



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 06:47 pm GMT

PDB ID : 7PNK
EMDB ID : EMD-13548
Title : Unstacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-09-07
Resolution : 3.61 Å(reported)
Based on initial model : 6KAC

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

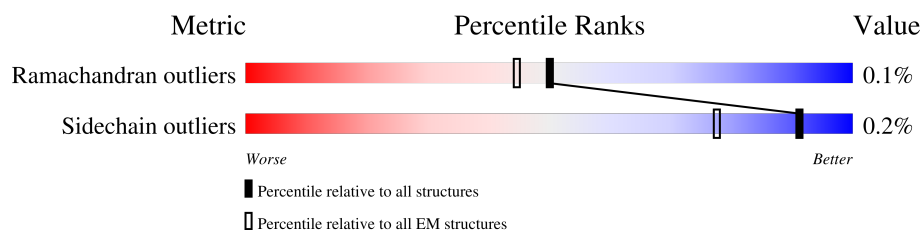
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.61 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.



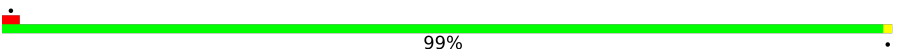
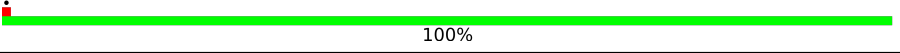
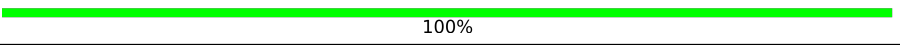
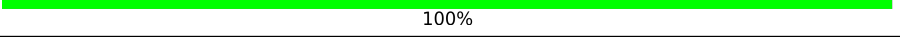
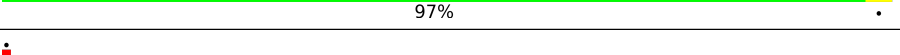
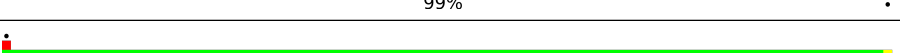
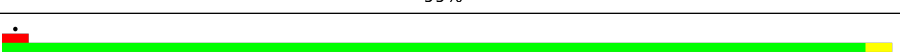
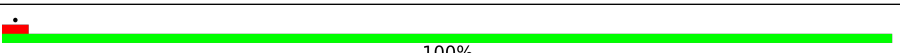
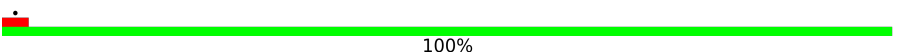
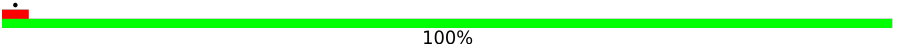
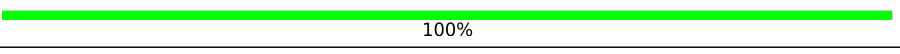
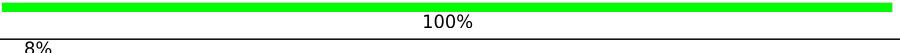
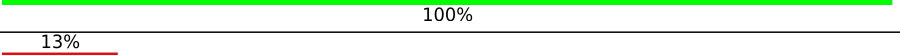
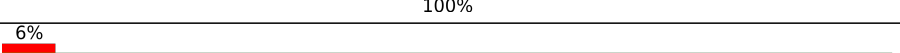
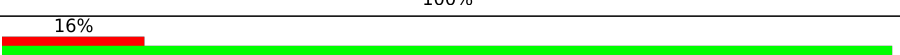
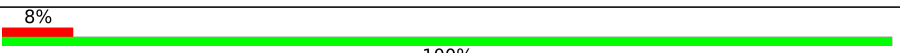

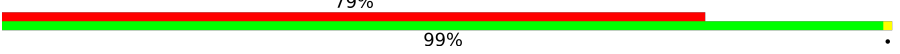
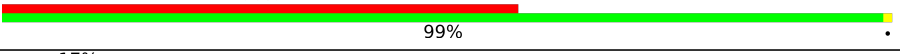
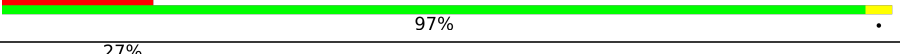
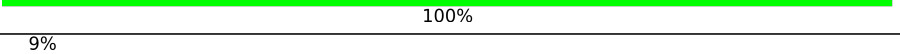
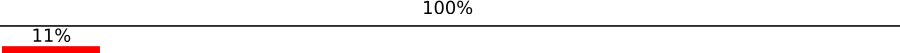
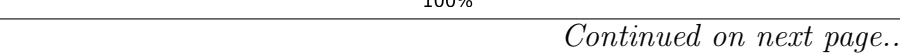


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	336	 8% 100%
1	a	336	 99%
2	B	484	 100%
2	b	484	 99%
3	V	32	 97%
3	v	32	 100%
4	C	449	 100%
4	c	449	 100%
5	D	348	 100%

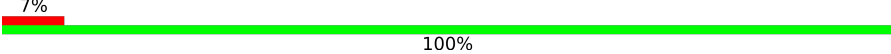
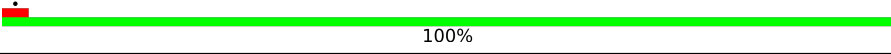
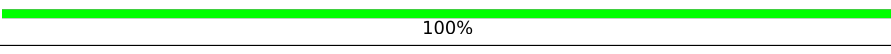
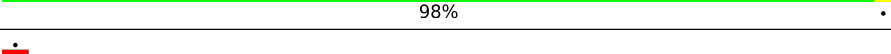
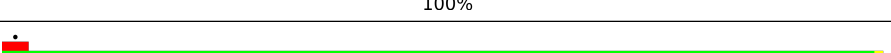
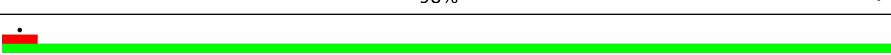
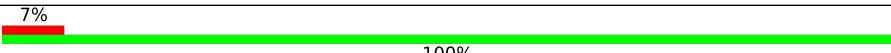


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	d	348	 99%
6	E	76	 100%
6	e	76	 100%
7	F	31	 100%
7	f	31	 97%
8	H	67	 99%
8	h	67	 99%
9	I	35	 97%
9	i	35	 100%
10	J	36	 100%
10	j	36	 100%
11	K	37	 100%
11	k	37	 100%
12	L	38	 8%100%
12	l	38	 13%100%
13	M	31	 6%100%
13	m	31	 16%100%
14	O	238	 8%100%
14	o	238	 6%99%
15	P	187	 79%99%
15	p	187	 58%99%
16	T	30	 17%97%
16	t	30	 27%100%
17	W	44	 9%100%
17	w	44	 11%100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	X	30	
18	x	30	
19	Z	61	
19	z	61	
20	N	222	
21	G	221	
22	S	243	
23	Y	222	
24	U	27	
24	u	27	

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
28	CLA	A	405	X	-	-	-
28	CLA	A	406	X	-	-	-
28	CLA	A	407	X	-	-	-
28	CLA	A	410	X	-	-	-
28	CLA	B	602	X	-	-	-
28	CLA	B	603	X	-	-	-
28	CLA	B	604	X	-	-	-
28	CLA	B	605	X	-	-	-
28	CLA	B	606	X	-	-	-
28	CLA	B	607	X	-	-	-
28	CLA	B	608	X	-	-	-
28	CLA	B	609	X	-	-	-
28	CLA	B	610	X	-	-	-
28	CLA	B	611	X	-	-	-
28	CLA	B	612	X	-	-	-
28	CLA	B	613	X	-	-	-
28	CLA	B	614	X	-	-	-
28	CLA	B	615	X	-	-	-
28	CLA	B	616	X	-	-	-
28	CLA	B	617	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	C	501	X	-	-	-
28	CLA	C	502	X	-	-	-
28	CLA	C	503	X	-	-	-
28	CLA	C	504	X	-	-	-
28	CLA	C	505	X	-	-	-
28	CLA	C	506	X	-	-	-
28	CLA	C	507	X	-	-	-
28	CLA	C	508	X	-	-	-
28	CLA	C	509	X	-	-	-
28	CLA	C	510	X	-	-	-
28	CLA	C	511	X	-	-	-
28	CLA	C	512	X	-	-	-
28	CLA	C	513	X	-	-	-
28	CLA	D	402	X	-	-	-
28	CLA	D	403	X	-	-	-
28	CLA	G	602	X	-	-	-
28	CLA	G	603	X	-	-	-
28	CLA	G	604	X	-	-	-
28	CLA	G	610	X	-	-	-
28	CLA	G	611	X	-	-	-
28	CLA	G	612	X	-	-	-
28	CLA	G	613	X	-	-	-
28	CLA	G	614	X	-	-	-
28	CLA	N	602	X	-	-	-
28	CLA	N	603	X	-	-	-
28	CLA	N	604	X	-	-	-
28	CLA	N	610	X	-	-	-
28	CLA	N	611	X	-	-	-
28	CLA	N	612	X	-	-	-
28	CLA	N	613	X	-	-	-
28	CLA	N	614	X	-	-	-
28	CLA	S	602	X	-	-	-
28	CLA	S	603	X	-	-	-
28	CLA	S	604	X	-	-	-
28	CLA	S	605	X	-	-	-
28	CLA	S	609	X	-	-	-
28	CLA	S	610	X	-	-	-
28	CLA	S	611	X	-	-	-
28	CLA	S	612	X	-	-	-
28	CLA	S	613	X	-	-	-
28	CLA	S	614	X	-	-	-
28	CLA	S	617	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	Y	602	X	-	-	-
28	CLA	Y	603	X	-	-	-
28	CLA	Y	604	X	-	-	-
28	CLA	Y	608	X	-	-	-
28	CLA	Y	610	X	-	-	-
28	CLA	Y	611	X	-	-	-
28	CLA	Y	612	X	-	-	-
28	CLA	Y	613	X	-	-	-
28	CLA	Y	614	X	-	-	-
28	CLA	a	405	X	-	-	-
28	CLA	a	406	X	-	-	-
28	CLA	a	407	X	-	-	-
28	CLA	a	410	X	-	-	-
28	CLA	b	602	X	-	-	-
28	CLA	b	603	X	-	-	-
28	CLA	b	604	X	-	-	-
28	CLA	b	605	X	-	-	-
28	CLA	b	606	X	-	-	-
28	CLA	b	607	X	-	-	-
28	CLA	b	608	X	-	-	-
28	CLA	b	609	X	-	-	-
28	CLA	b	610	X	-	-	-
28	CLA	b	611	X	-	-	-
28	CLA	b	612	X	-	-	-
28	CLA	b	613	X	-	-	-
28	CLA	b	614	X	-	-	-
28	CLA	b	615	X	-	-	-
28	CLA	b	616	X	-	-	-
28	CLA	b	617	X	-	-	-
28	CLA	c	501	X	-	-	-
28	CLA	c	502	X	-	-	-
28	CLA	c	503	X	-	-	-
28	CLA	c	504	X	-	-	-
28	CLA	c	505	X	-	-	-
28	CLA	c	506	X	-	-	-
28	CLA	c	507	X	-	-	-
28	CLA	c	508	X	-	-	-
28	CLA	c	509	X	-	-	-
28	CLA	c	510	X	-	-	-
28	CLA	c	511	X	-	-	-
28	CLA	c	512	X	-	-	-
28	CLA	c	513	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	CLA	d	402	X	-	-	-
28	CLA	d	403	X	-	-	-
34	C7Z	B	620	X	-	-	-
34	C7Z	b	620	X	-	-	-
39	LMK	C	527	X	-	-	-
39	LMK	c	527	X	-	-	-
43	RRX	H	101	X	-	-	-
43	RRX	h	101	X	-	-	-
46	CHL	G	601	X	-	-	-
46	CHL	G	605	X	-	-	-
46	CHL	G	606	X	-	-	-
46	CHL	G	607	X	-	-	-
46	CHL	G	608	X	-	-	-
46	CHL	G	609	X	-	-	-
46	CHL	N	601	X	-	-	-
46	CHL	N	605	X	-	-	-
46	CHL	N	606	X	-	-	-
46	CHL	N	607	X	-	-	-
46	CHL	N	608	X	-	-	-
46	CHL	N	609	X	-	-	-
46	CHL	S	601	X	-	-	-
46	CHL	S	606	X	-	-	-
46	CHL	S	607	X	-	-	-
46	CHL	S	608	X	-	-	-
46	CHL	Y	601	X	-	-	-
46	CHL	Y	605	X	-	-	-
46	CHL	Y	606	X	-	-	-
46	CHL	Y	607	X	-	-	-
46	CHL	Y	609	X	-	-	-
48	XAT	G	622	X	-	-	-
48	XAT	N	622	X	-	-	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 60673 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	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	76	Total	C	N	O	S	0	0
			621	404	102	115			
6	e	76	Total	C	N	O	S	0	0
			621	404	102	115			

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	36	Total	C	N	O	S	0	0
			266	183	40	43			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
10	j	36	Total	C	N	O	0	0
			266	183	40	43		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	conflict	UNP A0A1C8XRM8
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8
j	7	ILE	THR	conflict	UNP A0A1C8XRM8
j	42	LEU	GLN	conflict	UNP A0A1C8XRM8

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total	C	N	O	S	0	0
			313	209	51	52	1		
12	l	38	Total	C	N	O	S	0	0
			313	209	51	52	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			234	159	33	42		
13	m	31	Total	C	N	O	0	0
			234	159	33	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	conflict	UNP D0FXZ3
m	9	THR	ILE	conflict	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1822	1153	296	367	6		
14	o	238	Total	C	N	O	S	0	0
			1822	1153	296	367	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	30	Total	C	N	O		0	0
			201	132	32	37			
18	x	30	Total	C	N	O		0	0
			201	132	32	37			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
19	z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Chlorophyll a-b binding protein of LHCII type I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total	C	N	O	S	0	0
			1680	1085	271	321	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

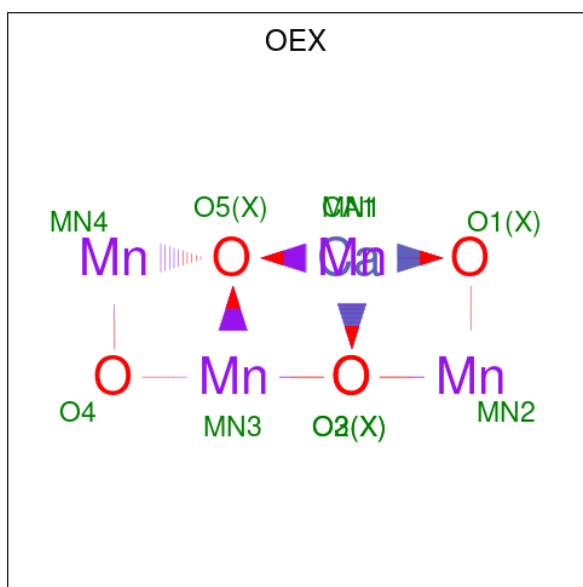
- Molecule 23 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	222	Total	C	N	O	S	0	0
			1670	1083	272	312	3		

- Molecule 24 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
24	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 25 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

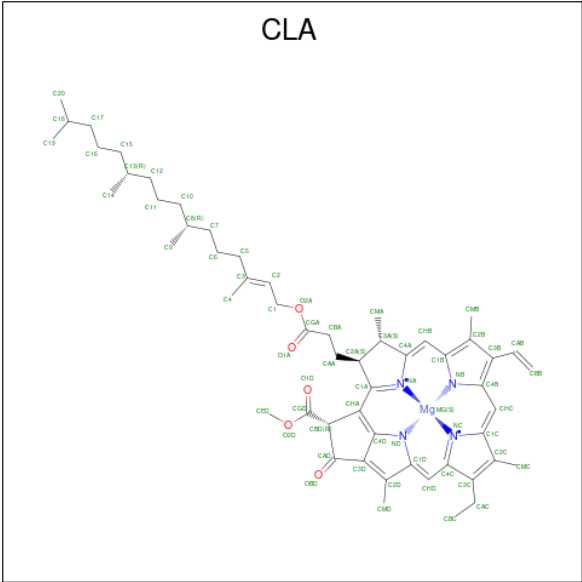
- Molecule 26 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 27 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Cl	0
			2	2	
27	a	2	Total	Cl	0
			2	2	

- Molecule 28 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	S	1	Total 60	C 50	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
28	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

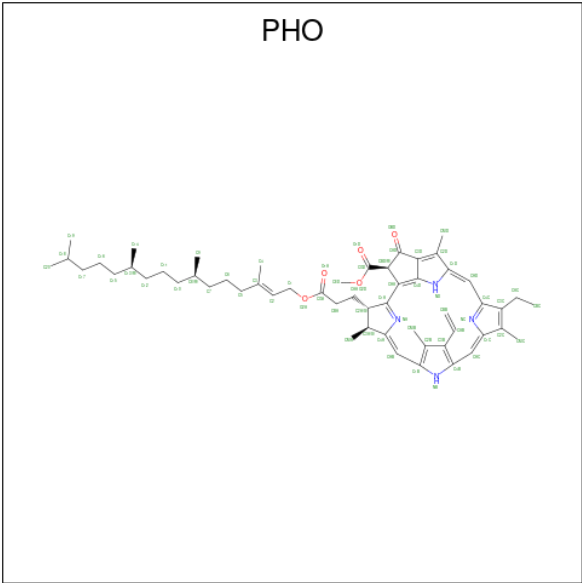
Mol	Chain	Residues	Atoms					AltConf
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 29 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



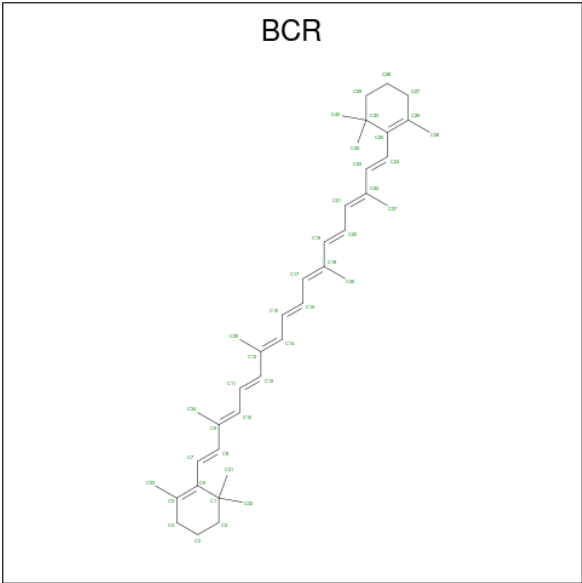
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	N	O	0
			64	55	4	5	
29	A	1	Total	C	N	O	0
			64	55	4	5	
29	a	1	Total	C	N	O	0
			64	55	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



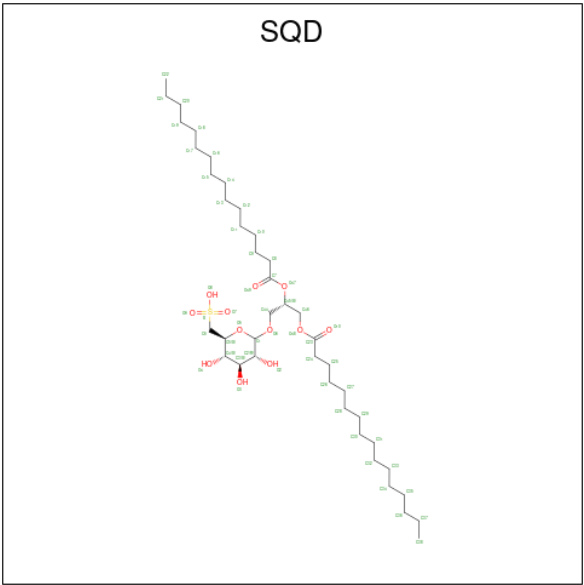
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	C	0
			40	40	
30	B	1	Total	C	0
			40	40	
30	B	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	D	1	Total	C	0
			40	40	
30	a	1	Total	C	0
			40	40	
30	b	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
30	b	1	Total	C	0
			40	40	
30	c	1	Total	C	0
			40	40	
30	c	1	Total	C	0
			40	40	
30	c	1	Total	C	0
			40	40	
30	c	1	Total	C	0
			40	40	
30	d	1	Total	C	0
			40	40	

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



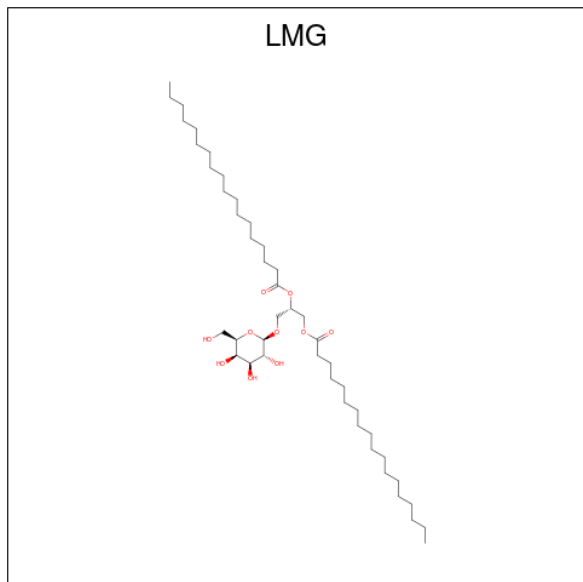
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	S	0
			51	38	12	1	
31	B	1	Total	C	O	S	0
			42	29	12	1	
31	B	1	Total	C	O	S	0
			54	41	12	1	
31	C	1	Total	C	O	S	0
			54	41	12	1	
31	M	1	Total	C	O	S	0
			42	29	12	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
31	a	1	Total	C	O	S	0
			51	38	12	1	
31	b	1	Total	C	O	S	0
			42	29	12	1	
31	b	1	Total	C	O	S	0
			54	41	12	1	
31	c	1	Total	C	O	S	0
			54	41	12	1	
31	m	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



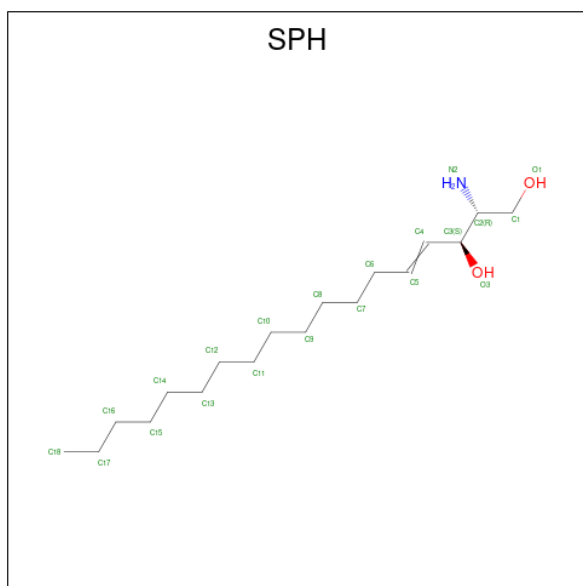
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			48	38	10	
32	B	1	Total	C	O	0
			44	34	10	
32	C	1	Total	C	O	0
			51	41	10	
32	C	1	Total	C	O	0
			55	45	10	
32	D	1	Total	C	O	0
			46	36	10	
32	H	1	Total	C	O	0
			48	38	10	

Continued on next page...

Continued from previous page...

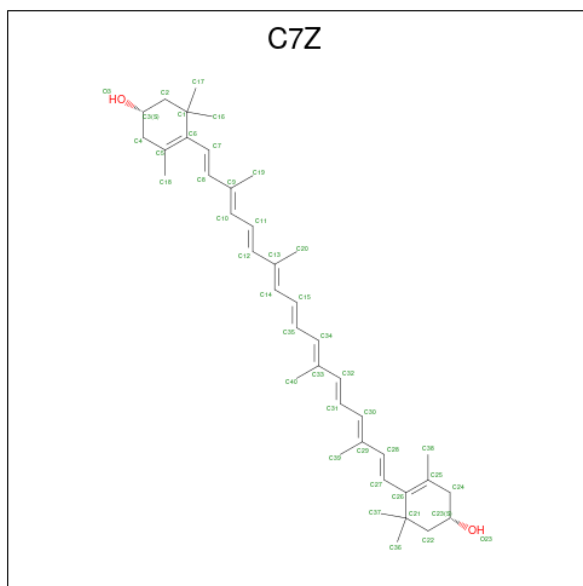
Mol	Chain	Residues	Atoms			AltConf
32	W	1	Total	C	O	0
			39	29	10	
32	a	1	Total	C	O	0
			48	38	10	
32	b	1	Total	C	O	0
			44	34	10	
32	c	1	Total	C	O	0
			51	41	10	
32	c	1	Total	C	O	0
			55	45	10	
32	d	1	Total	C	O	0
			46	36	10	
32	h	1	Total	C	O	0
			48	38	10	
32	w	1	Total	C	O	0
			39	29	10	

- Molecule 33 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



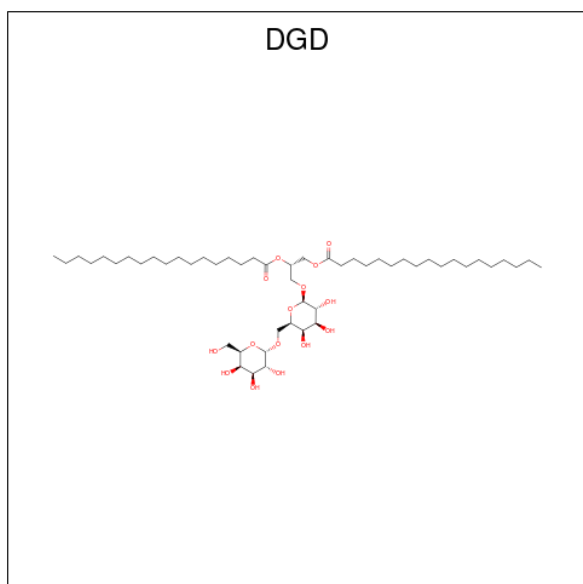
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			21	18	1	2	
33	Y	1	Total	C	N	O	0
			21	18	1	2	
33	a	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



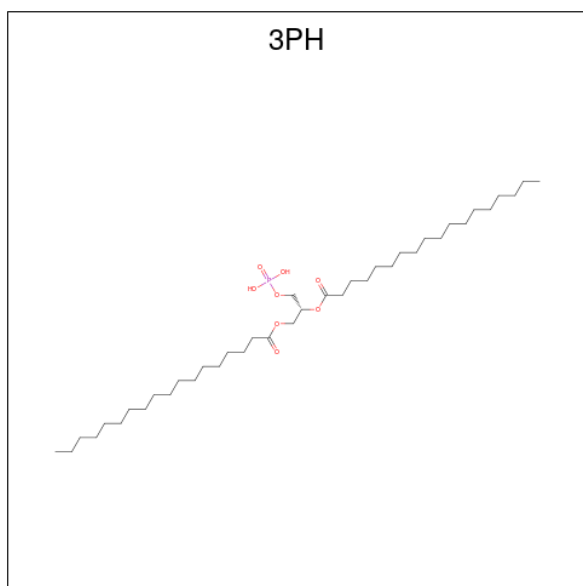
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			42	40	2	
34	b	1	Total	C	O	0
			42	40	2	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			43	28	15	
35	C	1	Total	C	O	0
			55	40	15	
35	C	1	Total	C	O	0
			62	47	15	
35	C	1	Total	C	O	0
			59	44	15	
35	b	1	Total	C	O	0
			43	28	15	
35	c	1	Total	C	O	0
			55	40	15	
35	c	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			59	44	15	

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



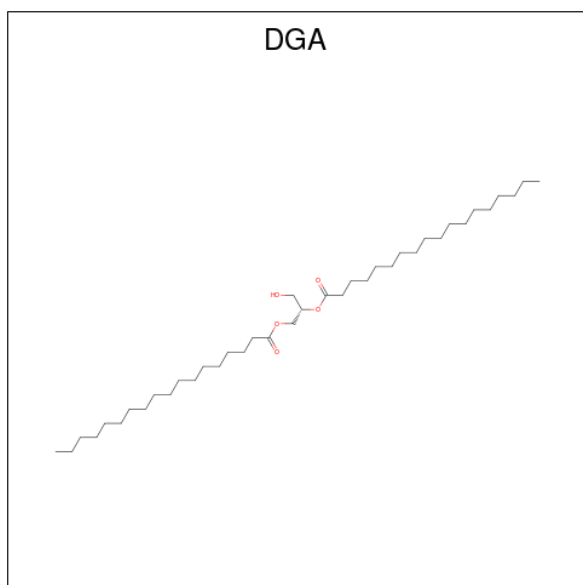
Mol	Chain	Residues	Atoms				AltConf
36	B	1	Total	C	O	P	0
			48	39	8	1	
36	T	1	Total	C	O	P	0
			48	39	8	1	
36	S	1	Total	C	O	P	0
			48	39	8	1	

Continued on next page...

Continued from previous page...

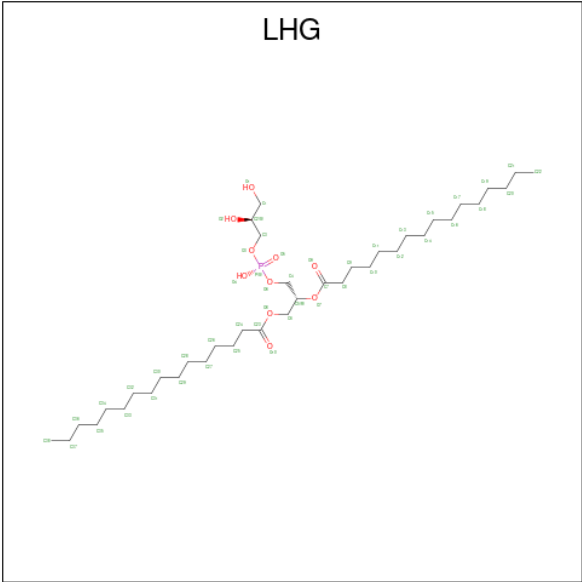
Mol	Chain	Residues	Atoms				AltConf
36	b	1	Total	C	O	P	0
			48	39	8	1	
36	t	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 37 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



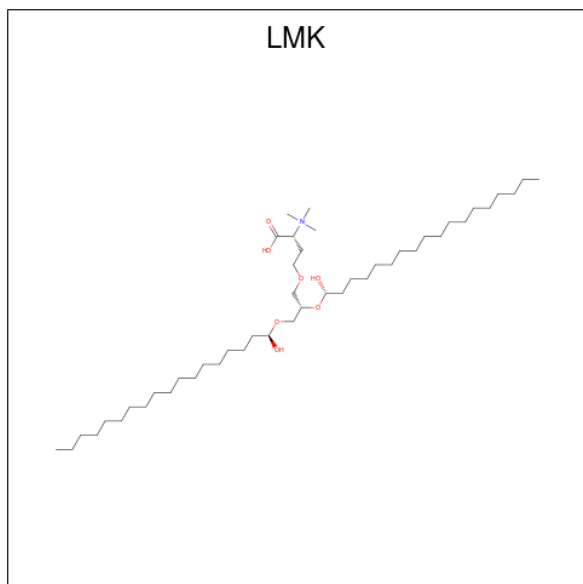
Mol	Chain	Residues	Atoms				AltConf
37	B	1	Total	C	O		0
			44	39	5		
37	C	1	Total	C	O		0
			44	39	5		
37	J	1	Total	C	O		0
			29	24	5		
37	b	1	Total	C	O		0
			44	39	5		
37	c	1	Total	C	O		0
			44	39	5		
37	j	1	Total	C	O		0
			29	24	5		

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



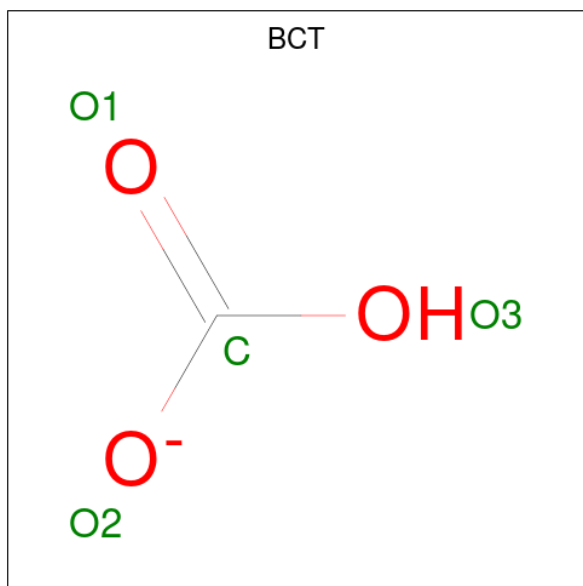
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	O	P	0
			47	36	10	1	
38	D	1	Total	C	O	P	0
			44	33	10	1	
38	D	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			39	28	10	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	N	1	Total	C	O	P	0
			49	38	10	1	
38	G	1	Total	C	O	P	0
			49	38	10	1	
38	S	1	Total	C	O	P	0
			45	34	10	1	
38	Y	1	Total	C	O	P	0
			49	38	10	1	
38	c	1	Total	C	O	P	0
			47	36	10	1	
38	d	1	Total	C	O	P	0
			44	33	10	1	
38	d	1	Total	C	O	P	0
			49	38	10	1	
38	d	1	Total	C	O	P	0
			39	28	10	1	
38	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 39 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxido-nyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (three-letter code: LMK) (formula: $C_{46}H_{94}NO_7$).



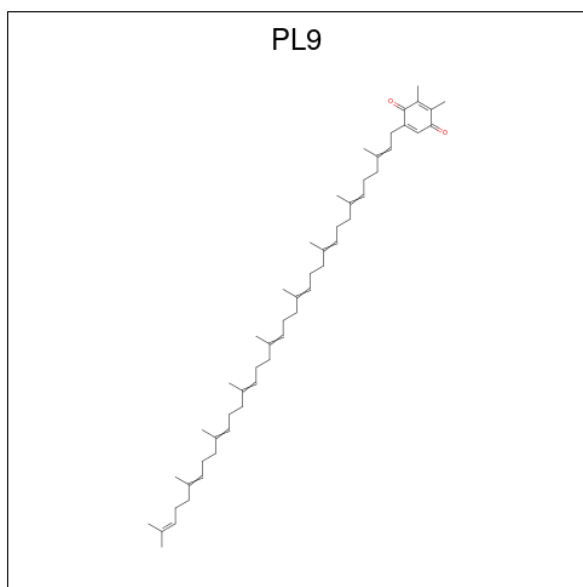
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	N	O	0
			40	32	1	7	
39	c	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 40 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



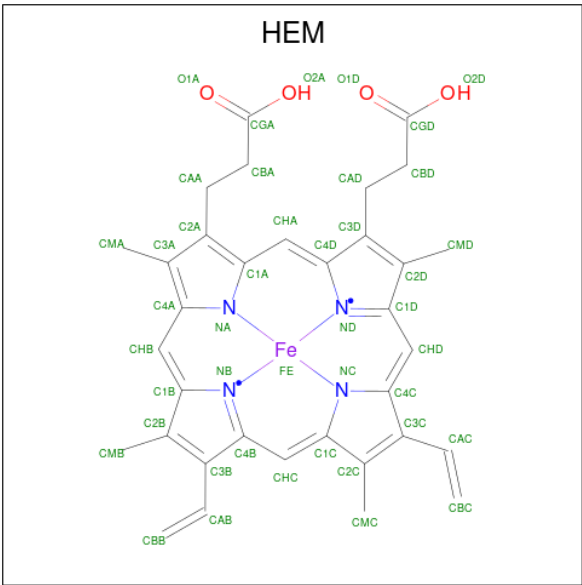
Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 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: $C_{53}H_{80}O_2$).



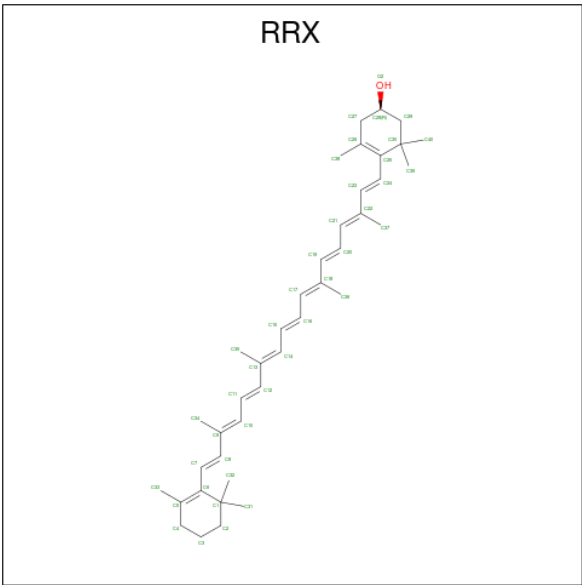
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			55	53	2	
41	d	1	Total	C	O	0
			55	53	2	

- Molecule 42 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



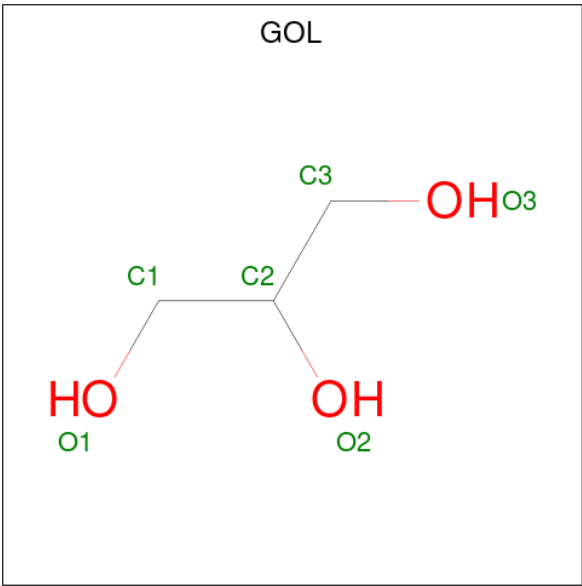
Mol	Chain	Residues	Atoms					AltConf
42	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
42	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 43 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



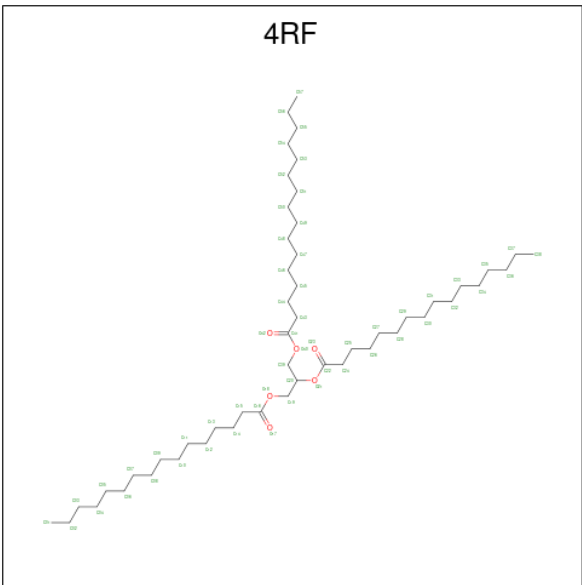
Mol	Chain	Residues	Atoms			AltConf
43	H	1	Total	C	O	0
			41	40	1	
43	h	1	Total	C	O	0
			41	40	1	

- Molecule 44 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			AltConf
44	I	1	Total	C	O	0
			6	3	3	

- Molecule 45 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: C₅₁H₉₈O₆).



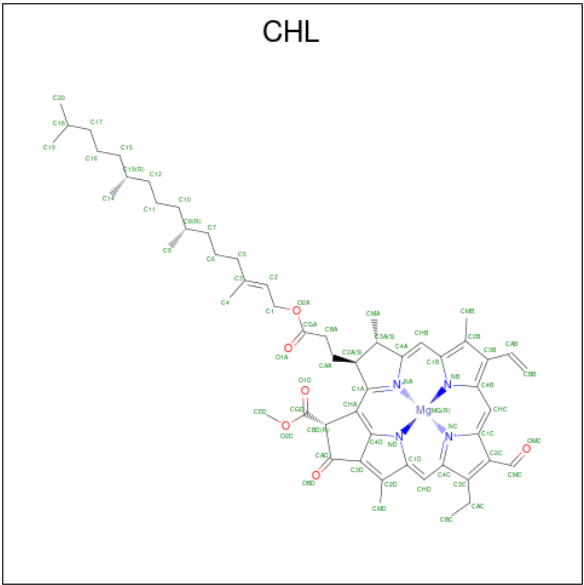
Mol	Chain	Residues	Atoms			AltConf
45	I	1	Total	C	O	0
			57	51	6	
45	K	1	Total	C	O	0
			57	51	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
45	i	1	Total	C	O	0
			57	51	6	
45	k	1	Total	C	O	0
			57	51	6	

- Molecule 46 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



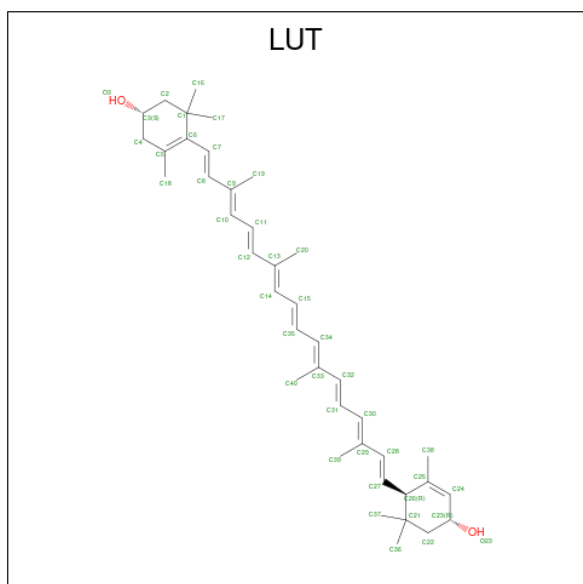
Mol	Chain	Residues	Atoms						AltConf
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			50	39	1	4	6		
46	N	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	G	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
46	G	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
46	G	1	Total	C	Mg	N	O	0	
			50	39	1	4	6		

Continued on next page...

Continued from previous page...

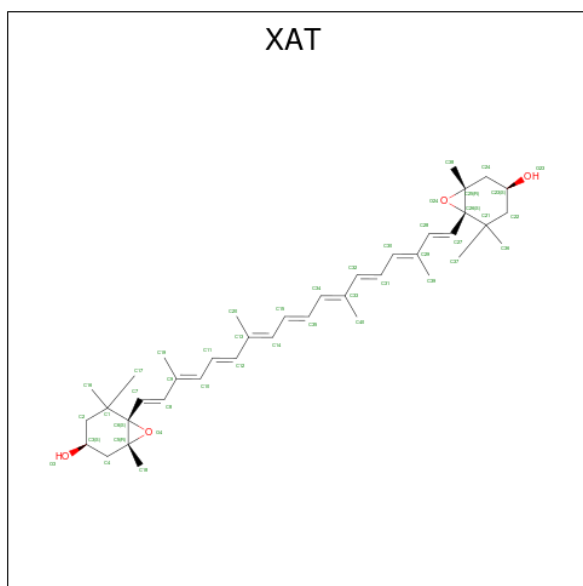
Mol	Chain	Residues	Atoms					AltConf
46	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
46	S	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 47 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



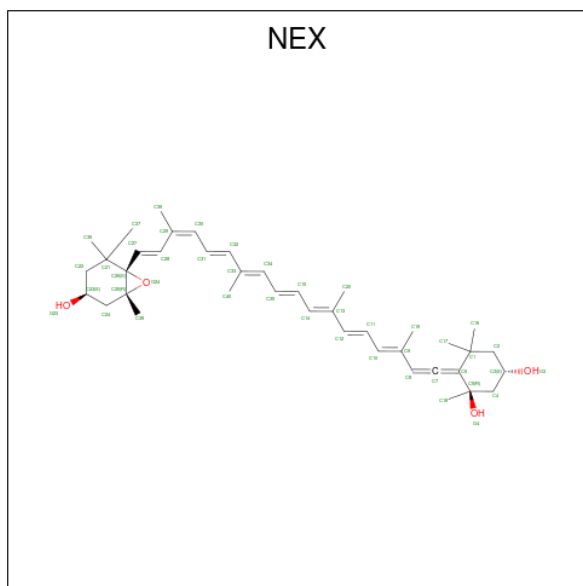
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			42	40	2	
47	N	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	

- Molecule 48 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



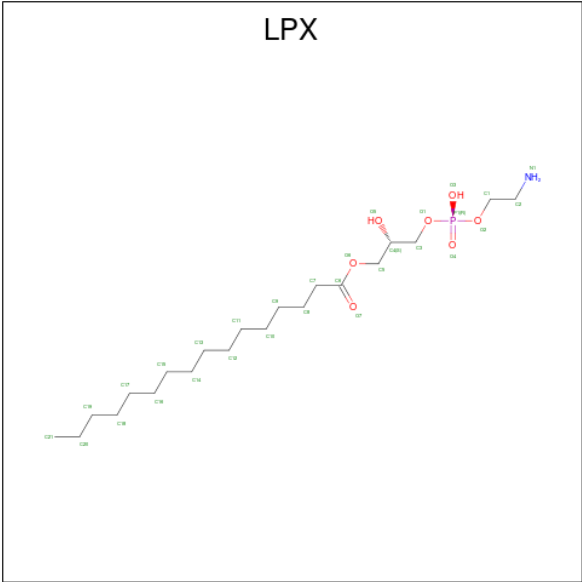
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	

- Molecule 49 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



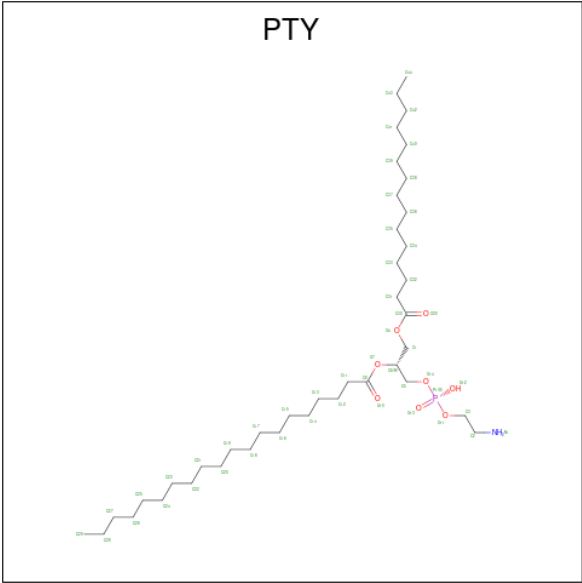
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	S	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	

- Molecule 50 is (2S)-3-[[[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-hydroxypropyl]hexadecanoate (three-letter code: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
50	S	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C₄₀H₈₀NO₈P).

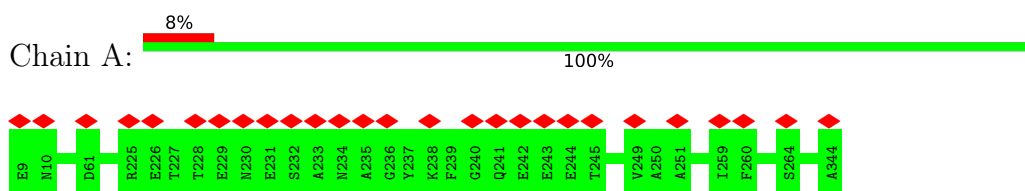


Mol	Chain	Residues	Atoms					AltConf
51	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
51	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	

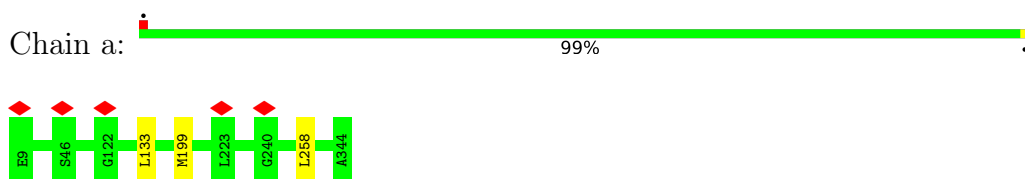
3 Residue-property plots [i](#)

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

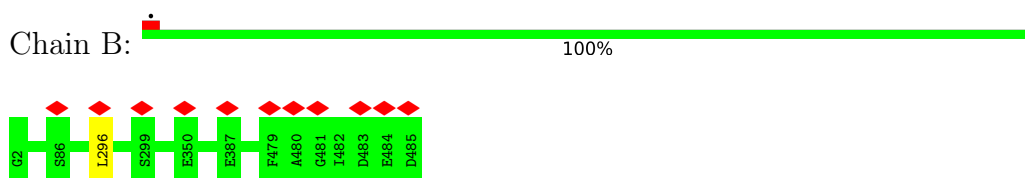
- Molecule 1: Photosystem II protein D1



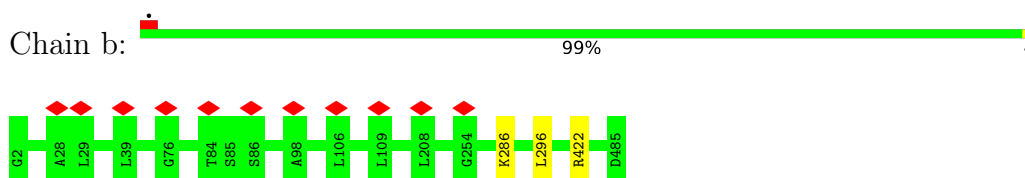
- Molecule 1: Photosystem II protein D1



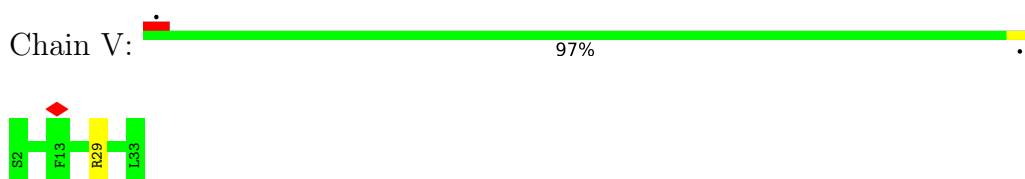
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II reaction center protein Ycf12



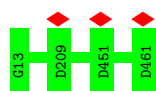
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  100%

There are no outlier residues recorded for this chain.

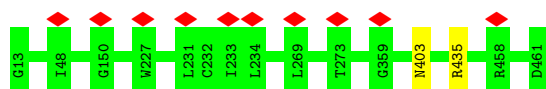
- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  100%



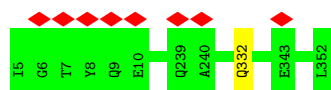
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c:  100%



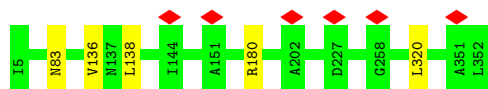
- Molecule 5: Photosystem II D2 protein

Chain D:  100%



- Molecule 5: Photosystem II D2 protein

Chain d:  99%



- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  100%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e:  100%

There are no outlier residues recorded for this chain.

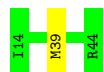
- Molecule 7: Cytochrome b559 subunit beta

Chain F:  100%

There are no outlier residues recorded for this chain.

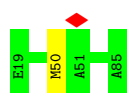
- Molecule 7: Cytochrome b559 subunit beta

Chain f:  97%



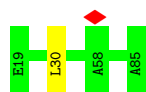
- Molecule 8: Photosystem II reaction center protein H

Chain H:  99%



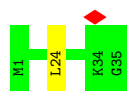
- Molecule 8: Photosystem II reaction center protein H

Chain h:  99%



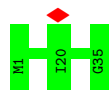
- Molecule 9: Photosystem II reaction center protein I

Chain I:  97%



- Molecule 9: Photosystem II reaction center protein I

Chain i:  100%



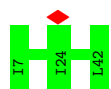
- Molecule 10: Photosystem II reaction center protein J

Chain J:  100%



- Molecule 10: Photosystem II reaction center protein J

Chain j:  100%



- Molecule 11: Photosystem II reaction center protein K

Chain K:  100%

There are no outlier residues recorded for this chain.

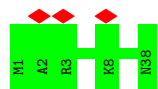
- Molecule 11: Photosystem II reaction center protein K

Chain k:  100%

There are no outlier residues recorded for this chain.

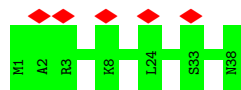
- Molecule 12: Photosystem II reaction center protein L

Chain L:  8% 100%



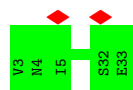
- Molecule 12: Photosystem II reaction center protein L

Chain l:  13% 100%



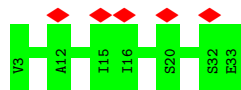
- Molecule 13: Photosystem II reaction center protein M

Chain M:  6% 100%



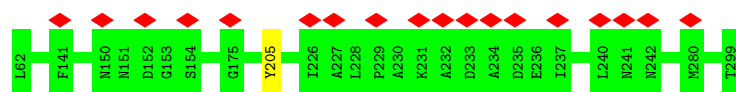
- Molecule 13: Photosystem II reaction center protein M

Chain m:  16% 100%

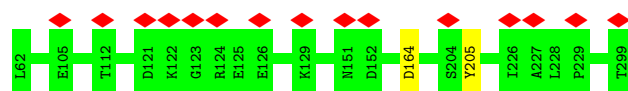


- Molecule 14: PsbO

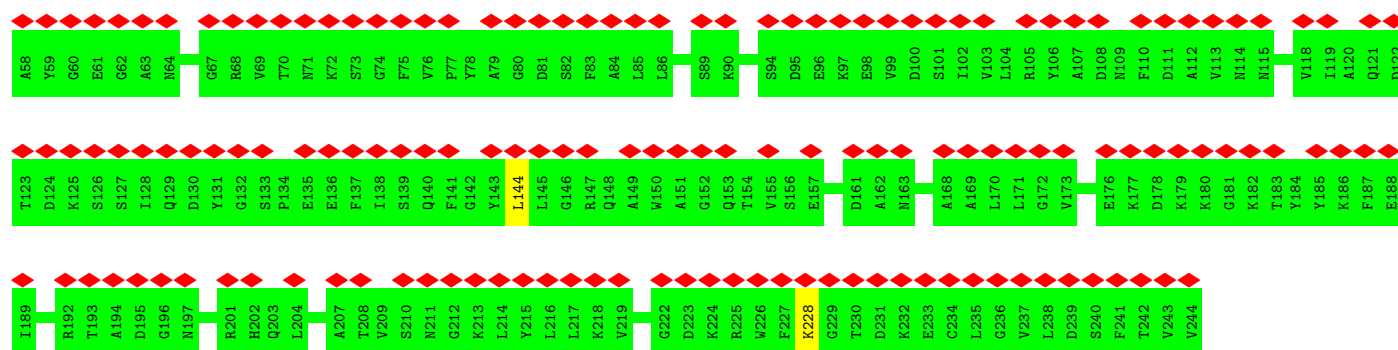
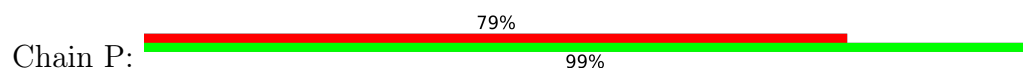
Chain O:  8% 100%



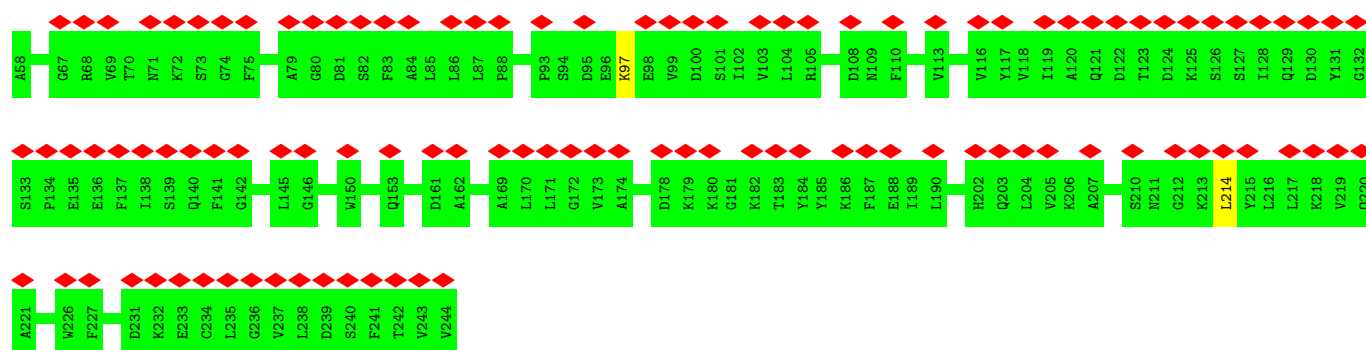
• Molecule 14: PsbO



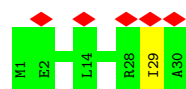
• Molecule 15: PsbP



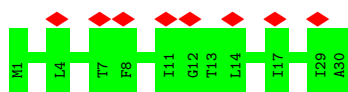
• Molecule 15: PsbP



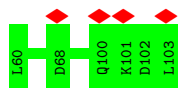
• Molecule 16: Photosystem II reaction center protein T



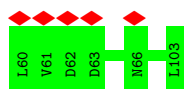
• Molecule 16: Photosystem II reaction center protein T



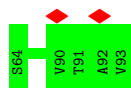
- Molecule 17: PsbW



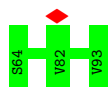
- Molecule 17: PsbW



- Molecule 18: PsbX



- Molecule 18: PsbX



- Molecule 19: Photosystem II reaction center protein Z



There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z



There are no outlier residues recorded for this chain.

- Molecule 20: Chlorophyll a-b binding protein of LHCII type I, chloroplastic





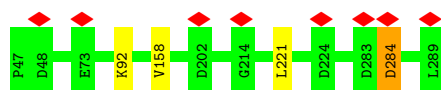
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G: 100%



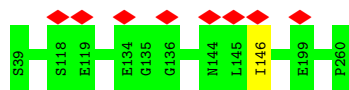
- Molecule 22: CP26

Chain S: 98%



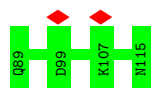
- Molecule 23: LHCII M1

Chain Y: 100%



- Molecule 24: PsbU

Chain U: 7% 100%



- Molecule 24: PsbU

Chain u: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	22.262	Depositor
Minimum map value	-13.270	Depositor
Average map value	0.035	Depositor
Map value standard deviation	1.121	Depositor
Recommended contour level	3.5	Depositor
Map size (\AA)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.896, 0.896, 0.896	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, OEX, LUT, BCT, 3PH, CSD, PHO, DGA, LMK, SPH, CHL, XAT, 4RF, PL9, DGD, SQD, RRX, C7Z, FE2, BCR, LMG, PTY, CL, HEM, LHG, LPX, NEX, CLA

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	0.29	0/2723	0.52	0/3715
1	a	0.33	0/2723	0.63	3/3715 (0.1%)
2	B	0.28	0/3906	0.53	1/5319 (0.0%)
2	b	0.29	0/3906	0.55	1/5319 (0.0%)
3	V	0.27	0/228	0.56	0/311
3	v	0.26	0/228	0.67	0/311
4	C	0.27	0/3602	0.51	0/4913
4	c	0.29	0/3602	0.55	0/4913
5	D	0.29	0/2860	0.53	0/3899
5	d	0.32	0/2860	0.60	2/3899 (0.1%)
6	E	0.27	0/639	0.53	0/870
6	e	0.30	0/639	0.53	0/870
7	F	0.27	0/259	0.50	0/351
7	f	0.27	0/259	0.75	1/351 (0.3%)
8	H	0.28	0/513	0.65	1/703 (0.1%)
8	h	0.29	0/513	0.69	1/703 (0.1%)
9	I	0.29	0/287	0.63	1/386 (0.3%)
9	i	0.33	0/287	0.58	0/386
10	J	0.26	0/272	0.45	0/369
10	j	0.25	0/272	0.57	0/369
11	K	0.31	0/308	0.54	0/423
11	k	0.38	0/308	0.62	0/423
12	L	0.30	0/321	0.49	0/435
12	l	0.30	0/321	0.57	0/435
13	M	0.32	0/237	0.51	0/323
13	m	0.30	0/237	0.61	0/323
14	O	0.28	0/1857	0.60	0/2508
14	o	0.27	0/1857	0.58	1/2508 (0.0%)
15	P	0.26	0/1473	0.53	1/1988 (0.1%)
15	p	0.26	0/1473	0.57	1/1988 (0.1%)
16	T	0.29	0/254	0.67	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.29	0/254	0.57	0/342
17	W	0.26	0/339	0.56	0/460
17	w	0.27	0/339	0.59	0/460
18	X	0.28	0/202	0.49	0/276
18	x	0.28	0/202	0.46	0/276
19	Z	0.26	0/469	0.42	0/641
19	z	0.31	0/469	0.54	0/641
20	N	0.27	0/1751	0.55	2/2386 (0.1%)
21	G	0.27	0/1725	0.51	0/2348
22	S	0.28	0/1903	0.59	2/2590 (0.1%)
23	Y	0.26	0/1719	0.49	0/2343
24	U	0.27	0/224	0.61	0/298
24	u	0.24	0/224	0.57	0/298
All	All	0.29	0/49044	0.56	18/66727 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	c	0	1
5	d	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	LEU	CA-CB-CG	7.80	133.23	115.30
2	b	296	LEU	CA-CB-CG	7.76	133.15	115.30
1	a	133	LEU	CB-CG-CD2	7.16	123.17	111.00
22	S	221	LEU	CA-CB-CG	7.05	131.51	115.30
1	a	199	MET	CB-CG-SD	6.42	131.66	112.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	c	435	ARG	Sidechain
5	d	136	VAL	Peptide

5.2 Too-close contacts

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	335/336 (100%)	323 (96%)	12 (4%)	0	100	100
1	a	335/336 (100%)	317 (95%)	18 (5%)	0	100	100
2	B	481/484 (99%)	463 (96%)	18 (4%)	0	100	100
2	b	481/484 (99%)	465 (97%)	16 (3%)	0	100	100
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	428 (96%)	19 (4%)	0	100	100
4	c	447/449 (100%)	420 (94%)	27 (6%)	0	100	100
5	D	346/348 (99%)	334 (96%)	12 (4%)	0	100	100
5	d	346/348 (99%)	329 (95%)	17 (5%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	e	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
9	i	33/35 (94%)	30 (91%)	3 (9%)	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	k	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m	29/31 (94%)	29 (100%)	0	0	100	100
14	O	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	30	62
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	30	62
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	p	185/187 (99%)	168 (91%)	17 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	3	23
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	14	48
21	G	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	S	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	11	43
23	Y	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	25	59
24	U	25/27 (93%)	25 (100%)	0	0	100	100
24	u	25/27 (93%)	25 (100%)	0	0	100	100
All	All	6054/6142 (99%)	5755 (95%)	290 (5%)	9 (0%)	50	79

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
22	S	284	ASP
23	Y	146	ILE

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	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	276 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	385 (100%)	2 (0%)	86	92
3	V	25/25 (100%)	24 (96%)	1 (4%)	27	55
3	v	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	349 (100%)	1 (0%)	91	96
5	D	279/279 (100%)	278 (100%)	1 (0%)	89	94
5	d	279/279 (100%)	277 (99%)	2 (1%)	81	89
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	197/197 (100%)	197 (100%)	0	100	100
14	o	197/197 (100%)	197 (100%)	0	100	100
15	P	151/151 (100%)	150 (99%)	1 (1%)	81	89
15	p	151/151 (100%)	150 (99%)	1 (1%)	81	89
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	167 (99%)	1 (1%)	84	91
22	S	190/190 (100%)	190 (100%)	0	100	100
23	Y	167/167 (100%)	167 (100%)	0	100	100
24	U	26/26 (100%)	26 (100%)	0	100	100
24	u	26/26 (100%)	26 (100%)	0	100	100
All	All	4942/4940 (100%)	4932 (100%)	10 (0%)	91	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	d	83	ASN
5	d	180	ARG
15	p	97	LYS
21	G	73	GLN
2	b	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	282	GLN
2	b	290	GLN
15	p	220	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	317	ASN
14	O	274	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	B	218	2	3,7,8	0.85	0	1,8,10	0.20	0
2	CSD	b	218	2	3,7,8	0.93	0	1,8,10	0.03	0

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
2	CSD	B	218	2	-	1/2/6/8	-
2	CSD	b	218	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	N-CA-CB-SG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	b	218	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 250 ligands modelled in this entry, 6 are monoatomic - leaving 244 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	$\# Z > 2$
28	CLA	B	612	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	18 (23%)
28	CLA	b	616	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	17 (22%)
28	CLA	Y	613	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	17 (22%)
28	CLA	S	610	-	65,73,73	1.37	8 (12%)	76,113,113	1.90	19 (25%)
28	CLA	c	505	-	65,73,73	1.35	8 (12%)	76,113,113	2.13	18 (23%)
30	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.29	15 (26%)
28	CLA	S	613	-	55,63,73	1.48	9 (16%)	64,101,113	2.15	18 (28%)
28	CLA	c	512	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	18 (23%)
32	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.17	4 (7%)
30	BCR	C	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.42	14 (25%)
28	CLA	G	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	21 (27%)
41	PL9	D	405	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
28	CLA	A	410	-	60,68,73	1.39	7 (11%)	70,107,113	2.12	18 (25%)
34	C7Z	B	620	-	43,43,43	5.35	26 (60%)	58,60,60	2.27	22 (37%)
28	CLA	c	504	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	b	606	-	65,73,73	1.34	7 (10%)	76,113,113	2.07	17 (22%)
31	SQD	M	101	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
28	CLA	Y	604	-	65,73,73	1.35	8 (12%)	76,113,113	1.96	18 (23%)
42	HEM	F	101	7,6	41,50,50	1.48	5 (12%)	45,82,82	1.38	6 (13%)
28	CLA	B	602	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	17 (22%)
28	CLA	c	510	-	65,73,73	1.32	8 (12%)	76,113,113	2.02	16 (21%)
28	CLA	B	617	-	65,73,73	1.35	7 (10%)	76,113,113	1.97	17 (22%)
28	CLA	S	604	-	55,63,73	1.47	8 (14%)	64,101,113	2.21	18 (28%)
35	DGD	c	520	-	60,60,67	1.09	6 (10%)	74,74,81	0.90	2 (2%)
28	CLA	B	614	-	65,73,73	1.33	6 (9%)	76,113,113	1.99	17 (22%)
46	CHL	G	608	-	44,52,74	1.03	3 (6%)	46,87,114	1.39	9 (19%)
28	CLA	G	614	-	49,57,73	1.54	9 (18%)	55,93,113	2.33	17 (30%)
30	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.50	16 (28%)
38	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
46	CHL	N	605	20	66,74,74	0.83	2 (3%)	73,114,114	1.19	8 (10%)
29	PHO	A	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.13	6 (12%)
28	CLA	C	513	-	65,73,73	1.38	8 (12%)	76,113,113	1.98	15 (19%)
33	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.05	1 (5%)
45	4RF	k	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.87	3 (5%)
28	CLA	a	405	-	65,73,73	1.30	7 (10%)	76,113,113	2.03	20 (26%)
28	CLA	c	502	-	65,73,73	1.33	6 (9%)	76,113,113	2.05	18 (23%)
32	LMG	H	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.11	2 (3%)
28	CLA	d	403	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	17 (22%)
31	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
51	PTY	Y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.41	2 (9%)
46	CHL	S	601	22	46,54,74	1.00	3 (6%)	49,90,114	1.39	9 (18%)
35	DGD	b	623	-	44,44,67	0.87	1 (2%)	58,58,81	1.23	5 (8%)
49	NEX	N	623	-	38,46,46	3.34	10 (26%)	50,70,70	1.49	9 (18%)
28	CLA	c	513	-	65,73,73	1.34	7 (10%)	76,113,113	2.09	22 (28%)
31	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)
28	CLA	B	611	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	16 (21%)
49	NEX	Y	623	-	38,46,46	3.29	9 (23%)	50,70,70	1.80	14 (28%)
46	CHL	Y	609	-	66,74,74	0.84	3 (4%)	73,114,114	1.25	11 (15%)
32	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.06	3 (4%)
29	PHO	A	409	-	51,69,69	1.01	4 (7%)	47,99,99	1.15	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	d	402	-	65,73,73	1.37	8 (12%)	76,113,113	1.92	19 (25%)
31	SQD	m	101	-	41,42,54	0.88	0	50,53,65	0.97	2 (4%)
32	LMG	W	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.15	2 (4%)
28	CLA	c	501	-	65,73,73	1.36	9 (13%)	76,113,113	1.99	17 (22%)
47	LUT	G	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.02	12 (23%)
32	LMG	w	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.05	2 (4%)
28	CLA	B	613	-	65,73,73	1.35	9 (13%)	76,113,113	1.93	14 (18%)
28	CLA	b	605	-	65,73,73	1.38	9 (13%)	76,113,113	1.99	16 (21%)
28	CLA	Y	612	-	65,73,73	1.36	9 (13%)	76,113,113	1.97	16 (21%)
28	CLA	G	613	-	65,73,73	1.37	9 (13%)	76,113,113	1.99	16 (21%)
28	CLA	B	615	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
28	CLA	B	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.13	19 (25%)
28	CLA	C	506	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	16 (21%)
28	CLA	c	508	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
30	BCR	D	404	-	41,41,41	1.82	4 (9%)	56,56,56	4.24	16 (28%)
34	C7Z	b	620	-	43,43,43	5.37	26 (60%)	58,60,60	2.26	19 (32%)
37	DGA	j	101	-	28,28,43	1.30	3 (10%)	30,30,45	1.20	2 (6%)
47	LUT	Y	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.02	14 (27%)
28	CLA	b	610	-	65,73,73	1.34	6 (9%)	76,113,113	1.99	18 (23%)
30	BCR	C	515	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	12 (21%)
38	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.45	5 (9%)
35	DGD	c	519	-	63,63,67	1.13	6 (9%)	77,77,81	0.94	2 (2%)
28	CLA	A	407	-	50,58,73	1.54	8 (16%)	58,95,113	2.25	18 (31%)
28	CLA	S	609	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	16 (22%)
28	CLA	S	602	-	60,68,73	1.39	8 (13%)	70,107,113	2.14	20 (28%)
30	BCR	a	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.31	16 (28%)
28	CLA	b	602	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	15 (19%)
37	DGA	b	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.52	3 (6%)
38	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.18	3 (7%)
46	CHL	N	606	-	66,74,74	0.87	3 (4%)	73,114,114	1.17	10 (13%)
47	LUT	G	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.96	13 (25%)
28	CLA	G	604	-	49,57,73	1.57	10 (20%)	55,93,113	2.27	19 (34%)
49	NEX	S	623	-	38,46,46	3.36	10 (26%)	50,70,70	1.72	12 (24%)
36	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
32	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.09	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	CHL	Y	606	-	66,74,74	0.84	3 (4%)	73,114,114	1.19	10 (13%)
46	CHL	S	606	-	44,52,74	1.06	3 (6%)	46,87,114	1.42	8 (17%)
50	LPX	S	625	-	29,29,29	1.00	2 (6%)	31,33,33	0.97	1 (3%)
28	CLA	A	405	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
28	CLA	C	510	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	15 (19%)
28	CLA	C	512	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	18 (23%)
28	CLA	c	511	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	17 (22%)
32	LMG	c	521	-	51,51,55	1.07	4 (7%)	59,59,63	1.01	2 (3%)
28	CLA	C	508	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	18 (23%)
28	CLA	N	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	16 (21%)
48	XAT	N	622	-	39,47,47	0.68	1 (2%)	54,74,74	1.96	12 (22%)
46	CHL	G	606	-	50,58,74	0.99	3 (6%)	52,94,114	1.38	8 (15%)
38	LHG	G	624	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
28	CLA	C	509	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	16 (21%)
47	LUT	S	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.99	15 (29%)
37	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.49	3 (6%)
46	CHL	S	607	-	43,51,74	1.02	3 (6%)	45,86,114	1.43	8 (17%)
28	CLA	Y	603	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	18 (23%)
37	DGA	c	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.48	3 (6%)
28	CLA	B	616	-	65,73,73	1.37	9 (13%)	76,113,113	1.90	15 (19%)
36	3PH	T	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.11	2 (3%)
41	PL9	d	405	-	55,55,55	1.16	5 (9%)	68,69,69	1.59	13 (19%)
28	CLA	c	509	-	65,73,73	1.35	6 (9%)	76,113,113	1.95	16 (21%)
47	LUT	N	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.04	11 (21%)
28	CLA	C	511	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	18 (23%)
39	LMK	C	527	-	38,39,53	1.51	2 (5%)	41,46,60	1.47	2 (4%)
47	LUT	N	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.92	12 (23%)
28	CLA	B	609	-	65,73,73	1.33	7 (10%)	76,113,113	2.05	19 (25%)
30	BCR	B	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.31	18 (32%)
30	BCR	c	517	-	41,41,41	1.88	4 (9%)	56,56,56	4.48	15 (26%)
35	DGD	B	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.14	3 (5%)
28	CLA	Y	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	20 (26%)
46	CHL	N	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.25	13 (17%)
46	CHL	S	608	-	61,69,74	0.86	3 (4%)	67,108,114	1.24	10 (14%)
40	BCT	d	401	26	2,3,3	1.16	0	2,3,3	4.43	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	Y	611	-	65,73,73	1.35	9 (13%)	76,113,113	1.94	16 (21%)
33	SPH	a	414	-	19,20,20	0.67	0	18,21,21	1.03	0
28	CLA	N	602	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	17 (22%)
28	CLA	b	612	-	65,73,73	1.33	6 (9%)	76,113,113	2.01	16 (21%)
28	CLA	S	611	38	65,73,73	1.37	9 (13%)	76,113,113	2.01	17 (22%)
28	CLA	A	406	-	65,73,73	1.33	6 (9%)	76,113,113	2.04	17 (22%)
28	CLA	B	606	-	65,73,73	1.33	7 (10%)	76,113,113	2.10	18 (23%)
30	BCR	C	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.41	15 (26%)
28	CLA	b	603	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	18 (23%)
38	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
51	PTY	Y	626	-	49,49,49	0.88	4 (8%)	52,54,54	1.06	2 (3%)
28	CLA	N	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	18 (23%)
28	CLA	C	507	-	65,73,73	1.37	9 (13%)	76,113,113	2.02	19 (25%)
46	CHL	N	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.23	10 (13%)
30	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.51	16 (28%)
30	BCR	c	514	-	41,41,41	1.83	4 (9%)	56,56,56	4.45	15 (26%)
48	XAT	Y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.70	19 (35%)
46	CHL	Y	601	23	66,74,74	0.80	2 (3%)	73,114,114	1.18	8 (10%)
29	PHO	a	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.04	4 (8%)
28	CLA	C	501	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	18 (23%)
28	CLA	Y	608	-	50,58,73	1.55	10 (20%)	58,95,113	2.19	16 (27%)
28	CLA	c	507	-	65,73,73	1.38	8 (12%)	76,113,113	1.99	17 (22%)
28	CLA	D	403	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	16 (21%)
46	CHL	G	609	-	66,74,74	0.86	3 (4%)	73,114,114	1.22	10 (13%)
28	CLA	b	609	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	18 (23%)
28	CLA	b	615	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	17 (22%)
29	PHO	a	409	-	51,69,69	0.99	3 (5%)	47,99,99	1.25	5 (10%)
38	LHG	d	410	-	38,38,48	0.42	0	41,44,54	1.13	3 (7%)
32	LMG	D	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.05	2 (3%)
30	BCR	A	411	-	41,41,41	1.85	4 (9%)	56,56,56	4.25	13 (23%)
38	LHG	C	525	-	46,46,48	0.40	0	49,52,54	1.02	2 (4%)
28	CLA	a	407	-	49,57,73	1.55	8 (16%)	55,93,113	2.44	18 (32%)
32	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.09	4 (6%)
28	CLA	N	612	-	45,53,73	1.63	9 (20%)	52,89,113	2.09	13 (25%)
45	4RF	K	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.86	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	N	611	-	49,57,73	1.57	9 (18%)	55,93,113	2.24	16 (29%)
28	CLA	C	505	-	65,73,73	1.38	9 (13%)	76,113,113	1.93	17 (22%)
28	CLA	G	612	-	43,51,73	1.66	8 (18%)	49,86,113	2.17	13 (26%)
30	BCR	b	619	-	41,41,41	1.87	4 (9%)	56,56,56	4.37	13 (23%)
31	SQD	b	621	-	41,42,54	0.89	0	50,53,65	0.93	2 (4%)
42	HEM	f	101	7,6	41,50,50	1.47	5 (12%)	45,82,82	1.35	5 (11%)
45	4RF	i	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.89	3 (5%)
46	CHL	G	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.22	11 (15%)
28	CLA	B	603	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	18 (23%)
25	OEX	a	401	4,1	0,15,15	-	-	-	-	-
32	LMG	h	102	-	48,48,55	1.01	6 (12%)	56,56,63	1.17	3 (5%)
31	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
38	LHG	N	624	-	48,48,48	0.38	0	51,54,54	1.07	3 (5%)
33	SPH	A	414	-	19,20,20	0.65	0	18,21,21	1.06	1 (5%)
46	CHL	Y	607	-	66,74,74	0.75	2 (3%)	73,114,114	1.20	9 (12%)
47	LUT	Y	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.96	12 (23%)
47	LUT	S	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.94	14 (27%)
38	LHG	D	408	-	43,43,48	0.40	0	46,49,54	1.00	2 (4%)
28	CLA	B	610	-	65,73,73	1.37	7 (10%)	76,113,113	1.84	14 (18%)
28	CLA	a	410	-	60,68,73	1.40	7 (11%)	70,107,113	2.05	17 (24%)
37	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
28	CLA	B	604	-	65,73,73	1.37	9 (13%)	76,113,113	1.93	16 (21%)
28	CLA	Y	602	-	65,73,73	1.34	8 (12%)	76,113,113	1.97	19 (25%)
28	CLA	G	602	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	18 (23%)
30	BCR	c	515	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	14 (25%)
46	CHL	N	601	-	66,74,74	0.81	3 (4%)	73,114,114	1.23	12 (16%)
32	LMG	B	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.09	2 (3%)
28	CLA	S	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.07	17 (22%)
35	DGD	c	518	-	56,56,67	0.98	3 (5%)	70,70,81	0.99	2 (2%)
38	LHG	S	624	28	44,44,48	0.41	0	47,50,54	1.12	3 (6%)
32	LMG	a	413	-	48,48,55	1.00	4 (8%)	56,56,63	1.14	3 (5%)
28	CLA	b	611	-	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
28	CLA	C	504	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	17 (22%)
28	CLA	C	503	-	65,73,73	1.36	9 (13%)	76,113,113	1.99	18 (23%)
43	RRX	H	101	-	42,42,42	4.83	24 (57%)	57,58,58	2.76	22 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	S	605	-	50,58,73	1.59	10 (20%)	58,95,113	2.25	16 (27%)
46	CHL	G	605	-	48,56,74	0.95	2 (4%)	51,92,114	1.41	8 (15%)
28	CLA	b	617	-	65,73,73	1.34	6 (9%)	76,113,113	1.95	17 (22%)
28	CLA	G	603	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	18 (23%)
48	XAT	G	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.90	13 (24%)
28	CLA	B	607	-	65,73,73	1.35	9 (13%)	76,113,113	2.00	19 (25%)
31	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.93	3 (5%)
46	CHL	G	601	21	66,74,74	0.82	3 (4%)	73,114,114	1.23	11 (15%)
45	4RF	I	102	-	56,56,56	1.05	3 (5%)	59,59,59	0.88	3 (5%)
36	3PH	S	626	-	47,47,47	0.86	4 (8%)	51,52,52	4.42	4 (7%)
31	SQD	B	626	-	53,54,54	0.80	0	62,65,65	0.91	2 (3%)
28	CLA	N	614	-	49,57,73	1.56	10 (20%)	55,93,113	2.31	16 (29%)
28	CLA	b	613	-	65,73,73	1.36	8 (12%)	76,113,113	1.87	16 (21%)
49	NEX	G	623	-	38,46,46	3.25	10 (26%)	50,70,70	1.87	9 (18%)
28	CLA	b	608	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	18 (23%)
25	OEX	A	401	4,1	0,15,15	-	-	-	-	-
28	CLA	Y	614	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	17 (22%)
36	3PH	t	101	-	47,47,47	0.87	4 (8%)	51,52,52	1.15	2 (3%)
38	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
32	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.03	2 (3%)
28	CLA	B	608	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	15 (19%)
28	CLA	S	614	-	55,63,73	1.47	8 (14%)	64,101,113	2.09	15 (23%)
35	DGD	C	518	-	56,56,67	1.00	4 (7%)	70,70,81	0.91	2 (2%)
28	CLA	C	502	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
28	CLA	N	613	-	65,73,73	1.37	10 (15%)	76,113,113	1.99	17 (22%)
28	CLA	a	406	-	65,73,73	1.34	7 (10%)	76,113,113	1.93	18 (23%)
46	CHL	Y	605	23	46,54,74	0.97	2 (4%)	49,90,114	1.34	8 (16%)
39	LMK	c	527	-	38,39,53	1.49	2 (5%)	41,46,60	1.26	2 (4%)
37	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.24	2 (6%)
28	CLA	b	604	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	17 (22%)
38	LHG	d	409	-	48,48,48	0.38	0	51,54,54	0.99	2 (3%)
31	SQD	b	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
28	CLA	G	611	-	65,73,73	1.38	9 (13%)	76,113,113	1.96	16 (21%)
35	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.92	2 (2%)
38	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.02	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	3PH	b	624	-	47,47,47	0.87	4 (8%)	51,52,52	1.11	2 (3%)
35	DGD	C	519	-	63,63,67	1.13	6 (9%)	77,77,81	0.97	3 (3%)
28	CLA	c	503	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
28	CLA	c	506	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	17 (22%)
28	CLA	N	604	-	65,73,73	1.35	9 (13%)	76,113,113	2.05	19 (25%)
31	SQD	B	621	-	41,42,54	0.88	0	50,53,65	0.94	2 (4%)
32	LMG	b	622	-	44,44,55	0.87	2 (4%)	52,52,63	1.11	2 (3%)
38	LHG	d	408	-	43,43,48	0.40	0	46,49,54	0.99	2 (4%)
28	CLA	D	402	-	65,73,73	1.37	8 (12%)	76,113,113	1.92	17 (22%)
28	CLA	b	614	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	18 (23%)
30	BCR	b	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.61	20 (35%)
46	CHL	N	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.40	10 (19%)
40	BCT	D	401	-	2,3,3	1.27	0	2,3,3	4.06	2 (100%)
30	BCR	d	404	-	41,41,41	1.87	4 (9%)	56,56,56	4.39	17 (30%)
44	GOL	I	101	-	5,5,5	0.55	0	5,5,5	0.29	0
28	CLA	S	617	-	50,58,73	1.55	9 (18%)	58,95,113	2.26	17 (29%)
28	CLA	S	612	-	45,53,73	1.60	7 (15%)	52,89,113	2.17	16 (30%)
28	CLA	b	607	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	17 (22%)
43	RRX	h	101	-	42,42,42	4.91	24 (57%)	57,58,58	2.40	20 (35%)

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
28	CLA	B	612	-	1/1/15/20	17/37/115/115	-
28	CLA	b	616	-	1/1/15/20	10/37/115/115	-
28	CLA	Y	613	-	1/1/15/20	20/37/115/115	-
28	CLA	S	610	-	1/1/15/20	21/37/115/115	-
28	CLA	c	505	-	1/1/15/20	17/37/115/115	-
30	BCR	C	517	-	-	10/29/63/63	0/2/2/2
28	CLA	S	613	-	1/1/13/20	9/25/103/115	-
28	CLA	c	512	-	1/1/15/20	21/37/115/115	-
32	LMG	A	413	-	-	14/43/63/70	0/1/1/1
30	BCR	C	516	-	-	15/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	G	610	-	1/1/15/20	18/37/115/115	-
41	PL9	D	405	-	-	7/53/73/73	0/1/1/1
28	CLA	A	410	-	1/1/14/20	11/31/109/115	-
34	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
28	CLA	c	504	-	1/1/15/20	21/37/115/115	-
28	CLA	b	606	-	1/1/15/20	14/37/115/115	-
31	SQD	M	101	-	-	18/37/57/69	0/1/1/1
28	CLA	Y	604	-	1/1/15/20	15/37/115/115	-
42	HEM	F	101	7,6	-	0/12/54/54	-
28	CLA	B	602	-	1/1/15/20	22/37/115/115	-
28	CLA	c	510	-	1/1/15/20	18/37/115/115	-
28	CLA	B	617	-	1/1/15/20	17/37/115/115	-
28	CLA	S	604	-	1/1/13/20	9/25/103/115	-
35	DGD	c	520	-	-	7/48/88/95	0/2/2/2
28	CLA	B	614	-	1/1/15/20	11/37/115/115	-
46	CHL	G	608	-	3/3/15/26	1/13/111/137	-
28	CLA	G	614	-	1/1/11/20	10/18/96/115	-
30	BCR	B	618	-	-	7/29/63/63	0/2/2/2
38	LHG	D	409	-	-	28/53/53/53	-
46	CHL	N	605	20	4/4/20/26	2/39/137/137	-
29	PHO	A	408	-	-	13/37/103/103	0/5/6/6
28	CLA	C	513	-	1/1/15/20	18/37/115/115	-
33	SPH	Y	625	-	-	11/21/21/21	-
45	4RF	k	101	-	-	30/59/59/59	-
28	CLA	a	405	-	1/1/15/20	13/37/115/115	-
28	CLA	c	502	-	1/1/15/20	9/37/115/115	-
32	LMG	H	102	-	-	9/43/63/70	0/1/1/1
28	CLA	d	403	-	1/1/15/20	21/37/115/115	-
31	SQD	C	526	-	-	17/49/69/69	0/1/1/1
51	PTY	Y	627	-	-	13/20/20/53	-
46	CHL	S	601	22	3/3/16/26	3/15/113/137	-
35	DGD	b	623	-	-	11/32/72/95	0/2/2/2
49	NEX	N	623	-	-	2/27/83/83	1/3/3/3
28	CLA	c	513	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	a	412	-	-	22/46/66/69	0/1/1/1
28	CLA	B	611	-	1/1/15/20	11/37/115/115	-
49	NEX	Y	623	-	-	5/27/83/83	0/3/3/3
46	CHL	Y	609	-	4/4/20/26	11/39/137/137	-
32	LMG	c	523	-	-	14/50/70/70	0/1/1/1
29	PHO	A	409	-	-	4/37/103/103	0/5/6/6
28	CLA	d	402	-	1/1/15/20	21/37/115/115	-
31	SQD	m	101	-	-	20/37/57/69	0/1/1/1
32	LMG	W	201	-	-	12/34/54/70	0/1/1/1
28	CLA	c	501	-	1/1/15/20	20/37/115/115	-
47	LUT	G	621	-	-	5/29/67/67	0/2/2/2
32	LMG	w	201	-	-	10/34/54/70	0/1/1/1
28	CLA	B	613	-	1/1/15/20	16/37/115/115	-
28	CLA	b	605	-	1/1/15/20	17/37/115/115	-
28	CLA	Y	612	-	1/1/15/20	13/37/115/115	-
28	CLA	G	613	-	1/1/15/20	15/37/115/115	-
28	CLA	B	615	-	1/1/15/20	11/37/115/115	-
28	CLA	B	605	-	1/1/15/20	14/37/115/115	-
28	CLA	C	506	-	1/1/15/20	14/37/115/115	-
28	CLA	c	508	-	1/1/15/20	10/37/115/115	-
34	C7Z	b	620	-	1/1/12/26	14/29/67/67	0/2/2/2
30	BCR	D	404	-	-	12/29/63/63	0/2/2/2
37	DGA	j	101	-	-	14/30/30/45	-
47	LUT	Y	621	-	-	3/29/67/67	0/2/2/2
28	CLA	b	610	-	1/1/15/20	14/37/115/115	-
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
38	LHG	L	101	-	-	42/53/53/53	-
35	DGD	c	519	-	-	19/51/91/95	0/2/2/2
28	CLA	A	407	-	1/1/12/20	7/19/97/115	-
28	CLA	S	609	-	1/1/14/20	10/31/109/115	-
28	CLA	S	602	-	1/1/14/20	18/31/109/115	-
46	CHL	N	606	-	4/4/20/26	11/39/137/137	-
28	CLA	b	602	-	1/1/15/20	26/37/115/115	-
30	BCR	a	411	-	-	10/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGA	b	625	-	-	28/45/45/45	-
38	LHG	D	410	-	-	30/43/43/53	-
47	LUT	G	620	-	-	4/29/67/67	0/2/2/2
28	CLA	G	604	-	1/1/11/20	10/18/96/115	-
49	NEX	S	623	-	-	2/27/83/83	0/3/3/3
36	3PH	B	624	-	-	28/49/49/49	-
32	LMG	C	521	-	-	13/46/66/70	0/1/1/1
46	CHL	Y	606	-	4/4/20/26	7/39/137/137	-
46	CHL	S	606	-	3/3/15/26	1/13/111/137	-
50	LPX	S	625	-	-	12/31/31/31	-
28	CLA	A	405	-	1/1/15/20	13/37/115/115	-
28	CLA	C	510	-	1/1/15/20	16/37/115/115	-
28	CLA	C	512	-	1/1/15/20	23/37/115/115	-
28	CLA	c	511	-	1/1/15/20	16/37/115/115	-
32	LMG	c	521	-	-	13/46/66/70	0/1/1/1
28	CLA	C	508	-	1/1/15/20	13/37/115/115	-
28	CLA	N	603	-	1/1/15/20	18/37/115/115	-
48	XAT	N	622	-	1/1/12/26	0/31/93/93	0/4/4/4
46	CHL	G	606	-	3/3/16/26	5/20/118/137	-
38	LHG	G	624	-	-	29/53/53/53	-
28	CLA	C	509	-	1/1/15/20	18/37/115/115	-
47	LUT	S	621	-	-	1/29/67/67	0/2/2/2
37	DGA	B	625	-	-	25/45/45/45	-
46	CHL	S	607	-	3/3/15/26	0/12/110/137	-
28	CLA	Y	603	-	1/1/15/20	15/37/115/115	-
37	DGA	c	524	-	-	25/45/45/45	-
28	CLA	B	616	-	1/1/15/20	15/37/115/115	-
36	3PH	T	101	-	-	22/49/49/49	-
41	PL9	d	405	-	-	21/53/73/73	0/1/1/1
28	CLA	c	509	-	1/1/15/20	14/37/115/115	-
47	LUT	N	621	-	-	2/29/67/67	0/2/2/2
28	CLA	C	511	-	1/1/15/20	11/37/115/115	-
39	LMK	C	527	-	2/2/6/6	15/46/46/60	-
47	LUT	N	620	-	-	3/29/67/67	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	609	-	1/1/15/20	15/37/115/115	-
46	CHL	N	609	-	4/4/20/26	6/39/137/137	-
46	CHL	S	608	-	4/4/19/26	8/33/131/137	-
30	BCR	B	619	-	-	6/29/63/63	0/2/2/2
28	CLA	Y	610	-	1/1/15/20	15/37/115/115	-
30	BCR	c	517	-	-	8/29/63/63	0/2/2/2
35	DGD	B	623	-	-	14/32/72/95	0/2/2/2
28	CLA	Y	611	-	1/1/15/20	16/37/115/115	-
33	SPH	a	414	-	-	13/21/21/21	-
28	CLA	N	602	-	1/1/15/20	16/37/115/115	-
28	CLA	b	612	-	1/1/15/20	15/37/115/115	-
28	CLA	S	611	38	1/1/15/20	15/37/115/115	-
28	CLA	A	406	-	1/1/15/20	19/37/115/115	-
28	CLA	B	606	-	1/1/15/20	15/37/115/115	-
30	BCR	C	514	-	-	13/29/63/63	0/2/2/2
28	CLA	b	603	-	1/1/15/20	16/37/115/115	-
38	LHG	Y	624	-	-	31/53/53/53	-
51	PTY	Y	626	-	-	21/53/53/53	-
28	CLA	N	610	-	1/1/15/20	22/37/115/115	-
28	CLA	C	507	-	1/1/15/20	20/37/115/115	-
46	CHL	N	607	-	4/4/20/26	11/39/137/137	-
30	BCR	c	516	-	-	14/29/63/63	0/2/2/2
30	BCR	c	514	-	-	12/29/63/63	0/2/2/2
48	XAT	Y	622	-	-	1/31/93/93	0/4/4/4
46	CHL	Y	601	23	4/4/20/26	5/39/137/137	-
29	PHO	a	408	-	-	6/37/103/103	0/5/6/6
28	CLA	C	501	-	1/1/15/20	16/37/115/115	-
28	CLA	Y	608	-	1/1/12/20	9/19/97/115	-
28	CLA	c	507	-	1/1/15/20	16/37/115/115	-
28	CLA	D	403	-	1/1/15/20	14/37/115/115	-
46	CHL	G	609	-	4/4/20/26	8/39/137/137	-
28	CLA	b	609	-	1/1/15/20	20/37/115/115	-
28	CLA	b	615	-	1/1/15/20	13/37/115/115	-
29	PHO	a	409	-	-	8/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	d	410	-	-	23/43/43/53	-
32	LMG	D	411	-	-	10/41/61/70	0/1/1/1
30	BCR	A	411	-	-	11/29/63/63	0/2/2/2
38	LHG	C	525	-	-	32/51/51/53	-
28	CLA	a	407	-	1/1/11/20	9/18/96/115	-
32	LMG	C	523	-	-	18/50/70/70	0/1/1/1
28	CLA	N	612	-	1/1/11/20	3/13/91/115	-
45	4RF	K	101	-	-	32/59/59/59	-
28	CLA	N	611	-	1/1/11/20	11/18/96/115	-
28	CLA	C	505	-	1/1/15/20	18/37/115/115	-
28	CLA	G	612	-	1/1/10/20	4/11/89/115	-
30	BCR	b	619	-	-	11/29/63/63	0/2/2/2
31	SQD	b	621	-	-	18/37/57/69	0/1/1/1
46	CHL	G	607	-	4/4/20/26	10/39/137/137	-
42	HEM	f	101	7,6	-	1/12/54/54	-
45	4RF	i	101	-	-	31/59/59/59	-
28	CLA	B	603	-	1/1/15/20	15/37/115/115	-
32	LMG	h	102	-	-	11/43/63/70	0/1/1/1
38	LHG	N	624	-	-	33/53/53/53	-
31	SQD	c	526	-	-	13/49/69/69	0/1/1/1
33	SPH	A	414	-	-	8/21/21/21	-
46	CHL	Y	607	-	4/4/20/26	7/39/137/137	-
47	LUT	Y	620	-	-	3/29/67/67	0/2/2/2
47	LUT	S	620	-	-	4/29/67/67	0/2/2/2
38	LHG	D	408	-	-	24/48/48/53	-
28	CLA	B	610	-	1/1/15/20	14/37/115/115	-
28	CLA	a	410	-	1/1/14/20	7/31/109/115	-
37	DGA	C	524	-	-	22/45/45/45	-
28	CLA	B	604	-	1/1/15/20	17/37/115/115	-
28	CLA	Y	602	-	1/1/15/20	17/37/115/115	-
28	CLA	G	602	-	1/1/15/20	19/37/115/115	-
30	BCR	c	515	-	-	15/29/63/63	0/2/2/2
46	CHL	N	601	-	4/4/20/26	8/39/137/137	-
32	LMG	B	622	-	-	12/39/59/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	S	603	-	1/1/15/20	18/37/115/115	-
35	DGD	c	518	-	-	19/44/84/95	0/2/2/2
38	LHG	S	624	28	-	31/49/49/53	-
32	LMG	a	413	-	-	13/43/63/70	0/1/1/1
28	CLA	b	611	-	1/1/15/20	11/37/115/115	-
28	CLA	C	504	-	1/1/15/20	13/37/115/115	-
28	CLA	C	503	-	1/1/15/20	17/37/115/115	-
43	RRX	H	101	-	1/1/11/25	6/29/65/65	0/2/2/2
28	CLA	S	605	-	1/1/12/20	10/19/97/115	-
46	CHL	G	605	-	4/4/16/26	6/18/116/137	-
28	CLA	b	617	-	1/1/15/20	13/37/115/115	-
28	CLA	G	603	-	1/1/15/20	17/37/115/115	-
48	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
28	CLA	B	607	-	1/1/15/20	13/37/115/115	-
31	SQD	A	412	-	-	16/46/66/69	0/1/1/1
46	CHL	G	601	21	4/4/20/26	11/39/137/137	-
45	4RF	I	102	-	-	28/59/59/59	-
36	3PH	S	626	-	-	25/49/49/49	-
31	SQD	B	626	-	-	22/49/69/69	0/1/1/1
28	CLA	N	614	-	1/1/11/20	7/18/96/115	-
28	CLA	b	613	-	1/1/15/20	17/37/115/115	-
49	NEX	G	623	-	-	6/27/83/83	0/3/3/3
28	CLA	b	608	-	1/1/15/20	26/37/115/115	-
28	CLA	Y	614	-	1/1/15/20	14/37/115/115	-
36	3PH	t	101	-	-	26/49/49/49	-
38	LHG	l	101	-	-	38/53/53/53	-
32	LMG	d	411	-	-	8/41/61/70	0/1/1/1
28	CLA	B	608	-	1/1/15/20	25/37/115/115	-
28	CLA	S	614	-	1/1/13/20	7/25/103/115	-
46	CHL	Y	605	23	3/3/16/26	4/15/113/137	-
28	CLA	C	502	-	1/1/15/20	15/37/115/115	-
28	CLA	N	613	-	1/1/15/20	17/37/115/115	-
28	CLA	a	406	-	1/1/15/20	15/37/115/115	-
35	DGD	C	518	-	-	15/44/84/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMK	c	527	-	2/2/6/6	12/46/46/60	-
37	DGA	J	101	-	-	10/30/30/45	-
28	CLA	b	604	-	1/1/15/20	19/37/115/115	-
38	LHG	d	409	-	-	28/53/53/53	-
31	SQD	b	626	-	-	21/49/69/69	0/1/1/1
28	CLA	G	611	-	1/1/15/20	14/37/115/115	-
35	DGD	C	520	-	-	8/48/88/95	0/2/2/2
38	LHG	c	525	-	-	31/51/51/53	-
36	3PH	b	624	-	-	21/49/49/49	-
35	DGD	C	519	-	-	14/51/91/95	0/2/2/2
28	CLA	c	503	-	1/1/15/20	20/37/115/115	-
28	CLA	c	506	-	1/1/15/20	17/37/115/115	-
28	CLA	N	604	-	1/1/15/20	13/37/115/115	-
31	SQD	B	621	-	-	13/37/57/69	0/1/1/1
32	LMG	b	622	-	-	11/39/59/70	0/1/1/1
38	LHG	d	408	-	-	30/48/48/53	-
28	CLA	D	402	-	1/1/15/20	20/37/115/115	-
28	CLA	b	614	-	1/1/15/20	12/37/115/115	-
30	BCR	b	618	-	-	7/29/63/63	0/2/2/2
46	CHL	N	608	-	3/3/16/26	3/20/118/137	-
30	BCR	d	404	-	-	13/29/63/63	0/2/2/2
44	GOL	I	101	-	-	2/4/4/4	-
28	CLA	S	617	-	1/1/12/20	5/19/97/115	-
28	CLA	S	612	-	1/1/11/20	5/13/91/115	-
28	CLA	b	607	-	1/1/15/20	9/37/115/115	-
43	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2

The worst 5 of 1292 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	620	C7Z	C25-C26	15.90	1.62	1.34
34	B	620	C7Z	C25-C26	15.72	1.61	1.34
43	h	101	RRX	C26-C25	15.50	1.61	1.34
43	H	101	RRX	C26-C25	15.18	1.60	1.34
34	b	620	C7Z	C5-C6	15.02	1.60	1.34

The worst 5 of 2768 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	l	101	LHG	O7-C7-C8	23.08	161.24	111.50
38	L	101	LHG	O7-C7-C8	22.88	160.81	111.50
36	S	626	3PH	O21-C21-C22	22.37	159.71	111.50
30	b	618	BCR	C10-C11-C12	18.18	179.96	123.22
36	S	626	3PH	O21-C21-O22	-18.16	79.82	123.70

5 of 194 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	A	405	CLA	ND
28	A	406	CLA	ND
28	A	407	CLA	ND
28	A	410	CLA	ND
28	B	602	CLA	ND

5 of 3369 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	405	CLA	C1A-C2A-CAA-CBA
28	A	405	CLA	C3A-C2A-CAA-CBA
28	A	405	CLA	CBD-CGD-O2D-CED
28	A	406	CLA	C1A-C2A-CAA-CBA
28	A	406	CLA	C3A-C2A-CAA-CBA

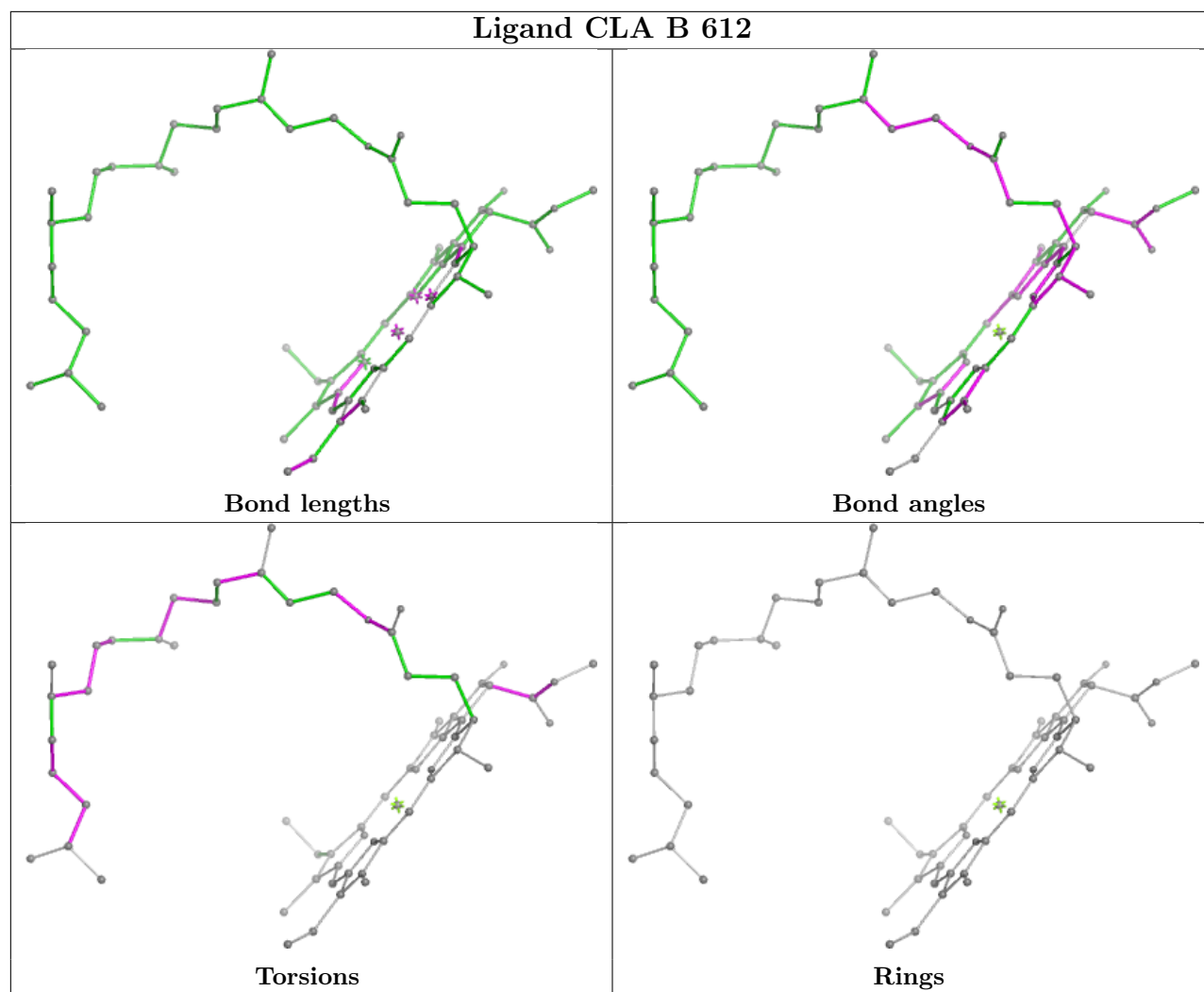
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	N	623	NEX	C1-C2-C3-C4-C5-C6

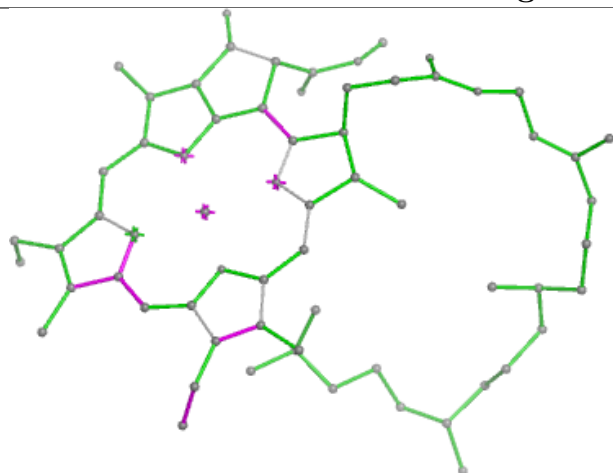
No monomer is involved in short contacts.

