



## wwPDB EM Validation Summary Report ⓘ

Dec 24, 2024 – 12:43 PM JST

PDB ID : 8XR6  
EMDB ID : EMD-38596  
Title : Cryo-EM structure of cryptophyte photosystem II  
Authors : Li, K.; Zhao, L.S.; Zhang, Y.Z.; Liu, L.N.  
Deposited on : 2024-01-06  
Resolution : 2.53 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

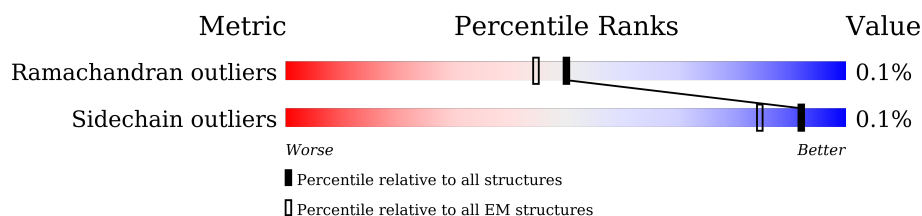
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.53 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.





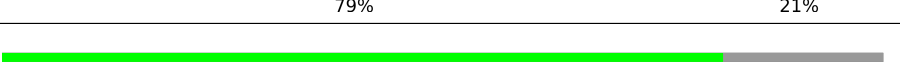
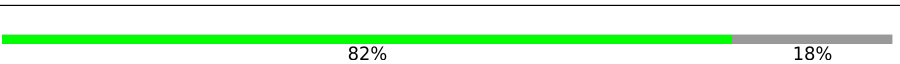
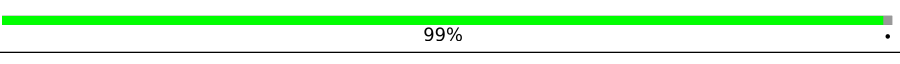
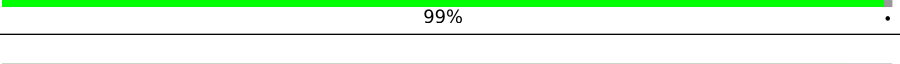
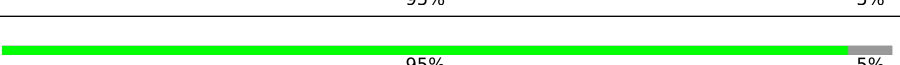
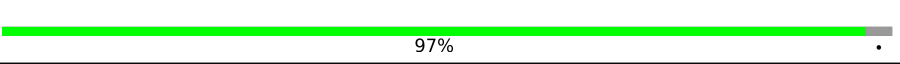
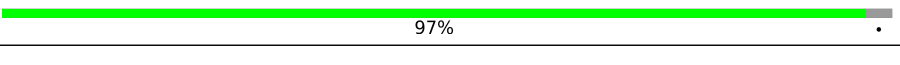
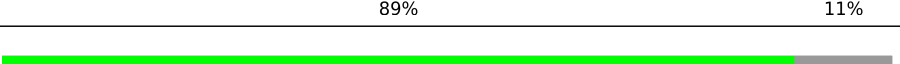


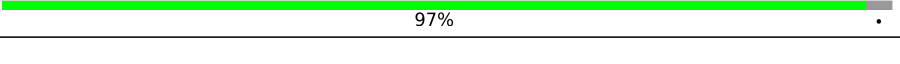
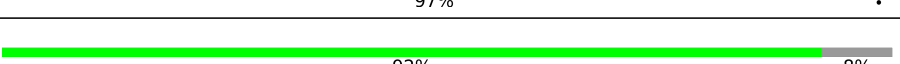
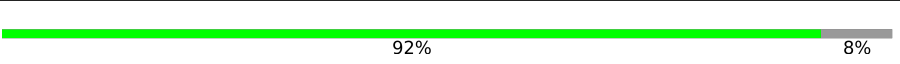
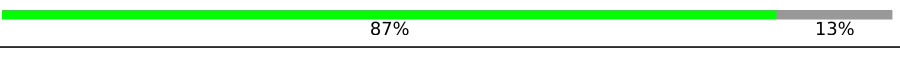

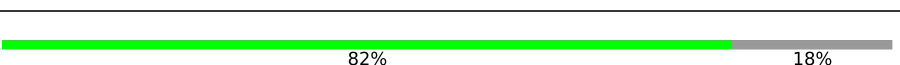
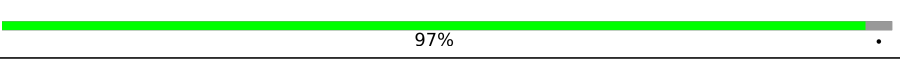
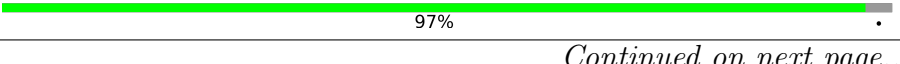



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	360	 93% 7%
1	a	360	 92% 7%
2	0	219	 80% 19%
2	4	219	 80% 19%
3	1	218	 80% 20%
3	7	218	 80% 20%
4	2	200	 94% 6%
4	8	200	 94% 6%
5	3	229	 80% 19%


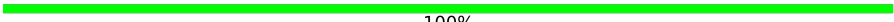




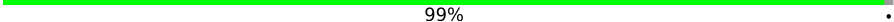
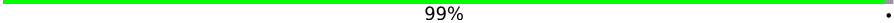
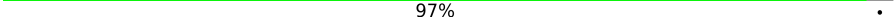
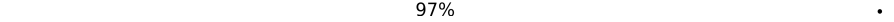






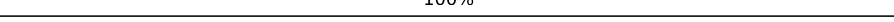
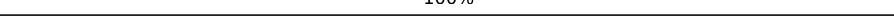
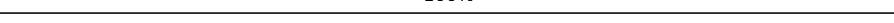



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Mol	Chain	Length	Quality of chain
5	9	229	
6	5	216	
6	g	216	
7	6	234	
7	p	234	
8	B	509	
8	b	509	
9	C	473	
9	c	473	
10	D	351	
10	d	351	
11	E	84	
11	e	84	
12	F	42	
12	f	42	
13	H	67	
13	h	67	
14	I	38	
14	i	38	
15	J	39	
15	j	39	
16	K	45	
16	k	45	
17	L	38	
17	l	38	

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Mol	Chain	Length	Quality of chain
18	M	37	 100%
18	m	37	 100%
19	N	297	 64% 36%
19	n	297	 64% 36%
20	O	300	 5% 87% 13%
20	o	300	 5% 87% 13%
21	Q	144	 10% 99%
21	q	144	 12% 99%
22	T	32	 97%
22	t	32	 97%
23	U	121	 77% 23%
23	u	121	 77% 23%
24	V	163	 84% 16%
24	v	163	 84% 16%
25	W	130	 38% 62%
25	w	130	 38% 62%
26	X	39	 100%
26	x	39	 100%
27	Y	34	 100%
27	y	34	 100%
28	Z	62	 98%
28	z	62	 98%

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
33	CLA	0	301	X	-	-	-
33	CLA	0	302	X	-	-	-
33	CLA	0	303	X	-	-	-
33	CLA	0	304	X	-	-	-
33	CLA	0	306	X	-	-	-
33	CLA	0	307	X	-	-	-
33	CLA	0	308	X	-	-	-
33	CLA	0	309	X	-	-	-
33	CLA	0	310	X	-	-	-
33	CLA	0	311	X	-	-	-
33	CLA	1	301	X	-	-	-
33	CLA	1	302	X	-	-	-
33	CLA	1	303	X	-	-	-
33	CLA	1	304	X	-	-	-
33	CLA	1	305	X	-	-	-
33	CLA	1	306	X	-	-	-
33	CLA	1	307	X	-	-	-
33	CLA	1	308	X	-	-	-
33	CLA	1	309	X	-	-	-
33	CLA	2	301	X	-	-	-
33	CLA	2	302	X	-	-	-
33	CLA	2	303	X	-	-	-
33	CLA	2	304	X	-	-	-
33	CLA	2	305	X	-	-	-
33	CLA	2	306	X	-	-	-
33	CLA	2	307	X	-	-	-
33	CLA	2	308	X	-	-	-
33	CLA	2	310	X	-	-	-
33	CLA	3	303	X	-	-	-
33	CLA	3	304	X	-	-	-
33	CLA	3	305	X	-	-	-
33	CLA	3	306	X	-	-	-
33	CLA	3	307	X	-	-	-
33	CLA	3	308	X	-	-	-
33	CLA	3	309	X	-	-	-
33	CLA	3	310	X	-	-	-
33	CLA	3	312	X	-	-	-
33	CLA	3	313	X	-	-	-
33	CLA	3	314	X	-	-	-
33	CLA	3	315	X	-	-	-
33	CLA	4	301	X	-	-	-
33	CLA	4	302	X	-	-	-
33	CLA	4	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	4	304	X	-	-	-
33	CLA	4	306	X	-	-	-
33	CLA	4	307	X	-	-	-
33	CLA	4	308	X	-	-	-
33	CLA	4	309	X	-	-	-
33	CLA	4	310	X	-	-	-
33	CLA	5	301	X	-	-	-
33	CLA	5	302	X	-	-	-
33	CLA	5	303	X	-	-	-
33	CLA	5	304	X	-	-	-
33	CLA	5	305	X	-	-	-
33	CLA	5	306	X	-	-	-
33	CLA	5	307	X	-	-	-
33	CLA	5	308	X	-	-	-
33	CLA	5	310	X	-	-	-
33	CLA	5	311	X	-	-	-
33	CLA	5	317	X	-	-	-
33	CLA	6	302	X	-	-	-
33	CLA	6	303	X	-	-	-
33	CLA	6	304	X	-	-	-
33	CLA	6	305	X	-	-	-
33	CLA	6	306	X	-	-	-
33	CLA	6	307	X	-	-	-
33	CLA	6	308	X	-	-	-
33	CLA	6	309	X	-	-	-
33	CLA	6	310	X	-	-	-
33	CLA	6	312	X	-	-	-
33	CLA	6	313	X	-	-	-
33	CLA	6	319	X	-	-	-
33	CLA	7	301	X	-	-	-
33	CLA	7	302	X	-	-	-
33	CLA	7	303	X	-	-	-
33	CLA	7	304	X	-	-	-
33	CLA	7	305	X	-	-	-
33	CLA	7	306	X	-	-	-
33	CLA	7	307	X	-	-	-
33	CLA	7	308	X	-	-	-
33	CLA	7	309	X	-	-	-
33	CLA	8	301	X	-	-	-
33	CLA	8	302	X	-	-	-
33	CLA	8	303	X	-	-	-
33	CLA	8	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	8	305	X	-	-	-
33	CLA	8	306	X	-	-	-
33	CLA	8	307	X	-	-	-
33	CLA	8	308	X	-	-	-
33	CLA	8	310	X	-	-	-
33	CLA	9	303	X	-	-	-
33	CLA	9	304	X	-	-	-
33	CLA	9	305	X	-	-	-
33	CLA	9	306	X	-	-	-
33	CLA	9	307	X	-	-	-
33	CLA	9	308	X	-	-	-
33	CLA	9	309	X	-	-	-
33	CLA	9	310	X	-	-	-
33	CLA	9	312	X	-	-	-
33	CLA	9	313	X	-	-	-
33	CLA	9	314	X	-	-	-
33	CLA	9	315	X	-	-	-
33	CLA	A	405	X	-	-	-
33	CLA	A	406	X	-	-	-
33	CLA	A	408	X	-	-	-
33	CLA	A	412	X	-	-	-
33	CLA	B	602	X	-	-	-
33	CLA	B	603	X	-	-	-
33	CLA	B	604	X	-	-	-
33	CLA	B	605	X	-	-	-
33	CLA	B	606	X	-	-	-
33	CLA	B	607	X	-	-	-
33	CLA	B	608	X	-	-	-
33	CLA	B	609	X	-	-	-
33	CLA	B	610	X	-	-	-
33	CLA	B	611	X	-	-	-
33	CLA	B	612	X	-	-	-
33	CLA	B	613	X	-	-	-
33	CLA	B	614	X	-	-	-
33	CLA	B	615	X	-	-	-
33	CLA	B	616	X	-	-	-
33	CLA	B	617	X	-	-	-
33	CLA	B	618	X	-	-	-
33	CLA	C	502	X	-	-	-
33	CLA	C	503	X	-	-	-
33	CLA	C	504	X	-	-	-
33	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	C	506	X	-	-	-
33	CLA	C	507	X	-	-	-
33	CLA	C	508	X	-	-	-
33	CLA	C	509	X	-	-	-
33	CLA	C	510	X	-	-	-
33	CLA	C	511	X	-	-	-
33	CLA	C	512	X	-	-	-
33	CLA	C	513	X	-	-	-
33	CLA	C	514	X	-	-	-
33	CLA	D	404	X	-	-	-
33	CLA	D	405	X	-	-	-
33	CLA	N	301	X	-	-	-
33	CLA	N	302	X	-	-	-
33	CLA	N	303	X	-	-	-
33	CLA	N	304	X	-	-	-
33	CLA	N	305	X	-	-	-
33	CLA	N	306	X	-	-	-
33	CLA	N	307	X	-	-	-
33	CLA	a	405	X	-	-	-
33	CLA	a	406	X	-	-	-
33	CLA	a	408	X	-	-	-
33	CLA	a	412	X	-	-	-
33	CLA	b	602	X	-	-	-
33	CLA	b	603	X	-	-	-
33	CLA	b	604	X	-	-	-
33	CLA	b	605	X	-	-	-
33	CLA	b	606	X	-	-	-
33	CLA	b	607	X	-	-	-
33	CLA	b	608	X	-	-	-
33	CLA	b	609	X	-	-	-
33	CLA	b	610	X	-	-	-
33	CLA	b	611	X	-	-	-
33	CLA	b	612	X	-	-	-
33	CLA	b	613	X	-	-	-
33	CLA	b	614	X	-	-	-
33	CLA	b	615	X	-	-	-
33	CLA	b	616	X	-	-	-
33	CLA	b	617	X	-	-	-
33	CLA	b	618	X	-	-	-
33	CLA	c	502	X	-	-	-
33	CLA	c	503	X	-	-	-
33	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CLA	c	505	X	-	-	-
33	CLA	c	506	X	-	-	-
33	CLA	c	507	X	-	-	-
33	CLA	c	508	X	-	-	-
33	CLA	c	509	X	-	-	-
33	CLA	c	510	X	-	-	-
33	CLA	c	511	X	-	-	-
33	CLA	c	512	X	-	-	-
33	CLA	c	513	X	-	-	-
33	CLA	c	514	X	-	-	-
33	CLA	d	404	X	-	-	-
33	CLA	d	405	X	-	-	-
33	CLA	g	301	X	-	-	-
33	CLA	g	302	X	-	-	-
33	CLA	g	303	X	-	-	-
33	CLA	g	304	X	-	-	-
33	CLA	g	305	X	-	-	-
33	CLA	g	306	X	-	-	-
33	CLA	g	307	X	-	-	-
33	CLA	g	308	X	-	-	-
33	CLA	g	310	X	-	-	-
33	CLA	g	311	X	-	-	-
33	CLA	g	317	X	-	-	-
33	CLA	n	301	X	-	-	-
33	CLA	n	302	X	-	-	-
33	CLA	n	303	X	-	-	-
33	CLA	n	304	X	-	-	-
33	CLA	n	305	X	-	-	-
33	CLA	n	306	X	-	-	-
33	CLA	p	302	X	-	-	-
33	CLA	p	303	X	-	-	-
33	CLA	p	304	X	-	-	-
33	CLA	p	305	X	-	-	-
33	CLA	p	306	X	-	-	-
33	CLA	p	307	X	-	-	-
33	CLA	p	308	X	-	-	-
33	CLA	p	309	X	-	-	-
33	CLA	p	310	X	-	-	-
33	CLA	p	312	X	-	-	-
33	CLA	p	313	X	-	-	-
33	CLA	p	319	X	-	-	-

## 2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 82310 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	334	Total	C	N	O	S	0	0
			2617	1712	430	463	12		
1	A	334	Total	C	N	O	S	0	0
			2617	1712	430	463	12		

- Molecule 2 is a protein called ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	177	Total	C	N	O	S	0	0
			1365	882	229	245	9		
2	4	177	Total	C	N	O	S	0	0
			1365	882	229	245	9		

- Molecule 3 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	175	Total	C	N	O	S	0	0
			1360	886	223	243	8		
3	7	175	Total	C	N	O	S	0	0
			1360	886	223	243	8		

- Molecule 4 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	187	Total	C	N	O	S	0	0
			1469	955	243	266	5		
4	8	187	Total	C	N	O	S	0	0
			1469	955	243	266	5		

- Molecule 5 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	185	Total	C	N	O	S	0	0
			1400	904	240	247	9		
5	9	185	Total	C	N	O	S	0	0
			1400	904	240	247	9		

- Molecule 6 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	170	Total	C	N	O	S	0	0
			1339	885	218	233	3		
6	g	170	Total	C	N	O	S	0	0
			1339	885	218	233	3		

- Molecule 7 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	192	Total	C	N	O	S	0	0
			1455	933	254	260	8		
7	p	192	Total	C	N	O	S	0	0
			1455	933	254	260	8		

- Molecule 8 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	503	Total	C	N	O	S	0	0
			3953	2581	674	687	11		
8	b	503	Total	C	N	O	S	0	0
			3953	2581	674	687	11		

- Molecule 9 is a protein called PsbC\_CP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	451	Total	C	N	O	S	0	0
			3503	2290	589	614	10		
9	c	451	Total	C	N	O	S	0	0
			3503	2290	589	614	10		

- Molecule 10 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	342	Total	C	N	O	S	0	0
			2713	1794	444	463	12		

- Molecule 11 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	75	Total	C	N	O		0	0
			616	402	102	112			
11	e	75	Total	C	N	O		0	0
			616	402	102	112			

- Molecule 12 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	29	Total	C	N	O	S	0	0
			235	159	40	35	1		
12	f	29	Total	C	N	O	S	0	0
			235	159	40	35	1		

- Molecule 13 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	65	Total	C	N	O	S	0	0
			515	344	81	88	2		
13	h	65	Total	C	N	O	S	0	0
			515	344	81	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	35	Total	C	N	O	S	0	0
			287	191	46	49	1		
14	i	35	Total	C	N	O	S	0	0
			287	191	46	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	34	Total	C	N	O		0	0
			249	168	38	43			
15	j	34	Total	C	N	O		0	0
			249	168	38	43			



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

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

- Molecule 17 is a protein called Photosystem II reaction center protein L.

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

- Molecule 18 is a protein called PsbM.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	37	Total	C	N	O	S	0	0
			276	182	43	50	1		
18	m	37	Total	C	N	O	S	0	0
			276	182	43	50	1		

- Molecule 19 is a protein called Psb-gama\_linker.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	190	Total	C	N	O	S	0	0
			1474	954	234	283	3		
19	n	190	Total	C	N	O	S	0	0
			1474	954	234	283	3		

- Molecule 20 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	262	Total	C	N	O	S	0	0
			1993	1253	326	408	6		
20	o	262	Total	C	N	O	S	0	0
			1993	1253	326	408	6		

- Molecule 21 is a protein called PsbQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	143	Total	C	N	O	S	0	0
			1102	698	190	211	3		
21	q	143	Total	C	N	O	S	0	0
			1102	698	190	211	3		

- Molecule 22 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	31	Total	C	N	O	S	0	0
			250	173	38	38	1		
22	t	31	Total	C	N	O	S	0	0
			250	173	38	38	1		

- Molecule 23 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	93	Total	C	N	O	S	0	0
			741	476	122	141	2		
23	u	93	Total	C	N	O	S	0	0
			741	476	122	141	2		

- Molecule 24 is a protein called Photosystem II cytochrome c550.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	137	Total	C	N	O	S	0	0
			1043	653	177	209	4		
24	v	137	Total	C	N	O	S	0	0
			1043	653	177	209	4		

- Molecule 25 is a protein called PsbW.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	49	Total	C	N	O	0	0
			391	251	61	79		
25	w	49	Total	C	N	O	0	0
			391	251	61	79		

- Molecule 26 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	39	Total	C	N	O	S	0	0
			291	192	47	51	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	x	39	Total	C	N	O	S	0	0
			291	192	47	51	1		

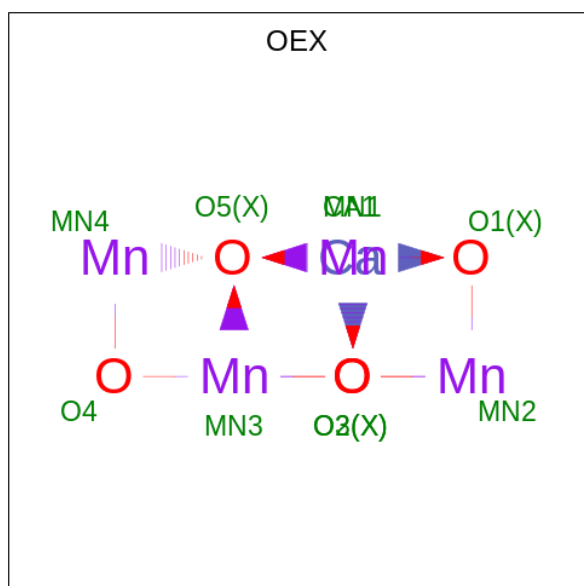
- Molecule 27 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	34	Total	C	N	O	S	0	0
			265	180	43	41	1		
27	y	34	Total	C	N	O	S	0	0
			265	180	43	41	1		

- Molecule 28 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		
28	z	61	Total	C	N	O	S	0	0
			457	315	67	74	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).

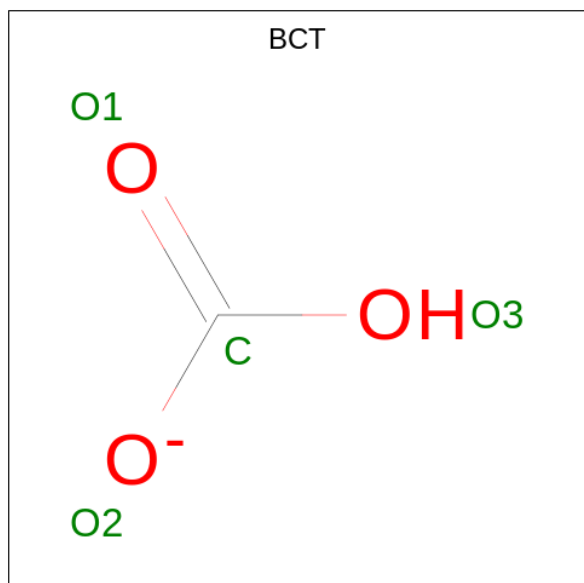


Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	Ca	Mn	O	0
			10	1	4	5	
29	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 30 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).

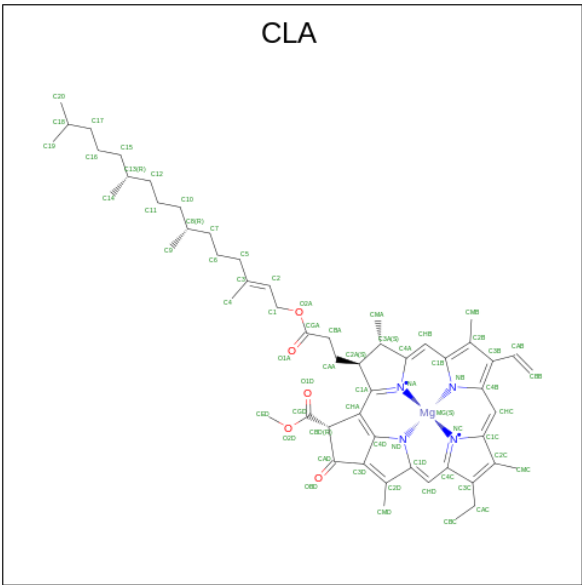


Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			4	1	3	
31	A	1	Total	C	O	0
			4	1	3	

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total	Cl	0
			1	1	
32	A	1	Total	Cl	0
			1	1	

- Molecule 33 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	0	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
33	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
33	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	0	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	1	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	2	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
33	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	3	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	3	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	4	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	4	1	Total 40	C 32	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
33	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
33	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
33	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
33	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	7	1	Total 64	C 54	Mg 1	N 4	O 5	0
33	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
33	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
33	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	8	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	9	1	Total 49	C 39	Mg 1	N 4	O 5	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	B	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	C	1	Total 56	C 46	Mg 1	N 4	O 5	0
33	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	N	1	Total 47	C 37	Mg 1	N 4	O 5	0
33	N	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
33	b	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	c	1	Total 56	C 46	Mg 1	N 4	O 5	0
33	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	g	1	Total 42	C 34	Mg 1	N 4	O 3	0

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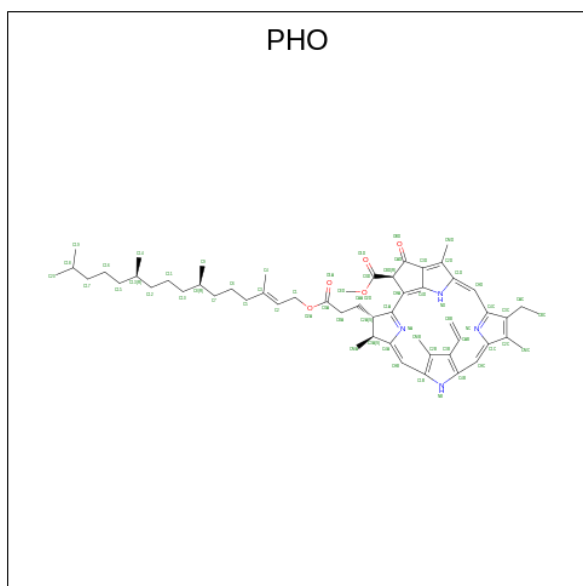
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	g	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	g	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	g	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
33	g	1	Total 40	C 32	Mg 1	N 4	O 3	0
33	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
33	n	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	n	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	n	1	Total 50	C 40	Mg 1	N 4	O 5	0
33	p	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	p	1	Total 41	C 33	Mg 1	N 4	O 3	0
33	p	1	Total 42	C 34	Mg 1	N 4	O 3	0
33	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
33	p	1	Total 45	C 35	Mg 1	N 4	O 5	0

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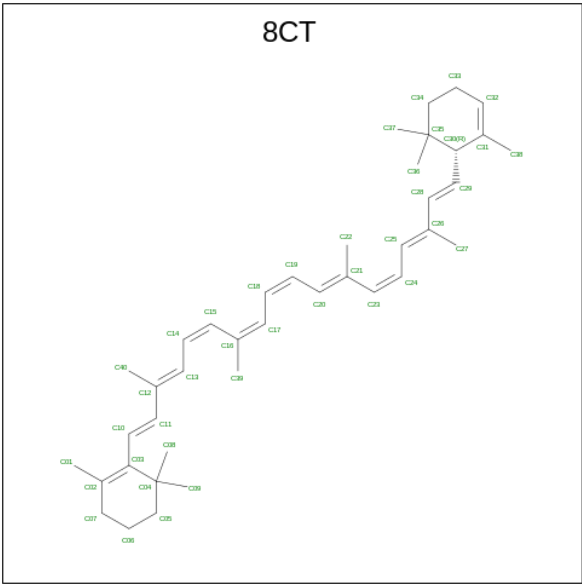
Mol	Chain	Residues	Atoms					AltConf
33	p	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
33	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 34 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 35 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	AltConf
35	a	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	0	1	Total C 40 40	0
35	1	1	Total C 40 40	0
35	4	1	Total C 40 40	0
35	7	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	C	1	Total C 40 40	0
35	C	1	Total C 40 40	0
35	C	1	Total C 40 40	0

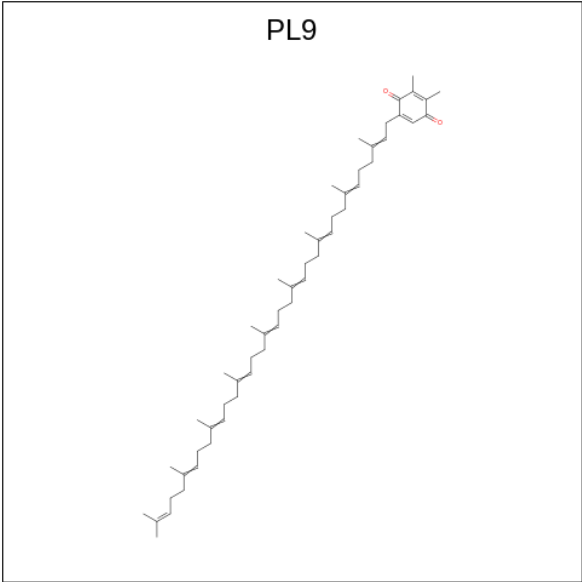
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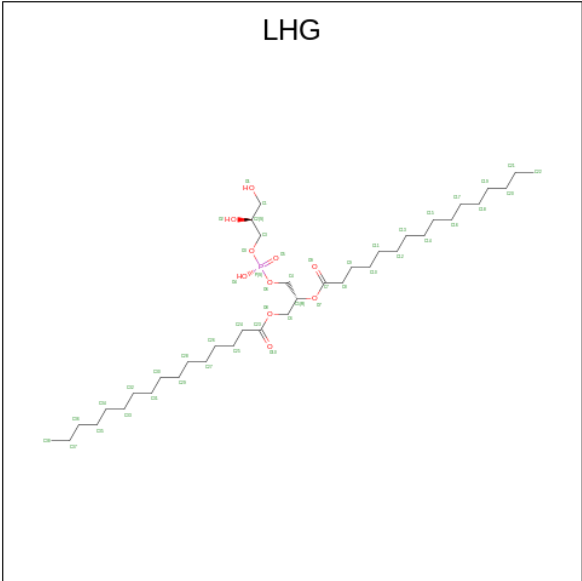
Mol	Chain	Residues	Atoms	AltConf
35	D	1	Total C 40 40	0
35	H	1	Total C 40 40	0
35	Y	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	b	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	c	1	Total C 40 40	0
35	d	1	Total C 40 40	0
35	h	1	Total C 40 40	0
35	y	1	Total C 40 40	0

- Molecule 36 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 (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	O	0
			30	28	2	
36	A	1	Total	C	O	0
			30	28	2	
36	D	1	Total	C	O	0
			55	53	2	
36	d	1	Total	C	O	0
			55	53	2	

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



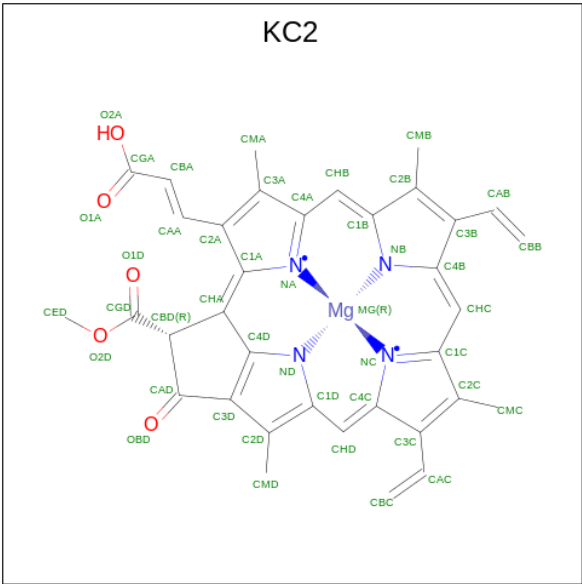
Mol	Chain	Residues	Atoms				AltConf
37	a	1	Total 24	C 13	O 10	P 1	0
37	A	1	Total 24	C 13	O 10	P 1	0
37	0	1	Total 24	C 13	O 10	P 1	0
37	1	1	Total 49	C 38	O 10	P 1	0
37	2	1	Total 46	C 35	O 10	P 1	0
37	3	1	Total 41	C 30	O 10	P 1	0
37	3	1	Total 24	C 13	O 10	P 1	0
37	3	1	Total 41	C 30	O 10	P 1	0
37	4	1	Total 24	C 13	O 10	P 1	0
37	5	1	Total 22	C 12	O 9	P 1	0
37	7	1	Total 49	C 38	O 10	P 1	0
37	8	1	Total 46	C 35	O 10	P 1	0
37	9	1	Total 41	C 30	O 10	P 1	0
37	9	1	Total 24	C 13	O 10	P 1	0
37	9	1	Total 41	C 30	O 10	P 1	0
37	B	1	Total 49	C 38	O 10	P 1	0
37	D	1	Total 46	C 35	O 10	P 1	0
37	D	1	Total 47	C 36	O 10	P 1	0
37	D	1	Total 49	C 38	O 10	P 1	0
37	b	1	Total 49	C 38	O 10	P 1	0
37	d	1	Total 46	C 35	O 10	P 1	0
37	d	1	Total 47	C 36	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
37	d	1	Total	C	O	P	0
			49	38	10	1	
37	g	1	Total	C	O	P	0
			22	12	9	1	

- Molecule 38 is Chlorophyll c2 (three-letter code: KC2) (formula: C<sub>35</sub>H<sub>28</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



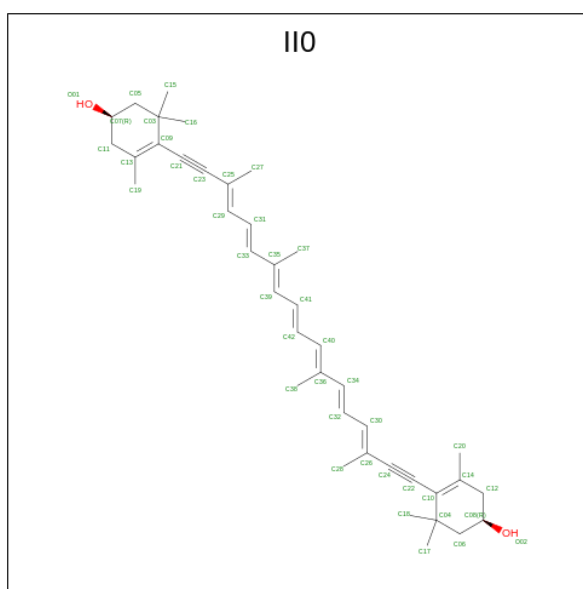
Mol	Chain	Residues	Atoms					AltConf
38	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
38	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	g	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	

- 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 (three-letter code: II0) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>2</sub>).



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

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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	1	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	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
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

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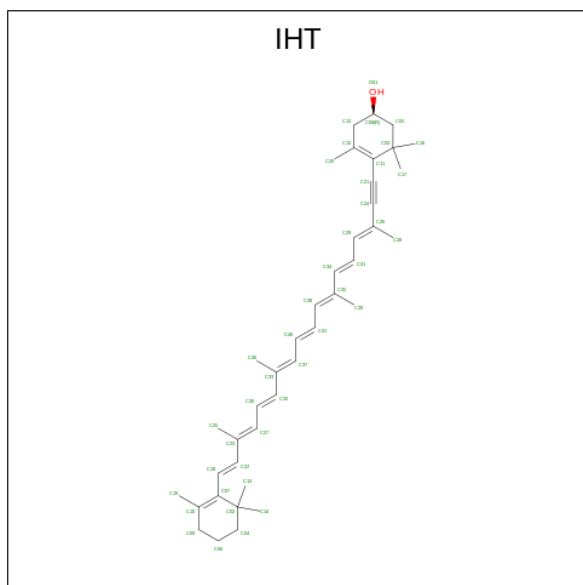
Mol	Chain	Residues	Atoms			AltConf
39	6	1	Total	C	O	0
			42	40	2	
39	6	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	7	1	Total	C	O	0
			42	40	2	
39	8	1	Total	C	O	0
			42	40	2	
39	8	1	Total	C	O	0
			42	40	2	
39	8	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	g	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	
39	p	1	Total	C	O	0
			42	40	2	

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

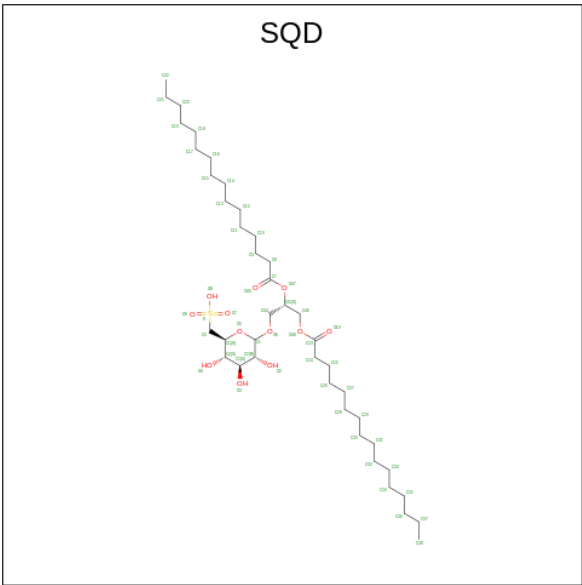
- Molecule 40 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: IHT) (formula: C<sub>40</sub>H<sub>54</sub>O).



Mol	Chain	Residues	Atoms			AltConf
40	2	1	Total	C	O	0
			41	40	1	
40	3	1	Total	C	O	0
			41	40	1	
40	5	1	Total	C	O	0
			41	40	1	
40	6	1	Total	C	O	0
			41	40	1	
40	8	1	Total	C	O	0
			41	40	1	
40	9	1	Total	C	O	0
			41	40	1	
40	g	1	Total	C	O	0
			41	40	1	
40	p	1	Total	C	O	0
			41	40	1	

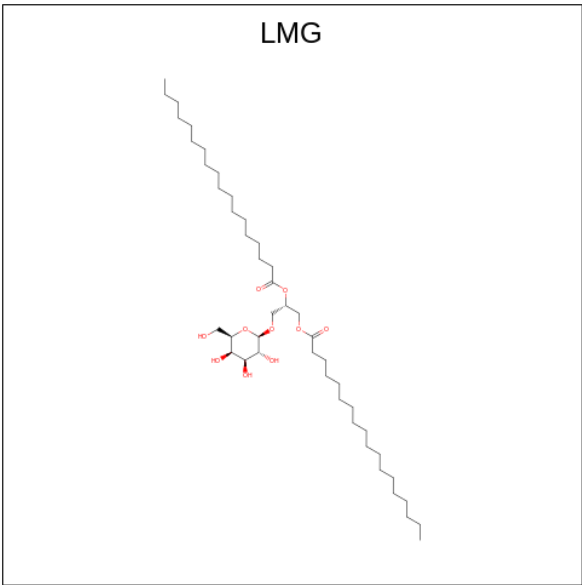
- Molecule 41 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).





Mol	Chain	Residues	Atoms				AltConf
41	B	1	Total	C	O	S	0
			38	25	12	1	
41	C	1	Total	C	O	S	0
			42	29	12	1	
41	J	1	Total	C	O	S	0
			46	33	12	1	
41	L	1	Total	C	O	S	0
			54	41	12	1	
41	b	1	Total	C	O	S	0
			38	25	12	1	
41	c	1	Total	C	O	S	0
			42	29	12	1	
41	j	1	Total	C	O	S	0
			46	33	12	1	
41	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



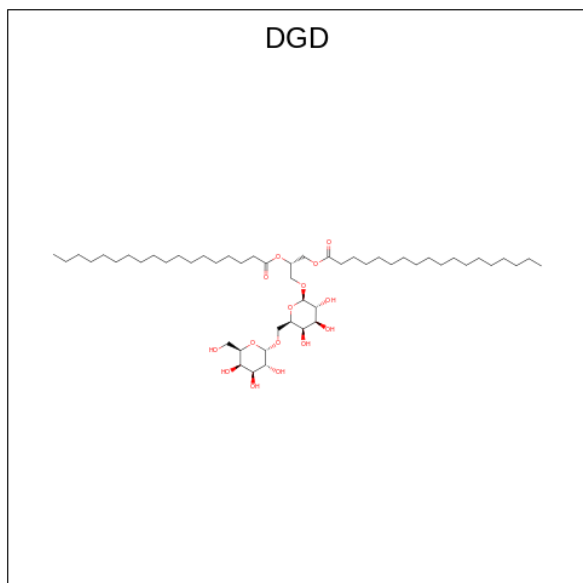
Mol	Chain	Residues	Atoms			AltConf
42	B	1	Total	C	O	0
			49	39	10	
42	B	1	Total	C	O	0
			43	33	10	
42	C	1	Total	C	O	0
			51	41	10	
42	D	1	Total	C	O	0
			46	36	10	
42	D	1	Total	C	O	0
			46	36	10	
42	T	1	Total	C	O	0
			43	33	10	
42	W	1	Total	C	O	0
			47	37	10	
42	b	1	Total	C	O	0
			49	39	10	
42	b	1	Total	C	O	0
			43	33	10	
42	c	1	Total	C	O	0
			51	41	10	
42	d	1	Total	C	O	0
			46	36	10	
42	d	1	Total	C	O	0
			46	36	10	
42	l	1	Total	C	O	0
			38	28	10	
42	m	1	Total	C	O	0
			38	28	10	

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Mol	Chain	Residues	Atoms			AltConf
42	t	1	Total	C	O	0
			43	33	10	
42	w	1	Total	C	O	0
			47	37	10	

- Molecule 43 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
43	C	1	Total	C	O	0
			55	40	15	
43	C	1	Total	C	O	0
			62	47	15	
43	C	1	Total	C	O	0
			62	47	15	
43	H	1	Total	C	O	0
			60	45	15	
43	c	1	Total	C	O	0
			55	40	15	
43	c	1	Total	C	O	0
			62	47	15	
43	c	1	Total	C	O	0
			62	47	15	
43	h	1	Total	C	O	0
			60	45	15	

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

# HEM

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

- | Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 45  | a     | 24       | Total O<br>24 24 | 0       |
| 45  | A     | 24       | Total O<br>24 24 | 0       |
| 45  | B     | 3        | Total O<br>3 3   | 0       |
| 45  | C     | 11       | Total O<br>11 11 | 0       |
| 45  | O     | 1        | Total O<br>1 1   | 0       |
| 45  | U     | 2        | Total O<br>2 2   | 0       |
| 45  | W     | 1        | Total O<br>1 1   | 0       |



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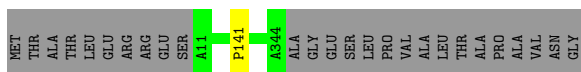
Mol	Chain	Residues	Atoms		AltConf
45	b	3	Total 3	O 3	0
45	c	11	Total 11	O 11	0
45	o	1	Total 1	O 1	0
45	u	2	Total 2	O 2	0
45	w	1	Total 1	O 1	0

### 3 Residue-property plots

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

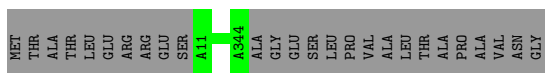
- Molecule 1: Photosystem II protein D1

Chain a: 




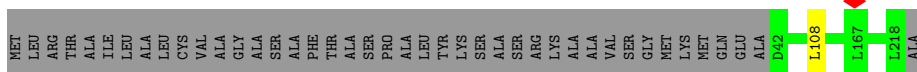
- Molecule 1: Photosystem II protein D1

Chain A: 




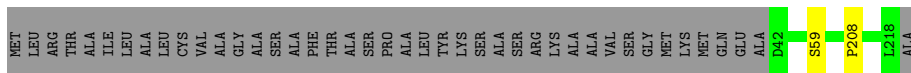
- Molecule 2: ACPII-4

Chain 0: 



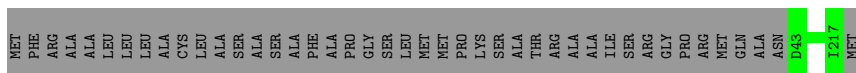
- Molecule 2: ACPII-4

Chain 4: 




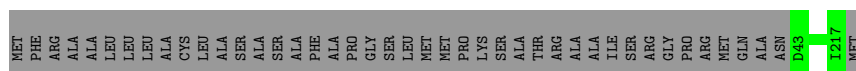
- Molecule 3: ACPII-1

Chain 1: 



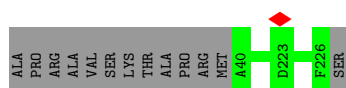
- Molecule 3: ACPII-1

Chain 7:  80% 20%



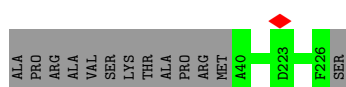
• Molecule 4: ACPII-2

Chain 2:  94% 6%



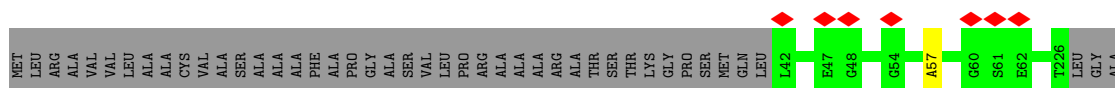
• Molecule 4: ACPII-2

Chain 8:  94% 6%




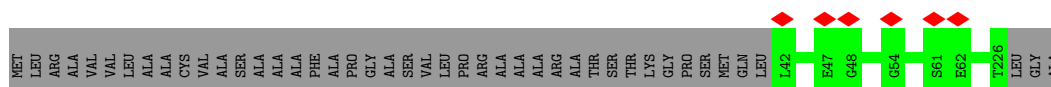
• Molecule 5: ACPII-3

Chain 3:  80% 19%




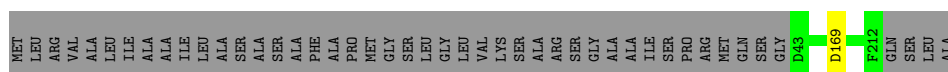
• Molecule 5: ACPII-3

Chain 9:  81% 19%




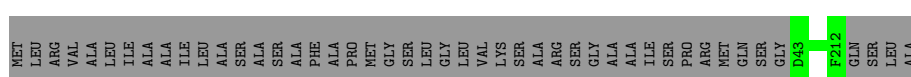
• Molecule 6: ACPII-5

Chain 5:  78% 21%




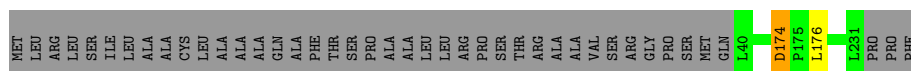
• Molecule 6: ACPII-5

Chain g:  79% 21%




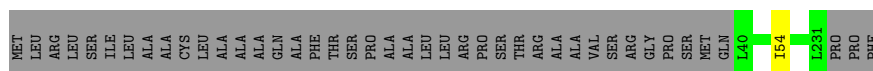
• Molecule 7: ACPII-6

Chain 6:  81% 18%



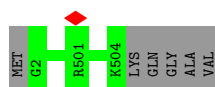
- Molecule 7: ACPII-6

Chain p:  82% 18%



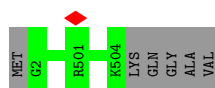
- Molecule 8: Photosystem II CP47 reaction center protein

Chain B:  99% .



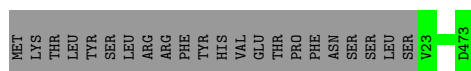
- Molecule 8: Photosystem II CP47 reaction center protein

Chain b:  99% .



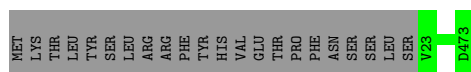
- Molecule 9: PsbC\_CP43

Chain C:  95% 5%



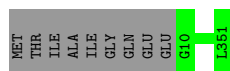
- Molecule 9: PsbC\_CP43

Chain c:  95% 5%



- Molecule 10: Photosystem II D2 protein

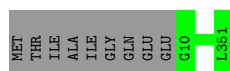
Chain D:  97% .




- Molecule 10: Photosystem II D2 protein

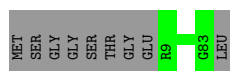


Chain d:  97% .




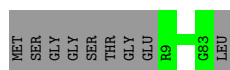
- Molecule 11: Cytochrome b559 subunit alpha

Chain E:  89% 11%



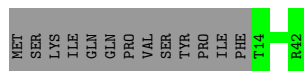
- Molecule 11: Cytochrome b559 subunit alpha

Chain e:  89% 11%



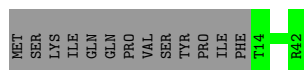
- Molecule 12: Cytochrome b559 subunit beta

Chain F:  69% 31%



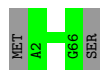
- Molecule 12: Cytochrome b559 subunit beta

Chain f:  69% 31%



- Molecule 13: Photosystem II reaction center protein H

Chain H:  97% .




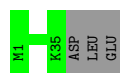
- Molecule 13: Photosystem II reaction center protein H

Chain h:  97% .



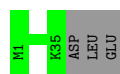
- Molecule 14: Photosystem II reaction center protein I

Chain I:  92% 8%




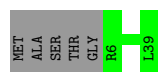
- Molecule 14: Photosystem II reaction center protein I

Chain i:  92% 8%




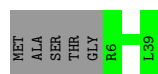
- Molecule 15: Photosystem II reaction center protein J

Chain J:  87% 13%




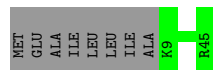
- Molecule 15: Photosystem II reaction center protein J

Chain j:  87% 13%




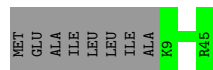
- Molecule 16: Photosystem II reaction center protein K

Chain K:  82% 18%



- Molecule 16: Photosystem II reaction center protein K

Chain k:  82% 18%



- Molecule 17: Photosystem II reaction center protein L

Chain L:  97% .



- Molecule 17: Photosystem II reaction center protein L

Chain l:  97%



- Molecule 18: PsbM

Chain M:  100%

There are no outlier residues recorded for this chain.

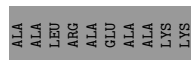
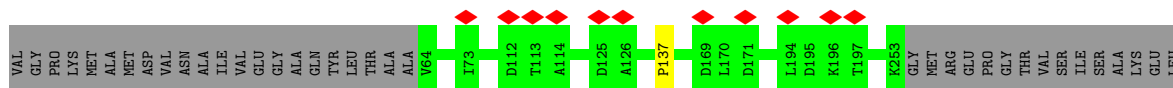
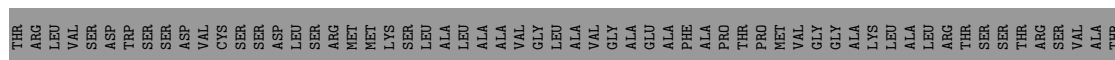
- Molecule 18: PsbM

Chain m:  100%

There are no outlier residues recorded for this chain.

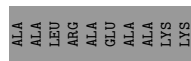
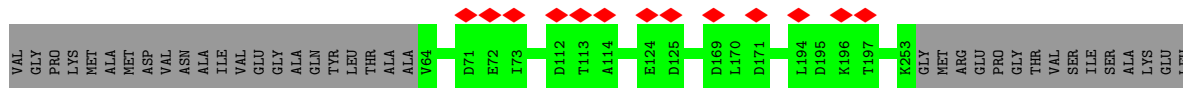
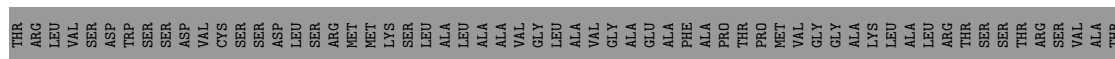
- Molecule 19: Psb-gama\_linker

Chain N:  64% 36%




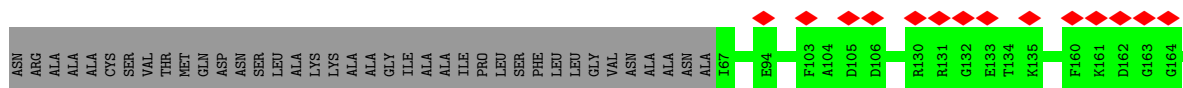
- Molecule 19: Psb-gama\_linker

Chain n:  64% 36%



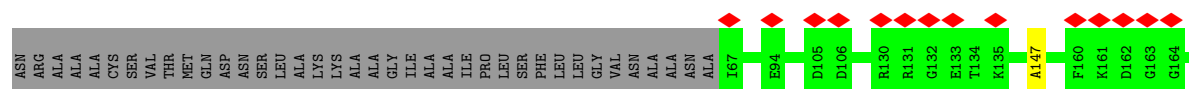
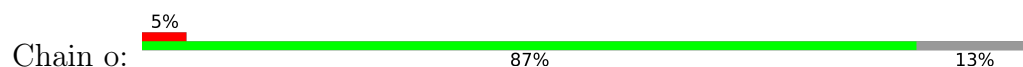
- Molecule 20: PsbO

Chain O:  5% 87% 13%

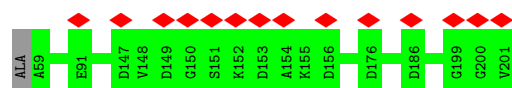




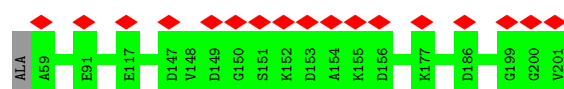
## • Molecule 20: PsbO



## • Molecule 21: PsbQ



## • Molecule 21: PsbQ



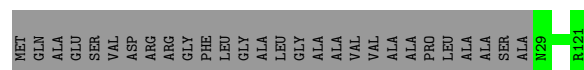
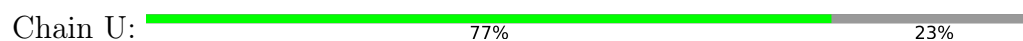
## • Molecule 22: Photosystem II reaction center protein T




## • Molecule 22: Photosystem II reaction center protein T

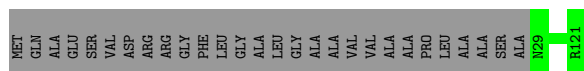


## • Molecule 23: PsbU




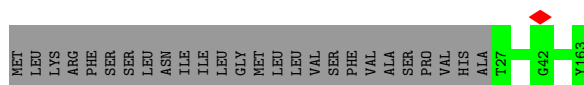
- Molecule 23: PsbU

Chain u:  77% 23%




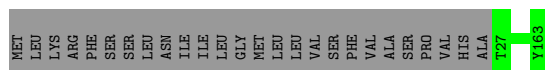
- Molecule 24: Photosystem II cytochrome c550

Chain V:  84% 16%



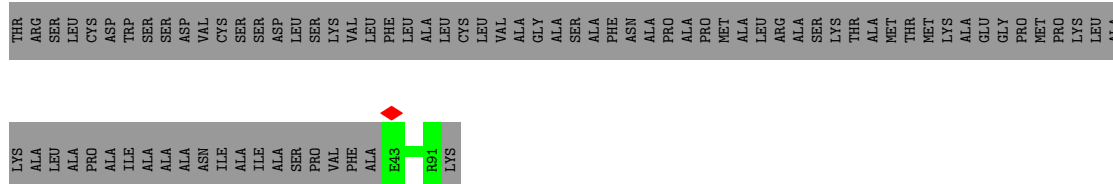
- Molecule 24: Photosystem II cytochrome c550

Chain v:  84% 16%



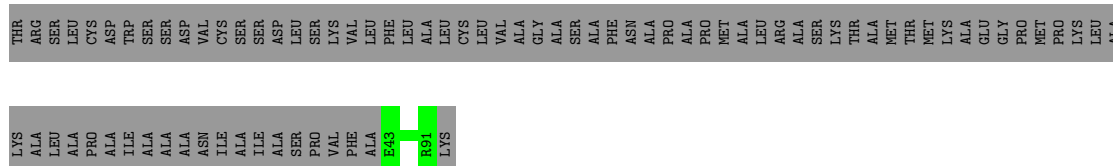
- Molecule 25: PsbW

Chain W:  38% 62%



- Molecule 25: PsbW

Chain w:  38% 62%



- Molecule 26: Photosystem II reaction center protein X

Chain X:  100%



- Molecule 26: Photosystem II reaction center protein X

Chain x:  100%



- Molecule 27: Photosystem II reaction center protein Psb30

Chain Y:  100%



- Molecule 27: Photosystem II reaction center protein Psb30

Chain y:  100%



- Molecule 28: Photosystem II reaction center protein Z

Chain Z:  98%



- Molecule 28: Photosystem II reaction center protein Z

Chain z:  98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	168683	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.868	Depositor
Minimum map value	0.000	Depositor
Average map value	0.088	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, FE2, HEM, OEX, CLA, II0, CL, PHO, 8CT, LHG, SQD, LMG, DGD, IHT, KC2, BCT

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	0.31	0/2701	0.54	0/3687
1	a	0.30	0/2701	0.55	0/3687
2	0	0.52	0/1398	0.77	0/1888
2	4	0.52	0/1398	0.73	0/1888
3	1	0.32	0/1396	0.58	0/1892
3	7	0.32	0/1396	0.58	0/1892
4	2	0.32	0/1508	0.57	0/2044
4	8	0.32	0/1508	0.57	0/2044
5	3	0.31	0/1434	0.58	0/1943
5	9	0.32	0/1434	0.61	0/1943
6	5	0.46	0/1376	0.60	0/1862
6	g	0.45	0/1376	0.58	0/1862
7	6	0.68	0/1487	0.86	0/2014
7	p	0.69	0/1487	0.82	0/2014
8	B	0.29	0/4084	0.56	0/5558
8	b	0.29	0/4084	0.56	0/5558
9	C	0.30	0/3618	0.53	0/4937
9	c	0.29	0/3618	0.53	0/4937
10	D	0.28	0/2806	0.53	0/3823
10	d	0.28	0/2806	0.53	0/3823
11	E	0.32	0/634	0.64	0/865
11	e	0.32	0/634	0.64	0/865
12	F	0.29	0/242	0.59	0/328
12	f	0.29	0/242	0.59	0/328
13	H	0.31	0/527	0.58	0/717
13	h	0.30	0/527	0.59	0/717
14	I	0.28	0/294	0.54	0/397
14	i	0.28	0/294	0.54	0/397
15	J	0.34	0/255	0.56	0/348
15	j	0.34	0/255	0.56	0/348
16	K	0.33	0/307	0.54	0/421
16	k	0.34	0/307	0.55	0/421



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	L	0.30	0/311	0.54	0/424
17	l	0.30	0/311	0.54	0/424
18	M	0.34	0/280	0.52	0/381
18	m	0.32	0/280	0.50	0/381
19	N	0.33	0/1516	0.65	0/2070
19	n	0.33	0/1516	0.64	0/2070
20	O	0.30	0/2024	0.58	0/2722
20	o	0.30	0/2024	0.59	0/2722
21	Q	0.28	0/1121	0.54	0/1508
21	q	0.28	0/1121	0.54	0/1508
22	T	0.30	0/257	0.54	0/348
22	t	0.30	0/257	0.54	0/348
23	U	0.29	0/757	0.55	0/1031
23	u	0.29	0/757	0.54	0/1031
24	V	0.27	0/1063	0.55	0/1443
24	v	0.27	0/1063	0.54	0/1443
25	W	0.31	0/398	0.56	0/541
25	w	0.31	0/398	0.56	0/541
26	X	0.29	0/295	0.61	0/402
26	x	0.29	0/295	0.61	0/402
27	Y	0.32	0/270	0.66	0/367
27	y	0.32	0/270	0.66	0/367
28	Z	0.28	0/467	0.45	0/638
28	z	0.28	0/467	0.45	0/638
All	All	0.35	0/65652	0.59	0/89198

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/360 (92%)	322 (97%)	10 (3%)	0	100	100
1	a	332/360 (92%)	322 (97%)	9 (3%)	1 (0%)	37	54
2	0	175/219 (80%)	167 (95%)	8 (5%)	0	100	100
2	4	175/219 (80%)	165 (94%)	9 (5%)	1 (1%)	22	37
3	1	173/218 (79%)	171 (99%)	2 (1%)	0	100	100
3	7	173/218 (79%)	171 (99%)	2 (1%)	0	100	100
4	2	185/200 (92%)	180 (97%)	5 (3%)	0	100	100
4	8	185/200 (92%)	181 (98%)	4 (2%)	0	100	100
5	3	183/229 (80%)	173 (94%)	9 (5%)	1 (0%)	25	42
5	9	183/229 (80%)	173 (94%)	10 (6%)	0	100	100
6	5	168/216 (78%)	164 (98%)	4 (2%)	0	100	100
6	g	168/216 (78%)	163 (97%)	5 (3%)	0	100	100
7	6	190/234 (81%)	181 (95%)	8 (4%)	1 (0%)	25	42
7	p	190/234 (81%)	183 (96%)	7 (4%)	0	100	100
8	B	501/509 (98%)	490 (98%)	11 (2%)	0	100	100
8	b	501/509 (98%)	488 (97%)	13 (3%)	0	100	100
9	C	449/473 (95%)	439 (98%)	10 (2%)	0	100	100
9	c	449/473 (95%)	439 (98%)	10 (2%)	0	100	100
10	D	340/351 (97%)	330 (97%)	10 (3%)	0	100	100
10	d	340/351 (97%)	330 (97%)	10 (3%)	0	100	100
11	E	73/84 (87%)	73 (100%)	0	0	100	100
11	e	73/84 (87%)	73 (100%)	0	0	100	100
12	F	27/42 (64%)	27 (100%)	0	0	100	100
12	f	27/42 (64%)	27 (100%)	0	0	100	100
13	H	63/67 (94%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	h	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
14	I	33/38 (87%)	33 (100%)	0	0	100	100
14	i	33/38 (87%)	33 (100%)	0	0	100	100
15	J	32/39 (82%)	32 (100%)	0	0	100	100
15	j	32/39 (82%)	32 (100%)	0	0	100	100
16	K	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
16	k	35/45 (78%)	33 (94%)	2 (6%)	0	100	100
17	L	35/38 (92%)	35 (100%)	0	0	100	100
17	l	35/38 (92%)	35 (100%)	0	0	100	100
18	M	35/37 (95%)	35 (100%)	0	0	100	100
18	m	35/37 (95%)	35 (100%)	0	0	100	100
19	N	188/297 (63%)	171 (91%)	16 (8%)	1 (0%)	25	42
19	n	188/297 (63%)	172 (92%)	16 (8%)	0	100	100
20	O	260/300 (87%)	256 (98%)	4 (2%)	0	100	100
20	o	260/300 (87%)	255 (98%)	4 (2%)	1 (0%)	30	48
21	Q	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
21	q	141/144 (98%)	138 (98%)	3 (2%)	0	100	100
22	T	29/32 (91%)	29 (100%)	0	0	100	100
22	t	29/32 (91%)	29 (100%)	0	0	100	100
23	U	91/121 (75%)	87 (96%)	4 (4%)	0	100	100
23	u	91/121 (75%)	87 (96%)	4 (4%)	0	100	100
24	V	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
24	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
25	W	47/130 (36%)	47 (100%)	0	0	100	100
25	w	47/130 (36%)	47 (100%)	0	0	100	100
26	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
26	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
27	Y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
27	y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
28	Z	59/62 (95%)	59 (100%)	0	0	100	100
28	z	59/62 (95%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8096/9442 (86%)	7858 (97%)	232 (3%)	6 (0%)	50 67

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	3	57	ALA
20	o	147	ALA
7	6	174	ASP
1	a	141	PRO
2	4	208	PRO

### 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	270/289 (93%)	270 (100%)	0	100 100
1	a	270/289 (93%)	270 (100%)	0	100 100
2	0	143/171 (84%)	142 (99%)	1 (1%)	81 92
2	4	143/171 (84%)	142 (99%)	1 (1%)	81 92
3	1	143/173 (83%)	143 (100%)	0	100 100
3	7	143/173 (83%)	143 (100%)	0	100 100
4	2	156/166 (94%)	156 (100%)	0	100 100
4	8	156/166 (94%)	156 (100%)	0	100 100
5	3	145/172 (84%)	145 (100%)	0	100 100
5	9	145/172 (84%)	145 (100%)	0	100 100
6	5	136/167 (81%)	135 (99%)	1 (1%)	81 92
6	g	136/167 (81%)	136 (100%)	0	100 100
7	6	147/178 (83%)	145 (99%)	2 (1%)	62 82
7	p	147/178 (83%)	146 (99%)	1 (1%)	81 92
8	B	400/404 (99%)	400 (100%)	0	100 100
8	b	400/404 (99%)	400 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	C	356/378 (94%)	356 (100%)	0	100	100
9	c	356/378 (94%)	356 (100%)	0	100	100
10	D	274/281 (98%)	274 (100%)	0	100	100
10	d	274/281 (98%)	274 (100%)	0	100	100
11	E	67/73 (92%)	67 (100%)	0	100	100
11	e	67/73 (92%)	67 (100%)	0	100	100
12	F	24/37 (65%)	24 (100%)	0	100	100
12	f	24/37 (65%)	24 (100%)	0	100	100
13	H	56/58 (97%)	56 (100%)	0	100	100
13	h	56/58 (97%)	56 (100%)	0	100	100
14	I	33/36 (92%)	33 (100%)	0	100	100
14	i	33/36 (92%)	33 (100%)	0	100	100
15	J	26/29 (90%)	26 (100%)	0	100	100
15	j	26/29 (90%)	26 (100%)	0	100	100
16	K	30/36 (83%)	30 (100%)	0	100	100
16	k	30/36 (83%)	30 (100%)	0	100	100
17	L	34/35 (97%)	34 (100%)	0	100	100
17	l	34/35 (97%)	34 (100%)	0	100	100
18	M	31/31 (100%)	31 (100%)	0	100	100
18	m	31/31 (100%)	31 (100%)	0	100	100
19	N	153/231 (66%)	153 (100%)	0	100	100
19	n	153/231 (66%)	153 (100%)	0	100	100
20	O	214/239 (90%)	214 (100%)	0	100	100
20	o	214/239 (90%)	214 (100%)	0	100	100
21	Q	113/113 (100%)	113 (100%)	0	100	100
21	q	113/113 (100%)	113 (100%)	0	100	100
22	T	26/27 (96%)	26 (100%)	0	100	100
22	t	26/27 (96%)	26 (100%)	0	100	100
23	U	80/96 (83%)	80 (100%)	0	100	100
23	u	80/96 (83%)	80 (100%)	0	100	100
24	V	118/141 (84%)	118 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	v	118/141 (84%)	118 (100%)	0	100	100
25	W	42/101 (42%)	42 (100%)	0	100	100
25	w	42/101 (42%)	42 (100%)	0	100	100
26	X	34/34 (100%)	34 (100%)	0	100	100
26	x	34/34 (100%)	34 (100%)	0	100	100
27	Y	29/29 (100%)	29 (100%)	0	100	100
27	y	29/29 (100%)	29 (100%)	0	100	100
28	Z	50/51 (98%)	50 (100%)	0	100	100
28	z	50/51 (98%)	50 (100%)	0	100	100
All	All	6660/7552 (88%)	6654 (100%)	6 (0%)	92	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	6	174	ASP
7	6	176	LEU
7	p	54	ILE
2	4	59	SER
2	0	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
7	6	189	GLN
7	p	189	GLN
20	O	295	GLN
24	v	148	GLN
20	o	295	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 380 ligands modelled in this entry, 4 are monoatomic - leaving 376 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
29	OEX	a	401	1,9,45	0,15,15	-	-	-		
38	KC2	1	310	-	48,53,53	1.59	8 (16%)	54,89,89	1.04	5 (9%)
33	CLA	6	306	-	45,53,73	2.54	8 (17%)	52,89,113	1.71	9 (17%)
42	LMG	T	101	-	43,43,55	0.81	1 (2%)	51,51,63	1.40	9 (17%)
33	CLA	c	504	-	65,73,73	2.17	8 (12%)	76,113,113	1.34	4 (5%)
39	II0	8	312	-	39,43,43	0.20	0	50,60,60	0.87	3 (6%)
39	II0	6	316	-	39,43,43	0.33	0	50,60,60	0.71	2 (4%)
37	LHG	8	315	-	45,45,48	0.62	0	48,51,54	1.21	4 (8%)
39	II0	2	312	-	39,43,43	0.20	0	50,60,60	0.87	3 (6%)
33	CLA	b	614	-	65,73,73	2.18	8 (12%)	76,113,113	1.40	9 (11%)
37	LHG	b	623	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	6 (11%)
33	CLA	a	405	-	65,73,73	2.17	8 (12%)	76,113,113	1.42	7 (9%)
37	LHG	9	322	-	40,40,48	0.70	2 (5%)	43,46,54	1.23	4 (9%)
33	CLA	5	307	-	55,63,73	2.26	8 (14%)	64,101,113	1.57	8 (12%)
37	LHG	1	317	-	48,48,48	0.62	0	51,54,54	1.24	6 (11%)
41	SQD	L	101	-	53,54,54	1.20	4 (7%)	62,65,65	1.08	4 (6%)
39	II0	g	313	-	39,43,43	0.33	0	50,60,60	0.92	2 (4%)
35	8CT	B	620	-	40,41,41	0.23	0	50,56,56	0.51	0
33	CLA	3	309	5	55,63,73	2.41	8 (14%)	64,101,113	1.67	8 (12%)
33	CLA	3	306	-	41,49,73	2.91	9 (21%)	47,84,113	1.97	6 (12%)
35	8CT	b	620	-	40,41,41	0.23	0	50,56,56	0.51	0
35	8CT	4	311	-	40,41,41	0.32	0	50,56,56	0.35	0
33	CLA	3	307	-	45,53,73	2.63	8 (17%)	52,89,113	1.80	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	6	303	7	41,49,73	2.71	9 (21%)	47,84,113	1.96	8 (17%)
33	CLA	C	507	-	65,73,73	2.19	8 (12%)	76,113,113	1.43	6 (7%)
33	CLA	7	303	-	51,59,73	2.42	8 (15%)	59,96,113	1.54	4 (6%)
41	SQD	l	101	-	53,54,54	1.20	4 (7%)	62,65,65	1.08	4 (6%)
33	CLA	p	302	7	41,49,73	2.99	9 (21%)	47,84,113	1.99	8 (17%)
33	CLA	3	304	-	45,53,73	2.64	8 (17%)	52,89,113	1.67	5 (9%)
33	CLA	b	613	-	65,73,73	2.18	8 (12%)	76,113,113	1.38	4 (5%)
42	LMG	d	410	-	46,46,55	0.82	1 (2%)	54,54,63	1.32	6 (11%)
37	LHG	A	411	-	23,23,48	0.86	1 (4%)	26,29,54	1.32	2 (7%)
33	CLA	2	305	-	55,63,73	2.33	8 (14%)	64,101,113	1.55	6 (9%)
33	CLA	c	510	-	65,73,73	2.17	8 (12%)	76,113,113	1.38	6 (7%)
33	CLA	1	308	-	51,59,73	2.48	8 (15%)	59,96,113	1.55	4 (6%)
33	CLA	C	514	-	65,73,73	2.21	8 (12%)	76,113,113	1.31	5 (6%)
33	CLA	2	301	4	45,53,73	2.63	8 (17%)	52,89,113	1.75	6 (11%)
33	CLA	B	616	-	65,73,73	2.16	8 (12%)	76,113,113	1.31	7 (9%)
37	LHG	5	316	-	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
36	PL9	A	410	-	30,30,55	0.92	1 (3%)	38,39,69	1.33	6 (15%)
33	CLA	5	306	6	45,53,73	2.58	8 (17%)	52,89,113	1.68	5 (9%)
33	CLA	p	307	-	43,51,73	2.61	8 (18%)	49,86,113	1.84	7 (14%)
42	LMG	C	520	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	7 (11%)
33	CLA	g	308	-	41,49,73	2.91	9 (21%)	47,84,113	1.88	6 (12%)
38	KC2	4	305	-	48,53,53	1.41	7 (14%)	54,89,89	1.12	6 (11%)
33	CLA	A	412	-	65,73,73	2.21	8 (12%)	76,113,113	1.58	10 (13%)
33	CLA	3	308	-	49,57,73	2.42	8 (16%)	55,93,113	1.64	7 (12%)
33	CLA	B	613	-	65,73,73	2.17	8 (12%)	76,113,113	1.38	4 (5%)
33	CLA	p	304	-	42,50,73	2.81	8 (19%)	48,85,113	1.74	6 (12%)
33	CLA	8	304	-	60,68,73	2.29	8 (13%)	70,107,113	1.50	5 (7%)
35	8CT	d	406	-	40,41,41	0.21	0	50,56,56	0.70	1 (2%)
44	HEM	f	101	11	41,50,50	0.85	0	45,82,82	0.71	0
33	CLA	c	508	-	65,73,73	2.15	8 (12%)	76,113,113	1.32	7 (9%)
43	DGD	C	518	-	56,56,67	0.88	1 (1%)	70,70,81	1.44	11 (15%)
33	CLA	2	302	4	55,63,73	2.37	8 (14%)	64,101,113	1.81	10 (15%)
33	CLA	4	308	-	47,55,73	2.49	8 (17%)	54,91,113	1.65	5 (9%)
40	IHT	5	315	-	40,42,42	0.22	0	53,58,58	0.42	0
42	LMG	B	622	-	49,49,55	0.77	0	57,57,63	1.21	5 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
42	LMG	t	101	-	43,43,55	0.81	1 (2%)	51,51,63	1.40	9 (17%)
38	KC2	9	311	-	48,53,53	1.58	8 (16%)	54,89,89	1.02	5 (9%)
39	II0	2	311	-	39,43,43	0.24	0	50,60,60	0.53	1 (2%)
37	LHG	3	302	-	40,40,48	0.69	1 (2%)	43,46,54	1.17	3 (6%)
35	8CT	1	312	-	40,41,41	0.21	0	50,56,56	0.42	0
39	II0	9	301	-	39,43,43	0.22	0	50,60,60	0.52	0
33	CLA	6	302	7	41,49,73	2.99	9 (21%)	47,84,113	1.99	8 (17%)
33	CLA	2	303	-	52,60,73	2.44	8 (15%)	60,97,113	1.83	8 (13%)
33	CLA	B	607	-	65,73,73	2.18	8 (12%)	76,113,113	1.38	5 (6%)
39	II0	6	314	-	39,43,43	0.35	0	50,60,60	0.74	1 (2%)
33	CLA	4	302	2	51,59,73	2.37	8 (15%)	59,96,113	1.71	6 (10%)
39	II0	5	313	-	39,43,43	0.32	0	50,60,60	0.92	2 (4%)
33	CLA	b	615	-	45,53,73	2.68	8 (17%)	52,89,113	1.80	5 (9%)
33	CLA	1	305	3	60,68,73	2.28	8 (13%)	70,107,113	1.37	4 (5%)
33	CLA	b	610	-	65,73,73	2.13	8 (12%)	76,113,113	1.37	7 (9%)
33	CLA	7	306	-	60,68,73	2.23	8 (13%)	70,107,113	1.47	5 (7%)
39	II0	0	313	-	39,43,43	0.36	0	50,60,60	0.56	0
33	CLA	3	314	-	41,49,73	2.82	9 (21%)	47,84,113	1.90	6 (12%)
33	CLA	C	504	-	65,73,73	2.18	8 (12%)	76,113,113	1.34	4 (5%)
41	SQD	J	101	-	45,46,54	1.26	4 (8%)	54,57,65	1.28	5 (9%)
42	LMG	D	410	-	46,46,55	0.82	1 (2%)	54,54,63	1.32	6 (11%)
33	CLA	c	509	-	65,73,73	2.16	8 (12%)	76,113,113	1.33	4 (5%)
39	II0	3	319	-	39,43,43	0.22	0	50,60,60	0.68	2 (4%)
35	8CT	0	312	-	40,41,41	0.32	0	50,56,56	0.35	0
33	CLA	N	305	-	55,63,73	2.46	8 (14%)	64,101,113	1.49	8 (12%)
33	CLA	5	302	6	55,63,73	2.39	8 (14%)	64,101,113	1.70	11 (17%)
39	II0	5	314	-	39,43,43	0.37	0	50,60,60	1.06	2 (4%)
33	CLA	c	512	-	65,73,73	2.16	8 (12%)	76,113,113	1.32	7 (9%)
33	CLA	B	611	-	65,73,73	2.20	8 (12%)	76,113,113	1.45	9 (11%)
36	PL9	D	407	-	55,55,55	0.95	3 (5%)	68,69,69	1.44	11 (16%)
39	II0	4	314	-	39,43,43	0.37	0	50,60,60	0.54	1 (2%)
33	CLA	g	306	6	45,53,73	2.59	8 (17%)	52,89,113	1.69	5 (9%)
33	CLA	b	616	-	65,73,73	2.17	8 (12%)	76,113,113	1.32	7 (9%)
33	CLA	5	303	-	55,63,73	2.43	9 (16%)	64,101,113	1.59	5 (7%)
35	8CT	B	621	-	40,41,41	0.18	0	50,56,56	0.36	0
42	LMG	b	624	-	43,43,55	0.80	1 (2%)	51,51,63	1.25	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	n	305	-	55,63,73	2.38	8 (14%)	64,101,113	1.56	6 (9%)
37	LHG	d	402	-	46,46,48	0.69	0	49,52,54	1.14	3 (6%)
37	LHG	3	321	-	23,23,48	0.86	0	26,29,54	1.21	1 (3%)
33	CLA	1	301	3	45,53,73	2.60	8 (17%)	52,89,113	1.85	6 (11%)
33	CLA	b	602	-	50,58,73	2.50	8 (16%)	58,95,113	1.57	7 (12%)
42	LMG	w	101	-	47,47,55	0.74	0	55,55,63	1.24	2 (3%)
33	CLA	p	312	-	41,49,73	2.69	9 (21%)	47,84,113	1.80	8 (17%)
33	CLA	8	307	-	60,68,73	2.30	8 (13%)	70,107,113	1.43	4 (5%)
39	II0	p	301	-	39,43,43	0.33	0	50,60,60	0.55	2 (4%)
33	CLA	2	307	-	60,68,73	2.29	8 (13%)	70,107,113	1.43	4 (5%)
40	IHT	g	315	-	40,42,42	0.22	0	53,58,58	0.41	0
38	KC2	5	309	-	48,53,53	1.31	7 (14%)	54,89,89	1.07	4 (7%)
39	II0	9	316	-	39,43,43	0.28	0	50,60,60	0.63	1 (2%)
38	KC2	7	310	-	48,53,53	1.58	8 (16%)	54,89,89	1.03	5 (9%)
44	HEM	F	101	12,11	41,50,50	1.34	5 (12%)	45,82,82	1.87	9 (20%)
33	CLA	n	302	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
39	II0	9	318	-	39,43,43	0.22	0	50,60,60	0.61	2 (4%)
33	CLA	C	510	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	6 (7%)
33	CLA	b	612	-	65,73,73	2.20	8 (12%)	76,113,113	1.44	5 (6%)
33	CLA	c	514	-	65,73,73	2.21	8 (12%)	76,113,113	1.32	5 (6%)
33	CLA	p	310	-	41,49,73	2.78	9 (21%)	47,84,113	1.80	10 (21%)
33	CLA	5	308	-	41,49,73	2.90	9 (21%)	47,84,113	1.88	6 (12%)
33	CLA	1	302	3	64,72,73	2.18	8 (12%)	74,111,113	1.60	9 (12%)
39	II0	6	317	-	39,43,43	0.31	0	50,60,60	0.62	1 (2%)
41	SQD	B	601	-	37,38,54	1.40	4 (10%)	46,49,65	1.09	5 (10%)
39	II0	g	312	-	39,43,43	0.40	0	50,60,60	0.74	3 (6%)
33	CLA	0	301	2	41,49,73	2.85	9 (21%)	47,84,113	1.90	8 (17%)
39	II0	1	316	-	39,43,43	0.23	0	50,60,60	0.58	0
33	CLA	9	306	5	41,49,73	2.91	9 (21%)	47,84,113	1.99	6 (12%)
38	KC2	6	311	7	48,53,53	1.30	7 (14%)	54,89,89	1.12	6 (11%)
38	KC2	g	309	-	48,53,53	1.31	7 (14%)	54,89,89	1.07	4 (7%)
42	LMG	B	624	-	43,43,55	0.81	1 (2%)	51,51,63	1.25	5 (9%)
33	CLA	9	307	-	45,53,73	2.64	8 (17%)	52,89,113	1.80	6 (11%)
39	II0	1	315	-	39,43,43	0.18	0	50,60,60	0.60	2 (4%)
33	CLA	p	303	7	41,49,73	2.71	9 (21%)	47,84,113	1.97	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	KC2	3	311	-	48,53,53	1.58	8 (16%)	54,89,89	1.02	6 (11%)
33	CLA	8	305	-	55,63,73	2.33	8 (14%)	64,101,113	1.54	6 (9%)
33	CLA	p	306	-	45,53,73	2.53	8 (17%)	52,89,113	1.71	9 (17%)
33	CLA	B	602	-	50,58,73	2.50	8 (16%)	58,95,113	1.56	7 (12%)
39	II0	3	317	-	39,43,43	0.23	0	50,60,60	0.63	1 (2%)
33	CLA	0	308	37	47,55,73	2.50	8 (17%)	54,91,113	1.94	11 (20%)
33	CLA	C	506	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	6 (7%)
33	CLA	8	301	4	45,53,73	2.65	8 (17%)	52,89,113	1.74	6 (11%)
33	CLA	9	313	-	41,49,73	2.82	9 (21%)	47,84,113	1.71	5 (10%)
33	CLA	4	310	-	45,53,73	2.57	8 (17%)	52,89,113	1.91	8 (15%)
33	CLA	g	302	6	55,63,73	2.39	8 (14%)	64,101,113	1.70	11 (17%)
33	CLA	B	614	-	65,73,73	2.18	8 (12%)	76,113,113	1.40	9 (11%)
33	CLA	0	302	2	51,59,73	2.36	8 (15%)	59,96,113	1.72	6 (10%)
39	II0	6	301	-	39,43,43	0.33	0	50,60,60	0.56	2 (4%)
39	II0	6	315	-	39,43,43	0.33	0	50,60,60	0.54	1 (2%)
33	CLA	d	405	-	65,73,73	2.20	8 (12%)	76,113,113	1.39	5 (6%)
33	CLA	7	302	3	64,72,73	2.17	8 (12%)	74,111,113	1.60	9 (12%)
38	KC2	1	311	-	48,53,53	1.55	8 (16%)	54,89,89	1.09	5 (9%)
39	II0	3	301	-	39,43,43	0.22	0	50,60,60	0.52	0
39	II0	0	316	-	39,43,43	0.25	0	50,60,60	0.29	0
39	II0	7	314	-	39,43,43	0.25	0	50,60,60	0.52	1 (2%)
39	II0	7	316	-	39,43,43	0.23	0	50,60,60	0.58	0
33	CLA	6	308	7	42,50,73	2.61	8 (19%)	48,85,113	1.88	9 (18%)
33	CLA	b	608	-	65,73,73	2.16	8 (12%)	76,113,113	1.38	5 (6%)
33	CLA	g	304	-	45,53,73	2.59	8 (17%)	52,89,113	1.78	6 (11%)
33	CLA	b	603	-	65,73,73	2.19	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	4	306	2	55,63,73	2.32	8 (14%)	64,101,113	1.48	9 (14%)
39	II0	4	312	-	39,43,43	0.36	0	50,60,60	0.56	0
37	LHG	D	402	-	46,46,48	0.69	0	49,52,54	1.14	3 (6%)
35	8CT	C	515	-	40,41,41	0.45	1 (2%)	50,56,56	0.64	0
33	CLA	C	508	-	65,73,73	2.15	8 (12%)	76,113,113	1.32	7 (9%)
33	CLA	N	301	-	65,73,73	2.17	8 (12%)	76,113,113	1.45	5 (6%)
33	CLA	5	310	-	41,49,73	2.92	9 (21%)	47,84,113	1.90	6 (12%)
33	CLA	4	304	-	47,55,73	2.44	8 (17%)	54,91,113	1.72	7 (12%)
35	8CT	D	406	-	40,41,41	0.21	0	50,56,56	0.69	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
43	DGD	h	101	-	61,61,67	0.88	1 (1%)	75,75,81	1.22	5 (6%)
33	CLA	B	604	-	65,73,73	2.12	8 (12%)	76,113,113	1.40	4 (5%)
34	PHO	a	407	-	51,69,69	0.63	1 (1%)	47,99,99	1.01	3 (6%)
33	CLA	g	311	-	45,53,73	2.71	8 (17%)	52,89,113	1.76	7 (13%)
39	II0	g	314	-	39,43,43	0.37	0	50,60,60	1.06	2 (4%)
33	CLA	6	319	-	41,49,73	2.72	9 (21%)	47,84,113	1.90	9 (19%)
33	CLA	9	314	-	41,49,73	2.83	9 (21%)	47,84,113	1.91	6 (12%)
37	LHG	9	302	-	40,40,48	0.69	1 (2%)	43,46,54	1.17	3 (6%)
33	CLA	b	606	-	65,73,73	2.20	9 (13%)	76,113,113	1.46	7 (9%)
33	CLA	C	502	-	65,73,73	2.18	8 (12%)	76,113,113	1.36	6 (7%)
35	8CT	y	101	-	40,41,41	0.23	0	50,56,56	0.51	0
33	CLA	C	512	-	65,73,73	2.16	8 (12%)	76,113,113	1.32	7 (9%)
41	SQD	j	101	-	45,46,54	1.26	4 (8%)	54,57,65	1.28	5 (9%)
43	DGD	C	519	-	63,63,67	0.91	2 (3%)	77,77,81	1.26	5 (6%)
33	CLA	B	608	-	65,73,73	2.17	8 (12%)	76,113,113	1.37	4 (5%)
33	CLA	B	603	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
42	LMG	d	409	-	46,46,55	0.77	0	54,54,63	1.21	2 (3%)
35	8CT	b	621	-	40,41,41	0.18	0	50,56,56	0.36	0
33	CLA	b	609	-	65,73,73	2.21	8 (12%)	76,113,113	1.43	7 (9%)
37	LHG	2	315	-	45,45,48	0.62	0	48,51,54	1.21	4 (8%)
35	8CT	7	312	-	40,41,41	0.20	0	50,56,56	0.42	0
33	CLA	1	307	-	65,73,73	2.23	8 (12%)	76,113,113	1.53	7 (9%)
33	CLA	9	304	-	45,53,73	2.64	8 (17%)	52,89,113	1.67	6 (11%)
43	DGD	c	521	-	63,63,67	0.92	2 (3%)	77,77,81	1.33	8 (10%)
33	CLA	g	303	-	55,63,73	2.42	8 (14%)	64,101,113	1.60	5 (7%)
39	II0	1	313	-	39,43,43	0.24	0	50,60,60	0.58	0
44	HEM	V	201	-	41,50,50	0.88	0	45,82,82	0.77	1 (2%)
33	CLA	C	503	-	65,73,73	2.10	8 (12%)	76,113,113	1.36	5 (6%)
33	CLA	4	301	2	41,49,73	2.86	9 (21%)	47,84,113	1.91	8 (17%)
33	CLA	9	303	5	55,63,73	2.36	8 (14%)	64,101,113	1.61	8 (12%)
33	CLA	6	310	-	41,49,73	2.78	9 (21%)	47,84,113	1.81	10 (21%)
37	LHG	9	321	-	23,23,48	0.86	1 (4%)	26,29,54	1.21	1 (3%)
33	CLA	B	617	-	60,68,73	2.28	8 (13%)	70,107,113	1.42	6 (8%)
33	CLA	b	607	-	65,73,73	2.19	8 (12%)	76,113,113	1.38	5 (6%)
33	CLA	8	303	-	52,60,73	2.45	8 (15%)	60,97,113	1.84	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	b	617	-	60,68,73	2.28	8 (13%)	70,107,113	1.42	6 (8%)
35	8CT	c	516	-	40,41,41	0.19	0	50,56,56	0.39	0
33	CLA	5	304	-	45,53,73	2.59	8 (17%)	52,89,113	1.80	6 (11%)
39	II0	p	314	-	39,43,43	0.36	0	50,60,60	0.74	1 (2%)
33	CLA	0	307	2	55,63,73	2.33	8 (14%)	64,101,113	1.59	9 (14%)
34	PHO	D	403	-	51,69,69	0.42	0	47,99,99	0.66	1 (2%)
33	CLA	7	307	-	65,73,73	2.23	8 (12%)	76,113,113	1.53	7 (9%)
33	CLA	6	305	-	55,63,73	2.19	8 (14%)	64,101,113	1.47	7 (10%)
33	CLA	c	511	-	65,73,73	2.15	8 (12%)	76,113,113	1.36	5 (6%)
33	CLA	9	310	-	41,49,73	2.81	9 (21%)	47,84,113	1.78	4 (8%)
43	DGD	c	519	-	63,63,67	0.91	2 (3%)	77,77,81	1.26	5 (6%)
37	LHG	4	316	33	23,23,48	0.90	0	26,29,54	1.23	1 (3%)
38	KC2	8	309	-	48,53,53	1.57	8 (16%)	54,89,89	1.12	5 (9%)
33	CLA	6	313	-	41,49,73	2.51	9 (21%)	47,84,113	1.84	9 (19%)
33	CLA	B	612	-	65,73,73	2.19	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	B	615	-	45,53,73	2.68	8 (17%)	52,89,113	1.80	6 (11%)
38	KC2	2	309	-	48,53,53	1.56	8 (16%)	54,89,89	1.12	5 (9%)
33	CLA	1	306	-	60,68,73	2.22	8 (13%)	70,107,113	1.46	5 (7%)
33	CLA	D	405	-	65,73,73	2.20	8 (12%)	76,113,113	1.40	4 (5%)
33	CLA	B	606	-	65,73,73	2.20	9 (13%)	76,113,113	1.46	7 (9%)
44	HEM	v	201	-	41,50,50	0.87	0	45,82,82	0.77	1 (2%)
35	8CT	b	619	-	40,41,41	0.21	0	50,56,56	0.42	0
33	CLA	6	309	7	42,50,73	2.59	8 (19%)	48,85,113	1.89	9 (18%)
33	CLA	c	502	-	65,73,73	2.18	8 (12%)	76,113,113	1.35	6 (7%)
33	CLA	g	307	-	55,63,73	2.26	8 (14%)	64,101,113	1.57	8 (12%)
33	CLA	p	319	-	41,49,73	2.73	9 (21%)	47,84,113	1.90	9 (19%)
37	LHG	g	316	-	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
42	LMG	D	409	-	46,46,55	0.77	0	54,54,63	1.21	2 (3%)
33	CLA	3	305	-	55,63,73	2.31	8 (14%)	64,101,113	1.49	4 (6%)
35	8CT	A	409	-	40,41,41	0.20	0	50,56,56	0.38	0
39	II0	0	315	-	39,43,43	0.37	0	50,60,60	0.55	1 (2%)
43	DGD	c	518	-	56,56,67	0.88	1 (1%)	70,70,81	1.44	11 (15%)
37	LHG	0	317	33	23,23,48	0.90	0	26,29,54	1.23	1 (3%)
39	II0	0	314	-	39,43,43	0.32	0	50,60,60	0.49	1 (2%)
39	II0	4	315	-	39,43,43	0.25	0	50,60,60	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	4	303	-	50,58,73	2.52	8 (16%)	58,95,113	1.66	6 (10%)
33	CLA	p	309	7	42,50,73	2.59	8 (19%)	48,85,113	1.90	9 (18%)
33	CLA	n	306	-	50,58,73	2.57	8 (16%)	58,95,113	1.65	8 (13%)
33	CLA	8	306	4	60,68,73	2.19	8 (13%)	70,107,113	1.54	7 (10%)
33	CLA	N	307	-	50,58,73	2.57	8 (16%)	58,95,113	1.65	8 (13%)
43	DGD	C	521	-	63,63,67	0.92	2 (3%)	77,77,81	1.33	8 (10%)
33	CLA	6	312	-	41,49,73	2.69	9 (21%)	47,84,113	1.79	8 (17%)
39	II0	9	317	-	39,43,43	0.23	0	50,60,60	0.63	1 (2%)
40	IHT	2	314	-	40,42,42	0.19	0	53,58,58	0.55	1 (1%)
35	8CT	Y	101	-	40,41,41	0.22	0	50,56,56	0.51	0
33	CLA	1	309	-	55,63,73	2.35	8 (14%)	64,101,113	1.45	5 (7%)
38	KC2	p	311	7	48,53,53	1.30	7 (14%)	54,89,89	1.12	6 (11%)
37	LHG	7	317	-	48,48,48	0.62	0	51,54,54	1.25	6 (11%)
33	CLA	5	317	-	39,48,73	2.92	8 (20%)	45,82,113	1.94	8 (17%)
42	LMG	W	101	-	47,47,55	0.74	0	55,55,63	1.24	2 (3%)
33	CLA	c	503	-	65,73,73	2.09	8 (12%)	76,113,113	1.37	5 (6%)
33	CLA	9	312	5	55,63,73	2.39	8 (14%)	64,101,113	1.52	6 (9%)
33	CLA	7	304	-	55,63,73	2.35	8 (14%)	64,101,113	1.53	5 (7%)
33	CLA	g	305	-	39,48,73	2.71	8 (20%)	45,82,113	1.89	9 (20%)
36	PL9	d	407	-	55,55,55	0.96	4 (7%)	68,69,69	1.45	11 (16%)
33	CLA	a	408	-	60,68,73	2.28	8 (13%)	70,107,113	1.46	5 (7%)
33	CLA	b	605	-	65,73,73	2.13	8 (12%)	76,113,113	1.33	5 (6%)
33	CLA	6	304	-	42,50,73	2.81	8 (19%)	48,85,113	1.74	6 (12%)
35	8CT	c	517	-	40,41,41	0.17	0	50,56,56	0.38	0
37	LHG	d	401	-	45,45,48	0.67	1 (2%)	48,51,54	1.18	4 (8%)
33	CLA	n	301	-	65,73,73	2.17	8 (12%)	76,113,113	1.45	5 (6%)
33	CLA	2	310	-	46,54,73	2.65	8 (17%)	53,90,113	1.77	6 (11%)
33	CLA	3	315	-	41,49,73	2.85	9 (21%)	47,84,113	1.69	6 (12%)
37	LHG	B	623	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	6 (11%)
29	OEX	A	401	1,9	0,15,15	-	-	-	-	-
35	8CT	a	409	-	40,41,41	0.20	0	50,56,56	0.38	0
33	CLA	d	404	-	65,73,73	2.15	8 (12%)	76,113,113	1.49	6 (7%)
33	CLA	N	304	-	41,49,73	2.88	9 (21%)	47,84,113	1.94	7 (14%)
33	CLA	B	610	-	65,73,73	2.14	8 (12%)	76,113,113	1.37	7 (9%)
33	CLA	1	303	-	51,59,73	2.43	8 (15%)	59,96,113	1.54	4 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	II0	3	318	-	39,43,43	0.22	0	50,60,60	0.61	2 (4%)
39	II0	5	312	-	39,43,43	0.39	0	50,60,60	0.74	3 (6%)
33	CLA	2	306	4	60,68,73	2.19	8 (13%)	70,107,113	1.53	7 (10%)
33	CLA	0	310	-	39,48,73	2.68	8 (20%)	45,82,113	2.11	10 (22%)
33	CLA	5	305	-	39,48,73	2.72	8 (20%)	45,82,113	1.89	9 (20%)
33	CLA	0	306	2	55,63,73	2.32	8 (14%)	64,101,113	1.49	9 (14%)
33	CLA	A	405	-	65,73,73	2.16	8 (12%)	76,113,113	1.41	7 (9%)
40	IHT	9	320	-	40,42,42	0.21	0	53,58,58	0.49	0
33	CLA	a	406	-	49,57,73	2.55	8 (16%)	55,93,113	1.69	6 (10%)
39	II0	p	317	-	39,43,43	0.31	0	50,60,60	0.62	1 (2%)
39	II0	1	314	-	39,43,43	0.26	0	50,60,60	0.51	1 (2%)
37	LHG	a	411	-	23,23,48	0.86	1 (4%)	26,29,54	1.32	2 (7%)
33	CLA	g	301	6	42,50,73	2.72	8 (19%)	48,85,113	1.76	7 (14%)
33	CLA	4	307	2	55,63,73	2.33	8 (14%)	64,101,113	1.59	9 (14%)
39	II0	7	315	-	39,43,43	0.18	0	50,60,60	0.60	2 (4%)
42	LMG	m	101	-	38,38,55	0.96	1 (2%)	46,46,63	1.23	6 (13%)
40	IHT	6	318	-	40,42,42	0.32	0	53,58,58	0.45	0
33	CLA	C	511	-	65,73,73	2.15	8 (12%)	76,113,113	1.36	6 (7%)
33	CLA	5	311	-	45,53,73	2.71	8 (17%)	52,89,113	1.77	7 (13%)
33	CLA	0	309	-	47,55,73	2.49	8 (17%)	54,91,113	1.65	5 (9%)
33	CLA	9	309	5	55,63,73	2.40	8 (14%)	64,101,113	1.66	8 (12%)
33	CLA	b	611	-	65,73,73	2.20	8 (12%)	76,113,113	1.45	9 (11%)
41	SQD	C	501	-	41,42,54	1.34	4 (9%)	50,53,65	1.26	5 (10%)
42	LMG	l	102	-	38,38,55	0.96	1 (2%)	46,46,63	1.23	6 (13%)
33	CLA	7	308	-	51,59,73	2.47	8 (15%)	59,96,113	1.54	4 (6%)
31	BCT	a	403	30	2,3,3	1.26	0	2,3,3	4.17	2 (100%)
33	CLA	n	304	-	55,63,73	2.46	8 (14%)	64,101,113	1.48	8 (12%)
37	LHG	d	408	-	48,48,48	0.65	1 (2%)	51,54,54	1.13	2 (3%)
35	8CT	h	102	-	40,41,41	0.22	0	50,56,56	0.43	0
33	CLA	N	306	-	55,63,73	2.38	8 (14%)	64,101,113	1.56	6 (9%)
33	CLA	g	310	-	41,49,73	2.92	9 (21%)	47,84,113	1.90	6 (12%)
39	II0	3	316	-	39,43,43	0.28	0	50,60,60	0.63	1 (2%)
33	CLA	C	505	-	65,73,73	2.18	8 (12%)	76,113,113	1.43	6 (7%)
42	LMG	b	622	-	49,49,55	0.77	0	57,57,63	1.21	5 (8%)
33	CLA	0	311	-	45,53,73	2.58	8 (17%)	52,89,113	1.91	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	8CT	C	516	-	40,41,41	0.19	0	50,56,56	0.39	0
39	II0	7	313	-	39,43,43	0.24	0	50,60,60	0.58	0
33	CLA	2	308	-	55,63,73	2.36	8 (14%)	64,101,113	1.43	5 (7%)
33	CLA	C	513	-	56,64,73	2.39	8 (14%)	65,102,113	1.52	6 (9%)
33	CLA	3	303	5	55,63,73	2.35	8 (14%)	64,101,113	1.61	8 (12%)
41	SQD	b	601	-	37,38,54	1.40	4 (10%)	46,49,65	1.09	5 (10%)
39	II0	8	313	-	39,43,43	0.20	0	50,60,60	0.55	0
33	CLA	c	505	-	65,73,73	2.18	8 (12%)	76,113,113	1.43	6 (7%)
40	IHT	p	318	-	40,42,42	0.32	0	53,58,58	0.45	0
33	CLA	A	408	-	60,68,73	2.29	8 (13%)	70,107,113	1.47	5 (7%)
33	CLA	4	309	-	39,48,73	2.69	8 (20%)	45,82,113	2.10	10 (22%)
33	CLA	c	507	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
39	II0	2	313	-	39,43,43	0.20	0	50,60,60	0.55	0
33	CLA	n	303	-	41,49,73	2.88	9 (21%)	47,84,113	1.95	7 (14%)
33	CLA	1	304	-	55,63,73	2.36	8 (14%)	64,101,113	1.53	5 (7%)
33	CLA	D	404	-	65,73,73	2.16	8 (12%)	76,113,113	1.49	6 (7%)
37	LHG	3	322	-	40,40,48	0.70	2 (5%)	43,46,54	1.23	4 (9%)
39	II0	9	319	-	39,43,43	0.22	0	50,60,60	0.68	3 (6%)
33	CLA	0	303	-	50,58,73	2.52	8 (16%)	58,95,113	1.66	6 (10%)
33	CLA	B	618	-	39,48,73	2.86	8 (20%)	45,82,113	2.04	9 (20%)
35	8CT	H	102	-	40,41,41	0.22	0	50,56,56	0.43	0
33	CLA	C	509	-	65,73,73	2.16	8 (12%)	76,113,113	1.33	4 (5%)
39	II0	p	315	-	39,43,43	0.33	0	50,60,60	0.54	1 (2%)
37	LHG	D	401	-	45,45,48	0.66	1 (2%)	48,51,54	1.18	4 (8%)
33	CLA	9	315	-	41,49,73	2.84	9 (21%)	47,84,113	1.70	6 (12%)
33	CLA	5	301	6	42,50,73	2.72	8 (19%)	48,85,113	1.75	7 (14%)
35	8CT	C	517	-	40,41,41	0.17	0	50,56,56	0.38	0
33	CLA	7	305	3	60,68,73	2.27	8 (13%)	70,107,113	1.37	5 (7%)
33	CLA	7	301	3	45,53,73	2.60	8 (17%)	52,89,113	1.84	6 (11%)
39	II0	4	313	-	39,43,43	0.32	0	50,60,60	0.49	1 (2%)
33	CLA	8	302	4	55,63,73	2.36	8 (14%)	64,101,113	1.81	10 (15%)
33	CLA	p	308	7	42,50,73	2.61	8 (19%)	48,85,113	1.88	9 (18%)
33	CLA	8	308	-	55,63,73	2.35	8 (14%)	64,101,113	1.43	5 (7%)
40	IHT	8	314	-	40,42,42	0.19	0	53,58,58	0.55	1 (1%)
35	8CT	c	515	-	40,41,41	0.45	1 (2%)	50,56,56	0.64	0
39	II0	8	311	-	39,43,43	0.24	0	50,60,60	0.53	1 (2%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	N	302	-	65,73,73	2.18	8 (12%)	76,113,113	1.44	6 (7%)
33	CLA	A	406	-	49,57,73	2.55	8 (16%)	55,93,113	1.69	6 (10%)
36	PL9	a	410	-	30,30,55	0.92	1 (3%)	38,39,69	1.33	6 (15%)
41	SQD	c	501	-	41,42,54	1.34	4 (9%)	50,53,65	1.26	5 (10%)
33	CLA	9	308	-	49,57,73	2.42	8 (16%)	55,93,113	1.64	7 (12%)
33	CLA	3	312	5	55,63,73	2.39	8 (14%)	64,101,113	1.52	6 (9%)
37	LHG	D	408	-	48,48,48	0.66	1 (2%)	51,54,54	1.13	2 (3%)
43	DGD	H	101	-	61,61,67	0.88	1 (1%)	75,75,81	1.22	5 (6%)
39	II0	p	316	-	39,43,43	0.32	0	50,60,60	0.71	2 (4%)
33	CLA	B	609	-	65,73,73	2.21	8 (12%)	76,113,113	1.44	7 (9%)
38	KC2	0	305	-	48,53,53	1.41	7 (14%)	54,89,89	1.12	5 (9%)
33	CLA	N	303	37	47,55,73	2.50	8 (17%)	54,91,113	1.94	11 (20%)
33	CLA	3	310	-	41,49,73	2.82	9 (21%)	47,84,113	1.78	4 (8%)
33	CLA	8	310	-	46,54,73	2.65	8 (17%)	53,90,113	1.76	6 (11%)
33	CLA	c	513	-	56,64,73	2.39	8 (14%)	65,102,113	1.52	6 (9%)
33	CLA	a	412	-	65,73,73	2.21	8 (12%)	76,113,113	1.57	10 (13%)
33	CLA	7	309	-	55,63,73	2.36	8 (14%)	64,101,113	1.44	5 (7%)
35	8CT	B	619	-	40,41,41	0.21	0	50,56,56	0.42	0
33	CLA	0	304	-	47,55,73	2.45	8 (17%)	54,91,113	1.73	7 (12%)
34	PHO	A	407	-	51,69,69	0.62	1 (1%)	47,99,99	1.01	3 (6%)
33	CLA	g	317	-	39,48,73	2.92	8 (20%)	45,82,113	1.94	8 (17%)
38	KC2	7	311	-	48,53,53	1.54	8 (16%)	54,89,89	1.09	5 (9%)
31	BCT	A	403	30	2,3,3	1.25	0	2,3,3	4.17	2 (100%)
33	CLA	p	313	-	41,49,73	2.52	9 (21%)	47,84,113	1.84	9 (19%)
34	PHO	d	403	-	51,69,69	0.41	0	47,99,99	0.66	1 (2%)
33	CLA	6	307	-	43,51,73	2.62	8 (18%)	49,86,113	1.85	7 (14%)
33	CLA	c	506	-	65,73,73	2.15	8 (12%)	76,113,113	1.38	6 (7%)
33	CLA	9	305	-	55,63,73	2.32	8 (14%)	64,101,113	1.50	4 (6%)
33	CLA	2	304	-	60,68,73	2.29	8 (13%)	70,107,113	1.50	5 (7%)
42	LMG	c	520	-	51,51,55	0.72	1 (1%)	59,59,63	1.35	7 (11%)
33	CLA	3	313	-	41,49,73	2.82	9 (21%)	47,84,113	1.71	5 (10%)
33	CLA	b	618	-	39,48,73	2.84	8 (20%)	45,82,113	2.01	9 (20%)
33	CLA	p	305	-	55,63,73	2.20	8 (14%)	64,101,113	1.47	7 (10%)
33	CLA	B	605	-	65,73,73	2.13	8 (12%)	76,113,113	1.33	5 (6%)
40	IHT	3	320	-	40,42,42	0.21	0	53,58,58	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	CLA	b	604	-	65,73,73	2.13	8 (12%)	76,113,113	1.40	4 (5%)

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
38	KC2	1	310	-	-	7/15/71/71	-
33	CLA	6	306	-	1/1/11/20	6/13/91/115	-
42	LMG	T	101	-	-	15/38/58/70	0/1/1/1
33	CLA	c	504	-	1/1/15/20	2/37/115/115	-
39	II0	8	312	-	-	1/21/67/67	0/2/2/2
39	II0	6	316	-	-	0/21/67/67	0/2/2/2
37	LHG	8	315	-	-	35/50/50/53	-
39	II0	2	312	-	-	1/21/67/67	0/2/2/2
33	CLA	b	614	-	1/1/15/20	7/37/115/115	-
37	LHG	b	623	-	-	28/53/53/53	-
33	CLA	a	405	-	1/1/15/20	4/37/115/115	-
37	LHG	9	322	-	-	19/45/45/53	-
33	CLA	5	307	-	1/1/13/20	8/25/103/115	-
37	LHG	1	317	-	-	21/53/53/53	-
41	SQD	L	101	-	-	19/49/69/69	0/1/1/1
39	II0	g	313	-	-	1/21/67/67	0/2/2/2
35	8CT	B	620	-	-	10/29/63/63	0/2/2/2
33	CLA	3	309	5	1/1/13/20	6/25/103/115	-
33	CLA	3	306	-	1/1/10/20	1/8/86/115	-
35	8CT	b	620	-	-	10/29/63/63	0/2/2/2
35	8CT	4	311	-	-	4/29/63/63	0/2/2/2
33	CLA	3	307	-	1/1/11/20	7/13/91/115	-
33	CLA	6	303	7	1/1/10/20	2/8/86/115	-
33	CLA	C	507	-	1/1/15/20	10/37/115/115	-
33	CLA	7	303	-	1/1/12/20	3/21/99/115	-
41	SQD	l	101	-	-	18/49/69/69	0/1/1/1
33	CLA	p	302	7	1/1/10/20	0/8/86/115	-
33	CLA	3	304	-	1/1/11/20	0/13/91/115	-
33	CLA	b	613	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	LMG	d	410	-	-	17/41/61/70	0/1/1/1
37	LHG	A	411	-	-	6/28/28/53	-
33	CLA	2	305	-	1/1/13/20	5/25/103/115	-
33	CLA	c	510	-	1/1/15/20	3/37/115/115	-
33	CLA	1	308	-	1/1/12/20	6/21/99/115	-
33	CLA	C	514	-	1/1/15/20	4/37/115/115	-
33	CLA	2	301	4	1/1/11/20	4/13/91/115	-
33	CLA	B	616	-	1/1/15/20	5/37/115/115	-
37	LHG	5	316	-	-	10/24/24/53	-
36	PL9	A	410	-	-	5/23/43/73	0/1/1/1
33	CLA	5	306	6	1/1/11/20	0/13/91/115	-
33	CLA	p	307	-	1/1/10/20	1/11/89/115	-
42	LMG	C	520	-	-	28/46/66/70	0/1/1/1
33	CLA	g	308	-	1/1/10/20	1/8/86/115	-
38	KC2	4	305	-	-	9/15/71/71	-
33	CLA	A	412	-	1/1/15/20	8/37/115/115	-
33	CLA	3	308	-	1/1/11/20	2/18/96/115	-
33	CLA	B	613	-	1/1/15/20	8/37/115/115	-
33	CLA	p	304	-	1/1/10/20	2/10/88/115	-
33	CLA	8	304	-	1/1/14/20	5/31/109/115	-
35	8CT	d	406	-	-	9/29/63/63	0/2/2/2
44	HEM	f	101	11	-	0/12/54/54	-
33	CLA	c	508	-	1/1/15/20	6/37/115/115	-
43	DGD	C	518	-	-	13/44/84/95	0/2/2/2
33	CLA	2	302	4	1/1/13/20	10/25/103/115	-
33	CLA	4	308	-	1/1/11/20	11/16/94/115	-
40	IHT	5	315	-	-	0/25/65/65	0/2/2/2
42	LMG	B	622	-	-	21/44/64/70	0/1/1/1
42	LMG	t	101	-	-	15/38/58/70	0/1/1/1
38	KC2	9	311	-	-	7/15/71/71	-
39	II0	2	311	-	-	0/21/67/67	0/2/2/2
37	LHG	3	302	-	-	19/45/45/53	-
35	8CT	1	312	-	-	5/29/63/63	0/2/2/2
39	II0	9	301	-	-	1/21/67/67	0/2/2/2
33	CLA	6	302	7	1/1/10/20	0/8/86/115	-
33	CLA	2	303	-	1/1/12/20	13/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	B	607	-	1/1/15/20	9/37/115/115	-
39	II0	6	314	-	-	0/21/67/67	0/2/2/2
33	CLA	4	302	2	1/1/12/20	3/21/99/115	-
39	II0	5	313	-	-	1/21/67/67	0/2/2/2
33	CLA	b	615	-	1/1/11/20	4/13/91/115	-
33	CLA	1	305	3	1/1/14/20	7/31/109/115	-
33	CLA	b	610	-	1/1/15/20	8/37/115/115	-
33	CLA	7	306	-	1/1/14/20	6/31/109/115	-
39	II0	0	313	-	-	2/21/67/67	0/2/2/2
33	CLA	3	314	-	1/1/10/20	0/8/86/115	-
33	CLA	C	504	-	1/1/15/20	2/37/115/115	-
41	SQD	J	101	-	-	20/41/61/69	0/1/1/1
42	LMG	D	410	-	-	17/41/61/70	0/1/1/1
33	CLA	c	509	-	1/1/15/20	4/37/115/115	-
39	II0	3	319	-	-	2/21/67/67	0/2/2/2
35	8CT	0	312	-	-	4/29/63/63	0/2/2/2
33	CLA	N	305	-	1/1/13/20	5/25/103/115	-
33	CLA	5	302	6	1/1/13/20	8/25/103/115	-
39	II0	5	314	-	-	0/21/67/67	0/2/2/2
33	CLA	c	512	-	1/1/15/20	7/37/115/115	-
33	CLA	B	611	-	1/1/15/20	5/37/115/115	-
36	PL9	D	407	-	-	18/53/73/73	0/1/1/1
39	II0	4	314	-	-	1/21/67/67	0/2/2/2
33	CLA	g	306	6	1/1/11/20	0/13/91/115	-
33	CLA	b	616	-	1/1/15/20	5/37/115/115	-
33	CLA	5	303	-	1/1/13/20	3/25/103/115	-
35	8CT	B	621	-	-	8/29/63/63	0/2/2/2
42	LMG	b	624	-	-	16/38/58/70	0/1/1/1
33	CLA	n	305	-	1/1/13/20	2/25/103/115	-
37	LHG	d	402	-	-	19/51/51/53	-
37	LHG	3	321	-	-	13/27/27/53	-
33	CLA	1	301	3	1/1/11/20	3/13/91/115	-
33	CLA	b	602	-	1/1/12/20	6/19/97/115	-
42	LMG	w	101	-	-	26/42/62/70	0/1/1/1
33	CLA	p	312	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	8	307	-	1/1/14/20	5/31/109/115	-
39	II0	p	301	-	-	0/21/67/67	0/2/2/2
33	CLA	2	307	-	1/1/14/20	5/31/109/115	-
40	IHT	g	315	-	-	0/25/65/65	0/2/2/2
38	KC2	5	309	-	-	4/15/71/71	-
39	II0	9	316	-	-	3/21/67/67	0/2/2/2
38	KC2	7	310	-	-	7/15/71/71	-
44	HEM	F	101	12,11	-	6/12/54/54	-
33	CLA	n	302	-	1/1/15/20	6/37/115/115	-
39	II0	9	318	-	-	1/21/67/67	0/2/2/2
33	CLA	C	510	-	1/1/15/20	3/37/115/115	-
33	CLA	b	612	-	1/1/15/20	3/37/115/115	-
33	CLA	c	514	-	1/1/15/20	4/37/115/115	-
33	CLA	p	310	-	1/1/10/20	5/8/86/115	-
33	CLA	5	308	-	1/1/10/20	1/8/86/115	-
33	CLA	1	302	3	1/1/14/20	7/36/114/115	-
39	II0	6	317	-	-	2/21/67/67	0/2/2/2
41	SQD	B	601	-	-	11/33/53/69	0/1/1/1
39	II0	g	312	-	-	1/21/67/67	0/2/2/2
33	CLA	0	301	2	1/1/10/20	3/8/86/115	-
39	II0	1	316	-	-	2/21/67/67	0/2/2/2
33	CLA	9	306	5	1/1/10/20	1/8/86/115	-
38	KC2	6	311	7	-	3/15/71/71	-
38	KC2	g	309	-	-	4/15/71/71	-
42	LMG	B	624	-	-	16/38/58/70	0/1/1/1
33	CLA	9	307	-	1/1/11/20	7/13/91/115	-
39	II0	1	315	-	-	2/21/67/67	0/2/2/2
33	CLA	p	303	7	1/1/10/20	2/8/86/115	-
38	KC2	3	311	-	-	7/15/71/71	-
33	CLA	8	305	-	1/1/13/20	5/25/103/115	-
33	CLA	p	306	-	1/1/11/20	6/13/91/115	-
33	CLA	B	602	-	1/1/12/20	6/19/97/115	-
39	II0	3	317	-	-	0/21/67/67	0/2/2/2
33	CLA	0	308	37	1/1/11/20	11/16/94/115	-
33	CLA	C	506	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	8	301	4	1/1/11/20	4/13/91/115	-
33	CLA	9	313	-	1/1/10/20	2/8/86/115	-
33	CLA	4	310	-	1/1/11/20	5/13/91/115	-
33	CLA	g	302	6	1/1/13/20	8/25/103/115	-
33	CLA	B	614	-	1/1/15/20	8/37/115/115	-
33	CLA	0	302	2	1/1/12/20	3/21/99/115	-
39	II0	6	301	-	-	0/21/67/67	0/2/2/2
39	II0	6	315	-	-	2/21/67/67	0/2/2/2
33	CLA	d	405	-	1/1/15/20	9/37/115/115	-
33	CLA	7	302	3	1/1/14/20	7/36/114/115	-
38	KC2	1	311	-	-	6/15/71/71	-
39	II0	3	301	-	-	1/21/67/67	0/2/2/2
39	II0	0	316	-	-	2/21/67/67	0/2/2/2
39	II0	7	314	-	-	1/21/67/67	0/2/2/2
39	II0	7	316	-	-	2/21/67/67	0/2/2/2
33	CLA	6	308	7	1/1/10/20	5/10/88/115	-
33	CLA	b	608	-	1/1/15/20	6/37/115/115	-
33	CLA	g	304	-	1/1/11/20	3/13/91/115	-
33	CLA	b	603	-	1/1/15/20	4/37/115/115	-
33	CLA	4	306	2	1/1/13/20	9/25/103/115	-
39	II0	4	312	-	-	2/21/67/67	0/2/2/2
37	LHG	D	402	-	-	19/51/51/53	-
35	8CT	C	515	-	-	8/29/63/63	0/2/2/2
33	CLA	C	508	-	1/1/15/20	6/37/115/115	-
33	CLA	N	301	-	1/1/15/20	12/37/115/115	-
33	CLA	5	310	-	1/1/10/20	0/8/86/115	-
33	CLA	4	304	-	1/1/11/20	4/16/94/115	-
35	8CT	D	406	-	-	9/29/63/63	0/2/2/2
43	DGD	h	101	-	-	13/49/89/95	0/2/2/2
33	CLA	B	604	-	1/1/15/20	3/37/115/115	-
34	PHO	a	407	-	-	10/37/103/103	0/5/6/6
33	CLA	g	311	-	1/1/11/20	7/13/91/115	-
39	II0	g	314	-	-	0/21/67/67	0/2/2/2
33	CLA	6	319	-	1/1/10/20	6/8/86/115	-
33	CLA	9	314	-	1/1/10/20	0/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	9	302	-	-	19/45/45/53	-
33	CLA	b	606	-	1/1/15/20	3/37/115/115	-
33	CLA	C	502	-	1/1/15/20	3/37/115/115	-
35	8CT	y	101	-	-	8/29/63/63	0/2/2/2
33	CLA	C	512	-	1/1/15/20	7/37/115/115	-
41	SQD	j	101	-	-	20/41/61/69	0/1/1/1
43	DGD	C	519	-	-	23/51/91/95	0/2/2/2
33	CLA	B	608	-	1/1/15/20	6/37/115/115	-
33	CLA	B	603	-	1/1/15/20	4/37/115/115	-
42	LMG	d	409	-	-	17/41/61/70	0/1/1/1
35	8CT	b	621	-	-	8/29/63/63	0/2/2/2
33	CLA	b	609	-	1/1/15/20	2/37/115/115	-
37	LHG	2	315	-	-	35/50/50/53	-
35	8CT	7	312	-	-	5/29/63/63	0/2/2/2
33	CLA	1	307	-	1/1/15/20	5/37/115/115	-
33	CLA	9	304	-	1/1/11/20	0/13/91/115	-
43	DGD	c	521	-	-	23/51/91/95	0/2/2/2
33	CLA	g	303	-	1/1/13/20	3/25/103/115	-
39	II0	1	313	-	-	1/21/67/67	0/2/2/2
44	HEM	V	201	-	-	3/12/54/54	-
33	CLA	C	503	-	1/1/15/20	8/37/115/115	-
33	CLA	4	301	2	1/1/10/20	3/8/86/115	-
33	CLA	9	303	5	1/1/13/20	6/25/103/115	-
33	CLA	6	310	-	1/1/10/20	5/8/86/115	-
37	LHG	9	321	-	-	13/27/27/53	-
33	CLA	B	617	-	1/1/14/20	3/31/109/115	-
33	CLA	b	607	-	1/1/15/20	9/37/115/115	-
33	CLA	8	303	-	1/1/12/20	13/22/100/115	-
33	CLA	b	617	-	1/1/14/20	3/31/109/115	-
35	8CT	c	516	-	-	5/29/63/63	0/2/2/2
33	CLA	5	304	-	1/1/11/20	3/13/91/115	-
39	II0	p	314	-	-	0/21/67/67	0/2/2/2
33	CLA	0	307	2	1/1/13/20	10/25/103/115	-
34	PHO	D	403	-	-	6/37/103/103	0/5/6/6
33	CLA	7	307	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	6	305	-	1/1/13/20	4/25/103/115	-
33	CLA	c	511	-	1/1/15/20	8/37/115/115	-
33	CLA	9	310	-	1/1/10/20	2/8/86/115	-
43	DGD	c	519	-	-	23/51/91/95	0/2/2/2
37	LHG	4	316	33	-	7/27/27/53	-
38	KC2	8	309	-	-	9/15/71/71	-
33	CLA	6	313	-	1/1/10/20	4/8/86/115	-
33	CLA	B	612	-	1/1/15/20	3/37/115/115	-
33	CLA	B	615	-	1/1/11/20	4/13/91/115	-
38	KC2	2	309	-	-	9/15/71/71	-
33	CLA	1	306	-	1/1/14/20	6/31/109/115	-
33	CLA	D	405	-	1/1/15/20	9/37/115/115	-
33	CLA	B	606	-	1/1/15/20	3/37/115/115	-
44	HEM	v	201	-	-	3/12/54/54	-
35	8CT	b	619	-	-	3/29/63/63	0/2/2/2
33	CLA	6	309	7	1/1/10/20	2/10/88/115	-
33	CLA	c	502	-	1/1/15/20	3/37/115/115	-
33	CLA	g	307	-	1/1/13/20	8/25/103/115	-
33	CLA	p	319	-	1/1/10/20	6/8/86/115	-
37	LHG	g	316	-	-	10/24/24/53	-
42	LMG	D	409	-	-	17/41/61/70	0/1/1/1
33	CLA	3	305	-	1/1/13/20	4/25/103/115	-
35	8CT	A	409	-	-	3/29/63/63	0/2/2/2
39	II0	0	315	-	-	1/21/67/67	0/2/2/2
43	DGD	c	518	-	-	12/44/84/95	0/2/2/2
37	LHG	0	317	33	-	7/27/27/53	-
39	II0	0	314	-	-	2/21/67/67	0/2/2/2
39	II0	4	315	-	-	3/21/67/67	0/2/2/2
33	CLA	4	303	-	1/1/12/20	5/19/97/115	-
33	CLA	p	309	7	1/1/10/20	2/10/88/115	-
33	CLA	n	306	-	1/1/12/20	4/19/97/115	-
33	CLA	8	306	4	1/1/14/20	3/31/109/115	-
33	CLA	N	307	-	1/1/12/20	4/19/97/115	-
43	DGD	C	521	-	-	23/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CLA	6	312	-	1/1/10/20	2/8/86/115	-
39	II0	9	317	-	-	0/21/67/67	0/2/2/2
40	IHT	2	314	-	-	0/25/65/65	0/2/2/2
35	8CT	Y	101	-	-	8/29/63/63	0/2/2/2
33	CLA	1	309	-	1/1/13/20	0/25/103/115	-
38	KC2	p	311	7	-	3/15/71/71	-
37	LHG	7	317	-	-	21/53/53/53	-
33	CLA	5	317	-	1/1/9/20	1/8/82/115	-
42	LMG	W	101	-	-	26/42/62/70	0/1/1/1
33	CLA	c	503	-	1/1/15/20	7/37/115/115	-
33	CLA	9	312	5	1/1/13/20	2/25/103/115	-
33	CLA	7	304	-	1/1/13/20	4/25/103/115	-
33	CLA	g	305	-	1/1/9/20	2/8/82/115	-
36	PL9	d	407	-	-	18/53/73/73	0/1/1/1
33	CLA	a	408	-	1/1/14/20	2/31/109/115	-
33	CLA	b	605	-	1/1/15/20	14/37/115/115	-
33	CLA	6	304	-	1/1/10/20	2/10/88/115	-
35	8CT	c	517	-	-	6/29/63/63	0/2/2/2
37	LHG	d	401	-	-	25/50/50/53	-
33	CLA	n	301	-	1/1/15/20	12/37/115/115	-
33	CLA	2	310	-	1/1/11/20	2/15/93/115	-
33	CLA	3	315	-	1/1/10/20	4/8/86/115	-
37	LHG	B	623	-	-	28/53/53/53	-
35	8CT	a	409	-	-	3/29/63/63	0/2/2/2
33	CLA	d	404	-	1/1/15/20	1/37/115/115	-
33	CLA	N	304	-	1/1/10/20	1/8/86/115	-
33	CLA	B	610	-	1/1/15/20	8/37/115/115	-
33	CLA	1	303	-	1/1/12/20	3/21/99/115	-
39	II0	3	318	-	-	1/21/67/67	0/2/2/2
39	II0	5	312	-	-	2/21/67/67	0/2/2/2
33	CLA	2	306	4	1/1/14/20	3/31/109/115	-
33	CLA	0	310	-	1/1/9/20	8/8/82/115	-
33	CLA	5	305	-	1/1/9/20	2/8/82/115	-
33	CLA	0	306	2	1/1/13/20	9/25/103/115	-
33	CLA	A	405	-	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	IHT	9	320	-	-	7/25/65/65	0/2/2/2
33	CLA	a	406	-	1/1/11/20	6/18/96/115	-
39	II0	p	317	-	-	2/21/67/67	0/2/2/2
39	II0	1	314	-	-	1/21/67/67	0/2/2/2
37	LHG	a	411	-	-	6/28/28/53	-
33	CLA	g	301	6	1/1/10/20	5/10/88/115	-
33	CLA	4	307	2	1/1/13/20	10/25/103/115	-
39	II0	7	315	-	-	2/21/67/67	0/2/2/2
42	LMG	m	101	-	-	9/33/53/70	0/1/1/1
40	IHT	6	318	-	-	2/25/65/65	0/2/2/2
33	CLA	C	511	-	1/1/15/20	8/37/115/115	-
33	CLA	5	311	-	1/1/11/20	7/13/91/115	-
33	CLA	0	309	-	1/1/11/20	11/16/94/115	-
33	CLA	9	309	5	1/1/13/20	6/25/103/115	-
33	CLA	b	611	-	1/1/15/20	5/37/115/115	-
41	SQD	C	501	-	-	9/37/57/69	0/1/1/1
42	LMG	l	102	-	-	9/33/53/70	0/1/1/1
33	CLA	7	308	-	1/1/12/20	6/21/99/115	-
33	CLA	n	304	-	1/1/13/20	5/25/103/115	-
37	LHG	d	408	-	-	20/53/53/53	-
35	8CT	h	102	-	-	7/29/63/63	0/2/2/2
33	CLA	N	306	-	1/1/13/20	2/25/103/115	-
33	CLA	g	310	-	1/1/10/20	0/8/86/115	-
39	II0	3	316	-	-	3/21/67/67	0/2/2/2
33	CLA	C	505	-	1/1/15/20	11/37/115/115	-
42	LMG	b	622	-	-	21/44/64/70	0/1/1/1
33	CLA	0	311	-	1/1/11/20	5/13/91/115	-
35	8CT	C	516	-	-	5/29/63/63	0/2/2/2
39	II0	7	313	-	-	1/21/67/67	0/2/2/2
33	CLA	2	308	-	1/1/13/20	1/25/103/115	-
33	CLA	C	513	-	1/1/13/20	6/27/105/115	-
33	CLA	3	303	5	1/1/13/20	6/25/103/115	-
41	SQD	b	601	-	-	11/33/53/69	0/1/1/1
39	II0	8	313	-	-	5/21/67/67	0/2/2/2
33	CLA	c	505	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	IHT	p	318	-	-	2/25/65/65	0/2/2/2
33	CLA	A	408	-	1/1/14/20	2/31/109/115	-
33	CLA	4	309	-	1/1/9/20	8/8/82/115	-
33	CLA	c	507	-	1/1/15/20	10/37/115/115	-
39	II0	2	313	-	-	5/21/67/67	0/2/2/2
33	CLA	n	303	-	1/1/10/20	1/8/86/115	-
33	CLA	1	304	-	1/1/13/20	4/25/103/115	-
33	CLA	D	404	-	1/1/15/20	1/37/115/115	-
37	LHG	3	322	-	-	19/45/45/53	-
39	II0	9	319	-	-	2/21/67/67	0/2/2/2
33	CLA	0	303	-	1/1/12/20	5/19/97/115	-
33	CLA	B	618	-	1/1/9/20	2/8/82/115	-
35	8CT	H	102	-	-	7/29/63/63	0/2/2/2
33	CLA	C	509	-	1/1/15/20	4/37/115/115	-
39	II0	p	315	-	-	2/21/67/67	0/2/2/2
37	LHG	D	401	-	-	25/50/50/53	-
33	CLA	9	315	-	1/1/10/20	4/8/86/115	-
33	CLA	5	301	6	1/1/10/20	5/10/88/115	-
35	8CT	C	517	-	-	6/29/63/63	0/2/2/2
33	CLA	7	305	3	1/1/14/20	7/31/109/115	-
33	CLA	7	301	3	1/1/11/20	3/13/91/115	-
39	II0	4	313	-	-	2/21/67/67	0/2/2/2
33	CLA	8	302	4	1/1/13/20	10/25/103/115	-
33	CLA	p	308	7	1/1/10/20	5/10/88/115	-
33	CLA	8	308	-	1/1/13/20	1/25/103/115	-
40	IHT	8	314	-	-	0/25/65/65	0/2/2/2
35	8CT	c	515	-	-	8/29/63/63	0/2/2/2
39	II0	8	311	-	-	0/21/67/67	0/2/2/2
33	CLA	N	302	-	1/1/15/20	6/37/115/115	-
33	CLA	A	406	-	1/1/11/20	6/18/96/115	-
36	PL9	a	410	-	-	5/23/43/73	0/1/1/1
41	SQD	c	501	-	-	9/37/57/69	0/1/1/1
33	CLA	9	308	-	1/1/11/20	2/18/96/115	-
33	CLA	3	312	5	1/1/13/20	2/25/103/115	-
37	LHG	D	408	-	-	21/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	DGD	H	101	-	-	13/49/89/95	0/2/2/2
39	II0	p	316	-	-	0/21/67/67	0/2/2/2
33	CLA	B	609	-	1/1/15/20	2/37/115/115	-
38	KC2	0	305	-	-	9/15/71/71	-
33	CLA	N	303	37	1/1/11/20	11/16/94/115	-
33	CLA	3	310	-	1/1/10/20	2/8/86/115	-
33	CLA	8	310	-	1/1/11/20	2/15/93/115	-
33	CLA	c	513	-	1/1/13/20	6/27/105/115	-
33	CLA	a	412	-	1/1/15/20	8/37/115/115	-
33	CLA	7	309	-	1/1/13/20	0/25/103/115	-
35	8CT	B	619	-	-	3/29/63/63	0/2/2/2
33	CLA	0	304	-	1/1/11/20	4/16/94/115	-
34	PHO	A	407	-	-	10/37/103/103	0/5/6/6
33	CLA	g	317	-	1/1/9/20	1/8/82/115	-
38	KC2	7	311	-	-	6/15/71/71	-
33	CLA	p	313	-	1/1/10/20	4/8/86/115	-
34	PHO	d	403	-	-	6/37/103/103	0/5/6/6
33	CLA	6	307	-	1/1/10/20	1/11/89/115	-
33	CLA	c	506	-	1/1/15/20	7/37/115/115	-
33	CLA	9	305	-	1/1/13/20	4/25/103/115	-
33	CLA	2	304	-	1/1/14/20	5/31/109/115	-
42	LMG	c	520	-	-	28/46/66/70	0/1/1/1
33	CLA	3	313	-	1/1/10/20	2/8/86/115	-
33	CLA	b	618	-	1/1/9/20	2/8/82/115	-
33	CLA	p	305	-	1/1/13/20	4/25/103/115	-
33	CLA	B	605	-	1/1/15/20	14/37/115/115	-
40	IHT	3	320	-	-	7/25/65/65	0/2/2/2
33	CLA	b	604	-	1/1/15/20	3/37/115/115	-

The worst 5 of 1906 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	p	302	CLA	C1B-NB	11.31	1.45	1.35
33	6	302	CLA	C1B-NB	11.28	1.45	1.35
33	g	308	CLA	C1B-NB	10.86	1.44	1.35
33	5	308	CLA	C1B-NB	10.86	1.44	1.35
33	5	310	CLA	C1B-NB	10.82	1.44	1.35

The worst 5 of 1835 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	p	302	CLA	C4A-NA-C1A	-8.29	102.98	106.71
33	6	302	CLA	C4A-NA-C1A	-8.28	102.98	106.71
33	2	302	CLA	C4A-NA-C1A	-8.27	102.99	106.71
33	0	310	CLA	C4A-NA-C1A	-8.25	103.00	106.71
33	8	302	CLA	C4A-NA-C1A	-8.23	103.01	106.71

5 of 210 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
33	a	405	CLA	ND
33	a	406	CLA	ND
33	a	408	CLA	ND
33	a	412	CLA	ND
33	A	405	CLA	ND

5 of 2423 torsion outliers are listed below:

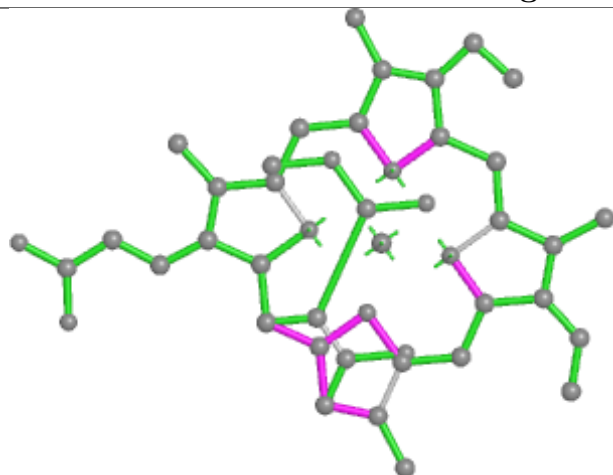
Mol	Chain	Res	Type	Atoms
33	a	412	CLA	C1A-C2A-CAA-CBA
33	a	412	CLA	C3A-C2A-CAA-CBA
33	A	412	CLA	C1A-C2A-CAA-CBA
33	A	412	CLA	C3A-C2A-CAA-CBA
33	0	306	CLA	C2-C3-C5-C6

There are no ring outliers.

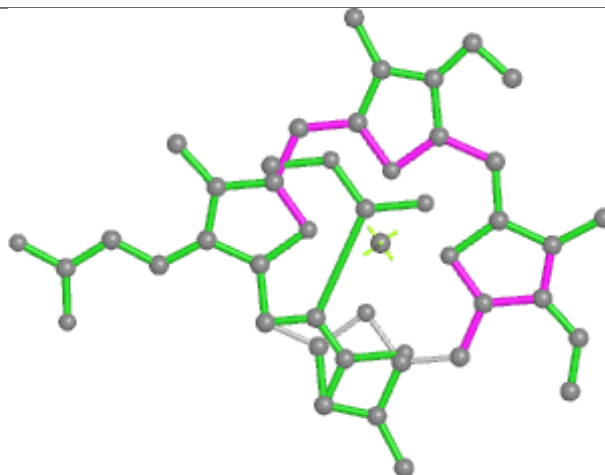
No monomer is involved in short contacts.

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.

