



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2025 – 04:52 PM JST

PDB ID : 9L5V / pdb\_00009l5v  
EMDB ID : EMD-62846  
Title : cryo-EM structure of PSII-ACPII from Rhodomonas sp. NIES-2332  
Authors : Yonehara, N.; Akita, F.; Shen, J.R.  
Deposited on : 2024-12-23  
Resolution : 2.17 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>.

---

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

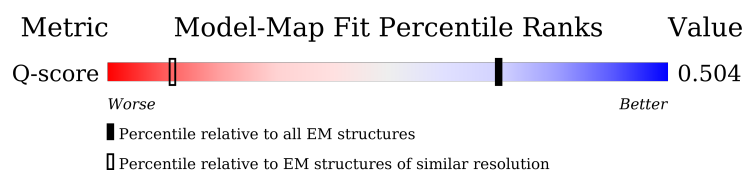
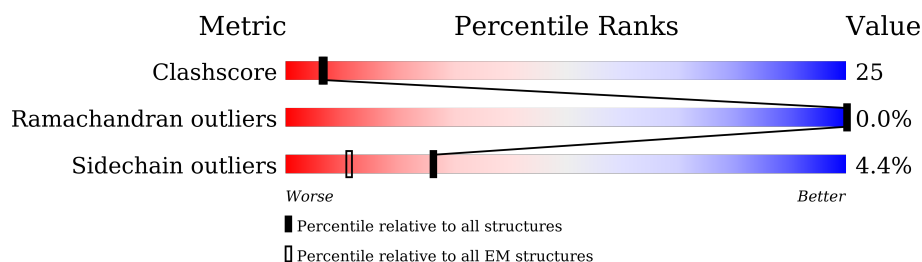
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





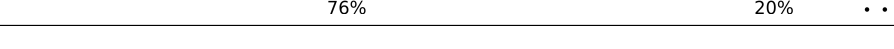
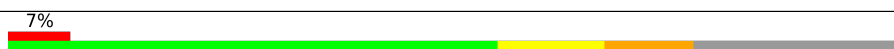

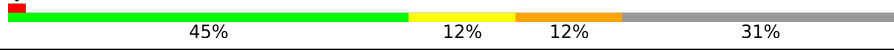

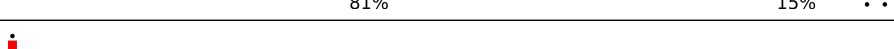



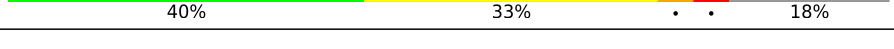




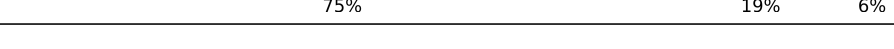







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	2651 ( 1.67 - 2.67 )

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	374	
1	a	374	
2	B	508	
2	b	508	






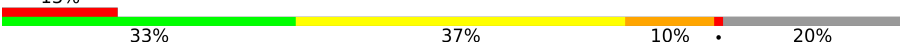
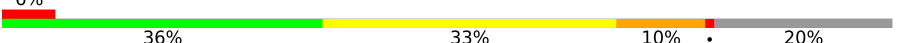
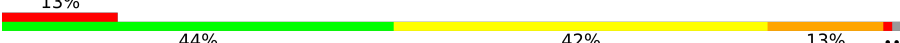
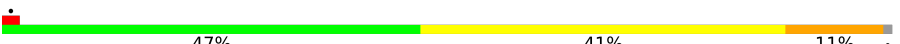

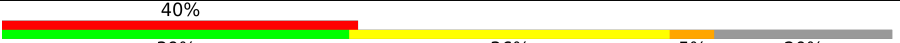

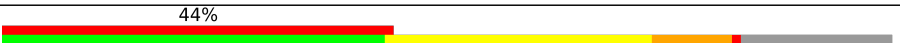



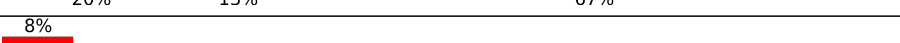
*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	486	
3	c	486	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	42	
6	f	42	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	118	
11	m	118	
12	T	32	
12	t	32	
13	W	121	
13	w	121	
14	X	39	
14	x	39	
15	Y	34	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	y	34	
16	Z	62	
16	z	62	
17	1	234	
17	N	234	
18	2	215	
18	O	215	
19	3	182	
19	P	182	
20	4	200	
20	Q	200	
21	5	228	
21	R	228	
22	6	174	
22	S	174	
23	G	292	
24	g	292	

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
26	CLA	1	601	X	-	-	-
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-
26	CLA	1	604	X	-	-	-
26	CLA	1	606	X	-	X	-
26	CLA	1	607	X	-	-	-
26	CLA	1	608	X	-	-	-
26	CLA	1	609	X	-	-	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	1	613	X	-	-	-
26	CLA	2	301	X	-	X	-
26	CLA	2	302	X	-	-	-
26	CLA	2	303	X	-	-	-
26	CLA	2	304	X	-	-	-
26	CLA	2	306	X	-	-	-
26	CLA	2	307	X	-	-	-
26	CLA	2	308	X	-	-	-
26	CLA	2	309	X	-	-	-
26	CLA	2	311	X	-	X	-
26	CLA	2	312	X	-	-	-
26	CLA	2	319	X	-	X	-
26	CLA	3	301	X	-	-	-
26	CLA	3	302	X	-	-	-
26	CLA	3	305	X	-	-	-
26	CLA	3	306	X	-	-	-
26	CLA	3	307	X	-	X	-
26	CLA	3	309	X	-	-	-
26	CLA	4	301	X	-	X	-
26	CLA	4	302	X	-	-	-
26	CLA	4	303	X	-	X	-
26	CLA	4	304	X	-	-	-
26	CLA	4	306	X	-	X	-
26	CLA	4	307	X	-	-	-
26	CLA	4	308	X	-	-	-
26	CLA	4	309	X	-	-	-
26	CLA	4	312	X	-	-	-
26	CLA	4	313	X	-	-	-
26	CLA	5	601	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	604	X	-	-	-
26	CLA	5	605	X	-	X	-
26	CLA	5	606	X	-	-	-
26	CLA	5	607	X	-	-	-
26	CLA	5	608	X	-	-	-
26	CLA	5	609	X	-	-	-
26	CLA	5	611	X	-	X	-
26	CLA	5	612	X	-	-	-
26	CLA	6	601	X	-	-	-
26	CLA	6	602	X	-	-	-
26	CLA	6	603	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	6	604	X	-	-	-
26	CLA	6	605	X	-	-	-
26	CLA	6	606	X	-	-	-
26	CLA	6	607	X	-	-	-
26	CLA	6	609	X	-	X	-
26	CLA	6	610	X	-	-	-
26	CLA	A	402	X	-	-	-
26	CLA	A	403	X	-	-	-
26	CLA	A	405	X	-	-	-
26	CLA	B	601	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	608	X	-	-	-
26	CLA	B	609	X	-	-	-
26	CLA	B	610	X	-	-	-
26	CLA	B	611	X	-	-	-
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	614	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	C	502	X	-	-	-
26	CLA	C	503	X	-	-	-
26	CLA	C	504	X	-	-	-
26	CLA	C	505	X	-	-	-
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	508	X	-	-	-
26	CLA	C	509	X	-	-	-
26	CLA	C	510	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	C	513	X	-	-	-
26	CLA	C	514	X	-	-	-
26	CLA	D	404	X	-	-	-
26	CLA	D	407	X	-	-	-
26	CLA	D	408	X	-	-	-
26	CLA	G	401	X	-	-	-
26	CLA	G	402	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	N	601	X	-	X	-
26	CLA	N	602	X	-	-	-
26	CLA	N	603	X	-	-	-
26	CLA	N	604	X	-	-	-
26	CLA	N	606	X	-	X	-
26	CLA	N	607	X	-	-	-
26	CLA	N	608	X	-	-	-
26	CLA	N	609	X	-	-	-
26	CLA	N	613	X	-	-	-
26	CLA	N	614	X	-	X	-
26	CLA	O	601	X	-	X	-
26	CLA	O	602	X	-	-	-
26	CLA	O	603	X	-	-	-
26	CLA	O	604	X	-	-	-
26	CLA	O	605	X	-	-	-
26	CLA	O	606	X	-	-	-
26	CLA	O	607	X	-	-	-
26	CLA	O	608	X	-	-	-
26	CLA	O	609	X	-	-	-
26	CLA	O	611	X	-	-	-
26	CLA	O	612	X	-	-	-
26	CLA	P	601	X	-	-	-
26	CLA	P	602	X	-	-	-
26	CLA	P	603	X	-	-	-
26	CLA	P	606	X	-	-	-
26	CLA	P	607	X	-	-	-
26	CLA	P	608	X	-	-	-
26	CLA	P	609	X	-	-	-
26	CLA	P	610	X	-	-	-
26	CLA	P	611	X	-	-	-
26	CLA	Q	301	X	-	-	-
26	CLA	Q	302	X	-	-	-
26	CLA	Q	303	X	-	-	-
26	CLA	Q	305	X	-	-	-
26	CLA	Q	306	X	-	-	-
26	CLA	Q	307	X	-	-	-
26	CLA	Q	308	X	-	-	-
26	CLA	Q	311	X	-	-	-
26	CLA	Q	312	X	-	-	-
26	CLA	R	302	X	-	-	-
26	CLA	R	303	X	-	-	-
26	CLA	R	304	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	R	305	X	-	-	-
26	CLA	R	306	X	-	X	-
26	CLA	R	307	X	-	-	-
26	CLA	R	308	X	-	-	-
26	CLA	R	309	X	-	-	-
26	CLA	R	310	X	-	-	-
26	CLA	R	312	X	-	-	-
26	CLA	R	313	X	-	-	-
26	CLA	S	601	X	-	-	-
26	CLA	S	602	X	-	-	-
26	CLA	S	603	X	-	-	-
26	CLA	S	604	X	-	-	-
26	CLA	S	605	X	-	-	-
26	CLA	S	606	X	-	-	-
26	CLA	S	607	X	-	-	-
26	CLA	S	609	X	-	-	-
26	CLA	S	610	X	-	-	-
26	CLA	a	402	X	-	-	-
26	CLA	a	403	X	-	-	-
26	CLA	a	405	X	-	-	-
26	CLA	b	601	X	-	-	-
26	CLA	b	603	X	-	-	-
26	CLA	b	604	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-
26	CLA	b	608	X	-	-	-
26	CLA	b	609	X	-	-	-
26	CLA	b	610	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	615	X	-	-	-
26	CLA	b	616	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-
26	CLA	c	507	X	-	-	-
26	CLA	c	508	X	-	-	-
26	CLA	c	509	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	c	510	X	-	-	-
26	CLA	c	511	X	-	-	-
26	CLA	c	512	X	-	-	-
26	CLA	c	513	X	-	-	-
26	CLA	c	514	X	-	-	-
26	CLA	c	515	X	-	-	-
26	CLA	d	402	X	-	-	-
26	CLA	d	405	X	-	-	-
26	CLA	d	406	X	-	-	-
26	CLA	g	401	X	-	-	-
26	CLA	g	402	X	-	-	-
28	WVN	3	313	-	-	X	-
28	WVN	C	516	-	X	-	-
34	LHG	1	620	-	-	X	-
34	LHG	2	321	-	-	X	-
34	LHG	N	621	-	-	X	-
38	KC2	N	612	-	-	X	-
38	KC2	Q	310	-	-	X	-
39	II0	3	310	-	-	X	-
39	II0	3	311	-	-	X	-
39	II0	4	320	-	-	X	-
40	IHT	1	619	-	X	-	-
40	IHT	2	317	-	-	X	-

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 69223 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	303	Total	C	N	O	S	1	0
			2377	1562	393	410	12		
1	a	311	Total	C	N	O	S	0	0
			2438	1603	401	422	12		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	482	Total	C	N	O	S	1	0
			3797	2479	650	656	12		
2	b	481	Total	C	N	O	S	0	0
			3782	2471	645	654	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	424	Total	C	N	O	S	1	0
			3331	2188	559	573	11		
3	c	421	Total	C	N	O	S	0	0
			3299	2164	555	569	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	1	0
			2713	1792	445	464	12		
4	d	341	Total	C	N	O	S	0	0
			2705	1788	443	462	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			525	345	85	95		
5	e	64	Total	C	N	O	0	0
			525	345	85	95		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			235	159	40	35	1		
6	f	30	Total	C	N	O	S	0	0
			246	168	41	36	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			508	337	81	88	2		
7	h	65	Total	C	N	O	S	0	0
			508	337	81	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			284	188	46	49	1		
8	i	35	Total	C	N	O	S	0	0
			284	188	46	49	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			296	209	44	43		
9	k	37	Total	C	N	O	0	0
			296	209	44	43		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	37	Total	C	N	O	0	0
			301	204	47	50		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	37	Total	C	N	O	0	0
			301	204	47	50		

- Molecule 11 is a protein called Photosystem II protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	36	Total	C	N	O	0	0
			271	181	42	48		
11	m	36	Total	C	N	O	0	0
			271	181	42	48		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	30	Total	C	N	O	S	0	0
			244	169	36	38	1		
12	t	30	Total	C	N	O	S	0	0
			244	169	36	38	1		

- Molecule 13 is a protein called Photosystem II protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	W	45	Total	C	N	O	0	0
			361	233	58	70		
13	w	45	Total	C	N	O	0	0
			361	233	58	70		

- Molecule 14 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	34	Total	C	N	O	S	0	0
			249	167	36	45	1		
14	x	34	Total	C	N	O	S	0	0
			249	167	36	45	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Y	28	Total	C	N	O	0	0
			209	140	36	33		
15	y	28	Total	C	N	O	0	0
			209	140	36	33		



- Molecule 16 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			451	305	67	76	3		
16	z	61	Total	C	N	O	S	0	0
			460	314	67	76	3		

- Molecule 17 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1	192	Total	C	N	O	S	0	0
			1477	944	262	263	8		
17	N	192	Total	C	N	O	S	0	0
			1477	944	262	263	8		

- Molecule 18 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2	172	Total	C	N	O	S	0	0
			1377	910	225	239	3		
18	O	172	Total	C	N	O	S	0	0
			1377	910	225	239	3		

- Molecule 19 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	180	Total	C	N	O	S	0	0
			1388	898	232	249	9		
19	P	180	Total	C	N	O	S	0	0
			1388	898	232	249	9		

- Molecule 20 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	160	Total	C	N	O	S	0	0
			1226	787	210	219	10		
20	Q	160	Total	C	N	O	S	0	0
			1226	787	210	219	10		

- Molecule 21 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	5	189	Total	C	N	O	S	0	0
			1481	972	242	264	3		
21	R	189	Total	C	N	O	S	0	0
			1481	972	242	264	3		

- Molecule 22 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	6	173	Total	C	N	O	S	0	0
			1327	856	227	236	8		
22	S	173	Total	C	N	O	S	0	0
			1327	856	227	236	8		

- Molecule 23 is a protein called Psb-gama\_linker.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	G	96	Total	C	N	O	0	0
			755	503	120	132		

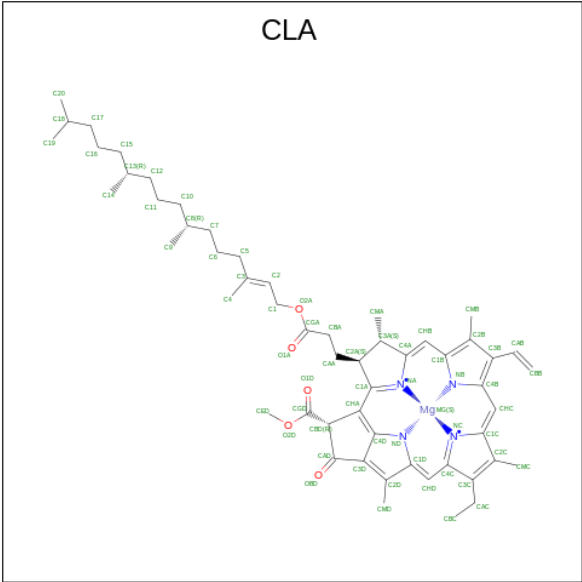
- Molecule 24 is a protein called Psb-gama\_linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	g	95	Total	C	N	O	S	0	0
			747	499	118	129	1		

- Molecule 25 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	Fe	0
			1	1	
25	a	1	Total	Fe	0
			1	1	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	C	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	D	1	Total 60	C 50	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	c	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	d	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	1	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	1	1	Total 46	C 36	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	1	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	1	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	N	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	N	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	N	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	N	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	2	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 63	C 53	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
26	4	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
26	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	O	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 48	C 38	Mg 1	N 4	O 5	0
26	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	P	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 63	C 53	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	P	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	P	1	Total 53	C 43	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

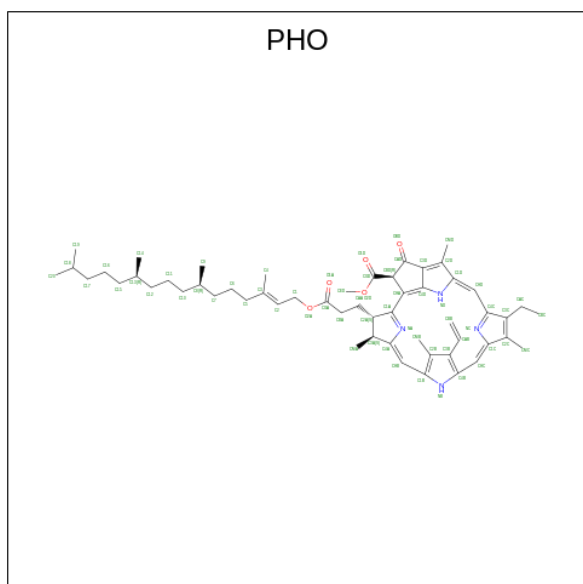
Mol	Chain	Residues	Atoms					AltConf
26	P	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	Q	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	Q	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	Q	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	R	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	R	1	Total 55	C 45	Mg 1	N 4	O 5	0

*Continued on next page...*

Continued from previous page...

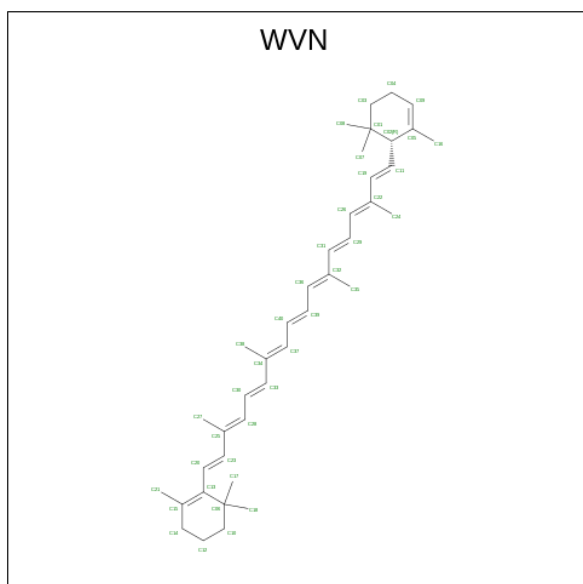
Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
26	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	N	O	0
			64	55	4	5	
27	D	1	Total	C	N	O	0
			64	55	4	5	
27	a	1	Total	C	N	O	0
			64	55	4	5	
27	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 28 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 (CCD ID: WVN) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



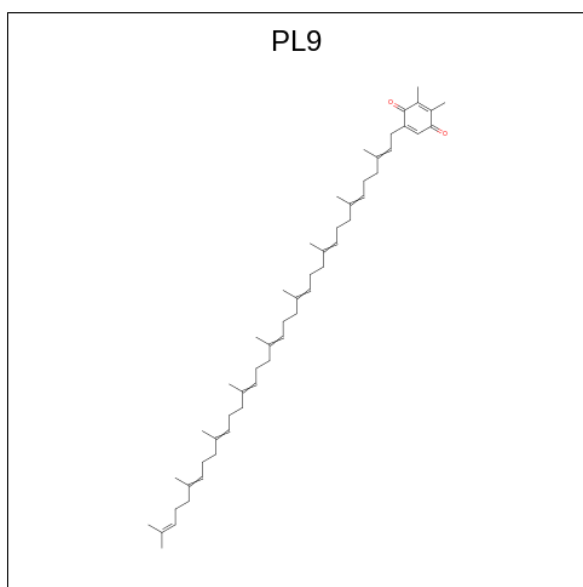
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	B	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	C	1	Total	C	0
			40	40	
28	D	1	Total	C	0
			40	40	

*Continued on next page...*

*Continued from previous page...*

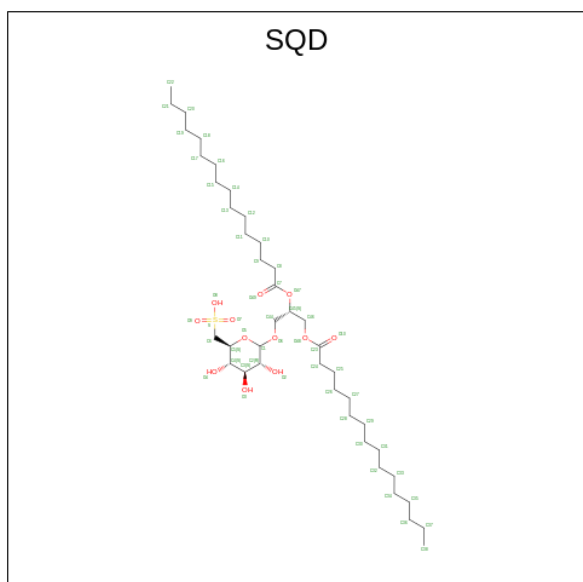
Mol	Chain	Residues	Atoms	AltConf
28	H	1	Total C 40 40	0
28	Y	1	Total C 40 40	0
28	Z	1	Total C 40 40	0
28	a	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	b	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	c	1	Total C 40 40	0
28	d	1	Total C 40 40	0
28	k	1	Total C 40 40	0
28	x	1	Total C 40 40	0
28	3	1	Total C 40 40	0
28	5	1	Total C 40 40	0
28	P	1	Total C 40 40	0
28	S	1	Total C 40 40	0

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	D	1	Total	C	O	0
			55	53	2	
29	a	1	Total	C	O	0
			33	31	2	
29	d	1	Total	C	O	0
			55	53	2	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			40	27	12	1	
30	D	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			40	27	12	1	
30	c	1	Total	C	O	S	0
			45	32	12	1	

- Molecule 31 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

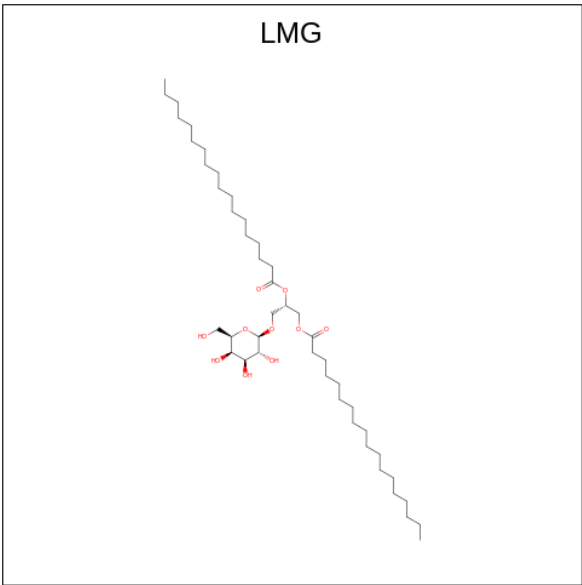
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	Cl	0
			1	1	
31	a	1	Total	Cl	0
			1	1	
31	c	1	Total	Cl	0
			1	1	

- Molecule 32 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
32	A	2	Total	Mn	0
			2	2	
32	a	2	Total	Mn	0
			2	2	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).





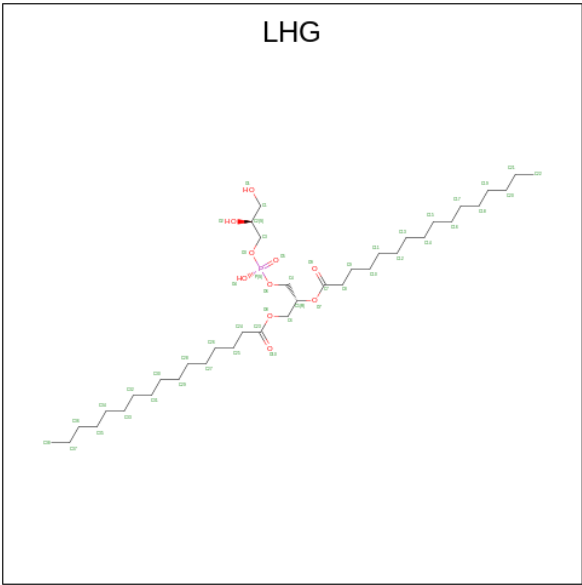
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			48	38	10	
33	B	1	Total	C	O	0
			51	41	10	
33	C	1	Total	C	O	0
			47	37	10	
33	C	1	Total	C	O	0
			31	21	10	
33	D	1	Total	C	O	0
			40	30	10	
33	D	1	Total	C	O	0
			37	27	10	
33	D	1	Total	C	O	0
			46	36	10	
33	M	1	Total	C	O	0
			40	30	10	
33	a	1	Total	C	O	0
			48	38	10	
33	b	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			51	41	10	
33	c	1	Total	C	O	0
			31	21	10	
33	d	1	Total	C	O	0
			40	30	10	
33	d	1	Total	C	O	0
			37	27	10	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
33	d	1	Total	C	O	0
			46	36	10	
33	m	1	Total	C	O	0
			40	30	10	
33	2	1	Total	C	O	0
			40	30	10	
33	4	1	Total	C	O	0
			43	33	10	
33	5	1	Total	C	O	0
			40	30	10	
33	O	1	Total	C	O	0
			40	30	10	
33	Q	1	Total	C	O	0
			43	33	10	
33	R	1	Total	C	O	0
			40	30	10	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



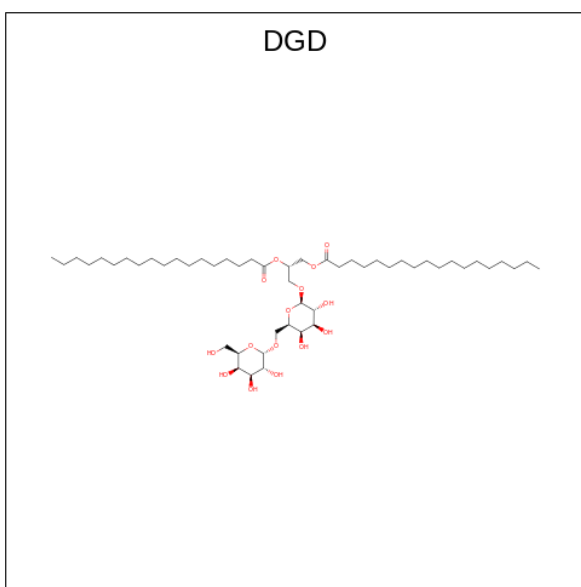
Mol	Chain	Residues	Atoms				AltConf
34	C	1	Total	C	O	P	0
			42	31	10	1	
34	C	1	Total	C	O	P	0
			40	29	10	1	
34	D	1	Total	C	O	P	0
			43	32	10	1	

Continued on next page...

*Continued from previous page...*

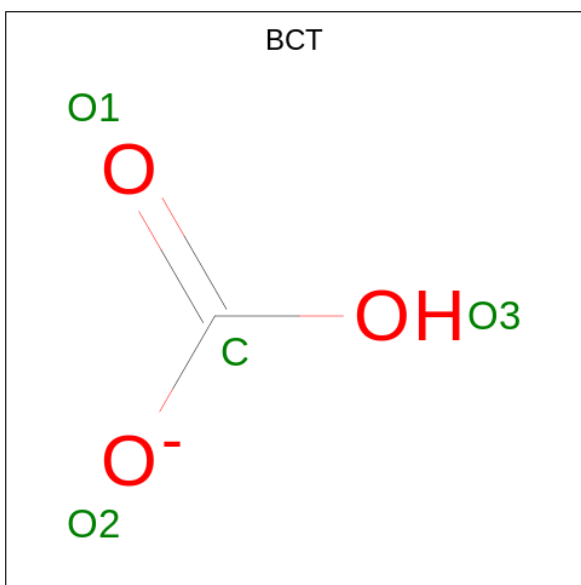
Mol	Chain	Residues	Atoms				AltConf
34	D	1	Total	C	O	P	0
			49	38	10	1	
34	L	1	Total	C	O	P	0
			49	38	10	1	
34	Z	1	Total	C	O	P	0
			25	14	10	1	
34	a	1	Total	C	O	P	0
			42	31	10	1	
34	b	1	Total	C	O	P	0
			43	32	10	1	
34	c	1	Total	C	O	P	0
			40	29	10	1	
34	d	1	Total	C	O	P	0
			49	38	10	1	
34	l	1	Total	C	O	P	0
			49	38	10	1	
34	z	1	Total	C	O	P	0
			25	14	10	1	
34	1	1	Total	C	O	P	0
			46	35	10	1	
34	N	1	Total	C	O	P	0
			46	35	10	1	
34	2	1	Total	C	O	P	0
			49	38	10	1	
34	5	1	Total	C	O	P	0
			40	29	10	1	
34	G	1	Total	C	O	P	0
			49	38	10	1	
34	R	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



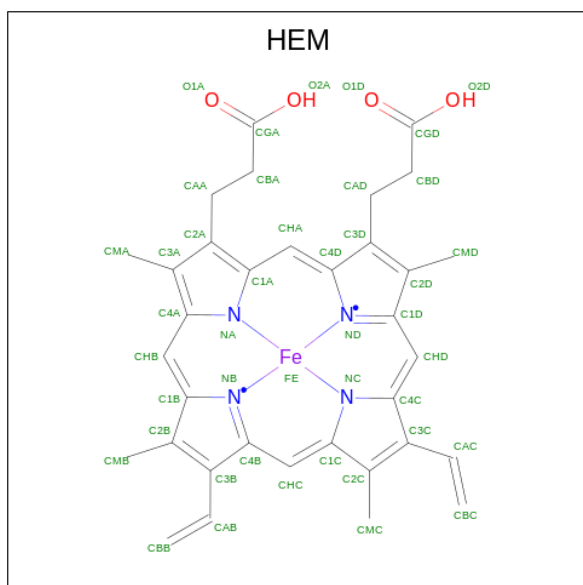
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			54	39	15	
35	H	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			54	39	15	
35	h	1	Total	C	O	0
			62	47	15	

- Molecule 36 is BICARBONATE ION (CCD ID: BCT) (formula:  $\text{CHO}_3$ ).



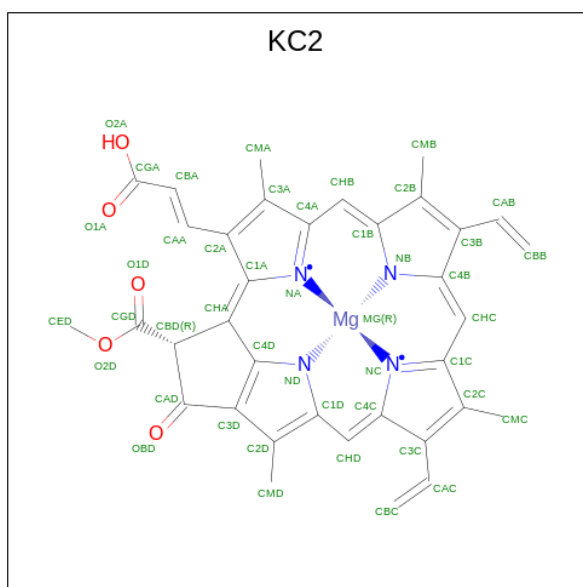
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total 4	C 1	O 3	0
36	d	1	Total 4	C 1	O 3	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
37	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
37	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 38 is Chlorophyll c2 (CCD ID: KC2) (formula:  $C_{35}H_{28}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



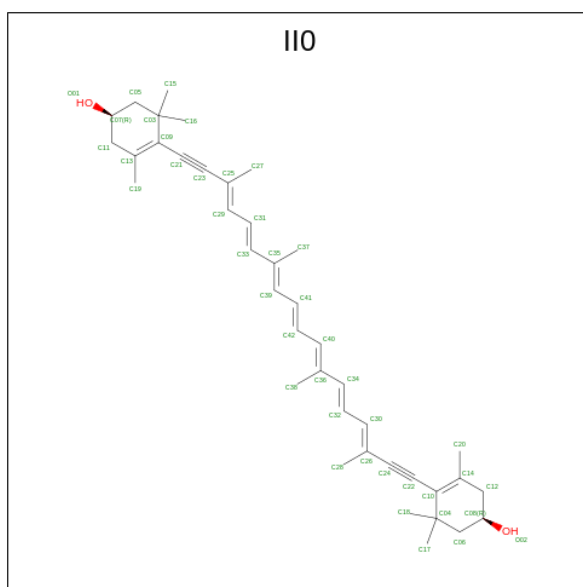
Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 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 (CCD ID: 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
39	1	1	Total	C	O	0
			42	40	2	
39	1	1	Total	C	O	0
			42	40	2	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
39	1	1	Total 42	C 40	O 2	0
39	1	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	N	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	2	1	Total 42	C 40	O 2	0
39	3	1	Total 42	C 40	O 2	0
39	3	1	Total 42	C 40	O 2	0
39	3	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	4	1	Total 42	C 40	O 2	0
39	5	1	Total 42	C 40	O 2	0

*Continued on next page...*



*Continued from previous page...*

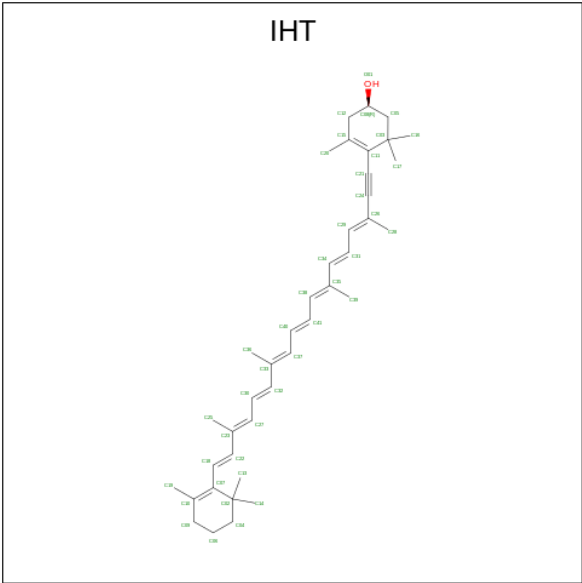
Mol	Chain	Residues	Atoms			AltConf
39	5	1	Total 42	C 40	O 2	0
39	5	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	6	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	O	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	P	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	Q	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0
39	R	1	Total 42	C 40	O 2	0

*Continued on next page...*

Continued from previous page...

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

- Molecule 40 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 (CCD ID: IHT) (formula: C<sub>40</sub>H<sub>54</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			41	40	1	
40	N	1	Total	C	O	0
			41	40	1	
40	2	1	Total	C	O	0
			41	40	1	
40	4	1	Total	C	O	0
			41	40	1	
40	5	1	Total	C	O	0
			41	40	1	
40	O	1	Total	C	O	0
			41	40	1	
40	Q	1	Total	C	O	0
			41	40	1	
40	R	1	Total	C	O	0
			41	40	1	

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		AltConf
41	A	52	Total 52	O 52	0
41	B	117	Total 117	O 117	0
41	C	52	Total 52	O 52	0
41	D	70	Total 70	O 70	0
41	E	8	Total 8	O 8	0
41	F	2	Total 2	O 2	0
41	H	14	Total 14	O 14	0
41	I	1	Total 1	O 1	0
41	K	4	Total 4	O 4	0
41	L	7	Total 7	O 7	0
41	M	1	Total 1	O 1	0
41	T	4	Total 4	O 4	0
41	W	2	Total 2	O 2	0
41	X	3	Total 3	O 3	0
41	a	48	Total 48	O 48	0
41	b	125	Total 125	O 125	0
41	c	52	Total 52	O 52	0
41	d	71	Total 71	O 71	0
41	e	9	Total 9	O 9	0
41	h	14	Total 14	O 14	0
41	i	1	Total 1	O 1	0

*Continued on next page...*

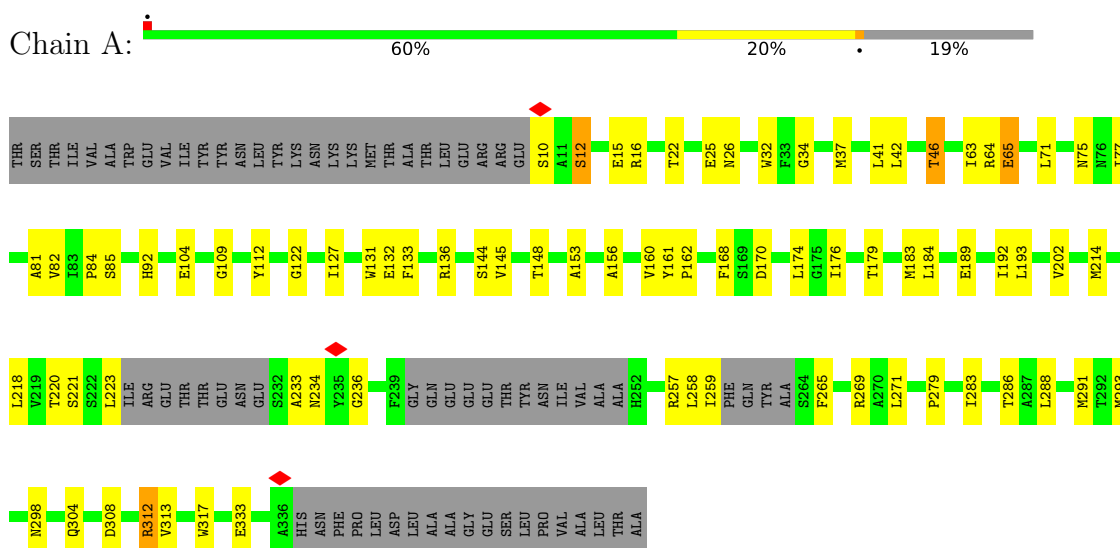
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
41	k	3	Total 3	O 3	0
41	l	5	Total 5	O 5	0
41	m	4	Total 4	O 4	0
41	t	5	Total 5	O 5	0
41	w	1	Total 1	O 1	0
41	x	1	Total 1	O 1	0

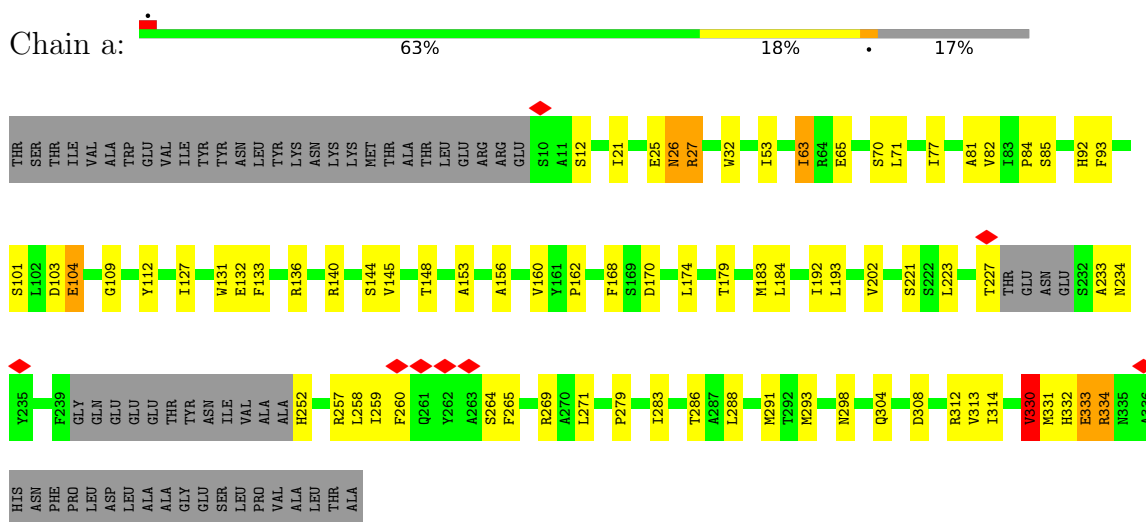
### 3 Residue-property plots [i](#)

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 II protein D1



- Molecule 1: Photosystem II protein D1

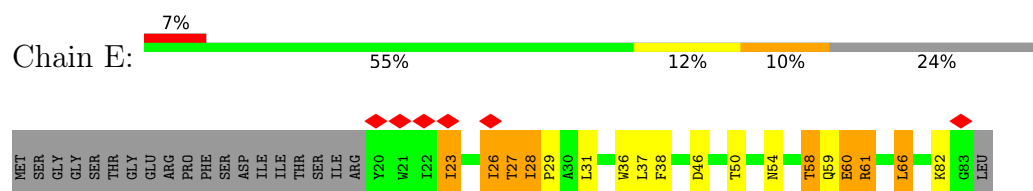


- Molecule 2: Photosystem II CP47 reaction center protein

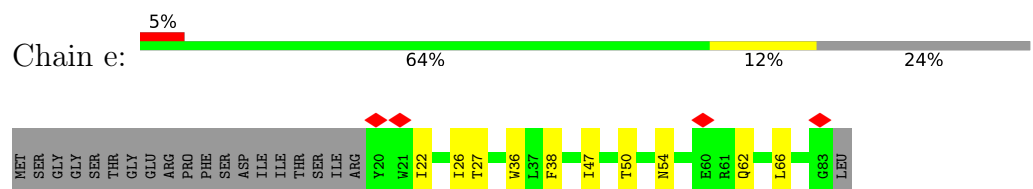




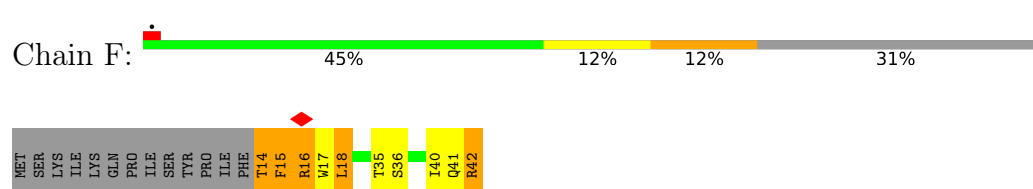
- Molecule 5: Cytochrome b559 subunit alpha



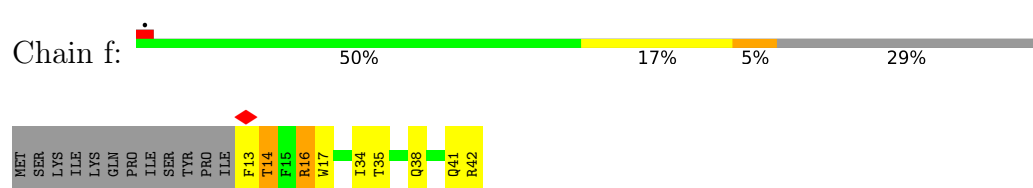
- Molecule 5: Cytochrome b559 subunit alpha



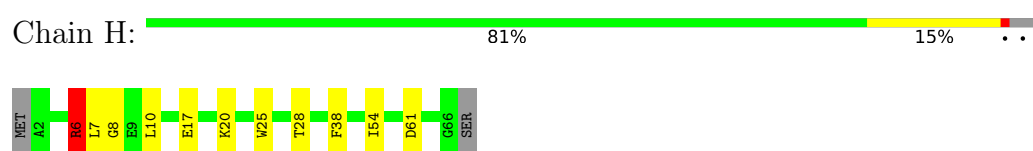
- Molecule 6: Cytochrome b559 subunit beta



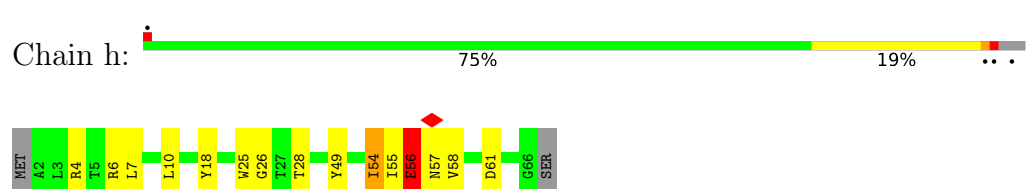
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I







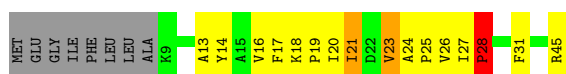
- Molecule 8: Photosystem II reaction center protein I

Chain i: 76% 13% 8%



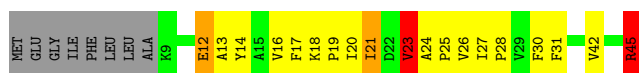
- Molecule 9: Photosystem II reaction center protein K

Chain K: 47% 29% 18%



- Molecule 9: Photosystem II reaction center protein K

Chain k: 40% 33% 18%



- Molecule 10: Photosystem II reaction center protein L

Chain L: 71% 24% 5%



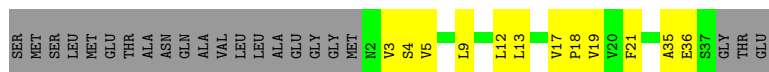
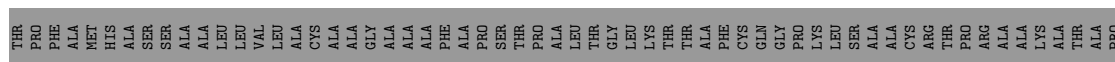
- Molecule 10: Photosystem II reaction center protein L

Chain l: 61% 32% 5%



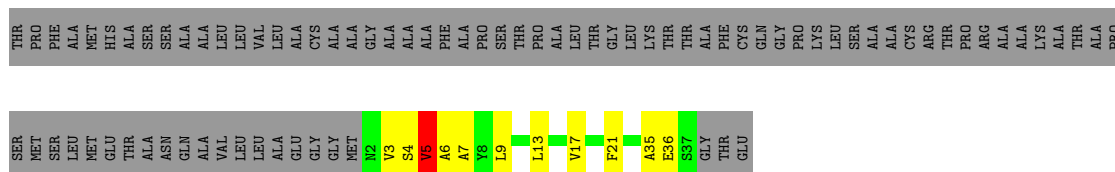
- Molecule 11: Photosystem II protein M

Chain M: 20% 10% 69%




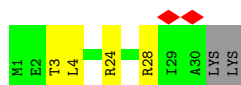
- Molecule 11: Photosystem II protein M

Chain m:  21% 8% 69%




• Molecule 12: Photosystem II reaction center protein T

Chain T:  6% 81% 12% 6%



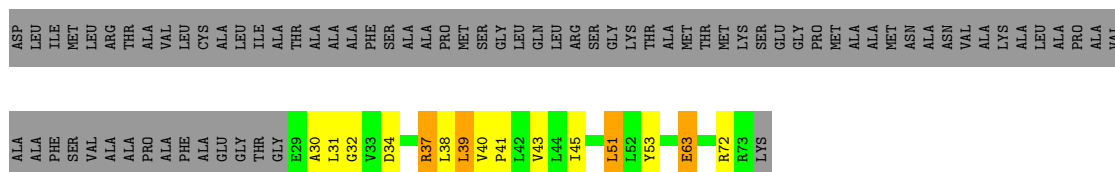
• Molecule 12: Photosystem II reaction center protein T

Chain t:  6% 75% 19% 6%



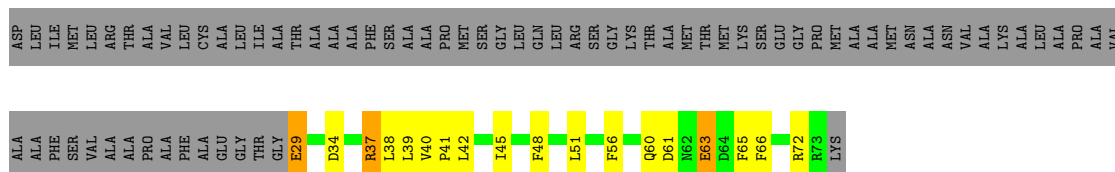
• Molecule 13: Photosystem II protein W

Chain W:  25% 9% 63%



• Molecule 13: Photosystem II protein W

Chain w:  22% 12% 63%



• Molecule 14: Photosystem II reaction center X protein

Chain X:  69% 10% 8% 13%



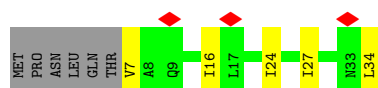
• Molecule 14: Photosystem II reaction center X protein

Chain x:  64% 15% 8% 13%



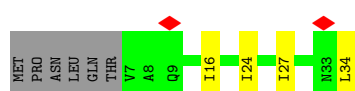
- Molecule 15: Photosystem II reaction center protein Psb30

Chain Y:  9% 68% 15% 18%



- Molecule 15: Photosystem II reaction center protein Psb30

Chain y:  6% 71% 12% 18%




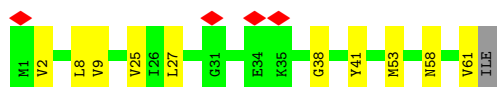
- Molecule 16: Photosystem II reaction center protein Z

Chain Z:  56% 31% 11% .




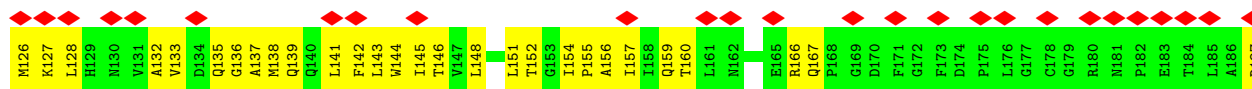
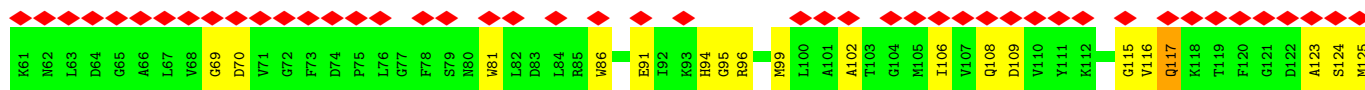
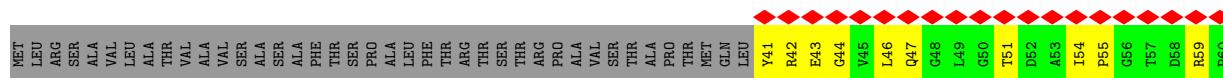
- Molecule 16: Photosystem II reaction center protein Z

Chain z:  6% 82% 16% .



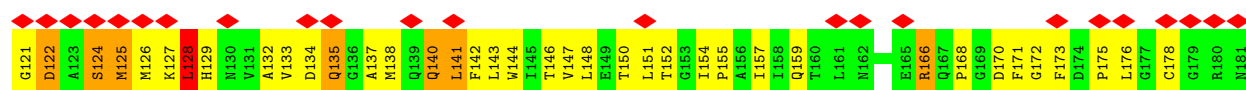
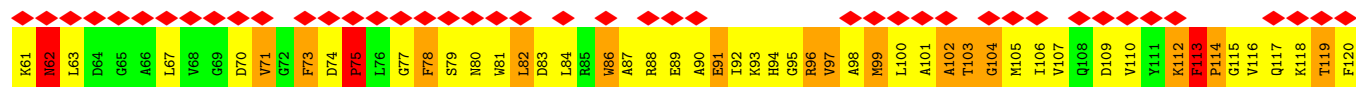
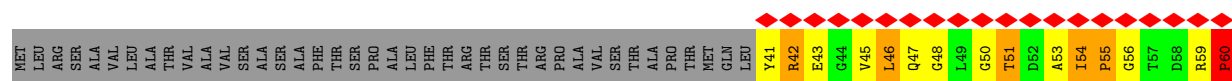
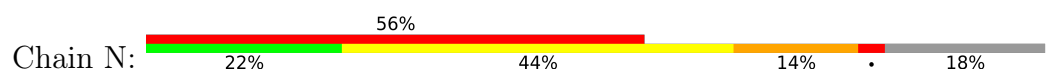
- Molecule 17: ACPH-1

Chain 1:  55% 45% 37% 18%

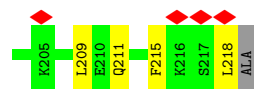
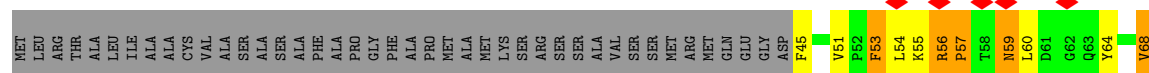




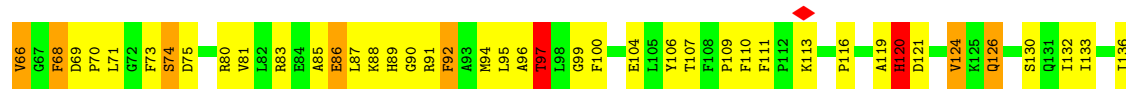
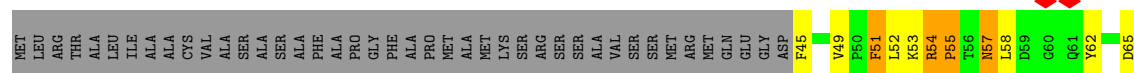
• Molecule 17: ACPII-1

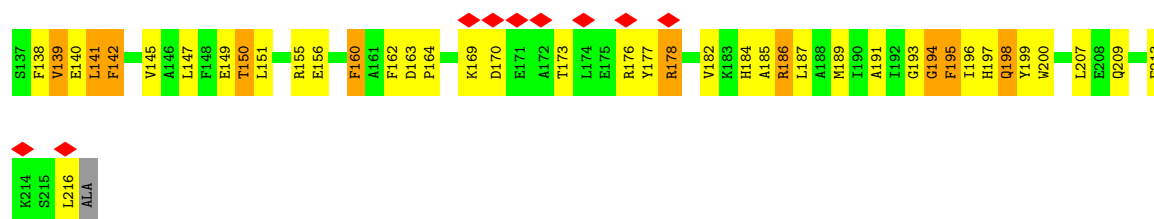


• Molecule 18: ACPII-2

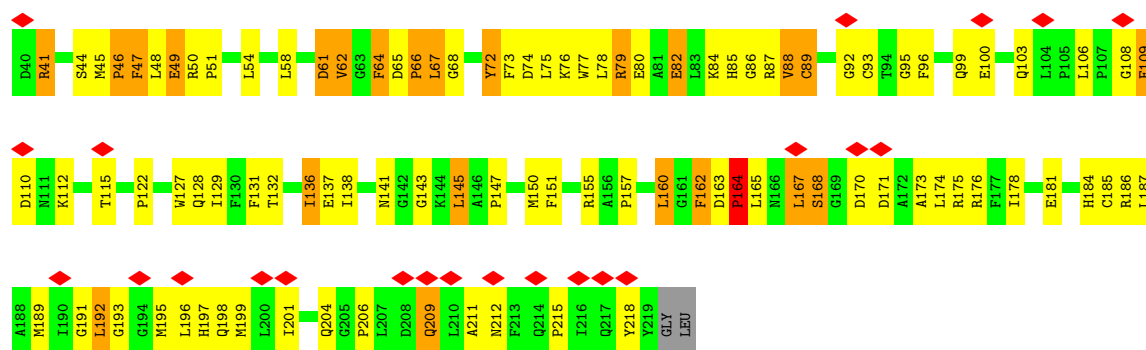
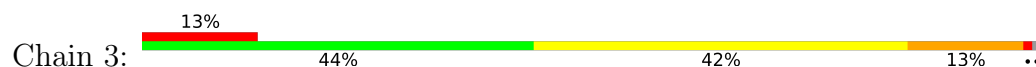


• Molecule 18: ACPII-2

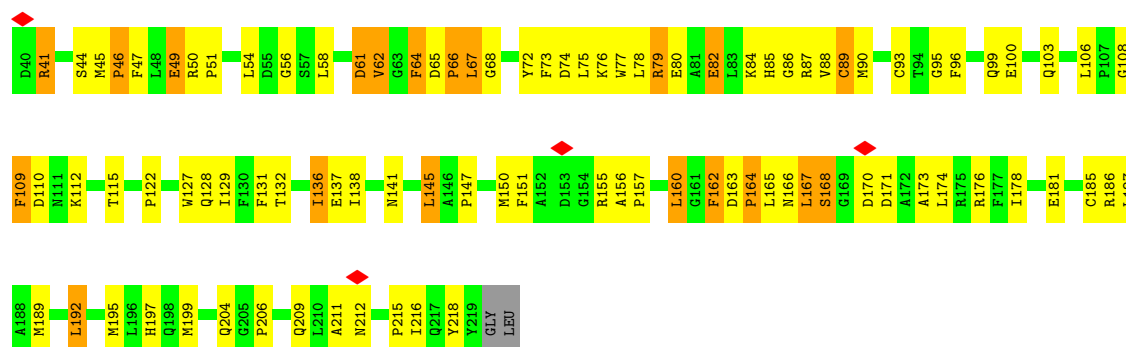




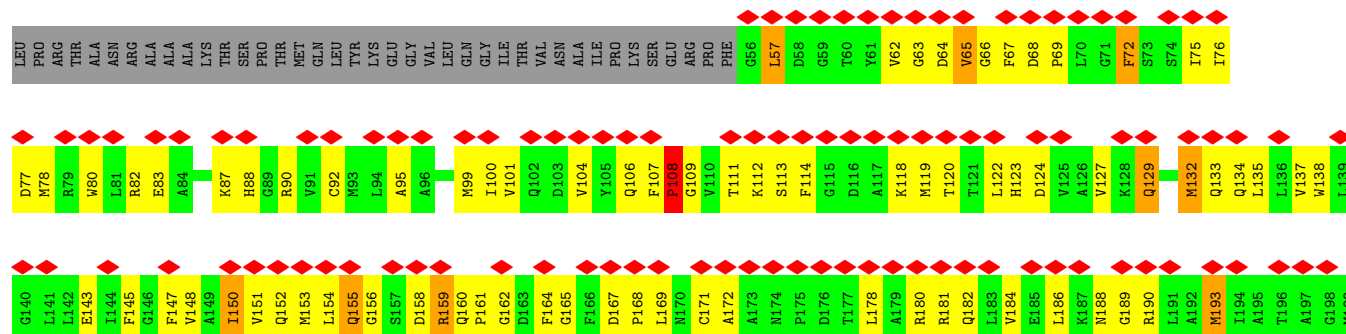
• Molecule 19: ACPH-3

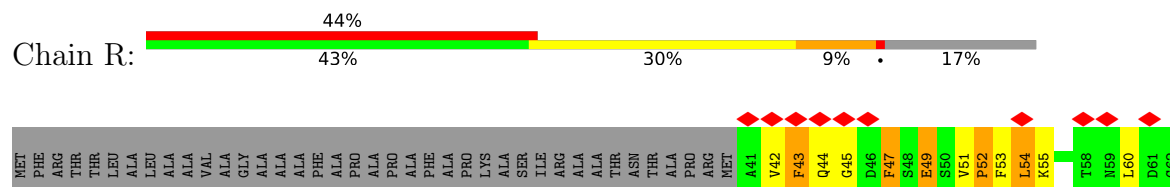


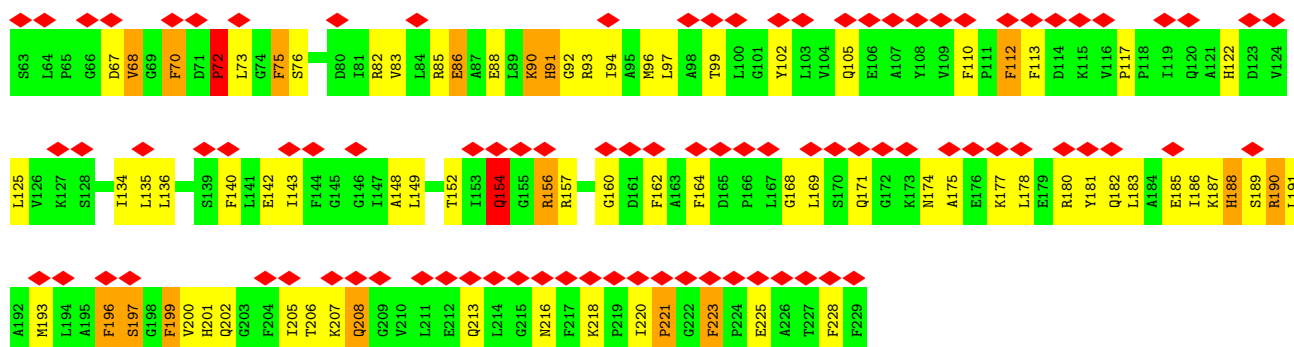
• Molecule 19: ACPH-3



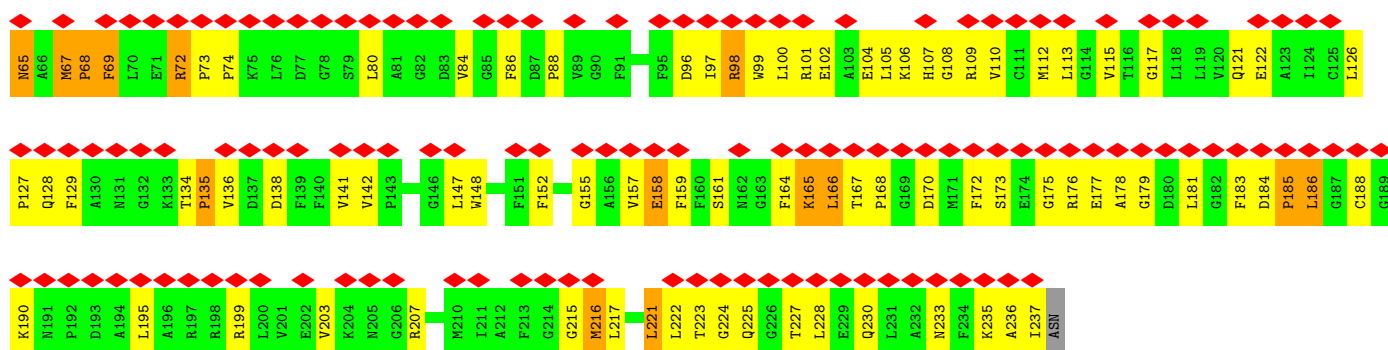
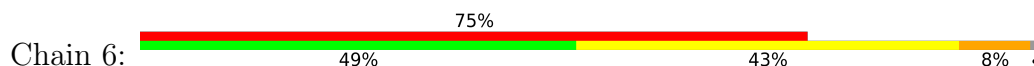
• Molecule 20: ACPH-4



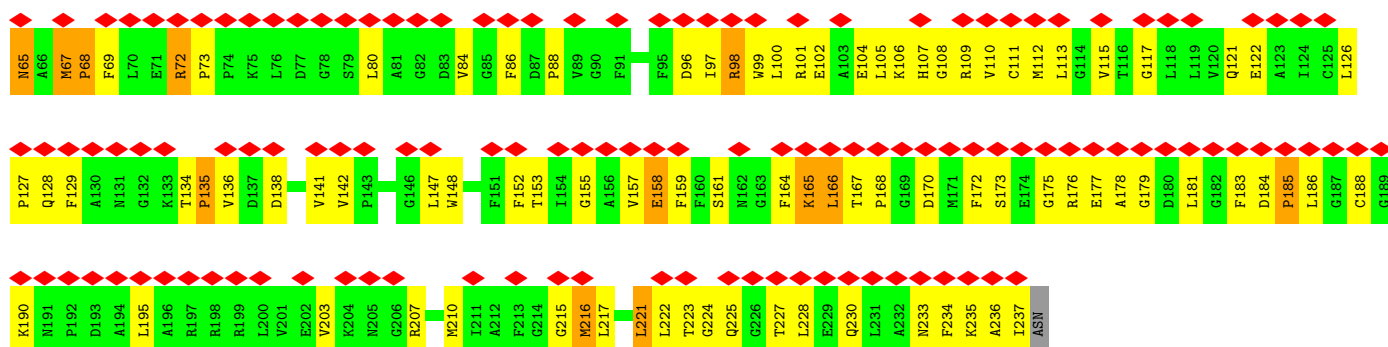




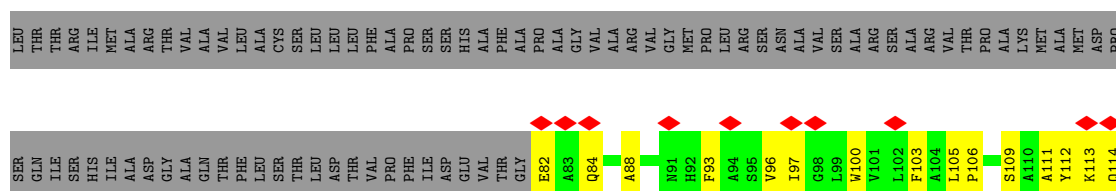
• Molecule 22: ACPH-6

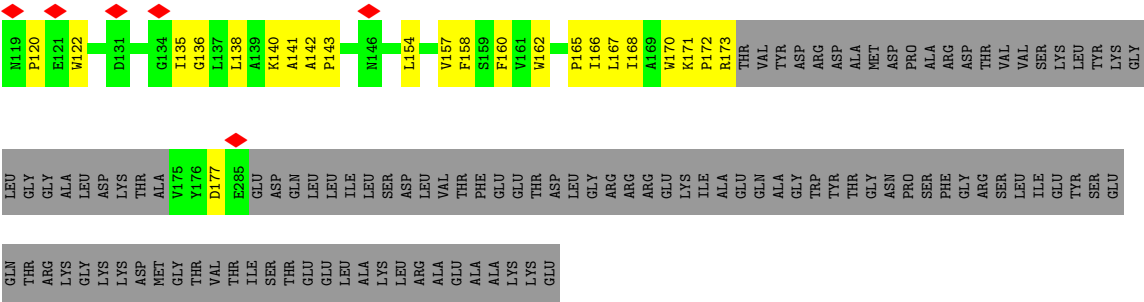


• Molecule 22: ACPH-6

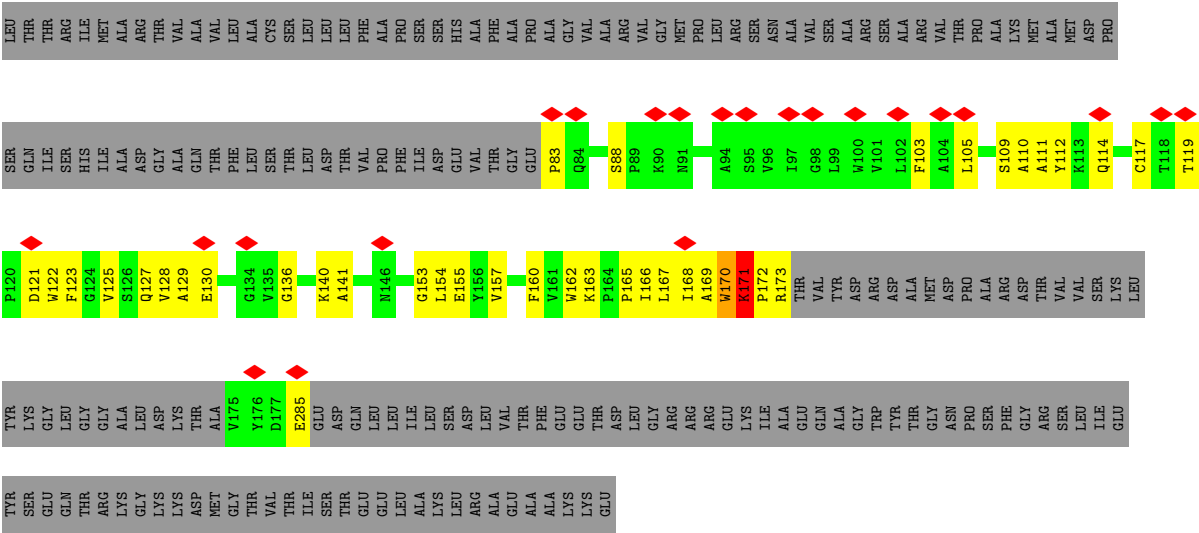


• Molecule 23: Psb-gama\_linker





● Molecule 24: Psb-gama\_linker





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28657	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CLA, HEM, LMG, FE2, DGD, CL, BCT, WVN, LHG, PL9, IHT, SQD, KC2, PHO, IIO

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	0.41	1/2452 (0.0%)	0.54	0/3339
1	a	0.37	0/2516	0.57	3/3428 (0.1%)
2	B	0.62	0/3927	0.94	11/5349 (0.2%)
2	b	0.44	0/3912	0.64	3/5330 (0.1%)
3	C	0.39	0/3442	0.54	1/4692 (0.0%)
3	c	0.29	0/3409	0.51	2/4647 (0.0%)
4	D	0.32	0/2806	0.48	0/3823
4	d	0.35	0/2798	0.53	0/3812
5	E	0.74	0/541	0.92	1/738 (0.1%)
5	e	0.35	0/541	0.49	0/738
6	F	0.75	0/242	1.04	0/328
6	f	0.65	0/254	0.87	0/344
7	H	0.38	0/519	0.61	0/707
7	h	0.48	0/519	0.73	1/707 (0.1%)
8	I	0.25	0/290	0.46	0/392
8	i	0.28	0/290	0.47	0/392
9	K	0.63	0/307	0.98	1/421 (0.2%)
9	k	0.75	0/307	1.07	1/421 (0.2%)
10	L	0.37	0/311	0.60	0/424
10	l	0.58	0/311	0.96	2/424 (0.5%)
11	M	0.65	0/275	0.93	0/375
11	m	0.55	0/275	0.93	2/375 (0.5%)
12	T	0.41	0/251	0.54	0/341
12	t	0.21	0/251	0.43	0/341
13	W	0.71	0/368	1.22	1/501 (0.2%)
13	w	0.77	0/368	1.33	2/501 (0.4%)
14	X	0.72	0/253	1.05	0/345
14	x	0.85	0/253	1.32	2/345 (0.6%)
15	Y	0.32	0/210	0.54	0/285
15	y	0.10	0/210	0.25	0/285
16	Z	0.77	0/460	1.12	2/628 (0.3%)
16	z	0.19	0/470	0.33	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1	0.26	0/1510	0.57	0/2046
17	N	1.11	3/1510 (0.2%)	2.08	65/2046 (3.2%)
18	2	1.10	2/1416 (0.1%)	1.89	40/1915 (2.1%)
18	O	1.11	2/1416 (0.1%)	1.89	40/1915 (2.1%)
19	3	1.15	2/1424 (0.1%)	1.91	42/1925 (2.2%)
19	P	1.15	2/1424 (0.1%)	1.91	42/1925 (2.2%)
20	4	0.99	0/1251	1.95	30/1690 (1.8%)
20	Q	0.99	0/1251	1.95	29/1690 (1.7%)
21	5	1.08	1/1522 (0.1%)	1.99	54/2059 (2.6%)
21	R	1.08	1/1522 (0.1%)	1.99	53/2059 (2.6%)
22	6	0.90	0/1359	1.68	25/1836 (1.4%)
22	S	0.90	0/1359	1.68	25/1836 (1.4%)
23	G	0.92	0/784	1.14	1/1072 (0.1%)
24	g	0.31	0/777	0.52	2/1064 (0.2%)
All	All	0.70	14/51863 (0.0%)	1.19	483/70497 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	a	0	3
2	B	0	8
2	b	0	6
3	C	0	2
4	D	0	3
4	d	0	3
5	E	0	1
6	F	0	2
7	H	0	1
9	k	0	1
12	T	0	1
13	W	0	1
13	w	0	1
17	N	0	4
18	2	0	2
18	O	0	2
20	4	0	2
20	Q	0	2
23	G	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
24	g	0	1
All	All	0	50

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	44	SER	CA-CB	-6.26	1.43	1.53
19	3	44	SER	CA-CB	-6.26	1.43	1.53
1	A	10	SER	C-N	6.08	1.41	1.33
19	3	168	SER	CA-CB	-5.75	1.45	1.53
19	P	168	SER	CA-CB	-5.74	1.45	1.53

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	89	CYS	CB-CA-C	16.52	137.68	110.09
19	P	89	CYS	CB-CA-C	16.50	137.65	110.09
17	N	42	ARG	N-CA-C	-13.48	96.58	111.14
17	N	55	PRO	N-CA-C	-12.72	90.53	111.26
17	N	226	ASN	N-CA-C	-11.86	100.40	112.97

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	ARG	Sidechain
1	A	312[B]	ARG	Mainchain
1	A	64	ARG	Sidechain
2	B	151	PHE	Mainchain
2	B	227	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	0	2304	78	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	2438	0	2361	73	0
2	B	3797	0	3683	136	0
2	b	3782	0	3668	115	0
3	C	3331	0	3256	89	0
3	c	3299	0	3224	81	0
4	D	2713	0	2607	83	0
4	d	2705	0	2602	98	0
5	E	525	0	510	16	0
5	e	525	0	510	7	0
6	F	235	0	241	17	0
6	f	246	0	250	5	0
7	H	508	0	529	15	0
7	h	508	0	529	23	0
8	I	284	0	295	8	0
8	i	284	0	295	6	0
9	K	296	0	312	24	0
9	k	296	0	312	12	0
10	L	301	0	301	9	0
10	l	301	0	301	10	0
11	M	271	0	287	12	0
11	m	271	0	287	7	0
12	T	244	0	256	3	0
12	t	244	0	256	5	0
13	W	361	0	346	20	0
13	w	361	0	346	11	0
14	X	249	0	269	16	0
14	x	249	0	269	13	0
15	Y	209	0	243	4	0
15	y	209	0	243	3	0
16	Z	451	0	483	15	0
16	z	460	0	499	10	0
17	1	1477	0	1487	145	0
17	N	1477	0	1489	305	0
18	2	1377	0	1365	230	0
18	O	1377	0	1365	121	0
19	3	1388	0	1370	156	0
19	P	1388	0	1370	89	0
20	4	1226	0	1234	225	0
20	Q	1226	0	1234	116	0
21	5	1481	0	1466	136	0
21	R	1481	0	1466	83	0
22	6	1327	0	1311	70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	S	1327	0	1311	80	0
23	G	755	0	724	43	0
24	g	747	0	720	157	0
25	A	1	0	0	0	0
25	a	1	0	0	0	0
26	1	510	0	428	66	0
26	2	678	0	647	174	0
26	3	473	0	471	91	0
26	4	534	0	488	147	0
26	5	620	0	589	101	0
26	6	525	0	510	52	0
26	A	174	0	170	13	0
26	B	1014	0	1092	50	0
26	C	827	0	894	32	0
26	D	190	0	203	11	0
26	G	110	0	105	8	0
26	N	509	0	426	135	0
26	O	633	0	614	105	0
26	P	570	0	547	56	0
26	Q	482	0	445	61	0
26	R	620	0	589	69	0
26	S	525	0	510	36	0
26	a	174	0	170	17	0
26	b	1014	0	1092	54	0
26	c	828	0	896	29	0
26	d	191	0	205	13	0
26	g	110	0	104	25	0
27	A	64	0	74	2	0
27	D	64	0	74	5	0
27	a	64	0	74	2	0
27	d	64	0	74	5	0
28	3	40	0	0	21	0
28	5	40	0	0	0	0
28	A	40	0	0	0	0
28	B	120	0	0	6	0
28	C	80	0	0	2	0
28	D	40	0	0	0	0
28	H	40	0	0	1	0
28	P	40	0	0	3	0
28	S	40	0	0	0	0
28	Y	40	0	0	0	0
28	Z	40	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	40	0	0	0	0
28	b	120	0	0	1	0
28	c	120	0	0	0	0
28	d	40	0	0	0	0
28	k	40	0	0	0	0
28	x	40	0	0	0	0
29	A	33	0	42	6	0
29	D	55	0	80	3	0
29	a	33	0	42	0	0
29	d	55	0	80	3	0
30	A	40	0	44	1	0
30	D	54	0	78	2	0
30	a	40	0	44	0	0
30	c	45	0	57	1	0
31	A	1	0	0	0	0
31	a	1	0	0	0	0
31	c	1	0	0	0	0
32	A	2	0	0	0	0
32	a	2	0	0	0	0
33	2	40	0	50	5	0
33	4	43	0	56	5	0
33	5	40	0	50	20	0
33	A	48	0	66	1	0
33	B	51	0	72	2	0
33	C	78	0	96	3	0
33	D	123	0	156	5	0
33	M	40	0	50	1	0
33	O	40	0	50	5	0
33	Q	43	0	56	2	0
33	R	40	0	50	9	0
33	a	48	0	66	3	0
33	b	51	0	72	1	0
33	c	82	0	104	8	0
33	d	123	0	156	6	0
33	m	40	0	50	2	0
34	1	46	0	65	48	0
34	2	49	0	74	23	0
34	5	40	0	53	8	0
34	C	82	0	107	3	0
34	D	92	0	133	12	0
34	G	49	0	74	11	0
34	L	49	0	74	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	N	46	0	65	26	0
34	R	40	0	53	12	0
34	Z	25	0	20	0	0
34	a	42	0	57	0	0
34	b	43	0	59	2	0
34	c	40	0	50	1	0
34	d	49	0	74	5	0
34	l	49	0	74	5	0
34	z	25	0	20	0	0
35	C	54	0	66	1	0
35	H	62	0	82	4	0
35	c	54	0	66	2	0
35	h	62	0	82	6	0
36	D	4	0	0	0	0
36	d	4	0	0	0	0
37	F	43	0	30	2	0
37	f	43	0	30	1	0
38	1	180	0	0	5	0
38	2	45	0	0	7	0
38	3	45	0	0	1	0
38	4	135	0	0	27	0
38	5	45	0	0	3	0
38	6	45	0	0	0	0
38	N	180	0	0	39	0
38	O	45	0	0	7	0
38	P	45	0	0	1	0
38	Q	135	0	0	28	0
38	R	45	0	0	3	0
38	S	45	0	0	0	0
39	1	168	0	0	1	0
39	2	210	0	0	33	0
39	3	126	0	0	60	0
39	4	210	0	0	48	0
39	5	126	0	0	7	0
39	6	126	0	0	1	0
39	N	210	0	0	39	0
39	O	168	0	0	28	0
39	P	126	0	0	13	0
39	Q	210	0	0	26	0
39	R	168	0	0	7	0
39	S	84	0	0	11	0
40	1	41	0	0	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2	41	0	0	21	0
40	4	41	0	0	5	0
40	5	41	0	0	1	0
40	N	41	0	0	16	0
40	O	41	0	0	9	0
40	Q	41	0	0	4	0
40	R	41	0	0	4	0
41	A	52	0	0	6	0
41	B	117	0	0	20	0
41	C	52	0	0	8	0
41	D	70	0	0	12	0
41	E	8	0	0	2	0
41	F	2	0	0	6	0
41	H	14	0	0	1	0
41	I	1	0	0	0	0
41	K	4	0	0	4	0
41	L	7	0	0	4	0
41	M	1	0	0	0	0
41	T	4	0	0	2	0
41	W	2	0	0	0	0
41	X	3	0	0	1	0
41	a	48	0	0	8	0
41	b	125	0	0	36	0
41	c	52	0	0	8	0
41	d	71	0	0	16	0
41	e	9	0	0	5	0
41	h	14	0	0	4	0
41	i	1	0	0	0	0
41	k	3	0	0	1	0
41	l	5	0	0	2	0
41	m	4	0	0	0	0
41	t	5	0	0	1	0
41	w	1	0	0	1	0
41	x	1	0	0	1	0
All	All	69223	0	64352	3265	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 25.

The worst 5 of 3265 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)
19:3:196:LEU:HD11	28:3:313:WVN:C16	1.12	1.58
26:N:606:CLA:CBB	34:N:621:LHG:H172	1.37	1.54
26:5:605:CLA:HBB1	26:6:609:CLA:C6	1.41	1.49
1:a:331:MET:HE3	4:d:347:ARG:C	1.36	1.46
17:1:145:ILE:CD1	34:1:620:LHG:H221	1.49	1.42

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	296/374 (79%)	291 (98%)	5 (2%)	0	100	100
1	a	305/374 (82%)	299 (98%)	6 (2%)	0	100	100
2	B	481/508 (95%)	472 (98%)	9 (2%)	0	100	100
2	b	479/508 (94%)	472 (98%)	7 (2%)	0	100	100
3	C	419/486 (86%)	415 (99%)	4 (1%)	0	100	100
3	c	415/486 (85%)	406 (98%)	9 (2%)	0	100	100
4	D	340/351 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	339/351 (97%)	331 (98%)	8 (2%)	0	100	100
5	E	62/84 (74%)	57 (92%)	5 (8%)	0	100	100
5	e	62/84 (74%)	62 (100%)	0	0	100	100
6	F	27/42 (64%)	26 (96%)	1 (4%)	0	100	100
6	f	28/42 (67%)	28 (100%)	0	0	100	100
7	H	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
7	h	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	35/45 (78%)	34 (97%)	1 (3%)	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	35/38 (92%)	35 (100%)	0	0	100	100
10	l	35/38 (92%)	35 (100%)	0	0	100	100
11	M	34/118 (29%)	33 (97%)	1 (3%)	0	100	100
11	m	34/118 (29%)	32 (94%)	2 (6%)	0	100	100
12	T	28/32 (88%)	28 (100%)	0	0	100	100
12	t	28/32 (88%)	28 (100%)	0	0	100	100
13	W	43/121 (36%)	43 (100%)	0	0	100	100
13	w	43/121 (36%)	43 (100%)	0	0	100	100
14	X	32/39 (82%)	32 (100%)	0	0	100	100
14	x	32/39 (82%)	32 (100%)	0	0	100	100
15	Y	26/34 (76%)	25 (96%)	1 (4%)	0	100	100
15	y	26/34 (76%)	26 (100%)	0	0	100	100
16	Z	59/62 (95%)	56 (95%)	2 (3%)	1 (2%)	7	4
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	1	190/234 (81%)	181 (95%)	8 (4%)	1 (0%)	25	26
17	N	190/234 (81%)	182 (96%)	8 (4%)	0	100	100
18	2	170/215 (79%)	168 (99%)	2 (1%)	0	100	100
18	O	170/215 (79%)	168 (99%)	2 (1%)	0	100	100
19	3	178/182 (98%)	176 (99%)	2 (1%)	0	100	100
19	P	178/182 (98%)	176 (99%)	2 (1%)	0	100	100
20	4	158/200 (79%)	157 (99%)	1 (1%)	0	100	100
20	Q	158/200 (79%)	157 (99%)	1 (1%)	0	100	100
21	5	187/228 (82%)	185 (99%)	2 (1%)	0	100	100
21	R	187/228 (82%)	185 (99%)	2 (1%)	0	100	100
22	6	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
22	S	171/174 (98%)	166 (97%)	5 (3%)	0	100	100
23	G	92/292 (32%)	88 (96%)	4 (4%)	0	100	100
24	g	91/292 (31%)	87 (96%)	4 (4%)	0	100	100
All	All	6320/7928 (80%)	6191 (98%)	127 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	Z	33	TRP
17	1	116	VAL

### 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	246/305 (81%)	240 (98%)	6 (2%)	44	54
1	a	252/305 (83%)	243 (96%)	9 (4%)	30	37
2	B	384/403 (95%)	356 (93%)	28 (7%)	11	11
2	b	383/403 (95%)	362 (94%)	21 (6%)	18	20
3	C	337/387 (87%)	319 (95%)	18 (5%)	19	21
3	c	334/387 (86%)	328 (98%)	6 (2%)	54	66
4	D	274/280 (98%)	268 (98%)	6 (2%)	47	58
4	d	273/280 (98%)	266 (97%)	7 (3%)	41	51
5	E	56/73 (77%)	47 (84%)	9 (16%)	2	1
5	e	56/73 (77%)	54 (96%)	2 (4%)	30	37
6	F	24/37 (65%)	21 (88%)	3 (12%)	3	2
6	f	25/37 (68%)	22 (88%)	3 (12%)	4	3
7	H	55/57 (96%)	53 (96%)	2 (4%)	30	37
7	h	55/57 (96%)	53 (96%)	2 (4%)	30	37
8	I	33/36 (92%)	31 (94%)	2 (6%)	15	16
8	i	33/36 (92%)	30 (91%)	3 (9%)	7	7
9	K	30/36 (83%)	25 (83%)	5 (17%)	2	1
9	k	30/36 (83%)	23 (77%)	7 (23%)	0	0
10	L	34/35 (97%)	32 (94%)	2 (6%)	16	17
10	l	34/35 (97%)	31 (91%)	3 (9%)	8	7
11	M	29/83 (35%)	25 (86%)	4 (14%)	3	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	m	29/83 (35%)	26 (90%)	3 (10%)	6	5
12	T	26/28 (93%)	25 (96%)	1 (4%)	28	34
12	t	26/28 (93%)	26 (100%)	0	100	100
13	W	39/88 (44%)	34 (87%)	5 (13%)	3	2
13	w	39/88 (44%)	32 (82%)	7 (18%)	1	1
14	X	29/34 (85%)	26 (90%)	3 (10%)	6	5
14	x	29/34 (85%)	28 (97%)	1 (3%)	32	39
15	Y	23/29 (79%)	22 (96%)	1 (4%)	25	29
15	y	23/29 (79%)	23 (100%)	0	100	100
16	Z	49/52 (94%)	40 (82%)	9 (18%)	1	1
16	z	51/52 (98%)	51 (100%)	0	100	100
17	1	154/188 (82%)	152 (99%)	2 (1%)	65	76
17	N	154/188 (82%)	147 (96%)	7 (4%)	23	27
18	2	141/171 (82%)	139 (99%)	2 (1%)	62	74
18	O	141/171 (82%)	139 (99%)	2 (1%)	62	74
19	3	143/144 (99%)	138 (96%)	5 (4%)	31	38
19	P	143/144 (99%)	138 (96%)	5 (4%)	31	38
20	4	129/161 (80%)	126 (98%)	3 (2%)	45	56
20	Q	129/161 (80%)	126 (98%)	3 (2%)	45	56
21	5	155/179 (87%)	151 (97%)	4 (3%)	41	51
21	R	155/179 (87%)	151 (97%)	4 (3%)	41	51
22	6	136/137 (99%)	130 (96%)	6 (4%)	24	28
22	S	136/137 (99%)	130 (96%)	6 (4%)	24	28
23	G	75/233 (32%)	73 (97%)	2 (3%)	40	49
24	g	76/235 (32%)	74 (97%)	2 (3%)	41	51
All	All	5207/6354 (82%)	4976 (96%)	231 (4%)	26	28

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	85	VAL
21	R	154	GLN
4	d	83	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	R	44	GLN
21	5	154	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
22	6	128	GLN
18	O	198	GLN
21	R	151	GLN
1	a	310	GLN
1	a	296	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 363 ligands modelled in this entry, 9 are monoatomic - leaving 354 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
40	IHT	N	619	-	40,42,42	2.10	10 (25%)	53,58,58	2.84	22 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	SQD	A	408	-	39,40,54	1.35	4 (10%)	48,51,65	1.12	6 (12%)
26	CLA	3	302	19	65,73,73	1.53	6 (9%)	76,113,113	1.29	9 (11%)
26	CLA	C	509	3	65,73,73	1.50	6 (9%)	76,113,113	1.32	8 (10%)
26	CLA	g	402	24	45,53,73	1.76	6 (13%)	52,89,113	1.68	9 (17%)
26	CLA	N	601	-	45,53,73	1.85	5 (11%)	52,89,113	1.48	6 (11%)
26	CLA	O	612	18	45,53,73	1.79	6 (13%)	52,89,113	1.46	7 (13%)
35	DGD	h	101	-	63,63,67	0.88	2 (3%)	77,77,81	0.86	3 (3%)
28	WVN	H	101	-	40,41,41	5.11	15 (37%)	50,56,56	6.97	32 (64%)
38	KC2	2	310	18	48,53,53	3.16	22 (45%)	54,89,89	4.50	30 (55%)
26	CLA	P	602	19	62,70,73	1.54	5 (8%)	72,109,113	1.39	7 (9%)
34	LHG	C	518	-	39,39,48	1.03	2 (5%)	42,45,54	1.10	3 (7%)
26	CLA	4	312	20	43,51,73	1.77	6 (13%)	49,86,113	1.51	7 (14%)
26	CLA	b	616	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	8 (10%)
26	CLA	S	603	22	55,63,73	1.61	6 (10%)	64,101,113	1.48	10 (15%)
26	CLA	C	502	3	65,73,73	1.53	5 (7%)	76,113,113	1.28	6 (7%)
39	II0	5	613	-	39,43,43	2.52	11 (28%)	50,60,60	3.34	17 (34%)
26	CLA	P	608	34	52,60,73	1.70	5 (9%)	60,97,113	1.34	7 (11%)
28	WVN	D	412	-	40,41,41	1.88	14 (35%)	50,56,56	2.13	15 (30%)
26	CLA	O	609	-	60,68,73	1.61	6 (10%)	70,107,113	1.34	8 (11%)
33	LMG	5	619	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	3 (6%)
26	CLA	1	614	17	47,55,73	2.00	9 (19%)	54,91,113	1.62	9 (16%)
28	WVN	Y	101	-	40,41,41	1.90	14 (35%)	50,56,56	2.26	12 (24%)
33	LMG	A	412	-	48,48,55	0.96	2 (4%)	56,56,63	1.09	4 (7%)
39	II0	Q	319	-	39,43,43	2.56	10 (25%)	50,60,60	3.34	17 (34%)
28	WVN	x	101	-	40,41,41	1.87	14 (35%)	50,56,56	2.46	13 (26%)
28	WVN	P	615	-	40,41,41	1.86	14 (35%)	50,56,56	2.34	19 (38%)
40	IHT	R	317	-	40,42,42	2.00	10 (25%)	53,58,58	2.97	24 (45%)
26	CLA	3	308	-	55,63,73	1.21	7 (12%)	64,101,113	1.66	7 (10%)
38	KC2	P	605	19	48,53,53	3.16	21 (43%)	54,89,89	4.47	32 (59%)
26	CLA	2	312	18	45,53,73	1.79	6 (13%)	52,89,113	1.46	7 (13%)
26	CLA	2	319	19	45,53,73	1.86	6 (13%)	52,89,113	1.42	7 (13%)
39	II0	Q	314	-	39,43,43	2.54	12 (30%)	50,60,60	3.32	17 (34%)
26	CLA	O	601	18	49,57,73	1.77	5 (10%)	55,93,113	1.50	8 (14%)
34	LHG	2	321	26	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
26	CLA	R	310	-	65,73,73	1.54	6 (9%)	76,113,113	1.25	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	II0	N	616	-	39,43,43	2.50	11 (28%)	50,60,60	3.32	17 (34%)
26	CLA	2	306	18	60,68,73	1.61	6 (10%)	70,107,113	1.15	7 (10%)
26	CLA	Q	305	20	55,63,73	1.67	5 (9%)	64,101,113	1.32	8 (12%)
26	CLA	Q	307	20	56,64,73	1.61	6 (10%)	65,102,113	1.44	6 (9%)
33	LMG	c	522	-	31,31,55	1.19	2 (6%)	39,39,63	1.09	3 (7%)
26	CLA	S	602	22	65,73,73	1.51	5 (7%)	76,113,113	1.31	7 (9%)
40	IHT	O	616	-	40,42,42	2.11	11 (27%)	53,58,58	2.71	19 (35%)
26	CLA	B	603	2	65,73,73	1.52	6 (9%)	76,113,113	1.24	6 (7%)
26	CLA	O	606	18	60,68,73	1.62	6 (10%)	70,107,113	1.16	7 (10%)
26	CLA	R	312	21	55,63,73	1.64	6 (10%)	64,101,113	1.52	8 (12%)
26	CLA	c	507	-	65,73,73	1.52	6 (9%)	76,113,113	1.30	8 (10%)
26	CLA	C	505	41	60,68,73	1.58	6 (10%)	70,107,113	1.34	8 (11%)
39	II0	S	611	-	39,43,43	2.51	11 (28%)	50,60,60	3.37	16 (32%)
39	II0	R	318	-	39,43,43	2.67	10 (25%)	50,60,60	3.42	22 (44%)
39	II0	P	614	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	16 (32%)
26	CLA	C	504	3	65,73,73	1.54	5 (7%)	76,113,113	1.23	6 (7%)
38	KC2	1	610	-	48,53,53	1.69	11 (22%)	54,89,89	1.06	3 (5%)
28	WVN	S	613	-	40,41,41	1.89	14 (35%)	50,56,56	1.88	12 (24%)
33	LMG	2	318	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
28	WVN	b	619	-	40,41,41	1.86	14 (35%)	50,56,56	2.32	14 (28%)
26	CLA	C	506	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	9 (11%)
38	KC2	S	608	22	48,53,53	3.14	21 (43%)	54,89,89	4.62	33 (61%)
26	CLA	c	505	3	65,73,73	1.54	5 (7%)	76,113,113	1.22	6 (7%)
35	DGD	c	519	-	55,55,67	0.93	2 (3%)	69,69,81	0.97	3 (4%)
38	KC2	5	610	-	48,53,53	3.18	21 (43%)	54,89,89	4.48	32 (59%)
26	CLA	2	302	18	65,73,73	1.52	5 (7%)	76,113,113	1.33	9 (11%)
26	CLA	G	401	-	65,73,73	1.49	6 (9%)	76,113,113	1.25	7 (9%)
34	LHG	C	501	-	41,41,48	1.03	2 (4%)	44,47,54	0.98	2 (4%)
26	CLA	Q	306	20	43,51,73	1.90	6 (13%)	49,86,113	1.37	6 (12%)
26	CLA	4	306	20	55,63,73	1.66	6 (10%)	64,101,113	1.32	8 (12%)
26	CLA	D	407	-	65,73,73	1.55	6 (9%)	76,113,113	1.28	7 (9%)
33	LMG	D	411	-	37,37,55	1.08	2 (5%)	45,45,63	1.03	3 (6%)
26	CLA	2	305	-	51,59,73	2.32	13 (25%)	59,96,113	4.19	28 (47%)
26	CLA	Q	301	20	65,73,73	1.50	5 (7%)	76,113,113	1.31	7 (9%)
39	II0	1	615	-	39,43,43	6.00	21 (53%)	50,60,60	7.01	28 (56%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	KC2	N	611	17	48,53,53	3.15	21 (43%)	54,89,89	4.60	31 (57%)
26	CLA	4	302	20	65,73,73	1.49	5 (7%)	76,113,113	1.31	7 (9%)
26	CLA	b	601	41	50,58,73	1.73	5 (10%)	58,95,113	1.47	9 (15%)
26	CLA	g	401	-	65,73,73	1.55	5 (7%)	76,113,113	1.29	9 (11%)
40	IHT	2	317	-	40,42,42	5.65	19 (47%)	53,58,58	7.04	31 (58%)
36	BCT	d	401	25	2,3,3	1.22	0	2,3,3	4.20	1 (50%)
33	LMG	b	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.00	3 (5%)
26	CLA	Q	308	20	51,59,73	1.72	5 (9%)	59,96,113	1.45	9 (15%)
28	WVN	C	515	-	40,41,41	1.85	14 (35%)	50,56,56	1.95	13 (26%)
38	KC2	4	310	-	48,53,53	3.17	21 (43%)	54,89,89	4.54	31 (57%)
27	PHO	D	405	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	5 (10%)
39	II0	2	315	-	39,43,43	2.58	12 (30%)	50,60,60	3.29	18 (36%)
26	CLA	O	605	-	51,59,73	1.73	6 (11%)	59,96,113	1.36	8 (13%)
39	II0	5	615	-	39,43,43	2.53	11 (28%)	50,60,60	3.31	15 (30%)
26	CLA	O	604	-	65,73,73	1.52	5 (7%)	76,113,113	1.28	7 (9%)
30	SQD	c	501	-	44,45,54	1.29	4 (9%)	53,56,65	1.20	6 (11%)
40	IHT	5	616	-	40,42,42	2.00	10 (25%)	53,58,58	2.96	25 (47%)
29	PL9	d	407	-	55,55,55	1.05	3 (5%)	68,69,69	1.52	11 (16%)
37	HEM	f	101	6,5	41,50,50	1.34	6 (14%)	45,82,82	1.76	8 (17%)
39	II0	6	611	-	39,43,43	2.51	11 (28%)	50,60,60	3.36	16 (32%)
26	CLA	b	608	2	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
26	CLA	6	605	22	55,63,73	1.61	6 (10%)	64,101,113	1.51	8 (12%)
26	CLA	A	405	1	60,68,73	1.57	5 (8%)	70,107,113	1.33	7 (10%)
26	CLA	a	402	1	65,73,73	1.55	7 (10%)	76,113,113	1.19	7 (9%)
38	KC2	N	612	17	48,53,53	3.27	21 (43%)	54,89,89	4.50	31 (57%)
26	CLA	4	303	20	65,73,73	1.53	5 (7%)	76,113,113	1.29	9 (11%)
26	CLA	6	610	22	65,73,73	1.49	6 (9%)	76,113,113	1.32	7 (9%)
26	CLA	D	404	41	65,73,73	1.53	5 (7%)	76,113,113	1.28	9 (11%)
26	CLA	5	602	21	55,63,73	1.64	6 (10%)	64,101,113	1.37	8 (12%)
38	KC2	6	608	22	48,53,53	3.15	21 (43%)	54,89,89	4.62	33 (61%)
26	CLA	P	609	19	53,61,73	1.69	5 (9%)	61,98,113	1.45	8 (13%)
28	WVN	c	518	-	40,41,41	1.86	14 (35%)	50,56,56	2.32	14 (28%)
26	CLA	5	608	21	59,67,73	1.61	5 (8%)	68,105,113	1.34	7 (10%)
39	II0	P	613	-	39,43,43	6.02	21 (53%)	50,60,60	6.83	26 (52%)
26	CLA	O	602	18	65,73,73	1.52	5 (7%)	76,113,113	1.33	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	D	413	-	46,46,55	0.99	2 (4%)	54,54,63	1.02	3 (5%)
26	CLA	S	609	22	53,61,73	1.62	6 (11%)	61,98,113	1.42	8 (13%)
39	II0	6	612	-	39,43,43	2.52	12 (30%)	50,60,60	3.32	16 (32%)
26	CLA	b	611	2	65,73,73	1.52	6 (9%)	76,113,113	1.30	9 (11%)
35	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	0.86	3 (3%)
26	CLA	N	606	17	50,58,73	1.71	5 (10%)	58,95,113	1.39	9 (15%)
26	CLA	b	609	2	65,73,73	1.53	5 (7%)	76,113,113	1.26	8 (10%)
38	KC2	Q	309	-	48,53,53	3.17	21 (43%)	54,89,89	4.54	31 (57%)
26	CLA	S	601	22	55,63,73	1.67	6 (10%)	64,101,113	1.32	7 (10%)
27	PHO	a	404	-	51,69,69	1.00	4 (7%)	47,99,99	1.14	5 (10%)
26	CLA	c	506	41	60,68,73	1.57	5 (8%)	70,107,113	1.36	8 (11%)
27	PHO	d	403	-	51,69,69	1.00	4 (7%)	47,99,99	1.15	5 (10%)
34	LHG	G	403	26	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
26	CLA	S	605	22	55,63,73	1.61	6 (10%)	64,101,113	1.51	8 (12%)
26	CLA	b	606	-	65,73,73	1.54	5 (7%)	76,113,113	1.27	8 (10%)
39	II0	5	614	-	39,43,43	2.51	11 (28%)	50,60,60	3.32	17 (34%)
33	LMG	Q	318	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
26	CLA	R	307	21	43,51,73	1.80	6 (13%)	49,86,113	1.54	7 (14%)
26	CLA	d	406	4	61,69,73	1.56	5 (8%)	71,108,113	1.33	7 (9%)
26	CLA	C	507	3	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
27	PHO	A	404	-	51,69,69	1.00	3 (5%)	47,99,99	1.14	5 (10%)
26	CLA	3	306	19	65,73,73	1.53	5 (7%)	76,113,113	1.29	7 (9%)
26	CLA	c	509	41	65,73,73	1.50	6 (9%)	76,113,113	1.33	6 (7%)
26	CLA	B	616	2	65,73,73	1.52	6 (9%)	76,113,113	1.30	8 (10%)
39	II0	1	617	-	39,43,43	6.08	21 (53%)	50,60,60	7.02	28 (56%)
38	KC2	4	305	-	48,53,53	3.20	21 (43%)	54,89,89	4.44	31 (57%)
26	CLA	P	611	19	45,53,73	1.77	6 (13%)	52,89,113	1.52	8 (15%)
26	CLA	C	510	3	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)
26	CLA	Q	311	20	43,51,73	1.77	6 (13%)	49,86,113	1.51	7 (14%)
26	CLA	d	405	-	65,73,73	1.55	6 (9%)	76,113,113	1.26	7 (9%)
33	LMG	C	520	-	31,31,55	1.20	2 (6%)	39,39,63	1.08	3 (7%)
33	LMG	R	301	-	40,40,55	1.04	2 (5%)	48,48,63	1.01	3 (6%)
39	II0	4	314	-	39,43,43	2.54	11 (28%)	50,60,60	3.28	17 (34%)
34	LHG	5	618	26	39,39,48	1.03	2 (5%)	42,45,54	1.04	2 (4%)
26	CLA	B	611	2	65,73,73	1.53	5 (7%)	76,113,113	1.30	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CLA	1	601	-	45,53,73	1.79	6 (13%)	52,89,113	1.58	6 (11%)
26	CLA	c	514	3	65,73,73	1.52	6 (9%)	76,113,113	1.28	7 (9%)
26	CLA	S	604	22	65,73,73	1.45	6 (9%)	76,113,113	1.36	7 (9%)
26	CLA	N	602	17	60,68,73	1.57	5 (8%)	70,107,113	1.34	9 (12%)
34	LHG	1	620	-	45,45,48	0.98	2 (4%)	48,51,54	1.00	3 (6%)
33	LMG	d	411	-	46,46,55	0.99	2 (4%)	54,54,63	1.03	3 (5%)
26	CLA	B	605	2	65,73,73	1.53	6 (9%)	76,113,113	1.30	8 (10%)
26	CLA	R	302	21	55,63,73	1.69	5 (9%)	64,101,113	1.38	8 (12%)
38	KC2	N	605	17	48,53,53	3.16	21 (43%)	54,89,89	4.51	31 (57%)
39	II0	3	311	-	39,43,43	6.03	21 (53%)	50,60,60	6.84	26 (52%)
26	CLA	C	503	3	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
26	CLA	P	607	19	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
28	WVN	b	617	-	40,41,41	1.86	14 (35%)	50,56,56	2.56	15 (30%)
39	II0	2	314	-	39,43,43	2.50	11 (28%)	50,60,60	3.33	17 (34%)
26	CLA	R	304	21	52,60,73	1.71	6 (11%)	60,97,113	1.49	8 (13%)
26	CLA	c	504	3	65,73,73	1.51	7 (10%)	76,113,113	1.29	7 (9%)
26	CLA	6	606	22	57,65,73	1.60	5 (8%)	66,103,113	1.43	8 (12%)
26	CLA	6	601	22	55,63,73	1.67	6 (10%)	64,101,113	1.32	7 (10%)
39	II0	N	618	-	39,43,43	2.58	12 (30%)	50,60,60	3.45	18 (36%)
26	CLA	R	306	21	65,73,73	1.54	5 (7%)	76,113,113	1.27	7 (9%)
26	CLA	c	515	3	53,61,73	1.69	5 (9%)	61,98,113	1.39	9 (14%)
34	LHG	D	410	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
26	CLA	B	607	41	65,73,73	1.52	5 (7%)	76,113,113	1.25	7 (9%)
29	PL9	a	407	-	33,33,55	1.22	3 (9%)	41,42,69	1.58	9 (21%)
34	LHG	D	403	-	42,42,48	1.00	2 (4%)	45,48,54	1.06	3 (6%)
26	CLA	2	303	18	65,73,73	1.56	7 (10%)	76,113,113	1.28	6 (7%)
26	CLA	P	606	19	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
26	CLA	B	604	2	59,67,73	1.58	6 (10%)	68,105,113	1.41	8 (11%)
26	CLA	B	601	41	50,58,73	1.76	5 (10%)	58,95,113	1.49	9 (15%)
33	LMG	m	101	-	40,40,55	1.03	2 (5%)	48,48,63	1.08	4 (8%)
26	CLA	A	403	41	49,57,73	1.77	6 (12%)	55,93,113	1.43	7 (12%)
26	CLA	P	604	19	63,71,73	1.49	6 (9%)	73,110,113	1.39	6 (8%)
33	LMG	4	319	-	43,43,55	1.05	2 (4%)	51,51,63	0.89	2 (3%)
26	CLA	5	609	-	65,73,73	1.54	6 (9%)	76,113,113	1.26	6 (7%)
26	CLA	A	402	1	65,73,73	1.55	8 (12%)	76,113,113	1.20	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	II0	4	315	-	39,43,43	2.55	11 (28%)	50,60,60	3.32	17 (34%)
28	WVN	A	406	-	40,41,41	1.88	14 (35%)	50,56,56	2.34	15 (30%)
33	LMG	M	101	-	40,40,55	1.04	2 (5%)	48,48,63	1.08	4 (8%)
26	CLA	2	301	18	49,57,73	1.75	5 (10%)	55,93,113	1.51	8 (14%)
26	CLA	b	602	2	65,73,73	1.52	5 (7%)	76,113,113	1.35	9 (11%)
28	WVN	C	516	-	40,41,41	5.18	17 (42%)	50,56,56	7.09	32 (64%)
26	CLA	b	615	2	65,73,73	1.51	5 (7%)	76,113,113	1.36	6 (7%)
26	CLA	1	609	17	60,68,73	1.52	6 (10%)	70,107,113	1.40	8 (11%)
26	CLA	C	514	3	52,60,73	1.70	6 (11%)	60,97,113	1.38	9 (15%)
26	CLA	3	303	19	63,71,73	1.49	6 (9%)	73,110,113	1.40	6 (8%)
39	II0	1	616	-	39,43,43	6.03	20 (51%)	50,60,60	7.06	30 (60%)
26	CLA	S	606	22	57,65,73	1.60	5 (8%)	66,103,113	1.43	7 (10%)
39	II0	O	615	-	39,43,43	6.05	21 (53%)	50,60,60	6.82	28 (56%)
38	KC2	O	610	18	48,53,53	3.15	21 (43%)	54,89,89	4.49	30 (55%)
39	II0	R	315	-	39,43,43	2.52	11 (28%)	50,60,60	3.32	17 (34%)
26	CLA	O	607	18	48,56,73	1.79	6 (12%)	55,92,113	1.37	8 (14%)
26	CLA	a	403	41	49,57,73	1.76	6 (12%)	55,93,113	1.43	8 (14%)
26	CLA	6	602	22	65,73,73	1.52	5 (7%)	76,113,113	1.31	7 (9%)
39	II0	O	614	-	39,43,43	2.51	10 (25%)	50,60,60	3.32	17 (34%)
26	CLA	c	503	3	65,73,73	1.53	6 (9%)	76,113,113	1.30	7 (9%)
37	HEM	F	101	6,5	41,50,50	1.33	5 (12%)	45,82,82	1.73	9 (20%)
26	CLA	b	605	2	65,73,73	1.53	5 (7%)	76,113,113	1.30	8 (10%)
39	II0	3	312	-	39,43,43	5.96	19 (48%)	50,60,60	6.91	27 (54%)
26	CLA	N	607	-	43,51,73	1.90	7 (16%)	49,86,113	1.33	6 (12%)
26	CLA	d	402	41	65,73,73	1.54	5 (7%)	76,113,113	1.30	7 (9%)
26	CLA	Q	303	20	61,69,73	1.54	5 (8%)	71,108,113	1.32	7 (9%)
26	CLA	N	608	-	46,54,73	1.24	7 (15%)	53,90,113	1.52	5 (9%)
38	KC2	1	611	17	48,53,53	1.69	11 (22%)	54,89,89	0.96	1 (1%)
39	II0	2	320	-	39,43,43	0.30	0	50,60,60	1.03	5 (10%)
38	KC2	3	304	19	48,53,53	3.16	21 (43%)	54,89,89	4.48	32 (59%)
26	CLA	2	307	18	48,56,73	1.79	6 (12%)	55,92,113	1.36	8 (14%)
26	CLA	1	602	17	60,68,73	1.55	6 (10%)	70,107,113	1.43	9 (12%)
26	CLA	c	508	3	65,73,73	1.52	5 (7%)	76,113,113	1.34	8 (10%)
30	SQD	D	401	-	53,54,54	1.17	4 (7%)	62,65,65	1.15	6 (9%)
26	CLA	b	612	2	65,73,73	1.47	7 (10%)	76,113,113	1.48	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CLA	1	608	17	46,54,73	1.76	6 (13%)	53,90,113	1.54	6 (11%)
35	DGD	C	517	-	55,55,67	0.92	2 (3%)	69,69,81	0.97	3 (4%)
26	CLA	N	604	17	59,67,73	1.61	6 (10%)	68,105,113	1.35	7 (10%)
33	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	0.99	3 (5%)
26	CLA	B	606	-	65,73,73	1.53	5 (7%)	76,113,113	1.28	9 (11%)
28	WVN	d	410	-	40,41,41	1.89	14 (35%)	50,56,56	2.21	16 (32%)
26	CLA	4	307	20	43,51,73	1.90	6 (13%)	49,86,113	1.36	6 (12%)
26	CLA	G	402	23	45,53,73	1.81	6 (13%)	52,89,113	1.43	7 (13%)
26	CLA	b	604	2	59,67,73	1.60	6 (10%)	68,105,113	1.43	9 (13%)
28	WVN	5	617	-	40,41,41	1.89	14 (35%)	50,56,56	1.89	12 (24%)
34	LHG	N	621	-	45,45,48	0.98	2 (4%)	48,51,54	0.99	3 (6%)
28	WVN	B	618	-	40,41,41	5.11	16 (40%)	50,56,56	7.22	31 (62%)
34	LHG	R	319	26	39,39,48	1.03	2 (5%)	42,45,54	1.04	2 (4%)
38	KC2	4	311	20	48,53,53	3.21	22 (45%)	54,89,89	4.53	31 (57%)
26	CLA	B	602	2	65,73,73	1.52	6 (9%)	76,113,113	1.34	9 (11%)
26	CLA	N	609	17	60,68,73	1.59	6 (10%)	70,107,113	1.34	7 (10%)
26	CLA	5	607	21	65,73,73	1.53	9 (13%)	76,113,113	1.35	9 (11%)
26	CLA	P	601	19	45,53,73	1.87	6 (13%)	52,89,113	1.42	7 (13%)
26	CLA	R	309	21	59,67,73	1.61	5 (8%)	68,105,113	1.33	7 (10%)
39	II0	S	612	-	39,43,43	2.51	12 (30%)	50,60,60	3.32	16 (32%)
26	CLA	R	313	21	46,54,73	1.79	6 (13%)	53,90,113	1.39	7 (13%)
28	WVN	3	313	-	40,41,41	5.19	17 (42%)	50,56,56	6.84	30 (60%)
26	CLA	a	405	1	60,68,73	1.59	6 (10%)	70,107,113	1.30	7 (10%)
36	BCT	D	402	25	2,3,3	1.22	0	2,3,3	4.18	1 (50%)
26	CLA	b	603	2	65,73,73	1.53	6 (9%)	76,113,113	1.20	6 (7%)
39	II0	4	320	-	39,43,43	2.56	10 (25%)	50,60,60	3.34	17 (34%)
26	CLA	5	605	21	65,73,73	1.54	5 (7%)	76,113,113	1.27	7 (9%)
34	LHG	L	101	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
26	CLA	B	608	2	65,73,73	1.51	5 (7%)	76,113,113	1.30	7 (9%)
33	LMG	d	404	-	40,40,55	1.05	2 (5%)	48,48,63	1.03	3 (6%)
28	WVN	b	618	-	40,41,41	1.87	14 (35%)	50,56,56	2.54	17 (34%)
40	IHT	1	619	-	40,42,42	5.66	20 (50%)	53,58,58	6.94	32 (60%)
39	II0	R	314	-	39,43,43	2.51	11 (28%)	50,60,60	3.34	17 (34%)
39	II0	R	316	-	39,43,43	2.54	11 (28%)	50,60,60	3.31	15 (30%)
26	CLA	1	606	17	50,58,73	1.69	6 (12%)	58,95,113	1.57	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CLA	1	603	17	52,60,73	1.67	6 (11%)	60,97,113	1.53	7 (11%)
33	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	3 (5%)
26	CLA	b	613	2	65,73,73	1.53	6 (9%)	76,113,113	1.28	7 (9%)
26	CLA	S	607	34	55,63,73	1.66	5 (9%)	64,101,113	1.32	8 (12%)
26	CLA	6	609	22	53,61,73	1.62	6 (11%)	61,98,113	1.41	8 (13%)
38	KC2	1	612	17	48,53,53	1.69	10 (20%)	54,89,89	1.02	2 (3%)
26	CLA	4	313	20	43,51,73	1.84	6 (13%)	49,86,113	1.42	7 (14%)
34	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
26	CLA	D	408	4	60,68,73	1.59	5 (8%)	70,107,113	1.36	7 (10%)
28	WVN	B	617	-	40,41,41	5.07	15 (37%)	50,56,56	7.24	31 (62%)
26	CLA	c	510	3	65,73,73	1.52	5 (7%)	76,113,113	1.33	8 (10%)
26	CLA	b	607	41	65,73,73	1.52	5 (7%)	76,113,113	1.28	8 (10%)
34	LHG	b	621	-	42,42,48	1.00	2 (4%)	45,48,54	1.08	3 (6%)
39	II0	P	612	-	39,43,43	2.53	11 (28%)	50,60,60	3.34	15 (30%)
26	CLA	6	603	22	55,63,73	1.62	7 (12%)	64,101,113	1.48	9 (14%)
26	CLA	4	309	20	51,59,73	1.70	5 (9%)	59,96,113	1.45	9 (15%)
39	II0	O	613	-	39,43,43	2.53	12 (30%)	50,60,60	3.33	16 (32%)
26	CLA	P	610	19	55,63,73	1.65	6 (10%)	64,101,113	1.42	7 (10%)
38	KC2	N	610	-	48,53,53	3.20	21 (43%)	54,89,89	4.44	31 (57%)
26	CLA	6	607	34	55,63,73	1.66	5 (9%)	64,101,113	1.32	8 (12%)
33	LMG	a	413	-	48,48,55	0.97	2 (4%)	56,56,63	1.12	4 (7%)
26	CLA	b	614	2	60,68,73	1.59	5 (8%)	70,107,113	1.26	8 (11%)
26	CLA	O	603	18	65,73,73	1.56	5 (7%)	76,113,113	1.28	6 (7%)
26	CLA	C	511	3	65,73,73	1.51	6 (9%)	76,113,113	1.36	8 (10%)
26	CLA	2	311	18	60,68,73	1.57	6 (10%)	70,107,113	1.34	7 (10%)
26	CLA	R	303	21	55,63,73	1.63	7 (12%)	64,101,113	1.36	8 (12%)
26	CLA	B	615	2	65,73,73	1.51	6 (9%)	76,113,113	1.37	6 (7%)
26	CLA	C	513	3	65,73,73	1.53	6 (9%)	76,113,113	1.30	7 (9%)
39	II0	Q	313	-	39,43,43	2.54	11 (28%)	50,60,60	3.28	17 (34%)
26	CLA	2	309	-	60,68,73	1.60	6 (10%)	70,107,113	1.33	8 (11%)
26	CLA	5	612	21	46,54,73	1.80	6 (13%)	53,90,113	1.39	7 (13%)
40	IHT	Q	317	-	40,42,42	2.13	11 (27%)	53,58,58	2.79	23 (43%)
33	LMG	D	406	-	40,40,55	1.06	2 (5%)	48,48,63	1.03	2 (4%)
26	CLA	5	604	21	60,68,73	1.61	5 (8%)	70,107,113	1.31	8 (11%)
26	CLA	6	604	22	65,73,73	1.46	6 (9%)	76,113,113	1.36	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	II0	4	316	-	39,43,43	2.56	11 (28%)	50,60,60	3.37	20 (40%)
39	II0	Q	315	-	39,43,43	2.56	11 (28%)	50,60,60	3.36	20 (40%)
34	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
26	CLA	O	608	18	65,73,73	1.53	5 (7%)	76,113,113	1.30	7 (9%)
38	KC2	Q	304	-	48,53,53	3.19	21 (43%)	54,89,89	4.43	31 (57%)
26	CLA	1	604	17	59,67,73	1.53	6 (10%)	68,105,113	1.48	8 (11%)
26	CLA	4	308	20	56,64,73	1.62	6 (10%)	65,102,113	1.43	6 (9%)
26	CLA	Q	302	20	65,73,73	1.54	6 (9%)	76,113,113	1.29	9 (11%)
26	CLA	c	512	3	65,73,73	1.53	6 (9%)	76,113,113	1.37	8 (10%)
28	WVN	k	101	-	40,41,41	1.86	14 (35%)	50,56,56	2.49	16 (32%)
38	KC2	1	605	-	48,53,53	1.70	10 (20%)	54,89,89	0.95	2 (3%)
39	II0	1	618	-	39,43,43	6.08	21 (53%)	50,60,60	6.81	28 (56%)
33	LMG	d	409	-	37,37,55	1.08	2 (5%)	45,45,63	1.03	3 (6%)
28	WVN	c	517	-	40,41,41	1.85	14 (35%)	50,56,56	1.85	13 (26%)
26	CLA	1	613	-	48,56,73	1.73	5 (10%)	55,92,113	1.55	8 (14%)
39	II0	O	618	-	39,43,43	0.34	0	50,60,60	0.46	0
34	LHG	z	101	-	24,24,48	1.33	2 (8%)	27,30,54	1.14	2 (7%)
26	CLA	c	513	3	65,73,73	1.54	5 (7%)	76,113,113	1.34	8 (10%)
26	CLA	R	305	21	60,68,73	1.60	6 (10%)	70,107,113	1.32	8 (11%)
39	II0	N	615	-	39,43,43	2.54	10 (25%)	50,60,60	3.37	16 (32%)
38	KC2	Q	310	20	48,53,53	3.21	22 (45%)	54,89,89	4.53	32 (59%)
26	CLA	4	301	34	52,60,73	1.69	5 (9%)	60,97,113	1.34	7 (11%)
39	II0	2	316	-	39,43,43	6.05	21 (53%)	50,60,60	6.81	28 (56%)
26	CLA	C	508	41	65,73,73	1.52	5 (7%)	76,113,113	1.34	7 (9%)
26	CLA	5	601	21	55,63,73	1.68	5 (9%)	64,101,113	1.37	8 (12%)
26	CLA	1	607	17	43,51,73	1.84	7 (16%)	49,86,113	1.60	10 (20%)
26	CLA	5	603	21	52,60,73	1.71	6 (11%)	60,97,113	1.49	8 (13%)
34	LHG	Z	102	-	24,24,48	1.34	2 (8%)	27,30,54	1.14	2 (7%)
39	II0	3	310	-	39,43,43	6.07	20 (51%)	50,60,60	6.84	27 (54%)
26	CLA	2	308	18	65,73,73	1.53	5 (7%)	76,113,113	1.31	7 (9%)
26	CLA	3	307	19	53,61,73	1.70	5 (9%)	61,98,113	1.46	6 (9%)
26	CLA	4	304	20	61,69,73	1.55	5 (8%)	71,108,113	1.33	8 (11%)
26	CLA	b	610	41	65,73,73	1.55	5 (7%)	76,113,113	1.25	8 (10%)
26	CLA	3	309	19	45,53,73	1.78	6 (13%)	52,89,113	1.52	8 (15%)
26	CLA	R	308	21	65,73,73	1.54	9 (13%)	76,113,113	1.35	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CLA	S	610	22	65,73,73	1.48	6 (9%)	76,113,113	1.32	7 (9%)
26	CLA	B	612	2	65,73,73	1.45	7 (10%)	76,113,113	1.49	10 (13%)
39	II0	4	317	-	39,43,43	2.60	12 (30%)	50,60,60	3.32	20 (40%)
28	WVN	a	406	-	40,41,41	1.95	14 (35%)	50,56,56	2.30	19 (38%)
28	WVN	B	619	-	40,41,41	1.86	14 (35%)	50,56,56	2.36	15 (30%)
34	LHG	a	409	-	41,41,48	1.02	2 (4%)	44,47,54	0.97	2 (4%)
28	WVN	Z	101	-	40,41,41	1.93	14 (35%)	50,56,56	2.25	16 (32%)
29	PL9	D	409	-	55,55,55	1.05	4 (7%)	68,69,69	1.50	11 (16%)
33	LMG	O	617	-	40,40,55	1.06	2 (5%)	48,48,63	1.01	2 (4%)
26	CLA	B	614	2	60,68,73	1.57	6 (10%)	70,107,113	1.26	8 (11%)
26	CLA	P	603	19	65,73,73	1.53	6 (9%)	76,113,113	1.29	9 (11%)
26	CLA	Q	312	20	43,51,73	1.83	6 (13%)	49,86,113	1.41	7 (14%)
30	SQD	a	408	-	39,40,54	1.36	4 (10%)	48,51,65	1.12	6 (12%)
26	CLA	5	606	21	43,51,73	1.79	6 (13%)	49,86,113	1.53	7 (14%)
26	CLA	B	613	2	65,73,73	1.53	6 (9%)	76,113,113	1.26	7 (9%)
33	LMG	C	519	-	47,47,55	0.97	2 (4%)	55,55,63	1.18	4 (7%)
26	CLA	2	304	-	65,73,73	1.52	5 (7%)	76,113,113	1.29	7 (9%)
26	CLA	3	305	19	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
26	CLA	B	609	2	65,73,73	1.53	5 (7%)	76,113,113	1.27	8 (10%)
29	PL9	A	407	-	33,33,55	1.21	3 (9%)	41,42,69	1.57	9 (21%)
39	II0	N	617	-	39,43,43	2.58	10 (25%)	50,60,60	3.33	19 (38%)
26	CLA	O	611	18	60,68,73	1.56	6 (10%)	70,107,113	1.34	8 (11%)
28	WVN	c	516	-	40,41,41	1.89	14 (35%)	50,56,56	2.15	15 (30%)
26	CLA	N	614	17	47,55,73	1.80	5 (10%)	54,91,113	1.48	8 (14%)
26	CLA	N	613	-	48,56,73	1.75	6 (12%)	55,92,113	1.51	8 (14%)
39	II0	Q	316	-	39,43,43	2.60	12 (30%)	50,60,60	3.32	20 (40%)
26	CLA	B	610	41	65,73,73	1.54	5 (7%)	76,113,113	1.25	8 (10%)
26	CLA	3	301	19	62,70,73	1.53	5 (8%)	72,109,113	1.39	7 (9%)
26	CLA	C	512	3	65,73,73	1.55	5 (7%)	76,113,113	1.34	8 (10%)
26	CLA	c	511	3	65,73,73	1.50	6 (9%)	76,113,113	1.39	6 (7%)
38	KC2	R	311	-	48,53,53	3.18	21 (43%)	54,89,89	4.48	31 (57%)
26	CLA	5	611	21	55,63,73	1.63	6 (10%)	64,101,113	1.52	8 (12%)
39	II0	2	313	-	39,43,43	2.52	12 (30%)	50,60,60	3.33	16 (32%)
34	LHG	c	520	-	39,39,48	1.04	2 (5%)	42,45,54	1.12	2 (4%)
39	II0	N	620	-	39,43,43	2.58	12 (30%)	50,60,60	3.29	18 (36%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	IHT	4	318	-	40,42,42	2.13	11 (27%)	53,58,58	2.80	23 (43%)
39	II0	6	613	-	39,43,43	2.67	10 (25%)	50,60,60	3.42	22 (44%)
26	CLA	N	603	-	51,59,73	1.71	6 (11%)	59,96,113	1.41	6 (10%)