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

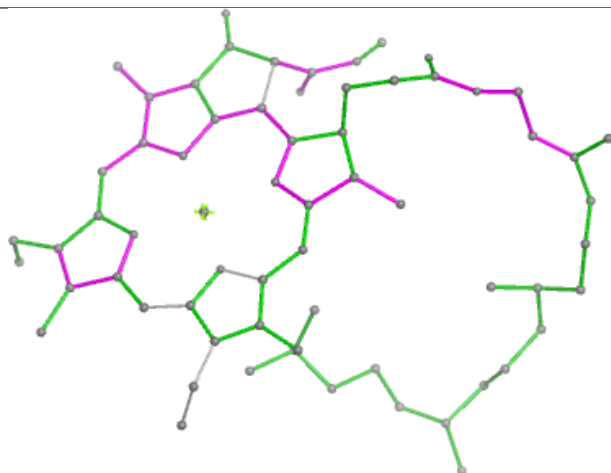
equivalents in the CSD to analyse the geometry.



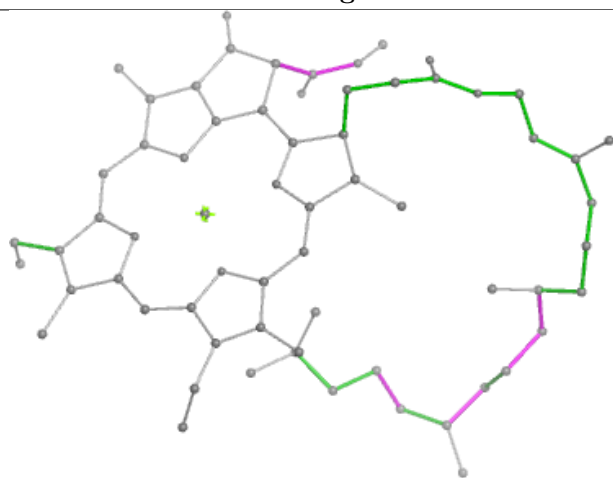
Ligand CLA b 616



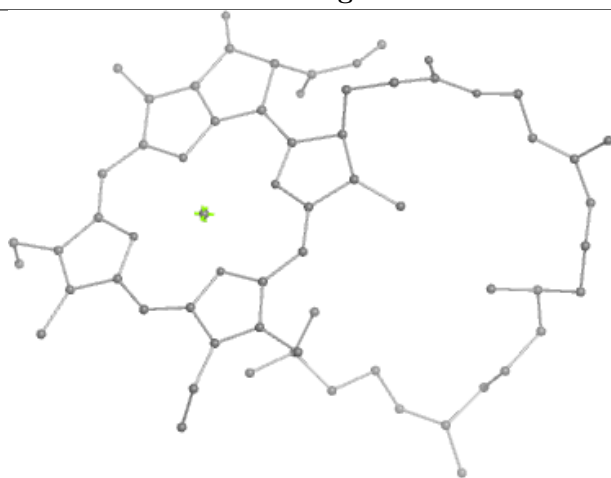
Bond lengths



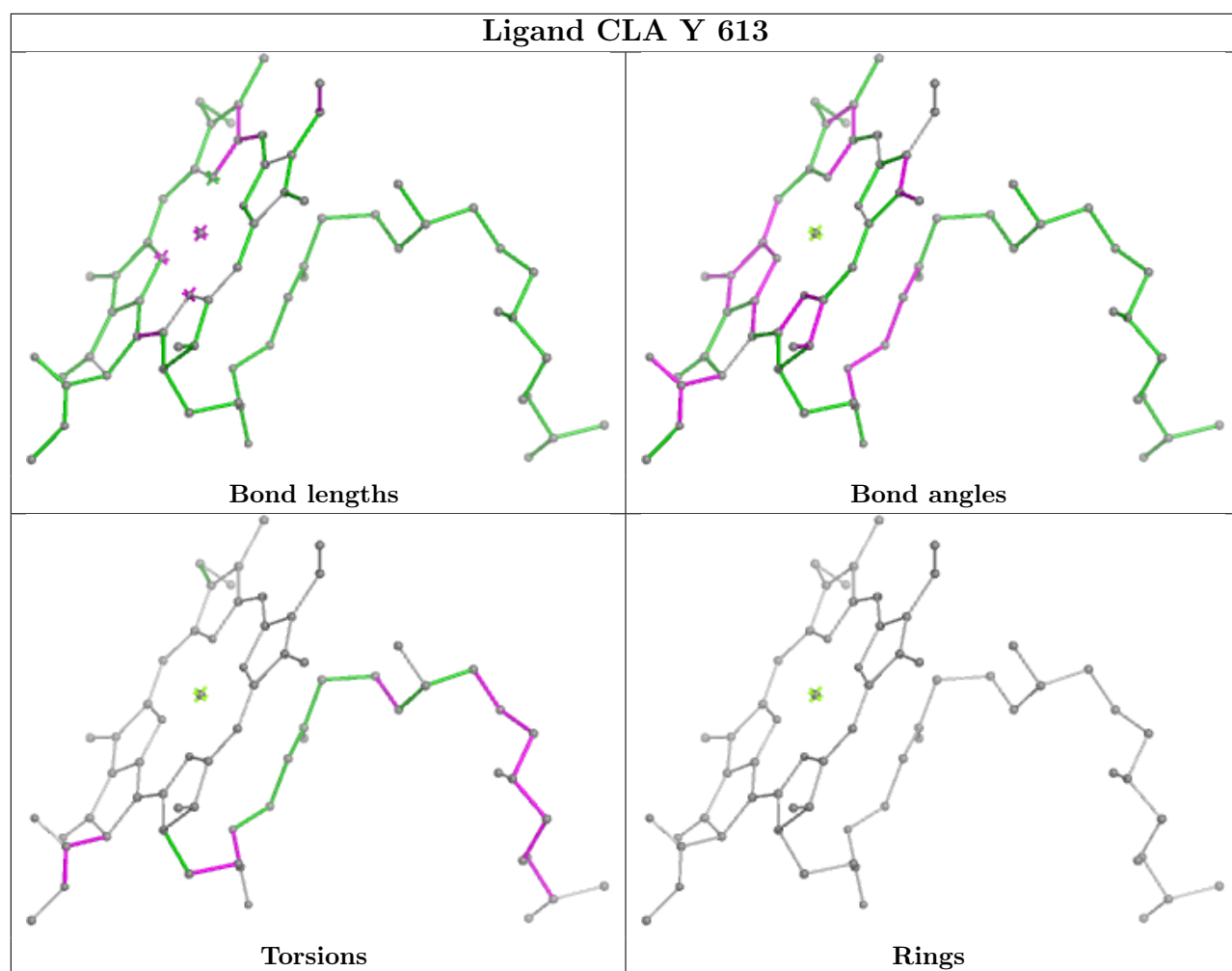
Bond angles

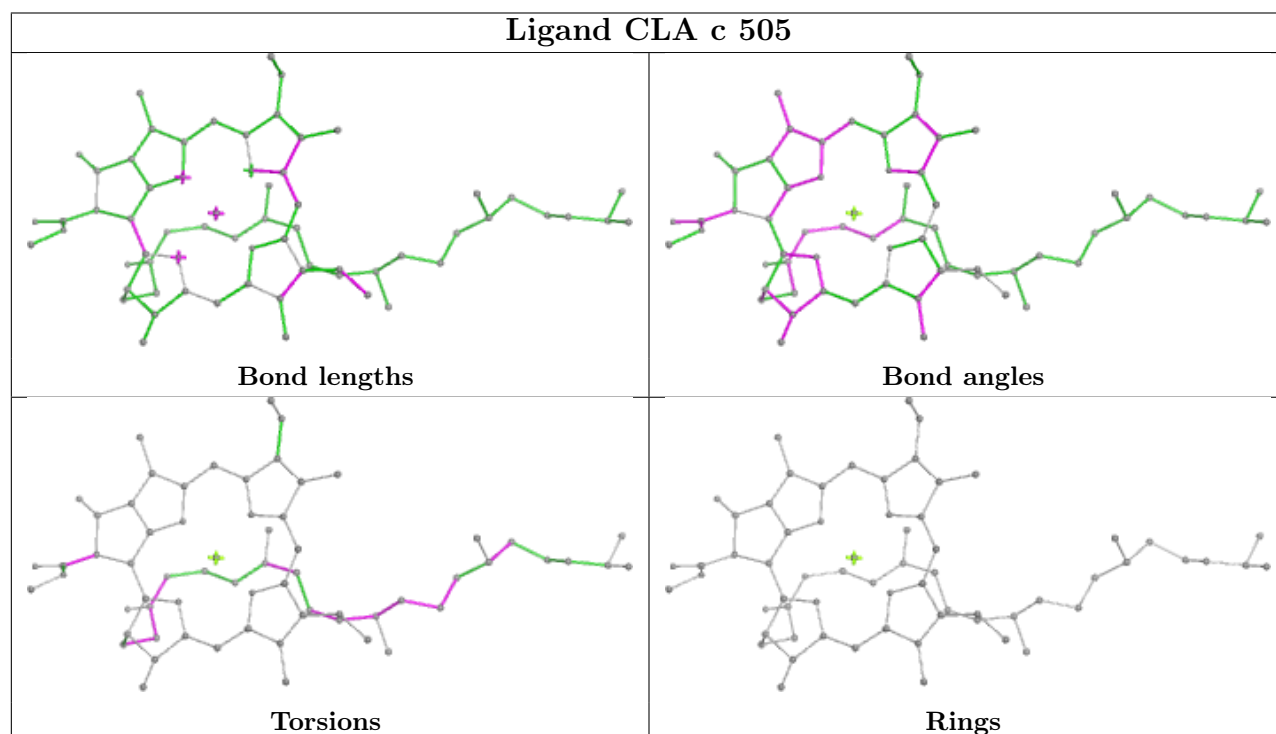
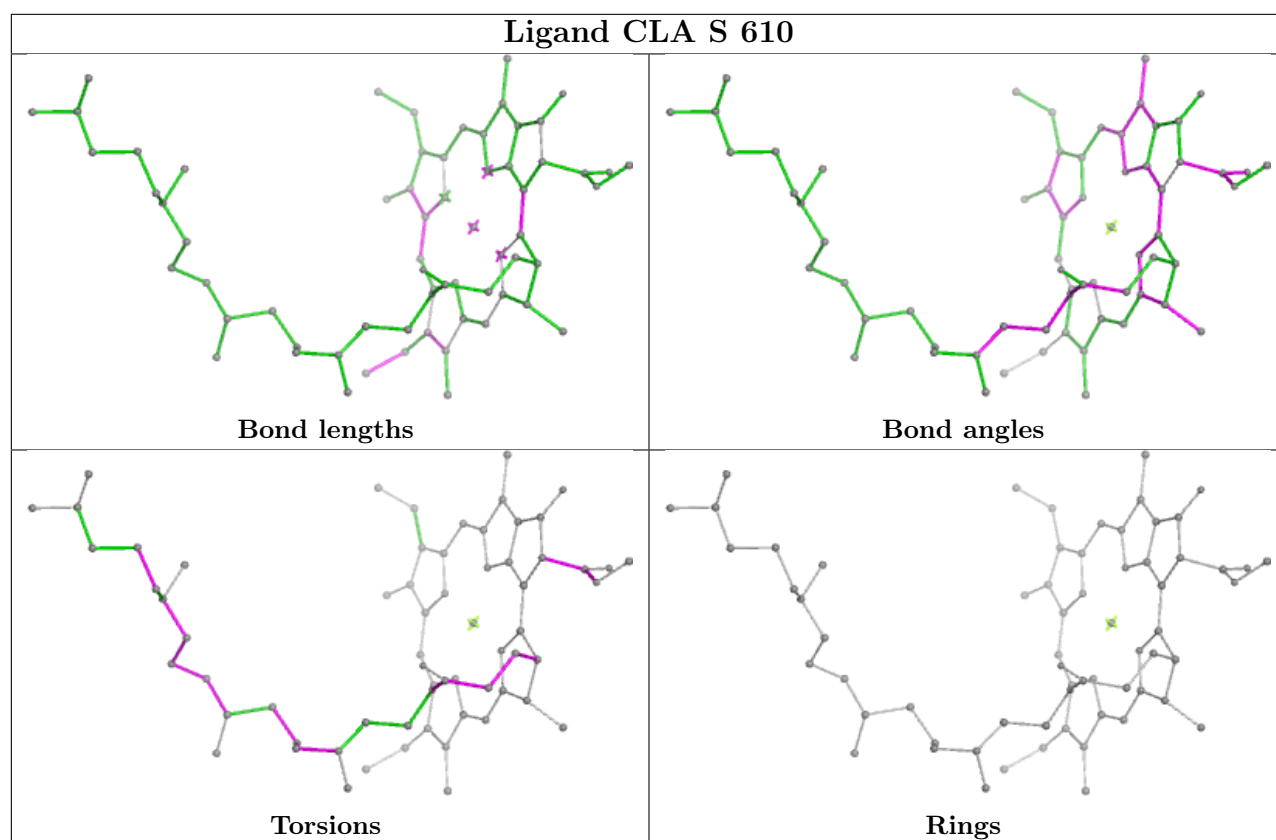


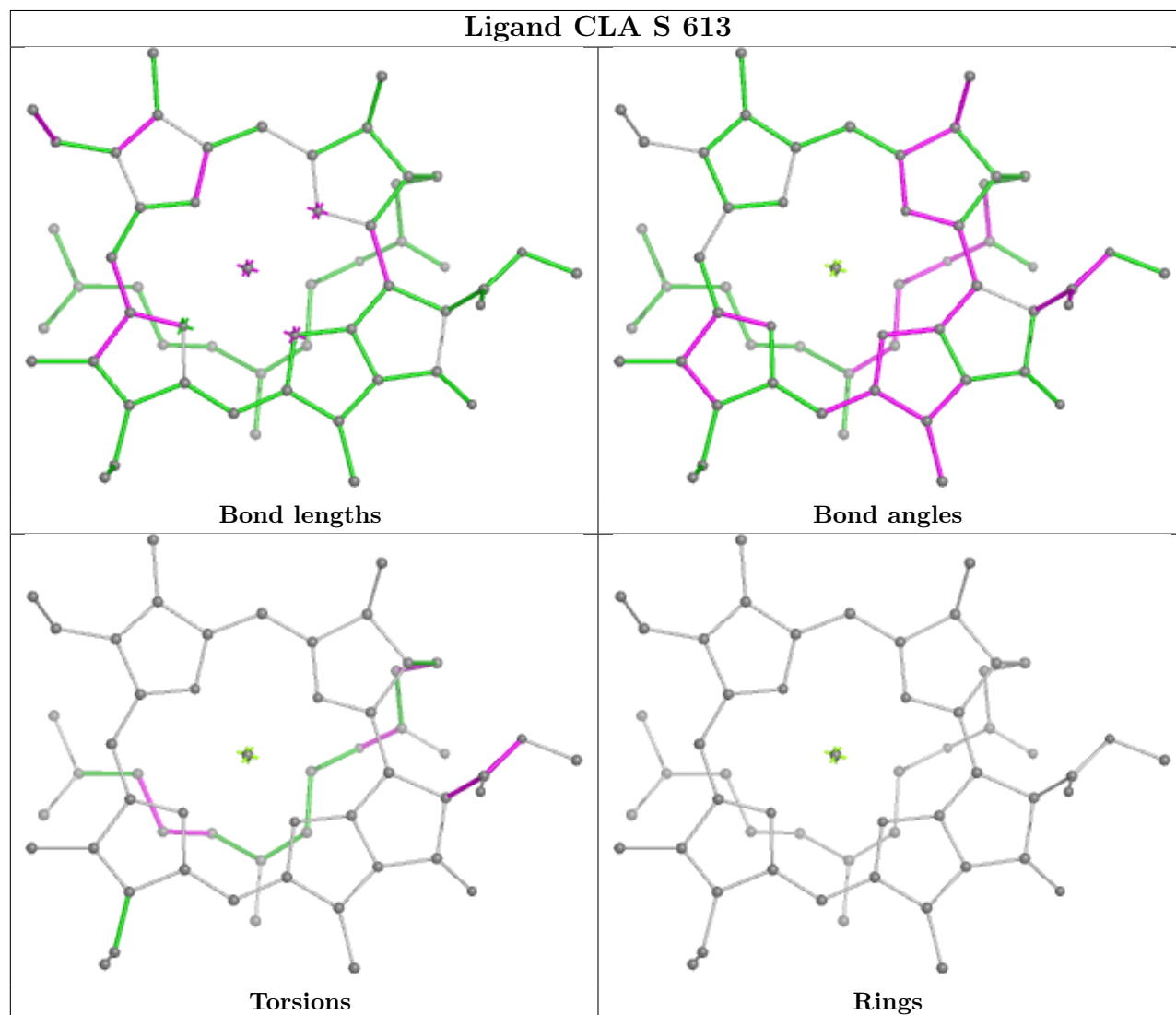
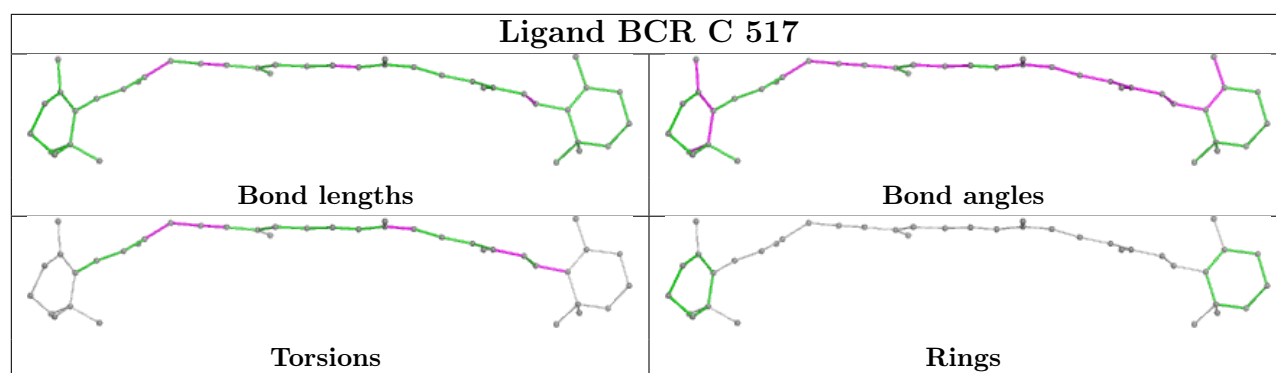
Torsions



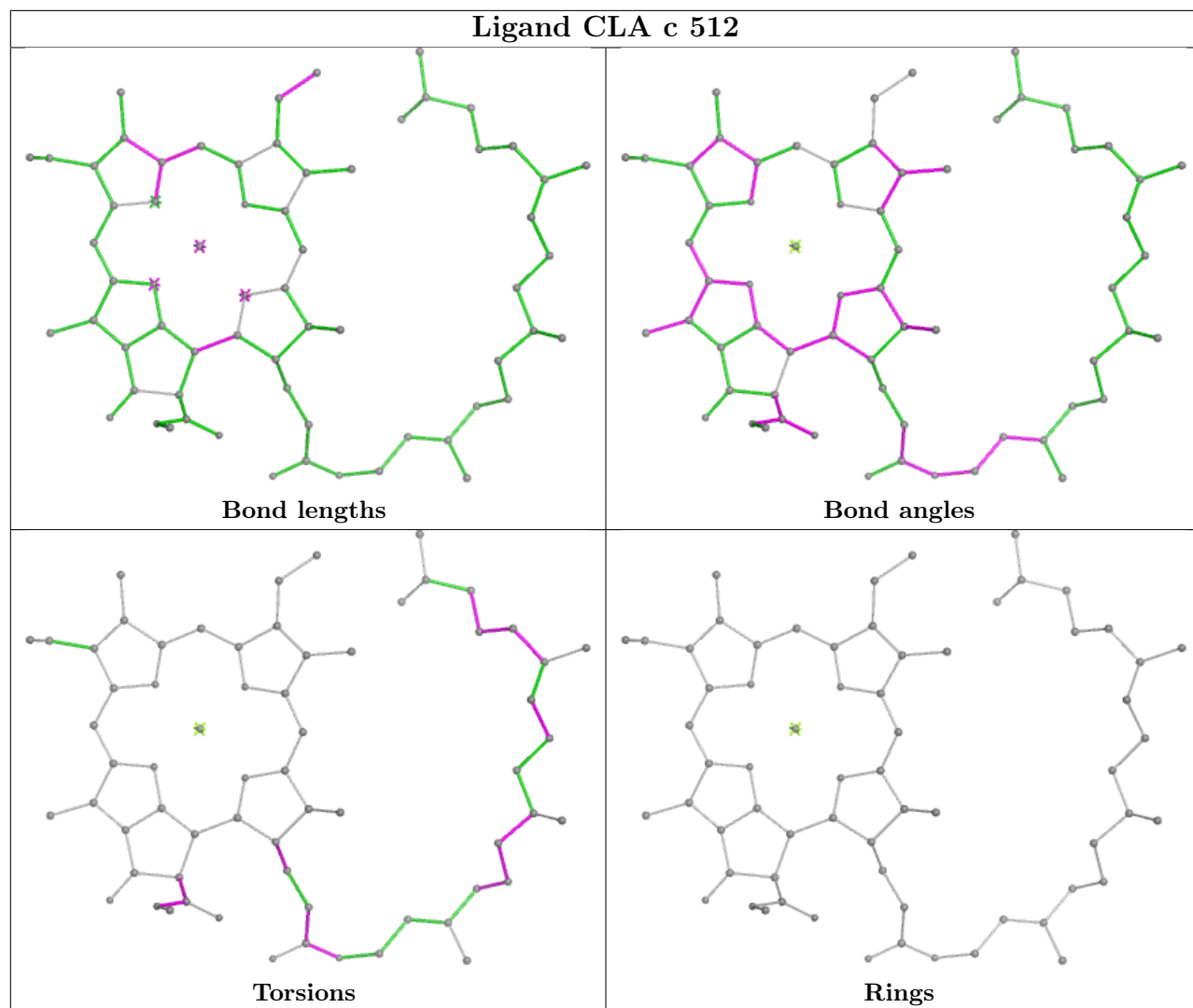
Rings

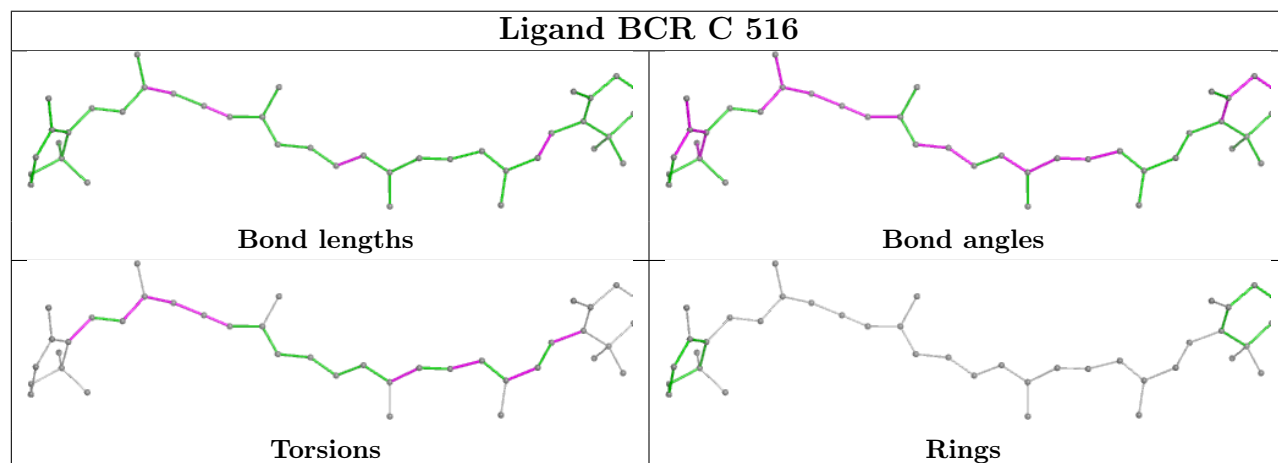
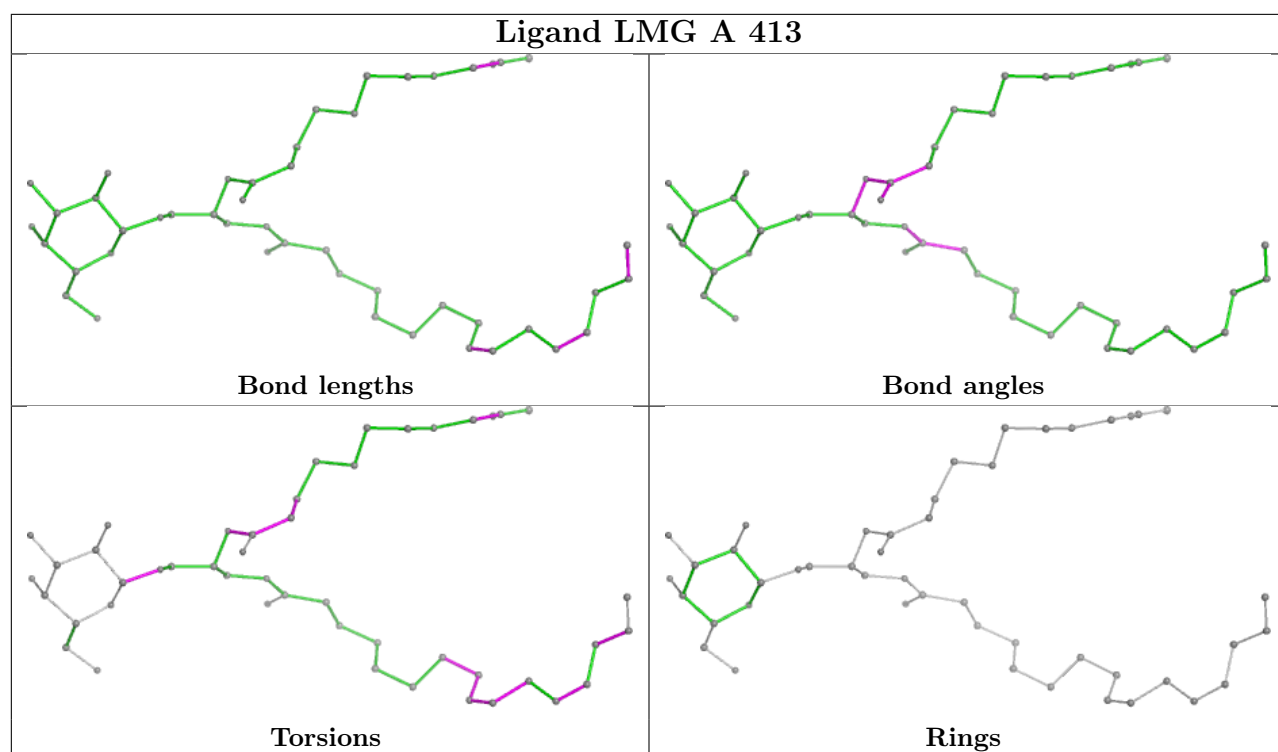




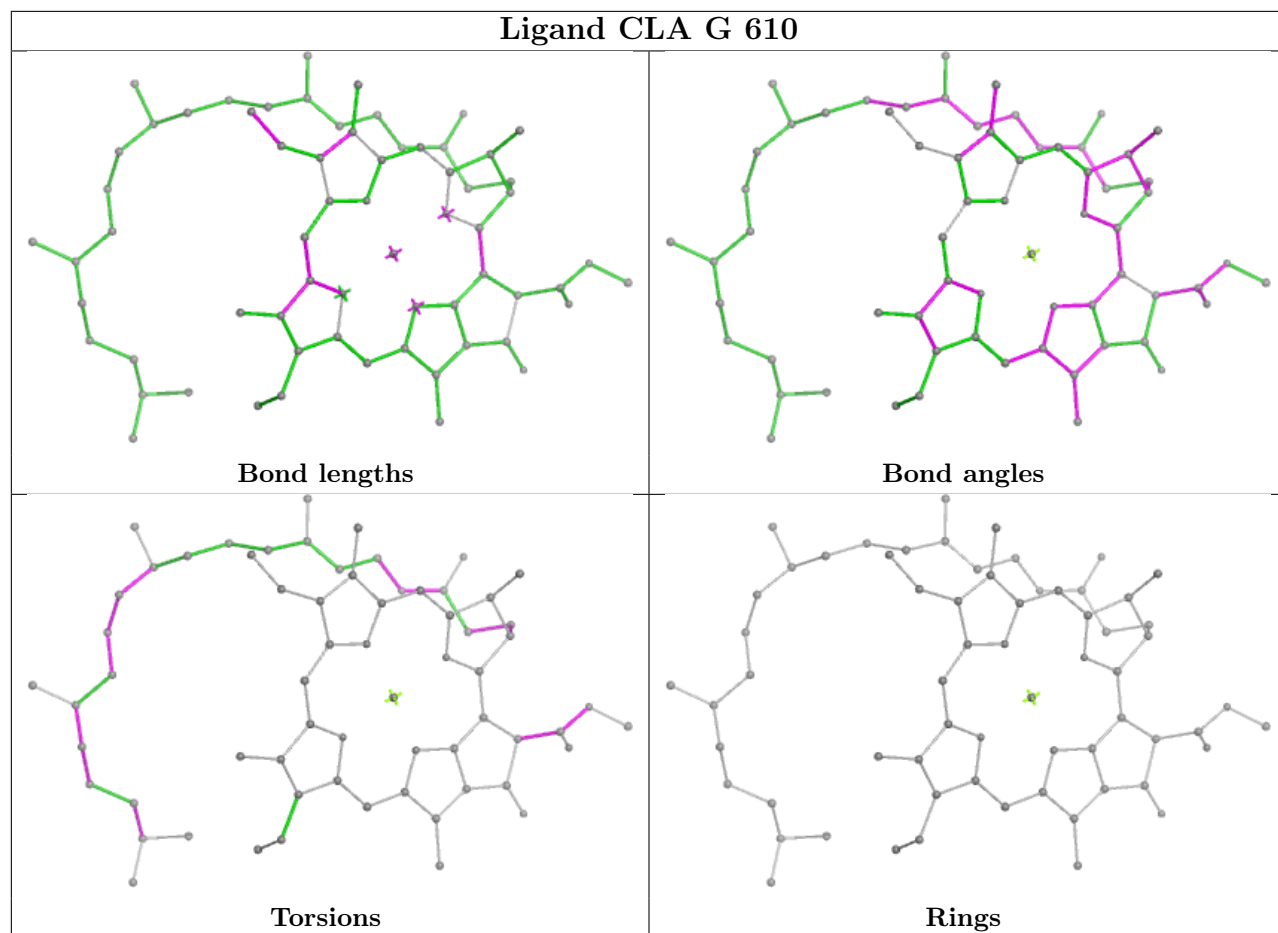


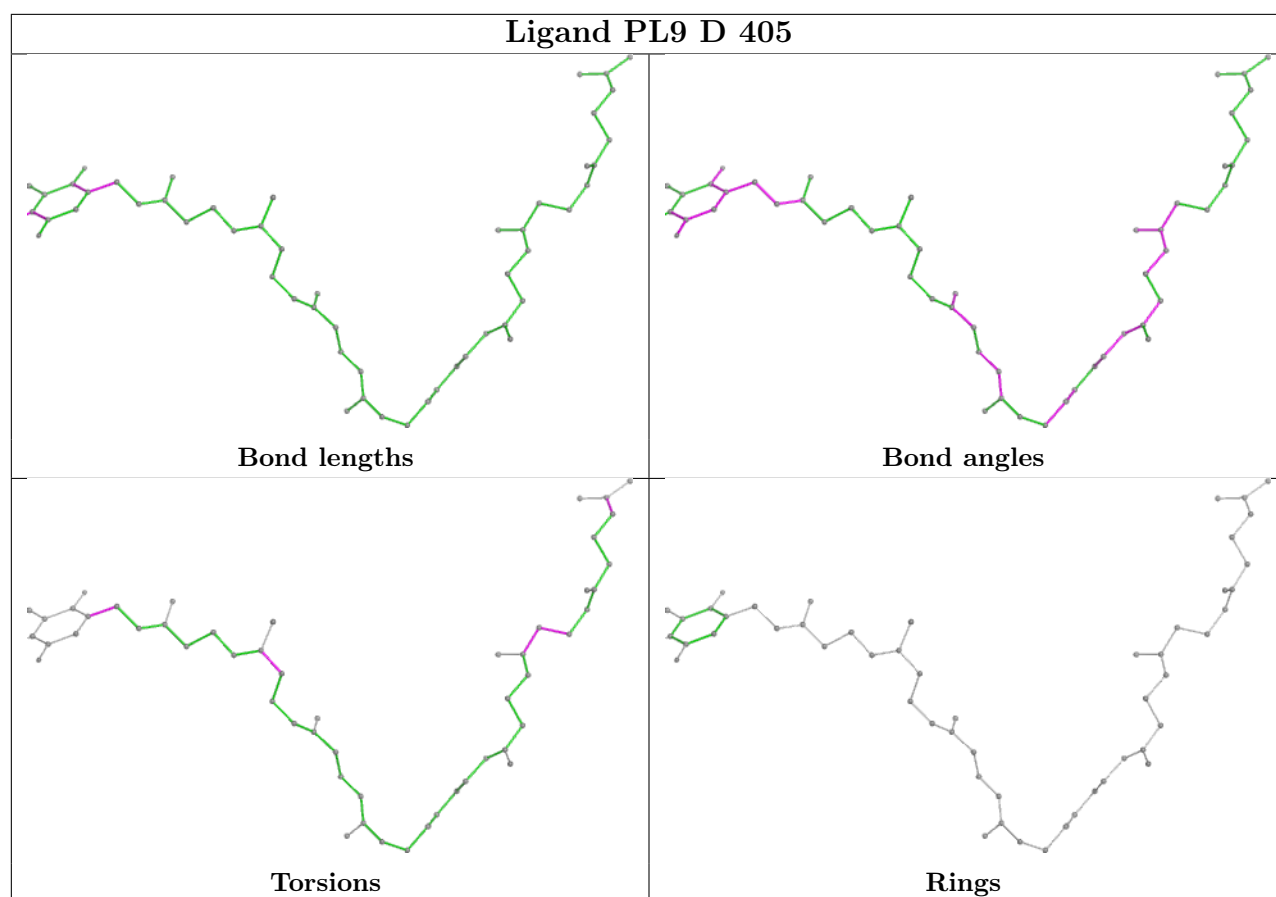
Ligand CLA c 512

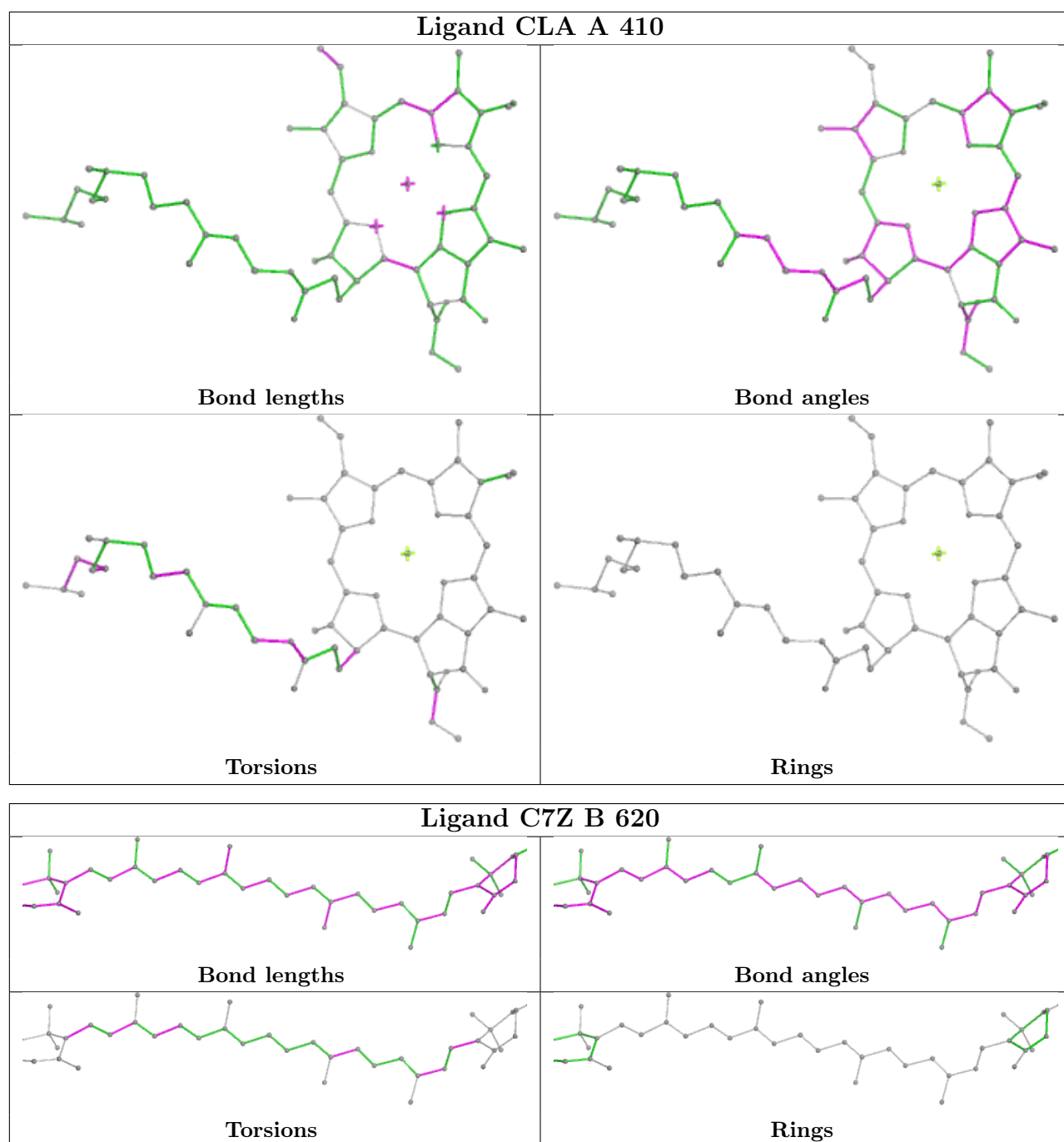


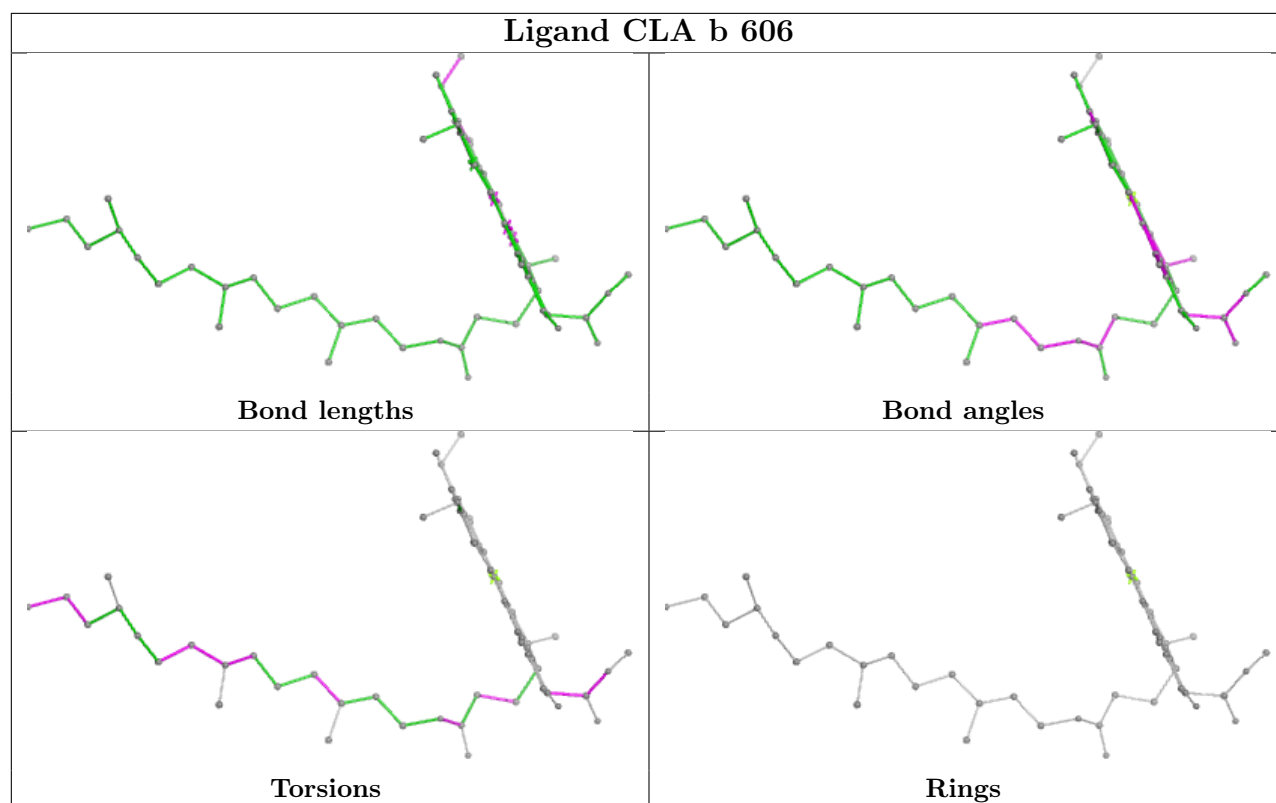
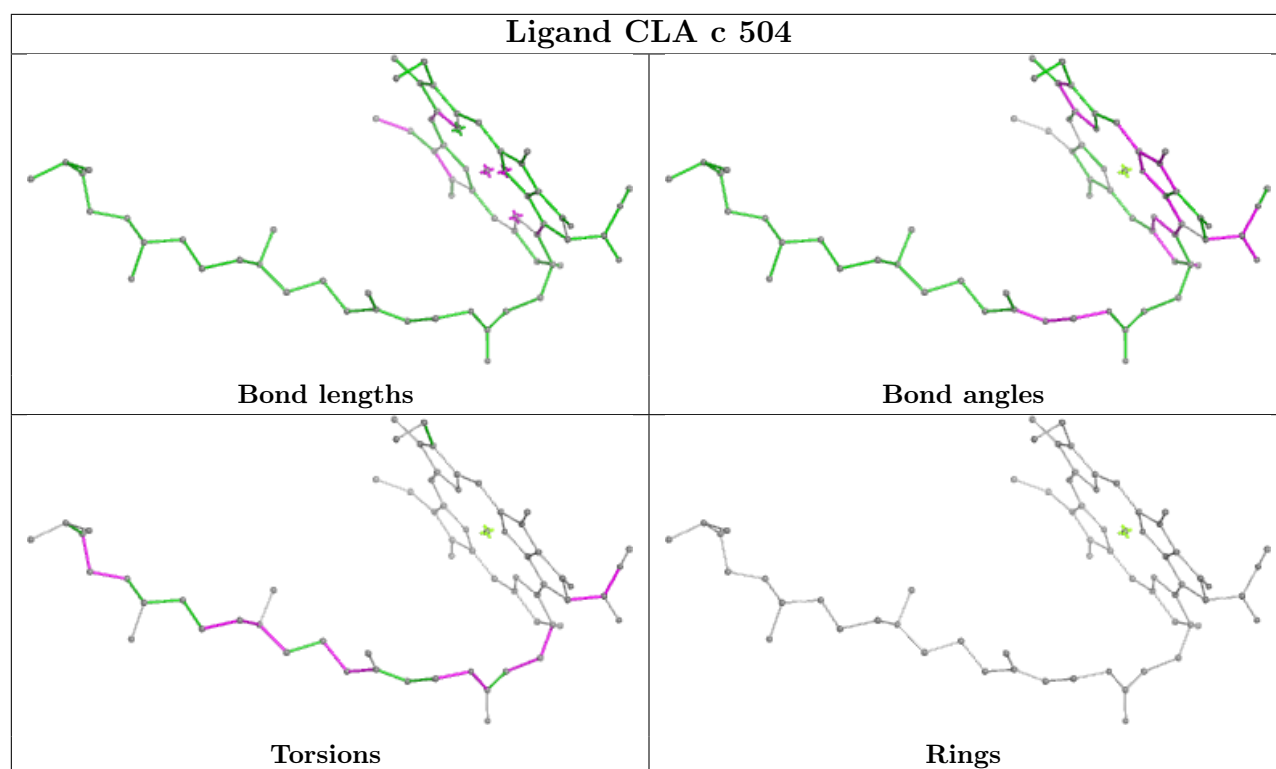


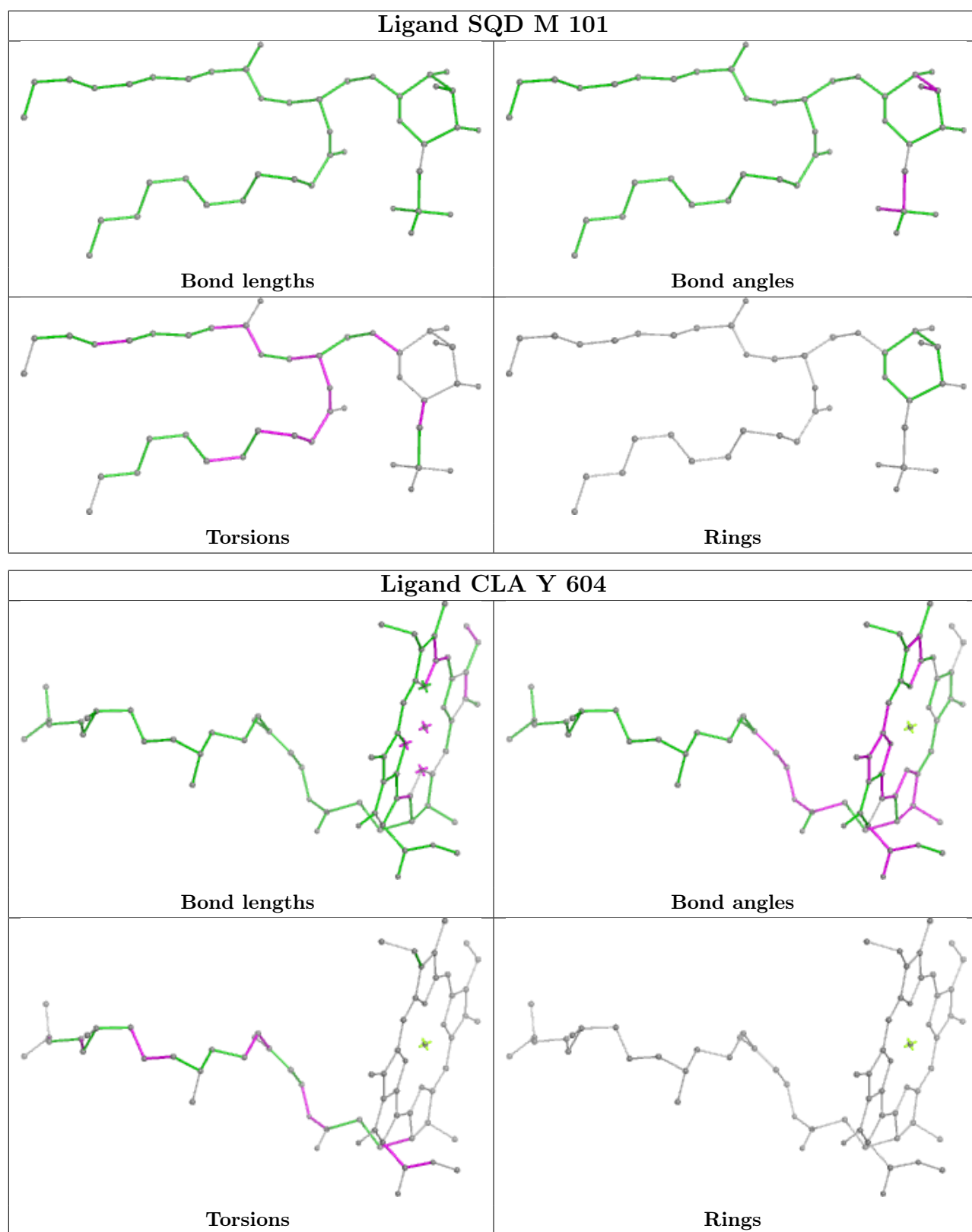
Ligand CLA G 610

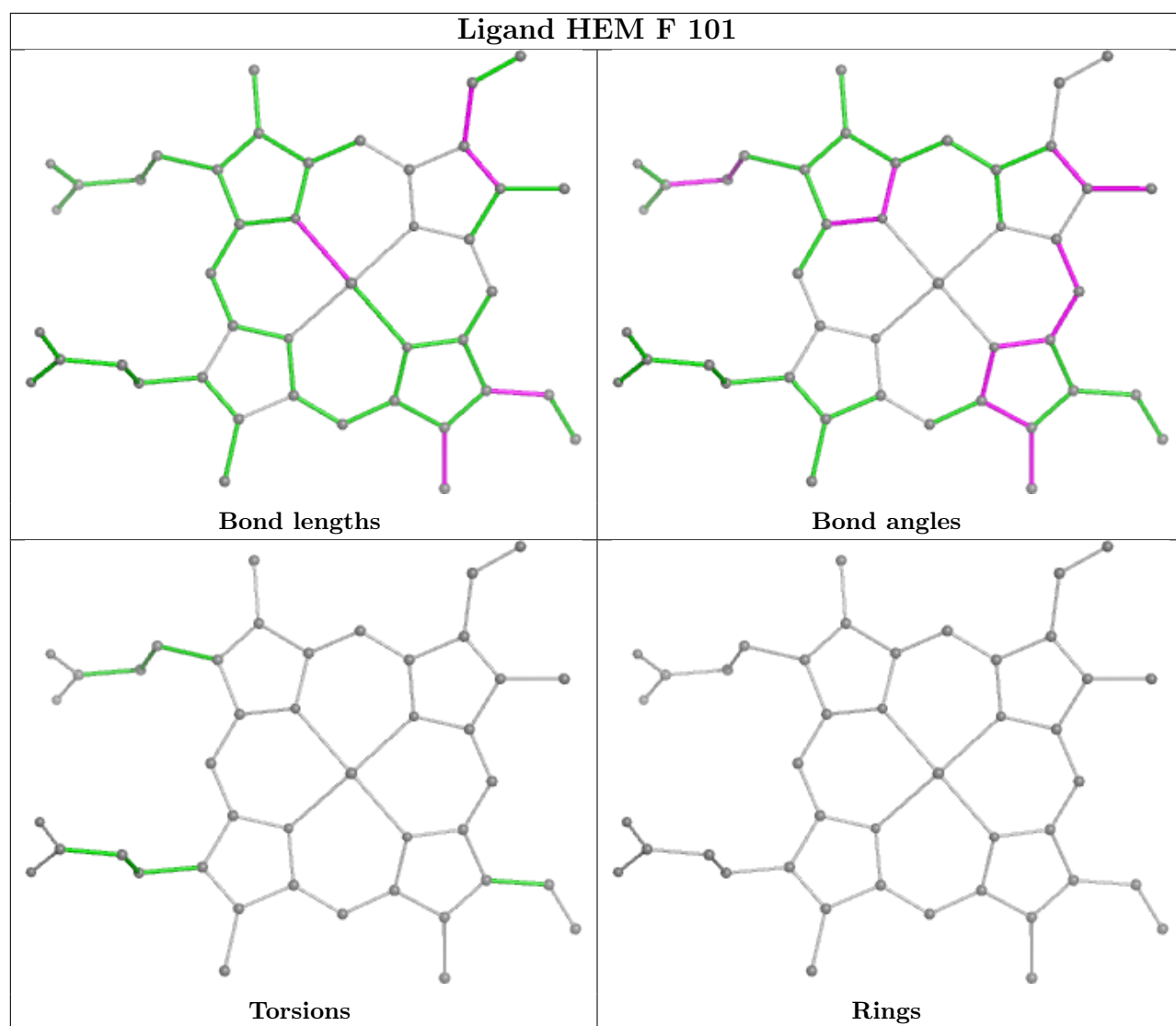




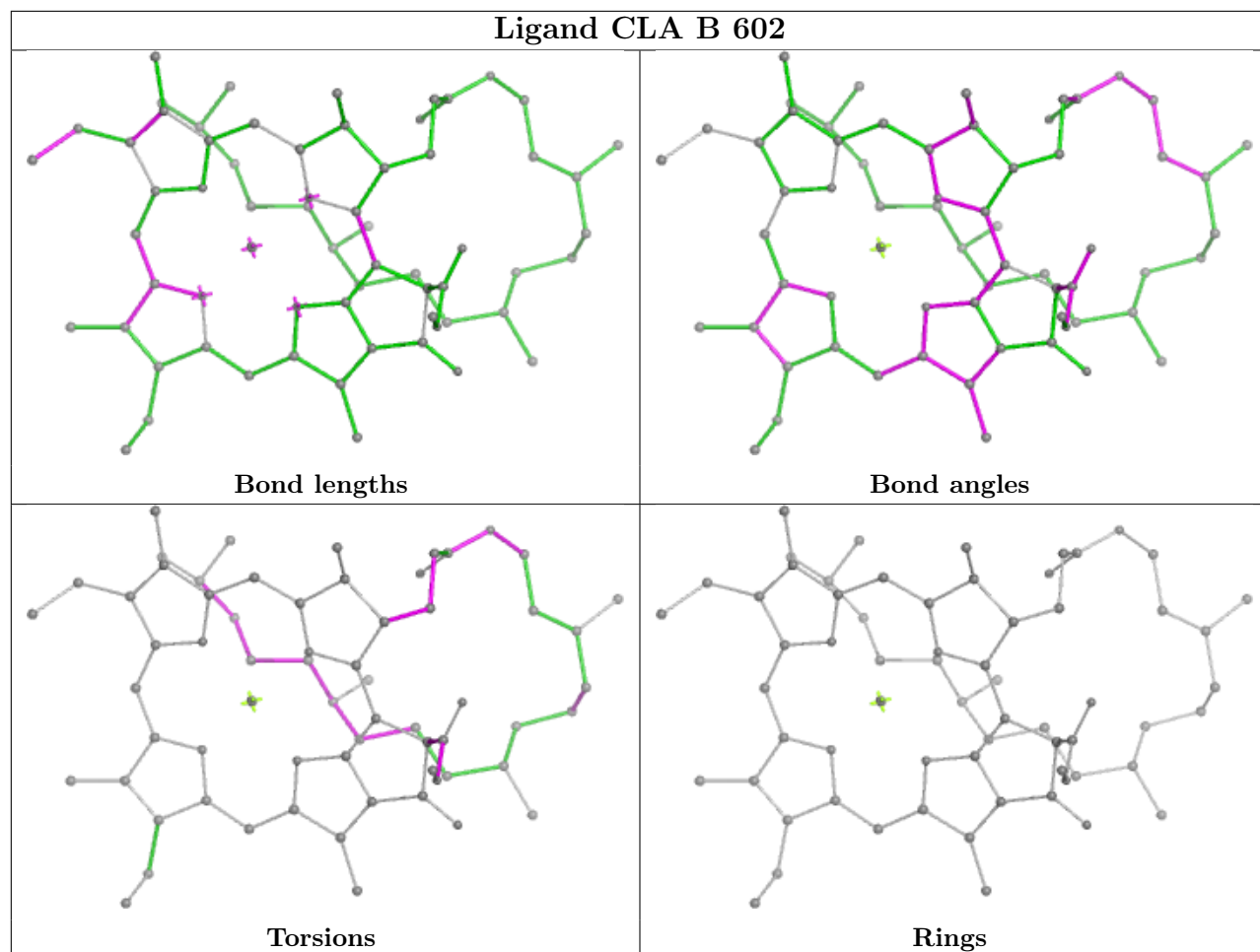




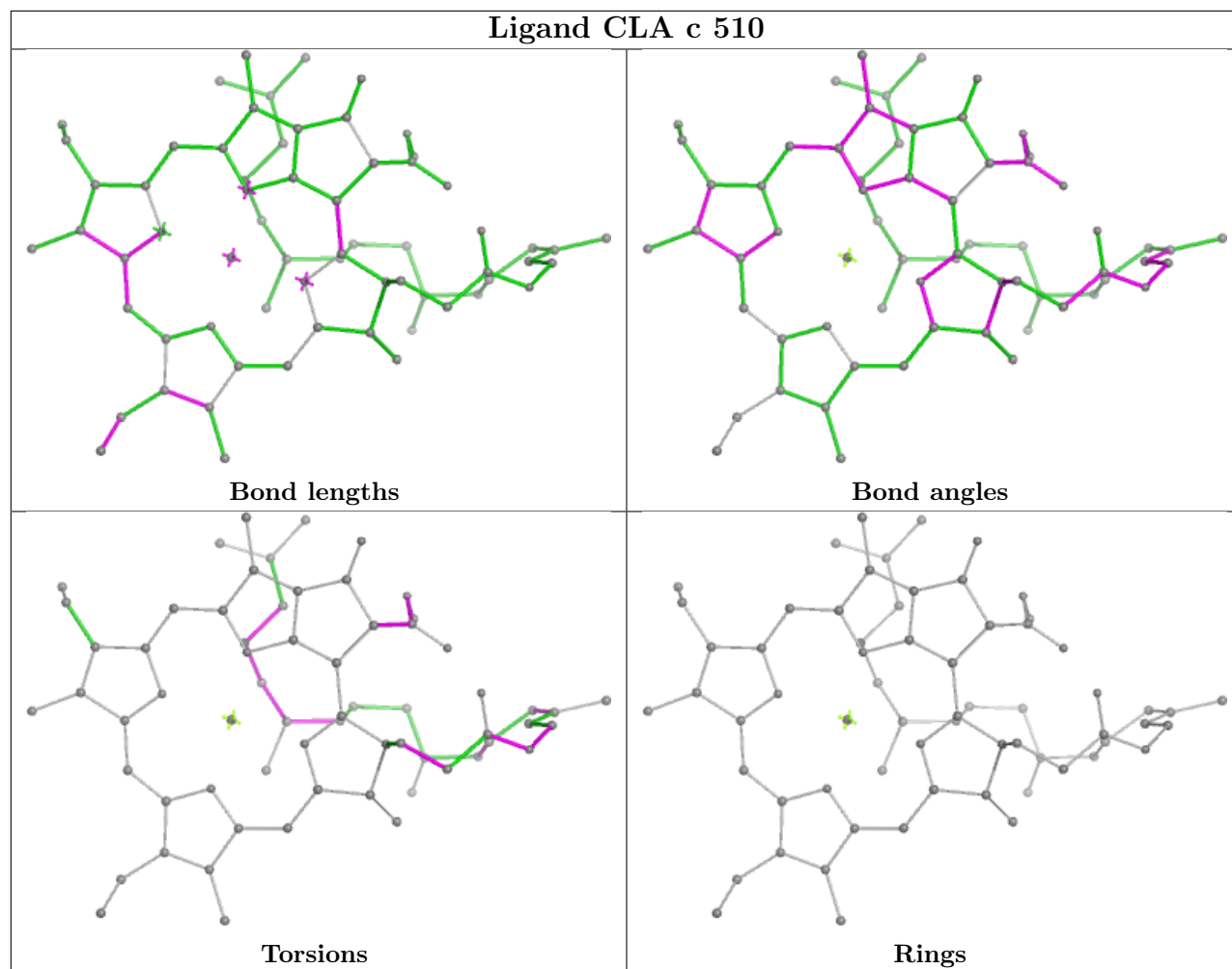


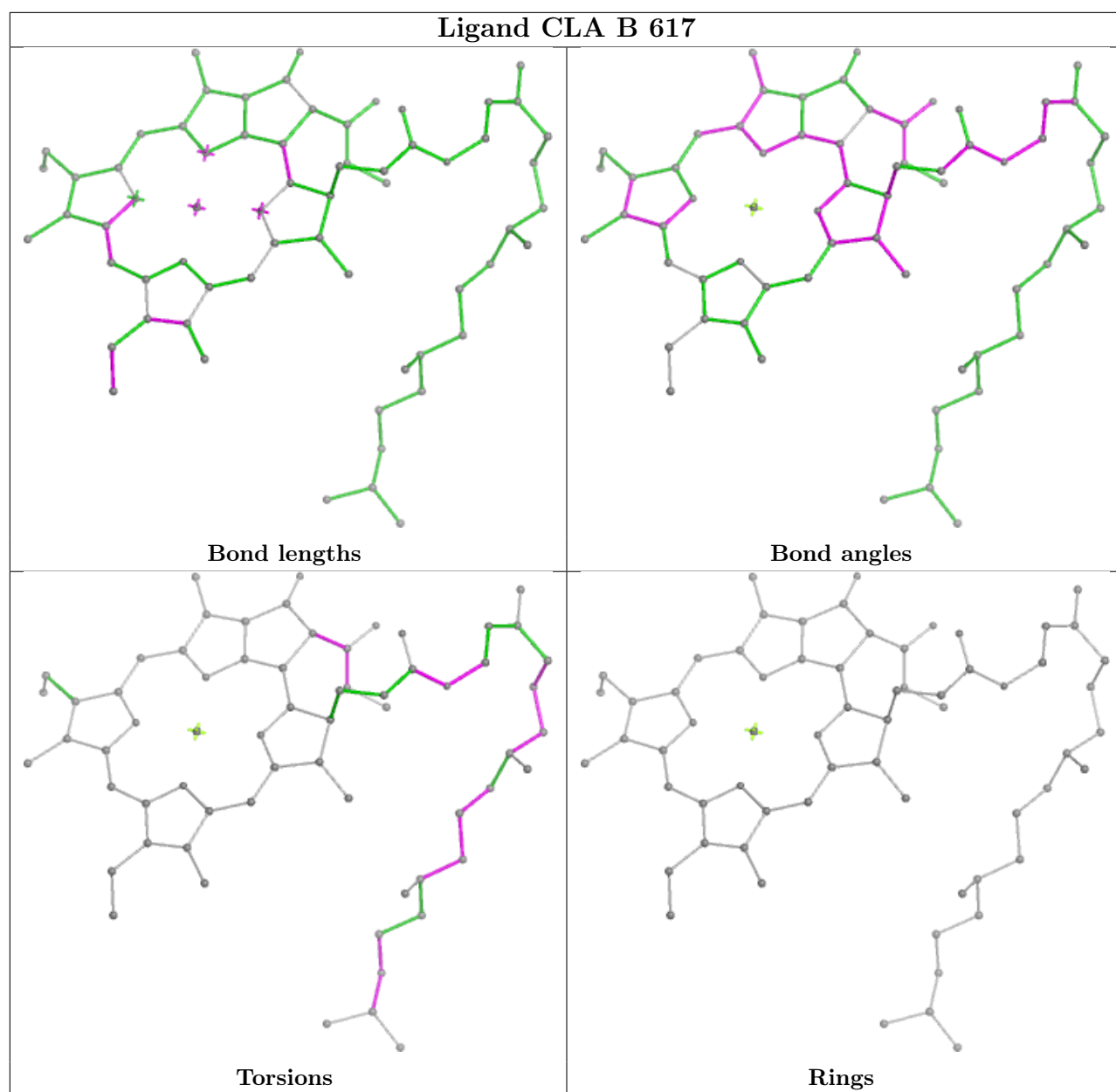


Ligand CLA B 602

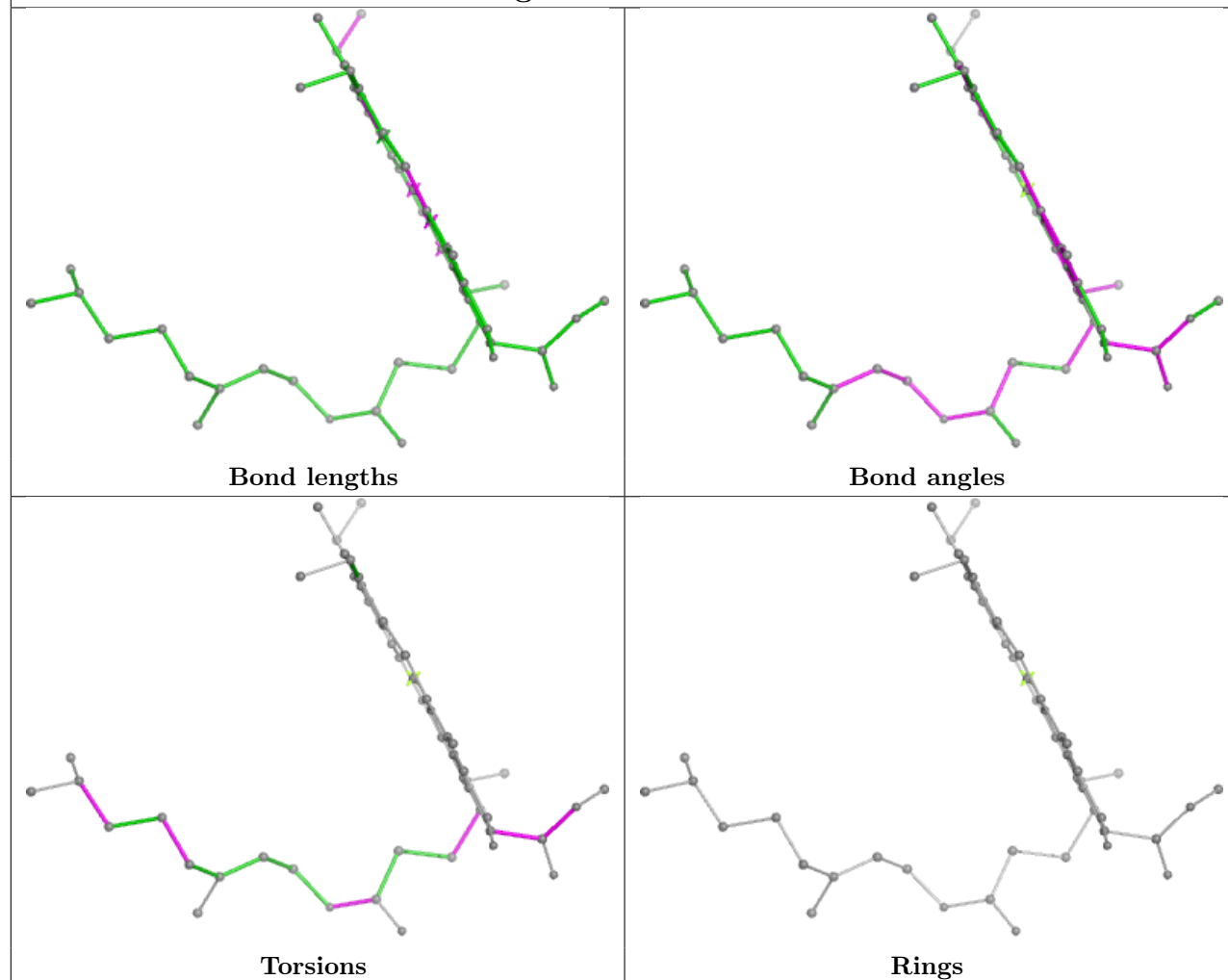


Ligand CLA c 510

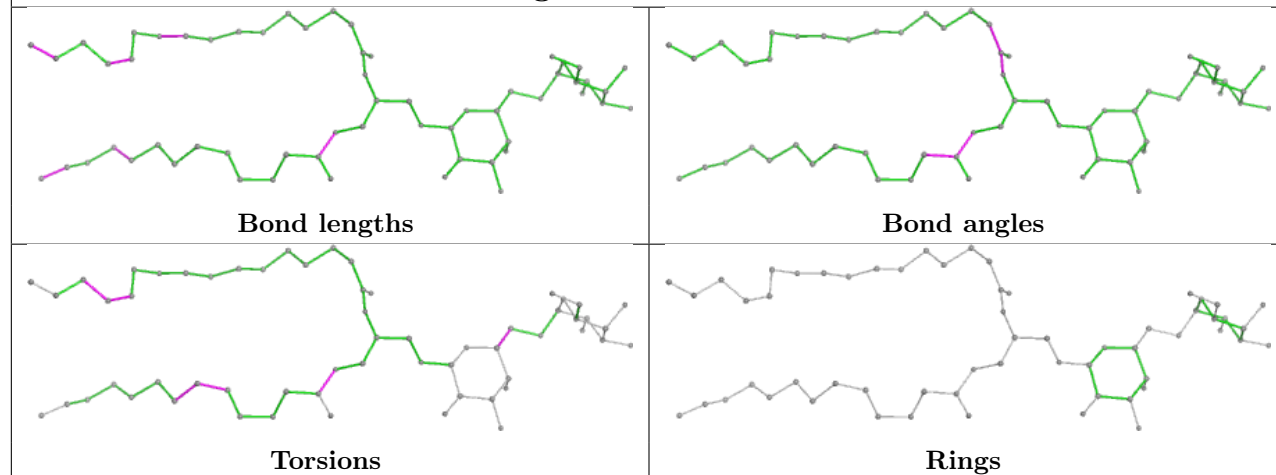


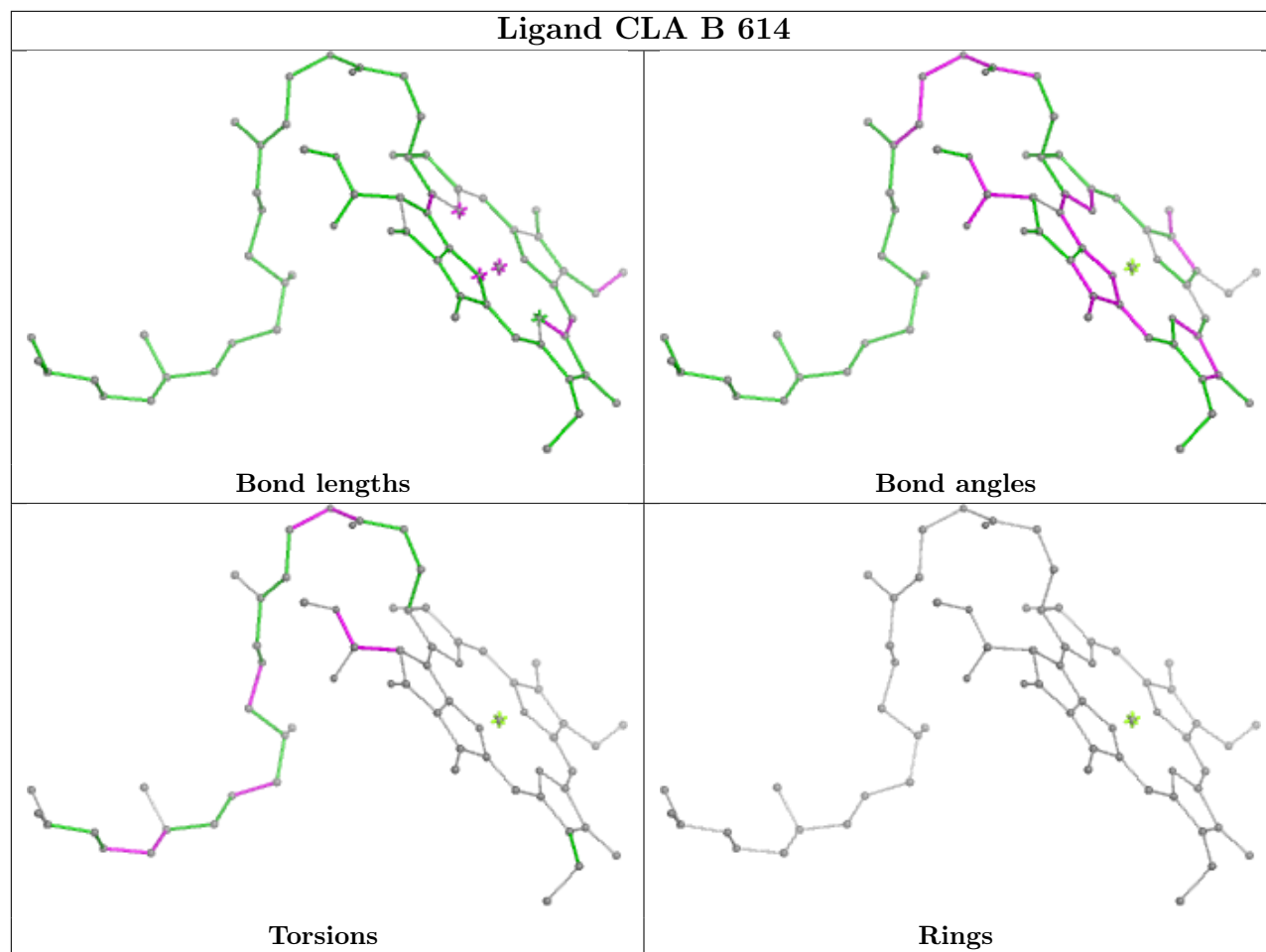


Ligand CLA S 604

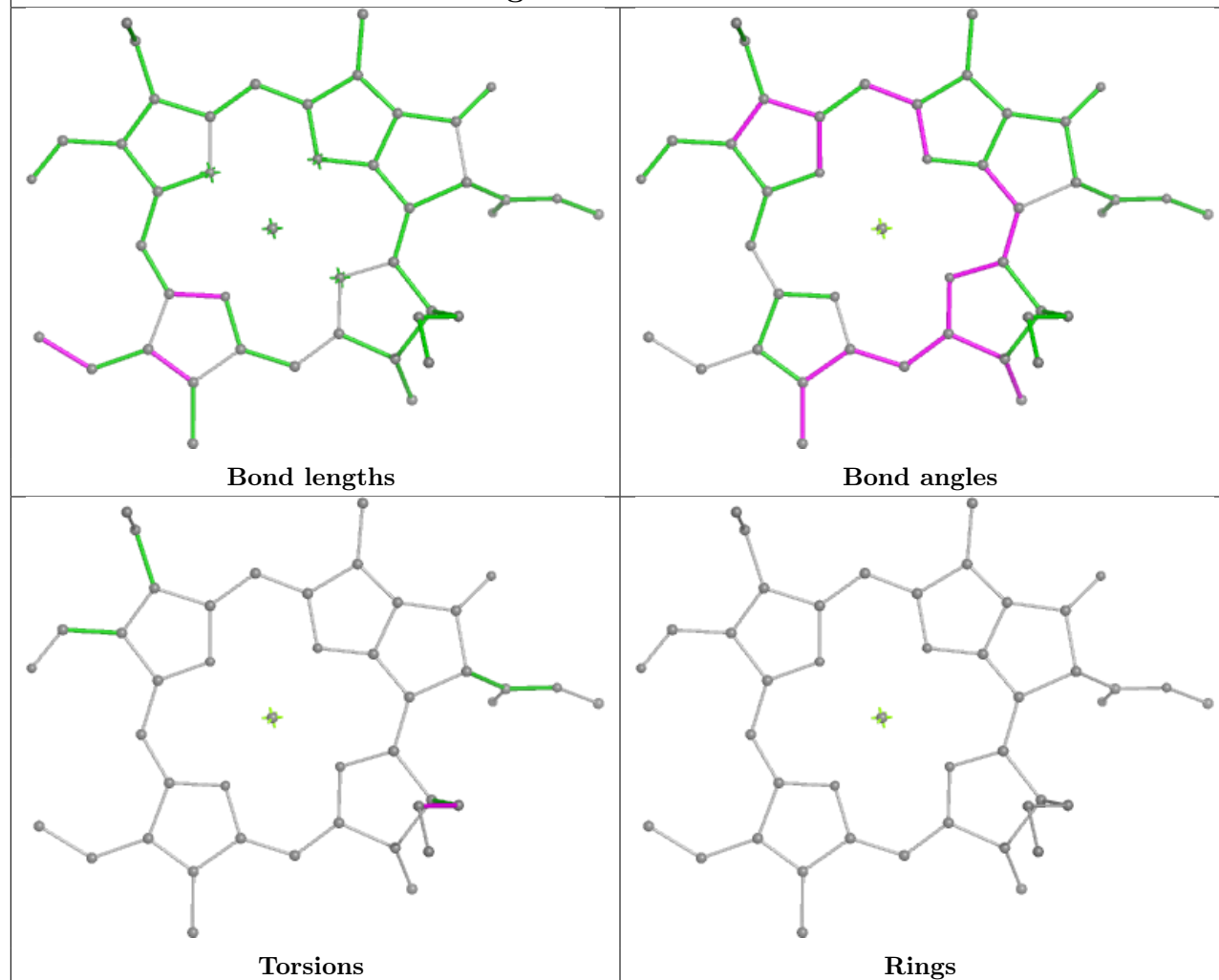


Ligand DGD c 520

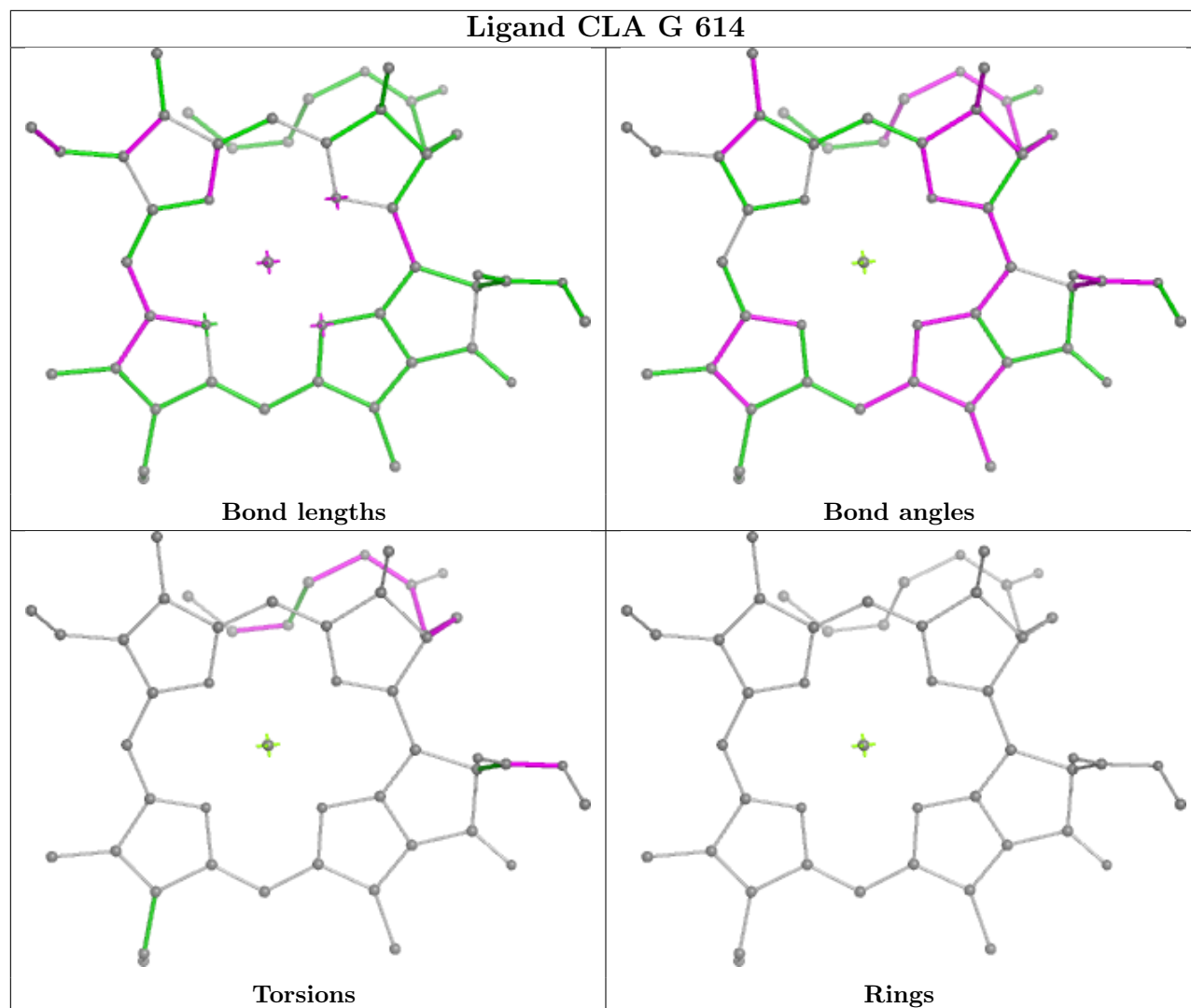




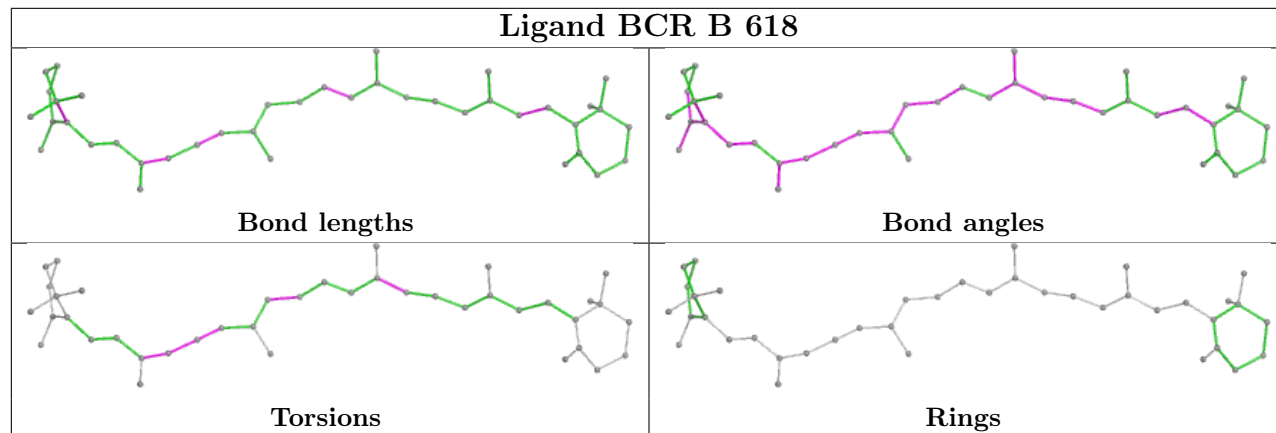
Ligand CHL G 608

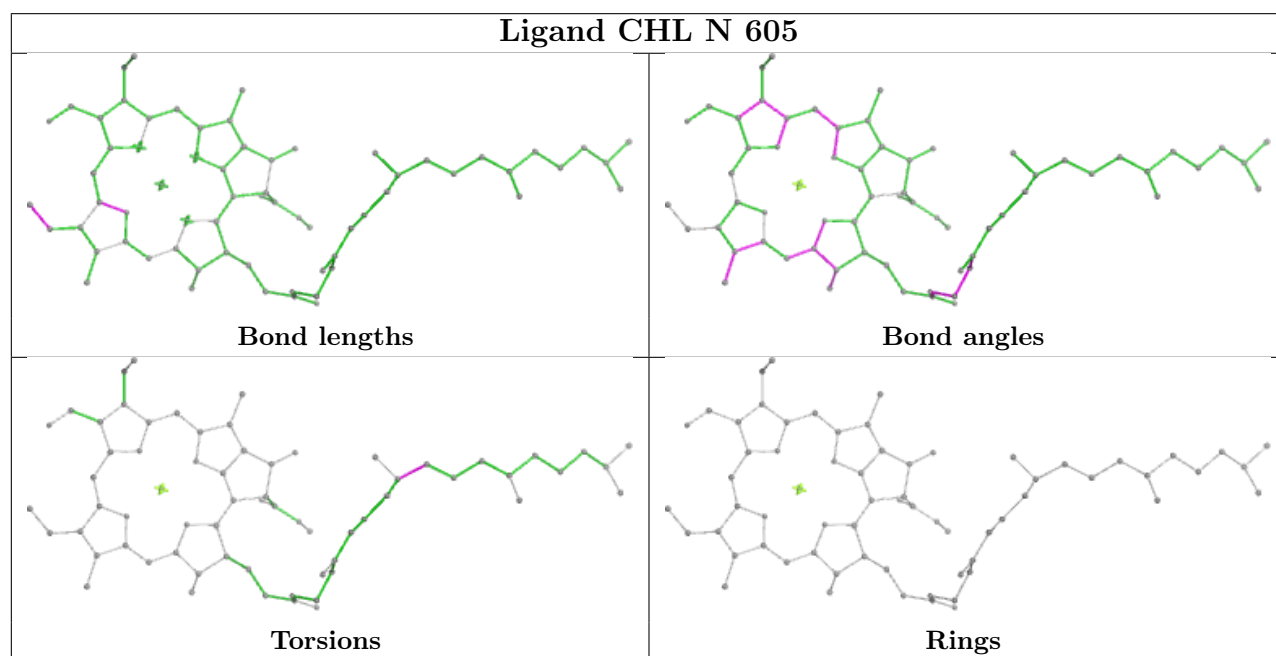
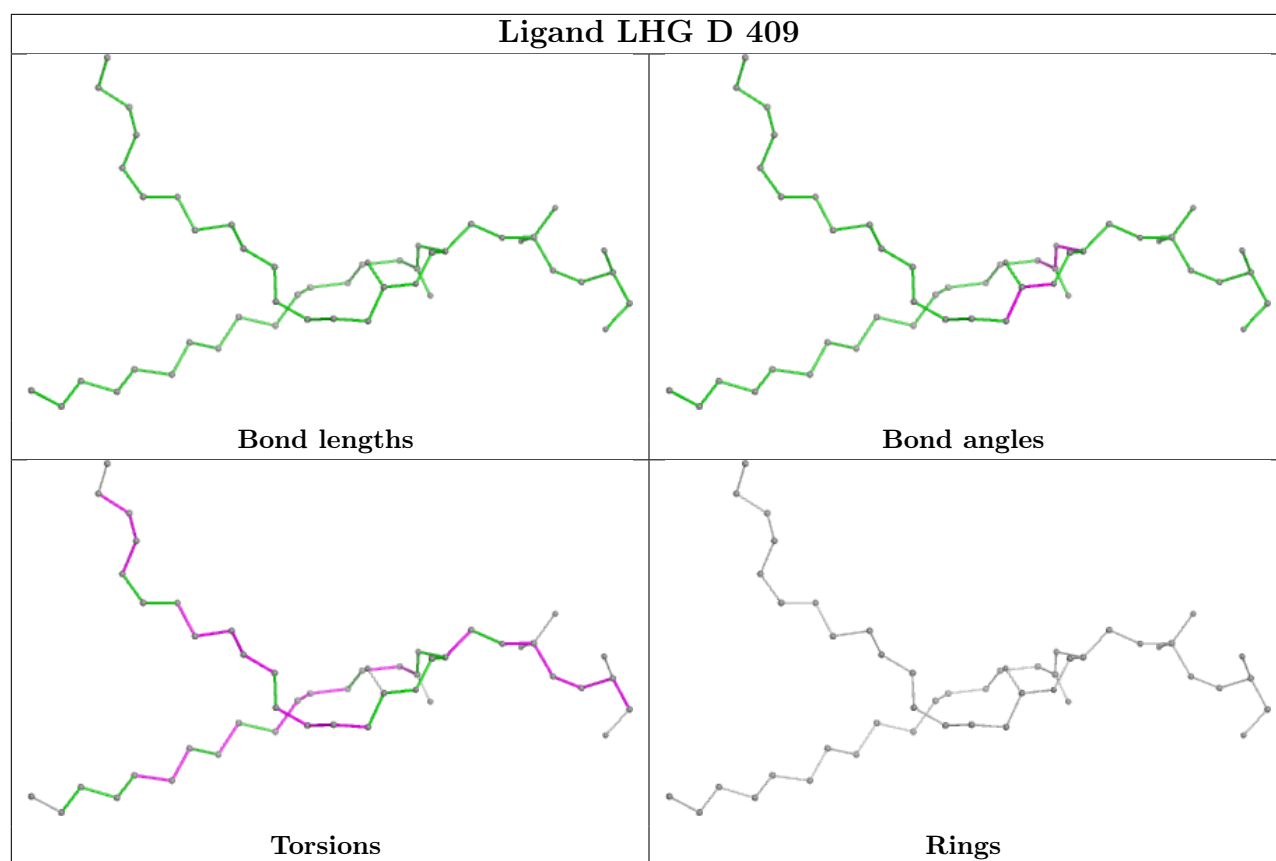