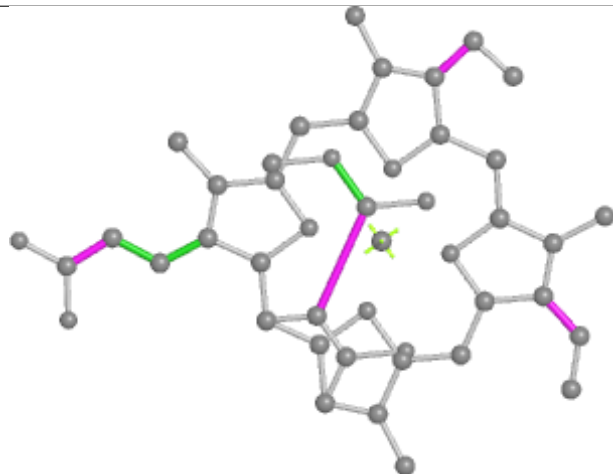
## Ligand KC2 1 310



Bond lengths



Bond angles

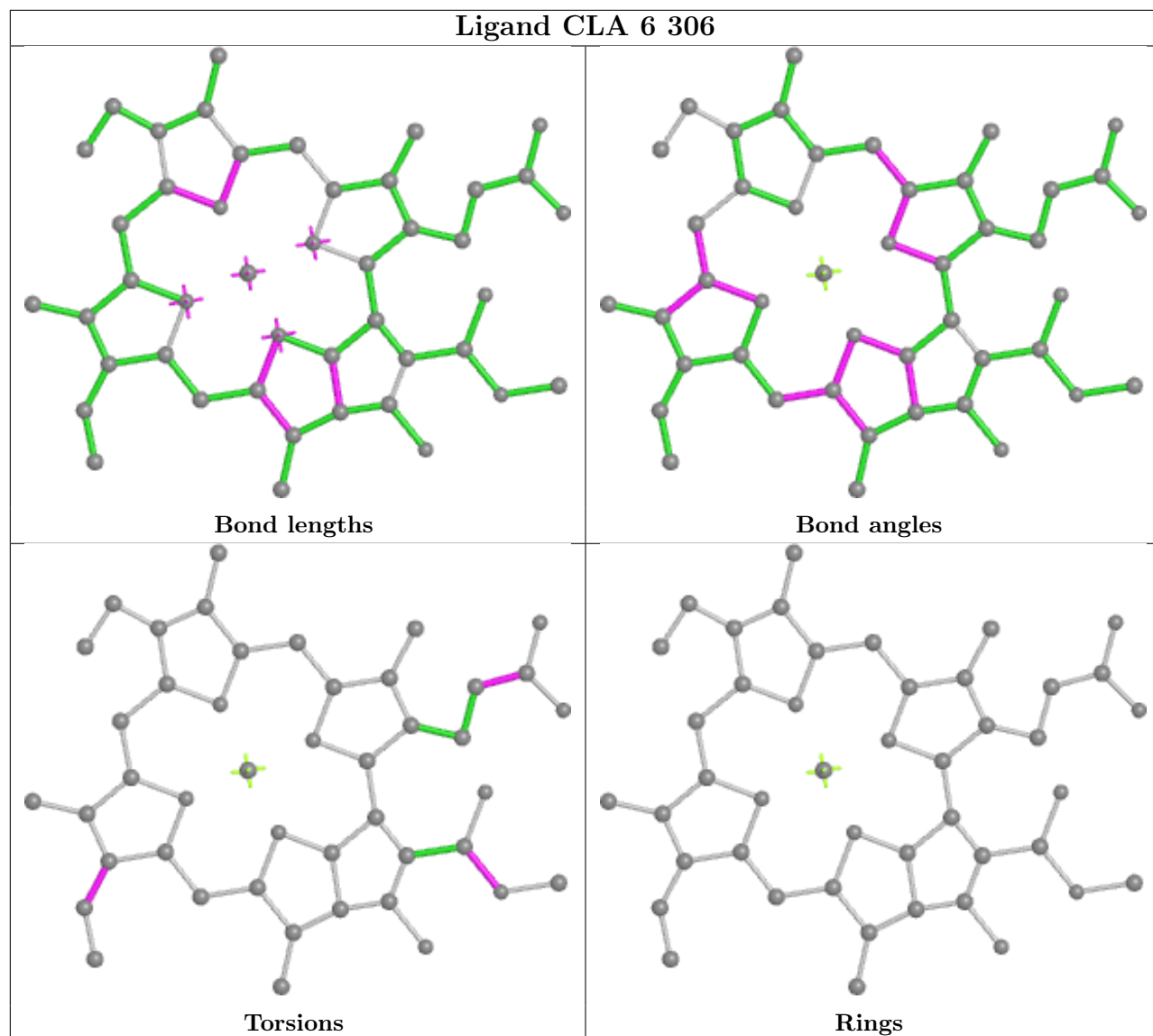


Torsions

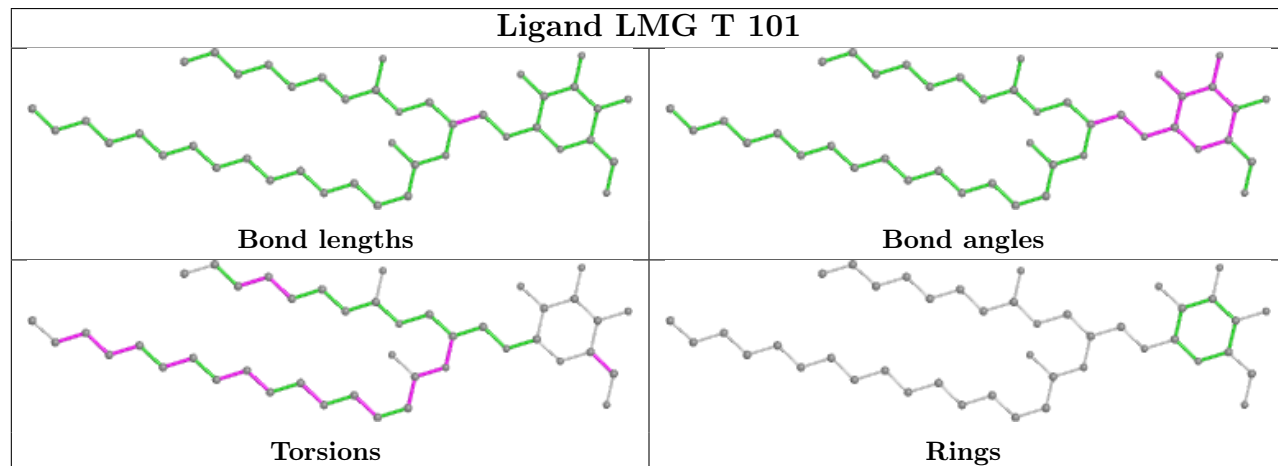


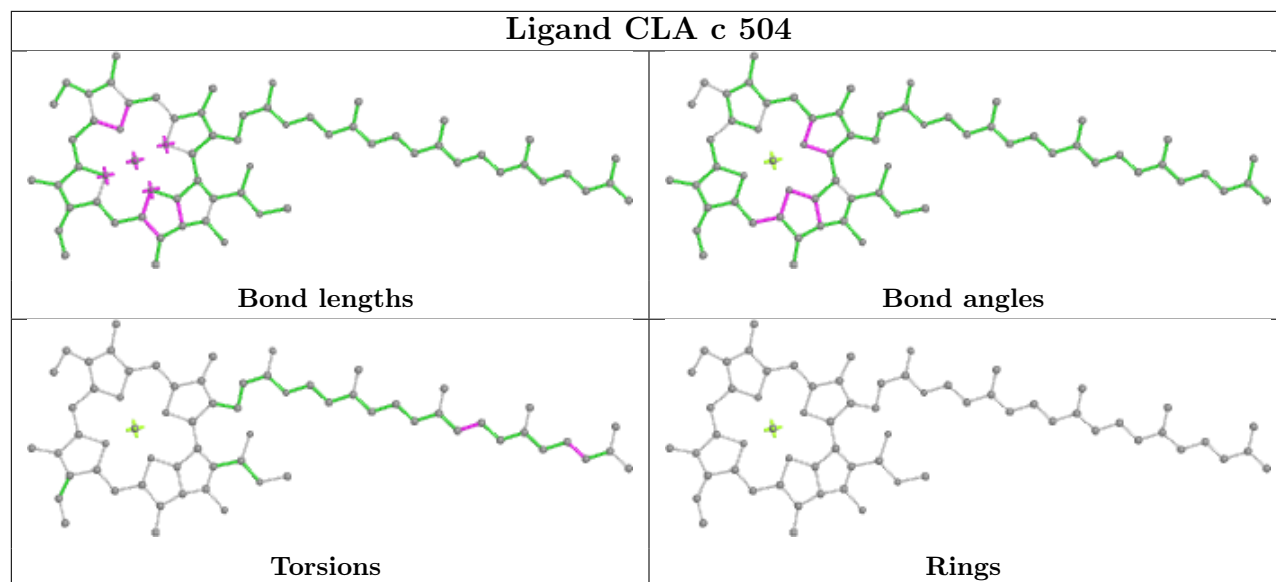
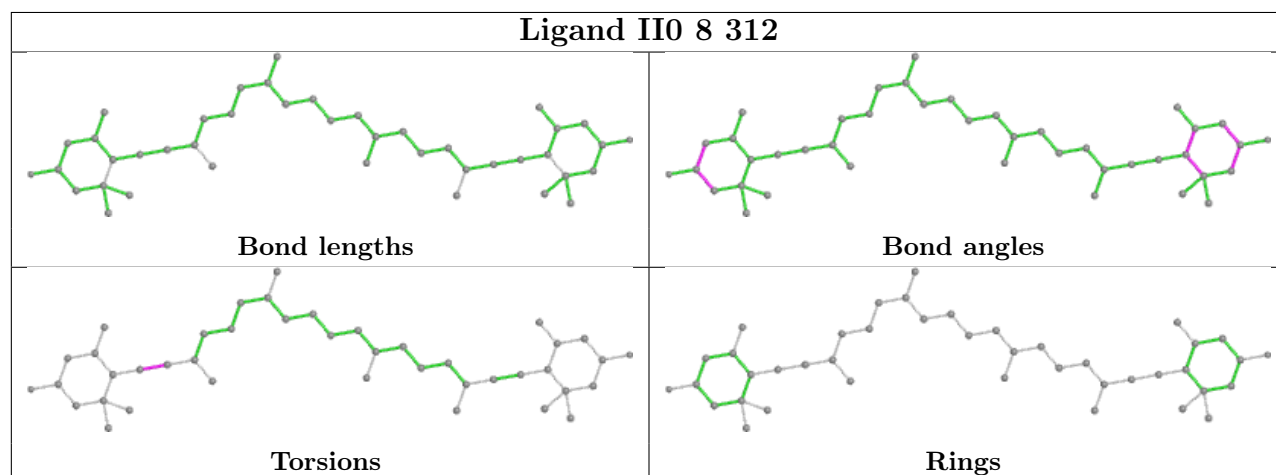
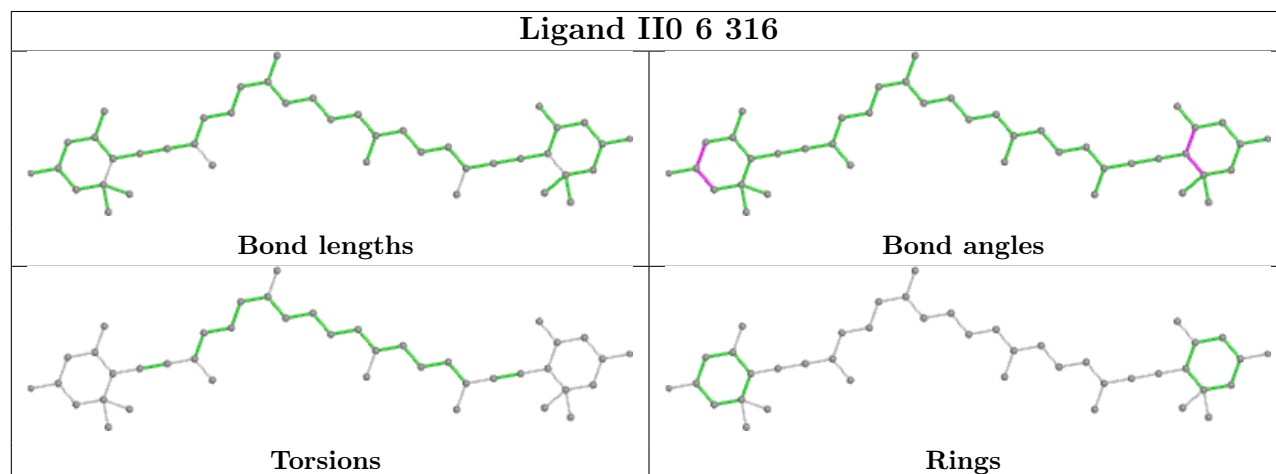
Rings

## Ligand CLA 6 306



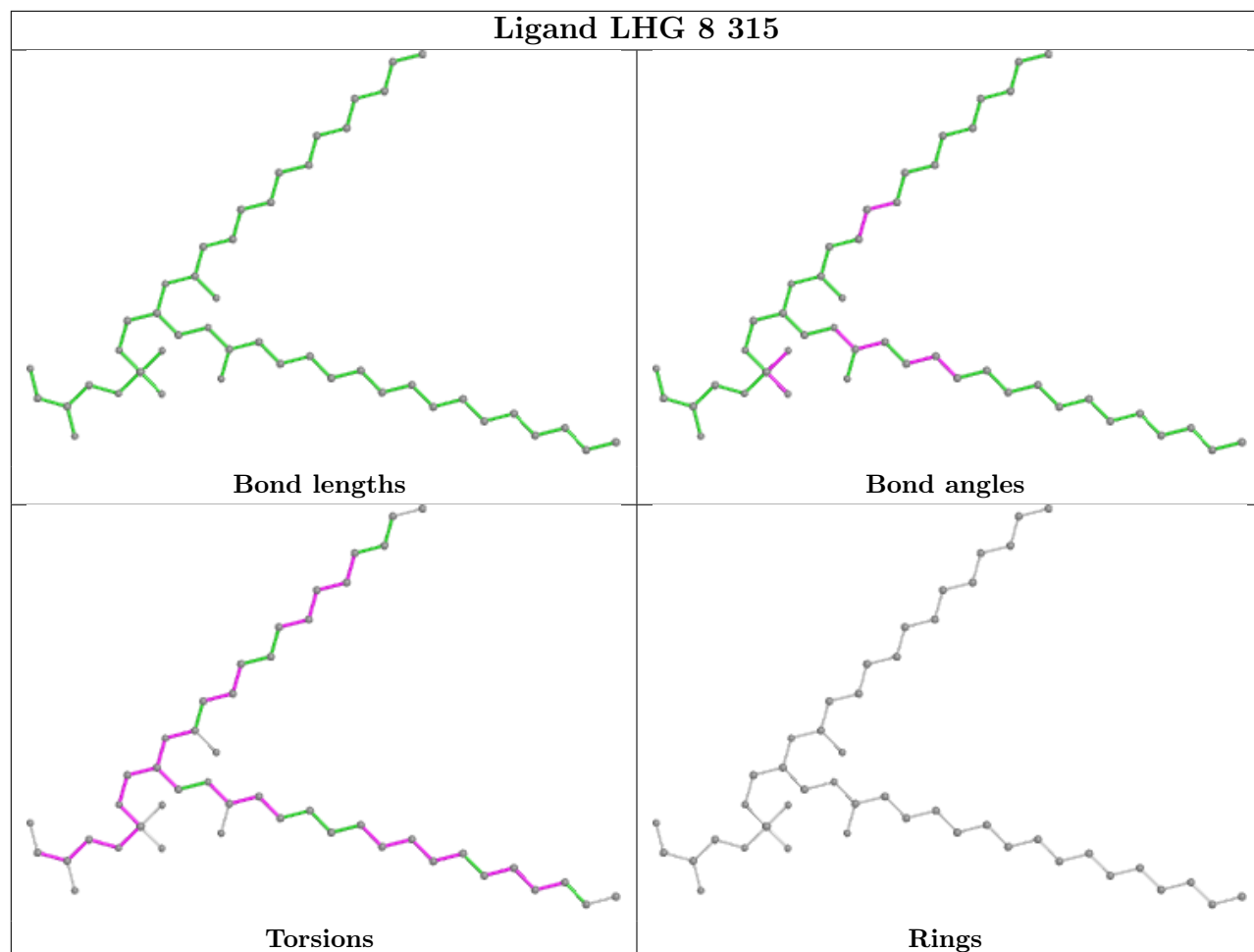
## Ligand LMG T 101



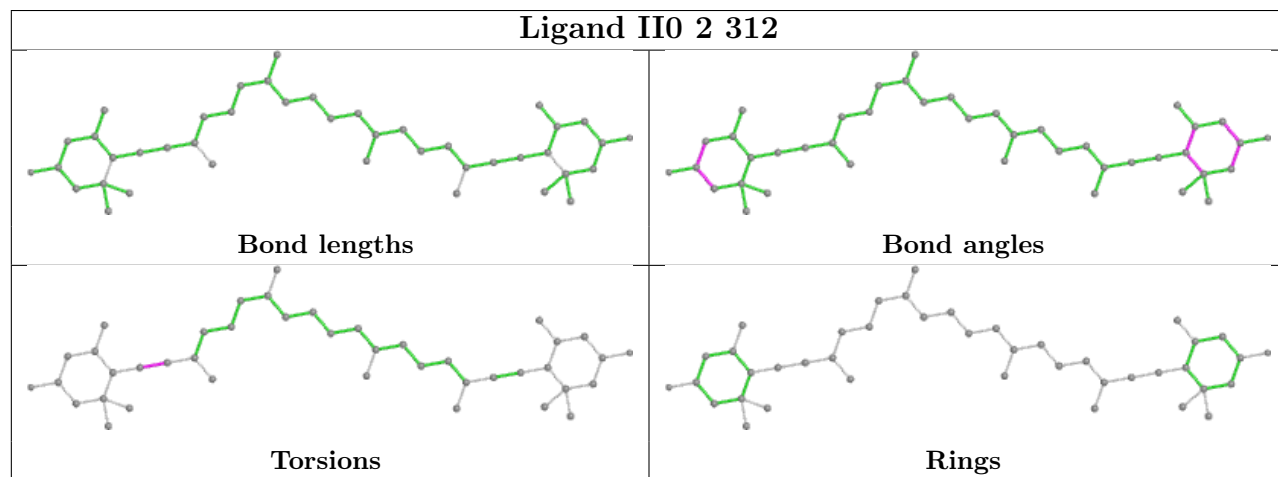
**Ligand CLA c 504****Ligand II0 8 312****Ligand II0 6 316**

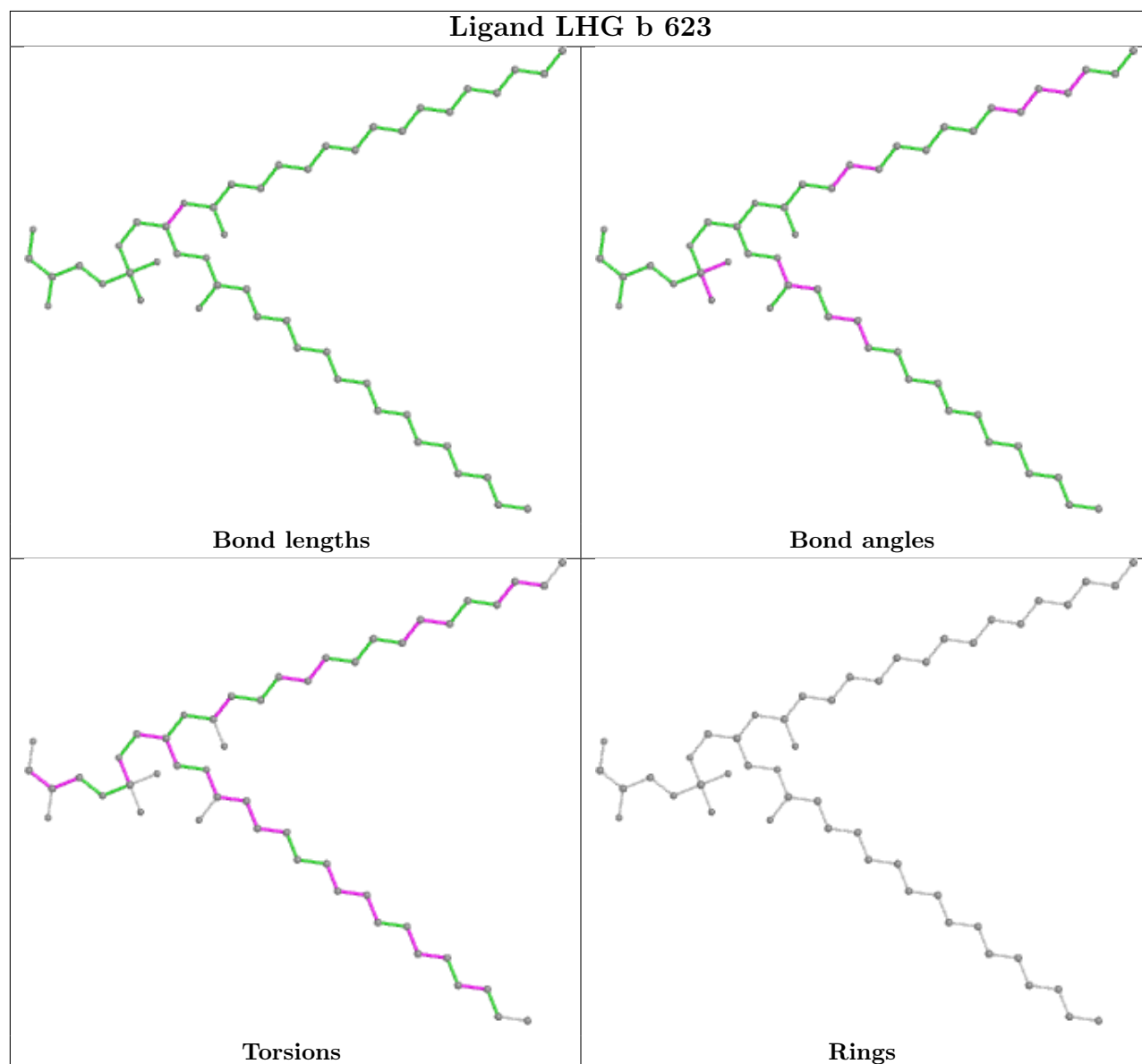
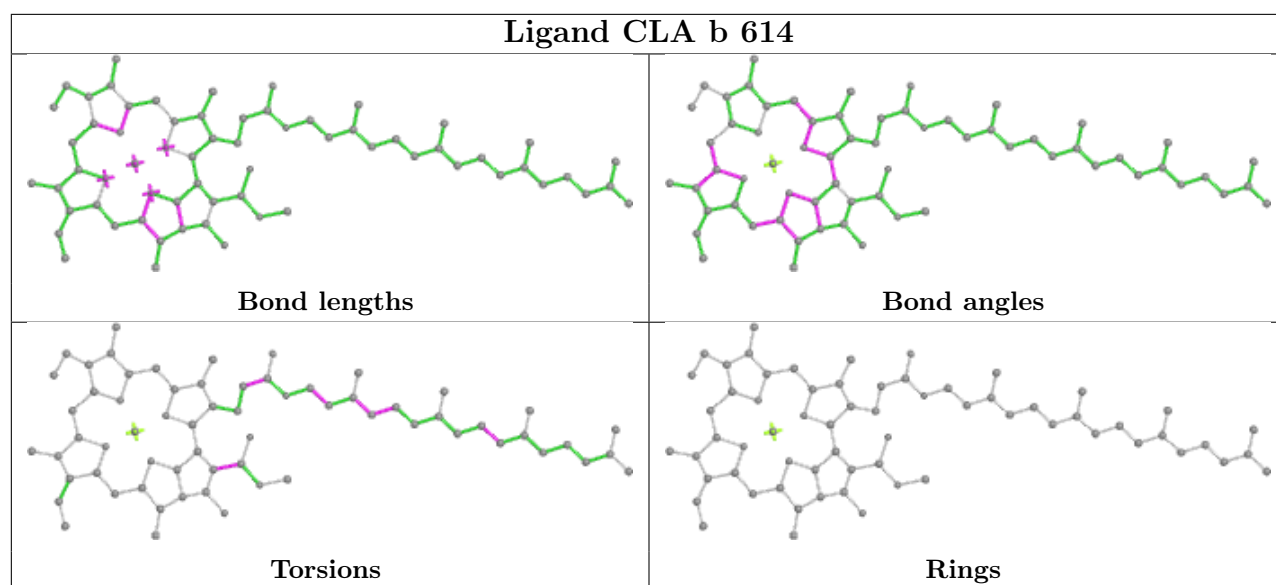


## Ligand LHG 8 315

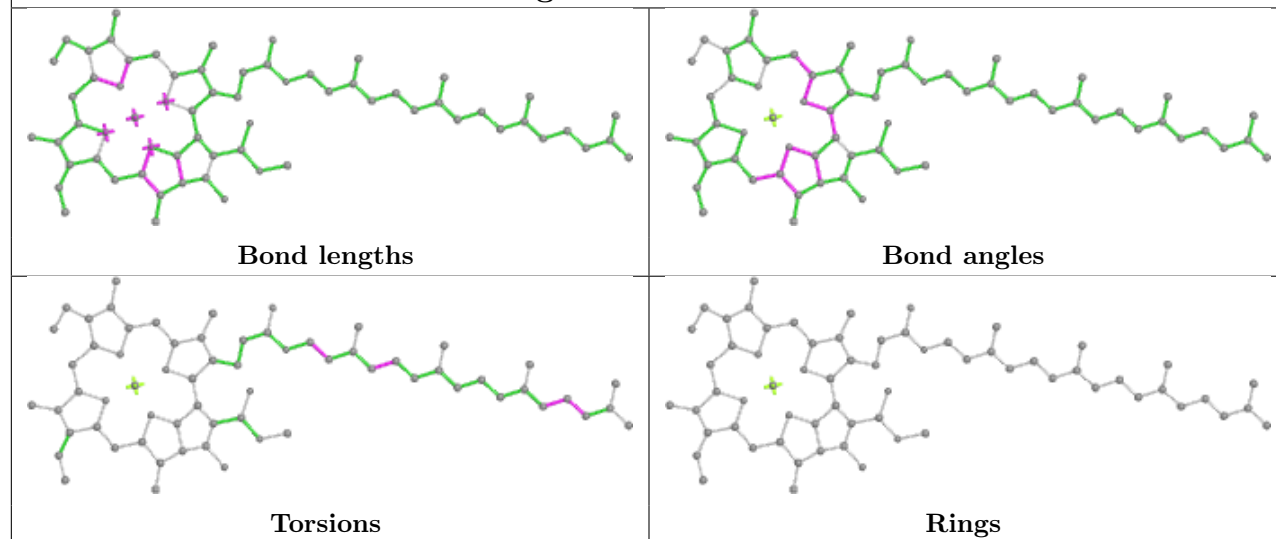


## Ligand II0 2 312

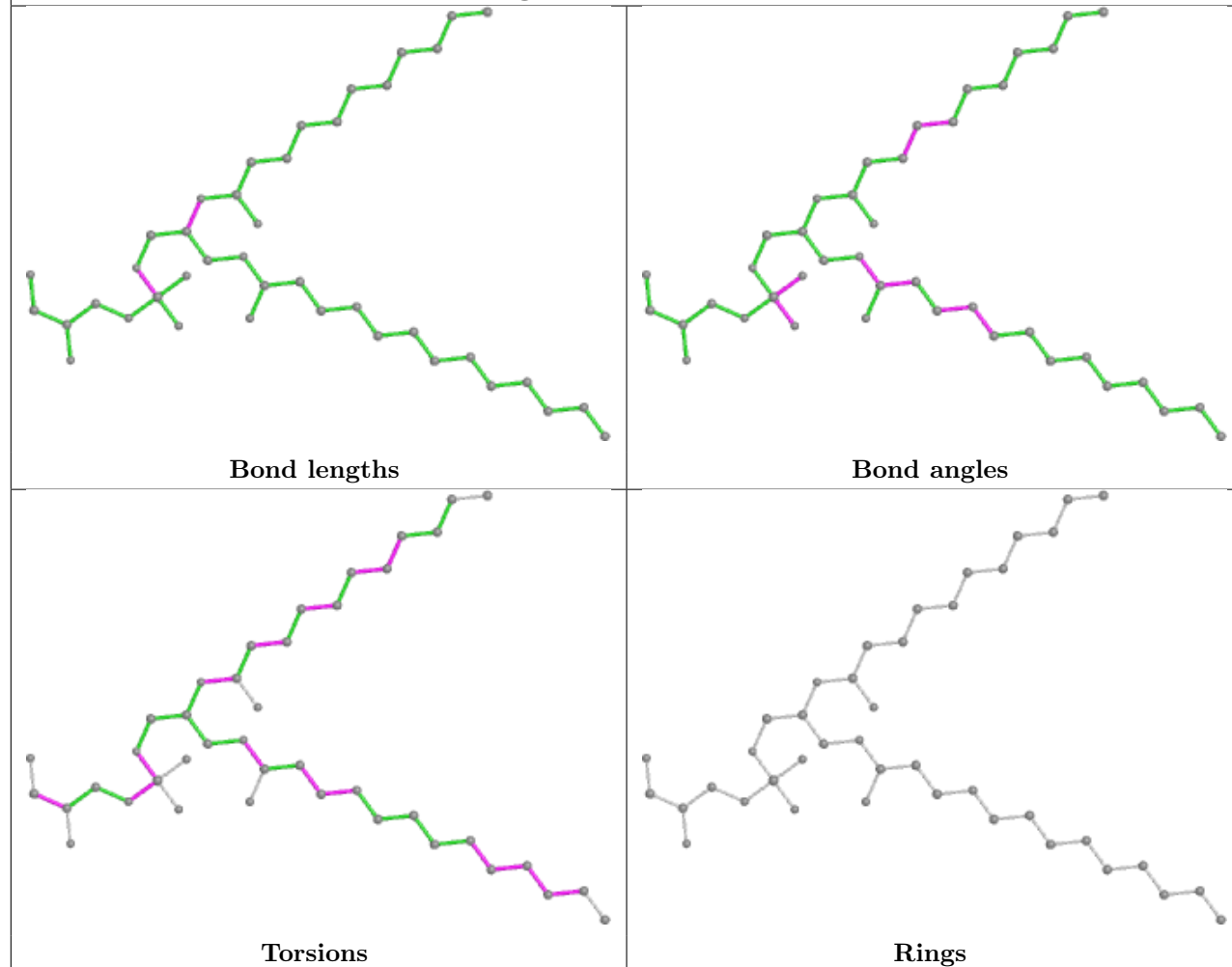


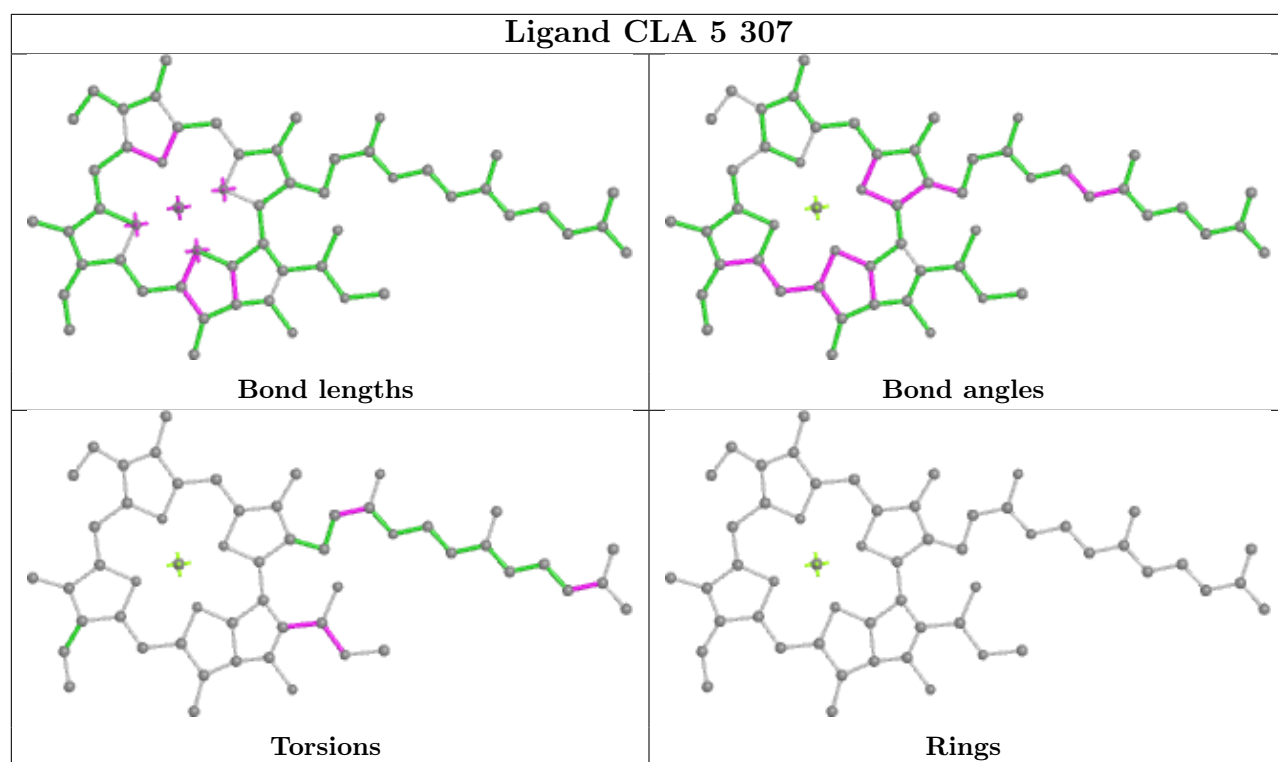


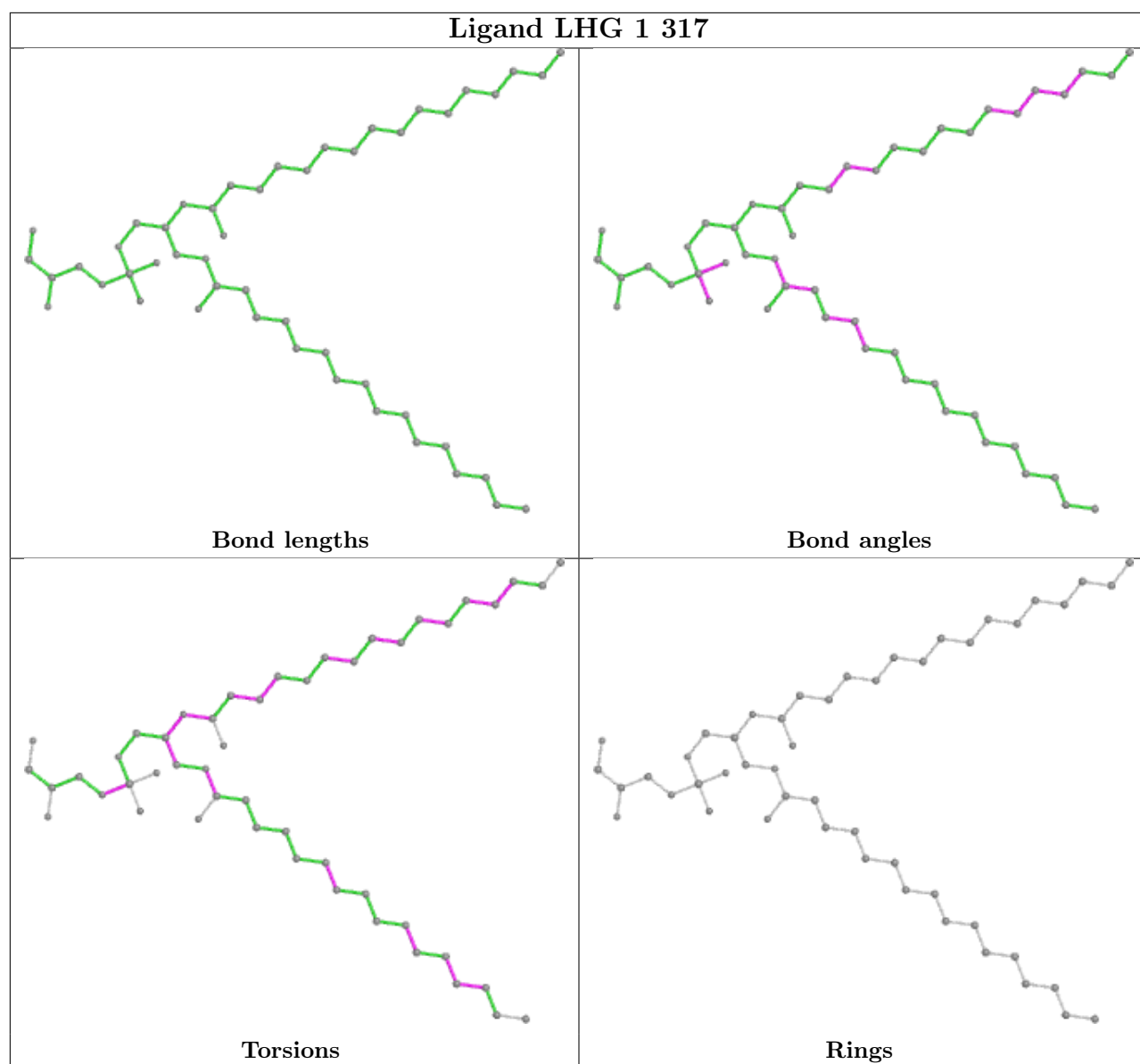
## Ligand CLA a 405

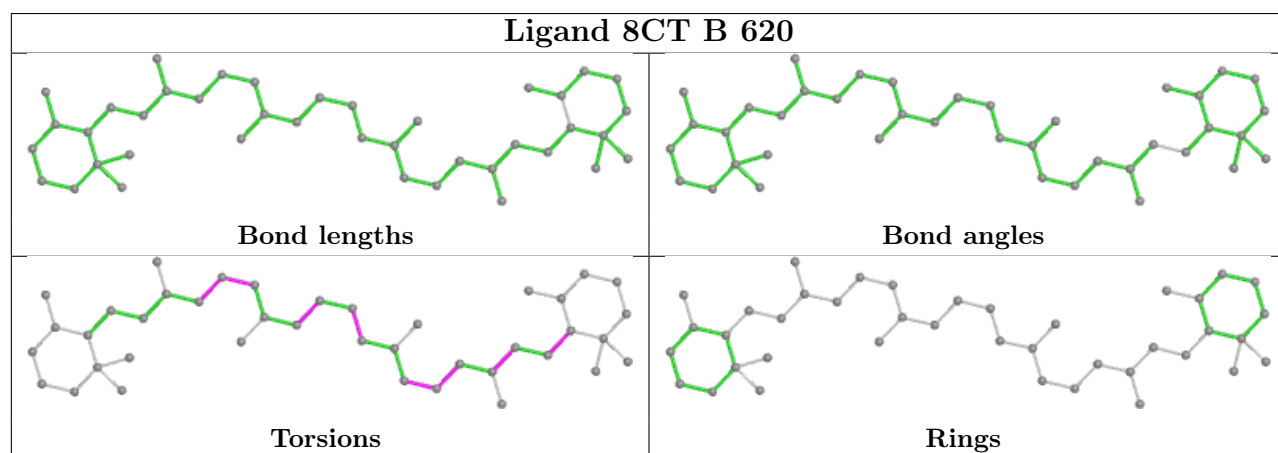
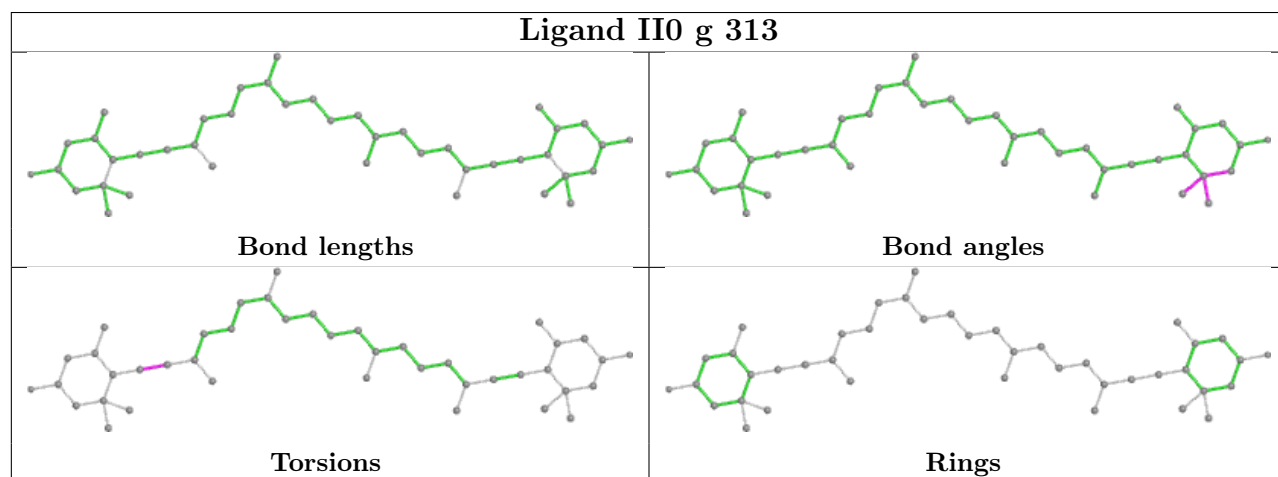
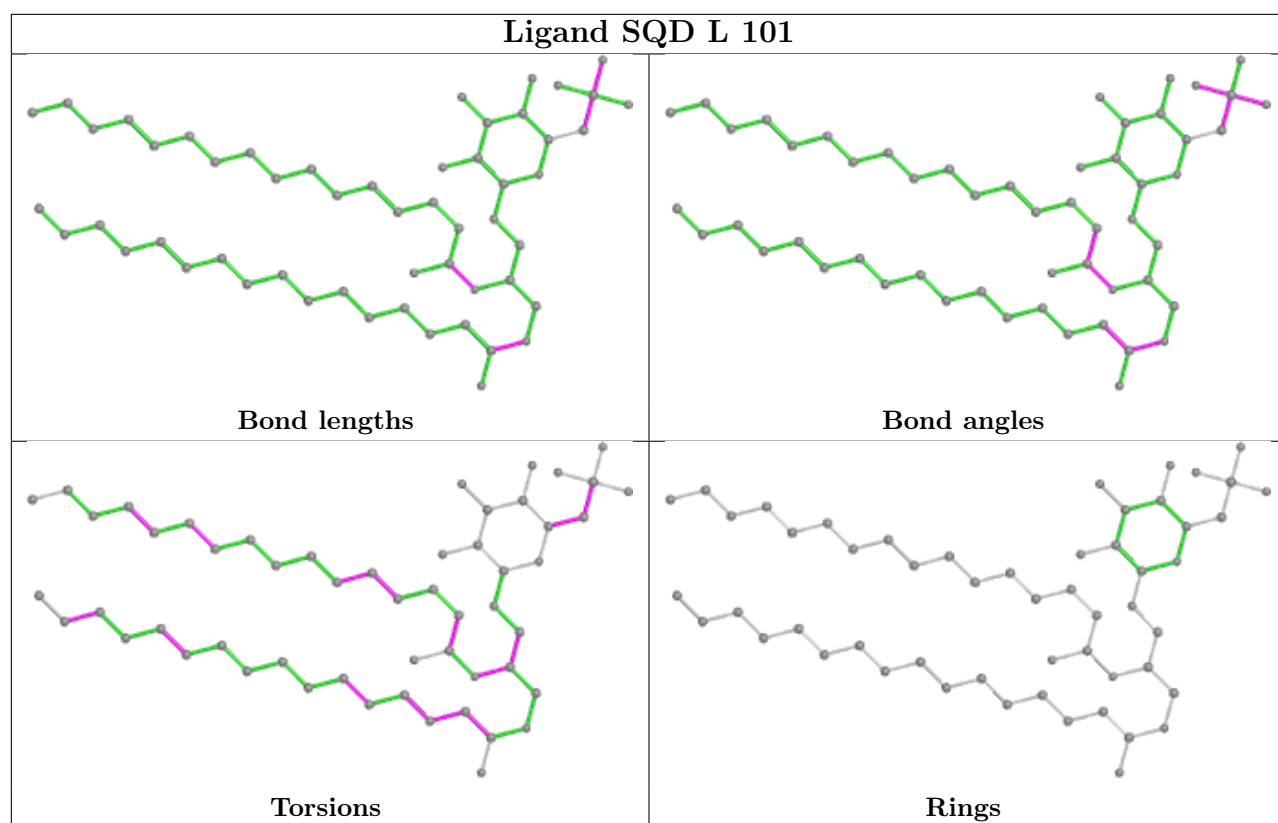


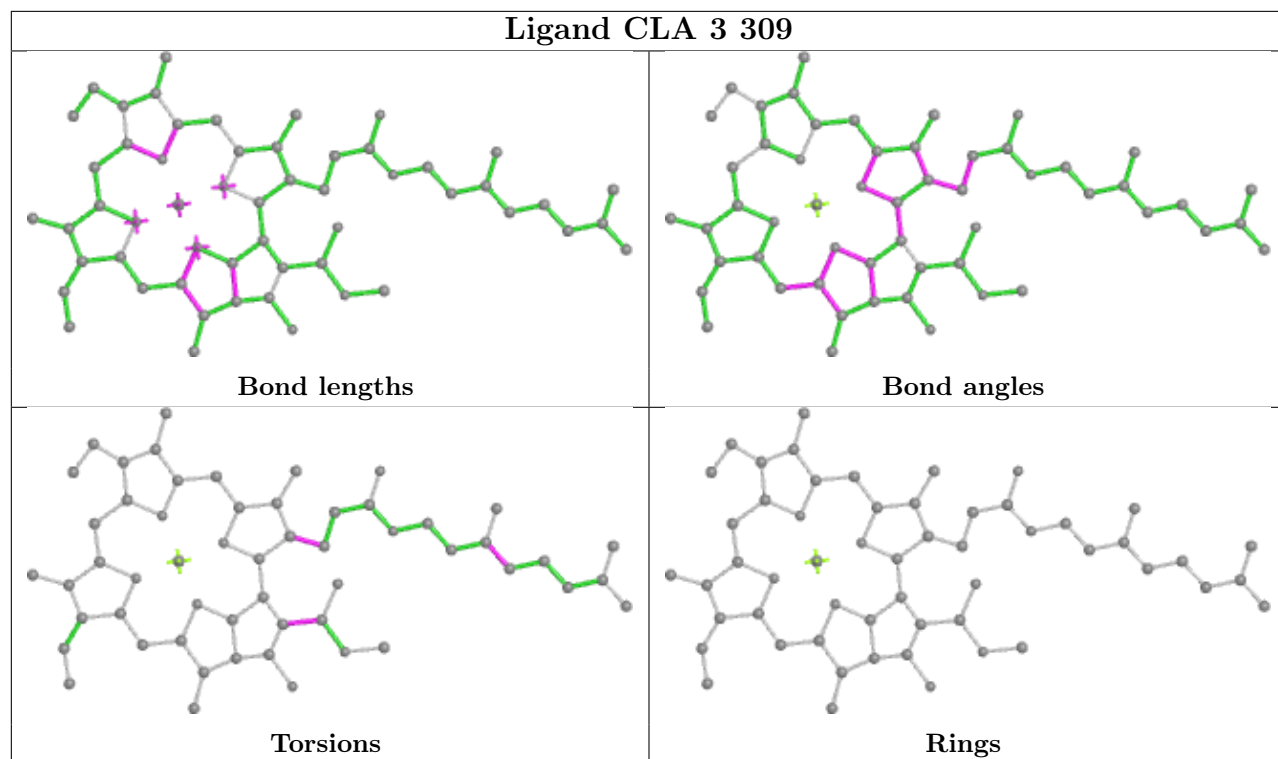
## Ligand LHG 9 322



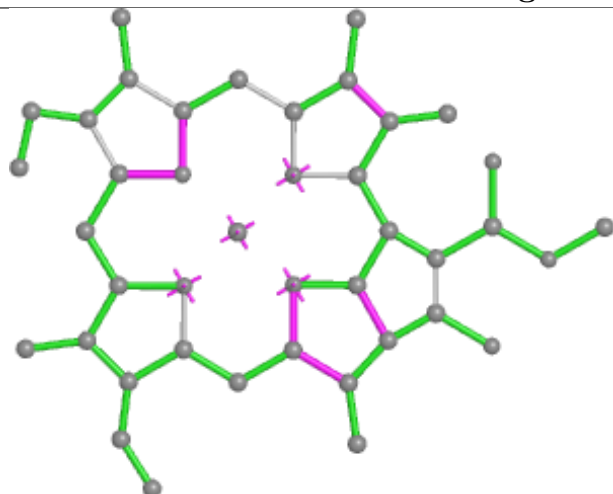




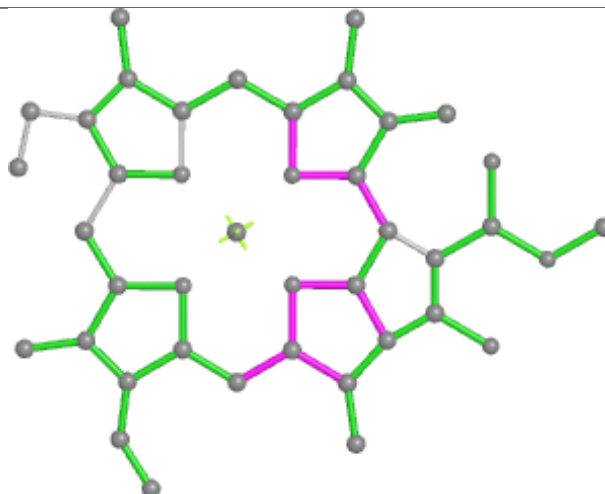




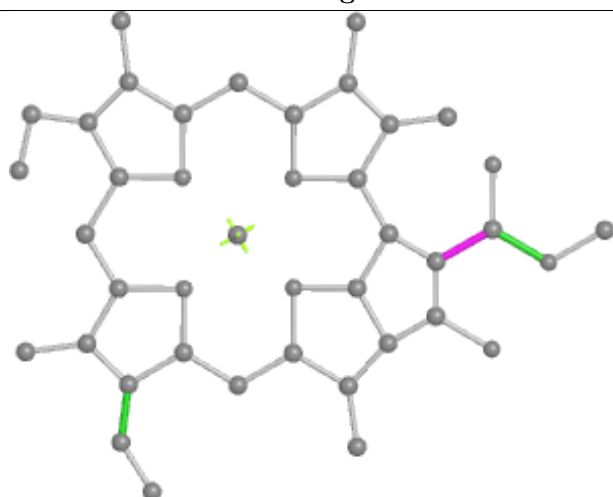
## Ligand CLA 3 306



Bond lengths



Bond angles

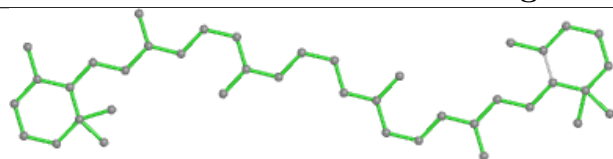


Torsions

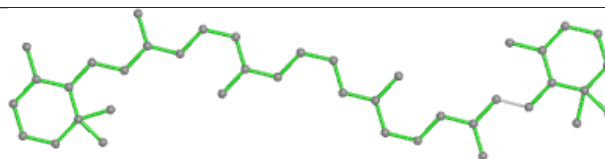


Rings

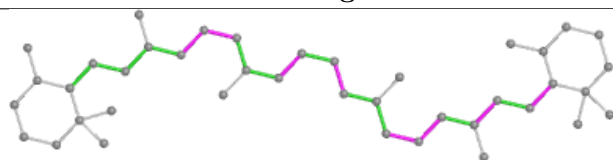
## Ligand 8CT b 620



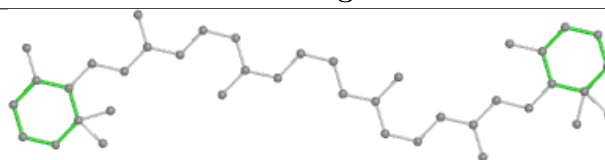
Bond lengths



Bond angles

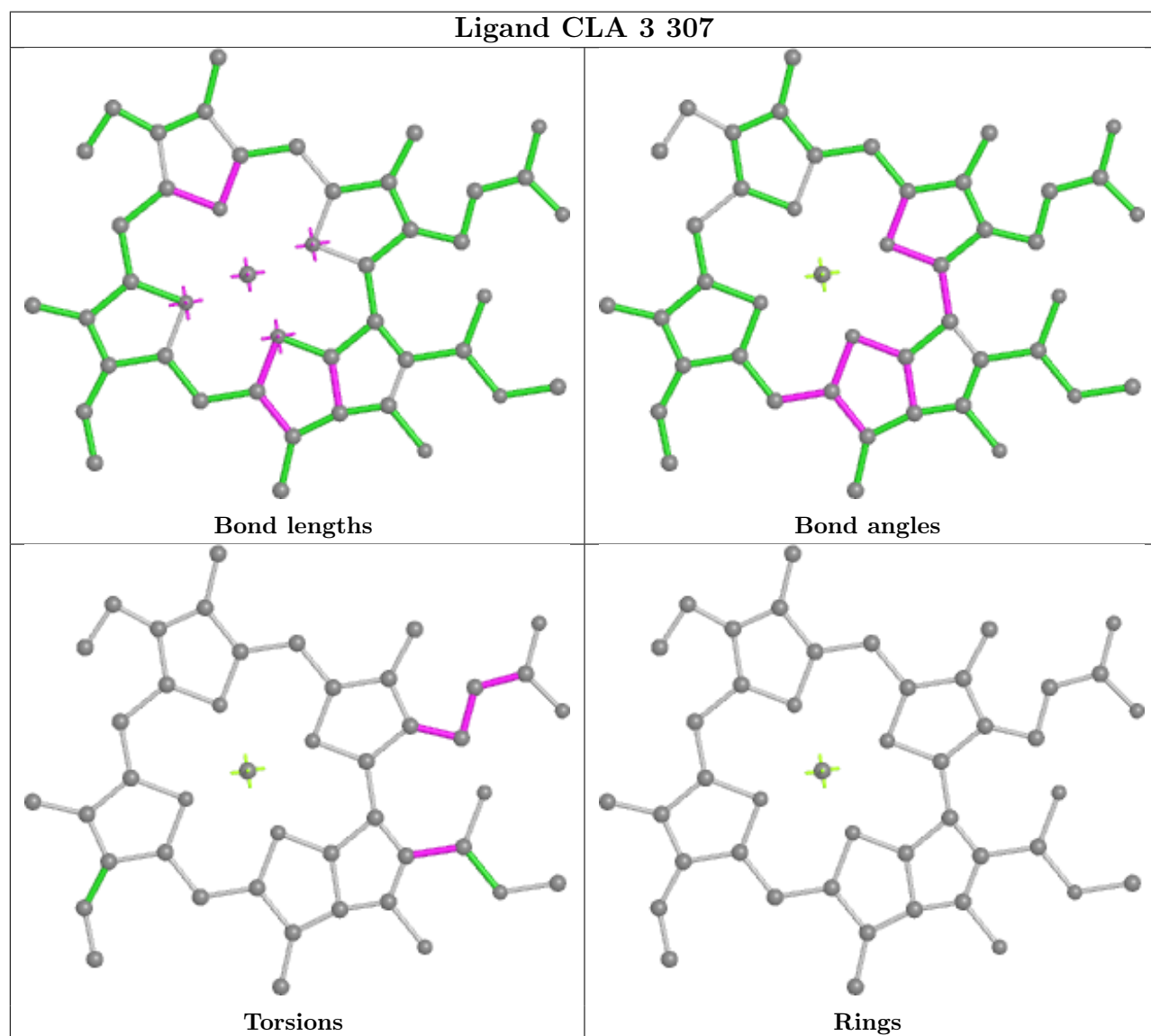
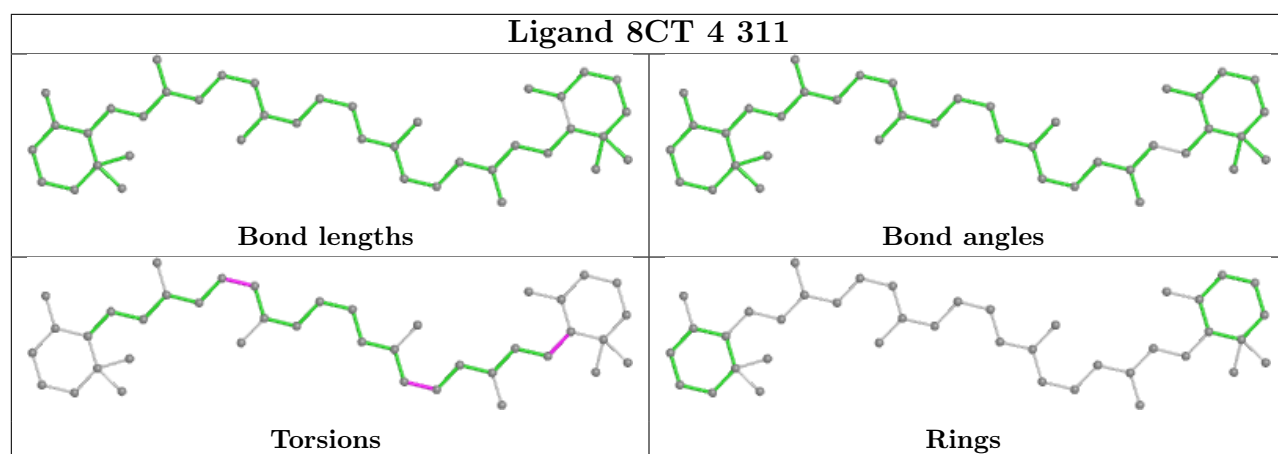


Torsions

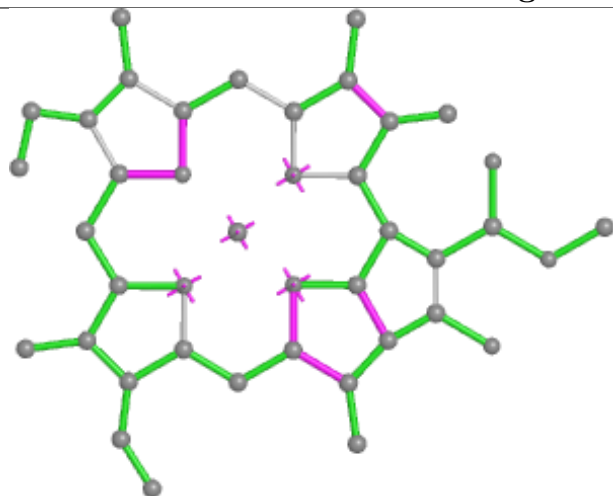


Rings

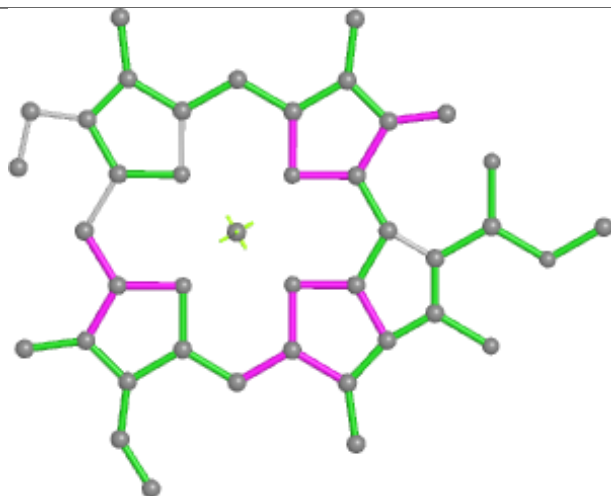




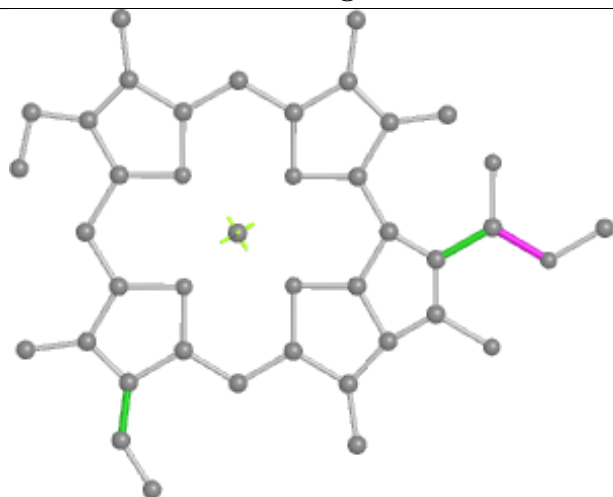
## Ligand CLA 6 303



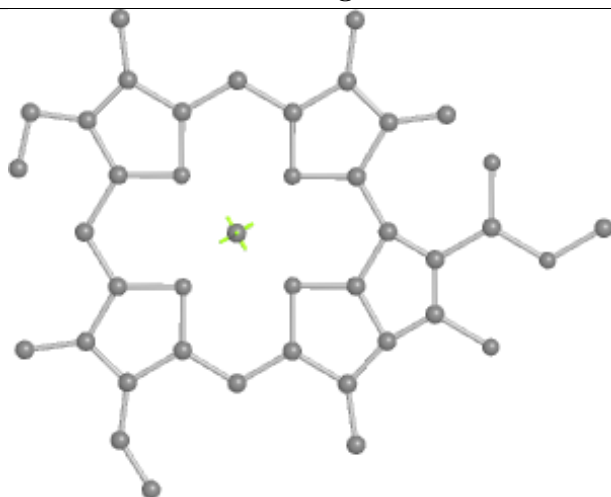
Bond lengths



Bond angles

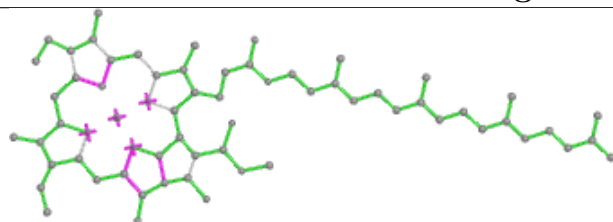


Torsions

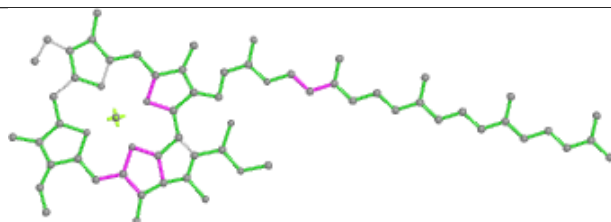


Rings

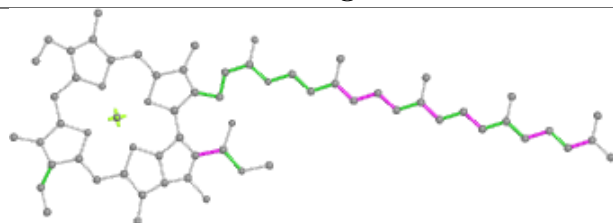
## Ligand CLA C 507



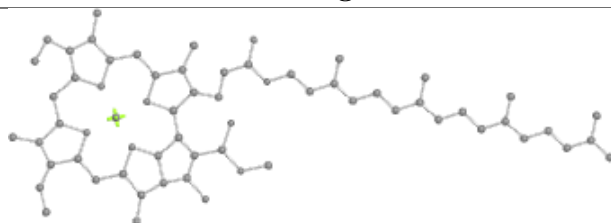
Bond lengths



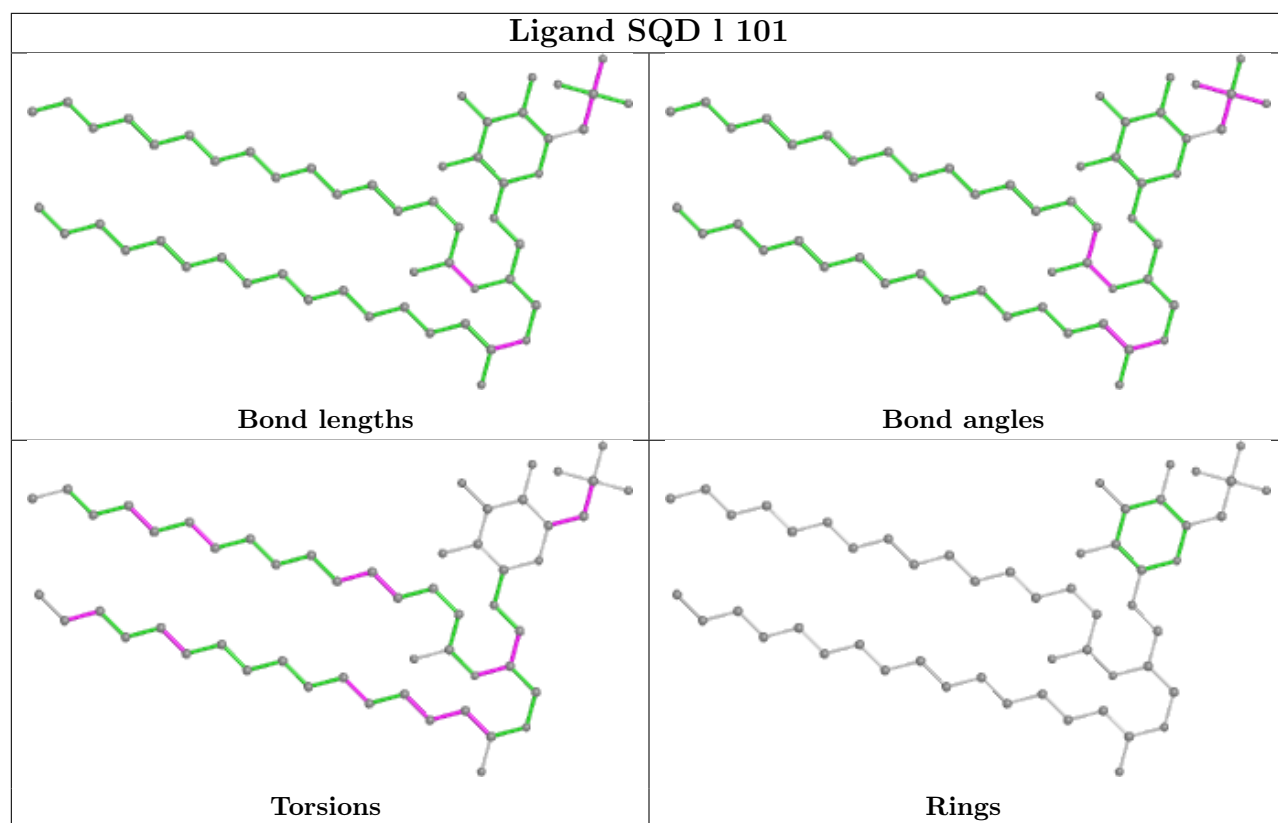
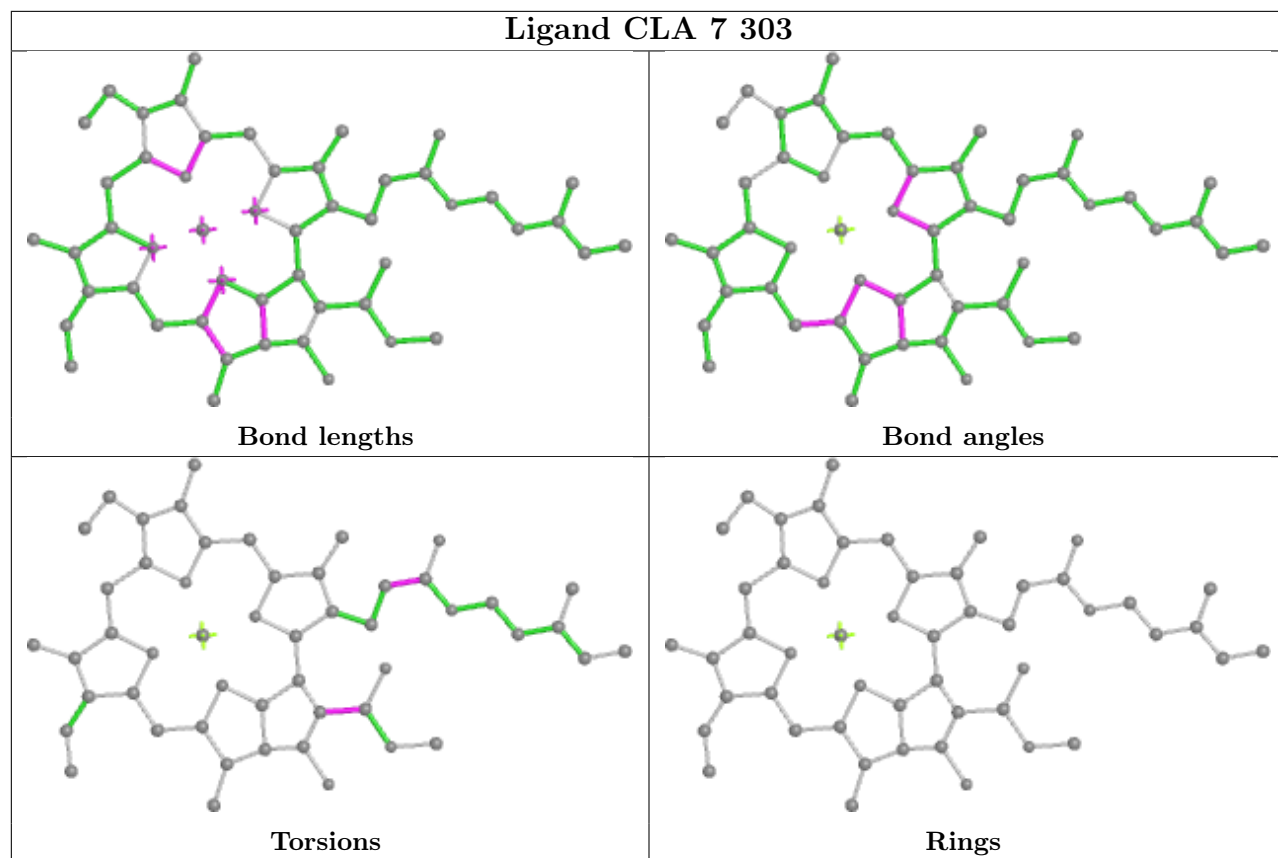
Bond angles



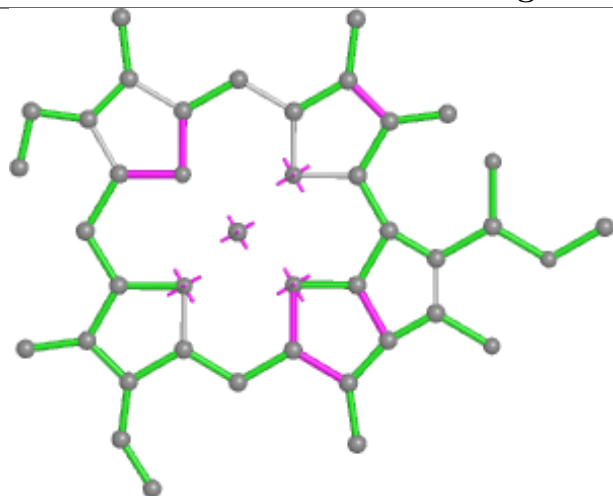
Torsions



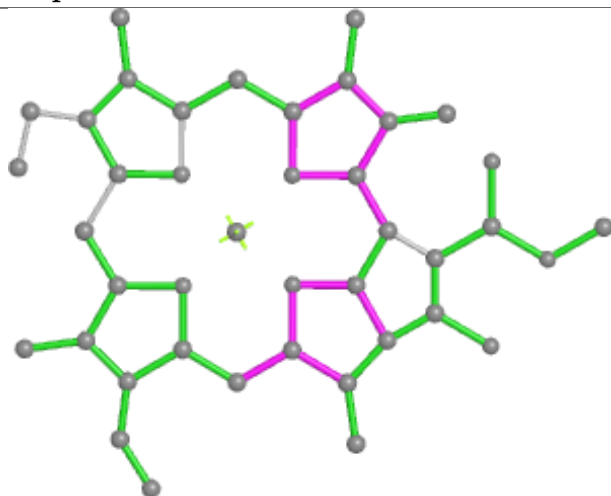
Rings



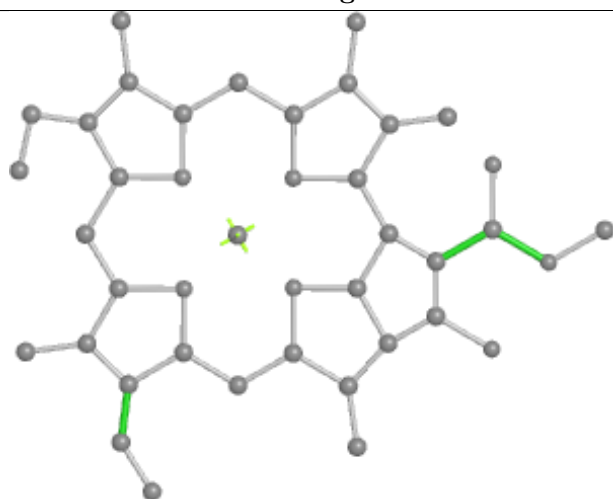
## Ligand CLA p 302



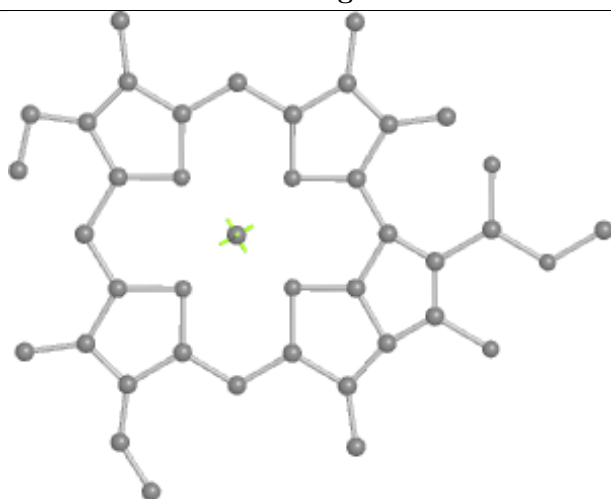
Bond lengths



Bond angles

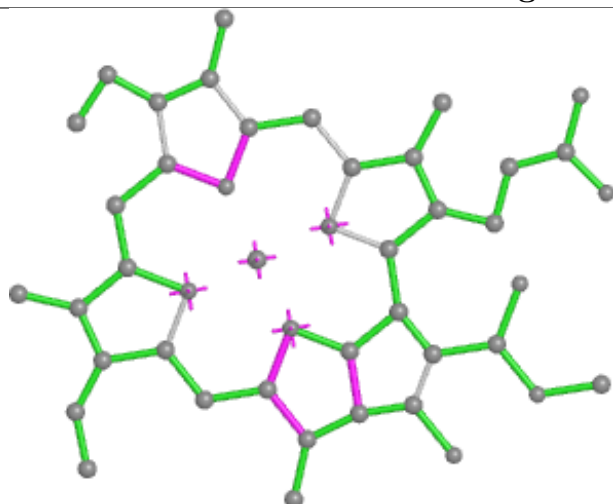


Torsions

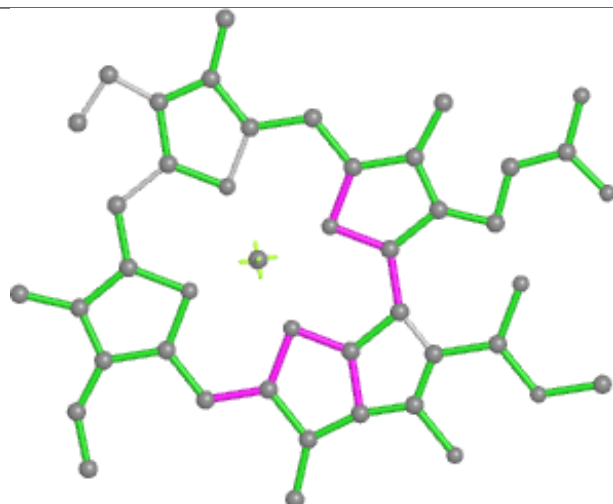


Rings

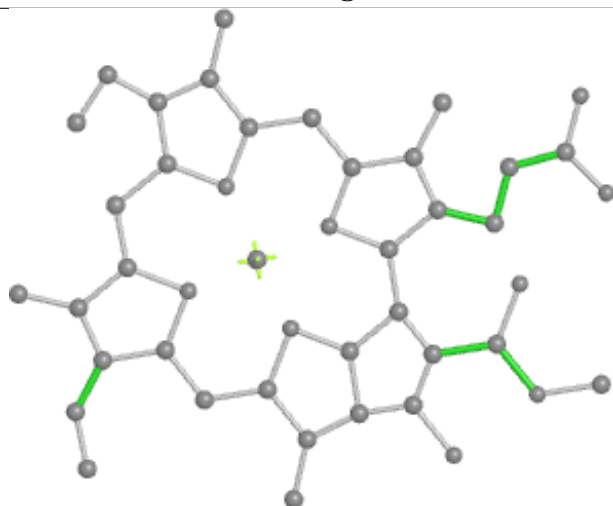
## Ligand CLA 3 304



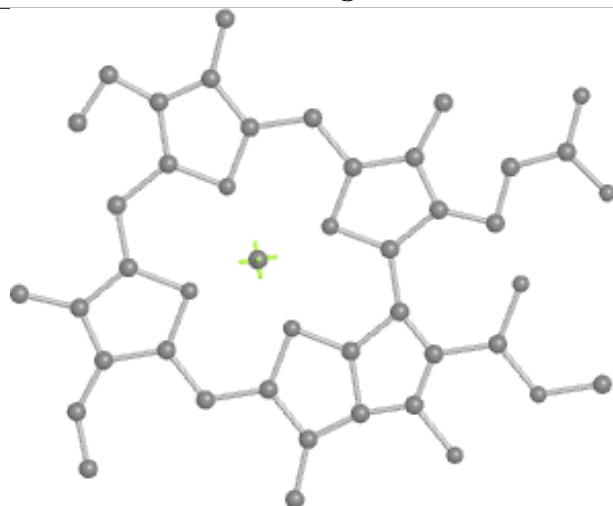
Bond lengths



Bond angles

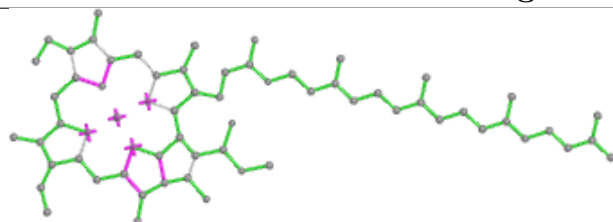


Torsions

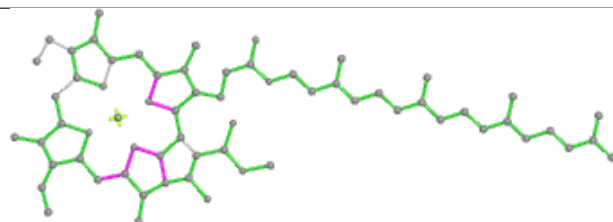


Rings

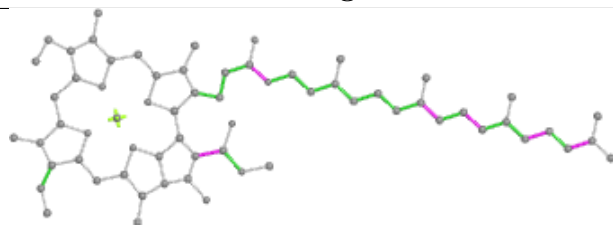
## Ligand CLA b 613



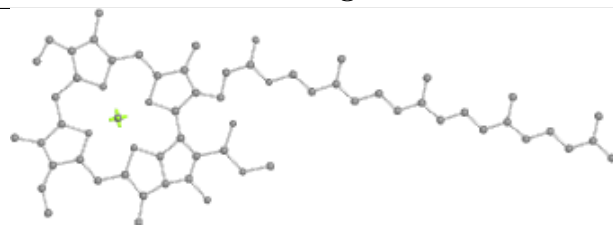
Bond lengths



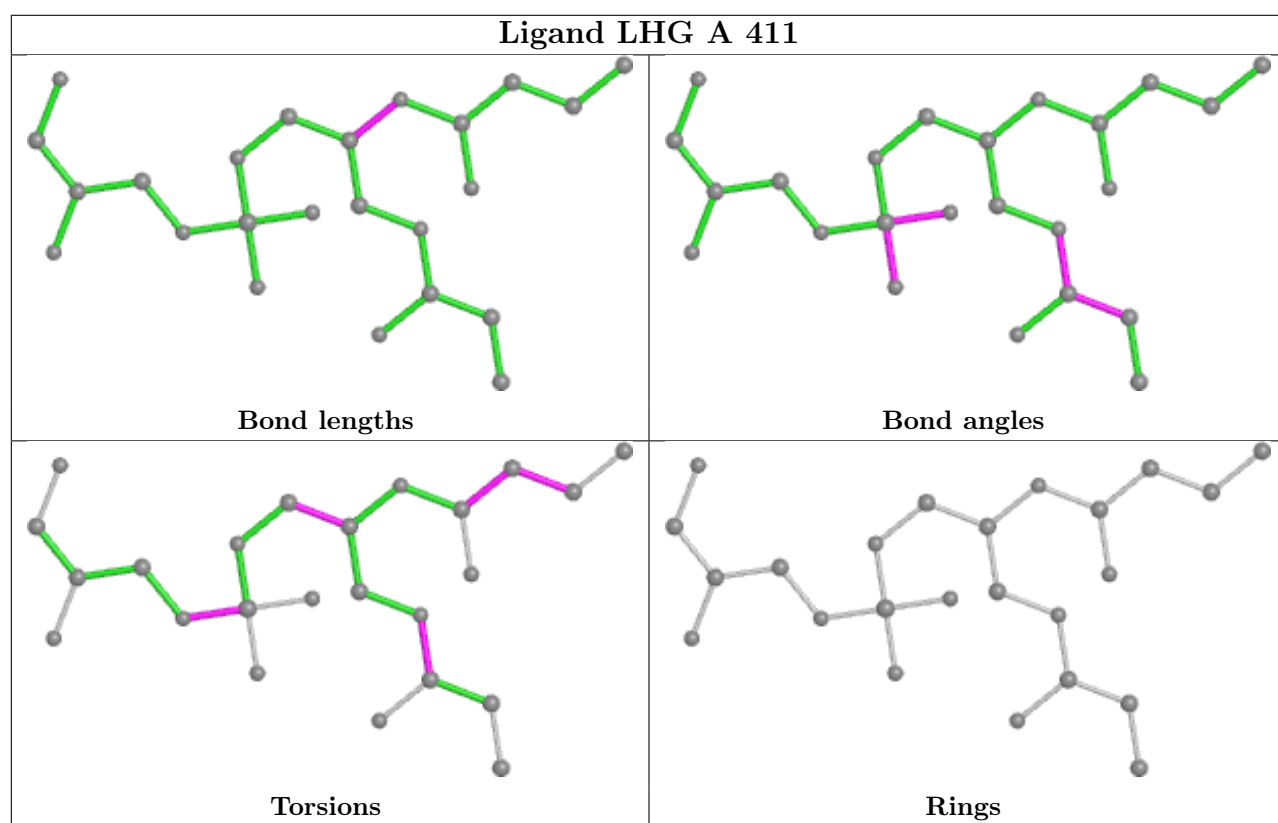
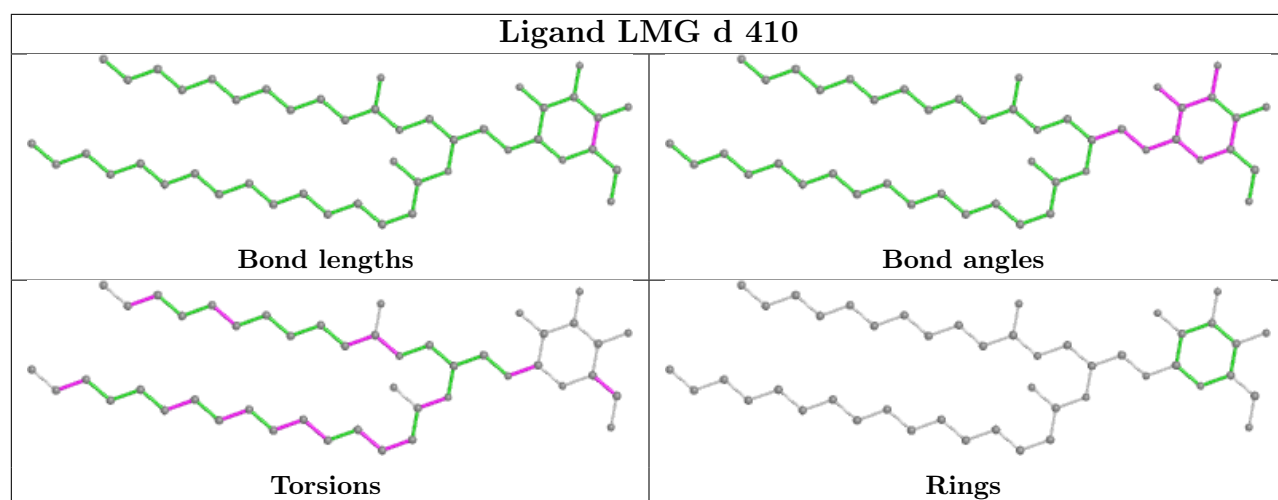
Bond angles

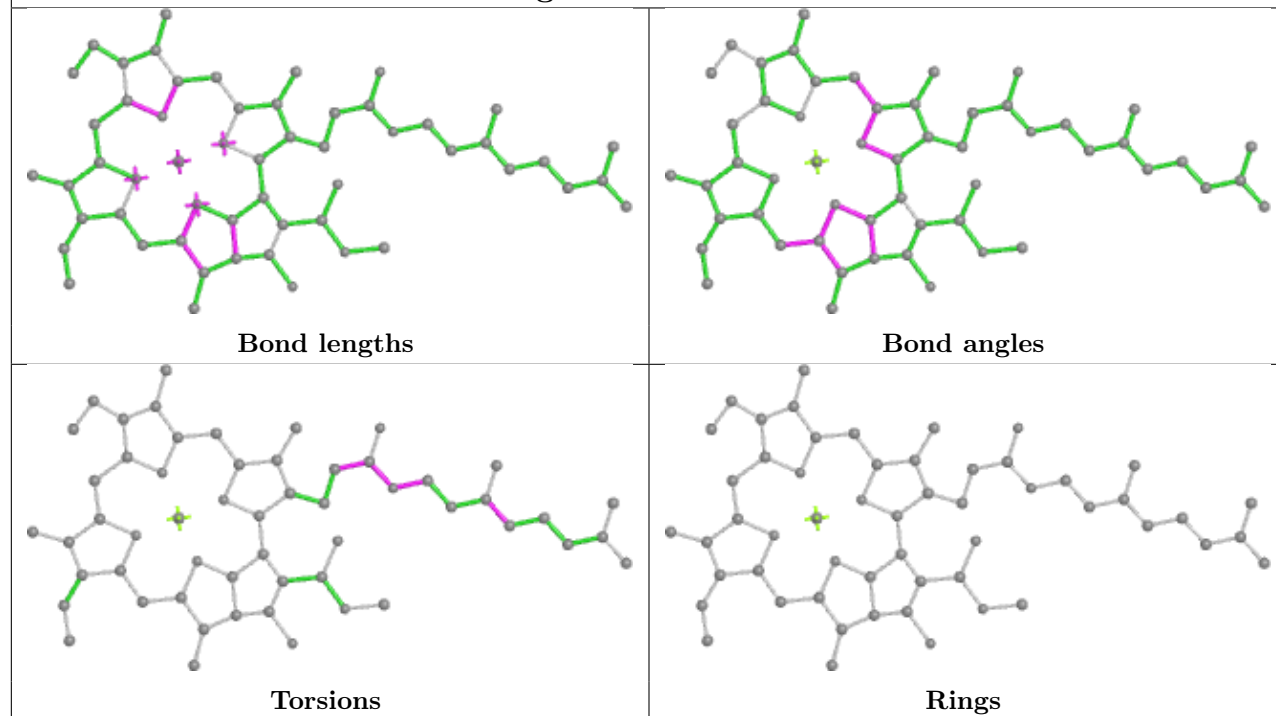
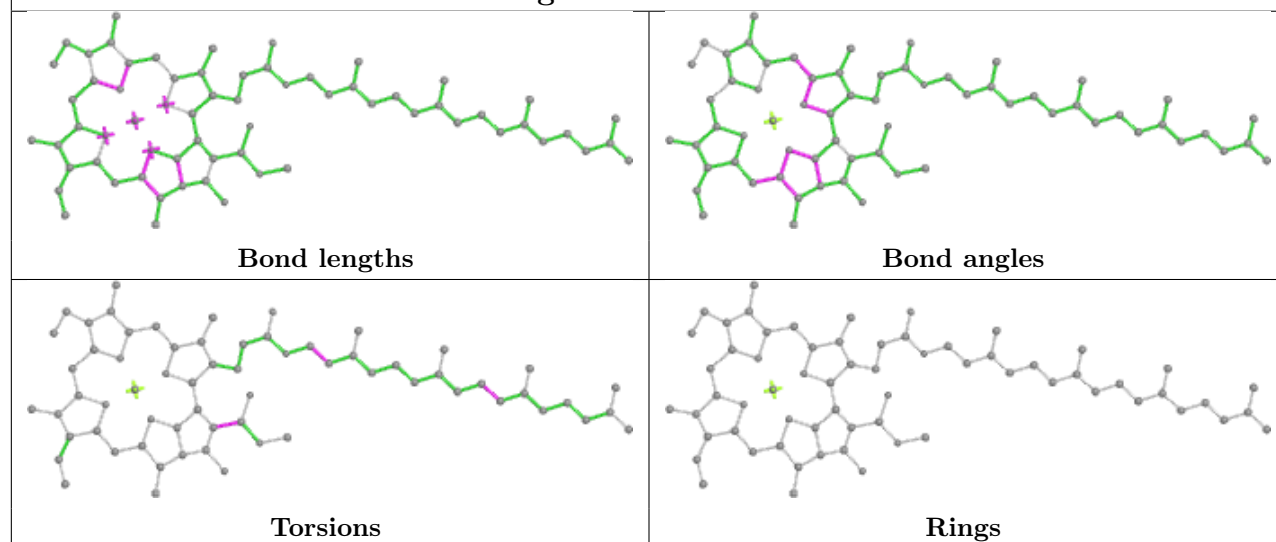


Torsions

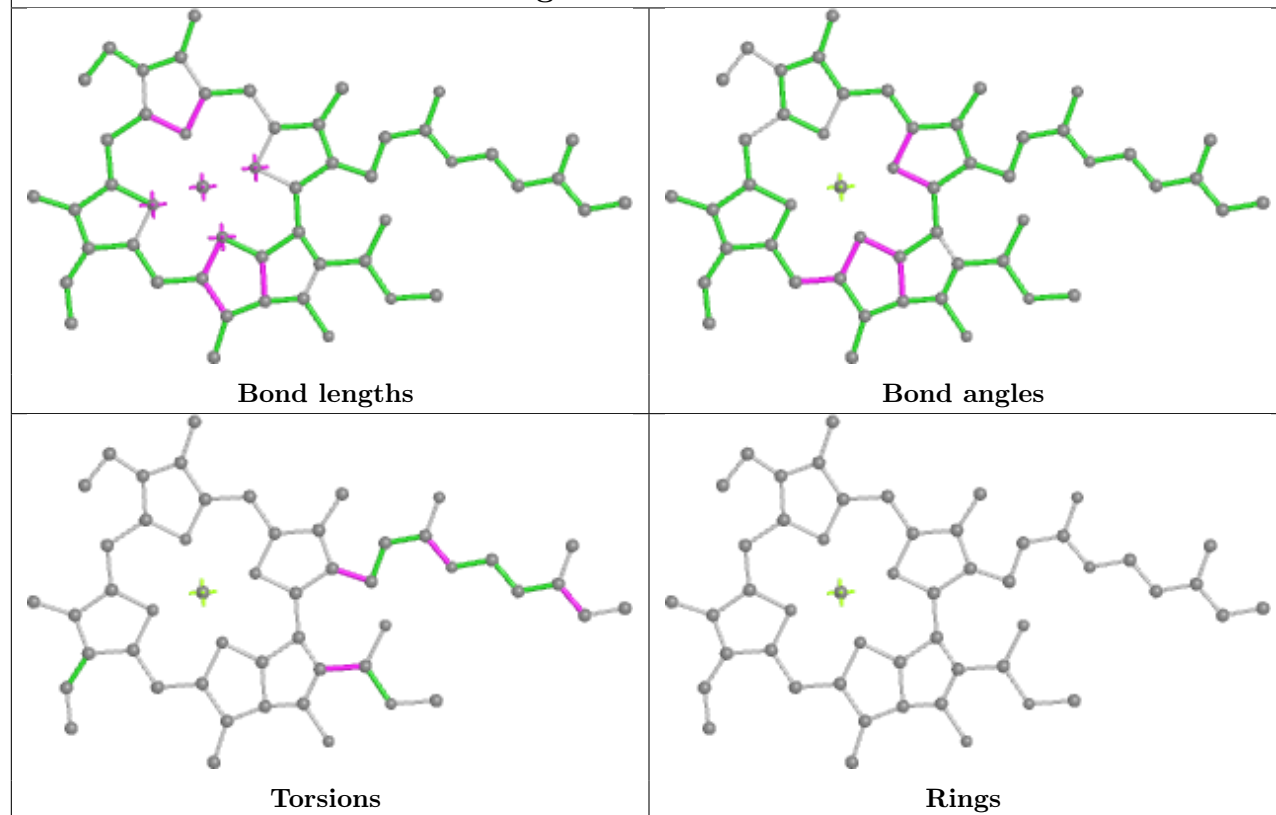


Rings

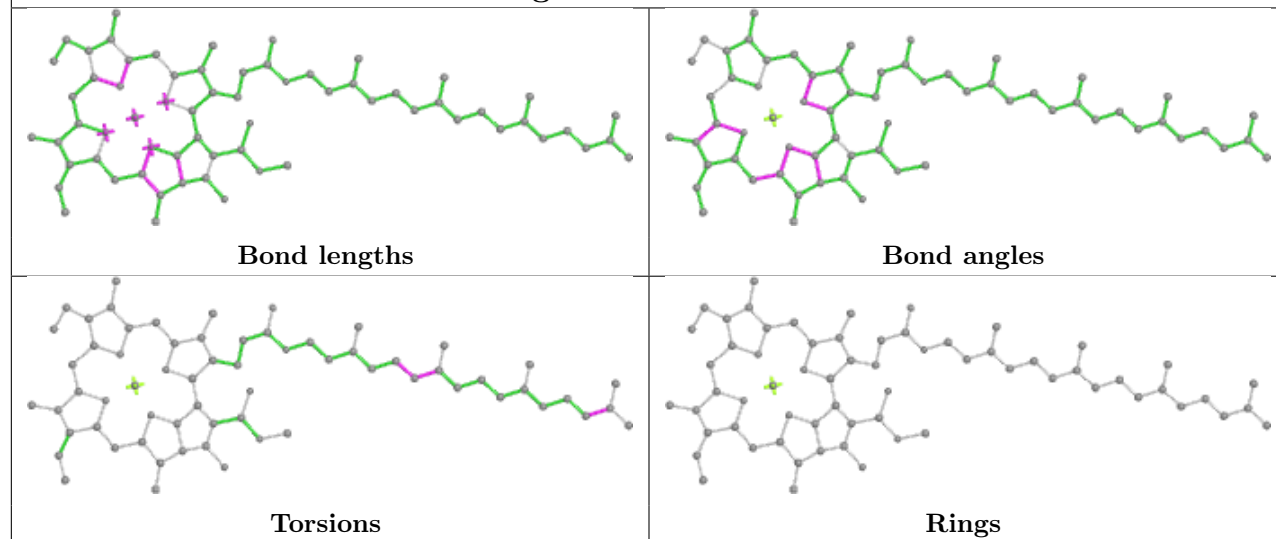


**Ligand CLA 2 305****Ligand CLA c 510**

## Ligand CLA 1 308

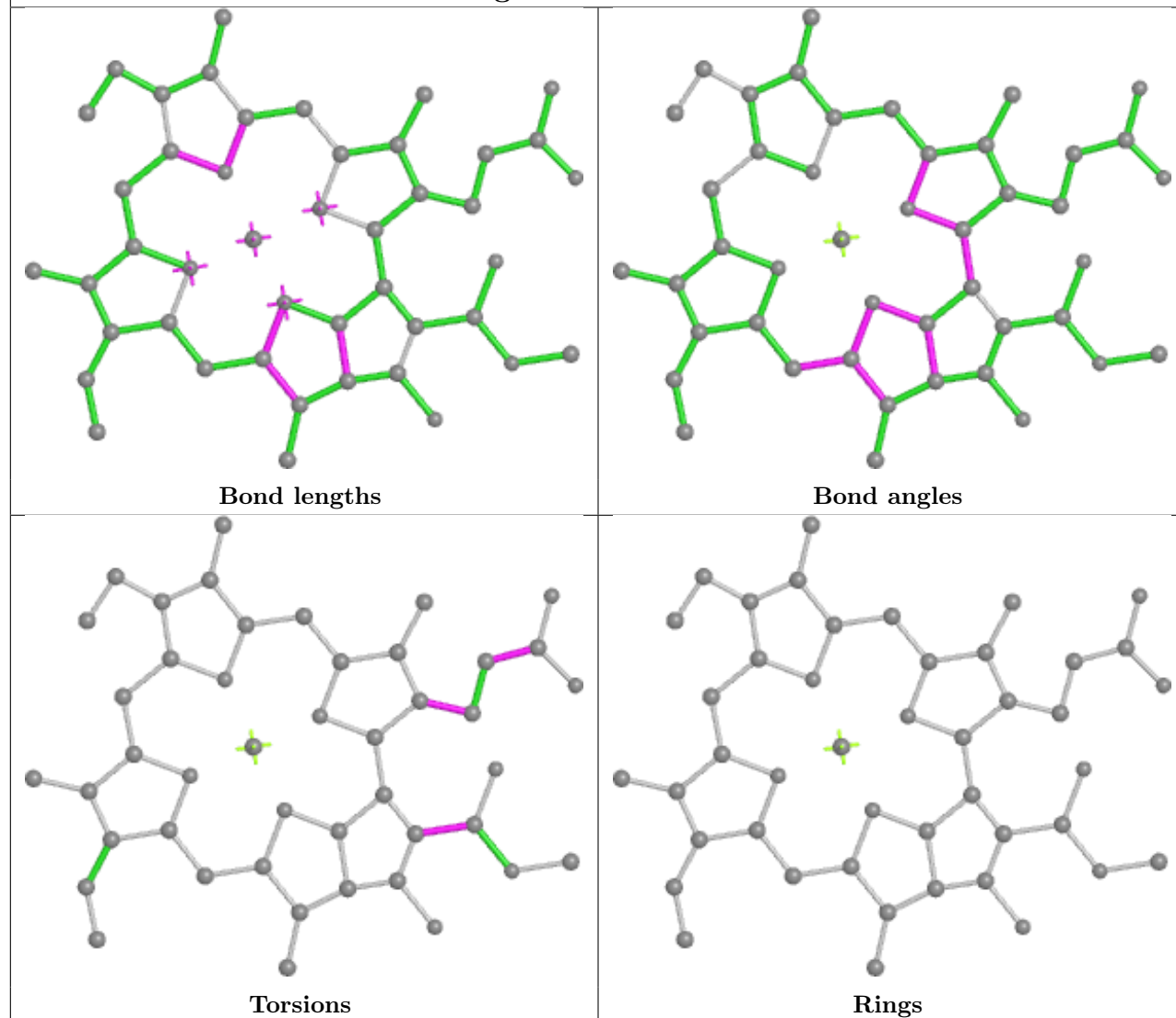


## Ligand CLA C 514

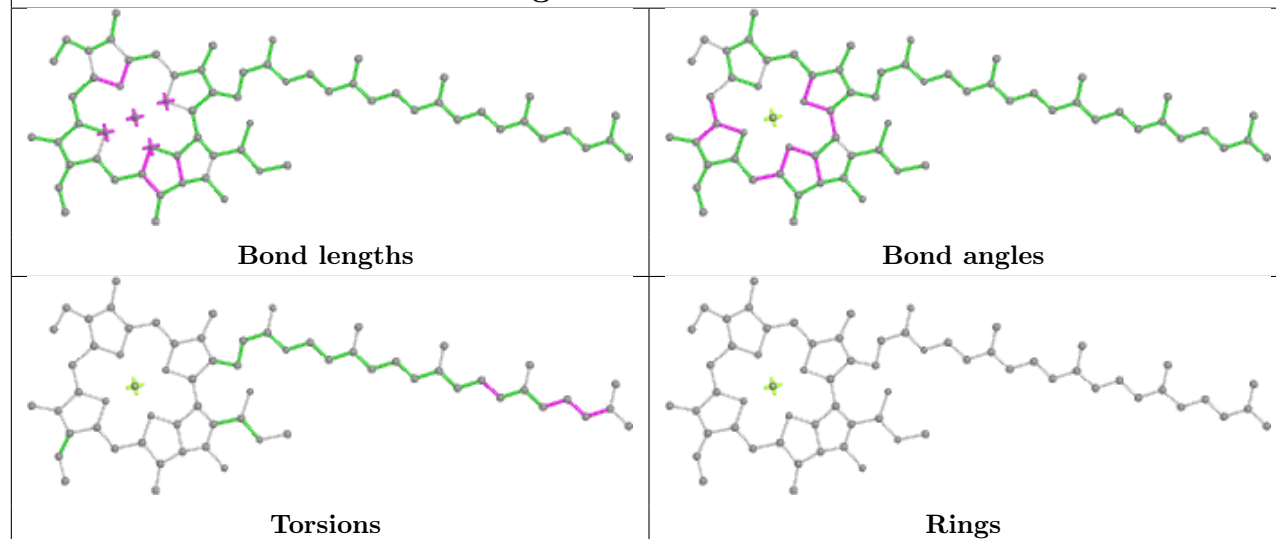




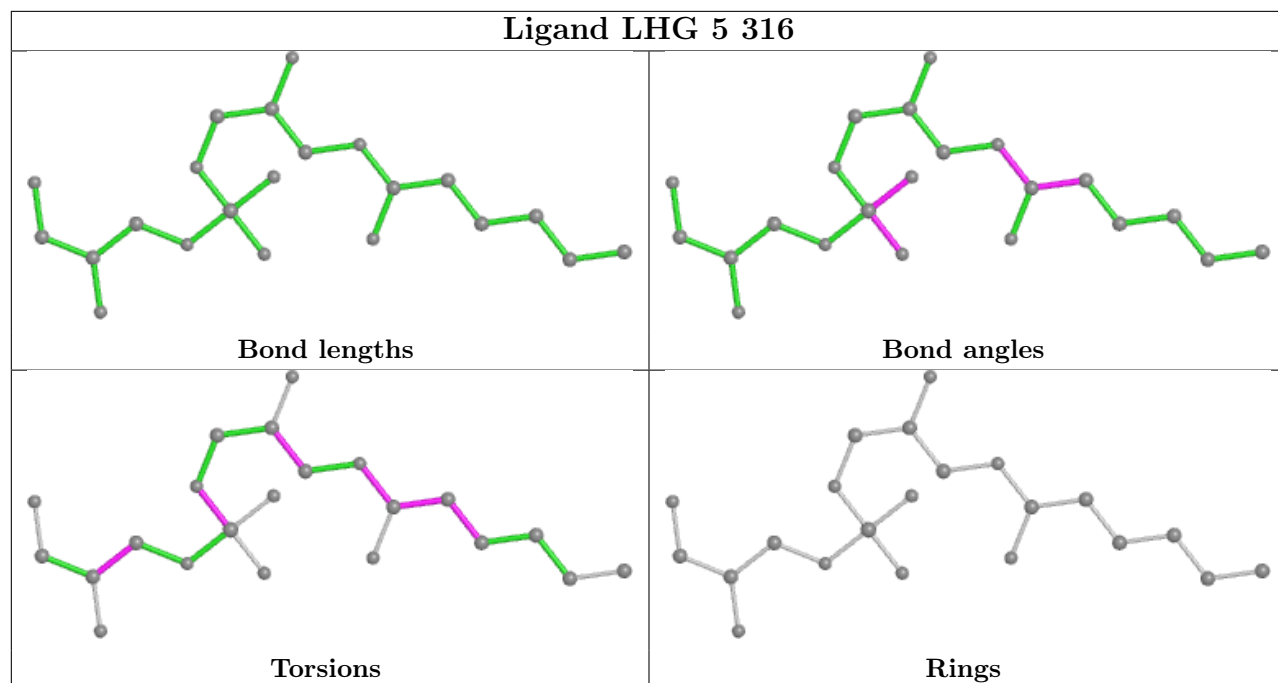
## Ligand CLA 2 301



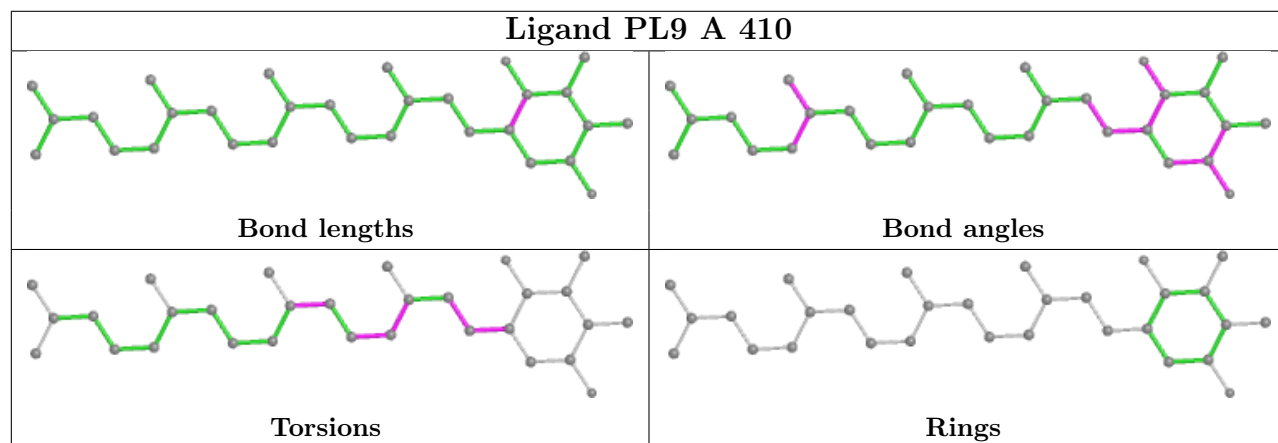
## Ligand CLA B 616



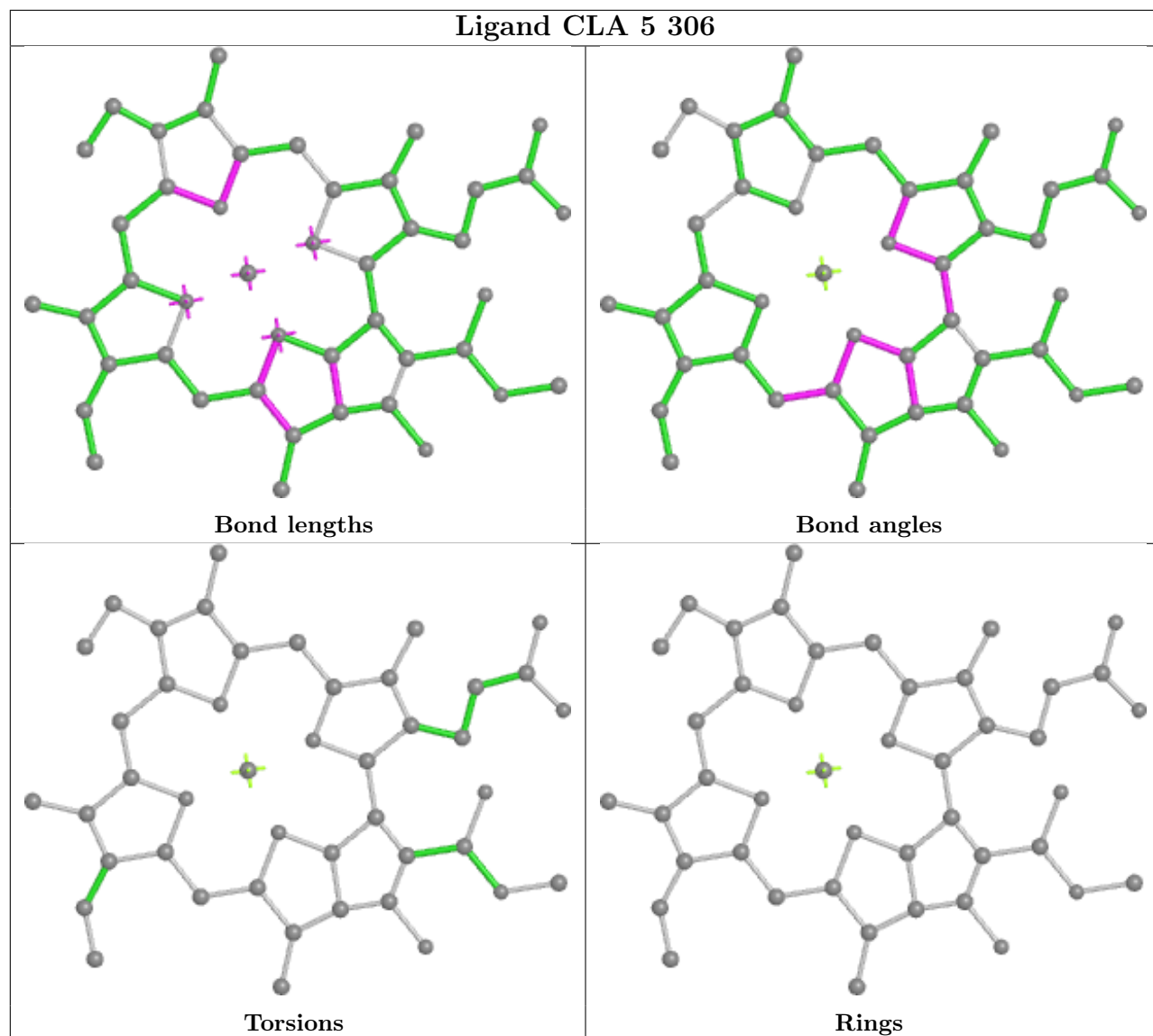
## Ligand LHG 5 316



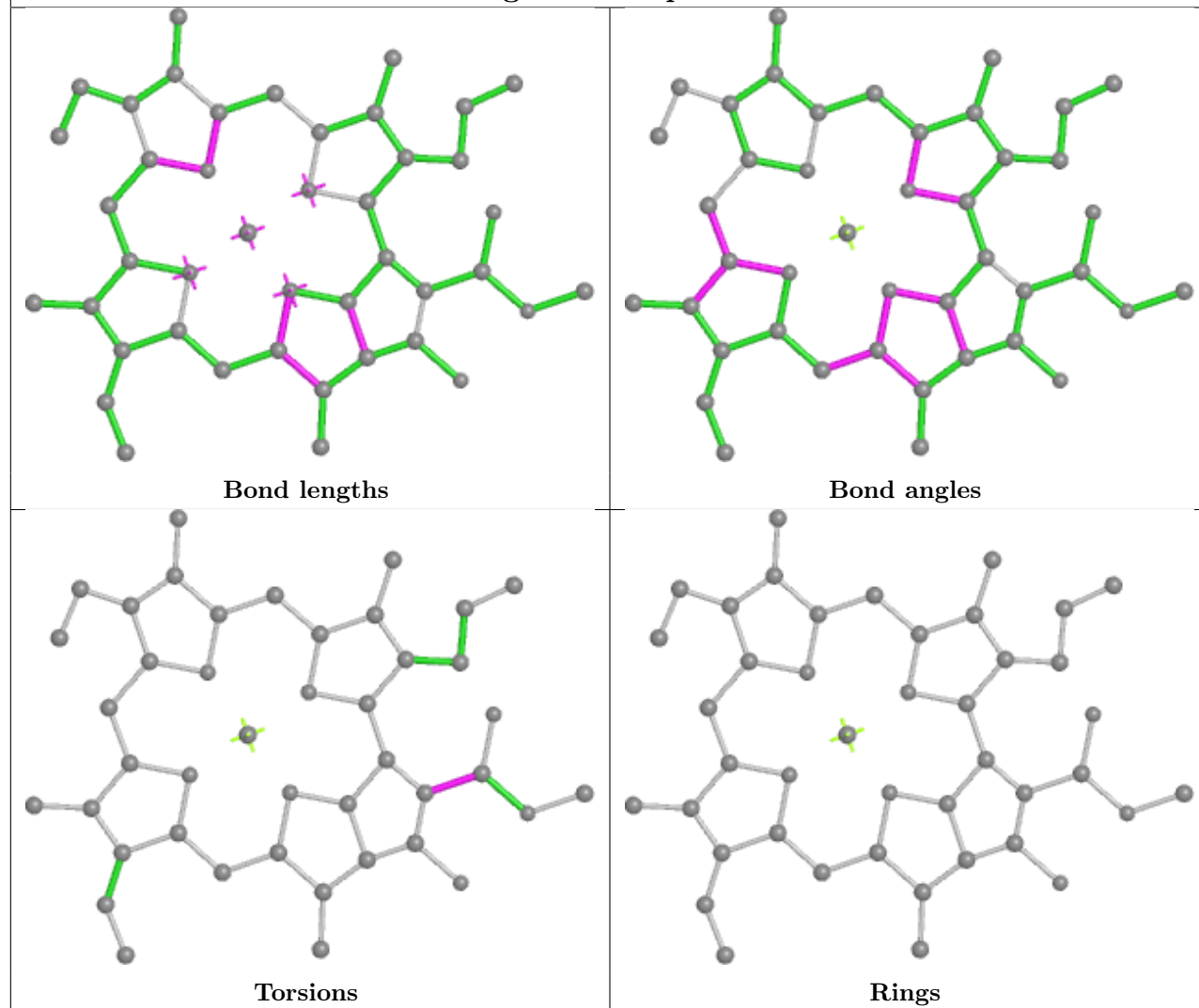
## Ligand PL9 A 410



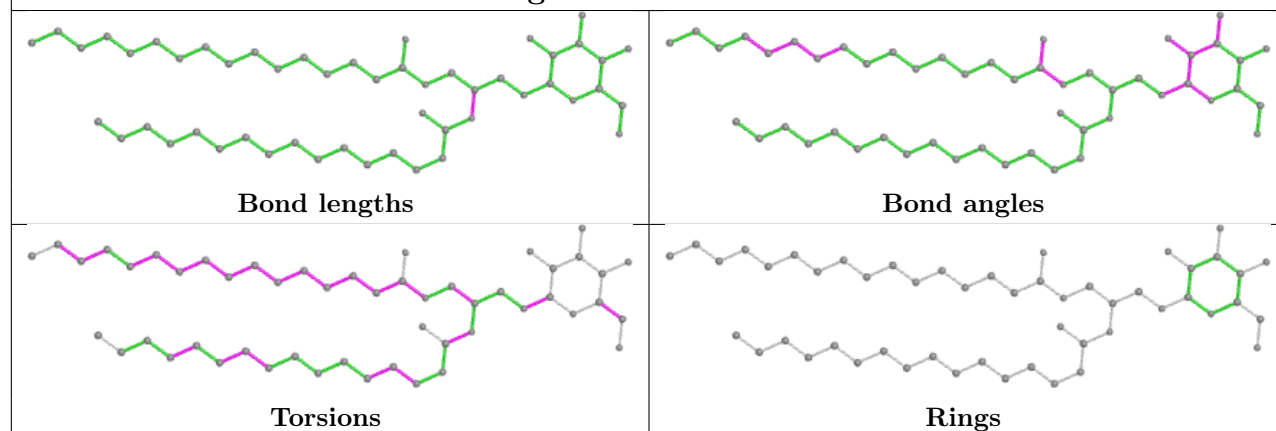
## Ligand CLA 5 306



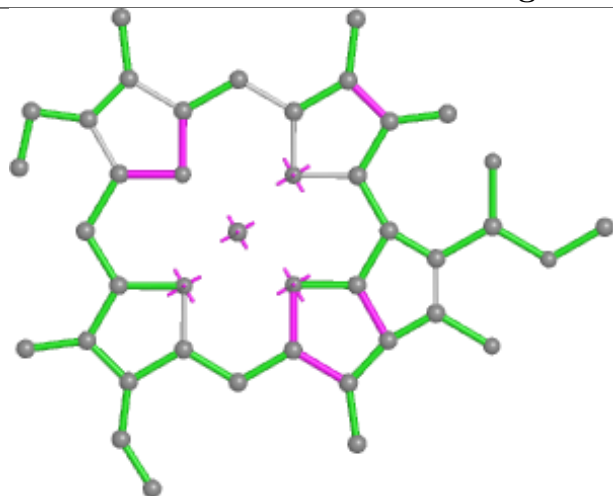
## Ligand CLA p 307



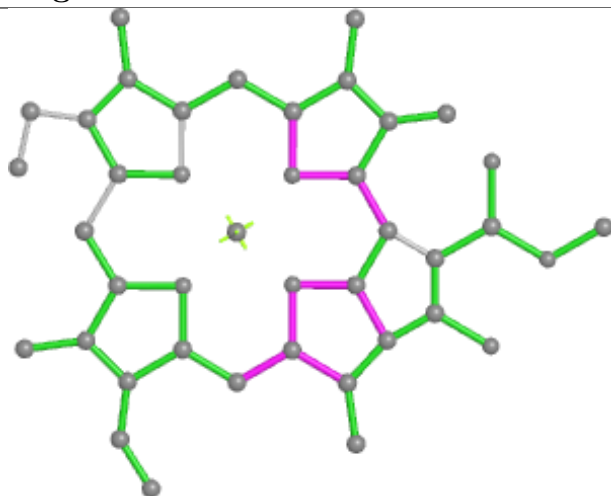
## Ligand LMG C 520



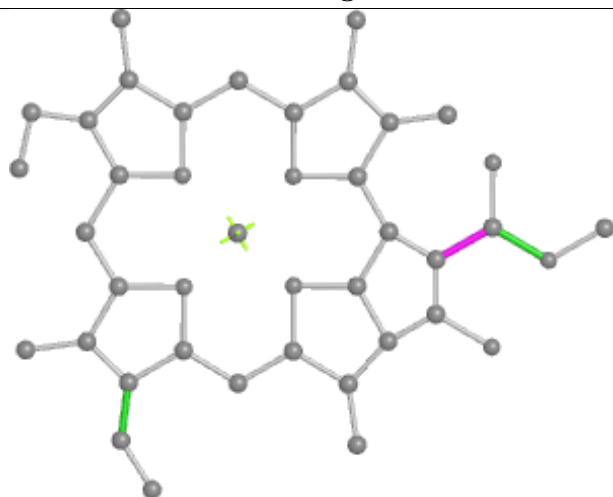
## Ligand CLA g 308



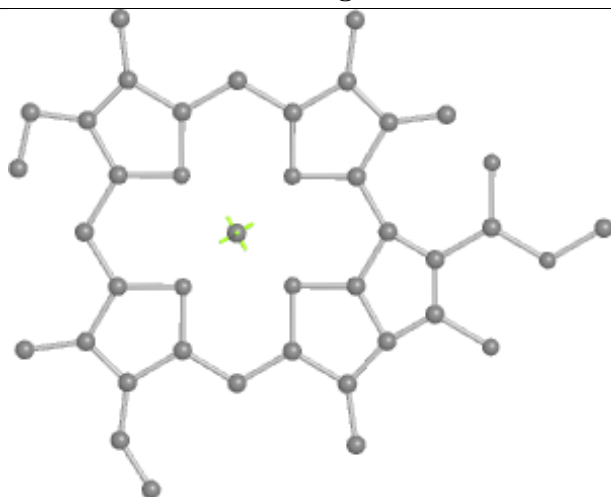
Bond lengths



Bond angles

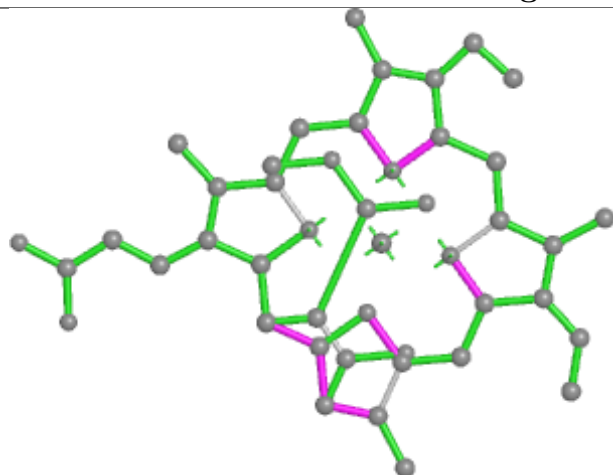


Torsions

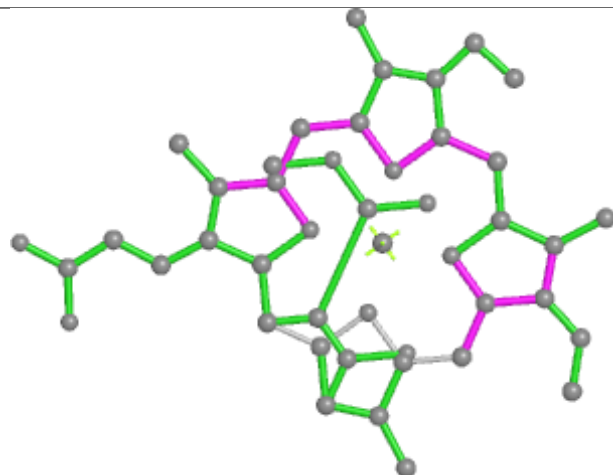


Rings

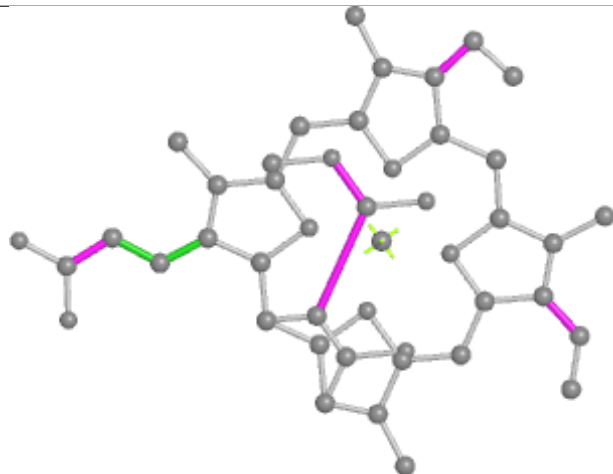
## Ligand KC2 4 305



Bond lengths



Bond angles

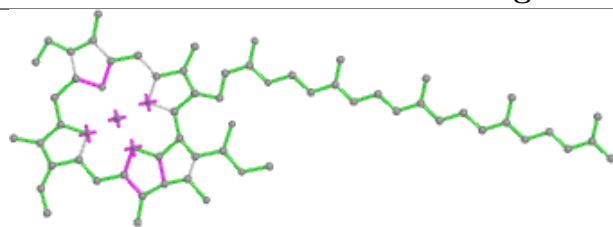


Torsions

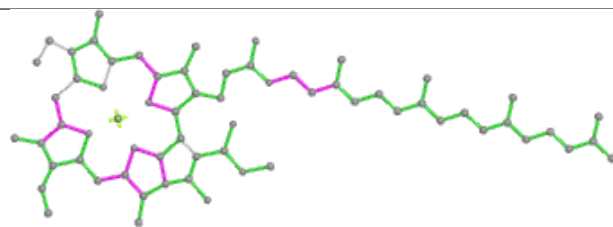


Rings

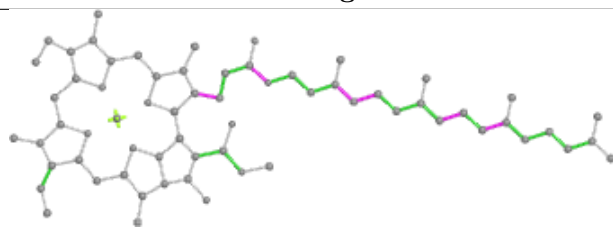
## Ligand CLA A 412



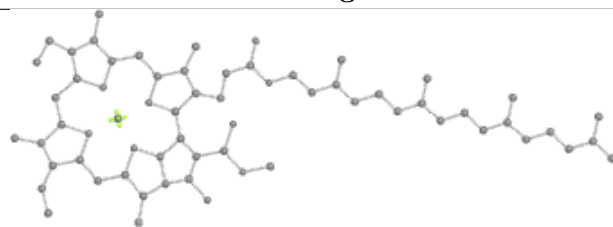
Bond lengths



Bond angles

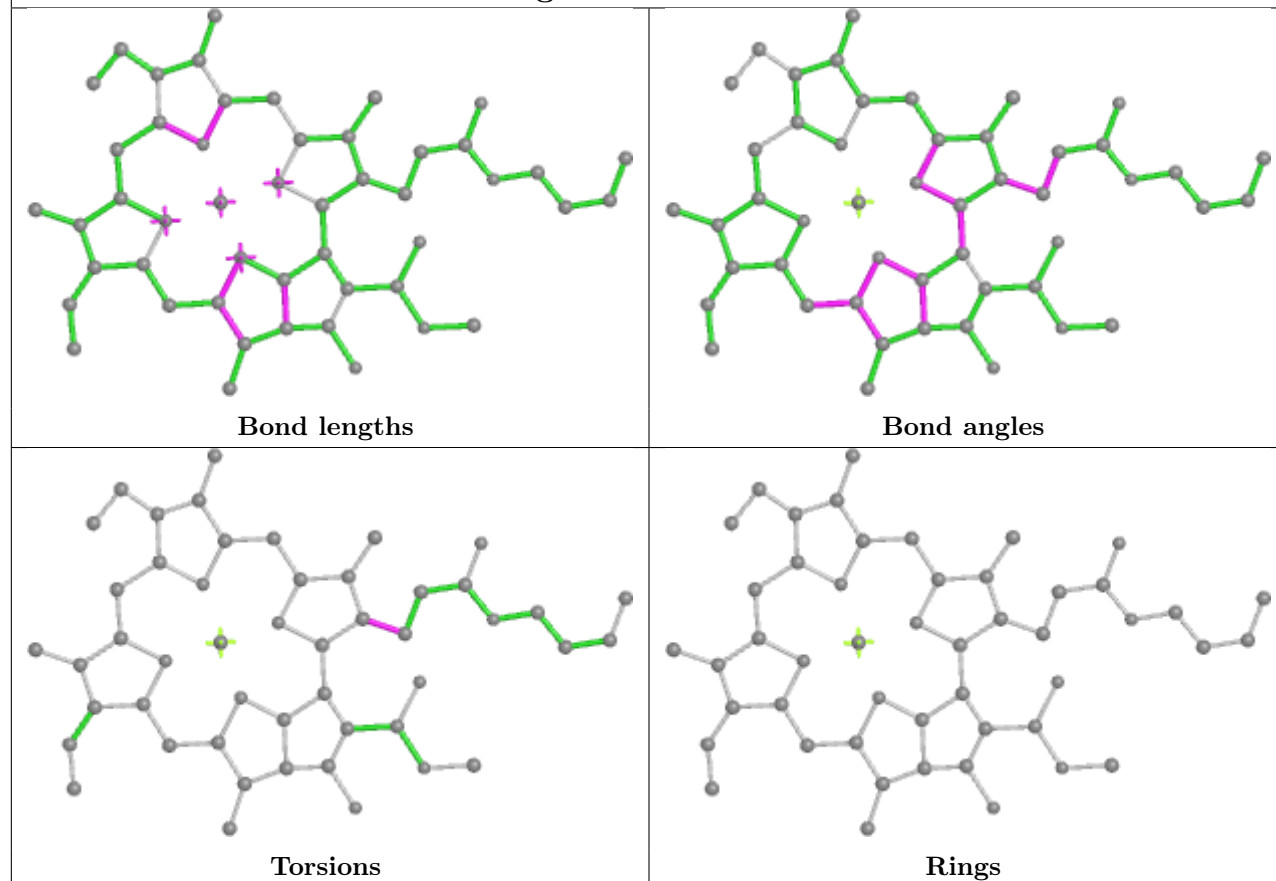


Torsions

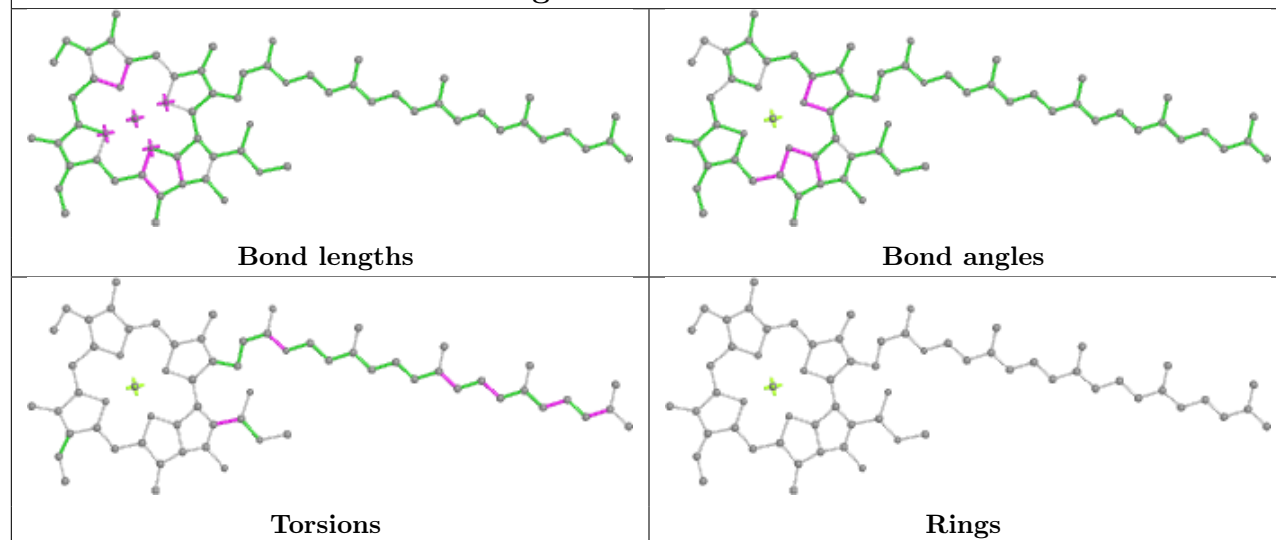


Rings

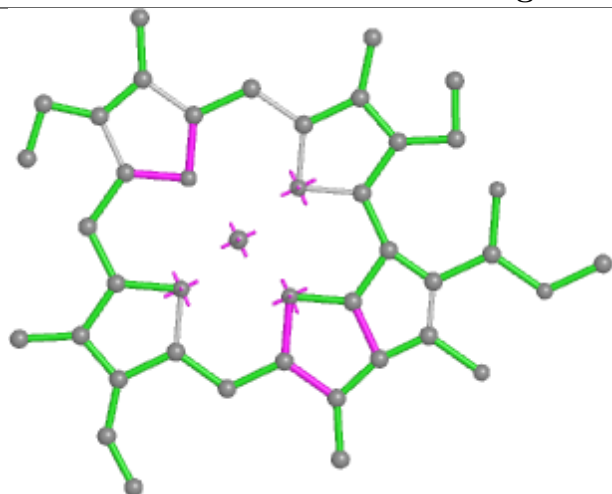
## Ligand CLA 3 308



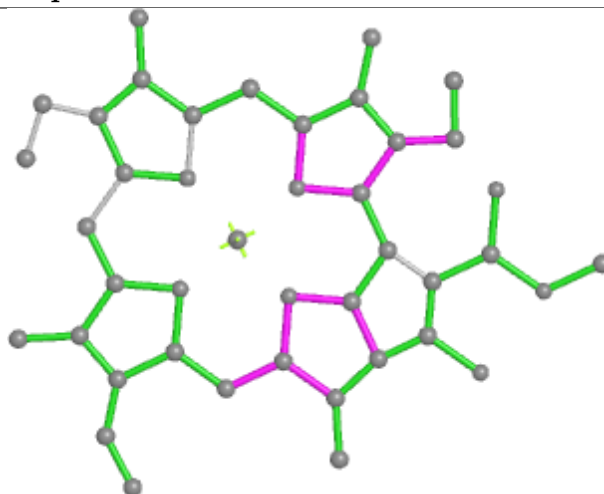
## Ligand CLA B 613



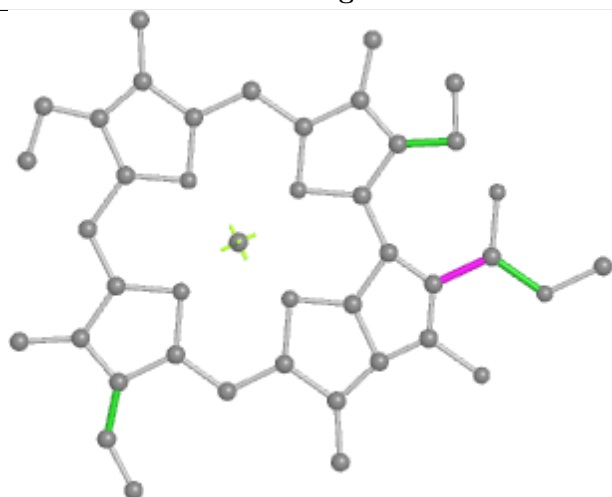
## Ligand CLA p 304



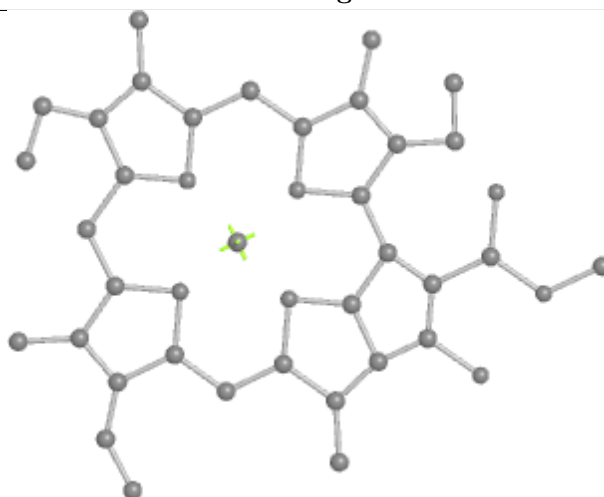
Bond lengths



Bond angles

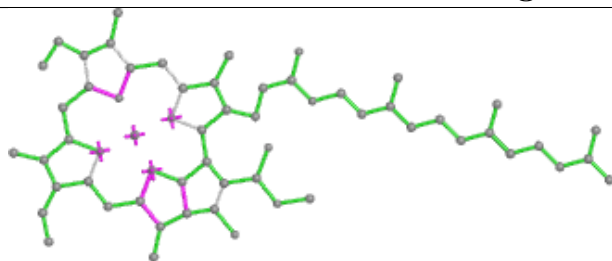


Torsions

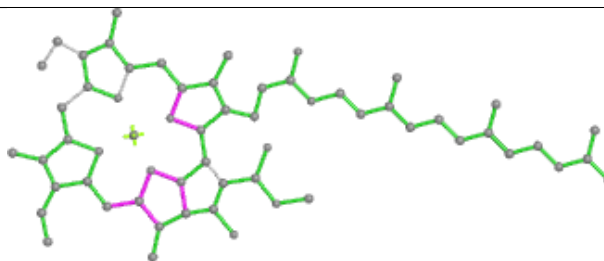


Rings

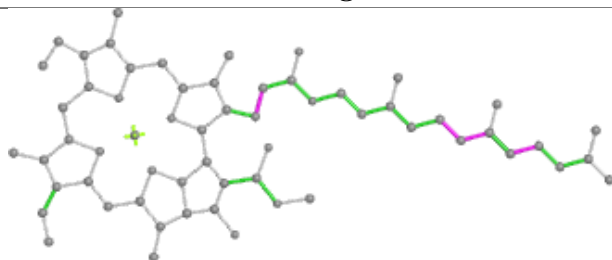
## Ligand CLA 8 304



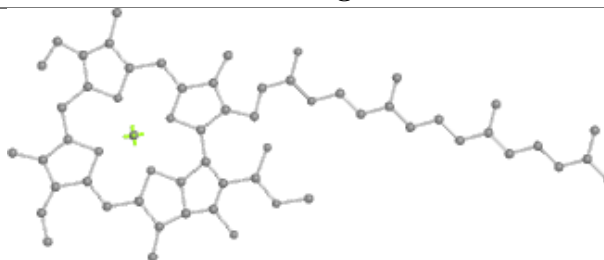
Bond lengths



Bond angles

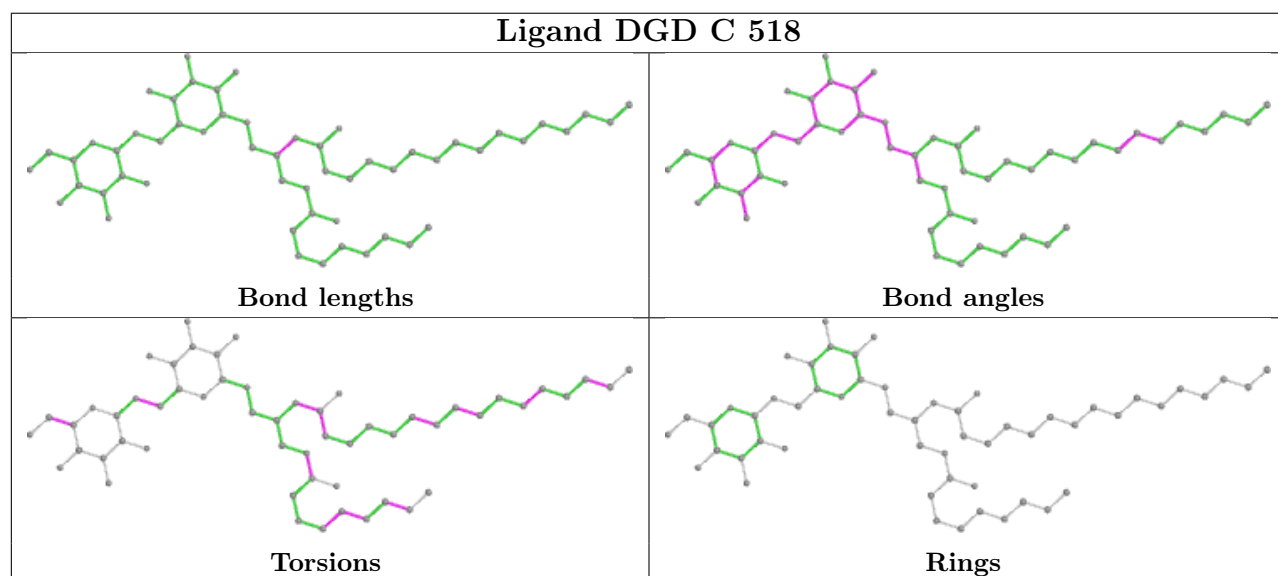
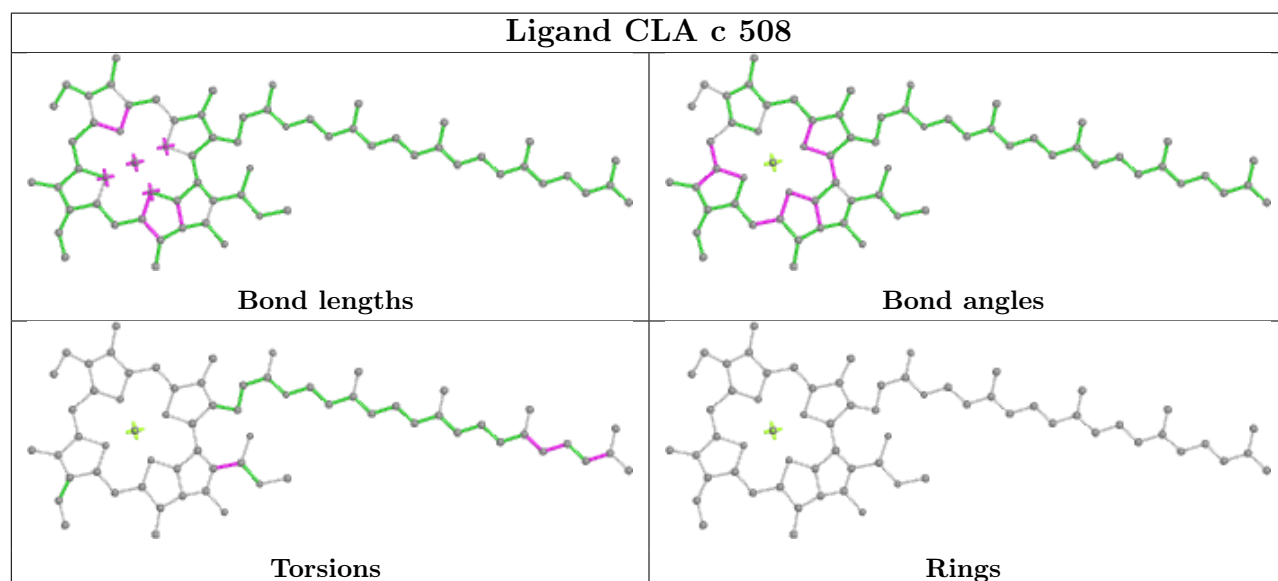
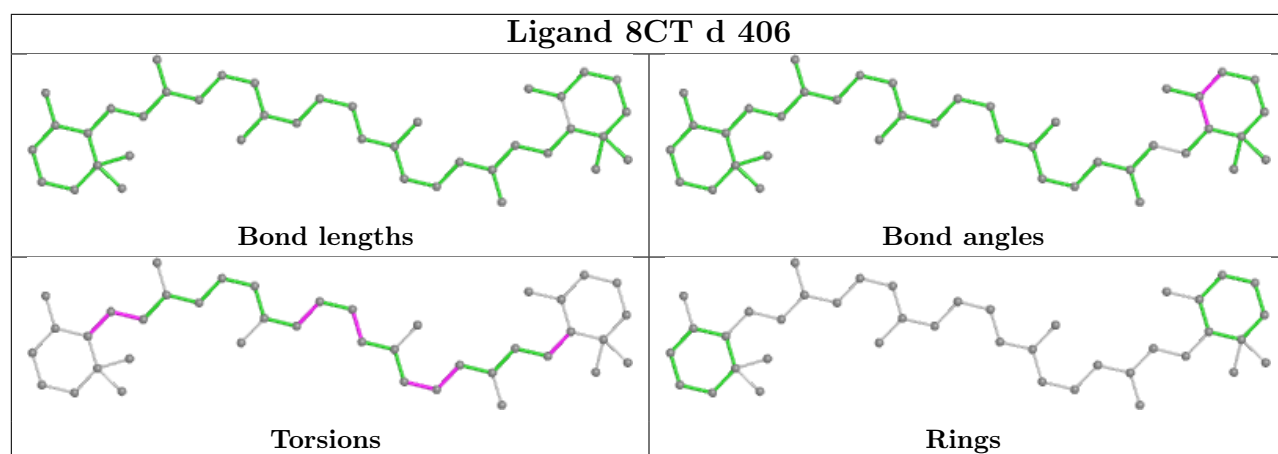