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
40	IHT	N	619	-	-	7/25/65/65	0/2/2/2
30	SQD	A	408	-	-	3/35/55/69	0/1/1/1
26	CLA	3	302	19	1/1/15/20	15/37/115/115	-
26	CLA	C	509	3	1/1/15/20	12/37/115/115	-
26	CLA	g	402	24	1/1/11/20	6/13/91/115	-
26	CLA	N	601	-	1/1/11/20	7/13/91/115	-
26	CLA	O	612	18	1/1/11/20	8/13/91/115	-
35	DGD	h	101	-	-	14/51/91/95	0/2/2/2
28	WVN	H	101	-	-	15/29/63/63	0/2/2/2
38	KC2	2	310	18	-	7/15/71/71	-
26	CLA	P	602	19	1/1/14/20	15/34/112/115	-
34	LHG	C	518	-	-	16/44/44/53	-
26	CLA	4	312	20	1/1/10/20	8/11/89/115	-
26	CLA	b	616	-	1/1/15/20	15/37/115/115	-
26	CLA	S	603	22	1/1/13/20	9/25/103/115	-
26	CLA	C	502	3	1/1/15/20	7/37/115/115	-
39	II0	5	613	-	-	0/21/67/67	0/2/2/2
26	CLA	P	608	34	1/1/12/20	6/22/100/115	-
28	WVN	D	412	-	-	9/29/63/63	0/2/2/2
26	CLA	O	609	-	1/1/14/20	15/31/109/115	-
33	LMG	5	619	-	-	8/35/55/70	0/1/1/1
26	CLA	1	614	17	-	9/16/94/115	-
28	WVN	Y	101	-	-	9/29/63/63	0/2/2/2
33	LMG	A	412	-	-	9/43/63/70	0/1/1/1
39	II0	Q	319	-	-	0/21/67/67	0/2/2/2
28	WVN	x	101	-	-	11/29/63/63	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	WVN	P	615	-	-	8/29/63/63	0/2/2/2
40	IHT	R	317	-	-	11/25/65/65	0/2/2/2
26	CLA	3	308	-	-	8/25/103/115	-
38	KC2	P	605	19	-	9/15/71/71	-
26	CLA	2	312	18	1/1/11/20	8/13/91/115	-
26	CLA	2	319	19	1/1/11/20	2/13/91/115	-
39	II0	Q	314	-	-	0/21/67/67	0/2/2/2
26	CLA	O	601	18	1/1/11/20	7/18/96/115	-
34	LHG	2	321	26	-	19/53/53/53	-
26	CLA	R	310	-	1/1/15/20	17/37/115/115	-
39	II0	N	616	-	-	1/21/67/67	0/2/2/2
26	CLA	2	306	18	1/1/14/20	14/31/109/115	-
26	CLA	Q	305	20	1/1/13/20	9/25/103/115	-
26	CLA	Q	307	20	1/1/13/20	9/27/105/115	-
33	LMG	c	522	-	-	5/26/46/70	0/1/1/1
26	CLA	S	602	22	1/1/15/20	17/37/115/115	-
40	IHT	O	616	-	-	6/25/65/65	0/2/2/2
26	CLA	B	603	2	1/1/15/20	9/37/115/115	-
26	CLA	O	606	18	1/1/14/20	14/31/109/115	-
26	CLA	R	312	21	1/1/13/20	14/25/103/115	-
26	CLA	c	507	-	1/1/15/20	8/37/115/115	-
26	CLA	C	505	41	1/1/14/20	12/31/109/115	-
39	II0	S	611	-	-	5/21/67/67	0/2/2/2
39	II0	R	318	-	-	4/21/67/67	0/2/2/2
39	II0	P	614	-	-	6/21/67/67	0/2/2/2
26	CLA	C	504	3	1/1/15/20	9/37/115/115	-
38	KC2	1	610	-	-	11/15/71/71	-
28	WVN	S	613	-	-	9/29/63/63	0/2/2/2
33	LMG	2	318	-	-	2/35/55/70	0/1/1/1
28	WVN	b	619	-	-	9/29/63/63	0/2/2/2
26	CLA	C	506	-	1/1/15/20	11/37/115/115	-
38	KC2	S	608	22	-	5/15/71/71	-
26	CLA	c	505	3	1/1/15/20	9/37/115/115	-
35	DGD	c	519	-	-	8/43/83/95	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC2	5	610	-	-	8/15/71/71	-
26	CLA	2	302	18	1/1/15/20	16/37/115/115	-
26	CLA	G	401	-	1/1/15/20	19/37/115/115	-
34	LHG	C	501	-	-	29/46/46/53	-
26	CLA	Q	306	20	1/1/10/20	3/11/89/115	-
26	CLA	4	306	20	1/1/13/20	9/25/103/115	-
26	CLA	D	407	-	1/1/15/20	5/37/115/115	-
33	LMG	D	411	-	-	2/32/52/70	0/1/1/1
26	CLA	2	305	-	-	5/21/99/115	-
26	CLA	Q	301	20	1/1/15/20	8/37/115/115	-
39	II0	1	615	-	-	14/21/67/67	0/2/2/2
38	KC2	N	611	17	-	4/15/71/71	-
26	CLA	4	302	20	1/1/15/20	8/37/115/115	-
26	CLA	b	601	41	1/1/12/20	9/19/97/115	-
26	CLA	g	401	-	1/1/15/20	9/37/115/115	-
40	IHT	2	317	-	-	16/25/65/65	0/2/2/2
33	LMG	b	620	-	-	6/46/66/70	0/1/1/1
26	CLA	Q	308	20	1/1/12/20	4/21/99/115	-
28	WVN	C	515	-	-	10/29/63/63	0/2/2/2
38	KC2	4	310	-	-	8/15/71/71	-
27	PHO	D	405	-	-	11/37/103/103	0/5/6/6
39	II0	2	315	-	-	3/21/67/67	0/2/2/2
26	CLA	O	605	-	1/1/12/20	6/21/99/115	-
39	II0	5	615	-	-	3/21/67/67	0/2/2/2
26	CLA	O	604	-	1/1/15/20	12/37/115/115	-
30	SQD	c	501	-	-	6/40/60/69	0/1/1/1
40	IHT	5	616	-	-	11/25/65/65	0/2/2/2
29	PL9	d	407	-	-	8/53/73/73	0/1/1/1
37	HEM	f	101	6,5	-	6/12/54/54	-
39	II0	6	611	-	-	6/21/67/67	0/2/2/2
26	CLA	b	608	2	1/1/15/20	6/37/115/115	-
26	CLA	6	605	22	1/1/13/20	14/25/103/115	-
26	CLA	A	405	1	1/1/14/20	10/31/109/115	-
26	CLA	a	402	1	1/1/15/20	8/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC2	N	612	17	-	10/15/71/71	-
26	CLA	4	303	20	1/1/15/20	14/37/115/115	-
26	CLA	6	610	22	1/1/15/20	10/37/115/115	-
26	CLA	D	404	41	1/1/15/20	10/37/115/115	-
26	CLA	5	602	21	1/1/13/20	12/25/103/115	-
38	KC2	6	608	22	-	5/15/71/71	-
26	CLA	P	609	19	1/1/12/20	5/23/101/115	-
28	WVN	c	518	-	-	11/29/63/63	0/2/2/2
26	CLA	5	608	21	1/1/13/20	10/30/108/115	-
39	II0	P	613	-	-	12/21/67/67	0/2/2/2
26	CLA	O	602	18	1/1/15/20	16/37/115/115	-
33	LMG	D	413	-	-	3/41/61/70	0/1/1/1
26	CLA	S	609	22	1/1/12/20	5/23/101/115	-
39	II0	6	612	-	-	1/21/67/67	0/2/2/2
26	CLA	b	611	2	1/1/15/20	10/37/115/115	-
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
26	CLA	N	606	17	1/1/12/20	6/19/97/115	-
26	CLA	b	609	2	1/1/15/20	8/37/115/115	-
38	KC2	Q	309	-	-	8/15/71/71	-
26	CLA	S	601	22	1/1/13/20	8/25/103/115	-
27	PHO	a	404	-	-	14/37/103/103	0/5/6/6
26	CLA	c	506	41	1/1/14/20	12/31/109/115	-
27	PHO	d	403	-	-	12/37/103/103	0/5/6/6
34	LHG	G	403	26	-	19/53/53/53	-
26	CLA	S	605	22	1/1/13/20	14/25/103/115	-
26	CLA	b	606	-	1/1/15/20	10/37/115/115	-
39	II0	5	614	-	-	1/21/67/67	0/2/2/2
33	LMG	Q	318	-	-	4/38/58/70	0/1/1/1
26	CLA	R	307	21	1/1/10/20	4/11/89/115	-
26	CLA	d	406	4	1/1/14/20	16/33/111/115	-
26	CLA	C	507	3	1/1/15/20	8/37/115/115	-
27	PHO	A	404	-	-	14/37/103/103	0/5/6/6
26	CLA	3	306	19	1/1/15/20	14/37/115/115	-
26	CLA	c	509	41	1/1/15/20	8/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	616	2	1/1/15/20	15/37/115/115	-
39	II0	1	617	-	-	10/21/67/67	0/2/2/2
38	KC2	4	305	-	-	7/15/71/71	-
26	CLA	P	611	19	1/1/11/20	8/13/91/115	-
26	CLA	C	510	3	1/1/15/20	13/37/115/115	-
26	CLA	Q	311	20	1/1/10/20	8/11/89/115	-
26	CLA	d	405	-	1/1/15/20	5/37/115/115	-
33	LMG	C	520	-	-	5/26/46/70	0/1/1/1
33	LMG	R	301	-	-	8/35/55/70	0/1/1/1
39	II0	4	314	-	-	2/21/67/67	0/2/2/2
34	LHG	5	618	26	-	11/44/44/53	-
26	CLA	B	611	2	1/1/15/20	10/37/115/115	-
26	CLA	1	601	-	1/1/11/20	6/13/91/115	-
26	CLA	c	514	3	1/1/15/20	12/37/115/115	-
26	CLA	S	604	22	1/1/15/20	18/37/115/115	-
26	CLA	N	602	17	1/1/14/20	7/31/109/115	-
34	LHG	1	620	-	-	9/50/50/53	-
33	LMG	d	411	-	-	3/41/61/70	0/1/1/1
26	CLA	B	605	2	1/1/15/20	9/37/115/115	-
26	CLA	R	302	21	1/1/13/20	6/25/103/115	-
38	KC2	N	605	17	-	12/15/71/71	-
39	II0	3	311	-	-	12/21/67/67	0/2/2/2
26	CLA	C	503	3	1/1/15/20	16/37/115/115	-
26	CLA	P	607	19	1/1/15/20	14/37/115/115	-
28	WVN	b	617	-	-	13/29/63/63	0/2/2/2
39	II0	2	314	-	-	1/21/67/67	0/2/2/2
26	CLA	R	304	21	1/1/12/20	9/22/100/115	-
26	CLA	c	504	3	1/1/15/20	16/37/115/115	-
26	CLA	6	606	22	1/1/13/20	11/28/106/115	-
26	CLA	6	601	22	1/1/13/20	8/25/103/115	-
39	II0	N	618	-	-	4/21/67/67	0/2/2/2
26	CLA	R	306	21	1/1/15/20	14/37/115/115	-
26	CLA	c	515	3	1/1/12/20	9/23/101/115	-
34	LHG	D	410	-	-	13/53/53/53	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	607	41	1/1/15/20	13/37/115/115	-
29	PL9	a	407	-	-	10/27/47/73	0/1/1/1
34	LHG	D	403	-	-	12/47/47/53	-
26	CLA	2	303	18	1/1/15/20	8/37/115/115	-
26	CLA	P	606	19	1/1/15/20	9/37/115/115	-
26	CLA	B	604	2	1/1/13/20	11/30/108/115	-
26	CLA	B	601	41	1/1/12/20	9/19/97/115	-
33	LMG	m	101	-	-	6/35/55/70	0/1/1/1
26	CLA	A	403	41	1/1/11/20	10/18/96/115	-
26	CLA	P	604	19	-	8/35/113/115	-
33	LMG	4	319	-	-	4/38/58/70	0/1/1/1
26	CLA	5	609	-	1/1/15/20	17/37/115/115	-
26	CLA	A	402	1	1/1/15/20	8/37/115/115	-
39	II0	4	315	-	-	0/21/67/67	0/2/2/2
28	WVN	A	406	-	-	2/29/63/63	0/2/2/2
33	LMG	M	101	-	-	7/35/55/70	0/1/1/1
26	CLA	2	301	18	1/1/11/20	7/18/96/115	-
26	CLA	b	602	2	-	6/37/115/115	-
28	WVN	C	516	-	-	16/29/63/63	0/2/2/2
26	CLA	b	615	2	1/1/15/20	9/37/115/115	-
26	CLA	1	609	17	1/1/14/20	15/31/109/115	-
26	CLA	C	514	3	1/1/12/20	9/22/100/115	-
26	CLA	3	303	19	-	8/35/113/115	-
39	II0	1	616	-	-	13/21/67/67	0/2/2/2
26	CLA	S	606	22	1/1/13/20	11/28/106/115	-
39	II0	O	615	-	-	11/21/67/67	0/2/2/2
38	KC2	O	610	18	-	7/15/71/71	-
39	II0	R	315	-	-	1/21/67/67	0/2/2/2
26	CLA	O	607	18	1/1/11/20	2/17/95/115	-
26	CLA	a	403	41	1/1/11/20	10/18/96/115	-
26	CLA	6	602	22	1/1/15/20	17/37/115/115	-
39	II0	O	614	-	-	1/21/67/67	0/2/2/2
26	CLA	c	503	3	1/1/15/20	8/37/115/115	-
37	HEM	F	101	6,5	-	6/12/54/54	-
26	CLA	b	605	2	1/1/15/20	9/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	II0	3	312	-	-	10/21/67/67	0/2/2/2
26	CLA	N	607	-	1/1/10/20	5/11/89/115	-
26	CLA	d	402	41	1/1/15/20	10/37/115/115	-
26	CLA	Q	303	20	1/1/14/20	16/33/111/115	-
26	CLA	N	608	-	1/1/11/20	5/15/93/115	-
38	KC2	1	611	17	-	8/15/71/71	-
39	II0	2	320	-	-	3/21/67/67	0/2/2/2
38	KC2	3	304	19	-	9/15/71/71	-
26	CLA	2	307	18	1/1/11/20	2/17/95/115	-
26	CLA	1	602	17	1/1/14/20	6/31/109/115	-
26	CLA	c	508	3	1/1/15/20	7/37/115/115	-
30	SQD	D	401	-	-	7/49/69/69	0/1/1/1
26	CLA	b	612	2	1/1/15/20	12/37/115/115	-
26	CLA	1	608	17	1/1/11/20	7/15/93/115	-
35	DGD	C	517	-	-	8/43/83/95	0/2/2/2
26	CLA	N	604	17	1/1/13/20	8/30/108/115	-
33	LMG	c	521	-	-	19/46/66/70	0/1/1/1
26	CLA	B	606	-	1/1/15/20	12/37/115/115	-
28	WVN	d	410	-	-	12/29/63/63	0/2/2/2
26	CLA	4	307	20	1/1/10/20	3/11/89/115	-
26	CLA	G	402	23	1/1/11/20	4/13/91/115	-
26	CLA	b	604	2	1/1/13/20	12/30/108/115	-
28	WVN	5	617	-	-	9/29/63/63	0/2/2/2
34	LHG	N	621	-	-	12/50/50/53	-
28	WVN	B	618	-	-	17/29/63/63	0/2/2/2
34	LHG	R	319	26	-	12/44/44/53	-
38	KC2	4	311	20	-	3/15/71/71	-
26	CLA	B	602	2	-	6/37/115/115	-
26	CLA	N	609	17	1/1/14/20	7/31/109/115	-
26	CLA	5	607	21	1/1/15/20	10/37/115/115	-
26	CLA	P	601	19	1/1/11/20	2/13/91/115	-
26	CLA	R	309	21	1/1/13/20	10/30/108/115	-
39	II0	S	612	-	-	1/21/67/67	0/2/2/2
26	CLA	R	313	21	1/1/11/20	5/15/93/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	WVN	3	313	-	-	16/29/63/63	0/2/2/2
26	CLA	a	405	1	1/1/14/20	11/31/109/115	-
26	CLA	b	603	2	1/1/15/20	9/37/115/115	-
39	II0	4	320	-	-	0/21/67/67	0/2/2/2
26	CLA	5	605	21	1/1/15/20	14/37/115/115	-
34	LHG	L	101	-	-	7/53/53/53	-
26	CLA	B	608	2	1/1/15/20	4/37/115/115	-
33	LMG	d	404	-	-	9/35/55/70	0/1/1/1
28	WVN	b	618	-	-	10/29/63/63	0/2/2/2
40	IHT	1	619	-	-	15/25/65/65	0/2/2/2
39	II0	R	314	-	-	0/21/67/67	0/2/2/2
39	II0	R	316	-	-	3/21/67/67	0/2/2/2
26	CLA	1	606	17	1/1/12/20	8/19/97/115	-
26	CLA	1	603	17	1/1/12/20	7/22/100/115	-
33	LMG	B	620	-	-	7/46/66/70	0/1/1/1
26	CLA	b	613	2	1/1/15/20	16/37/115/115	-
26	CLA	S	607	34	1/1/13/20	11/25/103/115	-
26	CLA	6	609	22	1/1/12/20	5/23/101/115	-
38	KC2	1	612	17	-	9/15/71/71	-
26	CLA	4	313	20	1/1/10/20	2/11/89/115	-
34	LHG	d	408	-	-	13/53/53/53	-
26	CLA	D	408	4	1/1/14/20	13/31/109/115	-
28	WVN	B	617	-	-	15/29/63/63	0/2/2/2
26	CLA	c	510	3	1/1/15/20	12/37/115/115	-
26	CLA	b	607	41	1/1/15/20	12/37/115/115	-
34	LHG	b	621	-	-	20/47/47/53	-
39	II0	P	612	-	-	2/21/67/67	0/2/2/2
26	CLA	6	603	22	1/1/13/20	9/25/103/115	-
26	CLA	4	309	20	1/1/12/20	4/21/99/115	-
39	II0	O	613	-	-	2/21/67/67	0/2/2/2
26	CLA	P	610	19	1/1/13/20	11/25/103/115	-
38	KC2	N	610	-	-	4/15/71/71	-
26	CLA	6	607	34	1/1/13/20	11/25/103/115	-
33	LMG	a	413	-	-	8/43/63/70	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	614	2	1/1/14/20	12/31/109/115	-
26	CLA	O	603	18	1/1/15/20	8/37/115/115	-
26	CLA	C	511	3	1/1/15/20	11/37/115/115	-
26	CLA	2	311	18	1/1/14/20	10/31/109/115	-
26	CLA	R	303	21	1/1/13/20	12/25/103/115	-
26	CLA	B	615	2	1/1/15/20	10/37/115/115	-
26	CLA	C	513	3	1/1/15/20	11/37/115/115	-
39	II0	Q	313	-	-	2/21/67/67	0/2/2/2
26	CLA	2	309	-	1/1/14/20	15/31/109/115	-
26	CLA	5	612	21	1/1/11/20	5/15/93/115	-
40	IHT	Q	317	-	-	10/25/65/65	0/2/2/2
33	LMG	D	406	-	-	9/35/55/70	0/1/1/1
26	CLA	5	604	21	1/1/14/20	11/31/109/115	-
26	CLA	6	604	22	1/1/15/20	18/37/115/115	-
39	II0	4	316	-	-	2/21/67/67	0/2/2/2
39	II0	Q	315	-	-	1/21/67/67	0/2/2/2
34	LHG	l	101	-	-	6/53/53/53	-
26	CLA	O	608	18	1/1/15/20	10/37/115/115	-
38	KC2	Q	304	-	-	7/15/71/71	-
26	CLA	1	604	17	1/1/13/20	15/30/108/115	-
26	CLA	4	308	20	1/1/13/20	9/27/105/115	-
26	CLA	Q	302	20	1/1/15/20	14/37/115/115	-
26	CLA	c	512	3	1/1/15/20	11/37/115/115	-
28	WVN	k	101	-	-	8/29/63/63	0/2/2/2
38	KC2	1	605	-	-	12/15/71/71	-
39	II0	1	618	-	-	14/21/67/67	0/2/2/2
33	LMG	d	409	-	-	2/32/52/70	0/1/1/1
28	WVN	c	517	-	-	10/29/63/63	0/2/2/2
26	CLA	1	613	-	1/1/11/20	8/17/95/115	-
39	II0	O	618	-	-	1/21/67/67	0/2/2/2
34	LHG	z	101	-	-	8/29/29/53	-
26	CLA	c	513	3	1/1/15/20	11/37/115/115	-
26	CLA	R	305	21	1/1/14/20	11/31/109/115	-
39	II0	N	615	-	-	4/21/67/67	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC2	Q	310	20	-	3/15/71/71	-
26	CLA	4	301	34	1/1/12/20	6/22/100/115	-
39	II0	2	316	-	-	11/21/67/67	0/2/2/2
26	CLA	C	508	41	1/1/15/20	8/37/115/115	-
26	CLA	5	601	21	1/1/13/20	6/25/103/115	-
26	CLA	1	607	17	1/1/10/20	5/11/89/115	-
26	CLA	5	603	21	1/1/12/20	9/22/100/115	-
34	LHG	Z	102	-	-	8/29/29/53	-
39	II0	3	310	-	-	10/21/67/67	0/2/2/2
26	CLA	2	308	18	1/1/15/20	10/37/115/115	-
26	CLA	3	307	19	1/1/12/20	5/23/101/115	-
26	CLA	4	304	20	1/1/14/20	17/33/111/115	-
26	CLA	b	610	41	1/1/15/20	9/37/115/115	-
26	CLA	3	309	19	1/1/11/20	8/13/91/115	-
26	CLA	R	308	21	1/1/15/20	10/37/115/115	-
26	CLA	S	610	22	1/1/15/20	10/37/115/115	-
26	CLA	B	612	2	1/1/15/20	12/37/115/115	-
39	II0	4	317	-	-	5/21/67/67	0/2/2/2
28	WVN	a	406	-	-	9/29/63/63	0/2/2/2
28	WVN	B	619	-	-	10/29/63/63	0/2/2/2
34	LHG	a	409	-	-	28/46/46/53	-
28	WVN	Z	101	-	-	10/29/63/63	0/2/2/2
29	PL9	D	409	-	-	7/53/73/73	0/1/1/1
33	LMG	O	617	-	-	2/35/55/70	0/1/1/1
26	CLA	B	614	2	1/1/14/20	11/31/109/115	-
26	CLA	P	603	19	1/1/15/20	15/37/115/115	-
26	CLA	Q	312	20	1/1/10/20	2/11/89/115	-
30	SQD	a	408	-	-	4/35/55/69	0/1/1/1
26	CLA	5	606	21	1/1/10/20	4/11/89/115	-
26	CLA	B	613	2	1/1/15/20	15/37/115/115	-
33	LMG	C	519	-	-	20/42/62/70	0/1/1/1
26	CLA	2	304	-	1/1/15/20	12/37/115/115	-
26	CLA	3	305	19	1/1/15/20	9/37/115/115	-
26	CLA	B	609	2	1/1/15/20	9/37/115/115	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PL9	A	407	-	-	10/27/47/73	0/1/1/1
39	II0	N	617	-	-	3/21/67/67	0/2/2/2
26	CLA	O	611	18	1/1/14/20	10/31/109/115	-
28	WVN	c	516	-	-	10/29/63/63	0/2/2/2
26	CLA	N	614	17	1/1/11/20	10/16/94/115	-
26	CLA	N	613	-	1/1/11/20	6/17/95/115	-
39	II0	Q	316	-	-	5/21/67/67	0/2/2/2
26	CLA	B	610	41	1/1/15/20	9/37/115/115	-
26	CLA	3	301	19	1/1/14/20	15/34/112/115	-
26	CLA	C	512	3	1/1/15/20	13/37/115/115	-
26	CLA	c	511	3	1/1/15/20	13/37/115/115	-
38	KC2	R	311	-	-	8/15/71/71	-
26	CLA	5	611	21	1/1/13/20	14/25/103/115	-
39	II0	2	313	-	-	1/21/67/67	0/2/2/2
34	LHG	c	520	-	-	13/44/44/53	-
39	II0	N	620	-	-	3/21/67/67	0/2/2/2
40	IHT	4	318	-	-	10/25/65/65	0/2/2/2
39	II0	6	613	-	-	4/21/67/67	0/2/2/2
26	CLA	N	603	-	1/1/12/20	7/21/99/115	-

The worst 5 of 2712 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	1	616	II0	C14-C10	18.08	1.55	1.34
39	2	316	II0	C14-C10	17.59	1.54	1.34
39	O	615	II0	C14-C10	17.57	1.54	1.34
40	1	619	IHT	C15-C11	17.56	1.54	1.34
39	1	618	II0	C14-C10	17.39	1.54	1.34

The worst 5 of 3792 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	617	WVN	C20-C23-C25	-27.60	84.52	126.23
28	B	618	WVN	C20-C23-C25	-26.81	85.73	126.23
28	C	516	WVN	C20-C23-C25	-26.79	85.76	126.23
39	3	312	II0	C24-C22-C10	-25.49	110.88	175.43
39	3	310	II0	C23-C21-C09	-25.28	111.43	175.43

5 of 187 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	402	CLA	ND
26	A	403	CLA	ND
26	A	405	CLA	ND
26	B	601	CLA	ND
26	B	603	CLA	ND

5 of 3158 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	403	CLA	C1A-C2A-CAA-CBA
26	A	403	CLA	C3A-C2A-CAA-CBA
26	A	405	CLA	C1A-C2A-CAA-CBA
26	A	405	CLA	C3A-C2A-CAA-CBA
26	A	405	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

301 monomers are involved in 1707 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	N	619	IHT	16	0
30	A	408	SQD	1	0
26	3	302	CLA	9	0
26	C	509	CLA	3	0
26	g	402	CLA	18	0
26	N	601	CLA	24	0
26	O	612	CLA	3	0
35	h	101	DGD	6	0
28	H	101	WVN	1	0
38	2	310	KC2	7	0
26	P	602	CLA	8	0
34	C	518	LHG	3	0
26	4	312	CLA	10	0
26	b	616	CLA	2	0
26	S	603	CLA	2	0
26	C	502	CLA	1	0
39	5	613	II0	2	0
26	P	608	CLA	5	0
26	O	609	CLA	1	0
33	5	619	LMG	20	0
26	1	614	CLA	4	0
33	A	412	LMG	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	Q	319	II0	10	0
28	P	615	WVN	3	0
40	R	317	IHT	4	0
26	3	308	CLA	8	0
38	P	605	KC2	1	0
26	2	312	CLA	6	0
26	2	319	CLA	26	0
39	Q	314	II0	4	0
26	O	601	CLA	25	0
34	2	321	LHG	23	0
26	R	310	CLA	2	0
39	N	616	II0	16	0
26	2	306	CLA	4	0
26	Q	305	CLA	6	0
26	Q	307	CLA	9	0
33	c	522	LMG	2	0
26	S	602	CLA	2	0
40	O	616	IHT	9	0
26	B	603	CLA	3	0
26	O	606	CLA	4	0
26	R	312	CLA	6	0
26	c	507	CLA	2	0
39	S	611	II0	11	0
39	P	614	II0	4	0
26	C	504	CLA	4	0
38	1	610	KC2	1	0
33	2	318	LMG	5	0
26	C	506	CLA	4	0
26	c	505	CLA	4	0
35	c	519	DGD	2	0
38	5	610	KC2	3	0
26	2	302	CLA	10	0
26	G	401	CLA	7	0
26	Q	306	CLA	8	0
26	4	306	CLA	45	0
26	D	407	CLA	7	0
33	D	411	LMG	2	0
26	2	305	CLA	14	0
26	Q	301	CLA	11	0
26	4	302	CLA	11	0
26	b	601	CLA	1	0
26	g	401	CLA	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	2	317	IHT	21	0
33	b	620	LMG	1	0
26	Q	308	CLA	10	0
38	4	310	KC2	12	0
27	D	405	PHO	5	0
39	2	315	II0	13	0
26	O	605	CLA	13	0
39	5	615	II0	4	0
26	O	604	CLA	2	0
30	c	501	SQD	1	0
40	5	616	IHT	1	0
29	d	407	PL9	3	0
37	f	101	HEM	1	0
39	6	611	II0	1	0
26	b	608	CLA	1	0
26	6	605	CLA	5	0
26	A	405	CLA	2	0
26	a	402	CLA	11	0
38	N	612	KC2	28	0
26	4	303	CLA	36	0
26	6	610	CLA	6	0
26	D	404	CLA	3	0
26	5	602	CLA	6	0
26	P	609	CLA	1	0
26	5	608	CLA	10	0
39	P	613	II0	6	0
26	O	602	CLA	8	0
33	D	413	LMG	1	0
26	S	609	CLA	9	0
26	b	611	CLA	5	0
35	H	102	DGD	4	0
26	N	606	CLA	21	0
26	b	609	CLA	4	0
38	Q	309	KC2	12	0
26	S	601	CLA	6	0
27	a	404	PHO	2	0
27	d	403	PHO	5	0
34	G	403	LHG	11	0
26	S	605	CLA	5	0
26	b	606	CLA	5	0
39	5	614	II0	1	0
33	Q	318	LMG	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	d	406	CLA	1	0
26	C	507	CLA	4	0
27	A	404	PHO	2	0
26	3	306	CLA	6	0
26	c	509	CLA	3	0
26	B	616	CLA	1	0
38	4	305	KC2	6	0
26	P	611	CLA	3	0
26	Q	311	CLA	9	0
26	d	405	CLA	8	0
33	C	520	LMG	3	0
33	R	301	LMG	9	0
39	4	314	II0	6	0
34	5	618	LHG	8	0
26	B	611	CLA	4	0
26	c	514	CLA	2	0
26	S	604	CLA	5	0
26	N	602	CLA	7	0
34	1	620	LHG	48	0
33	d	411	LMG	2	0
26	B	605	CLA	8	0
26	R	302	CLA	6	0
38	N	605	KC2	6	0
39	3	311	II0	26	0
26	C	503	CLA	4	0
26	P	607	CLA	3	0
28	b	617	WVN	1	0
39	2	314	II0	5	0
26	R	304	CLA	1	0
26	c	504	CLA	5	0
26	6	606	CLA	4	0
26	6	601	CLA	8	0
39	N	618	II0	2	0
26	R	306	CLA	21	0
26	c	515	CLA	2	0
34	D	410	LHG	5	0
26	B	607	CLA	2	0
34	D	403	LHG	7	0
26	2	303	CLA	19	0
26	P	606	CLA	5	0
26	B	604	CLA	3	0
26	B	601	CLA	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	m	101	LMG	2	0
26	A	403	CLA	2	0
26	P	604	CLA	3	0
33	4	319	LMG	5	0
26	5	609	CLA	2	0
26	A	402	CLA	10	0
39	4	315	II0	9	0
33	M	101	LMG	1	0
26	2	301	CLA	31	0
26	b	602	CLA	3	0
28	C	516	WVN	2	0
26	b	615	CLA	6	0
26	1	609	CLA	5	0
26	C	514	CLA	2	0
26	3	303	CLA	5	0
26	S	606	CLA	4	0
39	O	615	II0	8	0
38	O	610	KC2	7	0
39	R	315	II0	1	0
26	O	607	CLA	19	0
26	a	403	CLA	4	0
26	6	602	CLA	1	0
39	O	614	II0	6	0
26	c	503	CLA	2	0
37	F	101	HEM	2	0
26	b	605	CLA	7	0
39	3	312	II0	8	0
26	N	607	CLA	19	0
26	d	402	CLA	4	0
26	Q	303	CLA	1	0
26	N	608	CLA	3	0
38	1	611	KC2	3	0
39	2	320	II0	4	0
38	3	304	KC2	1	0
26	2	307	CLA	13	0
26	c	508	CLA	4	0
30	D	401	SQD	2	0
26	b	612	CLA	8	0
26	1	608	CLA	5	0
35	C	517	DGD	1	0
26	N	604	CLA	16	0
33	c	521	LMG	6	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	606	CLA	4	0
26	4	307	CLA	8	0
26	G	402	CLA	1	0
26	b	604	CLA	3	0
34	N	621	LHG	26	0
28	B	618	WVN	3	0
34	R	319	LHG	12	0
38	4	311	KC2	20	0
26	B	602	CLA	3	0
26	N	609	CLA	4	0
26	5	607	CLA	7	0
26	P	601	CLA	10	0
26	R	309	CLA	10	0
28	3	313	WVN	21	0
26	a	405	CLA	3	0
26	b	603	CLA	3	0
39	4	320	II0	29	0
26	5	605	CLA	31	0
34	L	101	LHG	7	0
26	B	608	CLA	1	0
33	d	404	LMG	4	0
40	1	619	IHT	1	0
39	R	314	II0	2	0
39	R	316	II0	4	0
26	1	606	CLA	42	0
26	1	603	CLA	8	0
33	B	620	LMG	2	0
26	b	613	CLA	8	0
26	S	607	CLA	2	0
26	6	609	CLA	24	0
38	1	612	KC2	1	0
34	d	408	LHG	5	0
26	D	408	CLA	1	0
28	B	617	WVN	3	0
26	c	510	CLA	3	0
26	b	607	CLA	2	0
34	b	621	LHG	2	0
39	P	612	II0	3	0
26	6	603	CLA	2	0
26	4	309	CLA	8	0
39	O	613	II0	12	0
26	P	610	CLA	15	0

*Continued on next page...*

*Continued from previous page...*

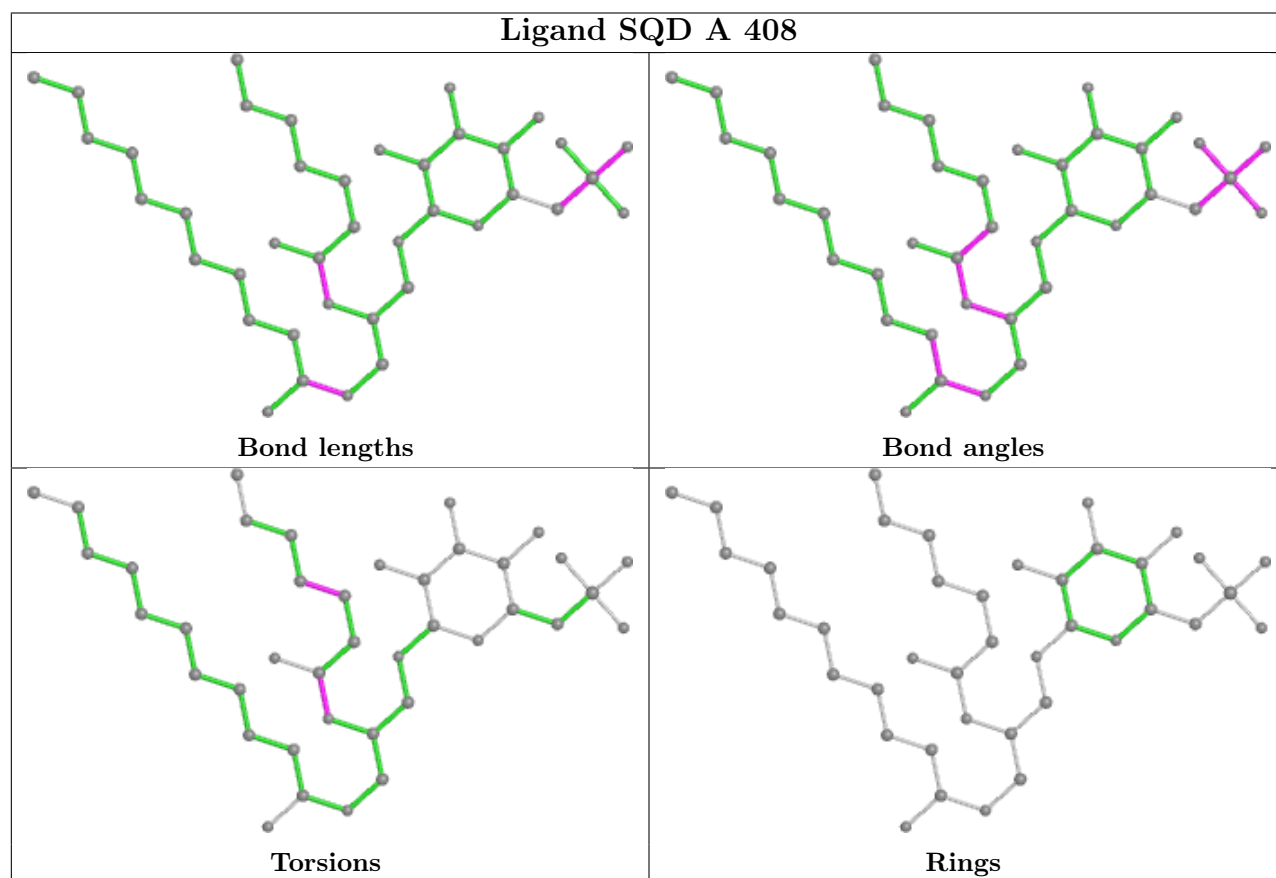
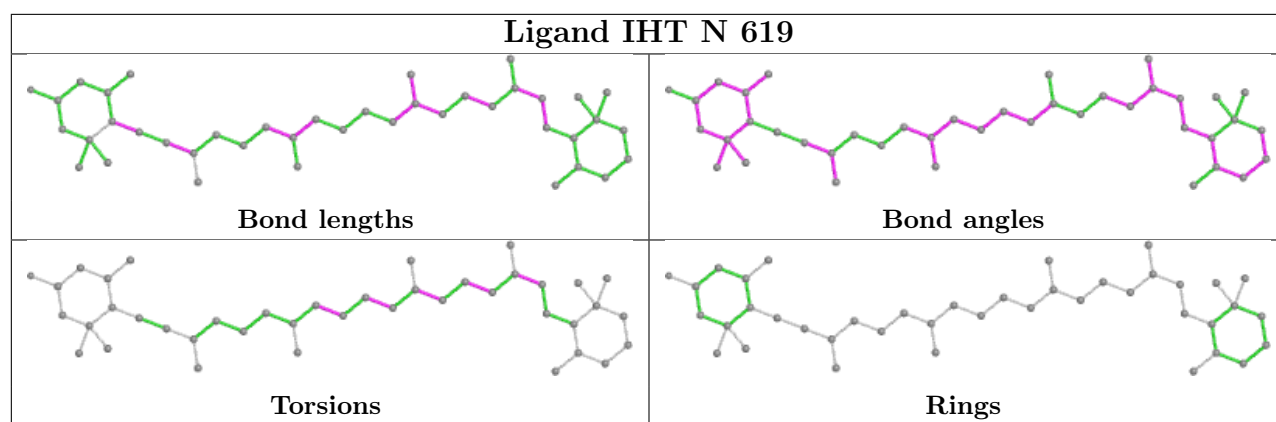
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	N	610	KC2	5	0
33	a	413	LMG	3	0
26	b	614	CLA	3	0
26	O	603	CLA	15	0
26	C	511	CLA	6	0
26	2	311	CLA	47	0
26	R	303	CLA	9	0
26	B	615	CLA	3	0
26	C	513	CLA	2	0
39	Q	313	II0	7	0
26	2	309	CLA	1	0
40	Q	317	IHT	4	0
33	D	406	LMG	4	0
26	5	604	CLA	4	0
26	6	604	CLA	5	0
34	l	101	LHG	5	0
26	O	608	CLA	15	0
38	Q	304	KC2	6	0
26	1	604	CLA	3	0
26	4	308	CLA	12	0
26	Q	302	CLA	7	0
26	c	512	CLA	6	0
39	1	618	II0	1	0
33	d	409	LMG	2	0
39	O	618	II0	2	0
26	c	513	CLA	1	0
26	R	305	CLA	4	0
39	N	615	II0	5	0
38	Q	310	KC2	21	0
26	4	301	CLA	31	0
39	2	316	II0	5	0
26	C	508	CLA	3	0
26	5	601	CLA	6	0
26	1	607	CLA	2	0
26	5	603	CLA	1	0
39	3	310	II0	26	0
26	2	308	CLA	12	0
26	3	307	CLA	43	0
26	4	304	CLA	1	0
26	b	610	CLA	5	0
26	3	309	CLA	2	0
26	R	308	CLA	11	0

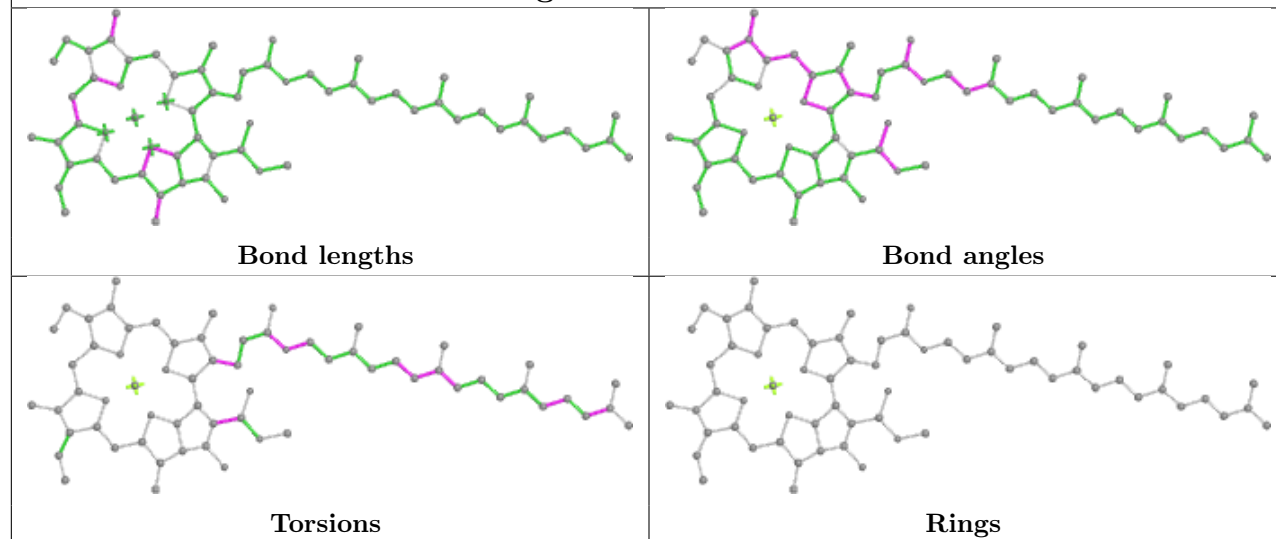
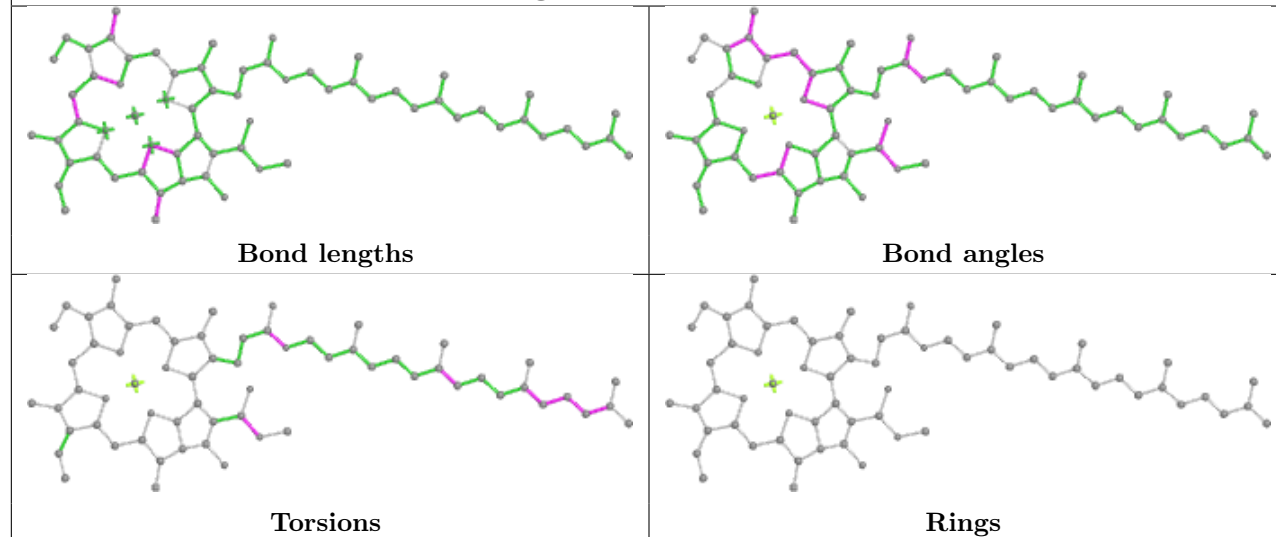
*Continued on next page...*

*Continued from previous page...*

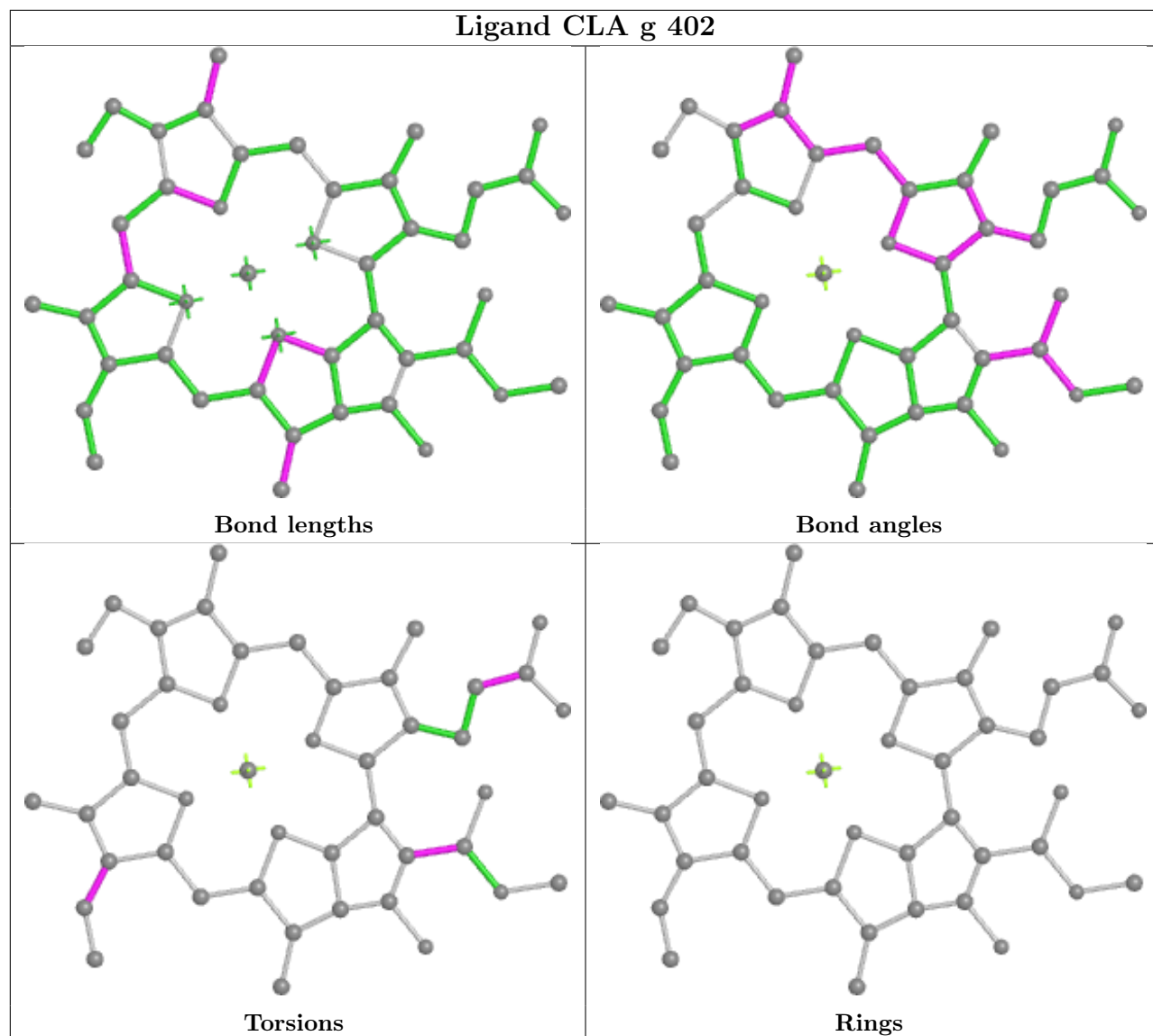
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	S	610	CLA	4	0
26	B	612	CLA	7	0
39	4	317	II0	4	0
29	D	409	PL9	3	0
33	O	617	LMG	5	0
26	B	614	CLA	2	0
26	P	603	CLA	5	0
26	B	613	CLA	6	0
26	2	304	CLA	4	0
26	3	305	CLA	7	0
26	B	609	CLA	5	0
29	A	407	PL9	6	0
39	N	617	II0	5	0
26	O	611	CLA	12	0
26	N	614	CLA	26	0
26	N	613	CLA	3	0
39	Q	316	II0	5	0
26	B	610	CLA	7	0
26	3	301	CLA	12	0
26	C	512	CLA	3	0
38	R	311	KC2	3	0
26	5	611	CLA	35	0
39	2	313	II0	6	0
34	c	520	LHG	1	0
39	N	620	II0	11	0
40	4	318	IHT	5	0
26	N	603	CLA	13	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.

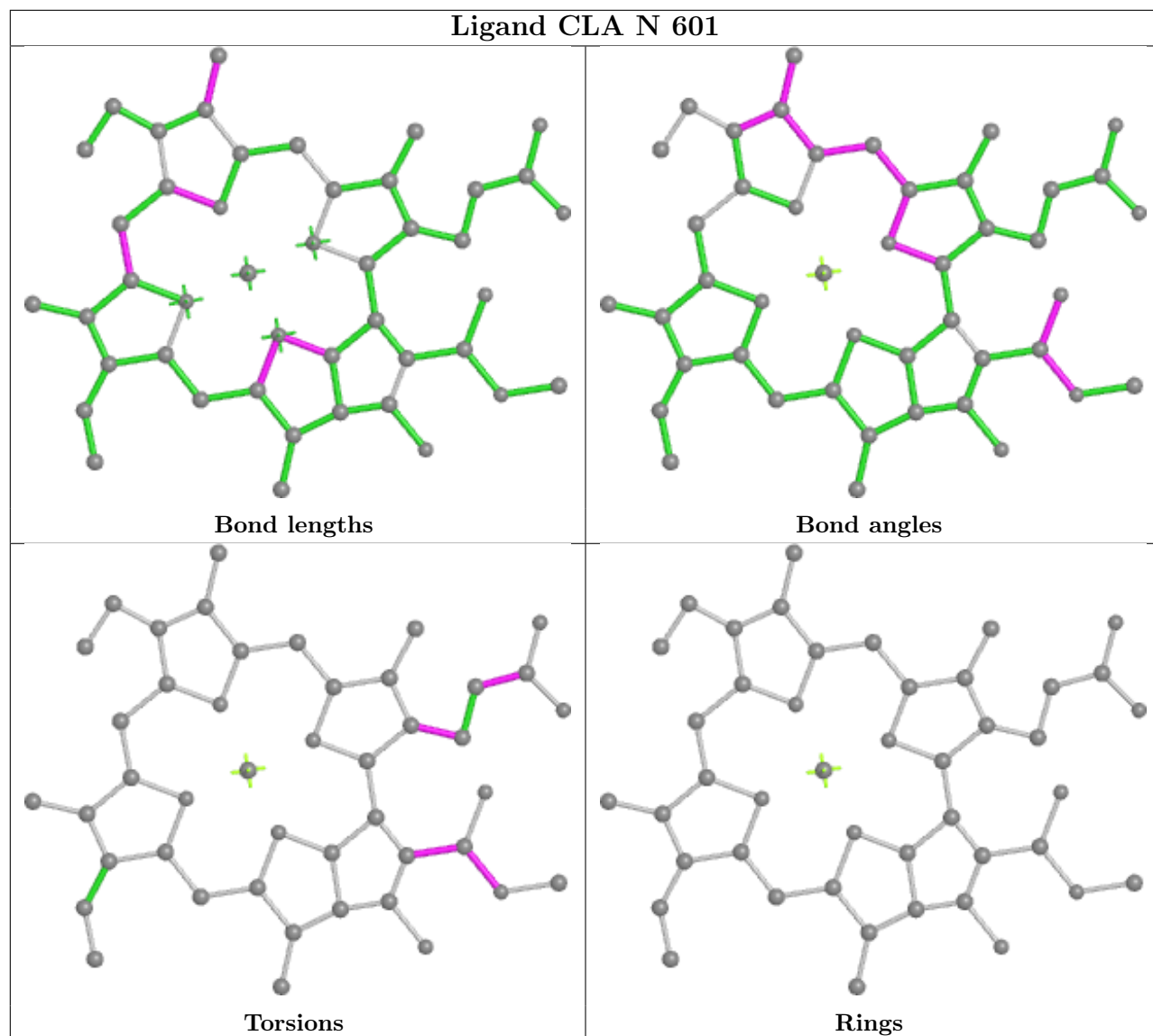


**Ligand CLA 3 302****Ligand CLA C 509**

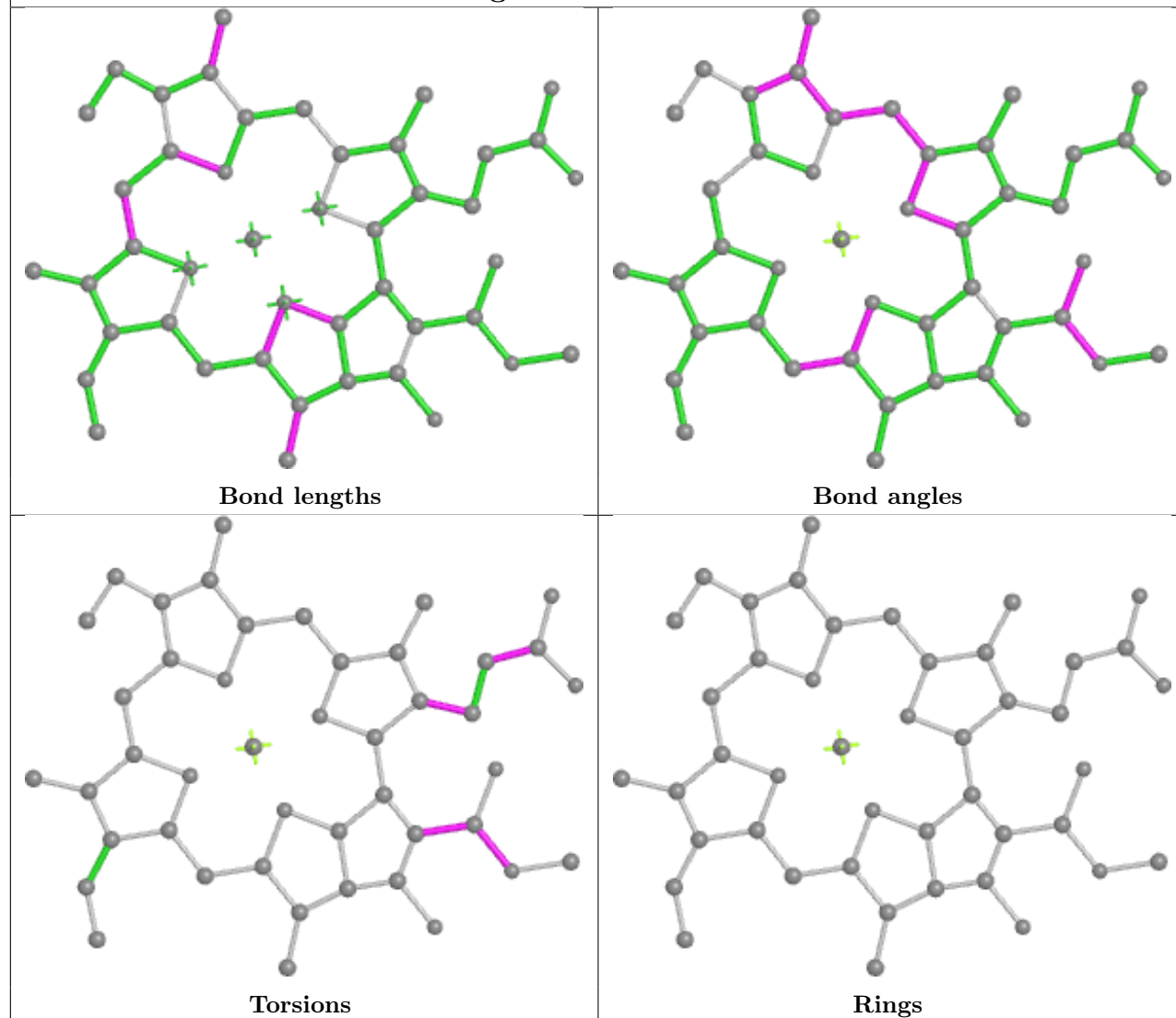
## Ligand CLA g 402



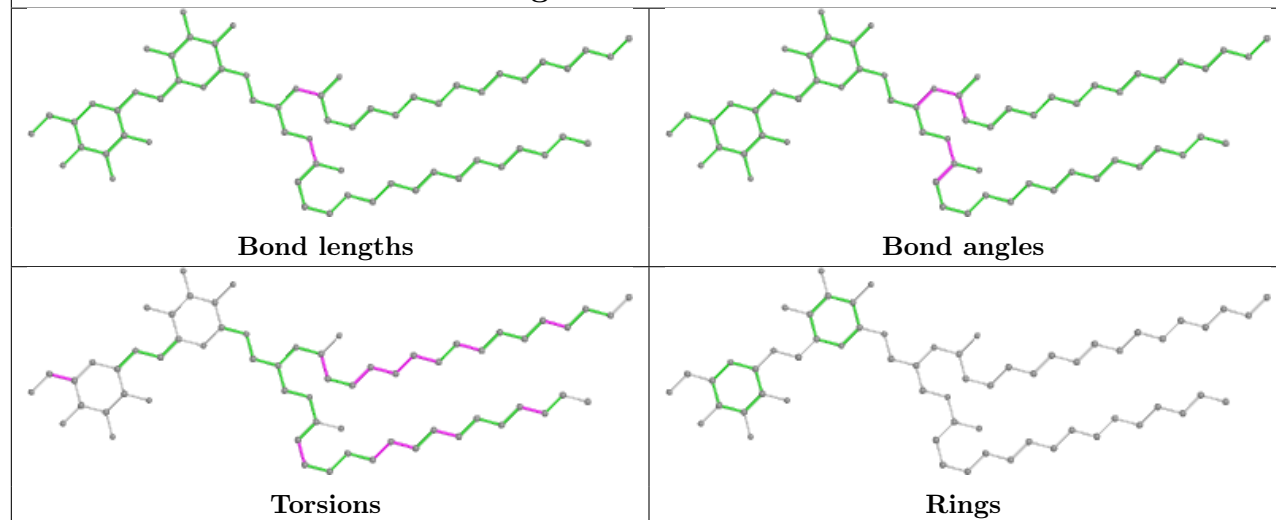
## Ligand CLA N 601



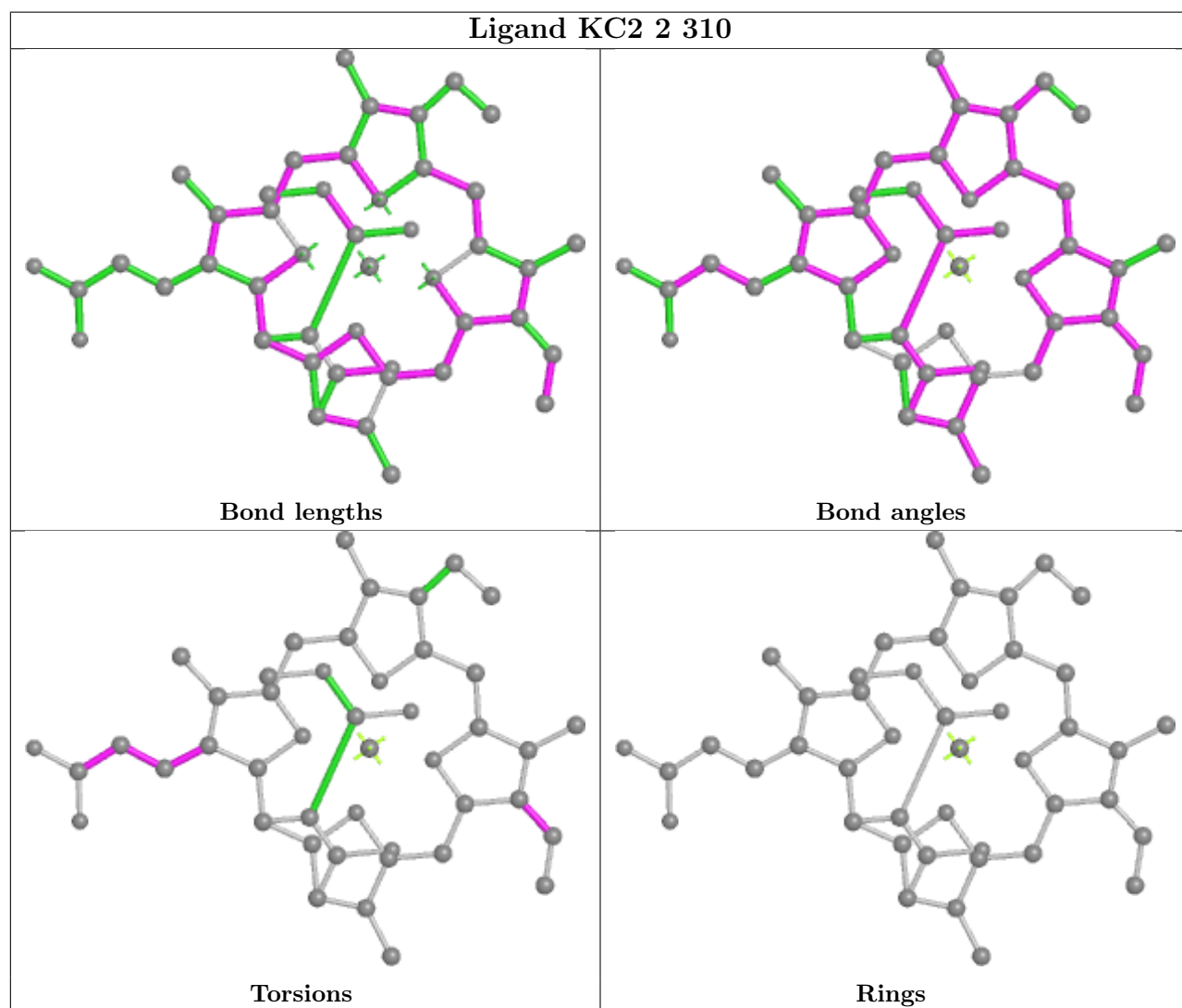
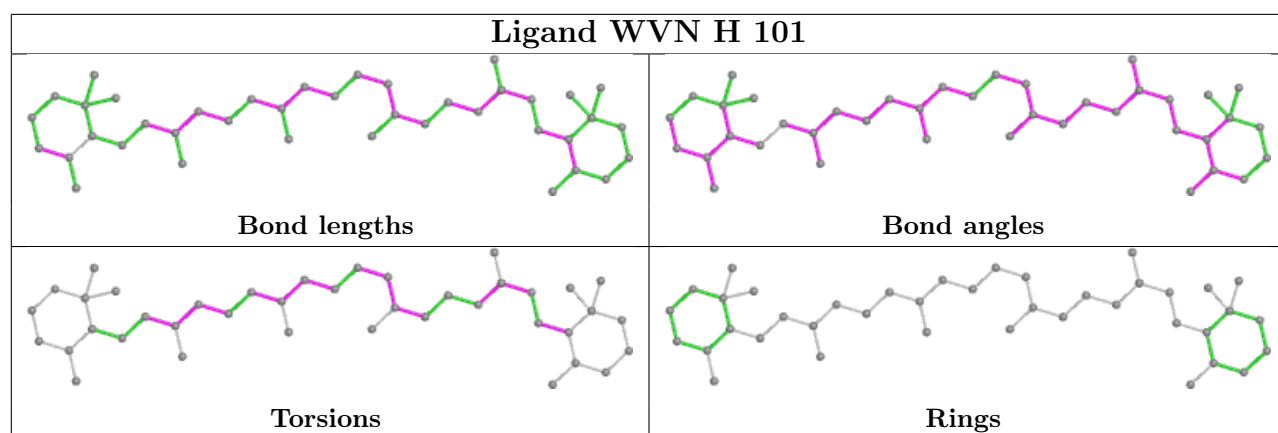
## Ligand CLA O 612

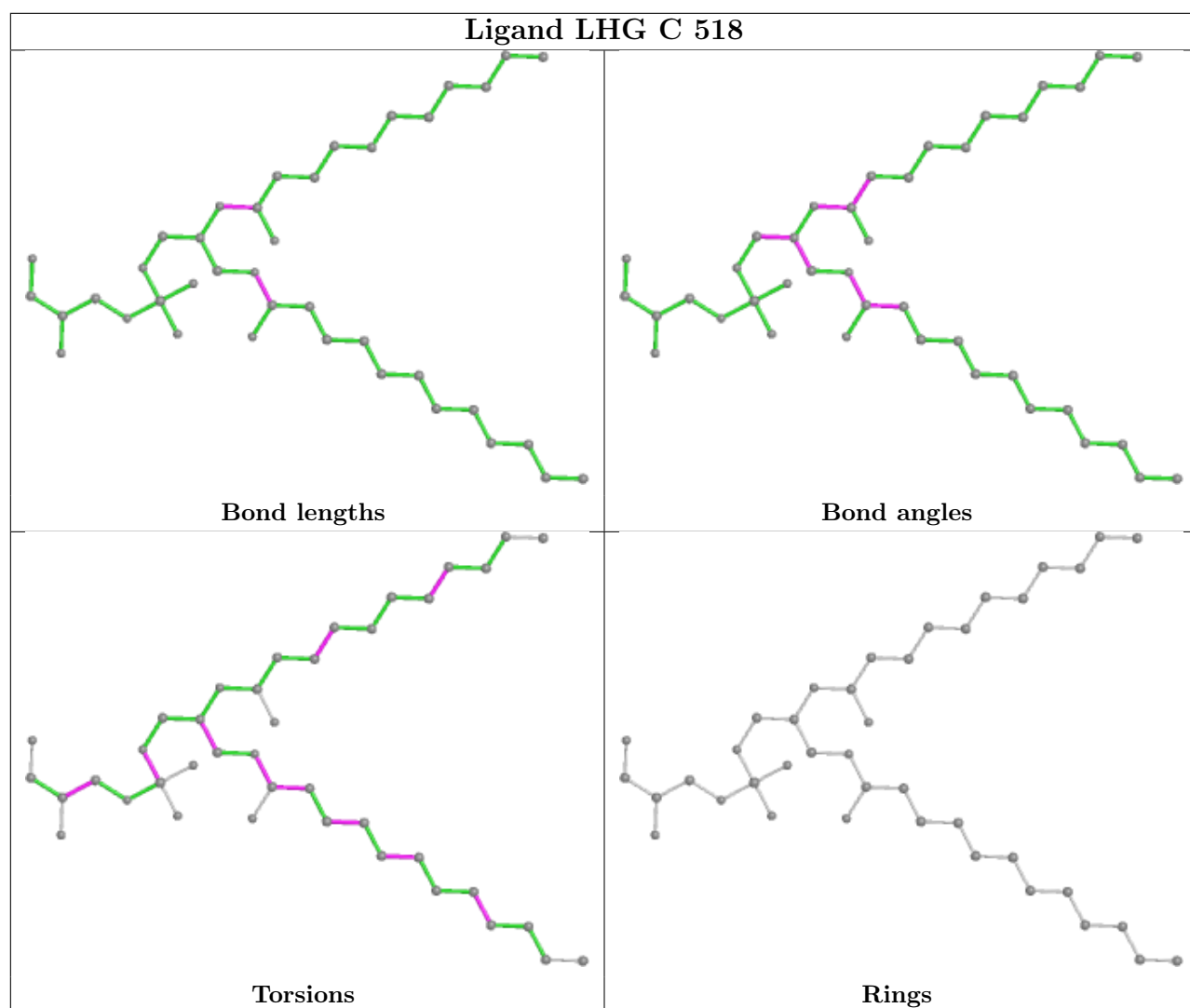
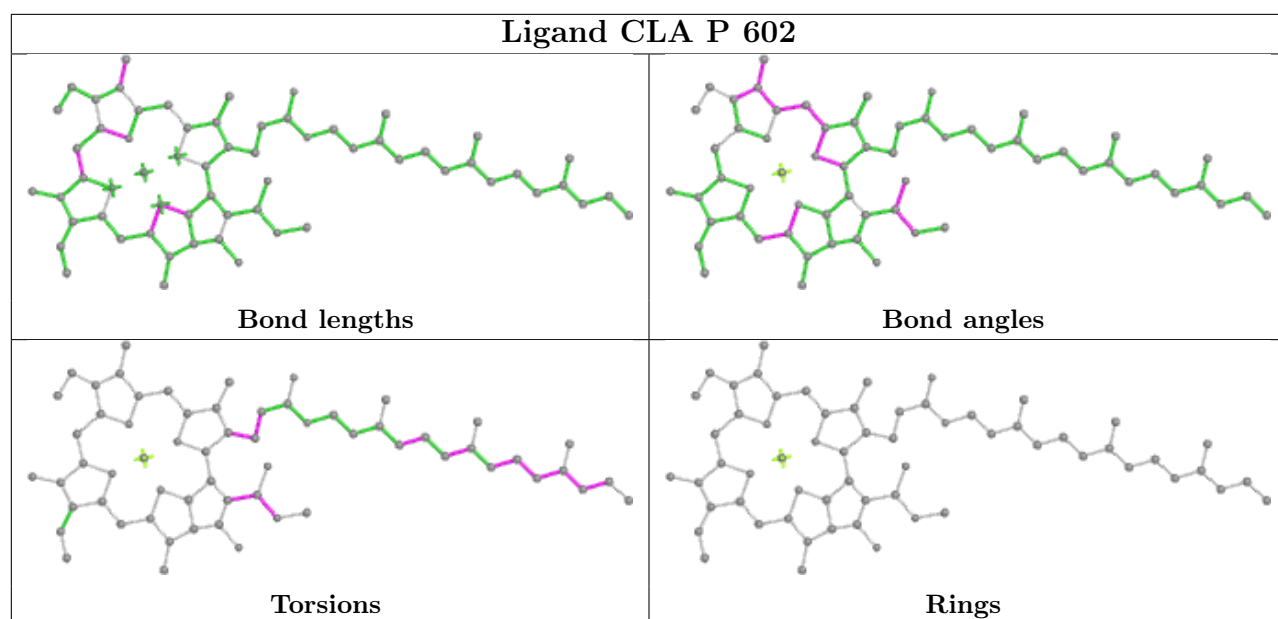


## Ligand DGD h 101

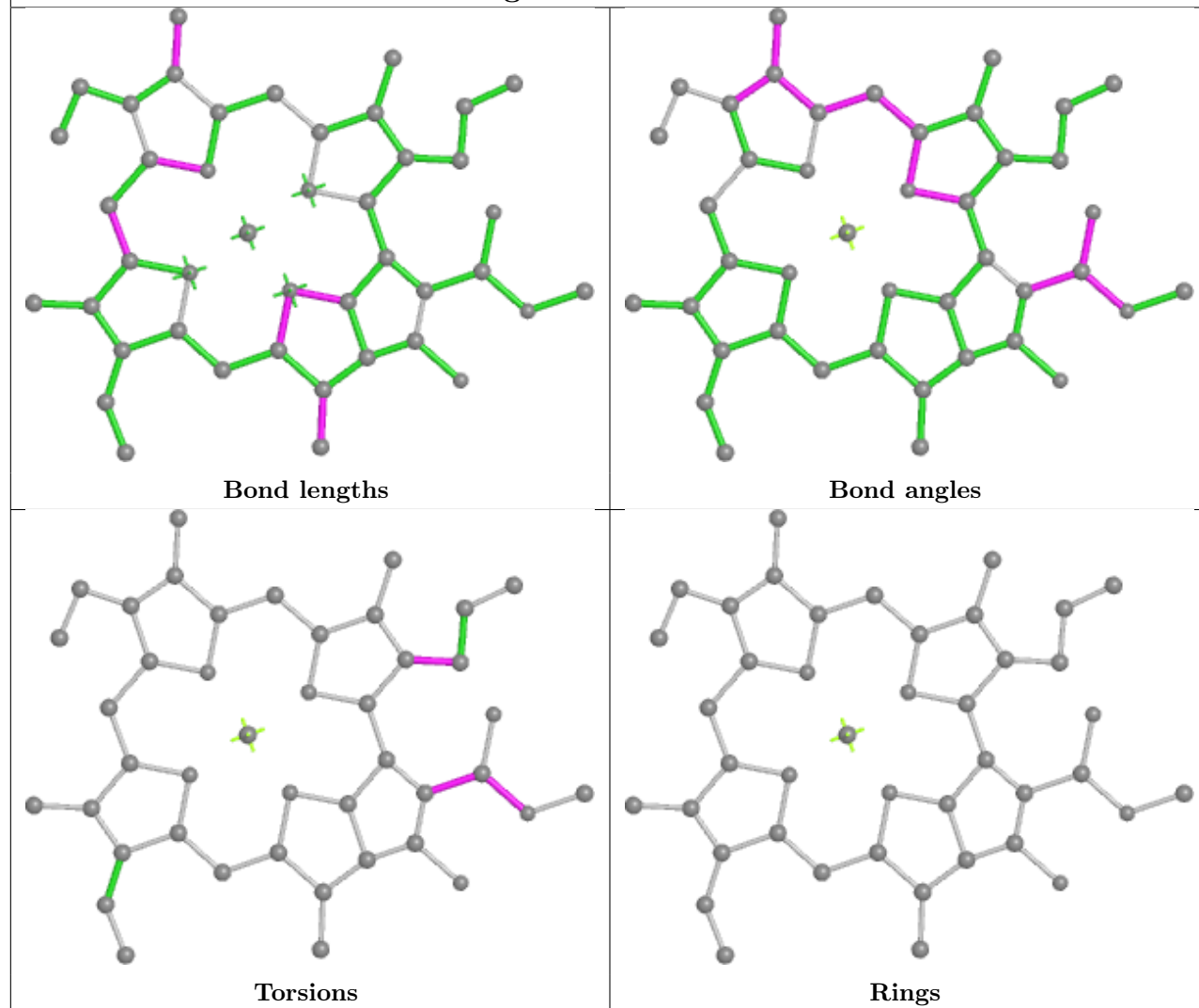




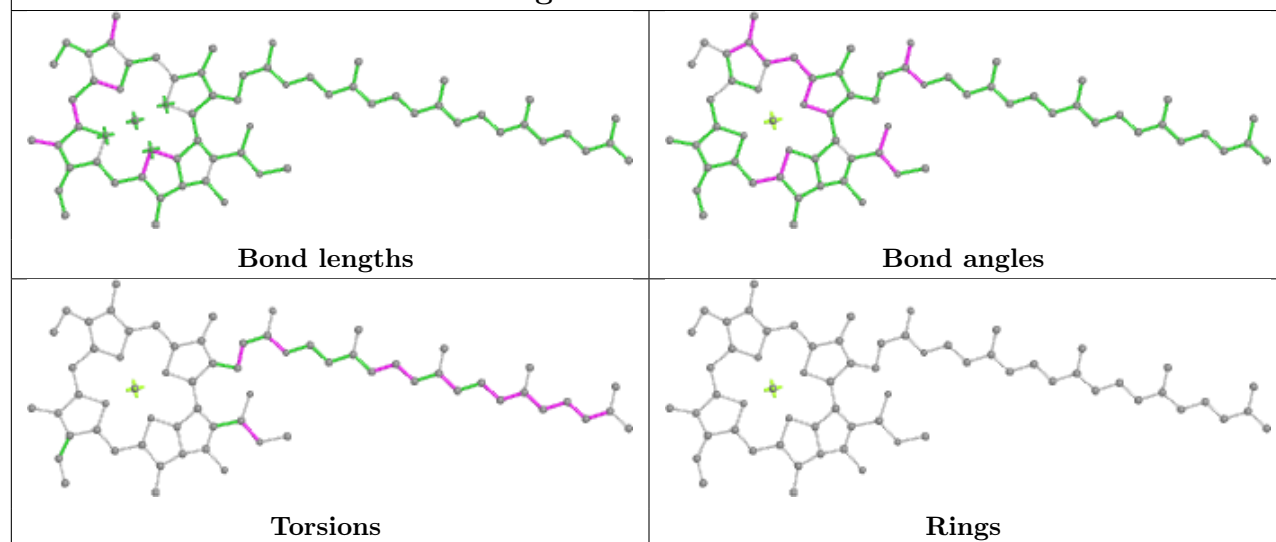


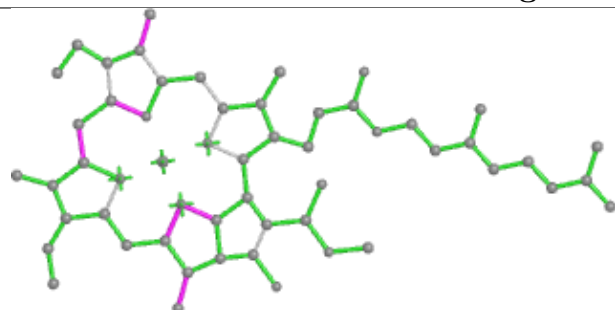


## Ligand CLA 4 312

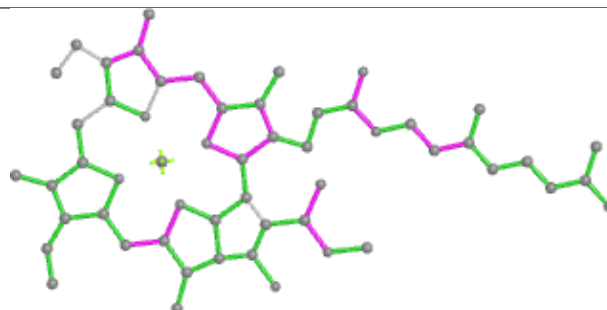


## Ligand CLA b 616

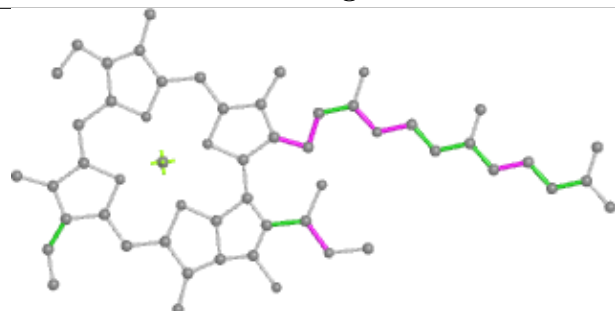


**Ligand CLA S 603**

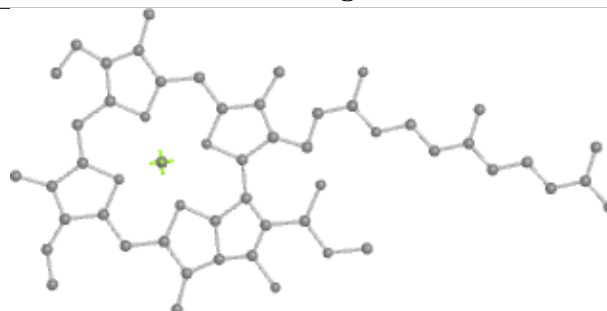
Bond lengths



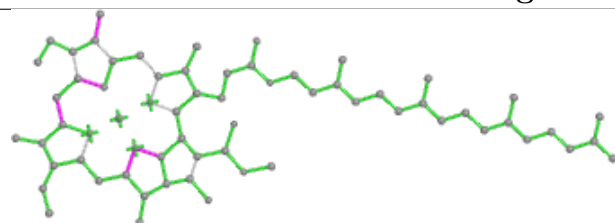
Bond angles



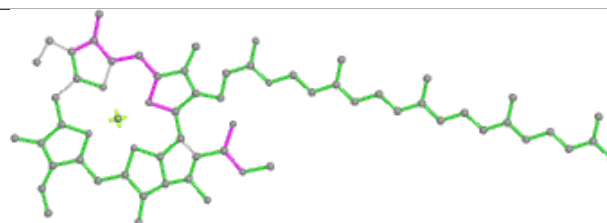
Torsions



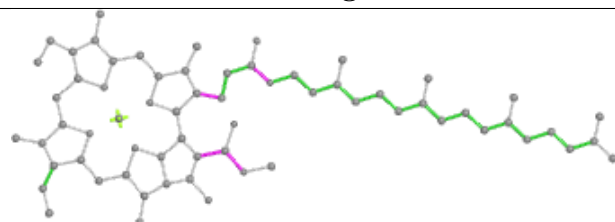
Rings

**Ligand CLA C 502**

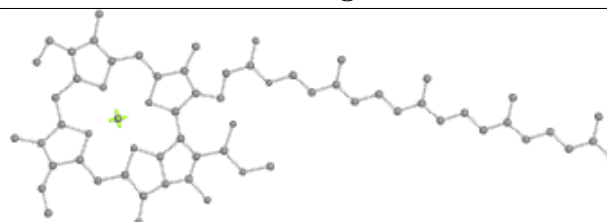
Bond lengths



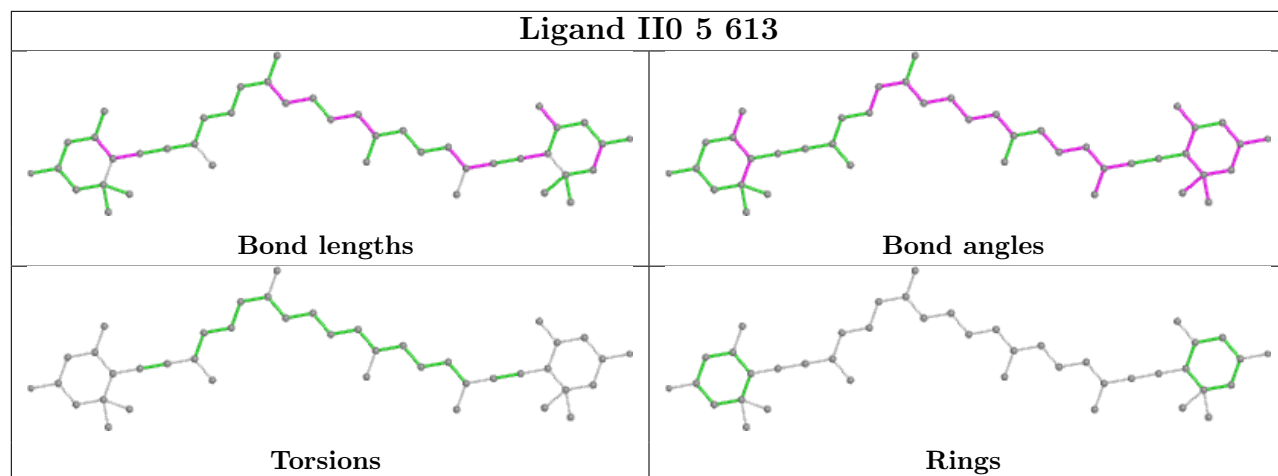
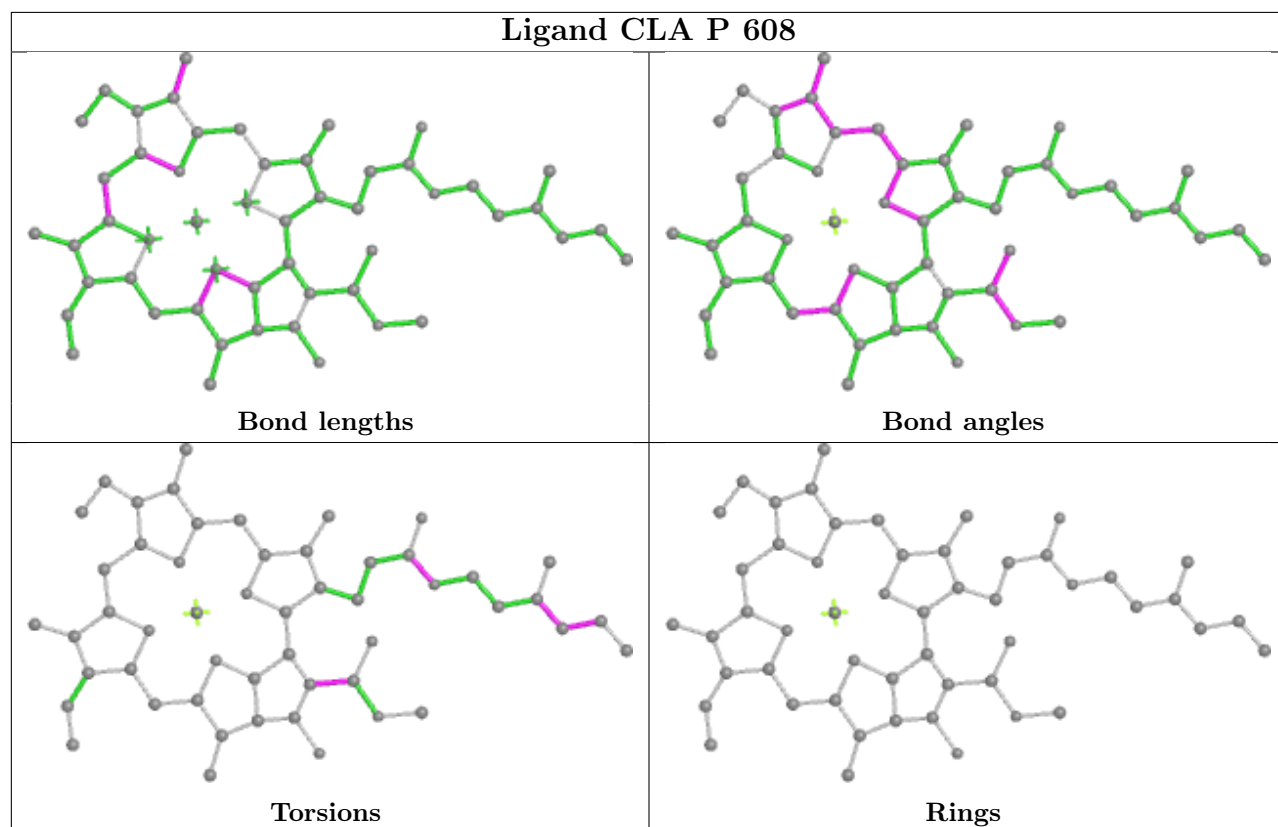
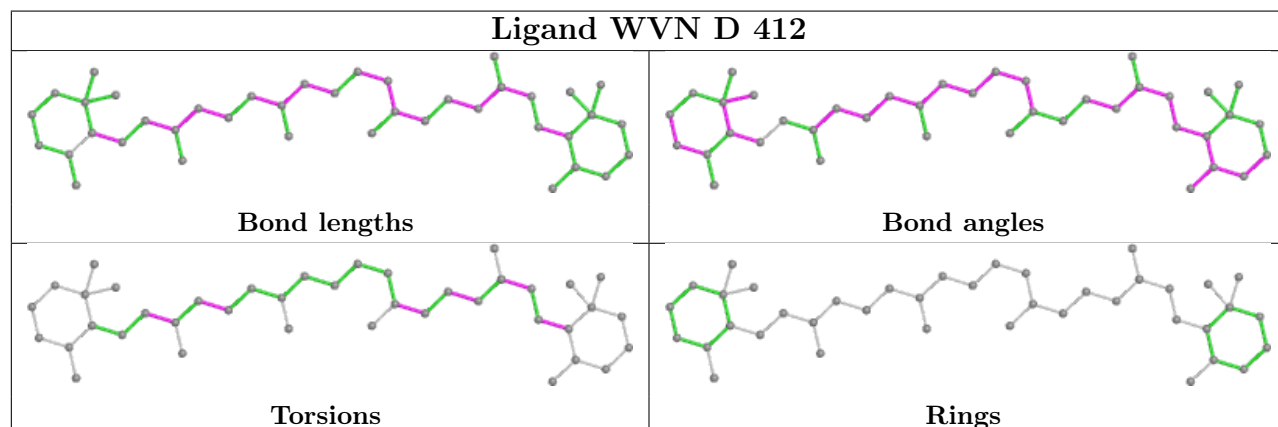
Bond angles

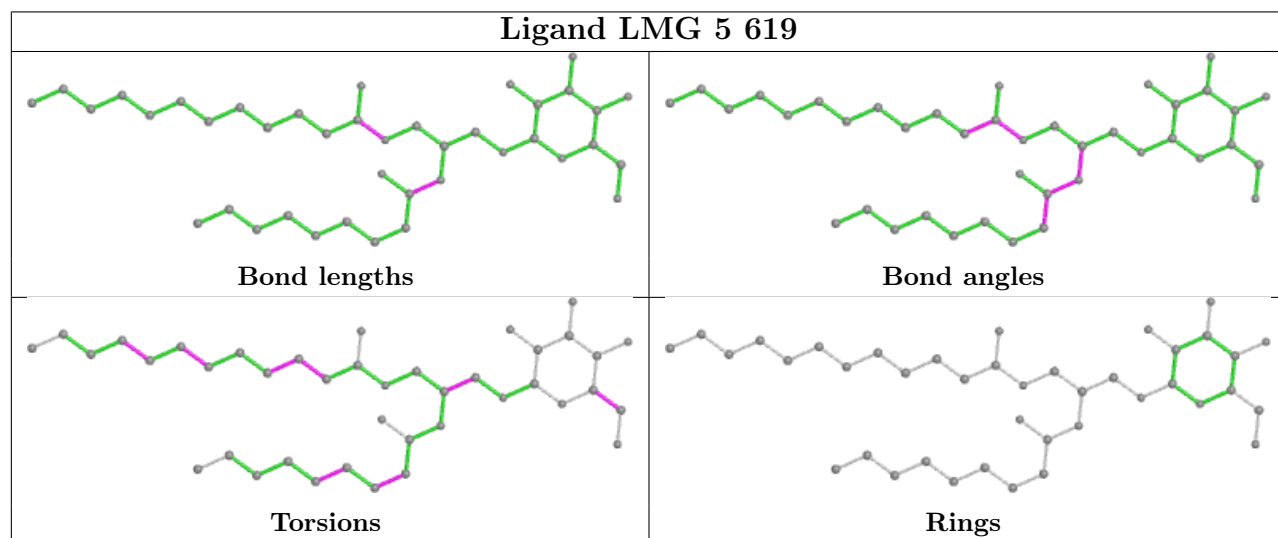
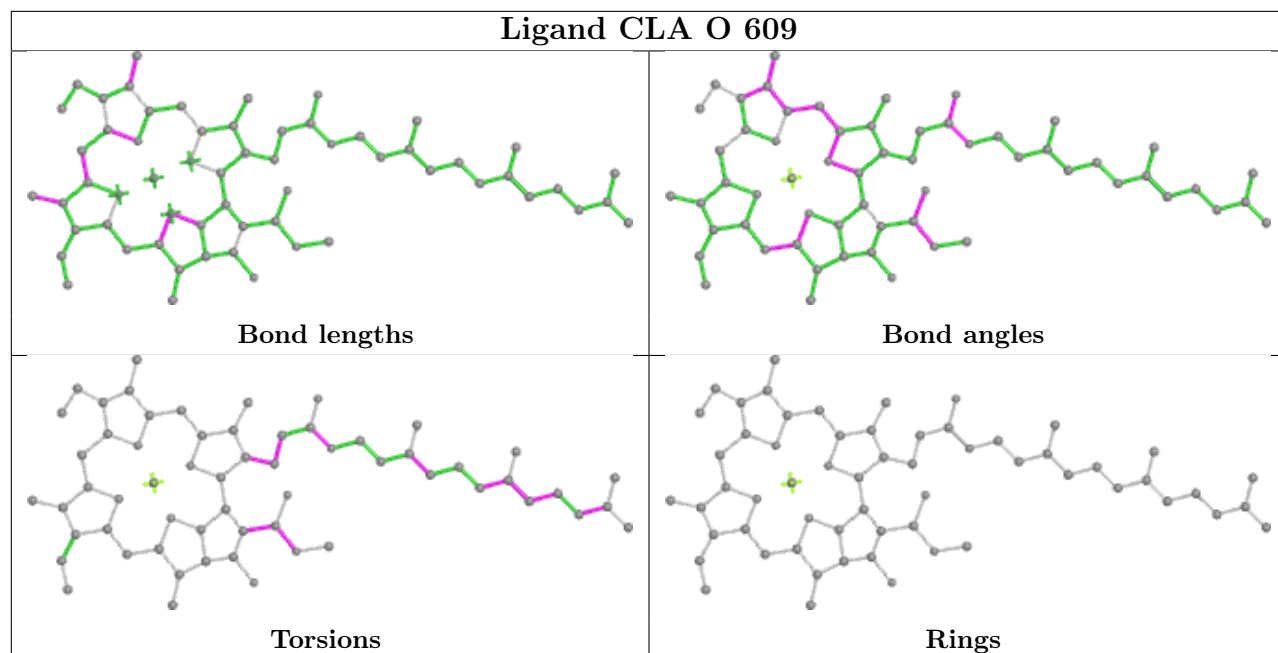


Torsions

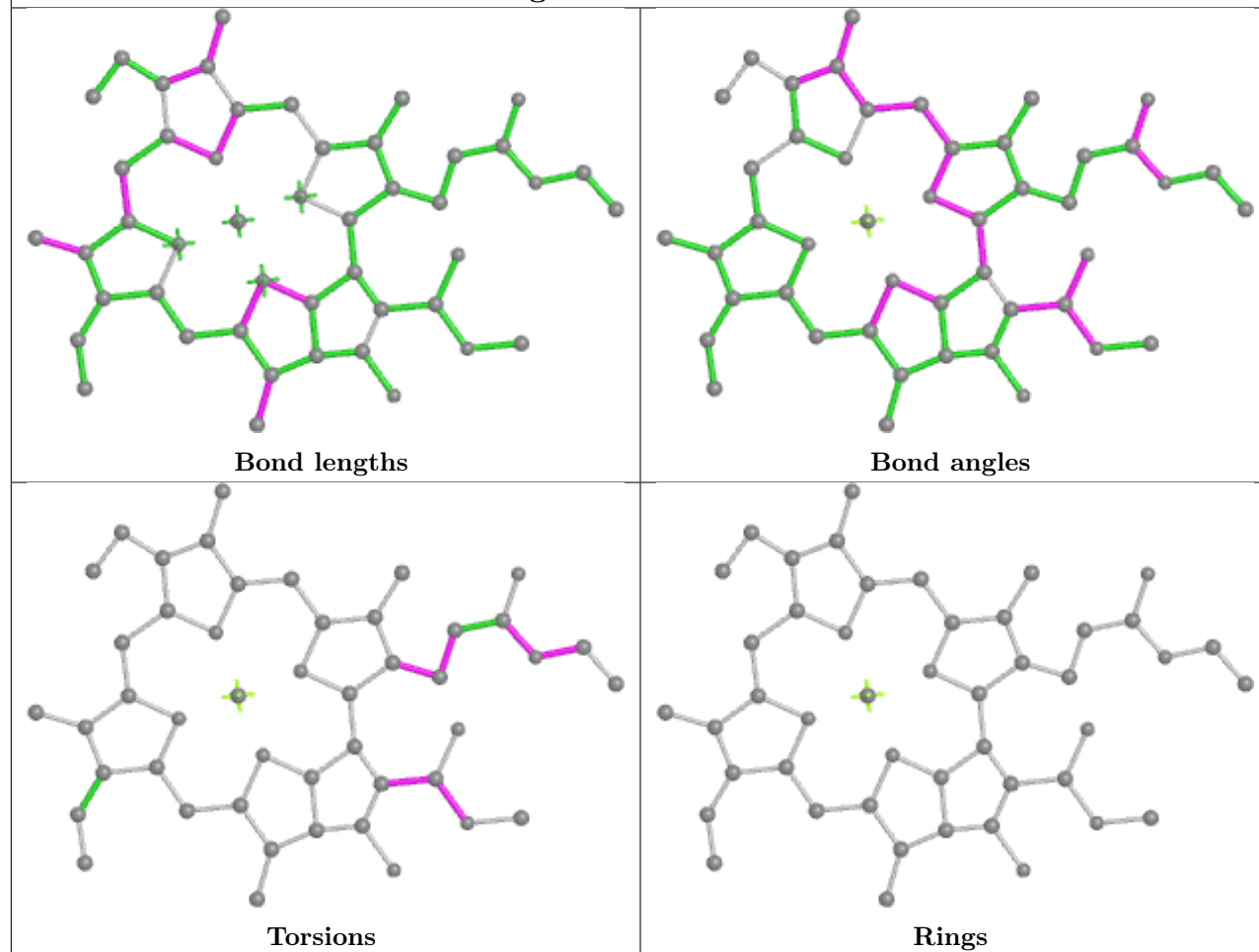


Rings

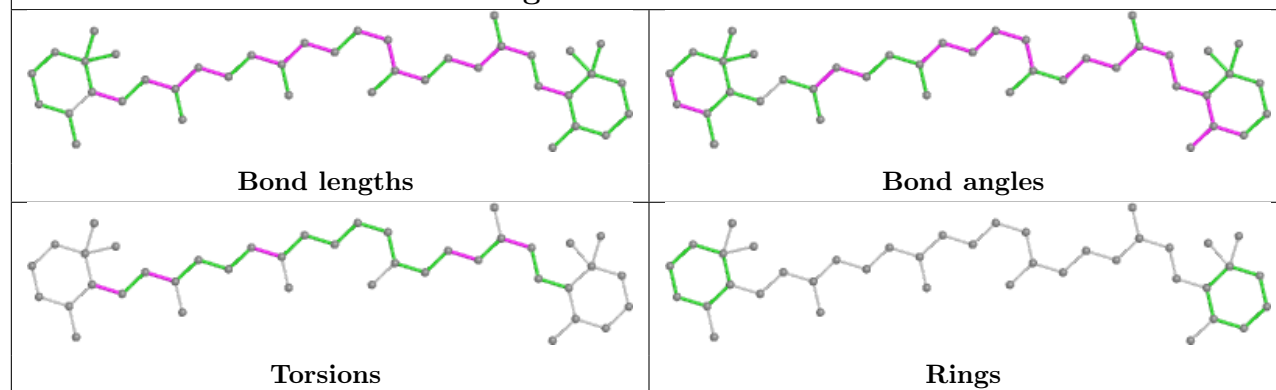
**Ligand II0 5 613****Ligand CLA P 608****Ligand WVN D 412**

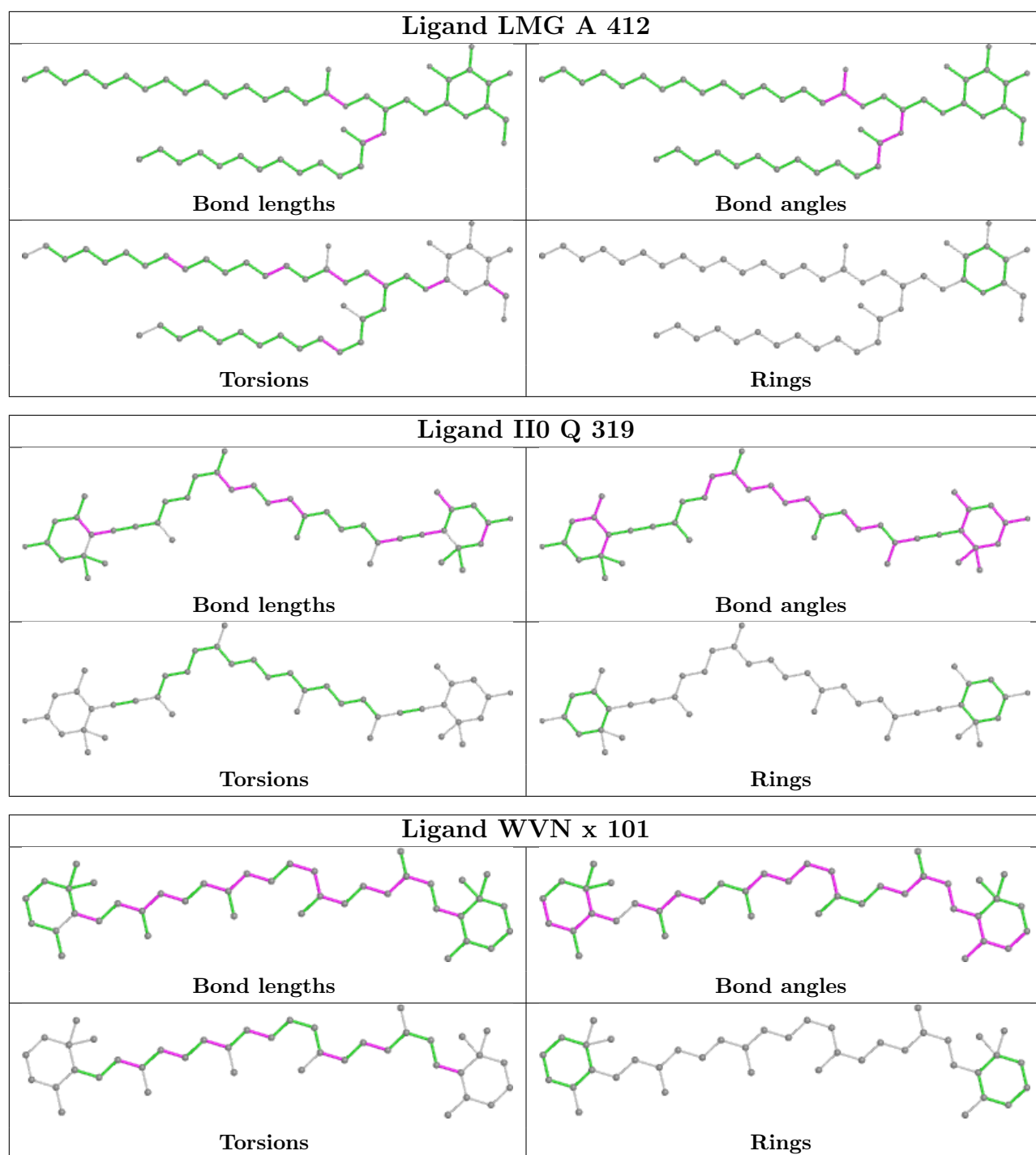


## Ligand CLA 1 614

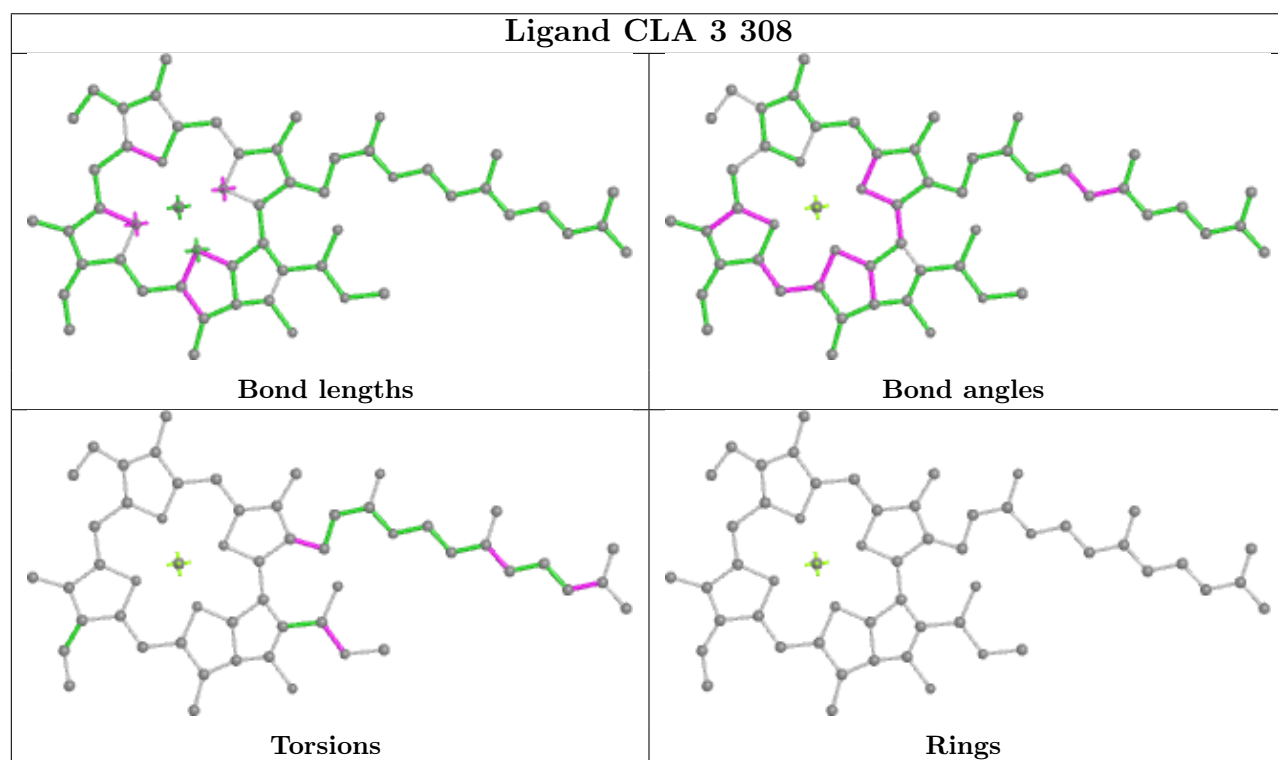
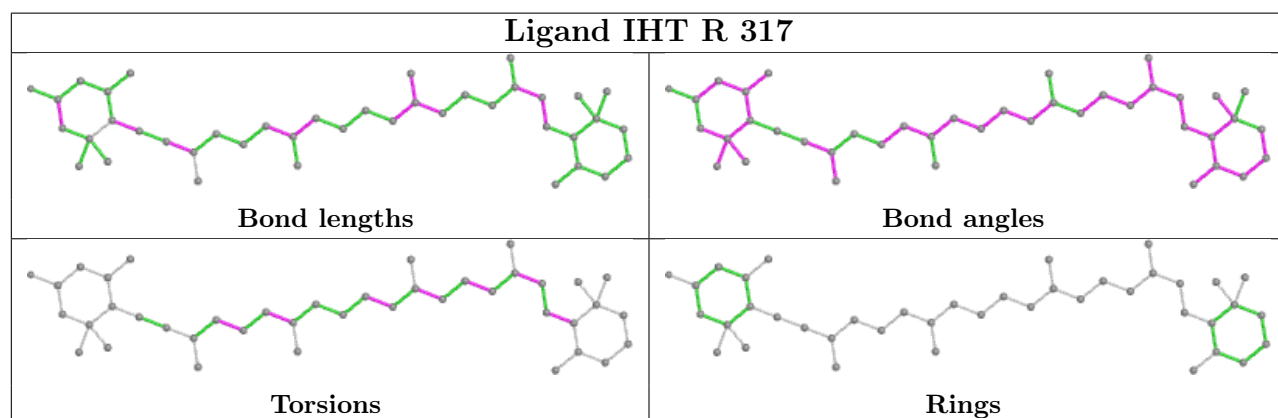
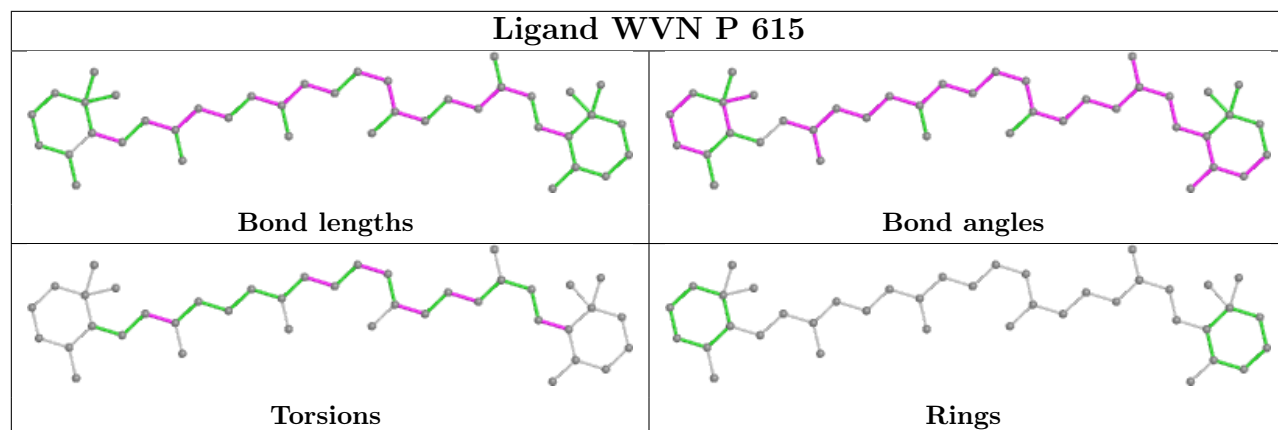


## Ligand WVN Y 101

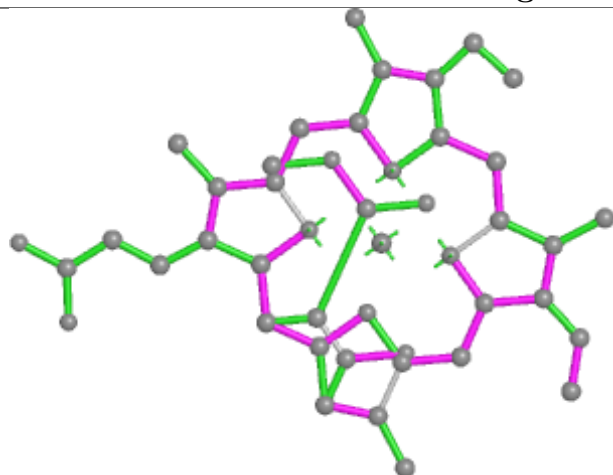




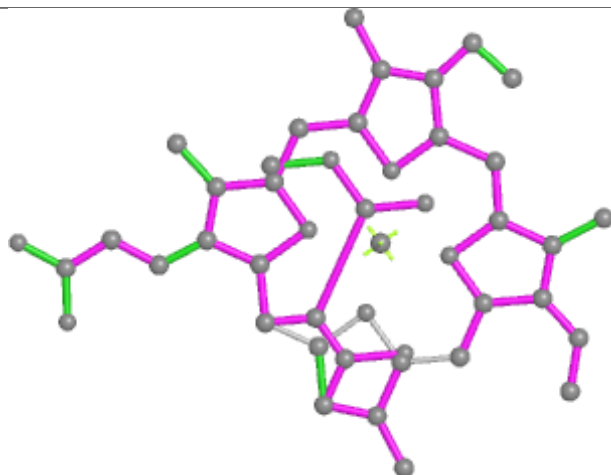




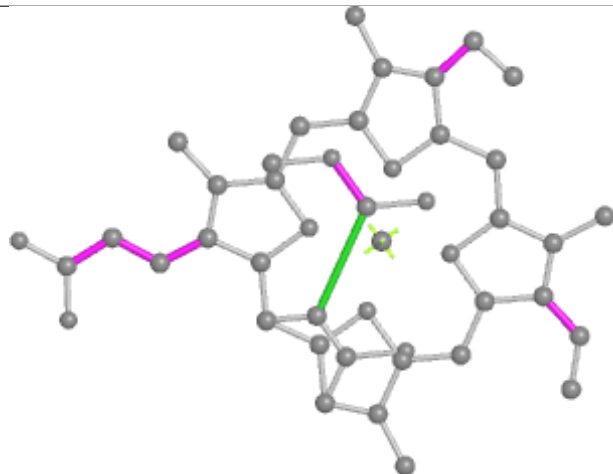
## Ligand KC2 P 605



Bond lengths



Bond angles

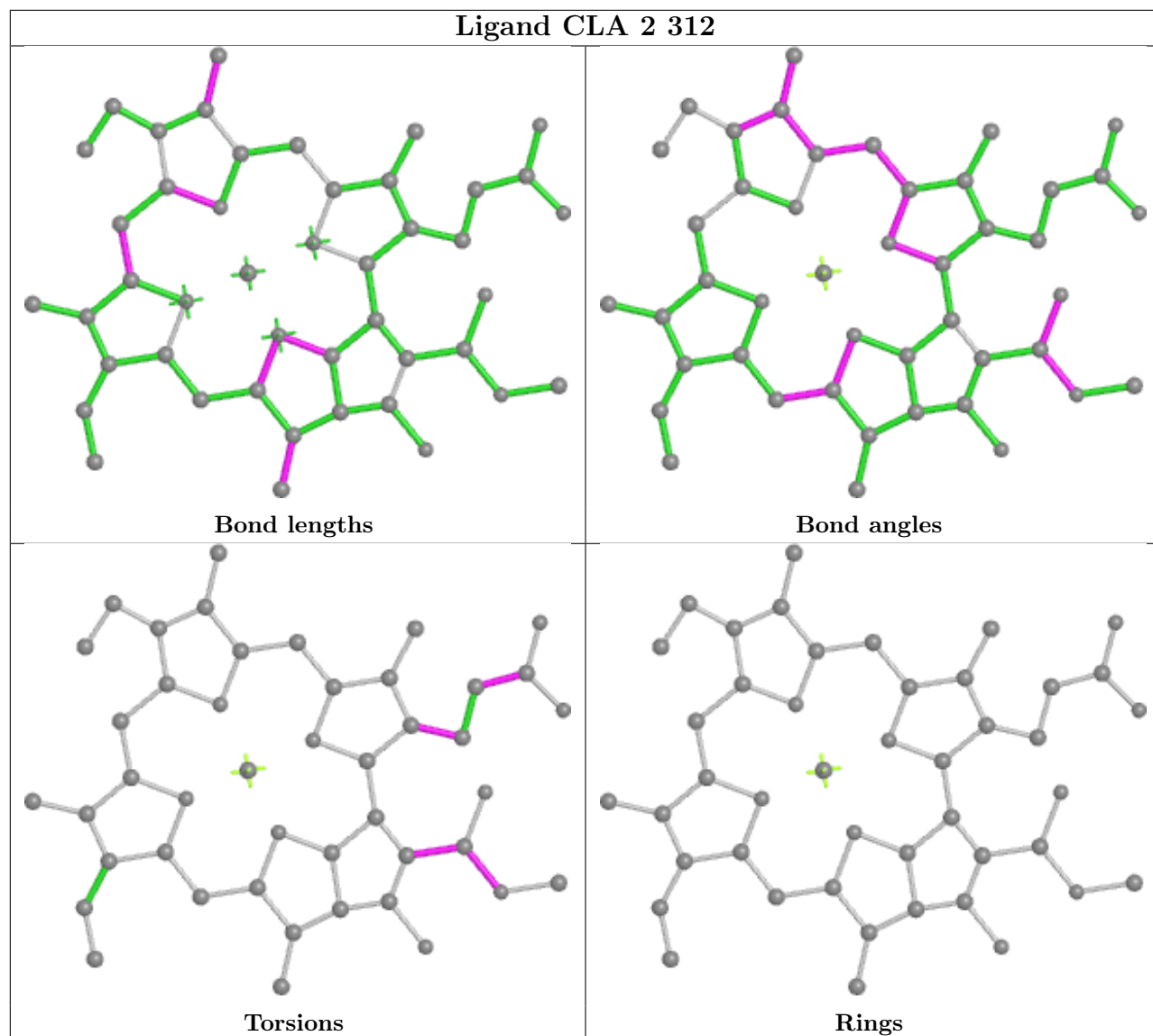


Torsions

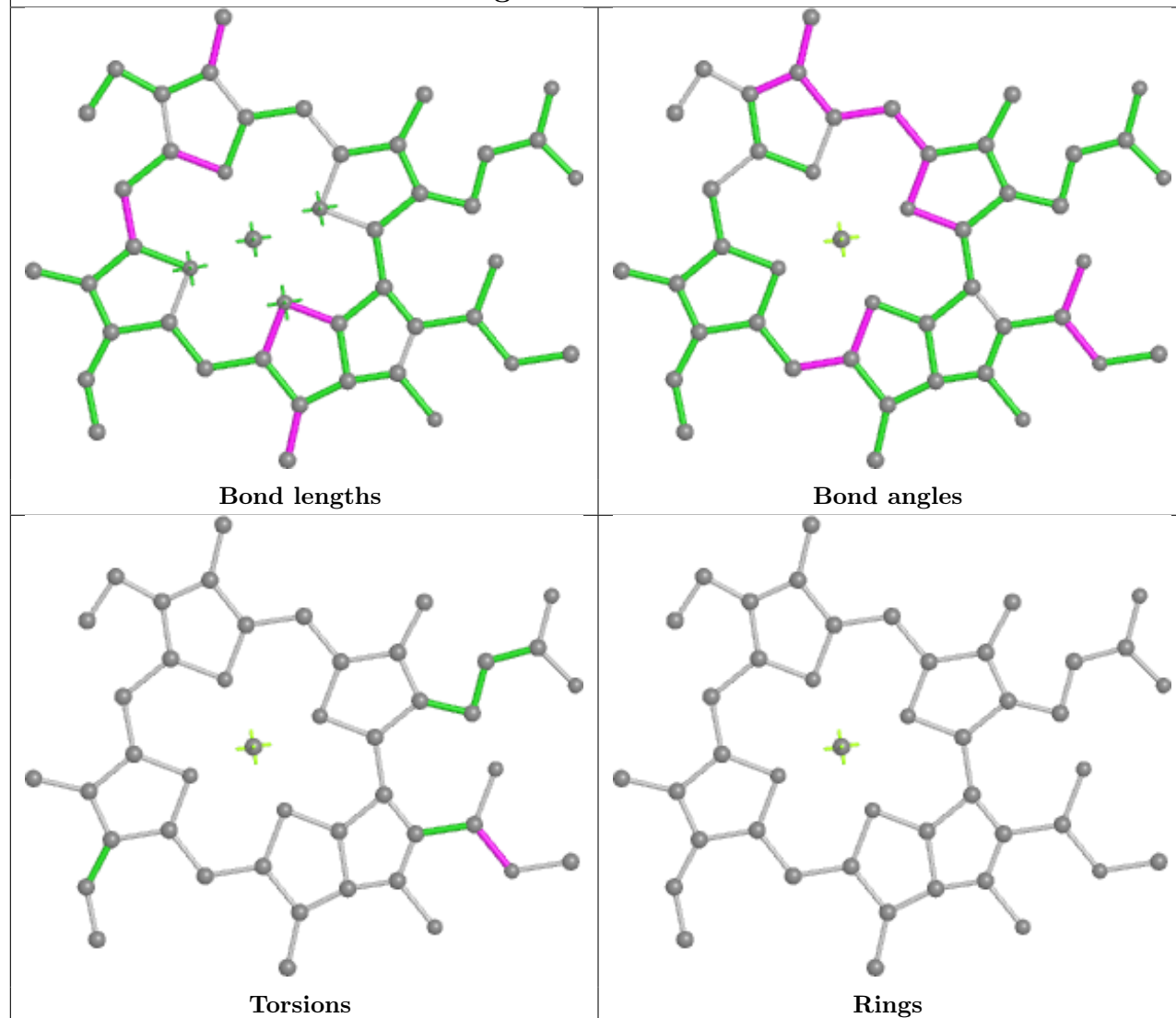


Rings

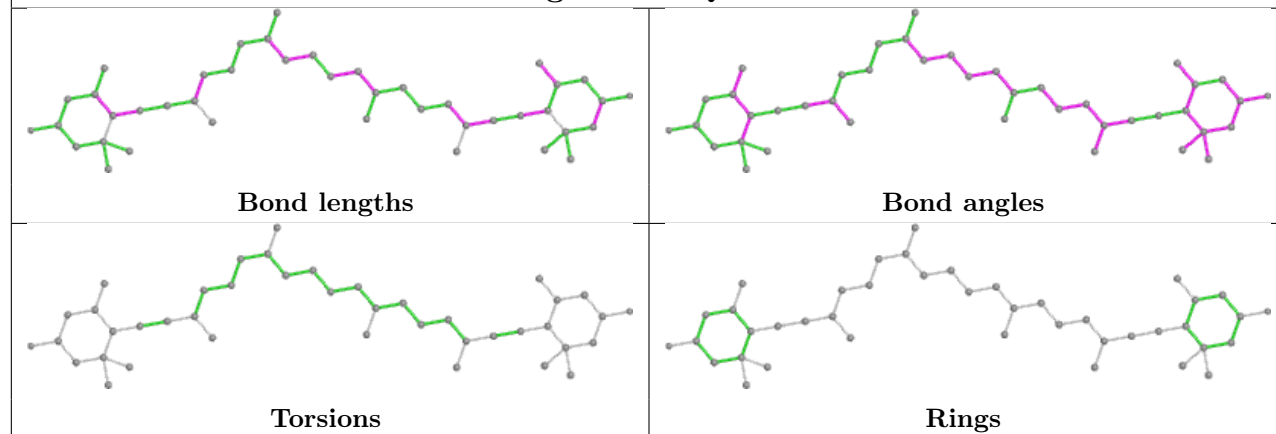
## Ligand CLA 2 312

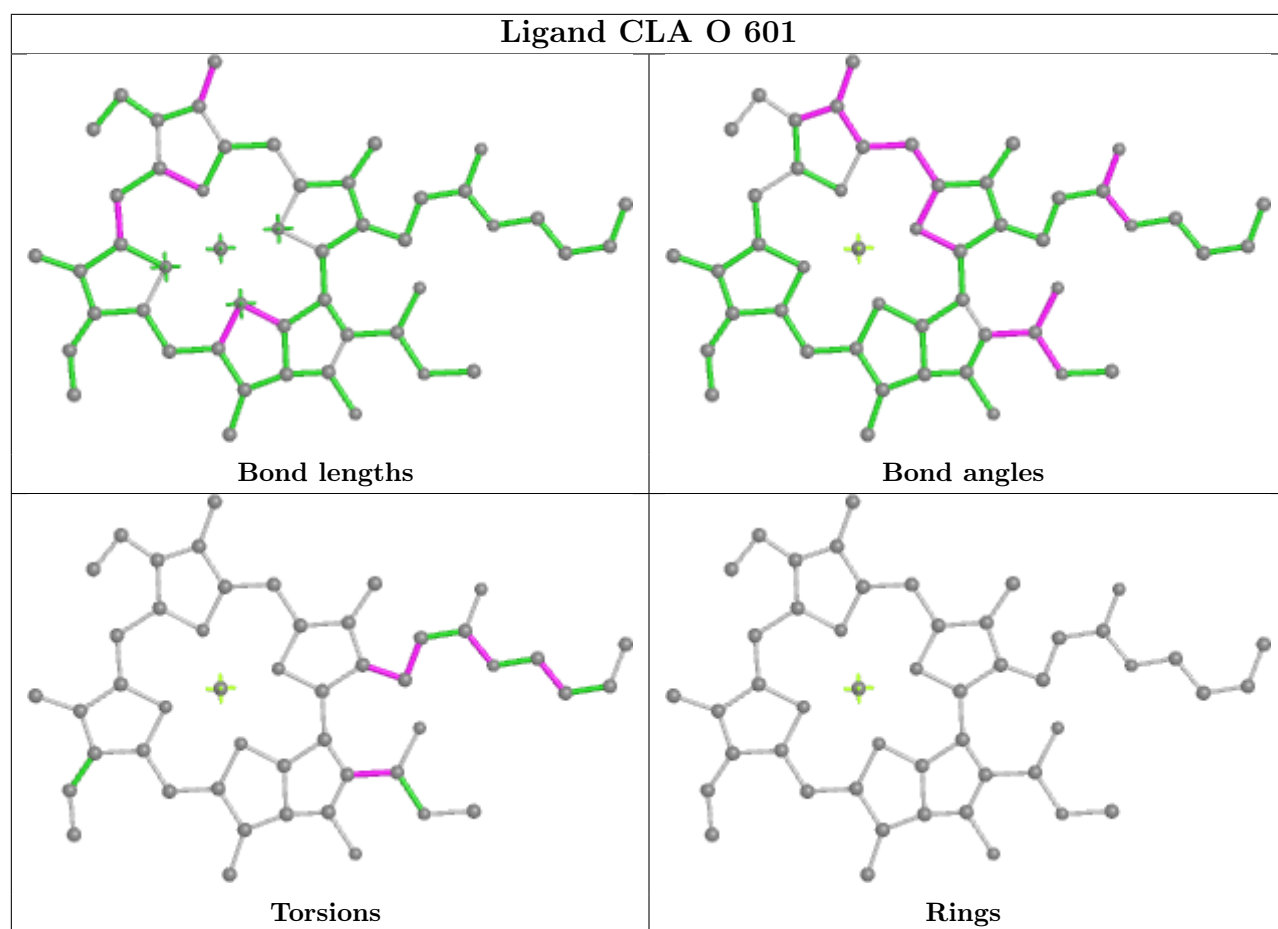


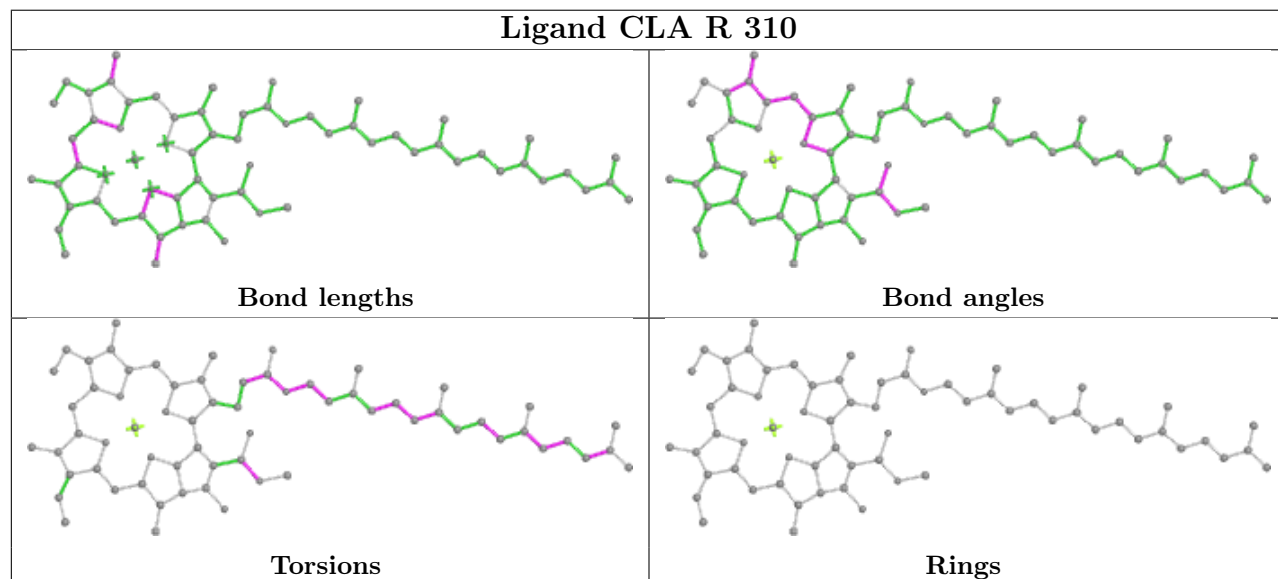
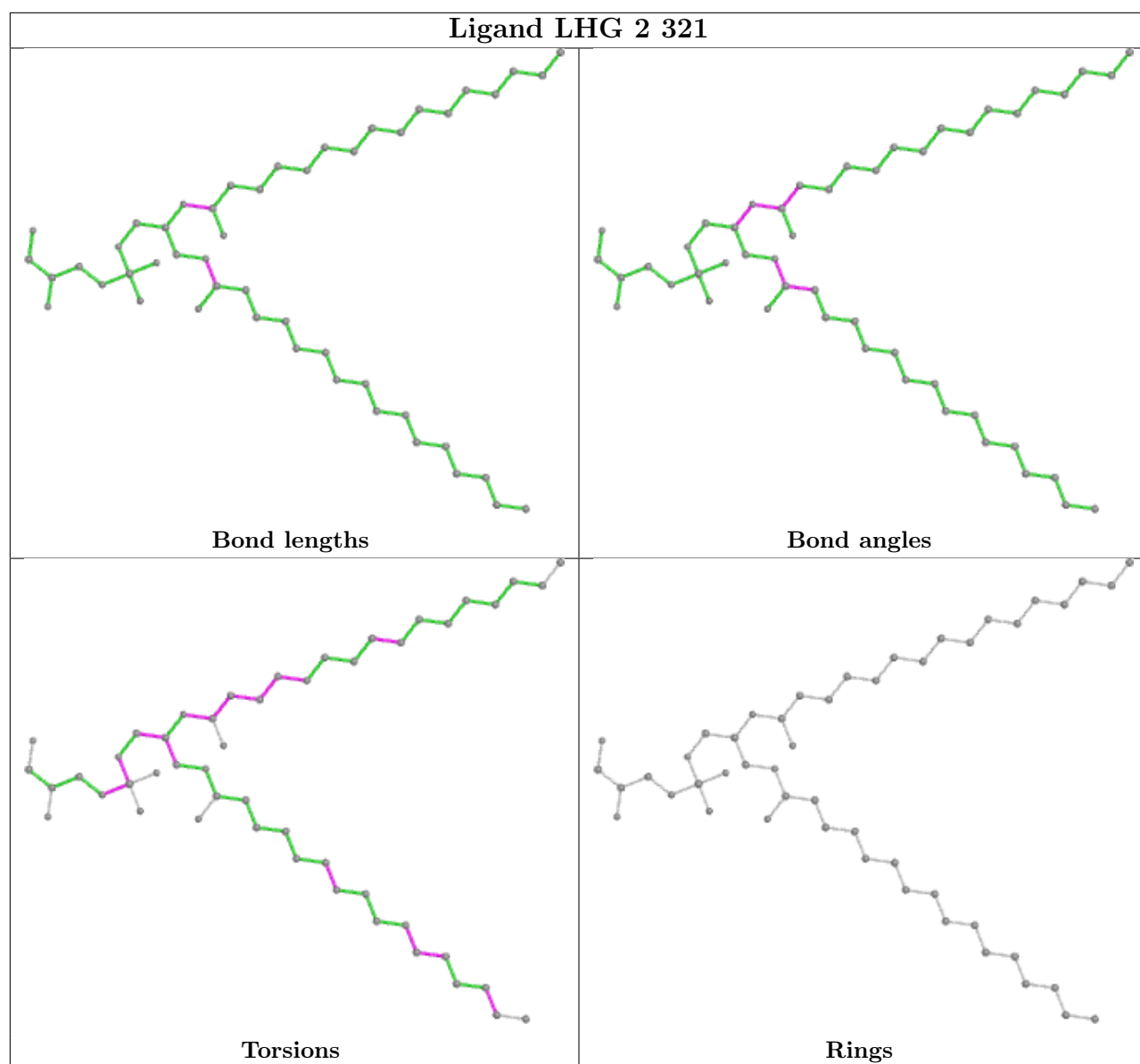
## Ligand CLA 2 319

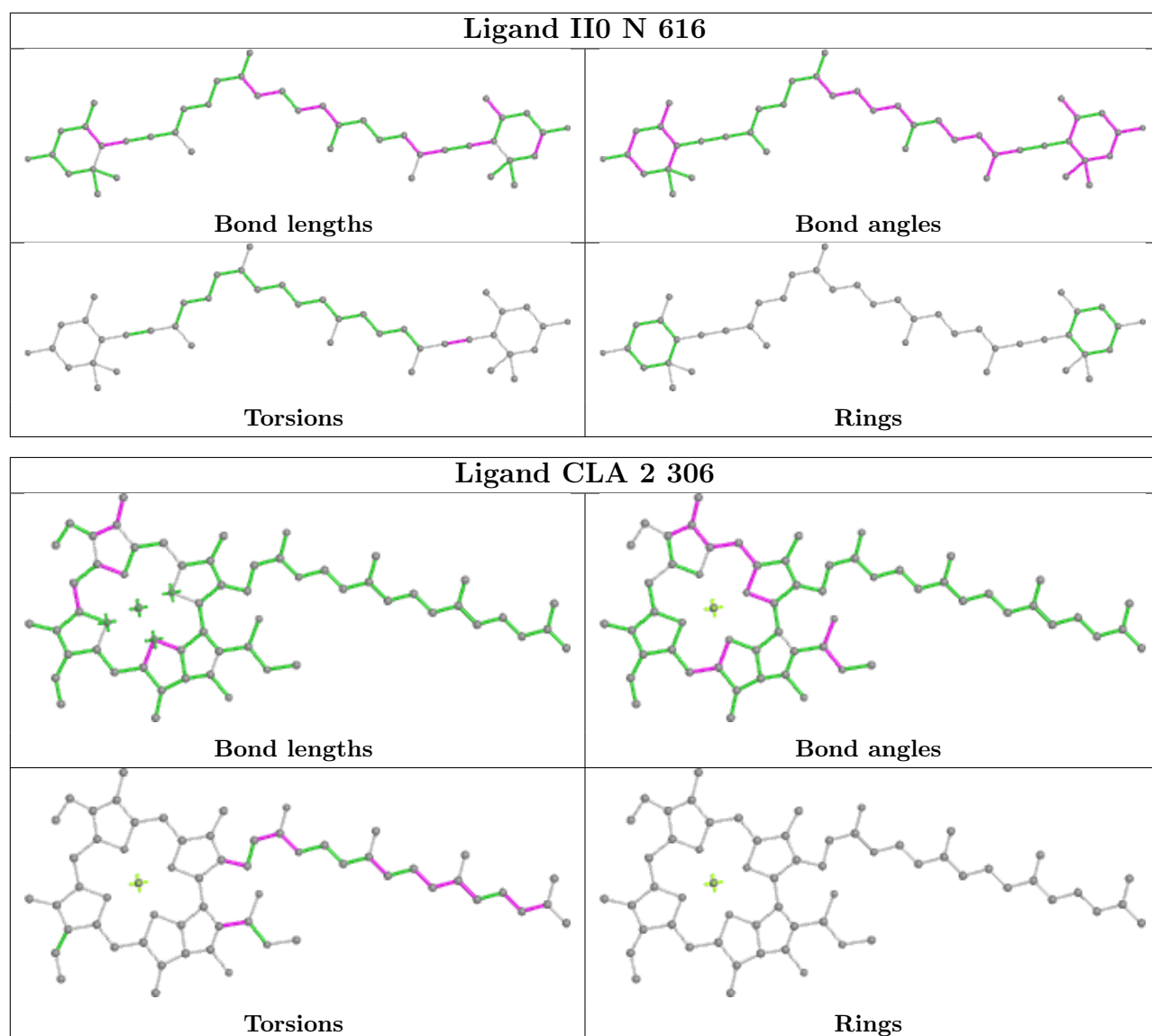


## Ligand II0 Q 314

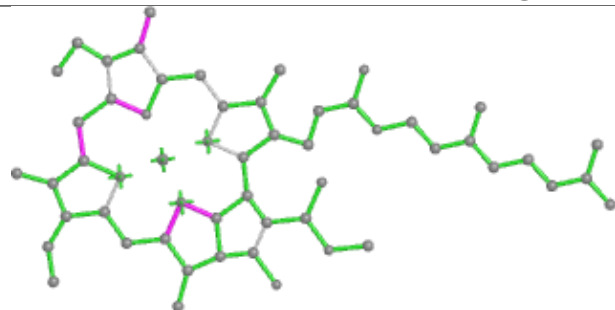




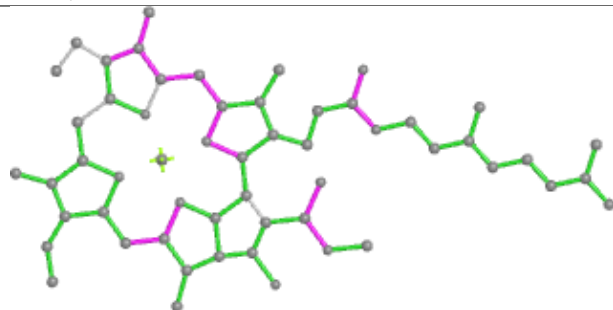




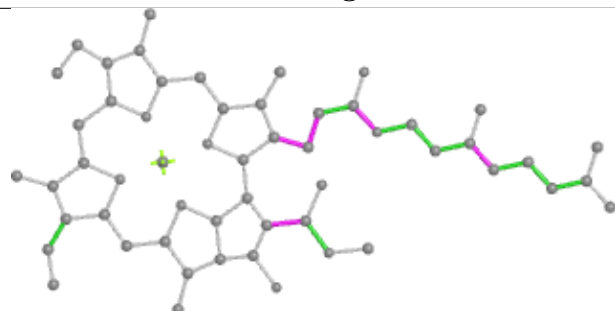
## Ligand CLA Q 305



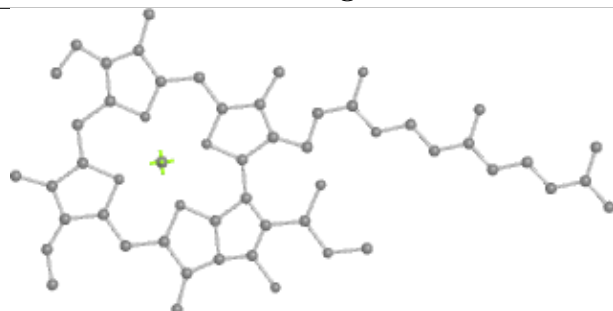
Bond lengths



Bond angles

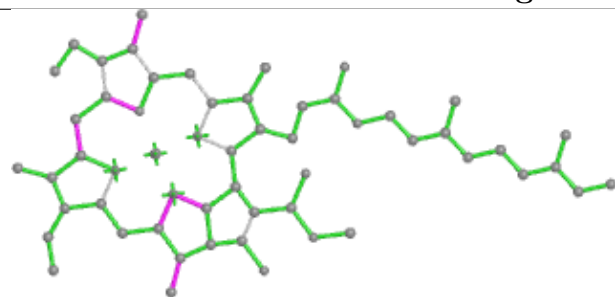


Torsions

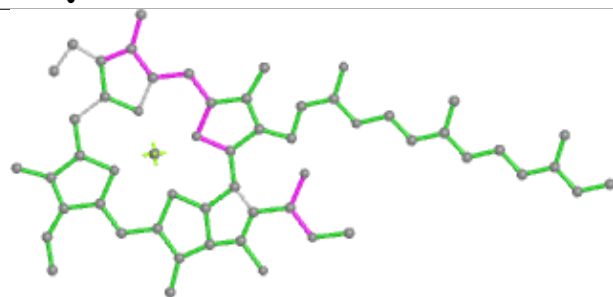


Rings

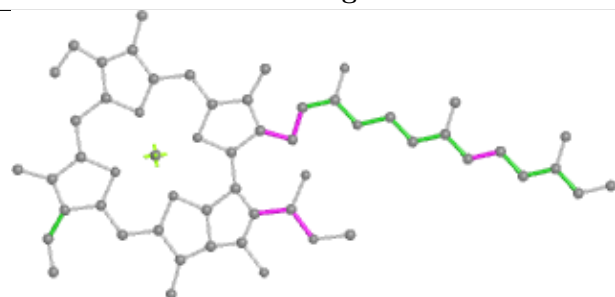
## Ligand CLA Q 307



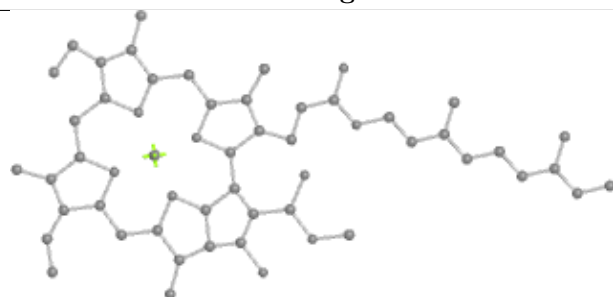
Bond lengths



Bond angles

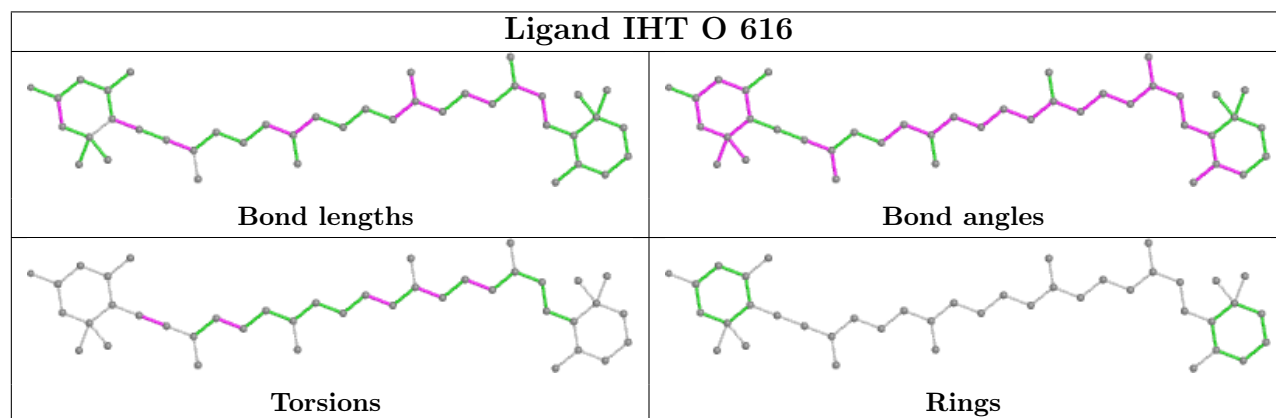
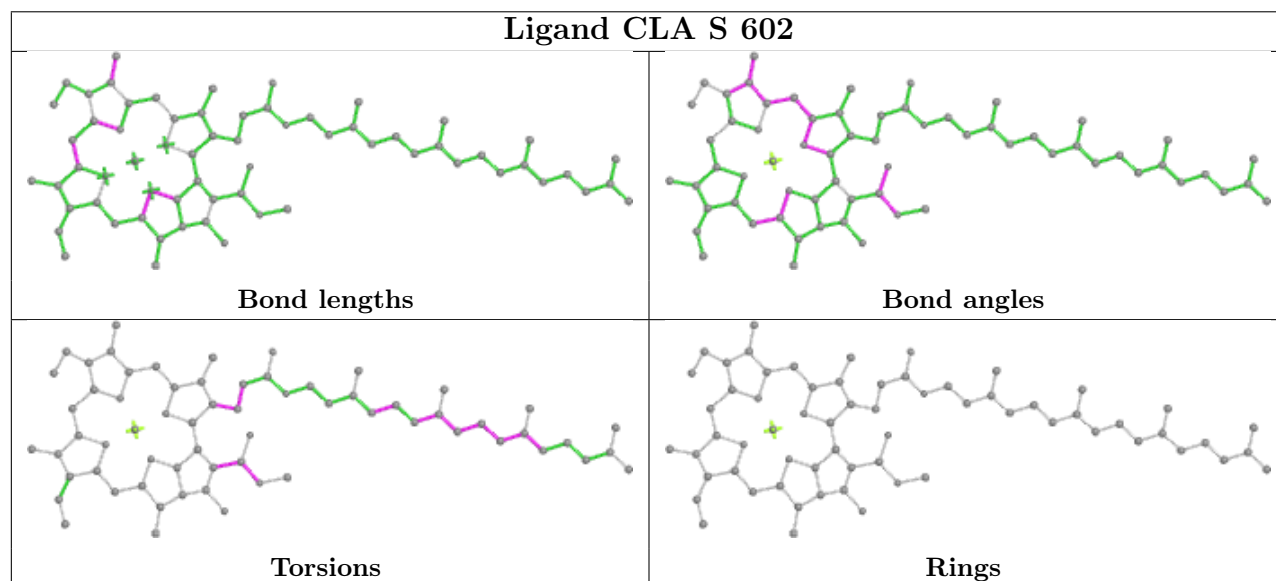
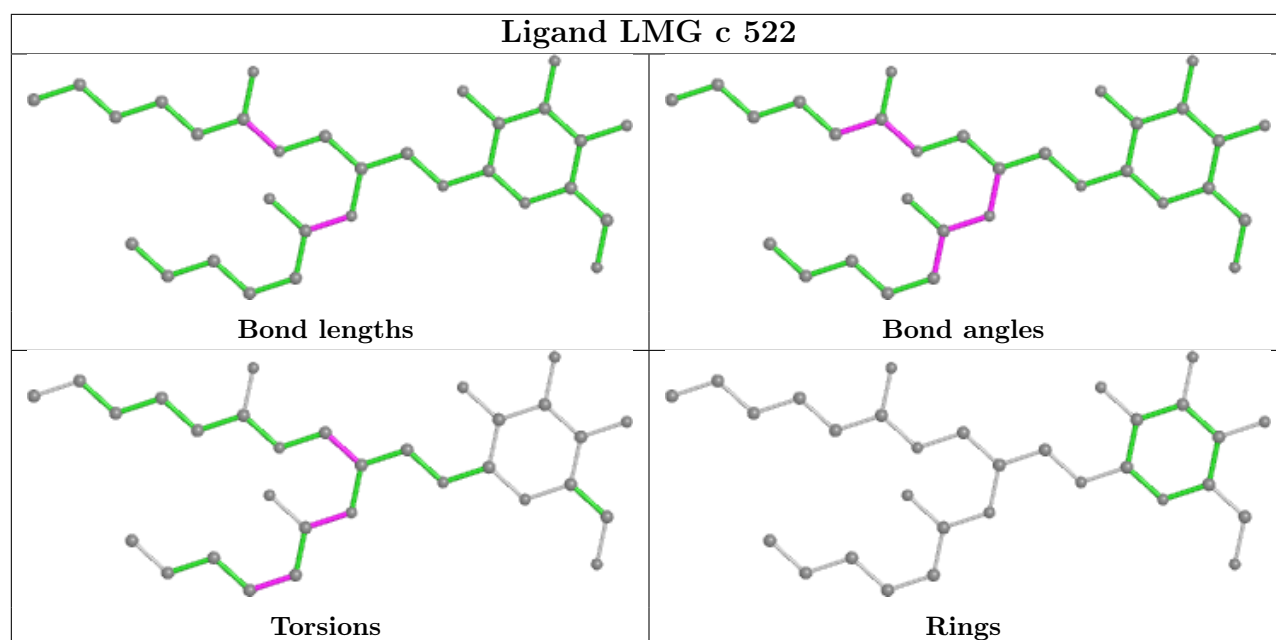