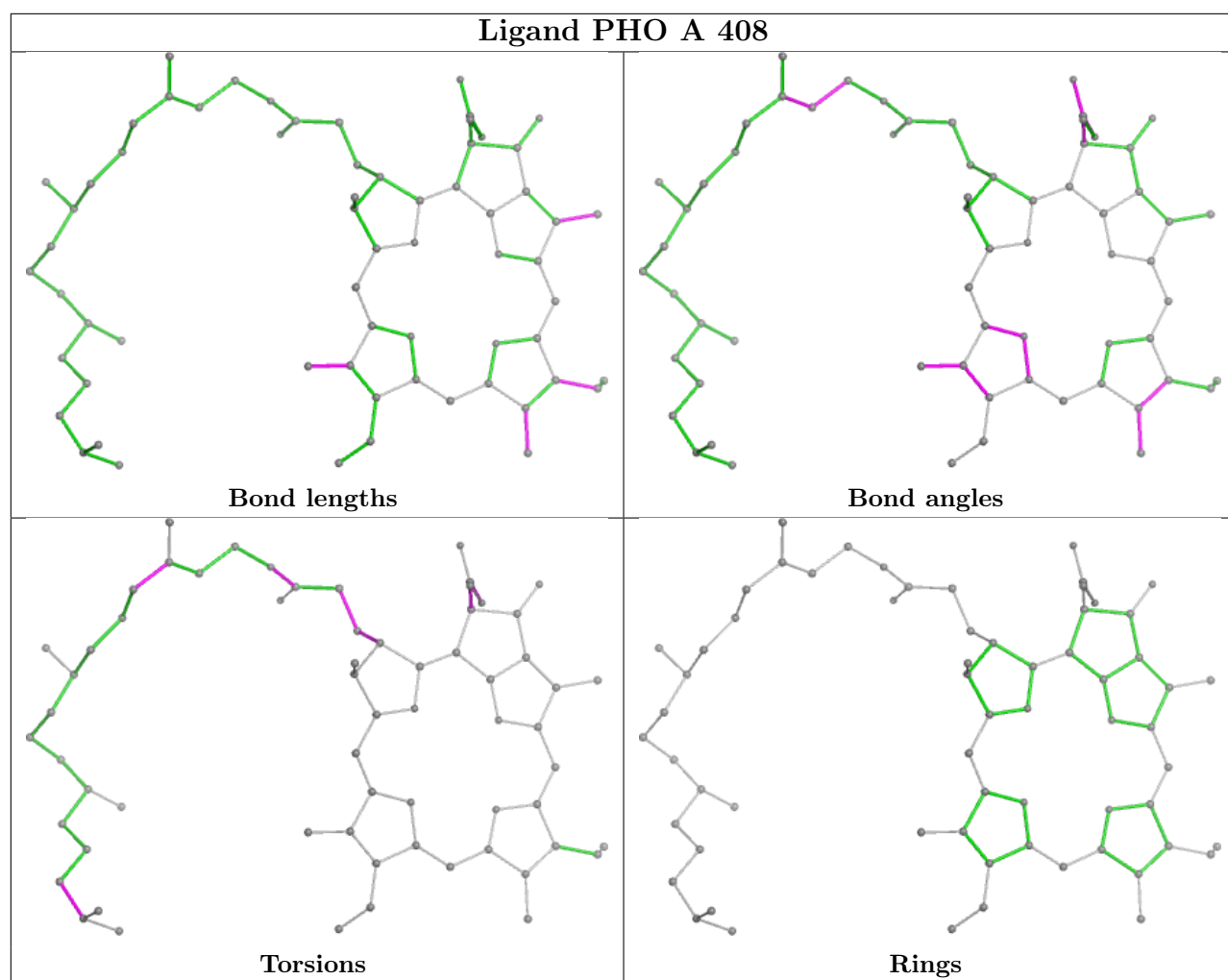
Ligand CLA G 614

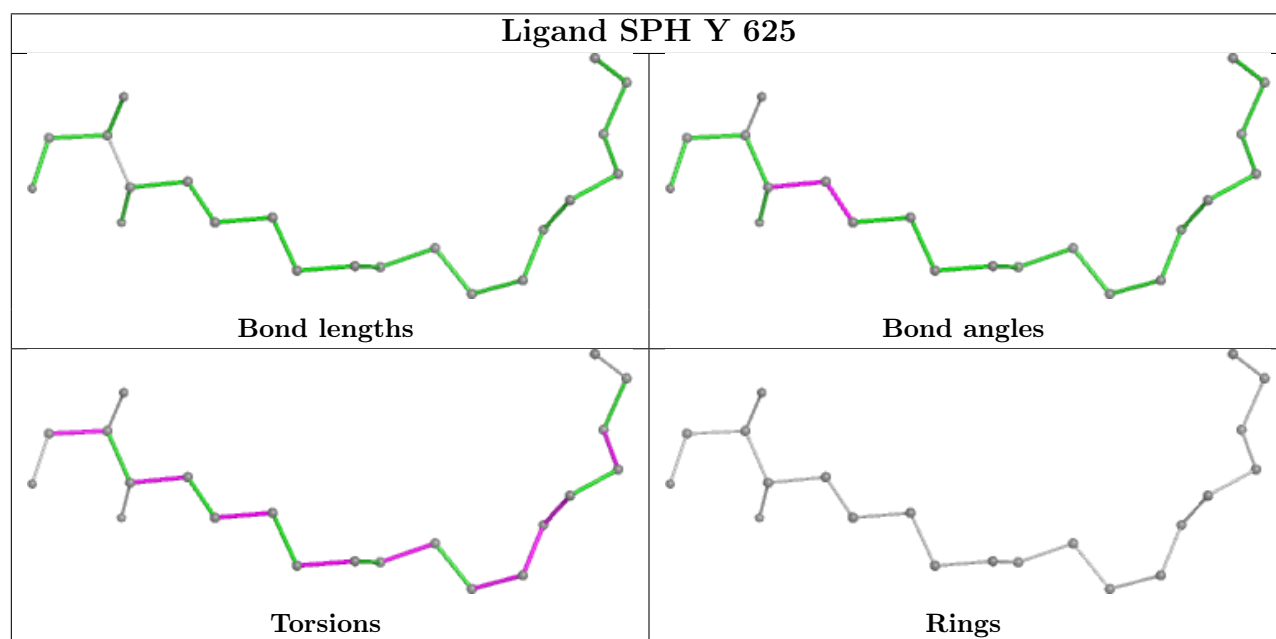
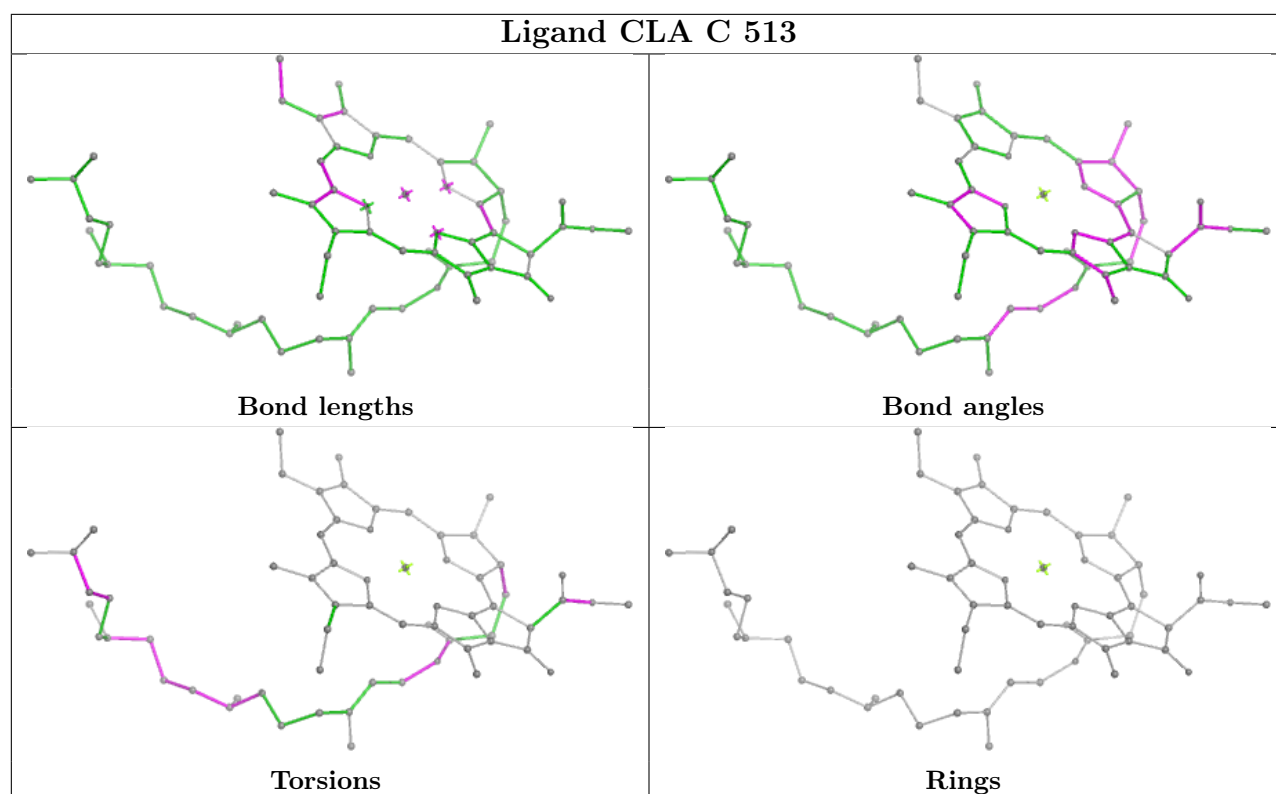


Ligand BCR B 618

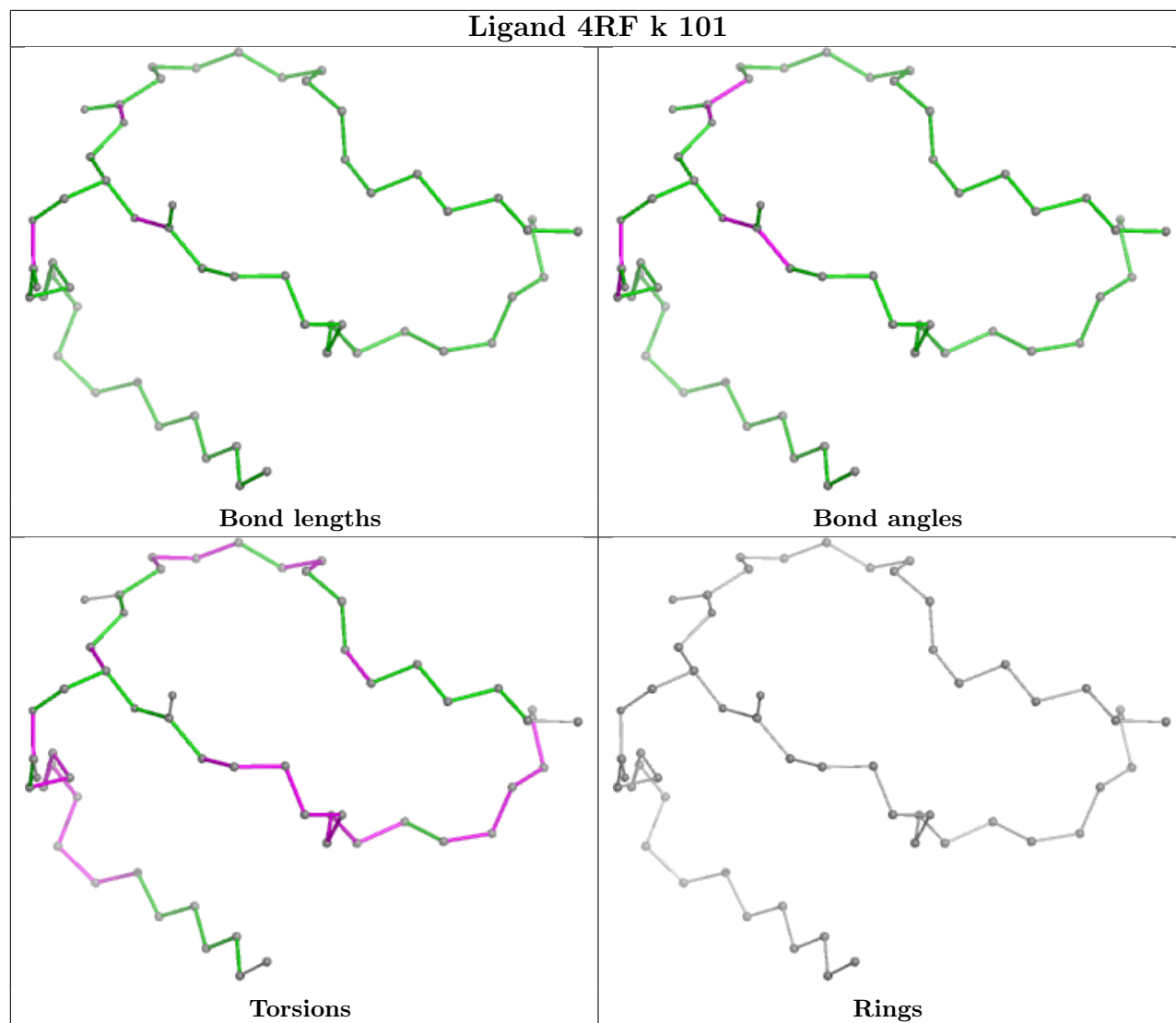


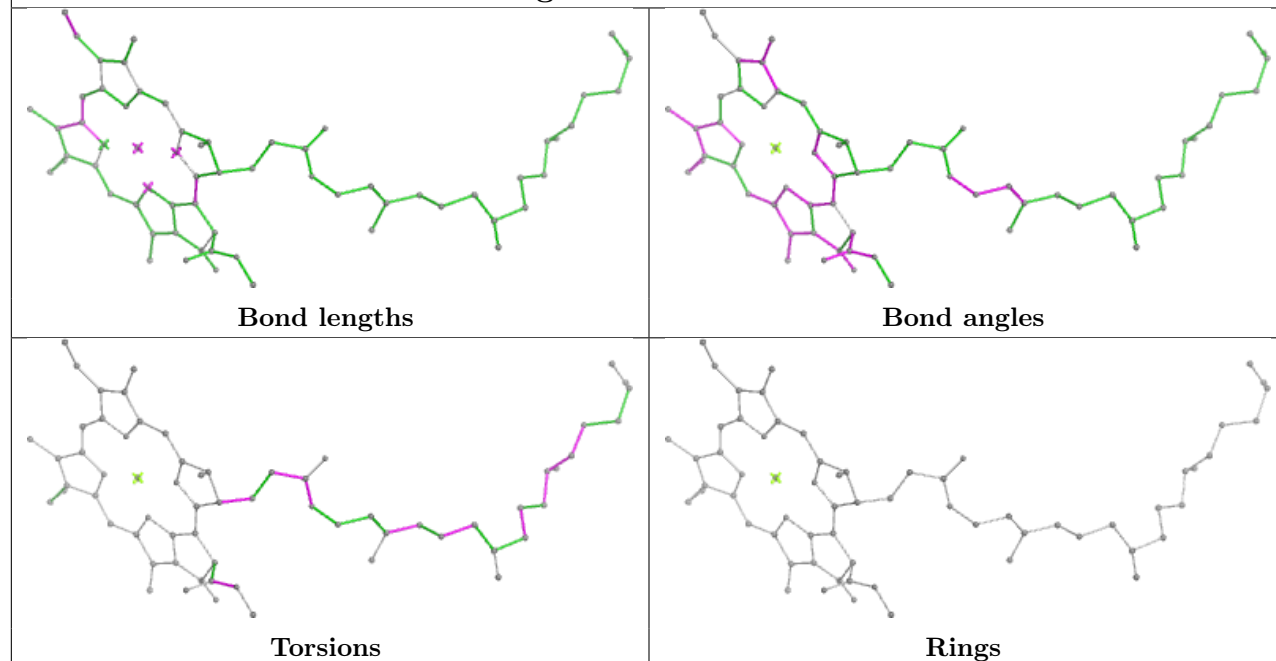
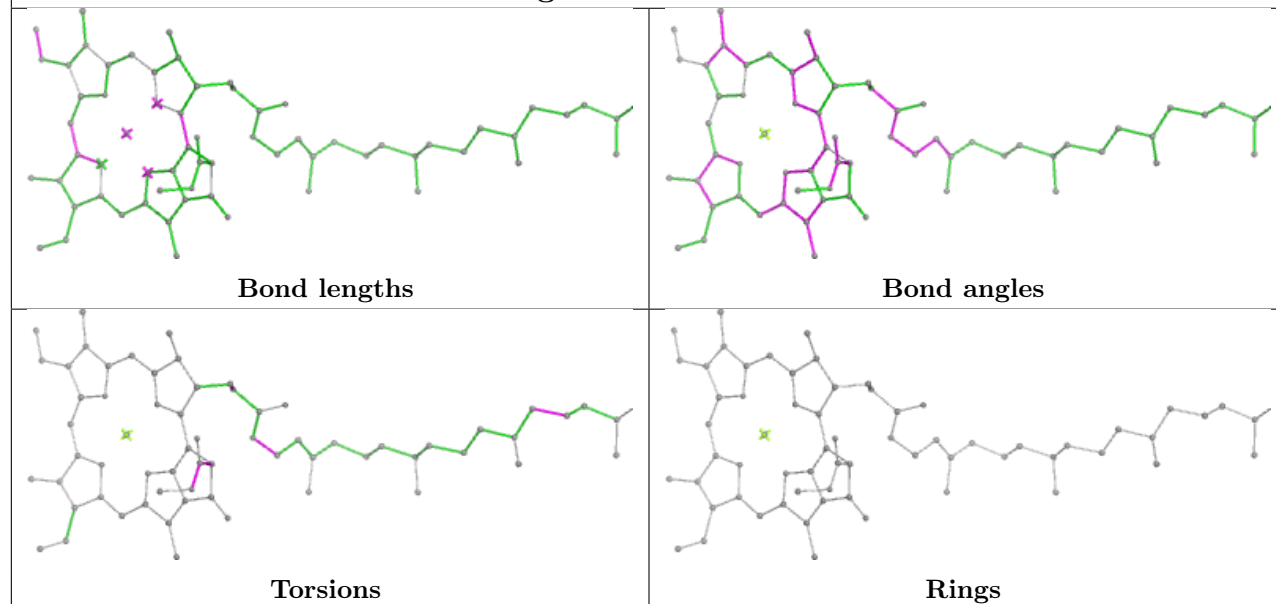


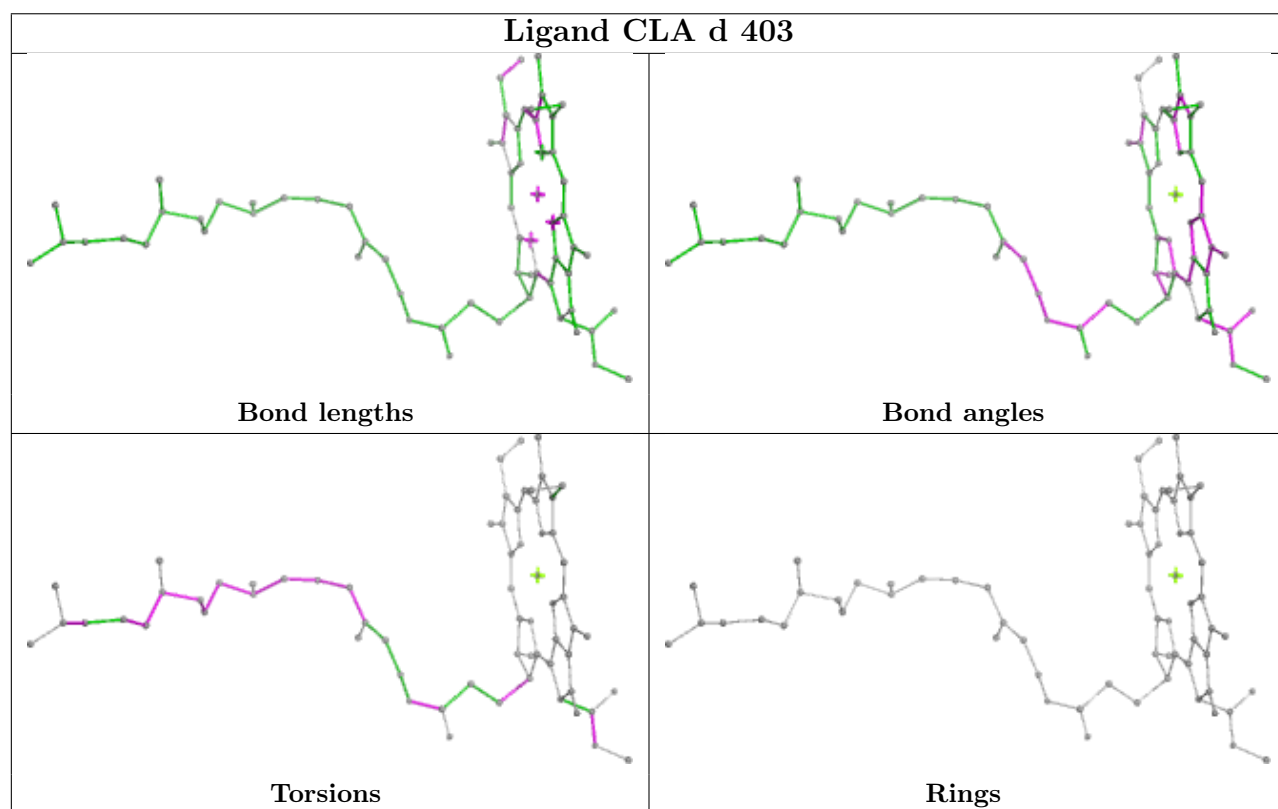
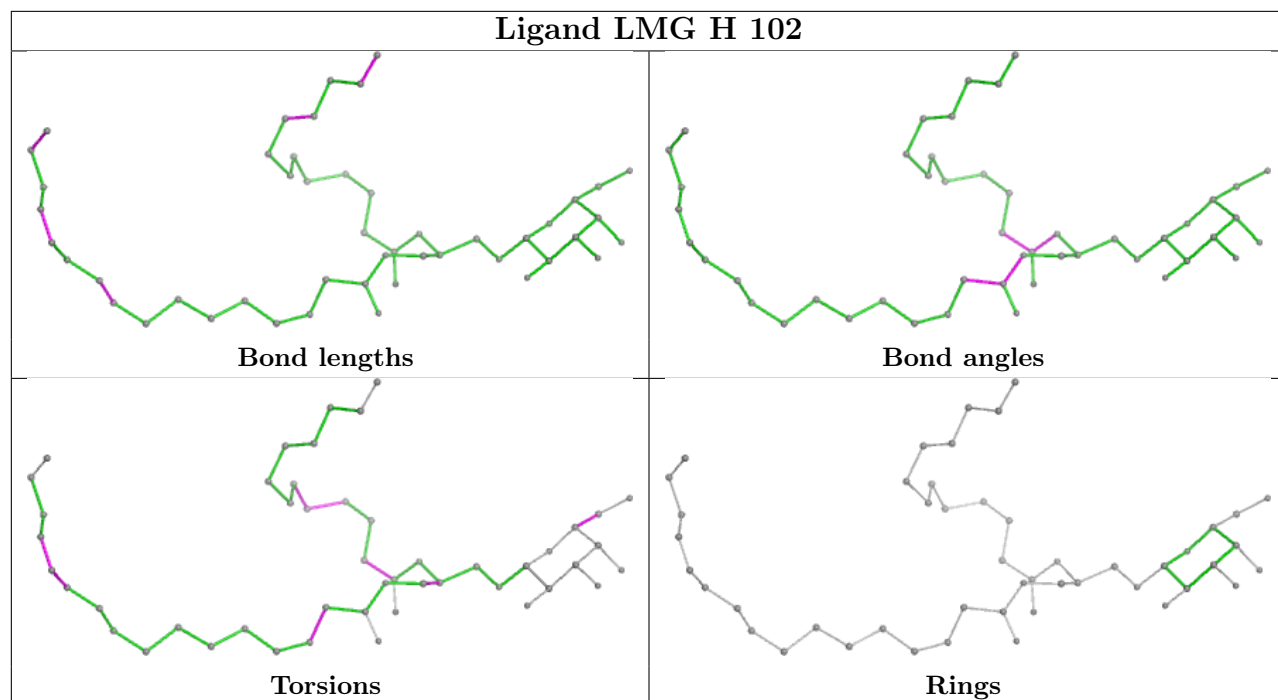


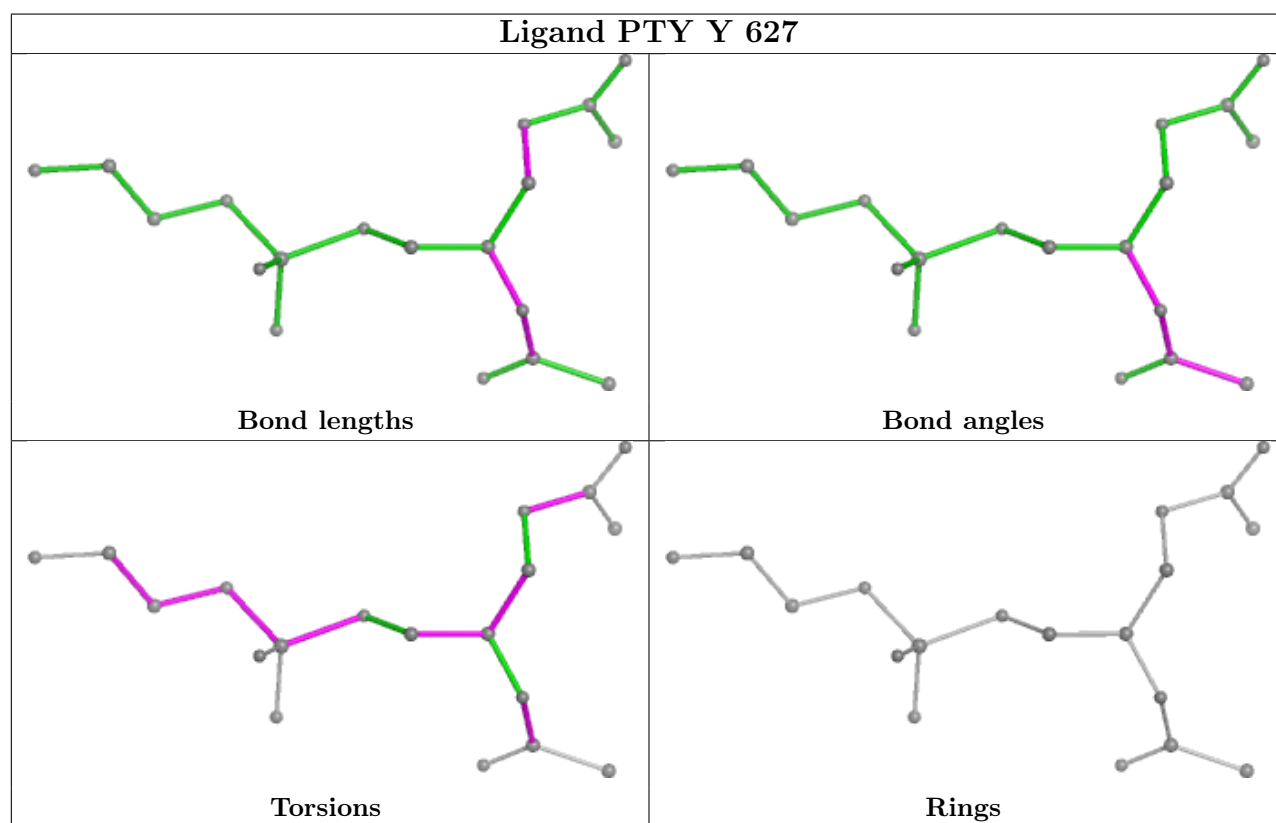
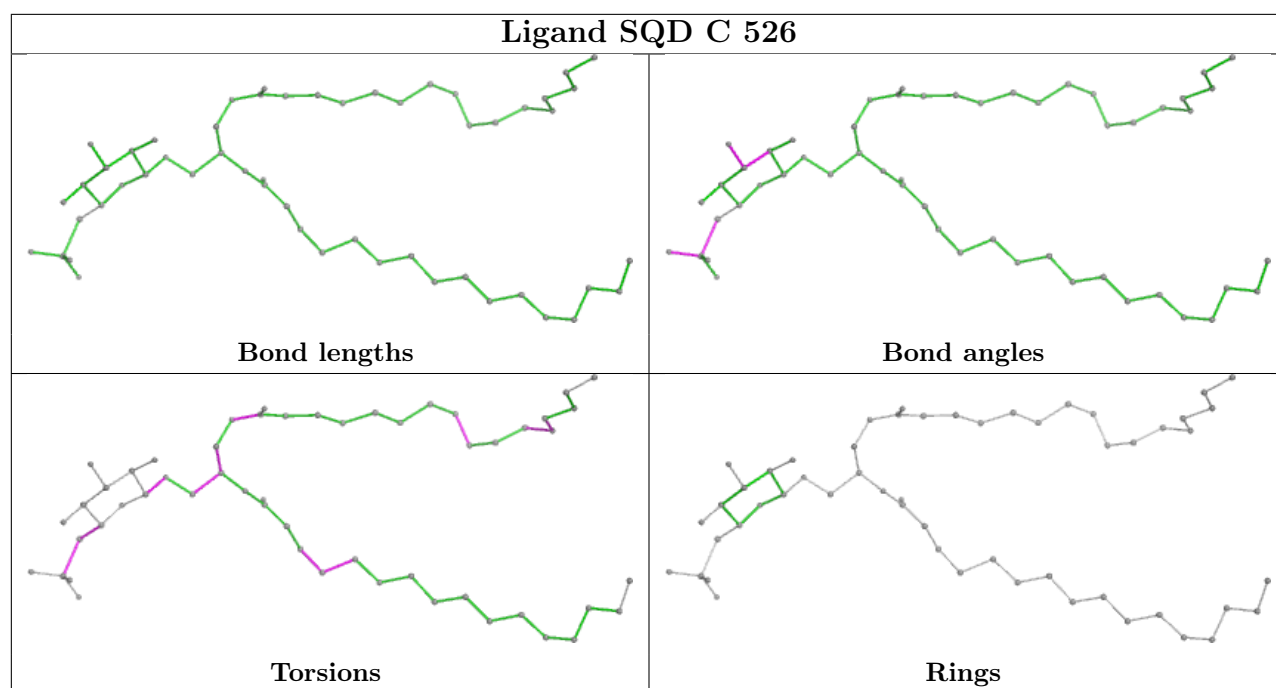


Ligand 4RF k 101

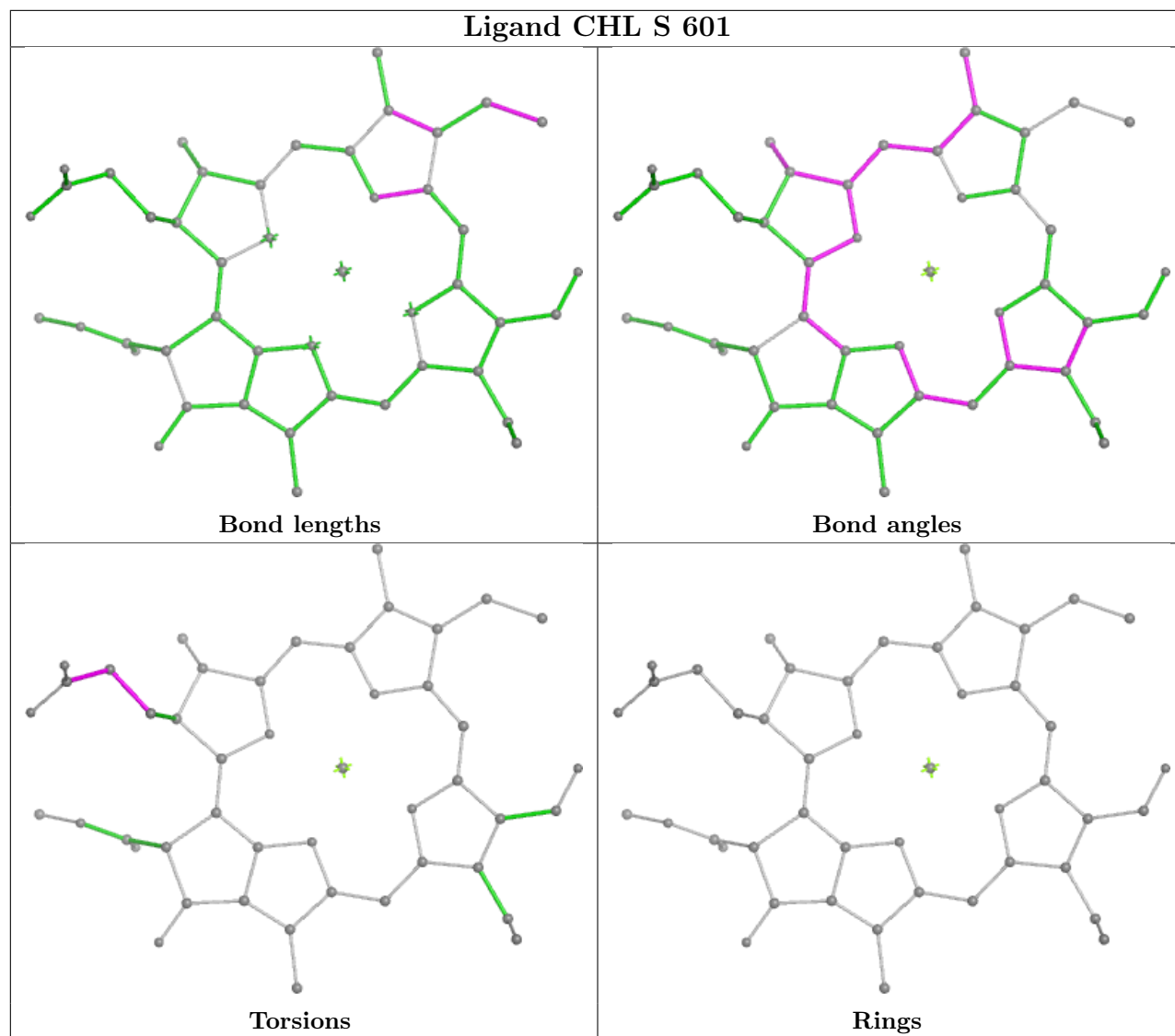


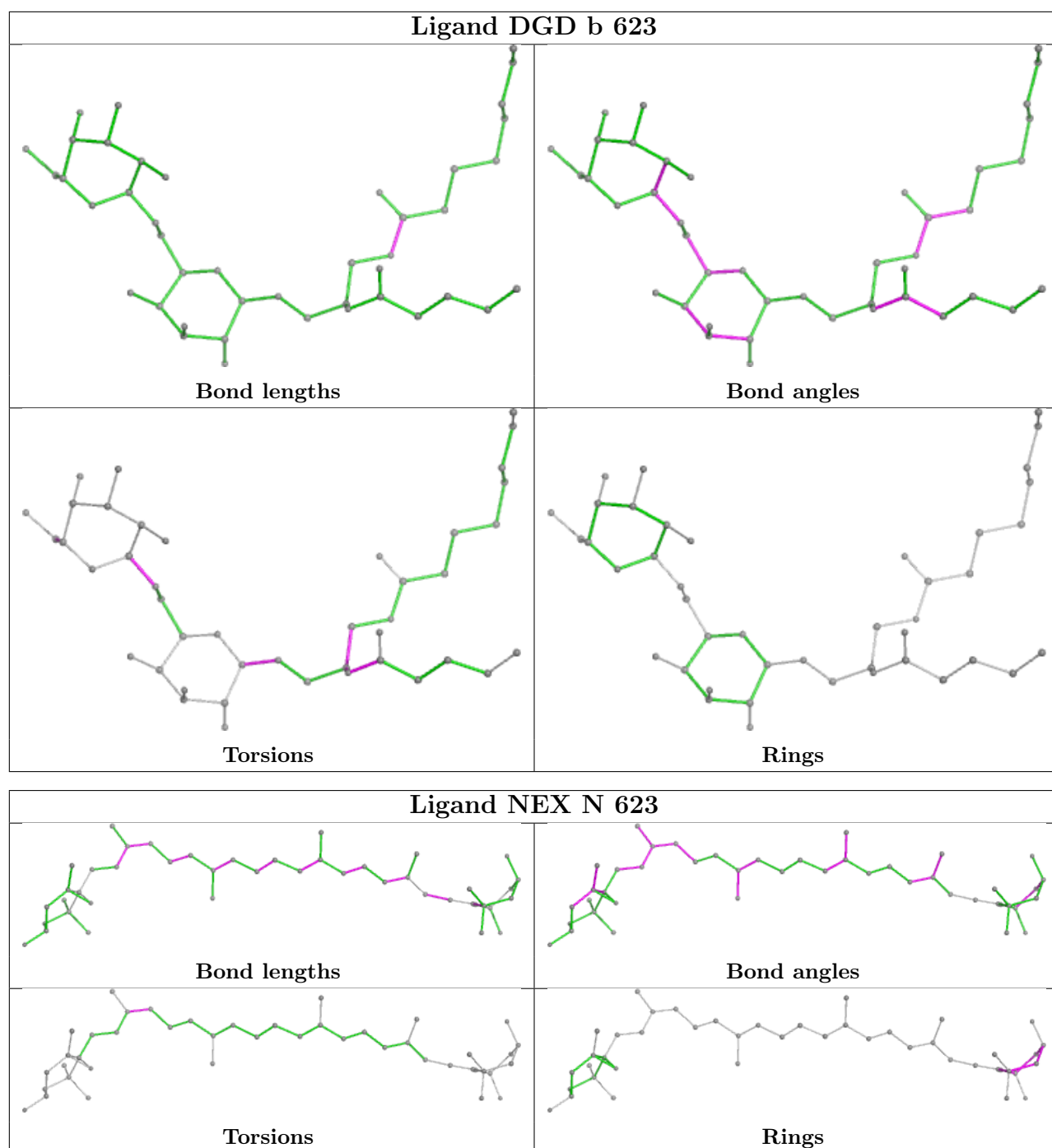
Ligand CLA a 405**Ligand CLA c 502**

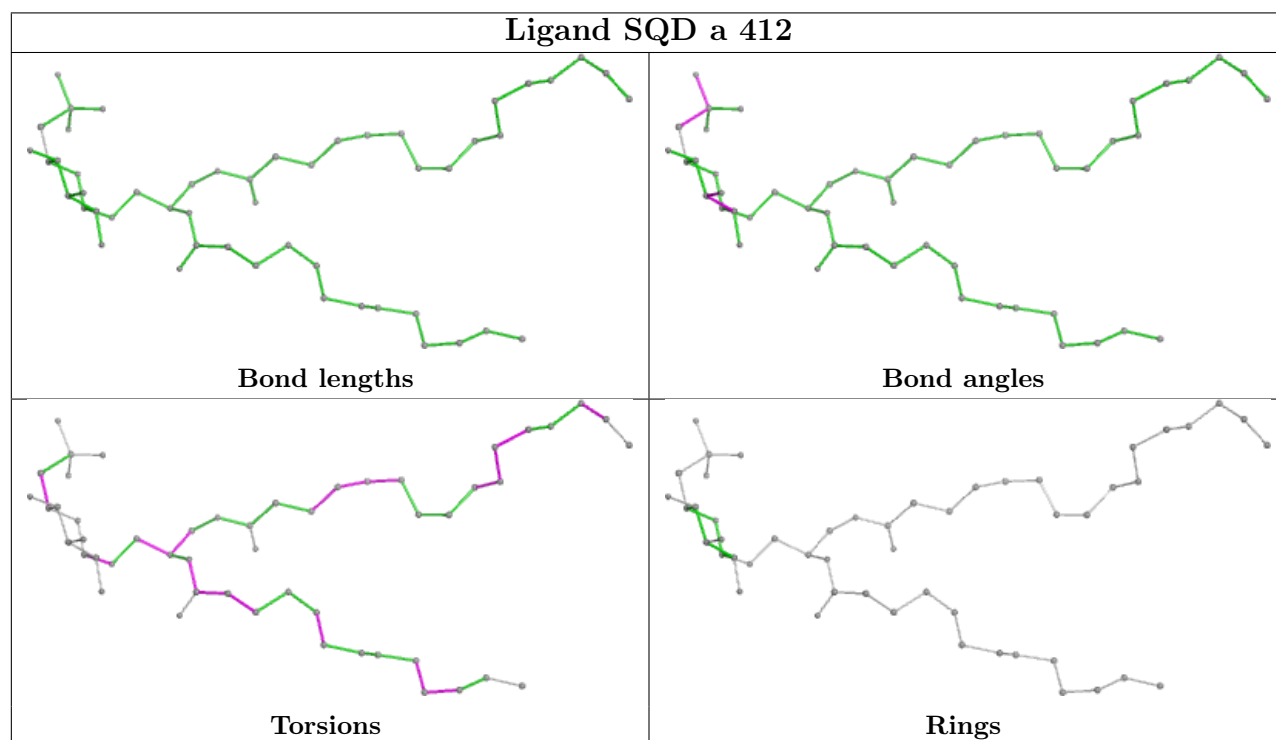
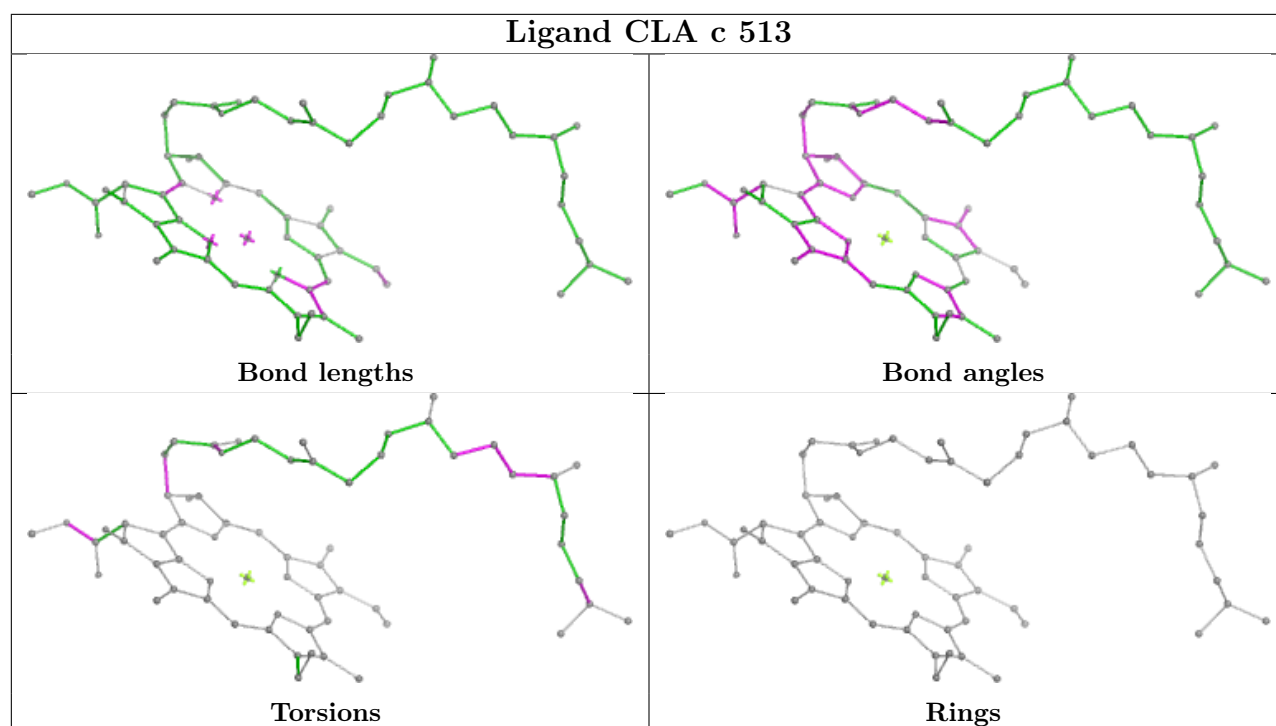




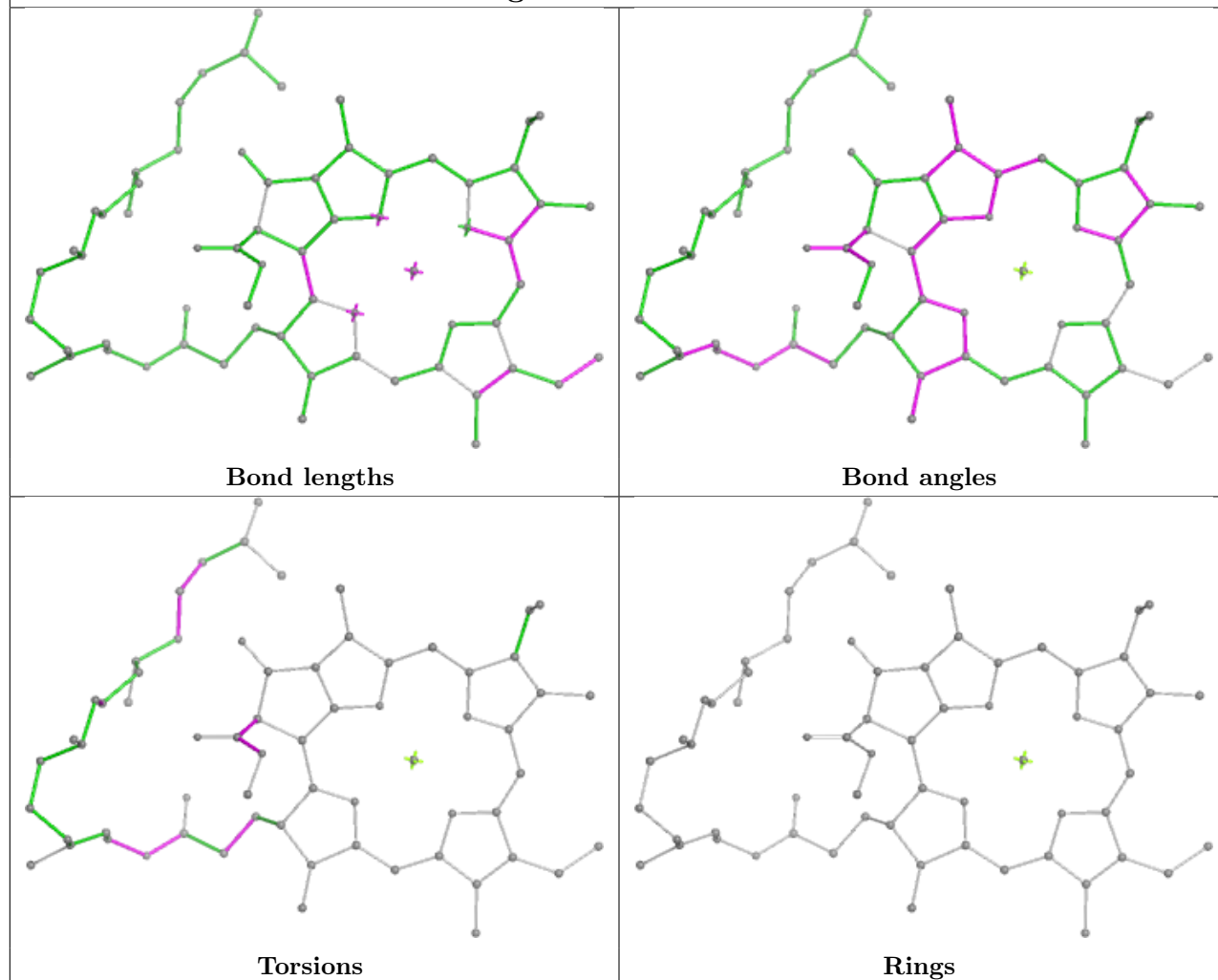
Ligand CHL S 601



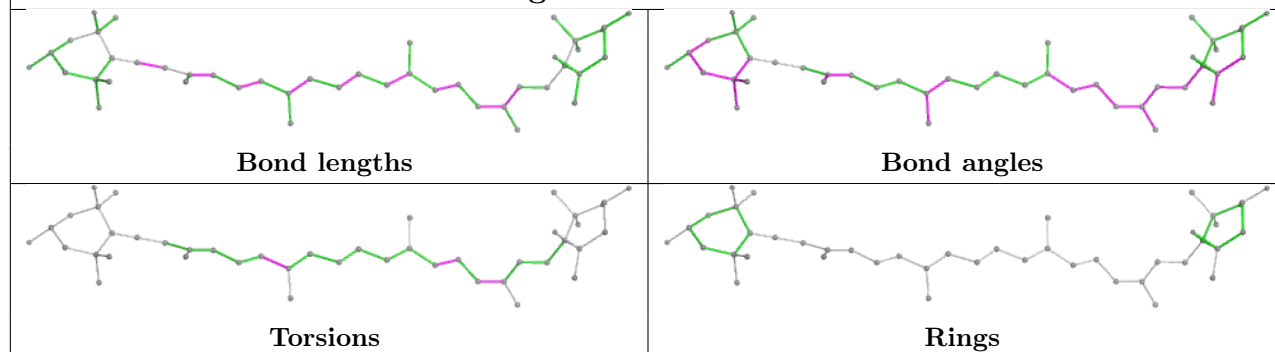


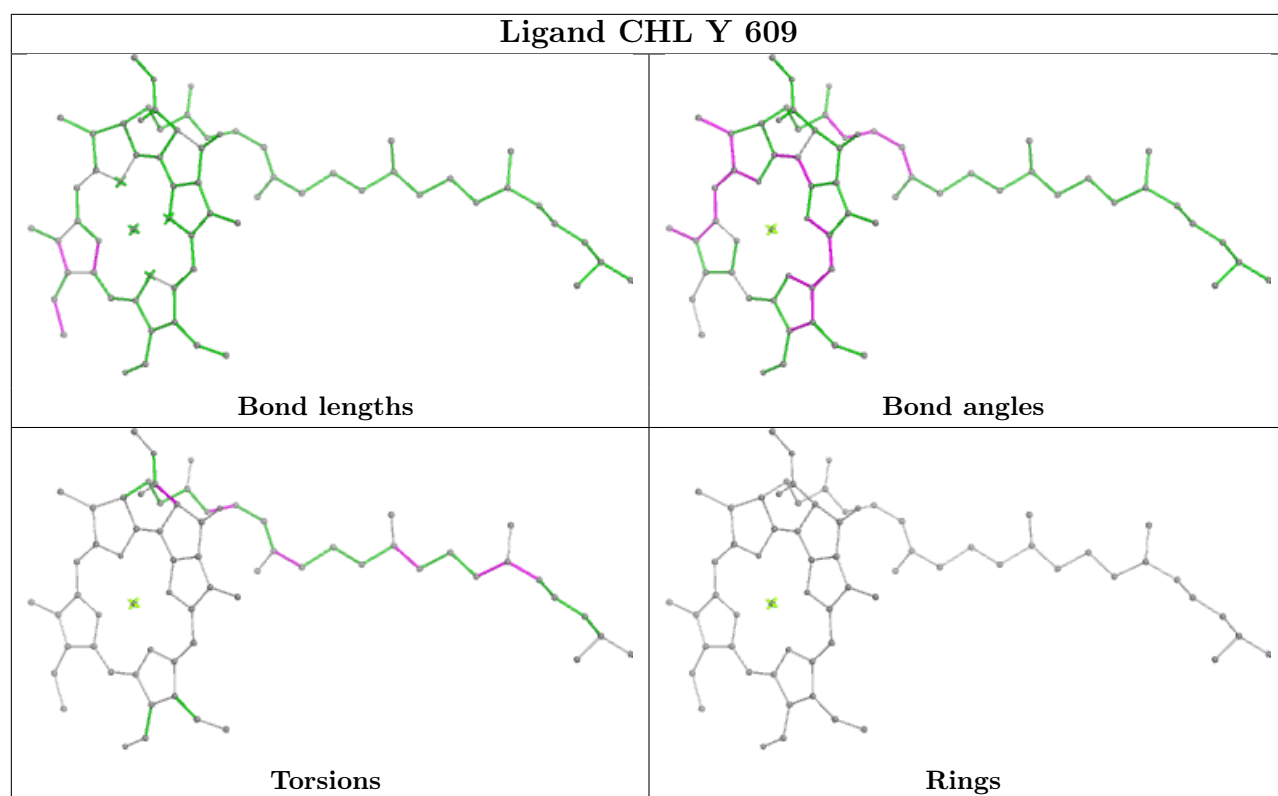


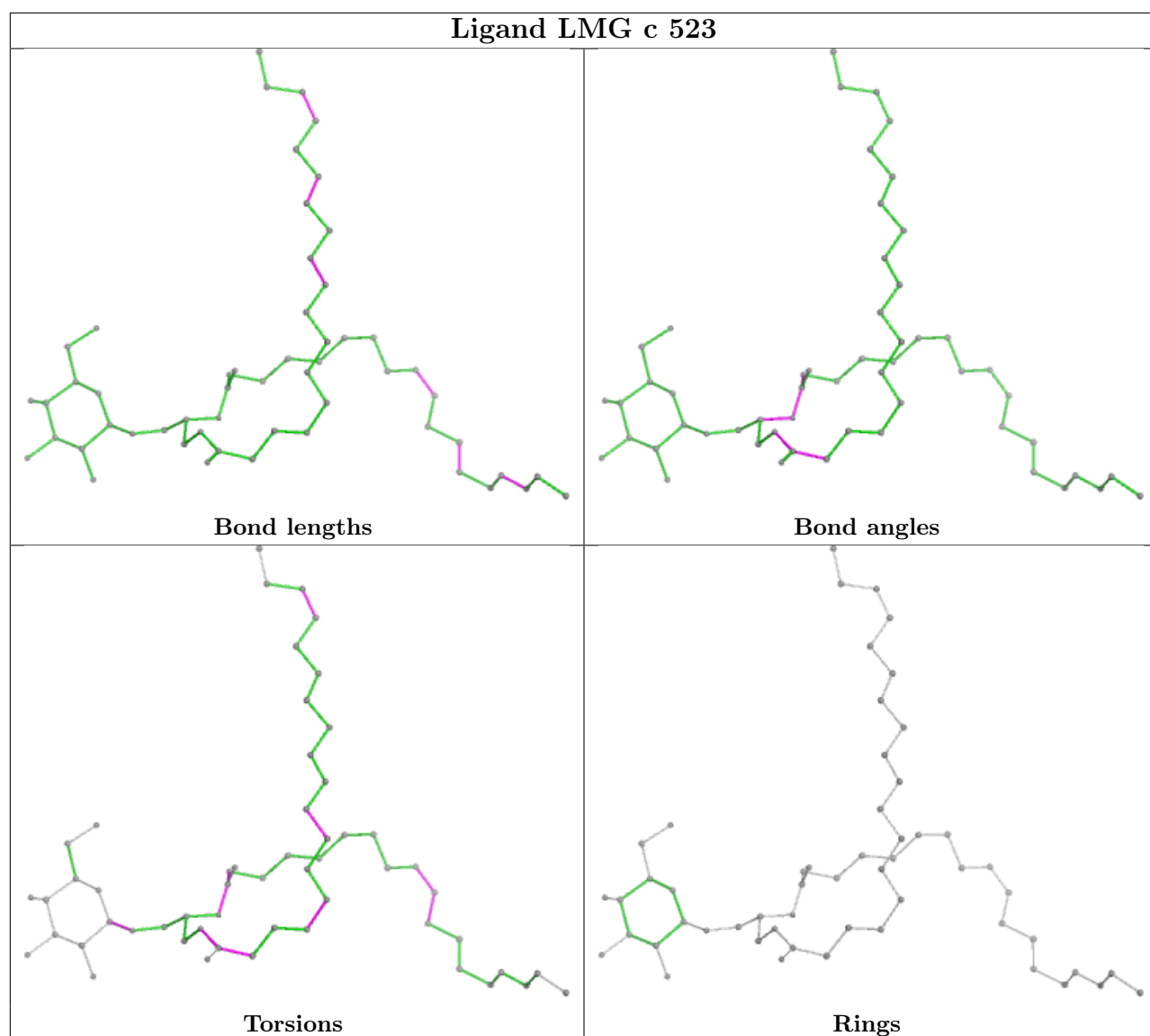
Ligand CLA B 611

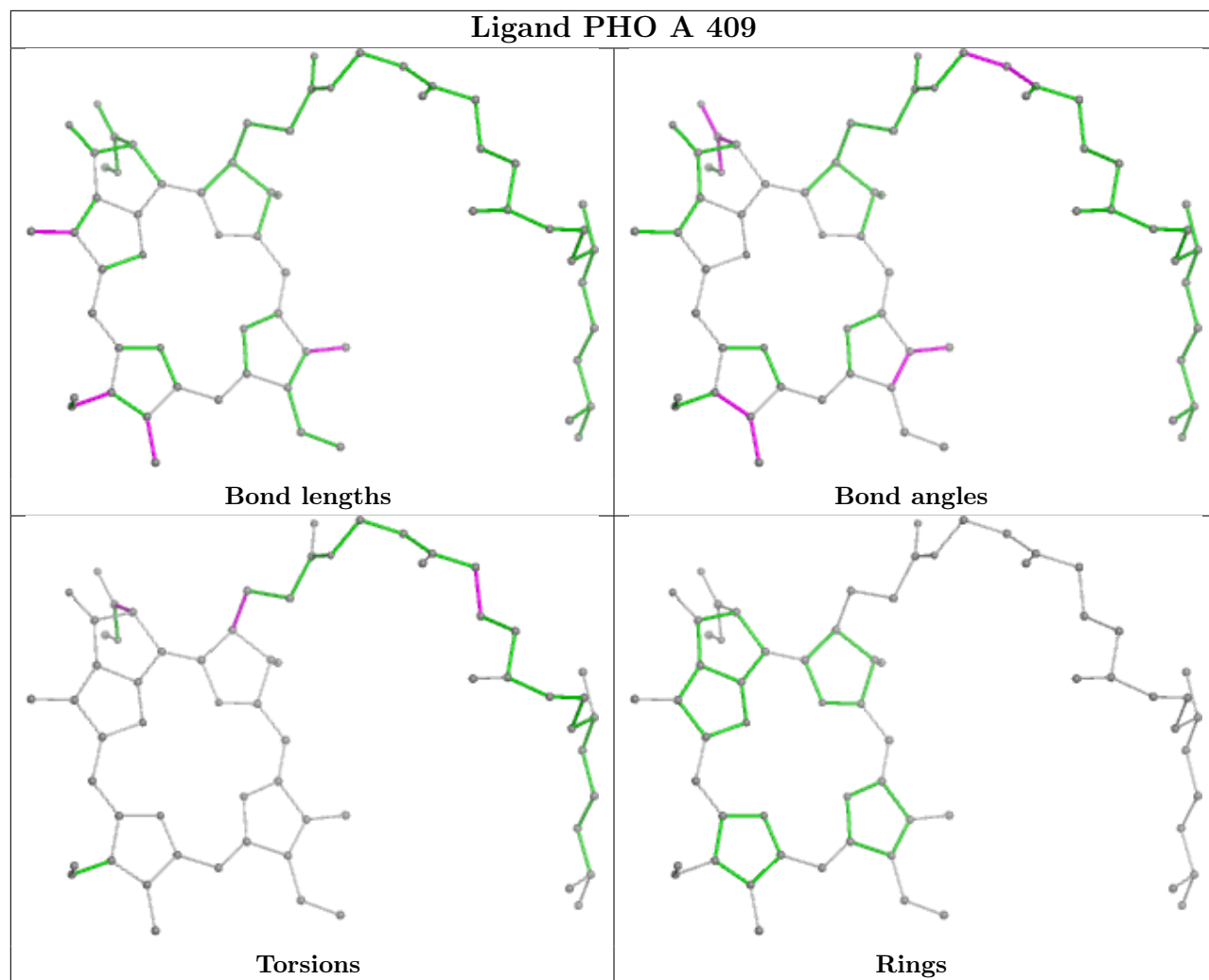


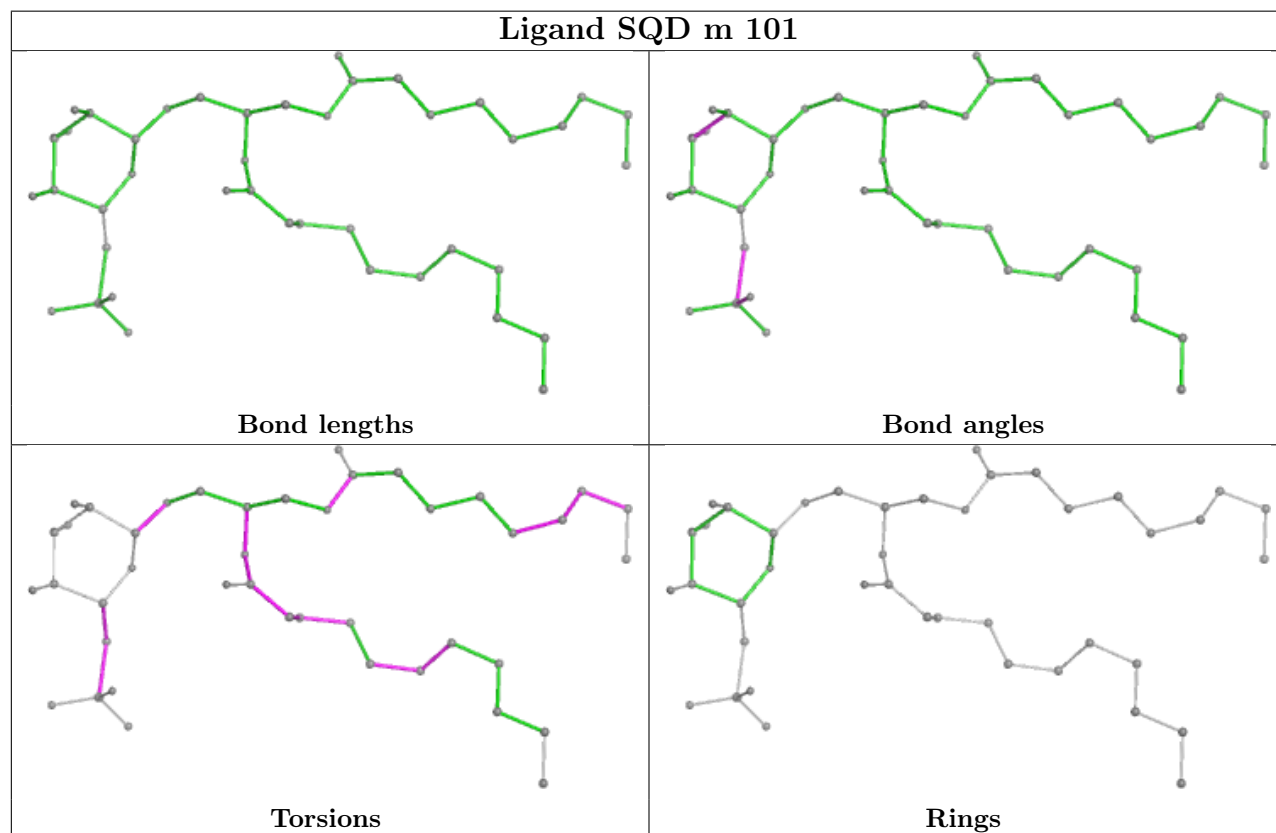
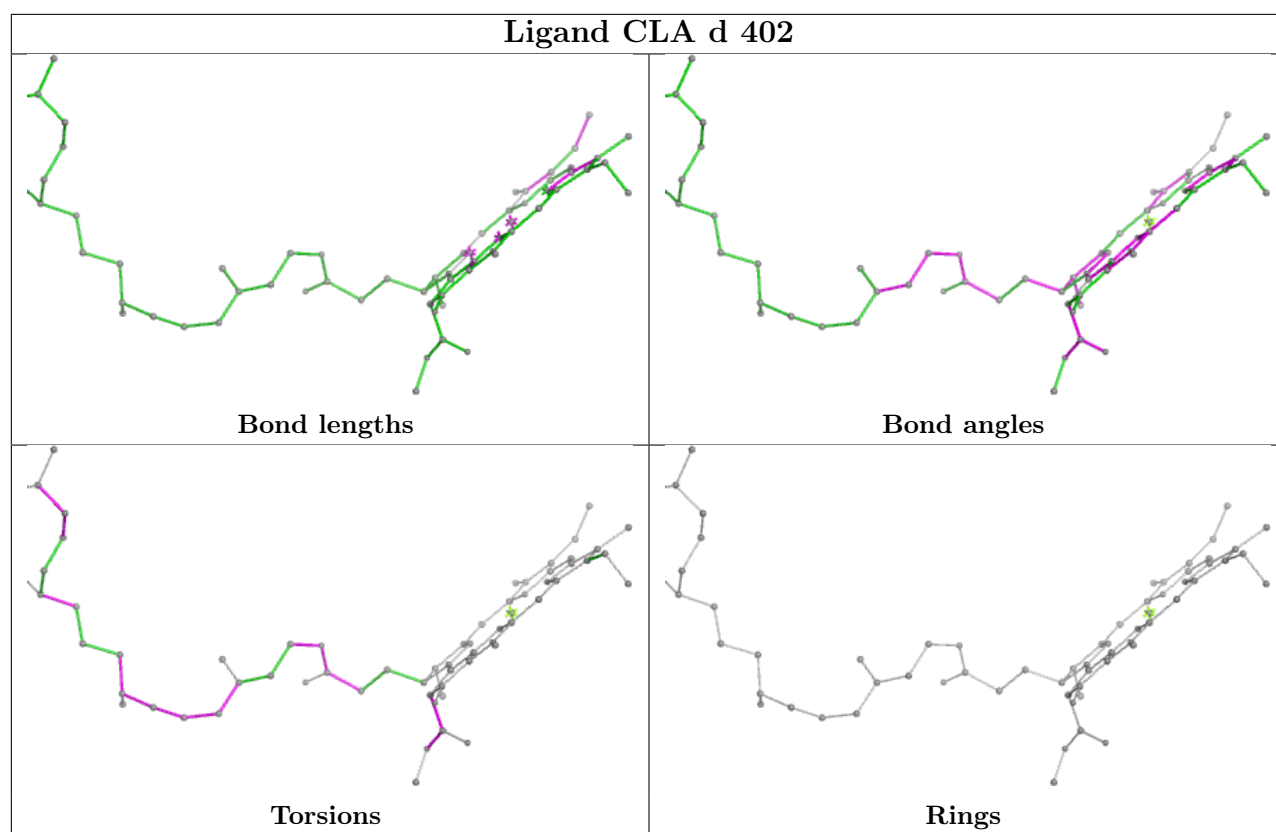
Ligand NEX Y 623

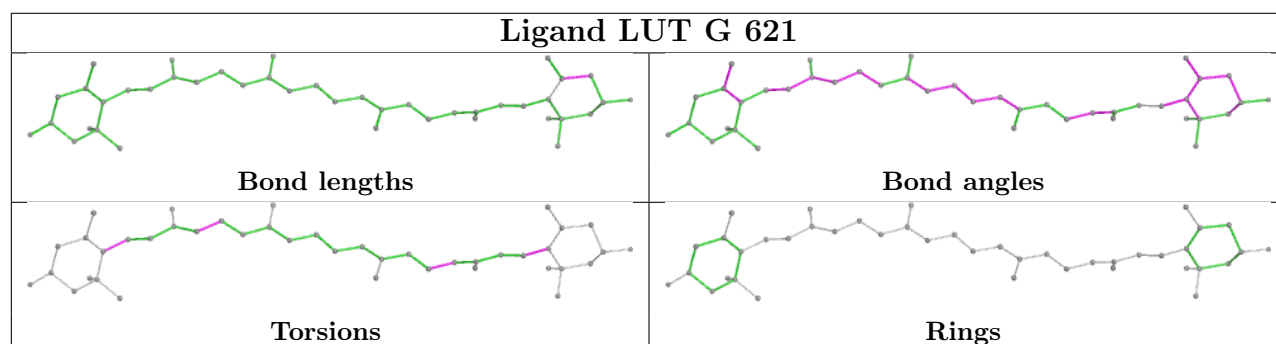
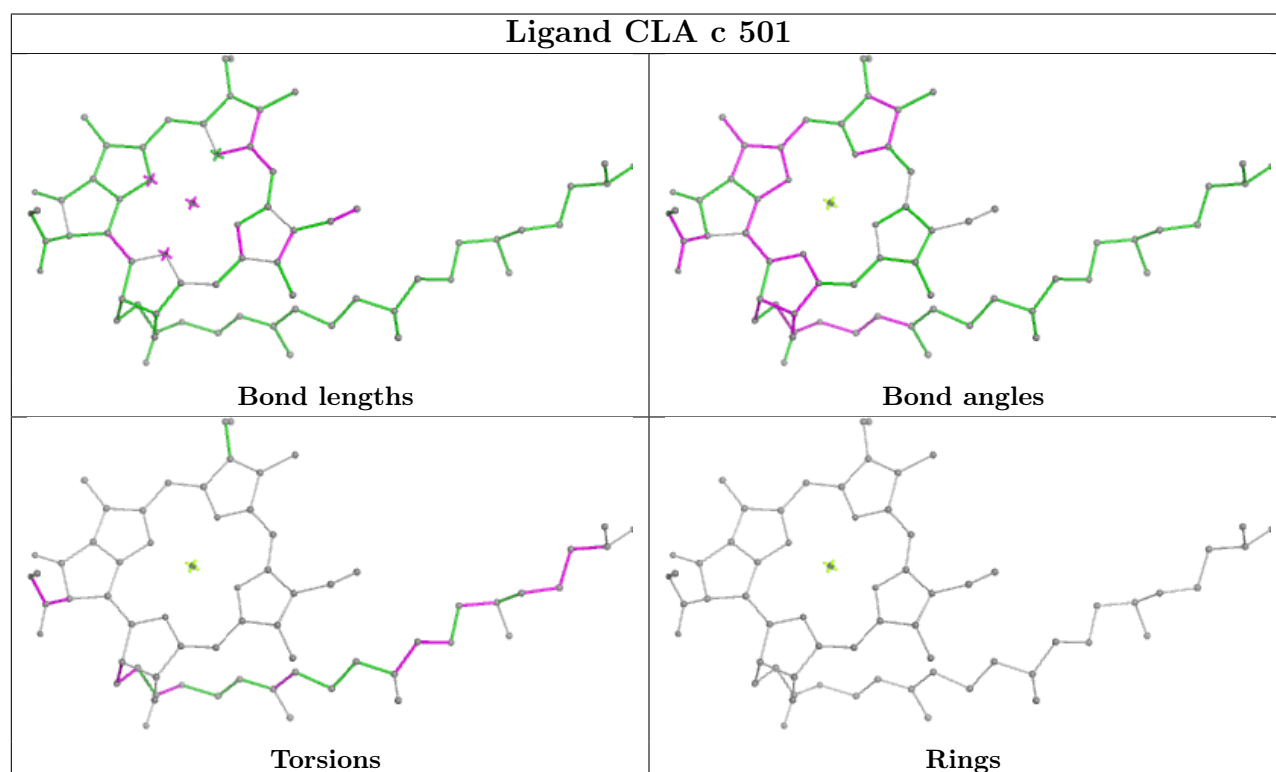
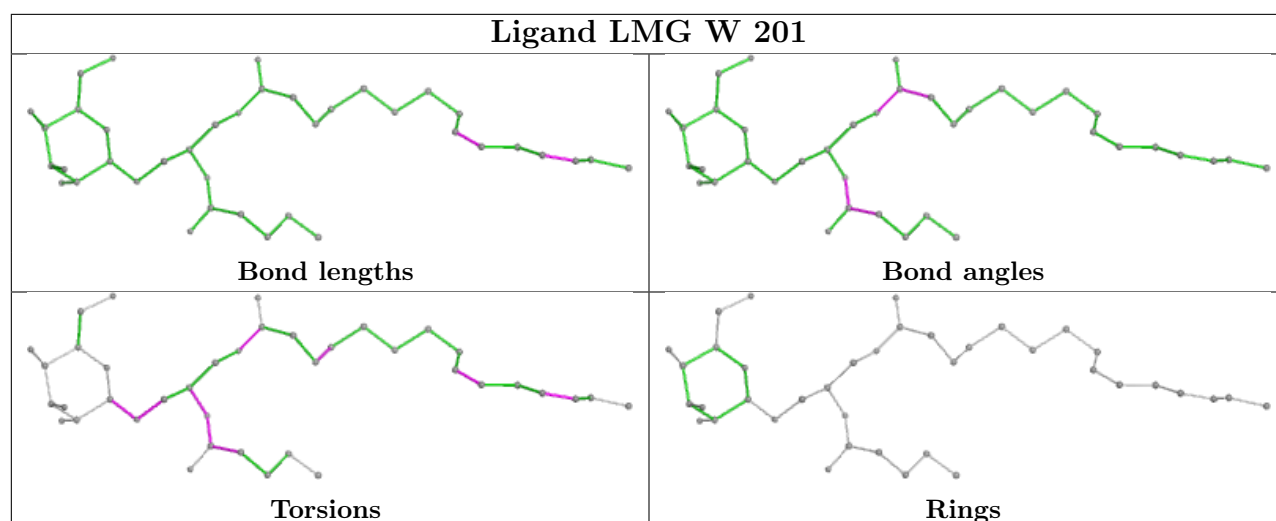


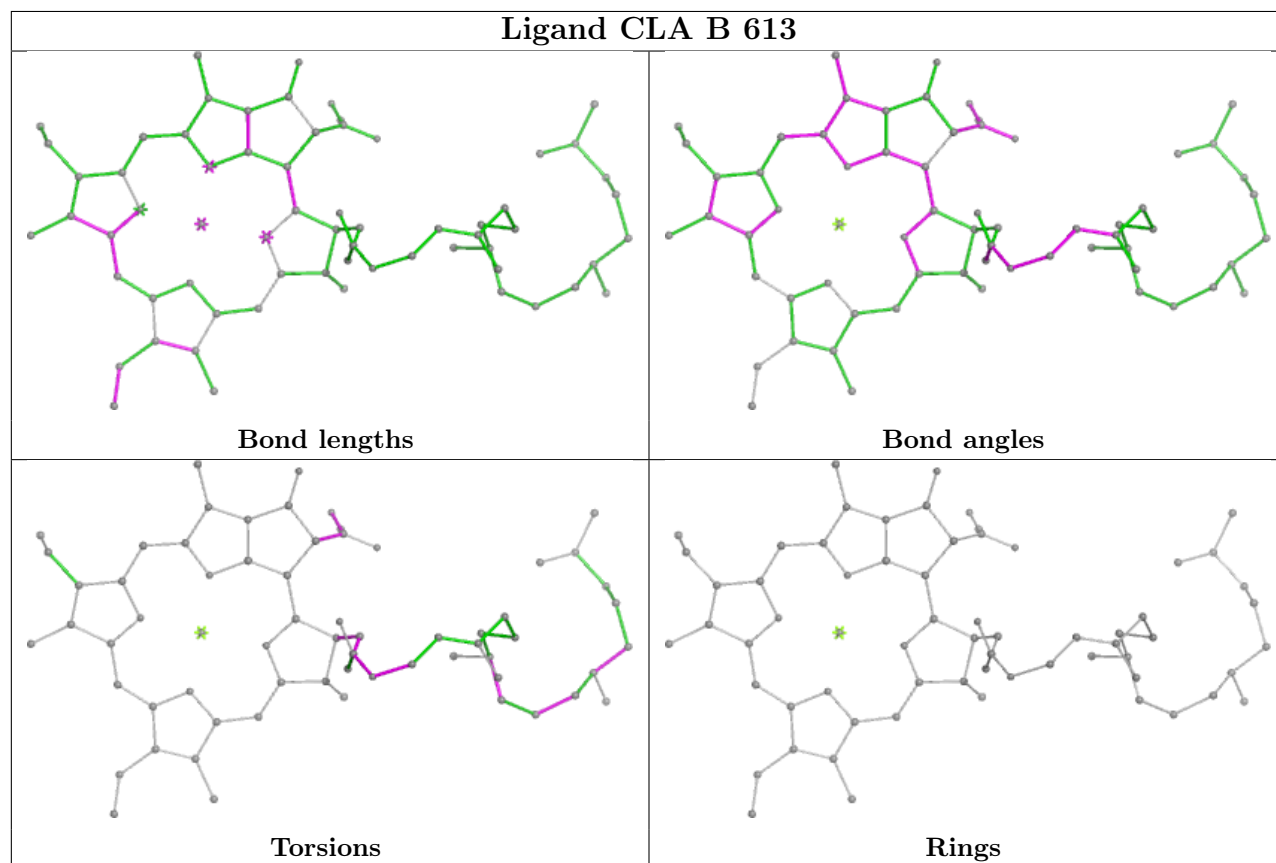
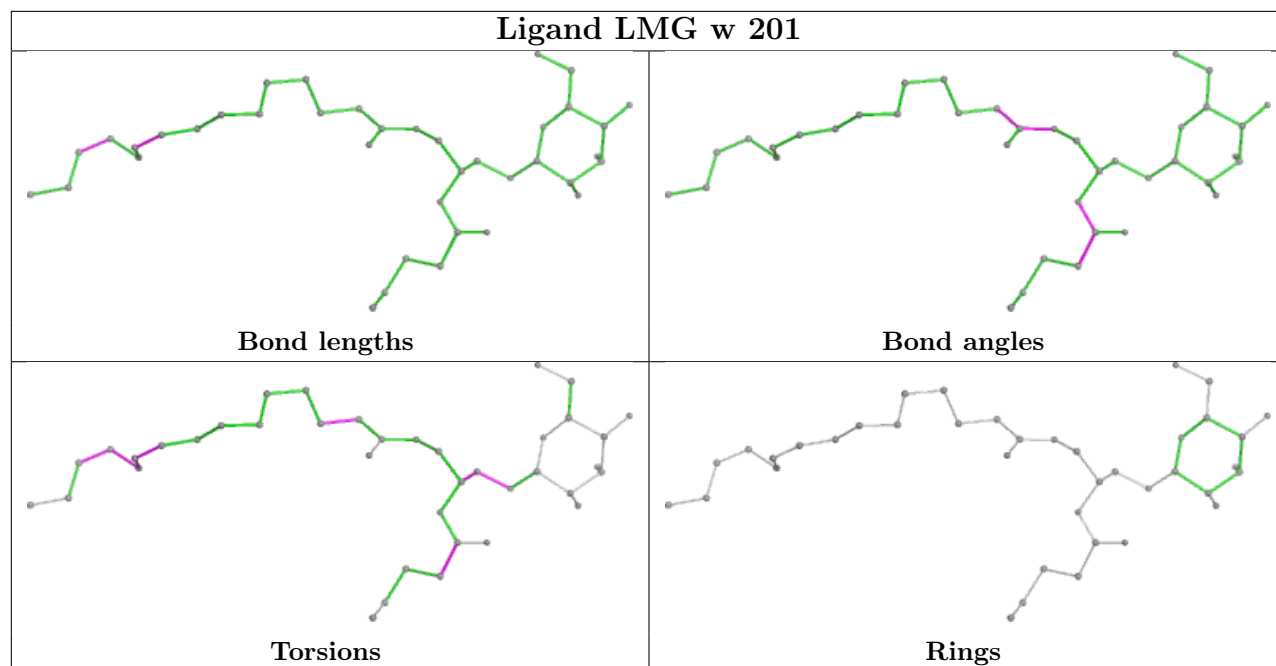


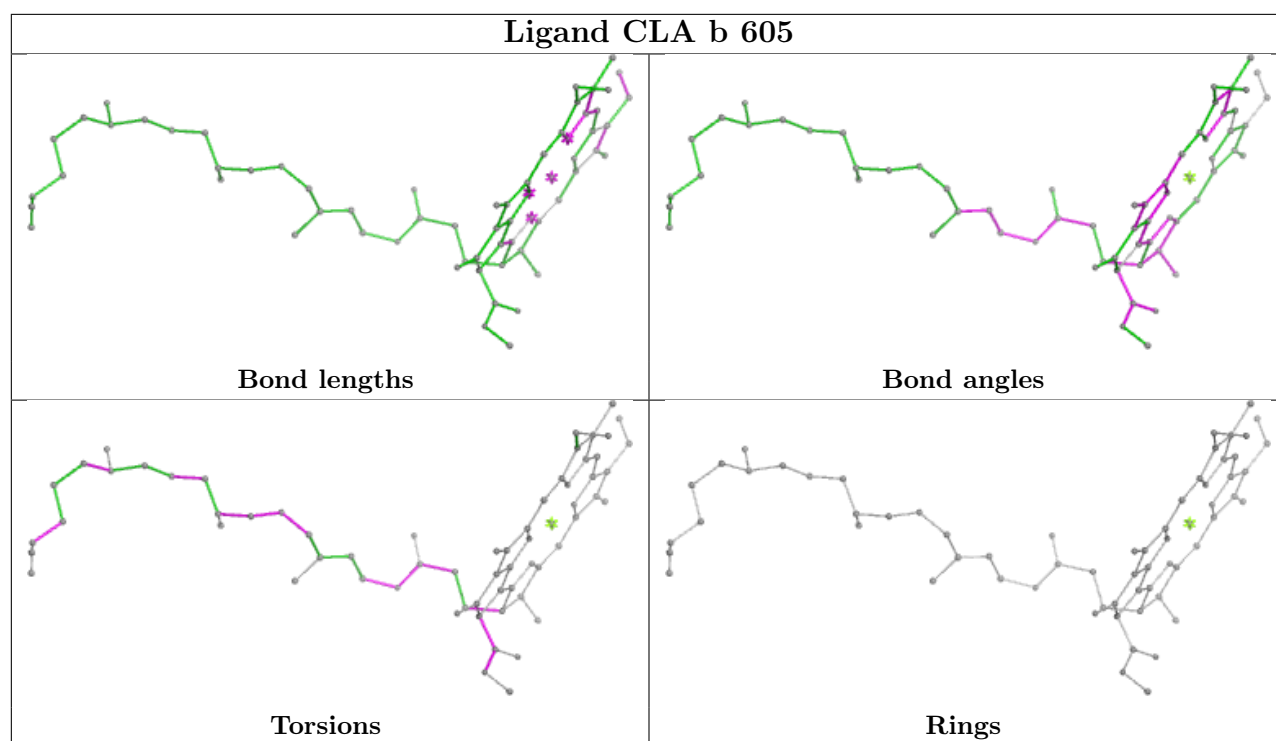




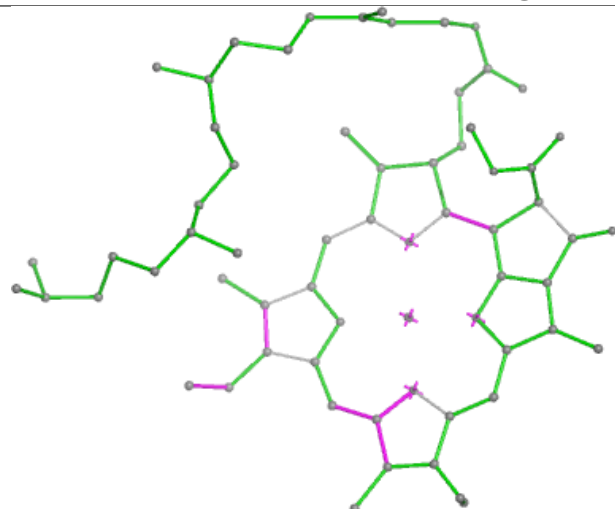




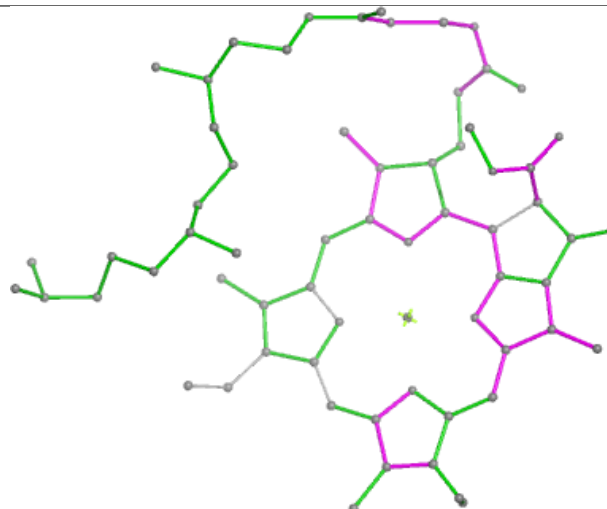




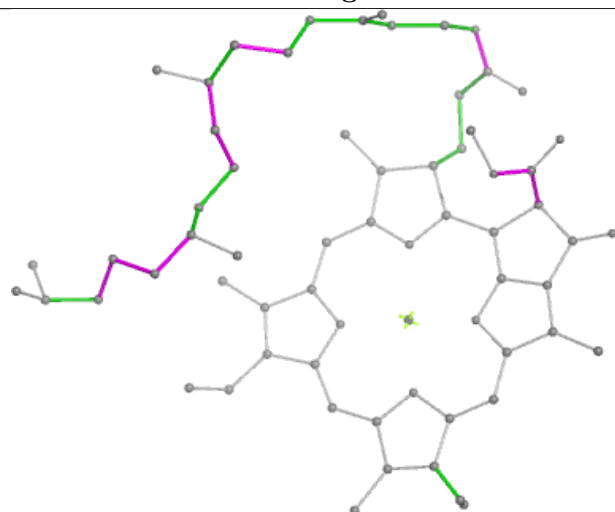
Ligand CLA Y 612



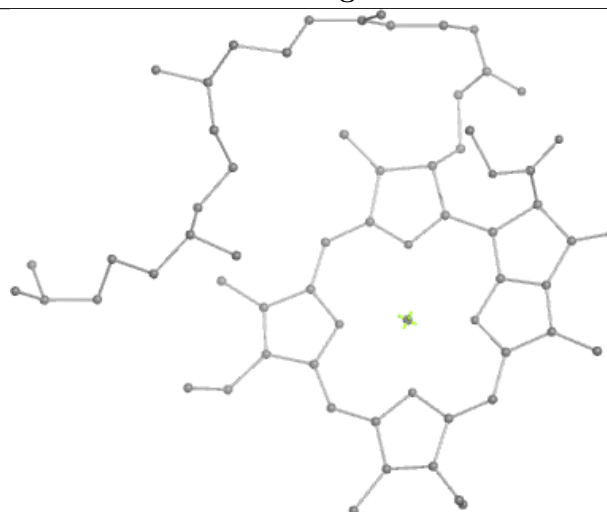
Bond lengths



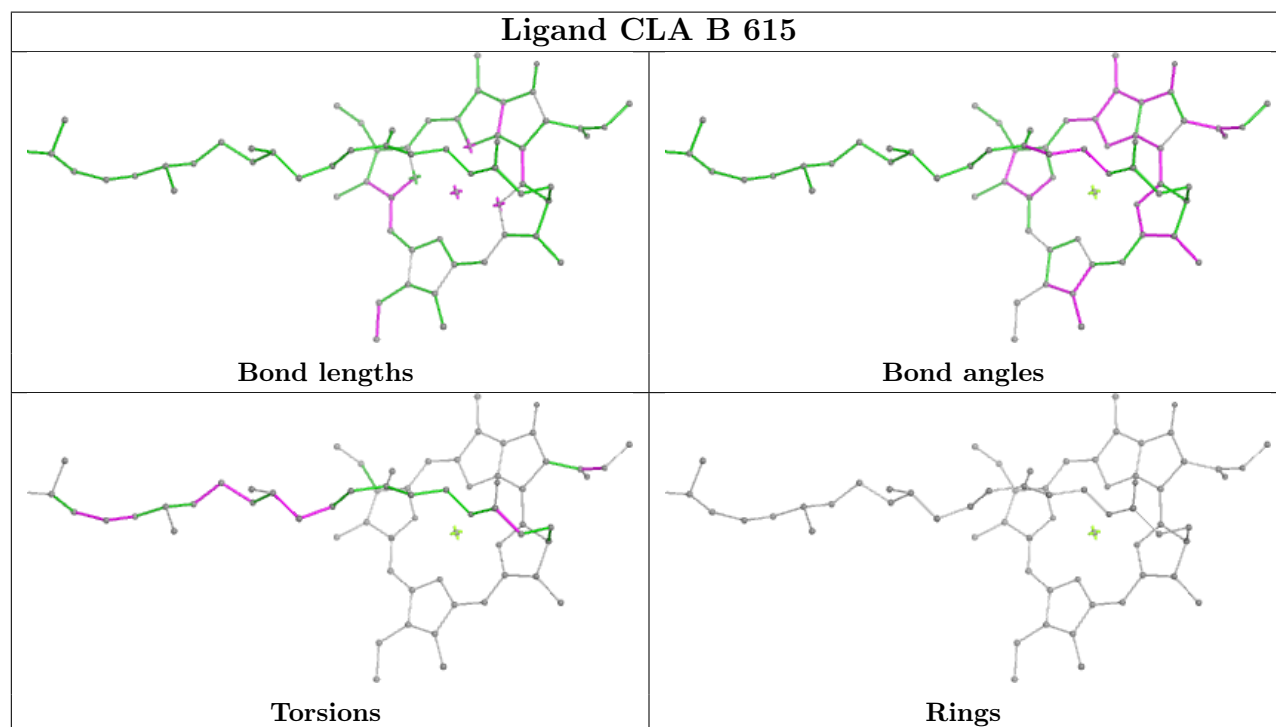
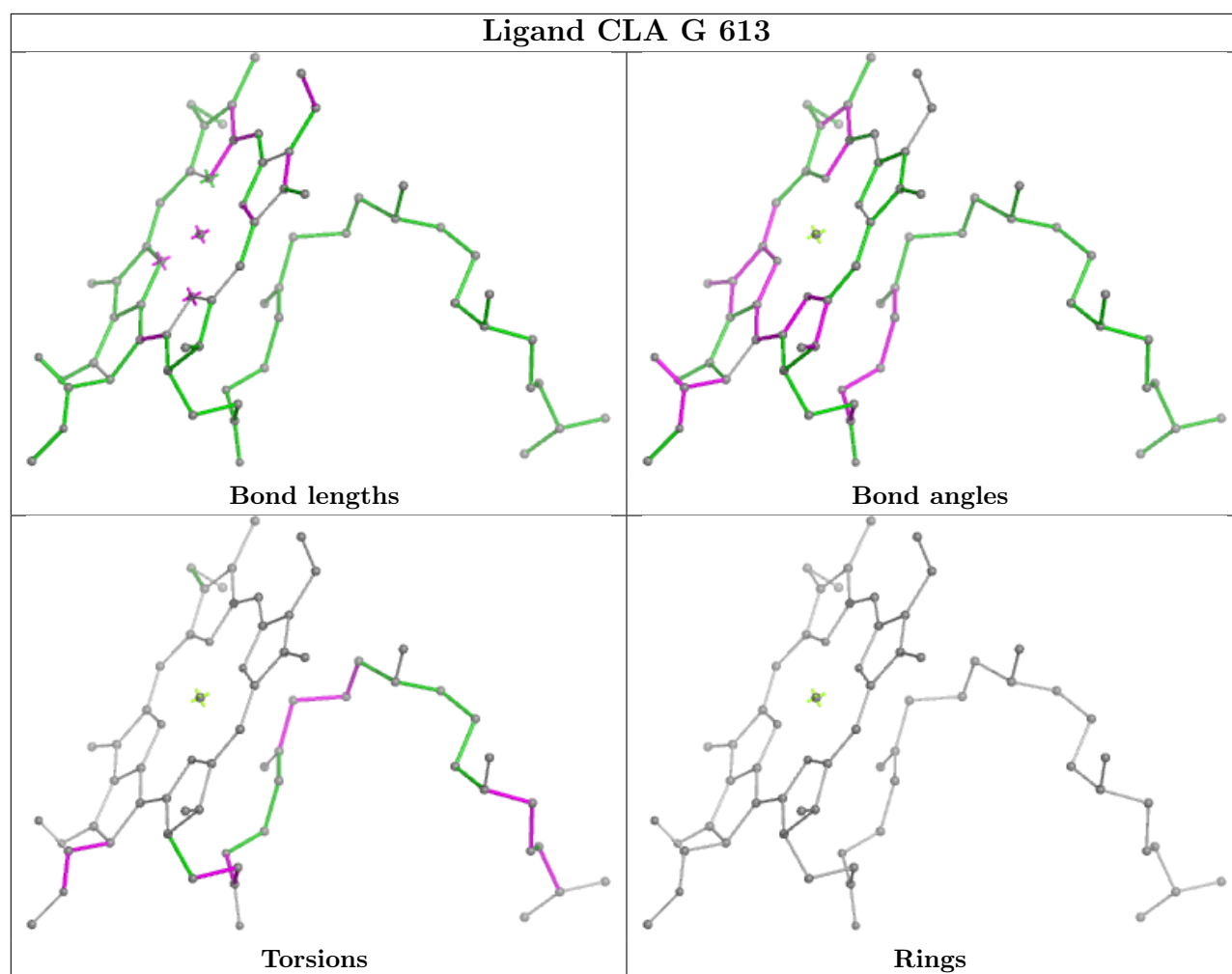
Bond angles