Torsions

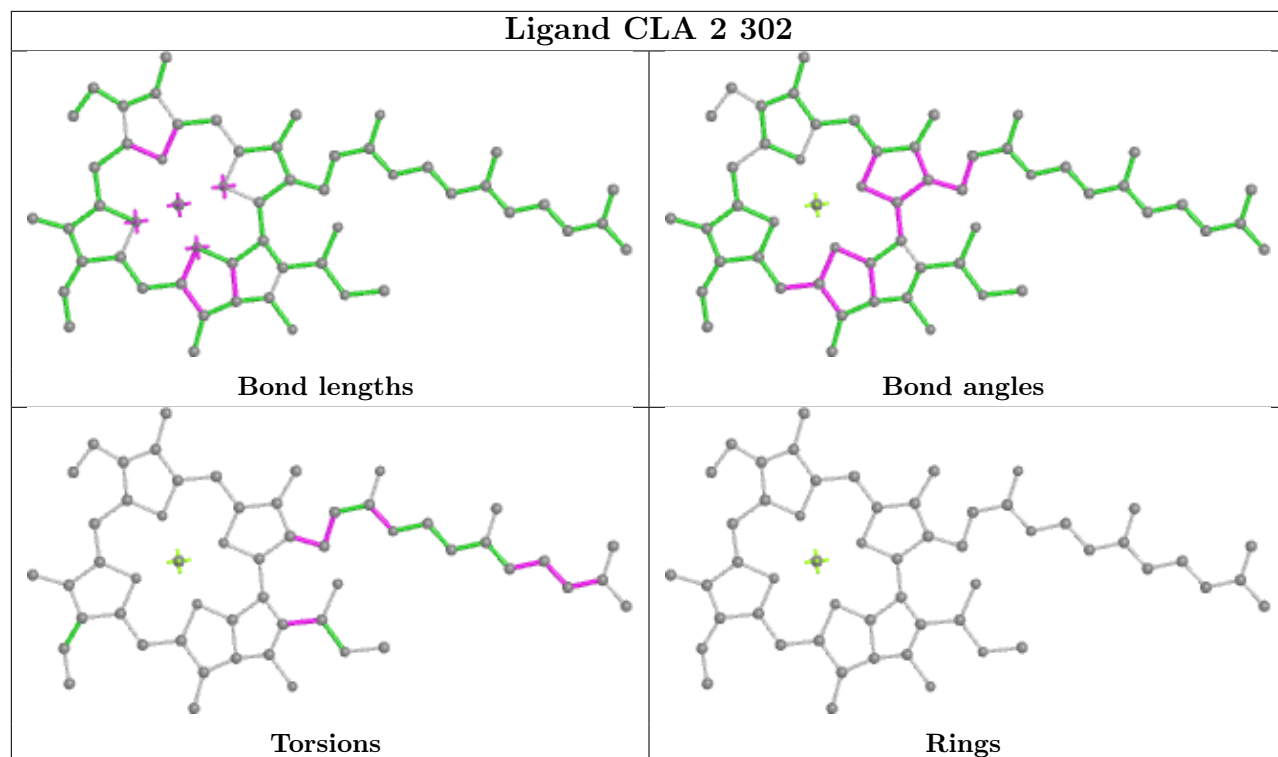


Rings

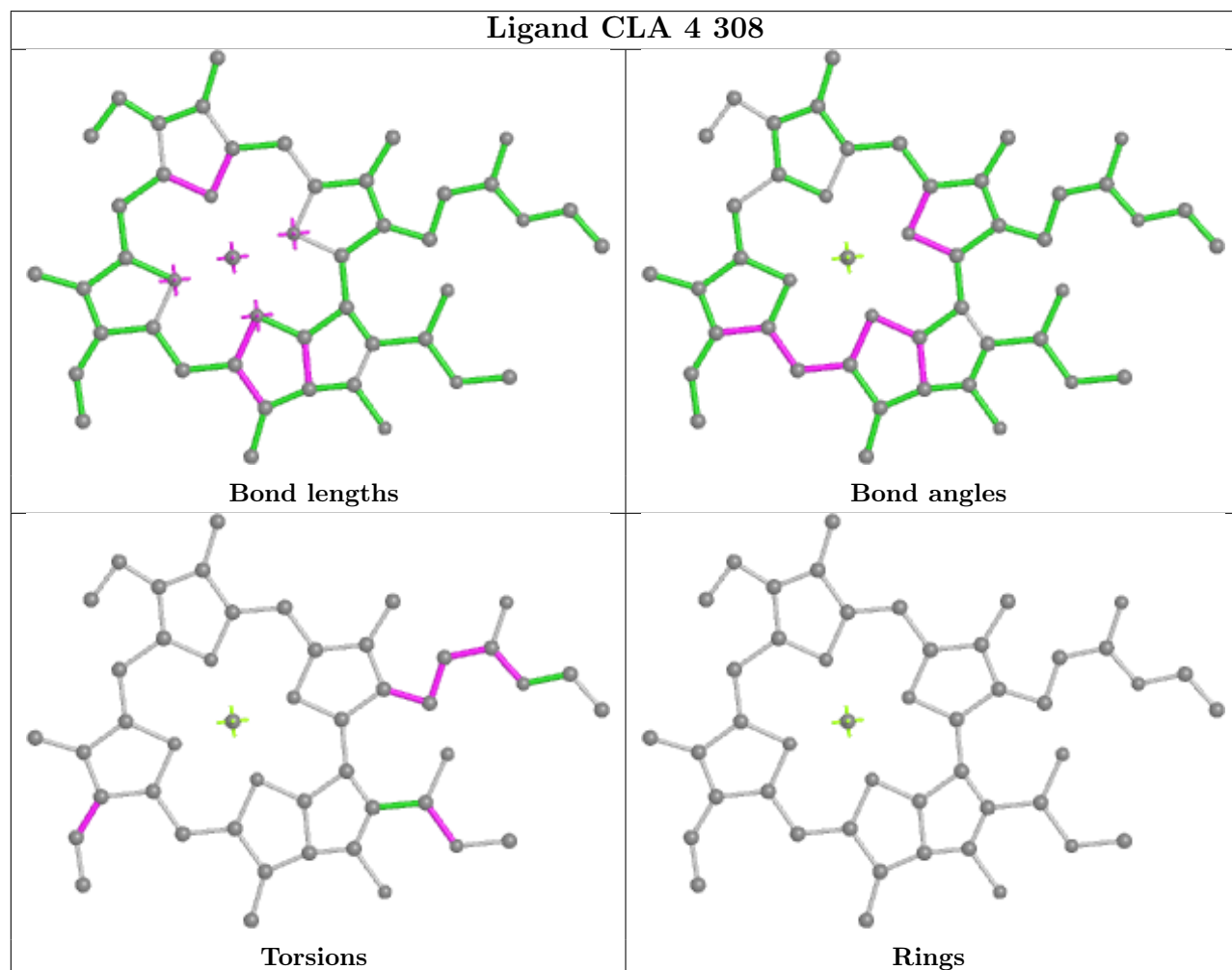


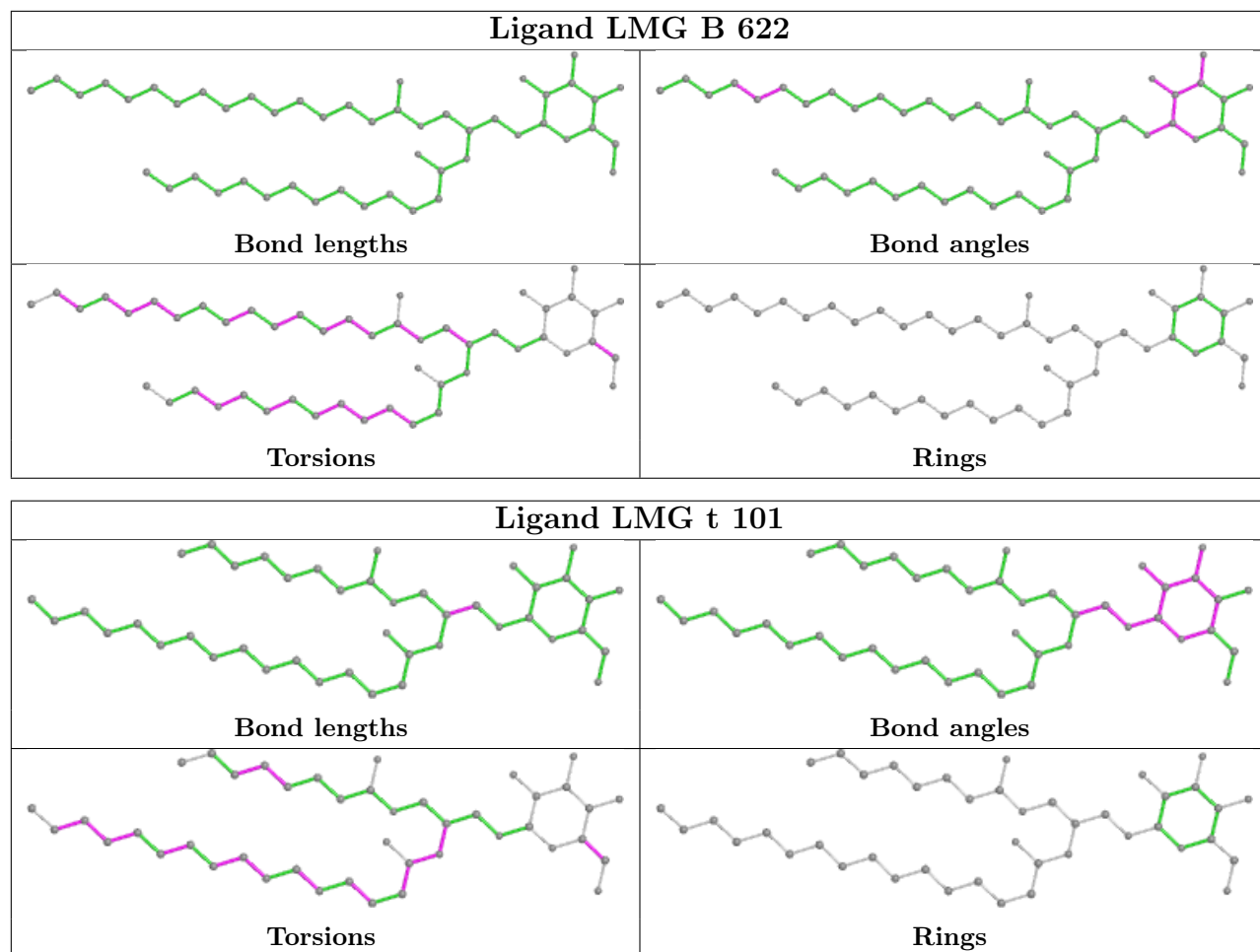


## Ligand CLA 2 302

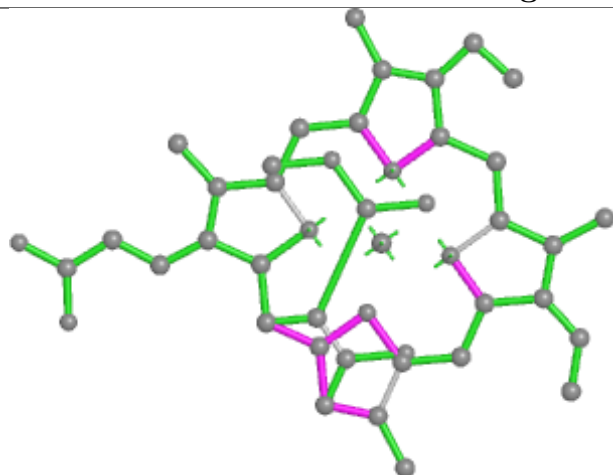


## Ligand CLA 4 308

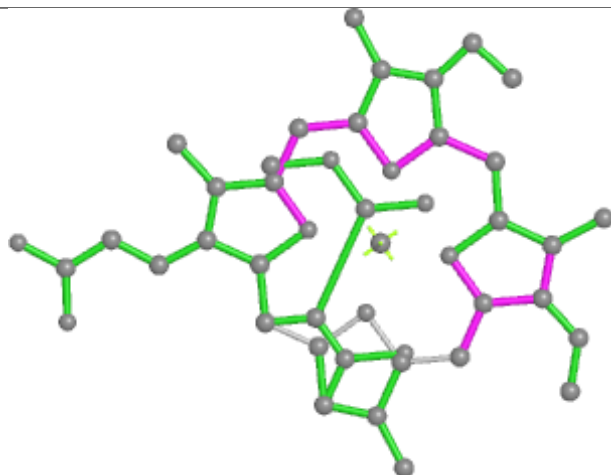




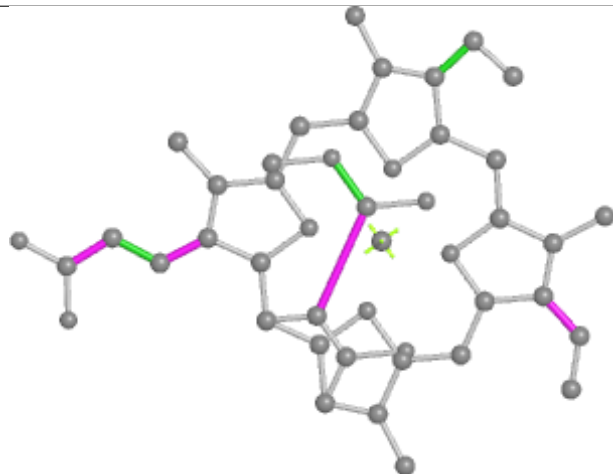
## Ligand KC2 9 311



Bond lengths



Bond angles

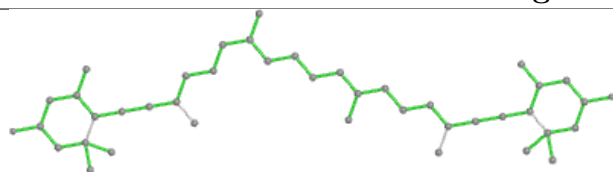


Torsions

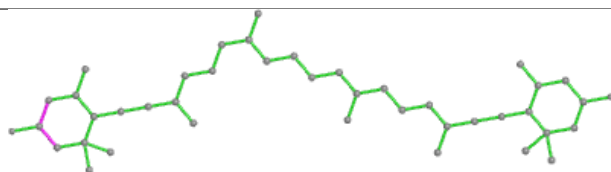


Rings

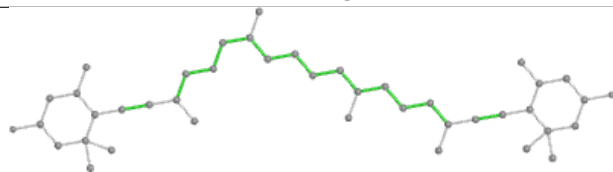
## Ligand II0 2 311



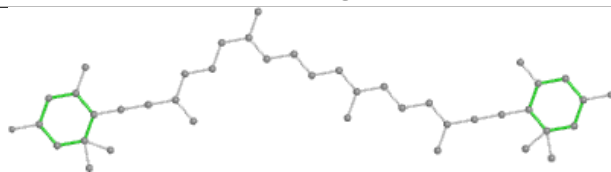
Bond lengths



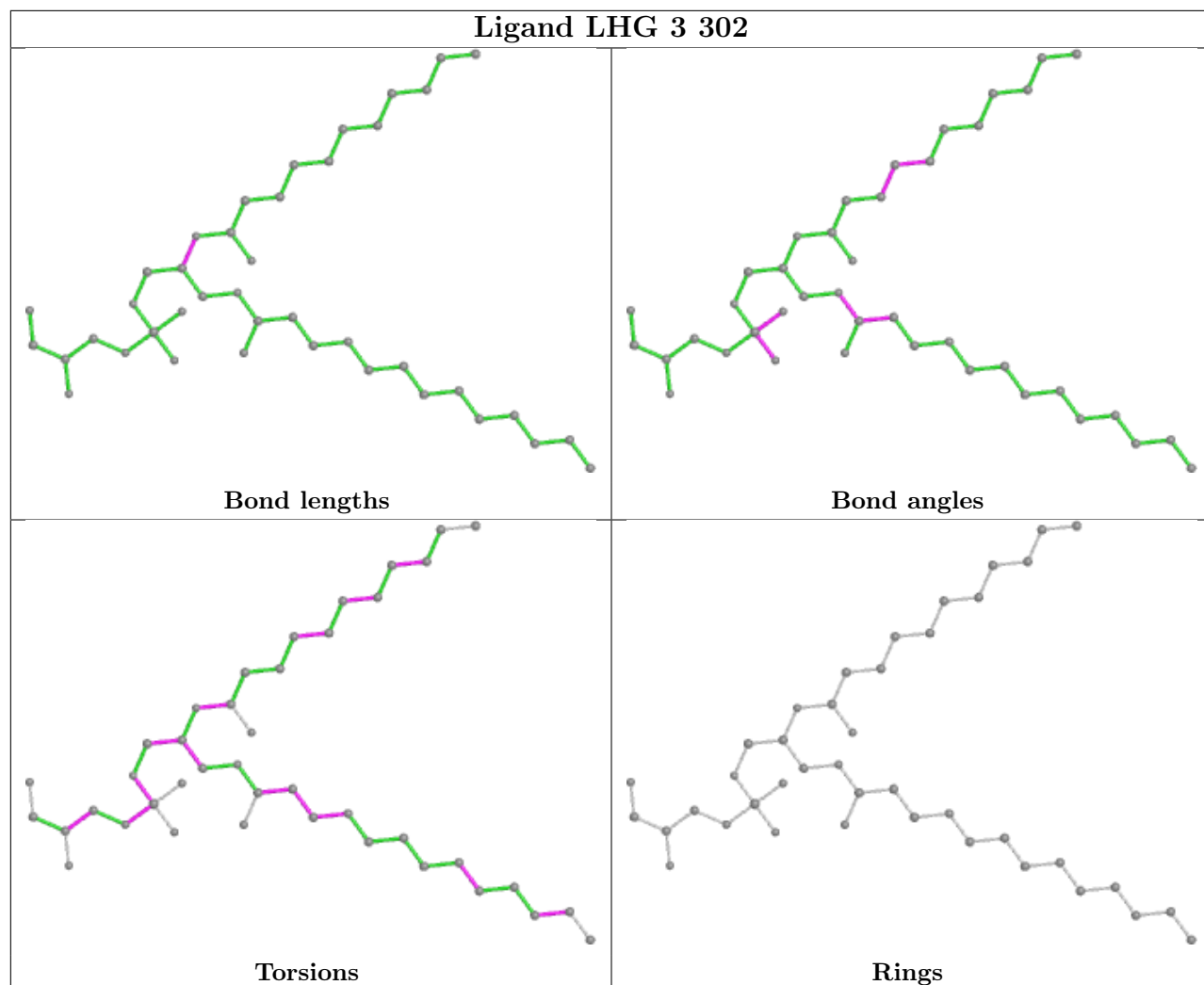
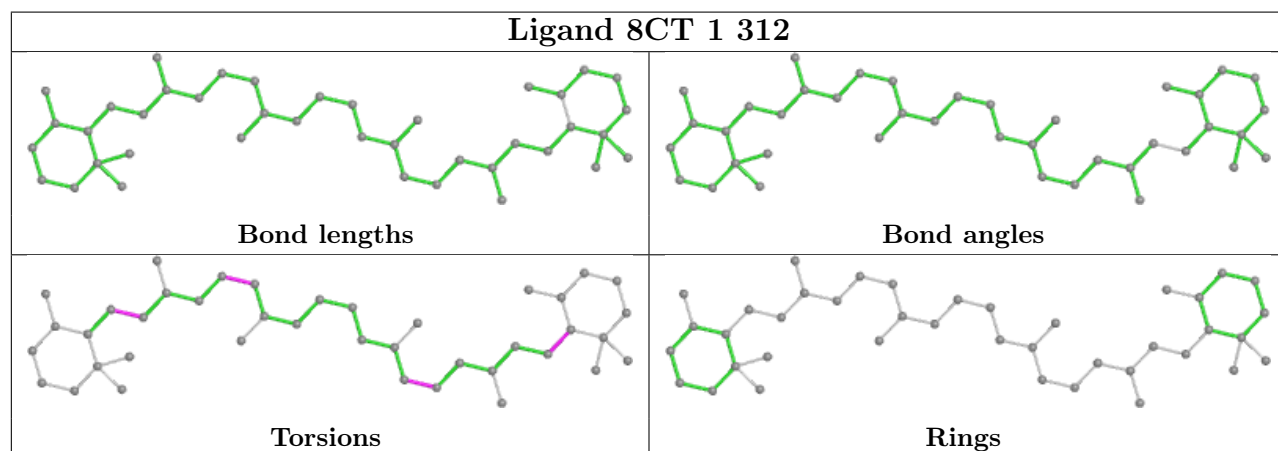
Bond angles



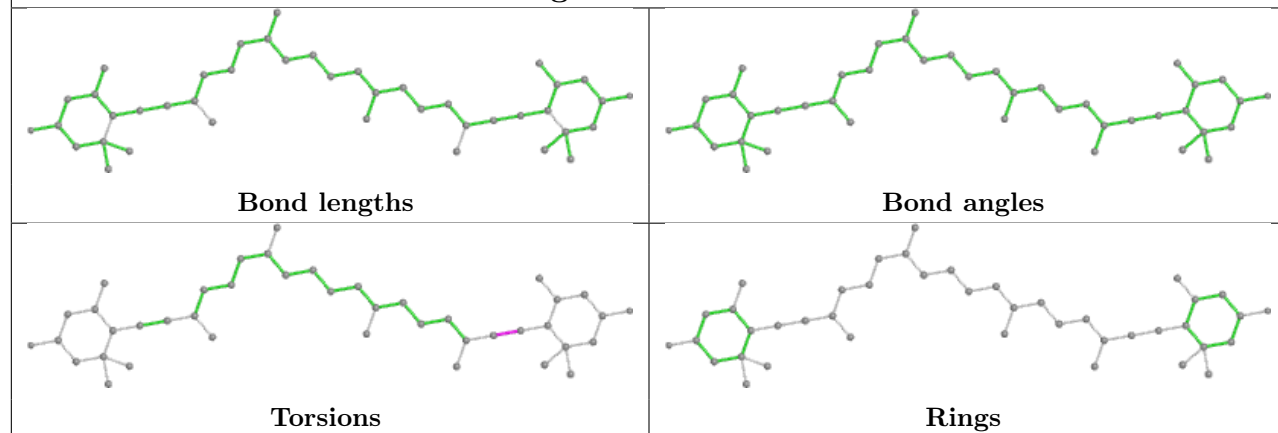
Torsions



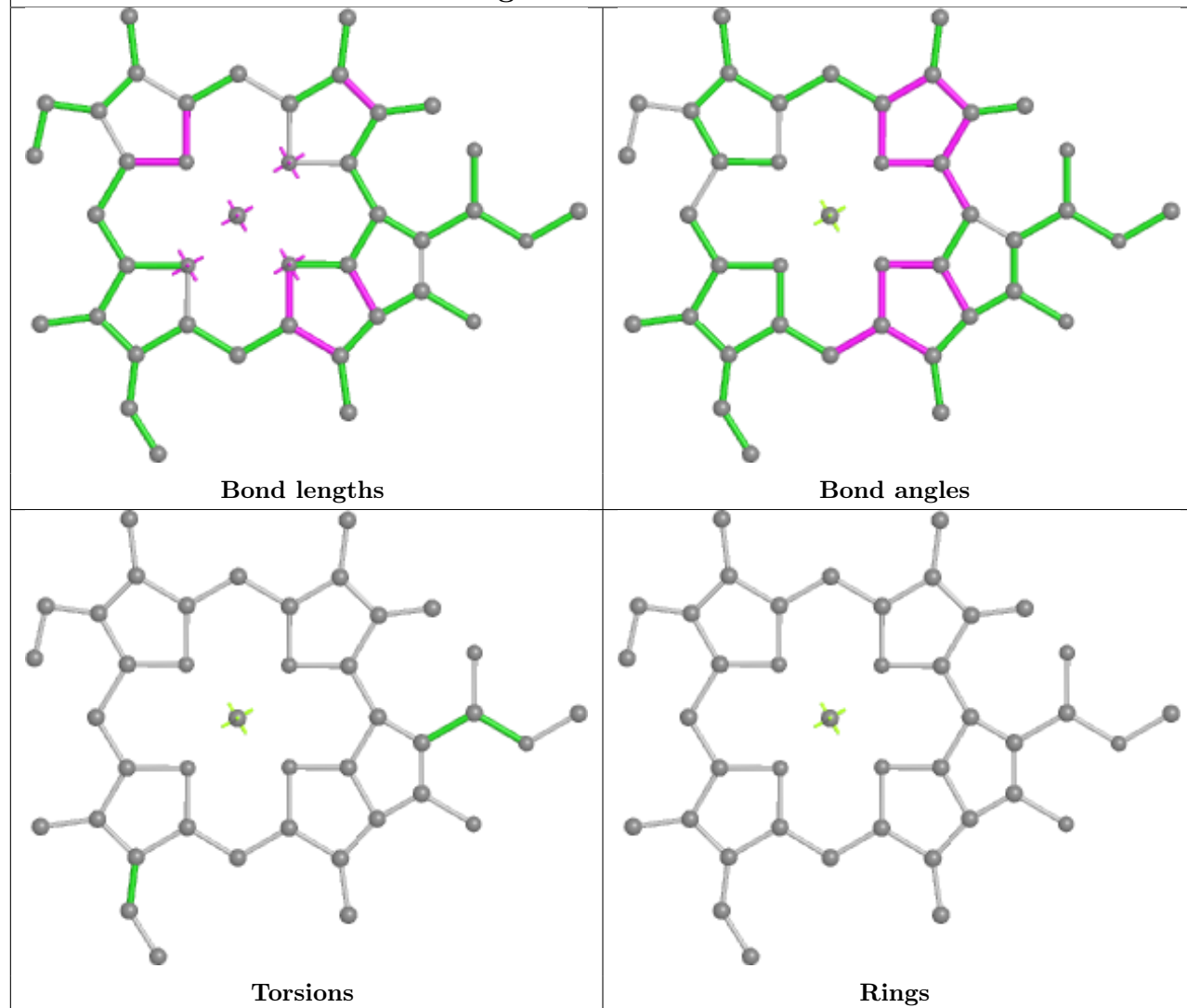
Rings

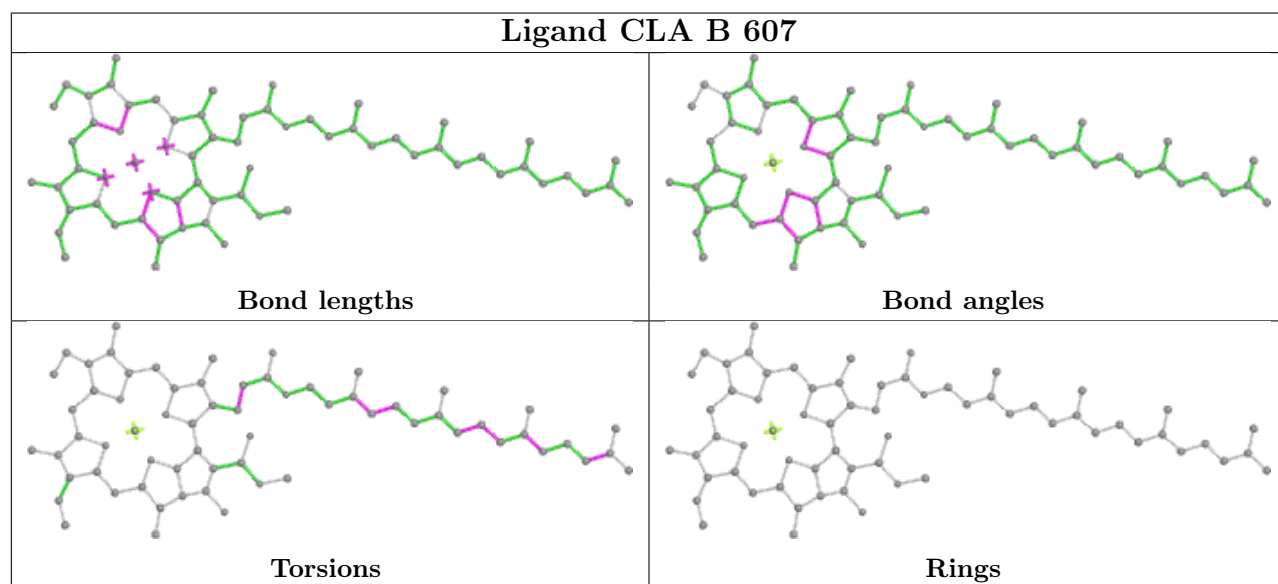
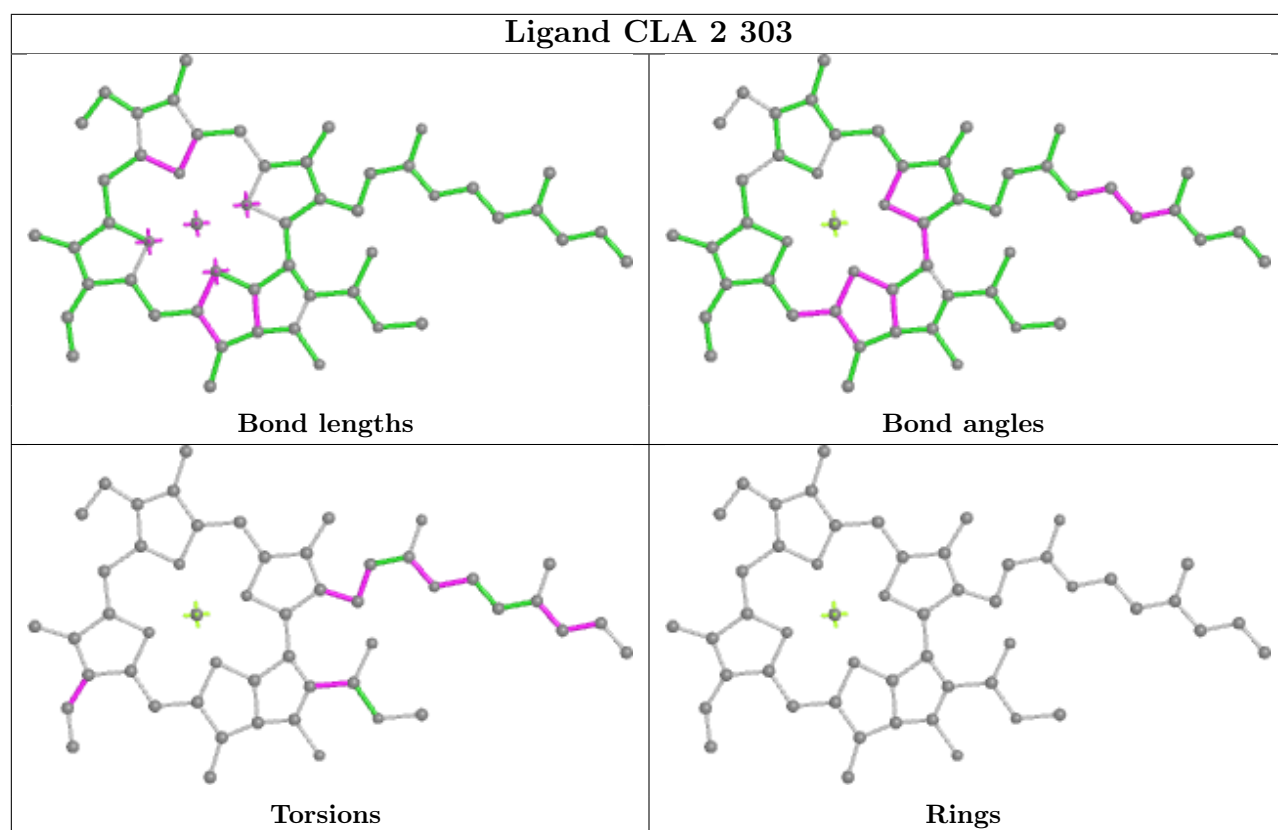
**Ligand LHG 3 302****Ligand 8CT 1 312**

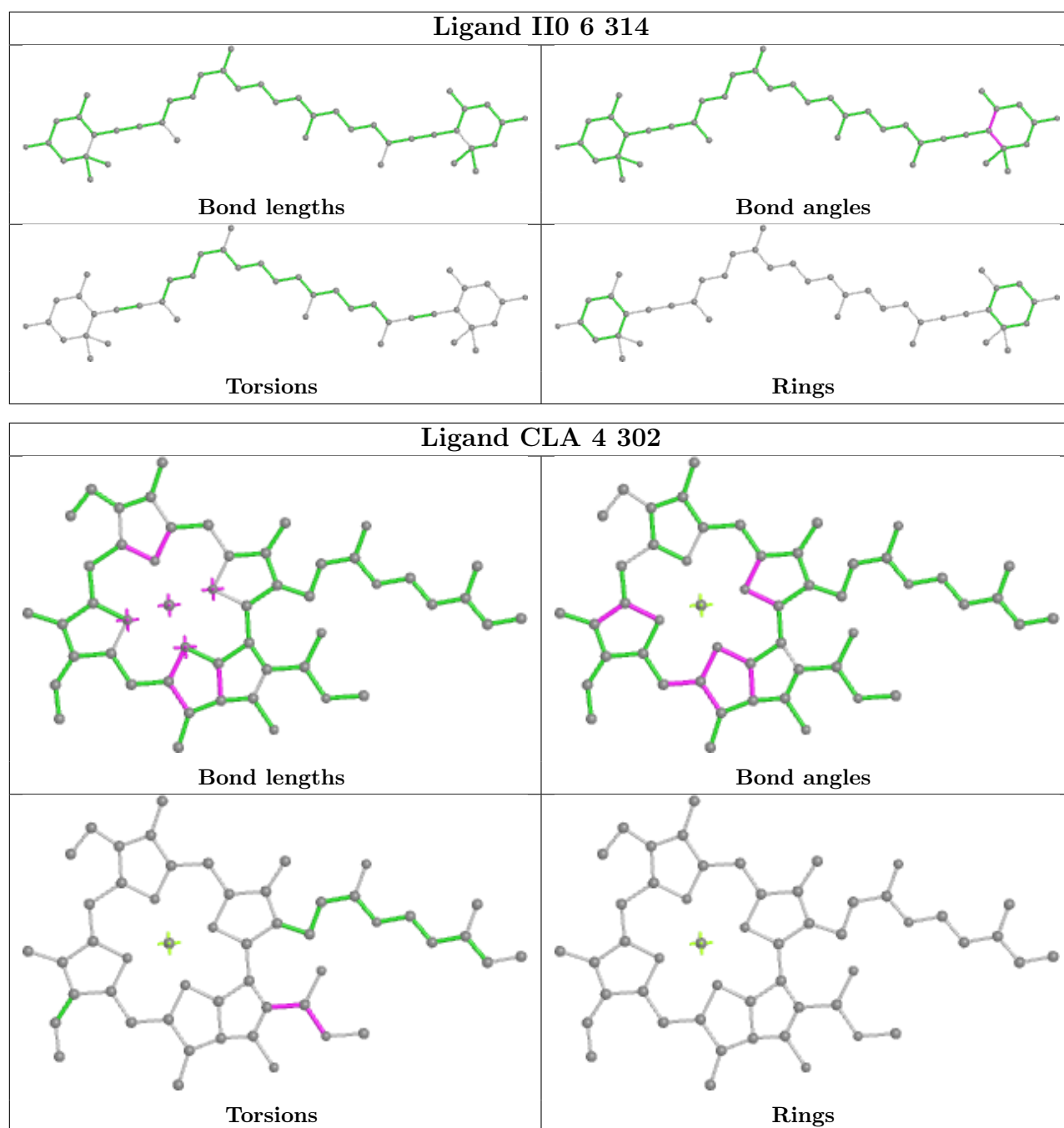
## Ligand II0 9 301



## Ligand CLA 6 302

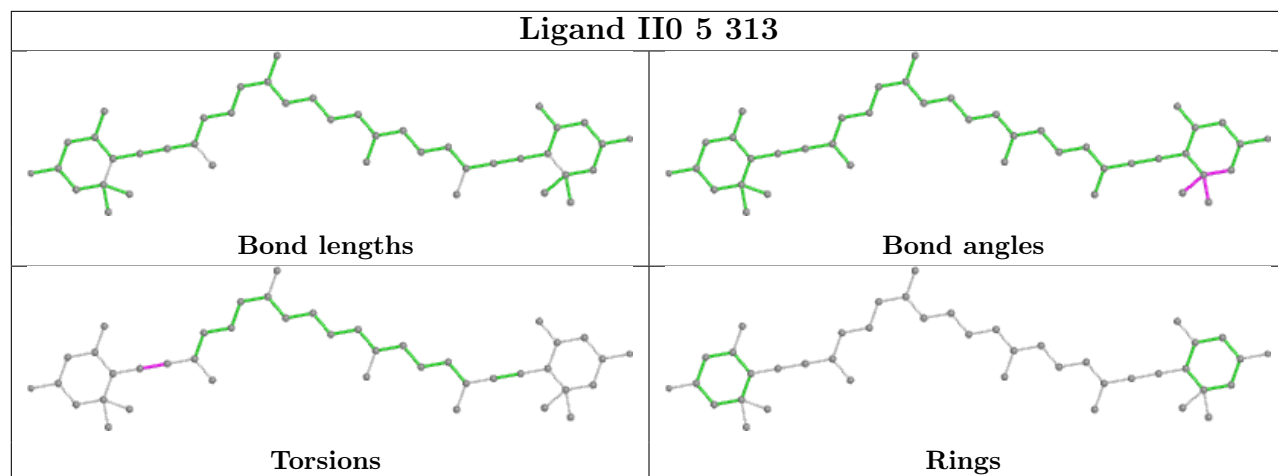




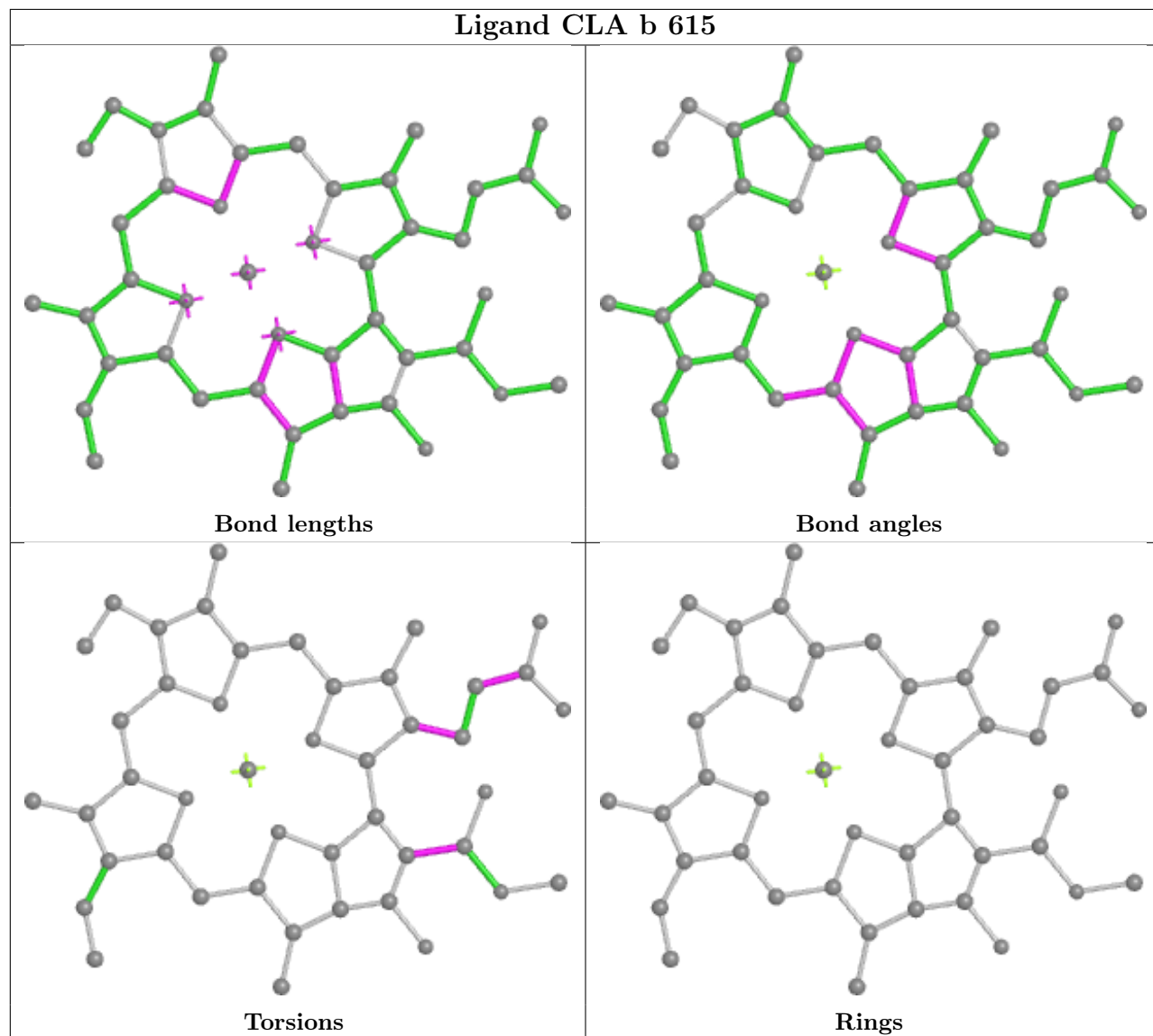


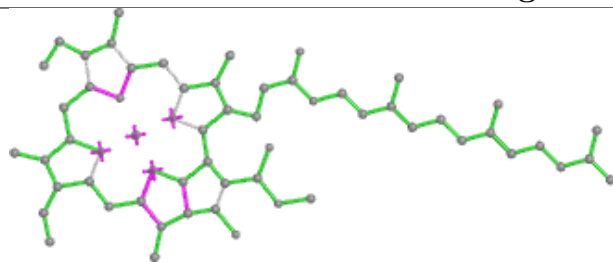
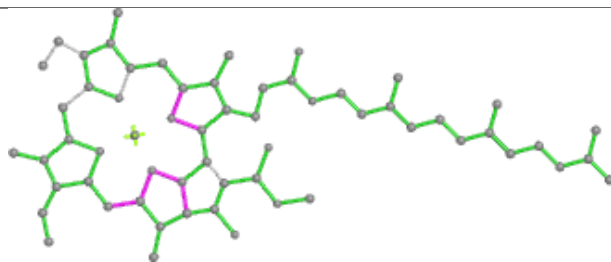
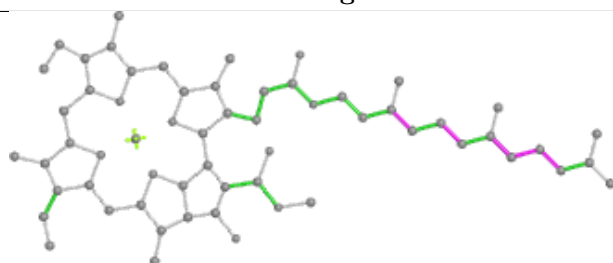
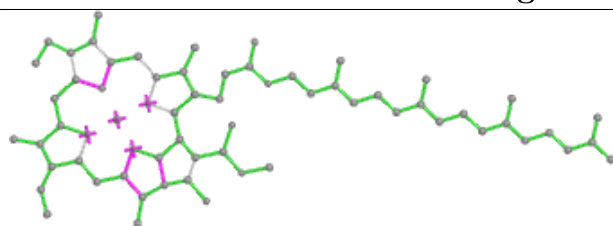
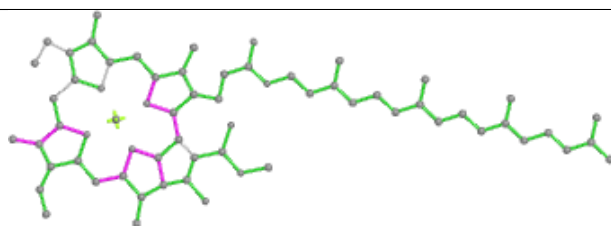
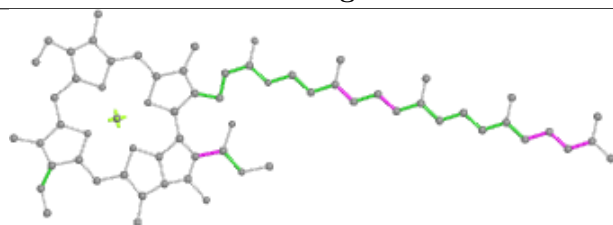
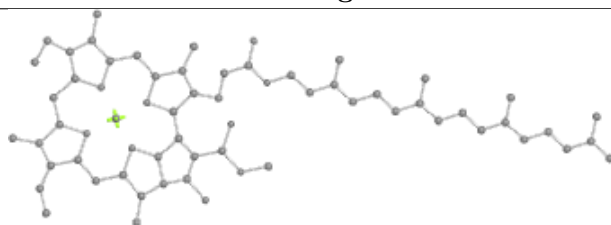


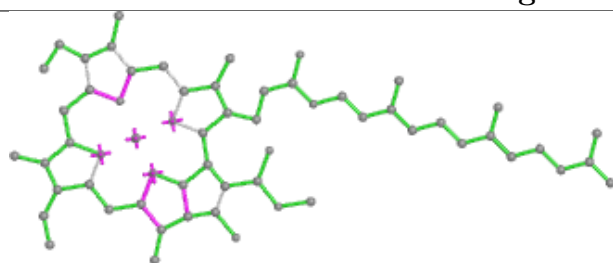
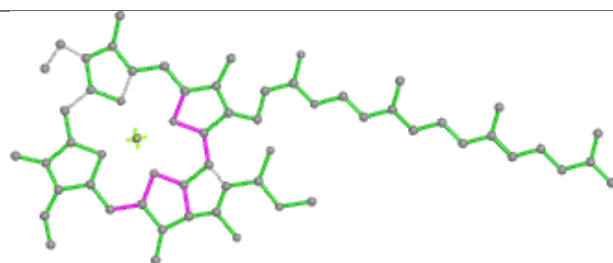
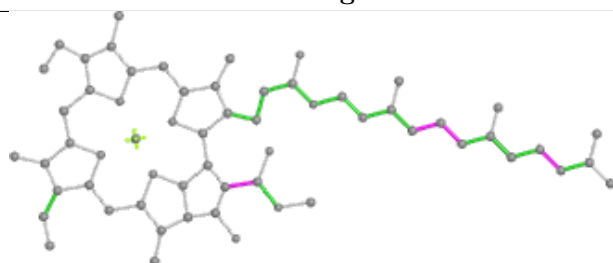
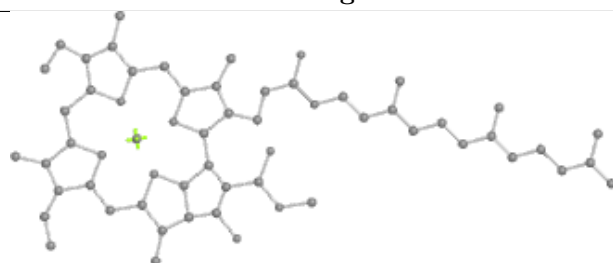
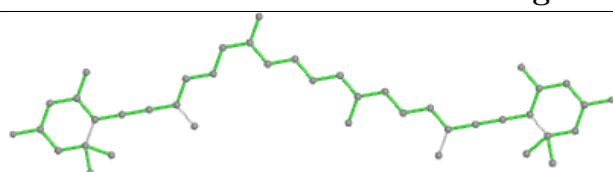
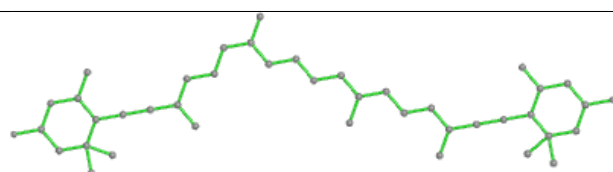
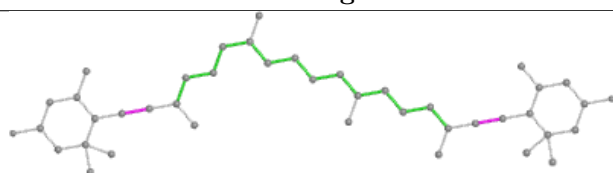
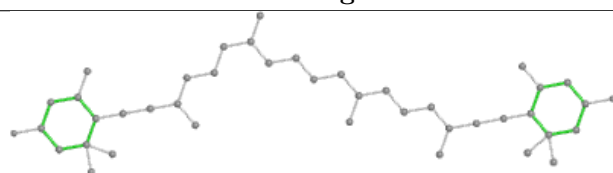
## Ligand II0 5 313



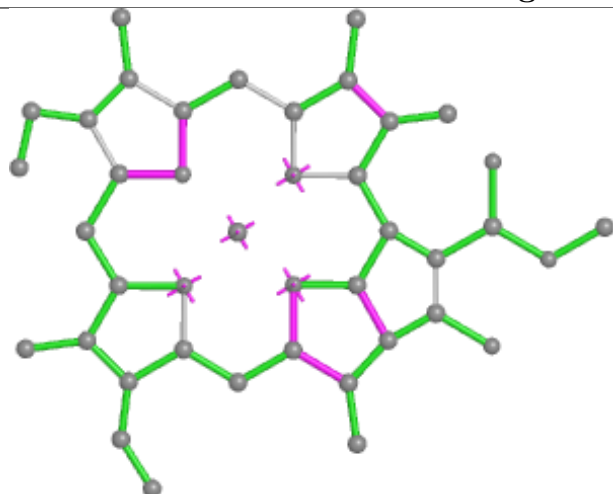
## Ligand CLA b 615



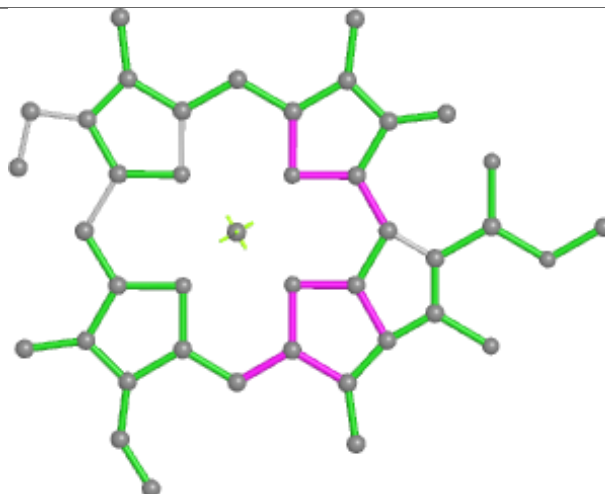
**Ligand CLA 1 305****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA b 610****Bond lengths****Bond angles****Torsions****Rings**

**Ligand CLA 7 306****Bond lengths****Bond angles****Torsions****Rings****Ligand II0 0 313****Bond lengths****Bond angles****Torsions****Rings**

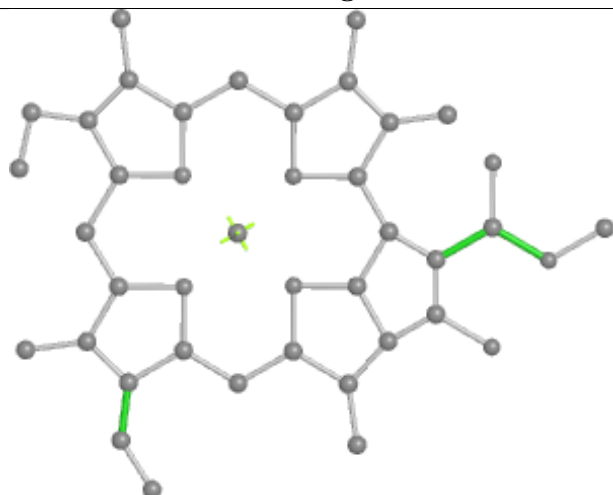
## Ligand CLA 3 314



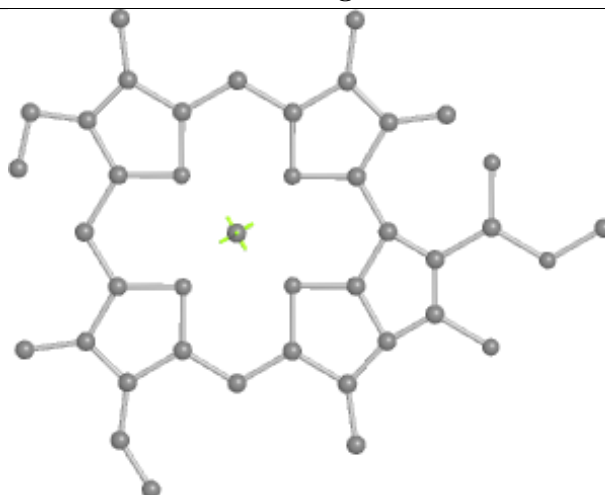
Bond lengths



Bond angles

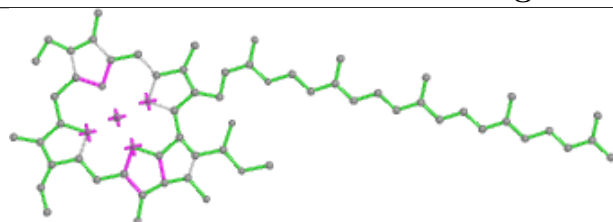


Torsions

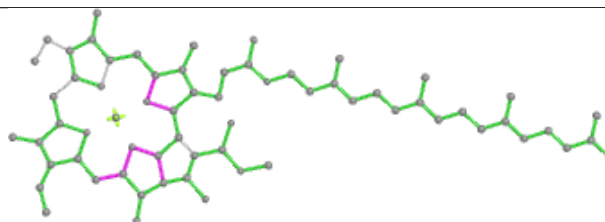


Rings

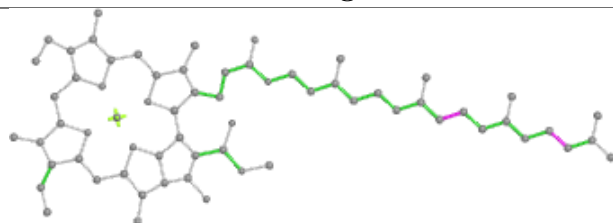
## Ligand CLA C 504



Bond lengths



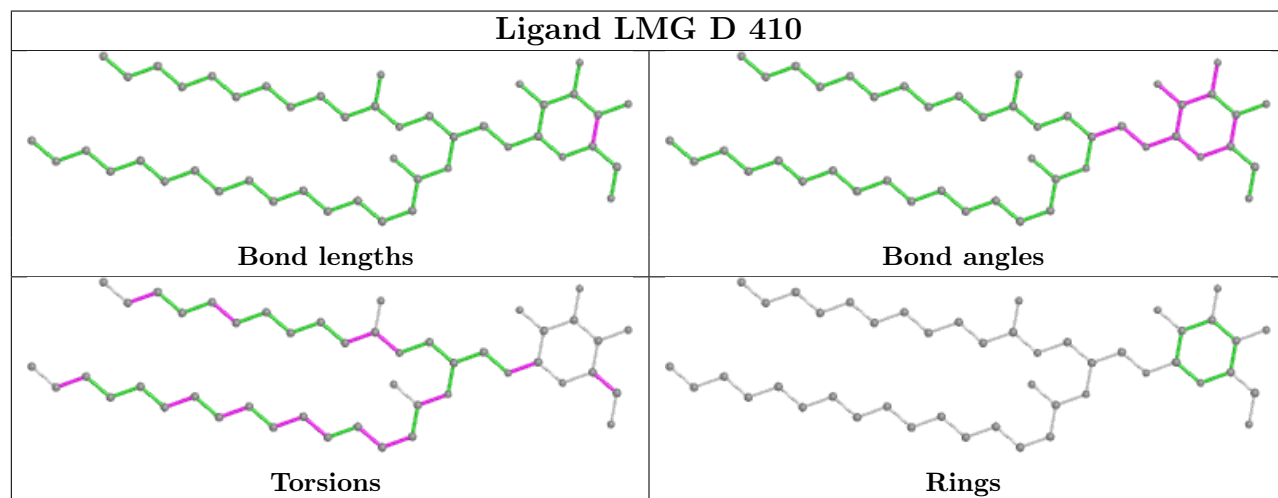
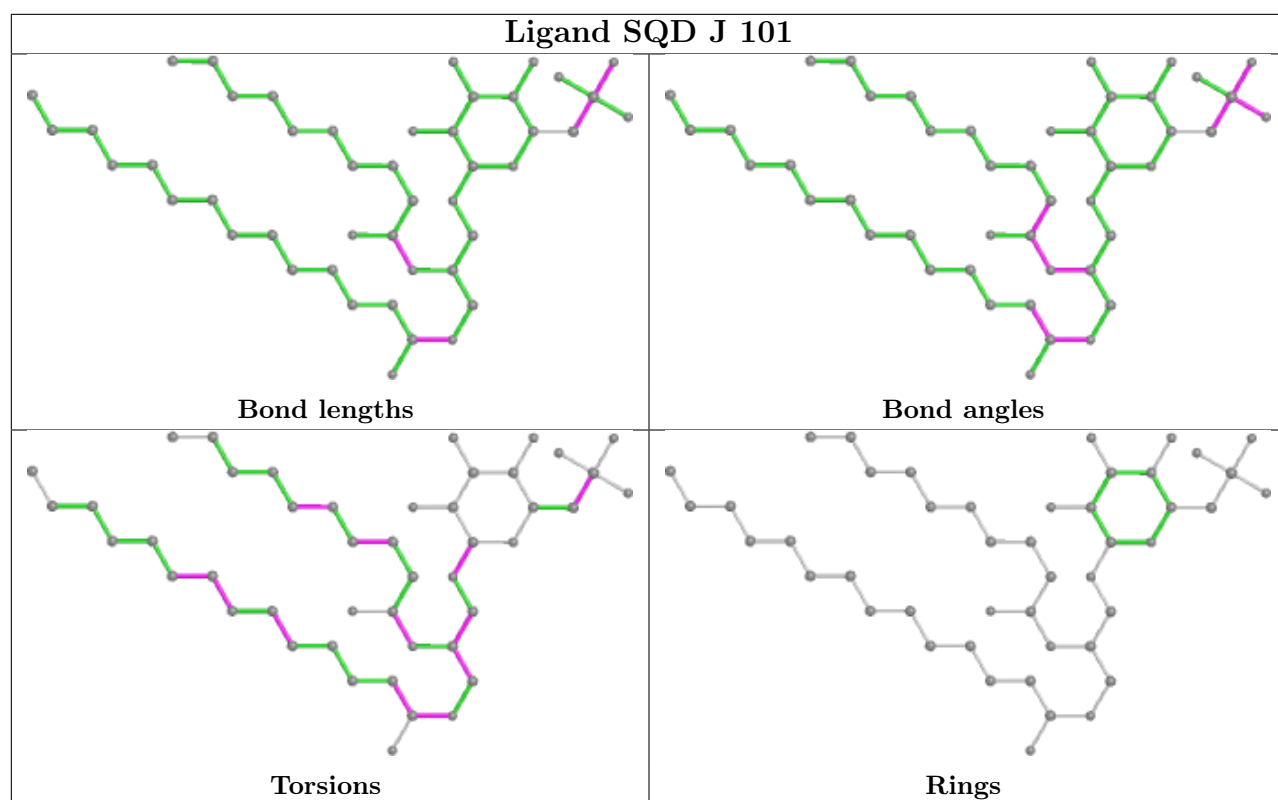
Bond angles

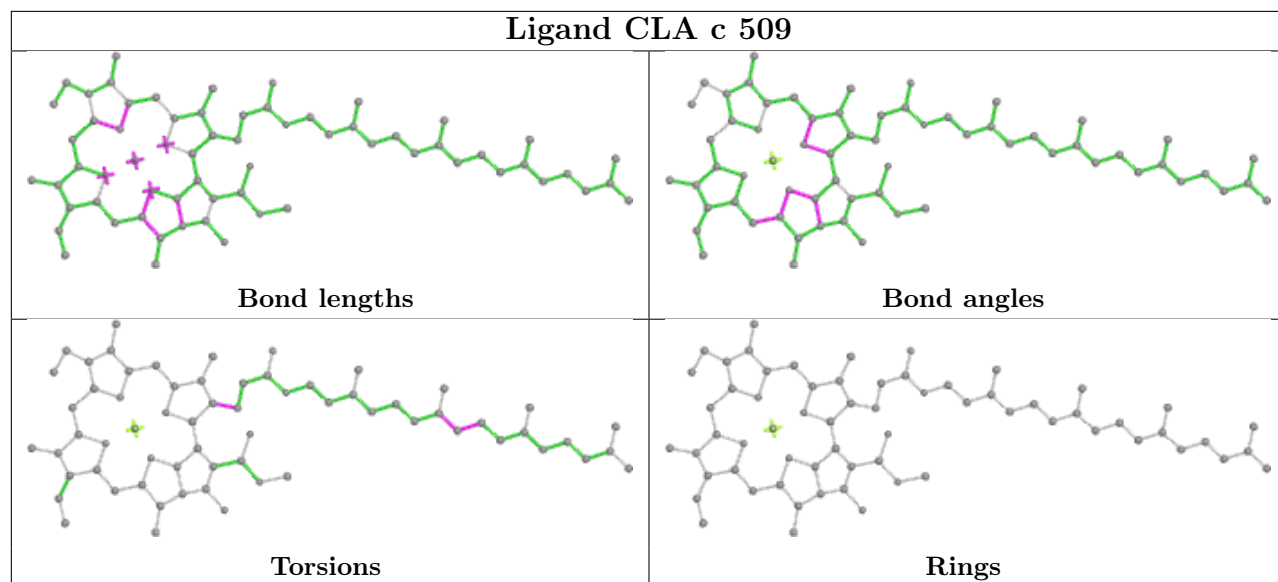
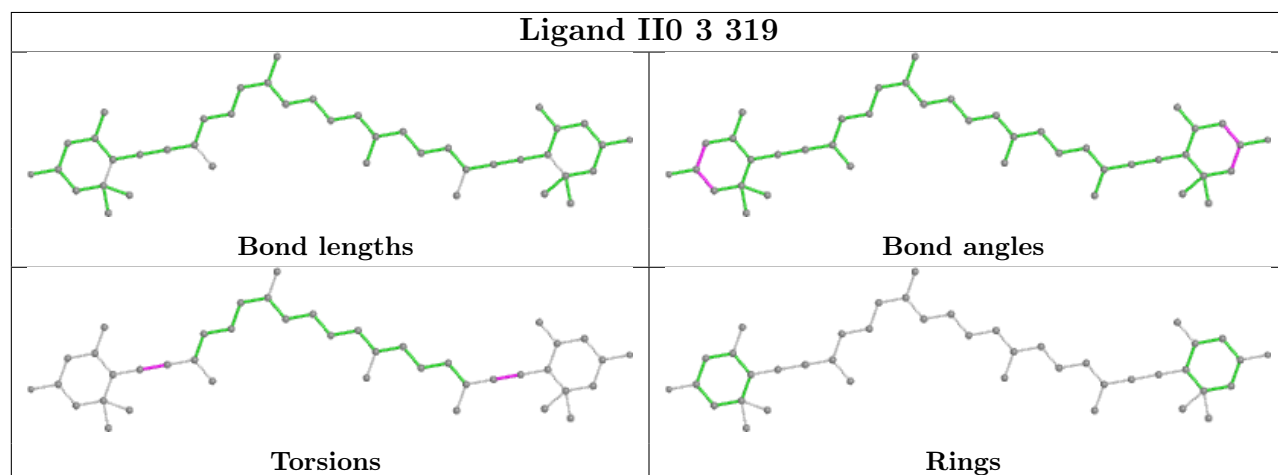
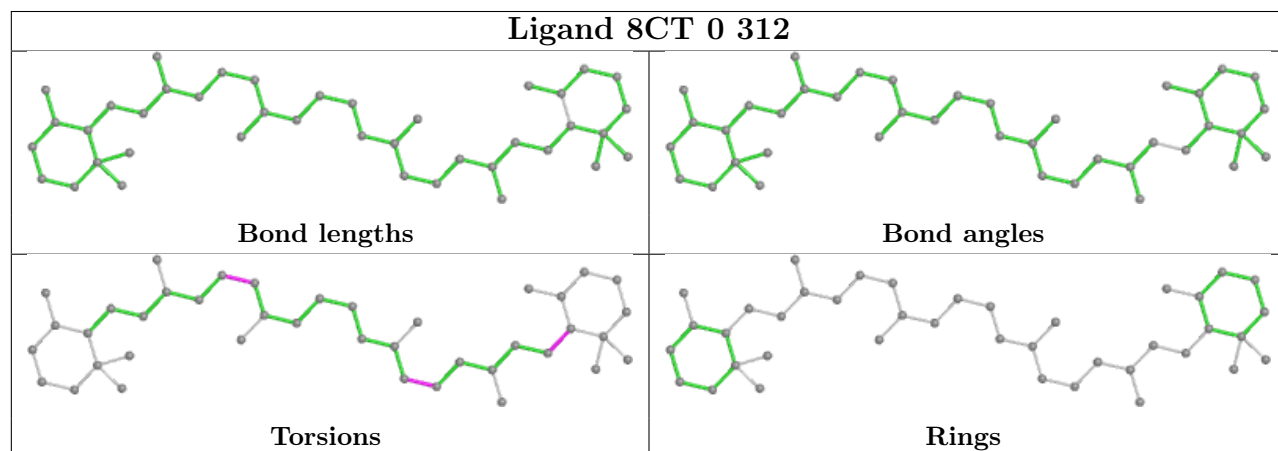


Torsions

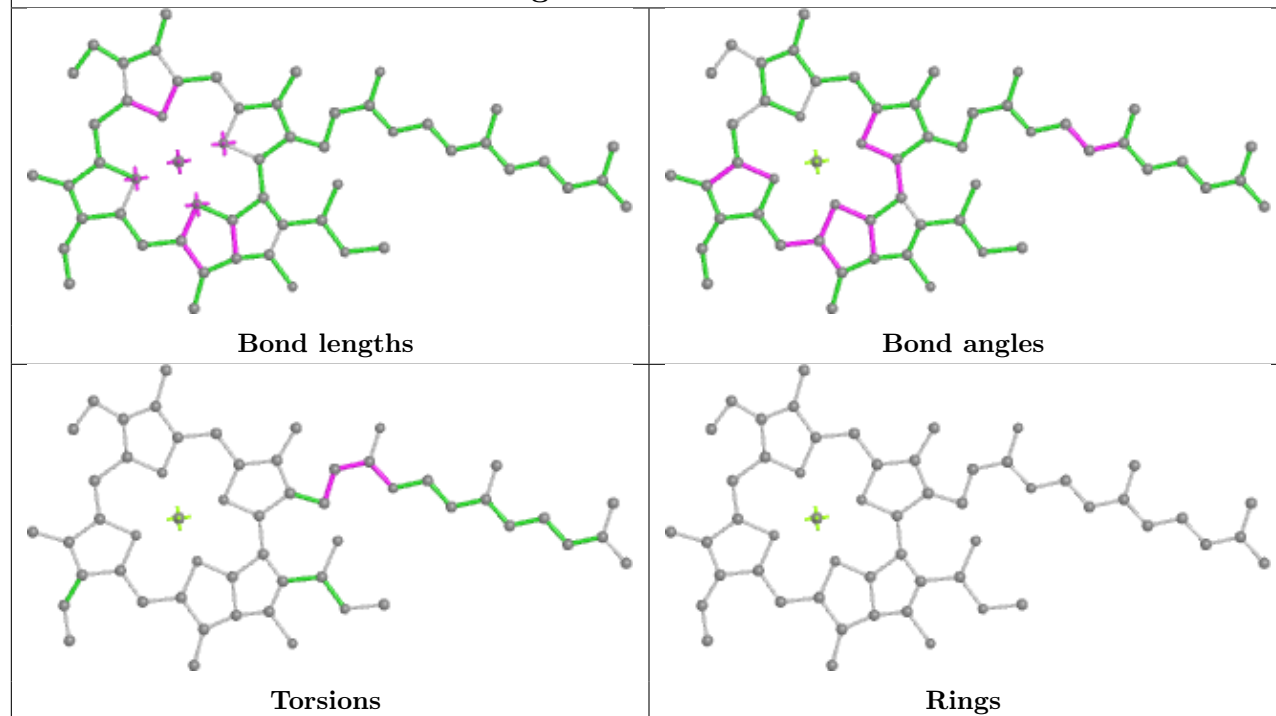


Rings

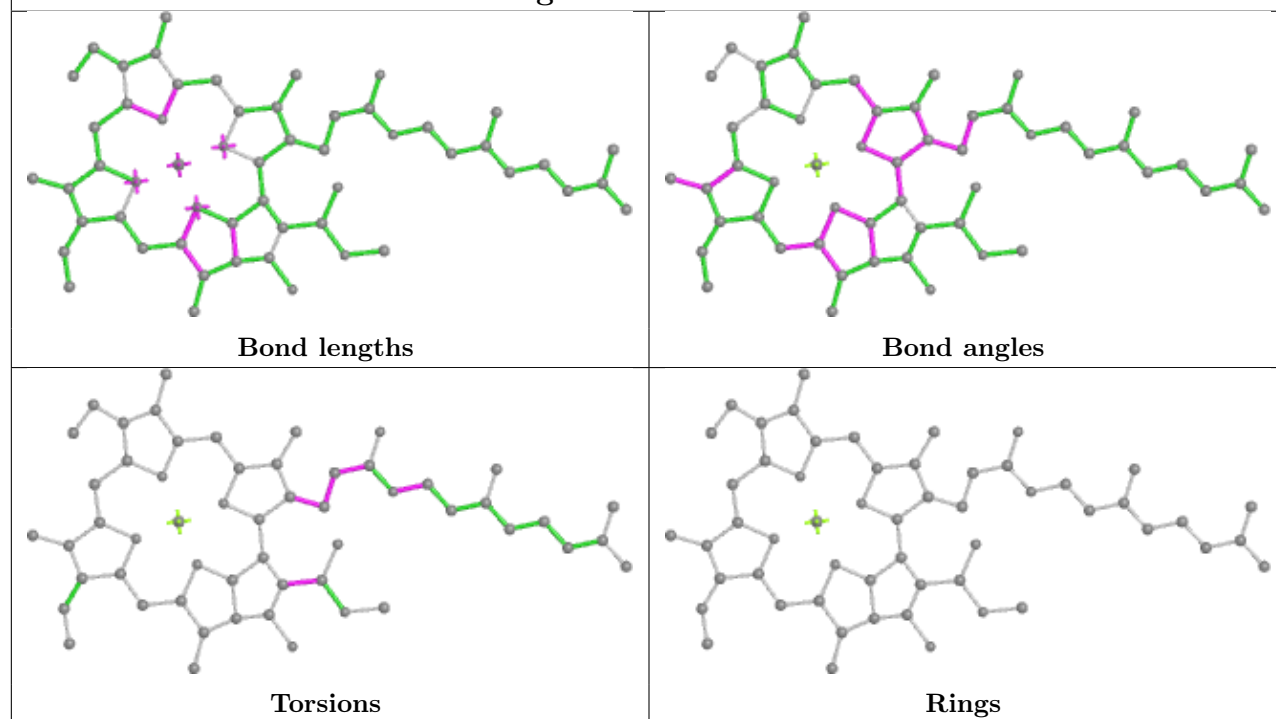


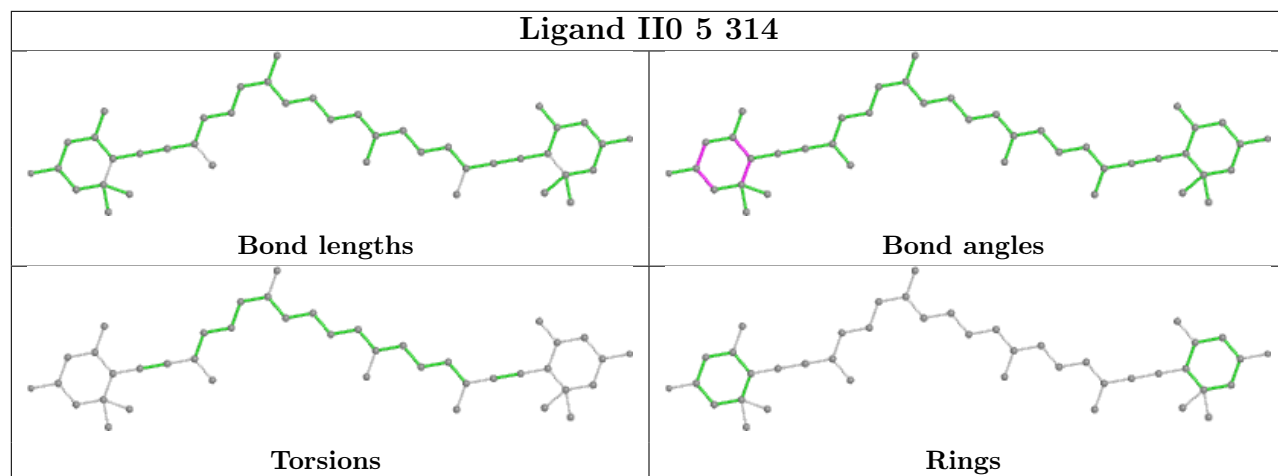
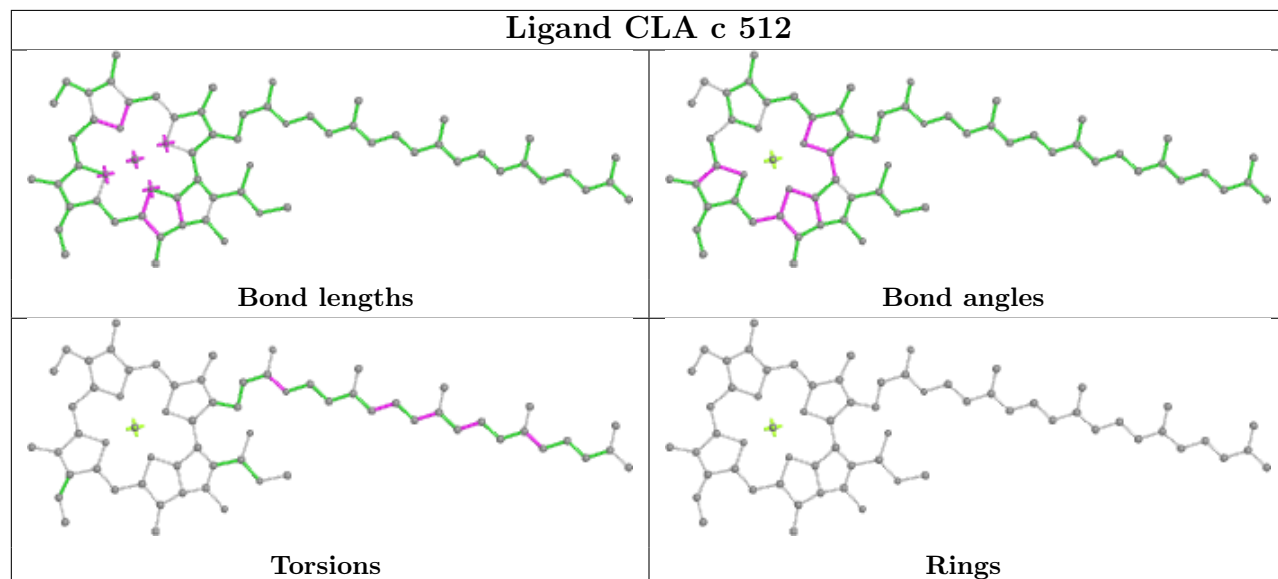
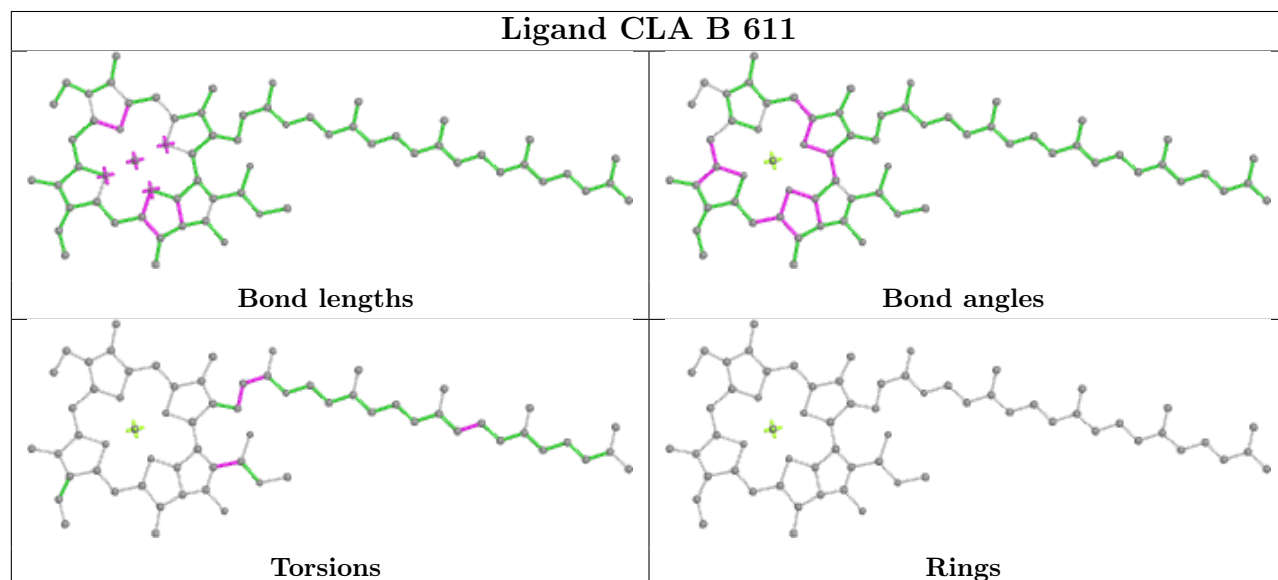
**Ligand CLA c 509****Ligand II0 3 319****Ligand 8CT 0 312**

## Ligand CLA N 305

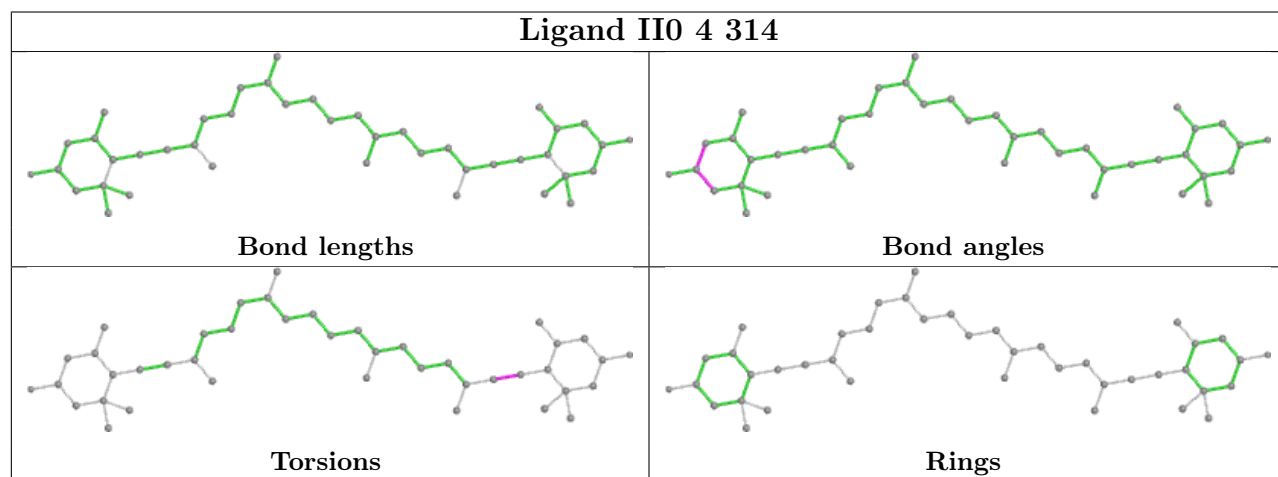
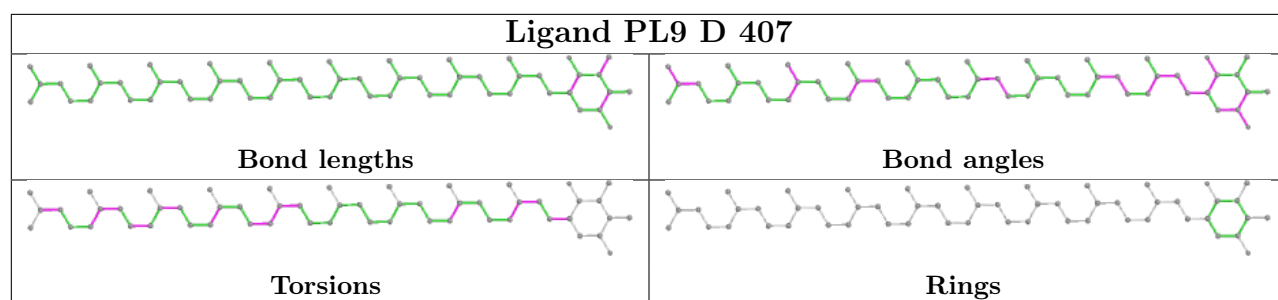


## Ligand CLA 5 302

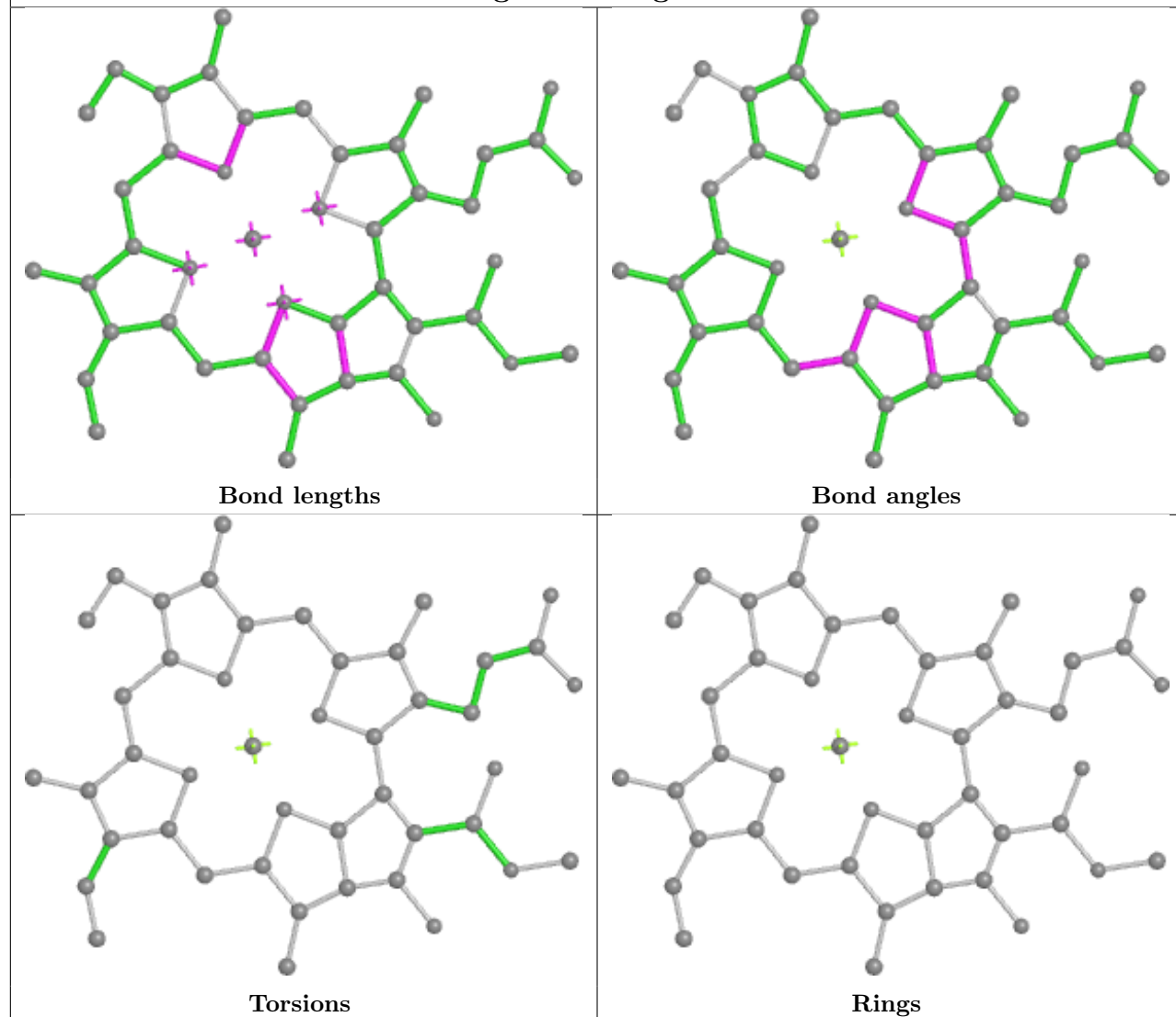


**Ligand II0 5 314****Ligand CLA c 512****Ligand CLA B 611**

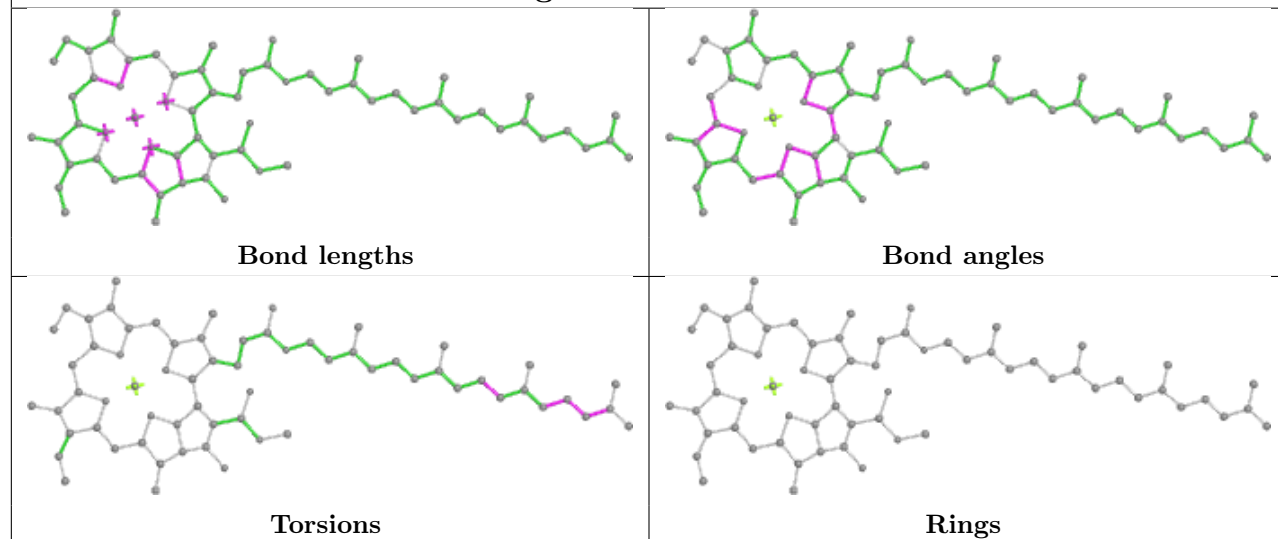


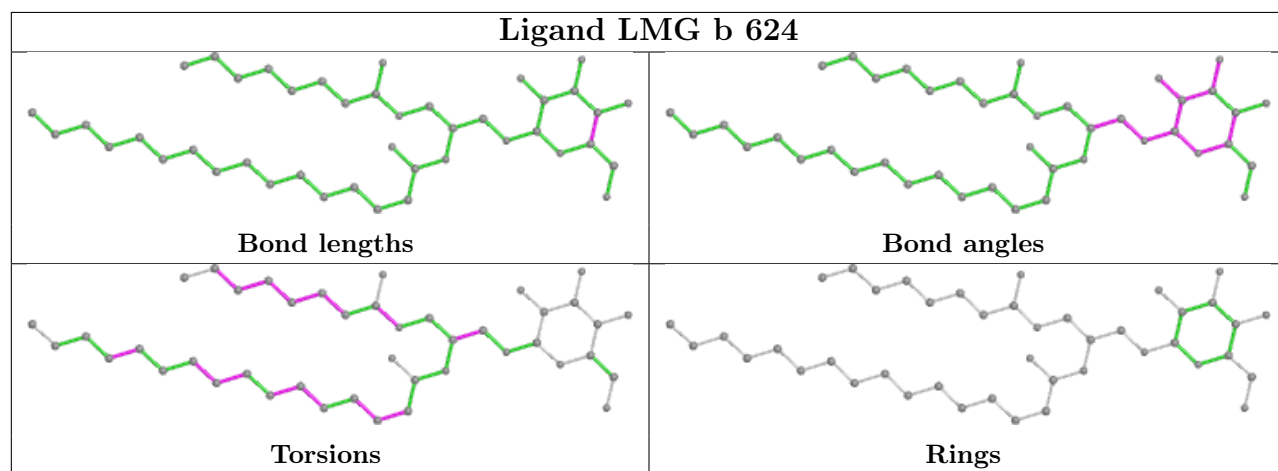
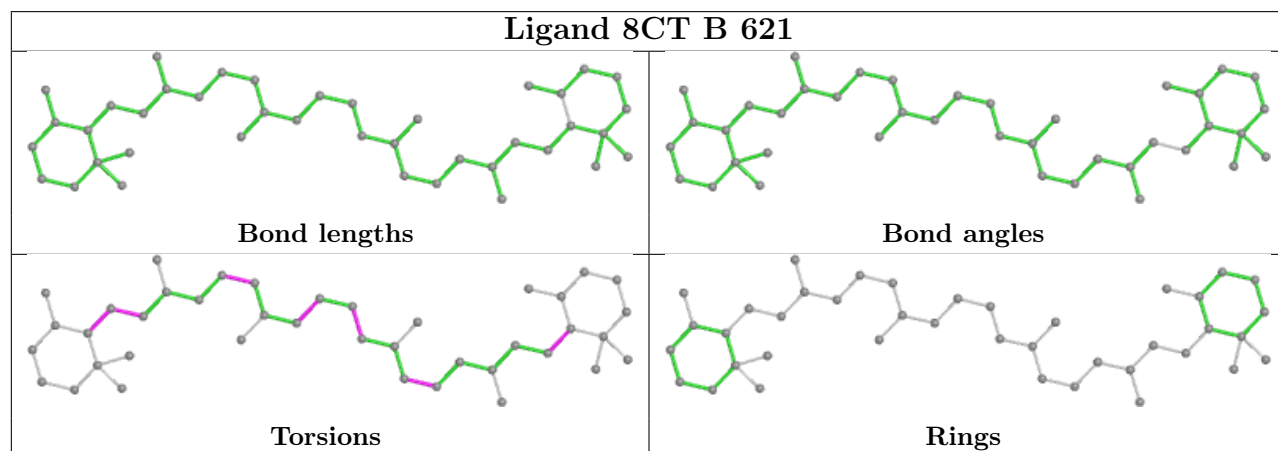
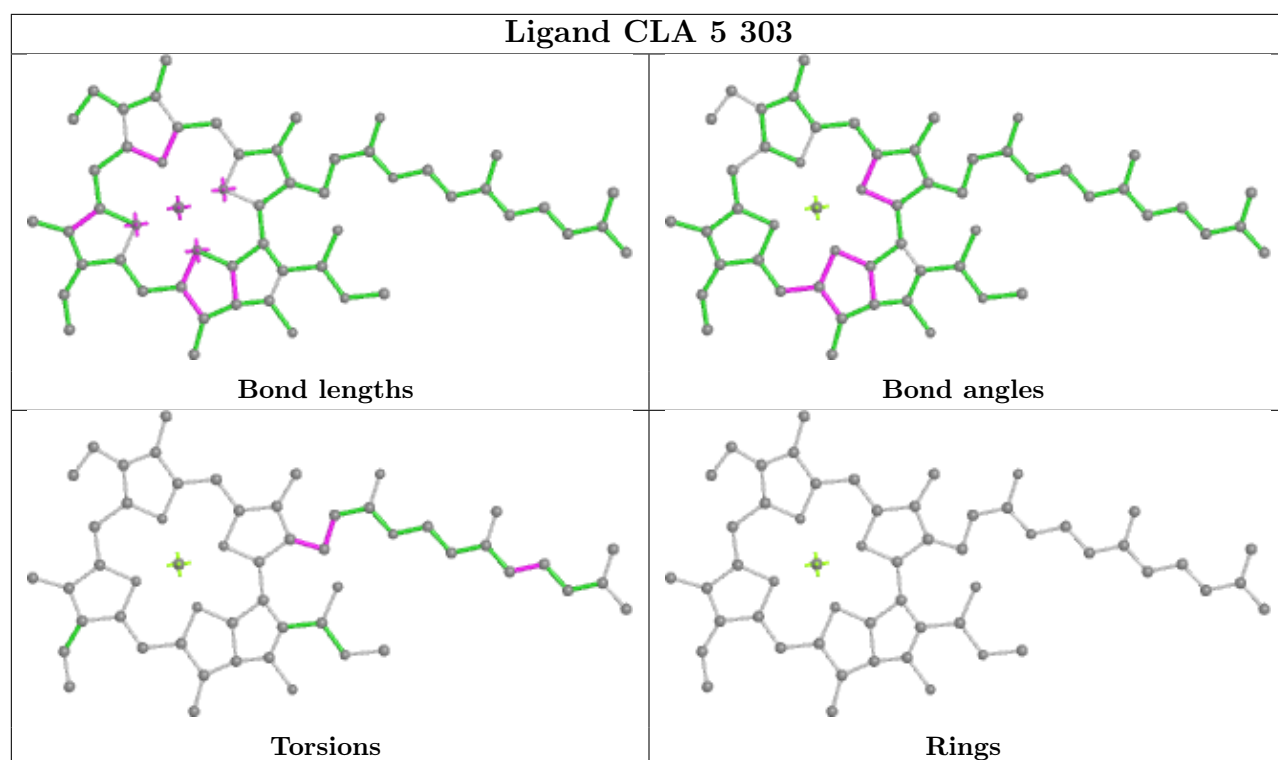


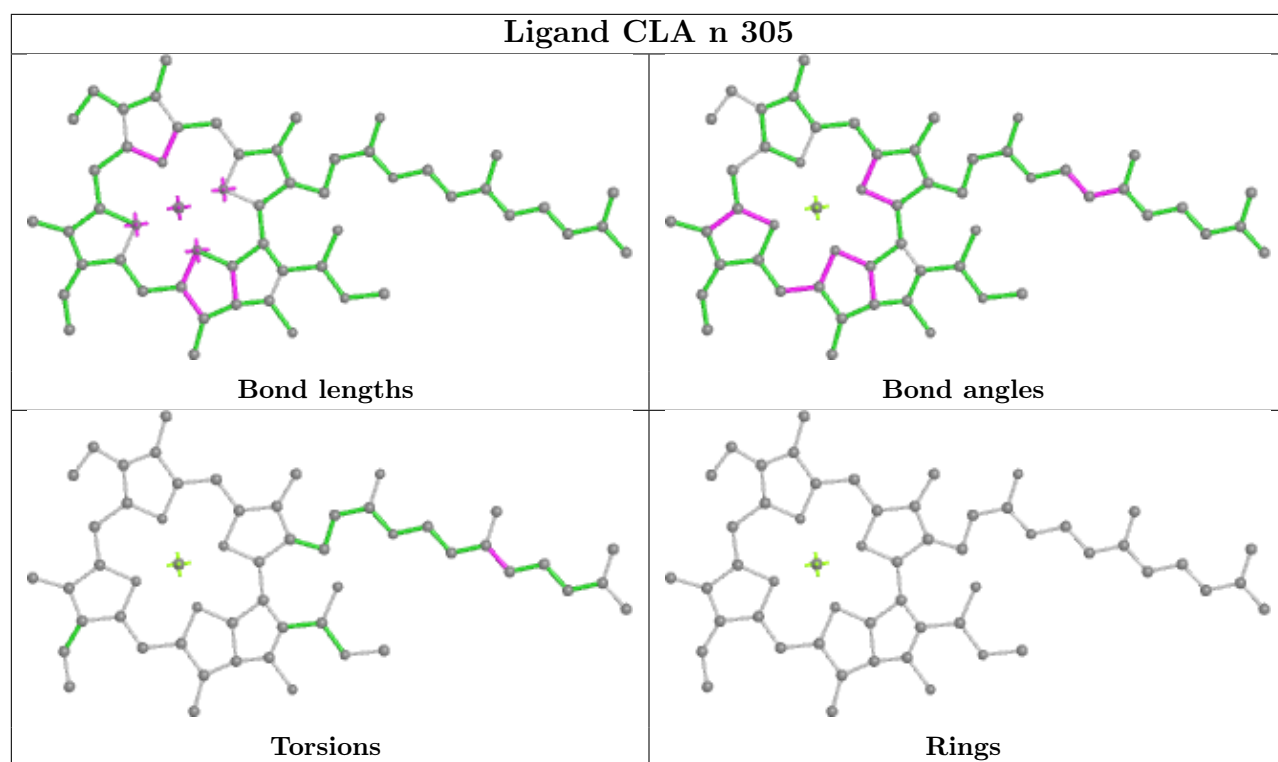
## Ligand CLA g 306

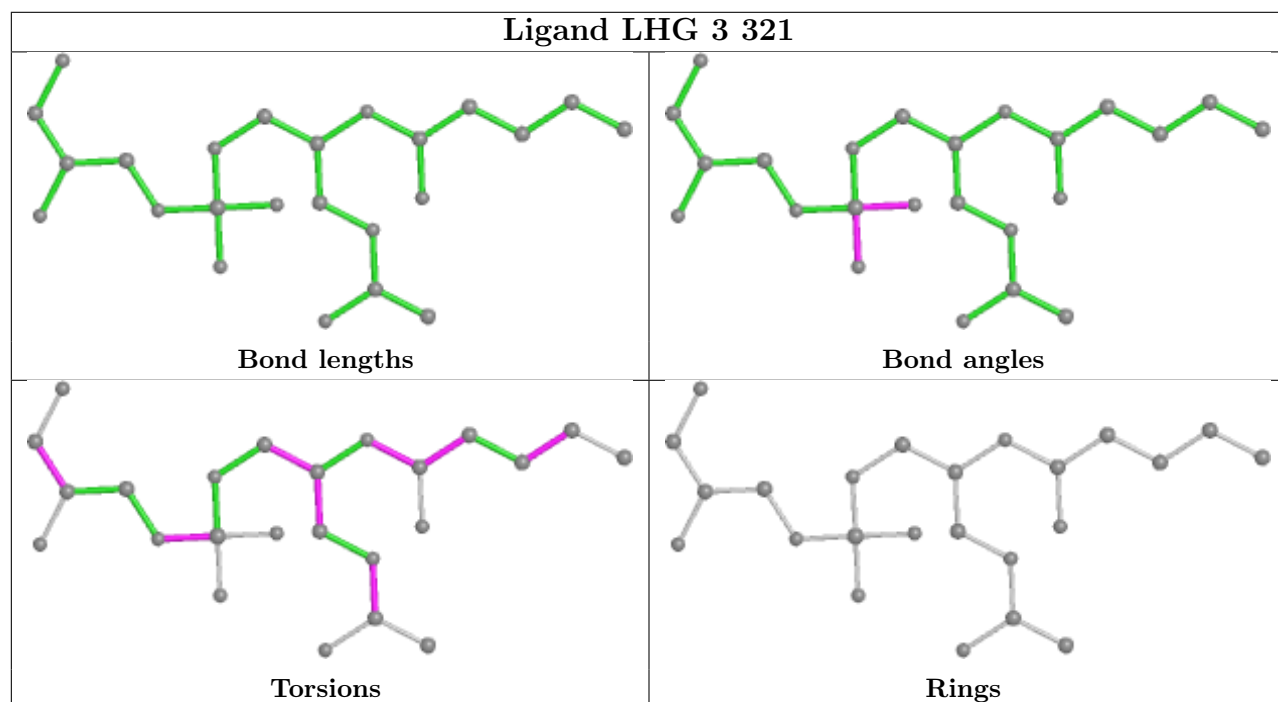
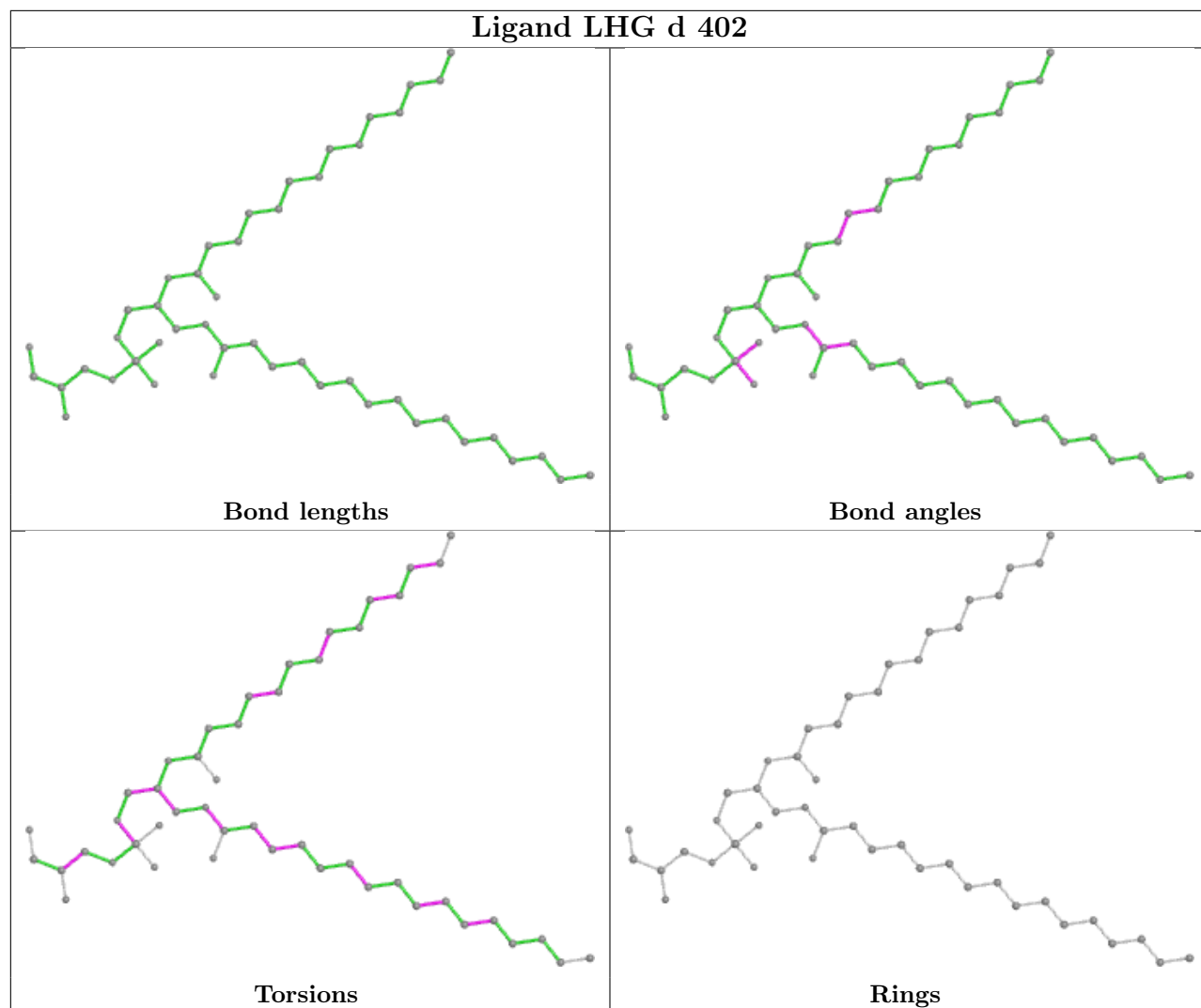


## Ligand CLA b 616

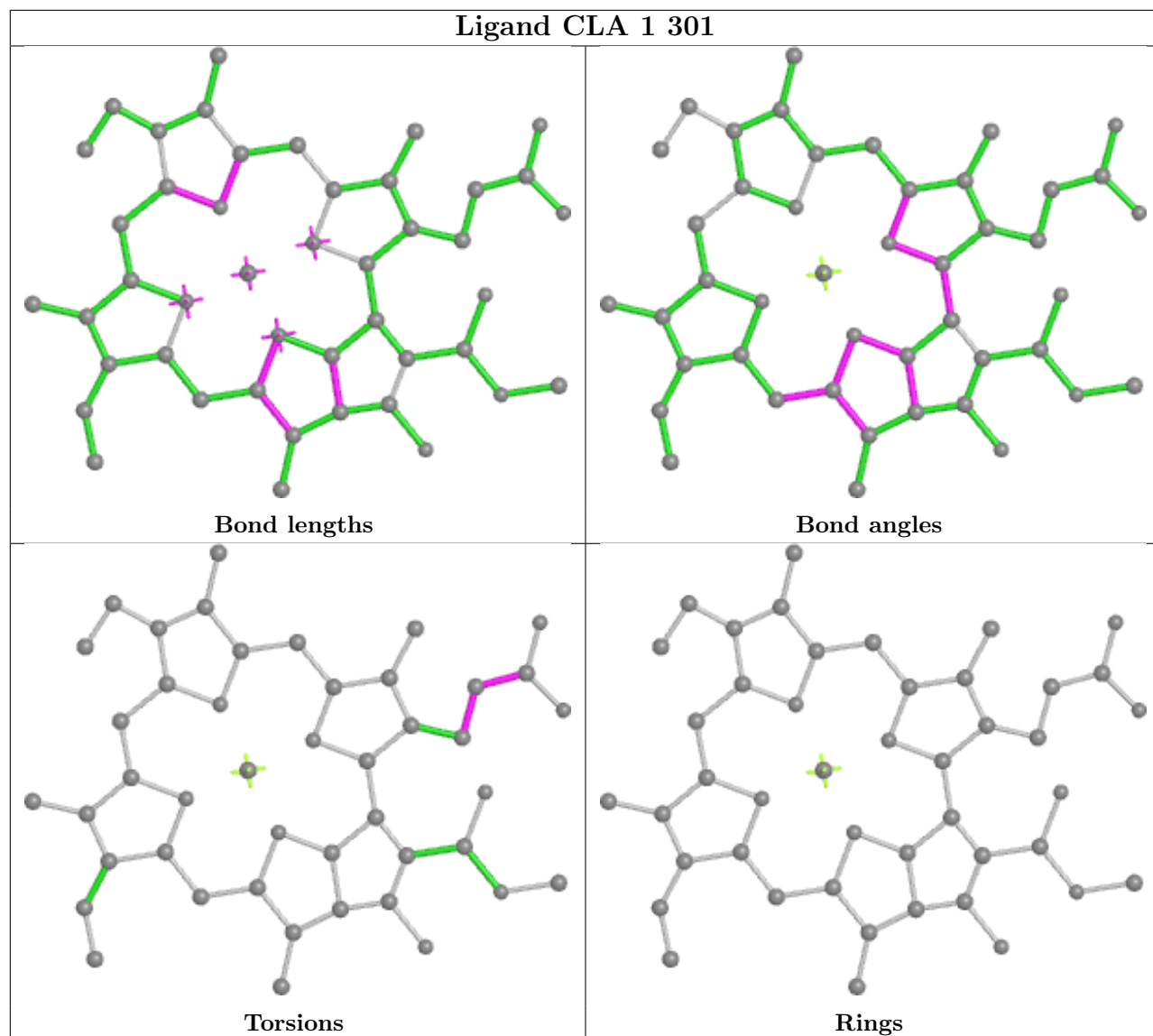




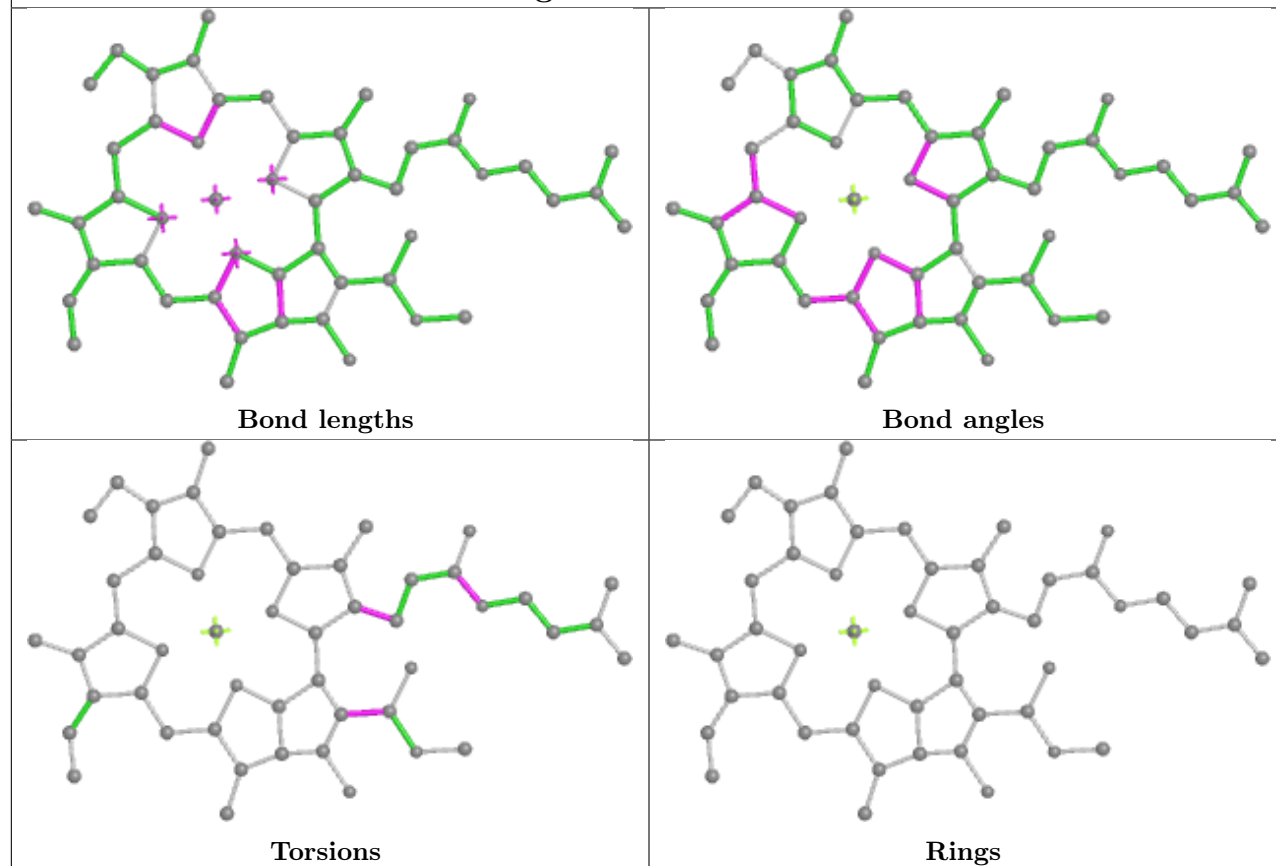




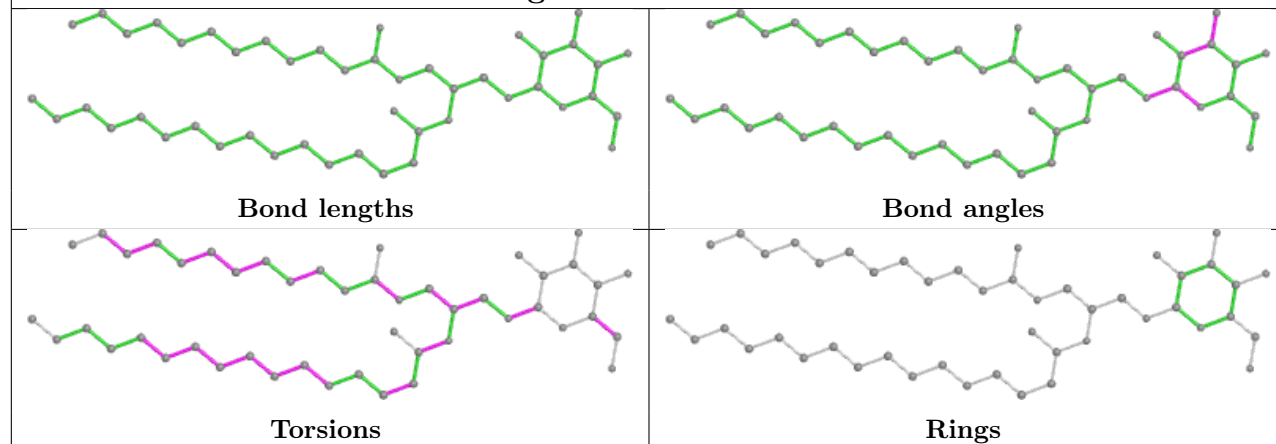
## Ligand CLA 1 301



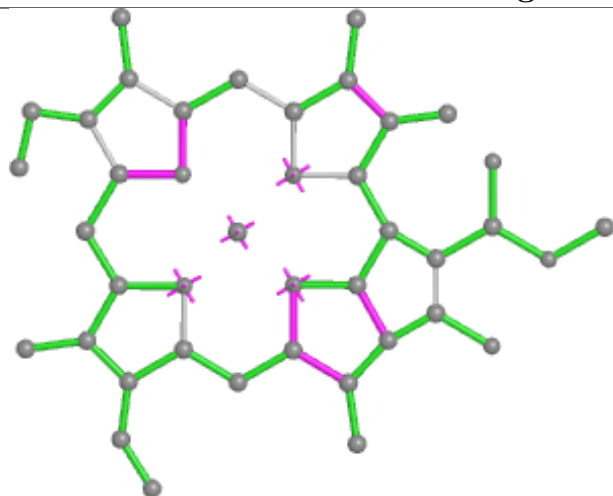
## Ligand CLA b 602



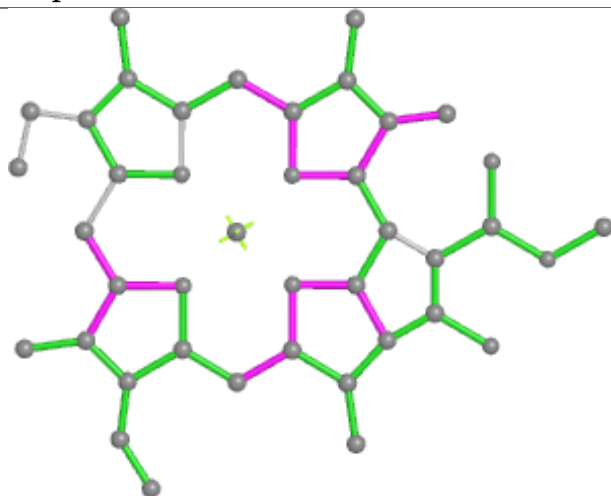
## Ligand LMG w 101



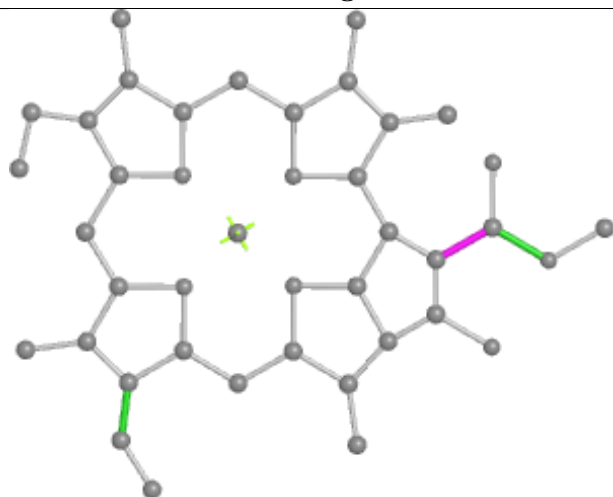
## Ligand CLA p 312



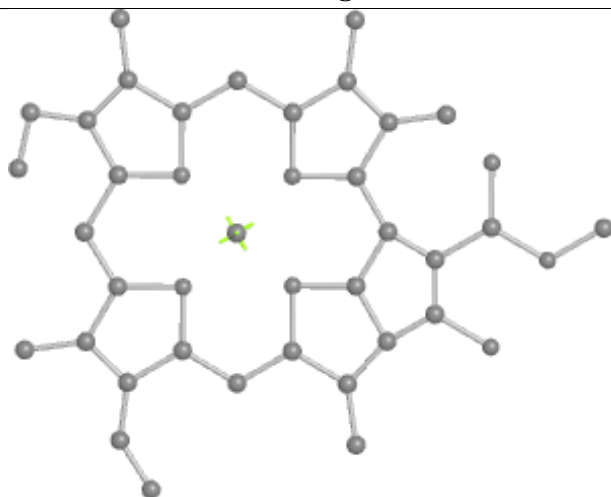
Bond lengths



Bond angles

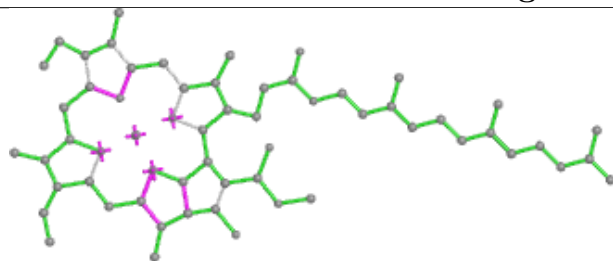


Torsions

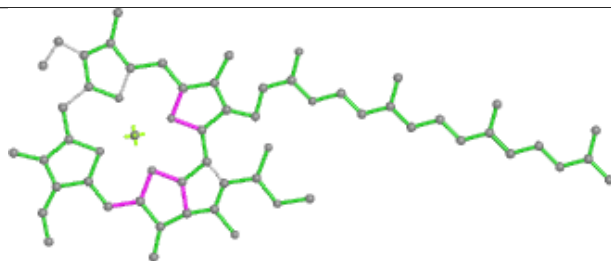


Rings

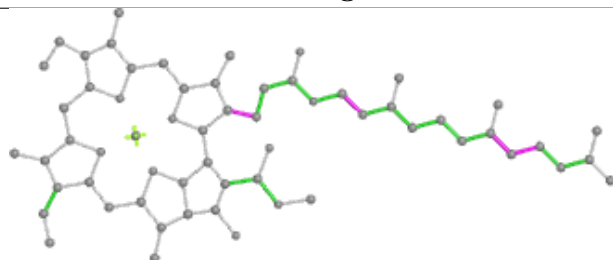
## Ligand CLA 8 307



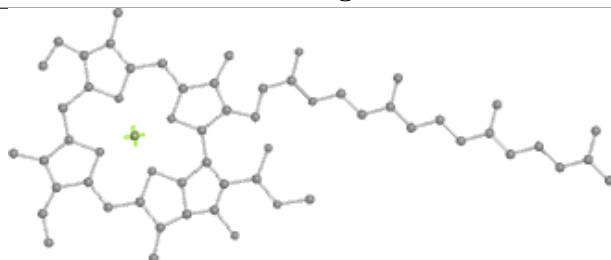
Bond lengths



Bond angles

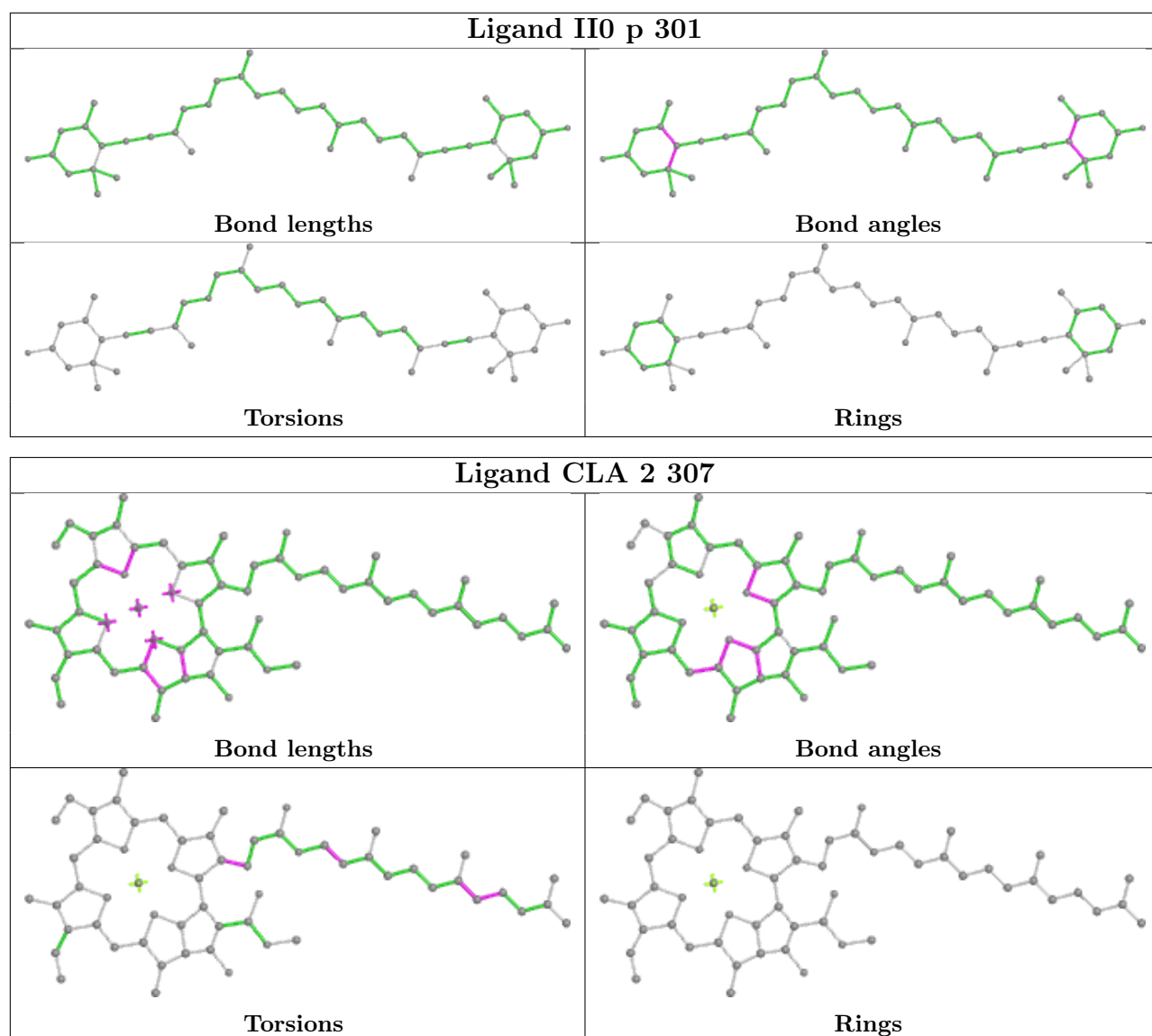


Torsions

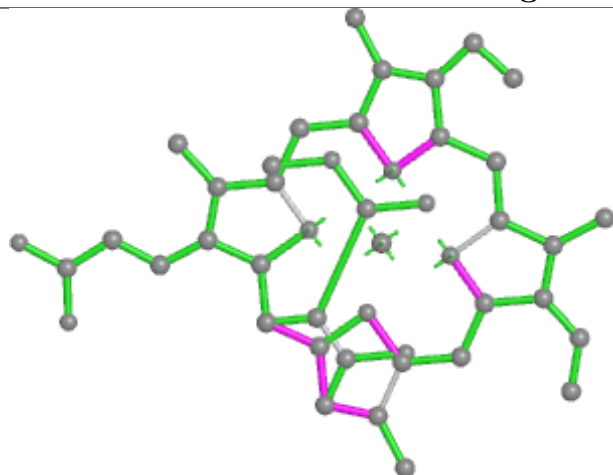


Rings

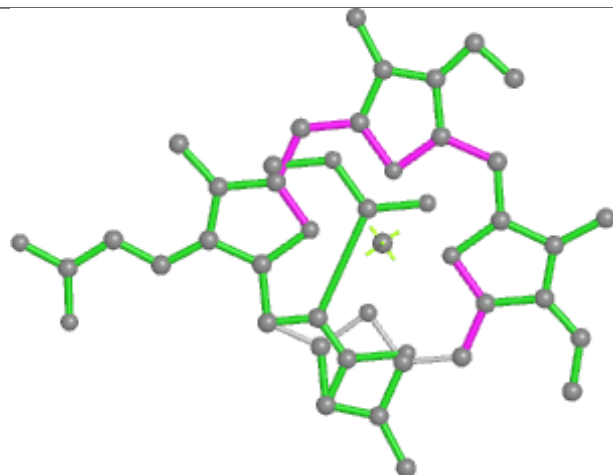




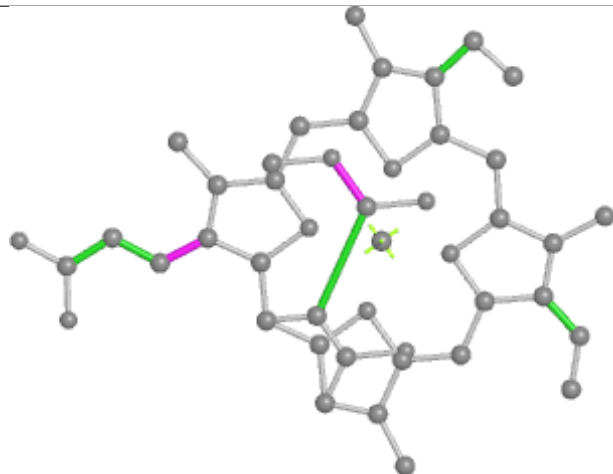
## Ligand KC2 5 309



Bond lengths



Bond angles

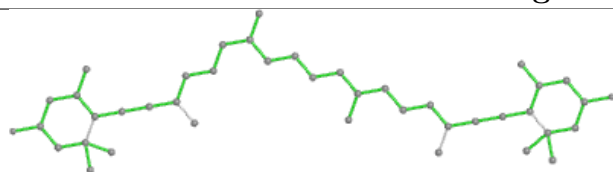


Torsions

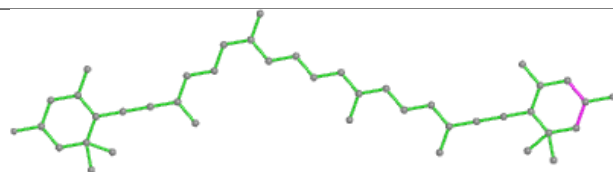


Rings

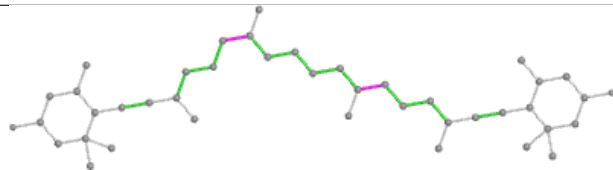
## Ligand II0 9 316



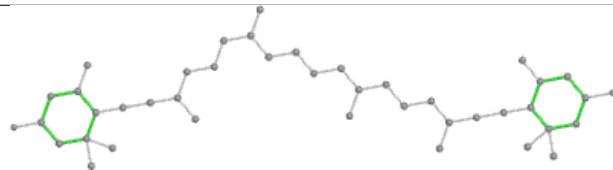
Bond lengths



Bond angles

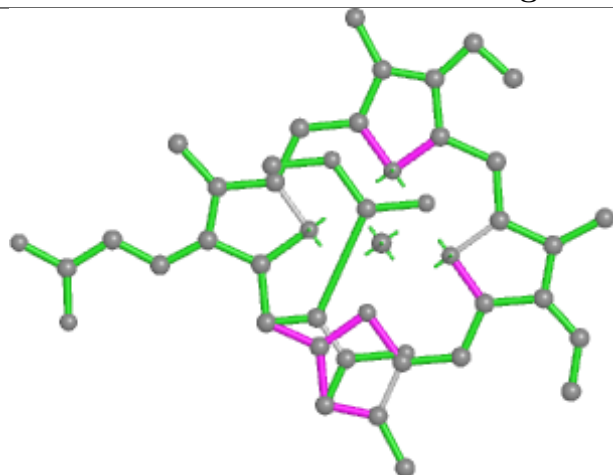


Torsions

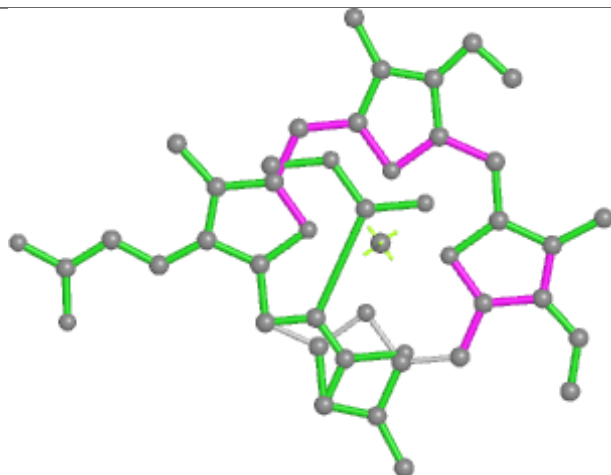


Rings

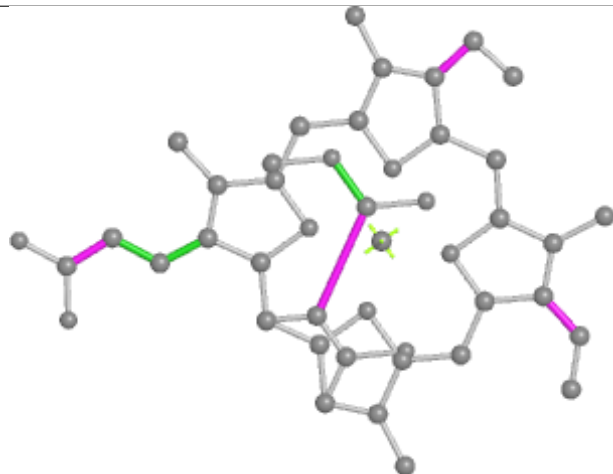
## Ligand KC2 7 310



Bond lengths



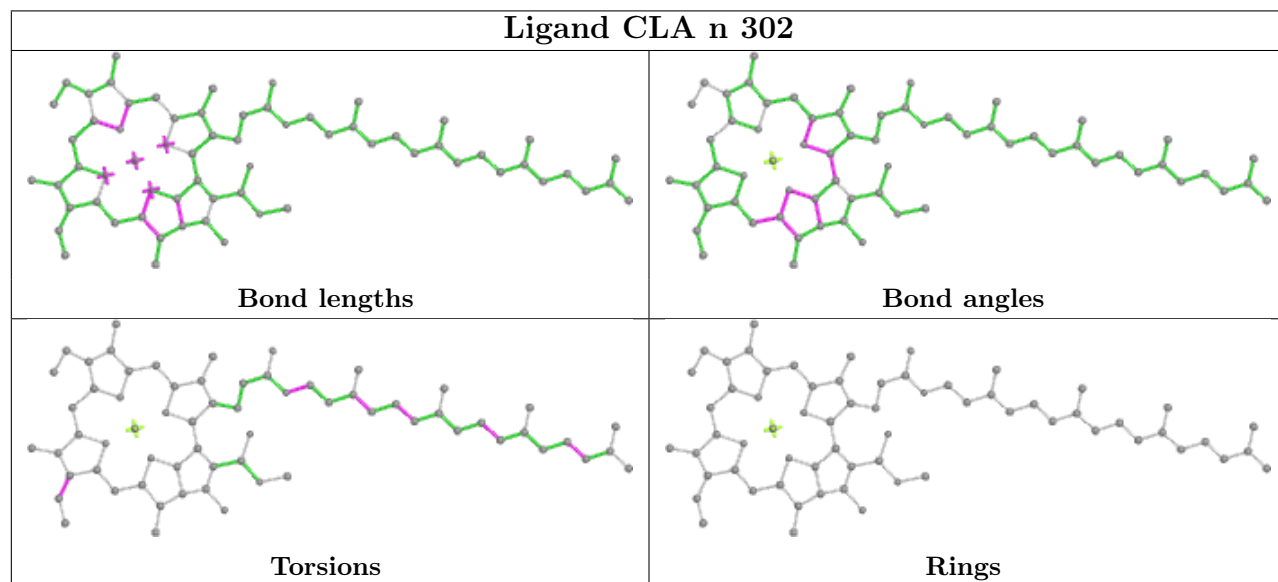
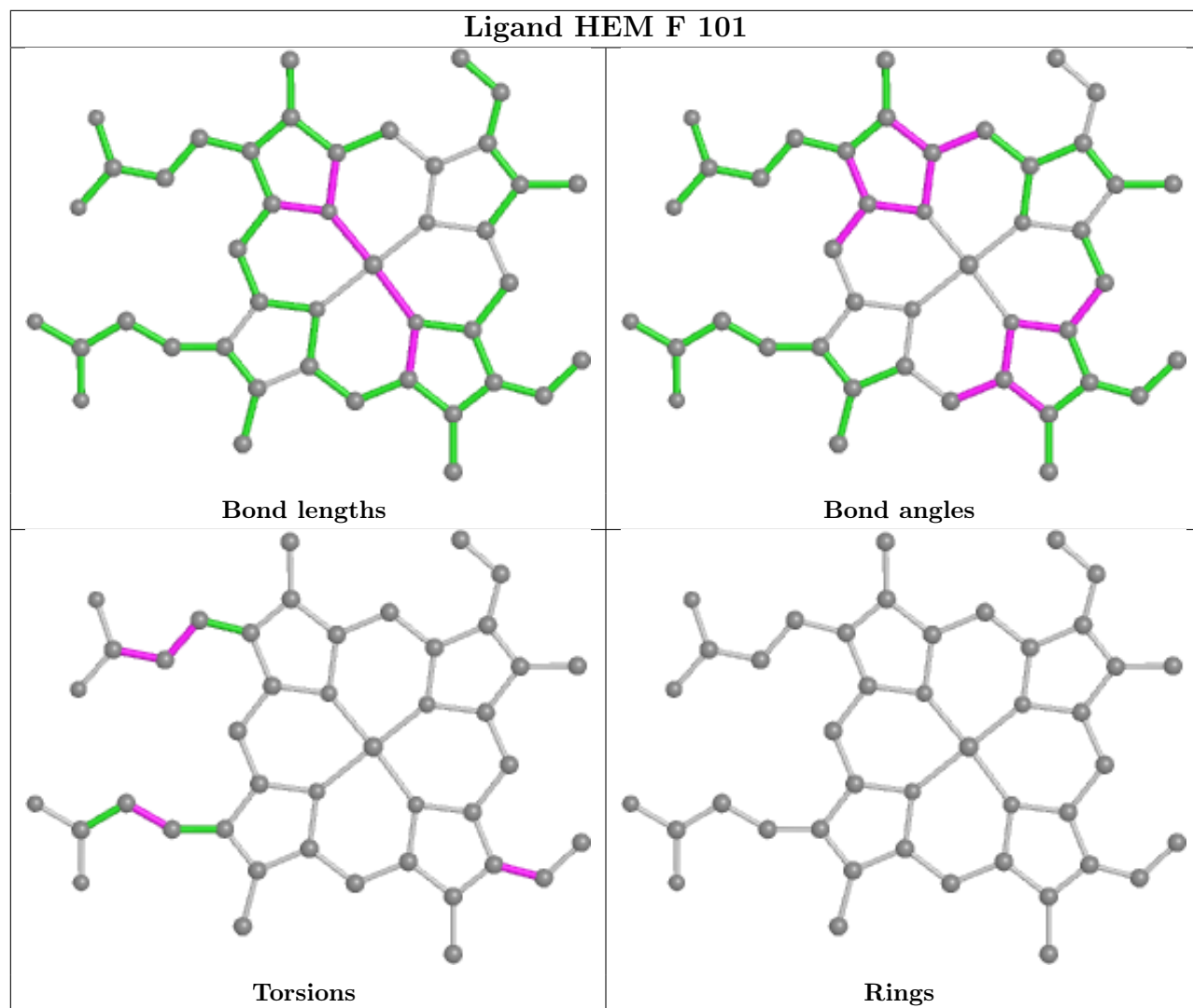
Bond angles

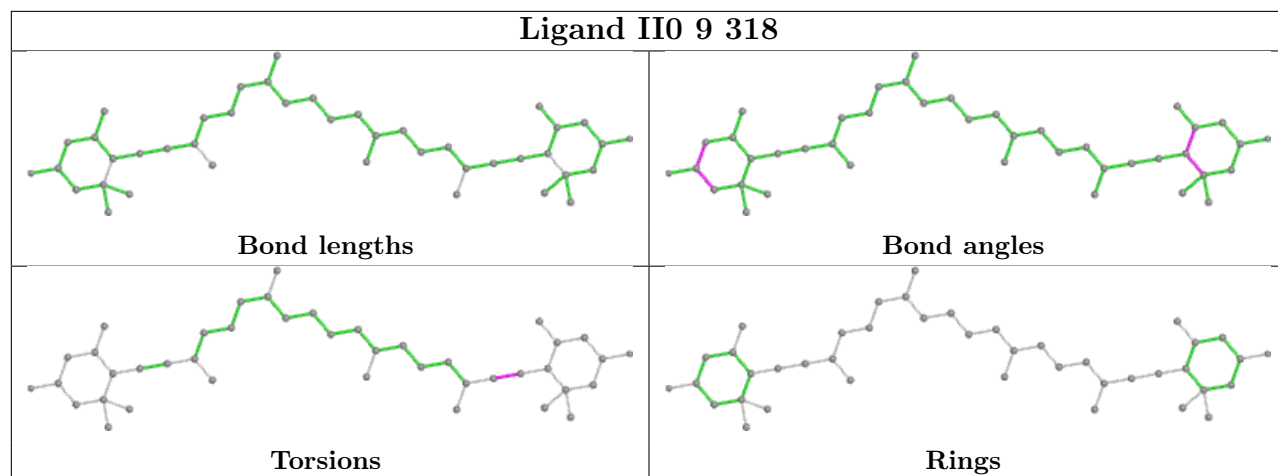
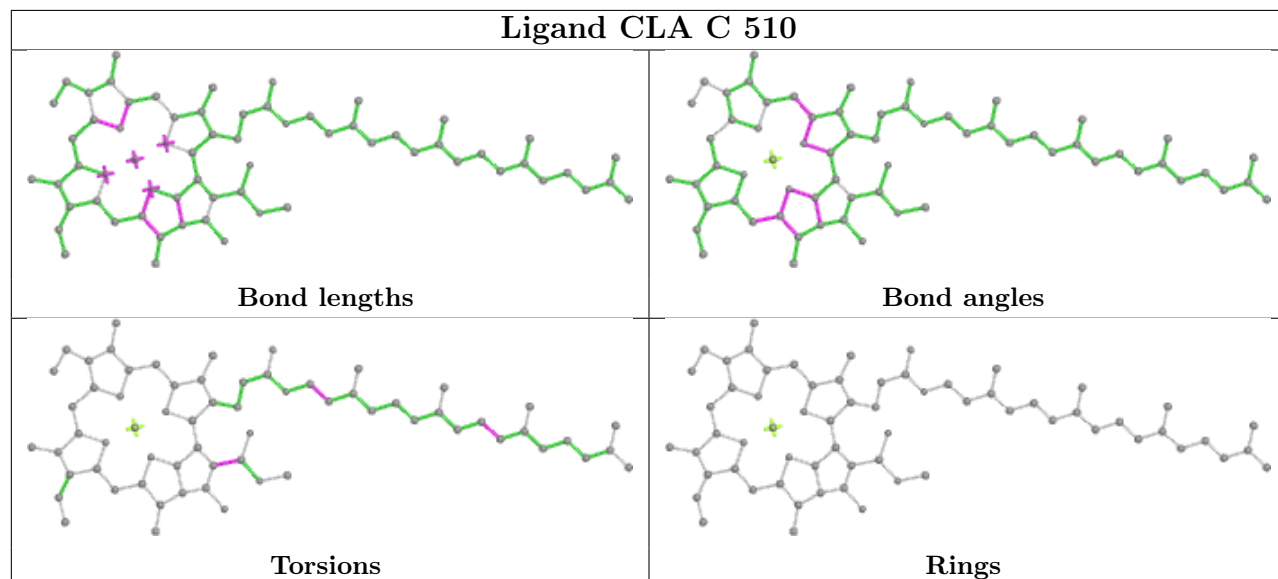
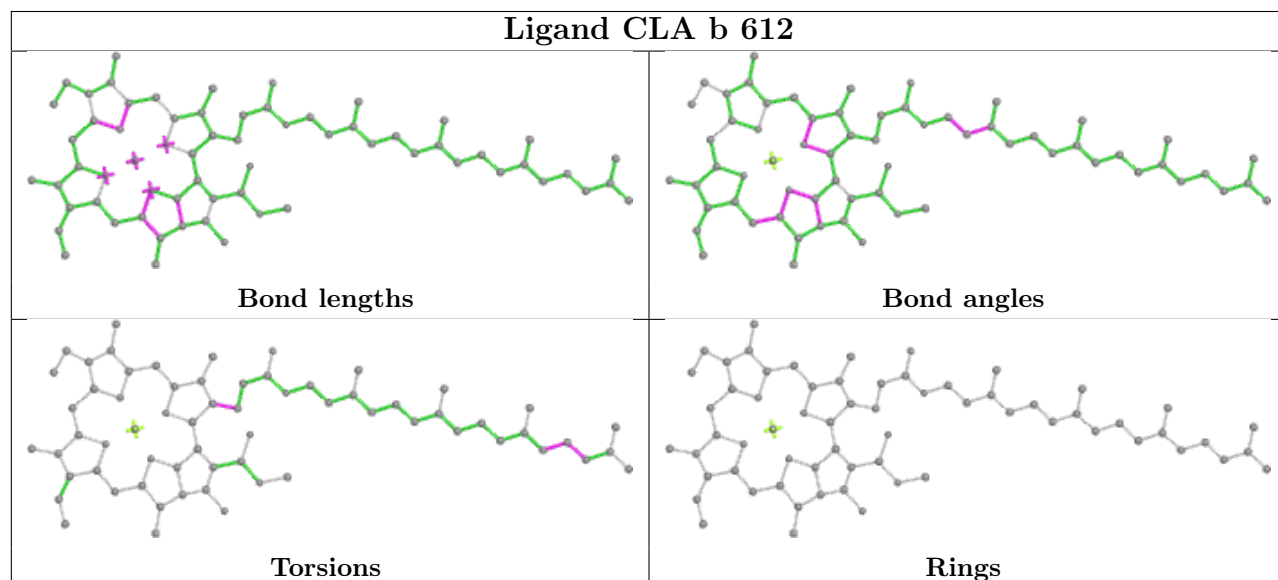