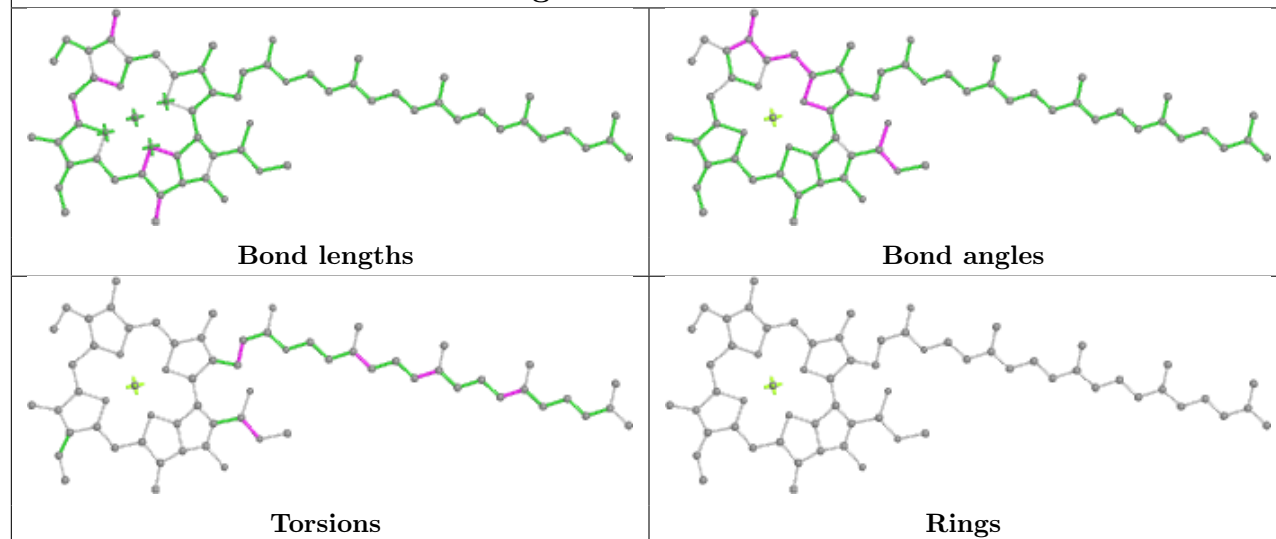
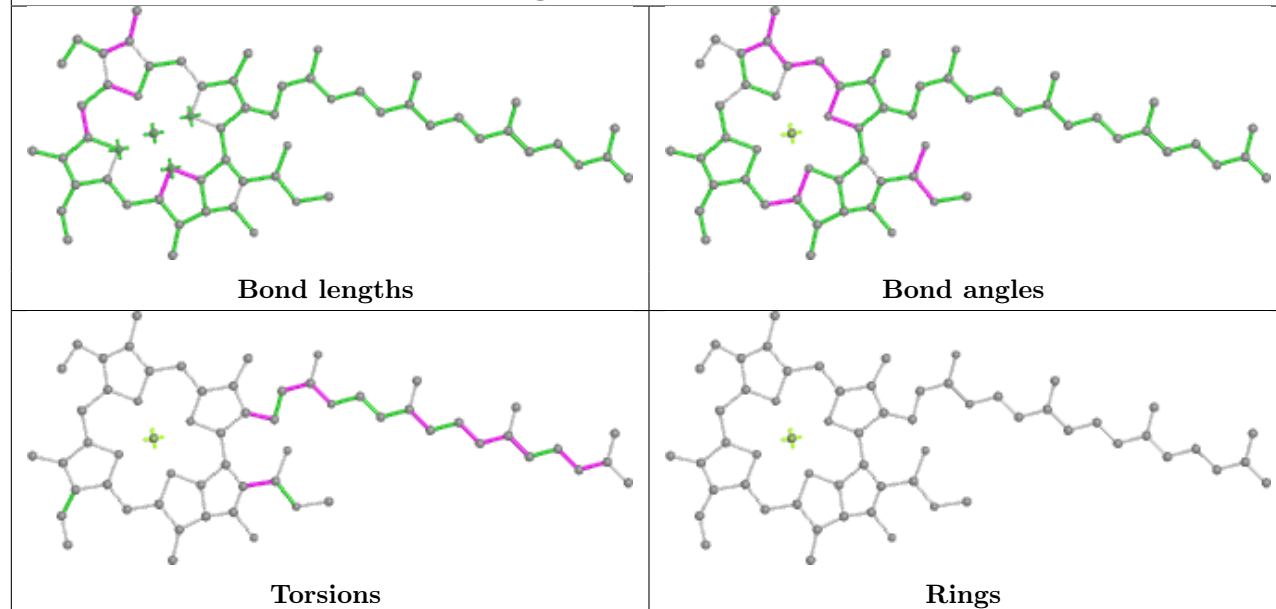
Torsions



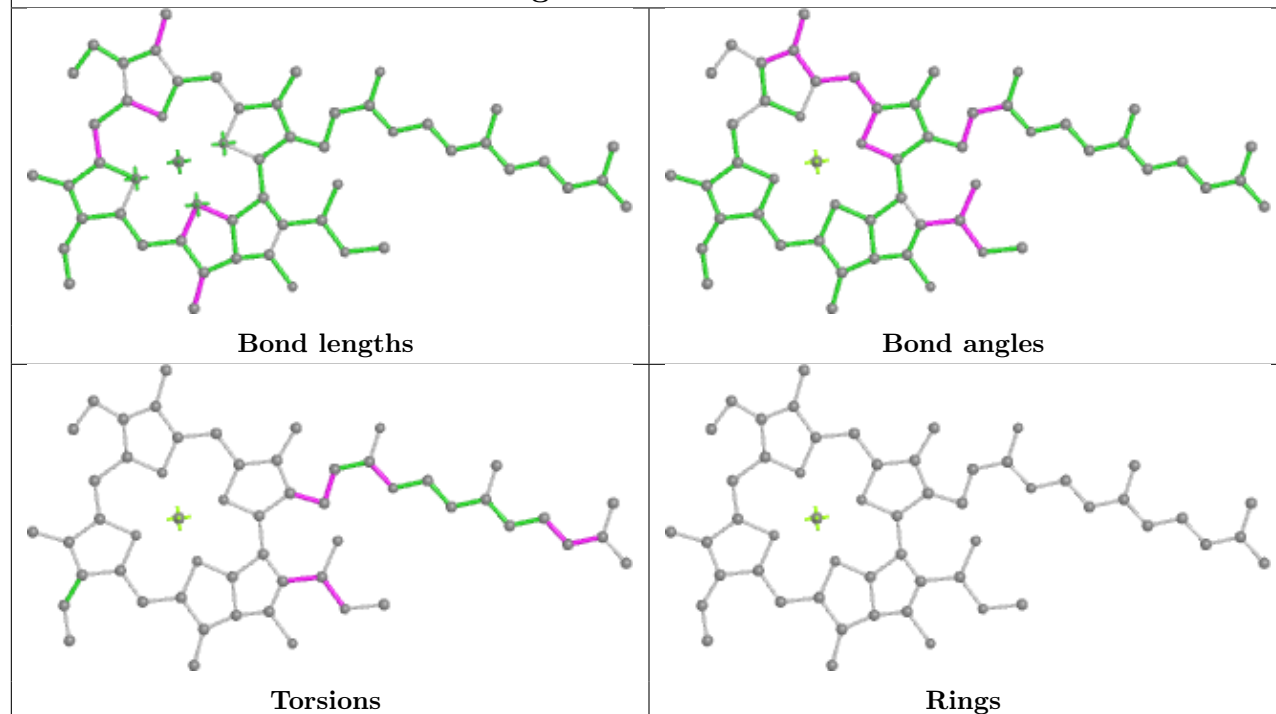
Rings



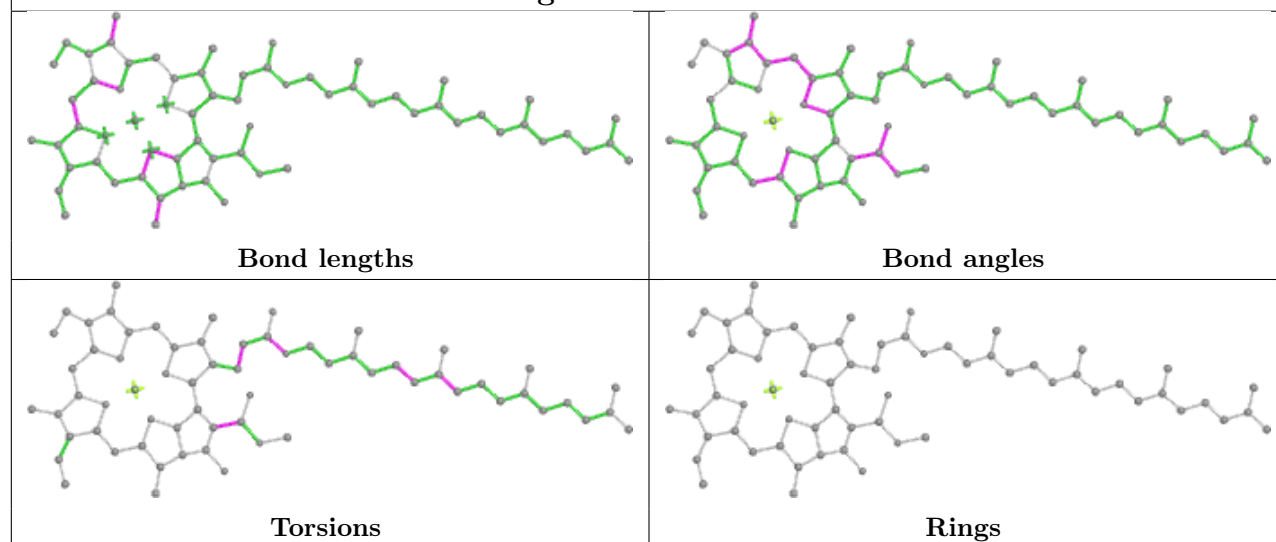


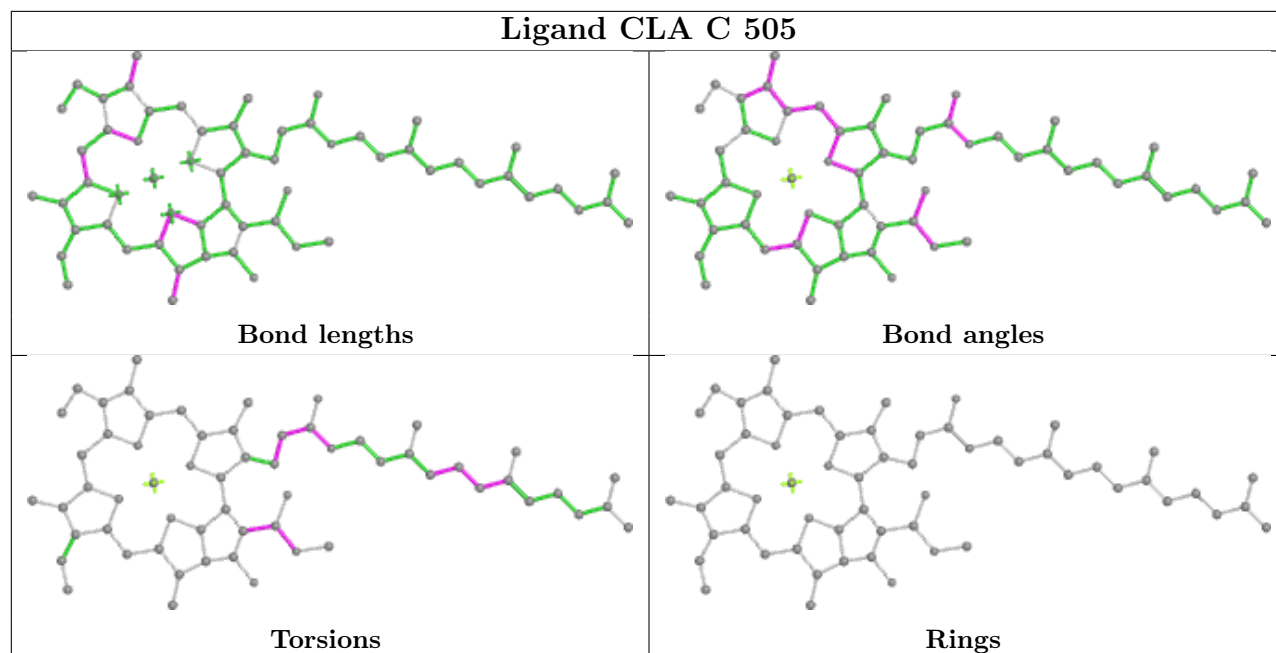
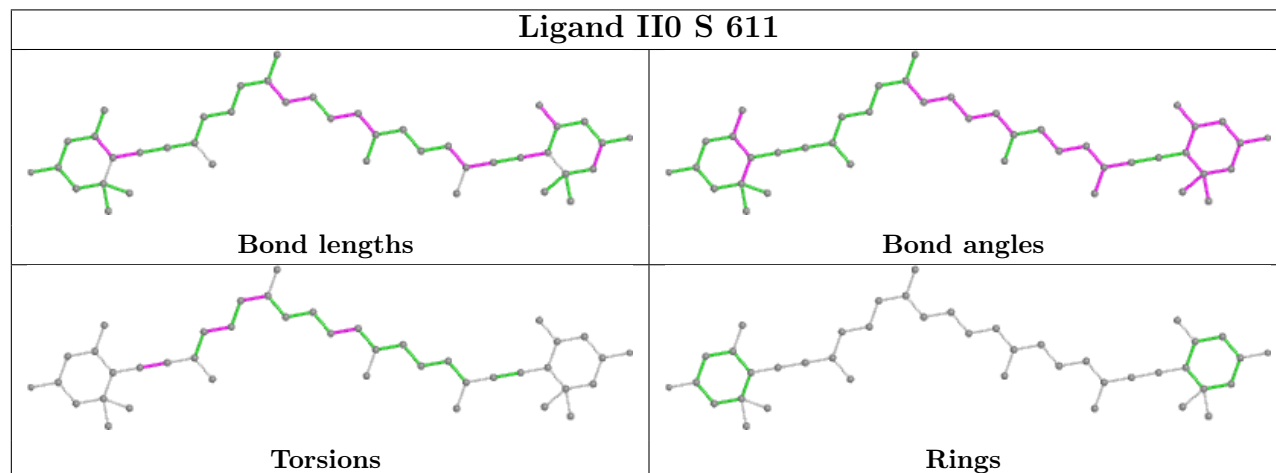
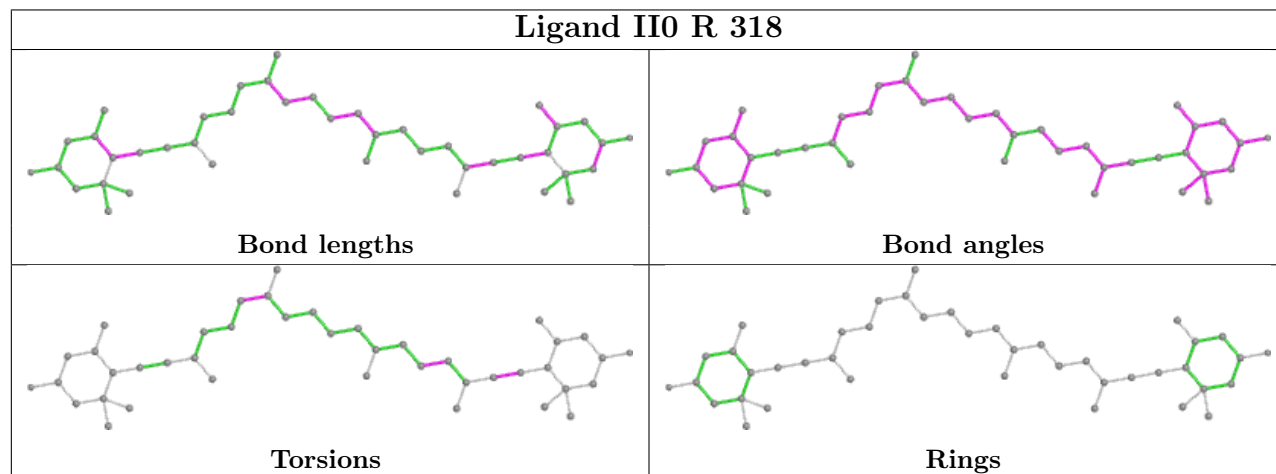
**Ligand CLA B 603****Ligand CLA O 606**

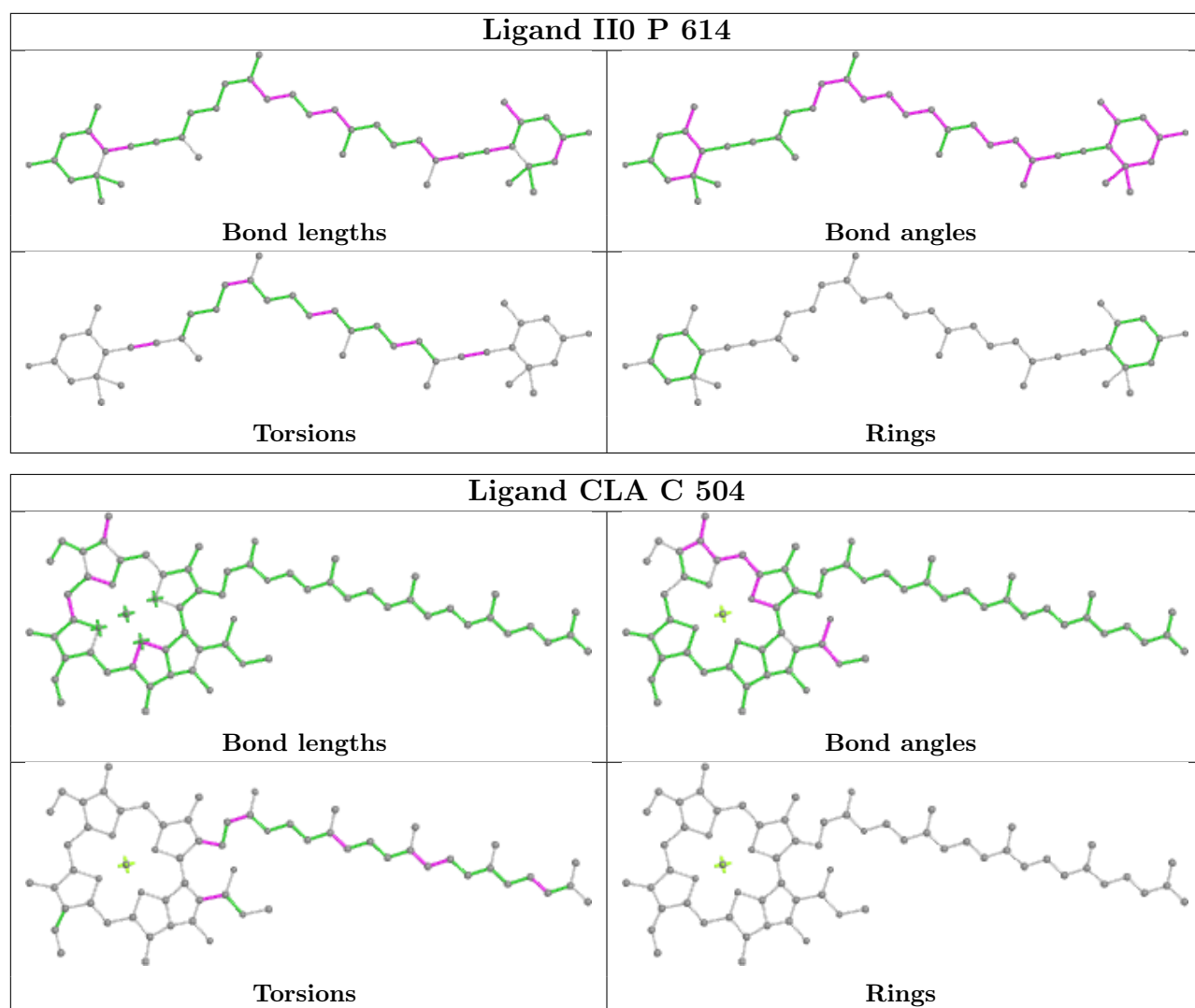
## Ligand CLA R 312



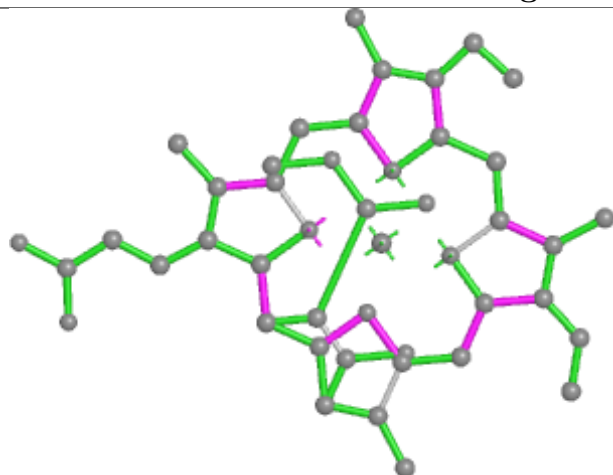
## Ligand CLA c 507



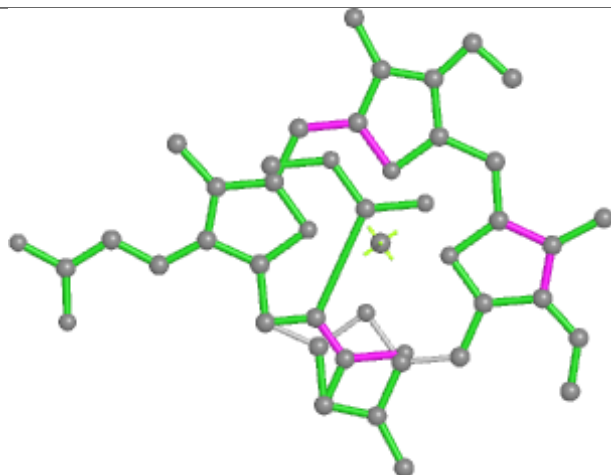
**Ligand CLA C 505****Ligand II0 S 611****Ligand II0 R 318**



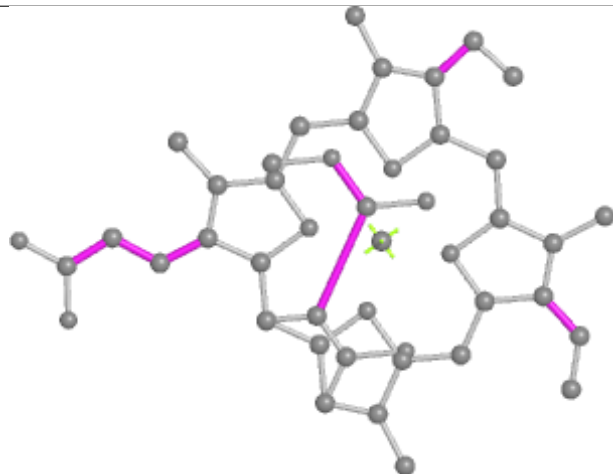
## Ligand KC2 1 610



Bond lengths



Bond angles

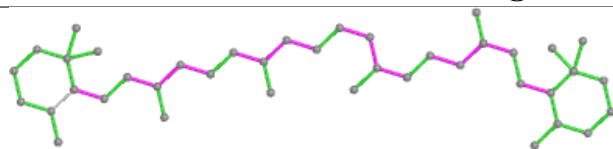


Torsions

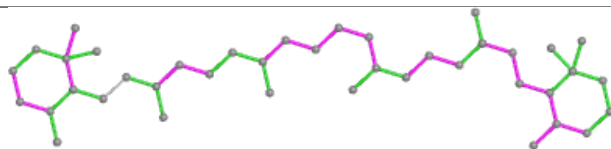


Rings

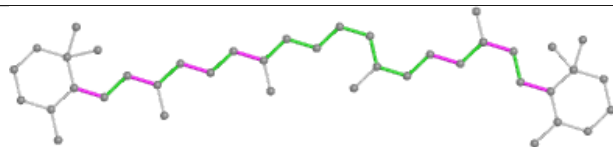
## Ligand WVN S 613



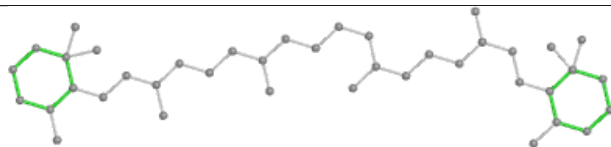
Bond lengths



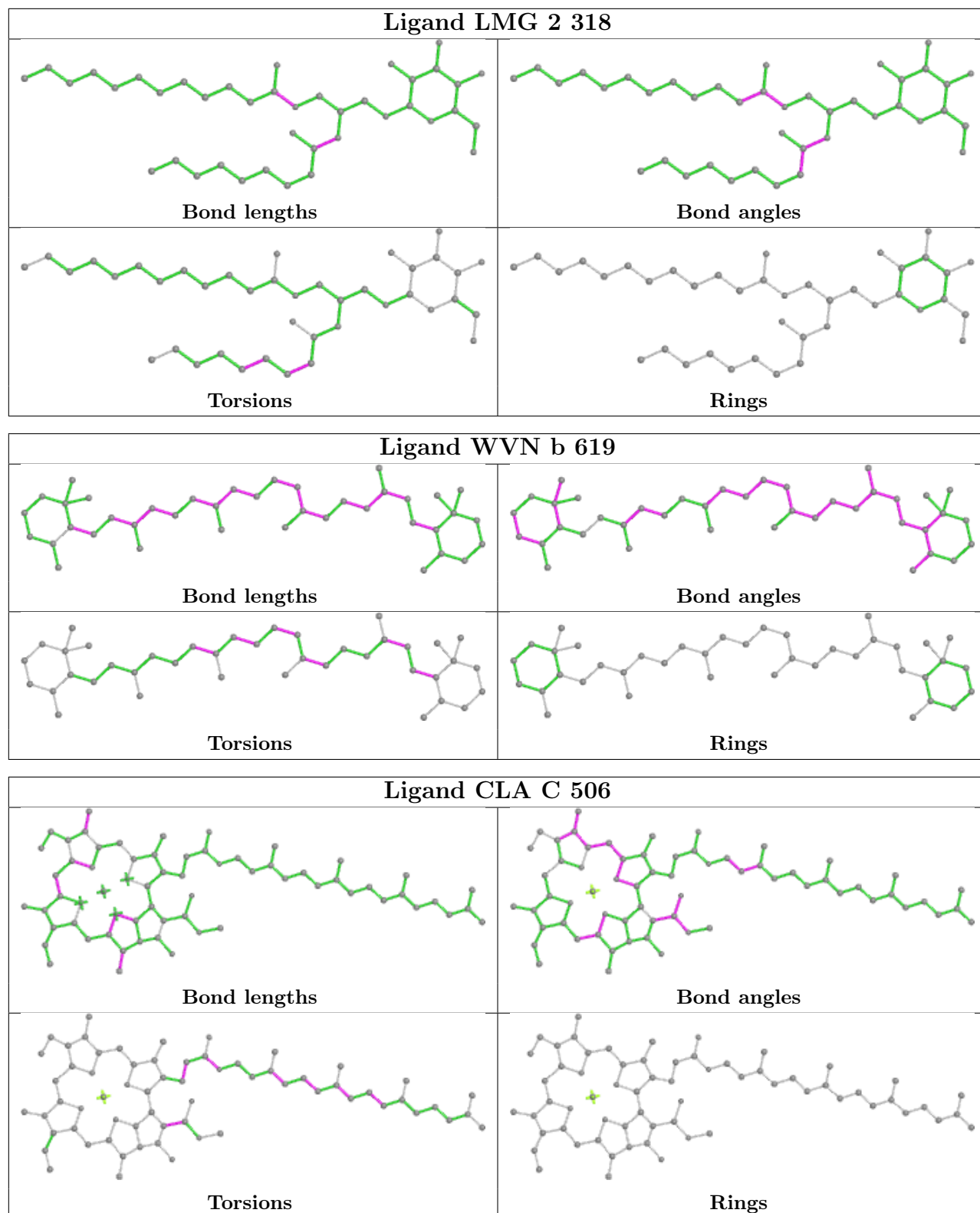
Bond angles



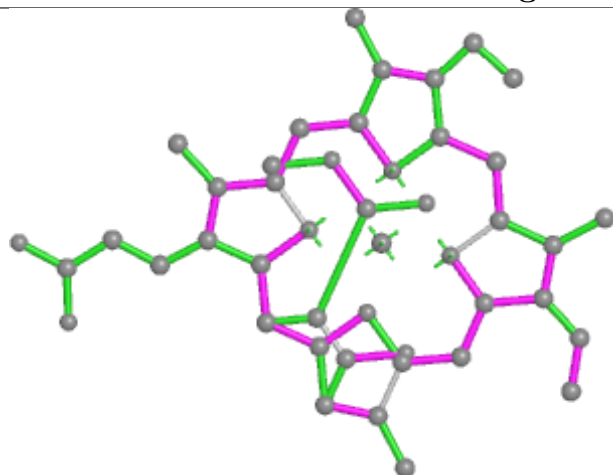
Torsions



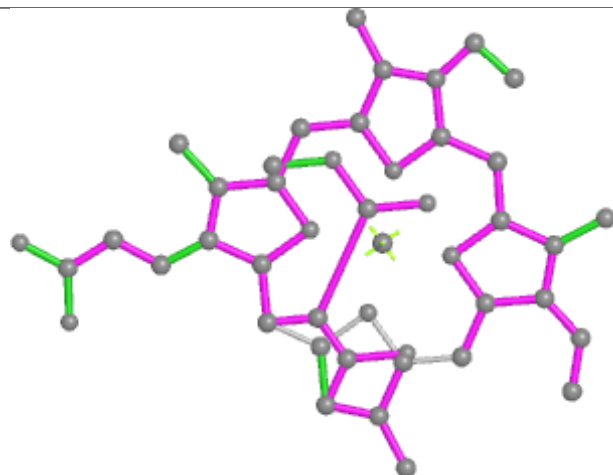
Rings



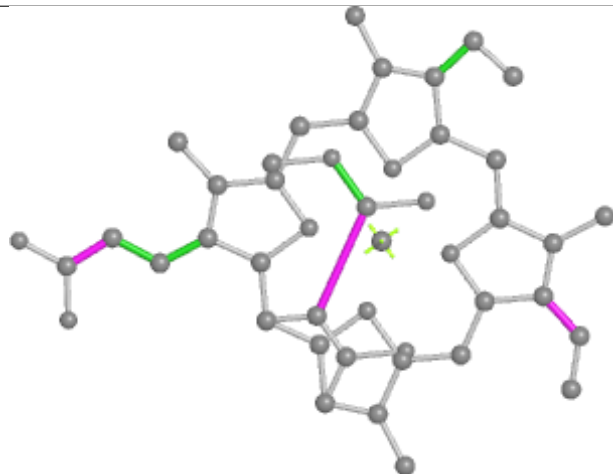
## Ligand KC2 S 608



Bond lengths



Bond angles

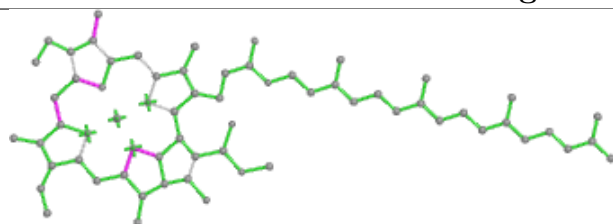


Torsions

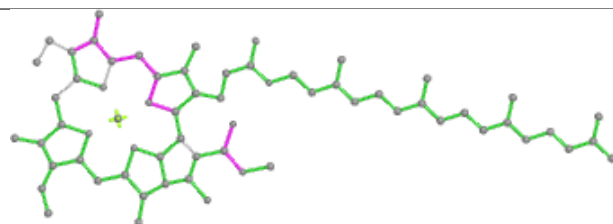


Rings

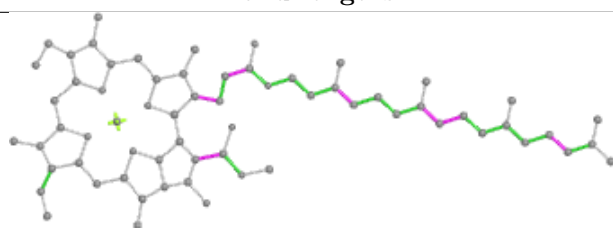
## Ligand CLA c 505



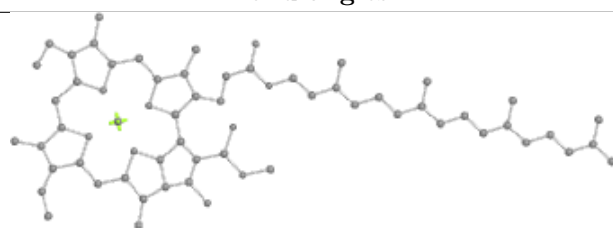
Bond lengths



Bond angles



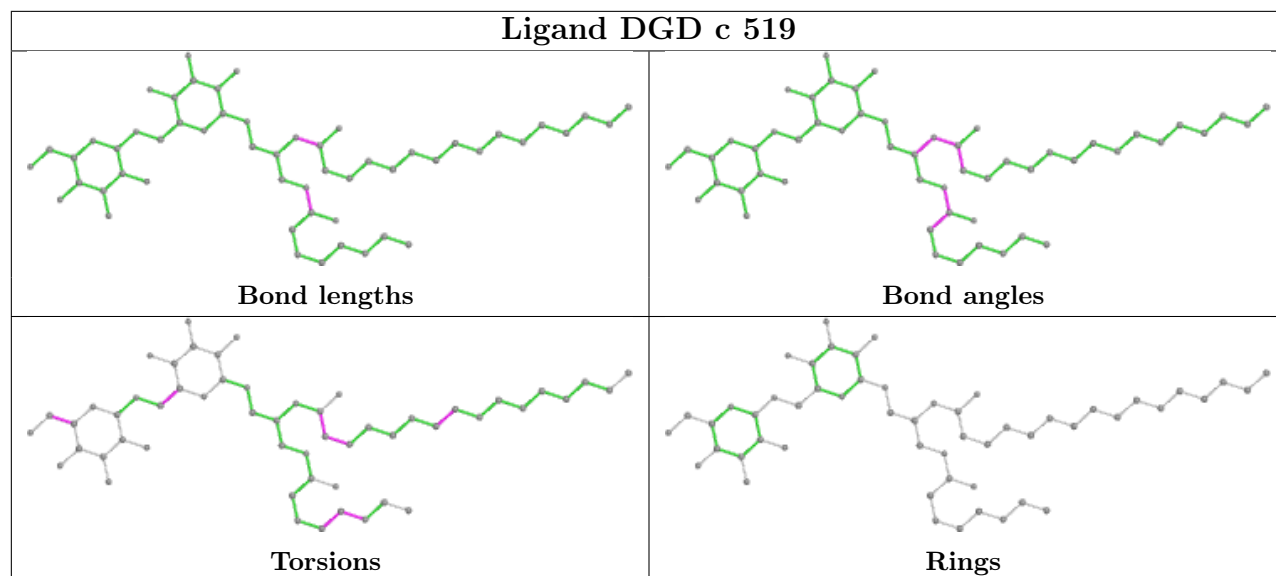
Torsions



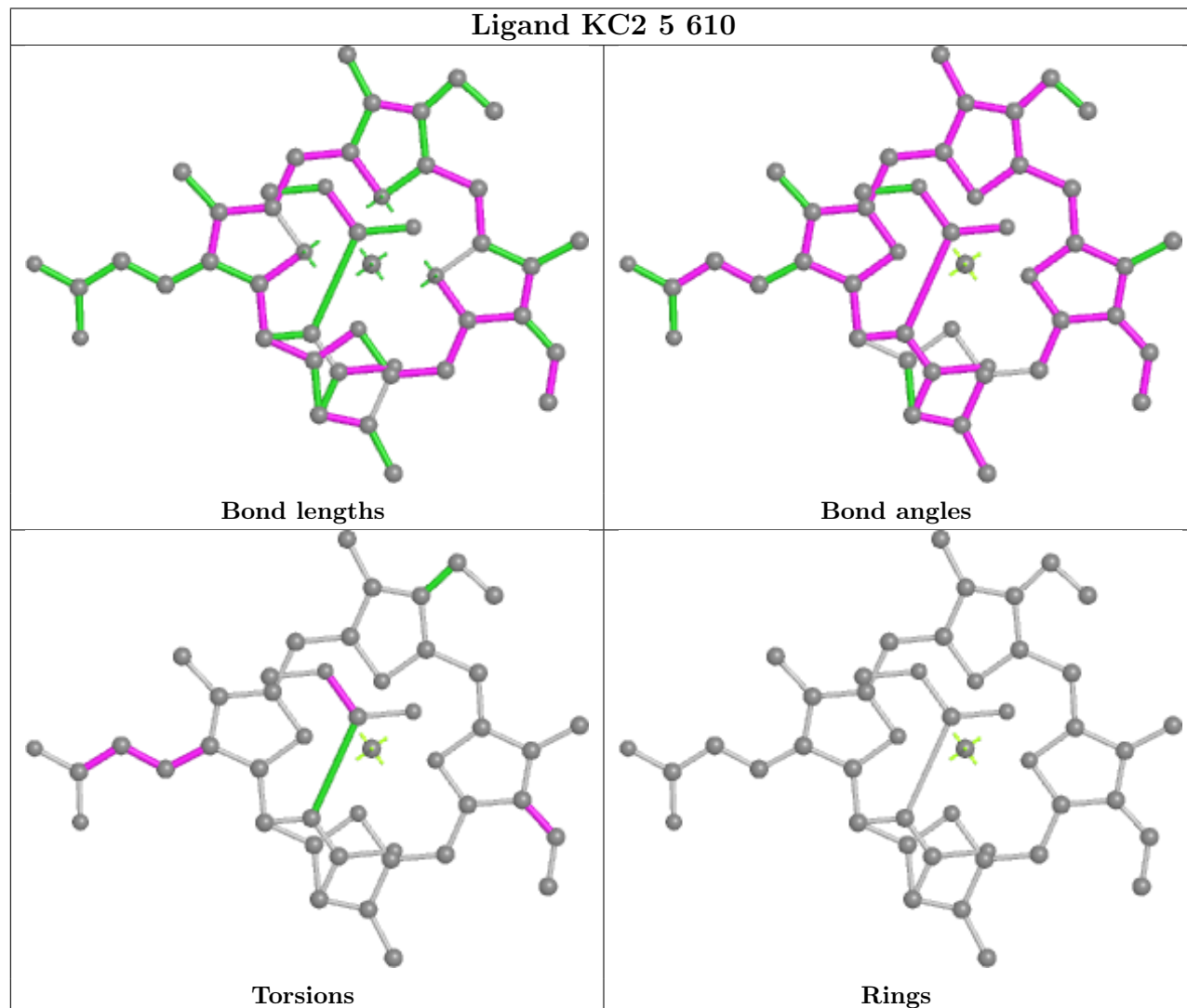
Rings

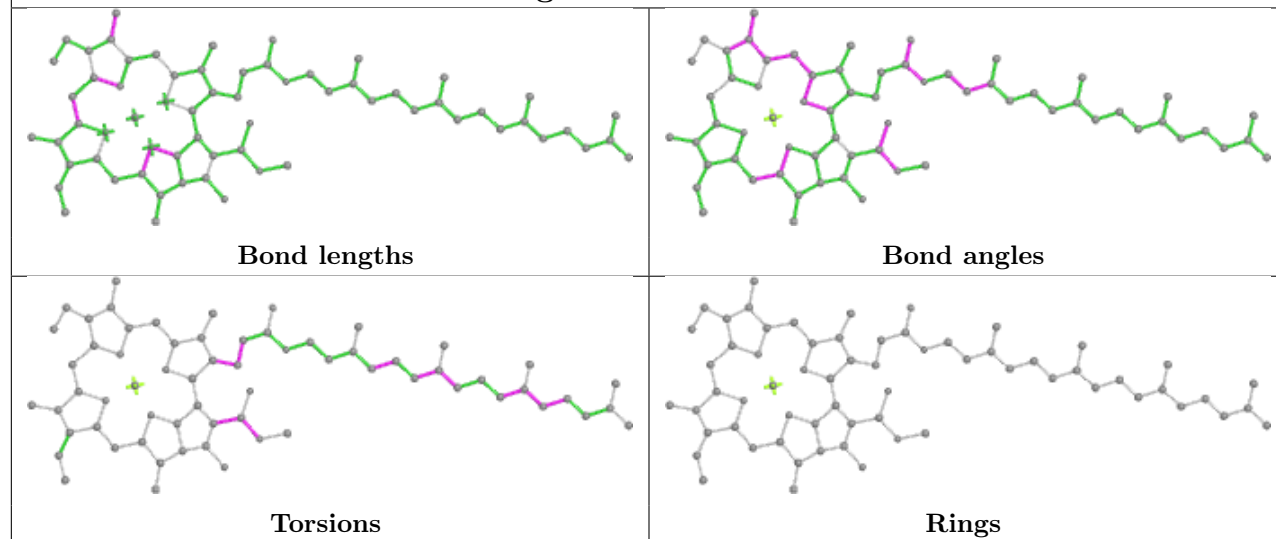
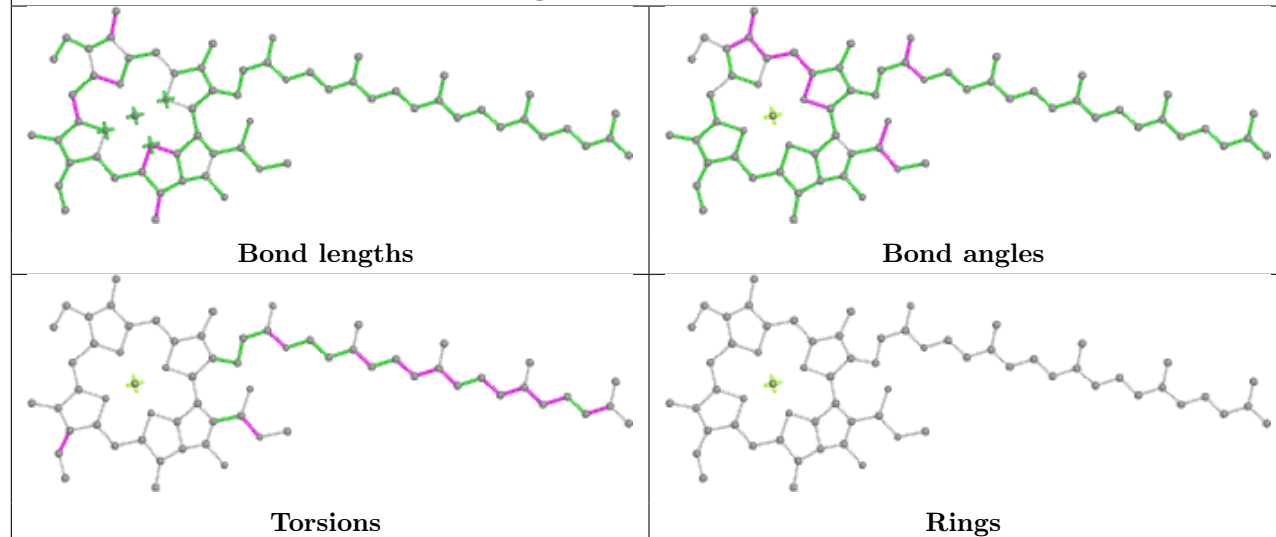


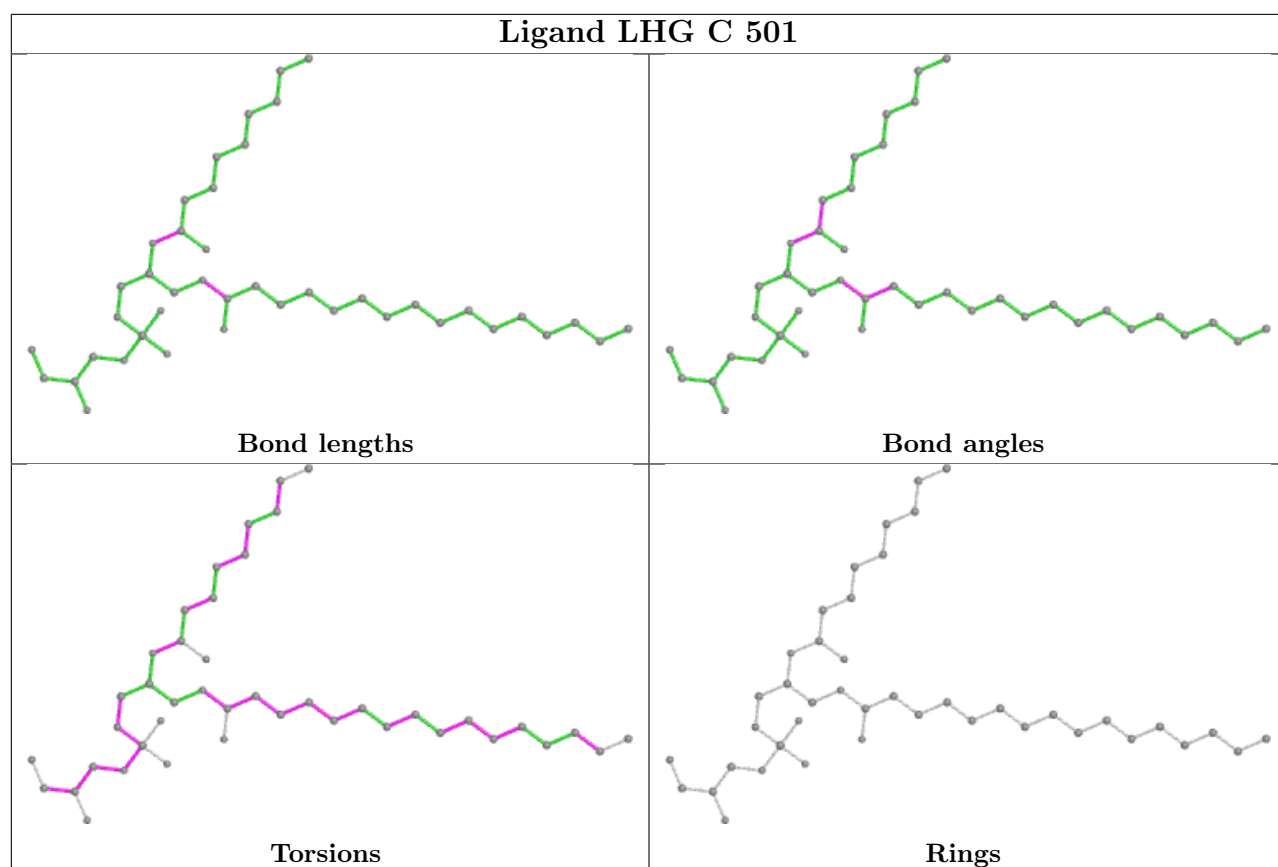
## Ligand DGD c 519



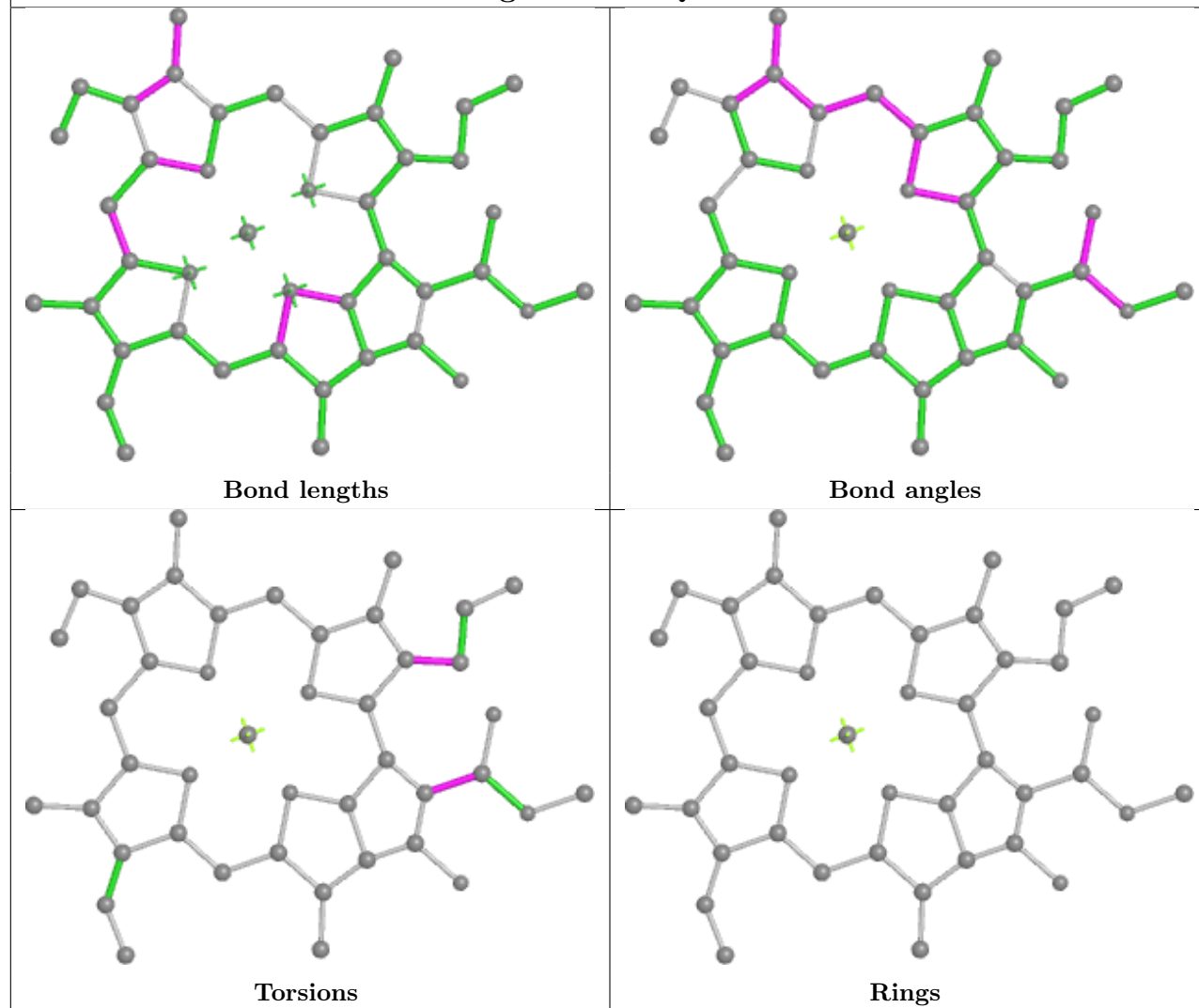
## Ligand KC2 5 610

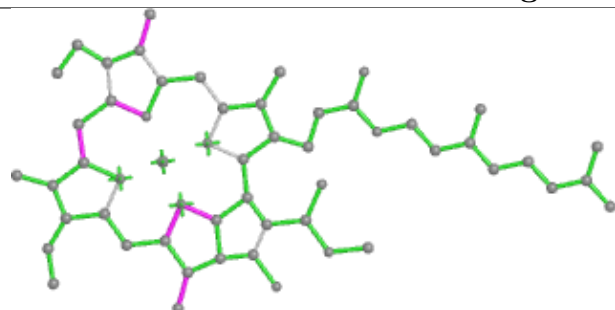
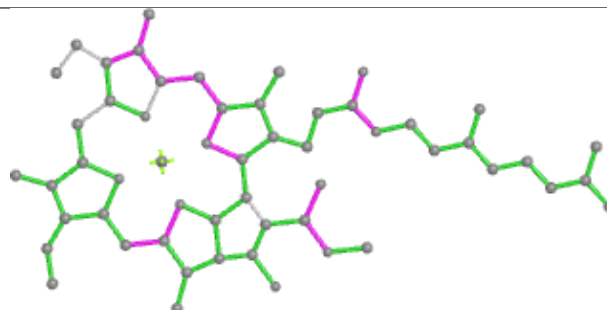
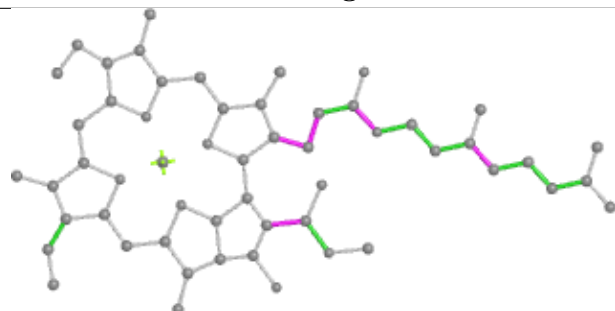
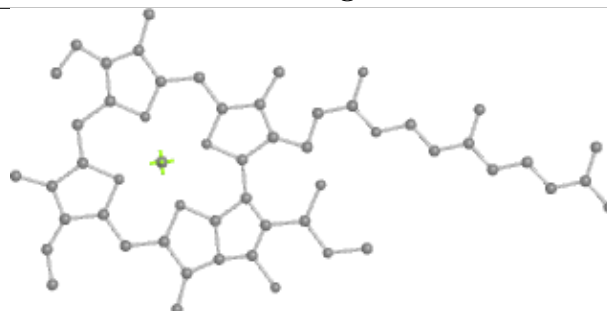
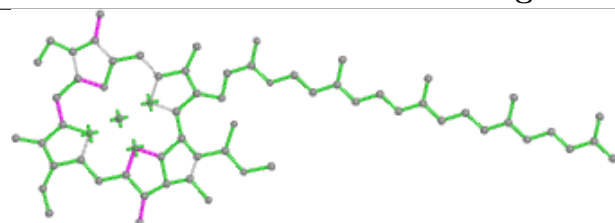
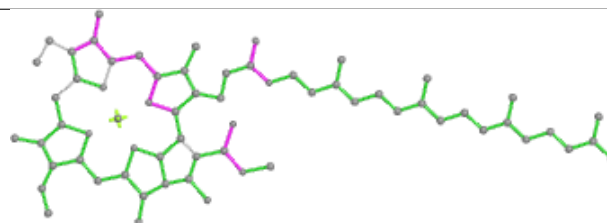
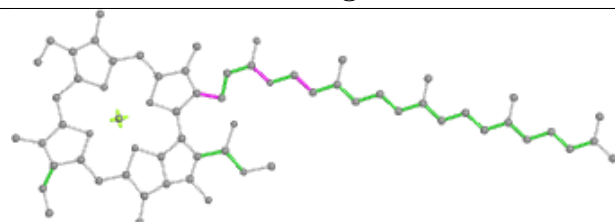
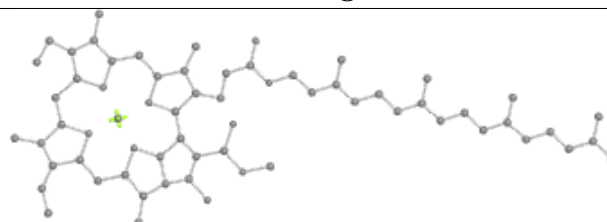


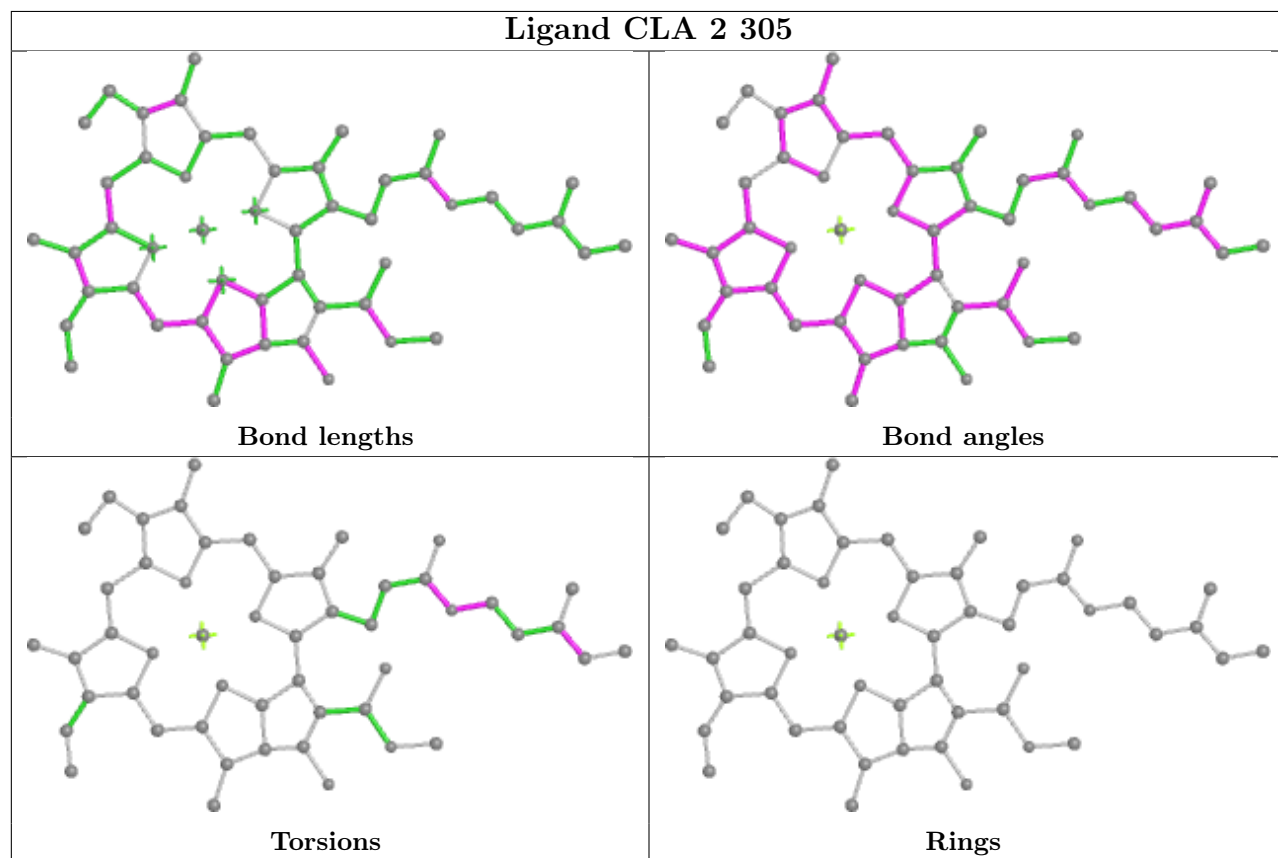
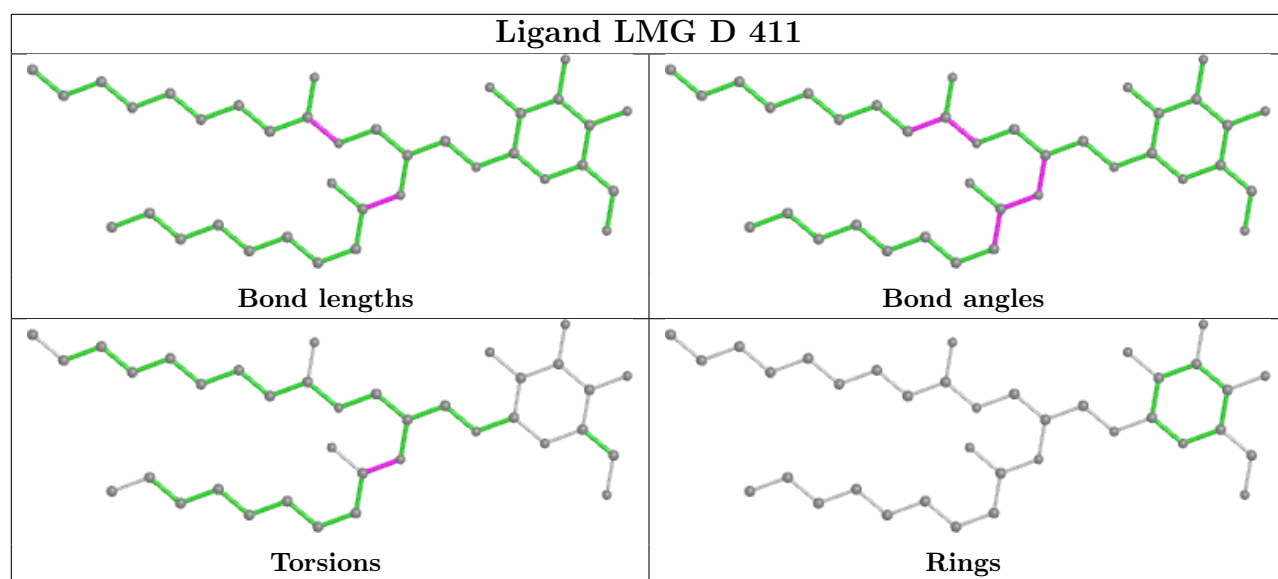
**Ligand CLA 2 302****Ligand CLA G 401**

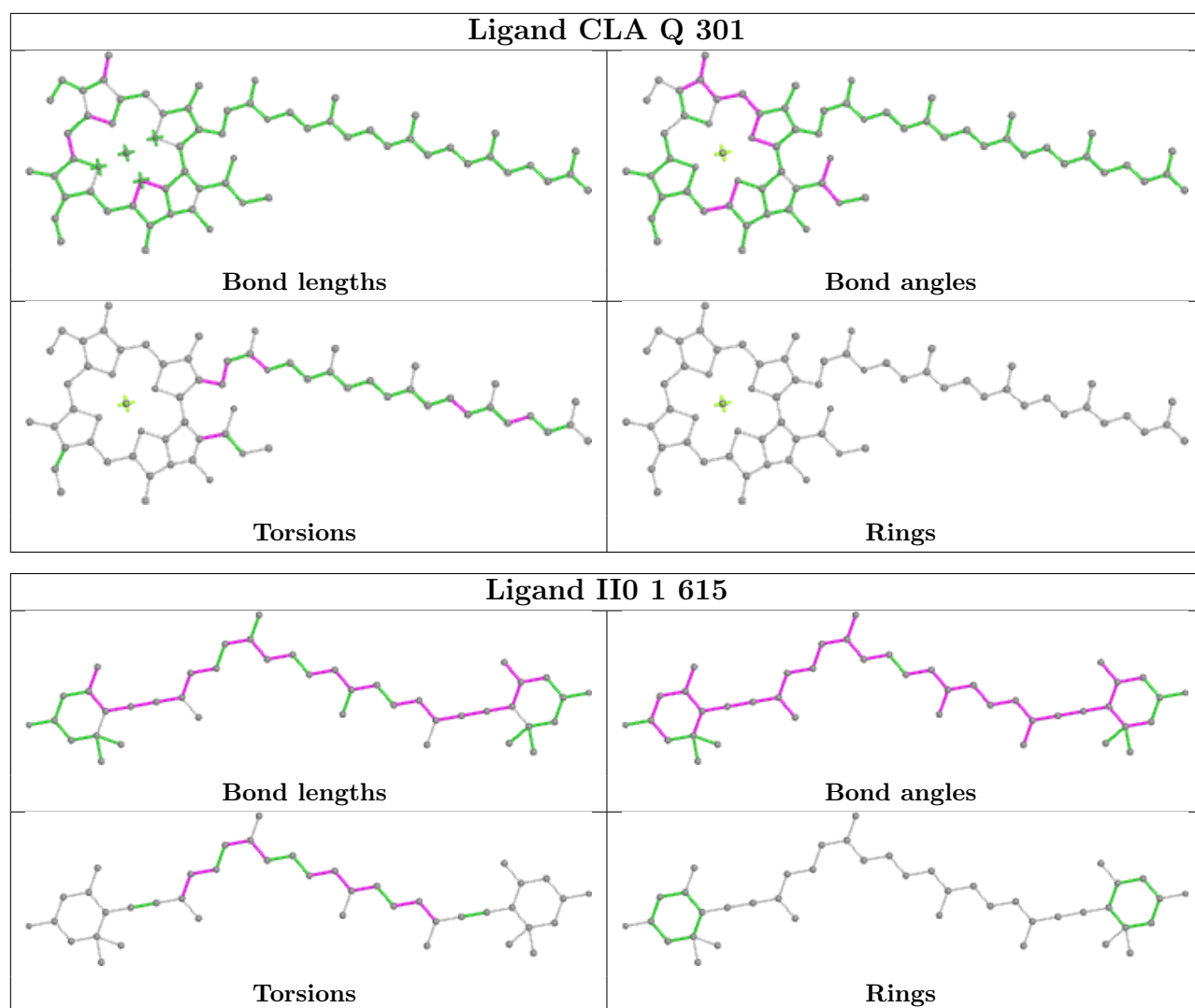


## Ligand CLA Q 306

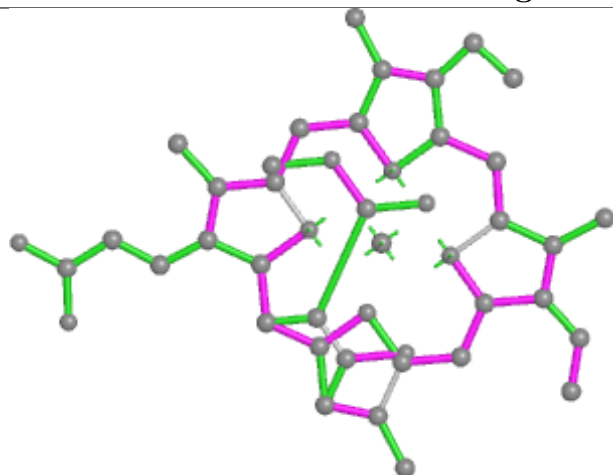


**Ligand CLA 4 306****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA D 407****Bond lengths****Bond angles****Torsions****Rings**

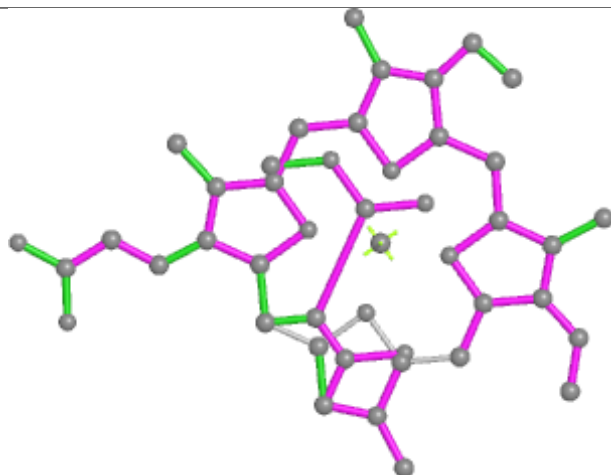




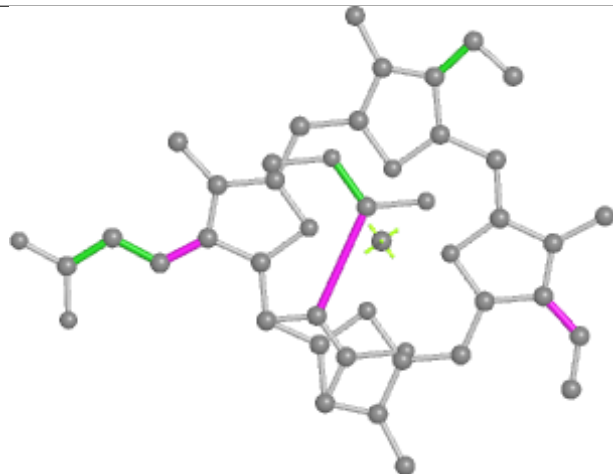
## Ligand KC2 N 611



Bond lengths



Bond angles

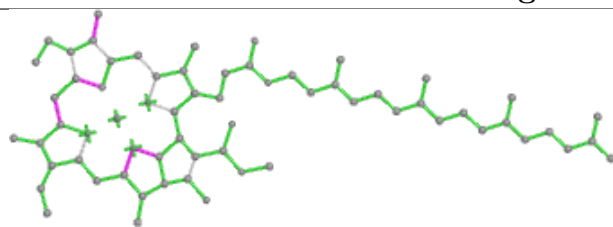


Torsions

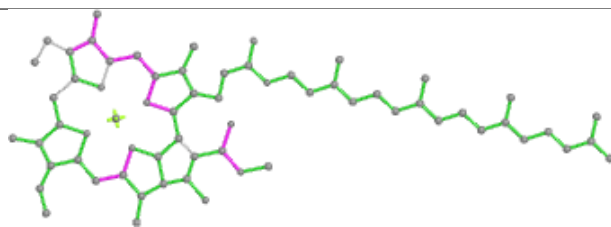


Rings

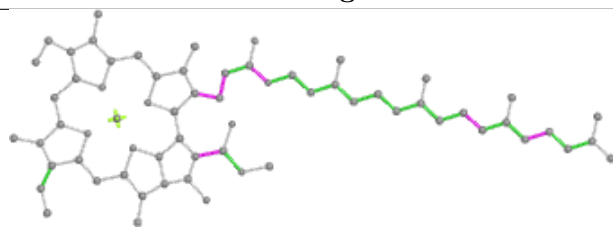
## Ligand CLA 4 302



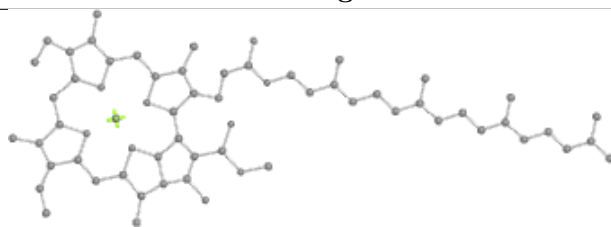
Bond lengths



Bond angles



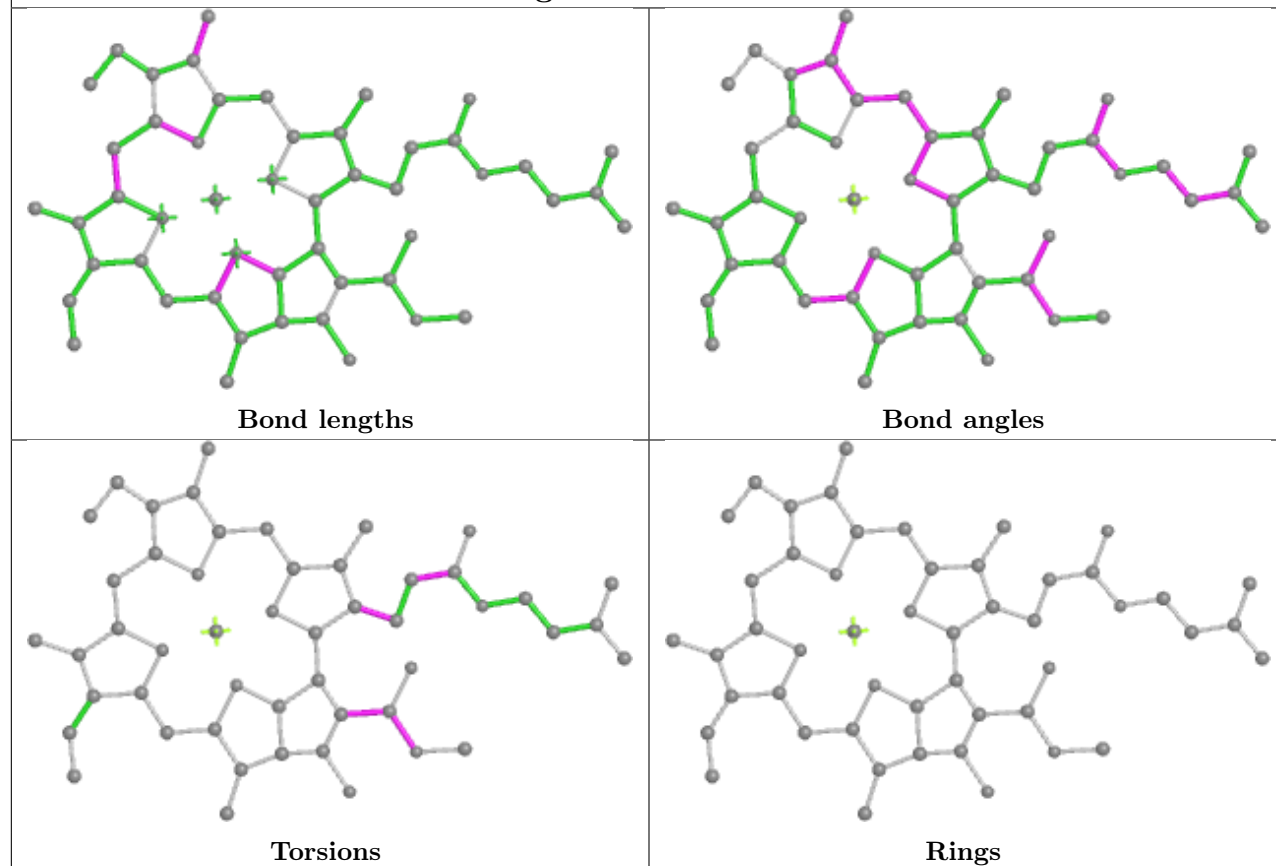
Torsions



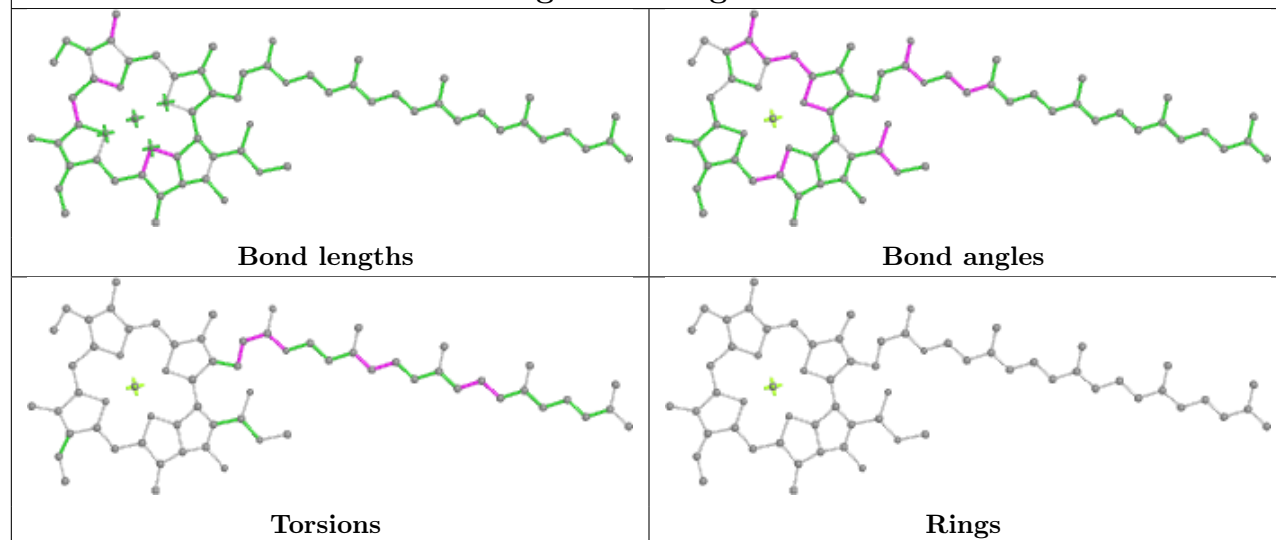
Rings

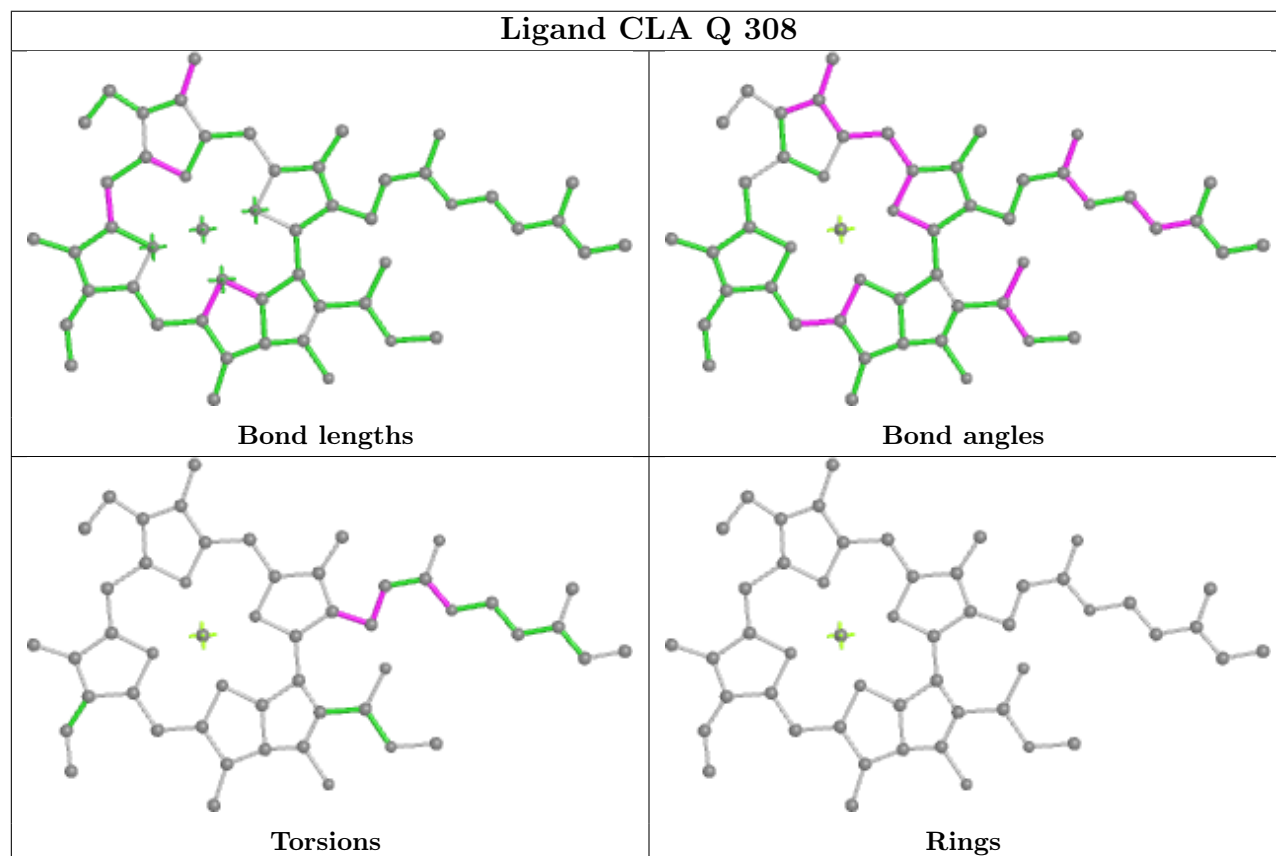
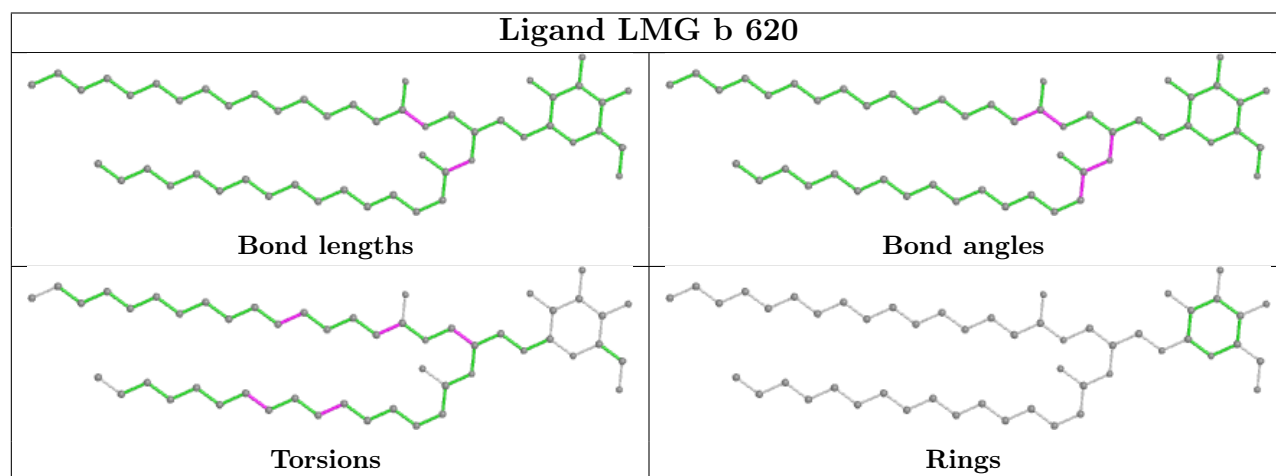
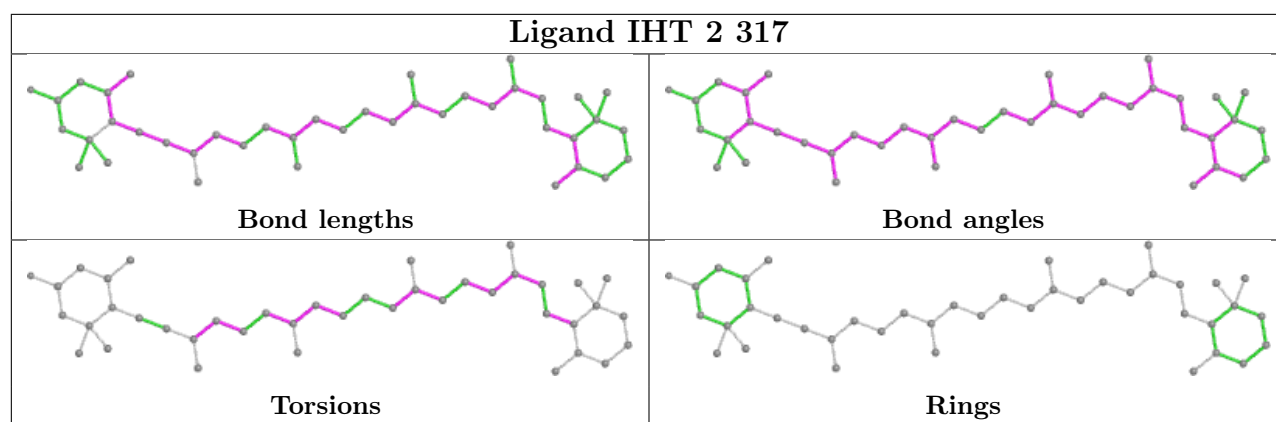


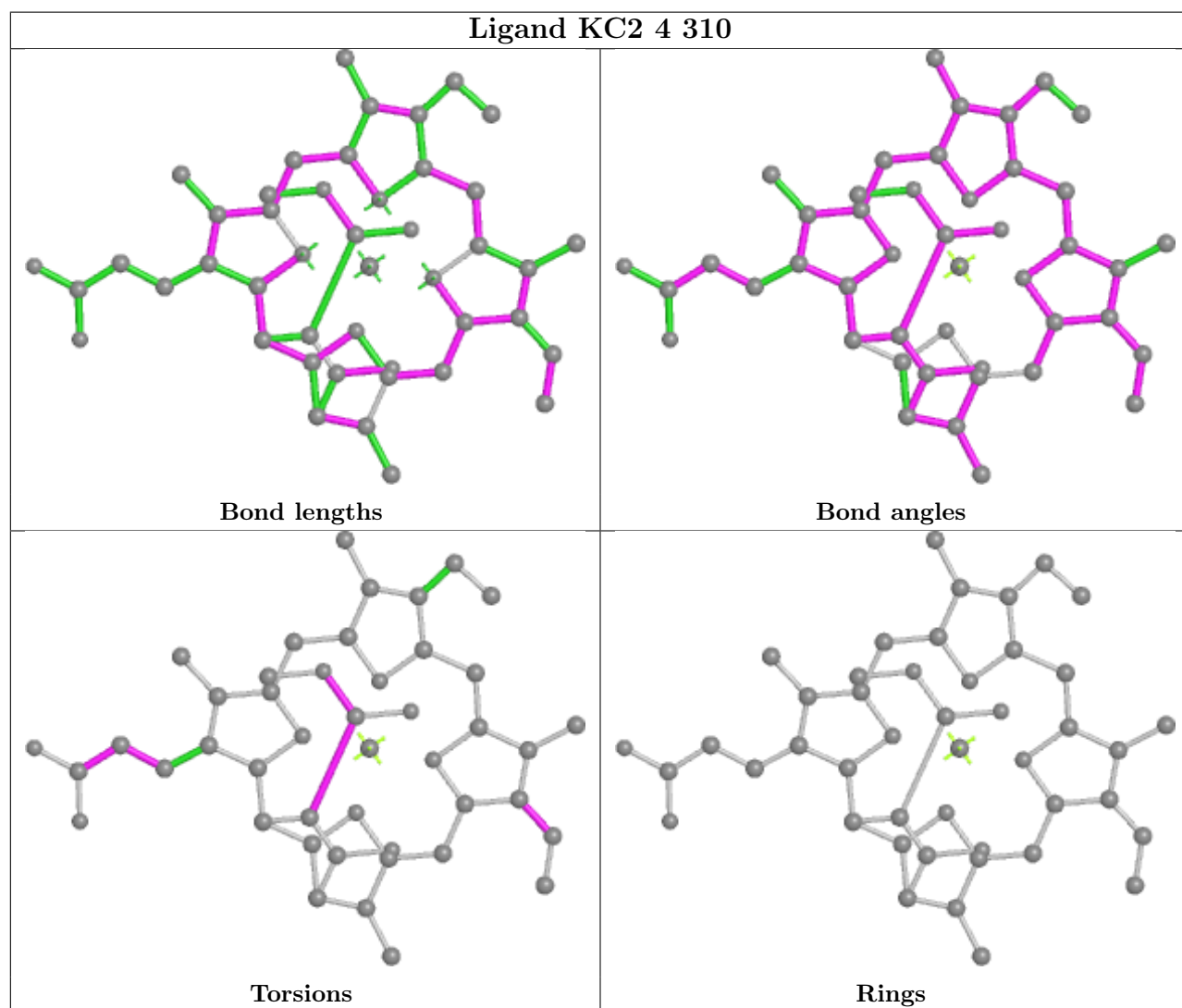
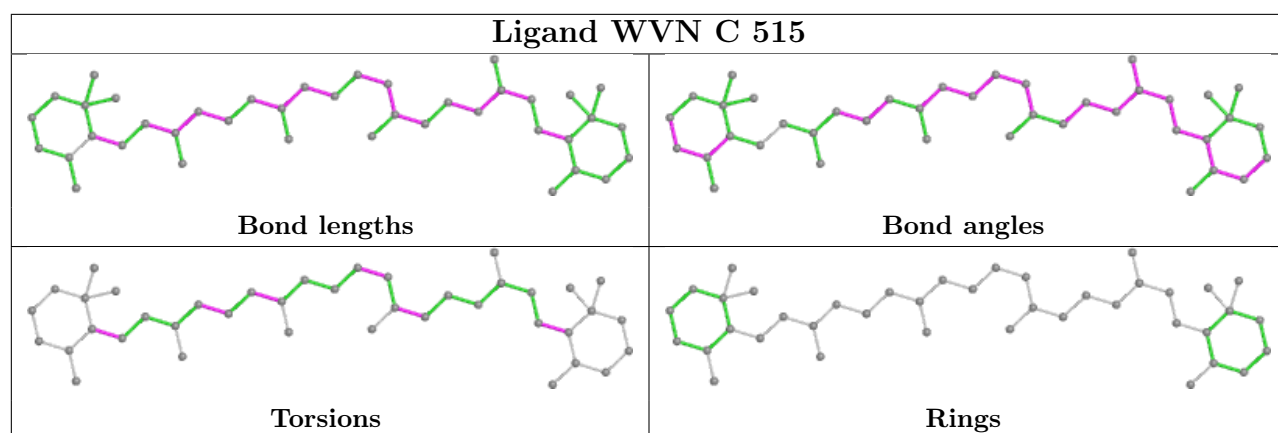
## Ligand CLA b 601

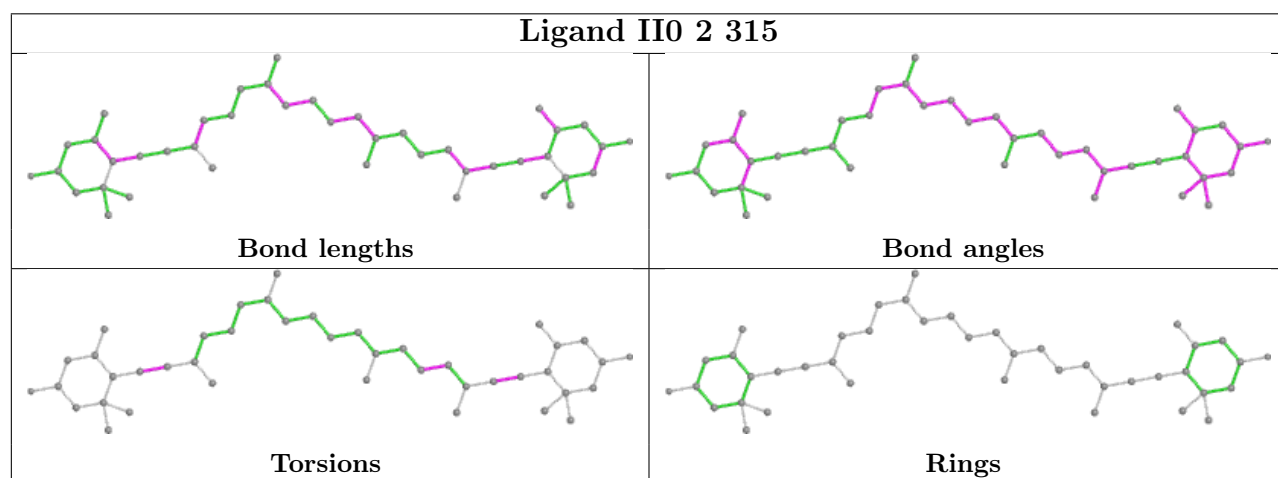
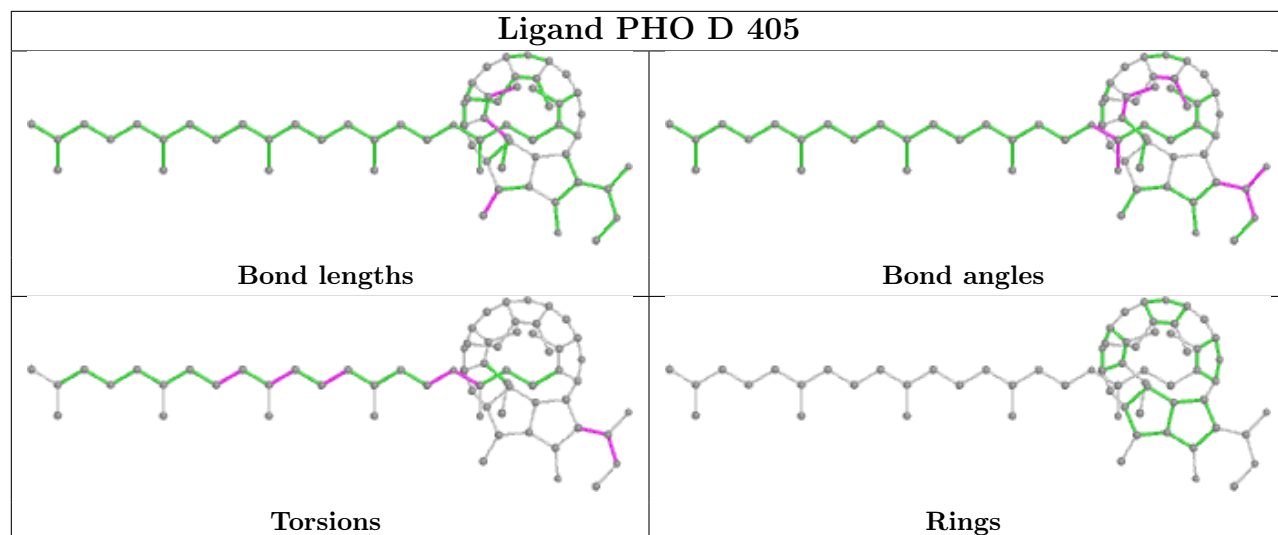


## Ligand CLA g 401

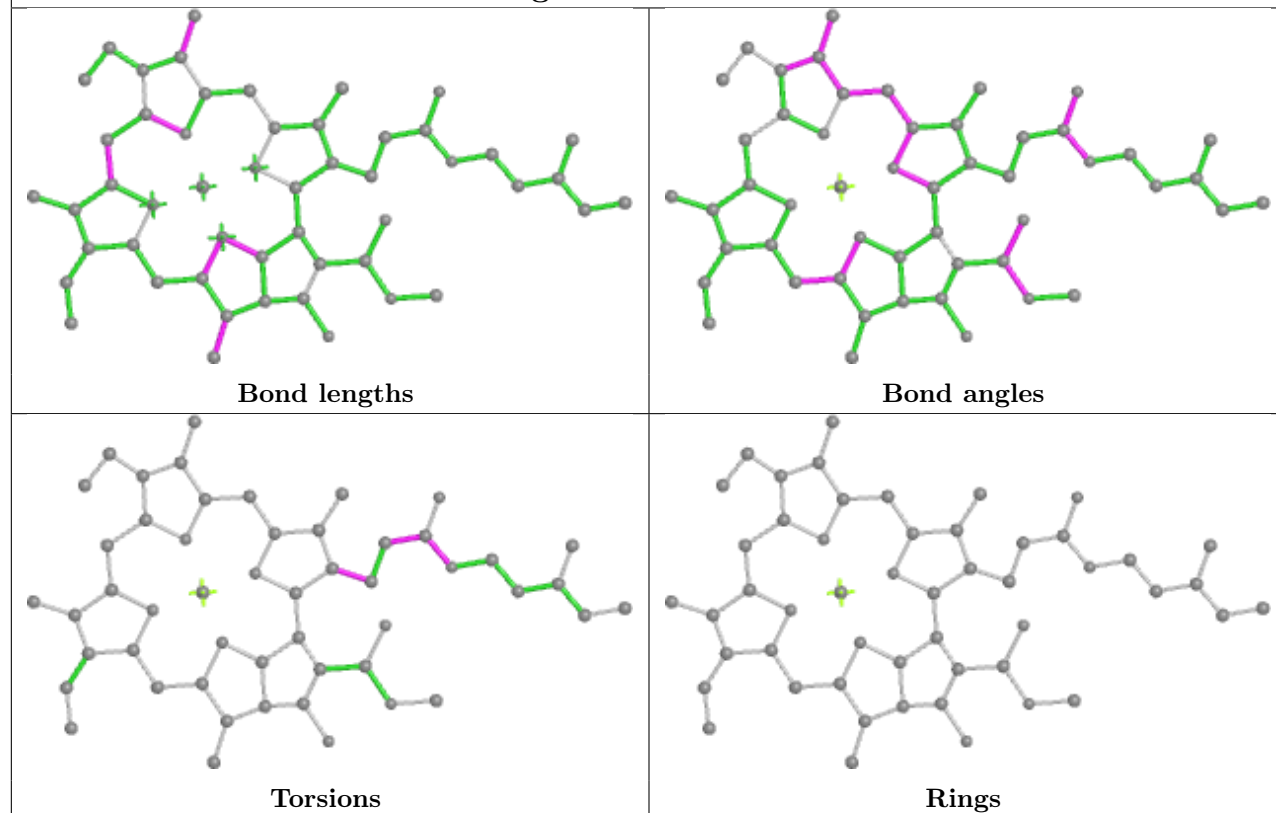




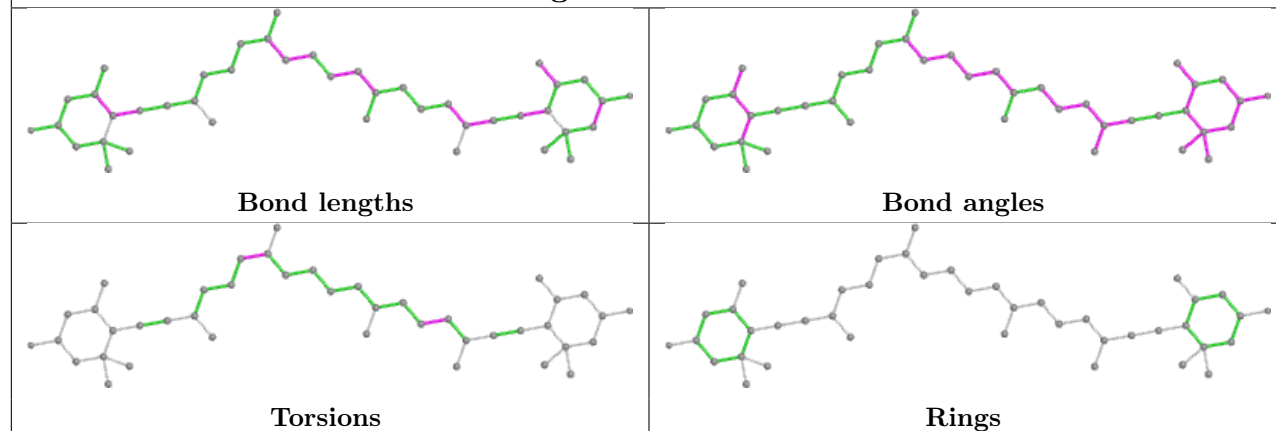


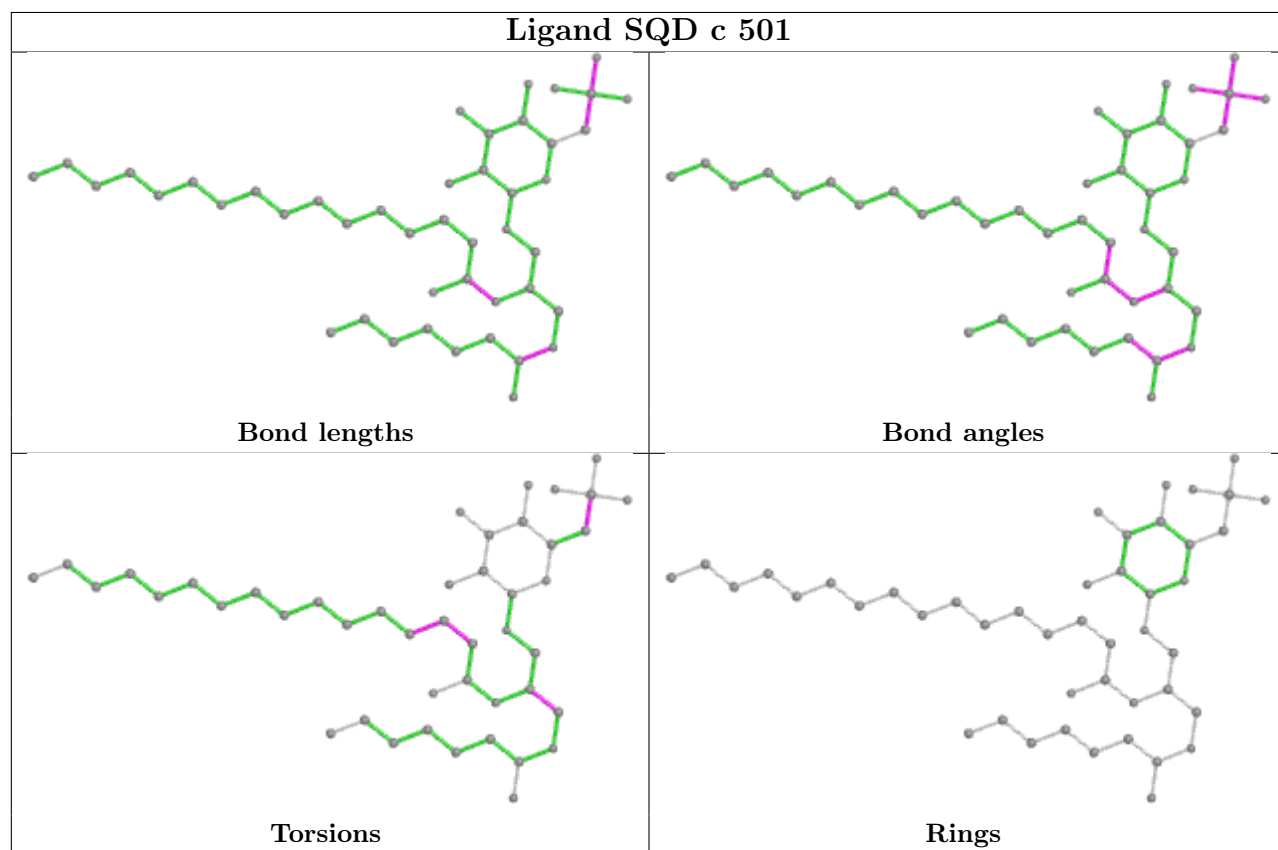
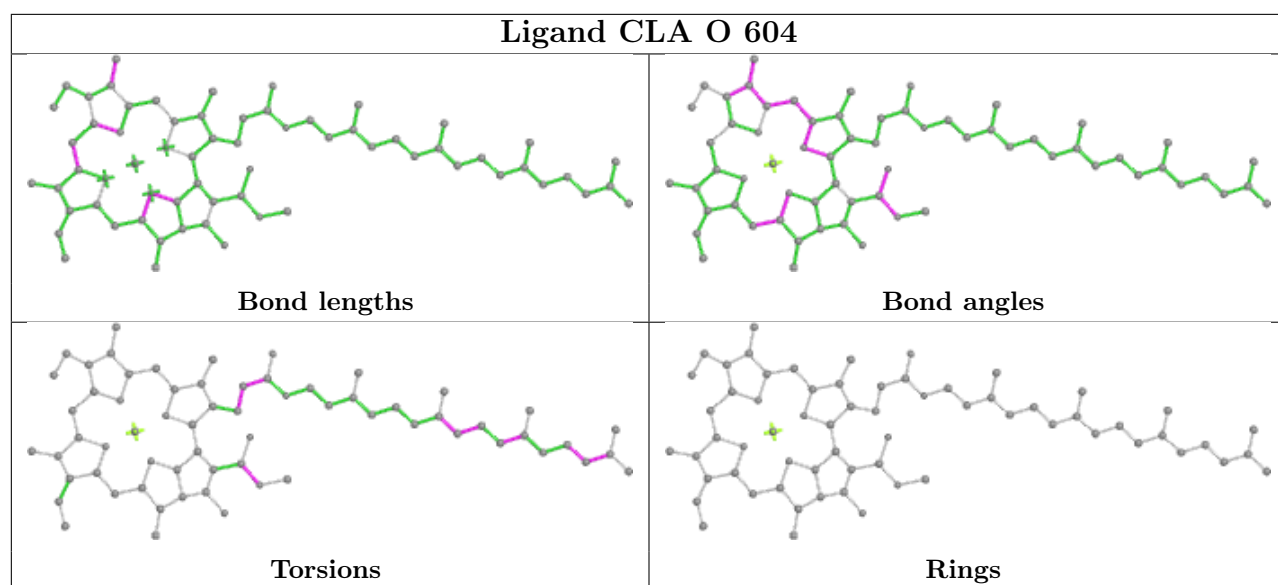


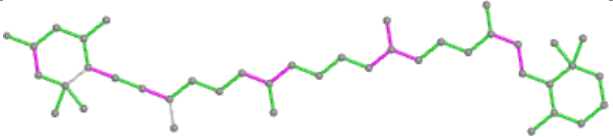
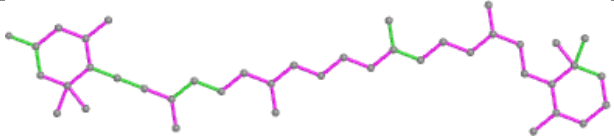
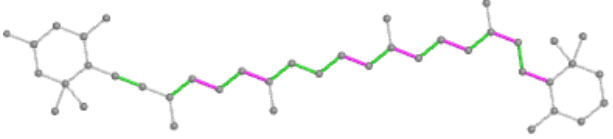
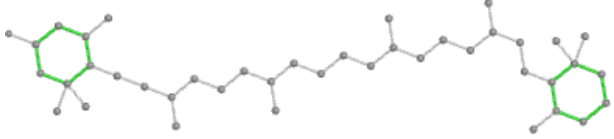
## Ligand CLA O 605

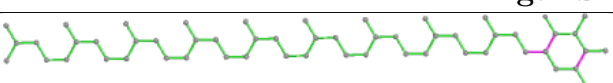
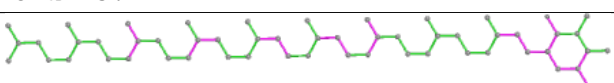
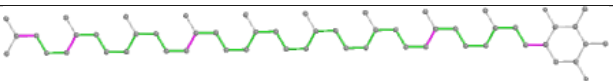
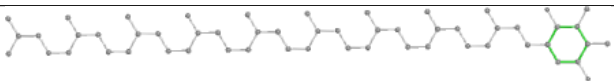


## Ligand II0 5 615

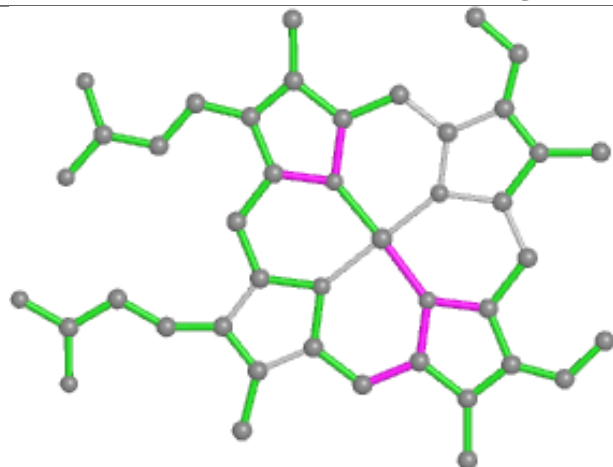




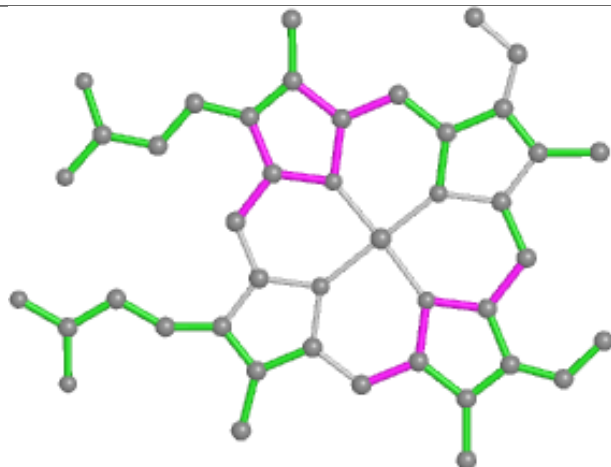
Ligand IHT 5 616	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand PL9 d 407	
	Bond lengths
	Bond angles
	Torsions
	Rings

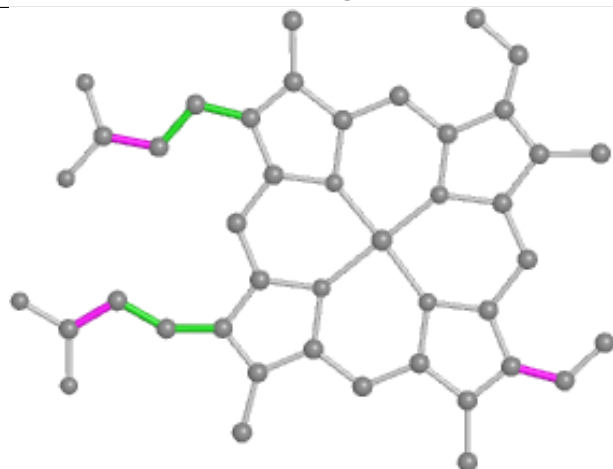
## Ligand HEM f 101



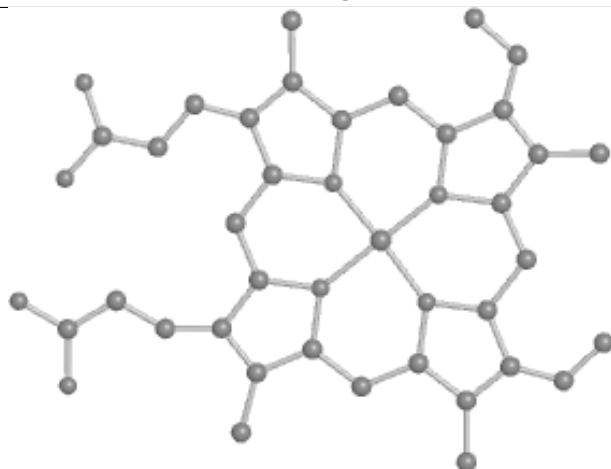
Bond lengths



Bond angles

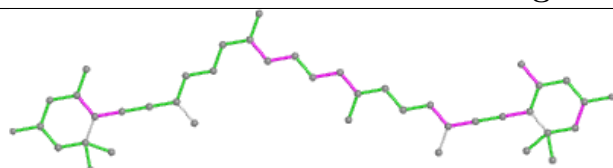


Torsions

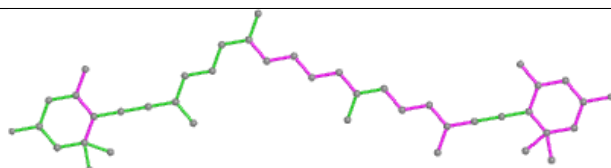


Rings

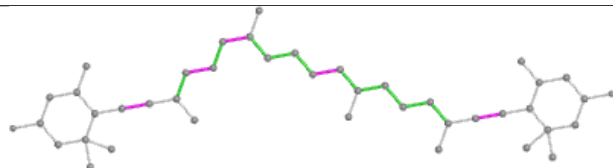
## Ligand II0 6 611



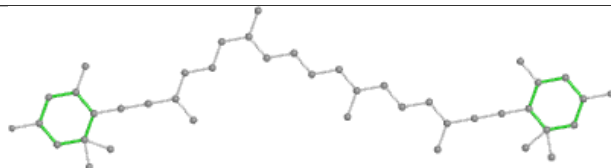
Bond lengths



Bond angles



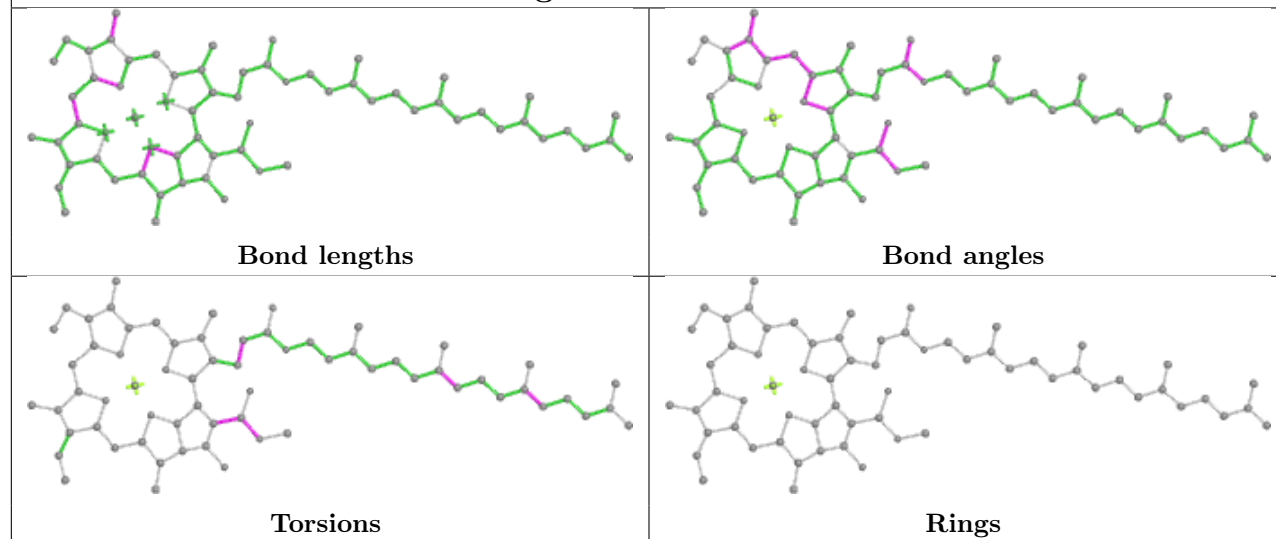
Torsions



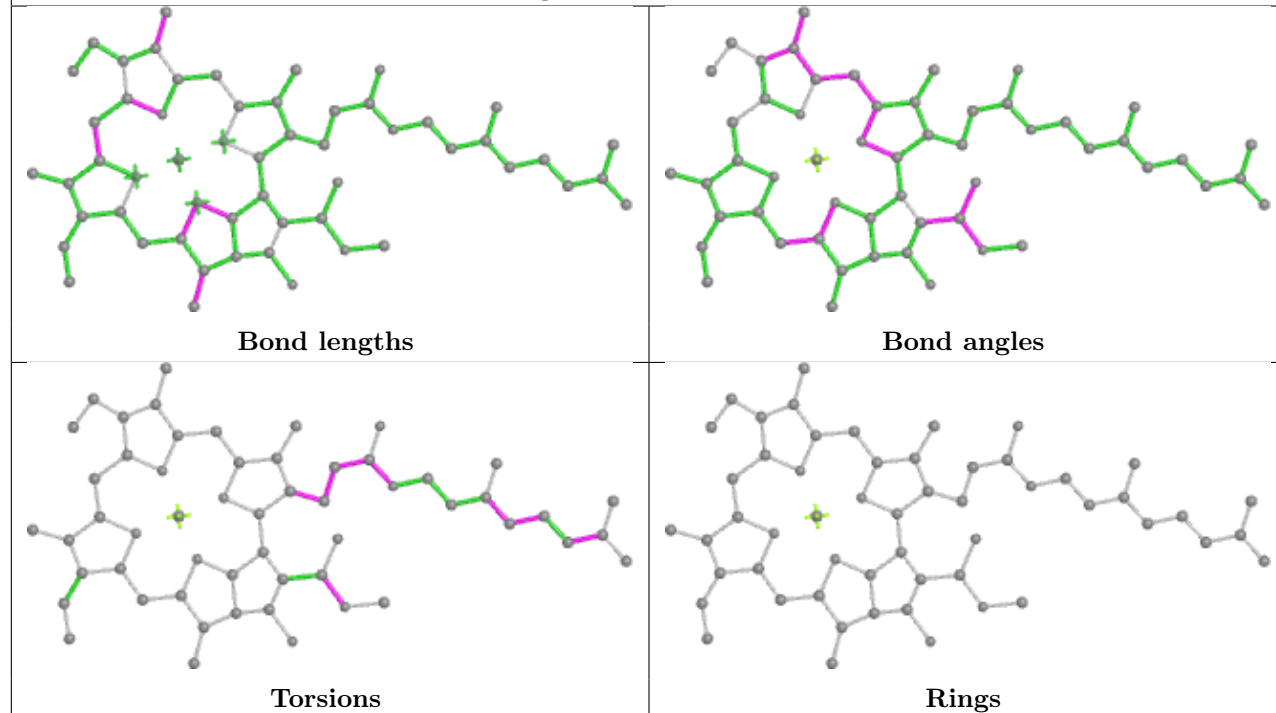
Rings

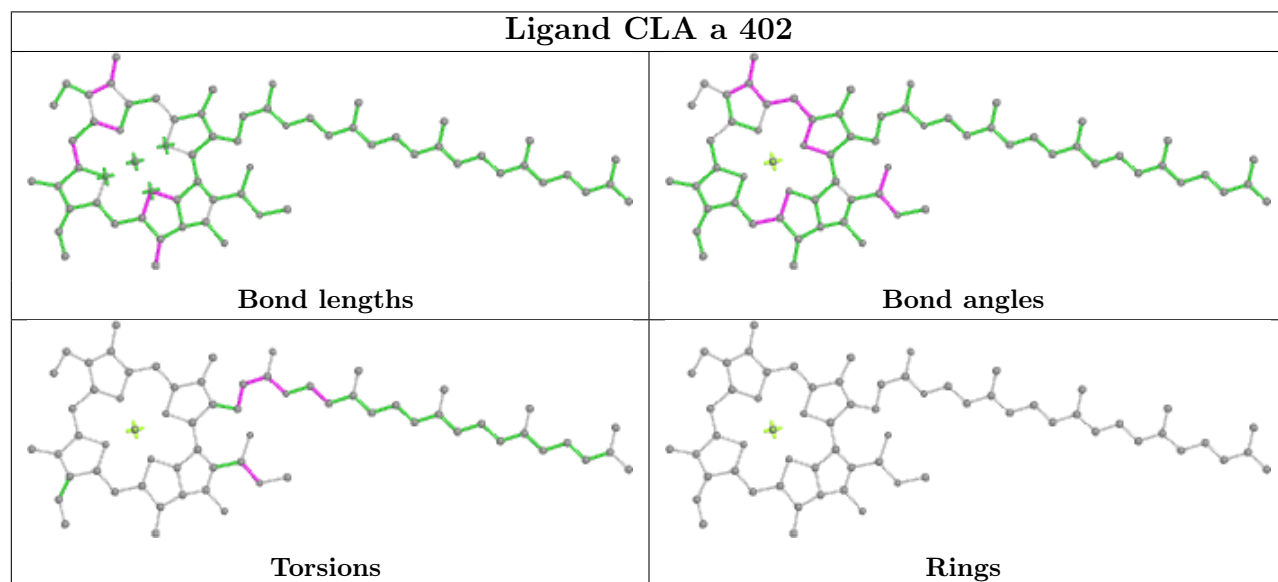
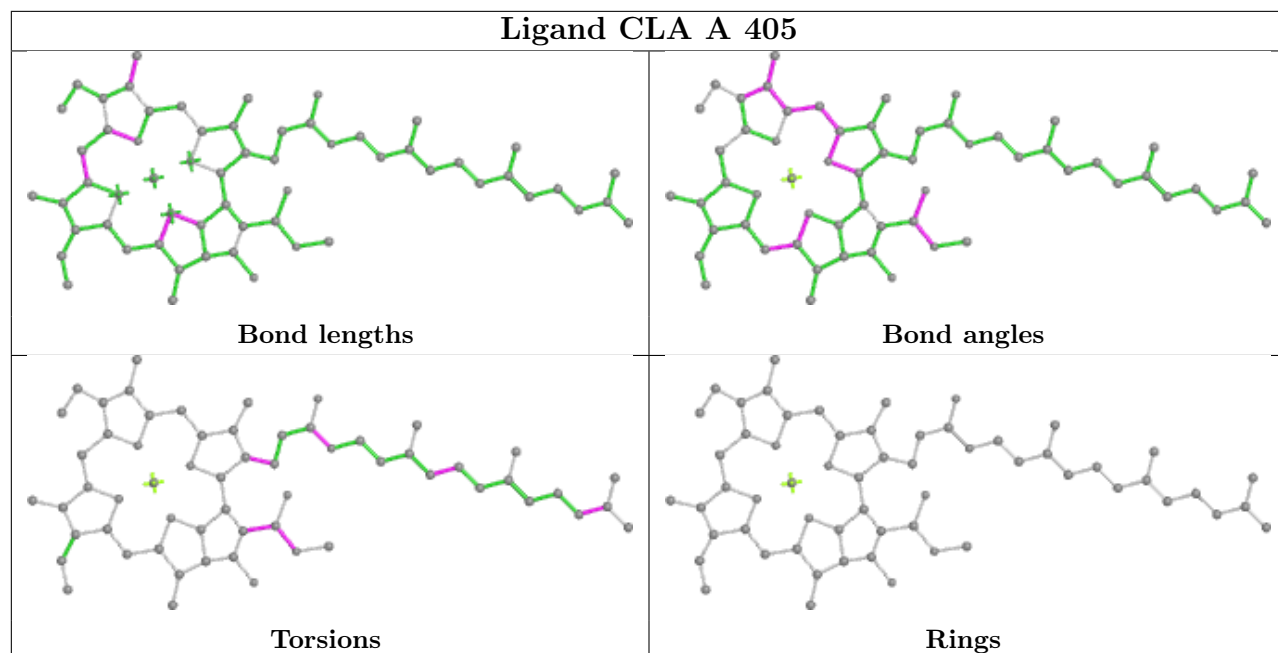


## Ligand CLA b 608

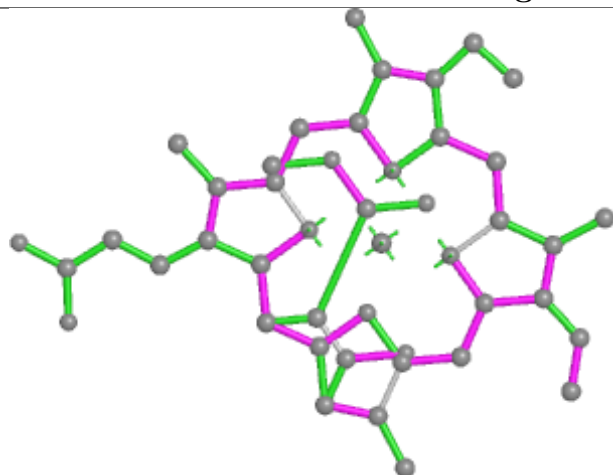


## Ligand CLA 6 605

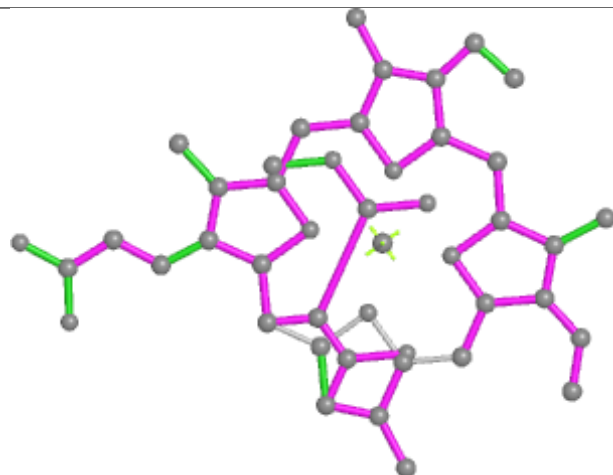




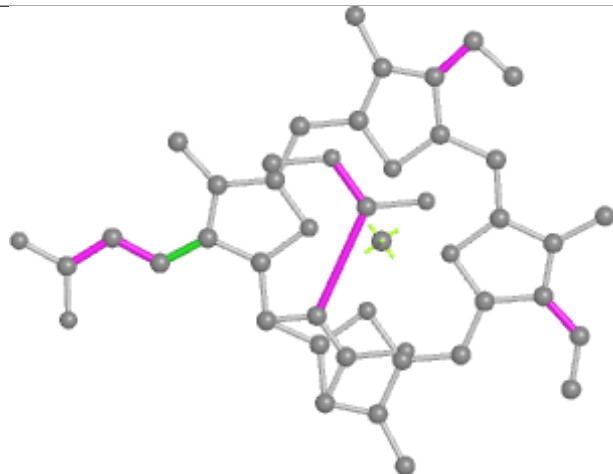
## Ligand KC2 N 612



Bond lengths



Bond angles

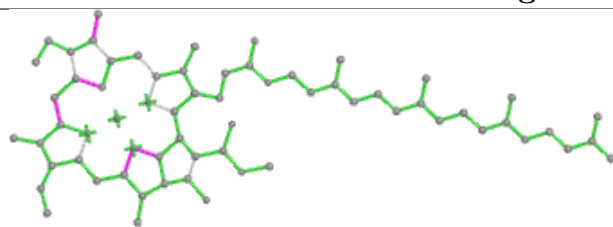


Torsions

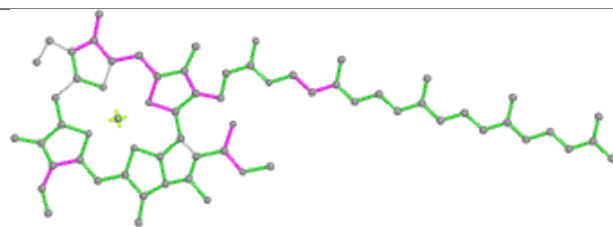


Rings

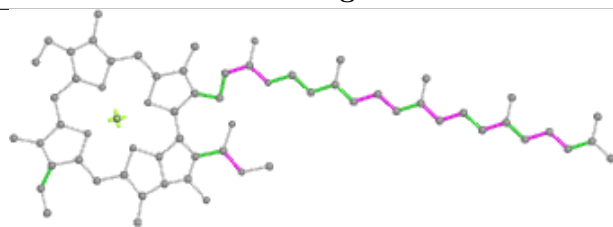
## Ligand CLA 4 303



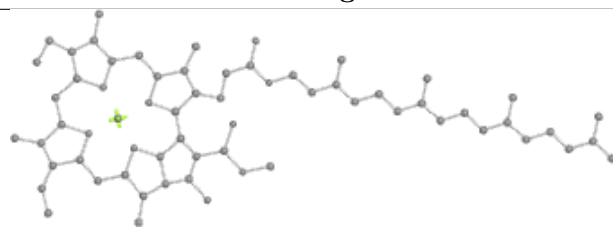
Bond lengths



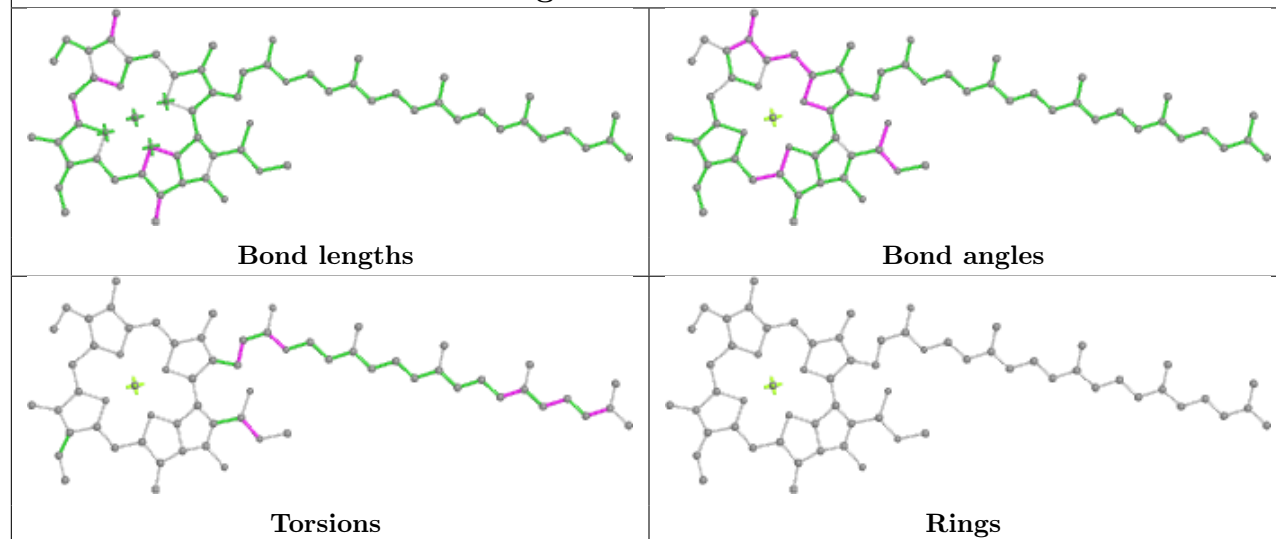
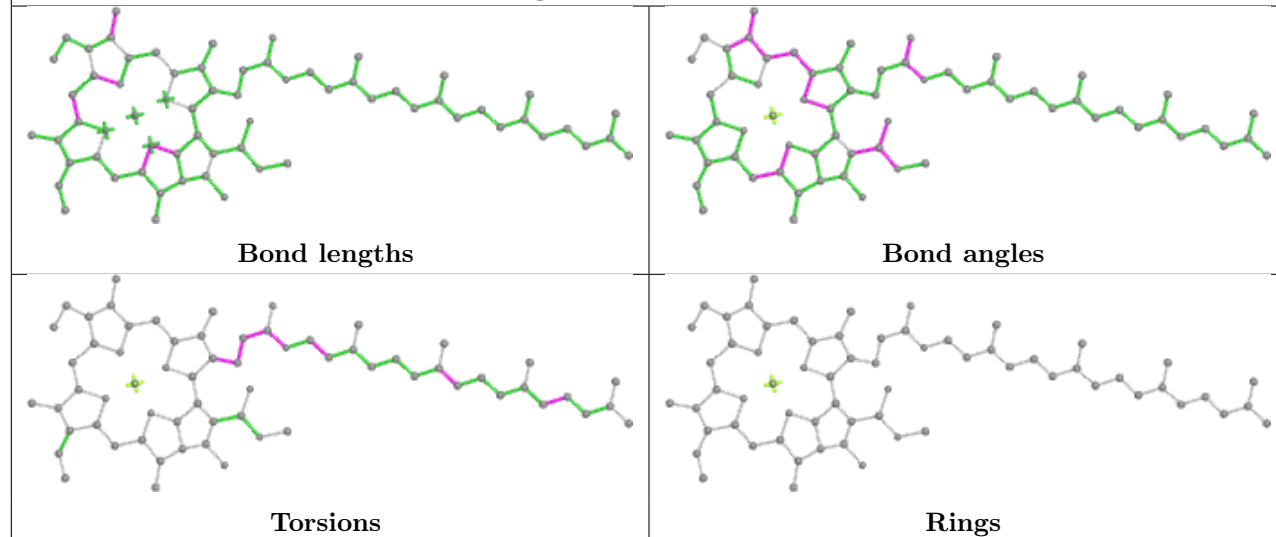
Bond angles

