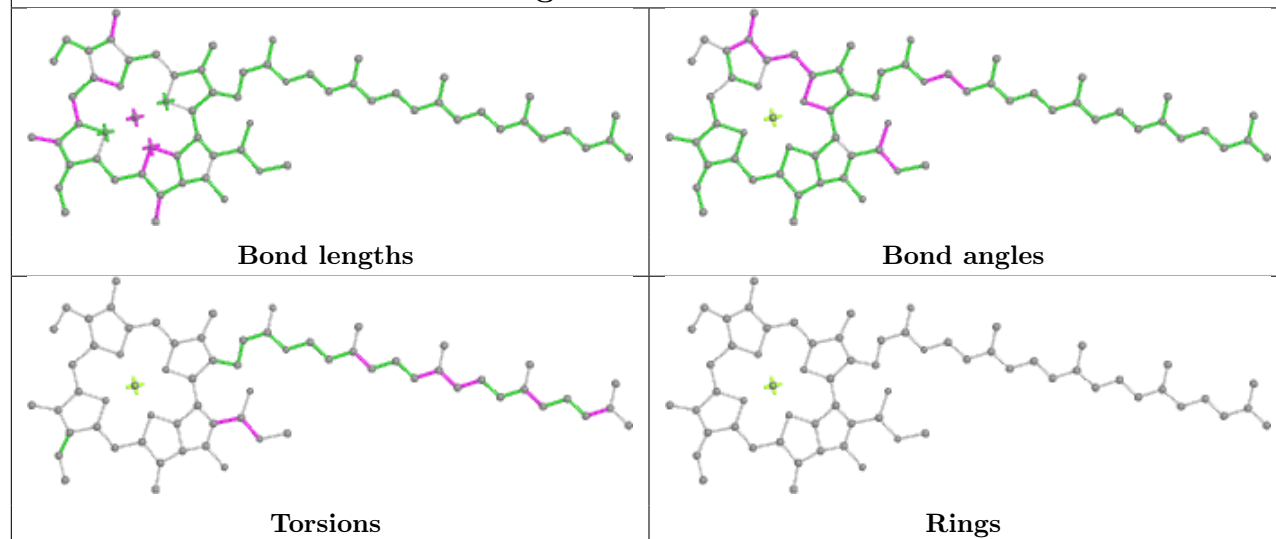
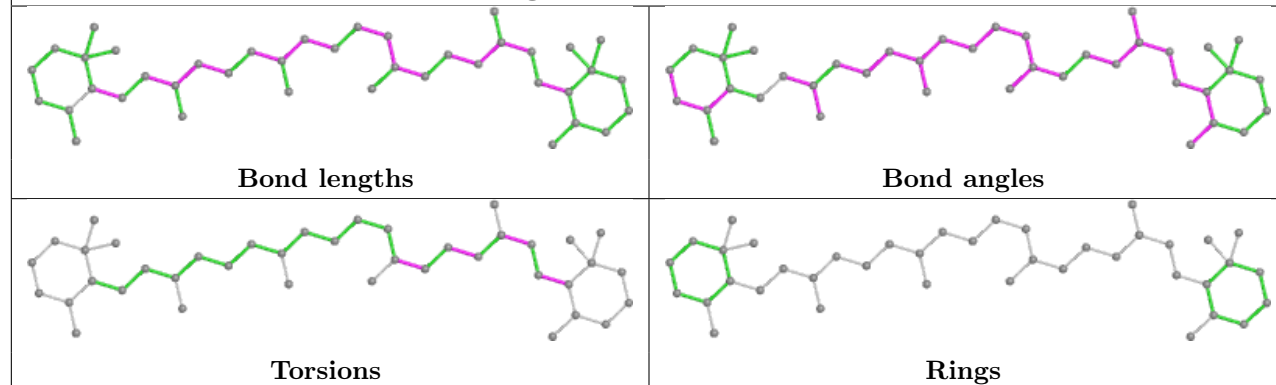
Bond angles



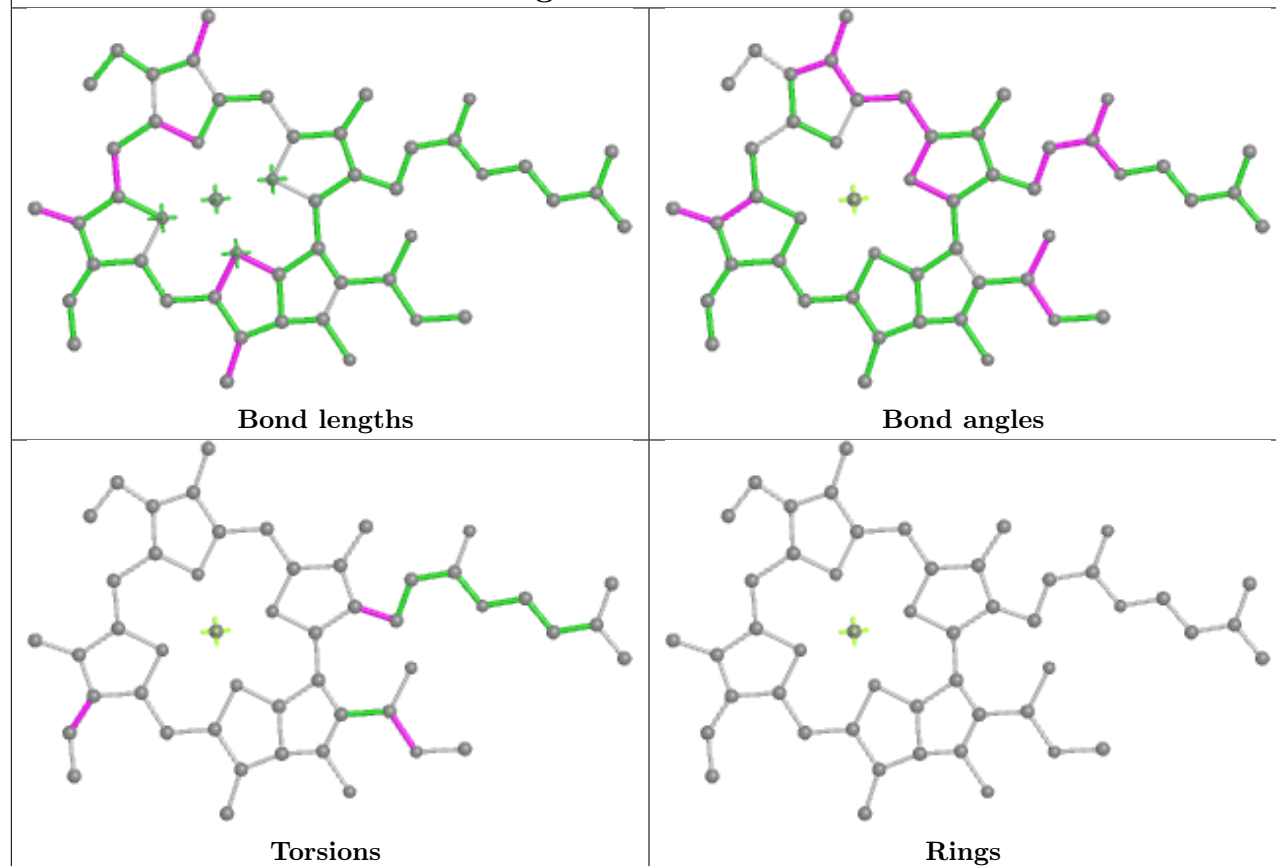
Torsions



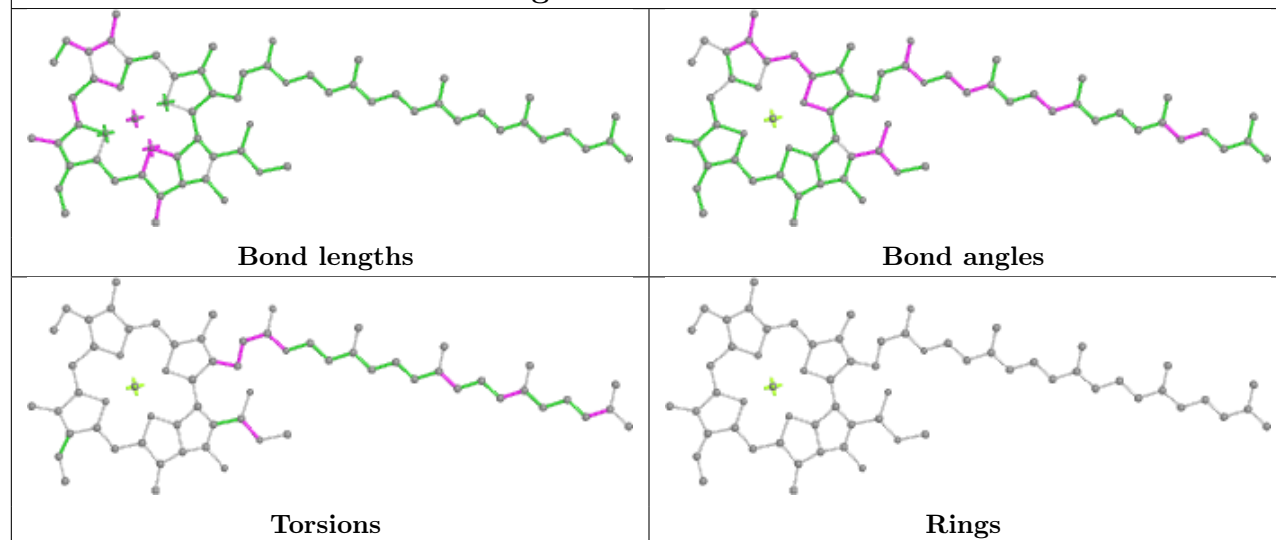
Rings

**Ligand CLA a 308****Ligand WVN B 848**

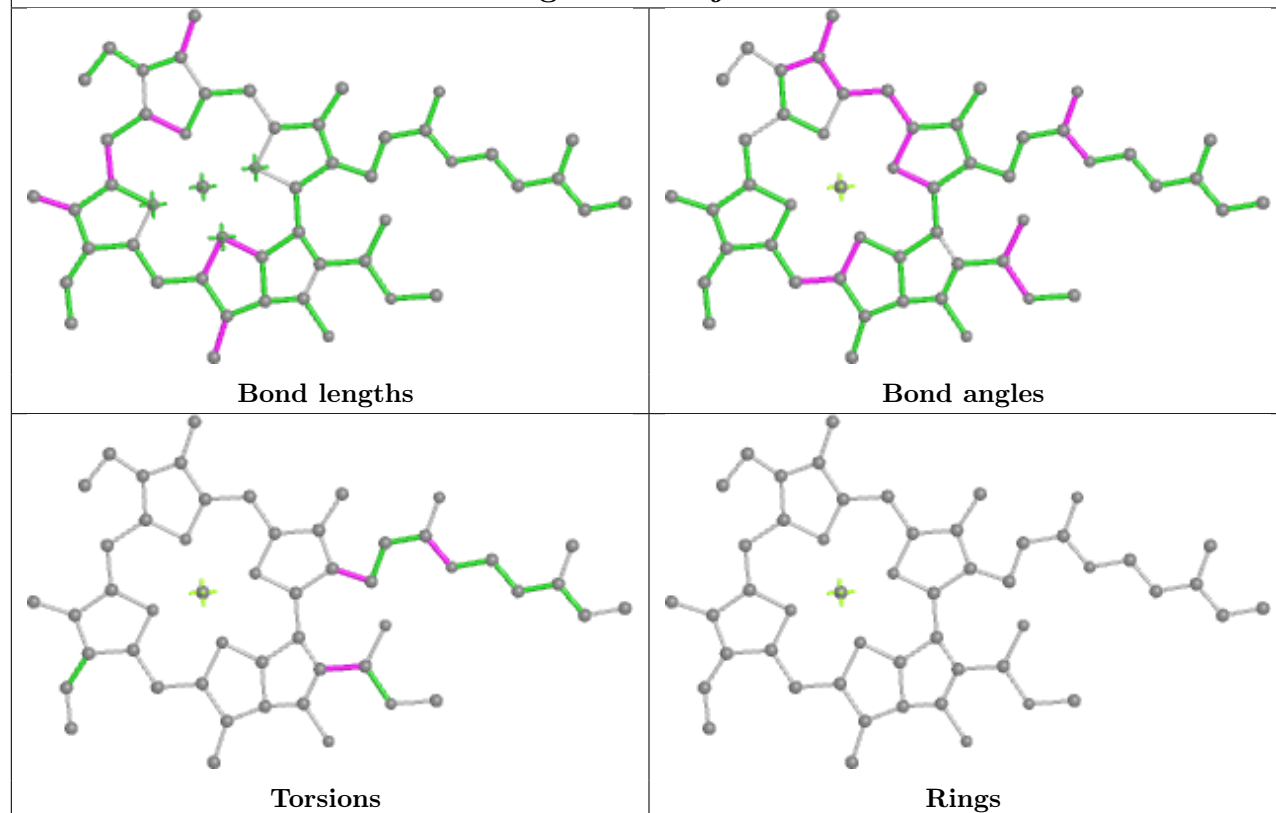
## Ligand CLA k 602



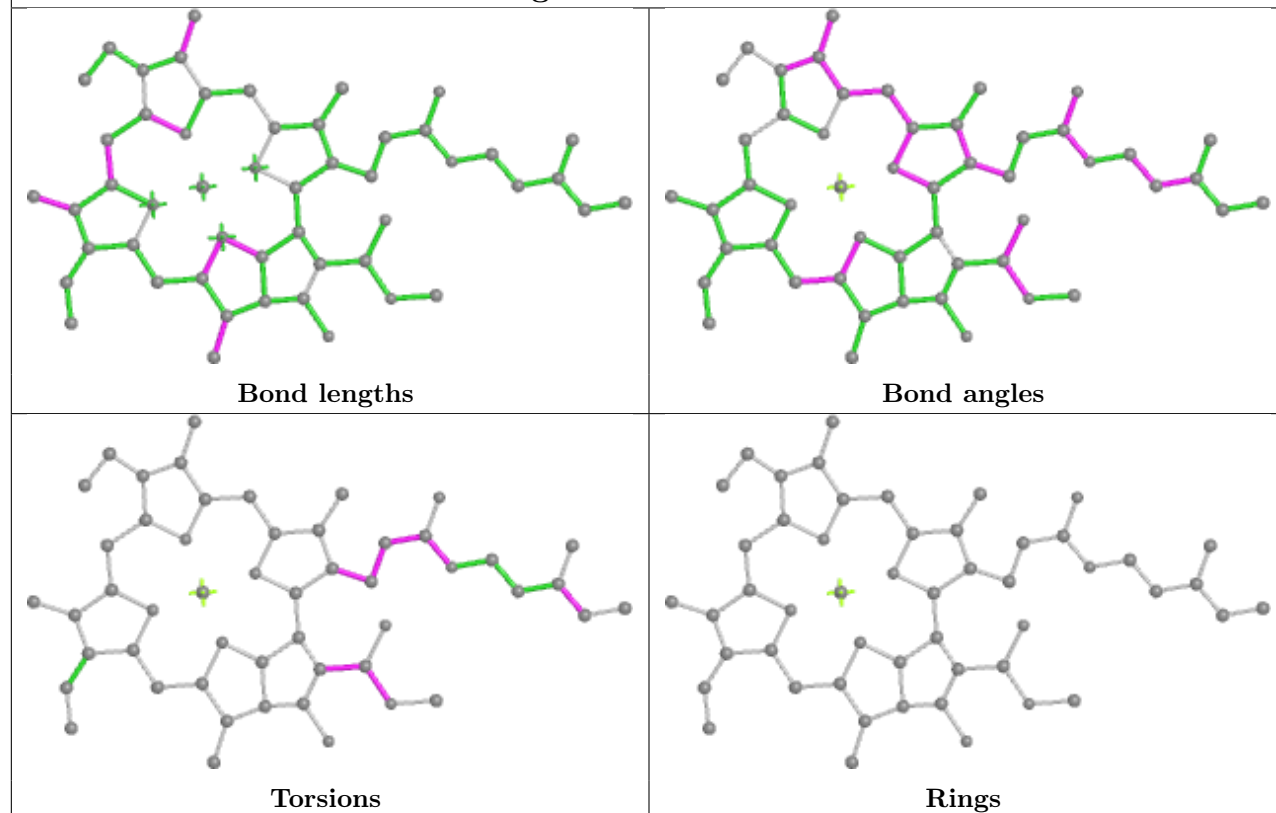
## Ligand CLA A 817



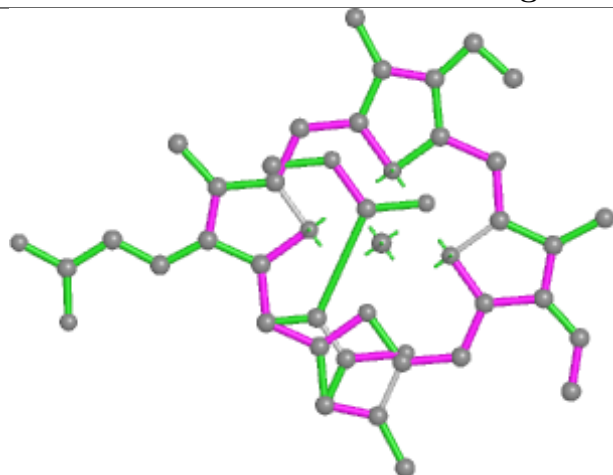
## Ligand CLA j 310



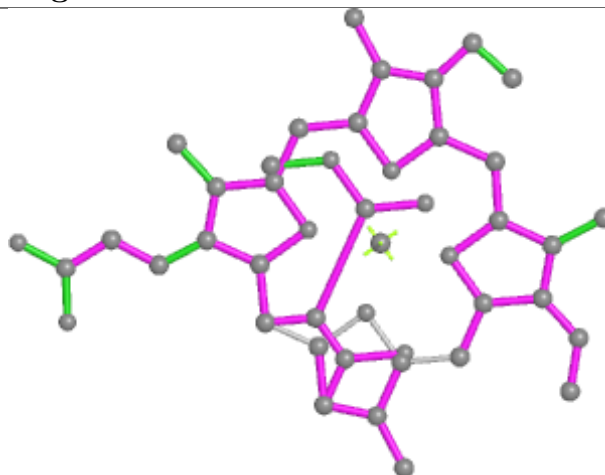
## Ligand CLA R 203



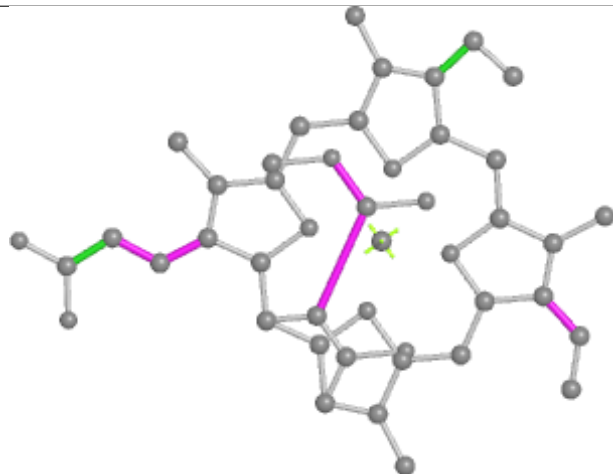
## Ligand KC2 g 312



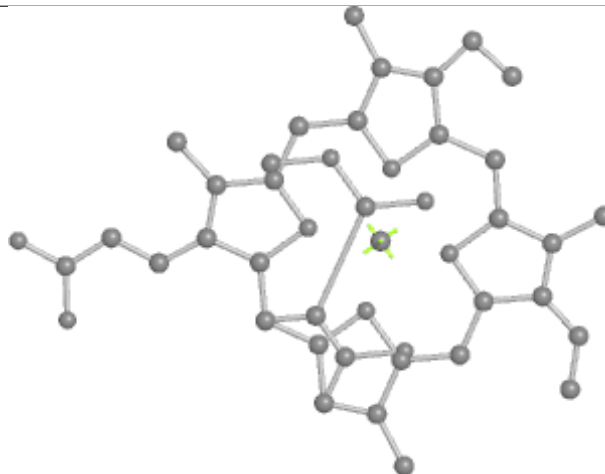
Bond lengths



Bond angles

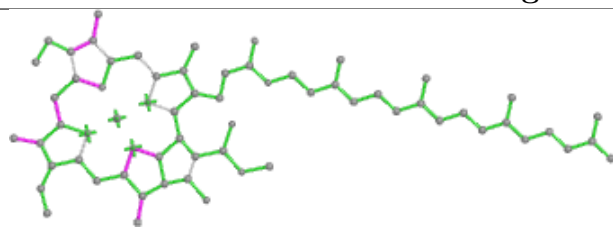


Torsions

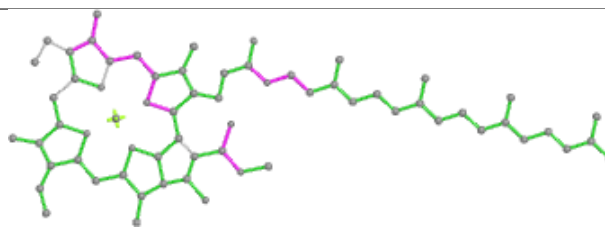


Rings

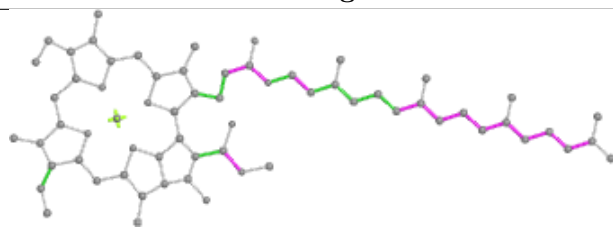
## Ligand CLA f 613



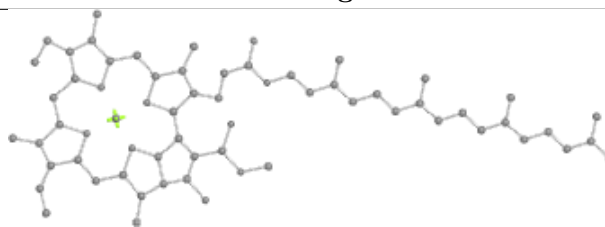
Bond lengths



Bond angles

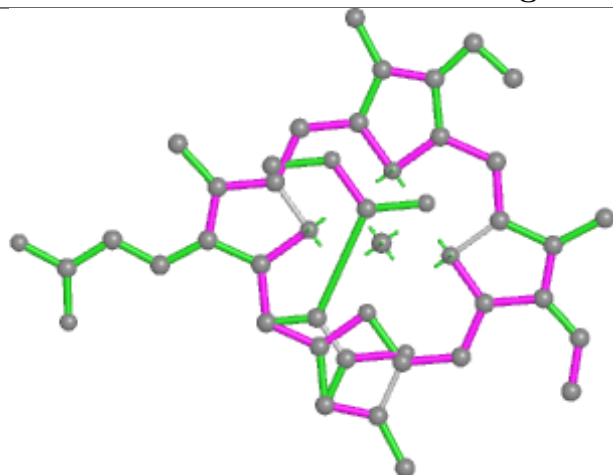


Torsions

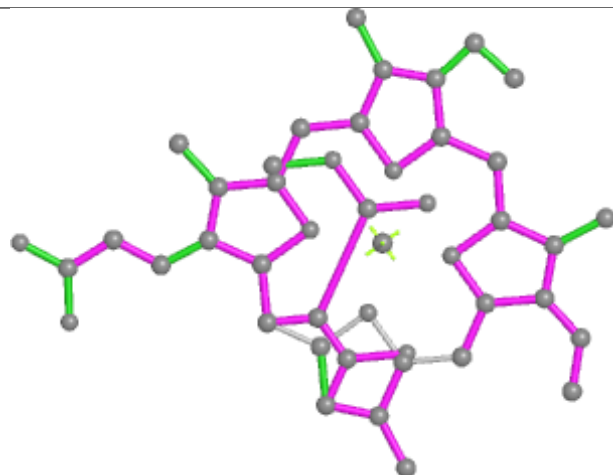


Rings

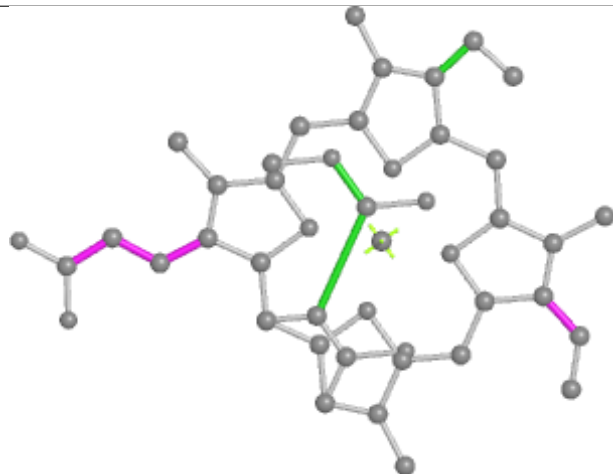
## Ligand KC2 k 613



Bond lengths



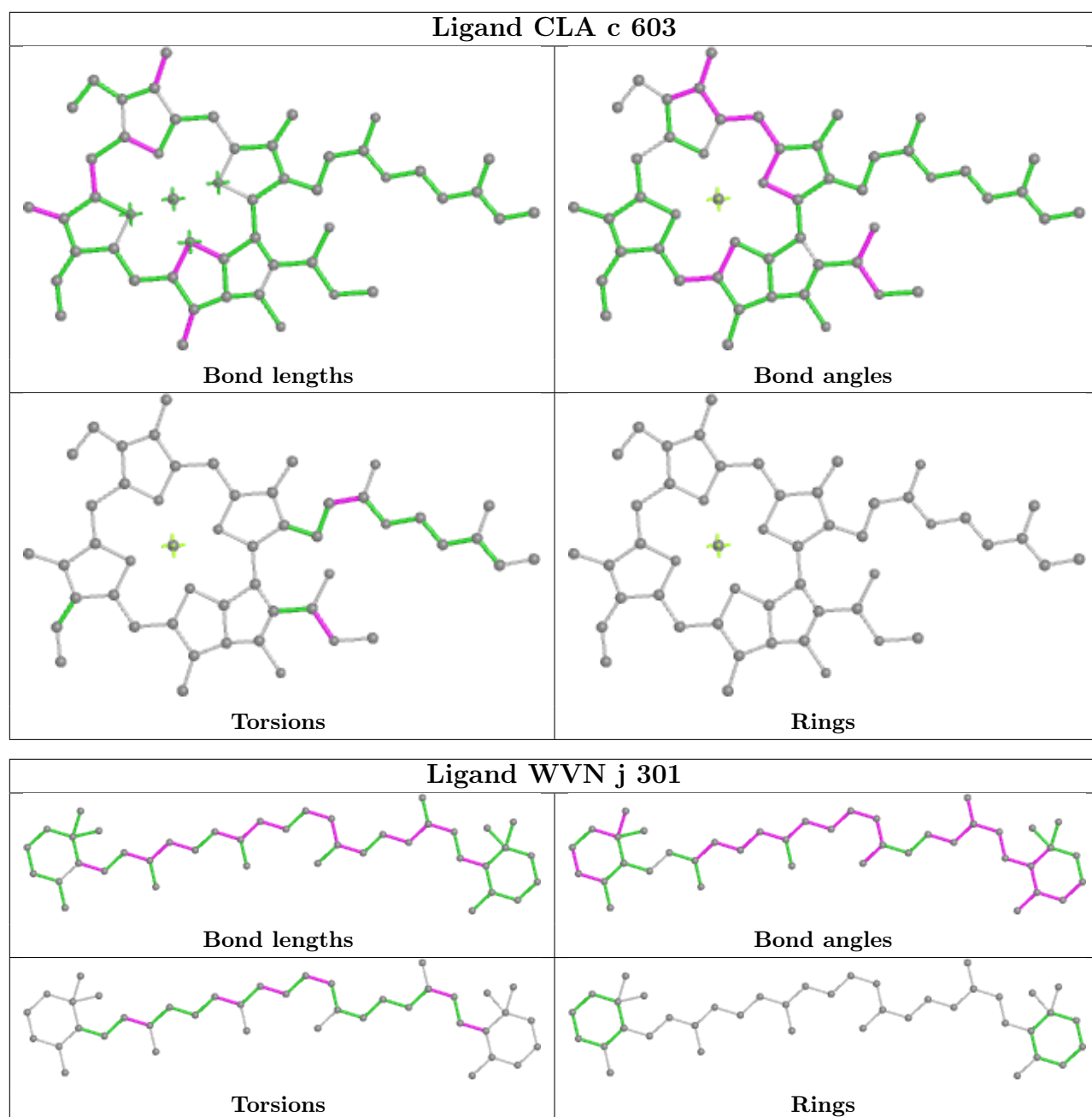
Bond angles

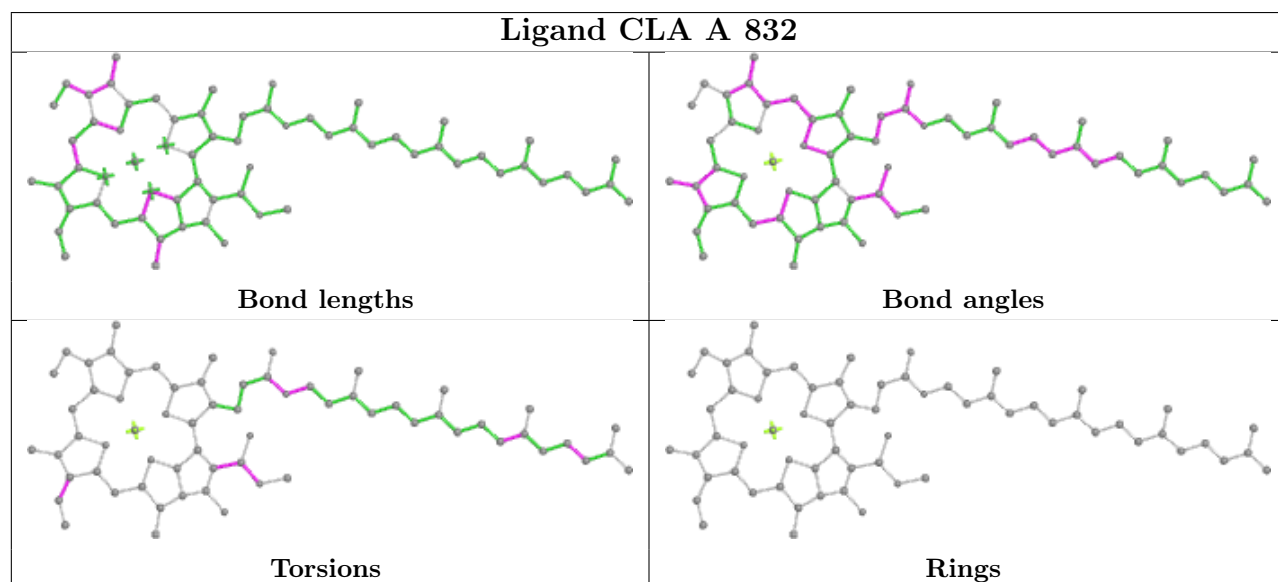
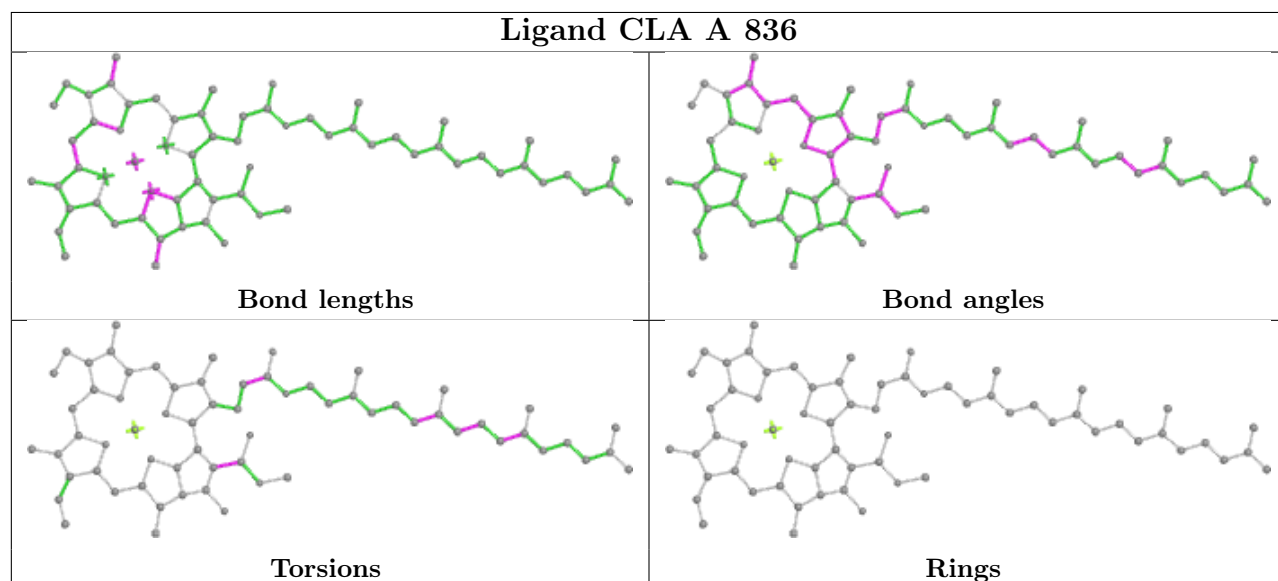
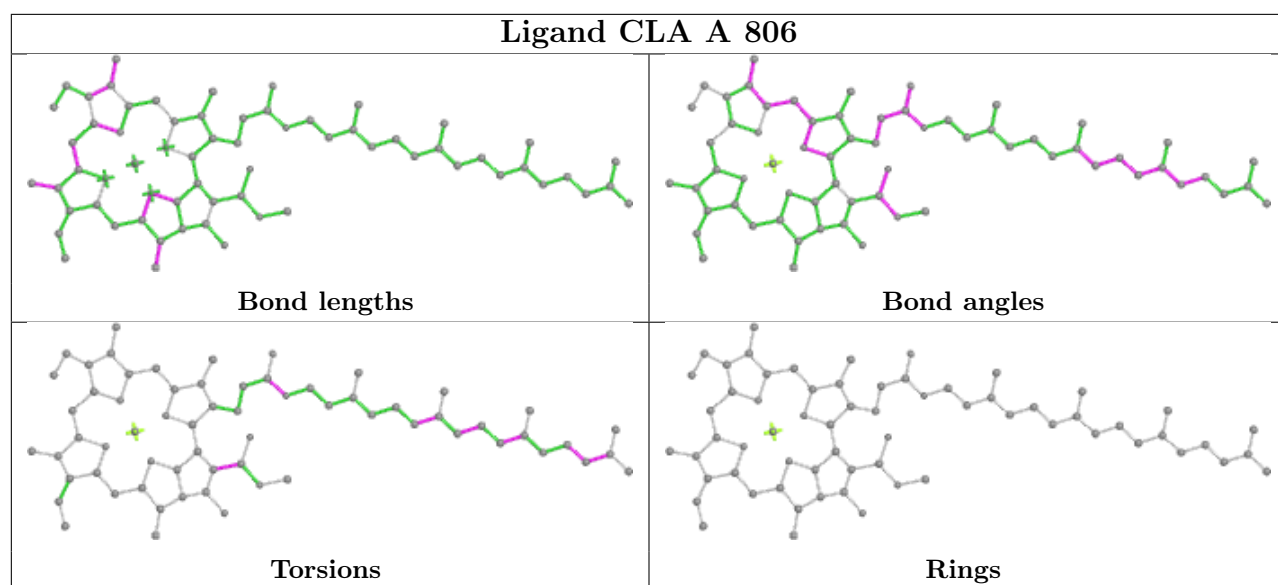


Torsions

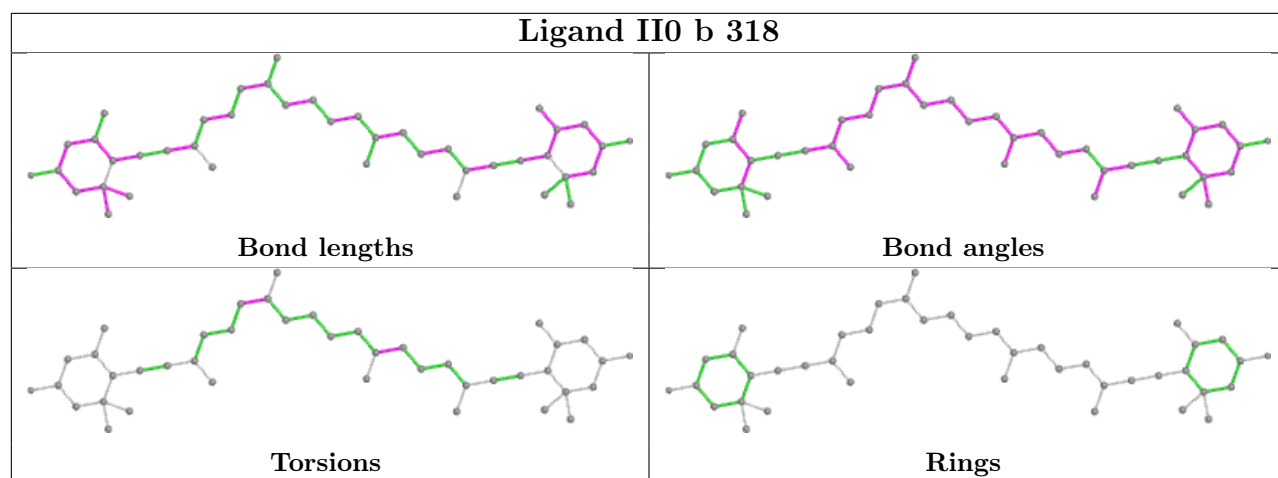
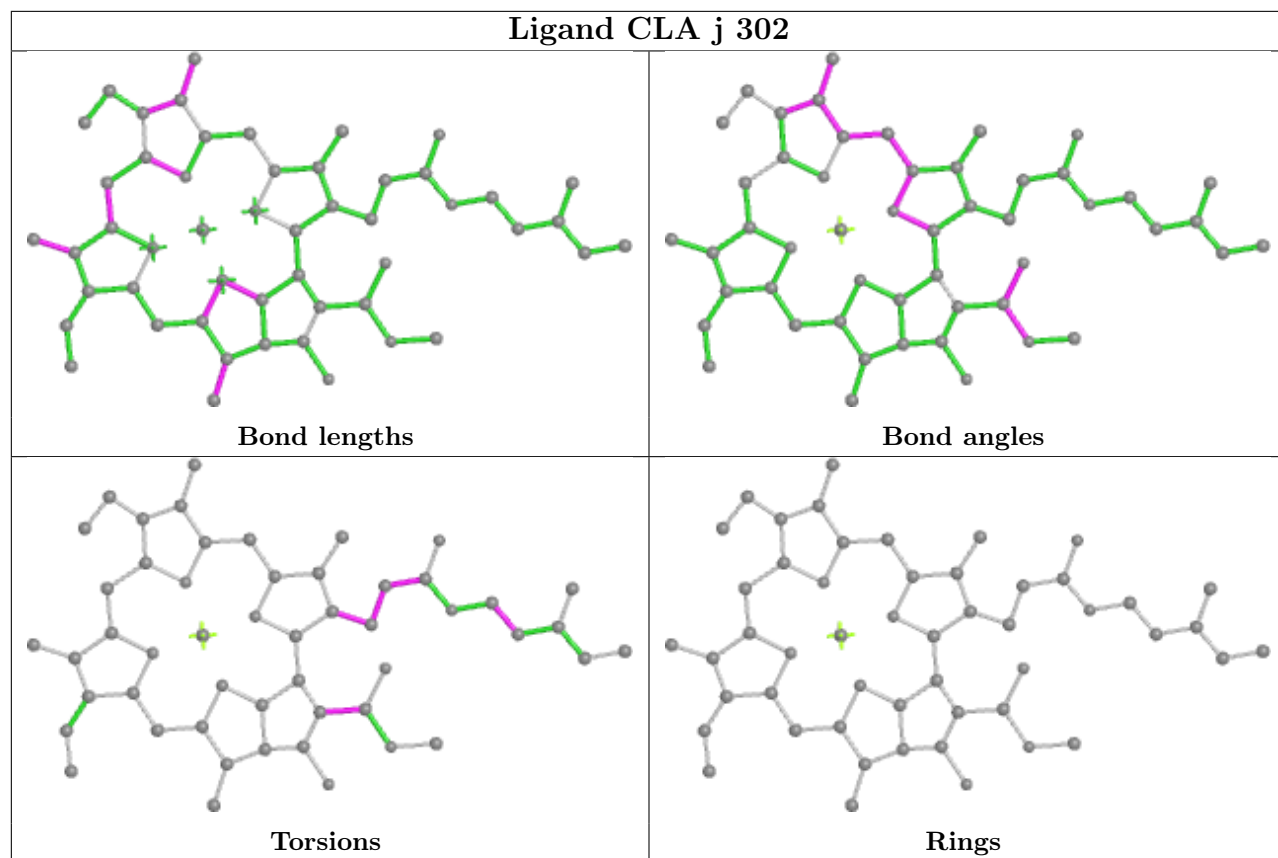