Torsions

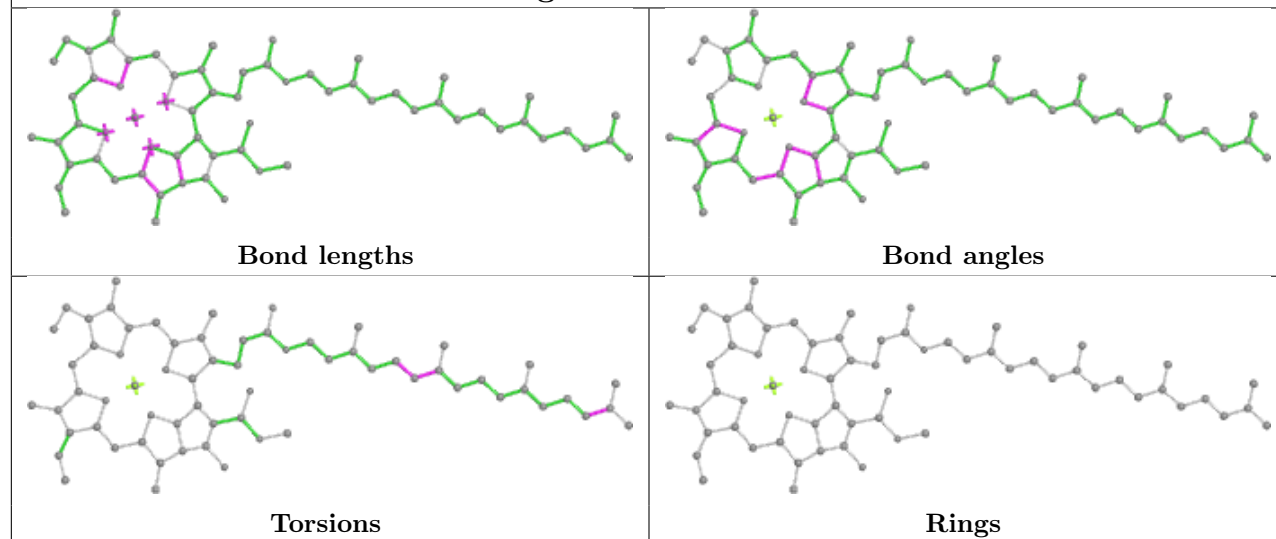


Rings

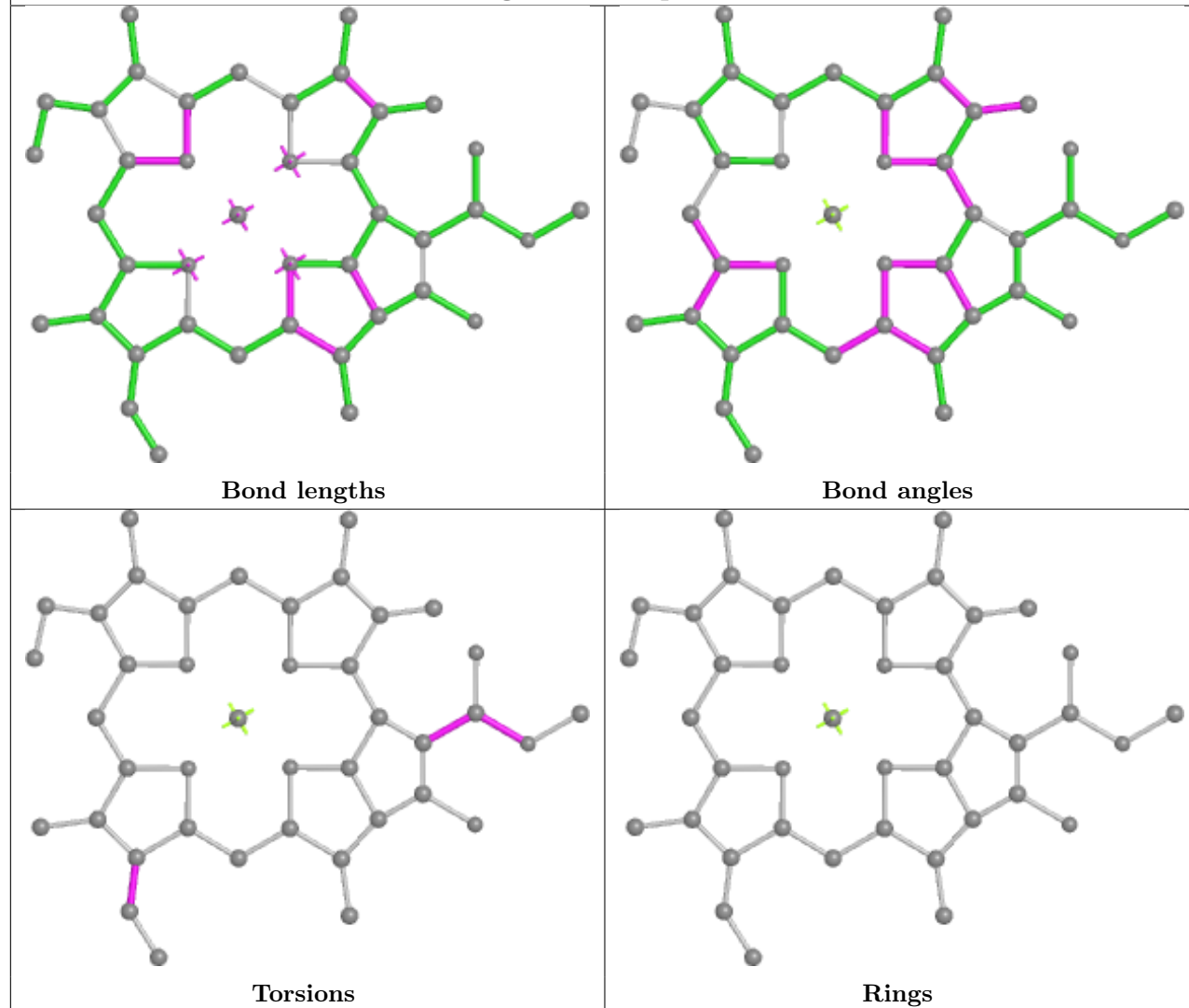


**Ligand II0 9 318****Ligand CLA C 510****Ligand CLA b 612**

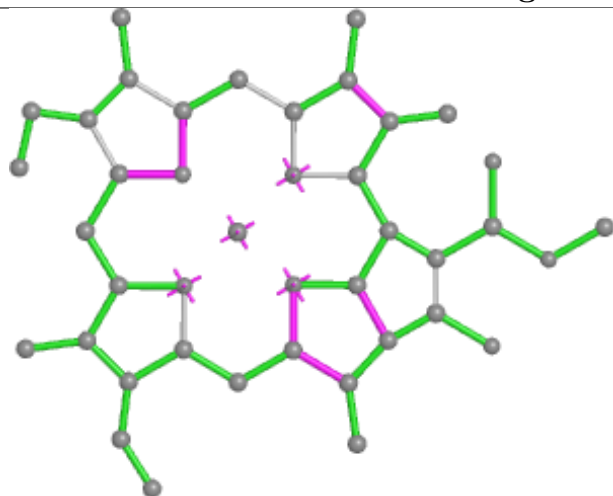
## Ligand CLA c 514



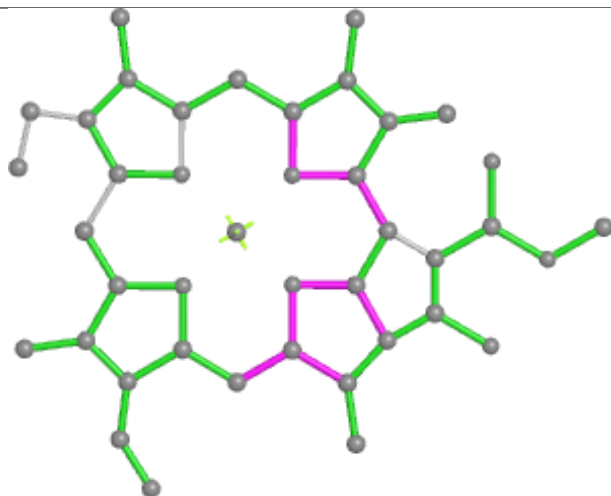
## Ligand CLA p 310



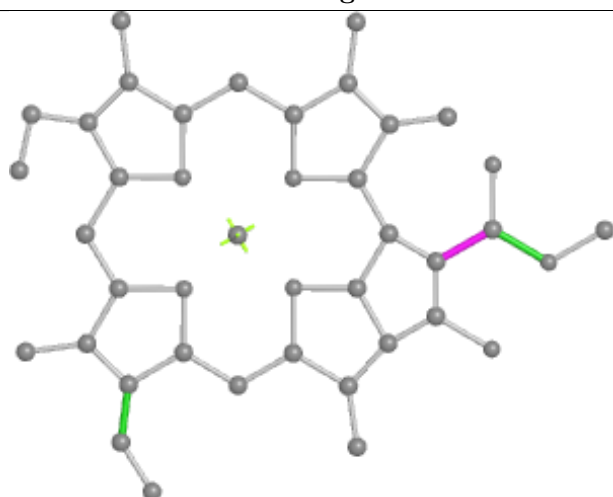
## Ligand CLA 5 308



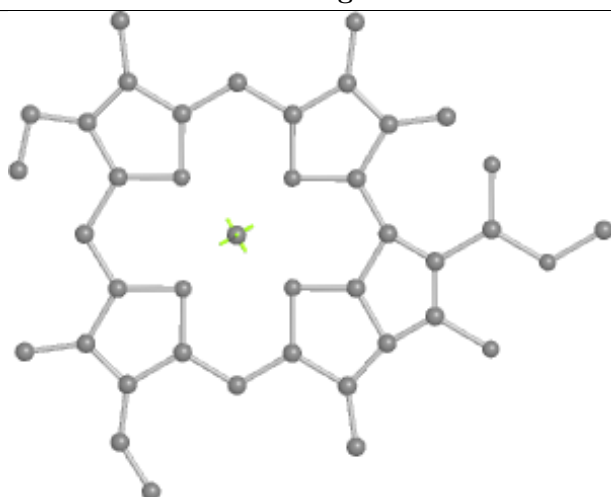
Bond lengths



Bond angles

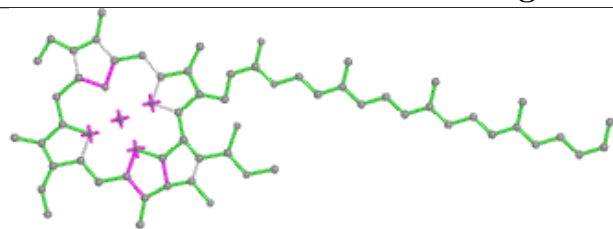


Torsions

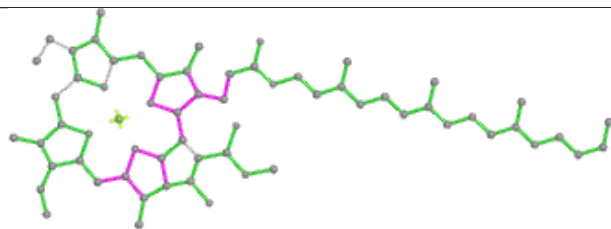


Rings

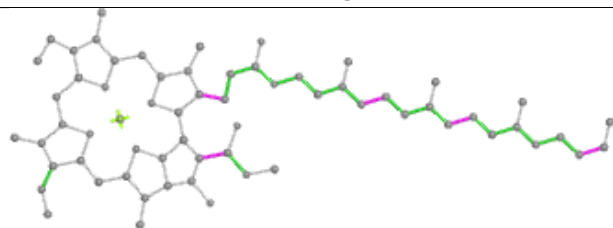
## Ligand CLA 1 302



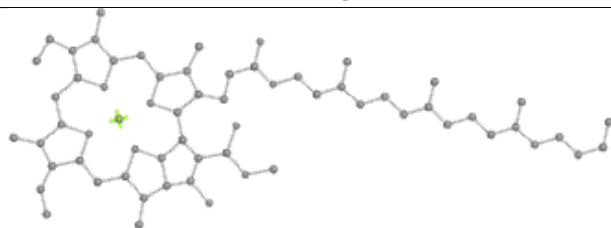
Bond lengths



Bond angles

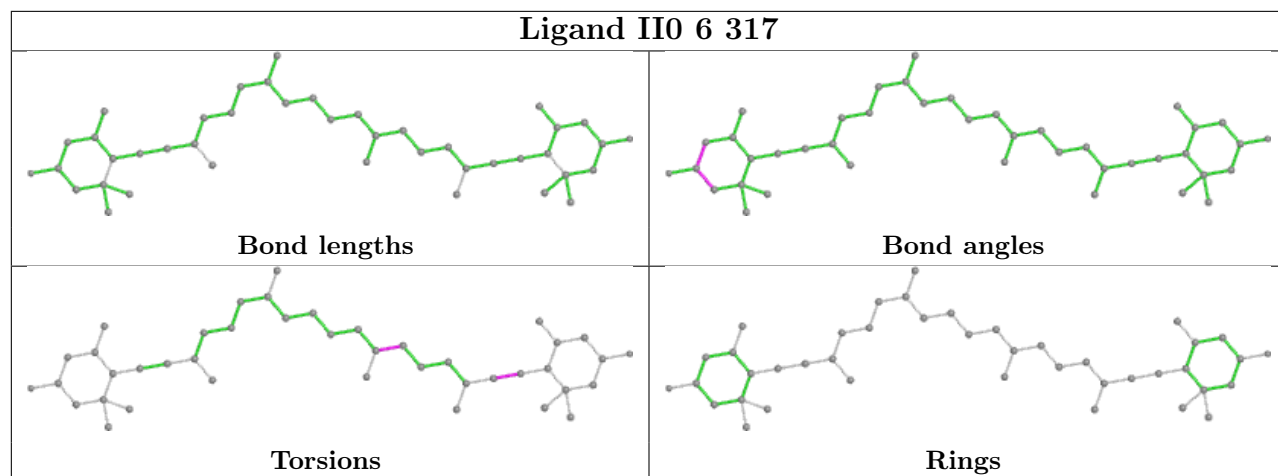


Torsions

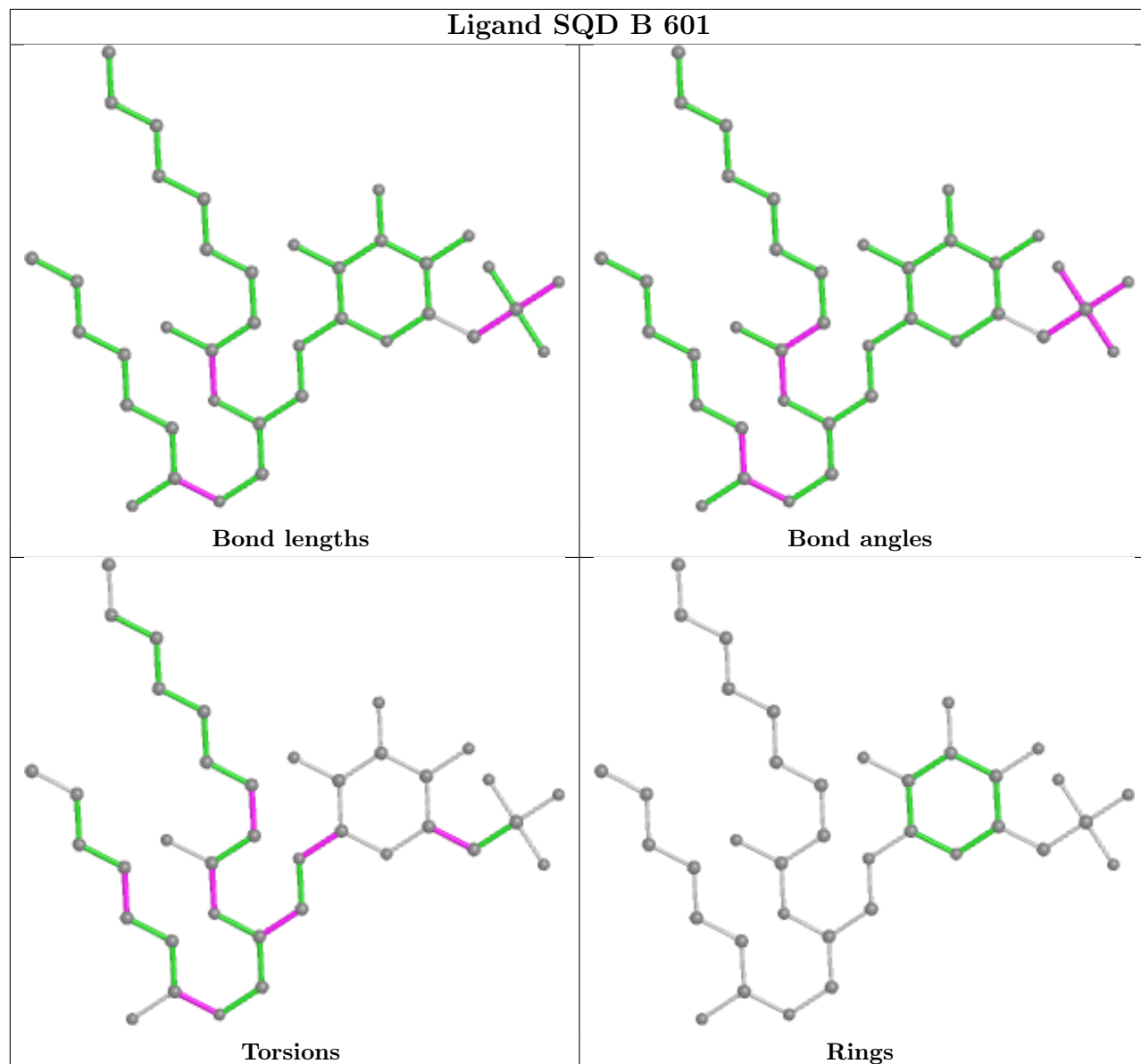


Rings

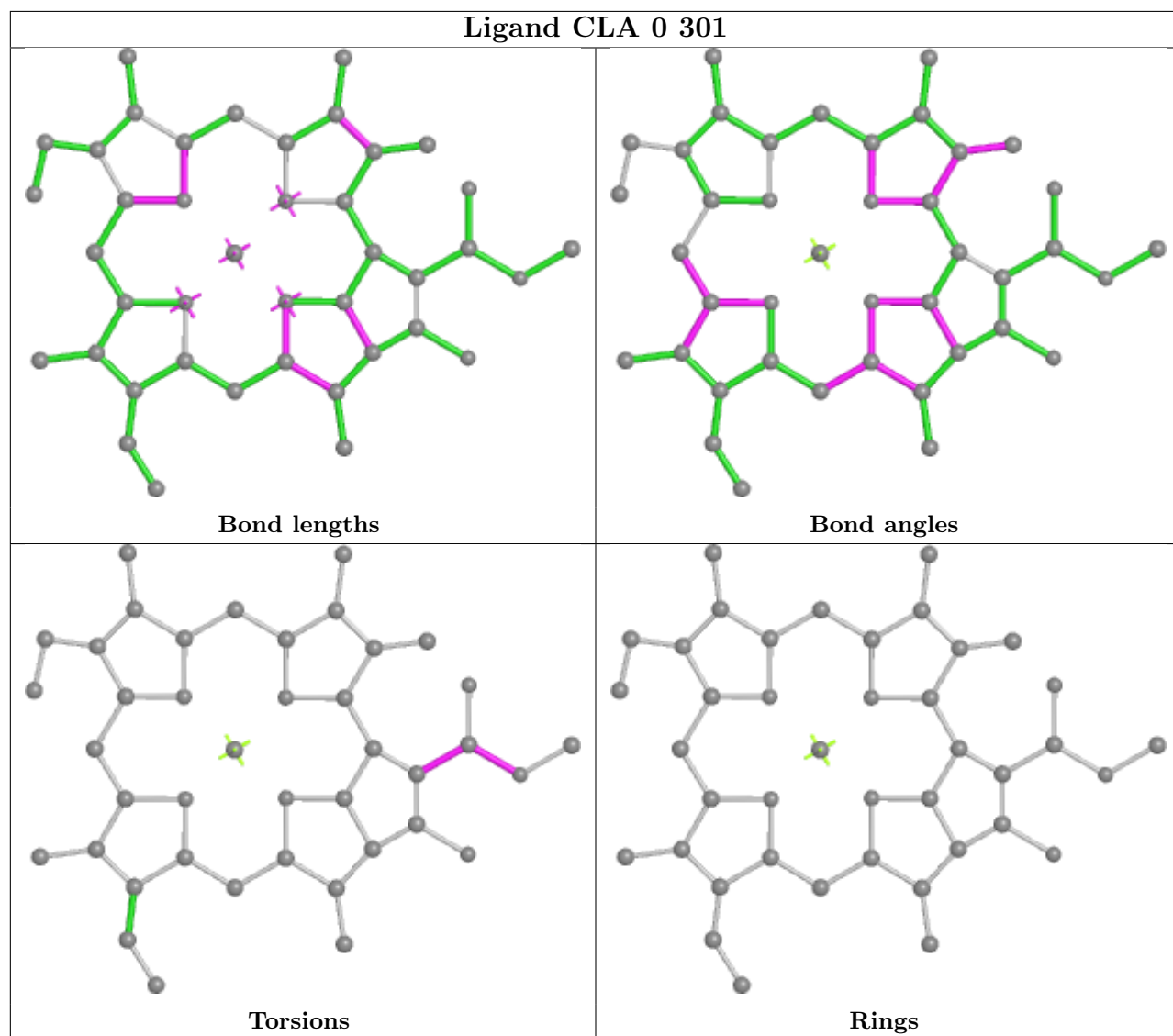
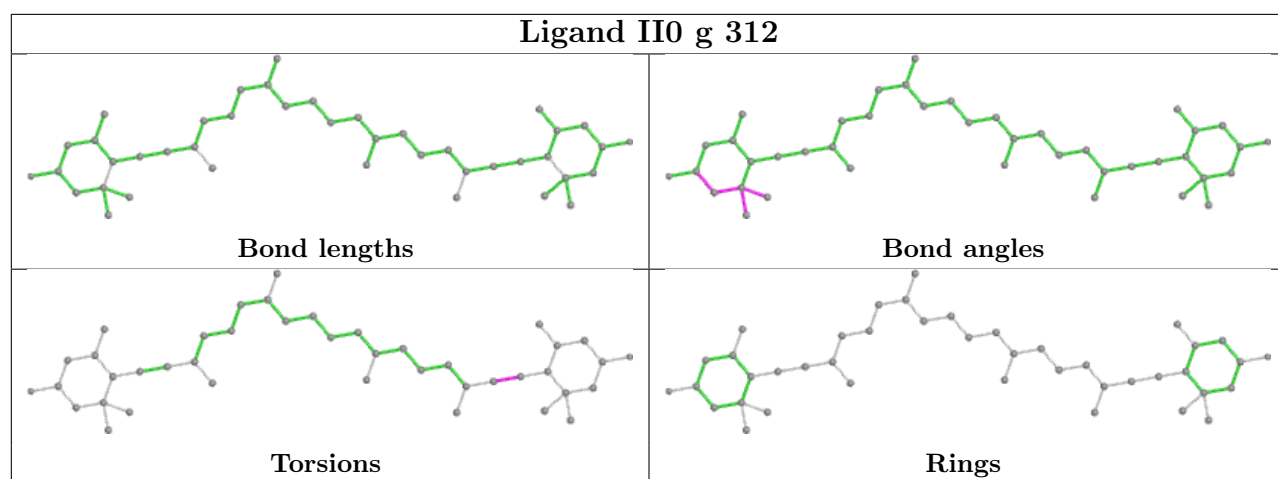
## Ligand II0 6 317



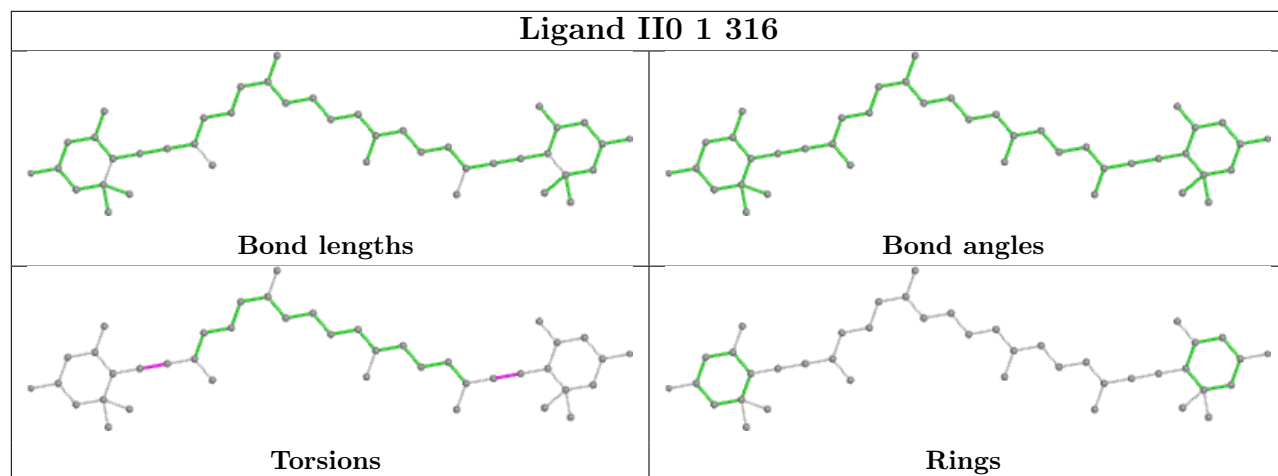
## Ligand SQD B 601



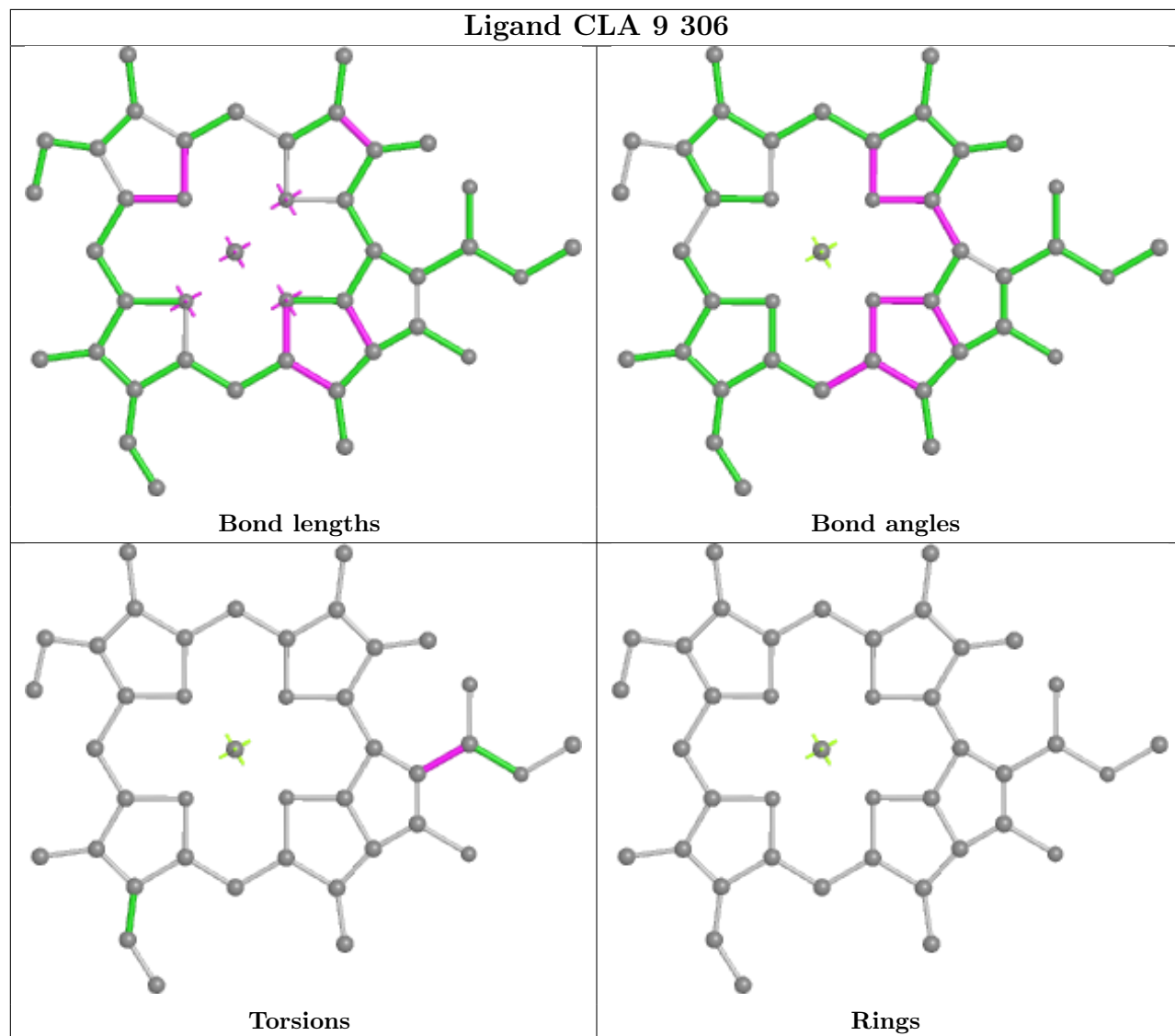




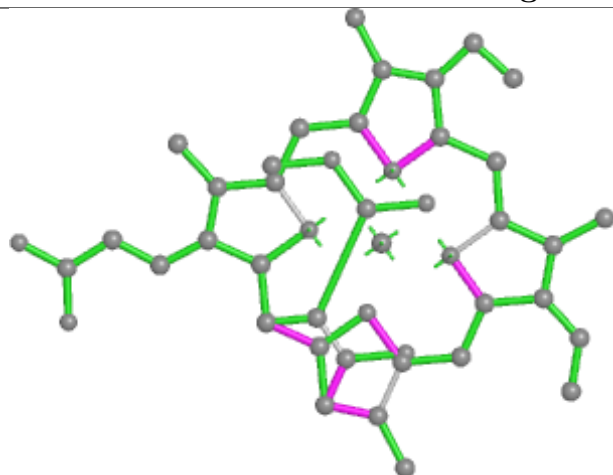
## Ligand II0 1 316



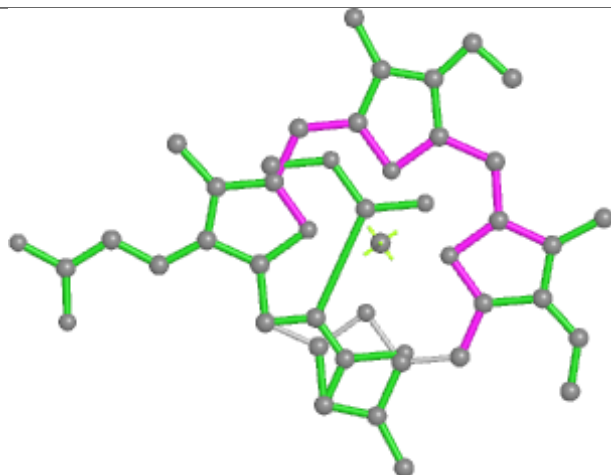
## Ligand CLA 9 306



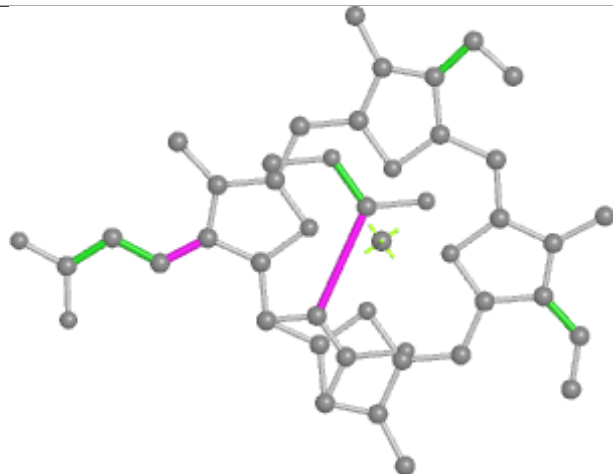
## Ligand KC2 6 311



Bond lengths



Bond angles

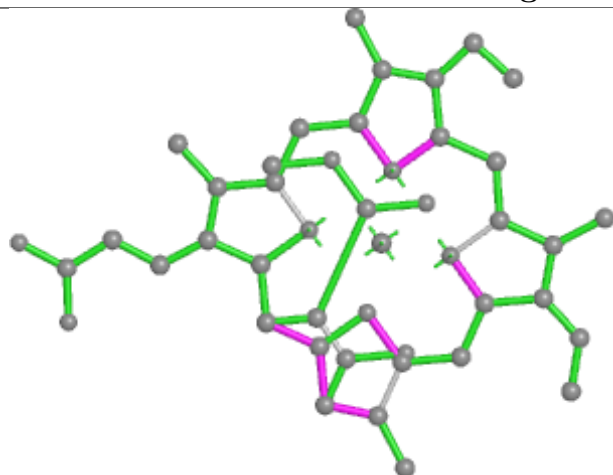


Torsions

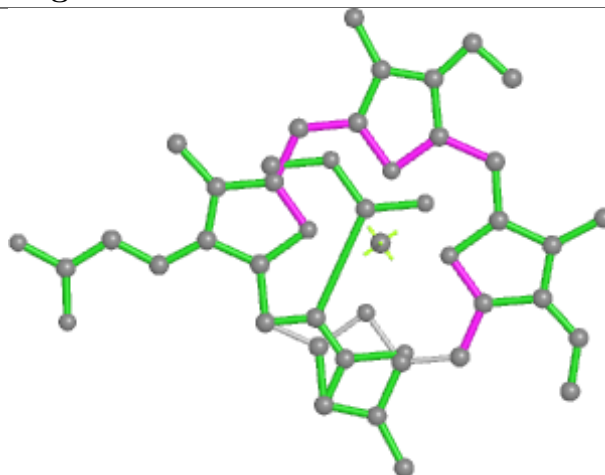


Rings

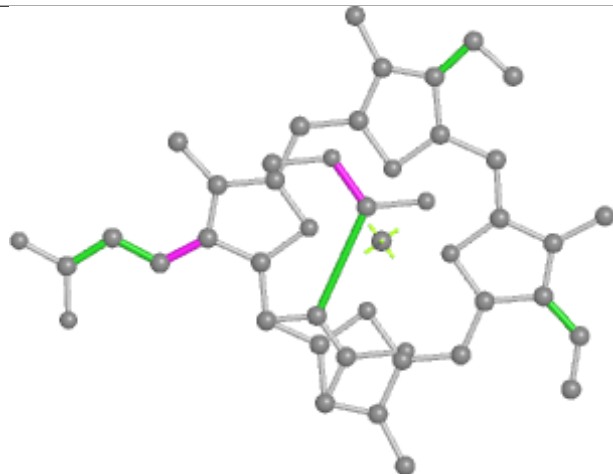
## Ligand KC2 g 309



Bond lengths



Bond angles

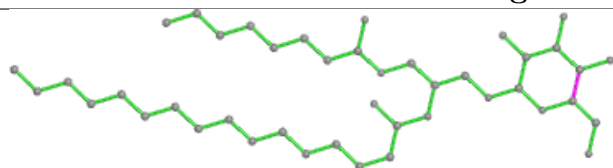


Torsions

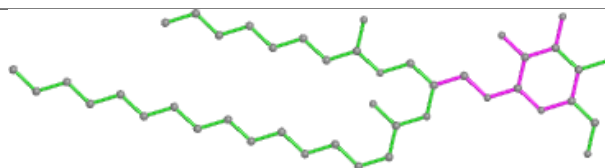


Rings

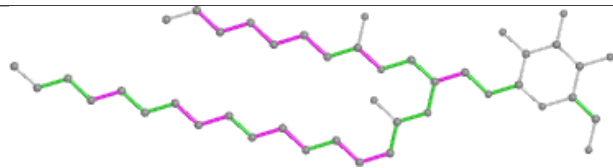
## Ligand LMG B 624



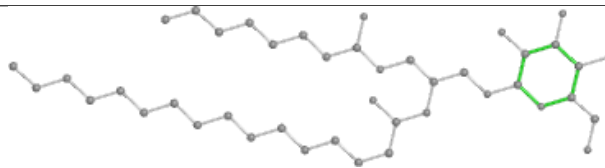
Bond lengths



Bond angles

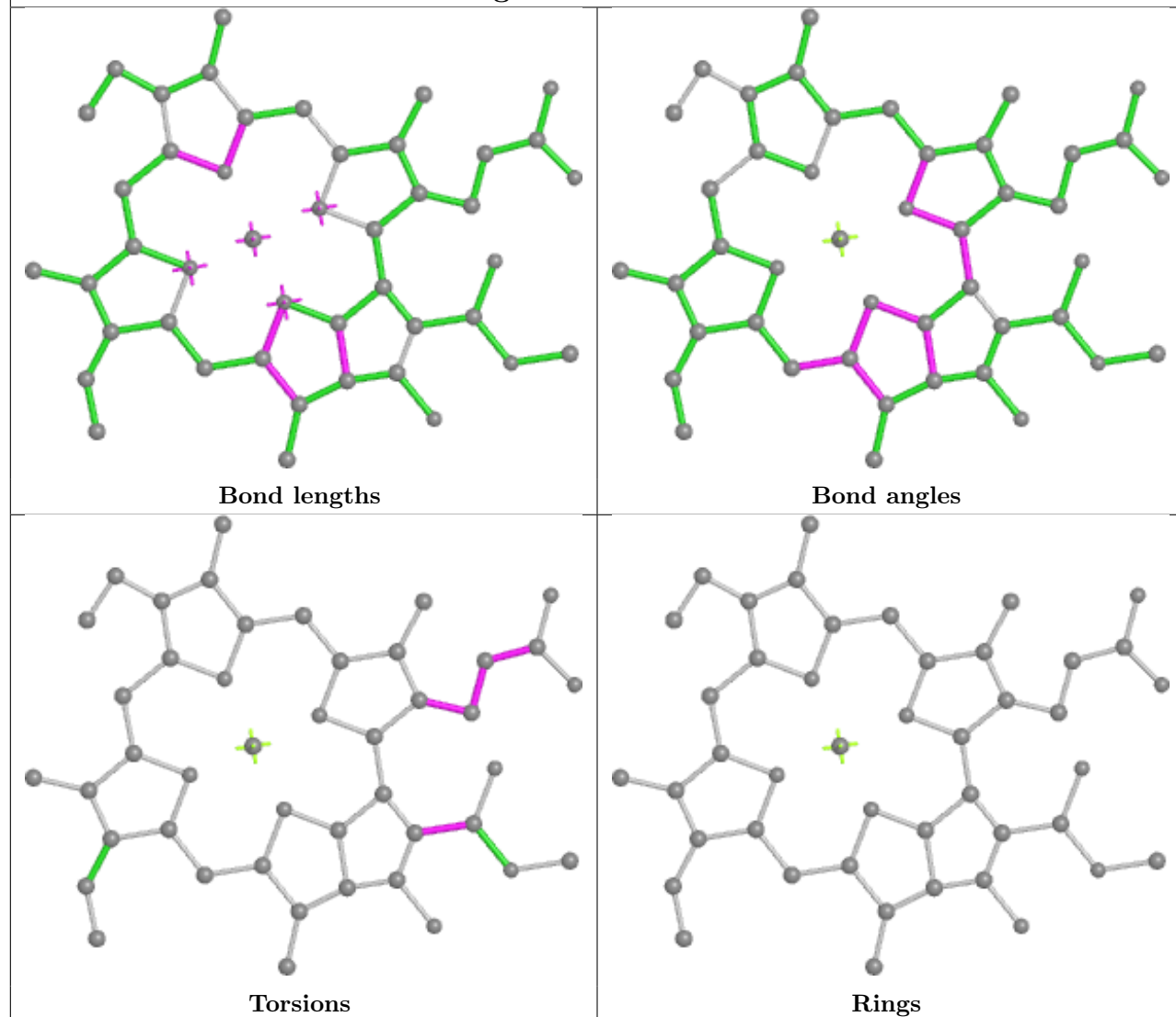


Torsions

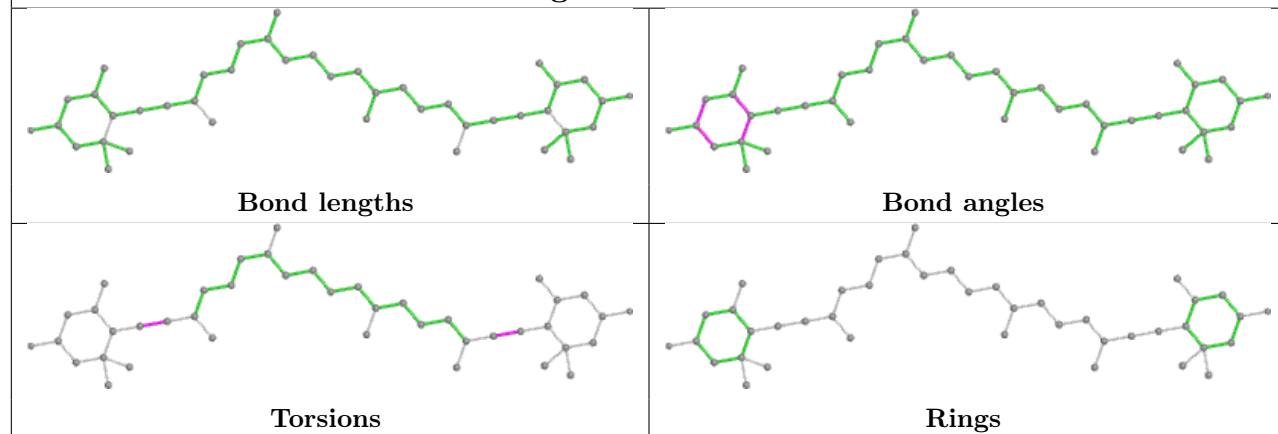


Rings

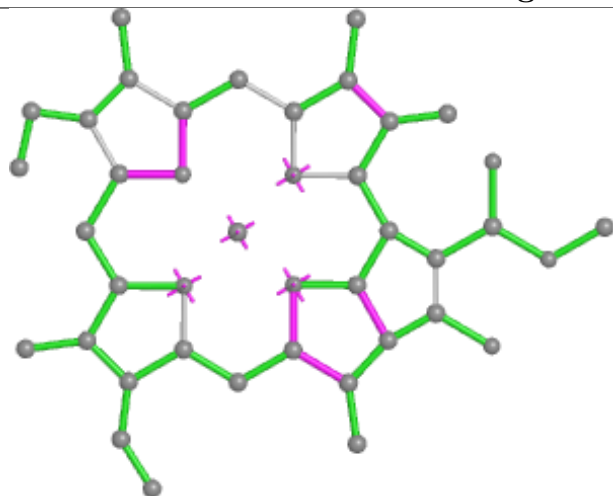
## Ligand CLA 9 307



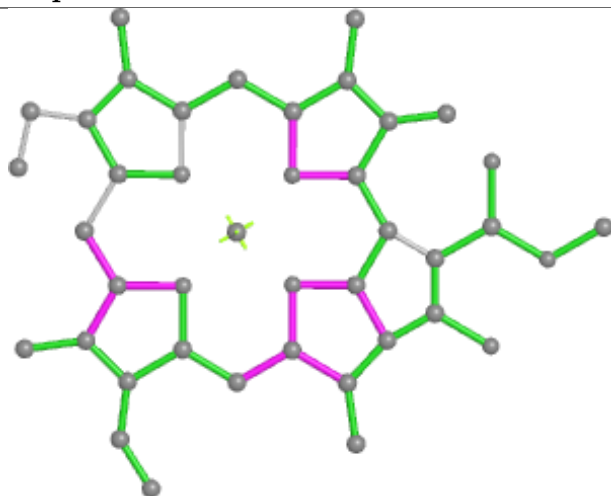
## Ligand II0 1 315



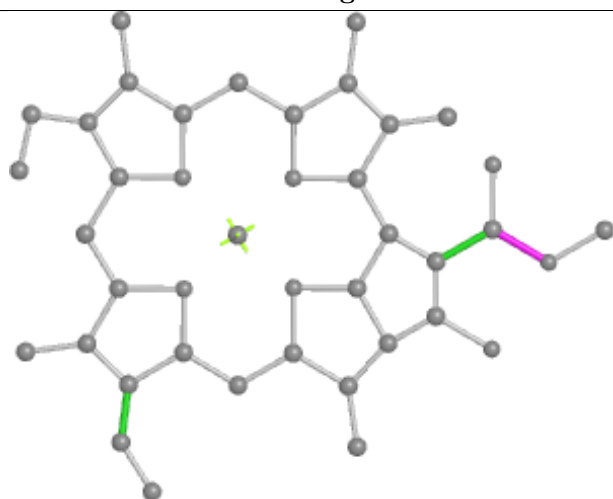
## Ligand CLA p 303



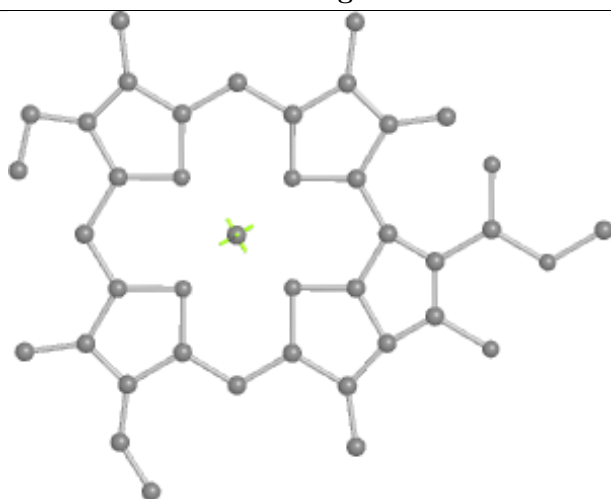
Bond lengths



Bond angles

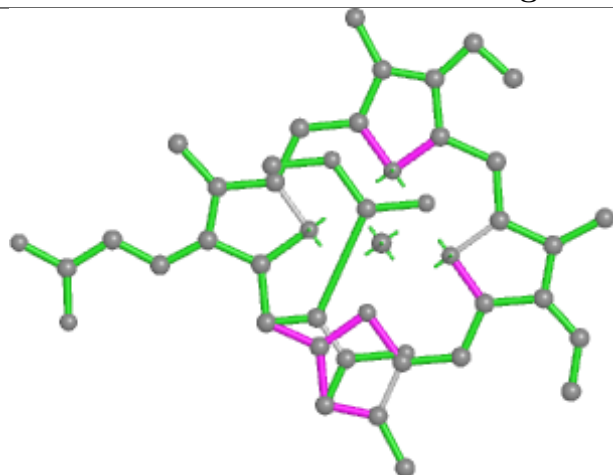


Torsions

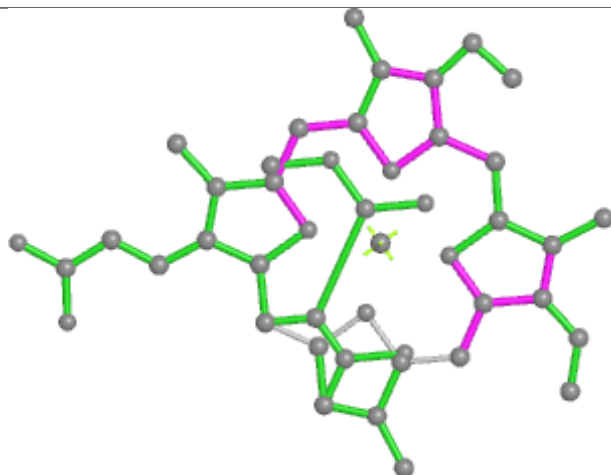


Rings

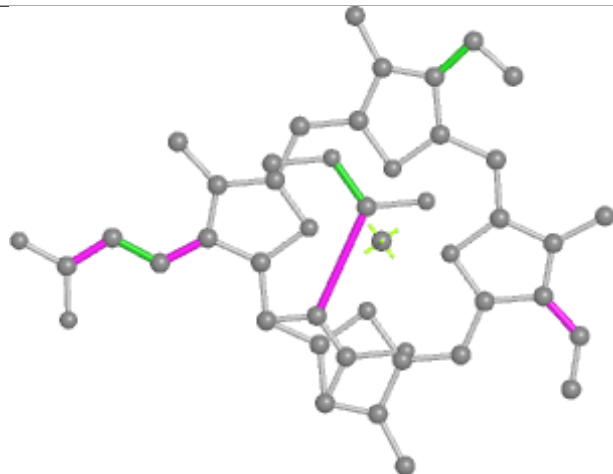
## Ligand KC2 3 311



Bond lengths



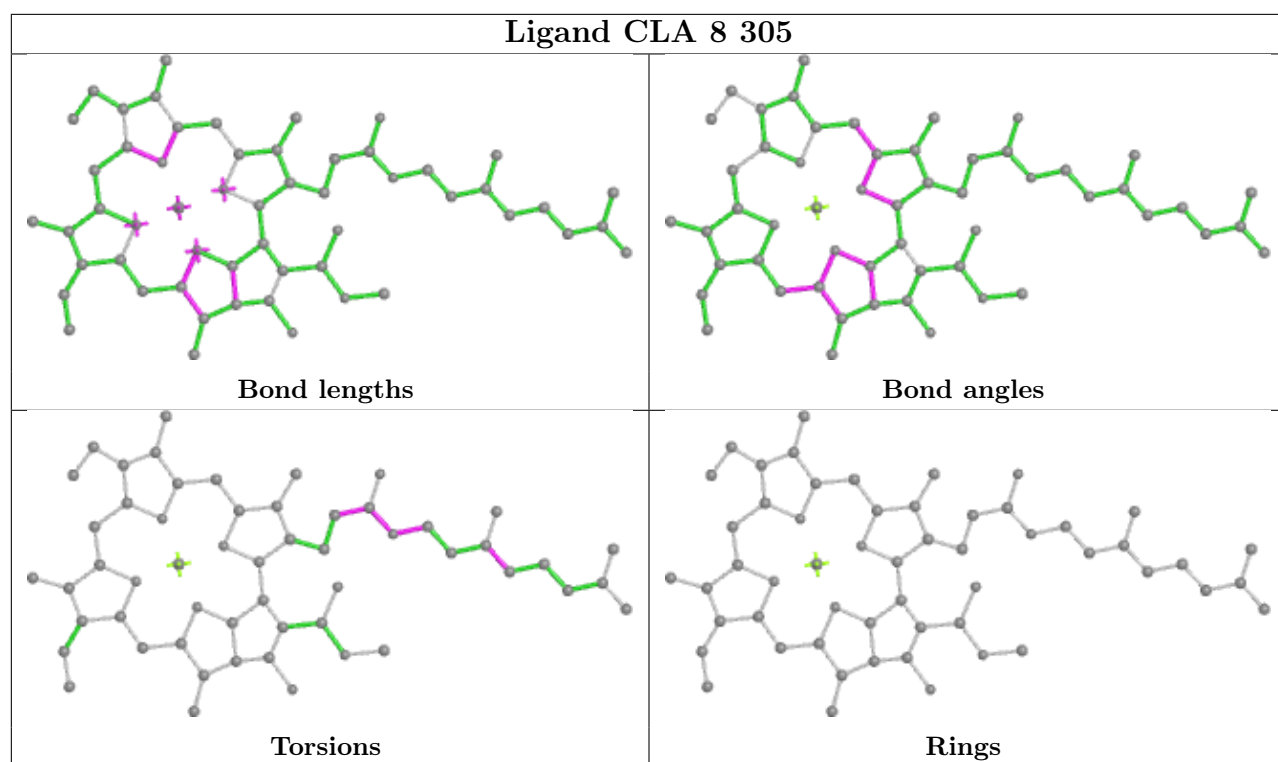
Bond angles



Torsions

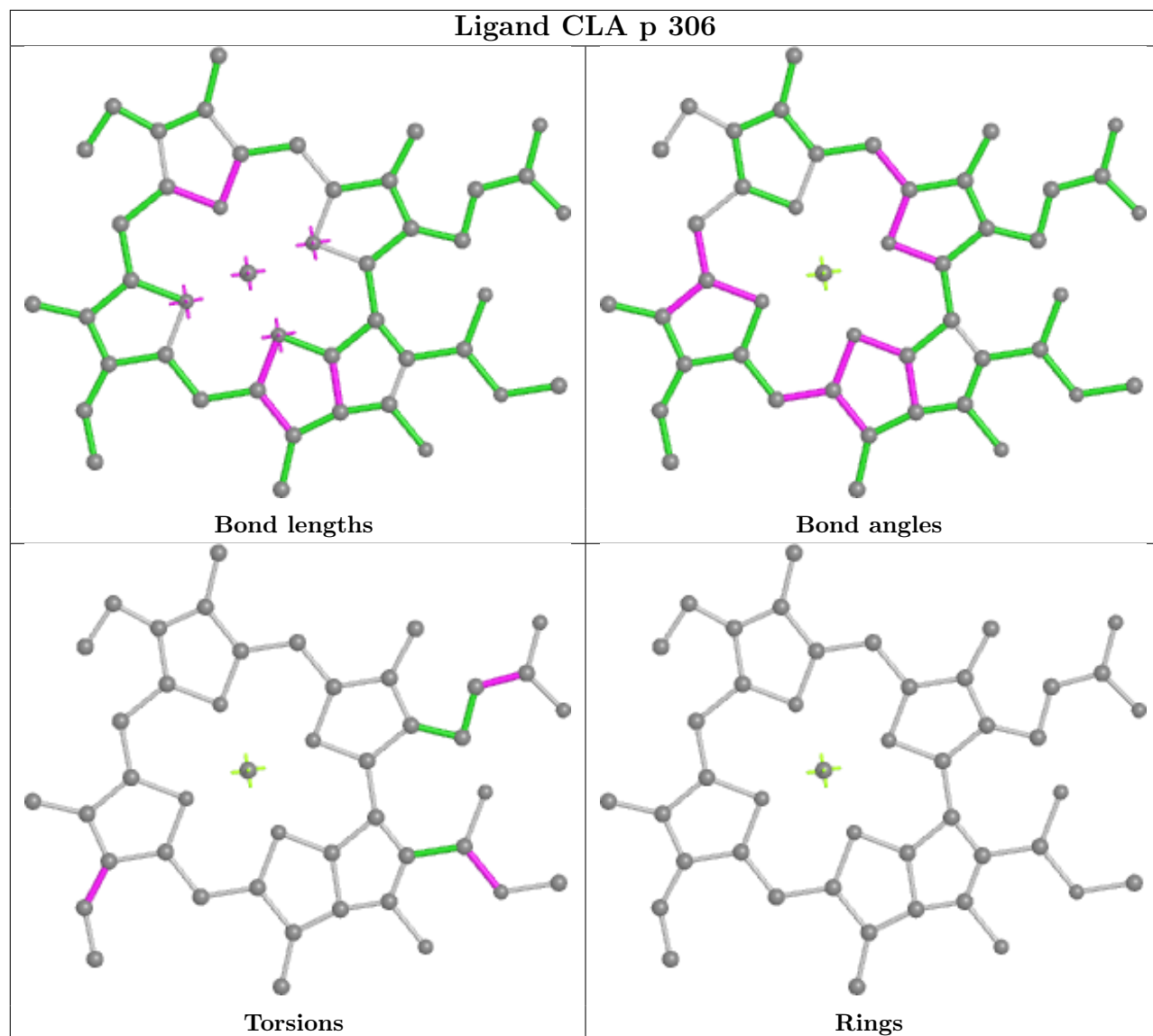


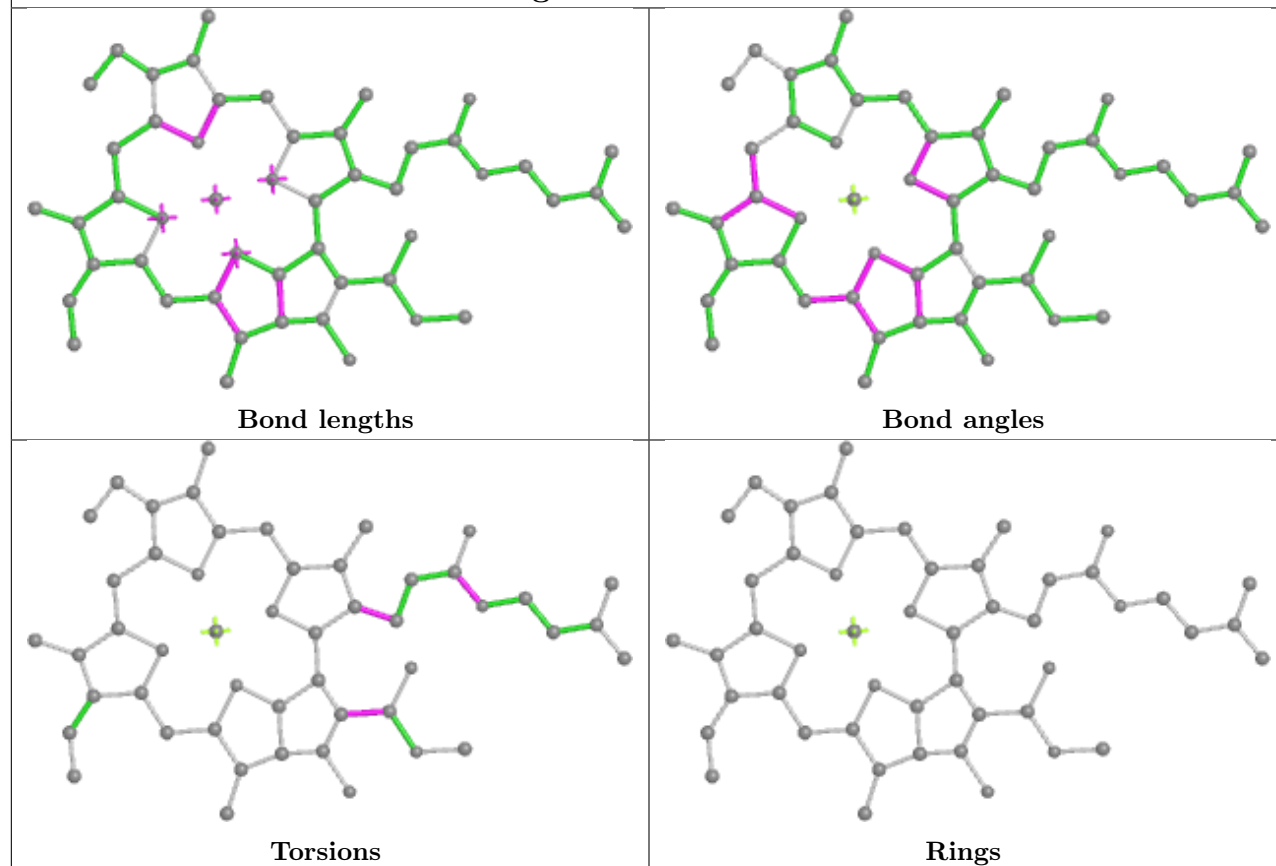
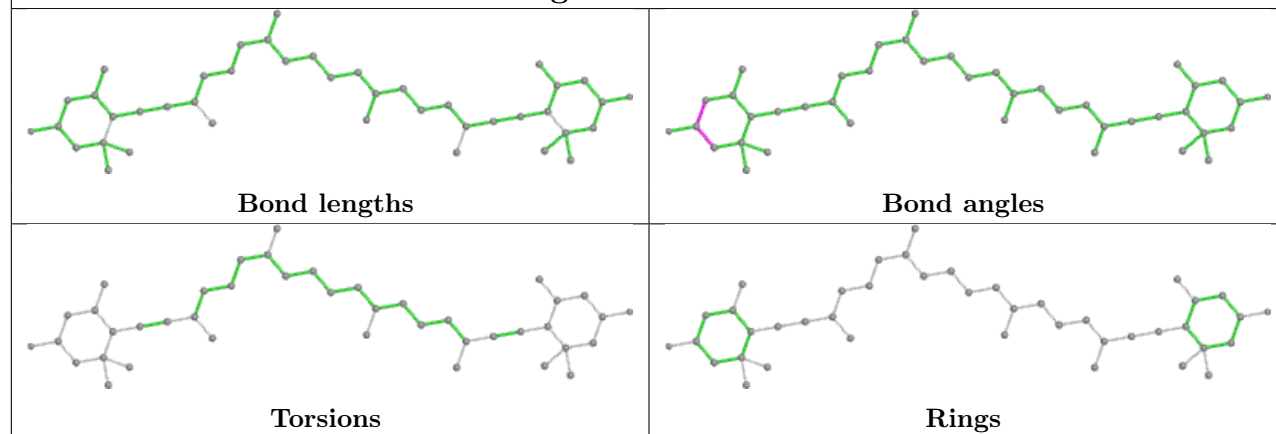
Rings



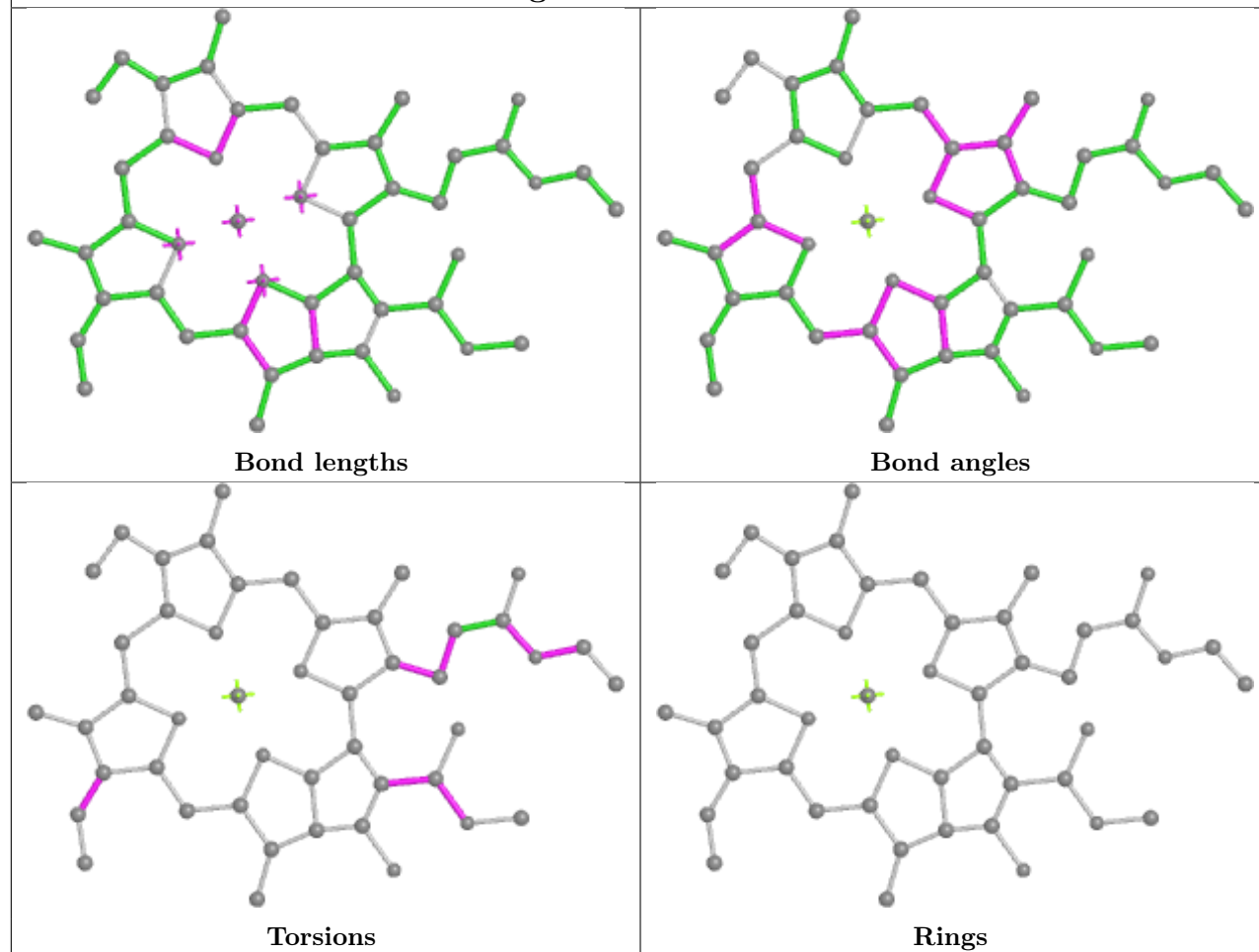


## Ligand CLA p 306

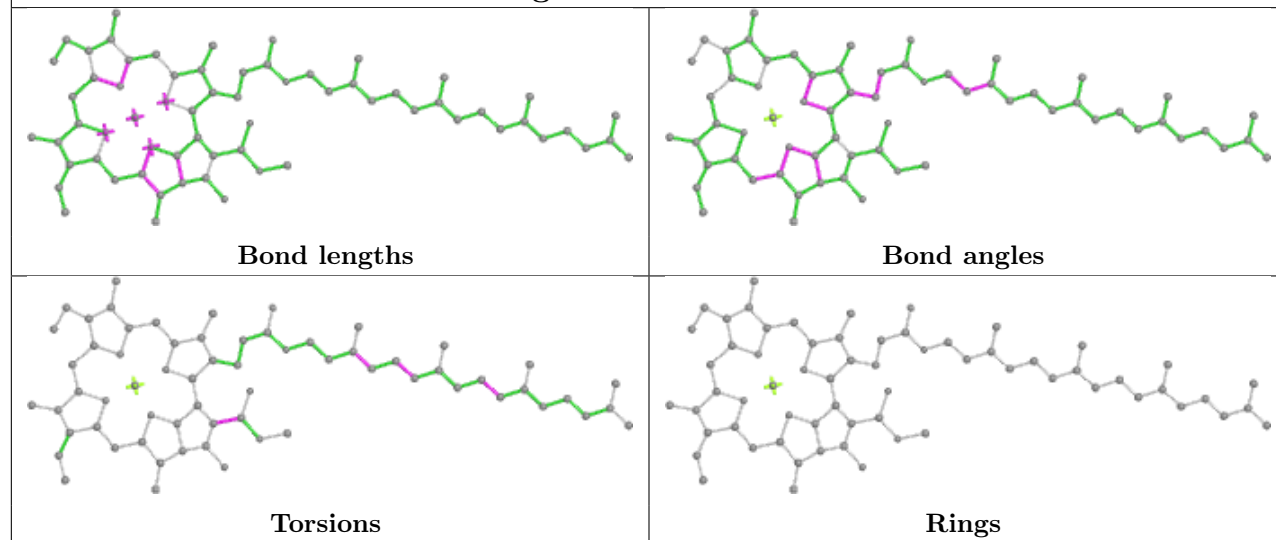


**Ligand CLA B 602****Ligand II0 3 317**

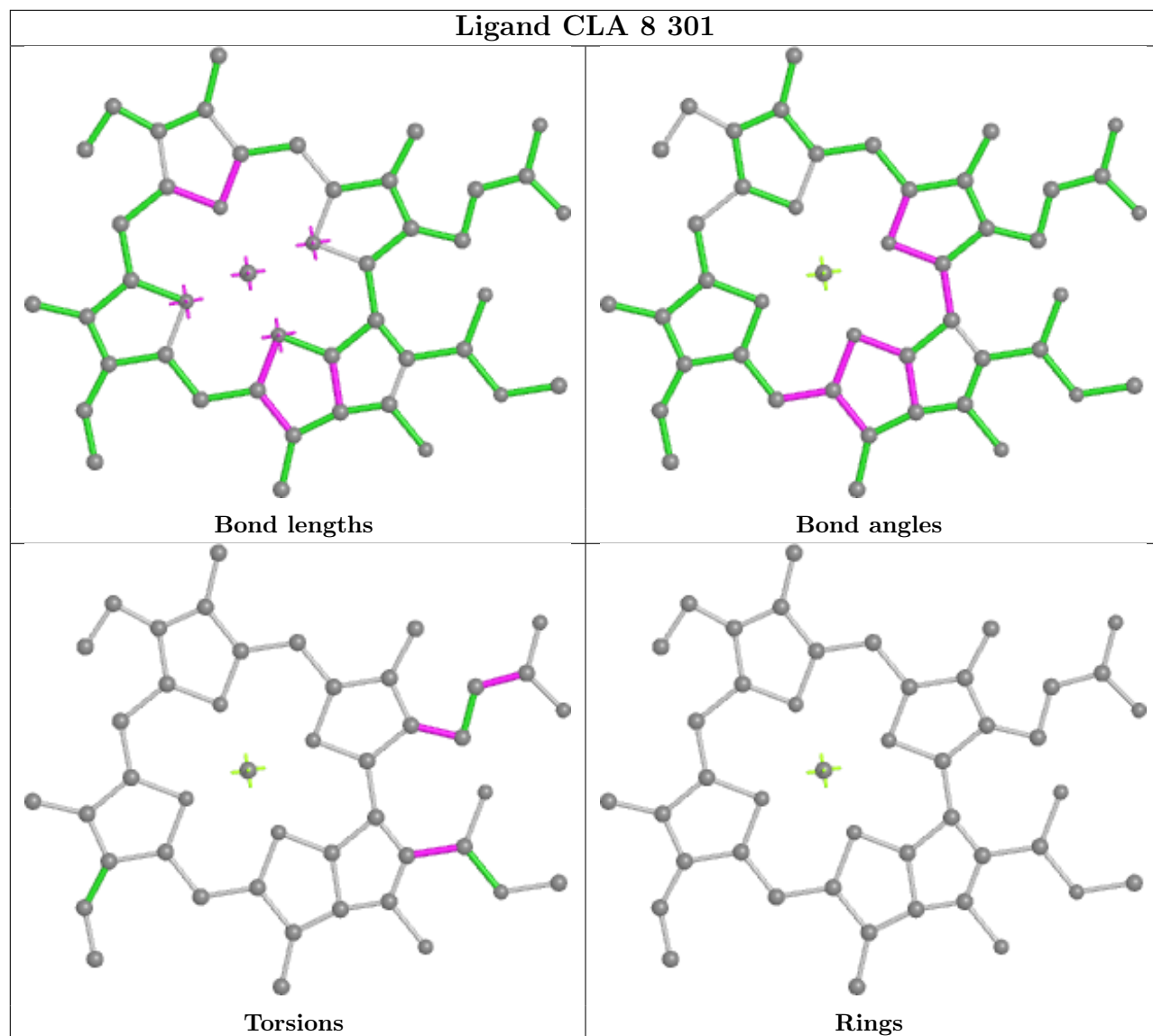
## Ligand CLA 0 308



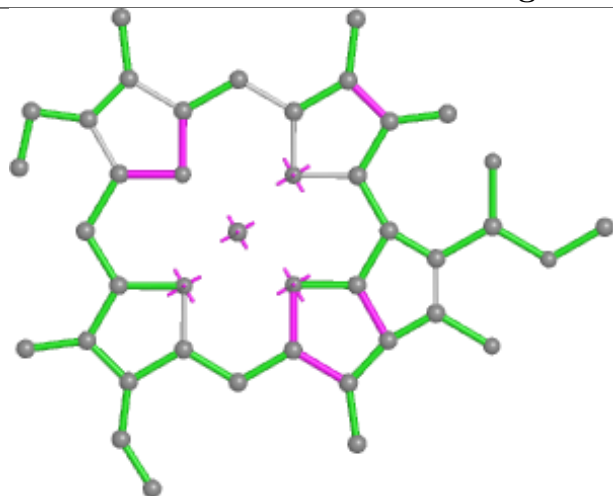
## Ligand CLA C 506



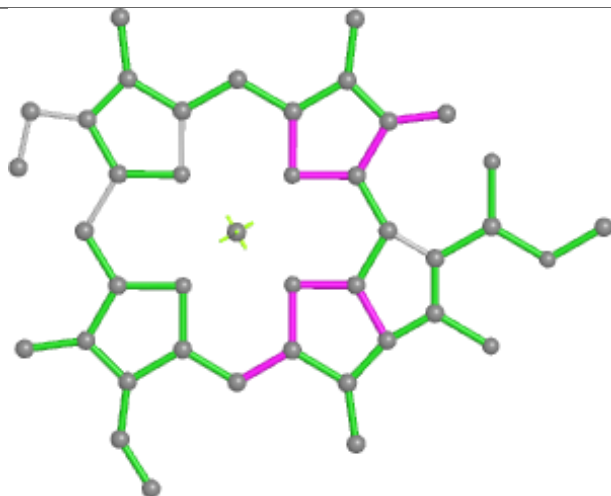
## Ligand CLA 8 301



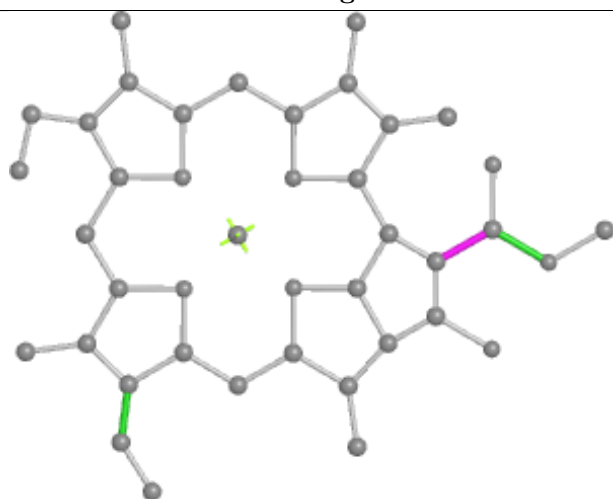
## Ligand CLA 9 313



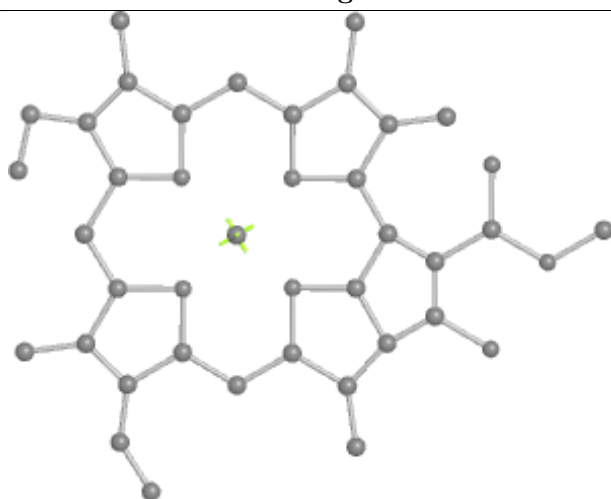
Bond lengths



Bond angles

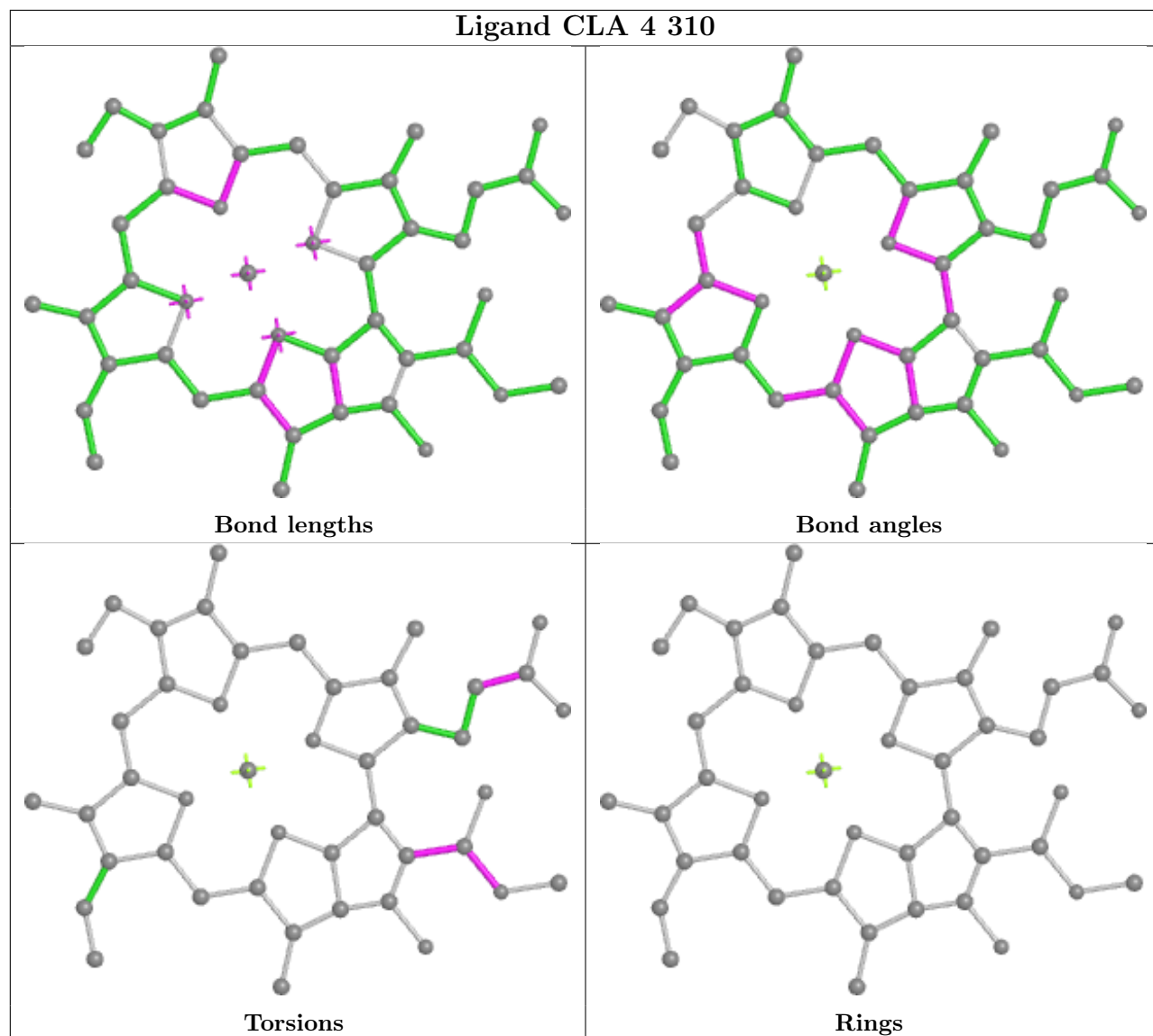


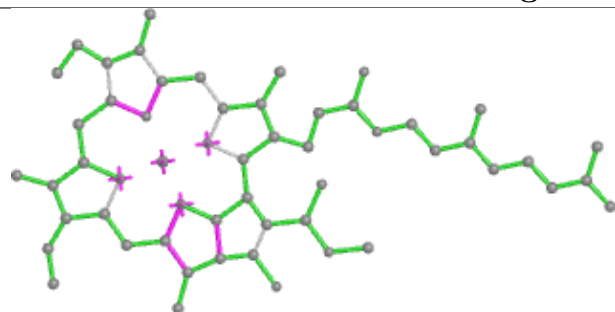
Torsions



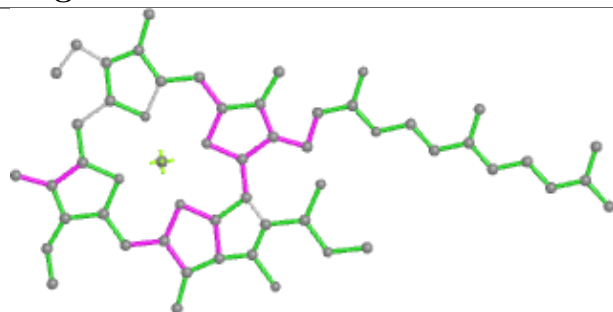
Rings

## Ligand CLA 4 310

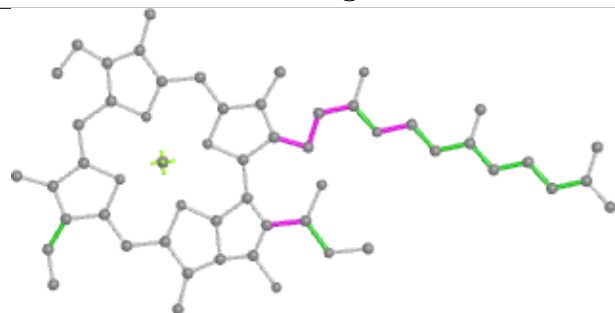


**Ligand CLA g 302**

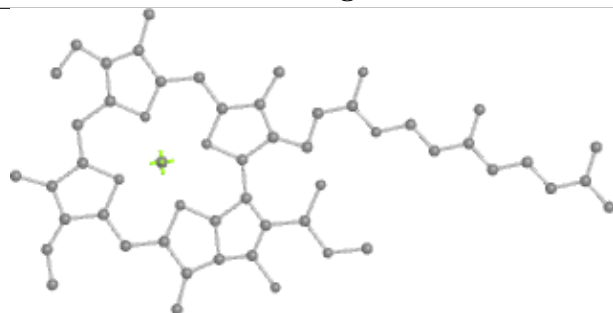
Bond lengths



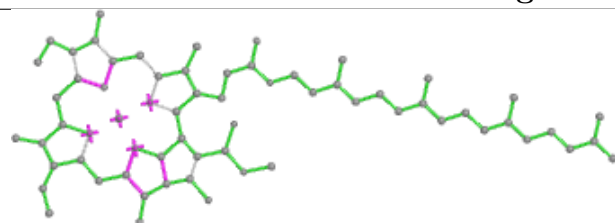
Bond angles



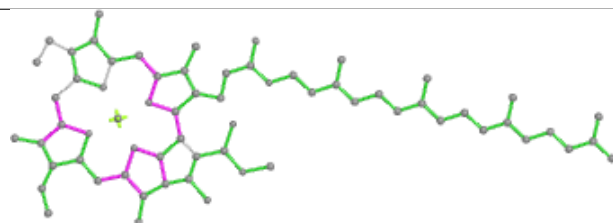
Torsions



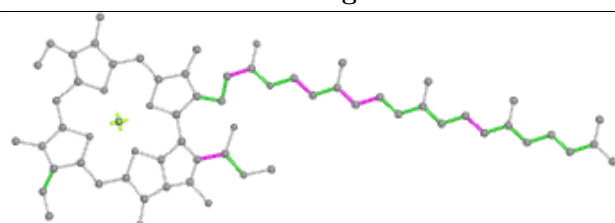
Rings

**Ligand CLA B 614**

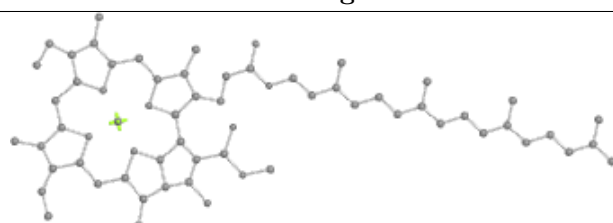
Bond lengths



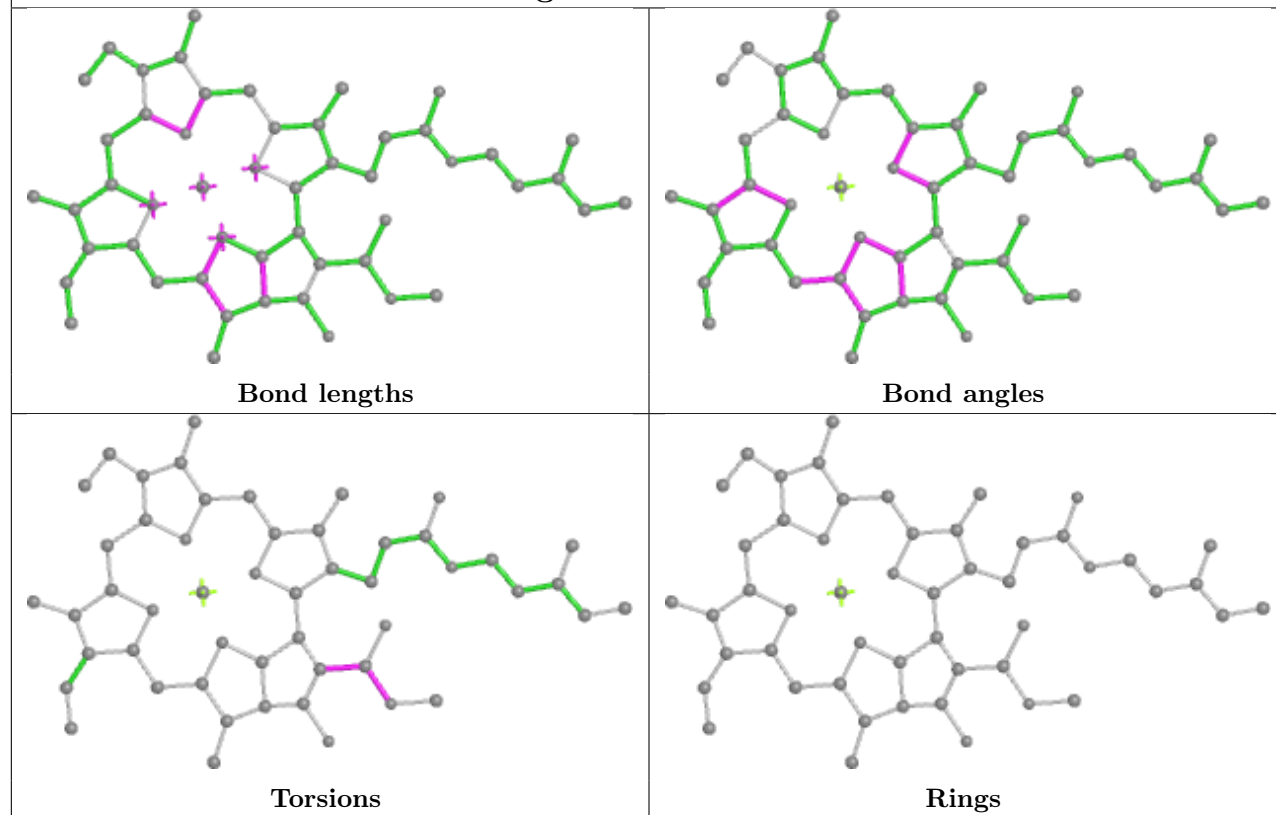
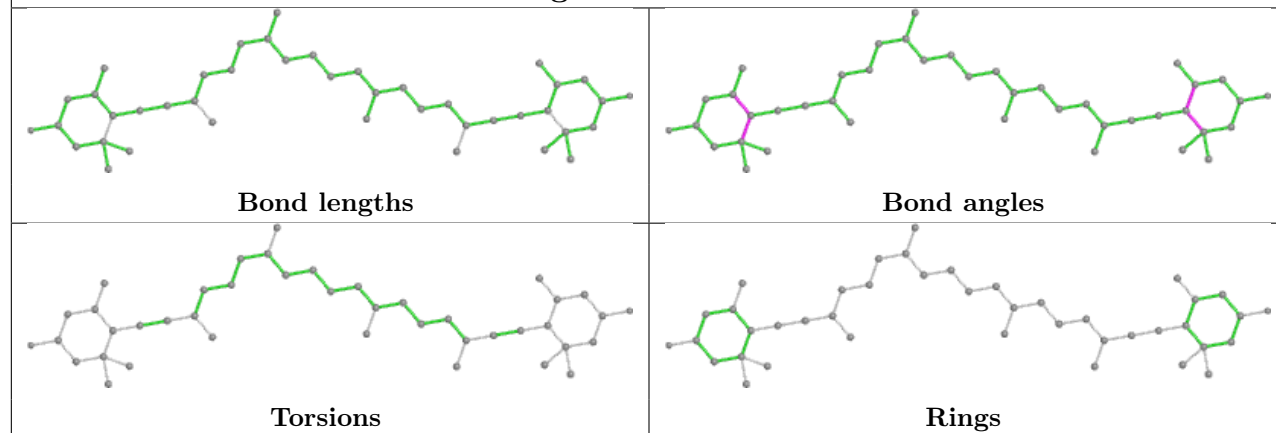
Bond angles



Torsions

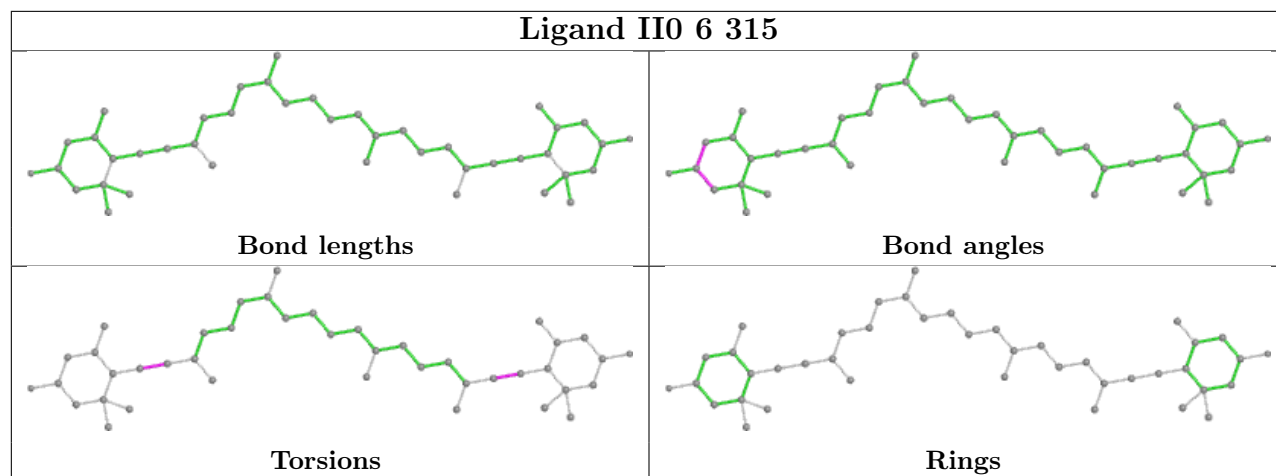


Rings

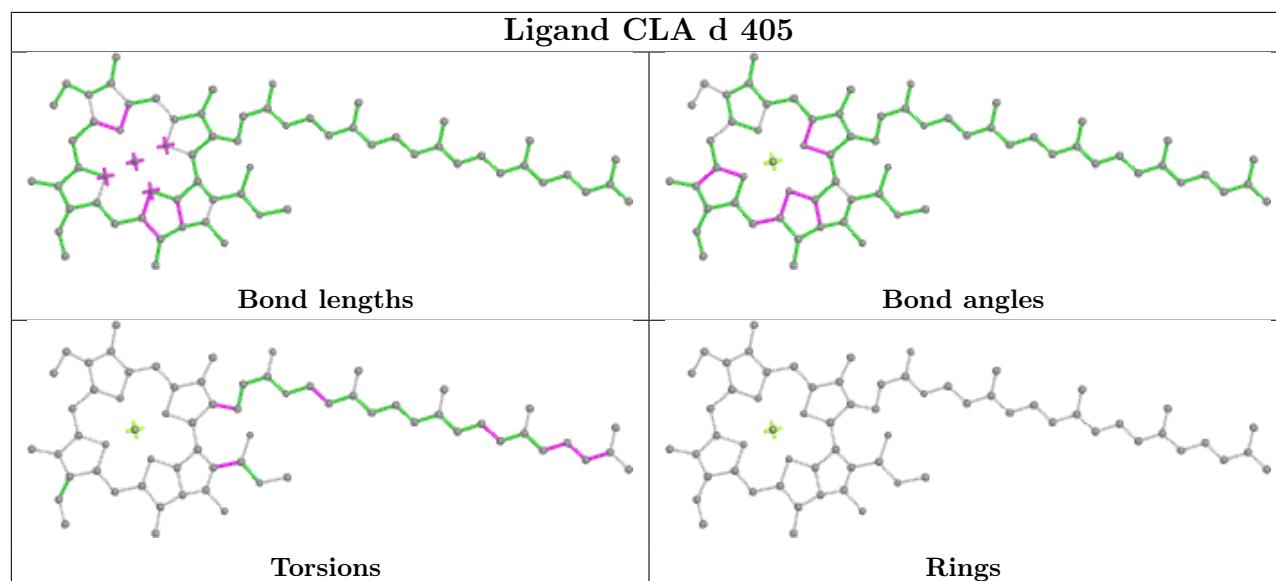
**Ligand CLA 0 302****Ligand II0 6 301**



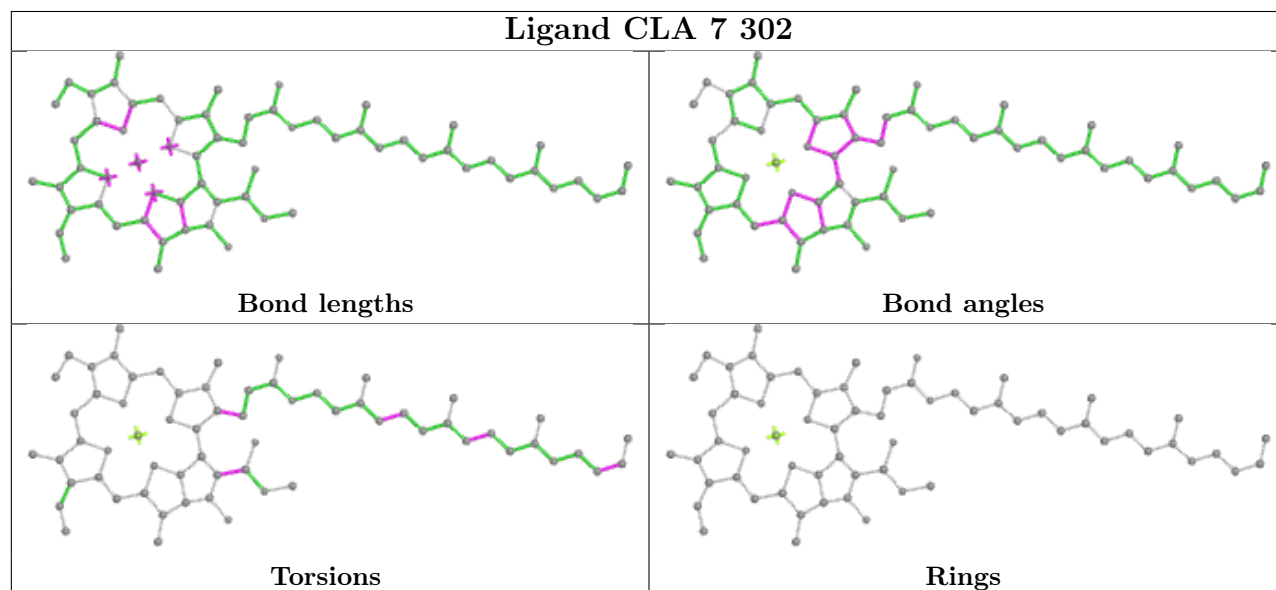
## Ligand II0 6 315



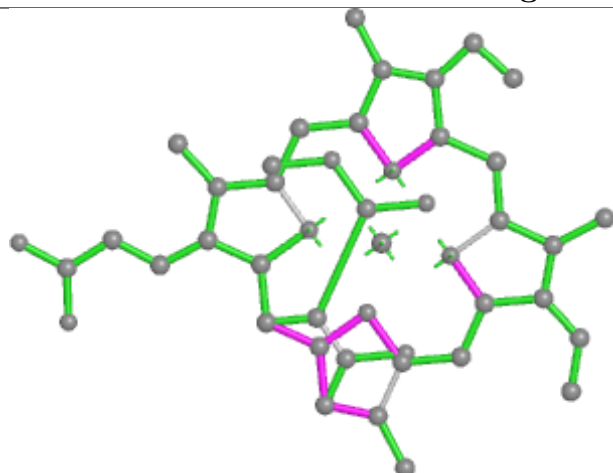
## Ligand CLA d 405



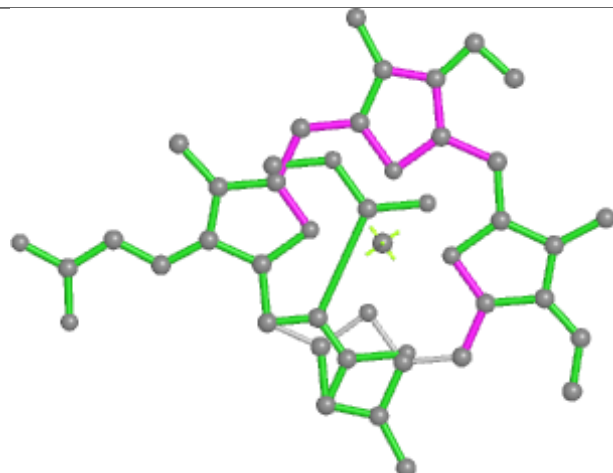
## Ligand CLA 7 302



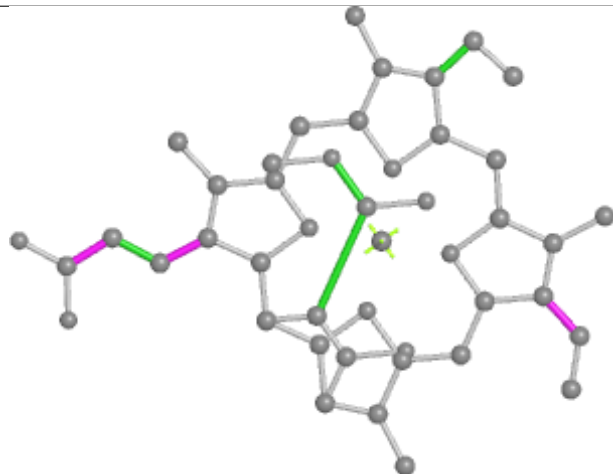
## Ligand KC2 1 311



Bond lengths



Bond angles

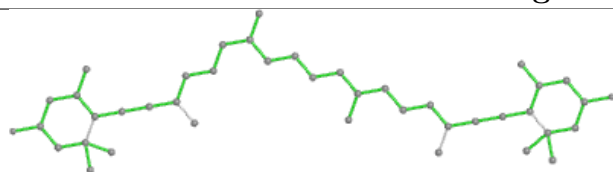


Torsions

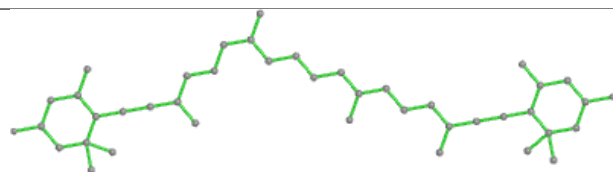


Rings

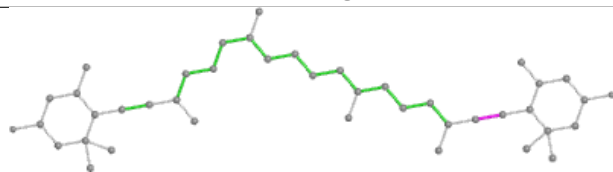
## Ligand II0 3 301



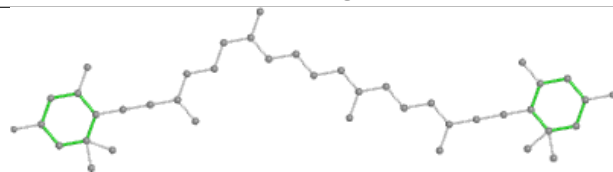
Bond lengths



Bond angles

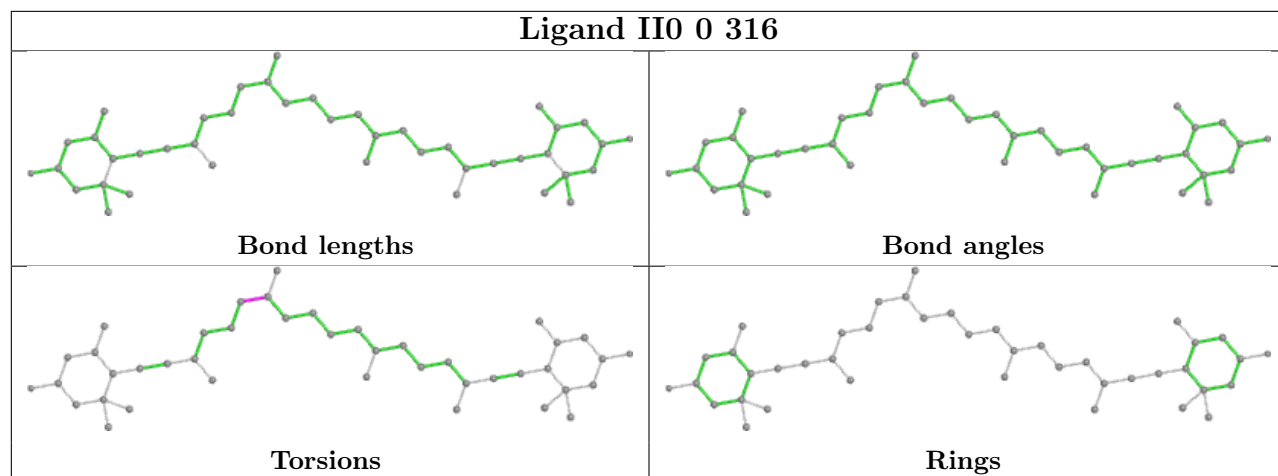


Torsions

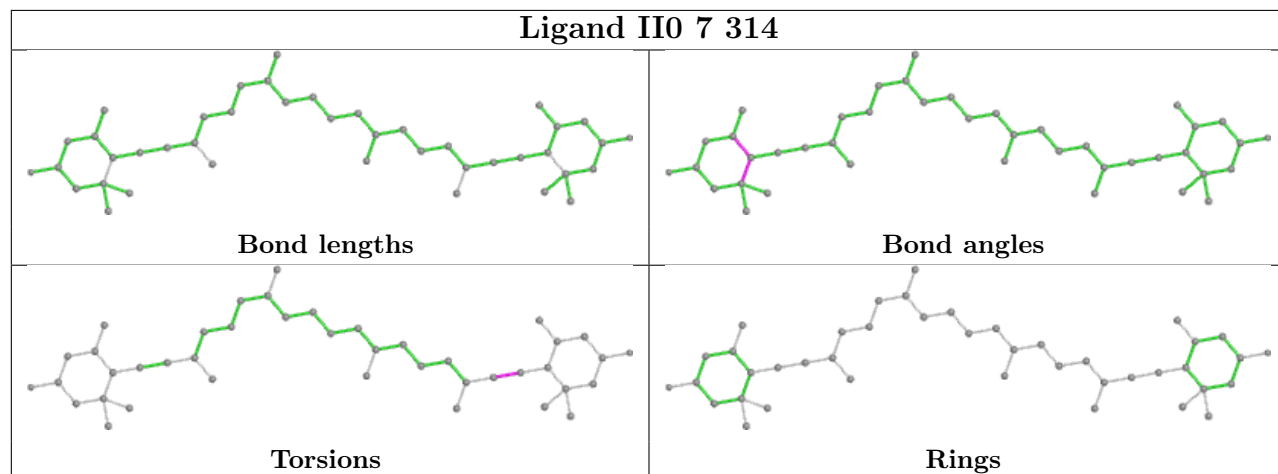


Rings

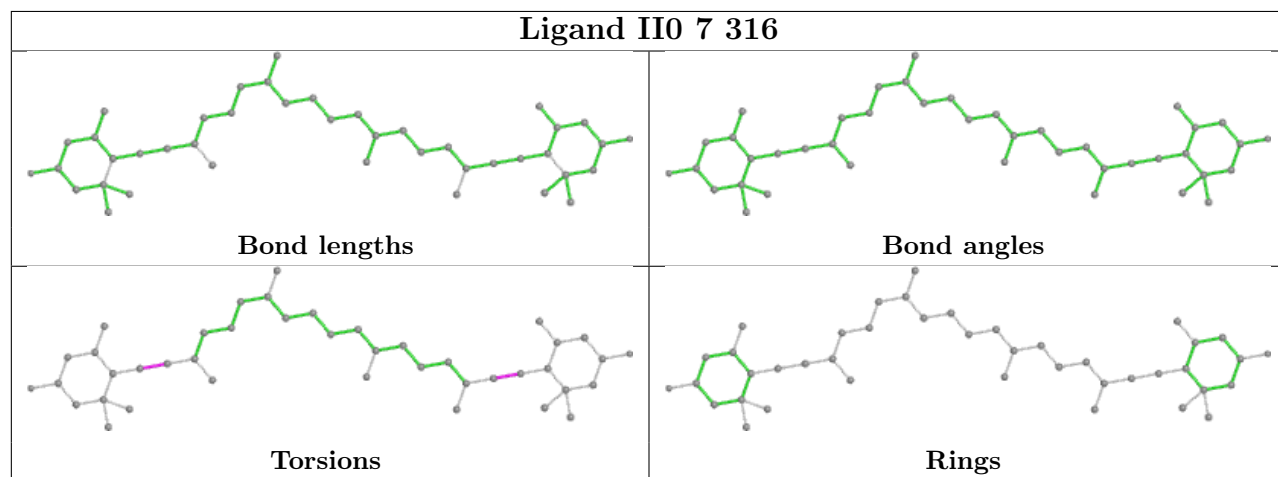
## Ligand II0 0 316



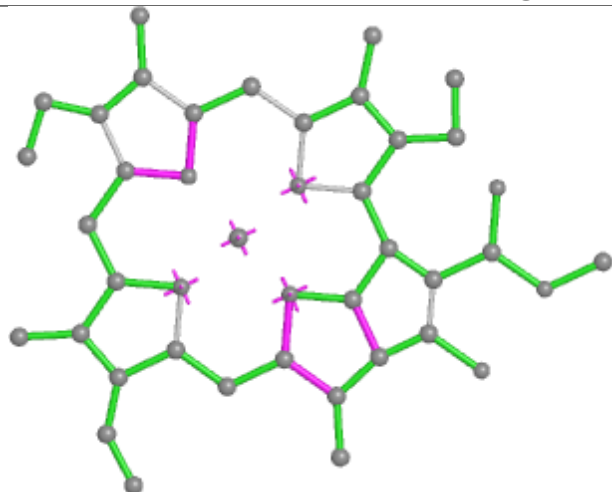
## Ligand II0 7 314



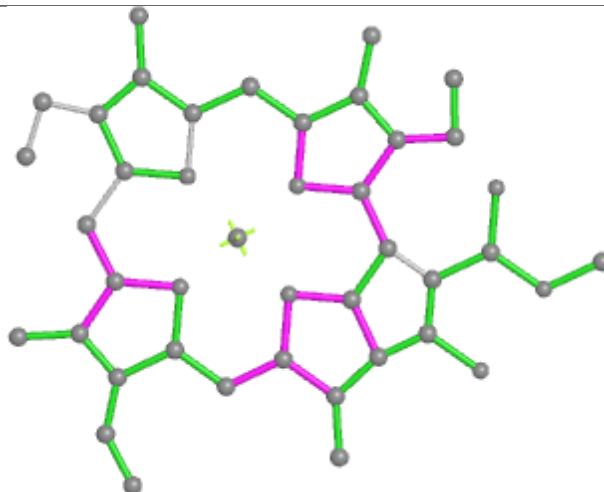
## Ligand II0 7 316



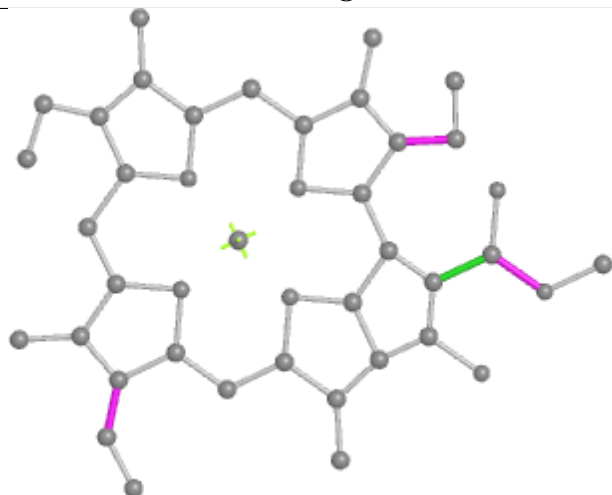
## Ligand CLA 6 308



Bond lengths



Bond angles

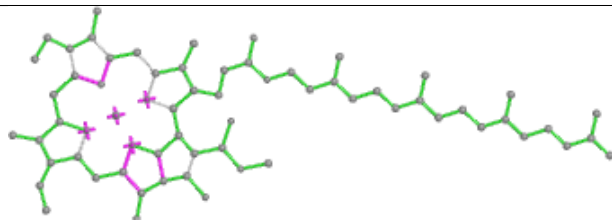


Torsions

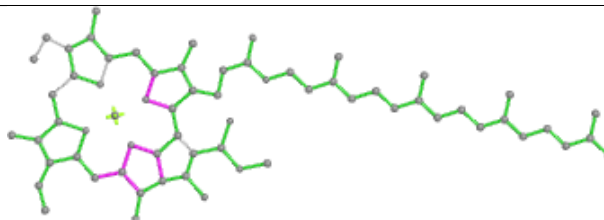


Rings

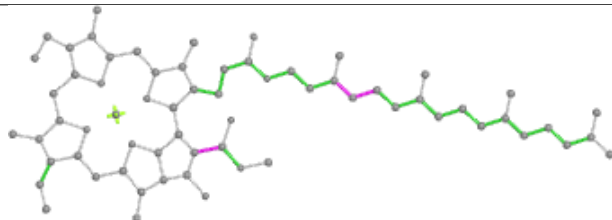
## Ligand CLA b 608



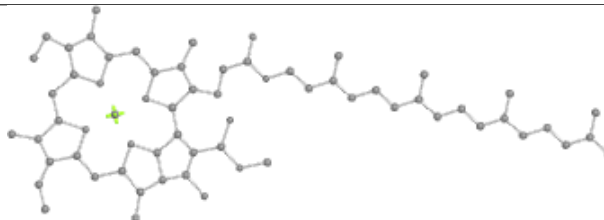
Bond lengths



Bond angles

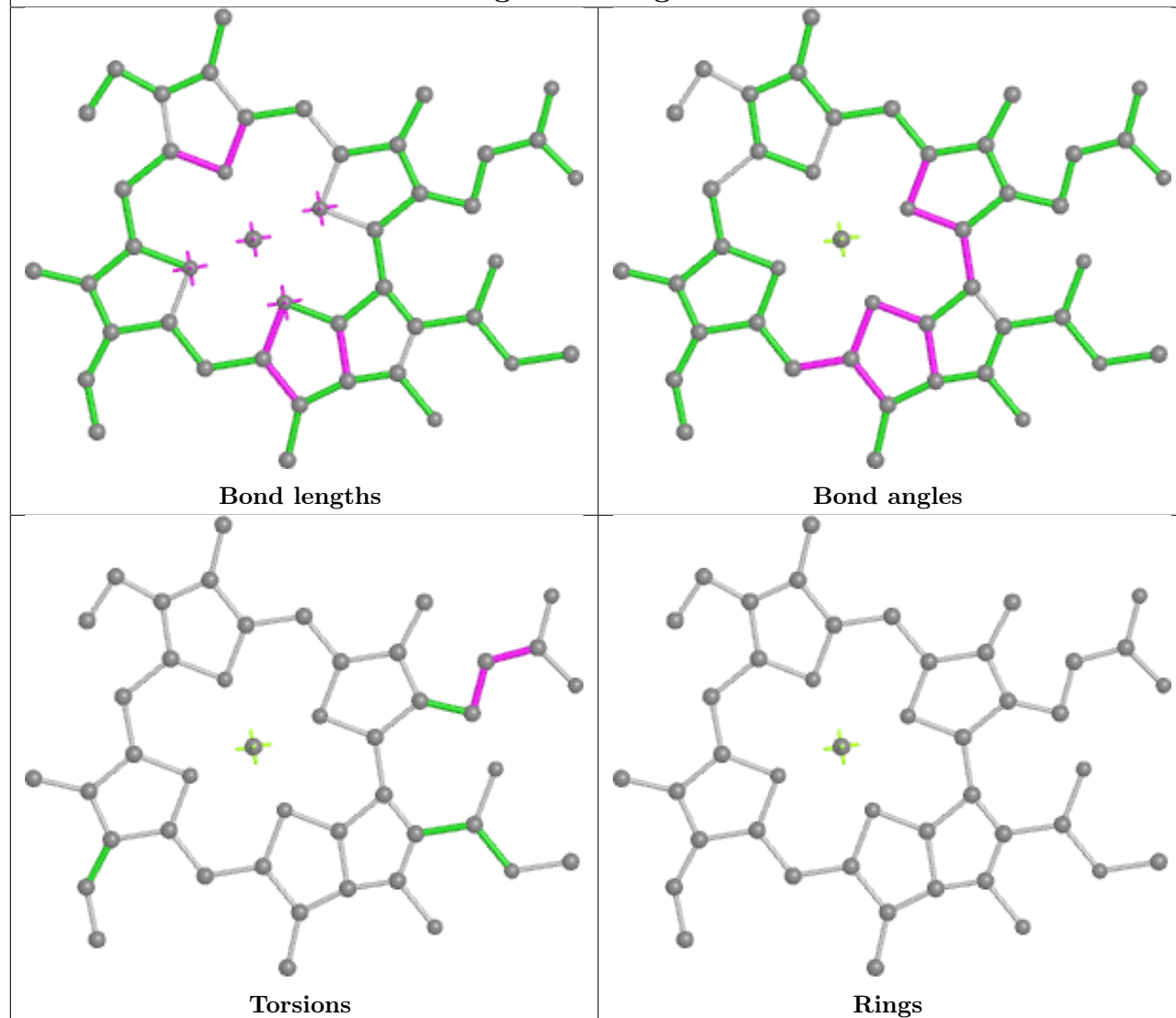


Torsions

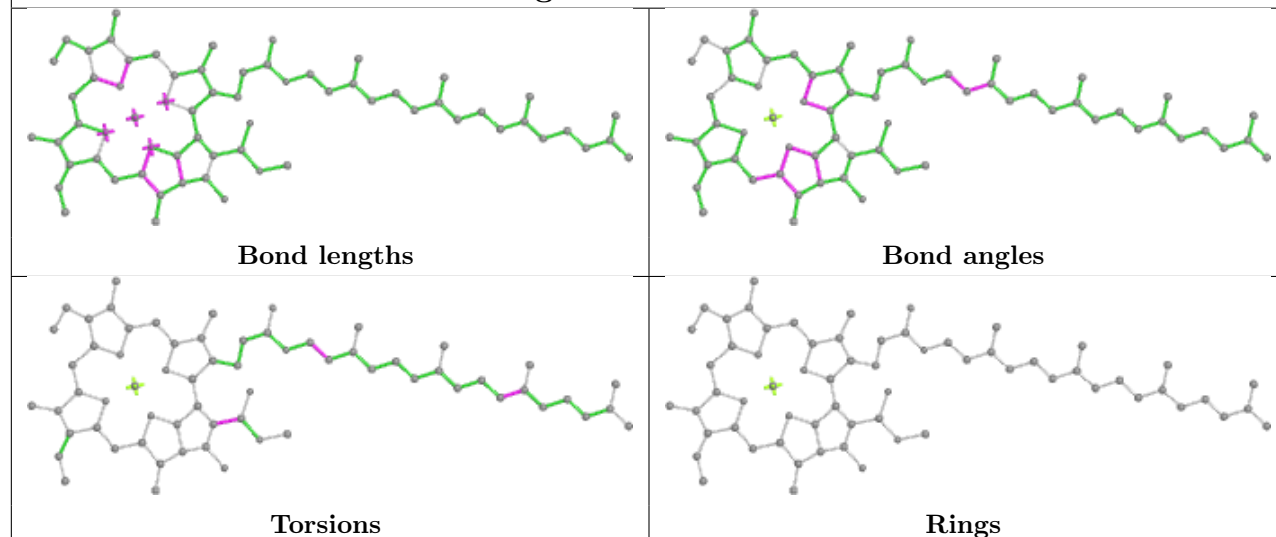


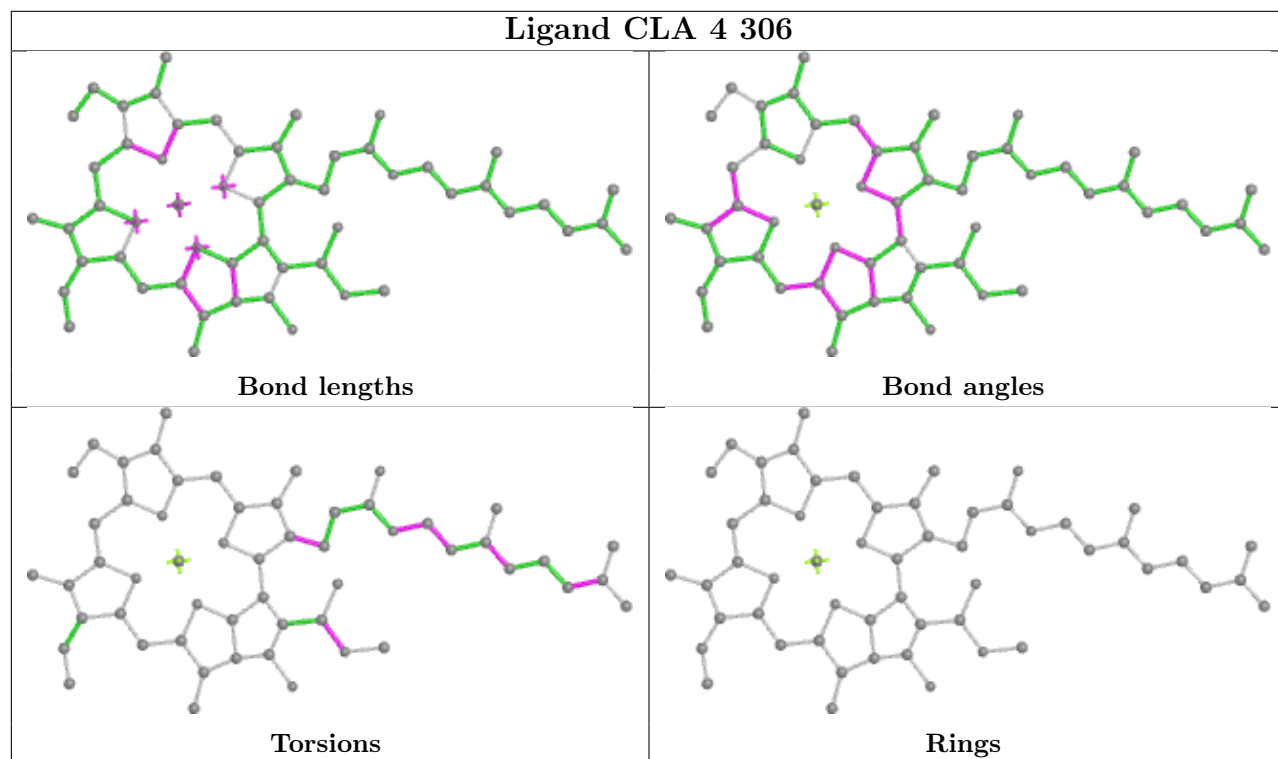
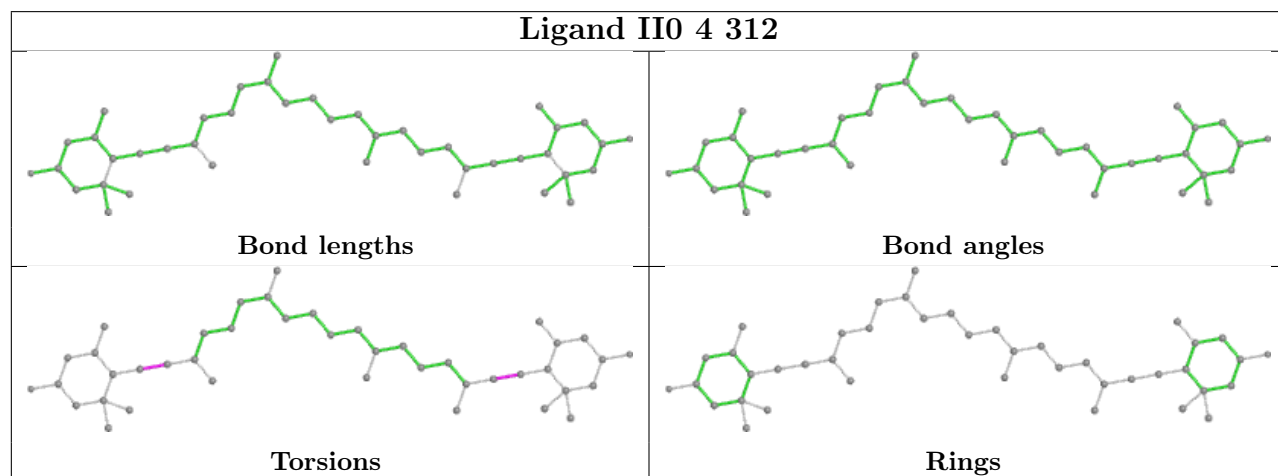
Rings

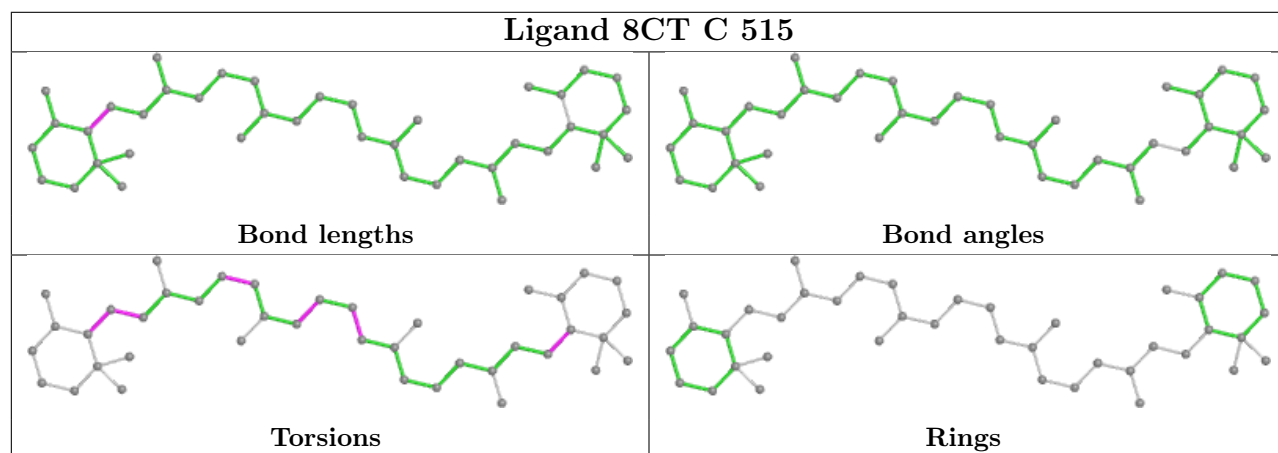
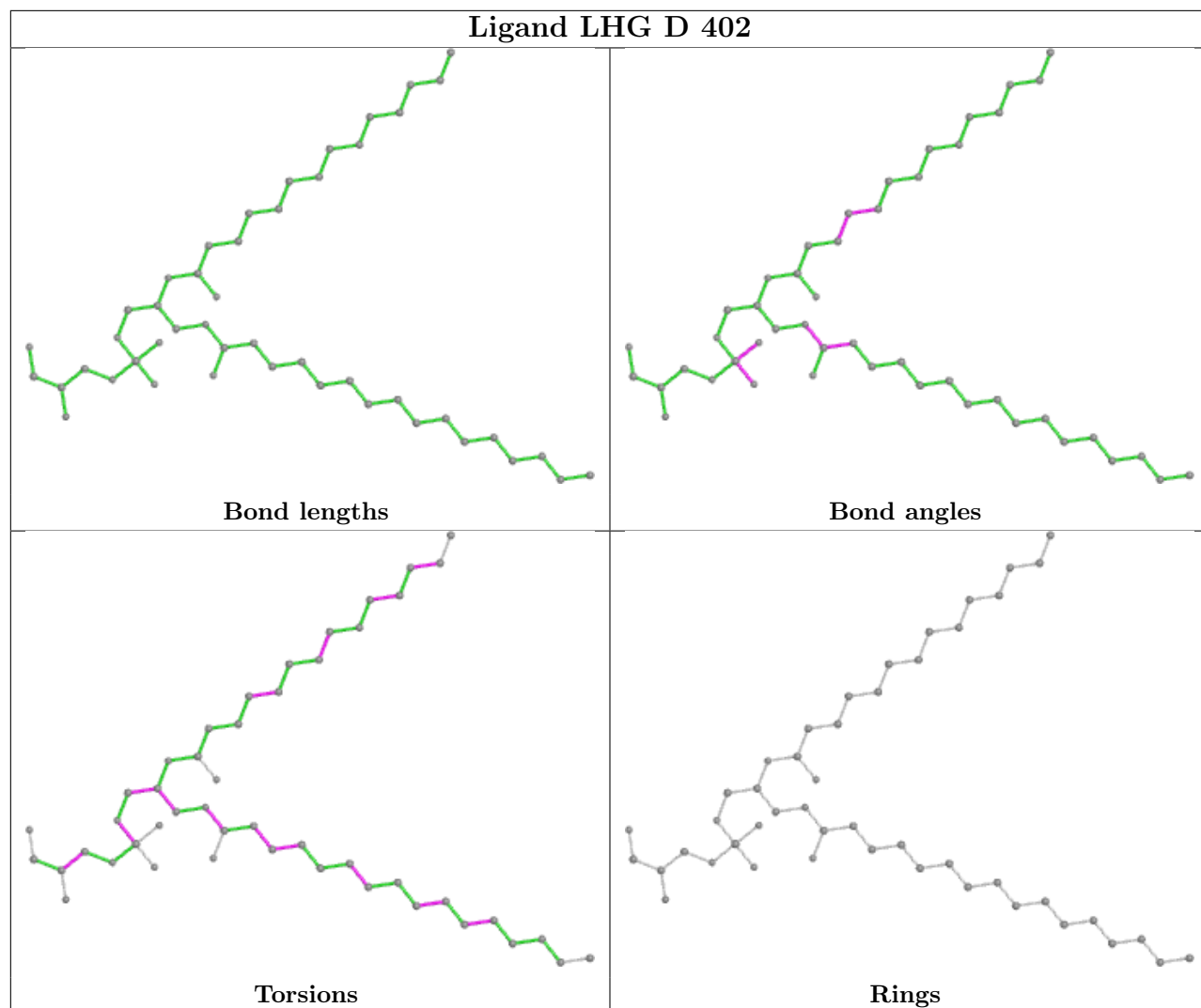
## Ligand CLA g 304

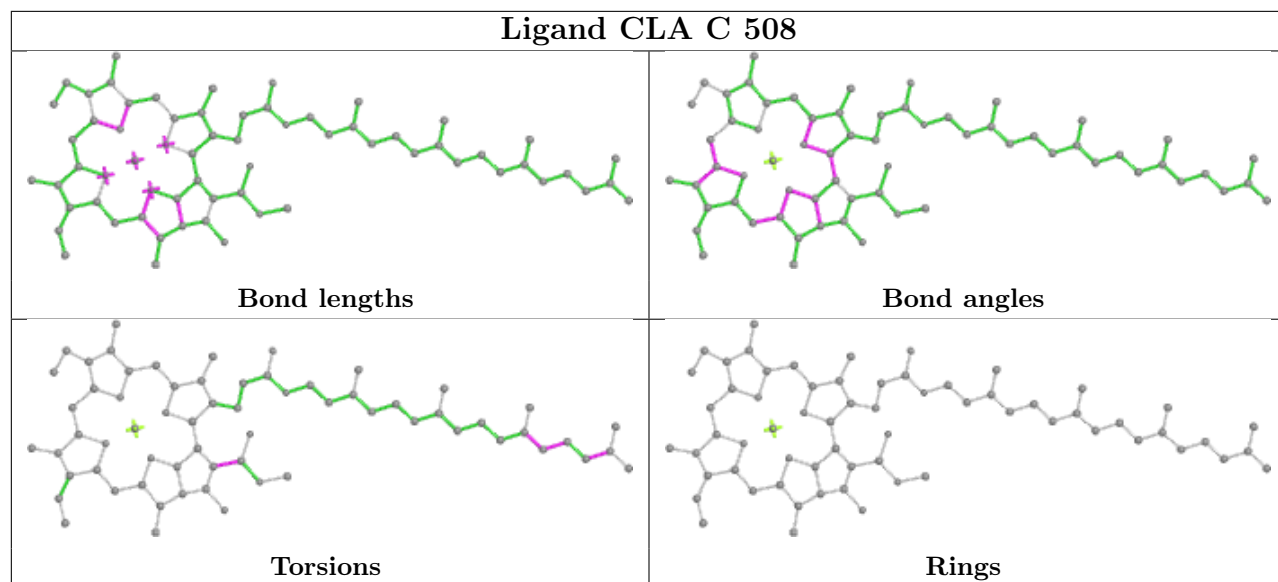
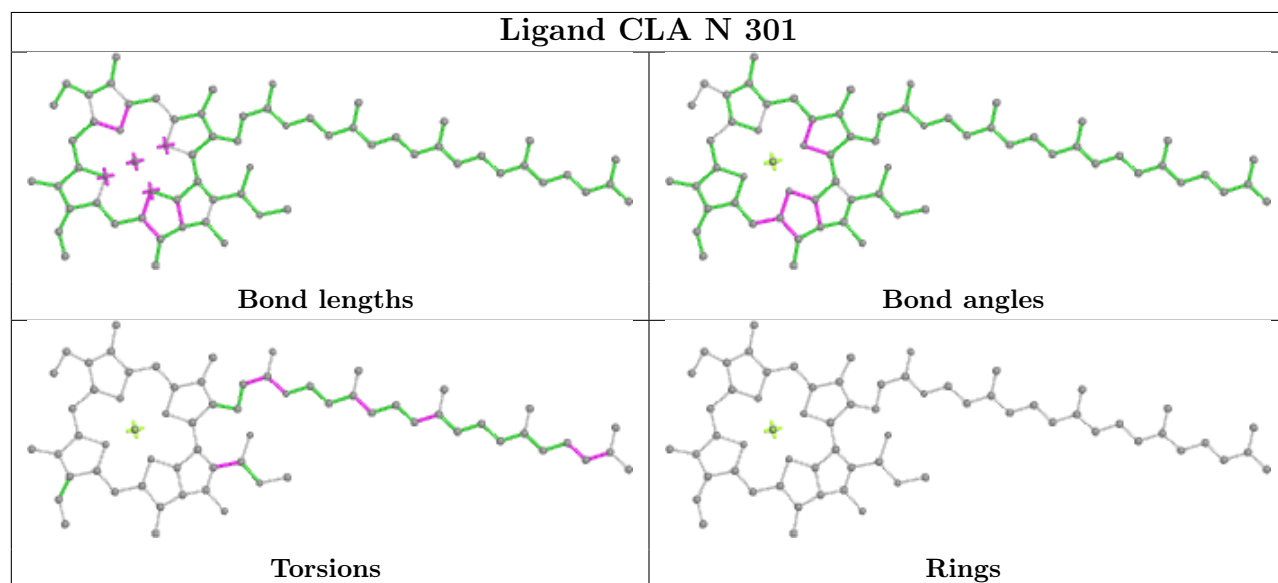


## Ligand CLA b 603



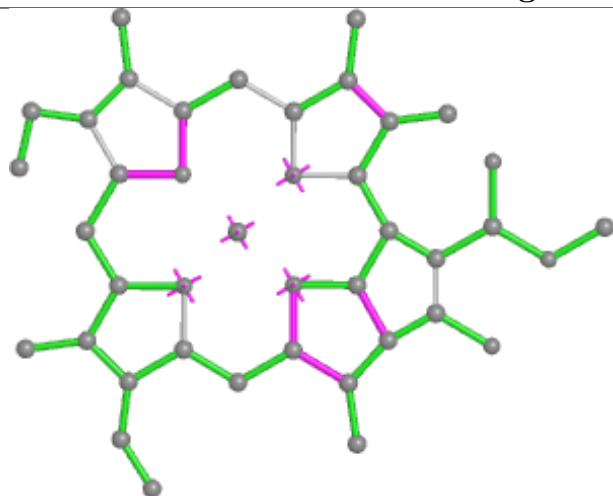
**Ligand CLA 4 306****Ligand II0 4 312**



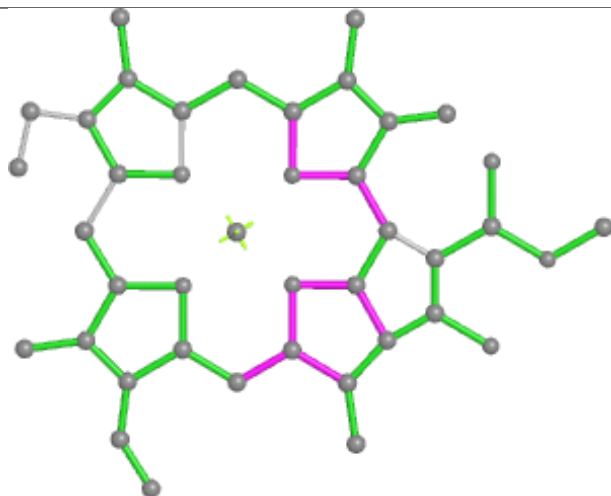
**Ligand CLA C 508****Ligand CLA N 301**



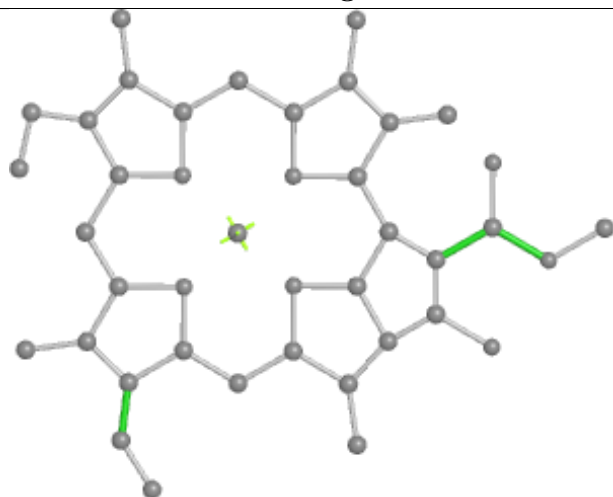
## Ligand CLA 5 310



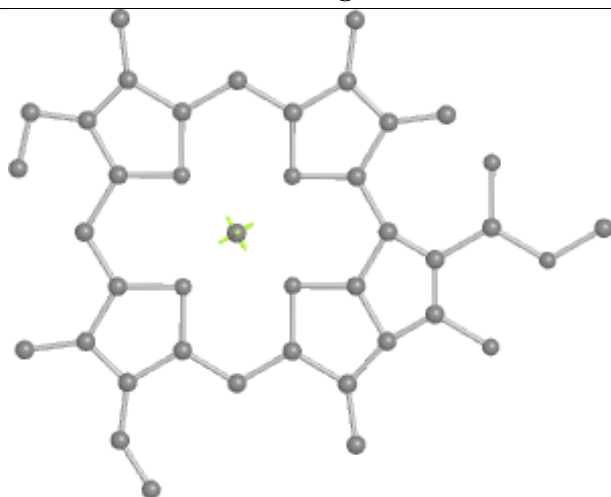
Bond lengths



Bond angles

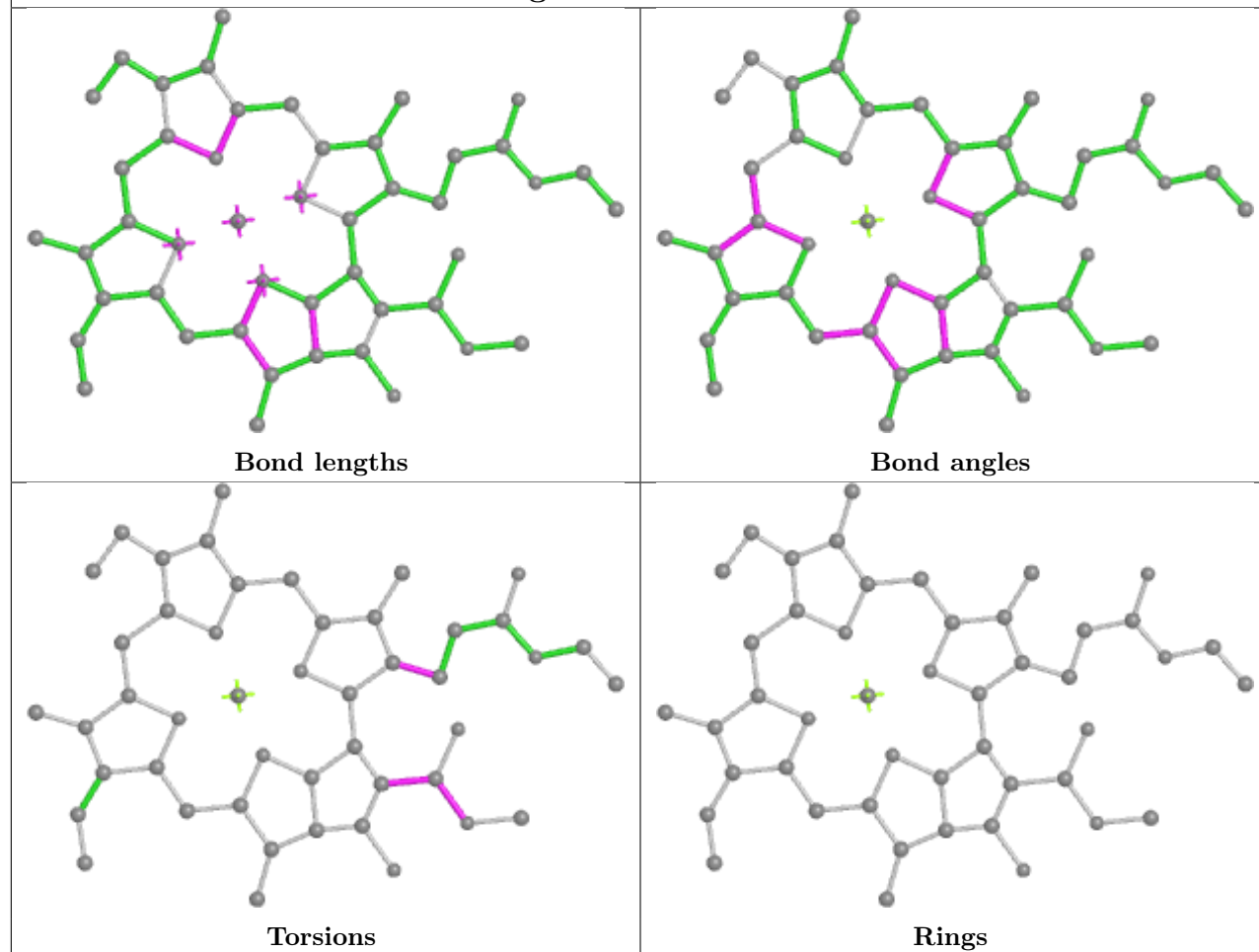


Torsions

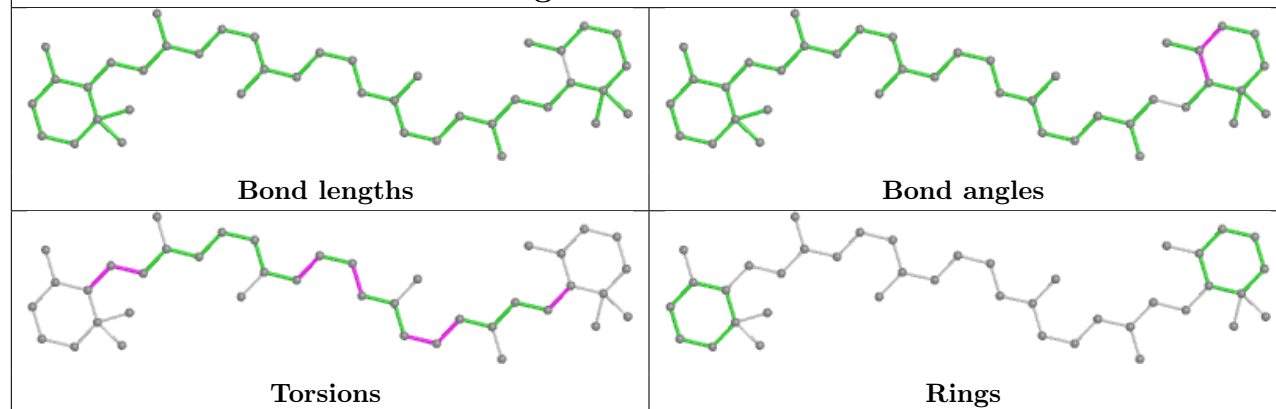


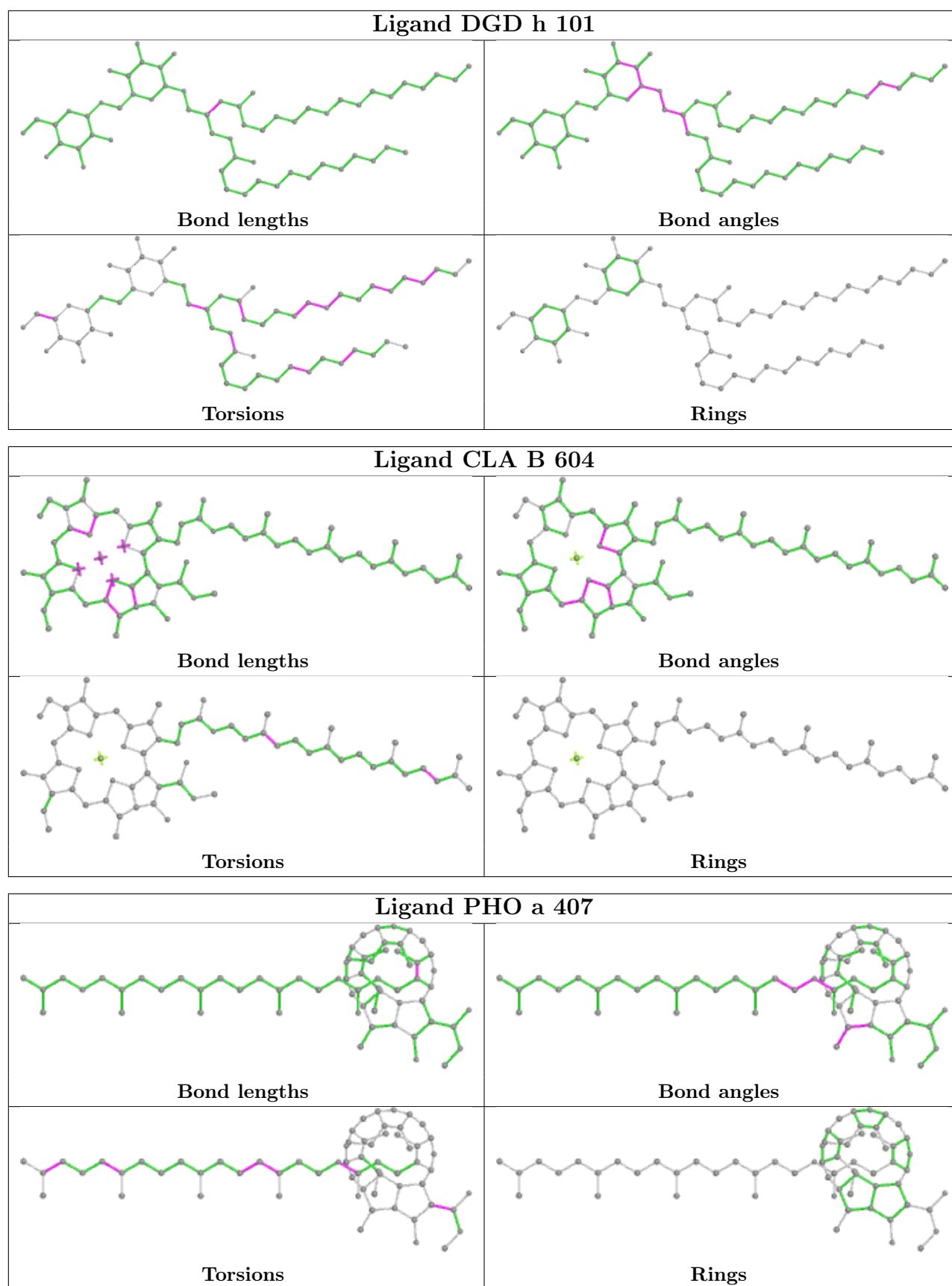
Rings

## Ligand CLA 4 304

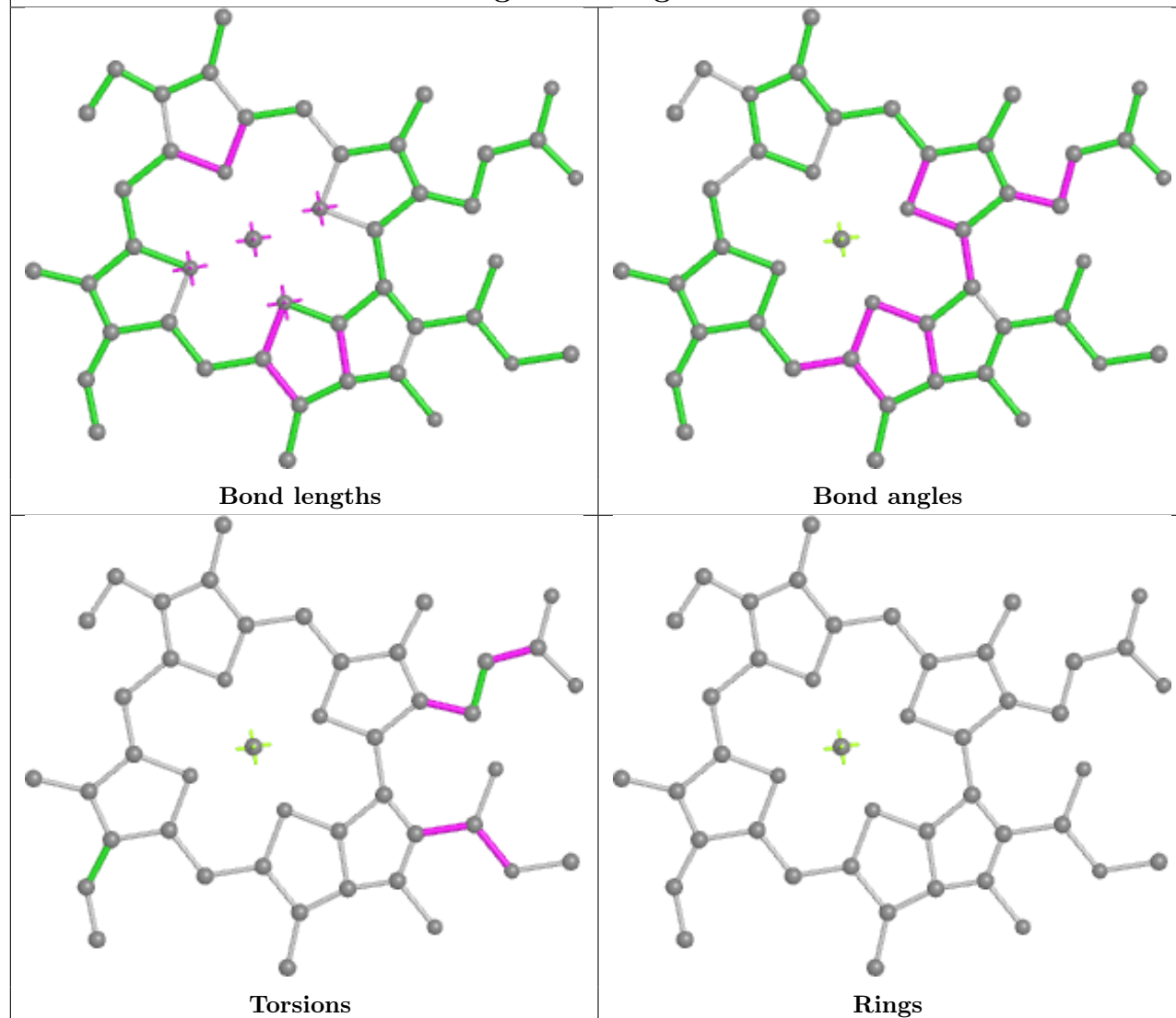


## Ligand 8CT D 406

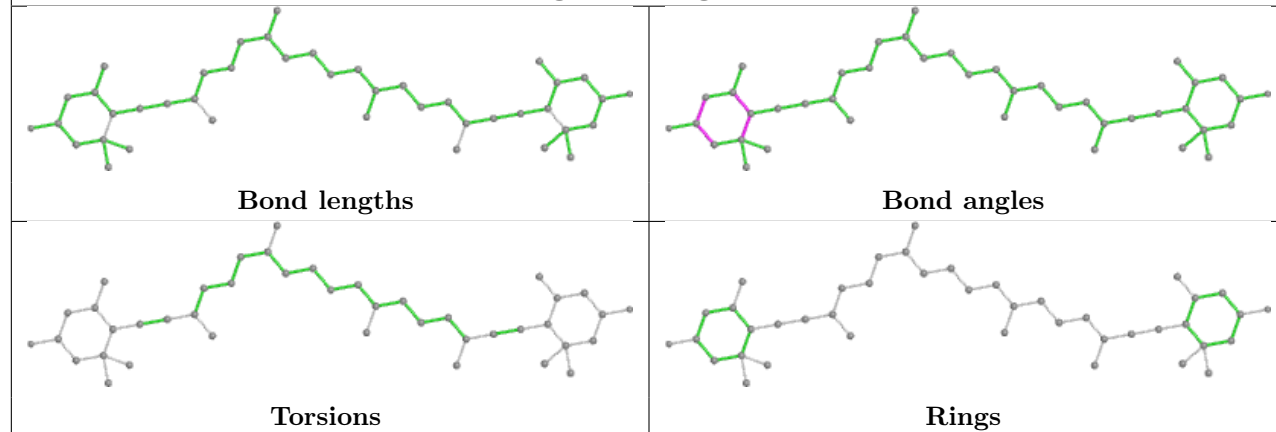




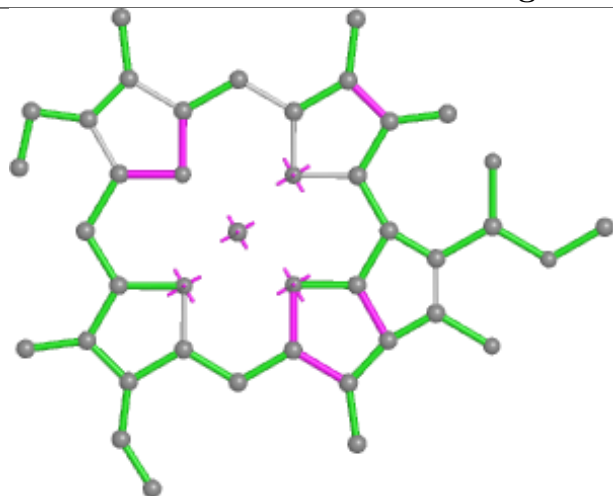
## Ligand CLA g 311



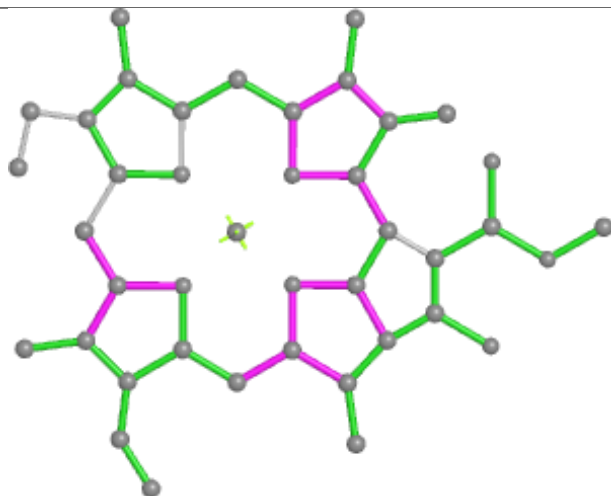
## Ligand II0 g 314



## Ligand CLA 6 319



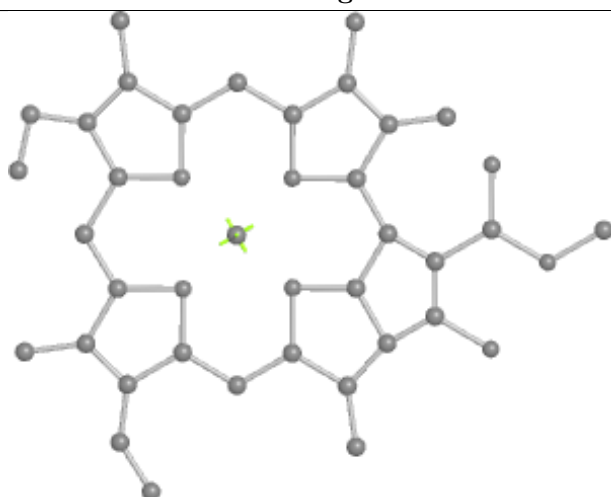
Bond lengths



Bond angles

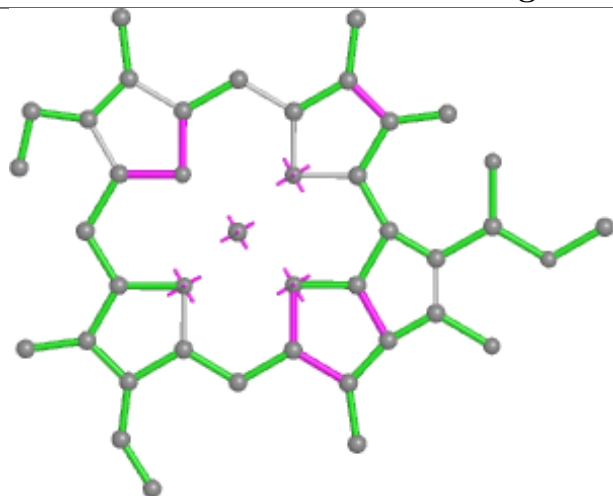


Torsions

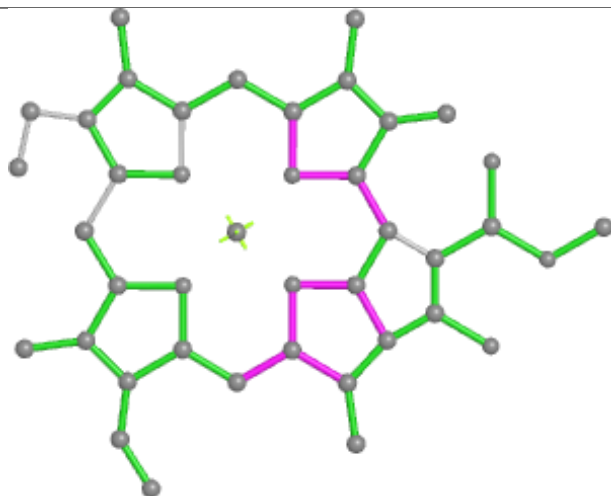


Rings

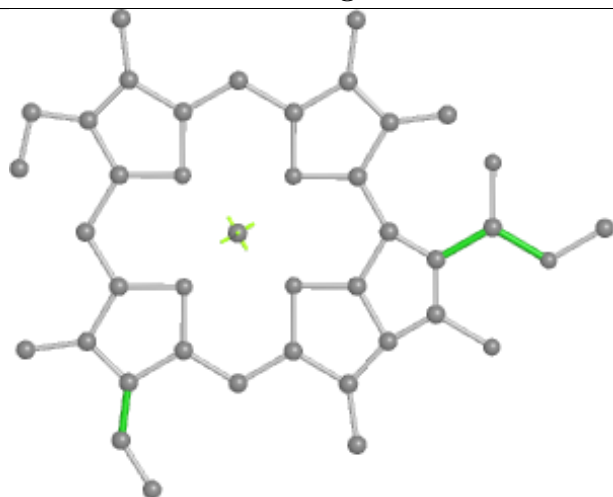
## Ligand CLA 9 314



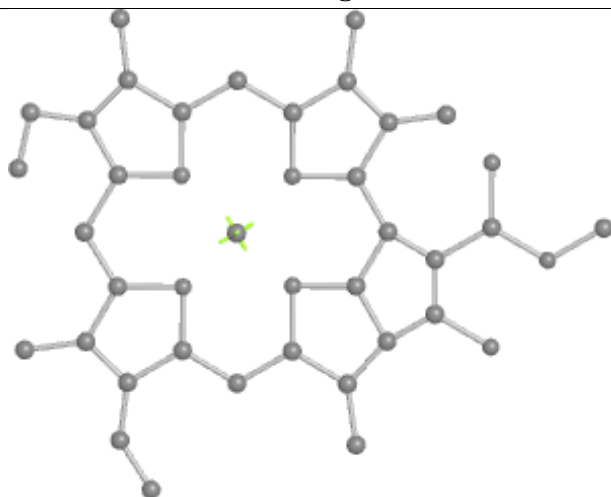
Bond lengths



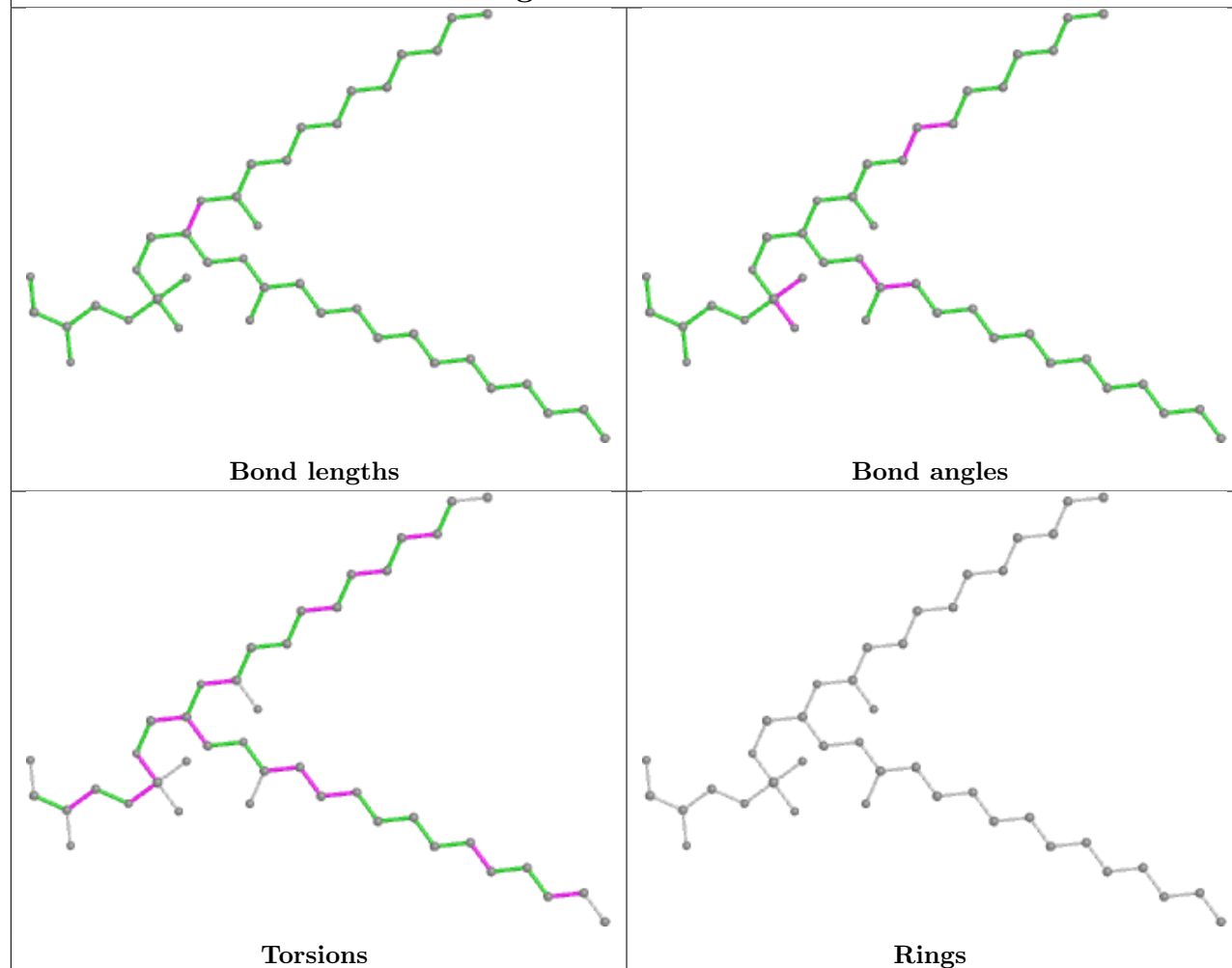
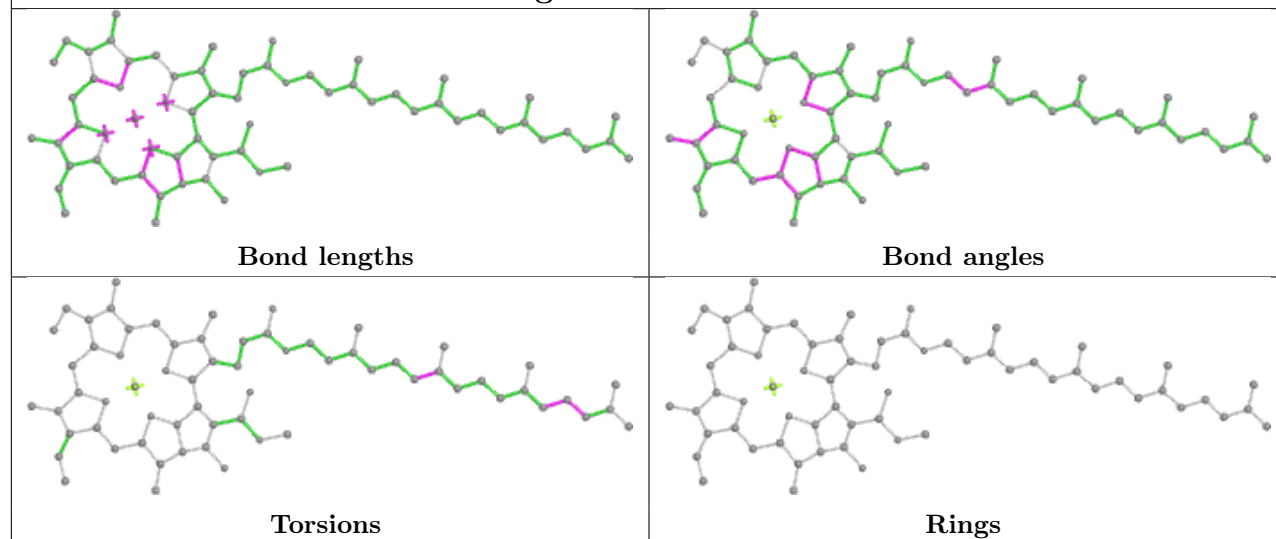
Bond angles