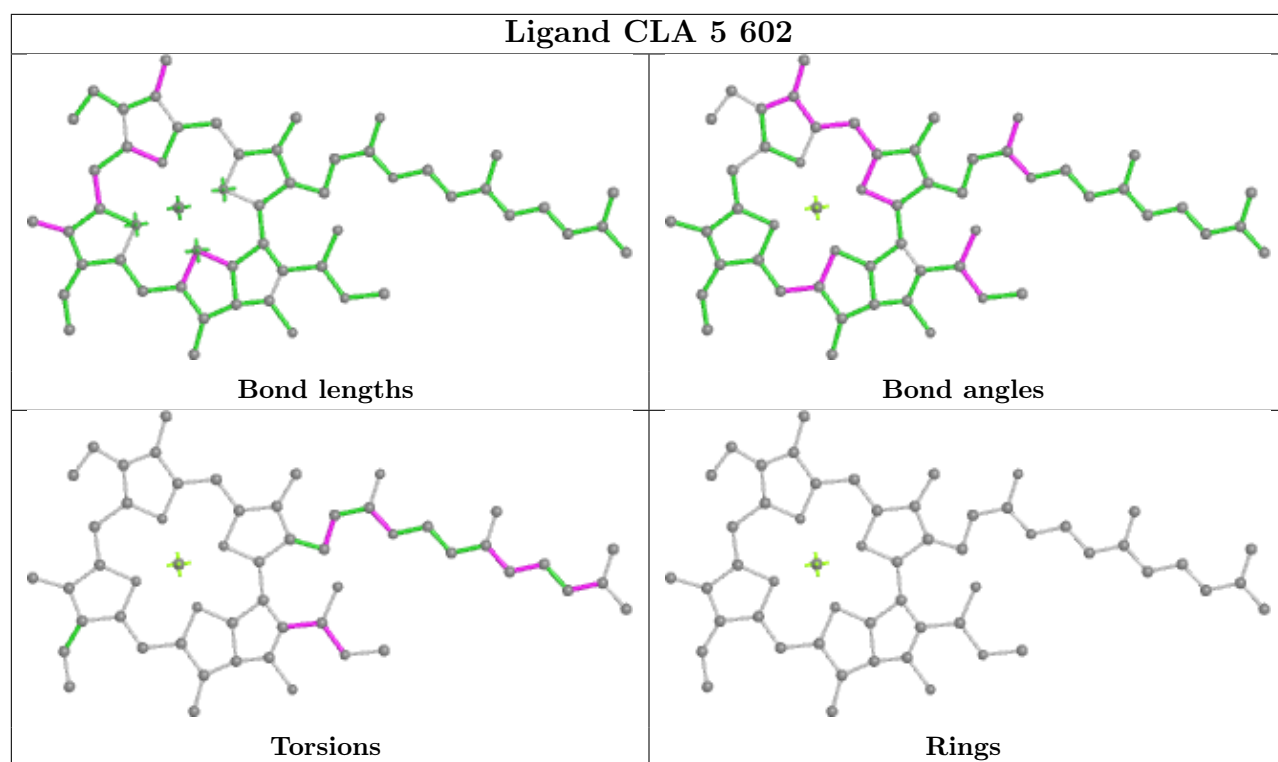


Torsions

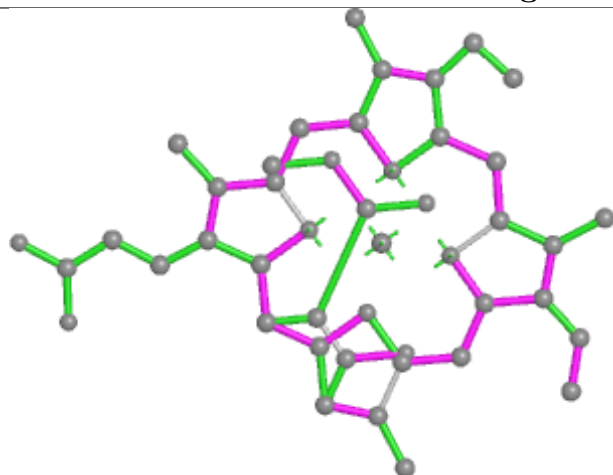


Rings

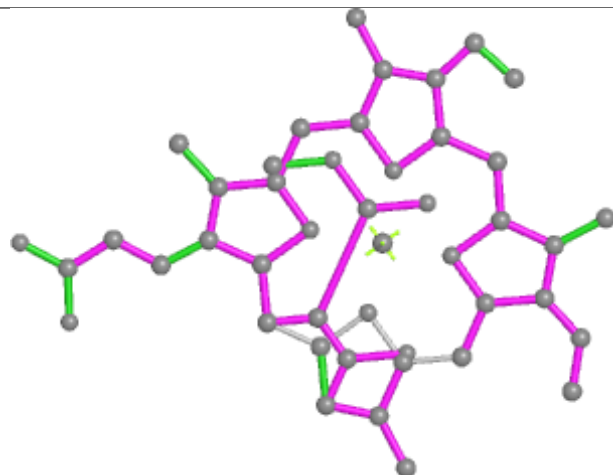
**Ligand CLA 6 610****Ligand CLA D 404**



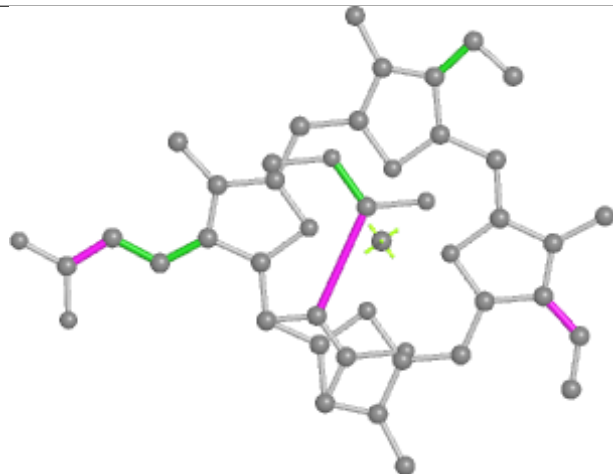
## Ligand KC2 6 608



Bond lengths



Bond angles

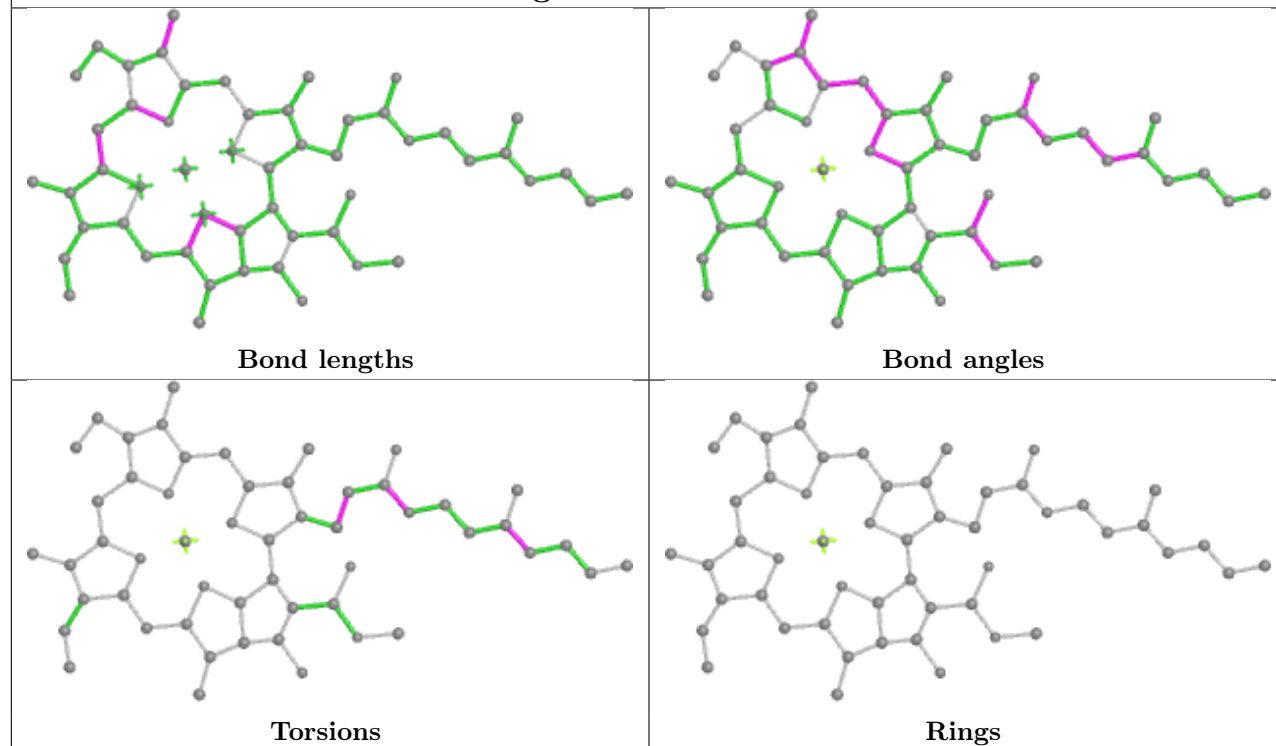


Torsions

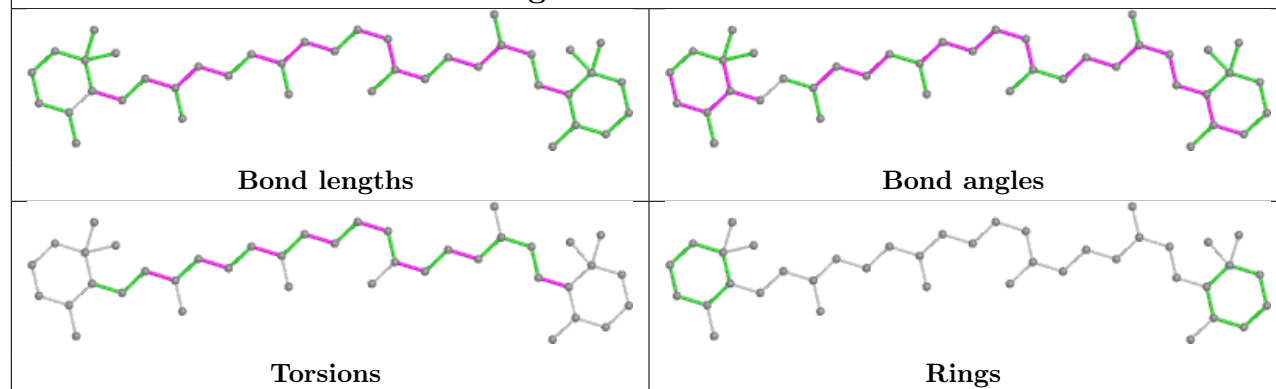


Rings

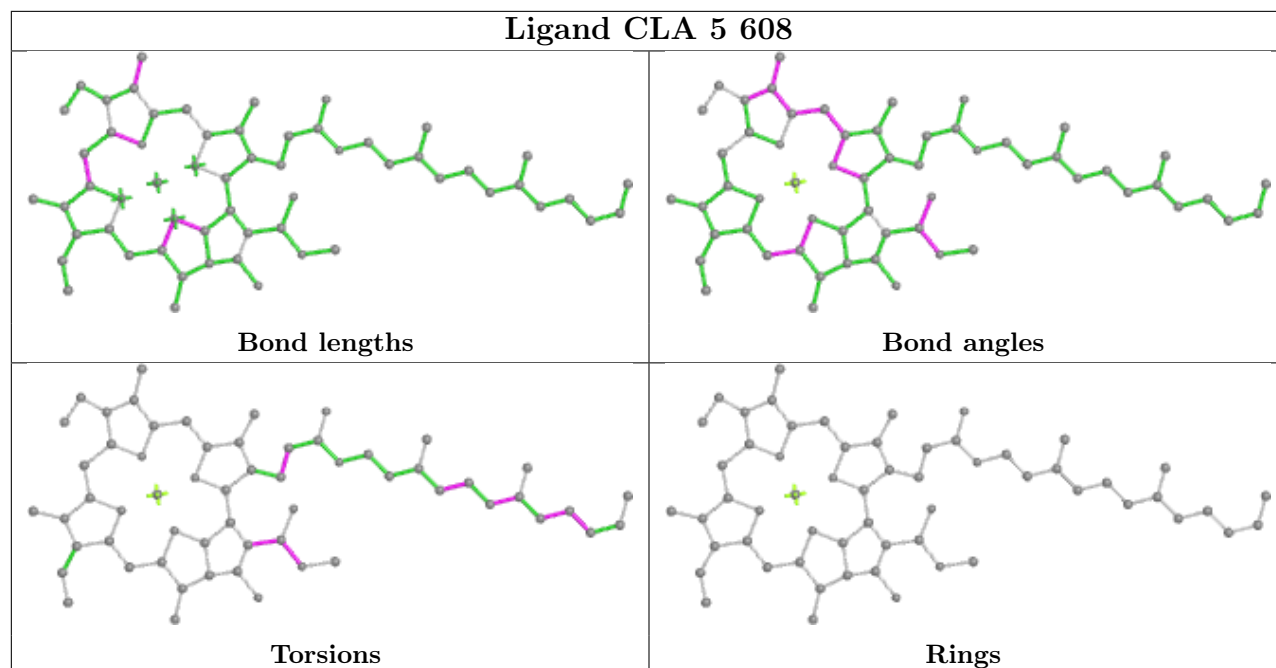
## Ligand CLA P 609



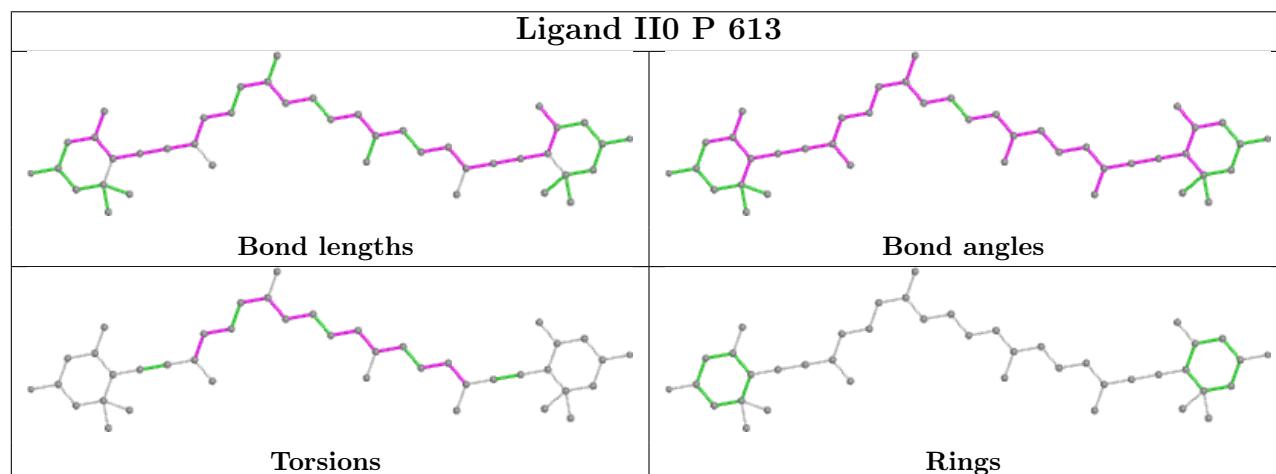
## Ligand WVN c 518



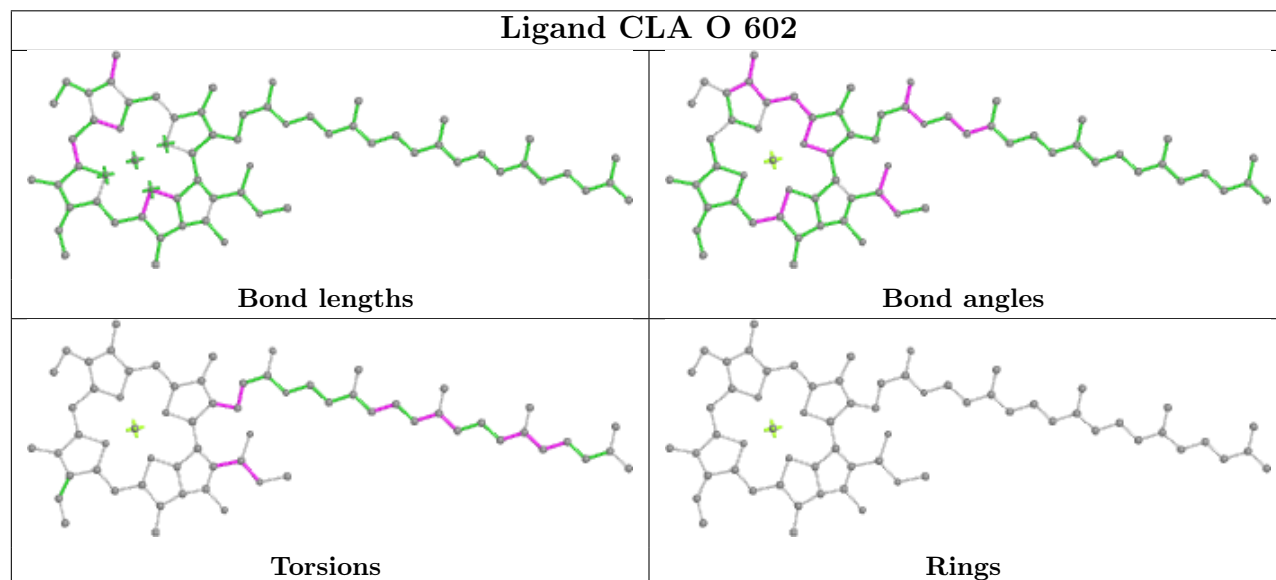
## Ligand CLA 5 608



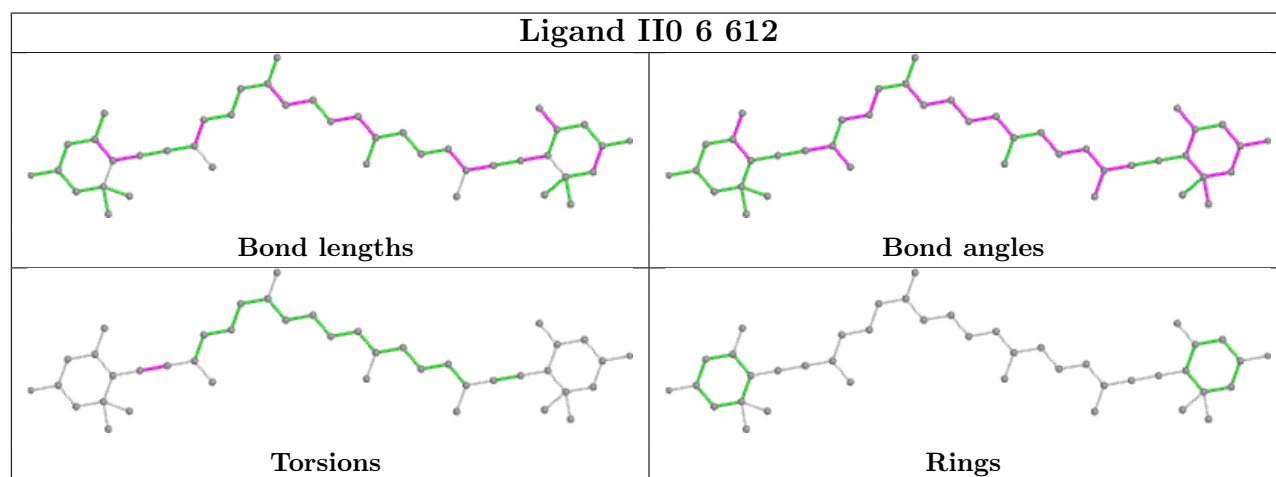
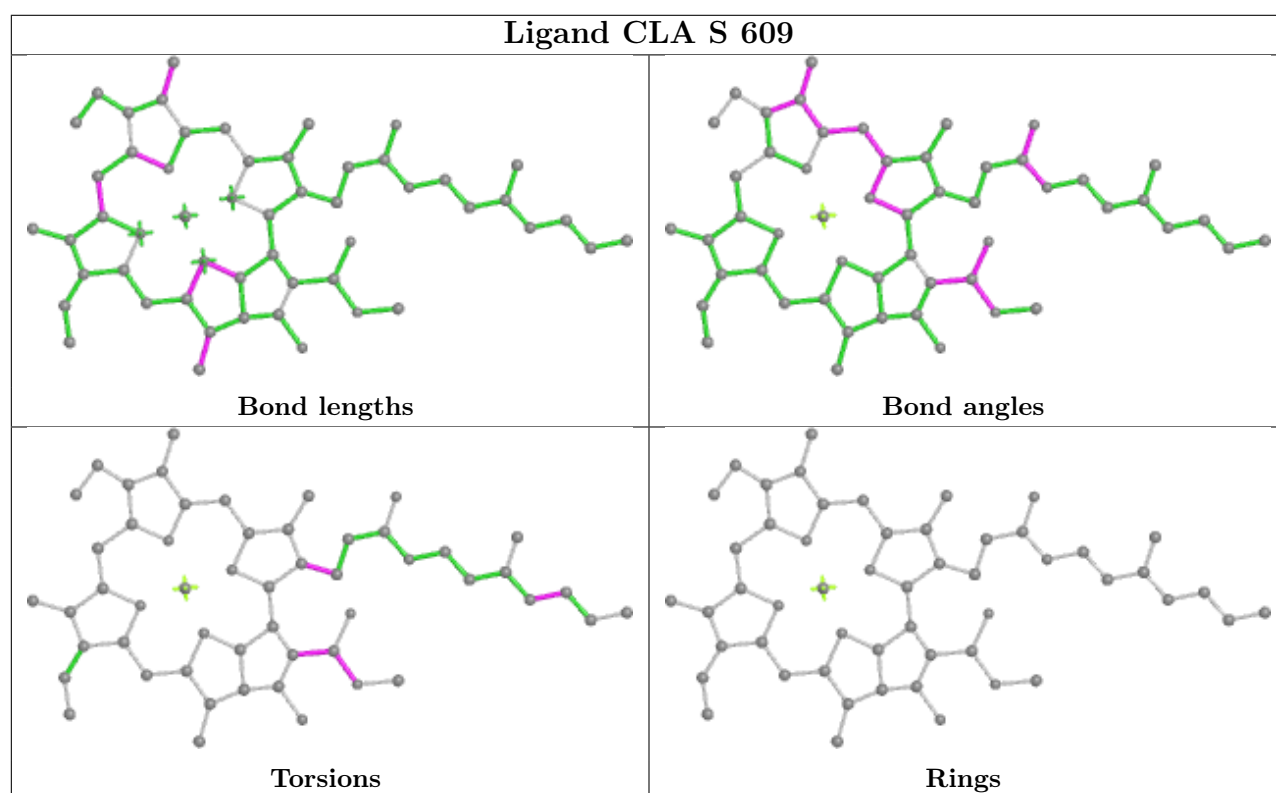
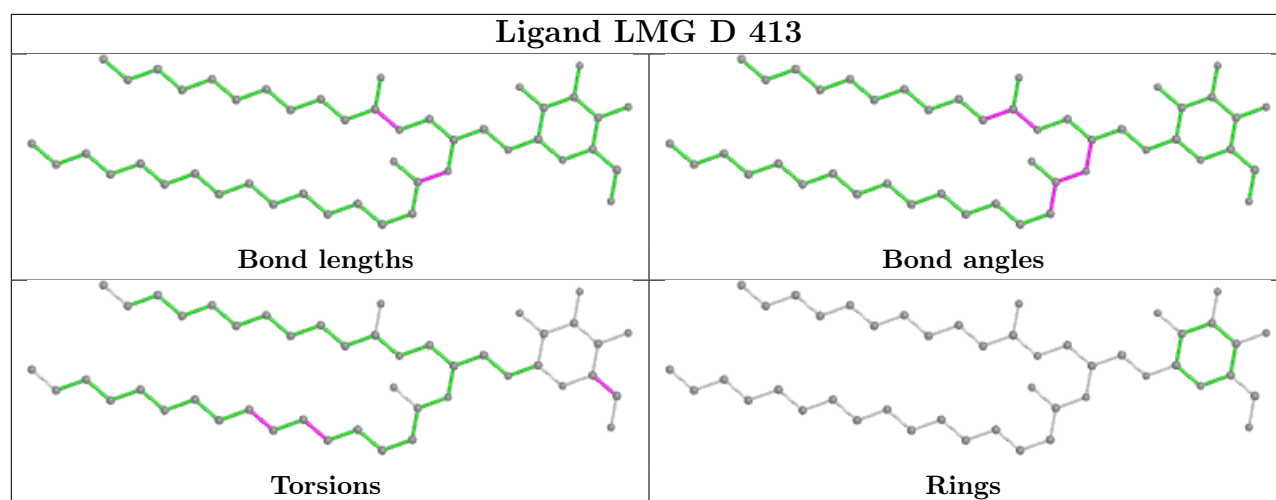
## Ligand II0 P 613

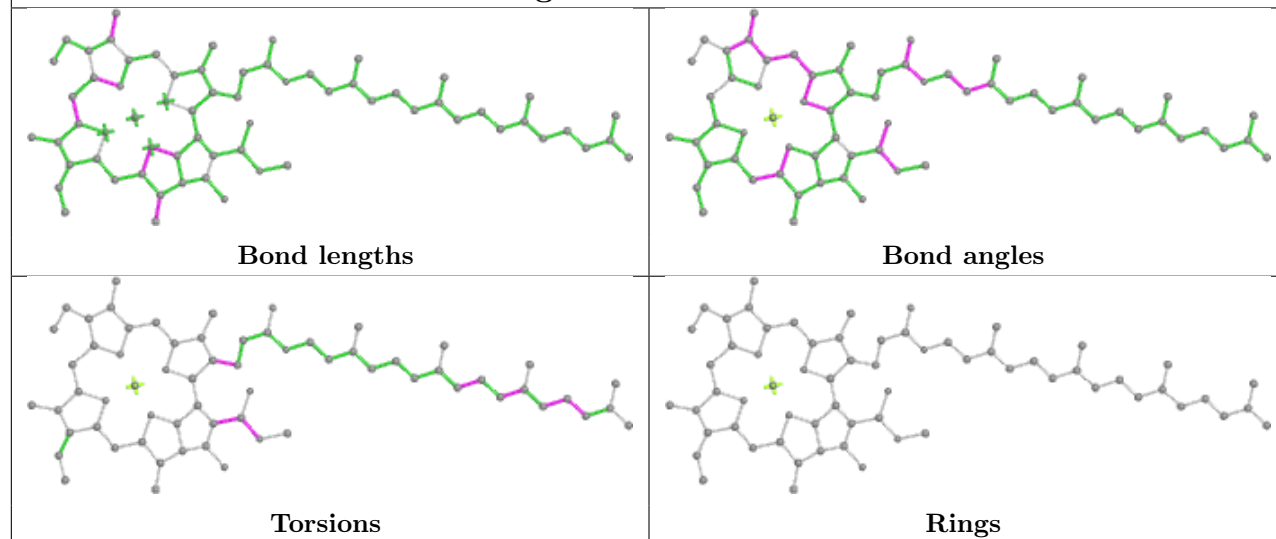
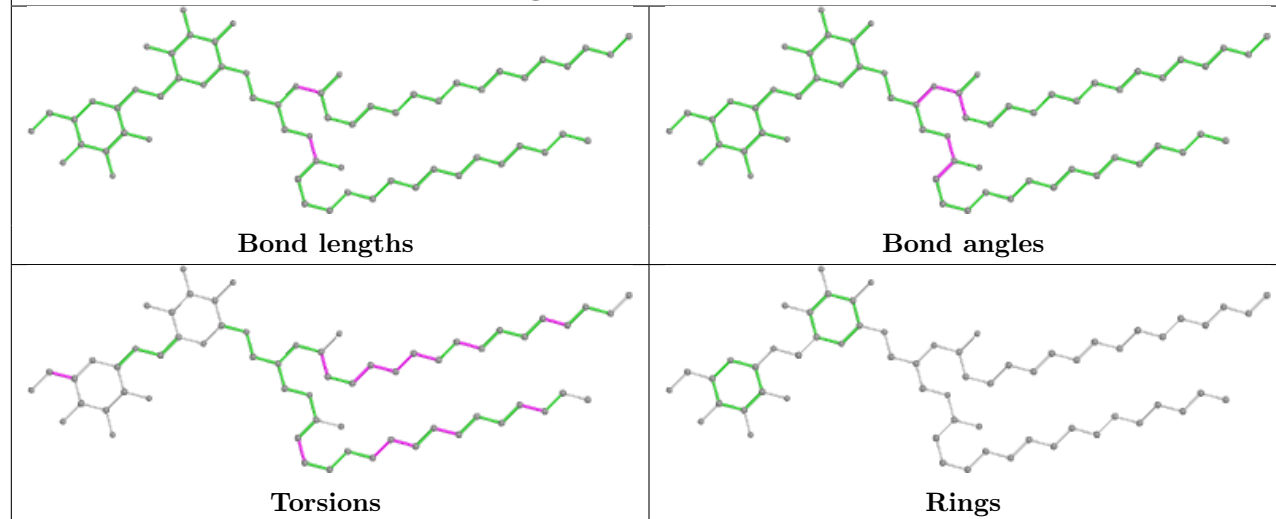


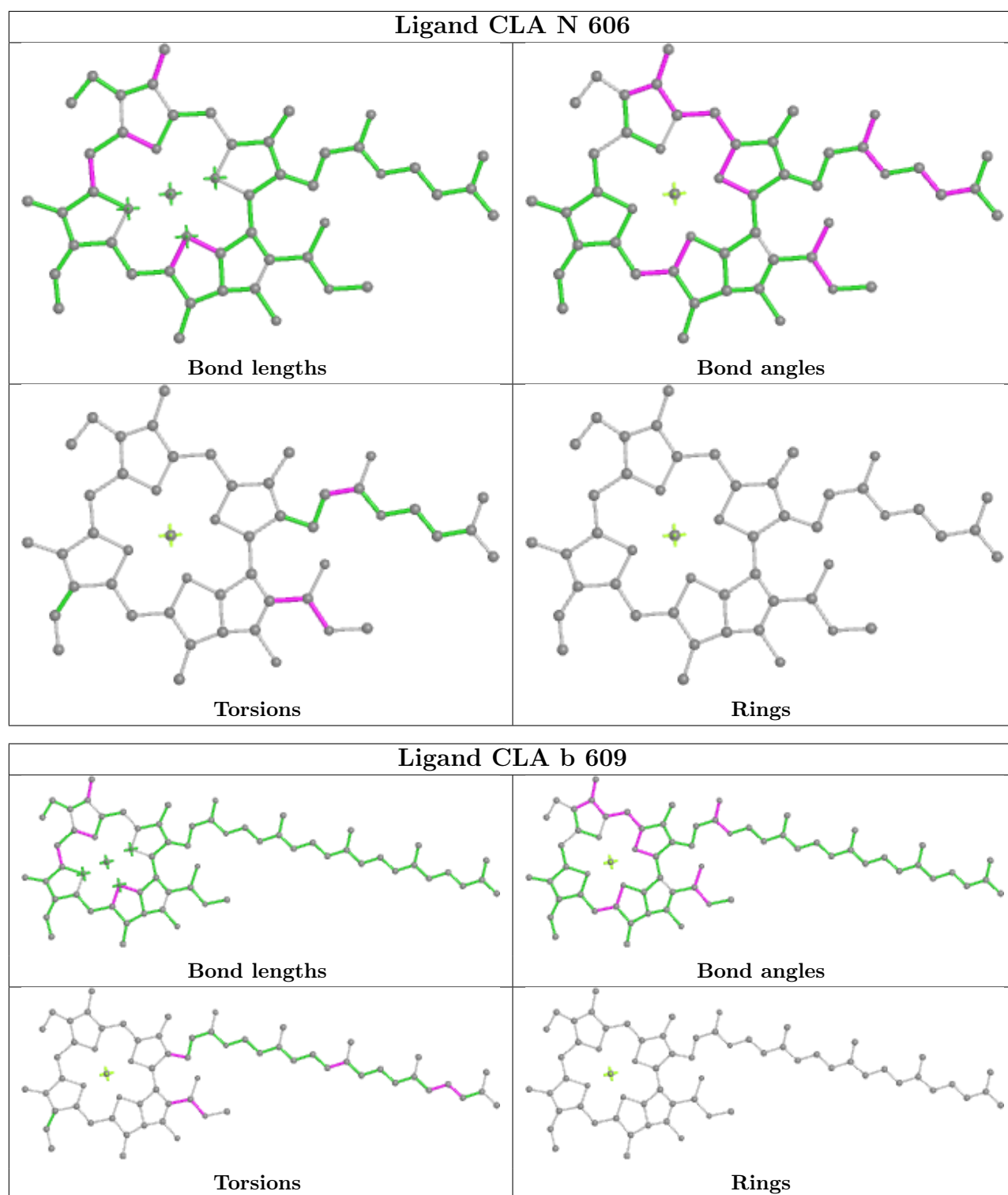
## Ligand CLA O 602



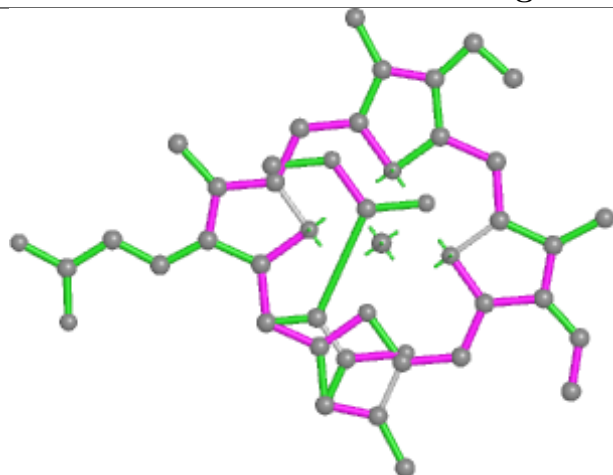




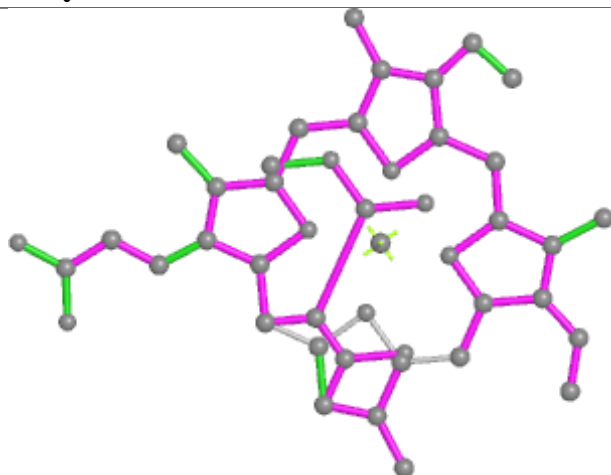
**Ligand CLA b 611****Ligand DGD H 102**



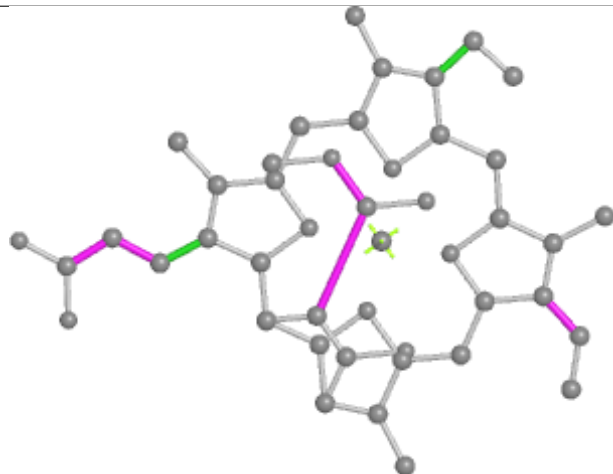
## Ligand KC2 Q 309



Bond lengths



Bond angles

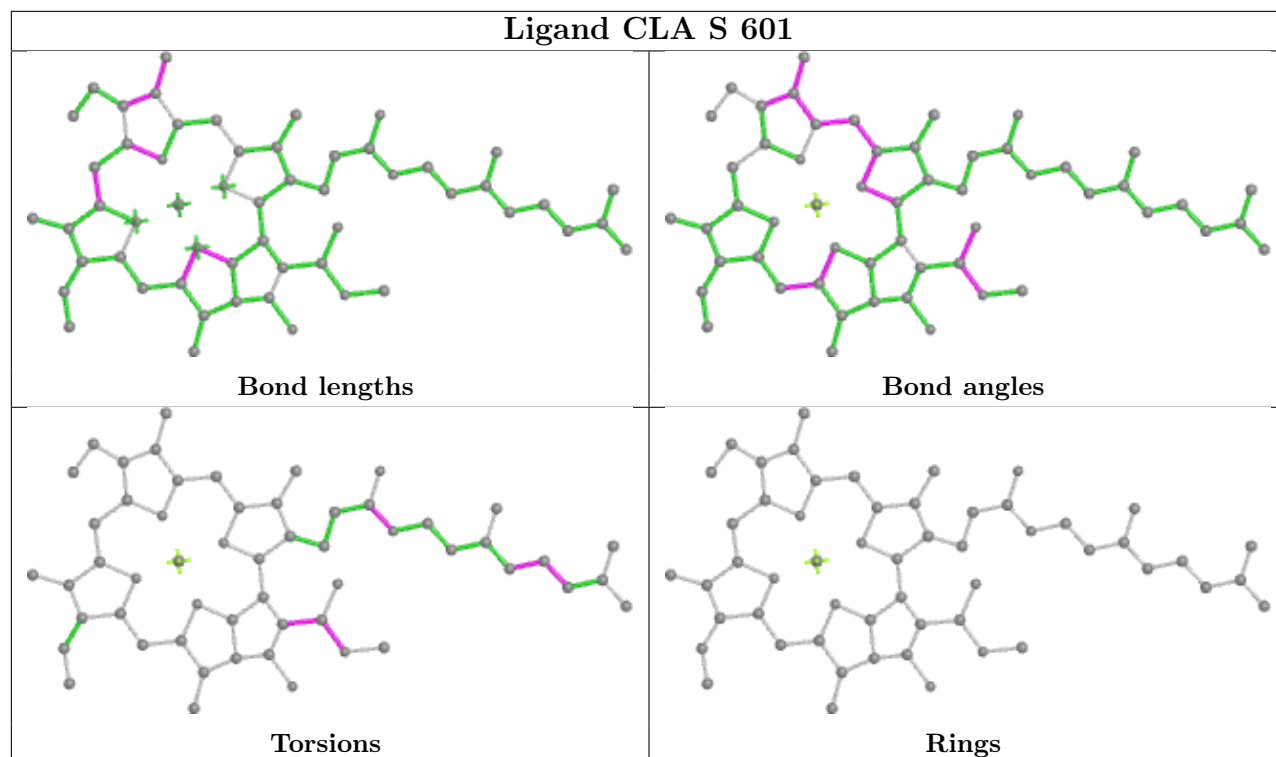


Torsions

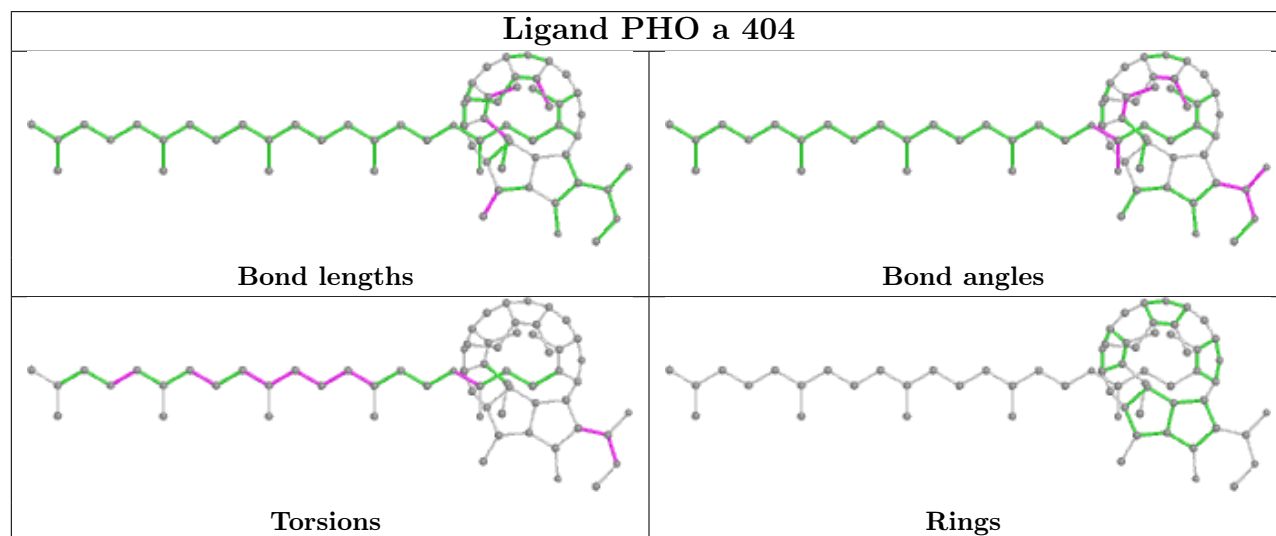


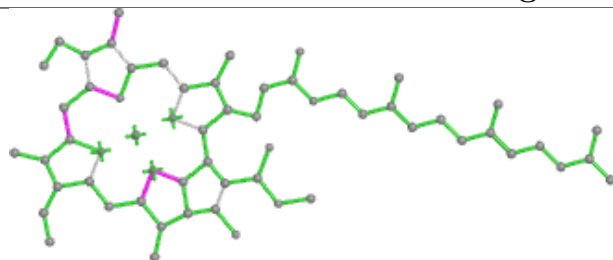
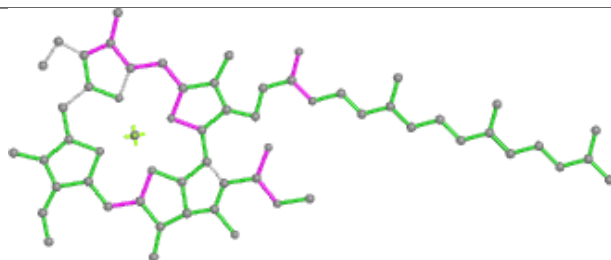
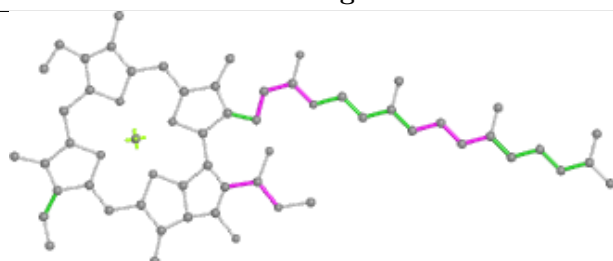
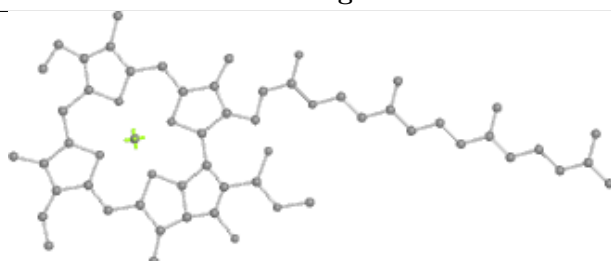
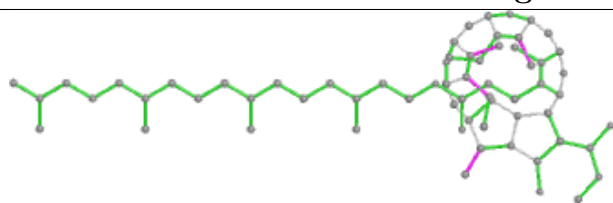
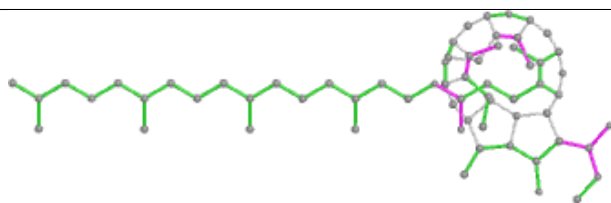
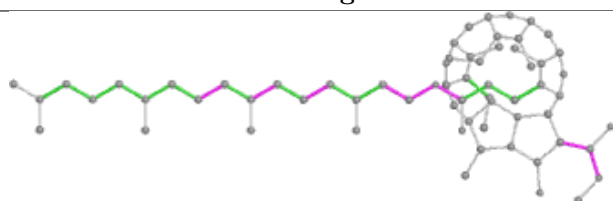
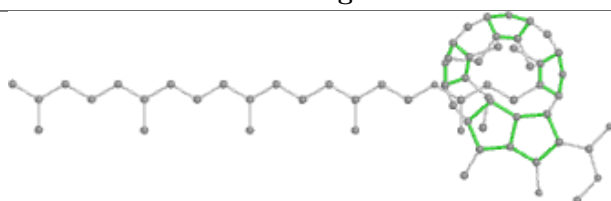
Rings

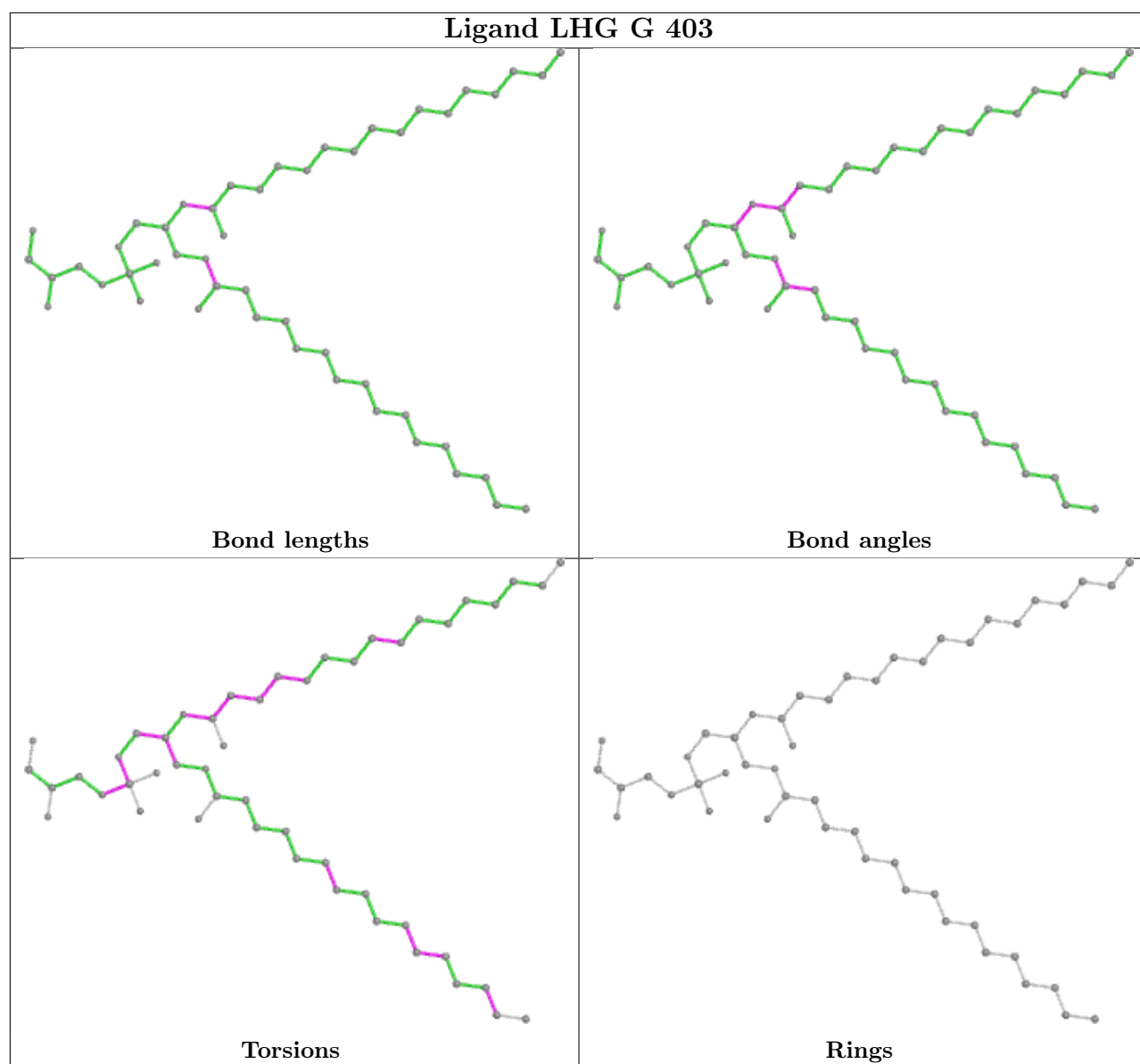
## Ligand CLA S 601

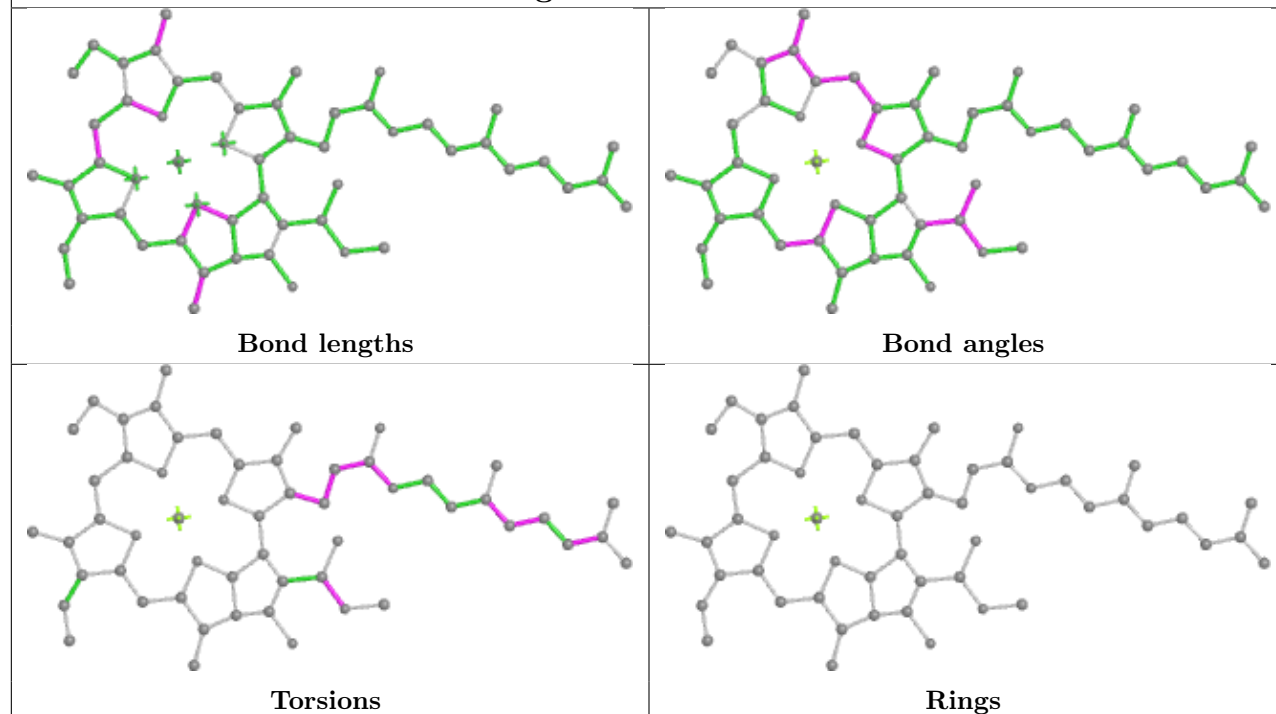
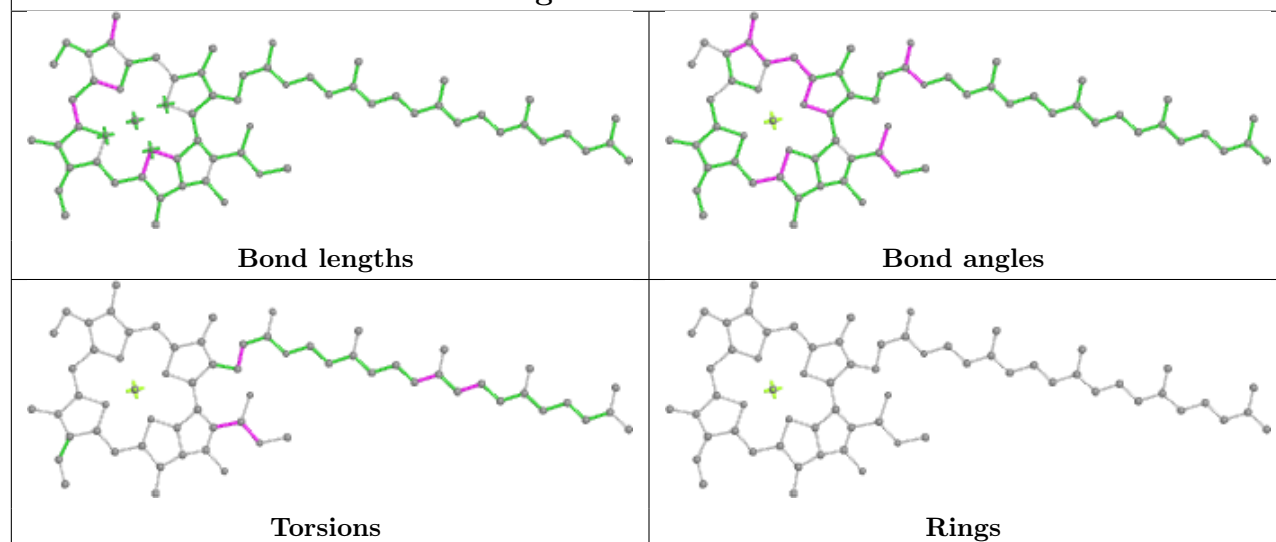


## Ligand PHO a 404

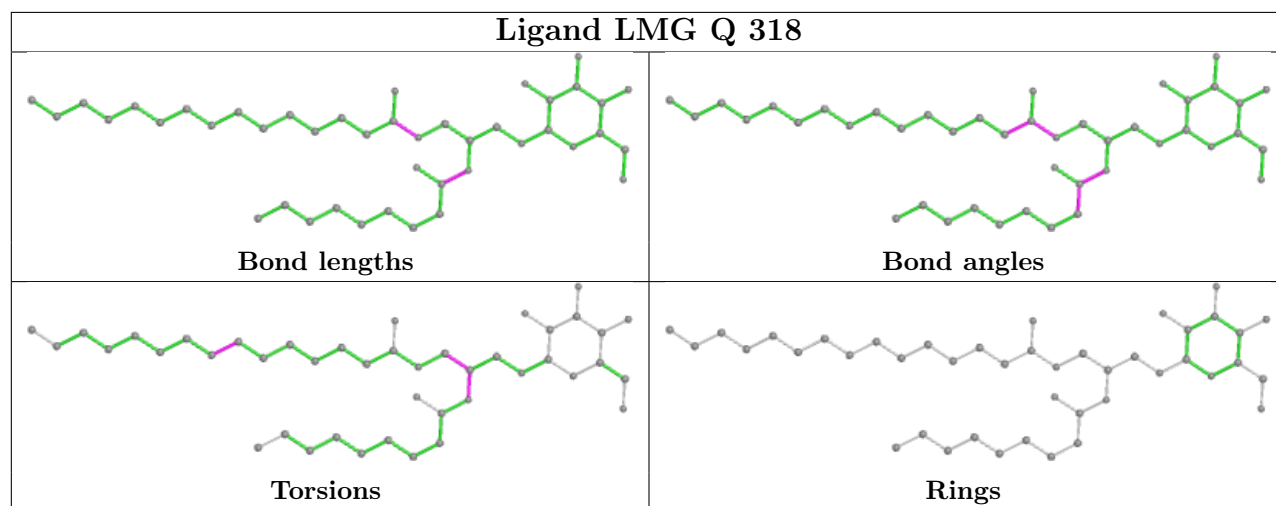
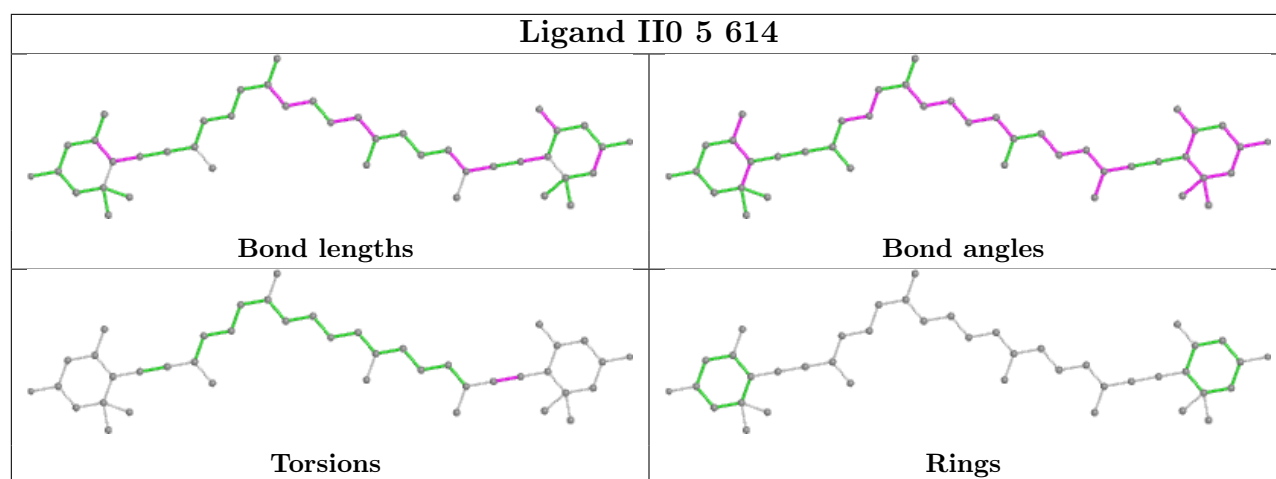


**Ligand CLA c 506****Bond lengths****Bond angles****Torsions****Rings****Ligand PHO d 403****Bond lengths****Bond angles****Torsions****Rings**

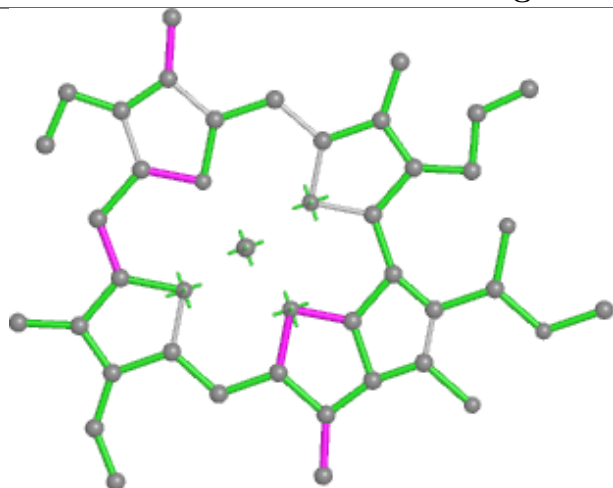


**Ligand CLA S 605****Ligand CLA b 606**

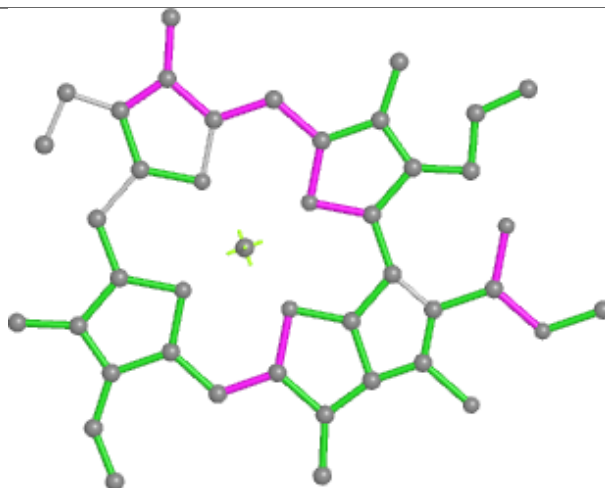




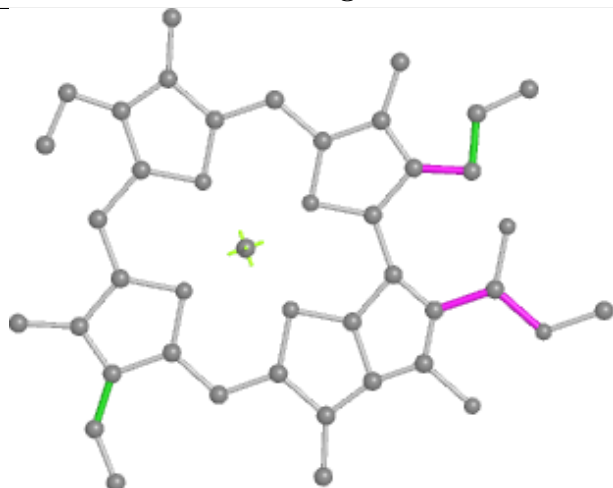
## Ligand CLA R 307



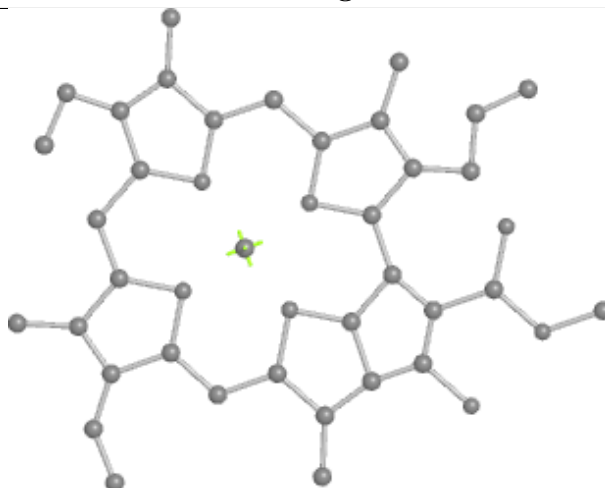
Bond lengths



Bond angles

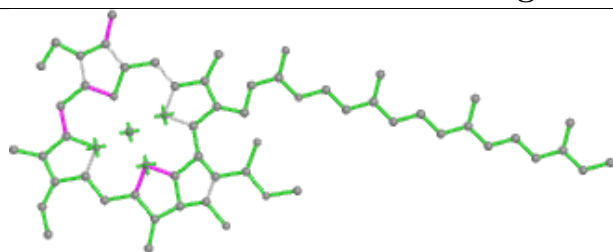


Torsions

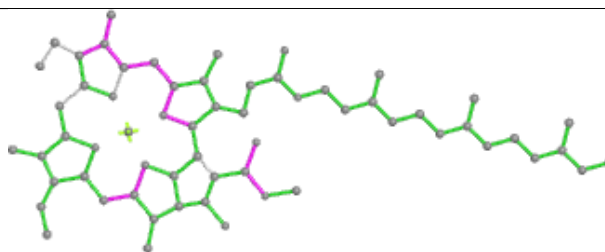


Rings

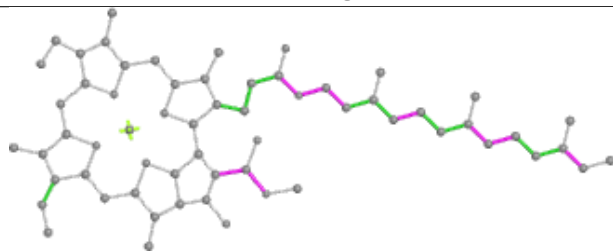
## Ligand CLA d 406



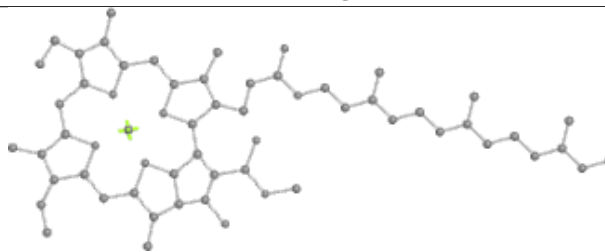
Bond lengths



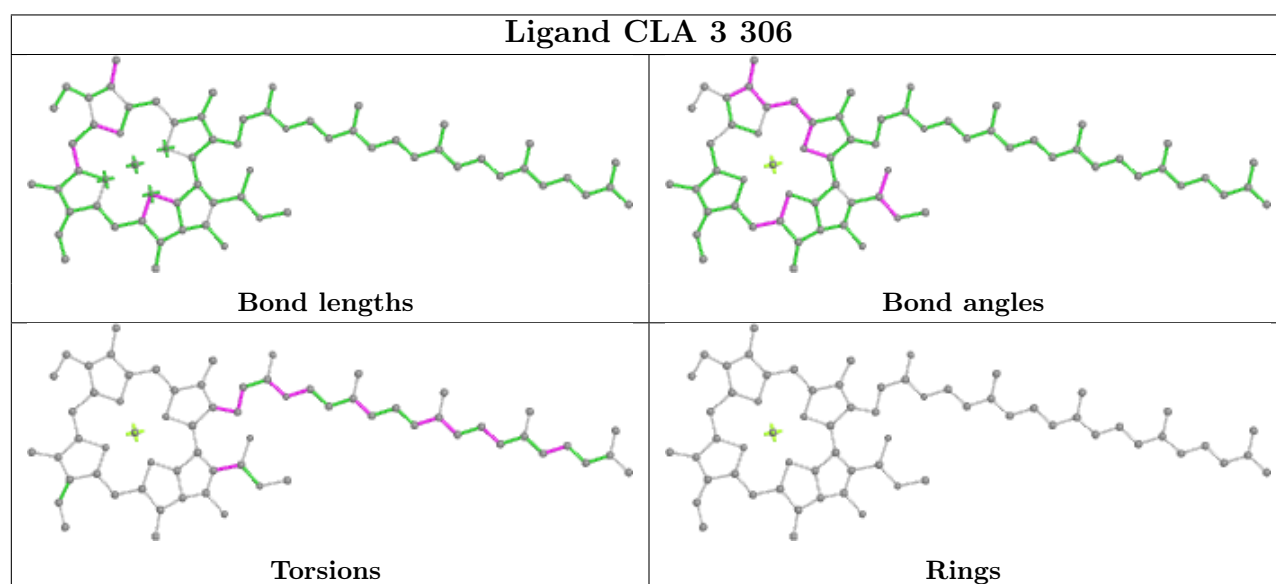
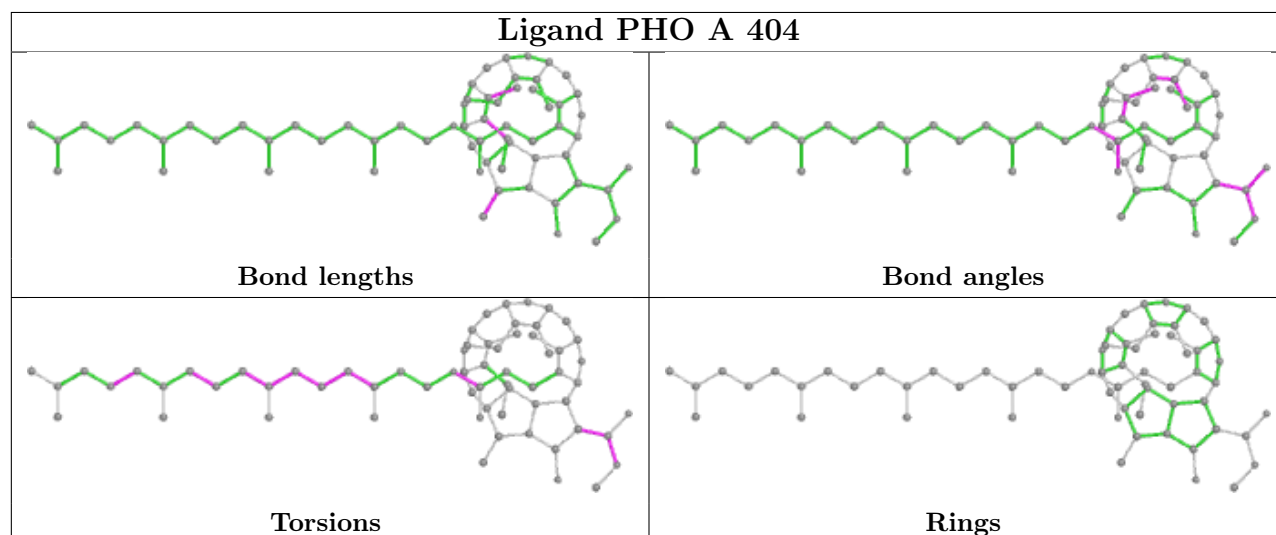
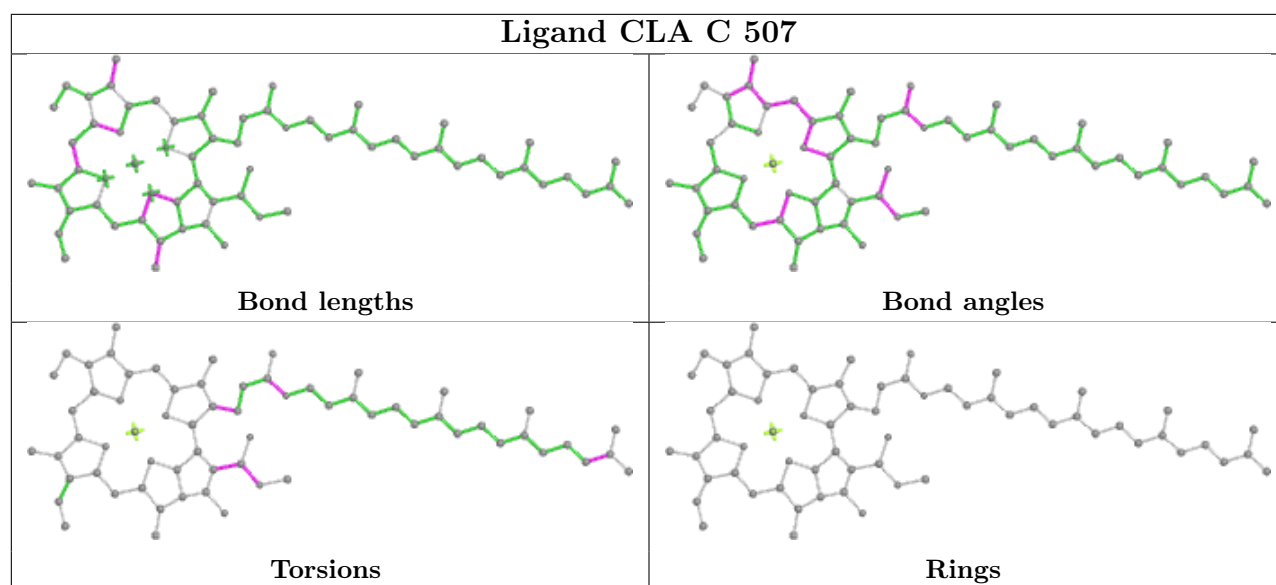
Bond angles

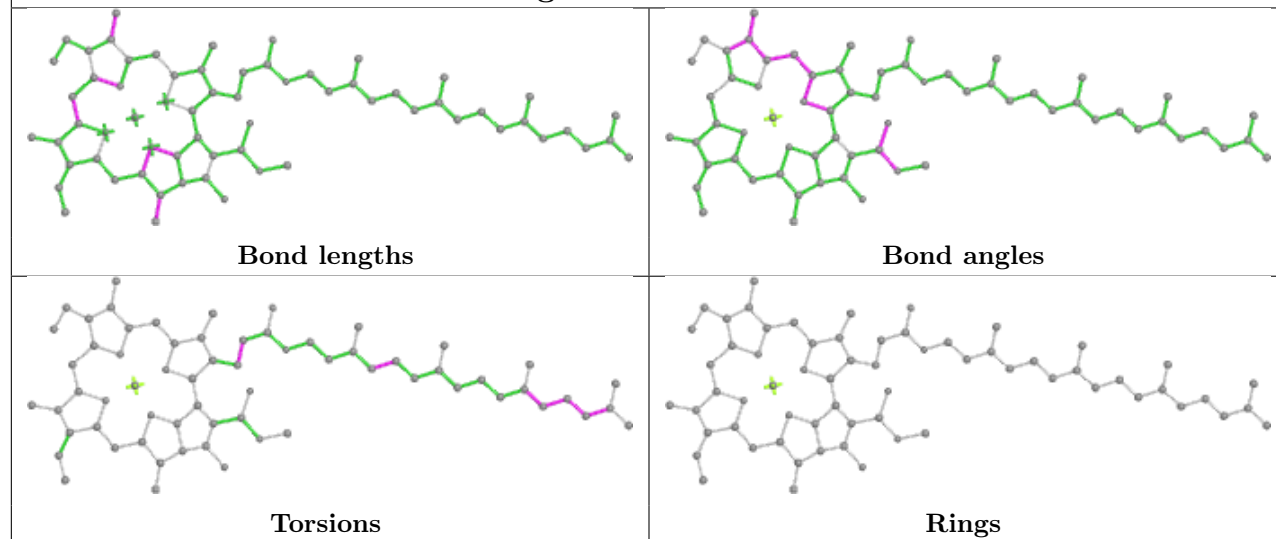
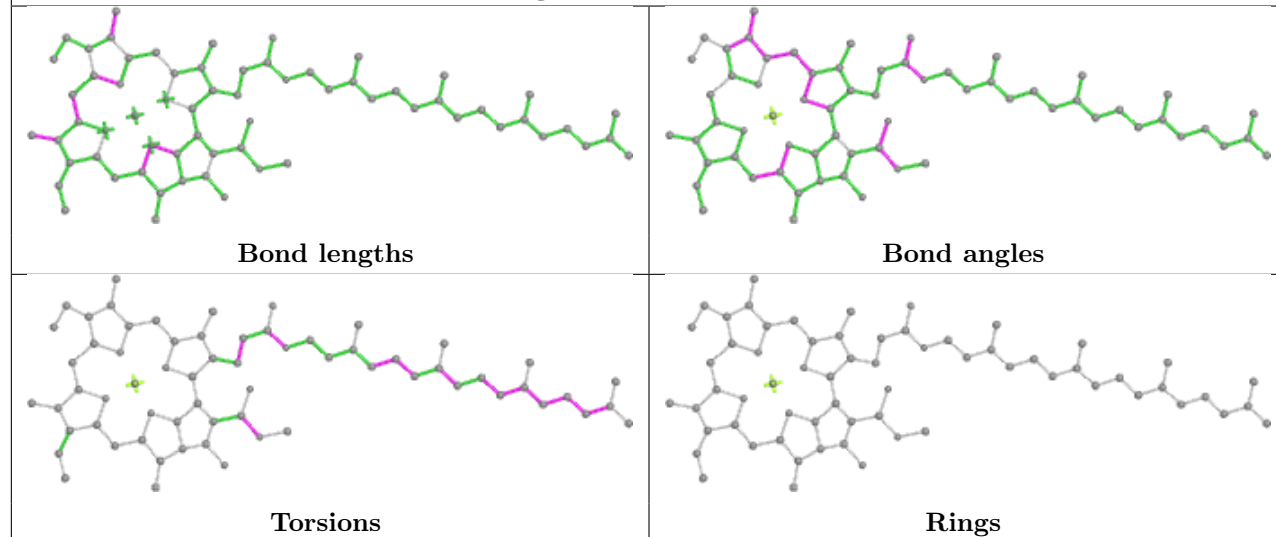
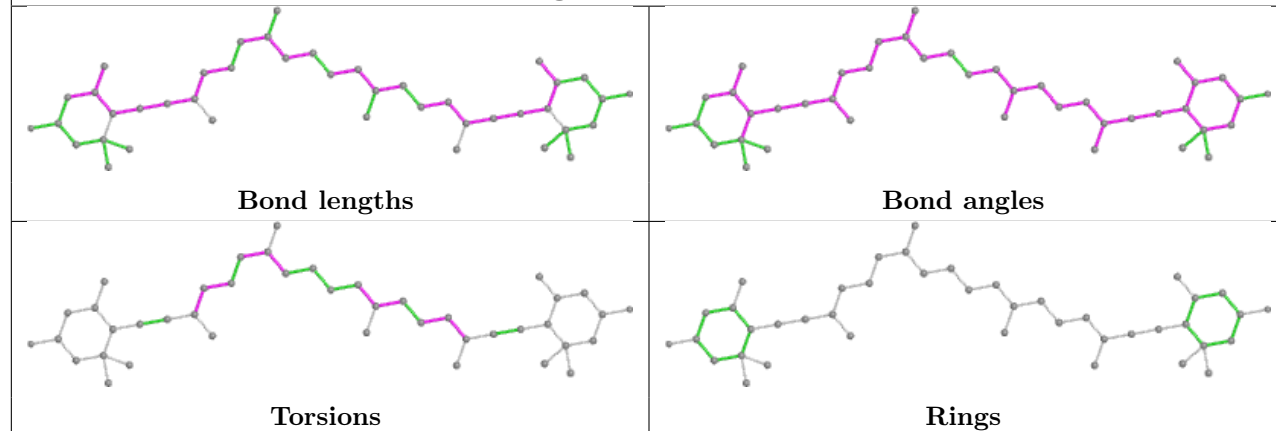


Torsions

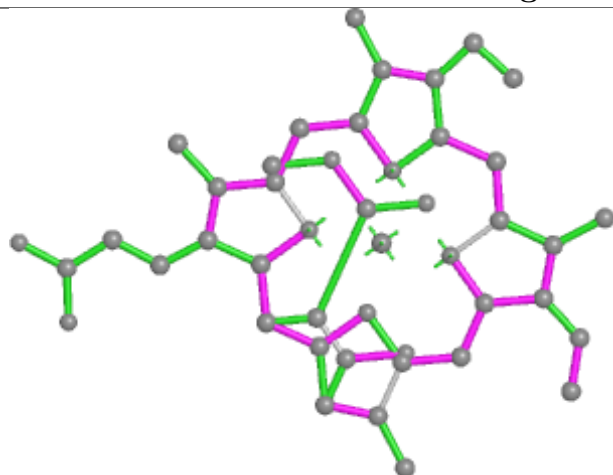


Rings

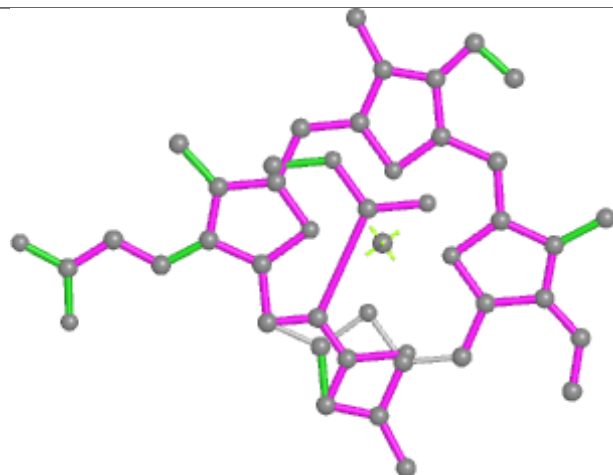


**Ligand CLA c 509****Ligand CLA B 616****Ligand II0 1 617**

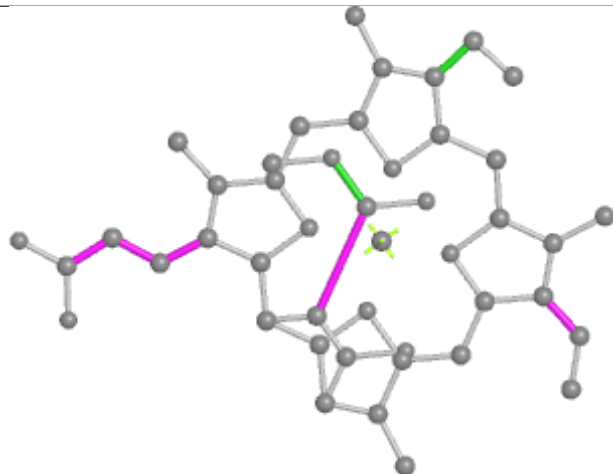
## Ligand KC2 4 305



Bond lengths



Bond angles

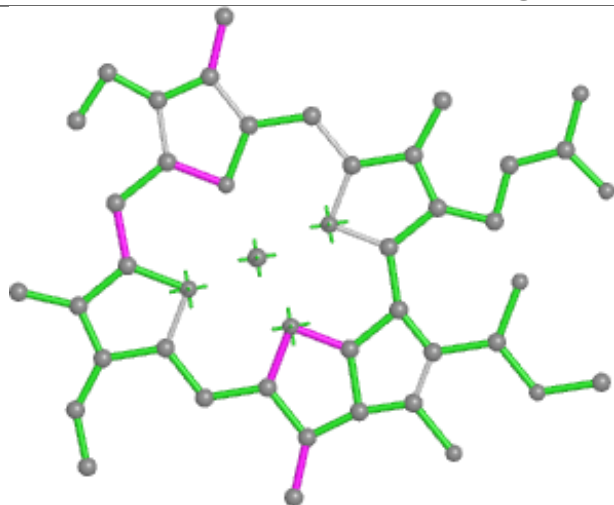


Torsions

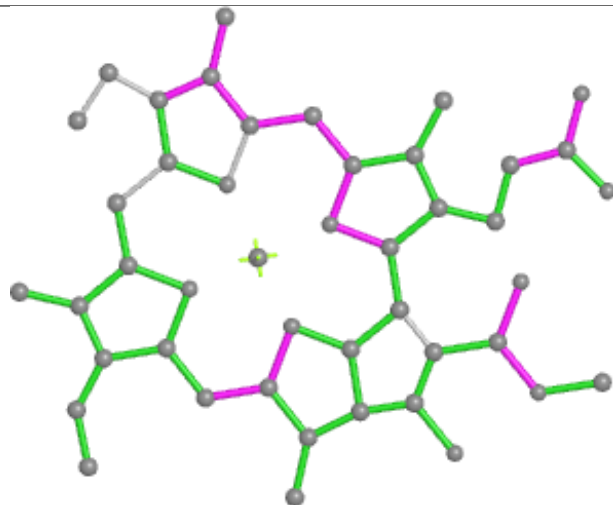


Rings

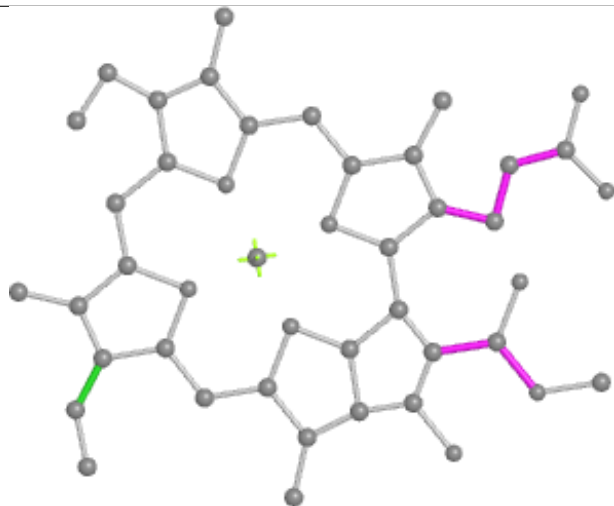
## Ligand CLA P 611



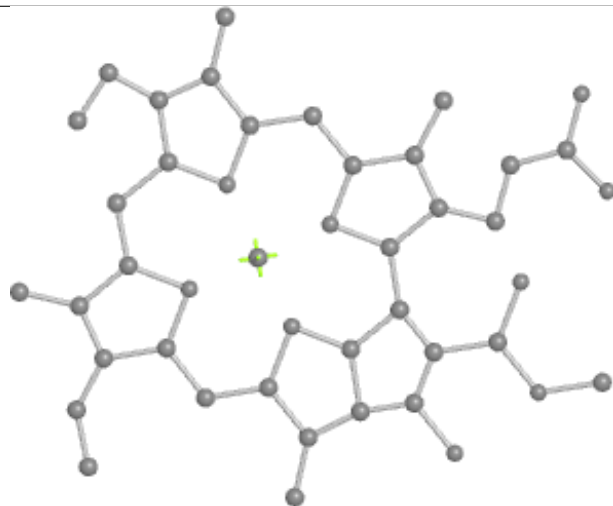
Bond lengths



Bond angles

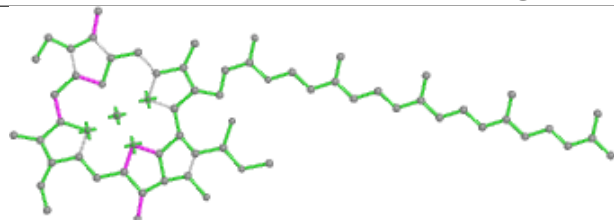


Torsions

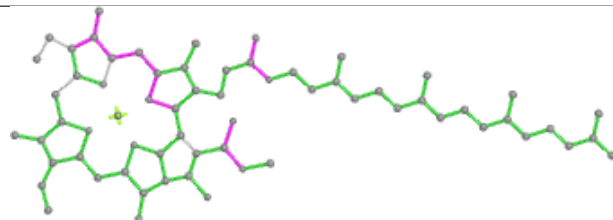


Rings

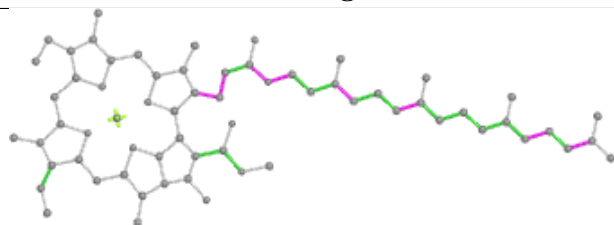
## Ligand CLA C 510



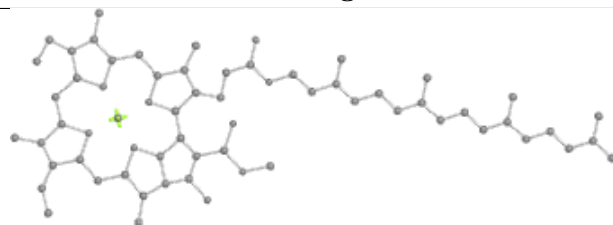
Bond lengths



Bond angles

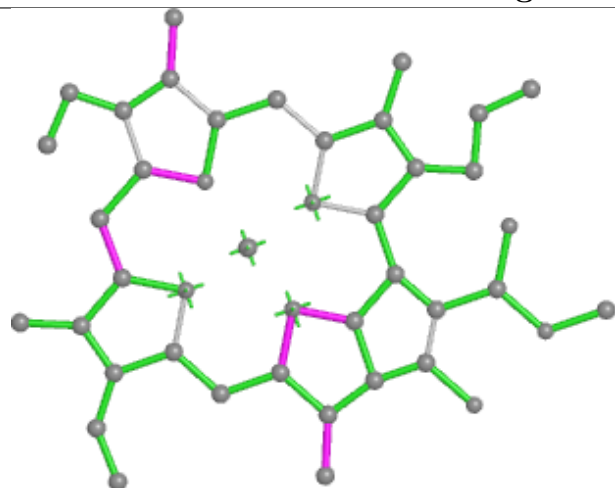


Torsions

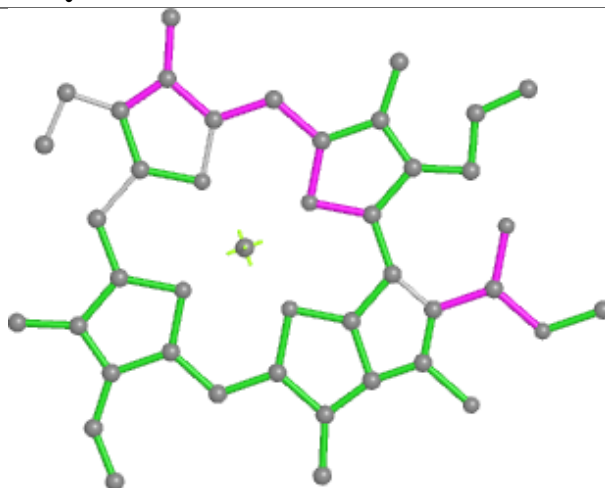


Rings

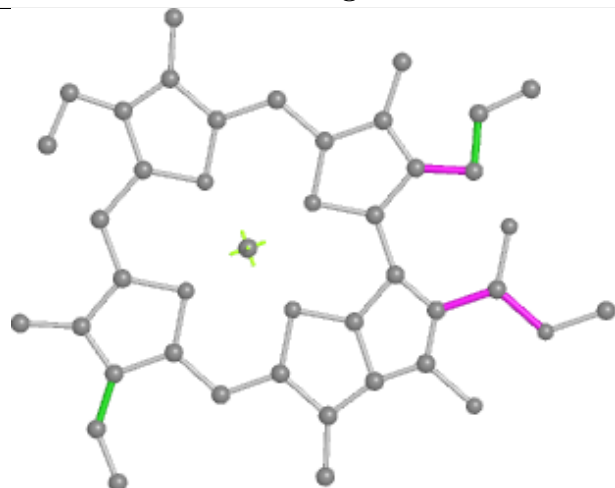
## Ligand CLA Q 311



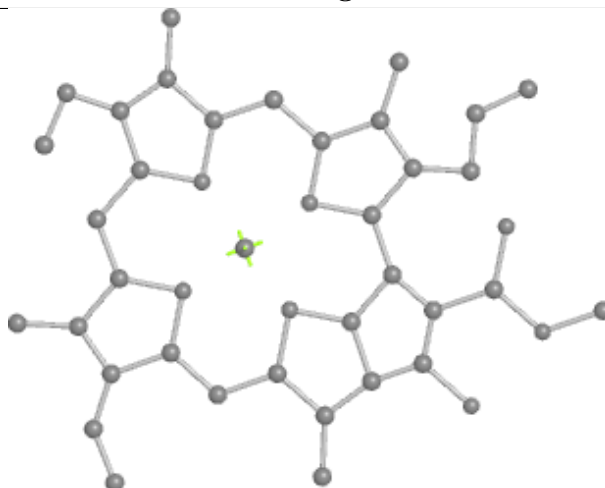
Bond lengths



Bond angles

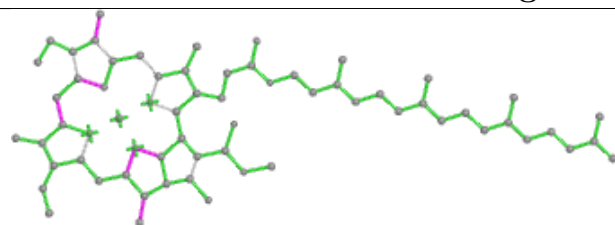


Torsions

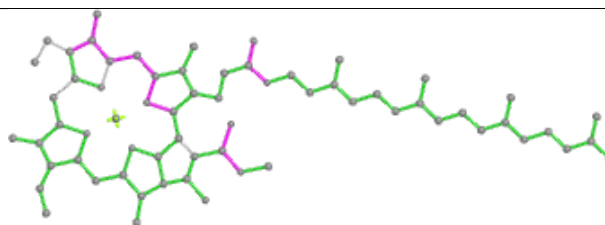


Rings

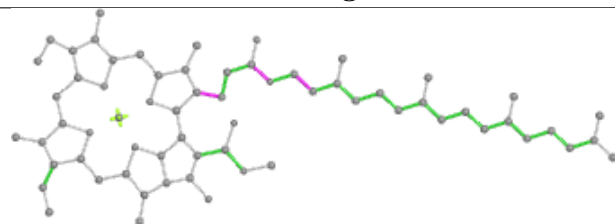
## Ligand CLA d 405



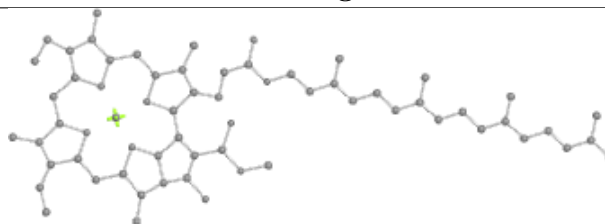
Bond lengths



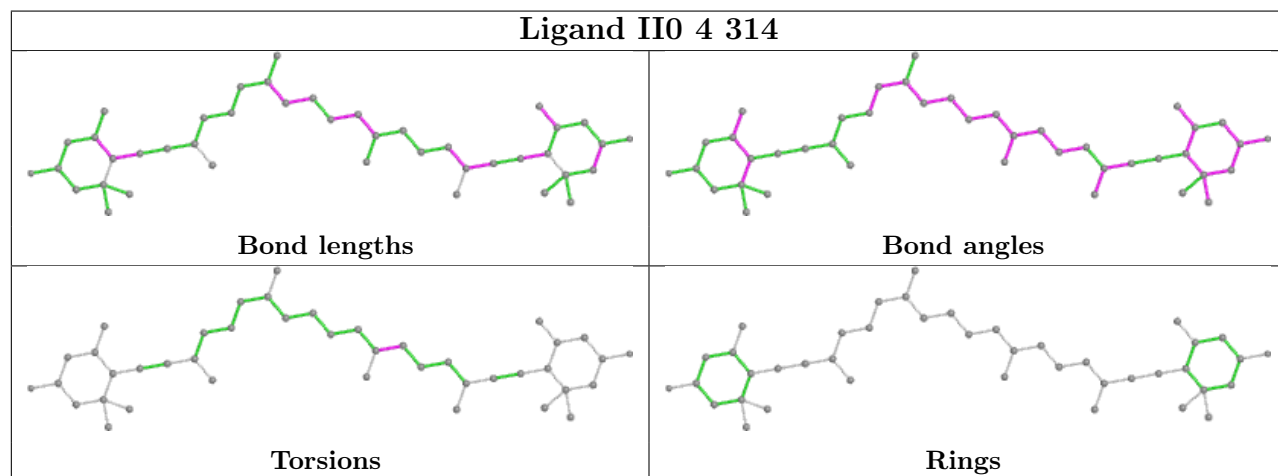
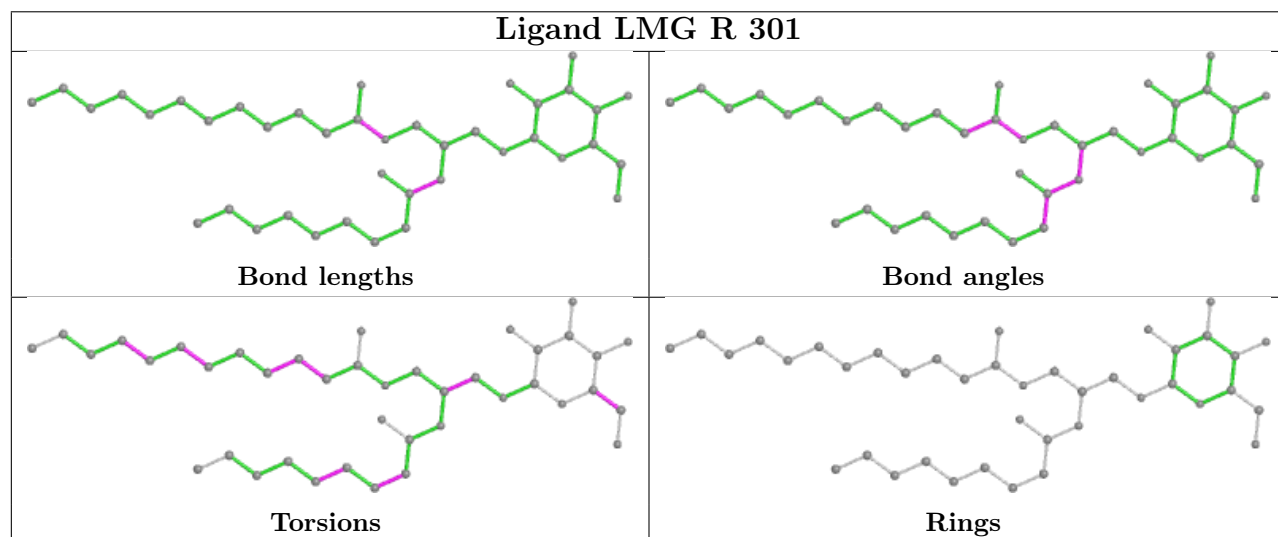
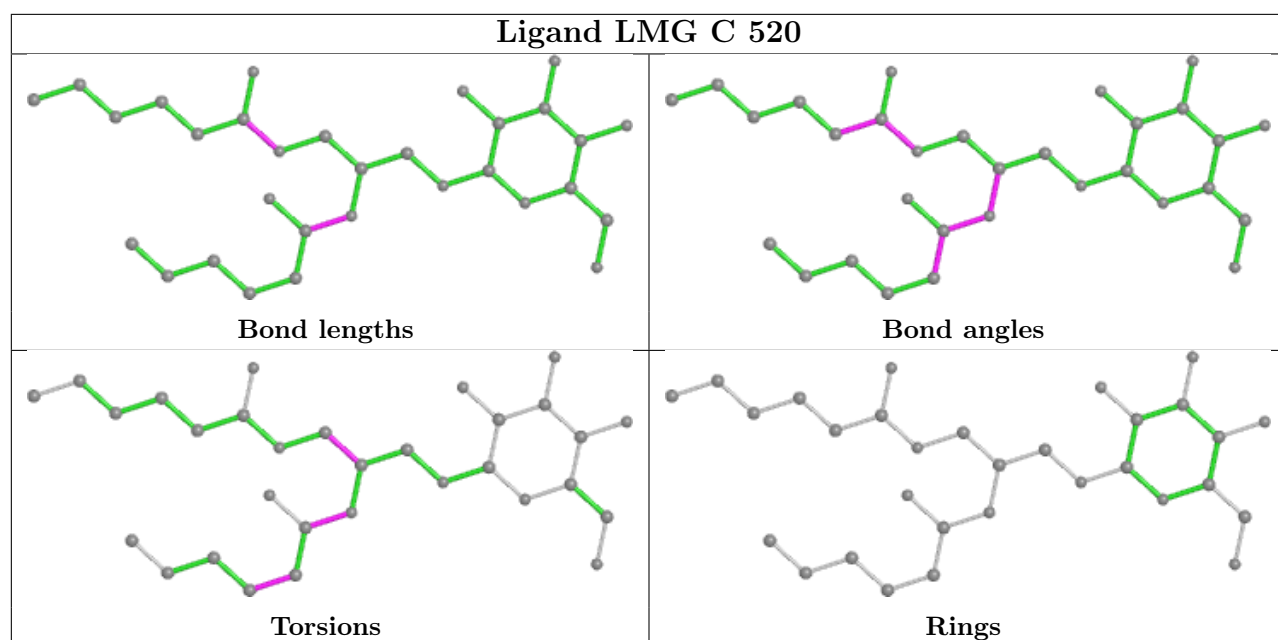
Bond angles



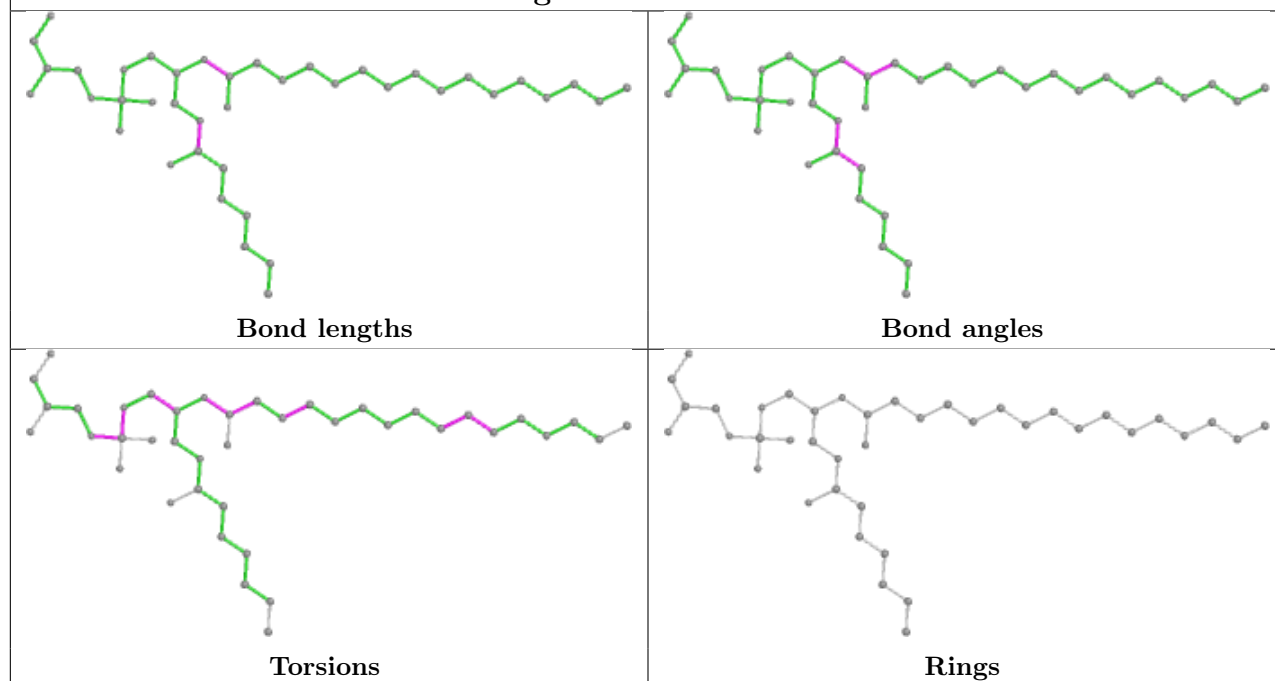
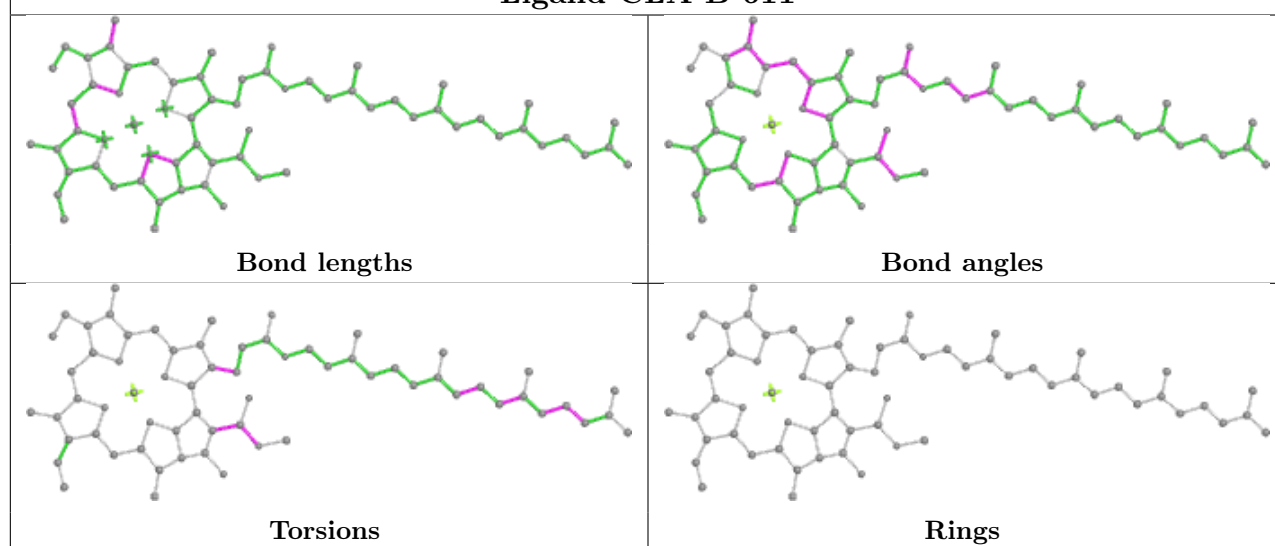
Torsions



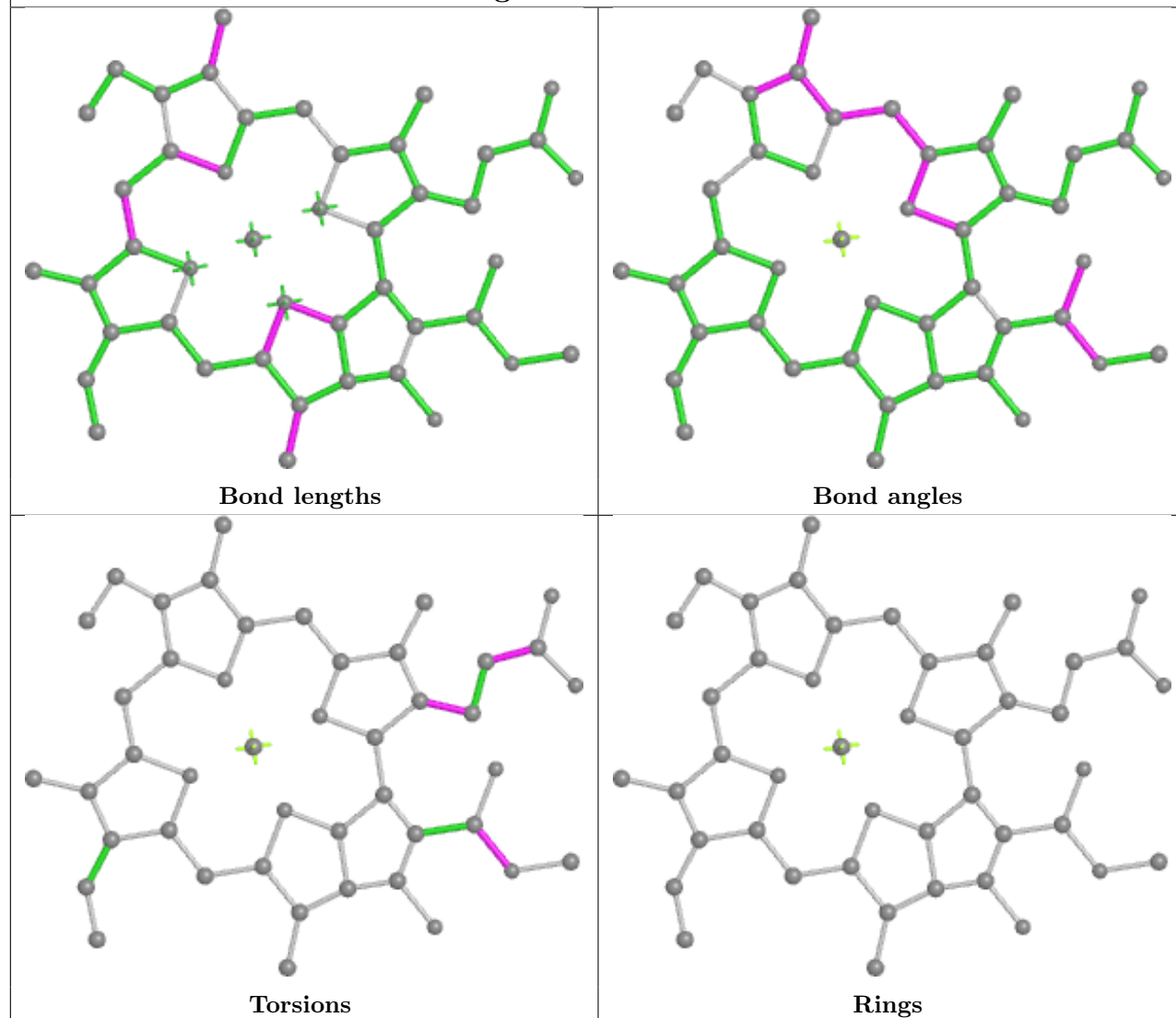
Rings



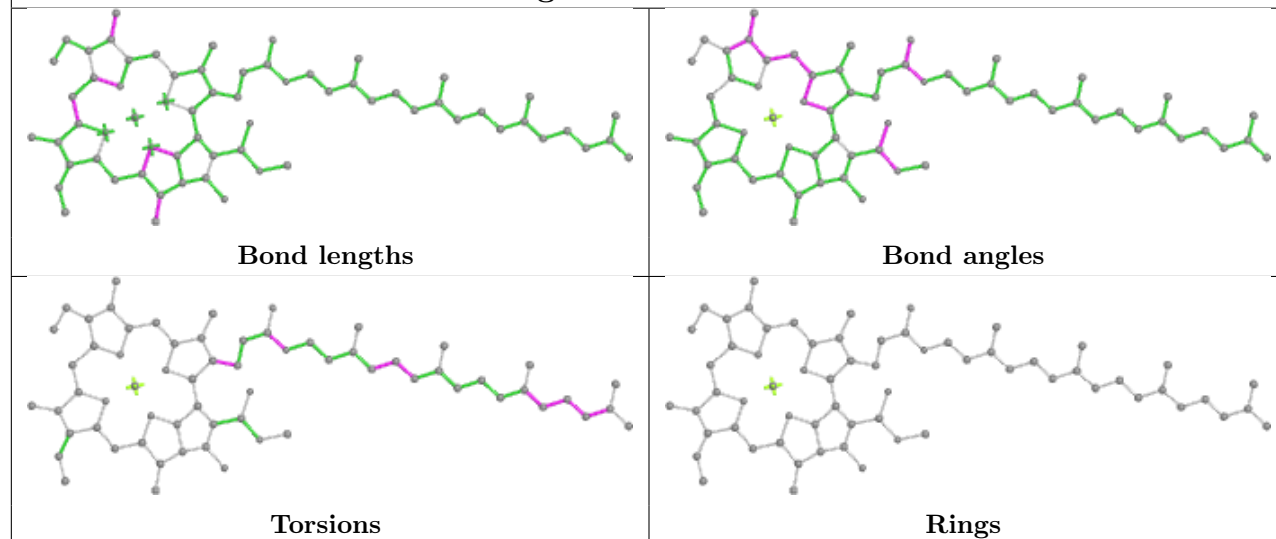


**Ligand LHG 5 618****Ligand CLA B 611**

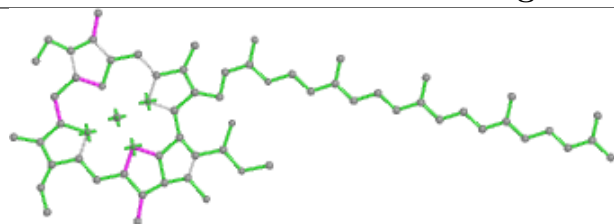
## Ligand CLA 1 601



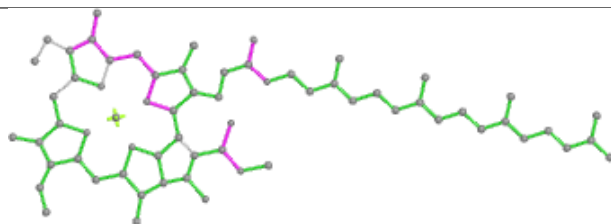
## Ligand CLA c 514



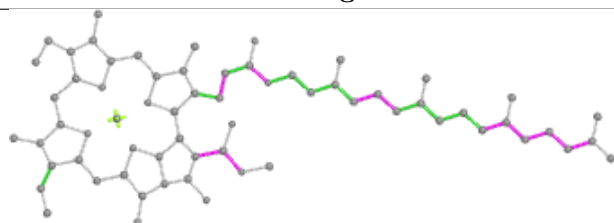
## Ligand CLA S 604



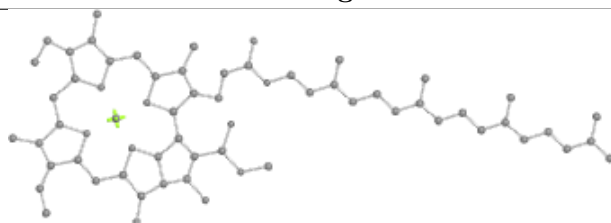
Bond lengths



Bond angles

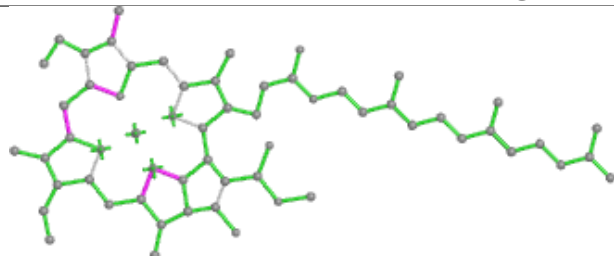


Torsions

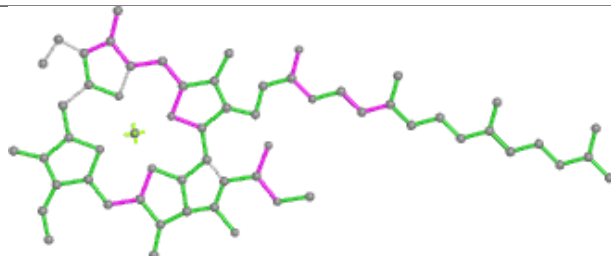


Rings

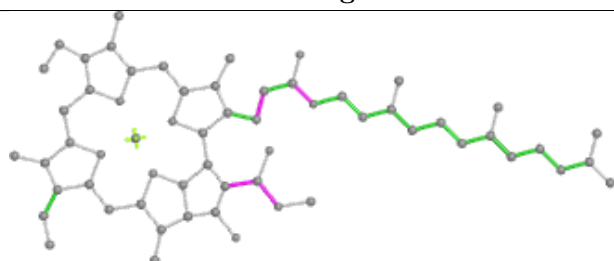
## Ligand CLA N 602



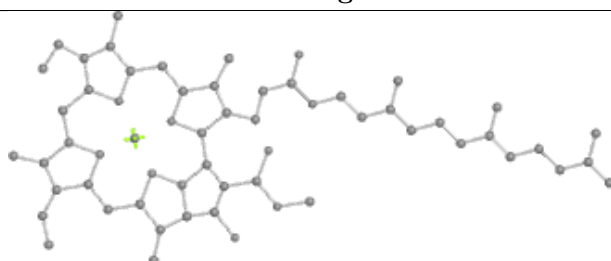
Bond lengths



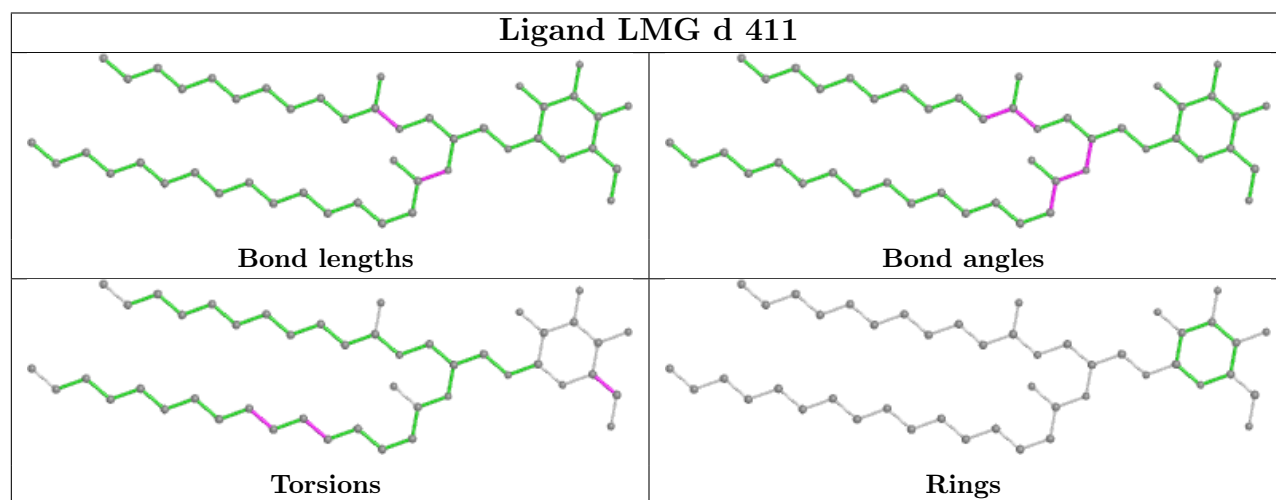
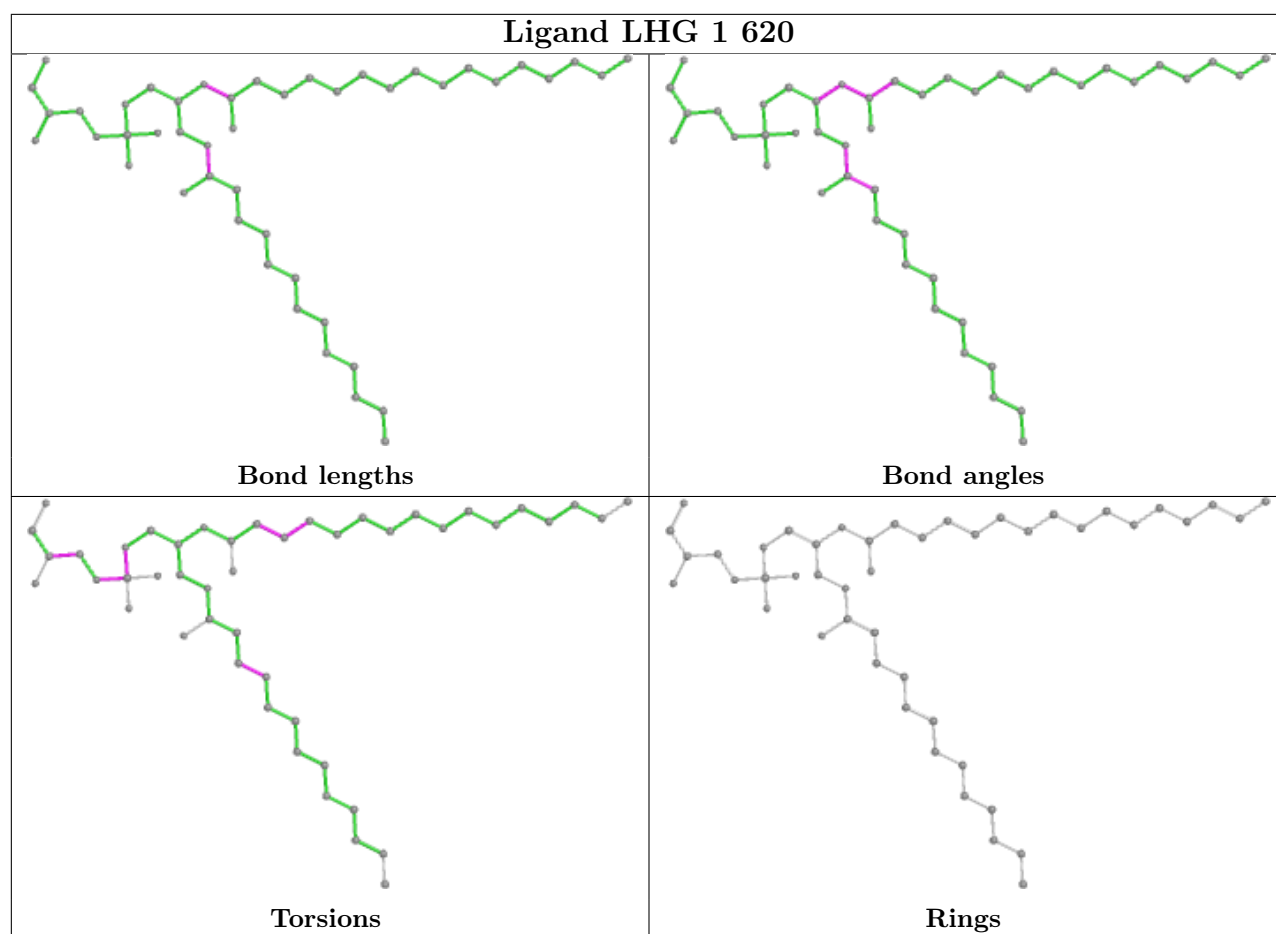
Bond angles

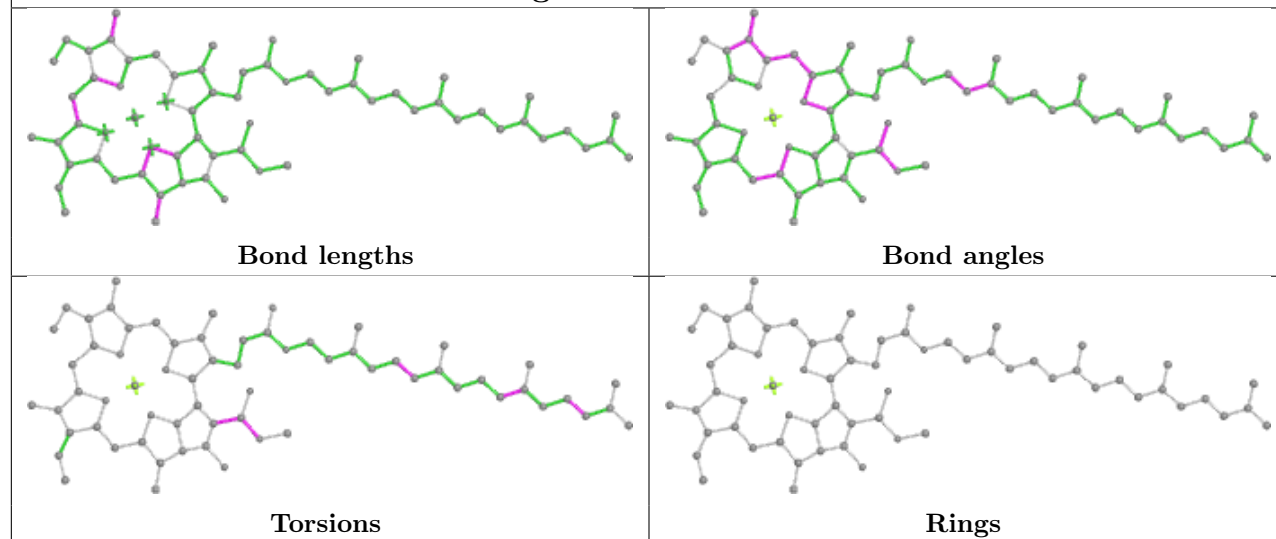
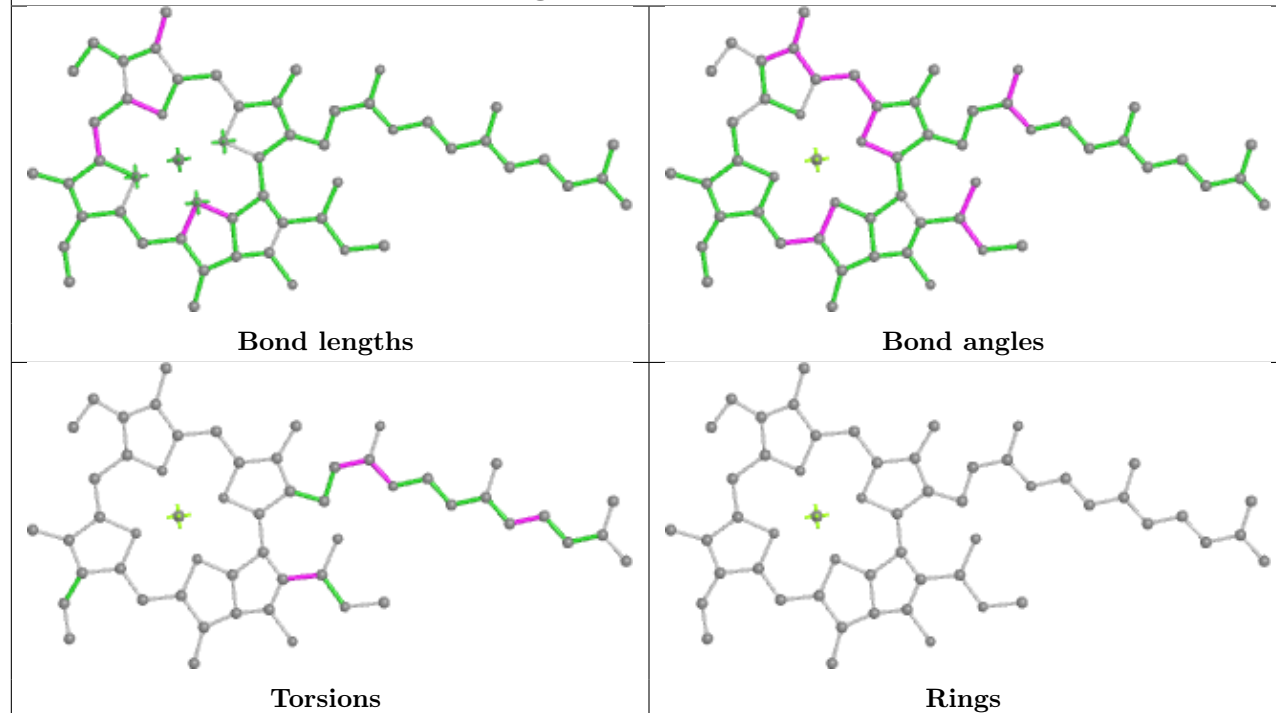


Torsions

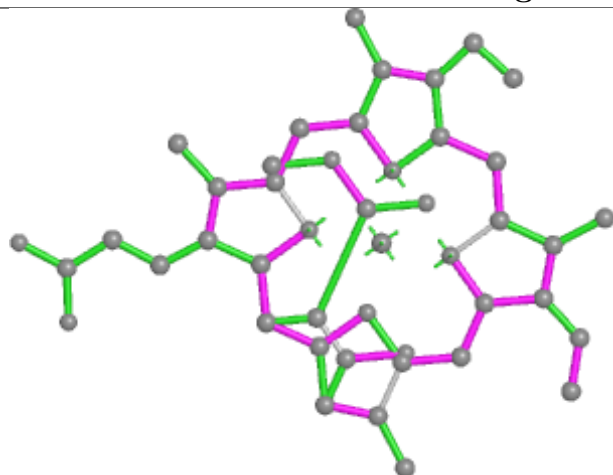


Rings

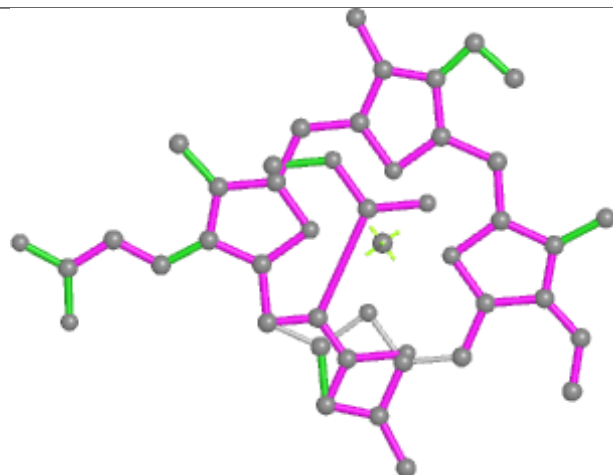


**Ligand CLA B 605****Ligand CLA R 302**

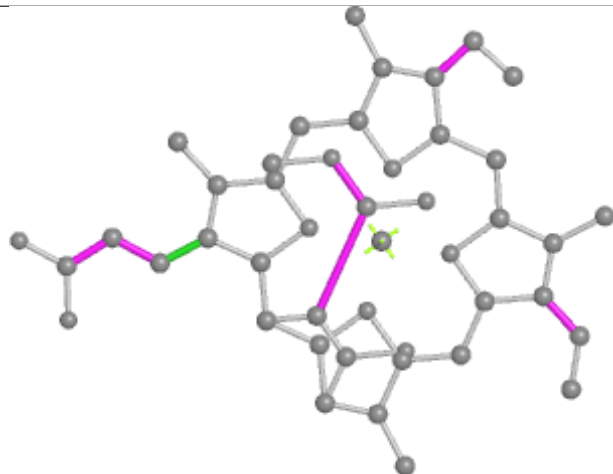
## Ligand KC2 N 605



Bond lengths



Bond angles

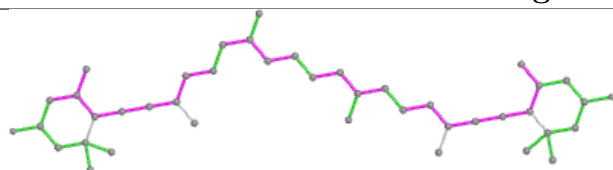


Torsions

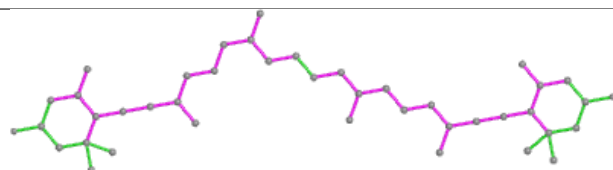


Rings

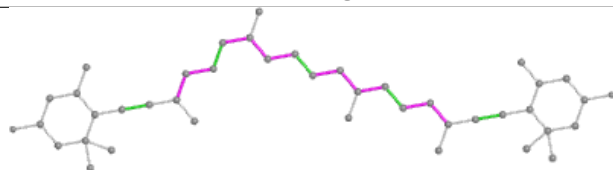
## Ligand II0 3 311



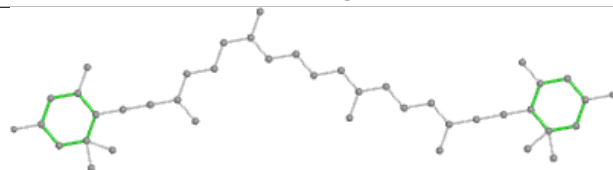
Bond lengths



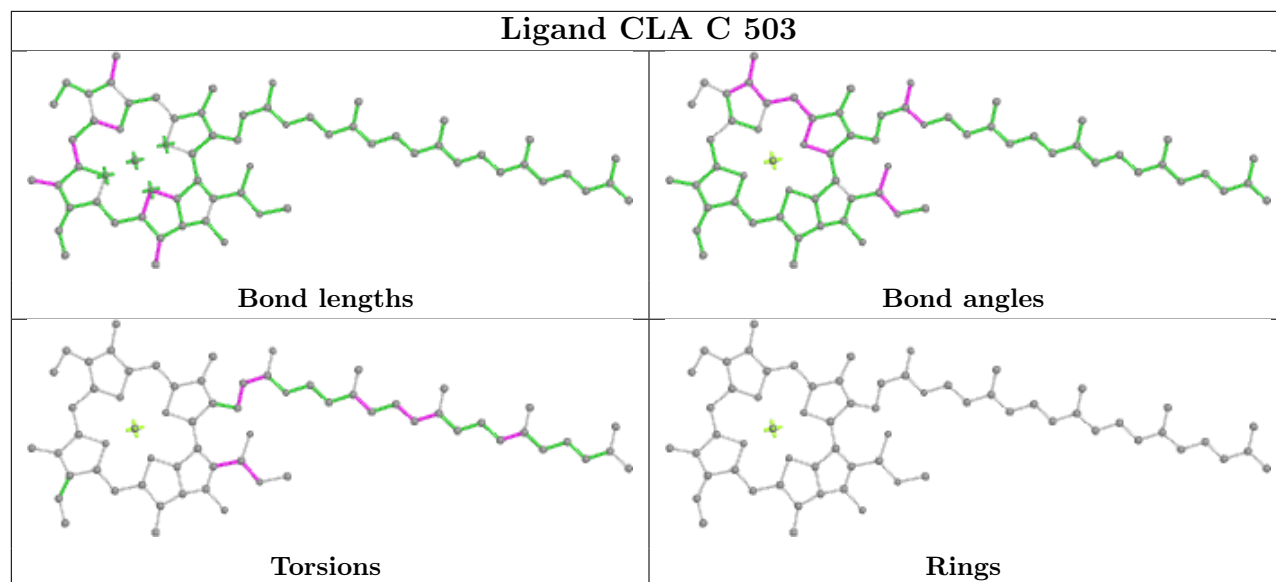
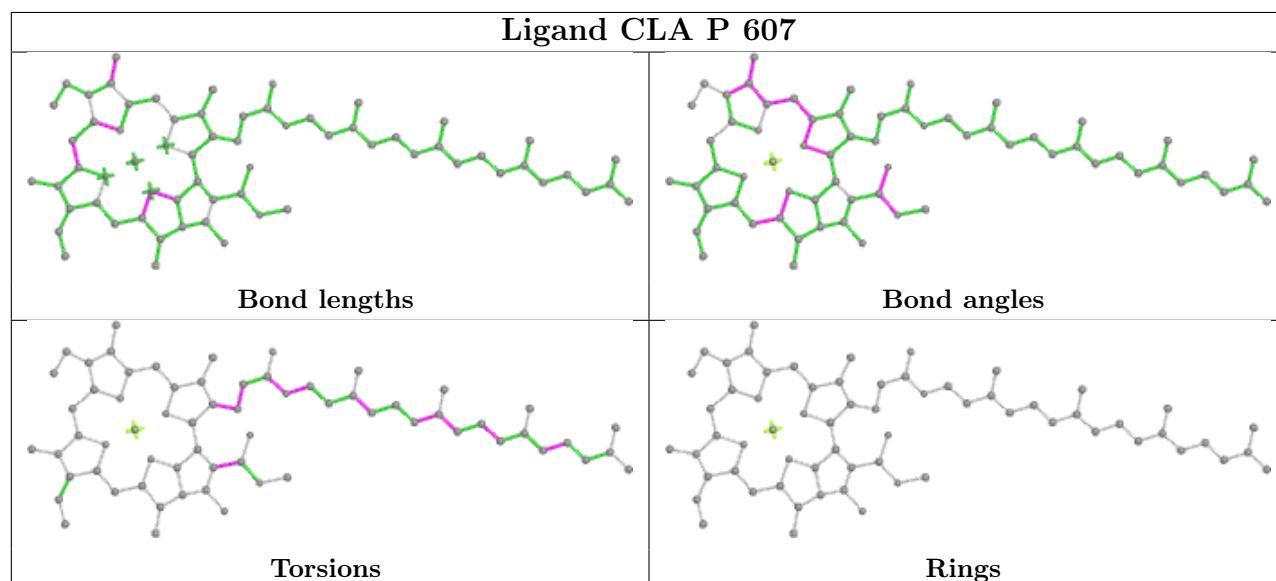
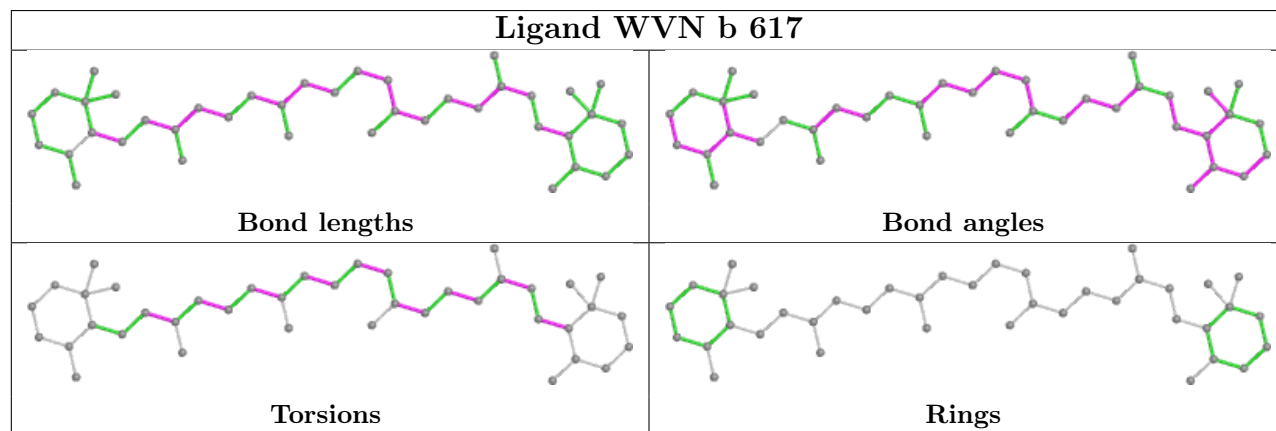
Bond angles