Rings

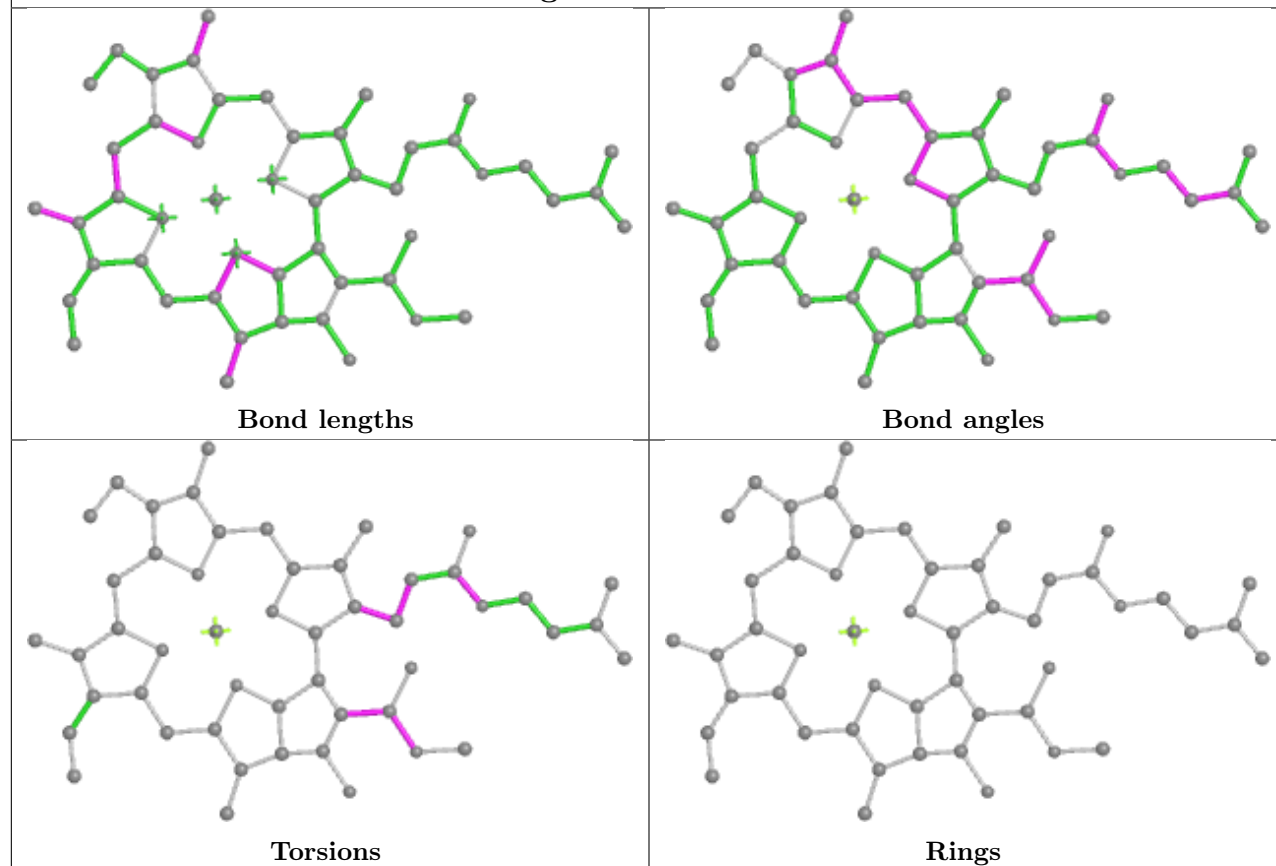




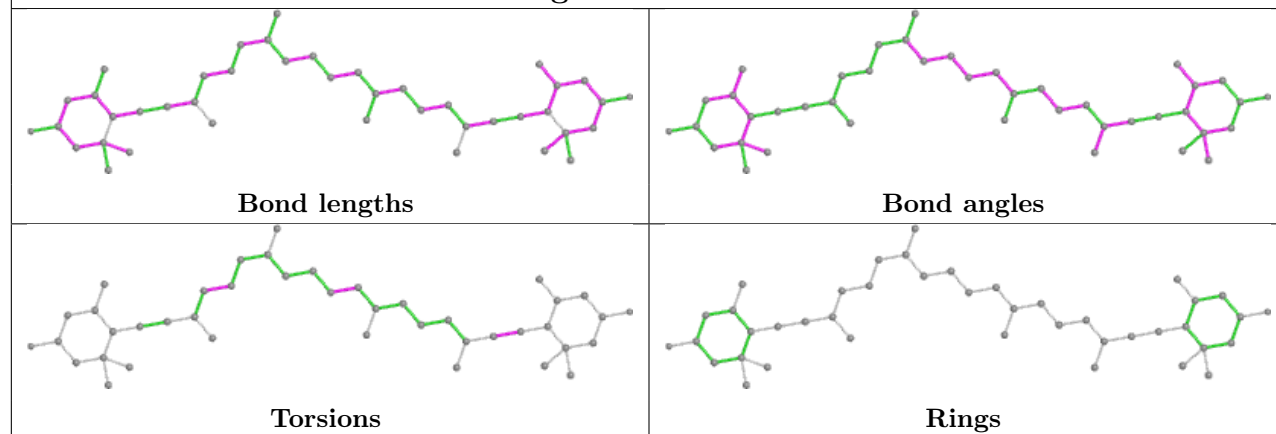




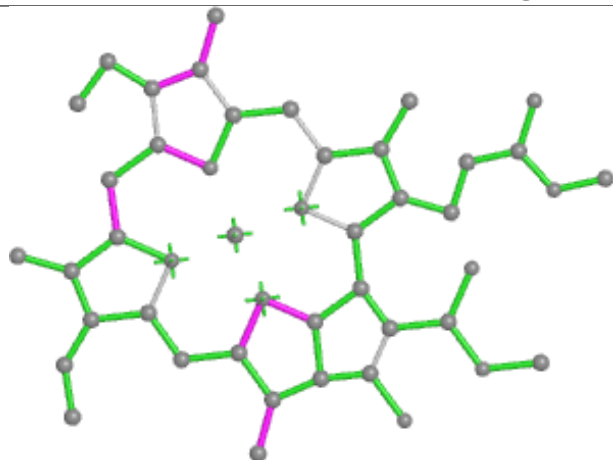
## Ligand CLA i 602



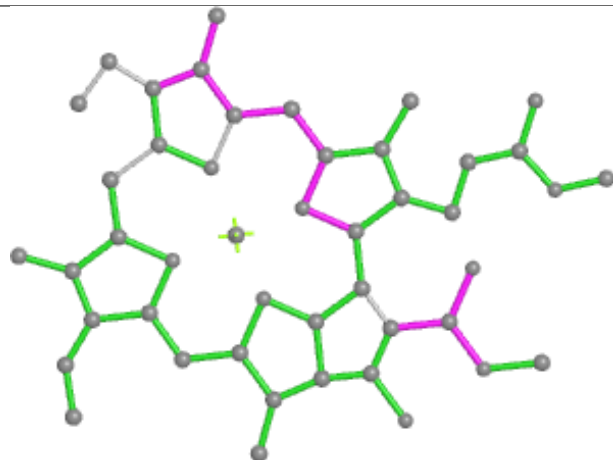
## Ligand II0 a 315



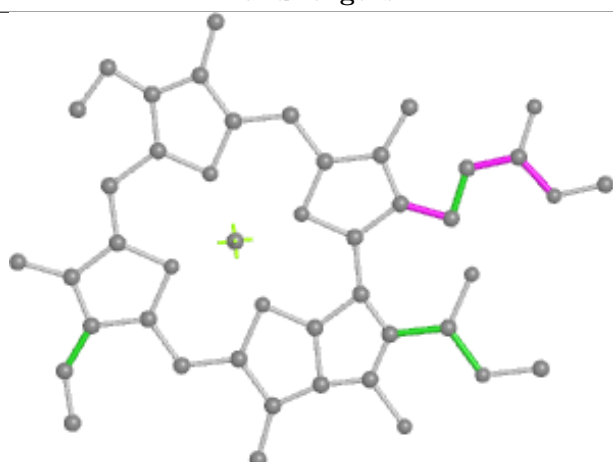
## Ligand CLA d 307



Bond lengths



Bond angles

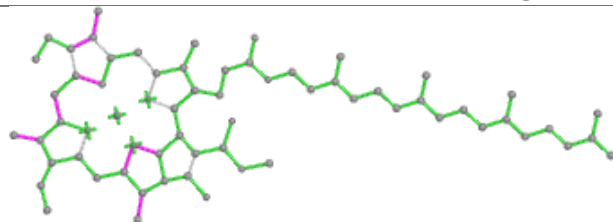


Torsions

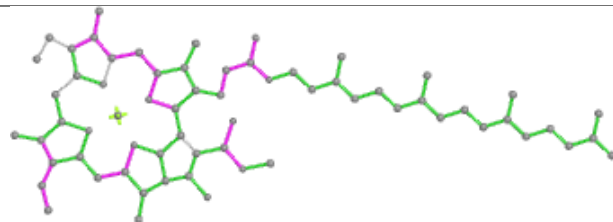


Rings

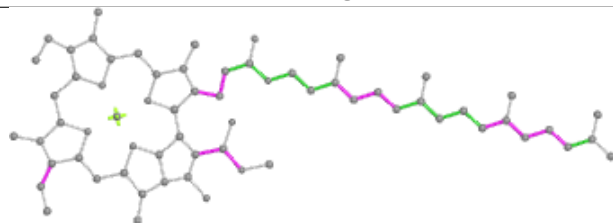
## Ligand CLA b 309



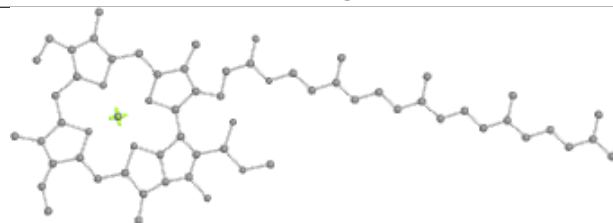
Bond lengths



Bond angles

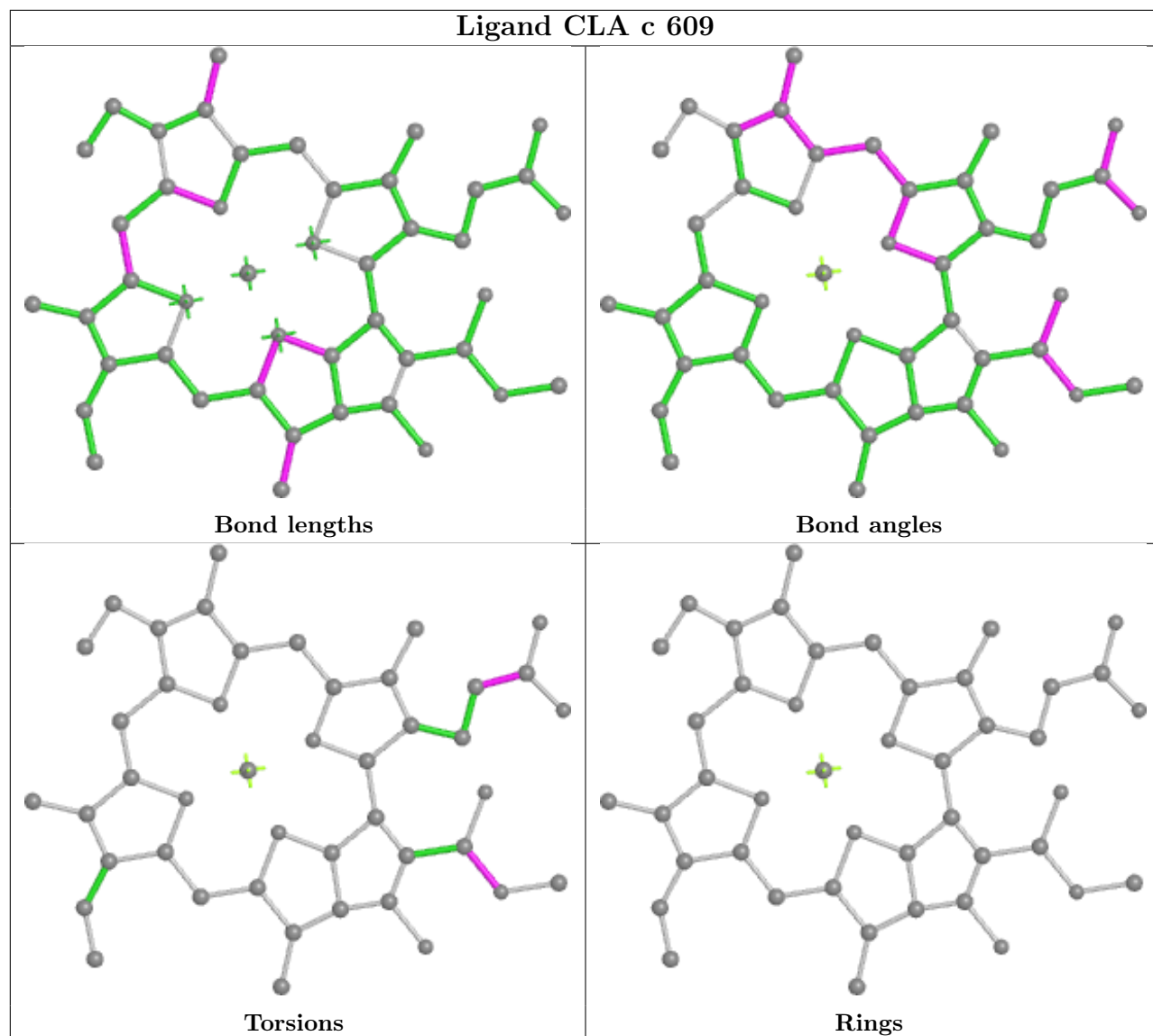


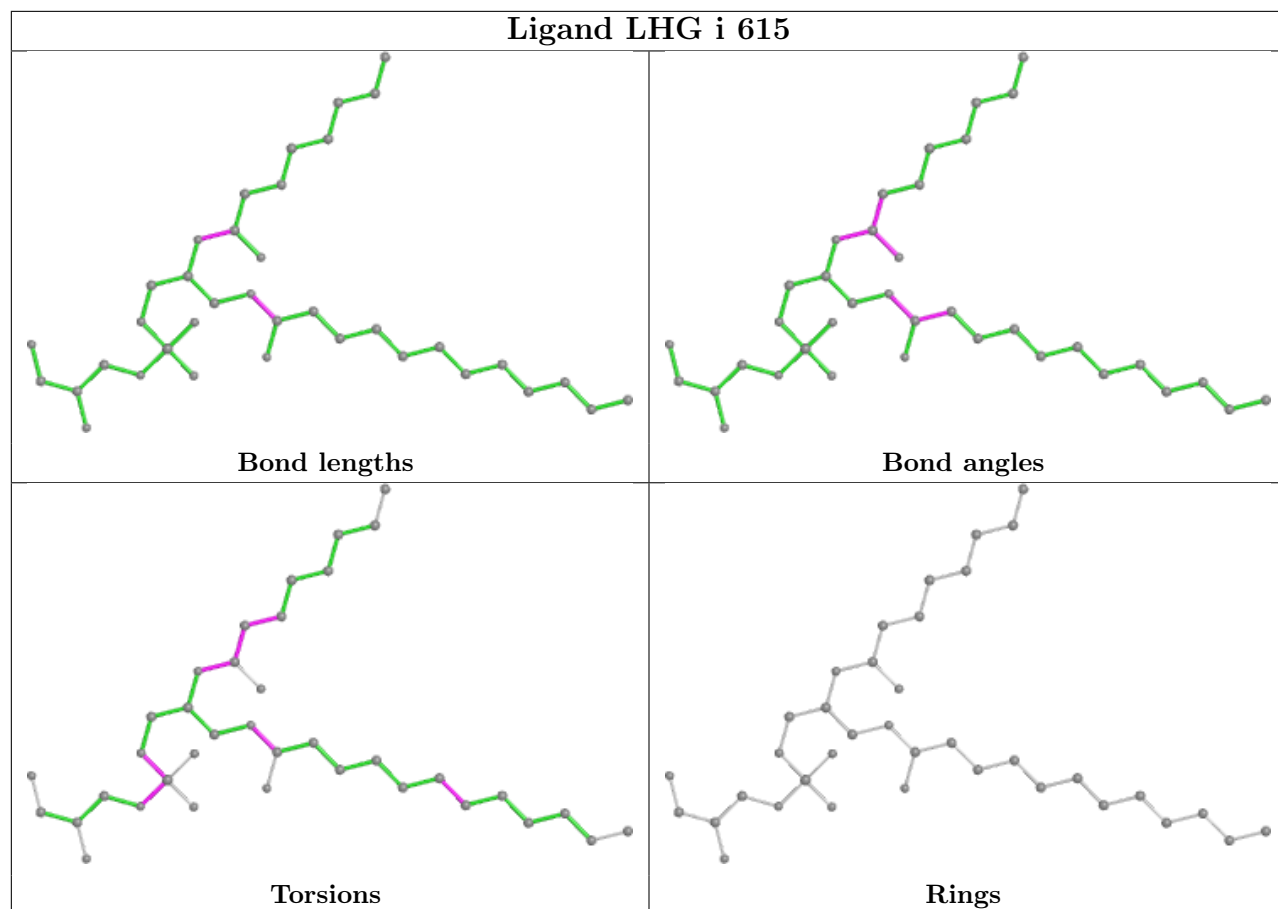
Torsions

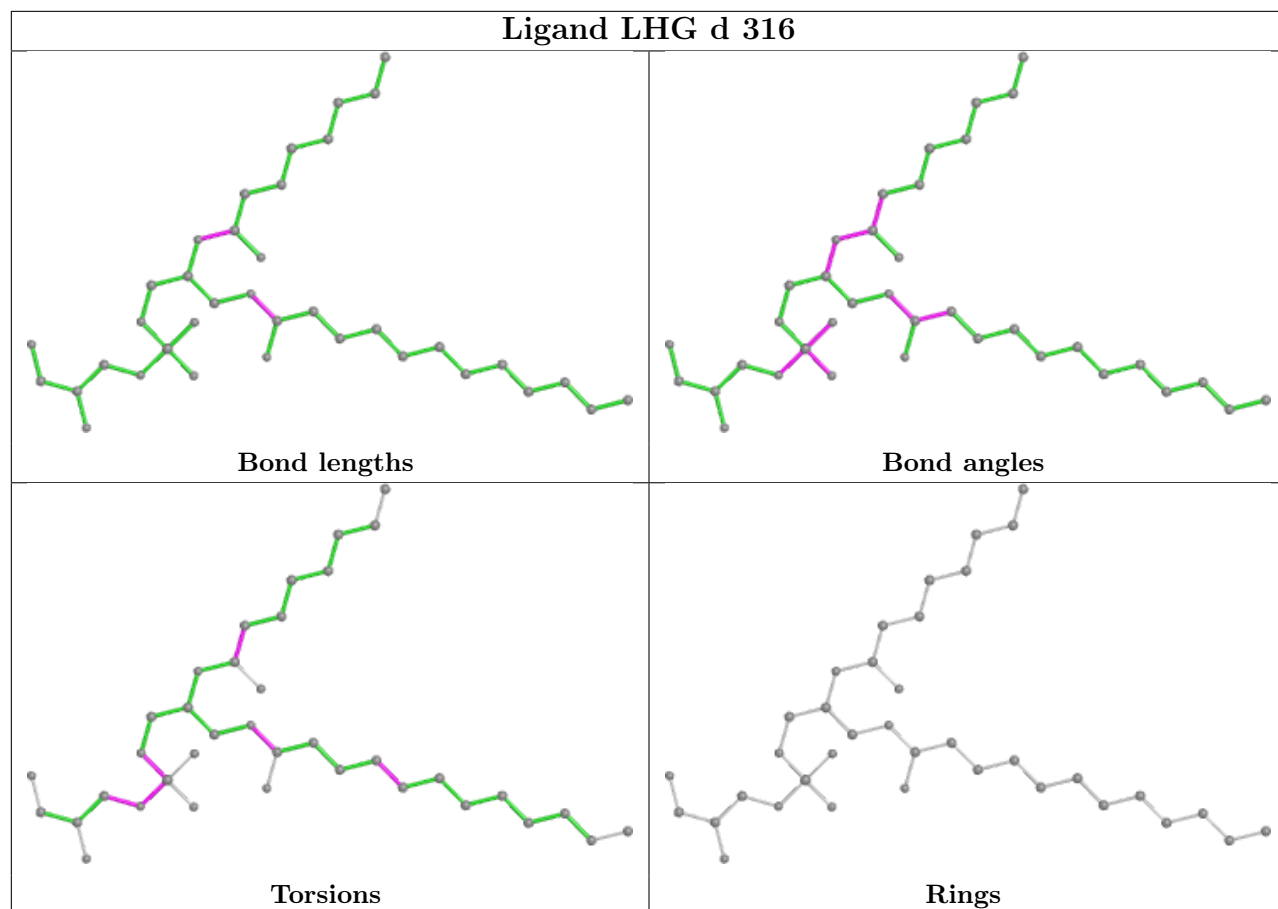


Rings

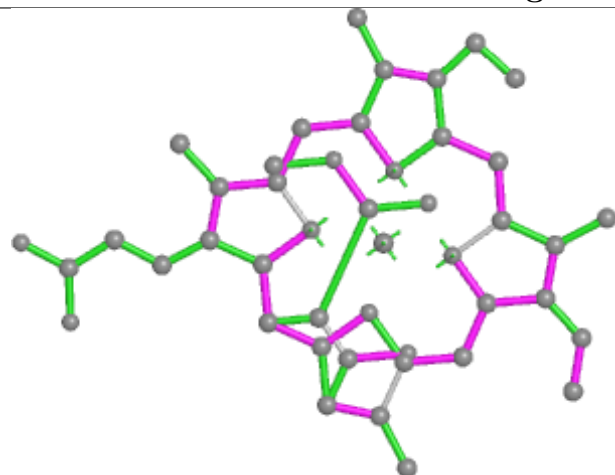
## Ligand CLA c 609



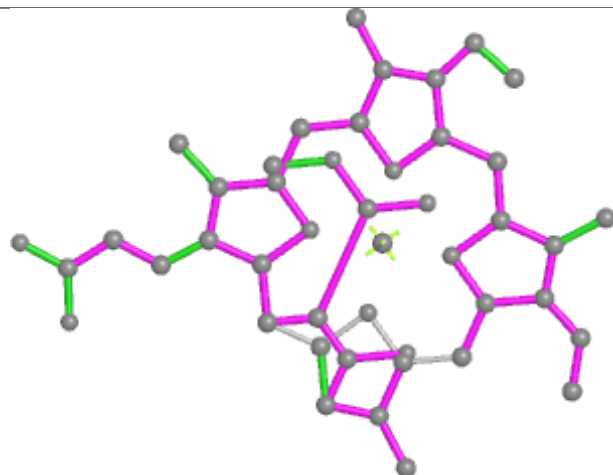




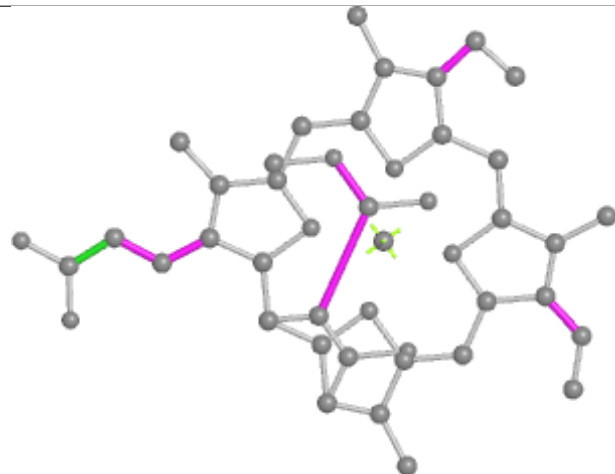
## Ligand KC2 i 616



Bond lengths



Bond angles

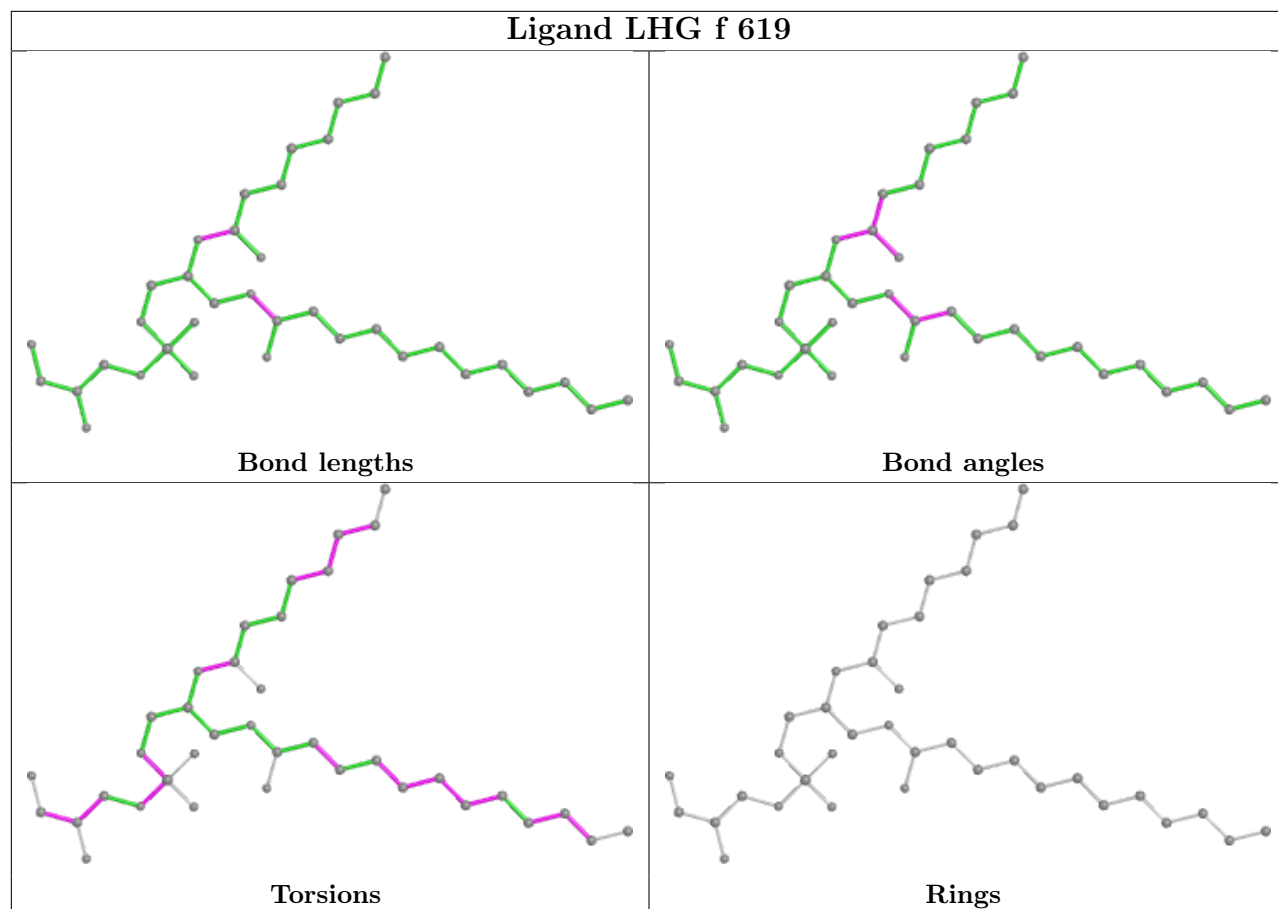


Torsions

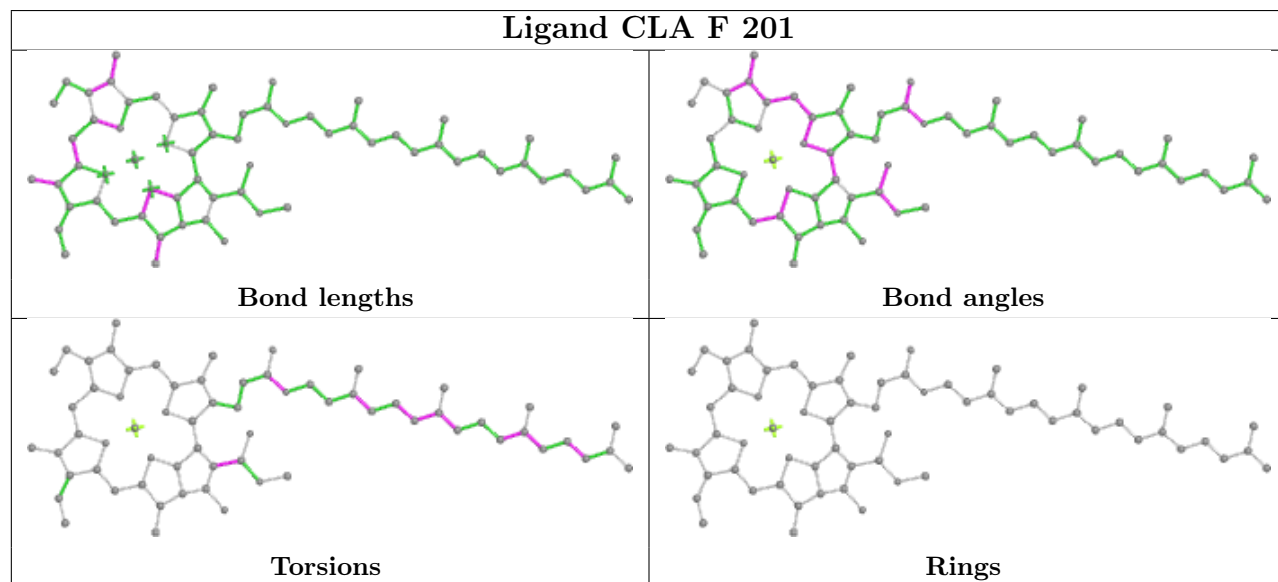


Rings

## Ligand LHG f 619

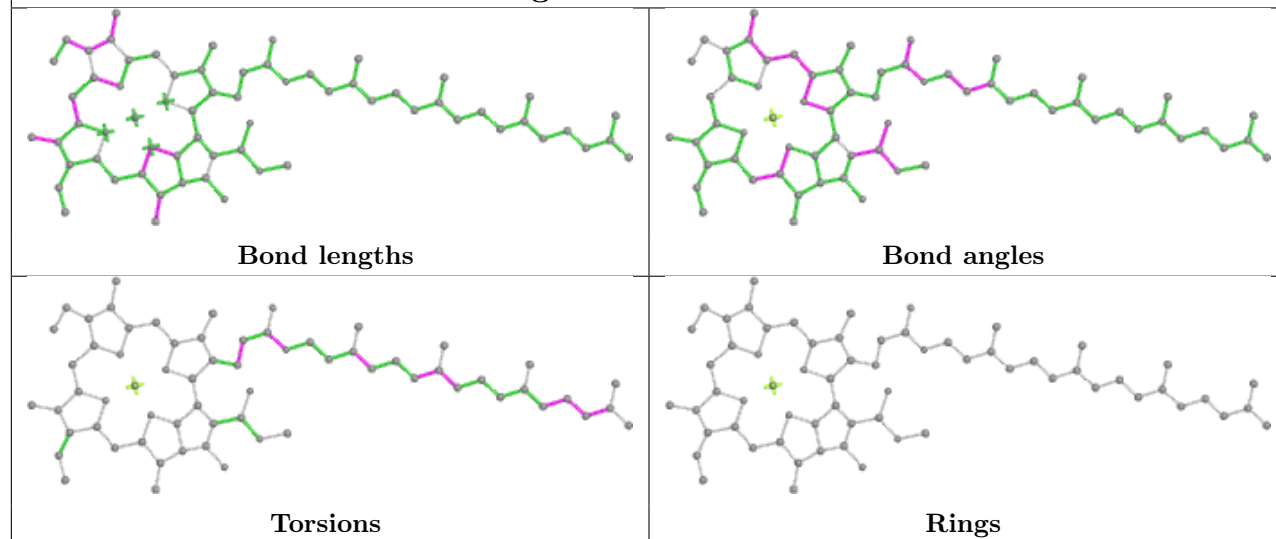


## Ligand CLA F 201

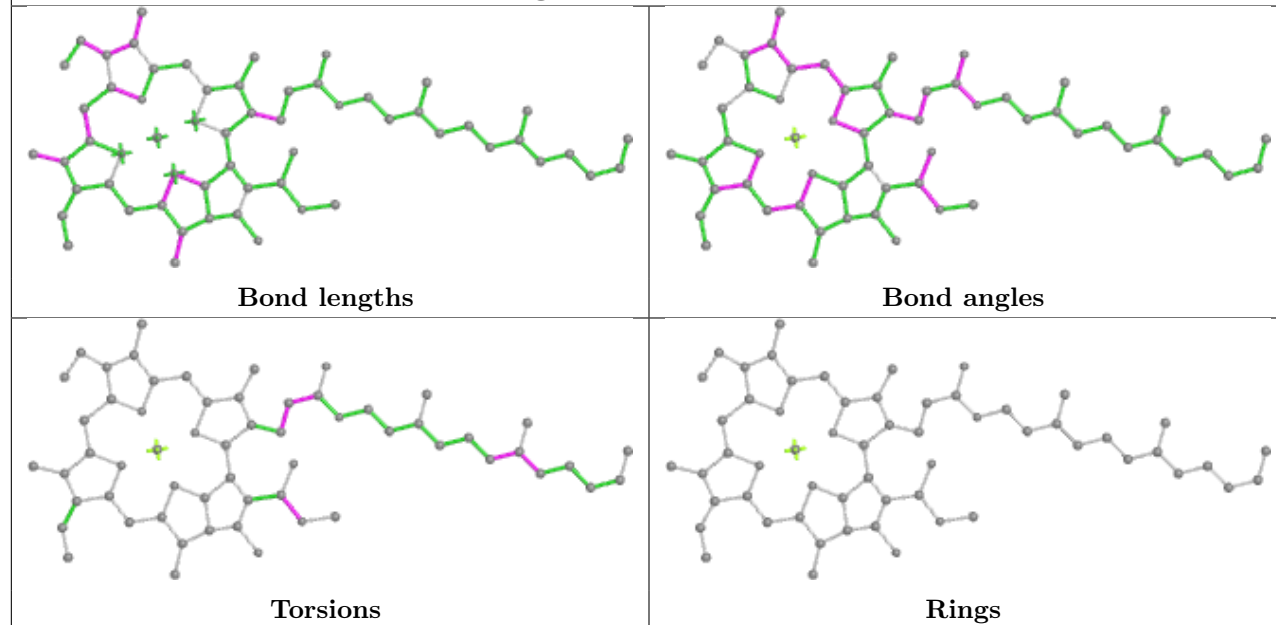




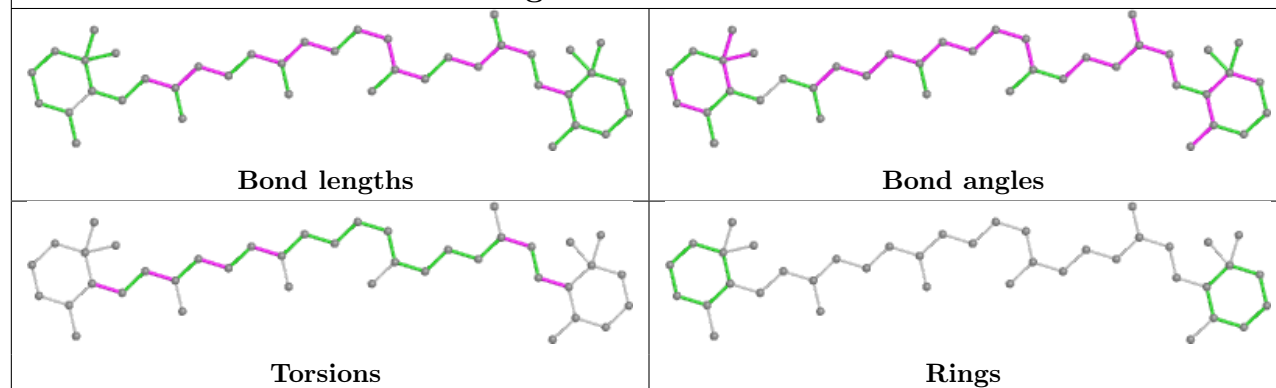
## Ligand CLA A 835

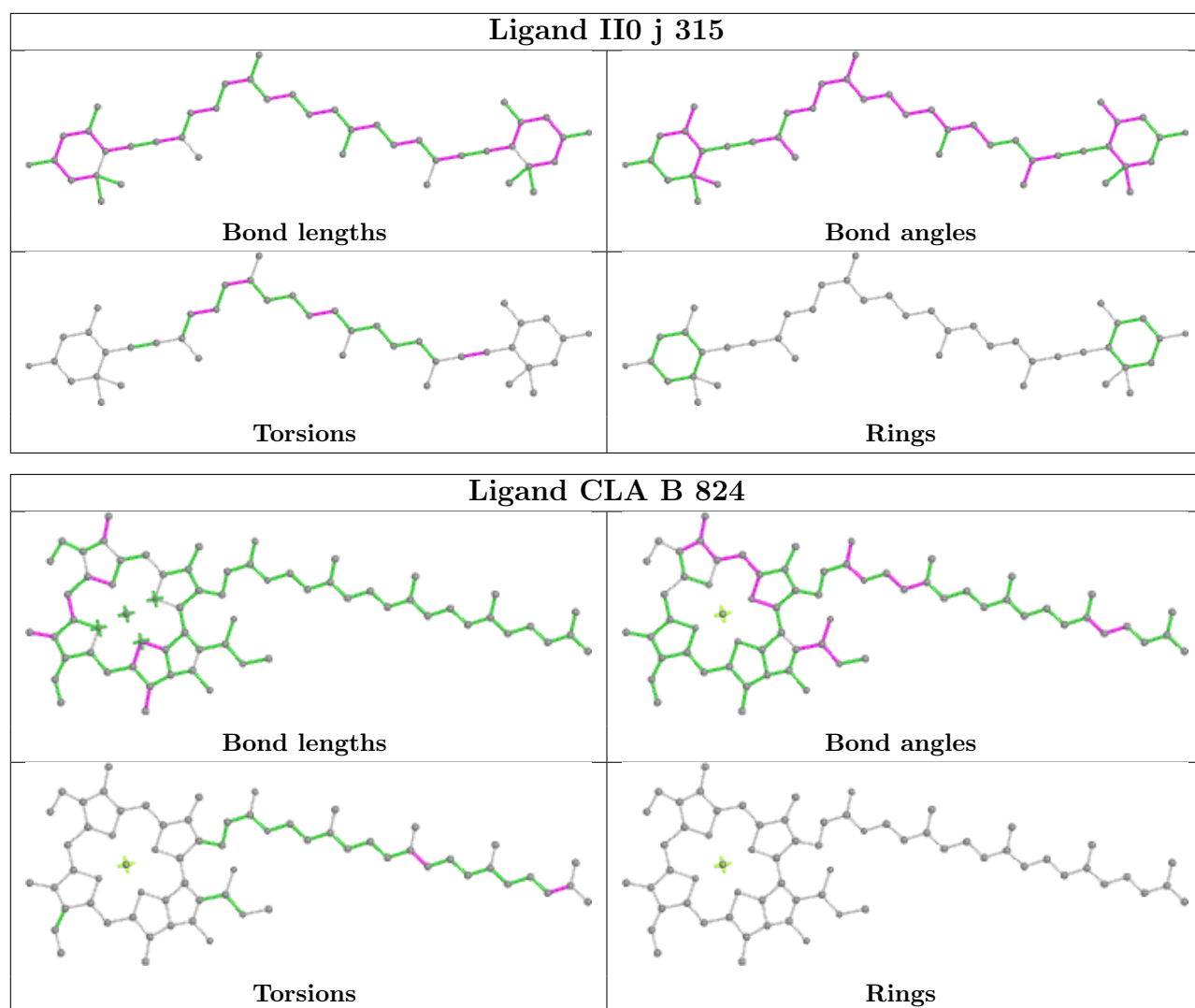


## Ligand CLA B 816

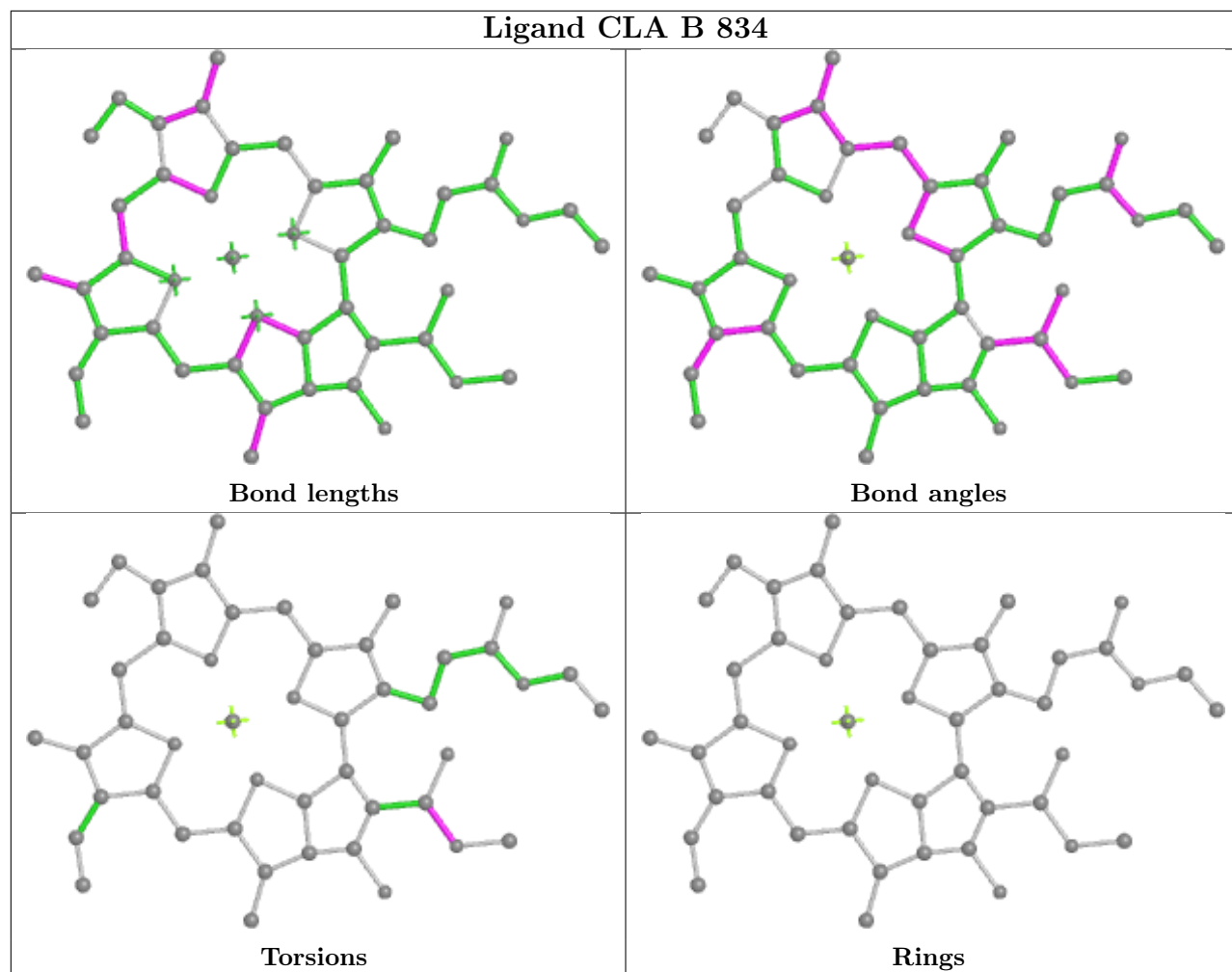


## Ligand WVN L 201

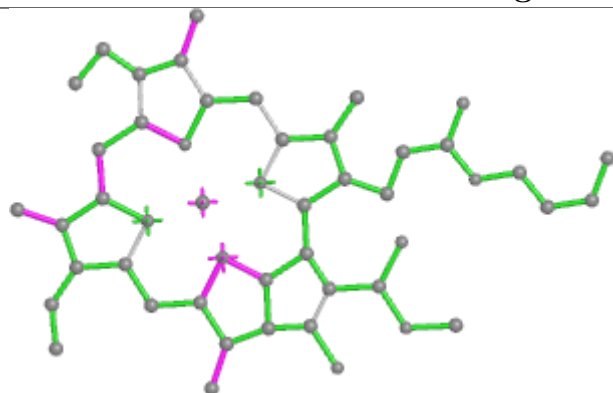




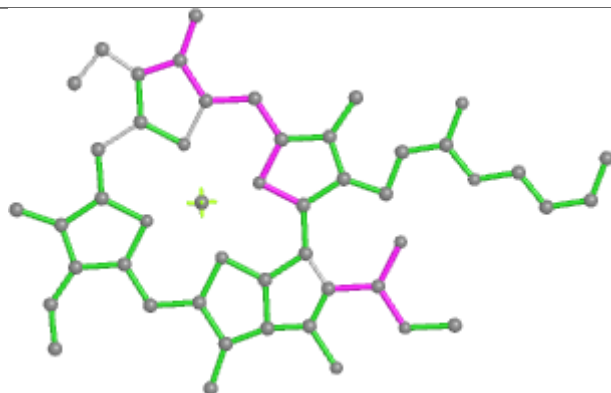
## Ligand CLA B 834



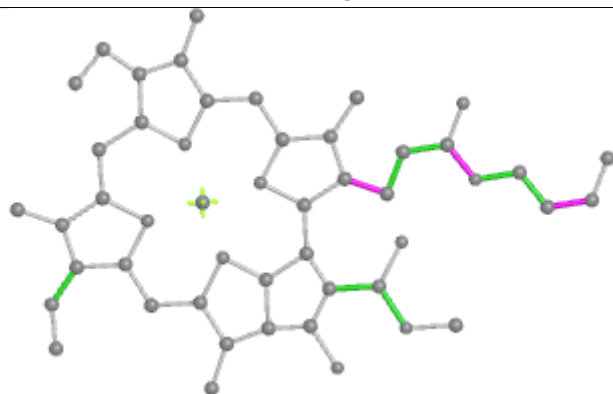
## Ligand CLA B 828



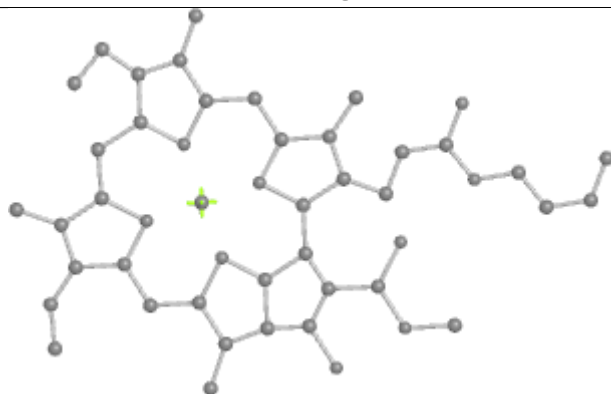
Bond lengths



Bond angles

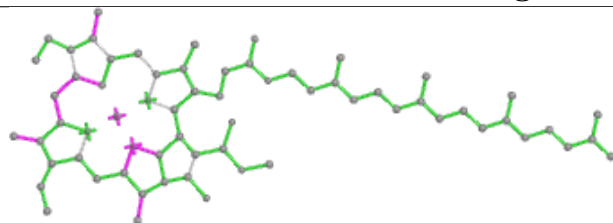


Torsions

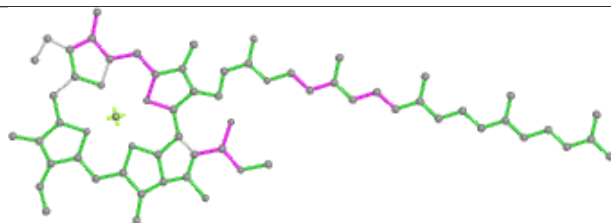


Rings

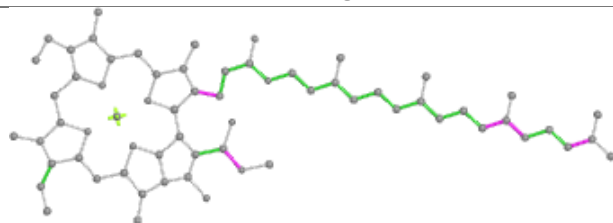
## Ligand CLA A 831



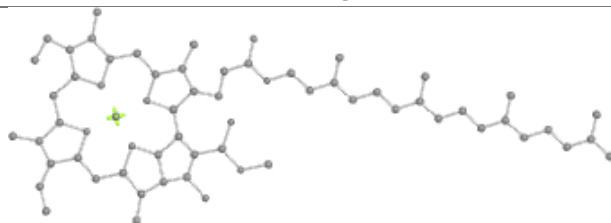
Bond lengths



Bond angles

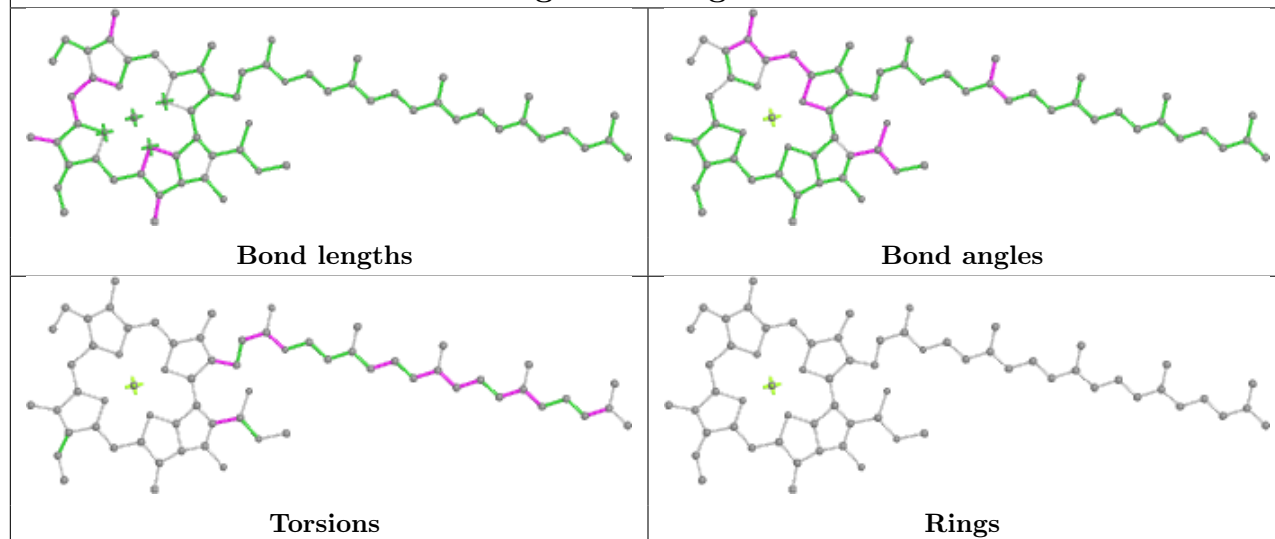


Torsions

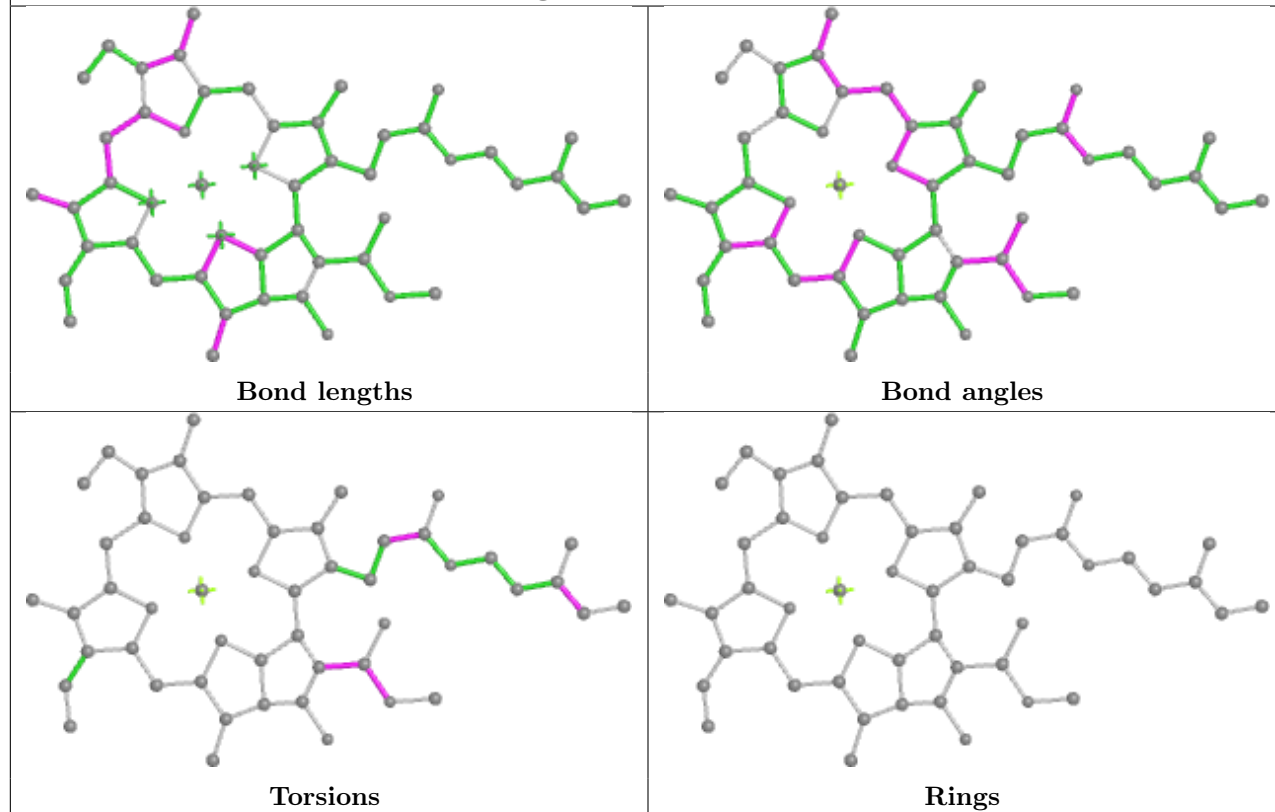


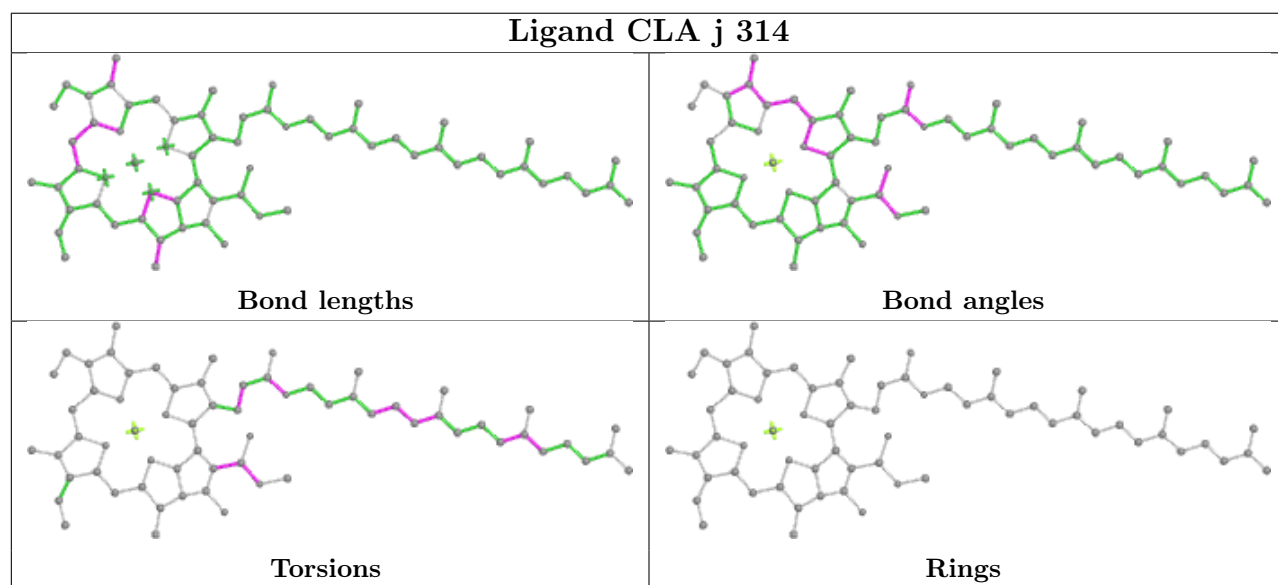
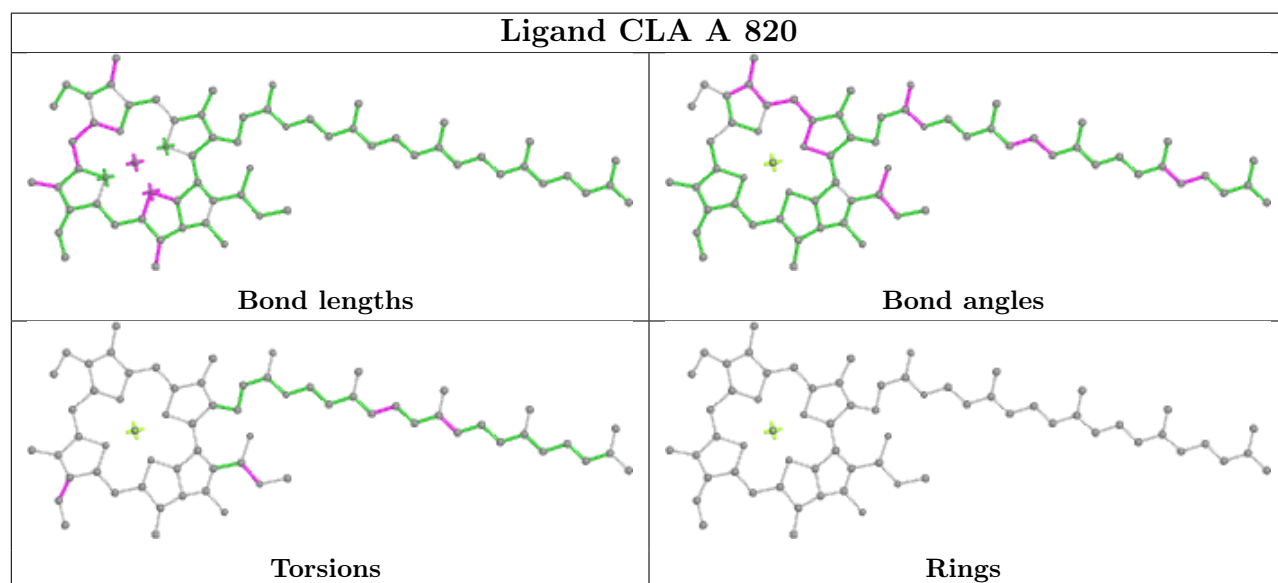
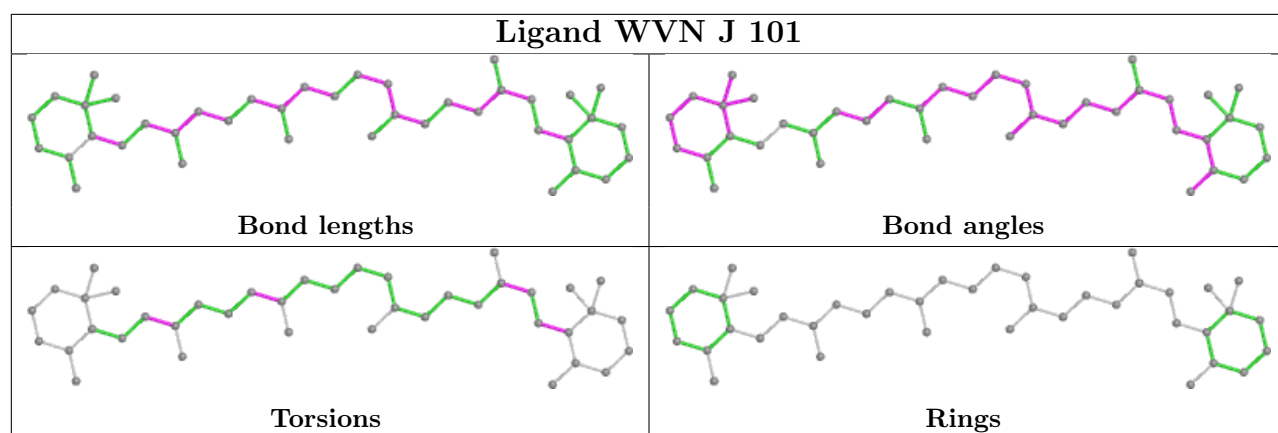
Rings

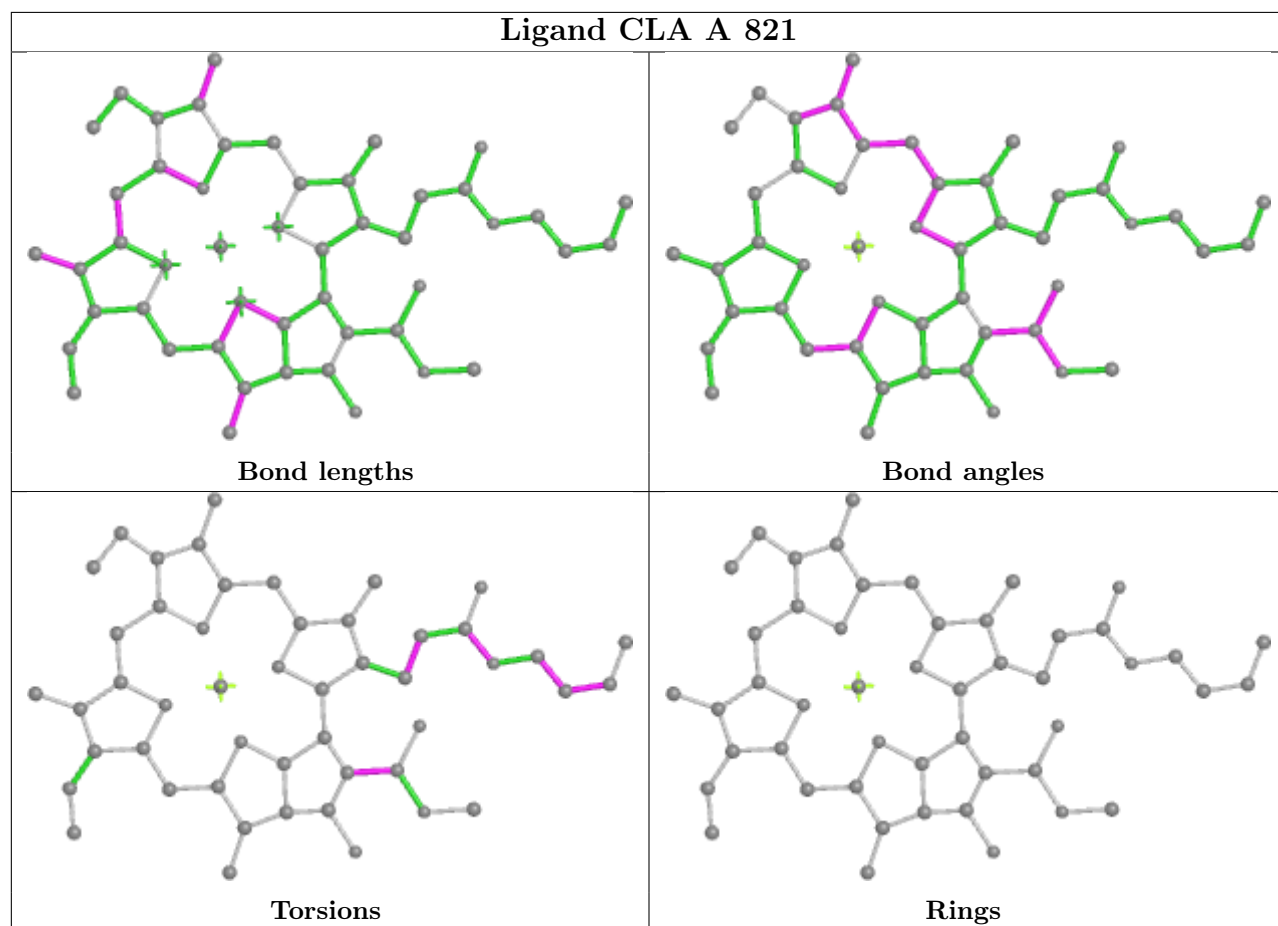
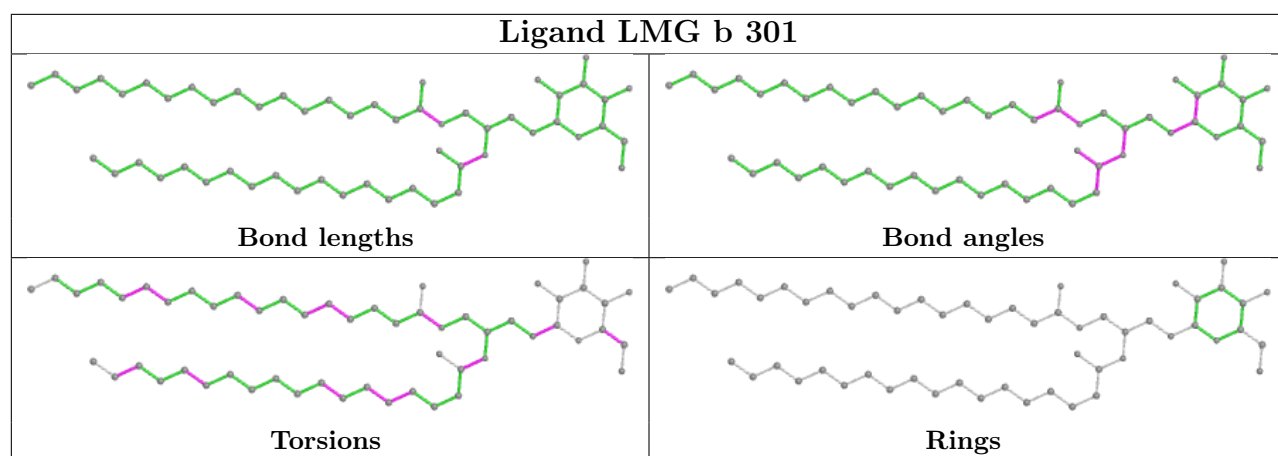
## Ligand CLA g 308

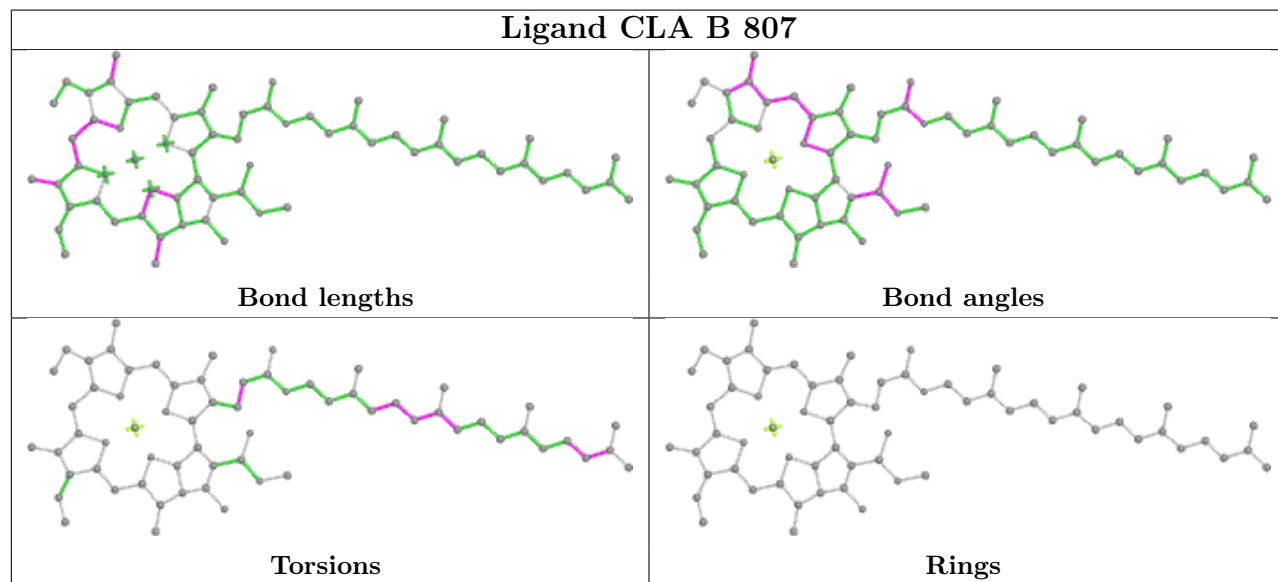
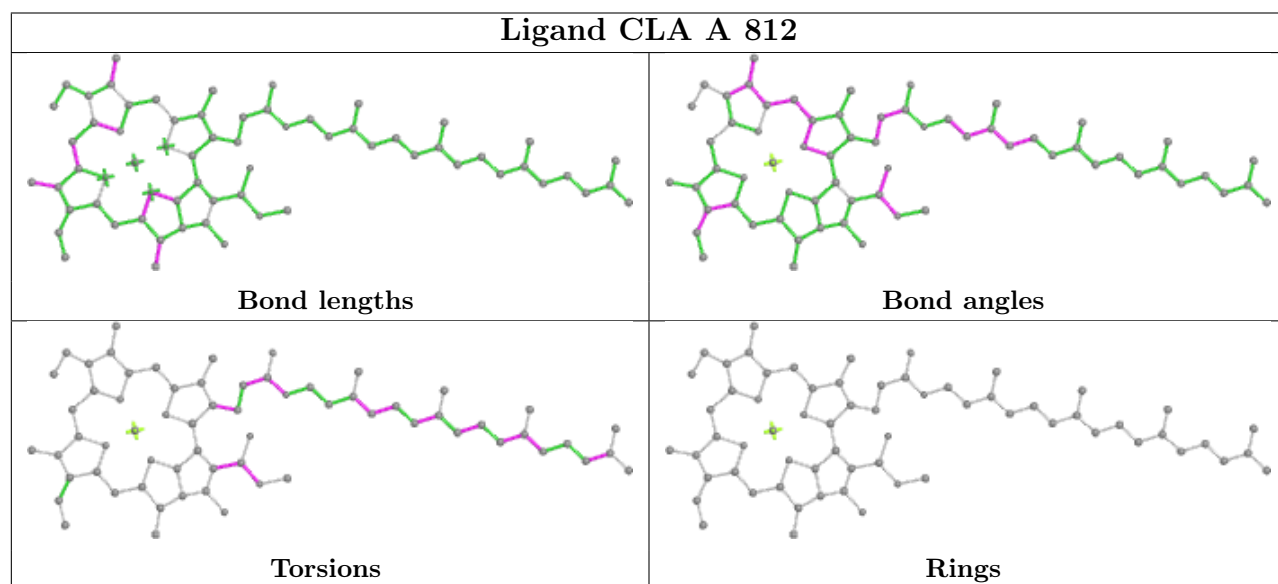
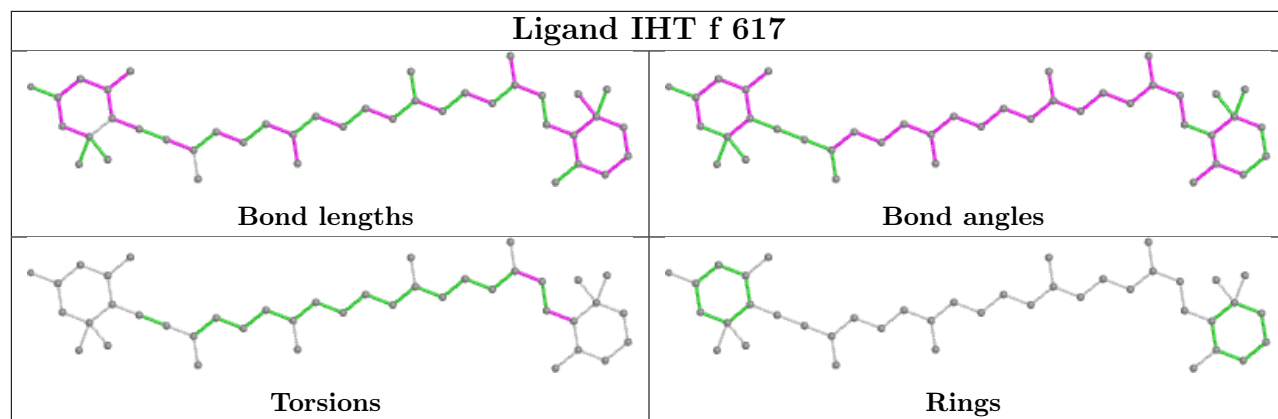


## Ligand CLA d 305

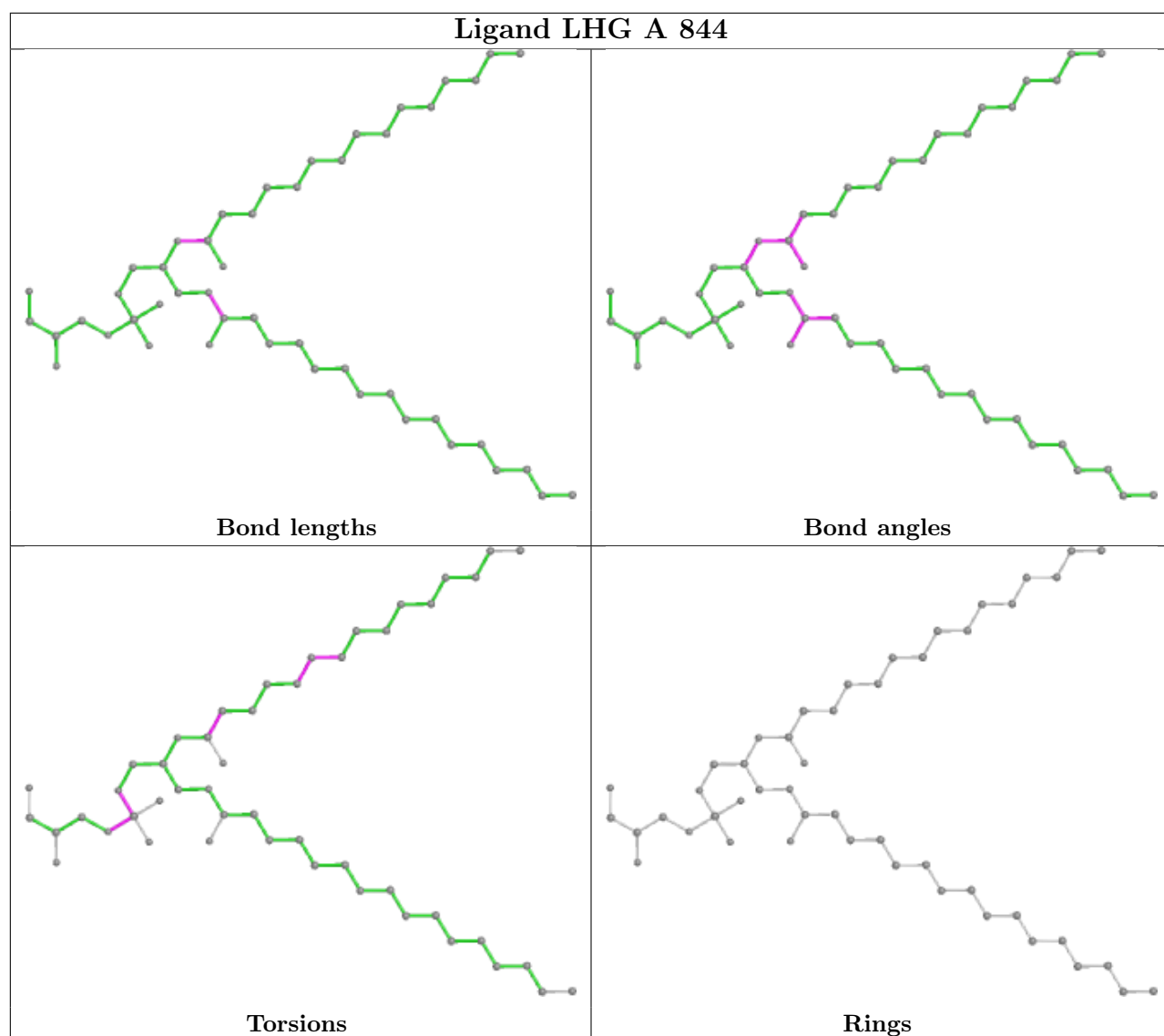


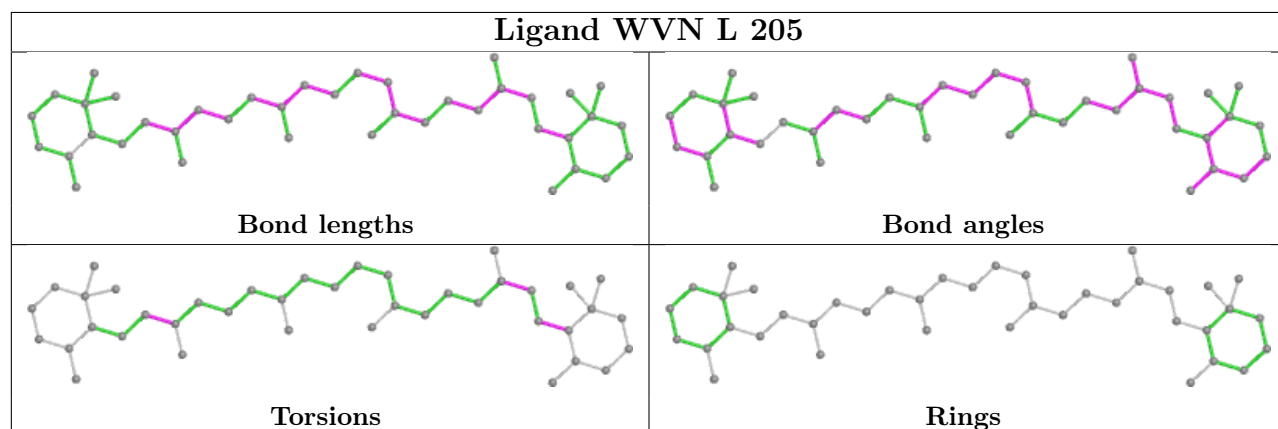
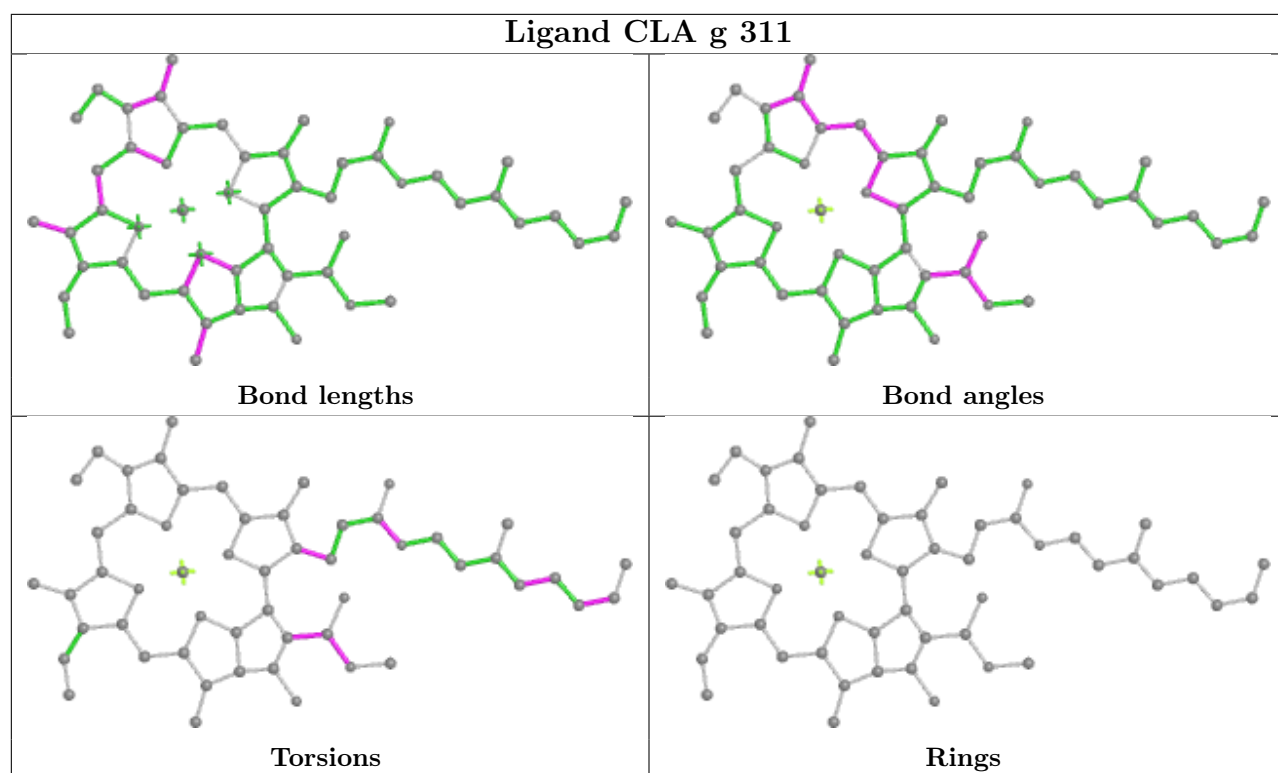


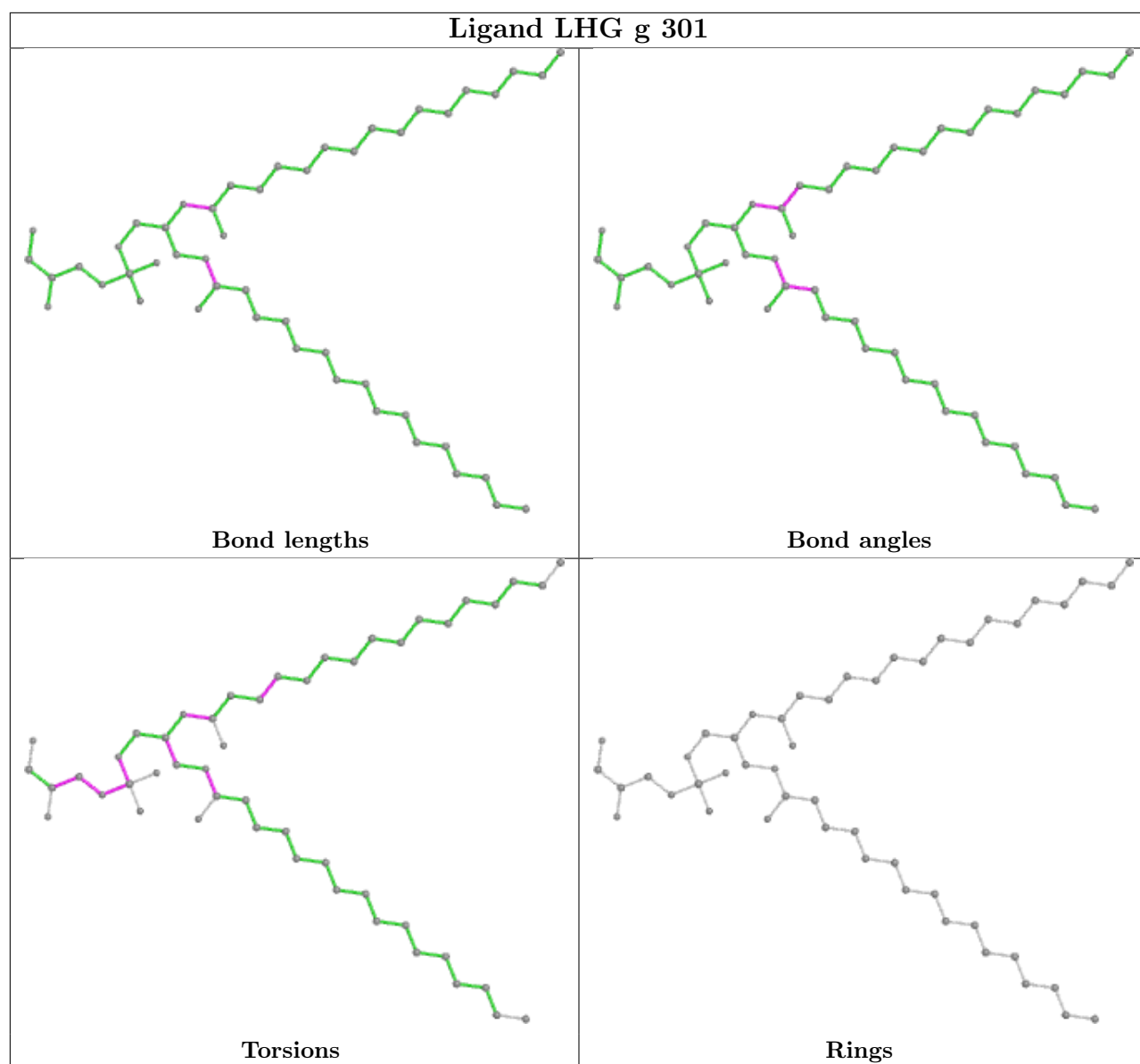




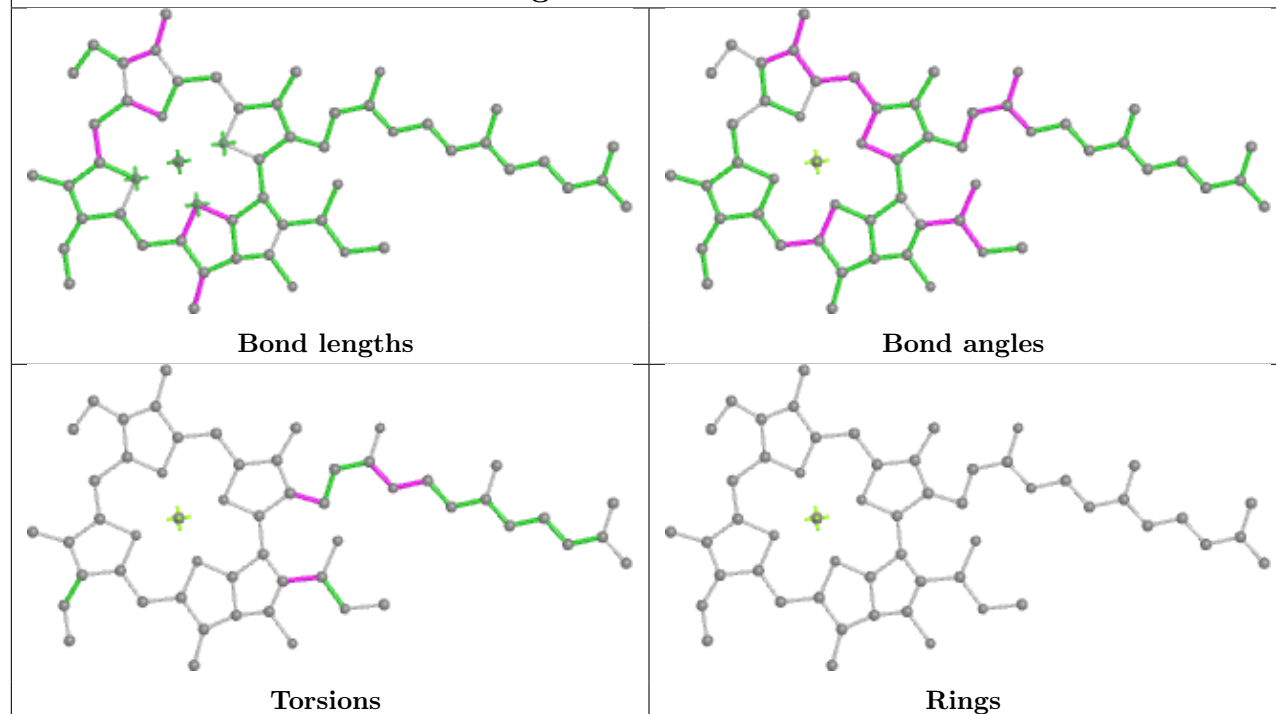




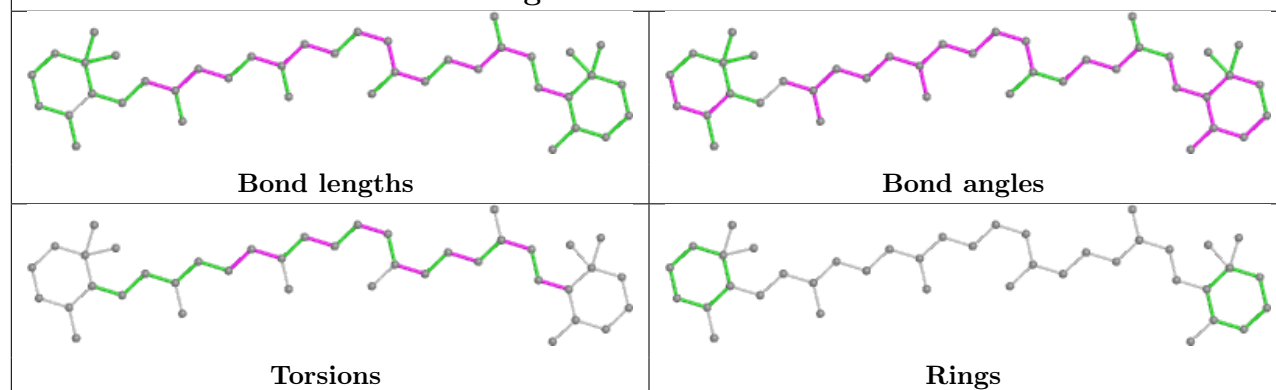




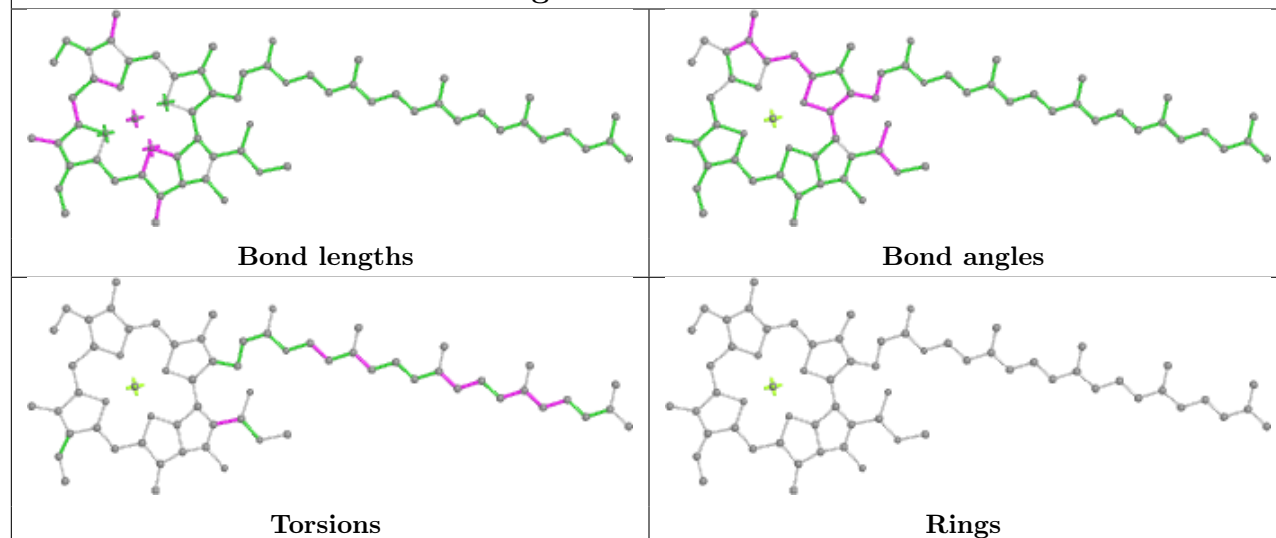
## Ligand CLA A 803



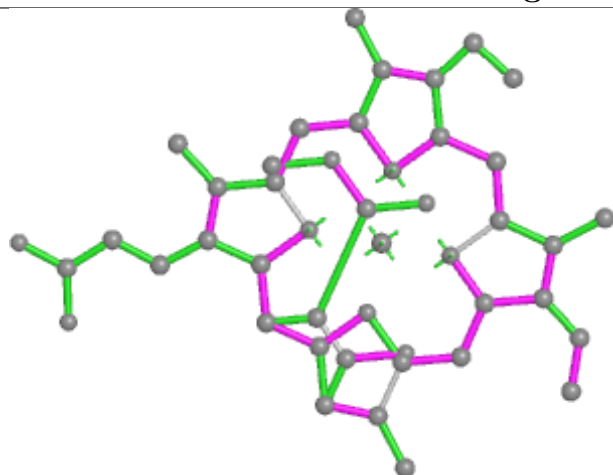
## Ligand WVN B 847



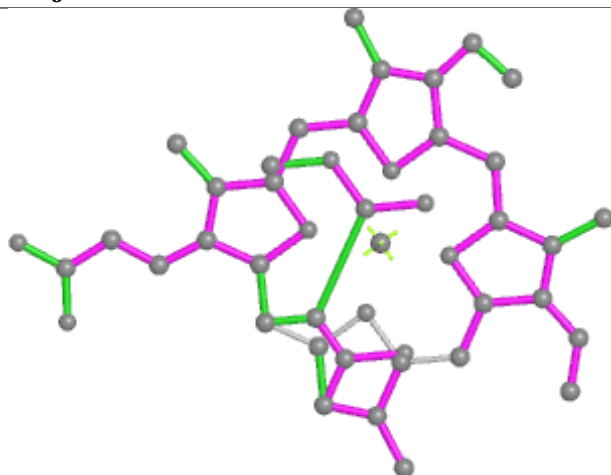
## Ligand CLA A 824



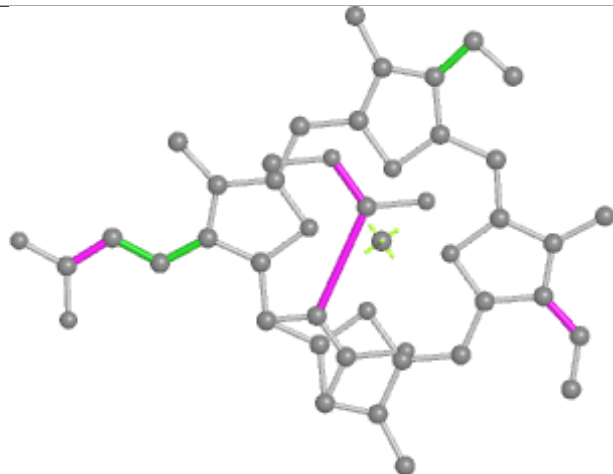
## Ligand KC2 j 312



Bond lengths



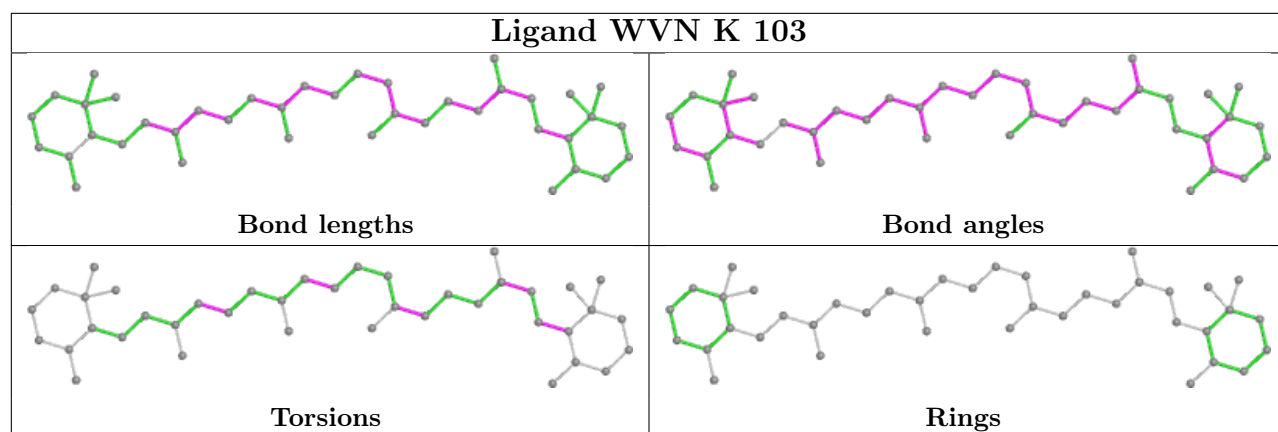
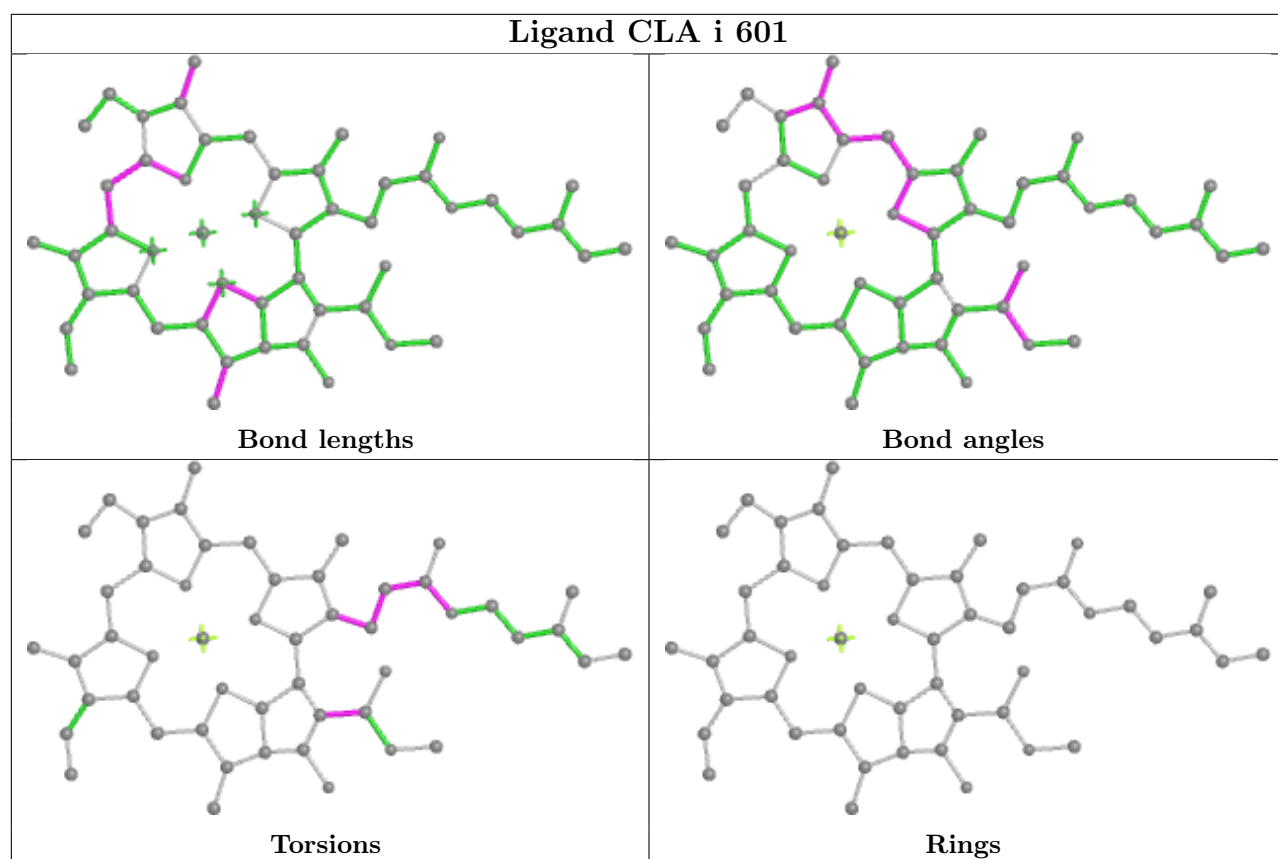
Bond angles

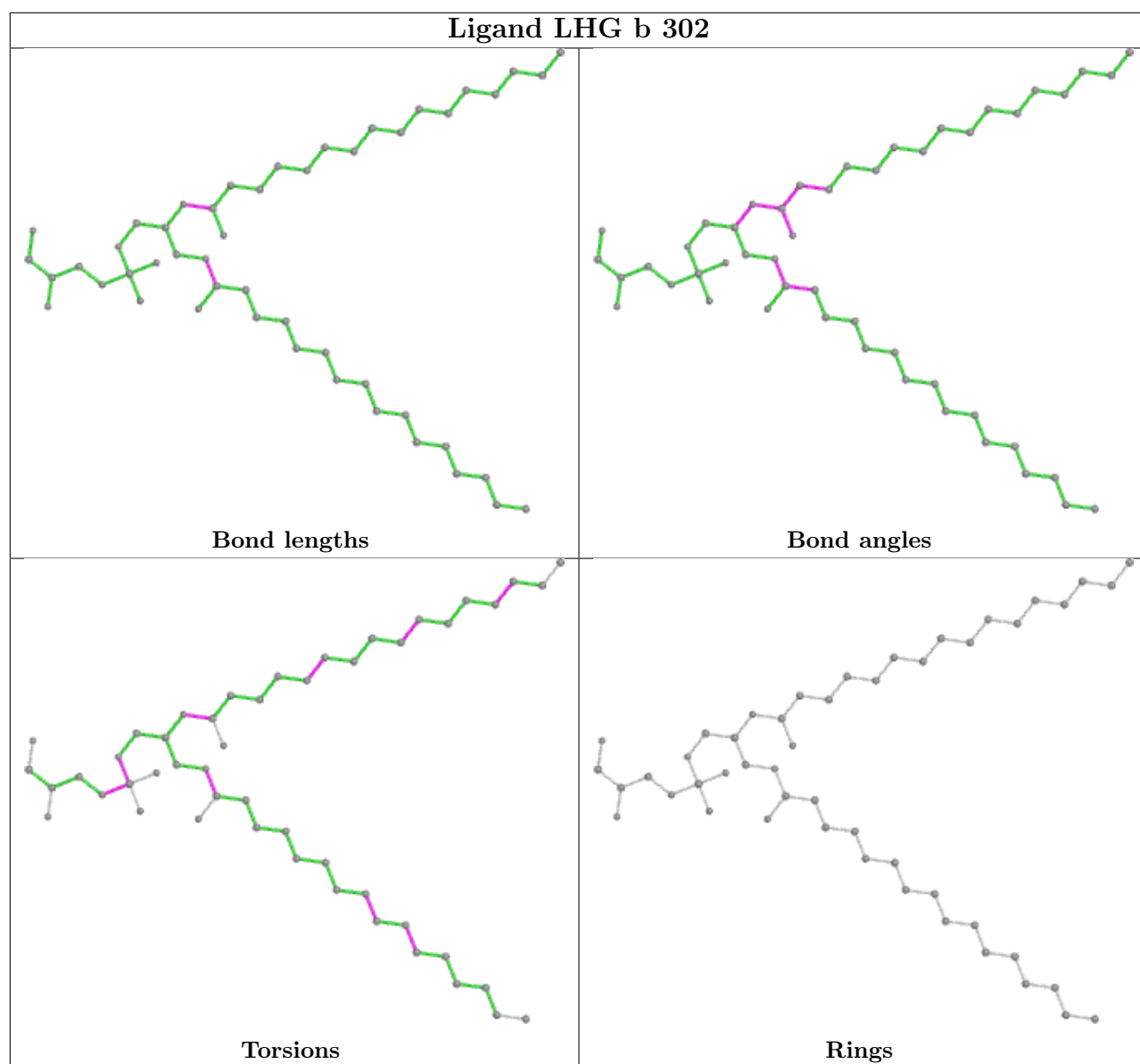


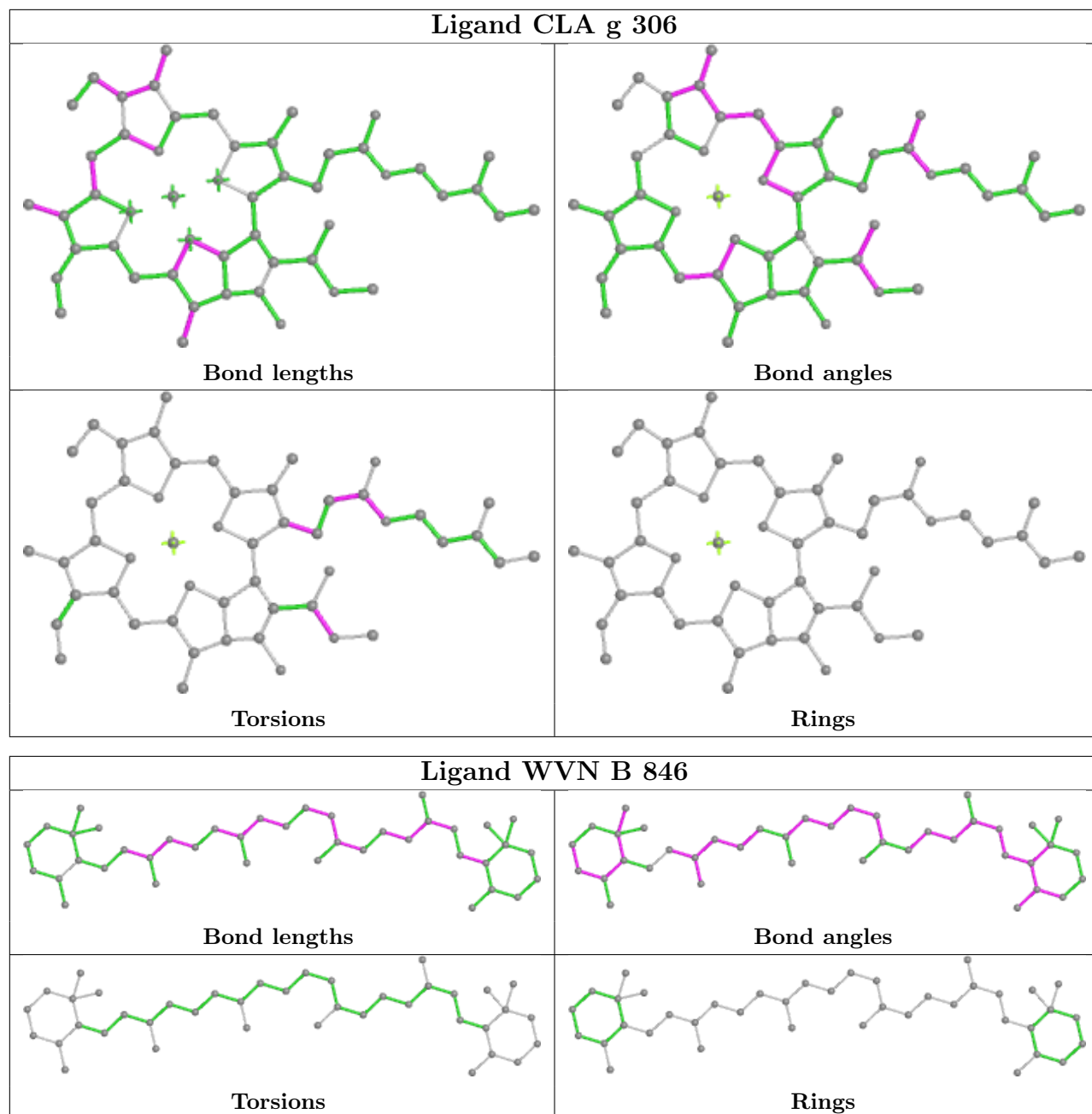
Torsions



Rings

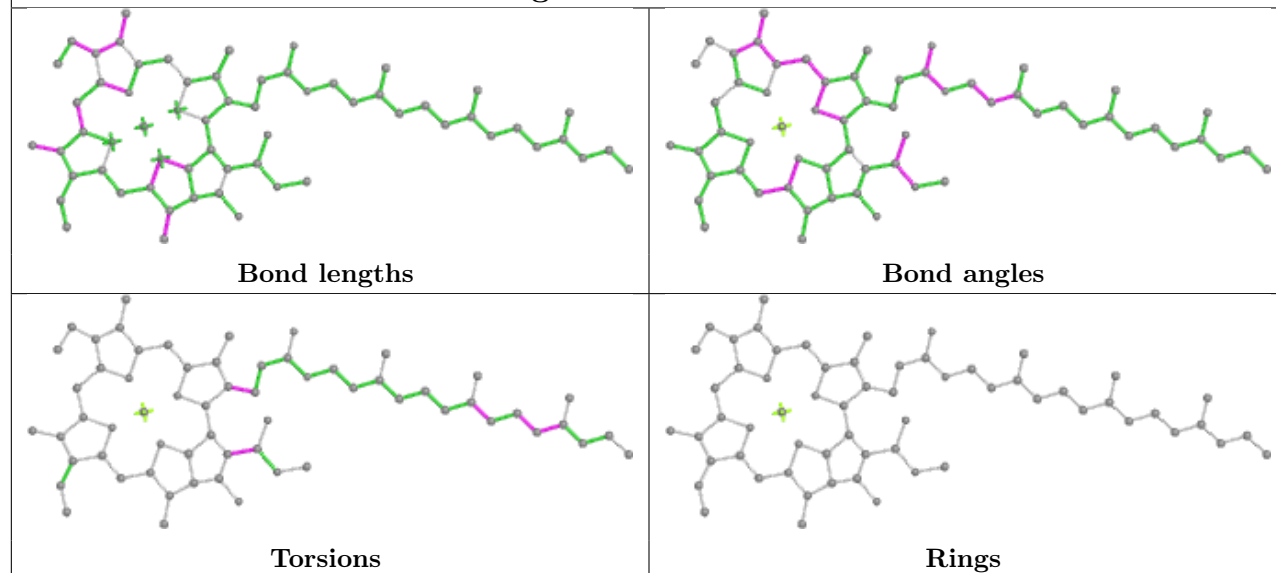




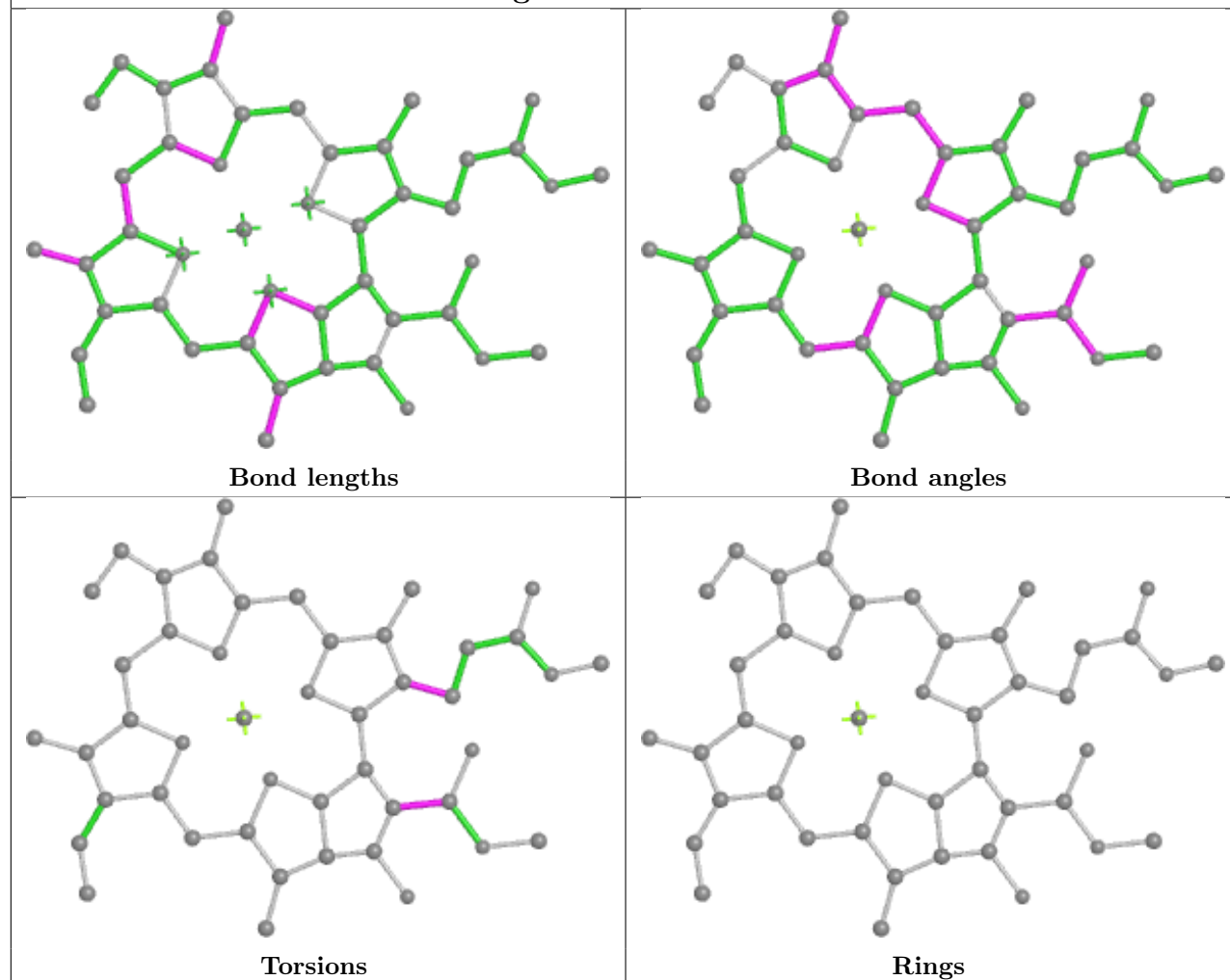


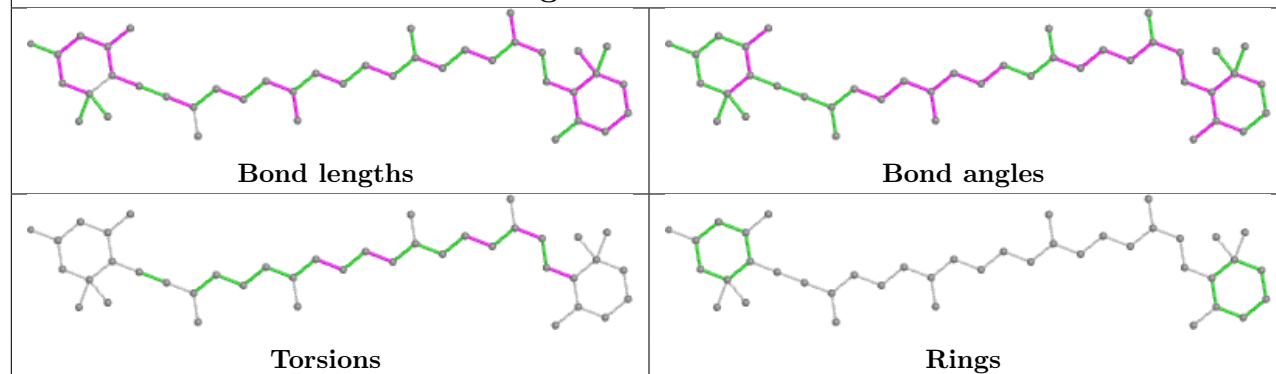
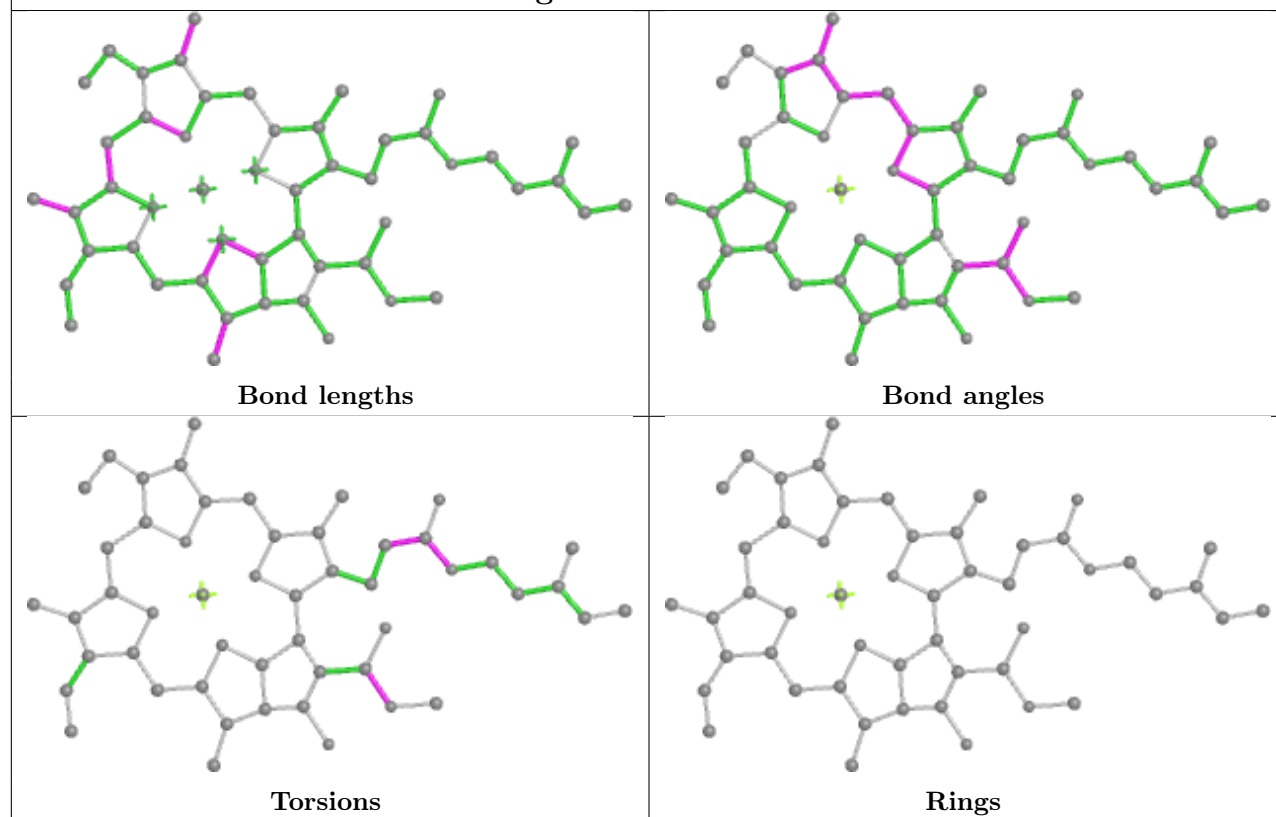
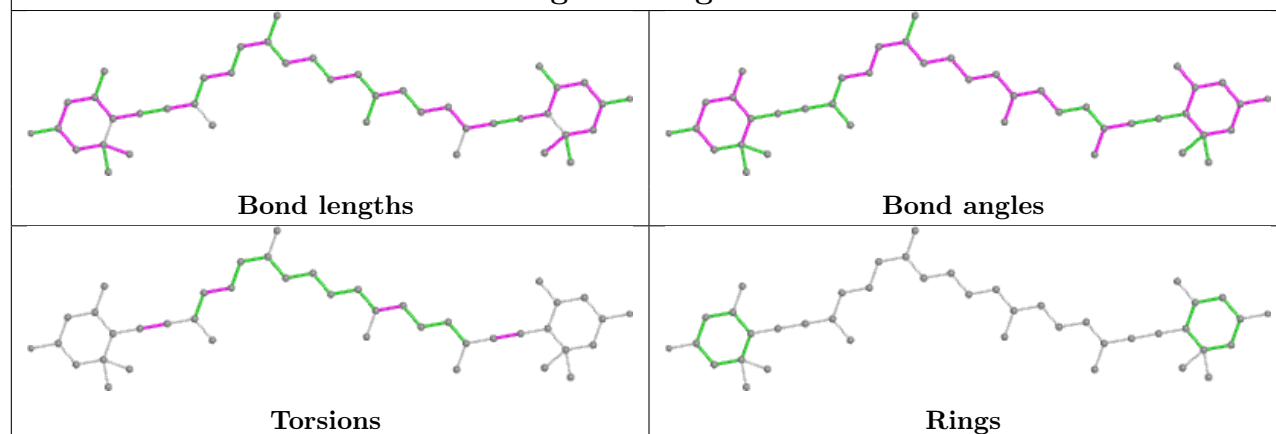