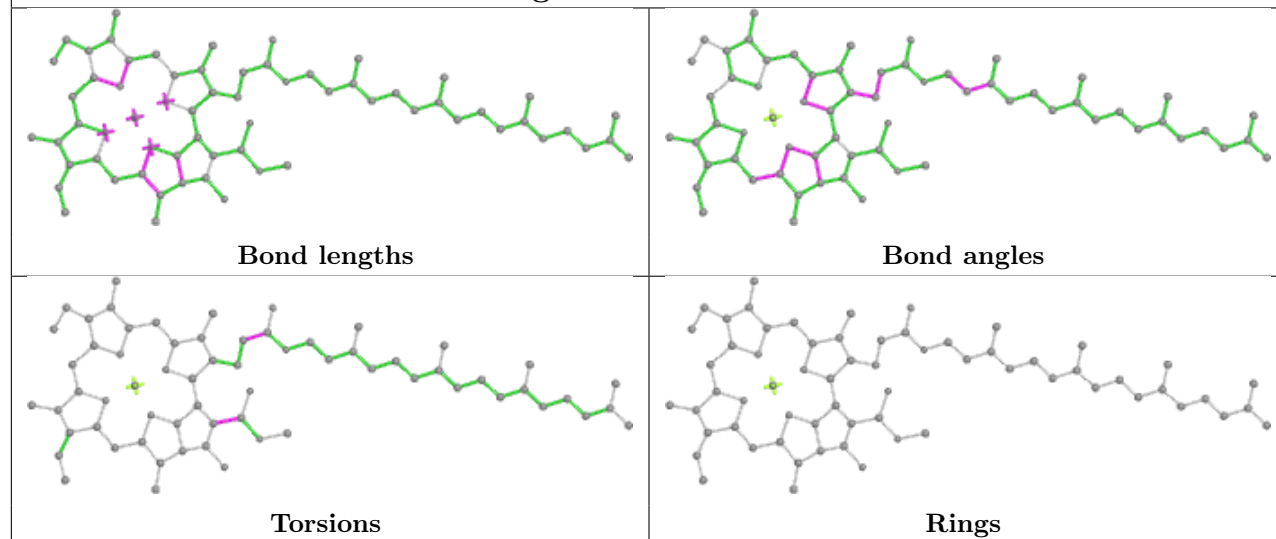
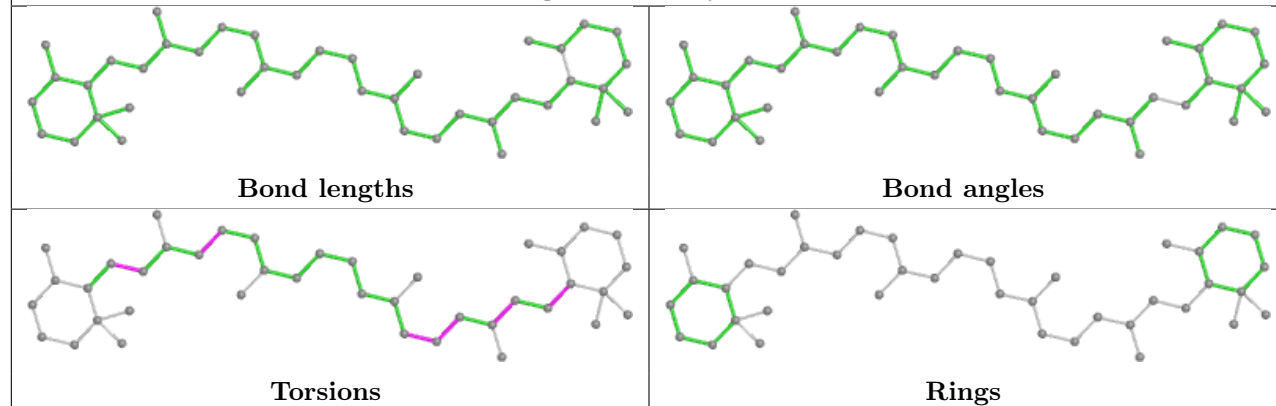
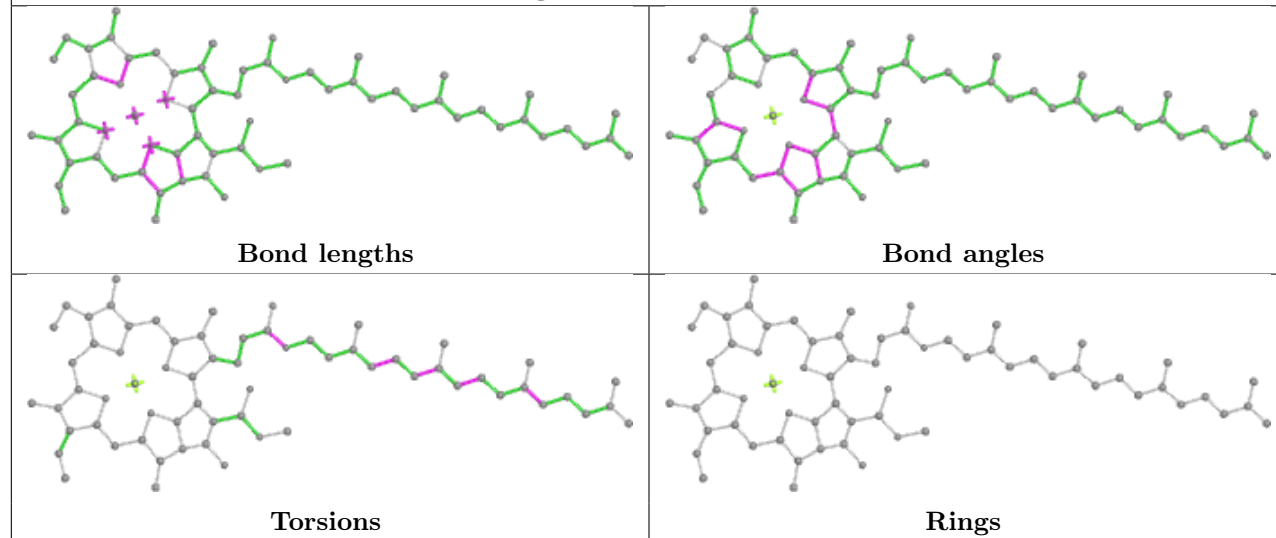


Torsions

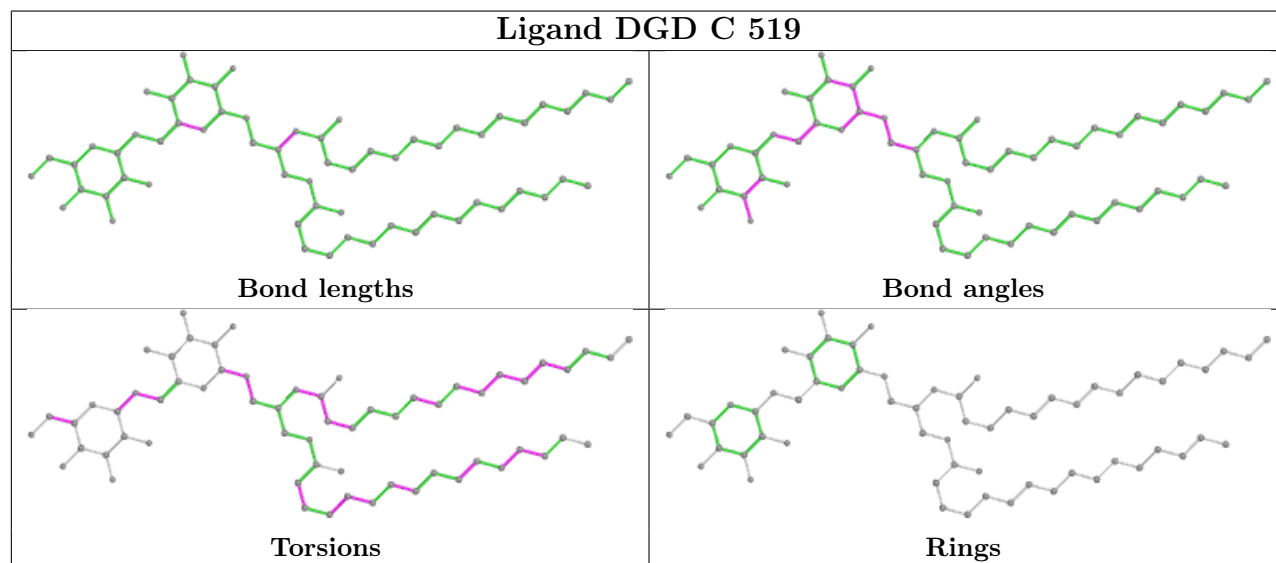
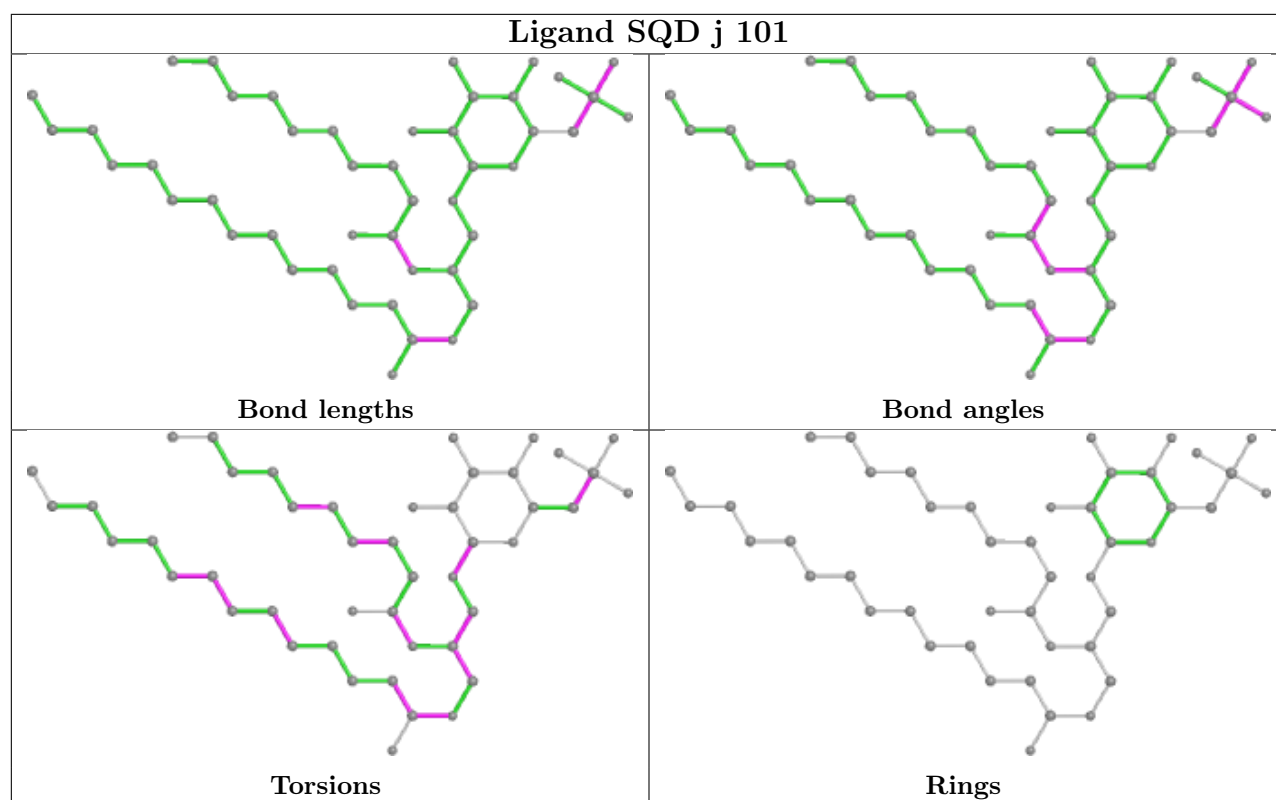


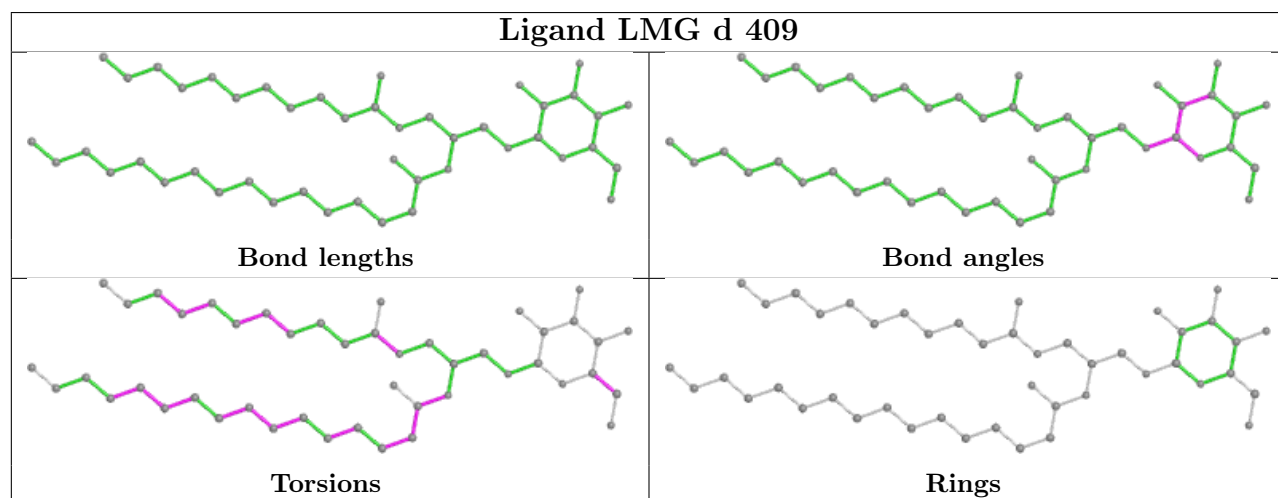
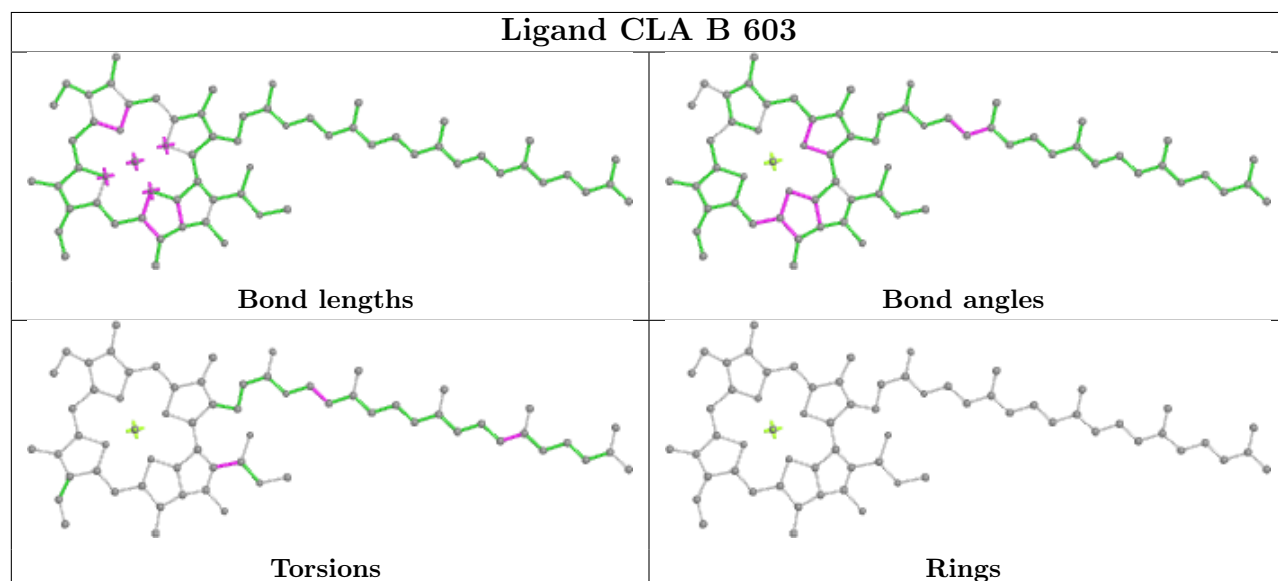
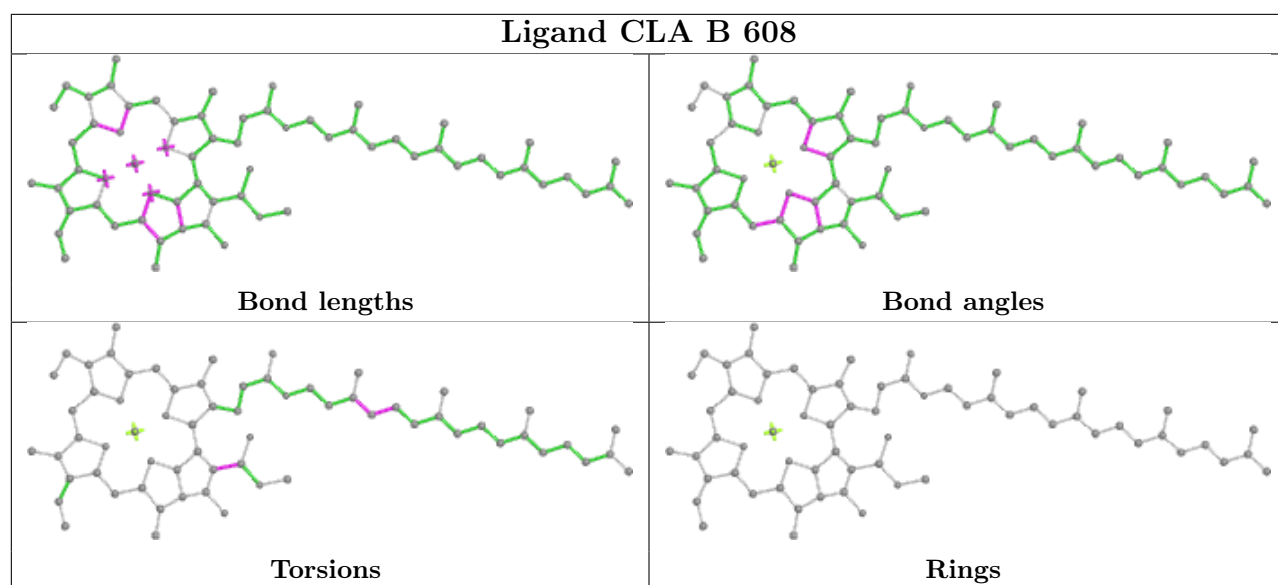
Rings

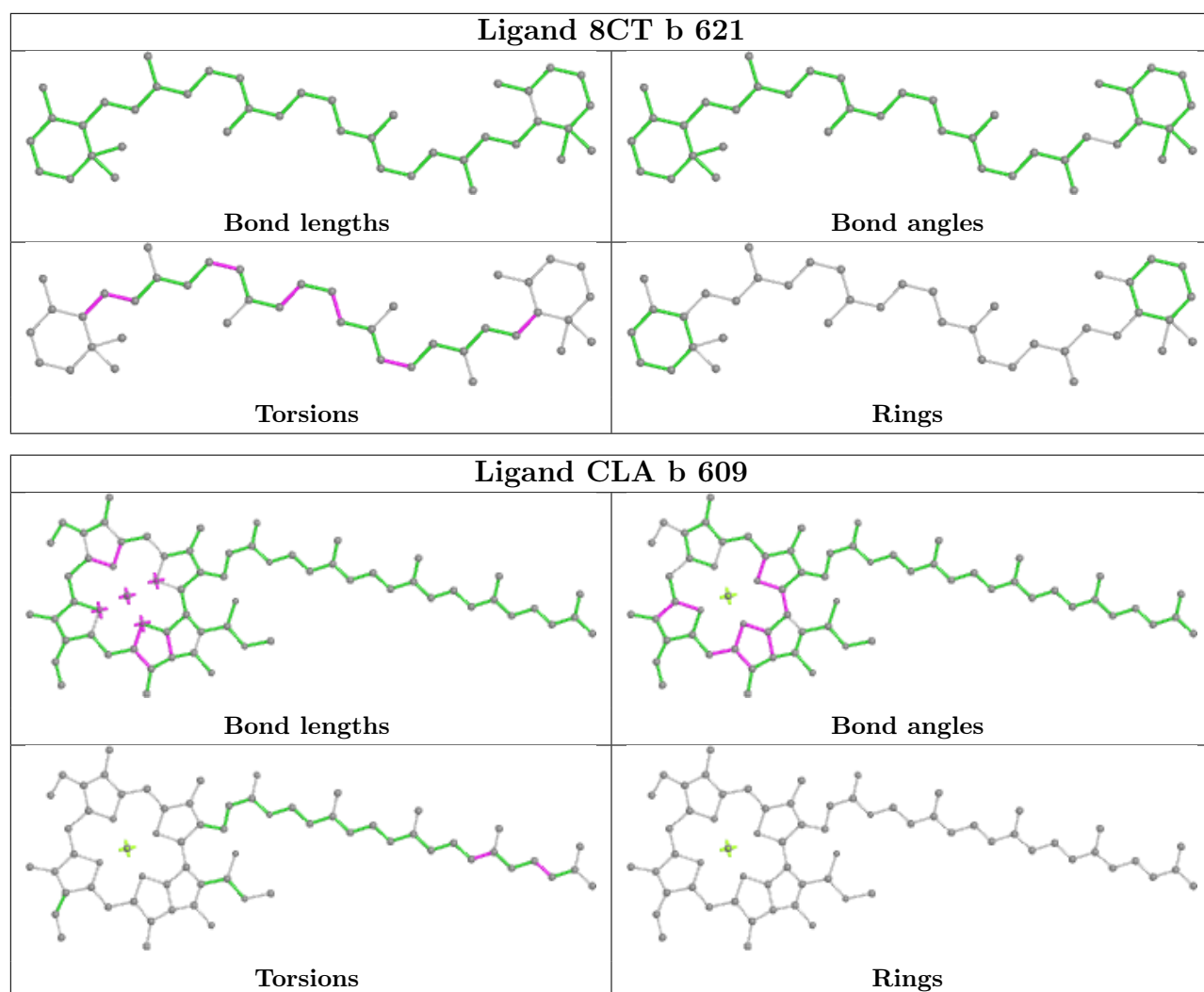
**Ligand LHG 9 302****Ligand CLA b 606**

**Ligand CLA C 502****Ligand 8CT y 101****Ligand CLA C 512**

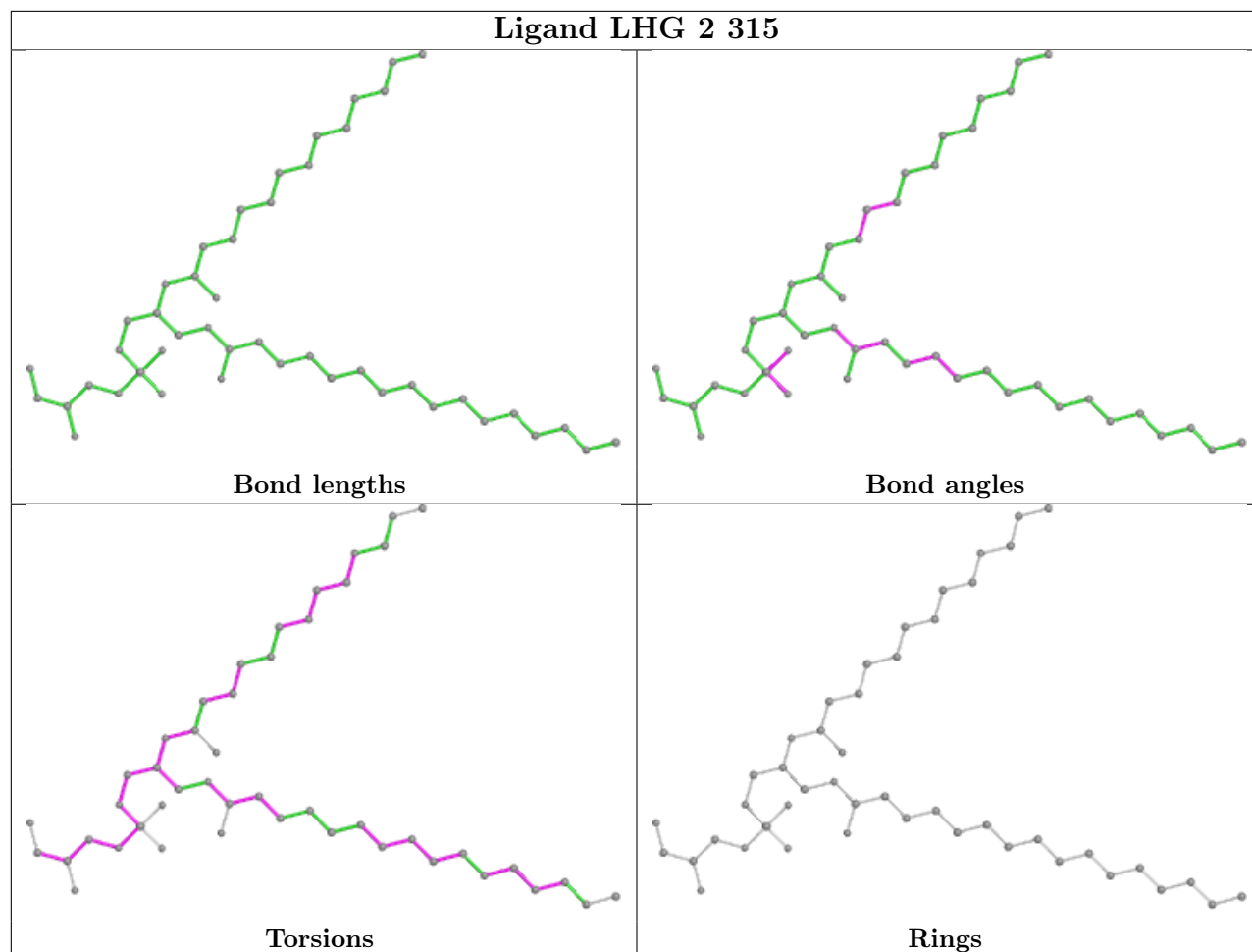




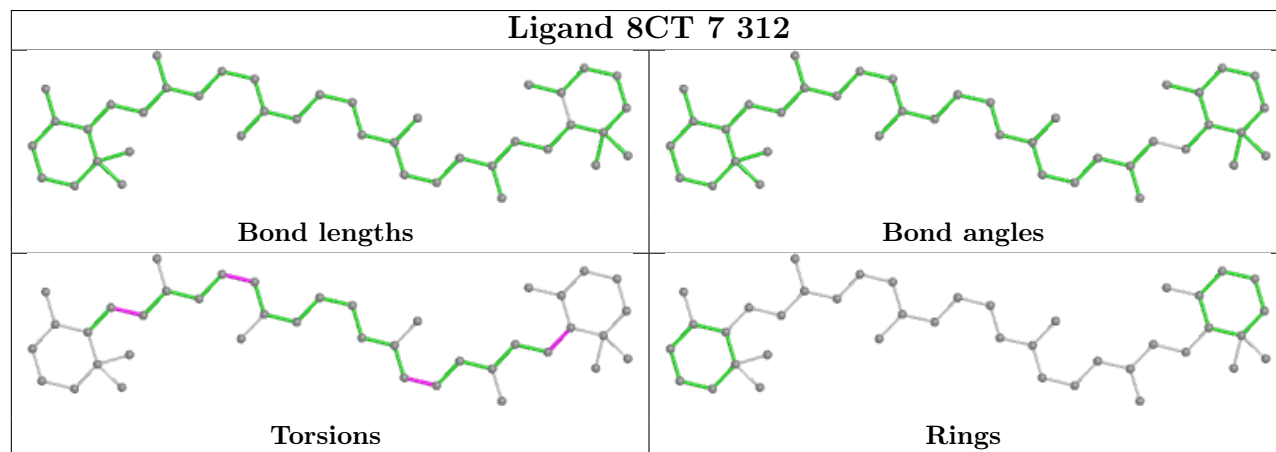




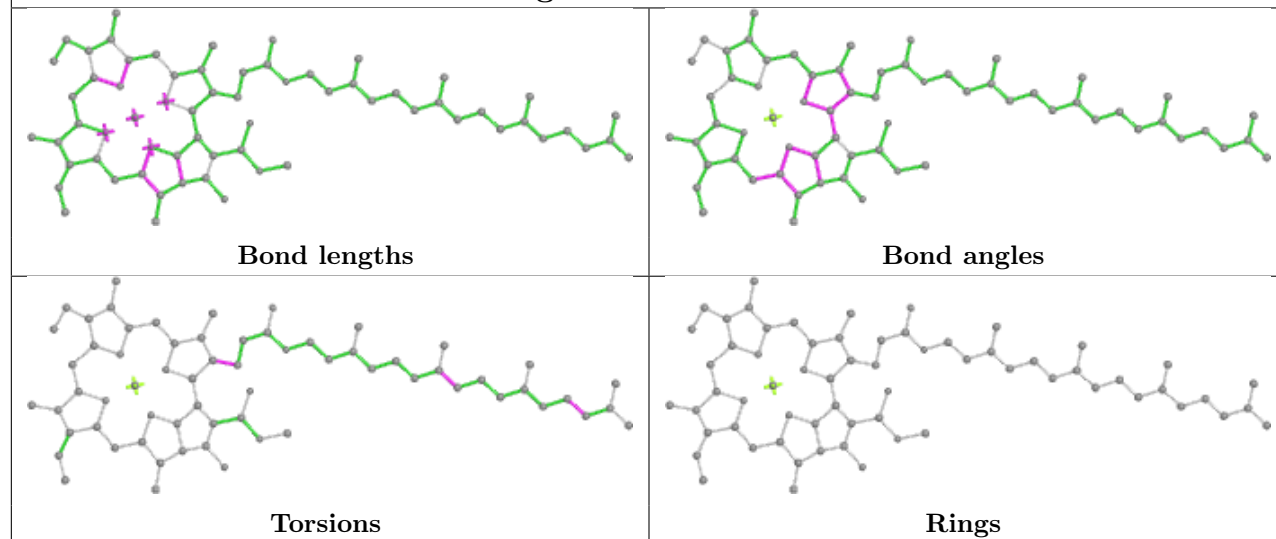
## Ligand LHG 2 315



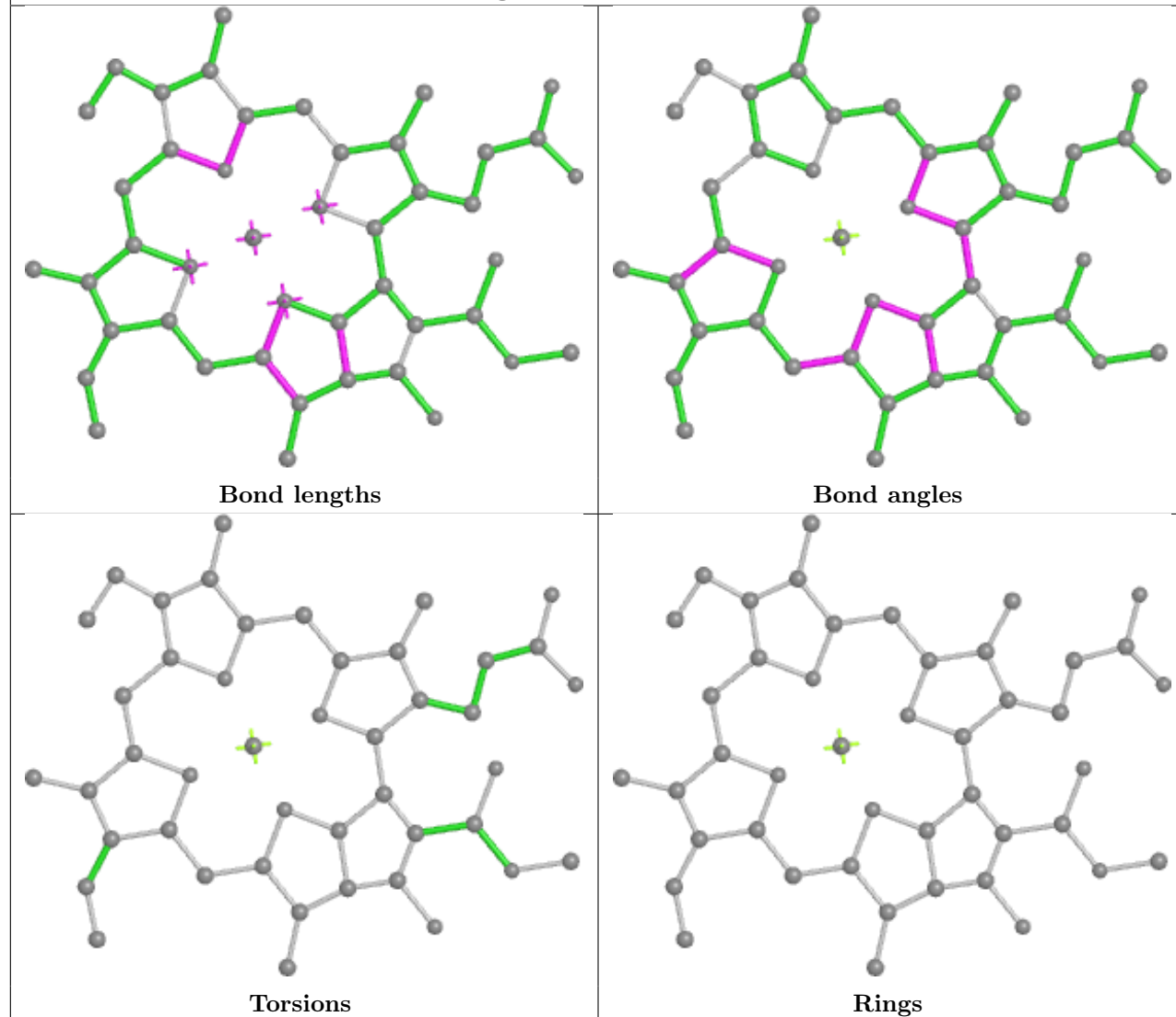
## Ligand 8CT 7 312

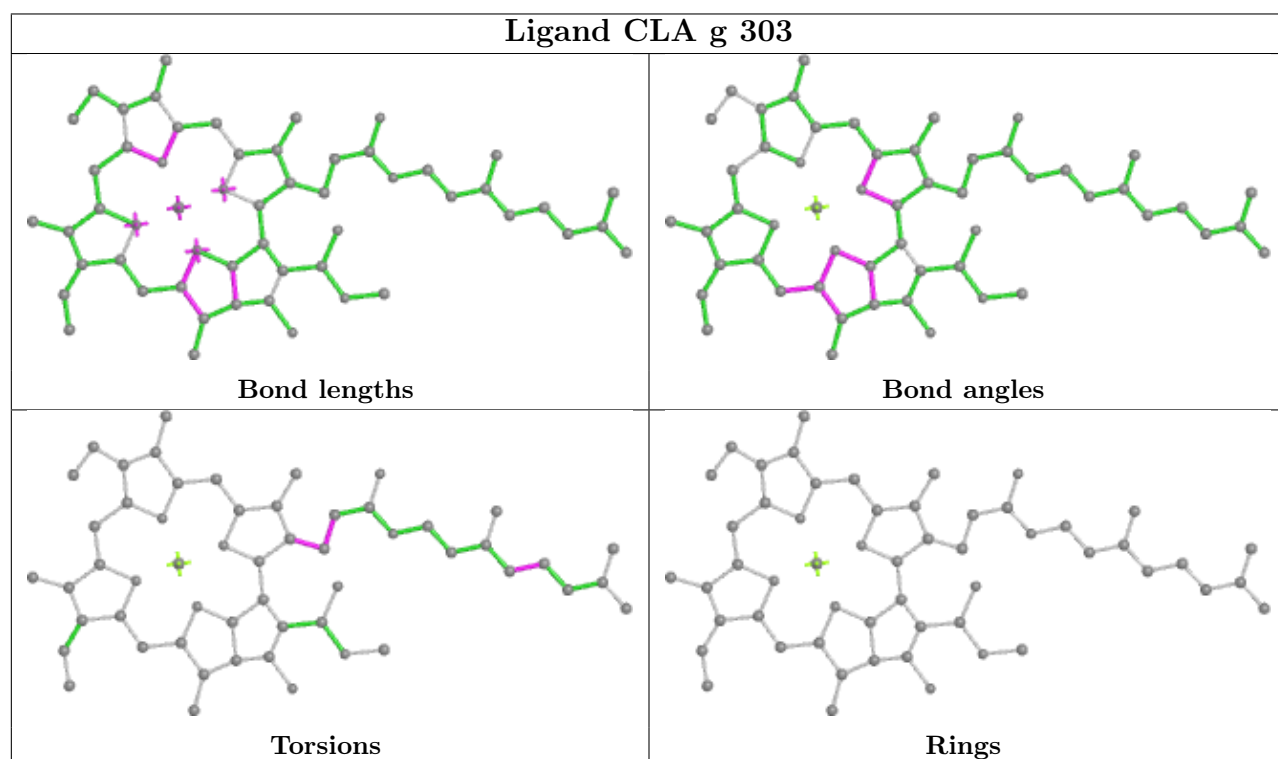
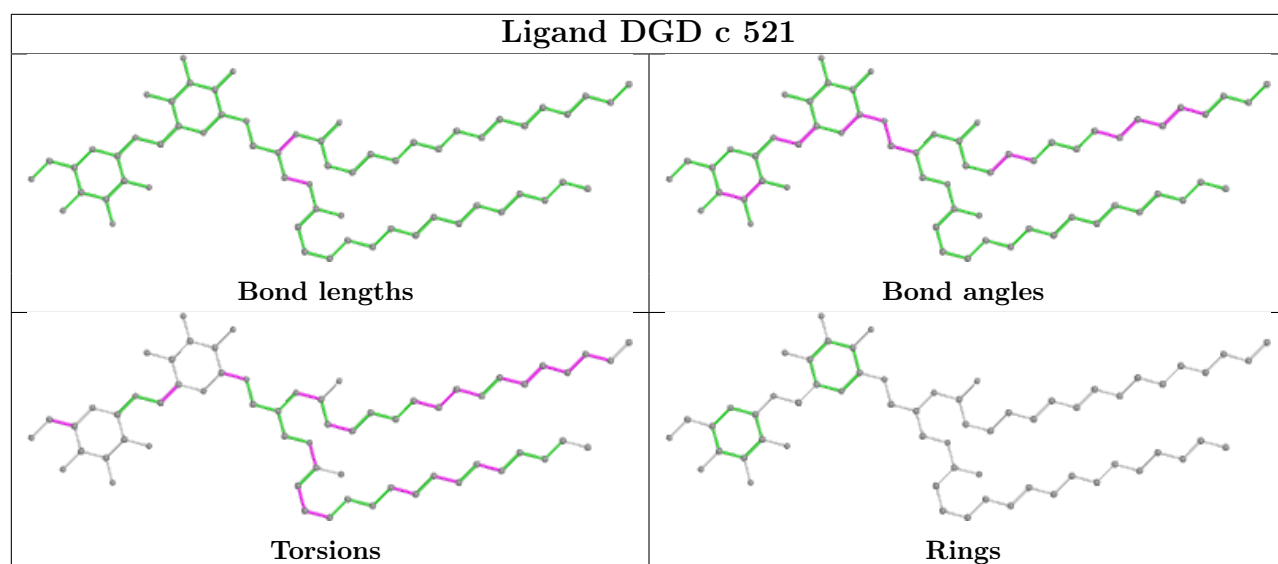


## Ligand CLA 1 307

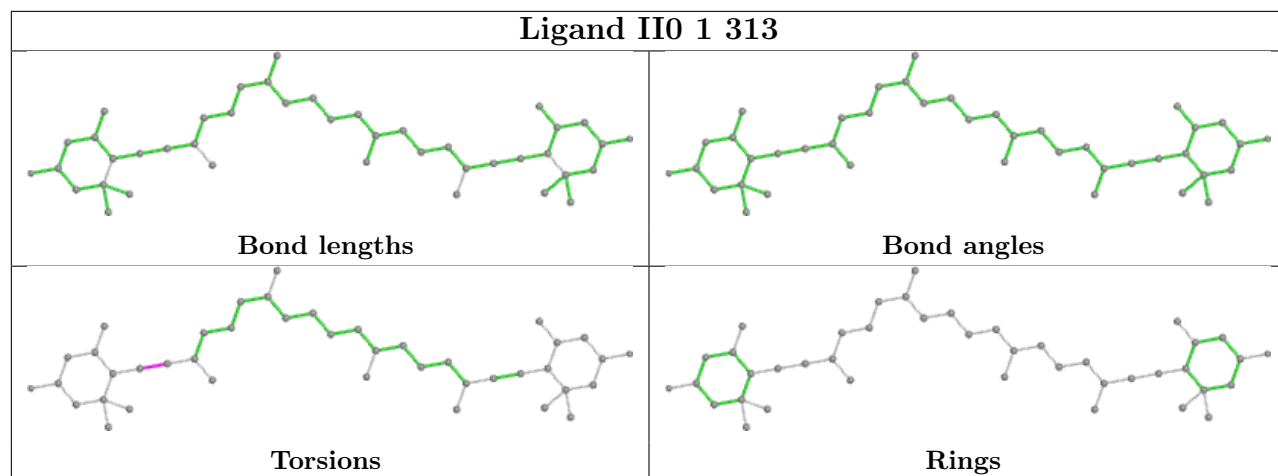


## Ligand CLA 9 304

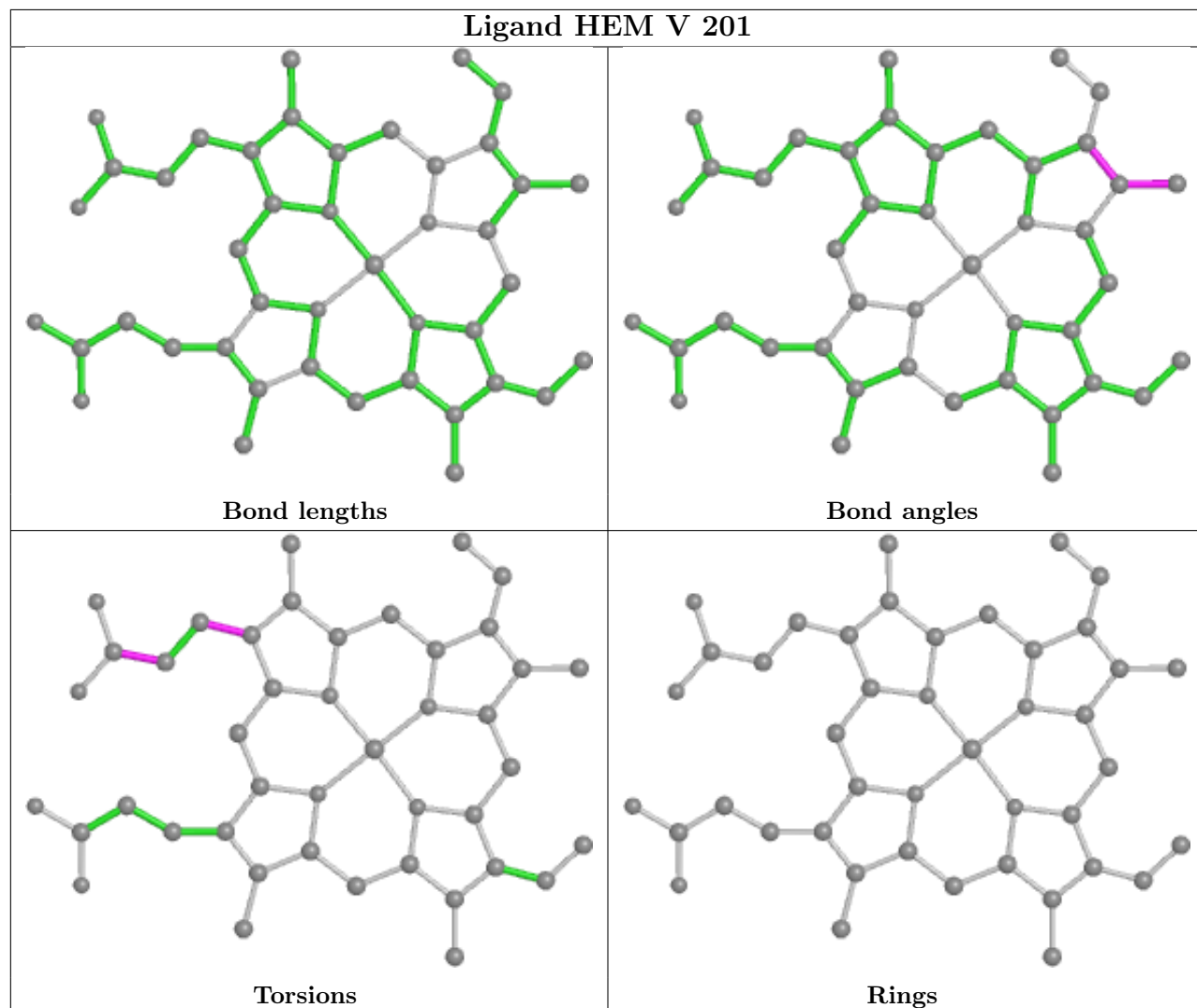




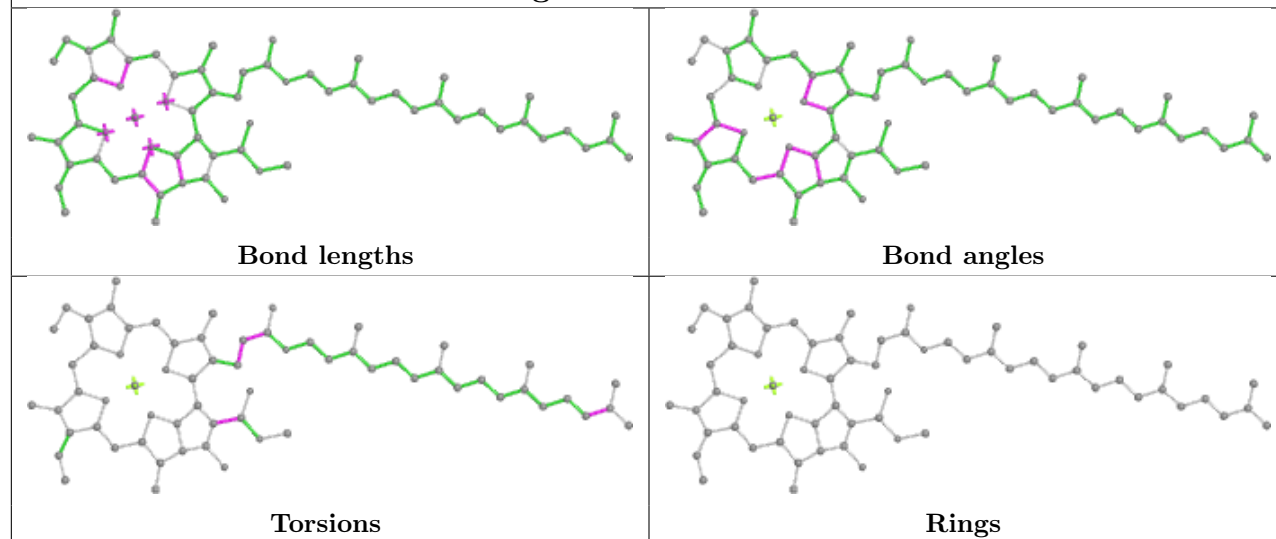
## Ligand II0 1 313



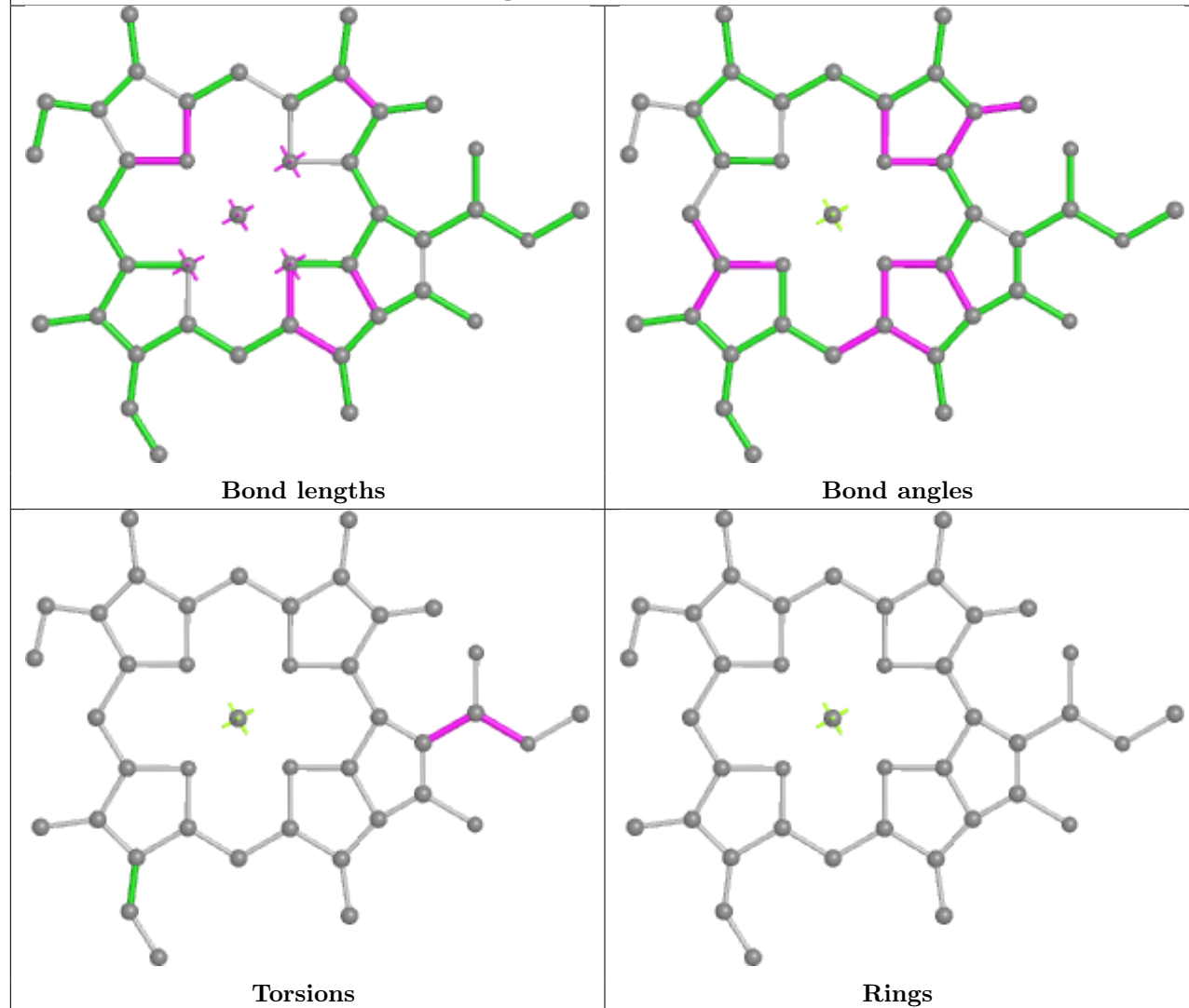
## Ligand HEM V 201



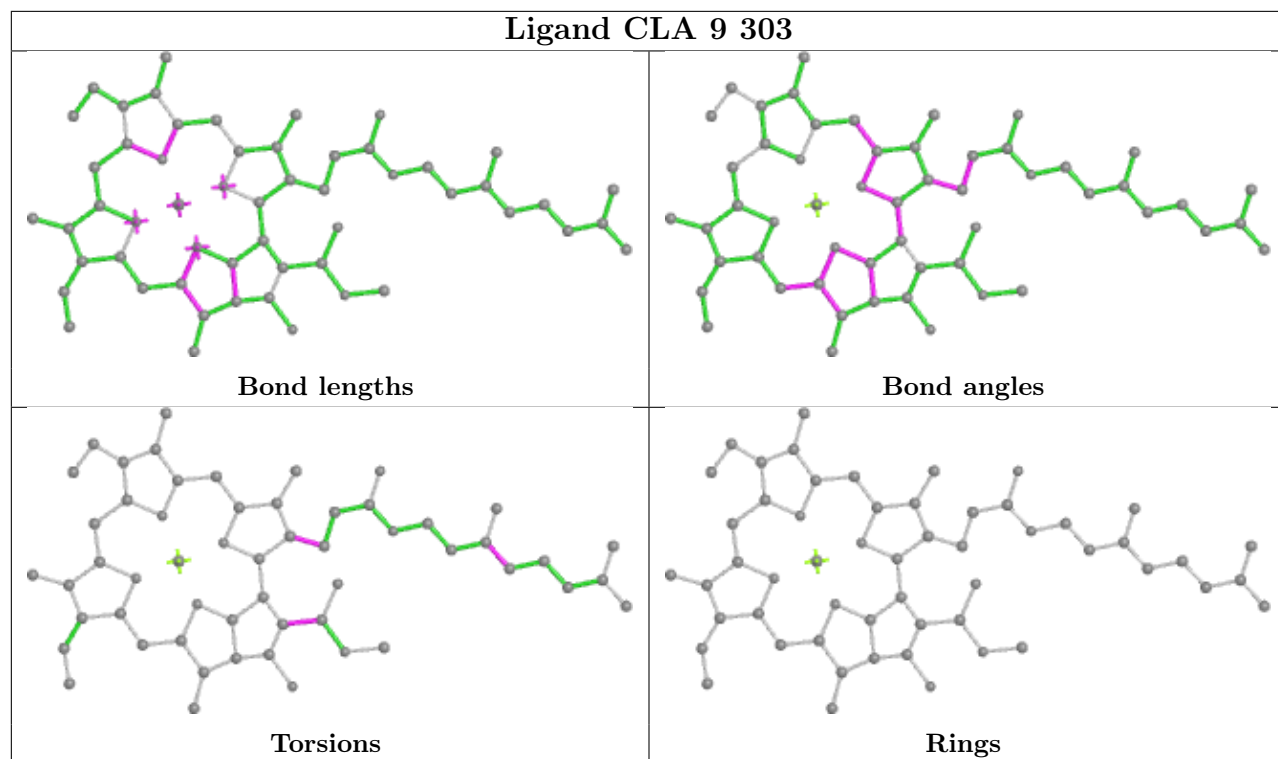
## Ligand CLA C 503



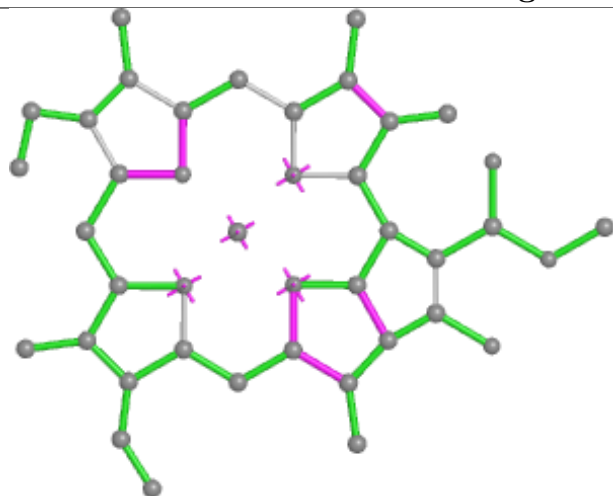
## Ligand CLA 4 301



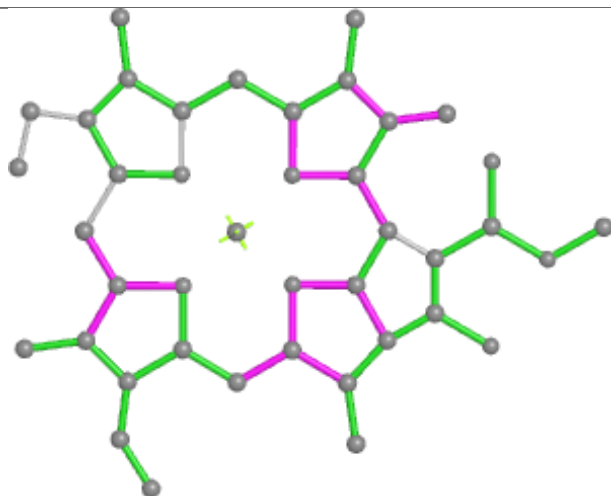




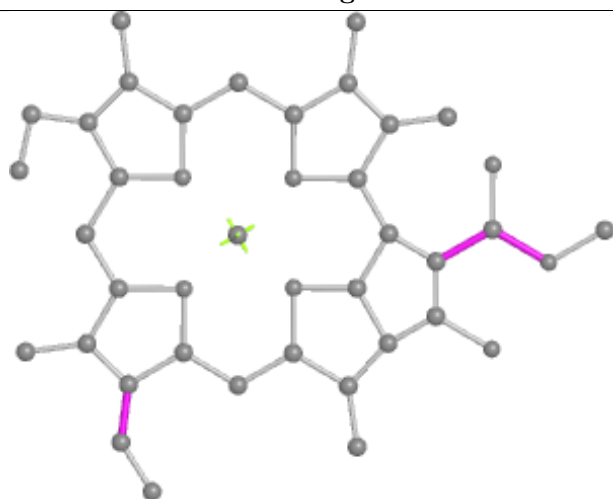
## Ligand CLA 6 310



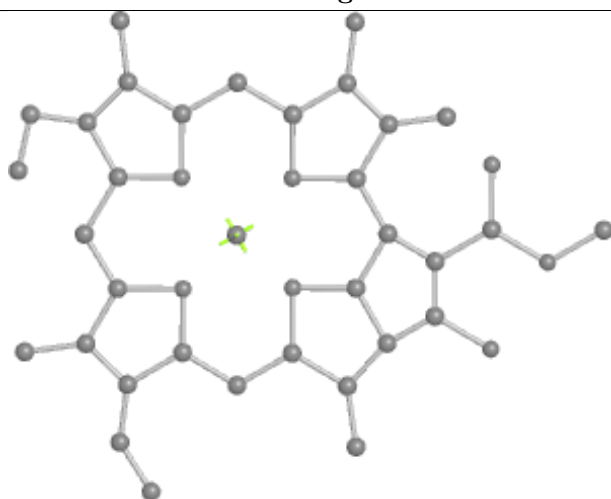
Bond lengths



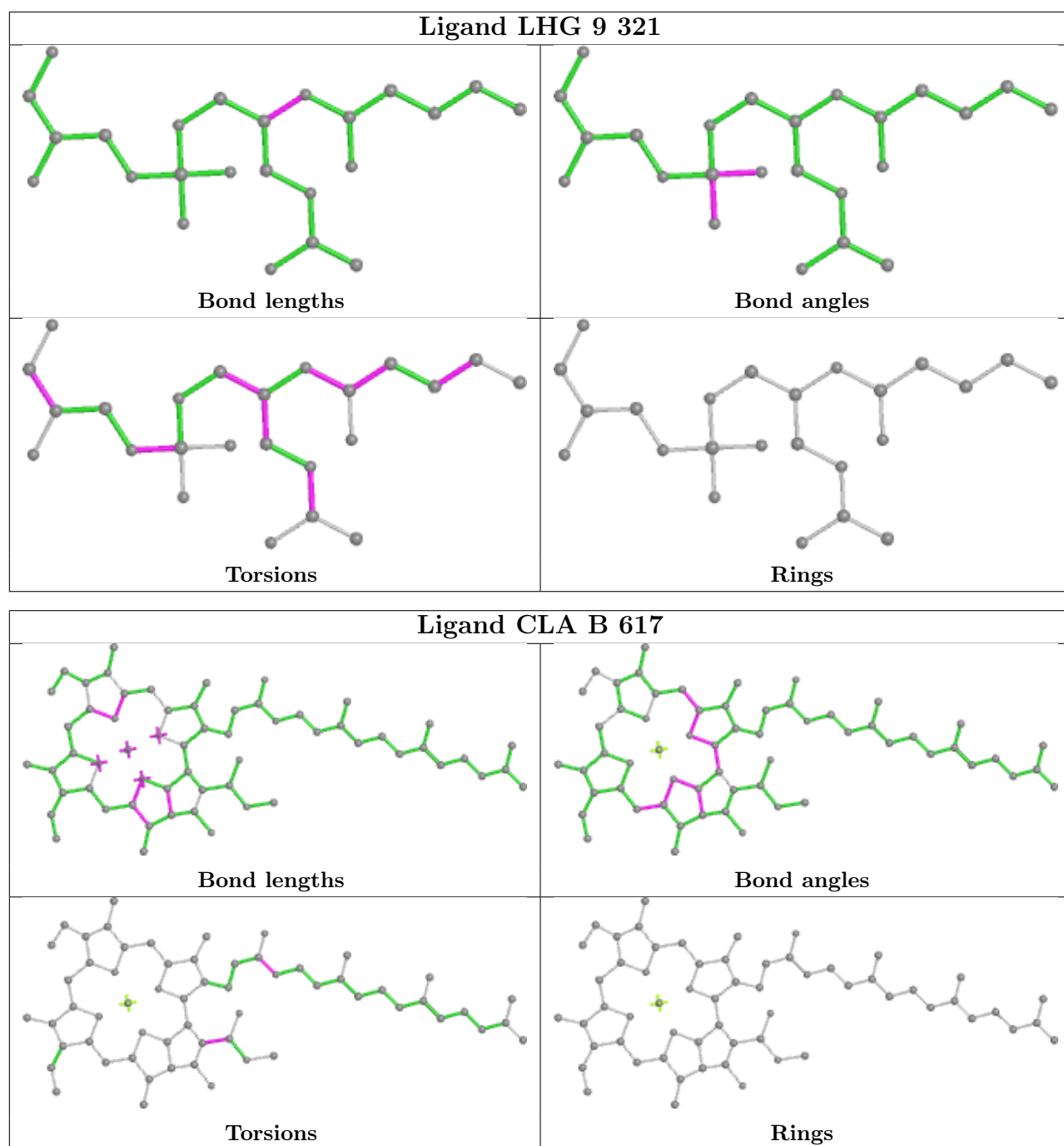
Bond angles



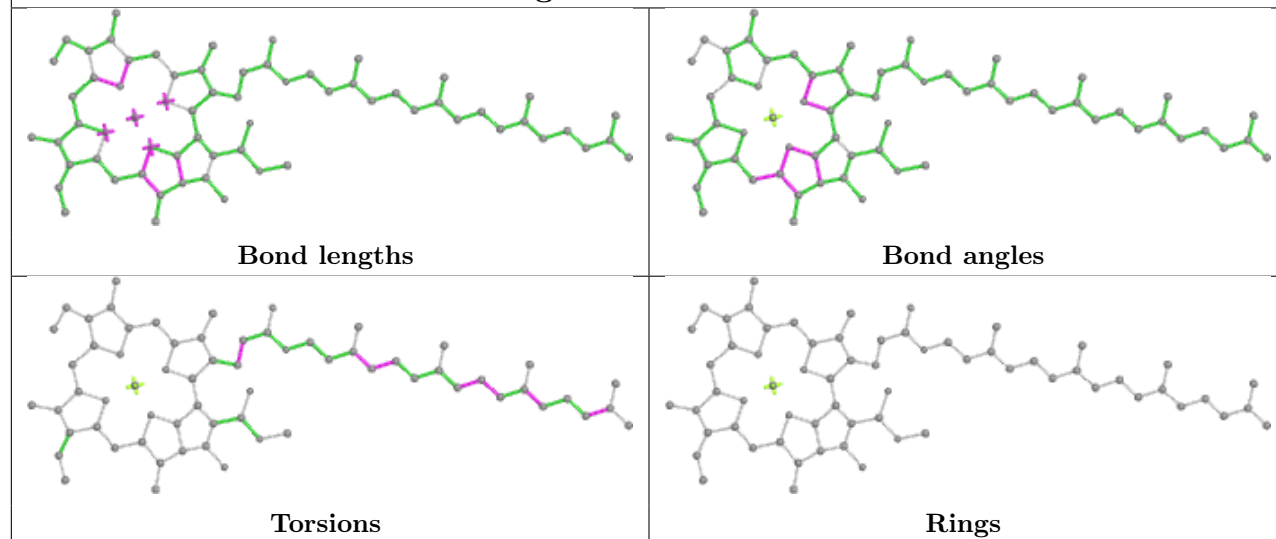
Torsions



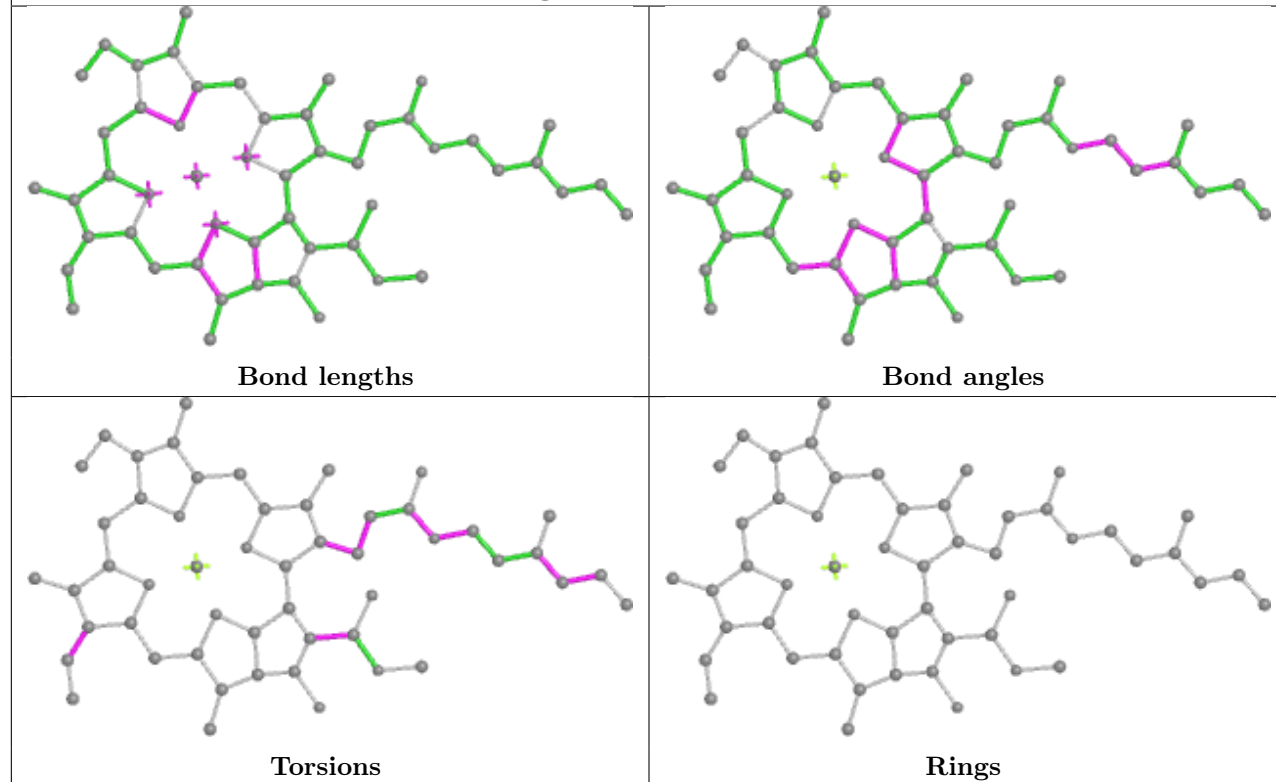
Rings

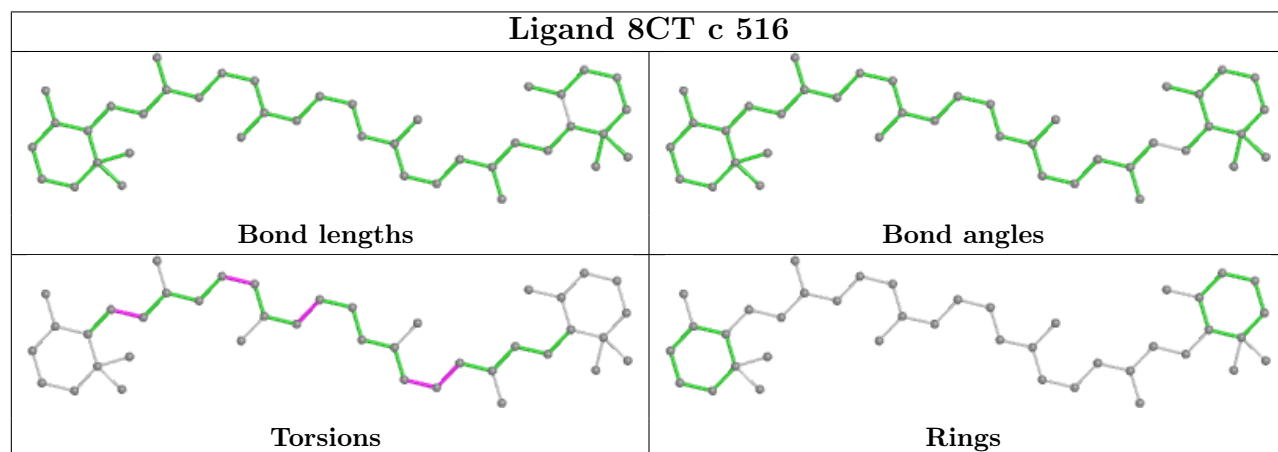
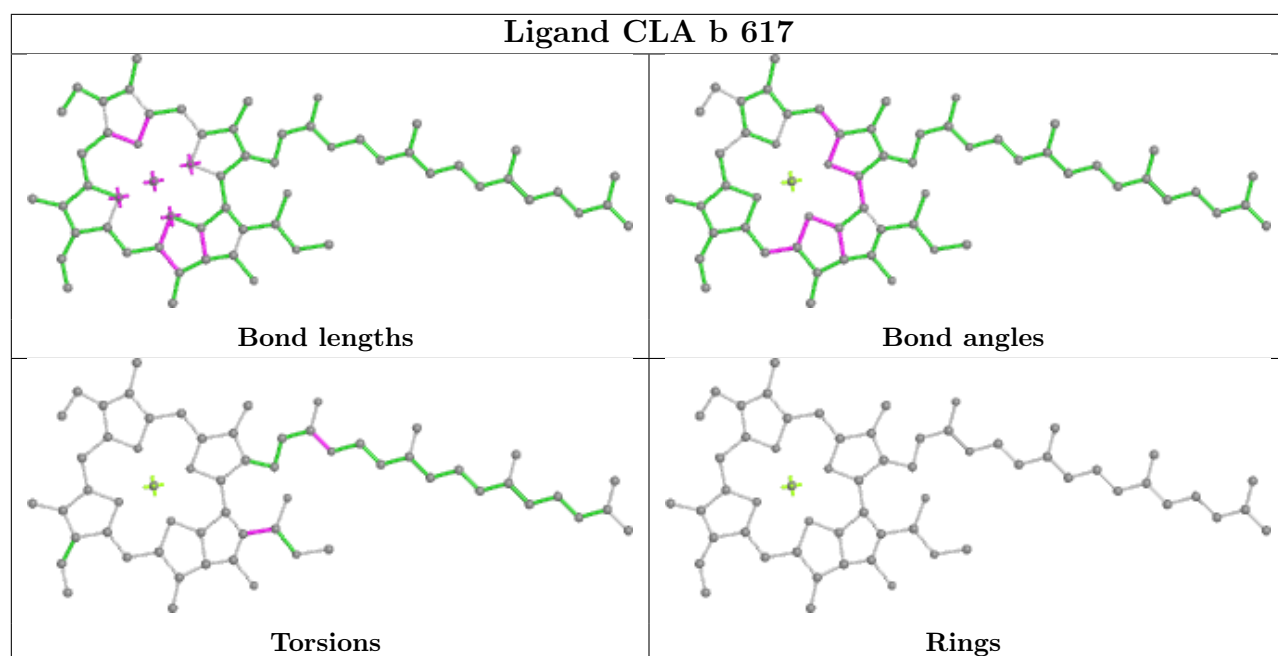


## Ligand CLA b 607

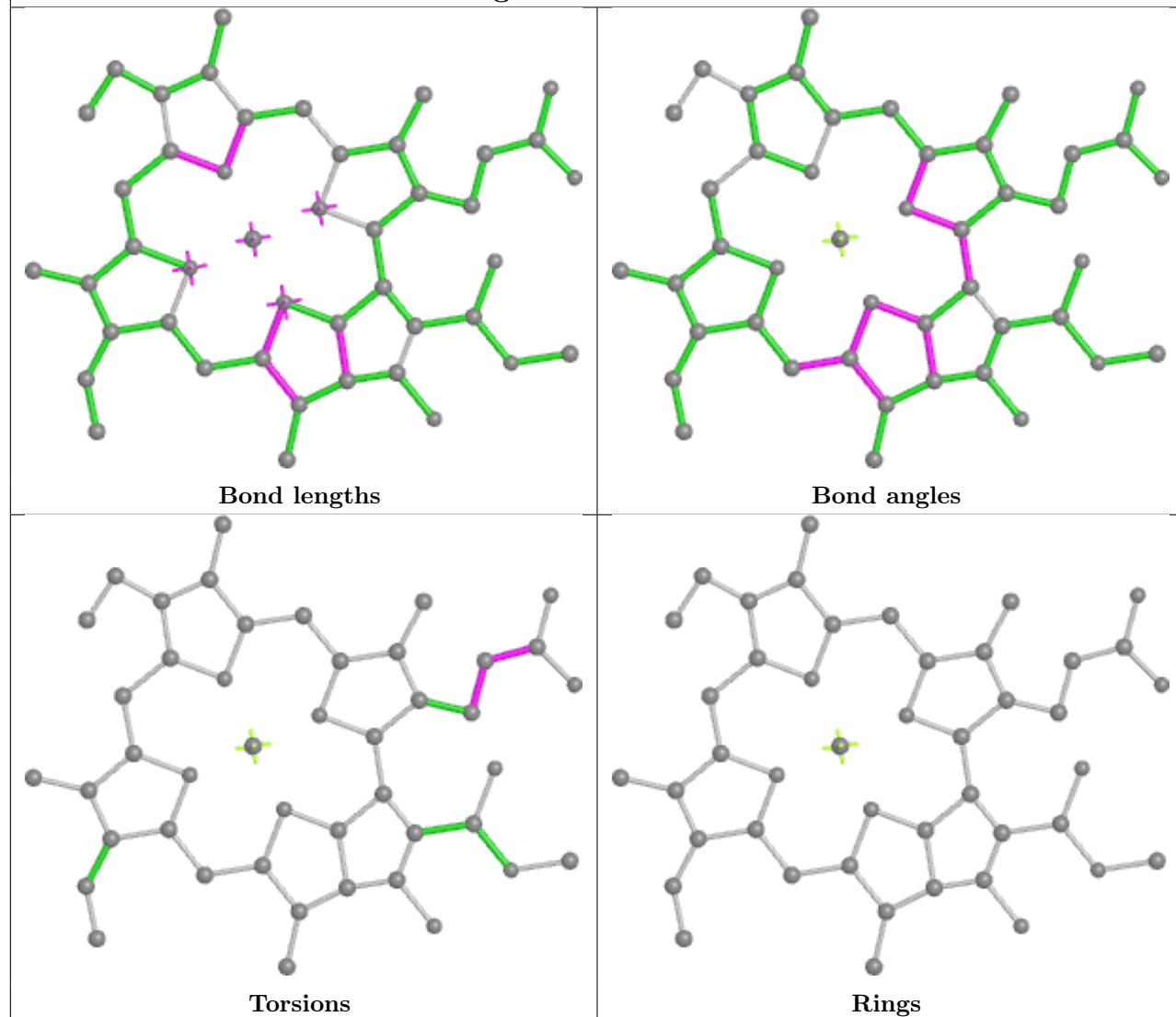


## Ligand CLA 8 303

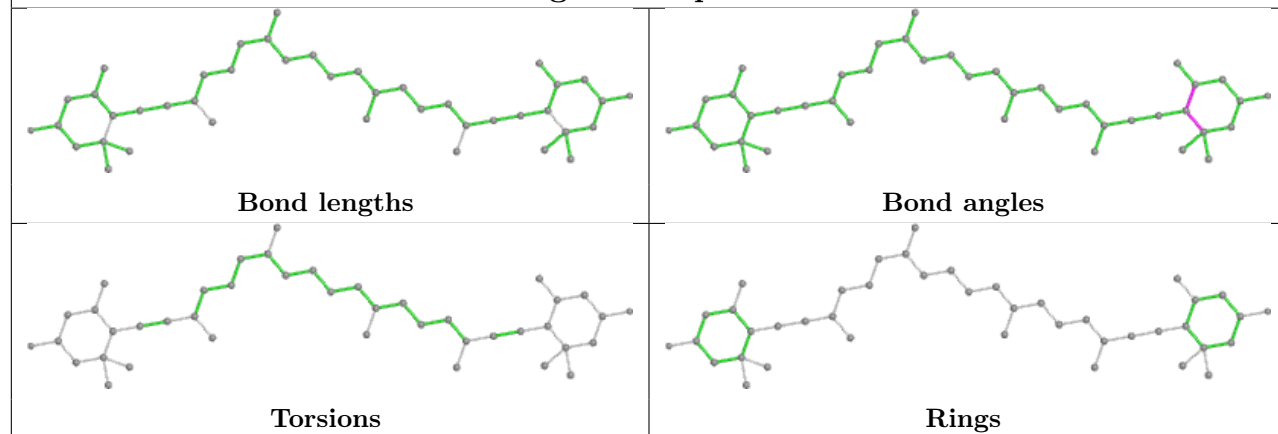


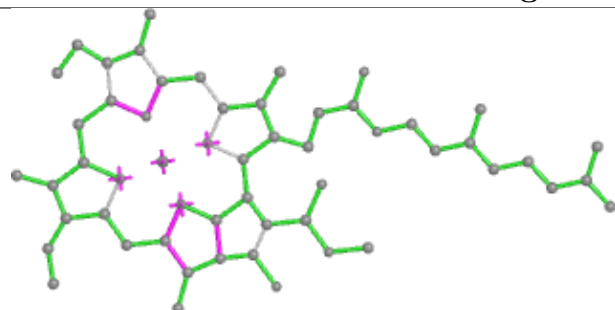


## Ligand CLA 5 304

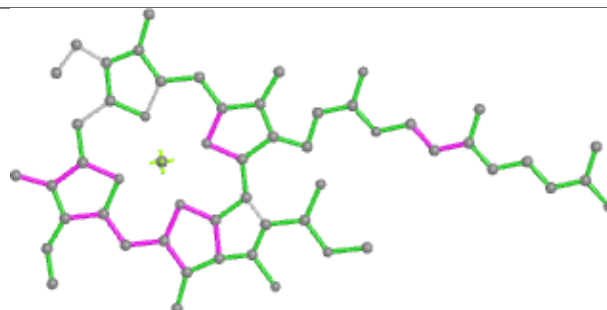


## Ligand II0 p 314

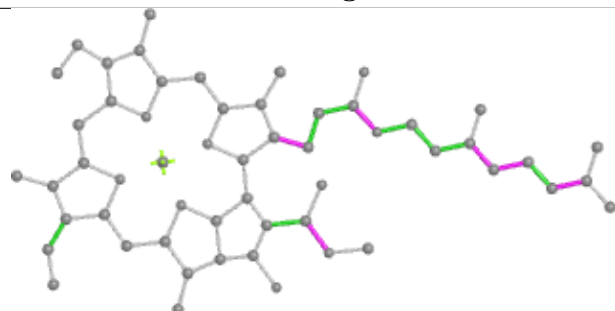


**Ligand CLA 0 307**

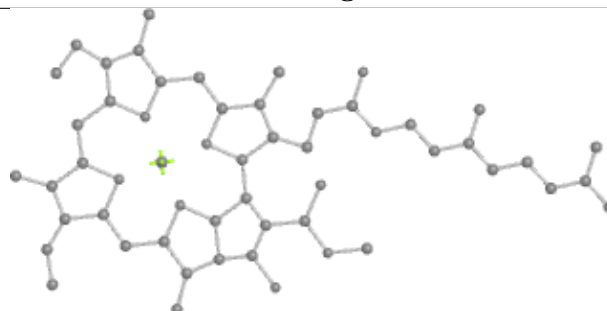
Bond lengths



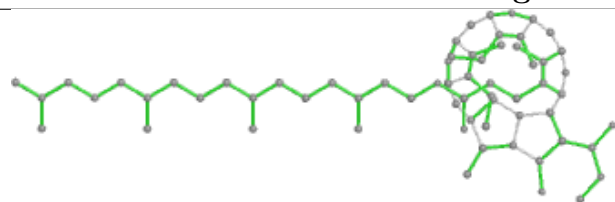
Bond angles



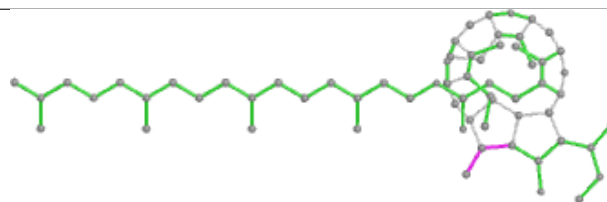
Torsions



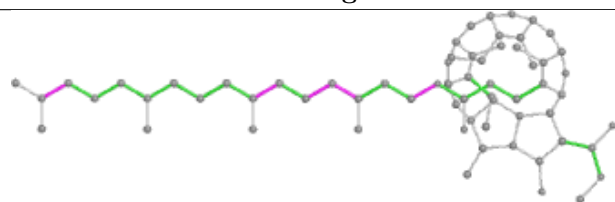
Rings

**Ligand PHO D 403**

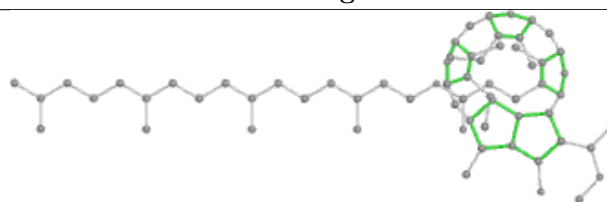
Bond lengths



Bond angles

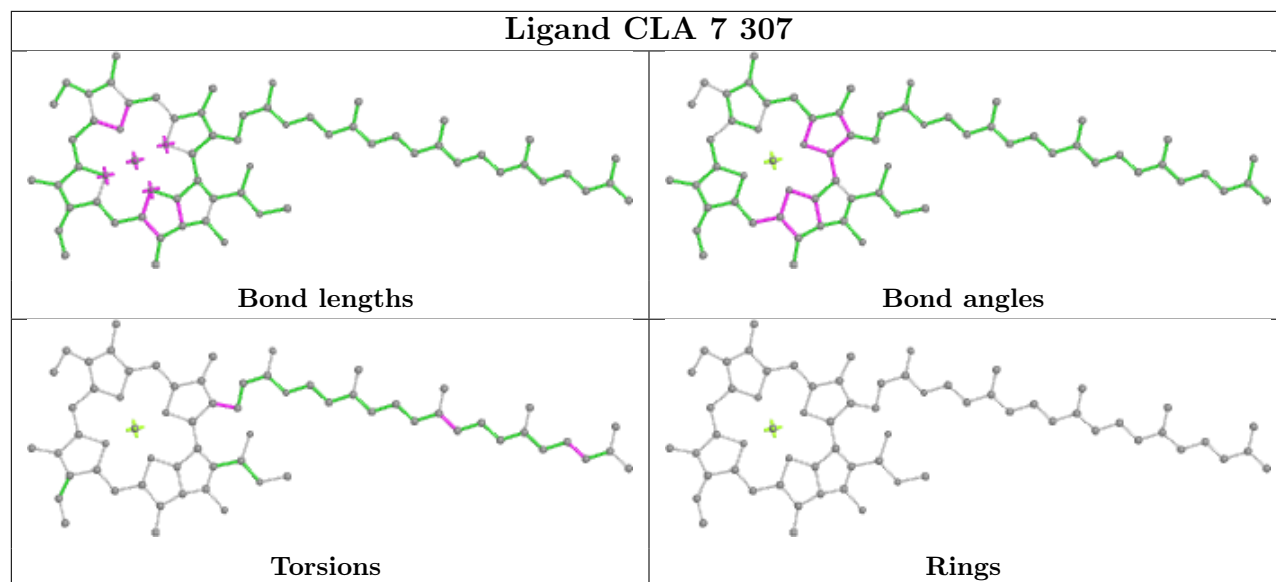


Torsions

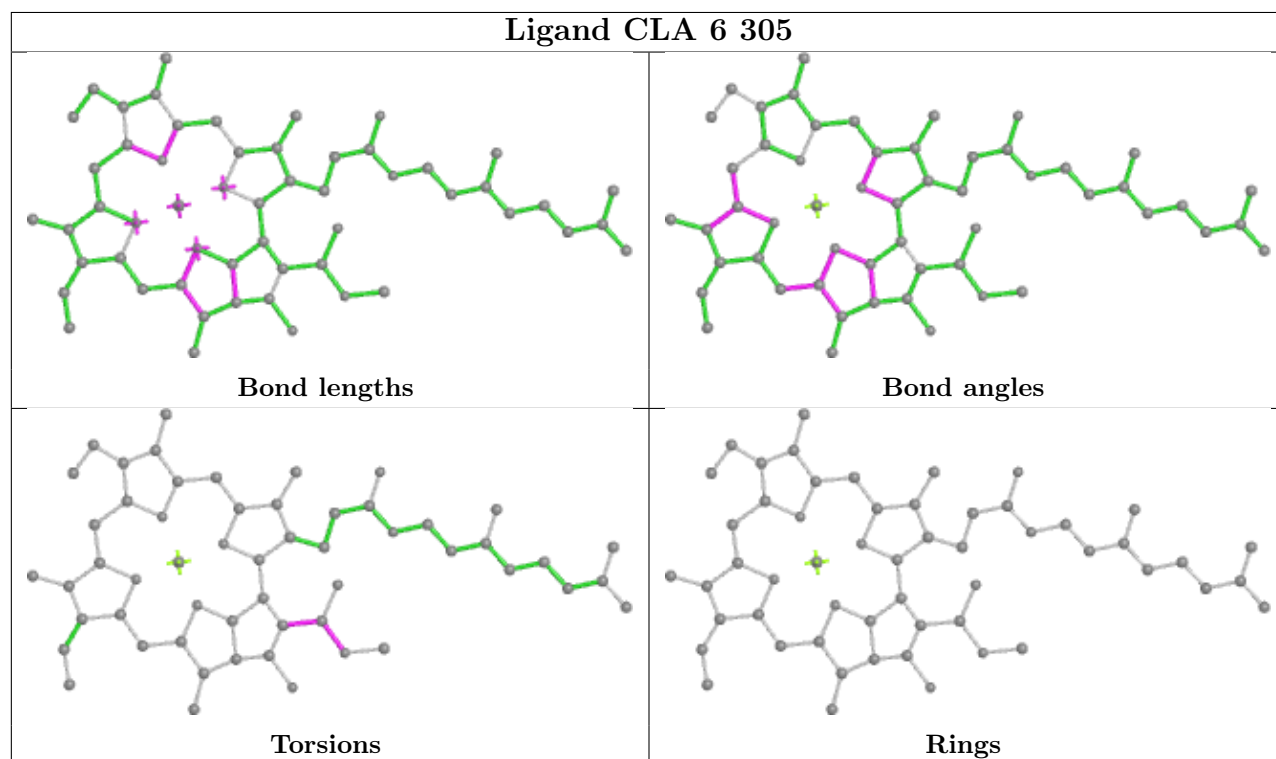


Rings

## Ligand CLA 7 307

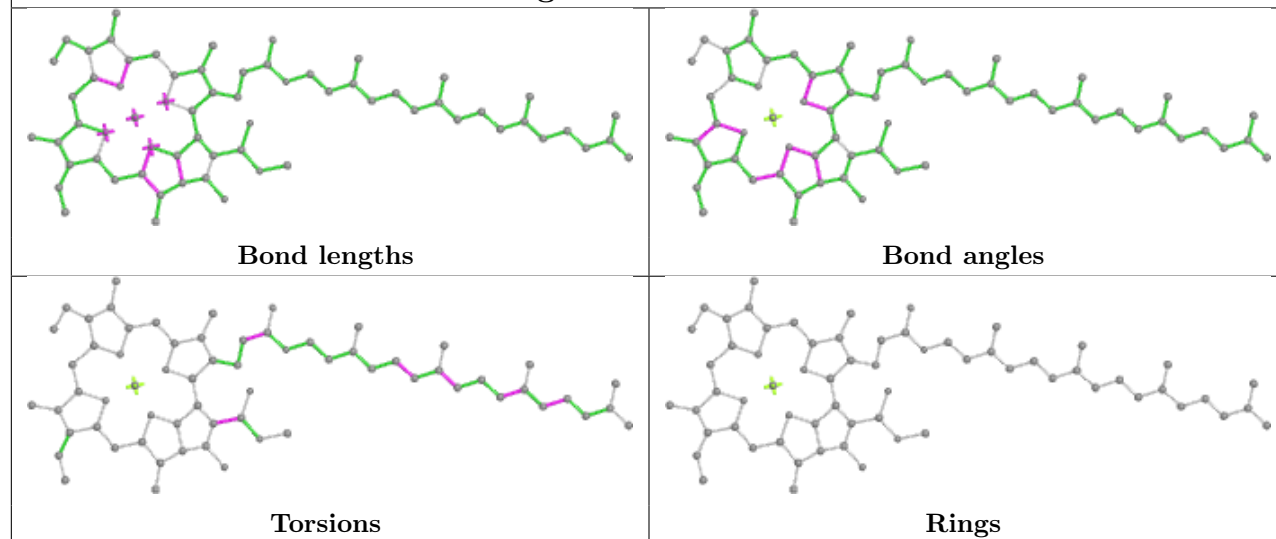


## Ligand CLA 6 305

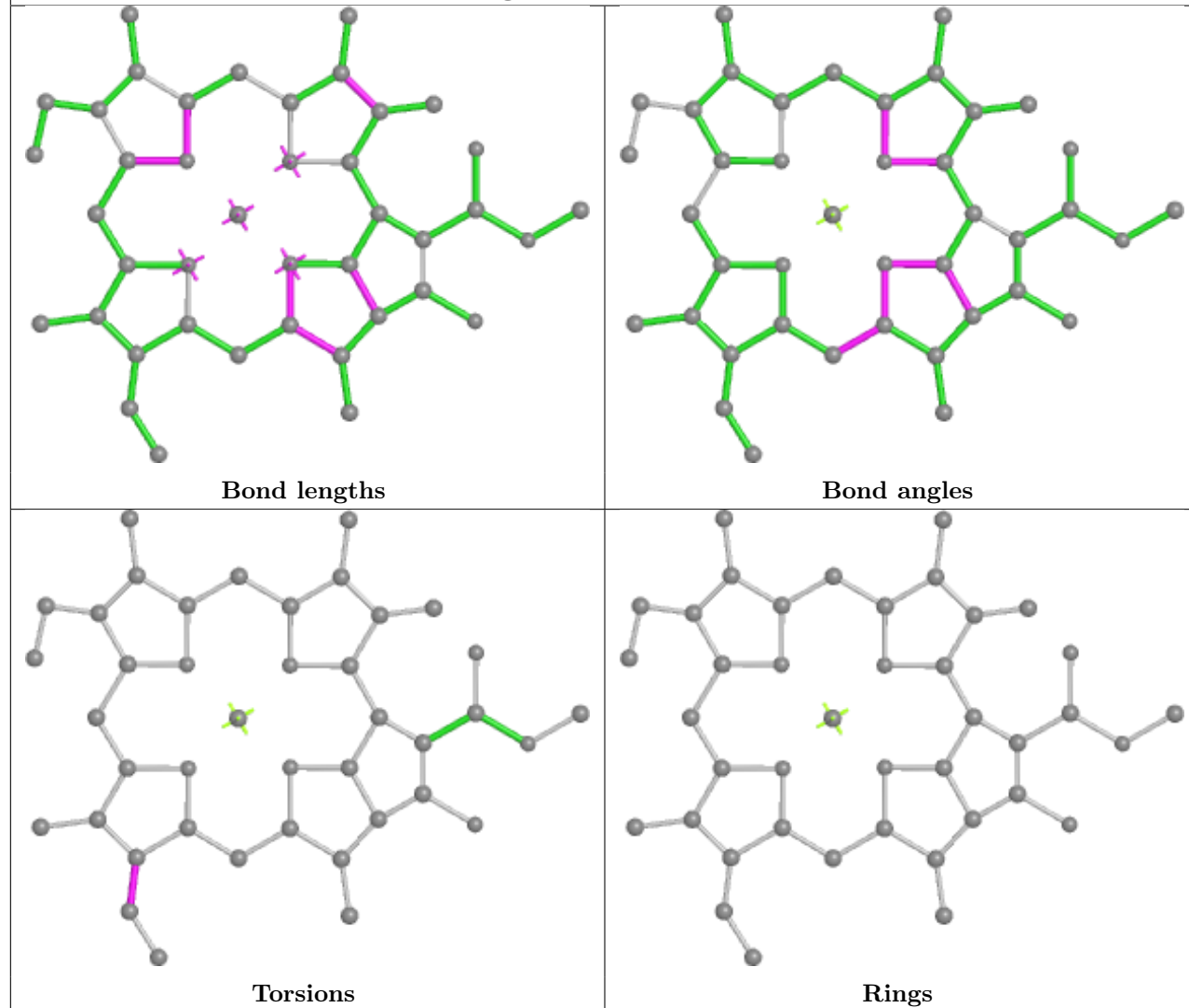


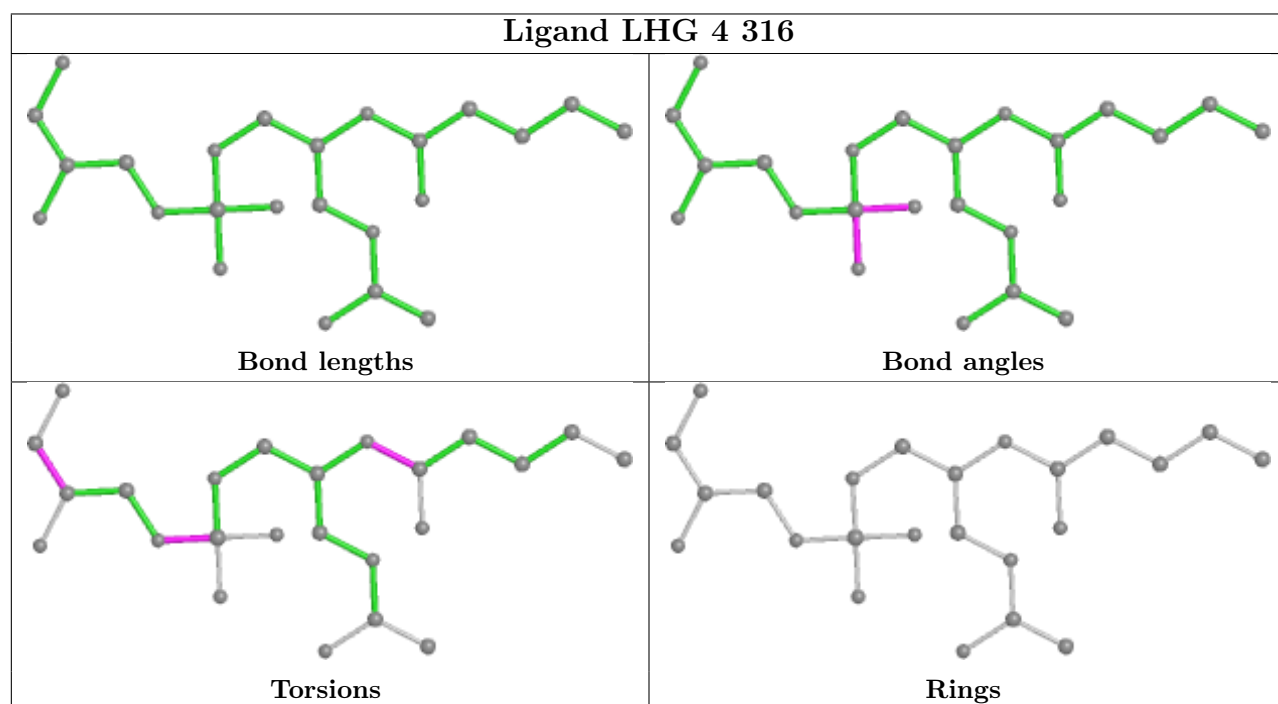
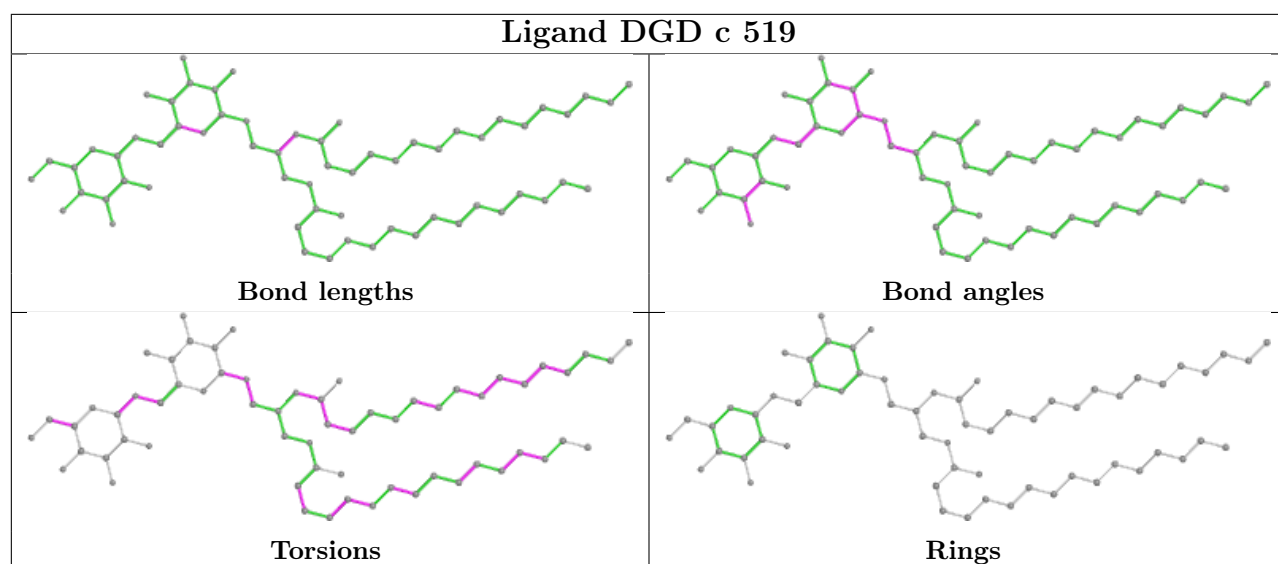


## Ligand CLA c 511

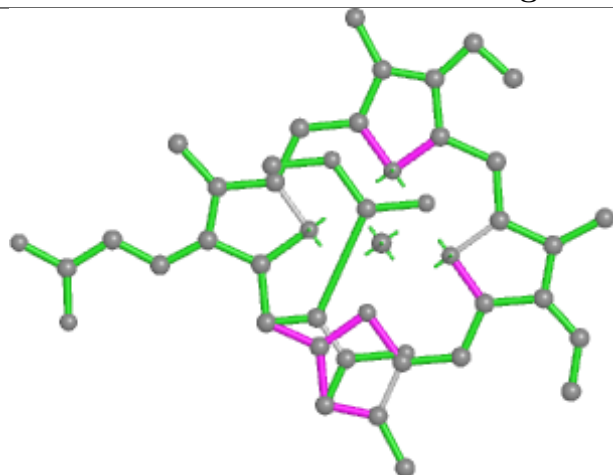


## Ligand CLA 9 310

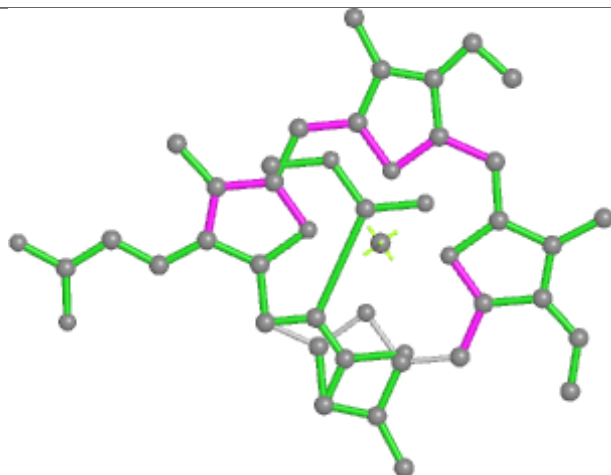




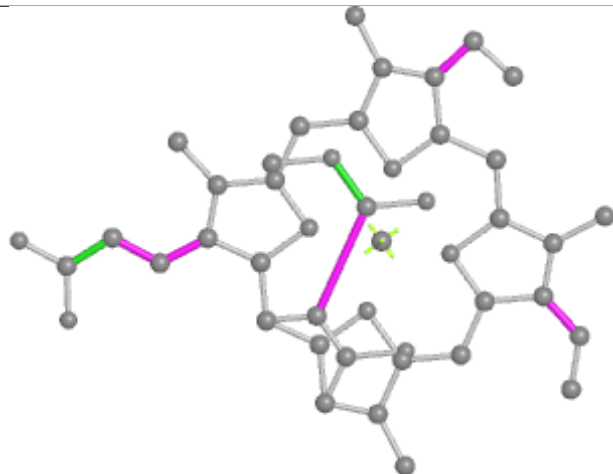
## Ligand KC2 8 309



Bond lengths



Bond angles

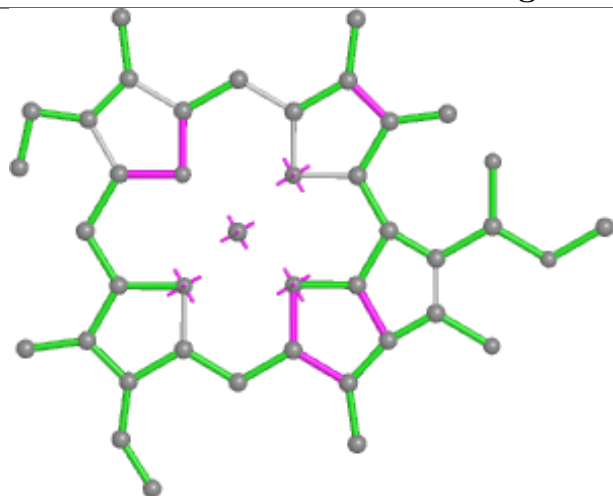


Torsions

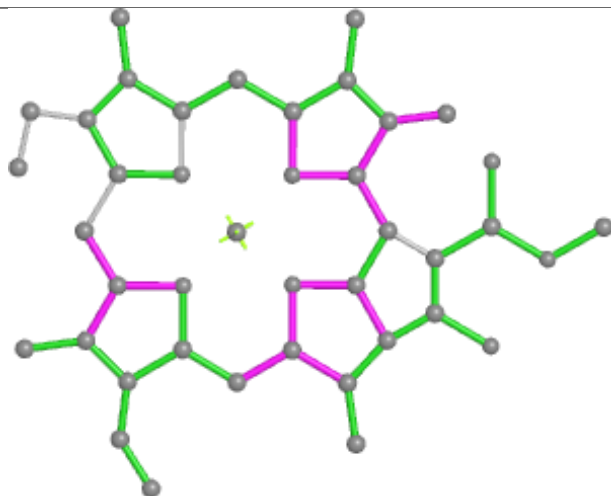


Rings

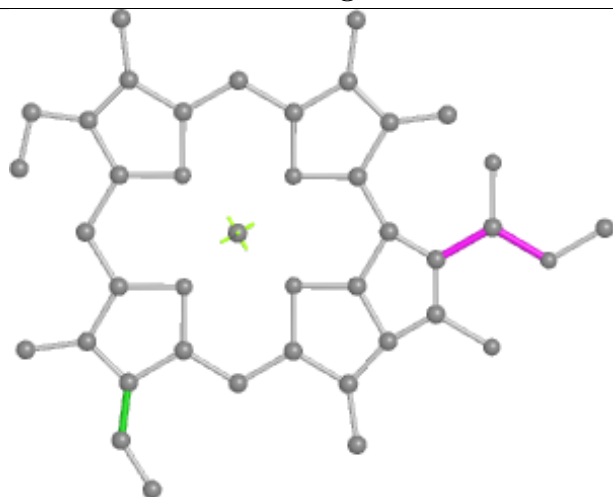
## Ligand CLA 6 313



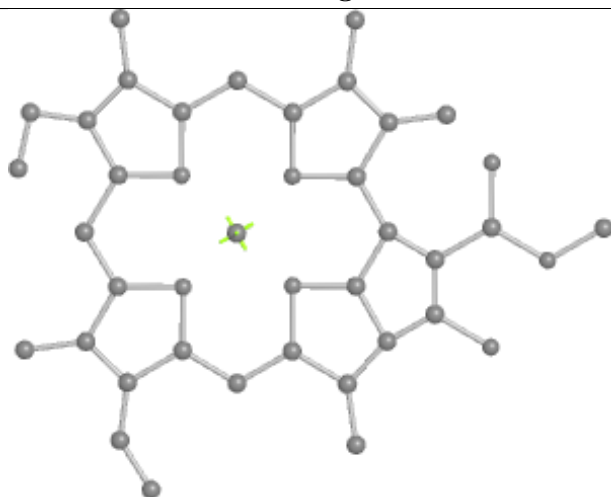
Bond lengths



Bond angles

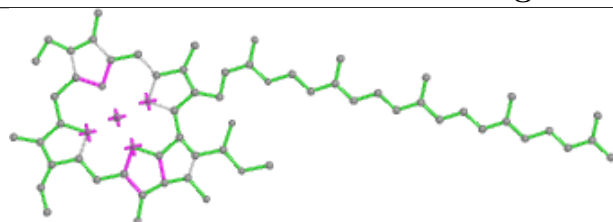


Torsions

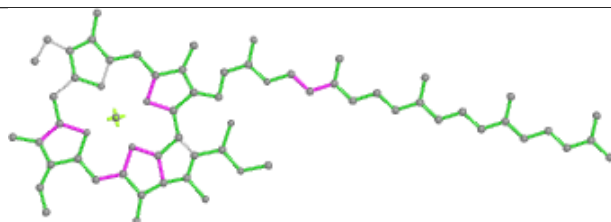


Rings

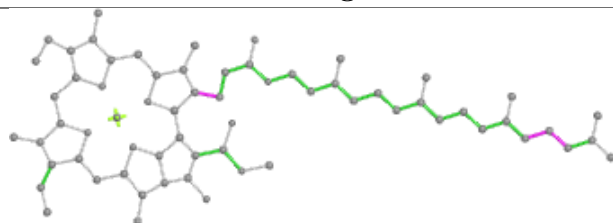
## Ligand CLA B 612



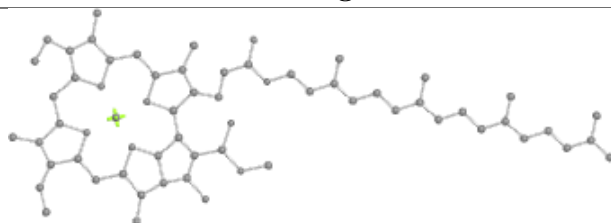
Bond lengths



Bond angles

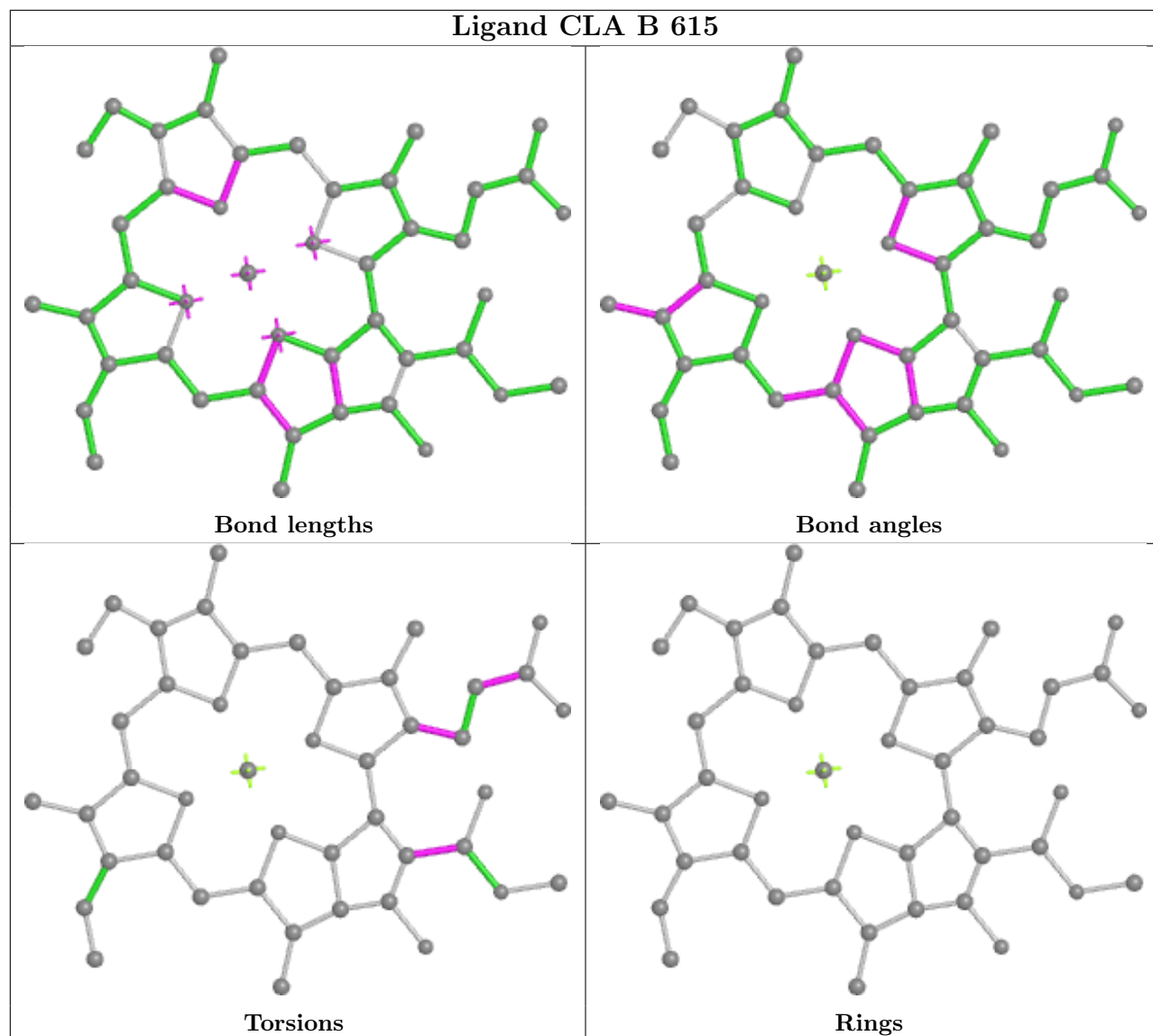


Torsions

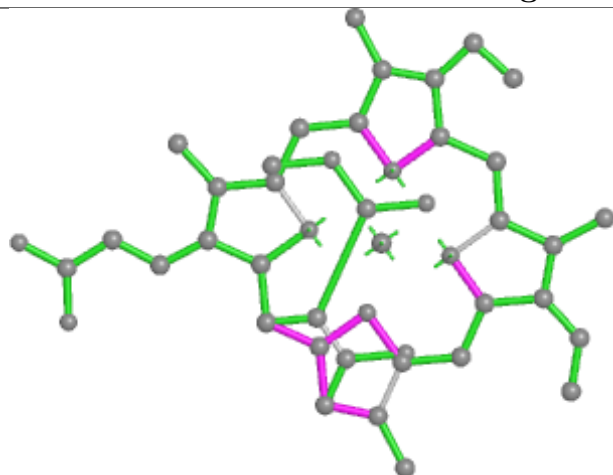


Rings

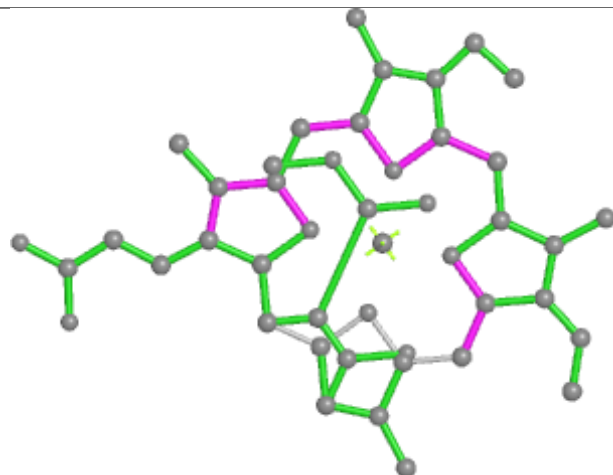
## Ligand CLA B 615



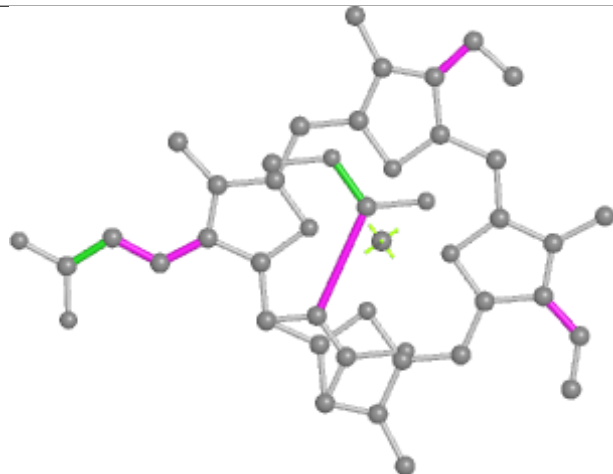
## Ligand KC2 2 309



Bond lengths



Bond angles

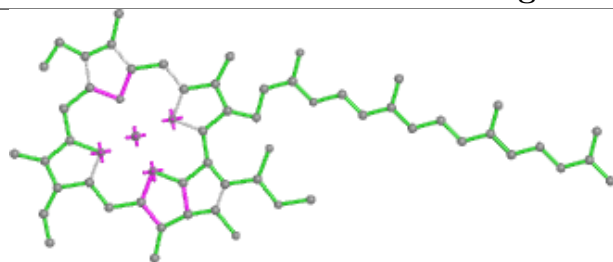


Torsions

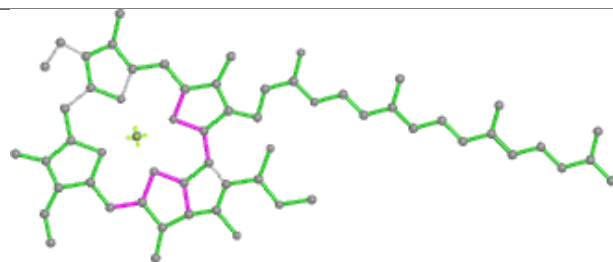


Rings

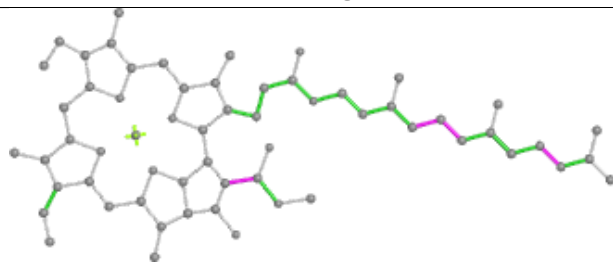
## Ligand CLA 1 306



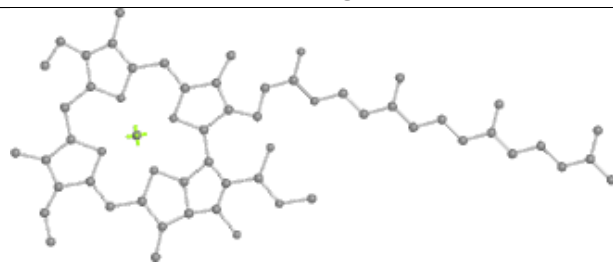
Bond lengths



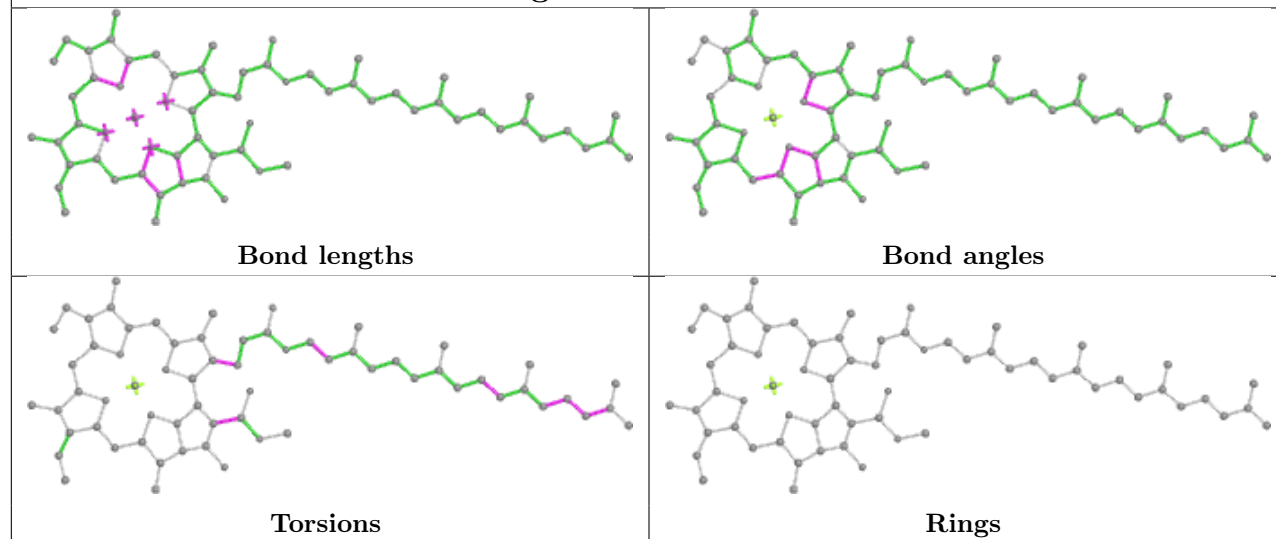
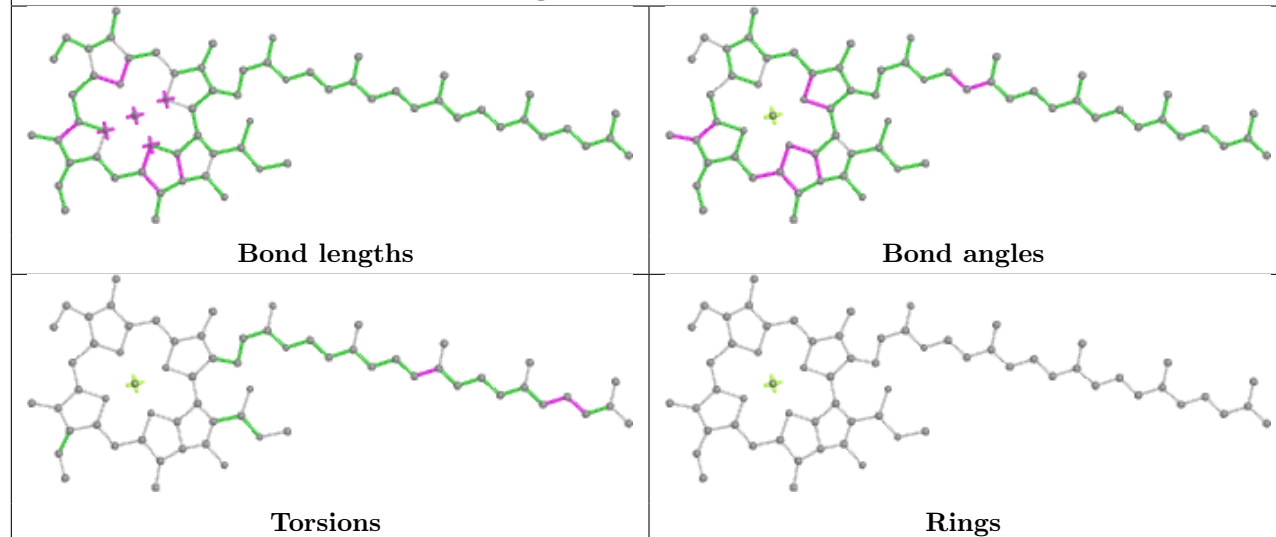
Bond angles

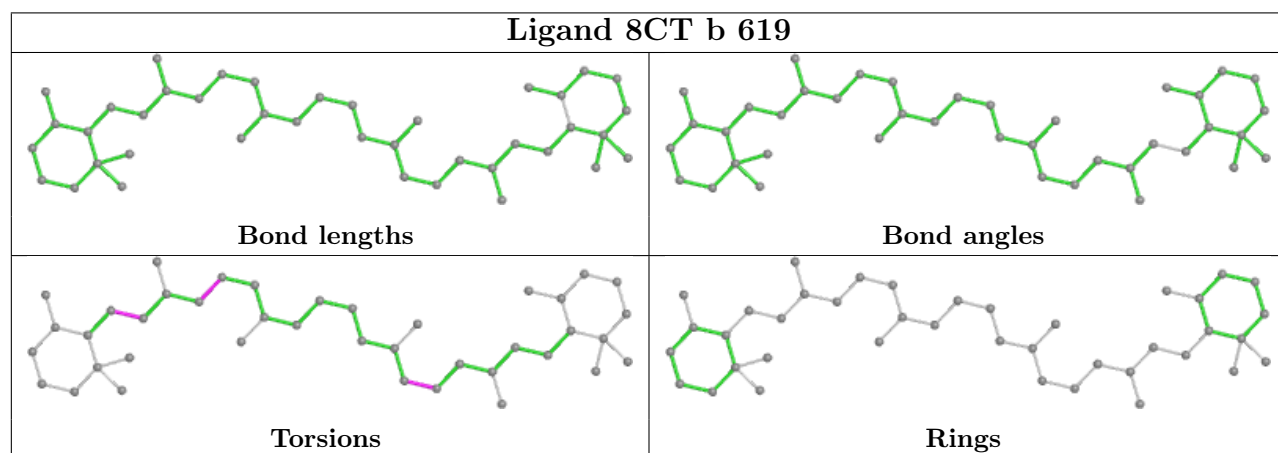
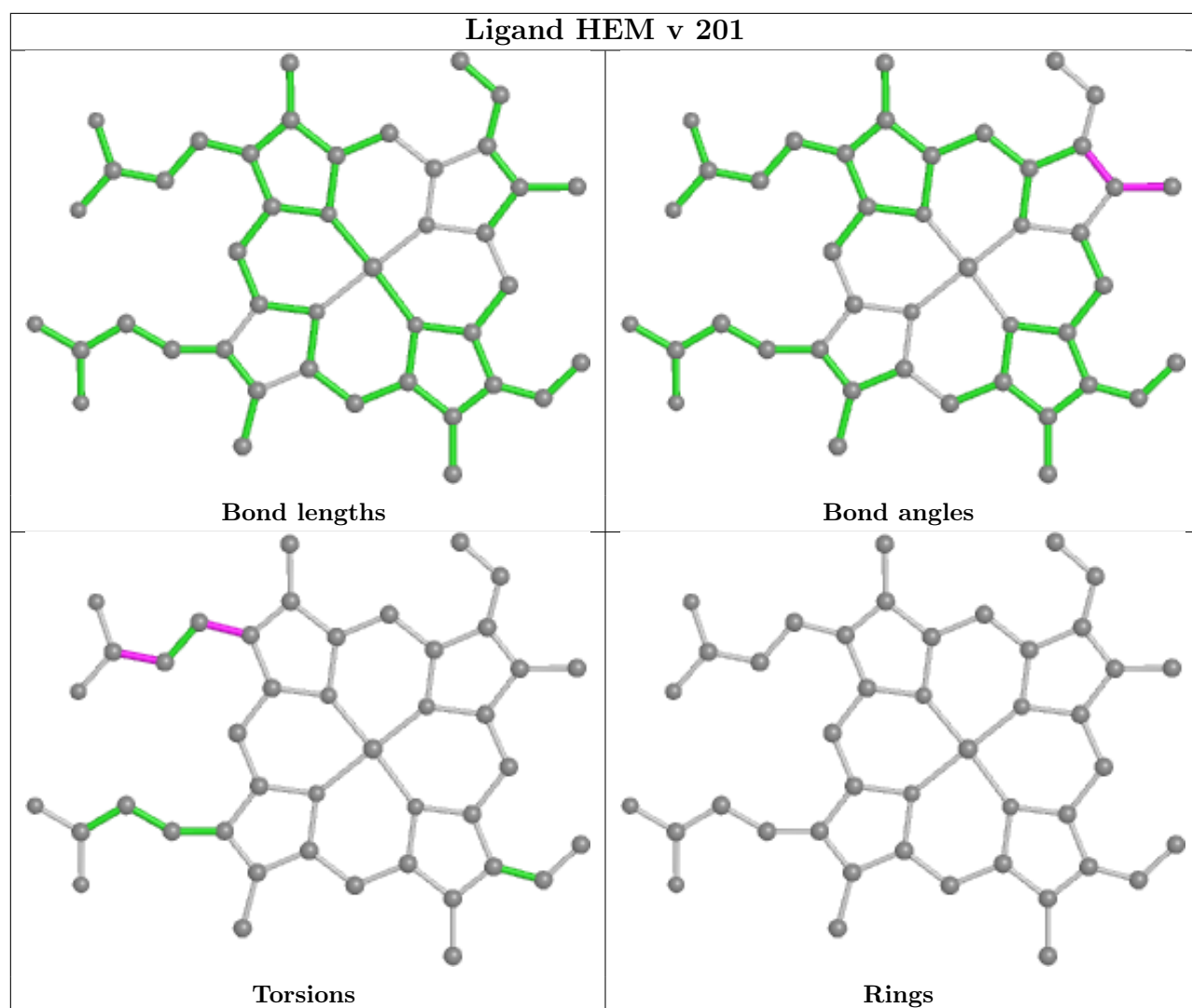