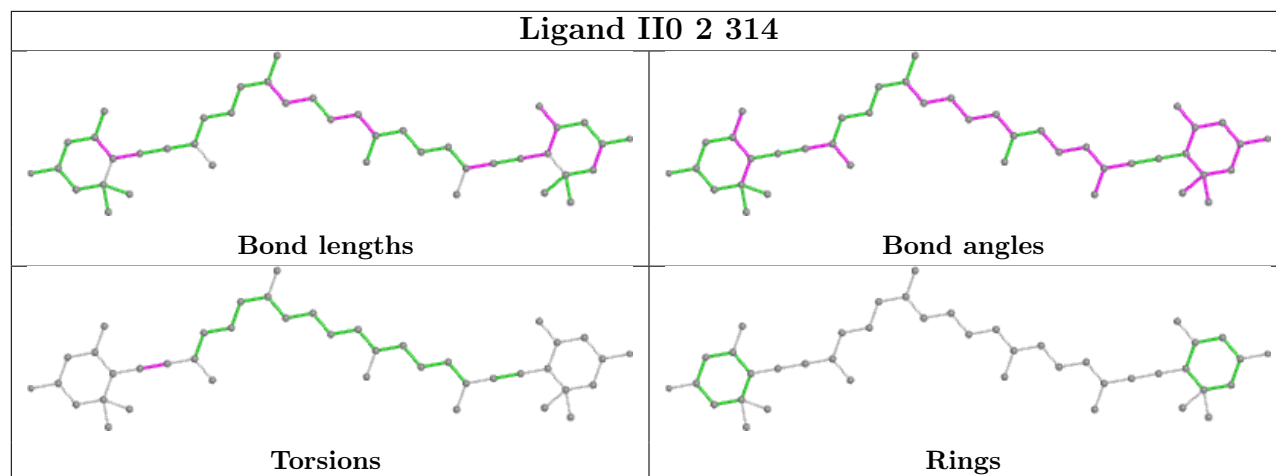
Torsions



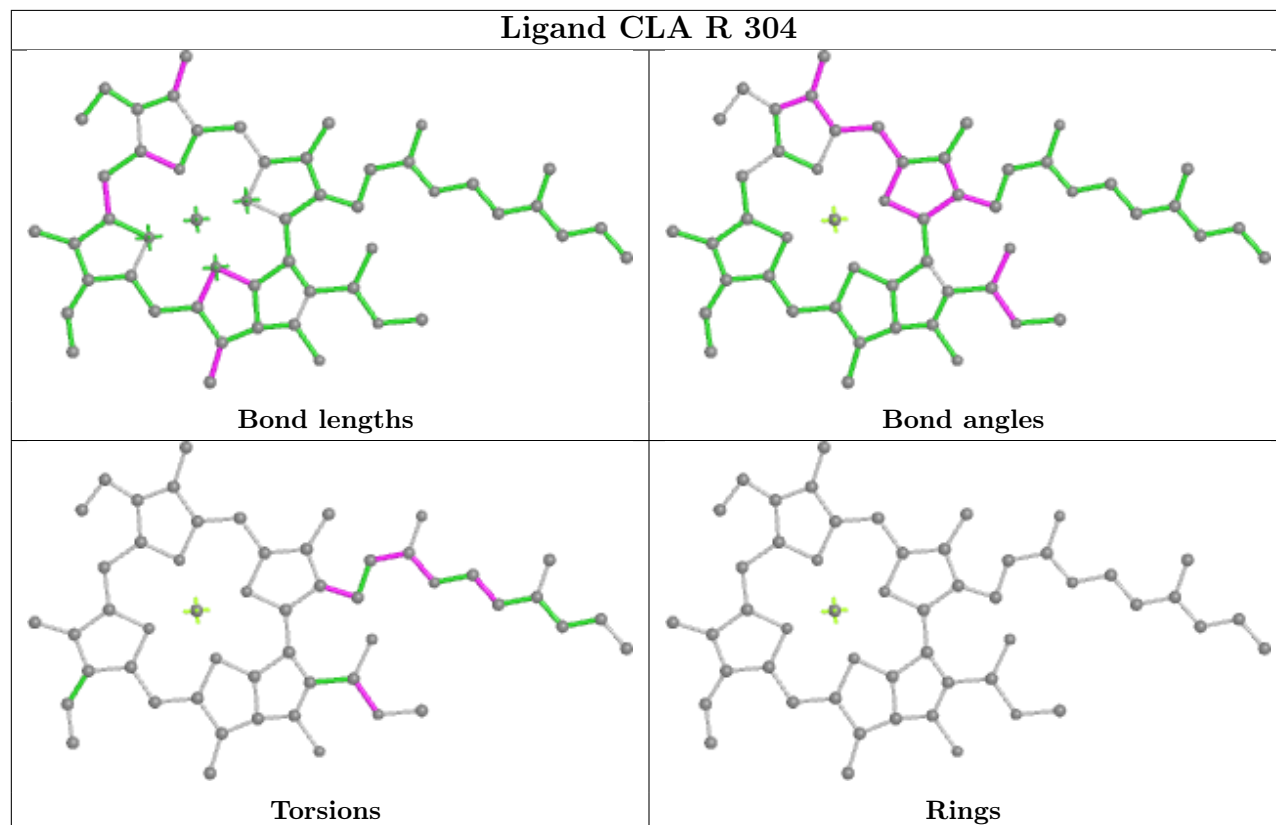
Rings

**Ligand CLA C 503****Ligand CLA P 607****Ligand WVN b 617**

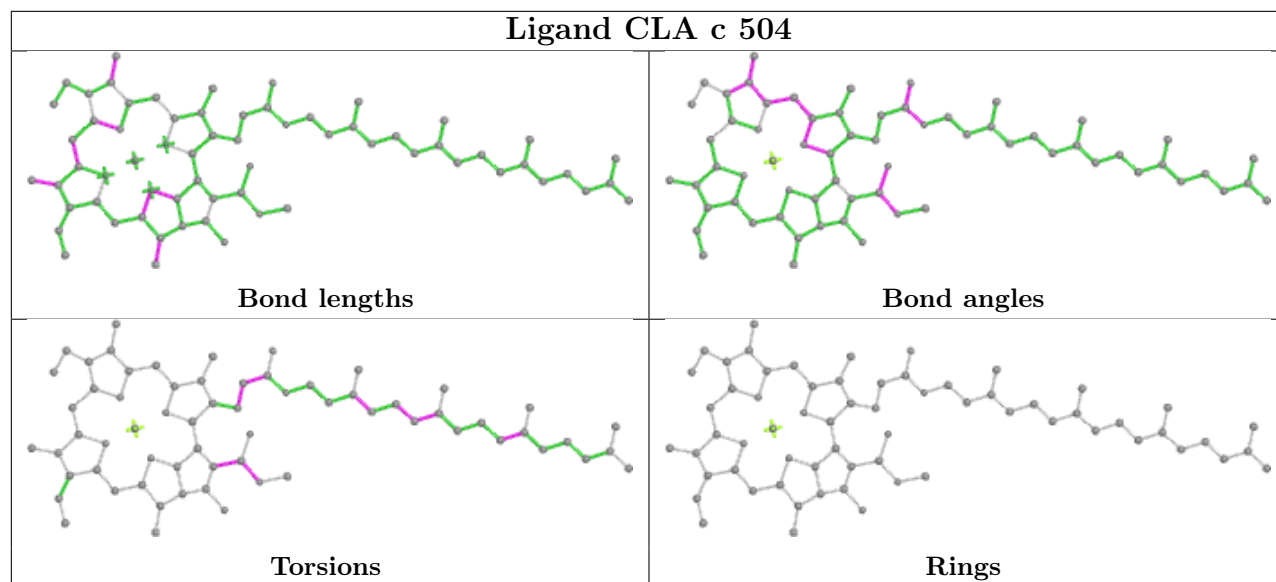
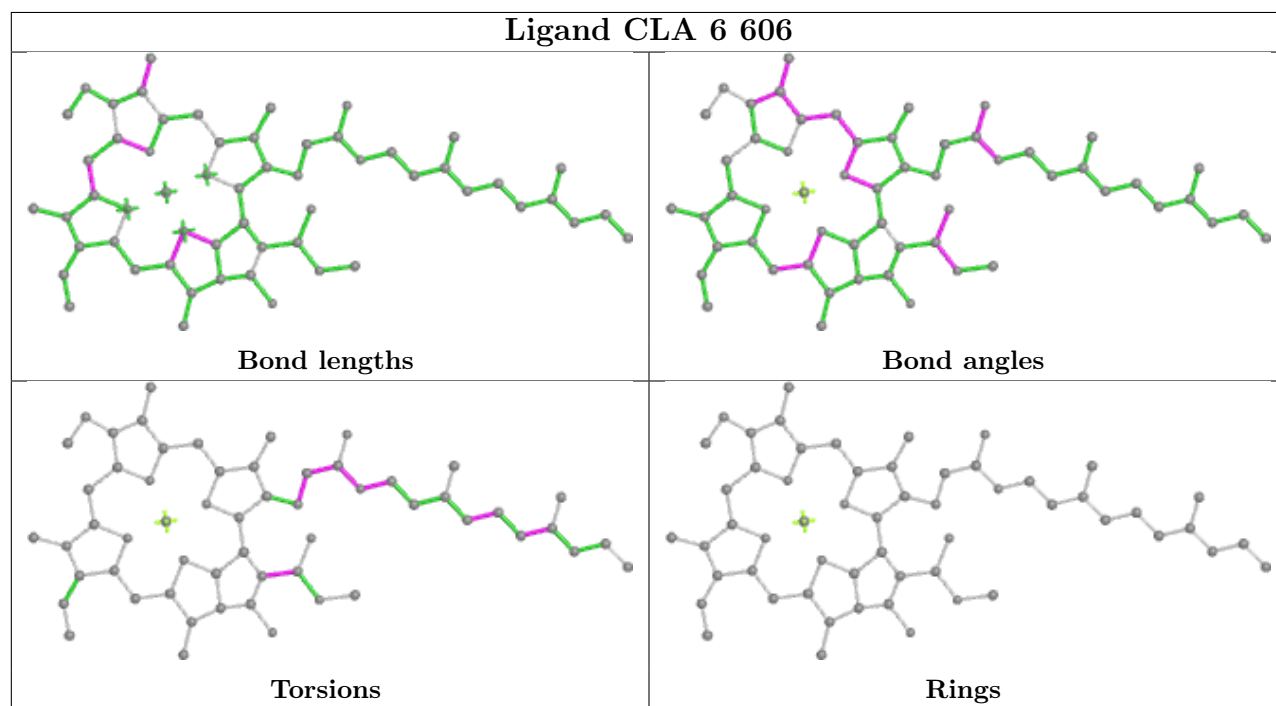
## Ligand II0 2 314

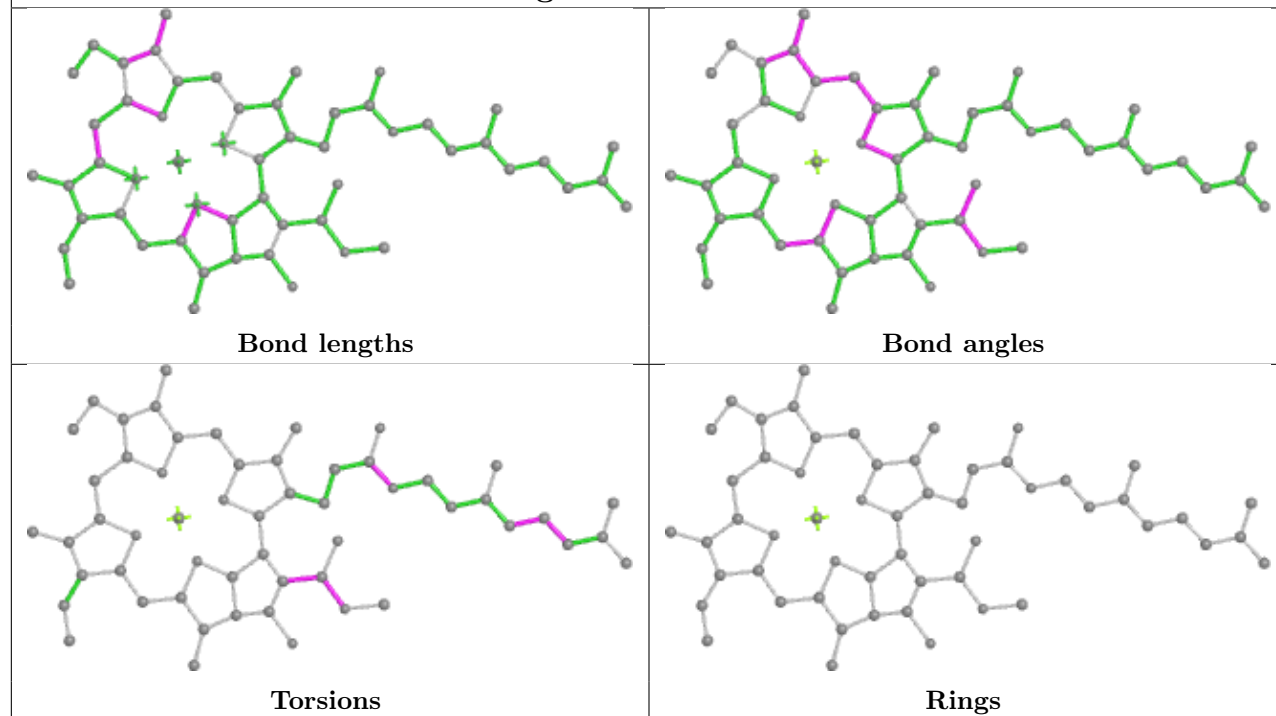
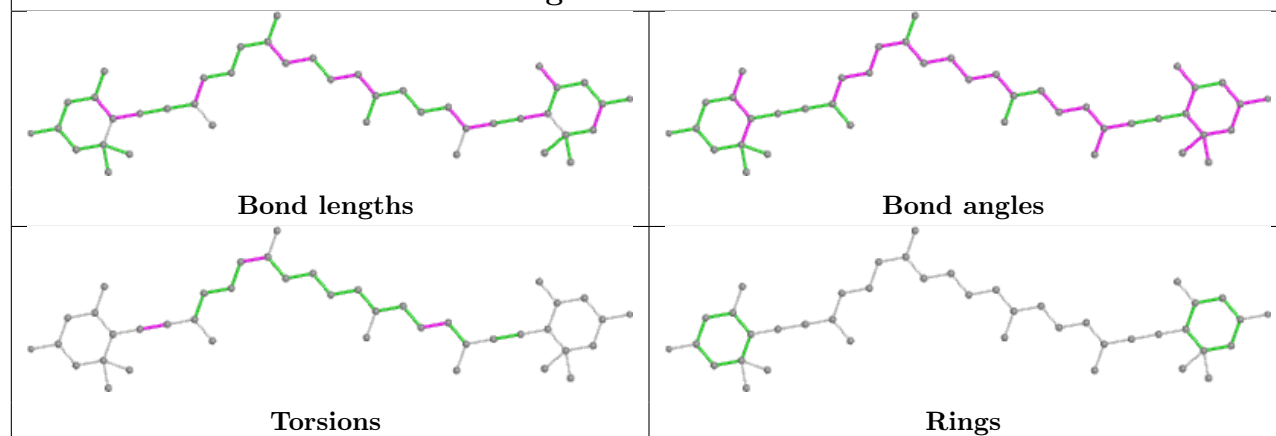


## Ligand CLA R 304

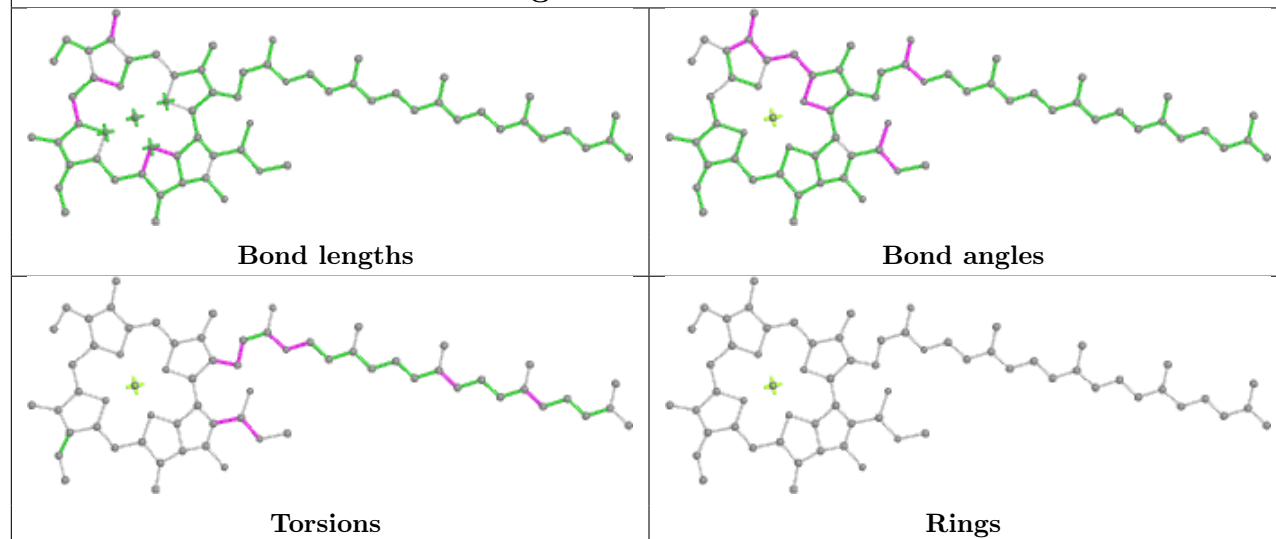




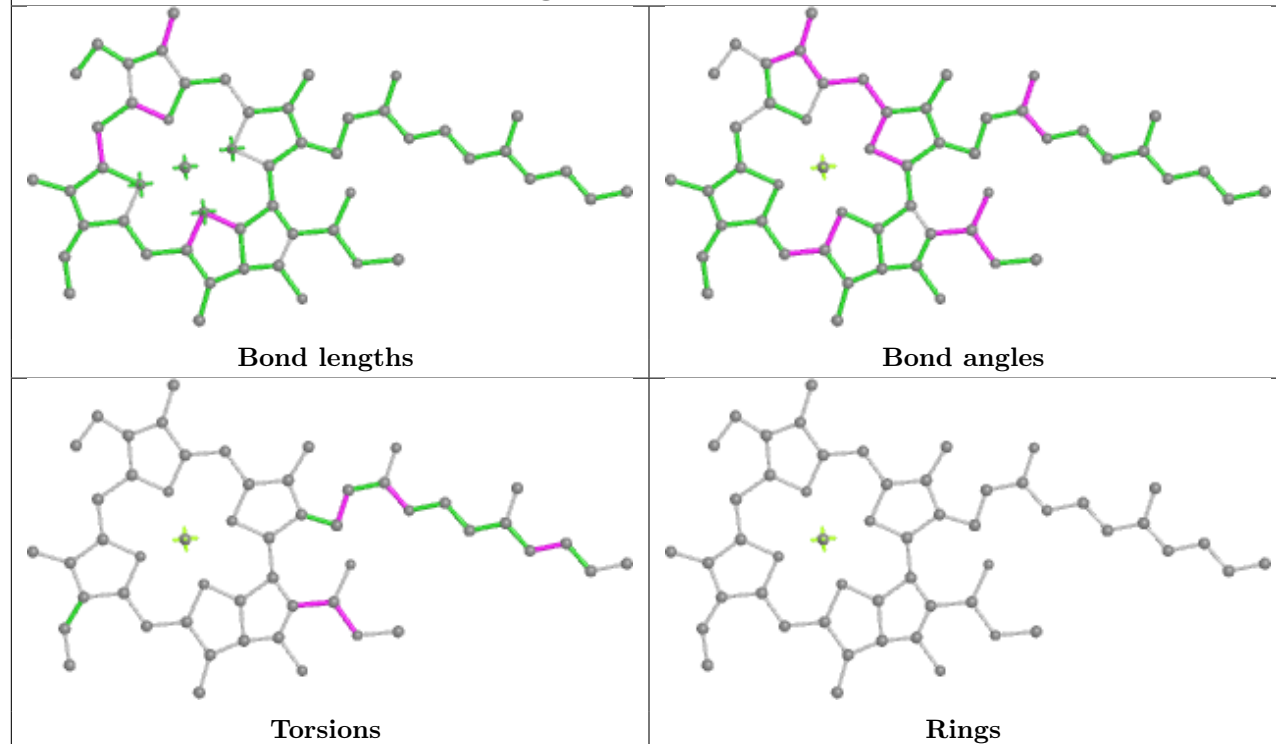
**Ligand CLA c 504****Ligand CLA 6 606**

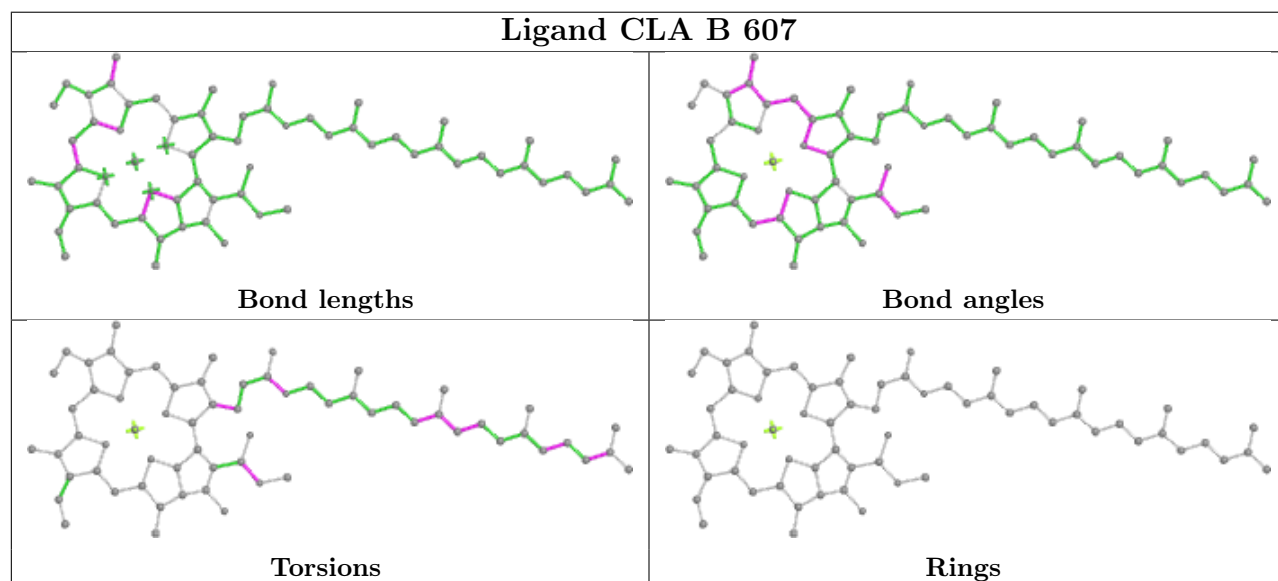
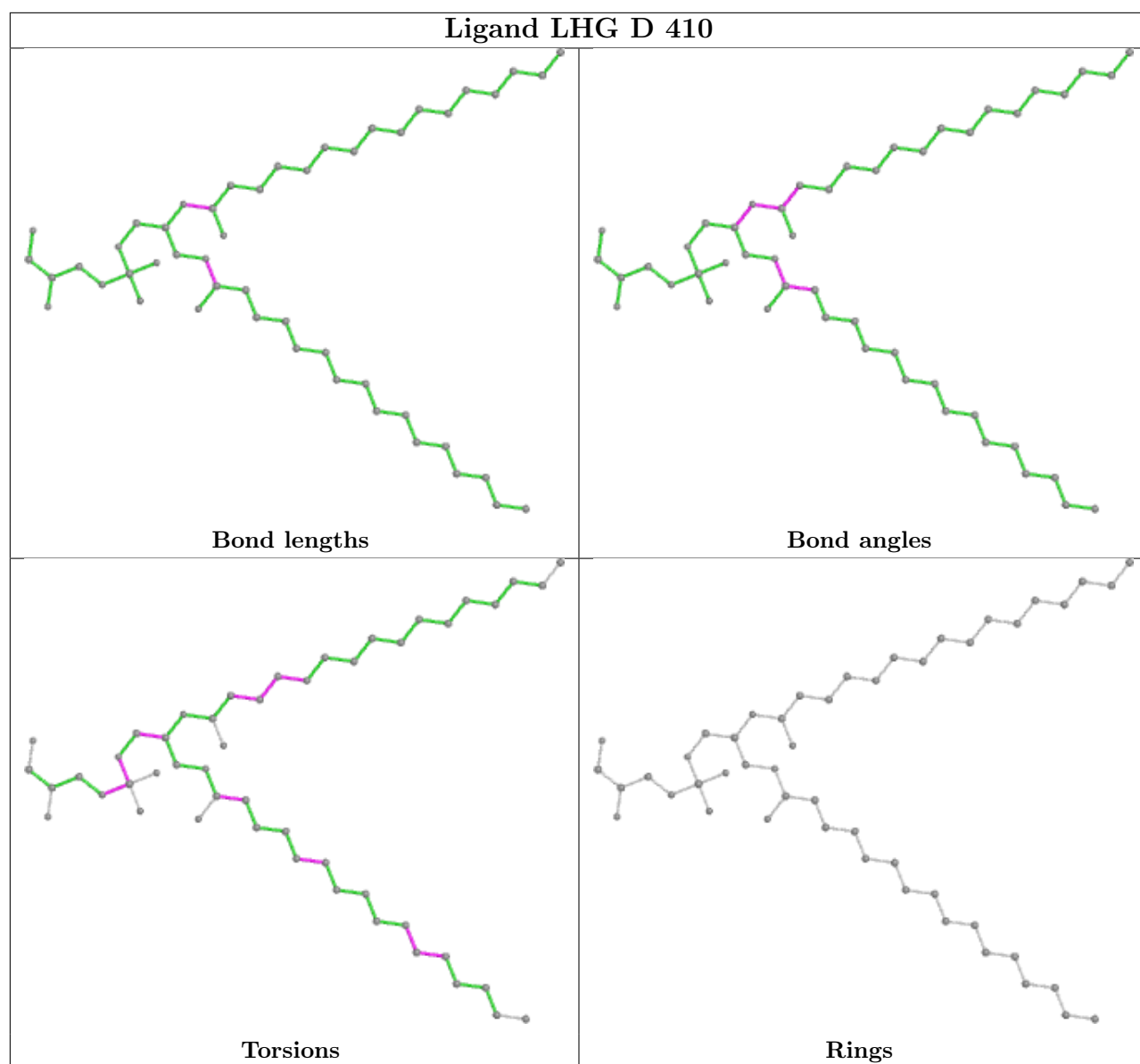
**Ligand CLA 6 601****Ligand II0 N 618**

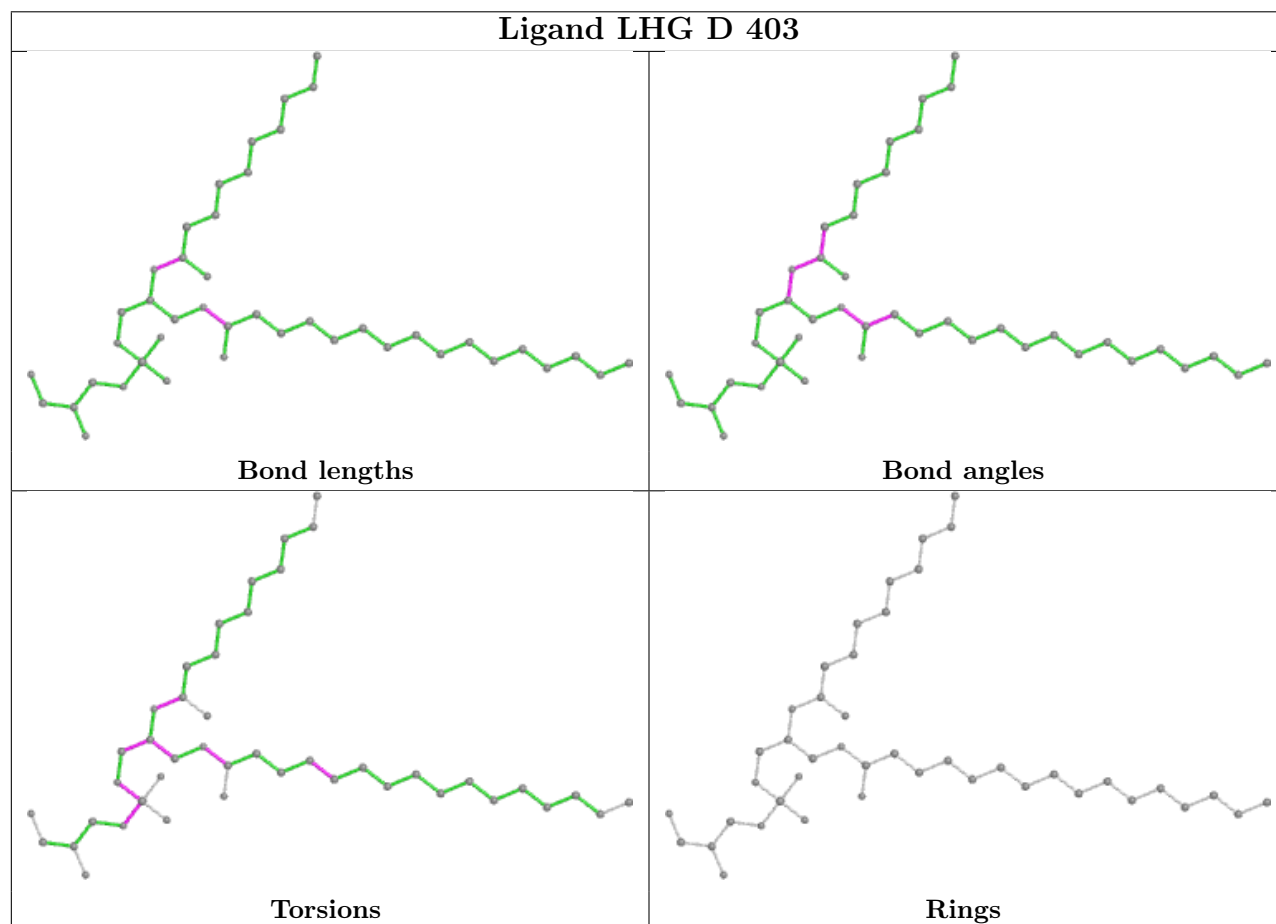
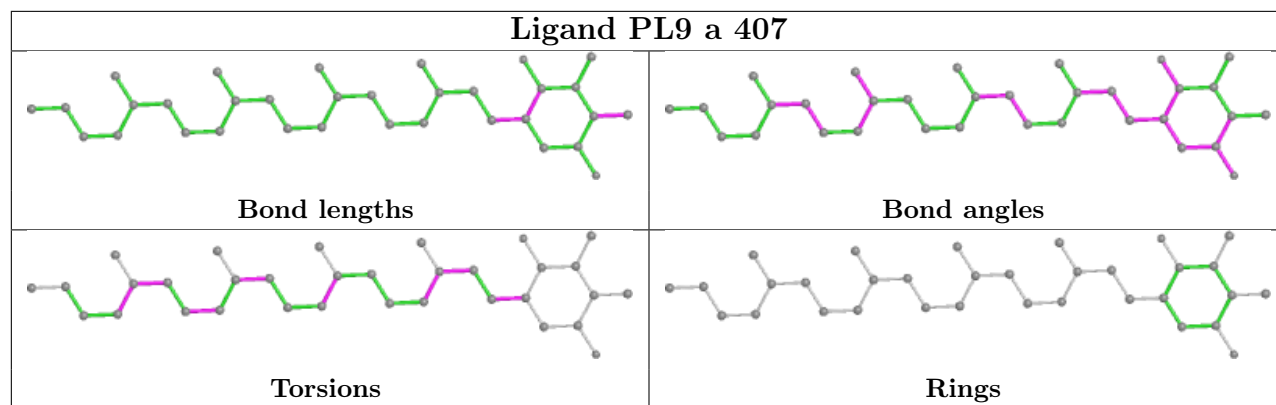
## Ligand CLA R 306

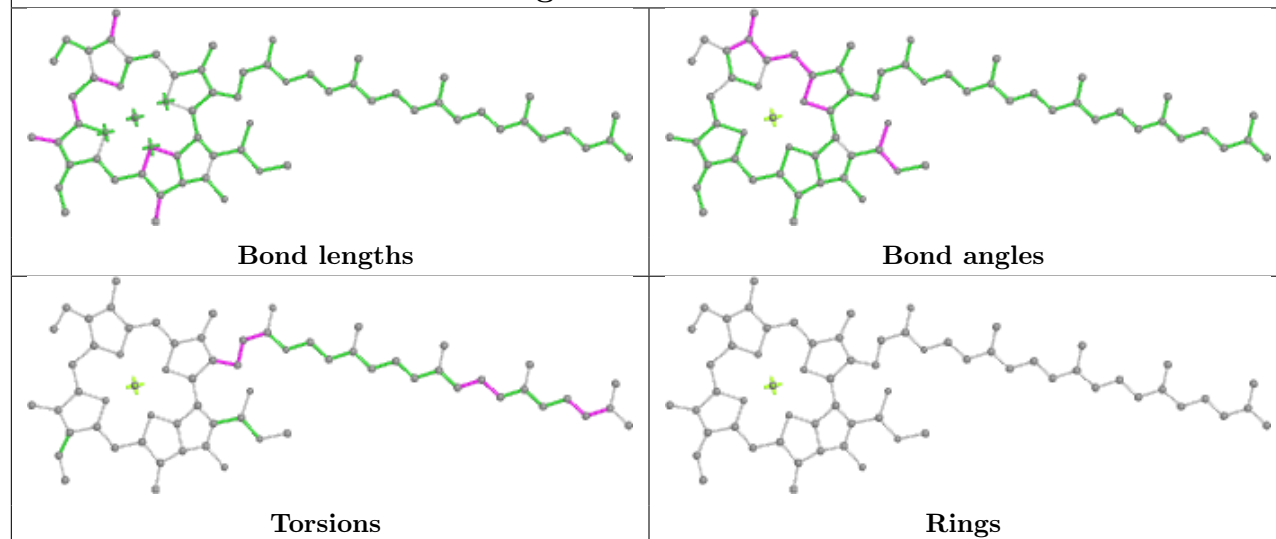
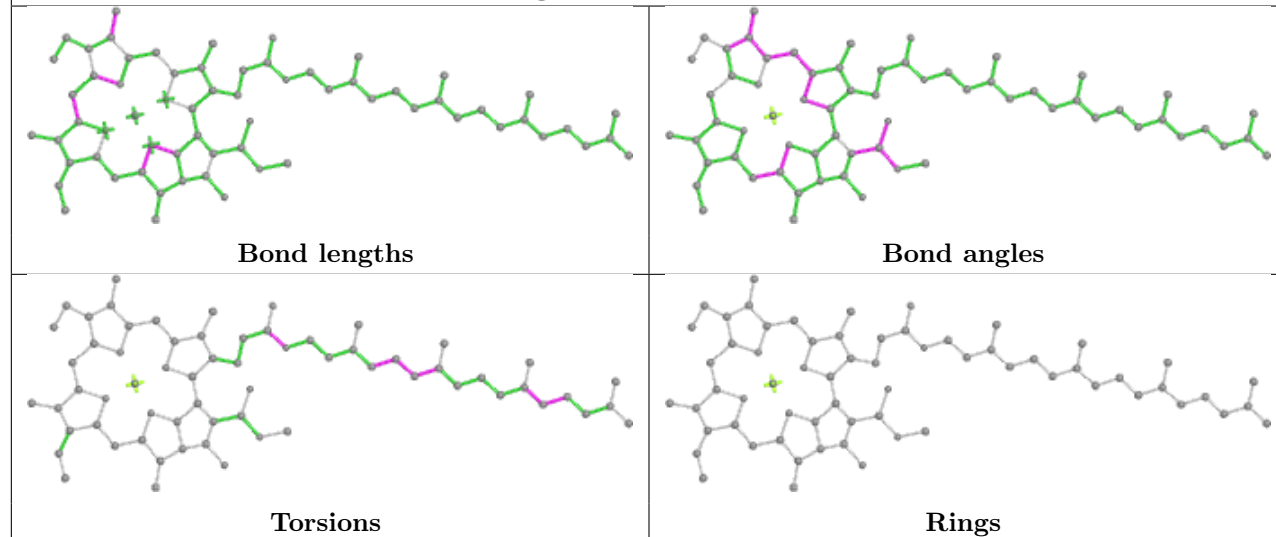


## Ligand CLA c 515

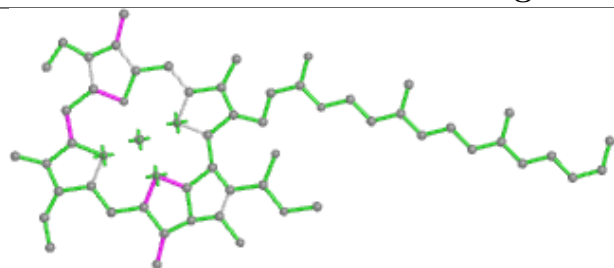




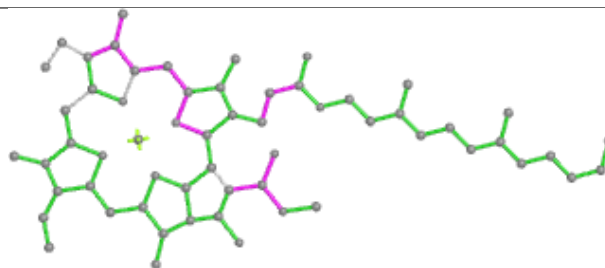


**Ligand CLA 2 303****Ligand CLA P 606**

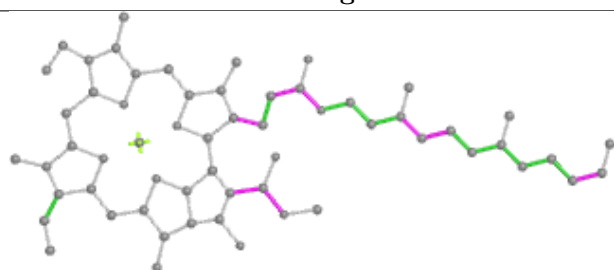
## Ligand CLA B 604



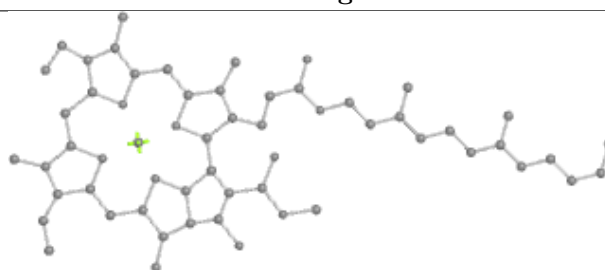
Bond lengths



Bond angles

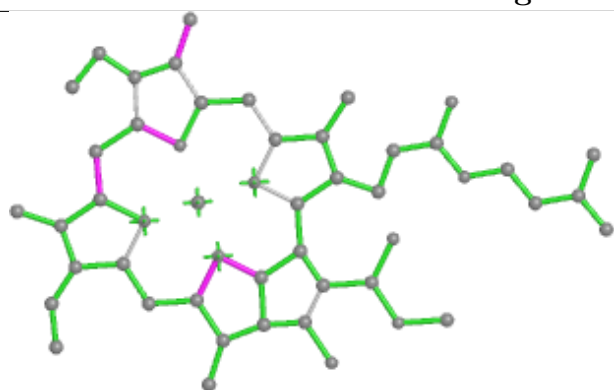


Torsions

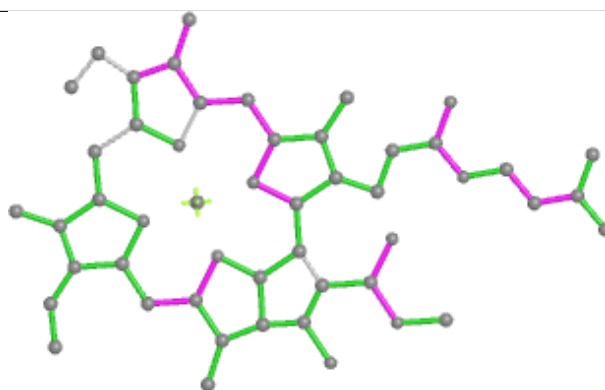


Rings

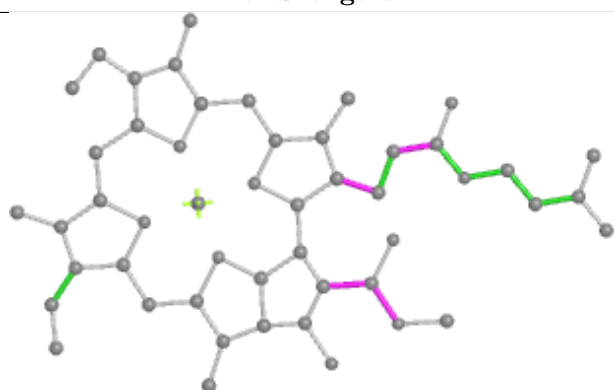
## Ligand CLA B 601



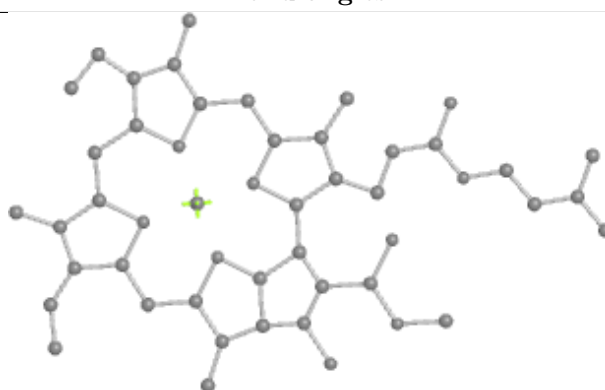
Bond lengths



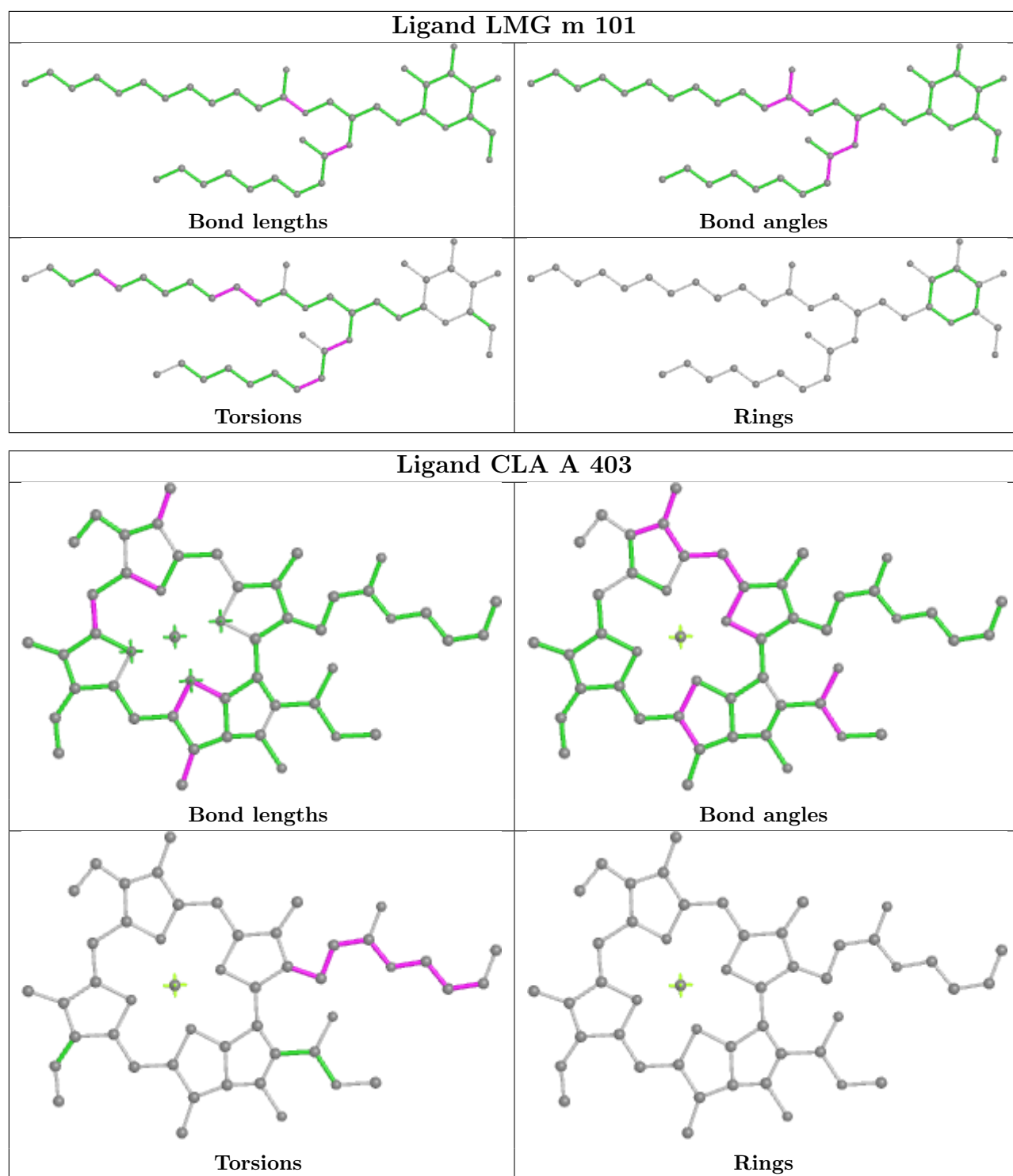
Bond angles



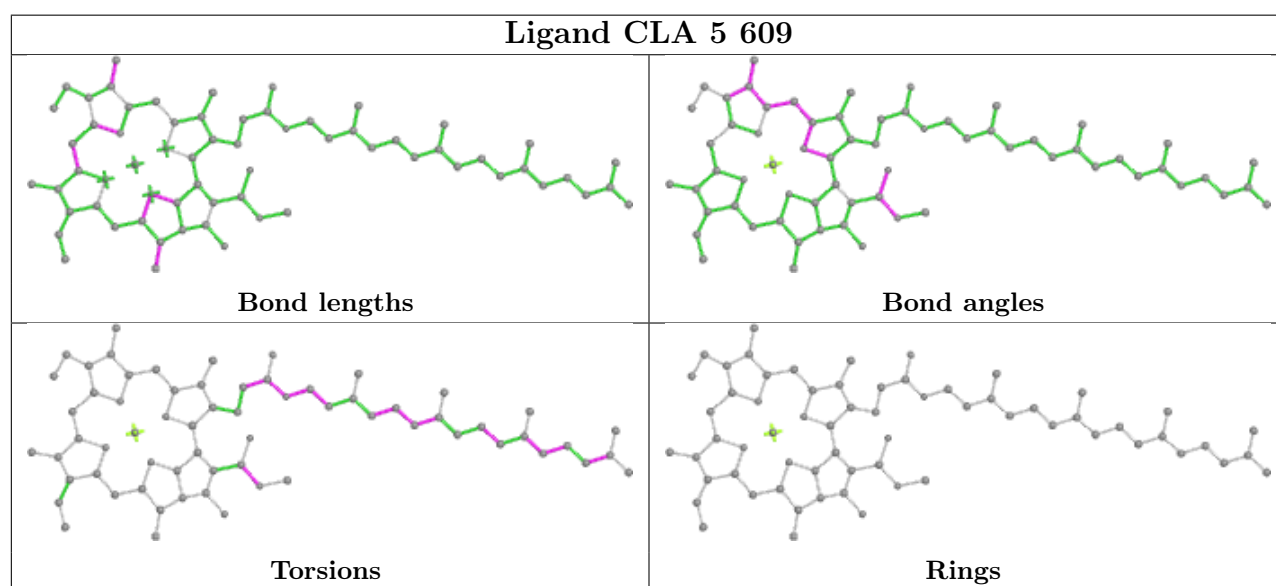
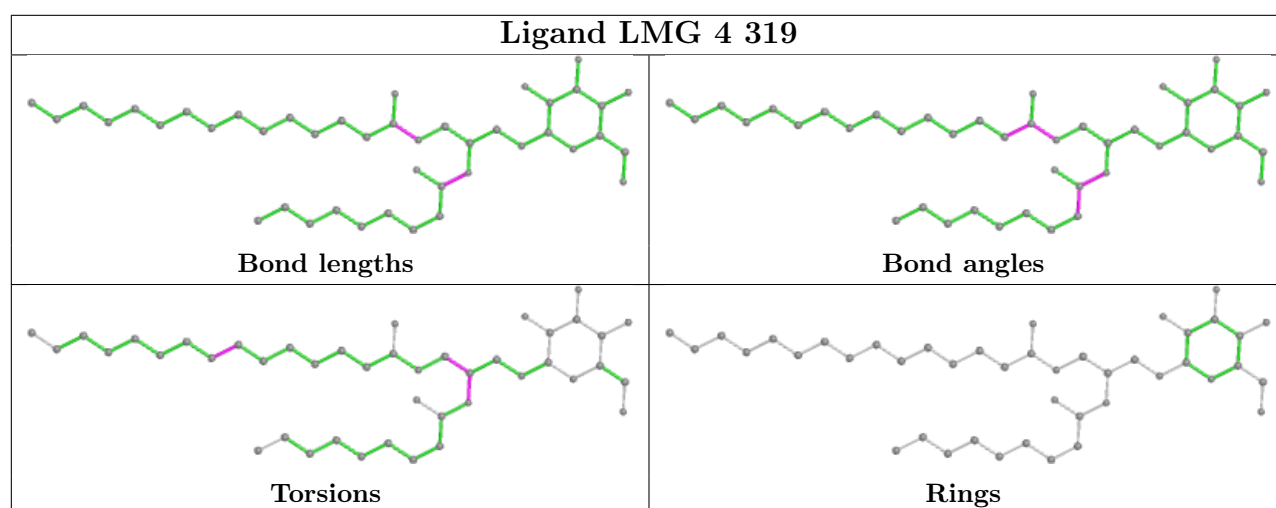
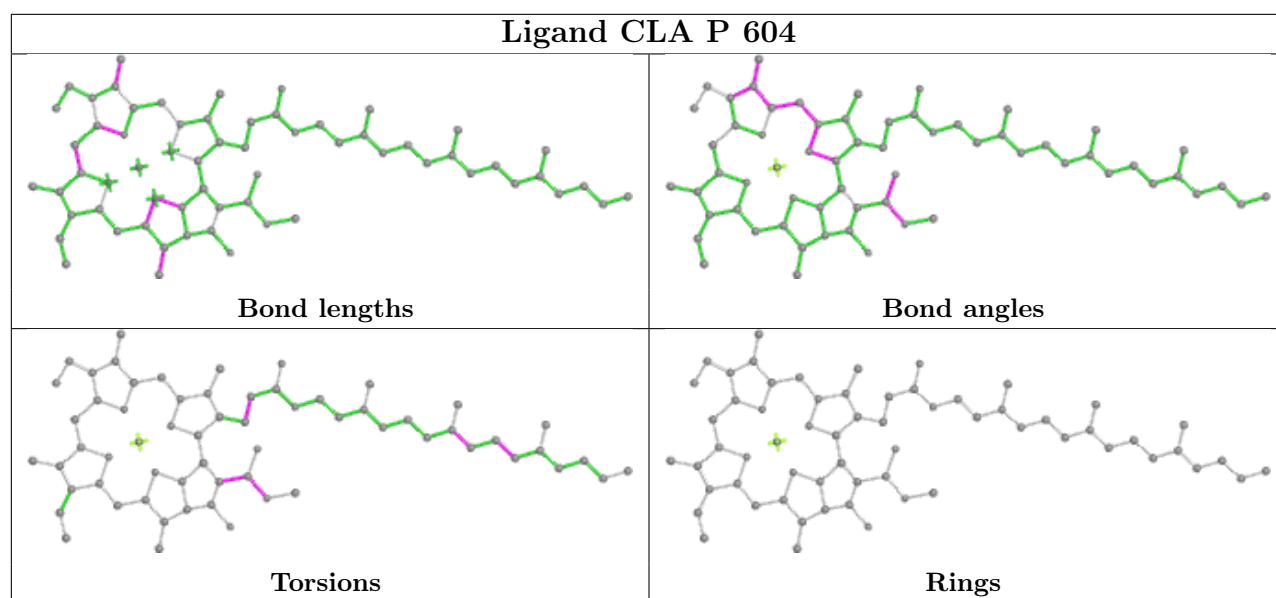
Torsions

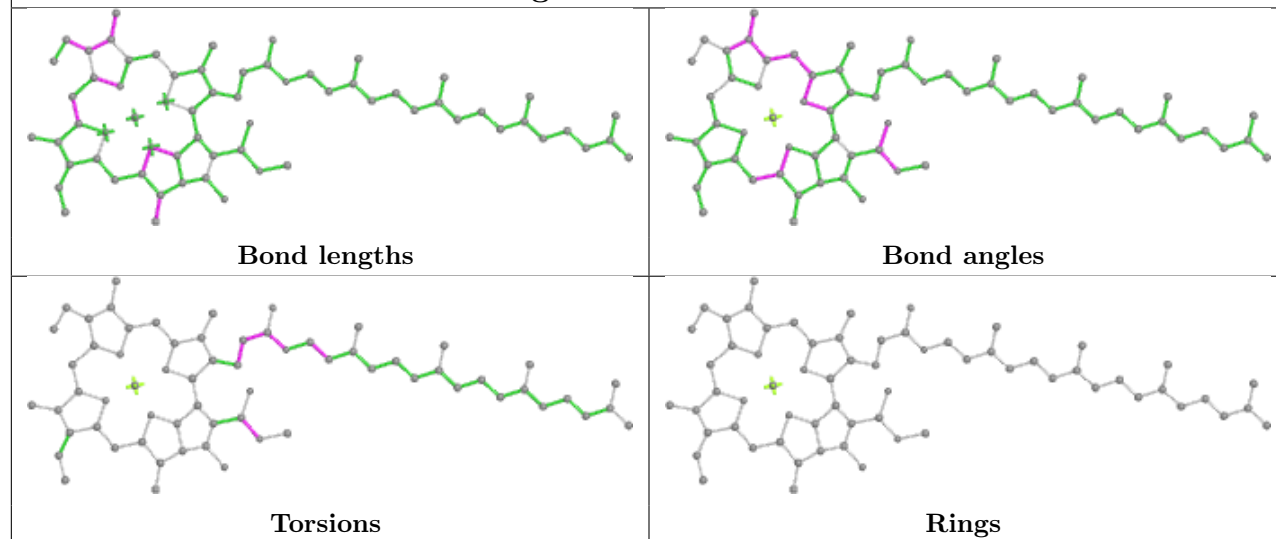
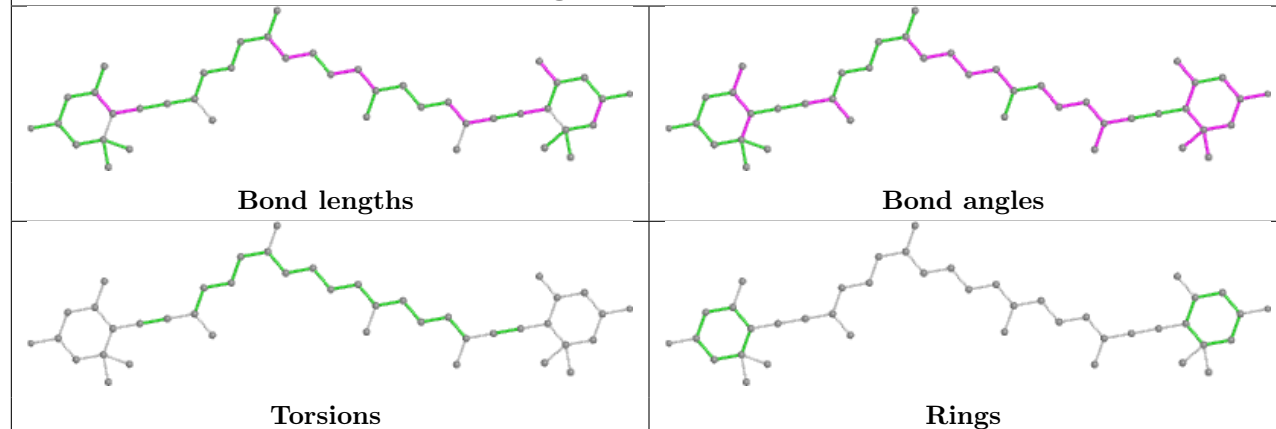
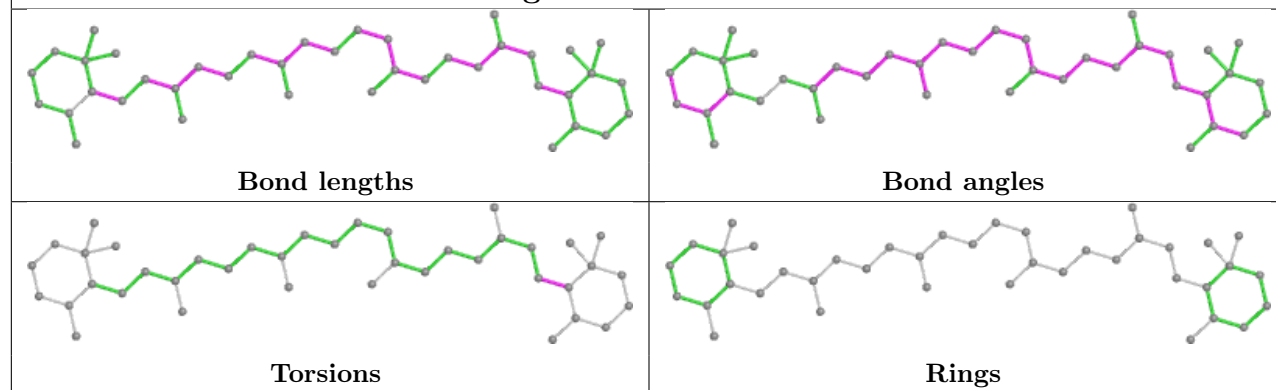


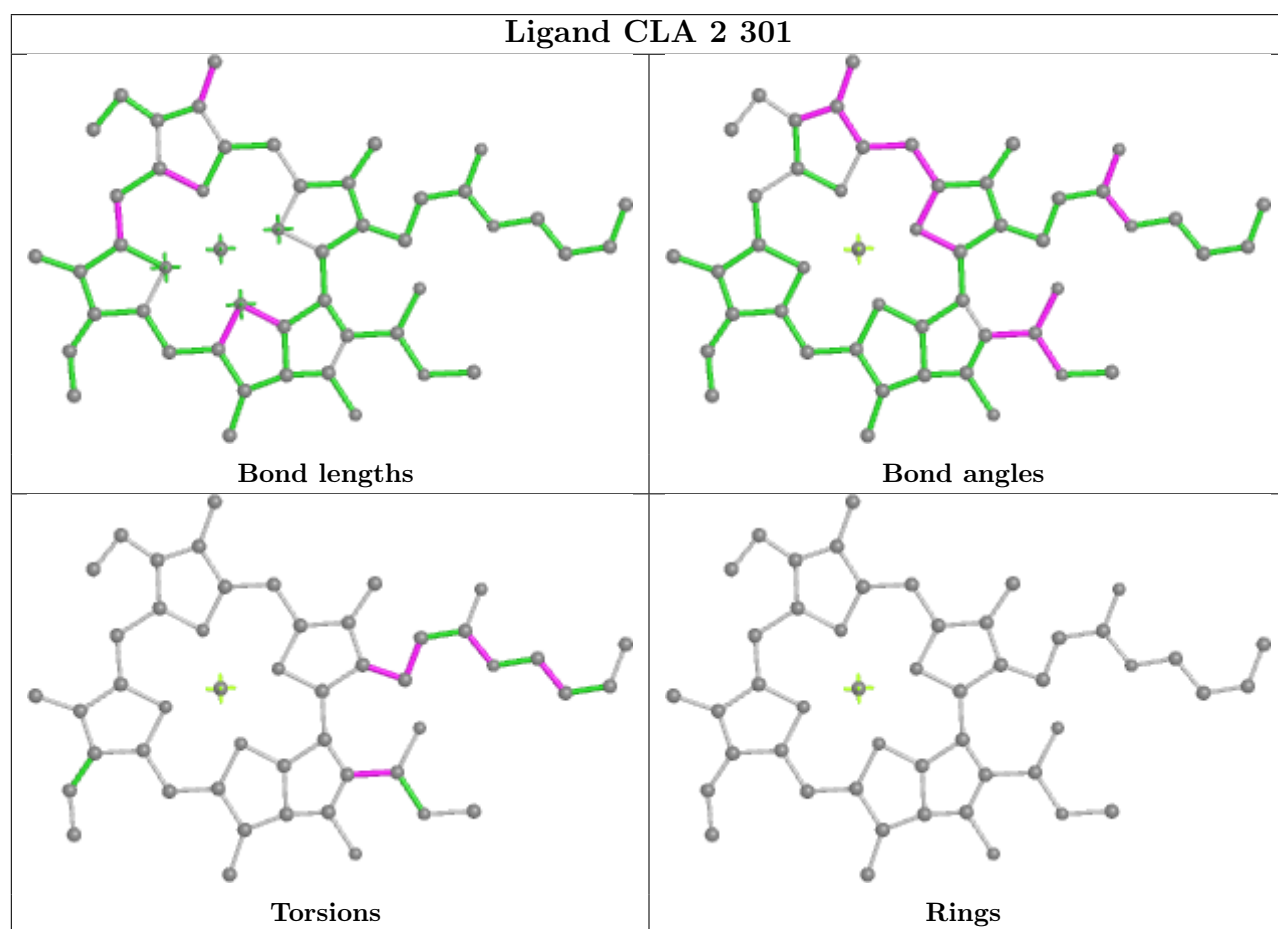
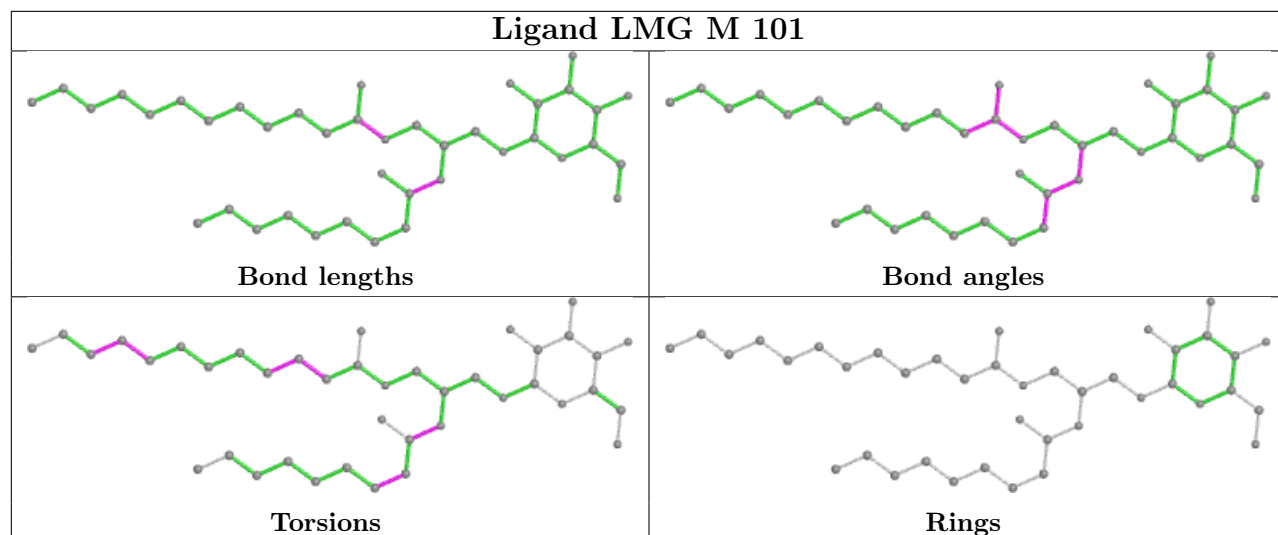
Rings



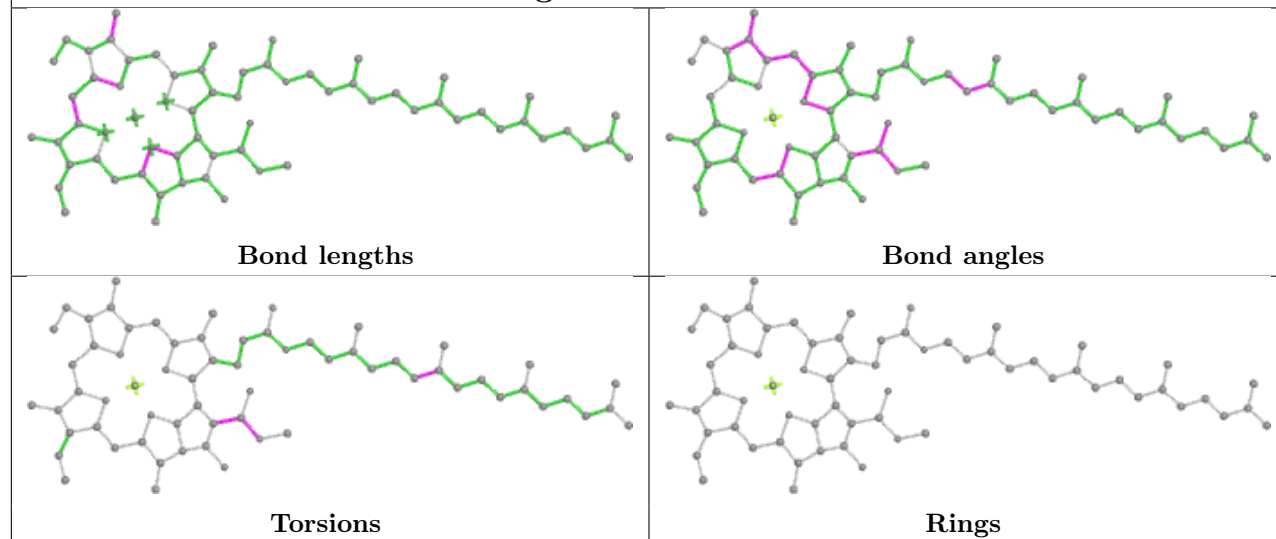




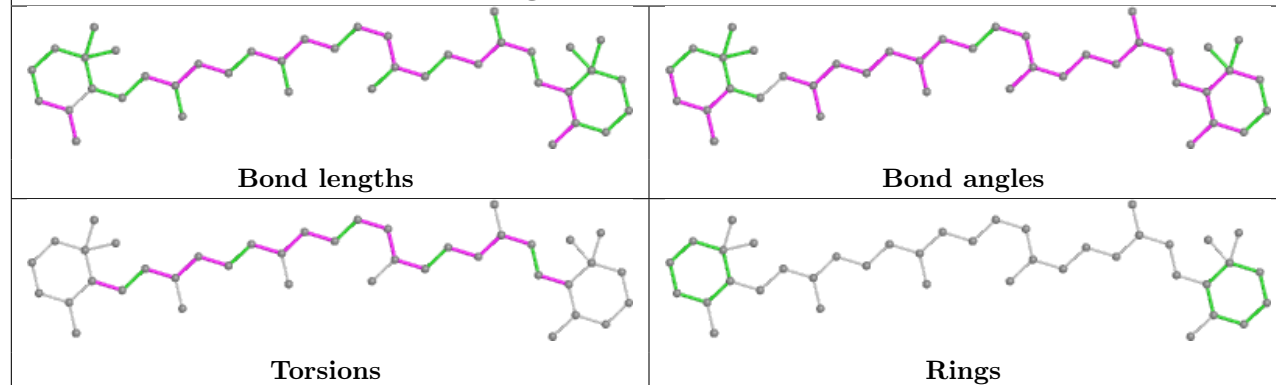
**Ligand CLA A 402****Ligand II0 4 315****Ligand WVN A 406**



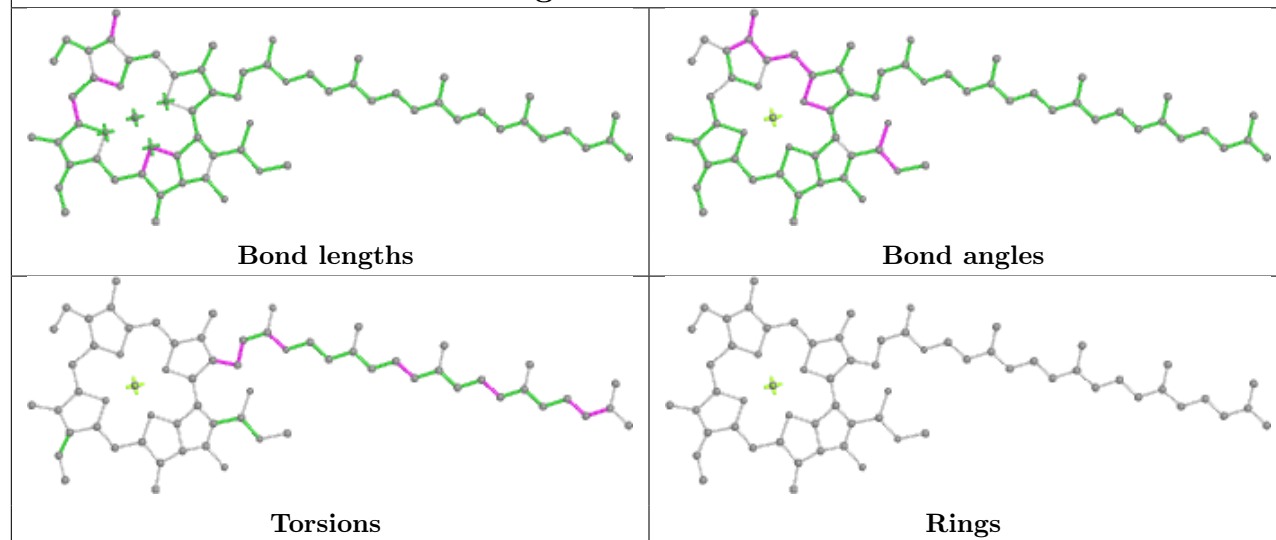
## Ligand CLA b 602



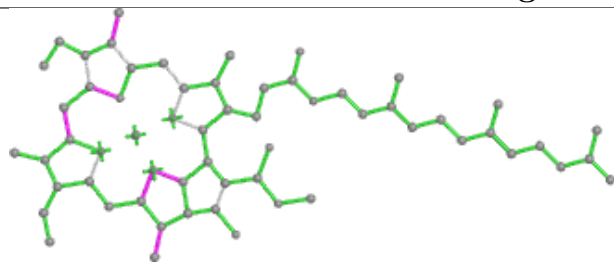
## Ligand WVN C 516



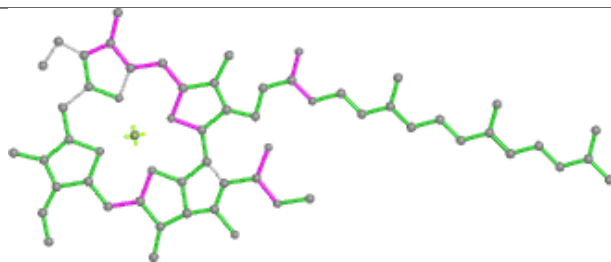
## Ligand CLA b 615



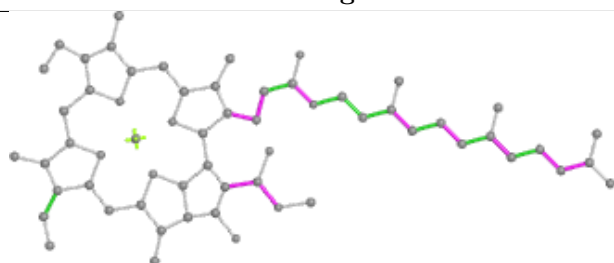
## Ligand CLA 1 609



Bond lengths



Bond angles

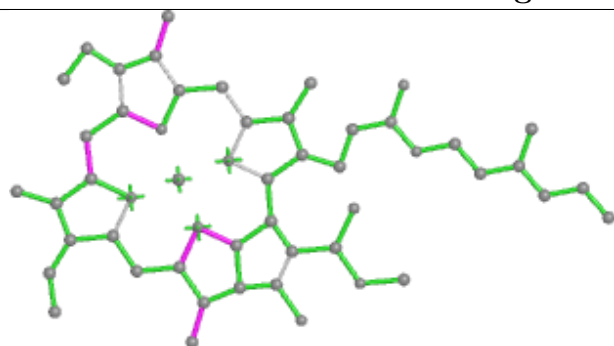


Torsions

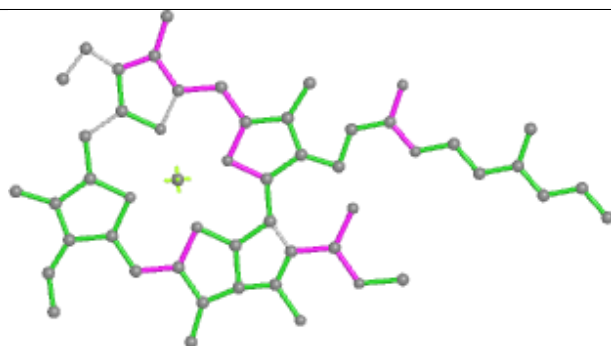


Rings

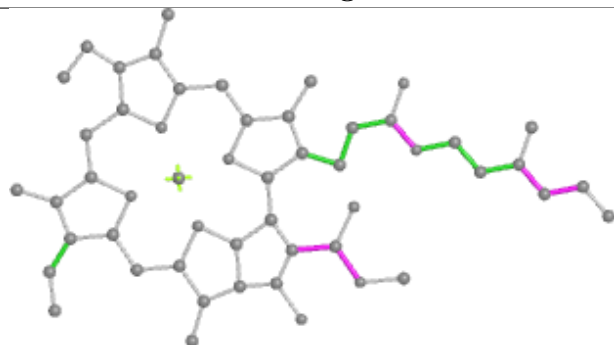
## Ligand CLA C 514



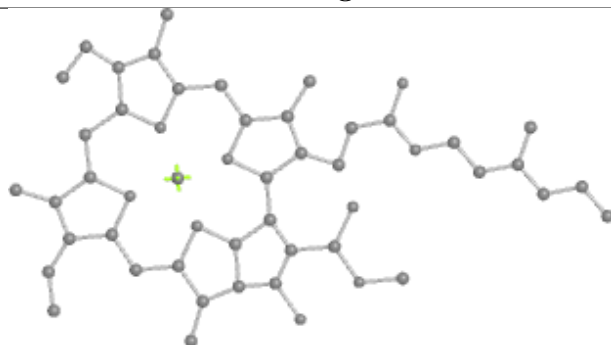
Bond lengths



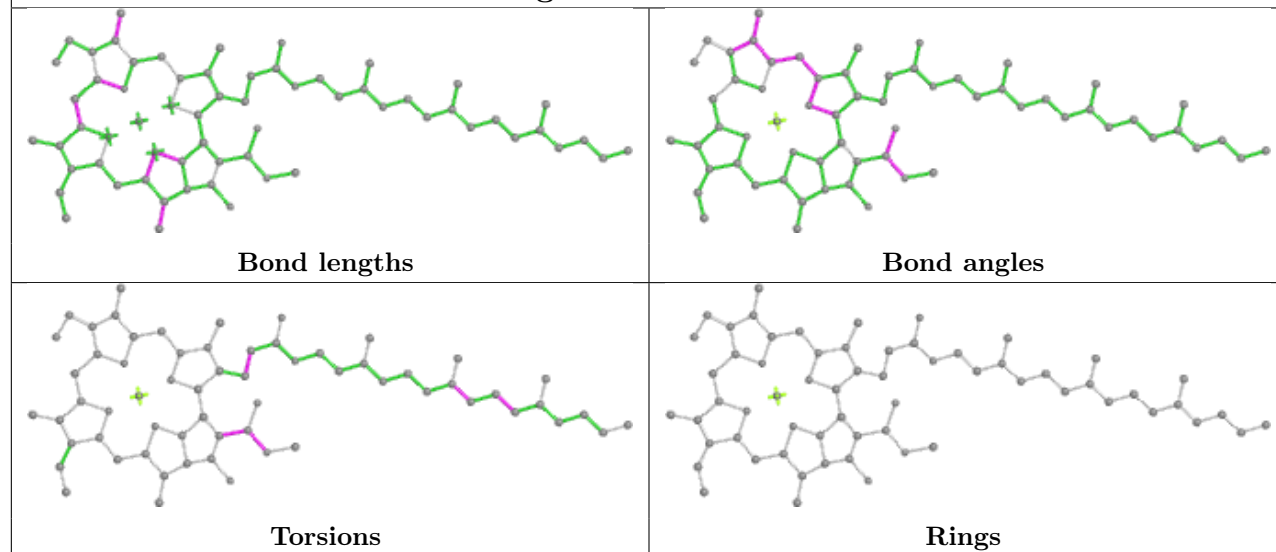
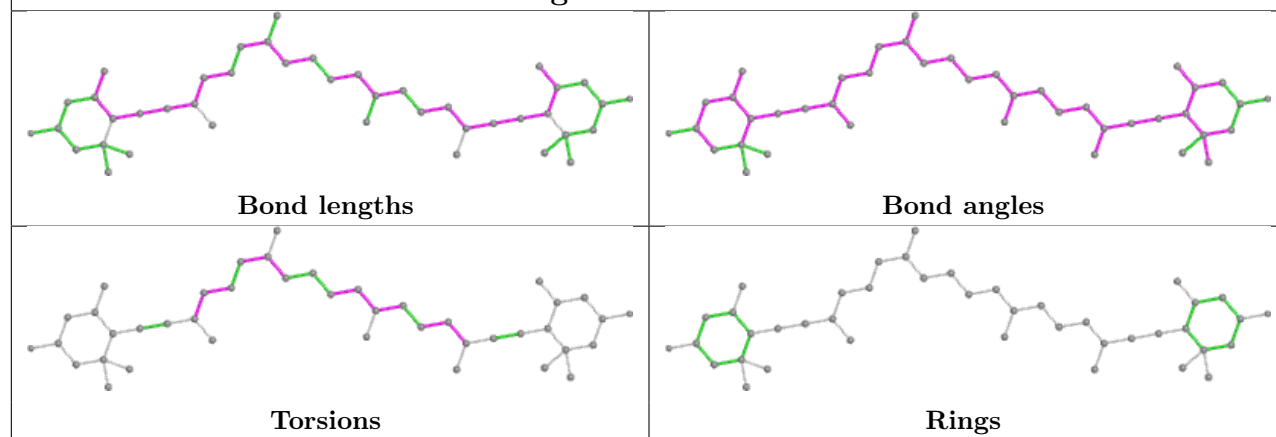
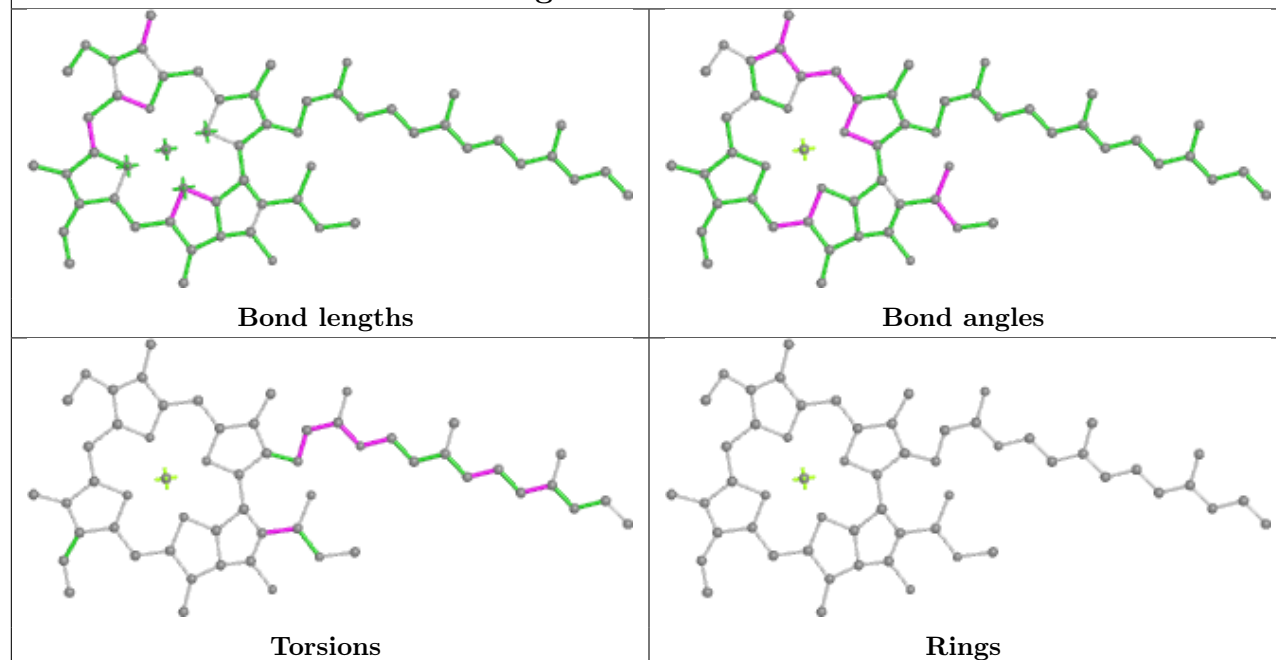
Bond angles



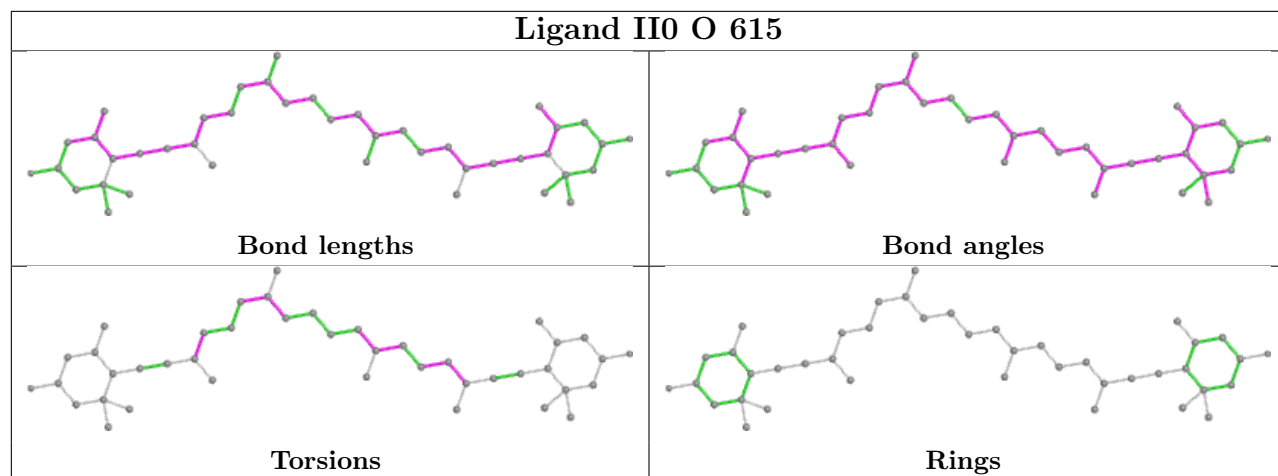
Torsions



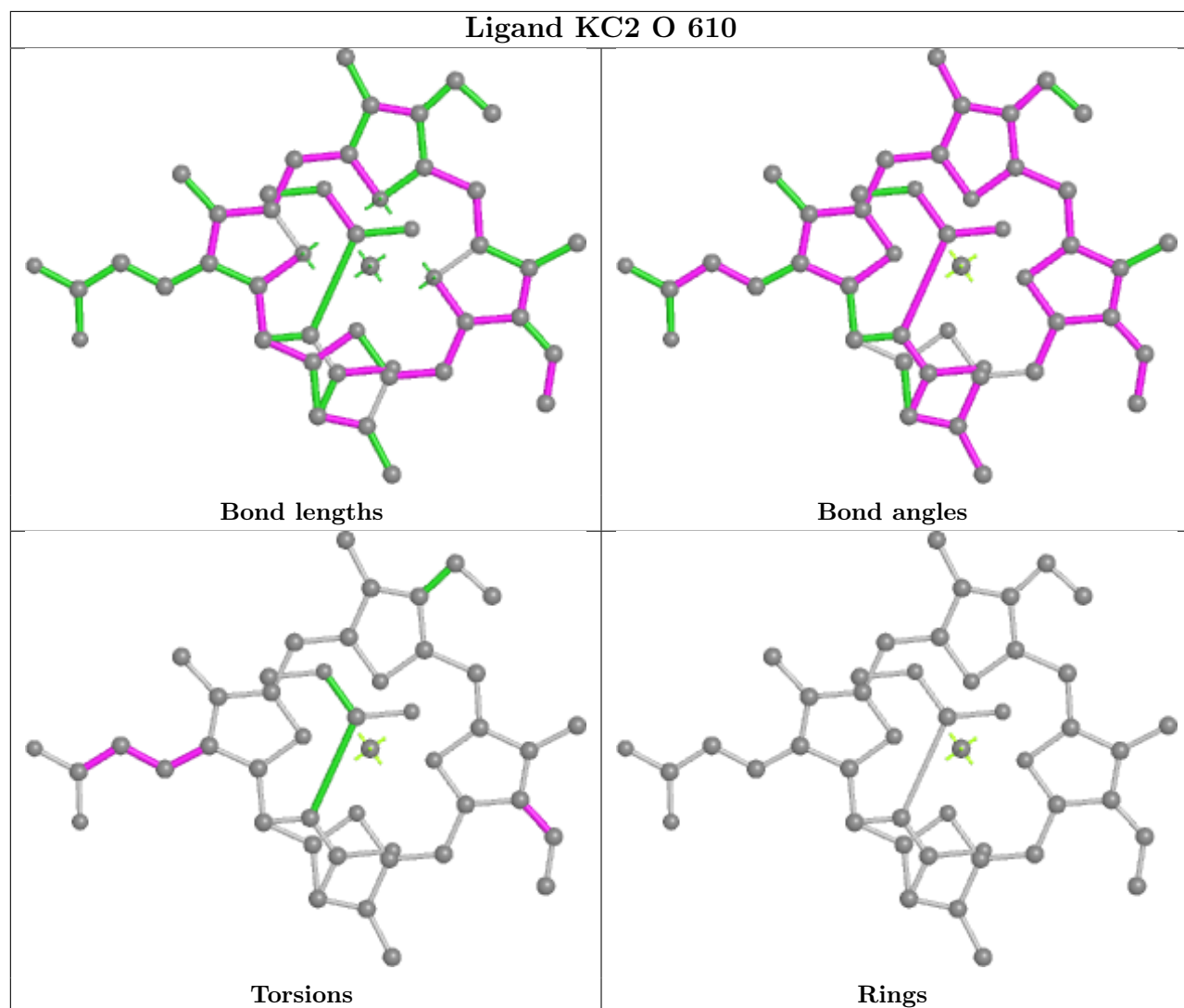
Rings

**Ligand CLA 3 303****Ligand II0 1 616****Ligand CLA S 606**

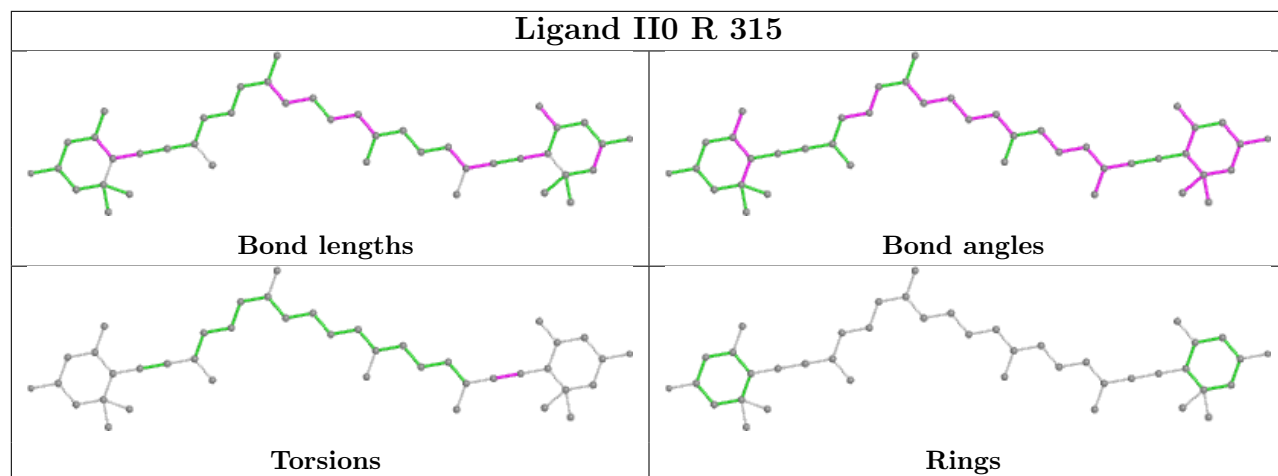
## Ligand II0 O 615



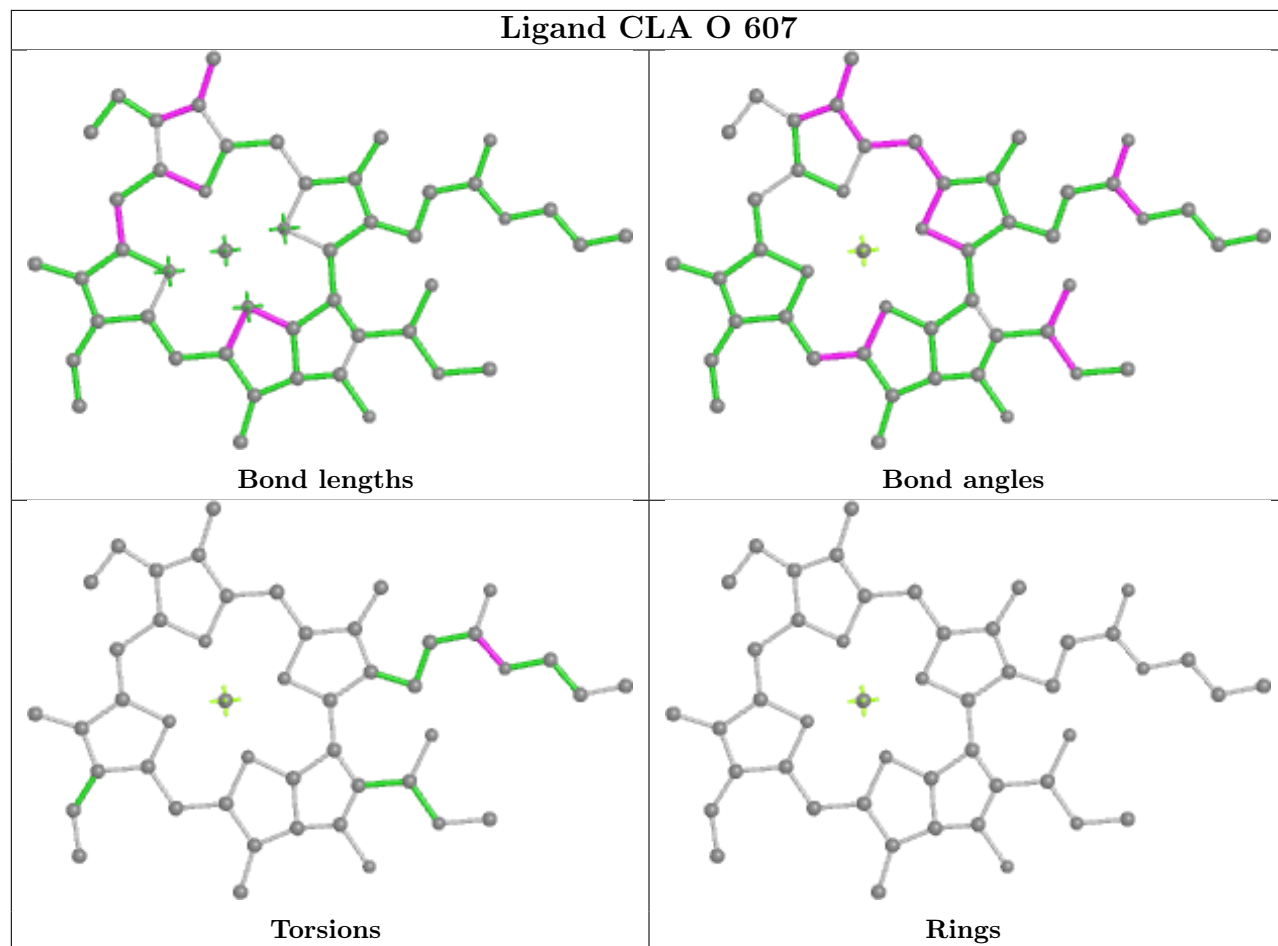
## Ligand KC2 O 610



## Ligand II0 R 315

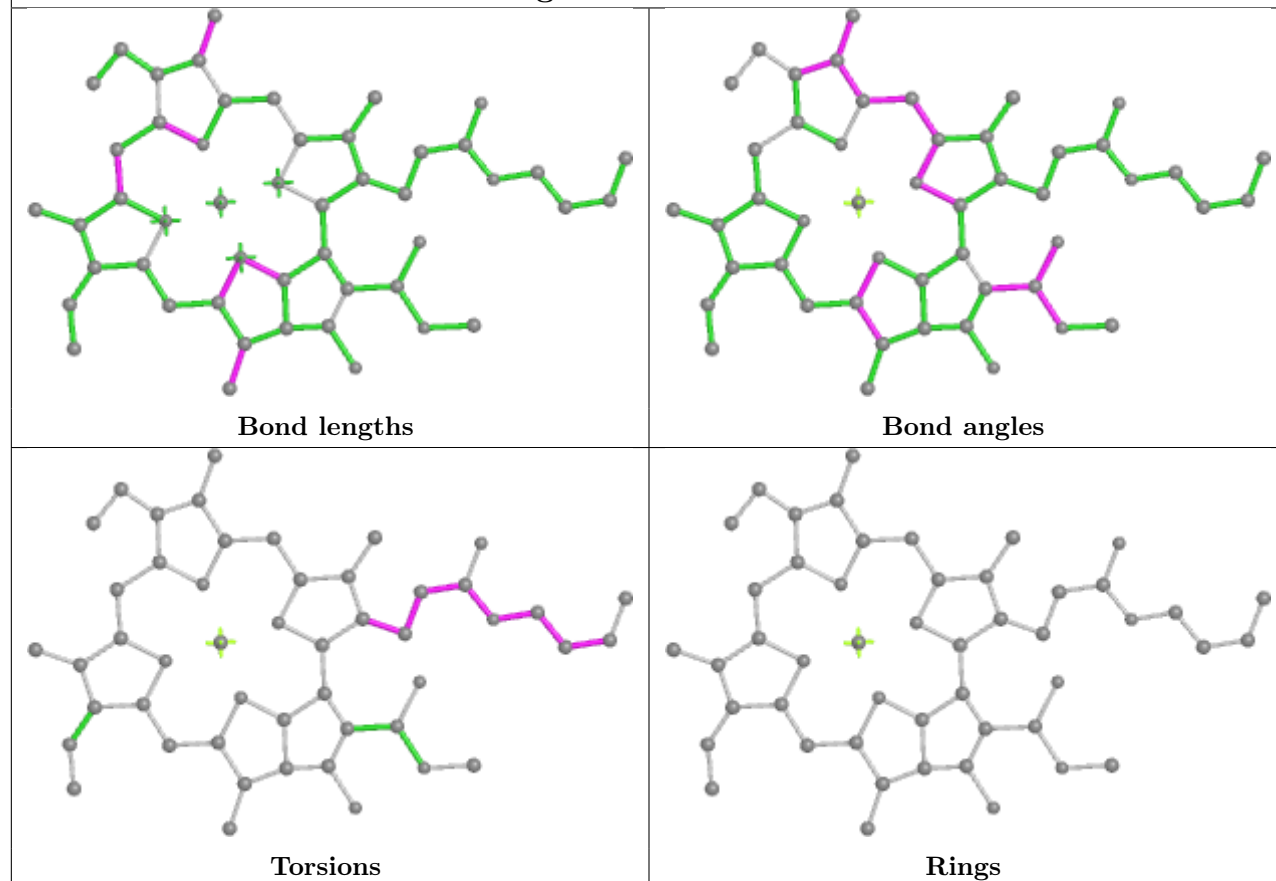


## Ligand CLA O 607

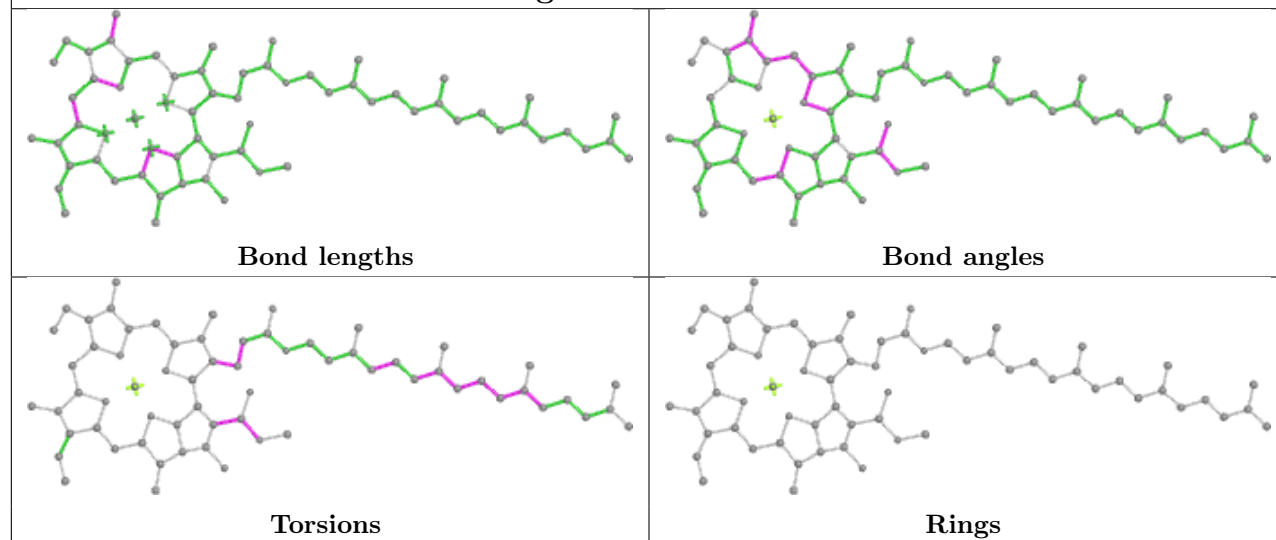


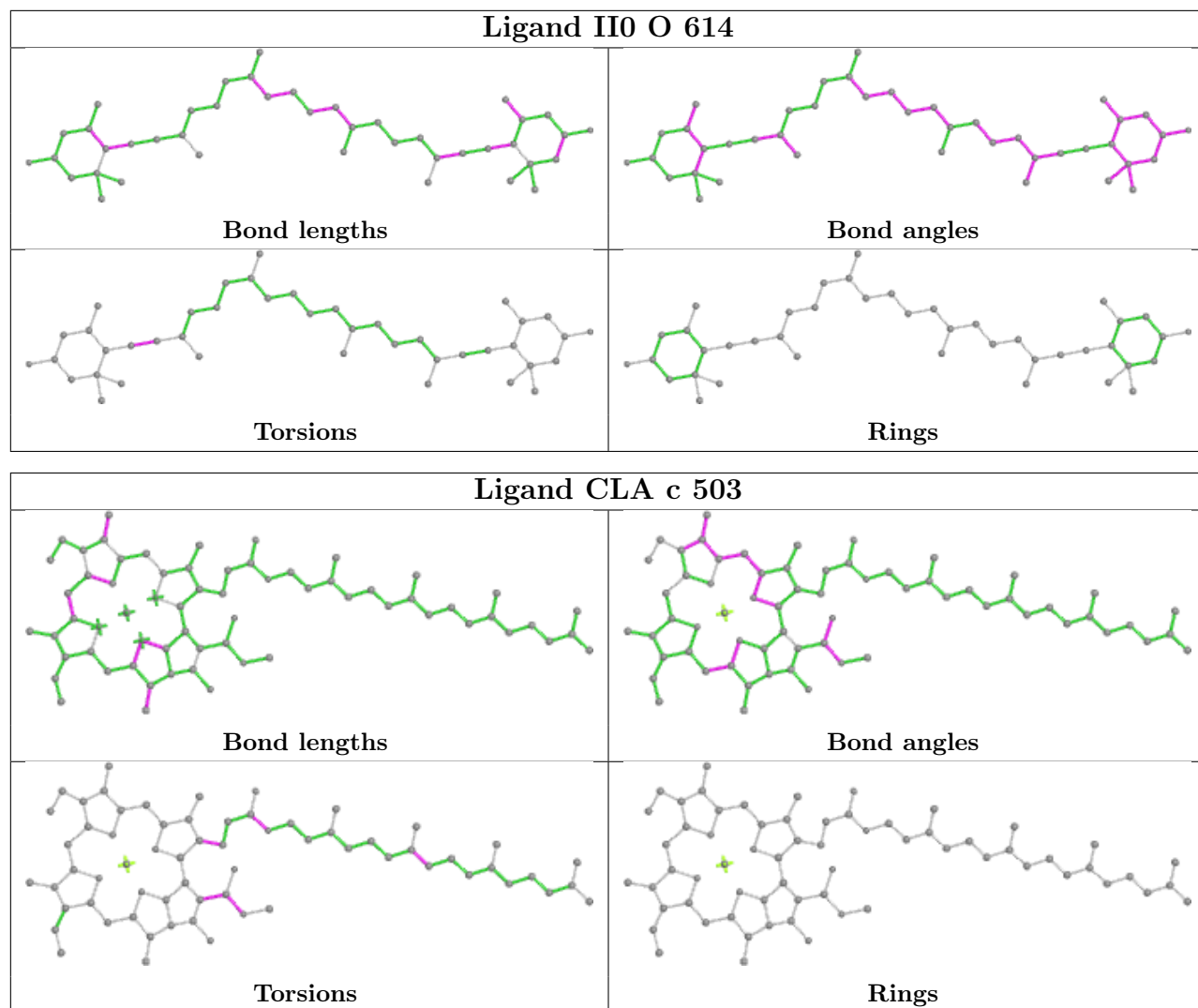


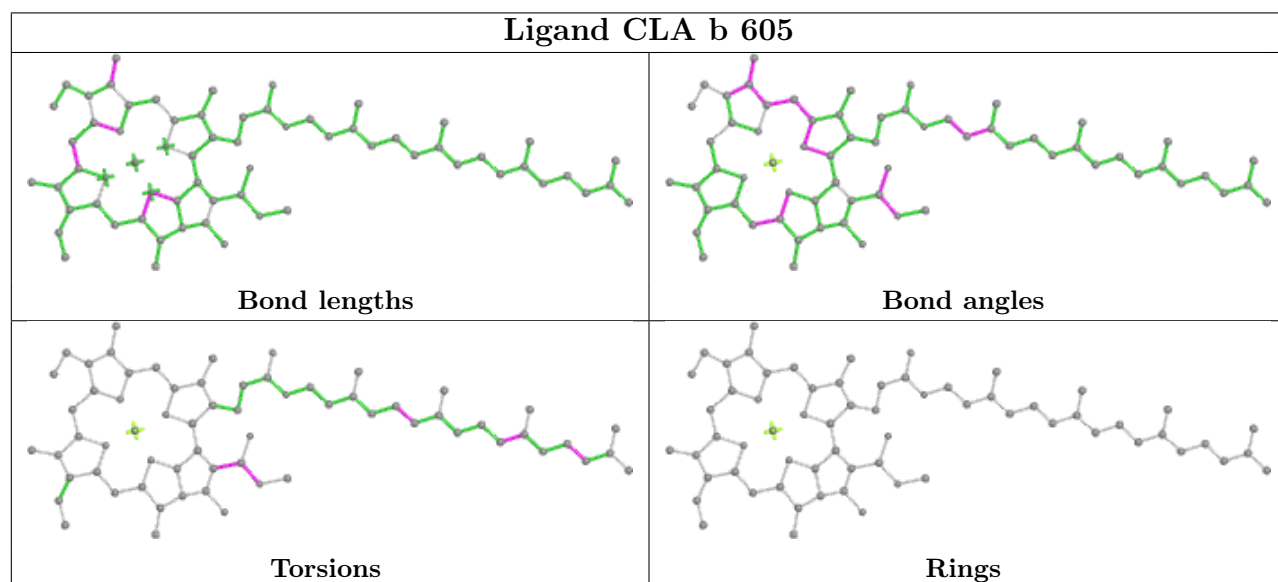
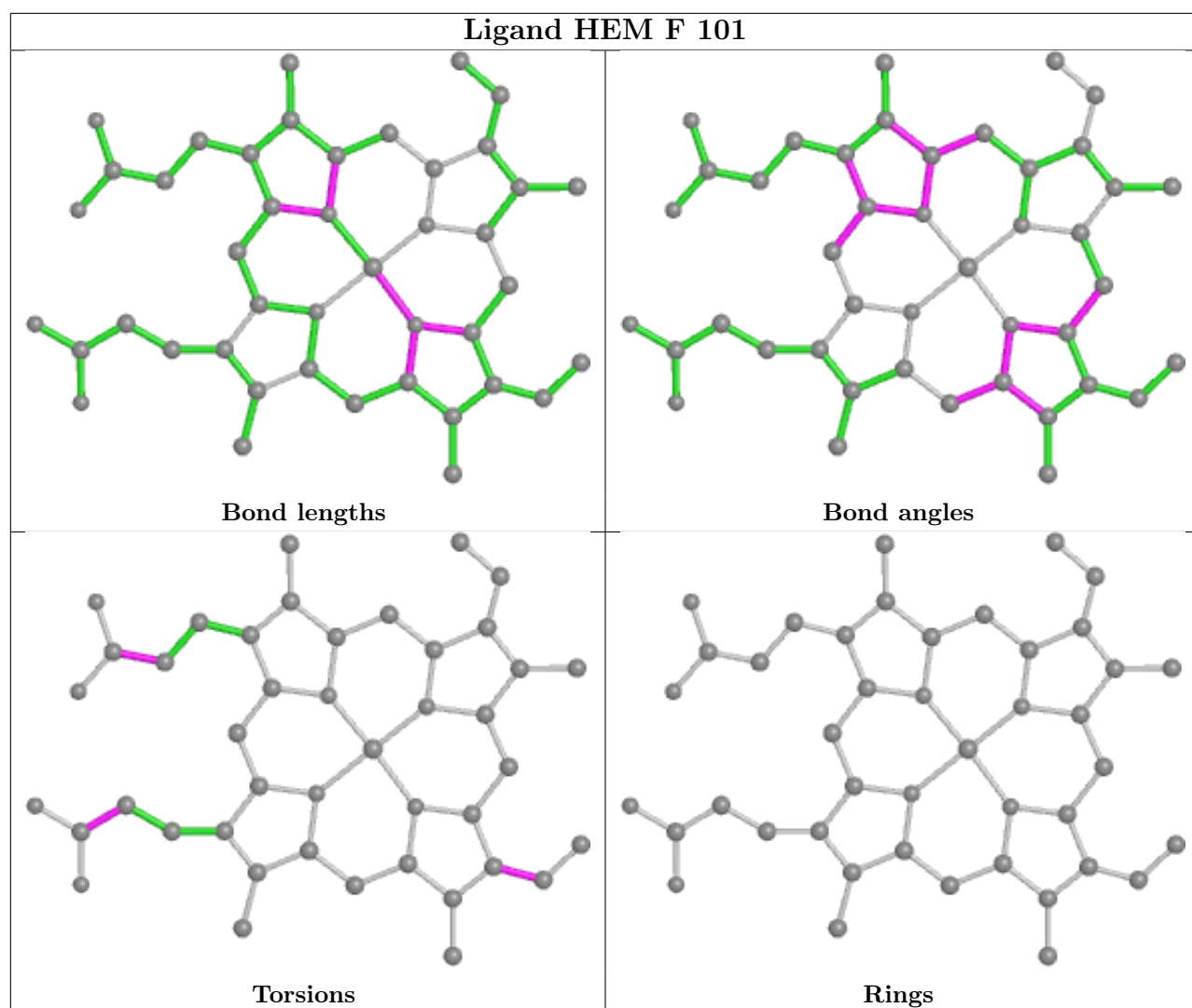
## Ligand CLA a 403



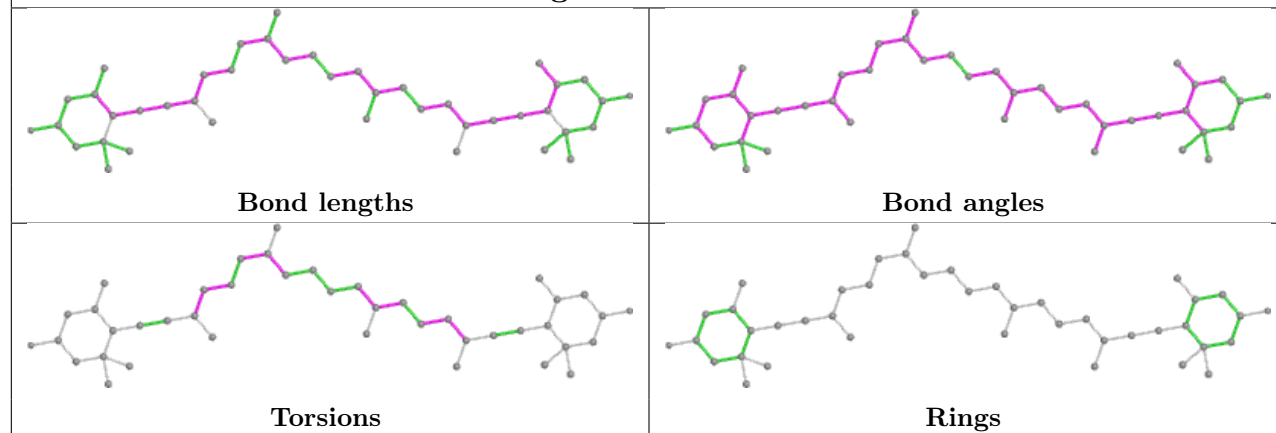
## Ligand CLA 6 602



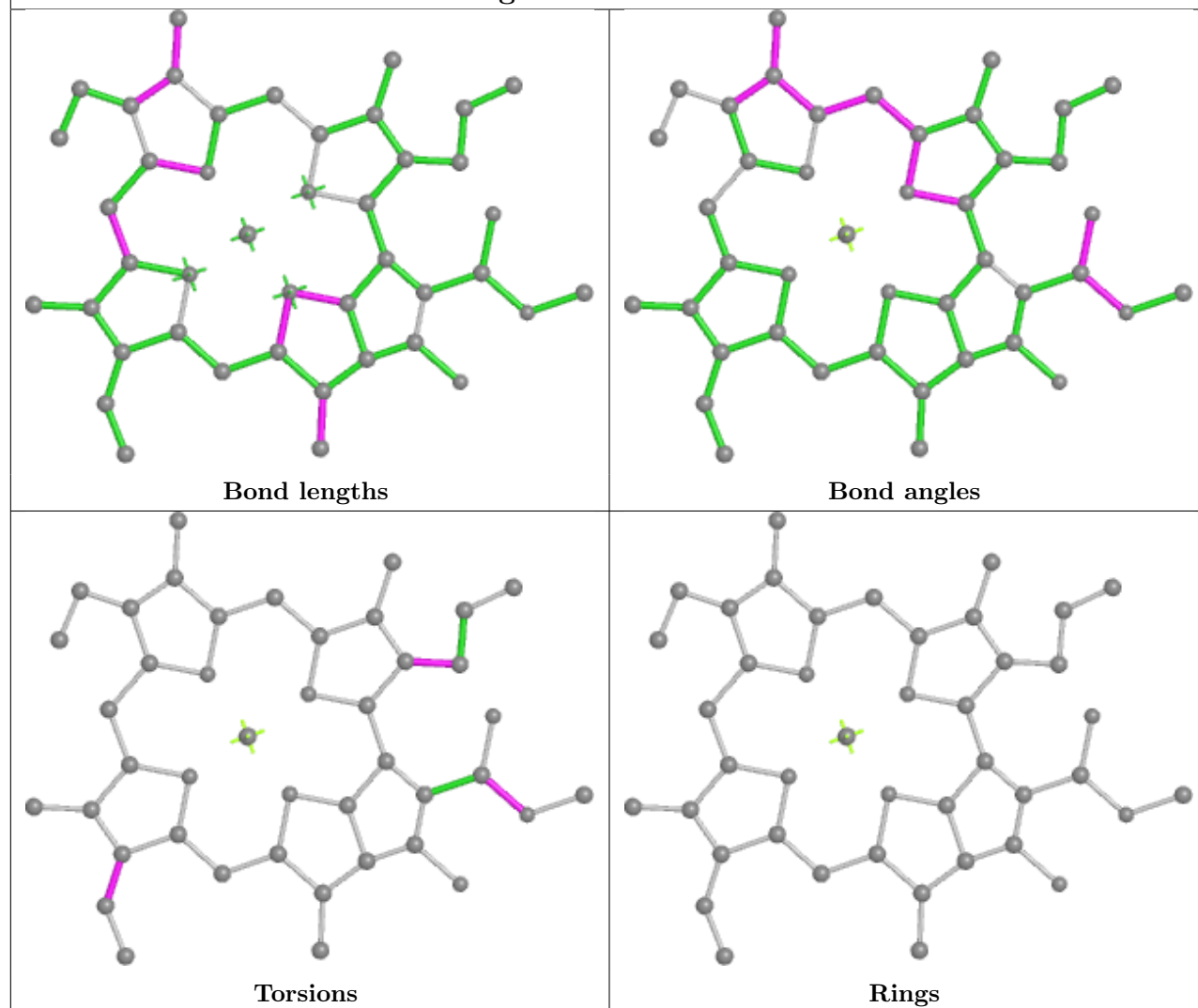




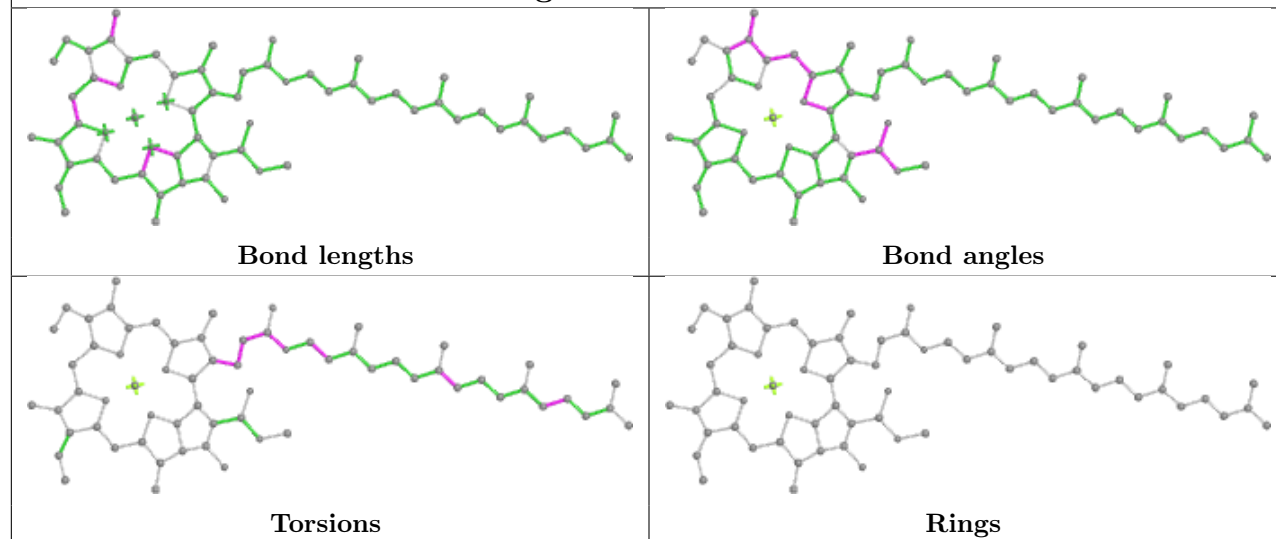
## Ligand II0 3 312



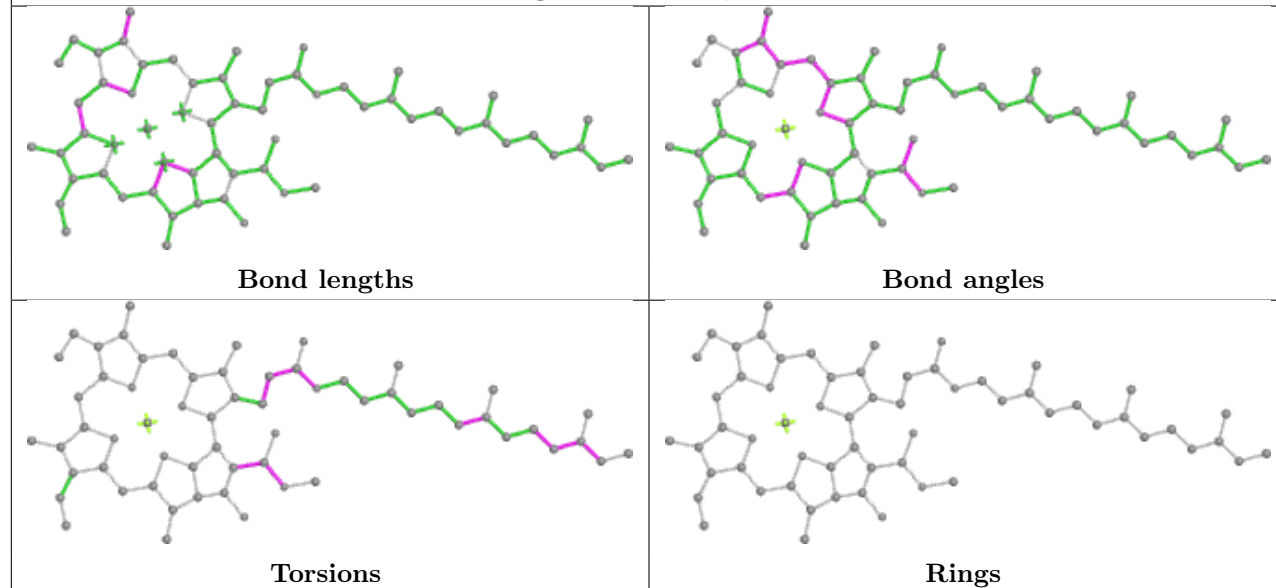
## Ligand CLA N 607

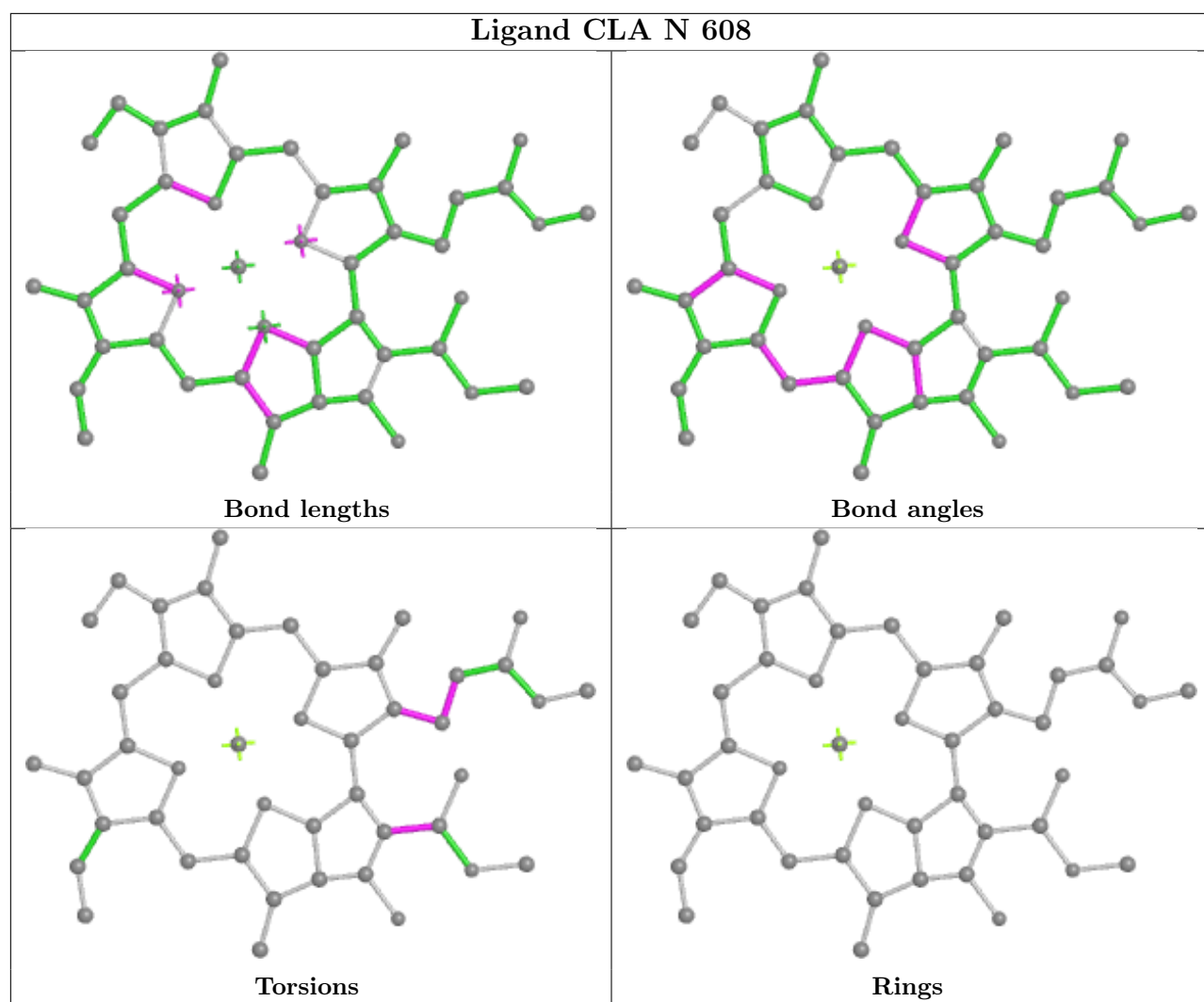


## Ligand CLA d 402

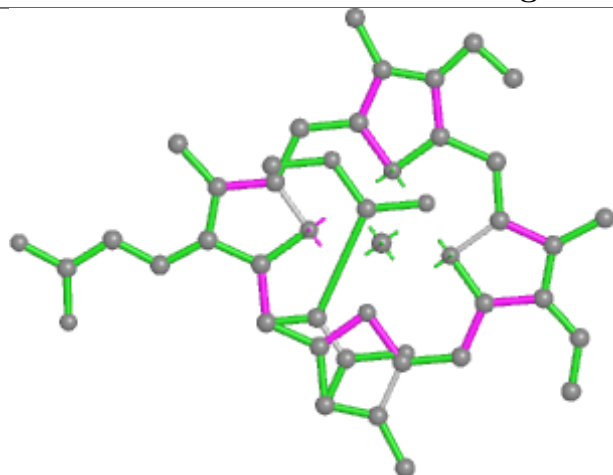


## Ligand CLA Q 303

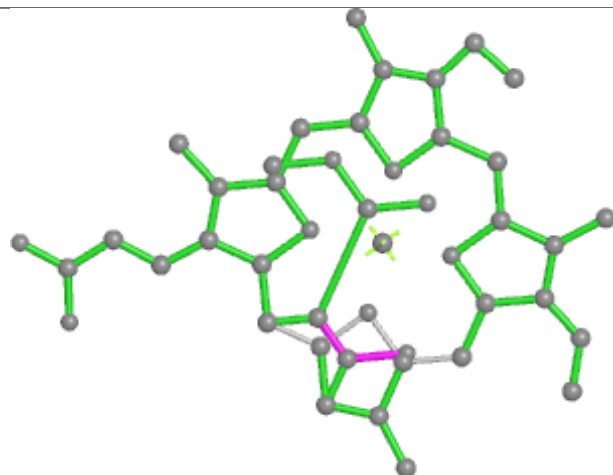




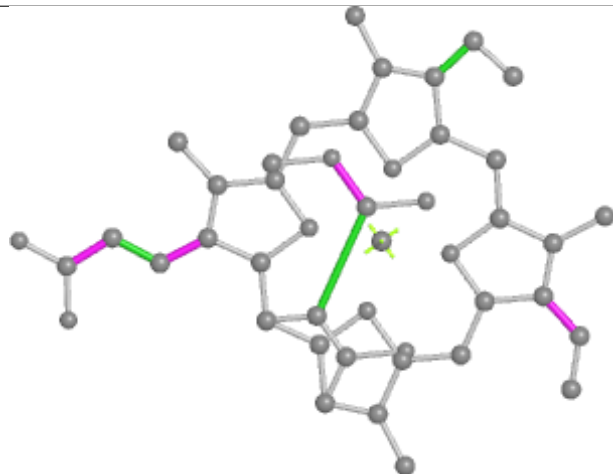
## Ligand KC2 1 611



Bond lengths



Bond angles

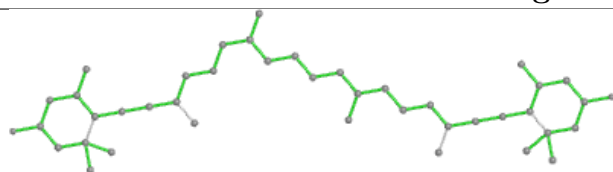


Torsions

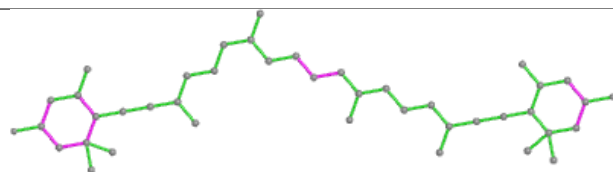


Rings

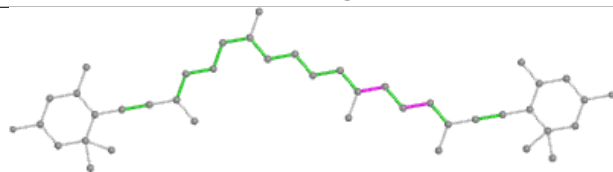
## Ligand II0 2 320



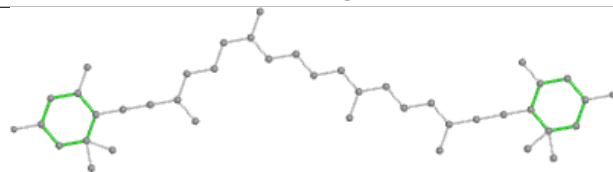
Bond lengths



Bond angles

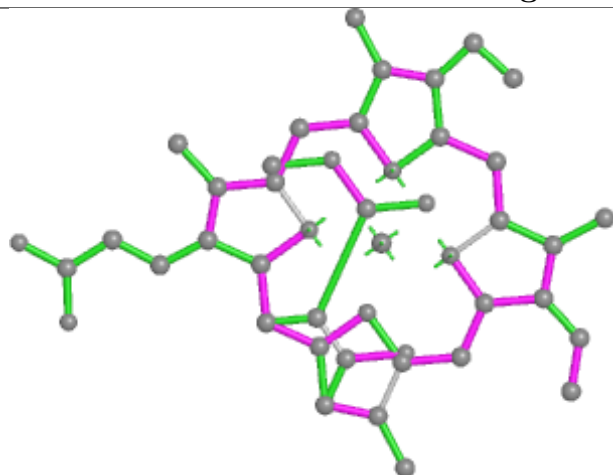


Torsions

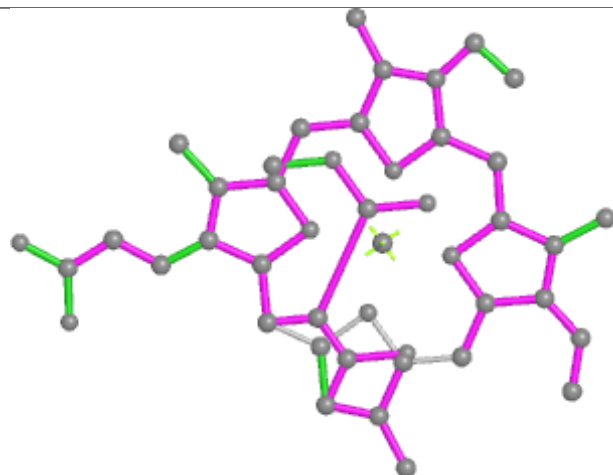


Rings

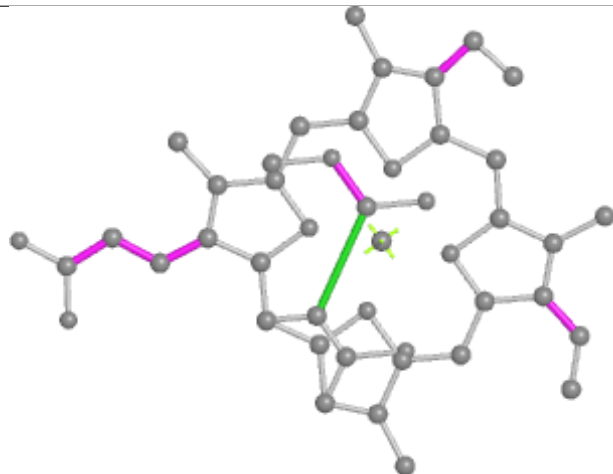
## Ligand KC2 3 304



Bond lengths



Bond angles



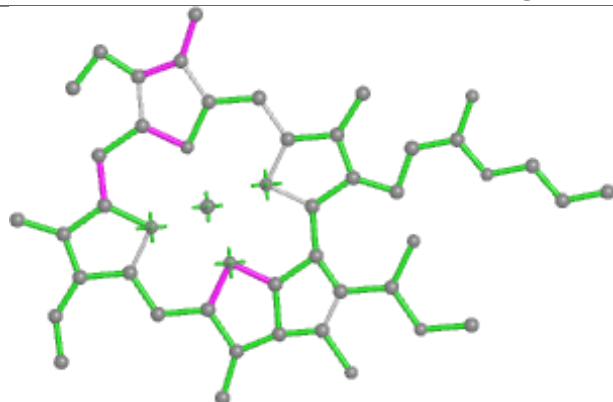
Torsions



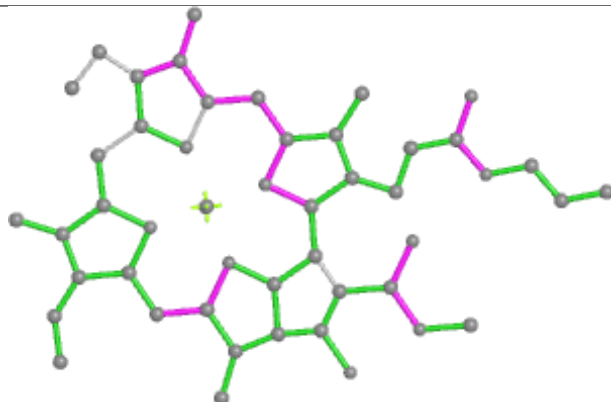
Rings



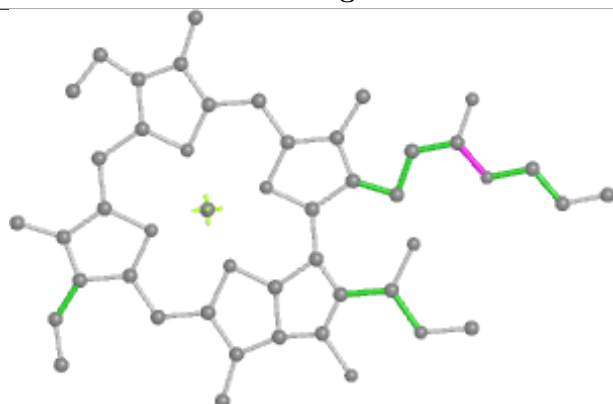
## Ligand CLA 2 307



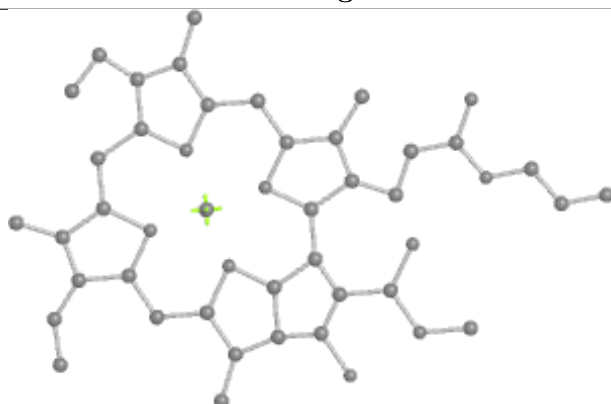
Bond lengths



Bond angles

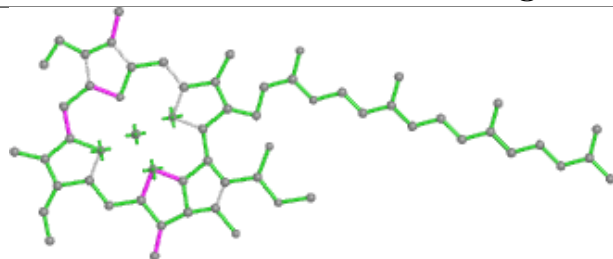


Torsions

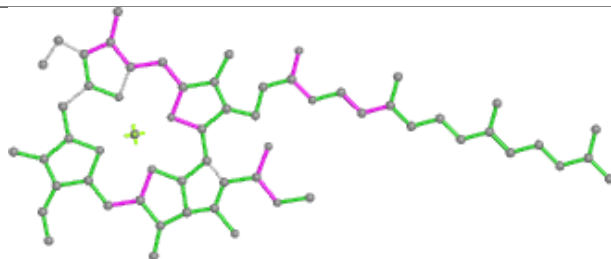


Rings

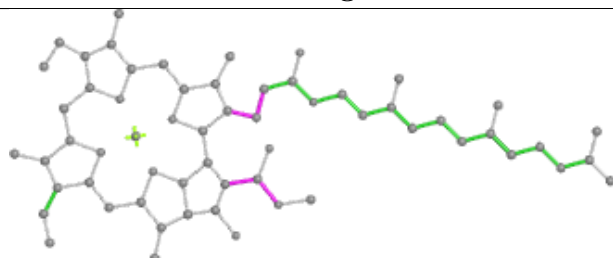
## Ligand CLA 1 602



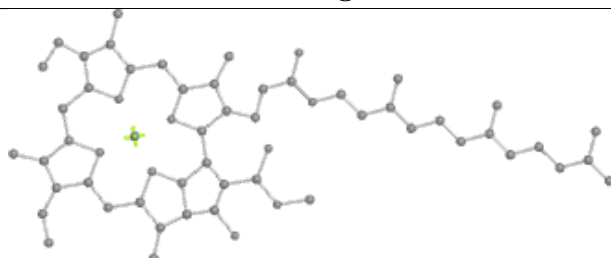
Bond lengths



Bond angles

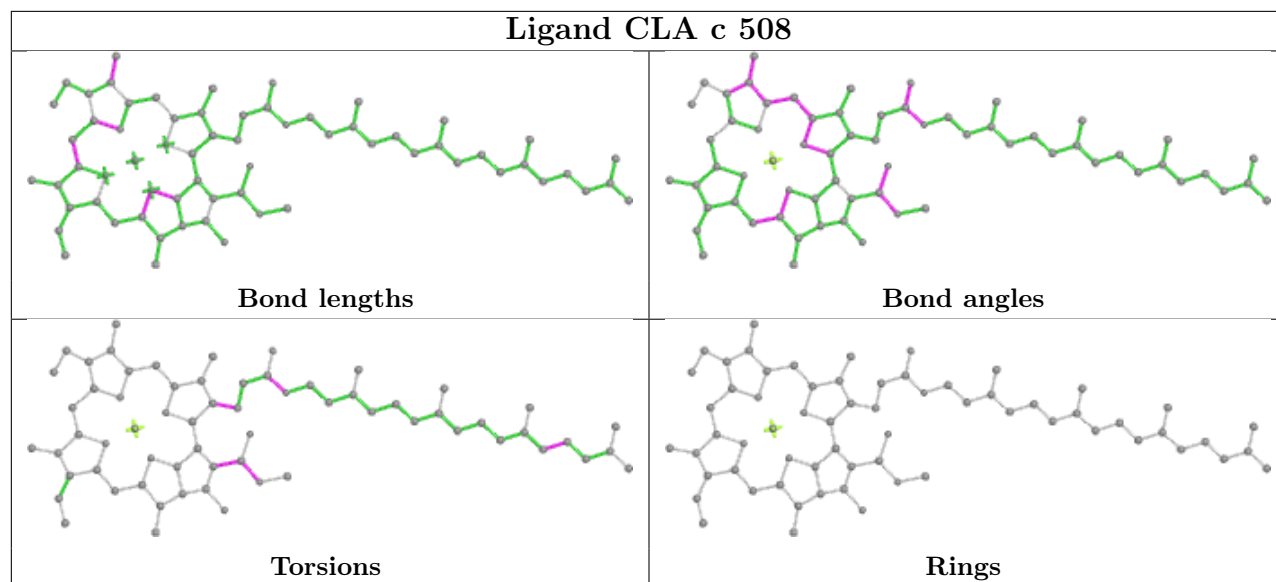


Torsions

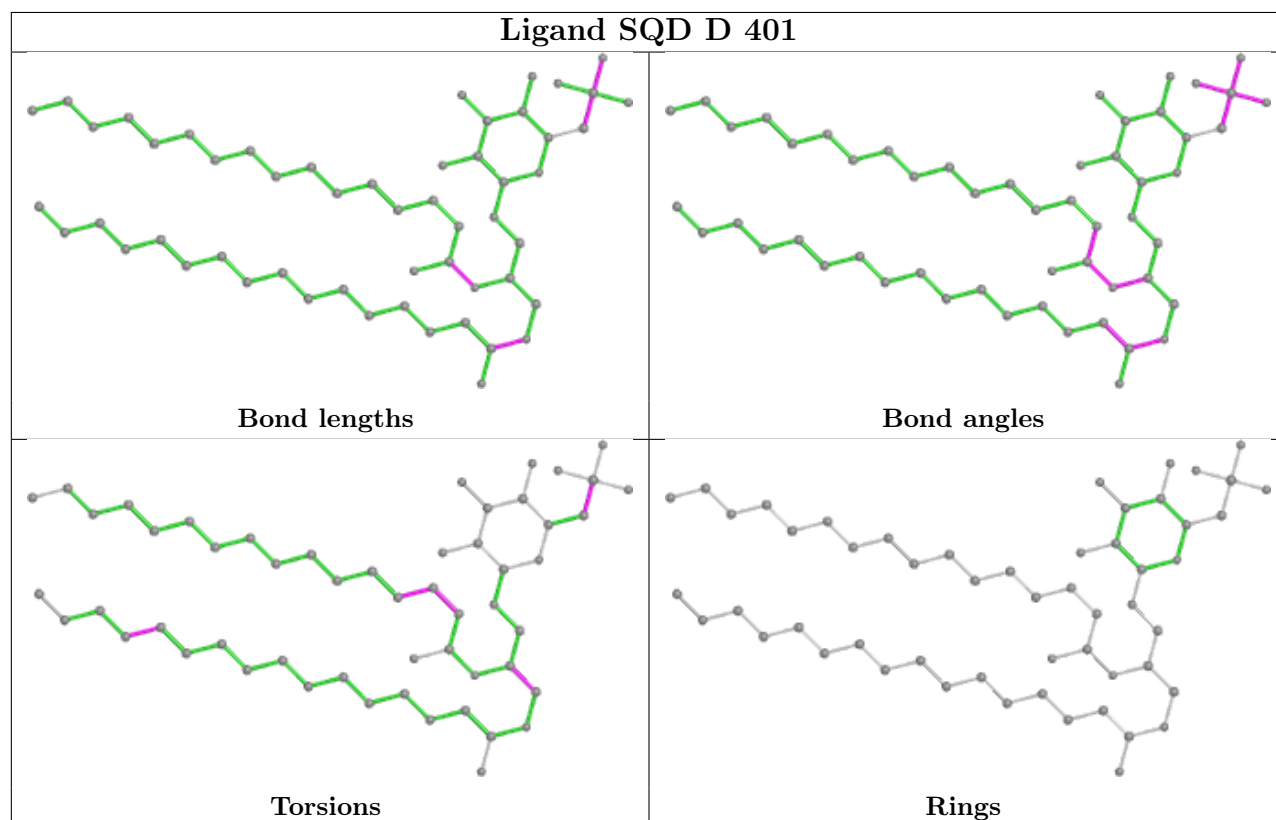


Rings

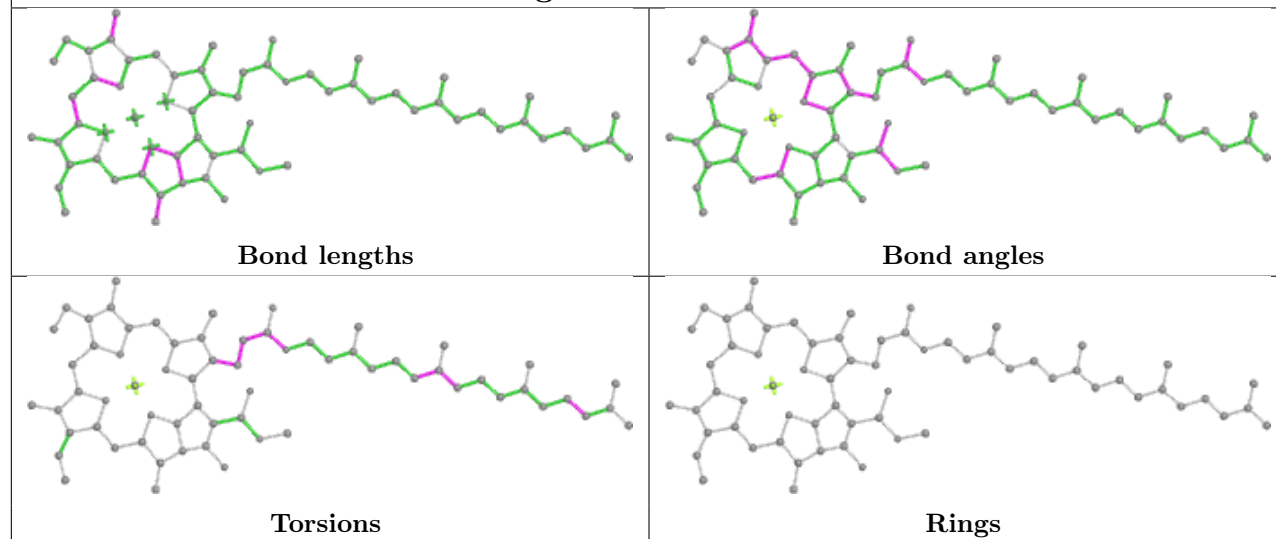
## Ligand CLA c 508



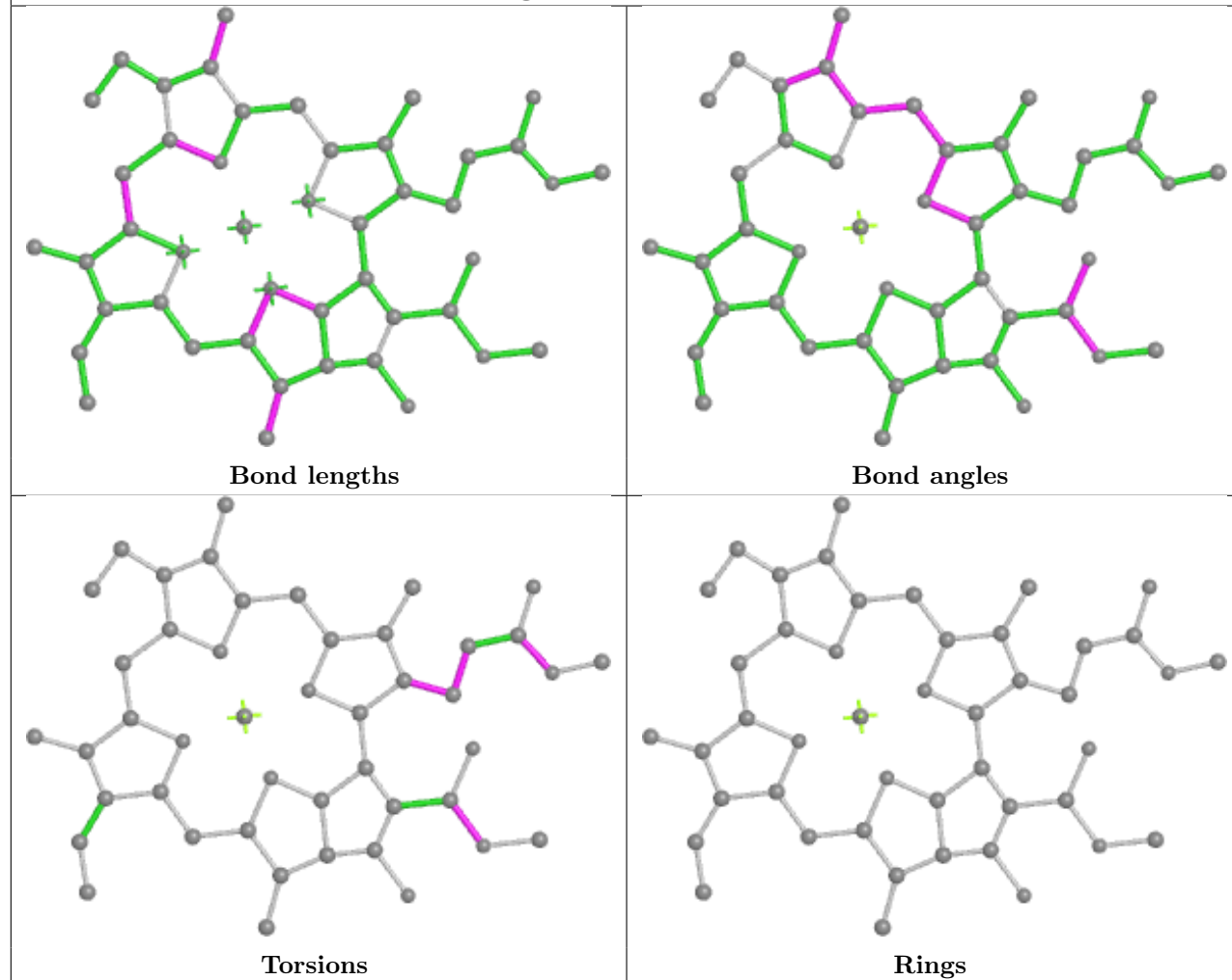
## Ligand SQD D 401

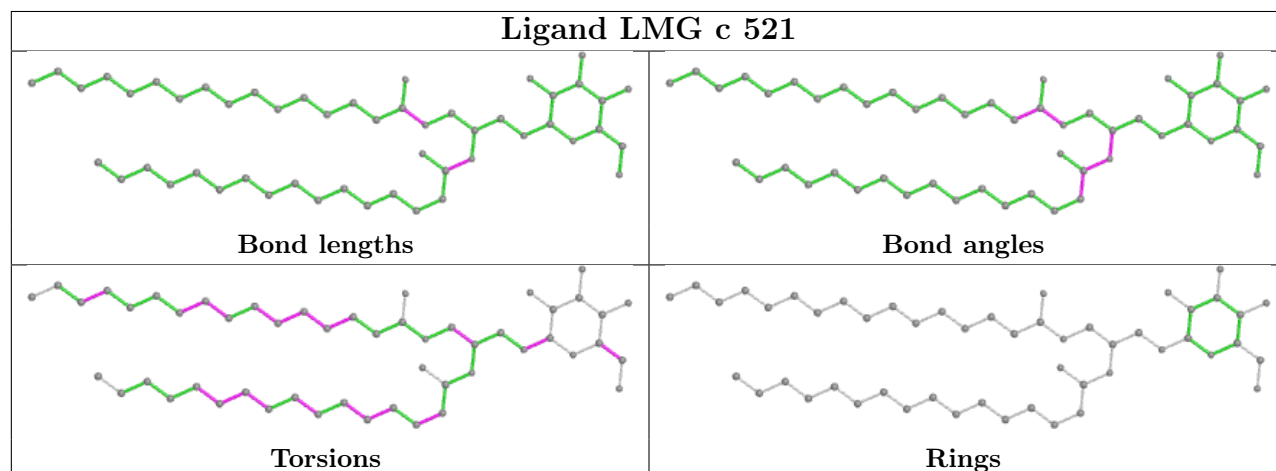
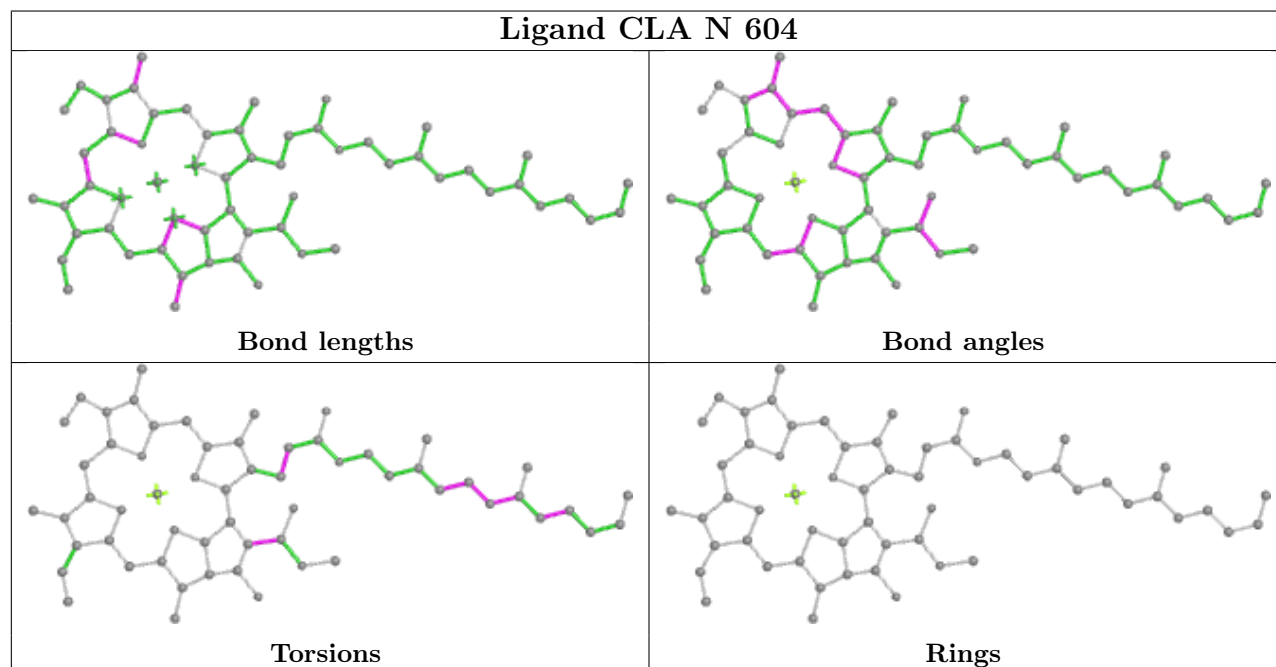
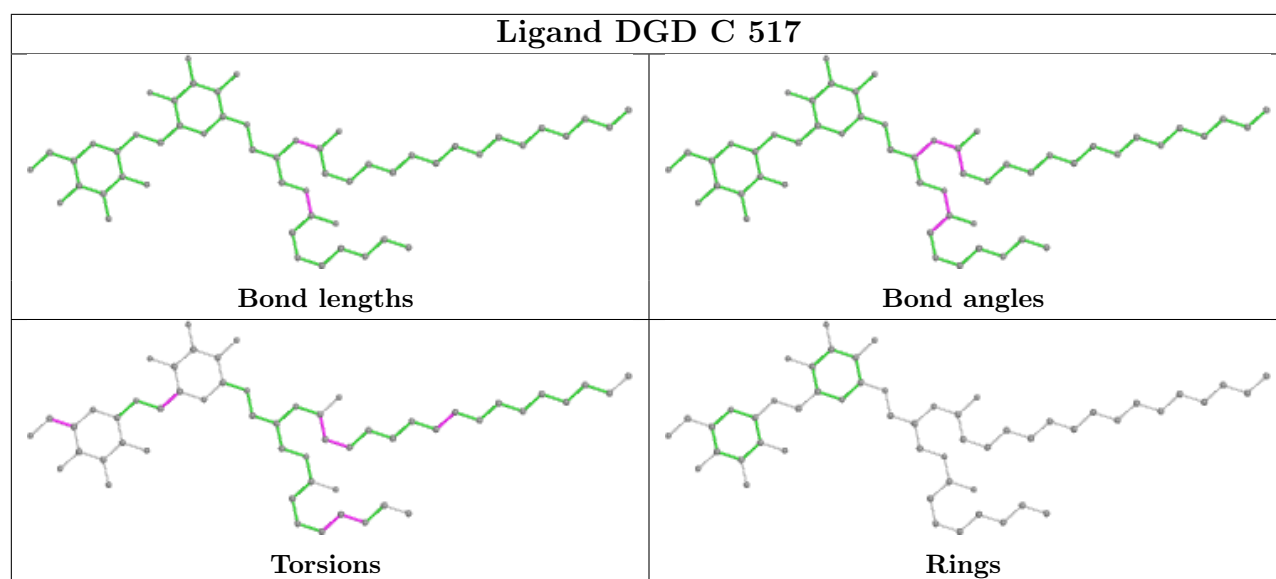