## Ligand CLA A 810

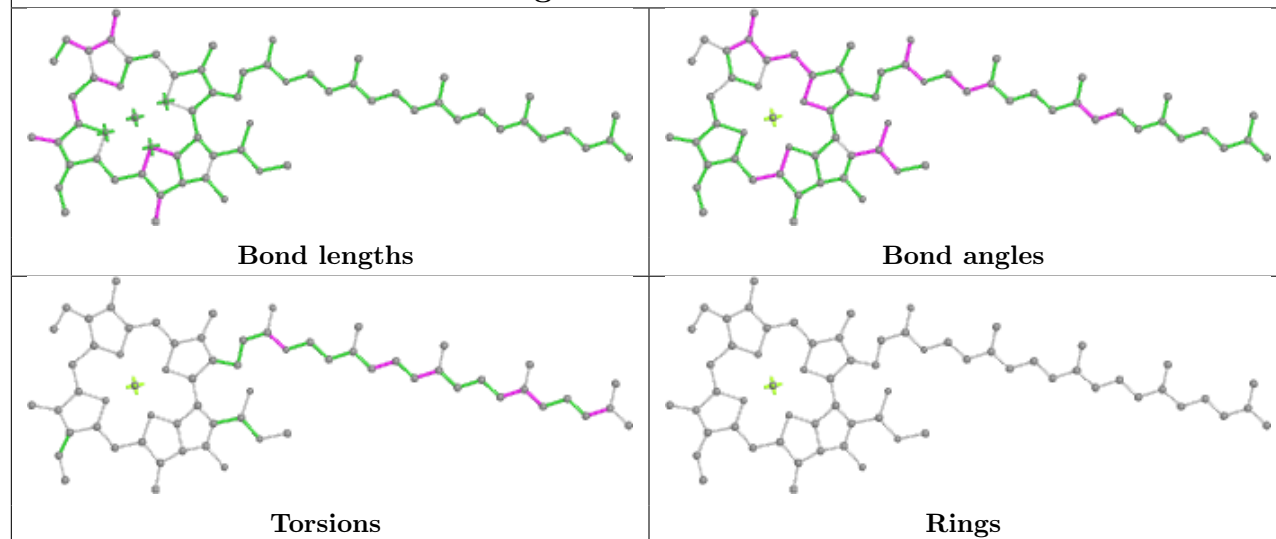


## Ligand CLA B 819

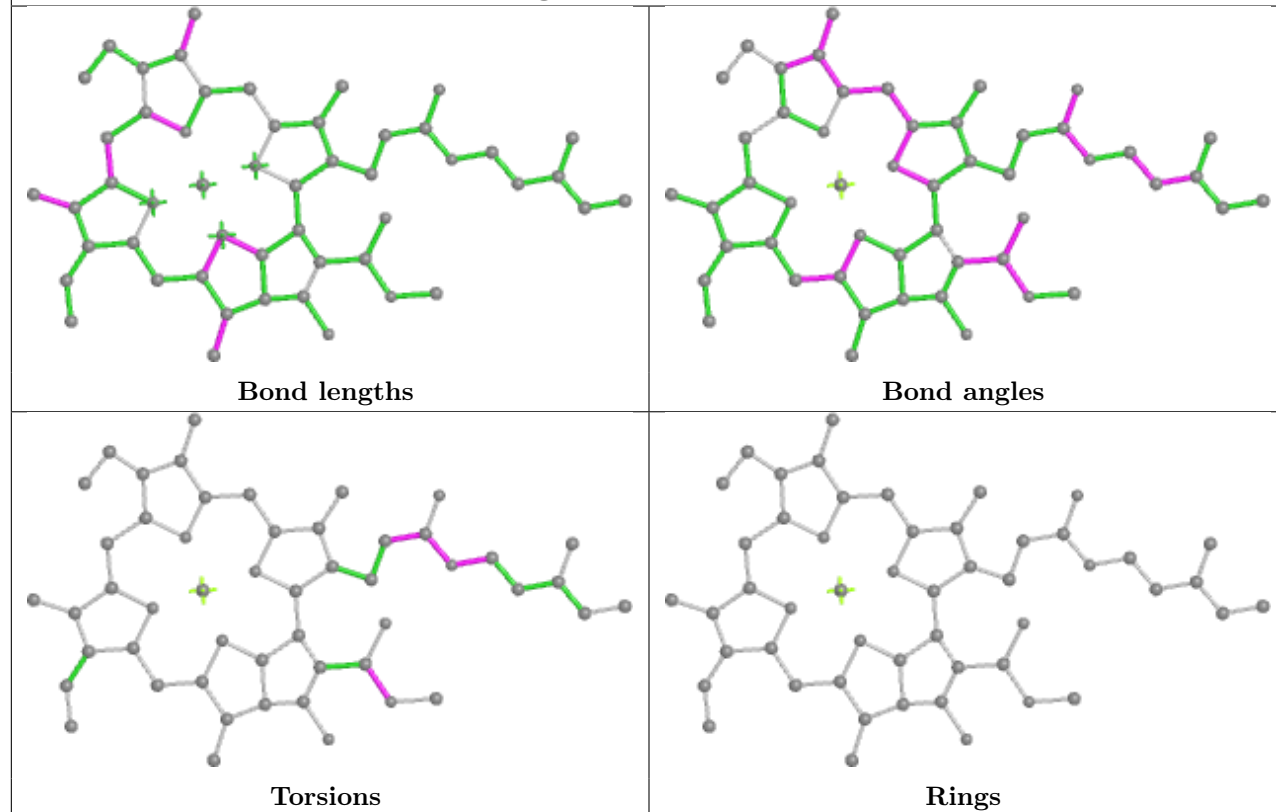


**Ligand IHT k 618****Ligand CLA k 606****Ligand II0 g 317**

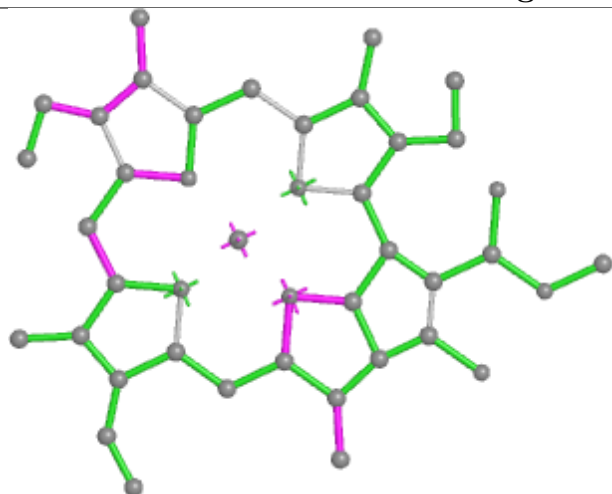
## Ligand CLA L 203



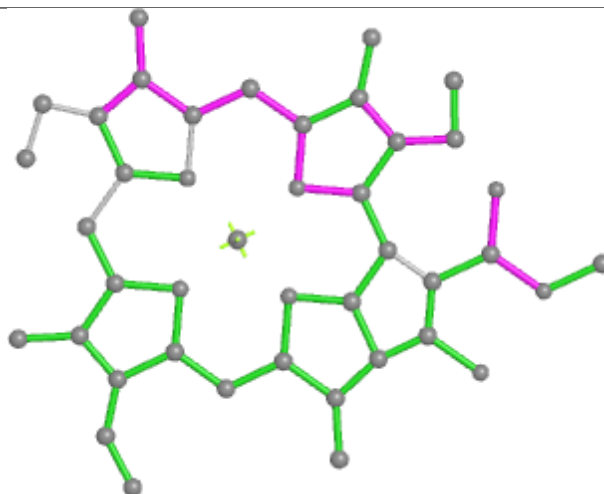
## Ligand CLA b 311



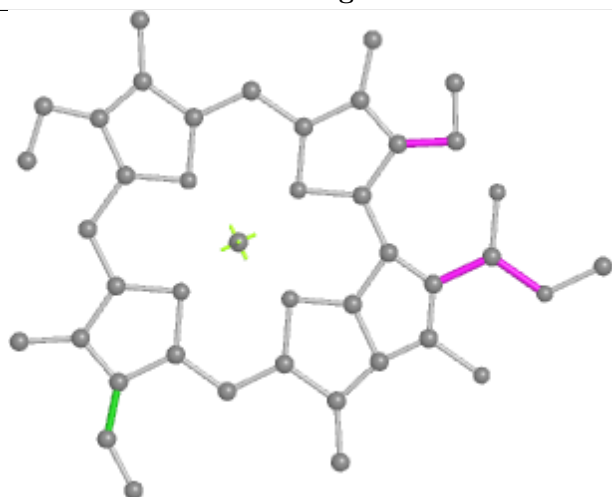
## Ligand CLA J 103



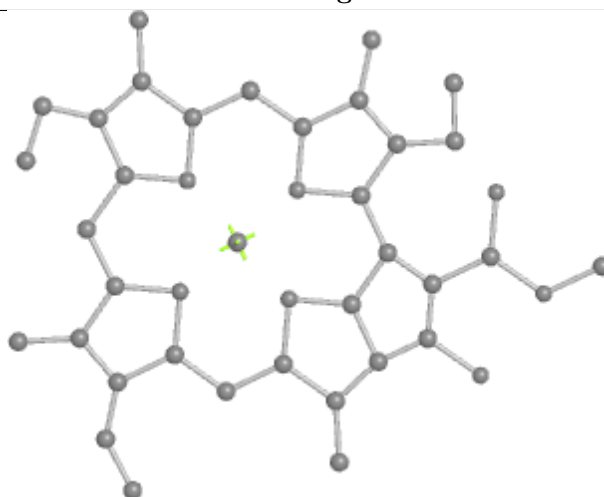
Bond lengths



Bond angles

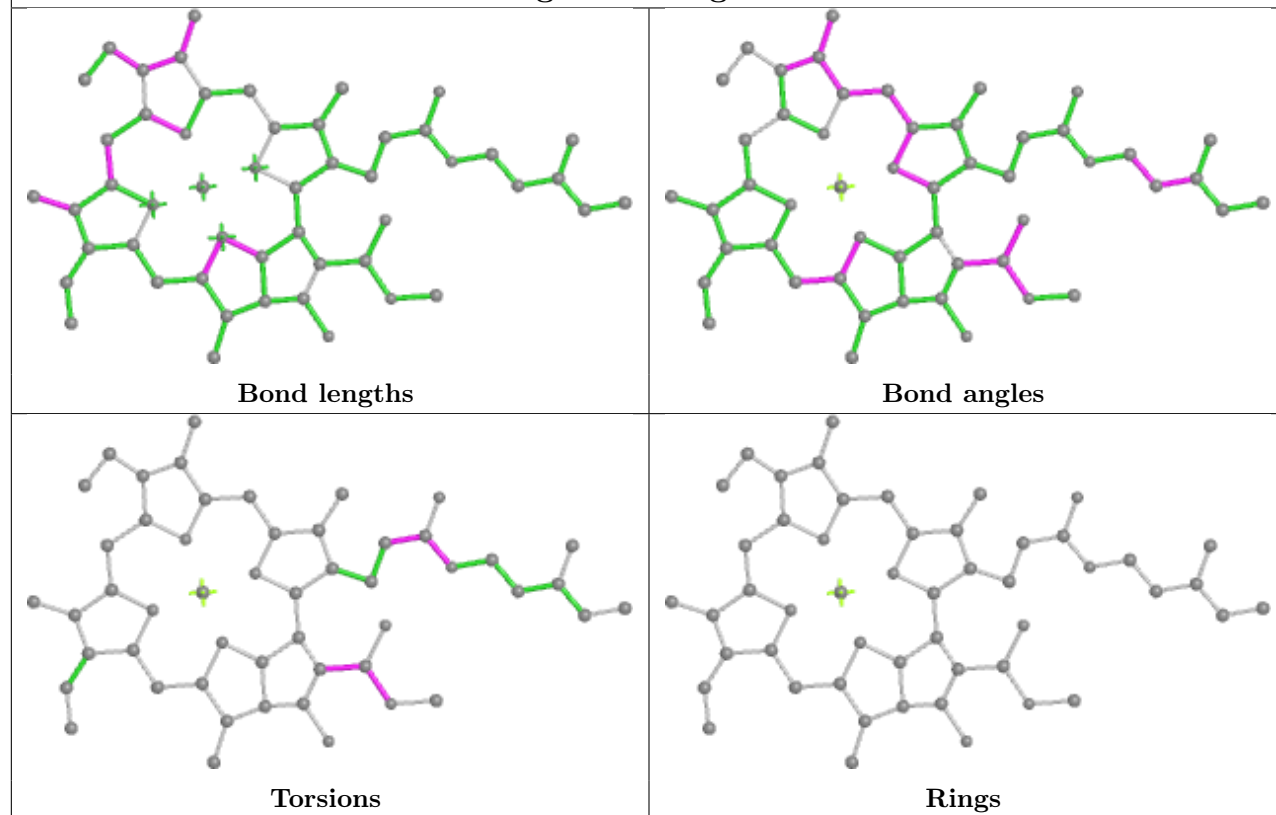


Torsions

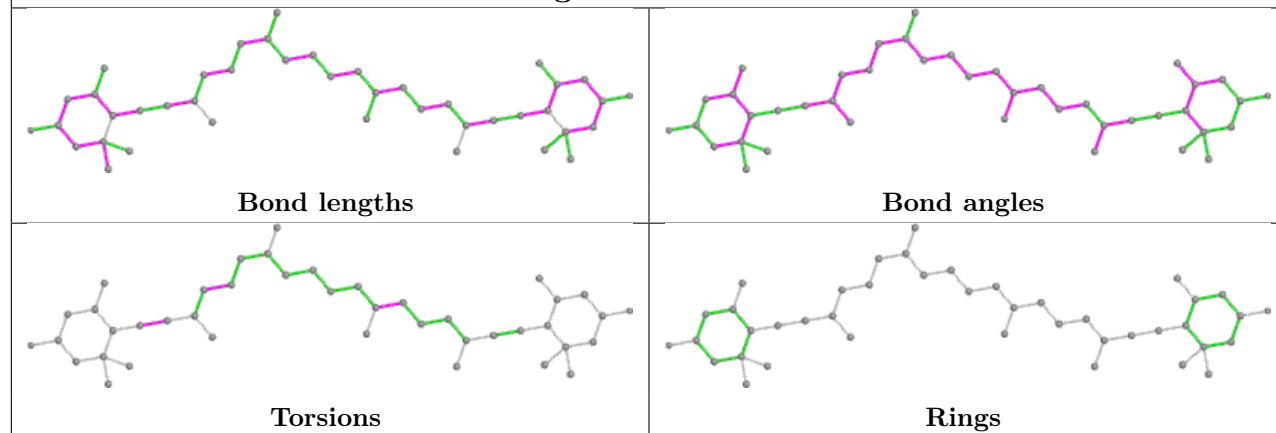


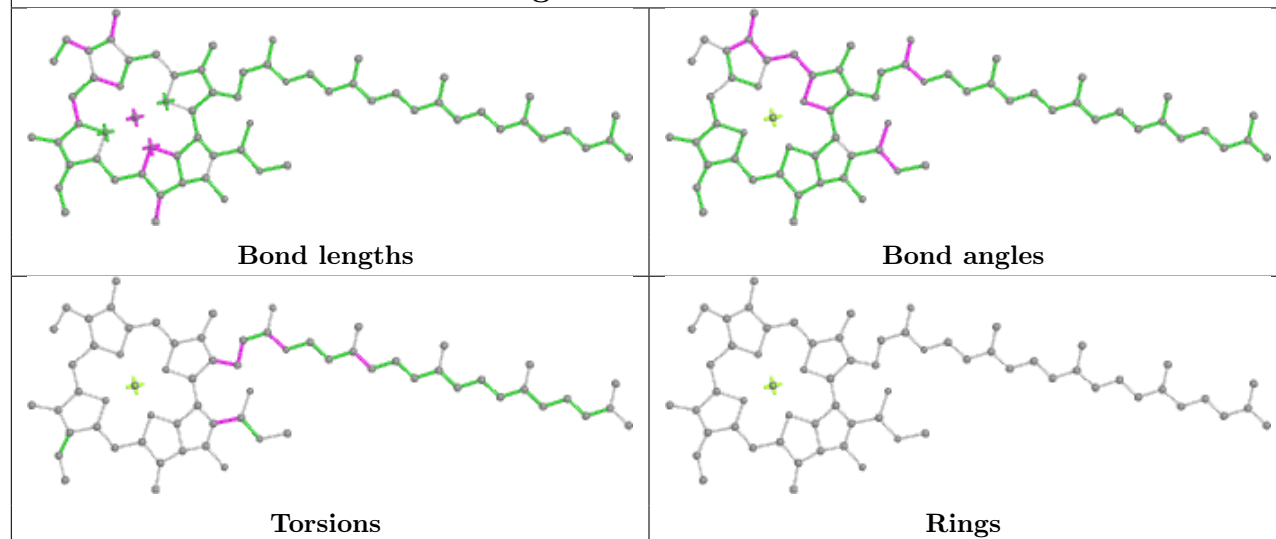
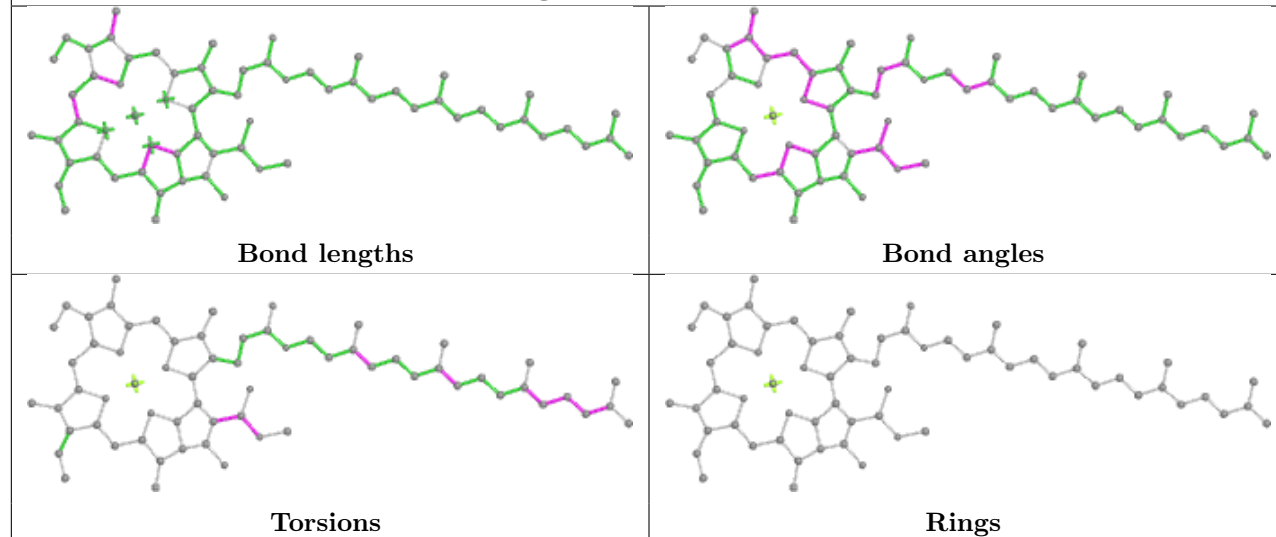
Rings

## Ligand CLA g 307

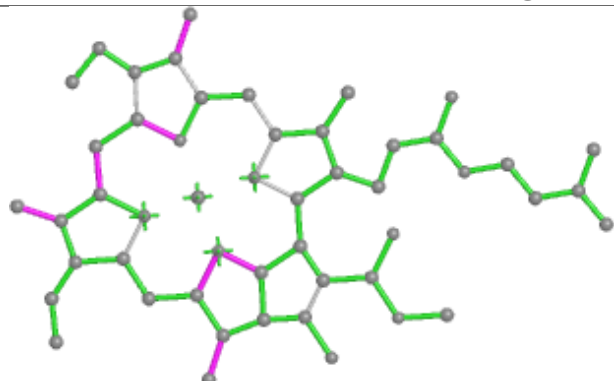


## Ligand II0 f 615

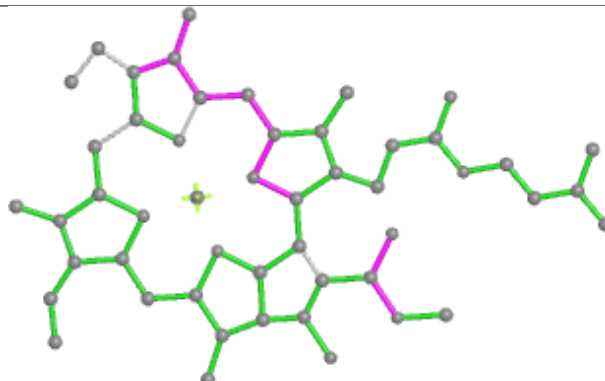


**Ligand CLA B 826****Ligand CLA b 310**

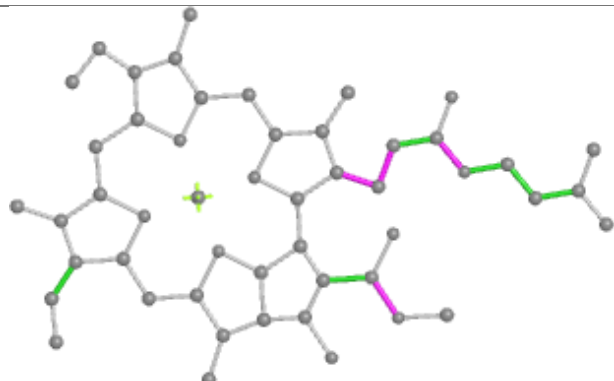
## Ligand CLA e 602



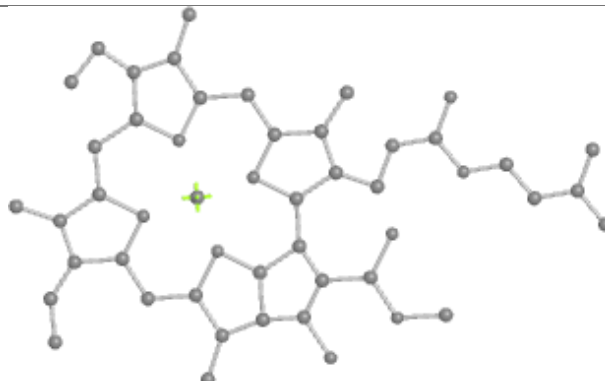
Bond lengths



Bond angles

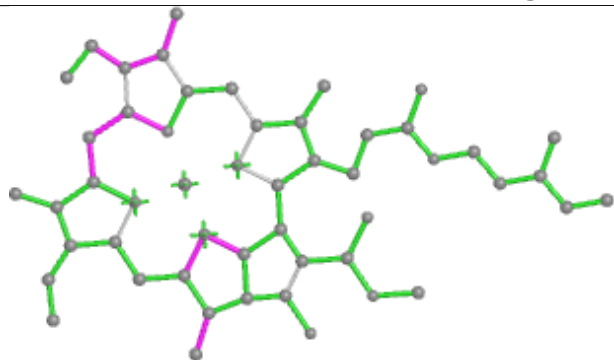


Torsions

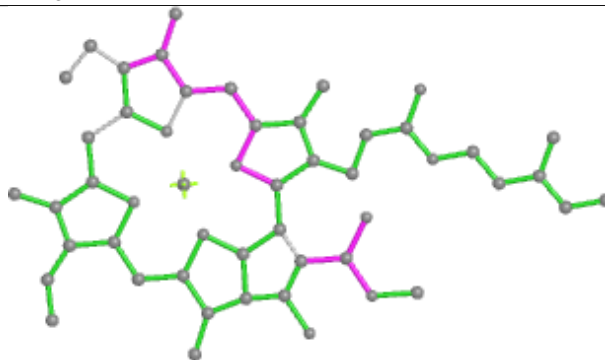


Rings

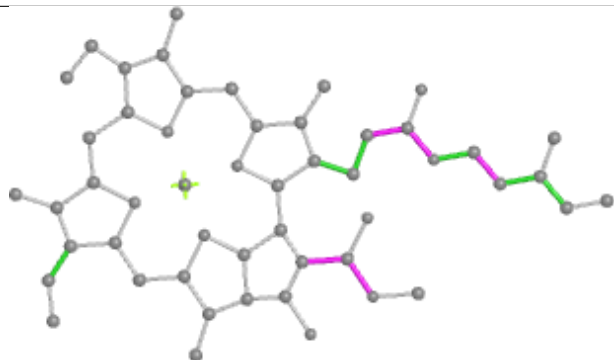
## Ligand CLA j 308



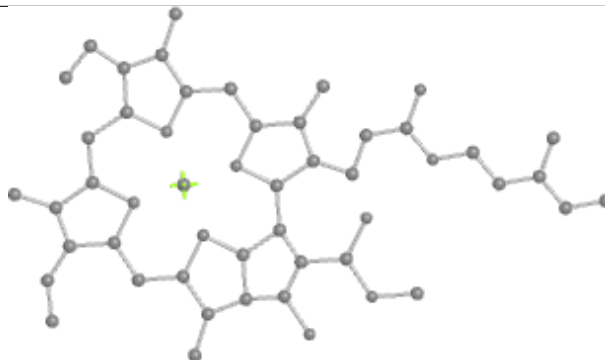
Bond lengths



Bond angles

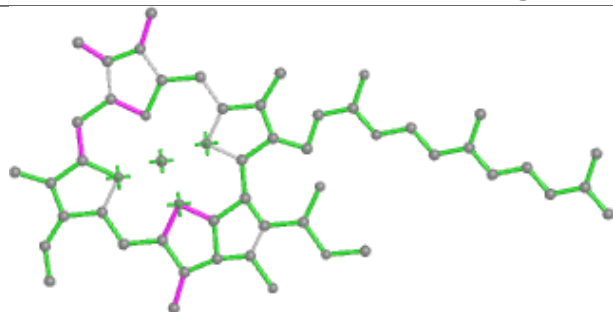


Torsions

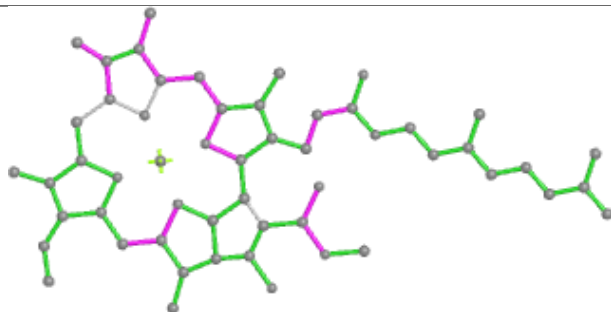


Rings

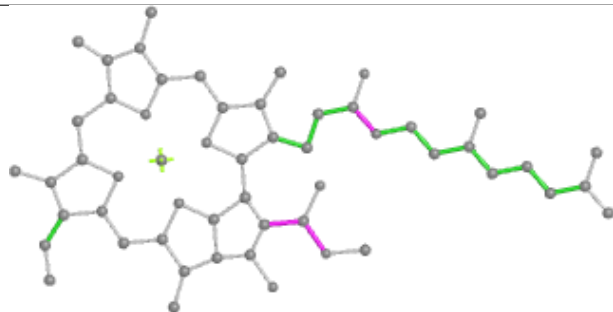
## Ligand CLA B 810



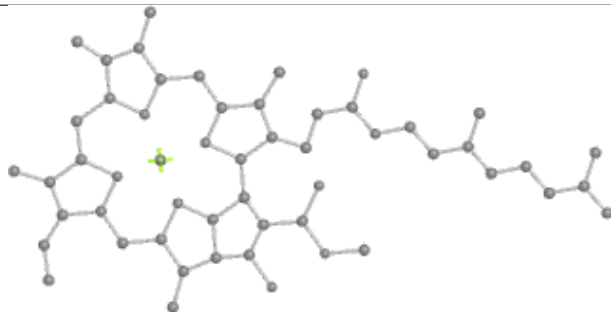
Bond lengths



Bond angles

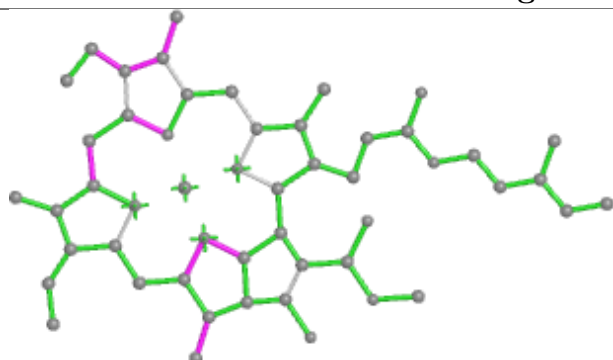


Torsions

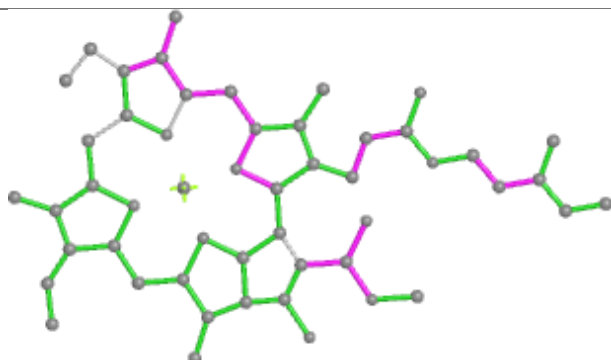


Rings

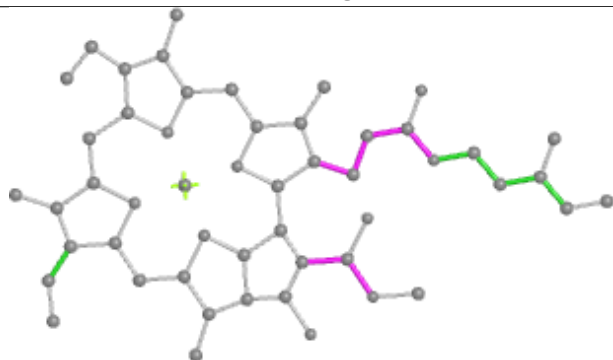
## Ligand CLA k 610



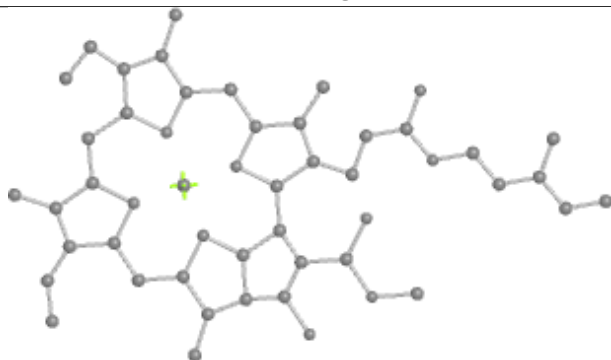
Bond lengths



Bond angles



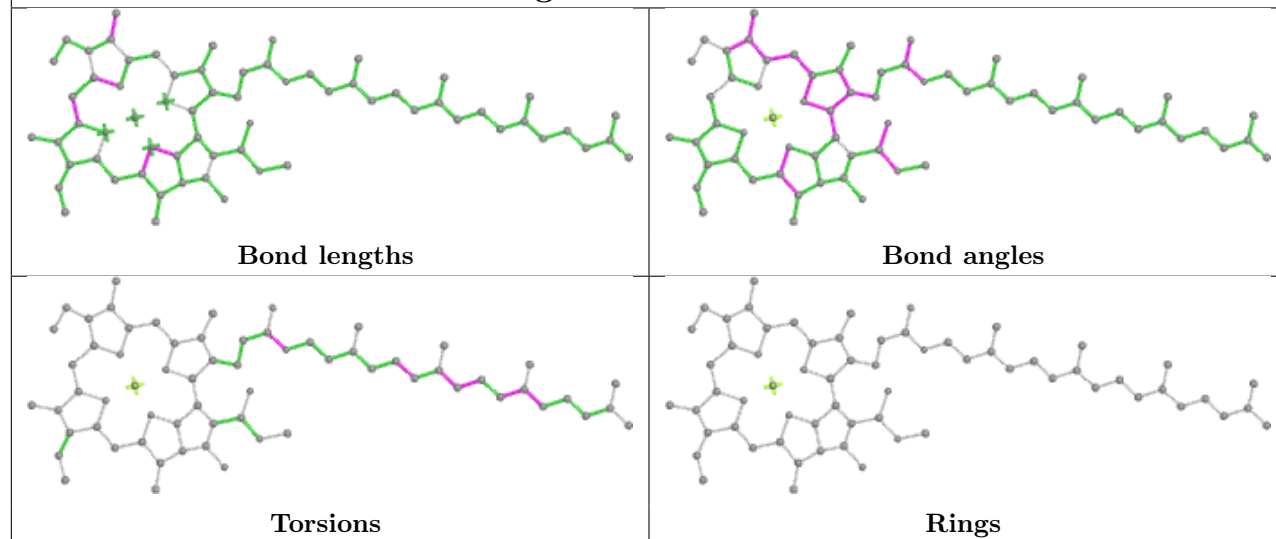
Torsions



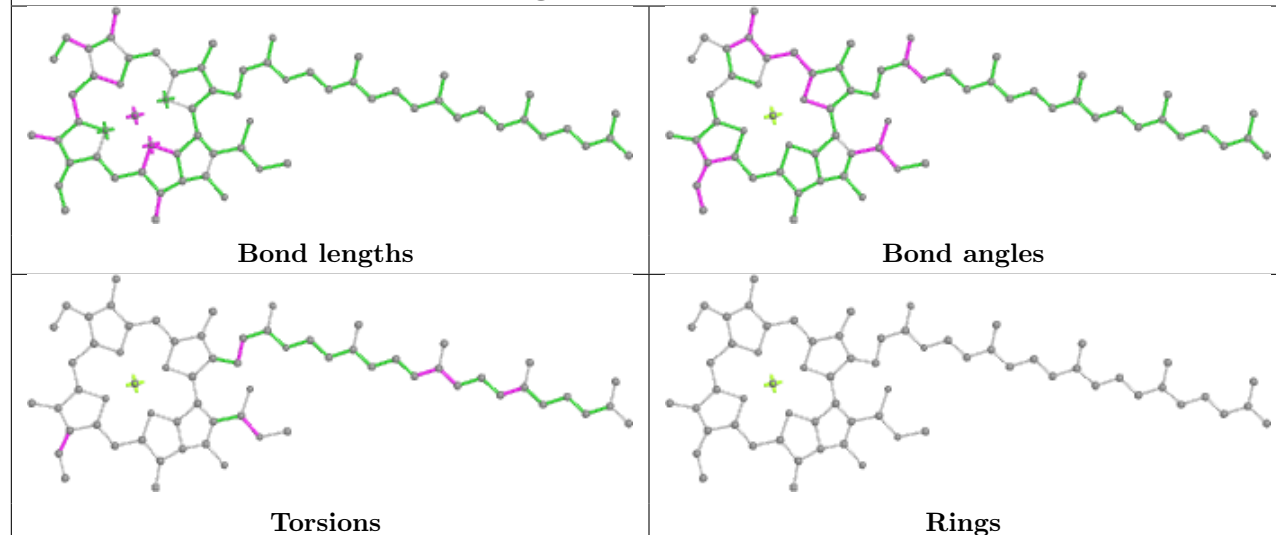
Rings



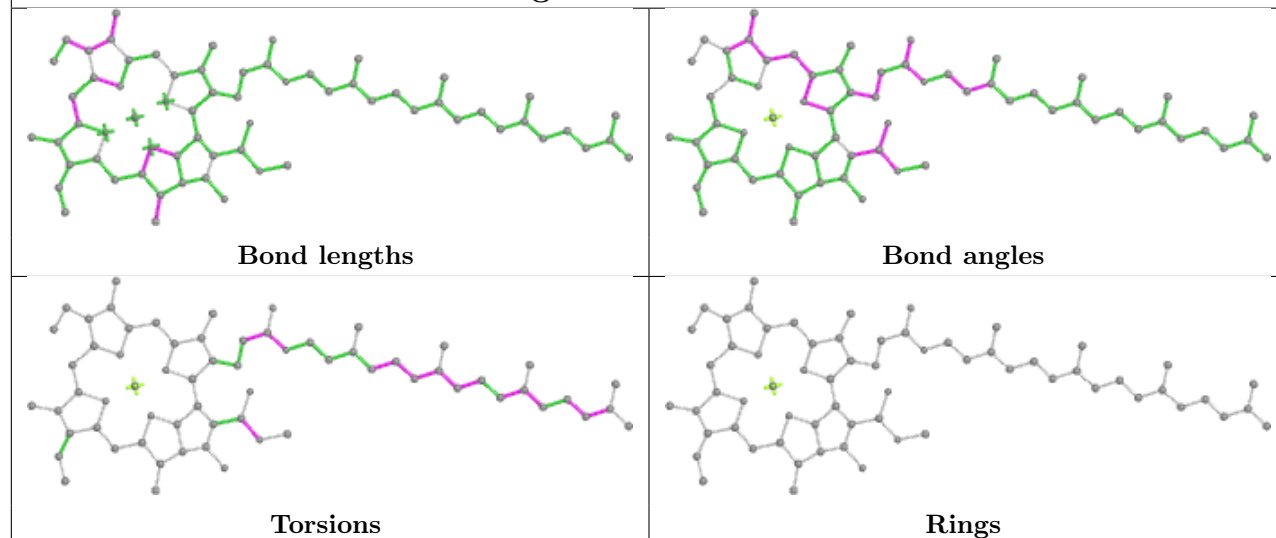
## Ligand CLA b 307

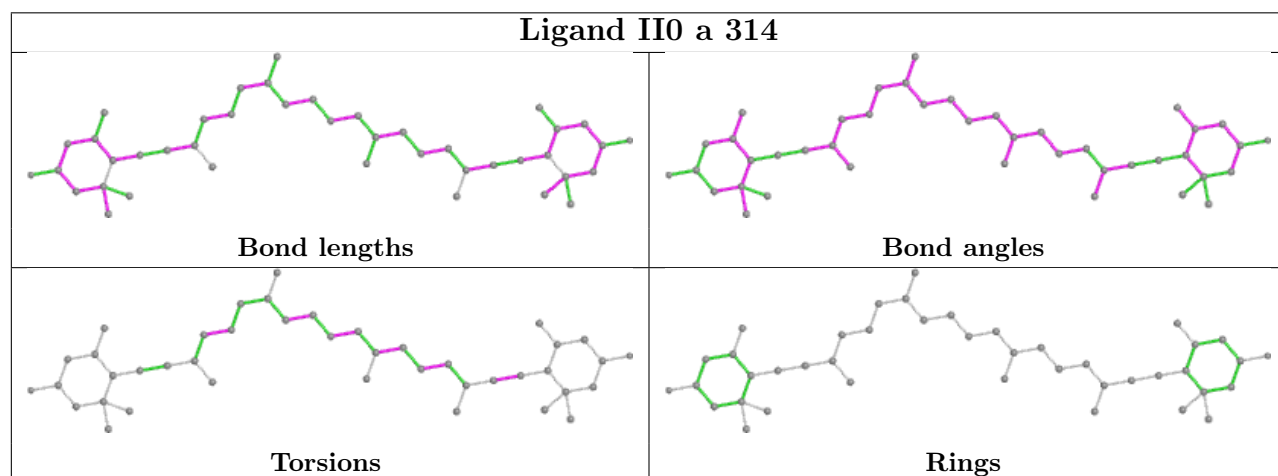
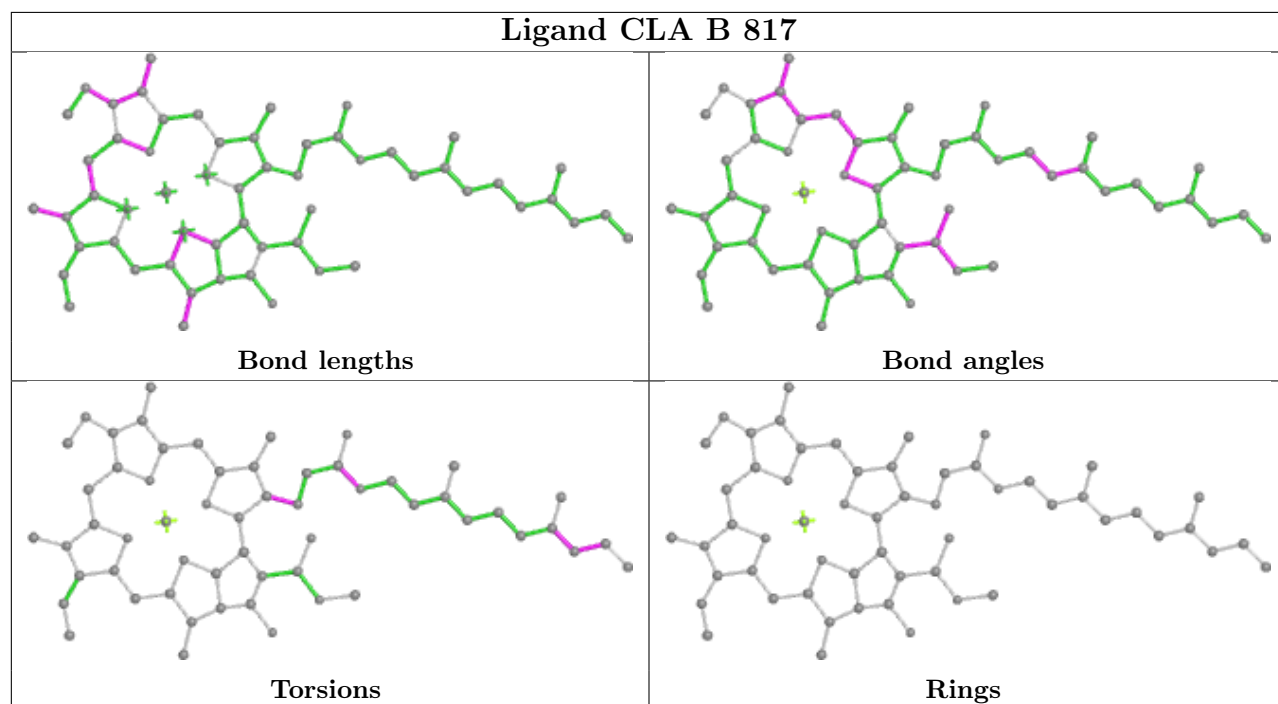
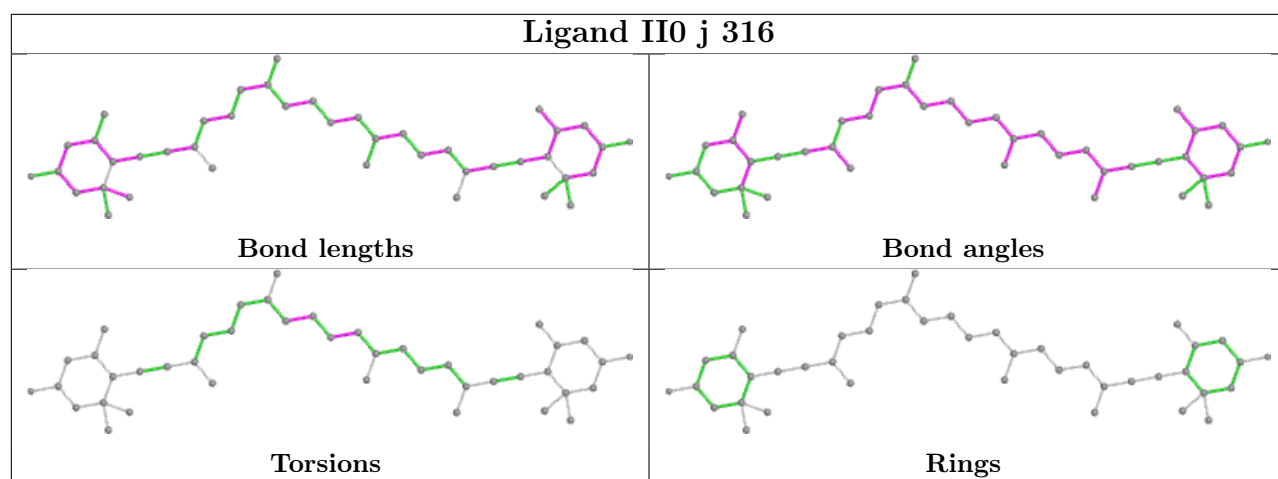


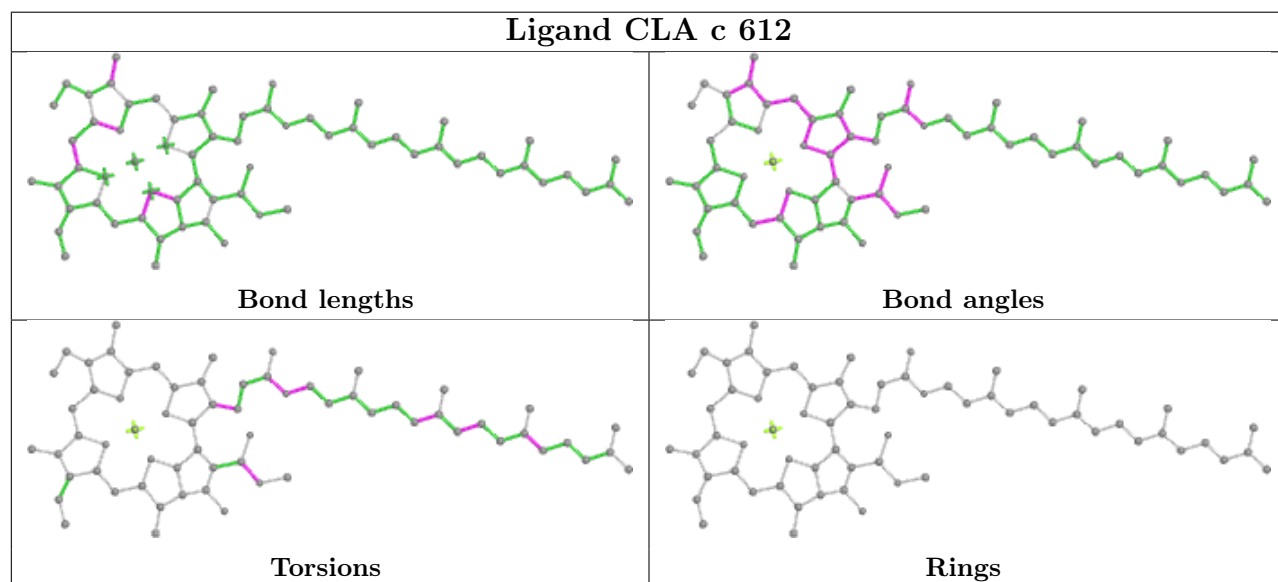
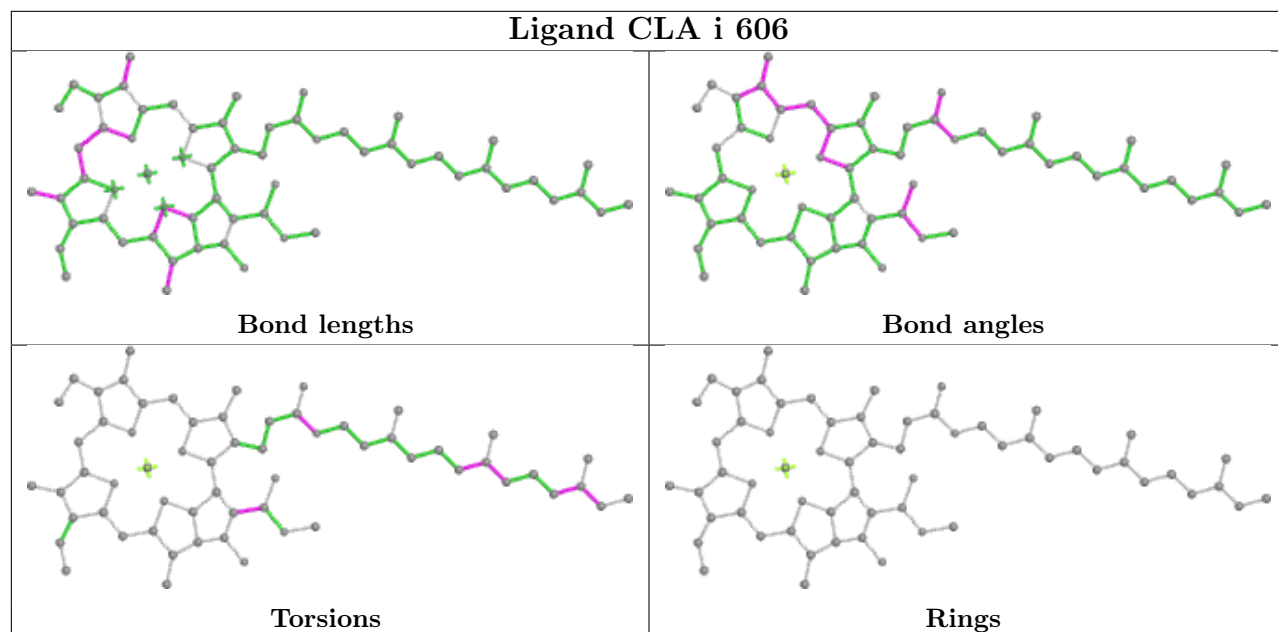
## Ligand CLA B 804

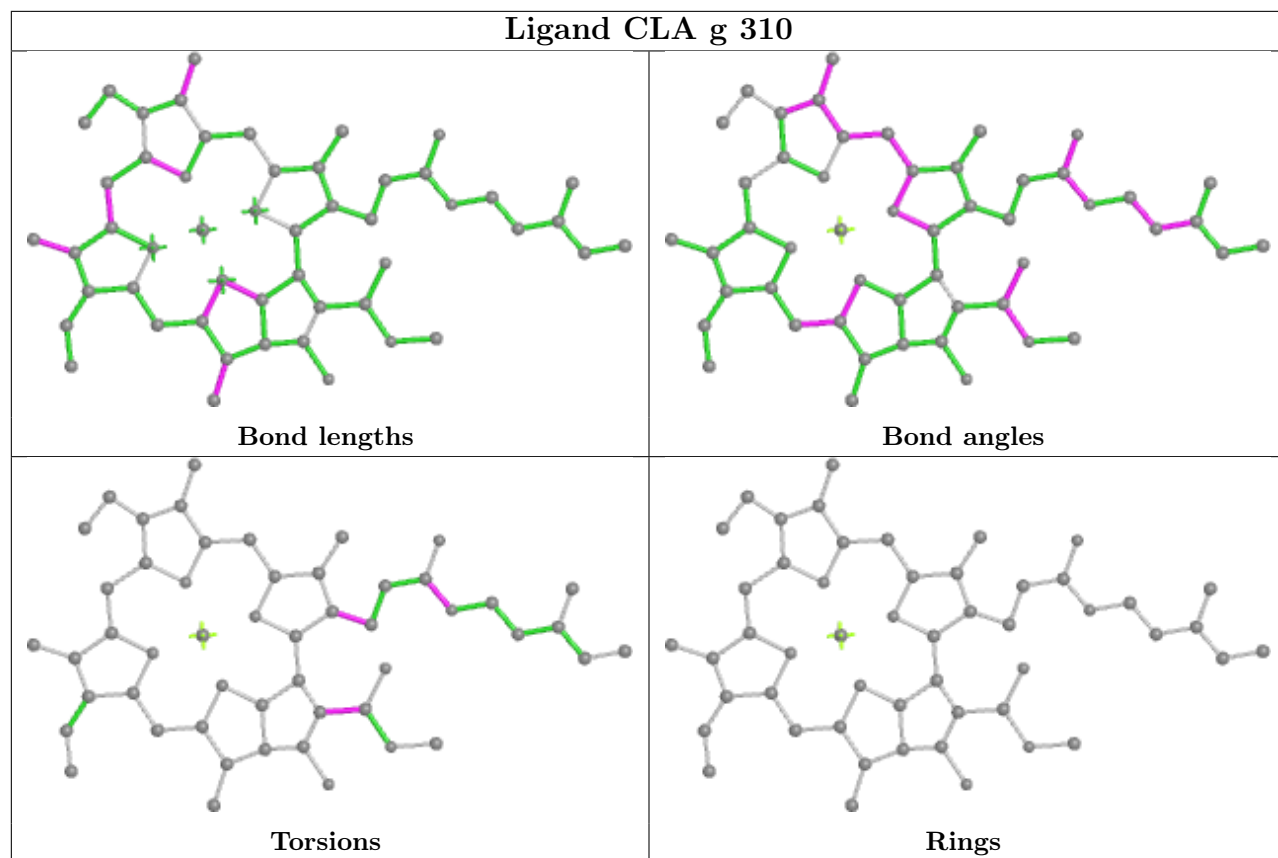


## Ligand CLA B 803

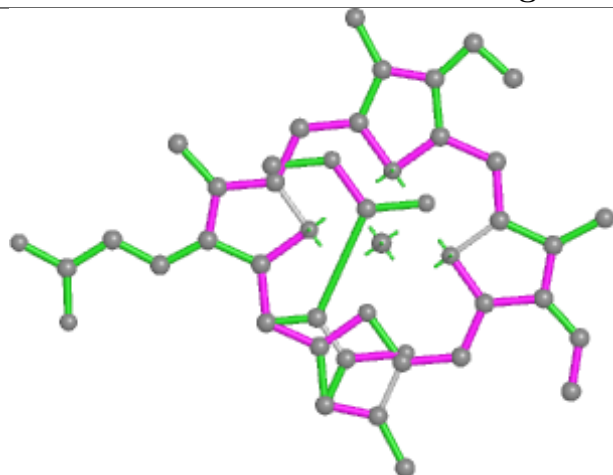




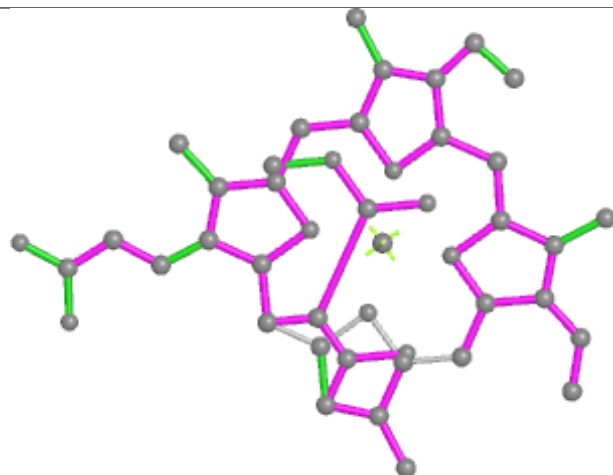




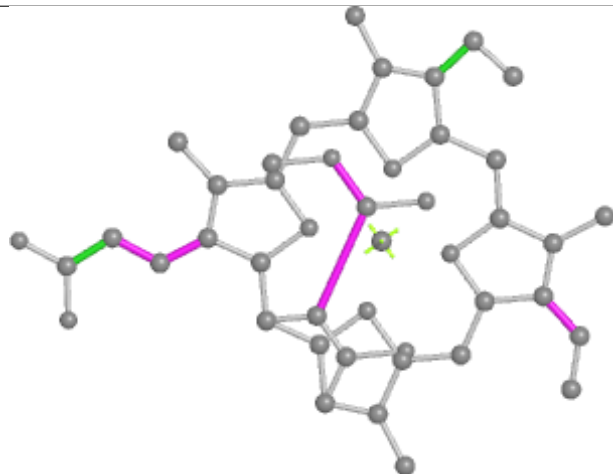
## Ligand KC2 d 311



Bond lengths



Bond angles

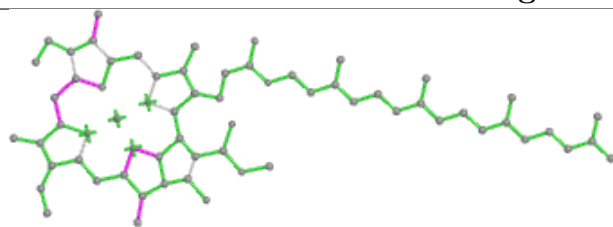


Torsions

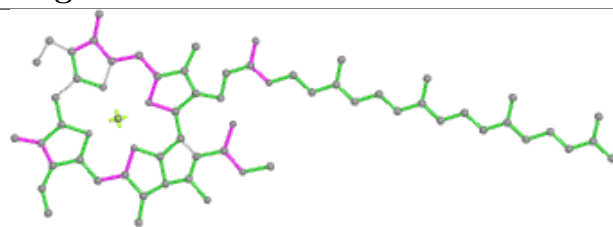


Rings

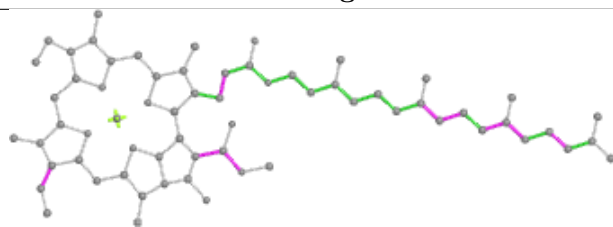
## Ligand CLA g 305



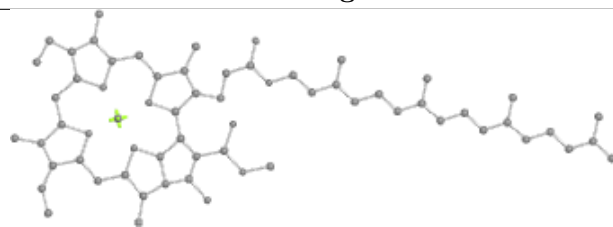
Bond lengths



Bond angles

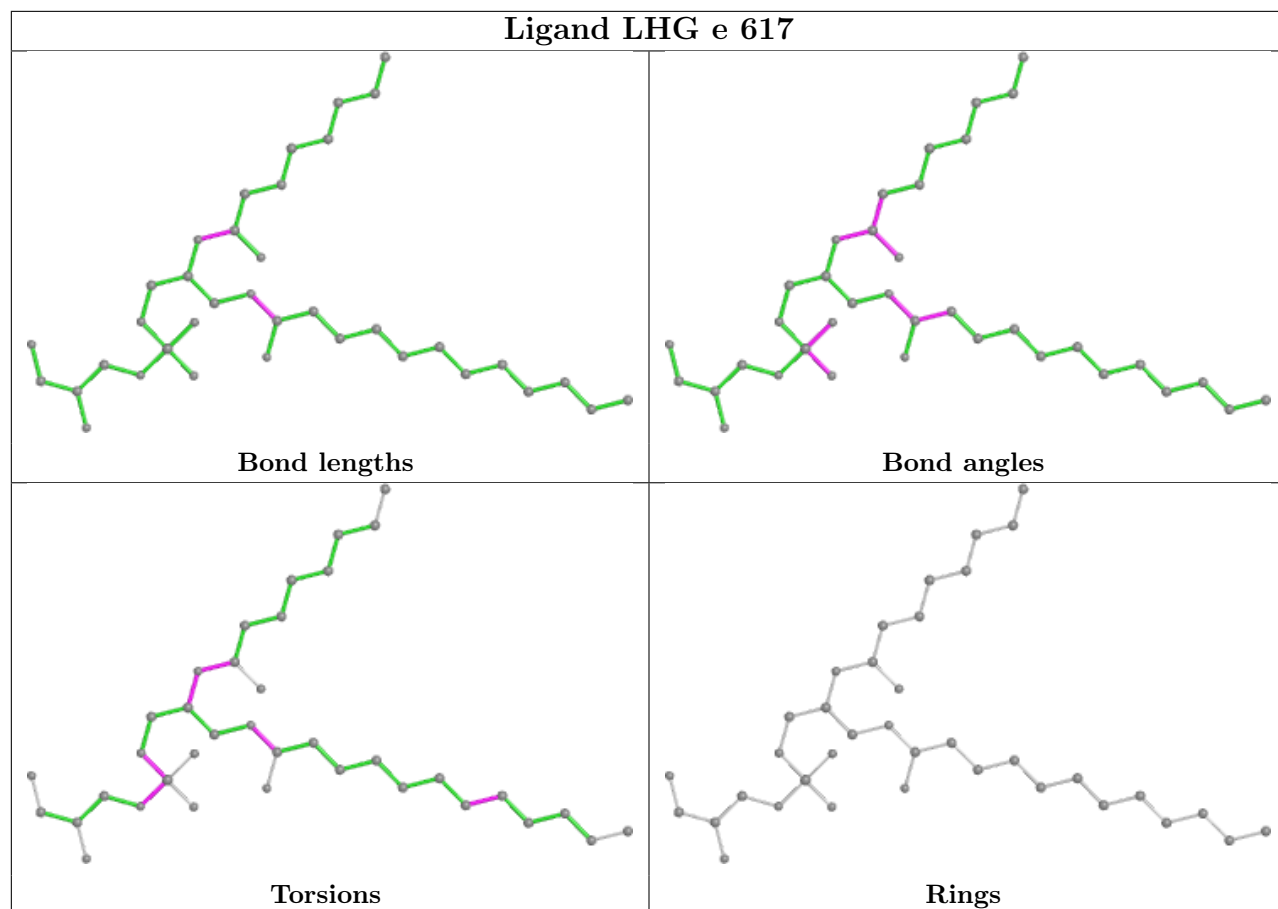


Torsions

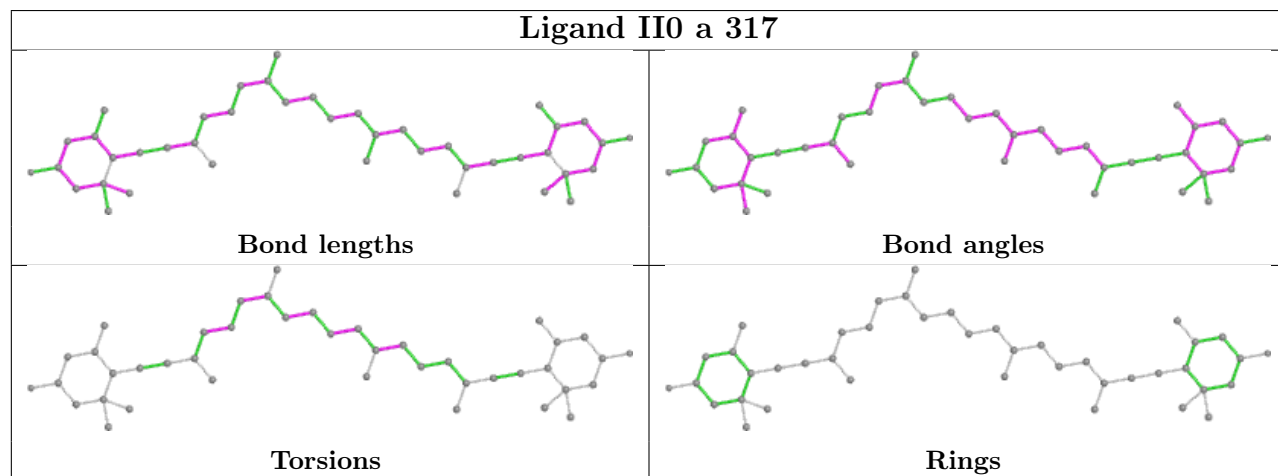


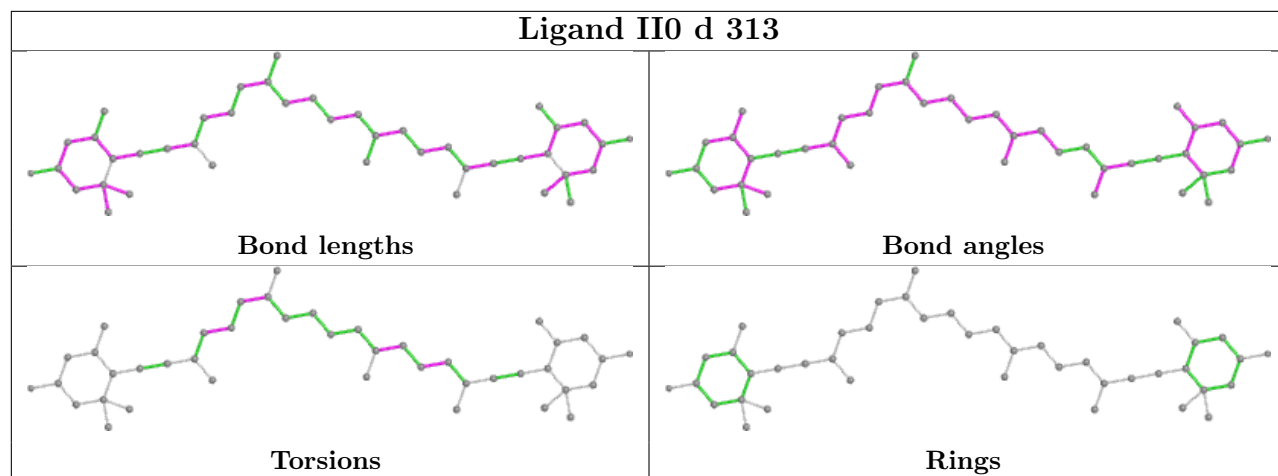
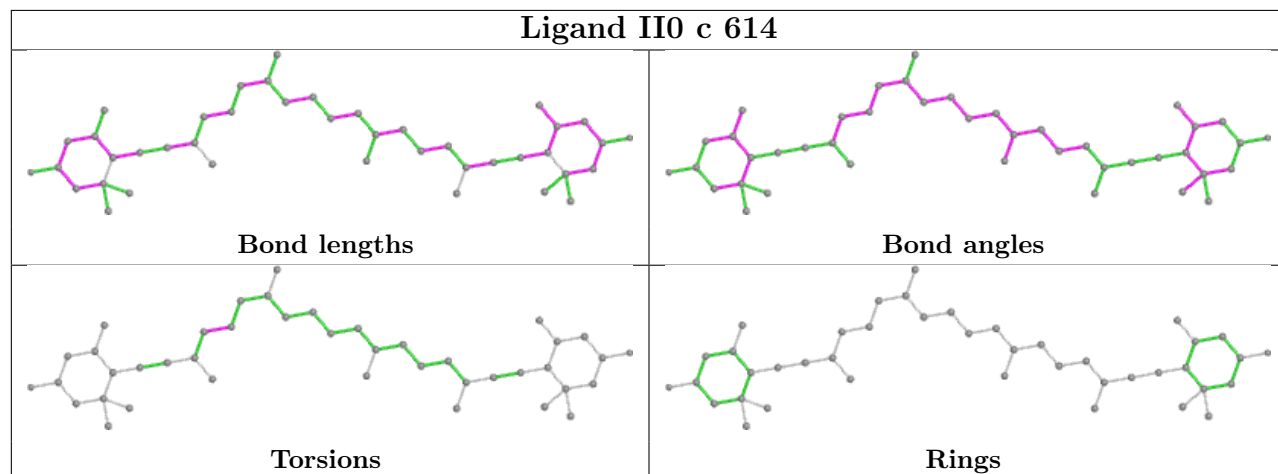
Rings