Torsions



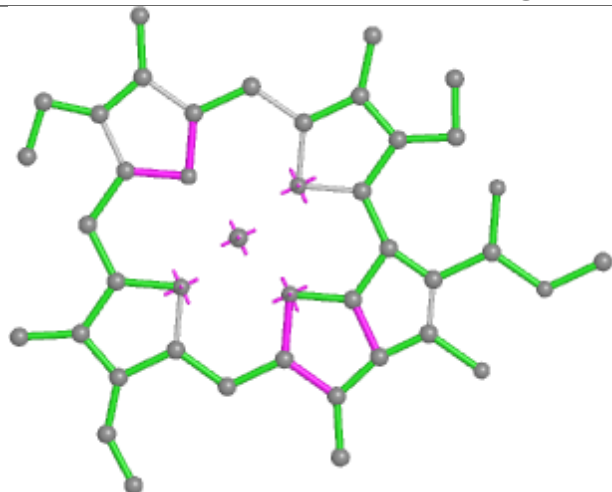
Rings

**Ligand CLA D 405****Ligand CLA B 606**

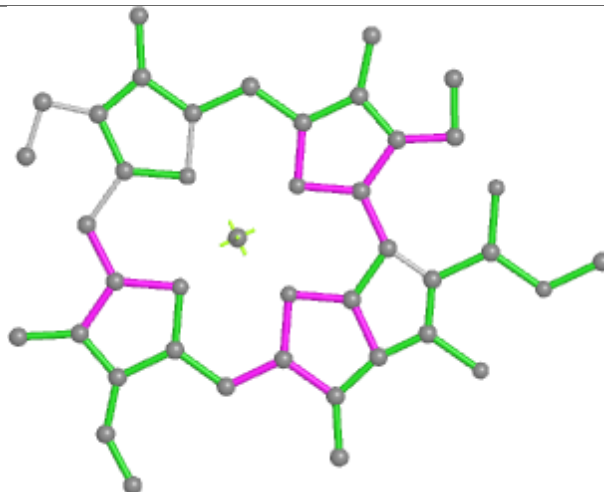




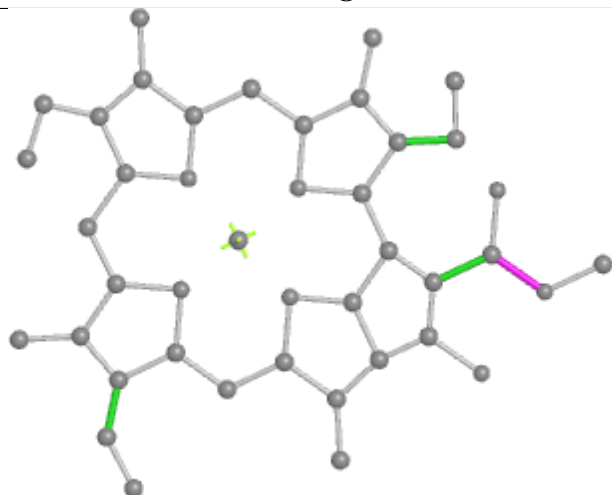
## Ligand CLA 6 309



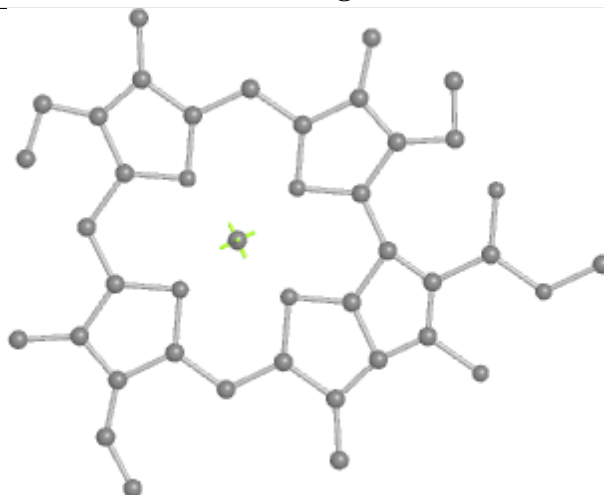
Bond lengths



Bond angles

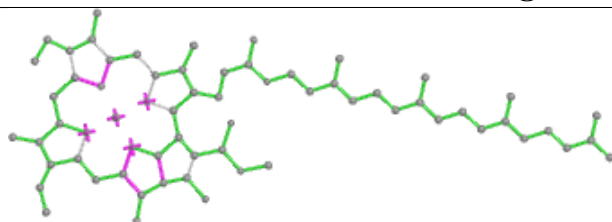


Torsions

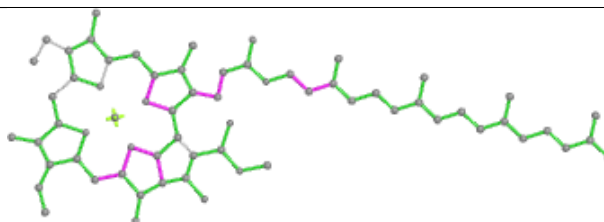


Rings

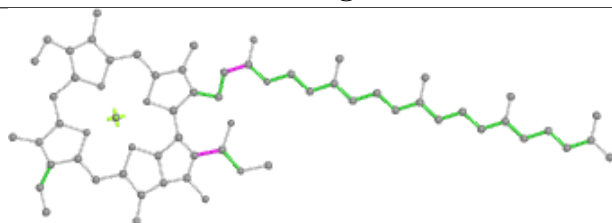
## Ligand CLA c 502



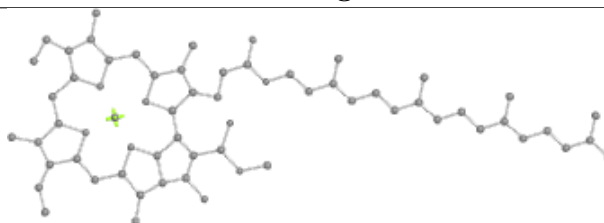
Bond lengths



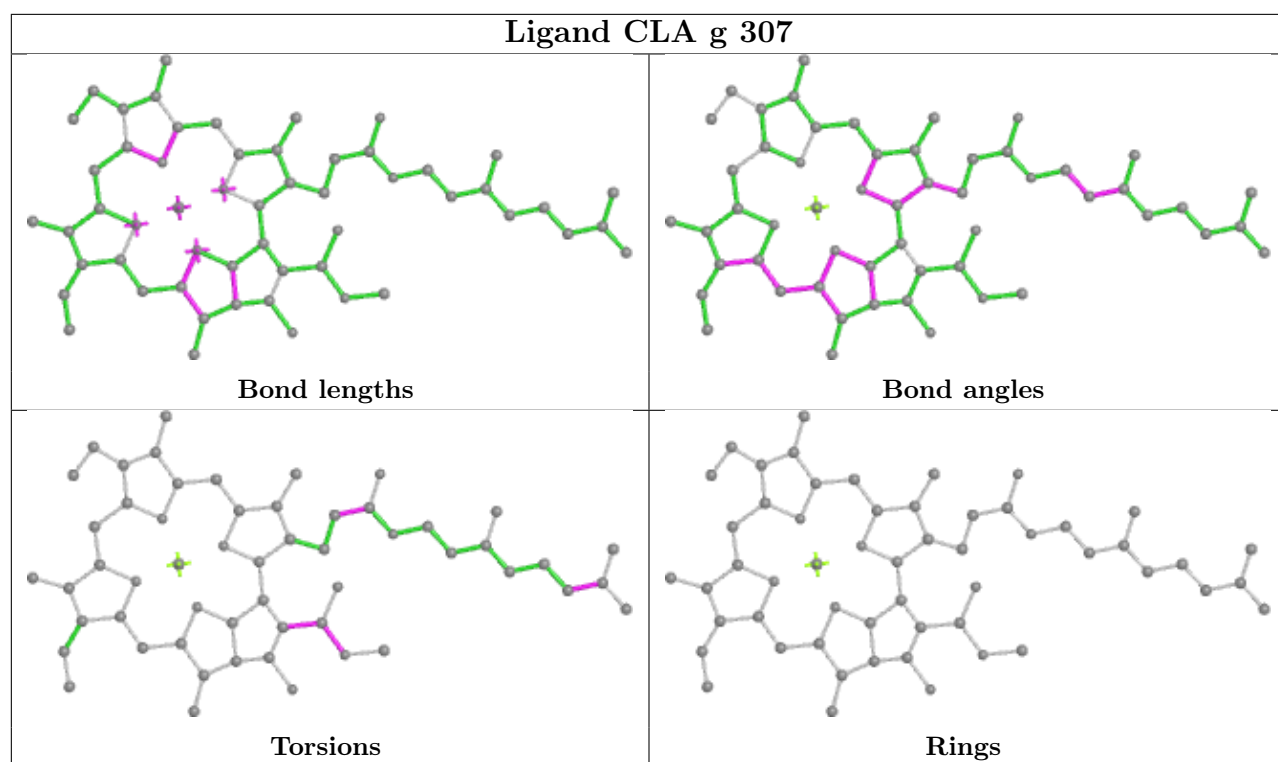
Bond angles



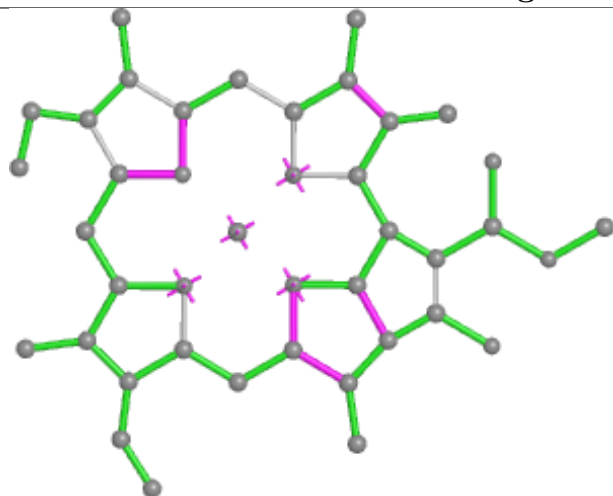
Torsions



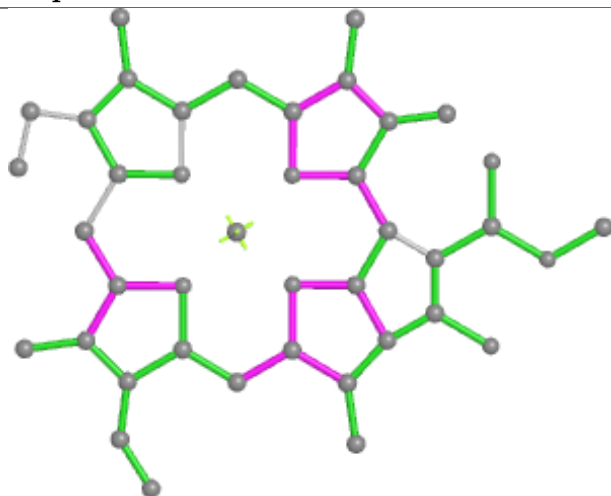
Rings



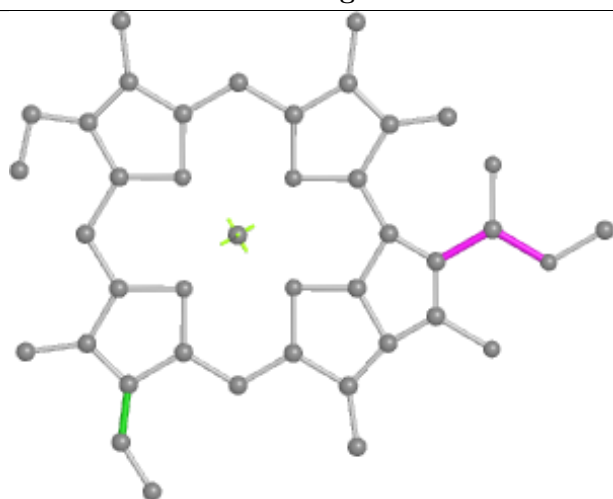
## Ligand CLA p 319



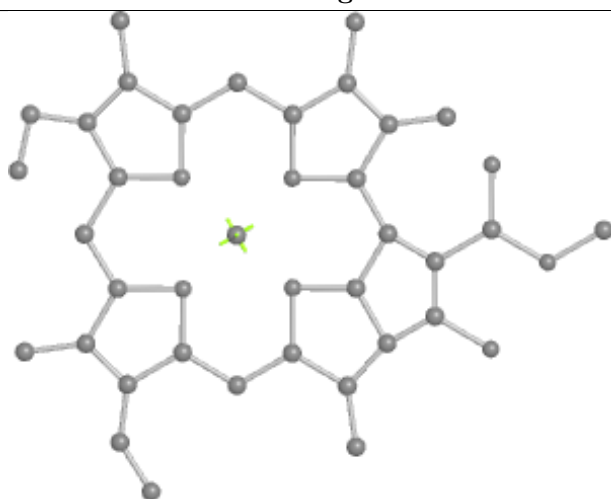
Bond lengths



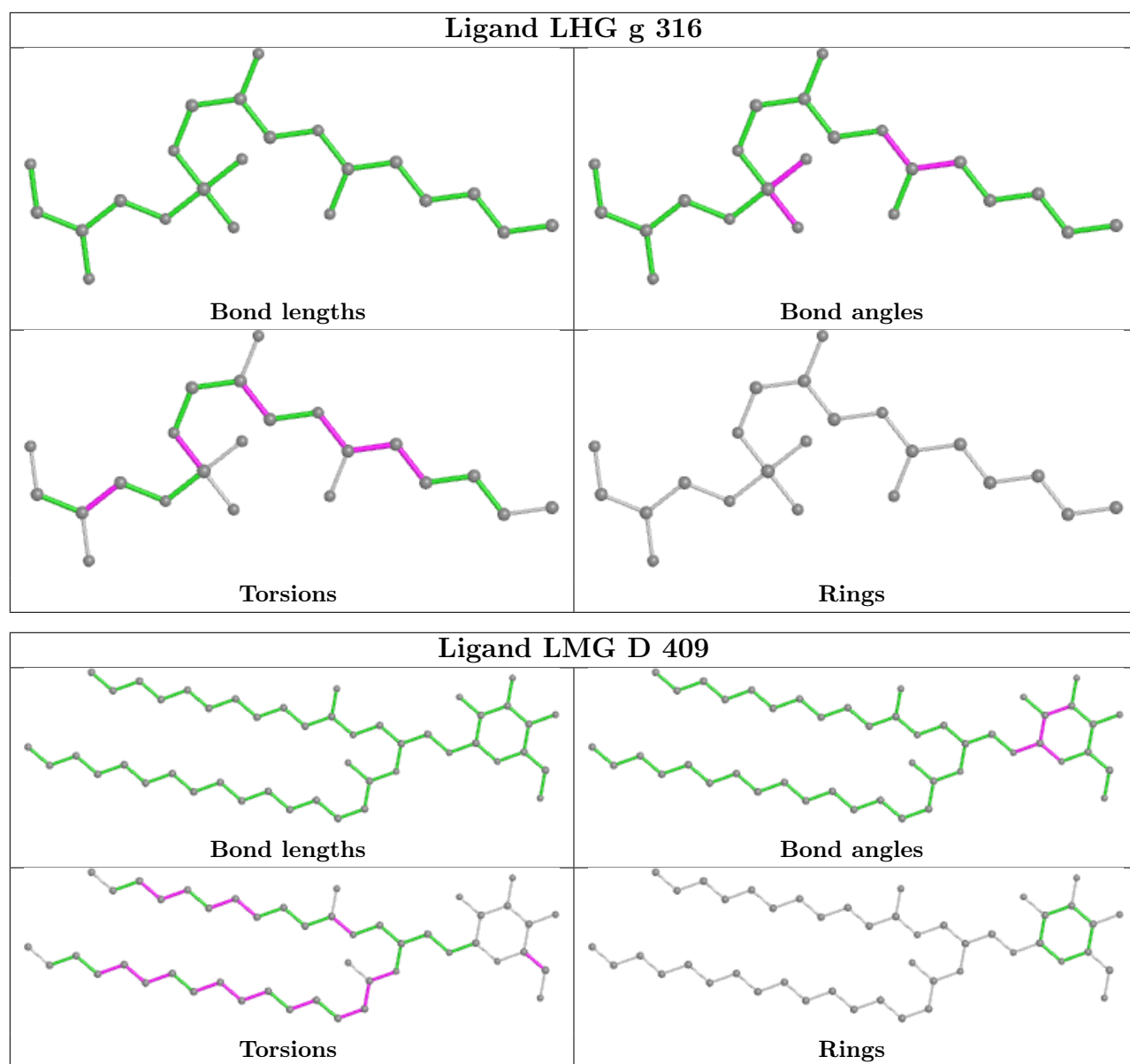
Bond angles

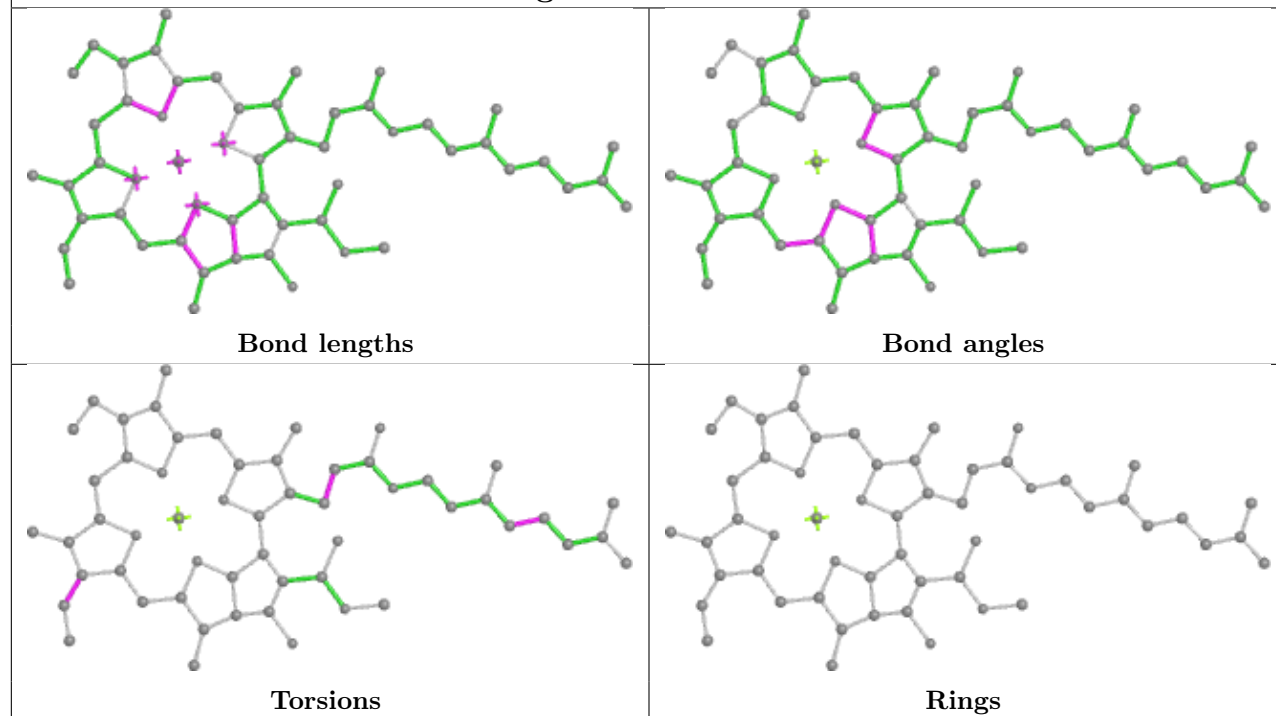
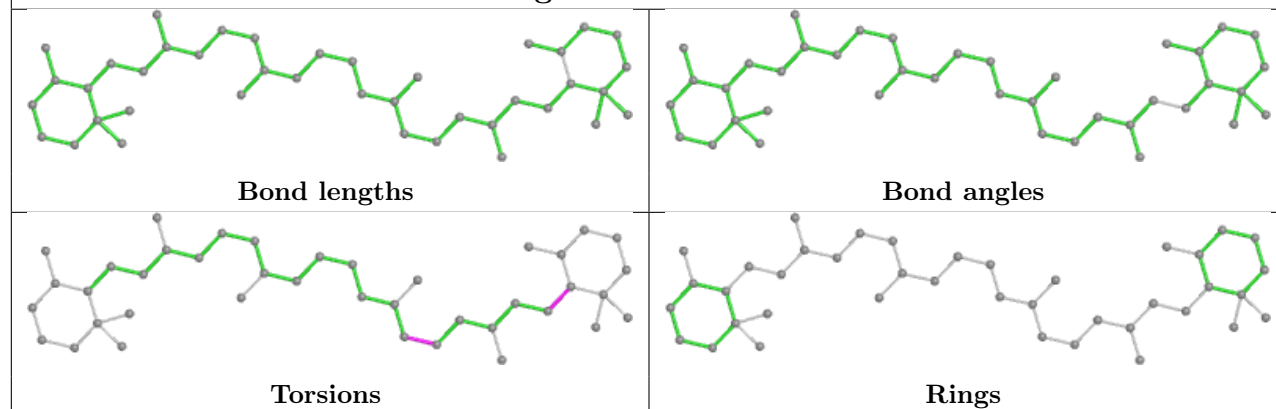
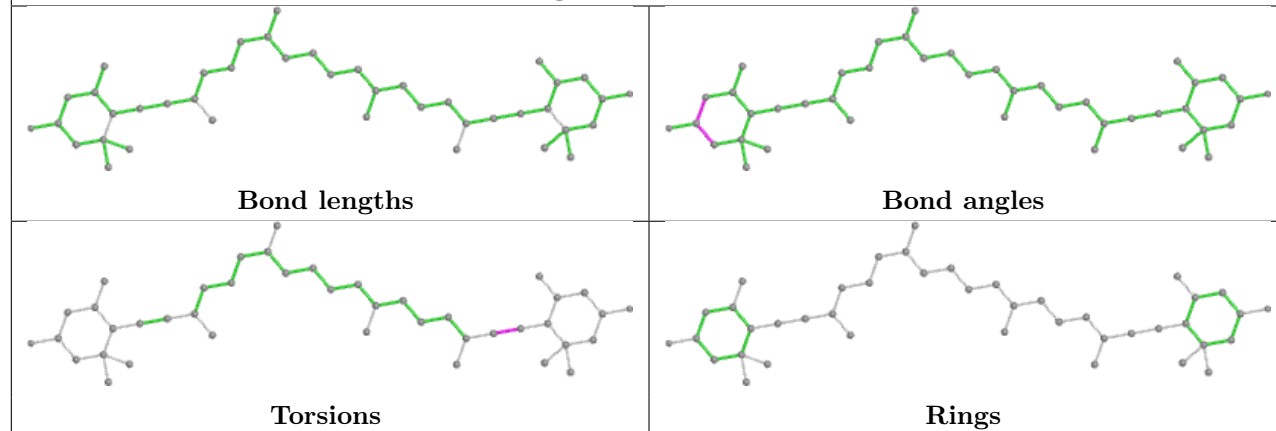


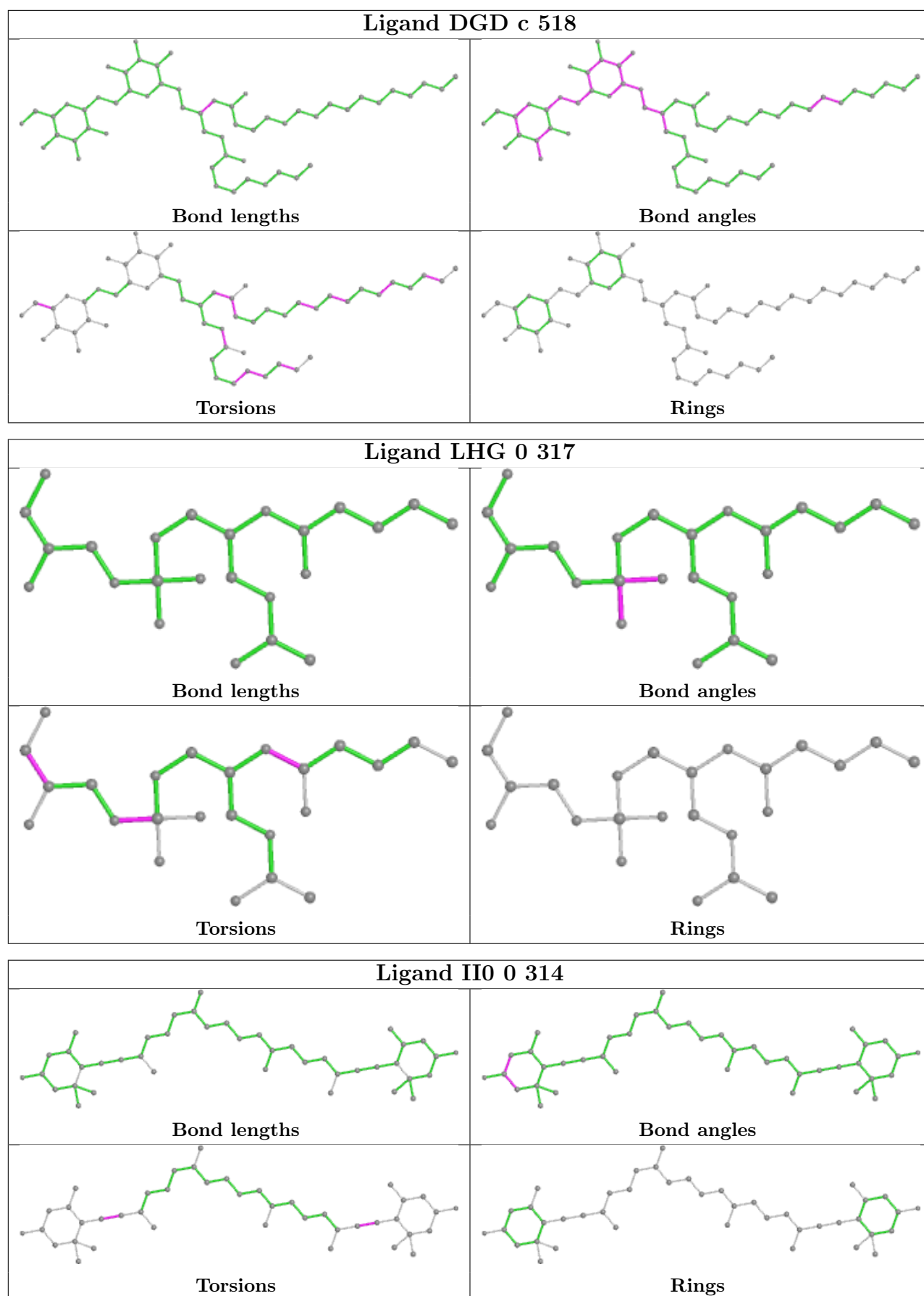
Torsions

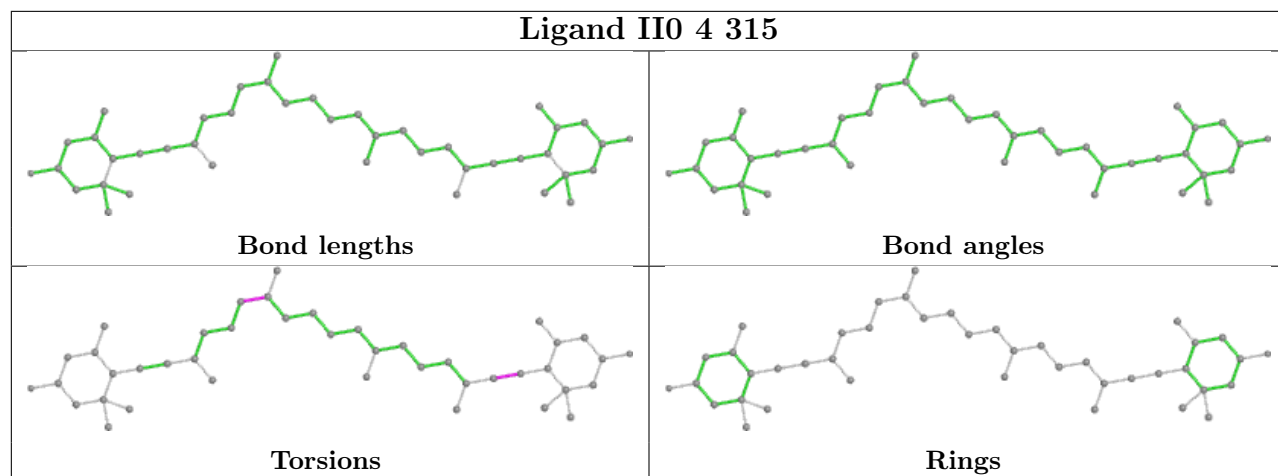
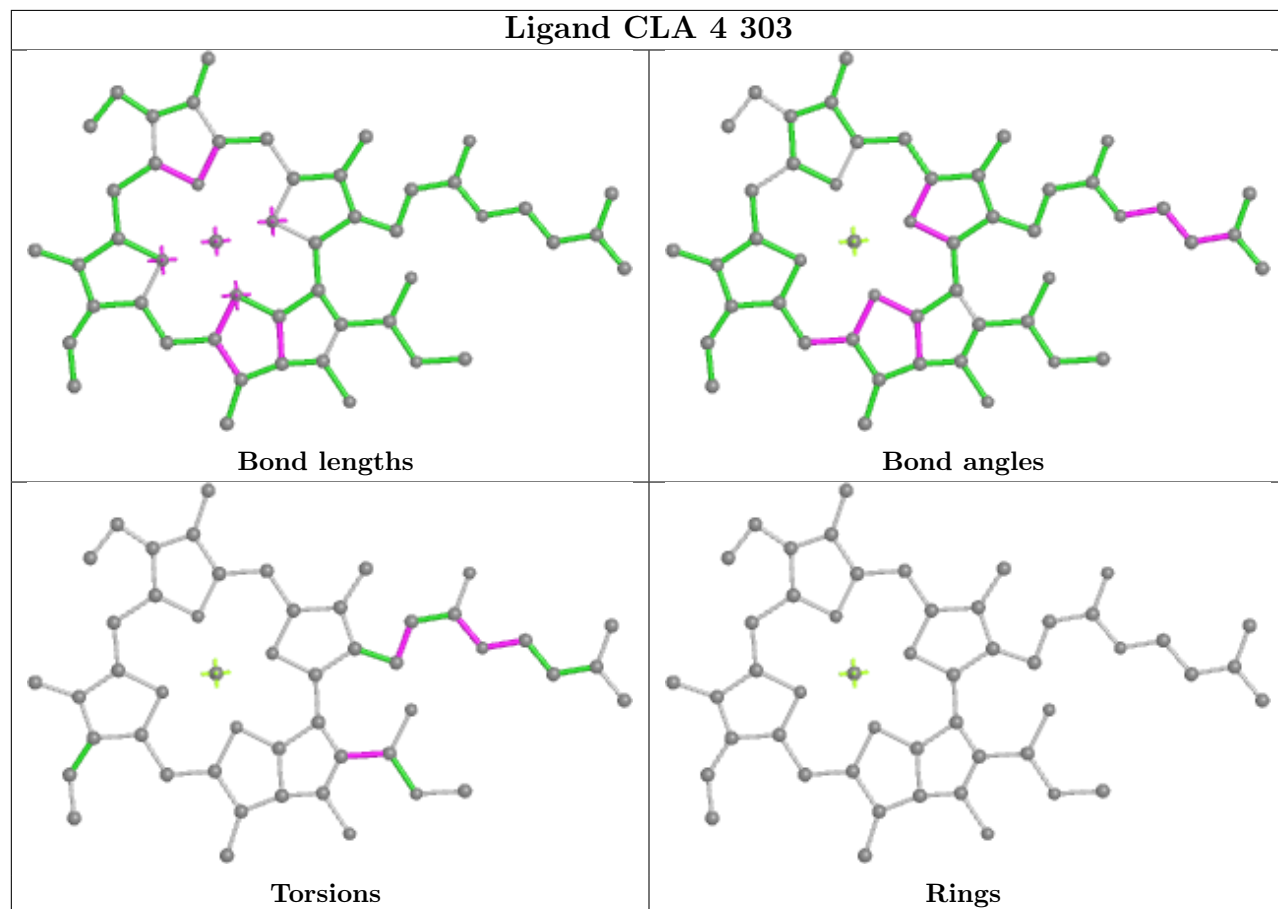


Rings

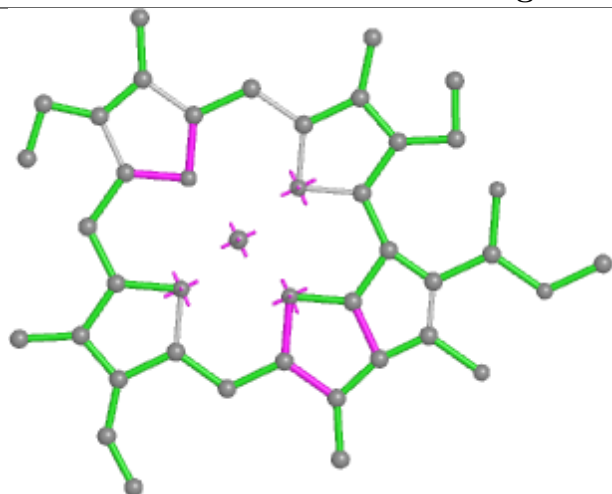


**Ligand CLA 3 305****Ligand 8CT A 409****Ligand II0 0 315**

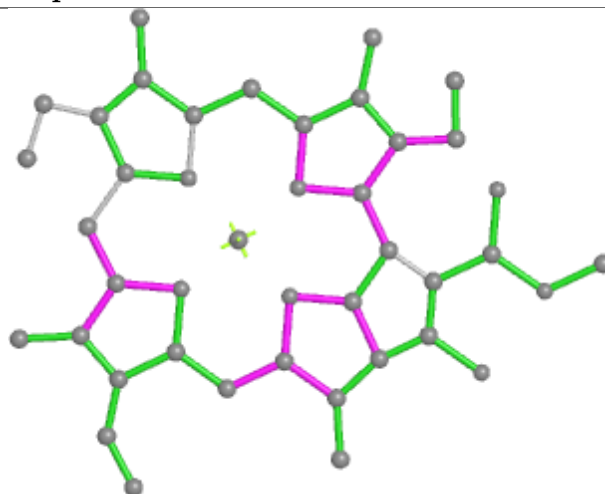


**Ligand II0 4 315****Ligand CLA 4 303**

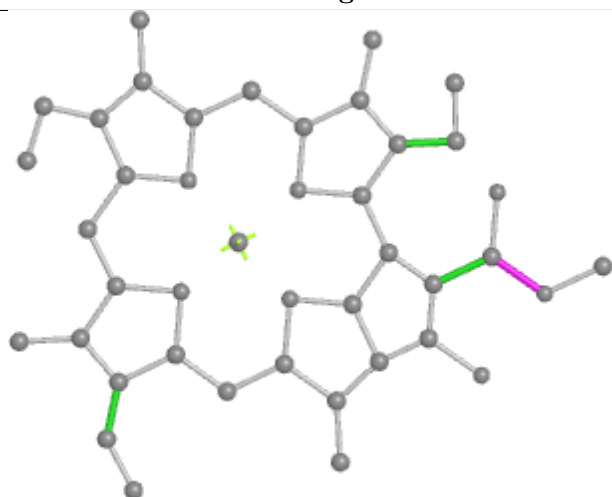
## Ligand CLA p 309



Bond lengths



Bond angles



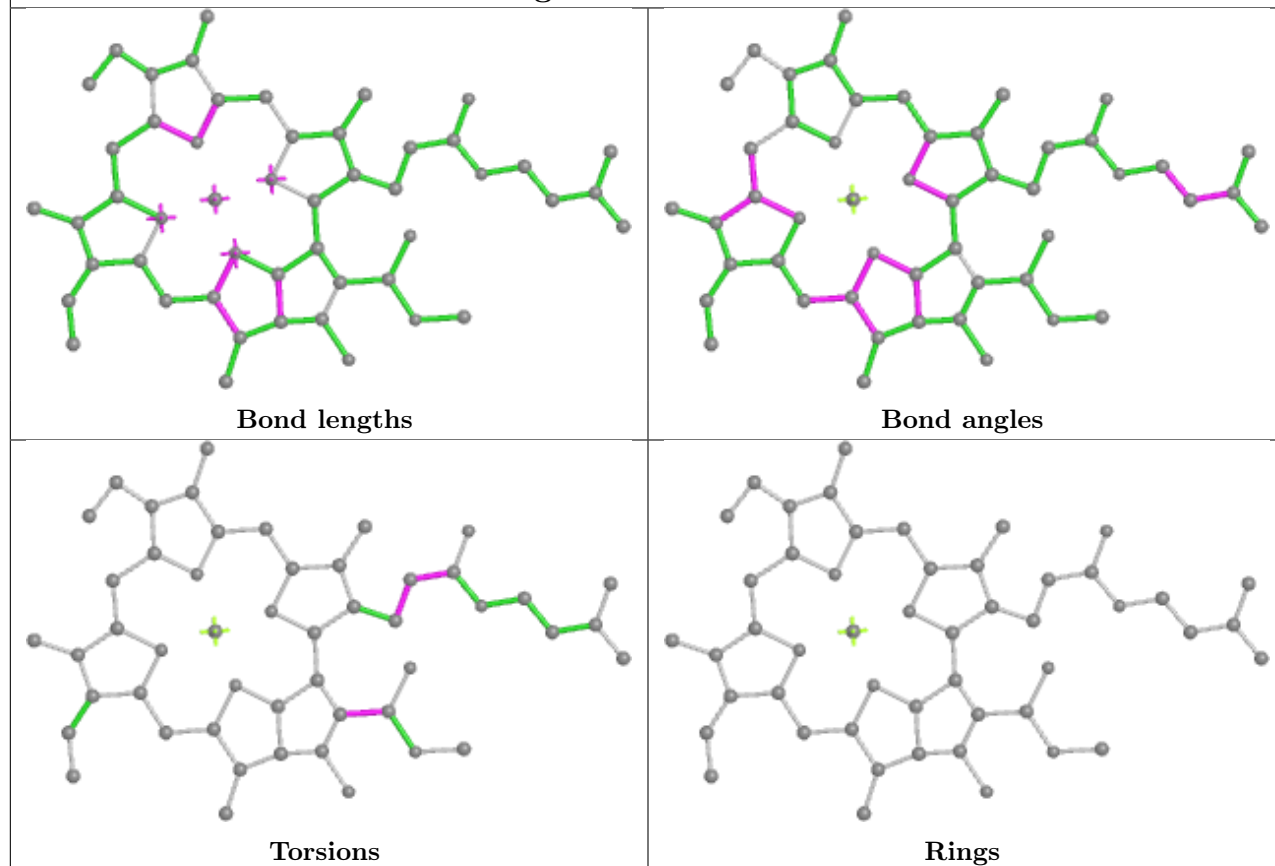
Torsions



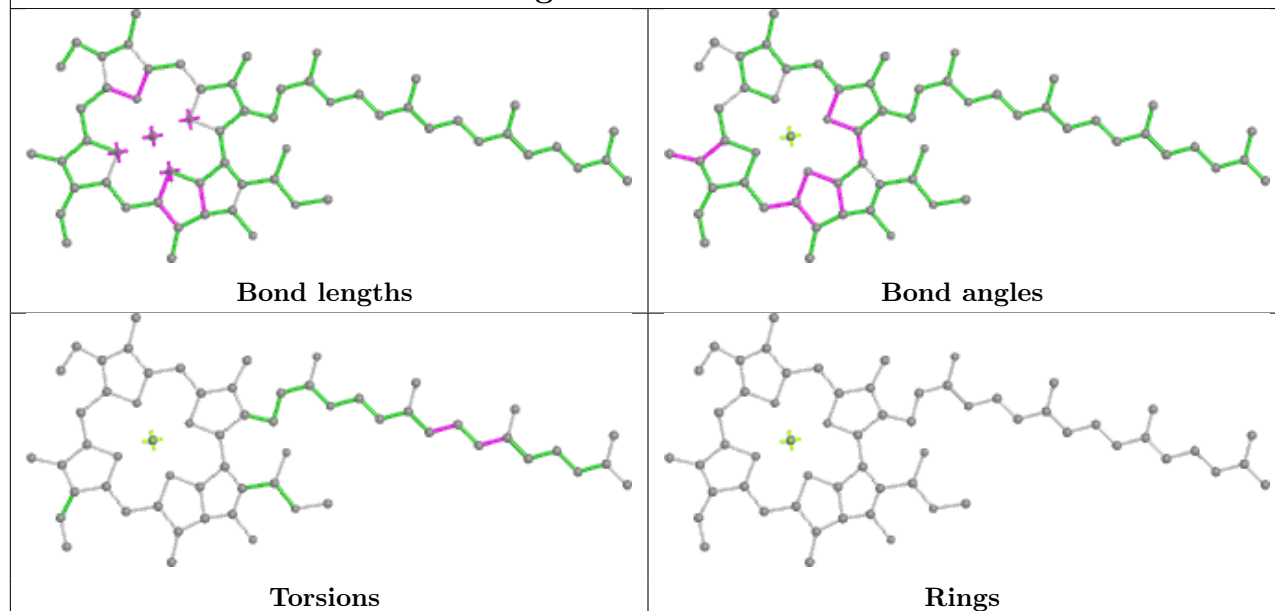
Rings

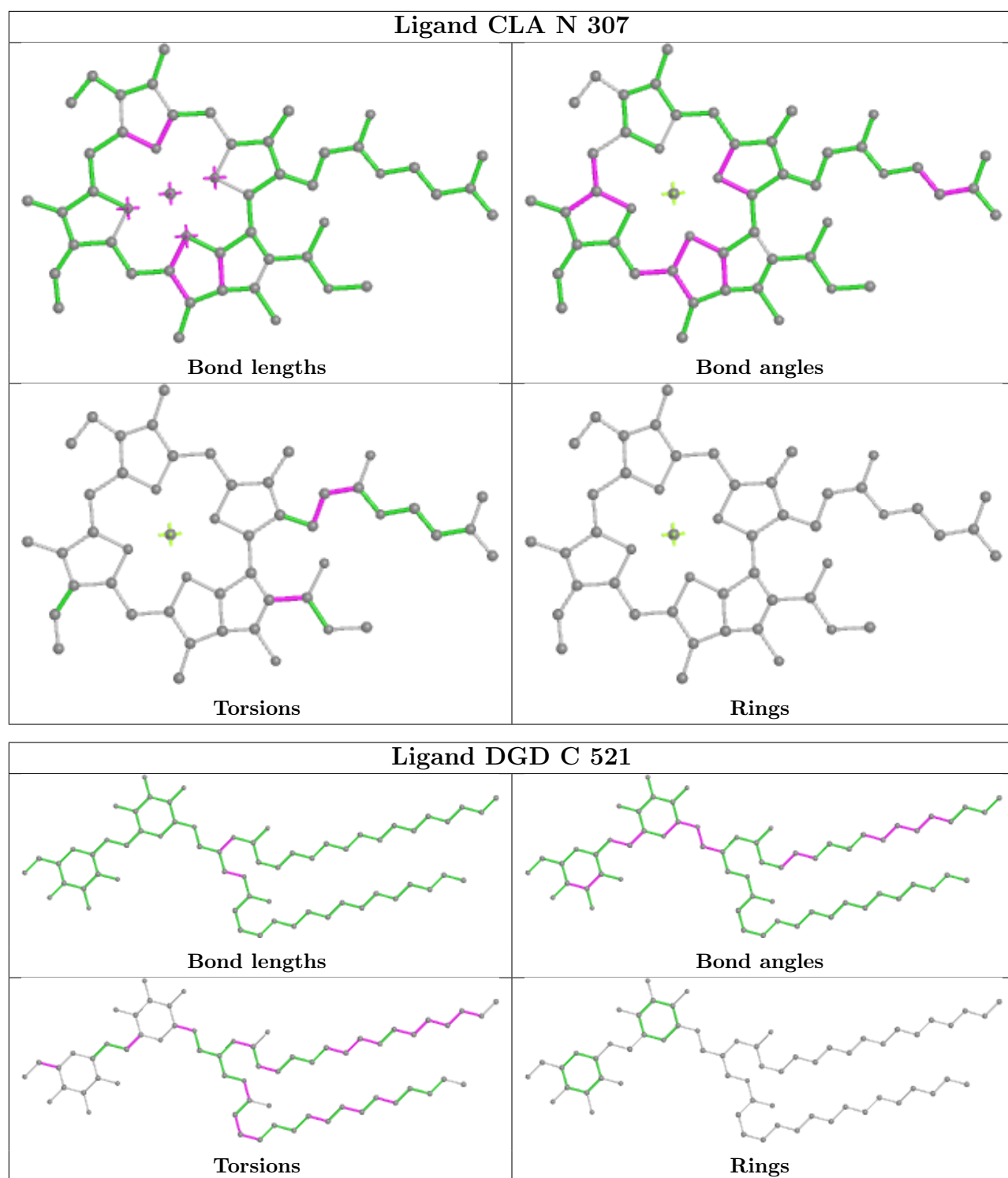


## Ligand CLA n 306

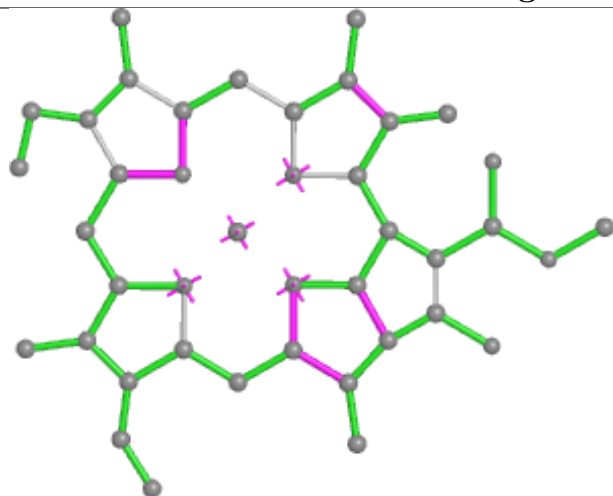


## Ligand CLA 8 306

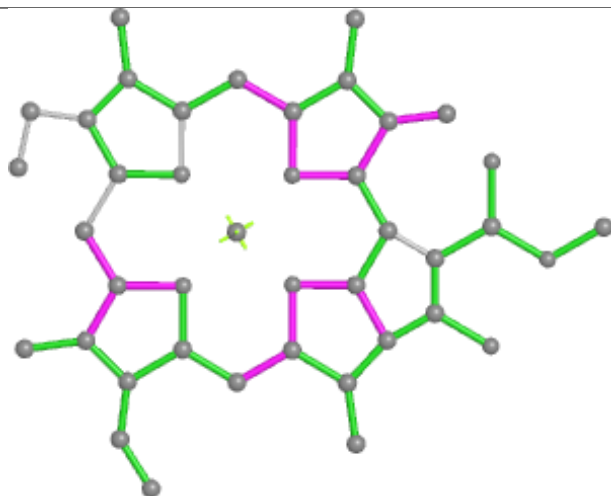




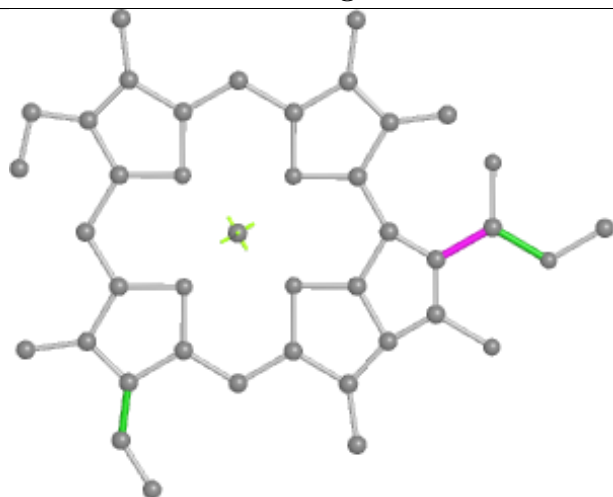
## Ligand CLA 6 312



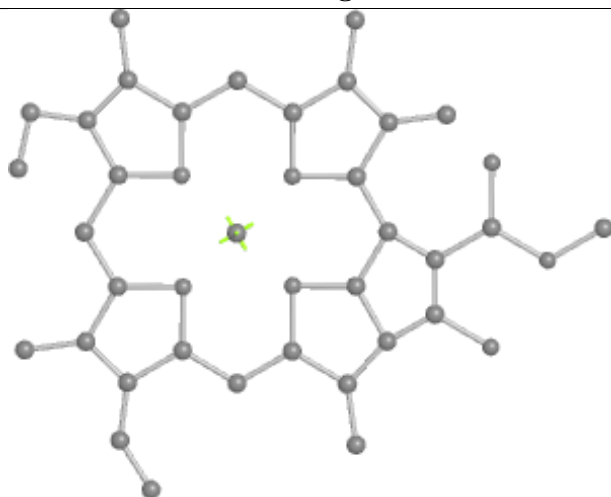
Bond lengths



Bond angles

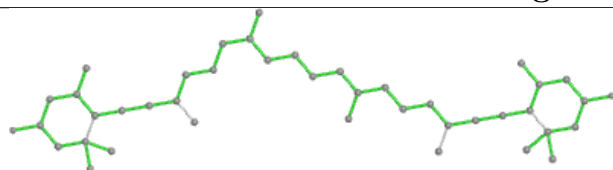


Torsions

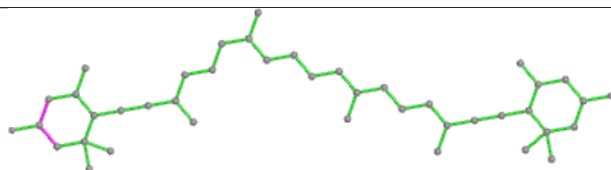


Rings

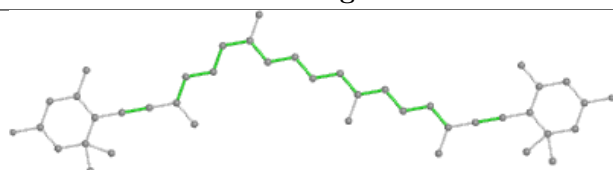
## Ligand II0 9 317



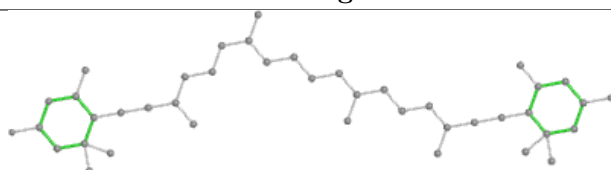
Bond lengths



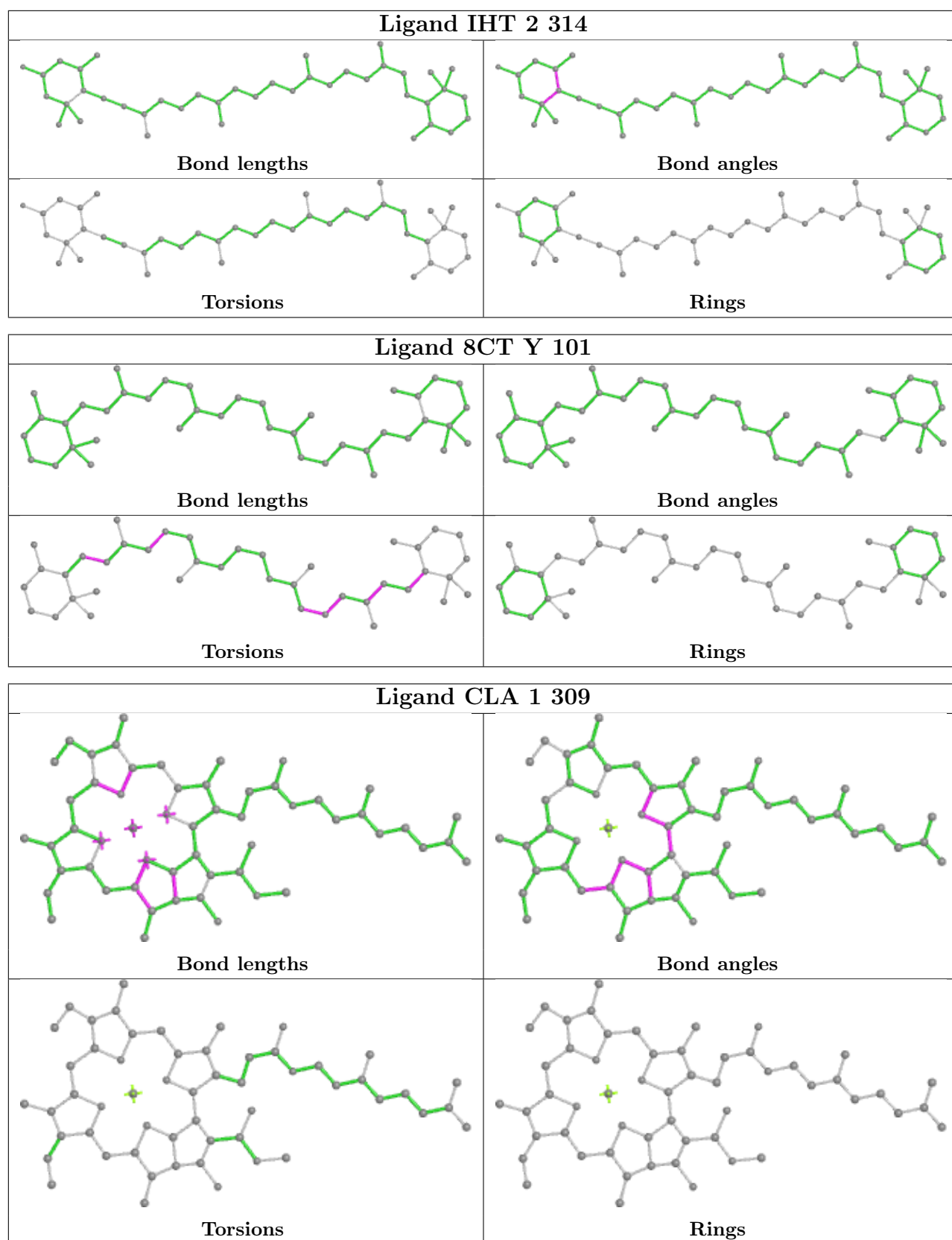
Bond angles



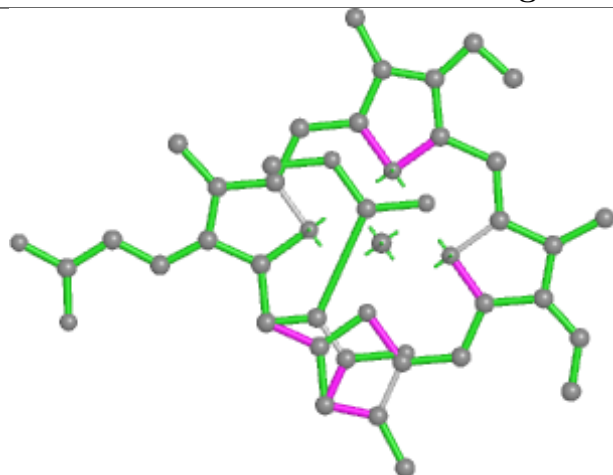
Torsions



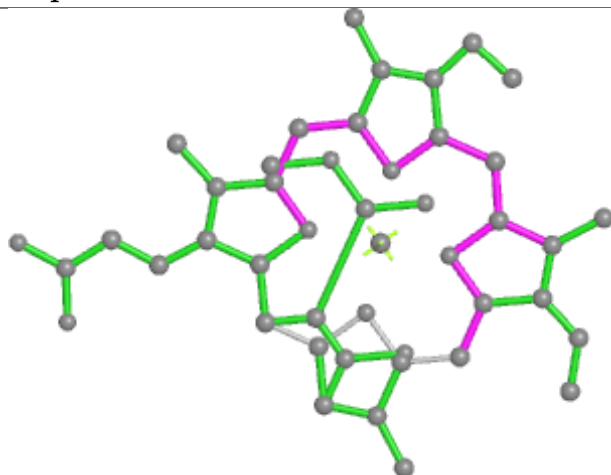
Rings



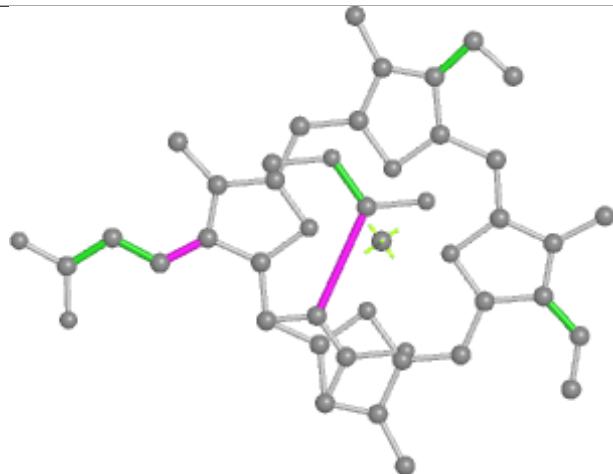
## Ligand KC2 p 311



Bond lengths



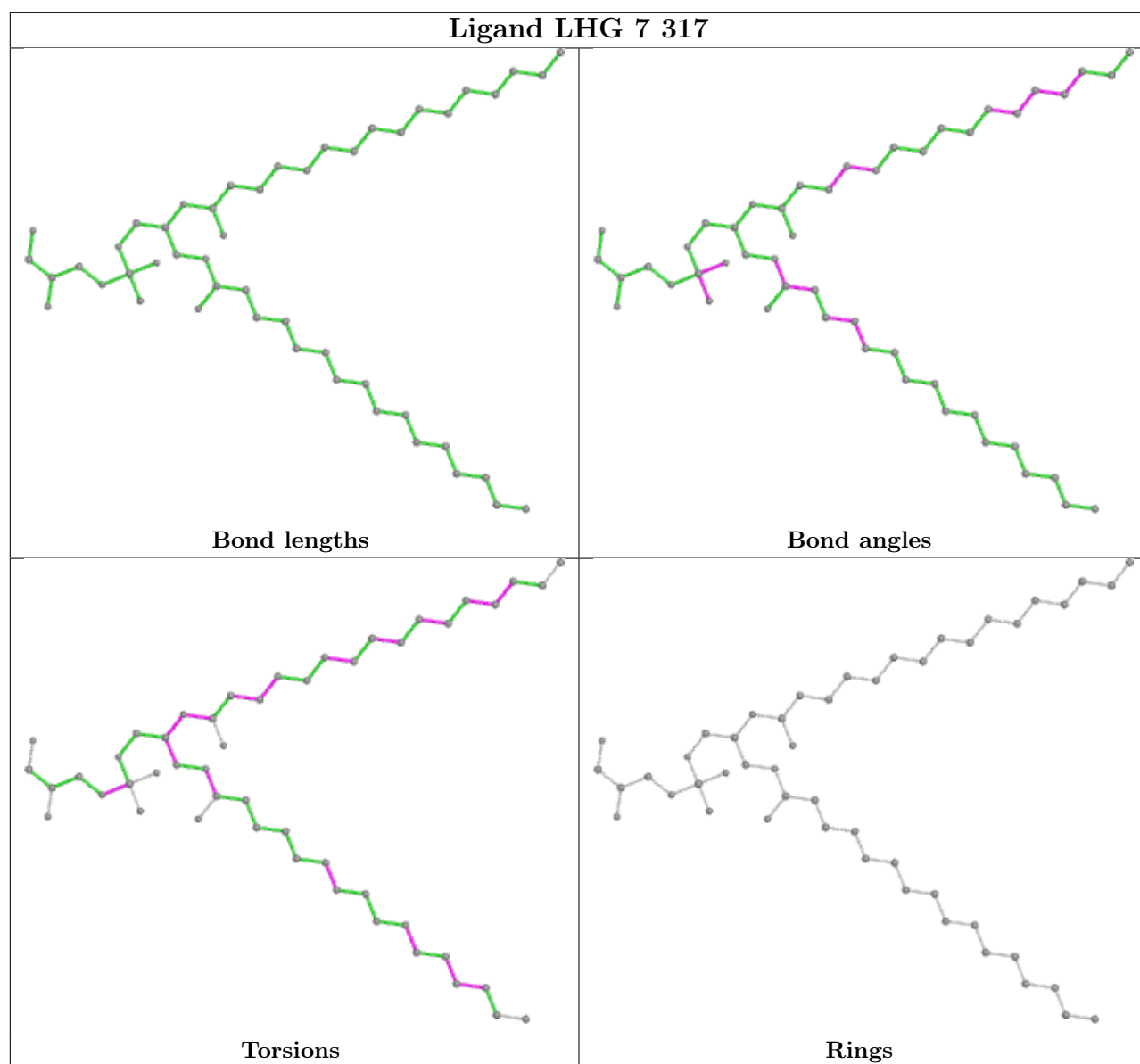
Bond angles



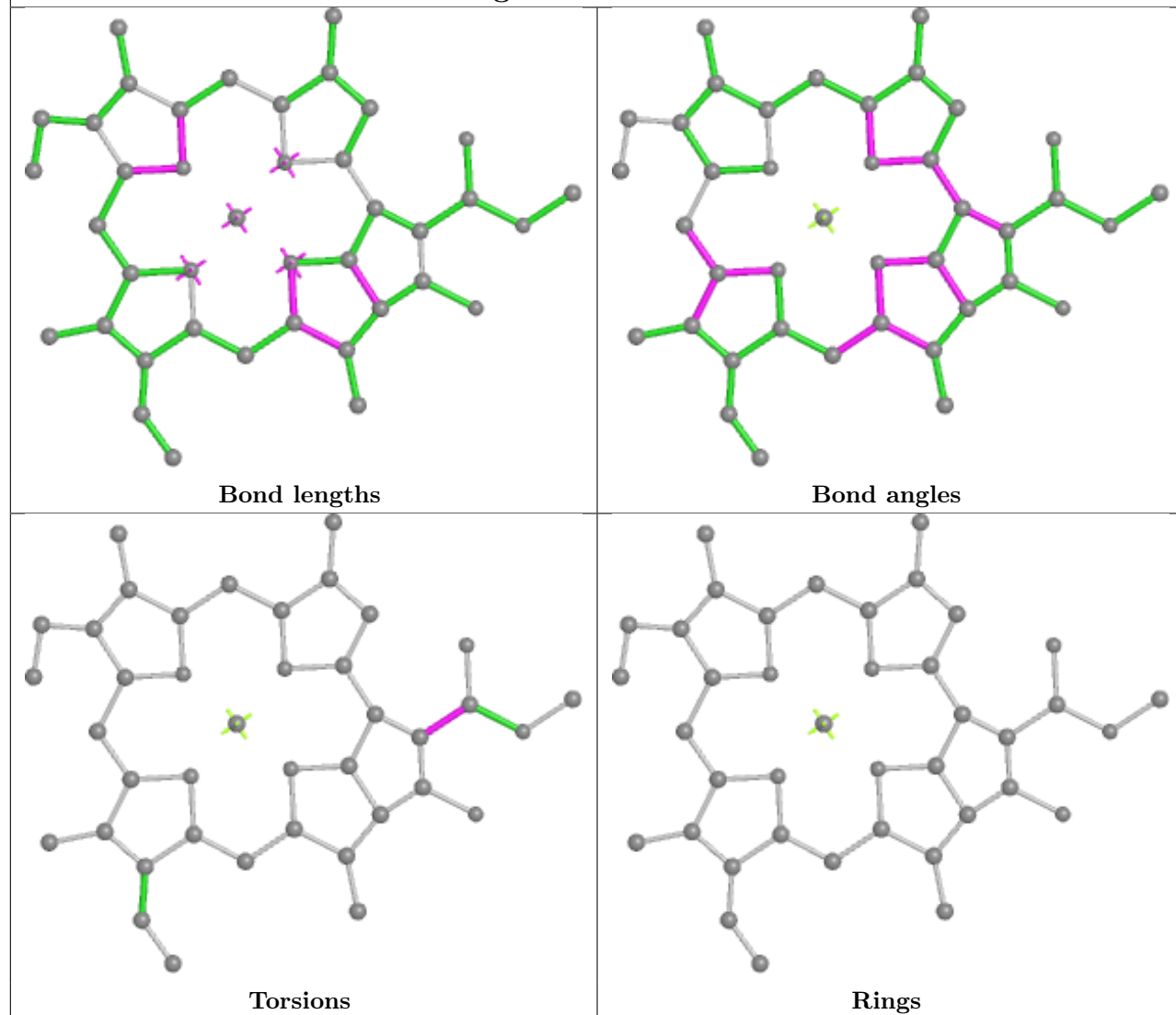
Torsions



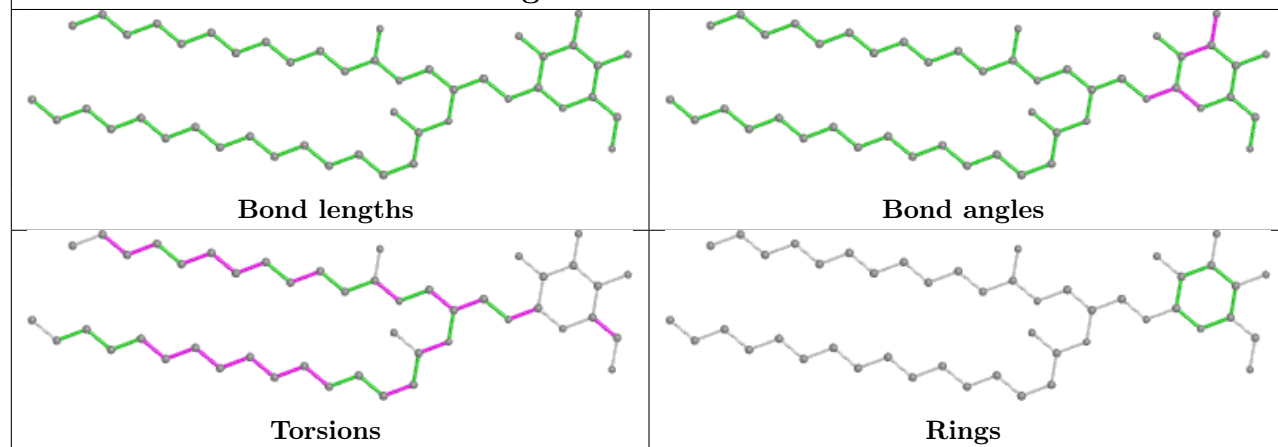
Rings



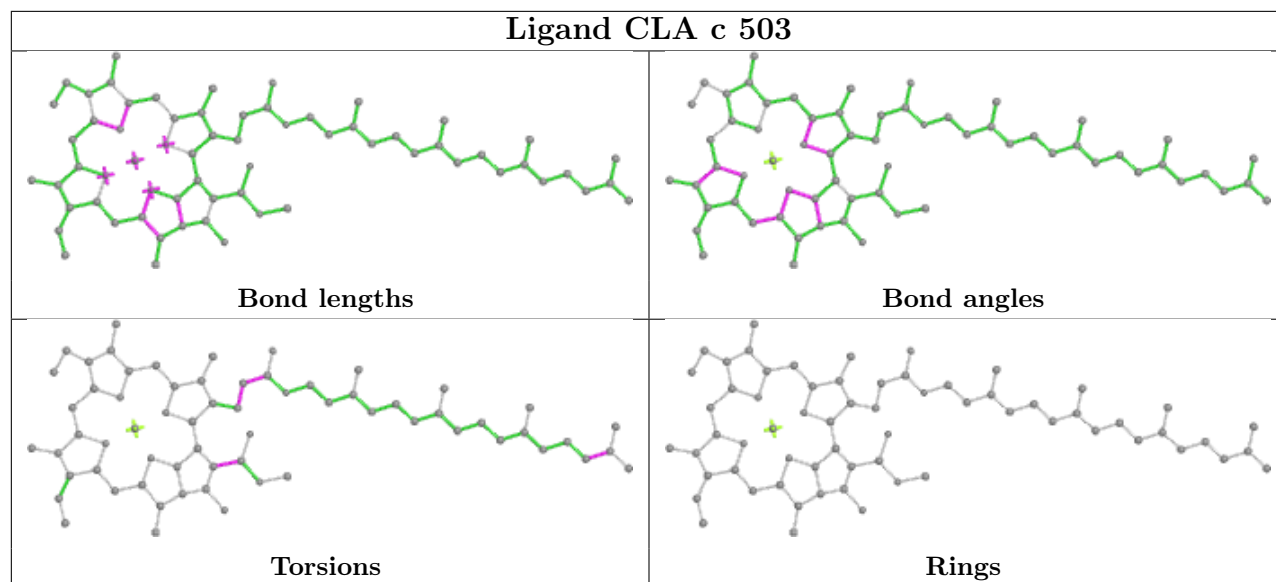
## Ligand CLA 5 317



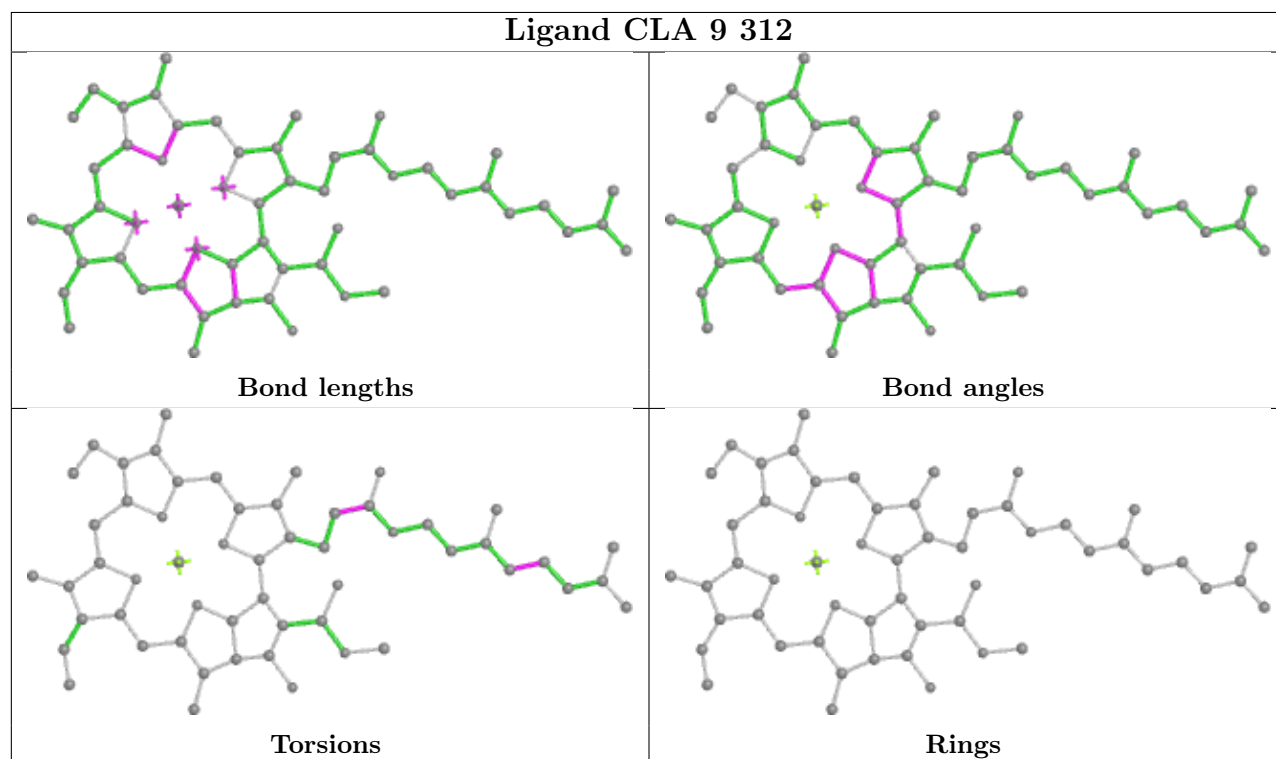
## Ligand LMG W 101



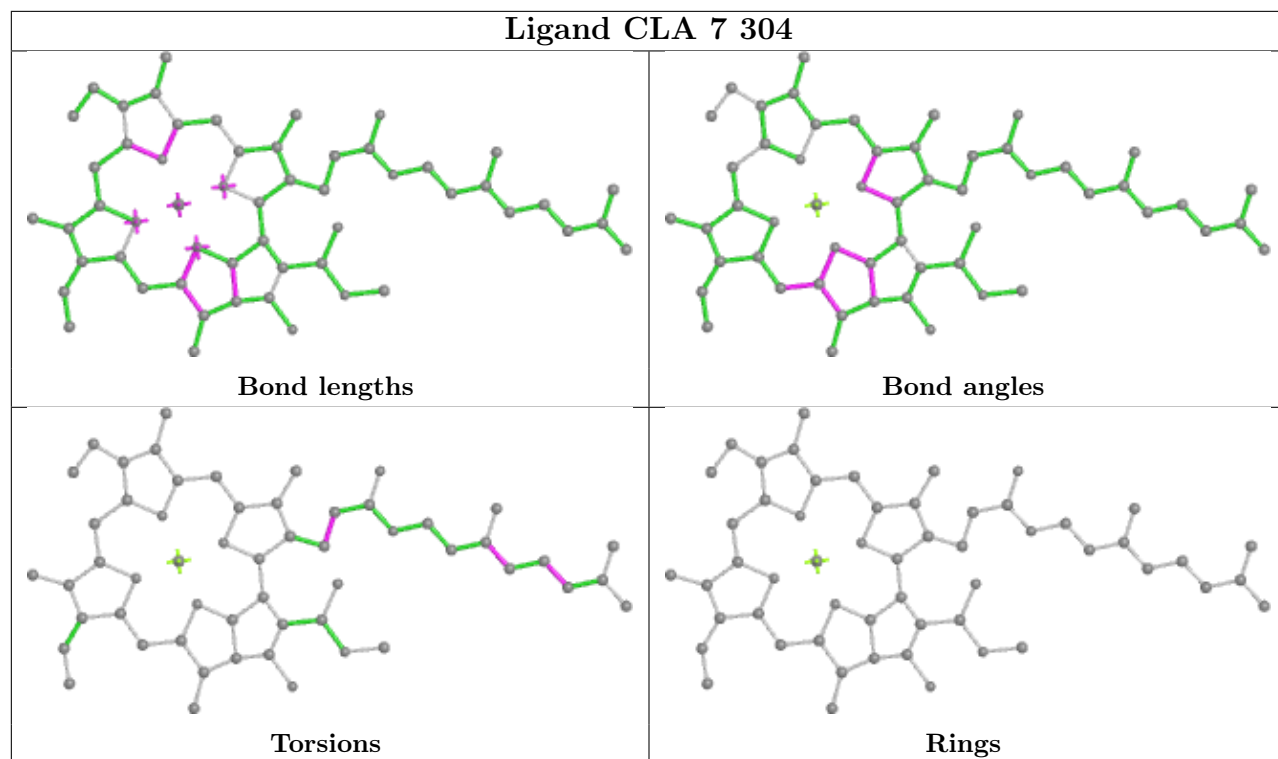
## Ligand CLA c 503

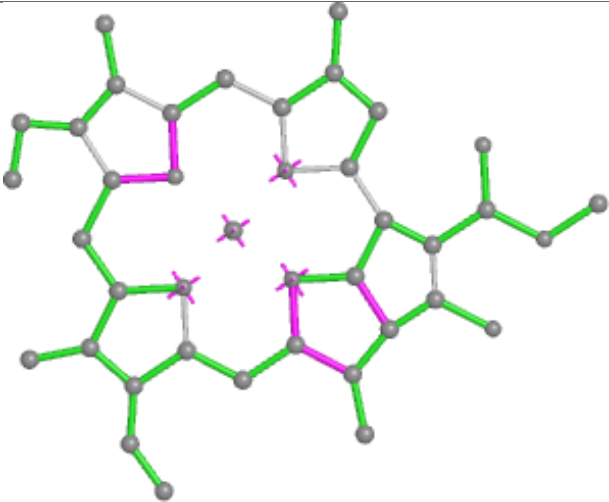
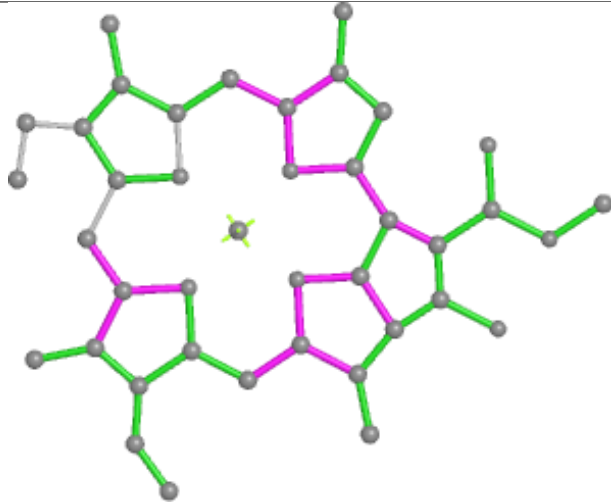
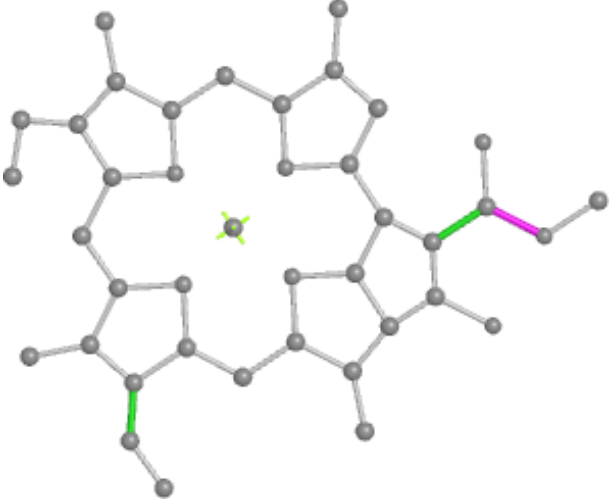
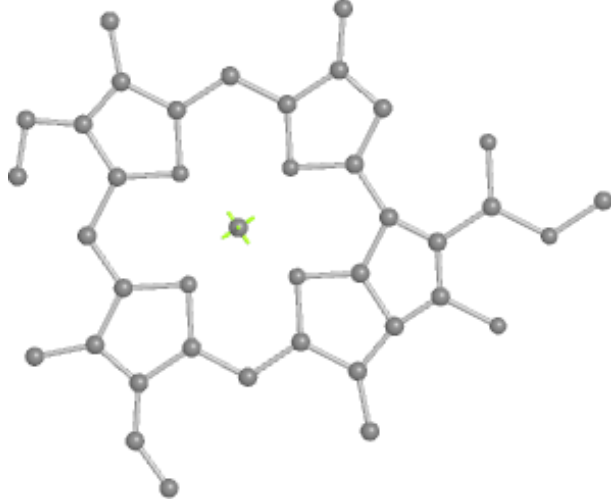
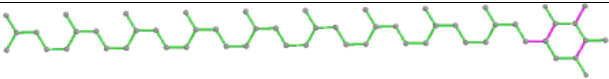
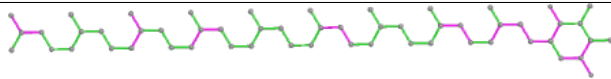
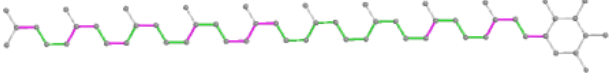
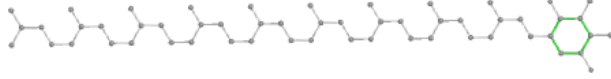


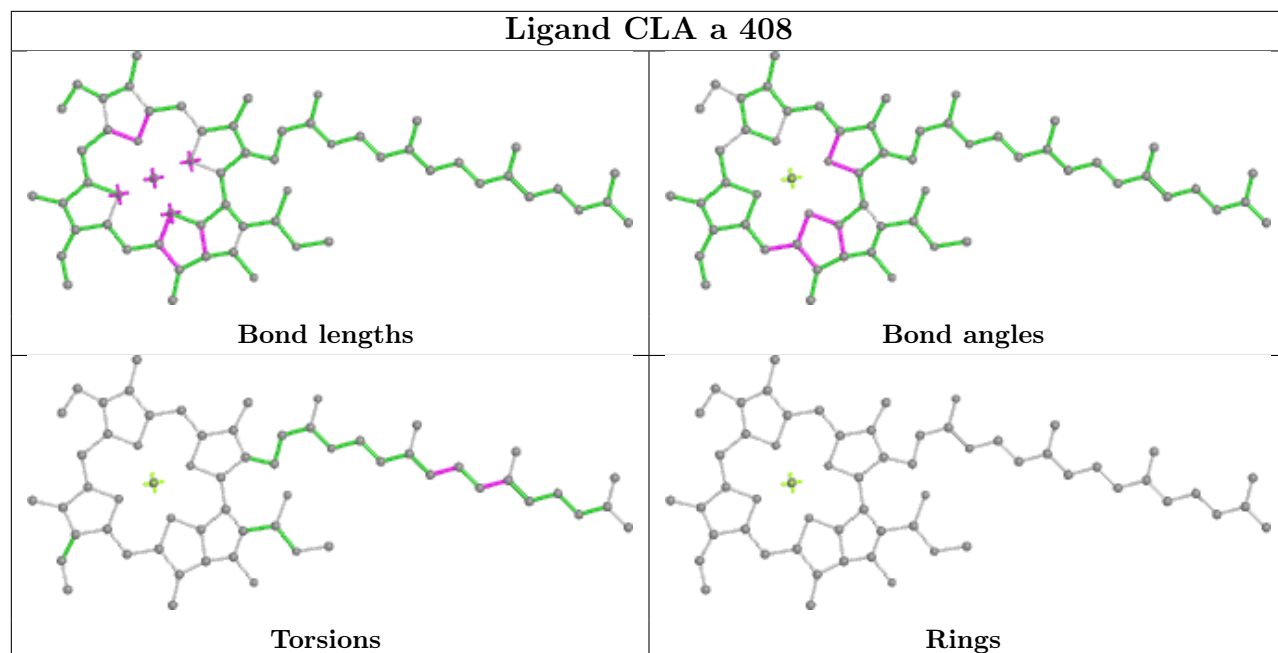
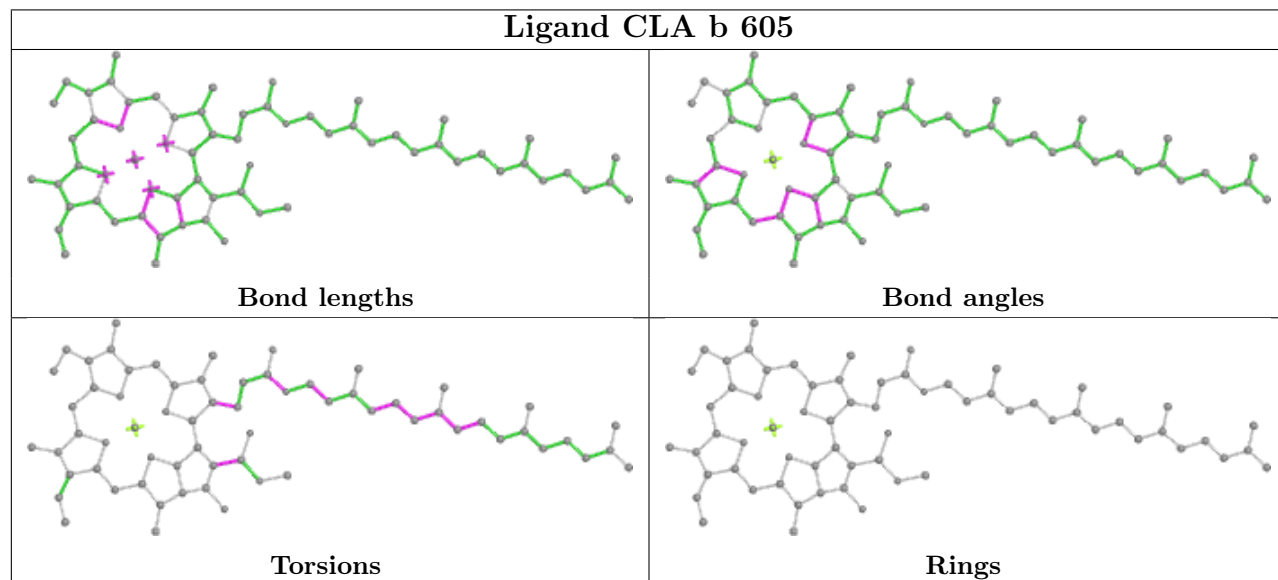
## Ligand CLA 9 312



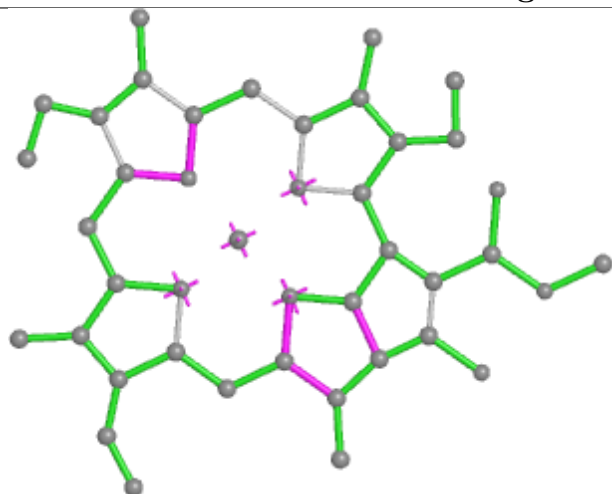




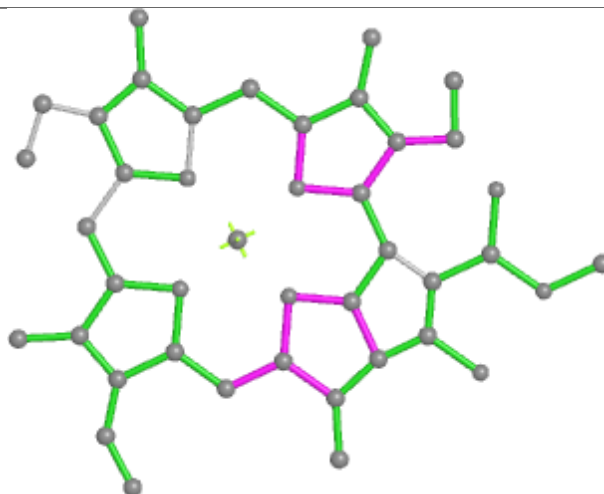
Ligand CLA g 305	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand PL9 d 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

**Ligand CLA a 408****Ligand CLA b 605**

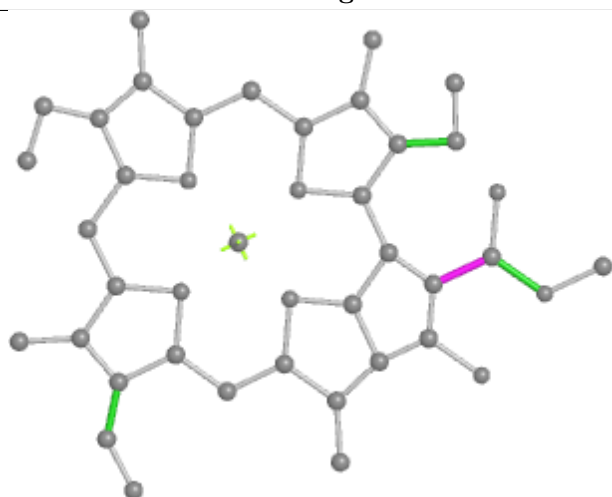
## Ligand CLA 6 304



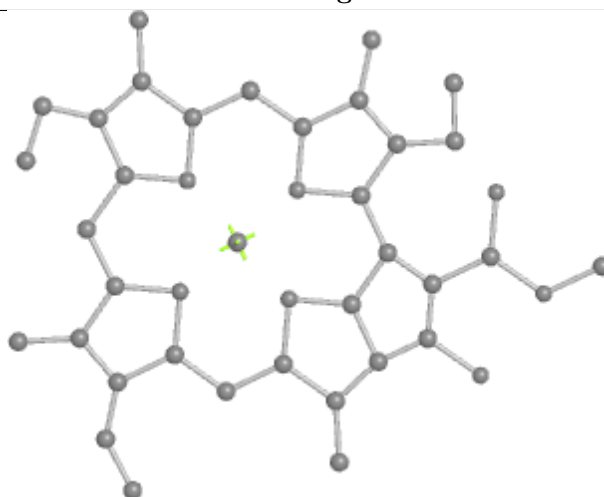
Bond lengths



Bond angles

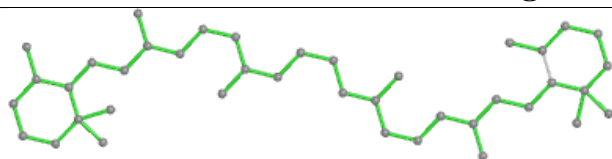


Torsions

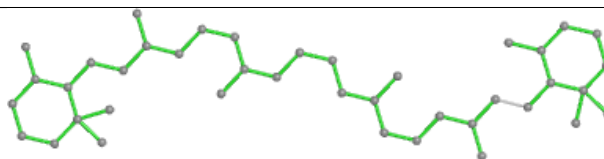


Rings

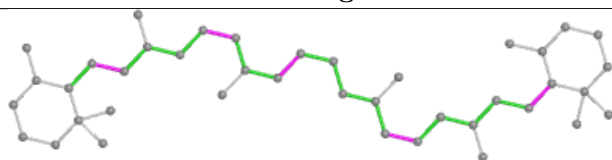
## Ligand 8CT c 517



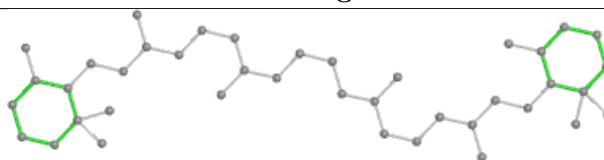
Bond lengths



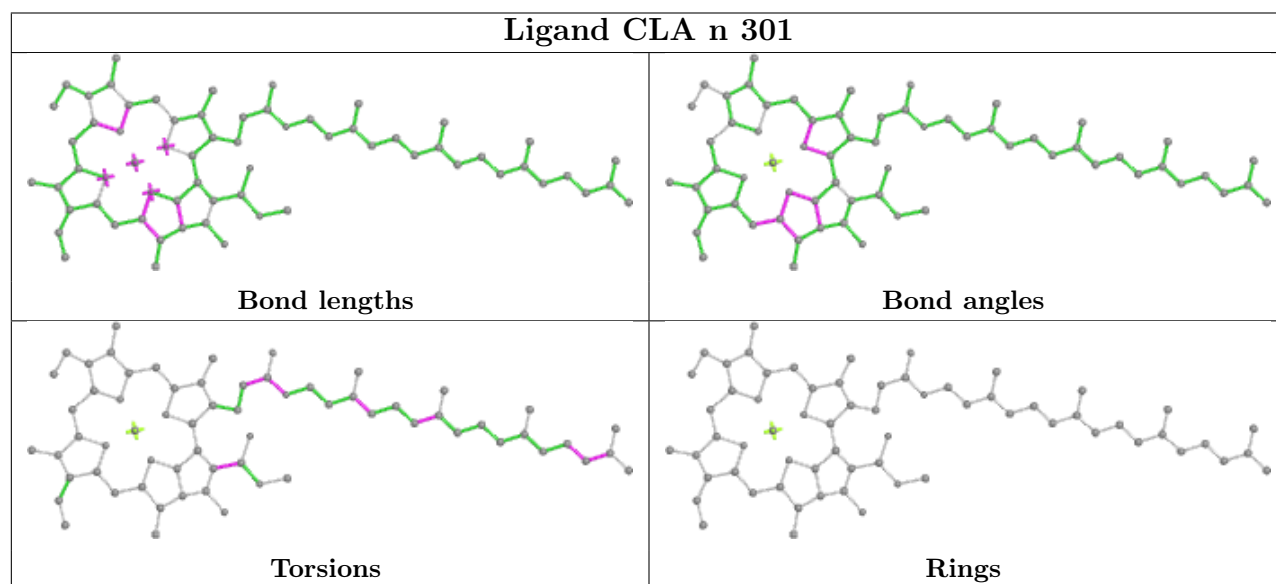
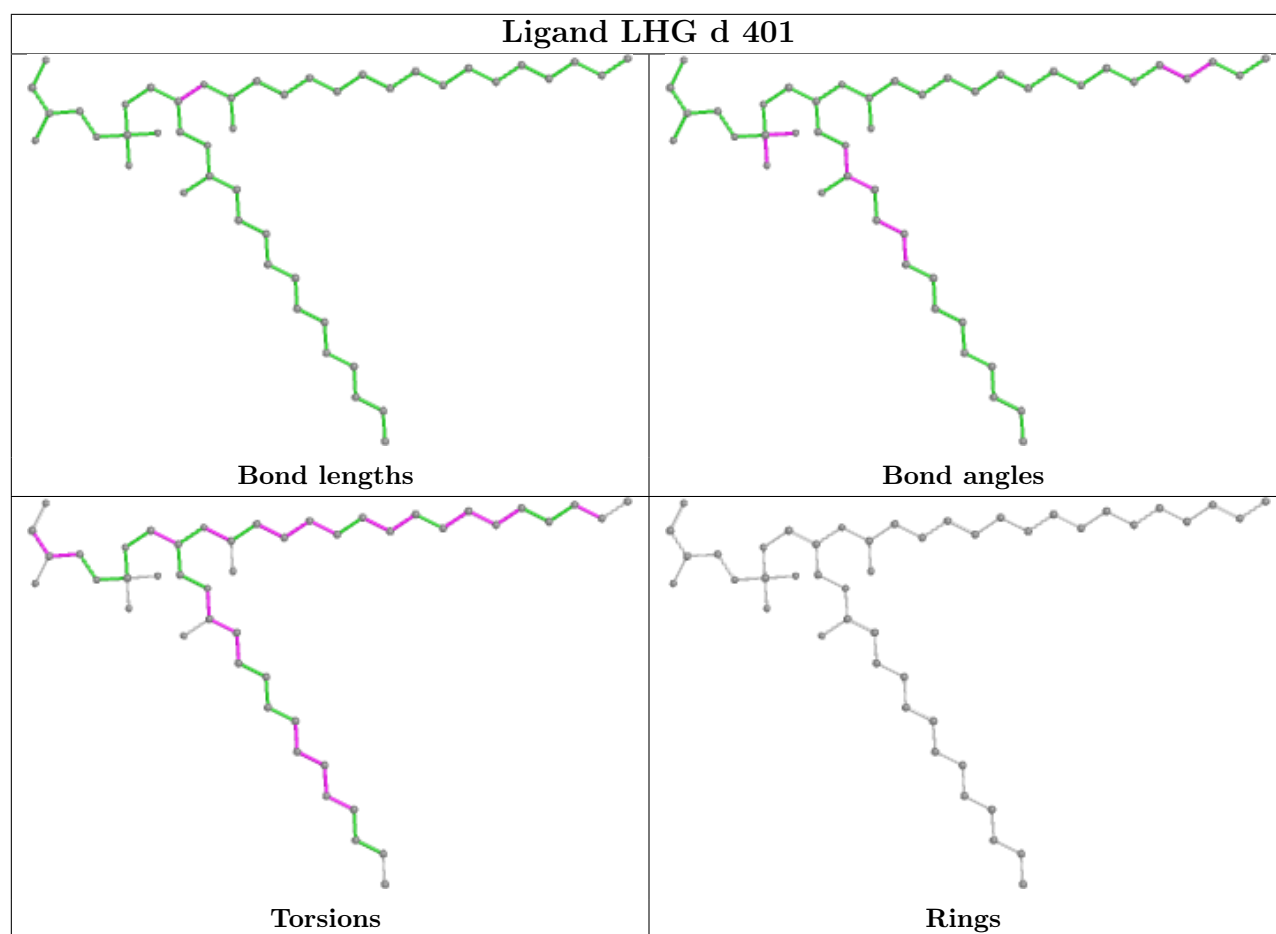
Bond angles



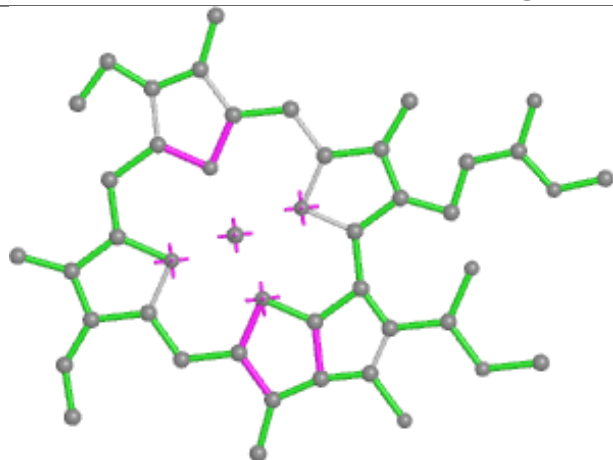
Torsions



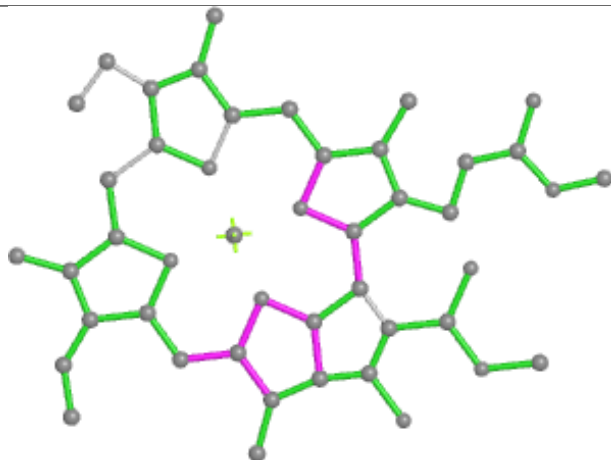
Rings



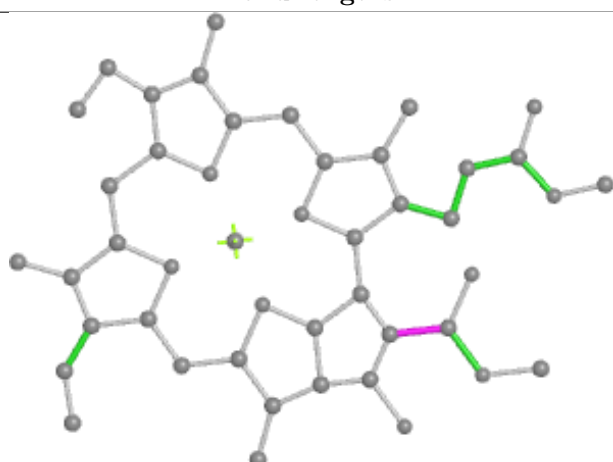
## Ligand CLA 2 310



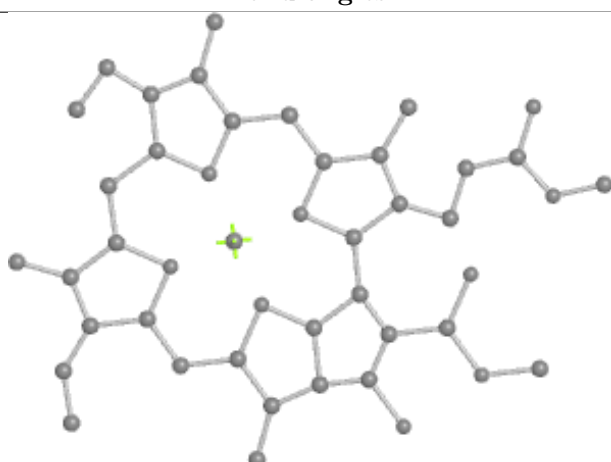
Bond lengths



Bond angles

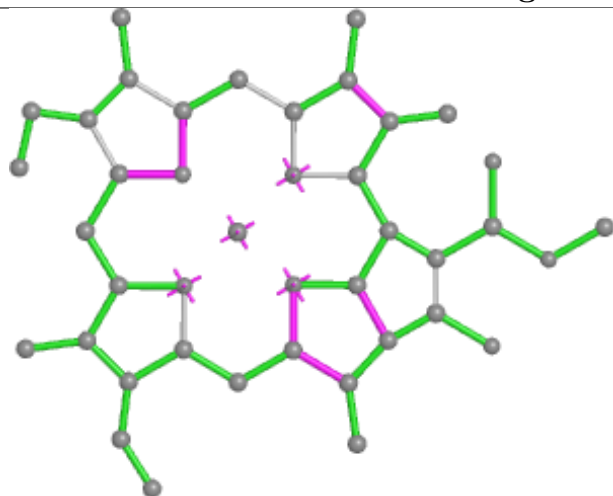


Torsions

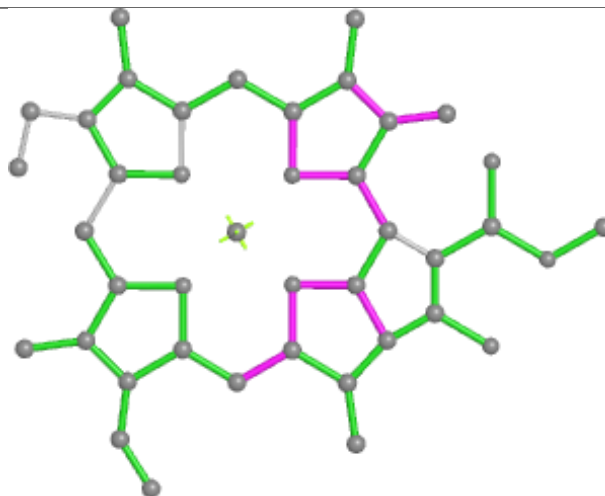


Rings

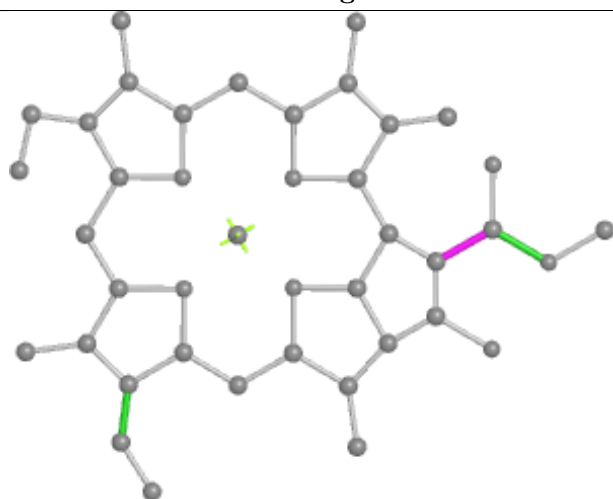
## Ligand CLA 3 315



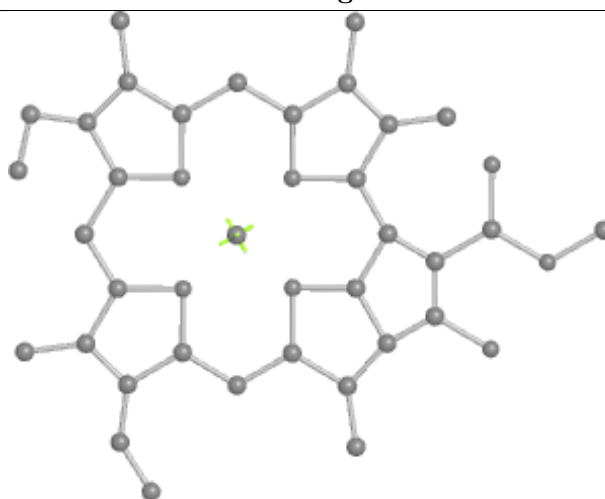
Bond lengths



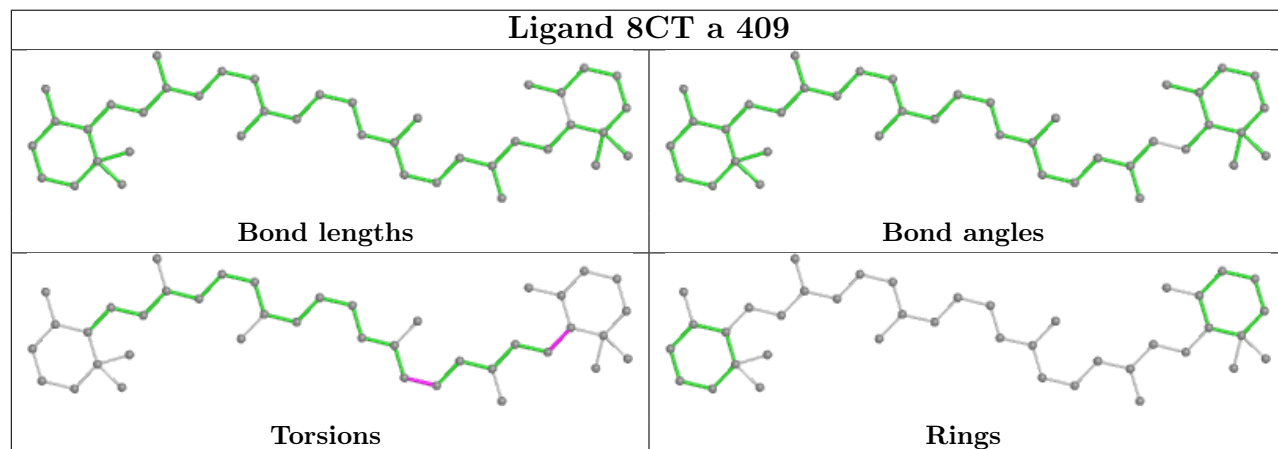
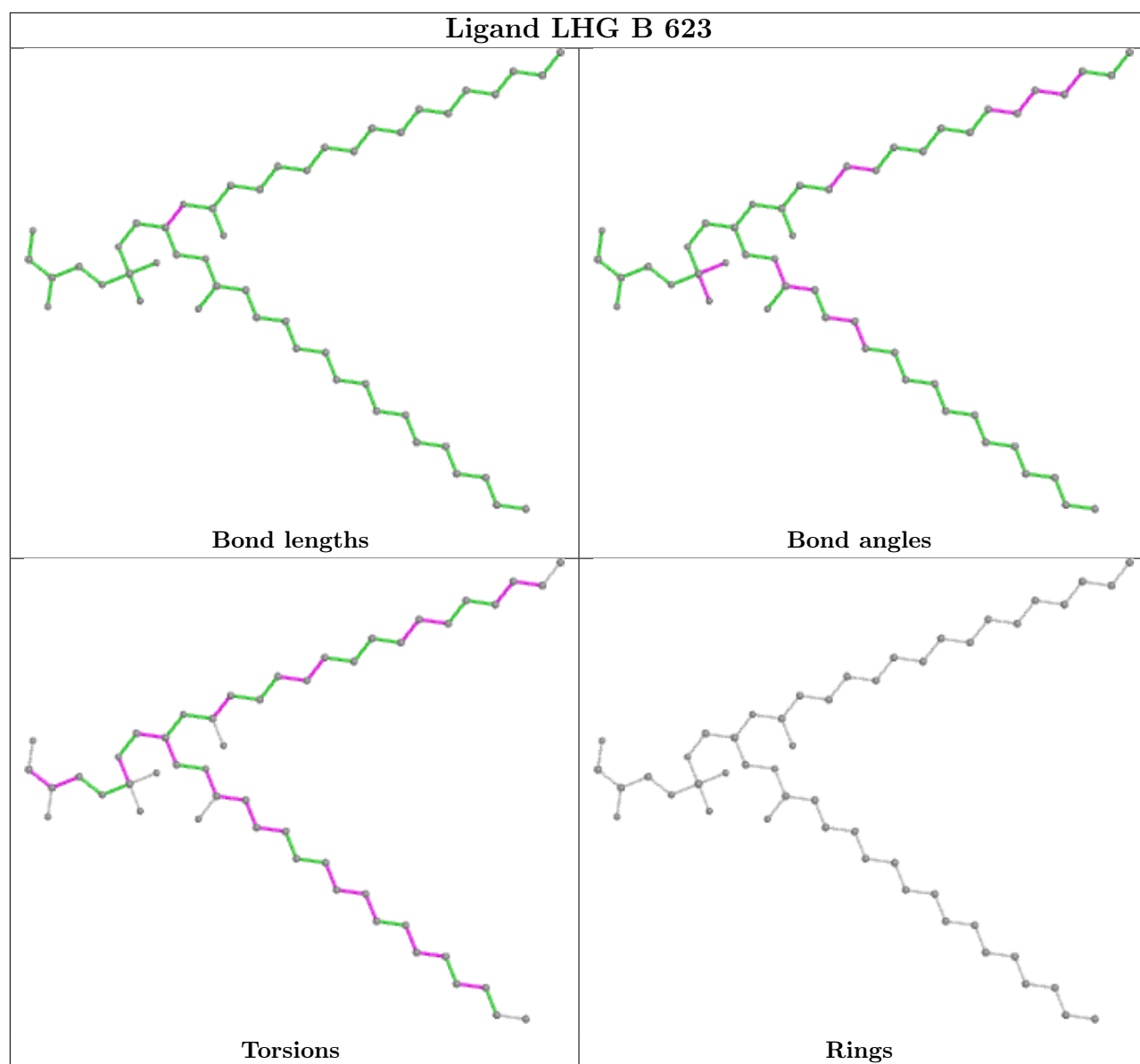
Bond angles



Torsions

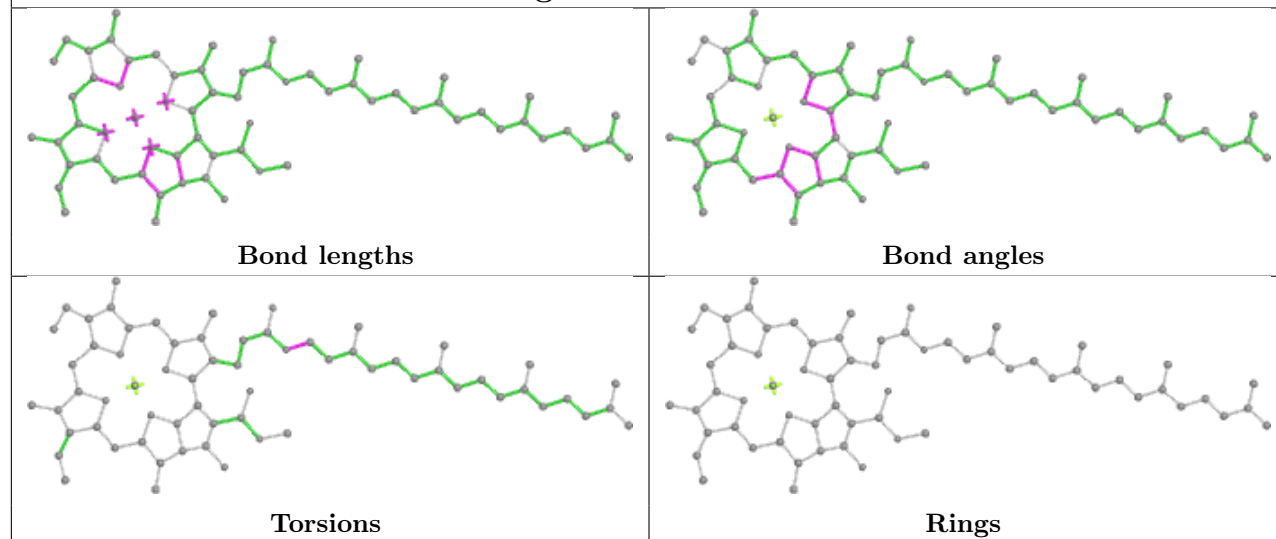


Rings

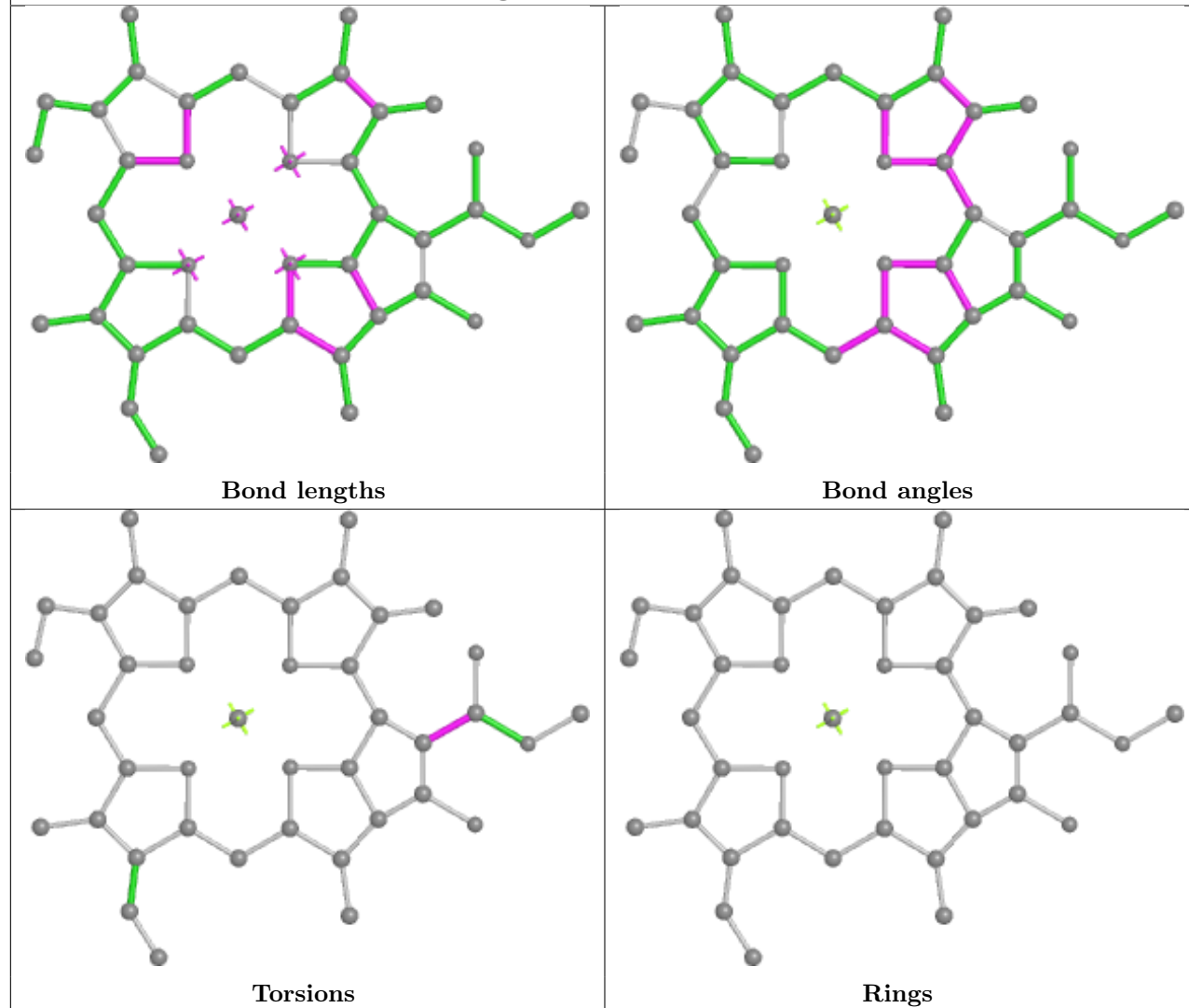




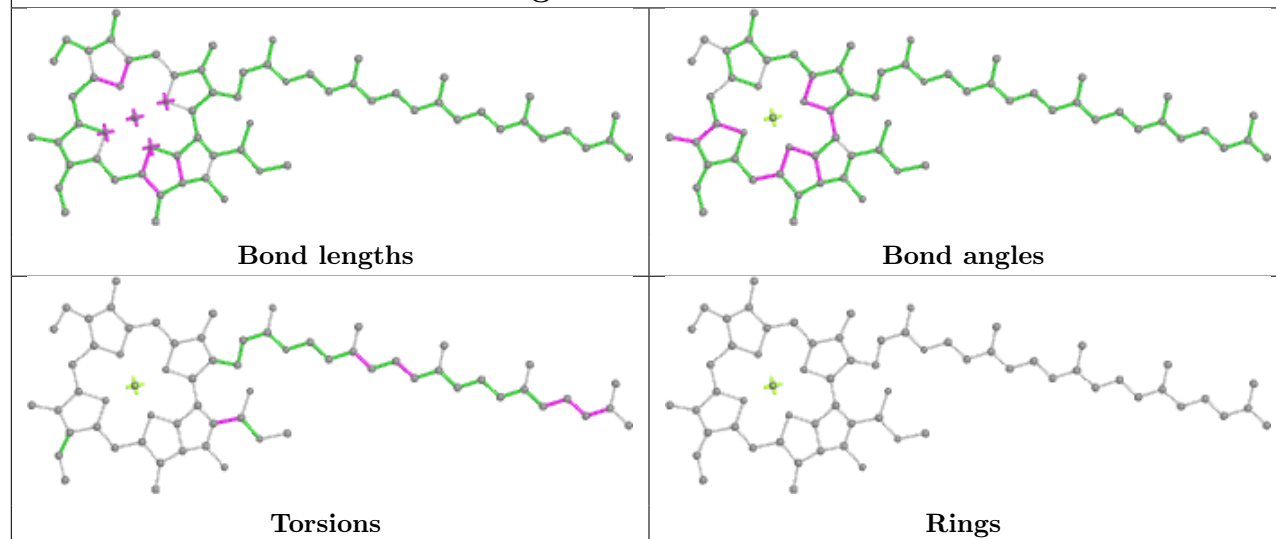
## Ligand CLA d 404



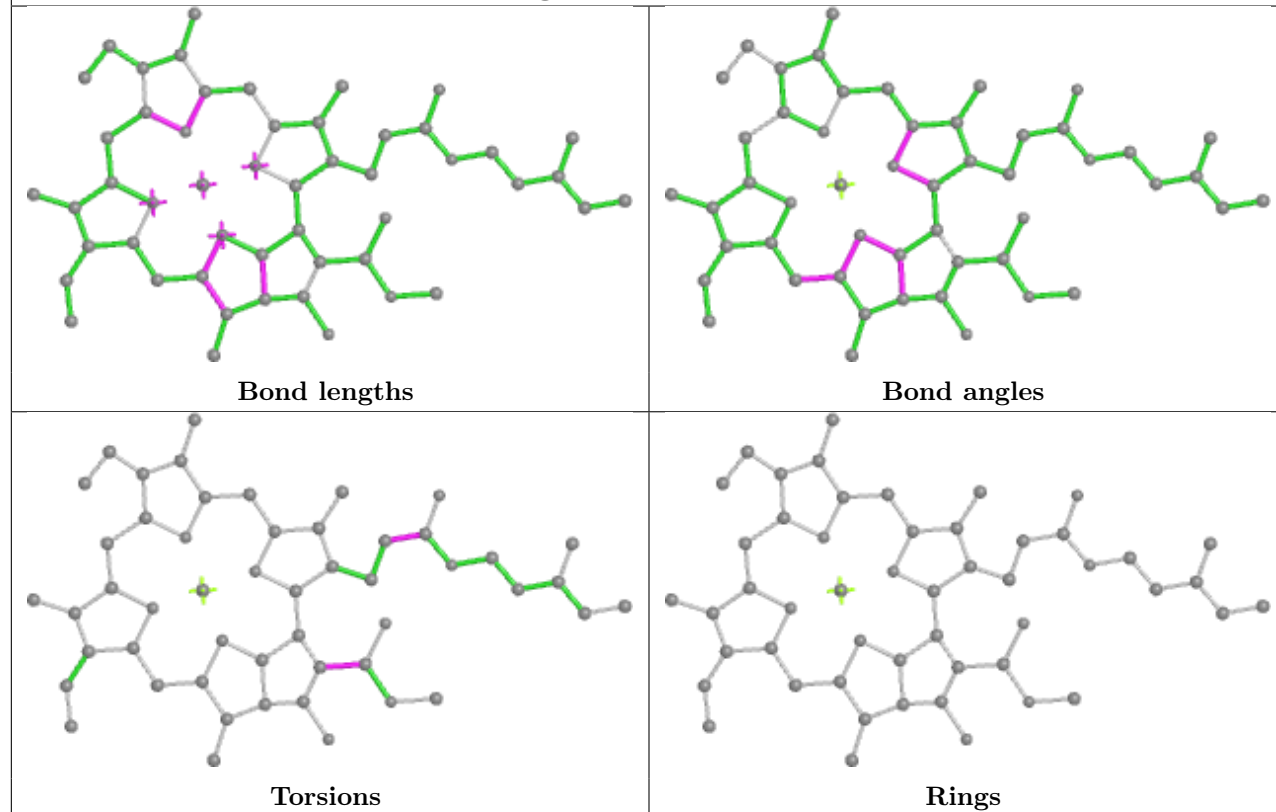
## Ligand CLA N 304

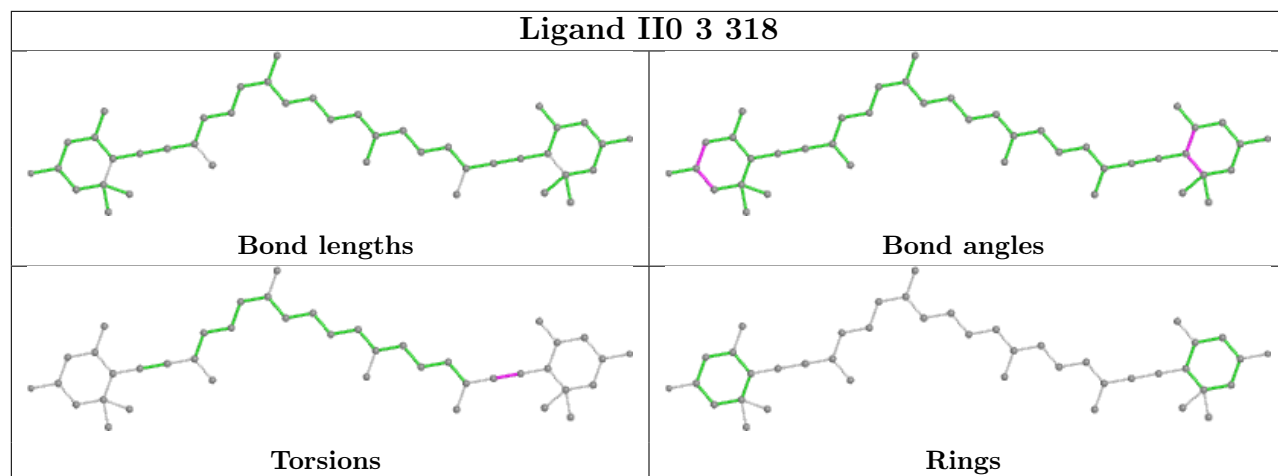
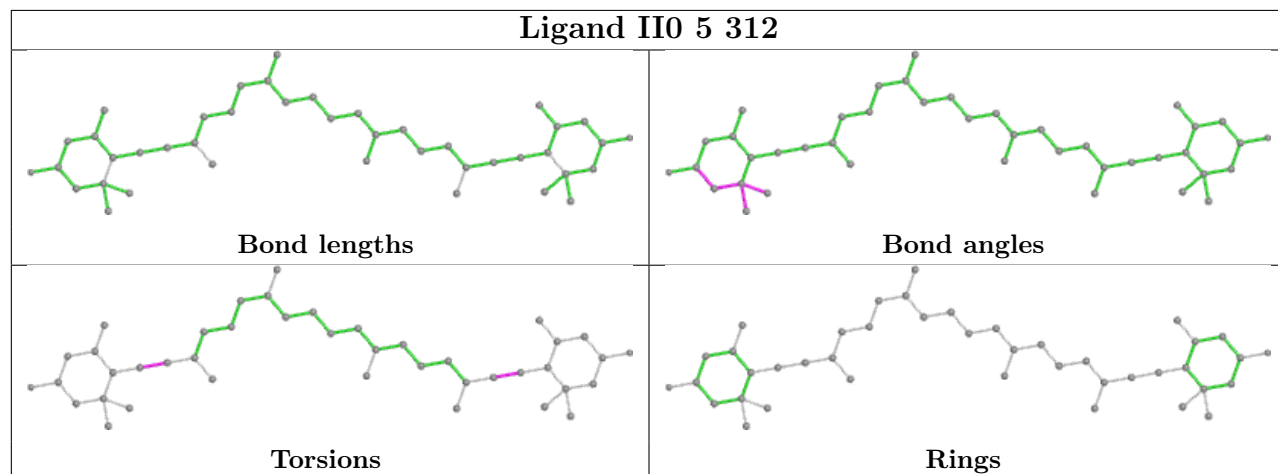
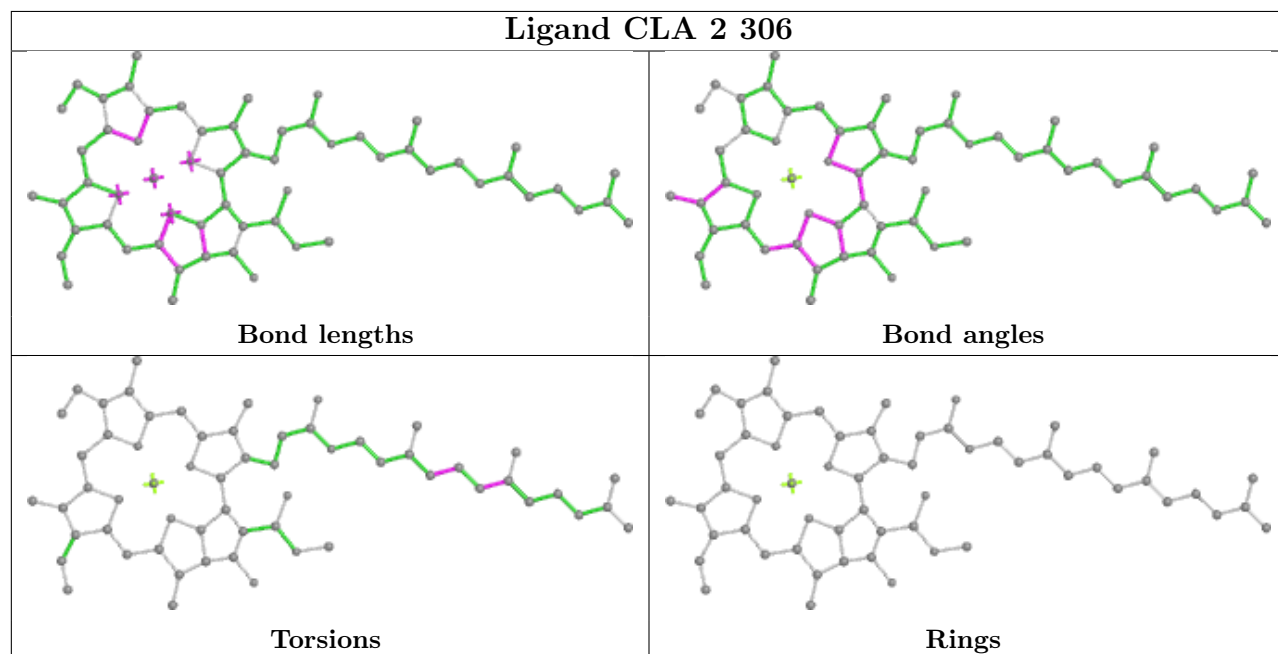


## Ligand CLA B 610

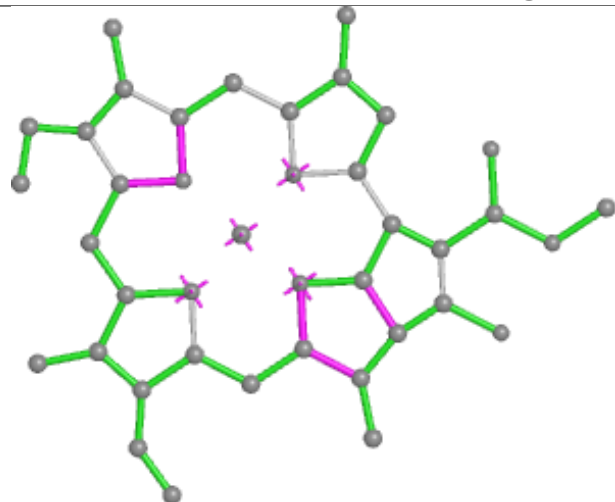


## Ligand CLA 1 303

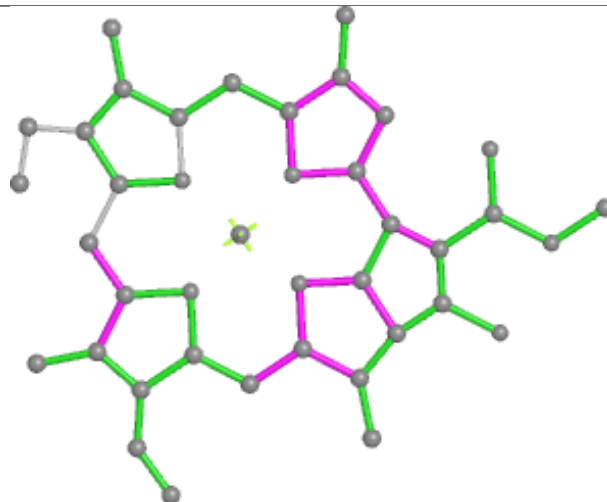


**Ligand II0 3 318****Ligand II0 5 312****Ligand CLA 2 306**

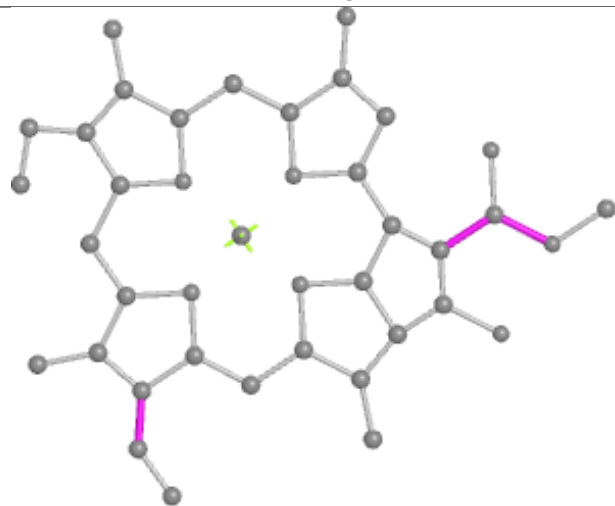
## Ligand CLA 0 310



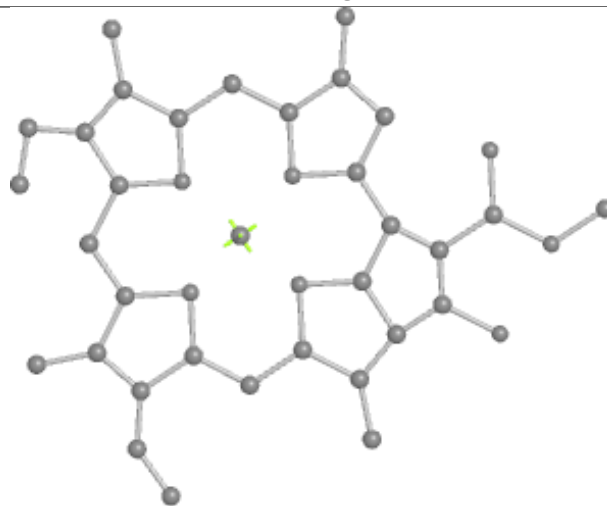
Bond lengths



Bond angles

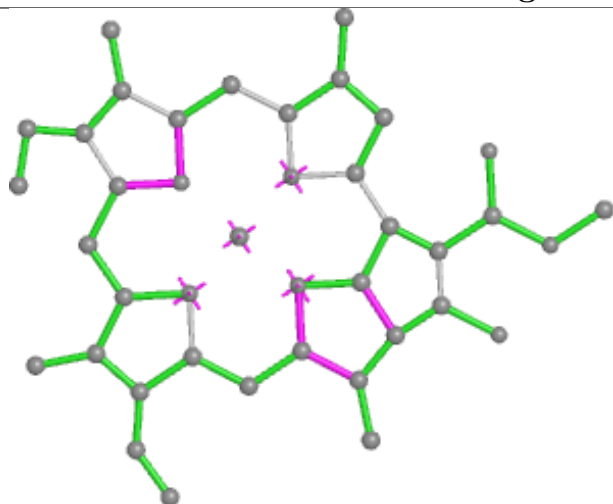


Torsions

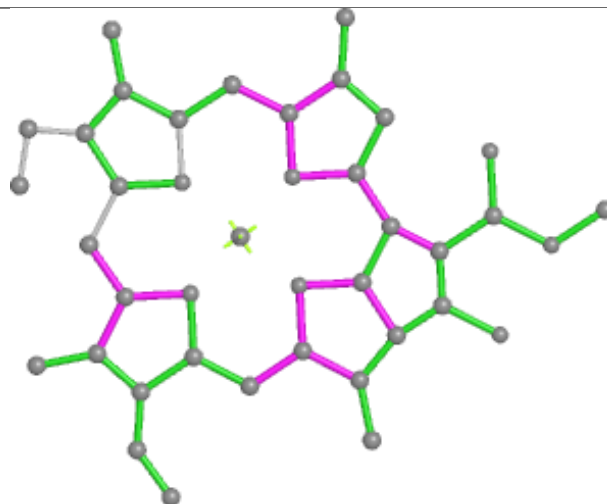


Rings

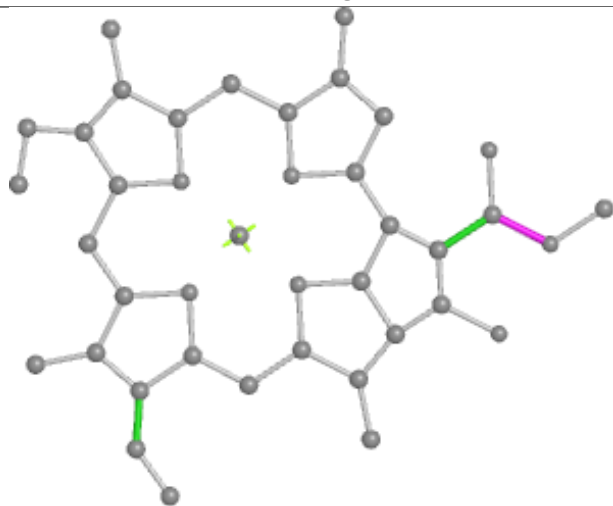
## Ligand CLA 5 305



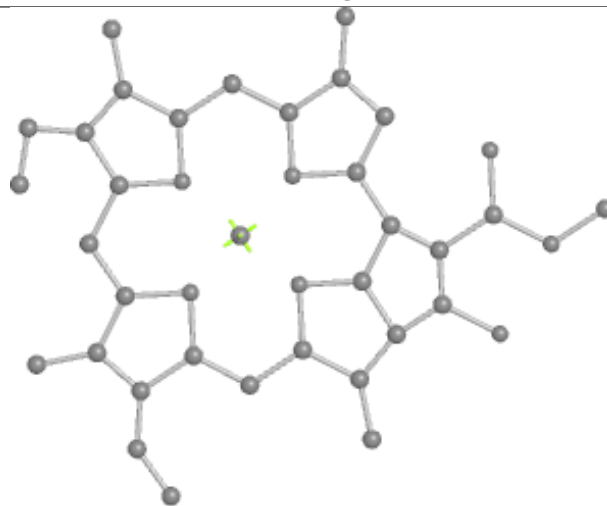
Bond lengths



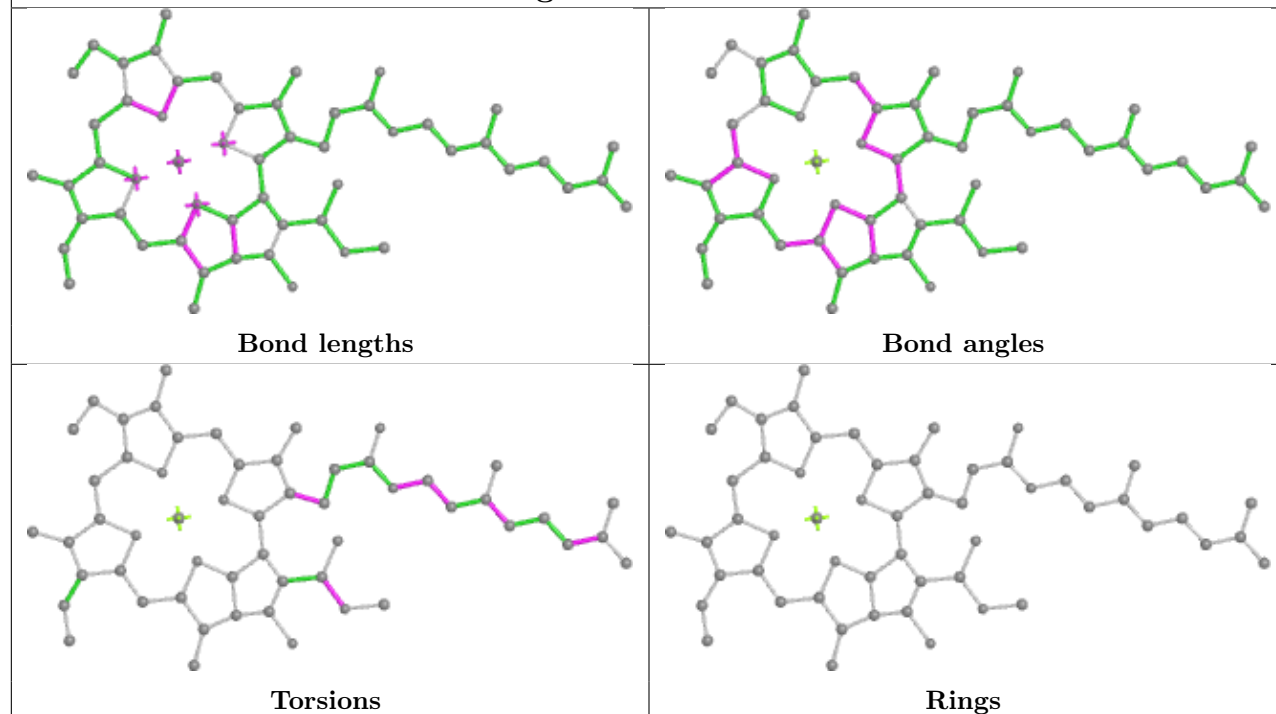
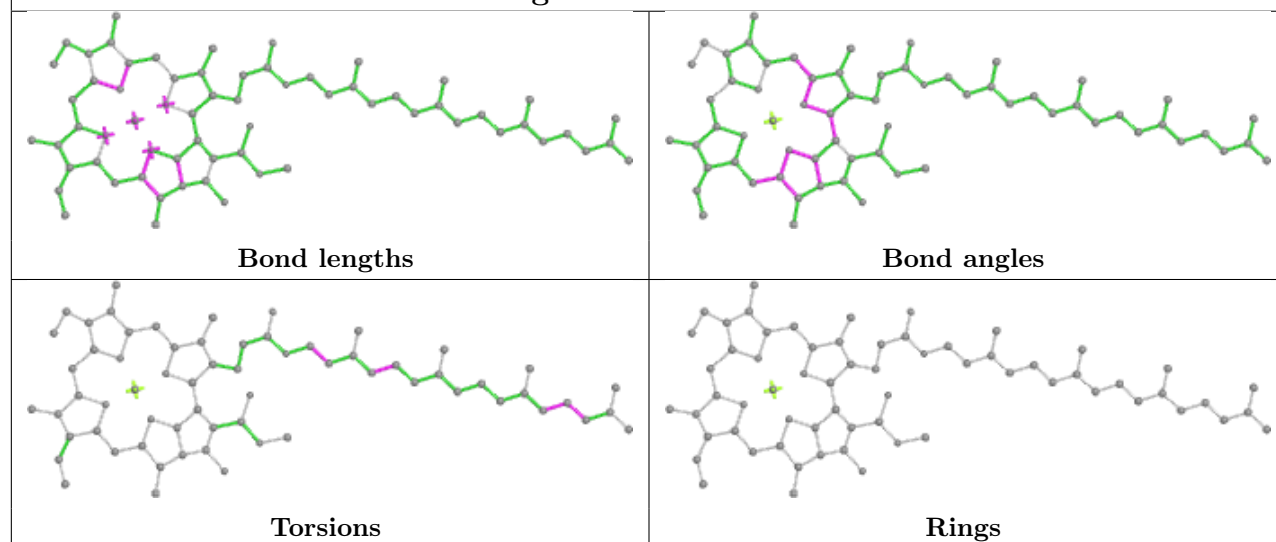
Bond angles



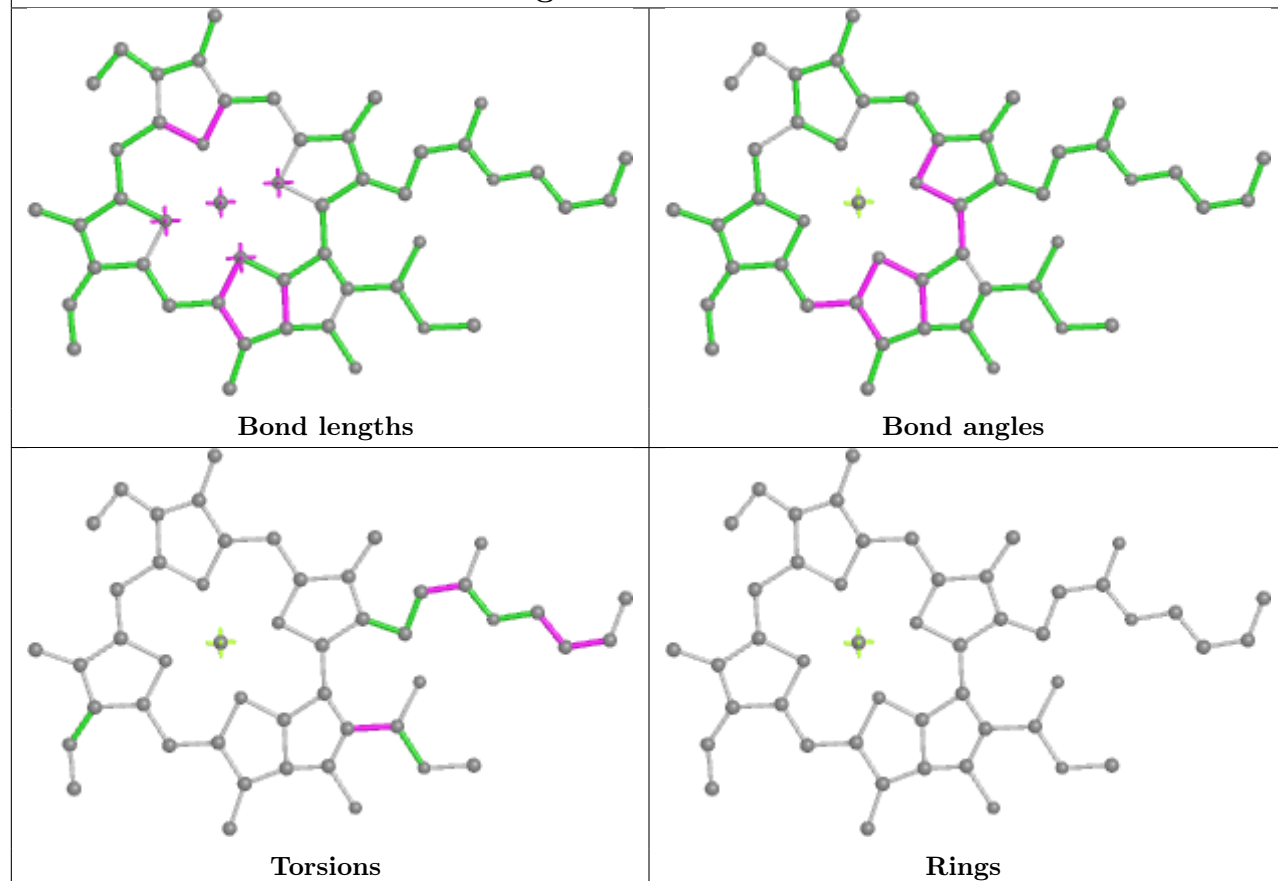
Torsions



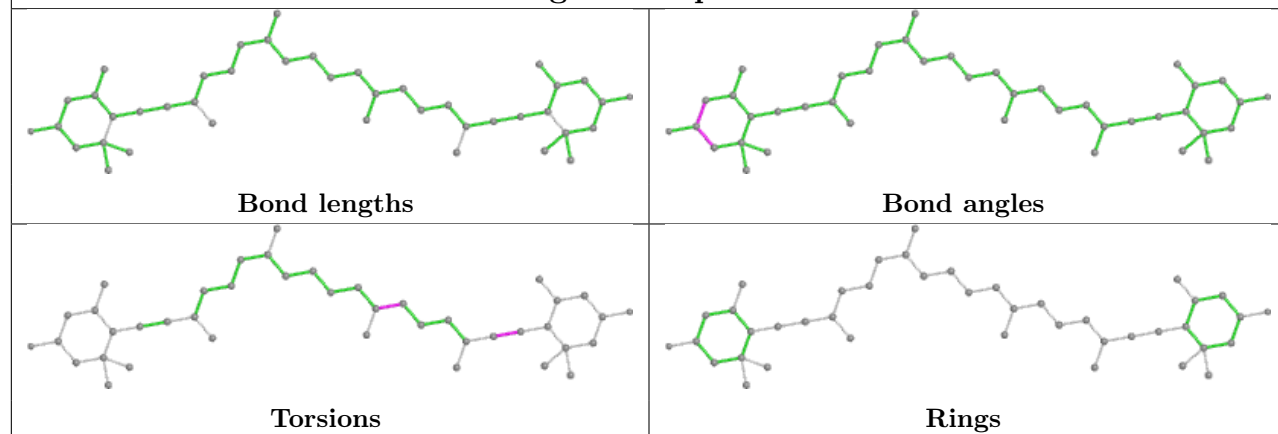
Rings

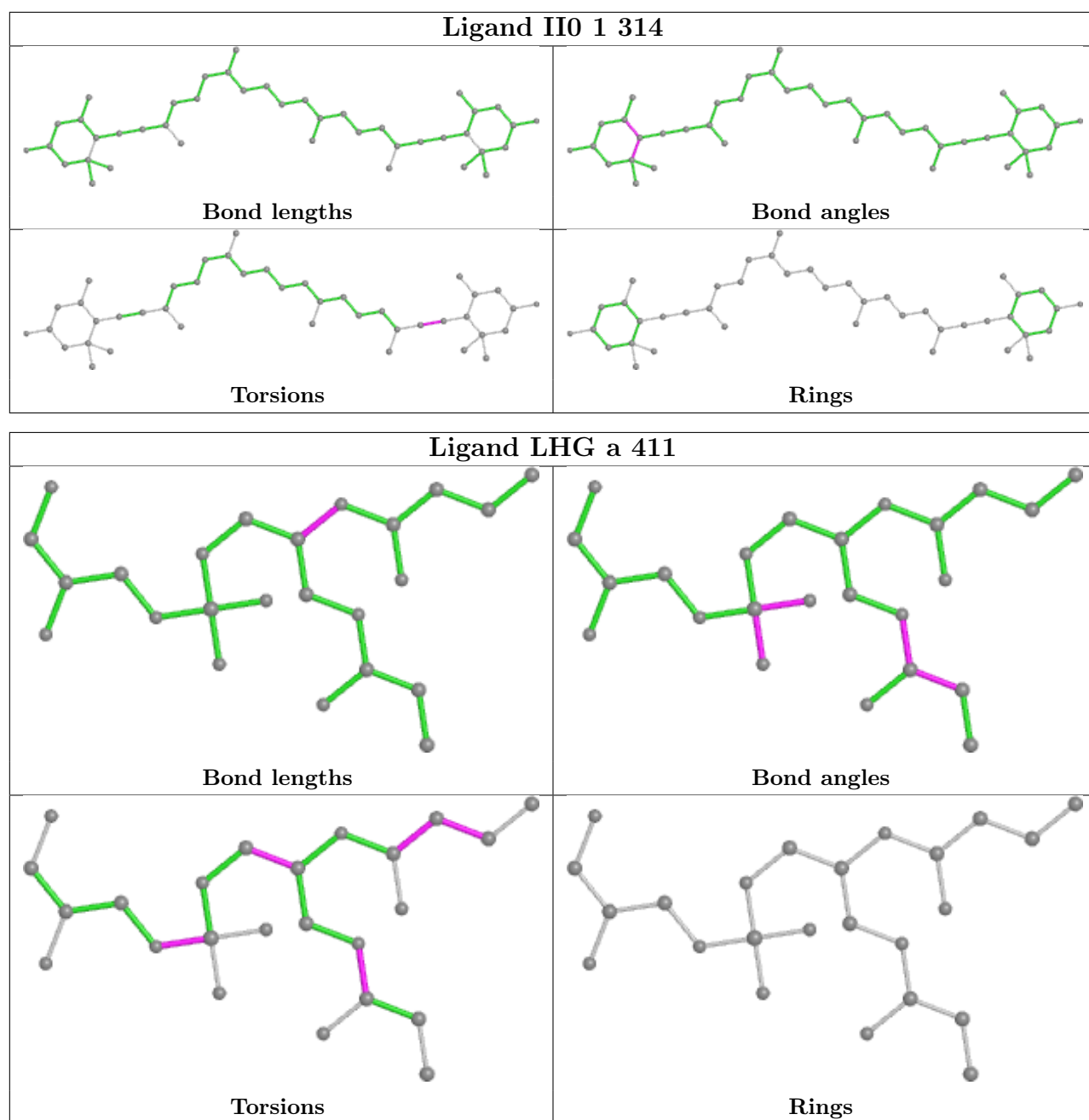
**Ligand CLA 0 306****Ligand CLA A 405****Ligand IHT 9 320**