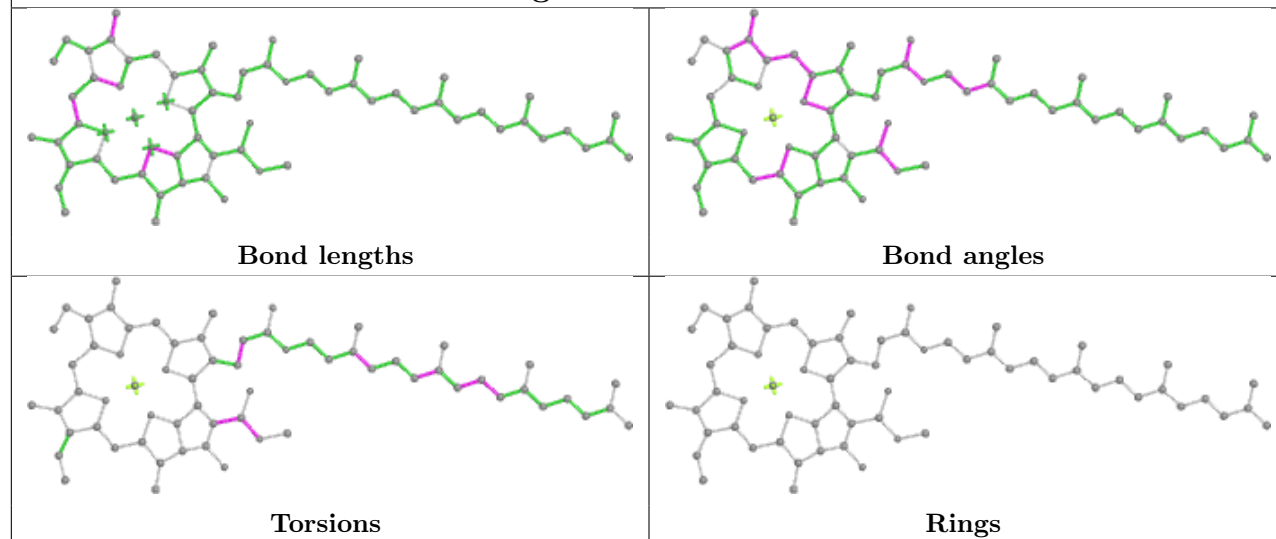
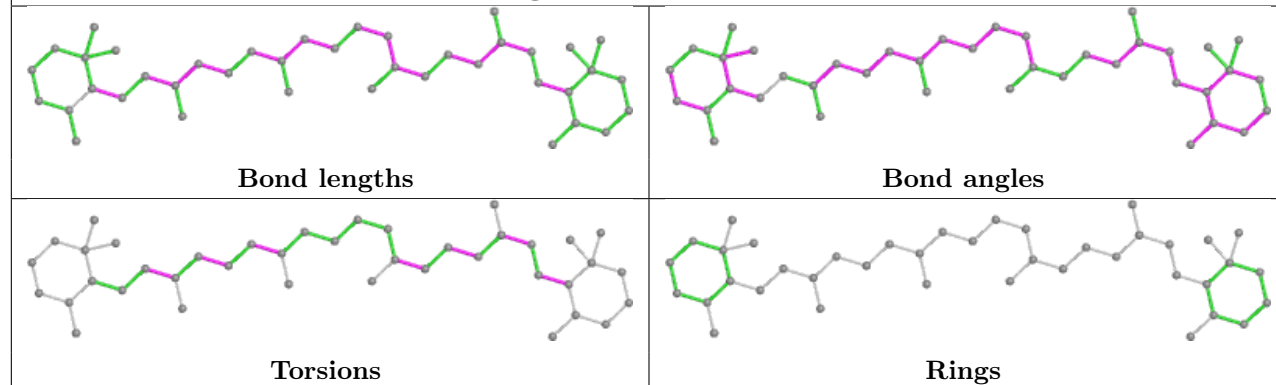
## Ligand CLA b 612



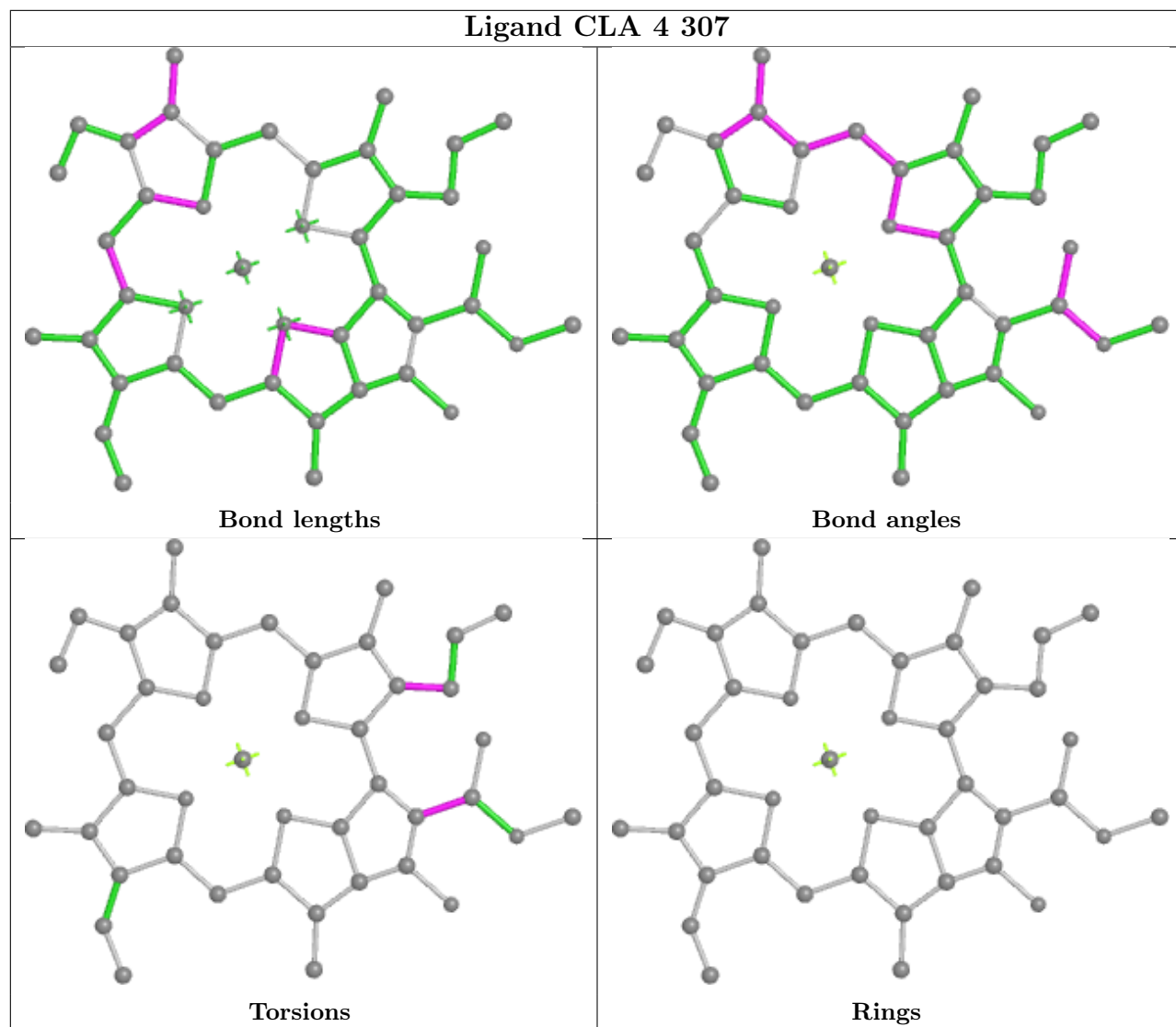
## Ligand CLA 1 608

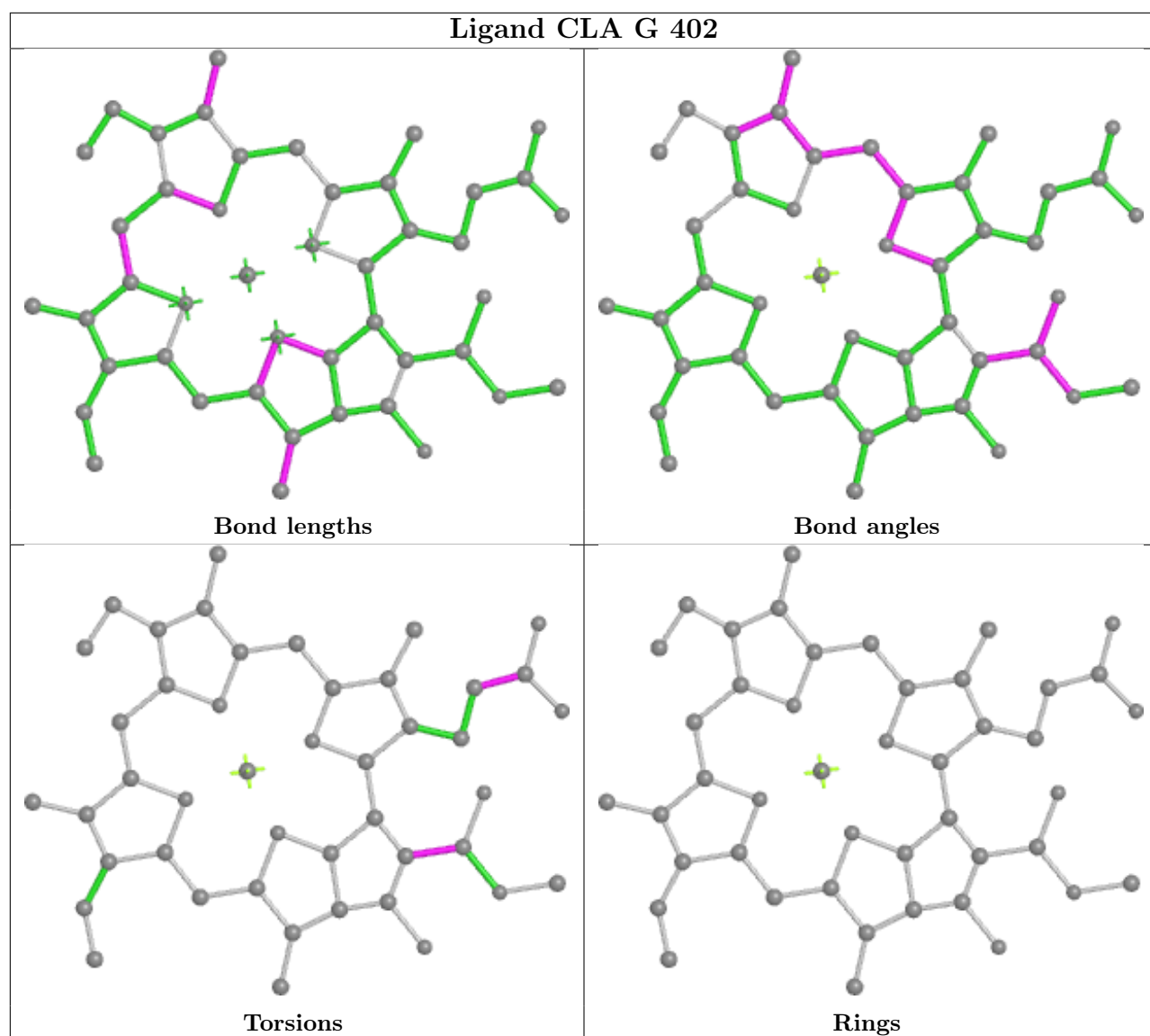


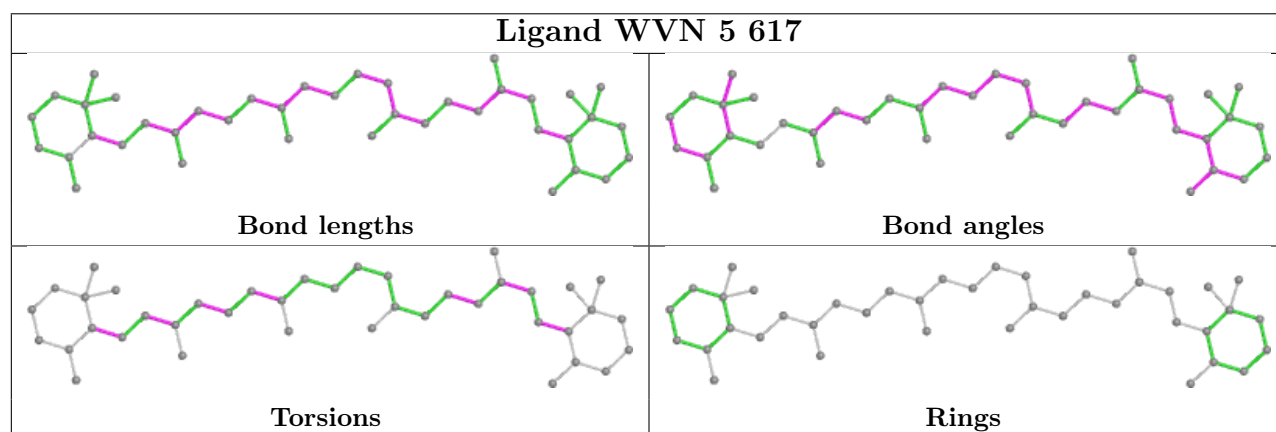
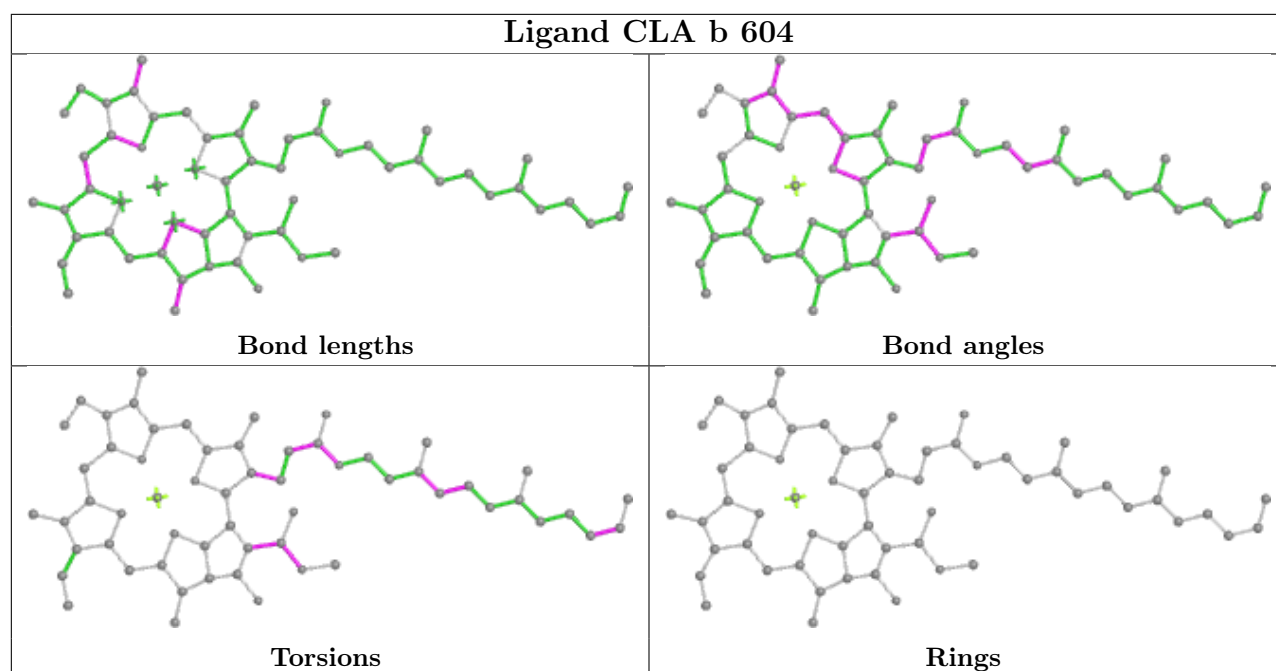


**Ligand CLA B 606****Ligand WVN d 410**

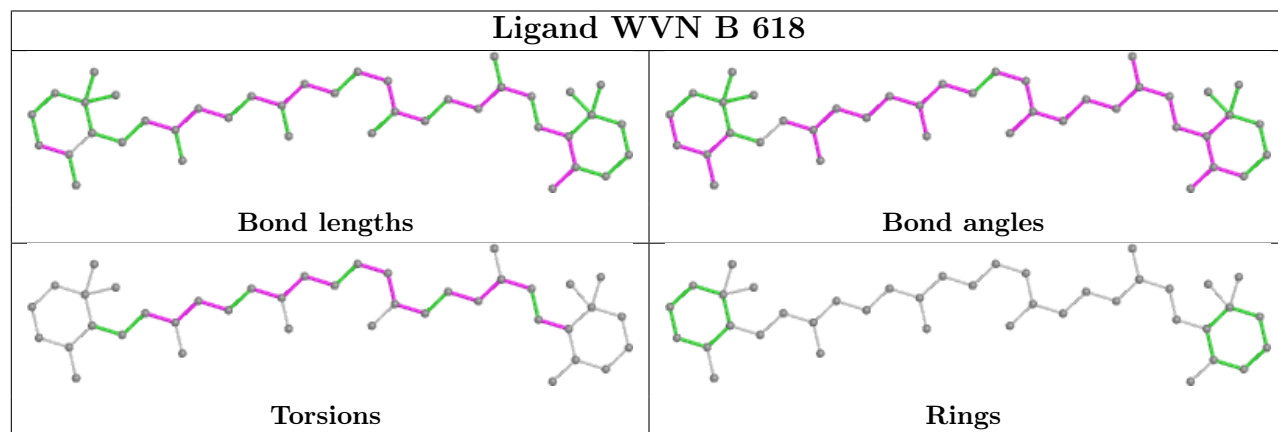
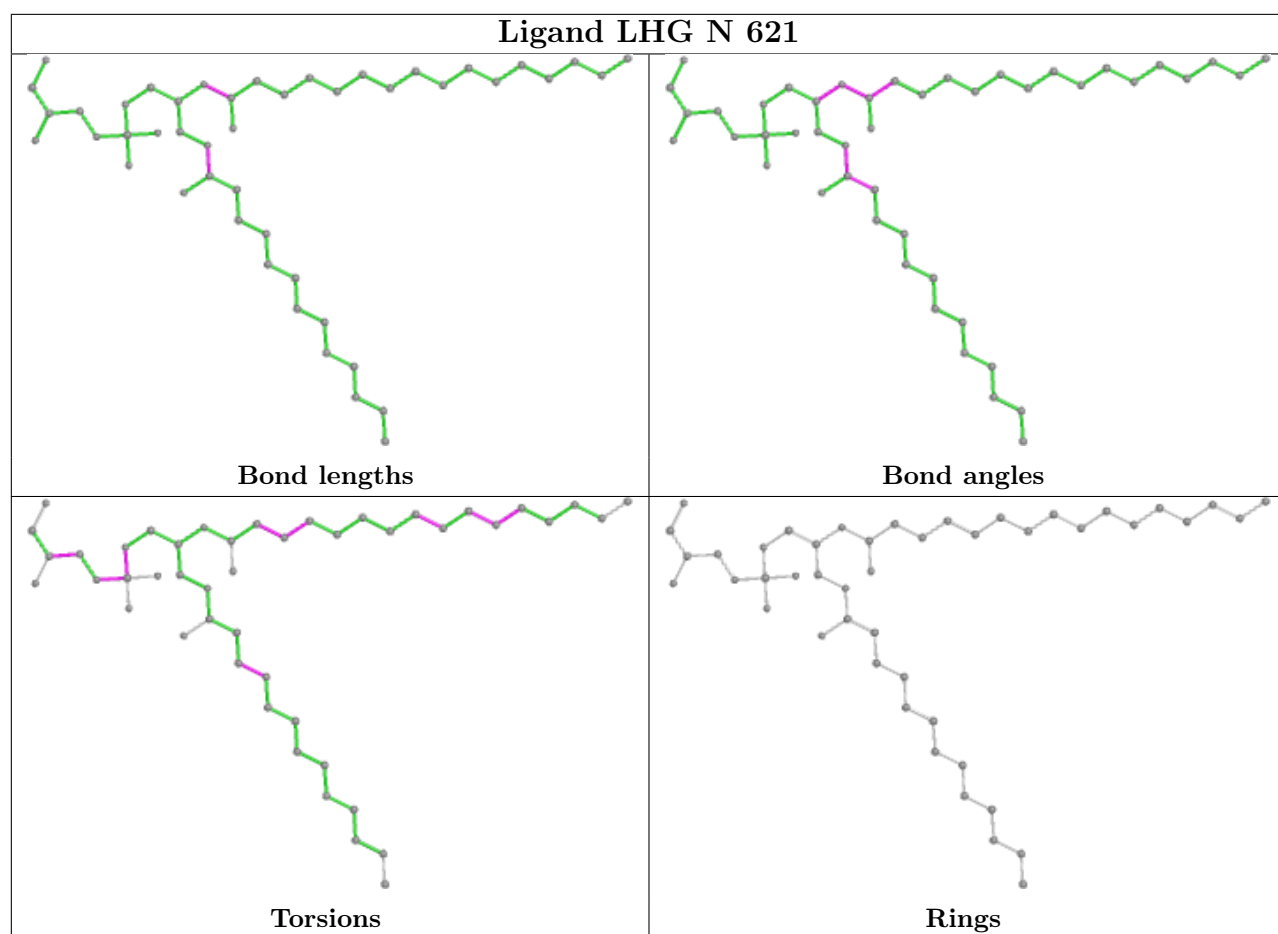
## Ligand CLA 4 307

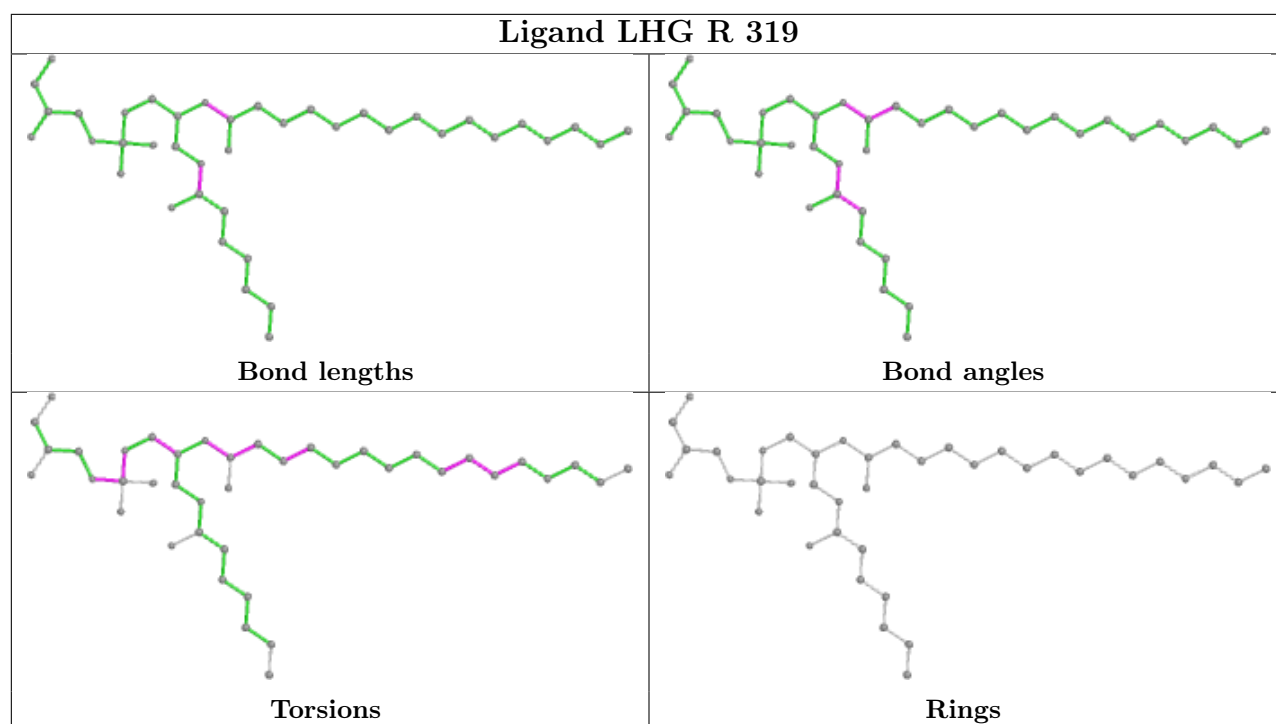




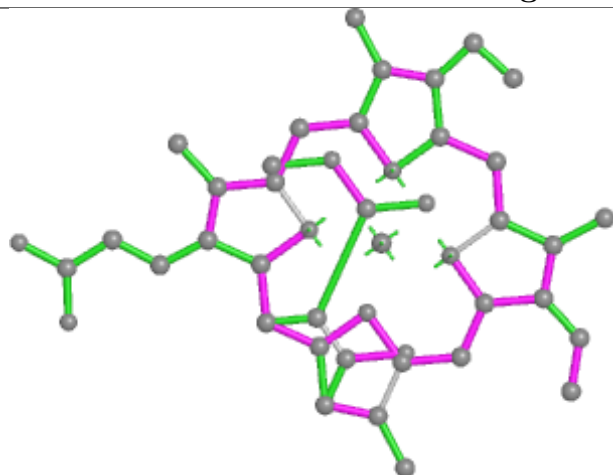




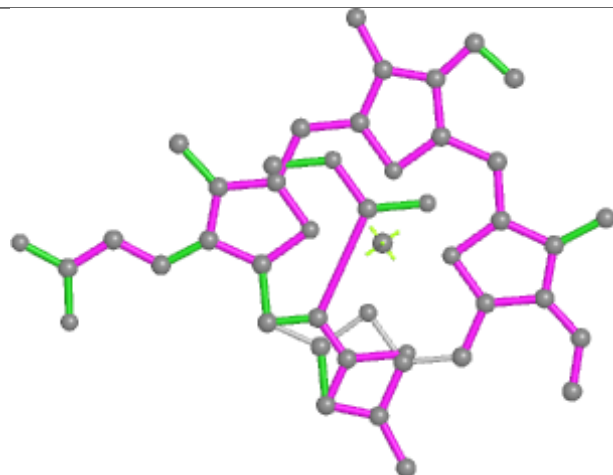




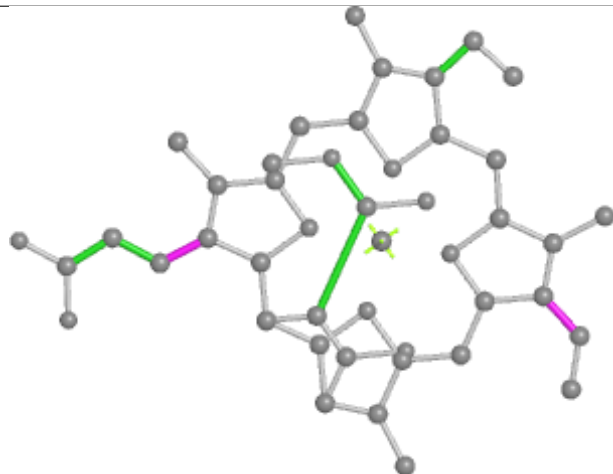
## Ligand KC2 4 311



Bond lengths



Bond angles

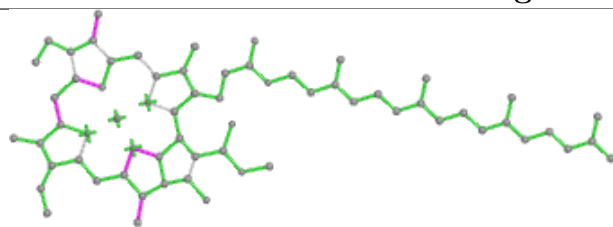


Torsions

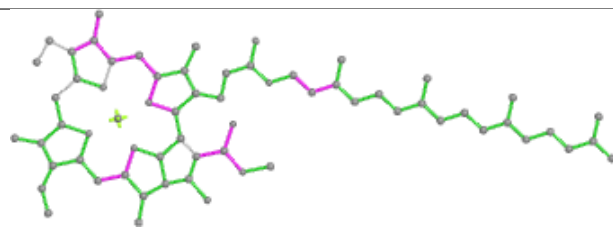


Rings

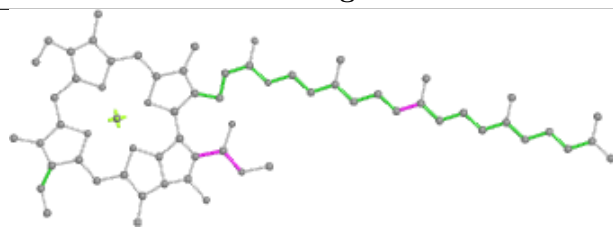
## Ligand CLA B 602



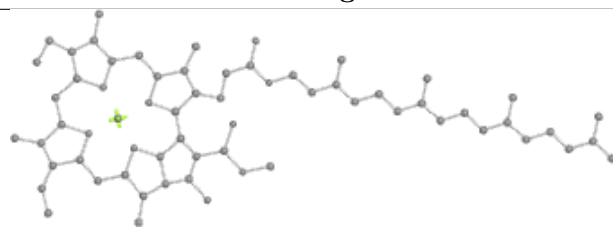
Bond lengths



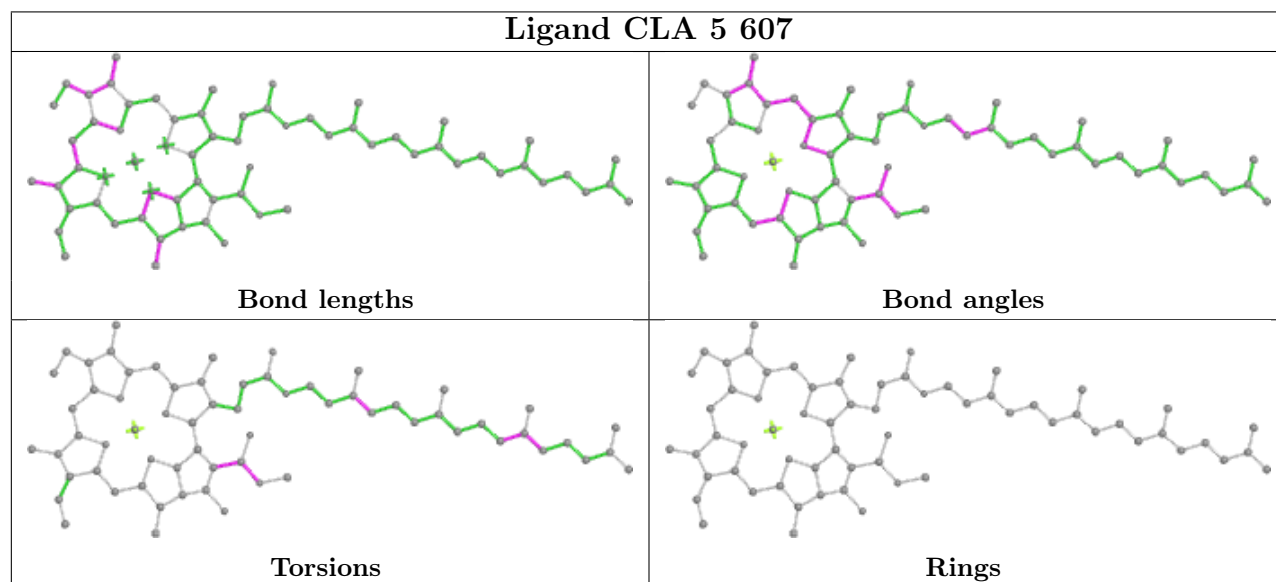
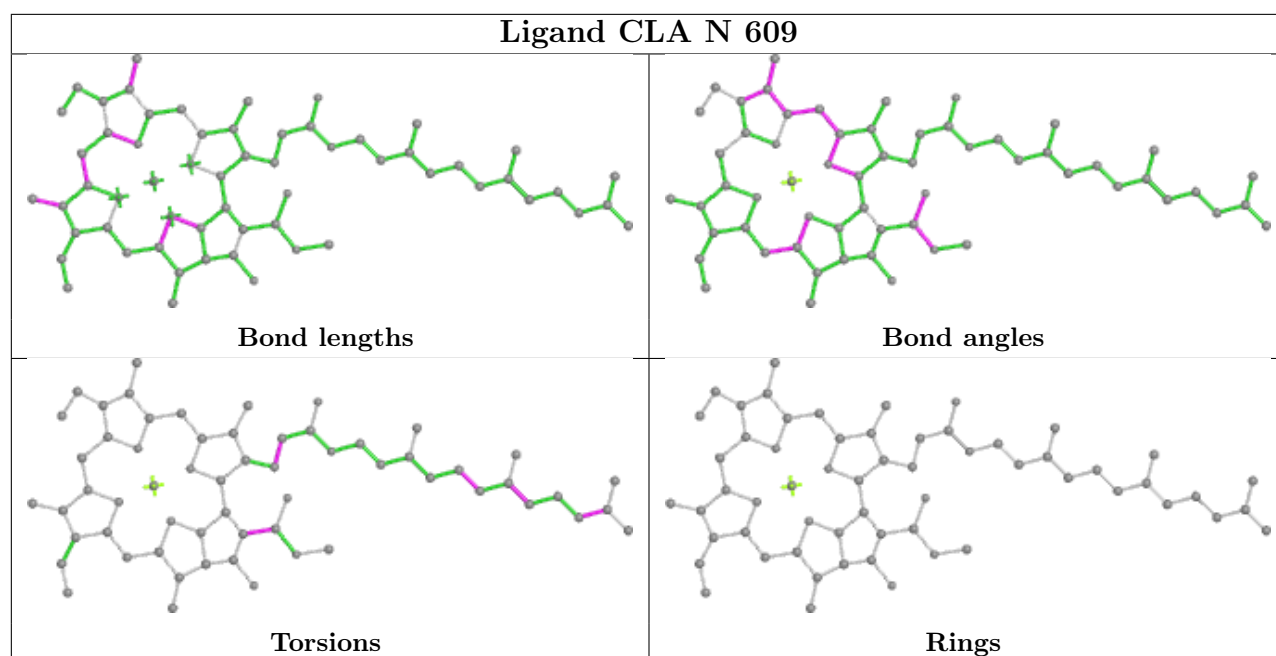
Bond angles



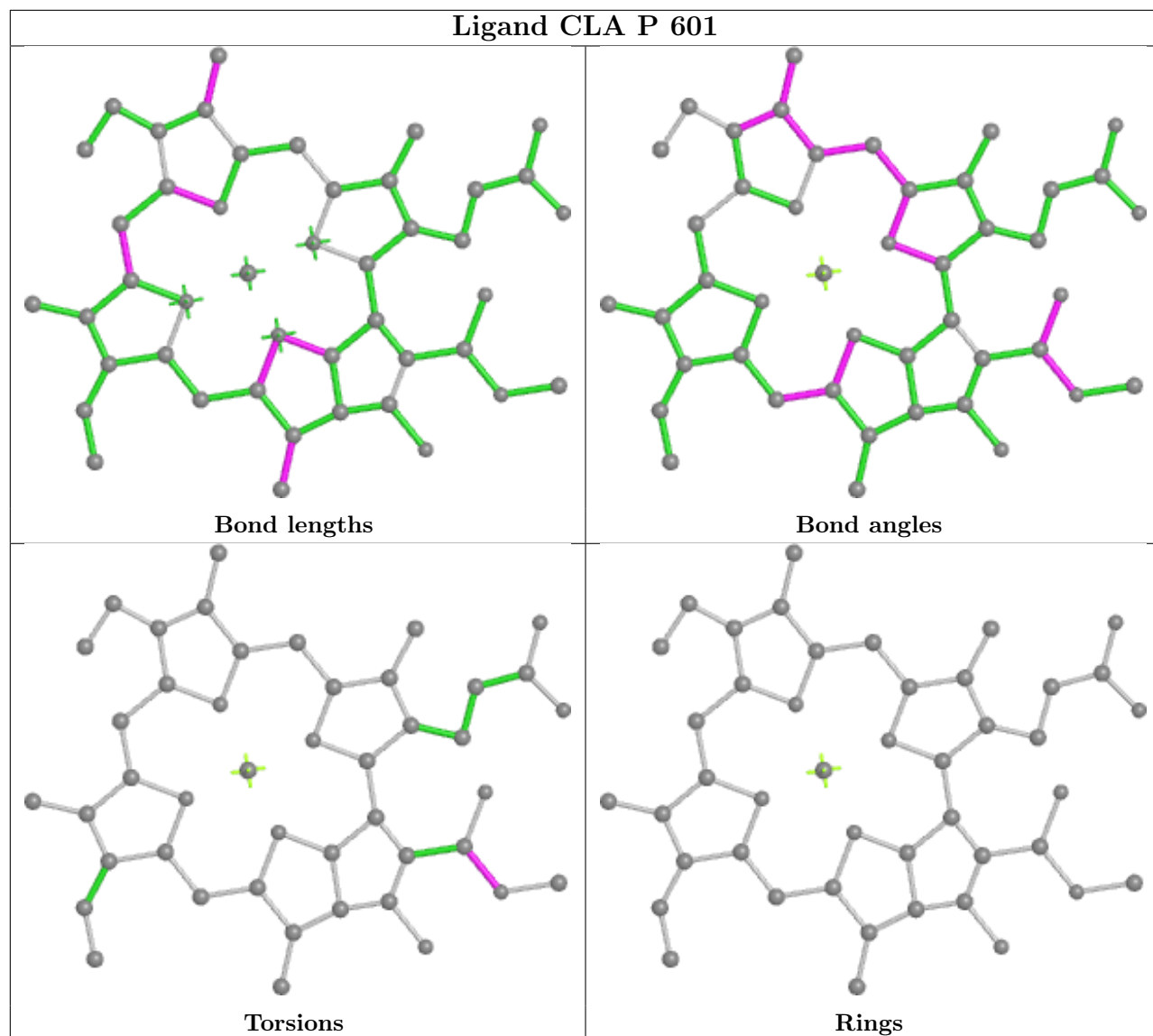
Torsions

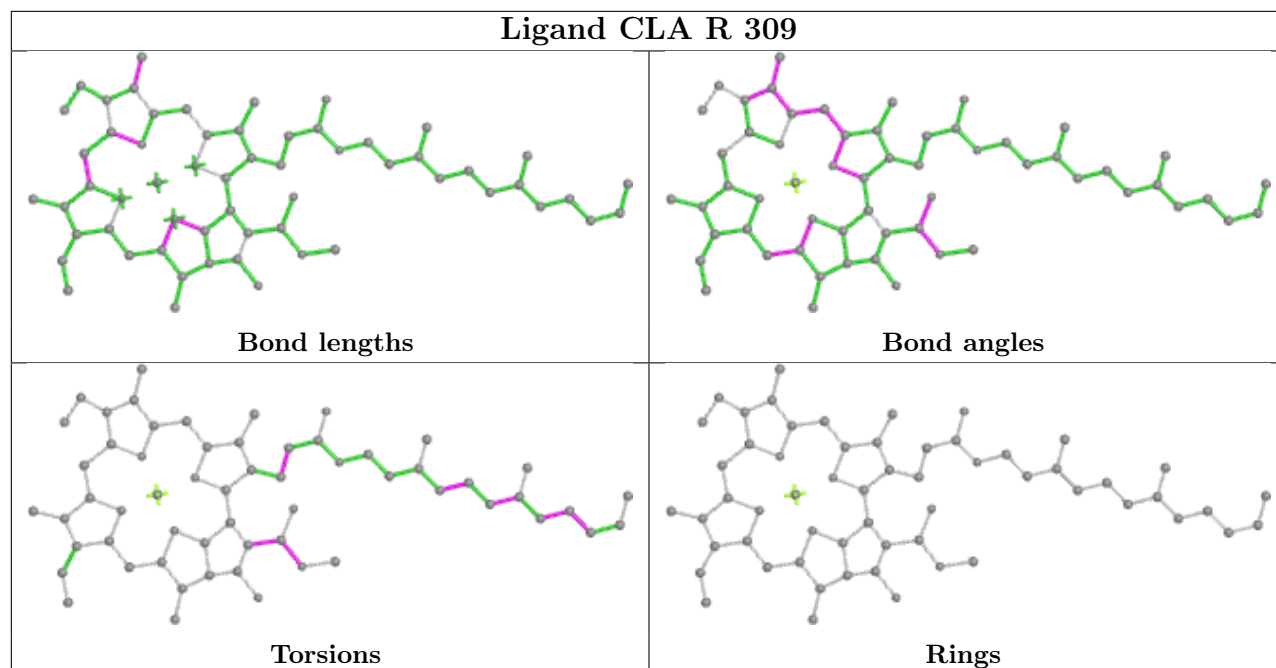
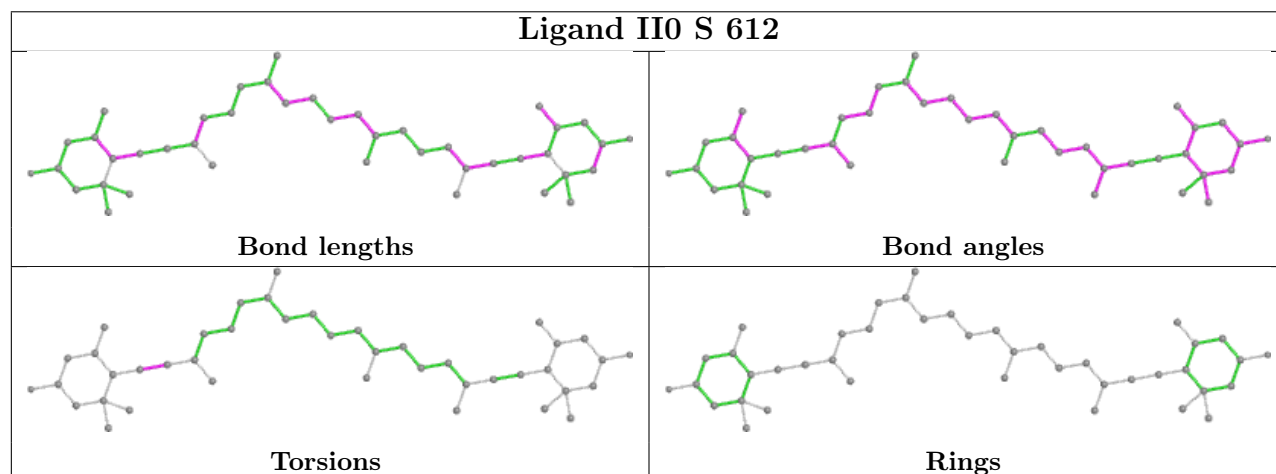


Rings

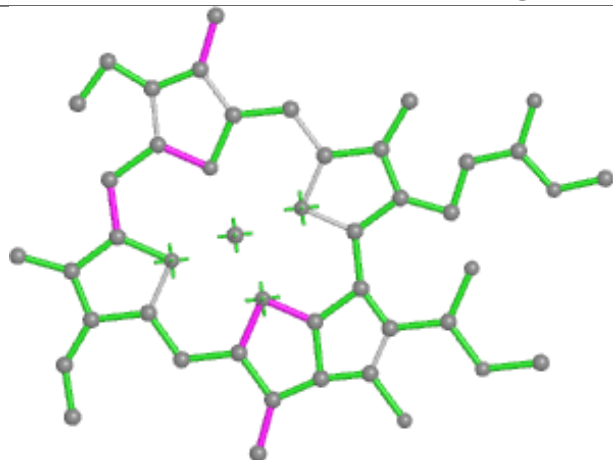


## Ligand CLA P 601

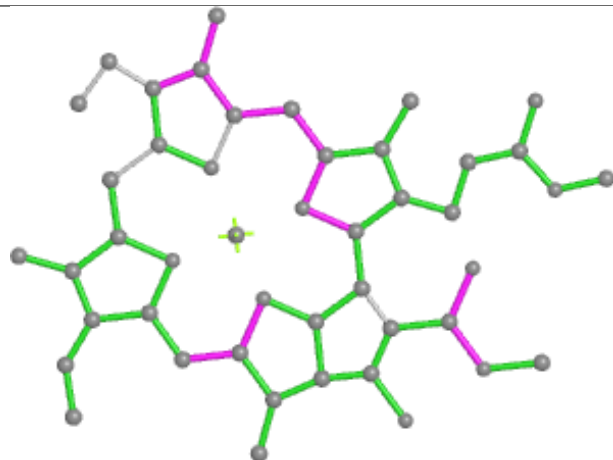


**Ligand CLA R 309****Ligand II0 S 612**

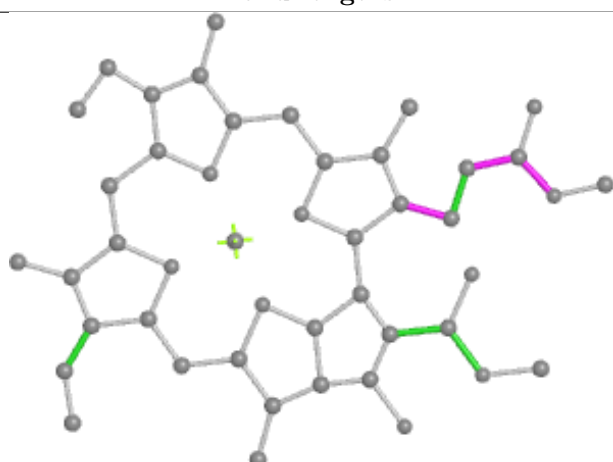
## Ligand CLA R 313



Bond lengths



Bond angles

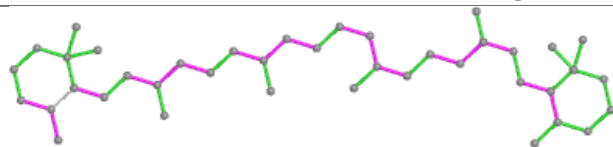


Torsions

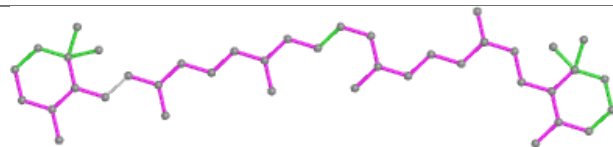


Rings

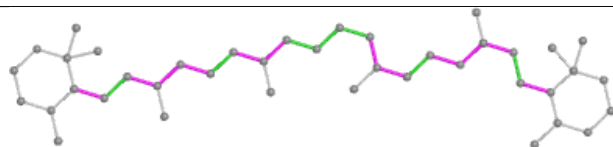
## Ligand WVN 3 313



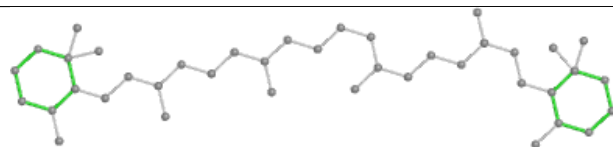
Bond lengths



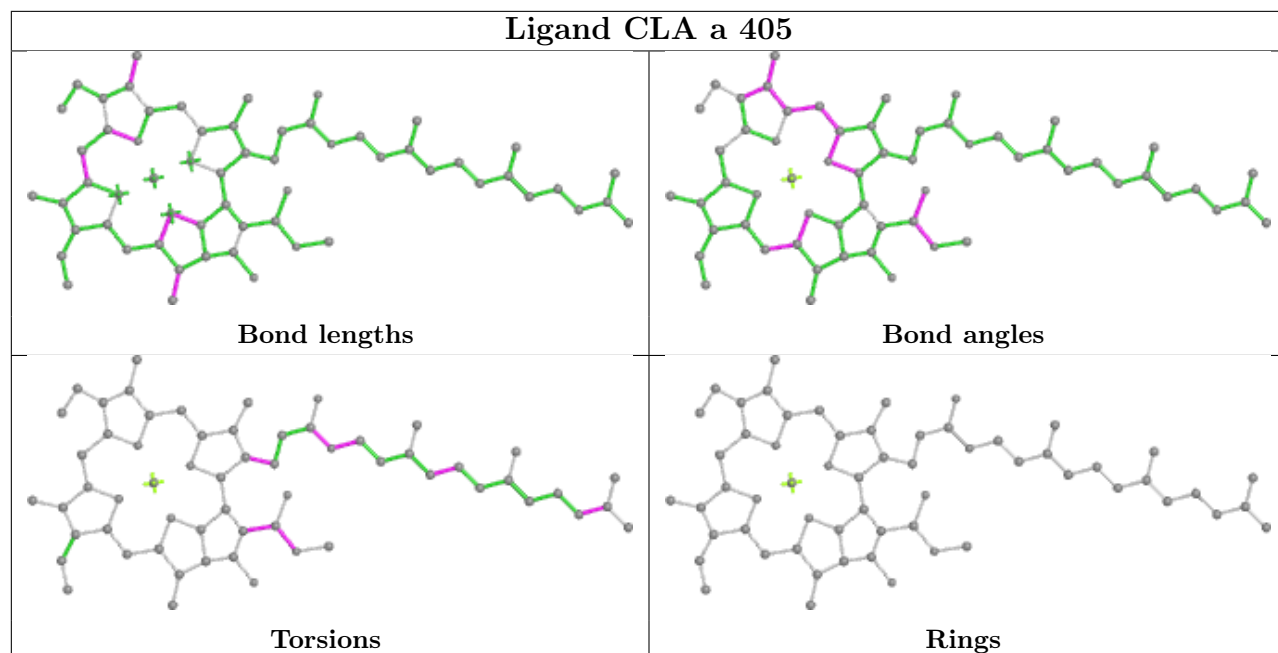
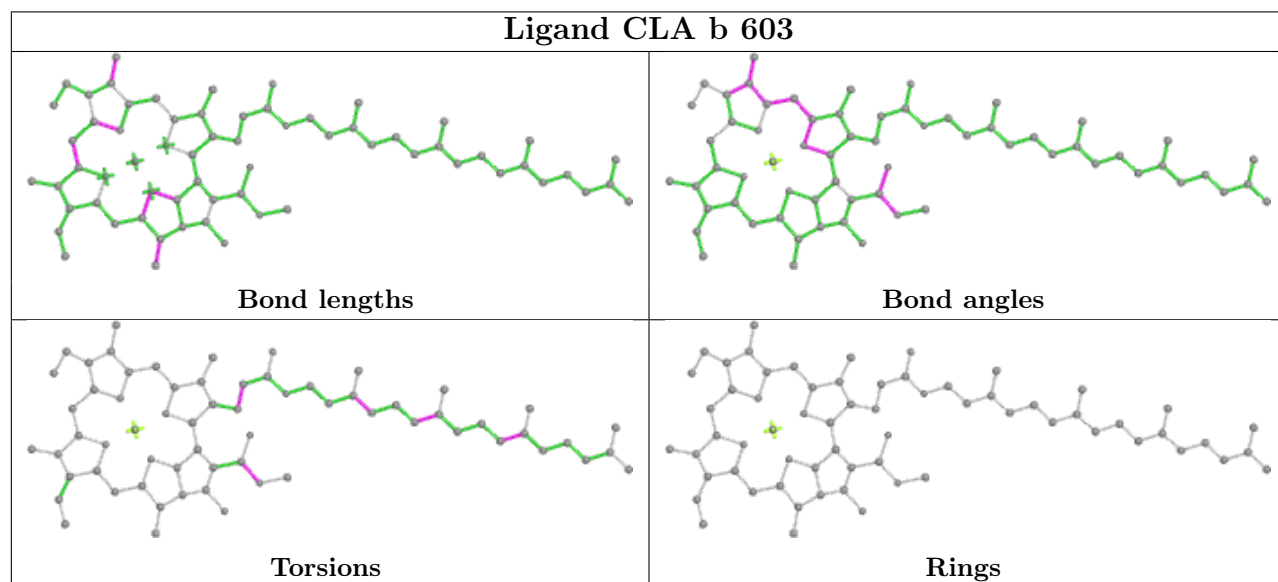
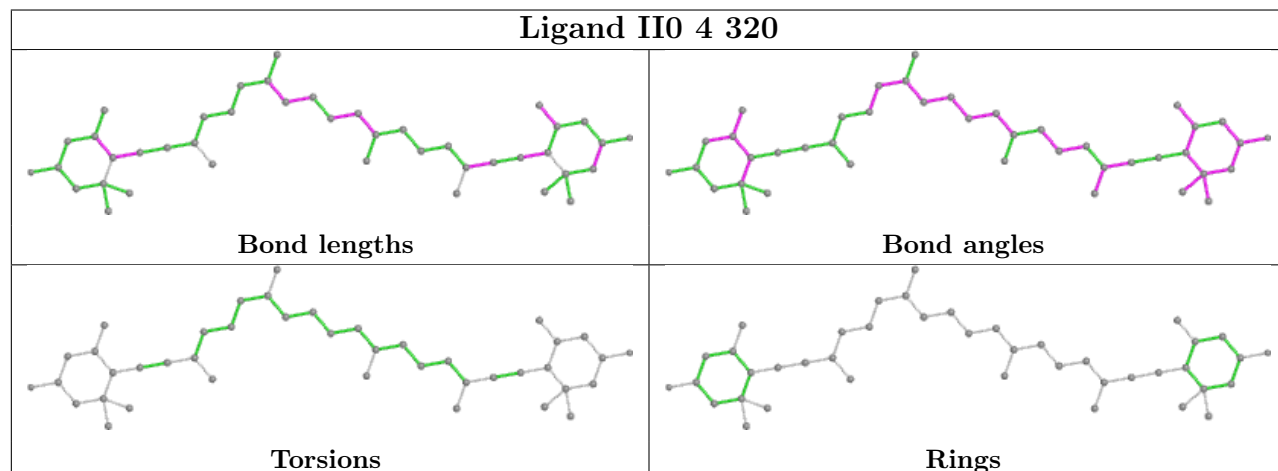
Bond angles



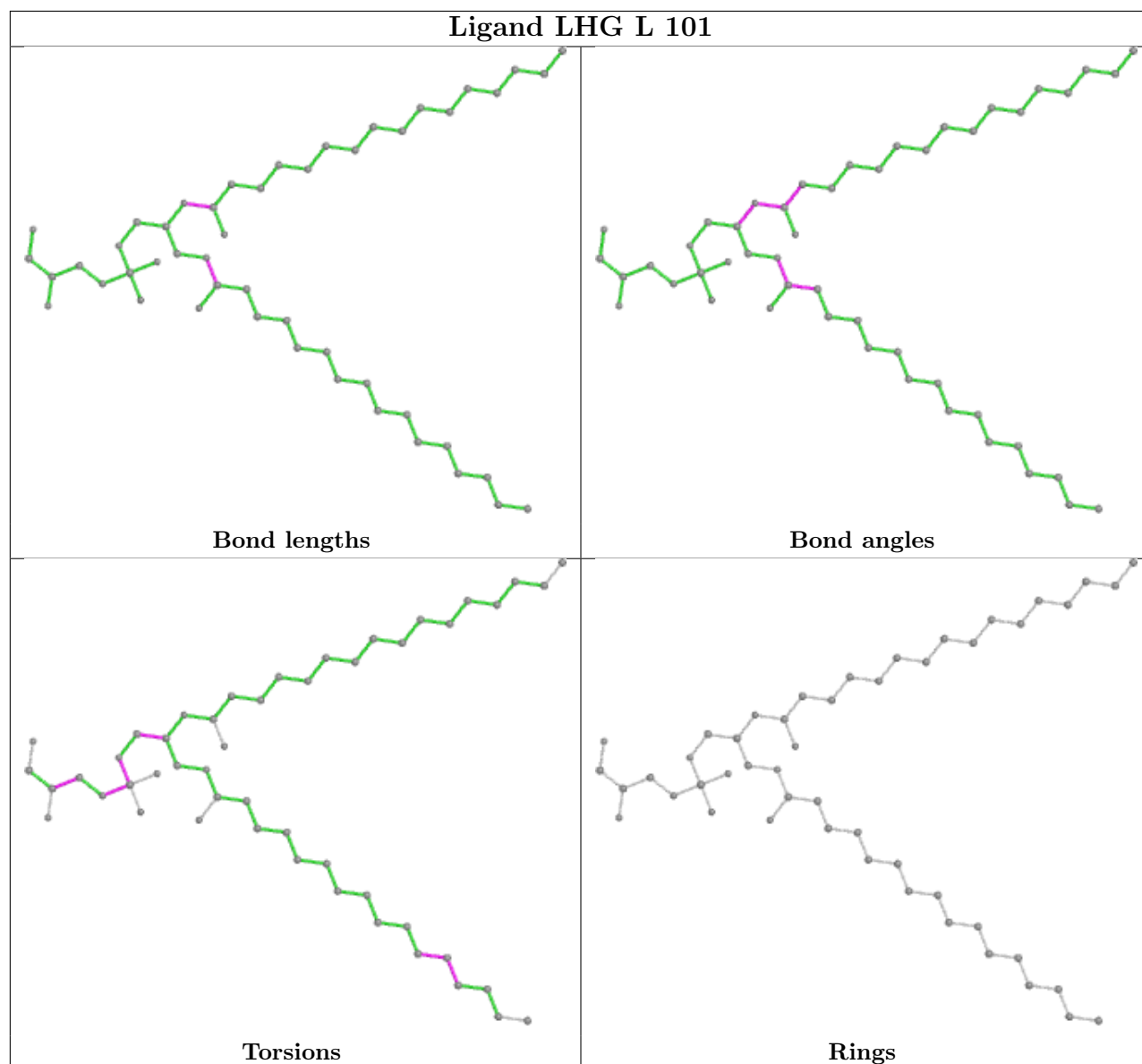
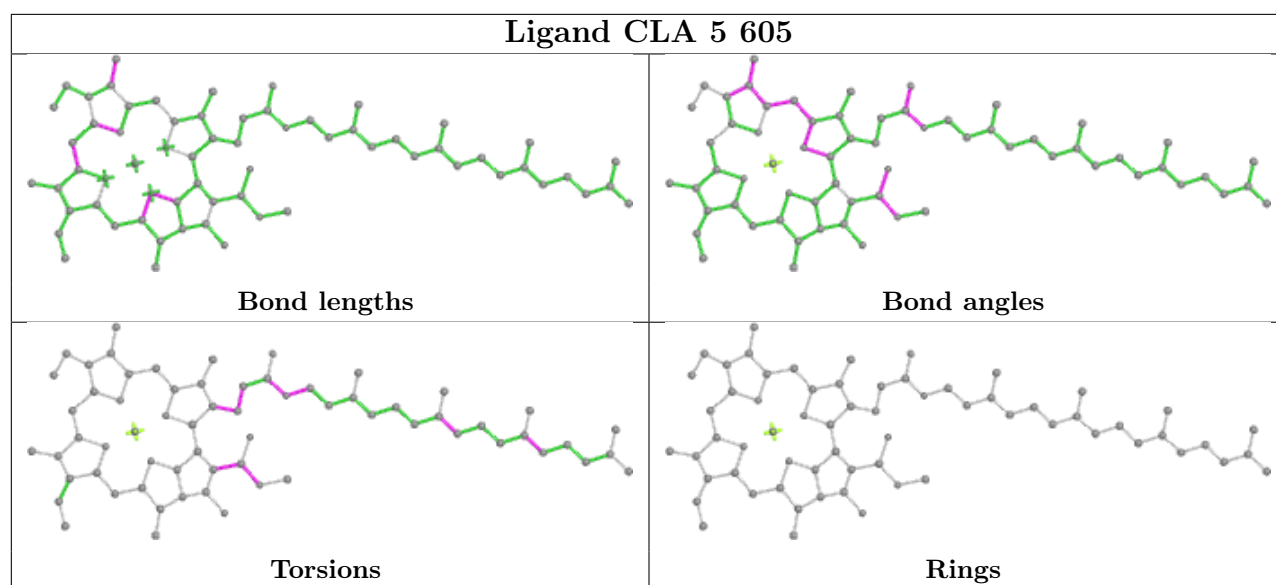
Torsions

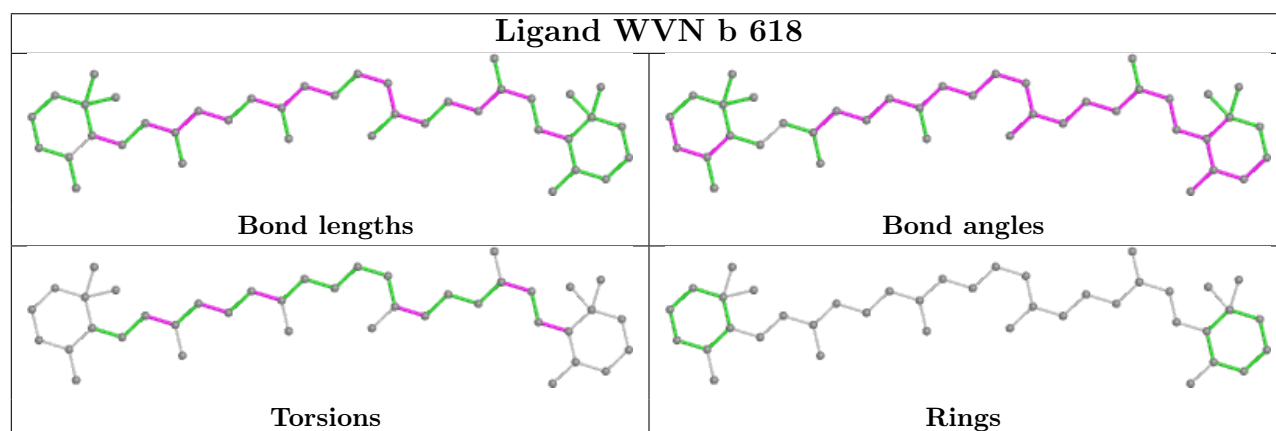
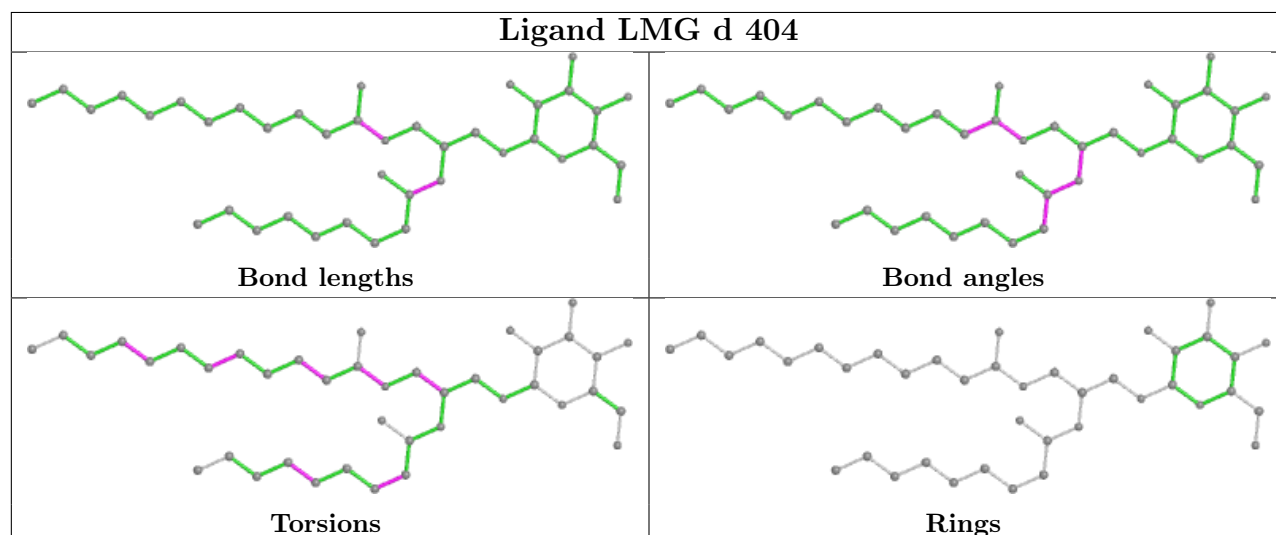
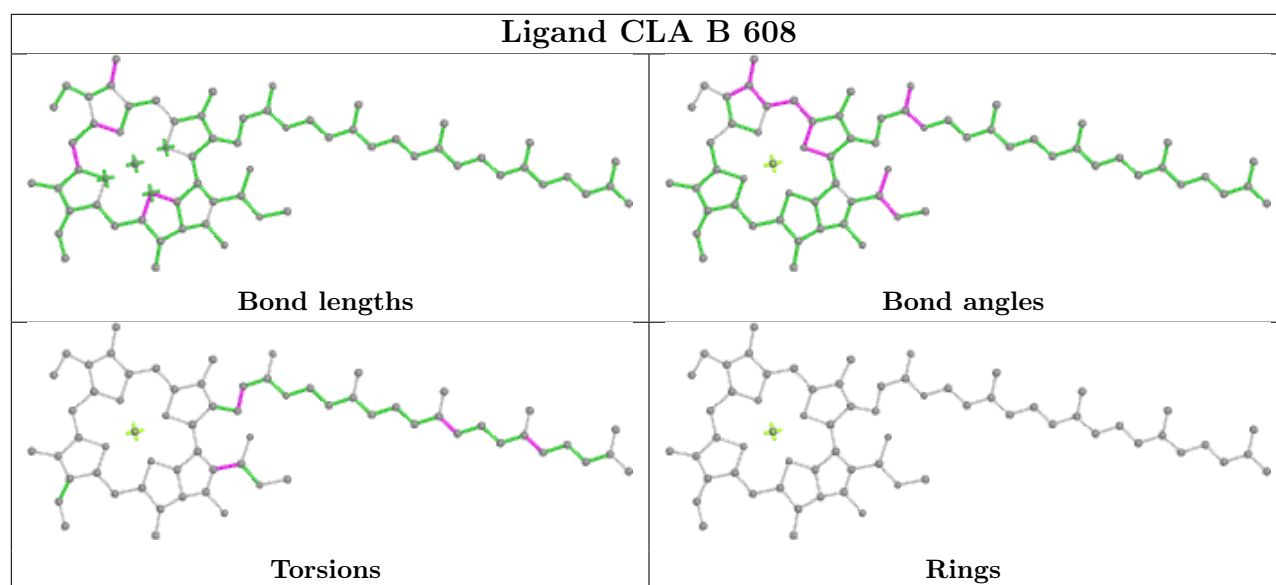


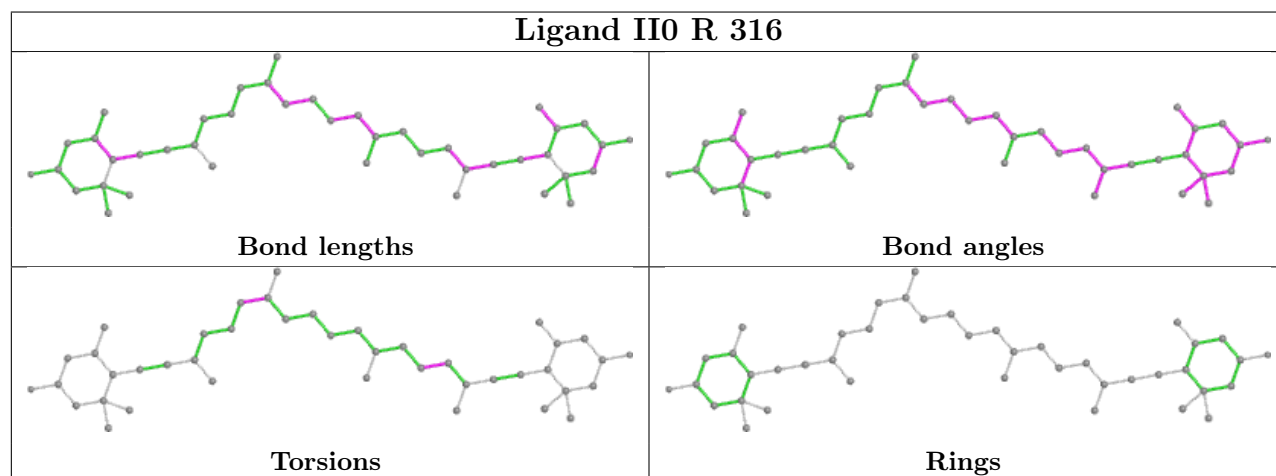
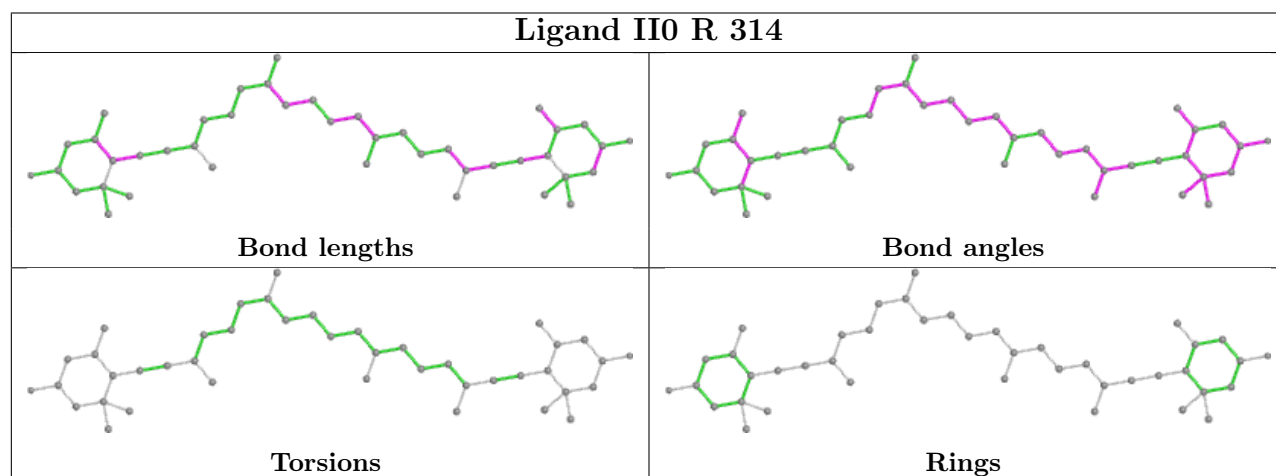
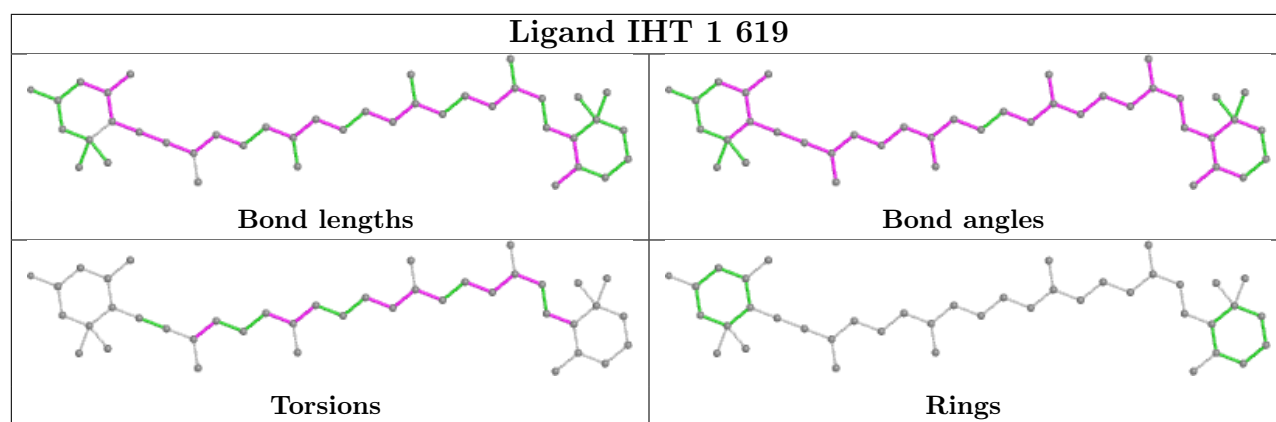
Rings

**Ligand CLA a 405****Ligand CLA b 603****Ligand II0 4 320**

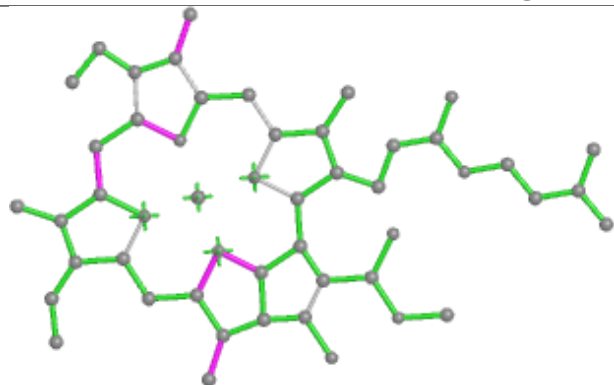




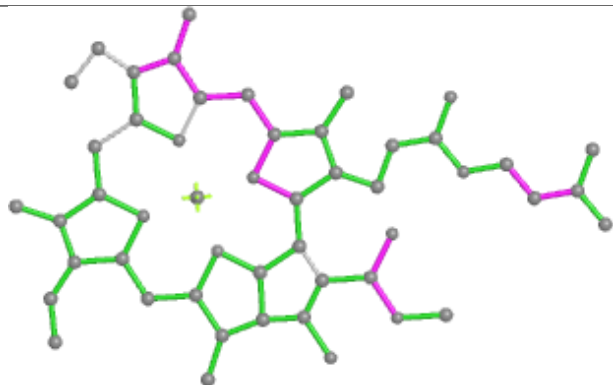




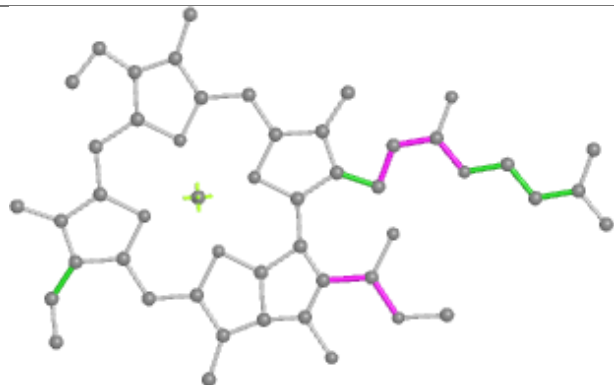
## Ligand CLA 1 606



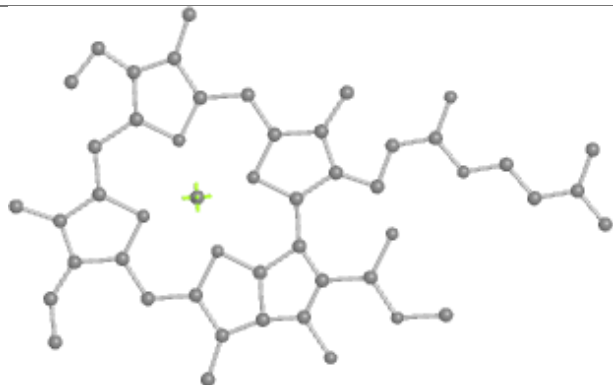
Bond lengths



Bond angles

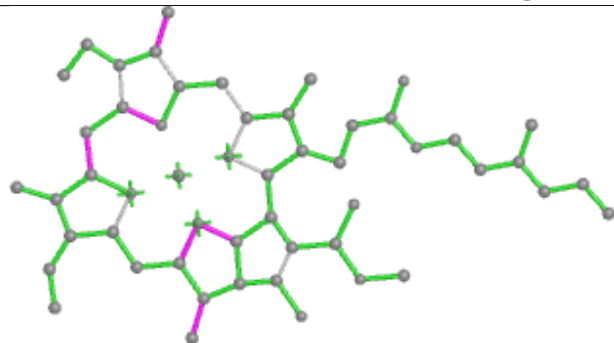


Torsions

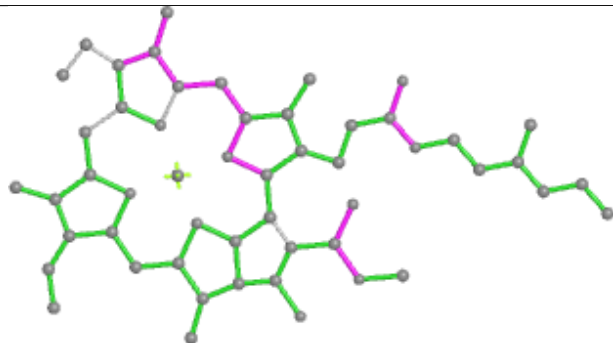


Rings

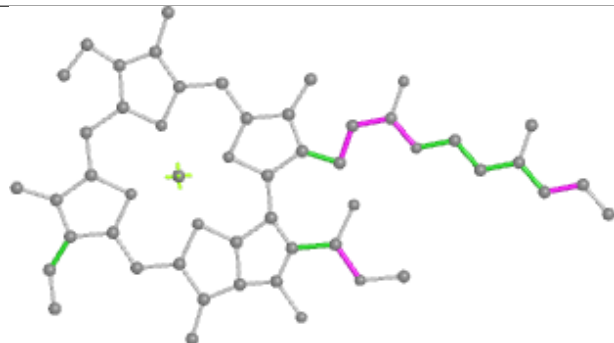
## Ligand CLA 1 603



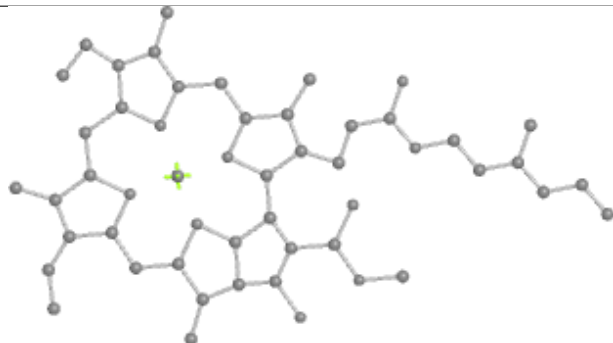
Bond lengths



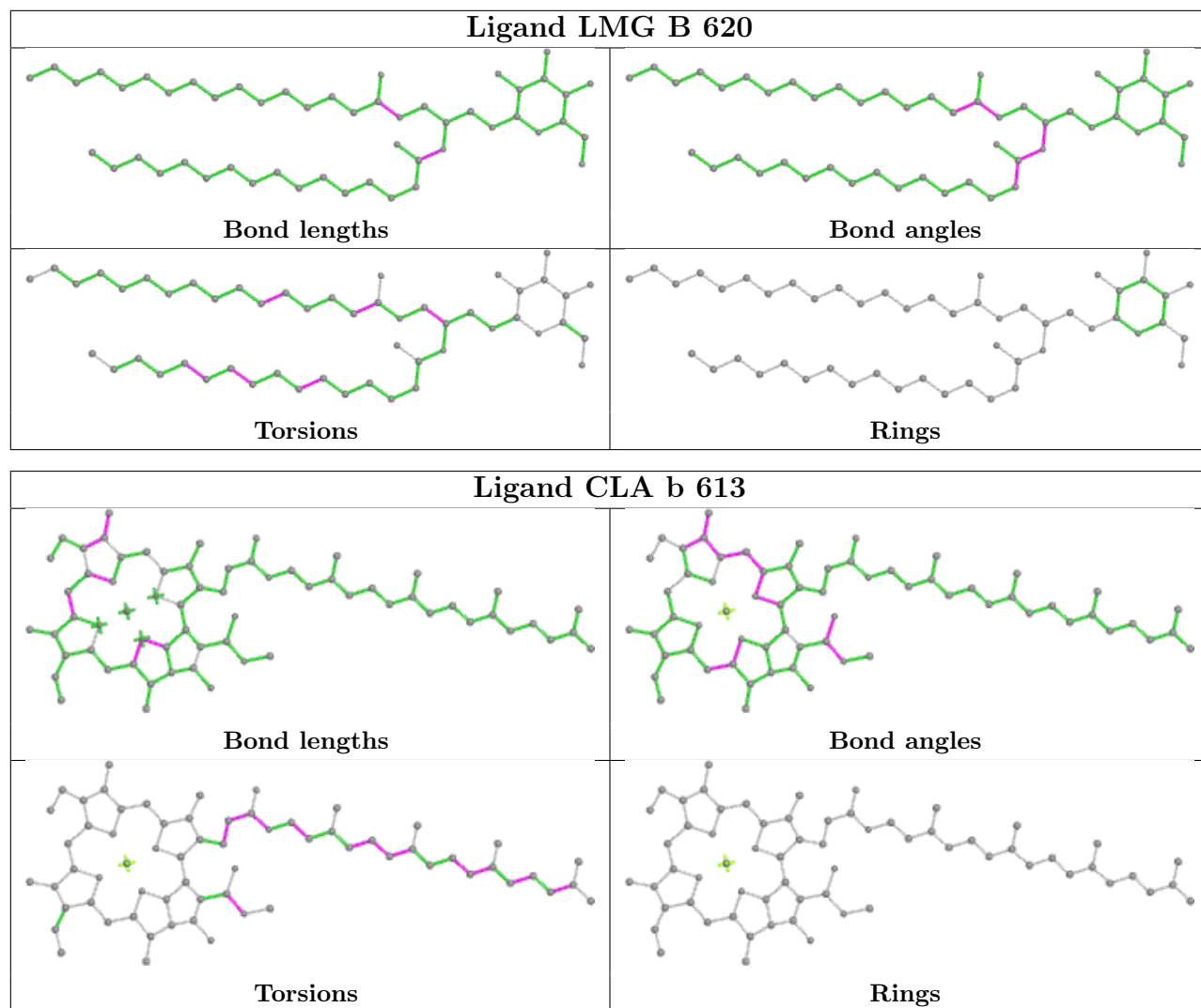
Bond angles



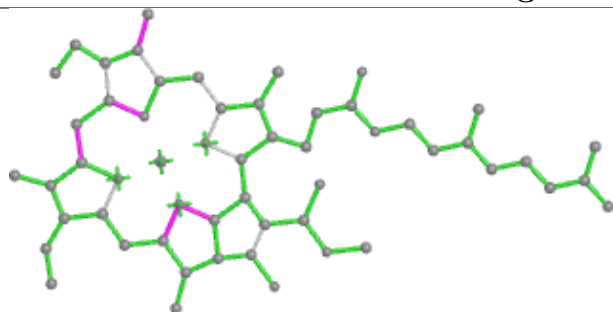
Torsions



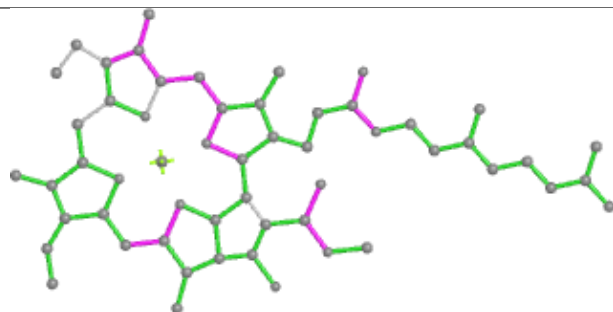
Rings



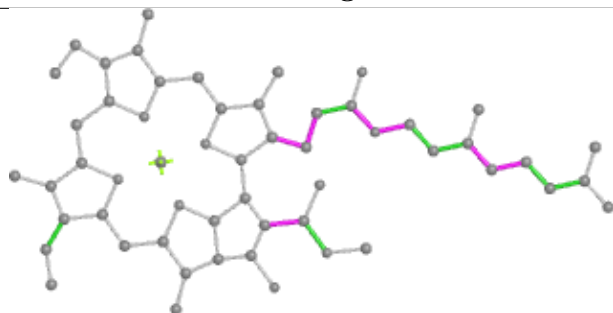
## Ligand CLA S 607



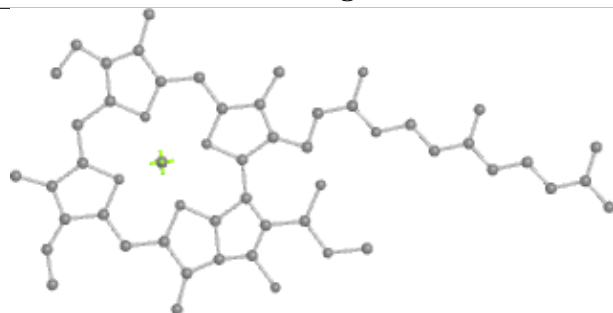
Bond lengths



Bond angles

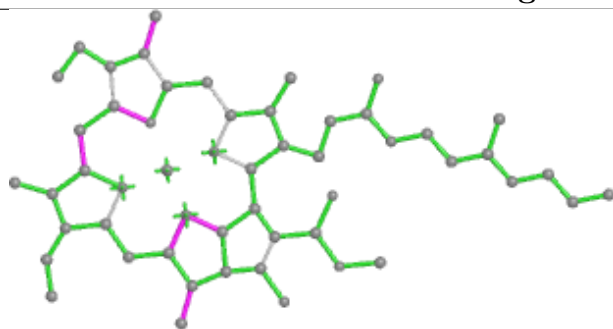


Torsions

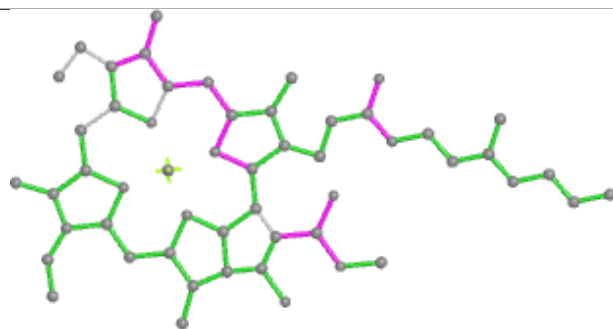


Rings

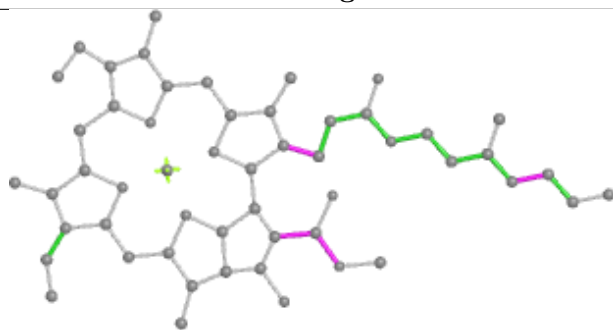
## Ligand CLA 6 609



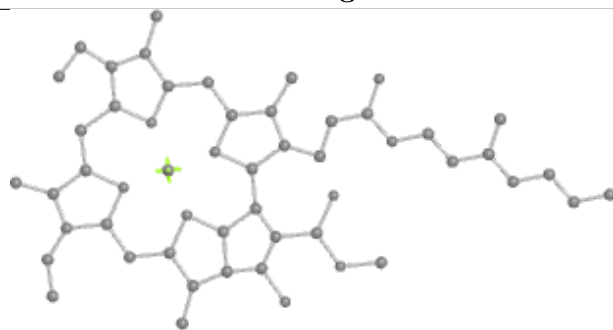
Bond lengths



Bond angles

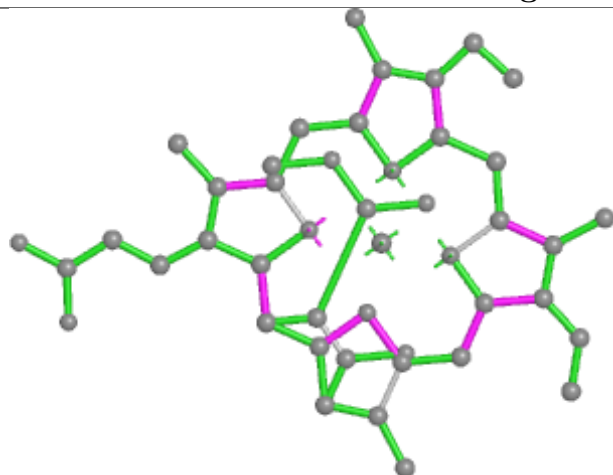


Torsions

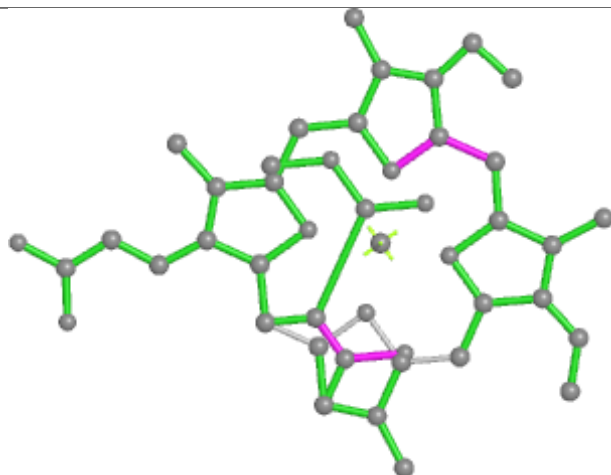


Rings

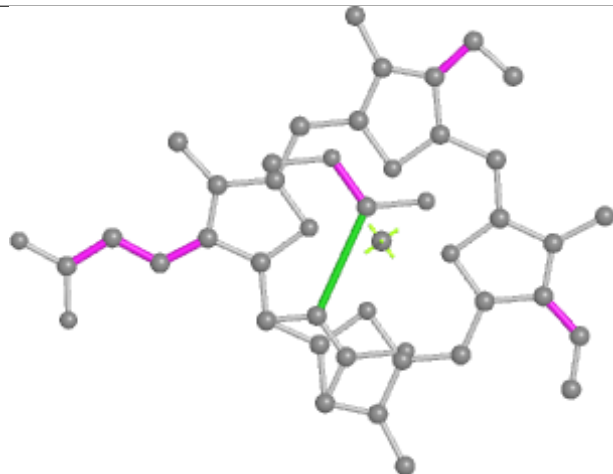
## Ligand KC2 1 612



Bond lengths



Bond angles

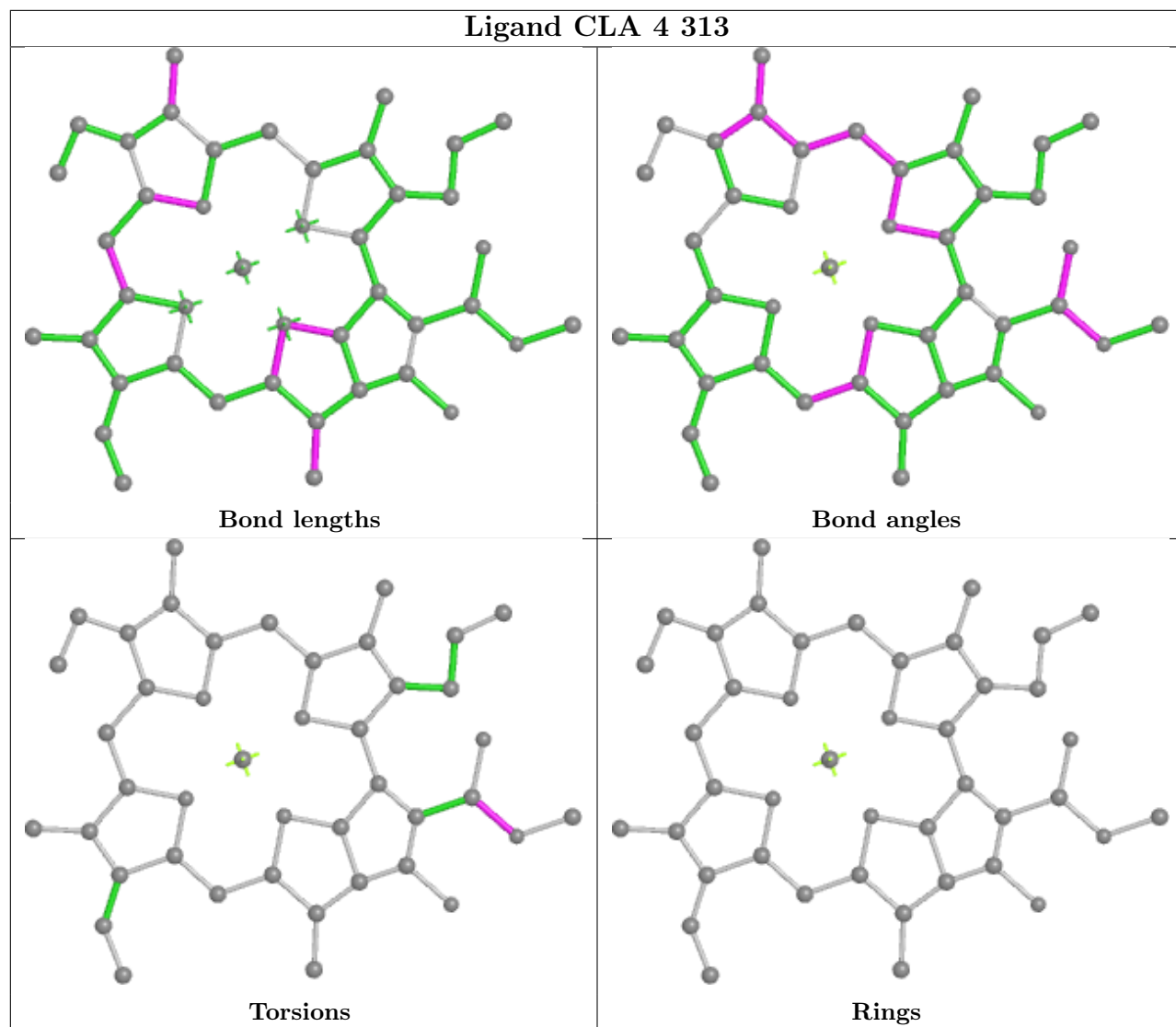


Torsions

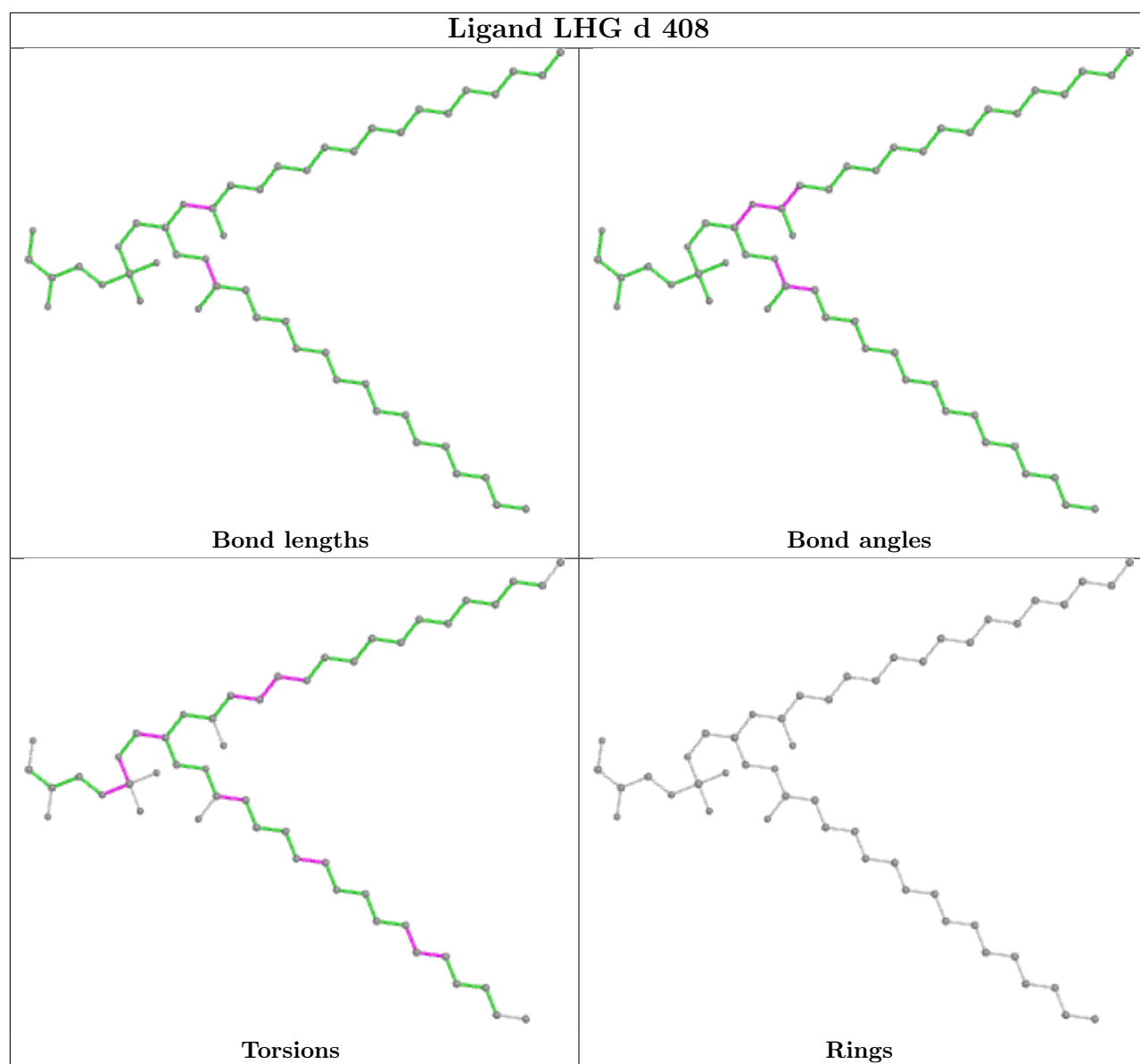


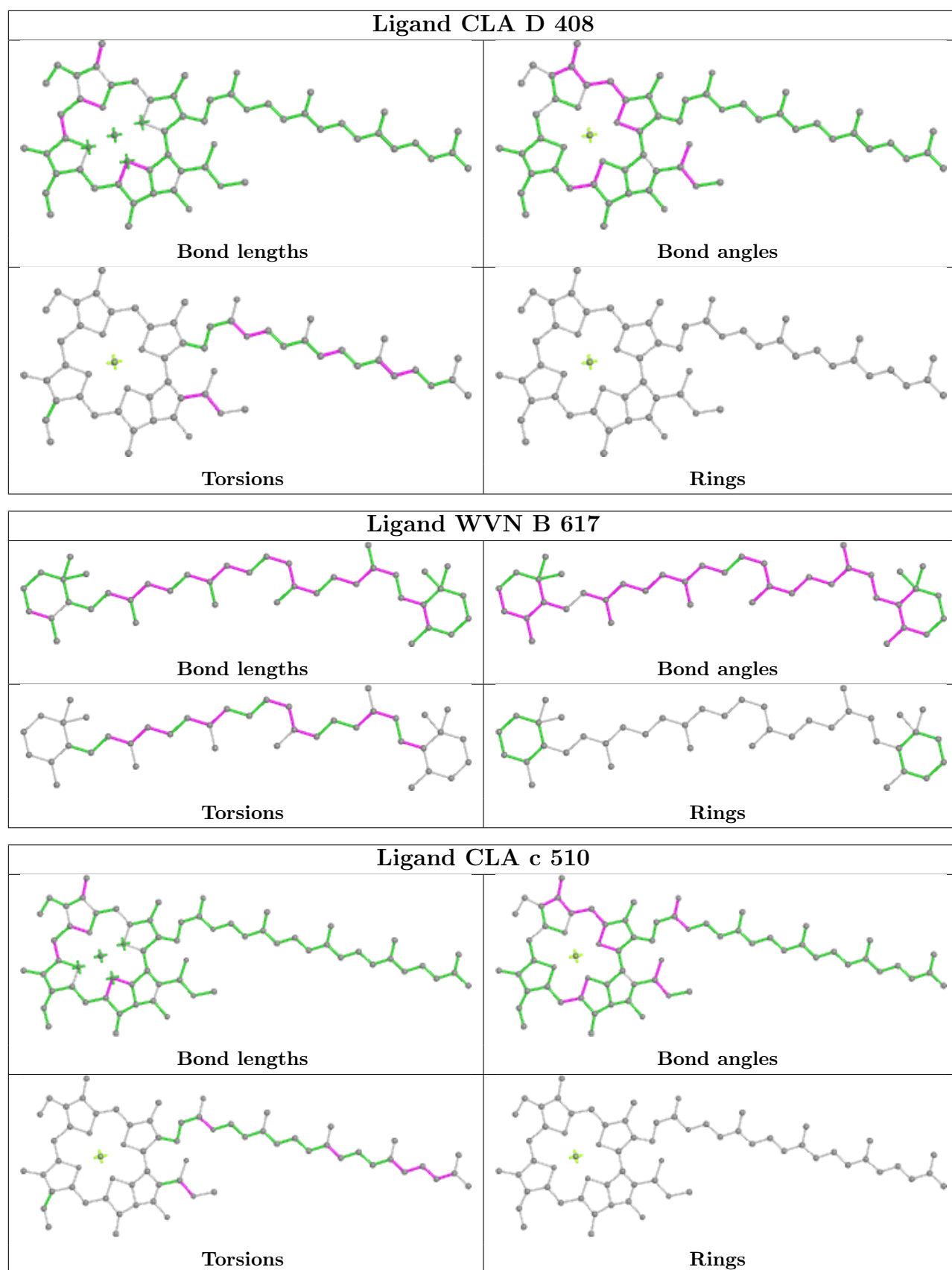
Rings

## Ligand CLA 4 313

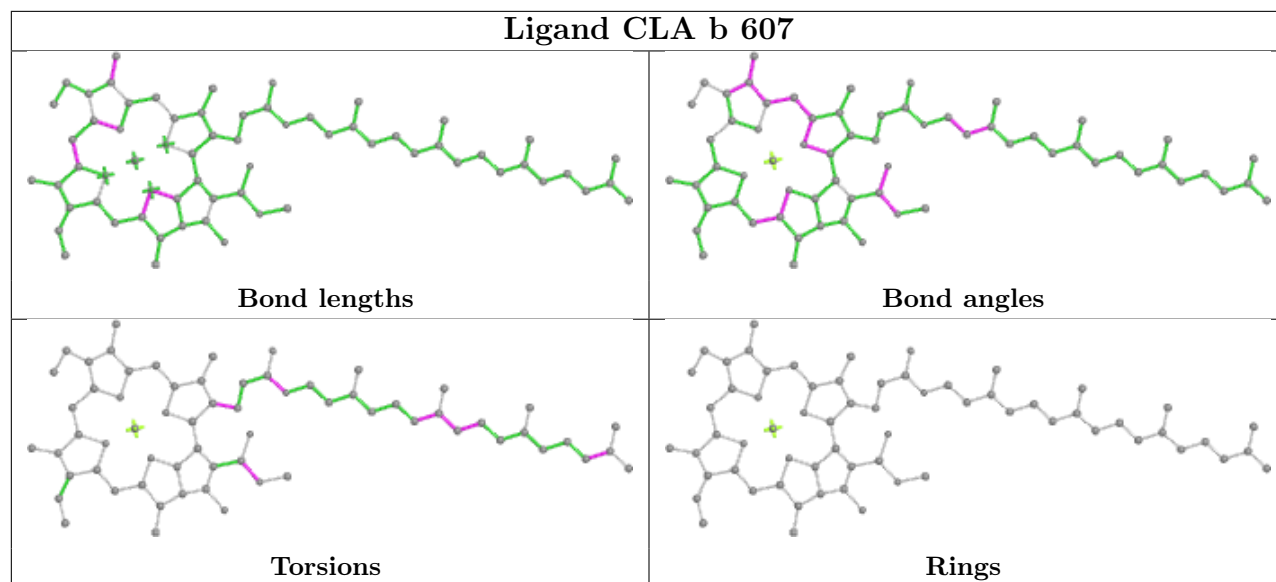




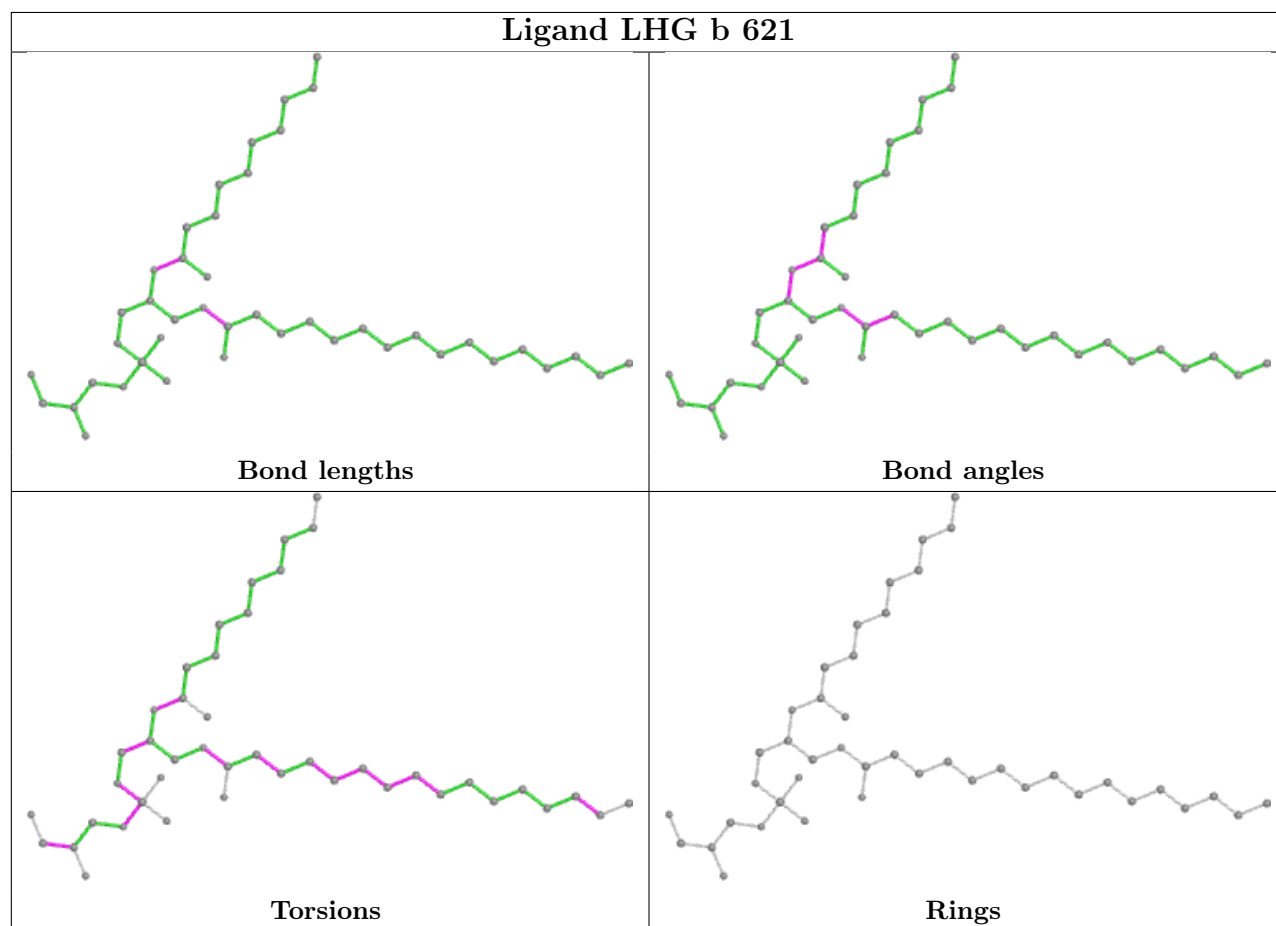




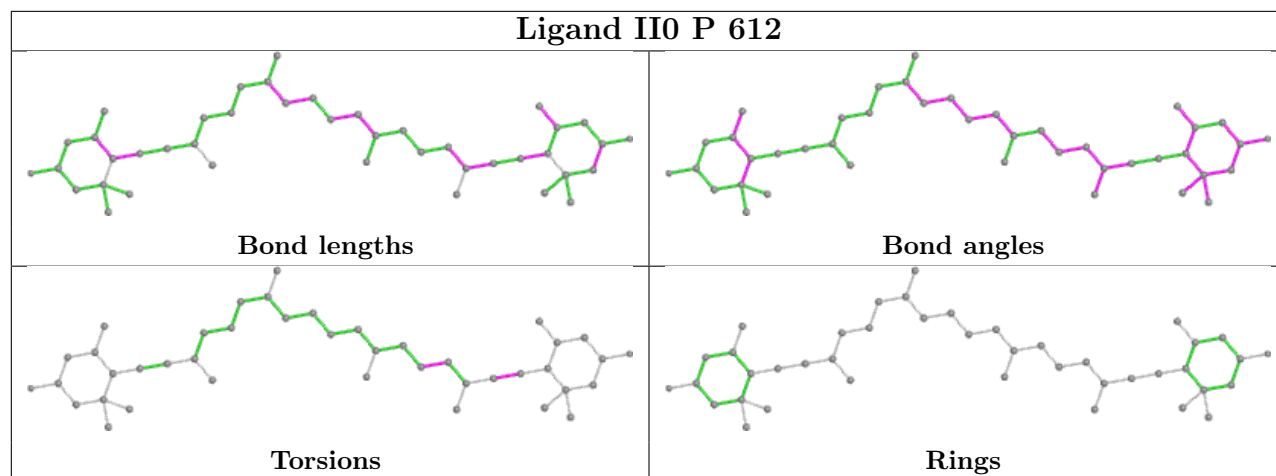
## Ligand CLA b 607



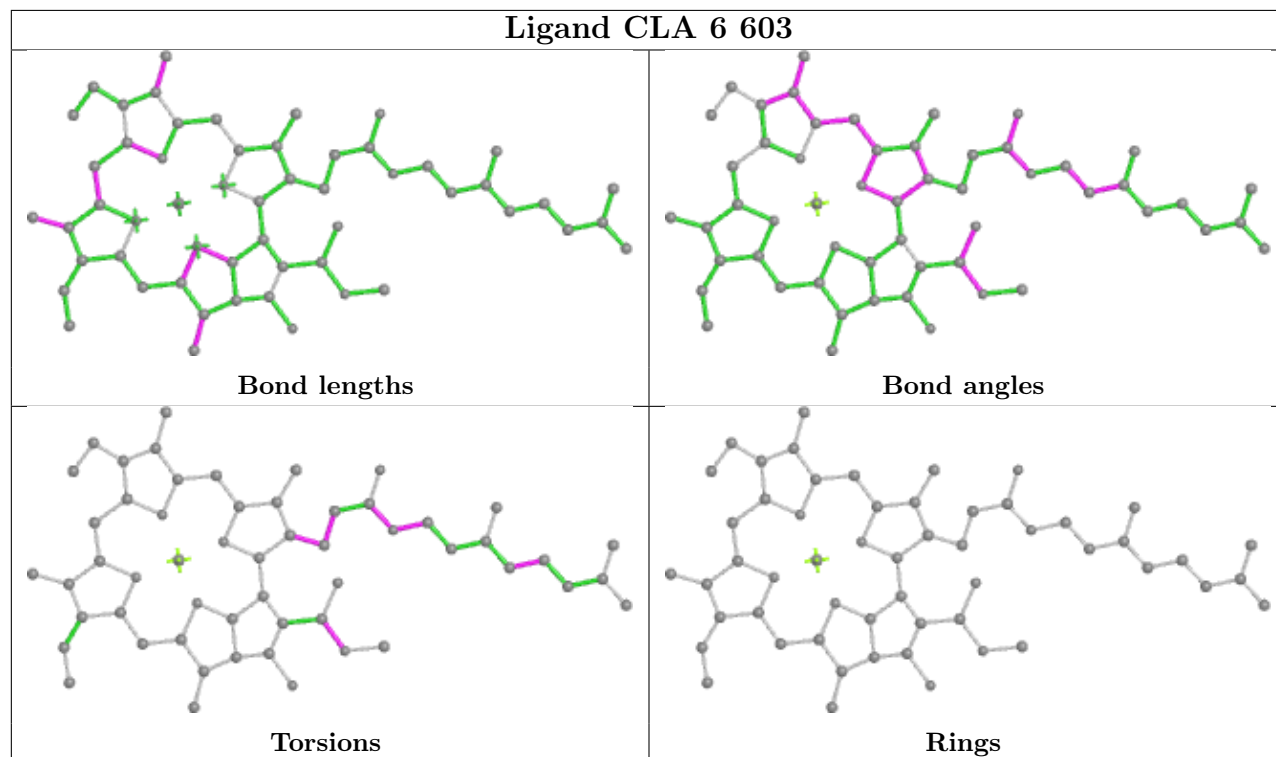
## Ligand LHG b 621



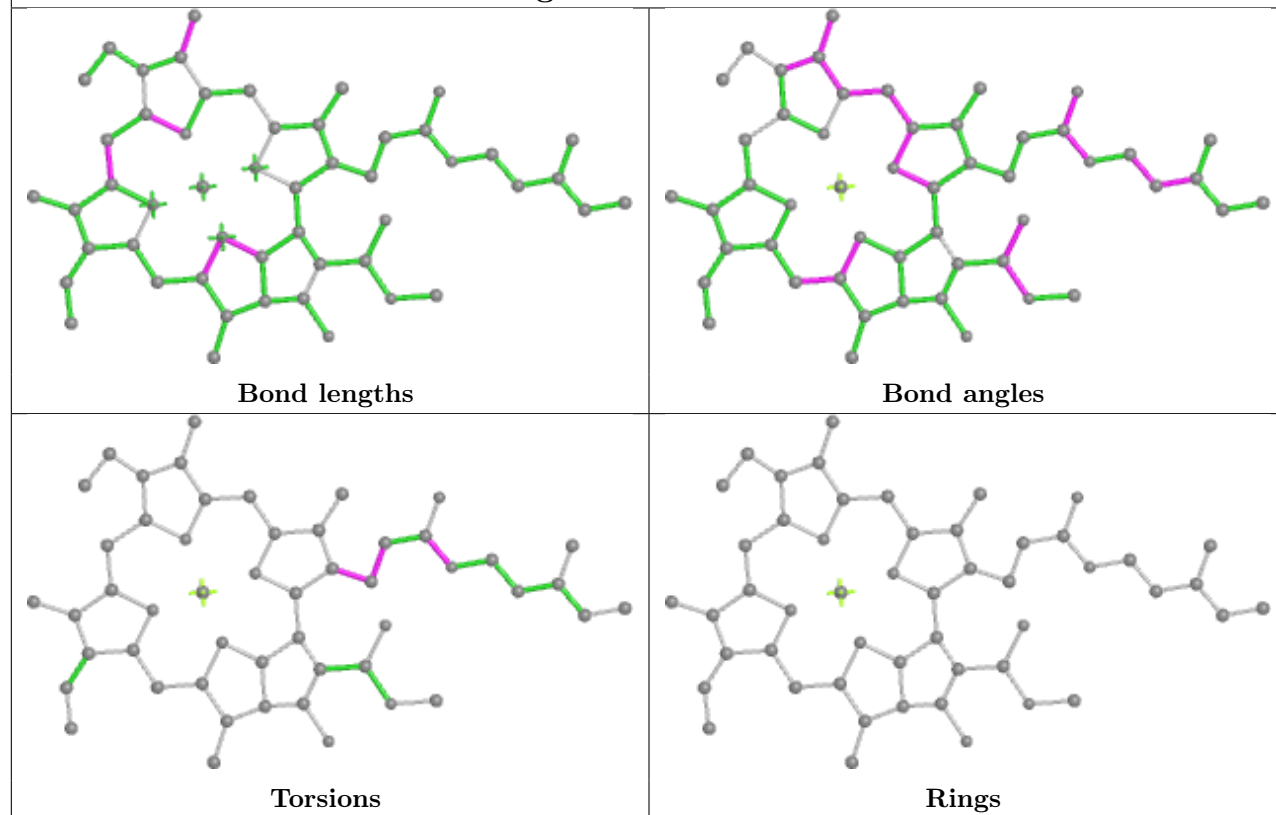
## Ligand II0 P 612



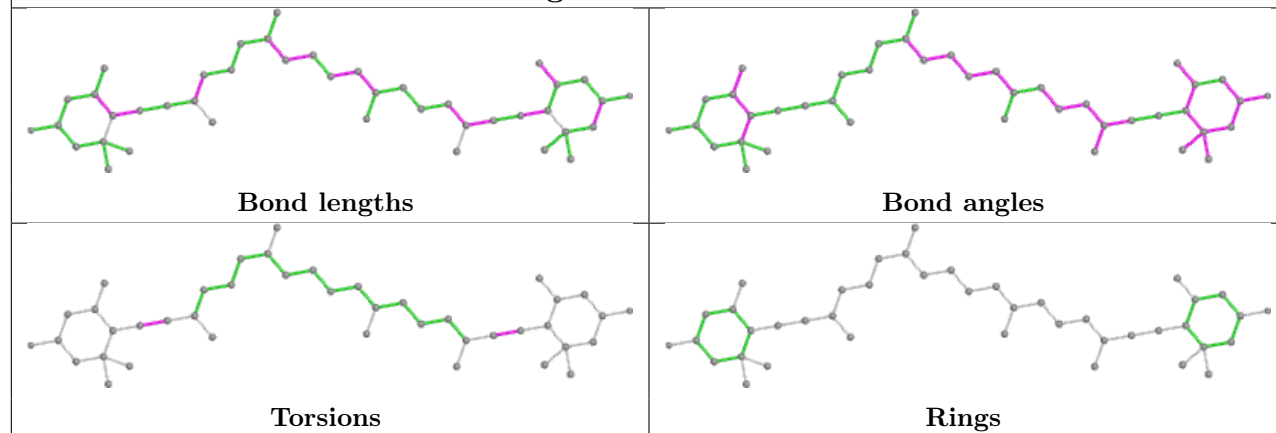
## Ligand CLA 6 603

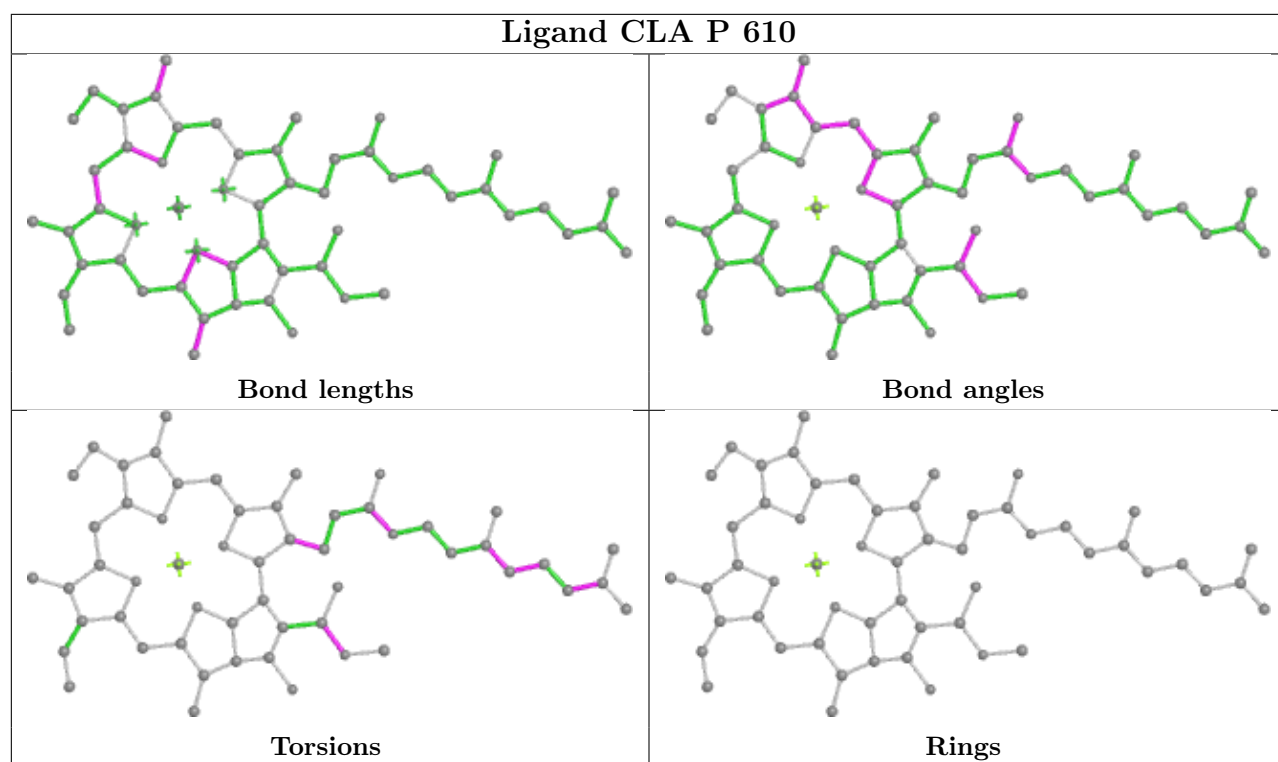


## Ligand CLA 4 309

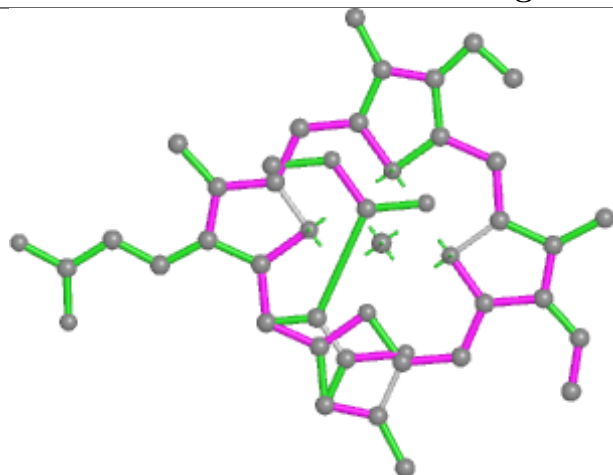


## Ligand II0 O 613

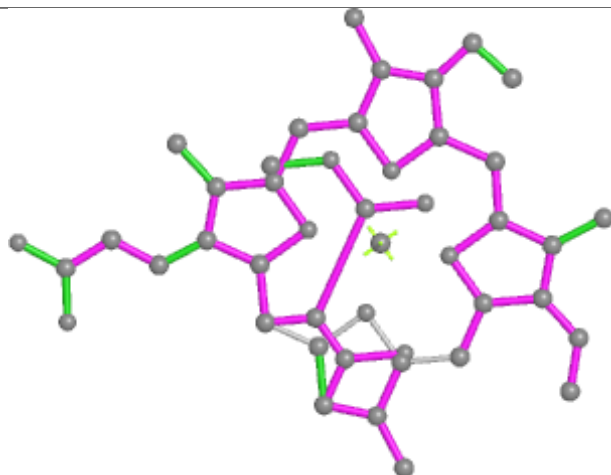




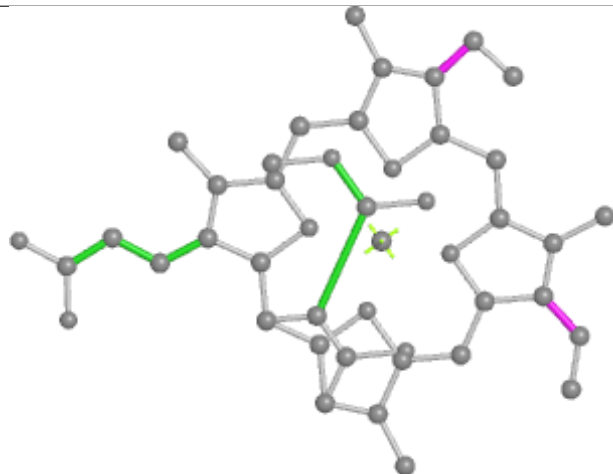
## Ligand KC2 N 610



Bond lengths



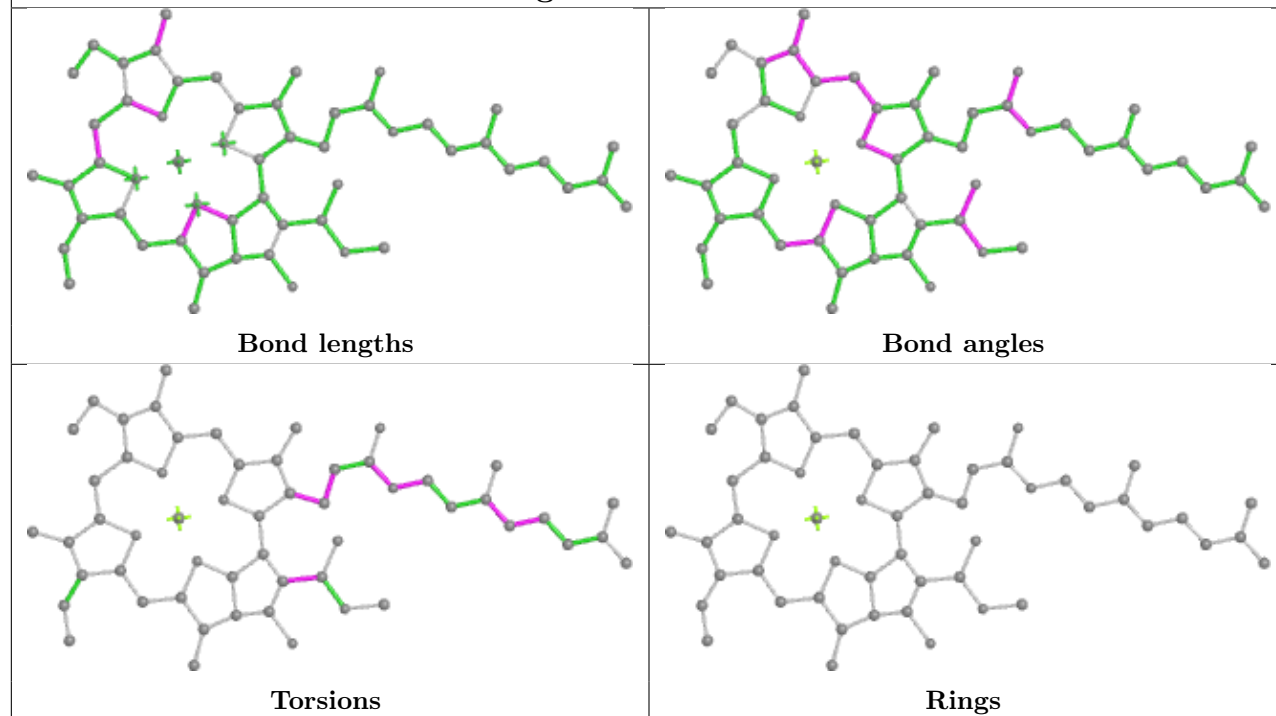
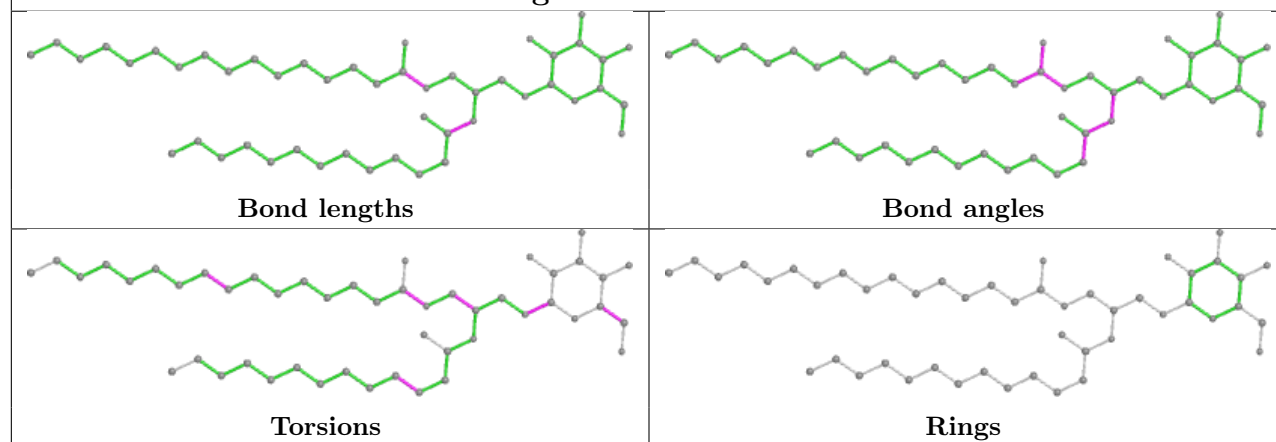
Bond angles