## Ligand LHG e 617

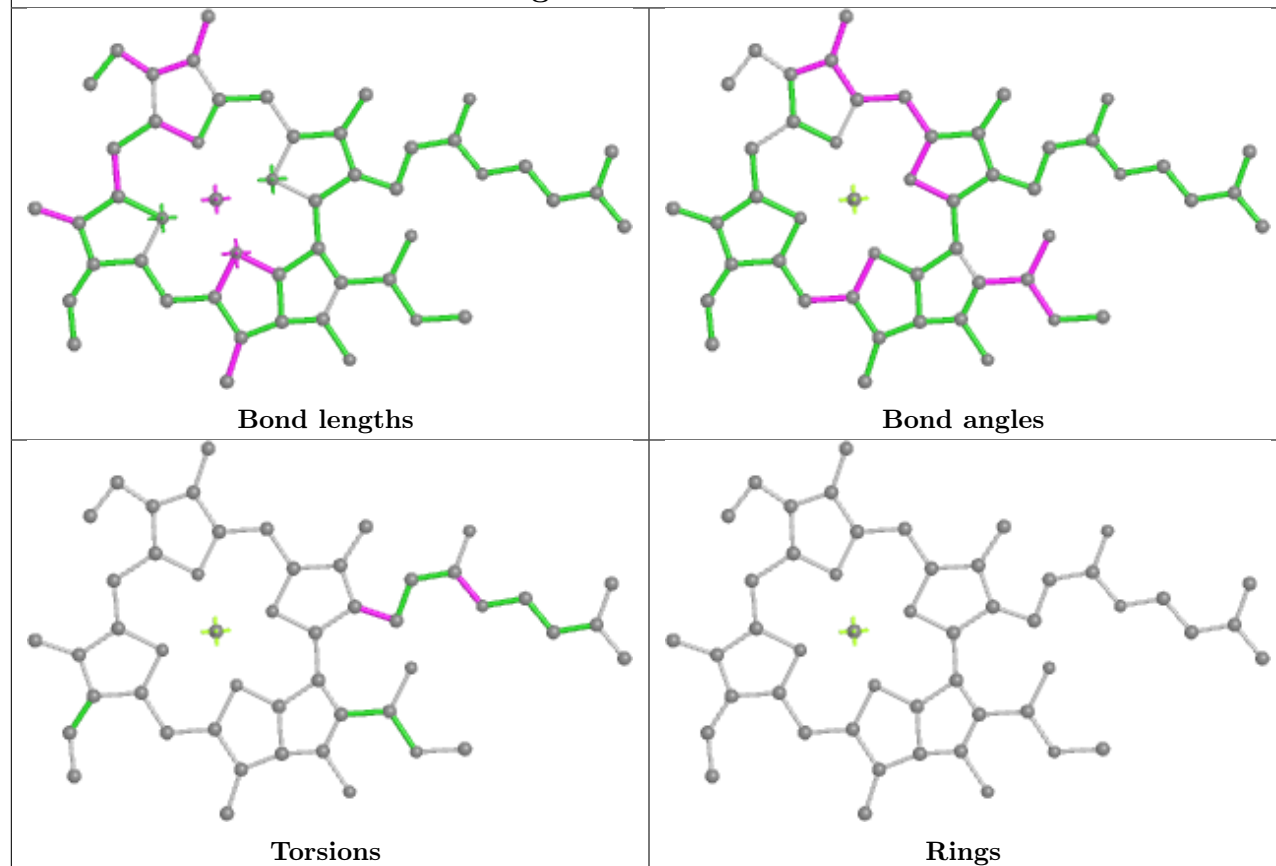


## Ligand II0 a 317

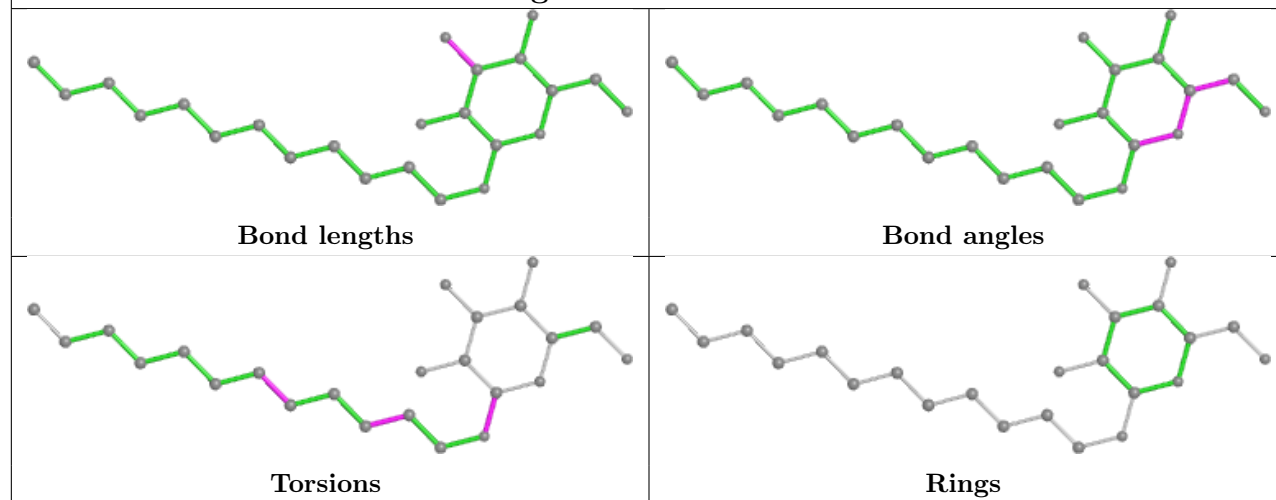


**Ligand II0 d 313****Ligand II0 c 614**

## Ligand CLA A 830

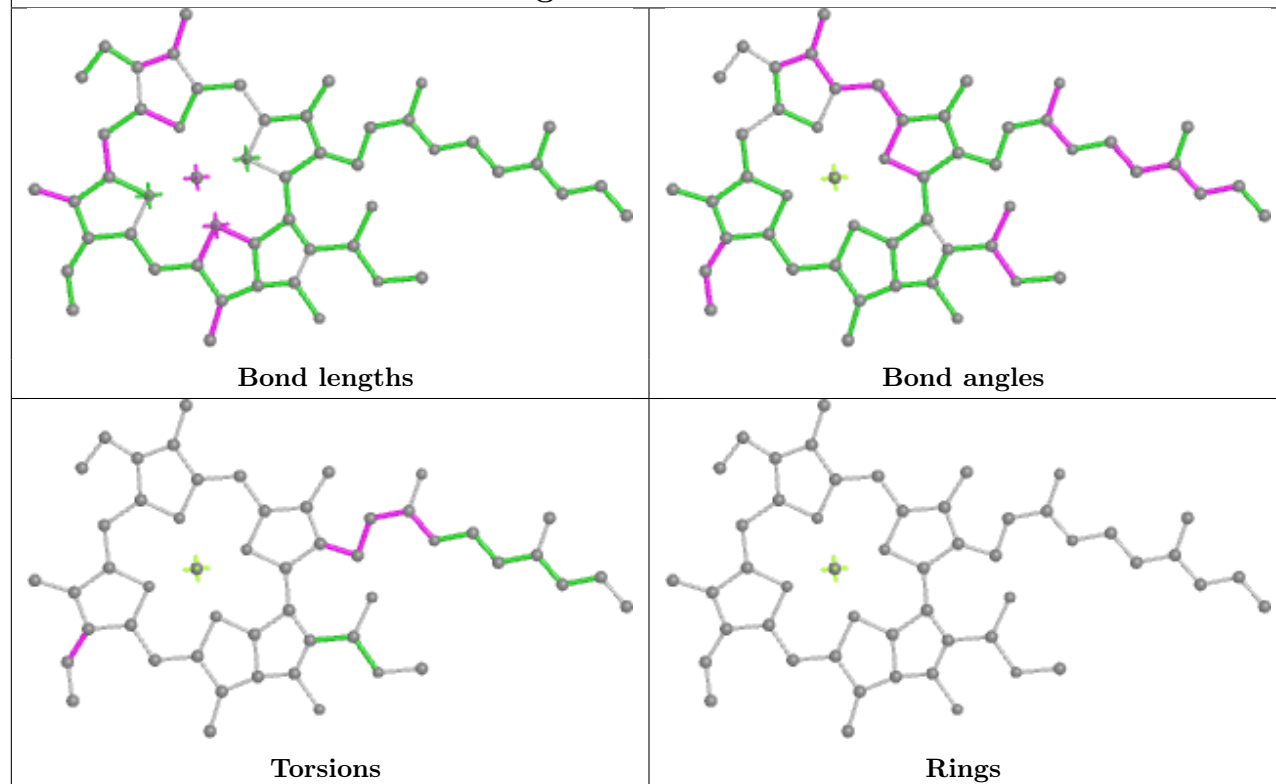


## Ligand LMT F 203

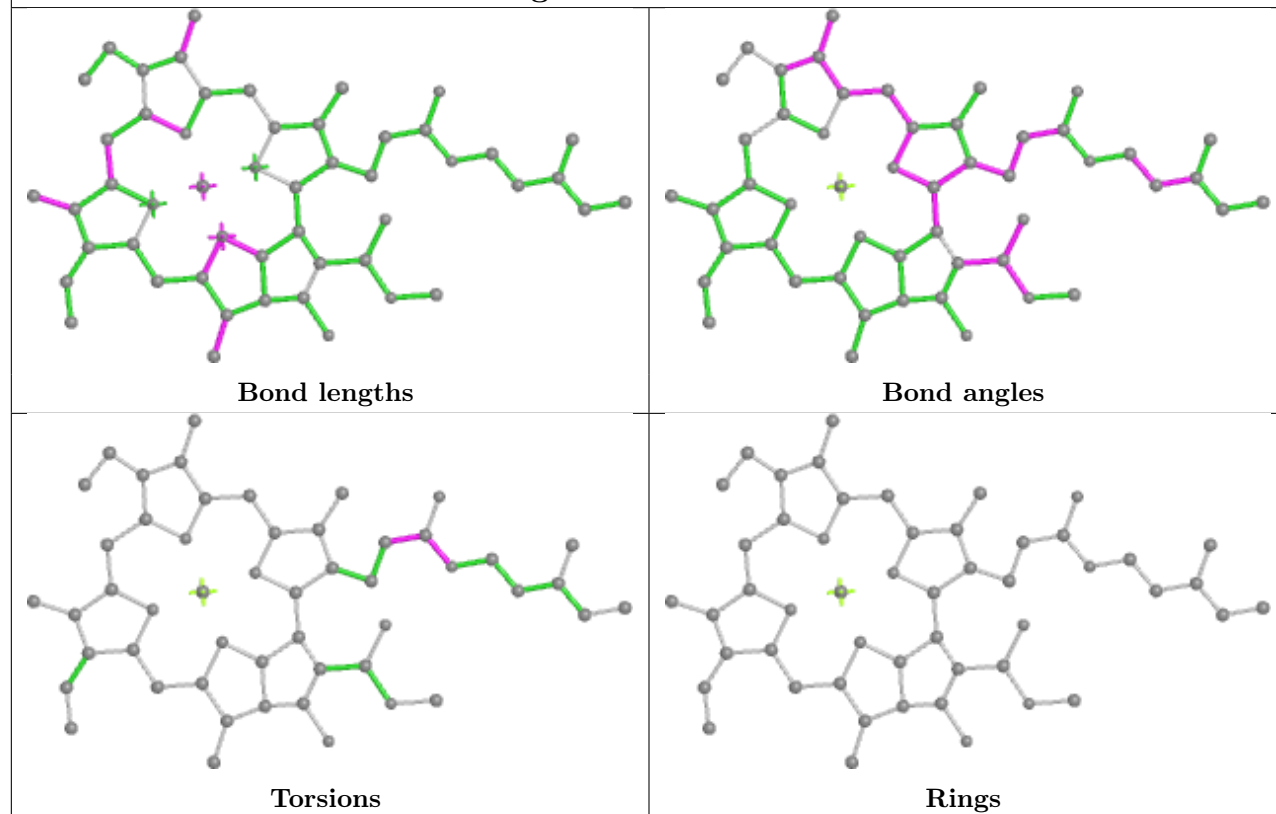




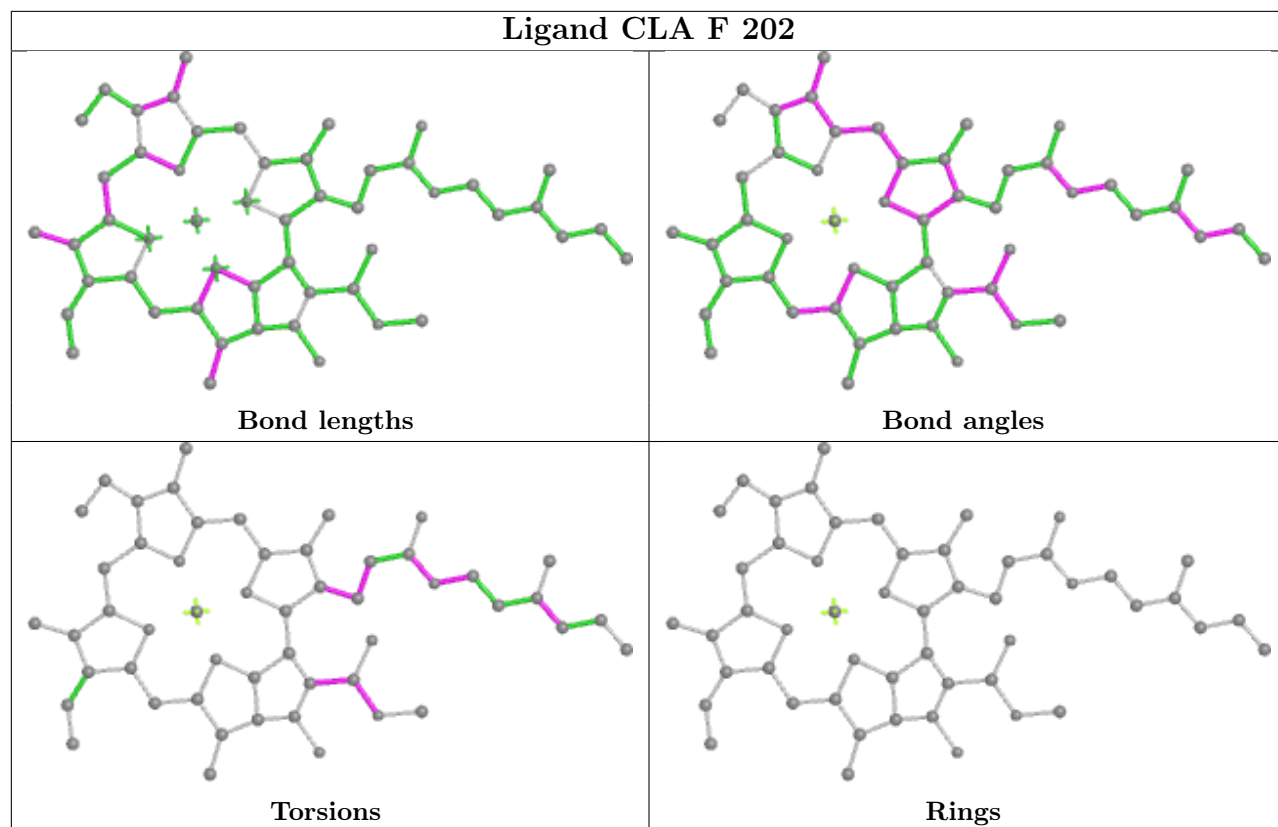
## Ligand CLA a 302



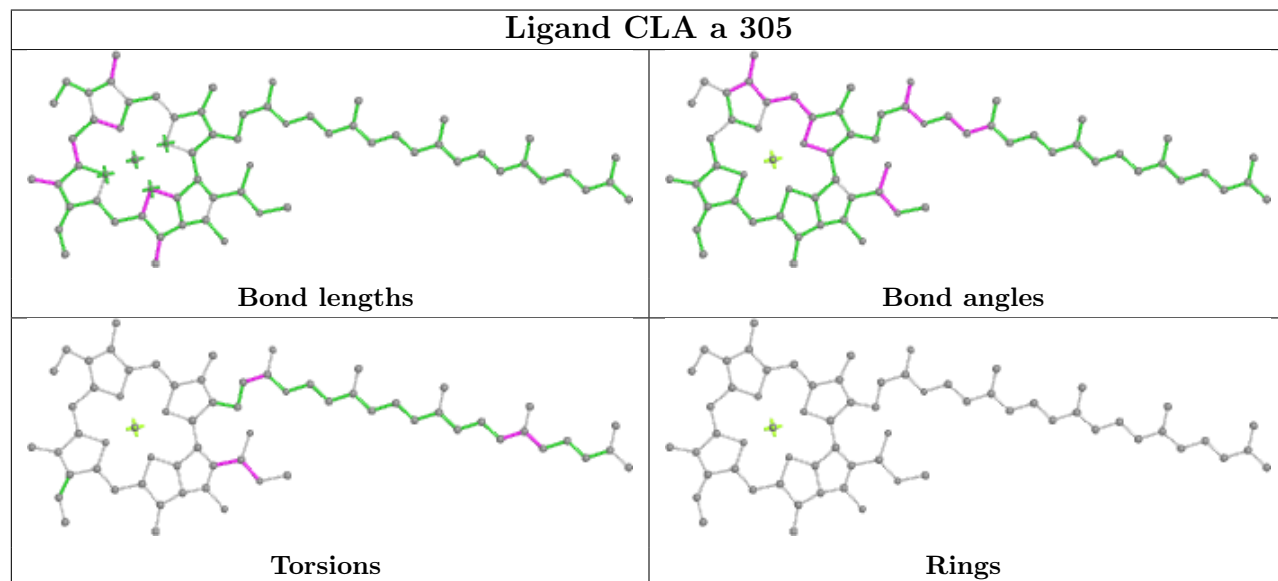
## Ligand CLA K 101



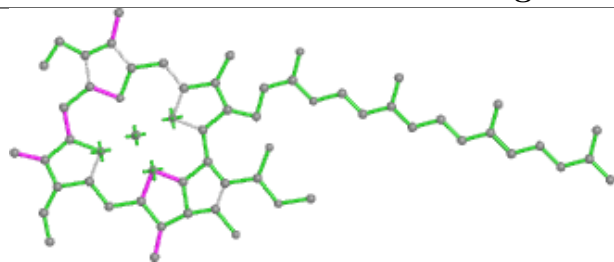
## Ligand CLA F 202



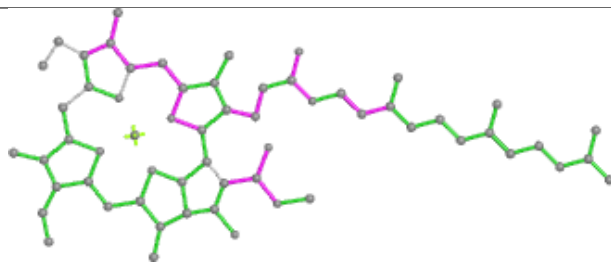
## Ligand CLA a 305



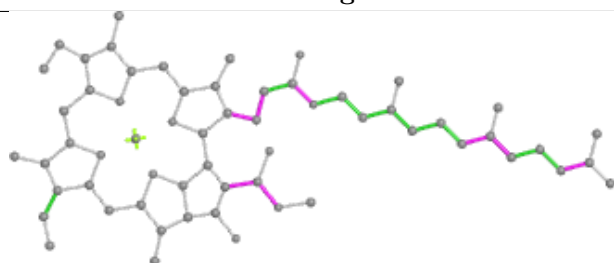
## Ligand CLA B 813



Bond lengths



Bond angles

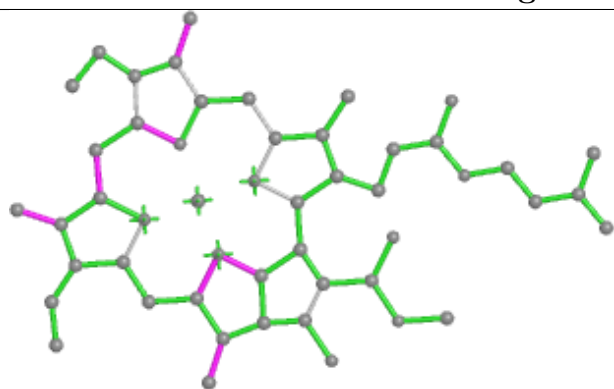


Torsions

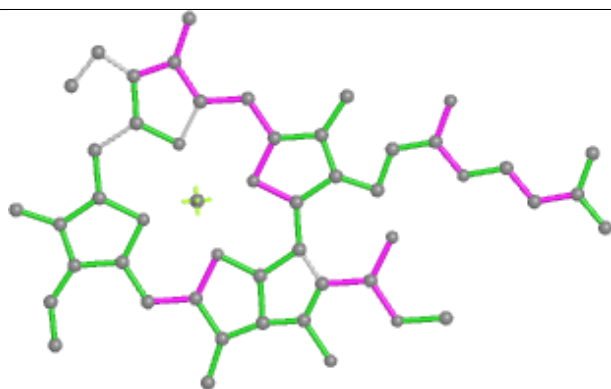


Rings

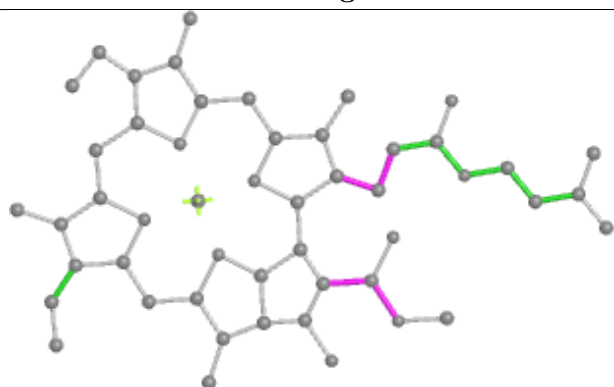
## Ligand CLA a 303



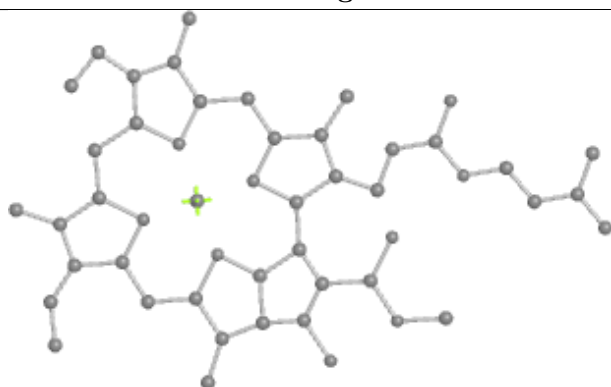
Bond lengths



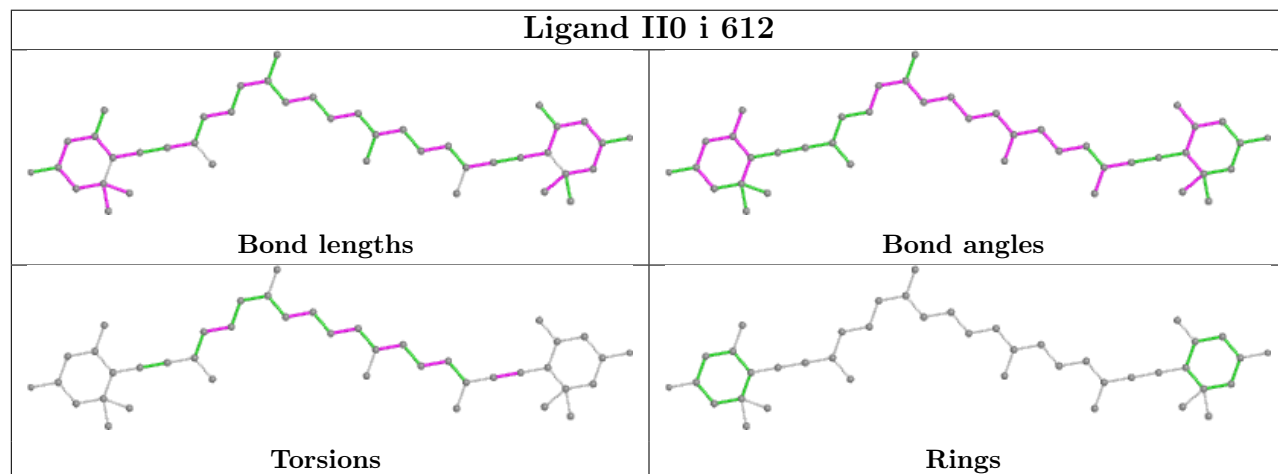
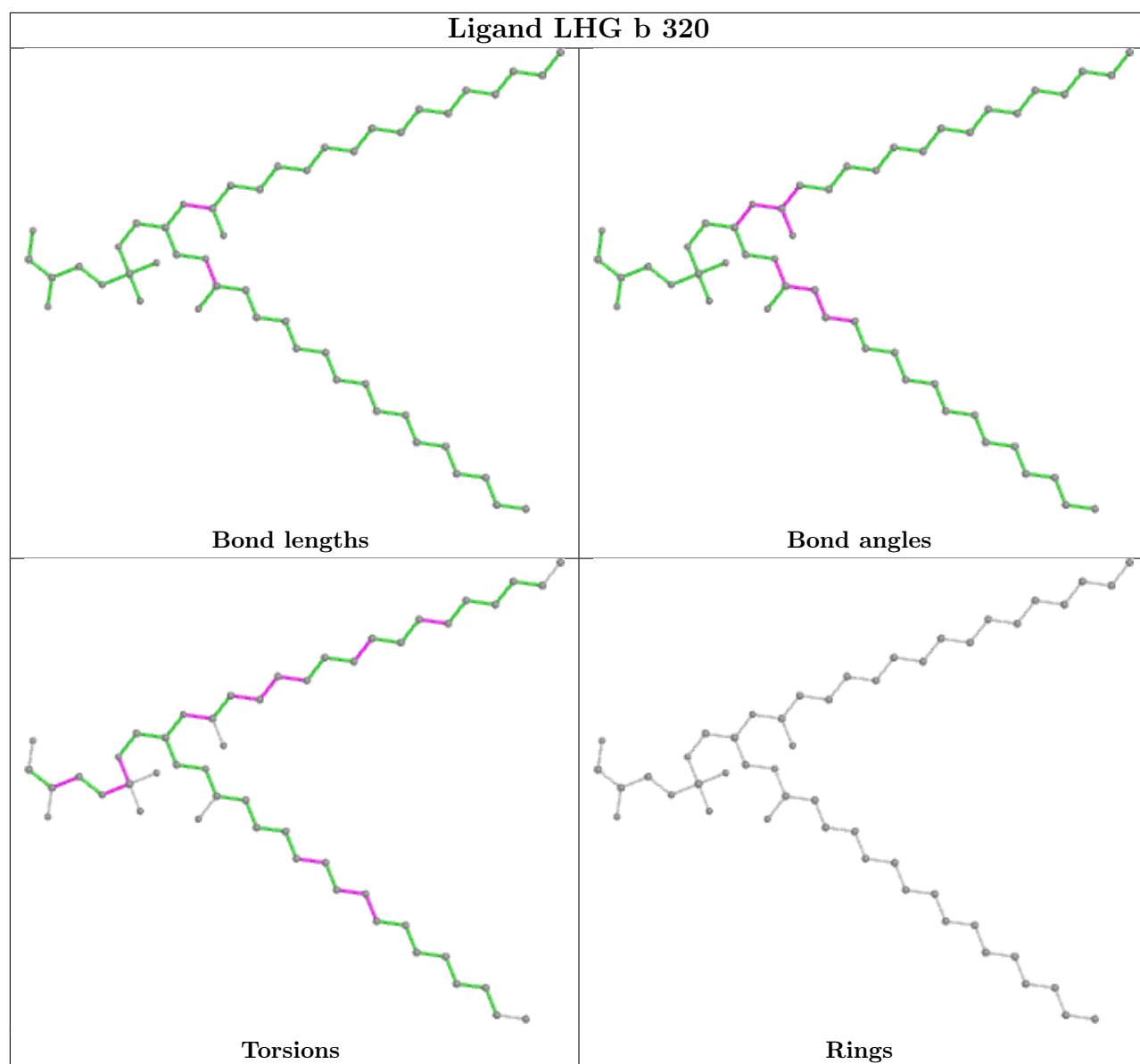
Bond angles

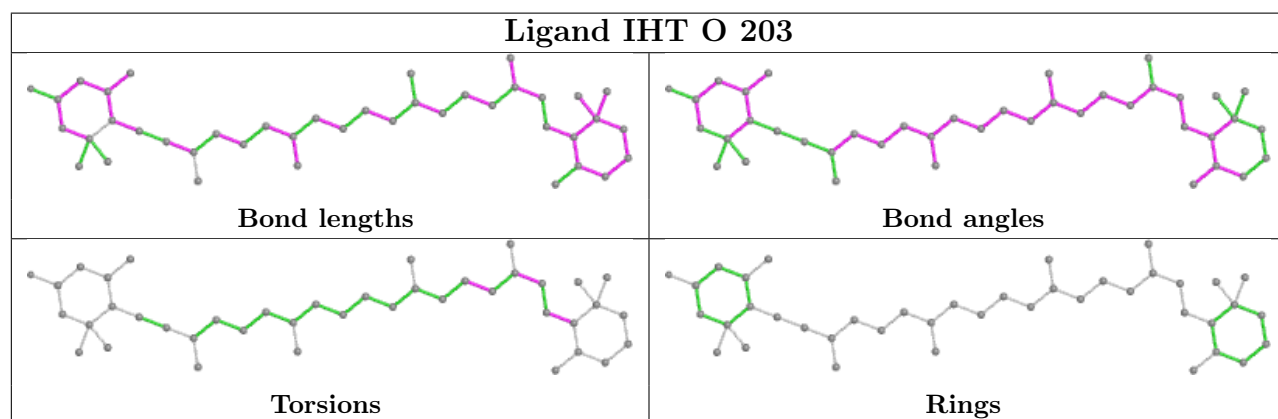
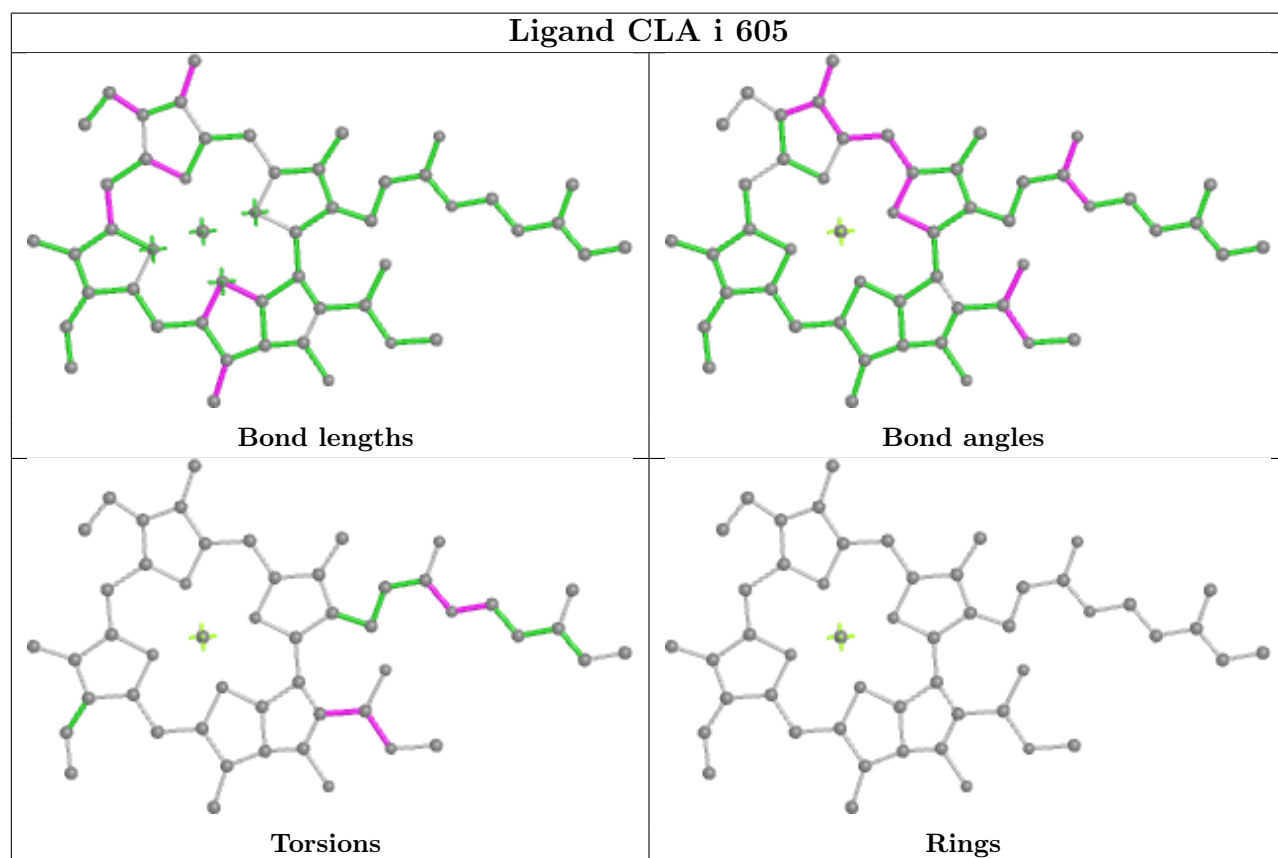
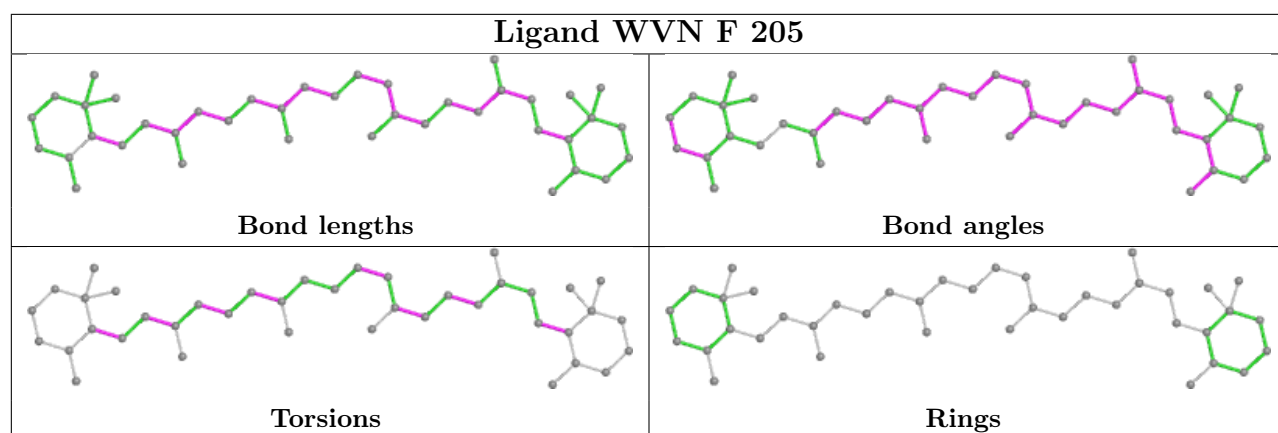


Torsions

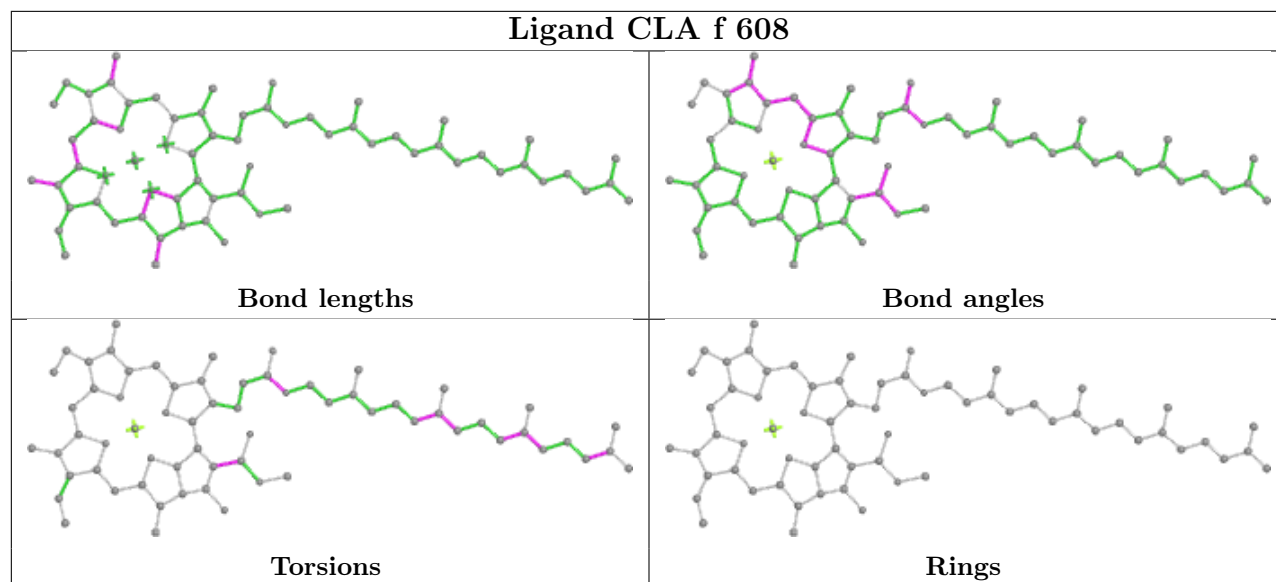


Rings

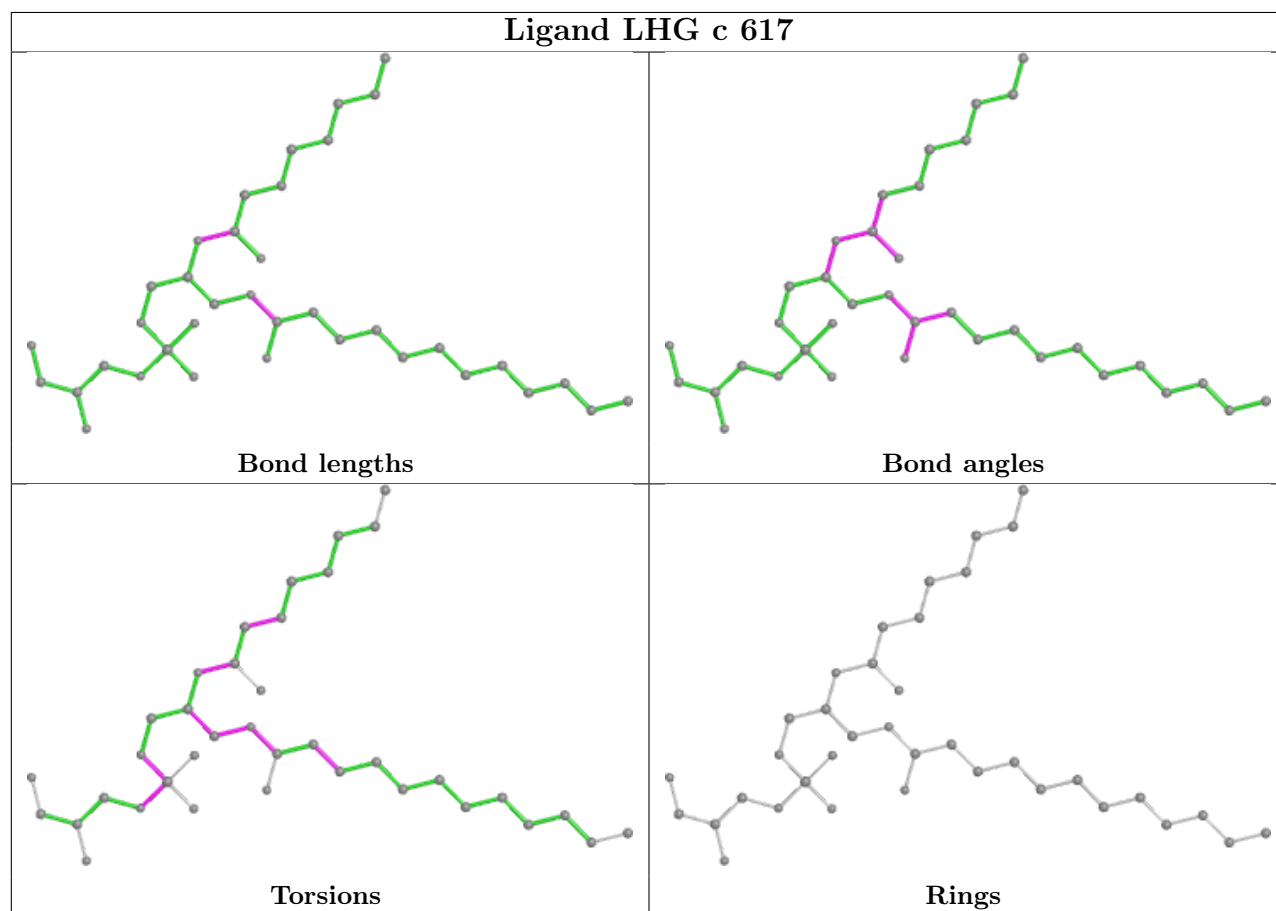




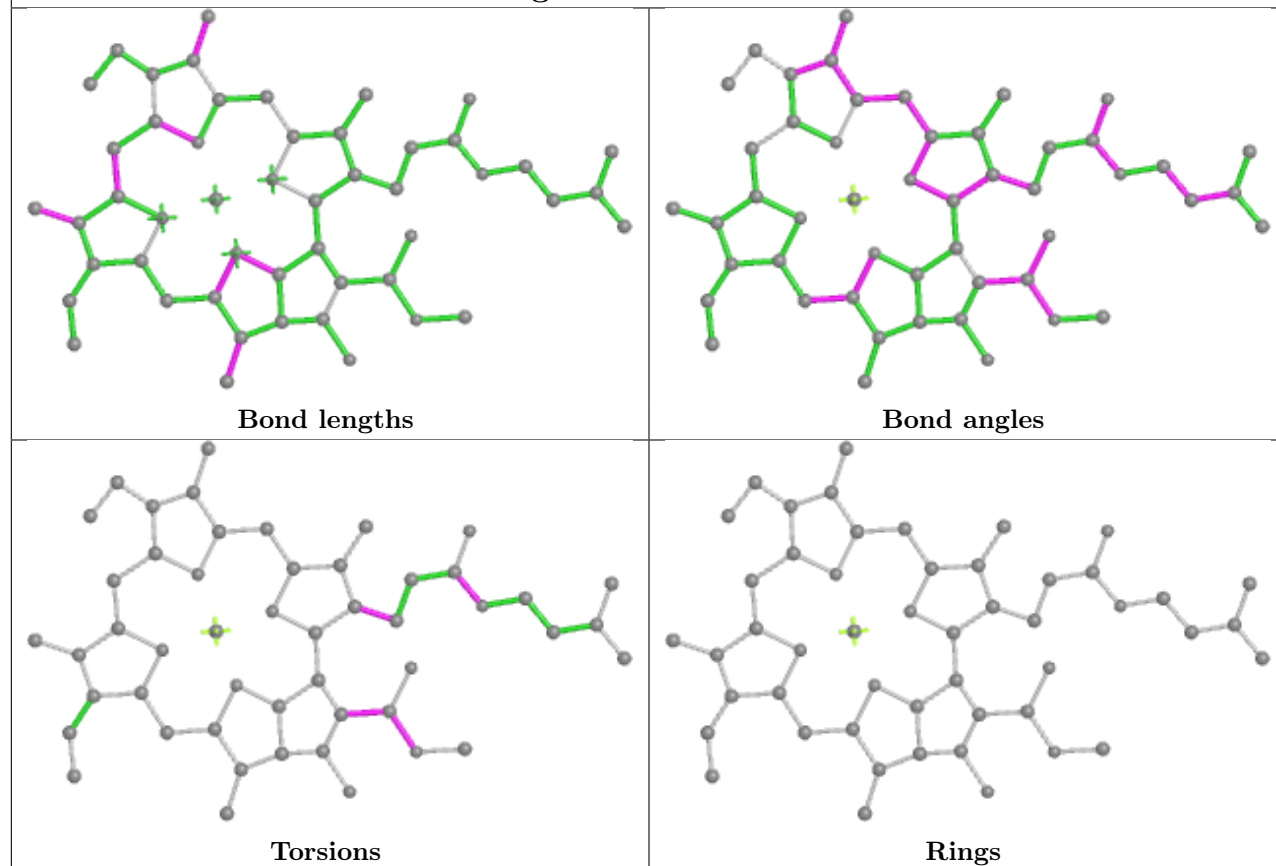
## Ligand CLA f 608



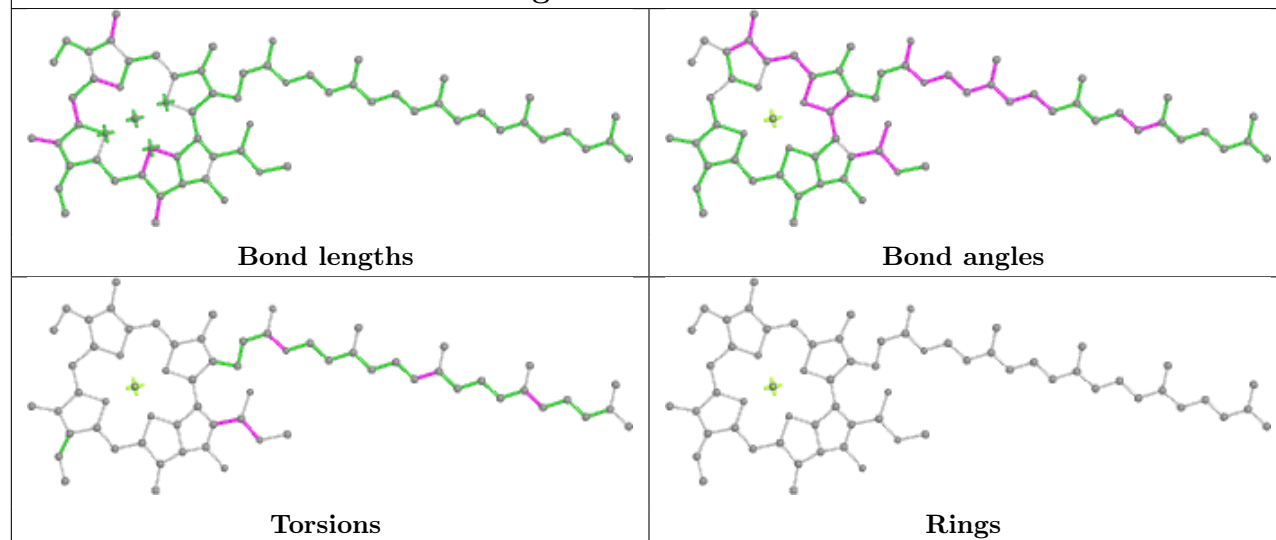
## Ligand LHG c 617



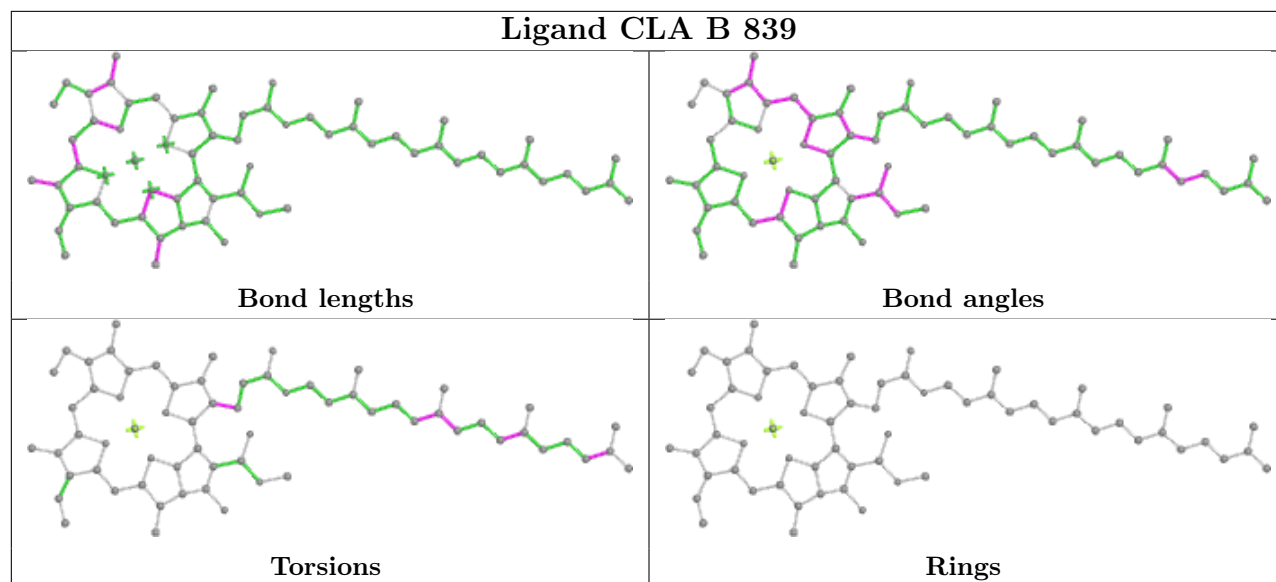
## Ligand CLA A 814



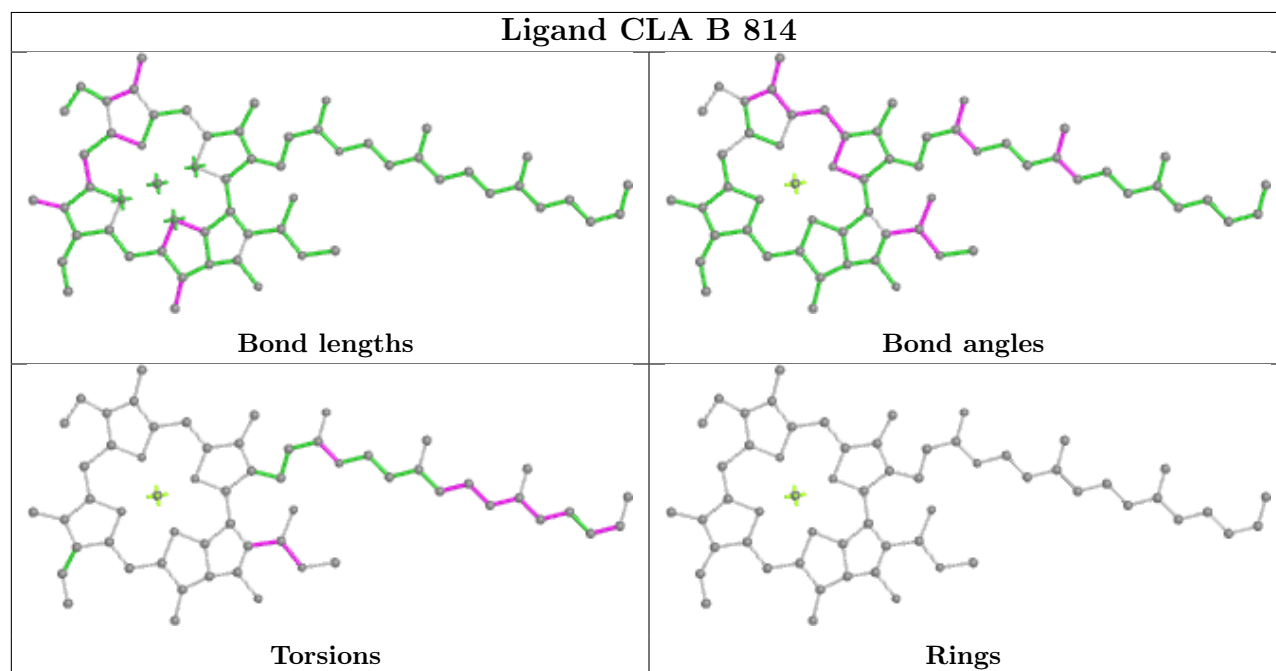
## Ligand CLA B 822



## Ligand CLA B 839

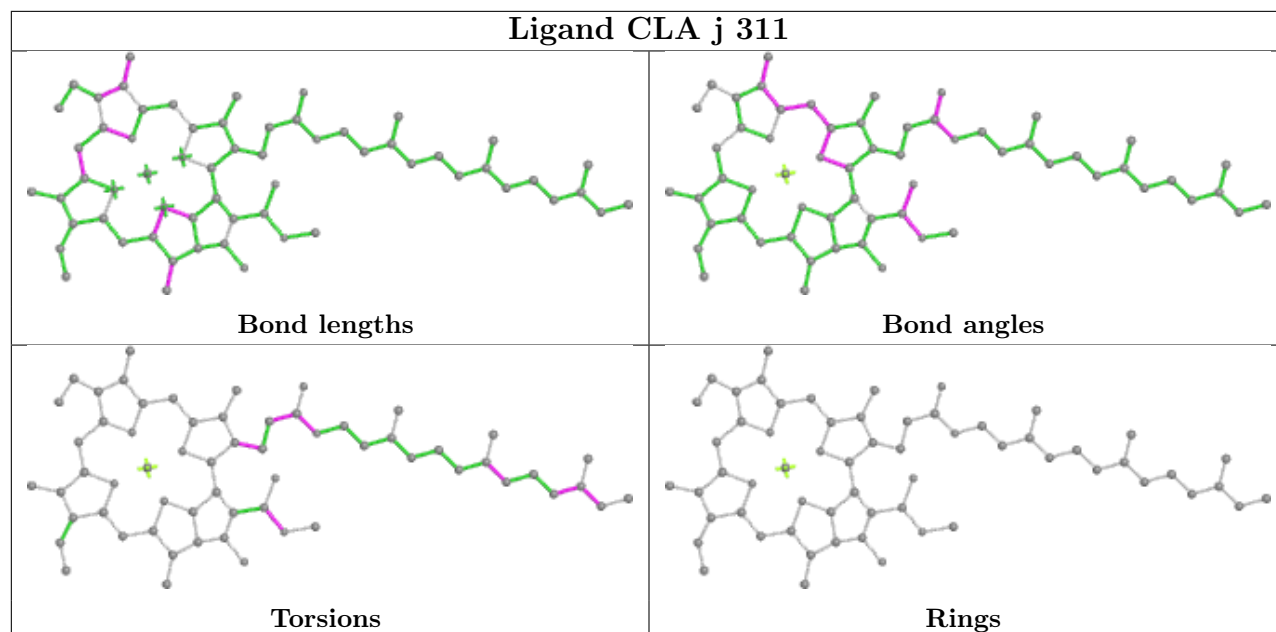


## Ligand CLA B 814

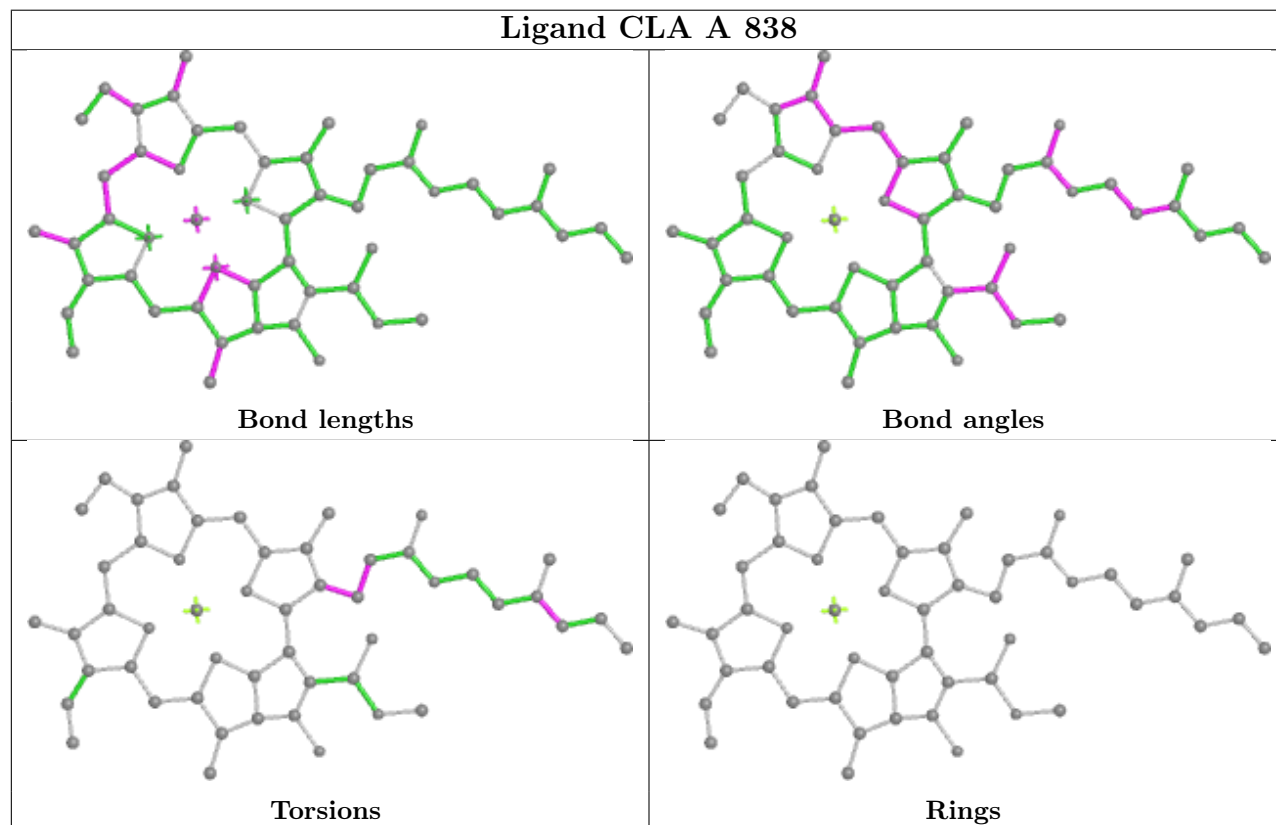




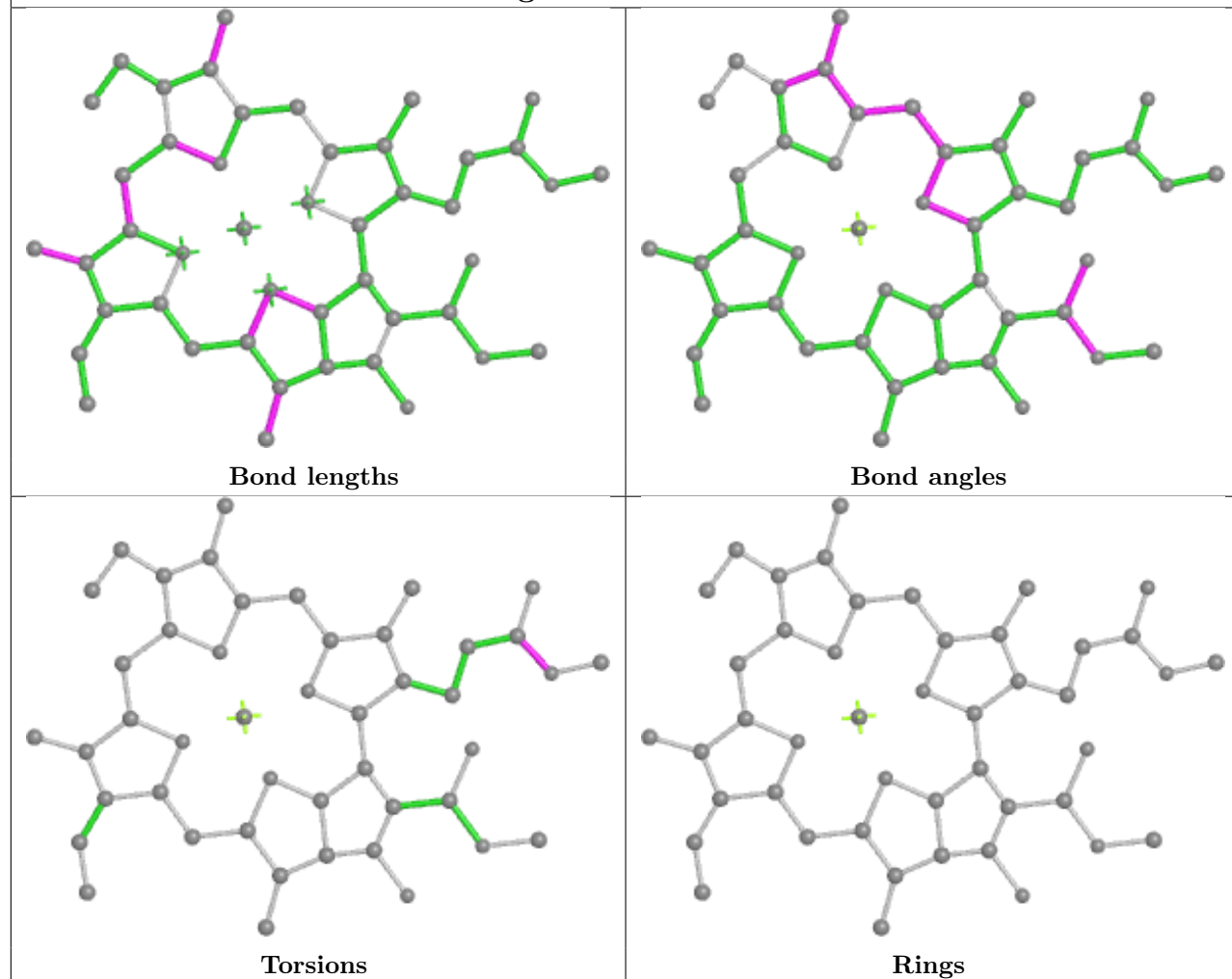
## Ligand CLA j 311



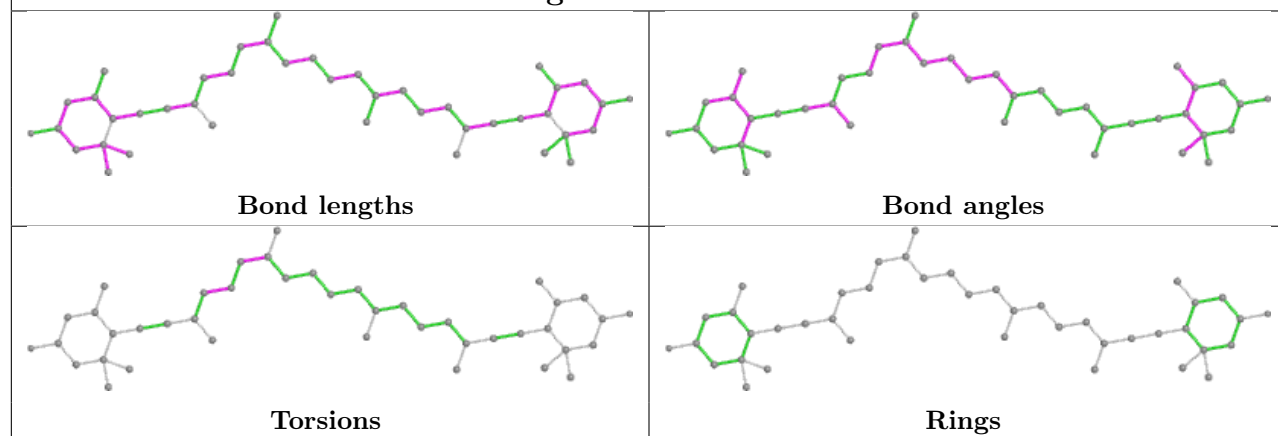
## Ligand CLA A 838



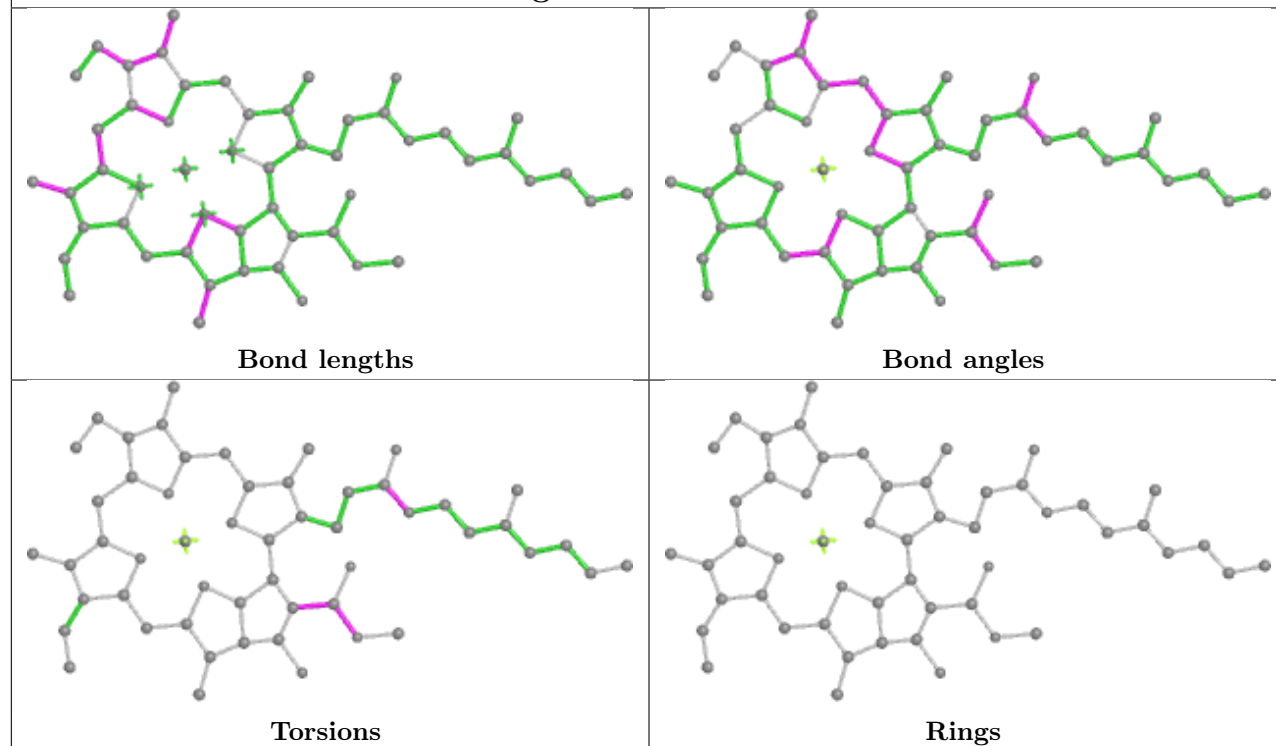
## Ligand CLA c 607



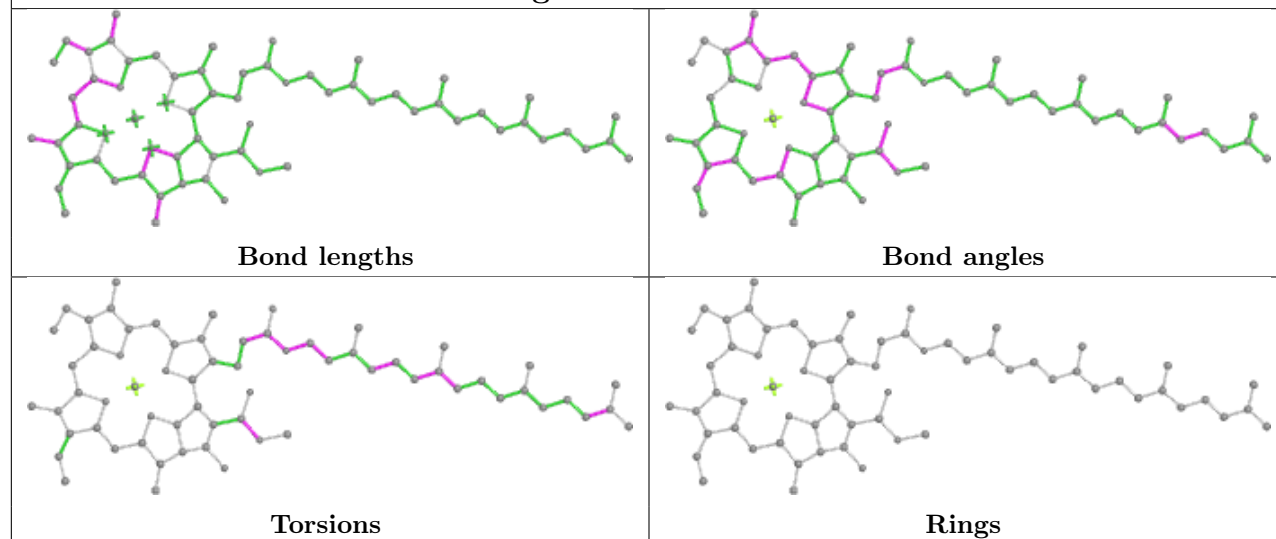
## Ligand II0 O 202

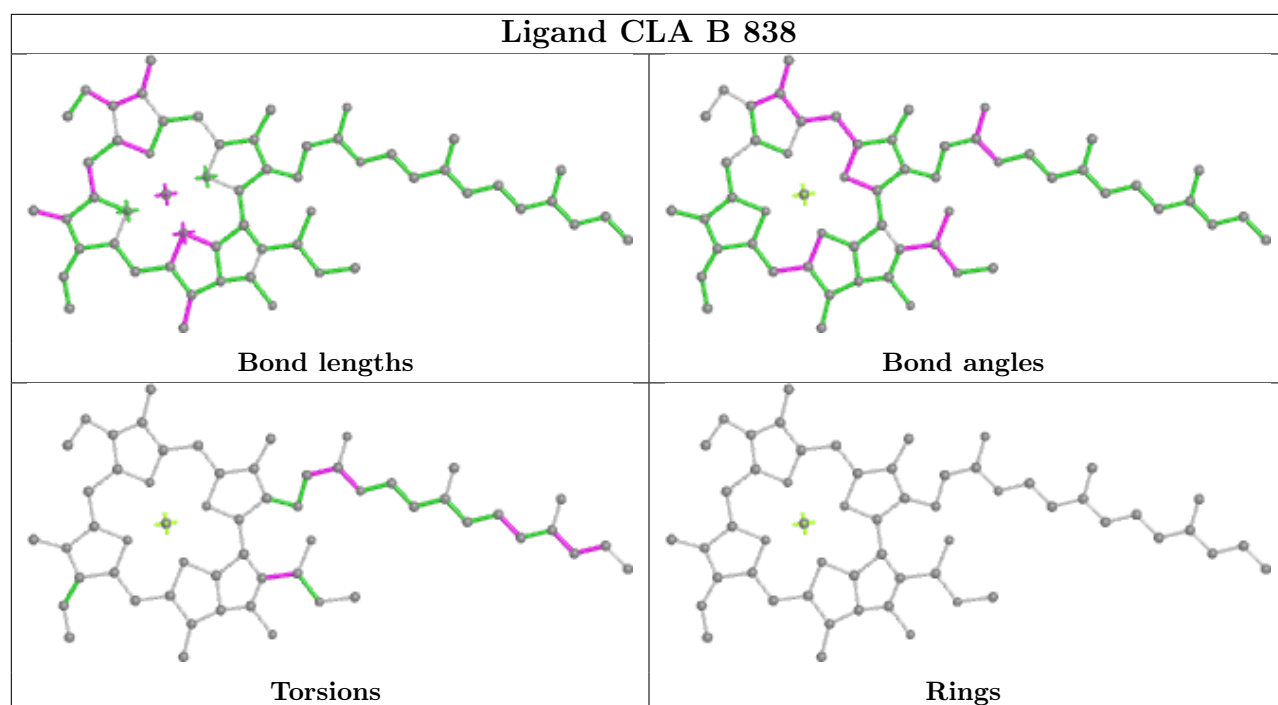


## Ligand CLA B 821

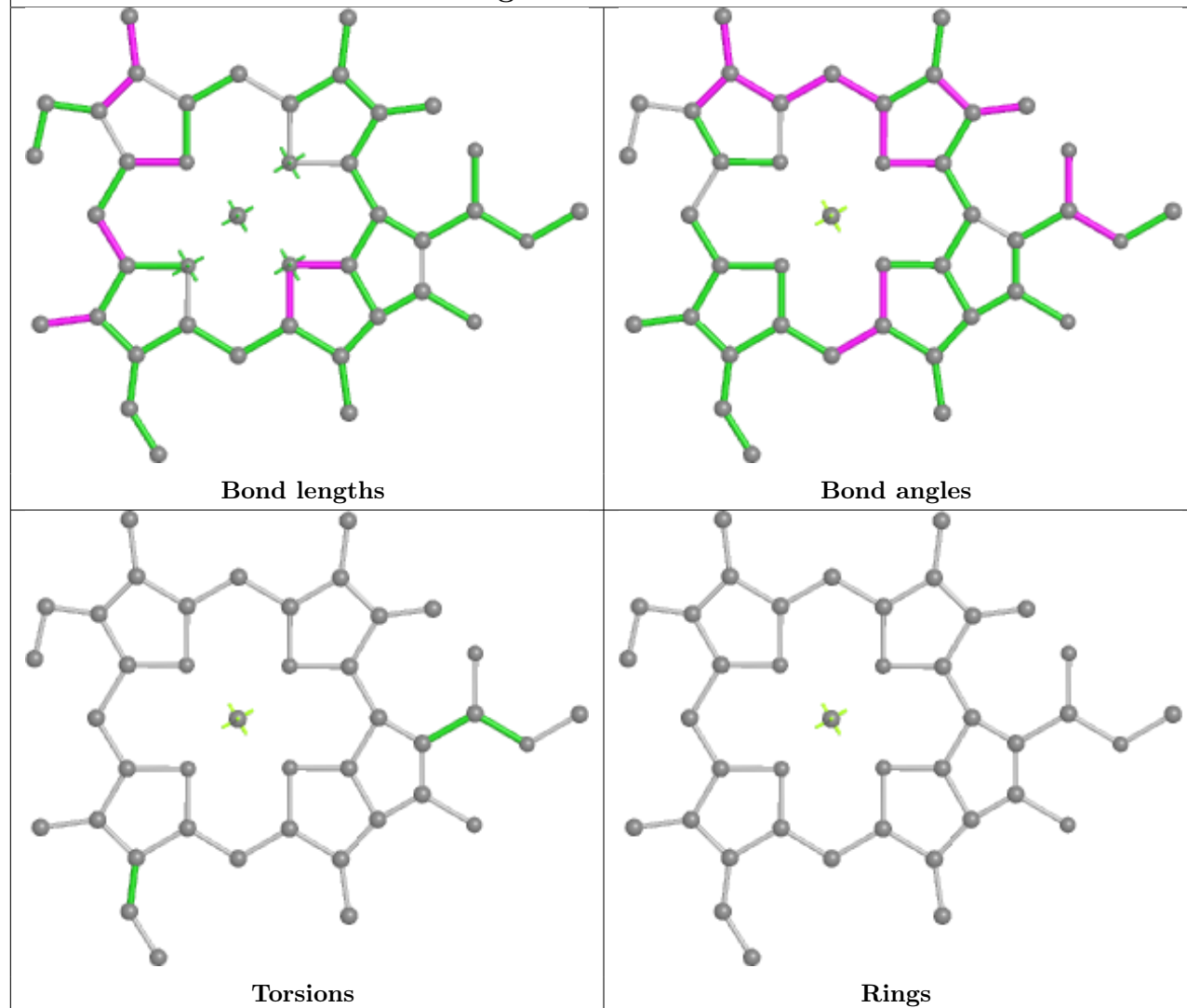


## Ligand CLA B 830

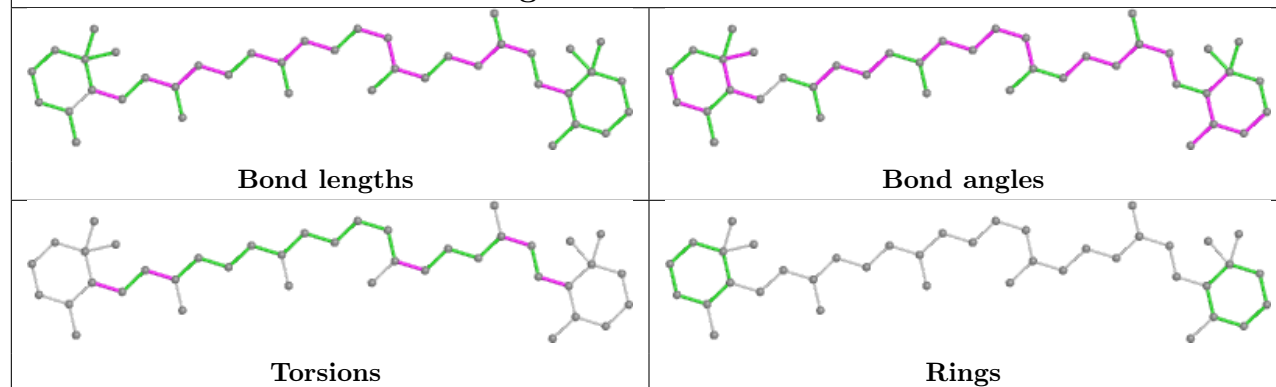


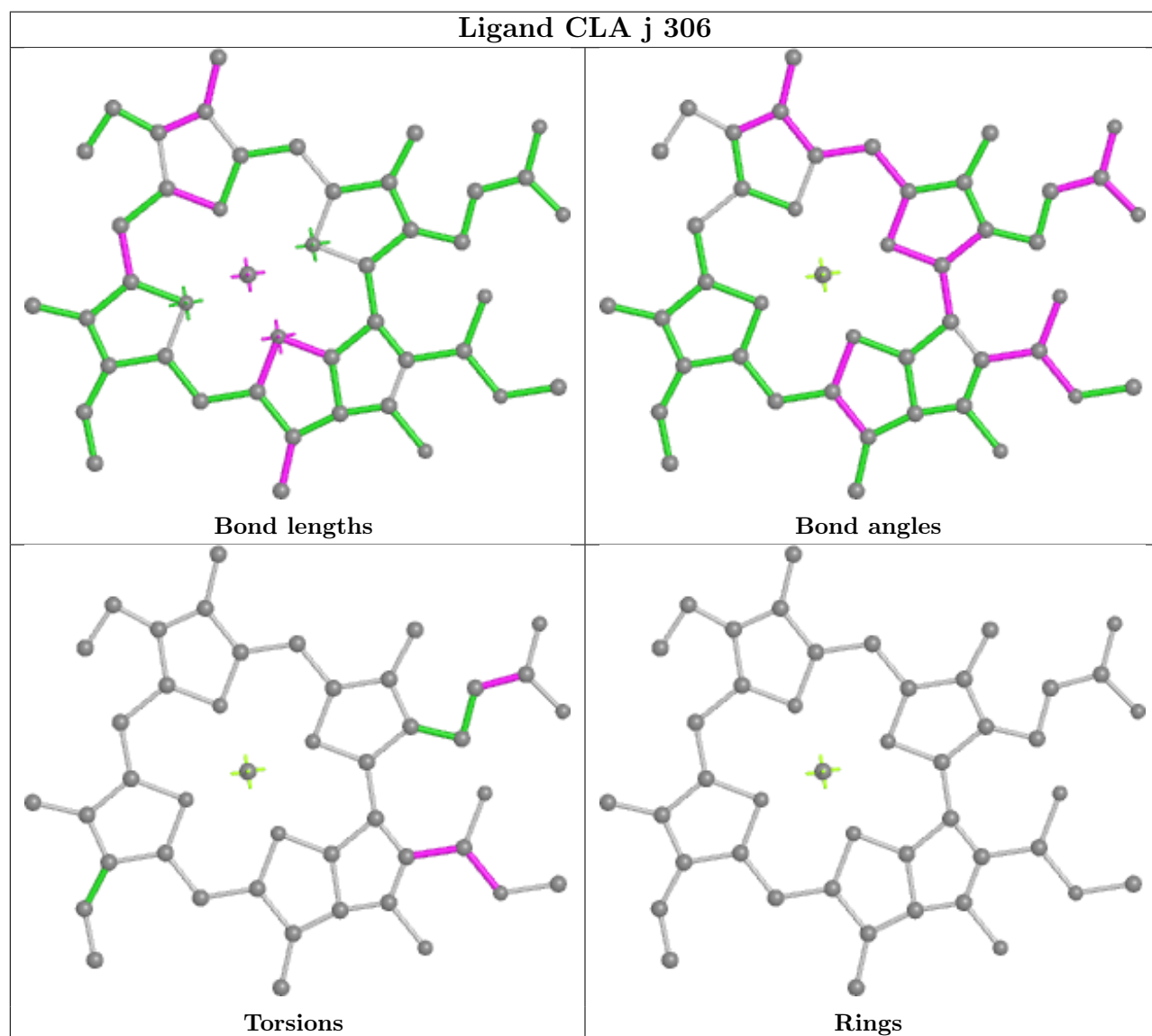
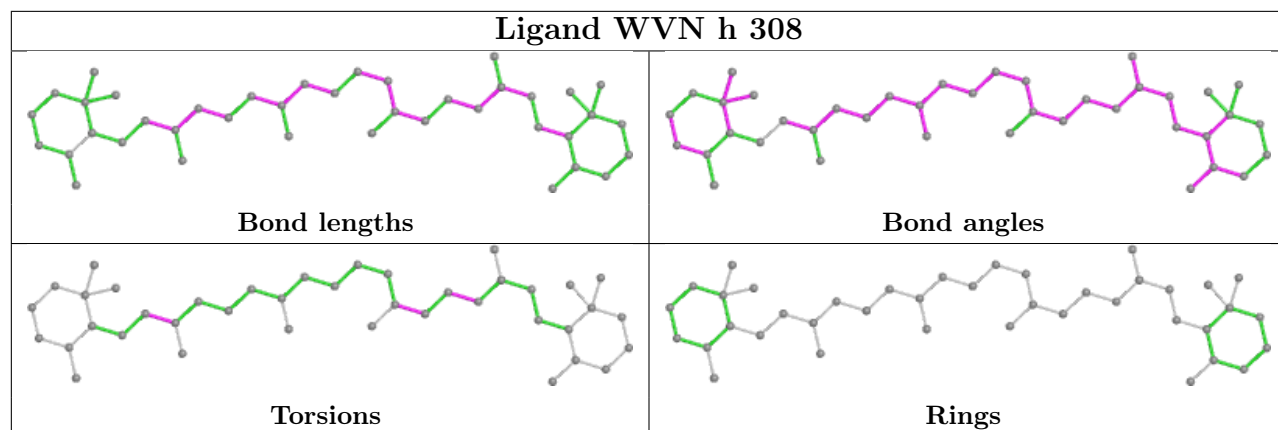