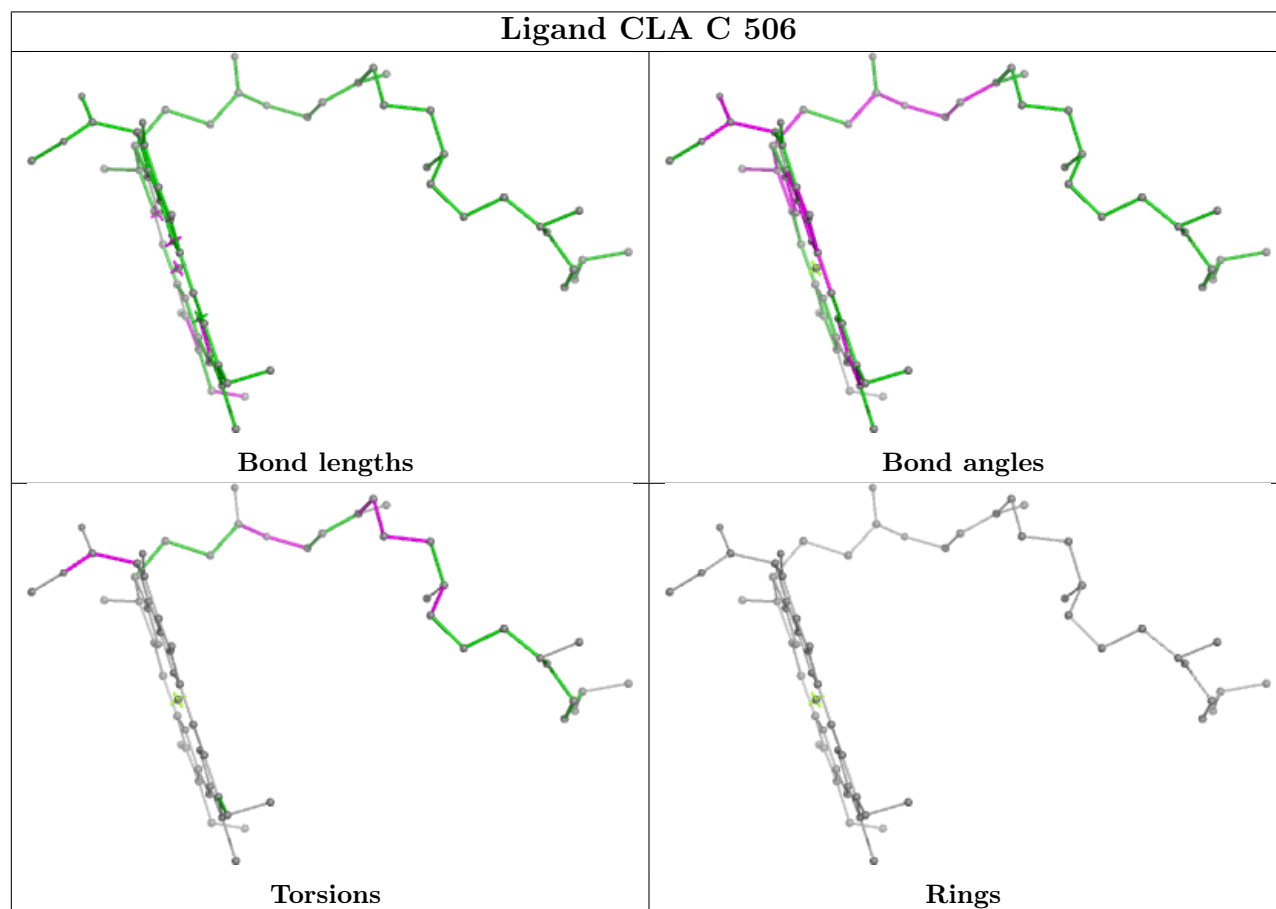
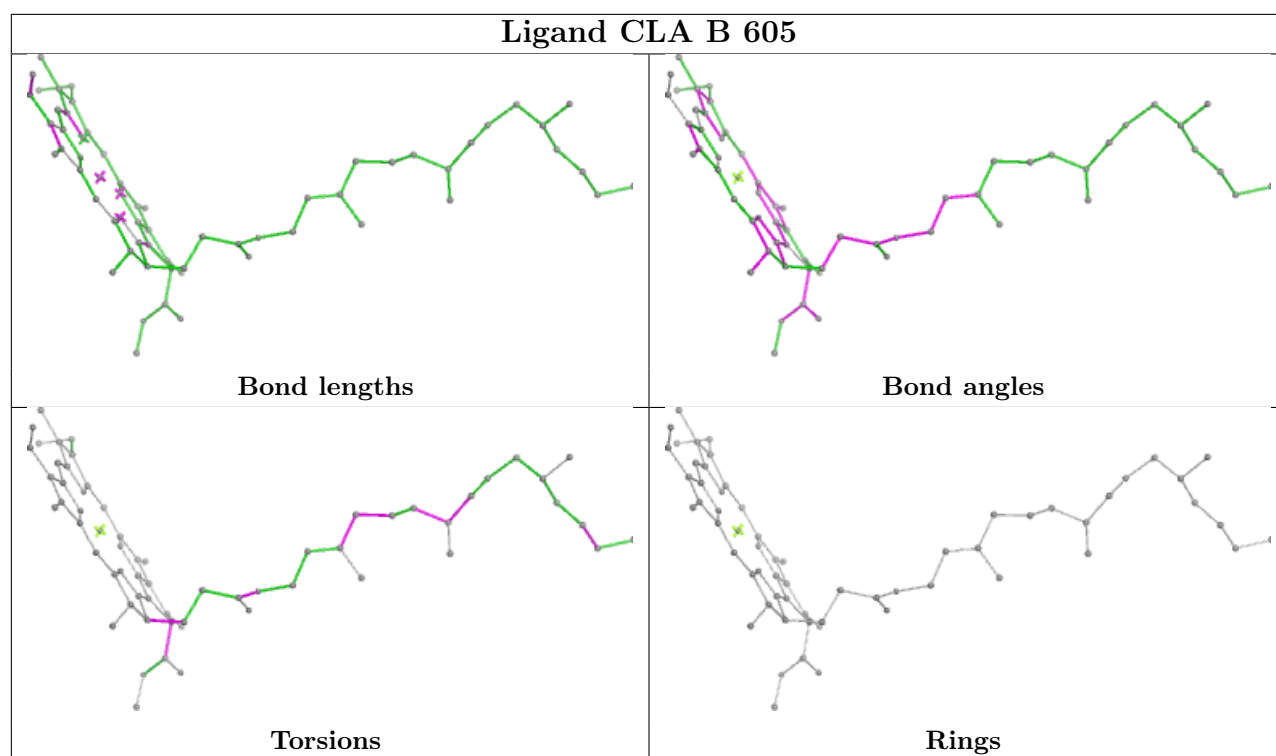


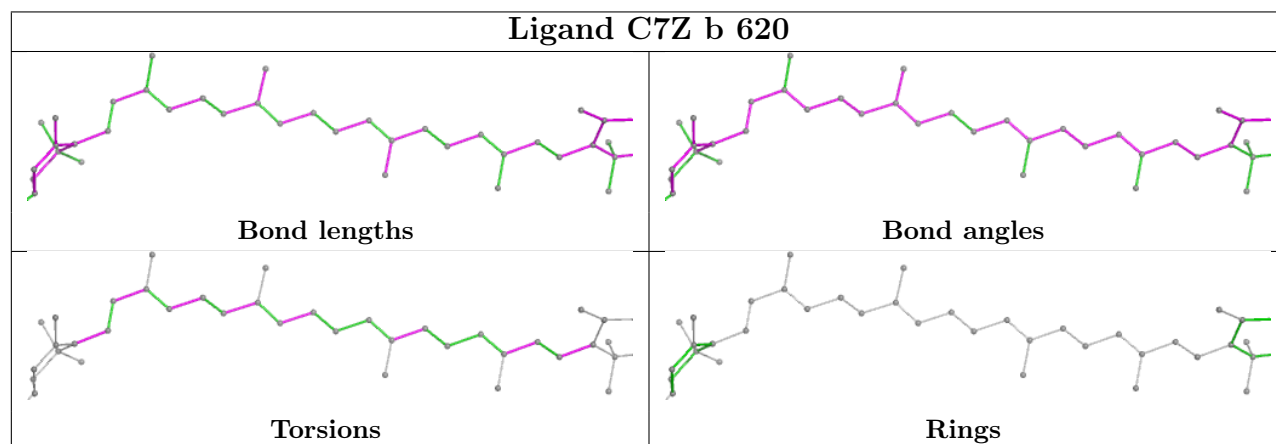
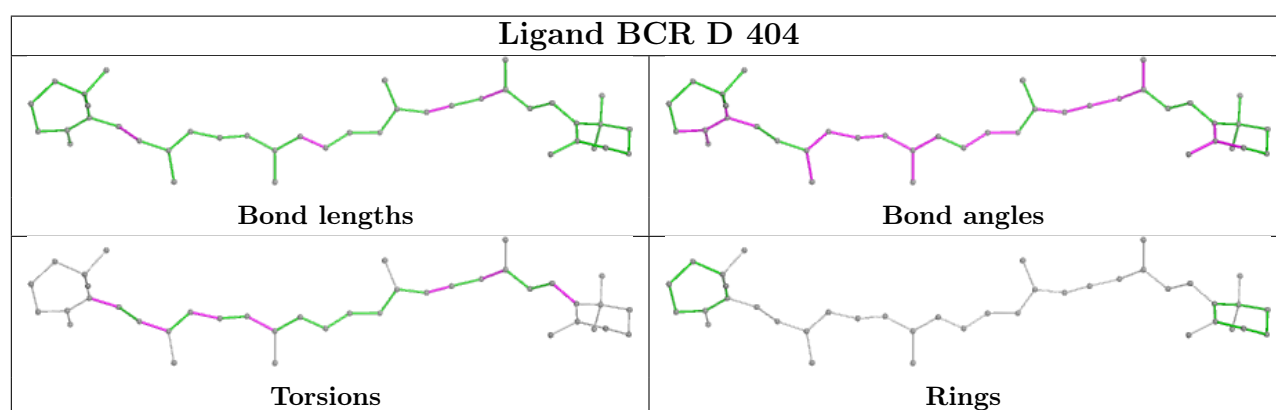
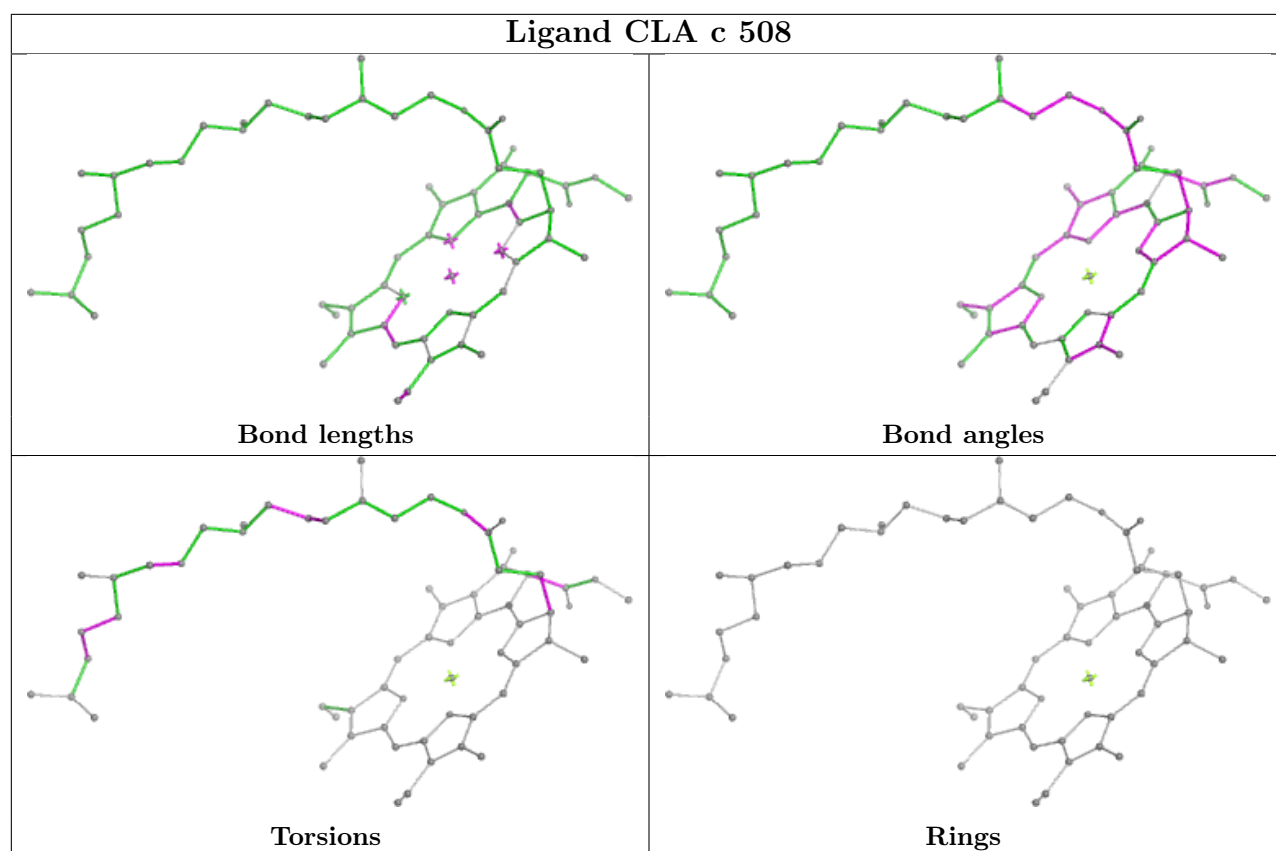
Torsions

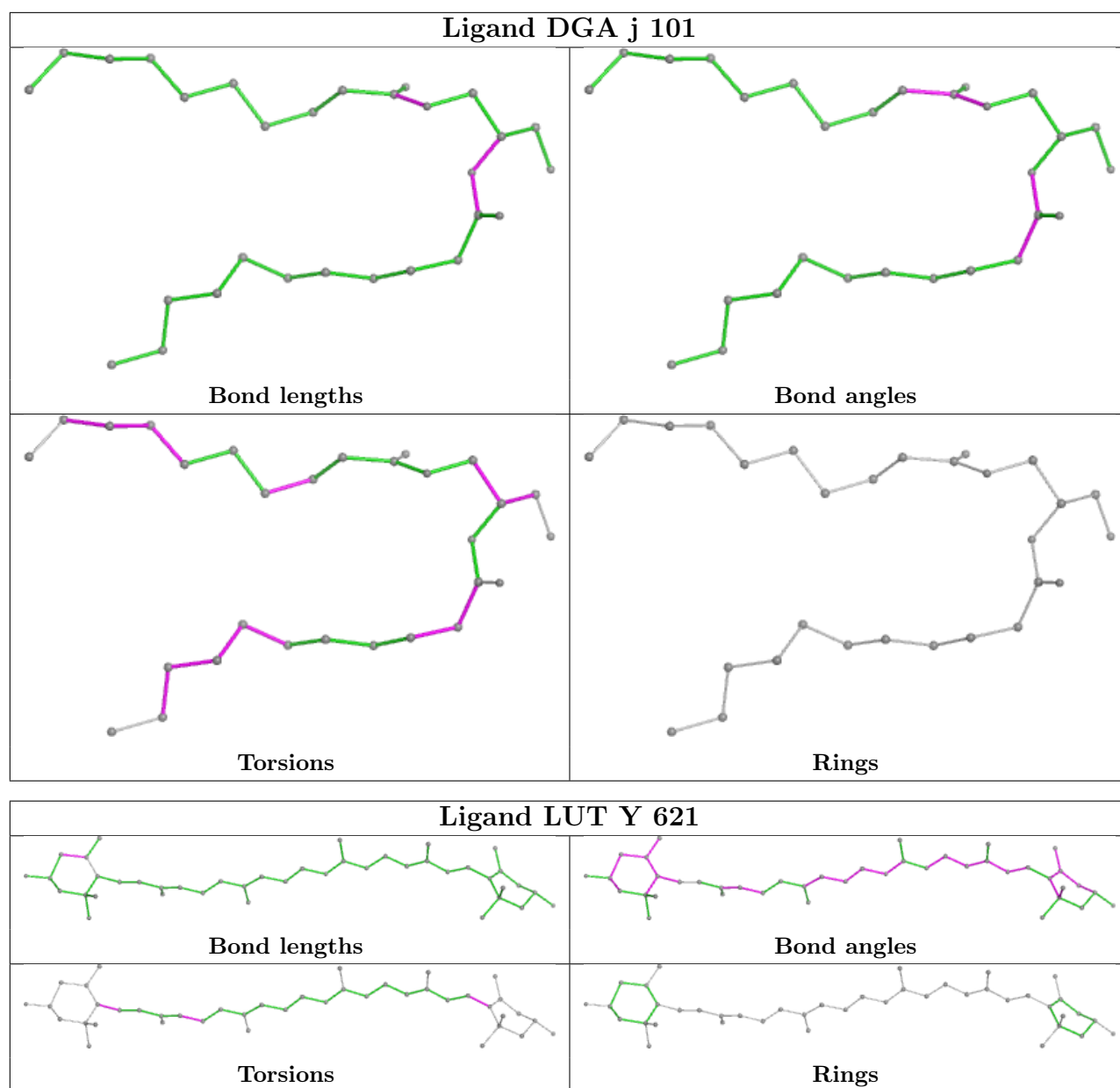


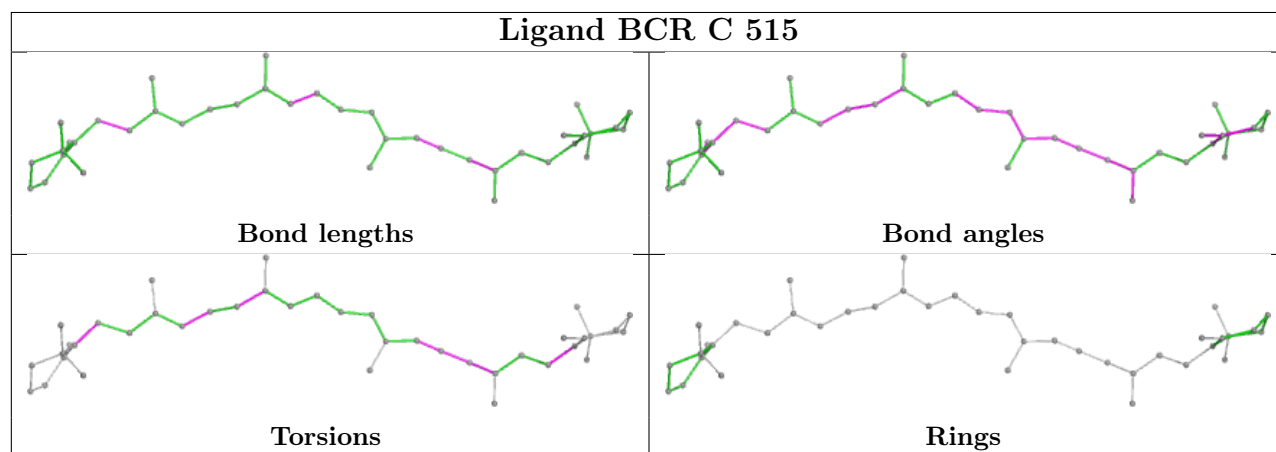
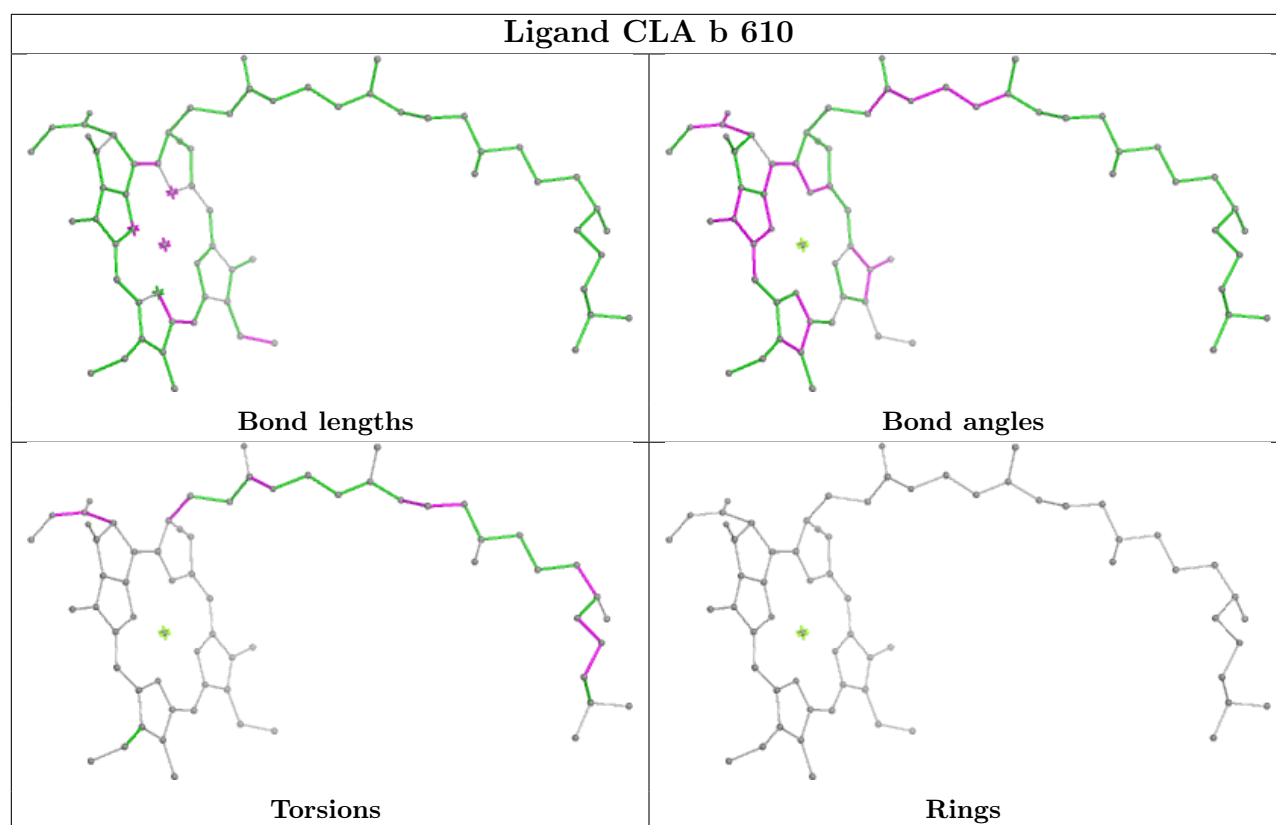
Rings

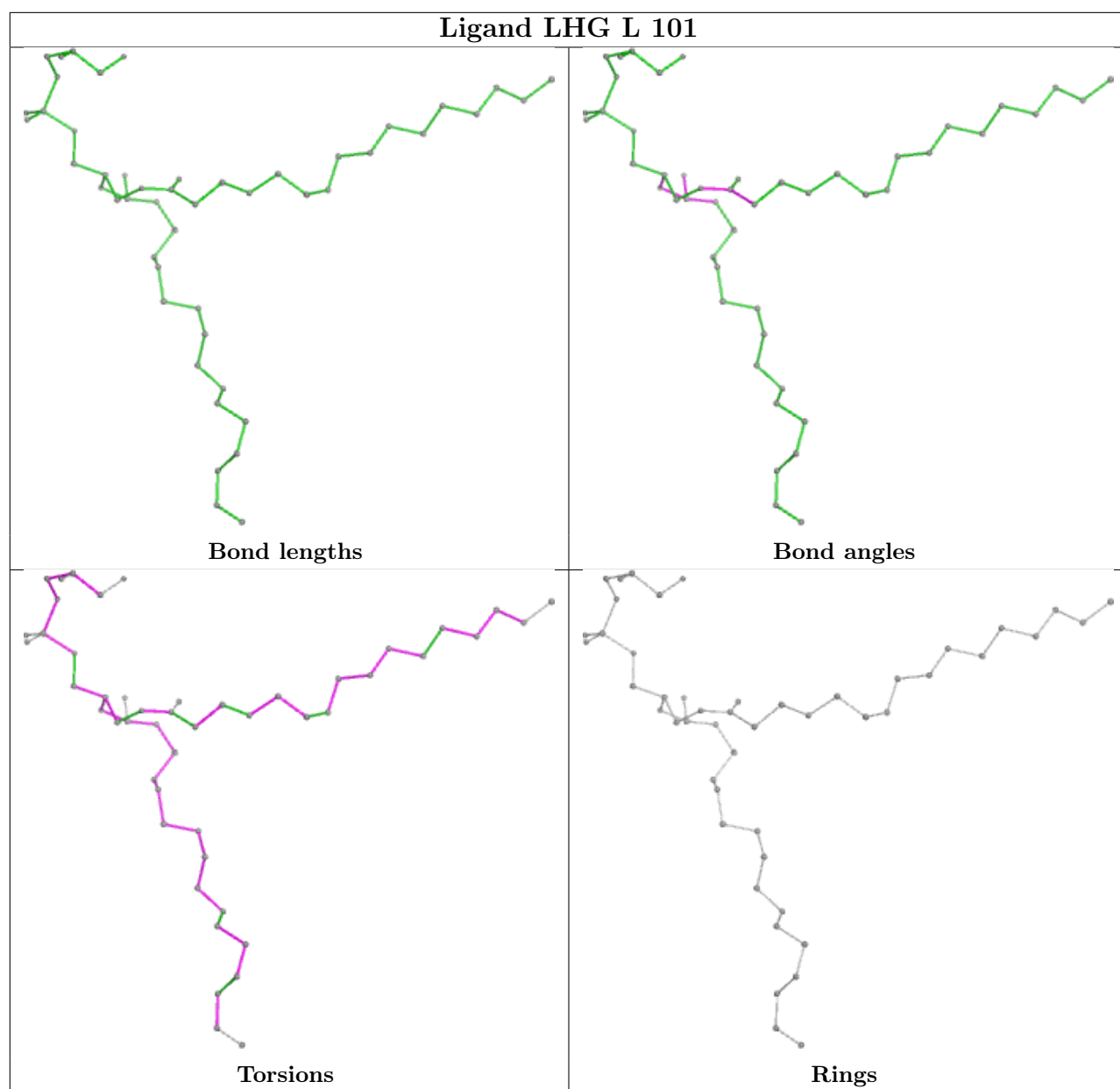


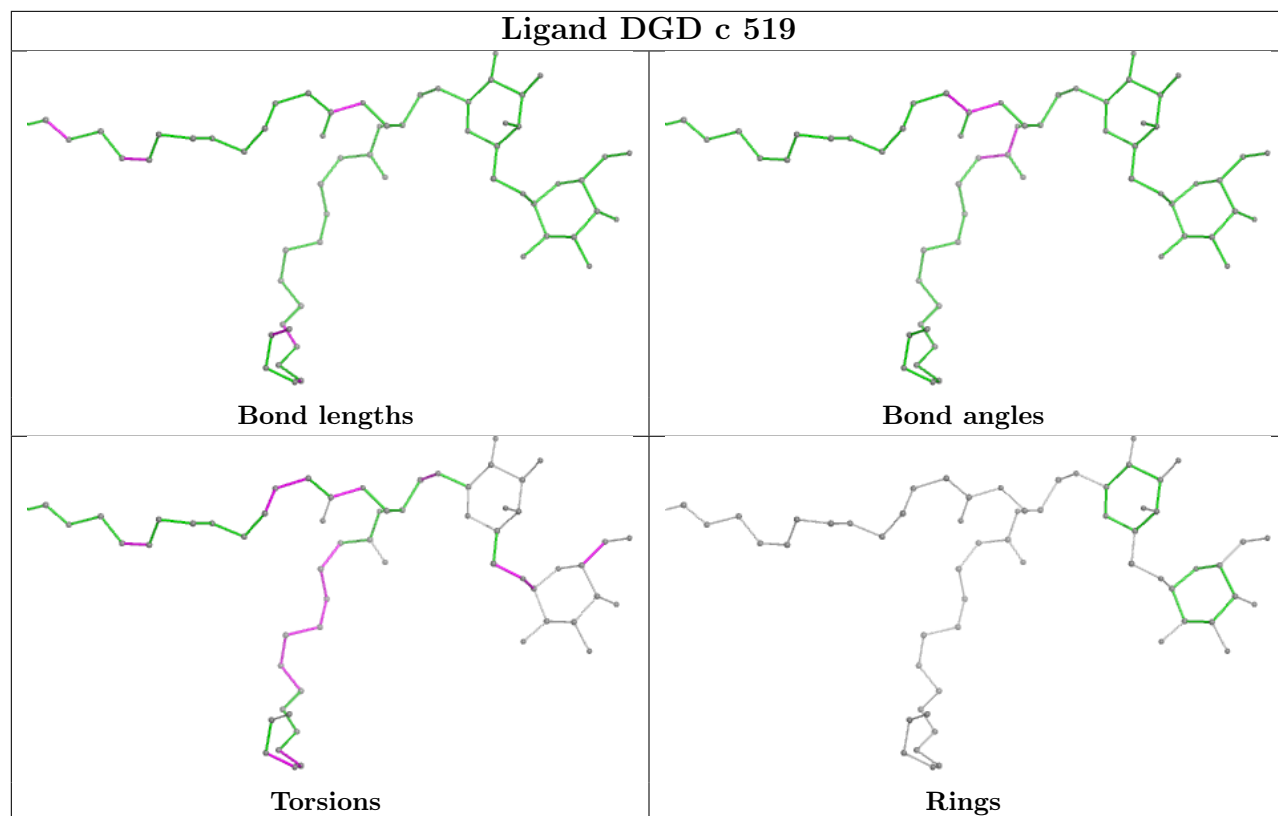




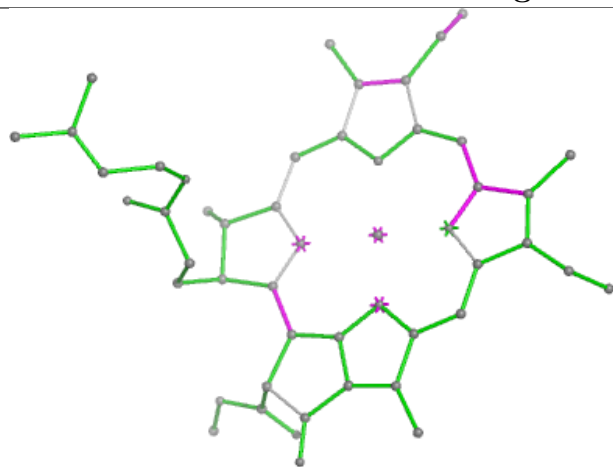




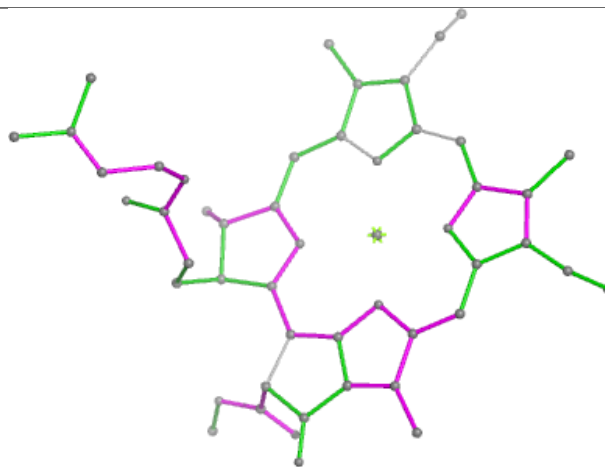




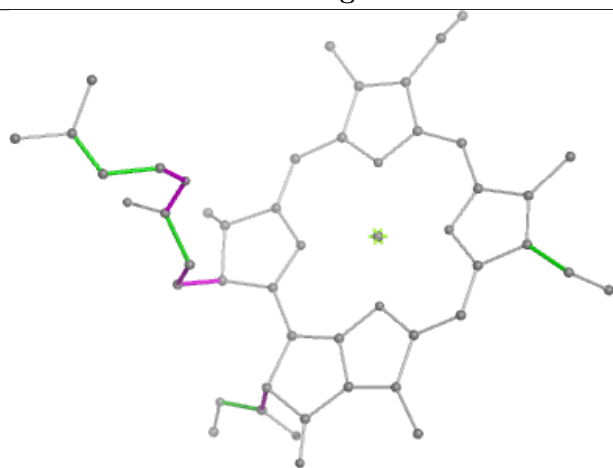
Ligand CLA A 407



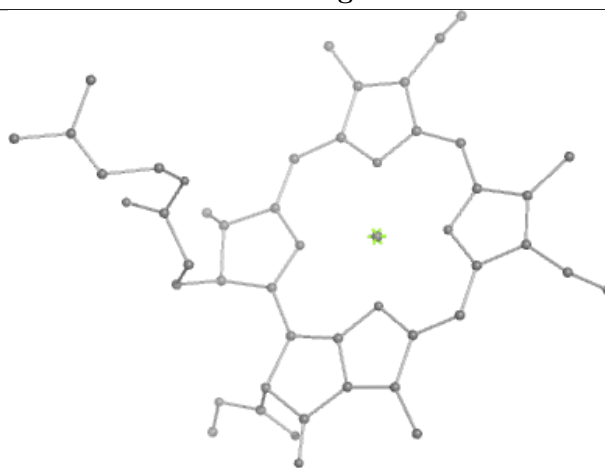
Bond lengths



Bond angles

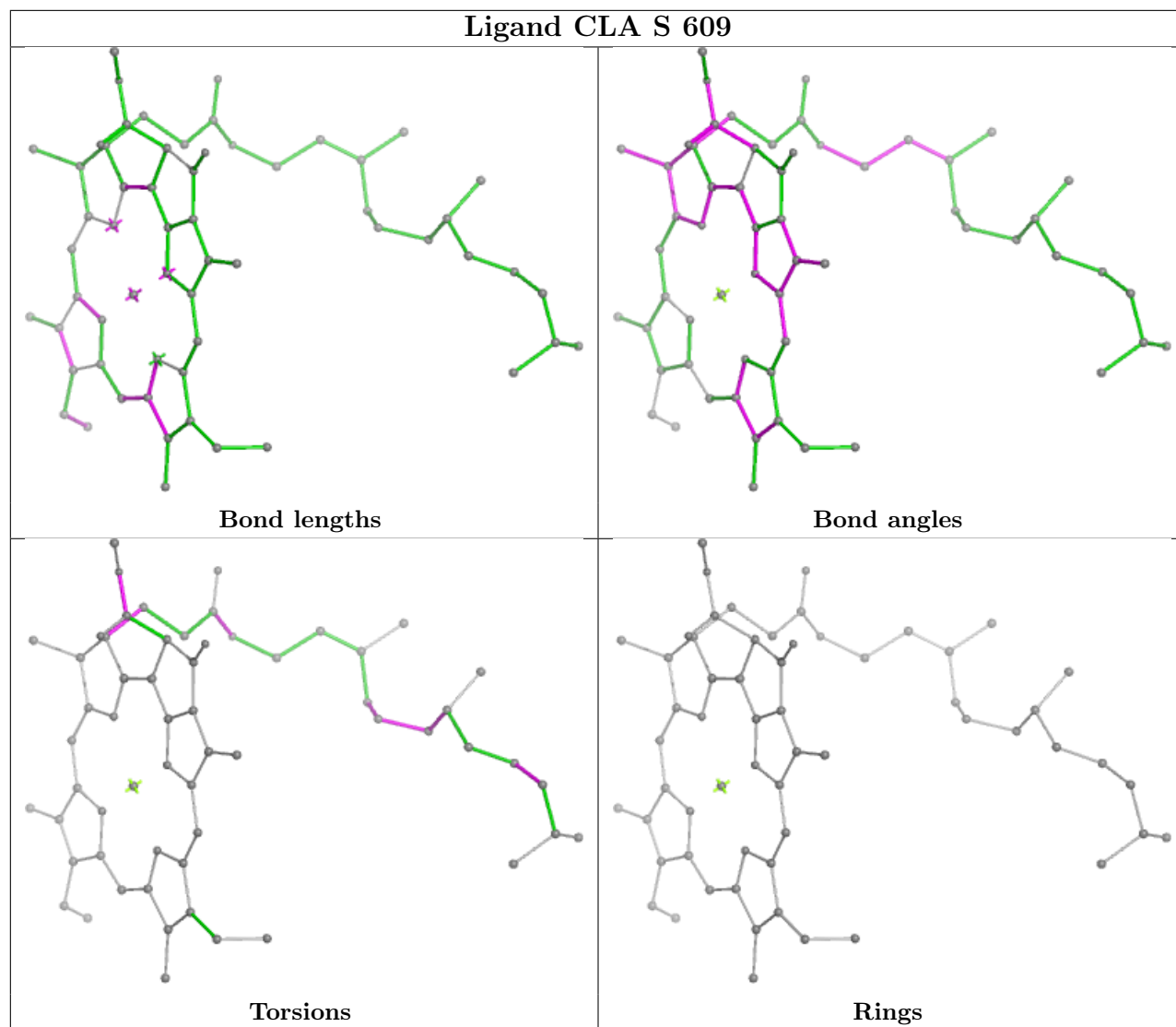


Torsions

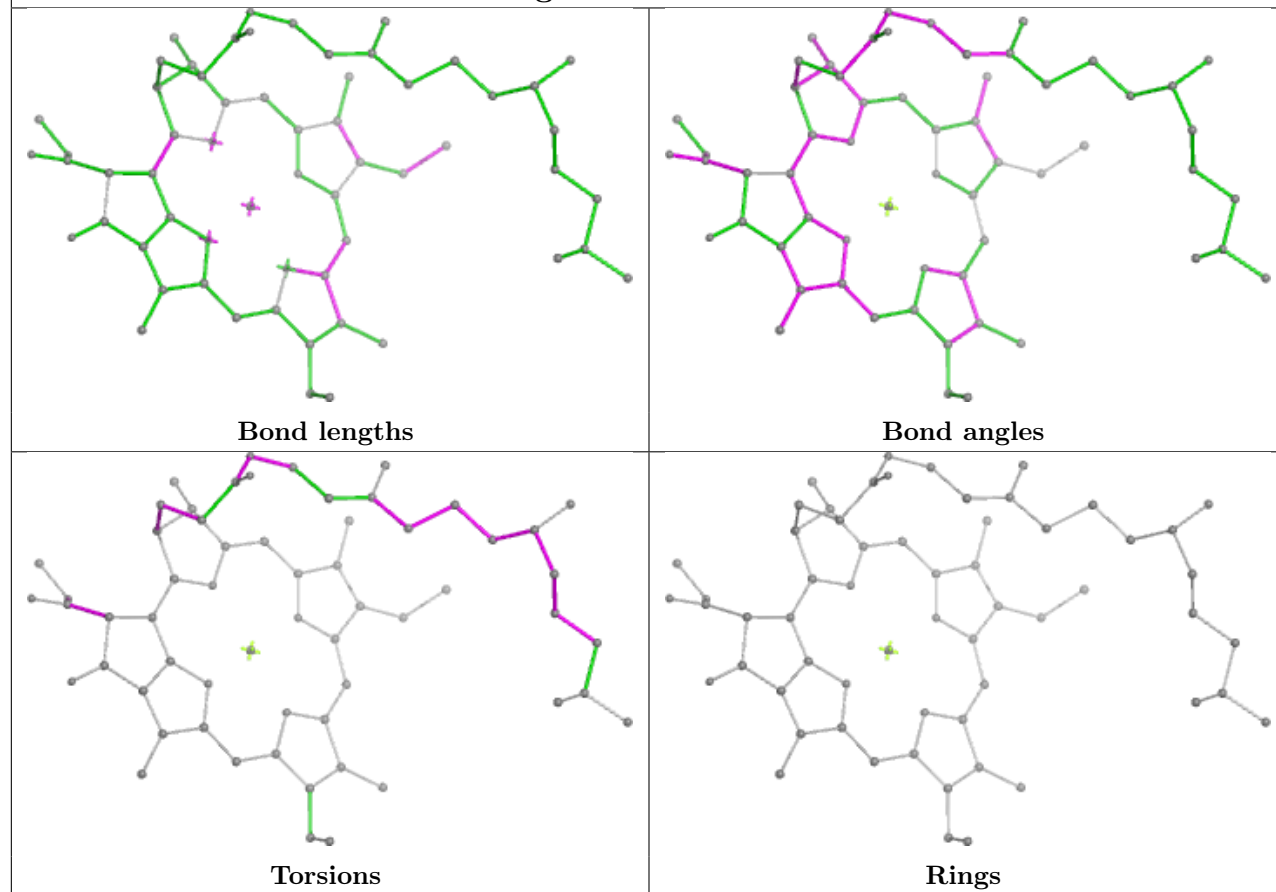


Rings

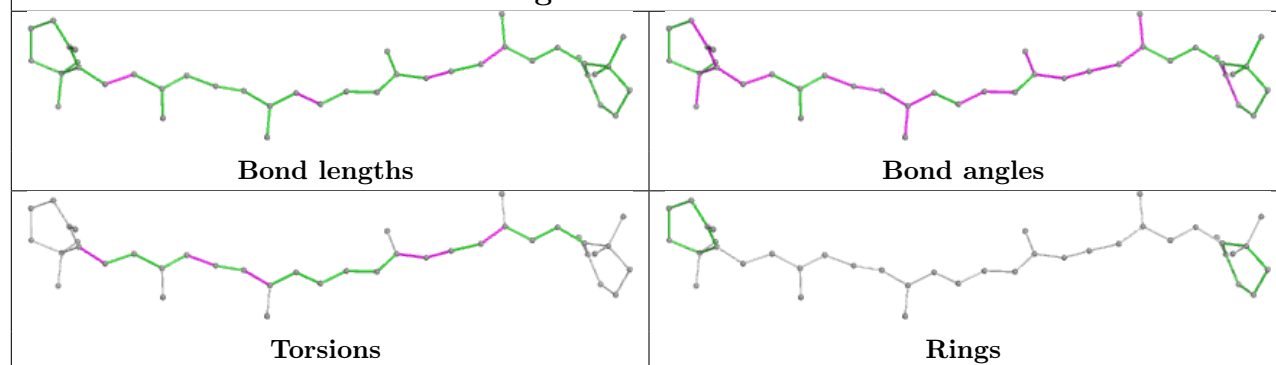
Ligand CLA S 609

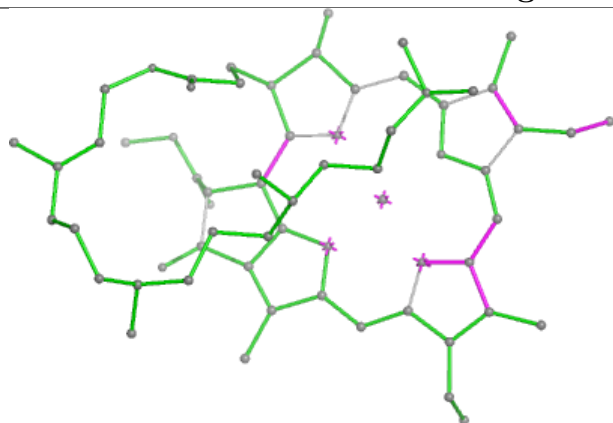
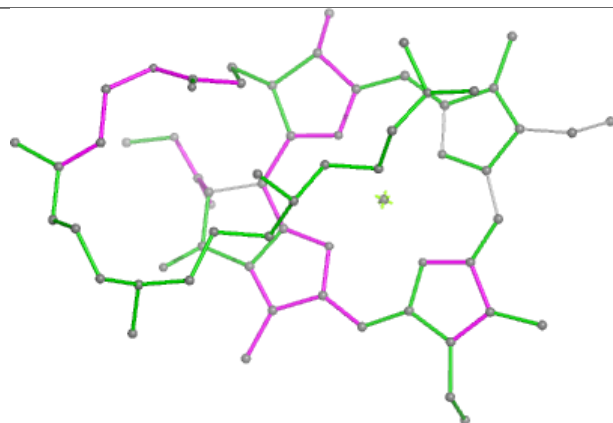
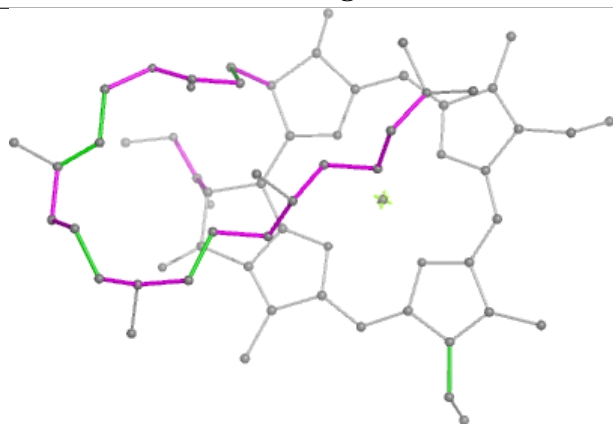
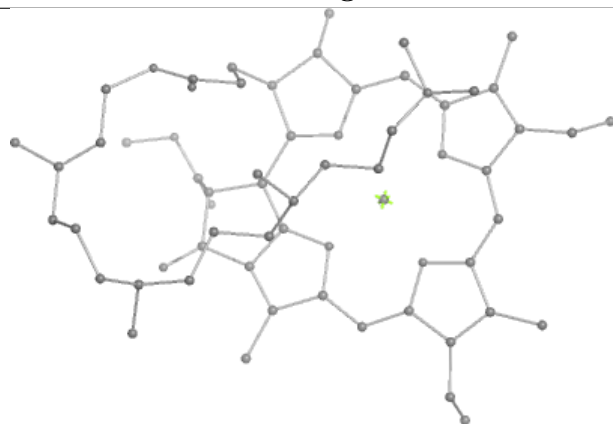
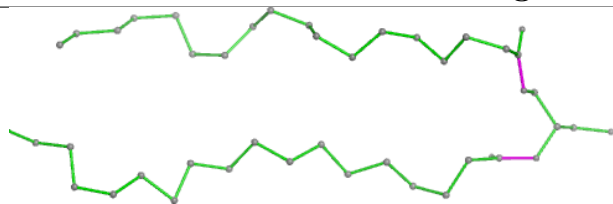
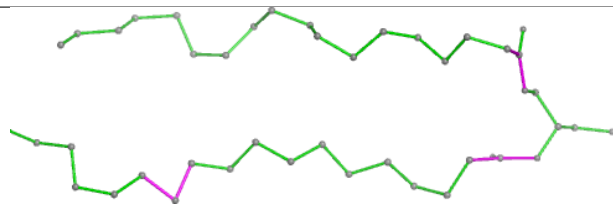
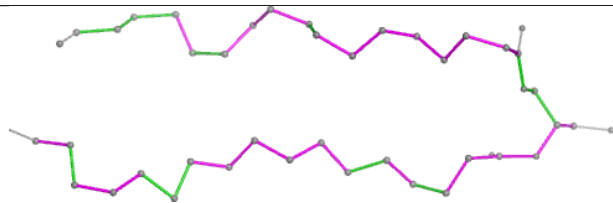
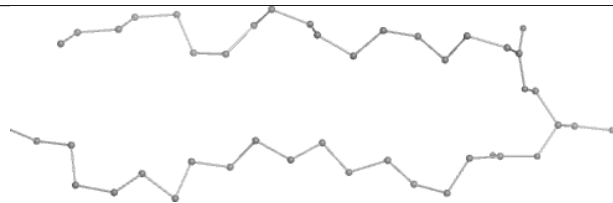


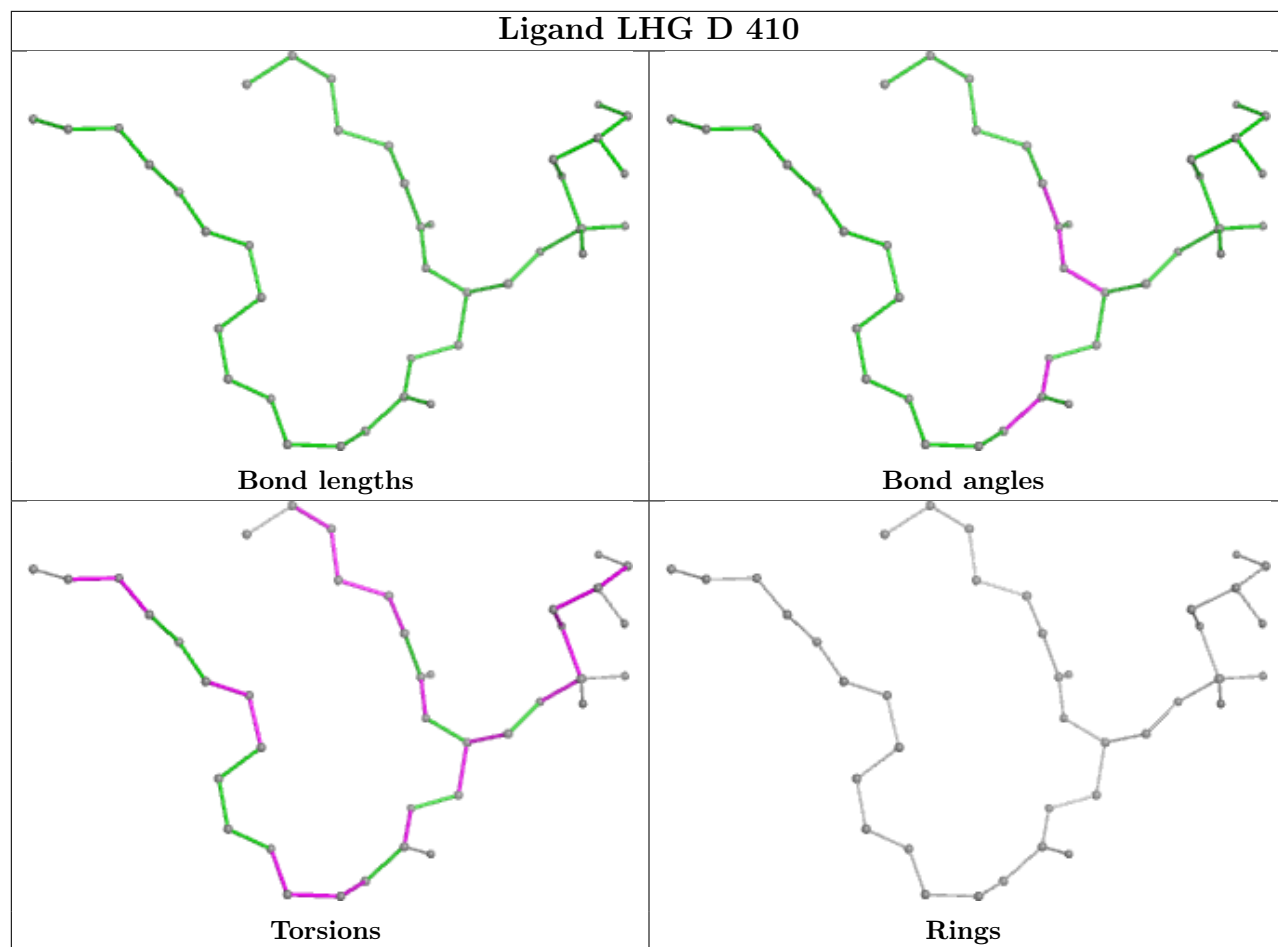
Ligand CLA S 602

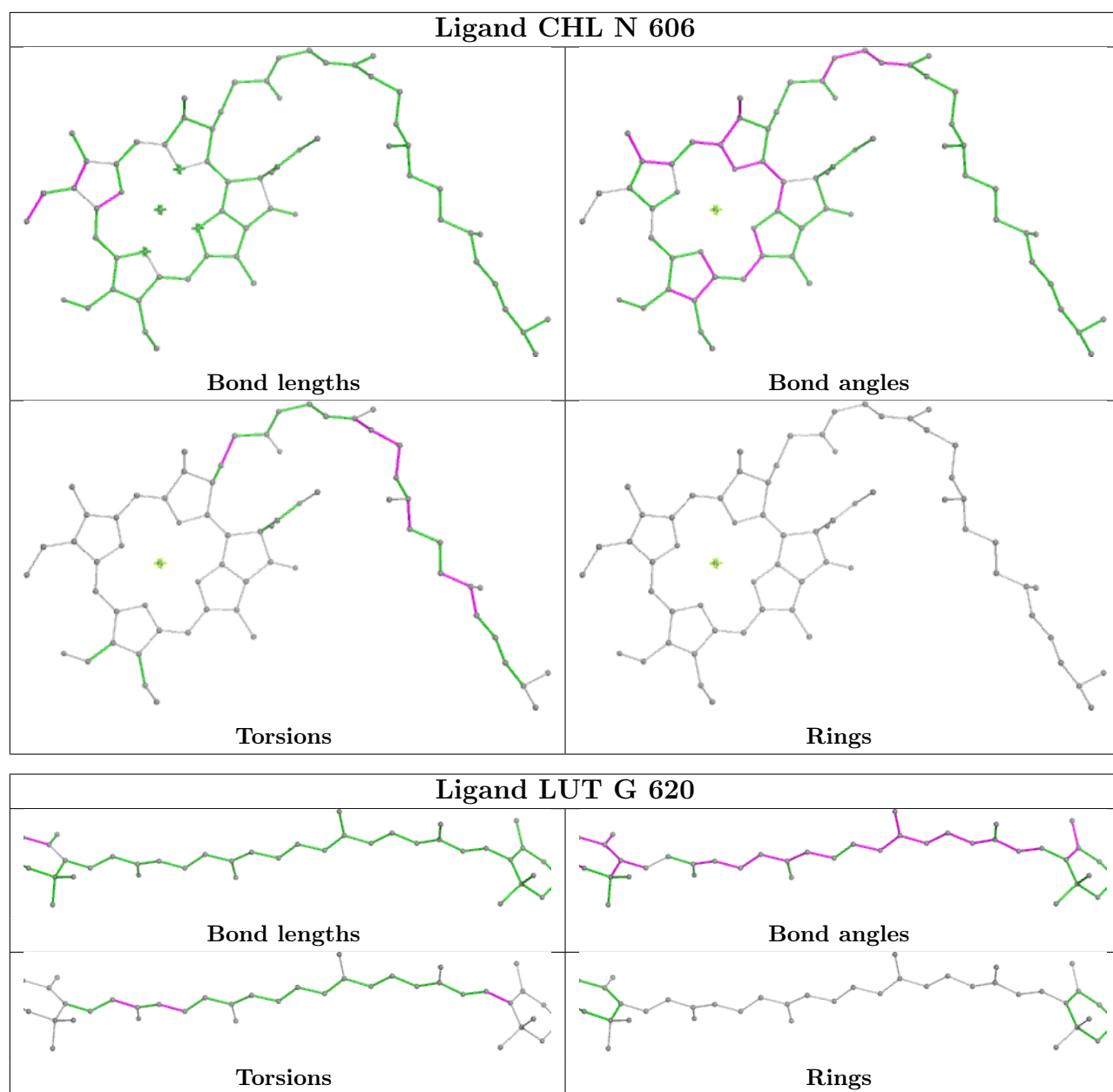


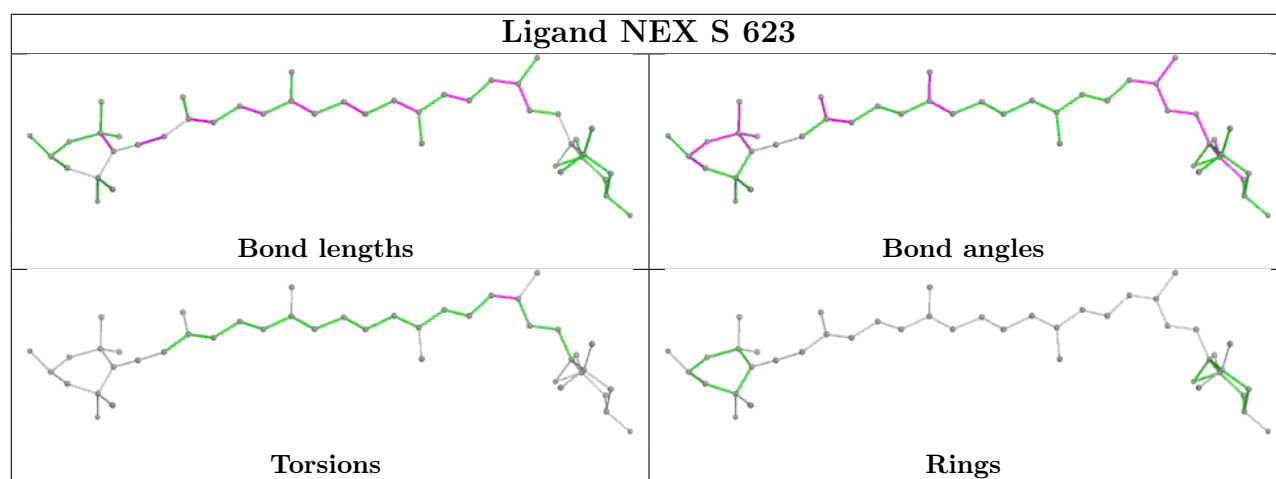
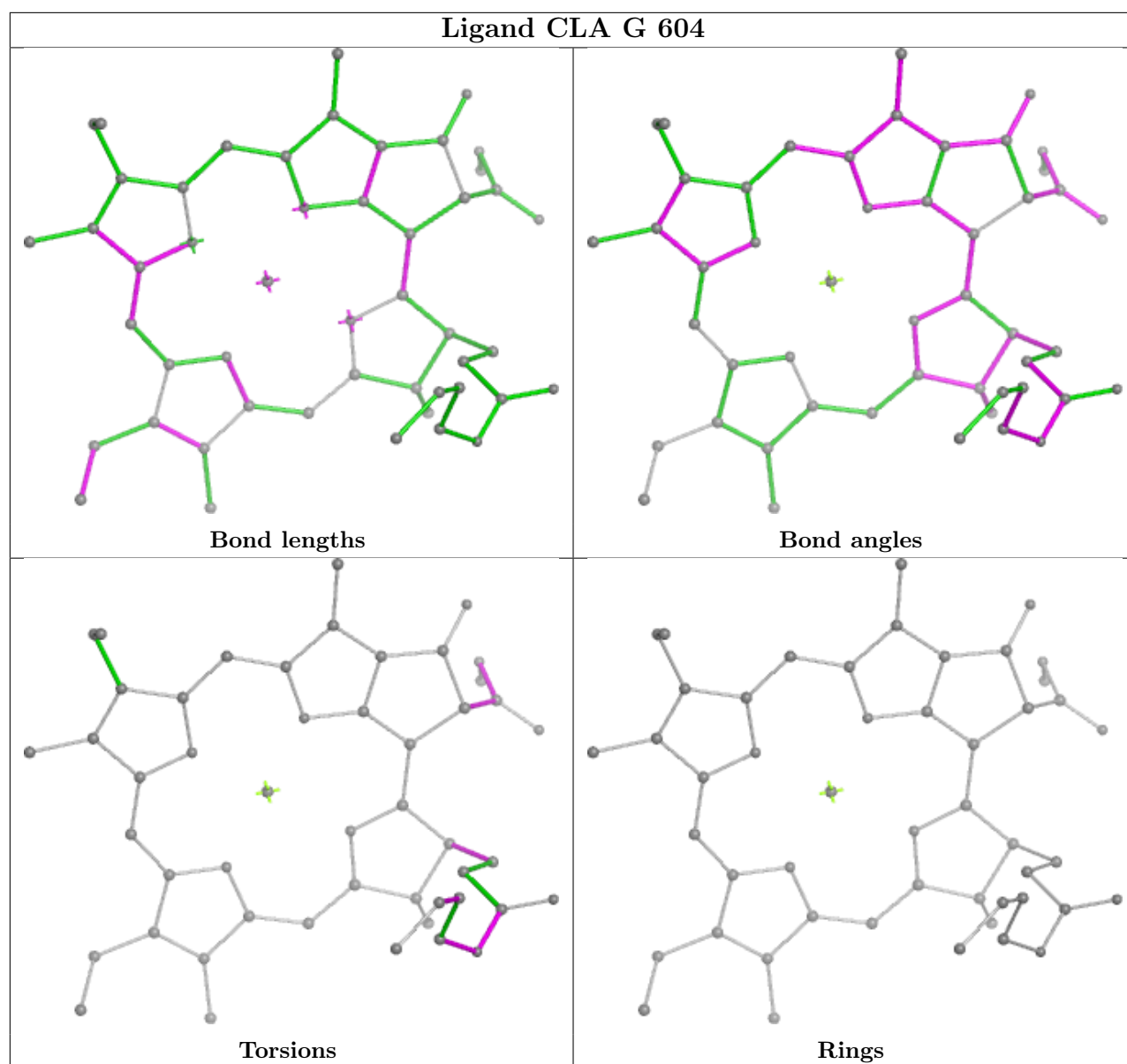
Ligand BCR a 411

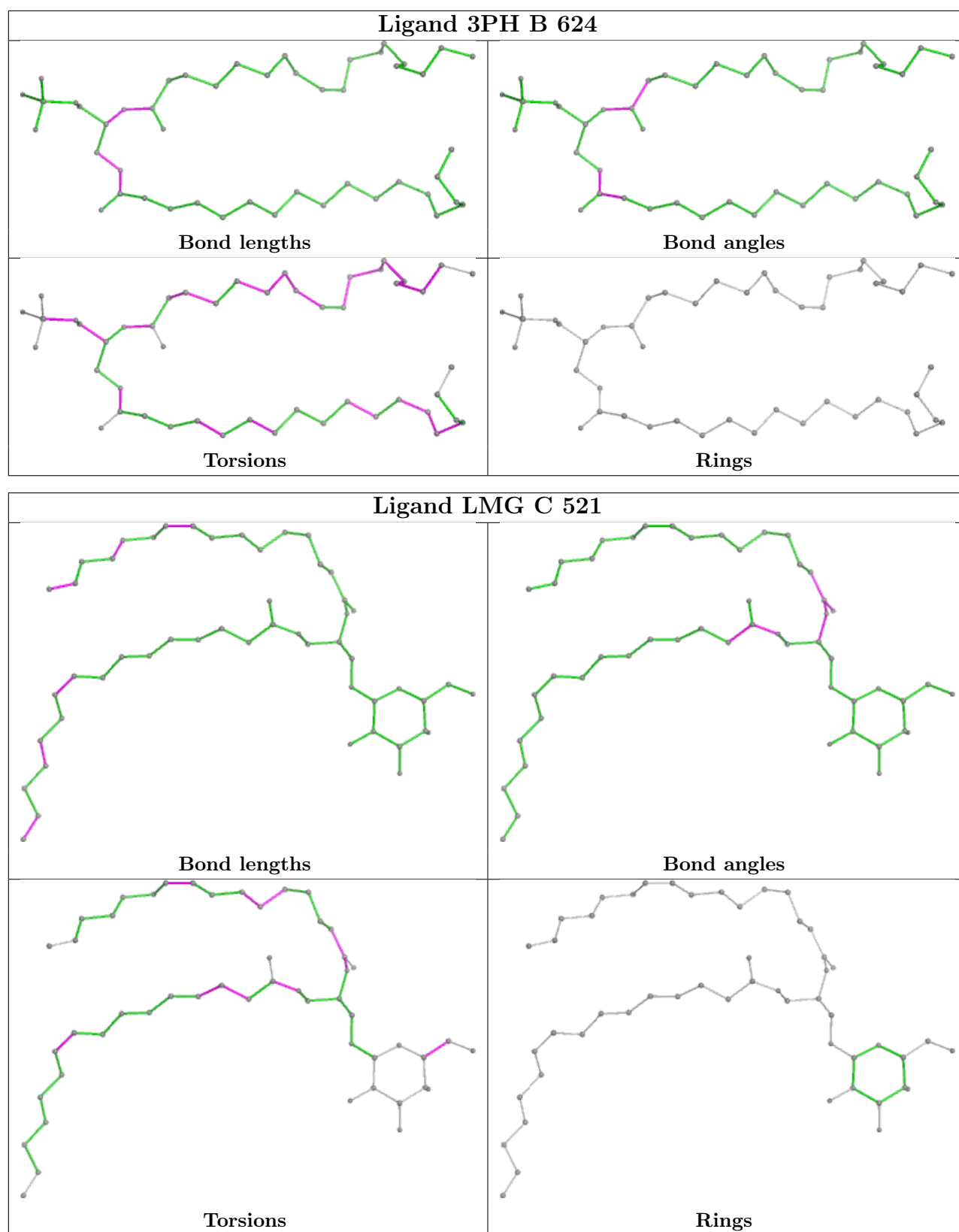


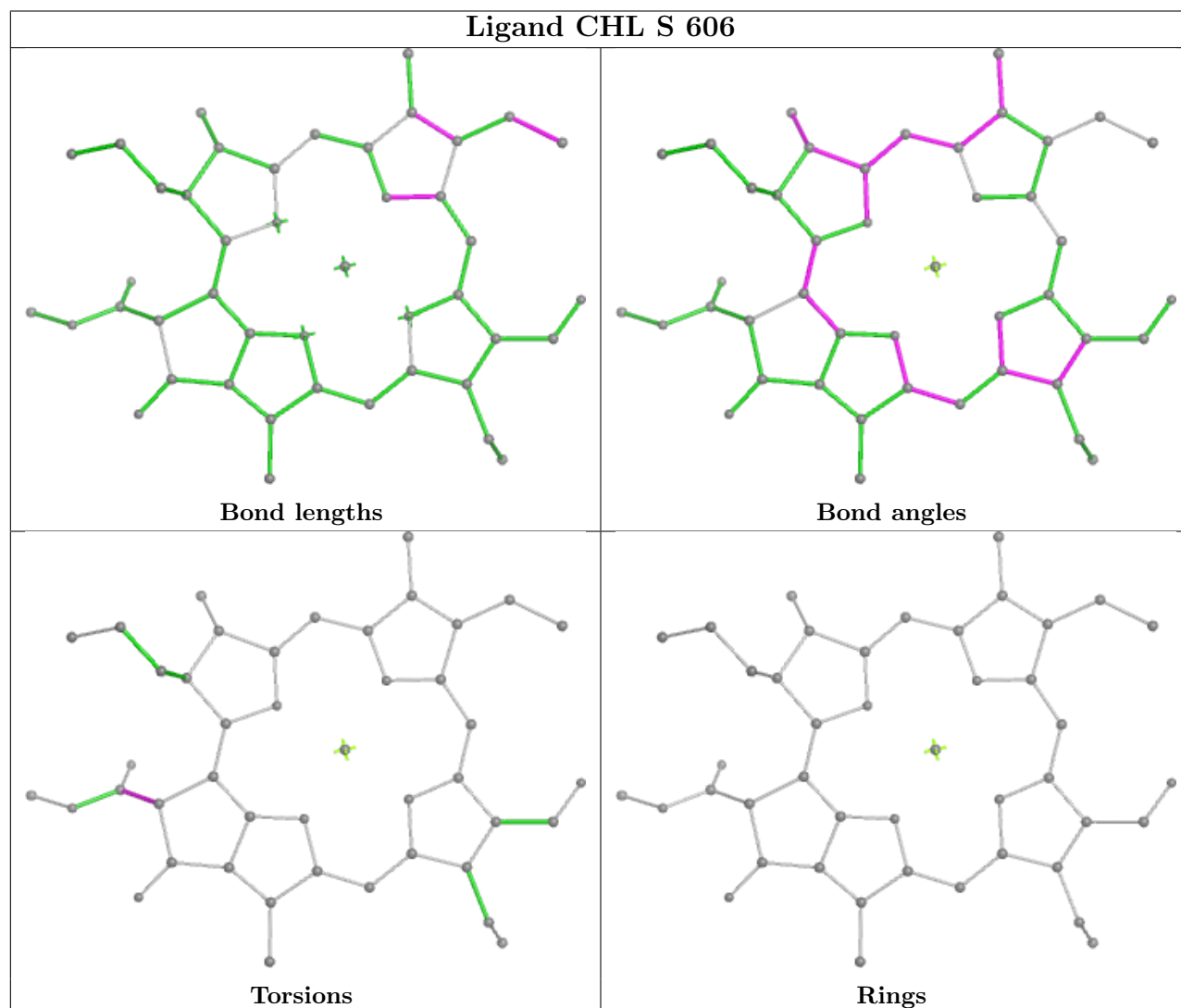
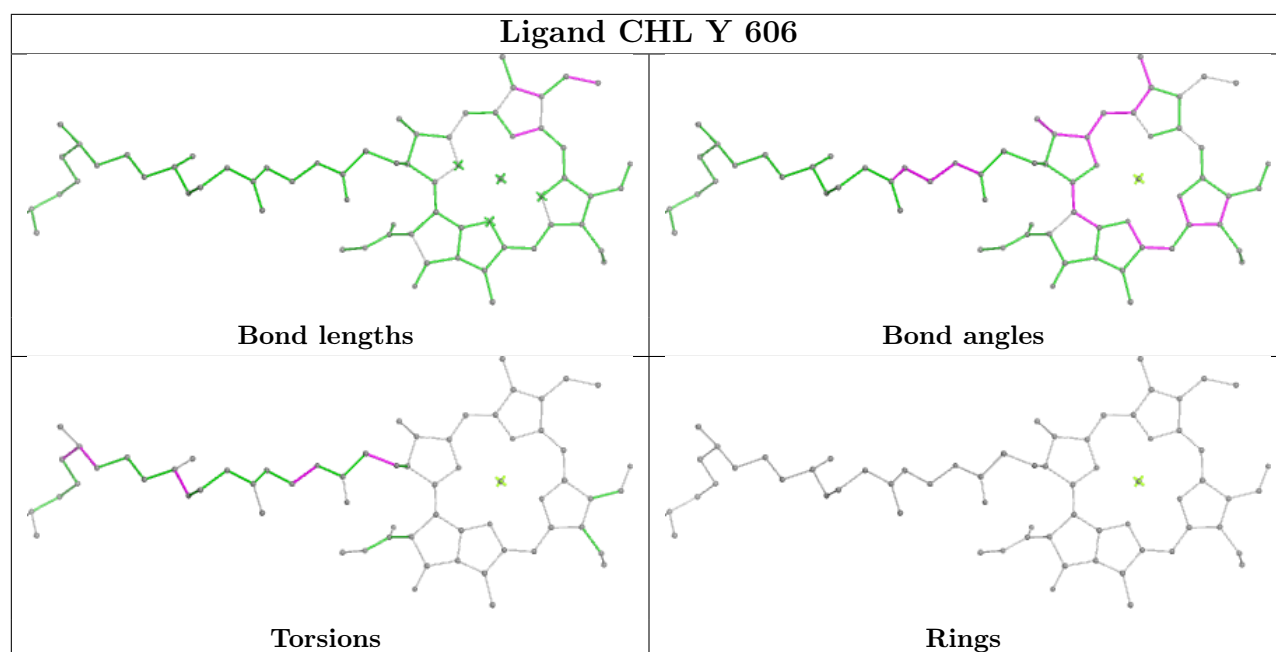
Ligand CLA b 602**Bond lengths****Bond angles****Torsions****Rings****Ligand DGA b 625****Bond lengths****Bond angles****Torsions****Rings**

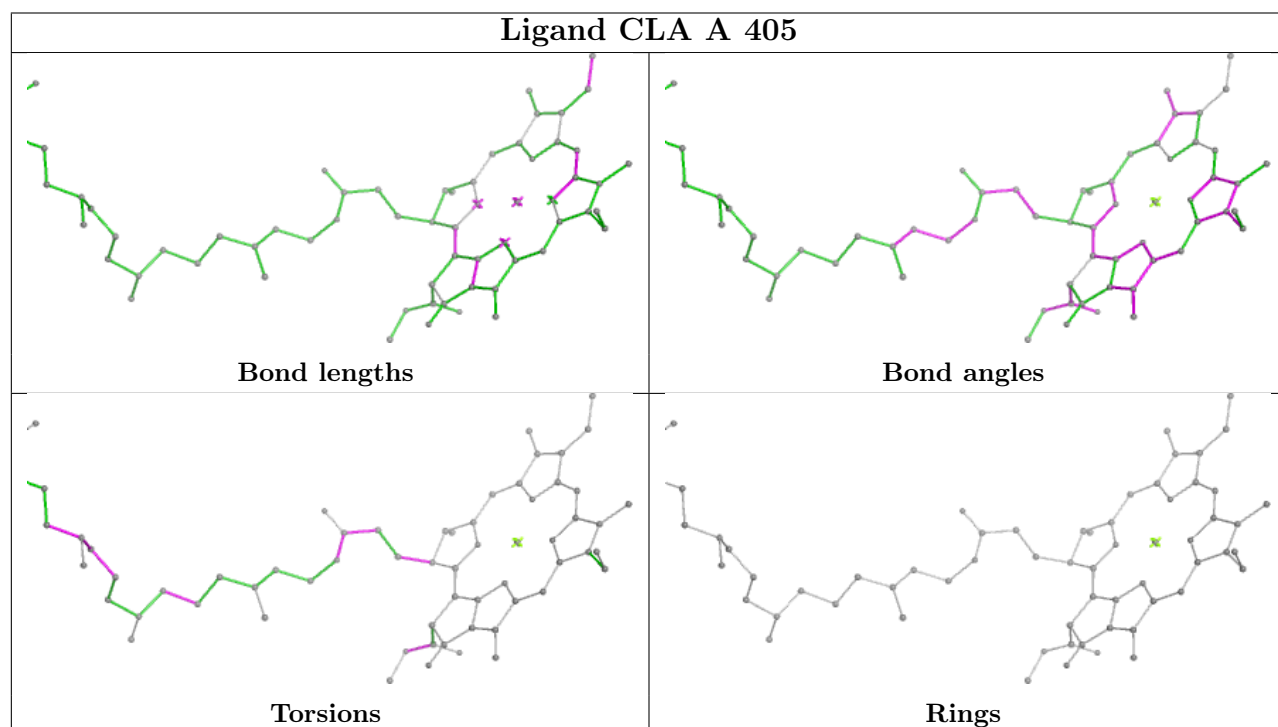
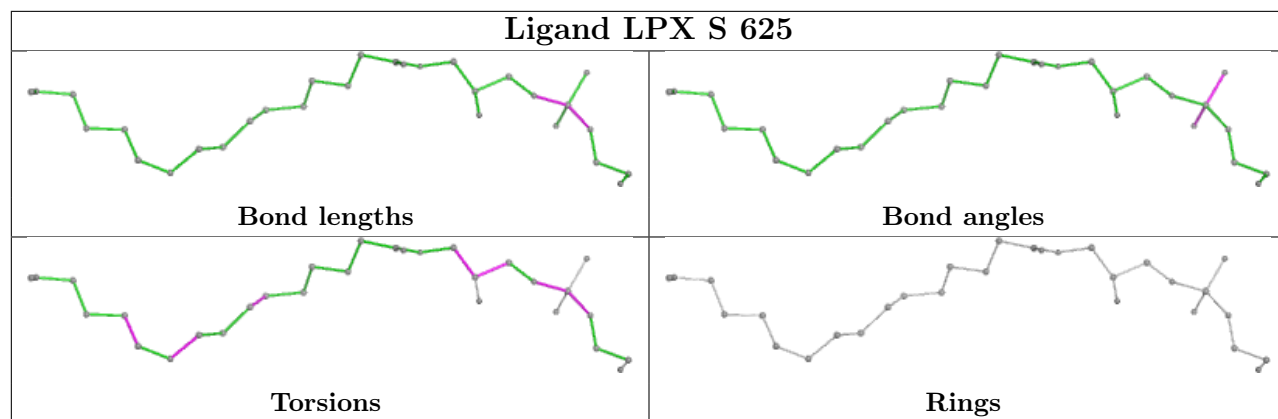




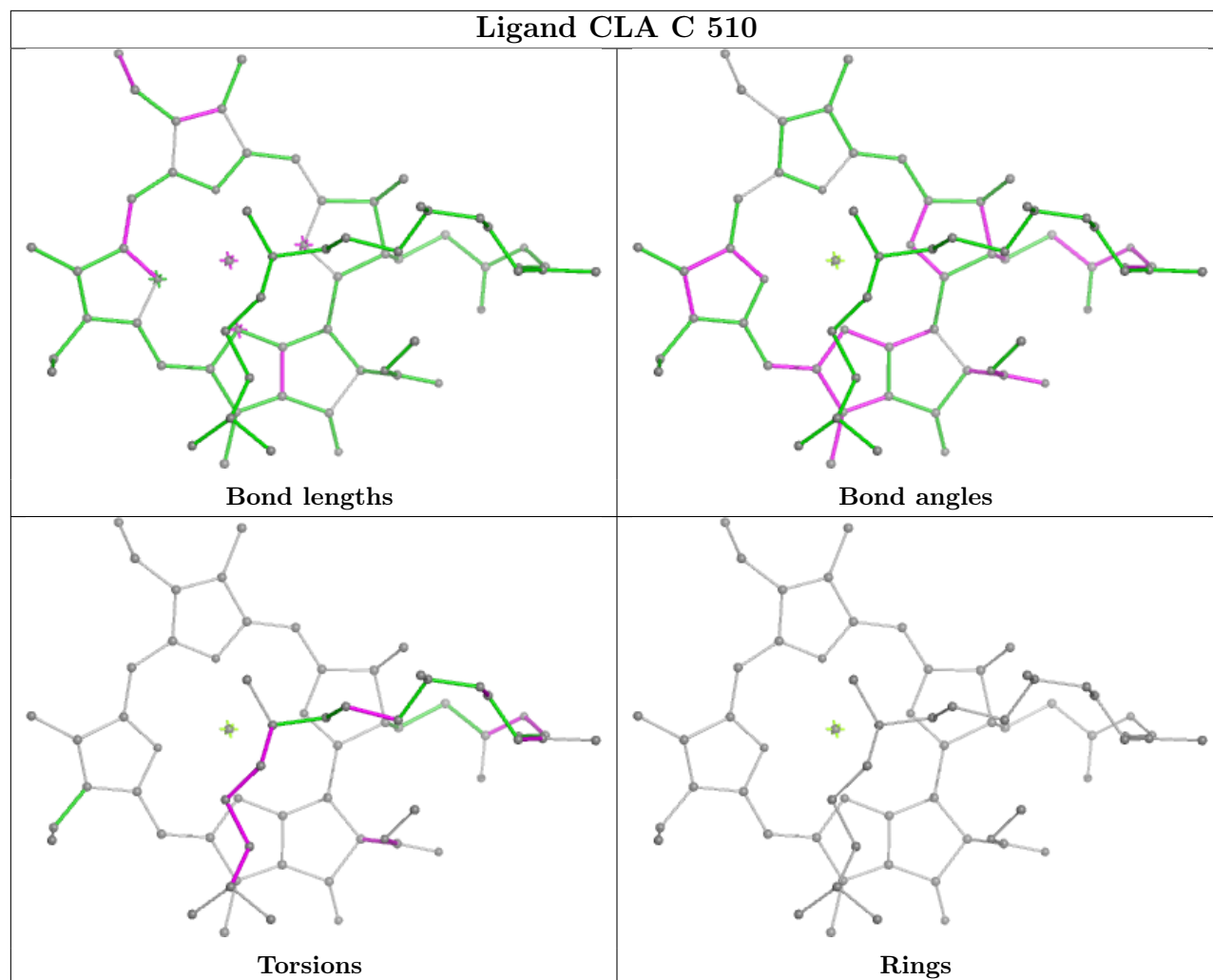


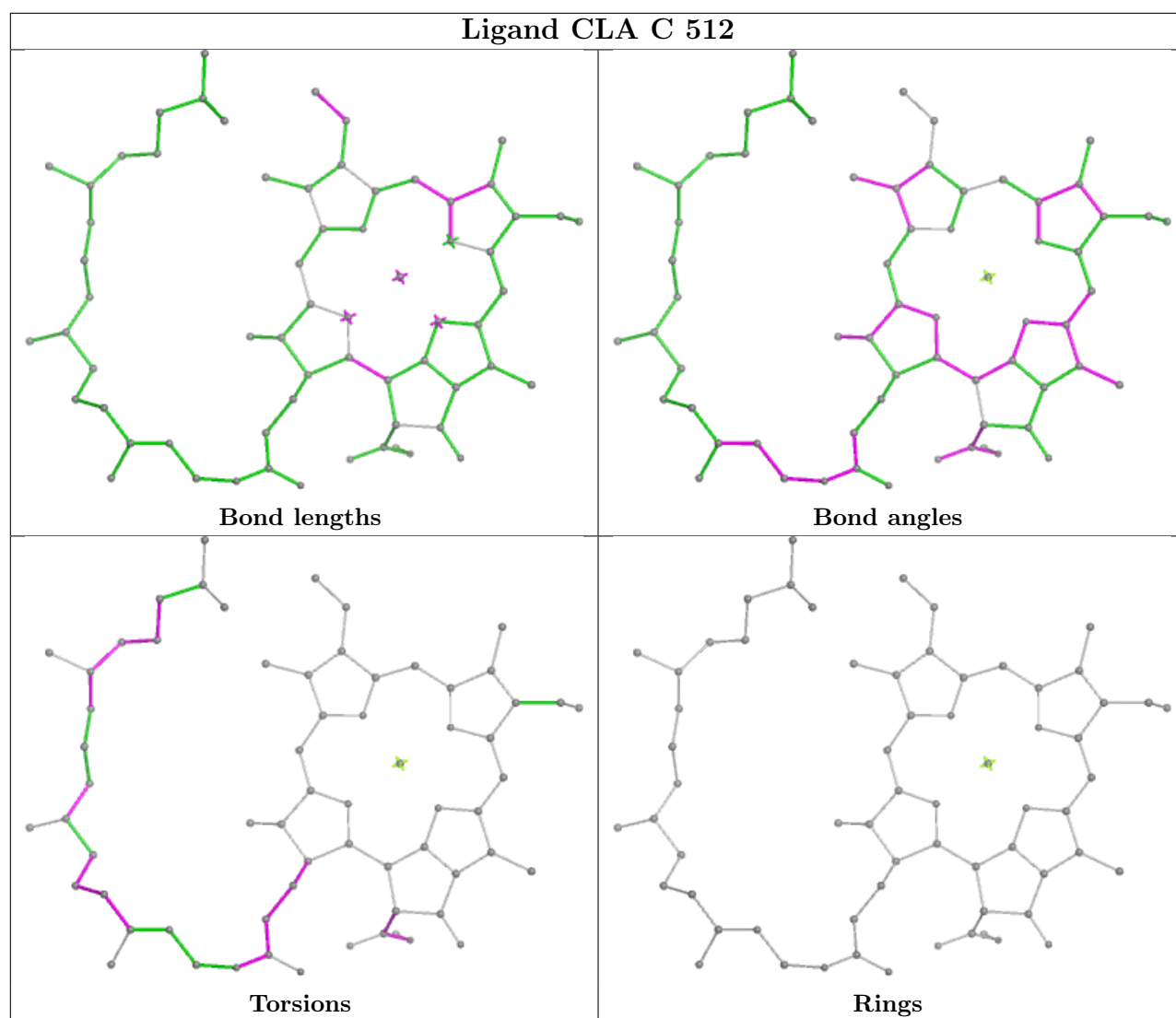


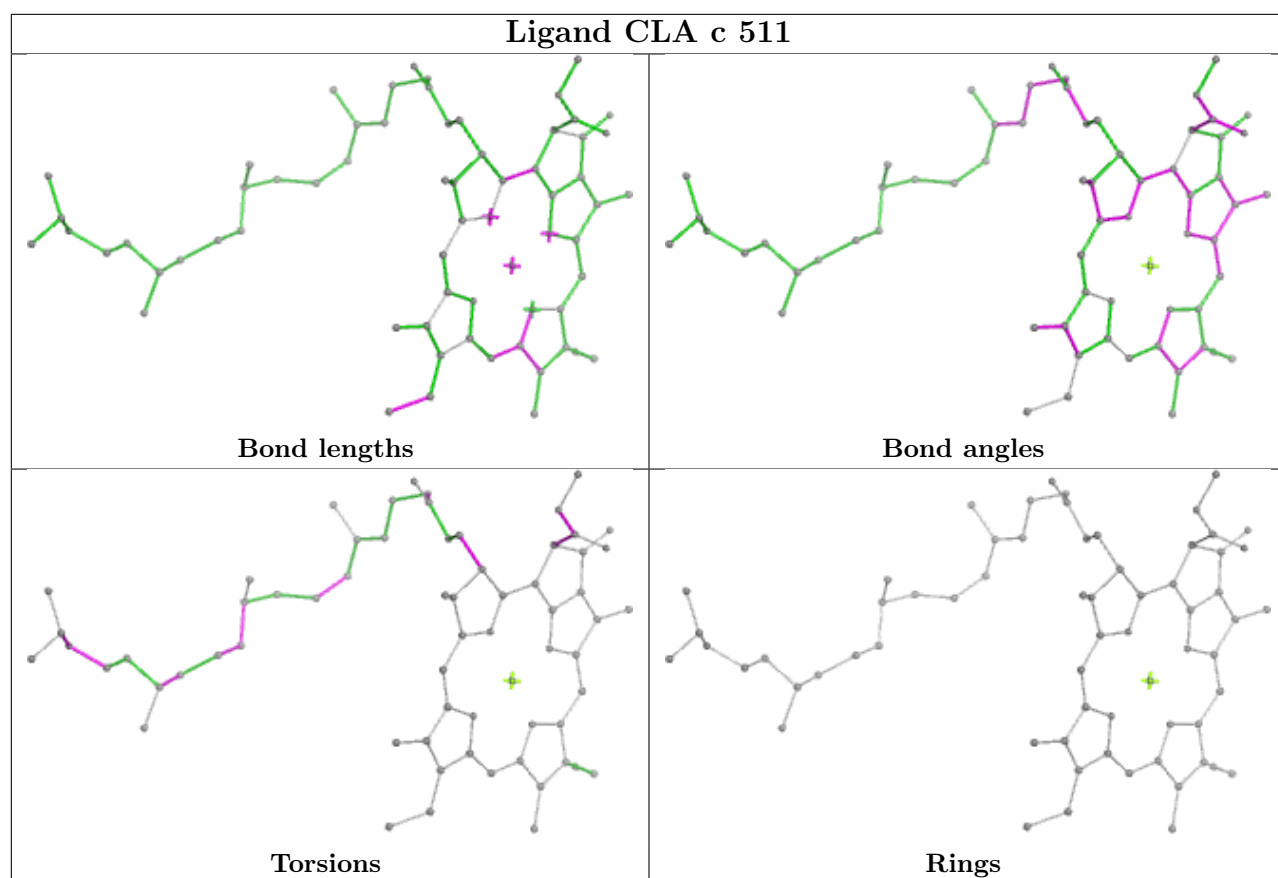


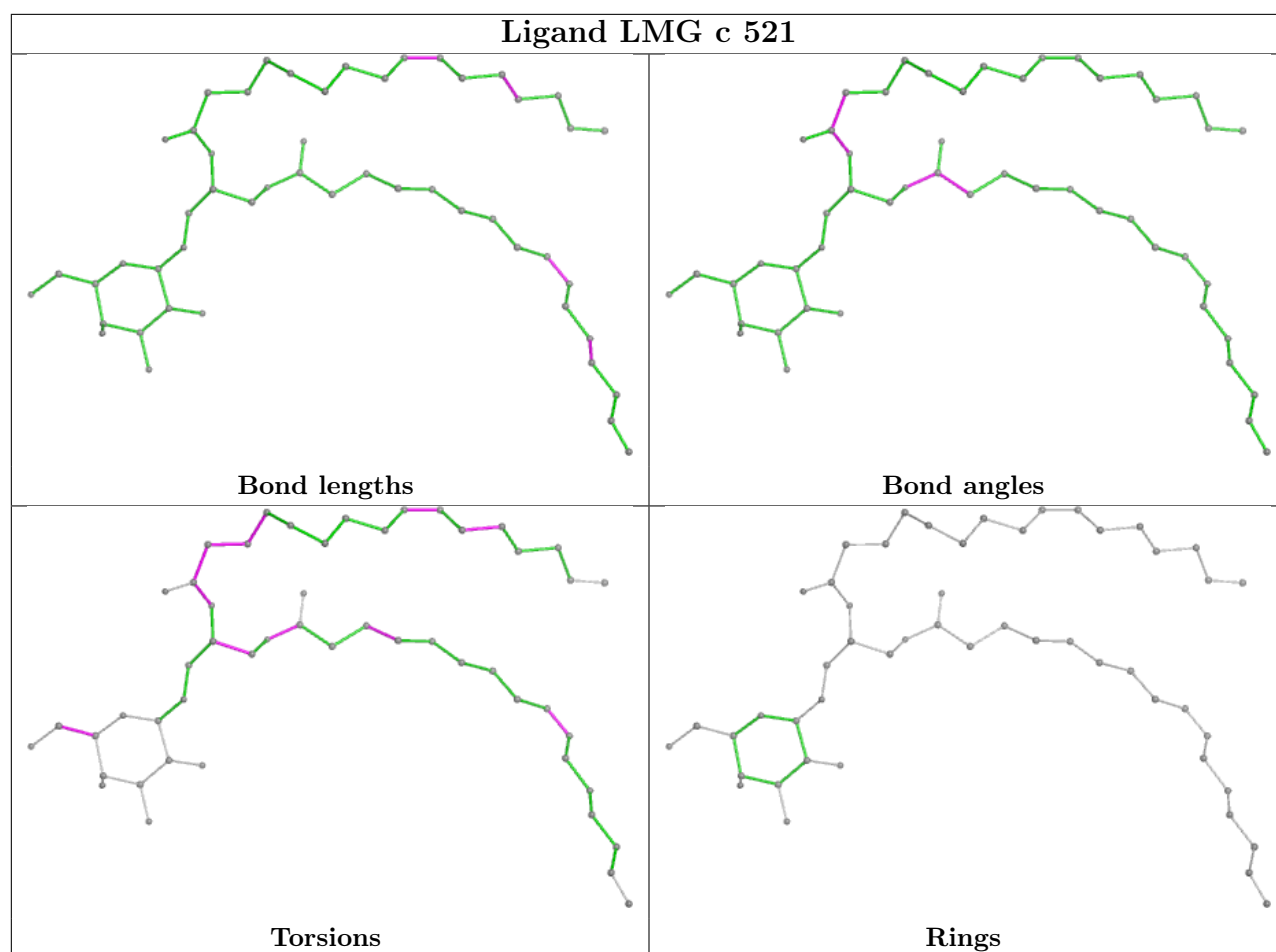


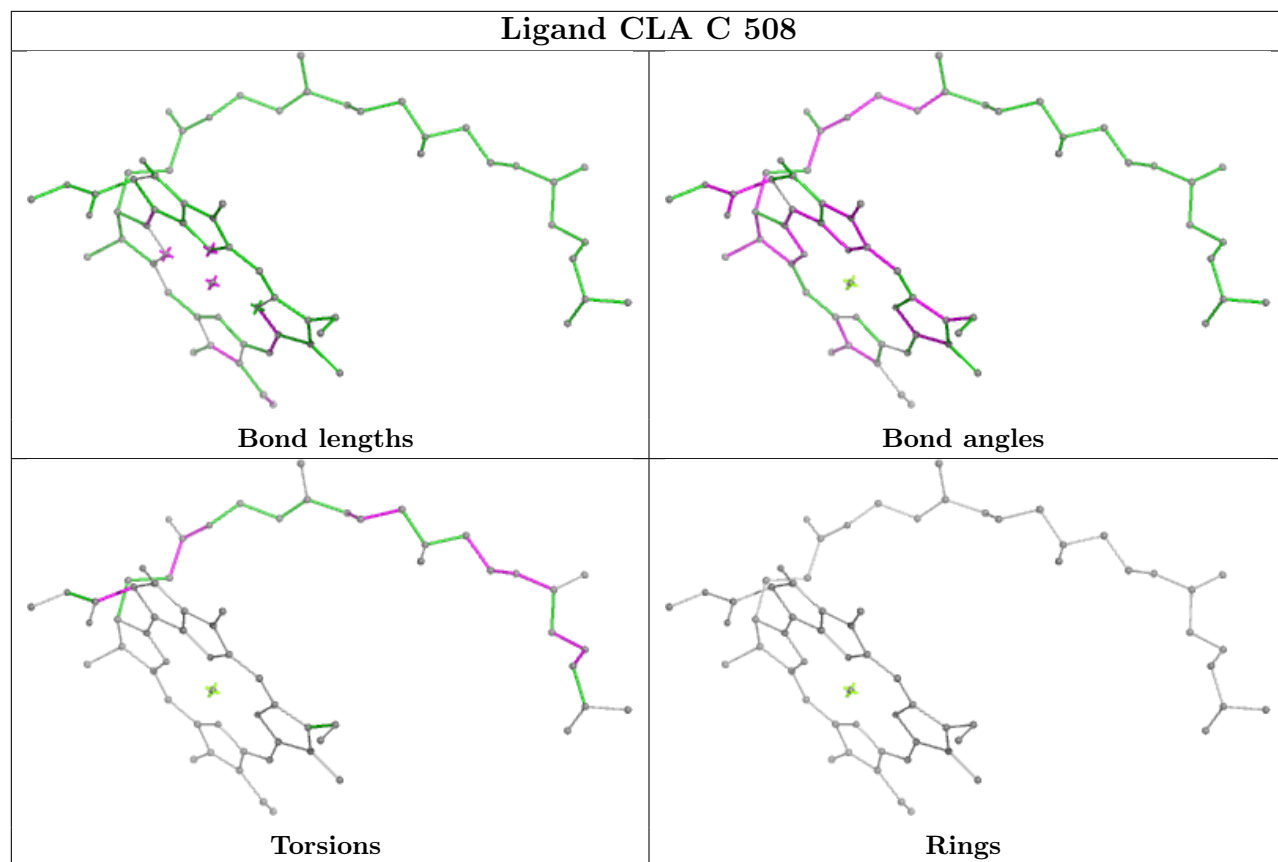
Ligand CLA C 510



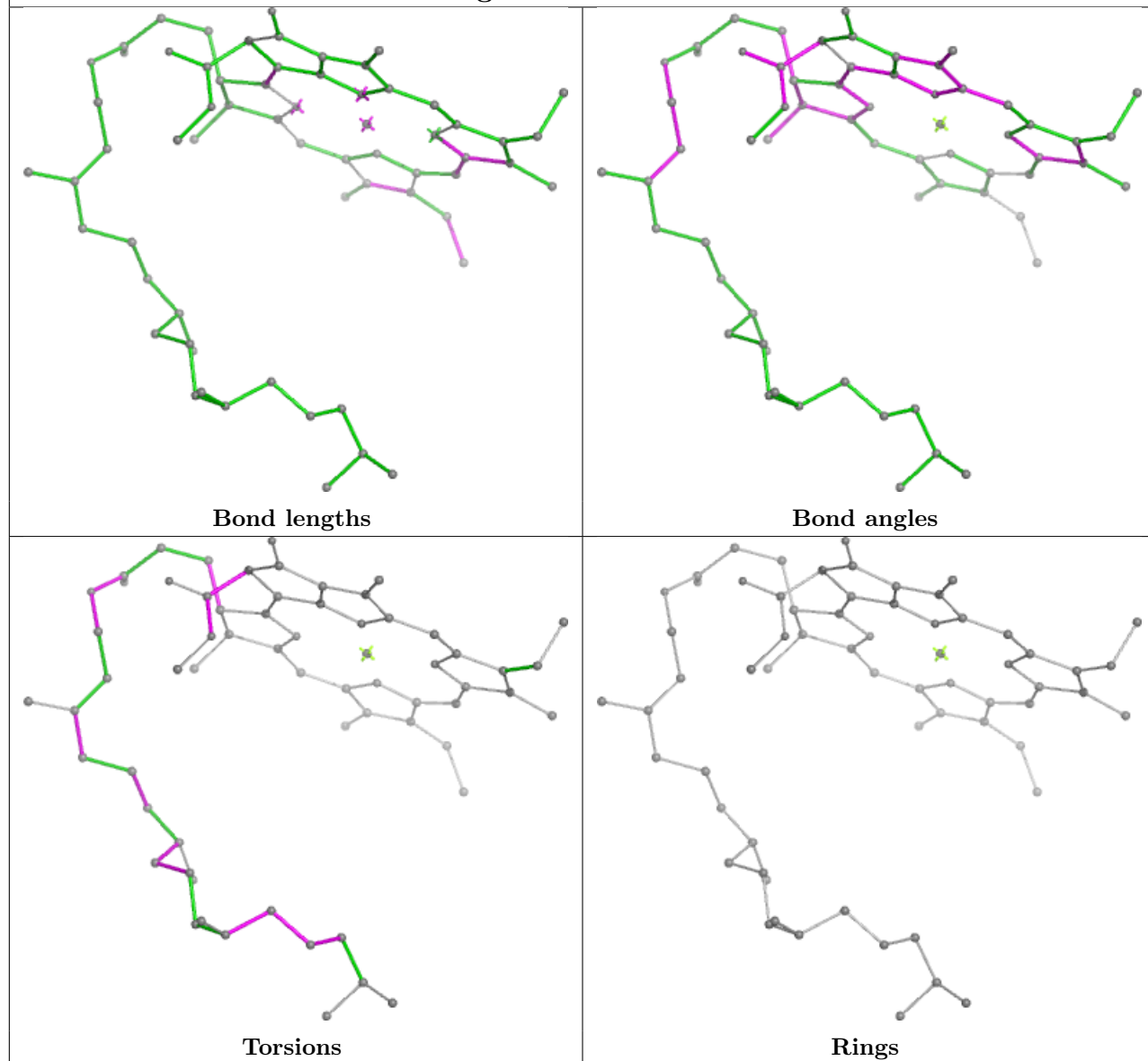




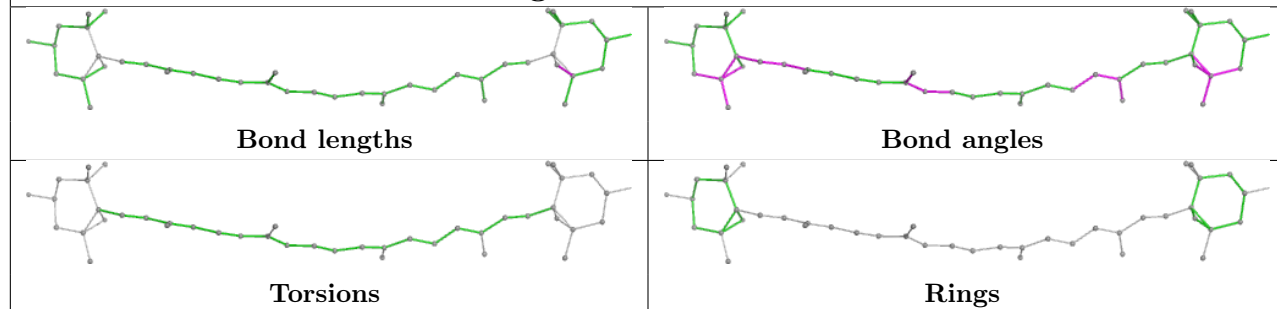


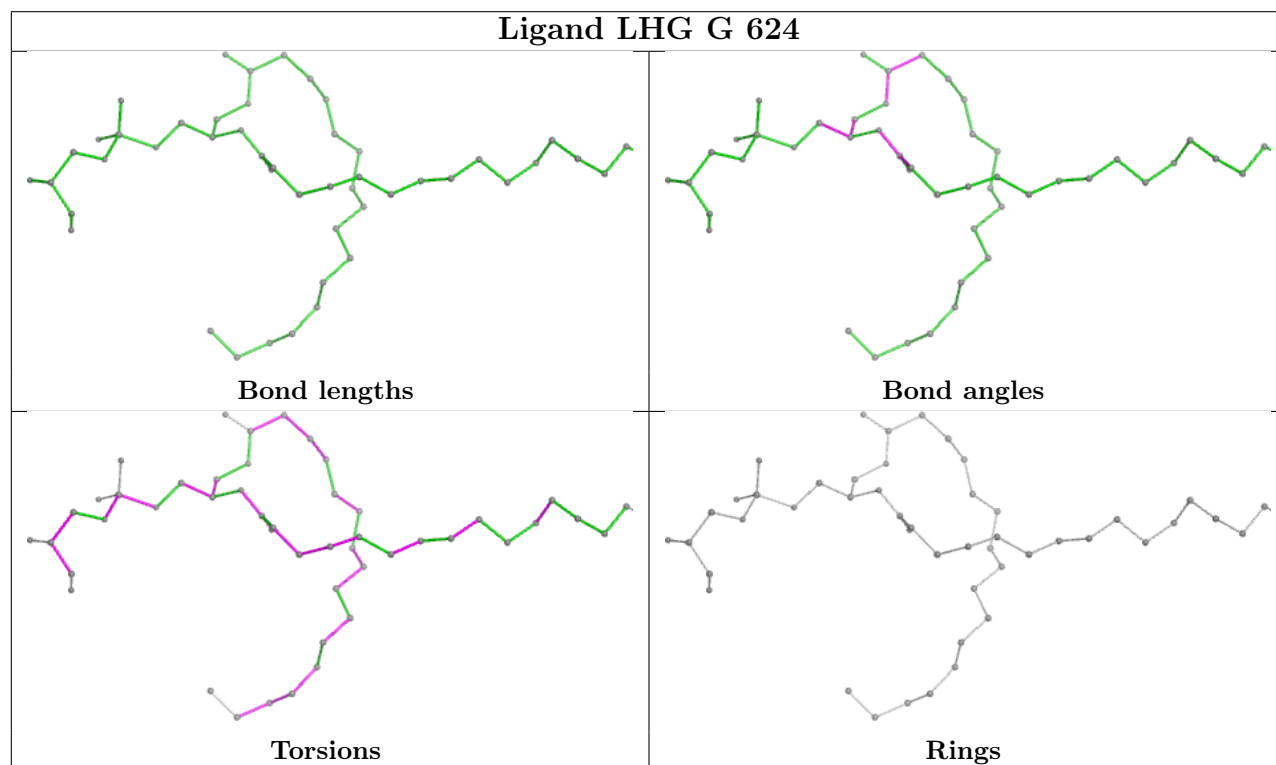
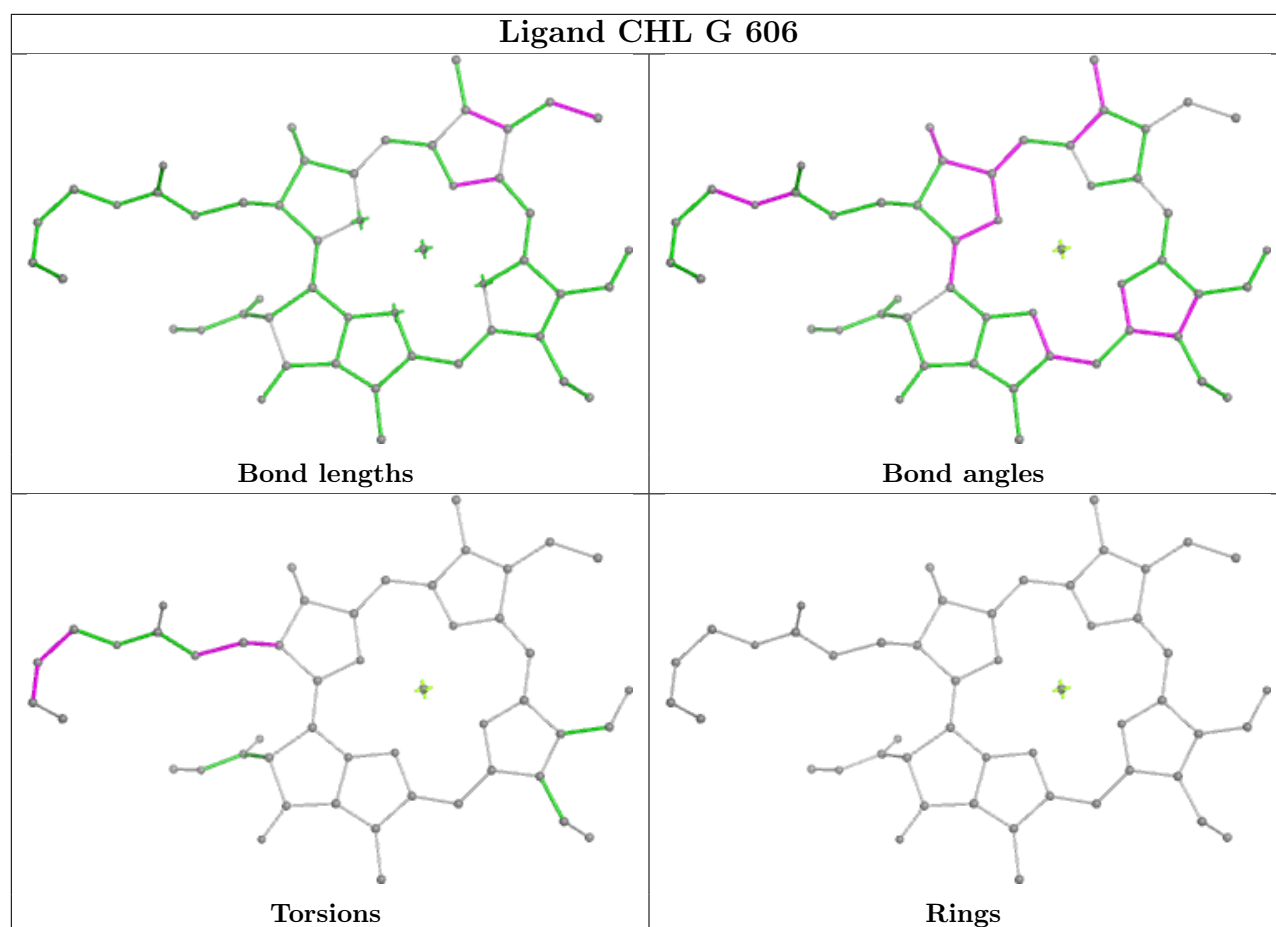