Torsions

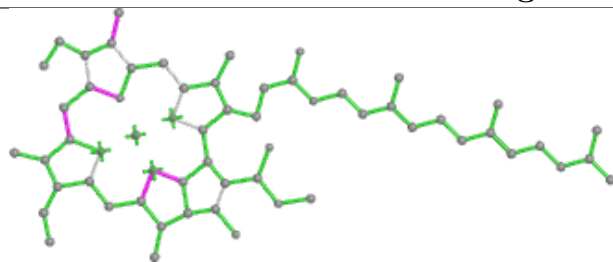


Rings

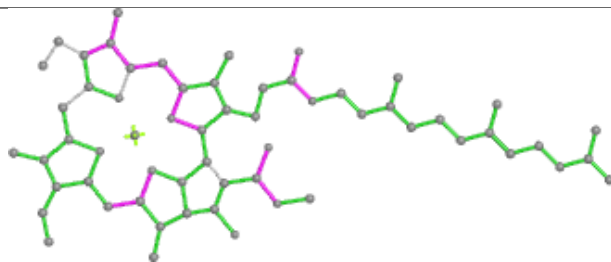
**Ligand CLA 6 607****Ligand LMG a 413**



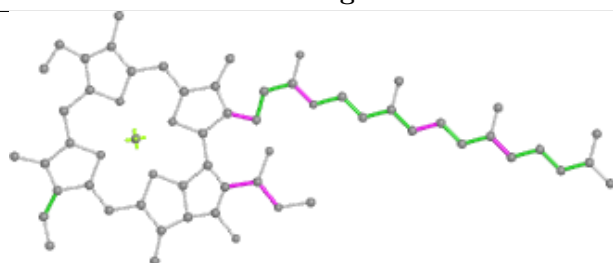
## Ligand CLA b 614



Bond lengths



Bond angles

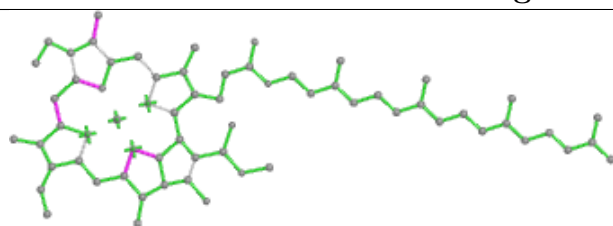


Torsions

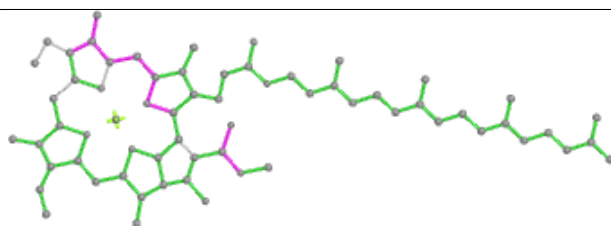


Rings

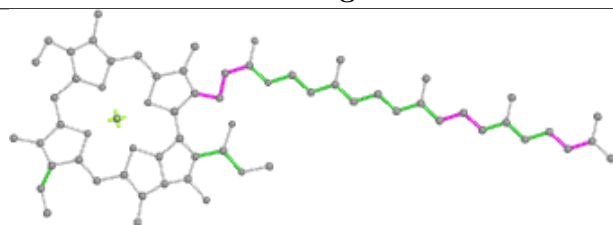
## Ligand CLA O 603



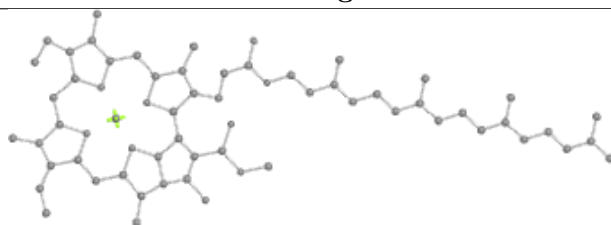
Bond lengths



Bond angles

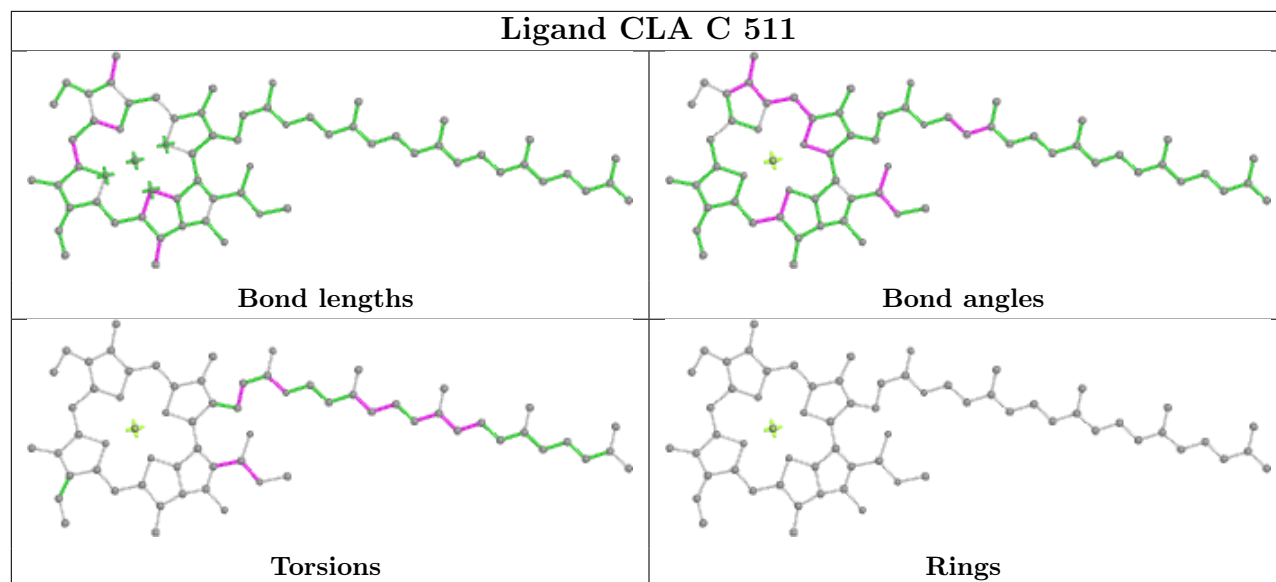


Torsions

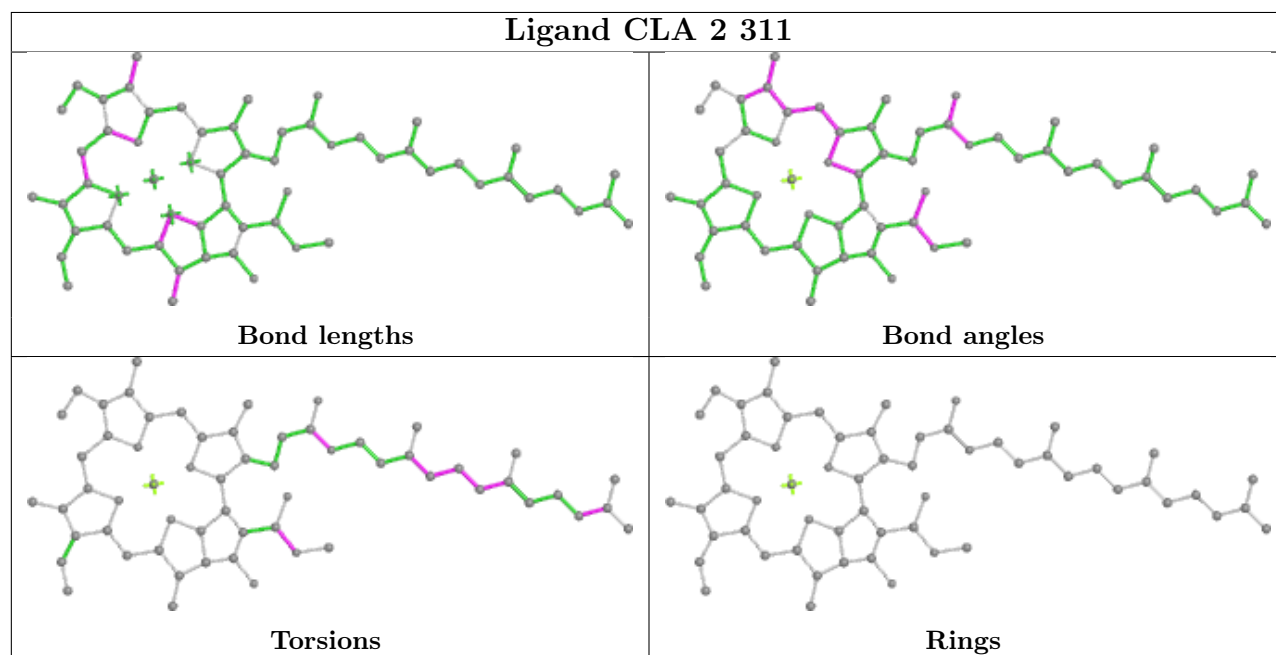


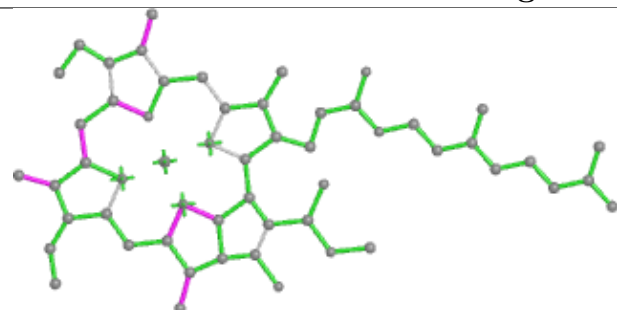
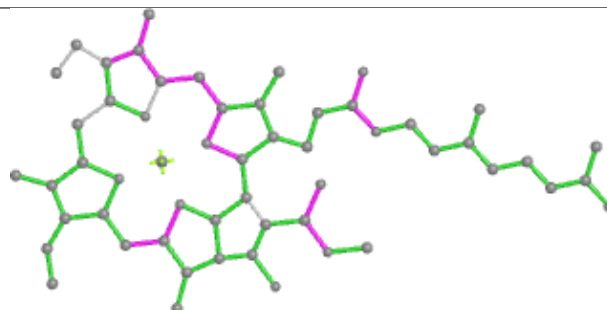
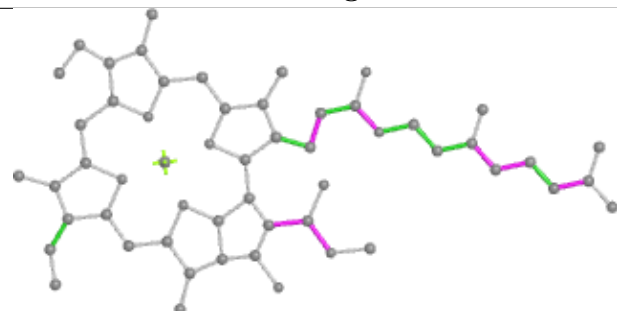
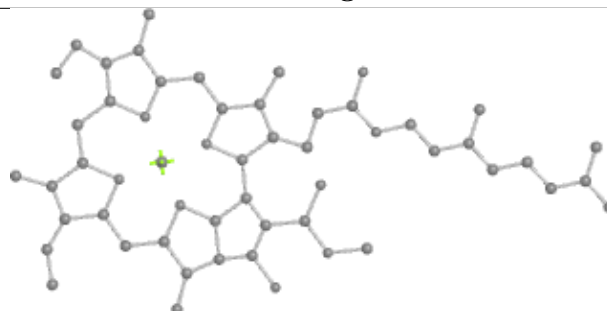
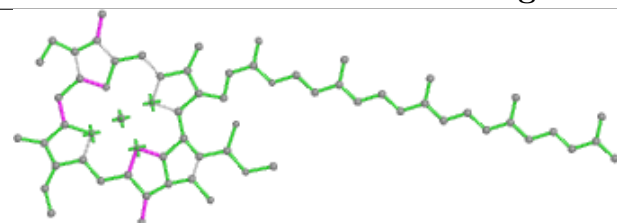
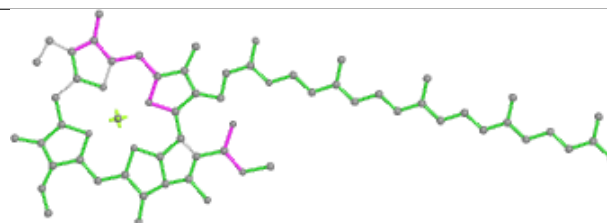
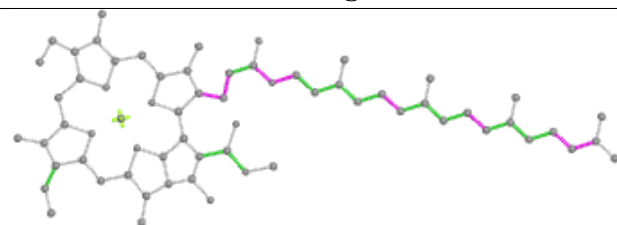
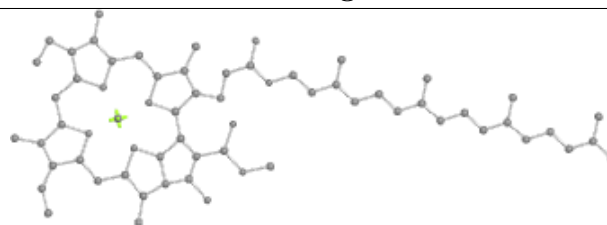
Rings

## Ligand CLA C 511

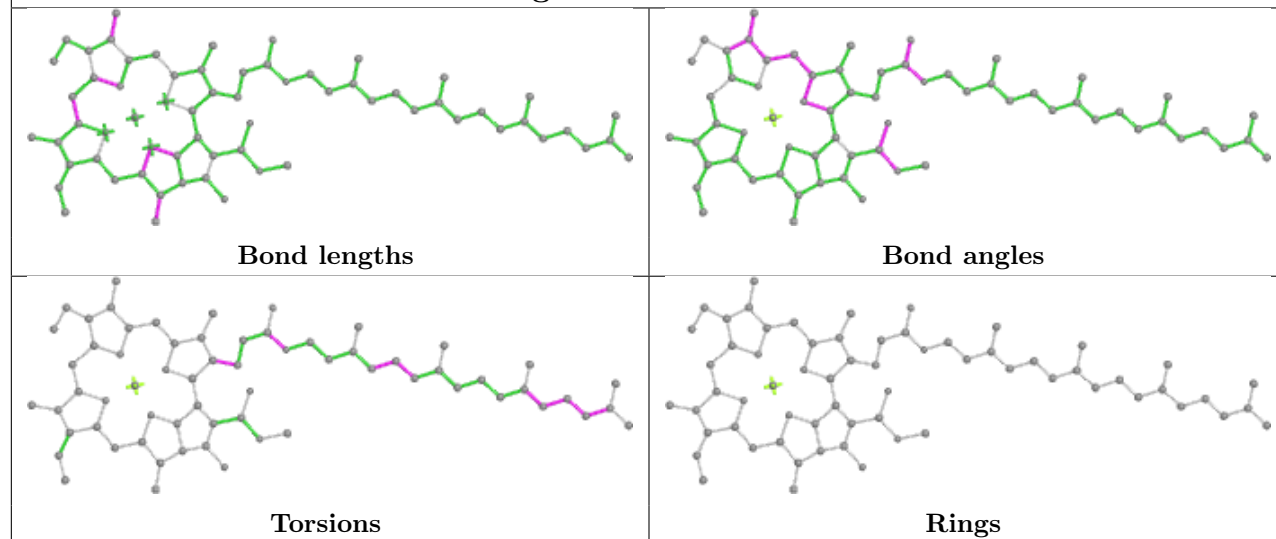


## Ligand CLA 2 311

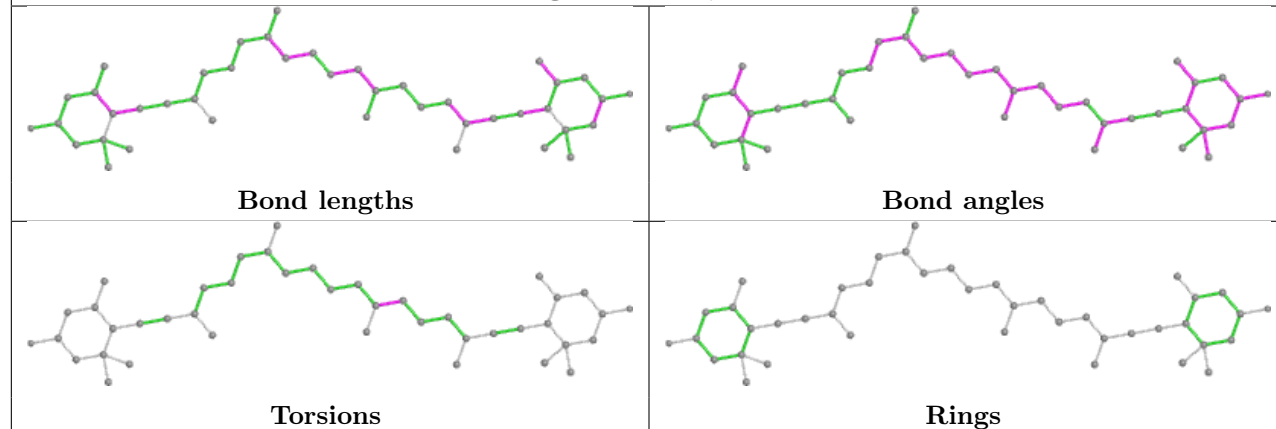


**Ligand CLA R 303****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 615****Bond lengths****Bond angles****Torsions****Rings**

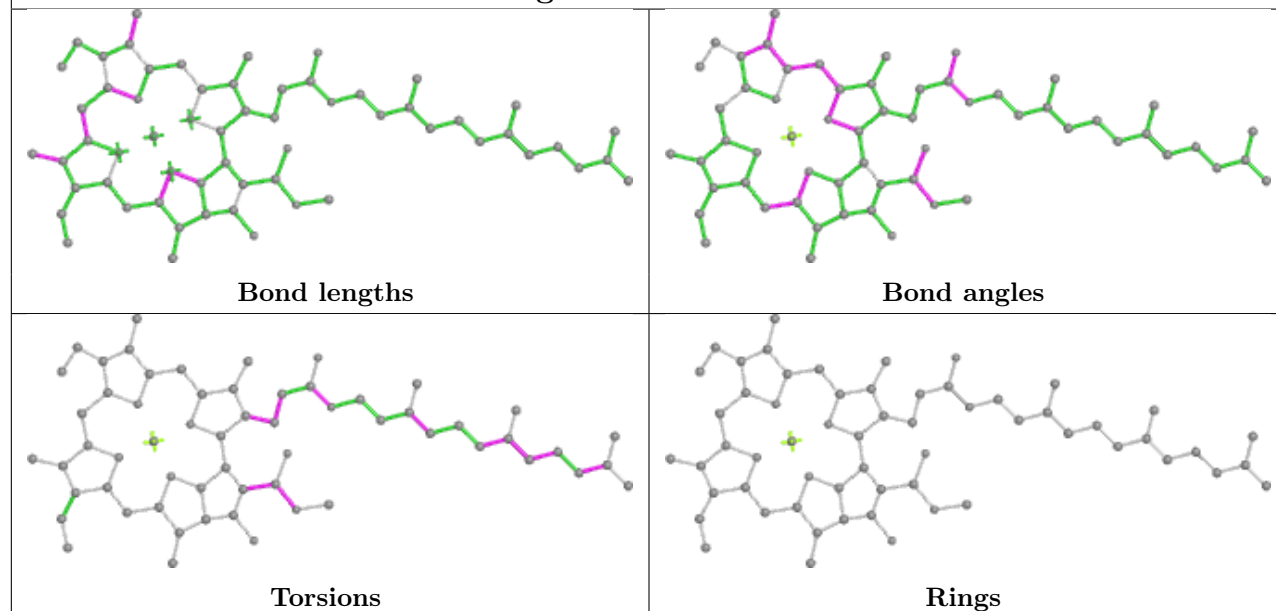
## Ligand CLA C 513



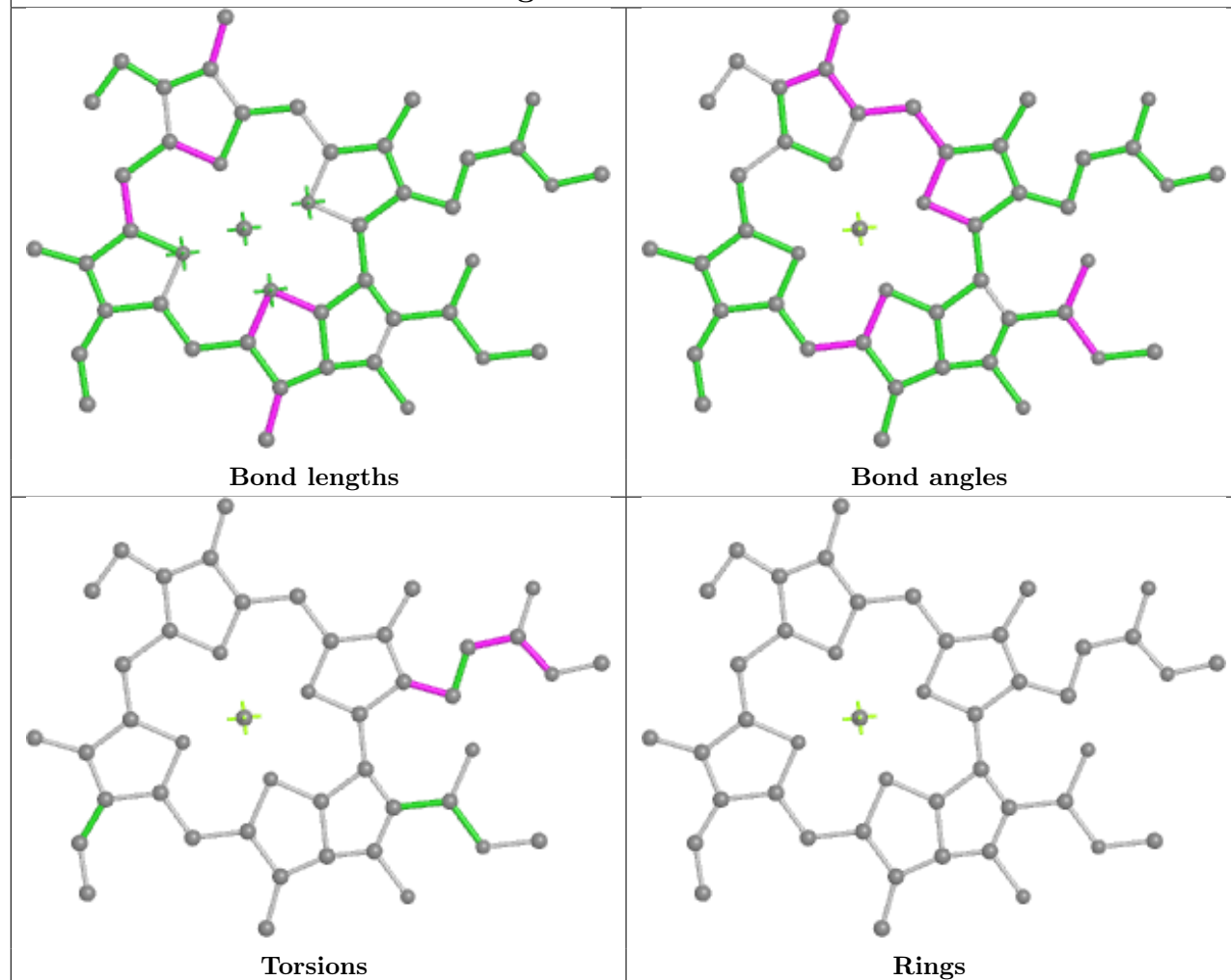
## Ligand II0 Q 313



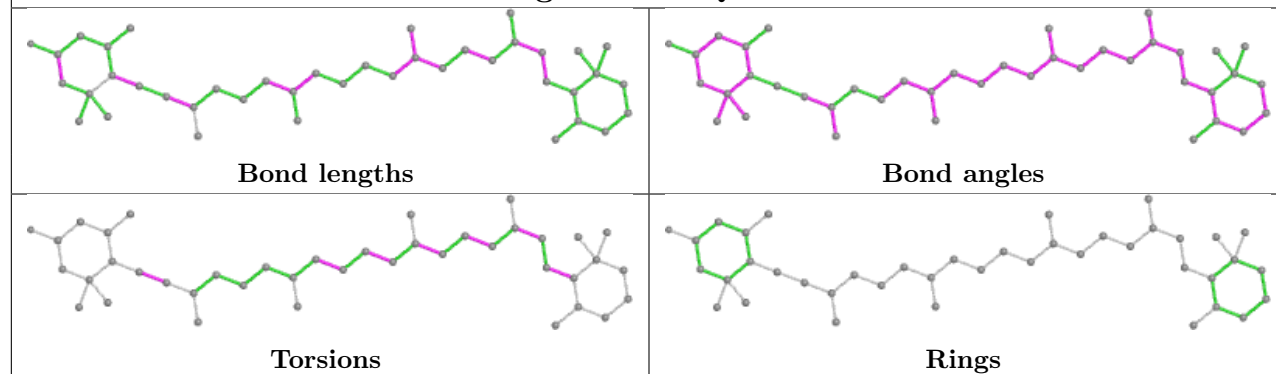
## Ligand CLA 2 309

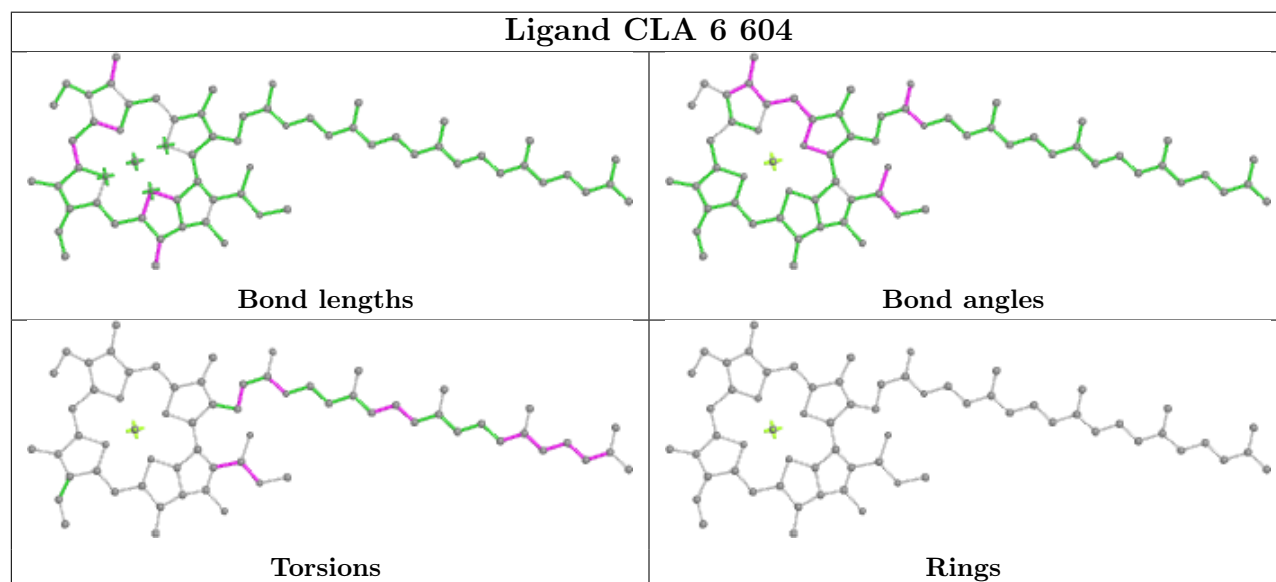
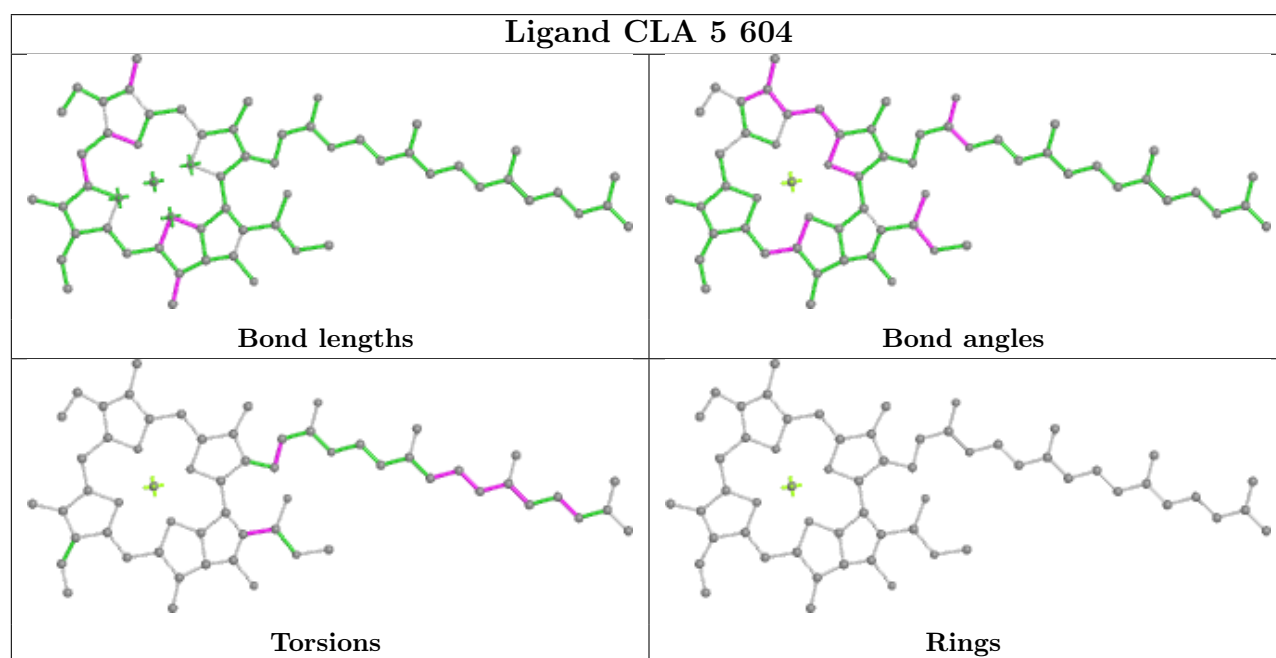
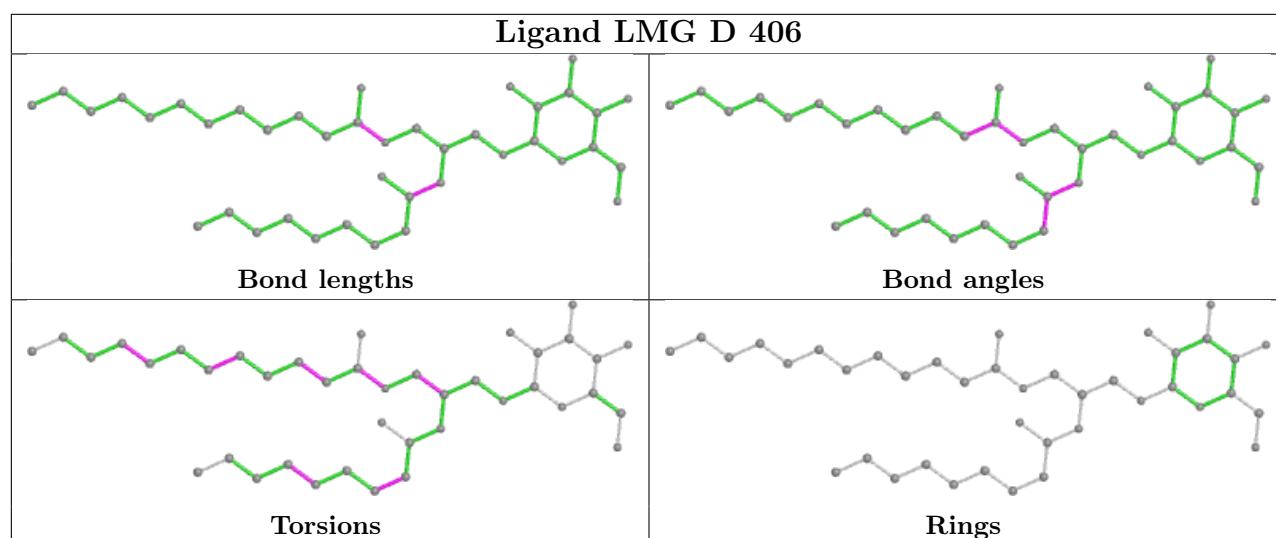


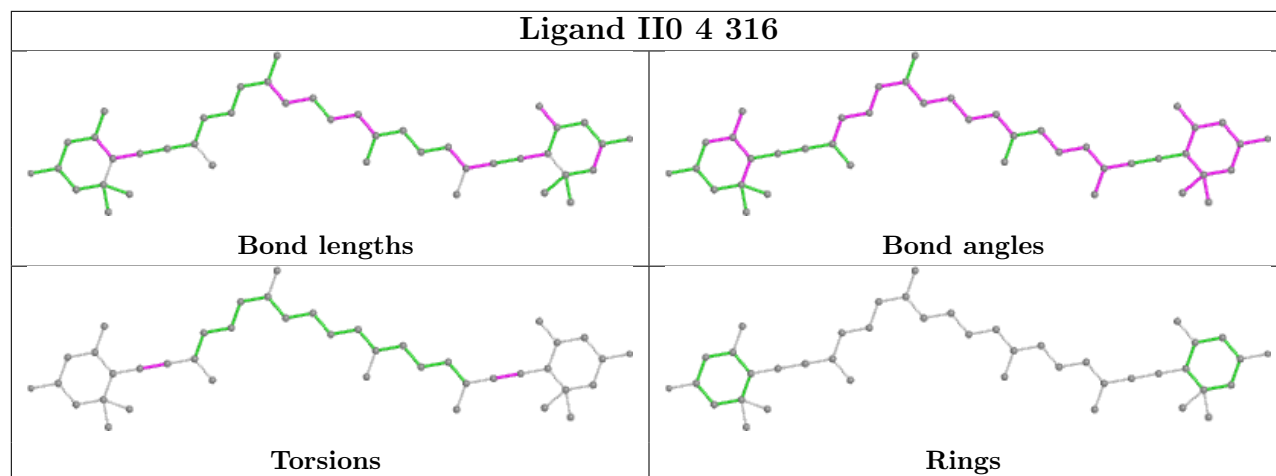
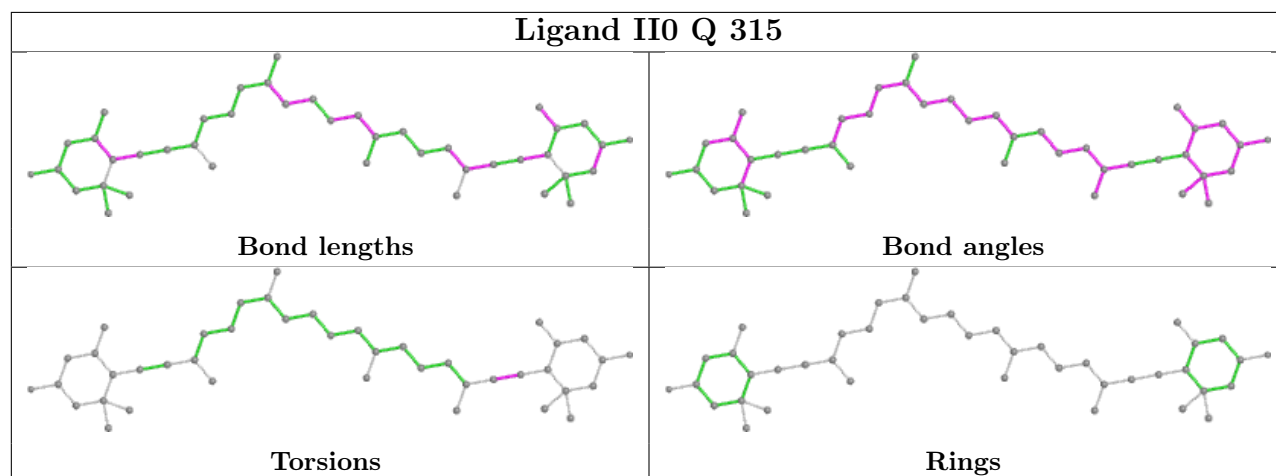
## Ligand CLA 5 612

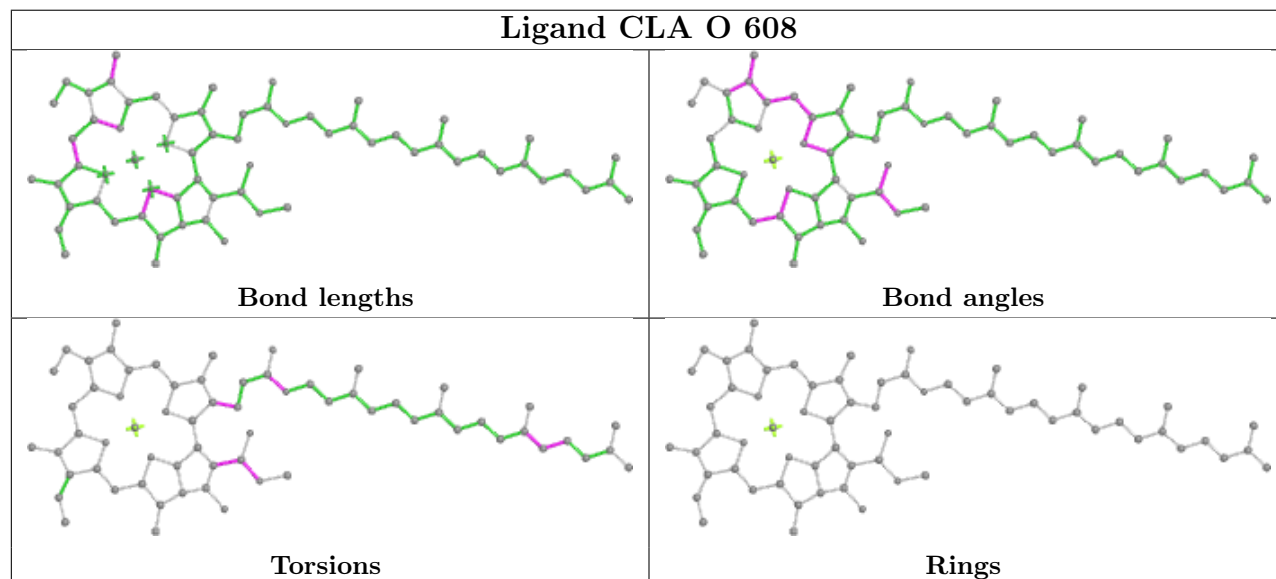
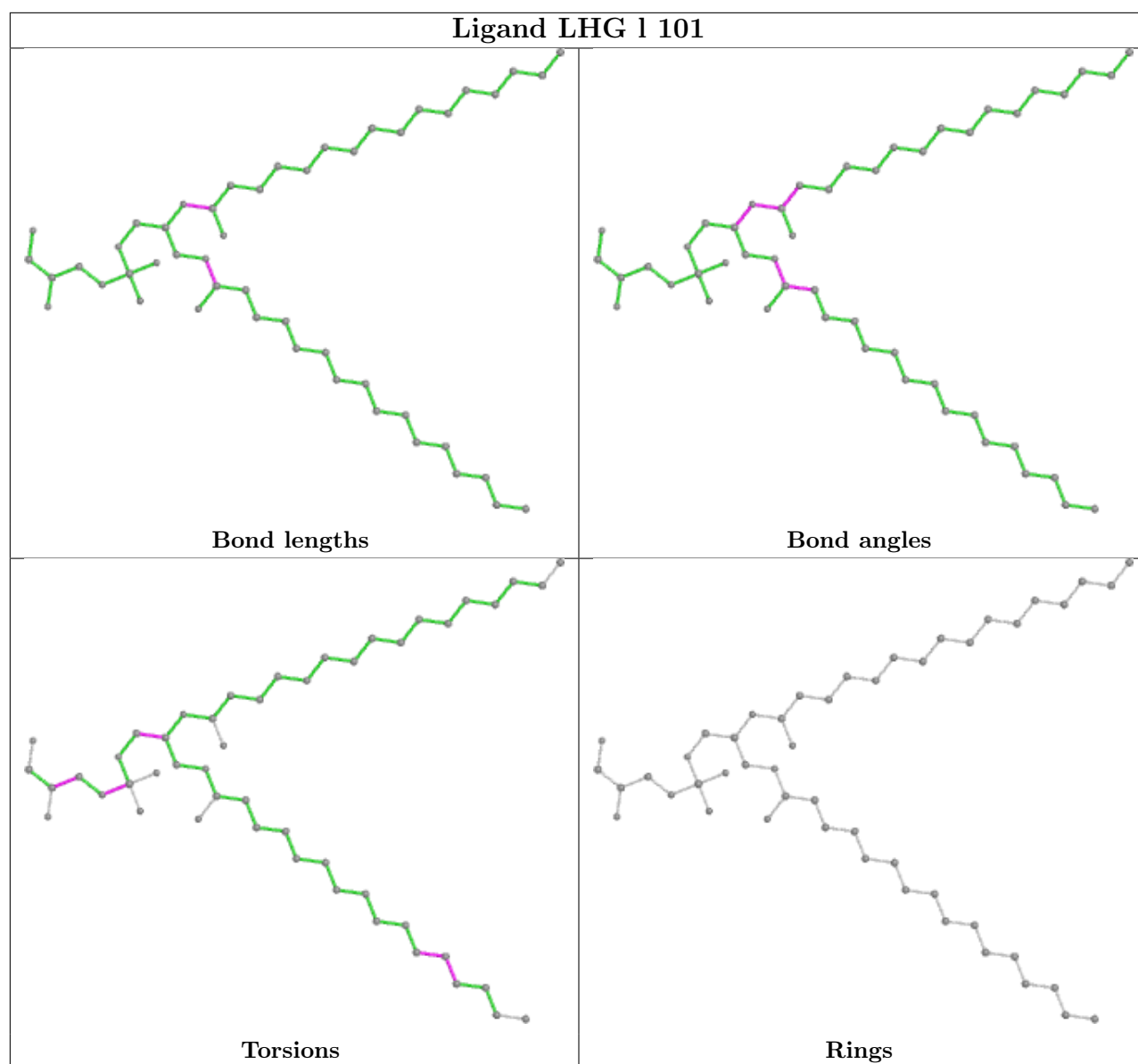


## Ligand IHT Q 317



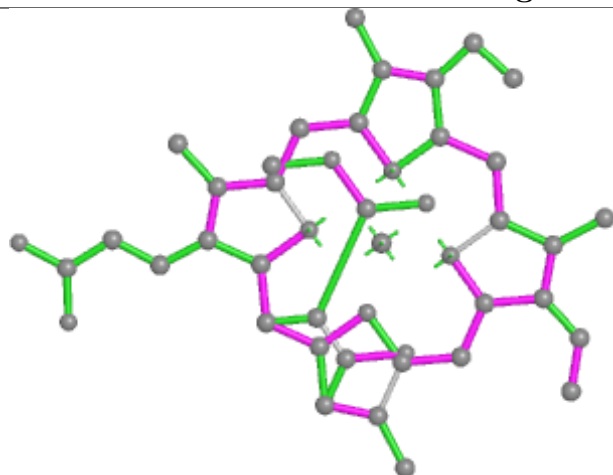


**Ligand II0 4 316****Ligand II0 Q 315**

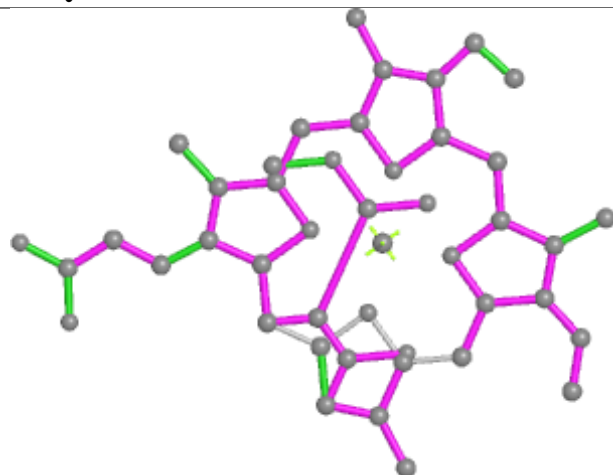




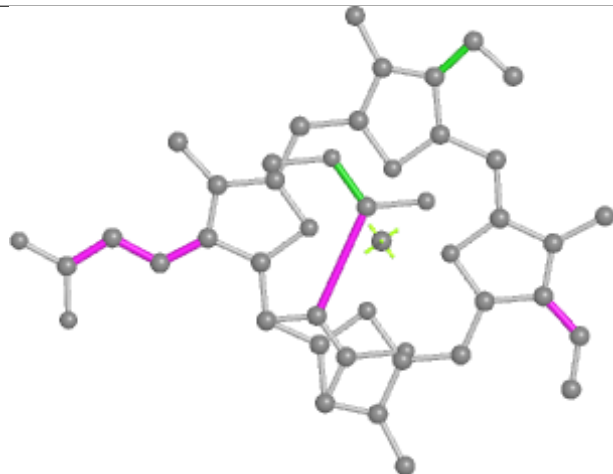
## Ligand KC2 Q 304



Bond lengths



Bond angles

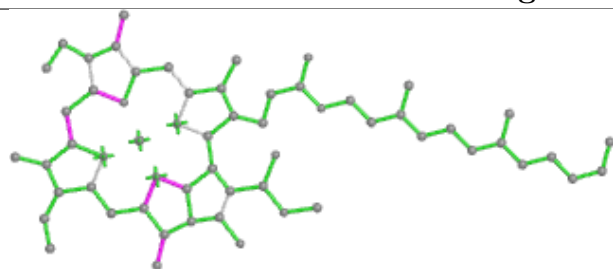


Torsions

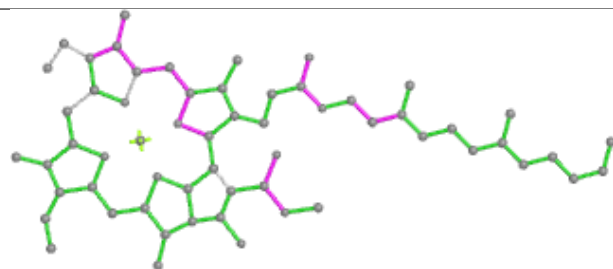


Rings

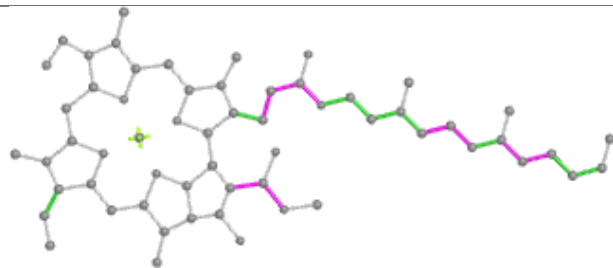
## Ligand CLA 1 604



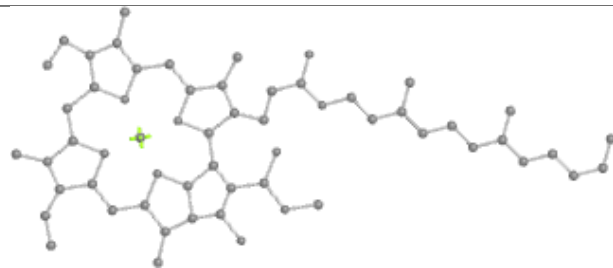
Bond lengths



Bond angles

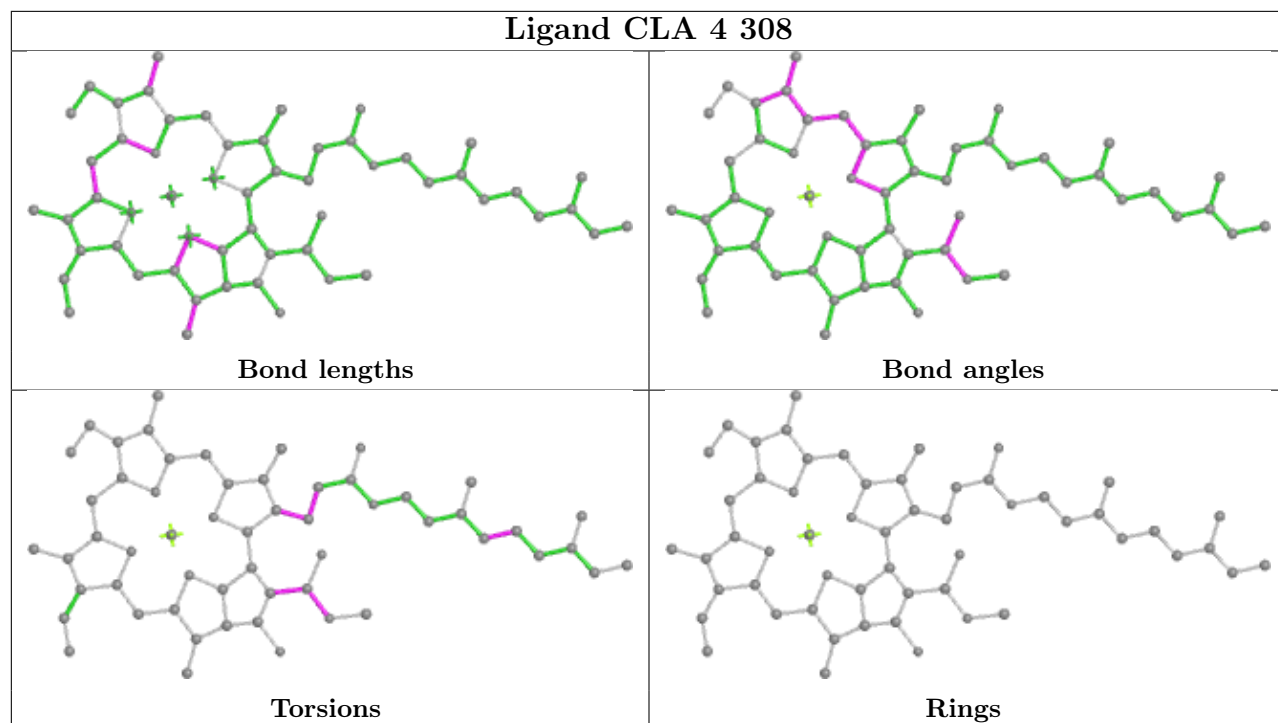


Torsions

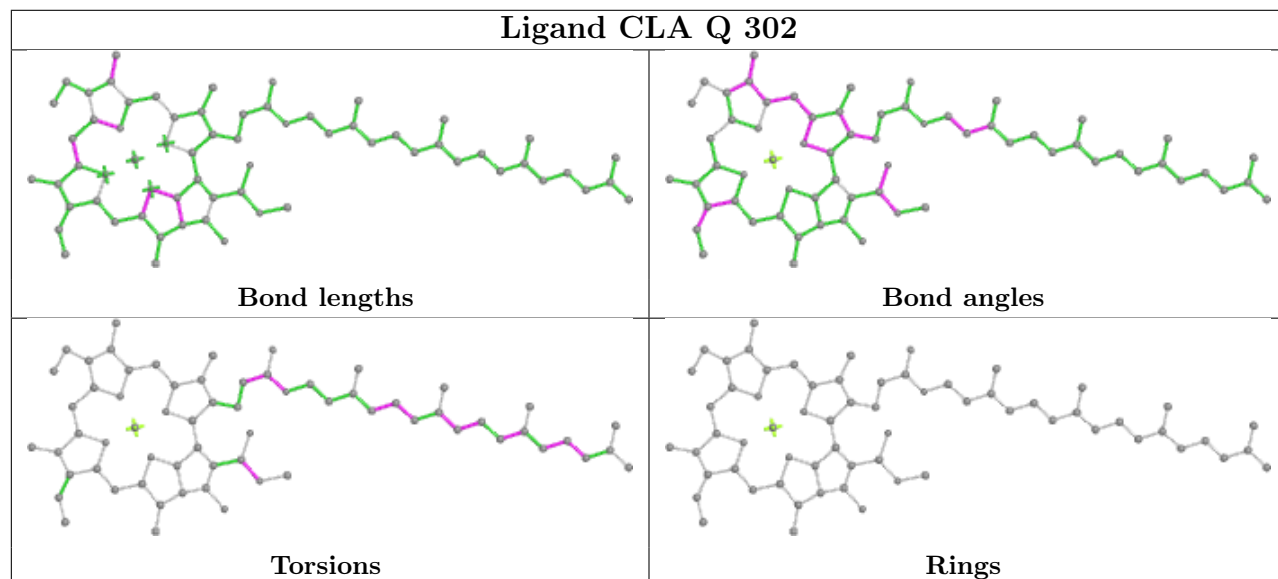


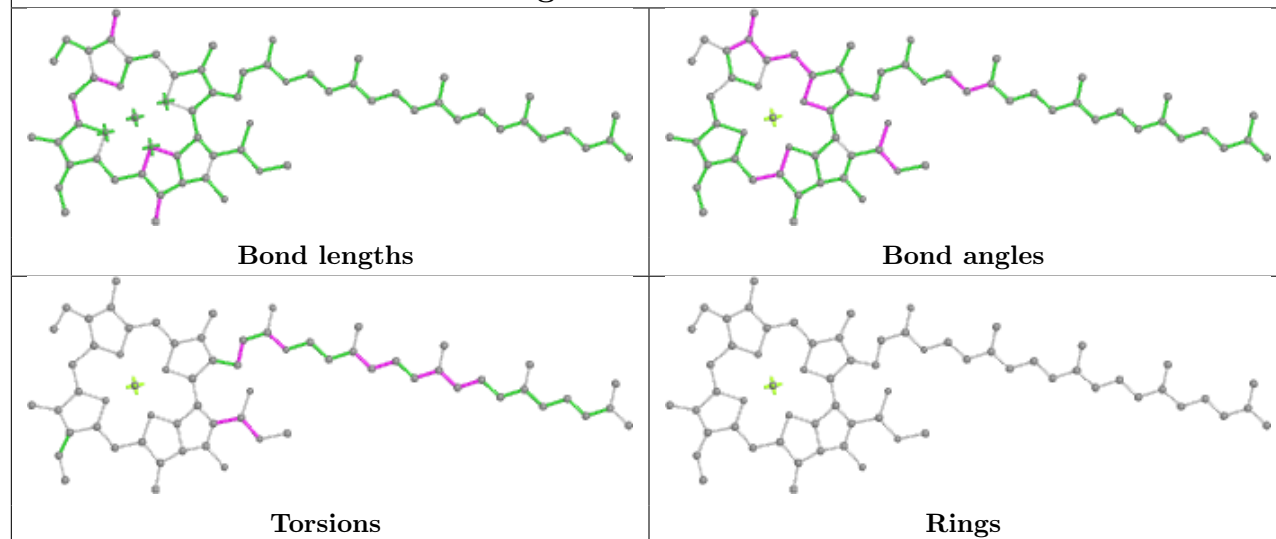
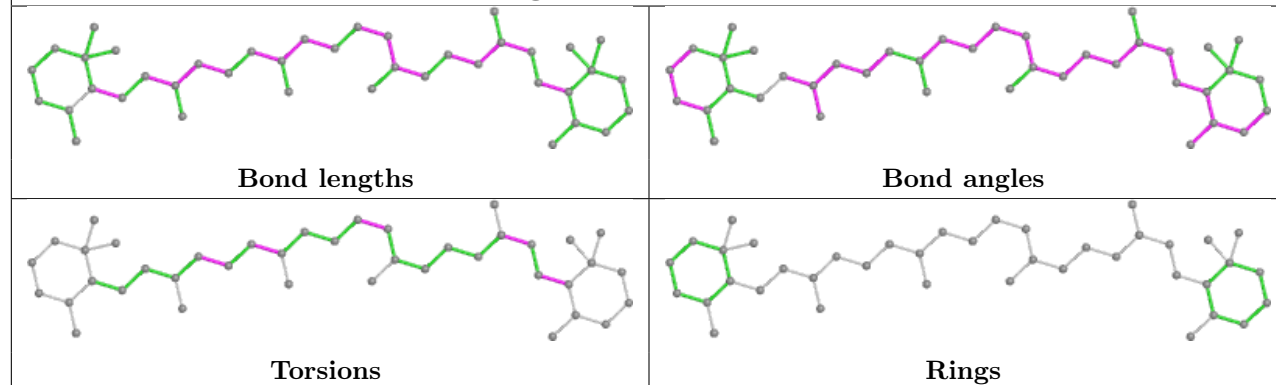
Rings

## Ligand CLA 4 308

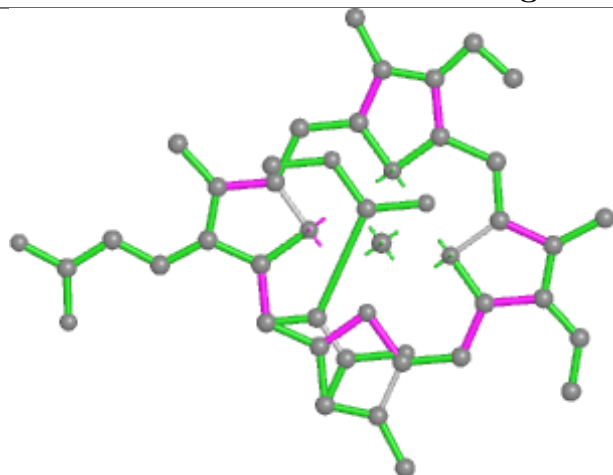


## Ligand CLA Q 302

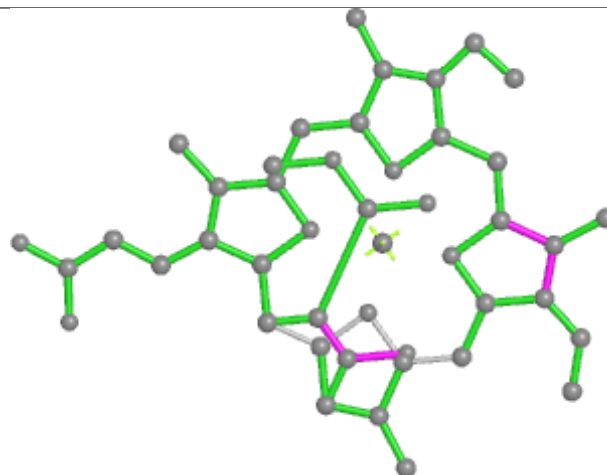


**Ligand CLA c 512****Ligand WVN k 101**

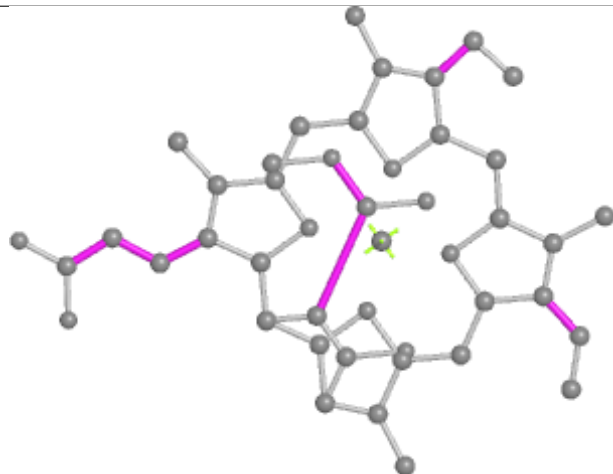
## Ligand KC2 1 605



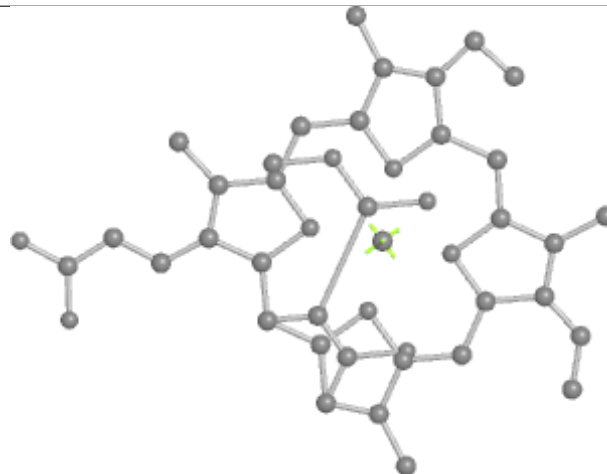
Bond lengths



Bond angles

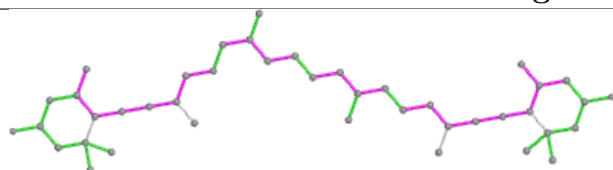


Torsions

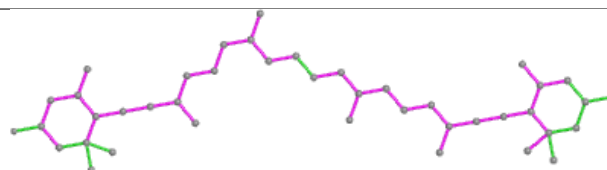


Rings

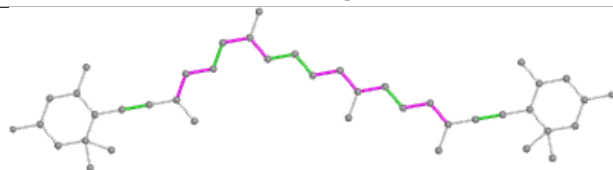
## Ligand II0 1 618



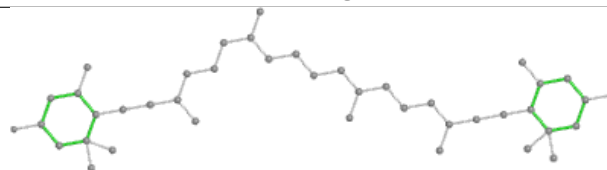
Bond lengths



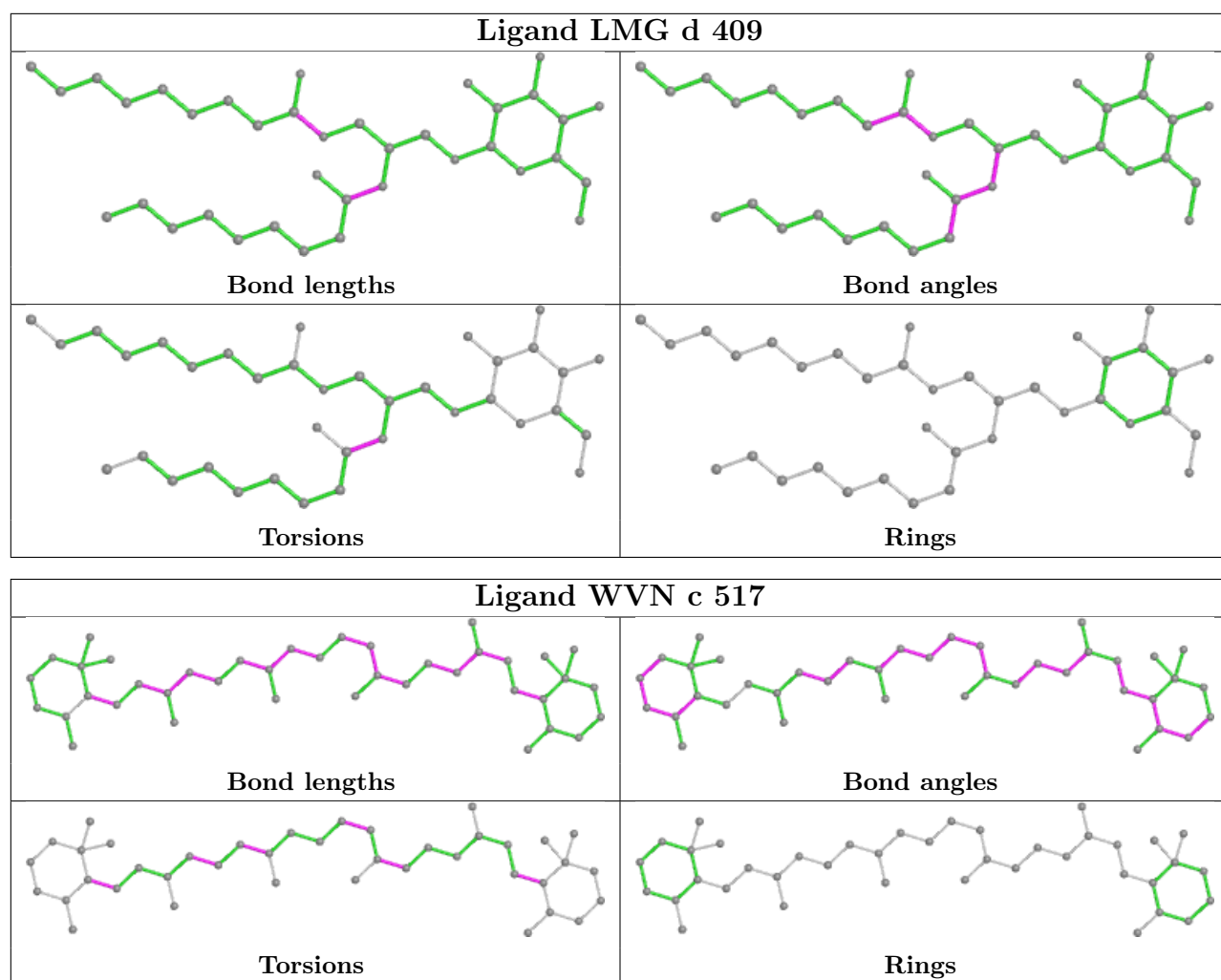
Bond angles



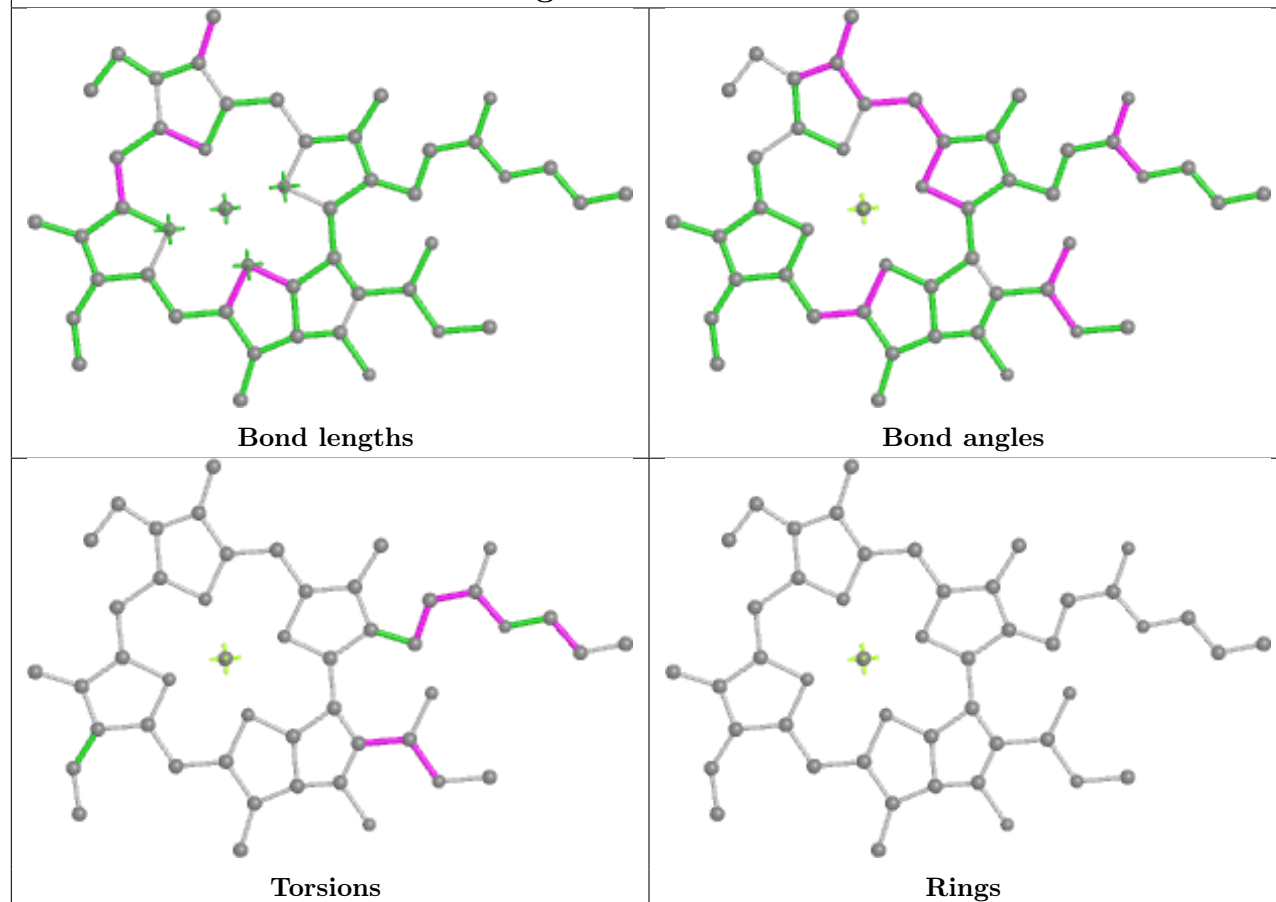
Torsions



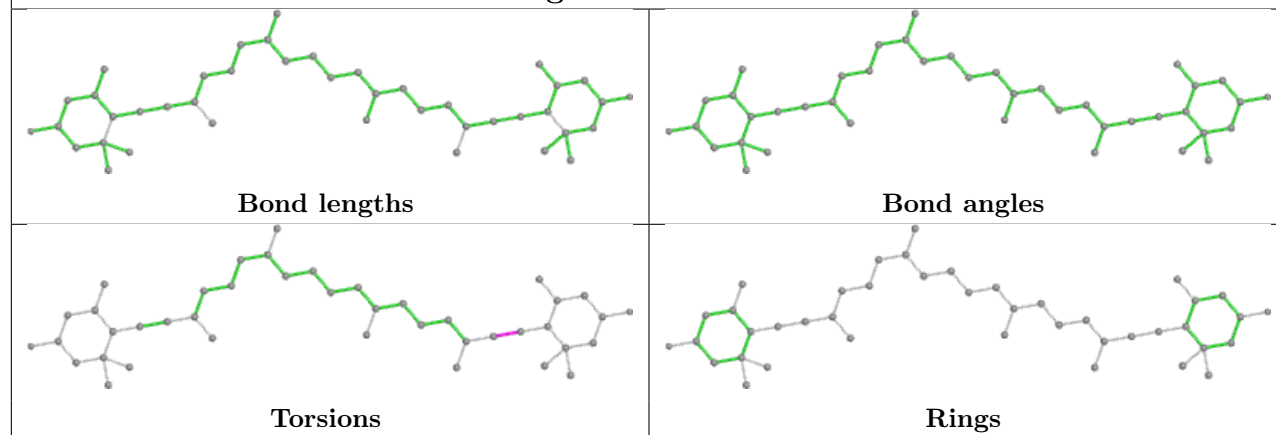
Rings



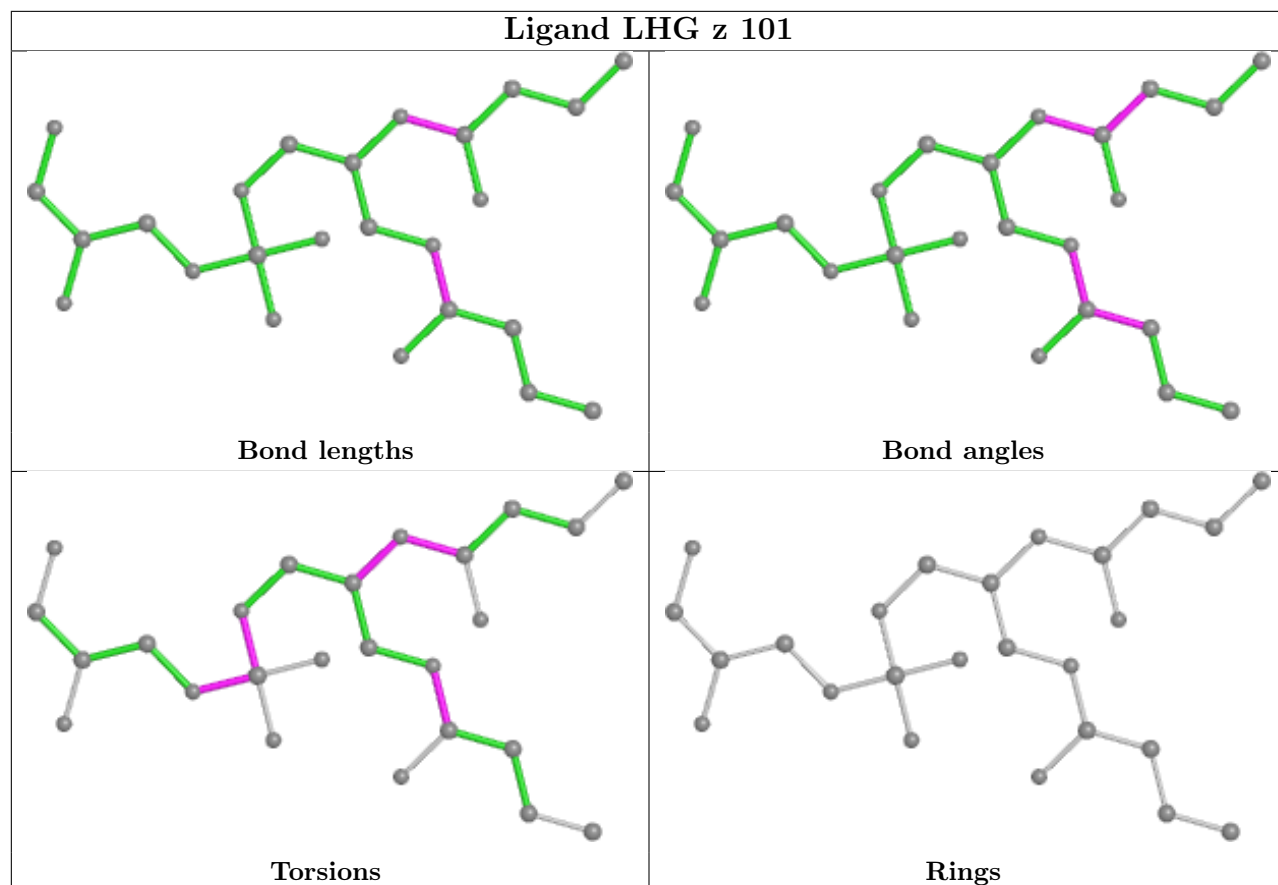
## Ligand CLA 1 613



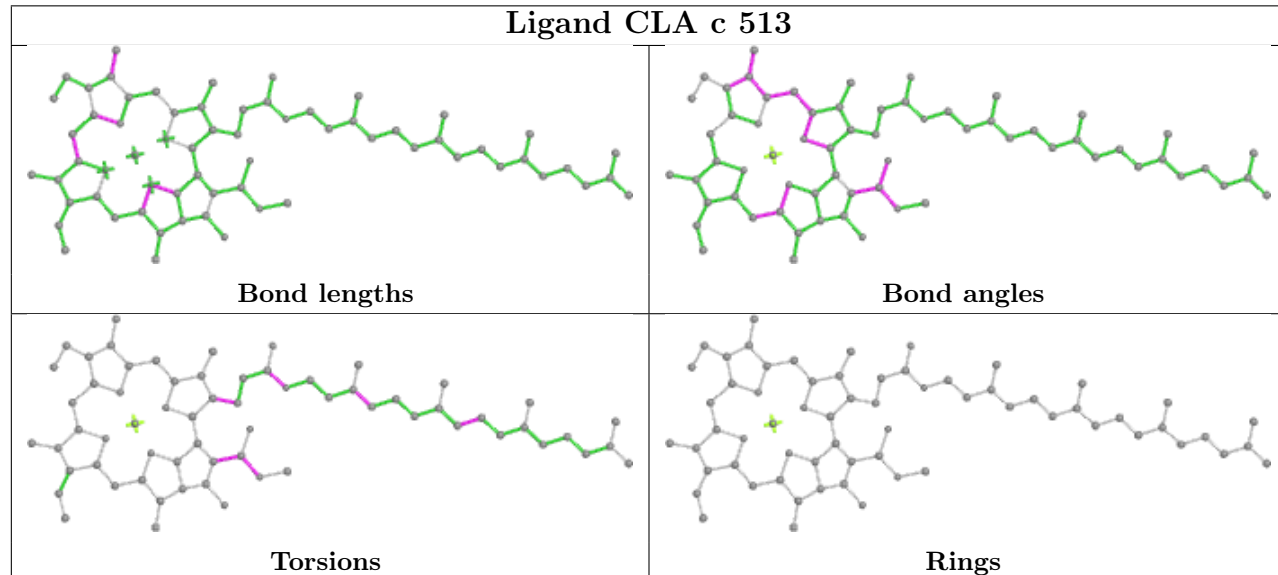
## Ligand II0 O 618

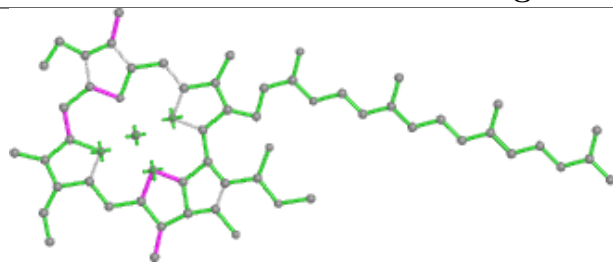
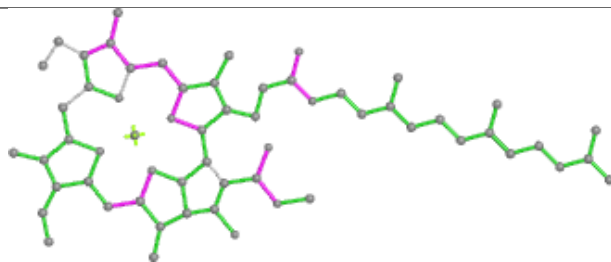
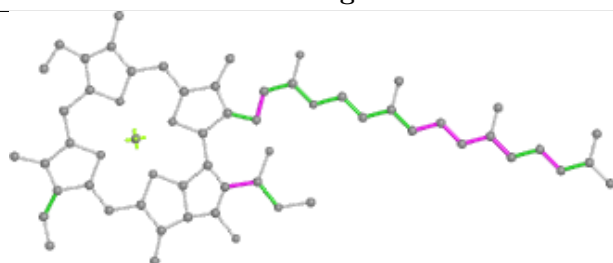
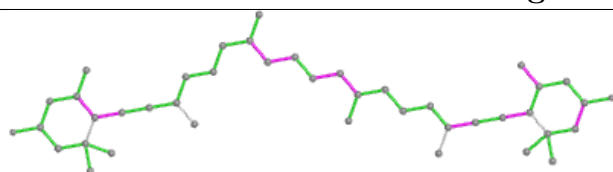
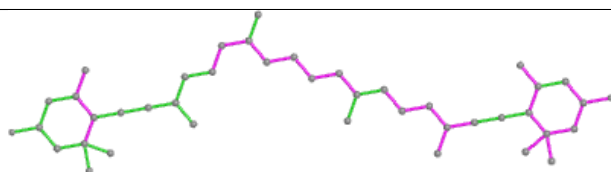
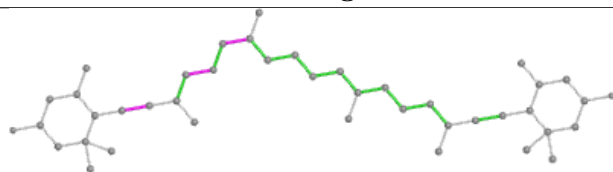
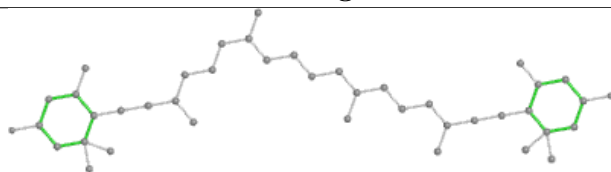


## Ligand LHG z 101



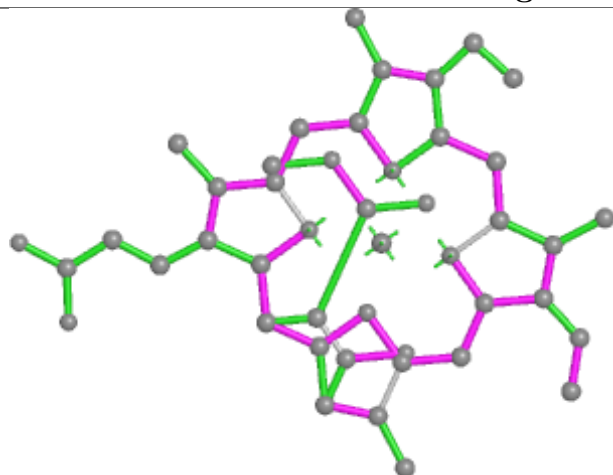
## Ligand CLA c 513



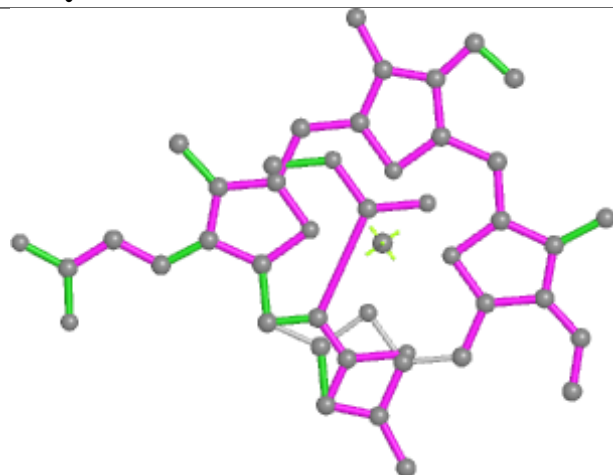
**Ligand CLA R 305****Bond lengths****Bond angles****Torsions****Rings****Ligand II0 N 615****Bond lengths****Bond angles****Torsions****Rings**