## Ligand CLA a 406



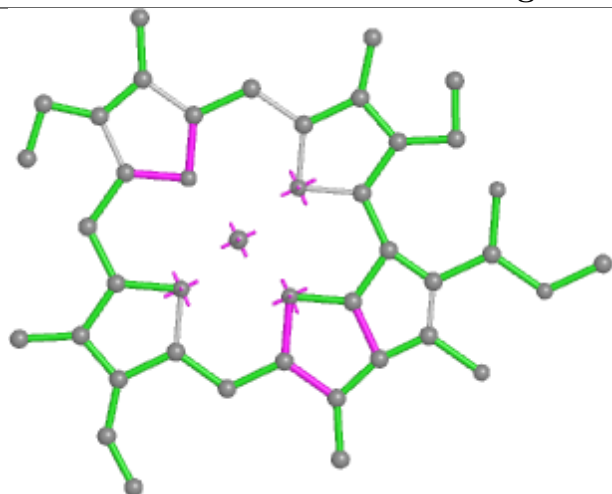
## Ligand II0 p 317



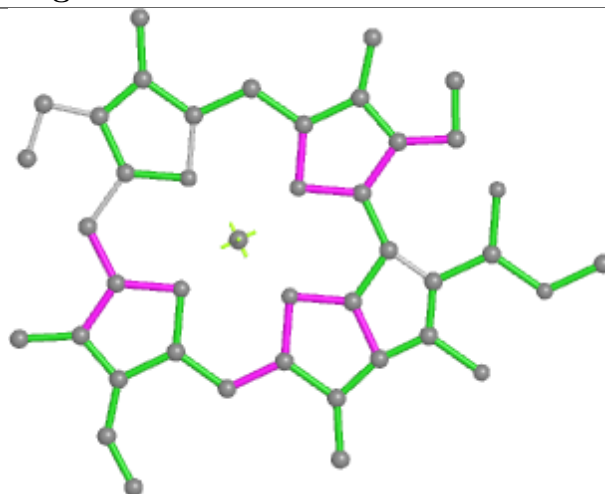




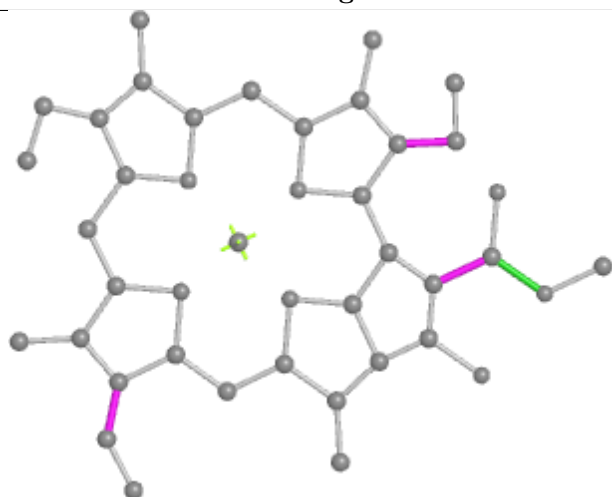
## Ligand CLA g 301



Bond lengths



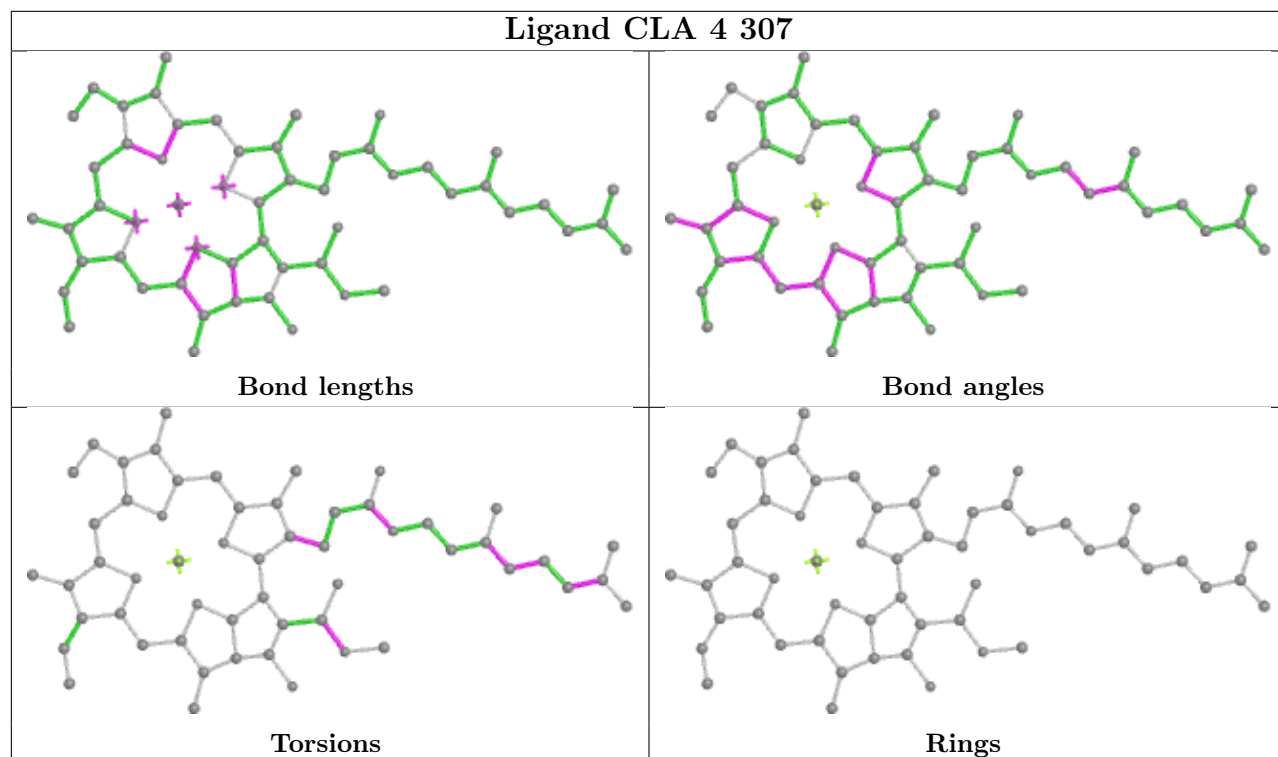
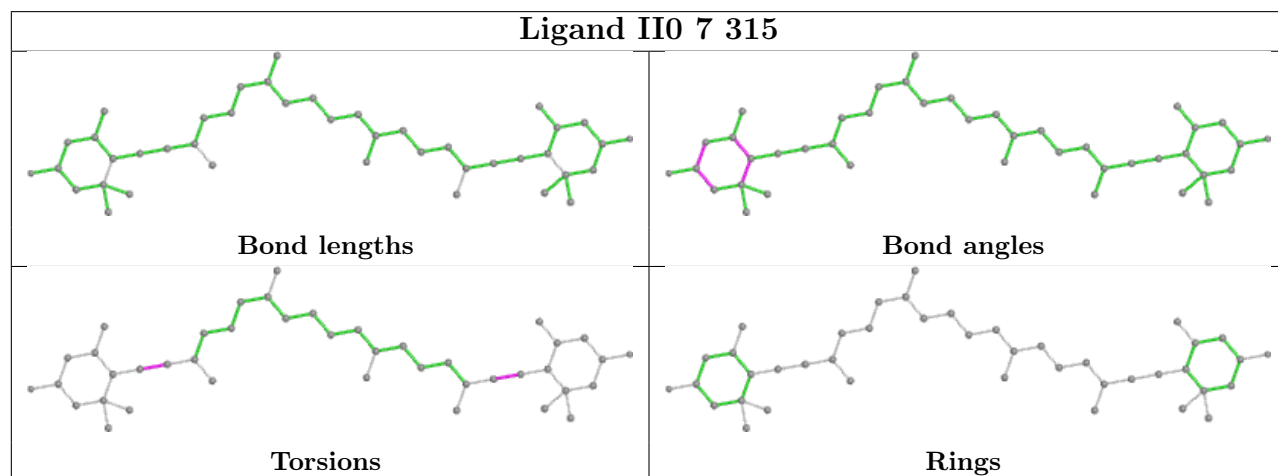
Bond angles

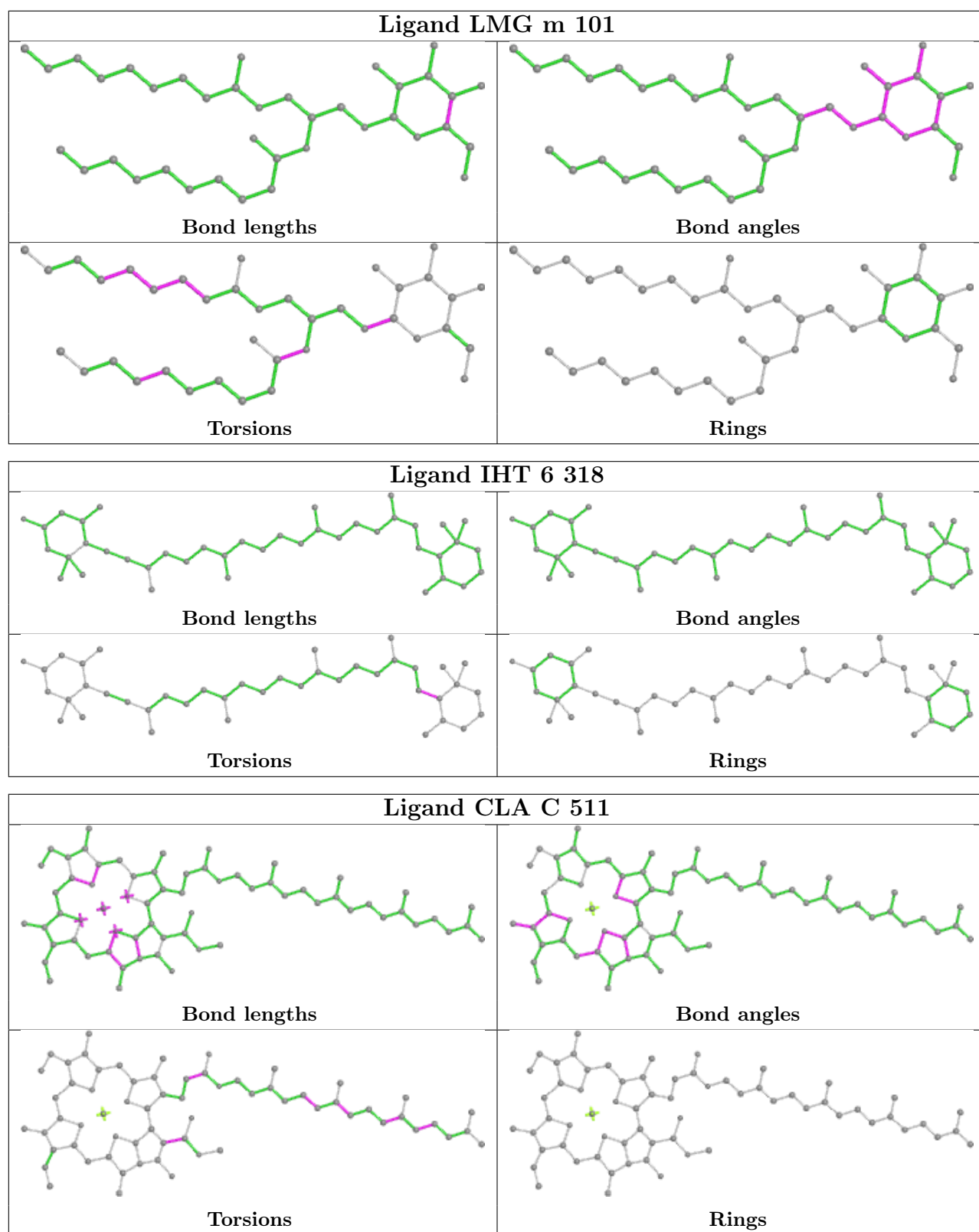


Torsions

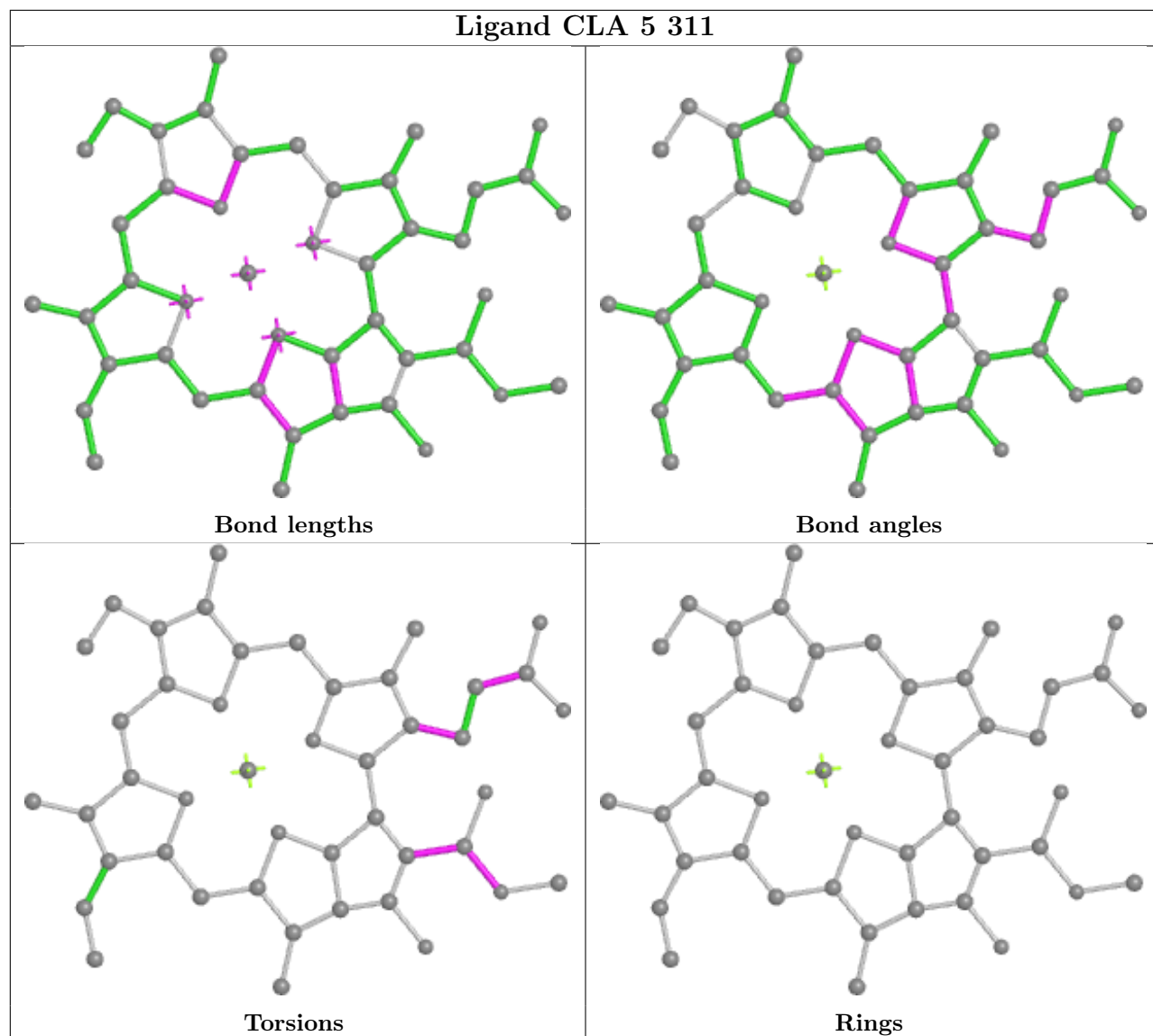


Rings

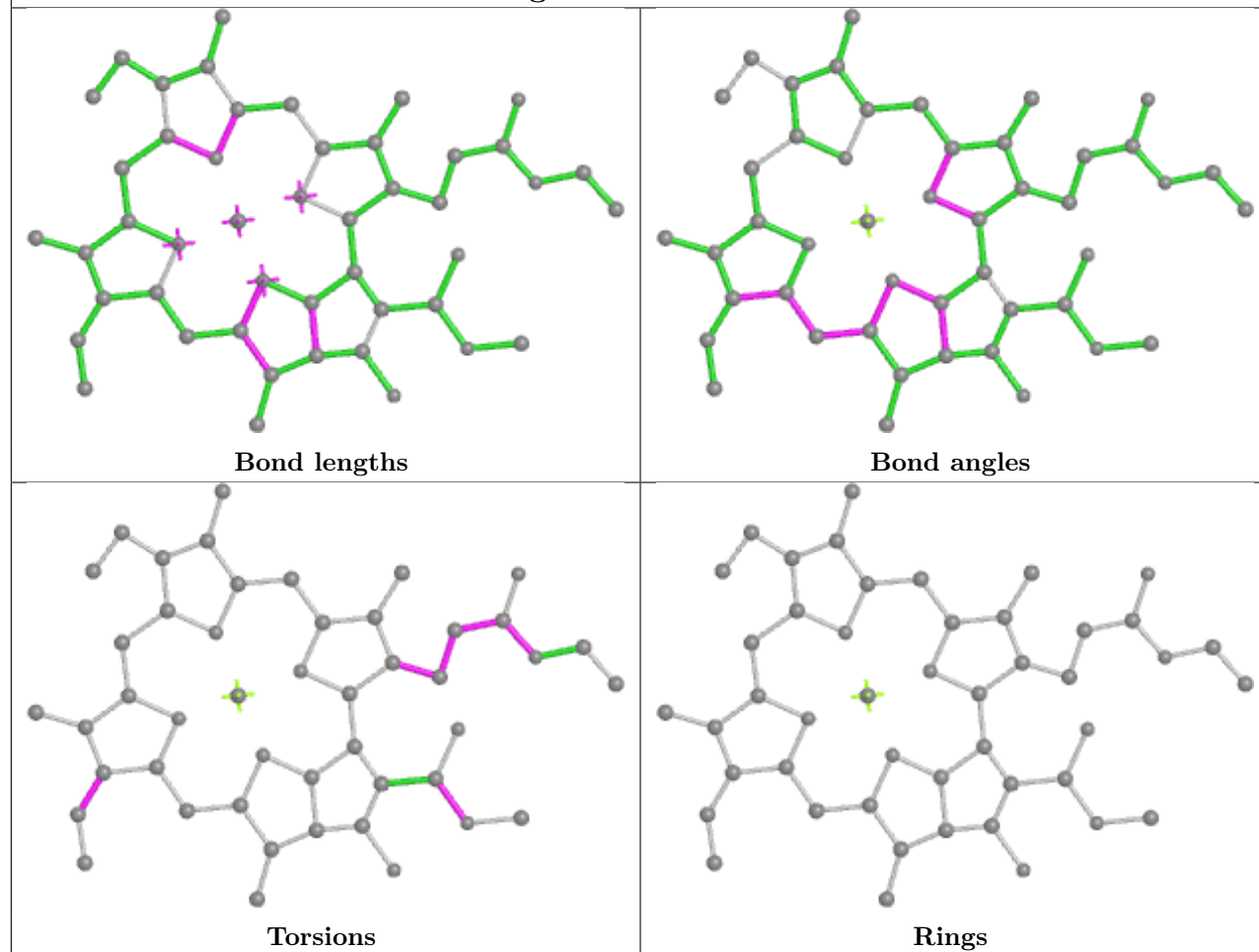
**Ligand CLA 4 307****Ligand II0 7 315**



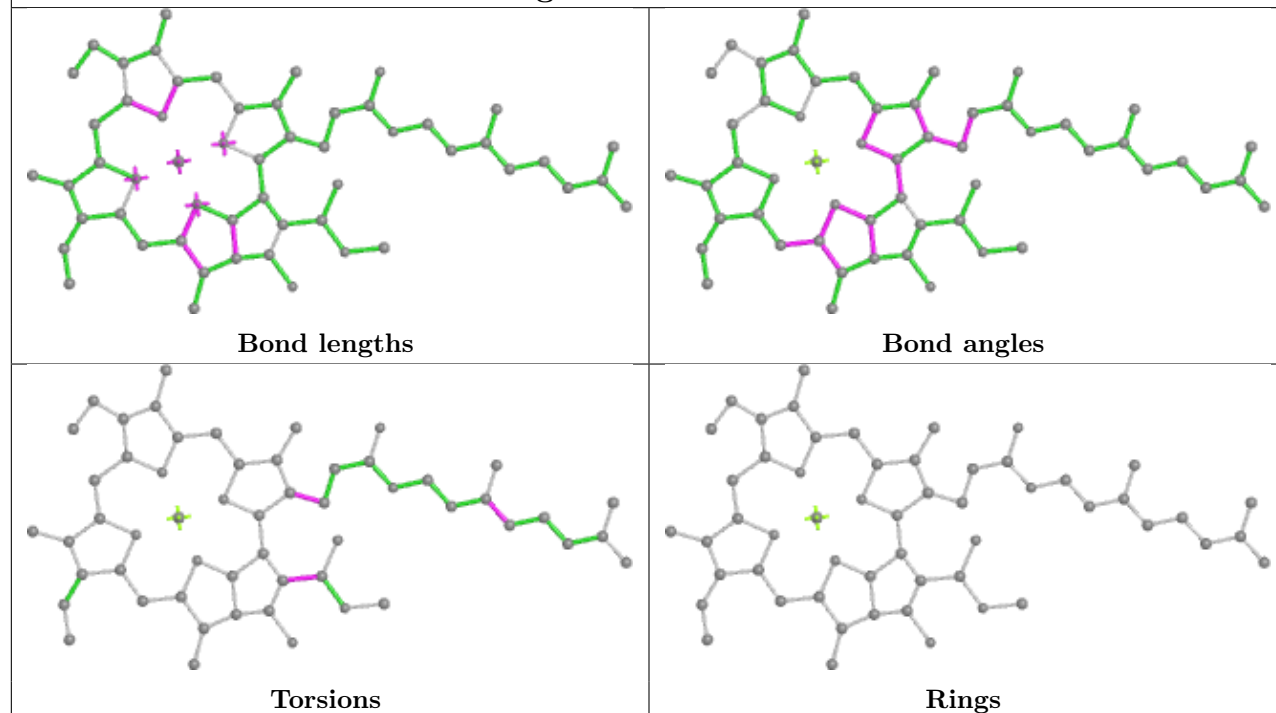
## Ligand CLA 5 311

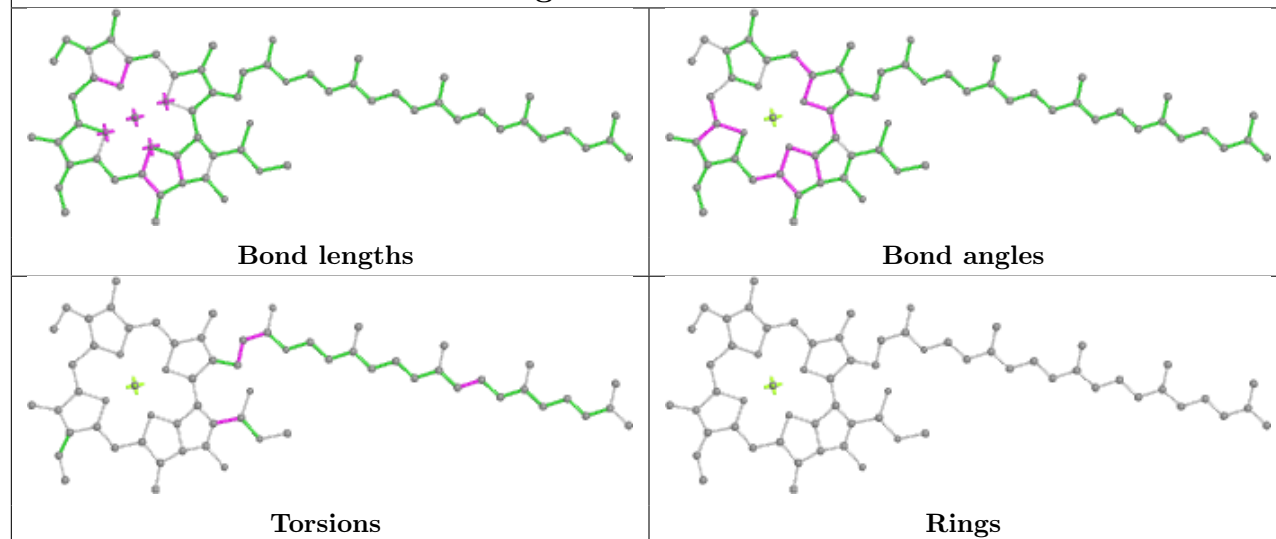
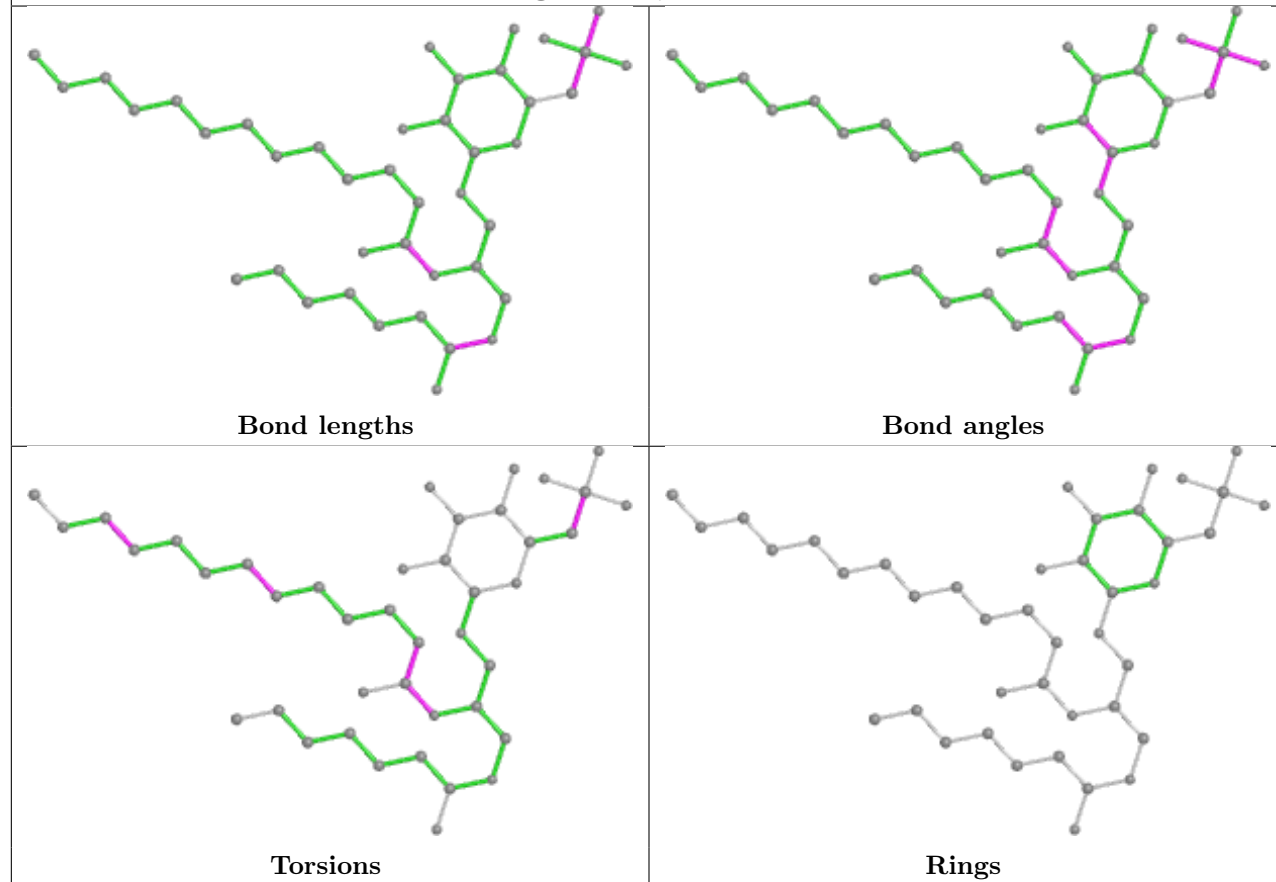


## Ligand CLA 0 309

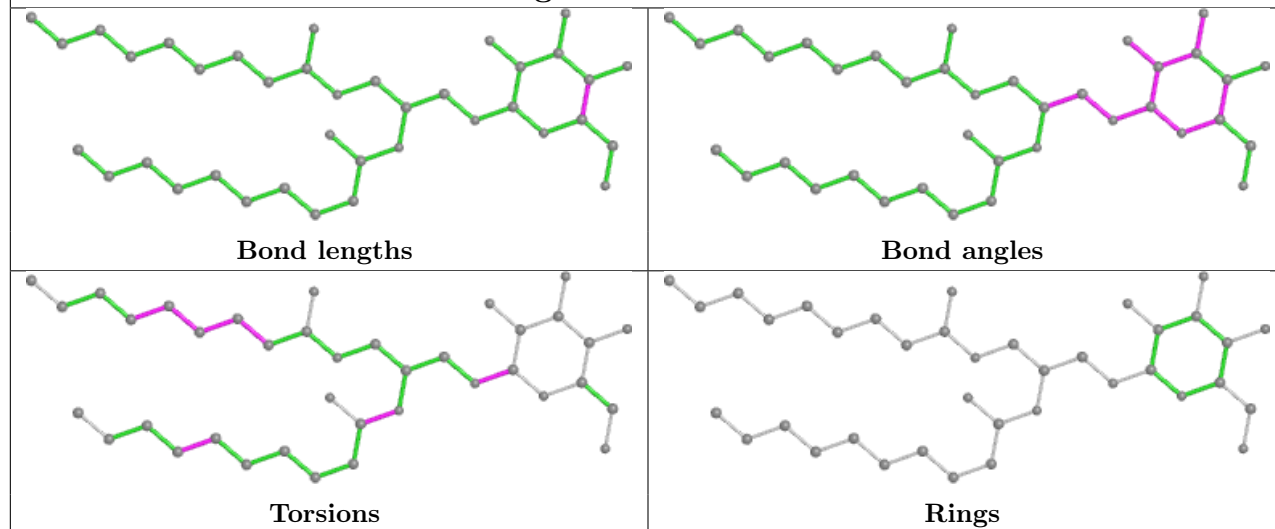


## Ligand CLA 9 309

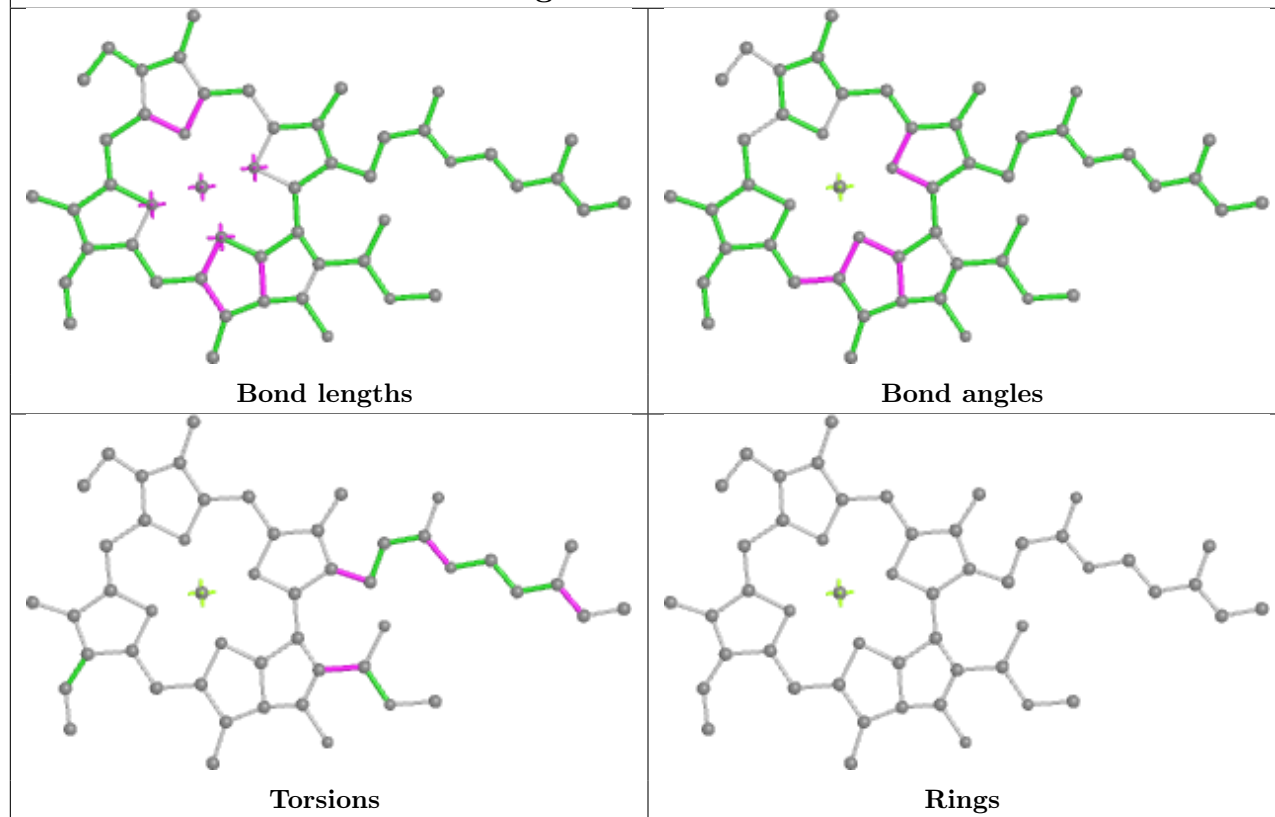


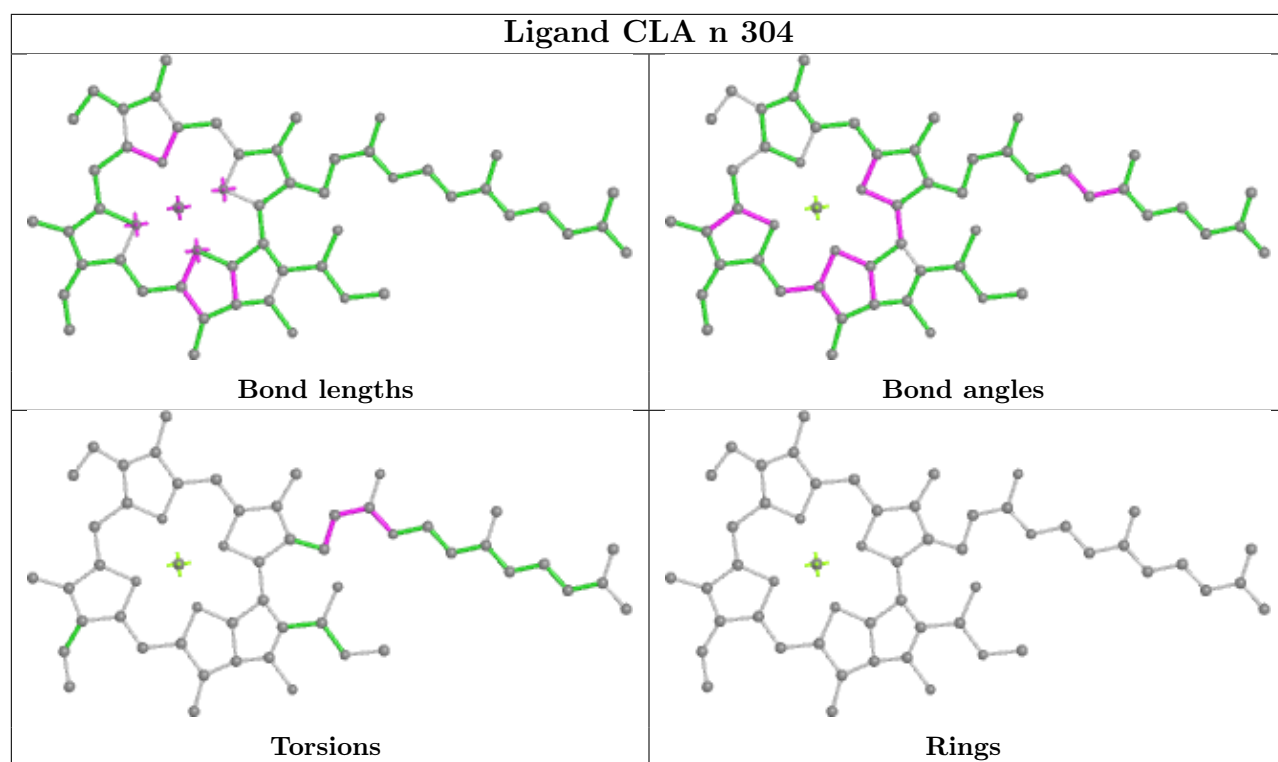
**Ligand CLA b 611****Ligand SQD C 501**

## Ligand LMG 1 102

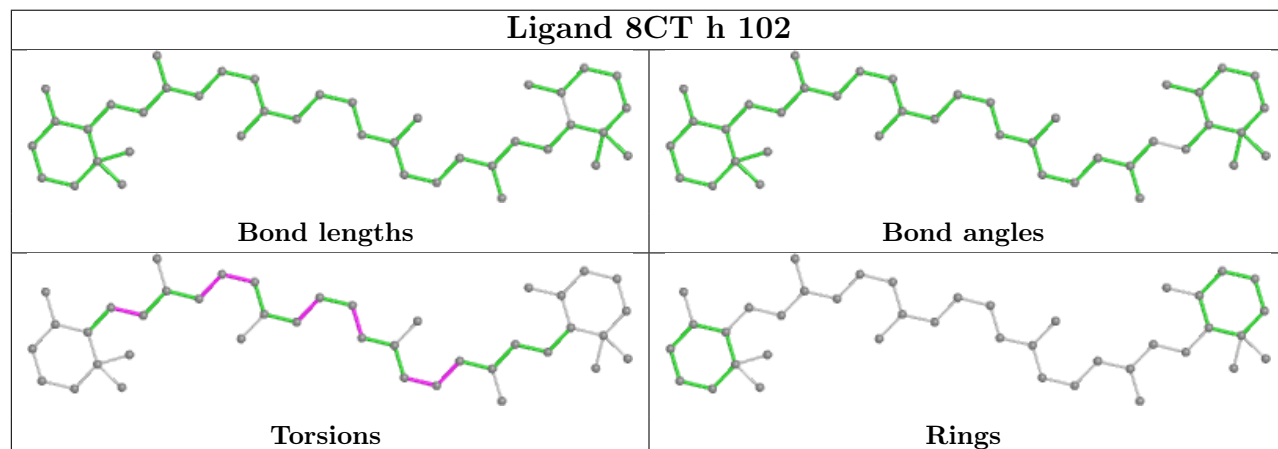
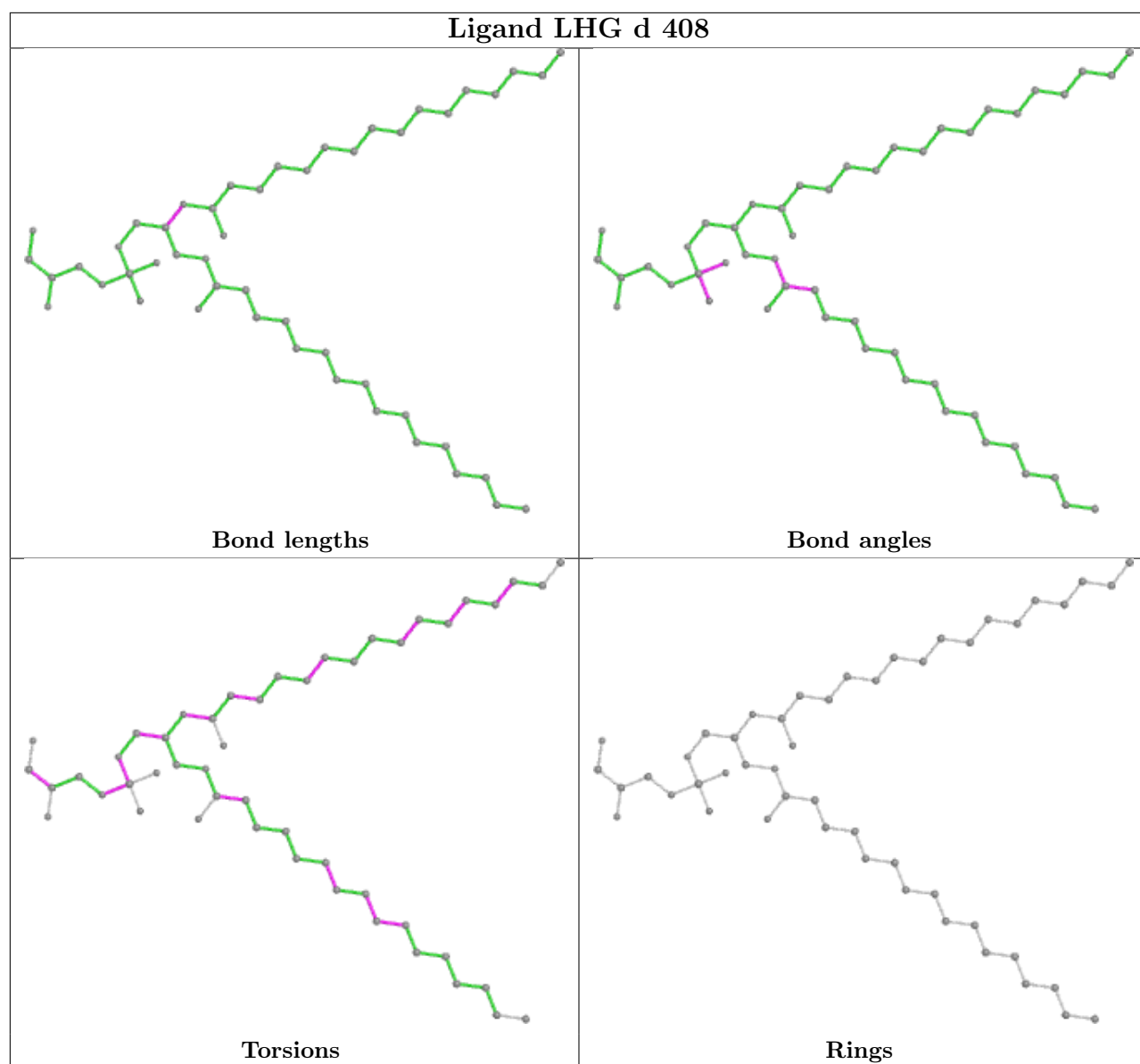


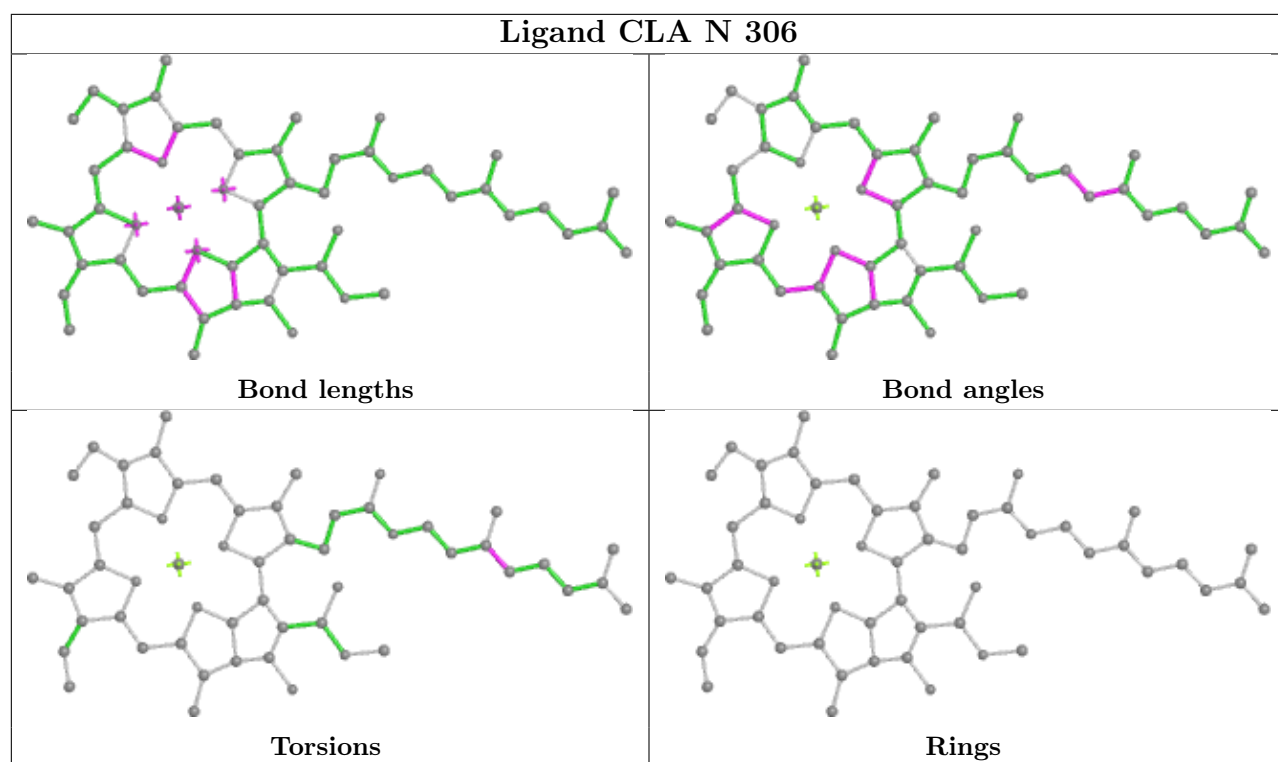
## Ligand CLA 7 308



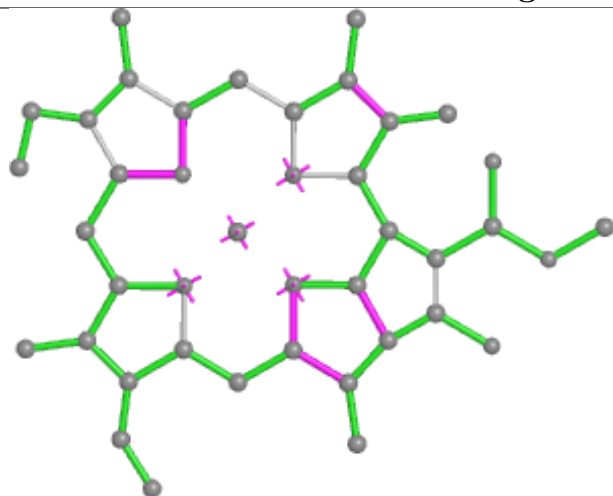




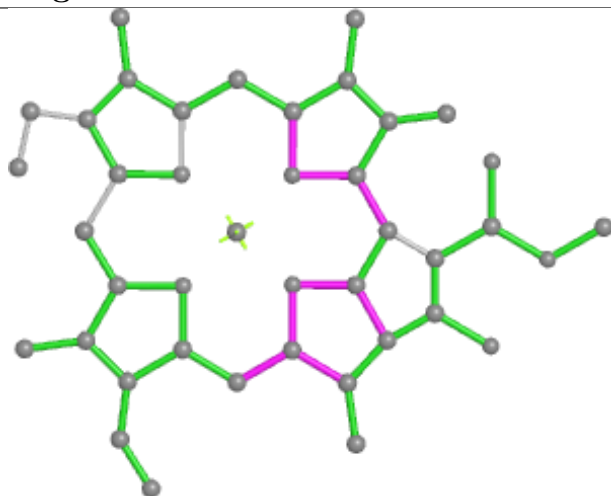




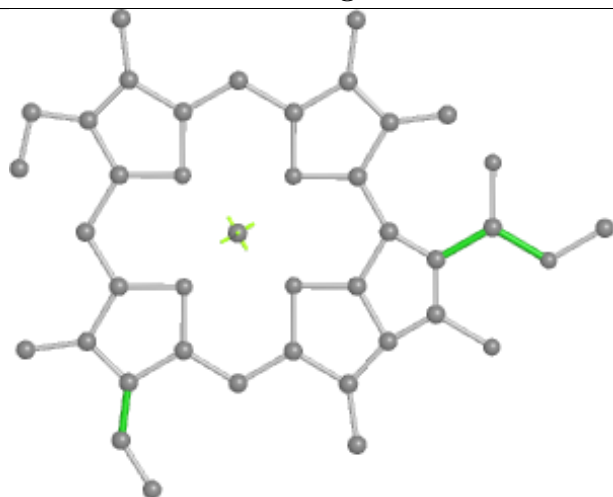
## Ligand CLA g 310



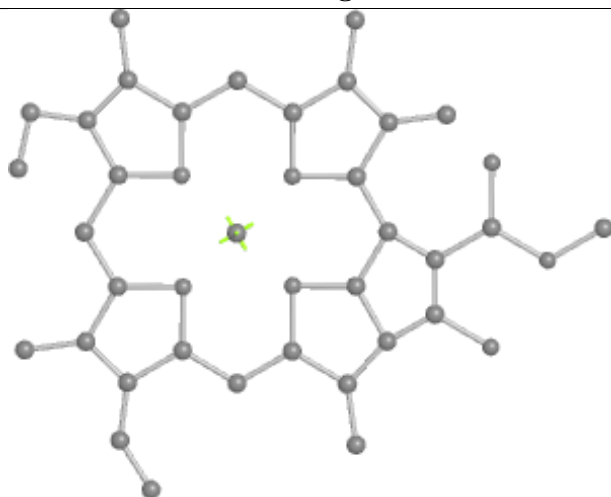
Bond lengths



Bond angles

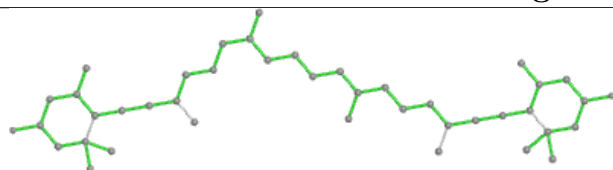


Torsions

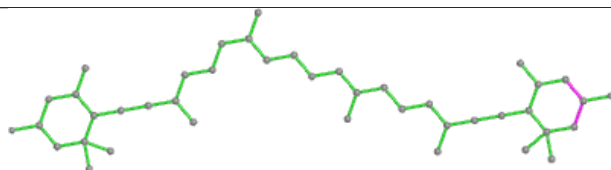


Rings

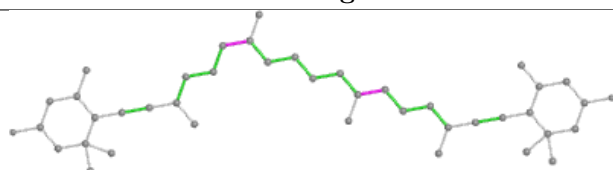
## Ligand II0 3 316



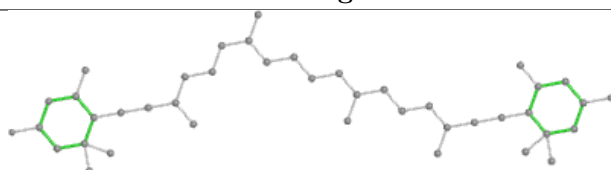
Bond lengths



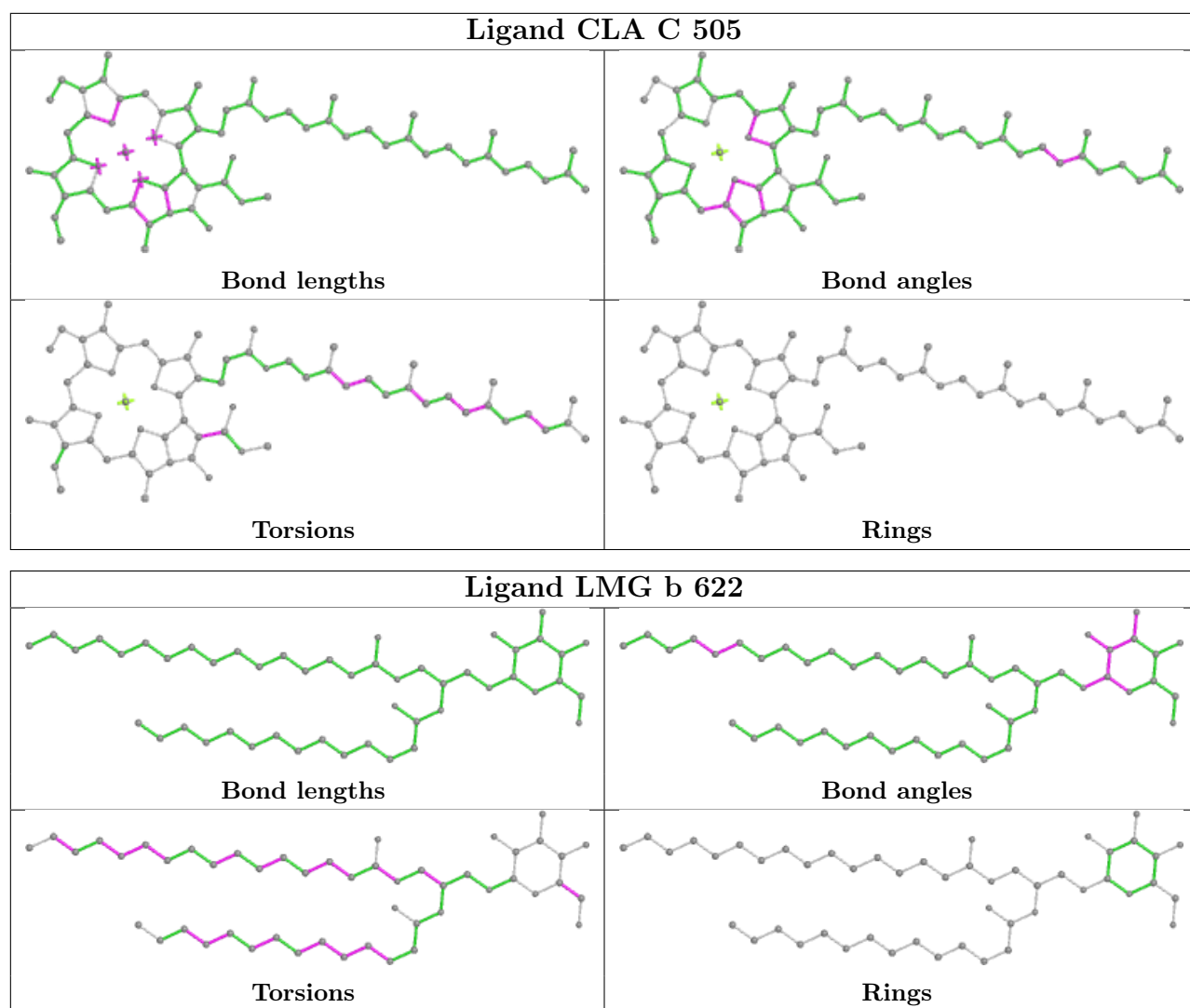
Bond angles



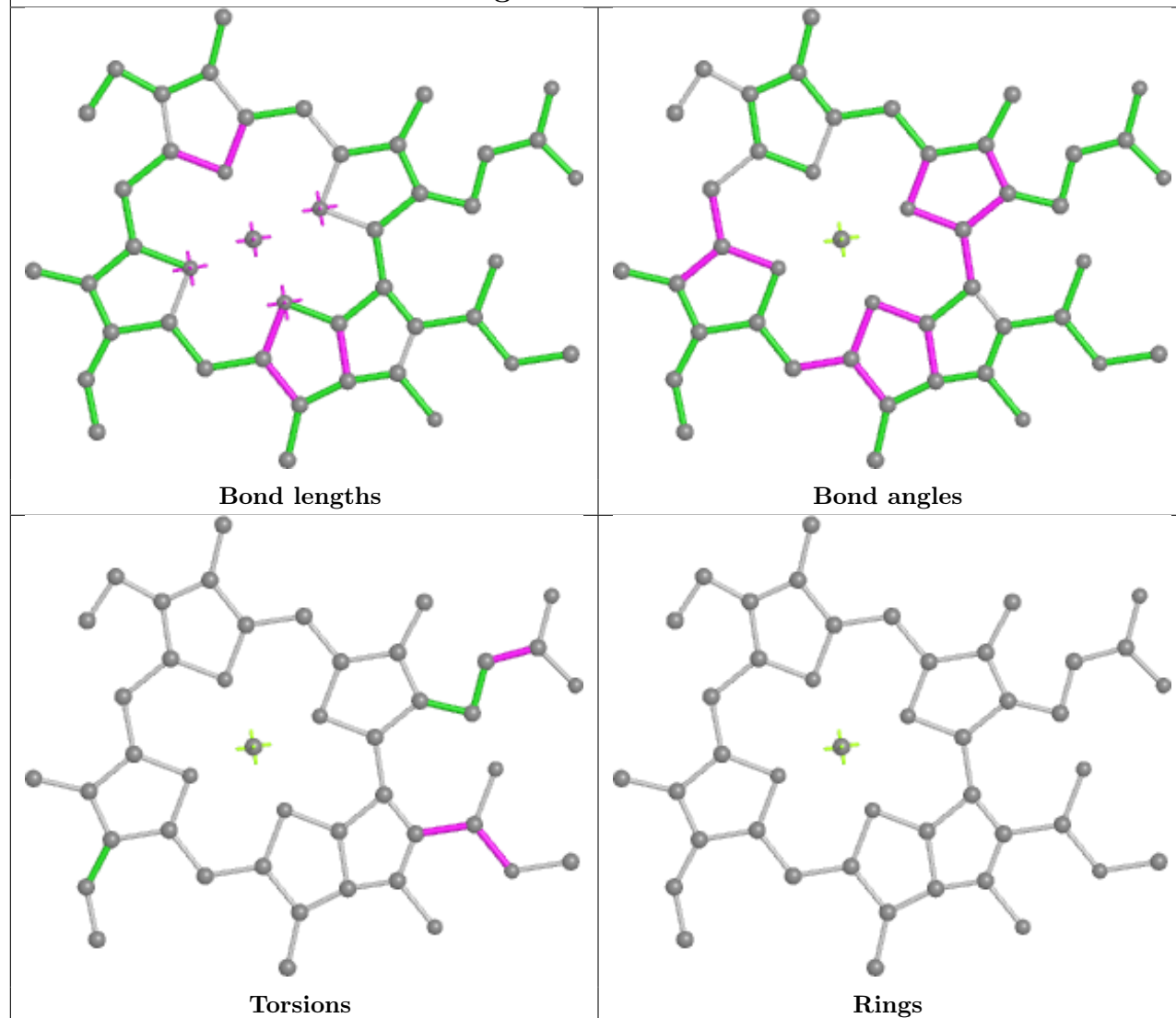
Torsions



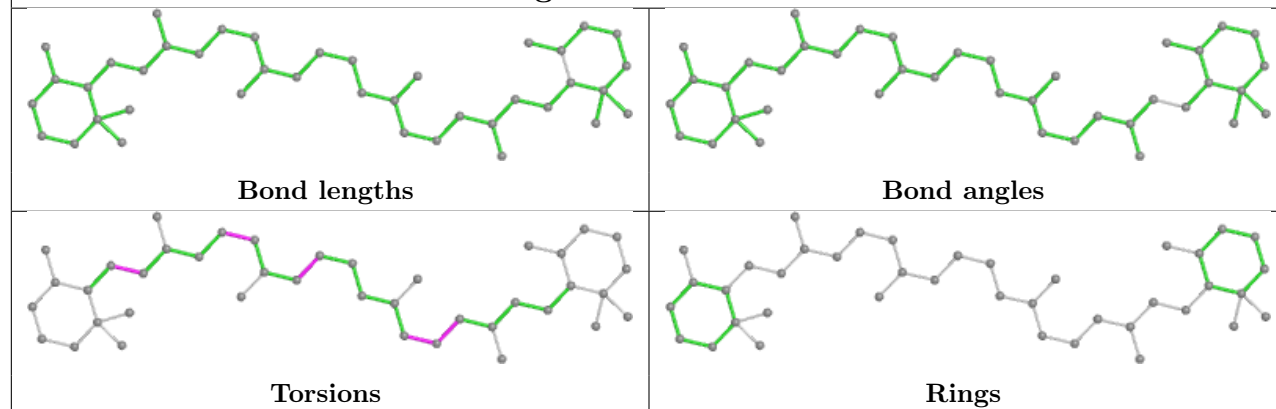
Rings

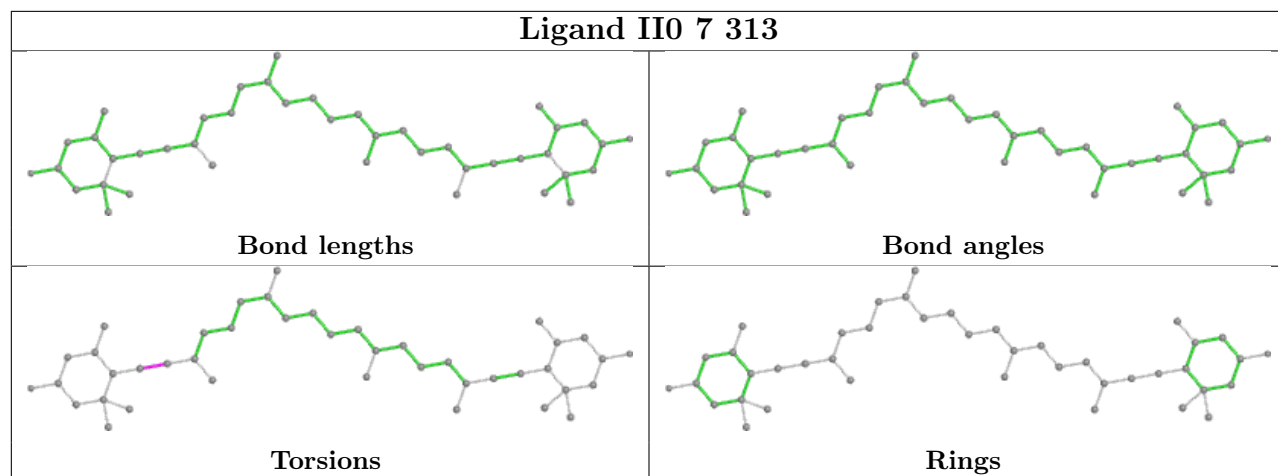
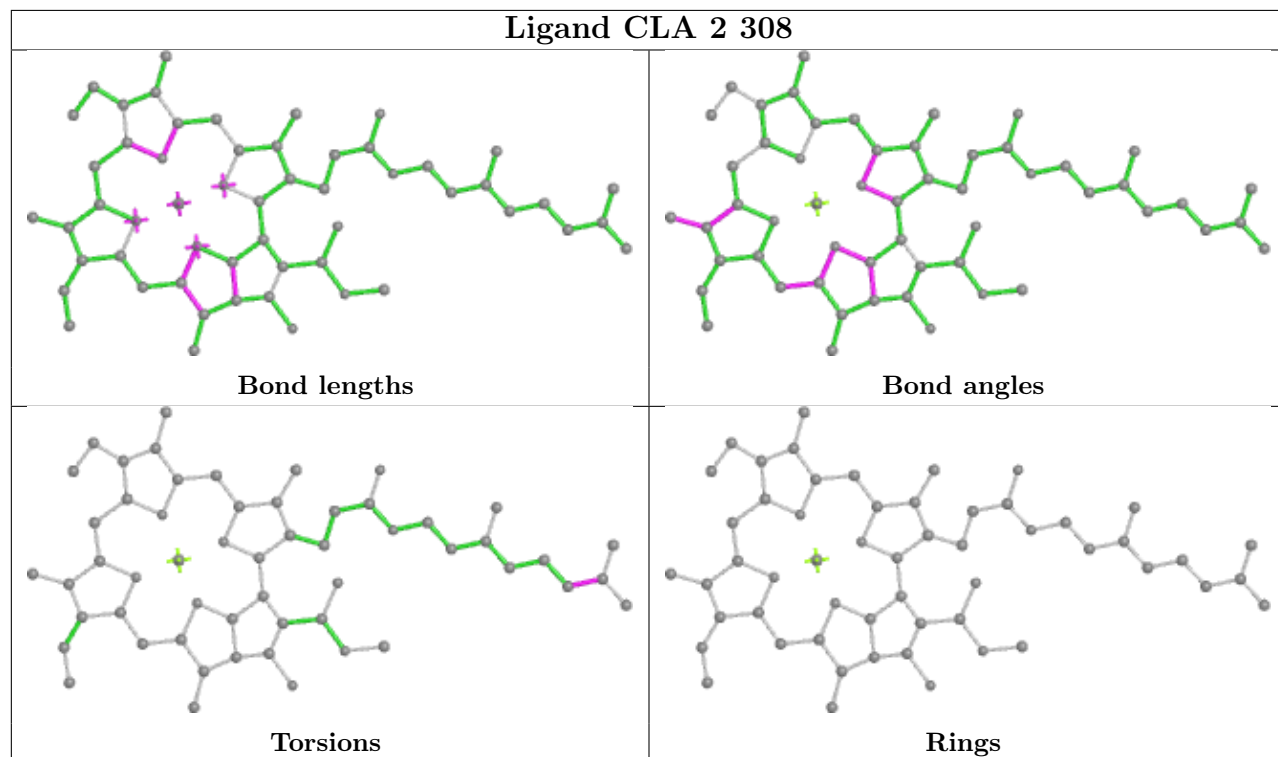


## Ligand CLA 0 311

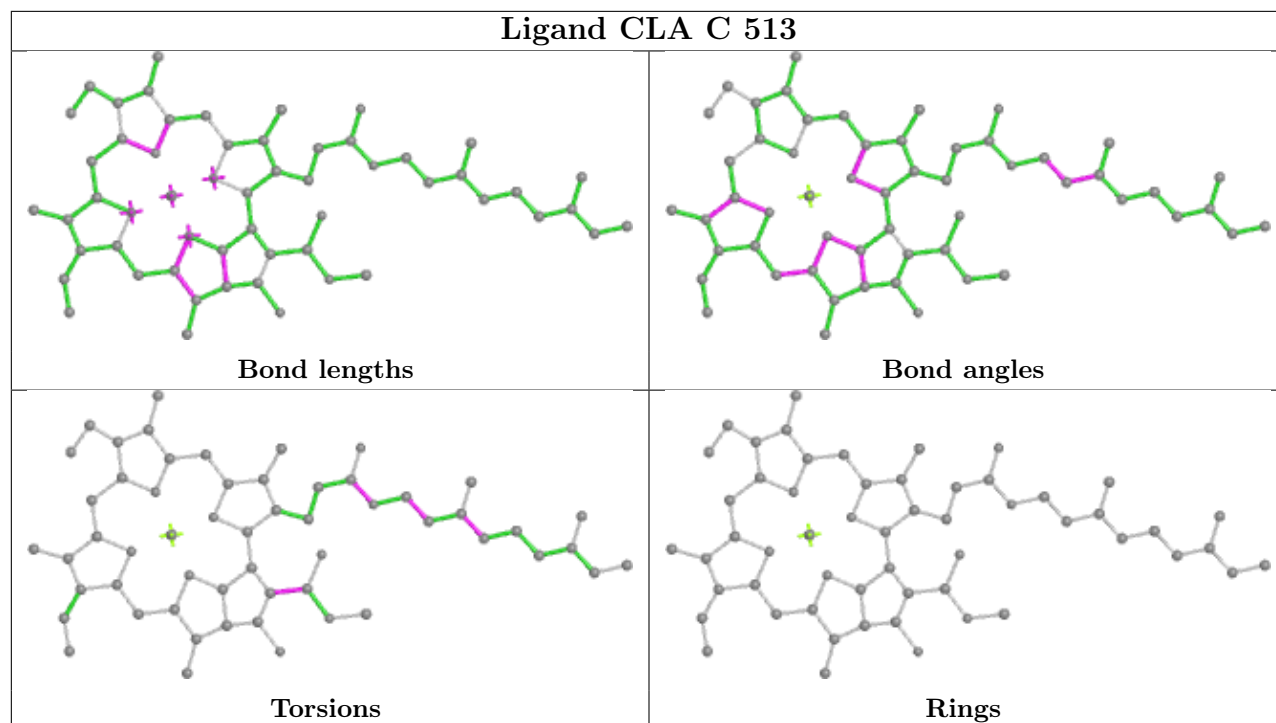


## Ligand 8CT C 516

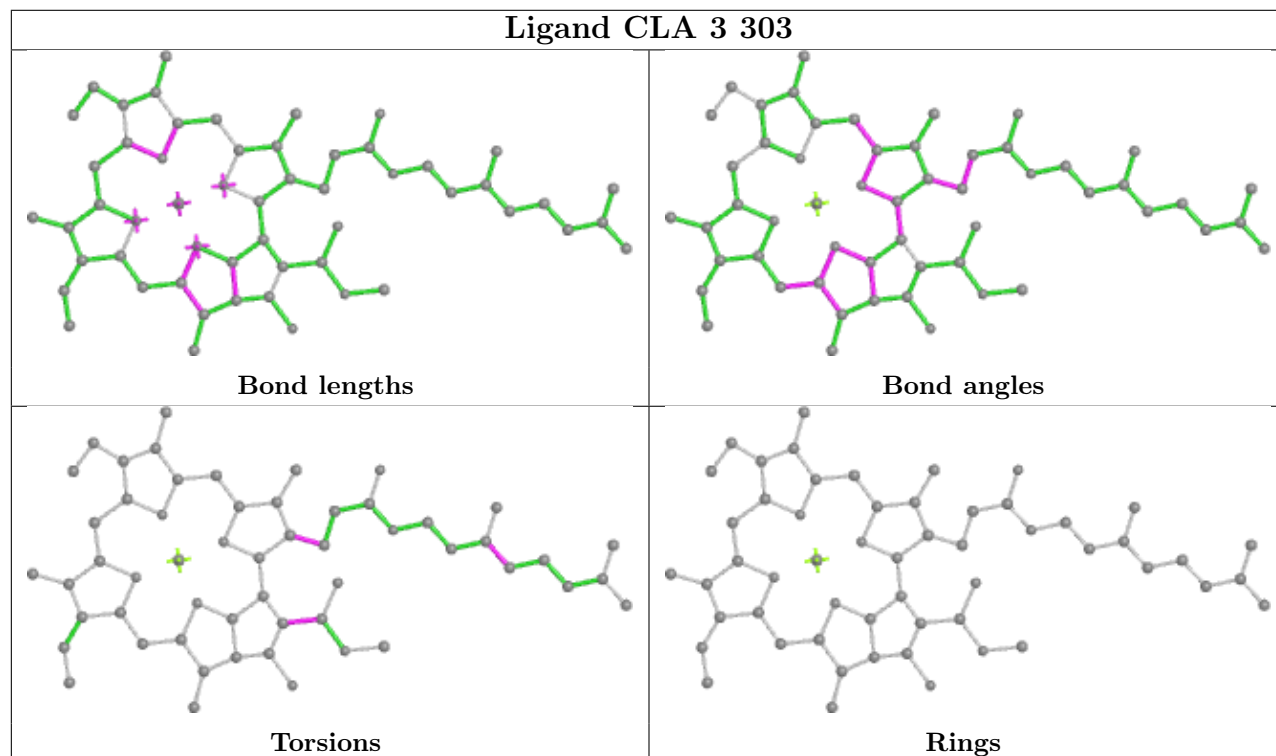


**Ligand II0 7 313****Ligand CLA 2 308**

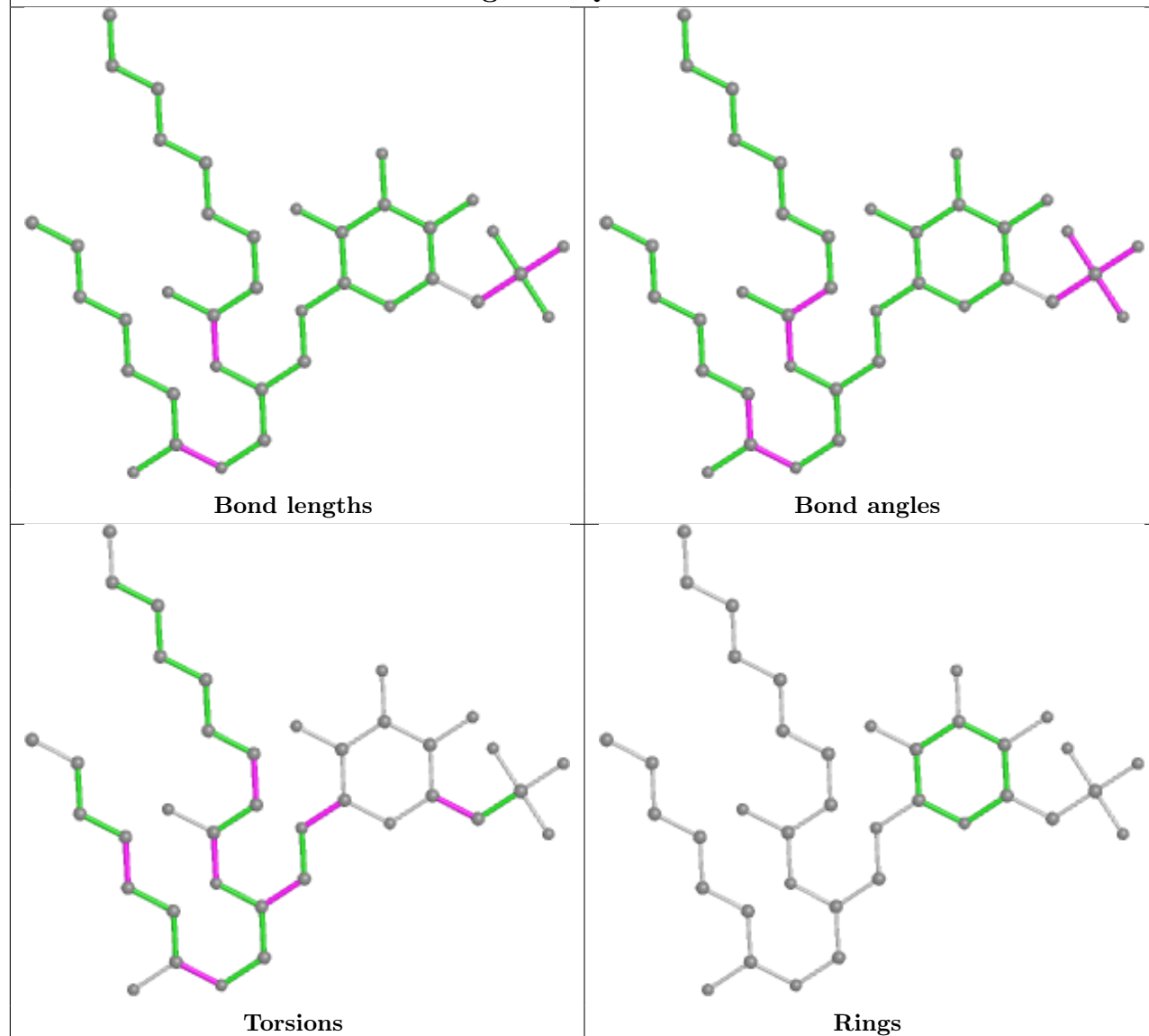
## Ligand CLA C 513



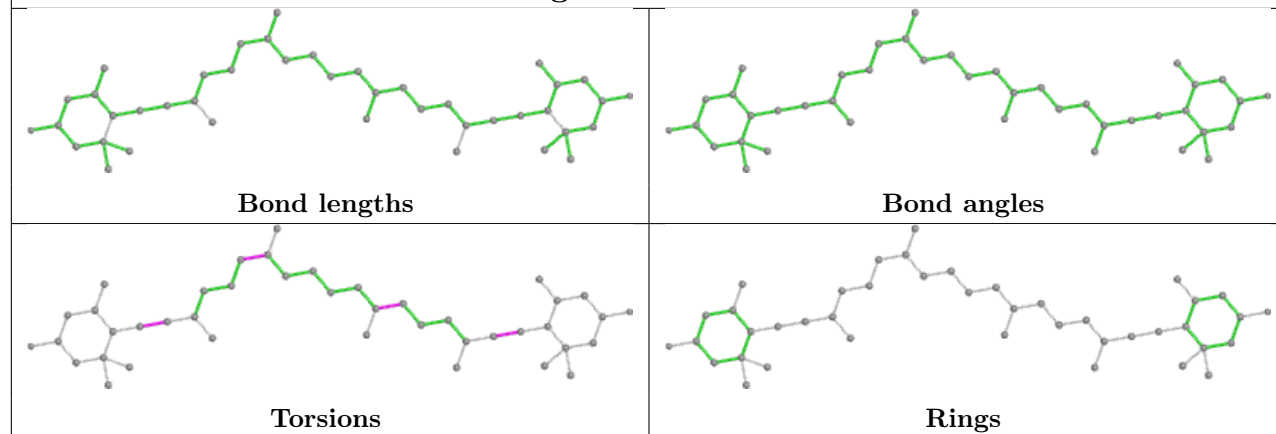
## Ligand CLA 3 303



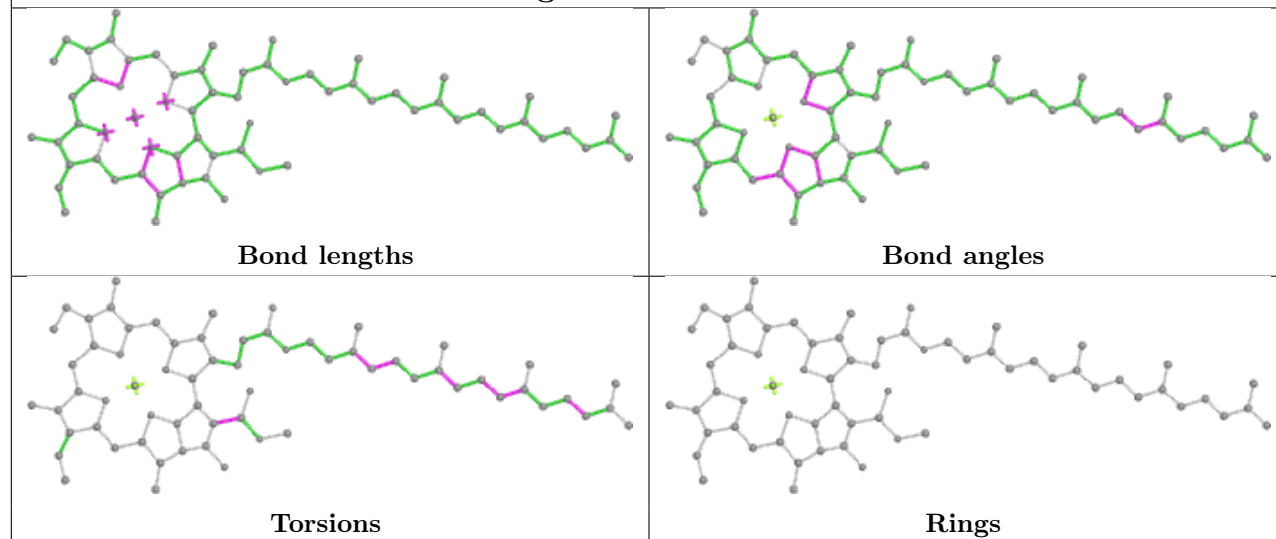
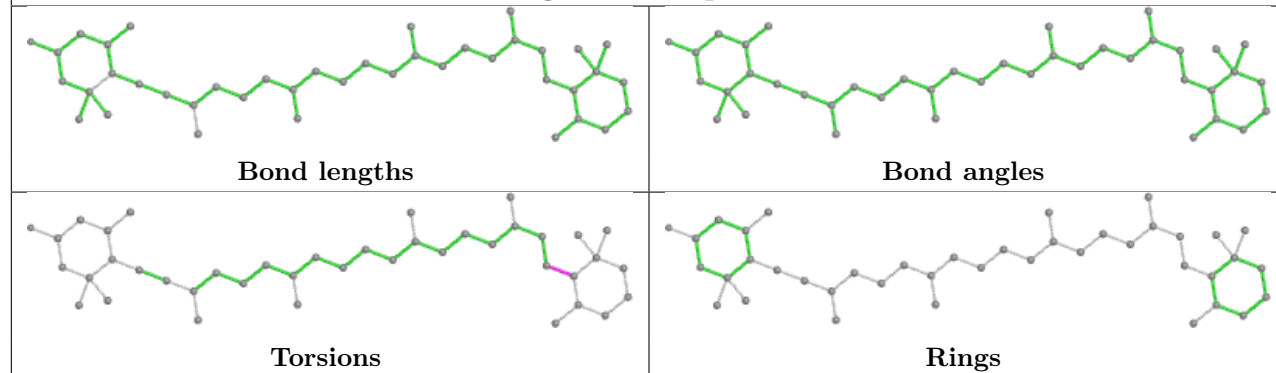
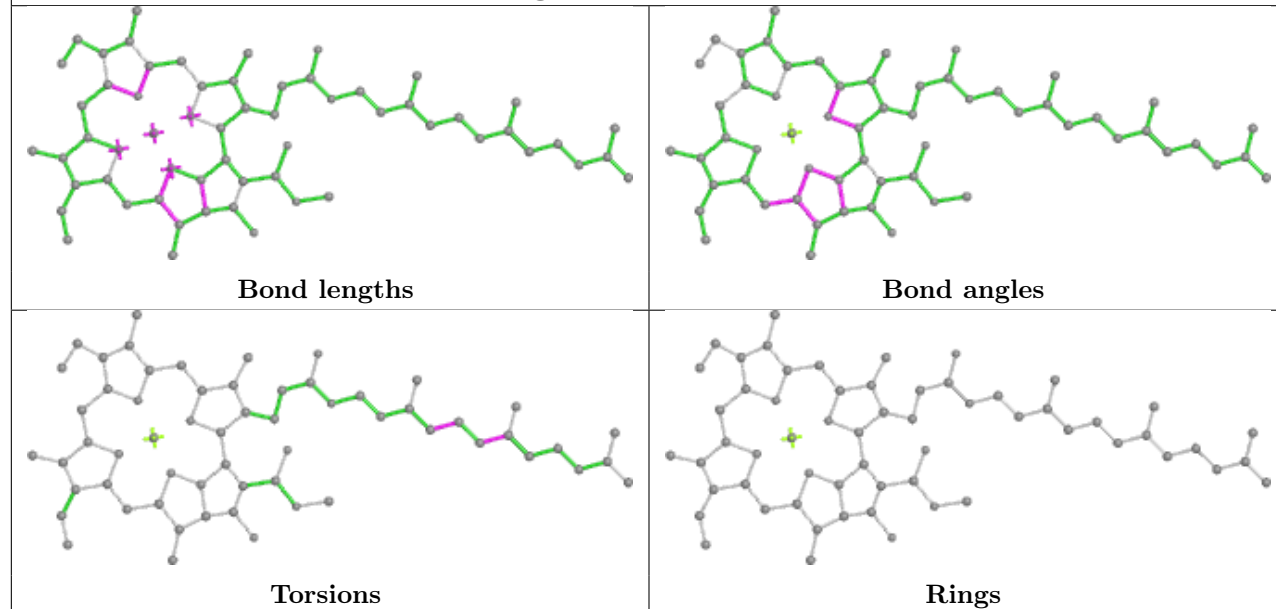
## Ligand SQD b 601



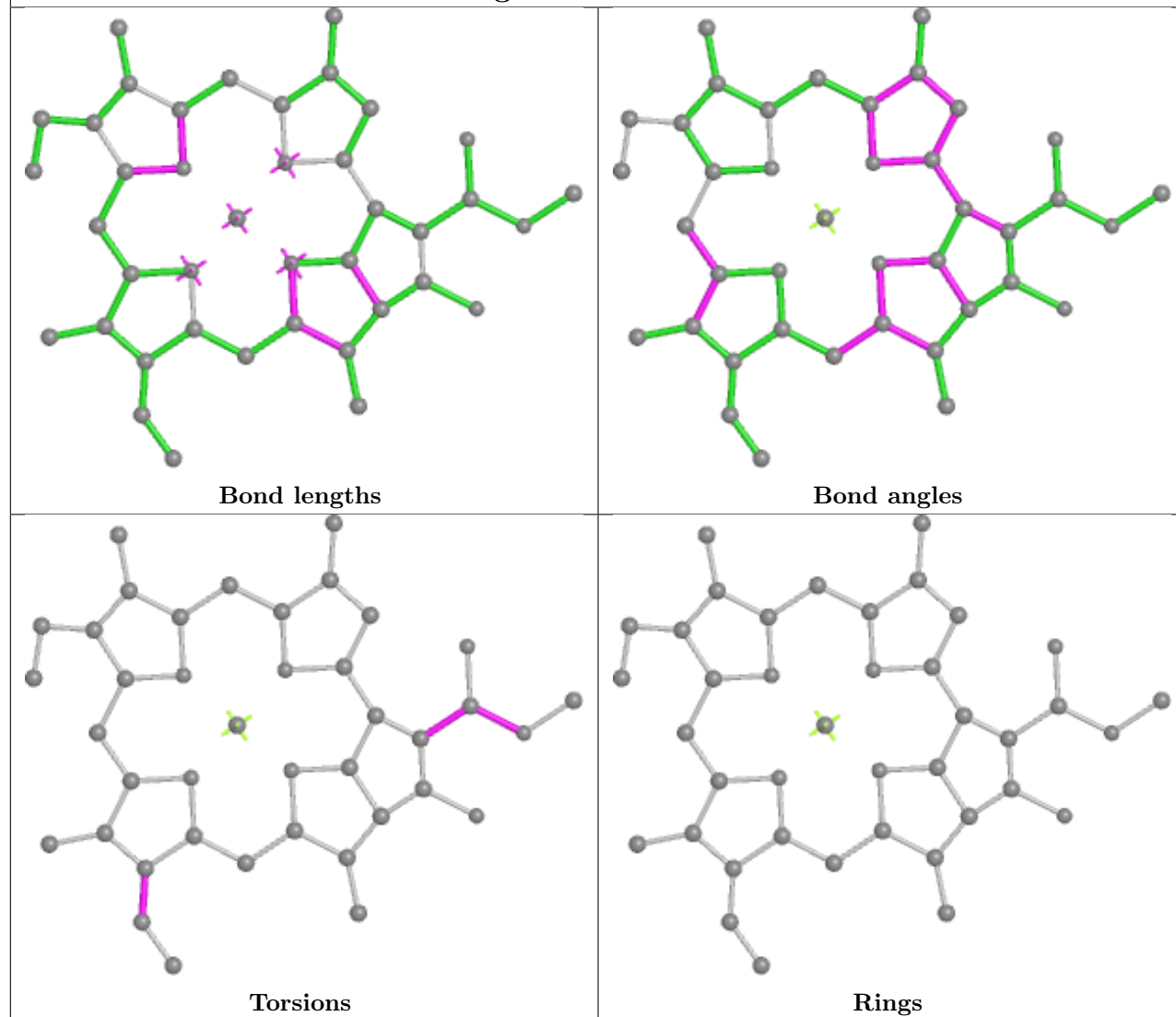
## Ligand II0 8 313



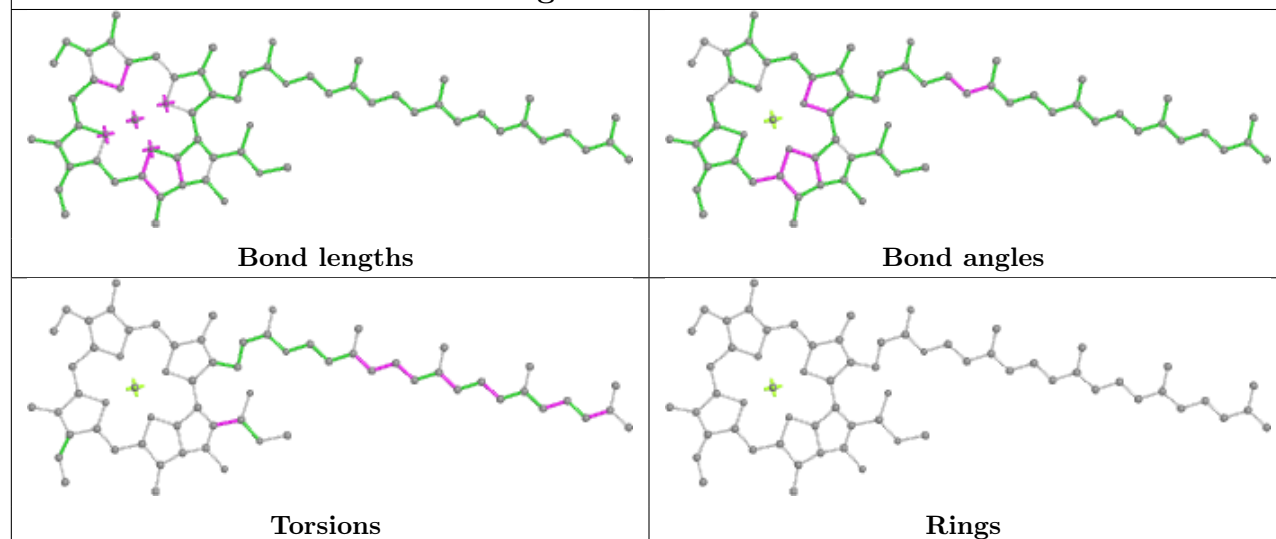


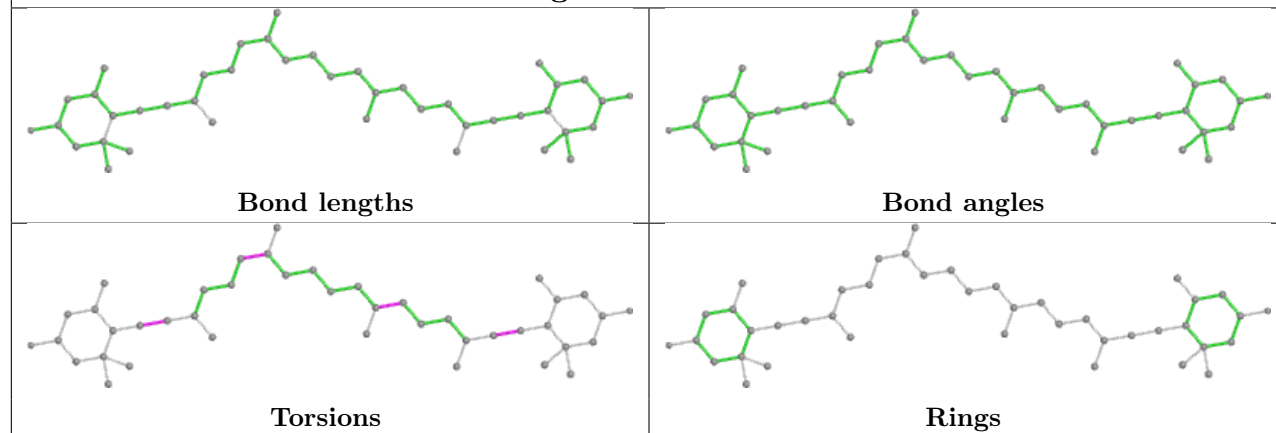
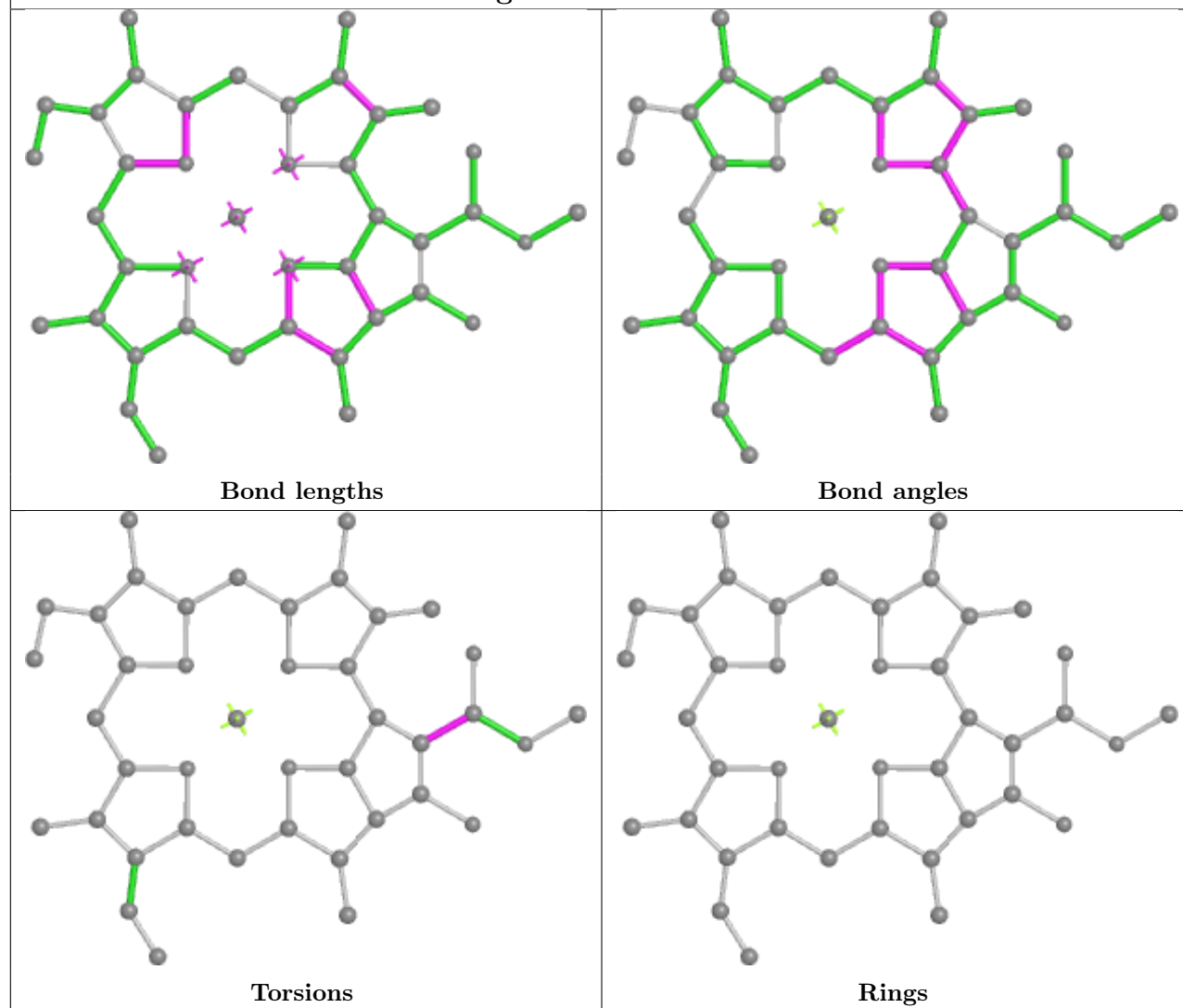
**Ligand CLA c 505****Ligand IHT p 318****Ligand CLA A 408**

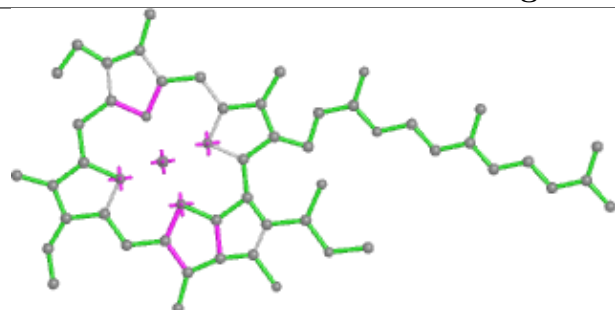
## Ligand CLA 4 309



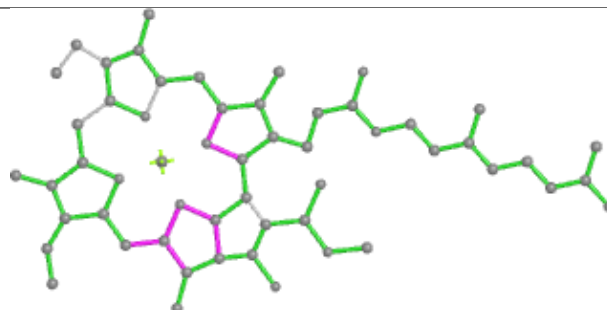
## Ligand CLA c 507



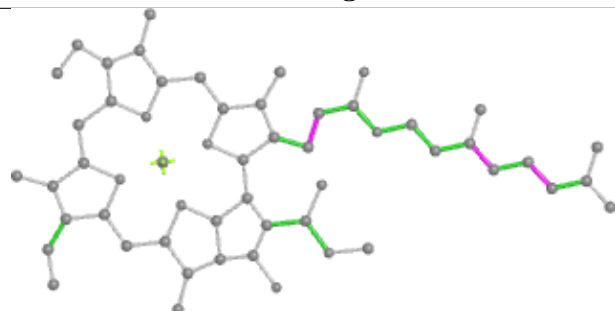
**Ligand II0 2 313****Ligand CLA n 303**

**Ligand CLA 1 304**

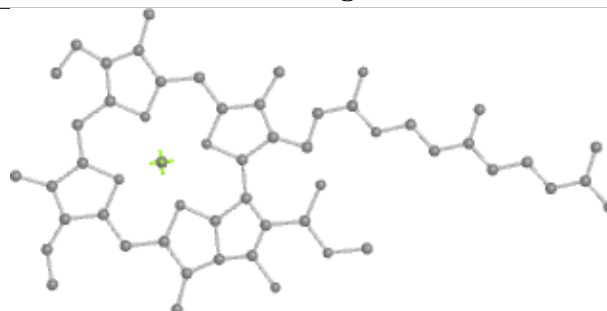
Bond lengths



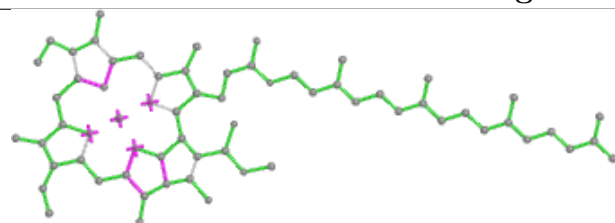
Bond angles



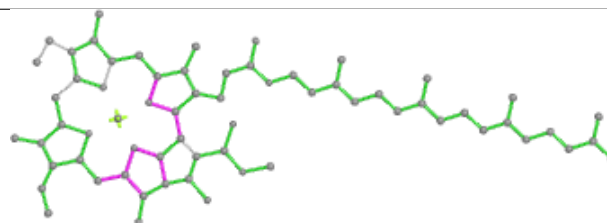
Torsions



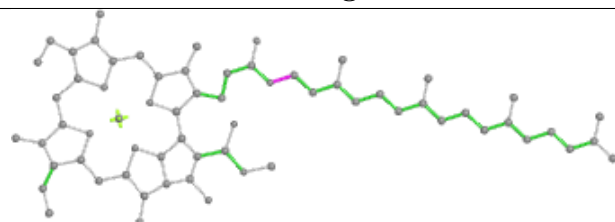
Rings

**Ligand CLA D 404**

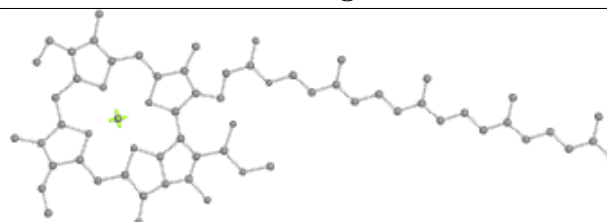
Bond lengths



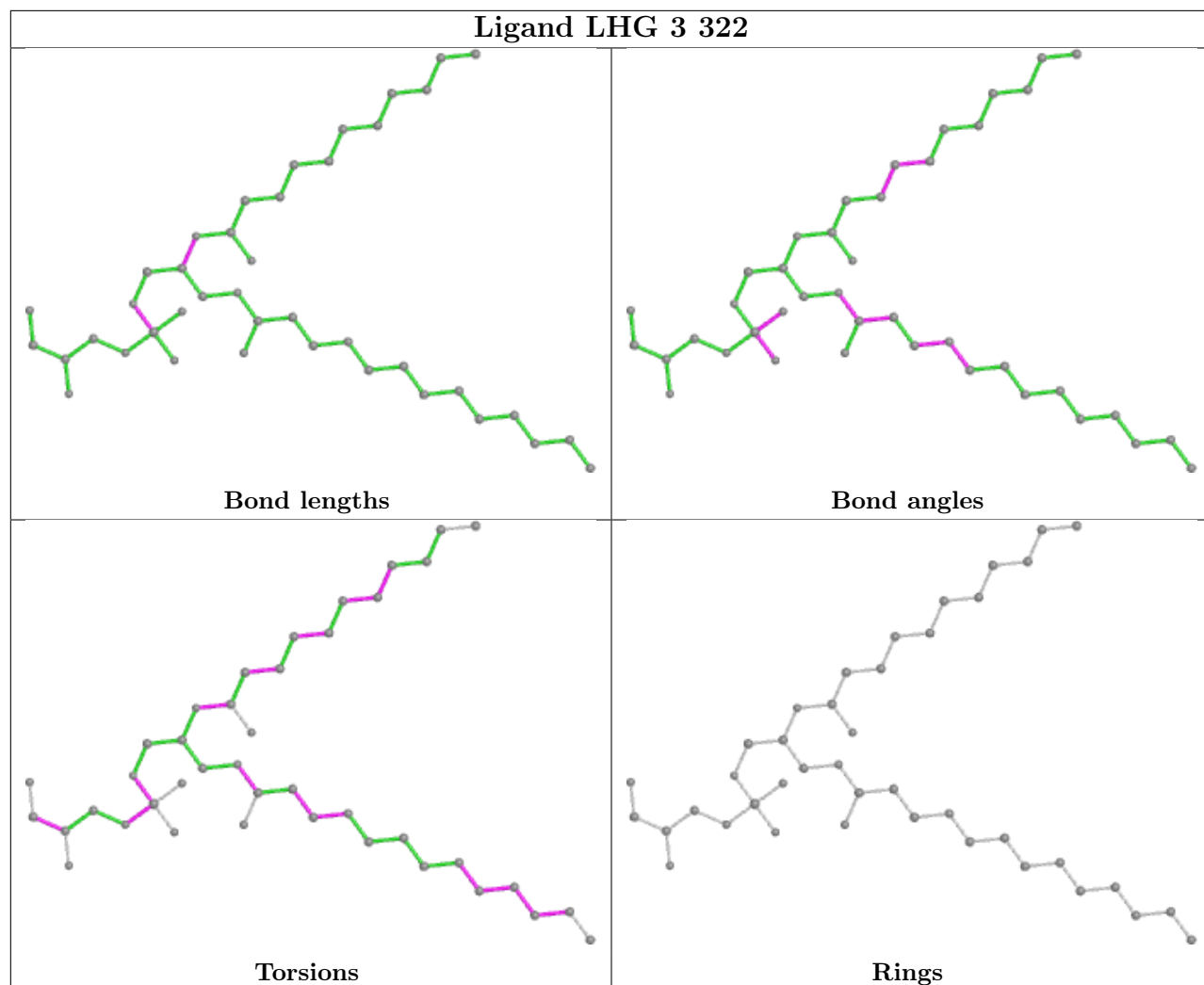
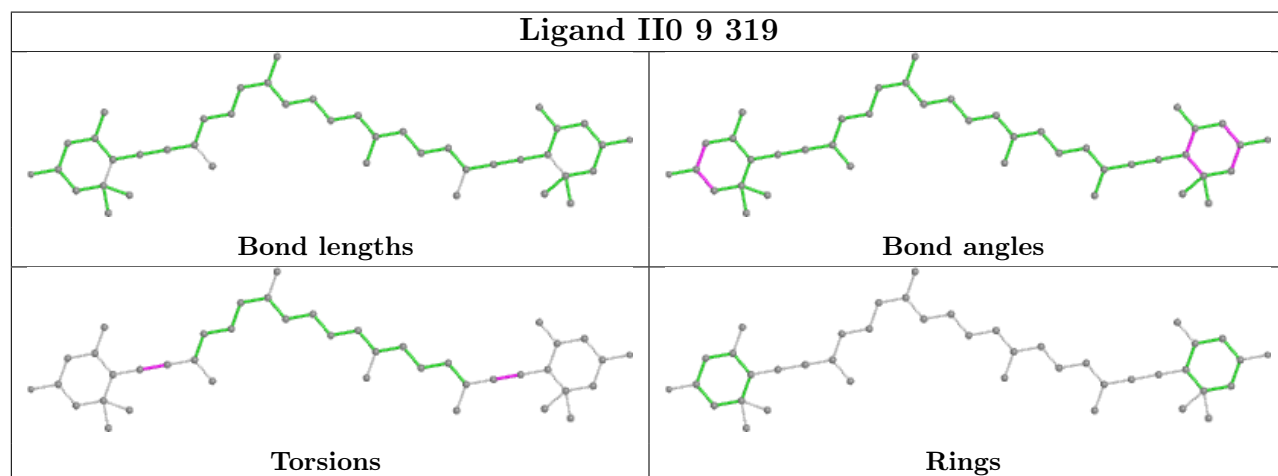
Bond angles



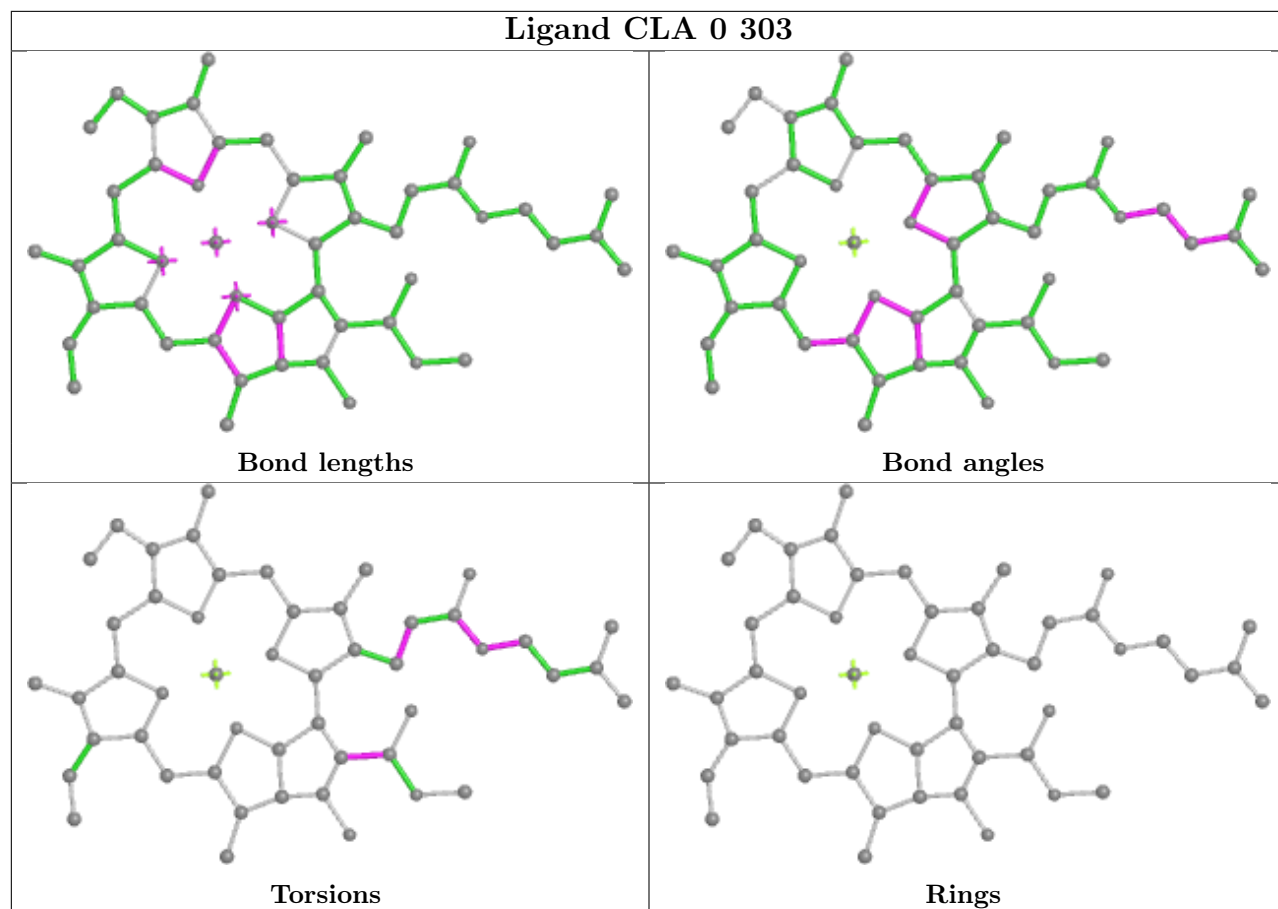
Torsions



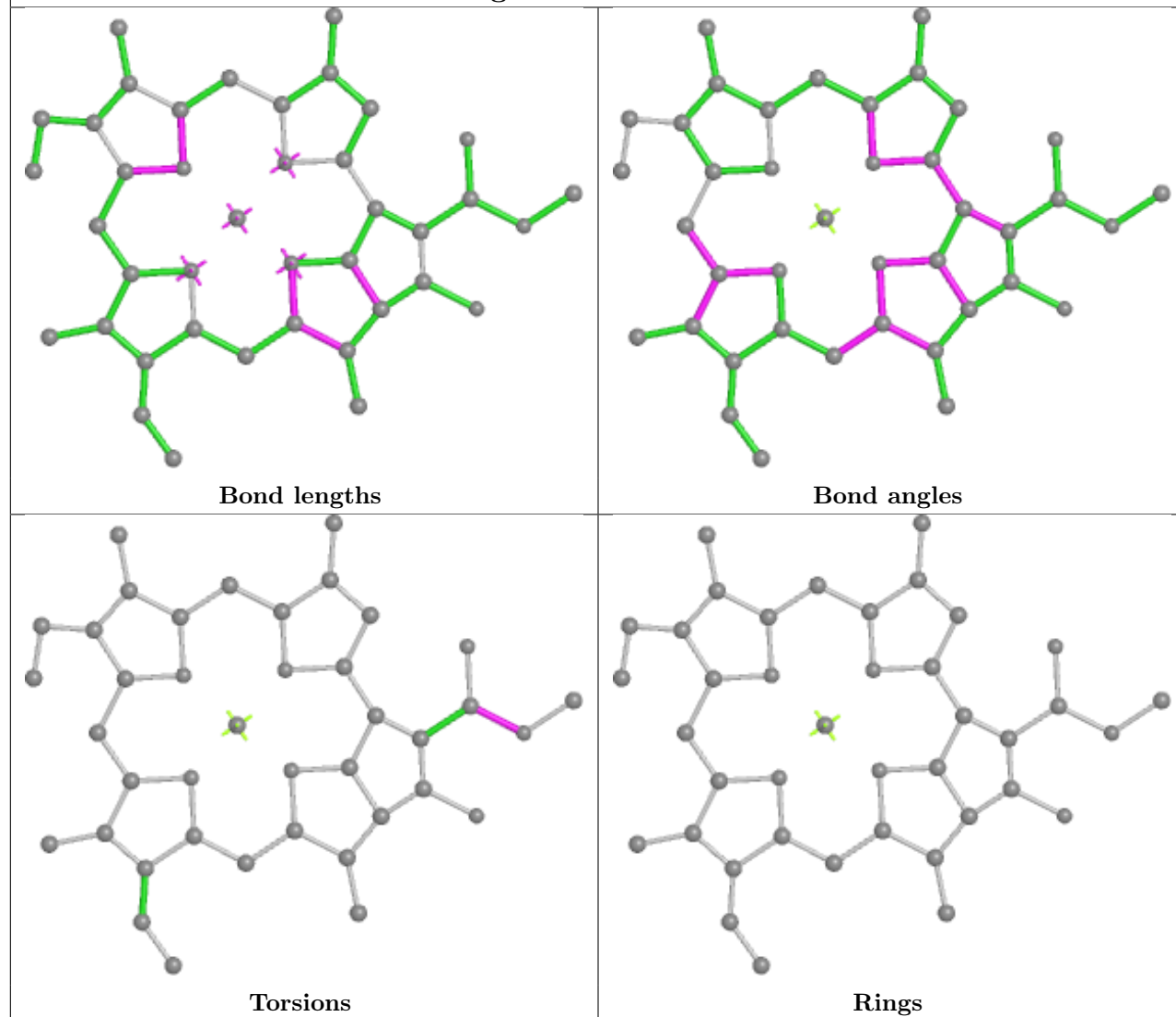
Rings

**Ligand LHG 3 322****Ligand II0 9 319**

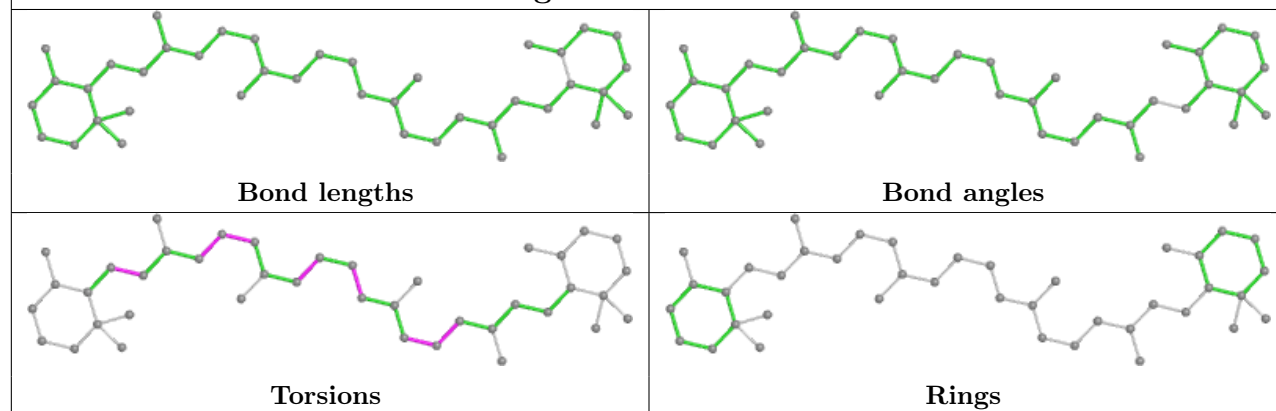
## Ligand CLA 0 303

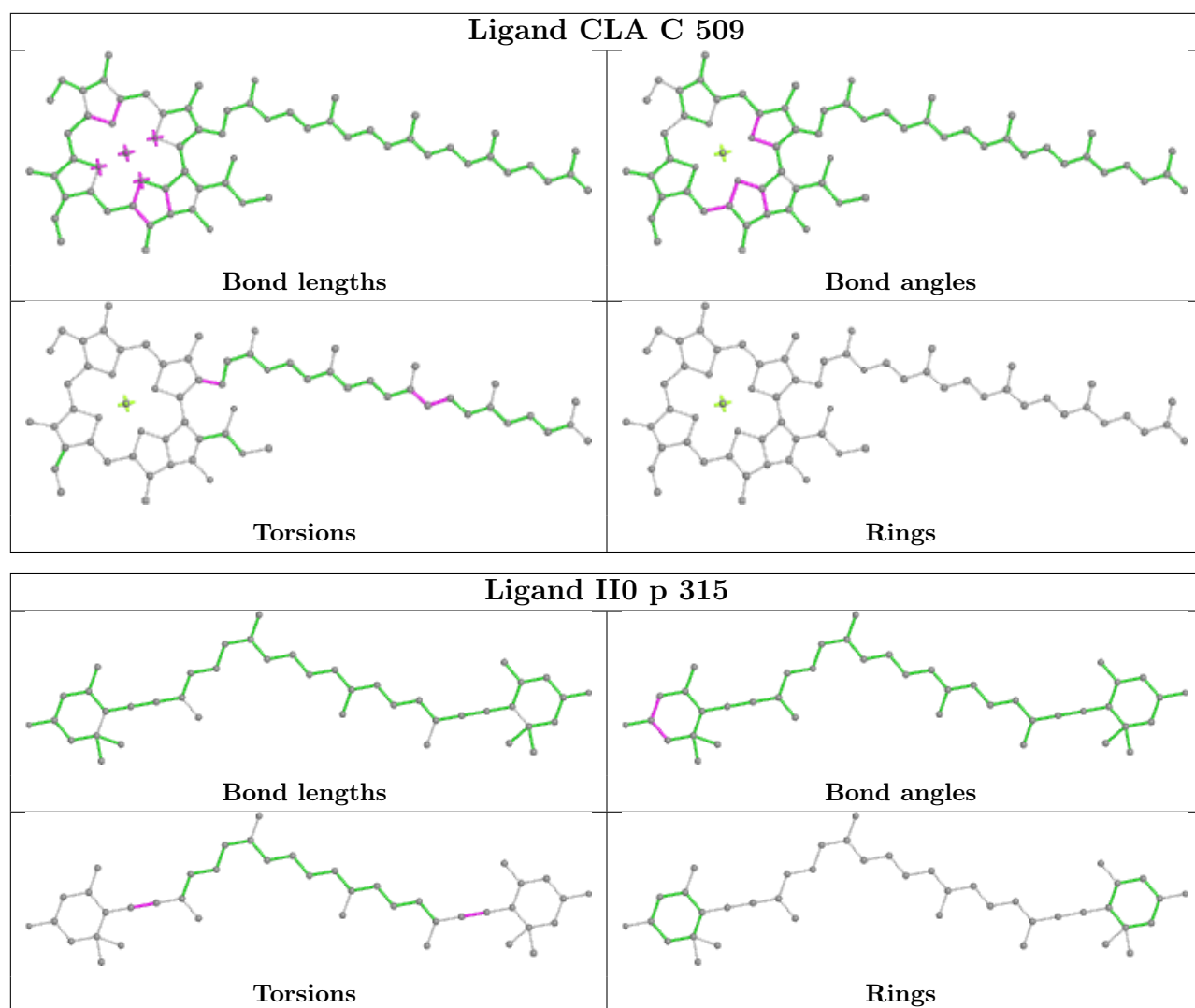


## Ligand CLA B 618

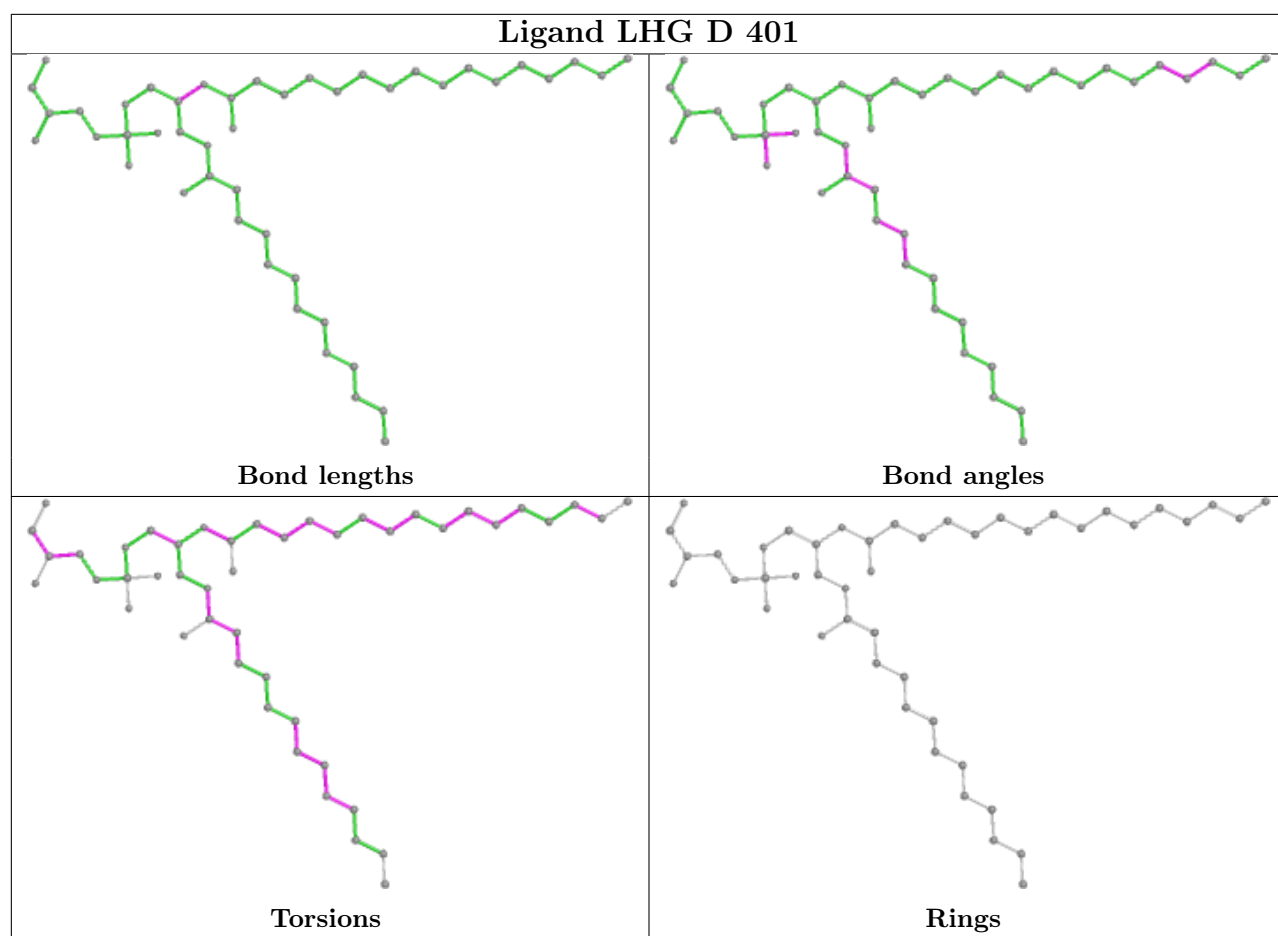


## Ligand 8CT H 102

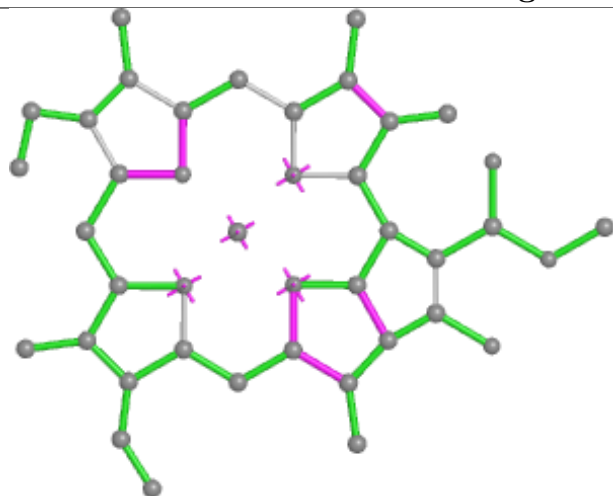




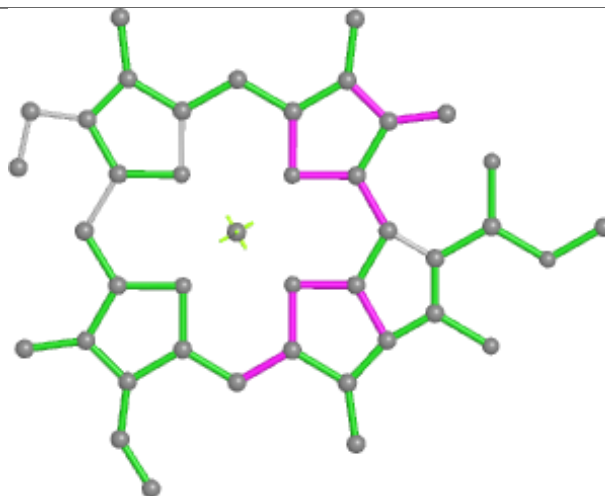




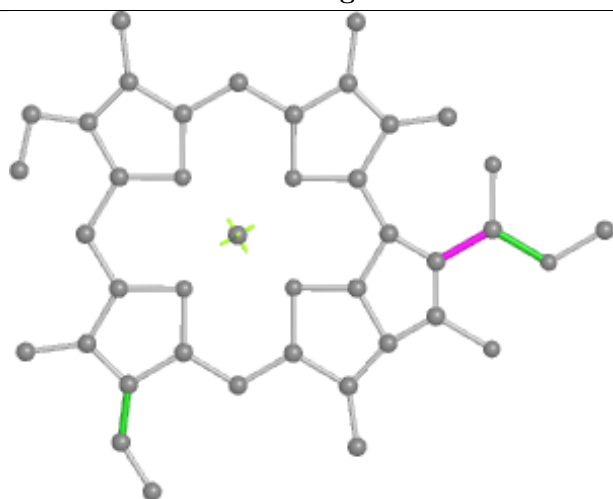
## Ligand CLA 9 315



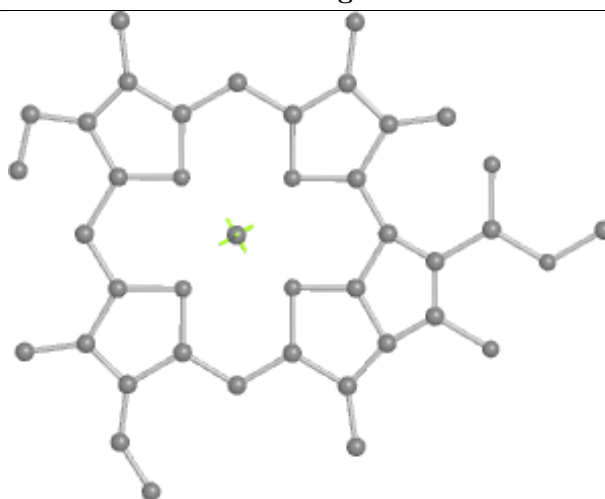
Bond lengths



Bond angles

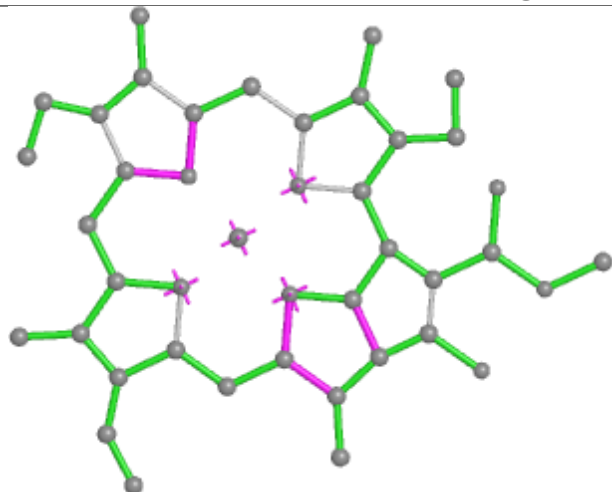


Torsions

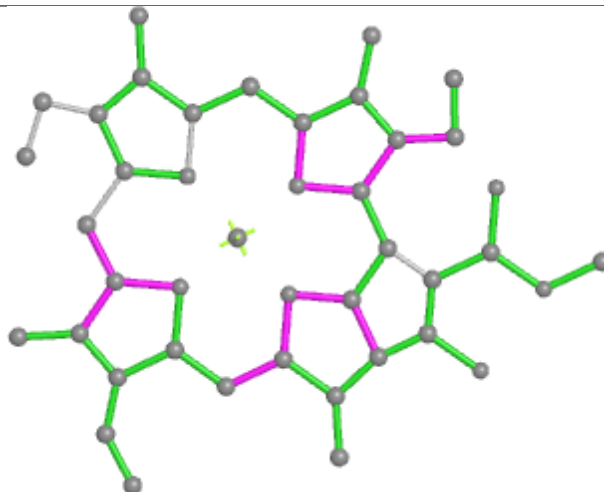


Rings

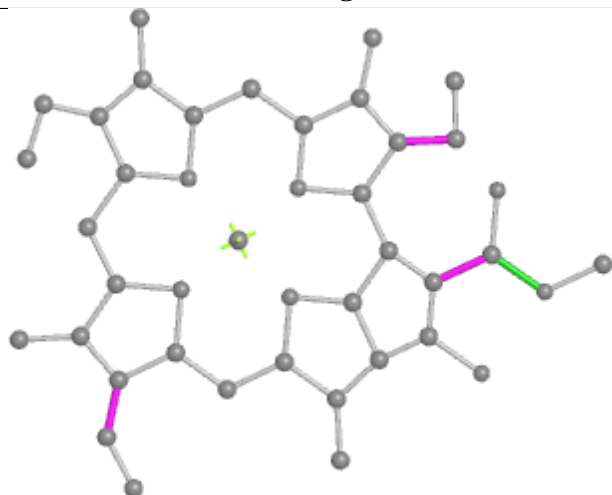
## Ligand CLA 5 301



Bond lengths



Bond angles

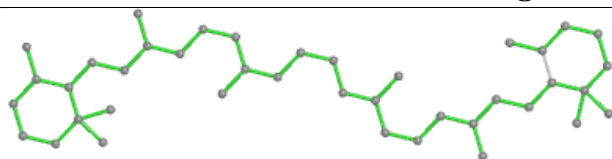


Torsions

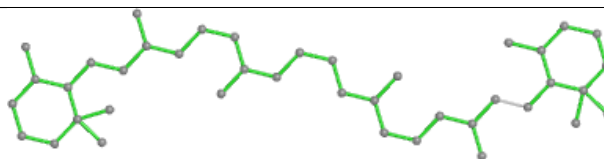


Rings

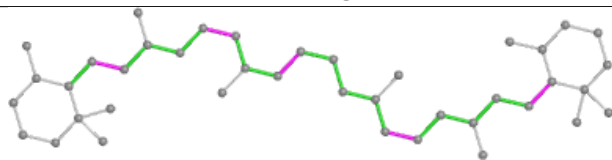
## Ligand 8CT C 517



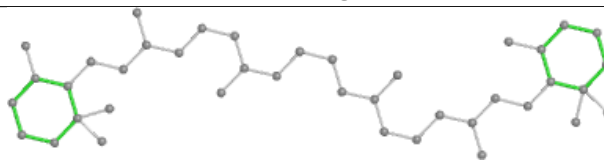
Bond lengths



Bond angles

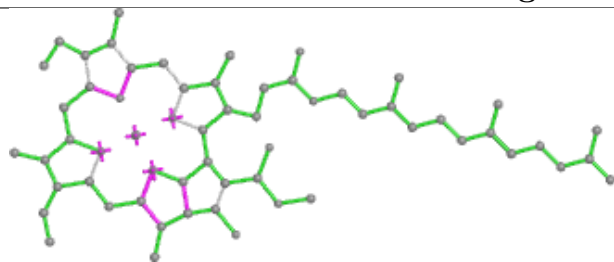


Torsions

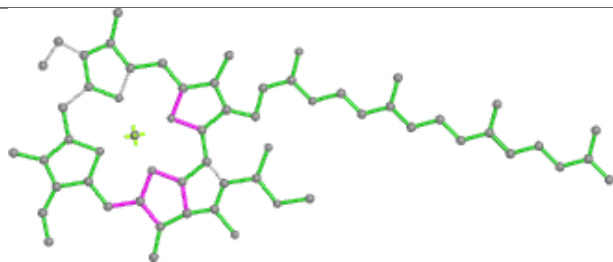


Rings

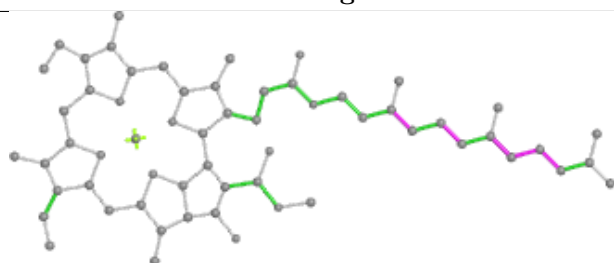
## Ligand CLA 7 305



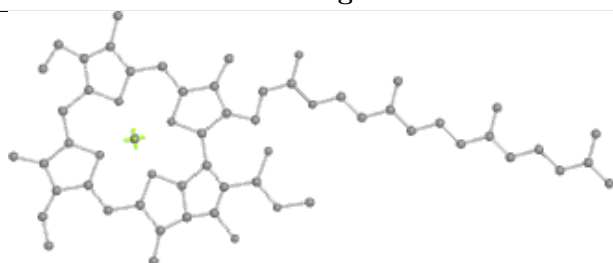
Bond lengths



Bond angles

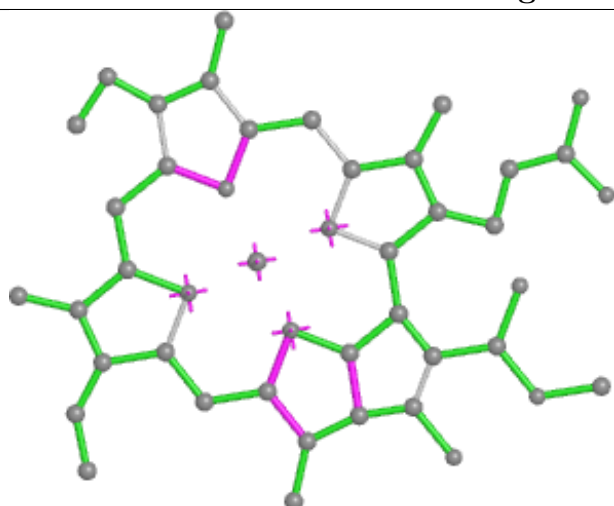


Torsions

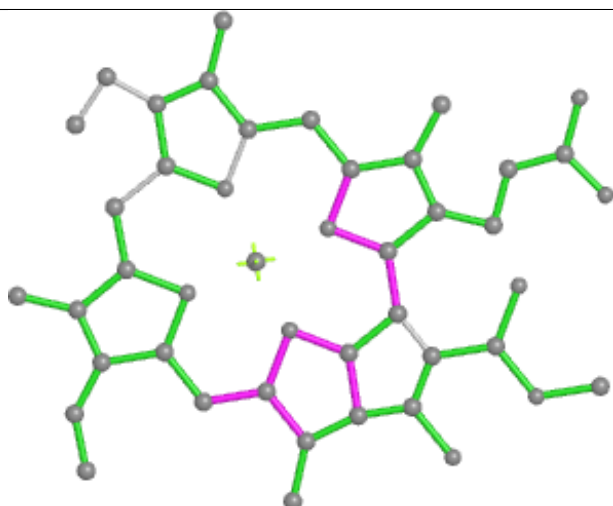


Rings

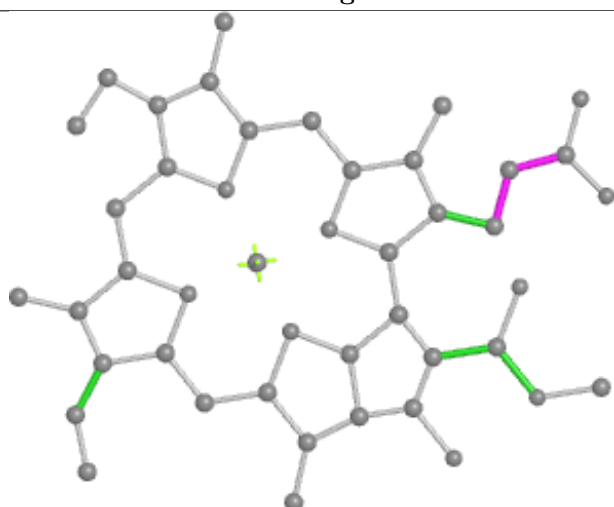
## Ligand CLA 7 301



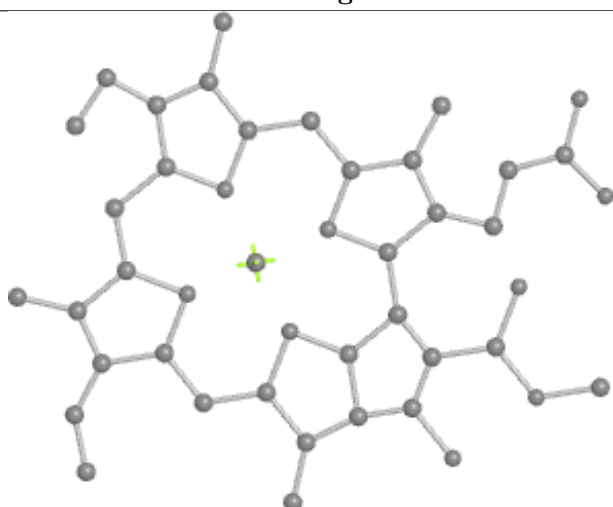
Bond lengths



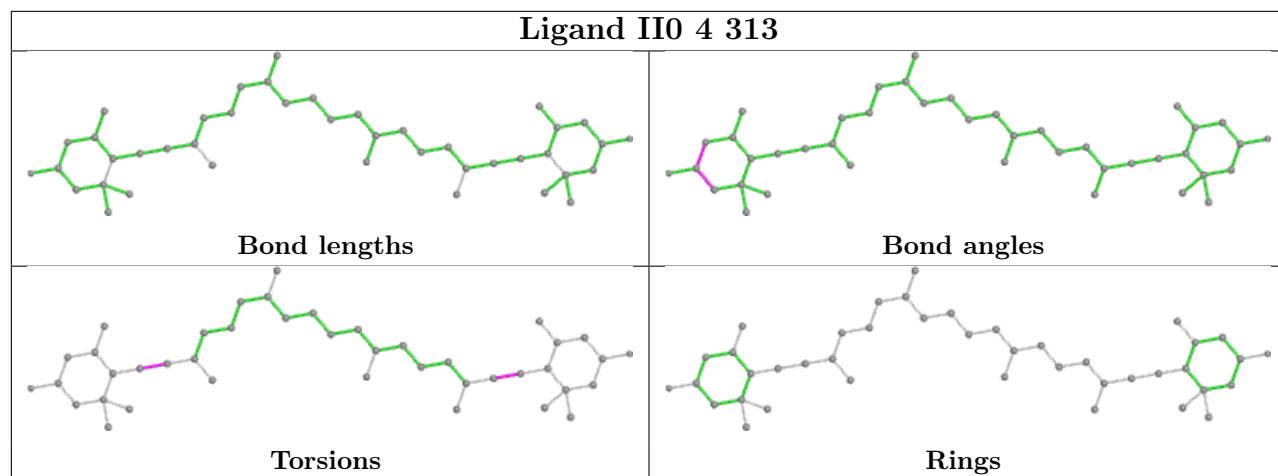
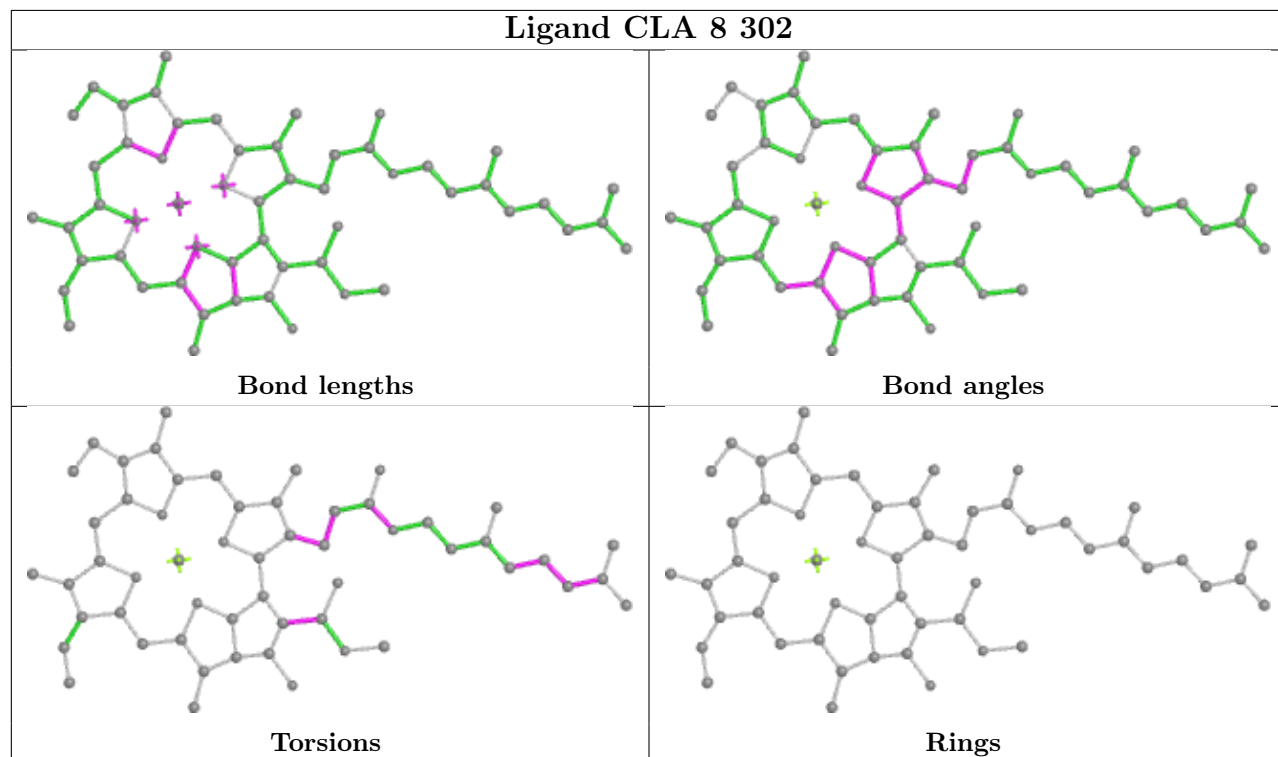
Bond angles