## Ligand CLA d 309

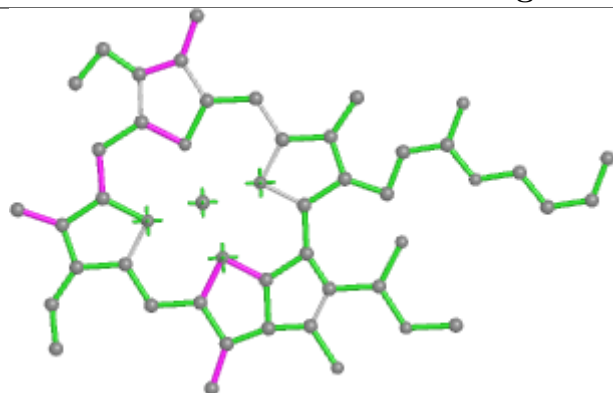


## Ligand WVN M 101

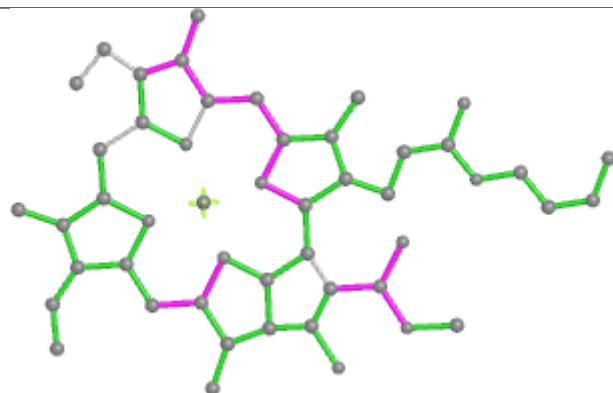




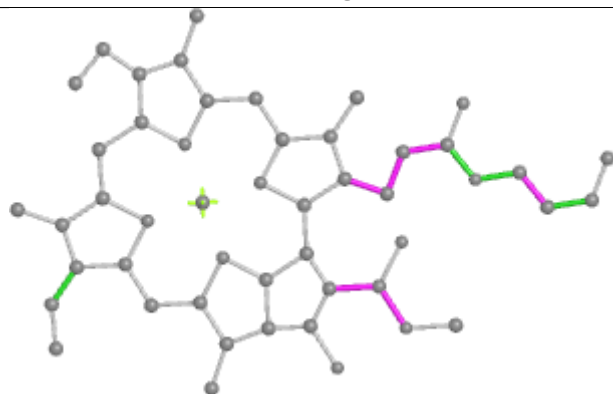
## Ligand CLA L 202



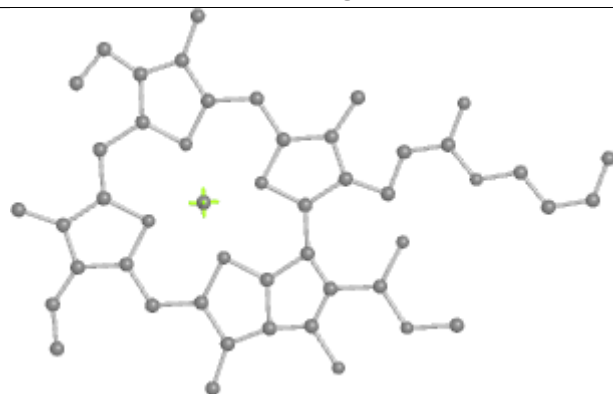
Bond lengths



Bond angles

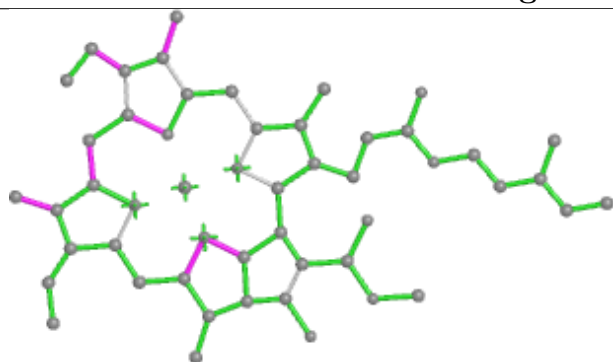


Torsions

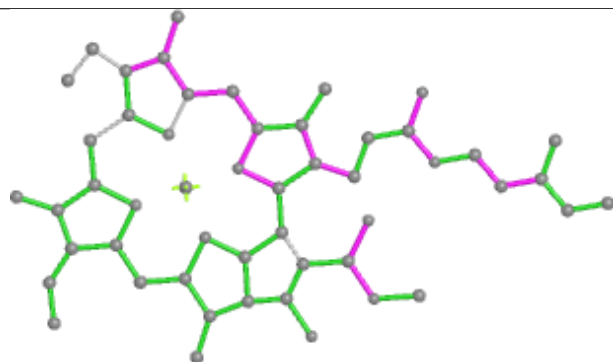


Rings

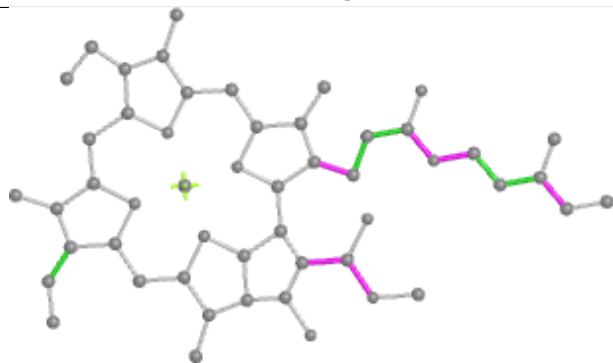
## Ligand CLA c 601



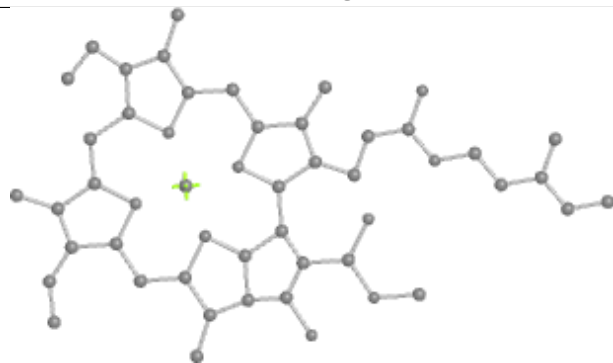
Bond lengths



Bond angles

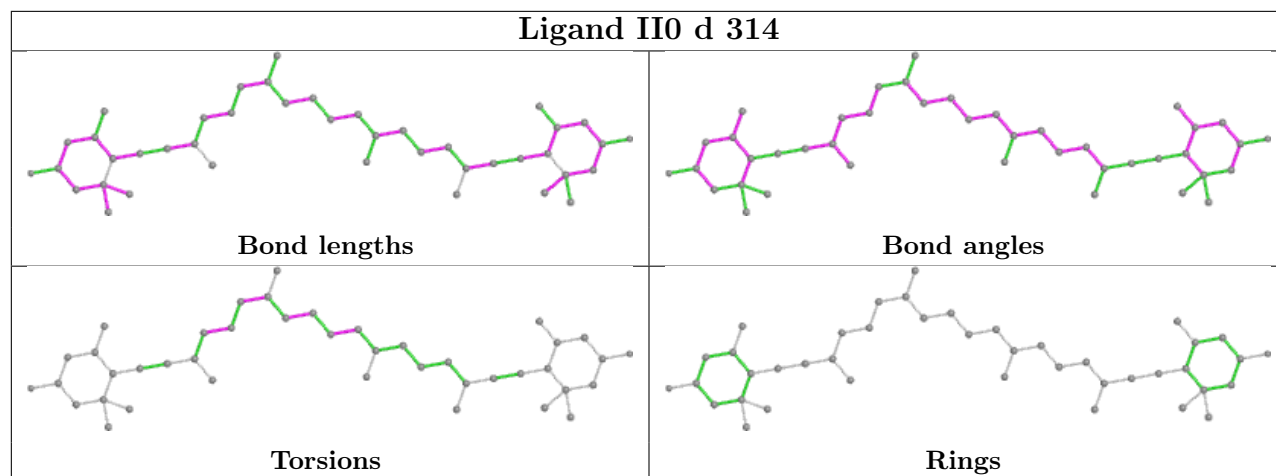


Torsions

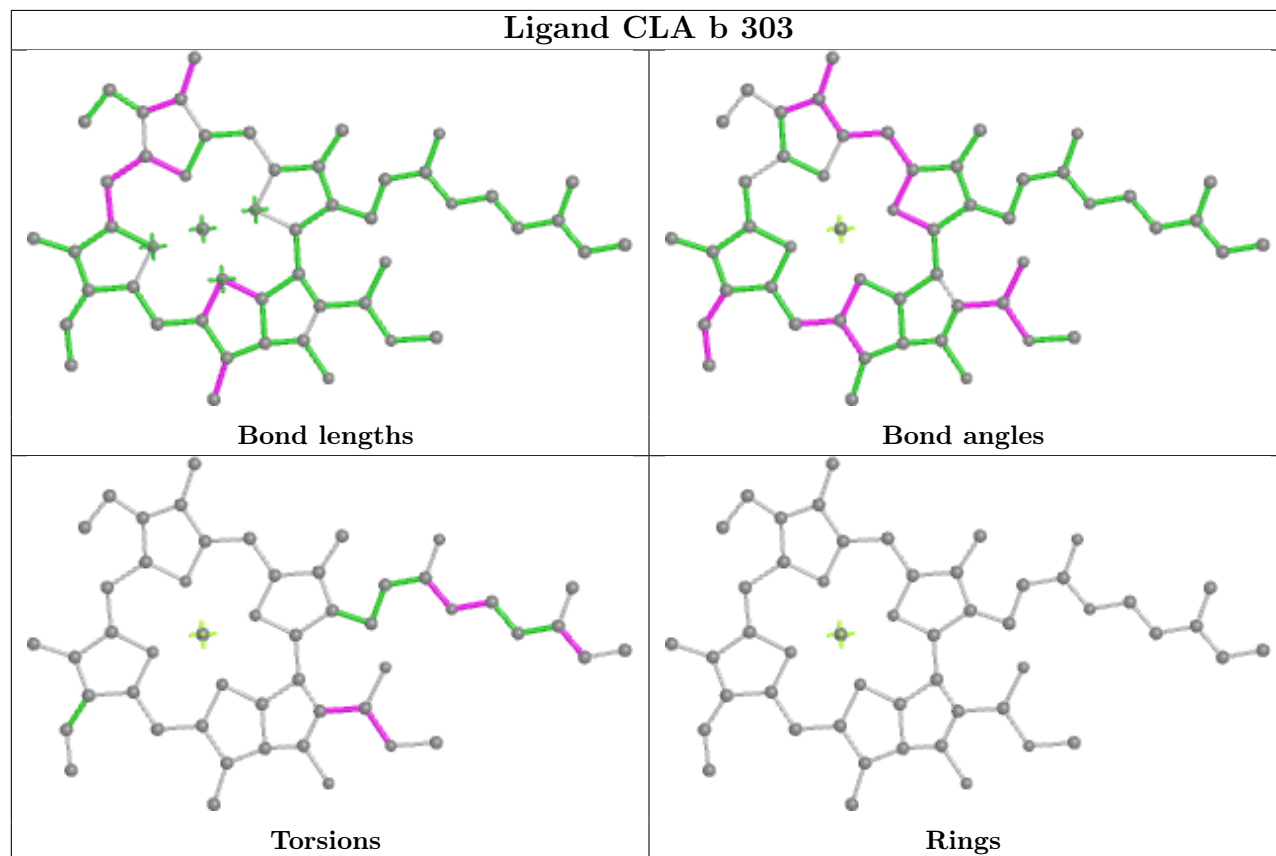


Rings

## Ligand II0 d 314

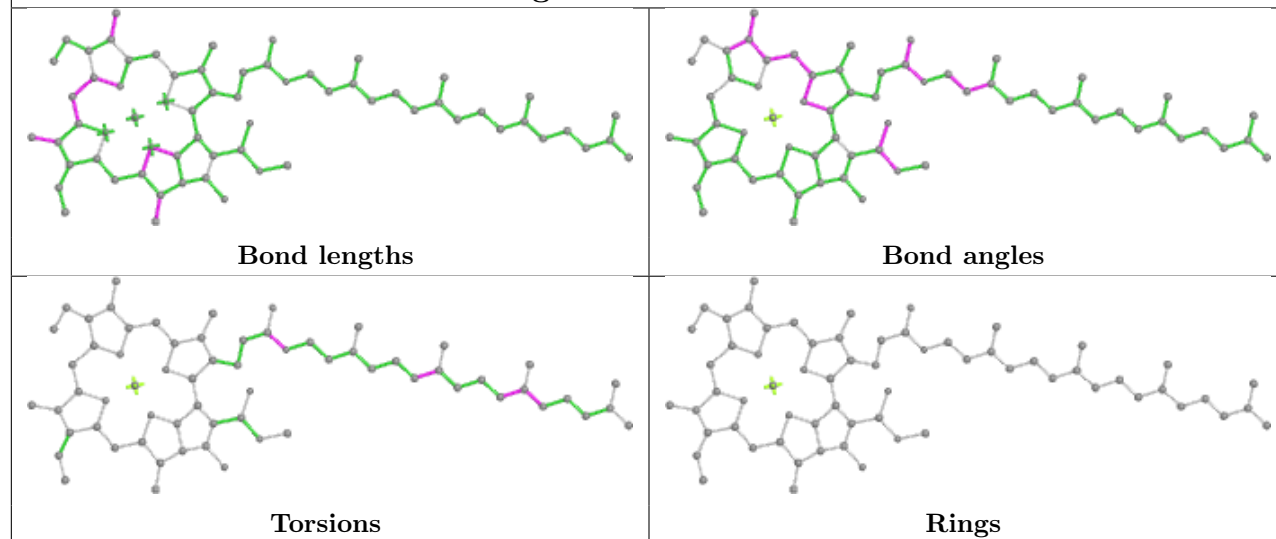


## Ligand CLA b 303

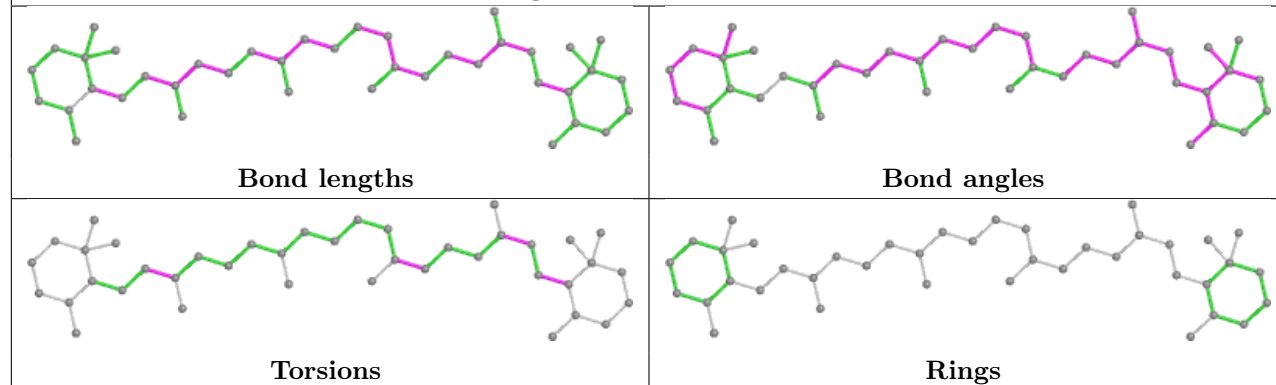




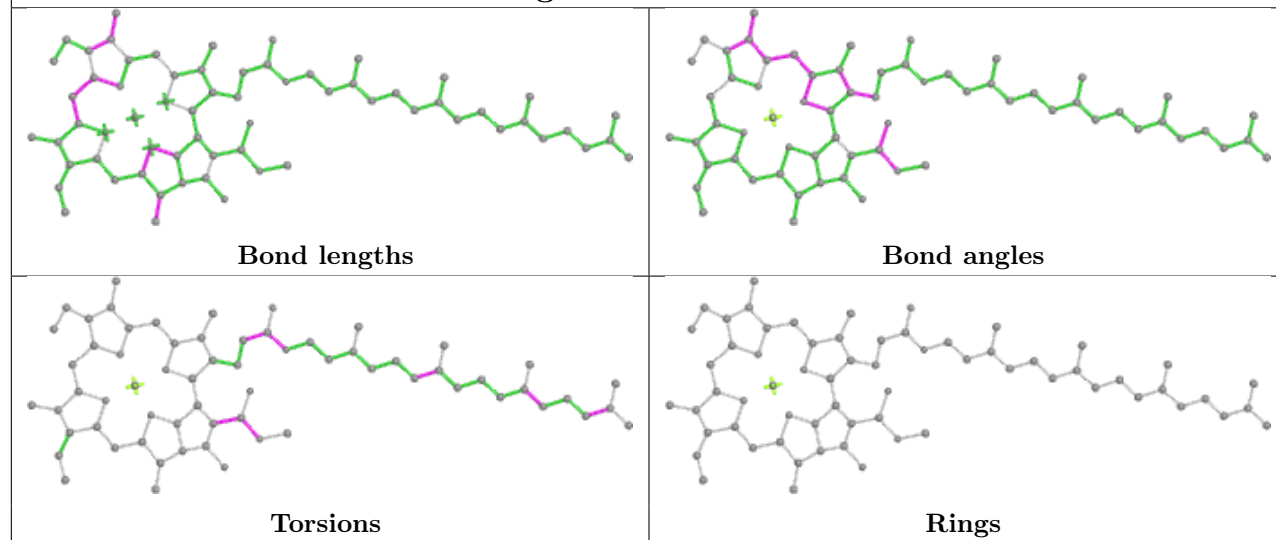
## Ligand CLA B 818

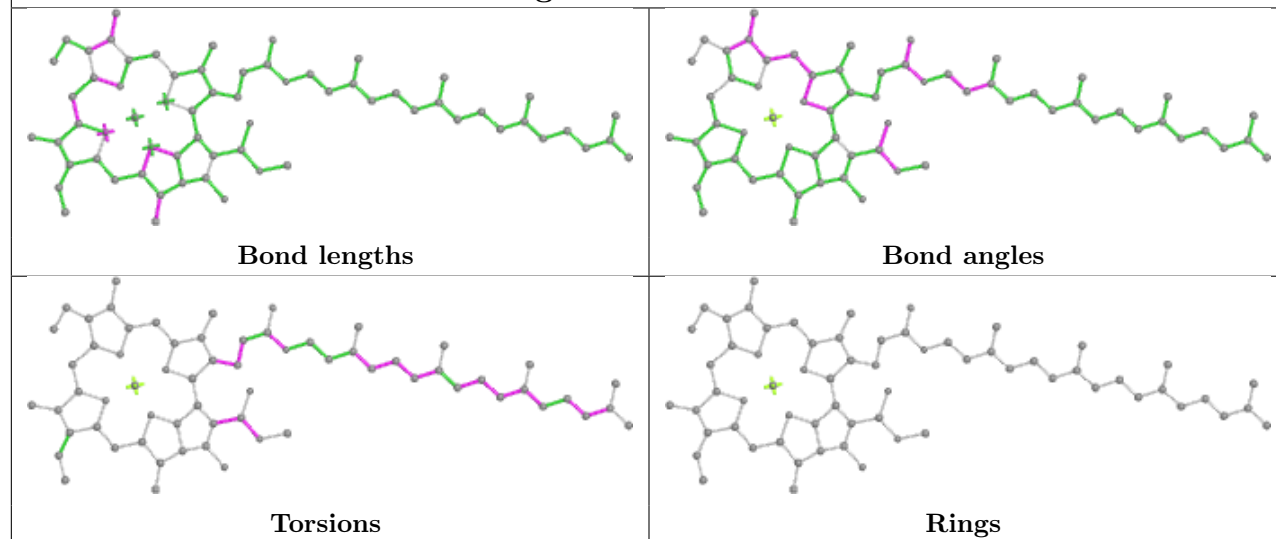
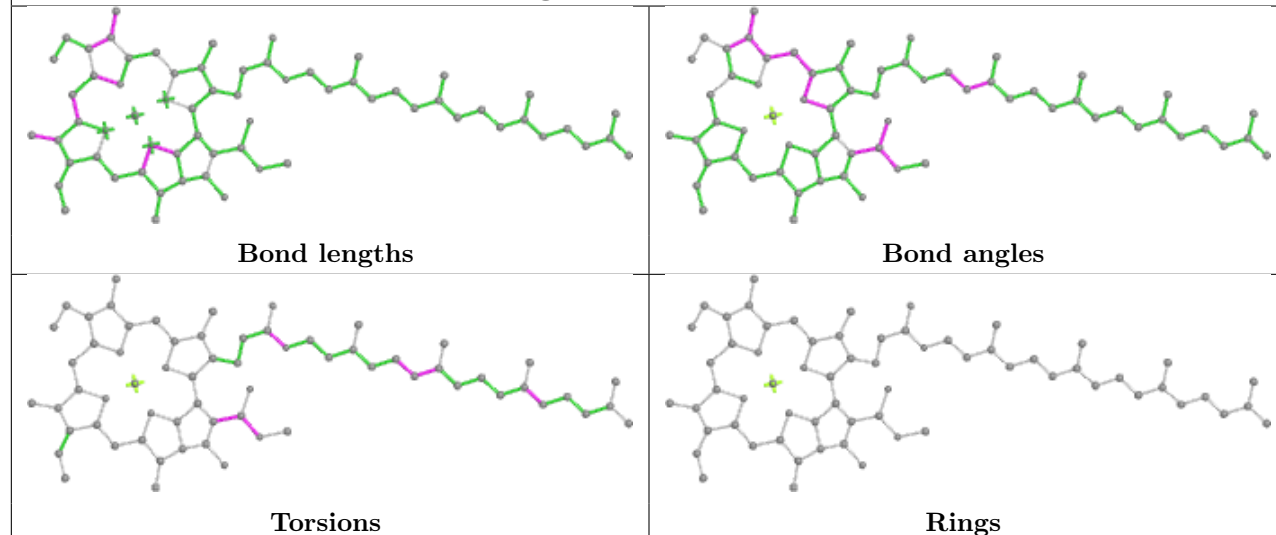
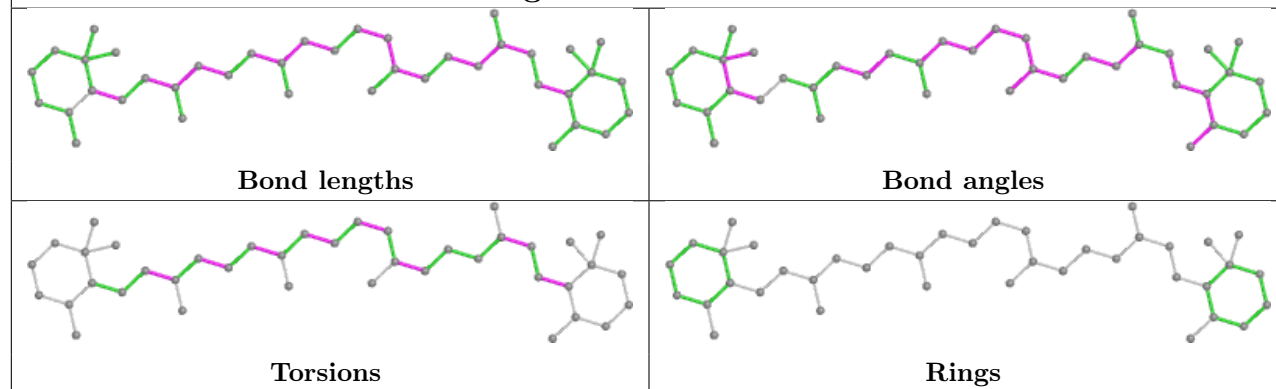


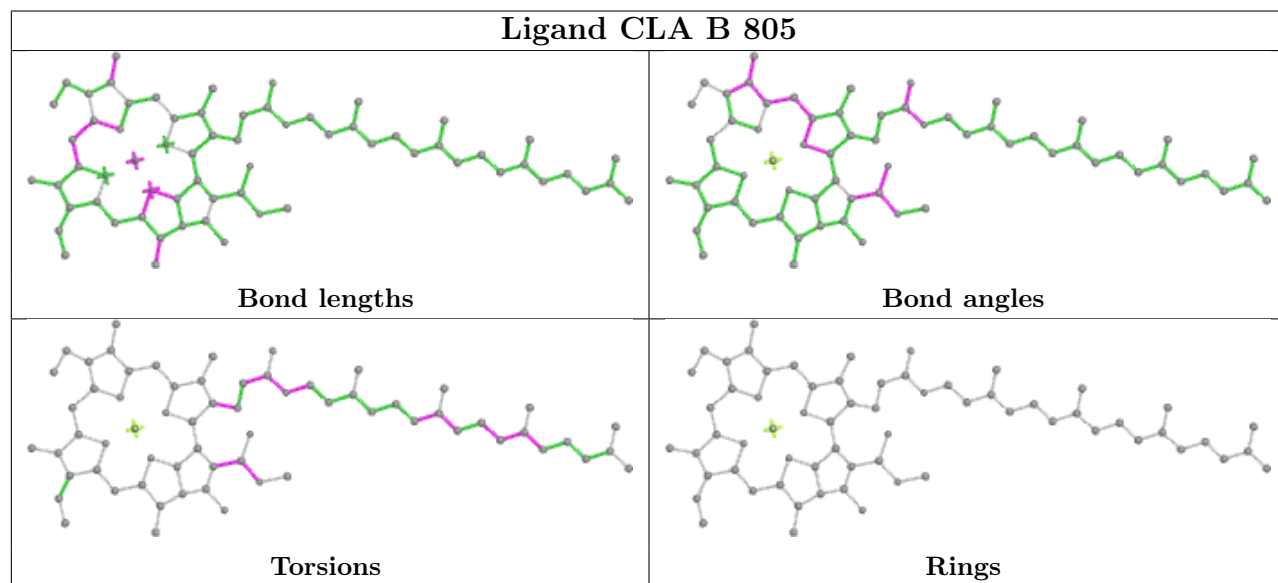
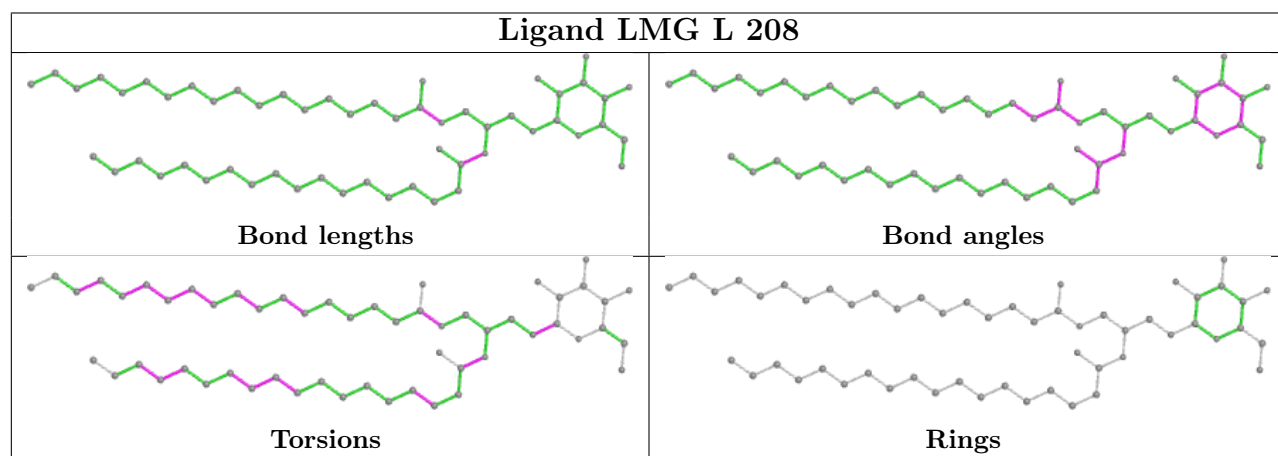
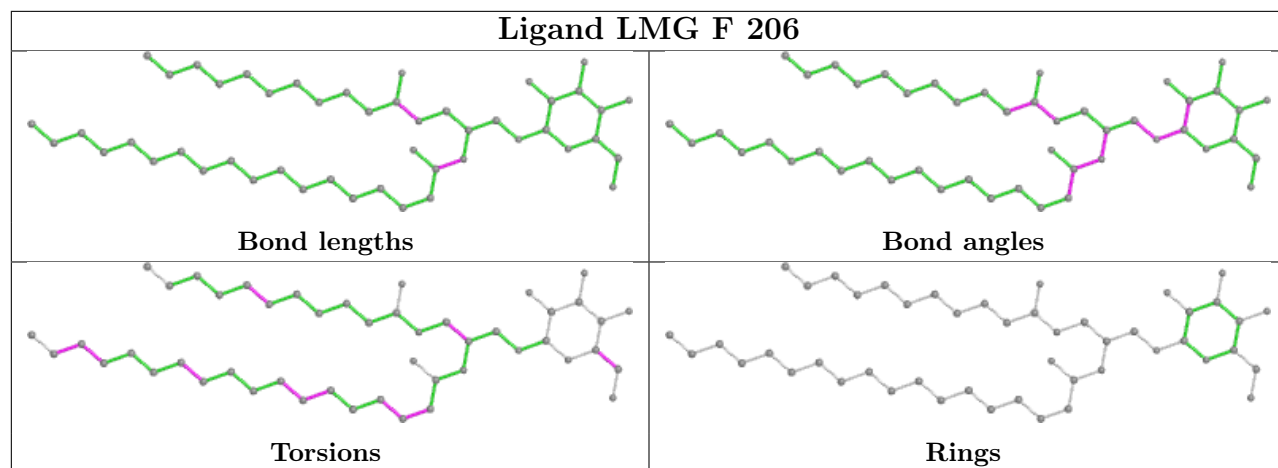
## Ligand WVN J 102

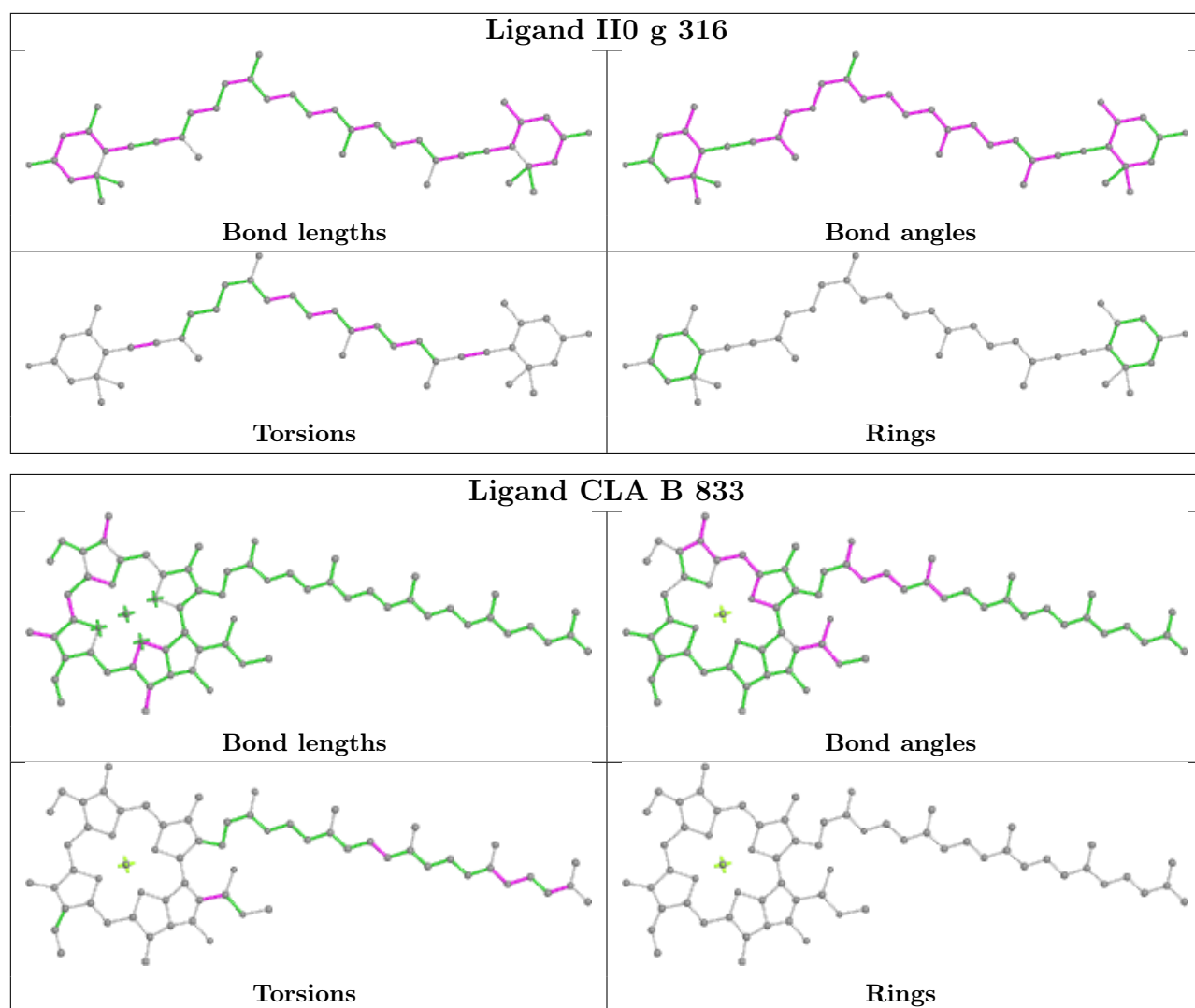


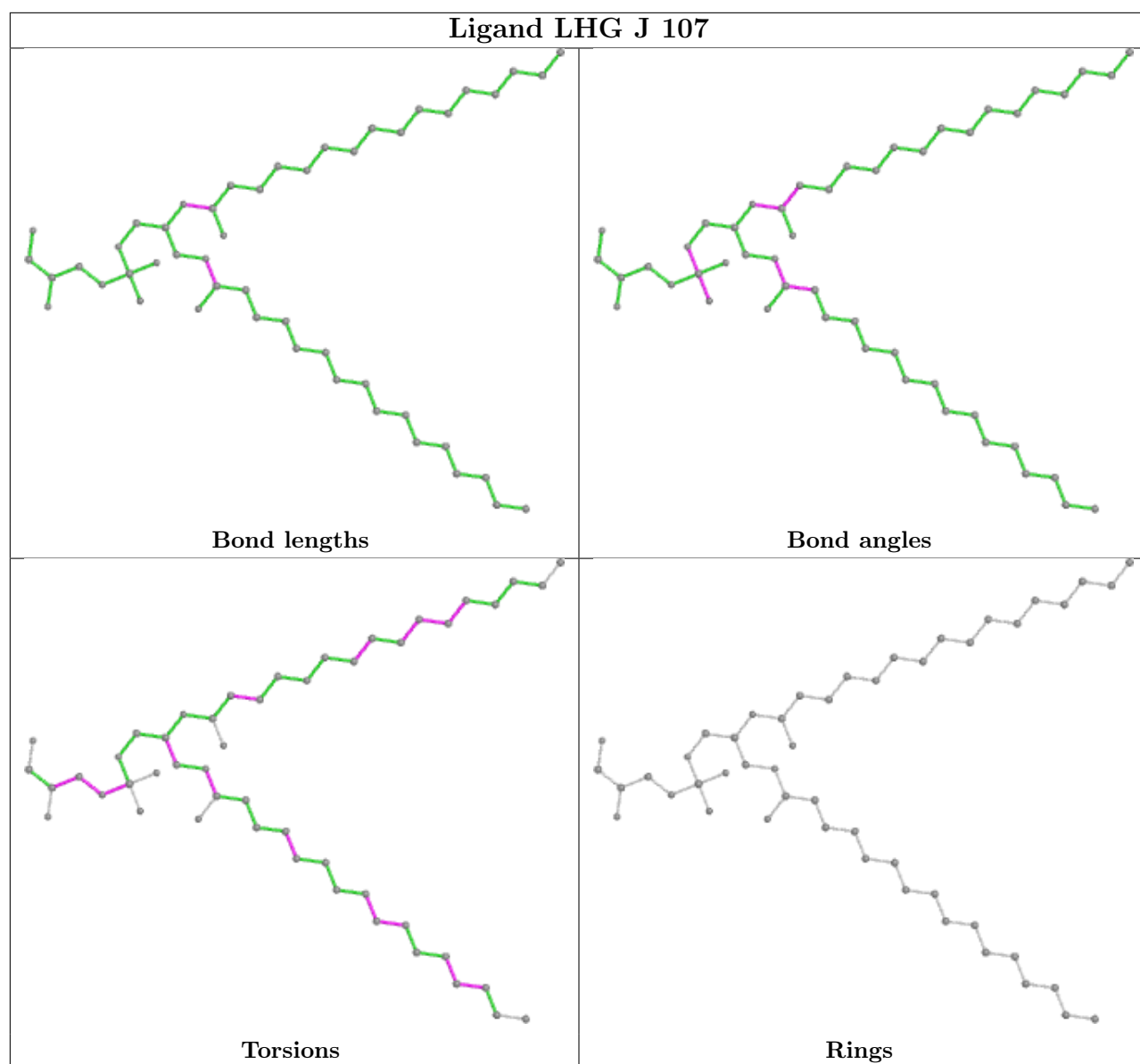
## Ligand CLA a 310



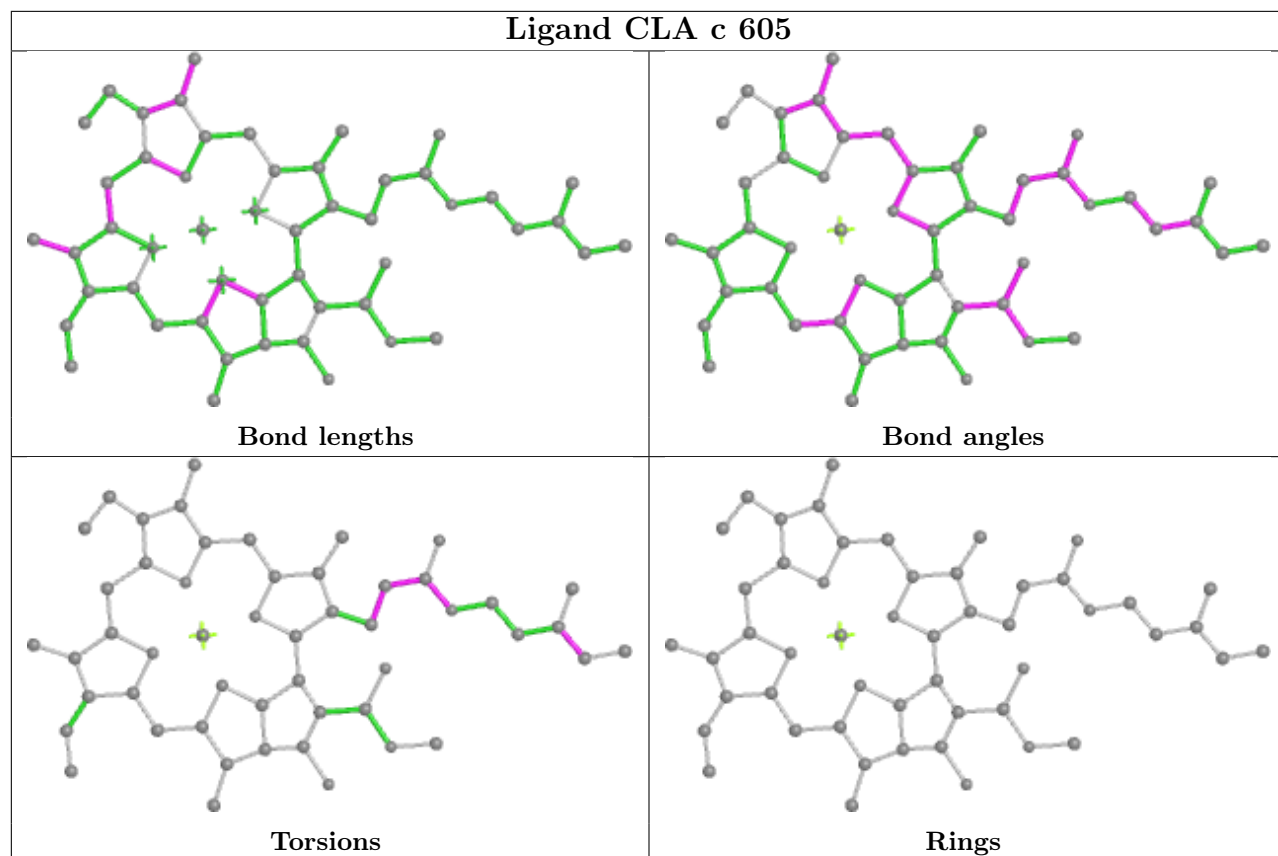
**Ligand CLA b 313****Ligand CLA e 607****Ligand WVN B 849**



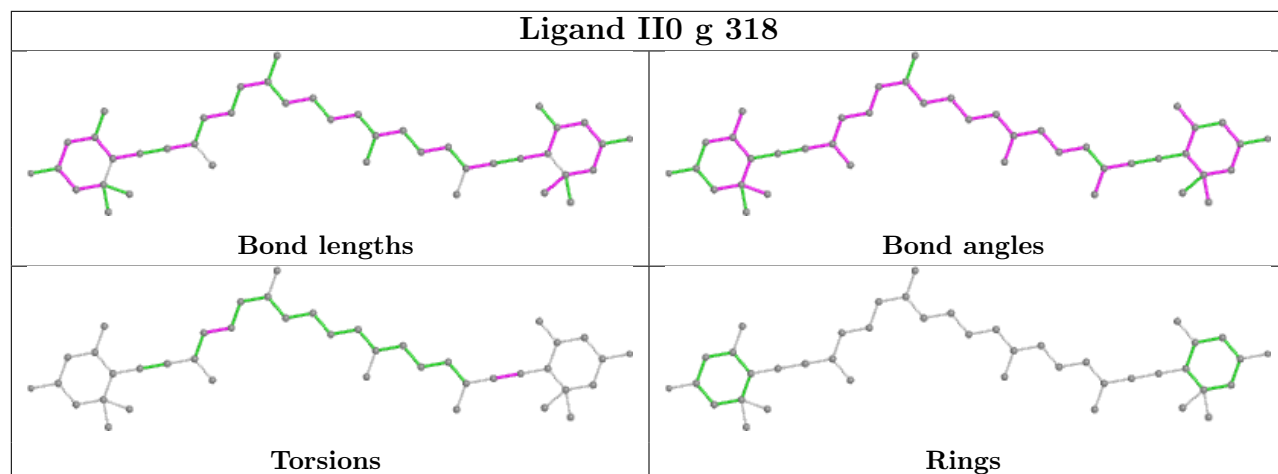


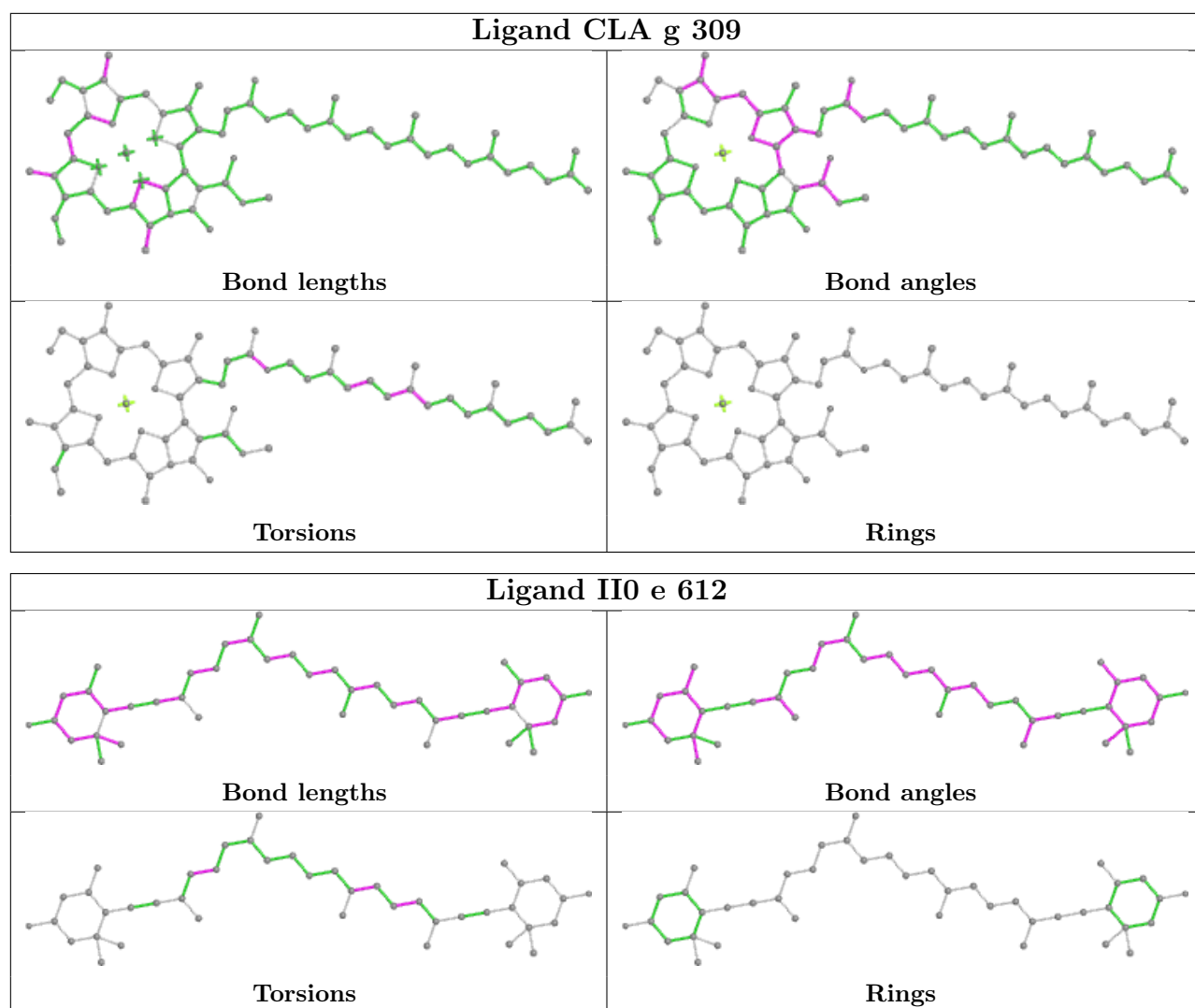


## Ligand CLA c 605

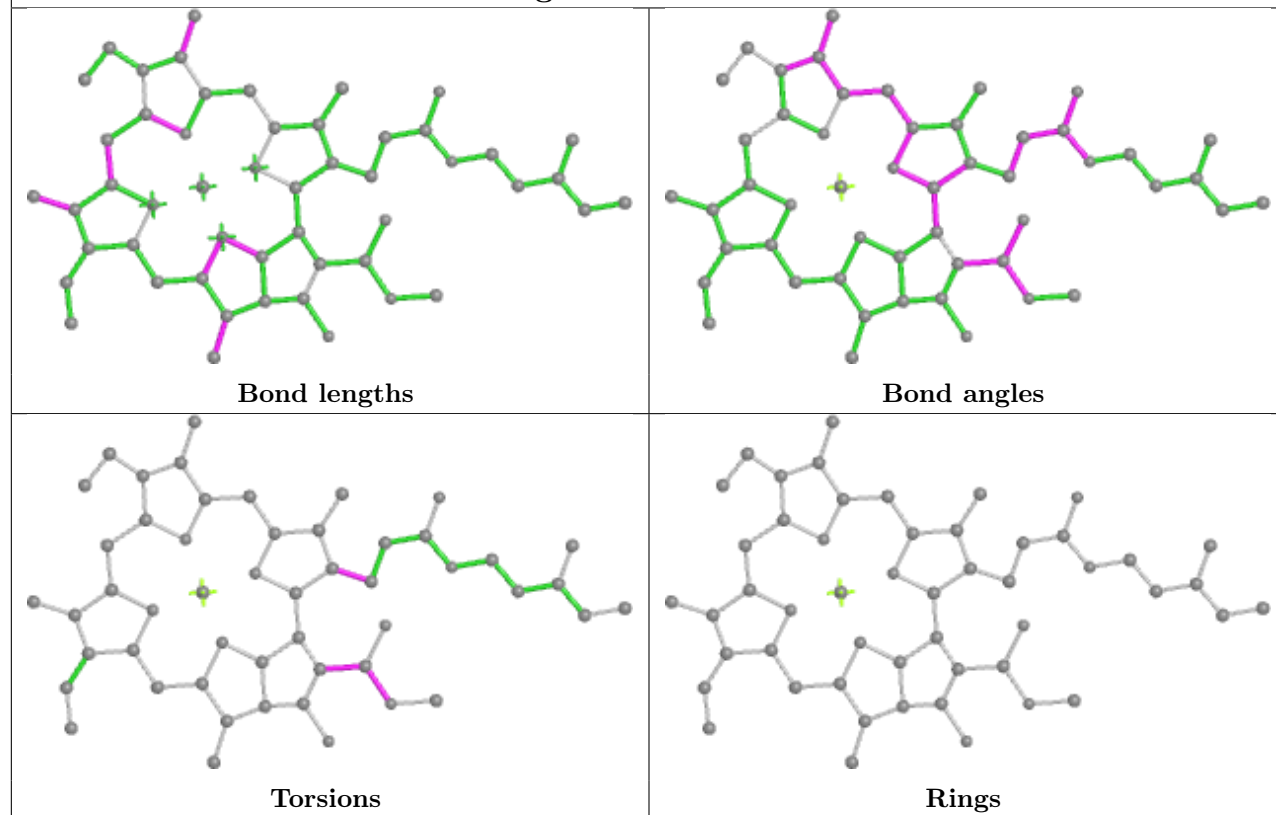


## Ligand II0 g 318

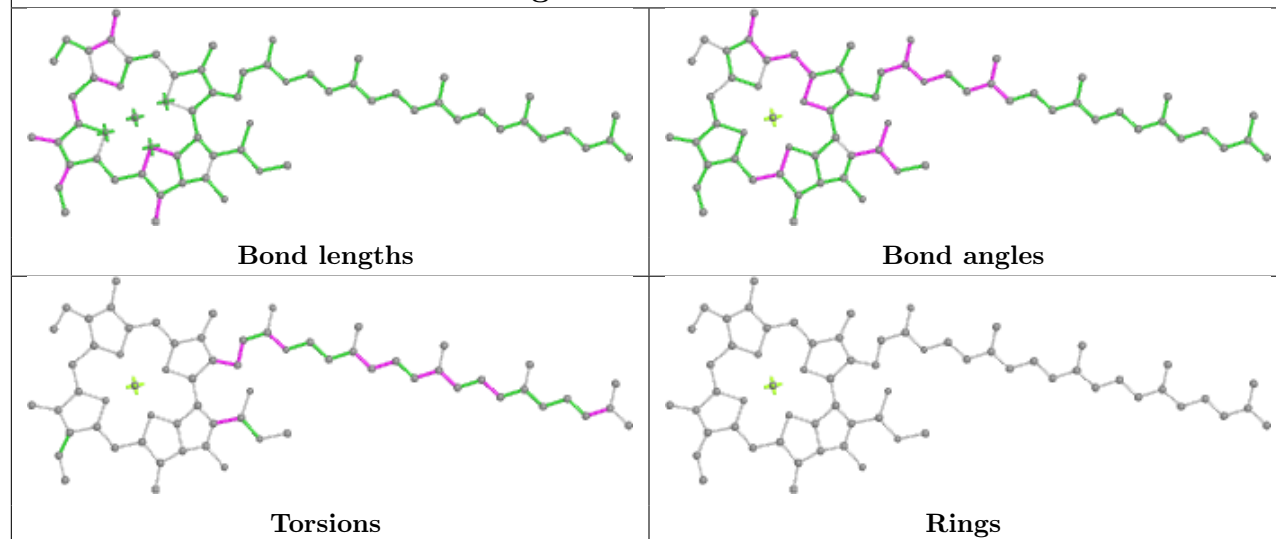




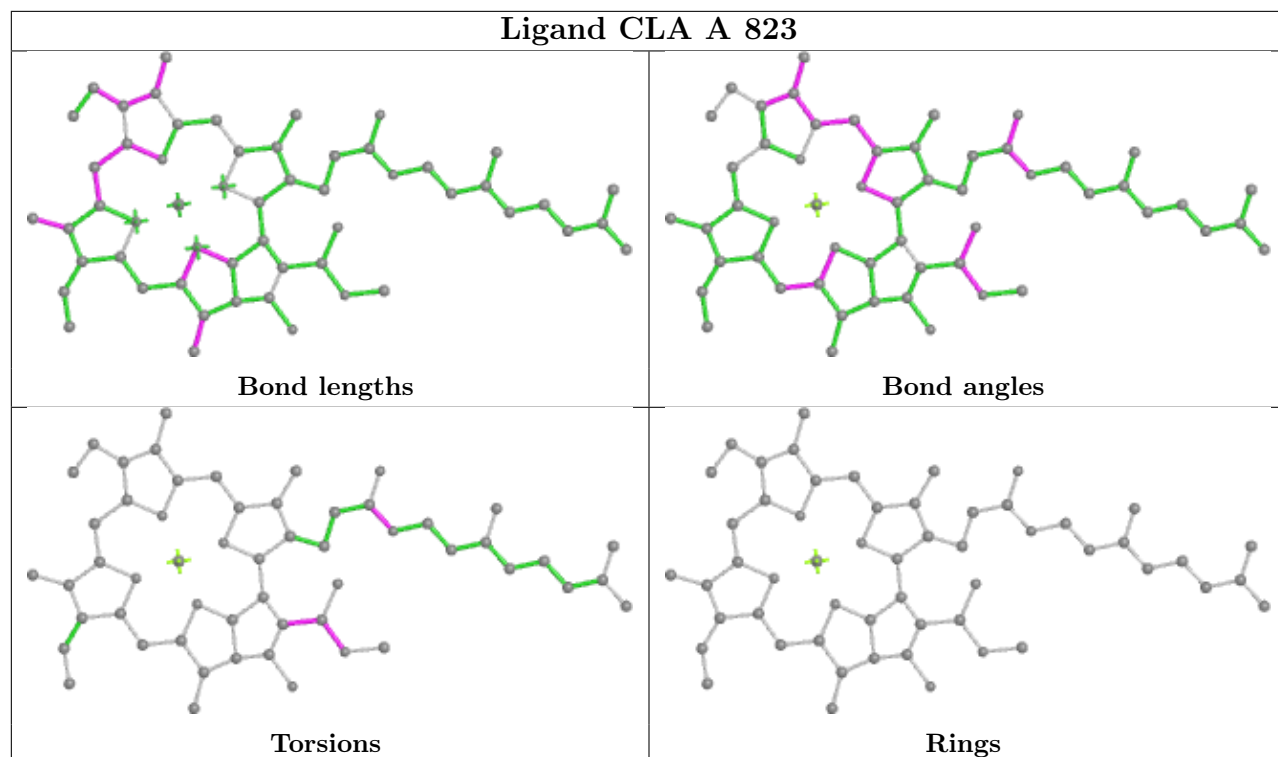
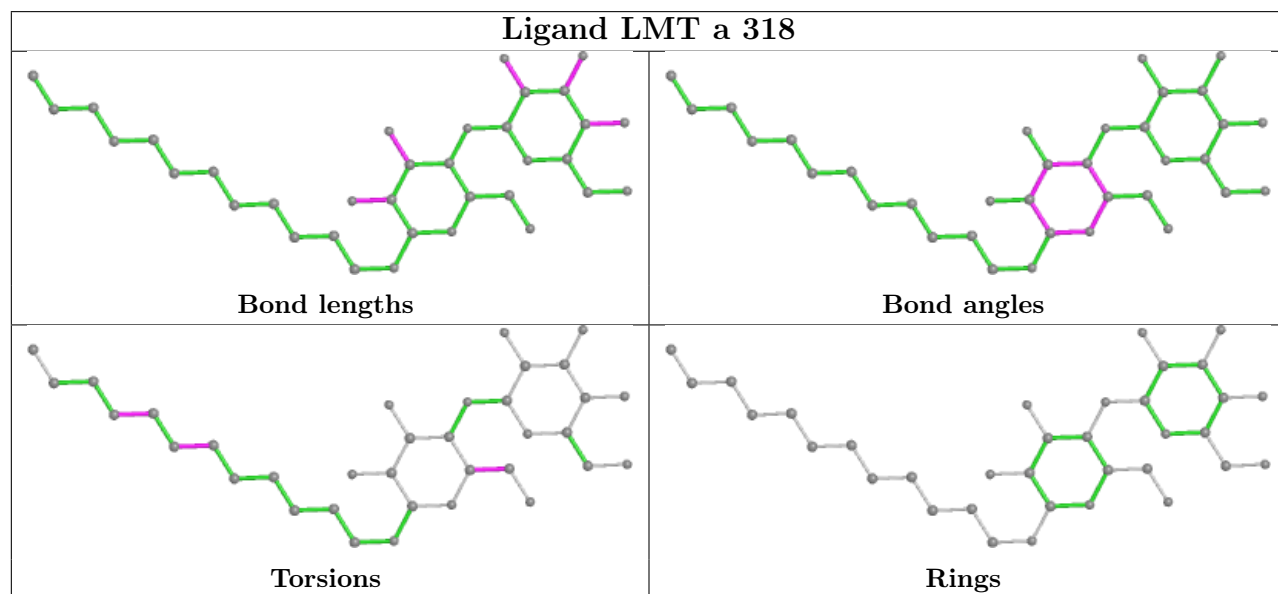
## Ligand CLA h 303

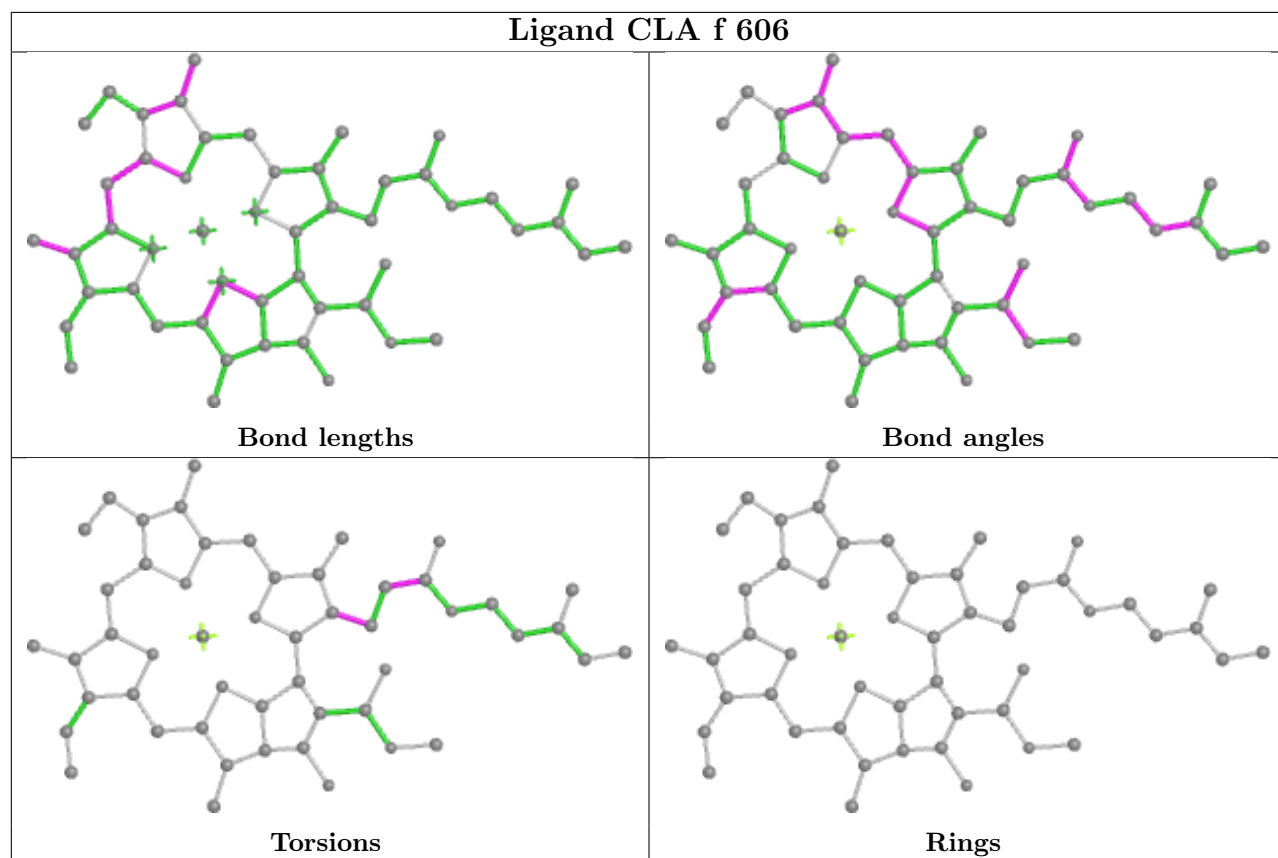
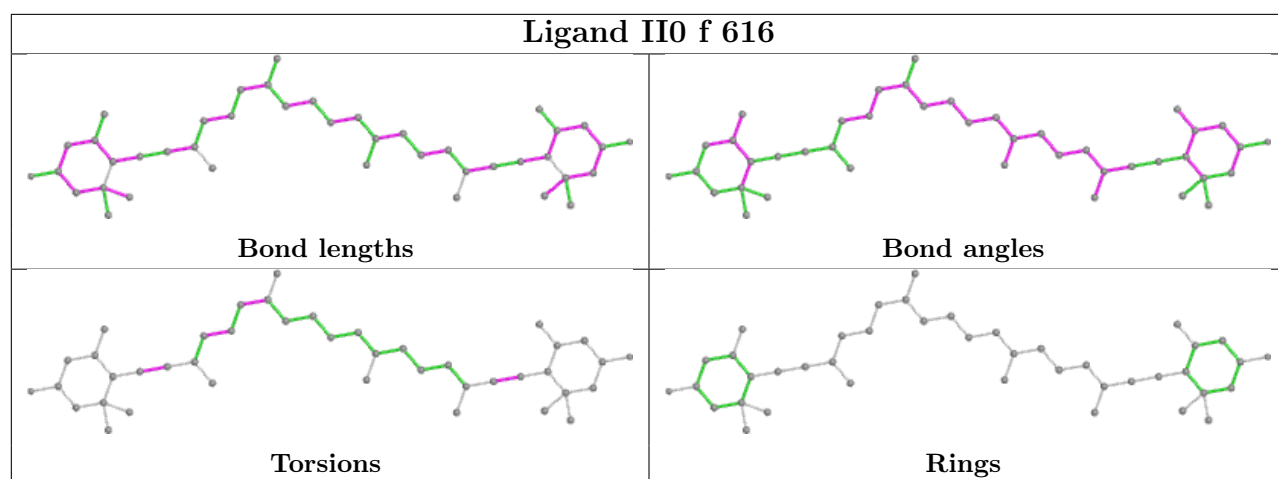


## Ligand CLA A 855

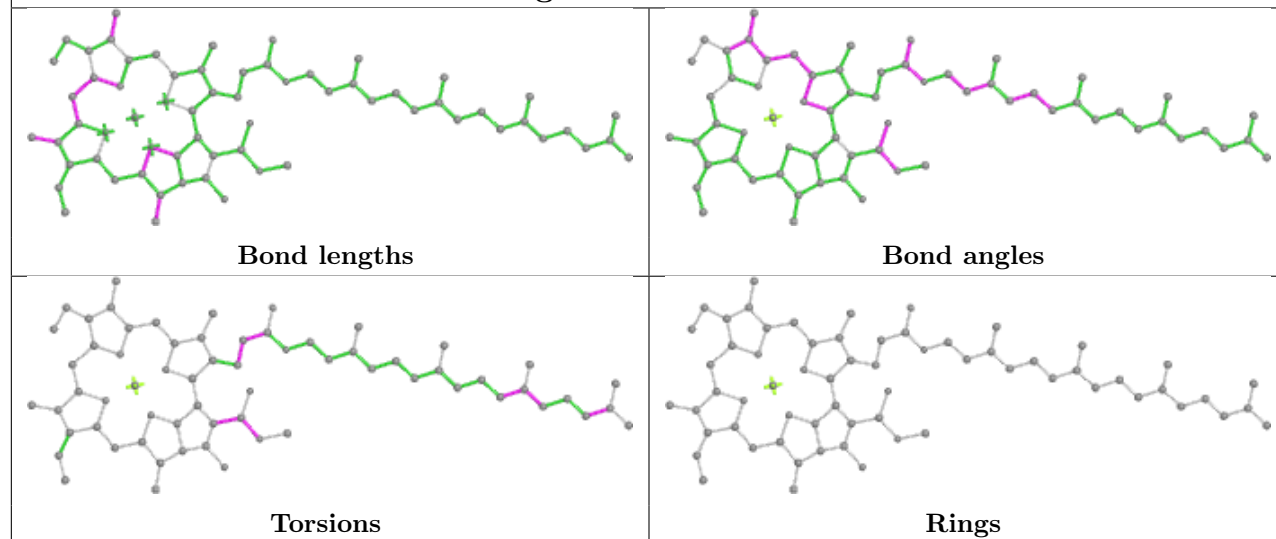




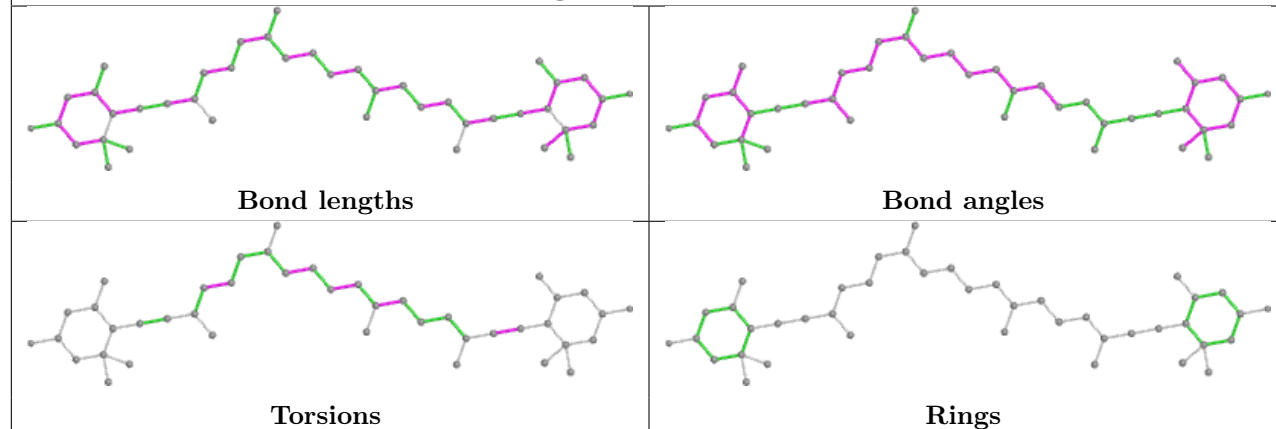
**Ligand CLA A 823****Ligand LMT a 318**



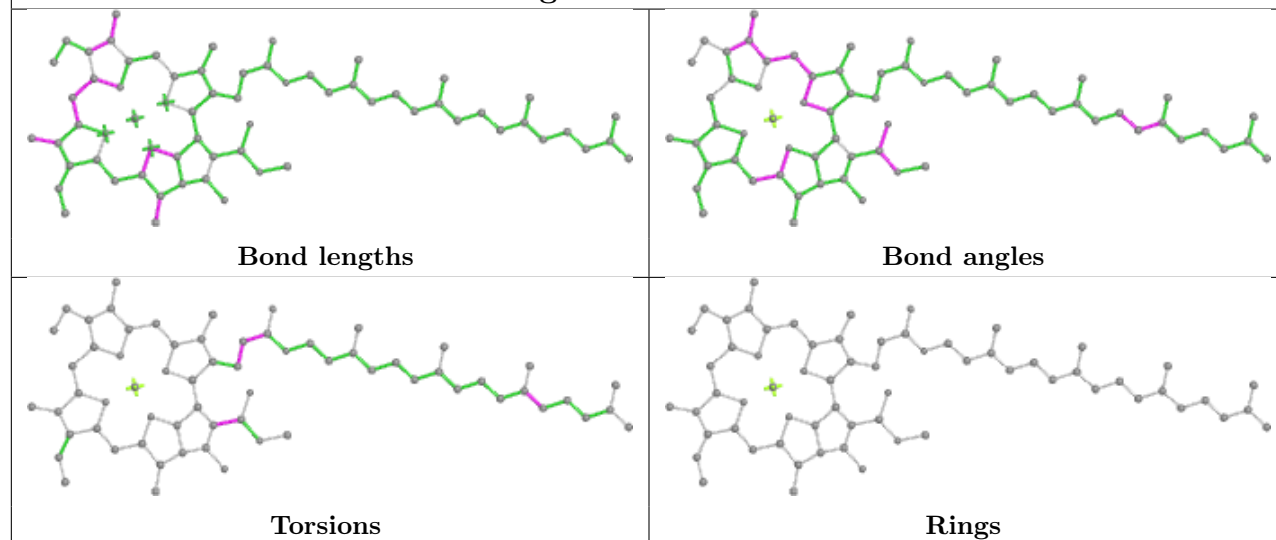
## Ligand CLA k 604



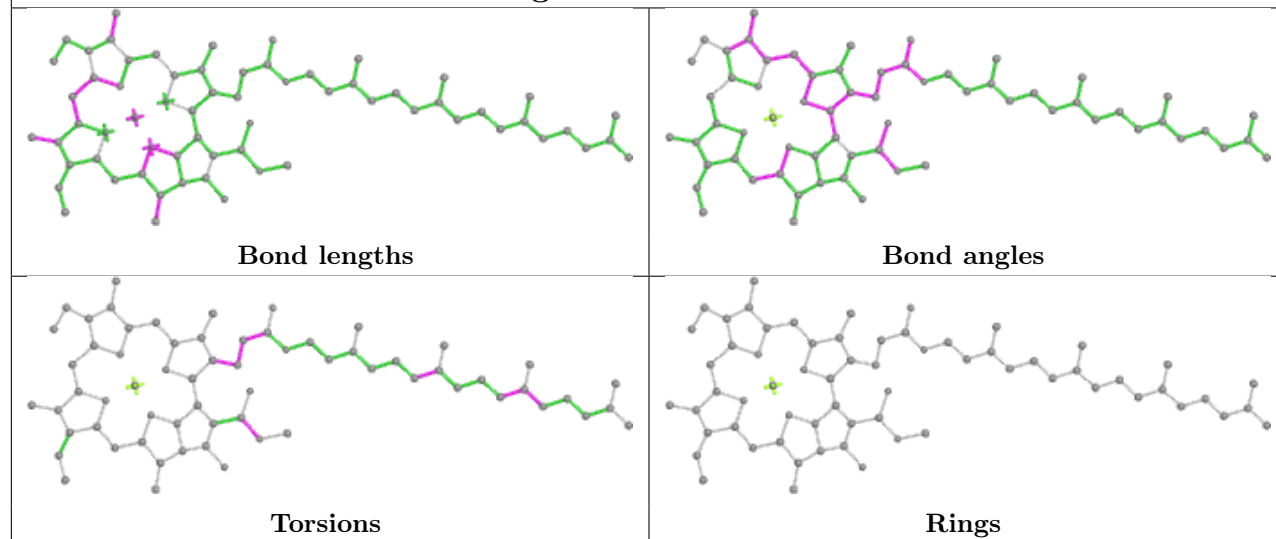
## Ligand II0 e 616



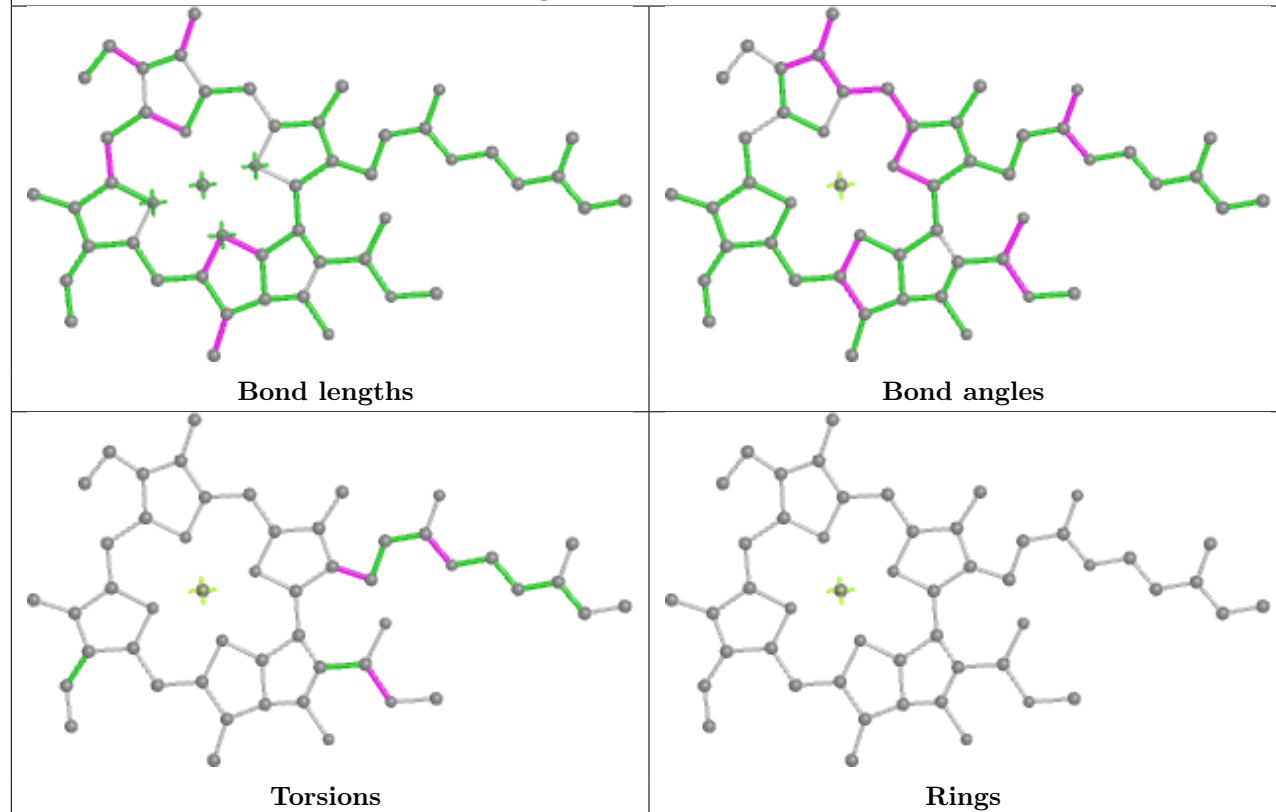
## Ligand CLA f 604

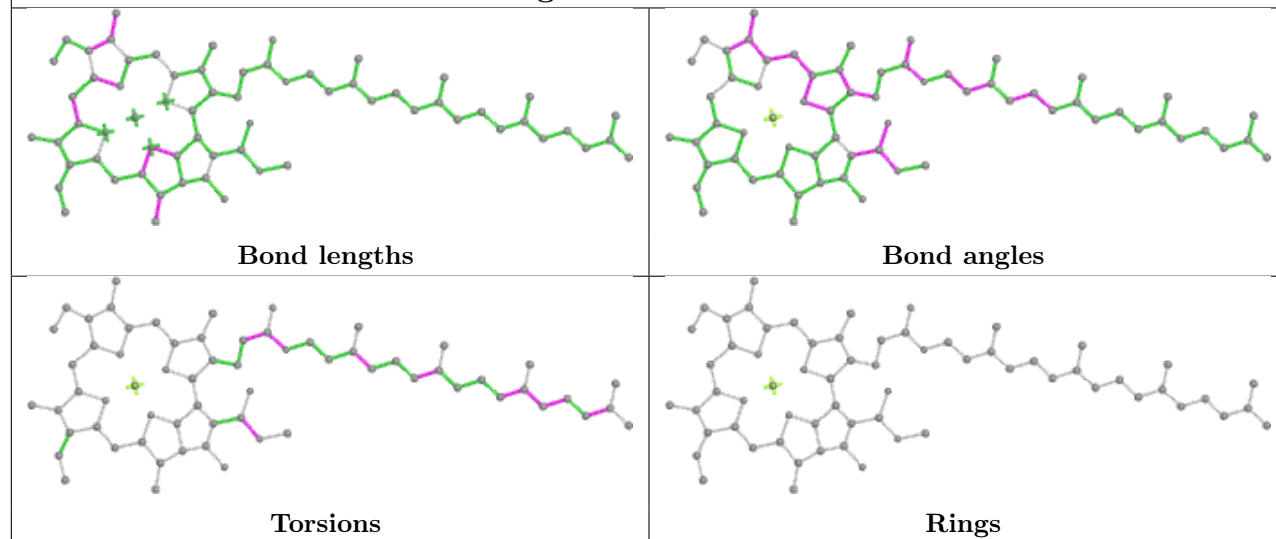
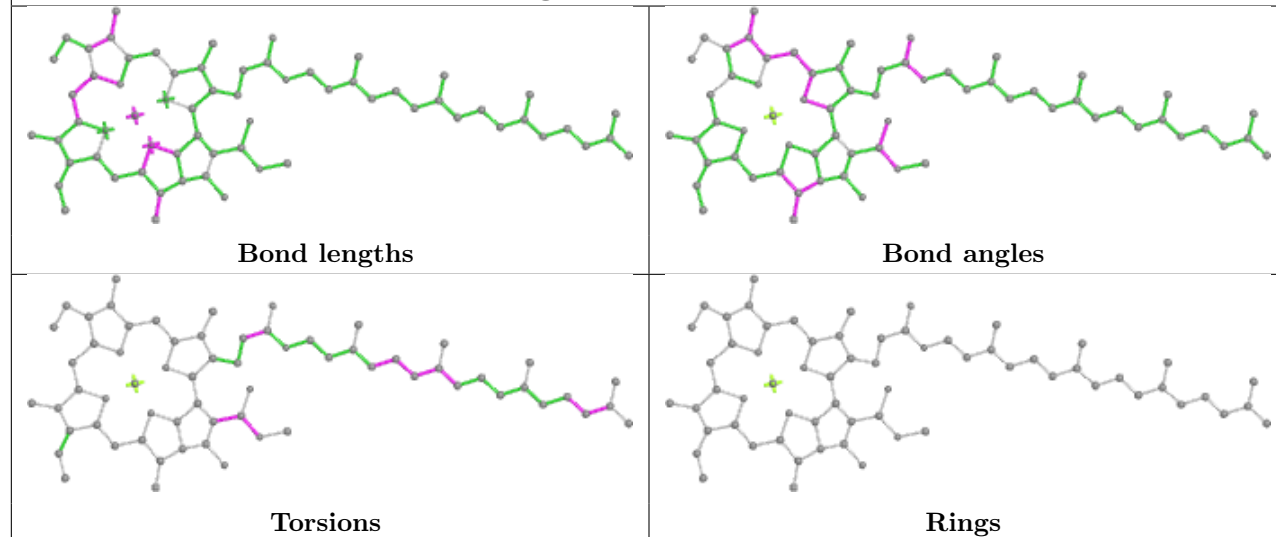
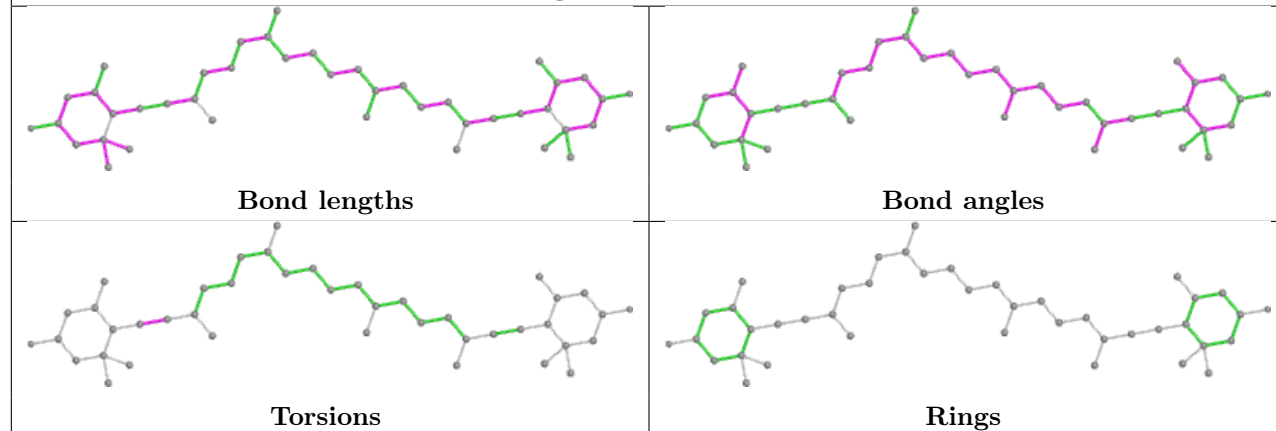


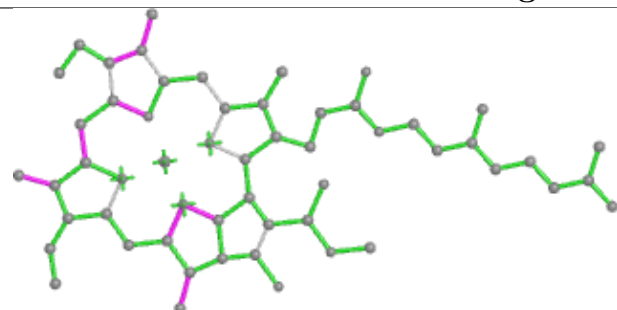
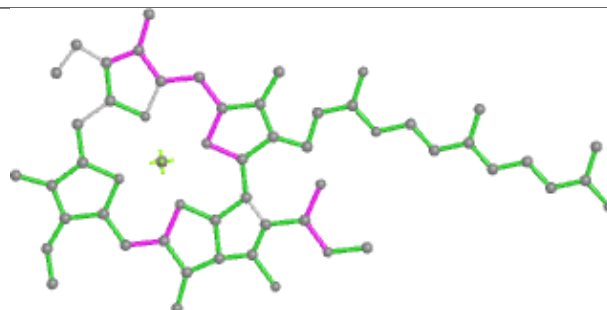
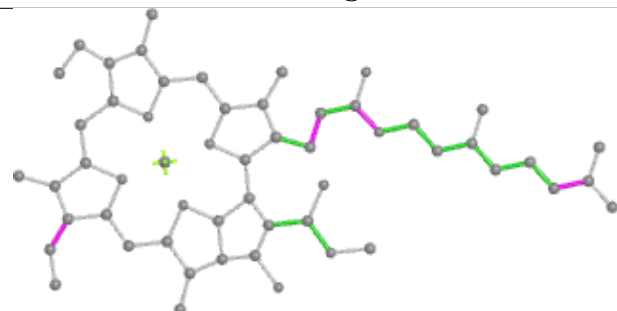
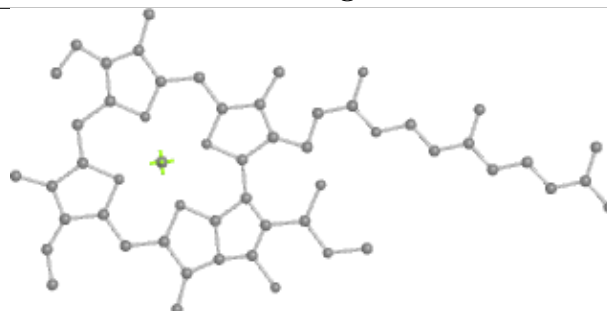
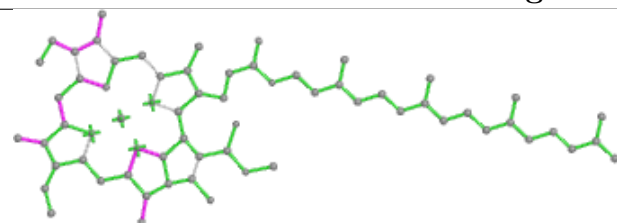
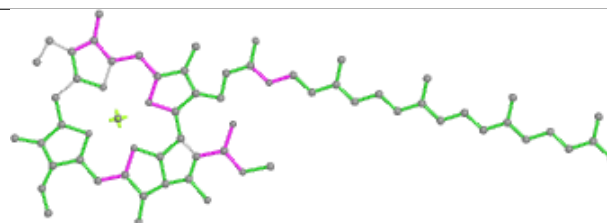
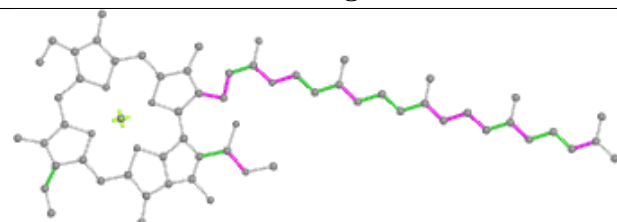
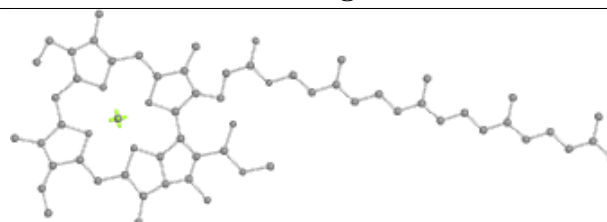
## Ligand CLA A 808