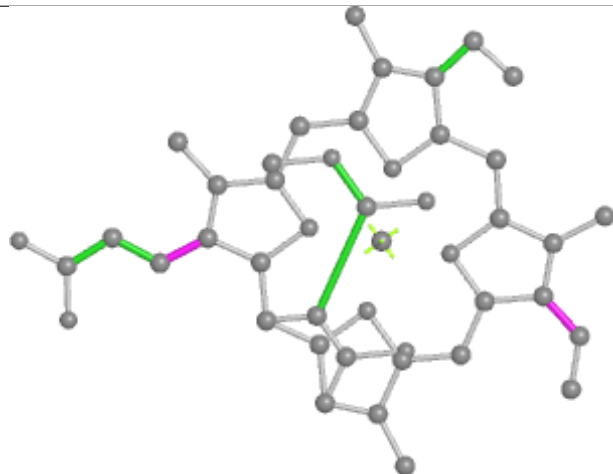
## Ligand KC2 Q 310



Bond lengths



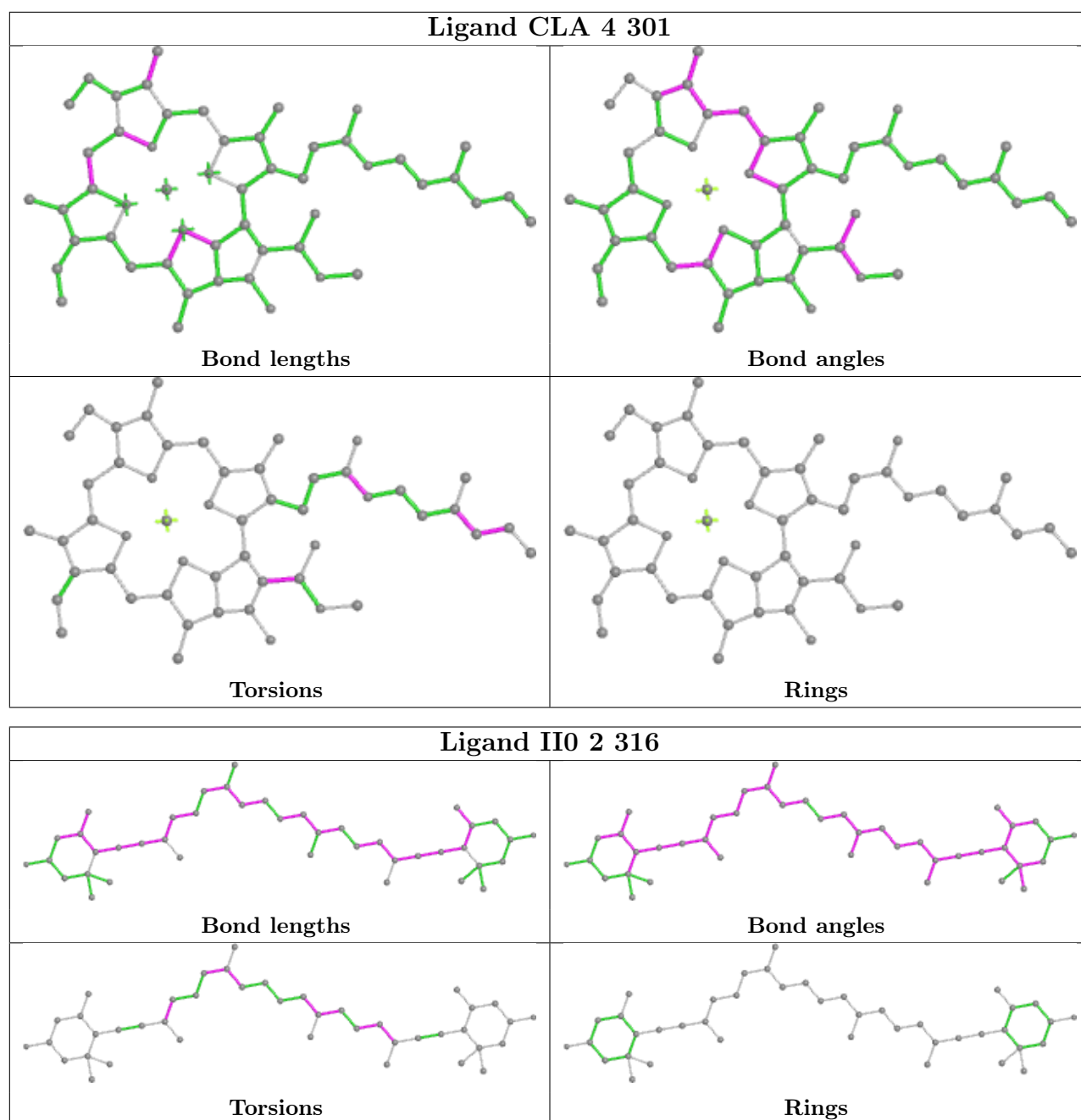
Bond angles



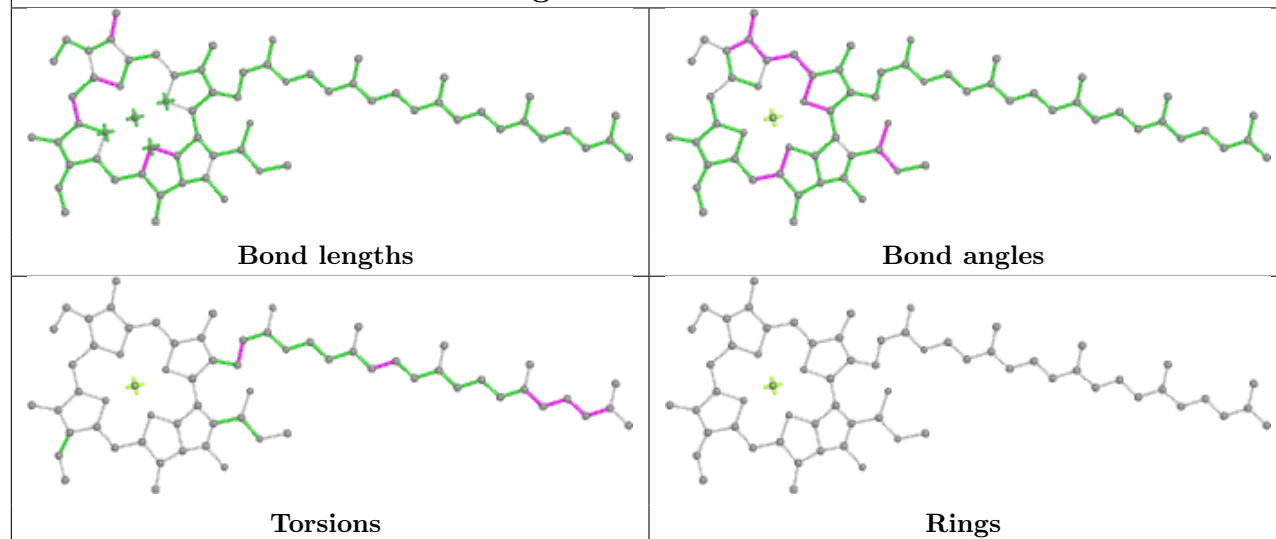
Torsions



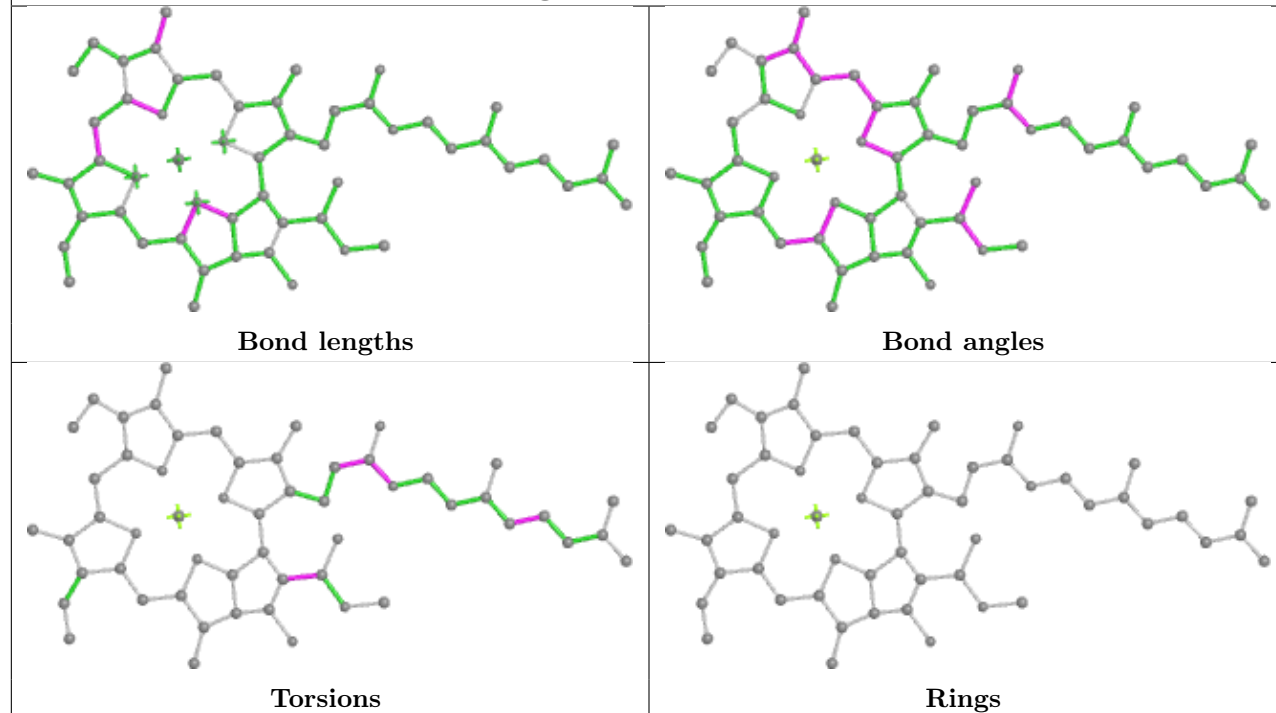
Rings



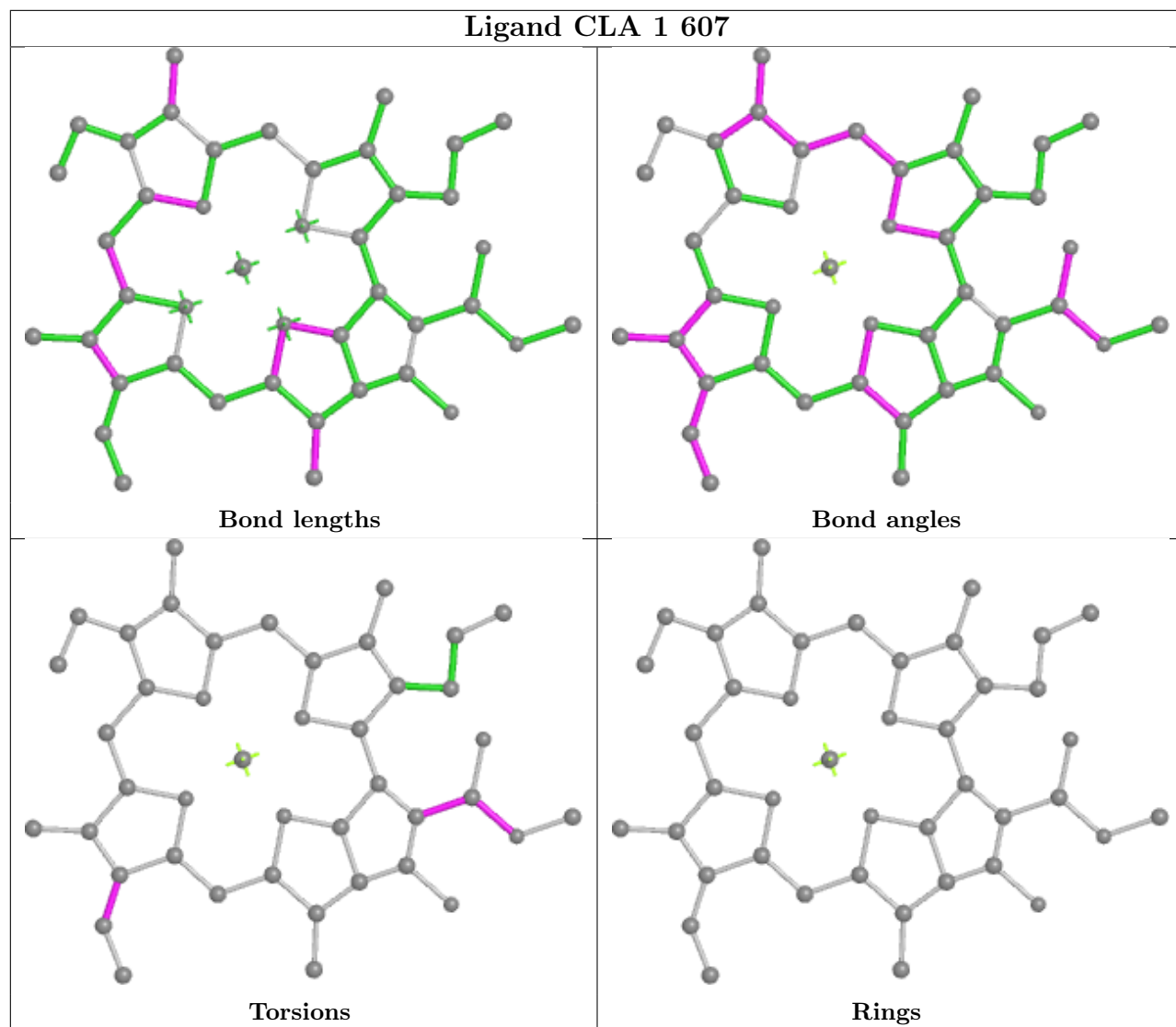
## Ligand CLA C 508



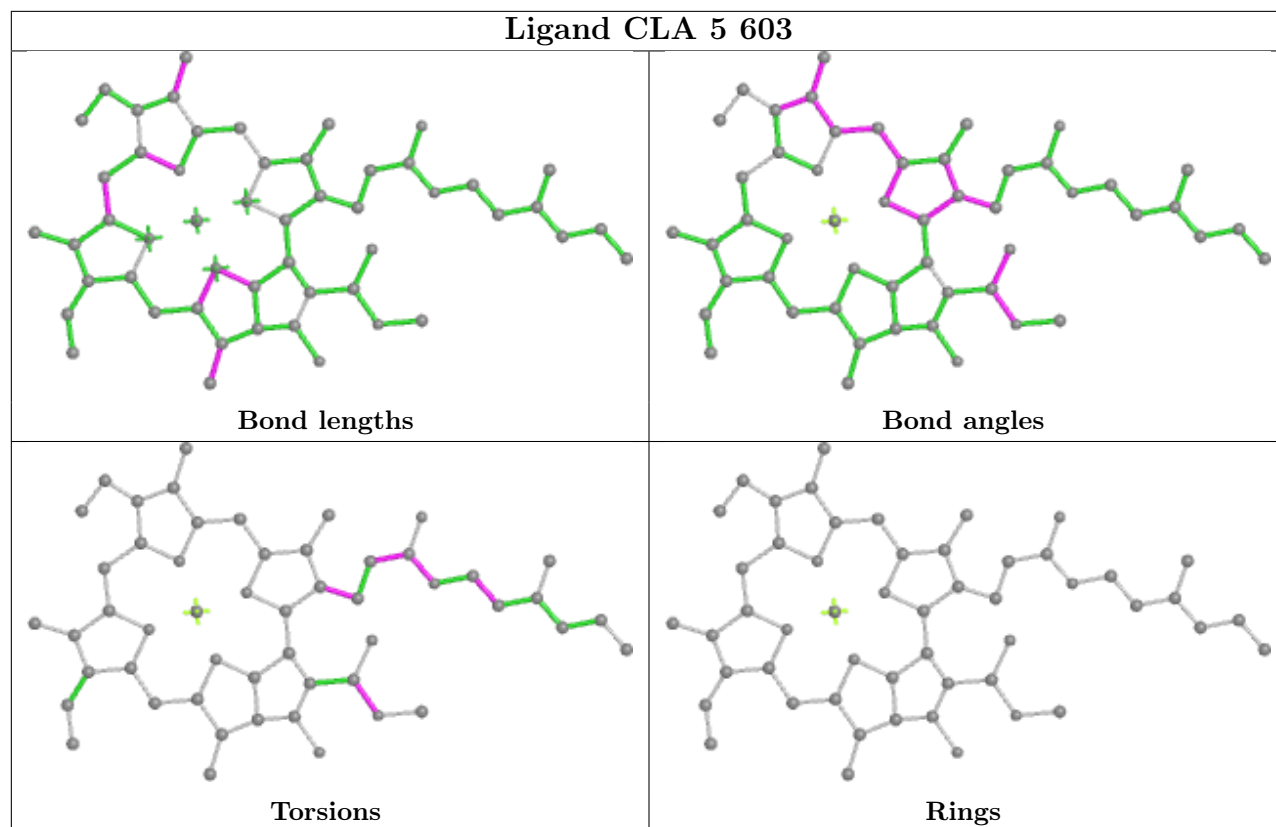
## Ligand CLA 5 601



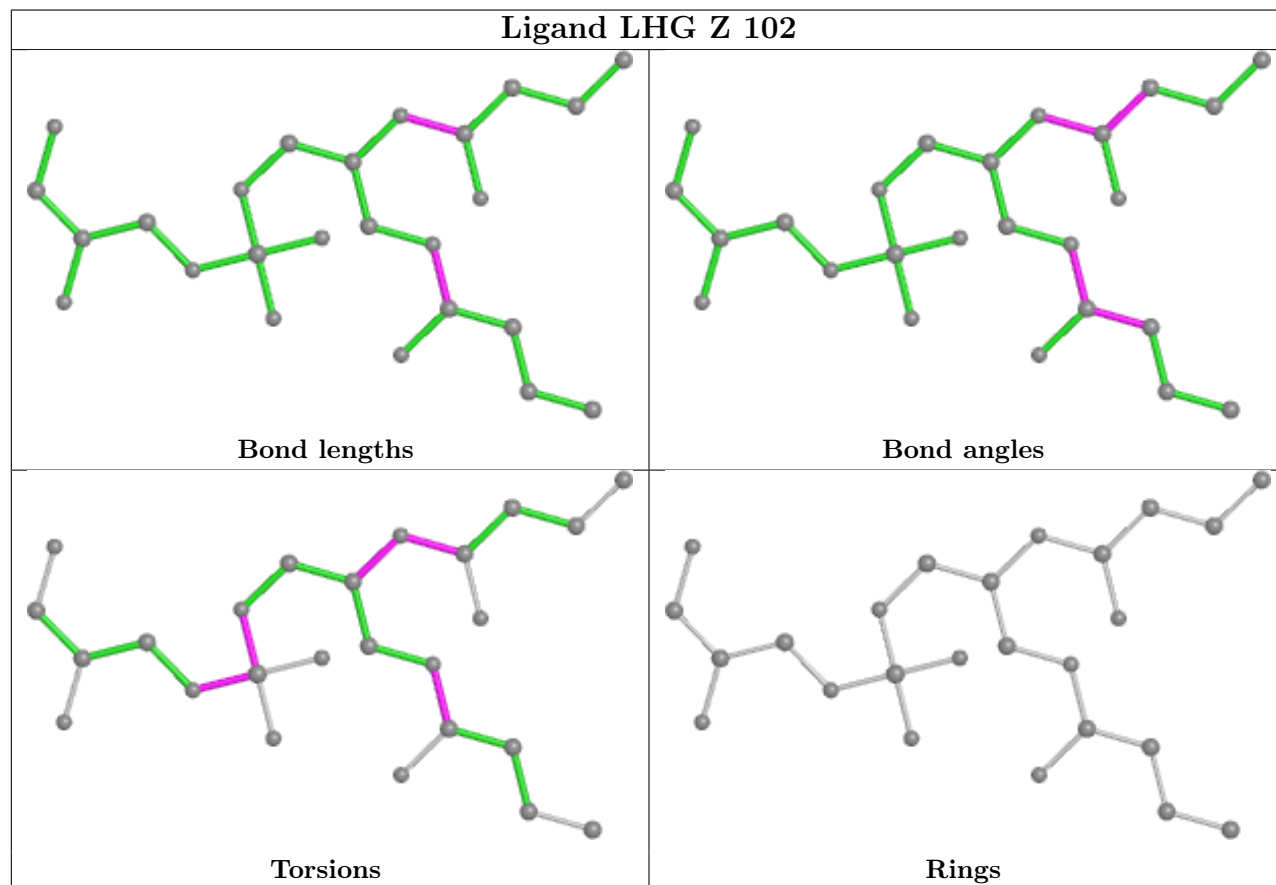
## Ligand CLA 1 607

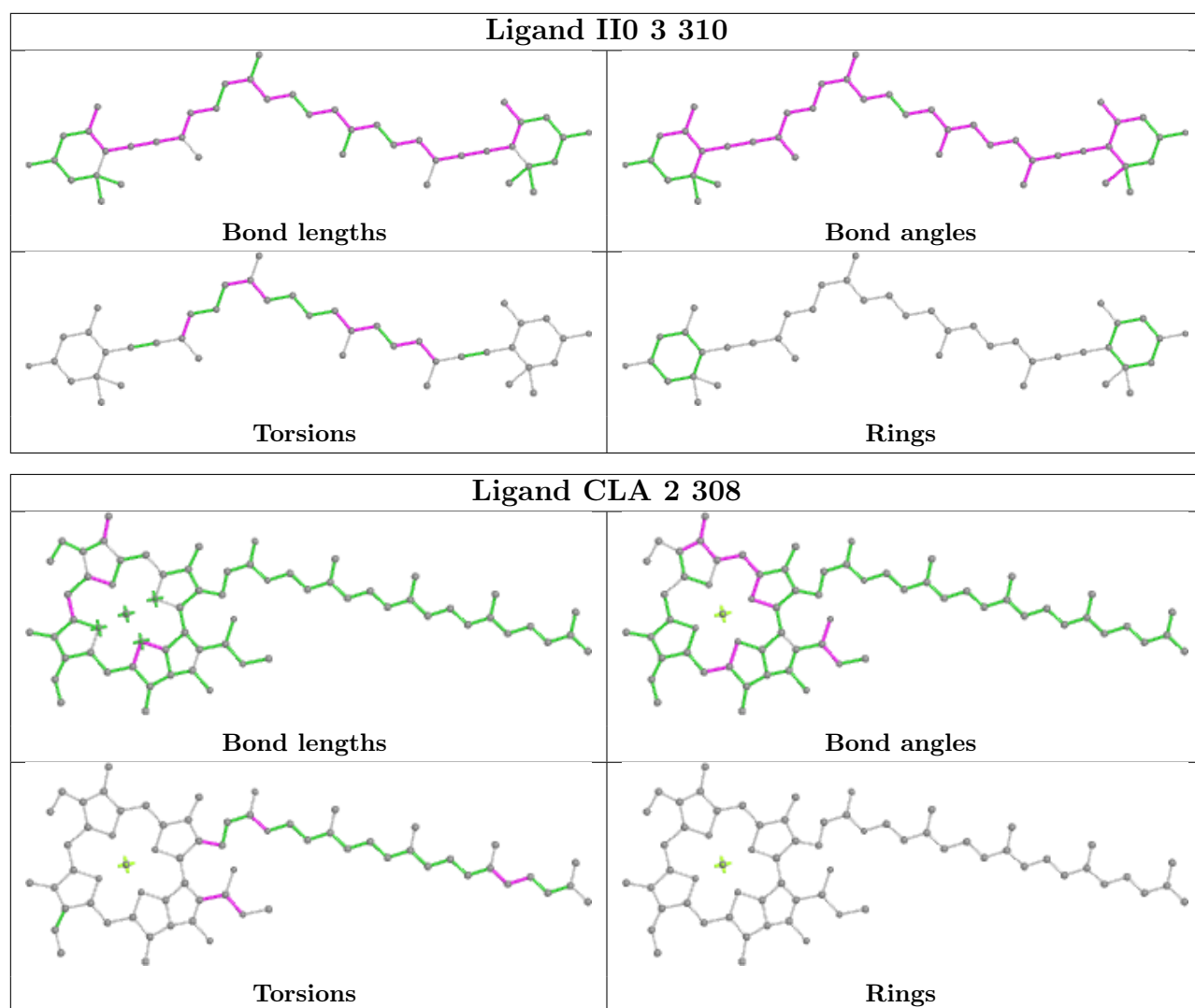


## Ligand CLA 5 603

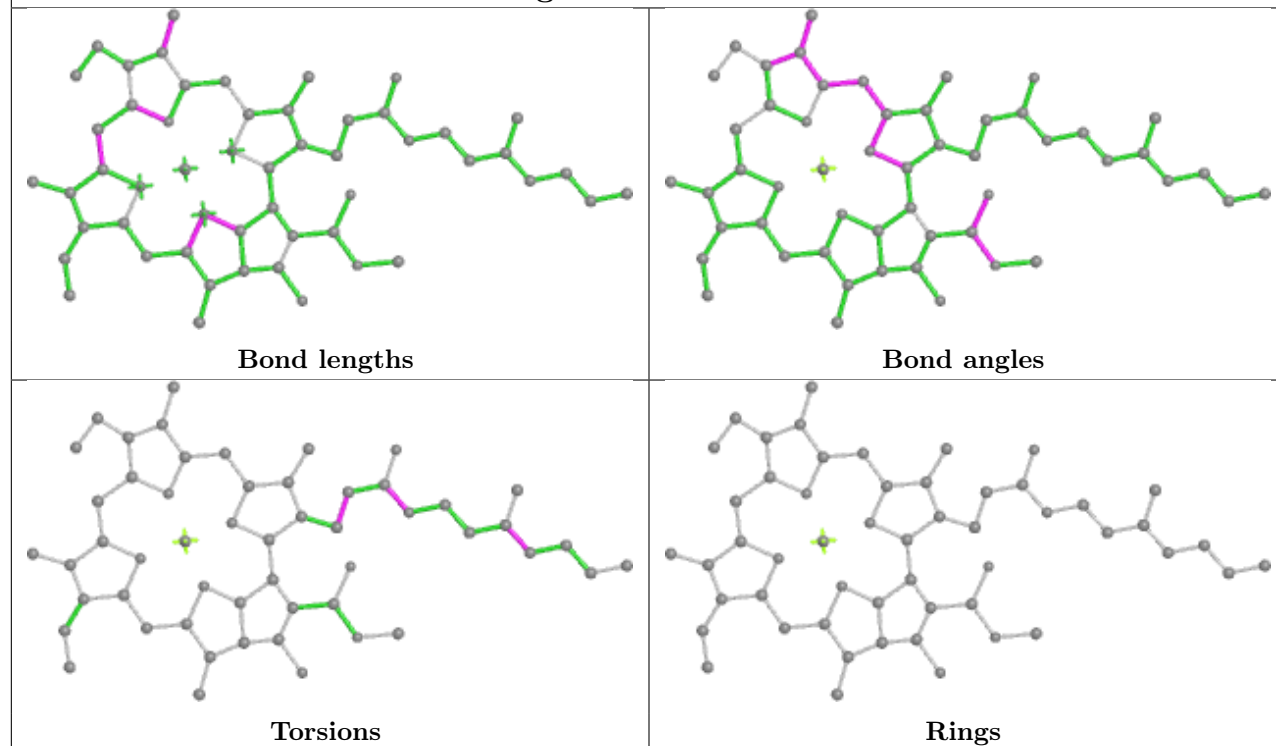


## Ligand LHG Z 102

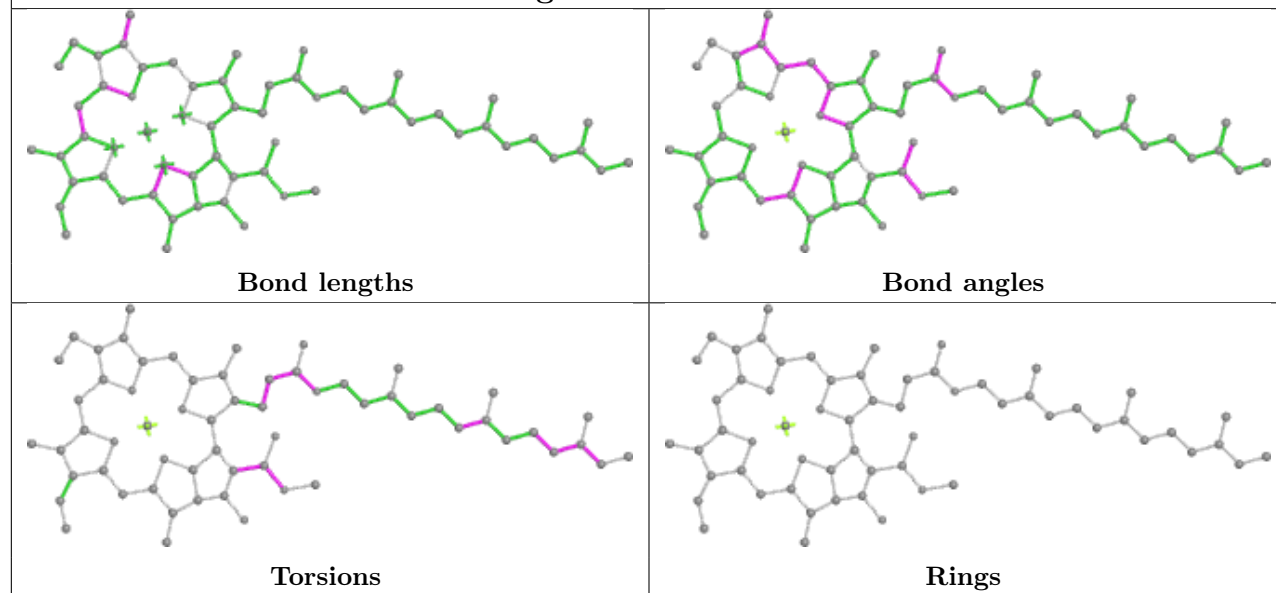




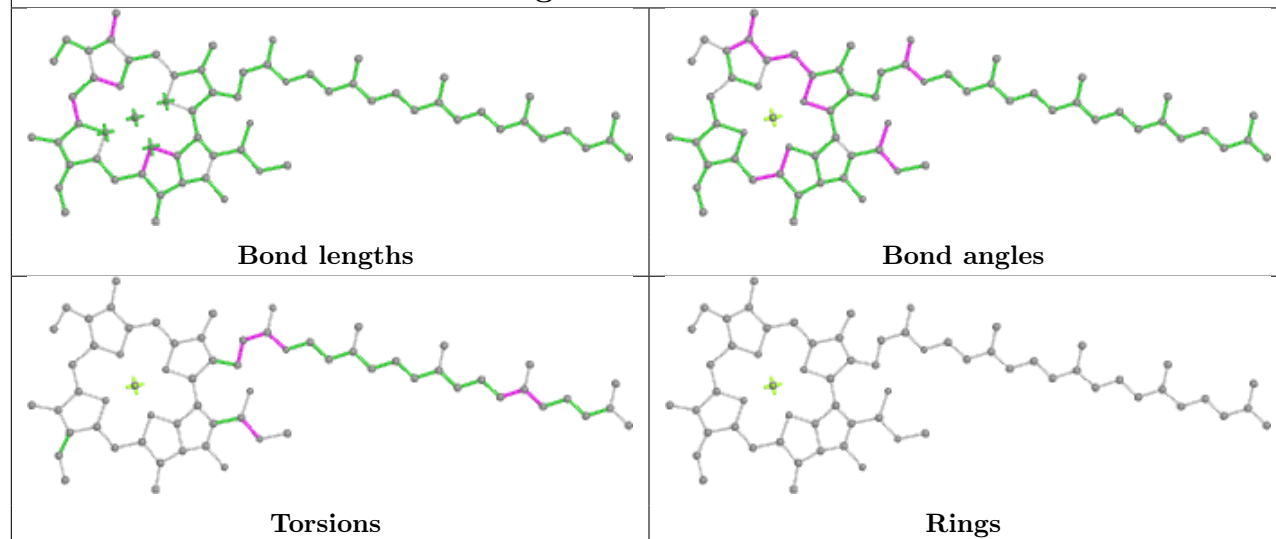
## Ligand CLA 3 307



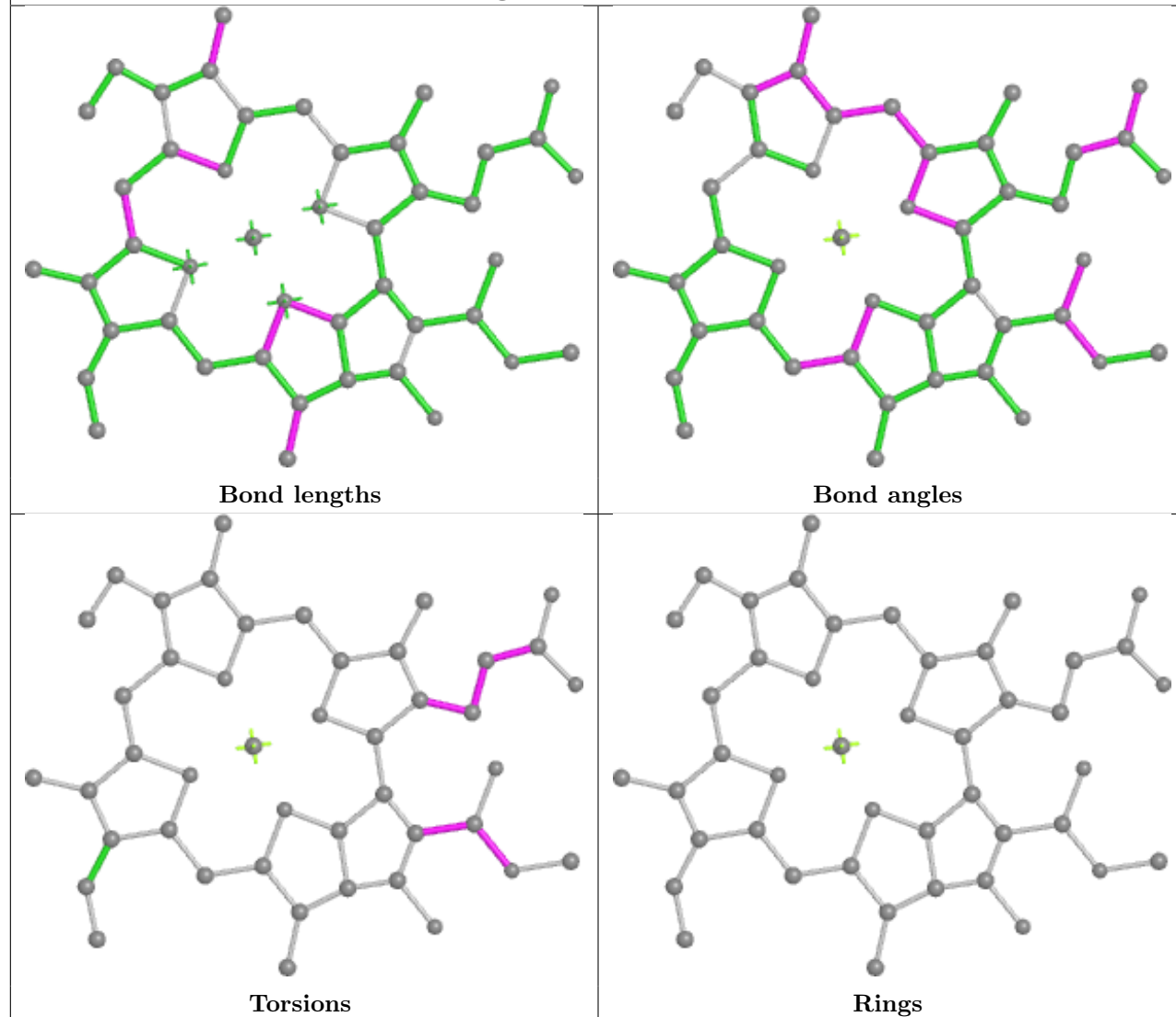
## Ligand CLA 4 304



## Ligand CLA b 610

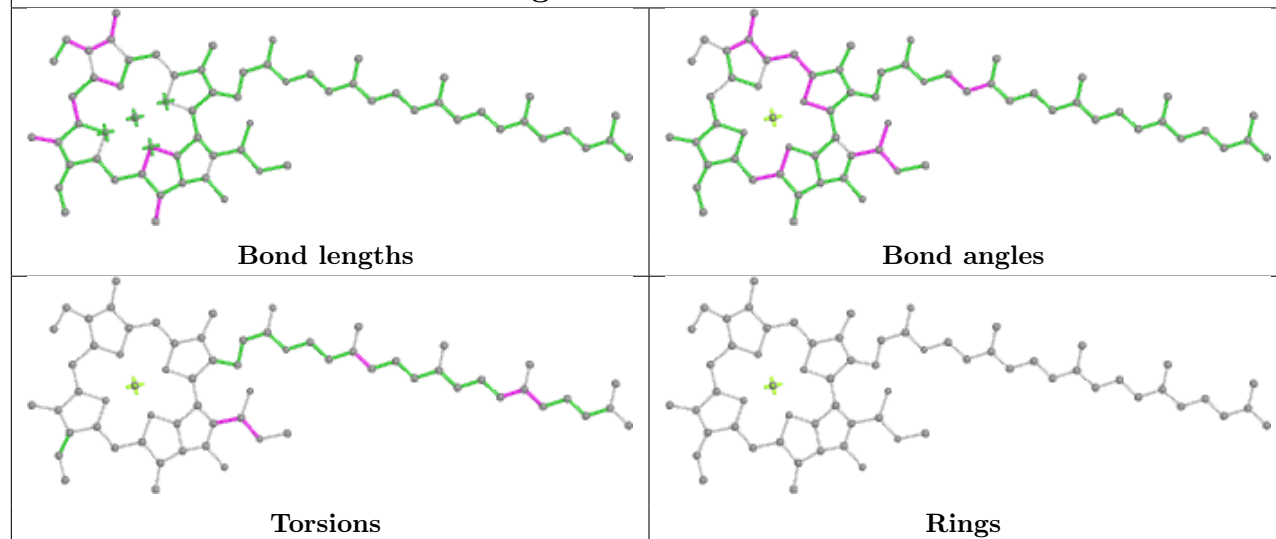


## Ligand CLA 3 309

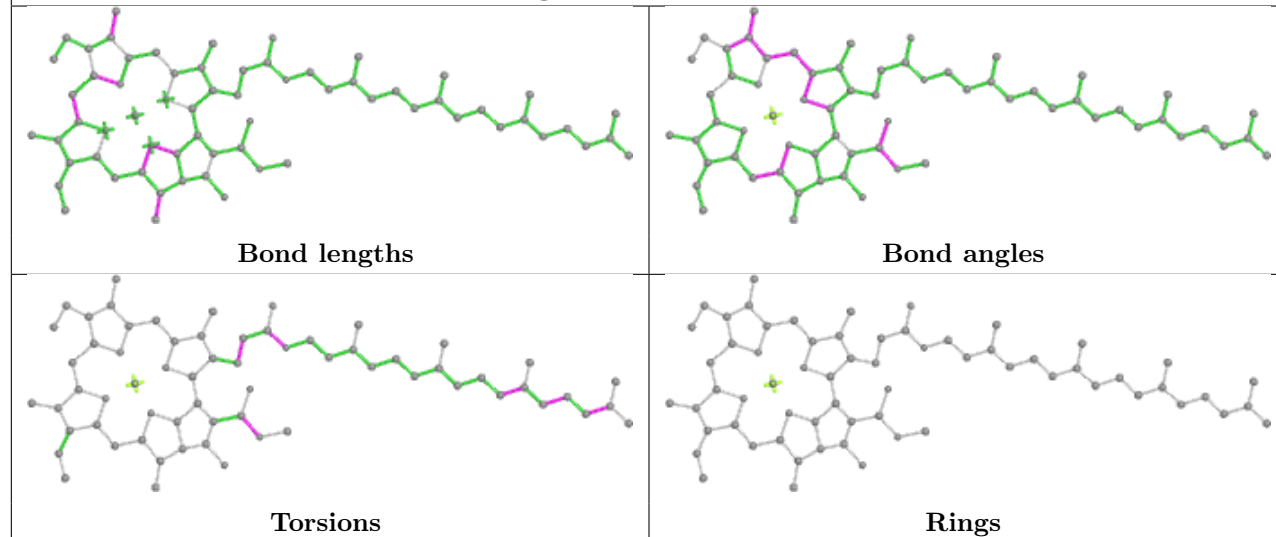




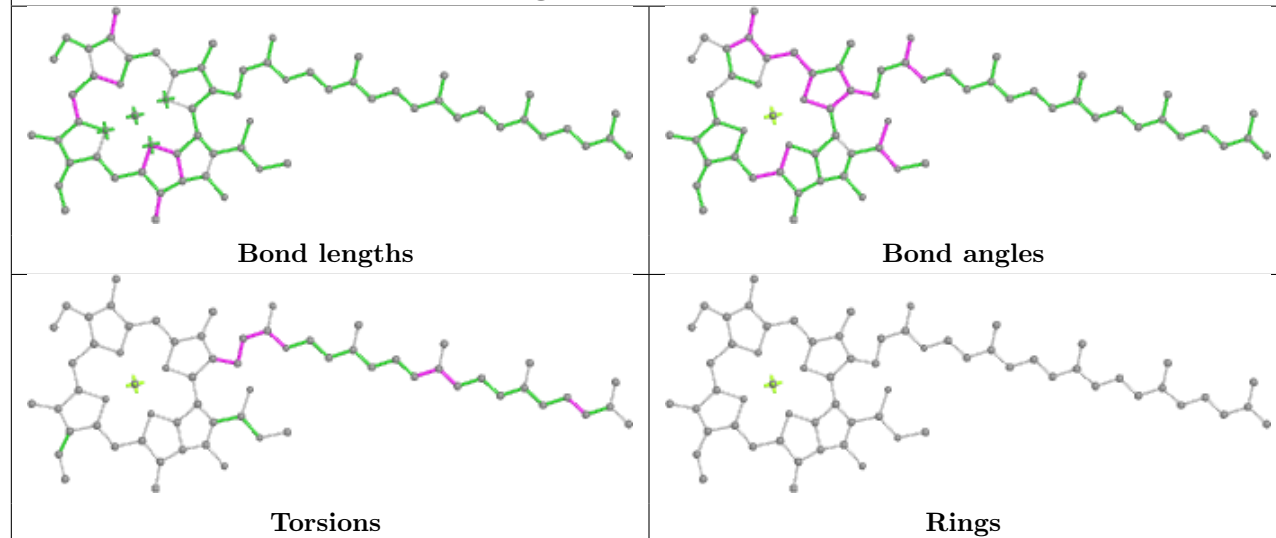
## Ligand CLA R 308

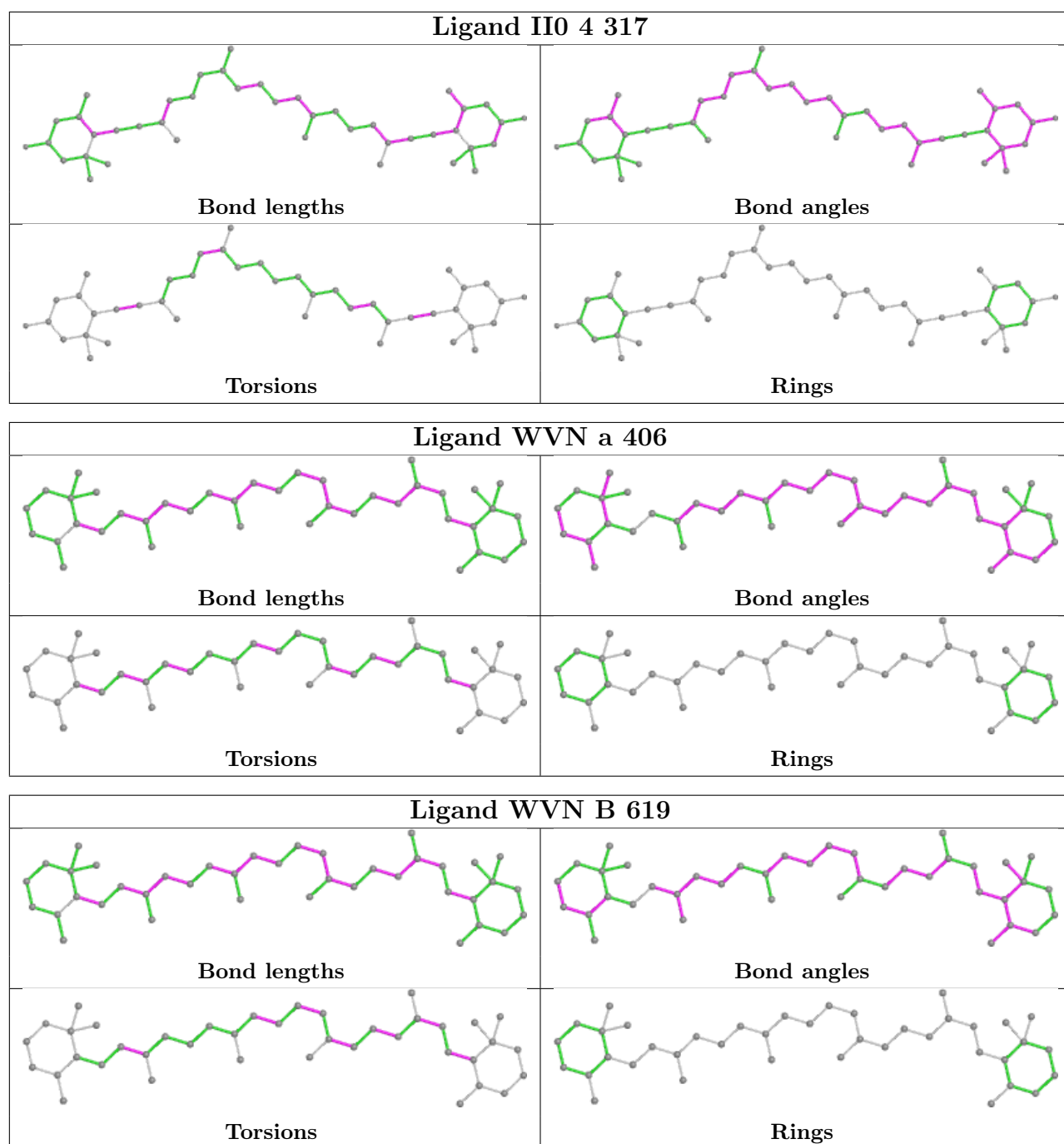


## Ligand CLA S 610

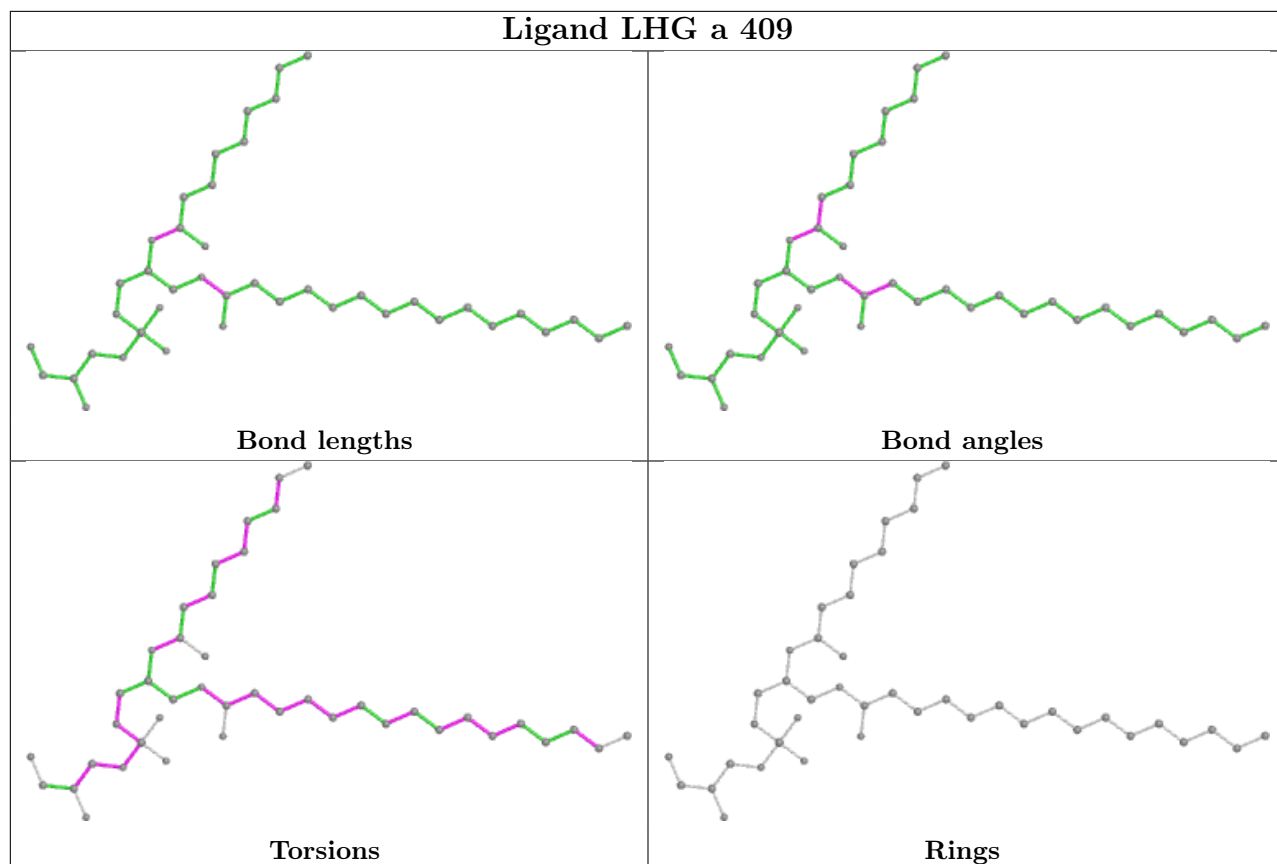


## Ligand CLA B 612

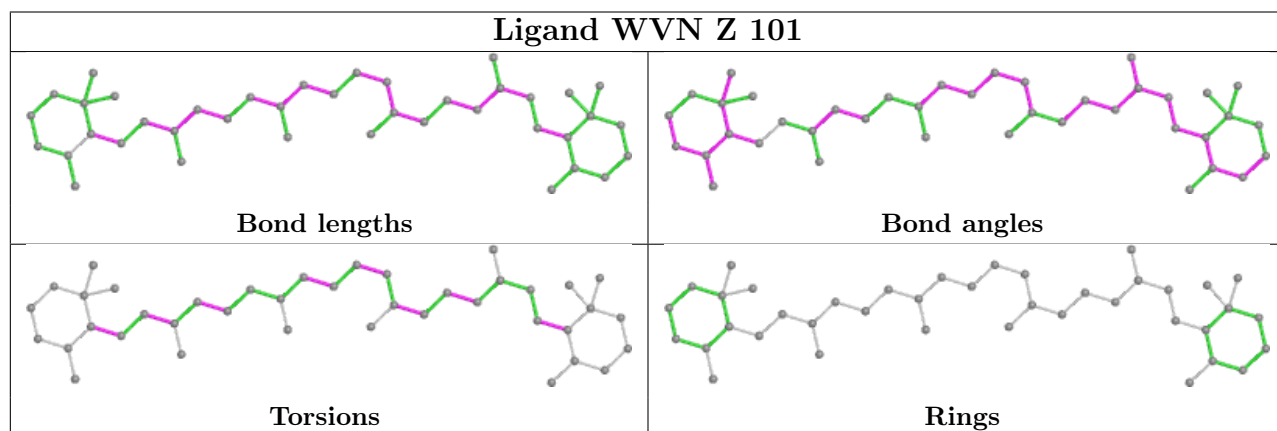




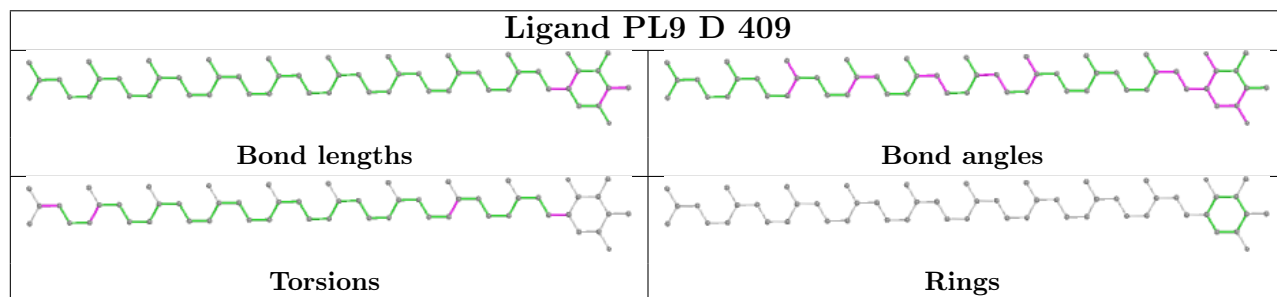
## Ligand LHG a 409

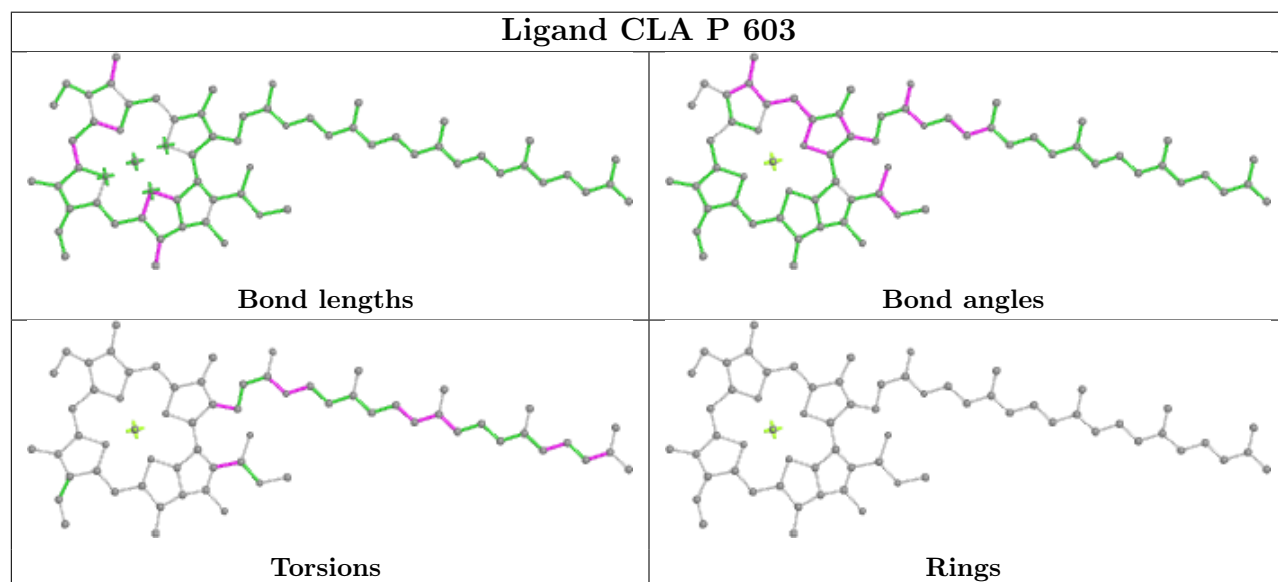
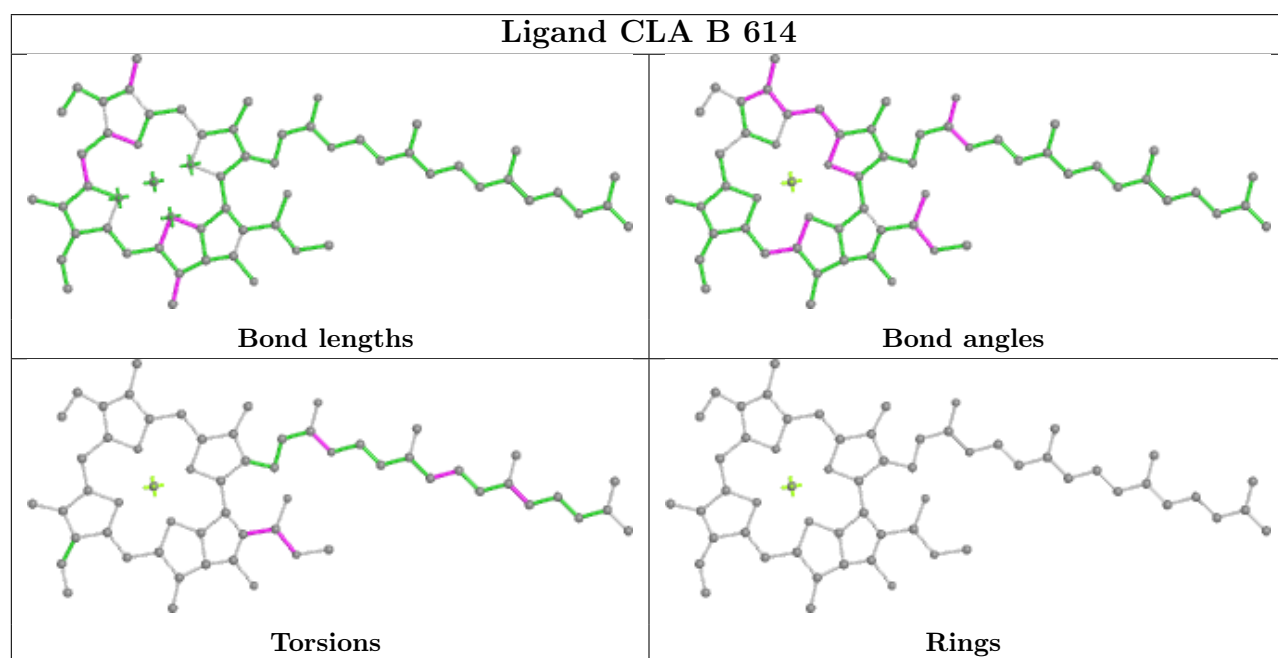
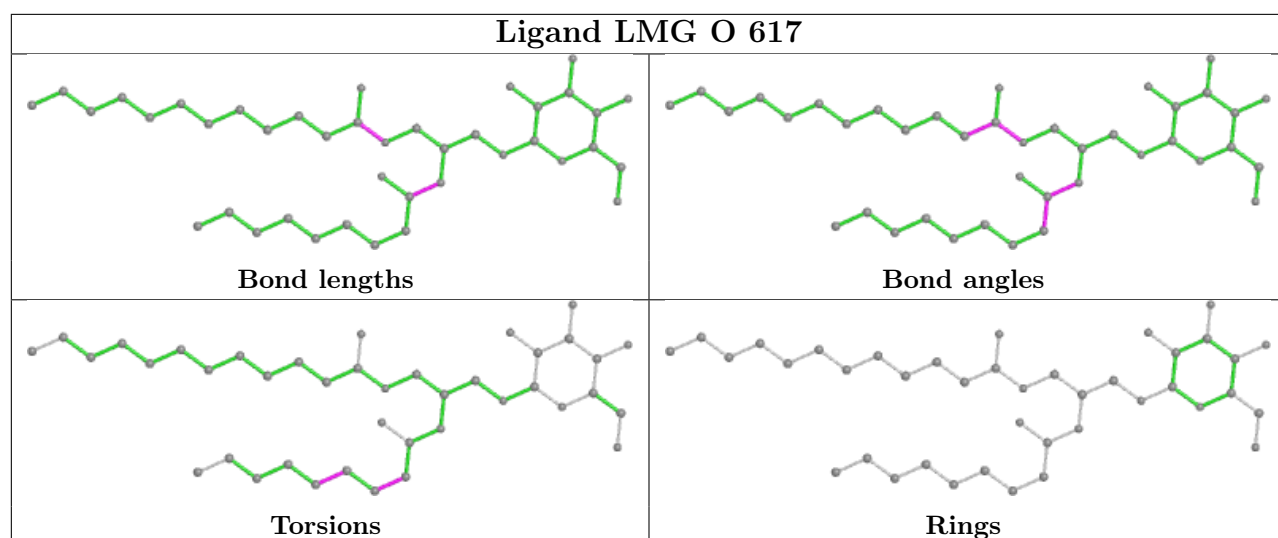


## Ligand WVN Z 101

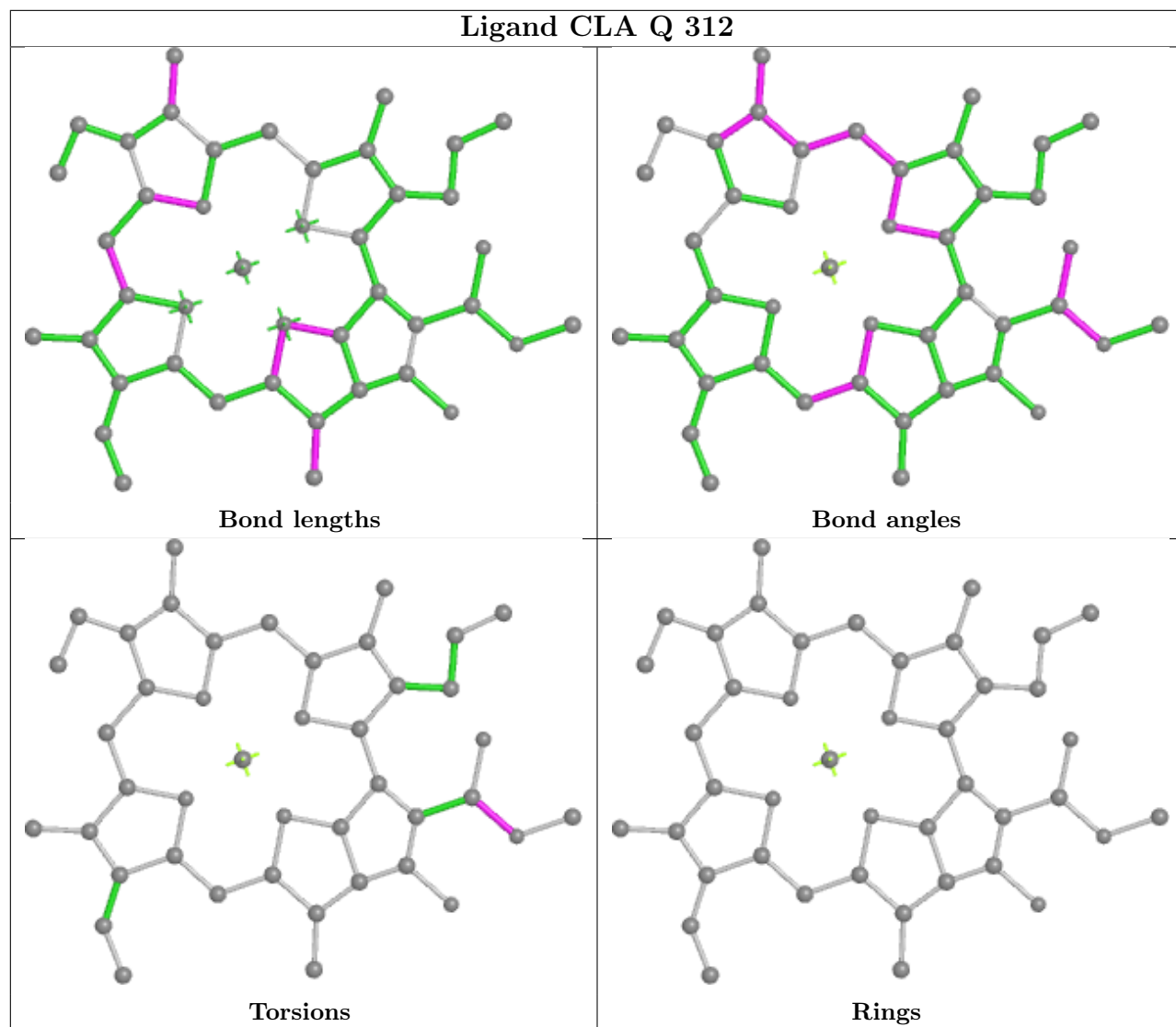


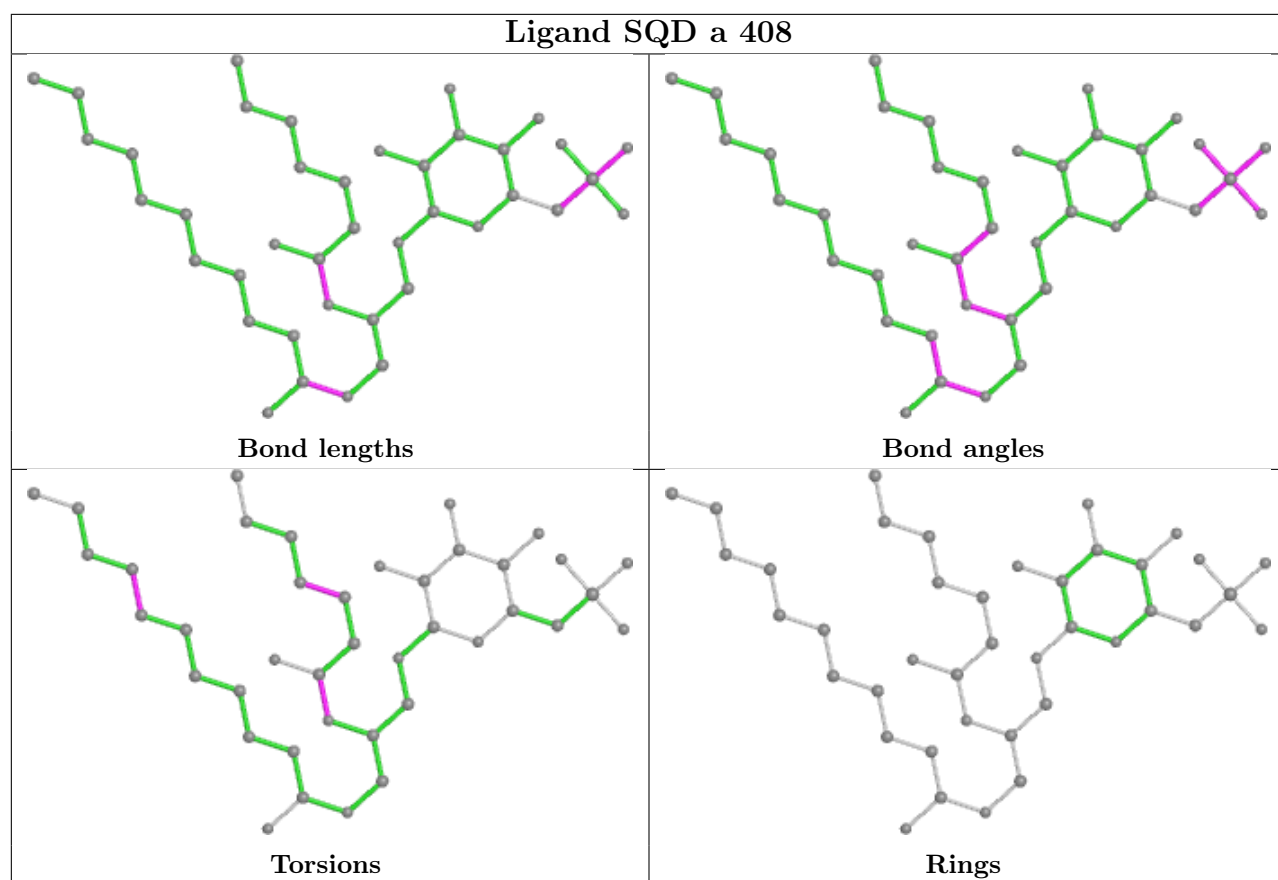
## Ligand PL9 D 409



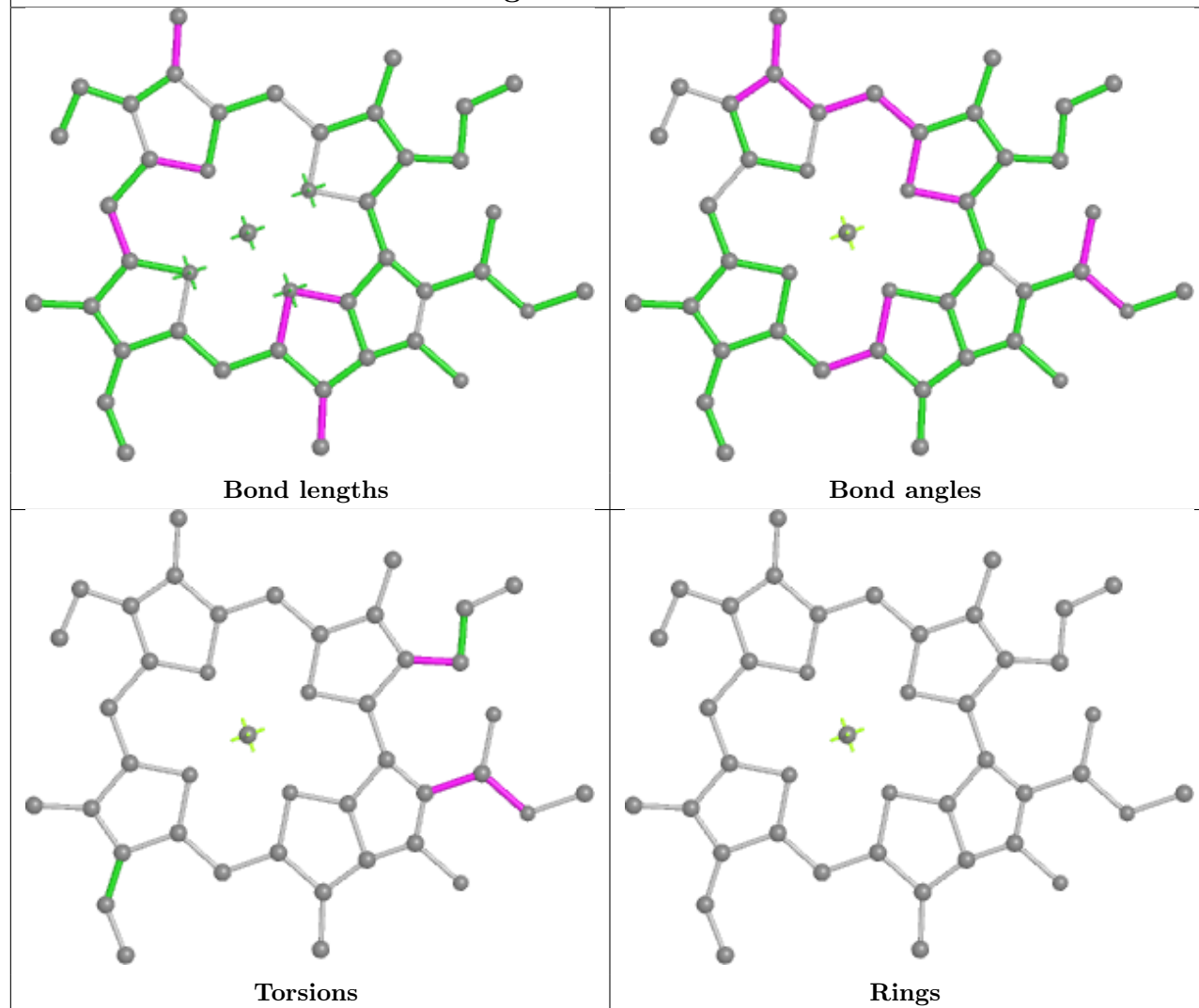


## Ligand CLA Q 312

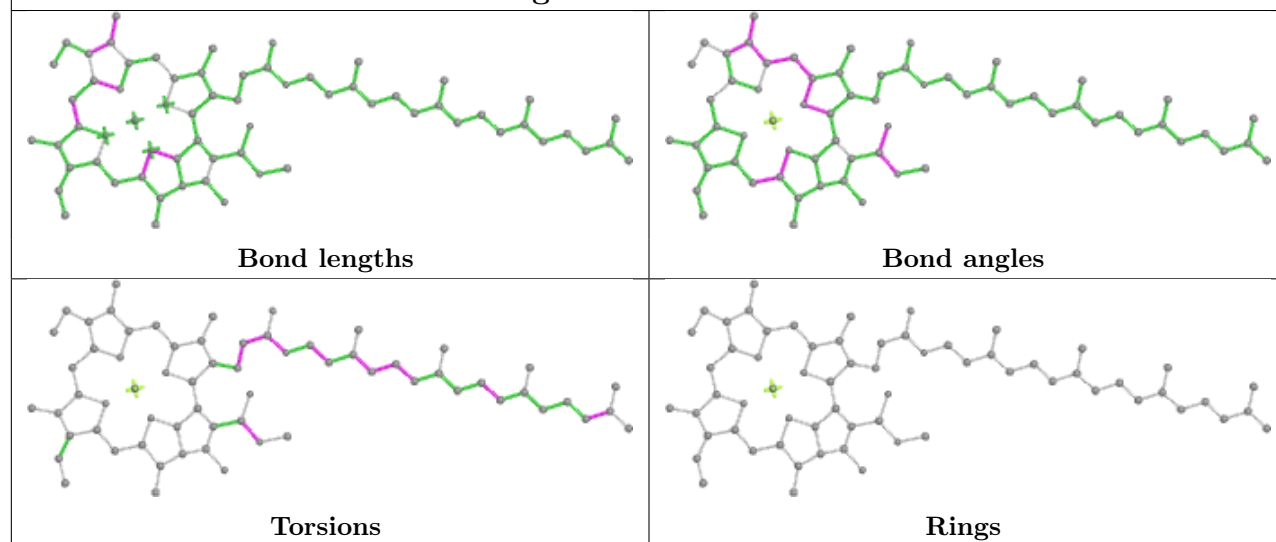


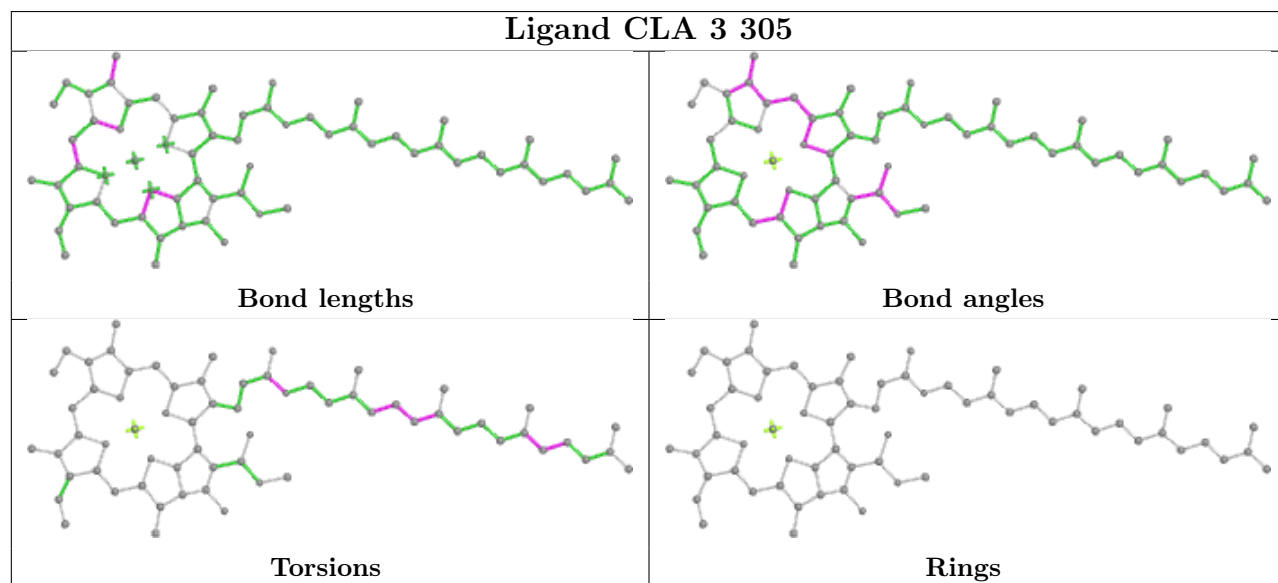
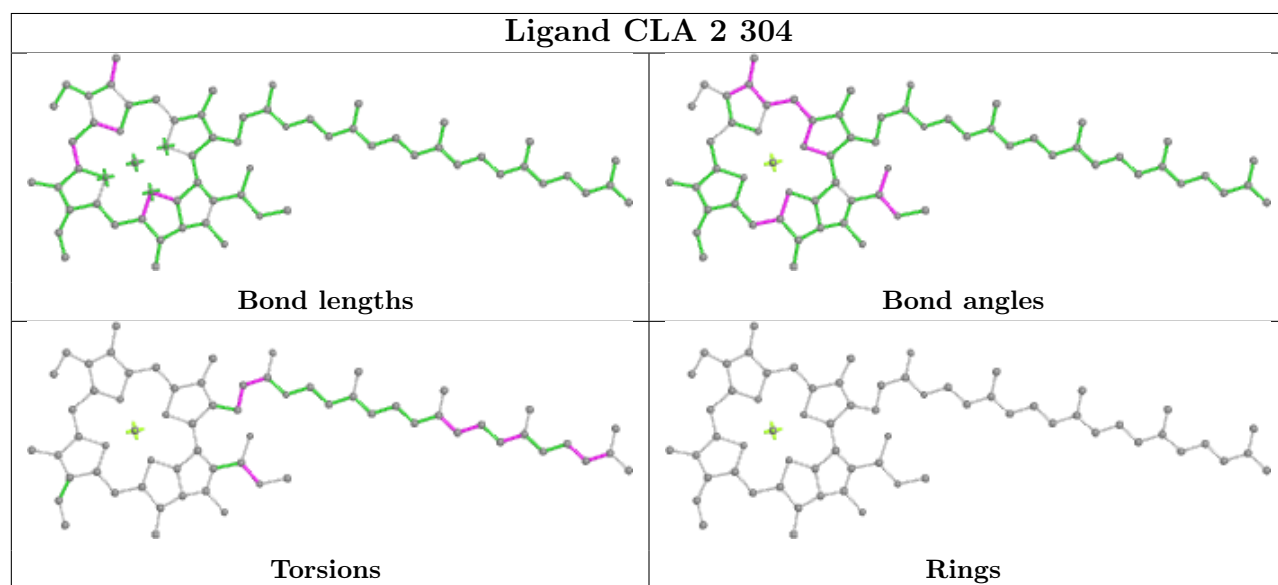
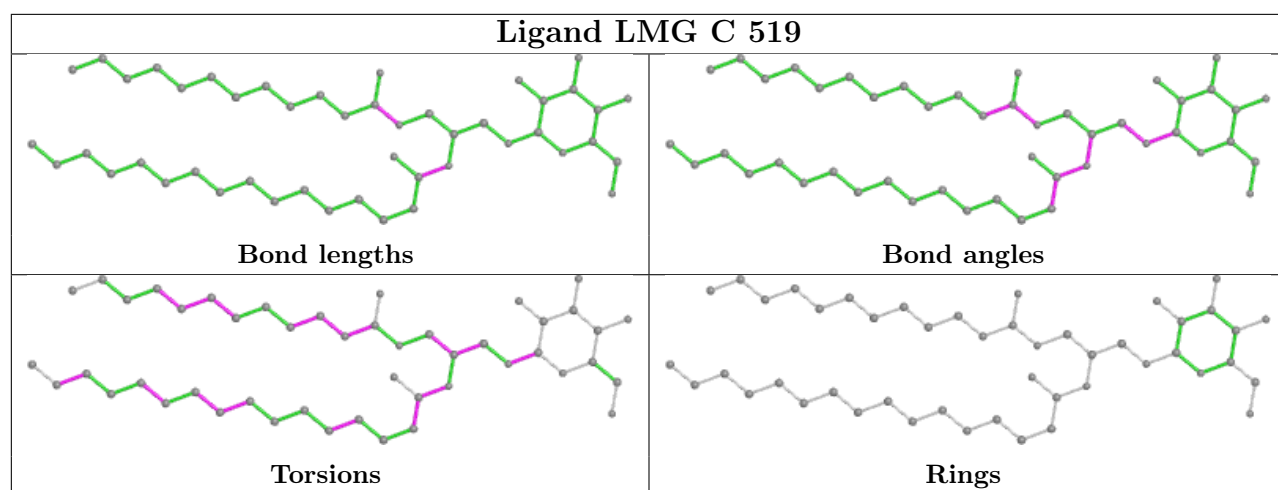


## Ligand CLA 5 606

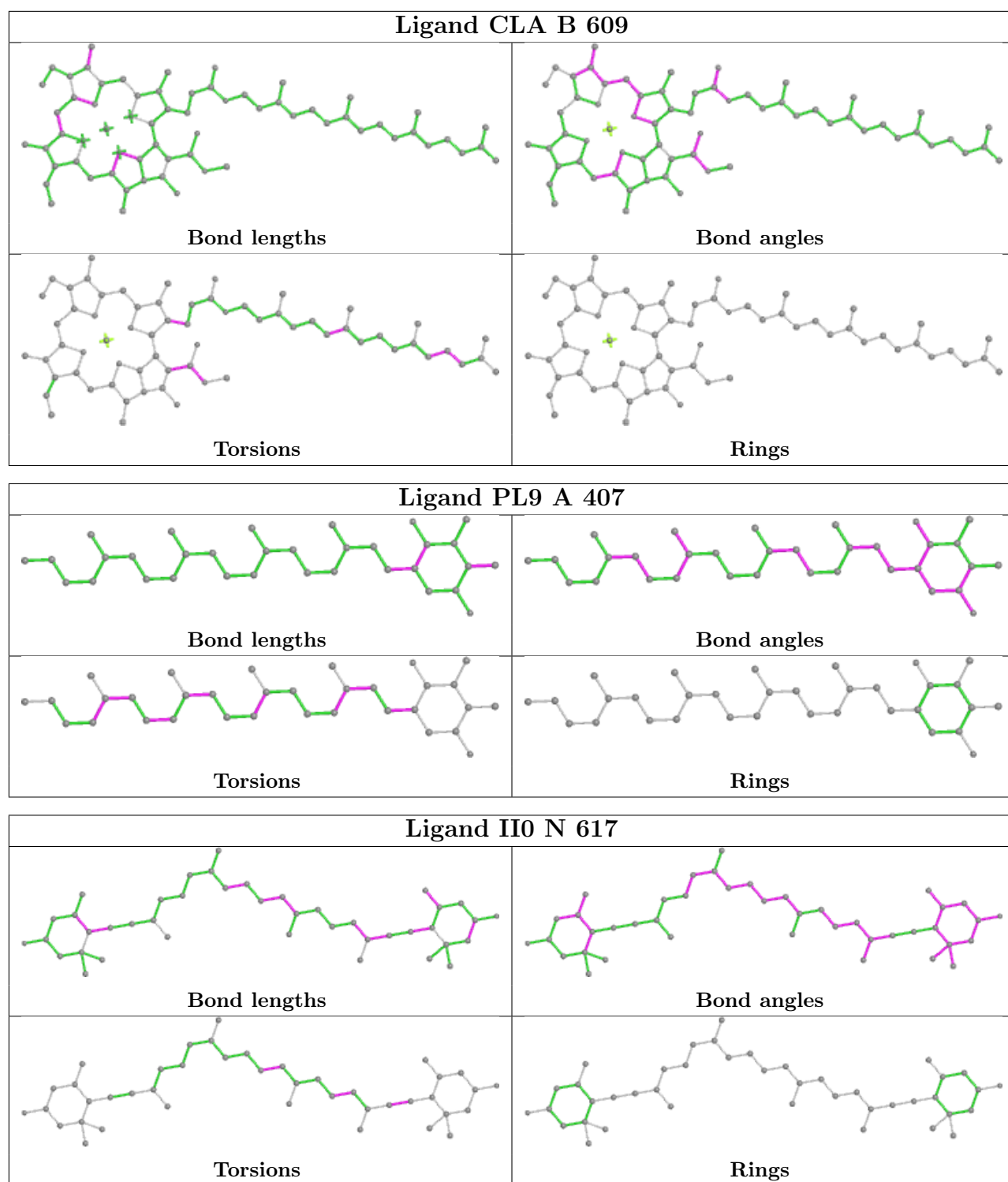


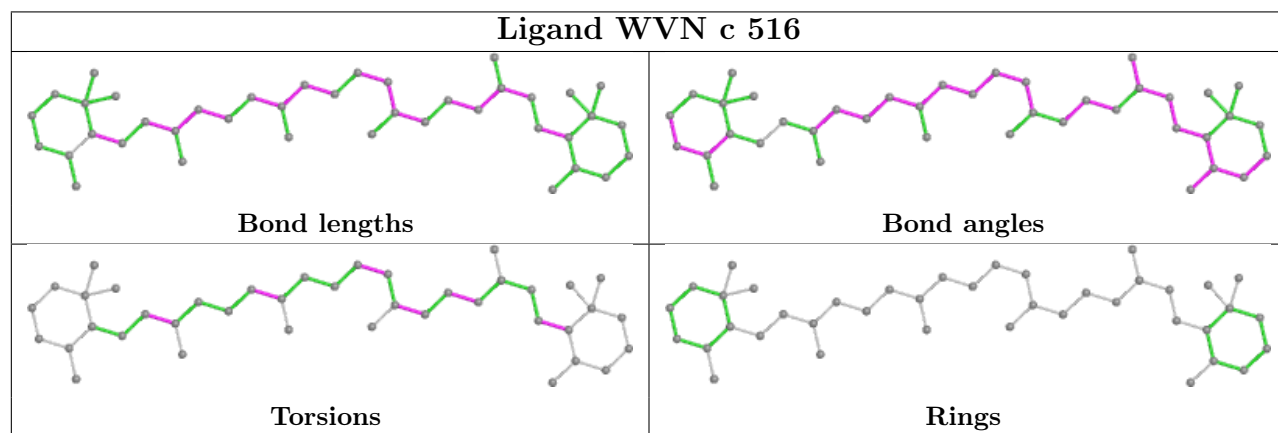
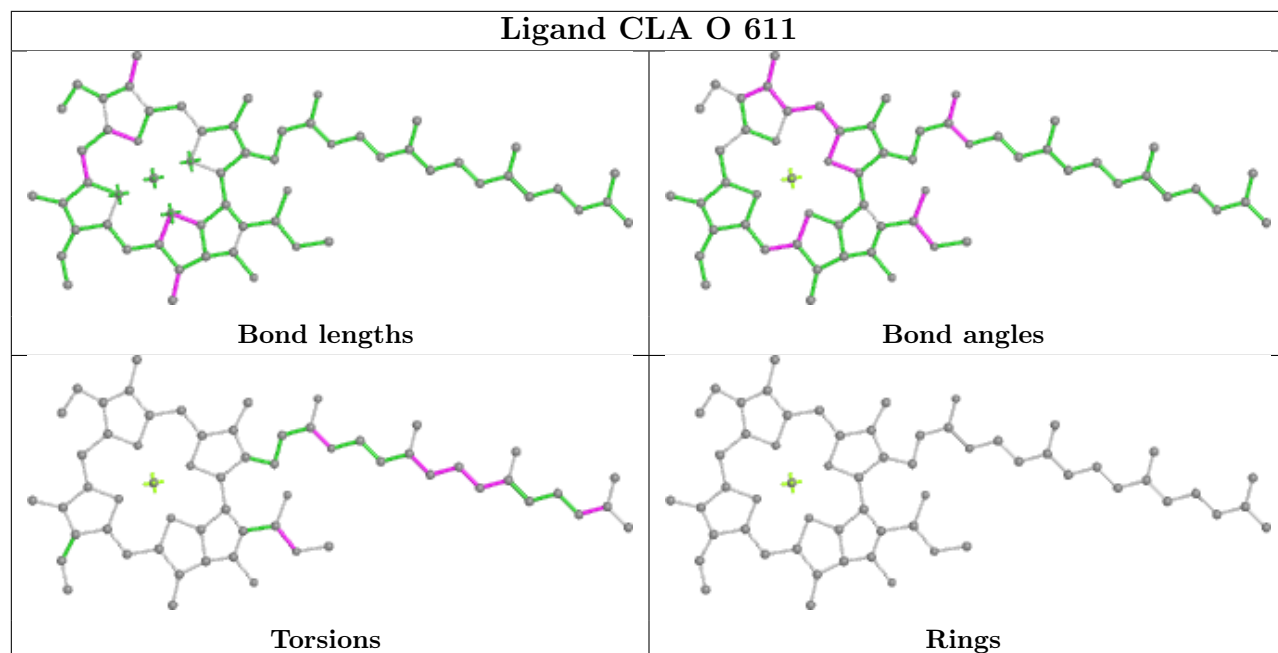
## Ligand CLA B 613



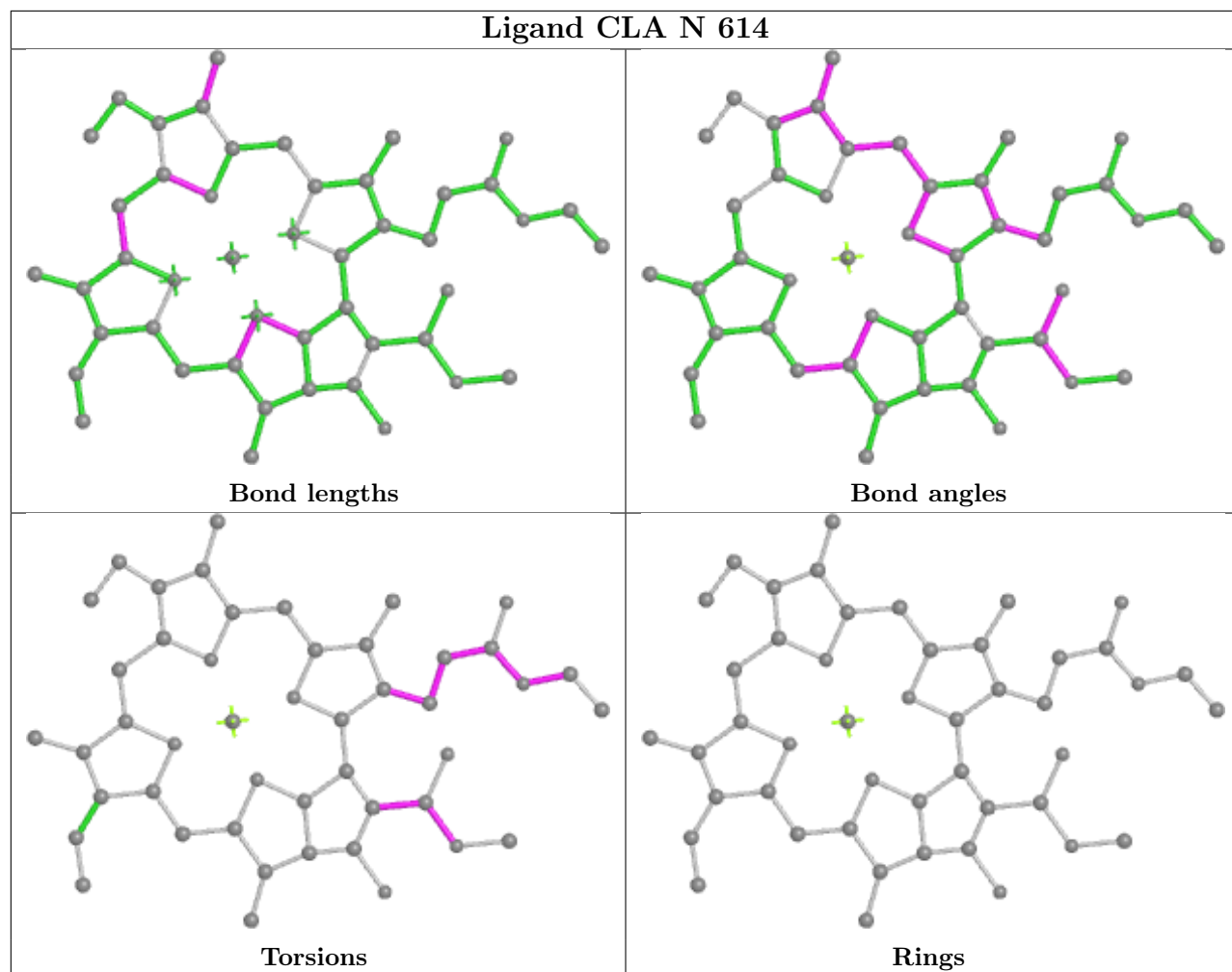




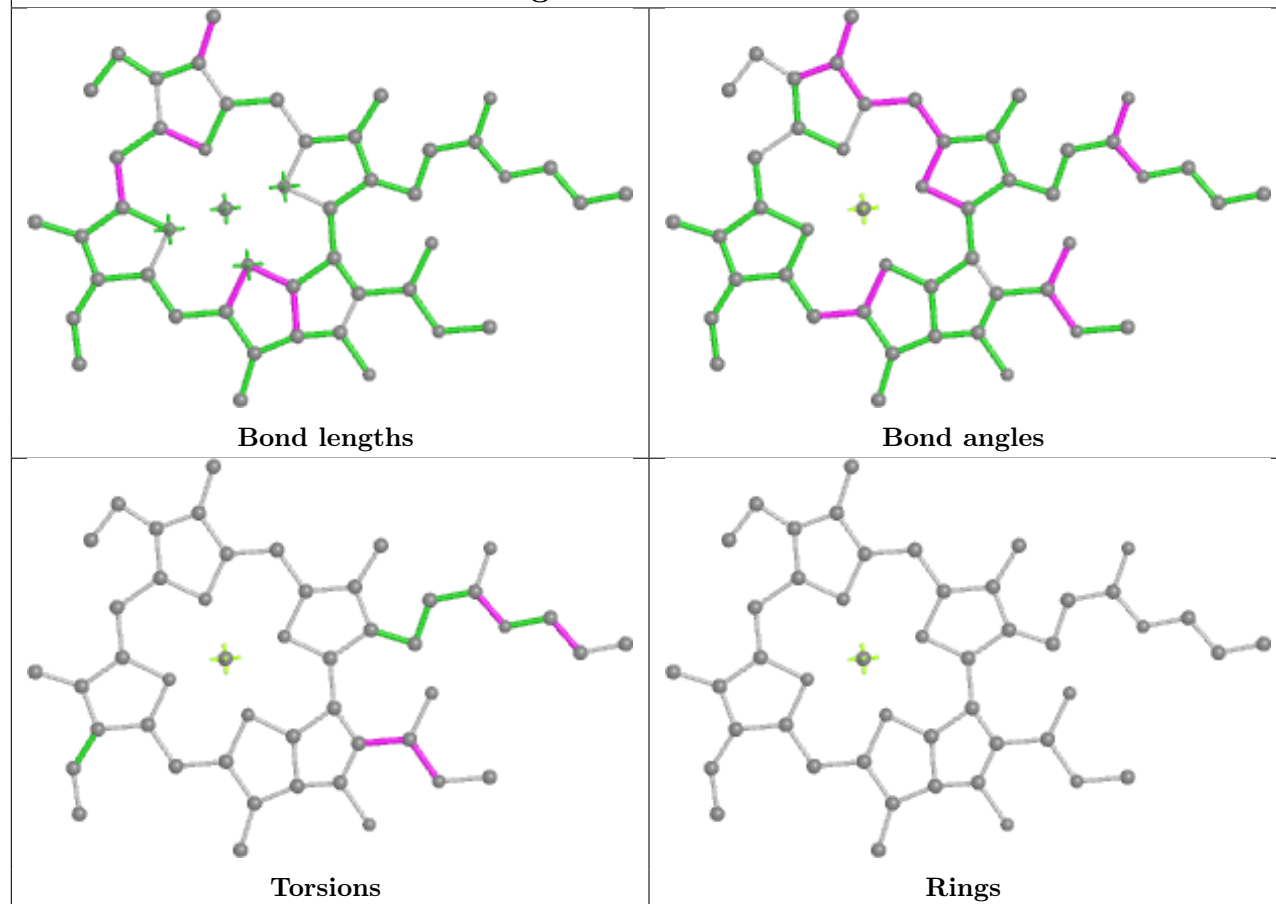




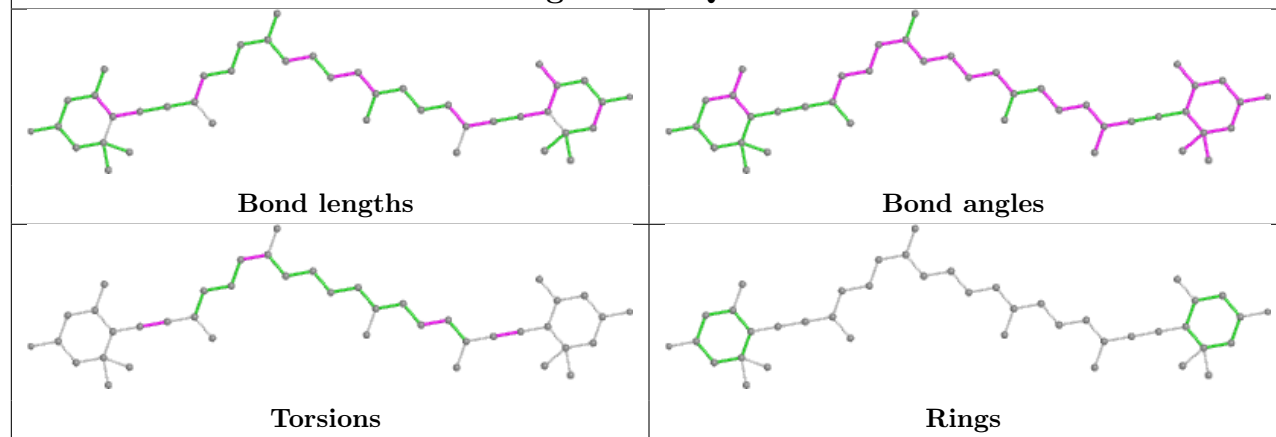
## Ligand CLA N 614



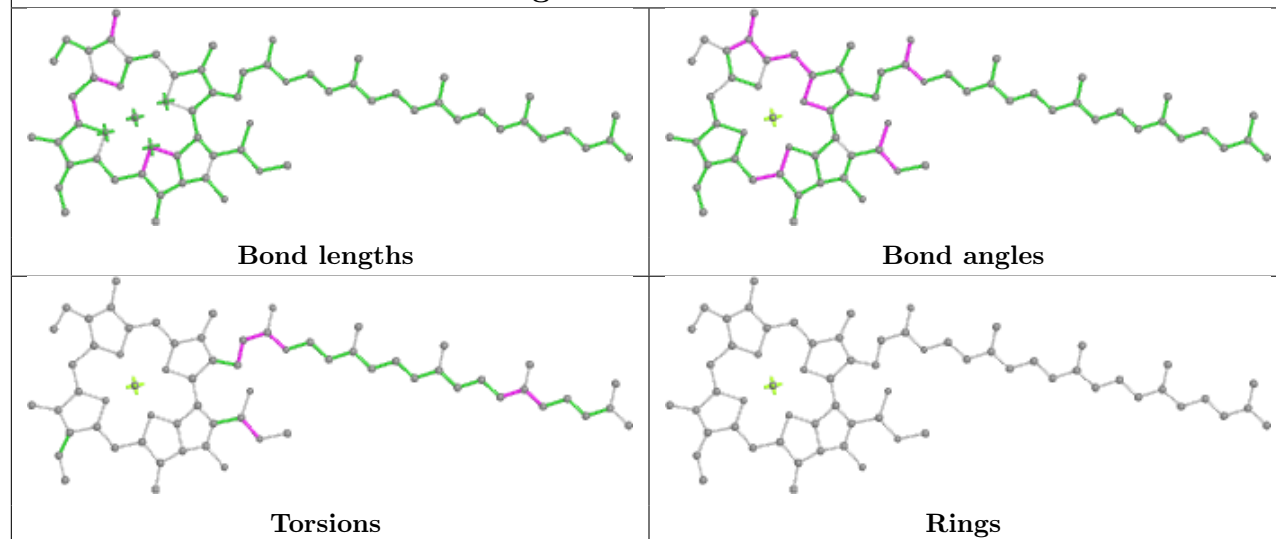
## Ligand CLA N 613



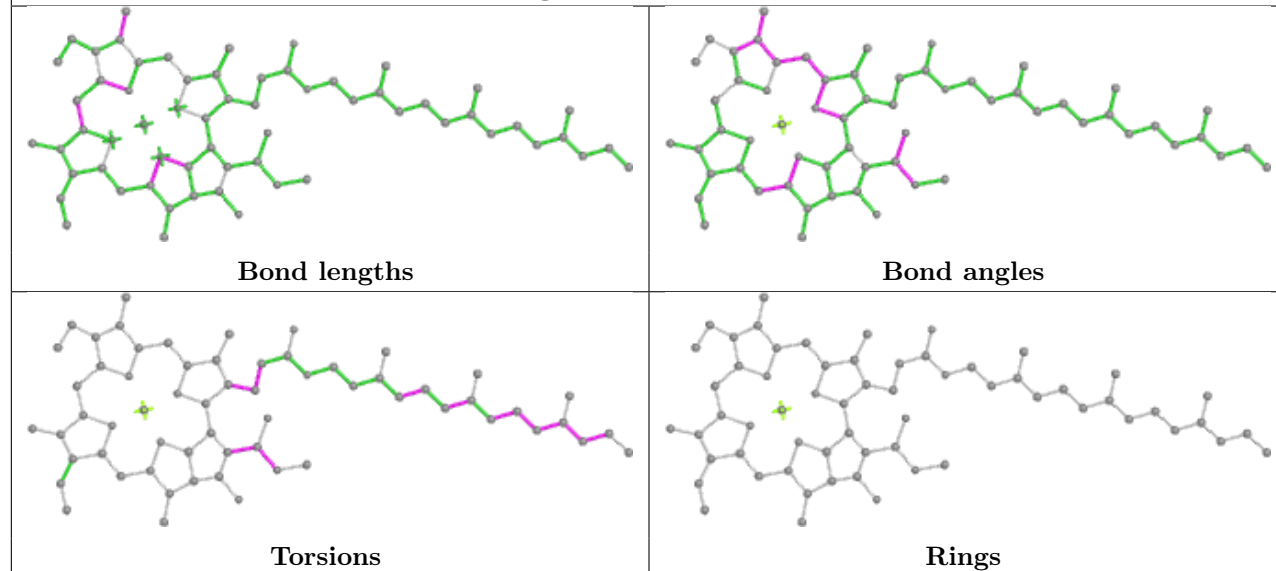
## Ligand II0 Q 316



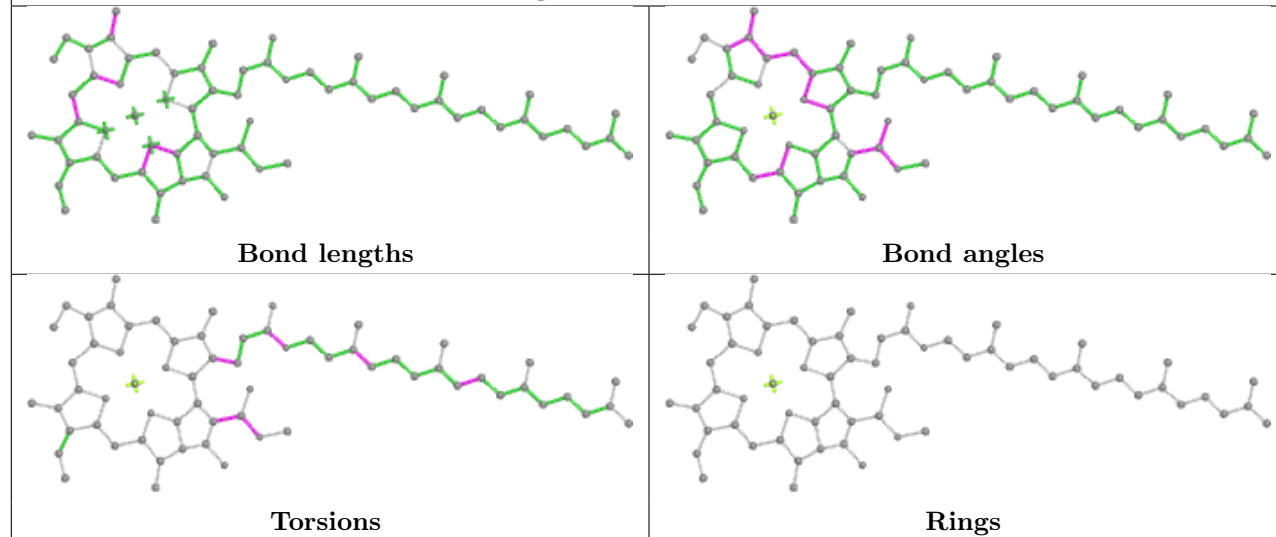
## Ligand CLA B 610



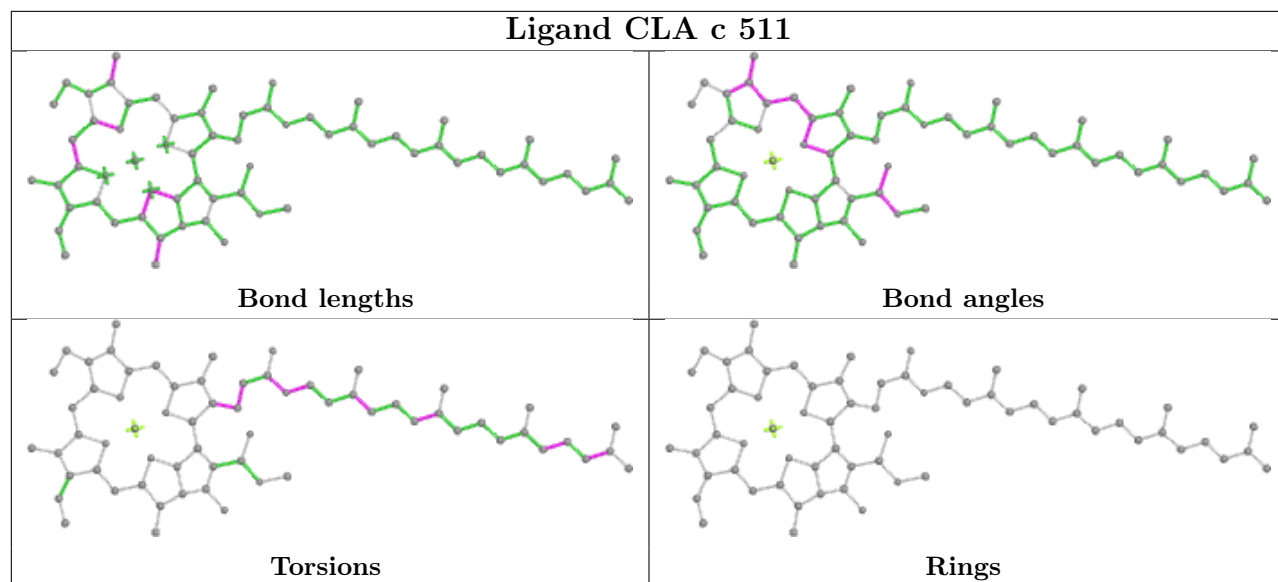
## Ligand CLA 3 301



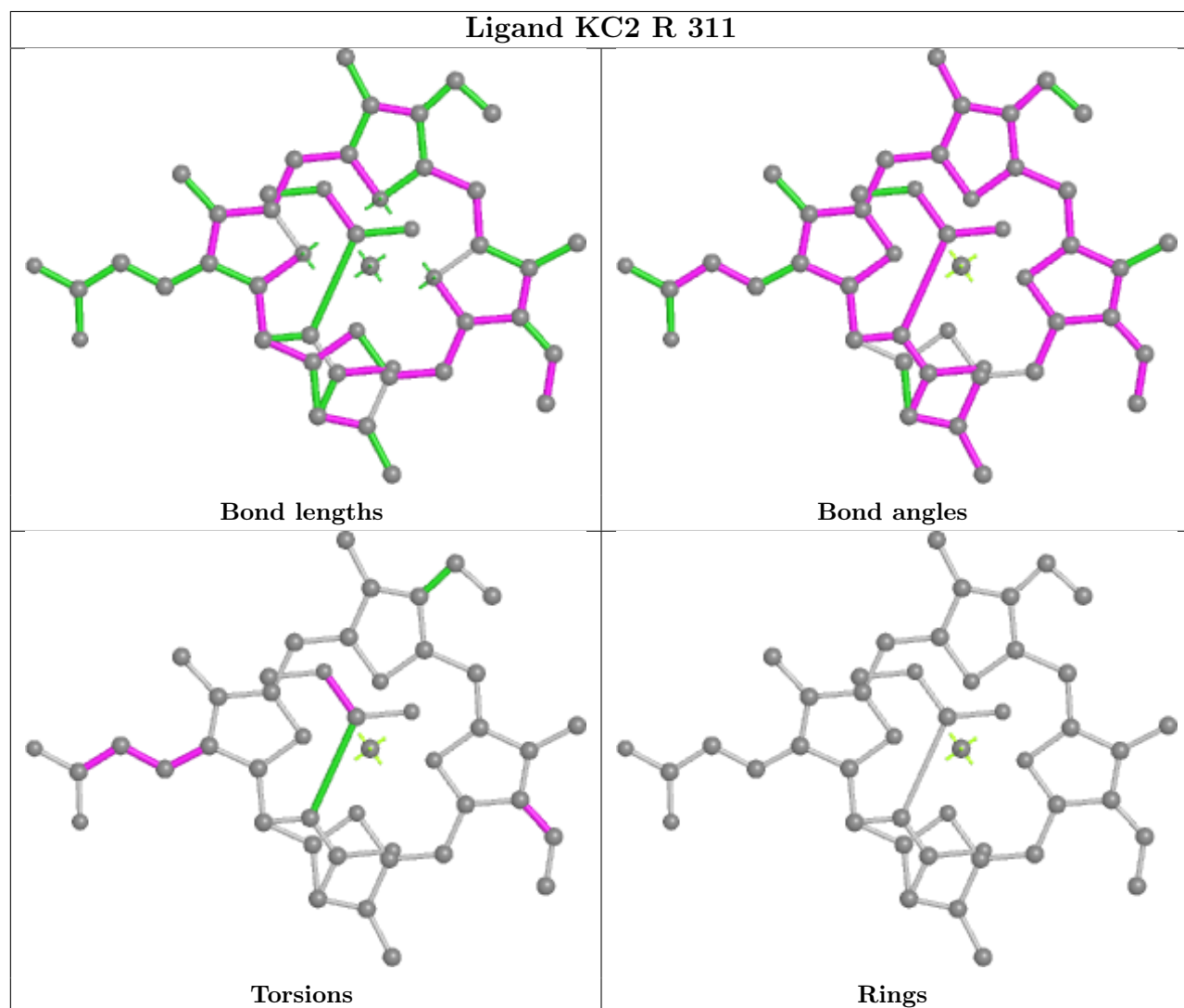
## Ligand CLA C 512

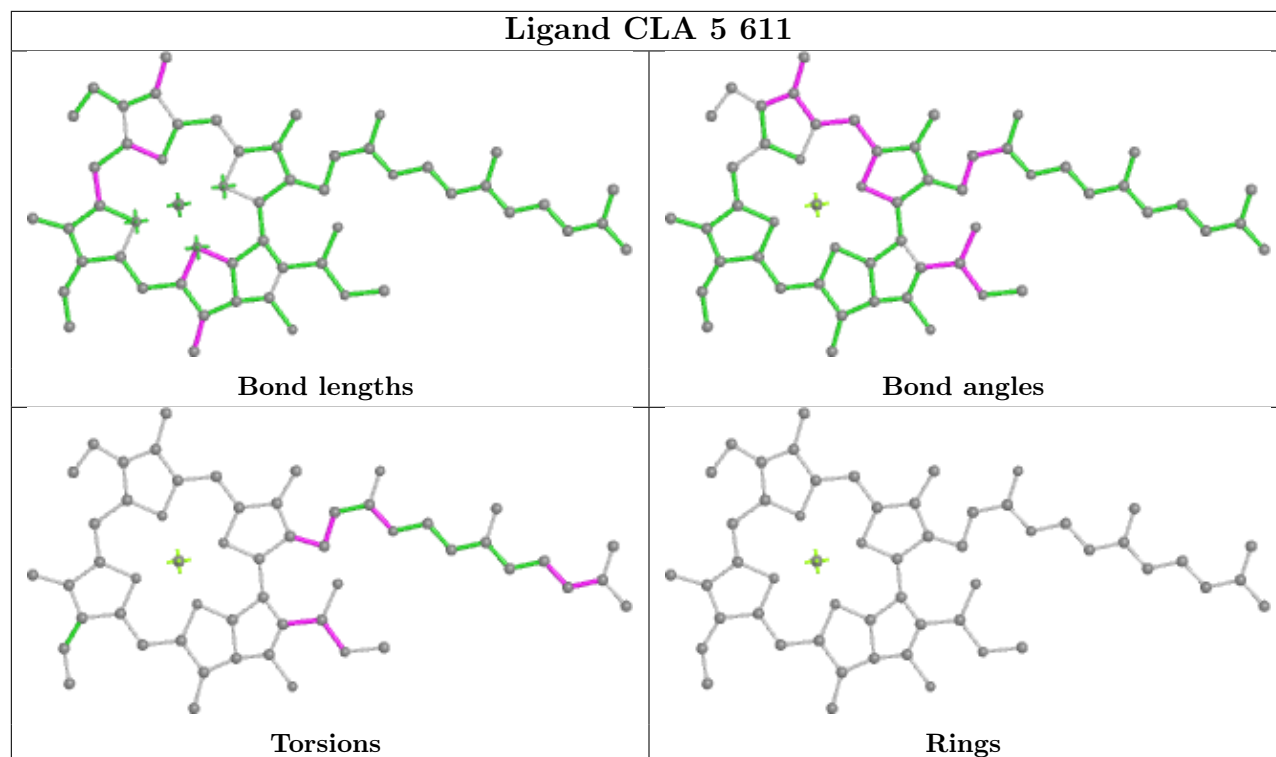
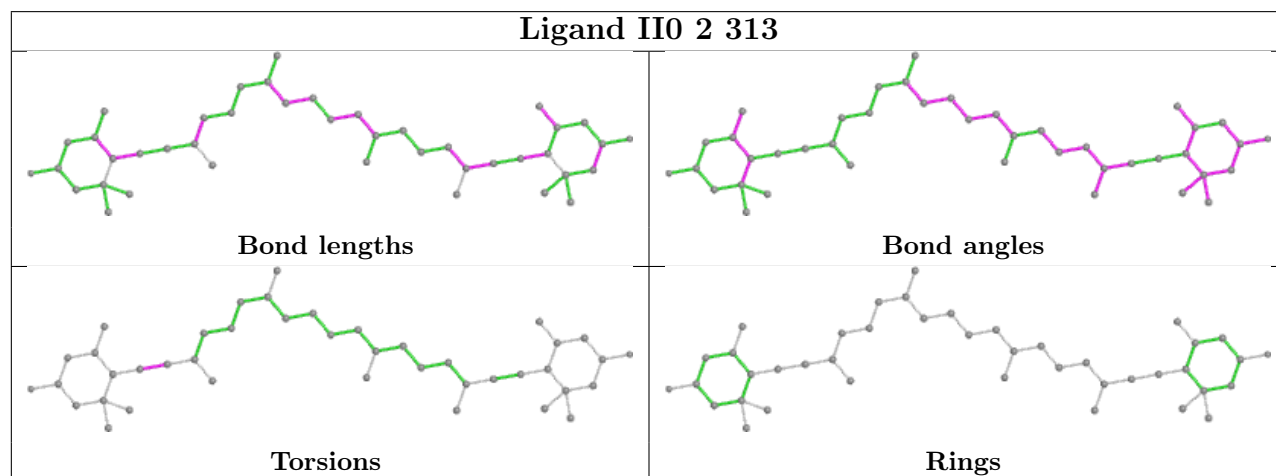


## Ligand CLA c 511

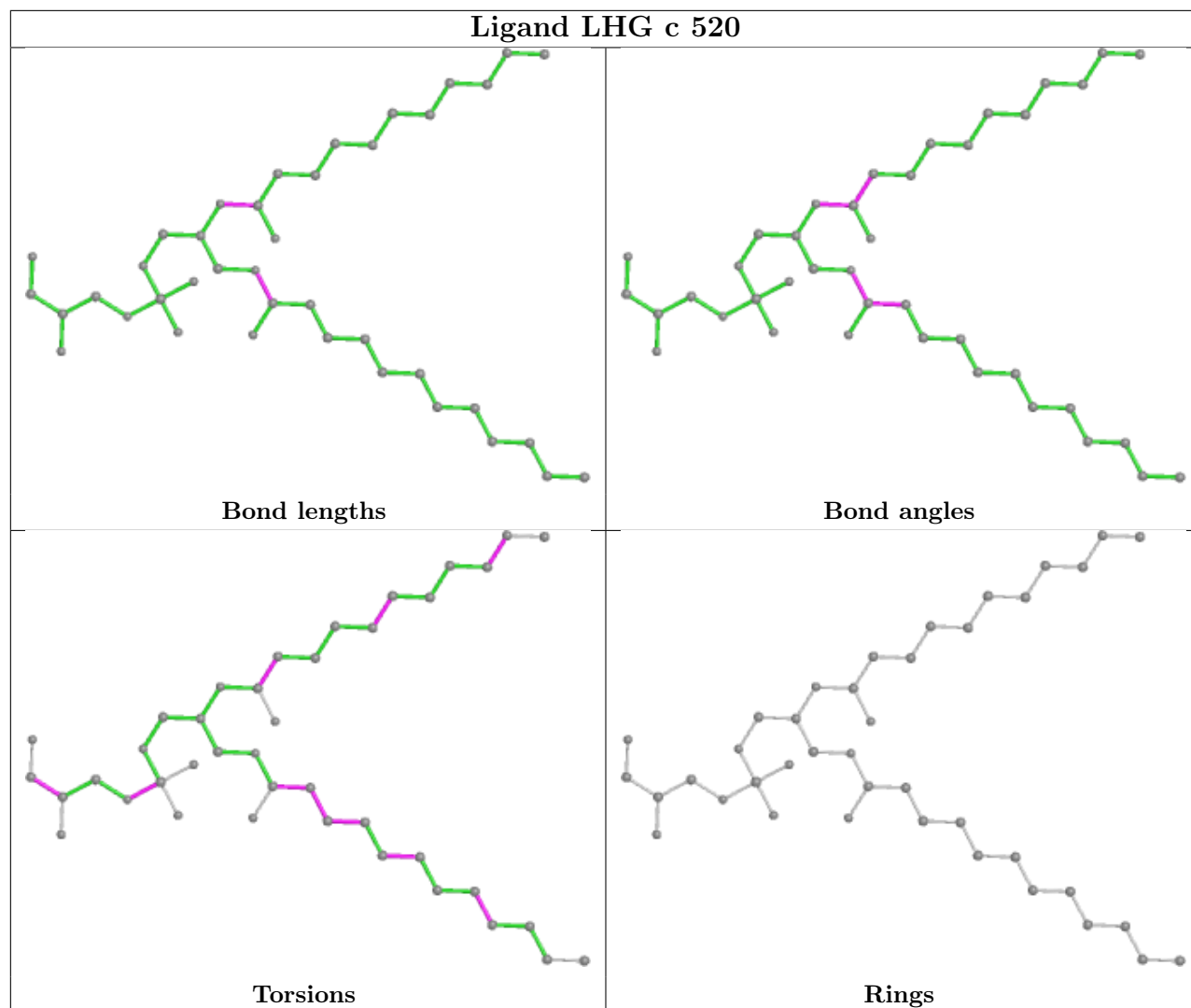


## Ligand KC2 R 311

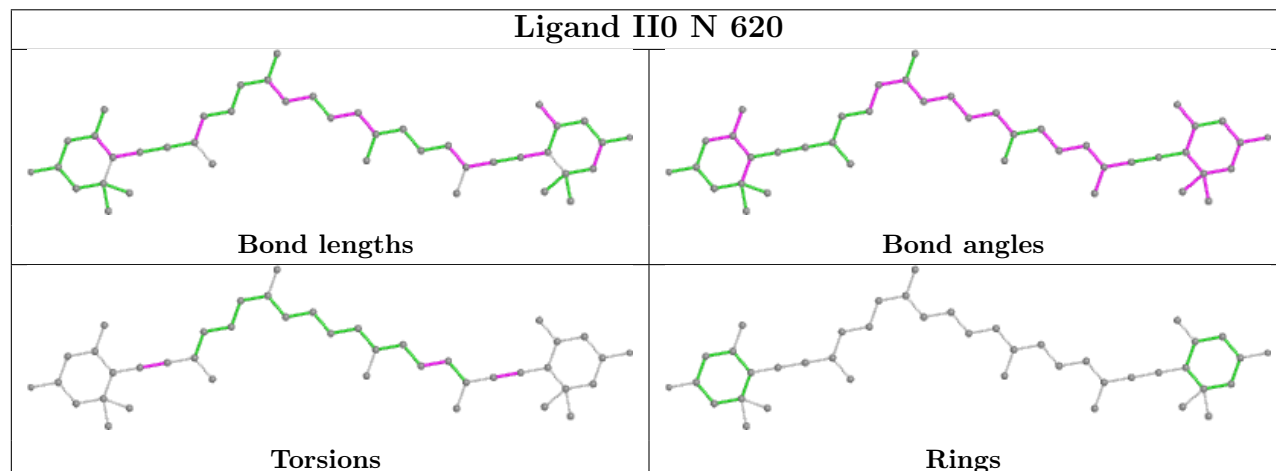


**Ligand CLA 5 611****Ligand II0 2 313**

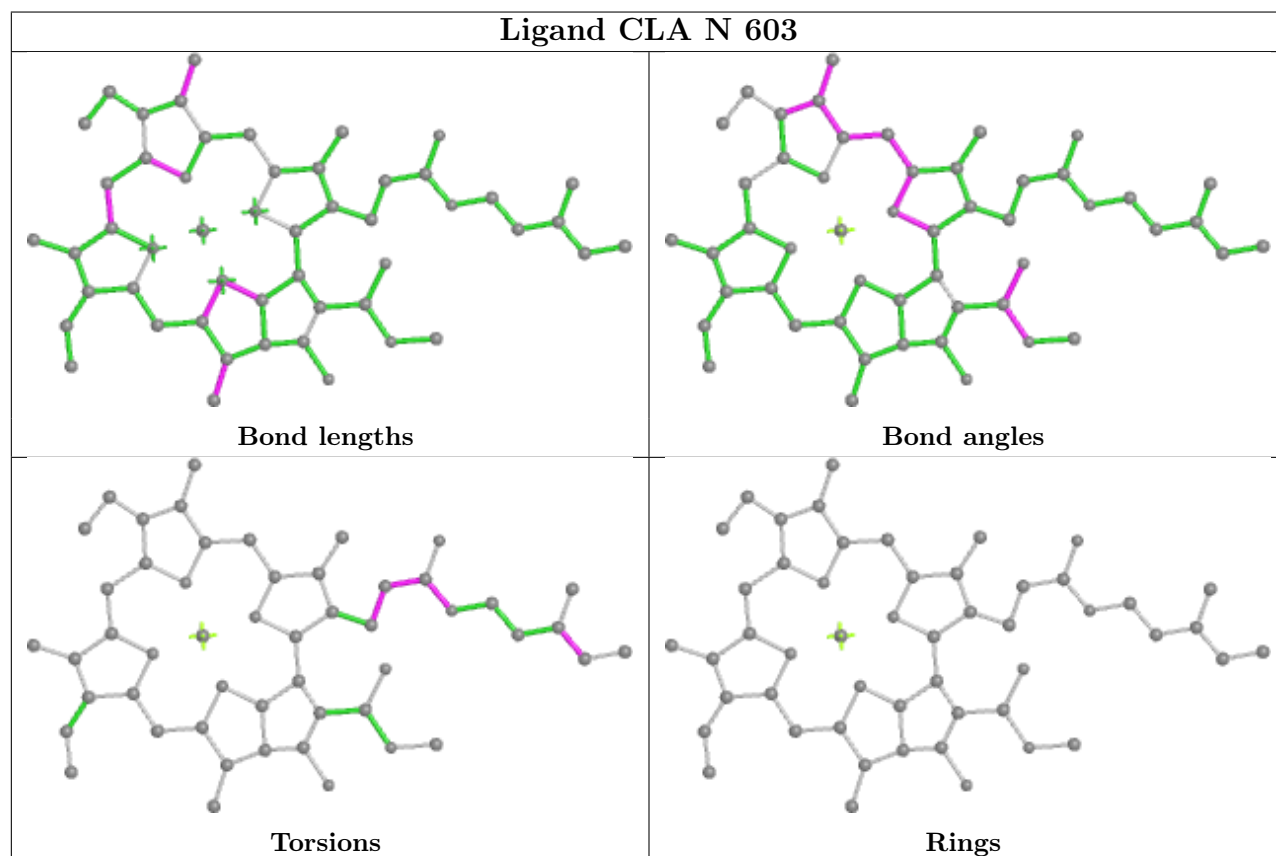
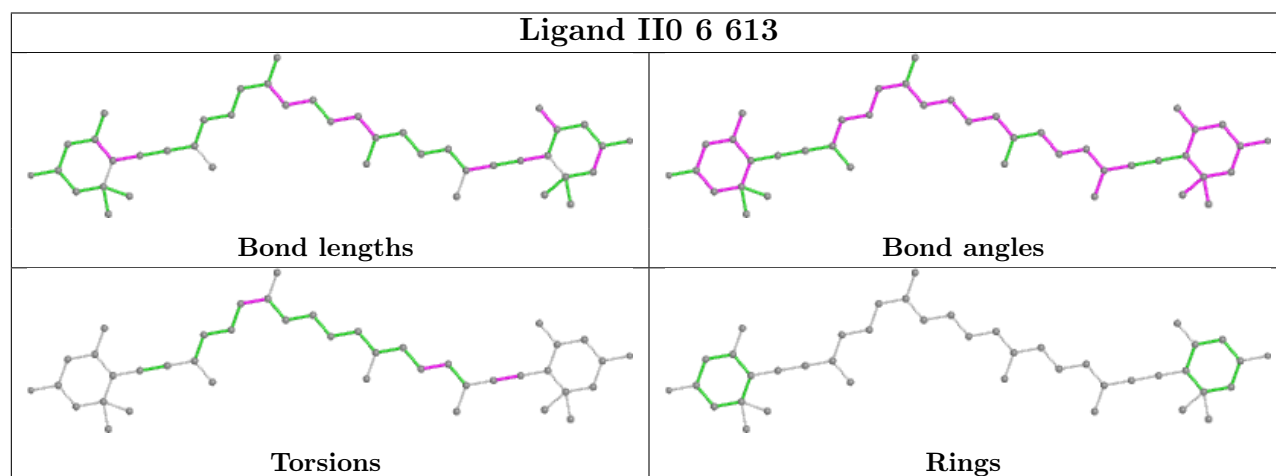
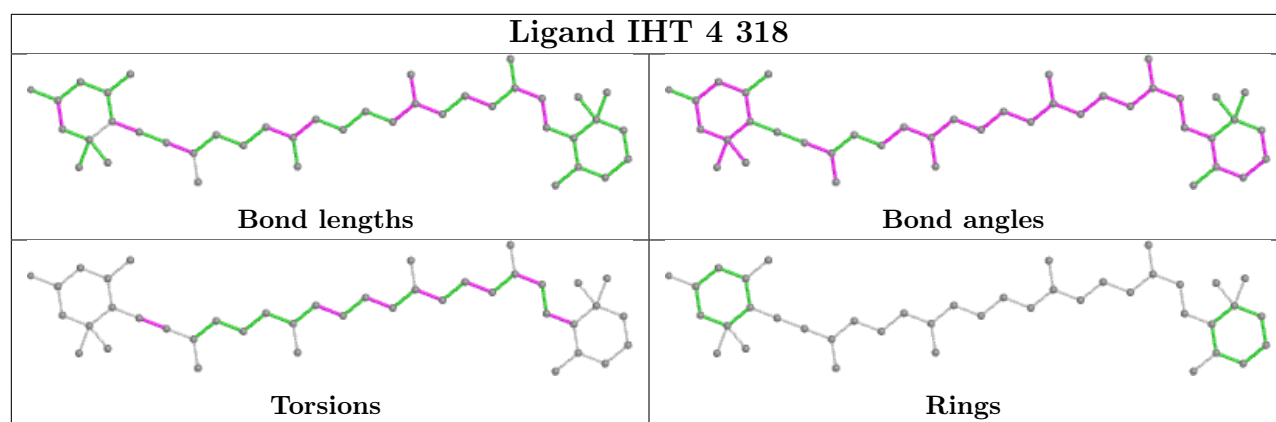
## Ligand LHG c 520



## Ligand II0 N 620







## 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.

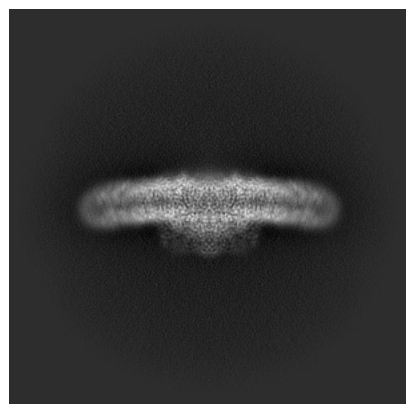
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62846. These allow visual inspection of the internal detail of the map and identification of artifacts.

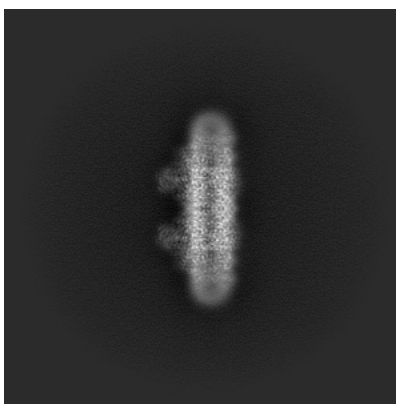
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

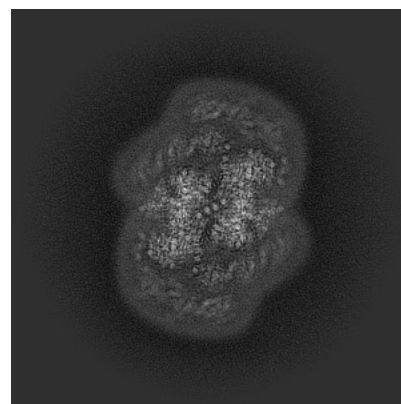
#### 6.1.1 Primary map



X

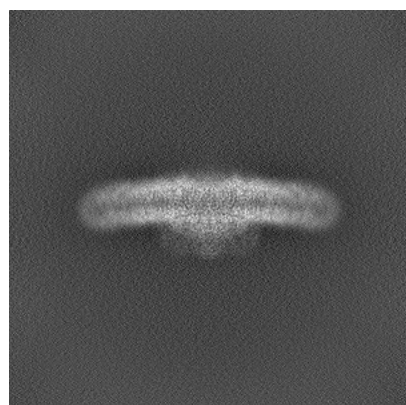


Y

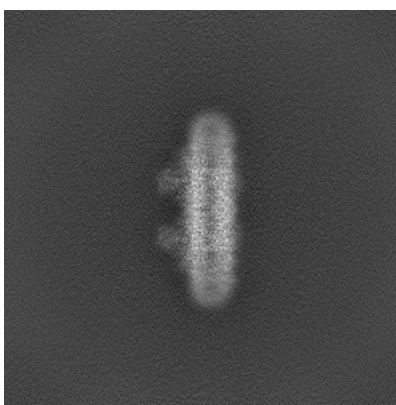


Z

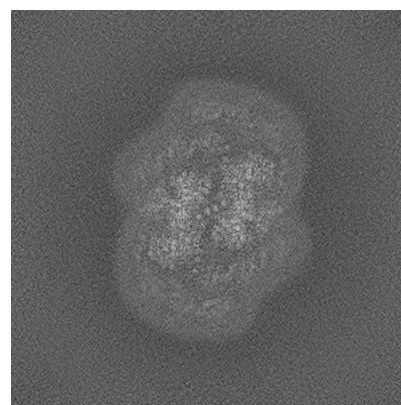
#### 6.1.2 Raw map



X



Y

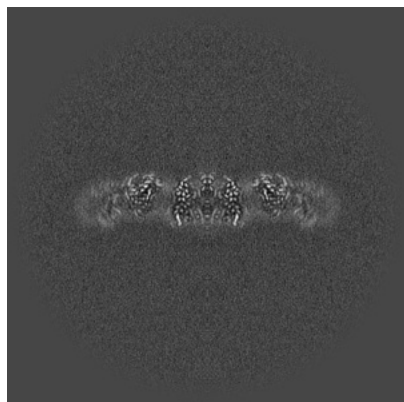


Z

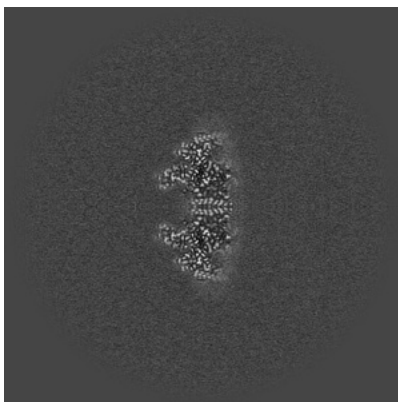
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

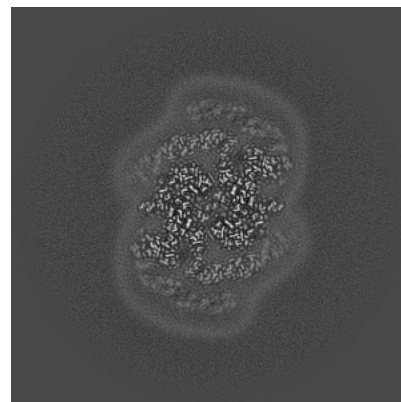
### 6.2.1 Primary map



X Index: 300

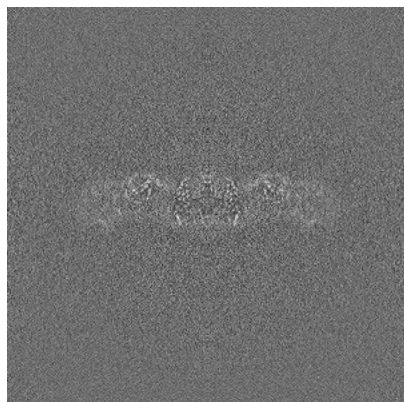


Y Index: 300

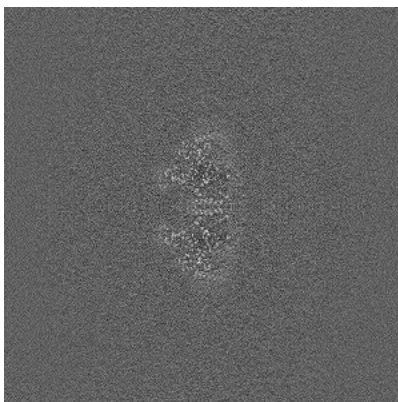


Z Index: 300

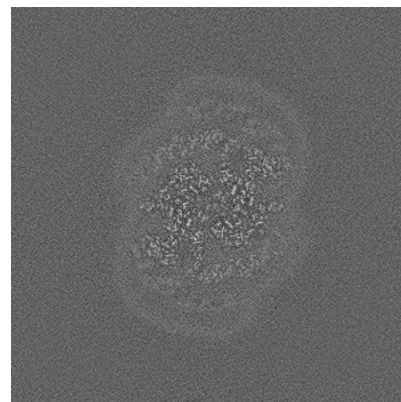
### 6.2.2 Raw map



X Index: 300



Y Index: 300

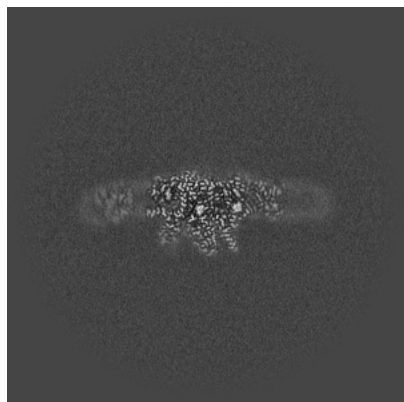


Z Index: 300

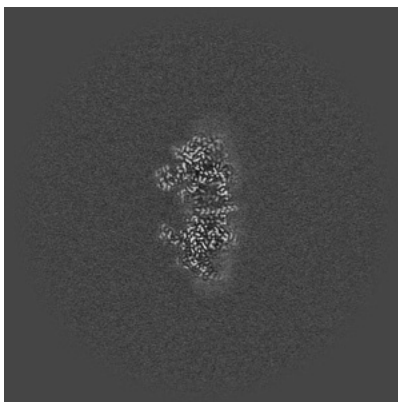
The images above show central slices of the map in three orthogonal directions.

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

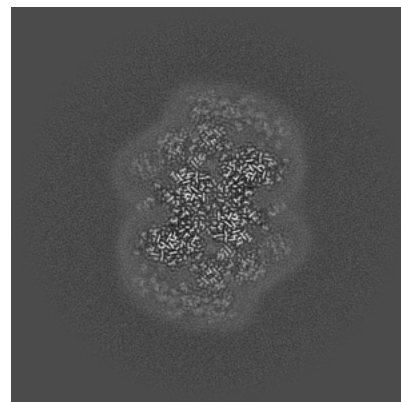
### 6.3.1 Primary map



X Index: 254

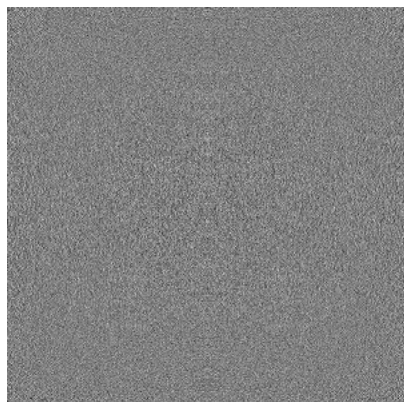


Y Index: 296

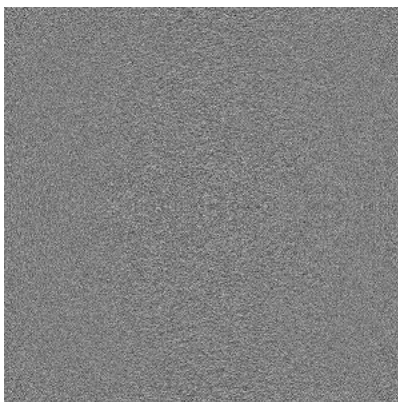


Z Index: 324

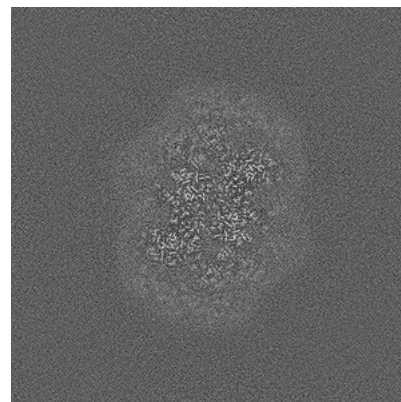
### 6.3.2 Raw map



X Index: 0



Y Index: 0



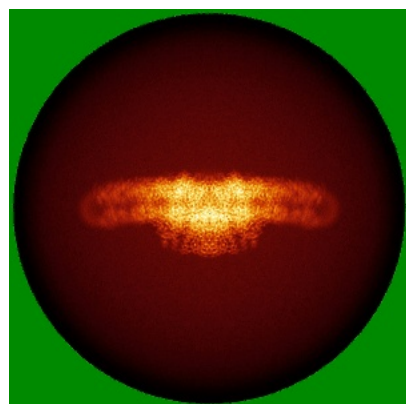
Z Index: 324

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

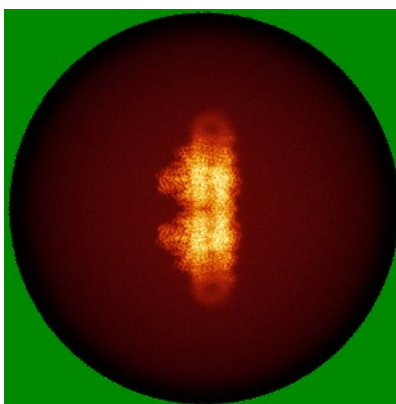


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

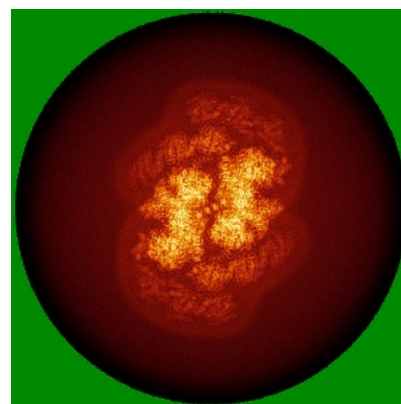
### 6.4.1 Primary map



X

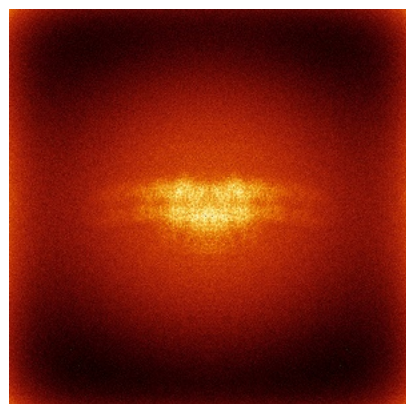


Y

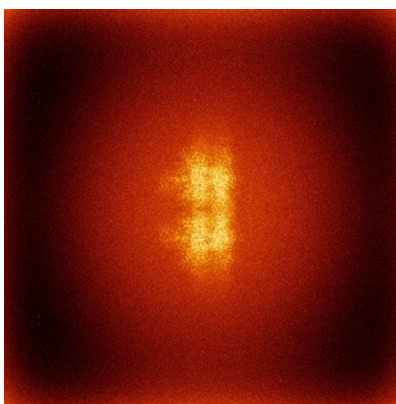


Z

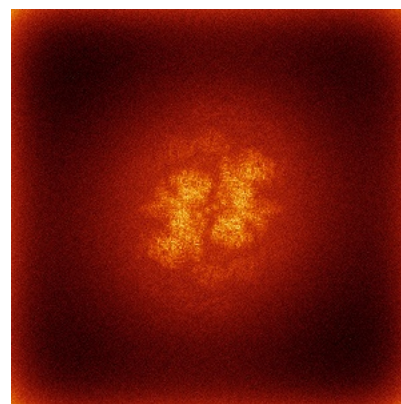
### 6.4.2 Raw map



X



Y

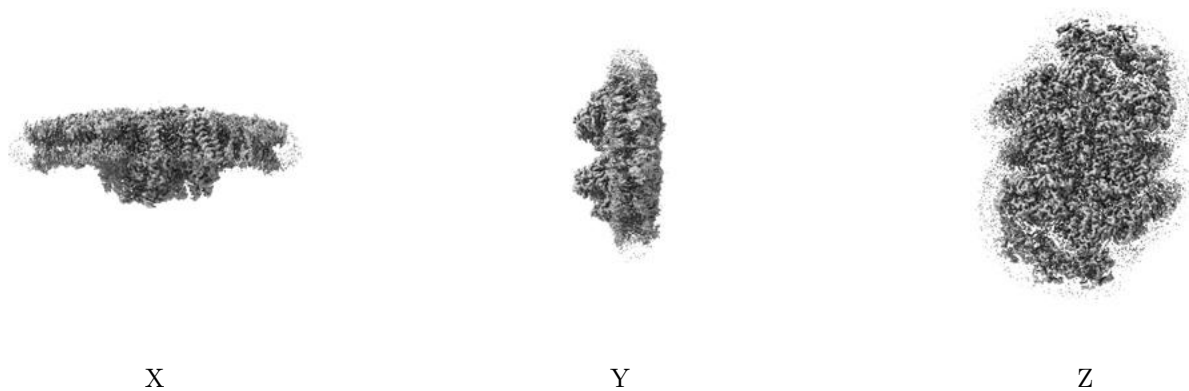


Z

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.

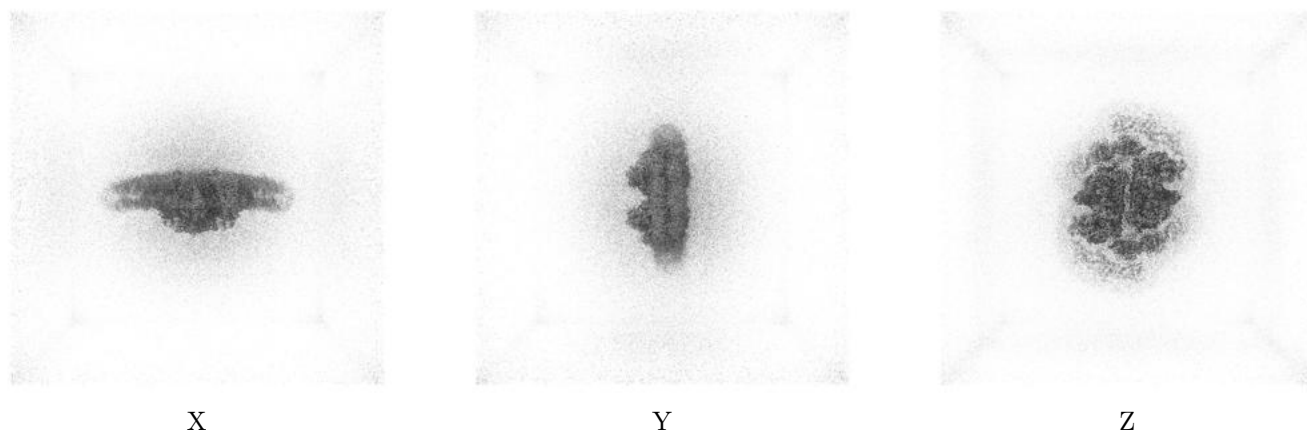
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

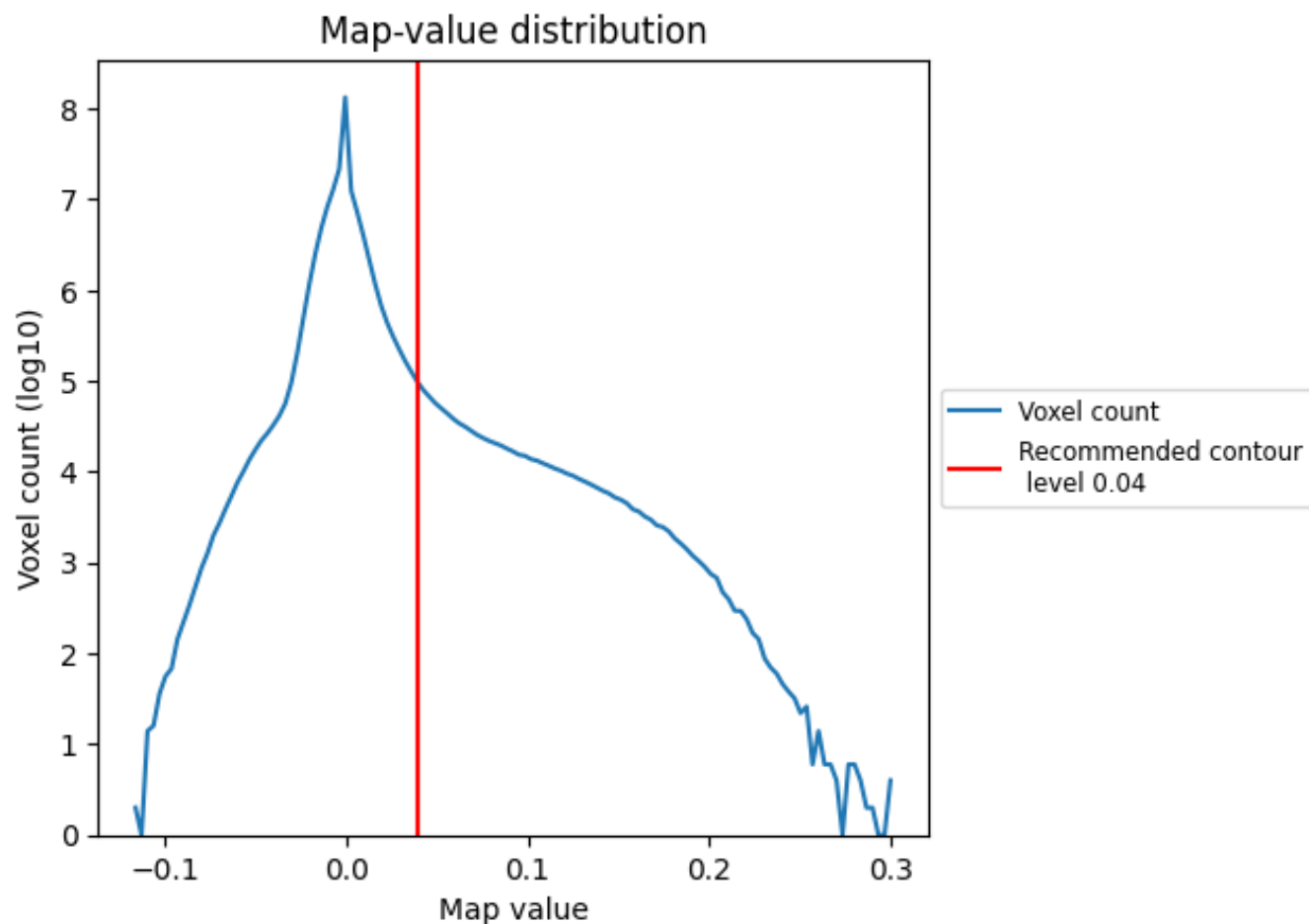
## 6.6 Mask visualisation [i](#)

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.

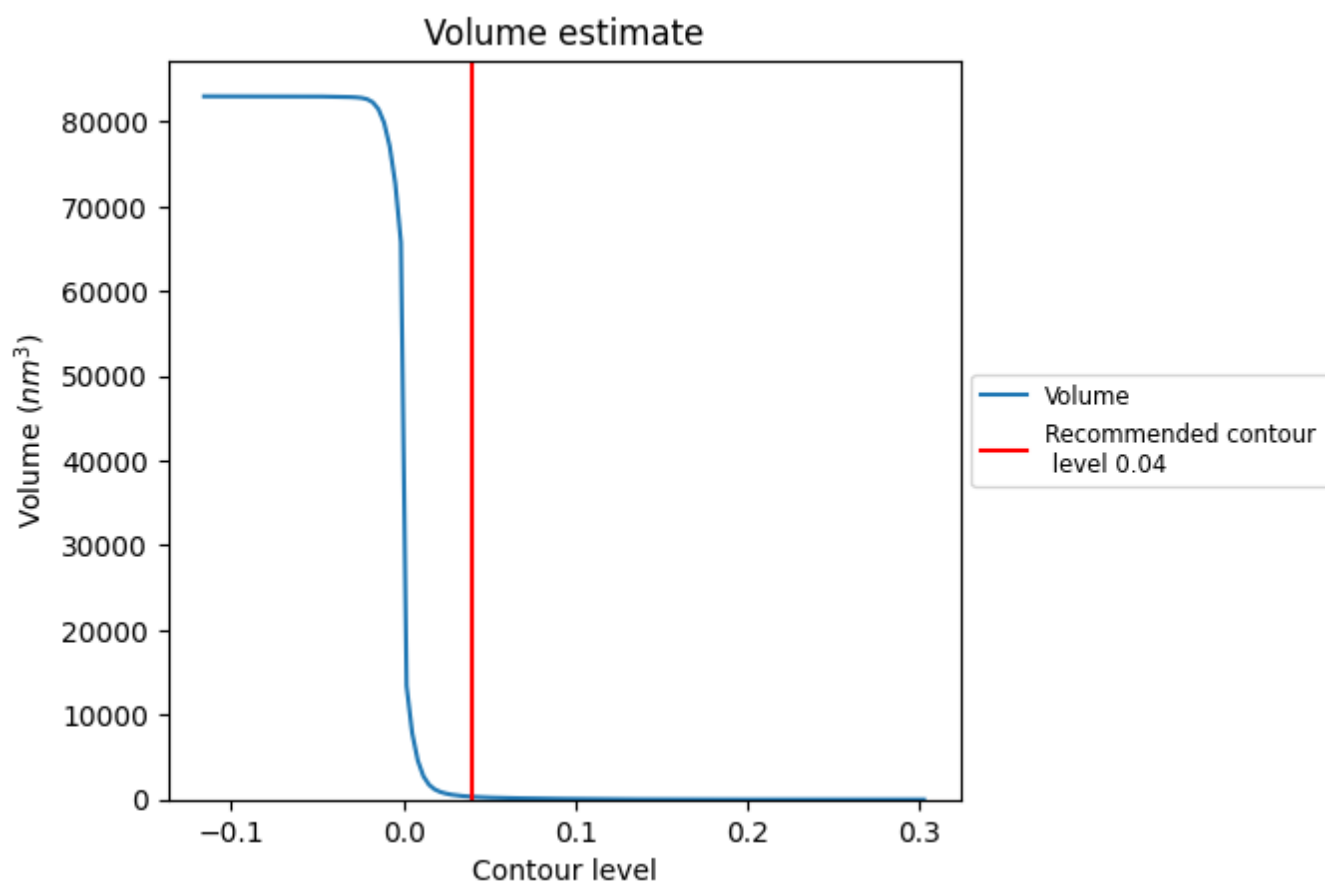
### 7.1 Map-value distribution [i](#)



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.



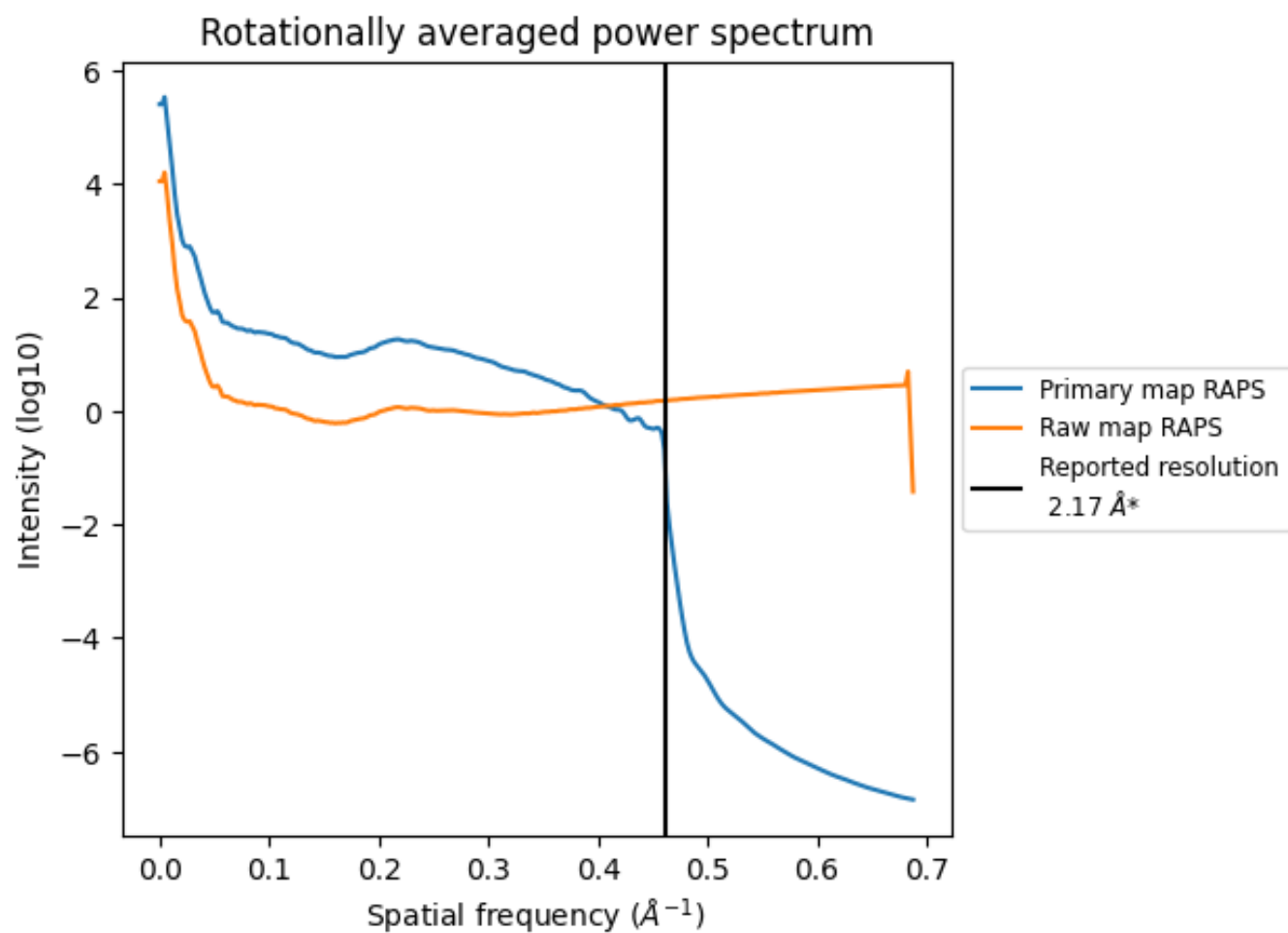
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332  $\text{nm}^3$ ; this corresponds to an approximate mass of 300 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 [i](#)

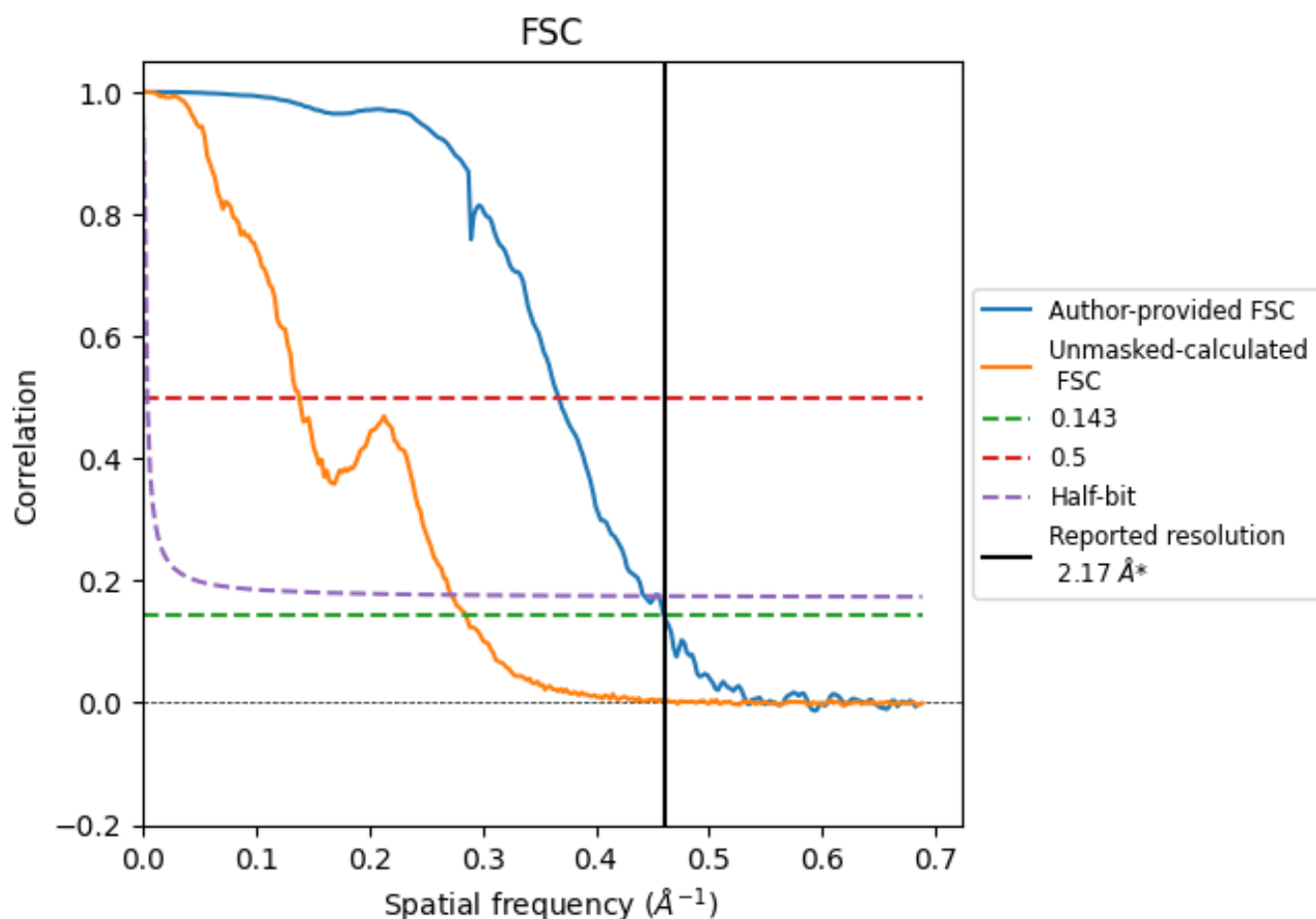


\*Reported resolution corresponds to spatial frequency of 0.461  $\text{\AA}^{-1}$

## 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 0.461  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

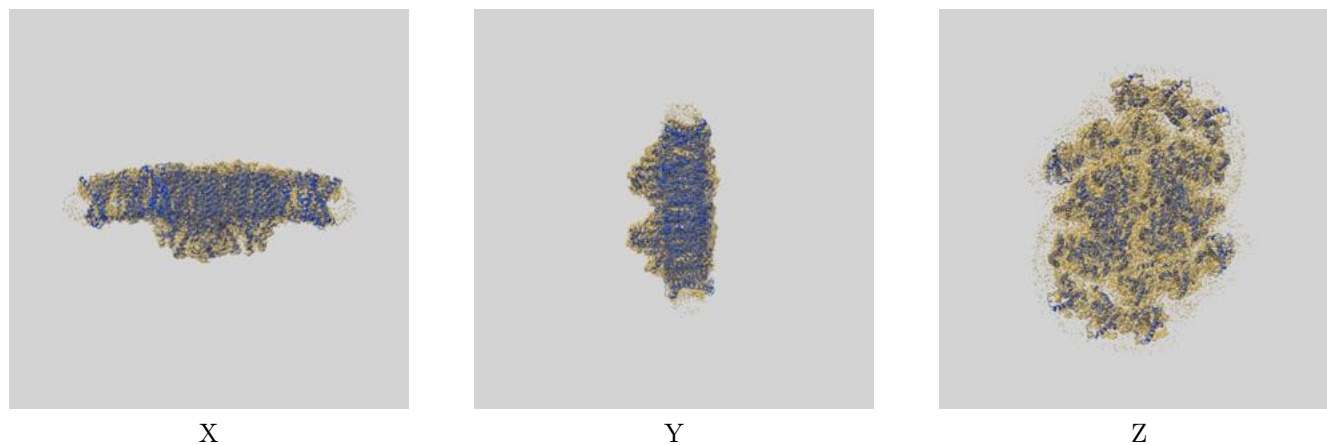
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	2.17	2.72	2.26
Unmasked-calculated*	3.51	7.23	3.67

\*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 3.51 differs from the reported value 2.17 by more than 10 %

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

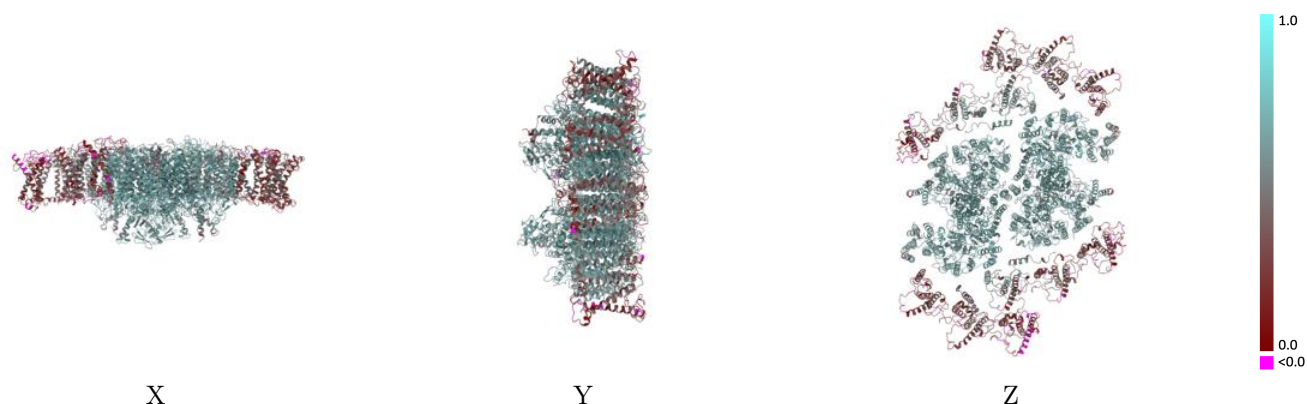
This section contains information regarding the fit between EMDB map EMD-62846 and PDB model 9L5V. Per-residue inclusion information can be found in section [3](#) on page [41](#).

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



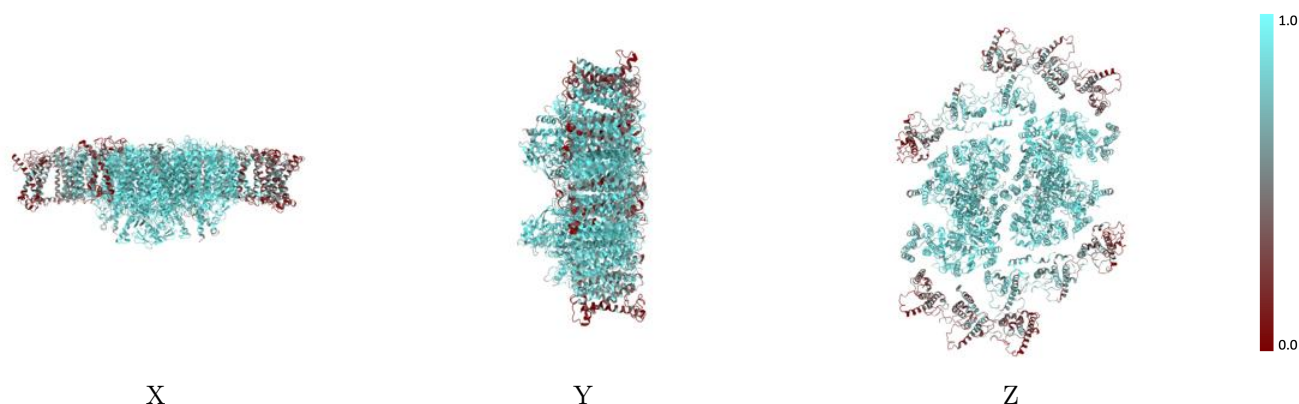
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



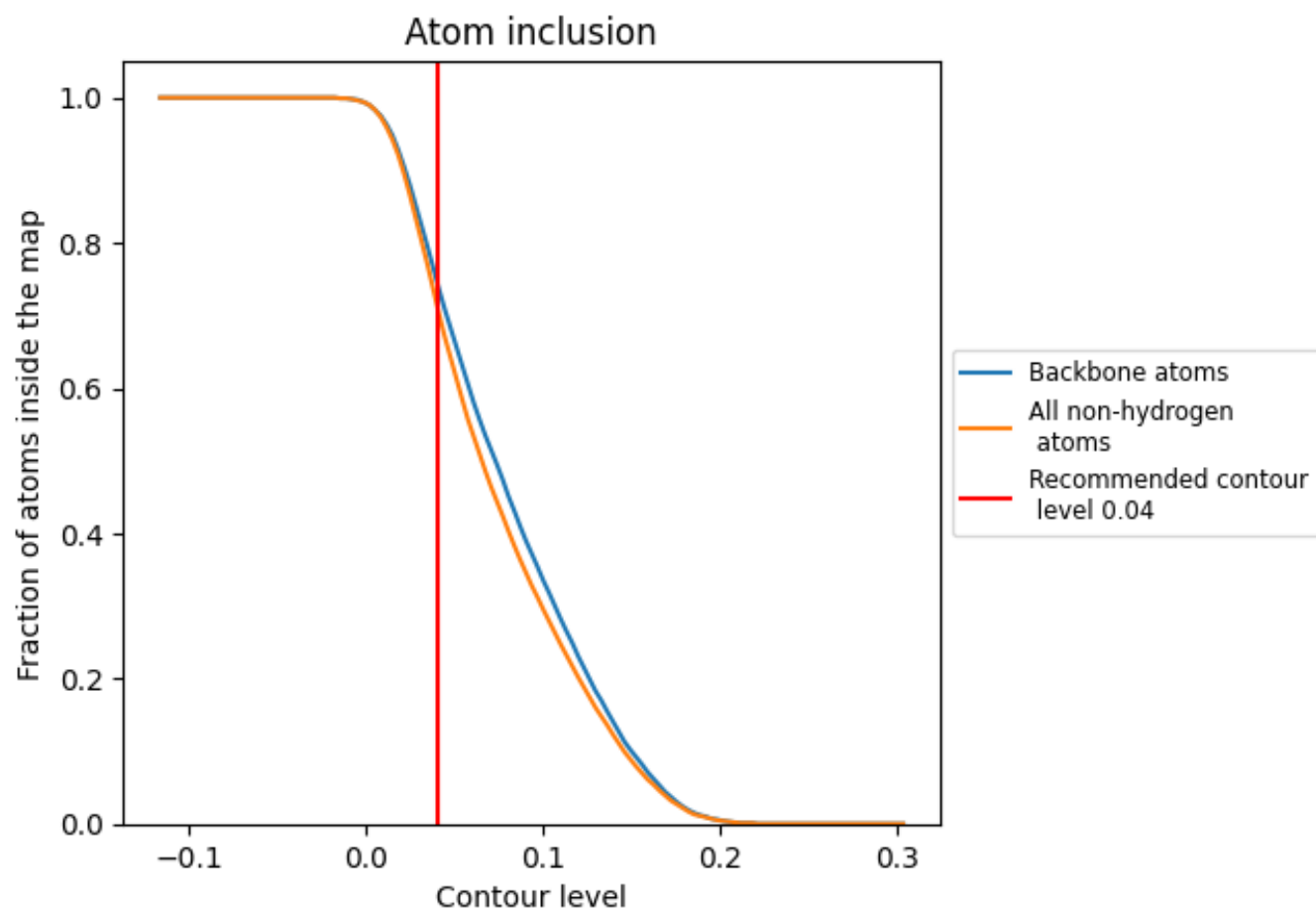
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (0.04) and Q-score for the entire model and for each chain.

























Chain	Atom inclusion	Q-score
All	 0.7150	 0.5040
1	 0.2870	 0.2650
2	 0.6190	 0.3710
3	 0.7070	 0.4300
4	 0.3100	 0.2220
5	 0.3450	 0.2950
6	 0.2880	 0.2460
A	 0.9230	 0.6450
B	 0.9300	 0.6430
C	 0.8890	 0.6090
D	 0.9250	 0.6420
E	 0.7920	 0.5590
F	 0.7880	 0.5400
G	 0.6010	 0.4290
H	 0.9420	 0.6420
I	 0.9710	 0.6660
K	 0.8900	 0.6090
L	 0.9480	 0.6420
M	 0.8310	 0.6070
N	 0.2850	 0.2380
O	 0.7210	 0.4800
P	 0.7860	 0.5300
Q	 0.4000	 0.3430
R	 0.3820	 0.3370
S	 0.2910	 0.2520
T	 0.8830	 0.6370
W	 0.9120	 0.6400
X	 0.8830	 0.6240
Y	 0.6410	 0.5270
Z	 0.6820	 0.5240
a	 0.9040	 0.6330
b	 0.9240	 0.6350
c	 0.8840	 0.6080
d	 0.9310	 0.6470
e	 0.7980	 0.5510



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
f	 0.7860	 0.5430
g	 0.5930	 0.3990
h	 0.9230	 0.6210
i	 0.9790	 0.6720
k	 0.8550	 0.6000
l	 0.9650	 0.6580
m	 0.8250	 0.6040
t	 0.8910	 0.6410
w	 0.9290	 0.6520
x	 0.8750	 0.6250
y	 0.6540	 0.5320
z	 0.6410	 0.4730