Ligand CLA N 603

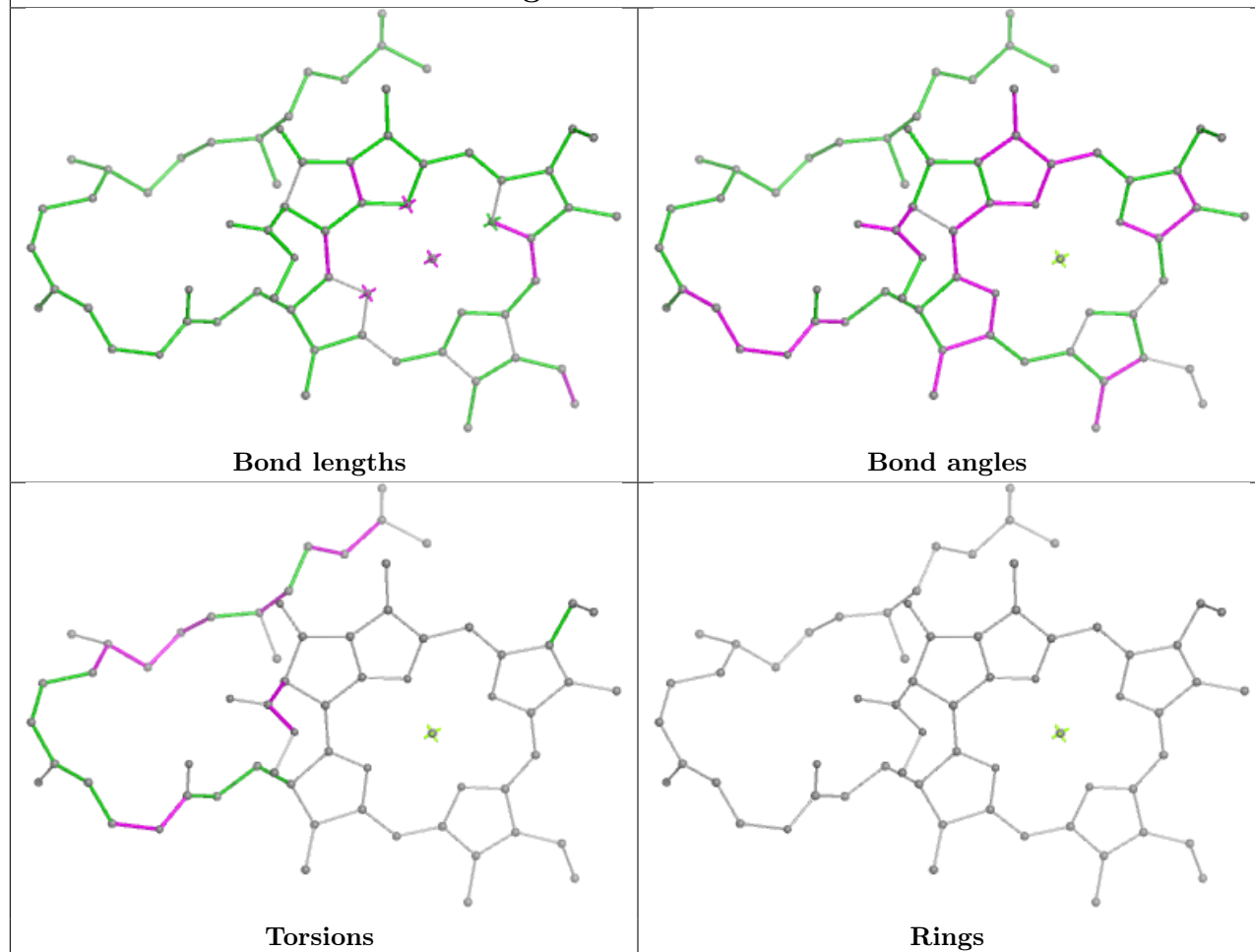


Ligand XAT N 622

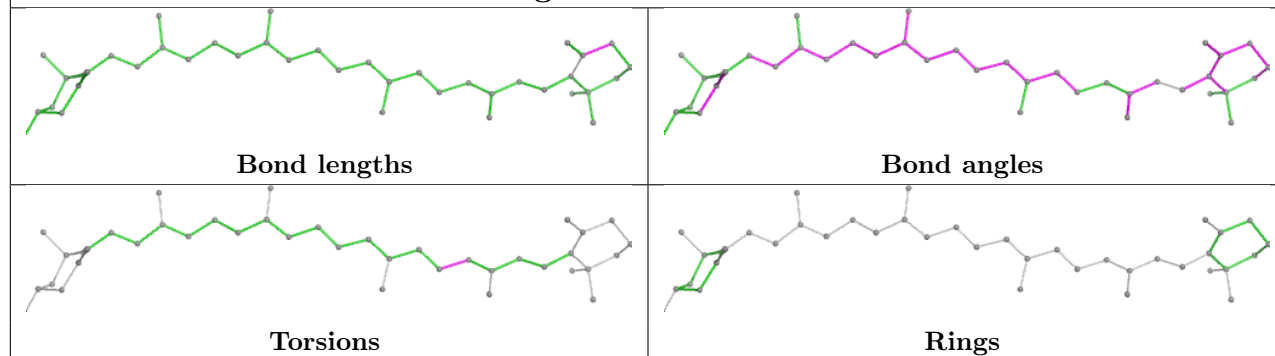


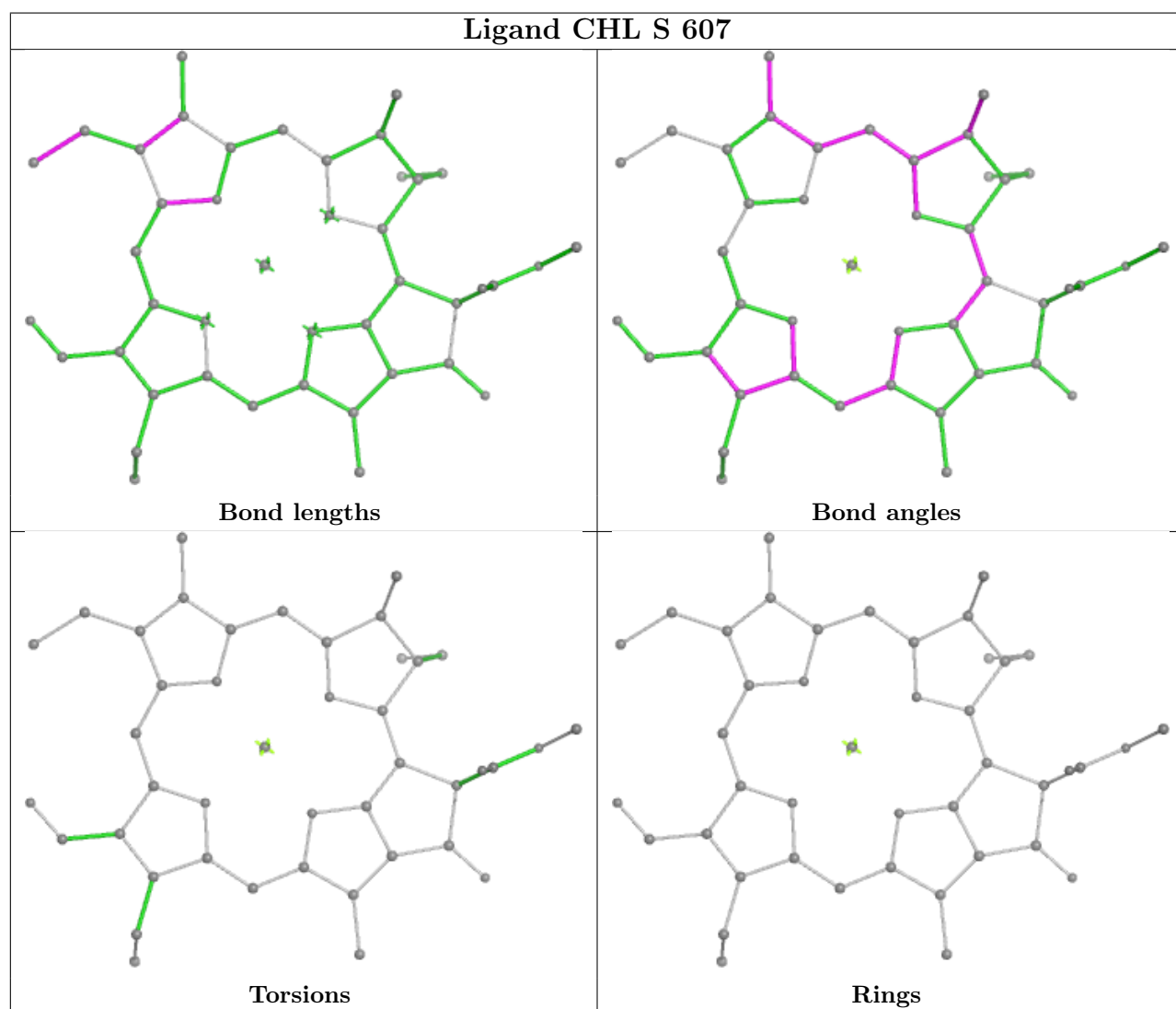
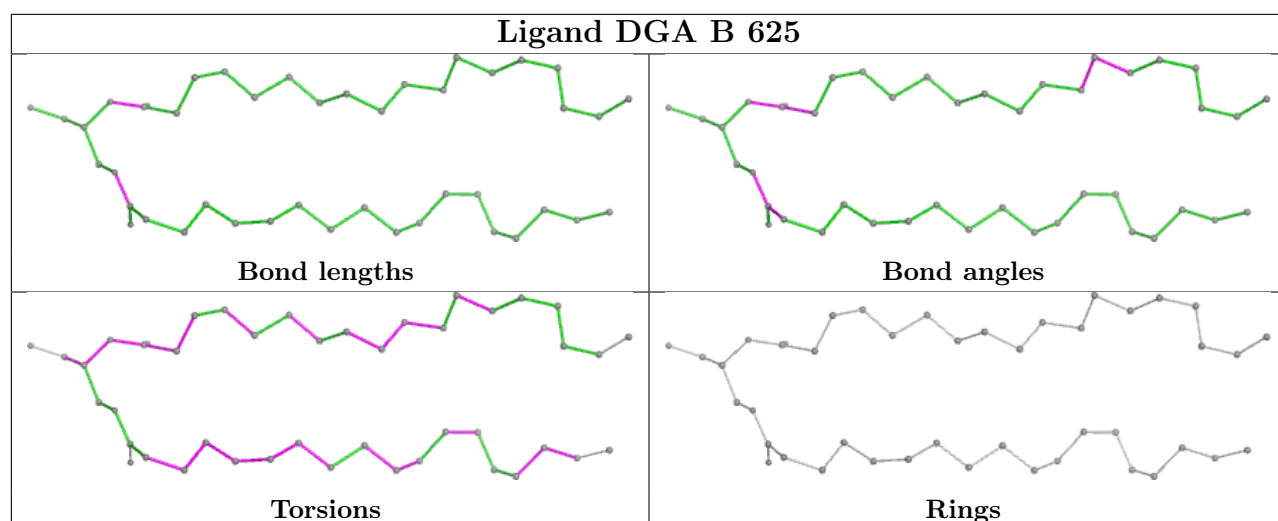


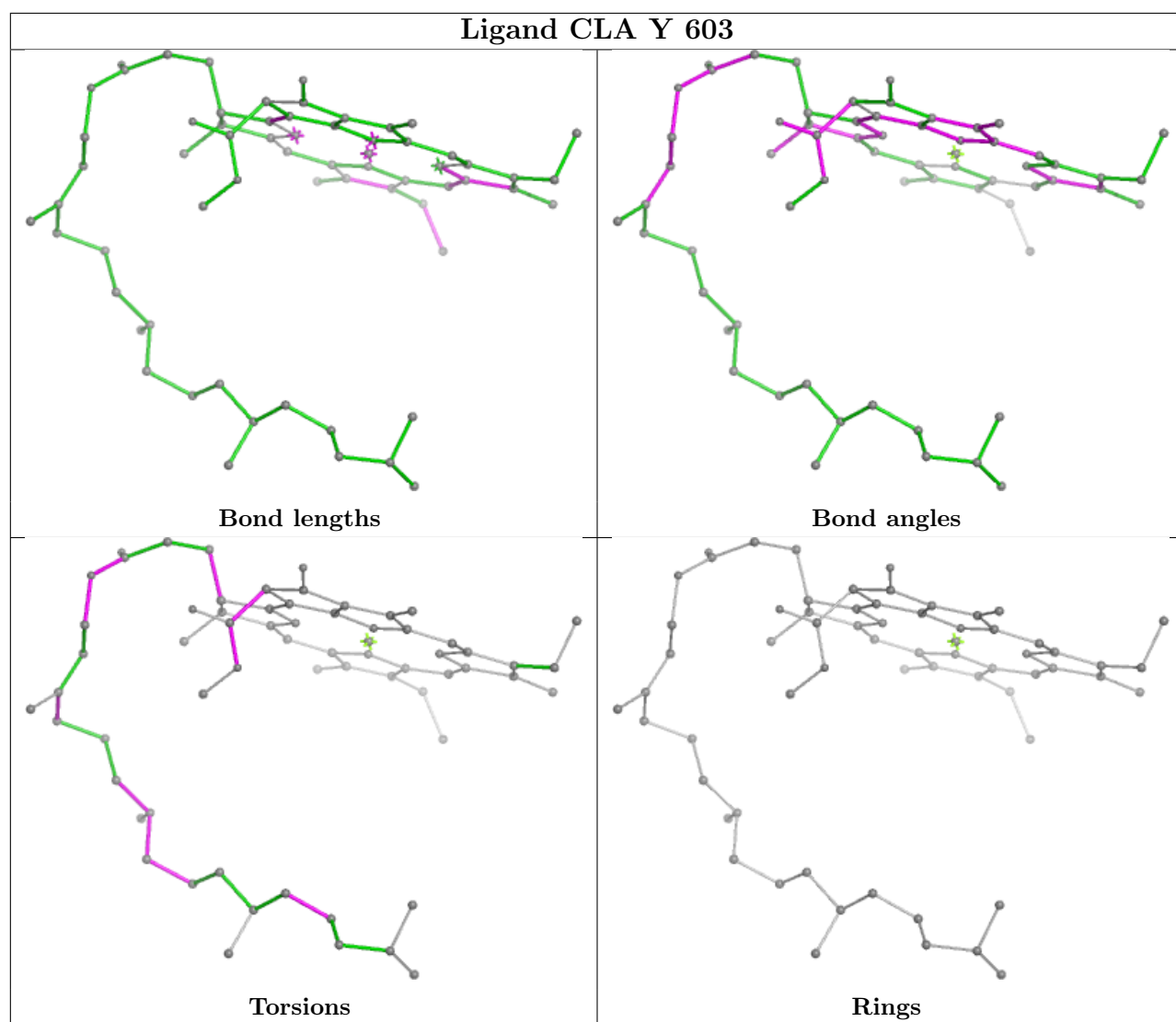
Ligand CLA C 509

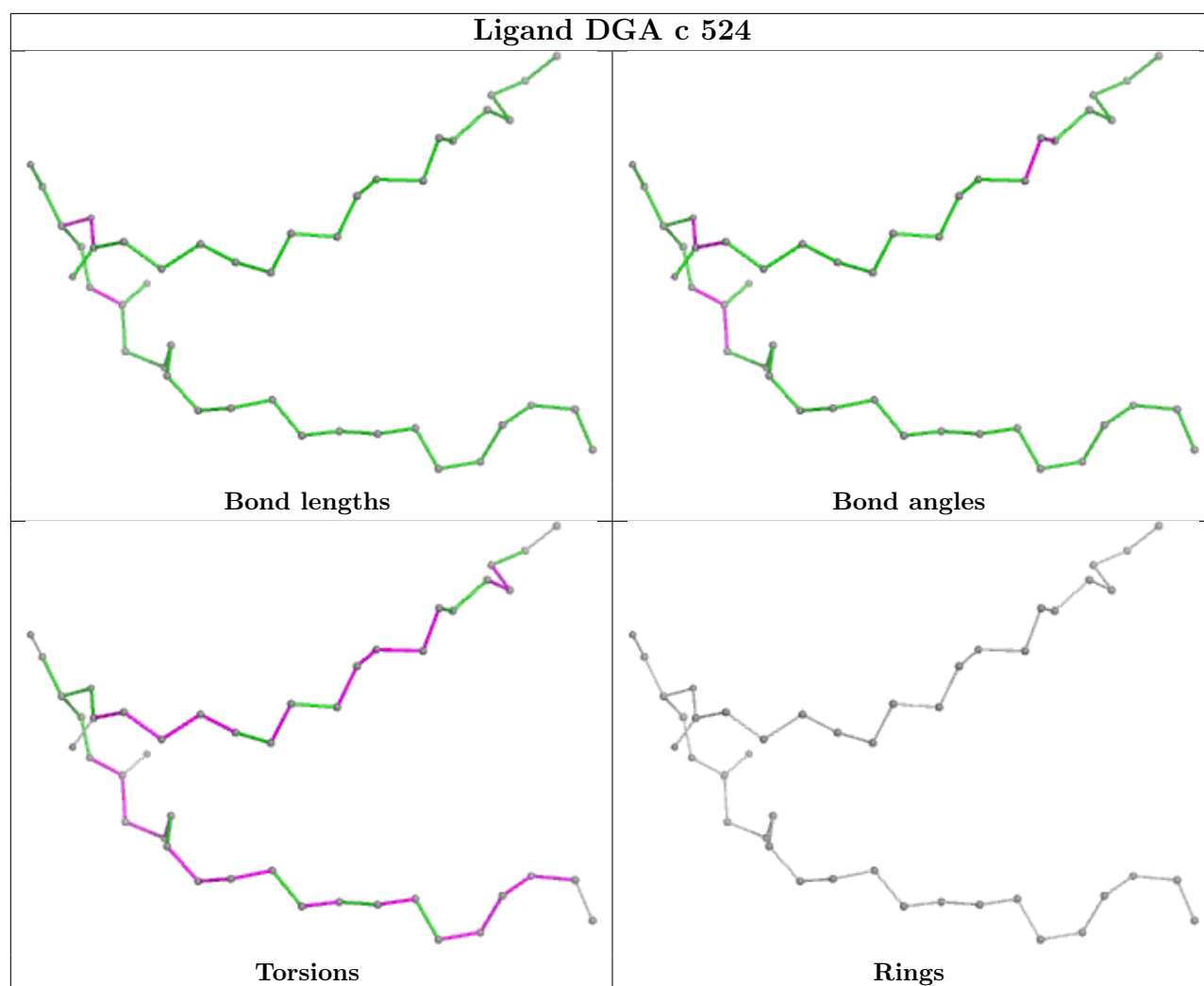


Ligand LUT S 621

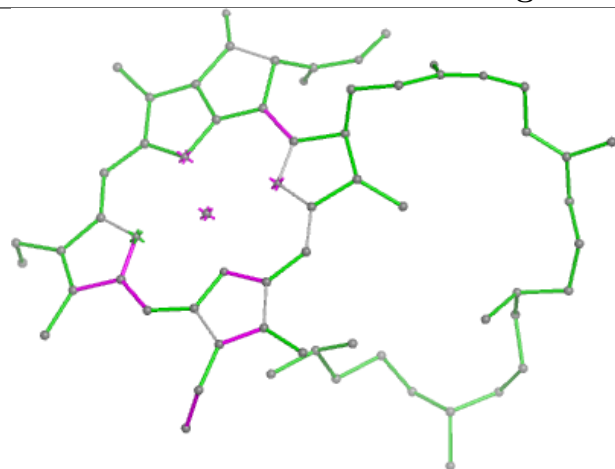




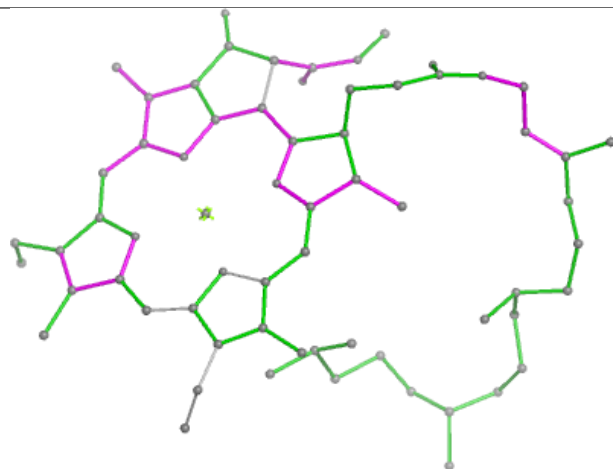




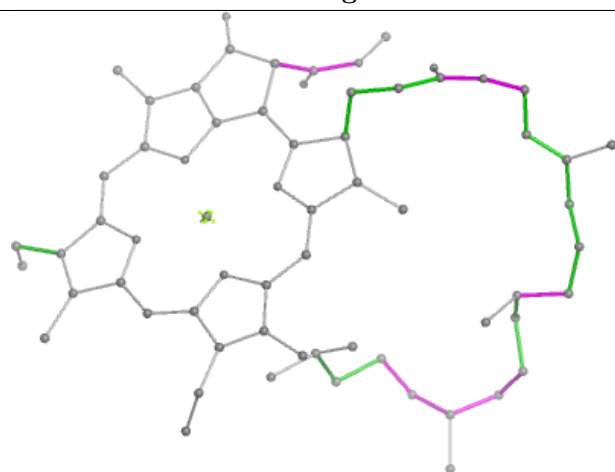
Ligand CLA B 616



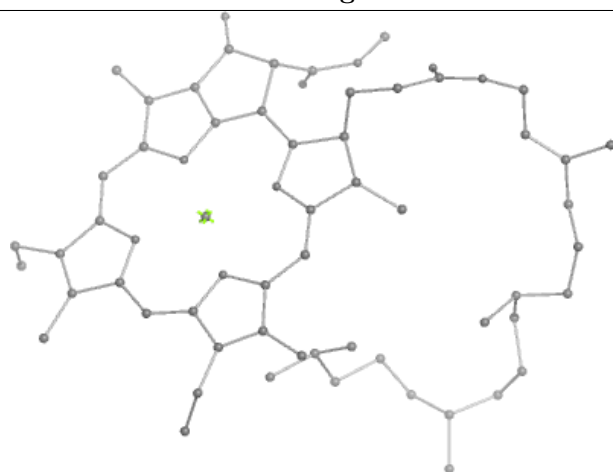
Bond lengths



Bond angles

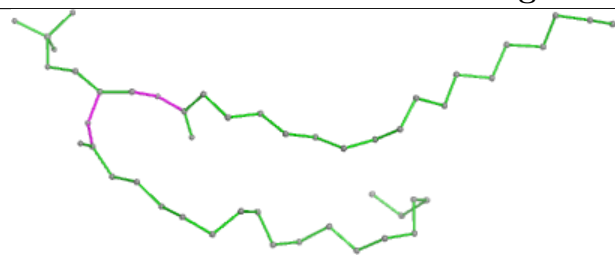


Torsions

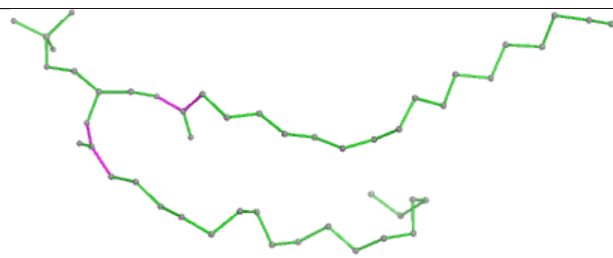


Rings

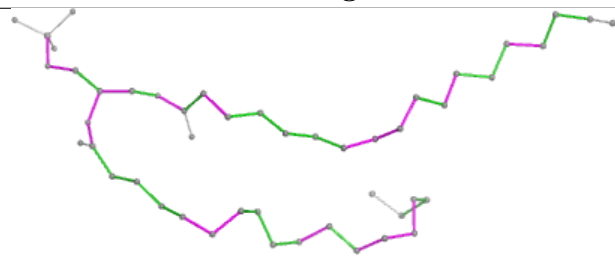
Ligand 3PH T 101



Bond lengths



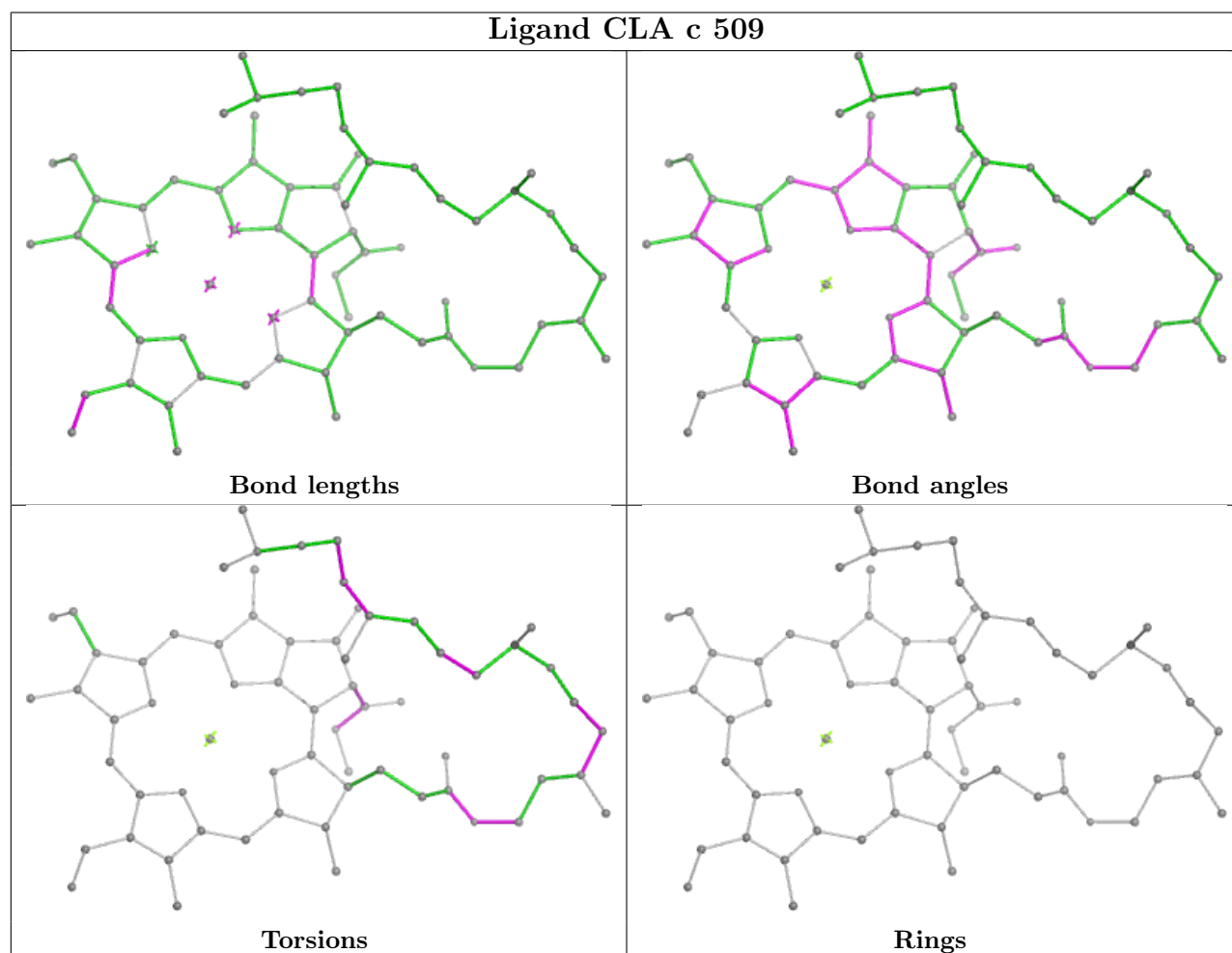
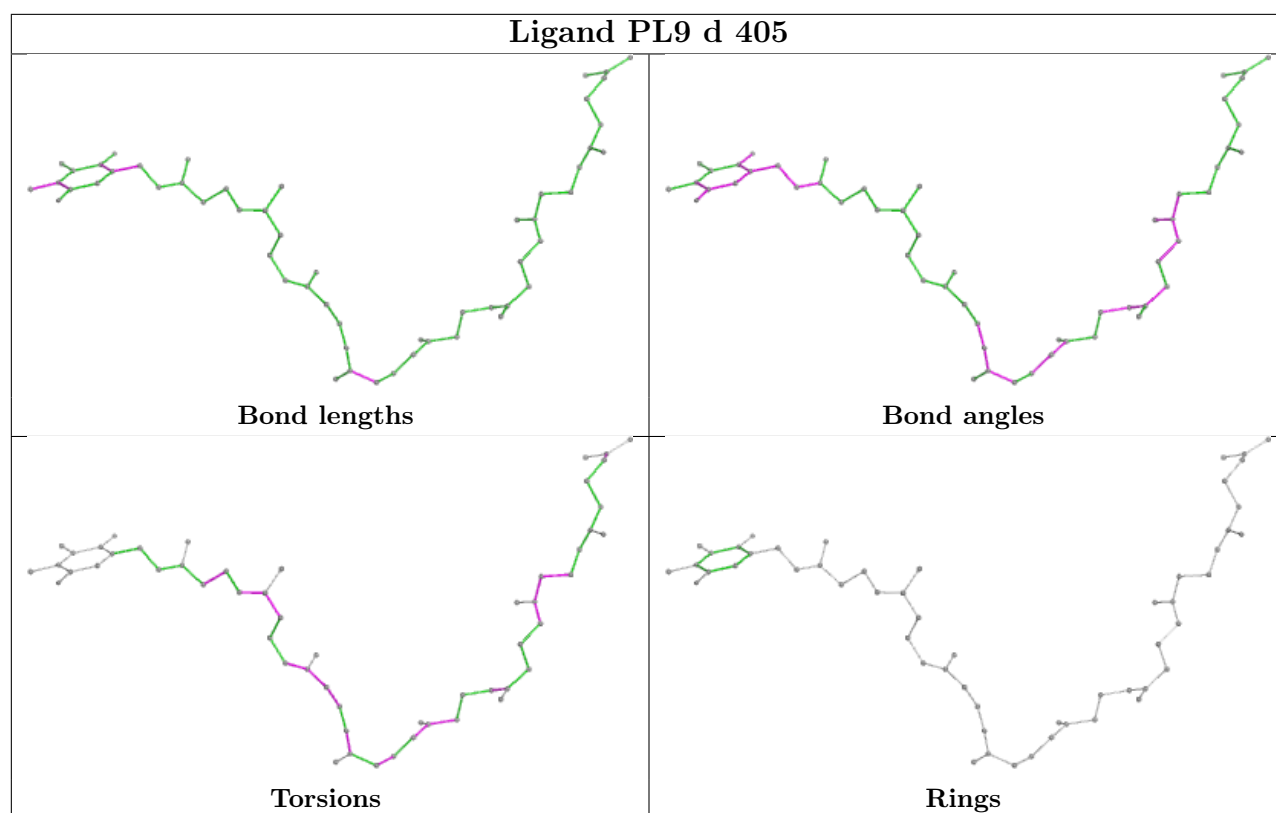
Bond angles

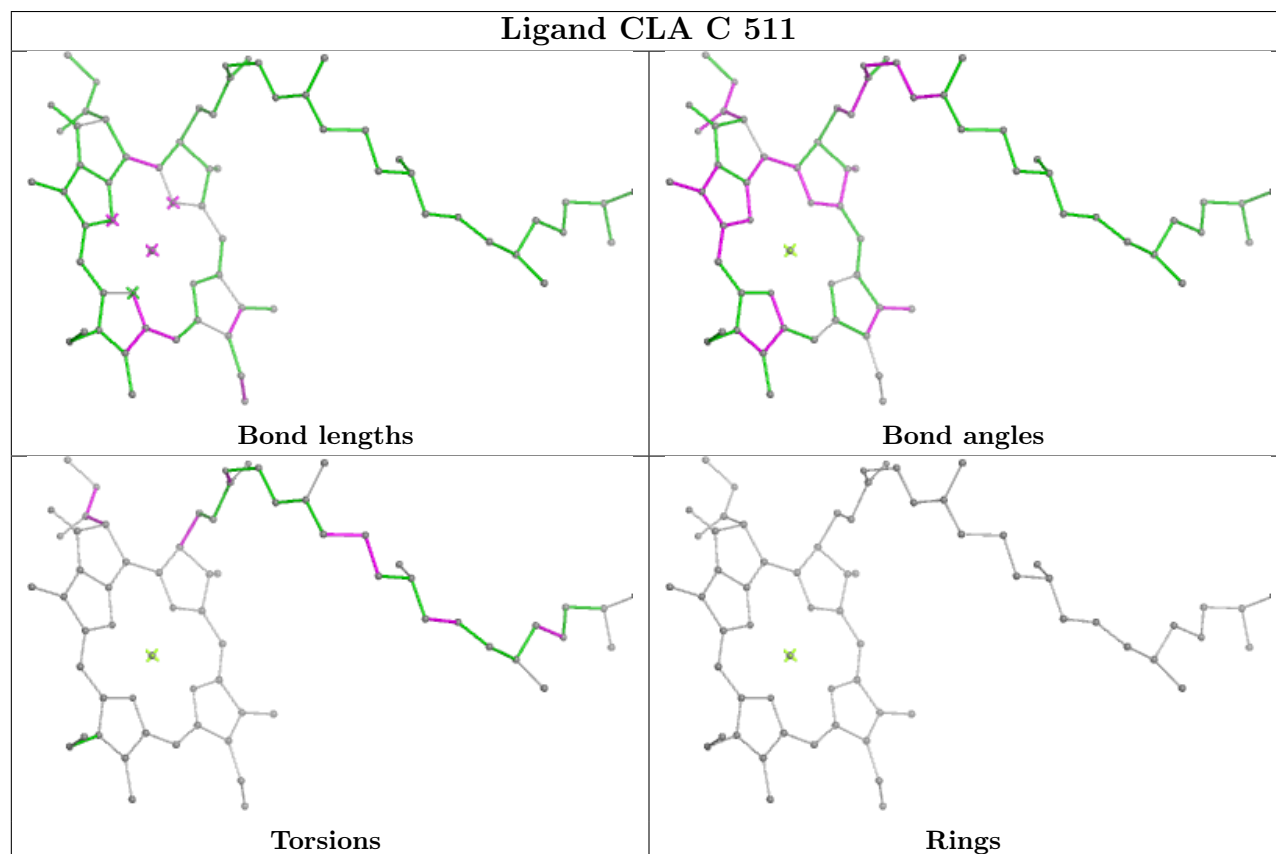
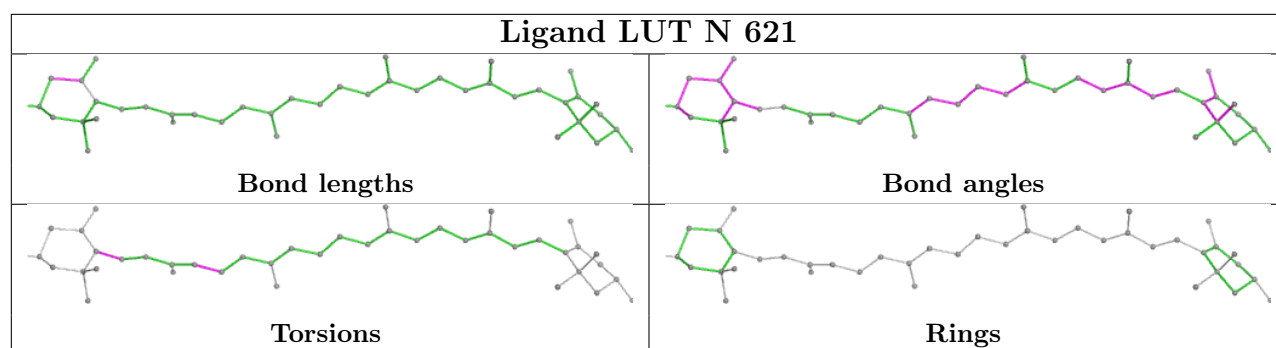


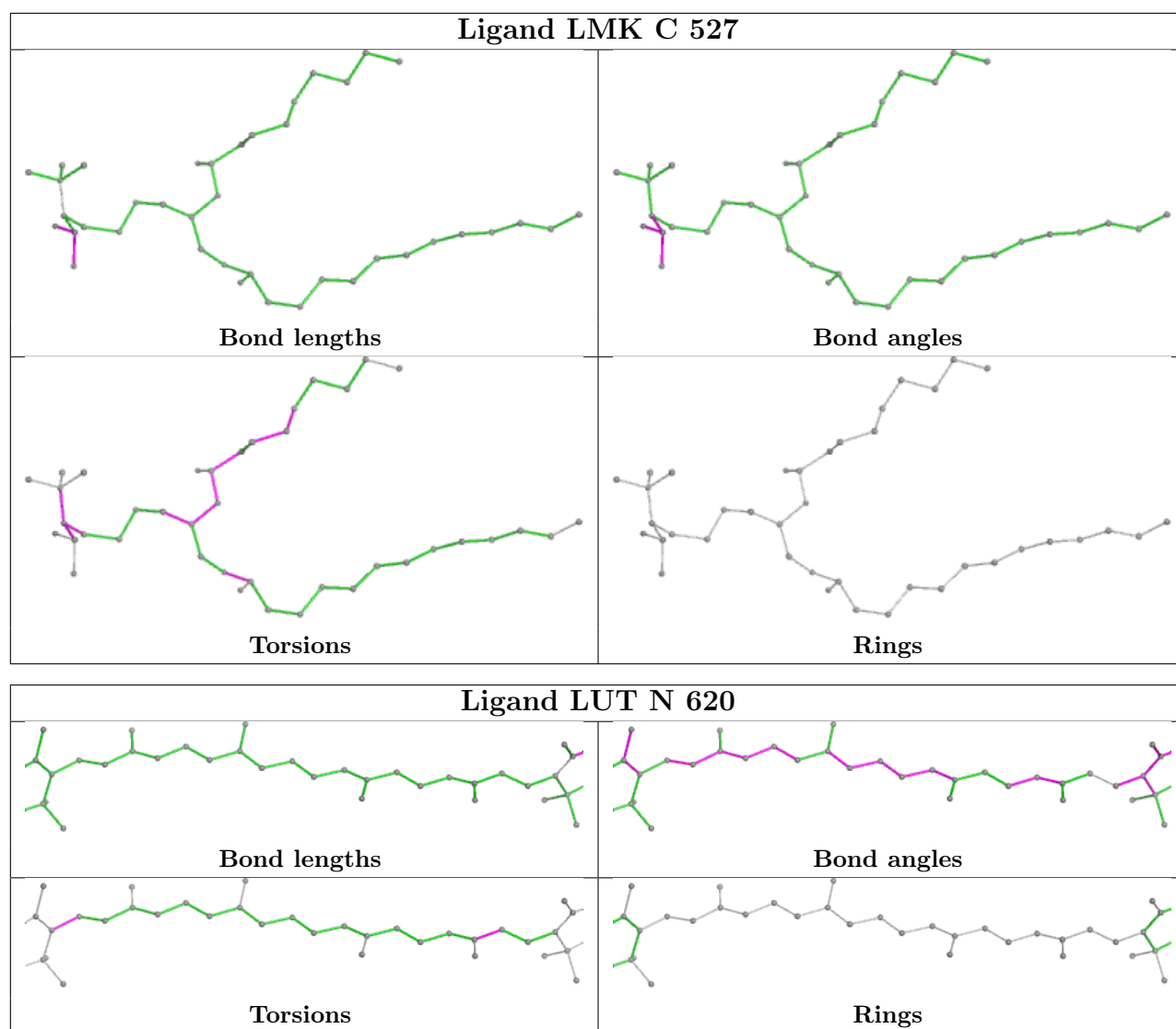
Torsions

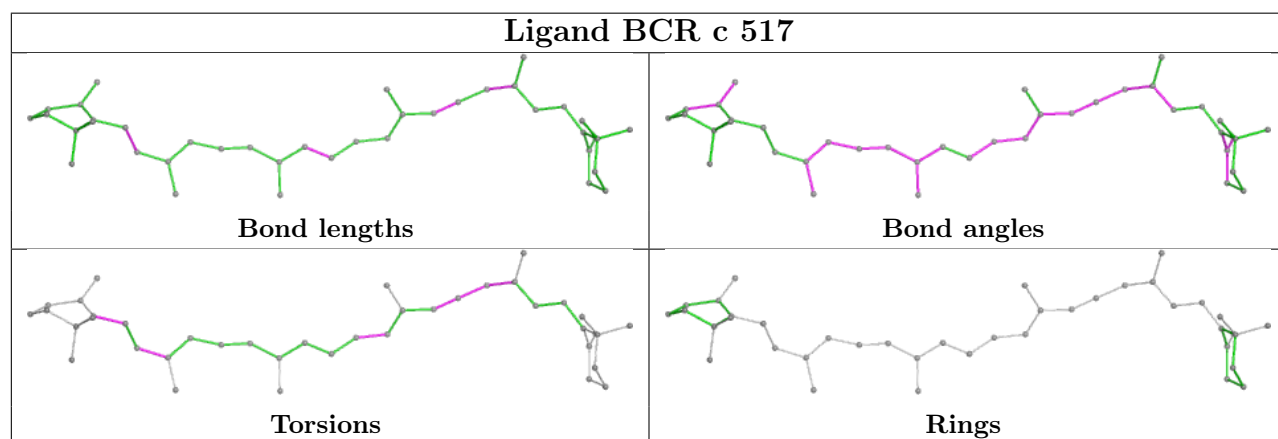
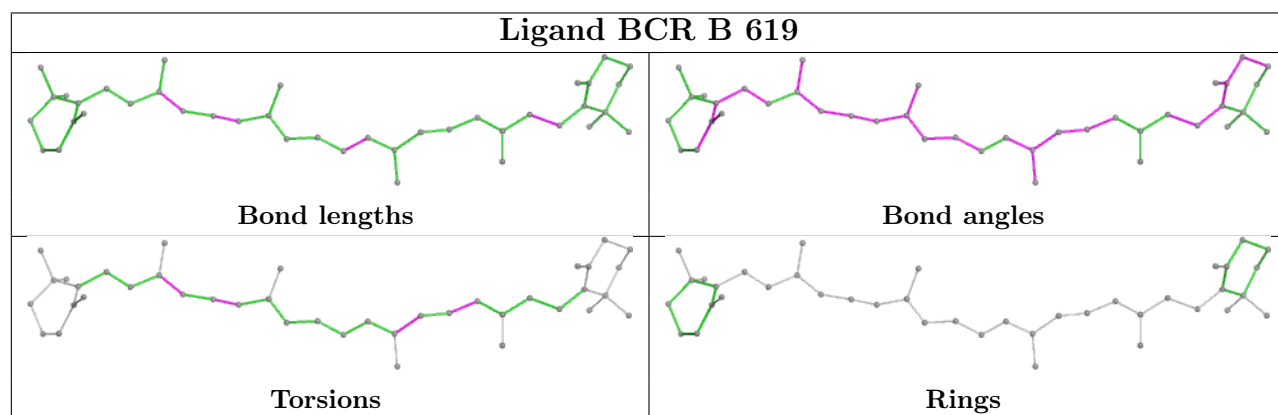
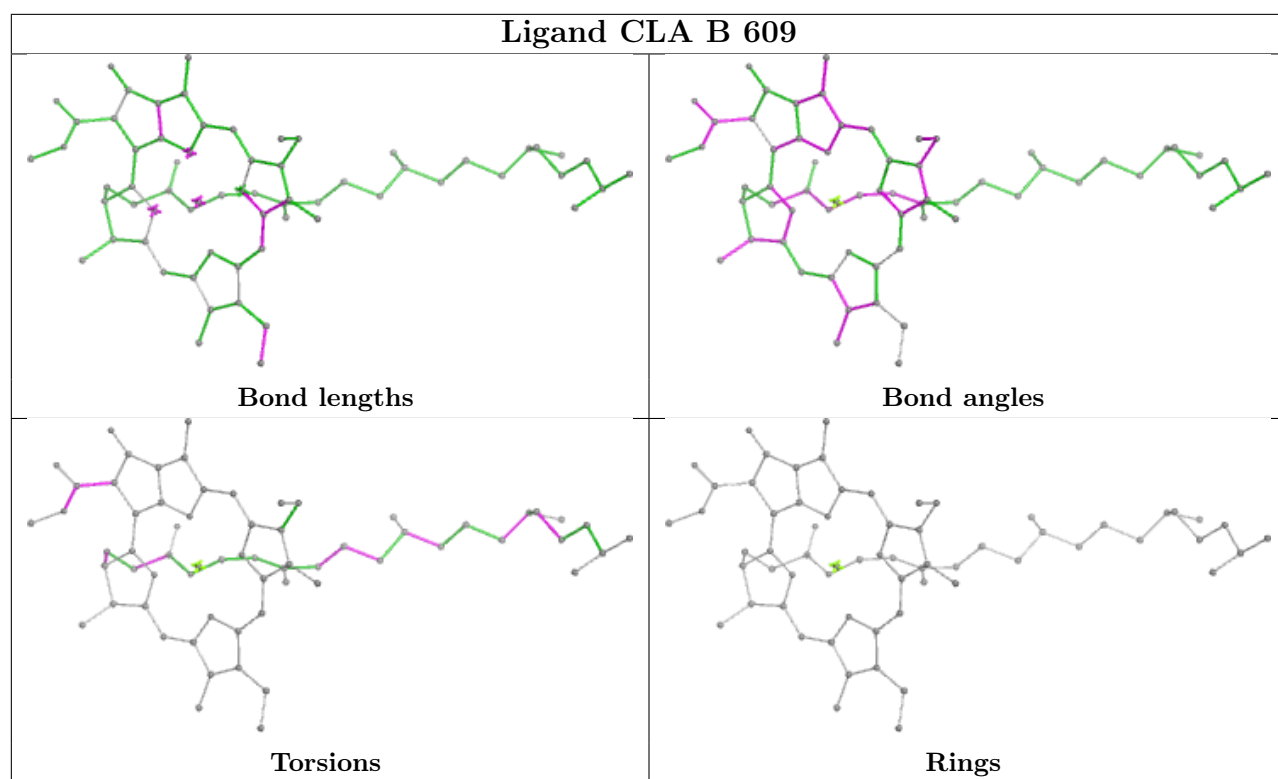


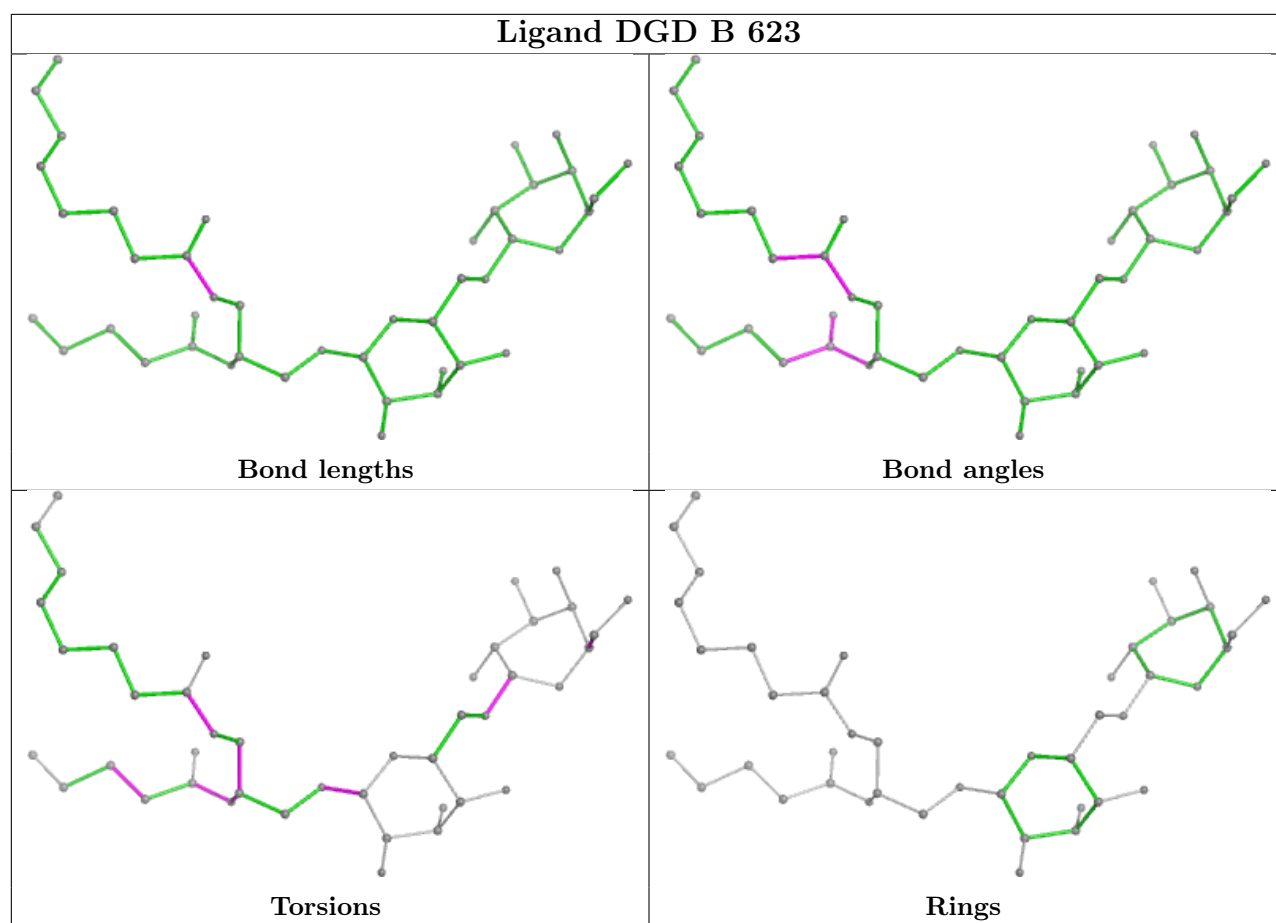
Rings



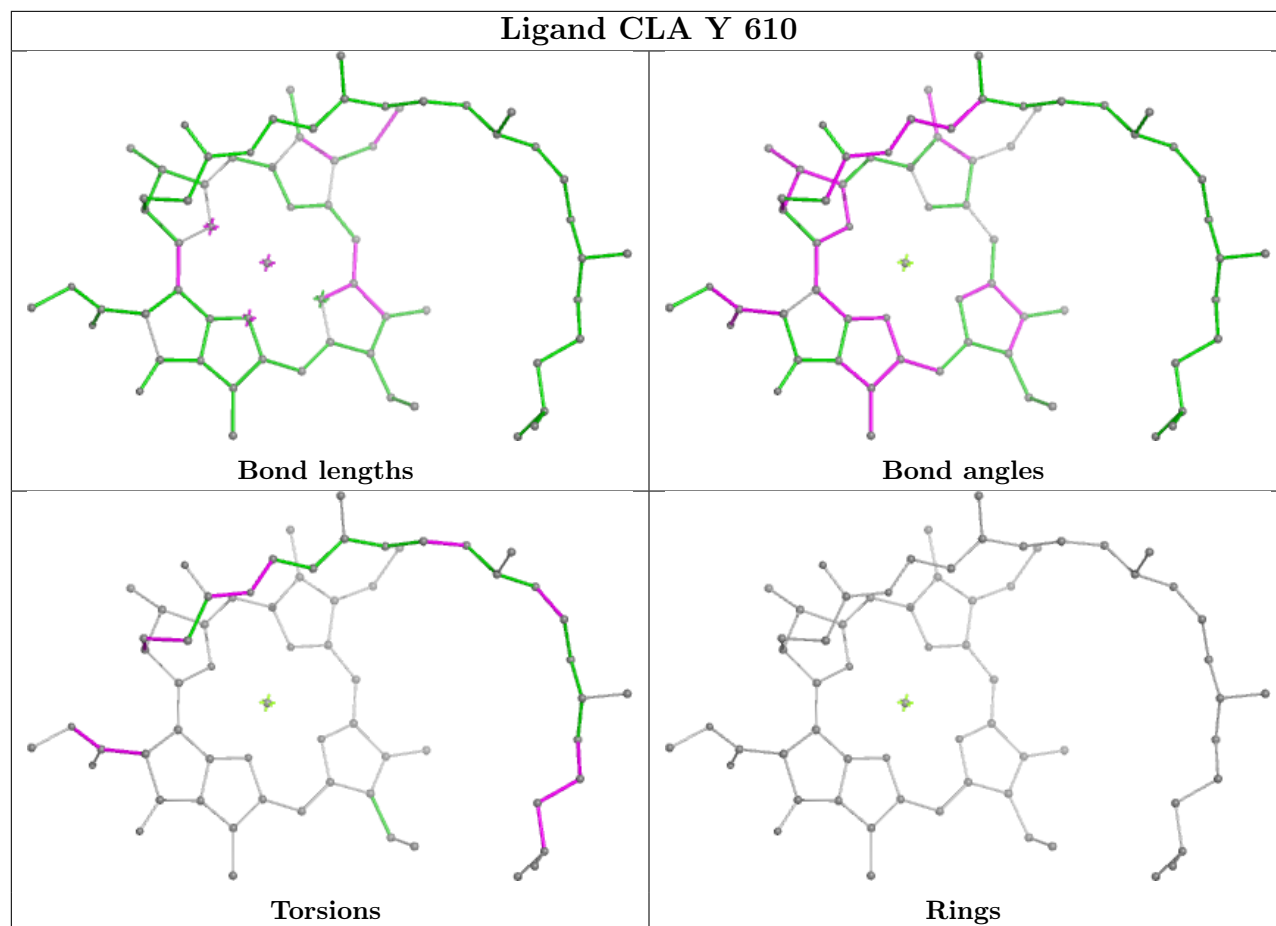




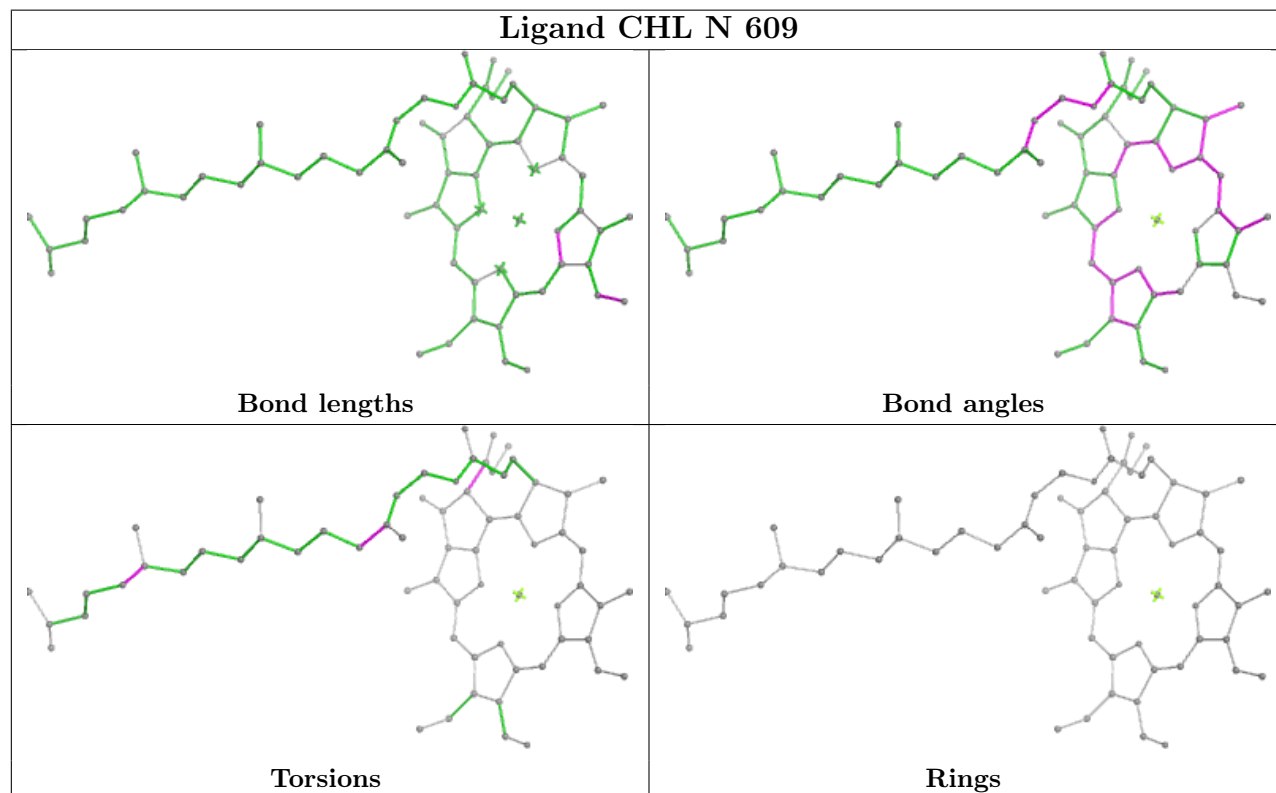


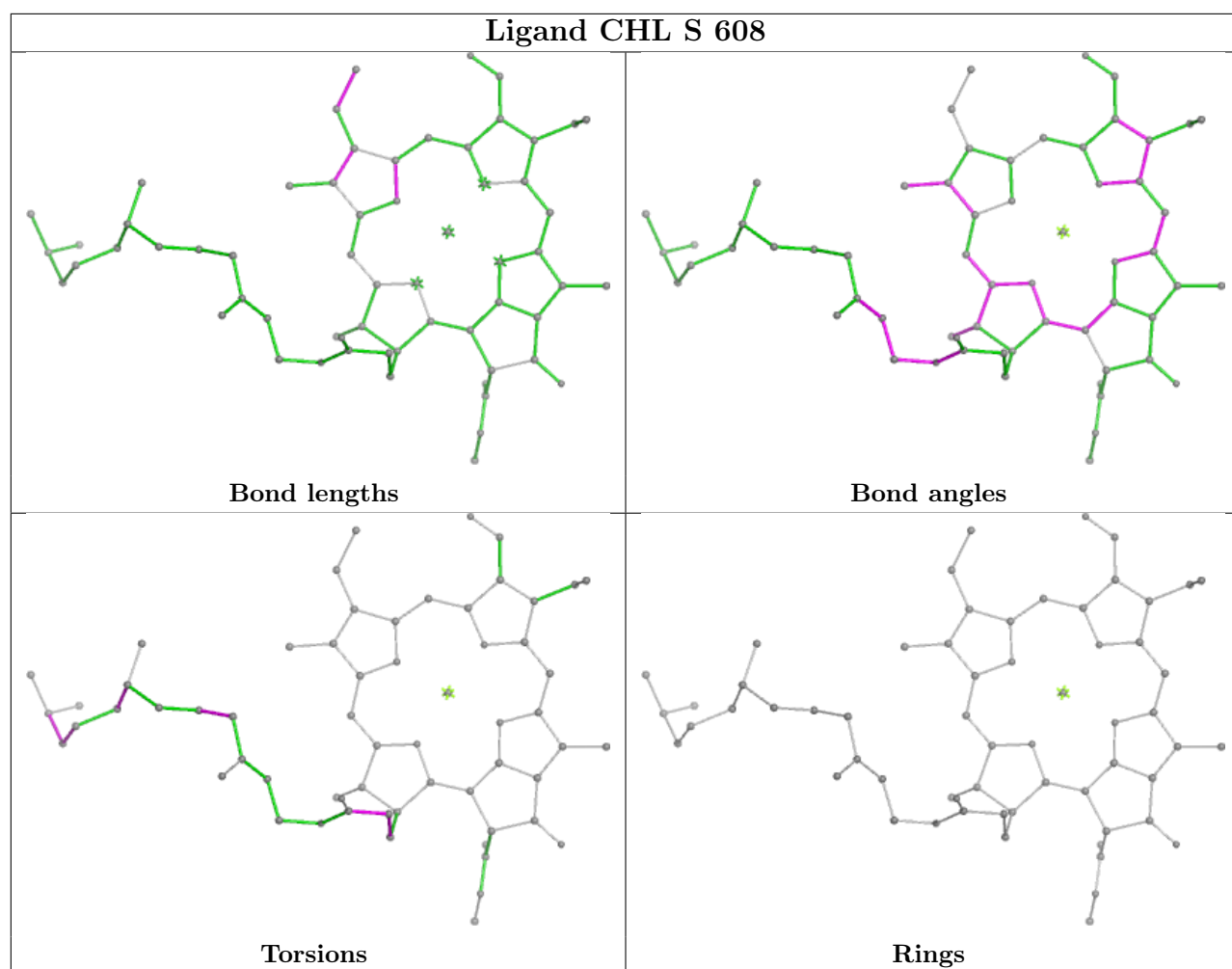


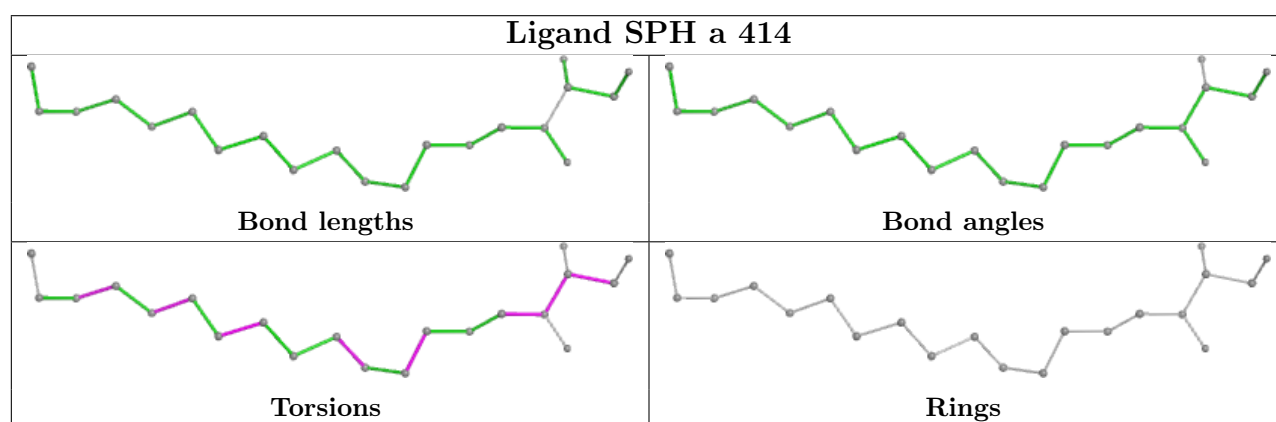
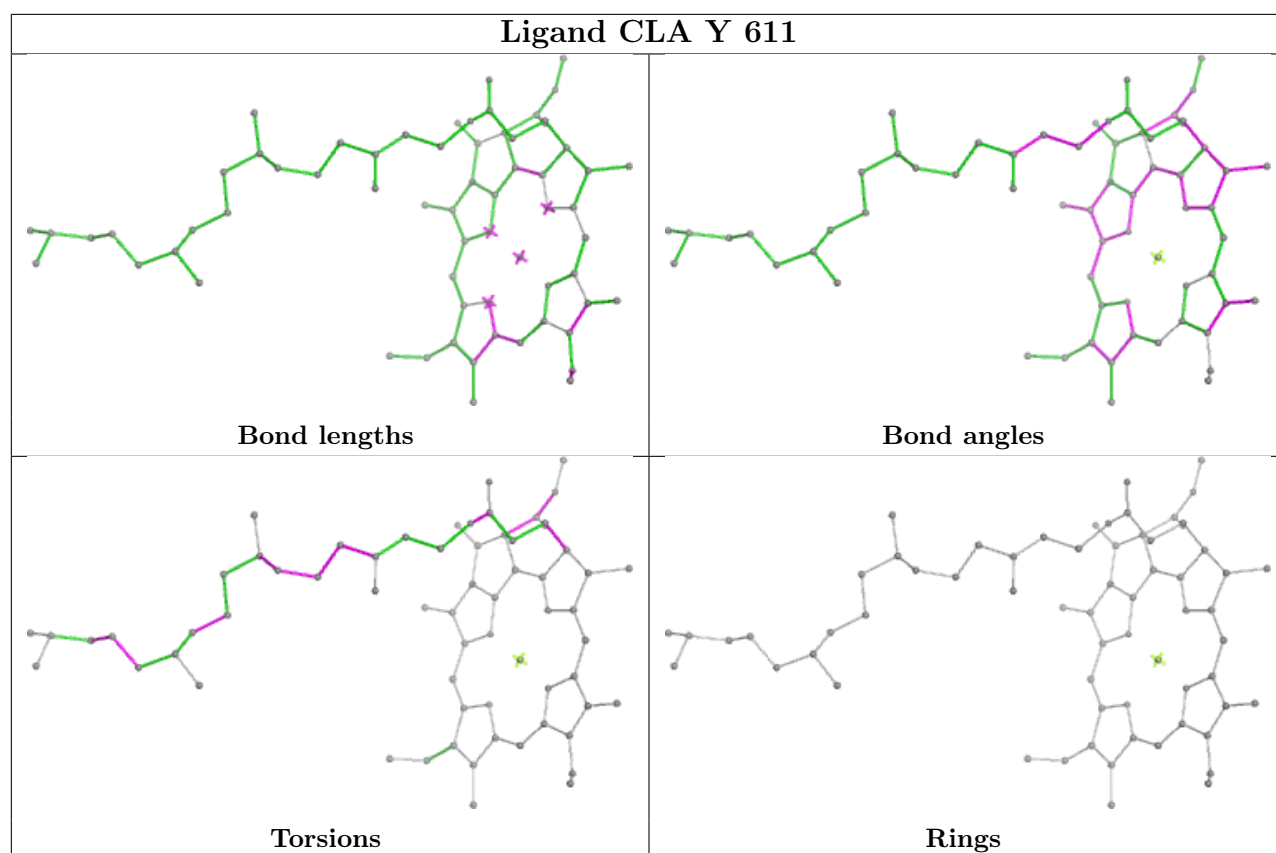
Ligand CLA Y 610

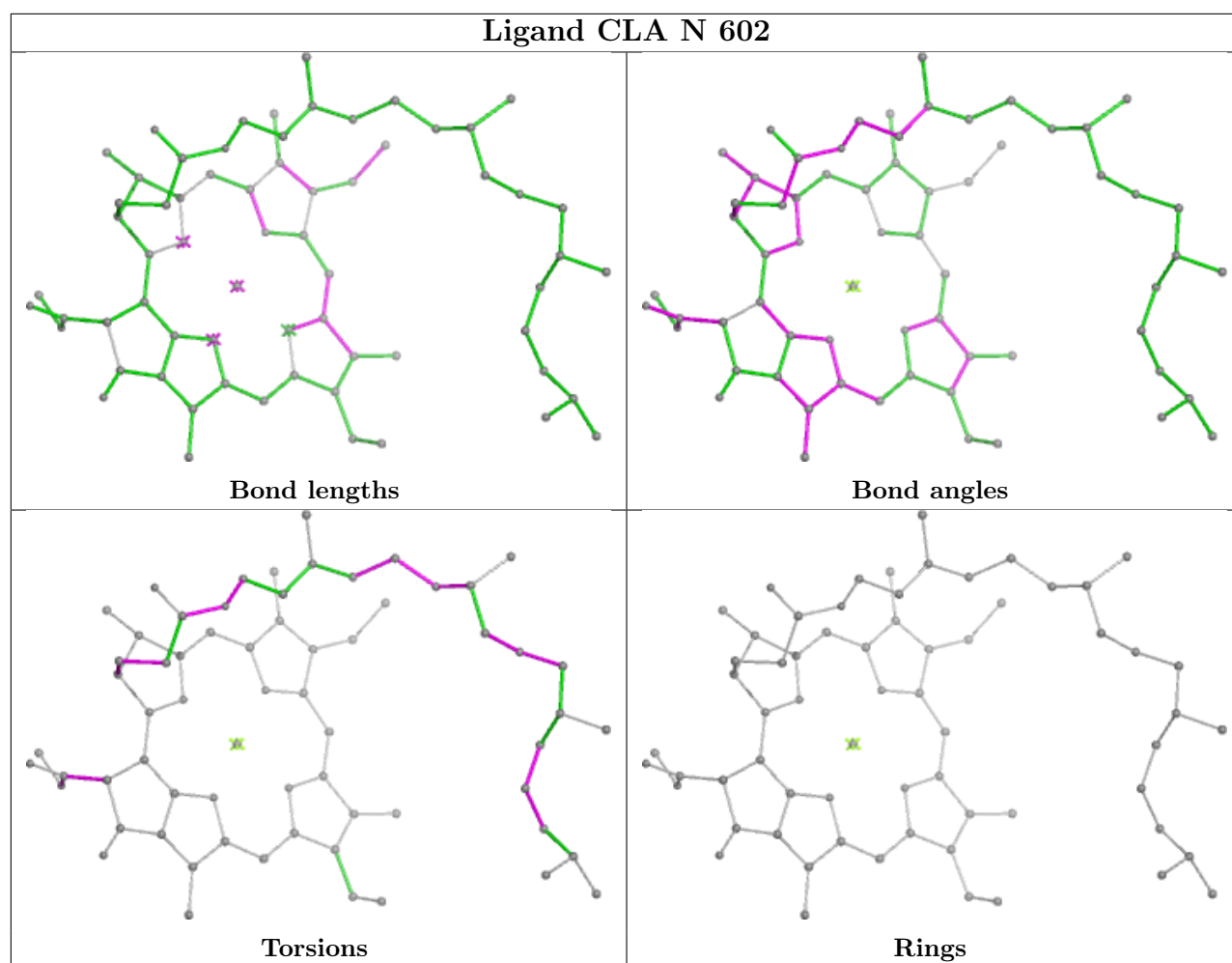


Ligand CHL N 609

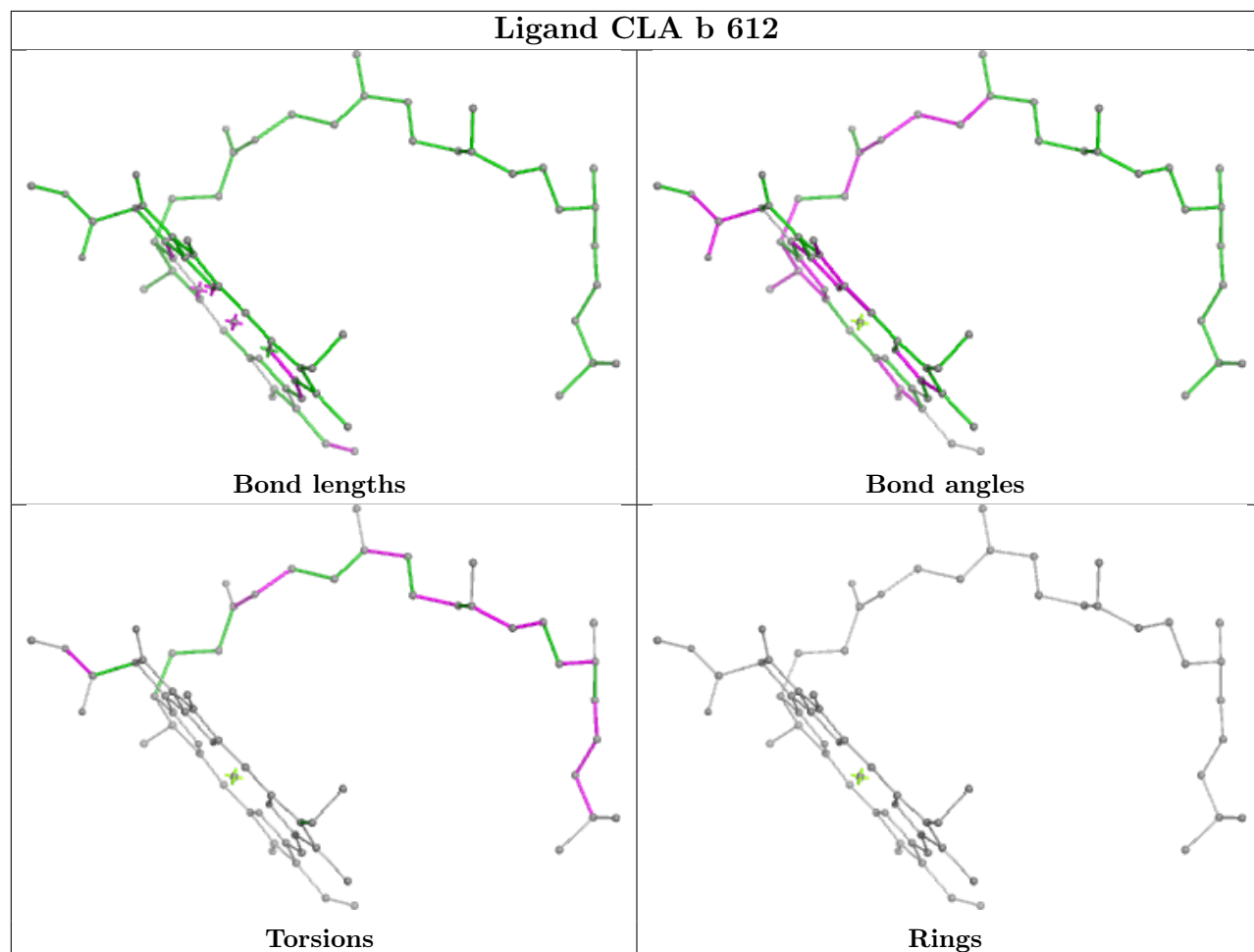




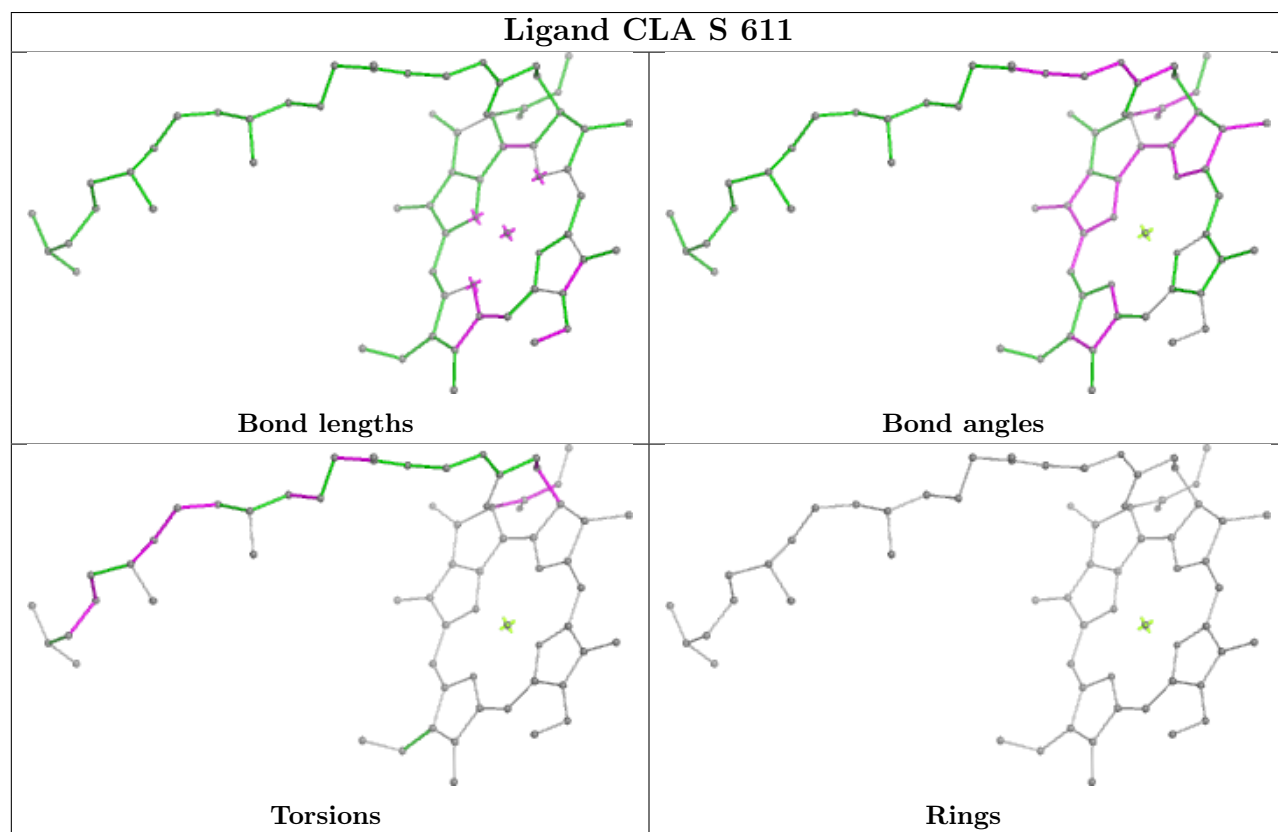


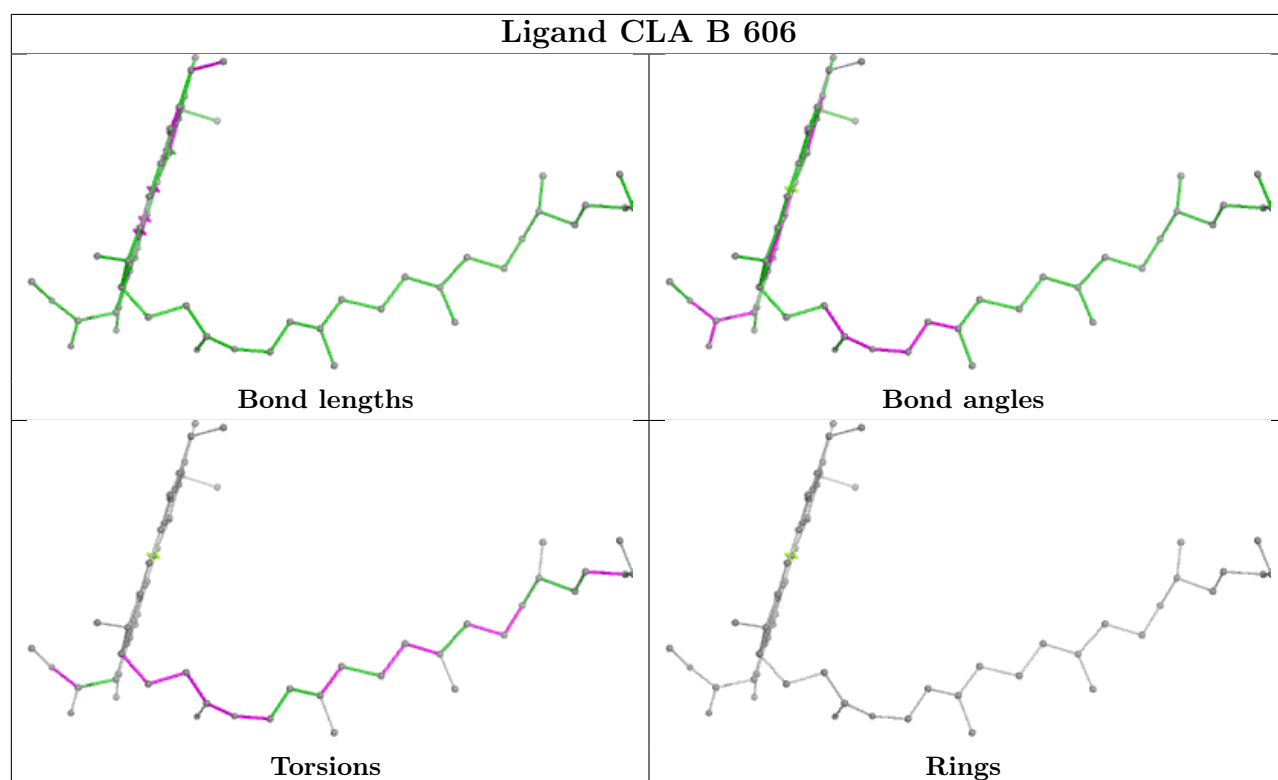
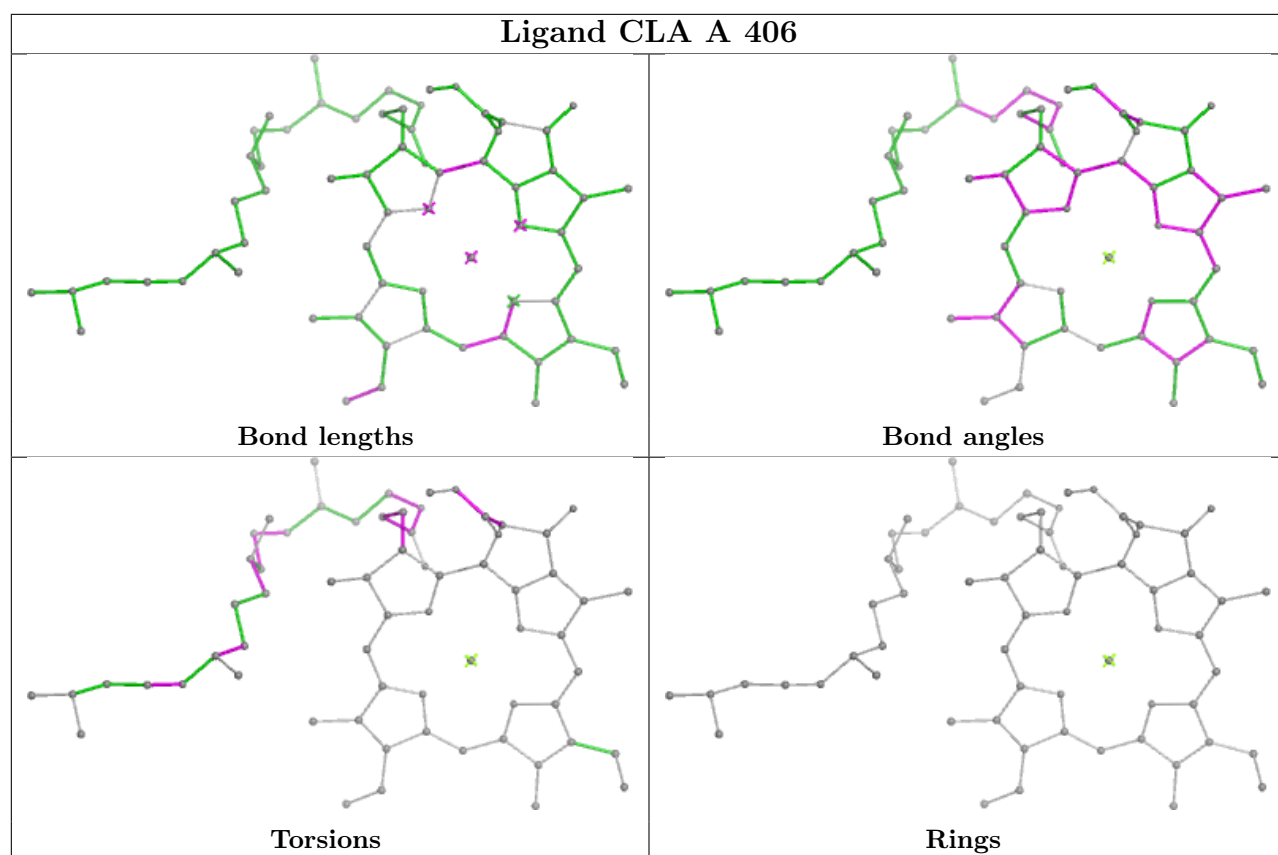