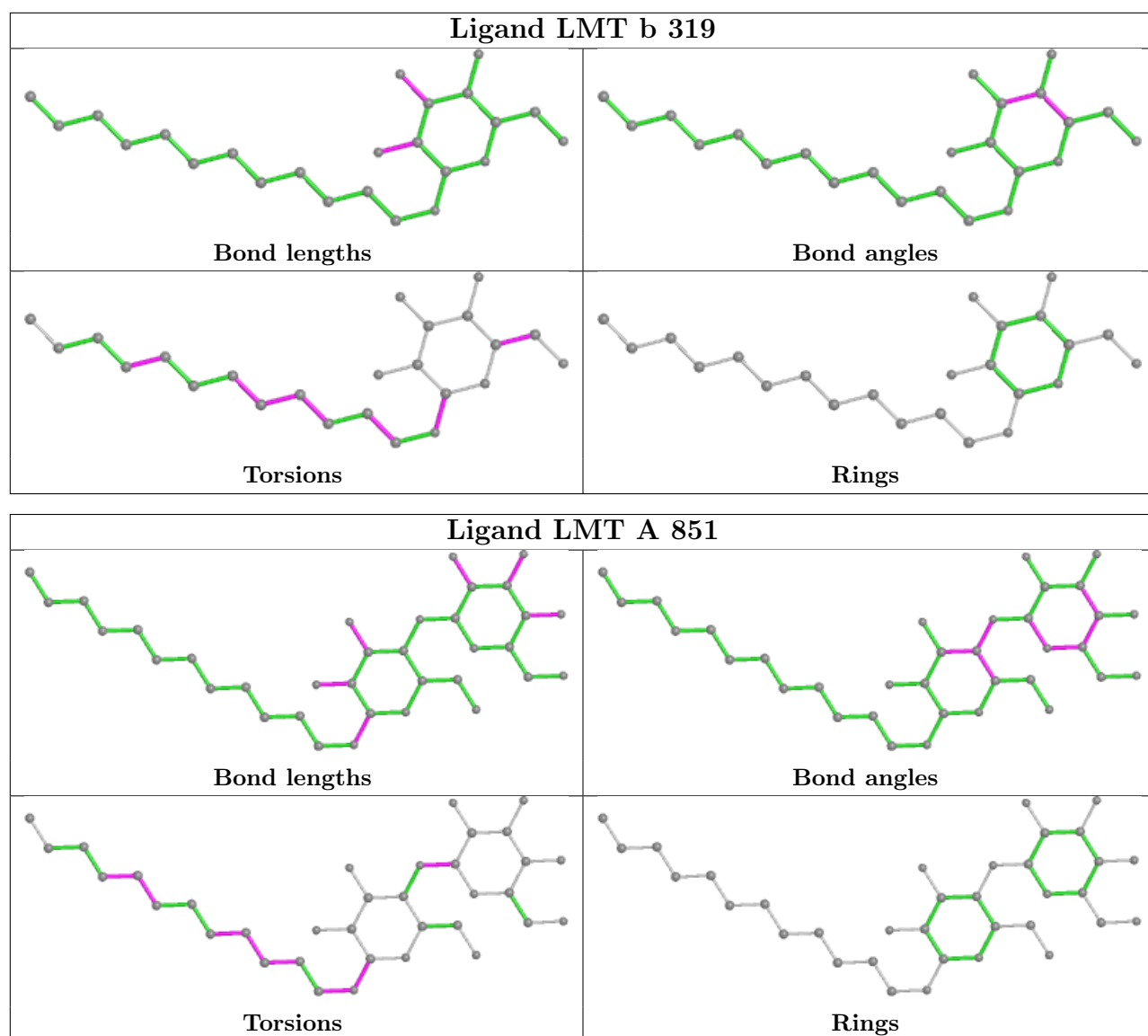


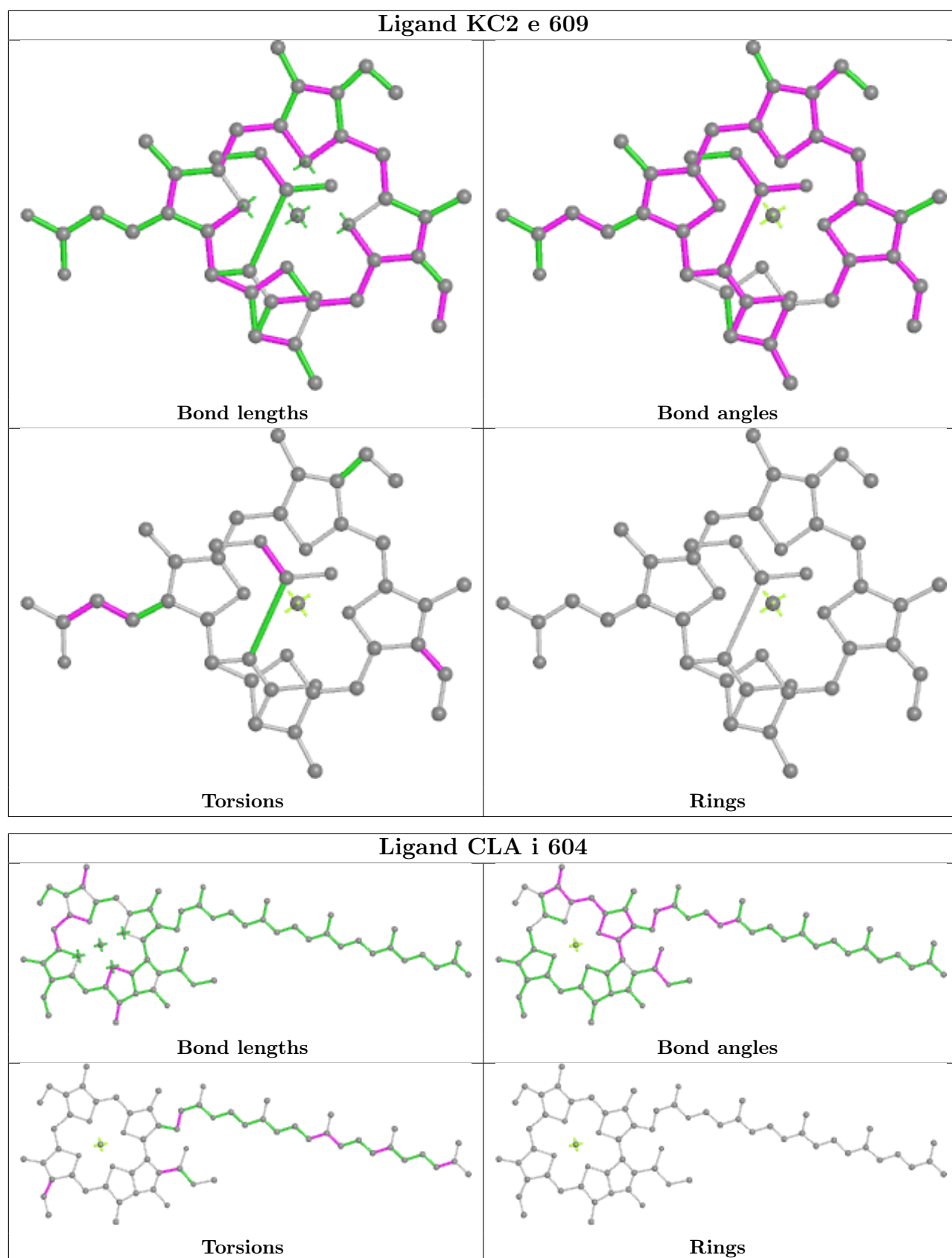
## Ligand CLA h 304



**Ligand CLA e 611****Ligand CLA e 605****Ligand II0 a 313**

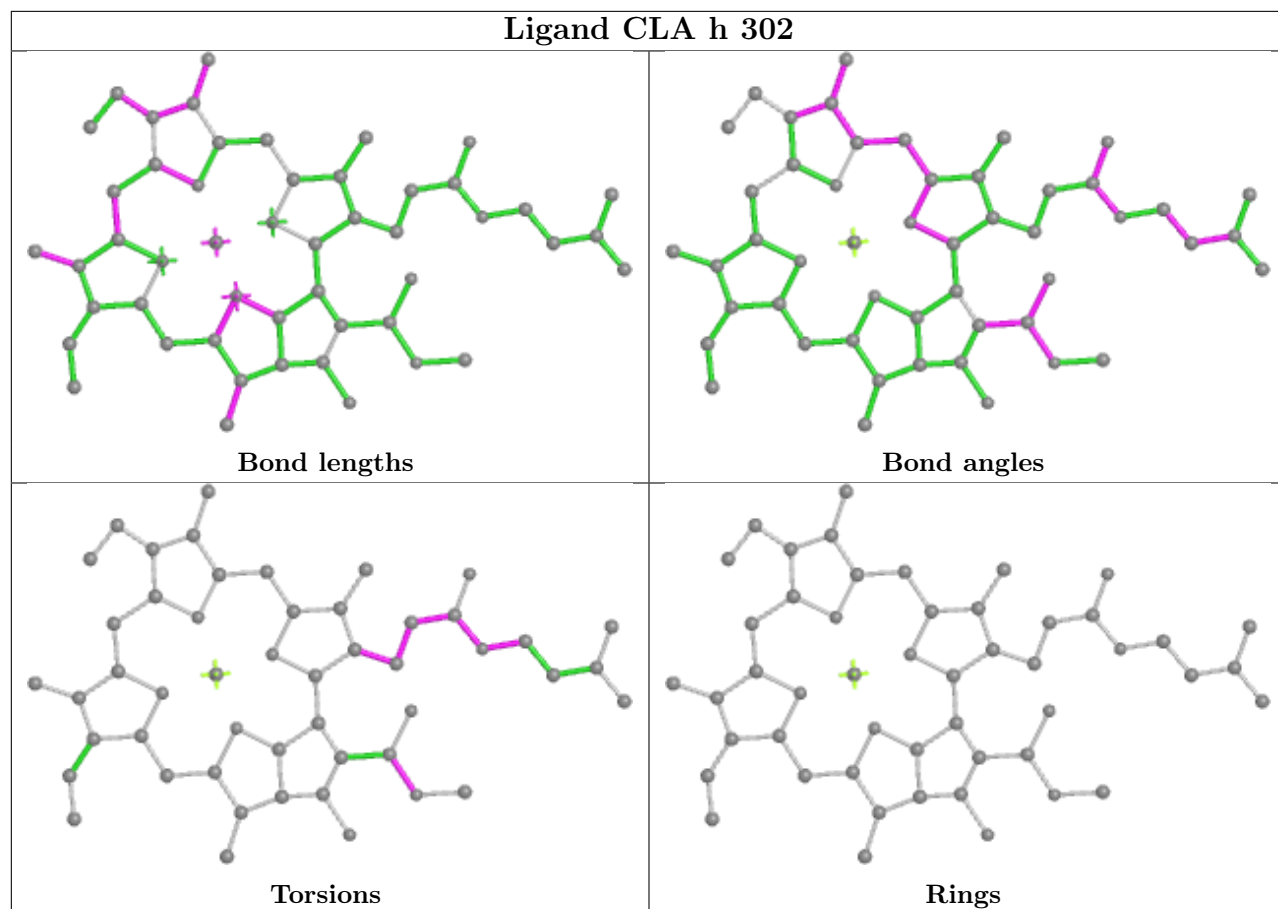
**Ligand CLA B 811****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA f 602****Bond lengths****Bond angles****Torsions****Rings**

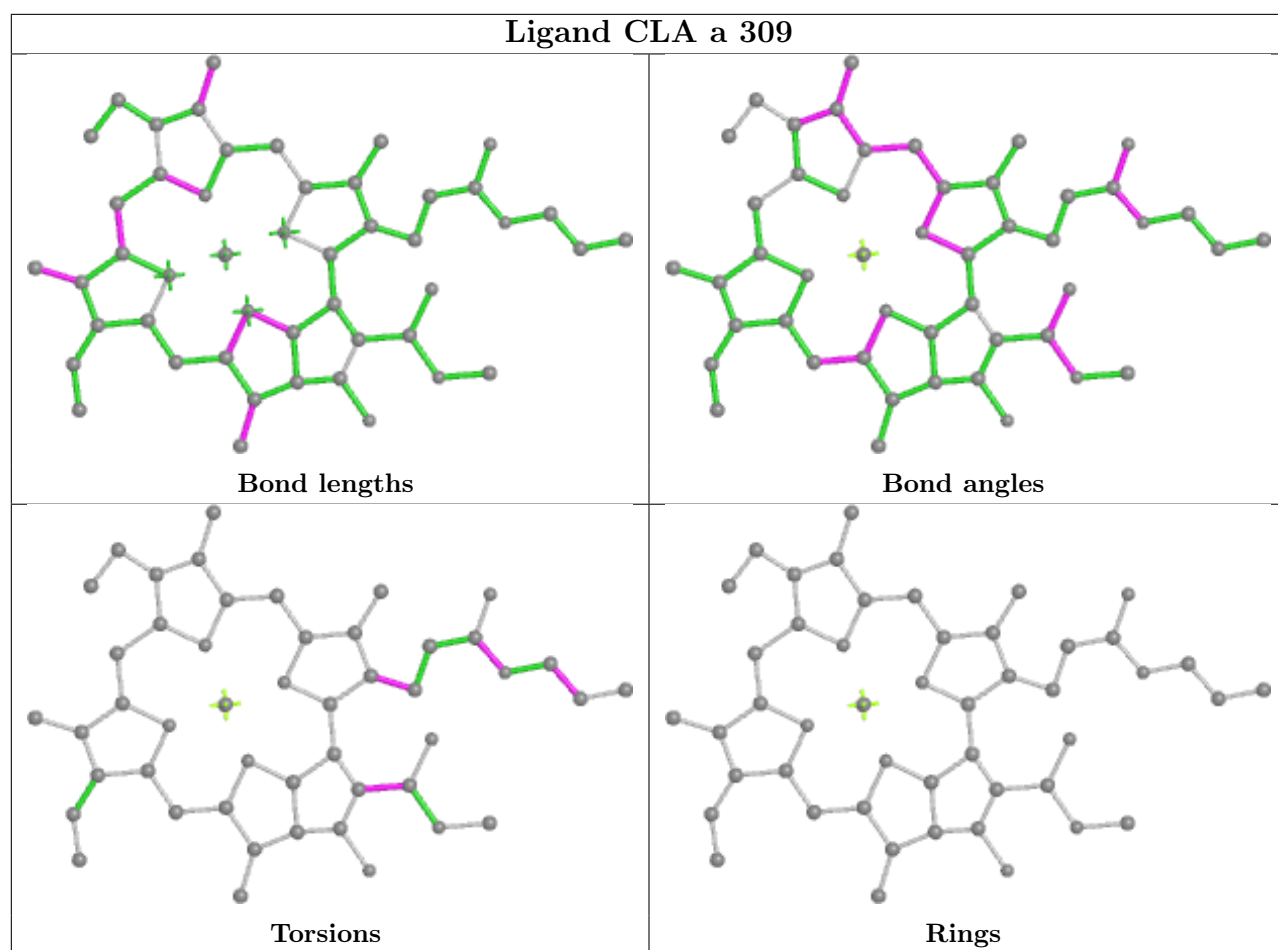




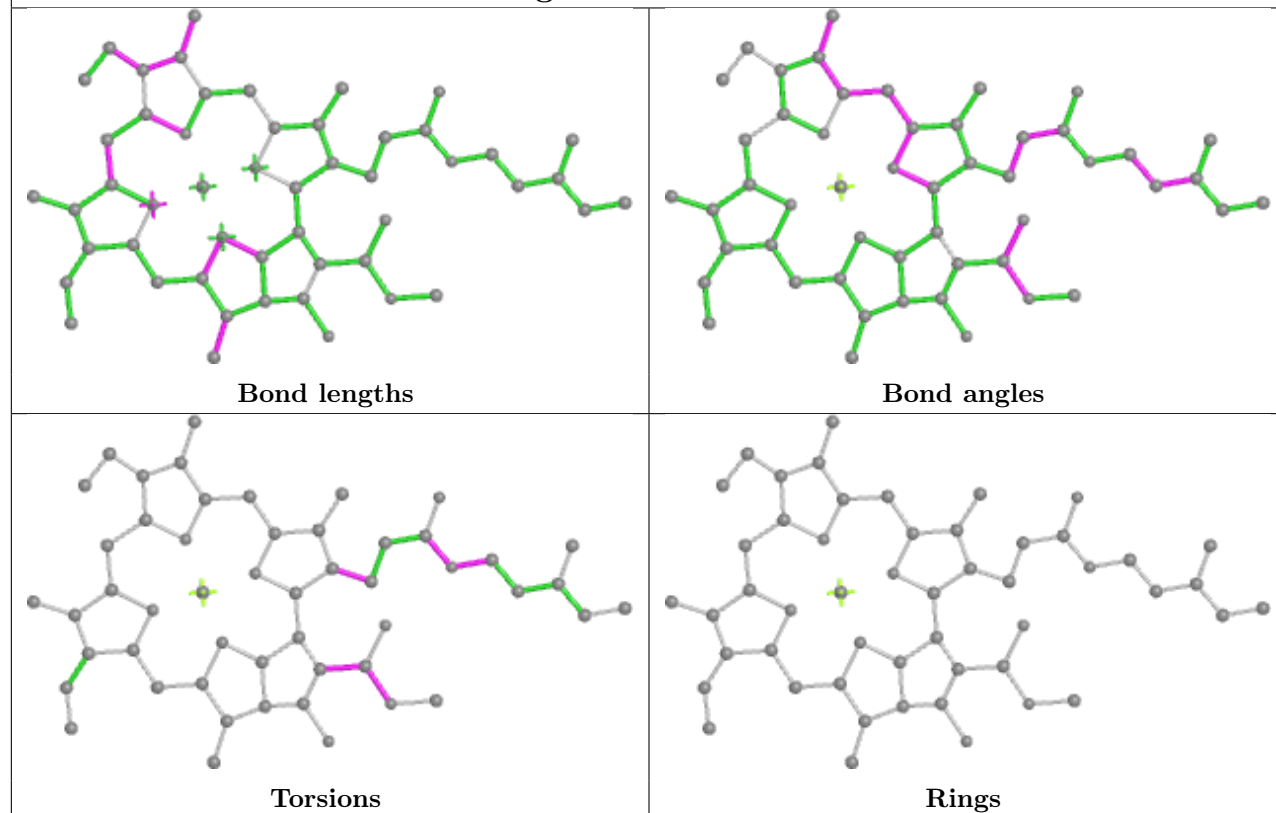


## Ligand CLA h 302

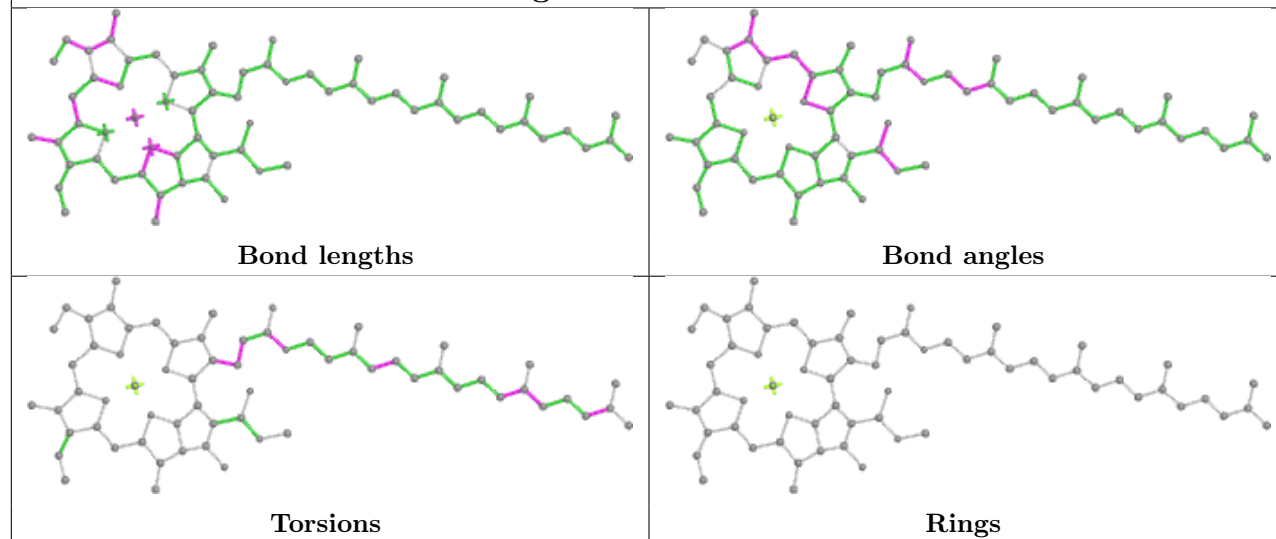




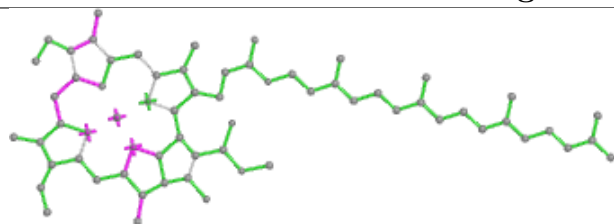
## Ligand CLA k 601



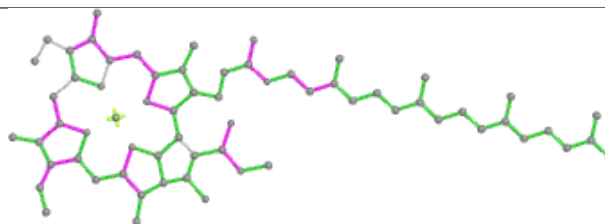
## Ligand CLA B 809



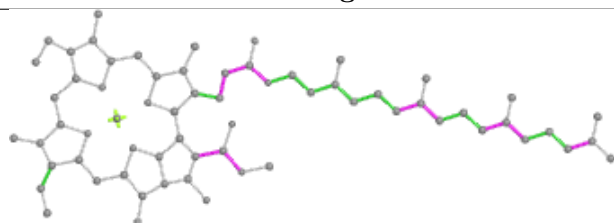
## Ligand CLA d 303



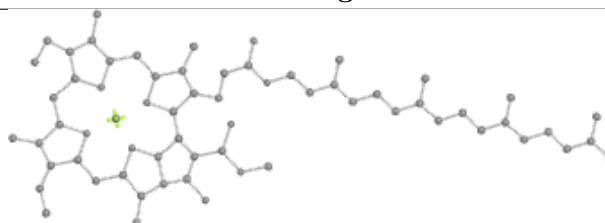
Bond lengths



Bond angles

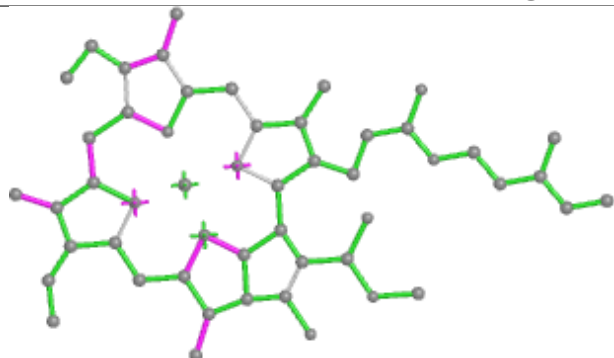


Torsions

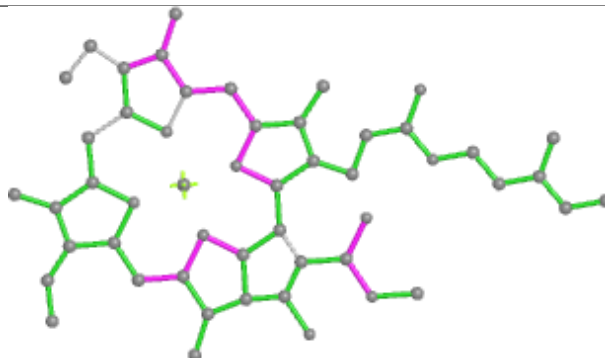


Rings

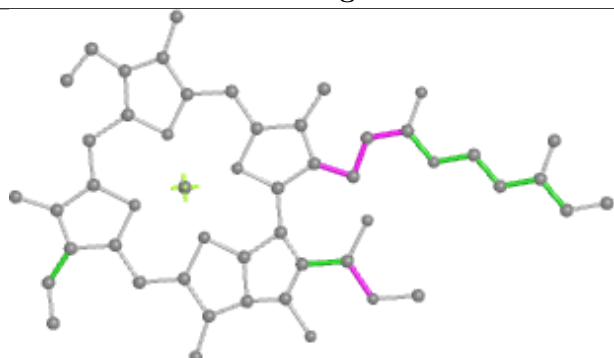
## Ligand CLA i 610



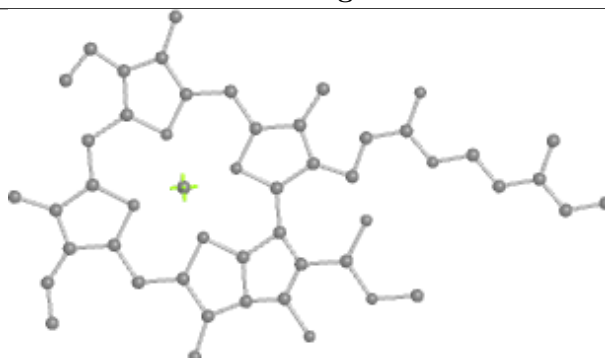
Bond lengths



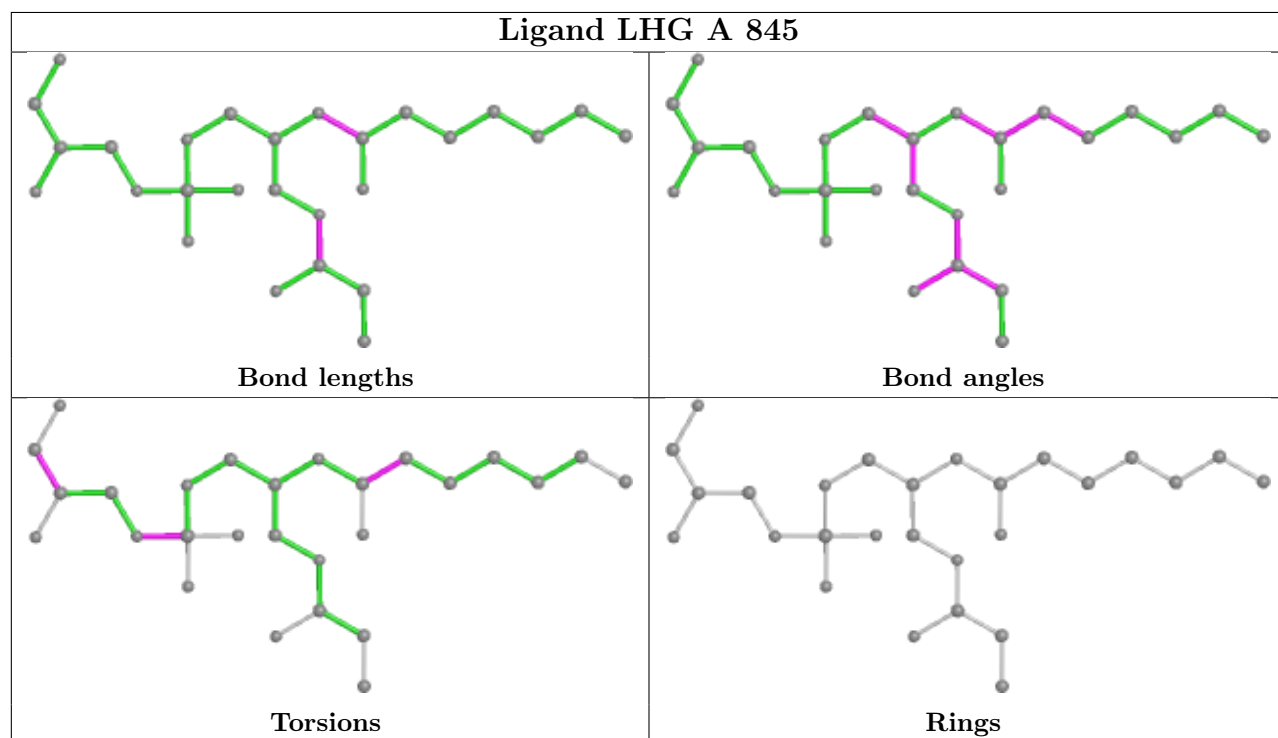
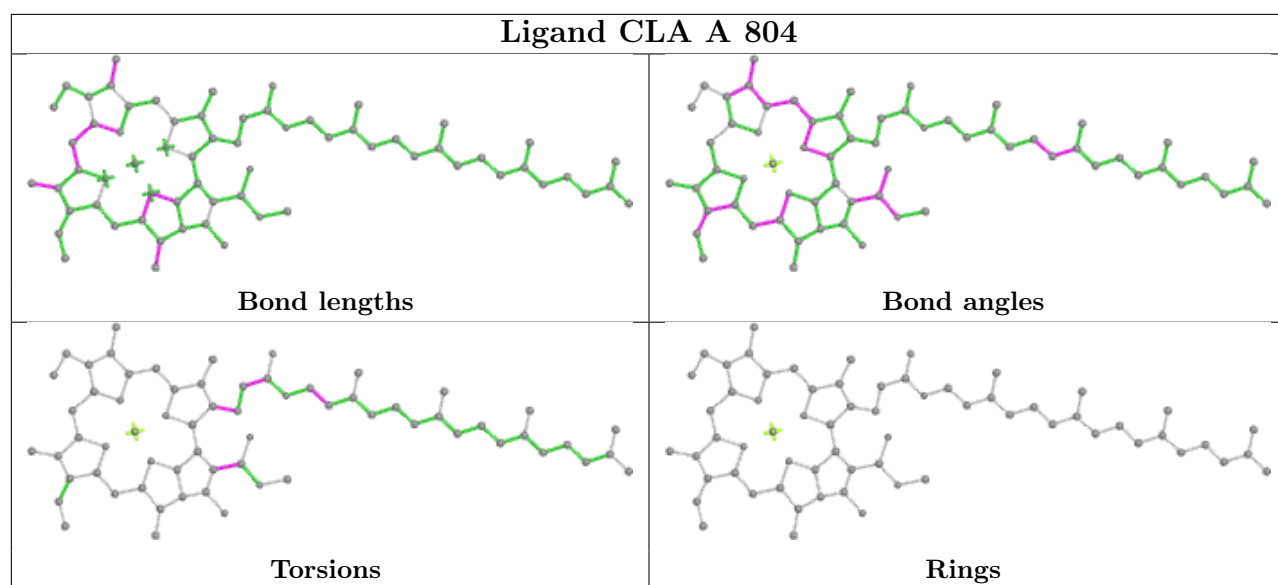
Bond angles



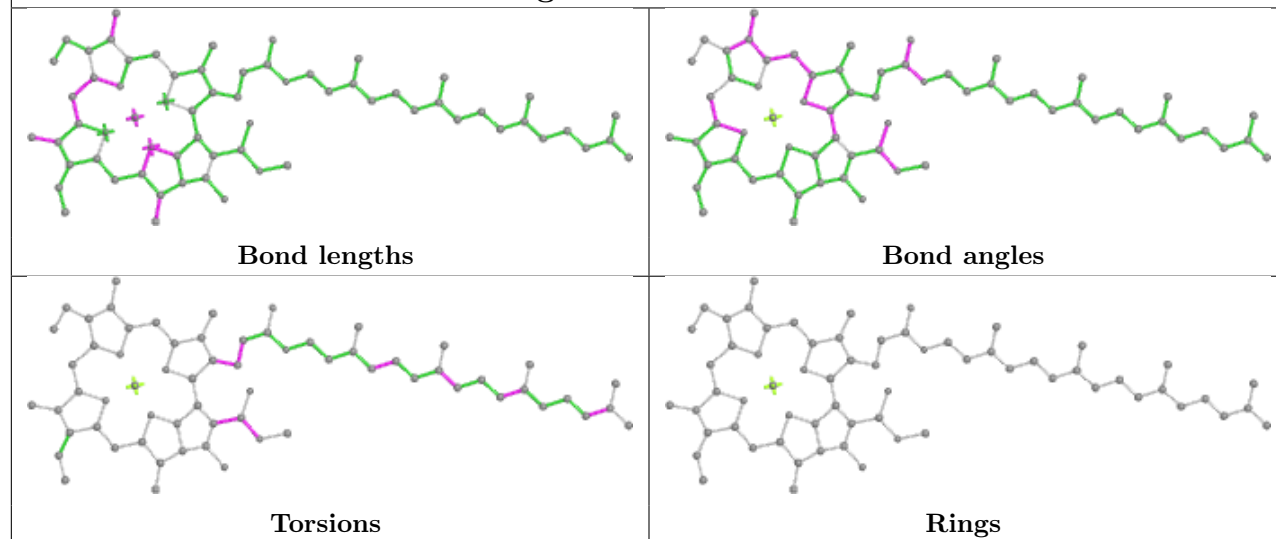
Torsions



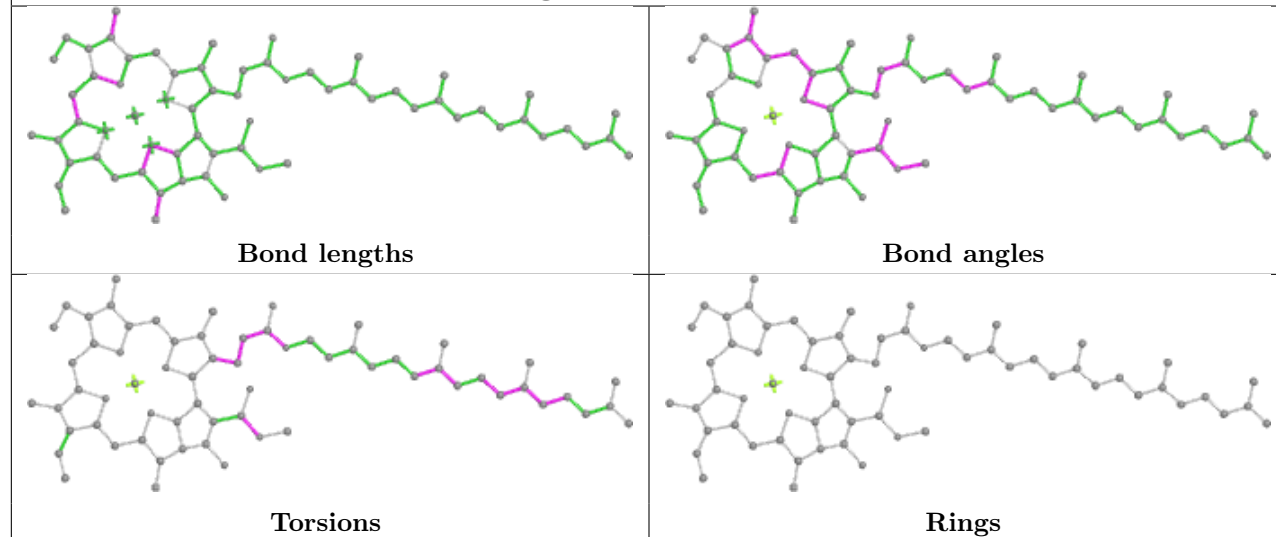
Rings



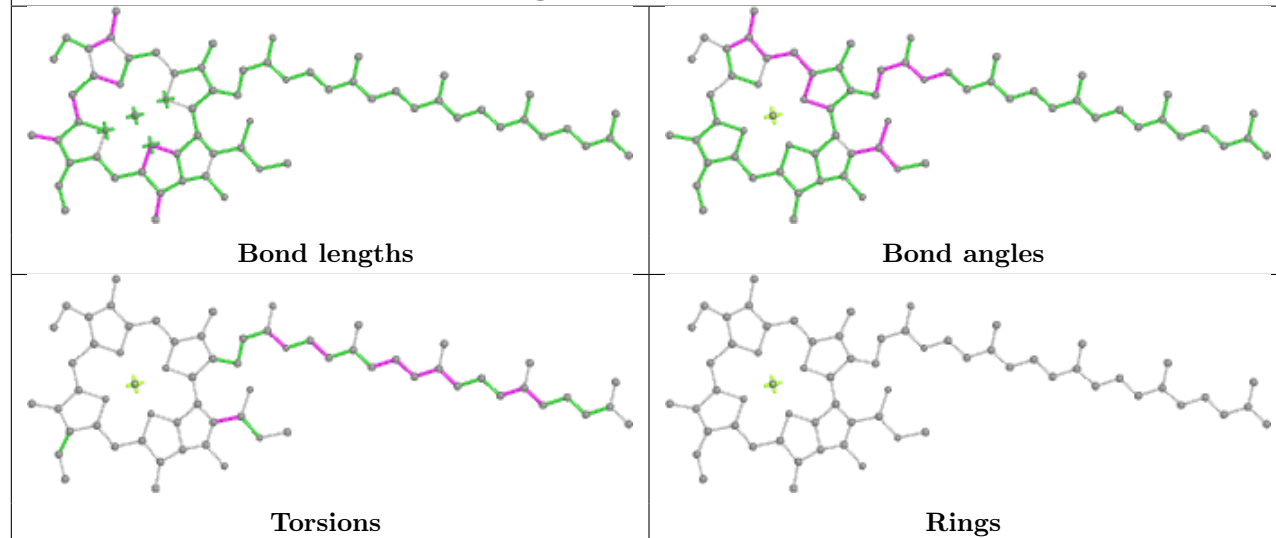
## Ligand CLA e 610



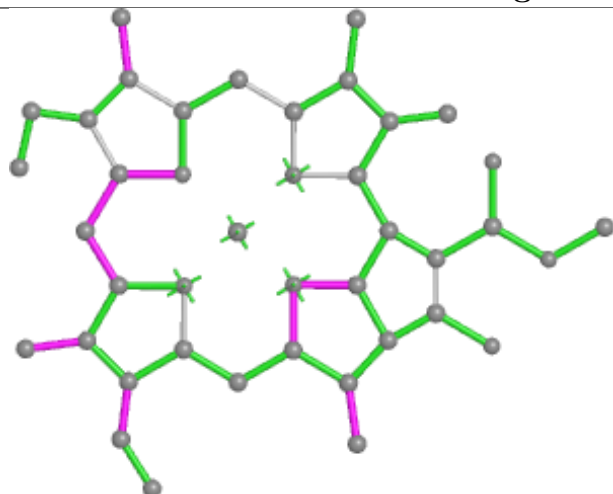
## Ligand CLA c 608



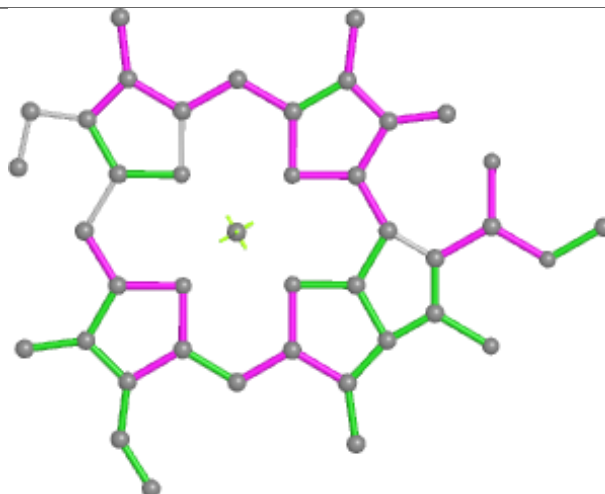
## Ligand CLA A 839



## Ligand CLA A 856



Bond lengths



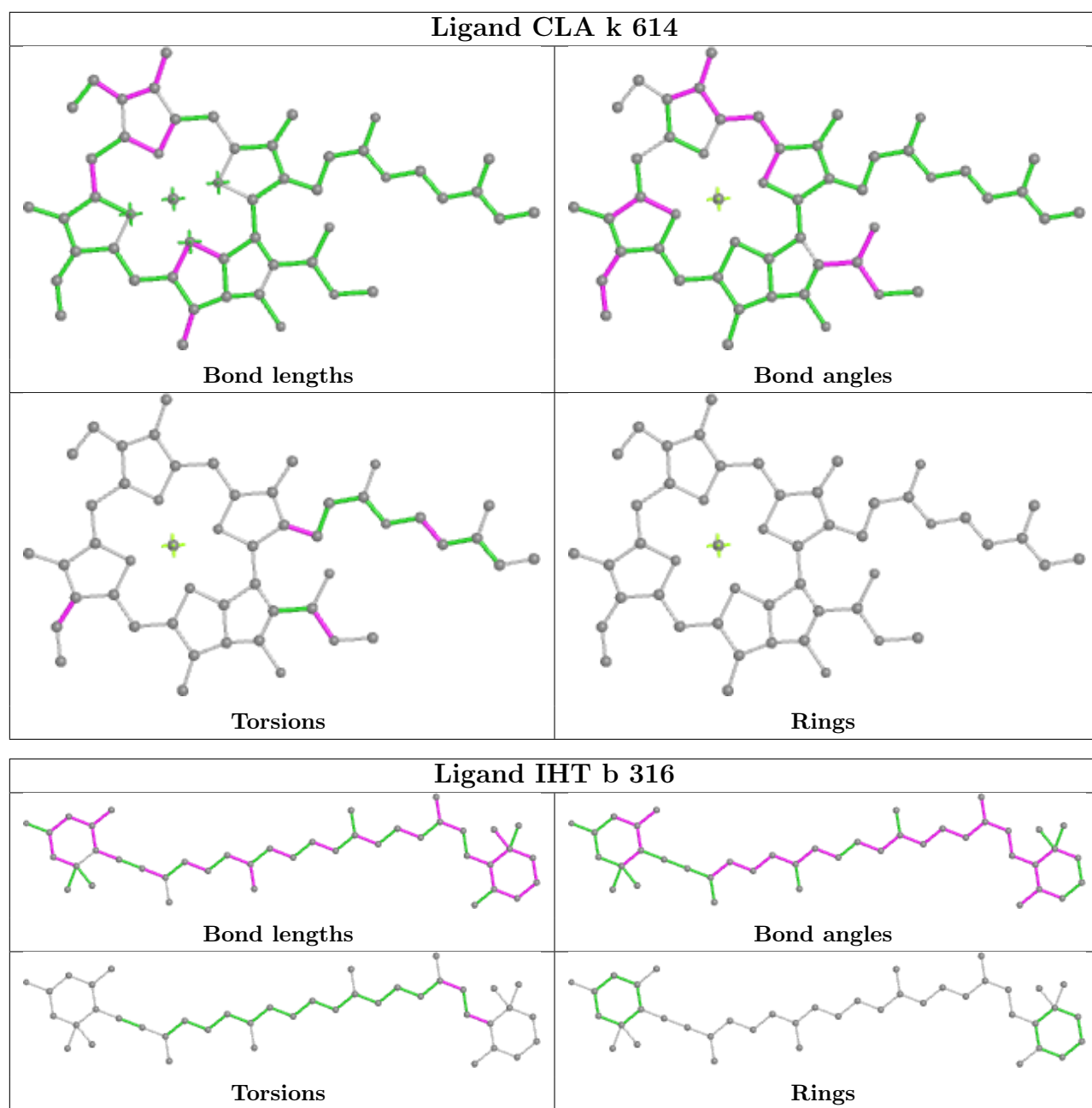
Bond angles



Torsions

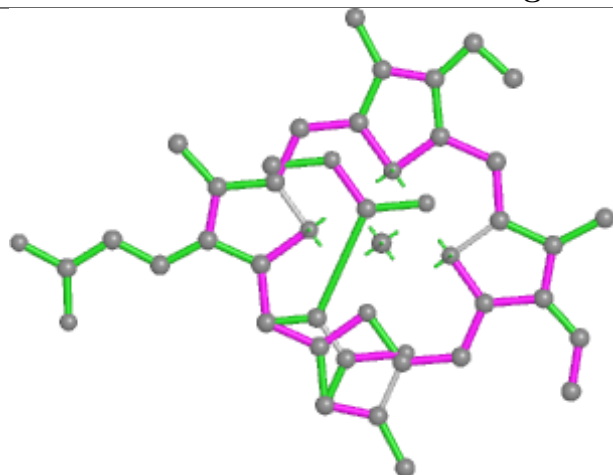


Rings

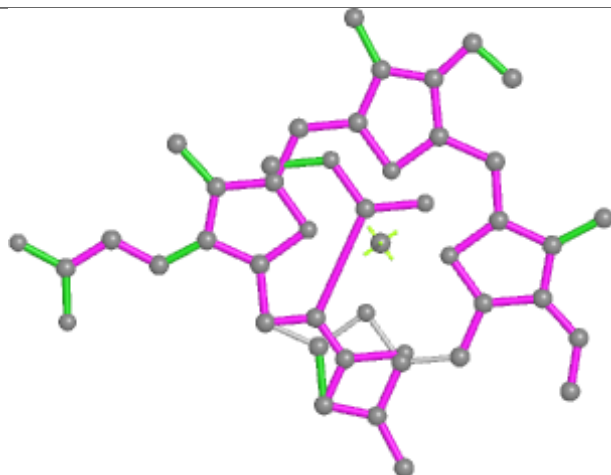




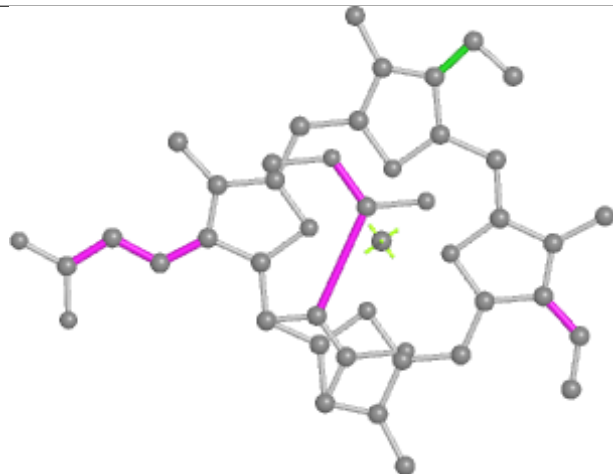
## Ligand KC2 f 611



Bond lengths



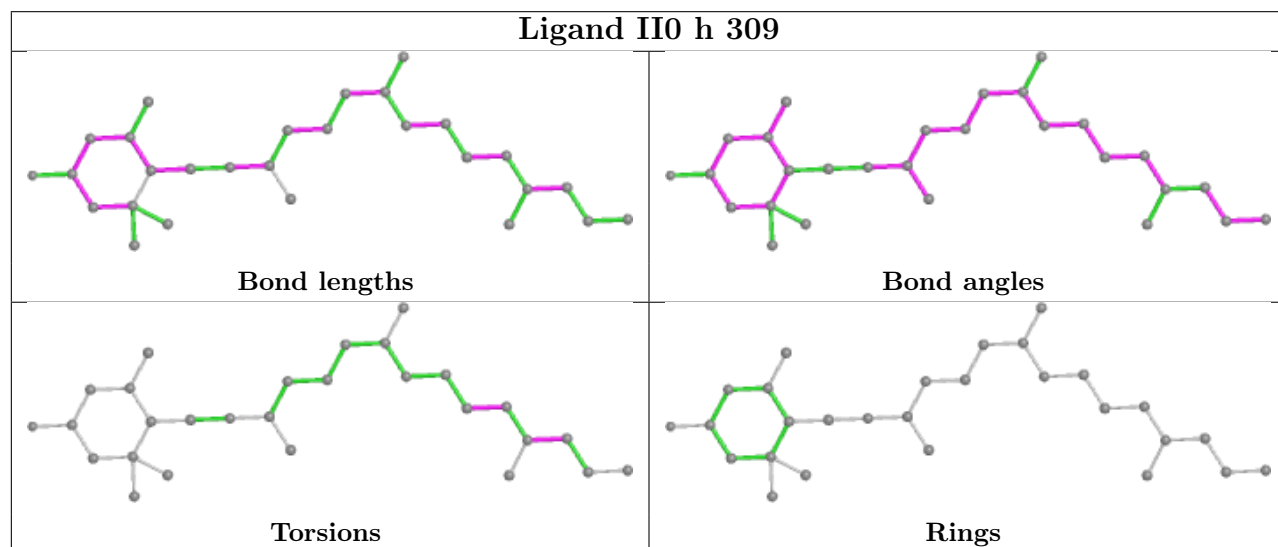
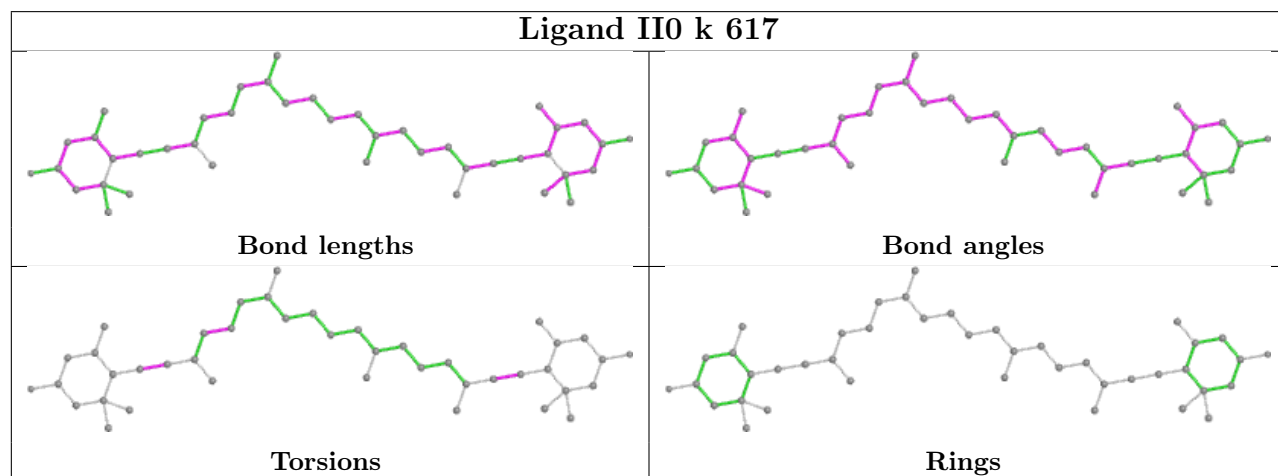
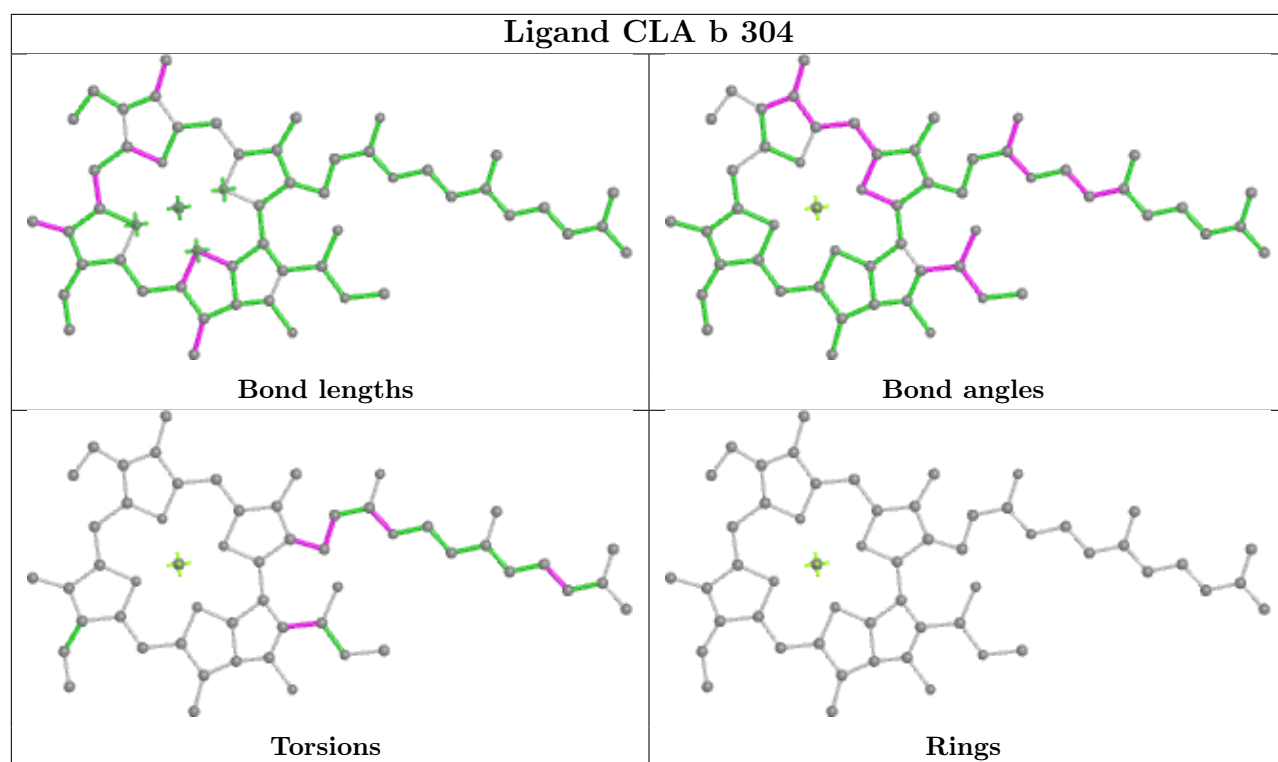
Bond angles

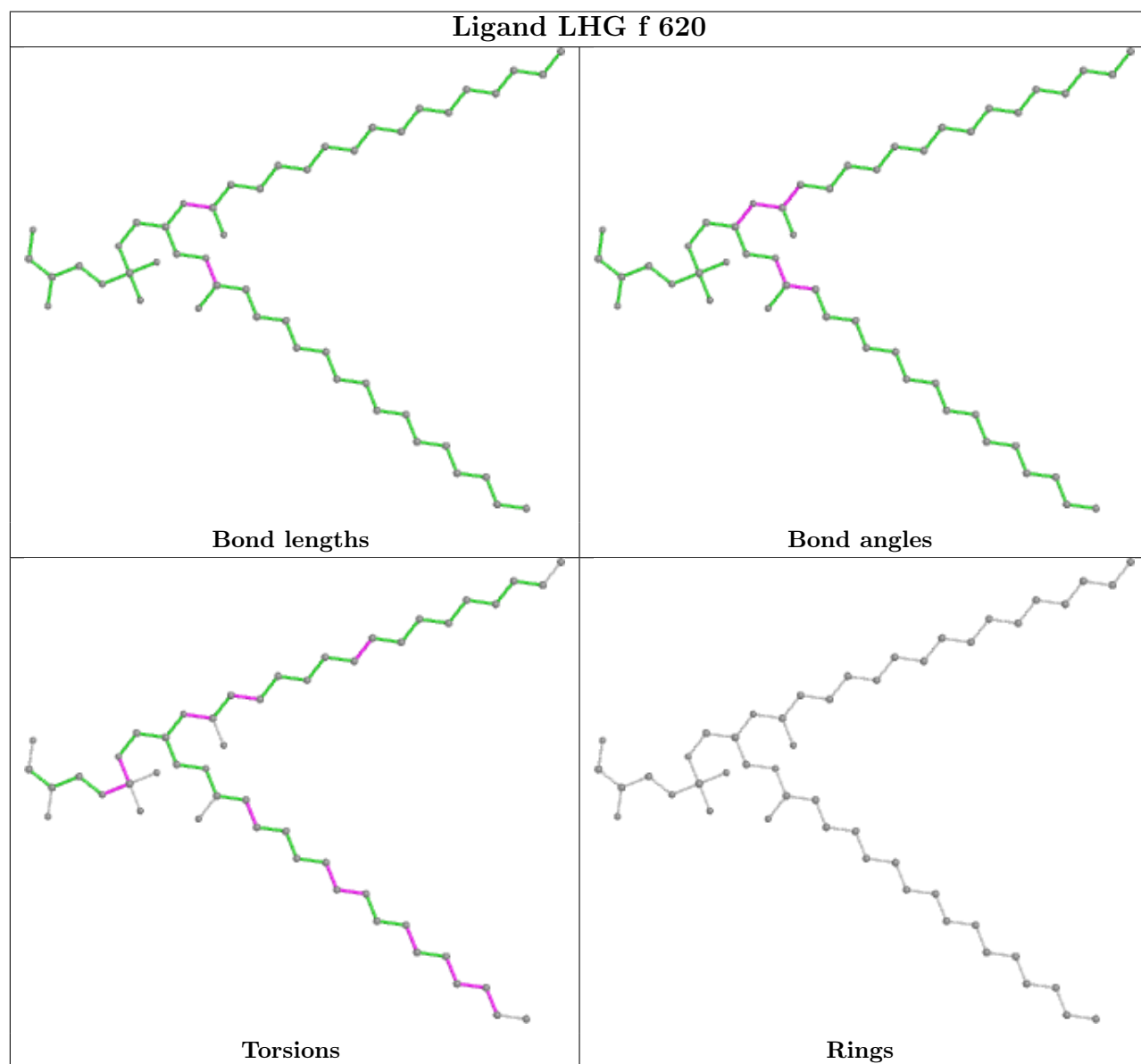
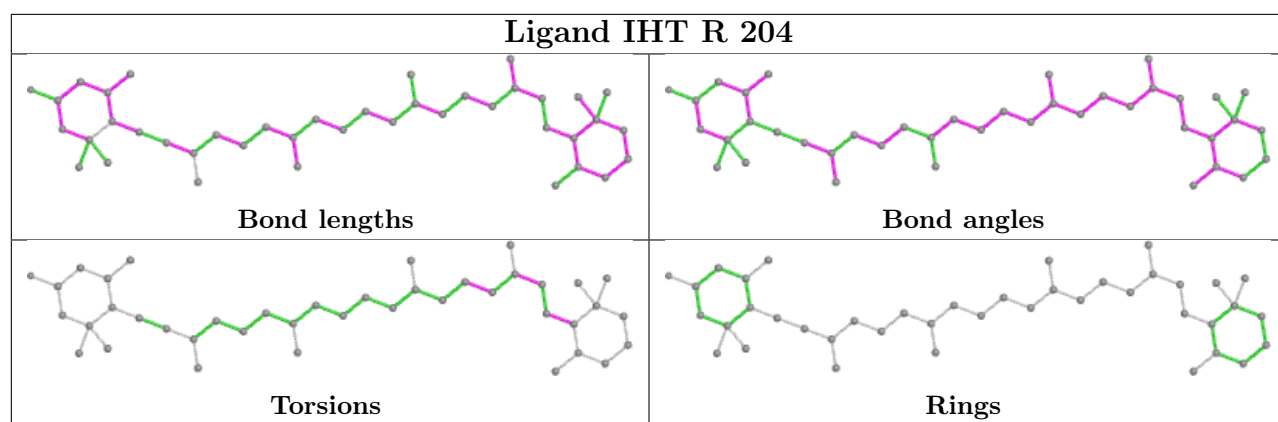


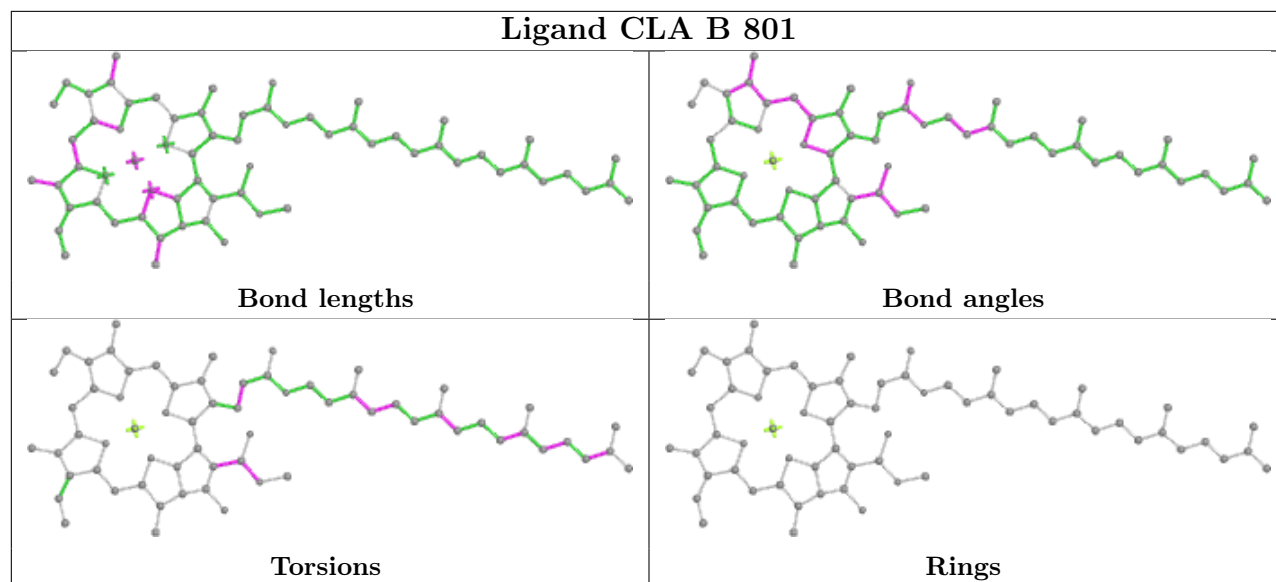
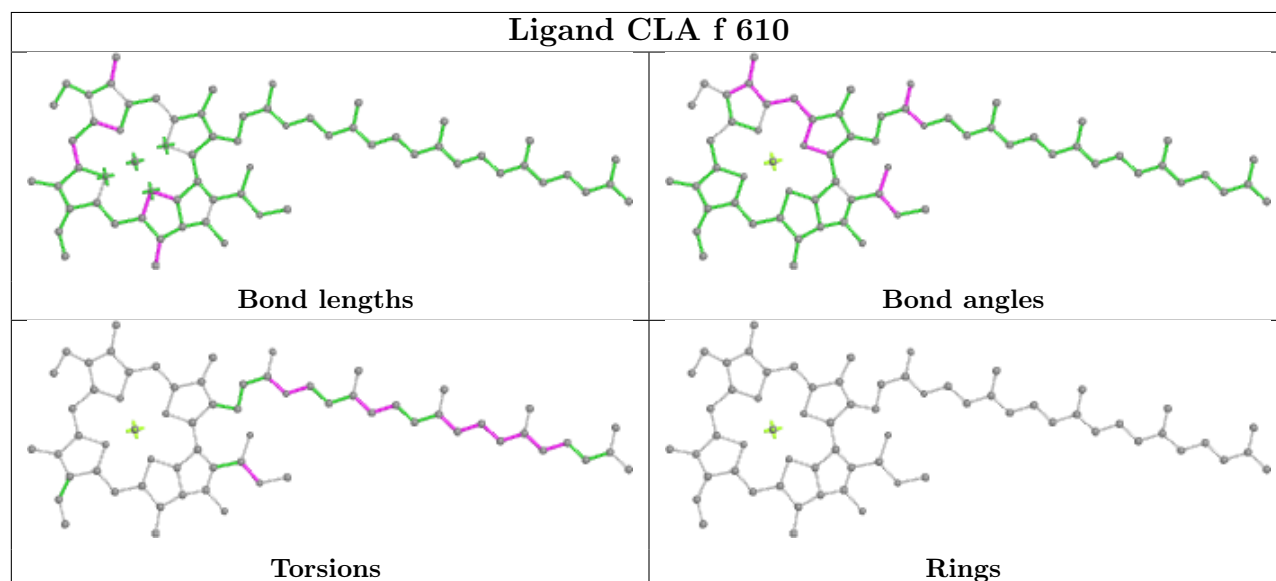
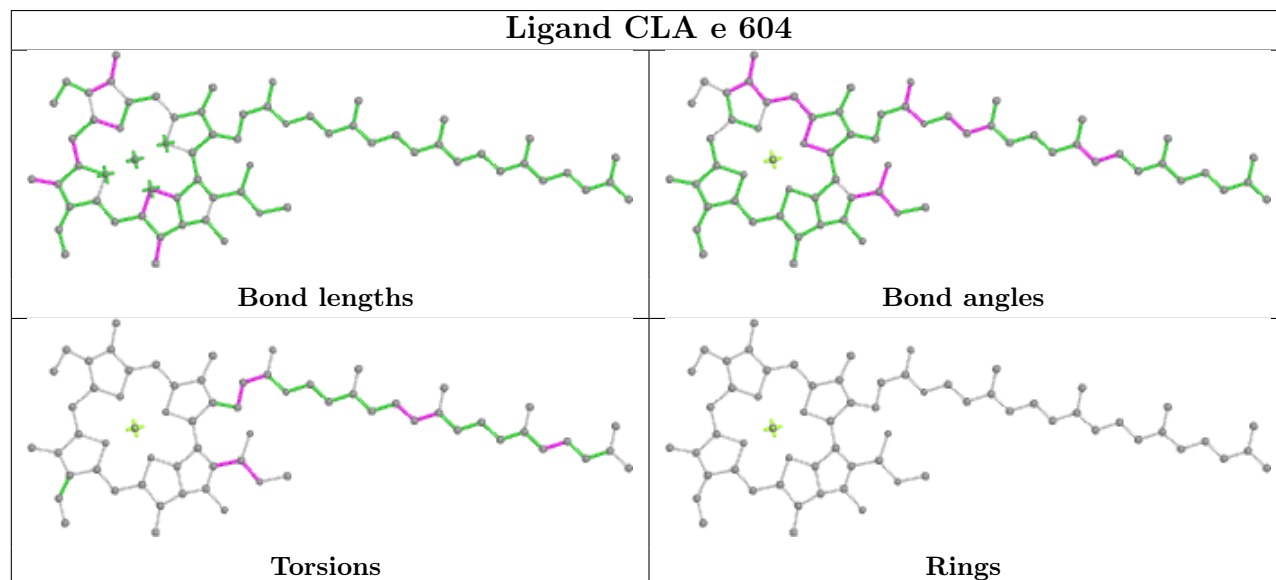
Torsions

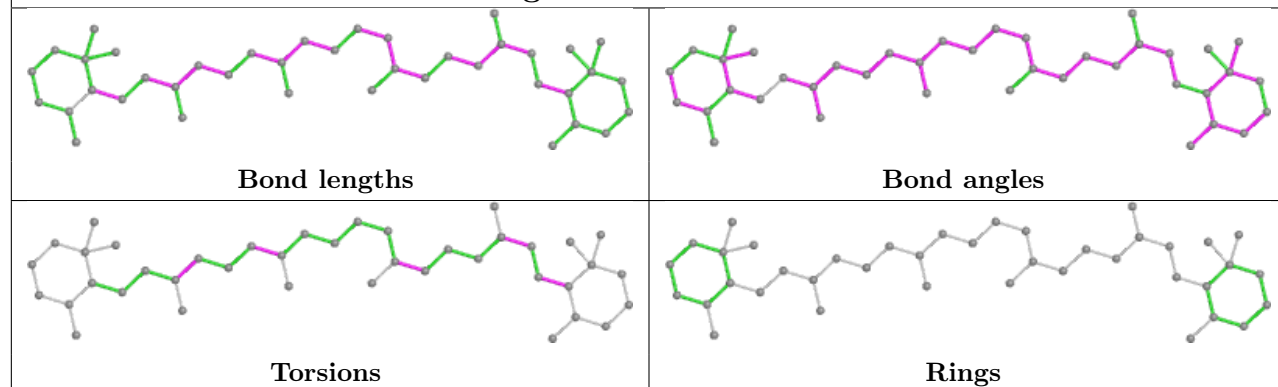
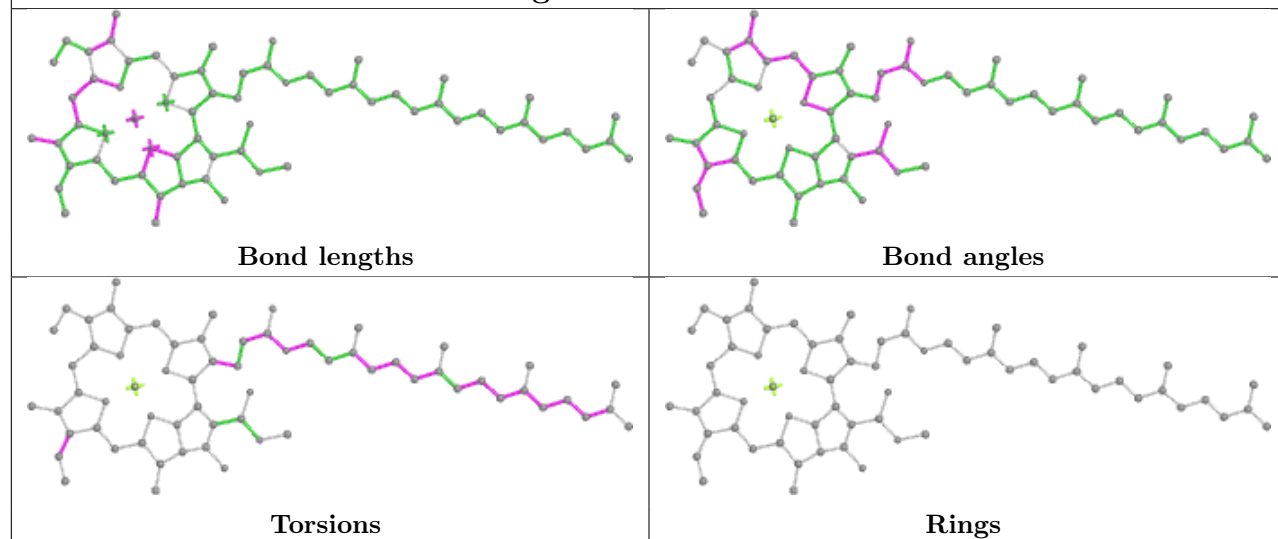
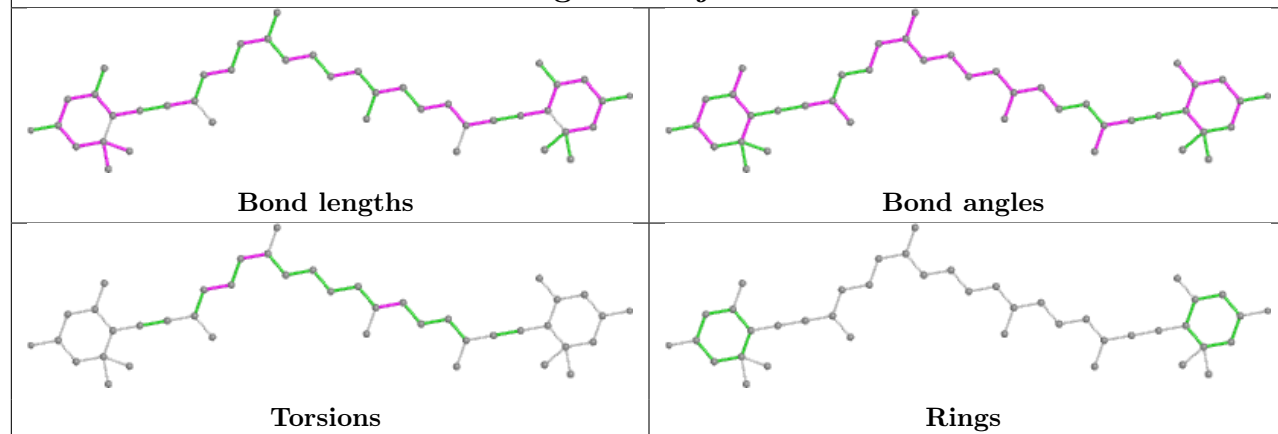


Rings

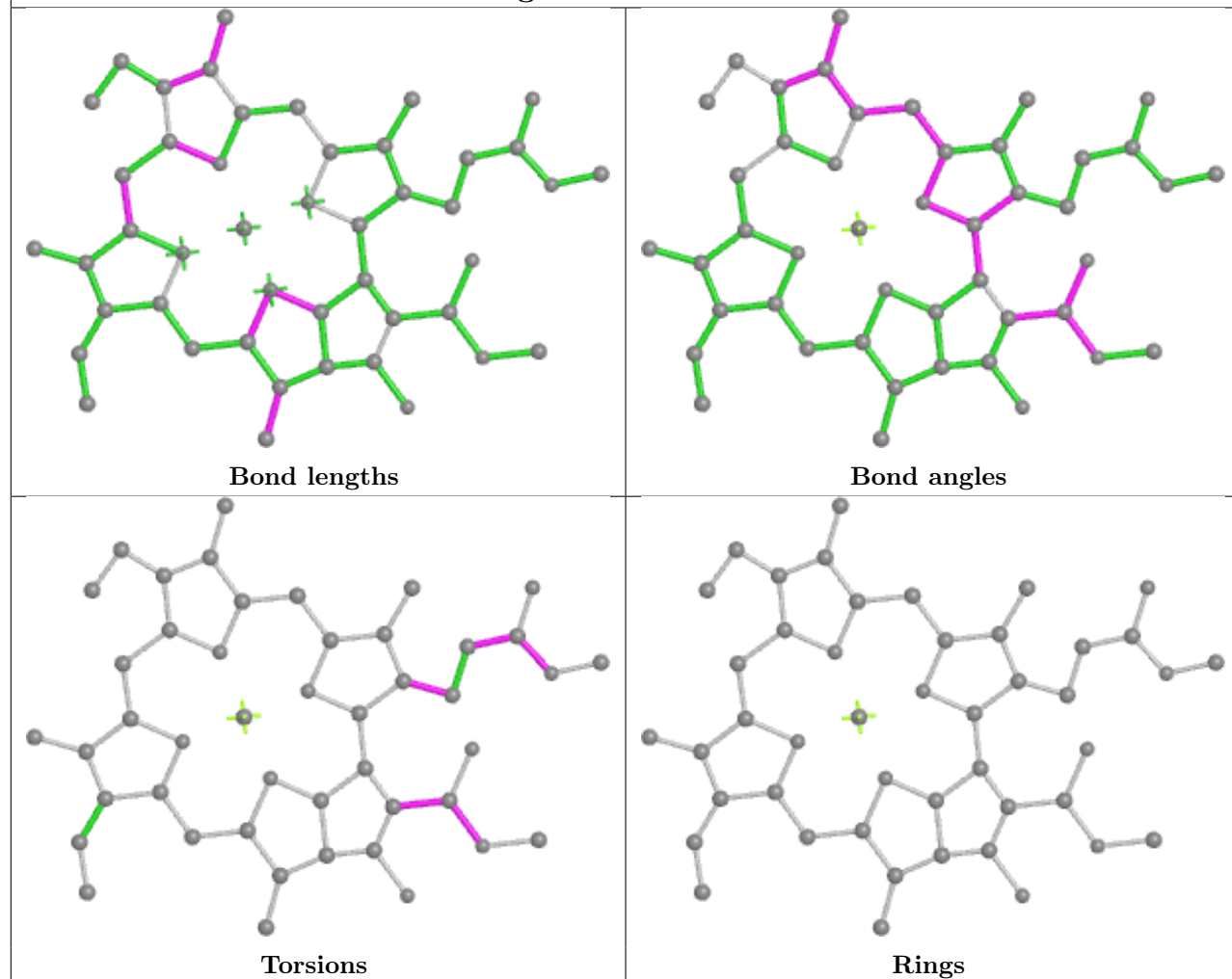




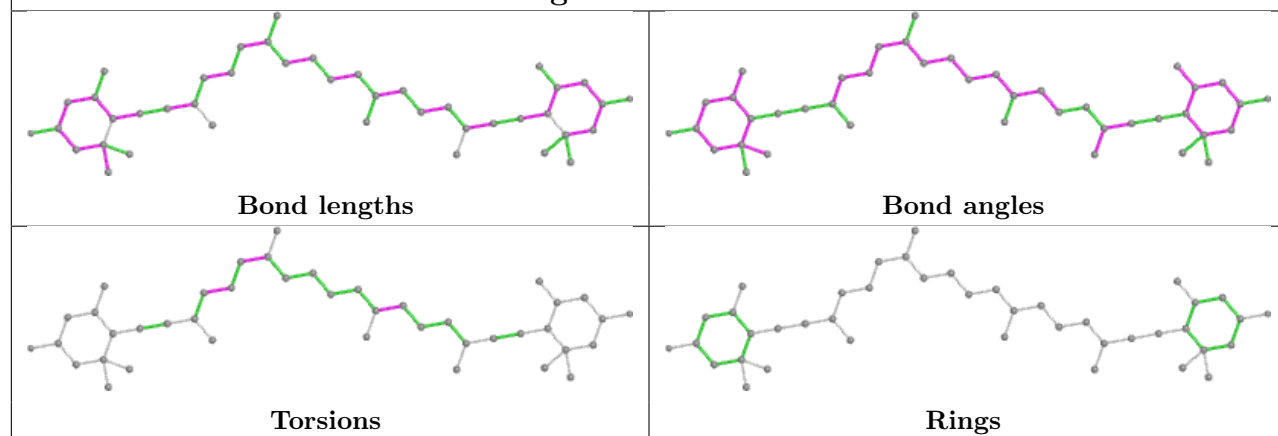
**Ligand CLA B 801****Ligand CLA f 610****Ligand CLA e 604**