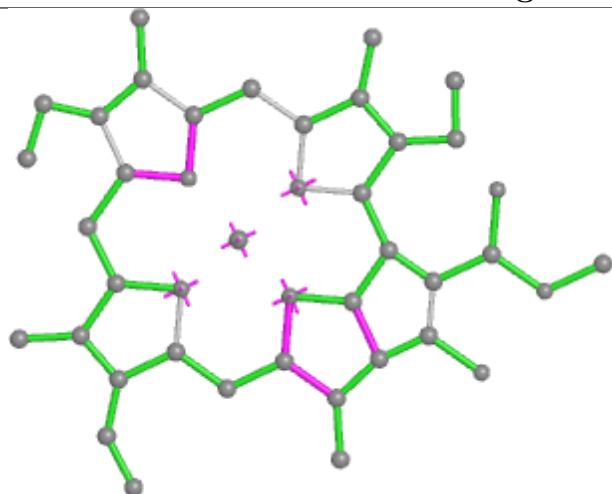
Torsions



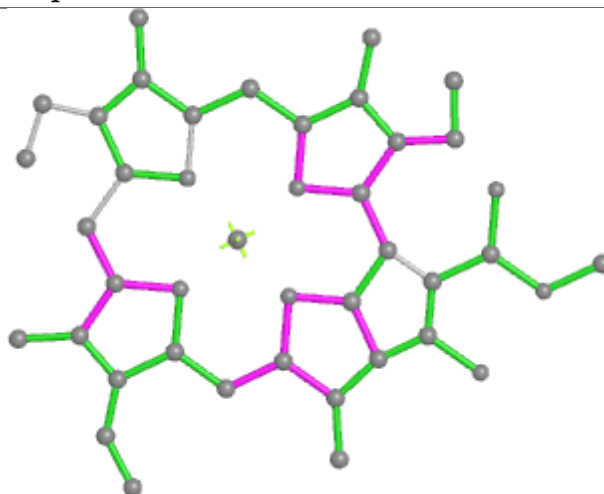
Rings

**Ligand II0 4 313****Ligand CLA 8 302**

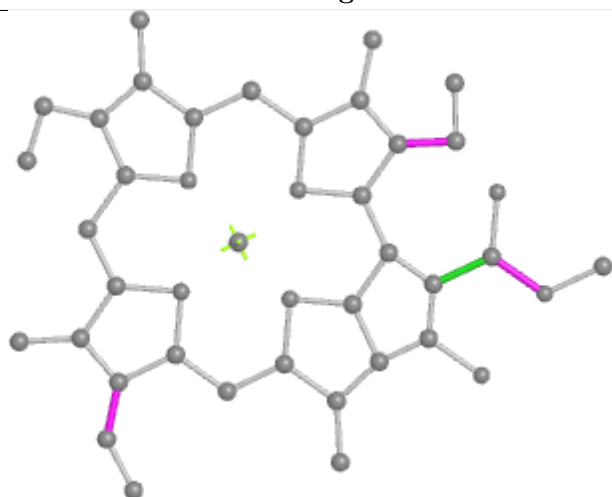
## Ligand CLA p 308



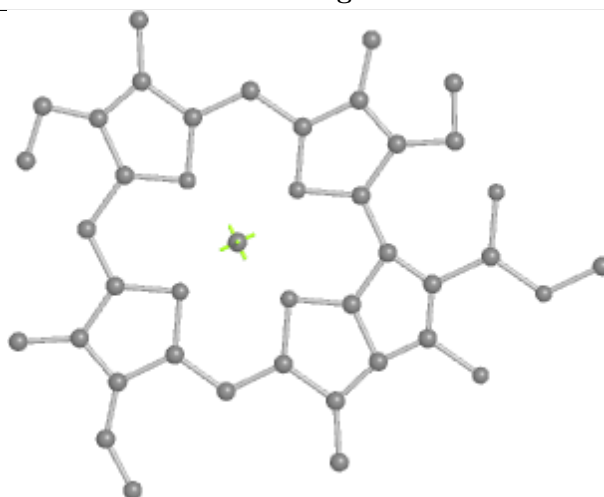
Bond lengths



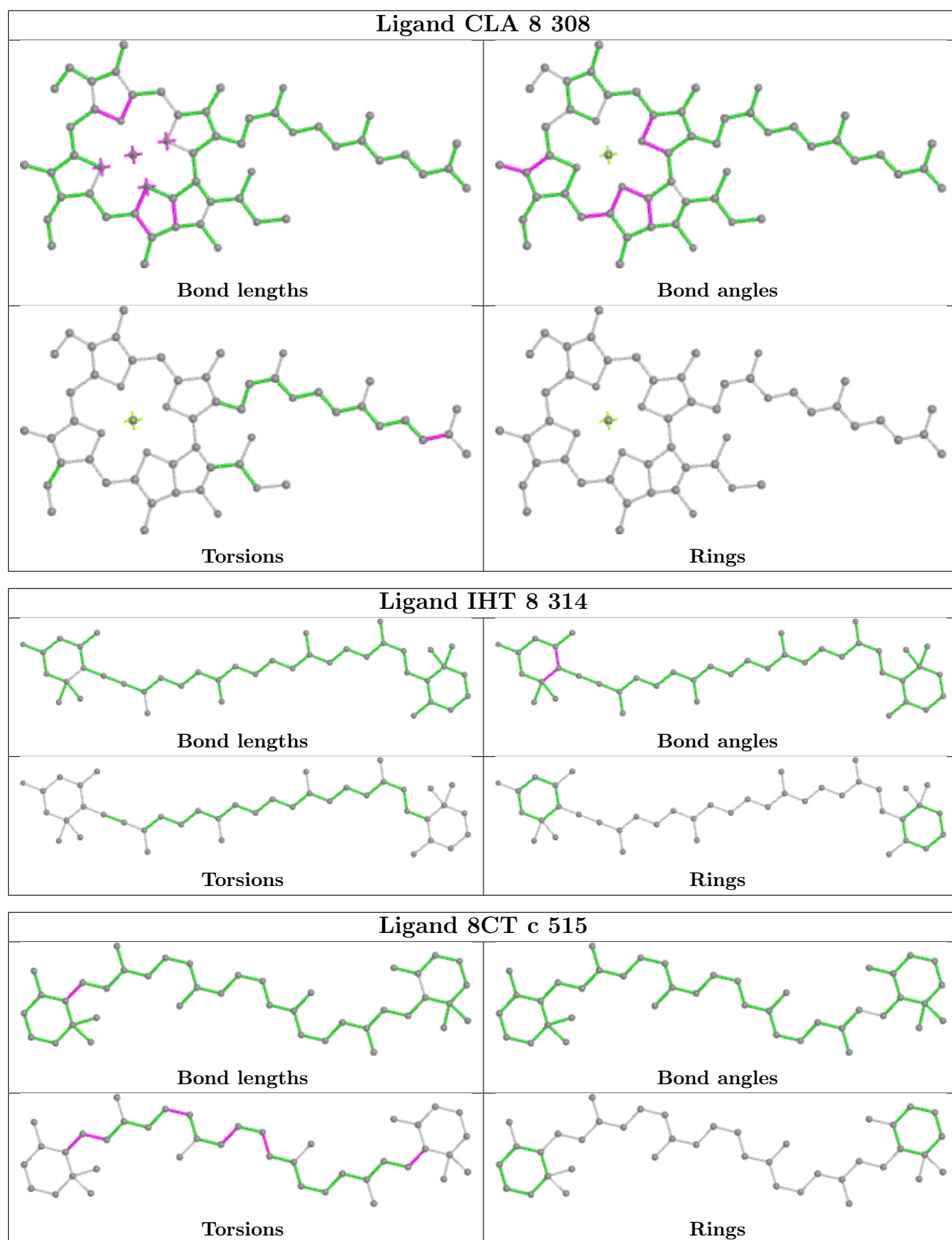
Bond angles

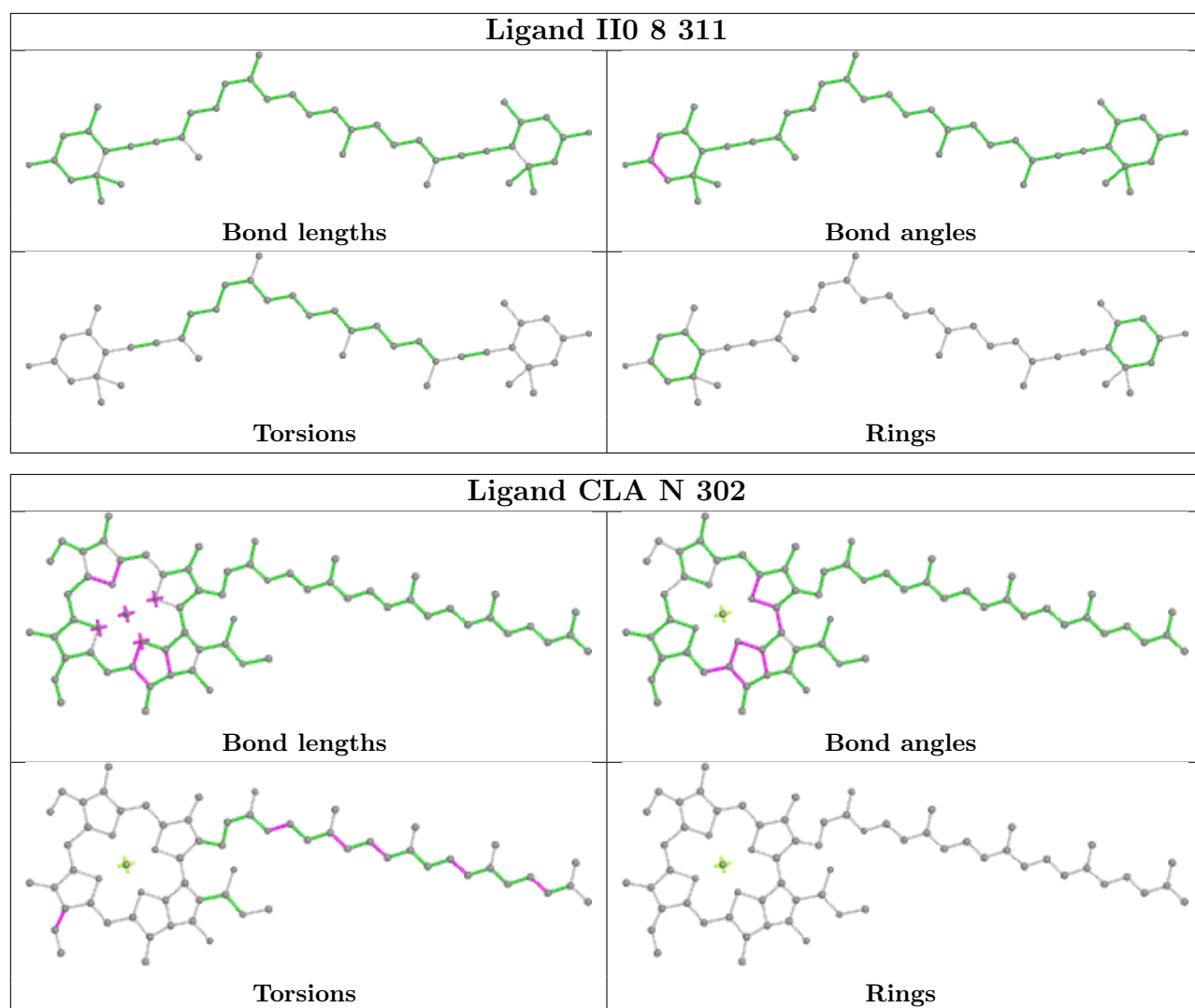


Torsions



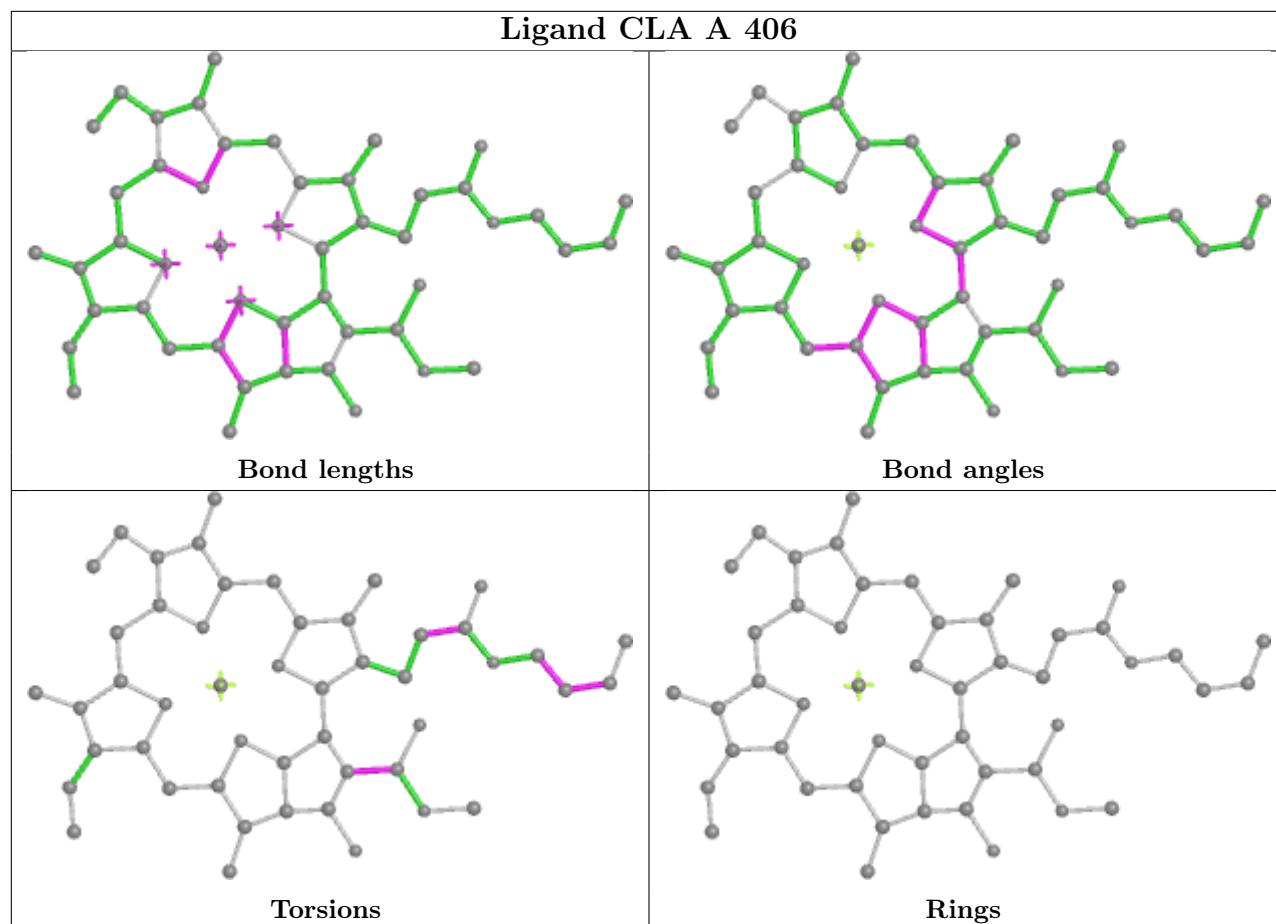
Rings



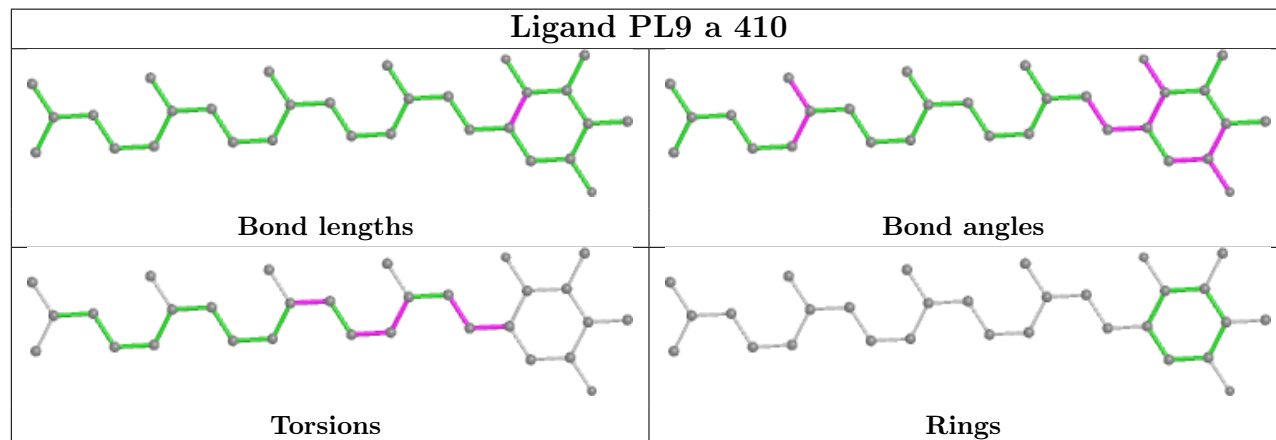


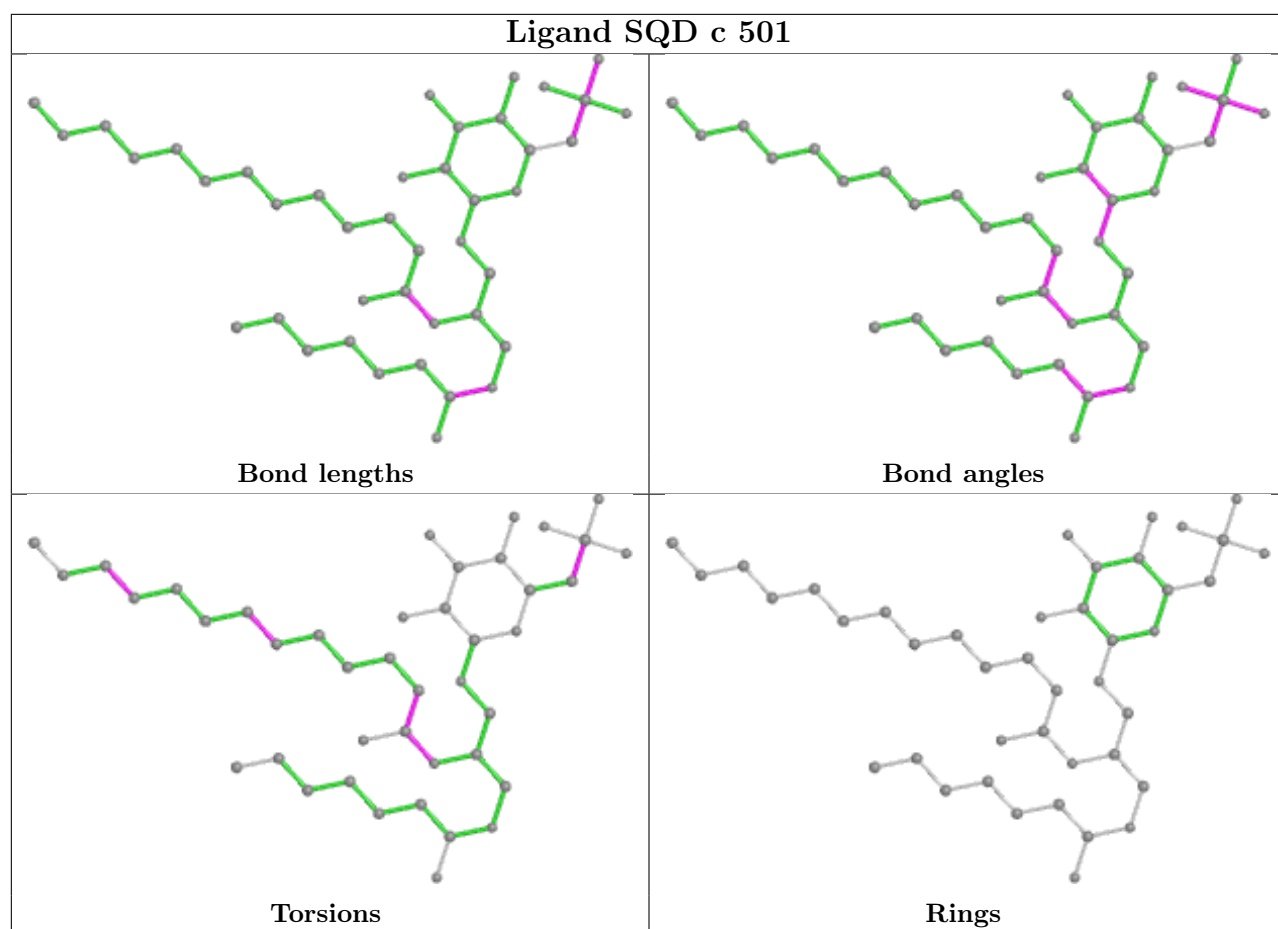


## Ligand CLA A 406

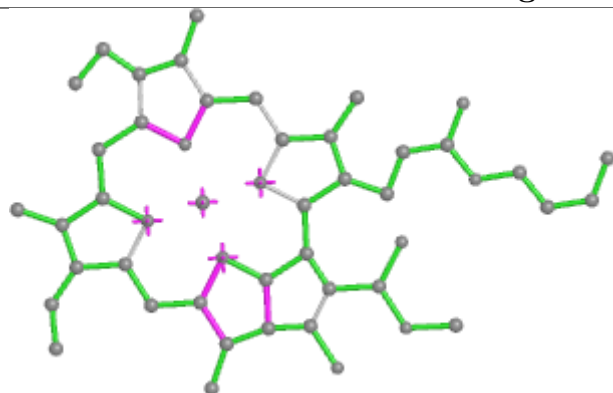


## Ligand PL9 a 410

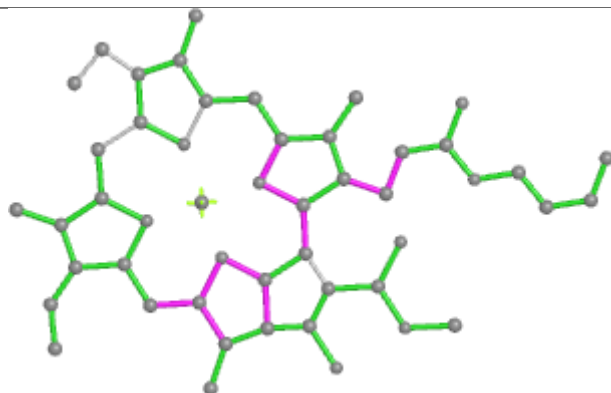




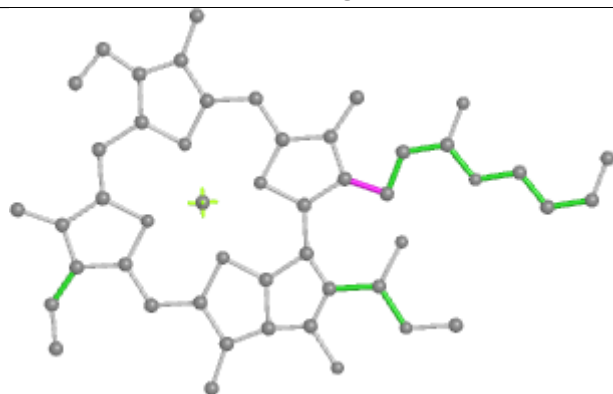
## Ligand CLA 9 308



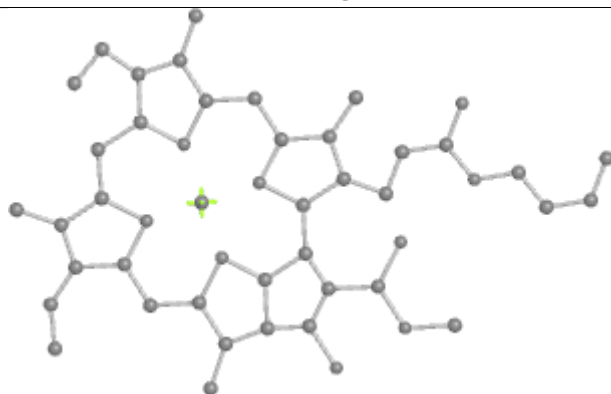
Bond lengths



Bond angles

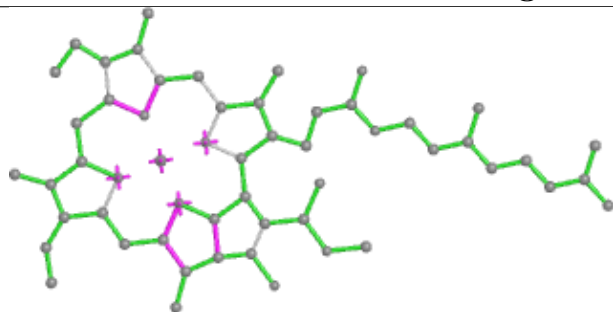


Torsions

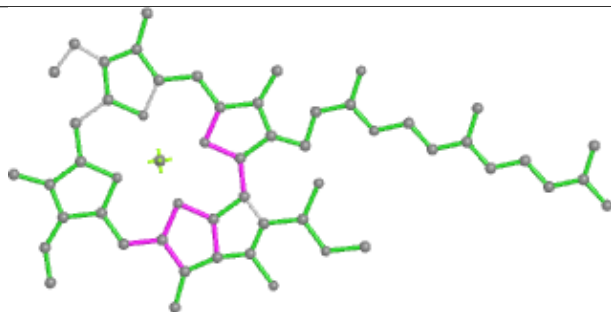


Rings

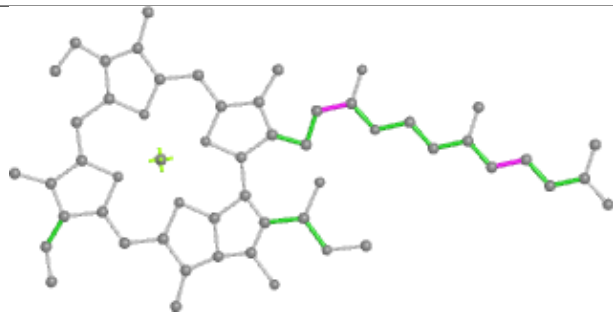
## Ligand CLA 3 312



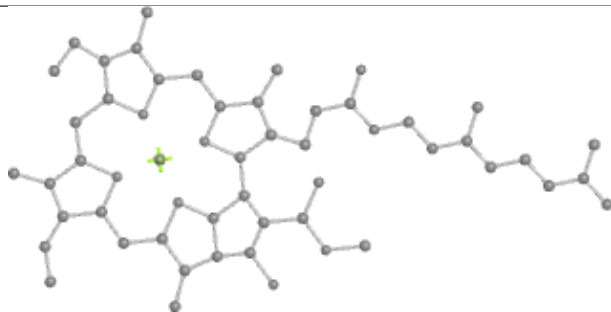
Bond lengths



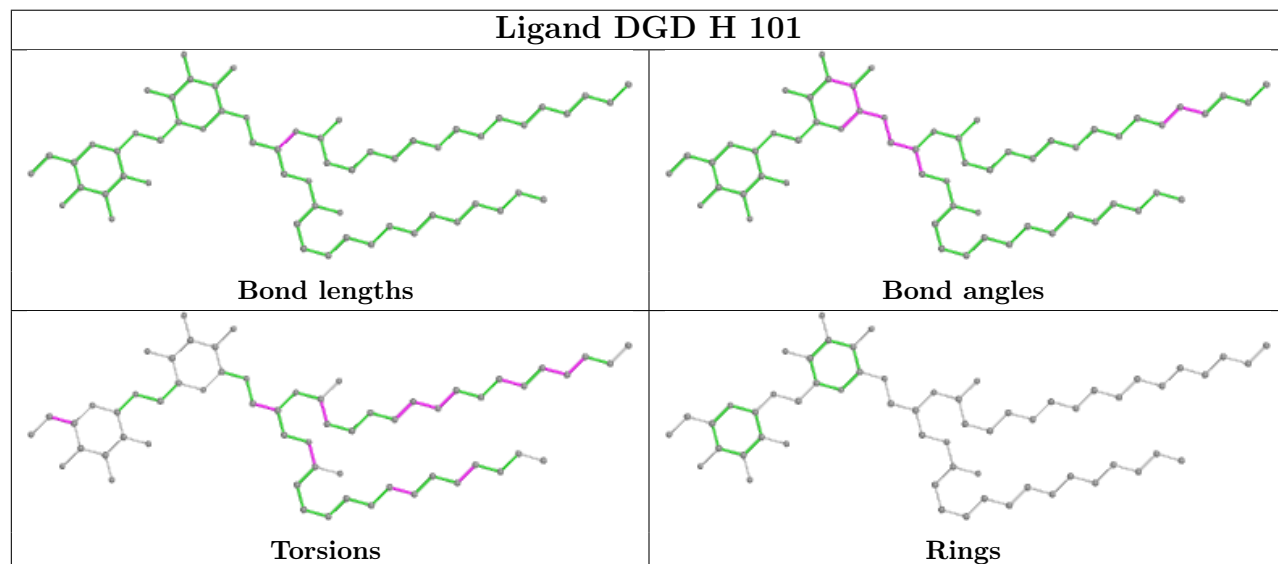
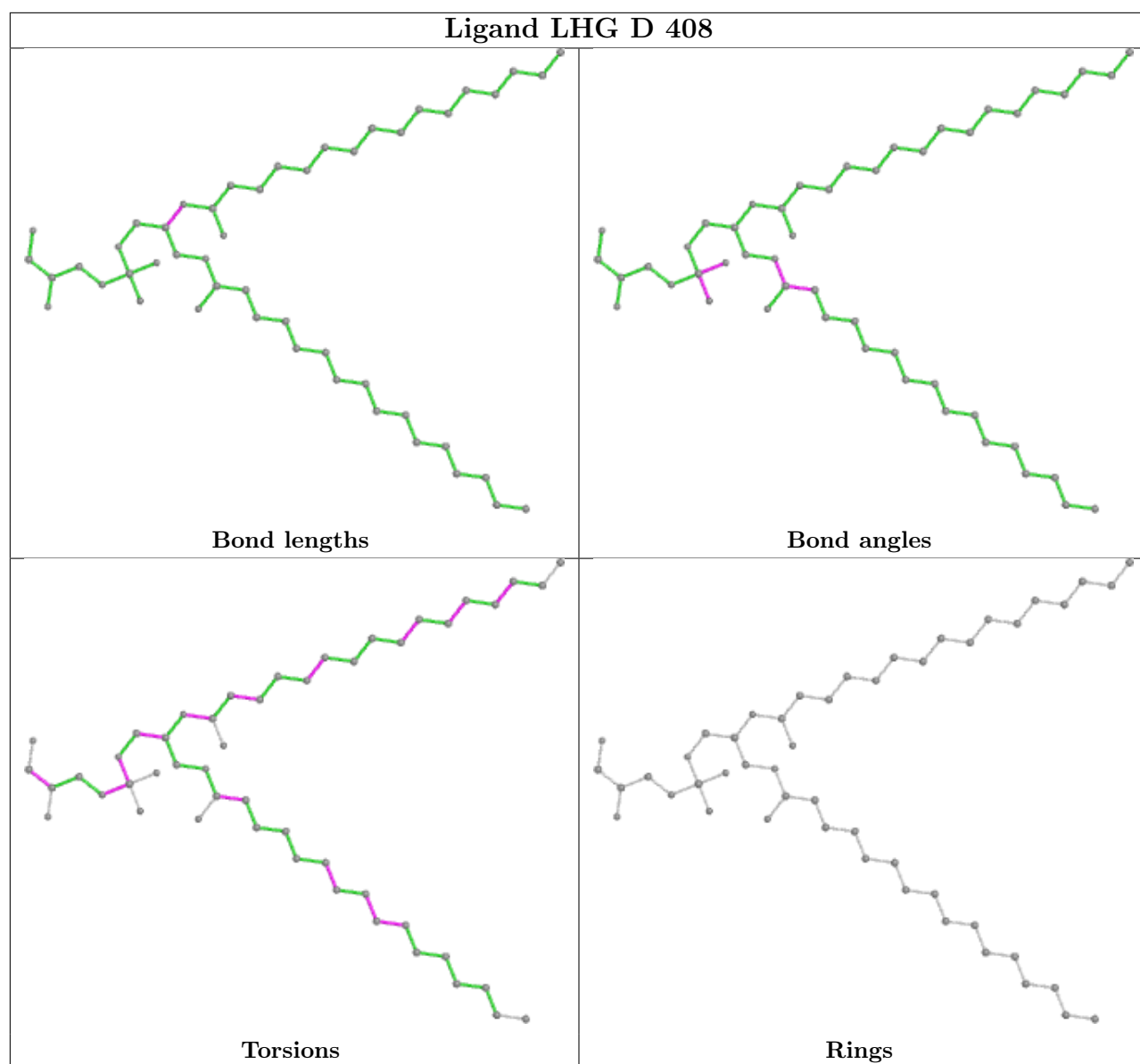
Bond angles

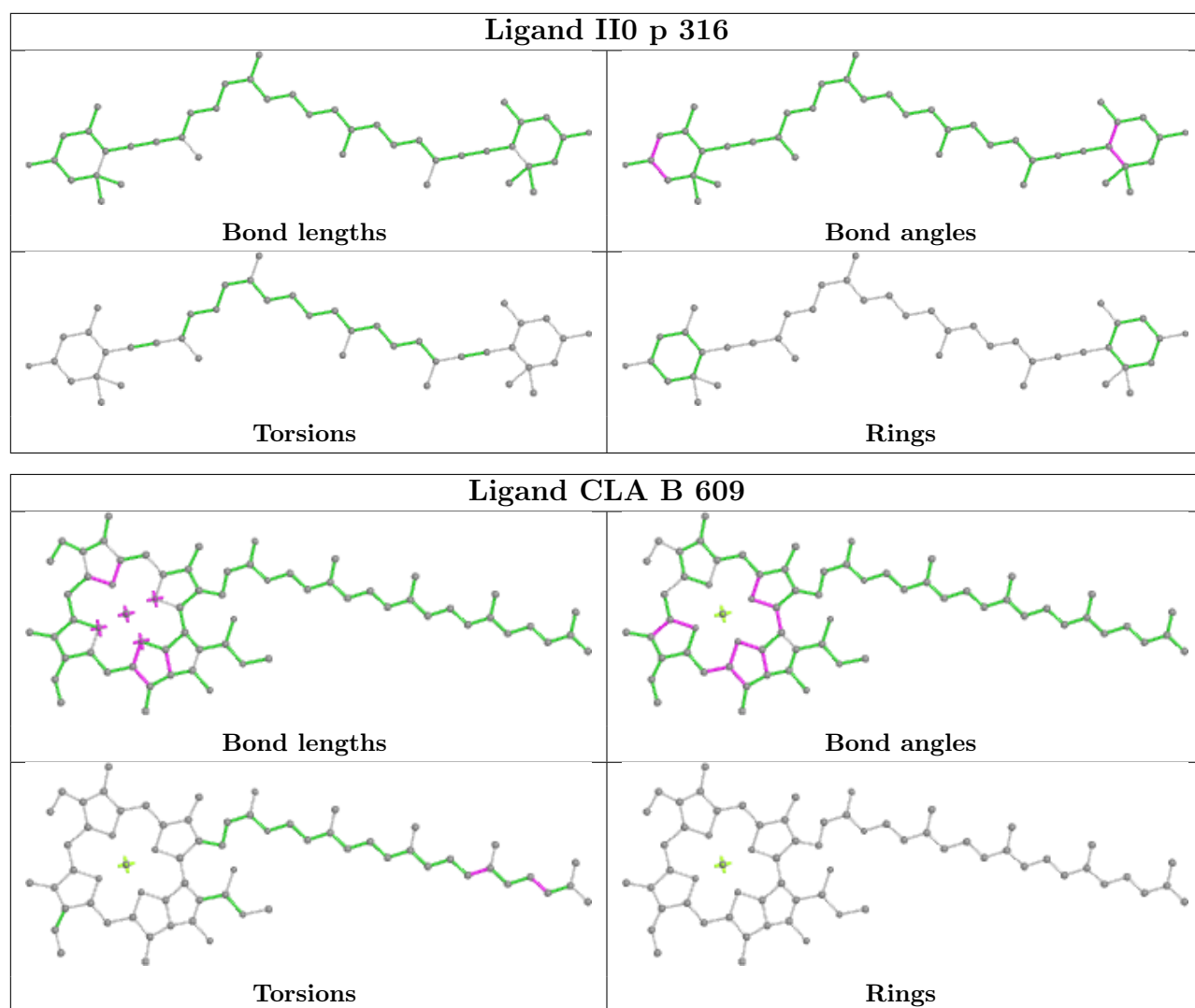


Torsions

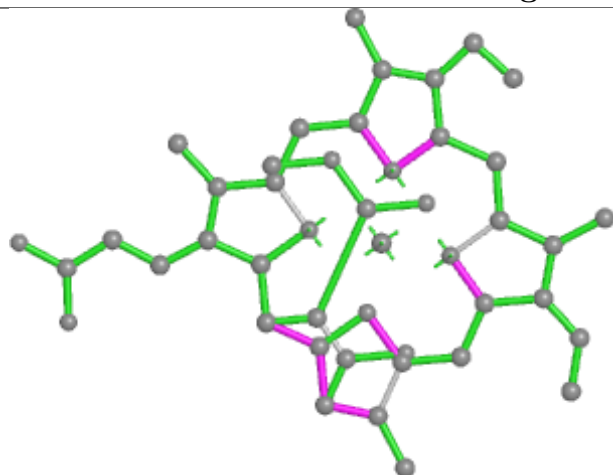


Rings

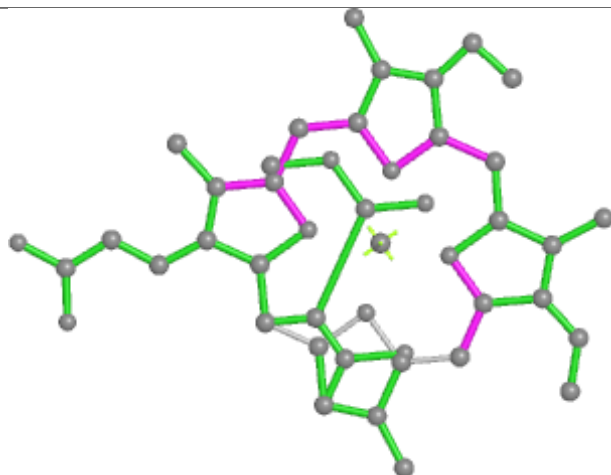




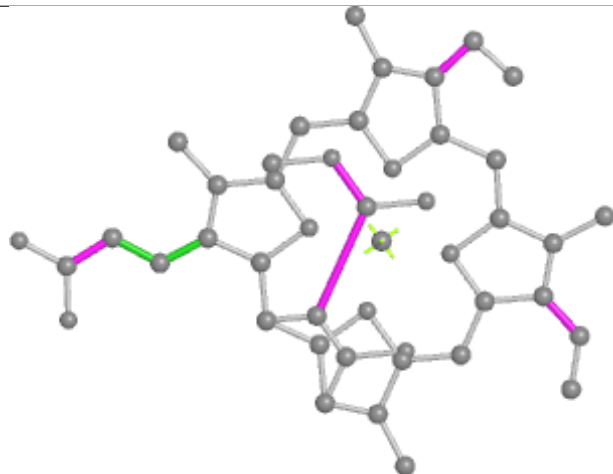
## Ligand KC2 0 305



Bond lengths



Bond angles

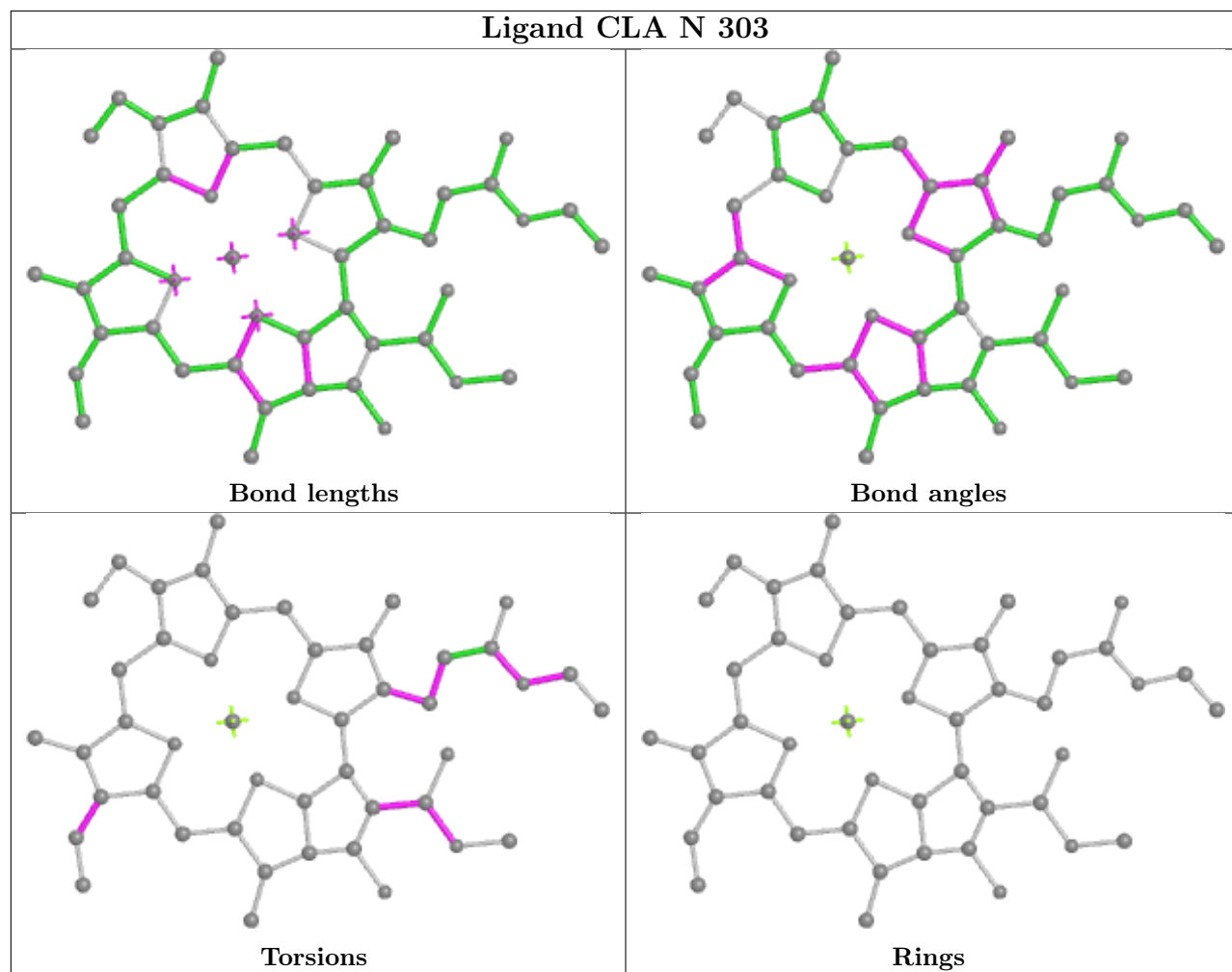


Torsions

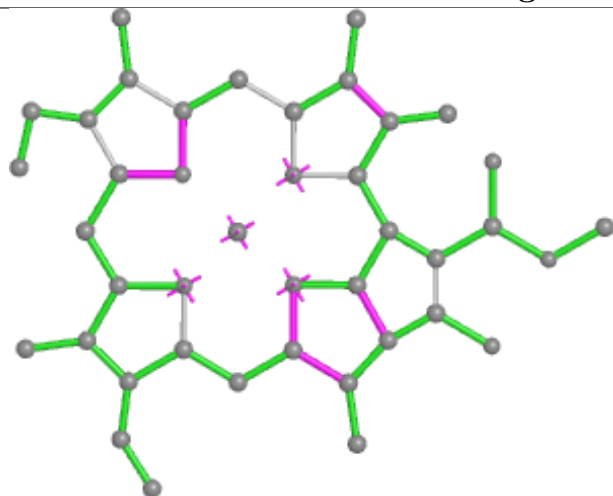


Rings

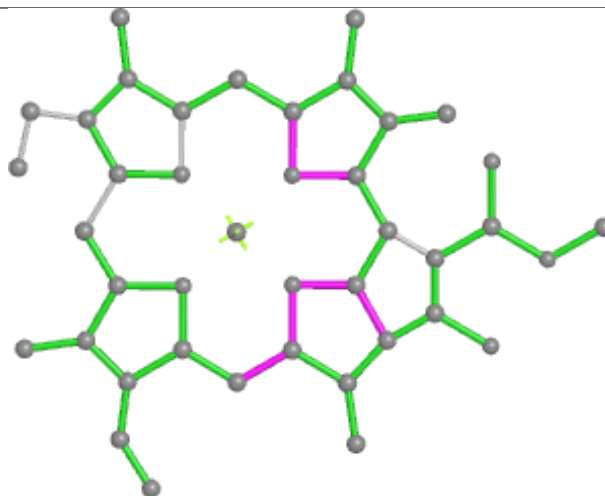
## Ligand CLA N 303



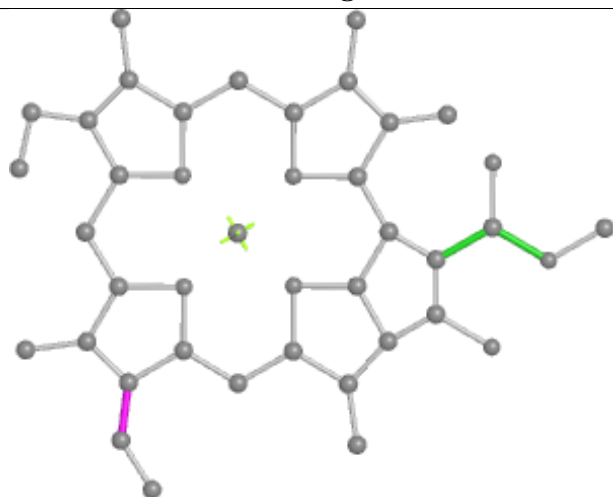
## Ligand CLA 3 310



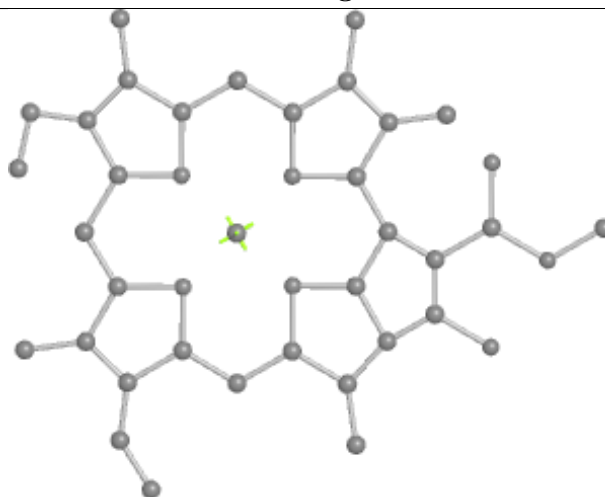
Bond lengths



Bond angles



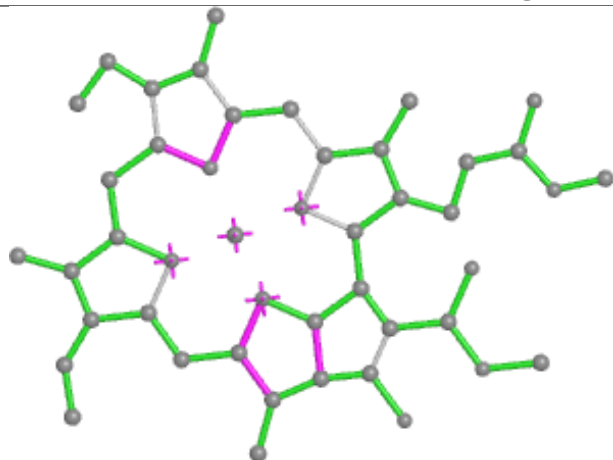
Torsions



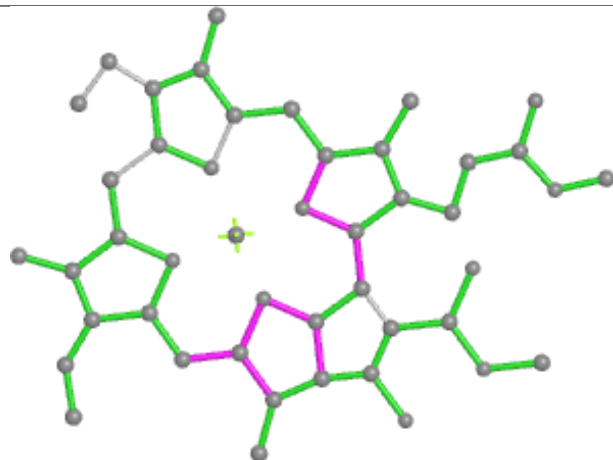
Rings



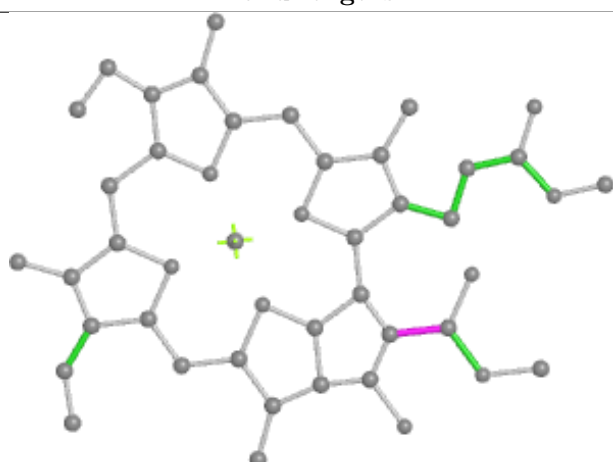
## Ligand CLA 8 310



Bond lengths



Bond angles

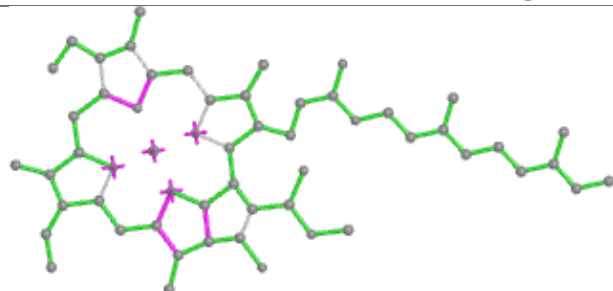


Torsions

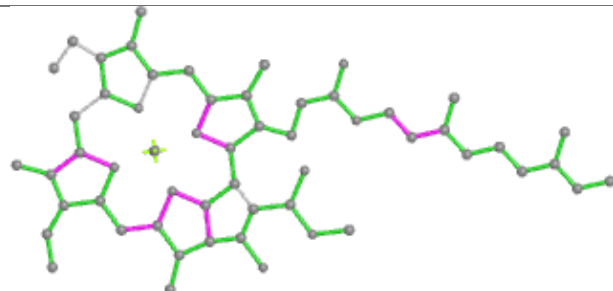


Rings

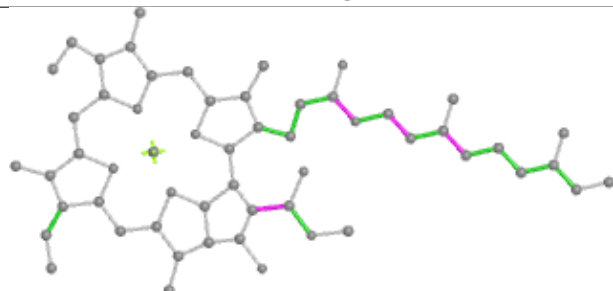
## Ligand CLA c 513



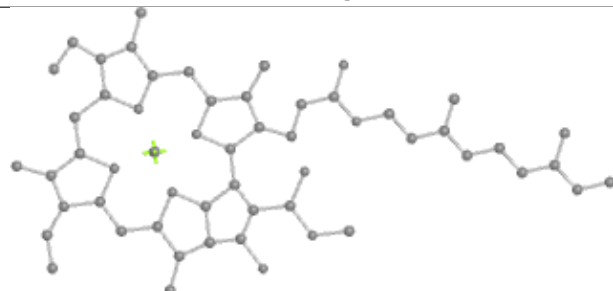
Bond lengths



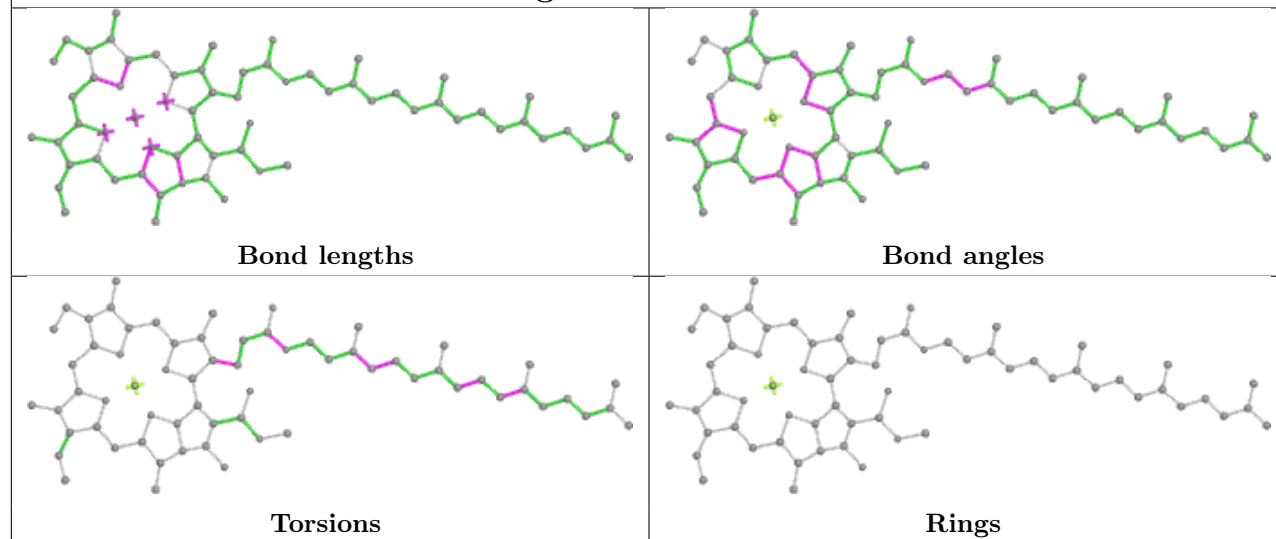
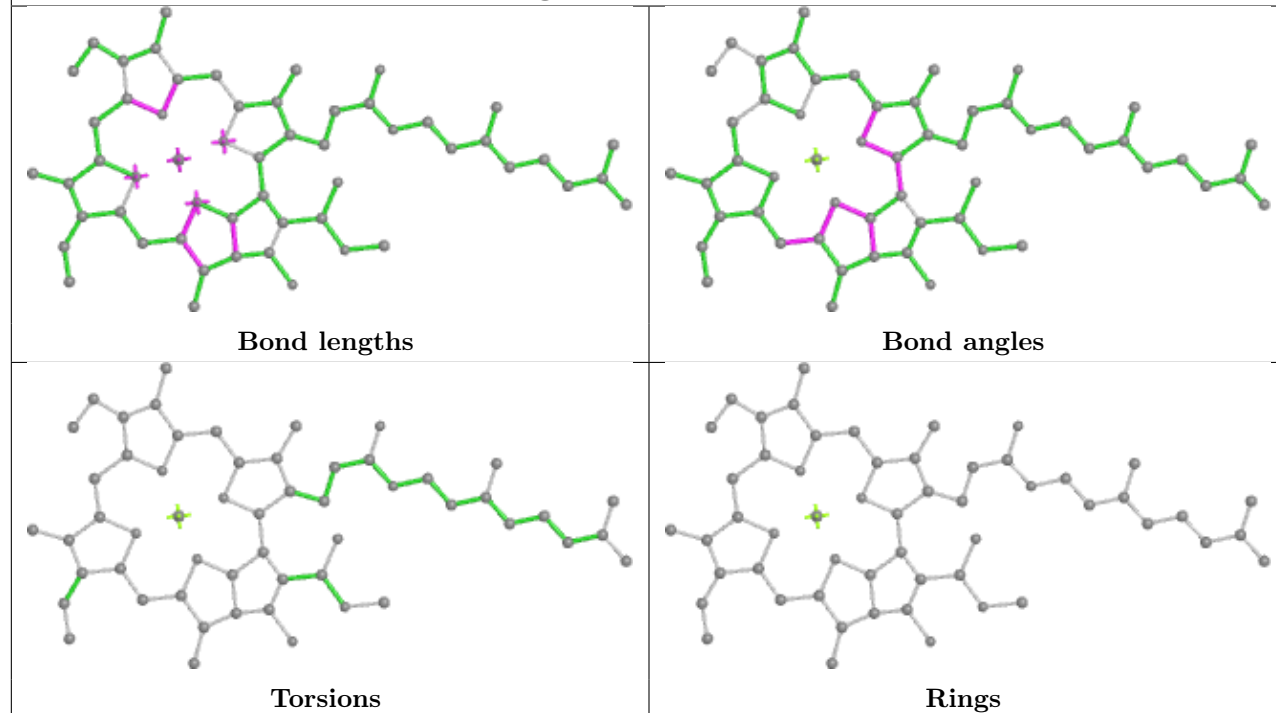
Bond angles

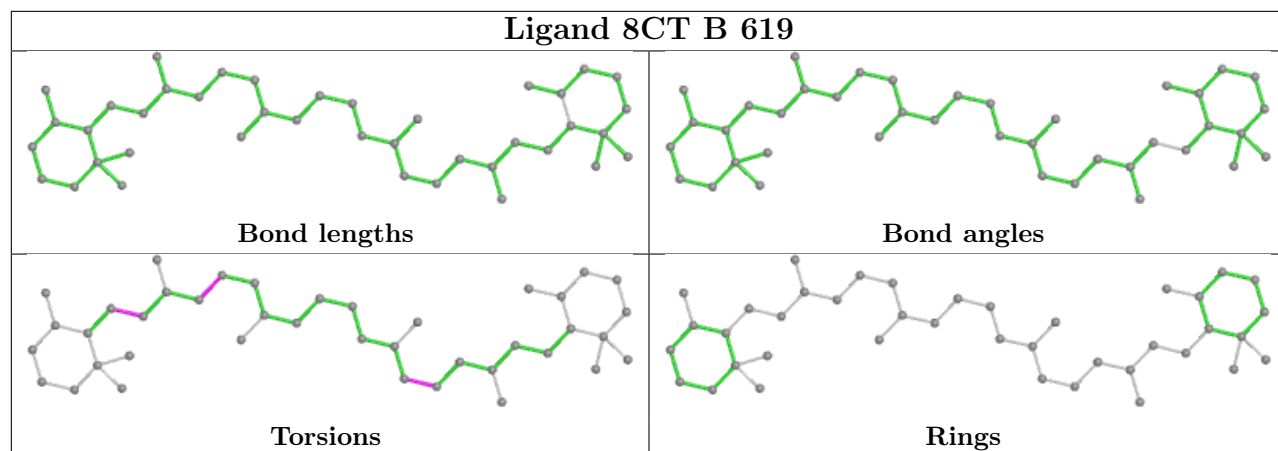
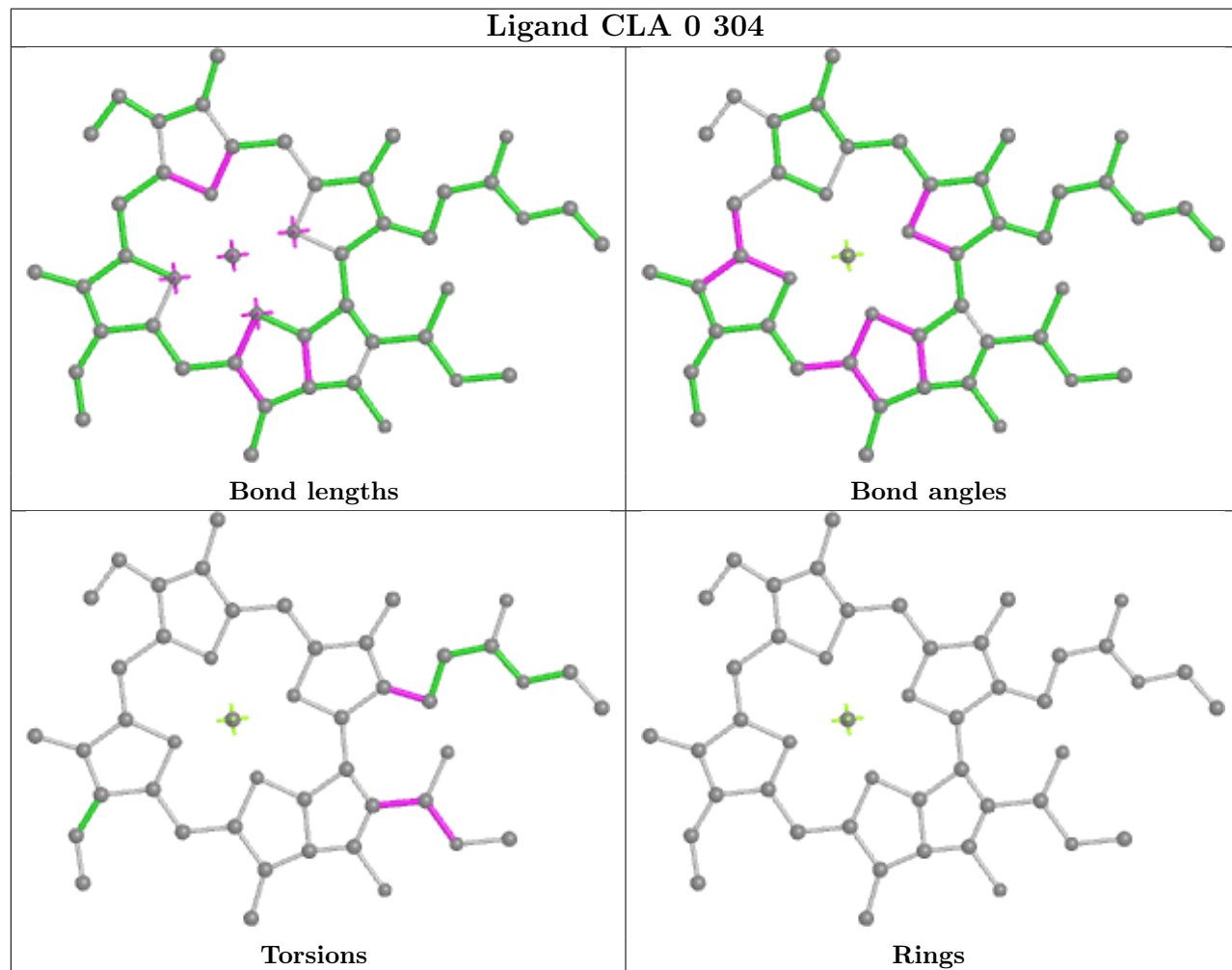


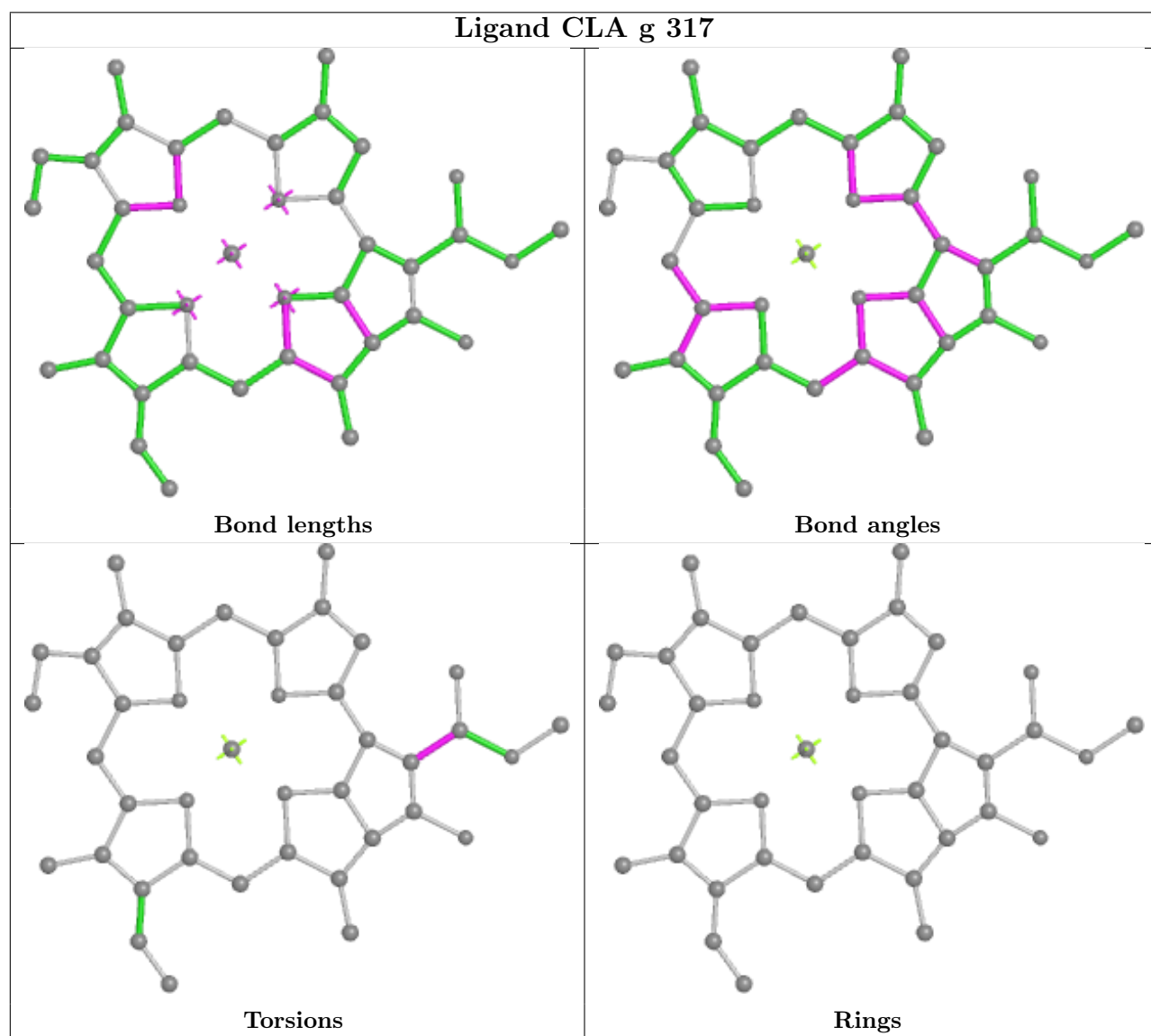
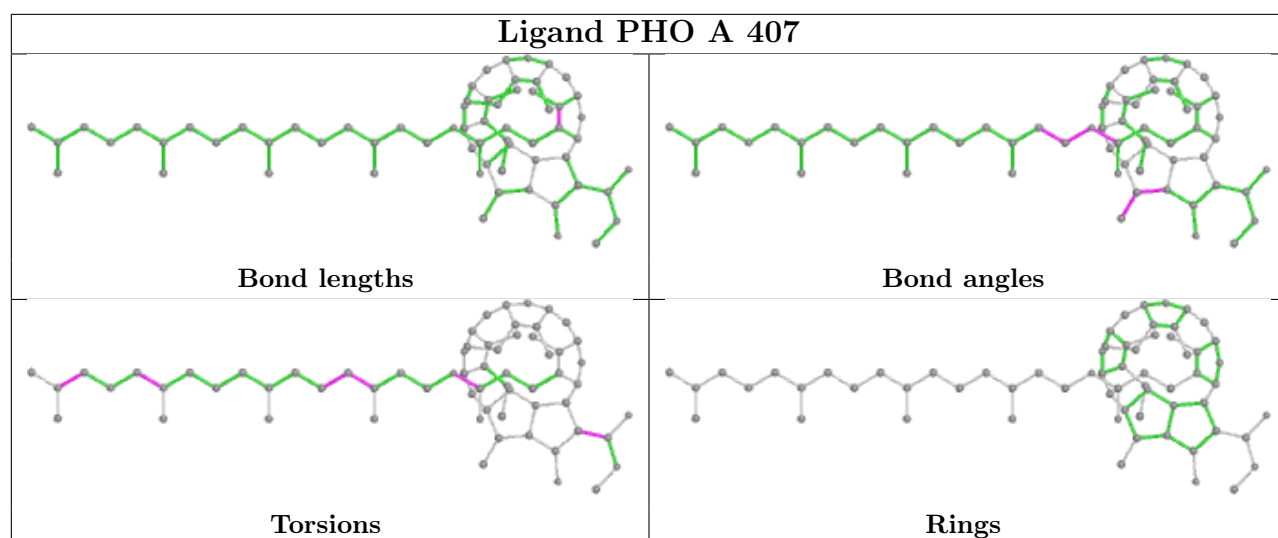
Torsions



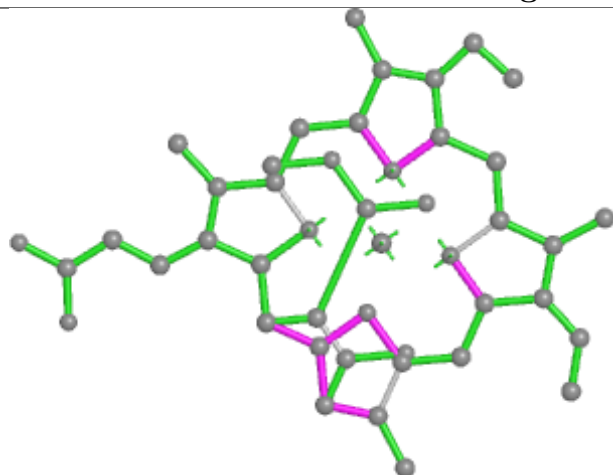
Rings

**Ligand CLA a 412****Ligand CLA 7 309**

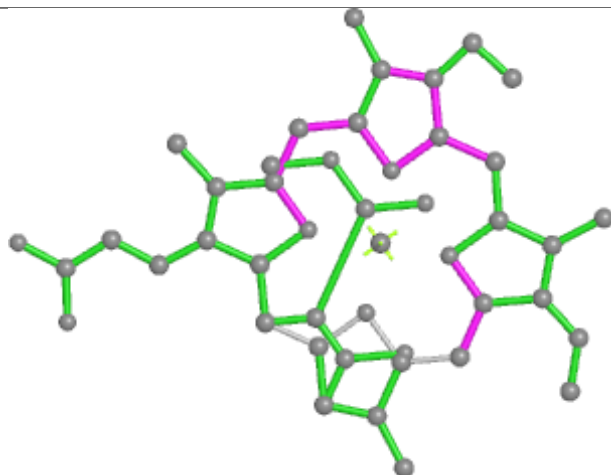
**Ligand 8CT B 619****Ligand CLA 0 304**



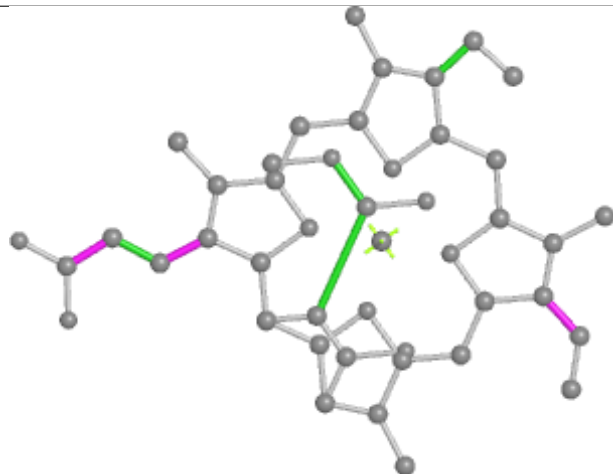
## Ligand KC2 7 311



Bond lengths



Bond angles

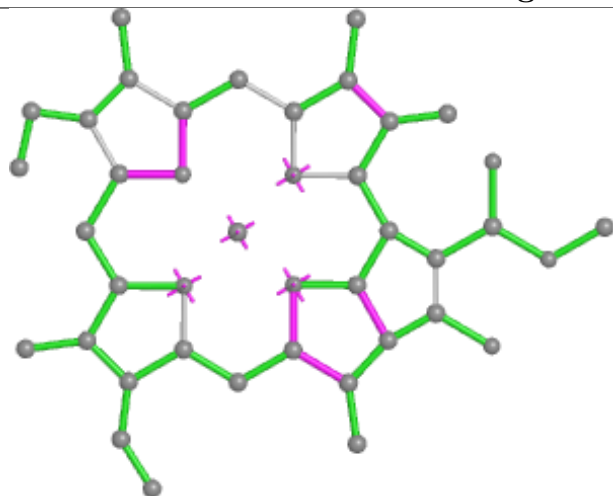


Torsions

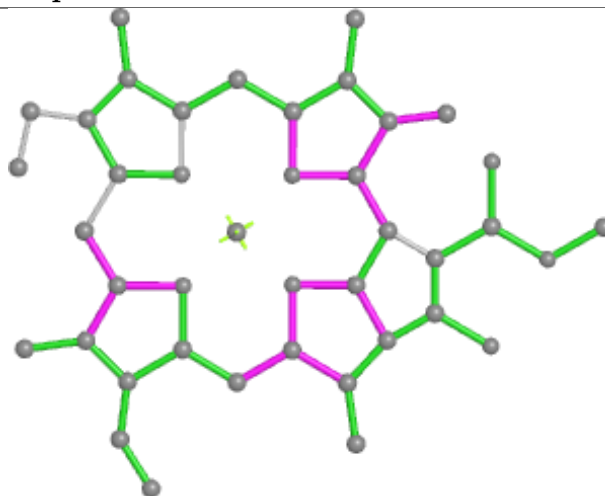


Rings

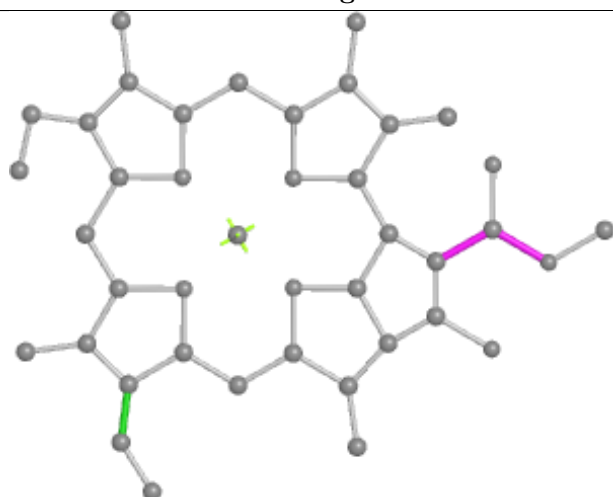
## Ligand CLA p 313



Bond lengths



Bond angles

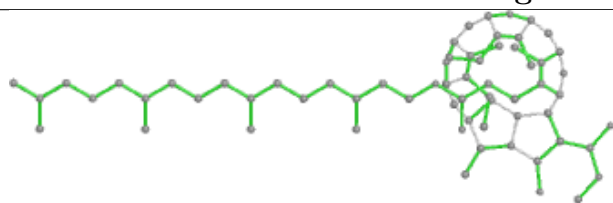


Torsions

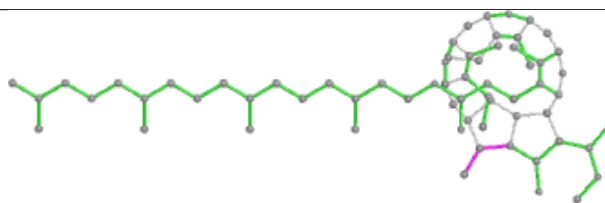


Rings

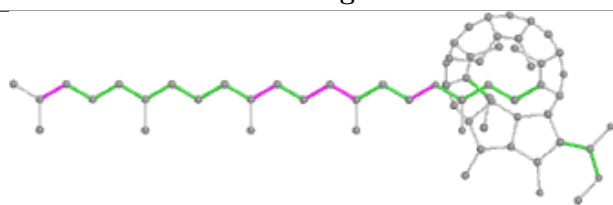
## Ligand PHO d 403



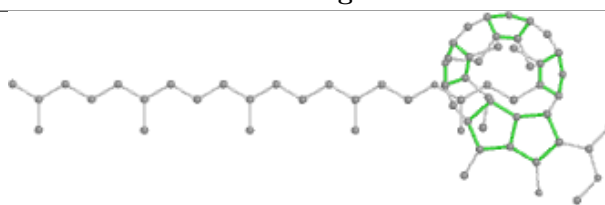
Bond lengths



Bond angles

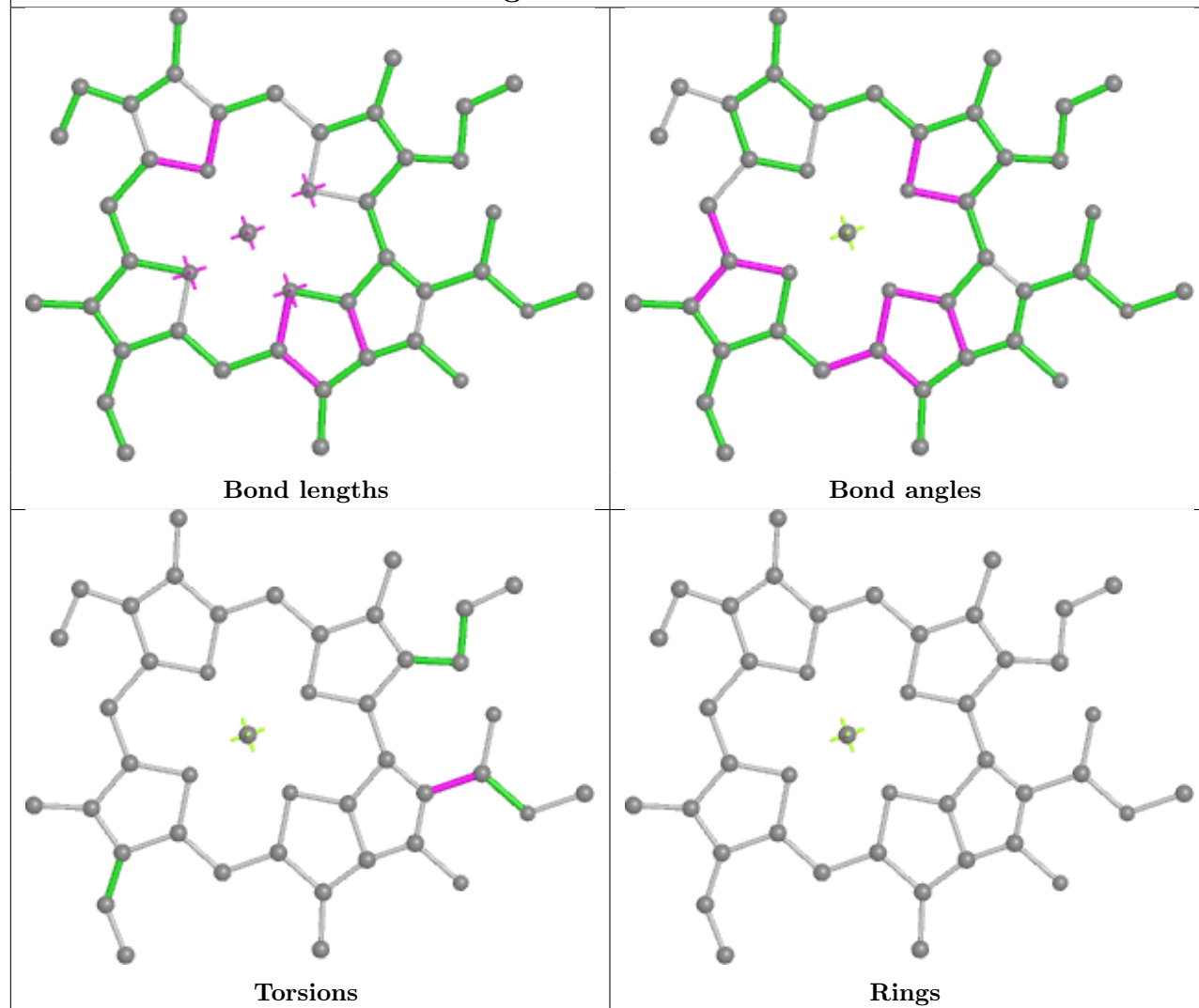


Torsions

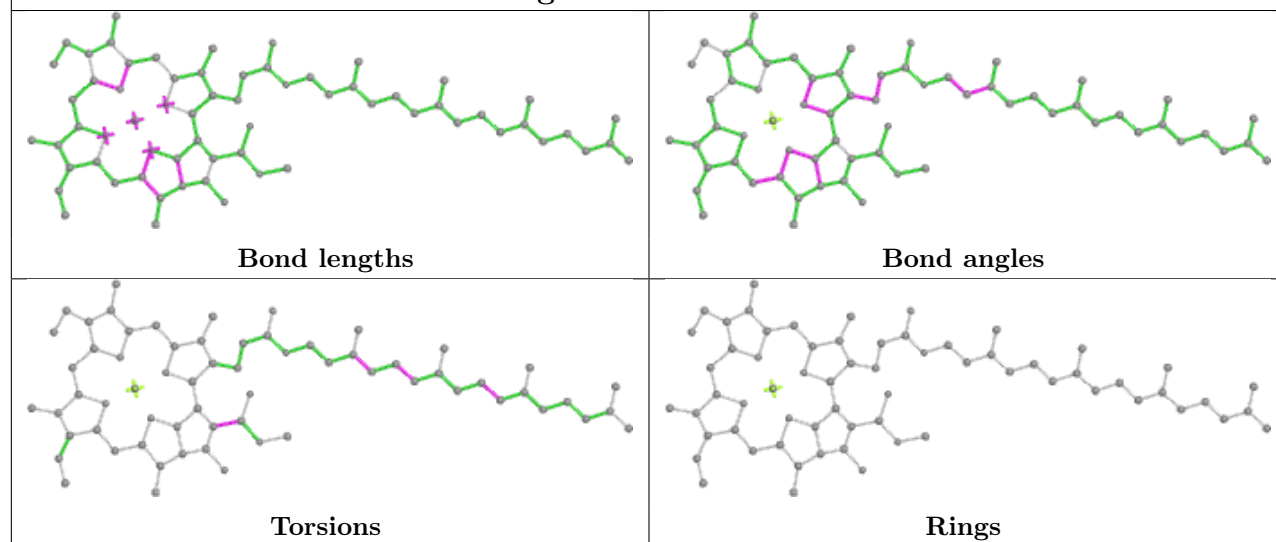


Rings

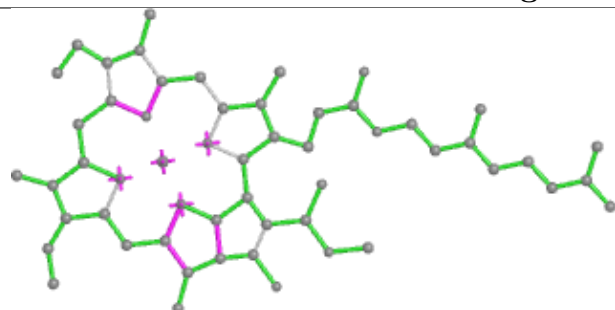
## Ligand CLA 6 307



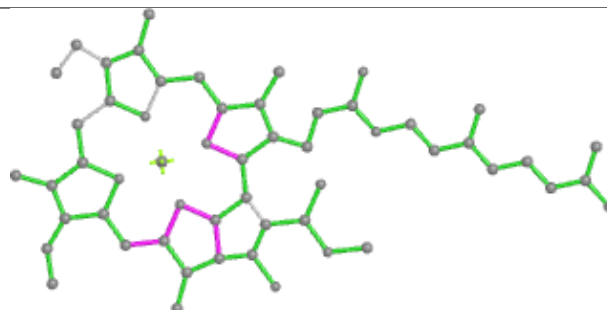
## Ligand CLA c 506



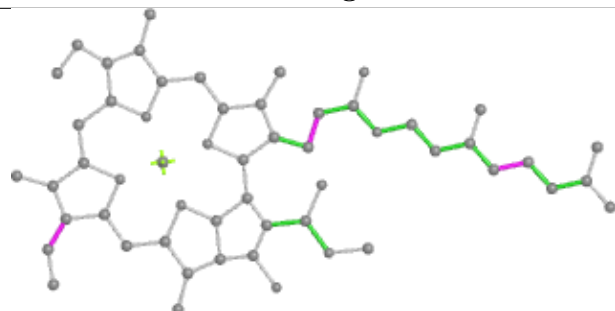
## Ligand CLA 9 305



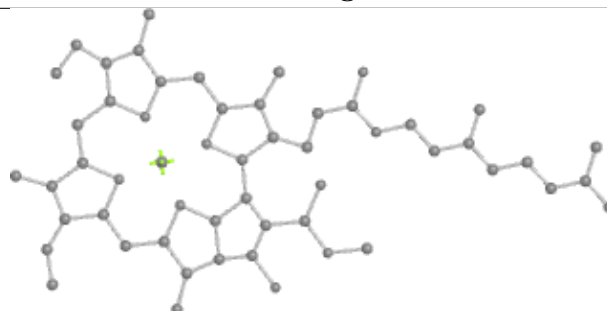
Bond lengths



Bond angles

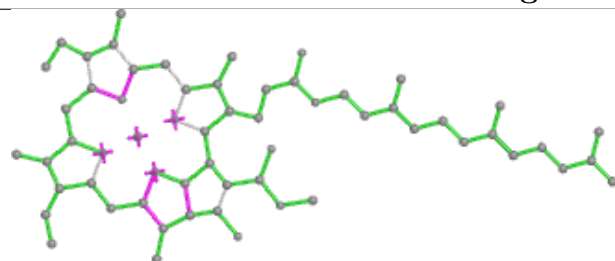


Torsions

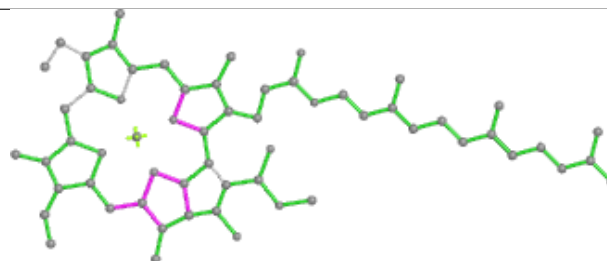


Rings

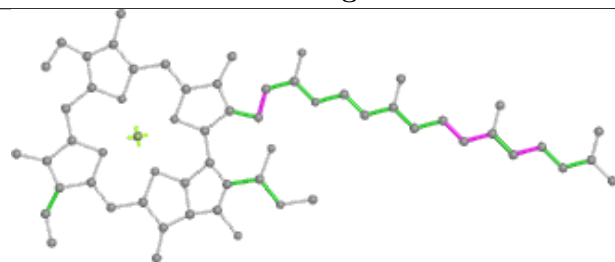
## Ligand CLA 2 304



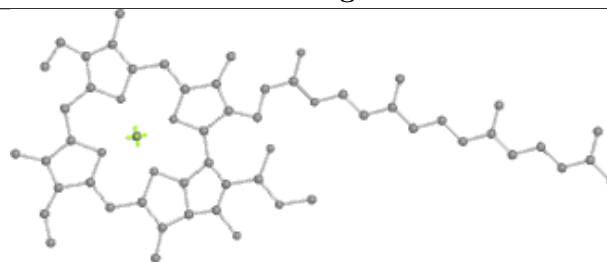
Bond lengths



Bond angles



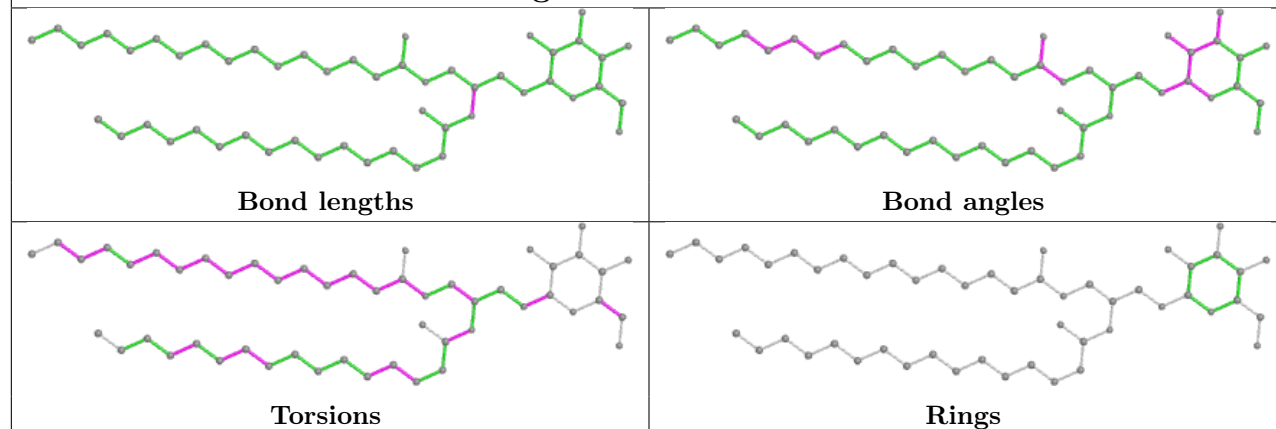
Torsions



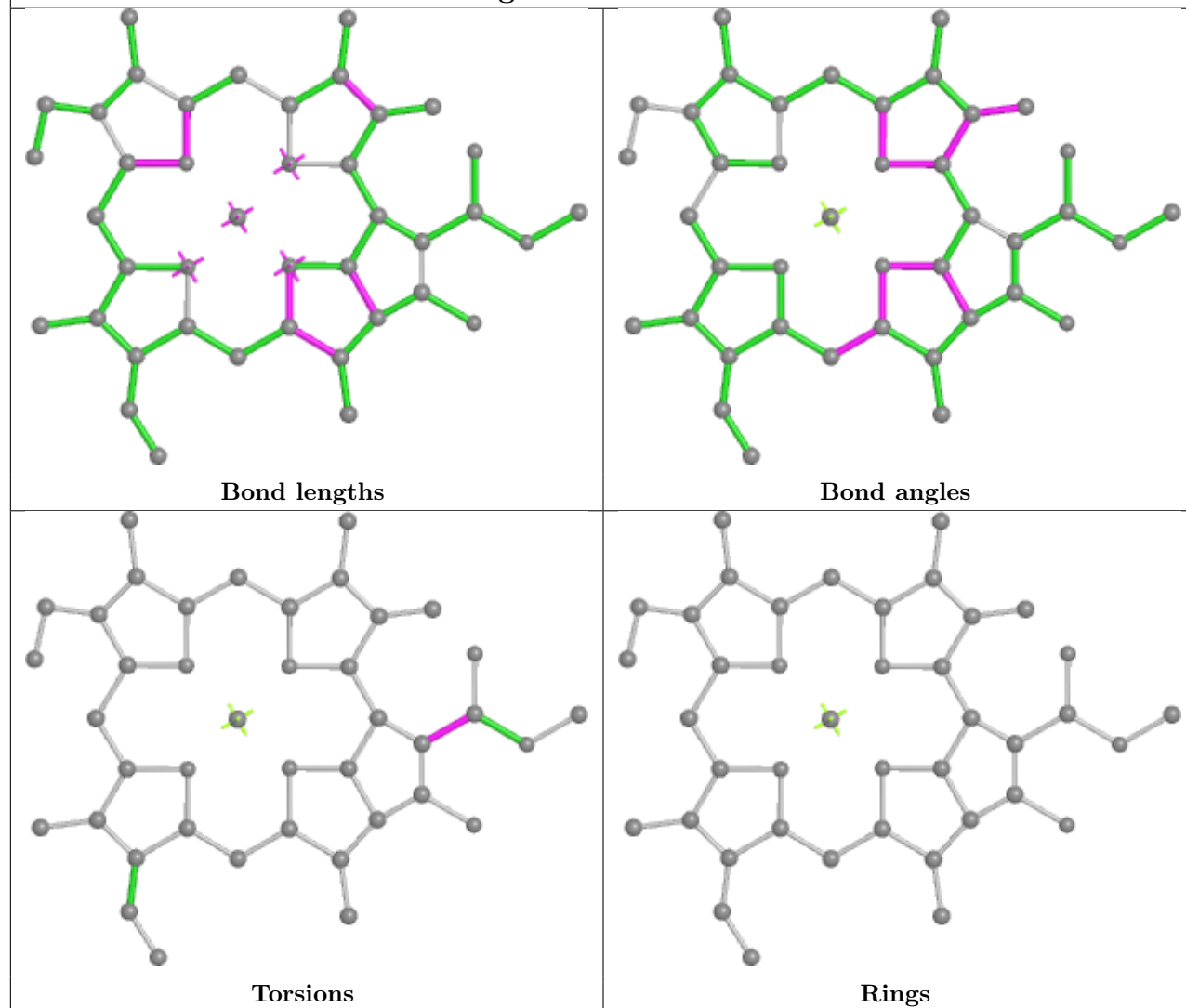
Rings



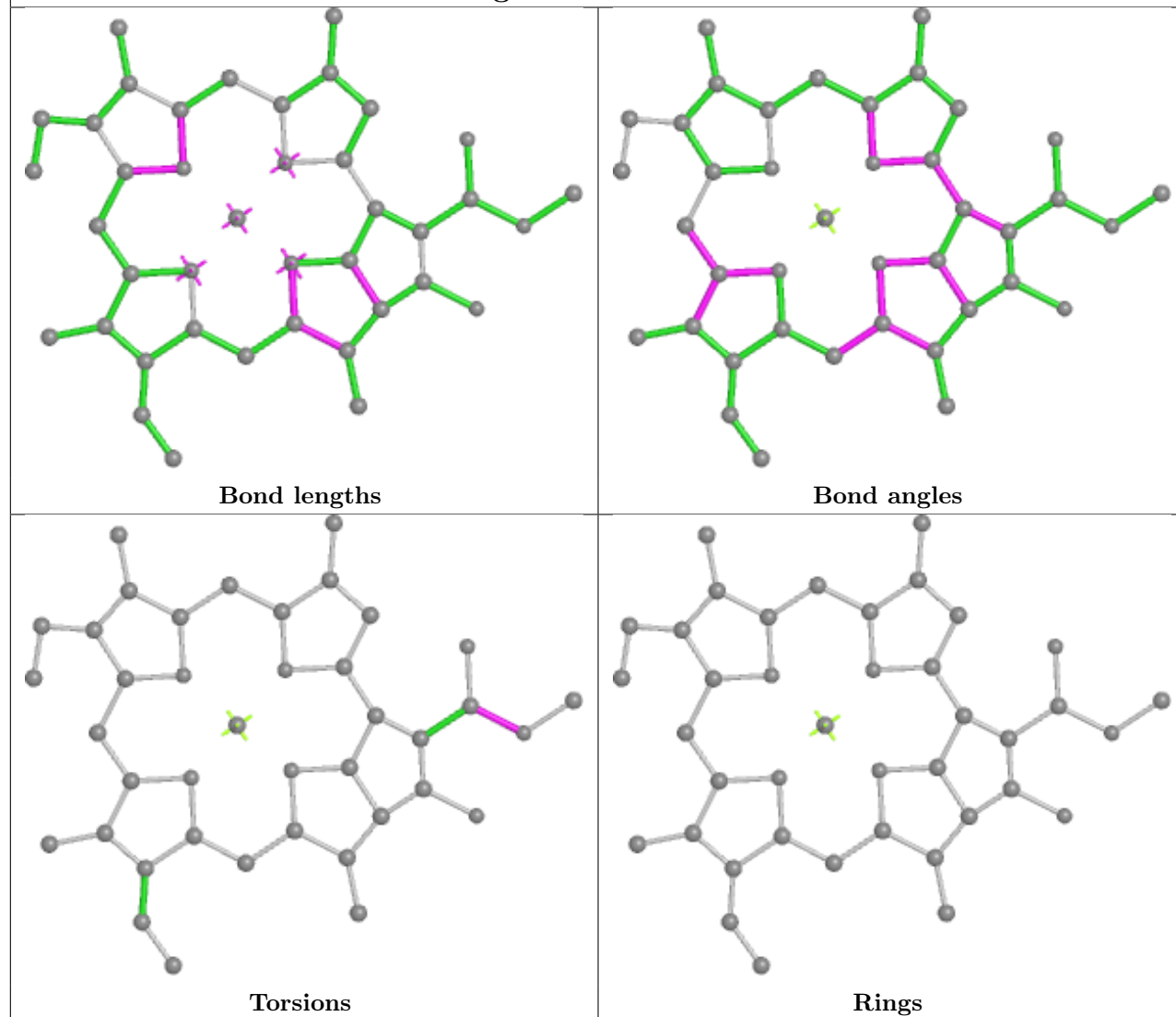
## Ligand LMG c 520

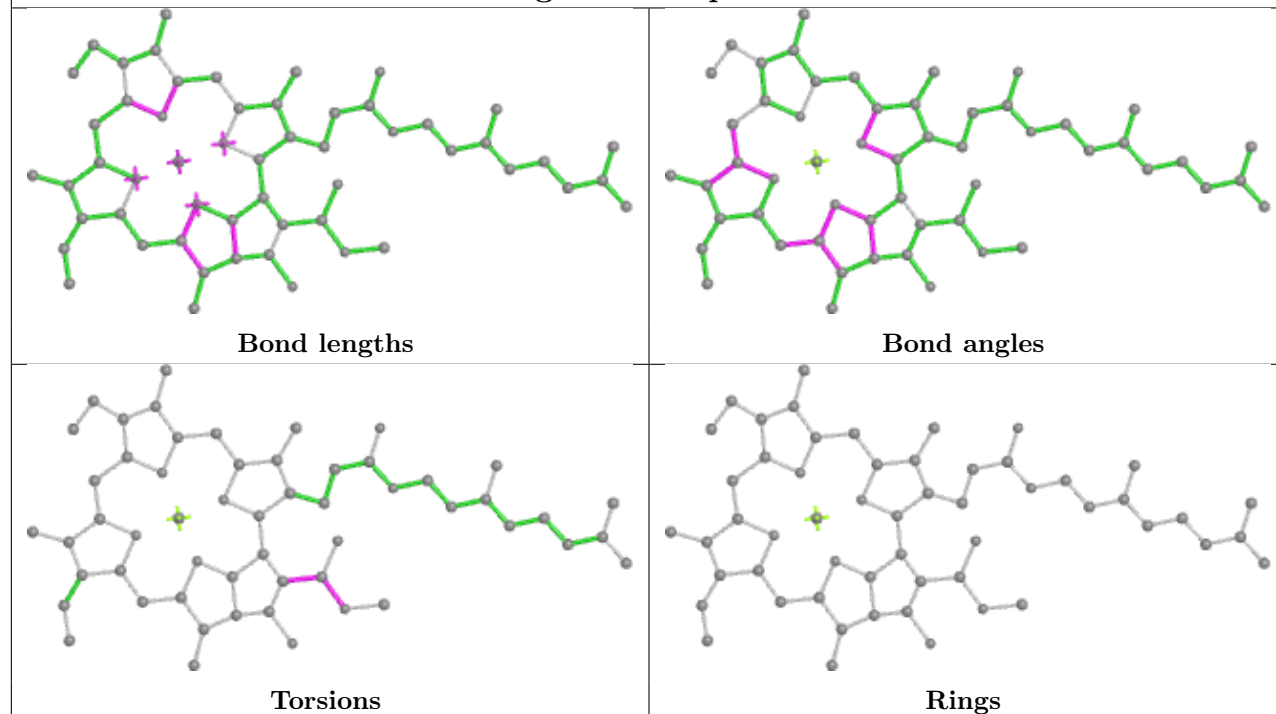
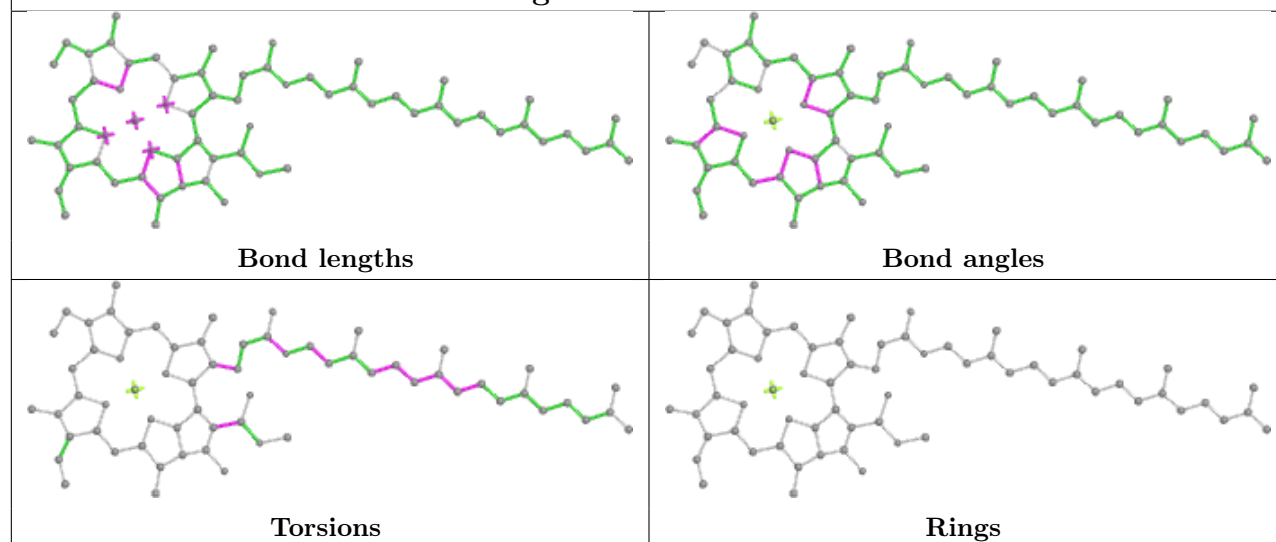
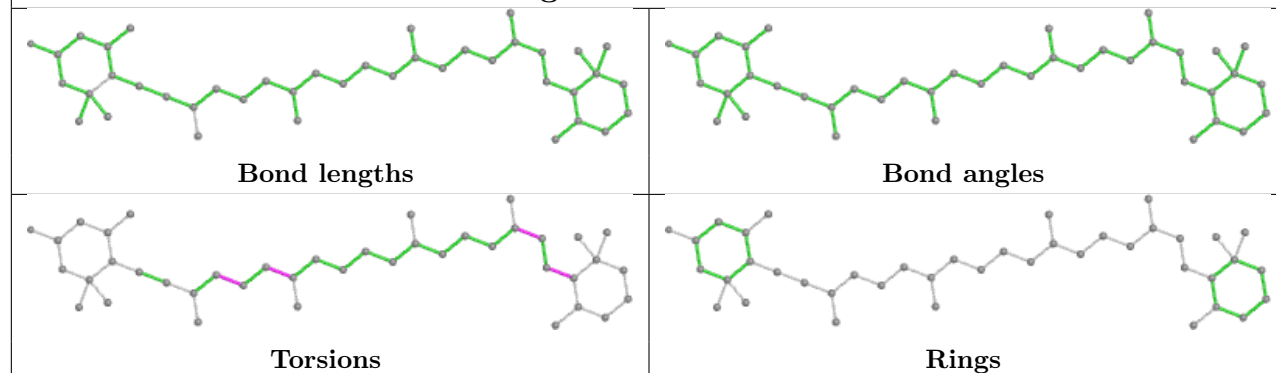


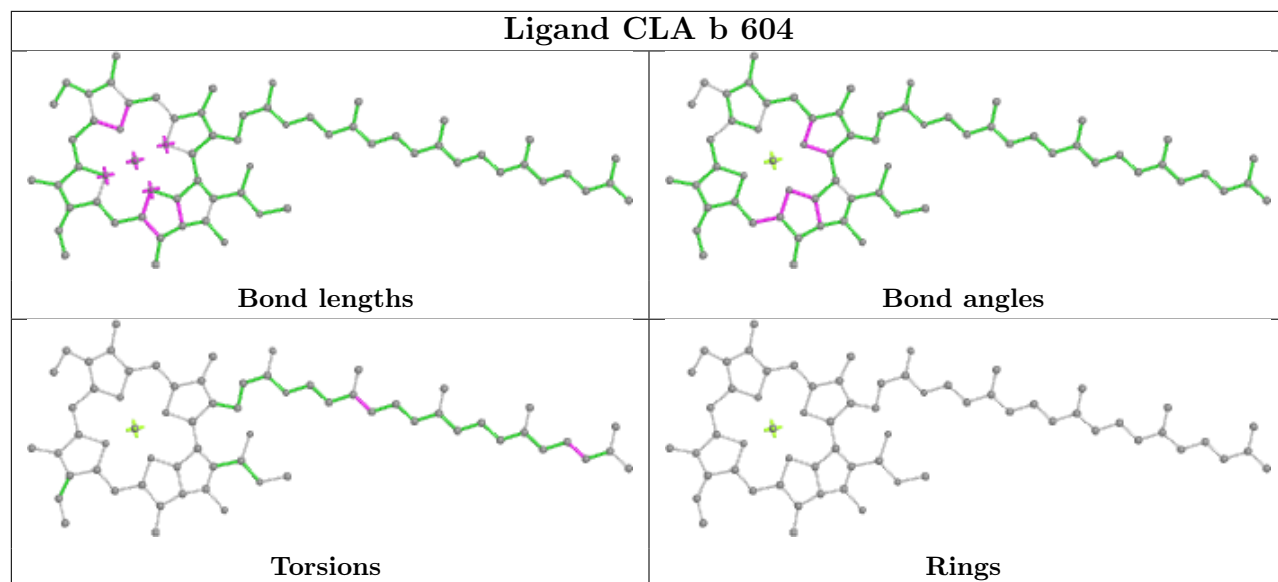
## Ligand CLA 3 313



## Ligand CLA b 618



**Ligand CLA p 305****Ligand CLA B 605****Ligand IHT 3 320**



## 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.

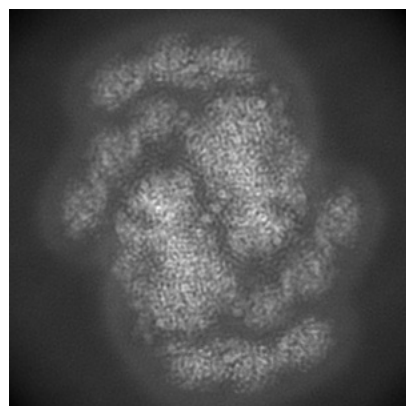
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38596. These allow visual inspection of the internal detail of the map and identification of artifacts.

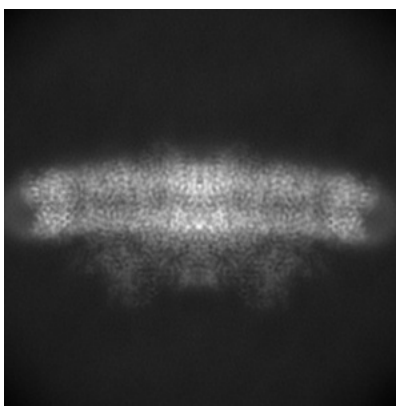
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

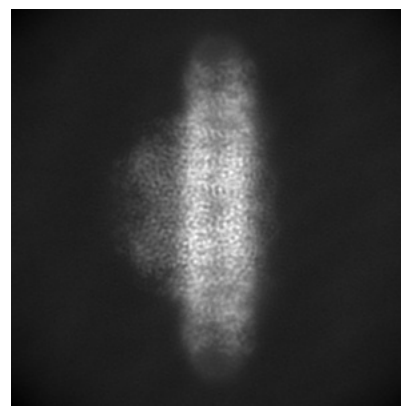
#### 6.1.1 Primary map



X

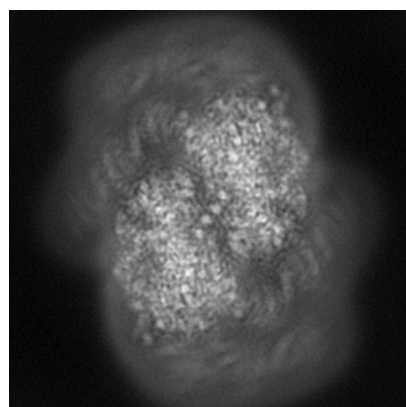


Y

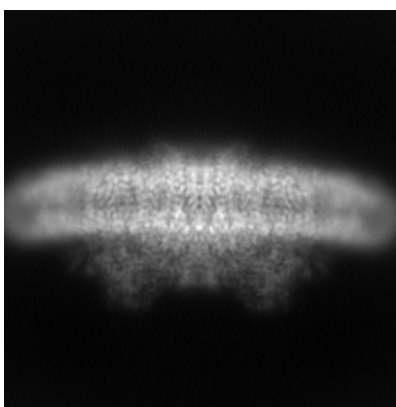


Z

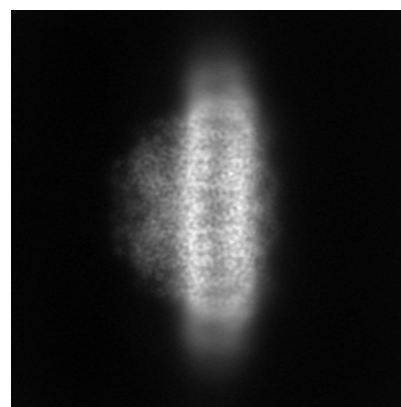
#### 6.1.2 Raw map



X



Y

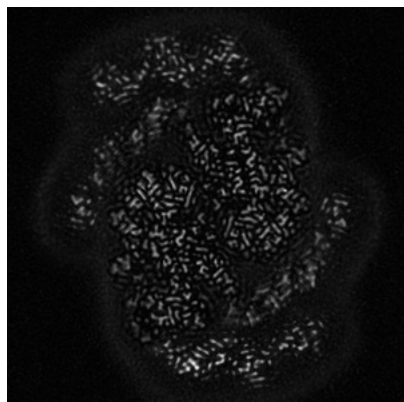


Z

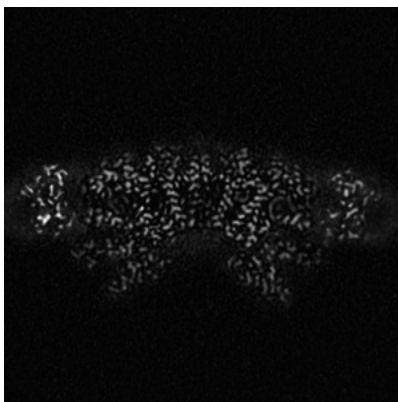
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

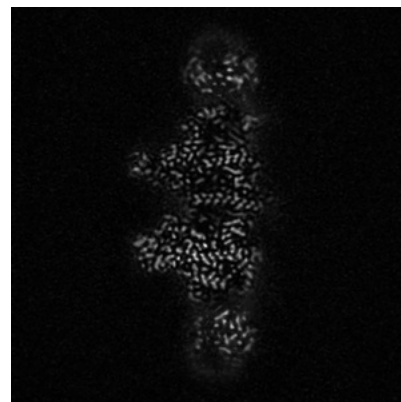
### 6.2.1 Primary map



X Index: 128

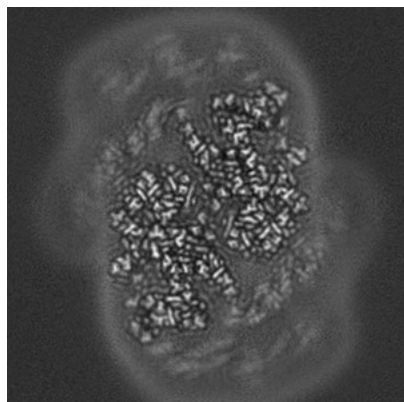


Y Index: 128

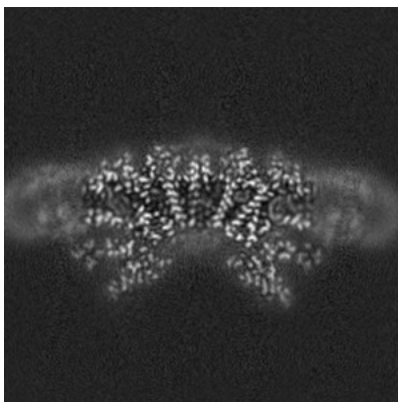


Z Index: 128

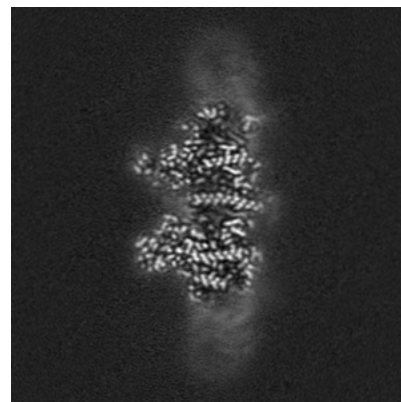
### 6.2.2 Raw map



X Index: 128



Y Index: 128

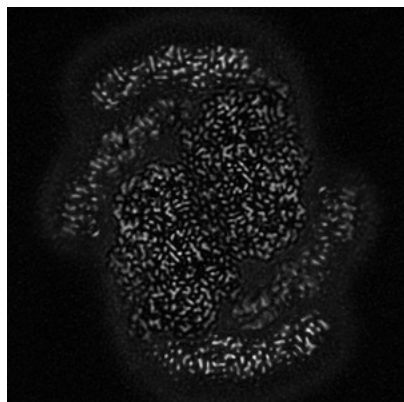


Z Index: 128

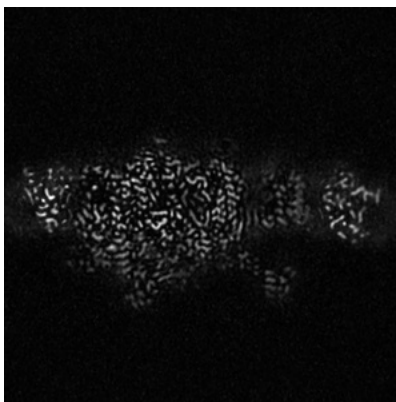
The images above show central slices of the map in three orthogonal directions.

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

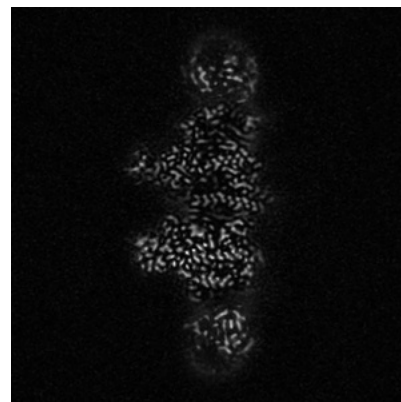
### 6.3.1 Primary map



X Index: 120

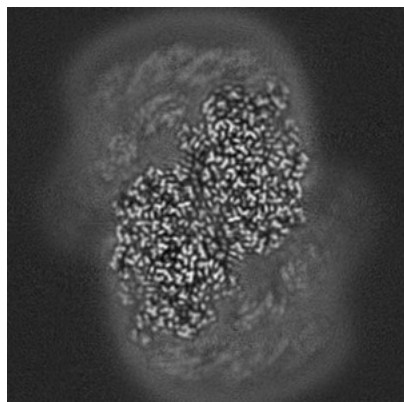


Y Index: 113

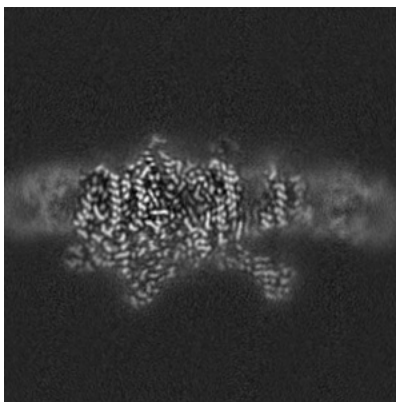


Z Index: 129

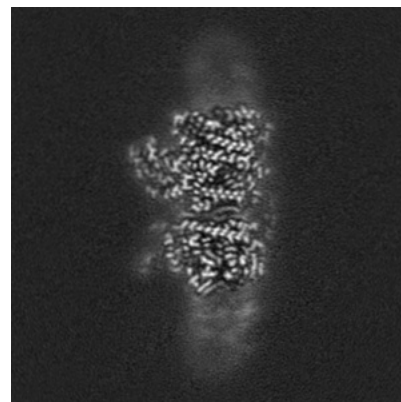
### 6.3.2 Raw map



X Index: 117



Y Index: 114



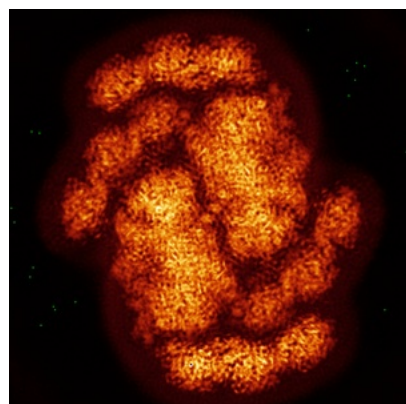
Z Index: 137

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

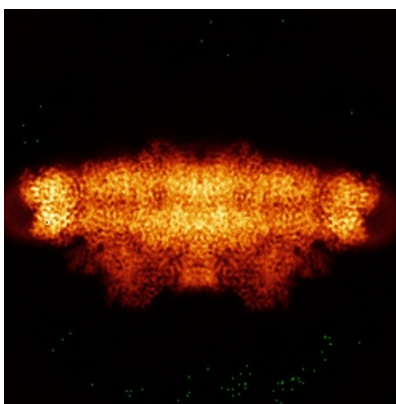


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

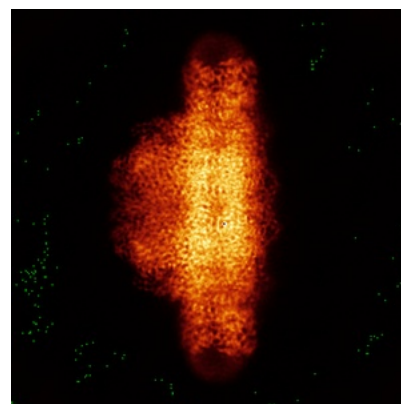
### 6.4.1 Primary map



X

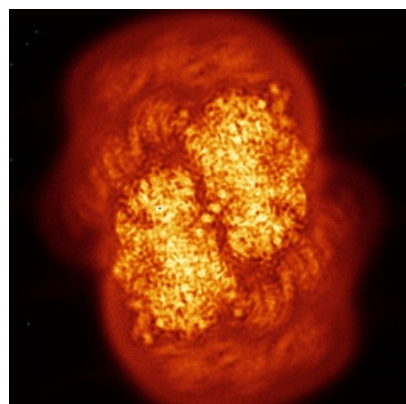


Y

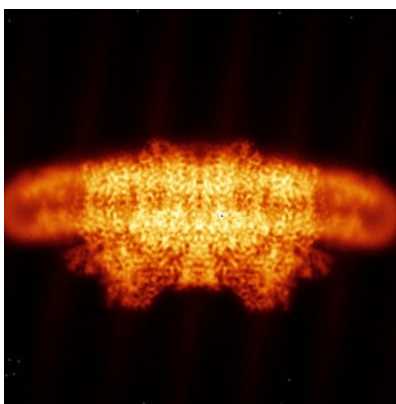


Z

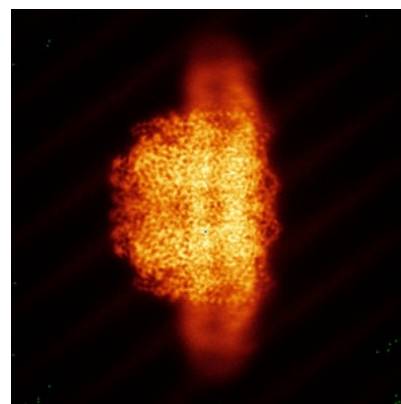
### 6.4.2 Raw map



X



Y



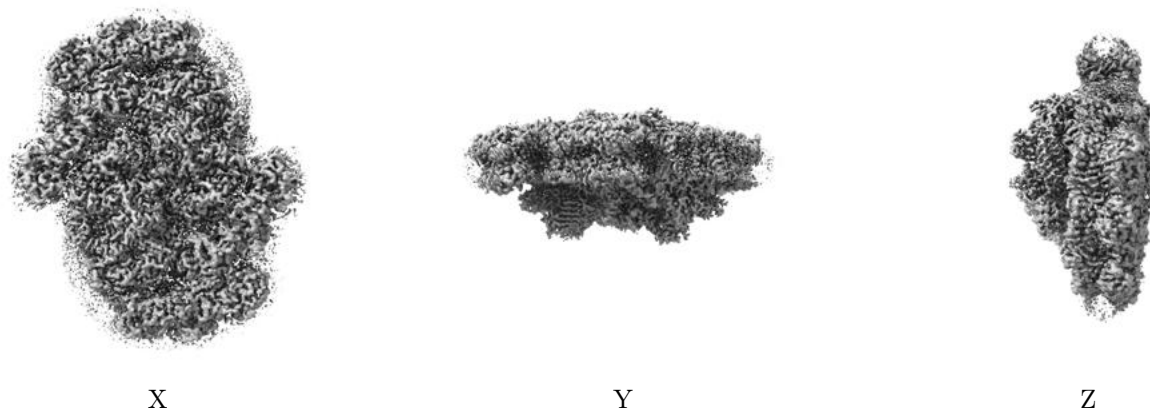
Z

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.



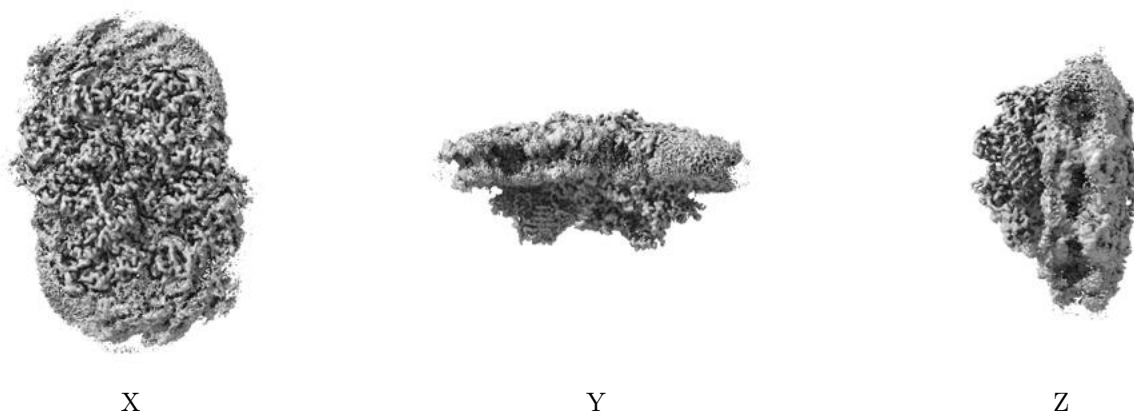
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. 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.

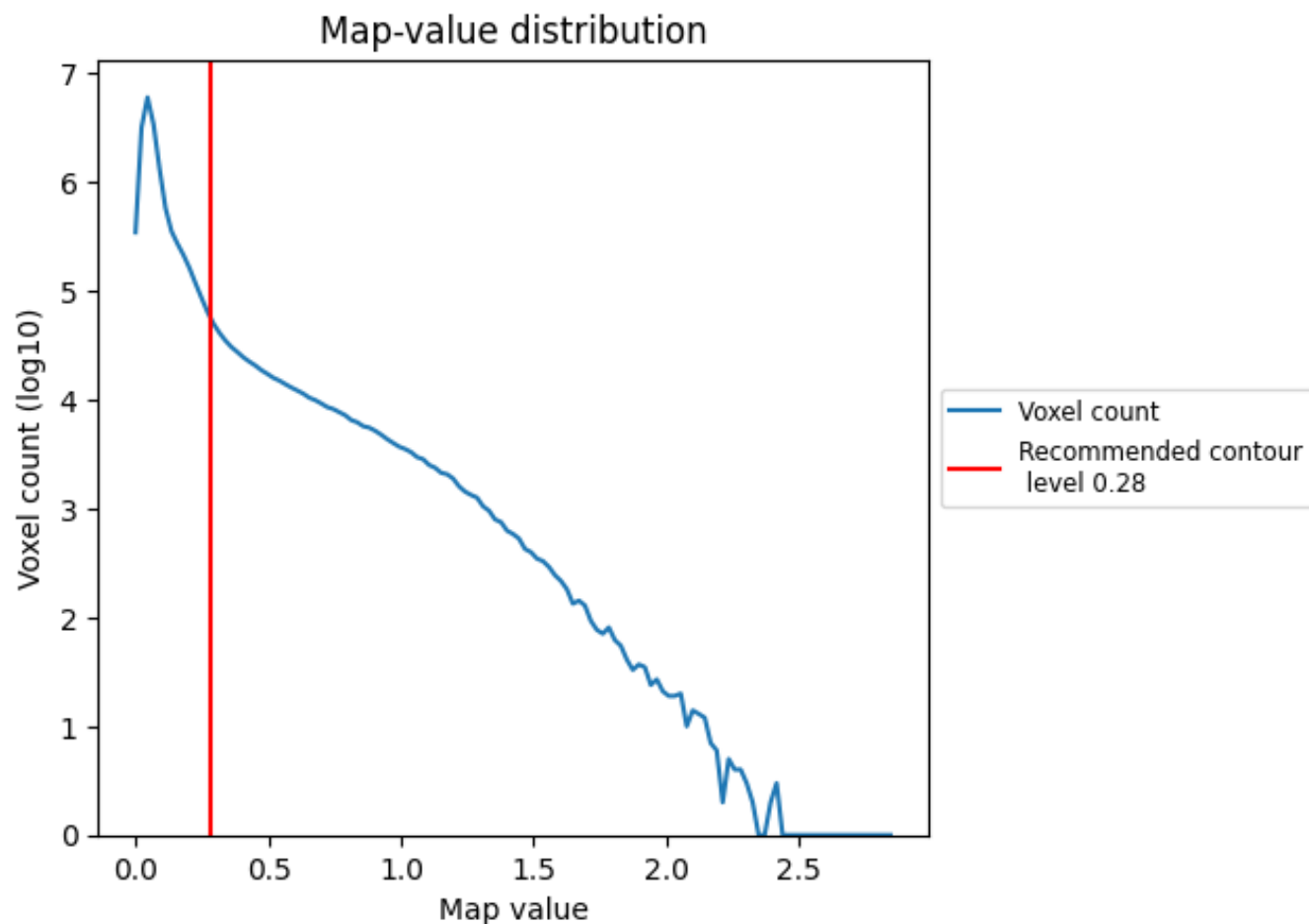
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

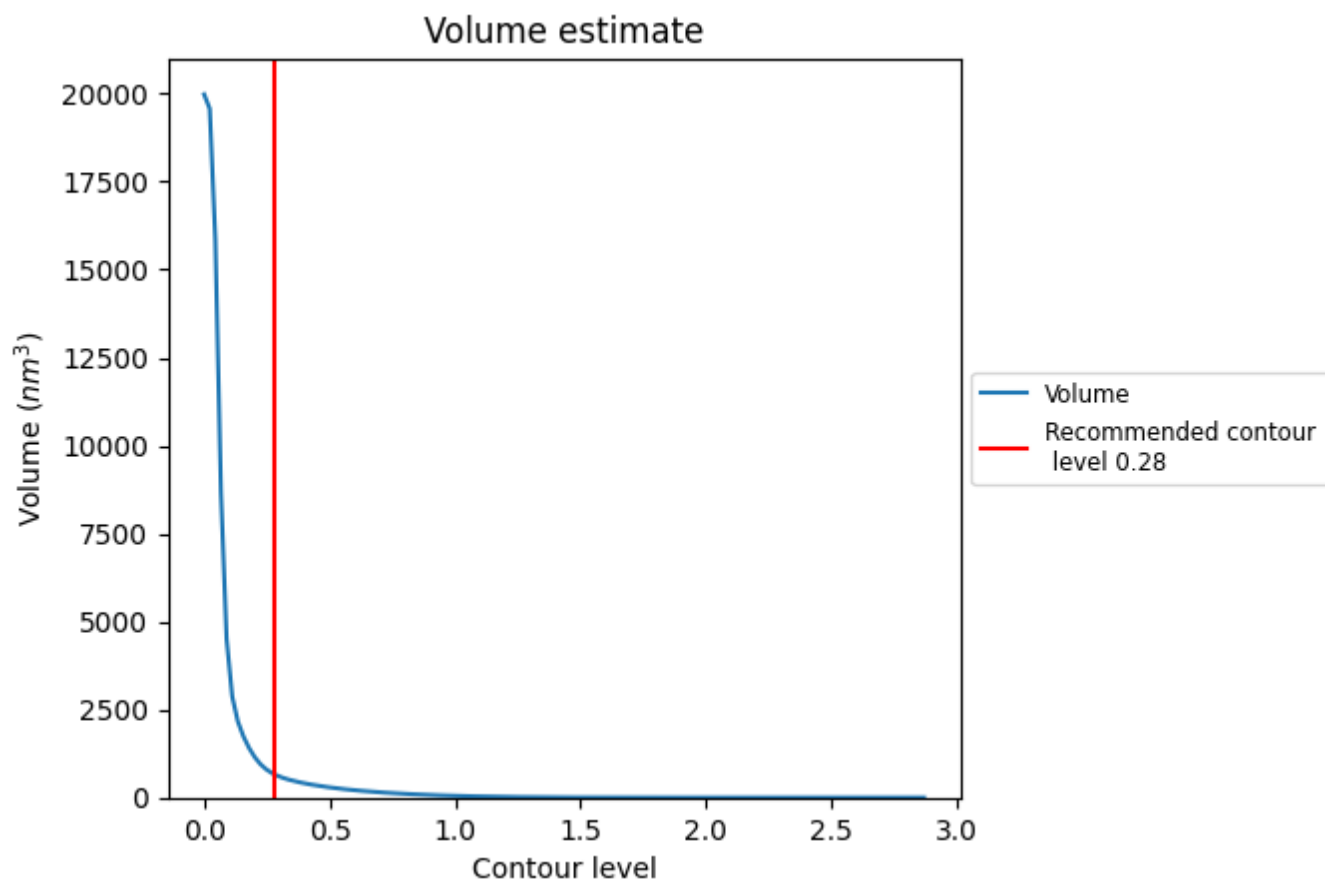
This section contains the results of statistical analysis of the map.

### 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.

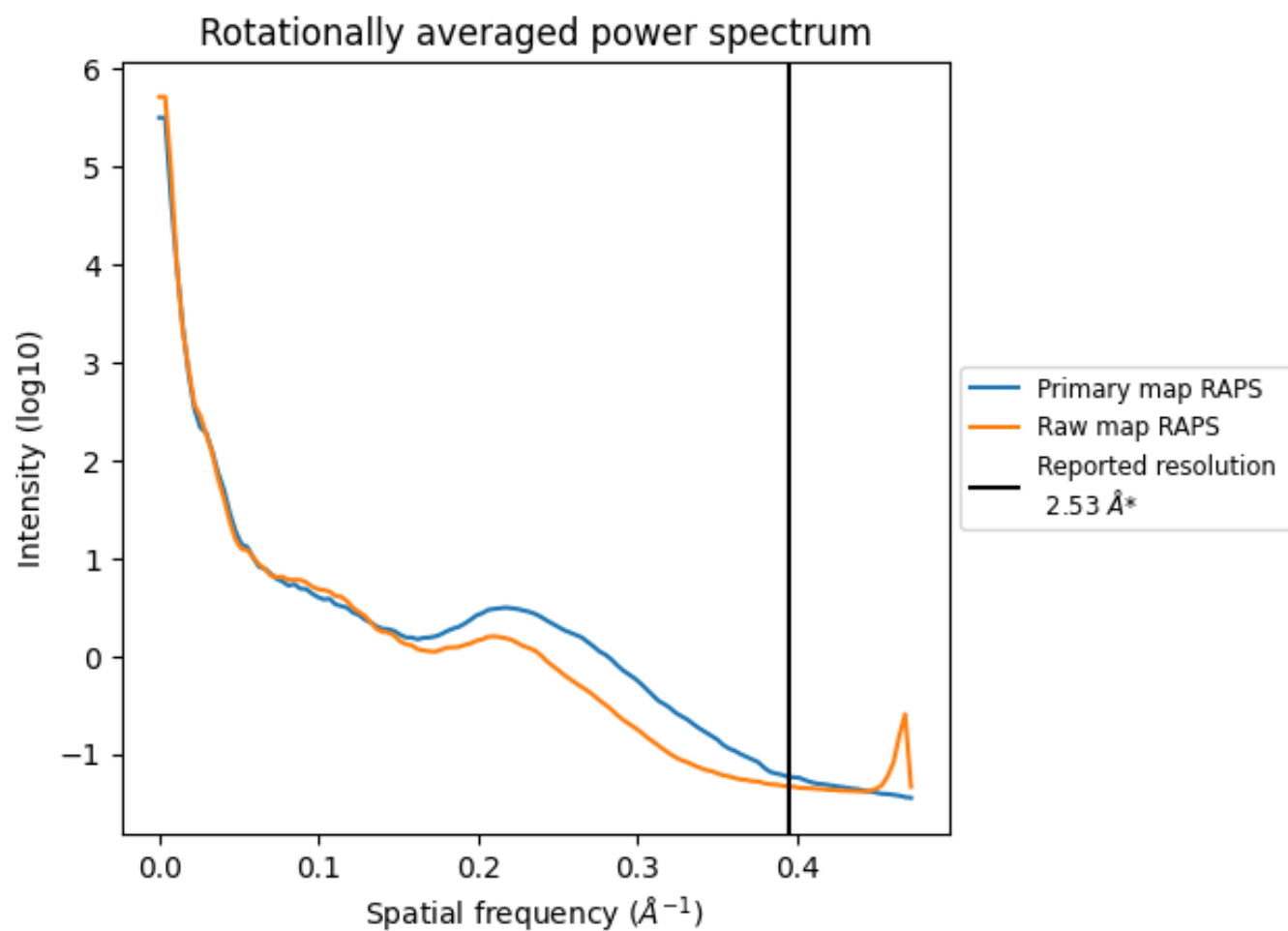
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 663 nm<sup>3</sup>; this corresponds to an approximate mass of 599 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

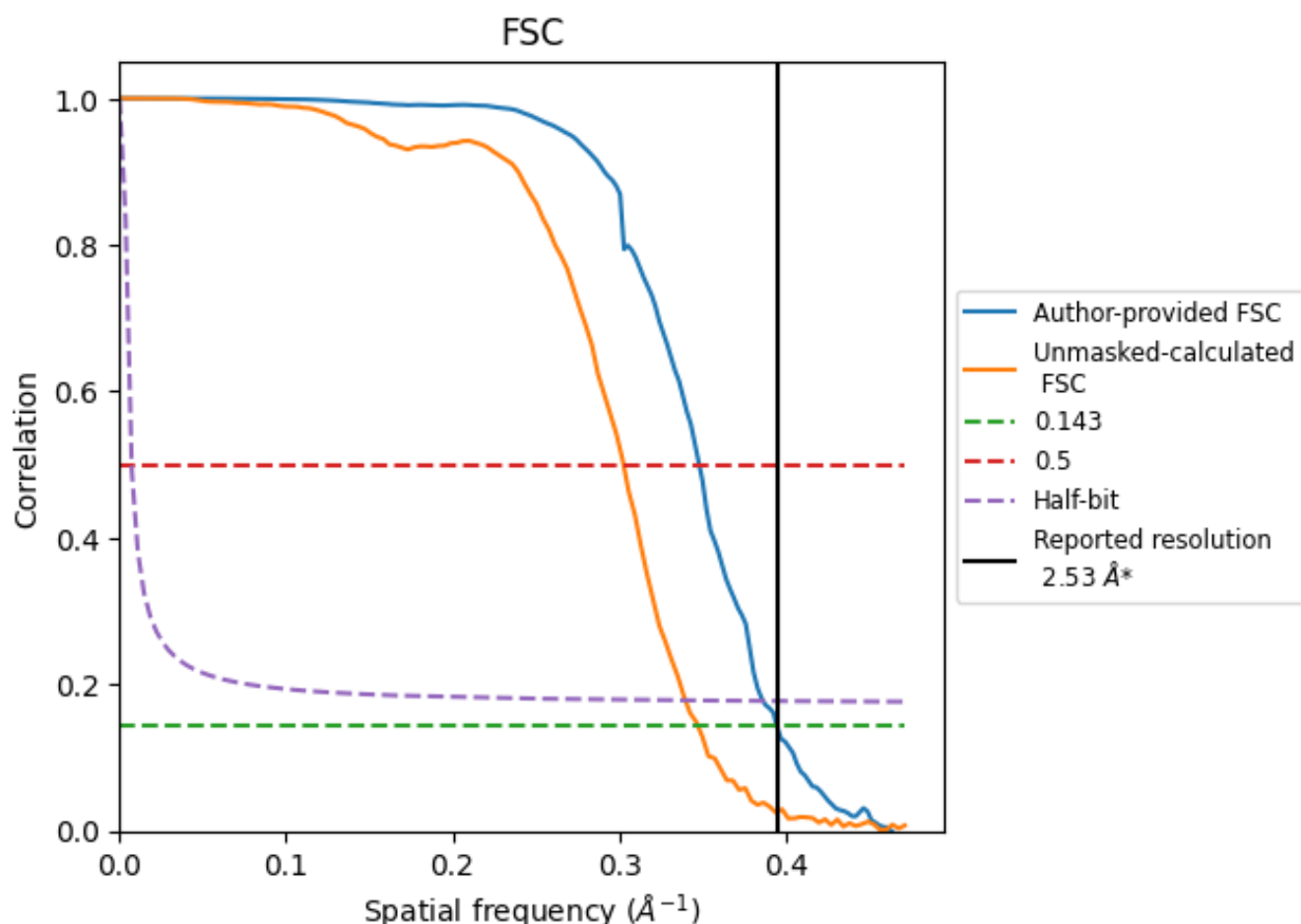


\*Reported resolution corresponds to spatial frequency of 0.395 Å<sup>-1</sup>

## 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 0.395 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

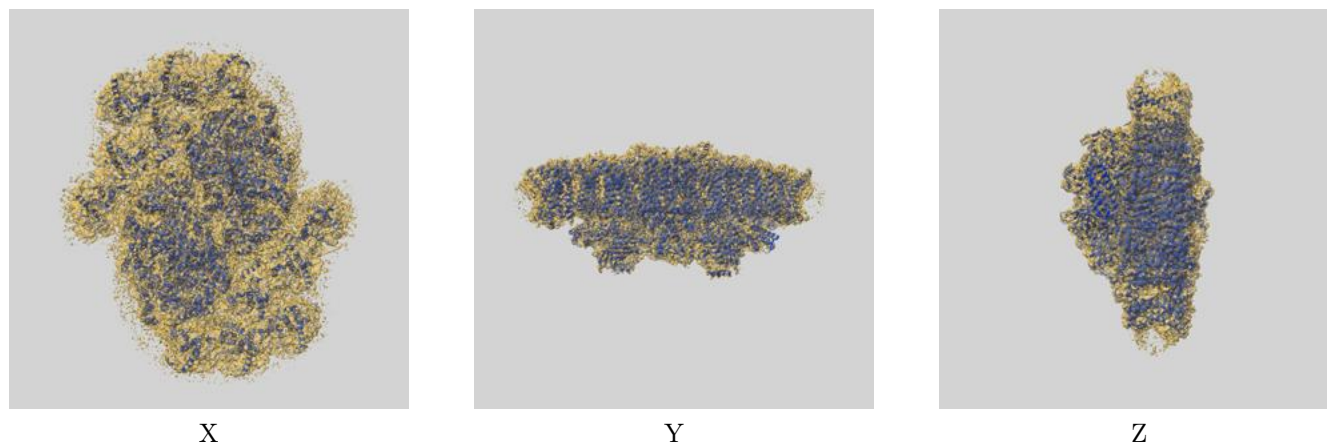
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.53	2.87	2.58
Unmasked-calculated*	2.88	3.30	2.94

\*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 2.88 differs from the reported value 2.53 by more than 10 %

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

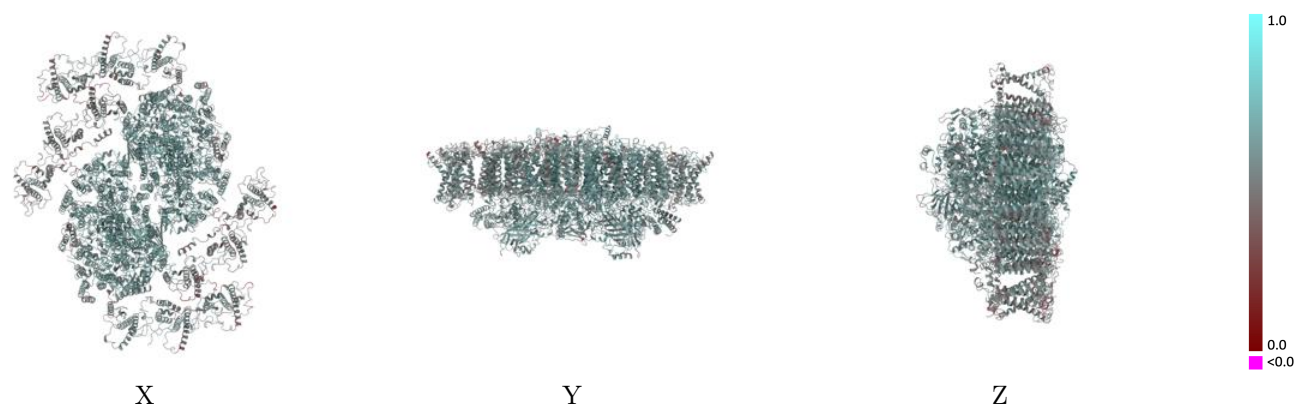
This section contains information regarding the fit between EMDB map EMD-38596 and PDB model 8XR6. Per-residue inclusion information can be found in [section 3](#) on [page 42](#).

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



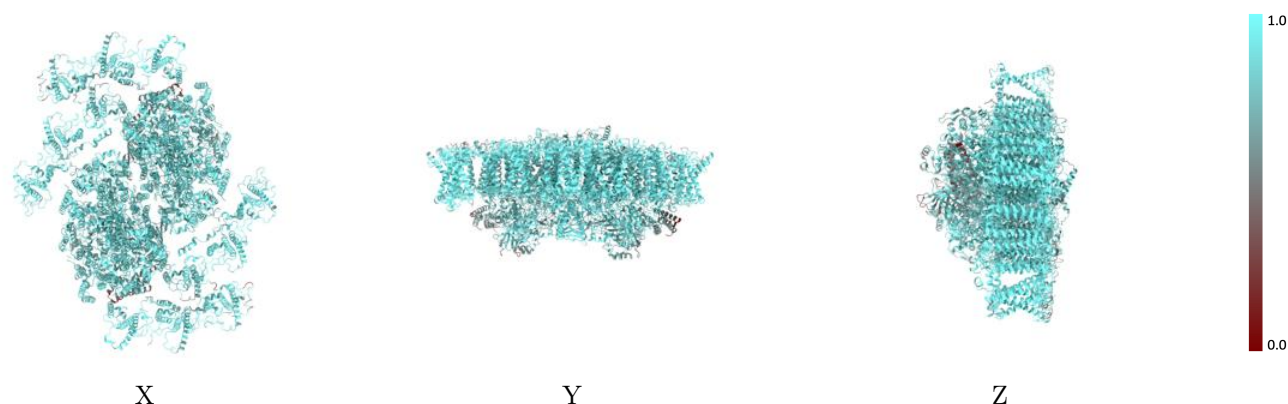
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

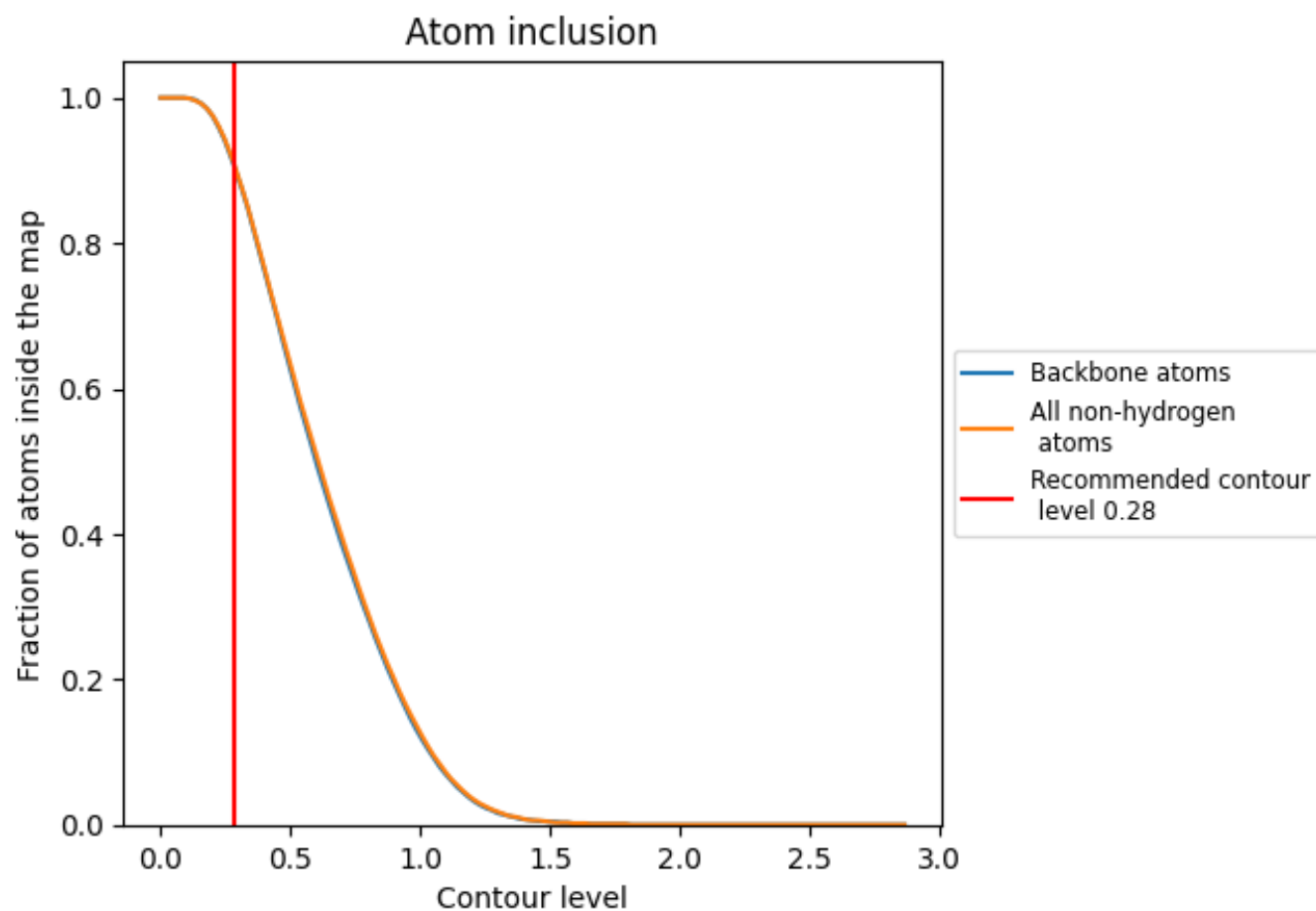
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.5740
0	 0.9020	 0.4810
1	 0.9410	 0.5430
2	 0.9370	 0.5470
3	 0.9060	 0.5260
4	 0.9110	 0.4900
5	 0.9330	 0.4860
6	 0.8940	 0.4950
7	 0.9330	 0.5320
8	 0.9330	 0.5380
9	 0.8910	 0.5130
A	 0.9770	 0.6470
B	 0.9650	 0.6220
C	 0.9710	 0.6230
D	 0.9780	 0.6400
E	 0.8900	 0.5270
F	 0.8810	 0.4910
H	 0.9720	 0.5900
I	 0.9930	 0.6410
J	 0.8830	 0.5920
K	 0.9660	 0.5930
L	 0.9490	 0.6280
M	 0.9410	 0.6170
N	 0.8100	 0.5080
O	 0.7700	 0.5860
Q	 0.6440	 0.5550
T	 0.9410	 0.6320
U	 0.8080	 0.5790
V	 0.8390	 0.5930
W	 0.8880	 0.5950
X	 0.9130	 0.5520
Y	 0.8070	 0.5410
Z	 0.8440	 0.5250
a	 0.9790	 0.6480
b	 0.9610	 0.6220



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Chain	Atom inclusion	Q-score
c	 0.9660	 0.6210
d	 0.9780	 0.6490
e	 0.8830	 0.5340
f	 0.8920	 0.5070
g	 0.9380	 0.4850
h	 0.9670	 0.5910
i	 0.9930	 0.6280
j	 0.8860	 0.5910
k	 0.9660	 0.5930
l	 0.9540	 0.6220
m	 0.9290	 0.6140
n	 0.8110	 0.5030
o	 0.7570	 0.5870
p	 0.8960	 0.4850
q	 0.6280	 0.5630
t	 0.9440	 0.6370
u	 0.7990	 0.5820
v	 0.8430	 0.5960
w	 0.8980	 0.6000
x	 0.9230	 0.5670
y	 0.8240	 0.5470
z	 0.8440	 0.5290