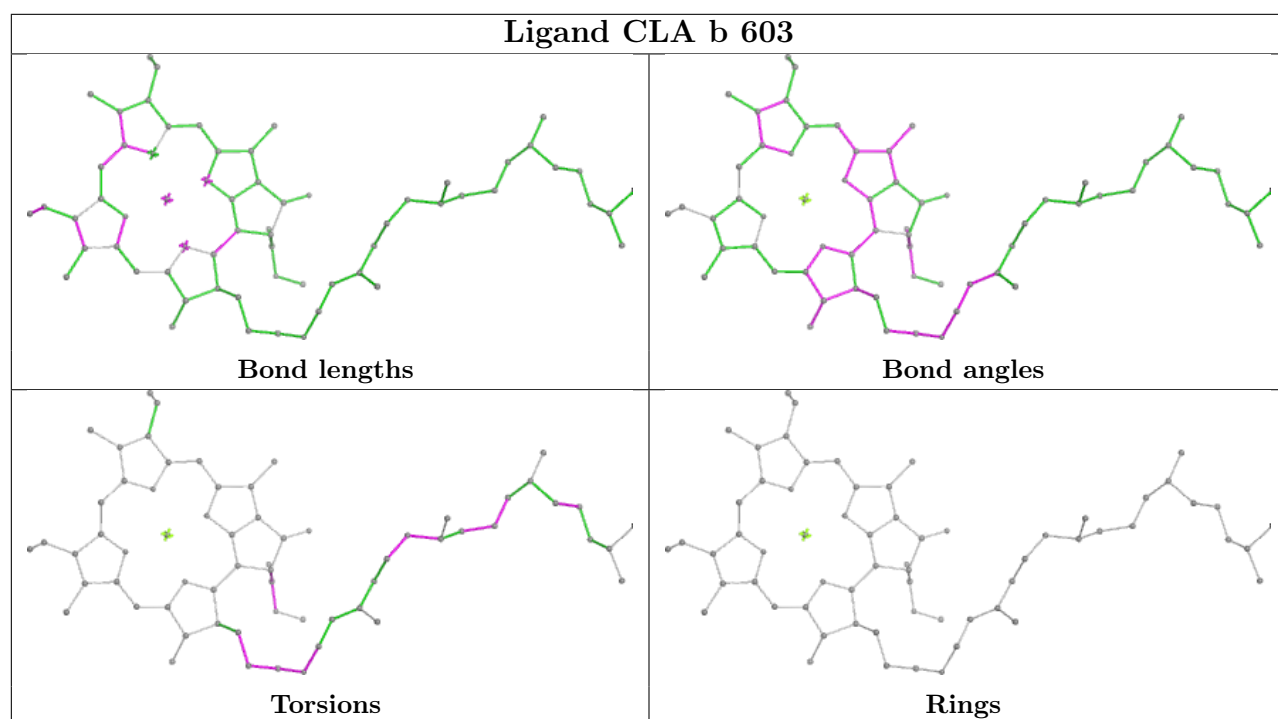
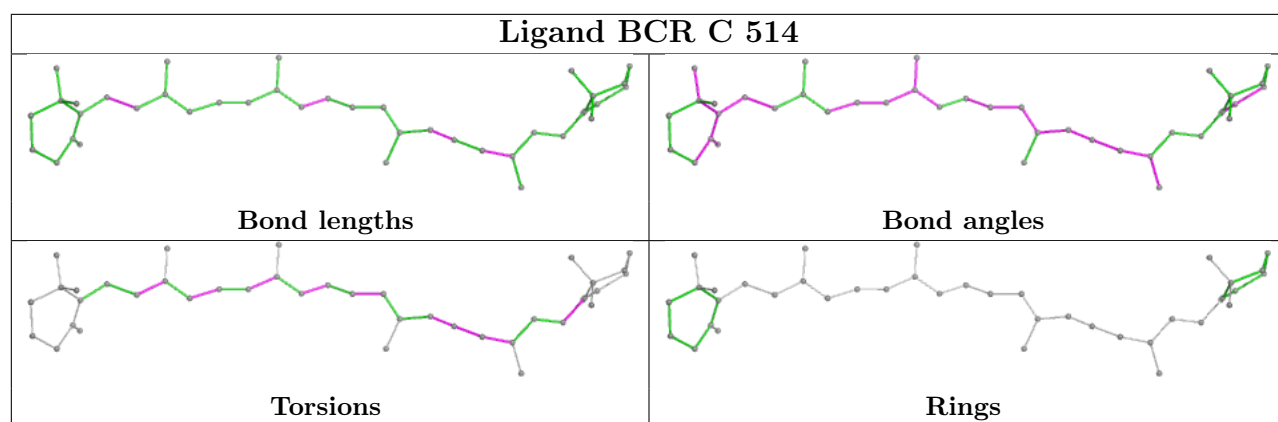
Ligand CLA b 612

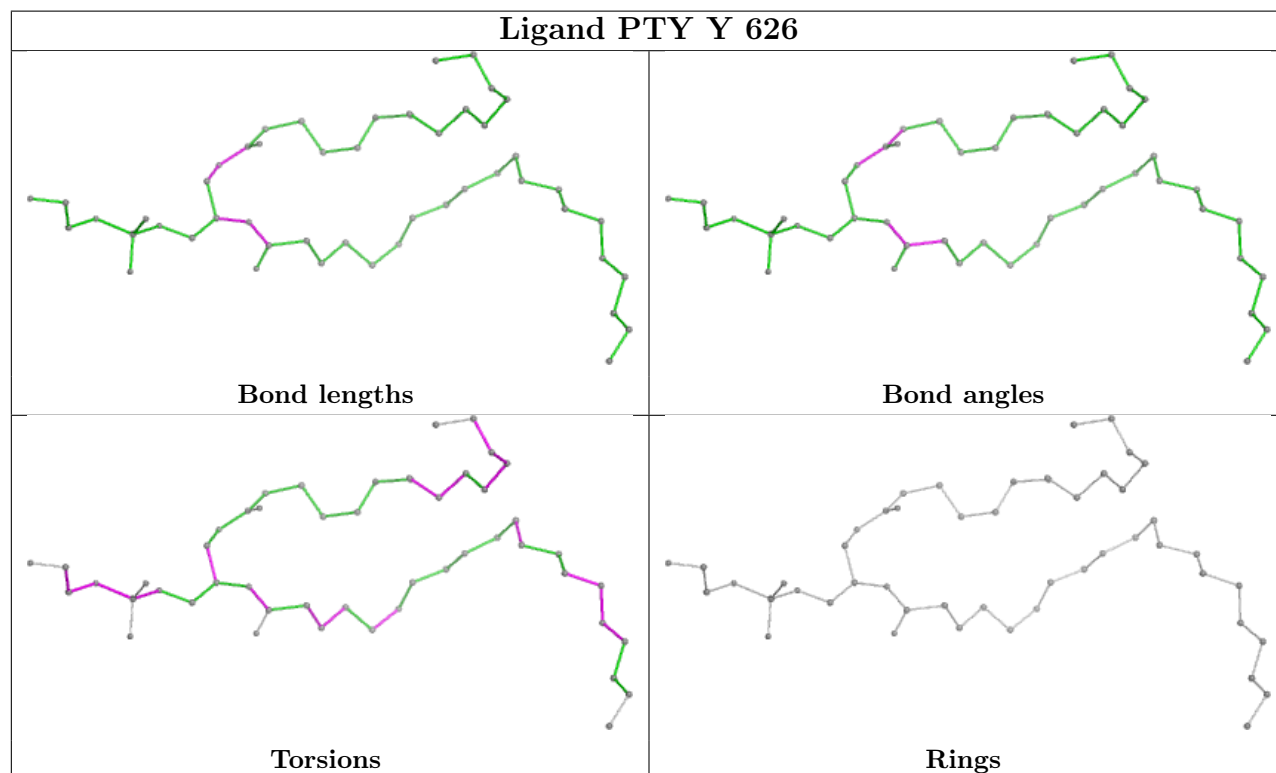
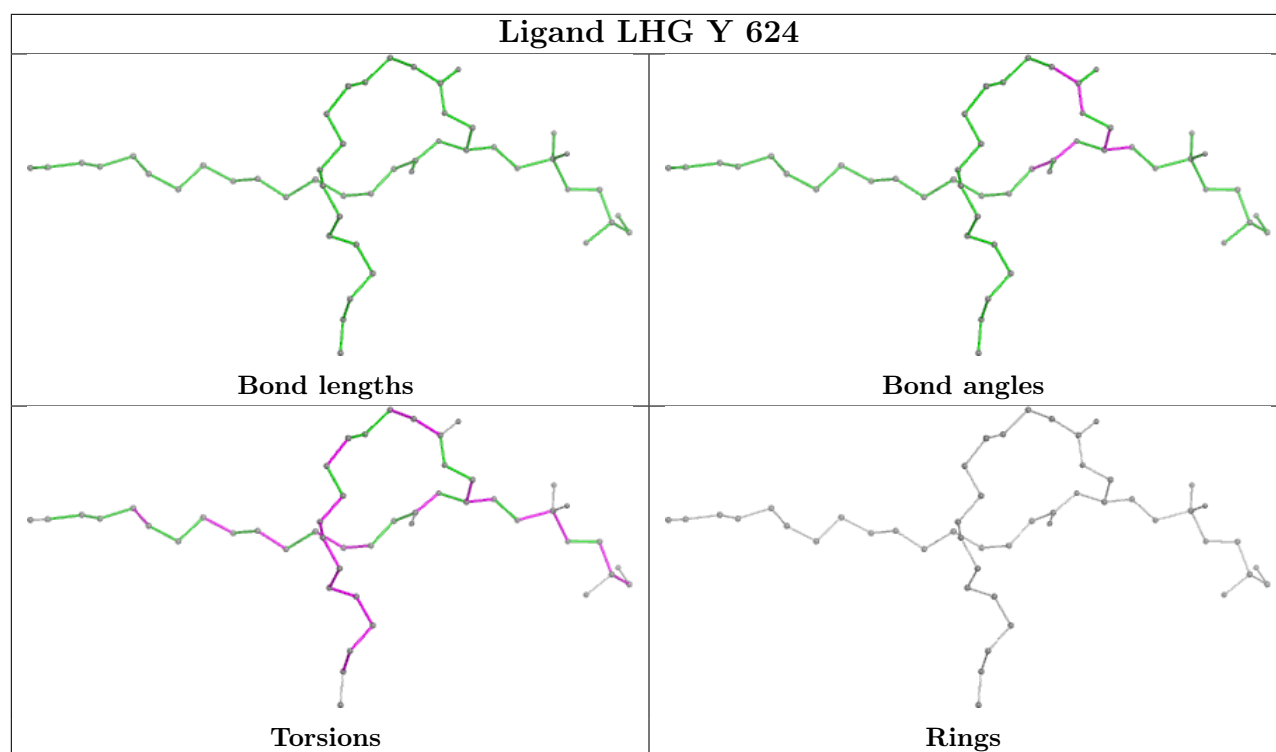


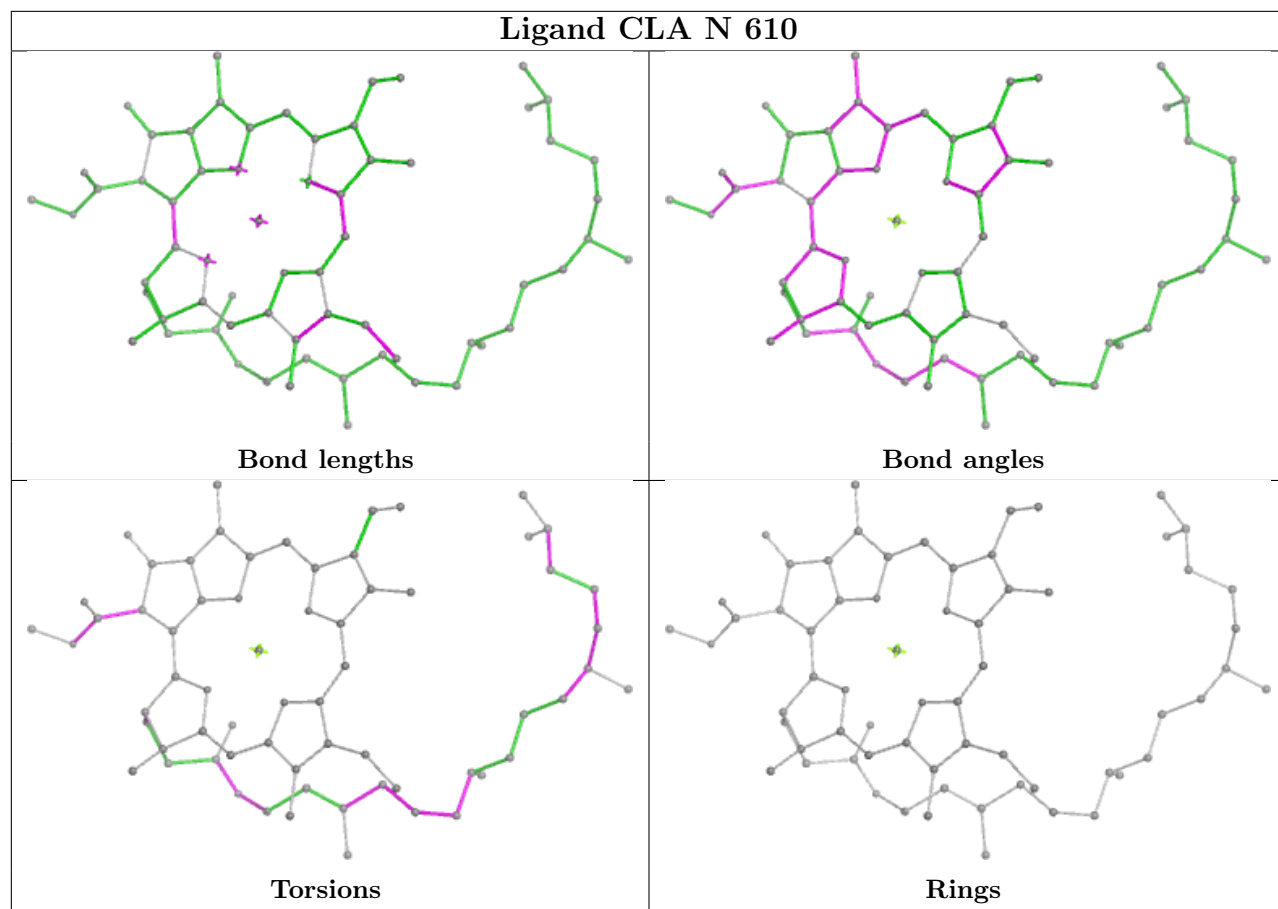
Ligand CLA S 611

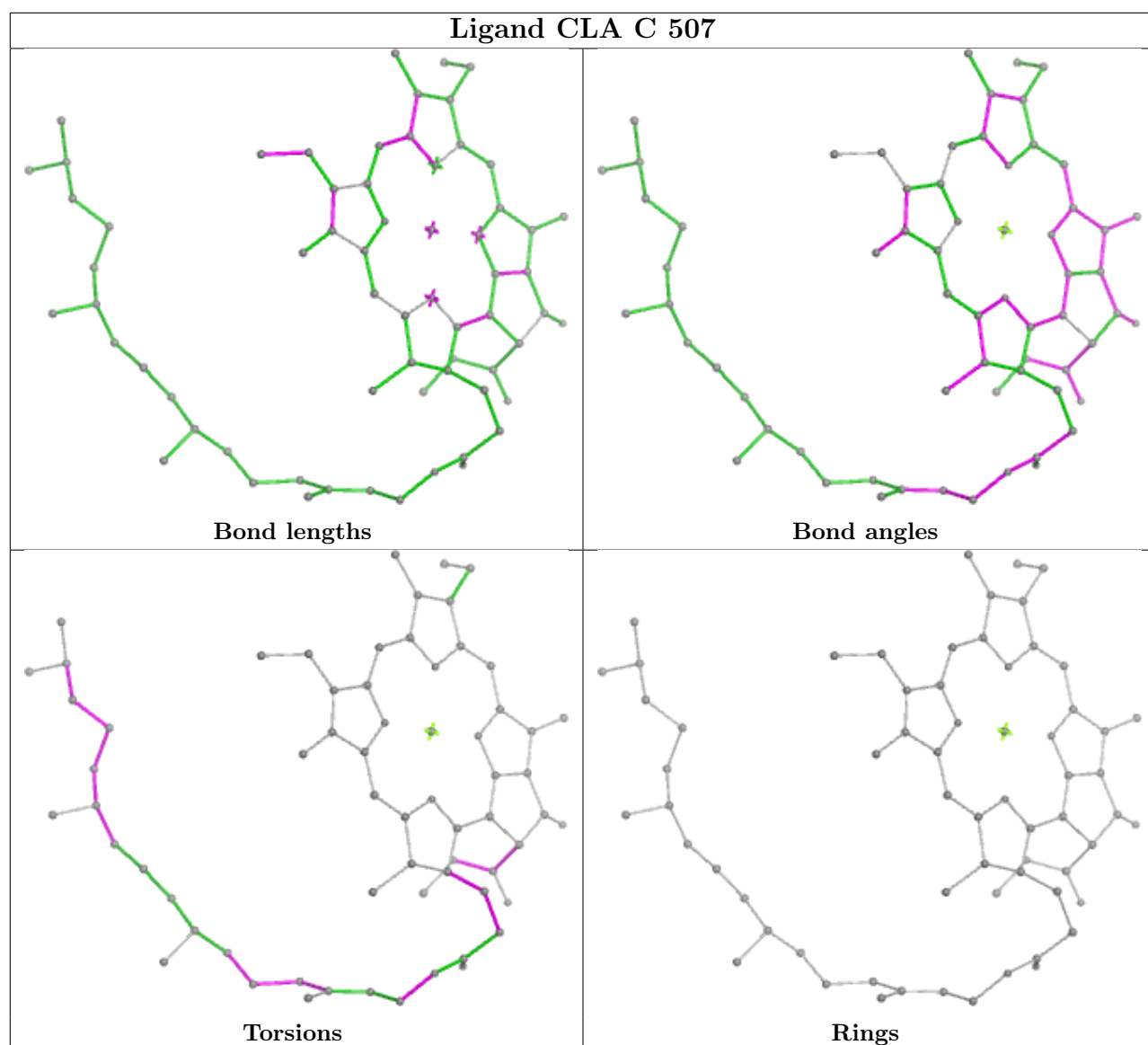




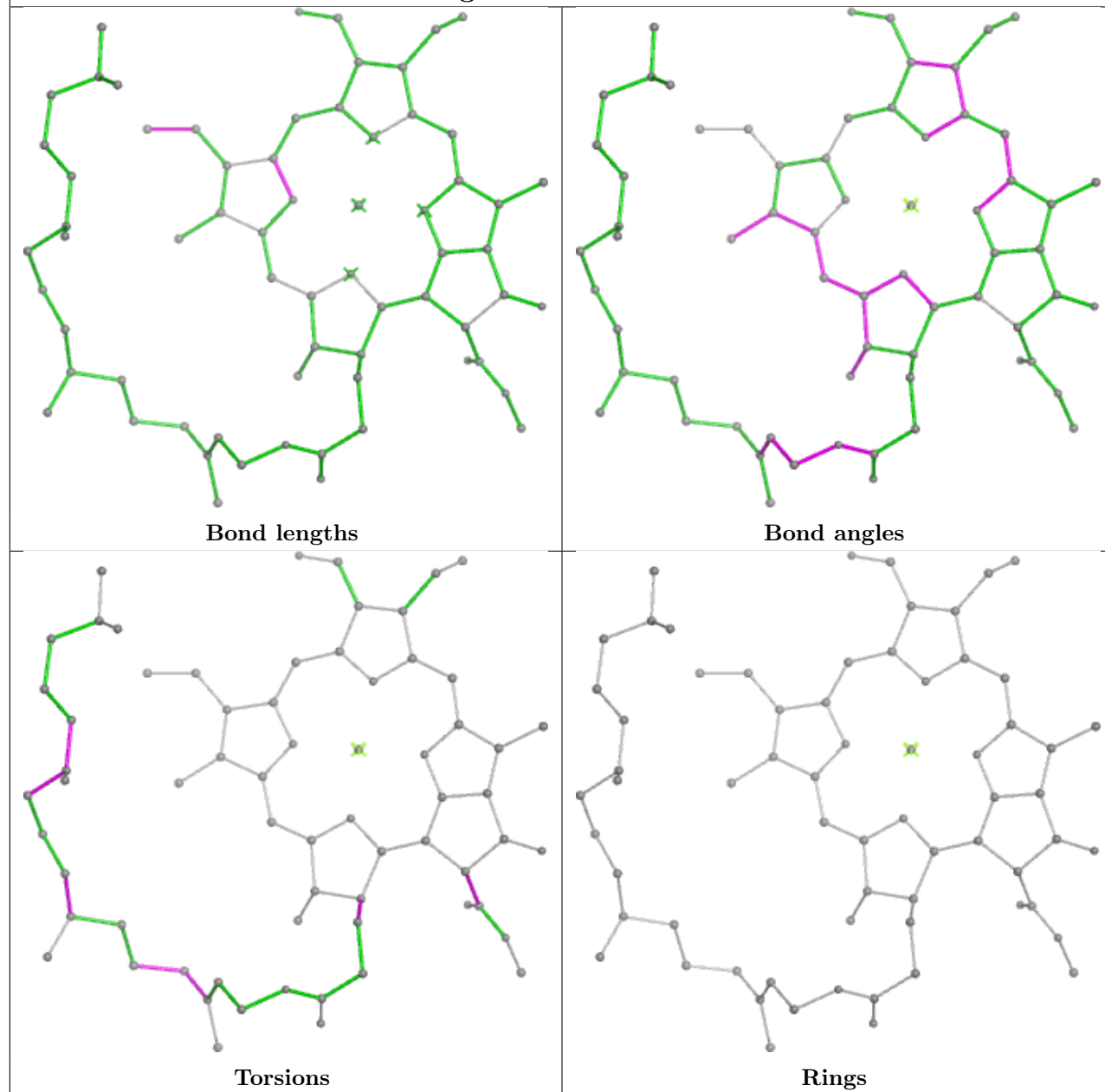




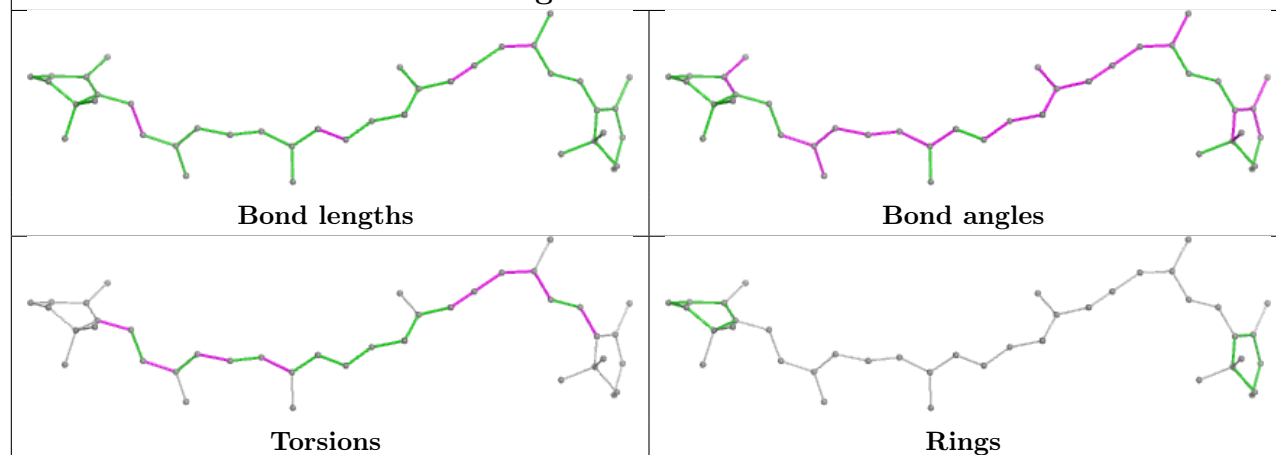


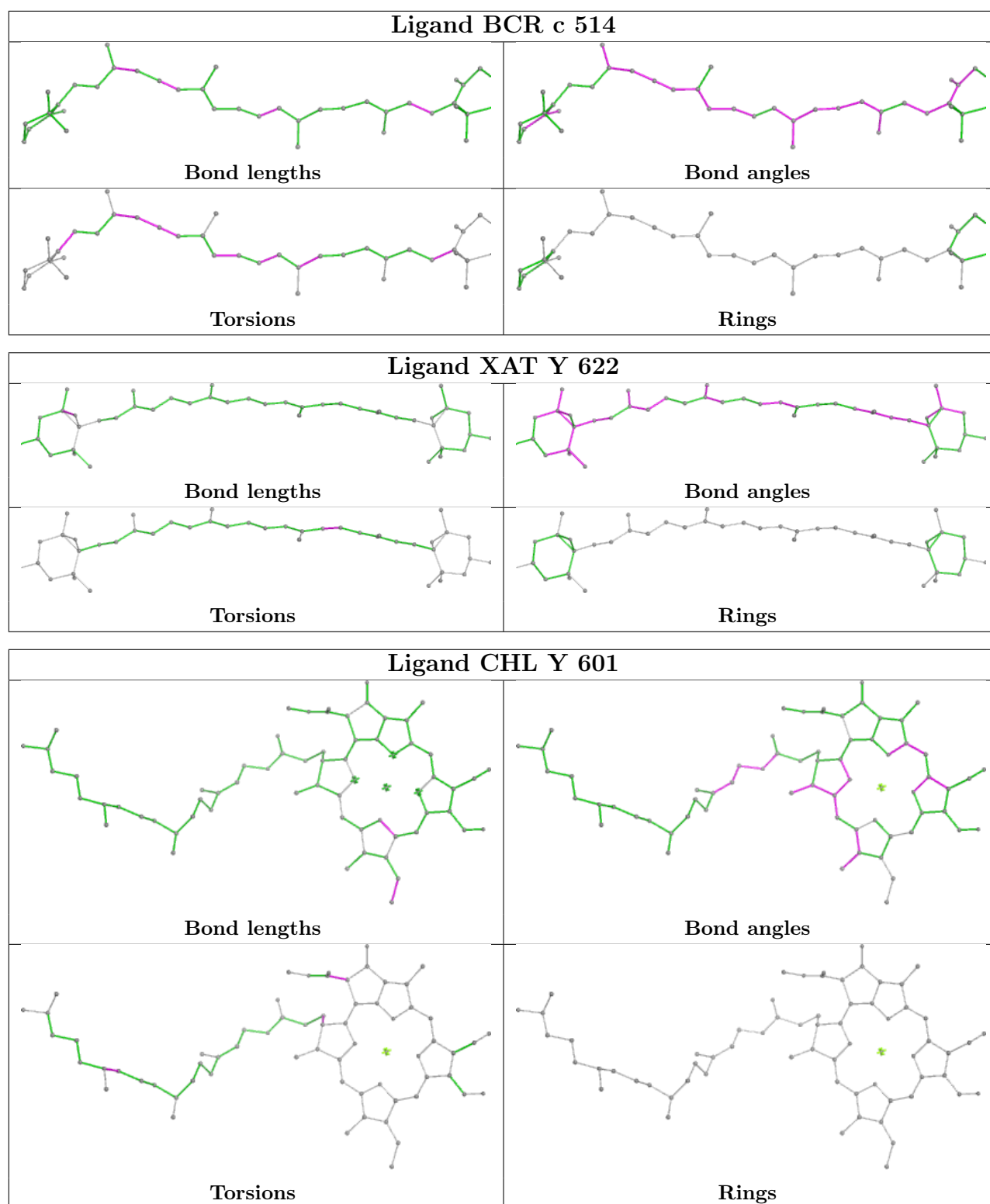


Ligand CHL N 607

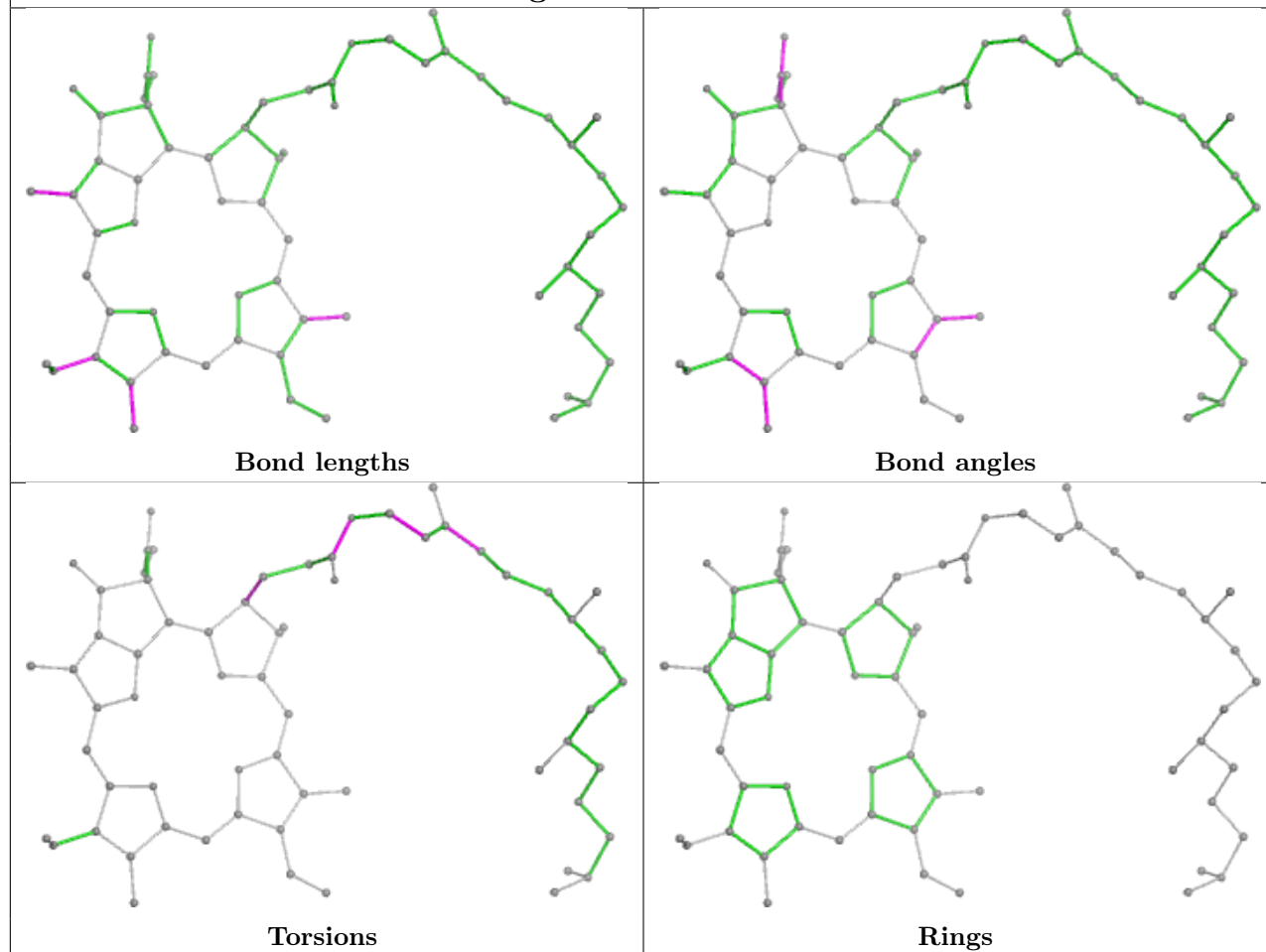


Ligand BCR c 516

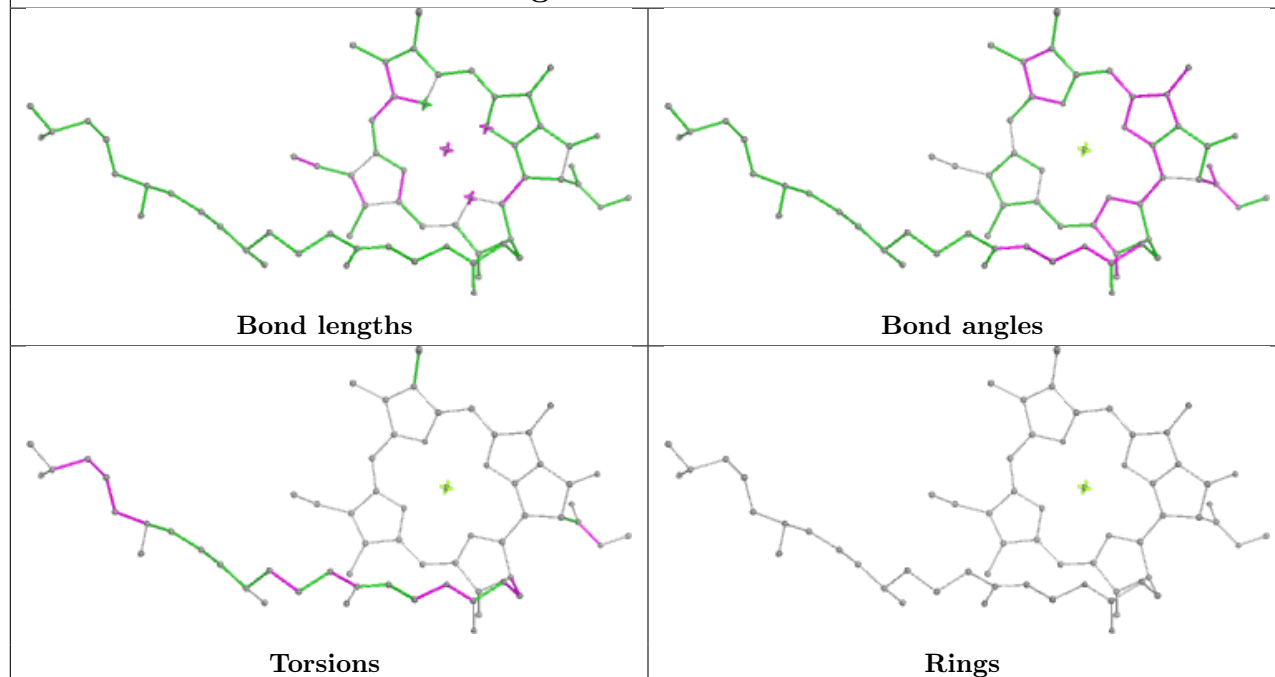




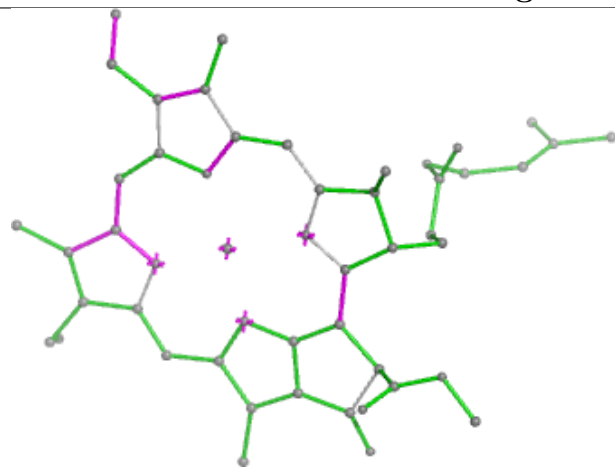
Ligand PHO a 408



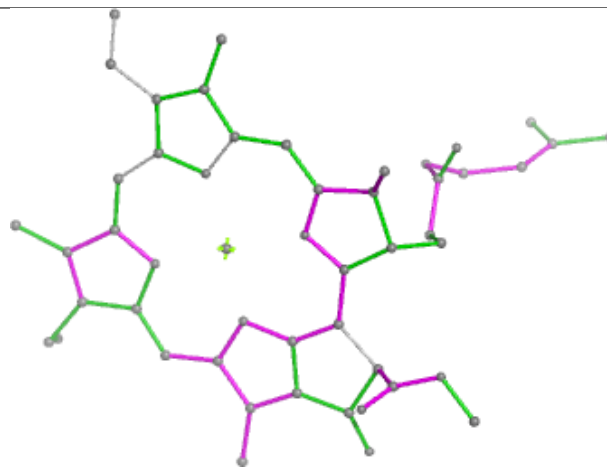
Ligand CLA C 501



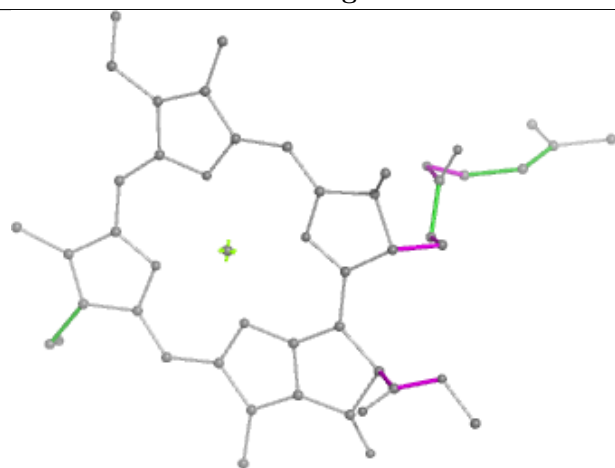
Ligand CLA Y 608



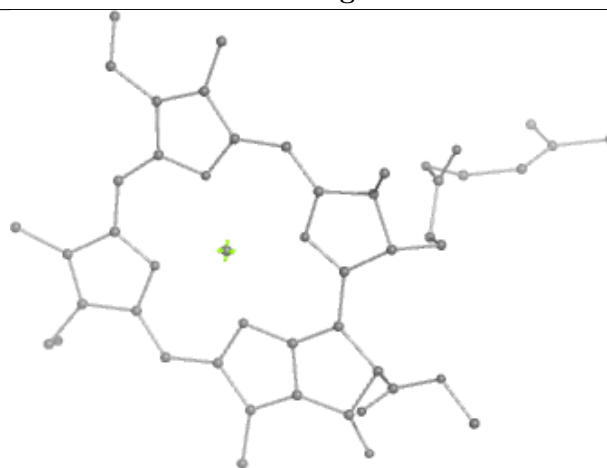
Bond lengths



Bond angles

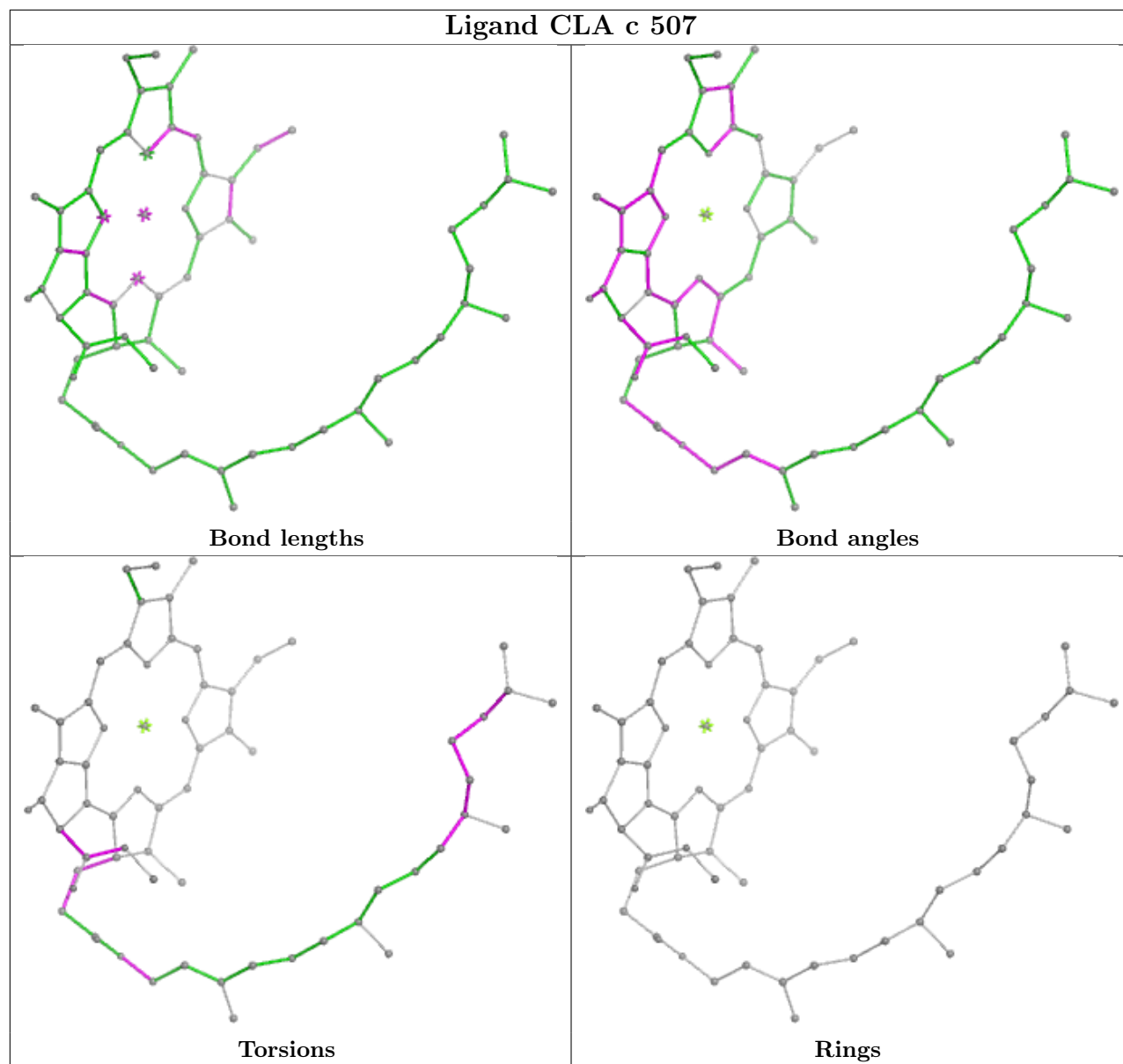


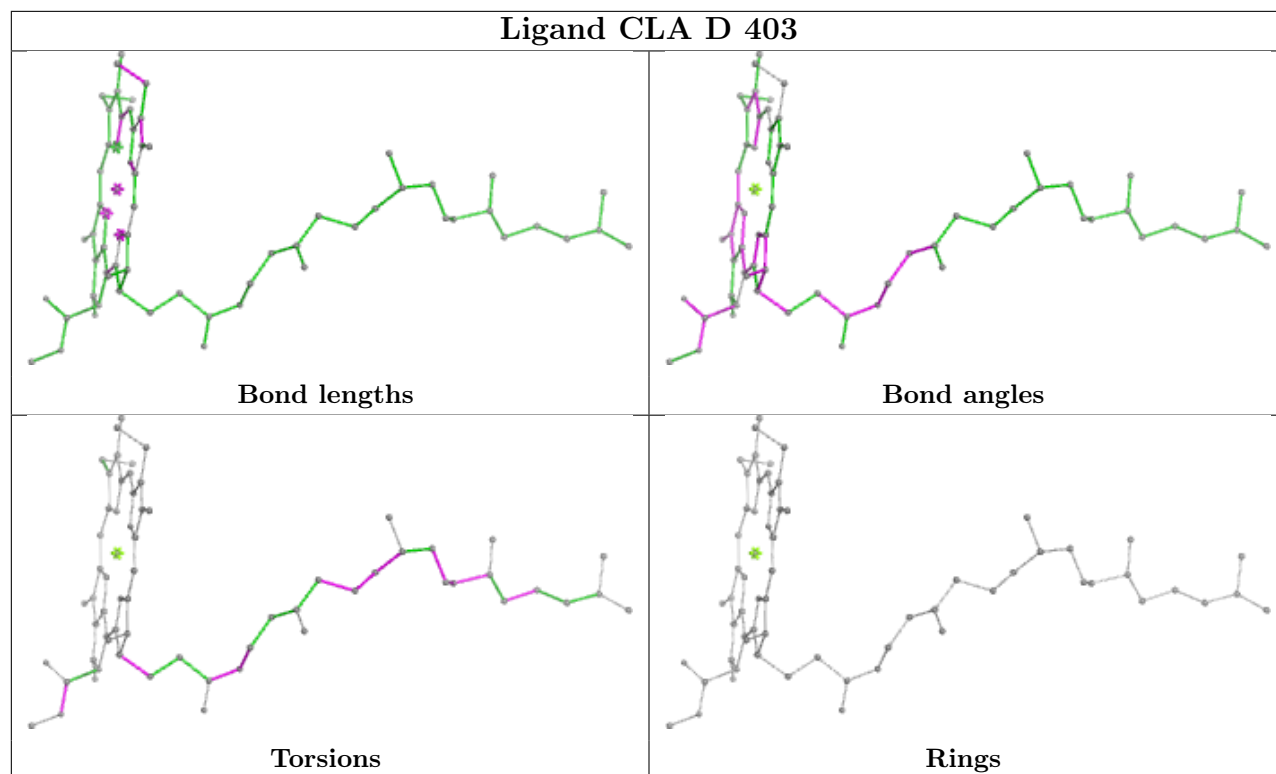
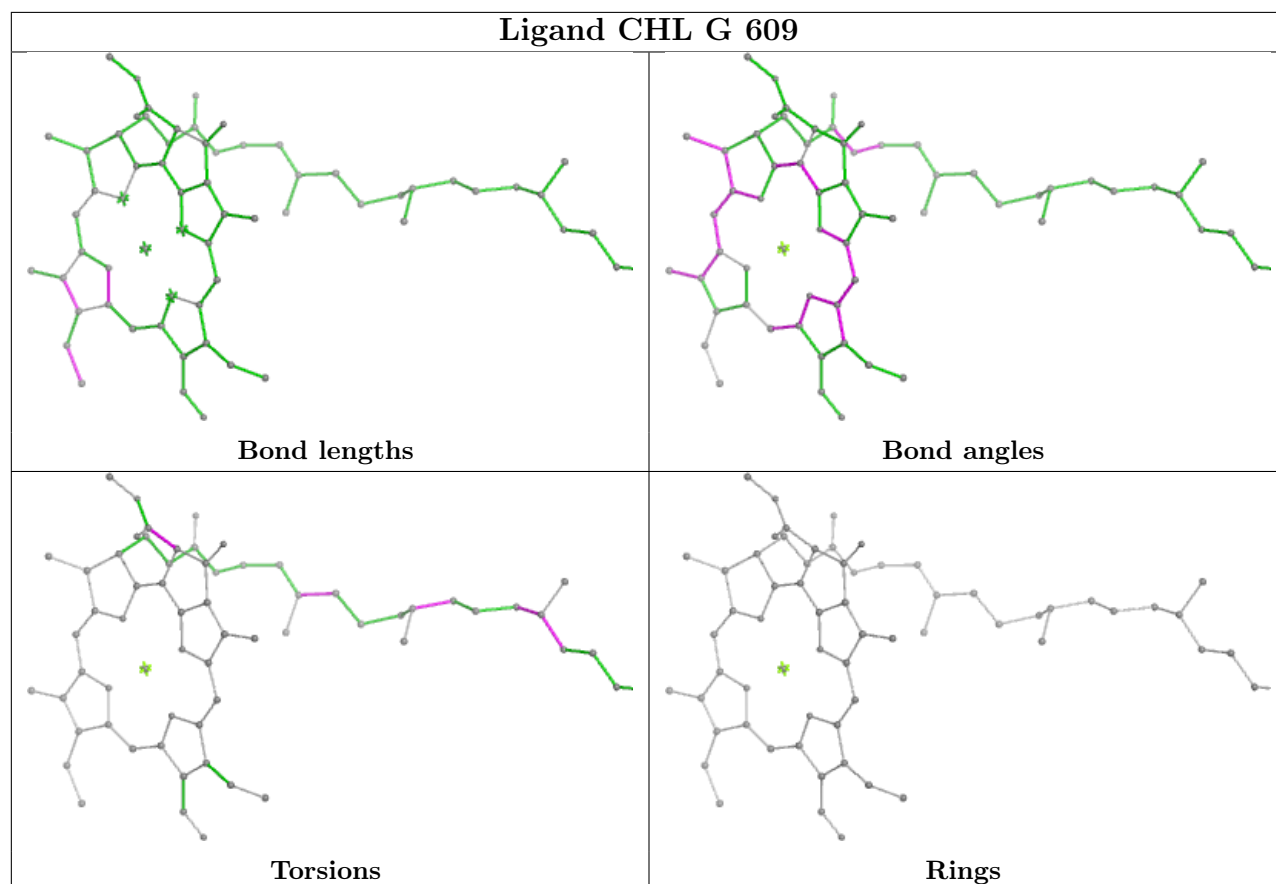
Torsions

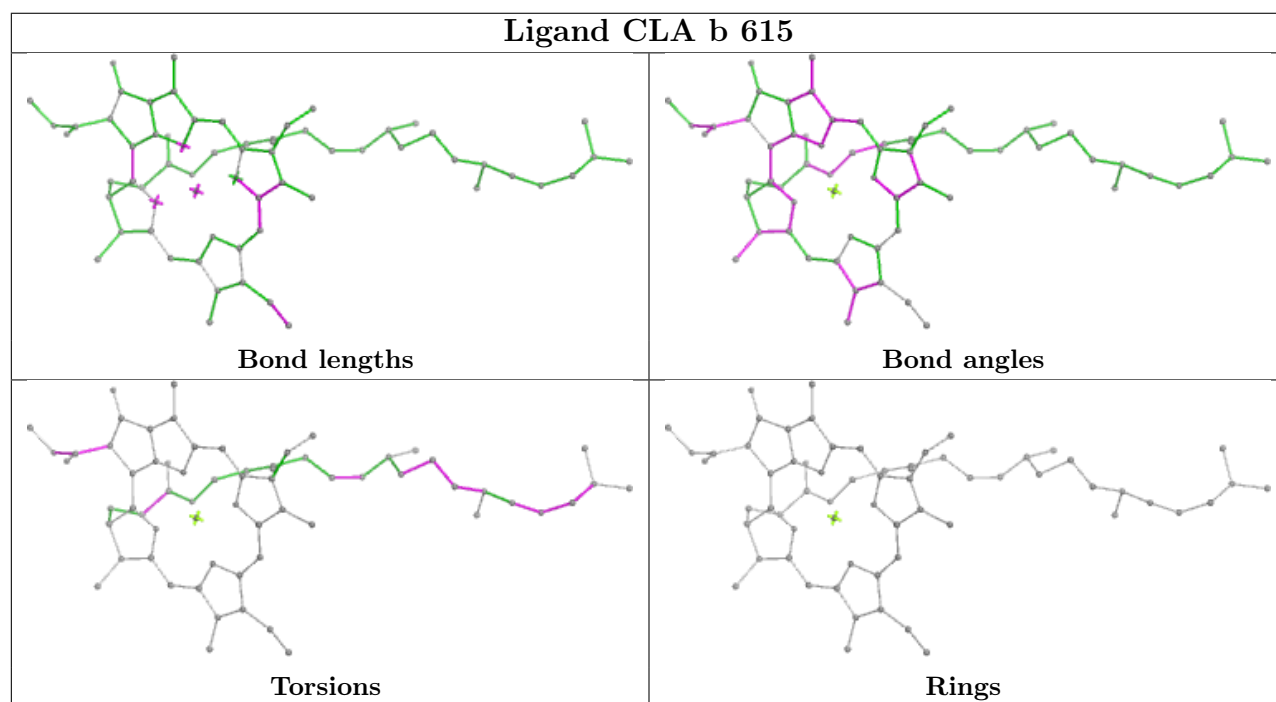
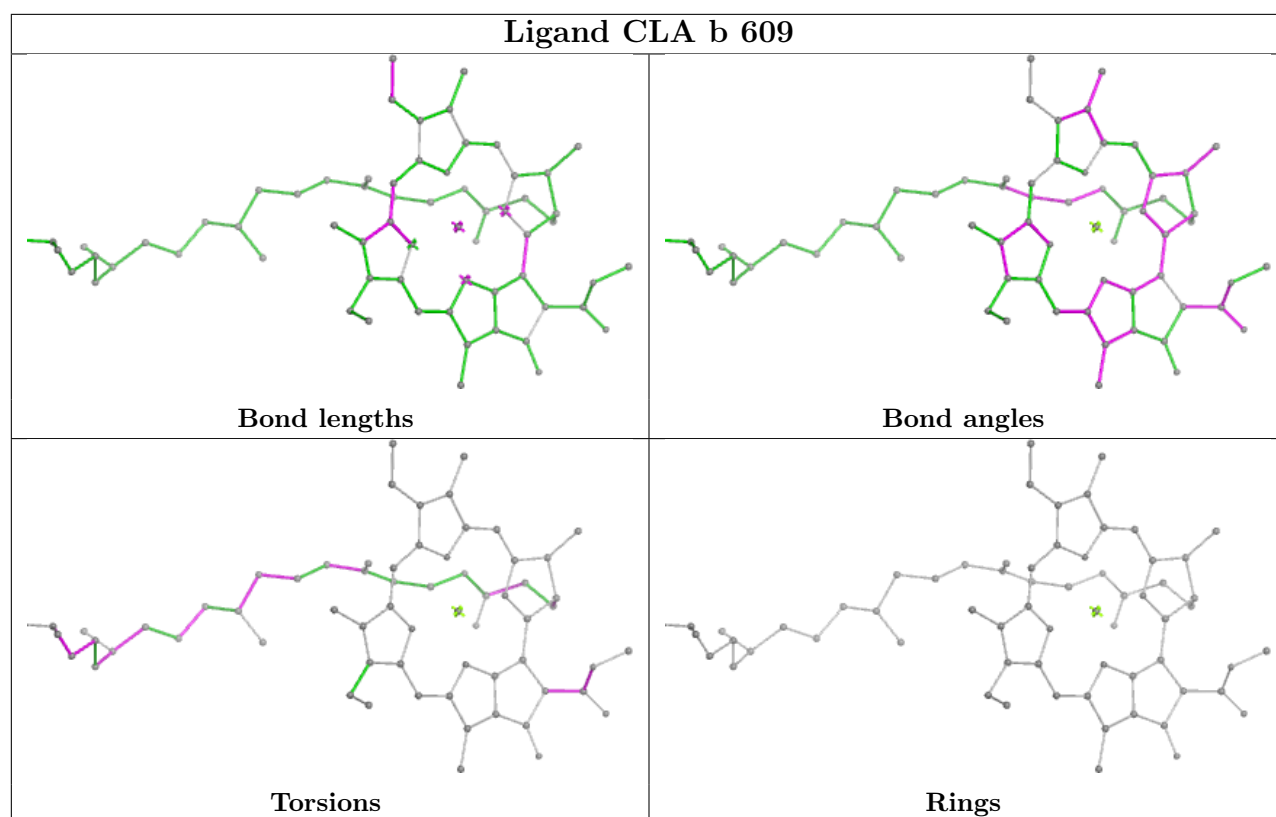


Rings

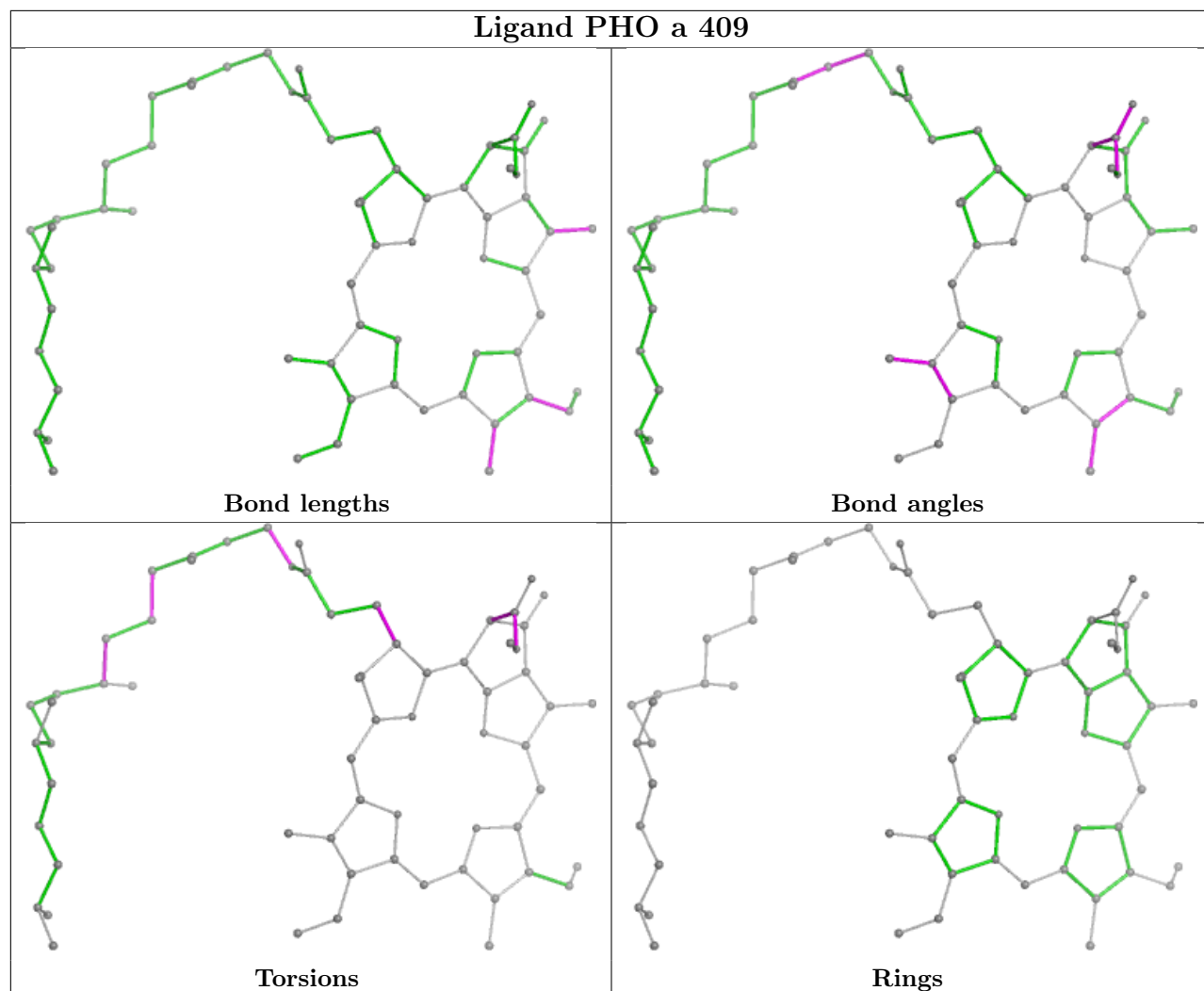
Ligand CLA c 507

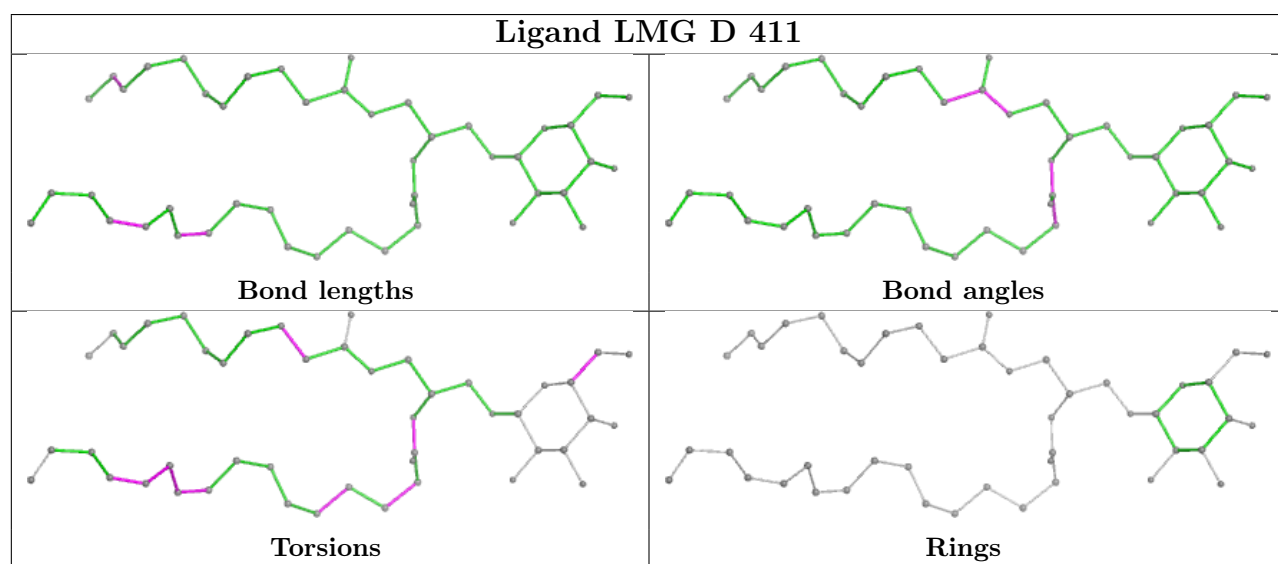
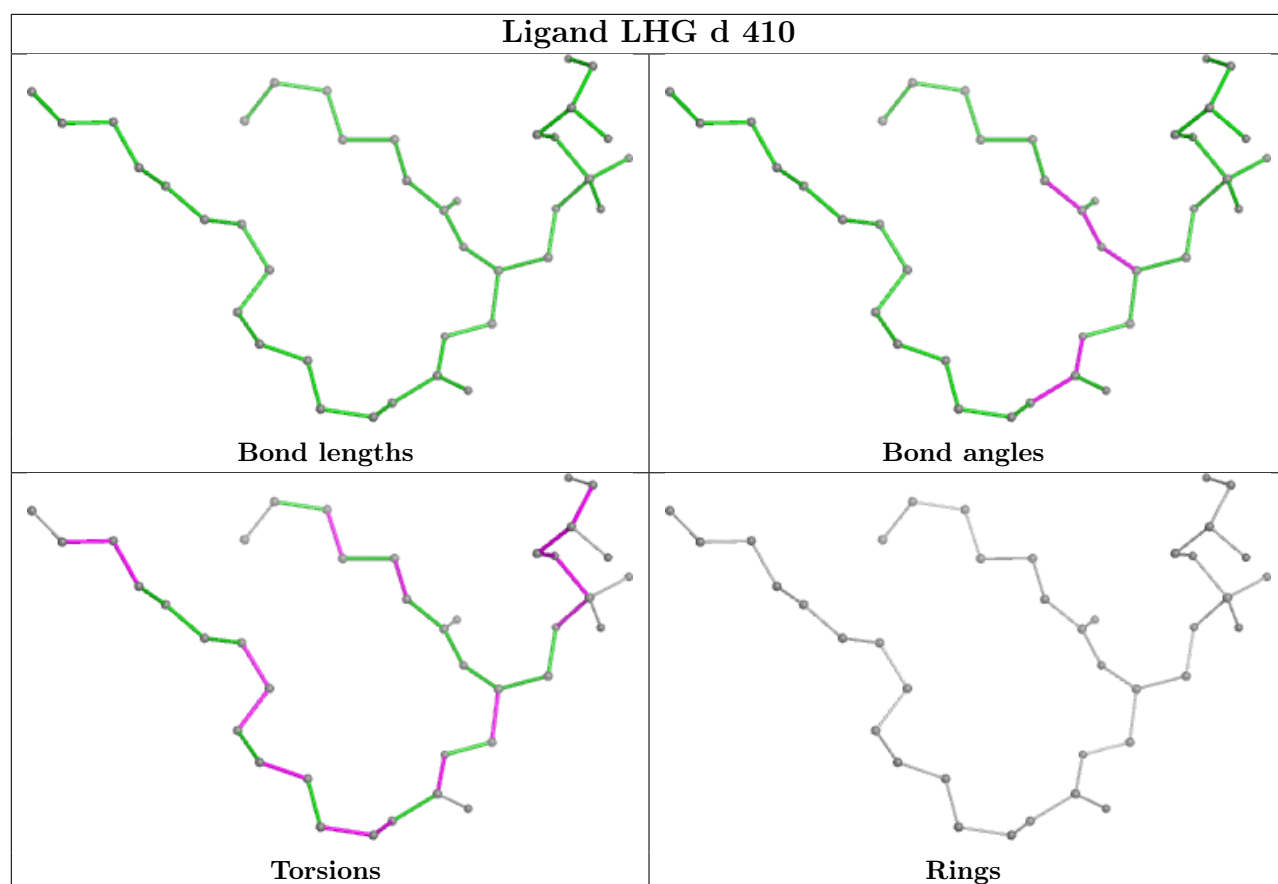


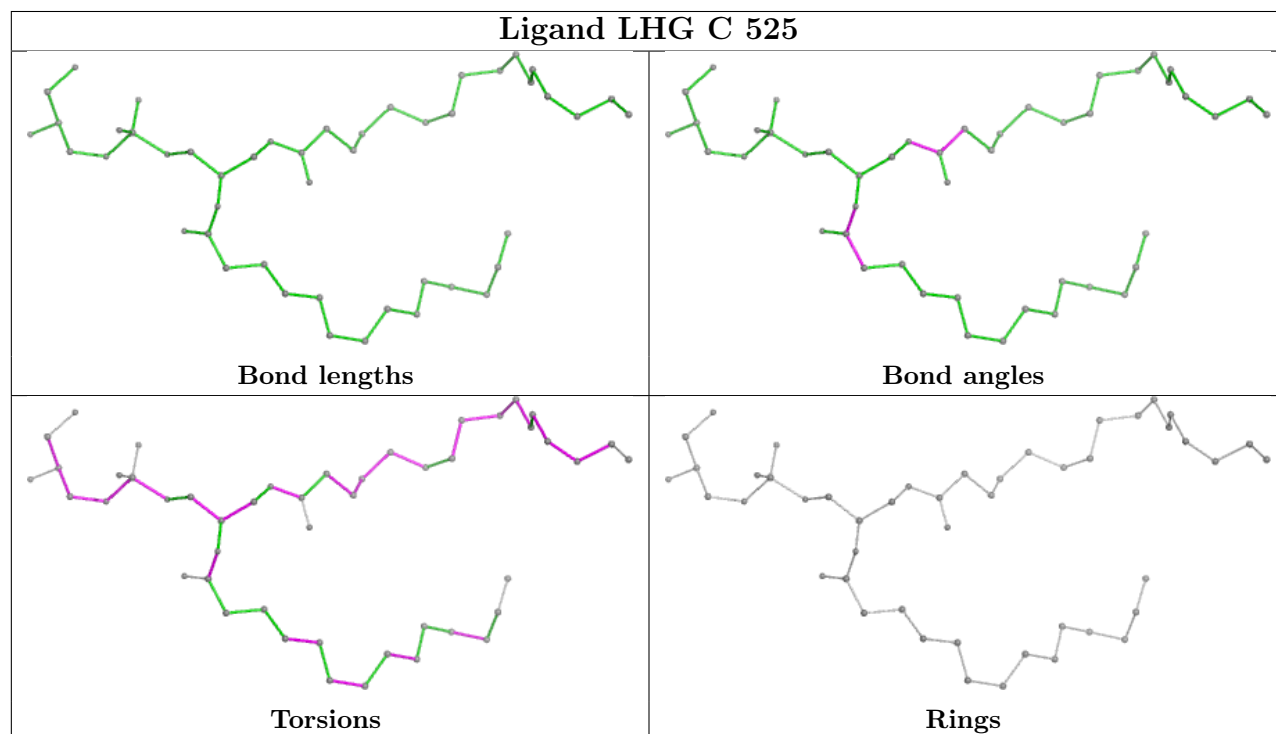
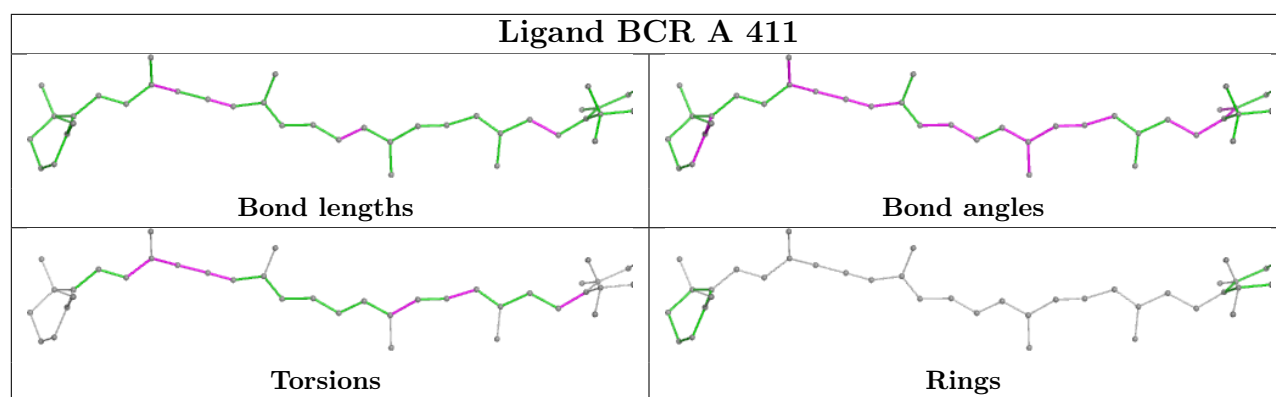
Ligand CLA D 403**Ligand CHL G 609**



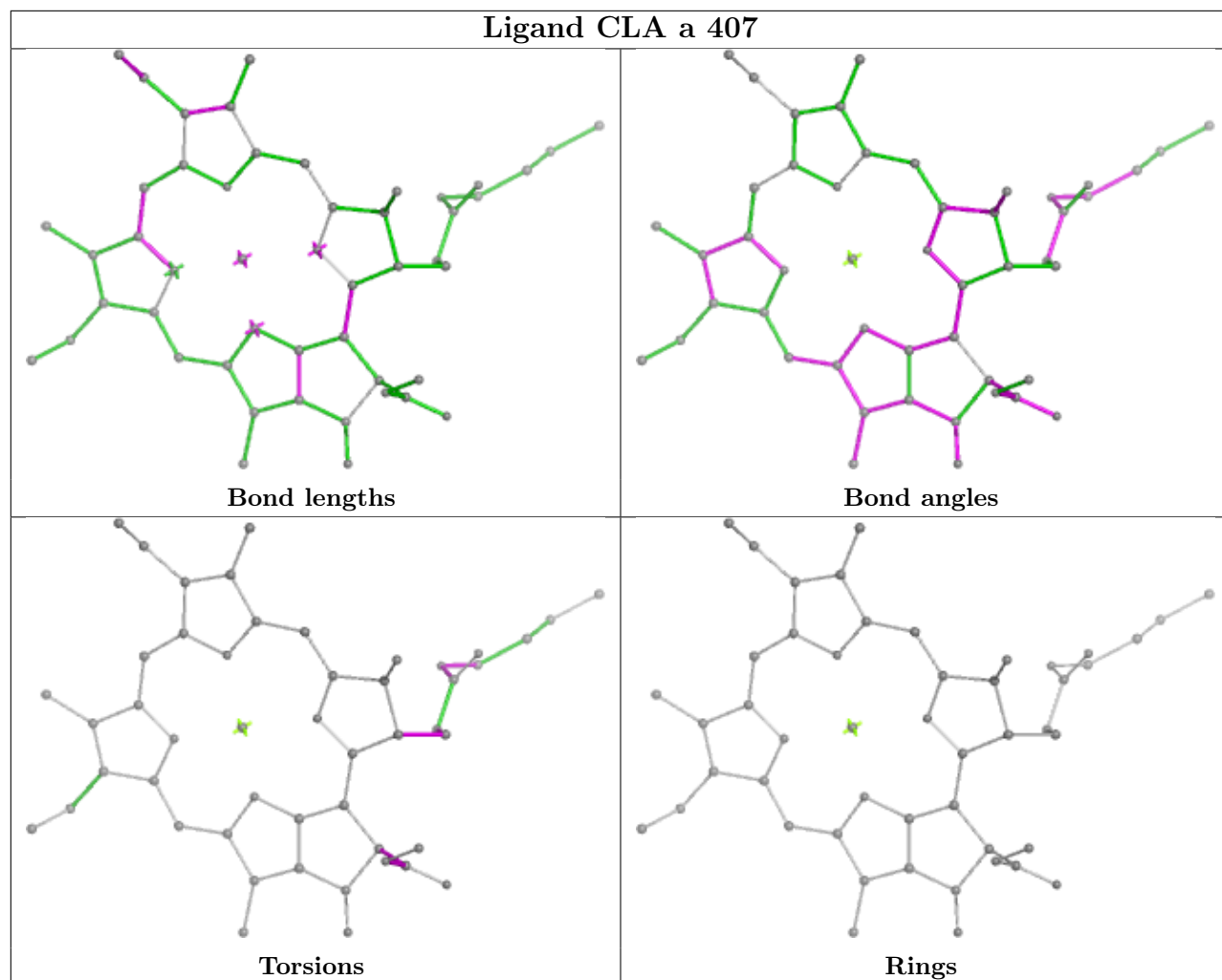
Ligand PHO a 409

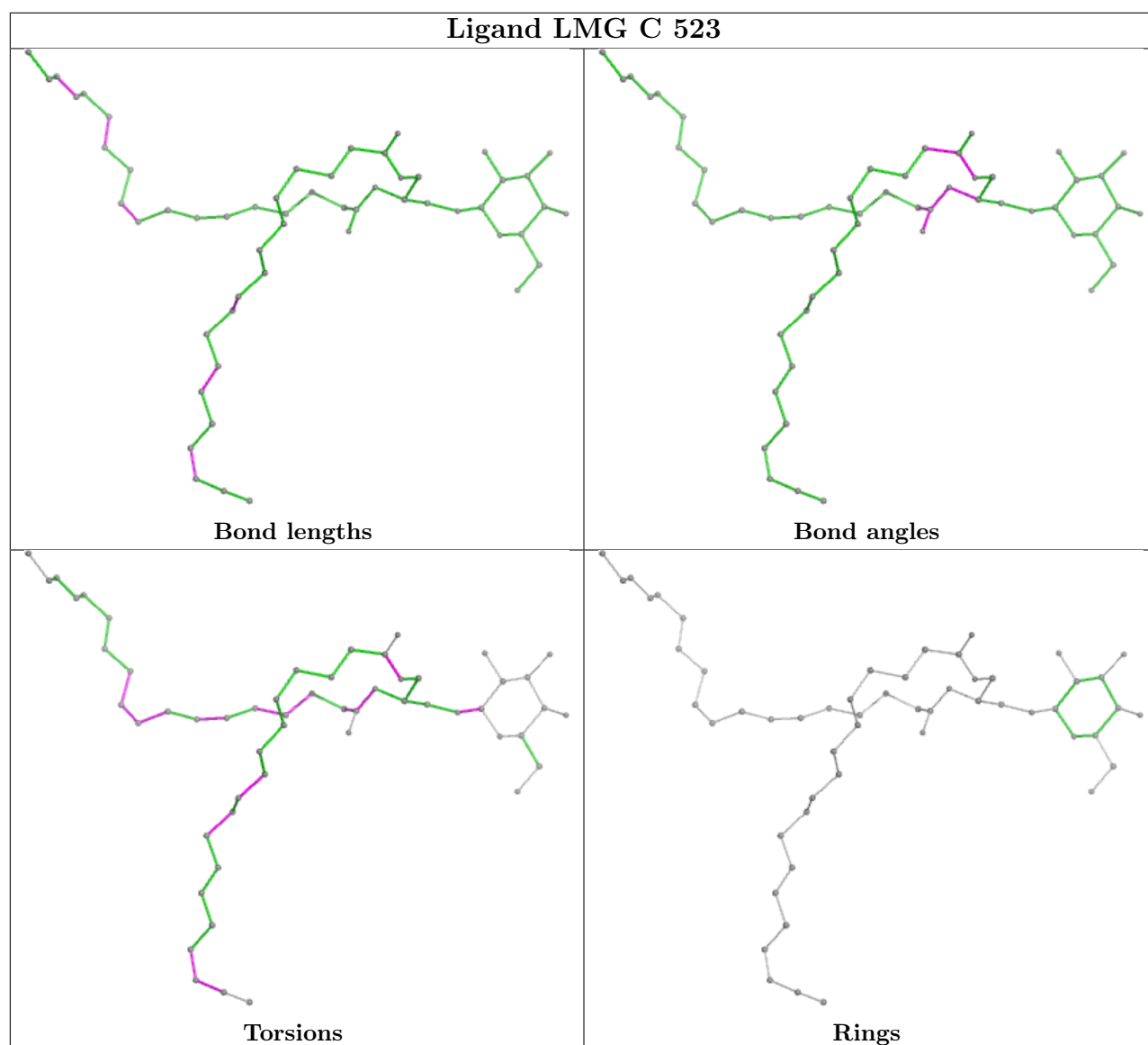




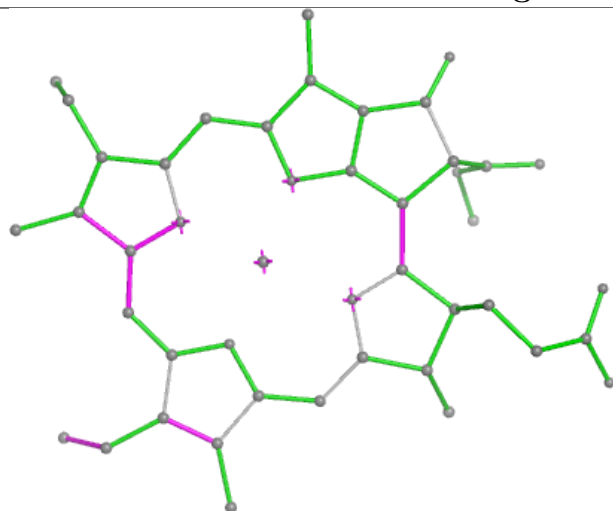


Ligand CLA a 407

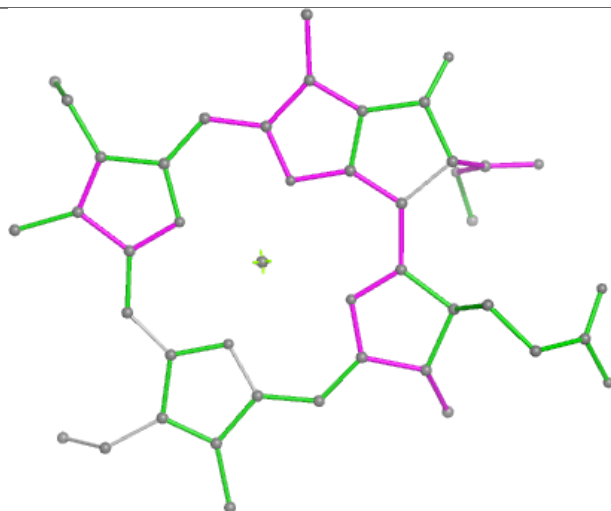




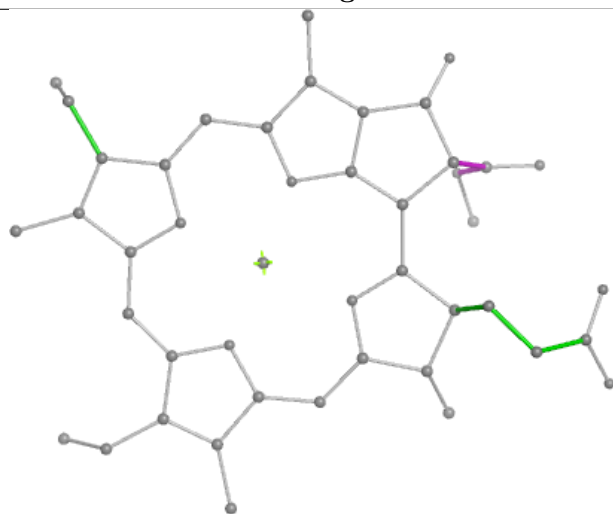
Ligand CLA N 612



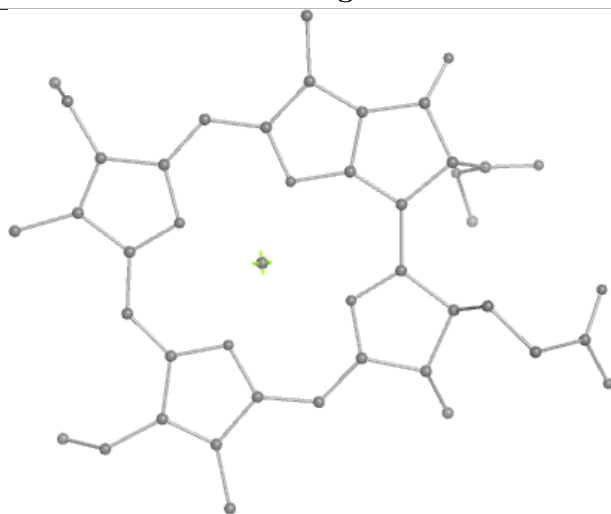
Bond lengths



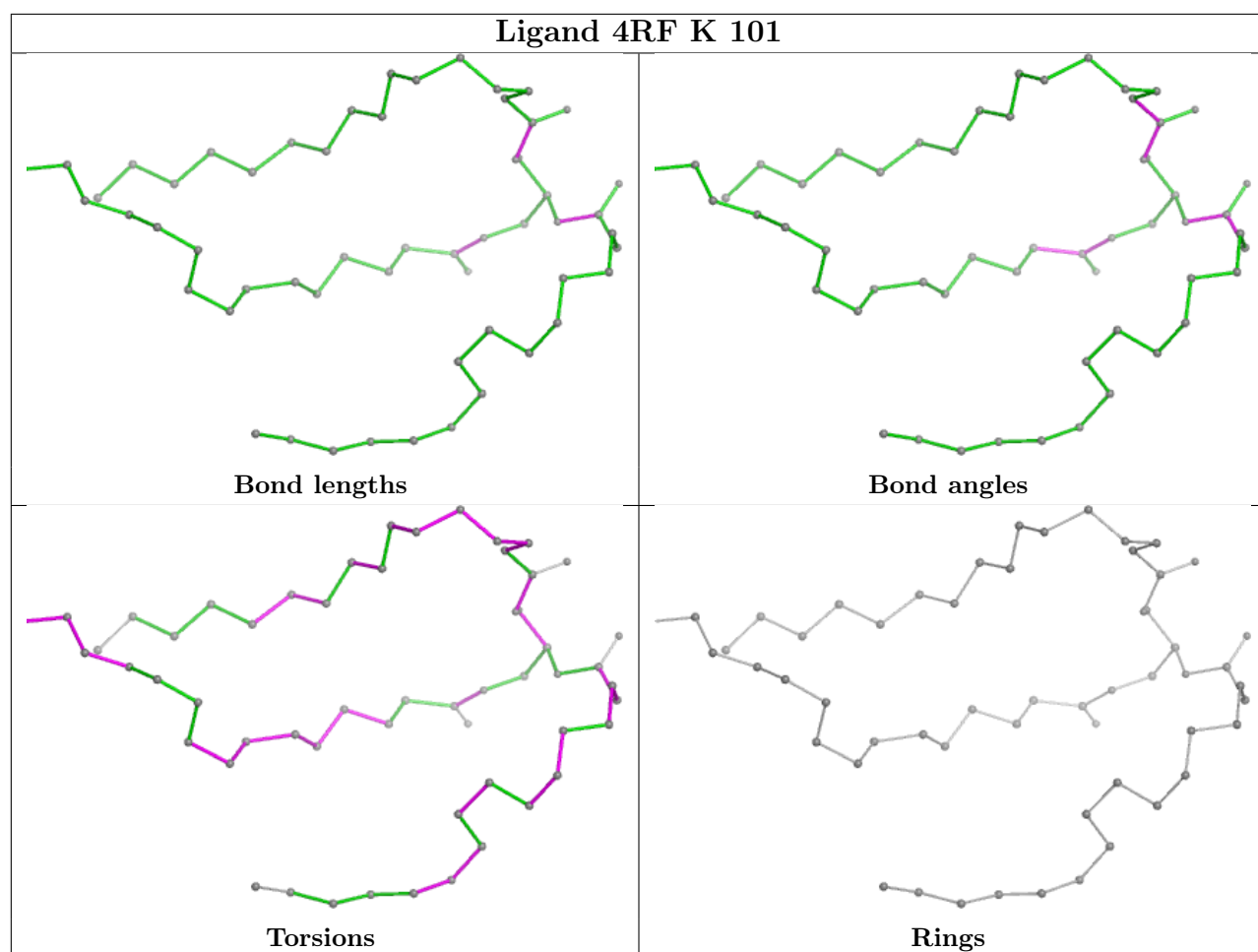
Bond angles

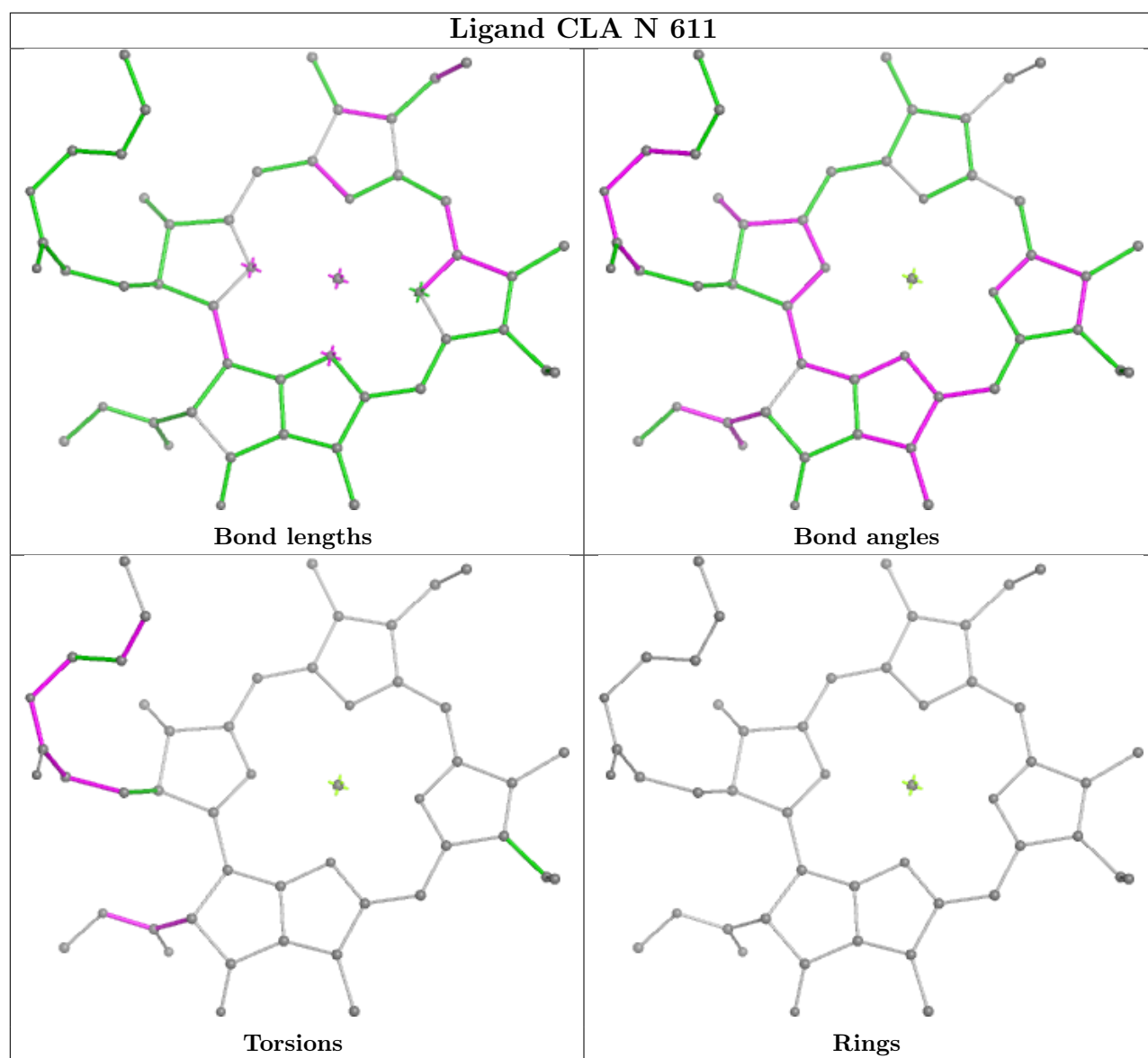


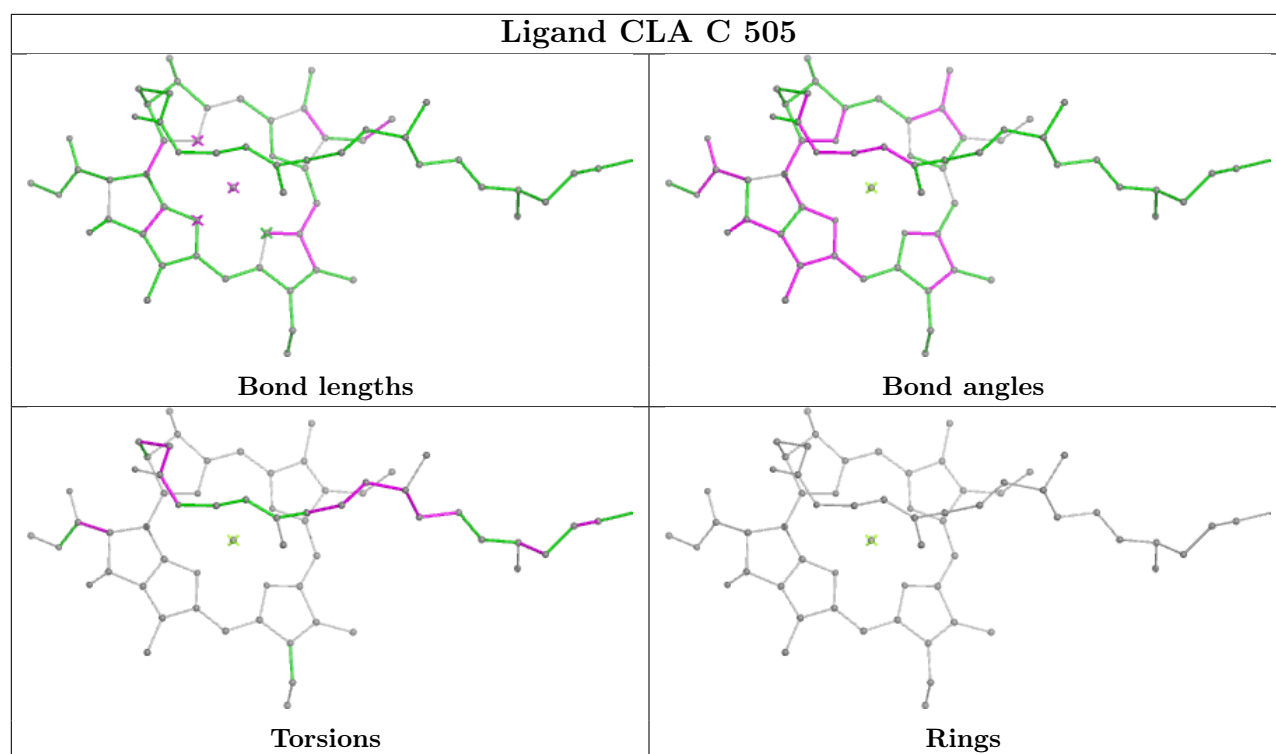
Torsions

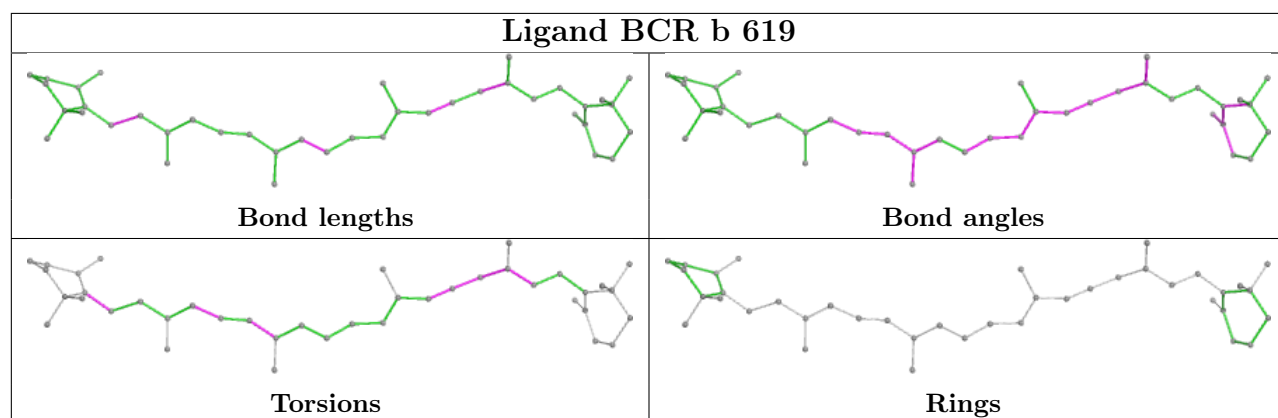
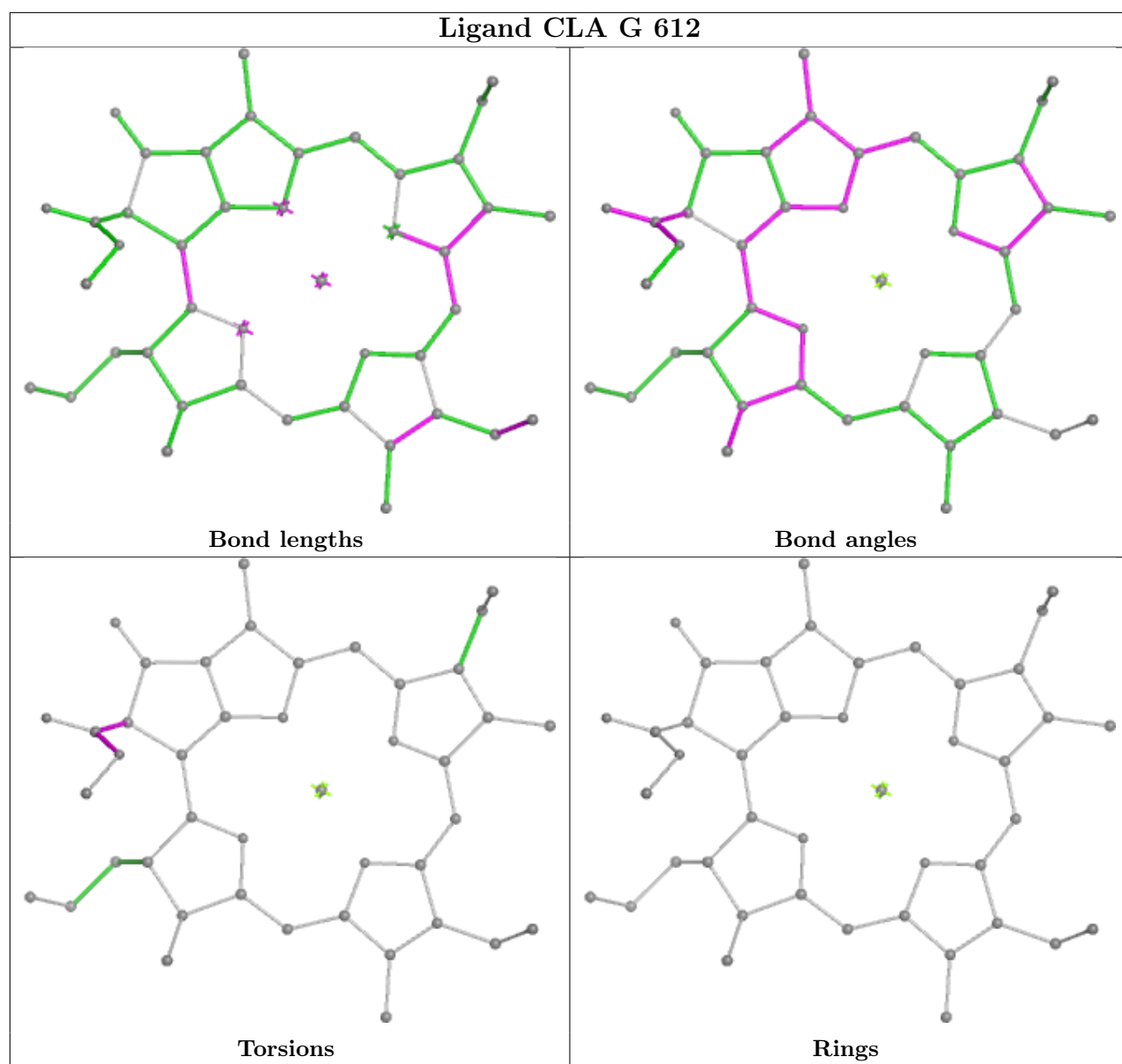