**Ligand WVN A 847****Ligand CLA B 836****Ligand II0 j 318**

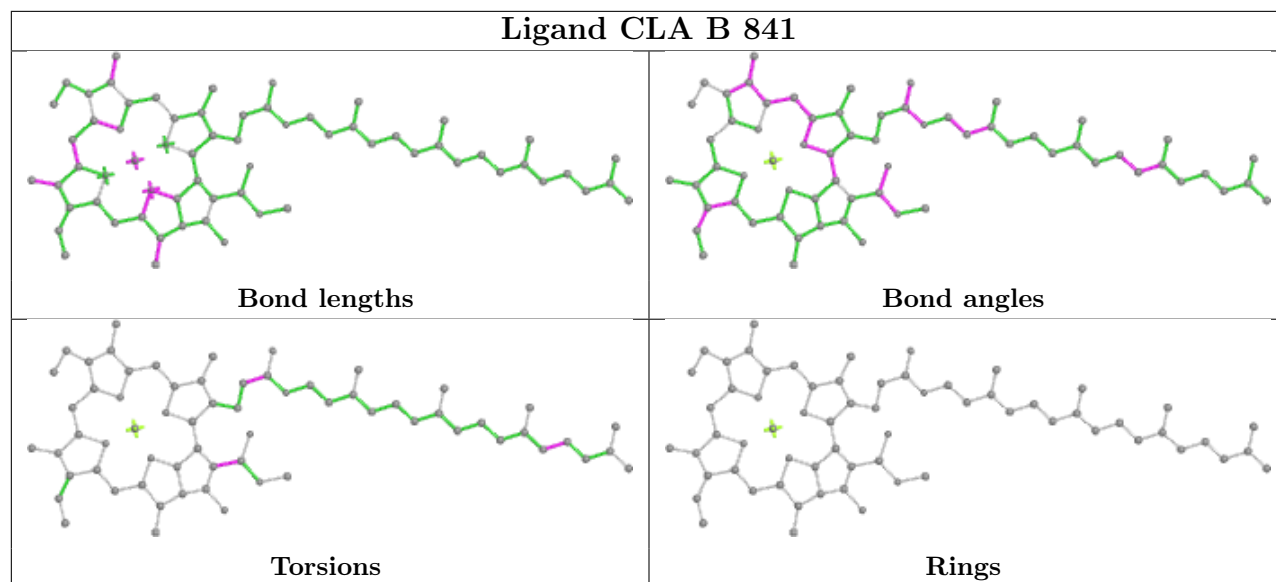
## Ligand CLA e 608



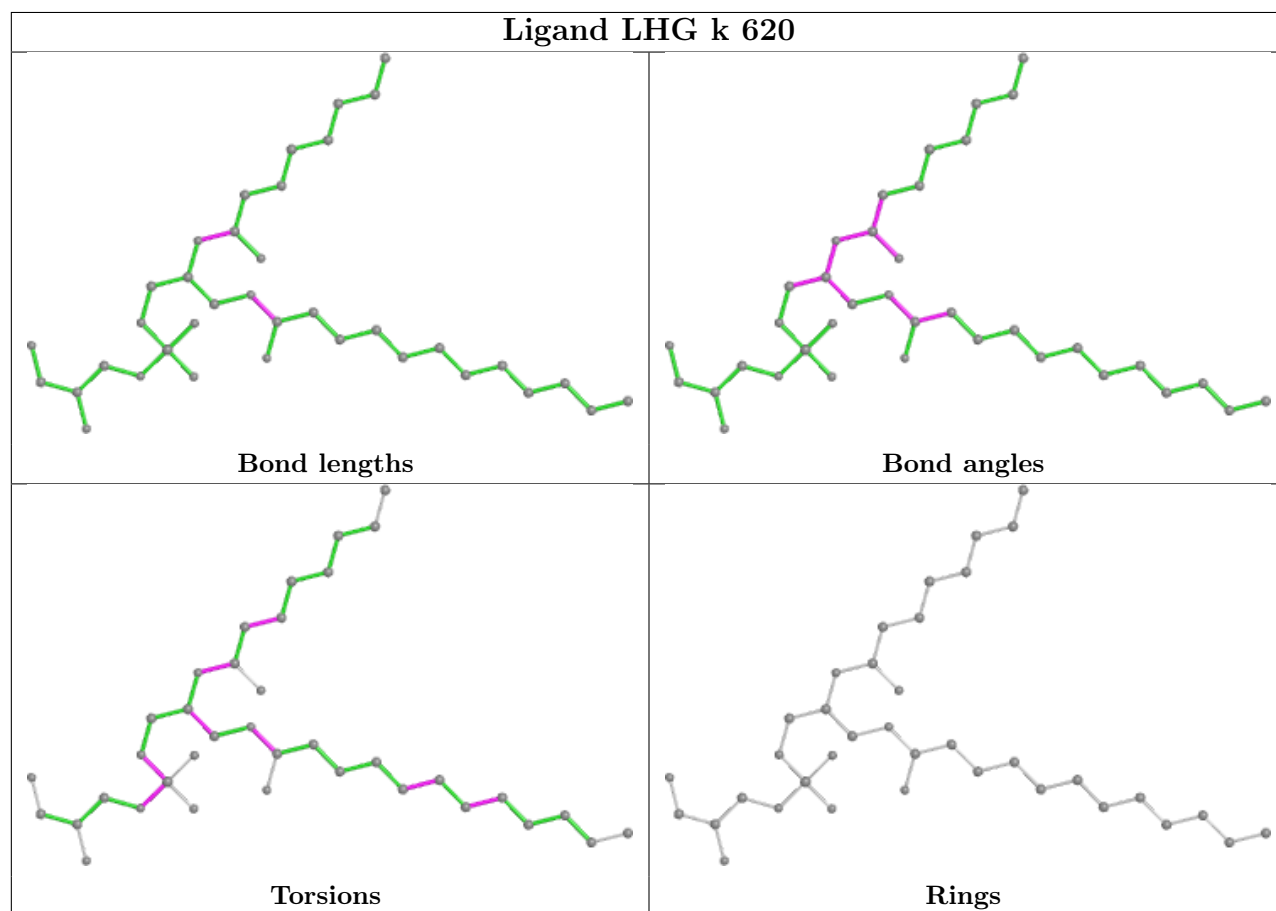
## Ligand II0 k 619

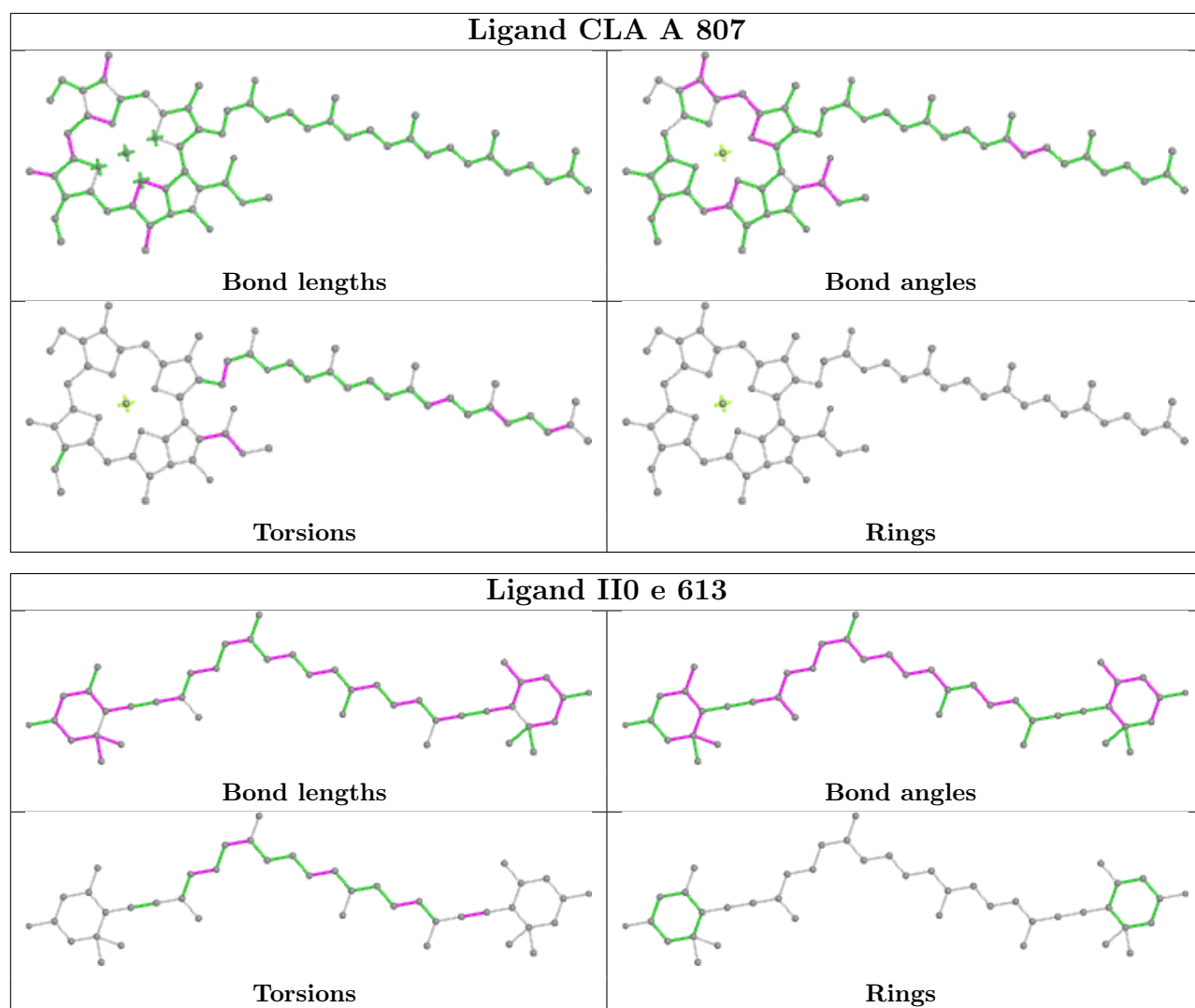


## Ligand CLA B 841



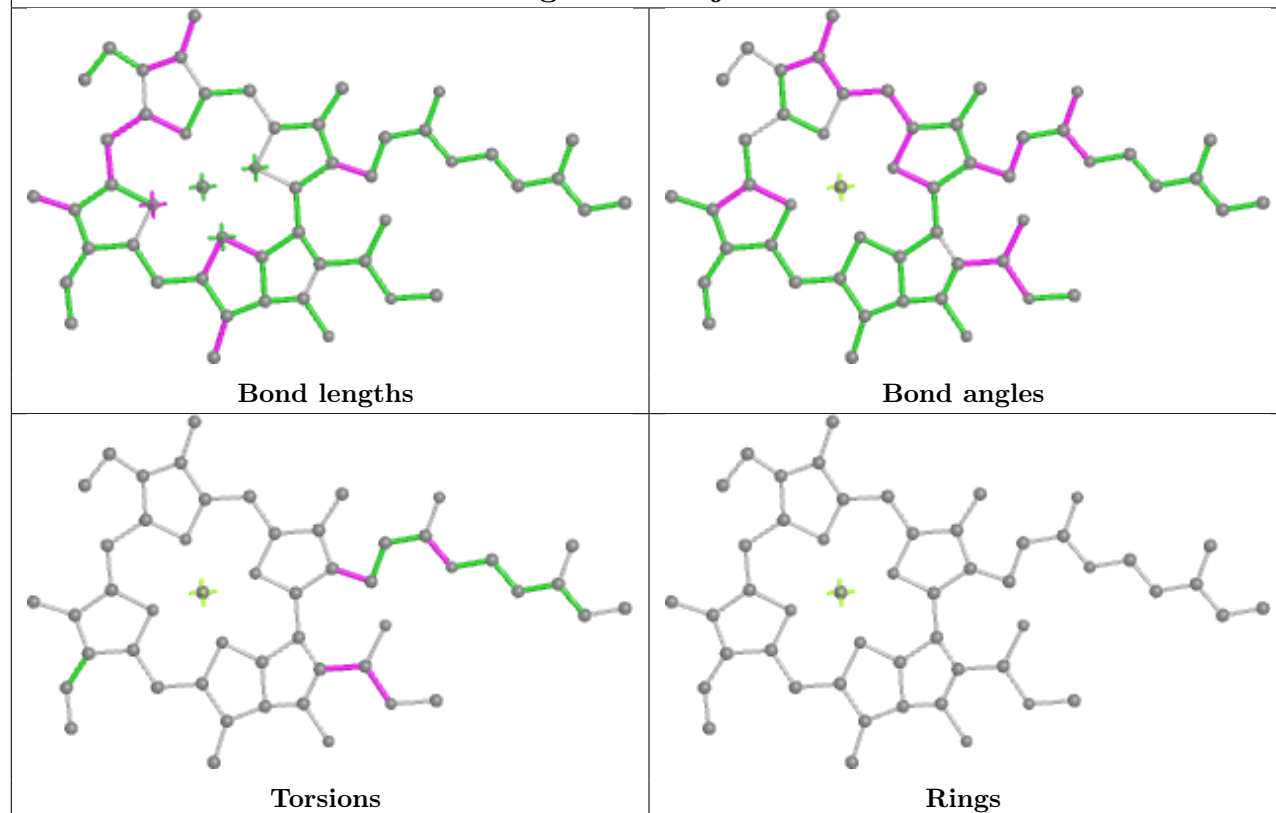
## Ligand LHG k 620



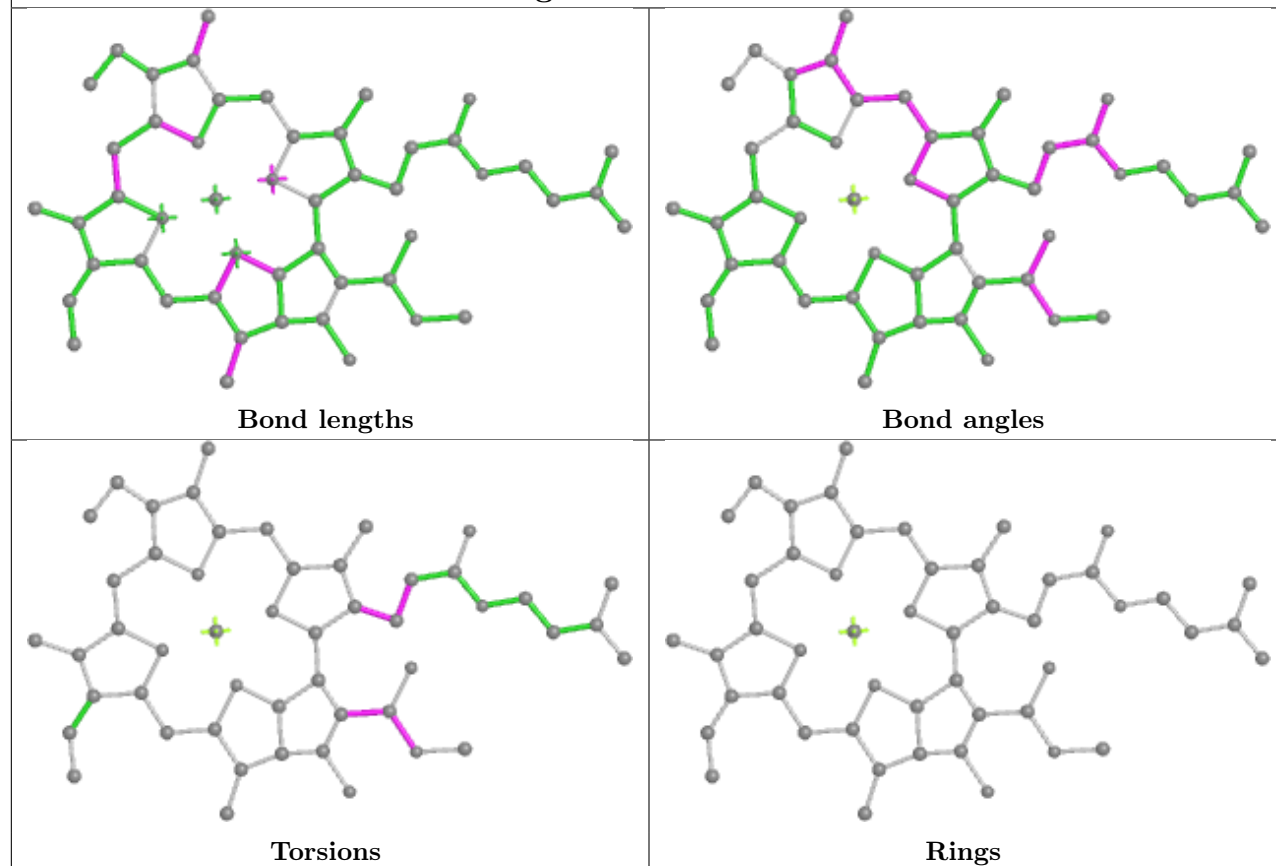


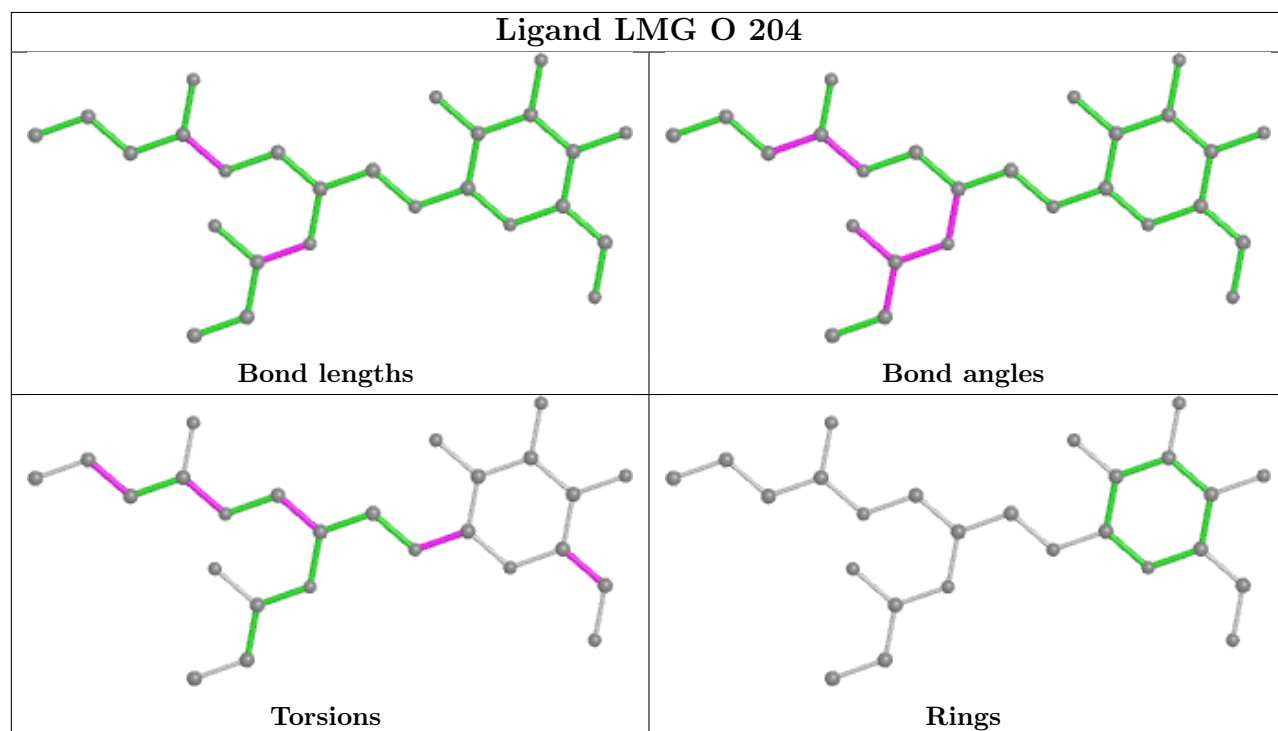
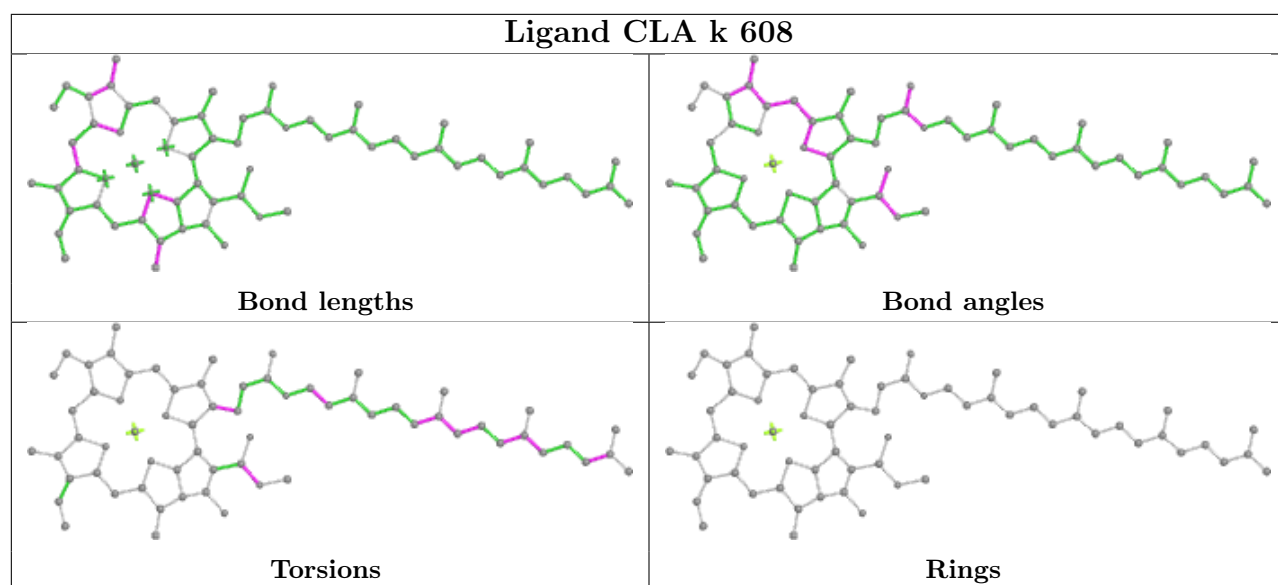


## Ligand CLA j 307

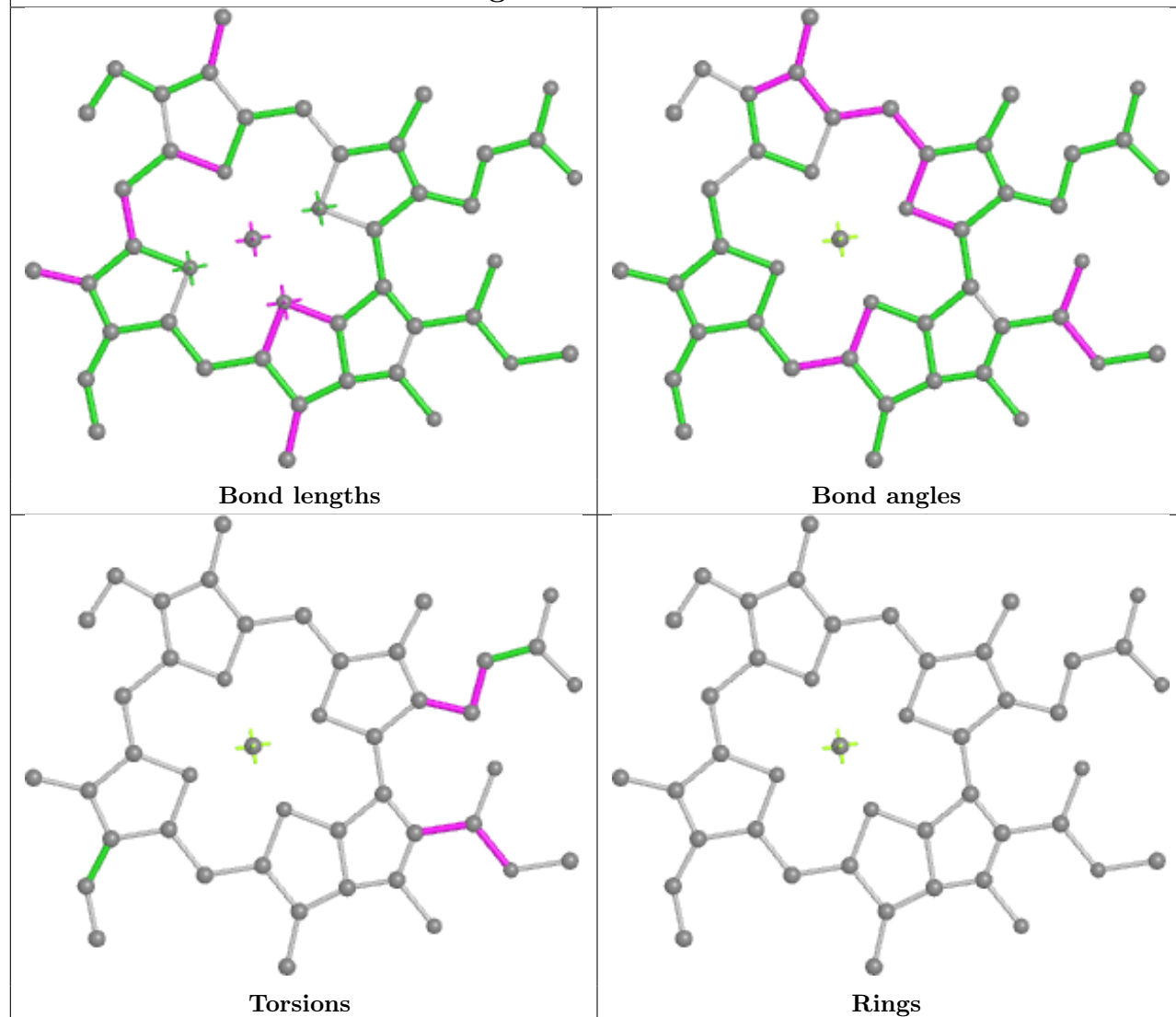


## Ligand CLA d 301

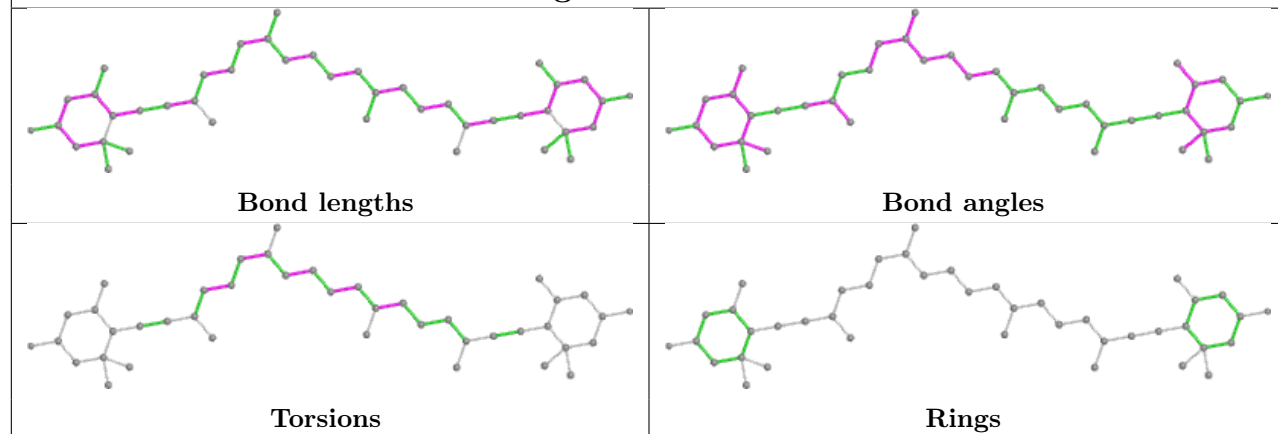


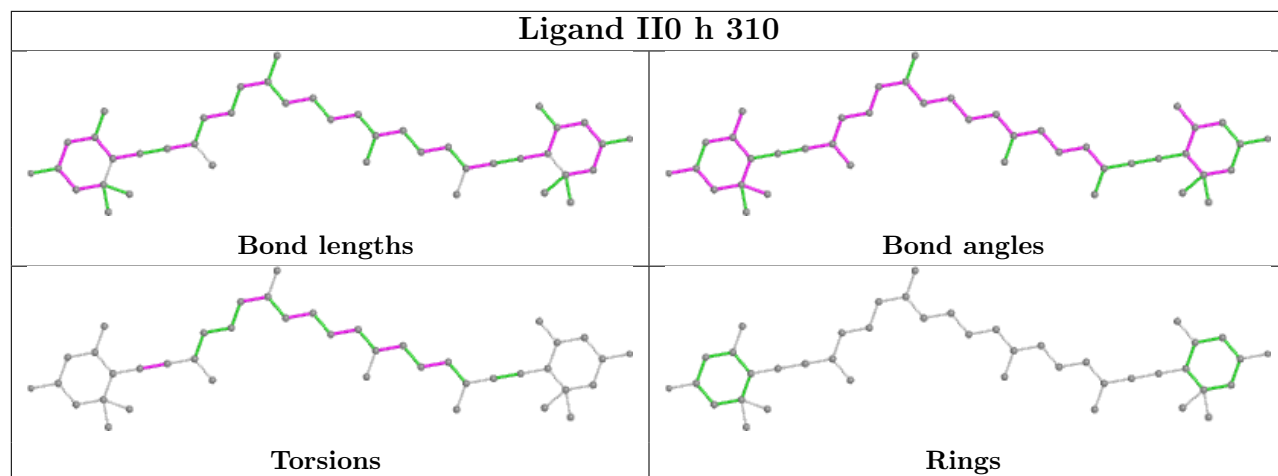
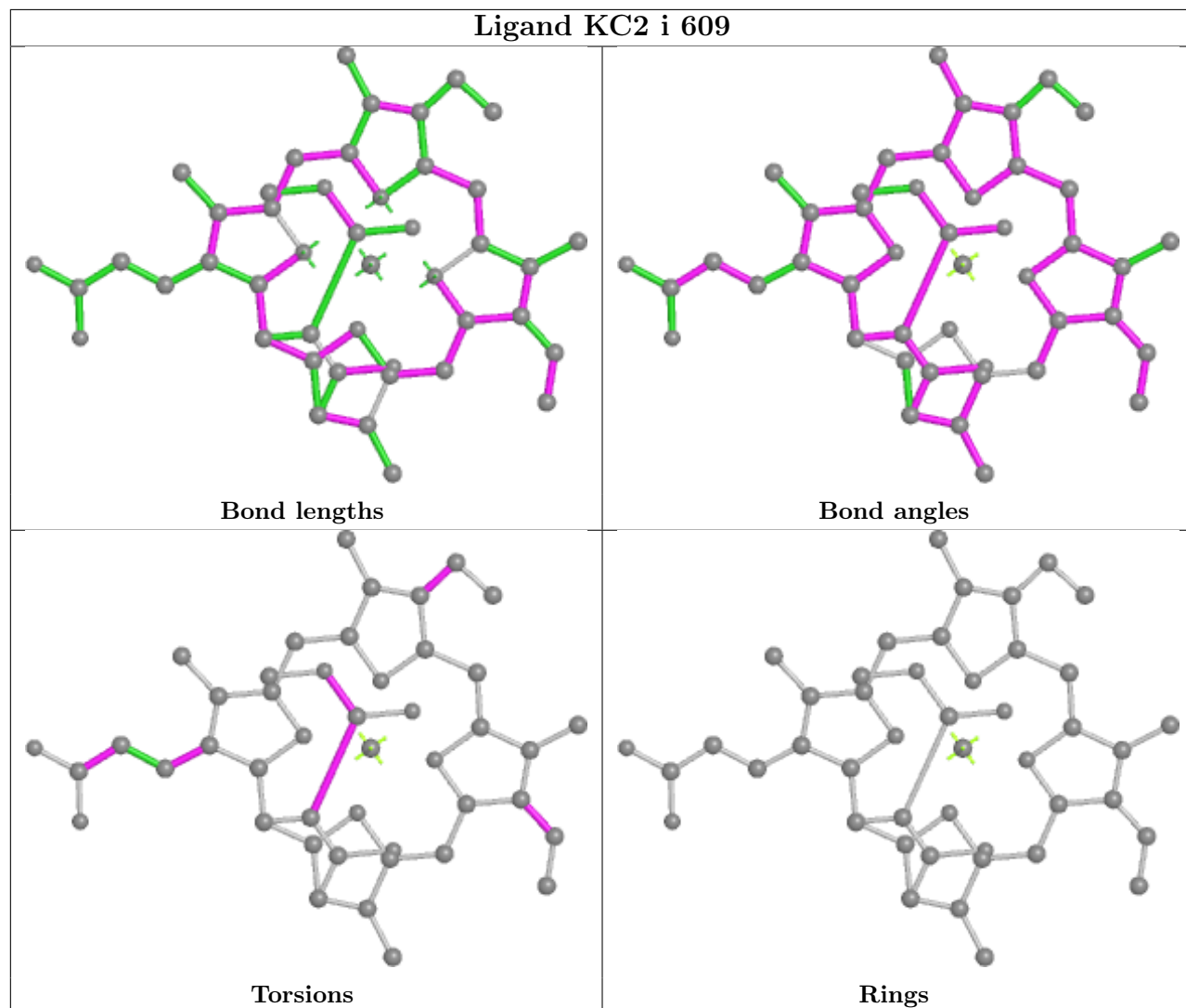


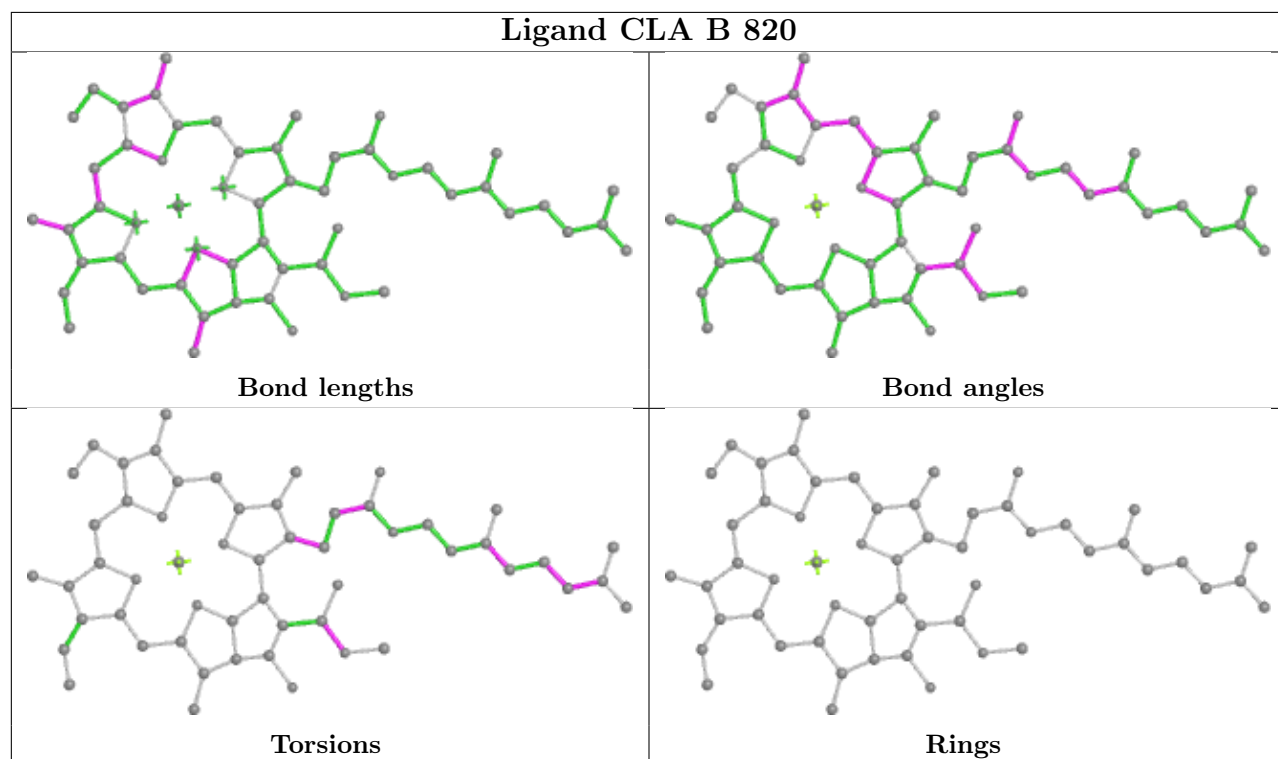
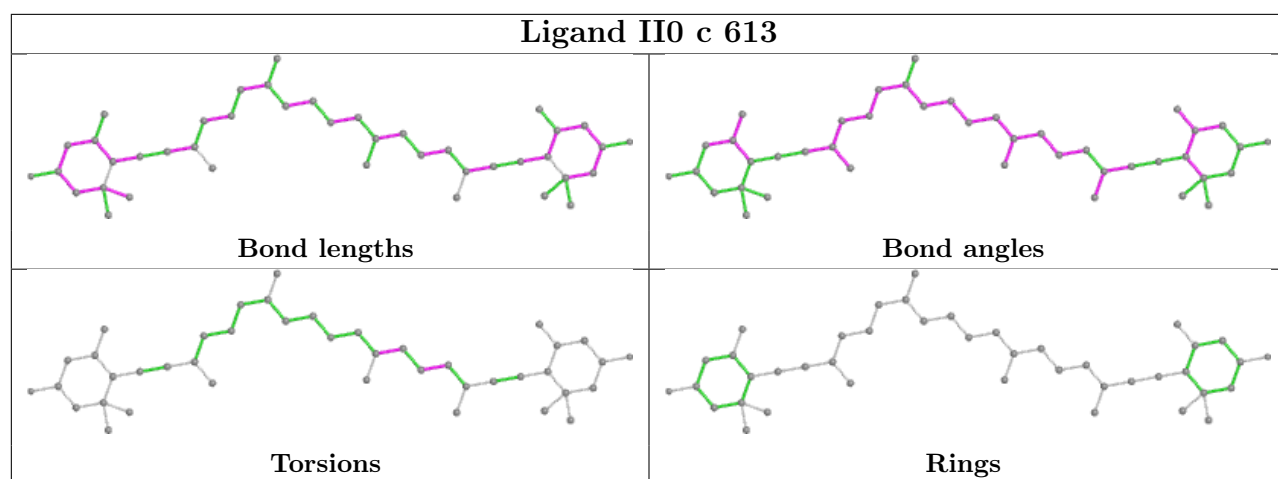
## Ligand CLA A 815



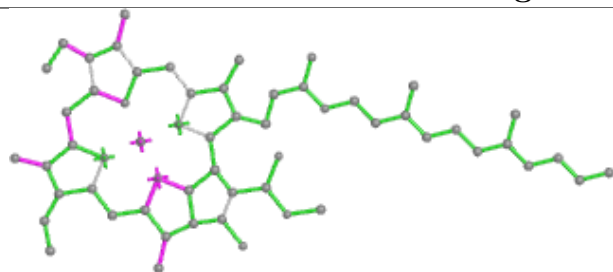
## Ligand II0 f 618



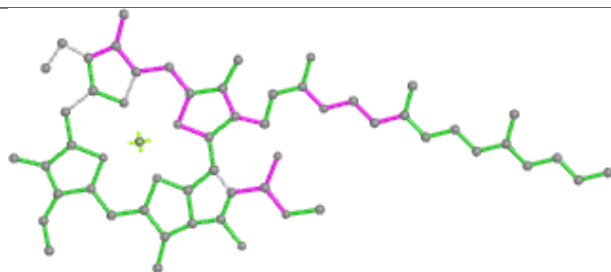
**Ligand II0 h 310****Ligand KC2 i 609**



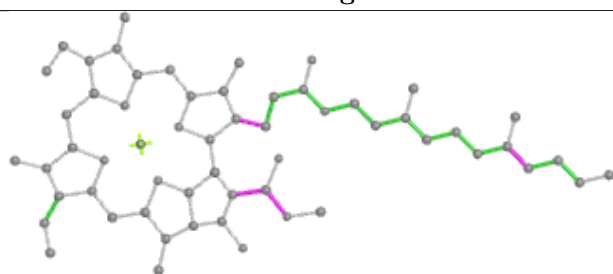
## Ligand CLA B 832



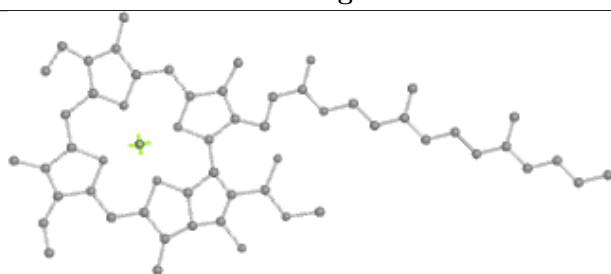
Bond lengths



Bond angles

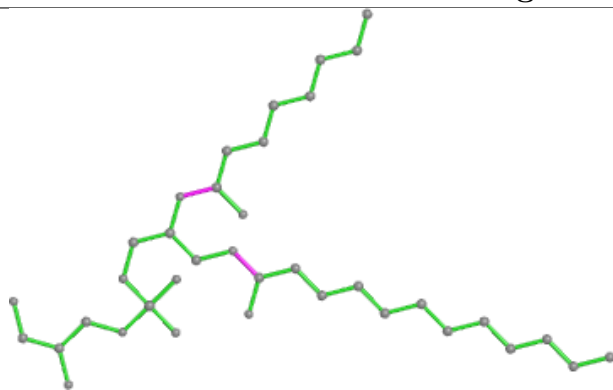


Torsions

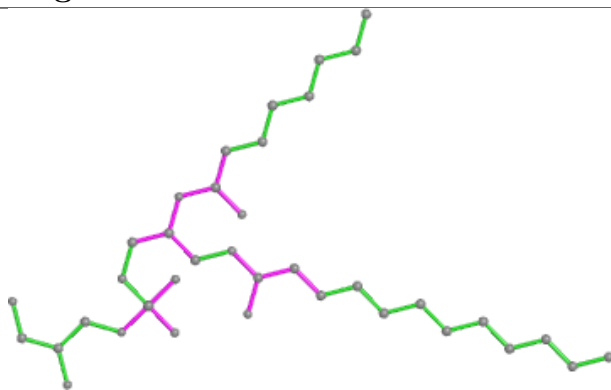


Rings

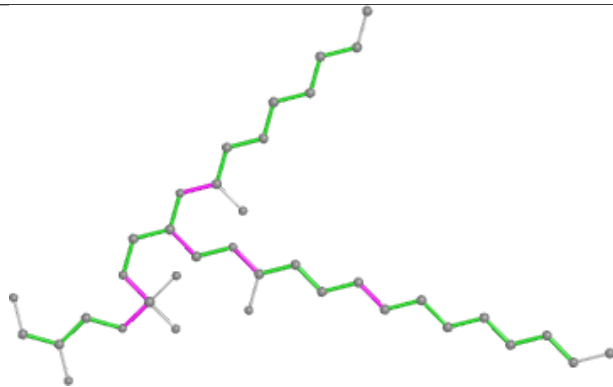
## Ligand LHG g 321



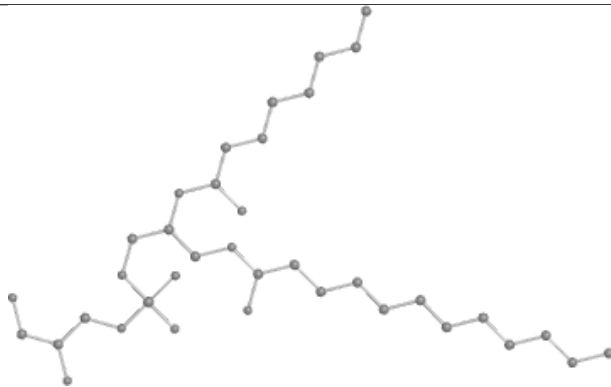
Bond lengths



Bond angles

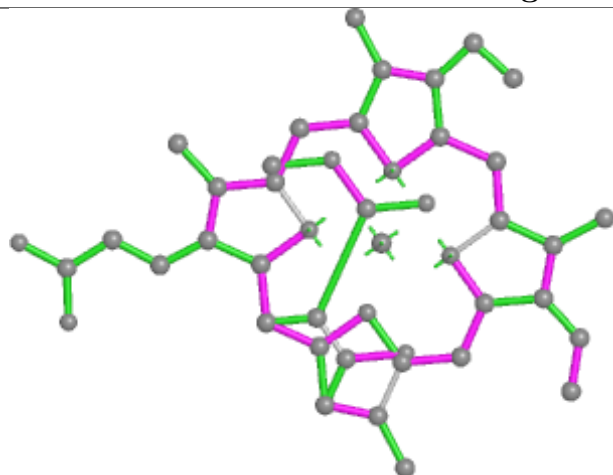


Torsions

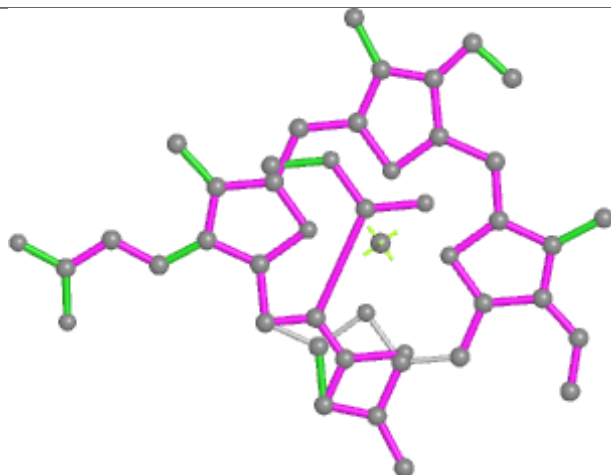


Rings

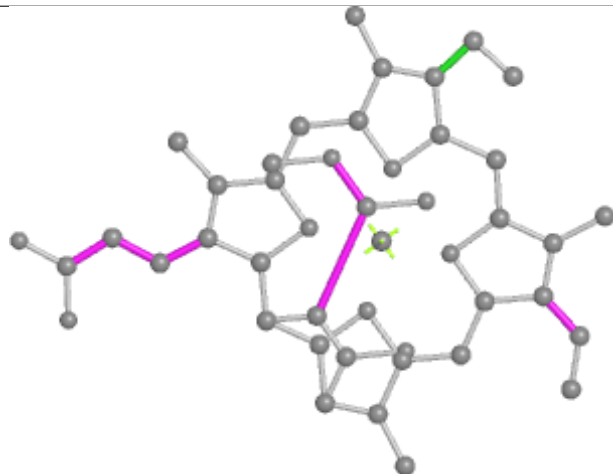
## Ligand KC2 c 610



Bond lengths



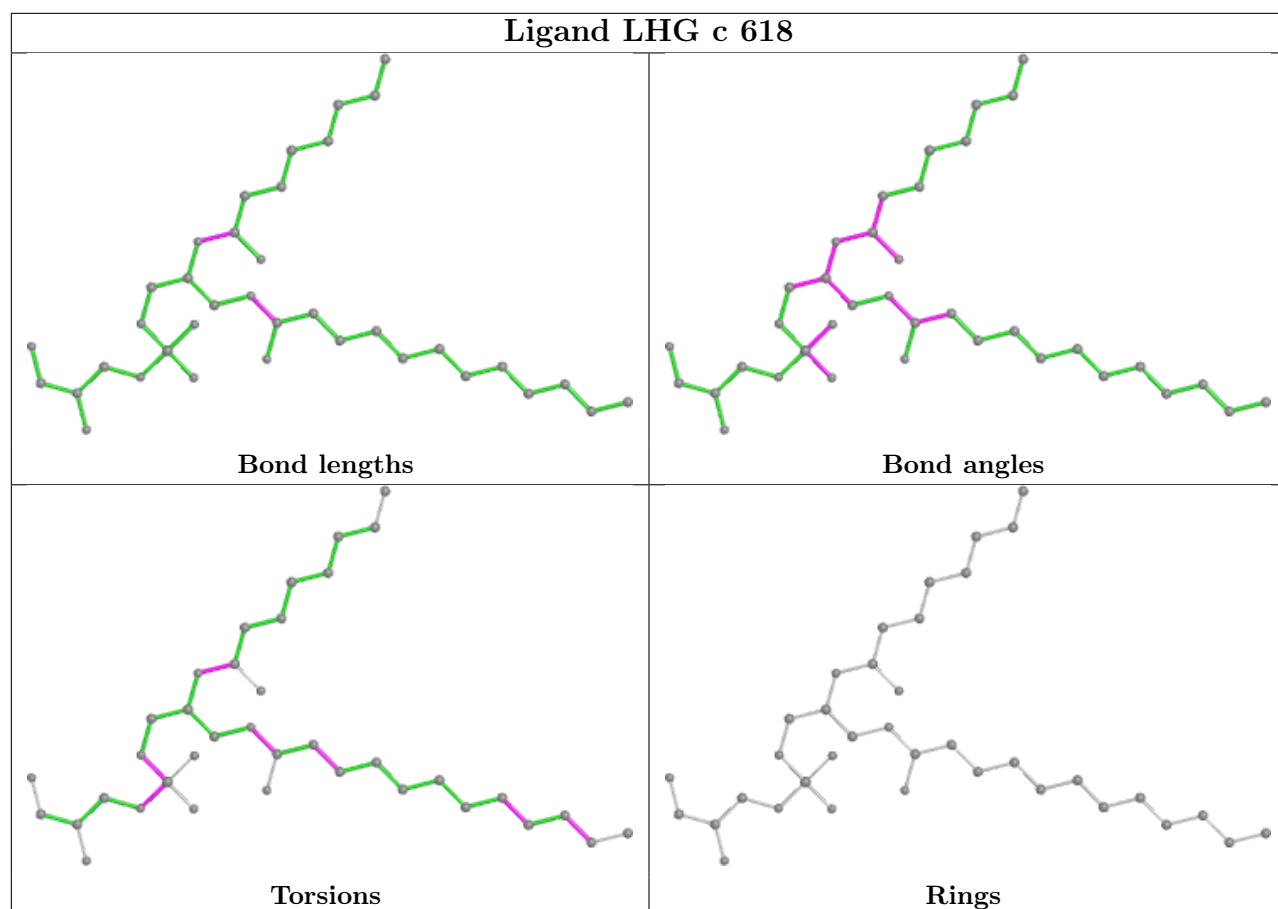
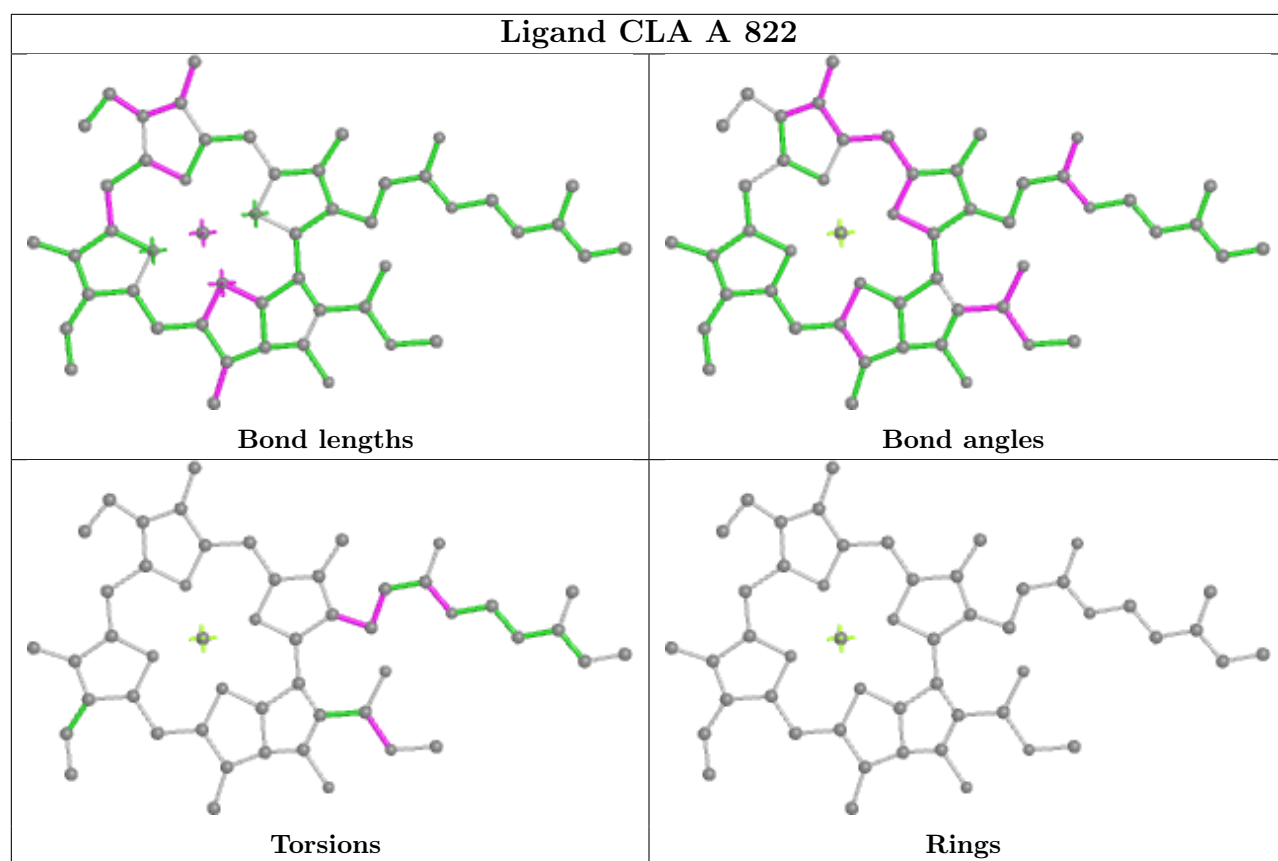
Bond angles



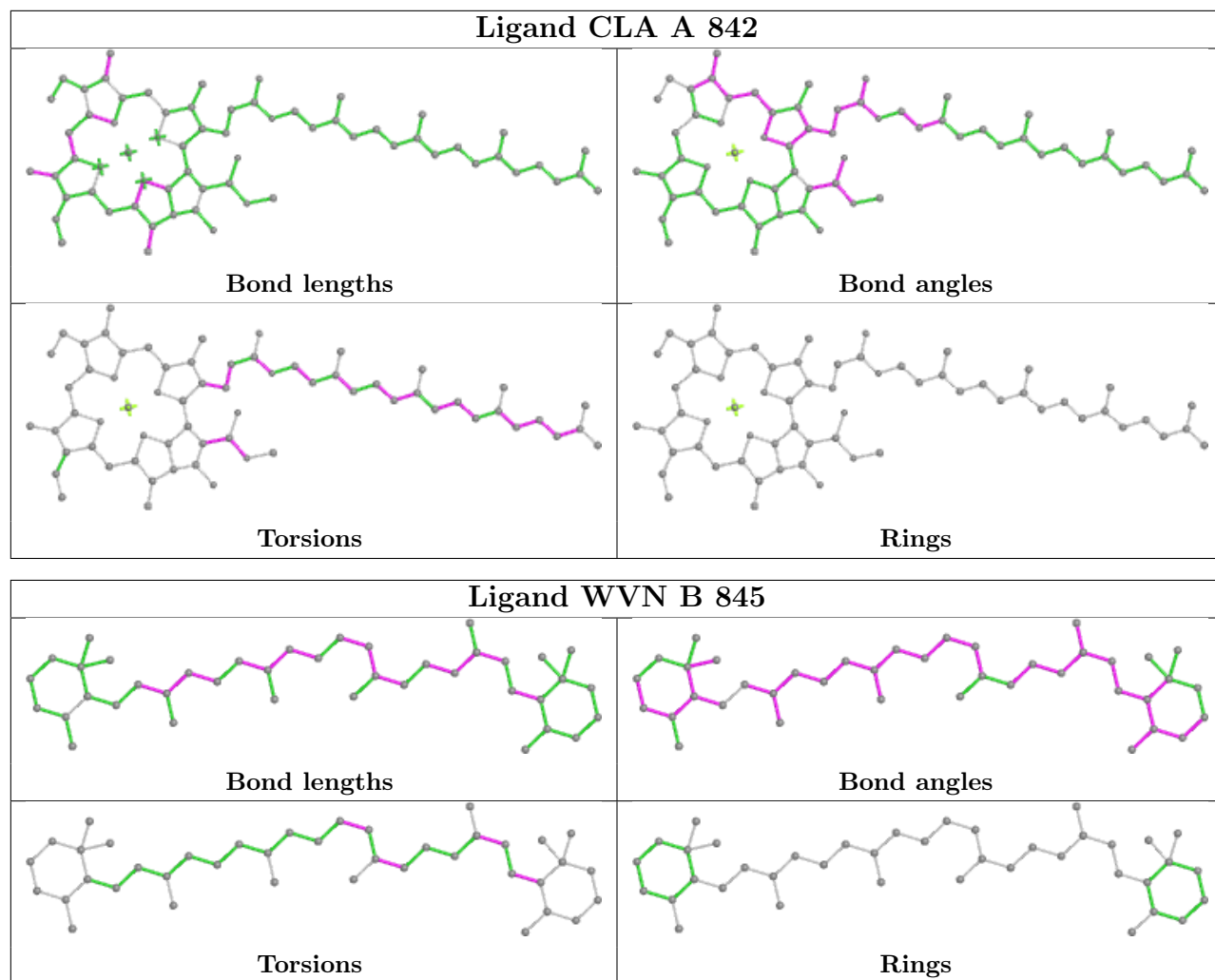
Torsions



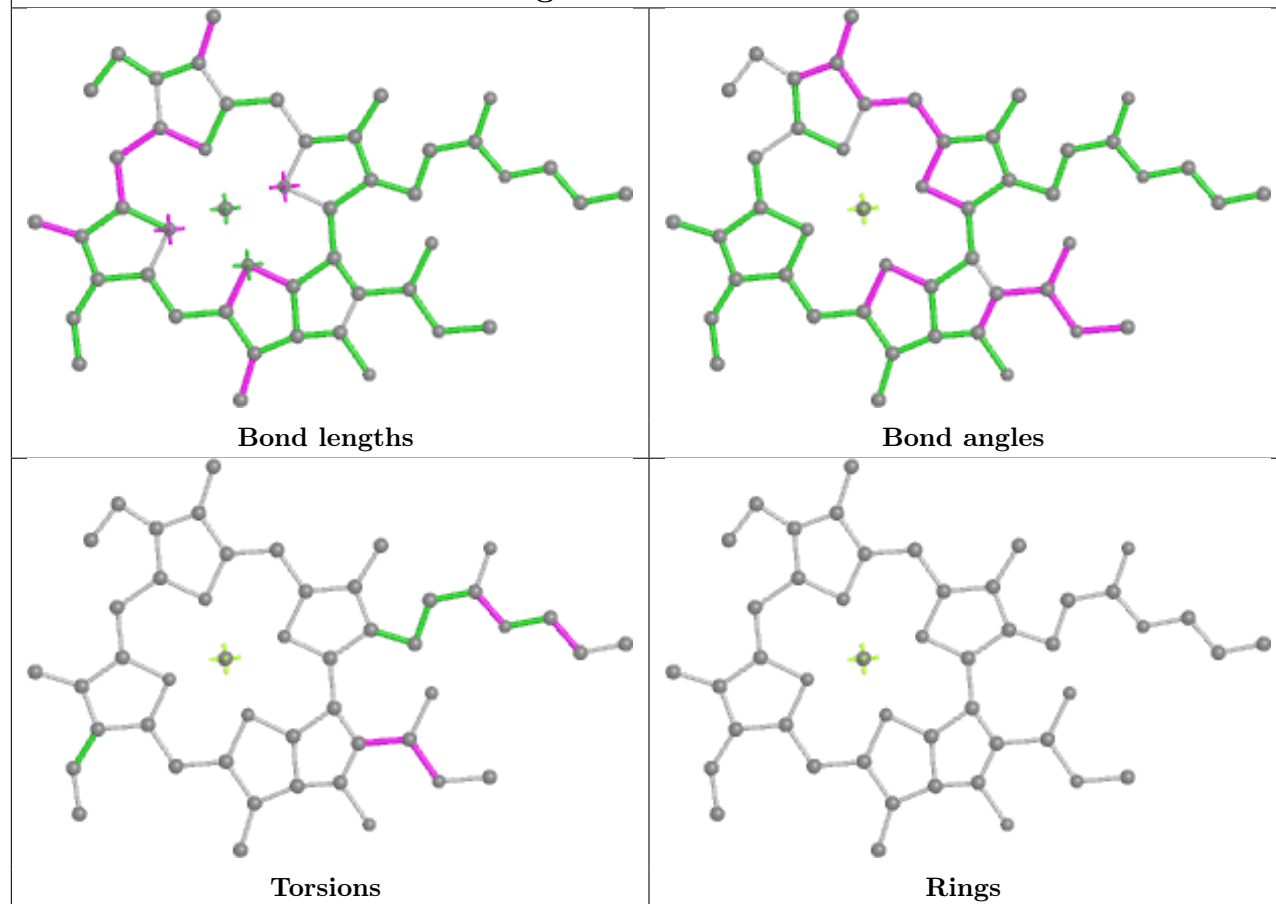
Rings



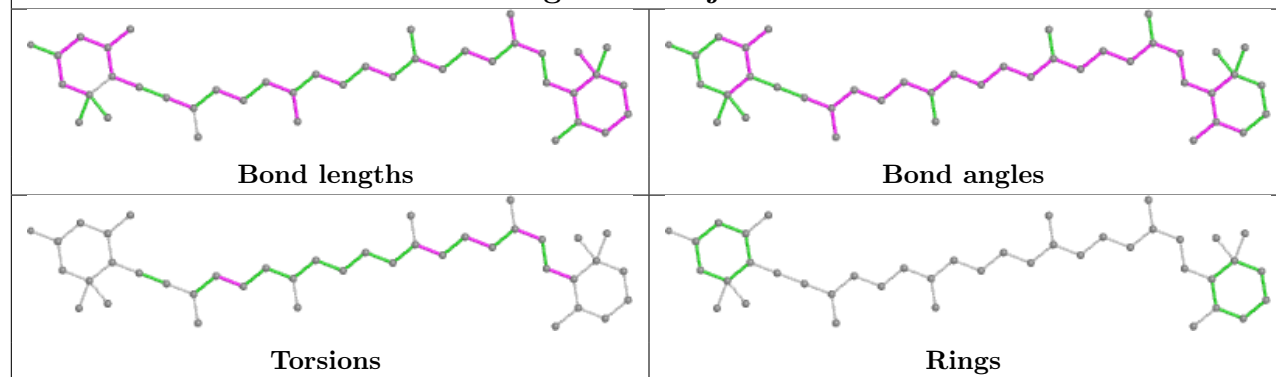




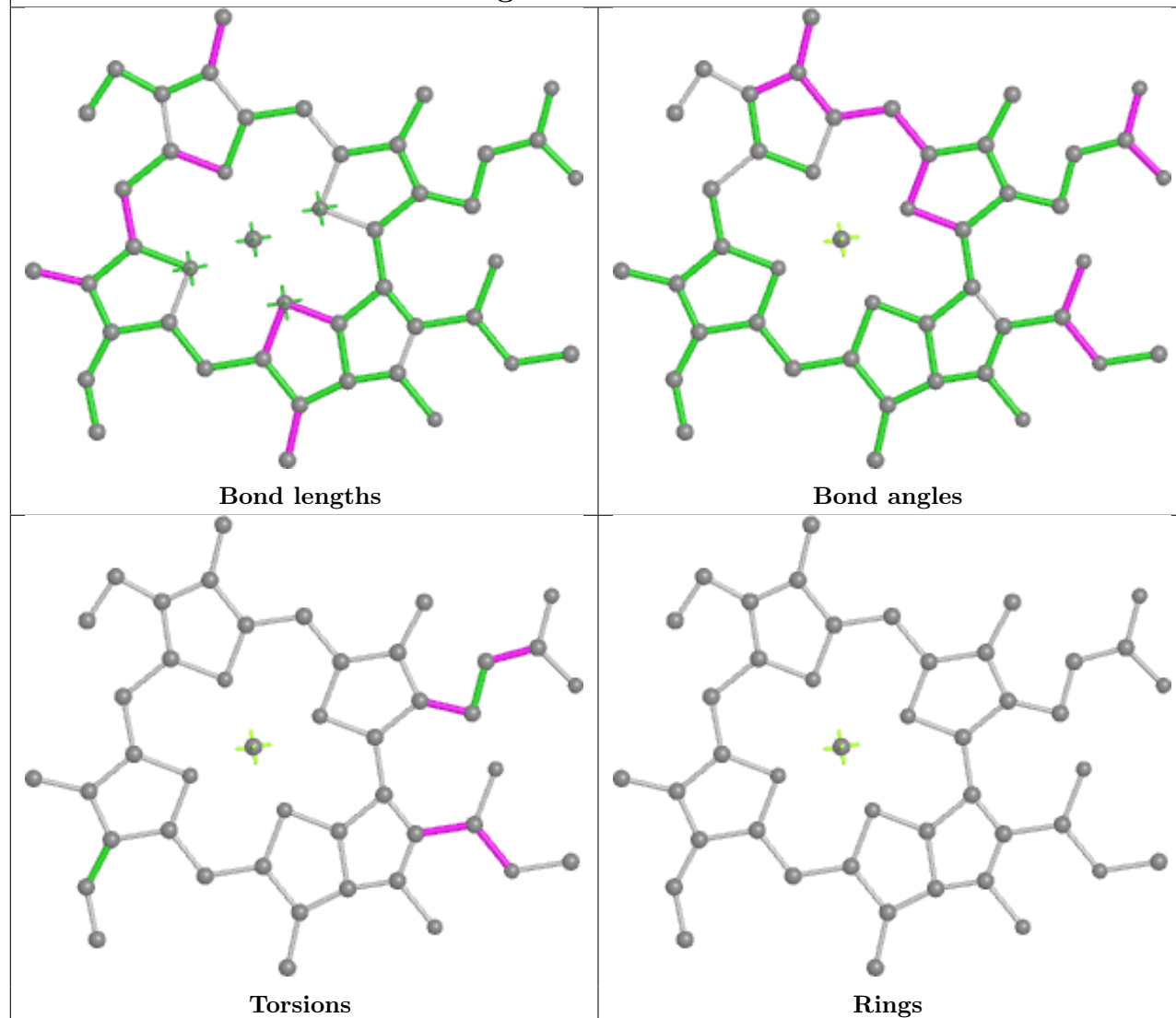
## Ligand CLA a 312



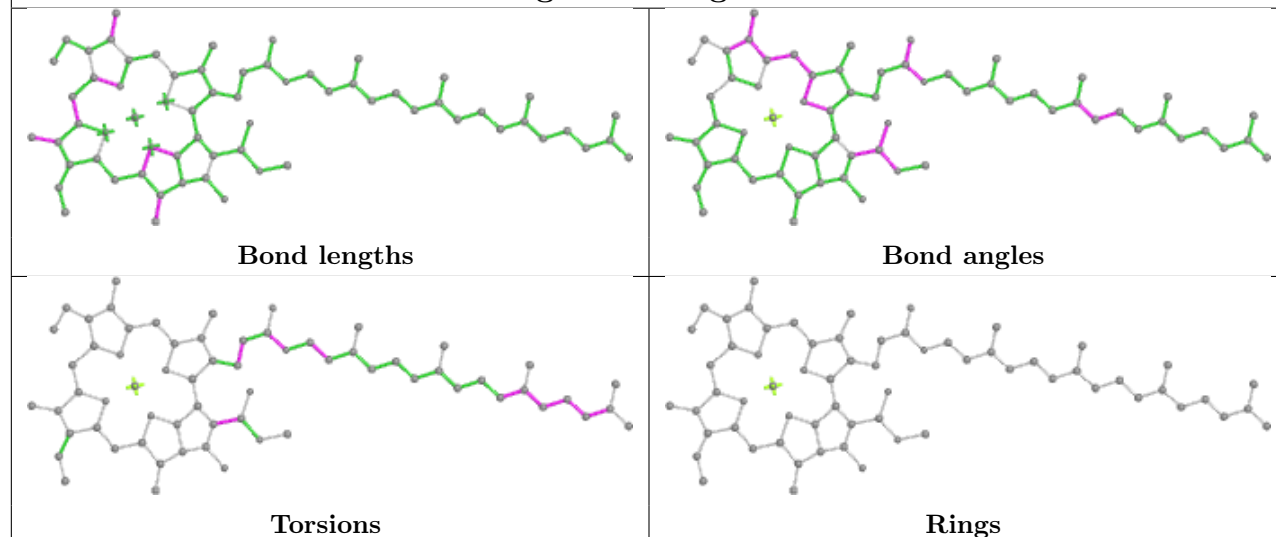
## Ligand IHT j 317

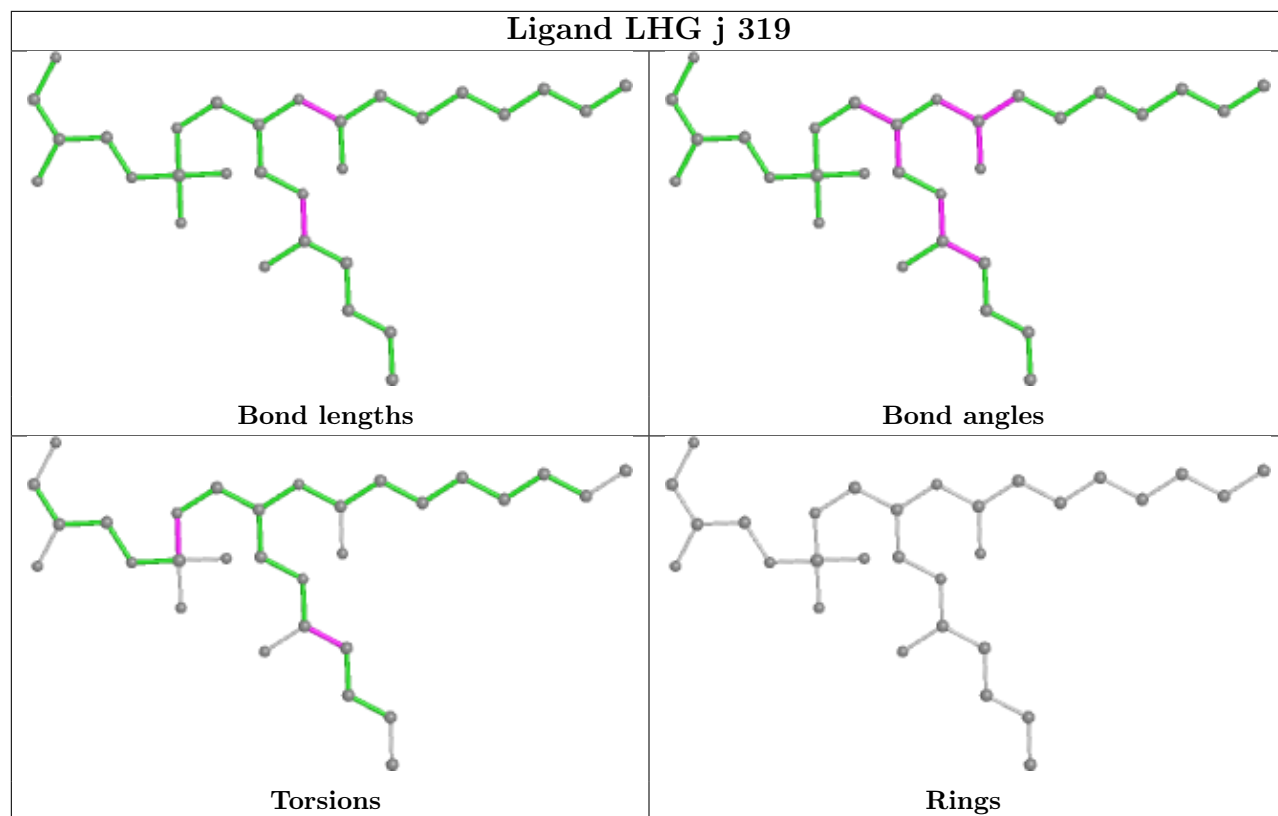


## Ligand CLA f 605

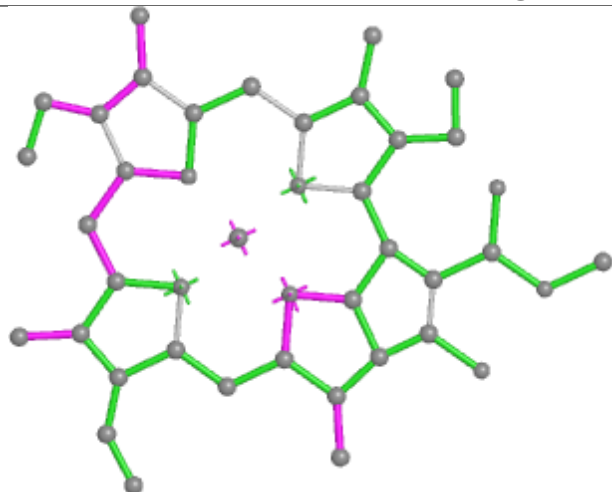


## Ligand CLA g 322

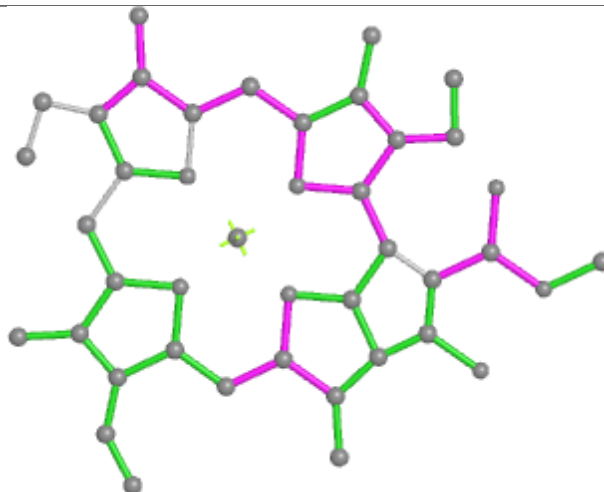




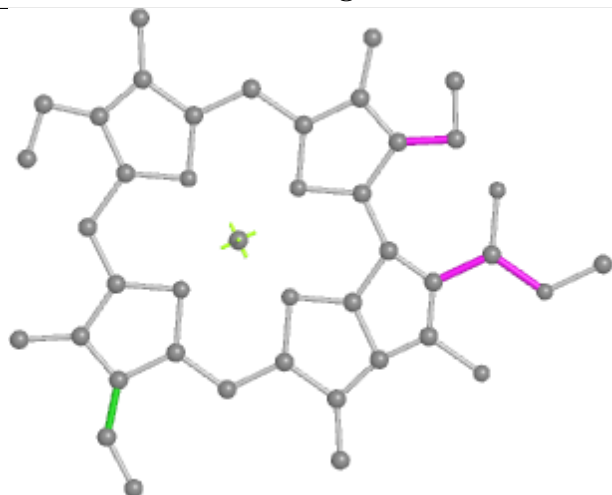
## Ligand CLA K 102



Bond lengths



Bond angles

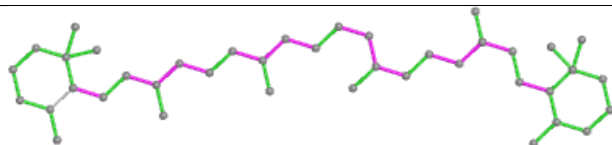


Torsions

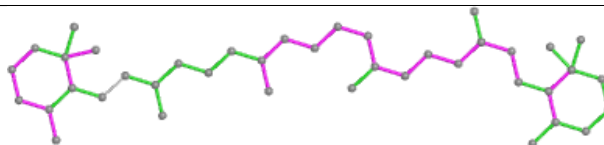


Rings

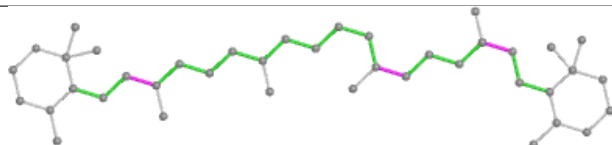
## Ligand WVN R 201



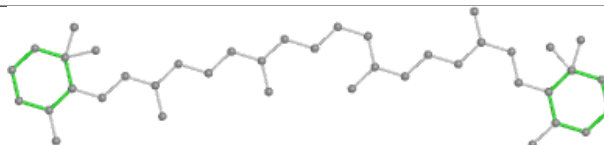
Bond lengths



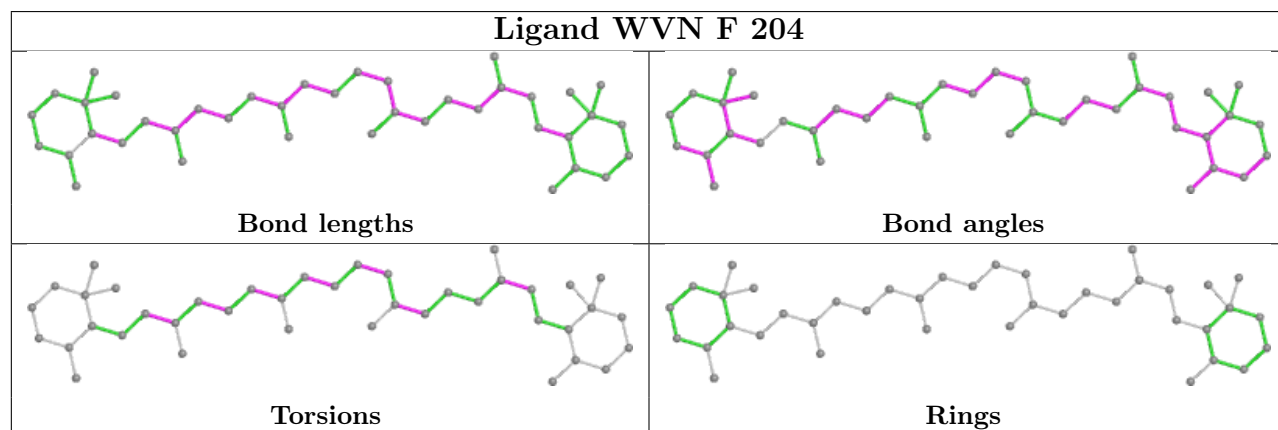
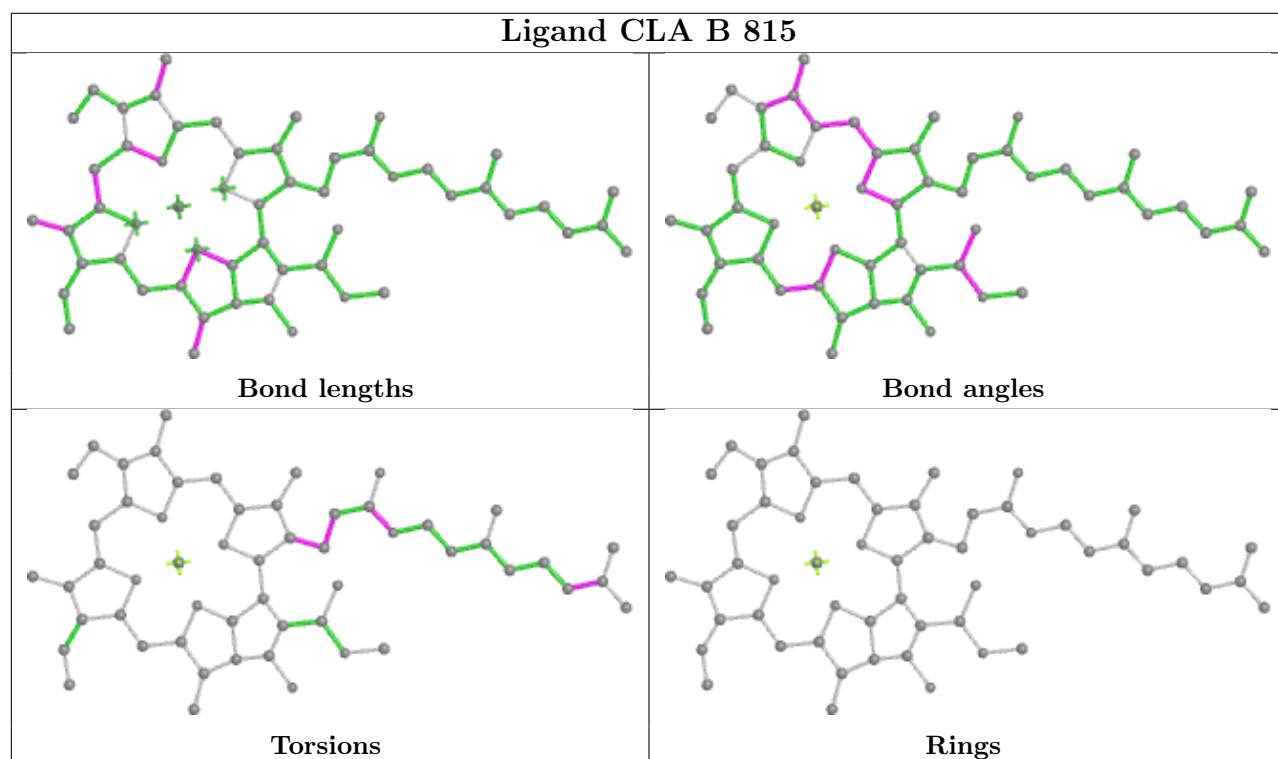
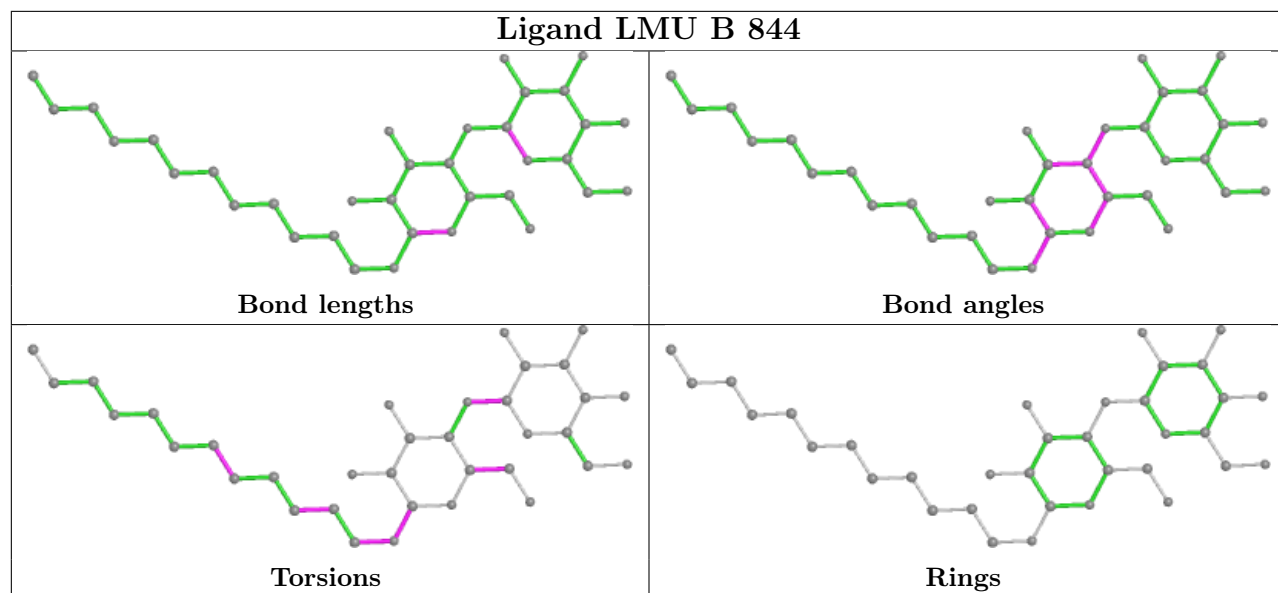
Bond angles