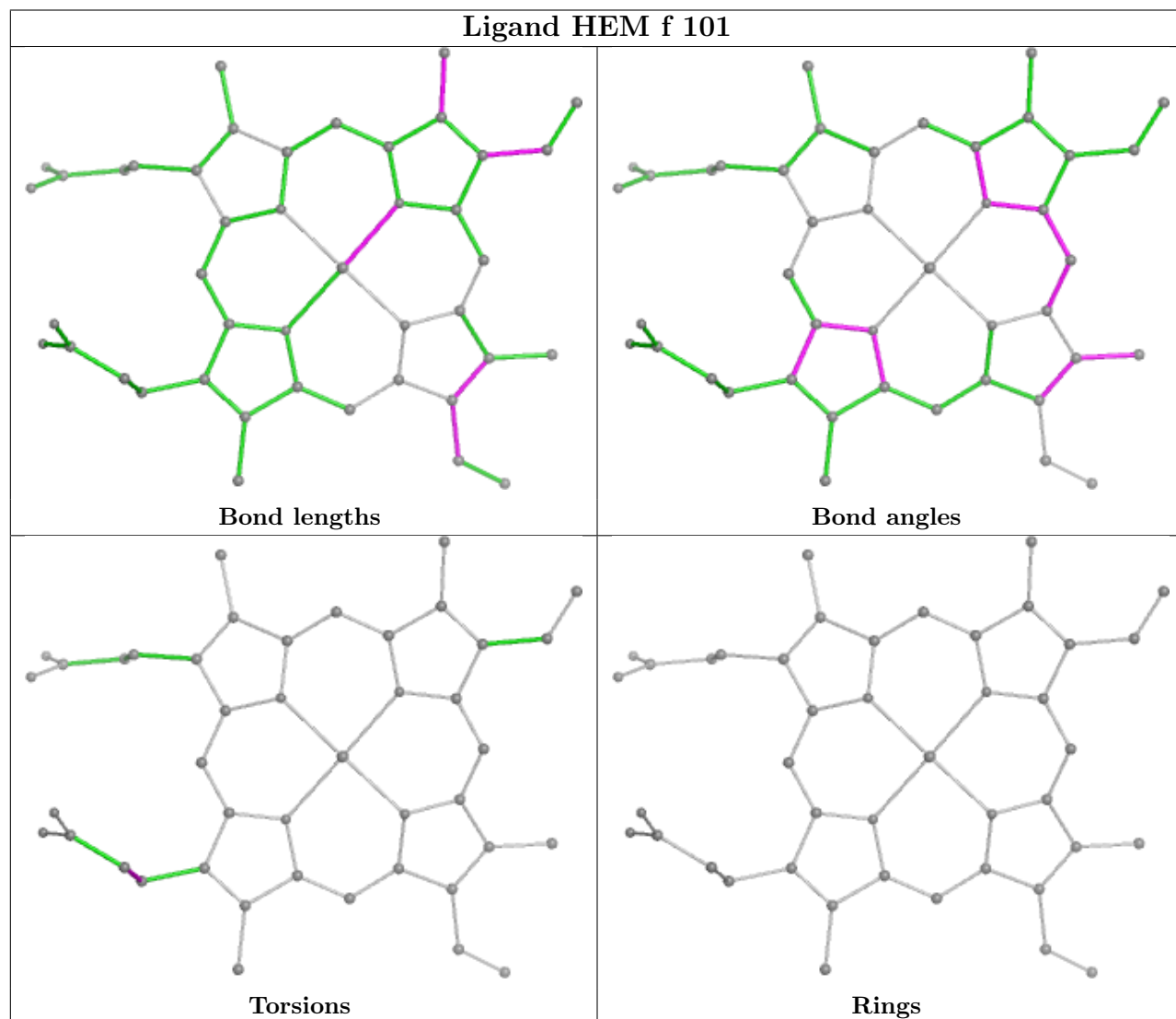
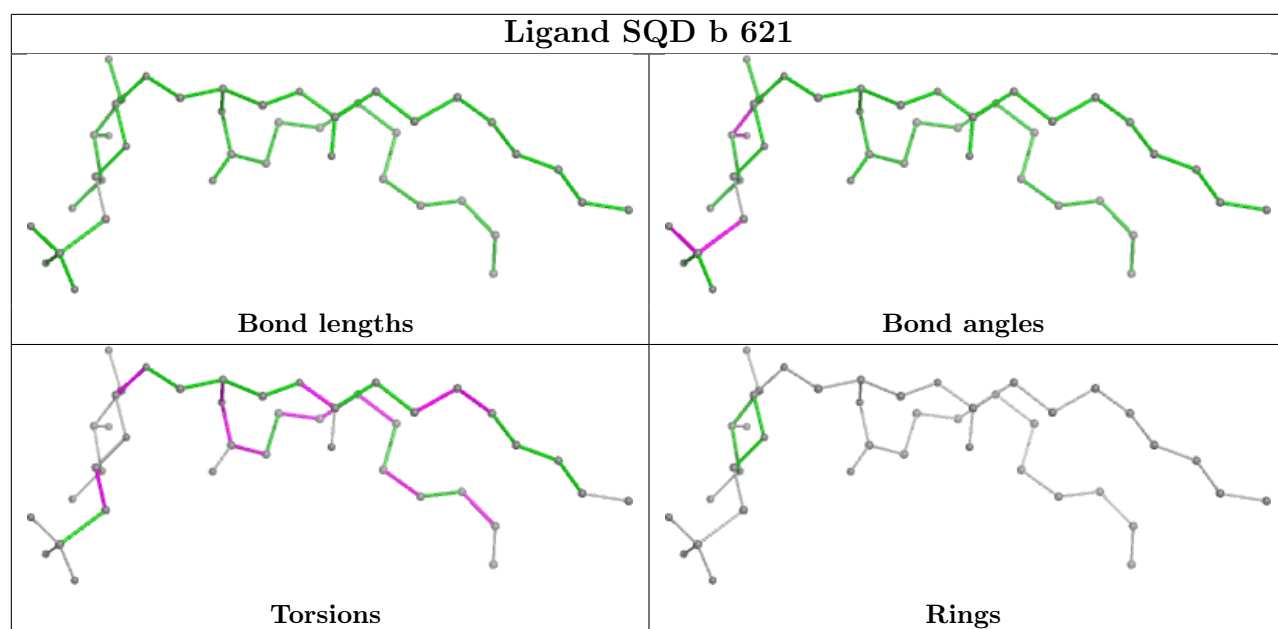
Rings

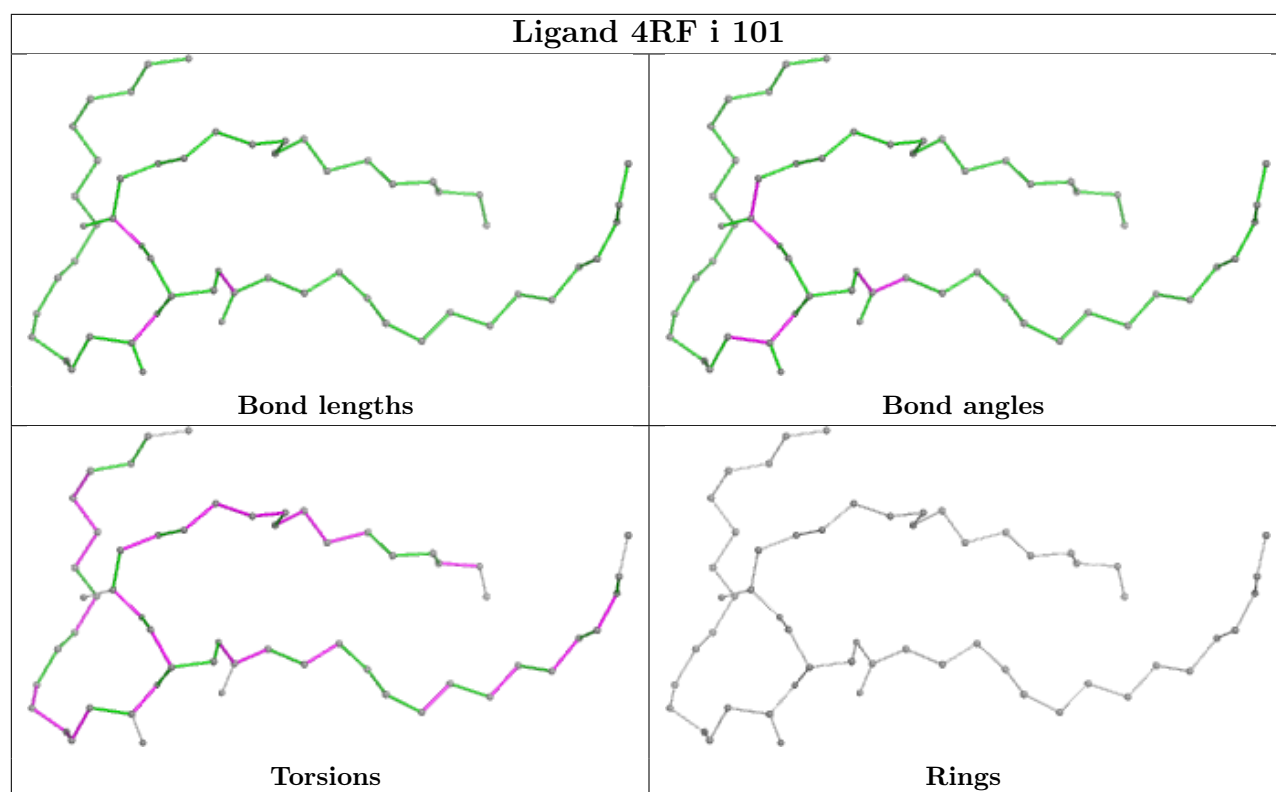


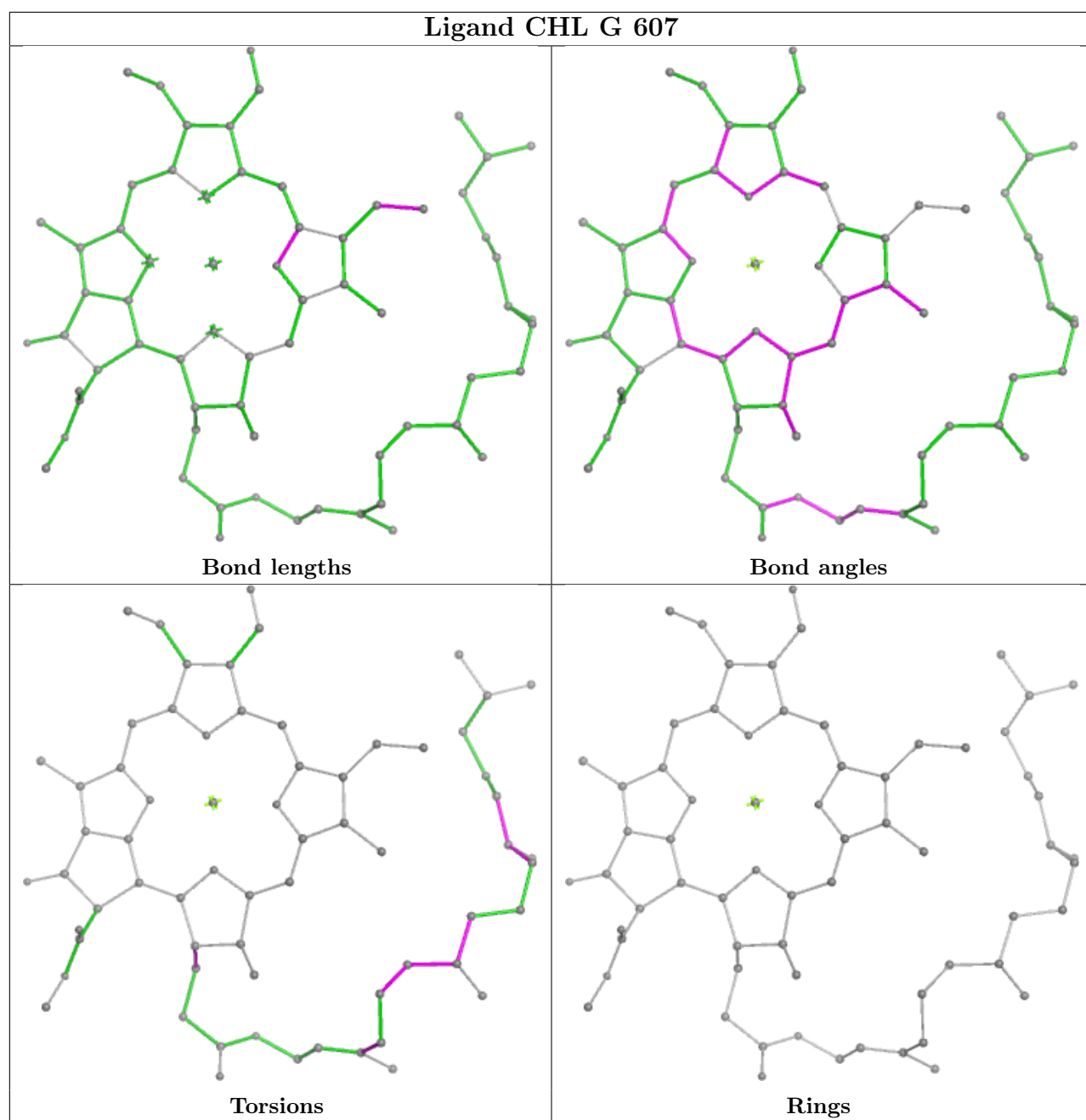


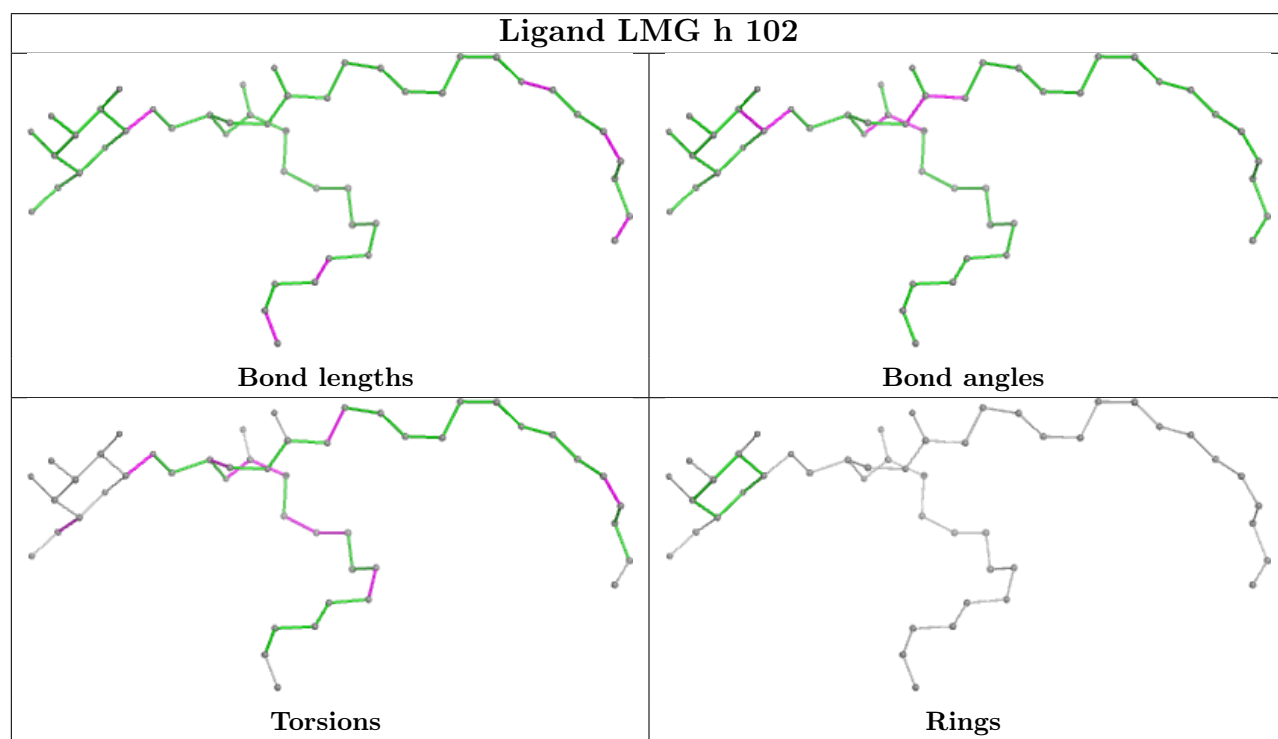
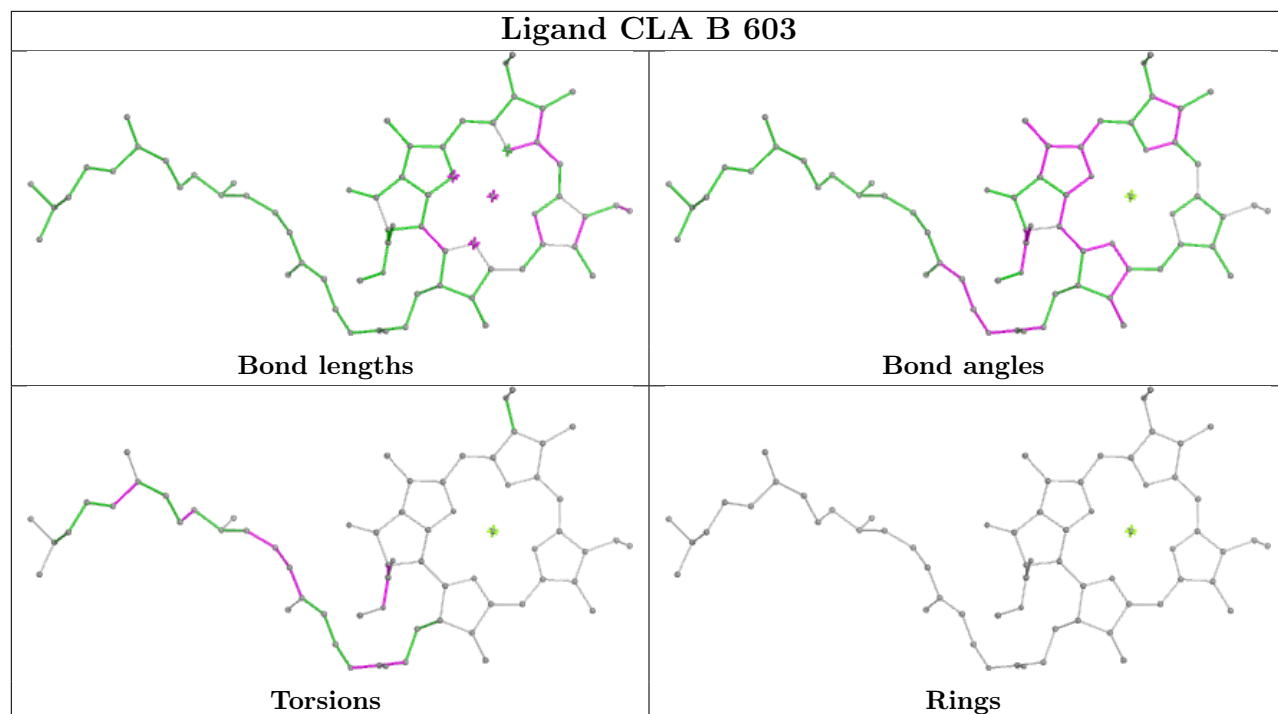


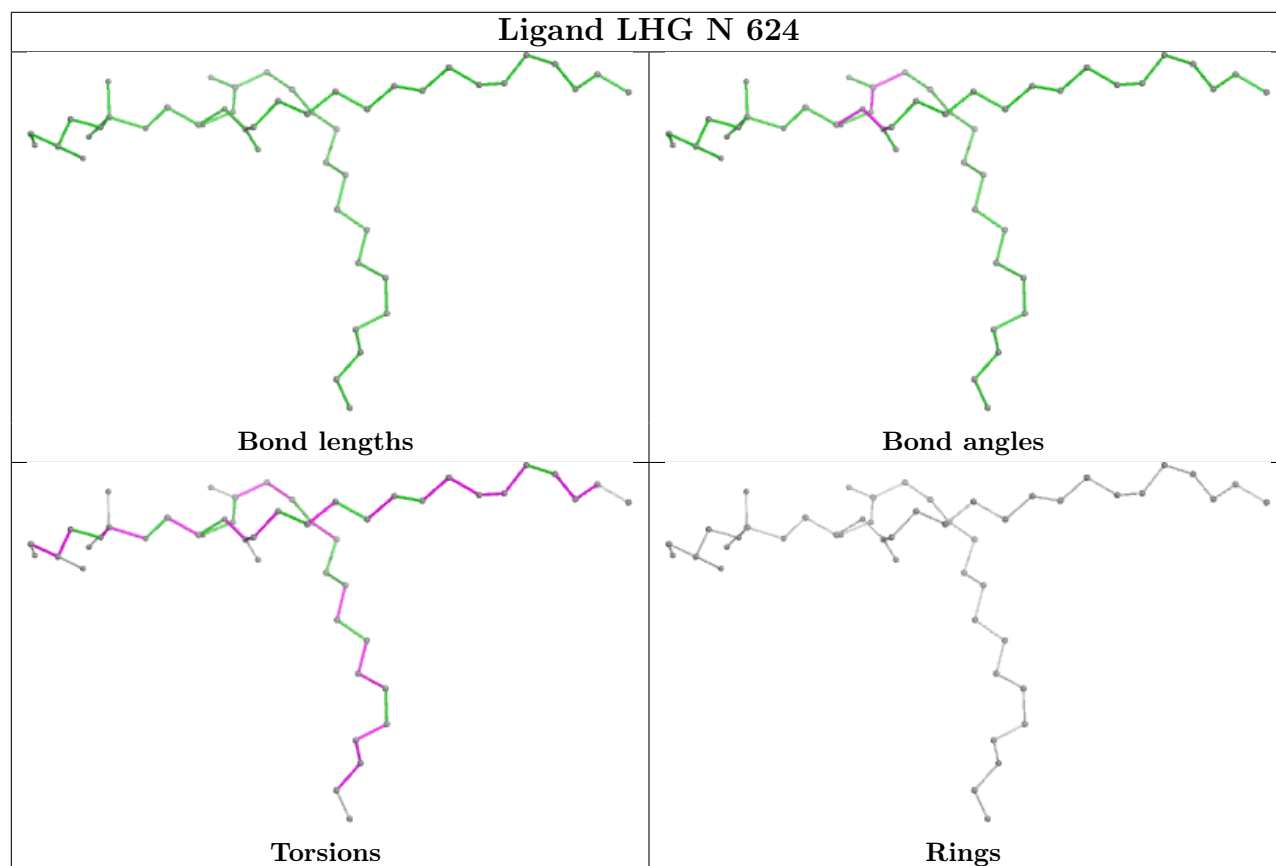
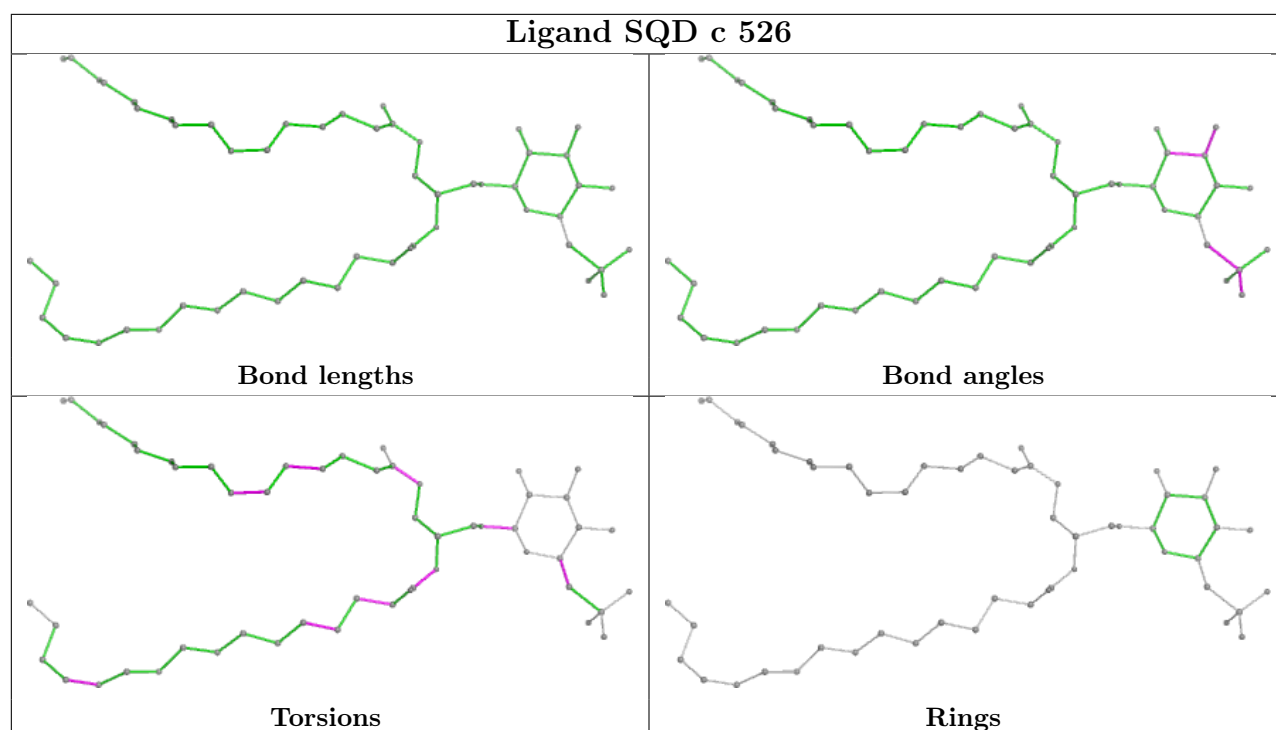


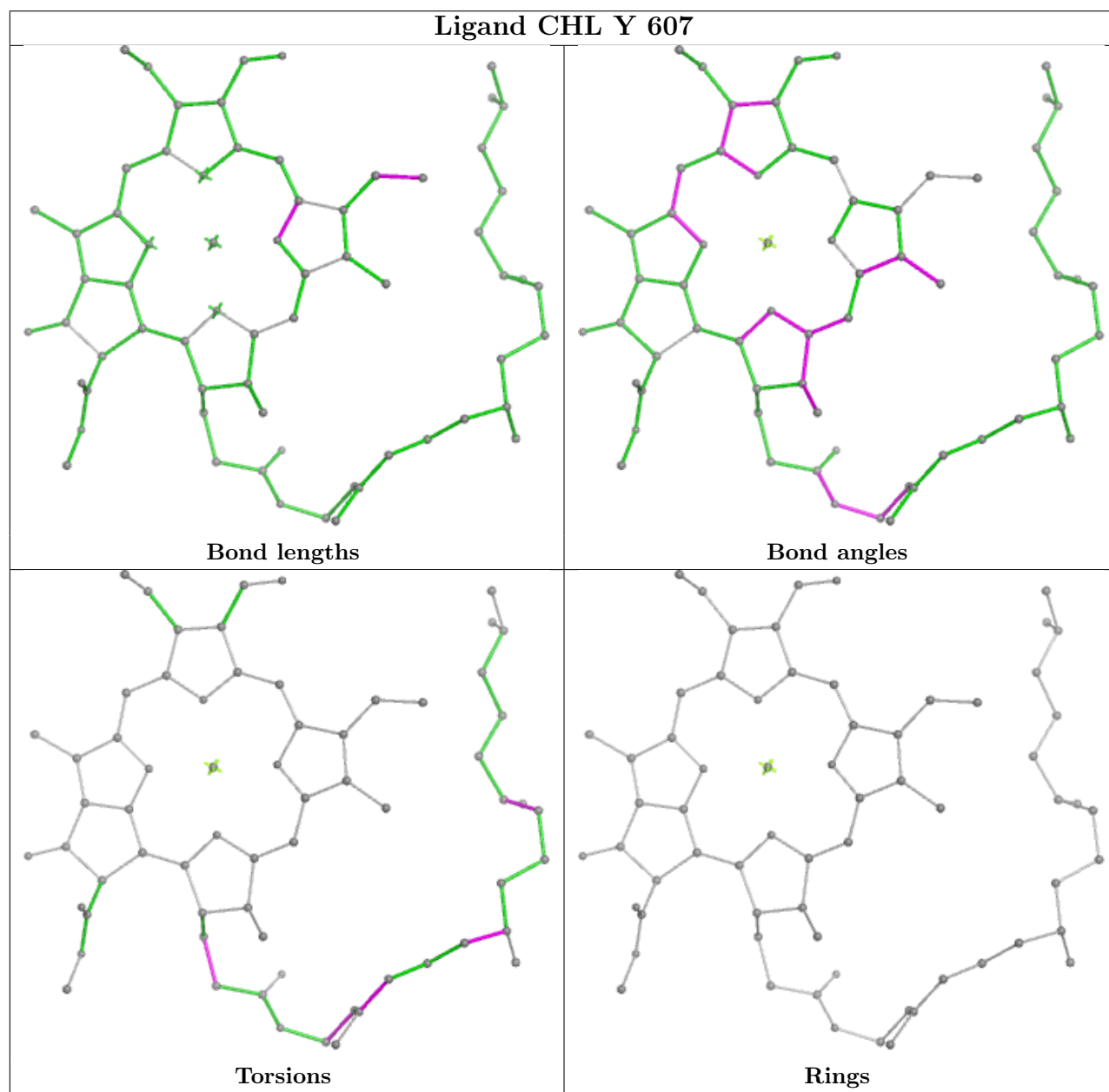
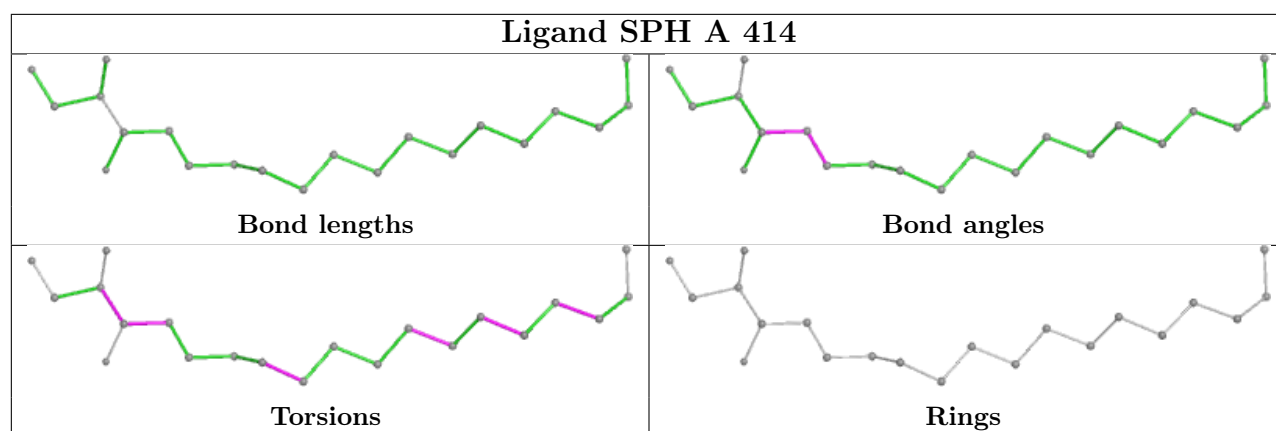


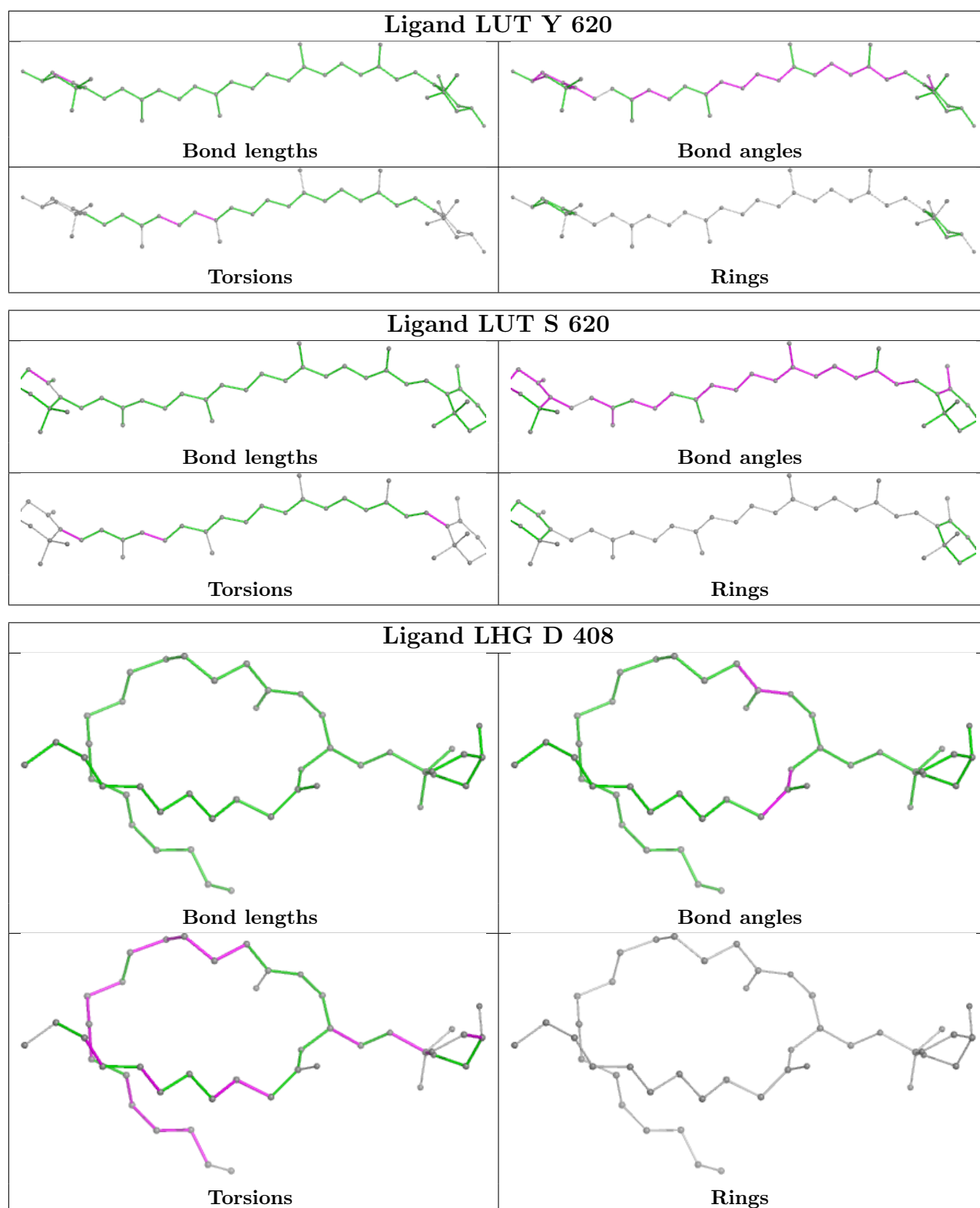


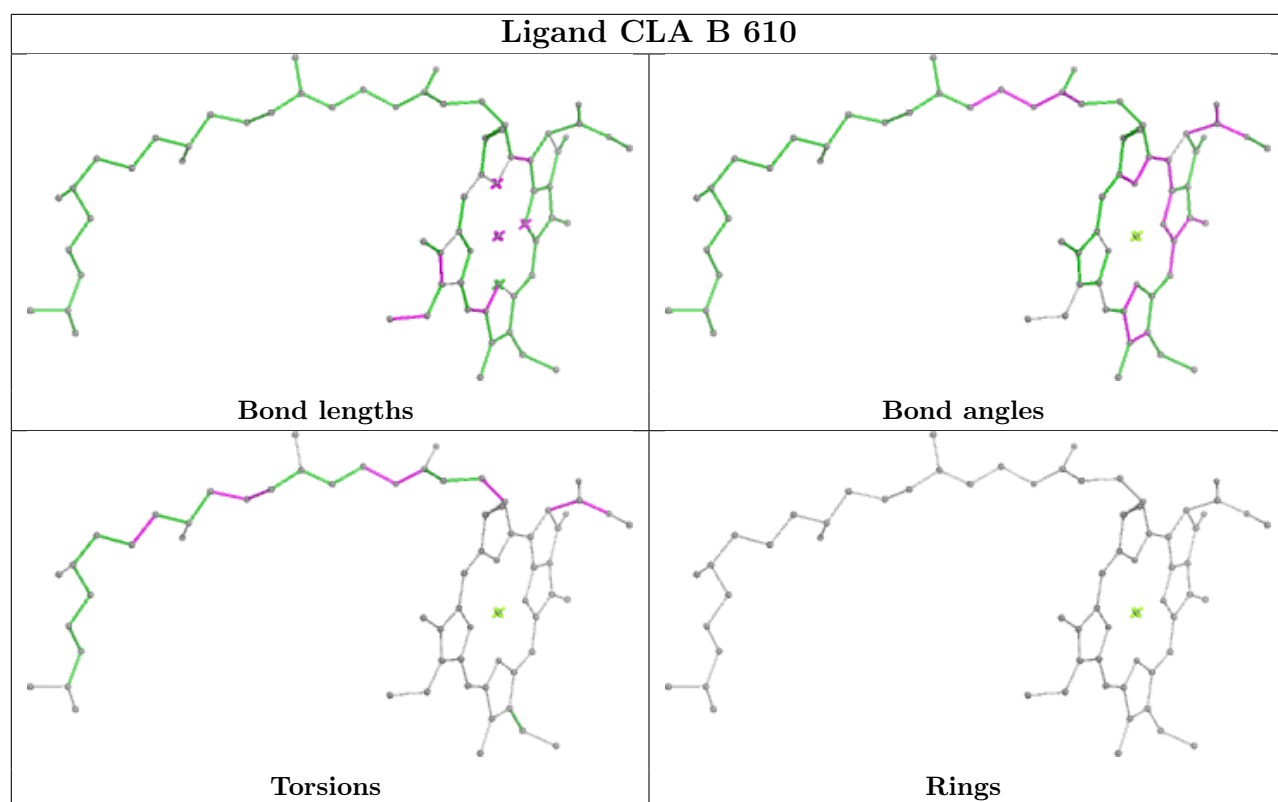


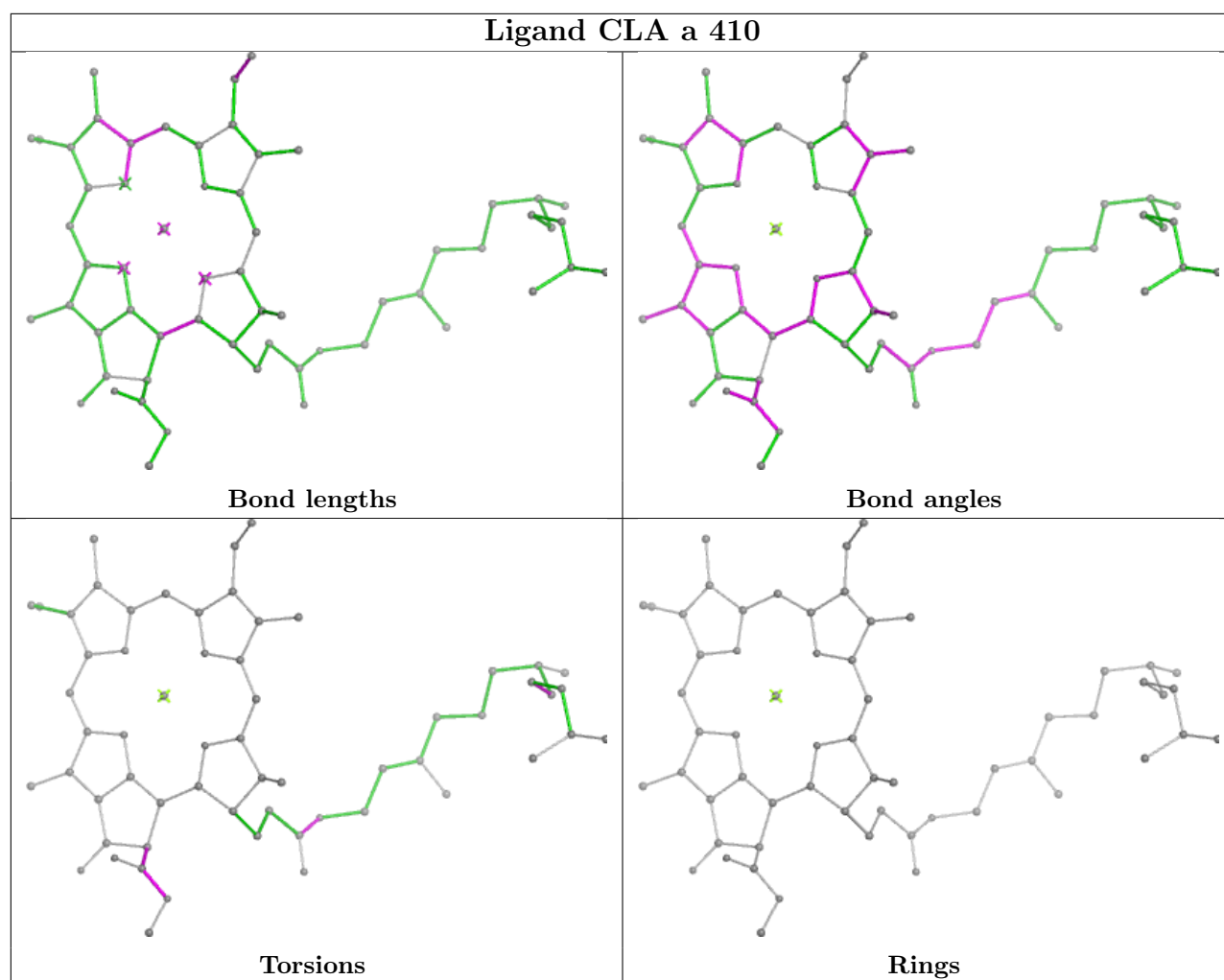


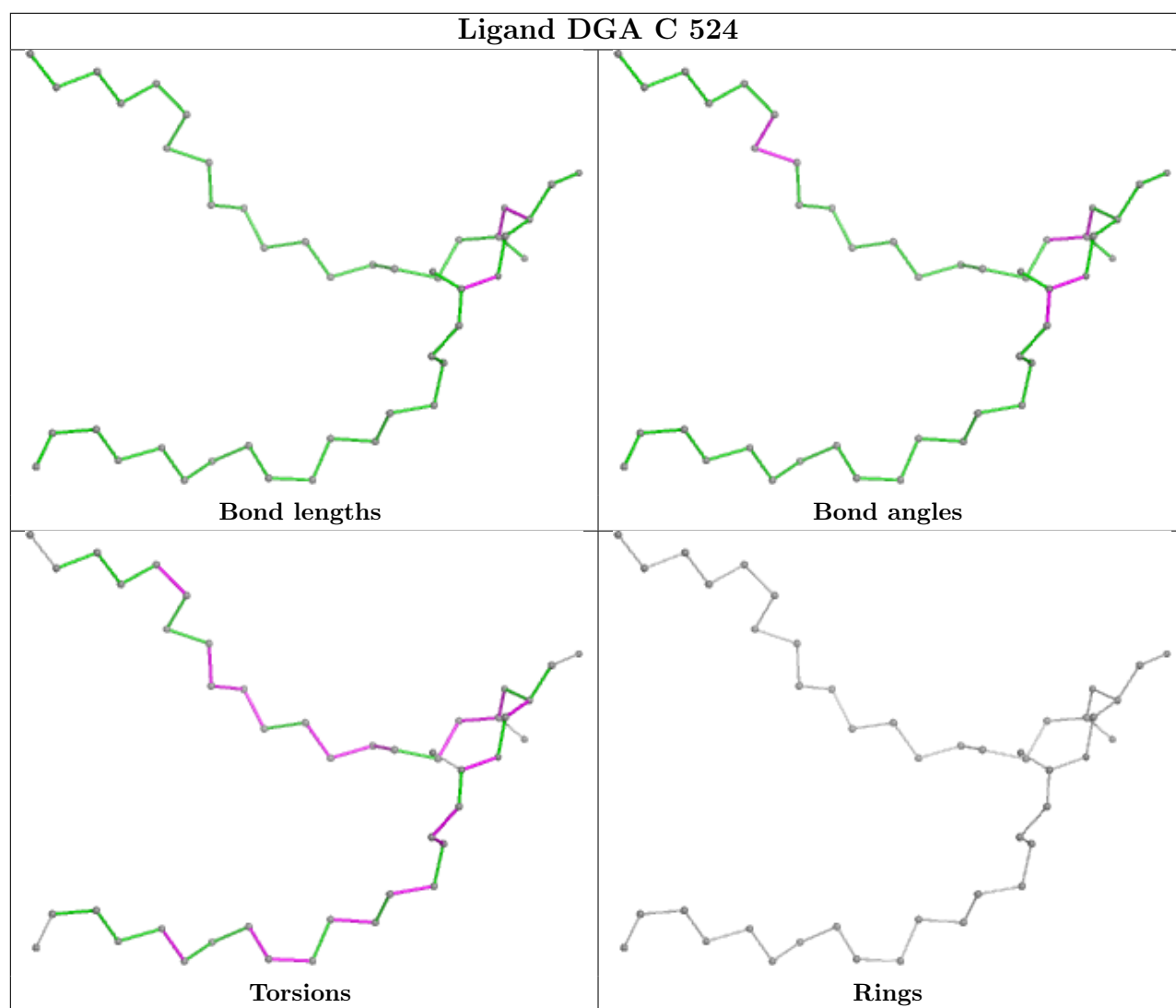


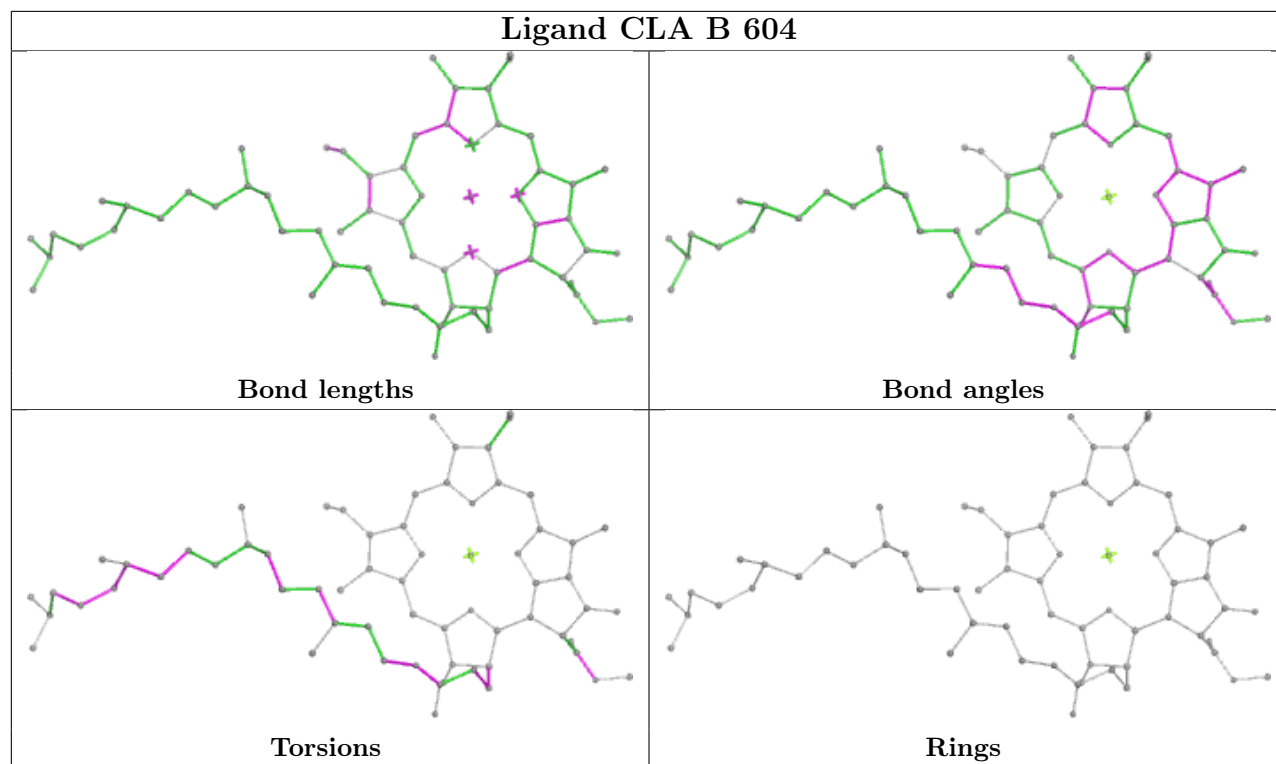
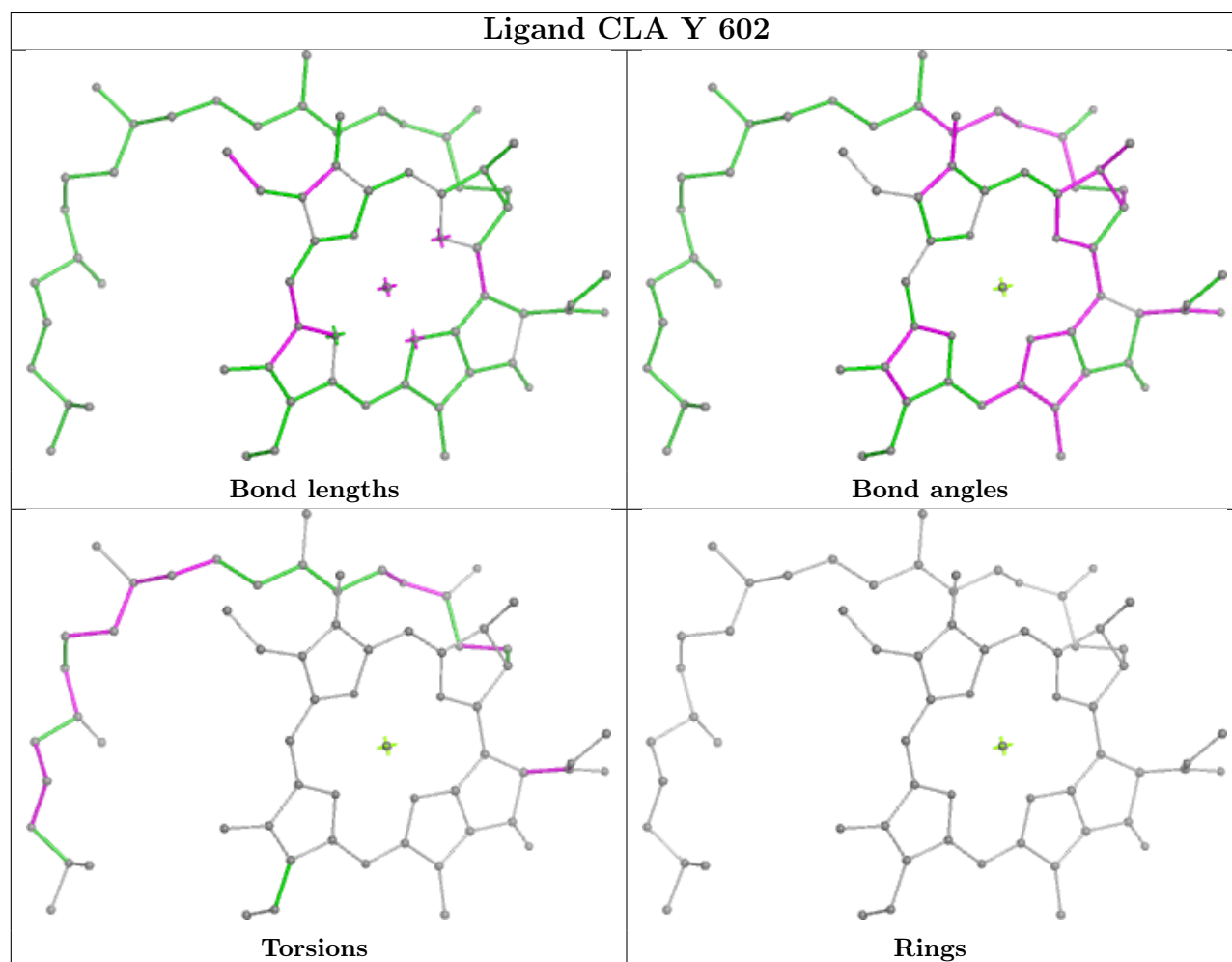


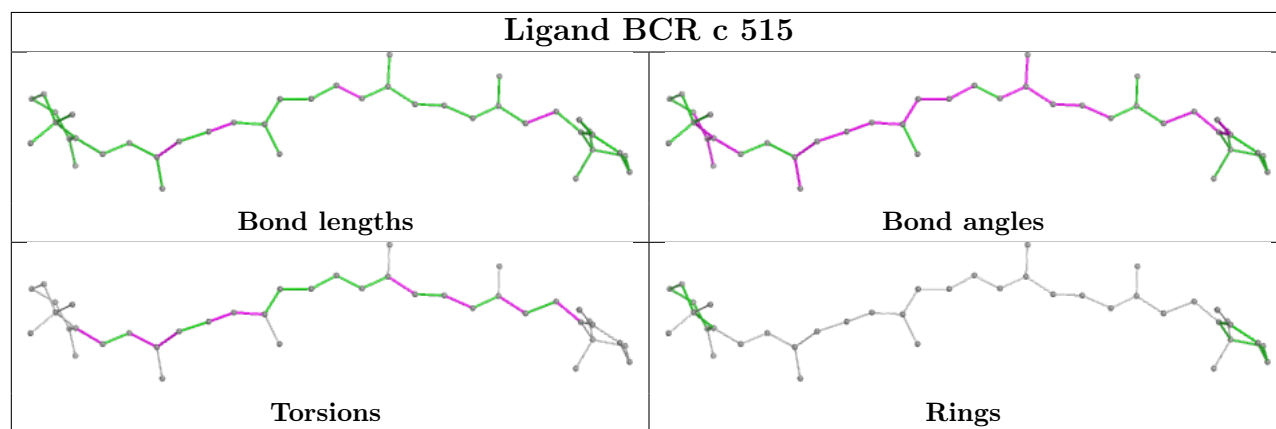
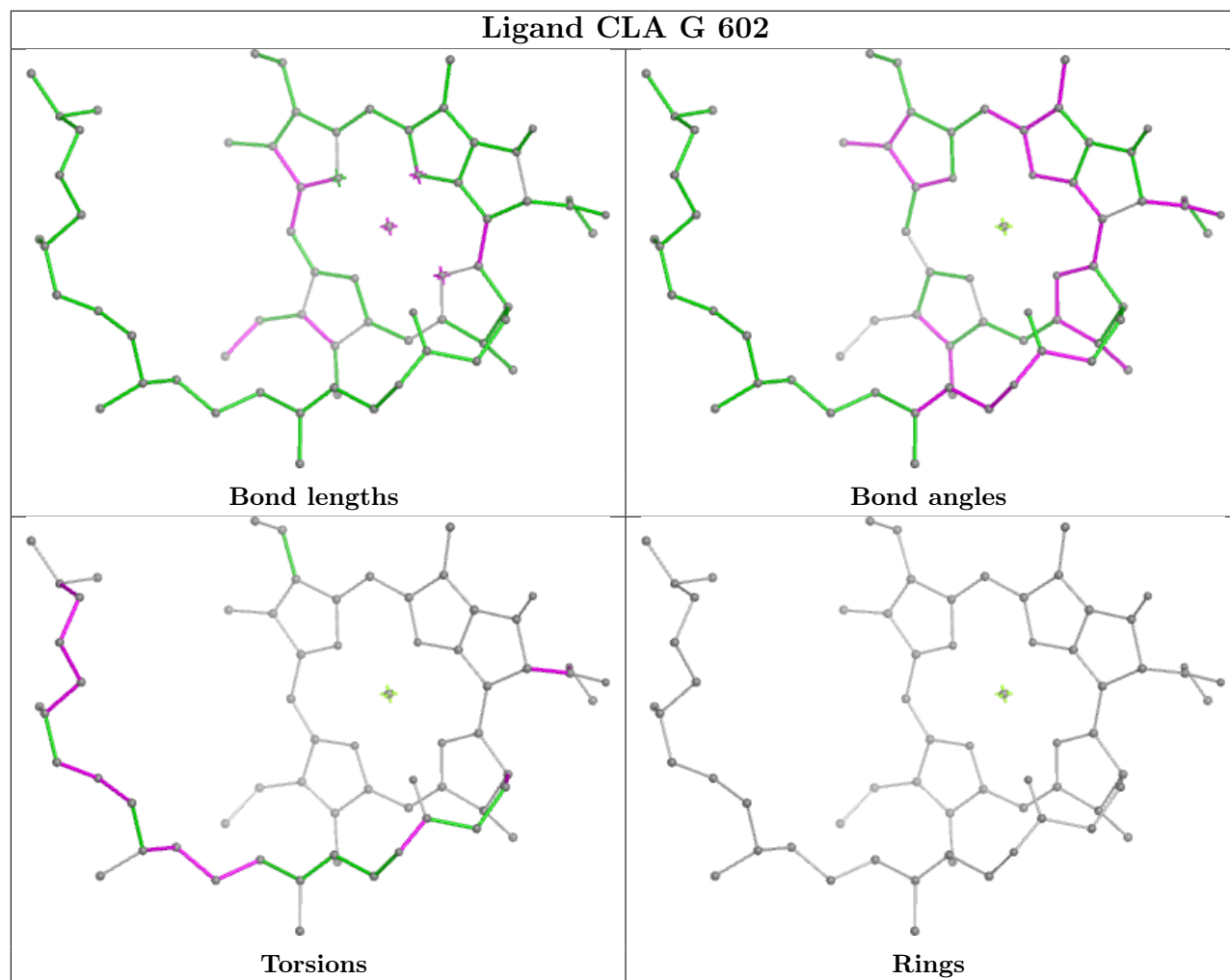


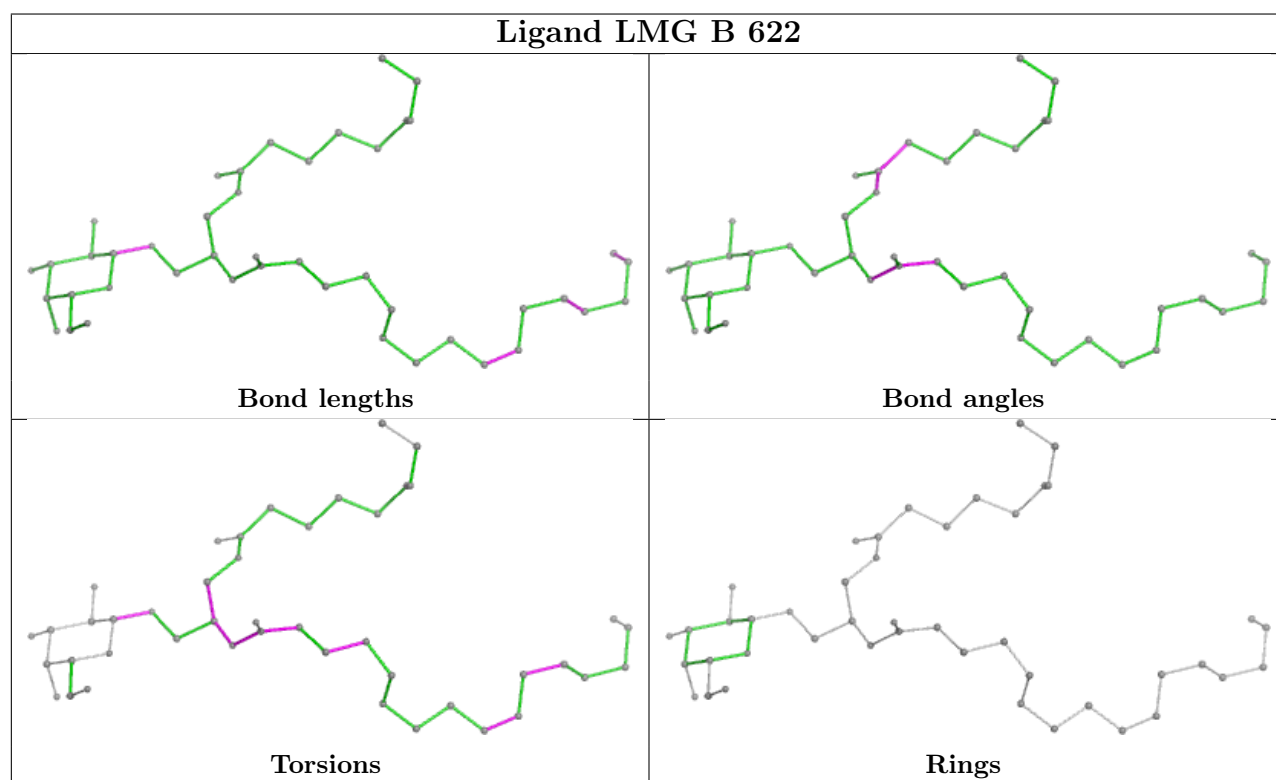
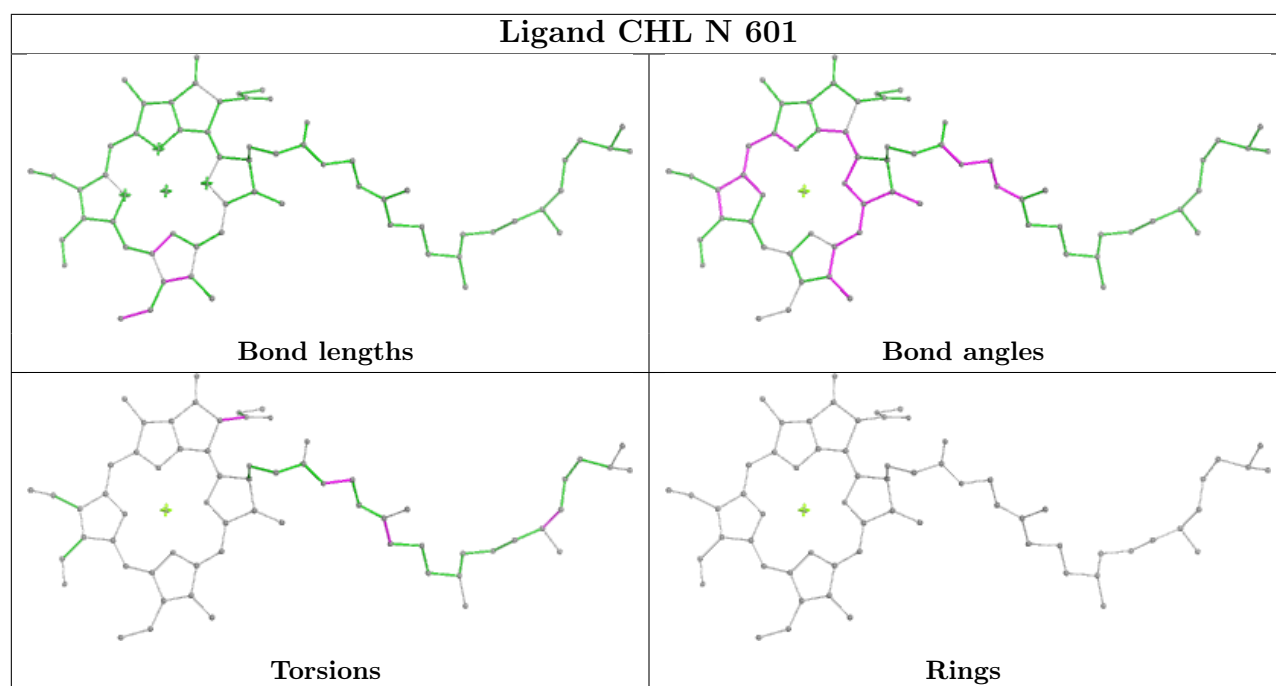




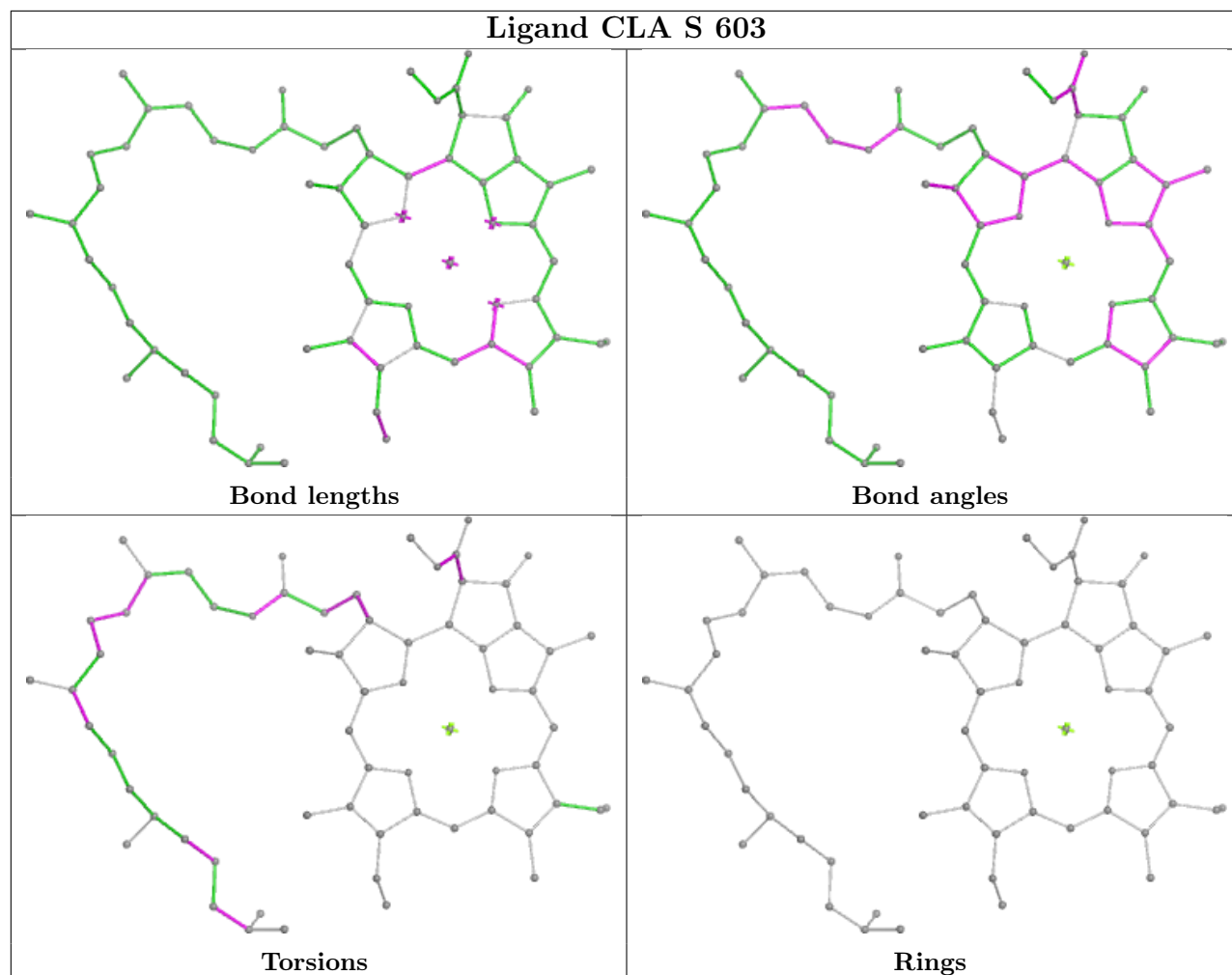


Ligand CLA B 604**Ligand CLA Y 602**

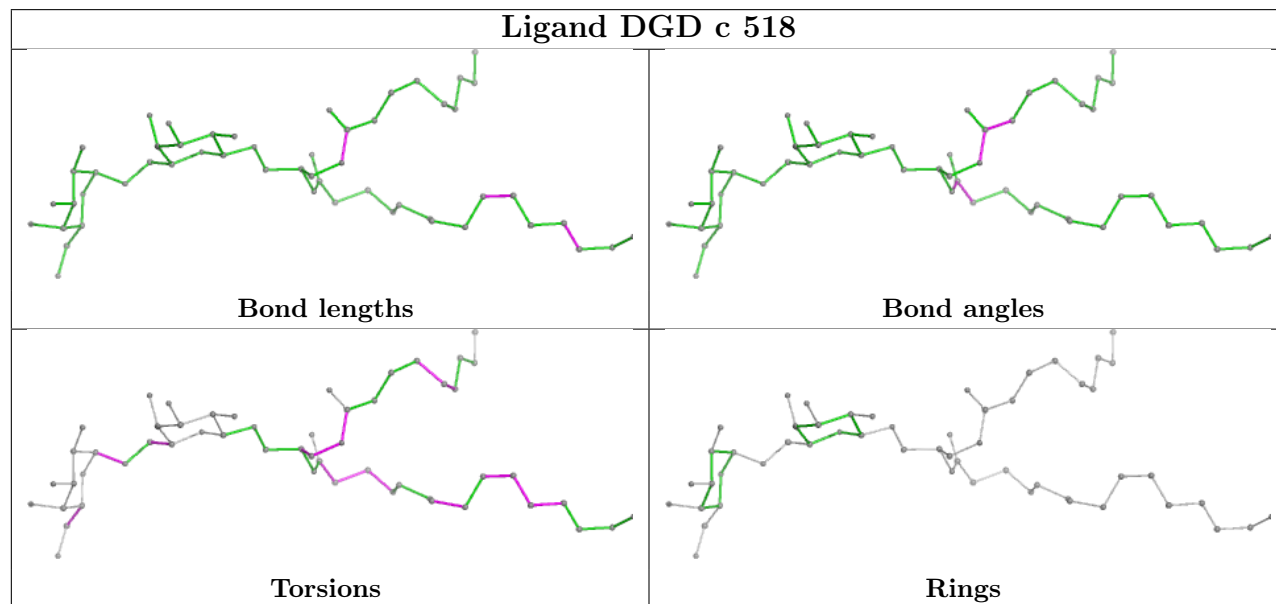


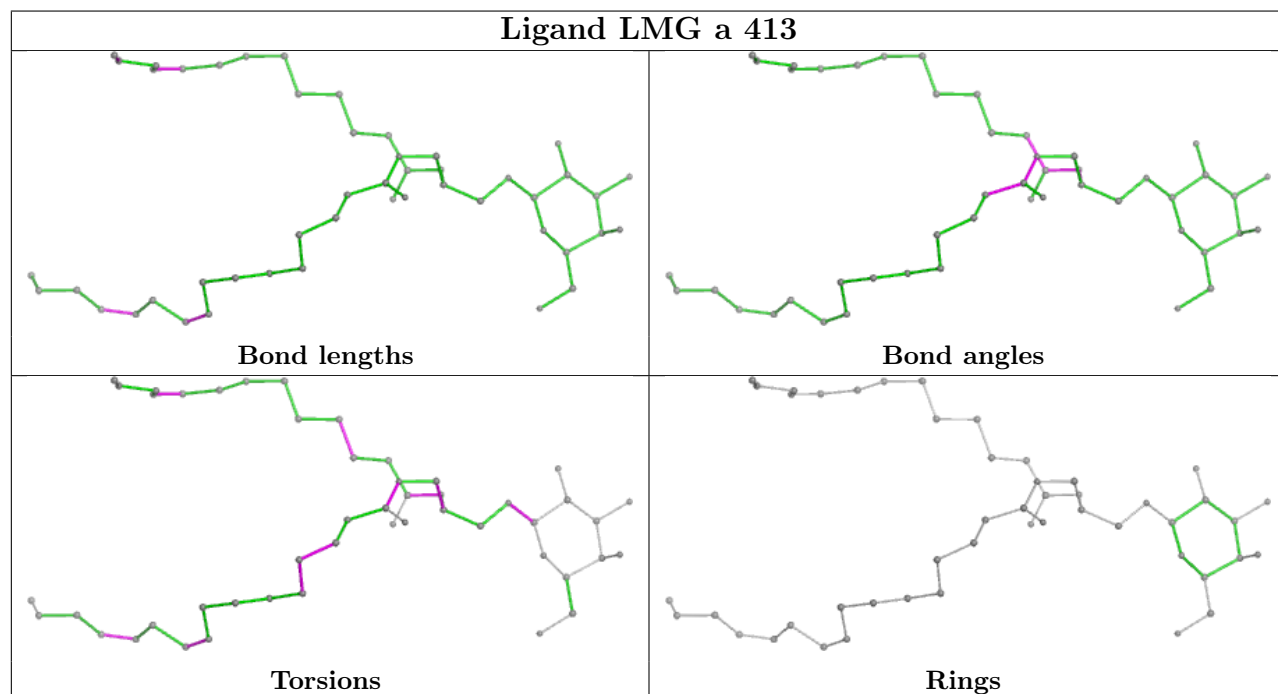
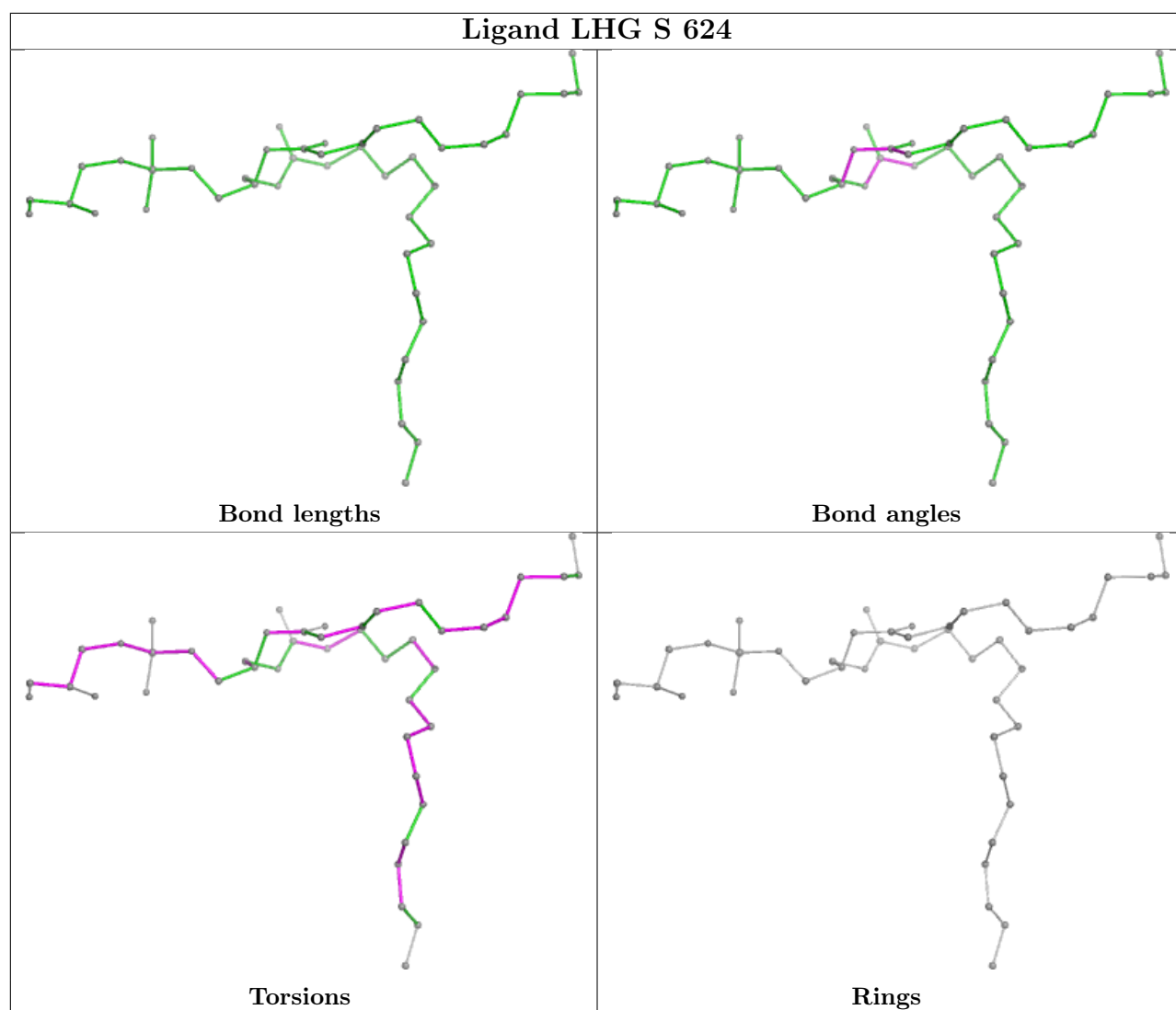


Ligand CLA S 603

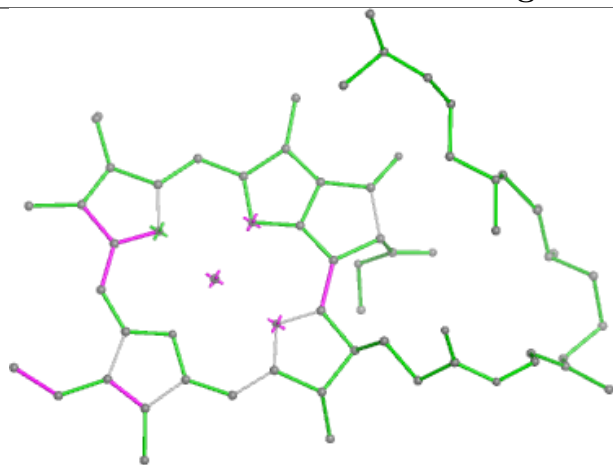


Ligand DGD c 518

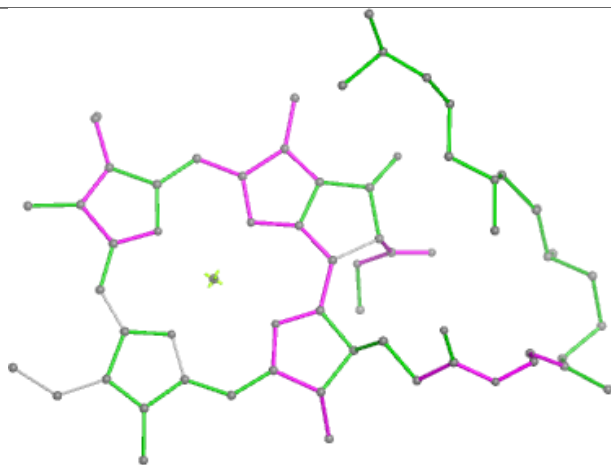




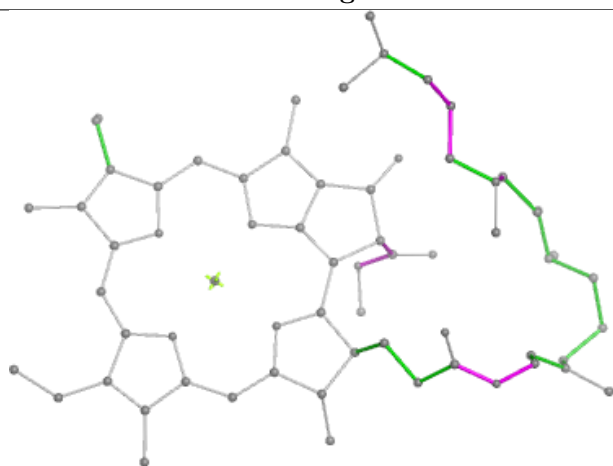
Ligand CLA b 611



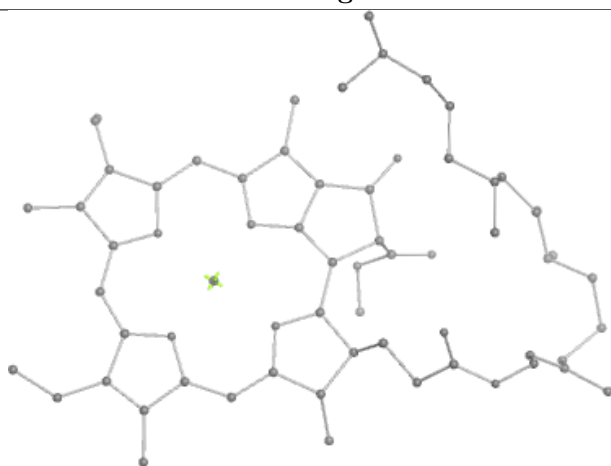
Bond lengths



Bond angles

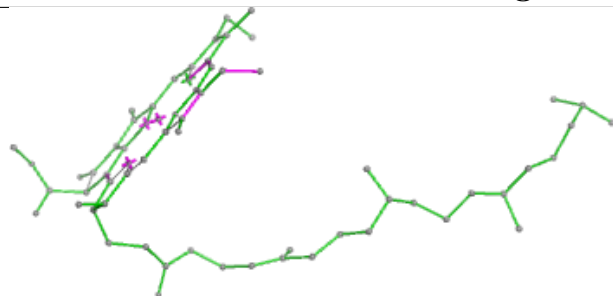


Torsions

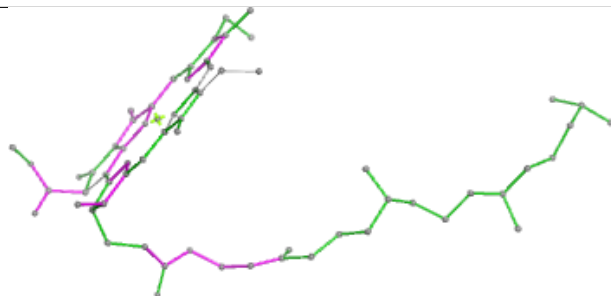


Rings

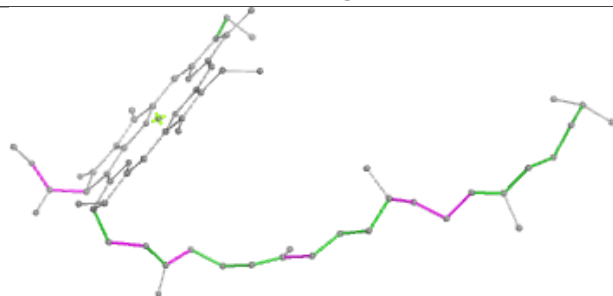
Ligand CLA C 504



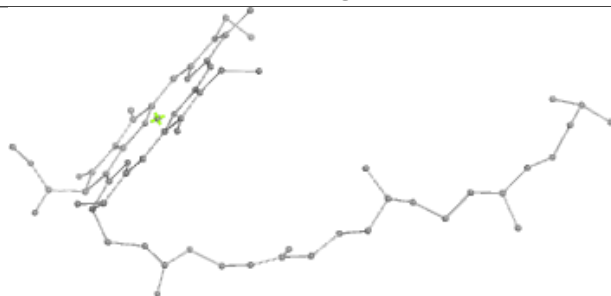
Bond lengths



Bond angles

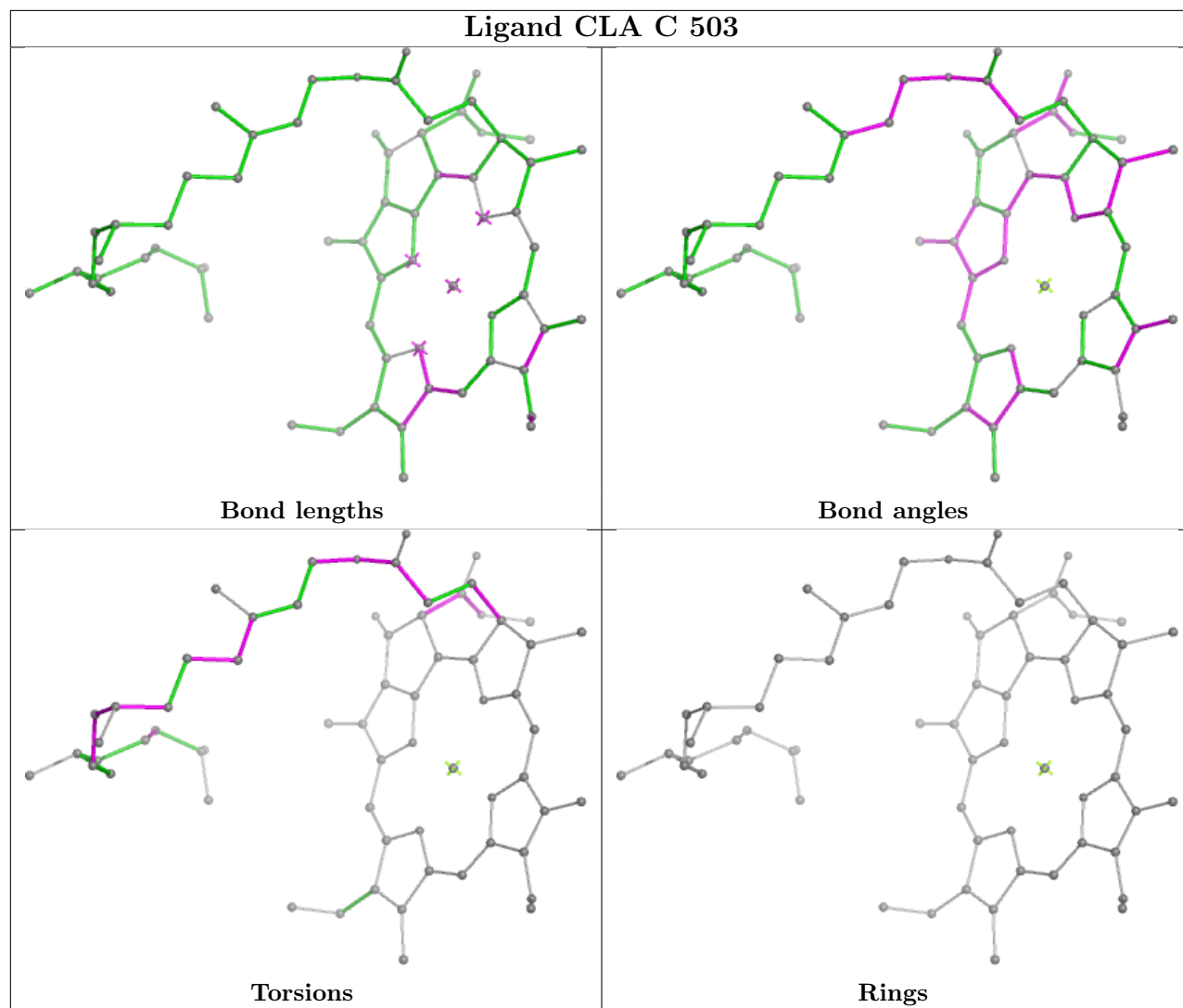


Torsions

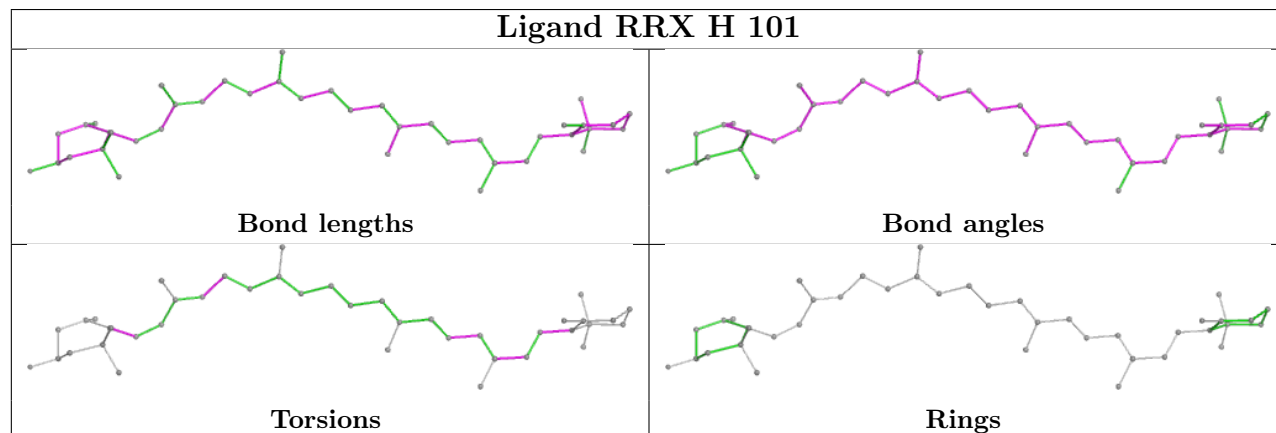


Rings

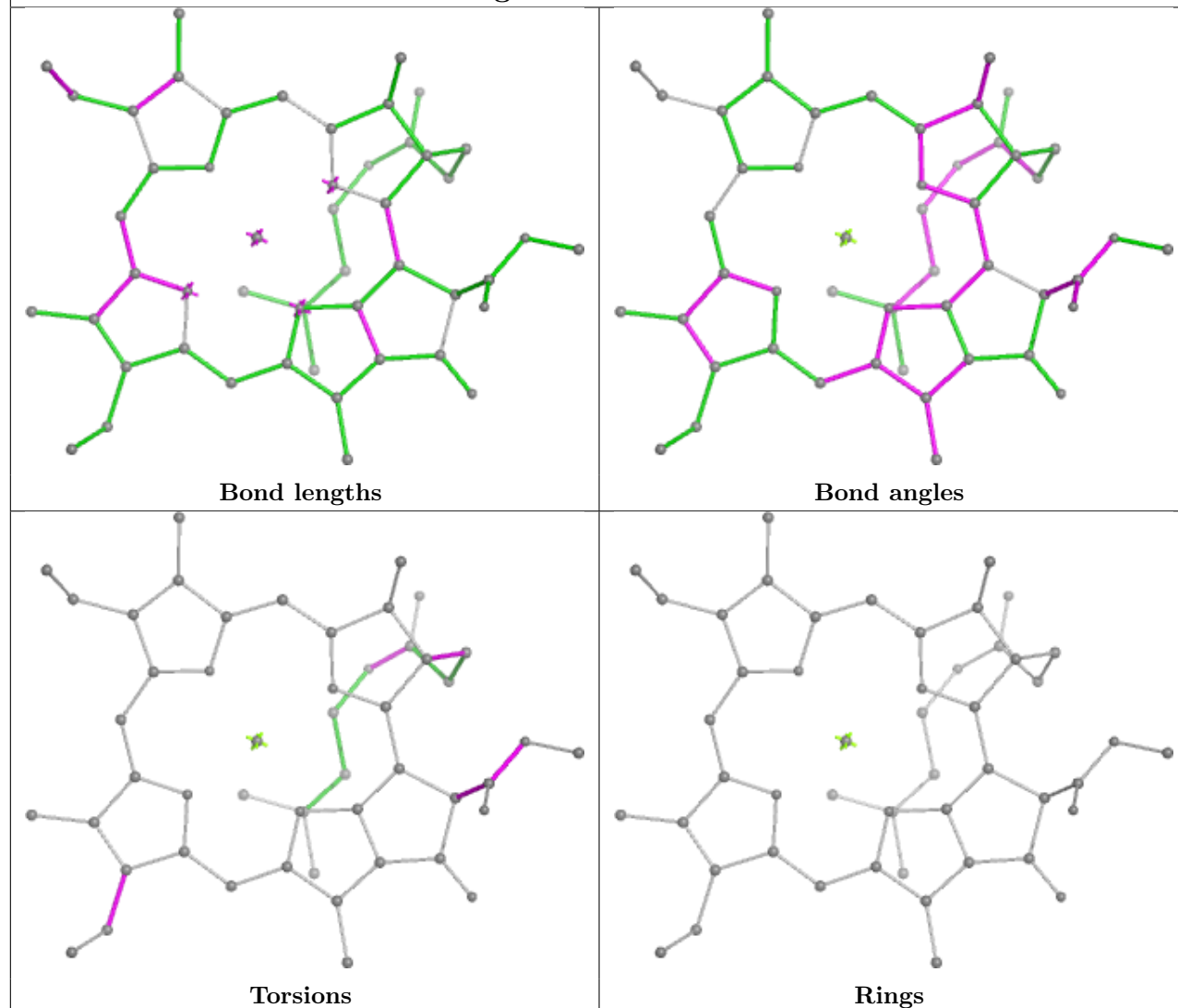
Ligand CLA C 503



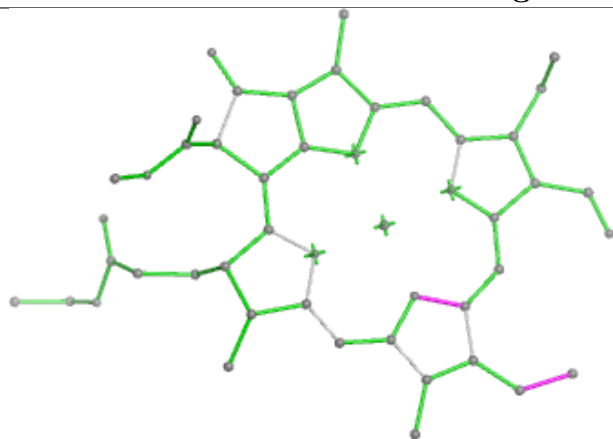
Ligand RRX H 101



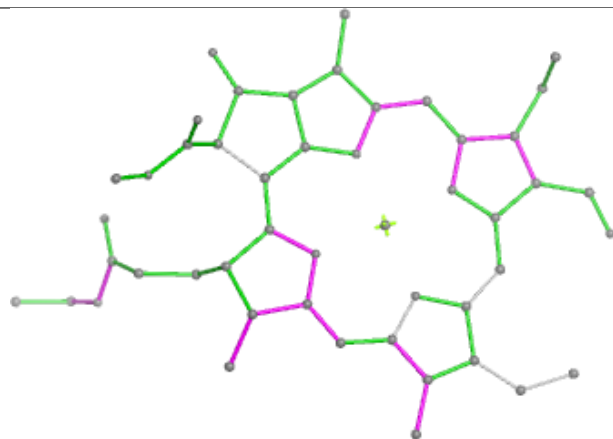
Ligand CLA S 605



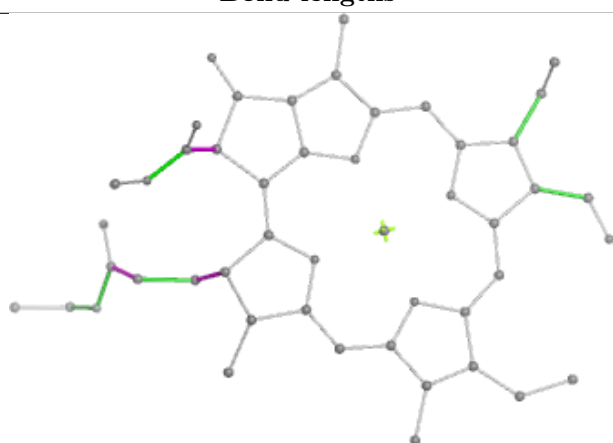
Ligand CHL G 605



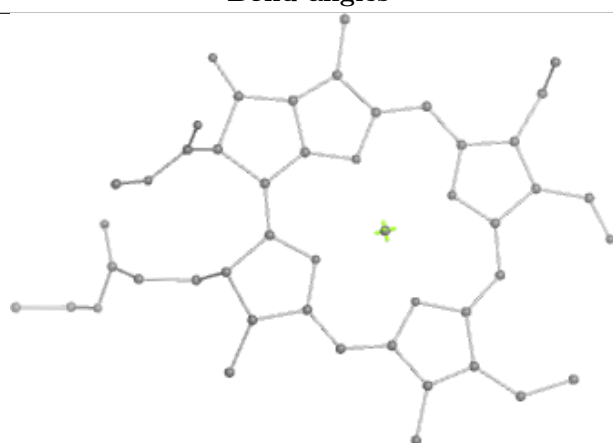
Bond lengths



Bond angles

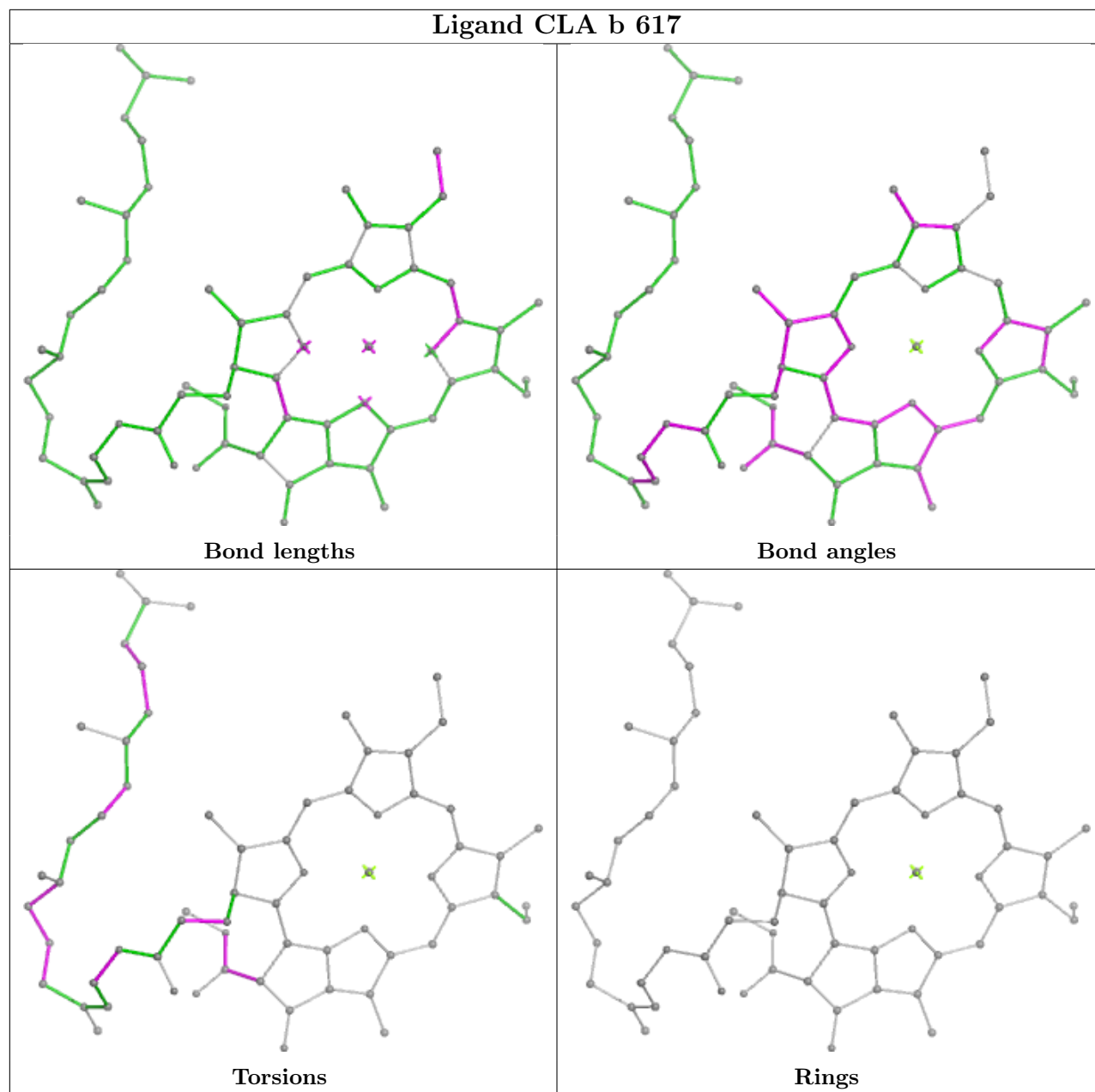


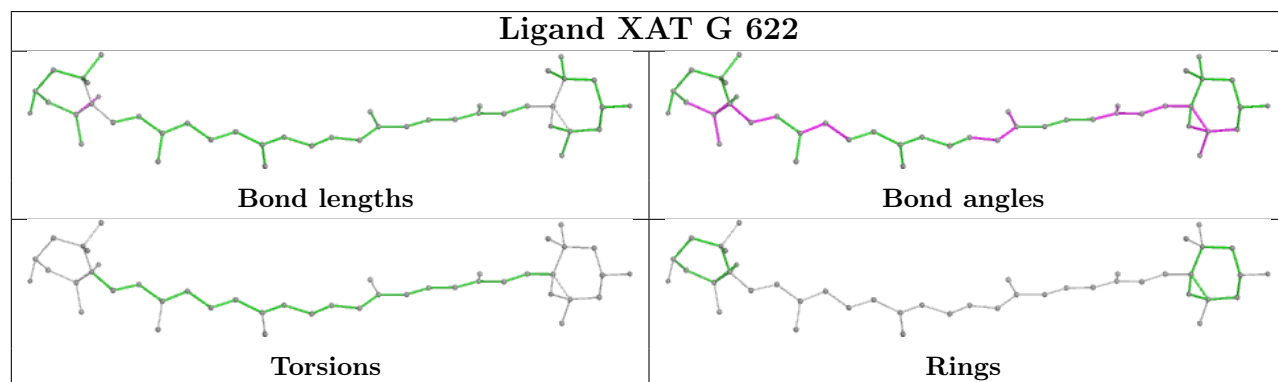
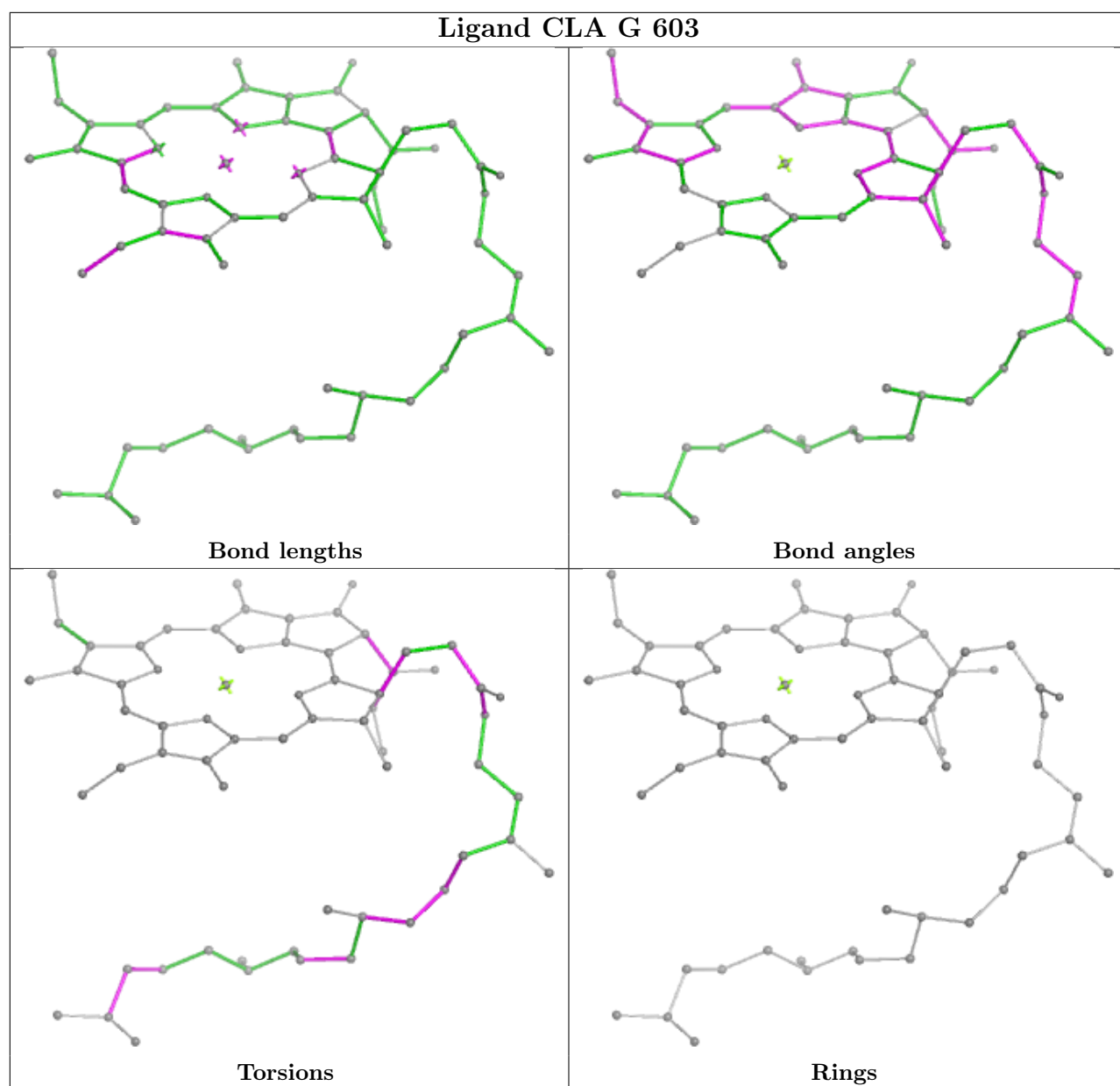
Torsions