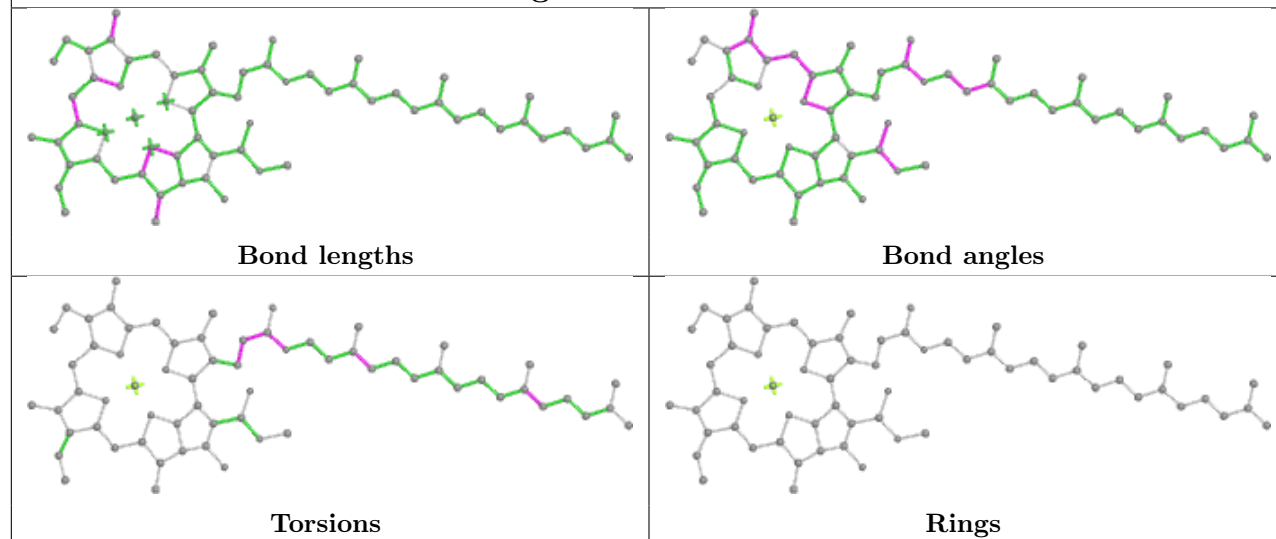
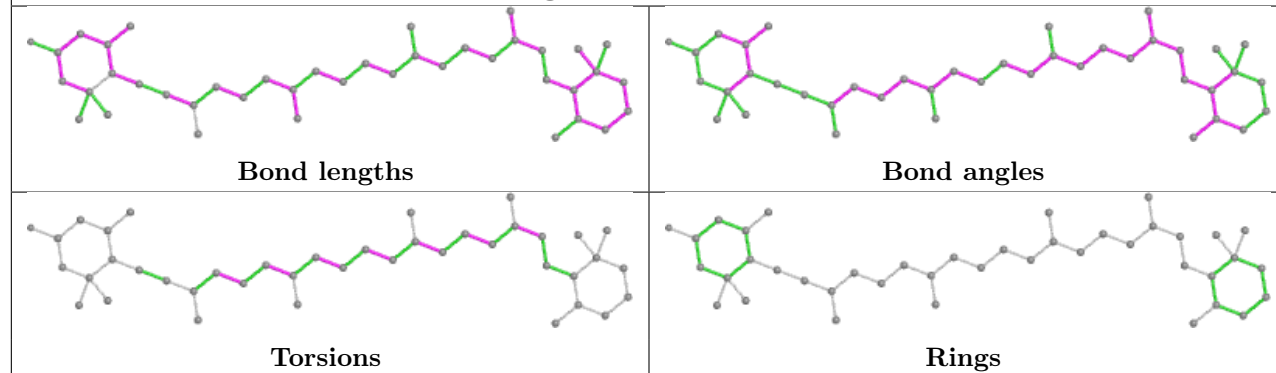
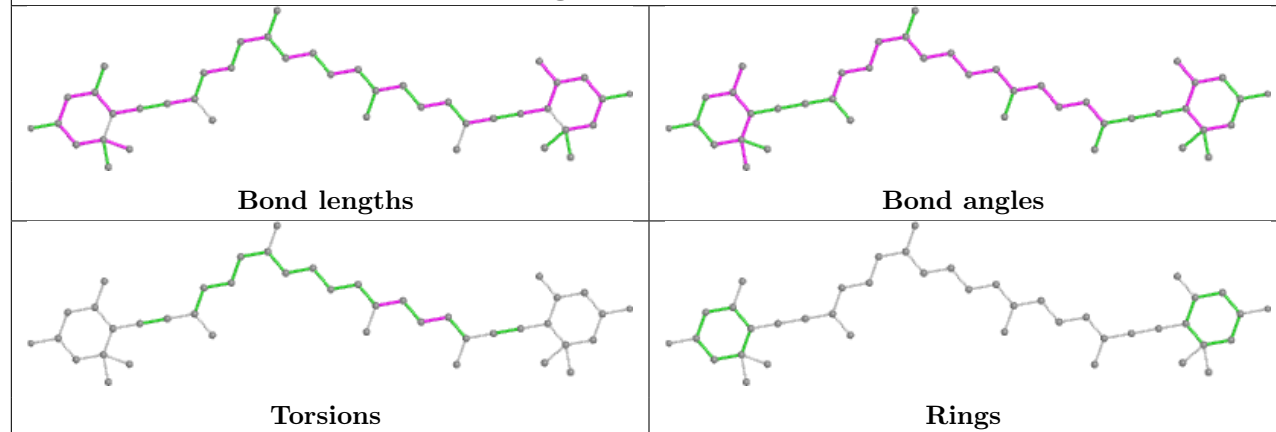


Torsions

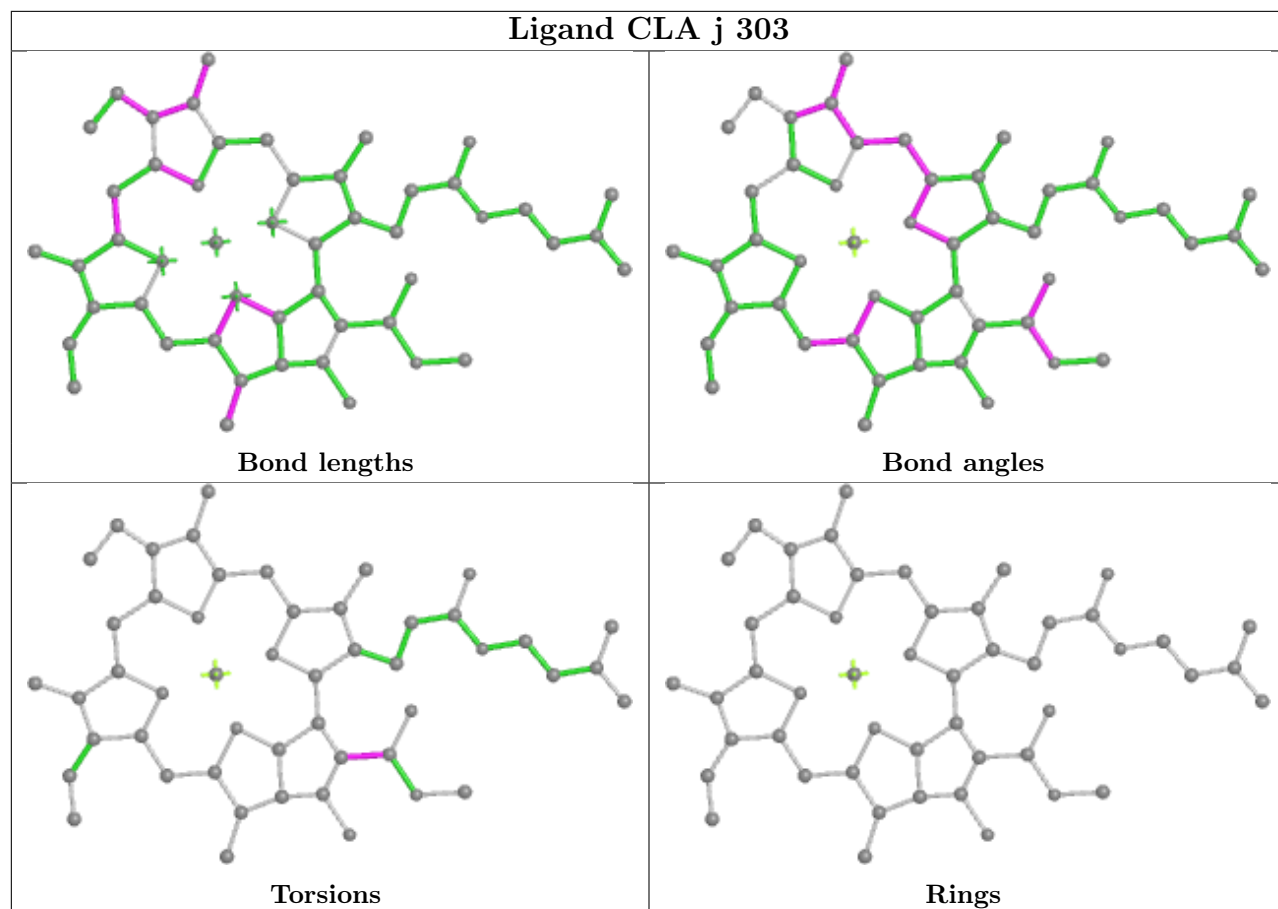


Rings



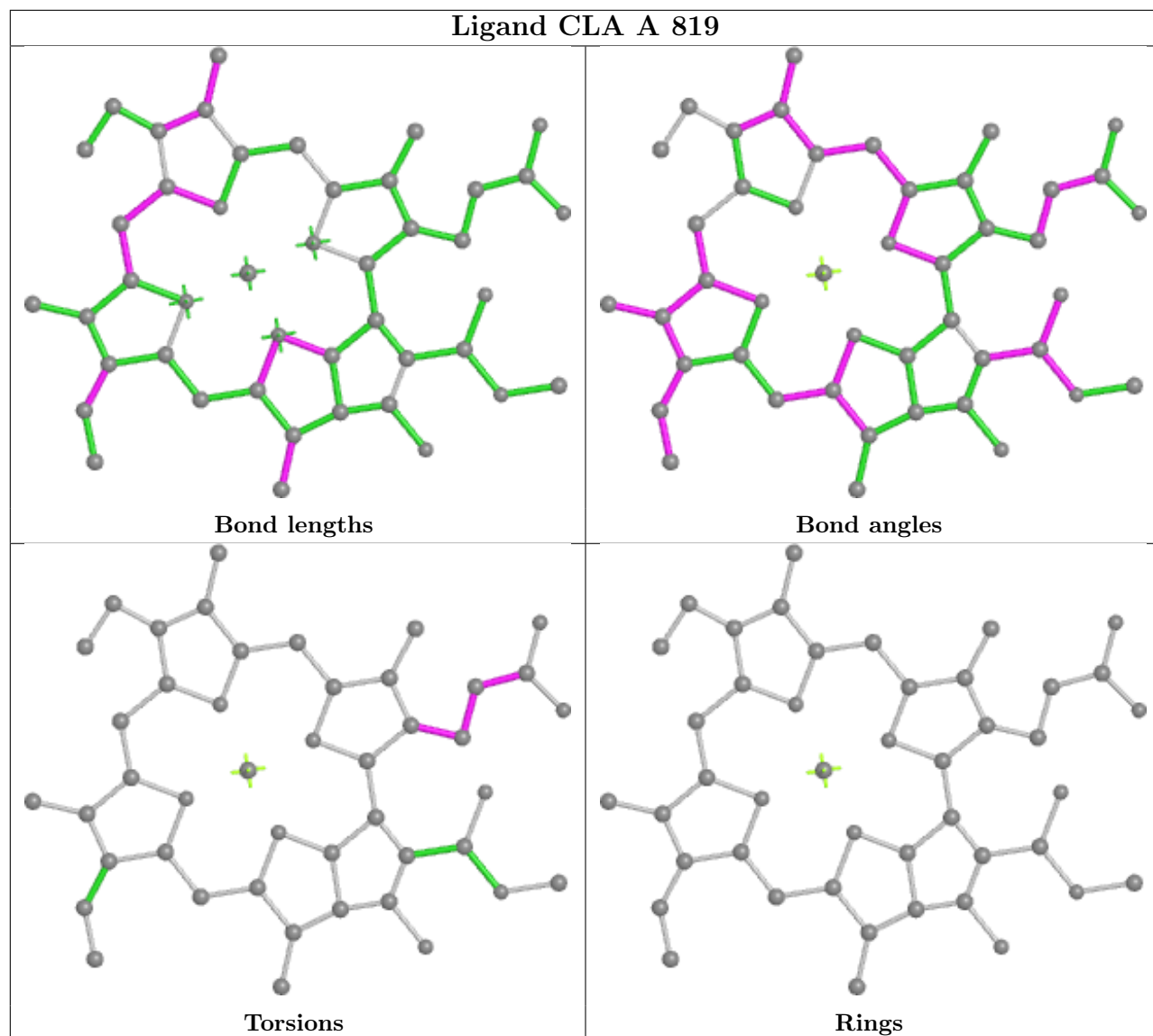
**Ligand CLA A 828****Ligand IHT c 615****Ligand II0 c 616**

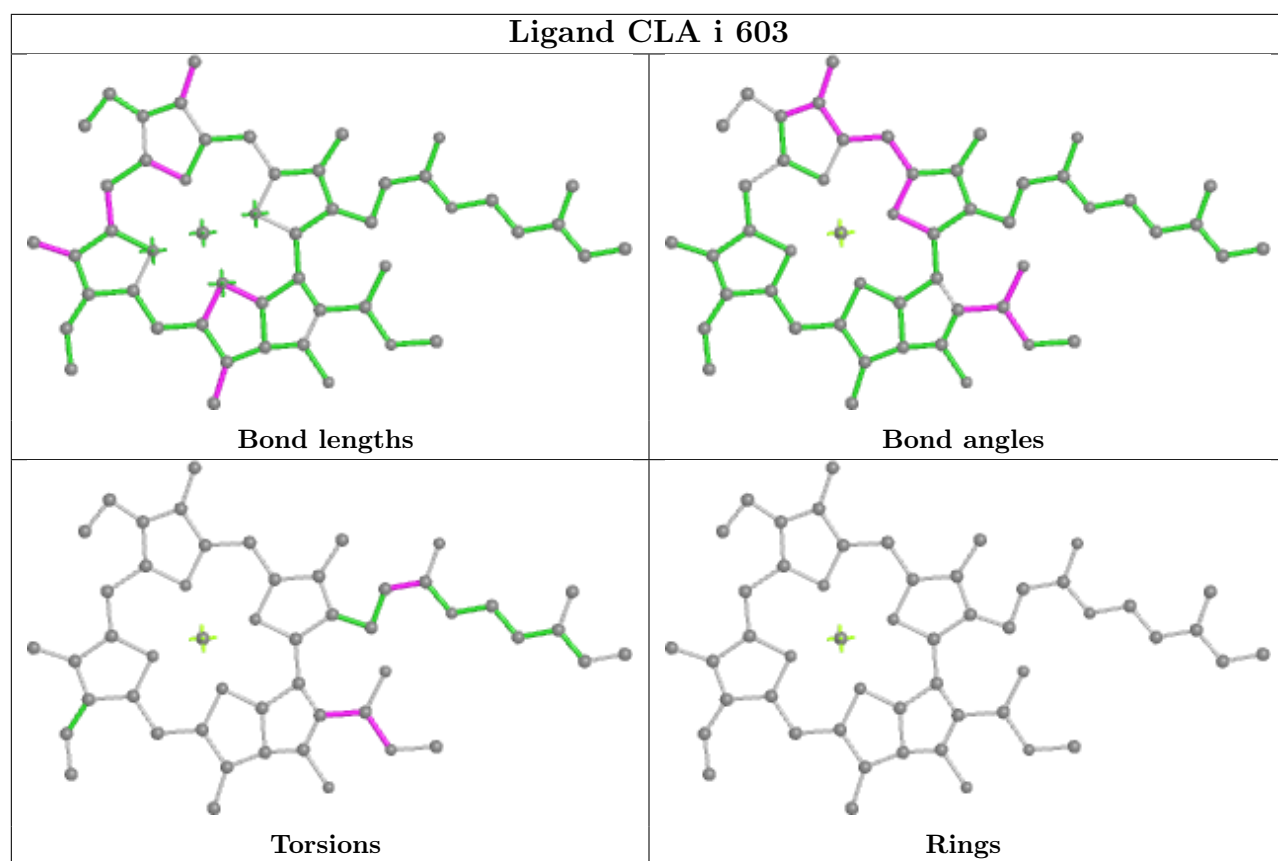
## Ligand CLA j 303



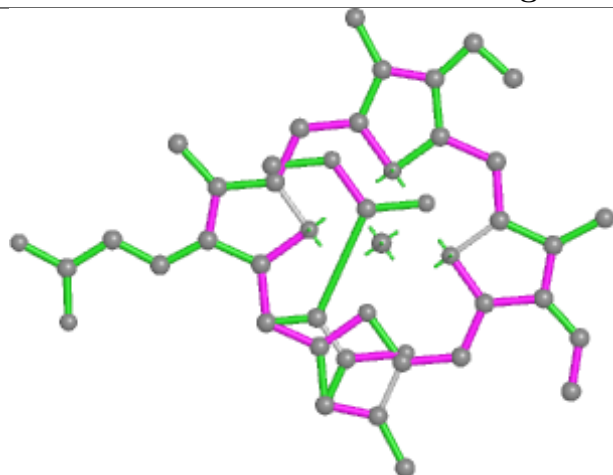


## Ligand CLA A 819

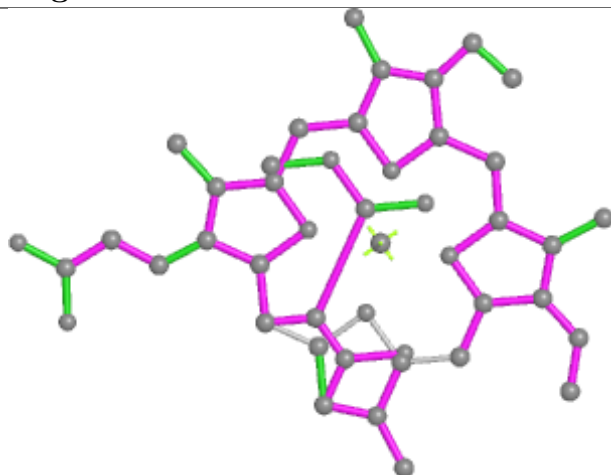




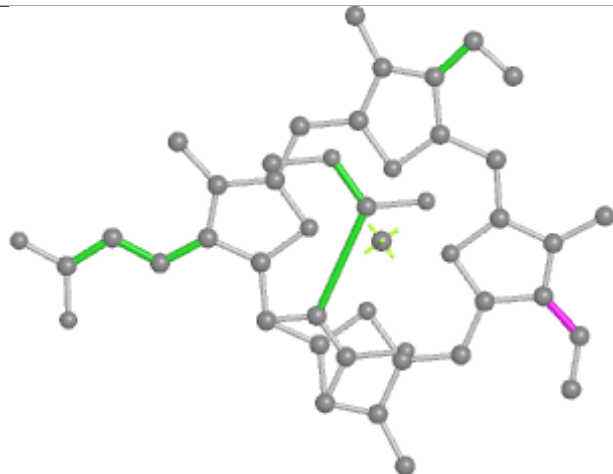
## Ligand KC2 g 313



Bond lengths



Bond angles

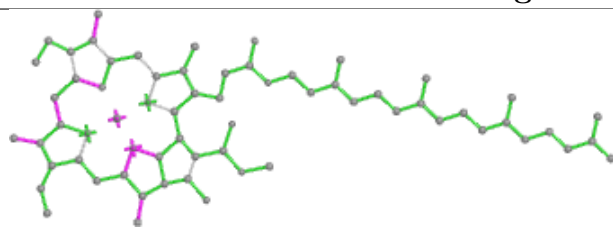


Torsions

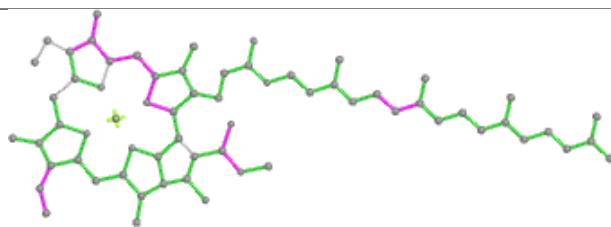


Rings

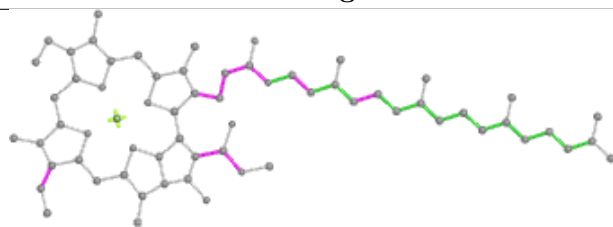
## Ligand CLA B 840



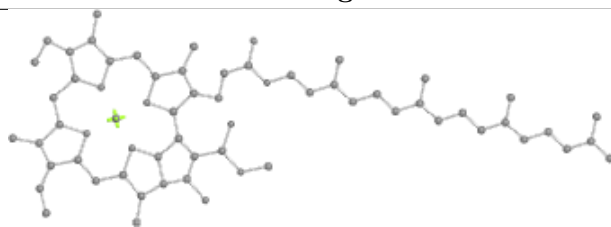
Bond lengths



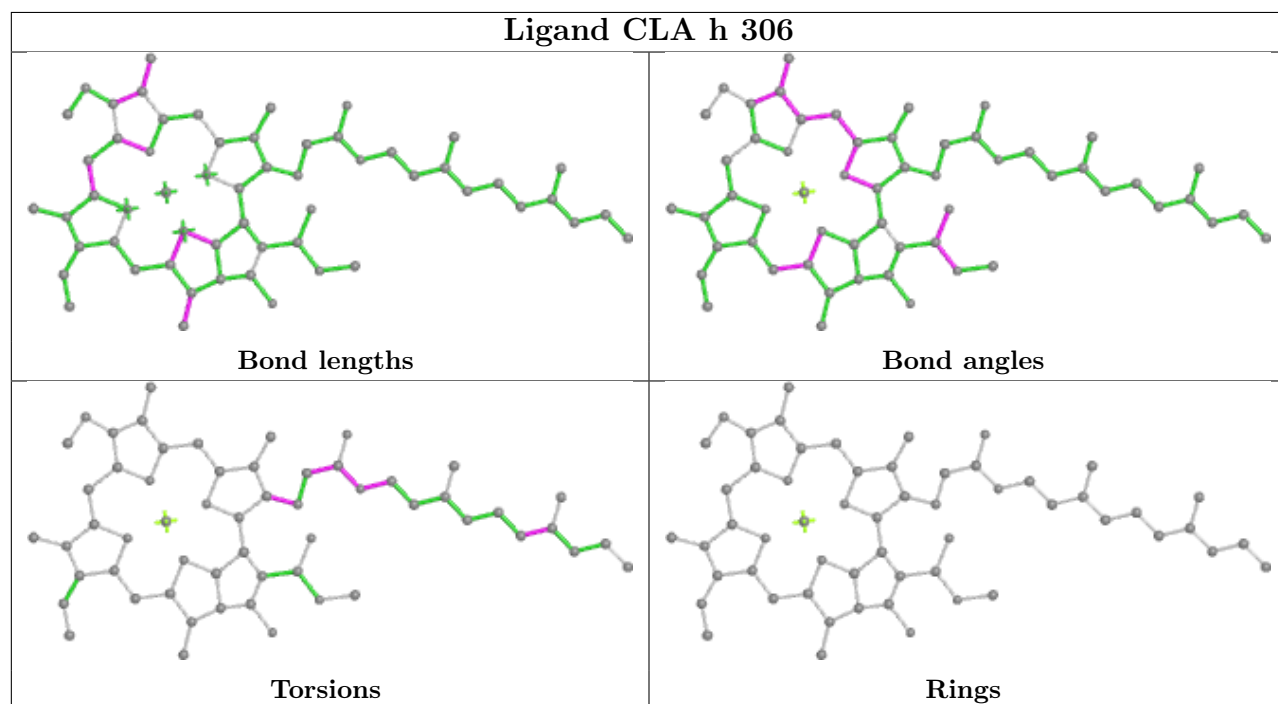
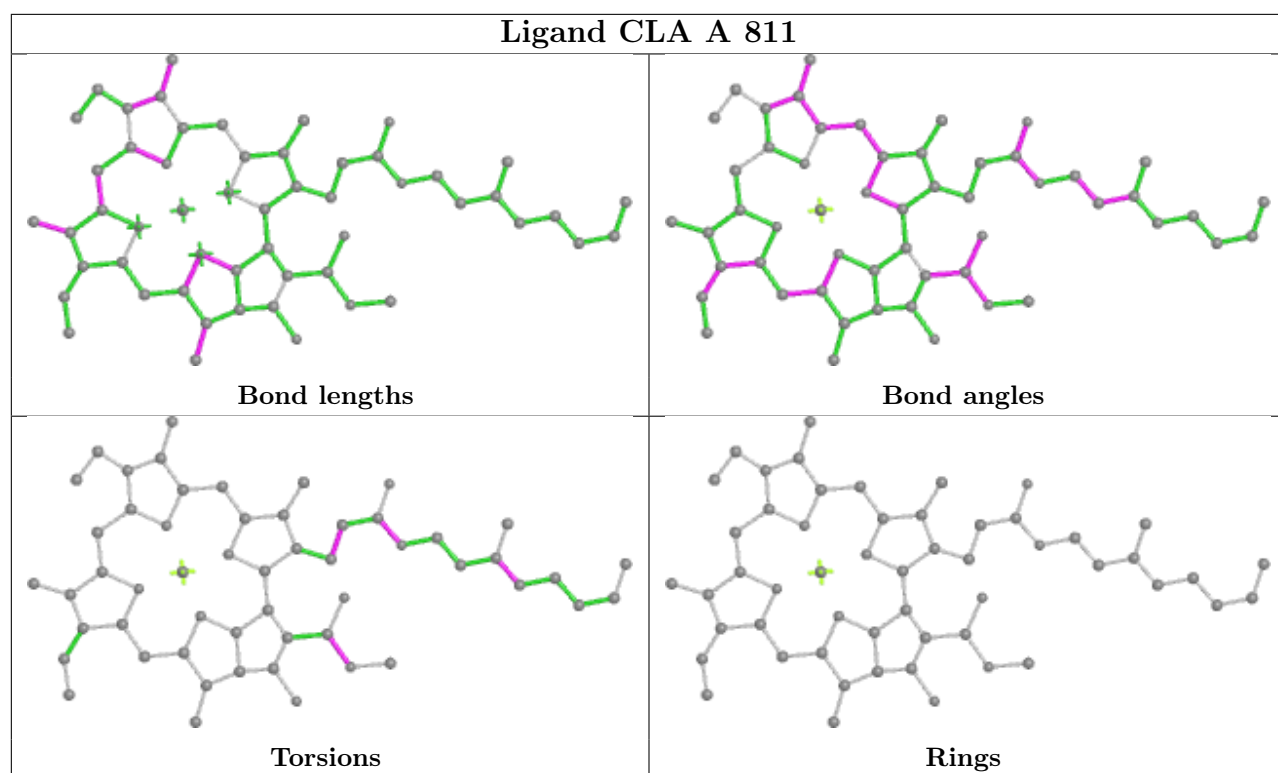
Bond angles



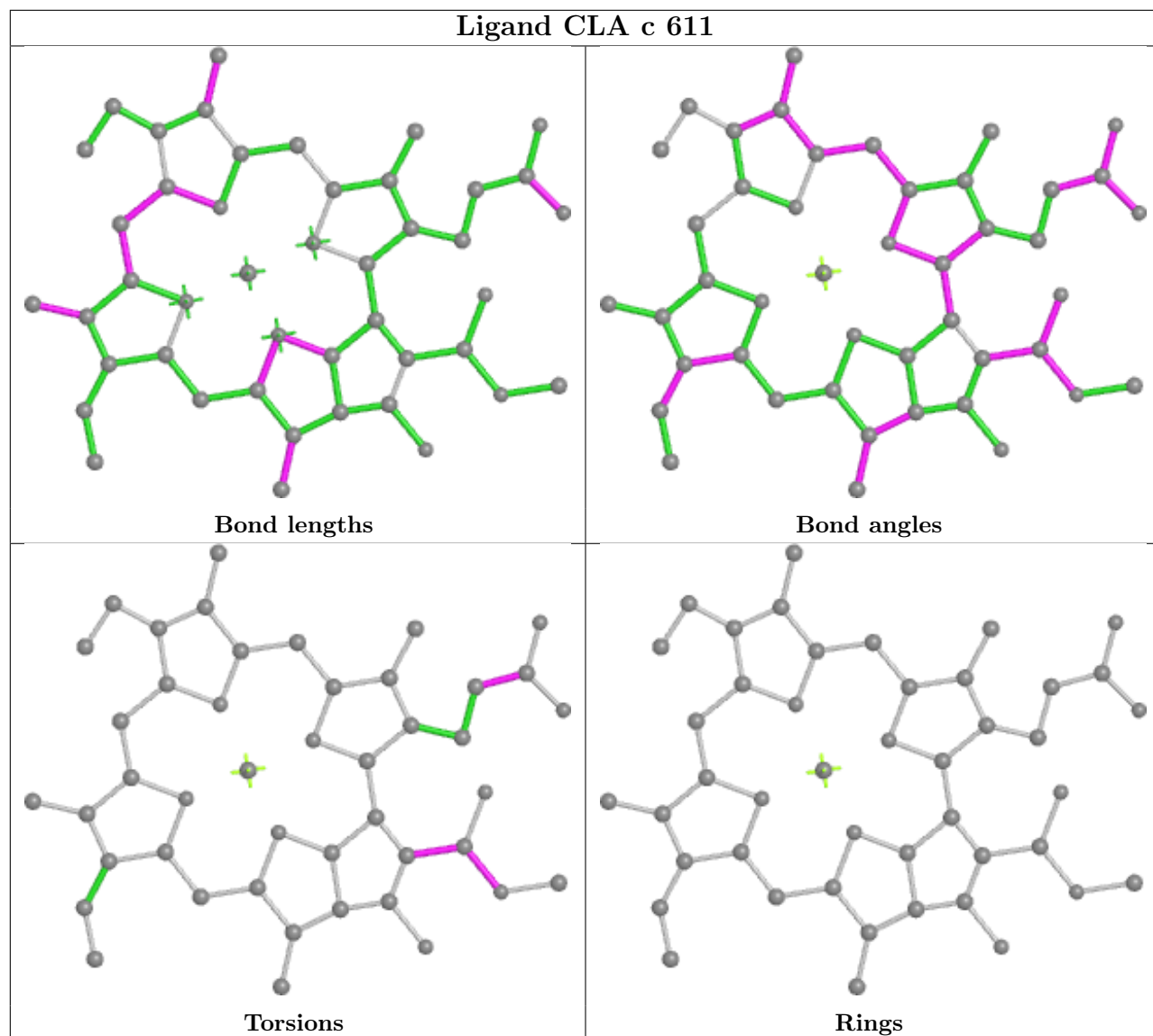
Torsions

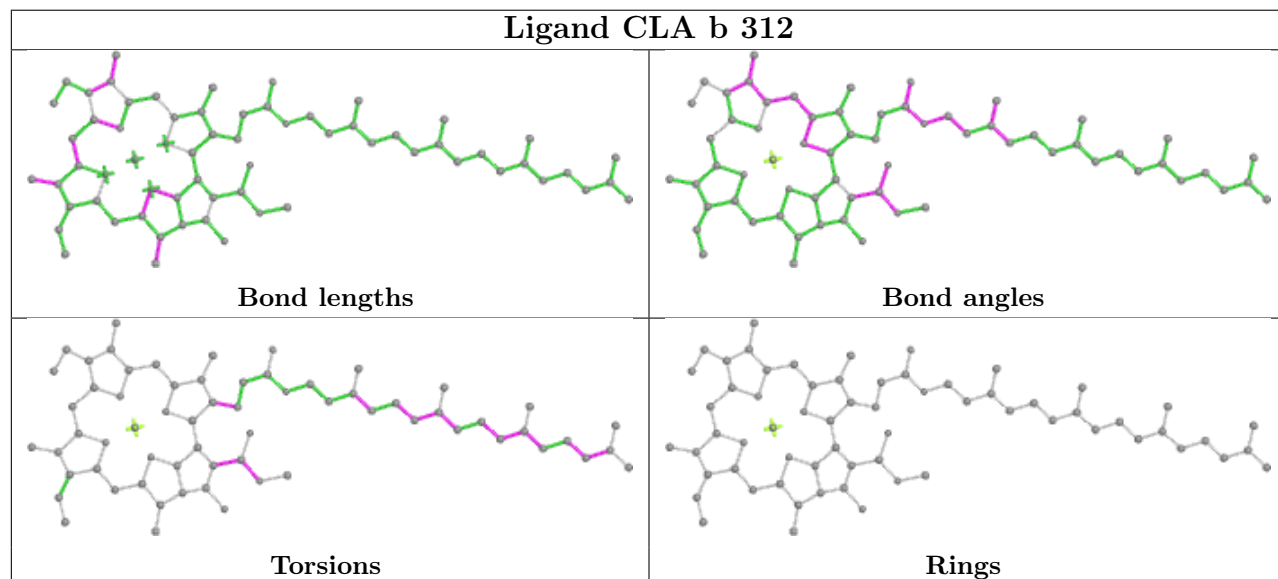
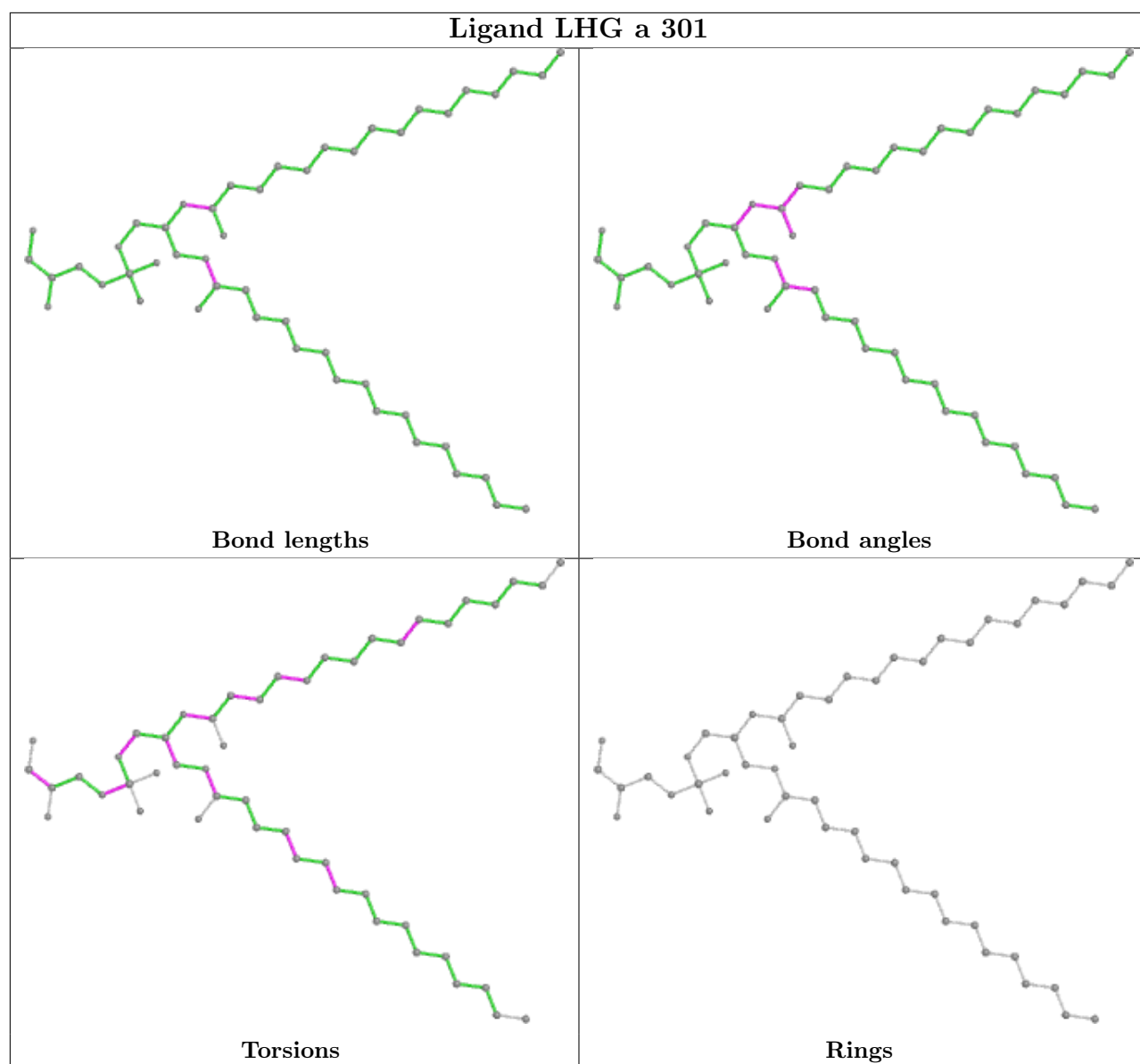


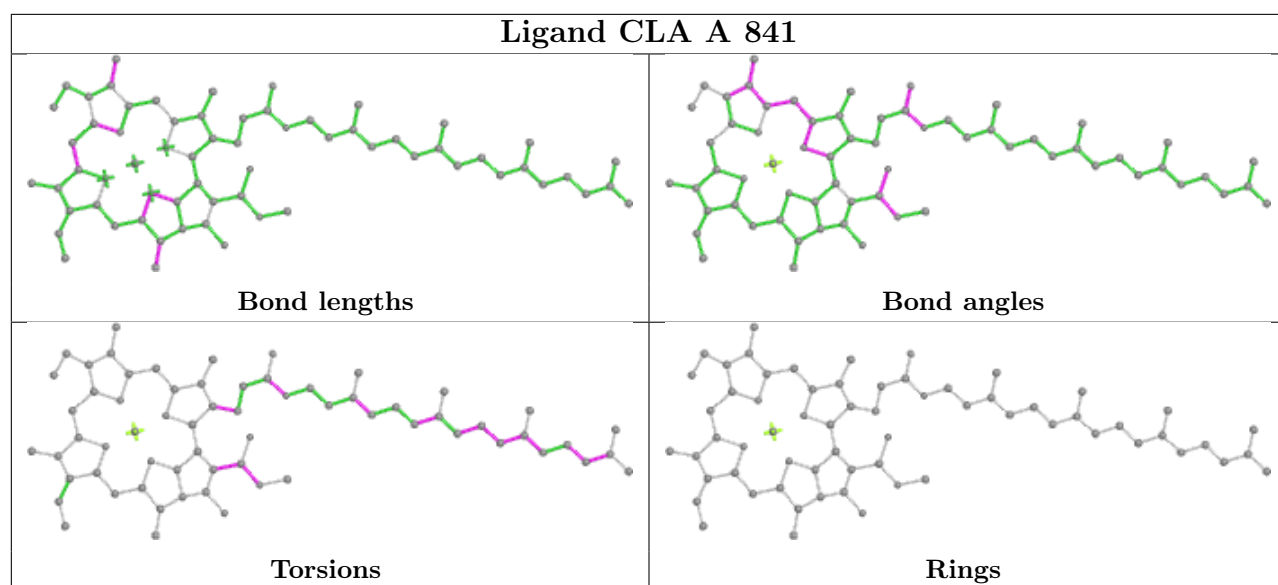
Rings



## Ligand CLA c 611







## 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.

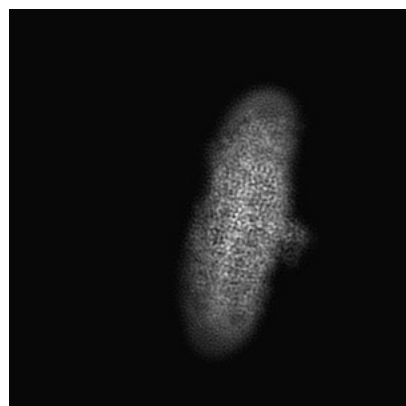
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37660. These allow visual inspection of the internal detail of the map and identification of artifacts.

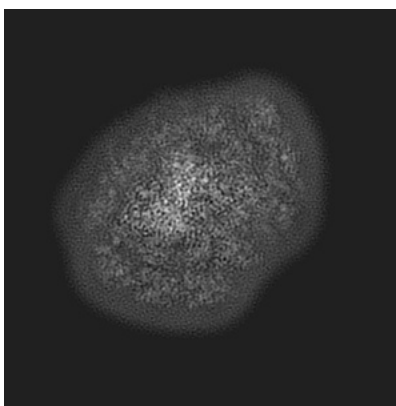
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

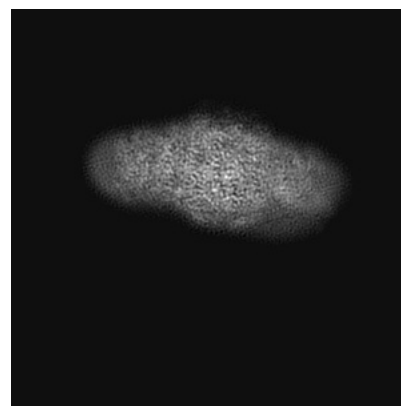
#### 6.1.1 Primary map



X

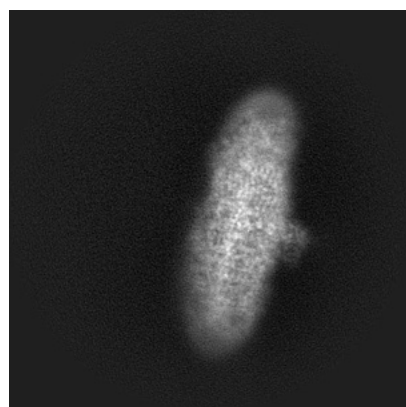


Y

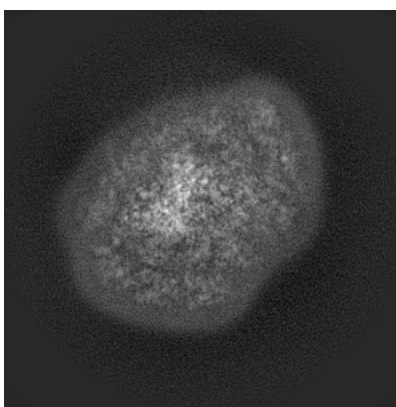


Z

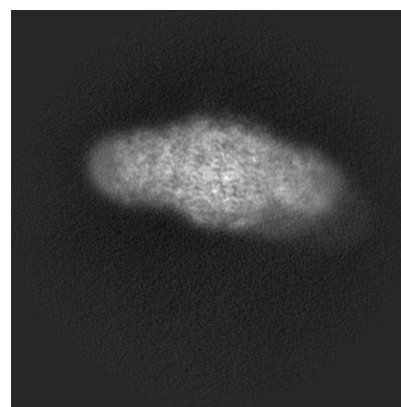
#### 6.1.2 Raw map



X



Y



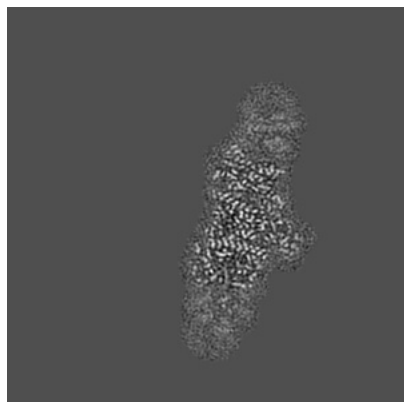
Z

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

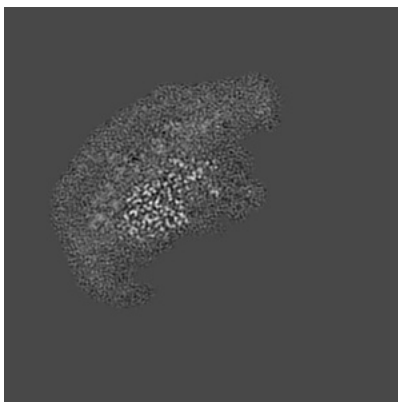


## 6.2 Central slices [i](#)

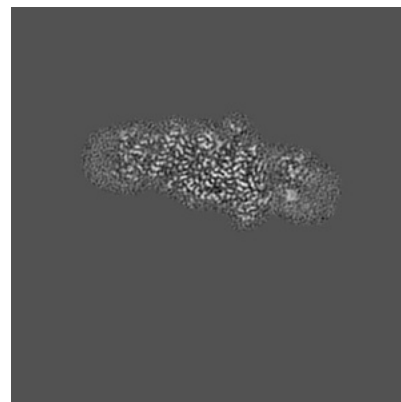
### 6.2.1 Primary map



X Index: 160

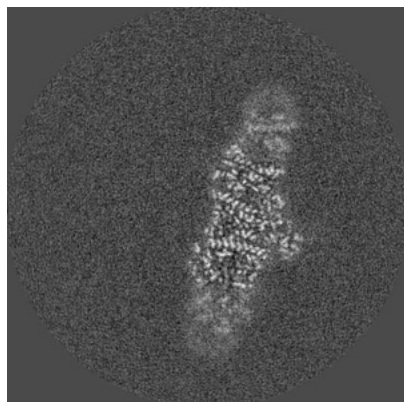


Y Index: 160

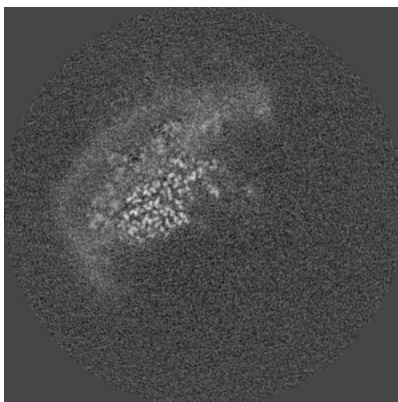


Z Index: 160

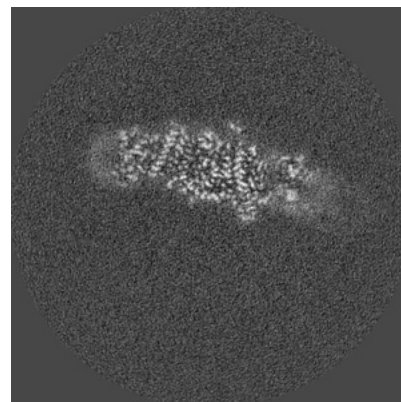
### 6.2.2 Raw map



X Index: 160



Y Index: 160

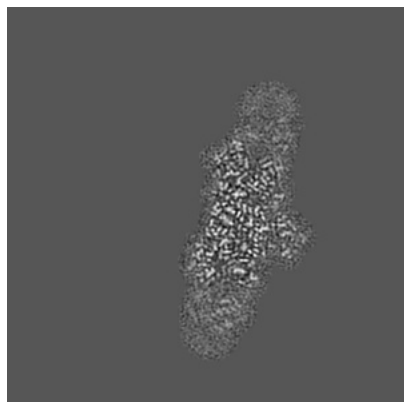


Z Index: 160

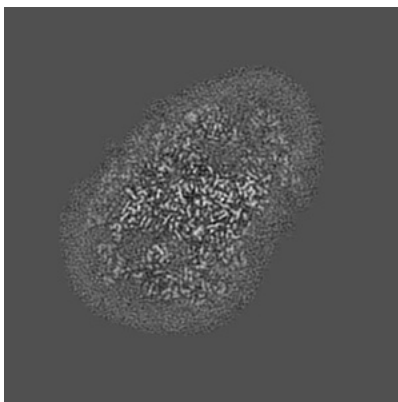
The images above show central slices of the map in three orthogonal directions.

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

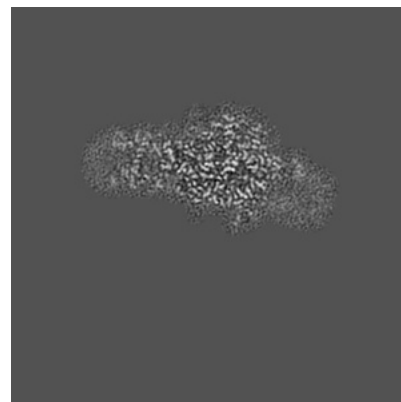
### 6.3.1 Primary map



X Index: 164

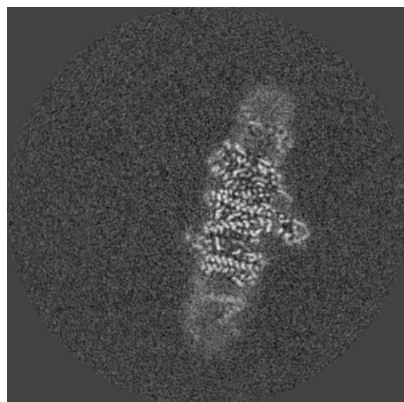


Y Index: 185

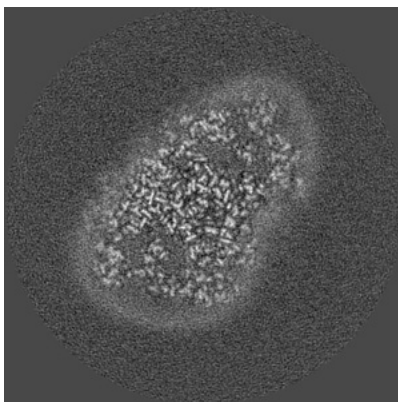


Z Index: 148

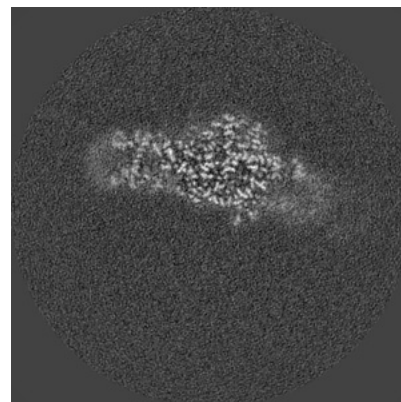
### 6.3.2 Raw map



X Index: 173



Y Index: 189

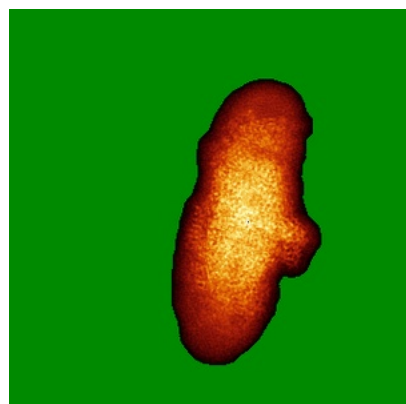


Z Index: 148

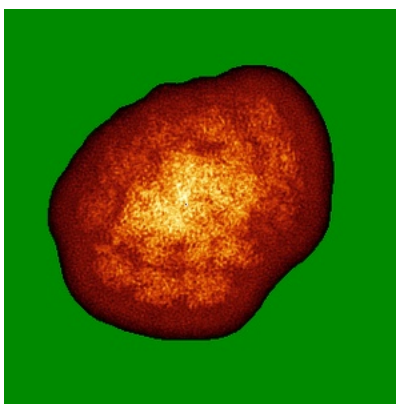
The images above show the largest variance slices of the map in three orthogonal directions.

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

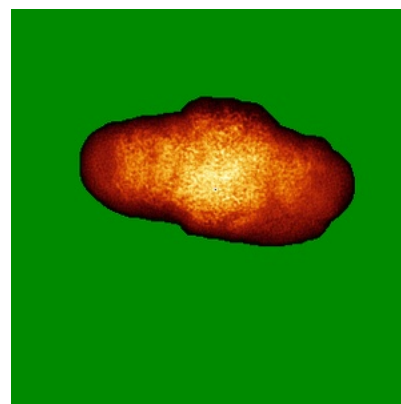
### 6.4.1 Primary map



X

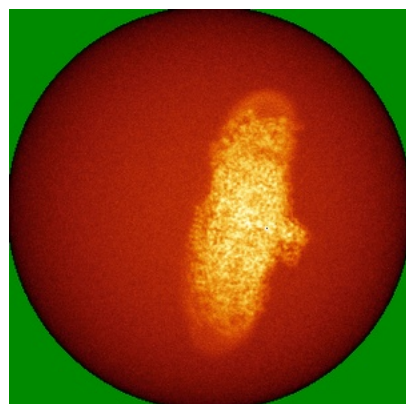


Y

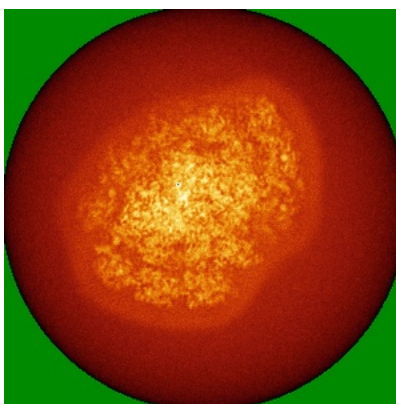


Z

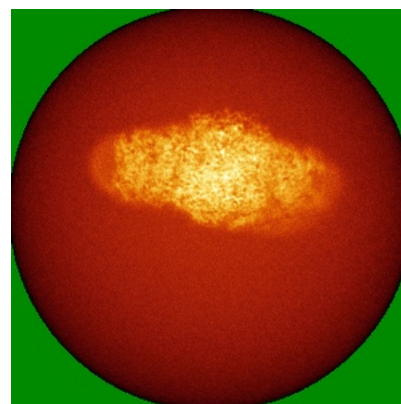
### 6.4.2 Raw map



X



Y

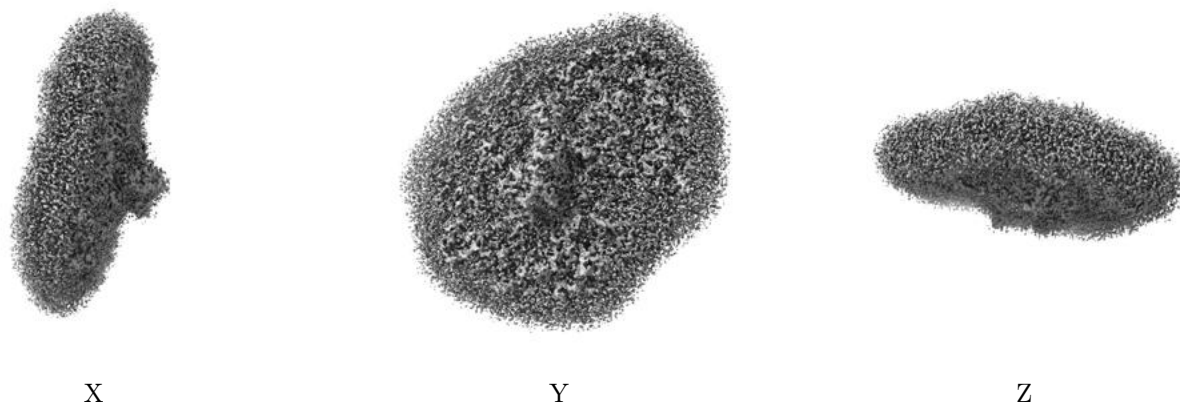


Z

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.

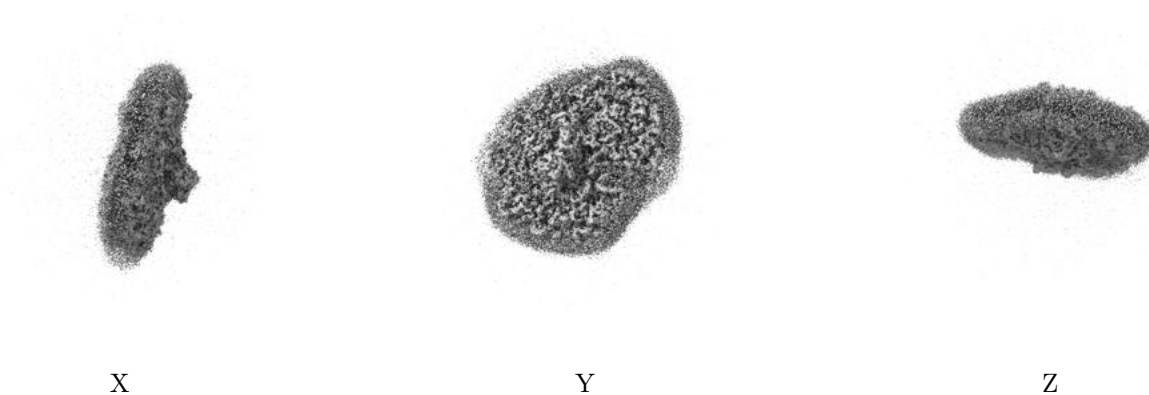
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

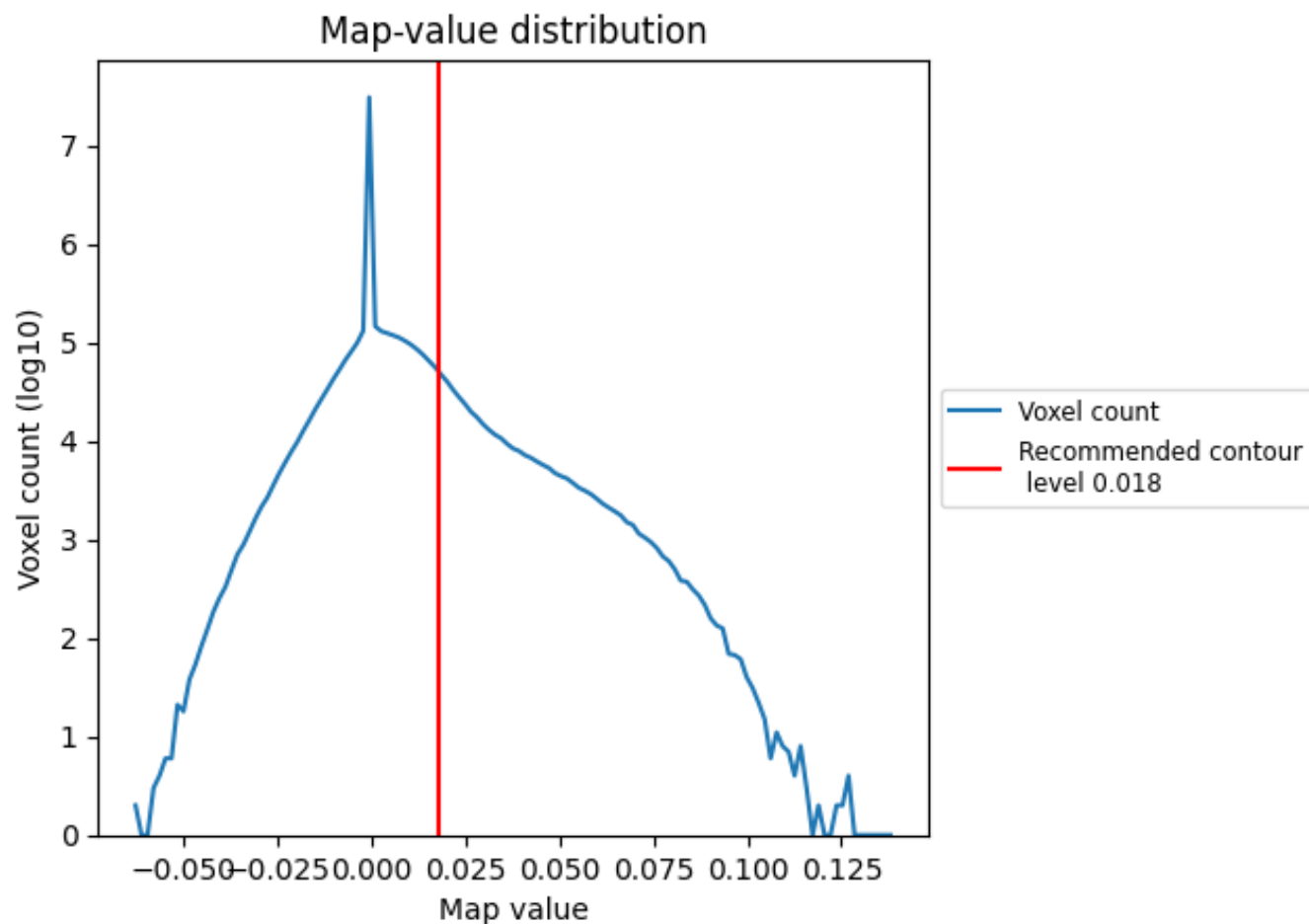
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

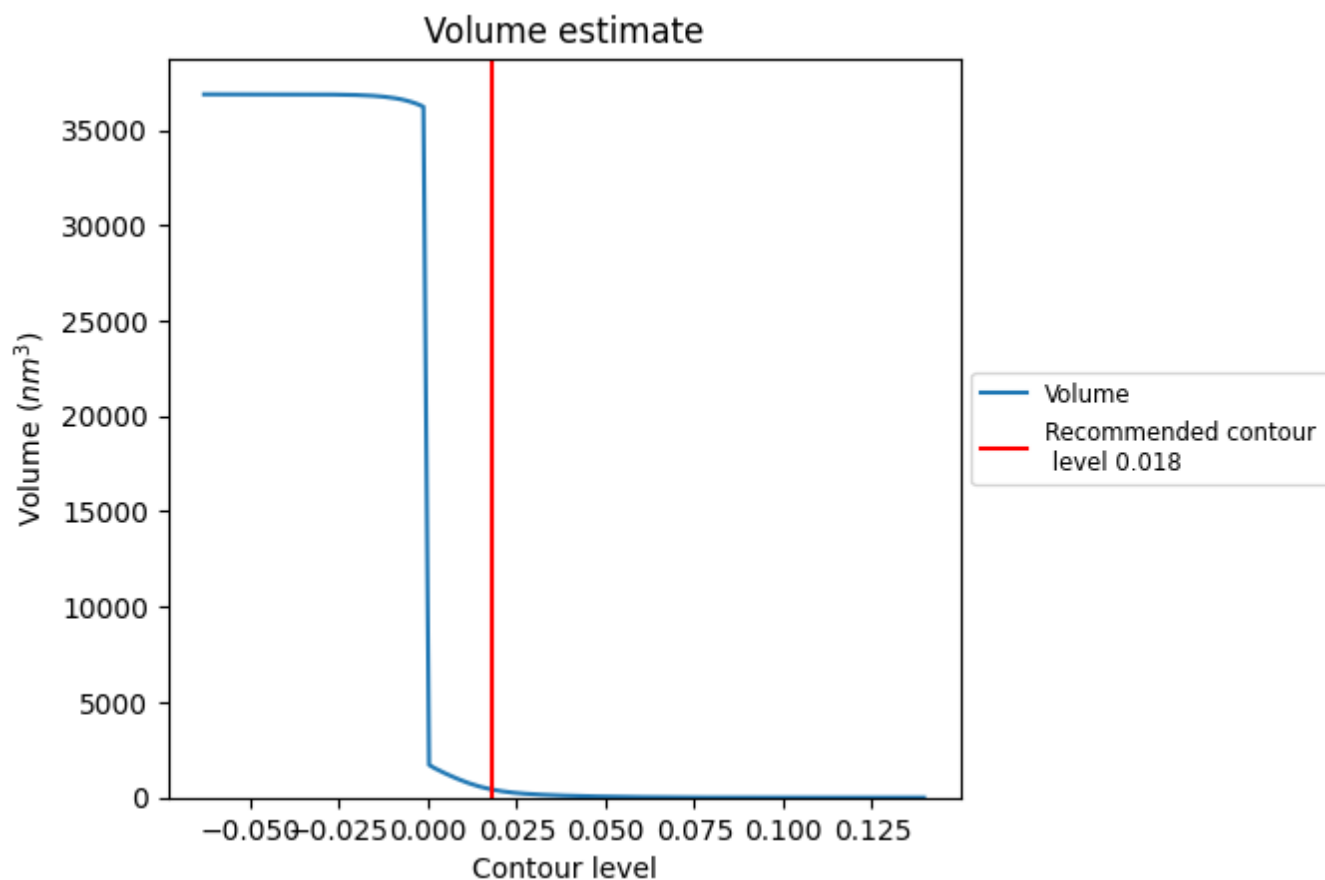
This section contains the results of statistical analysis of the map.

### 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.

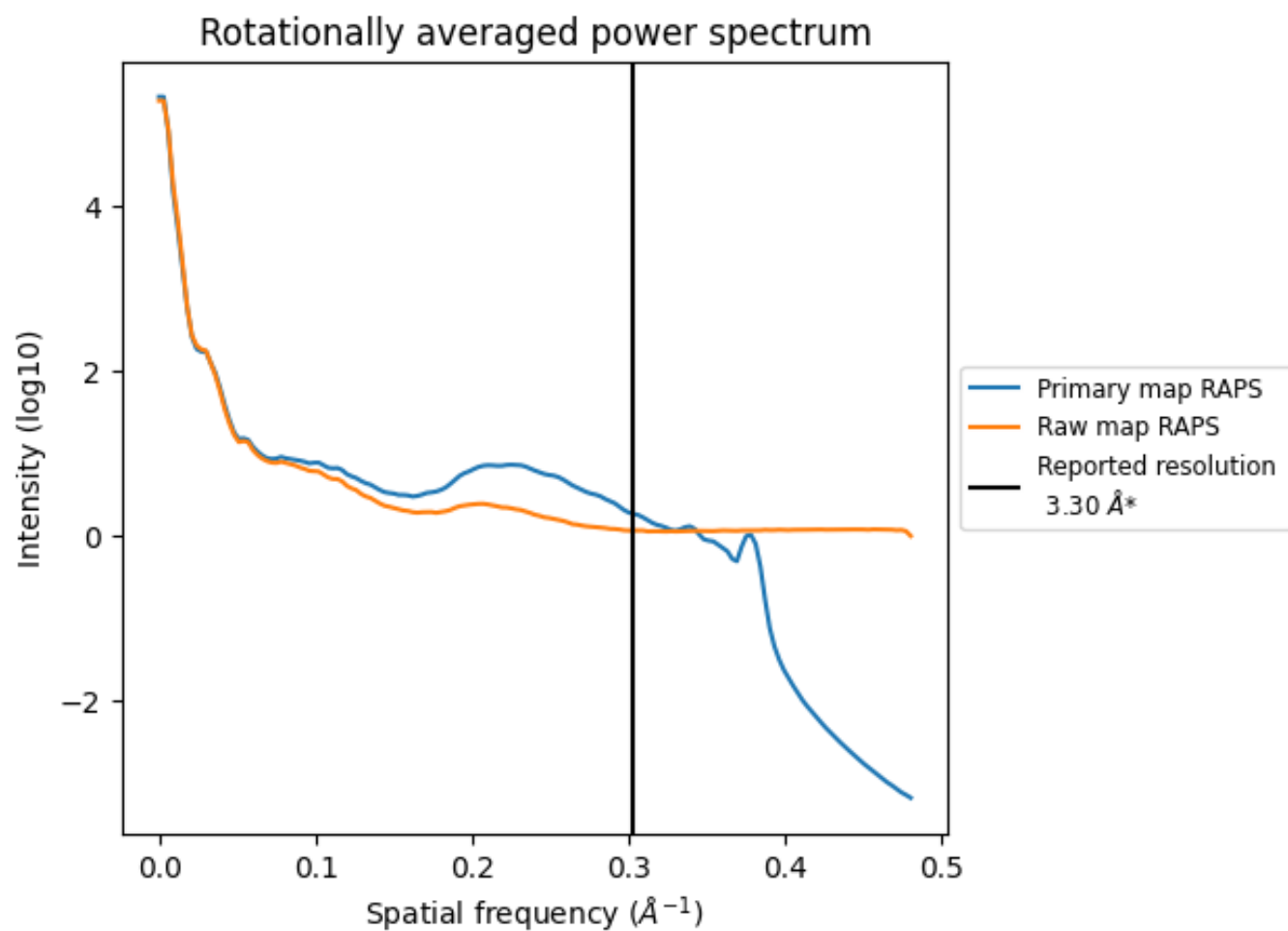
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm<sup>3</sup>; this corresponds to an approximate mass of 384 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 ⓘ



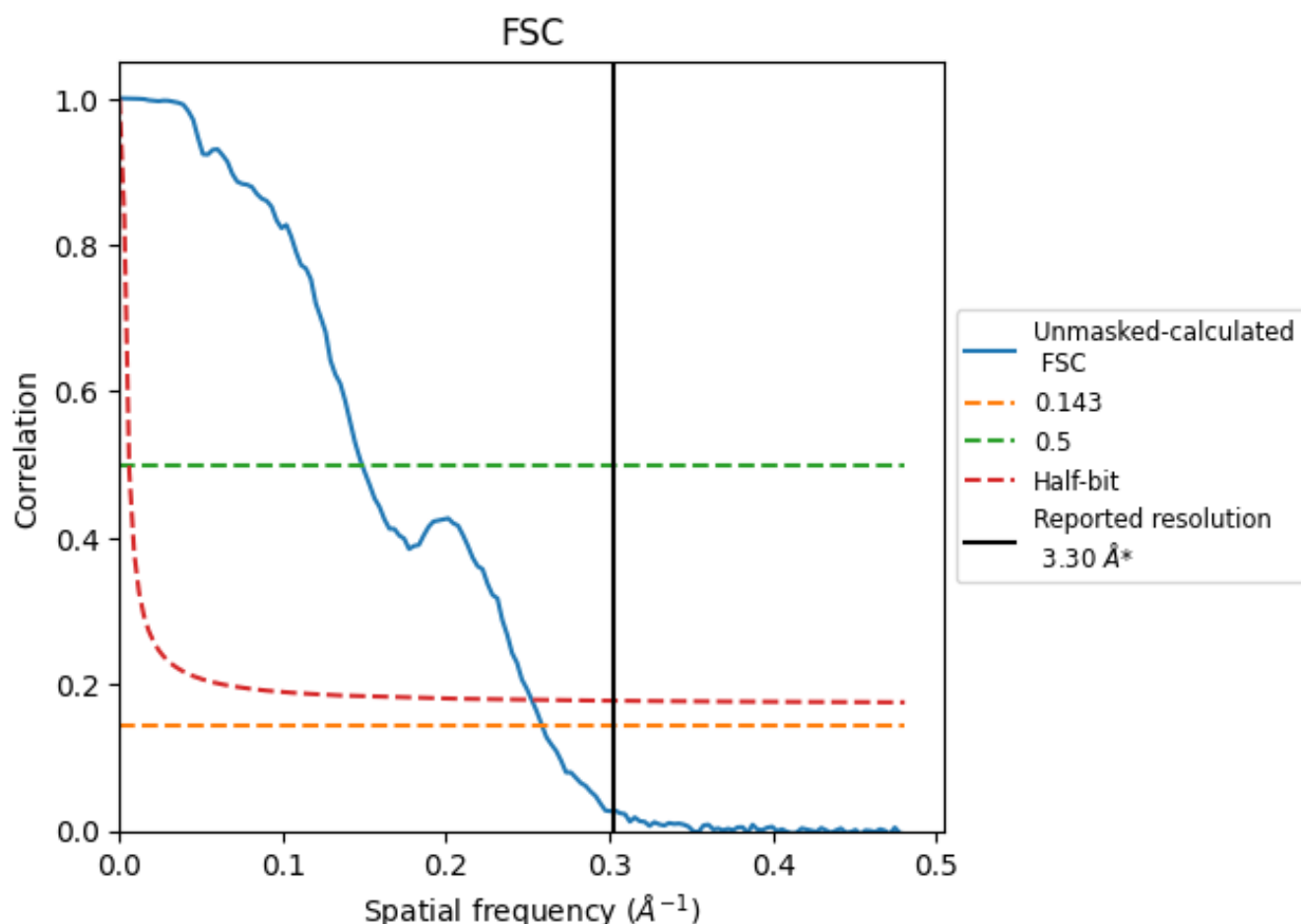
\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

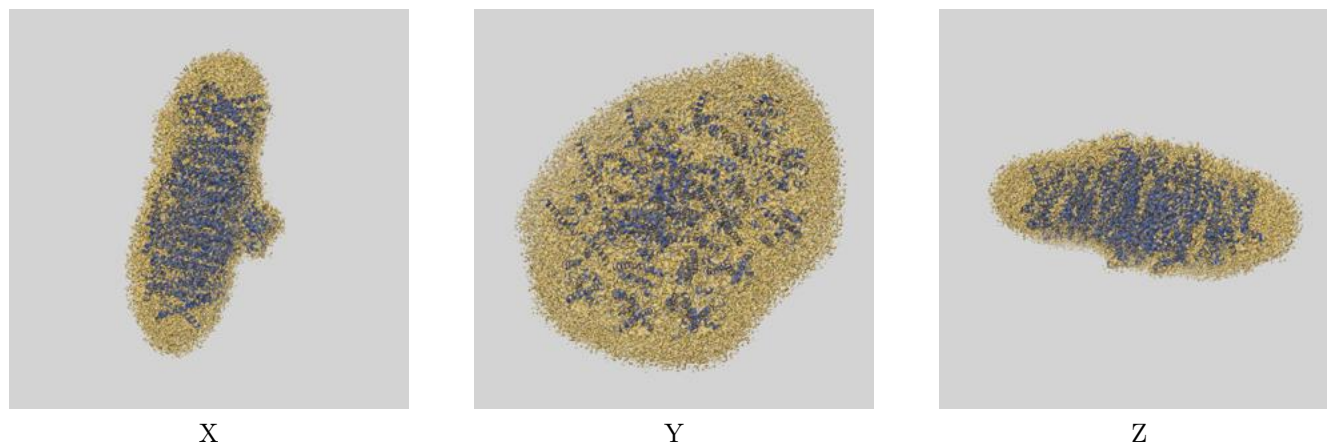
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.73	3.96

\*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 3.86 differs from the reported value 3.3 by more than 10 %

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

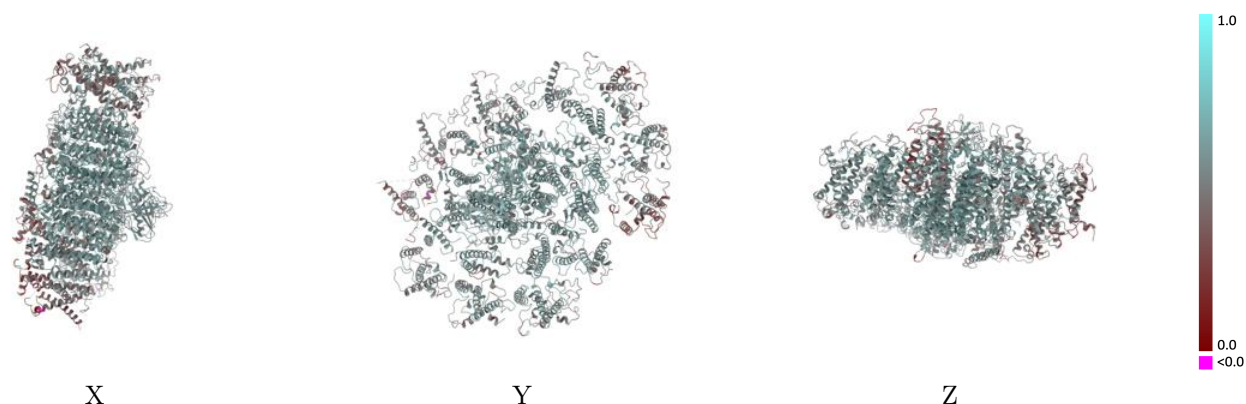
This section contains information regarding the fit between EMDB map EMD-37660 and PDB model 8WMW. Per-residue inclusion information can be found in section [3](#) on page [36](#).

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



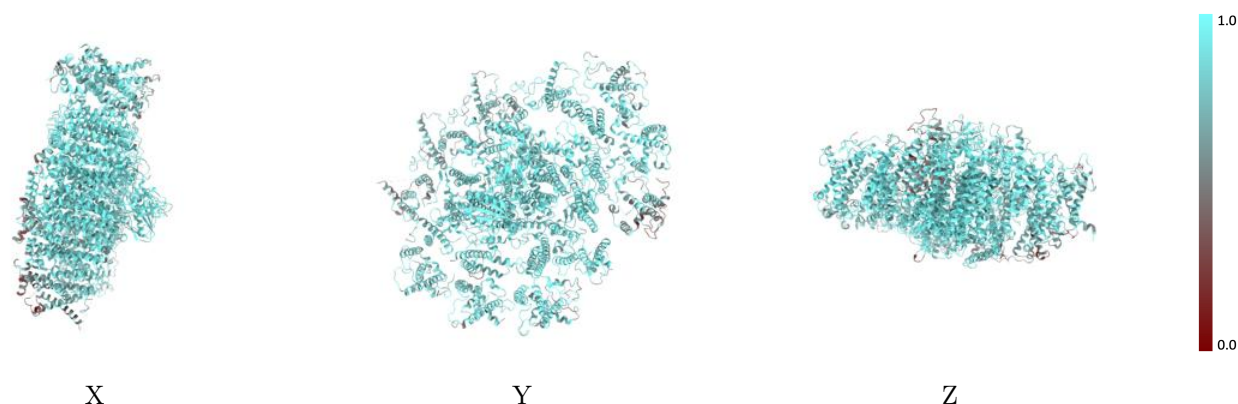
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



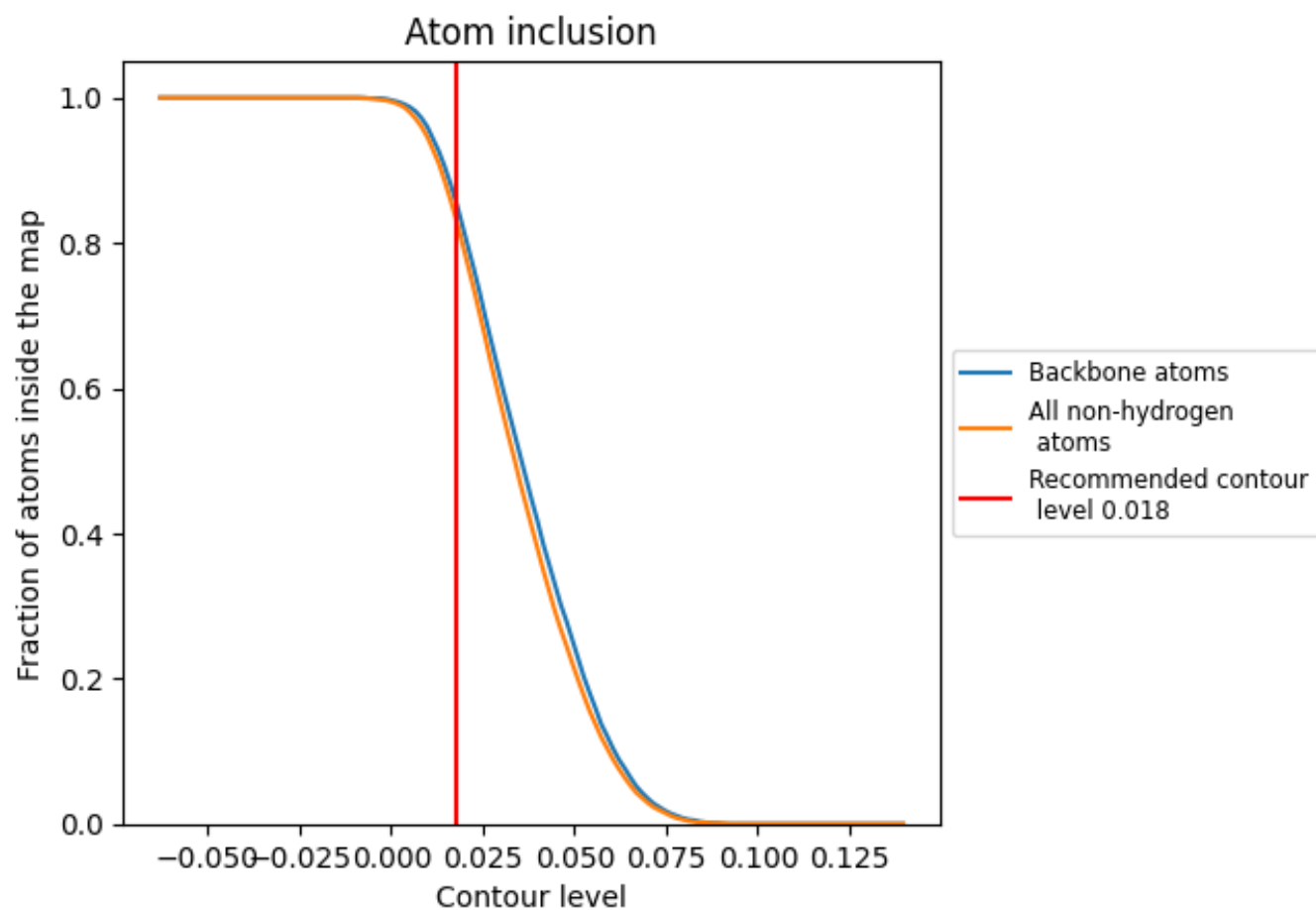
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5260
A	 0.9240	 0.5940
B	 0.9400	 0.6010
C	 0.9580	 0.5970
D	 0.8850	 0.5460
E	 0.8530	 0.5280
F	 0.8620	 0.5410
I	 0.9090	 0.5670
J	 0.7980	 0.5290
K	 0.8520	 0.5270
L	 0.8780	 0.5610
M	 0.8990	 0.5650
O	 0.8330	 0.5300
R	 0.8860	 0.5630
a	 0.7950	 0.4970
b	 0.6090	 0.4170
c	 0.6560	 0.4220
d	 0.6030	 0.3760
e	 0.7660	 0.4850
f	 0.8260	 0.5290
g	 0.8100	 0.5240
h	 0.8530	 0.5400
i	 0.6260	 0.3890
j	 0.8120	 0.5130
k	 0.7100	 0.4220