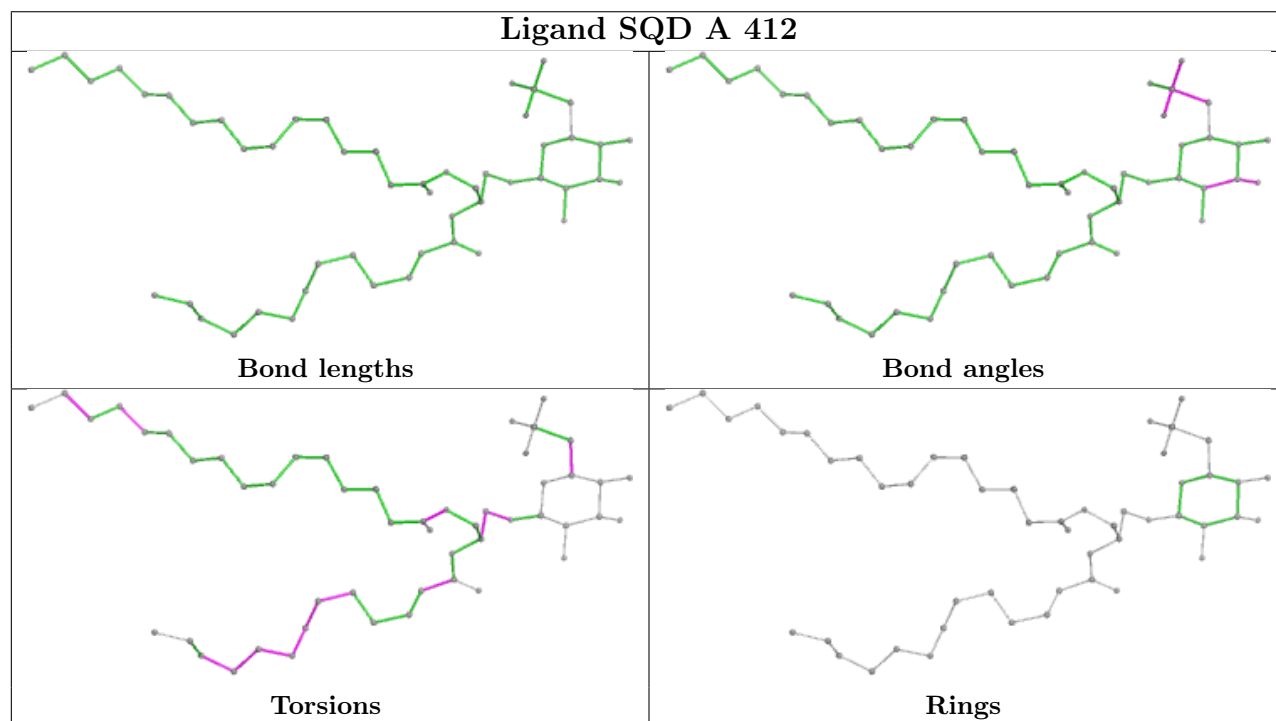
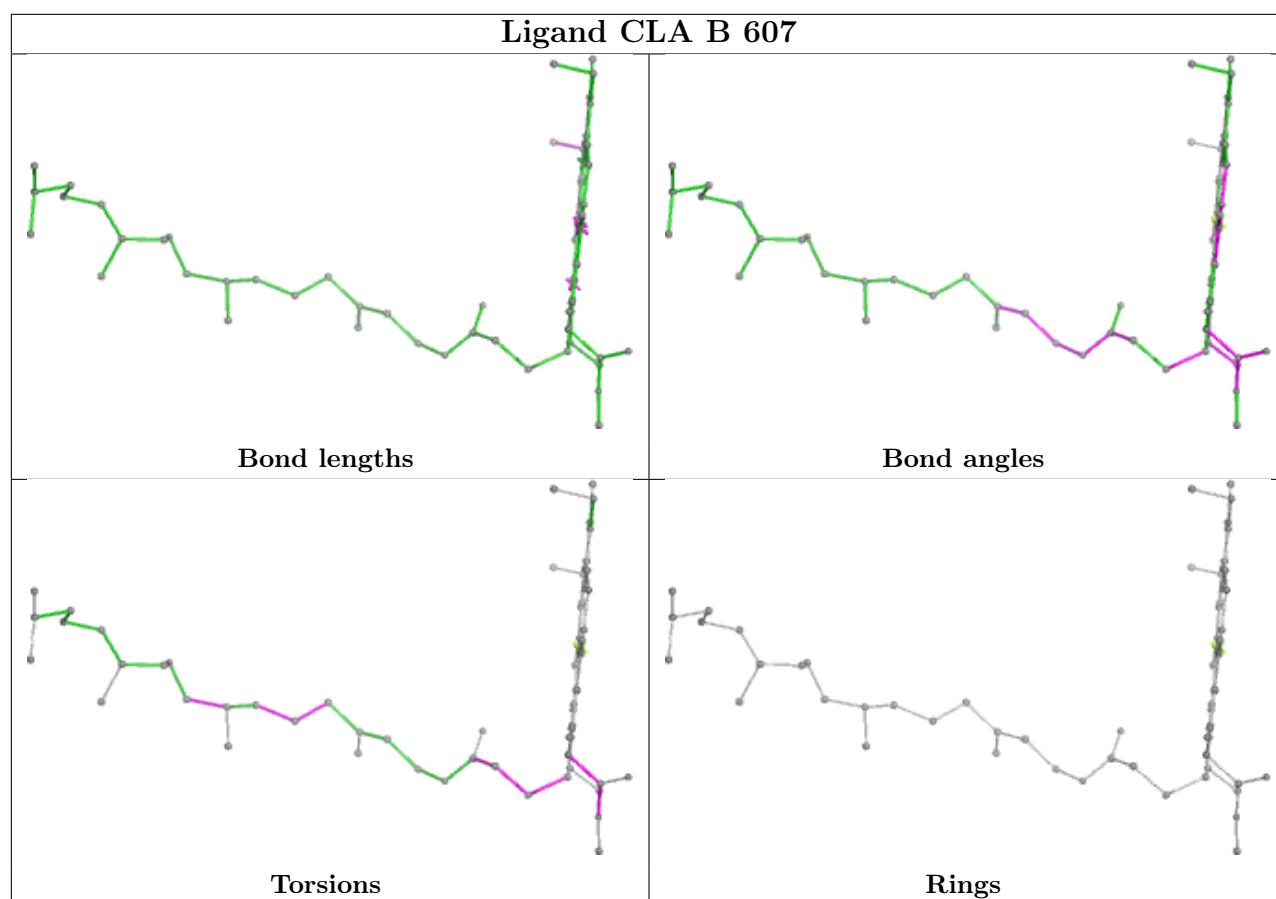


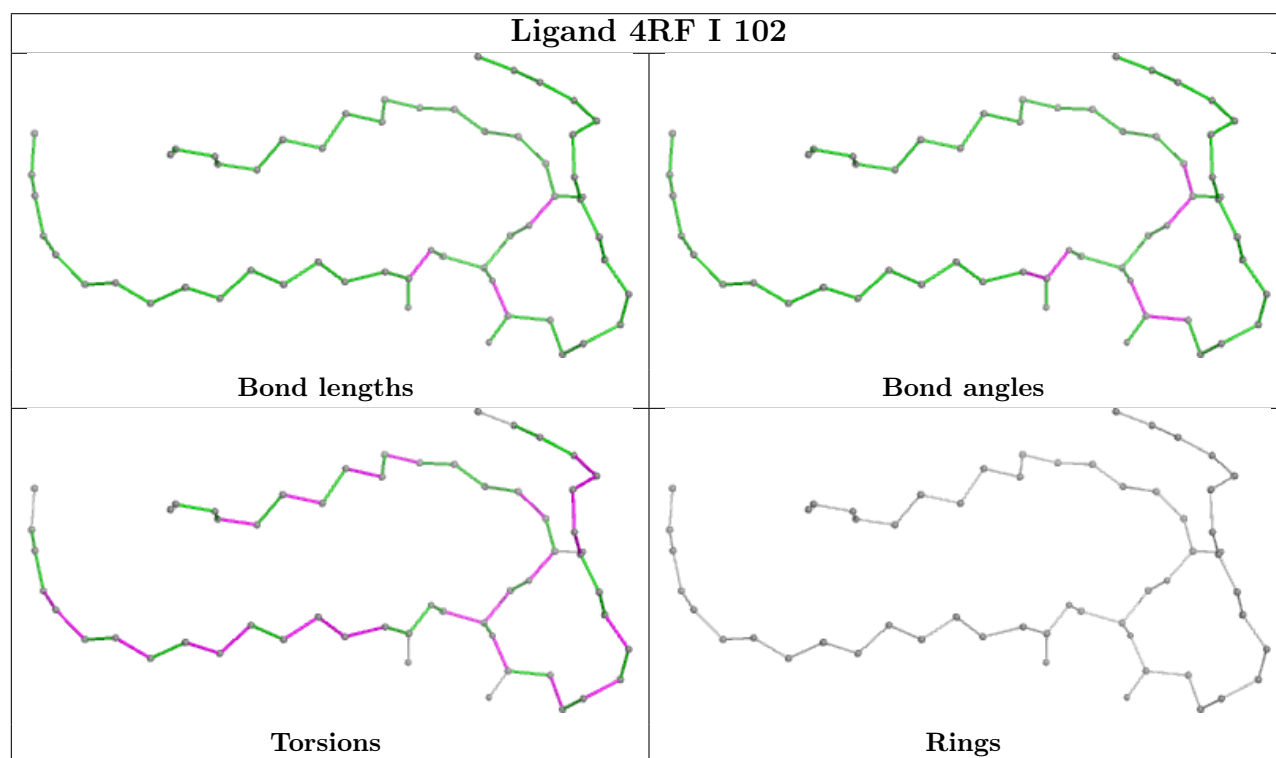
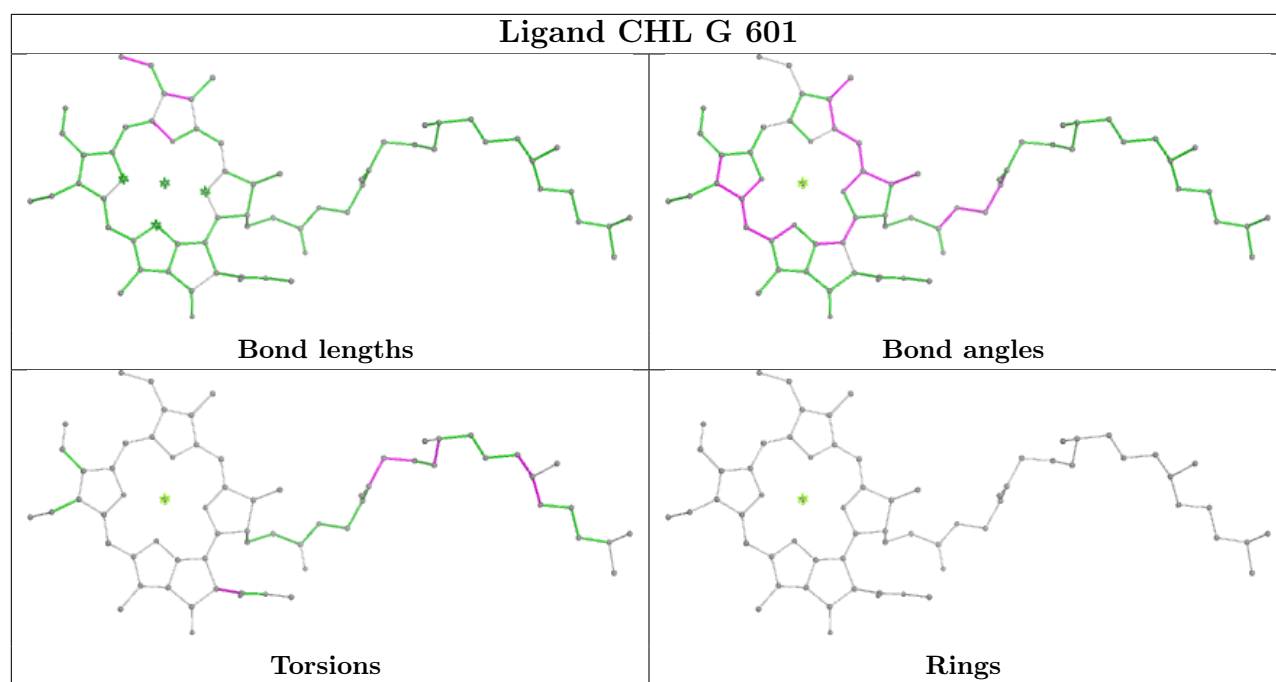
Rings

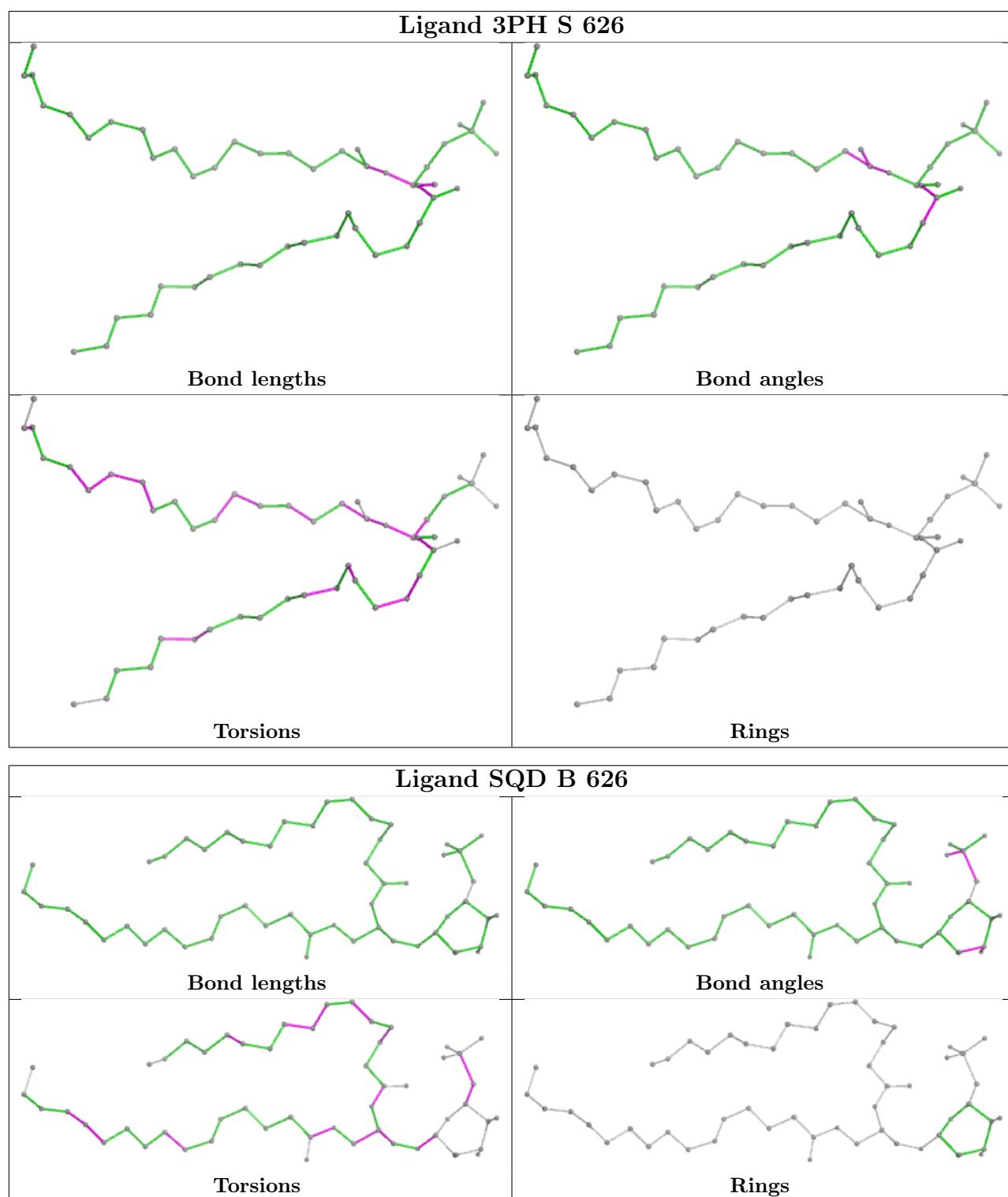
Ligand CLA b 617

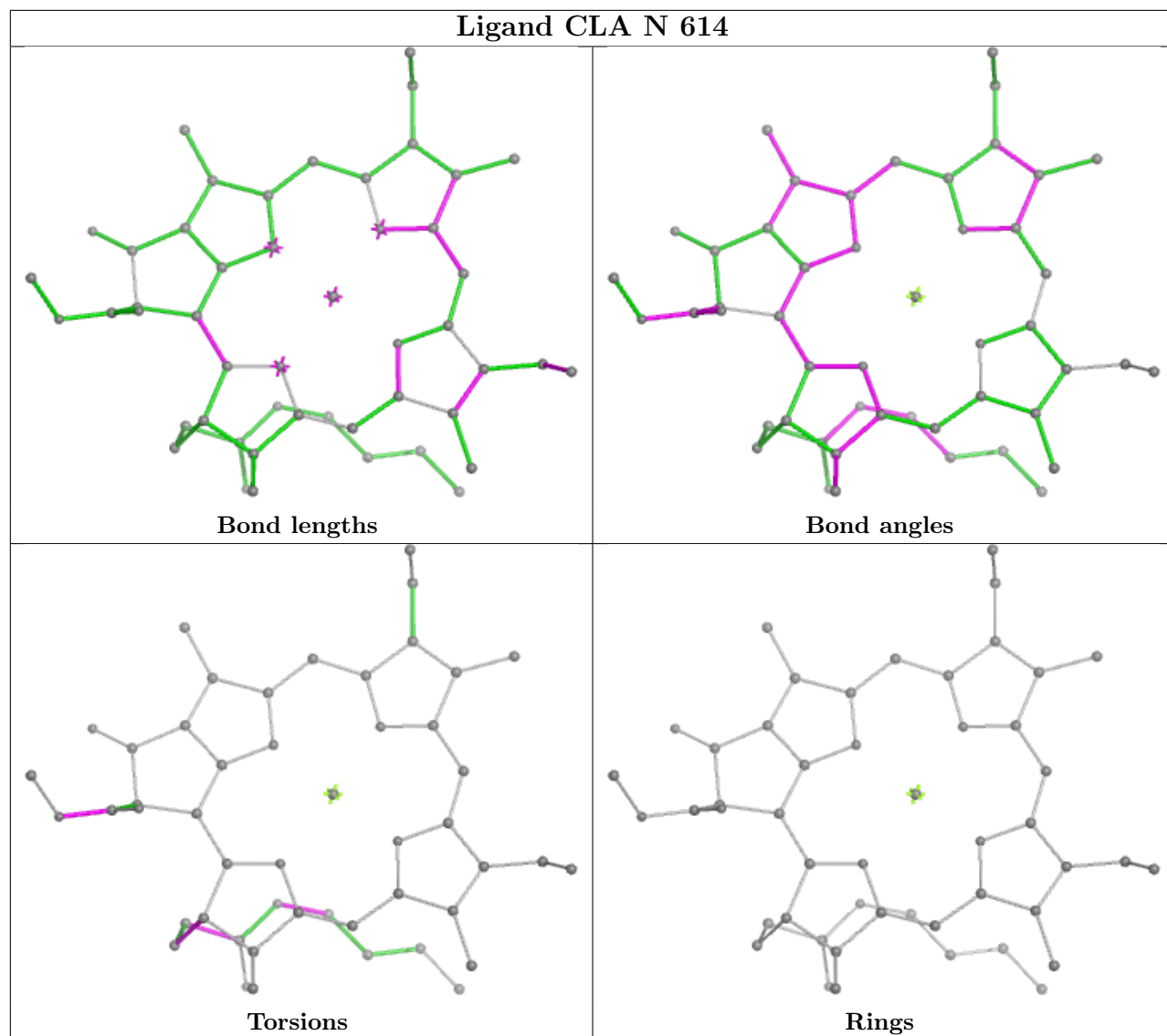


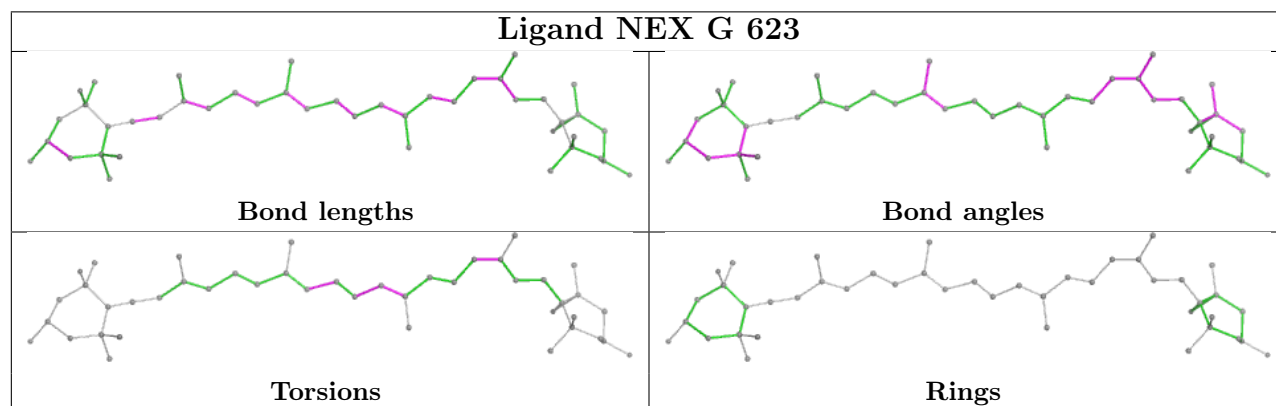
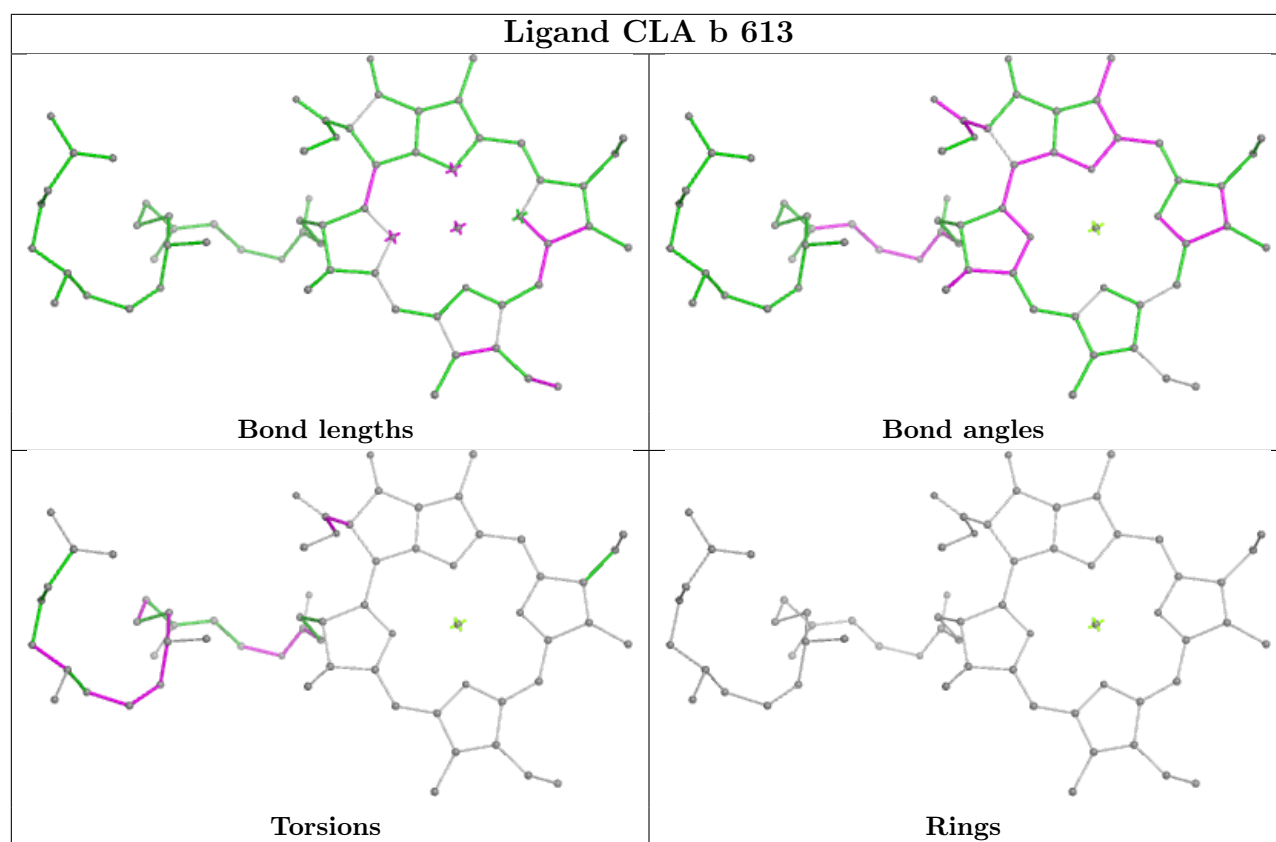


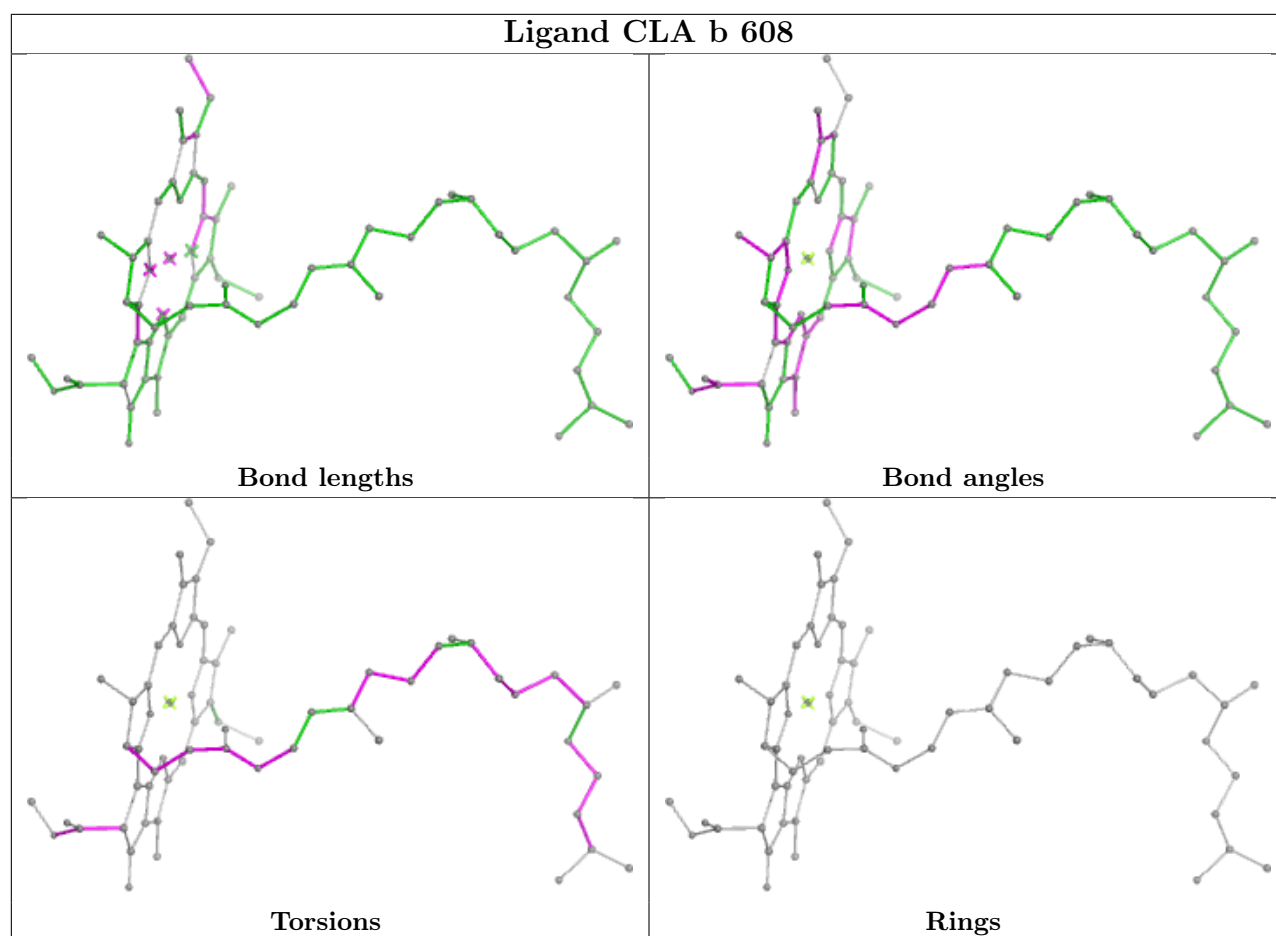




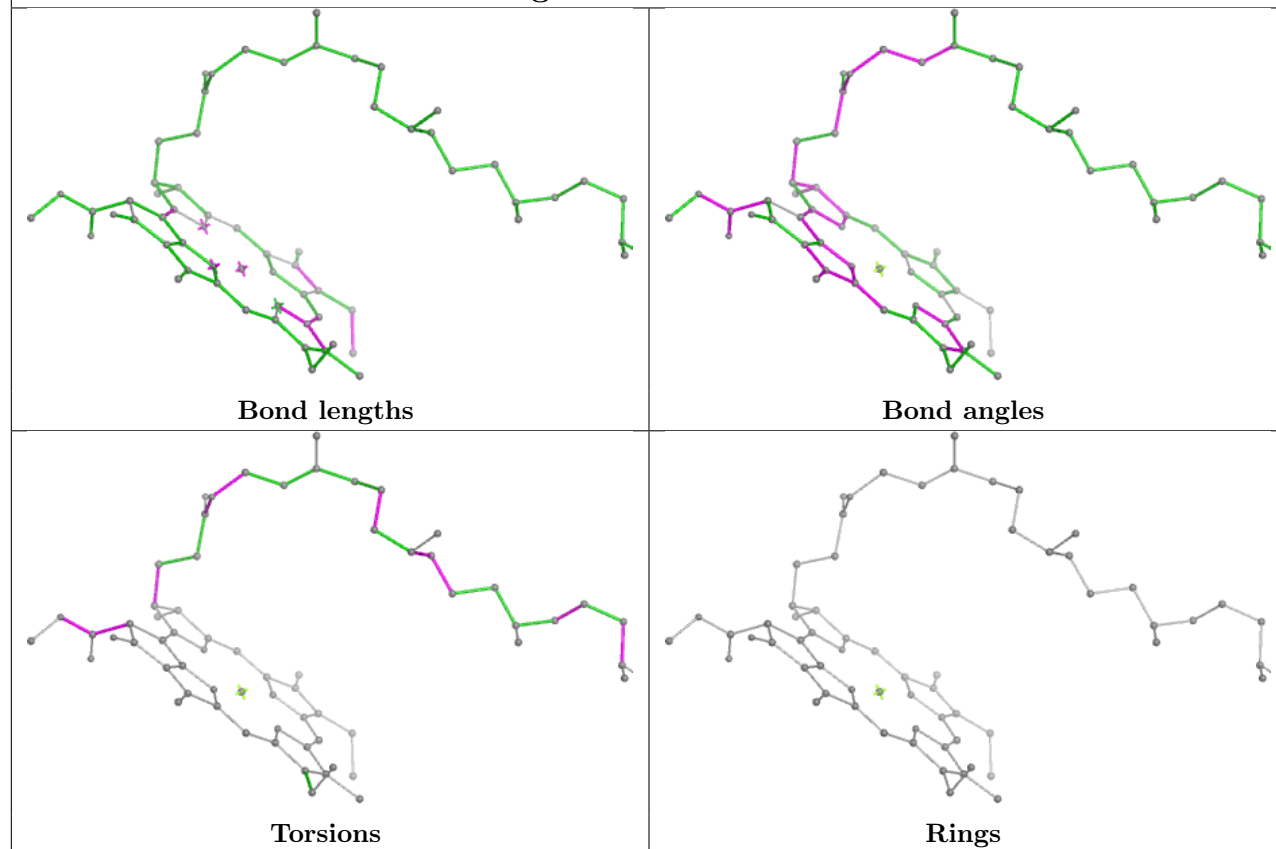




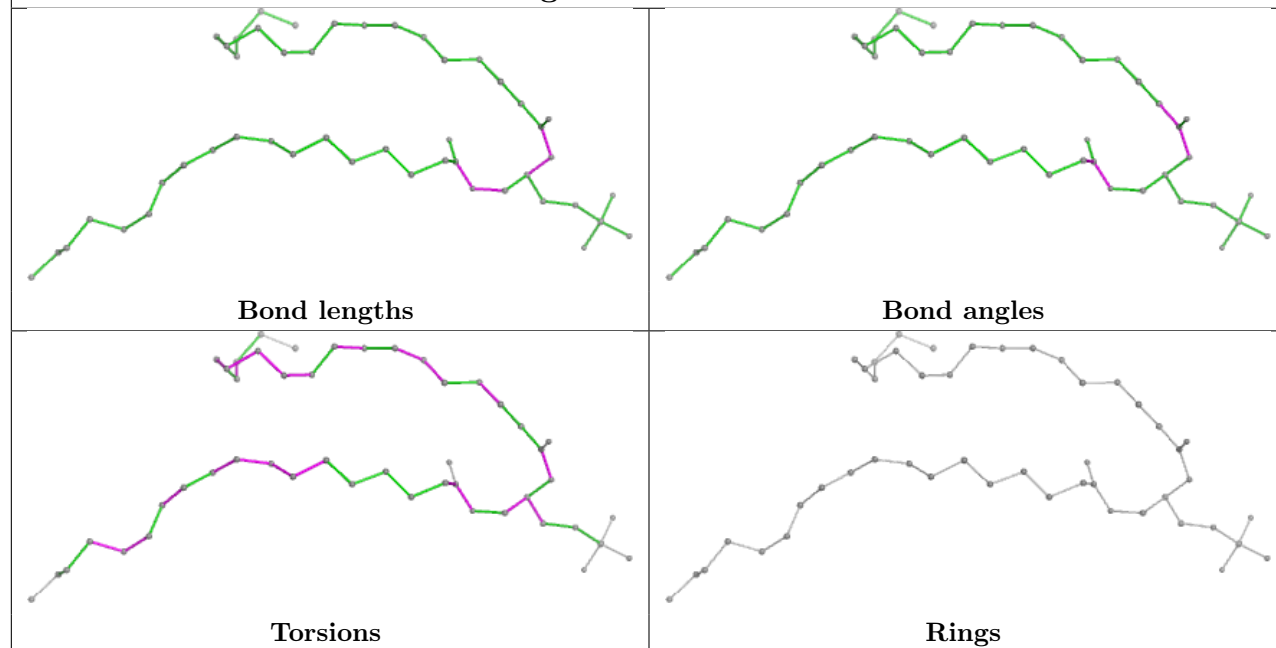


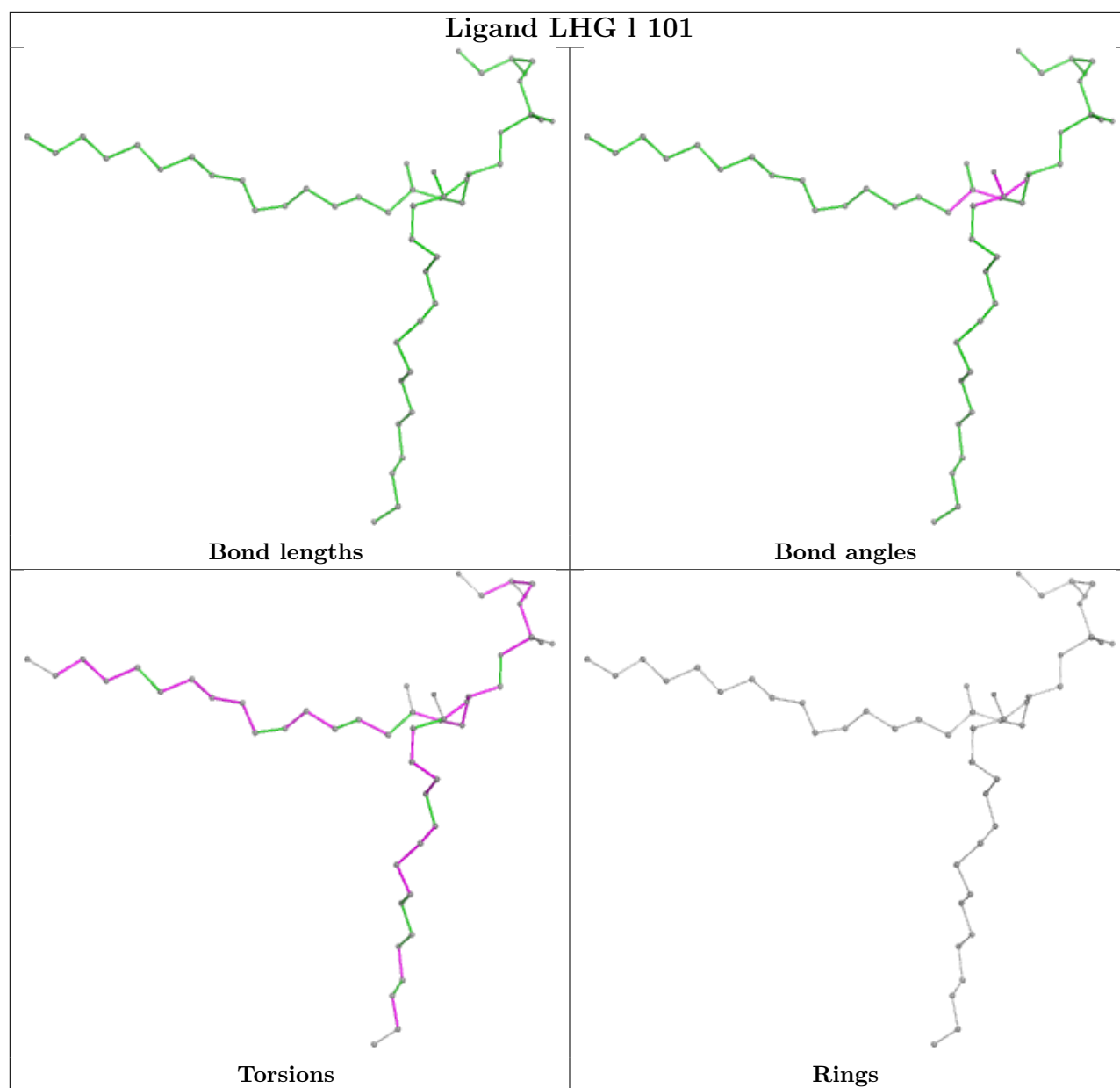


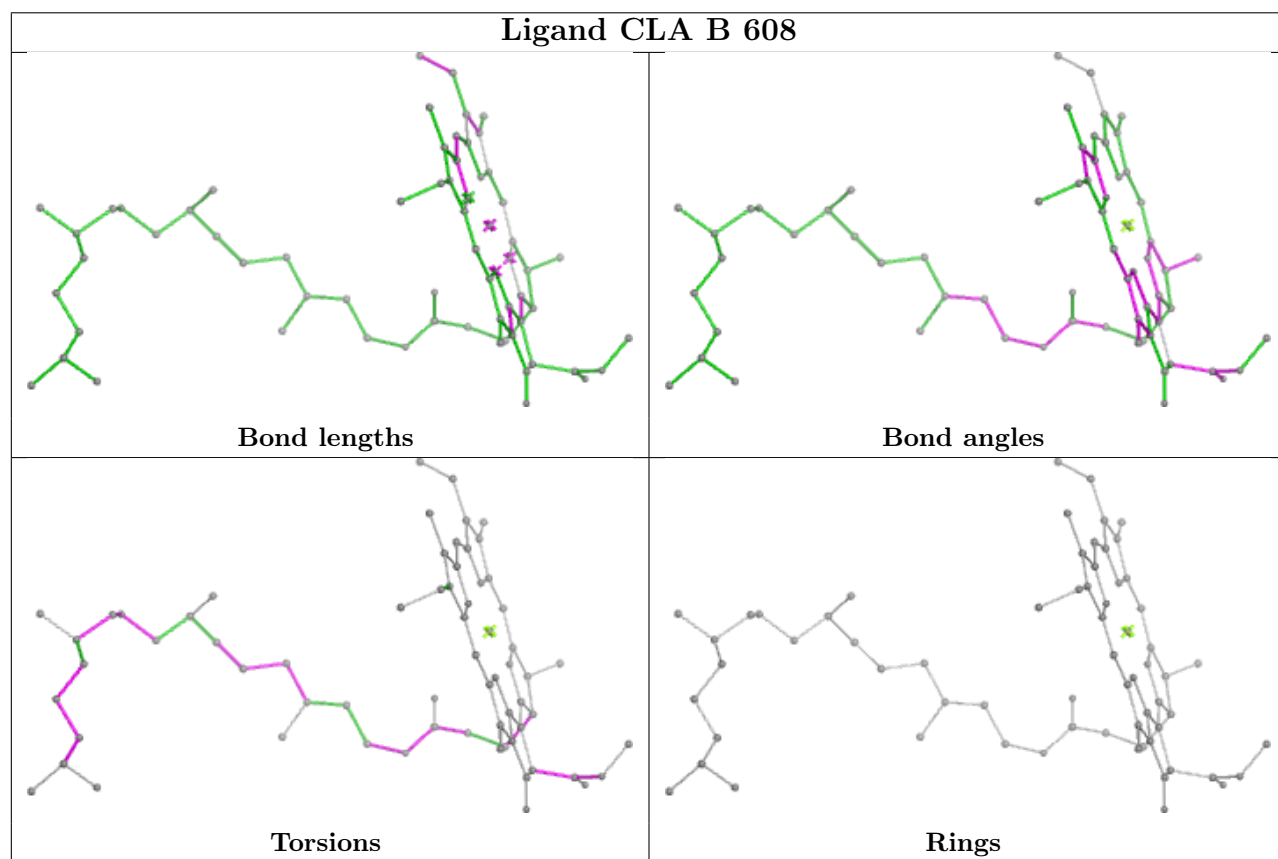
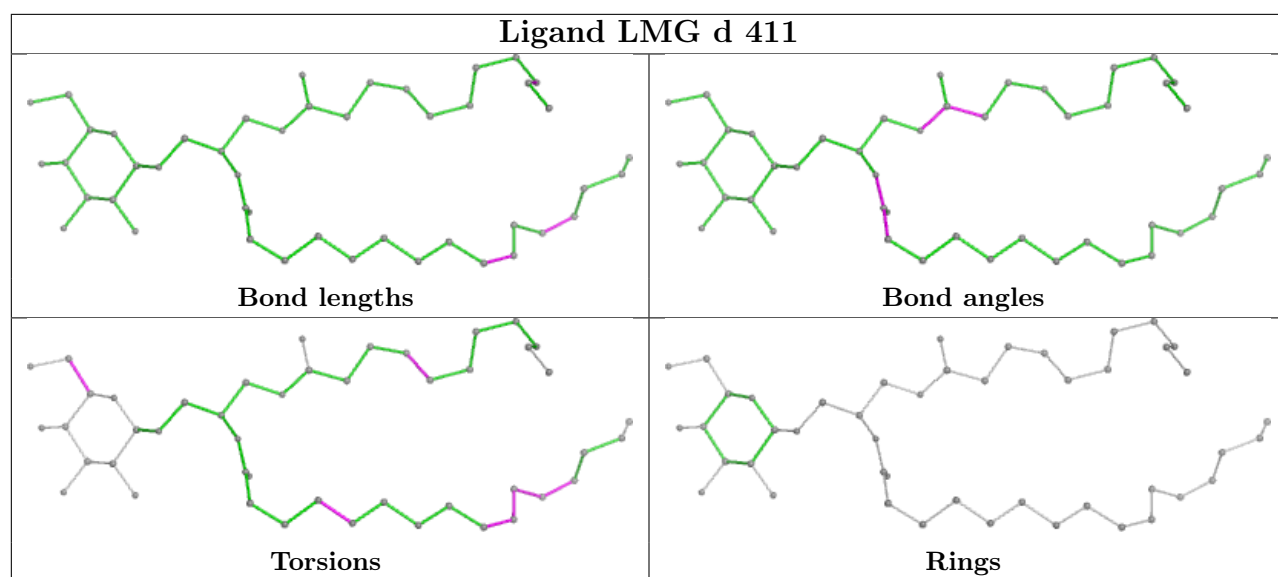
Ligand CLA Y 614



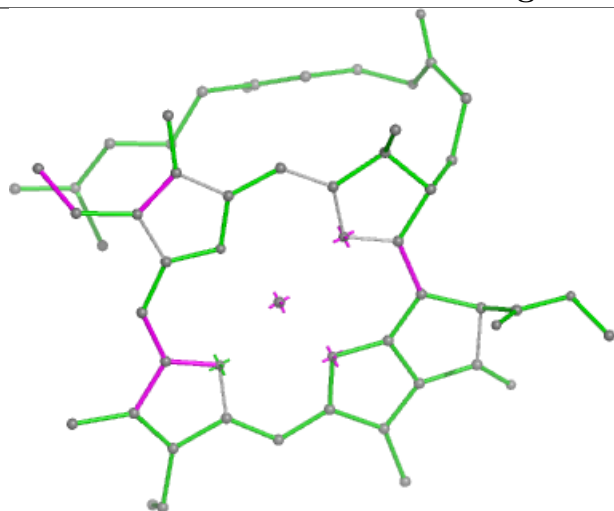
Ligand 3PH t 101



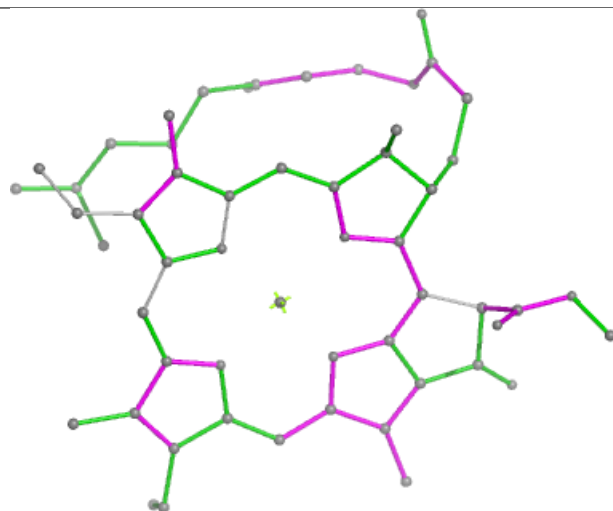




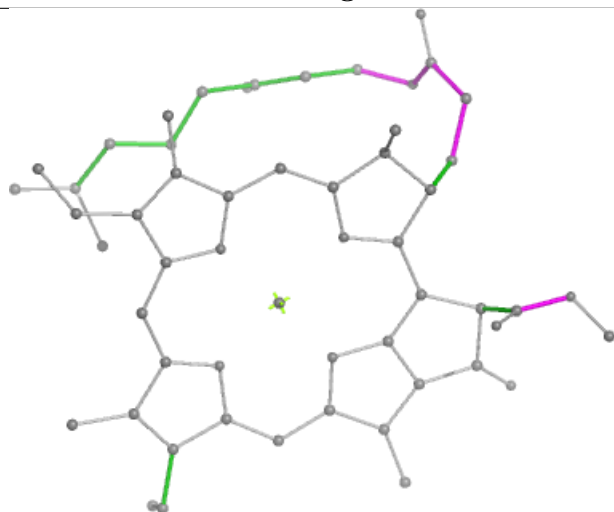
Ligand CLA S 614



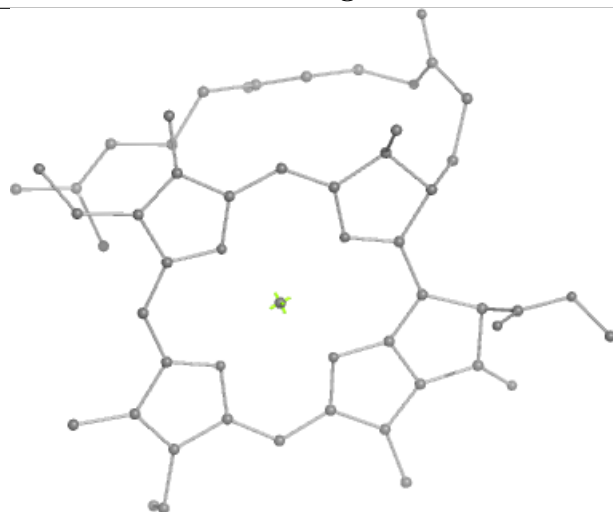
Bond lengths



Bond angles

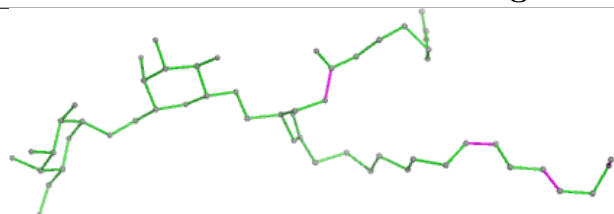


Torsions

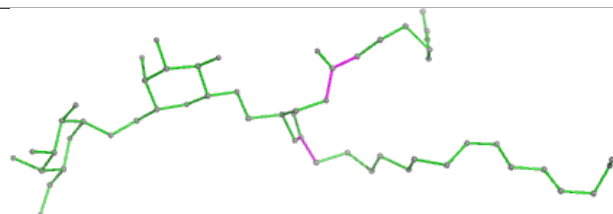


Rings

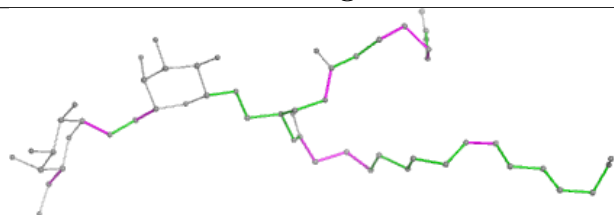
Ligand DGD C 518



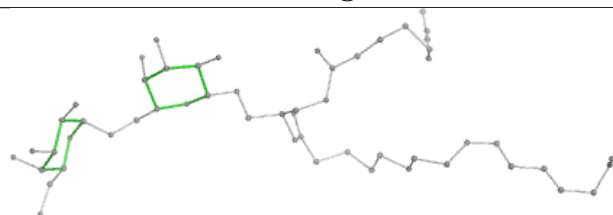
Bond lengths



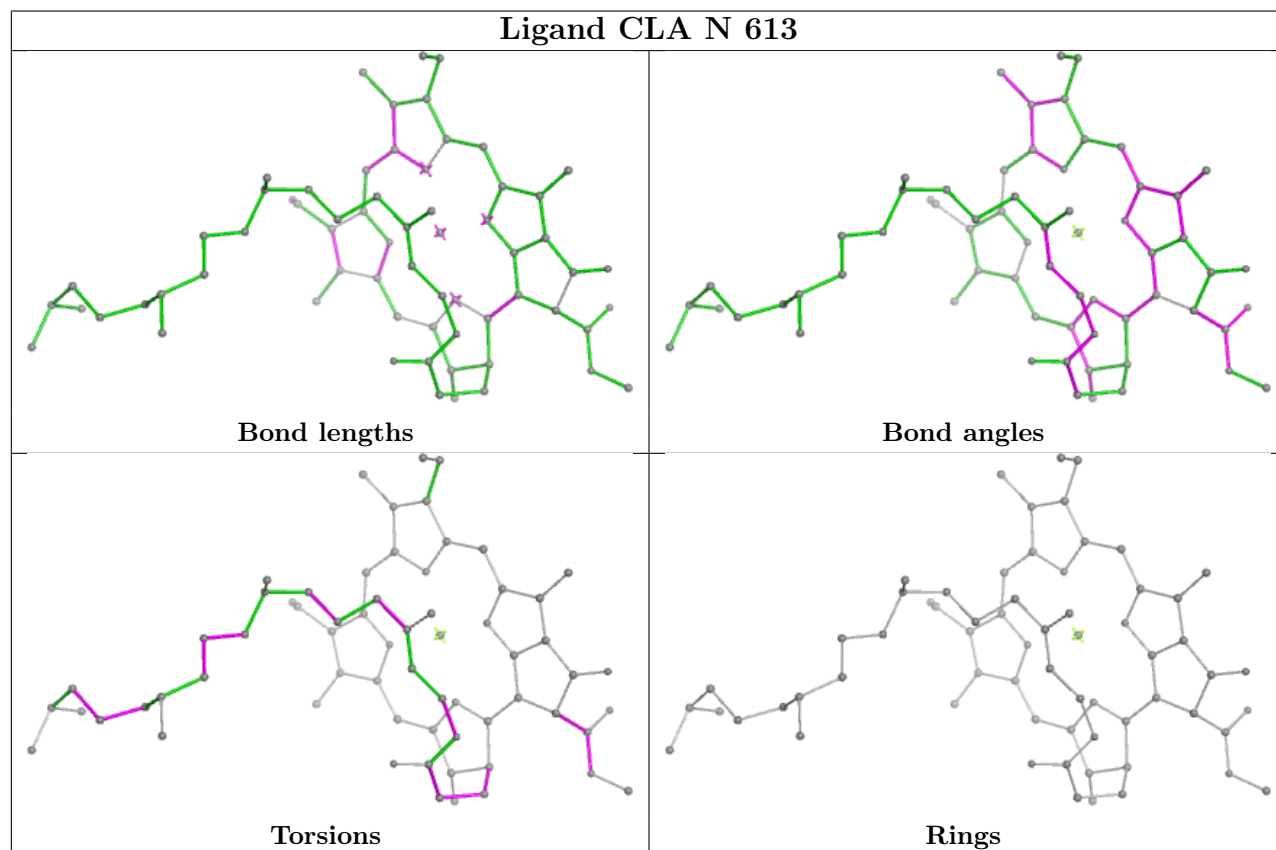
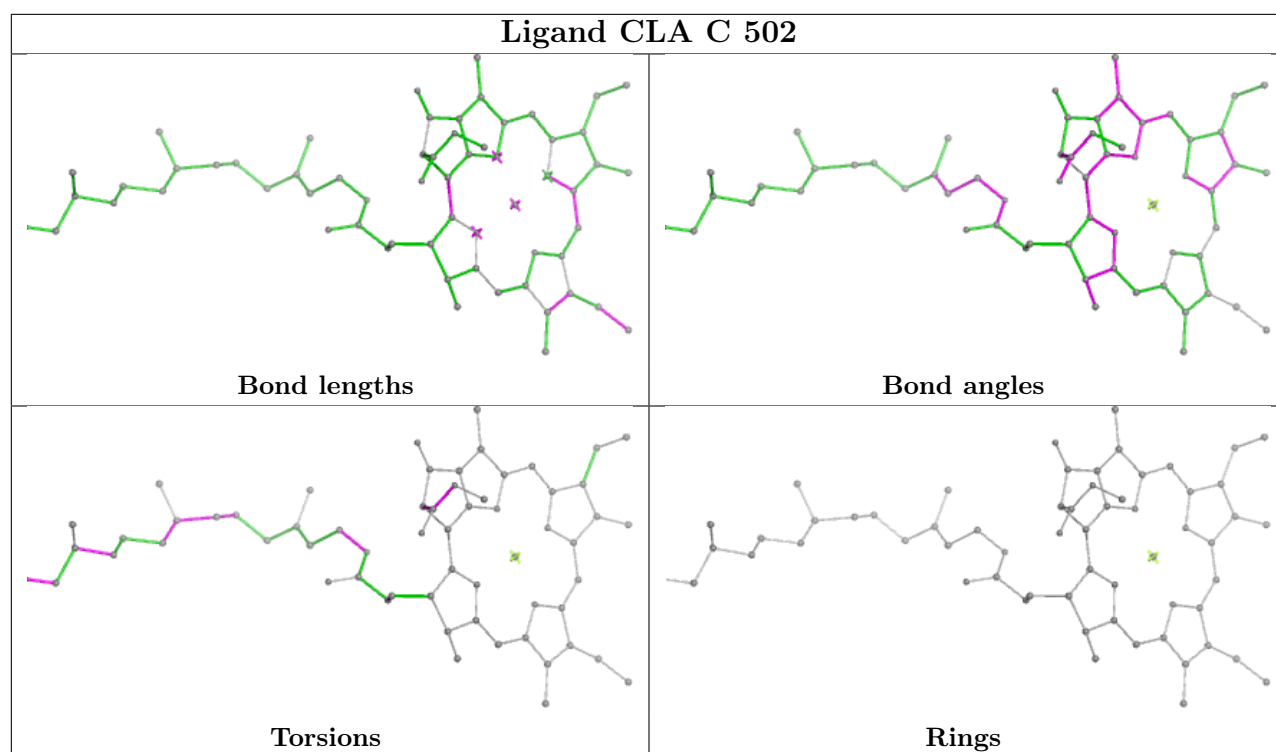
Bond angles

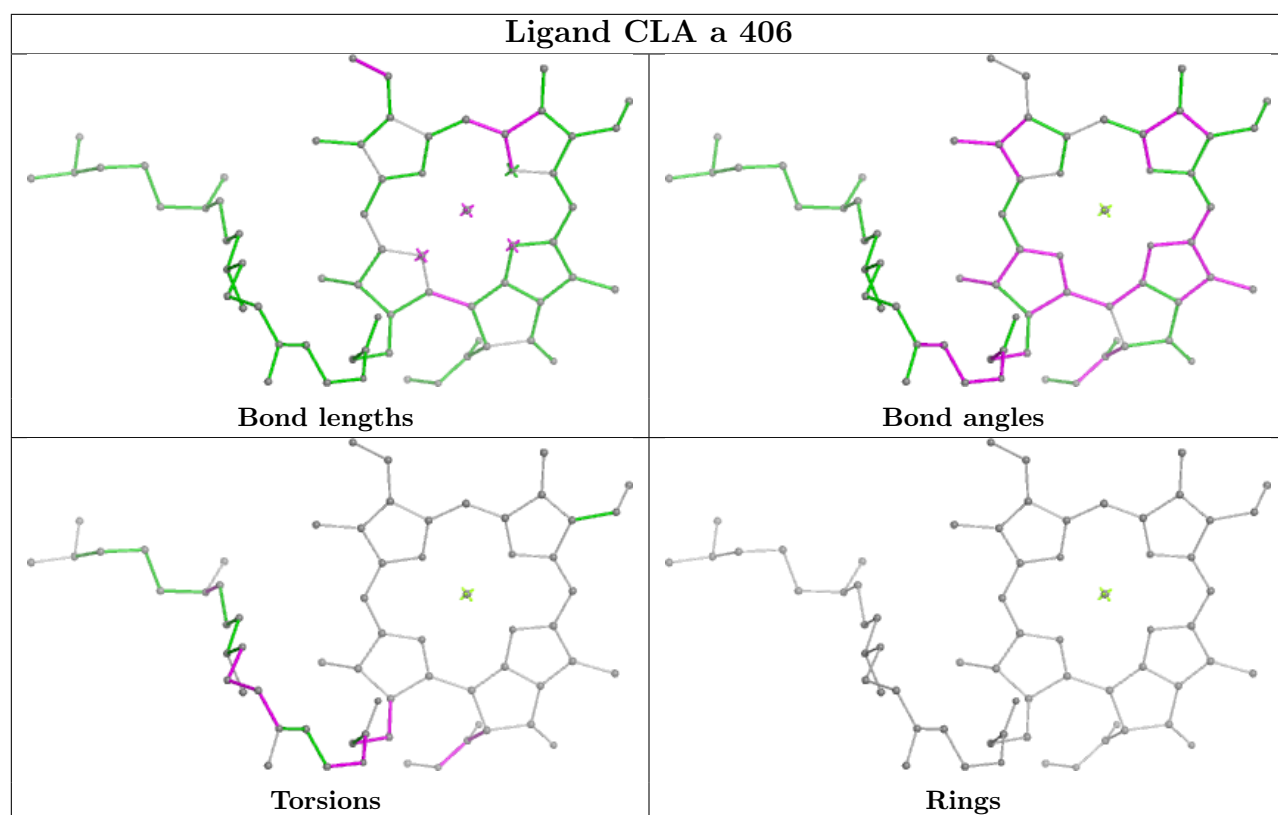


Torsions

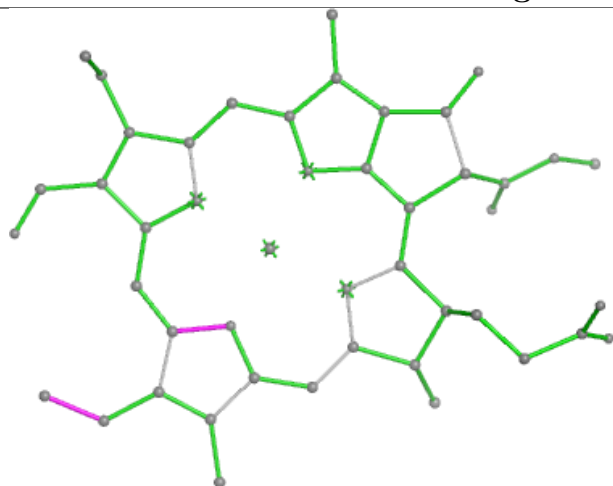


Rings

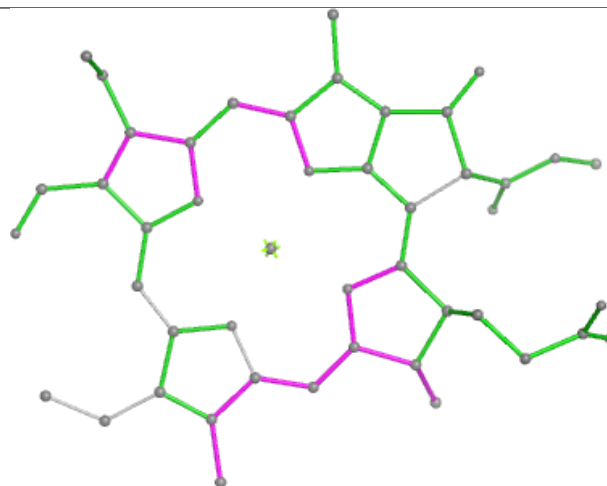




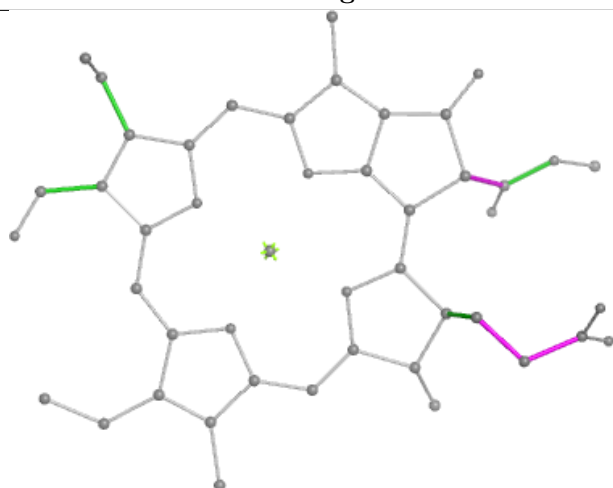
Ligand CHL Y 605



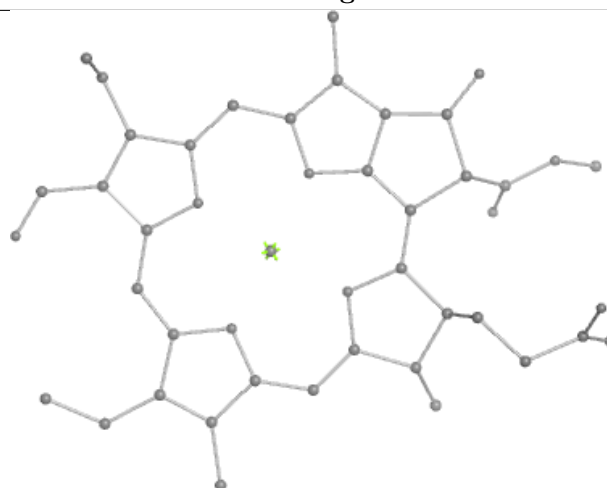
Bond lengths



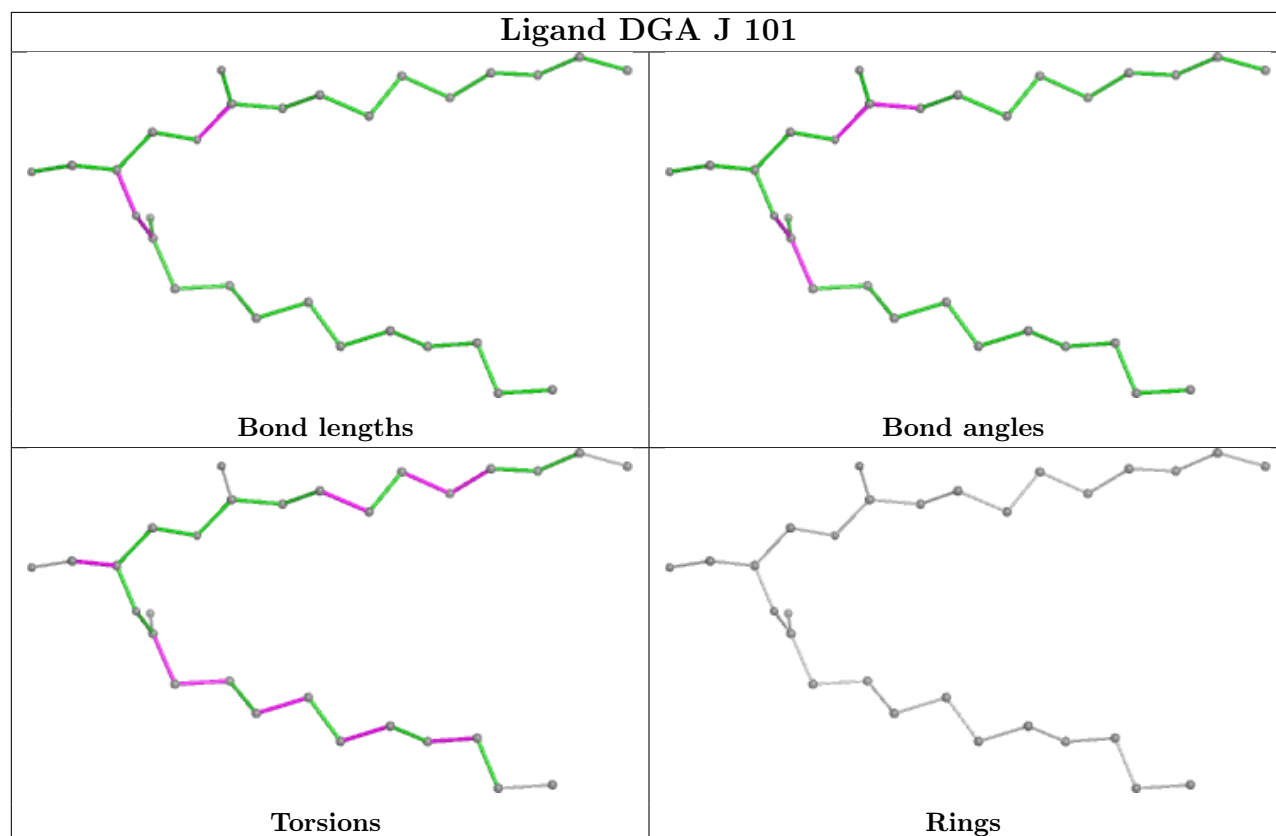
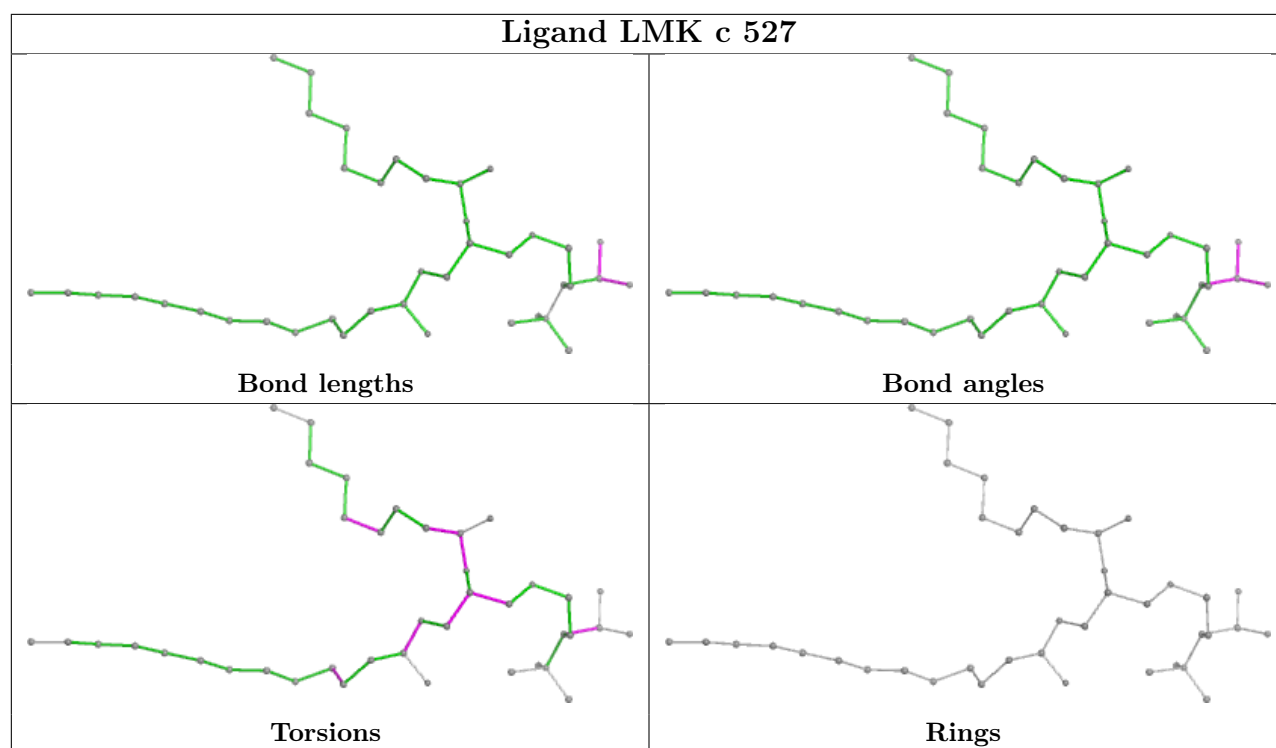
Bond angles

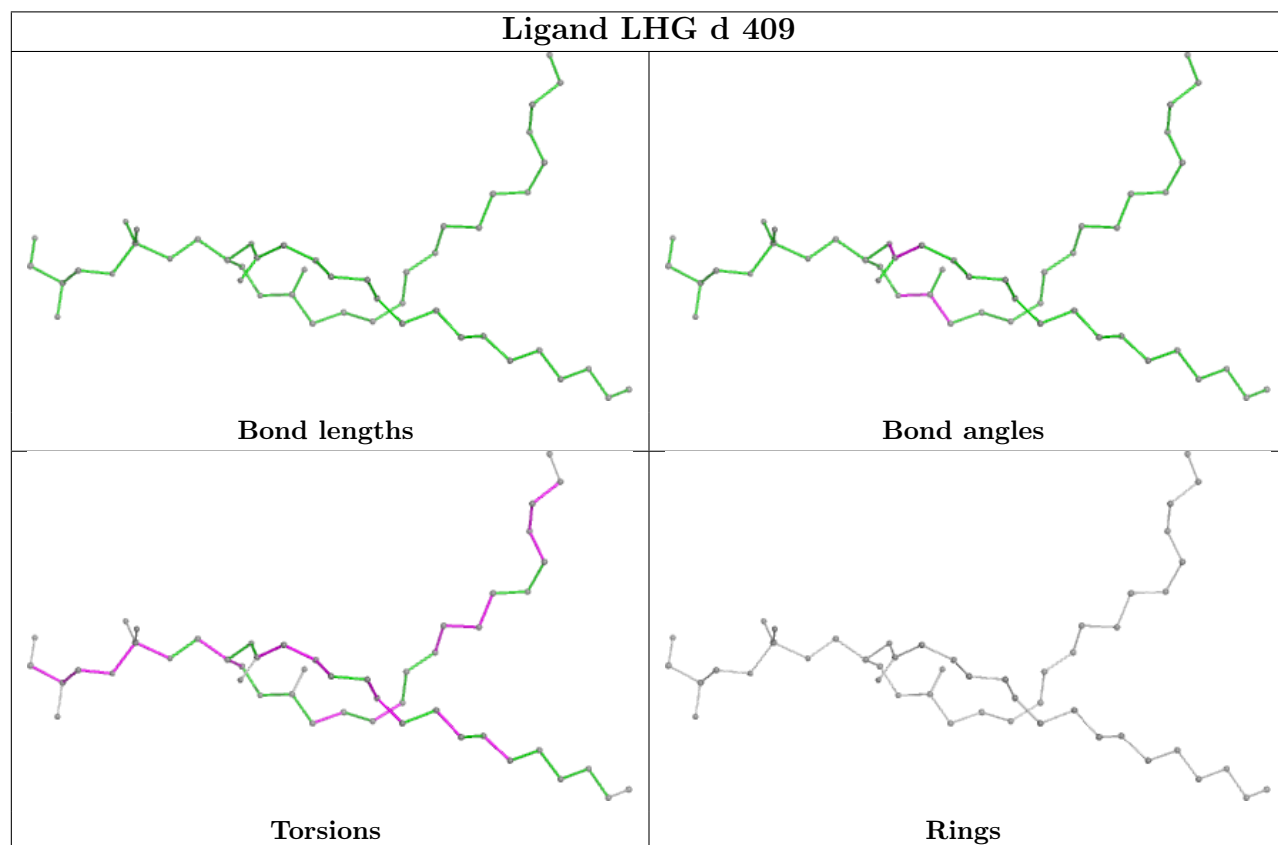
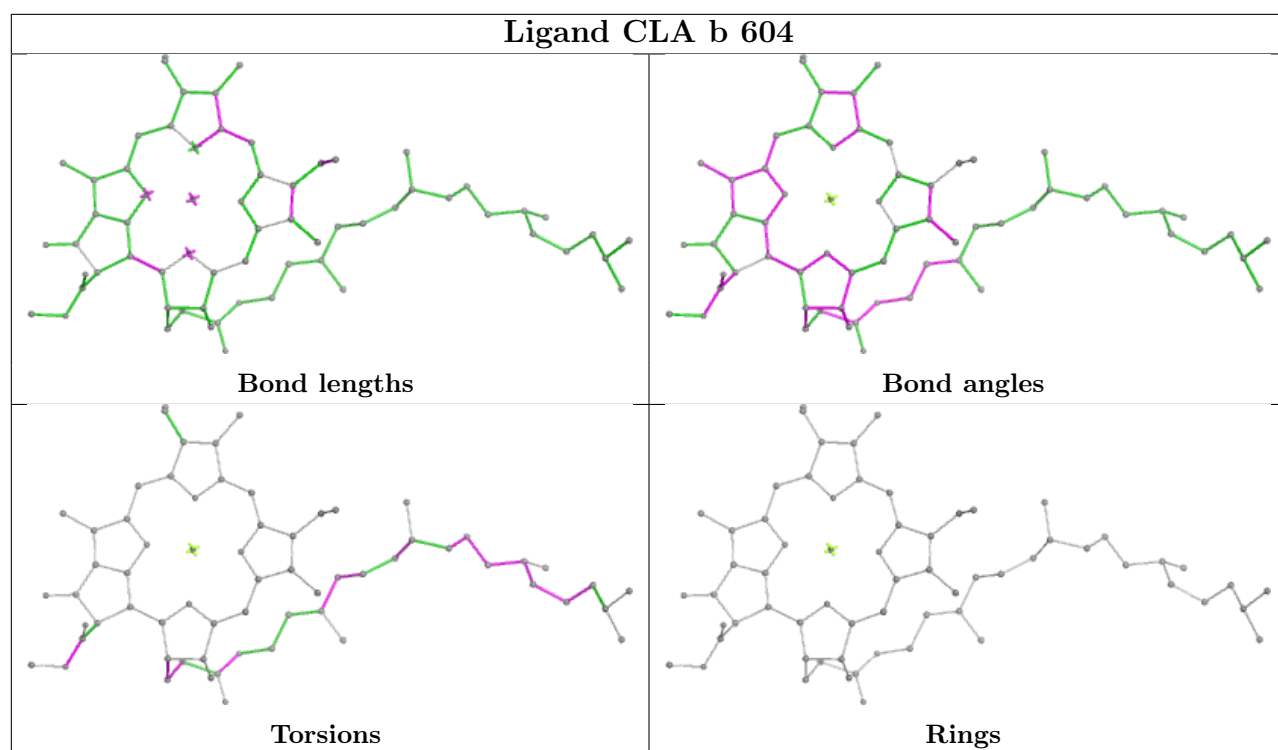


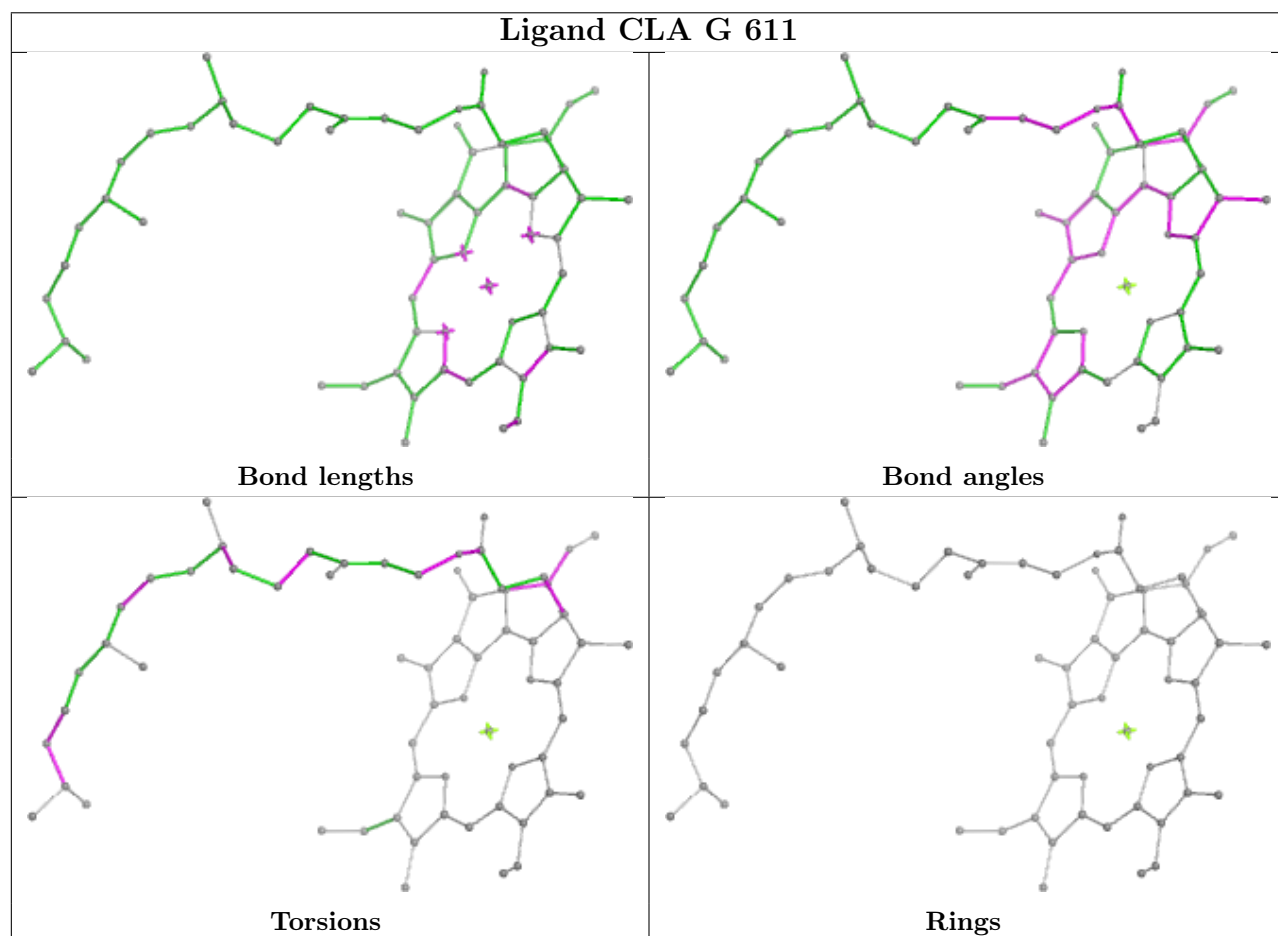
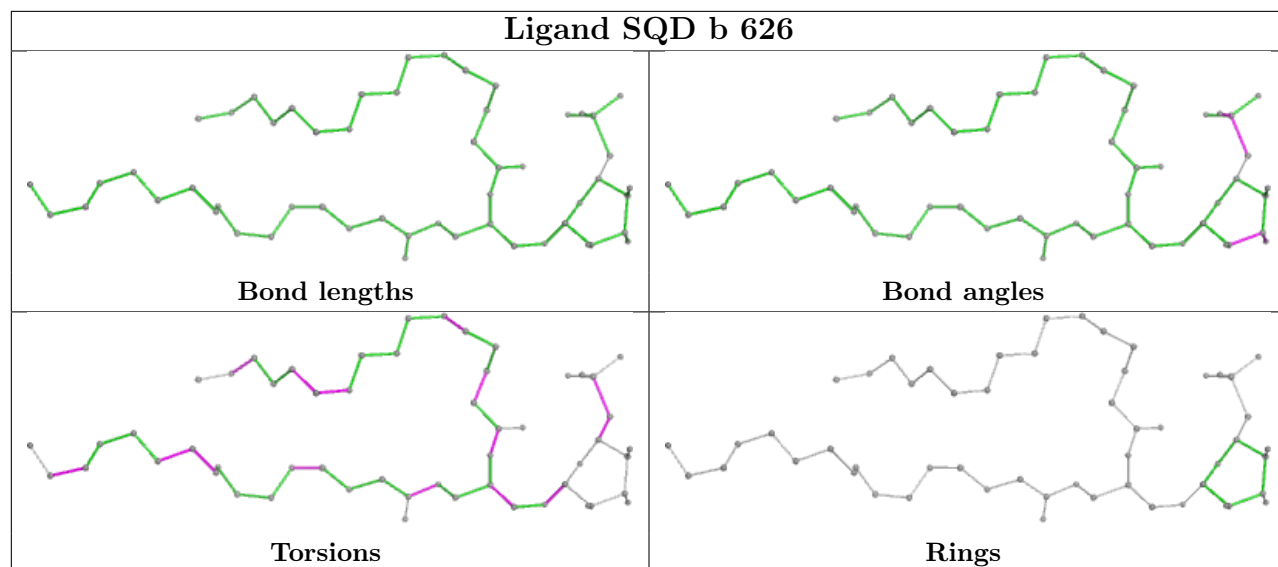
Torsions

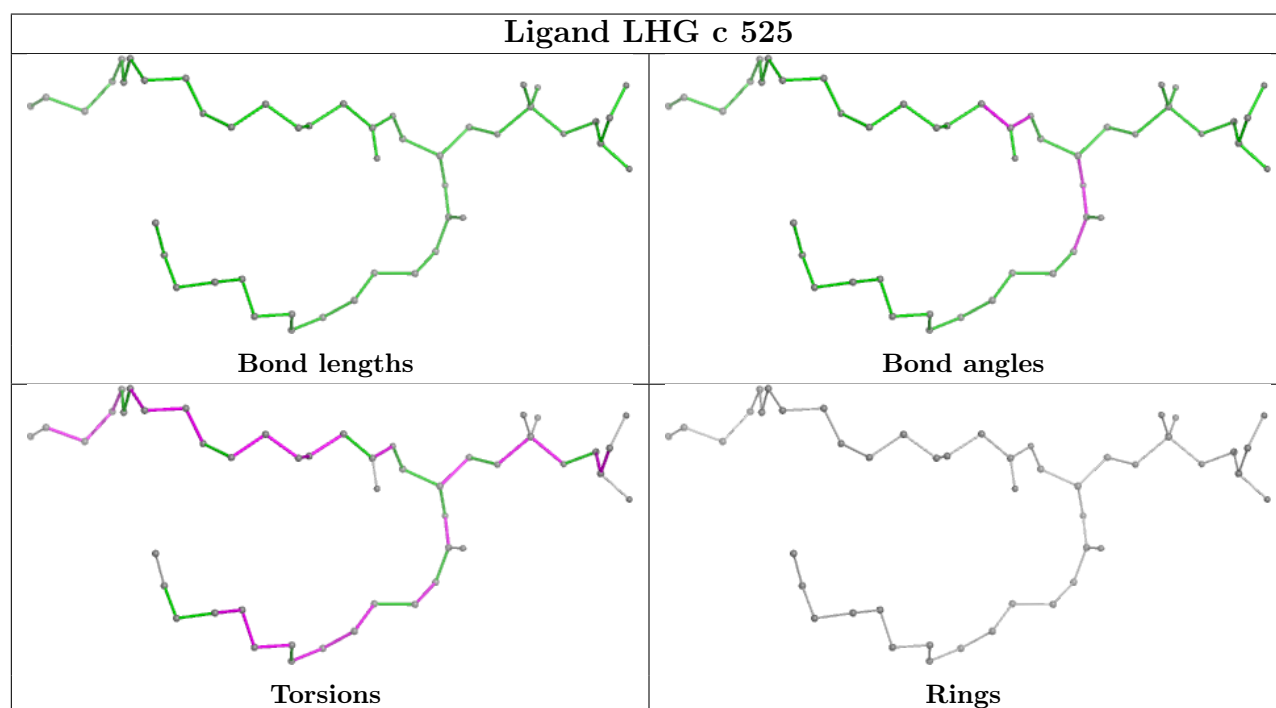
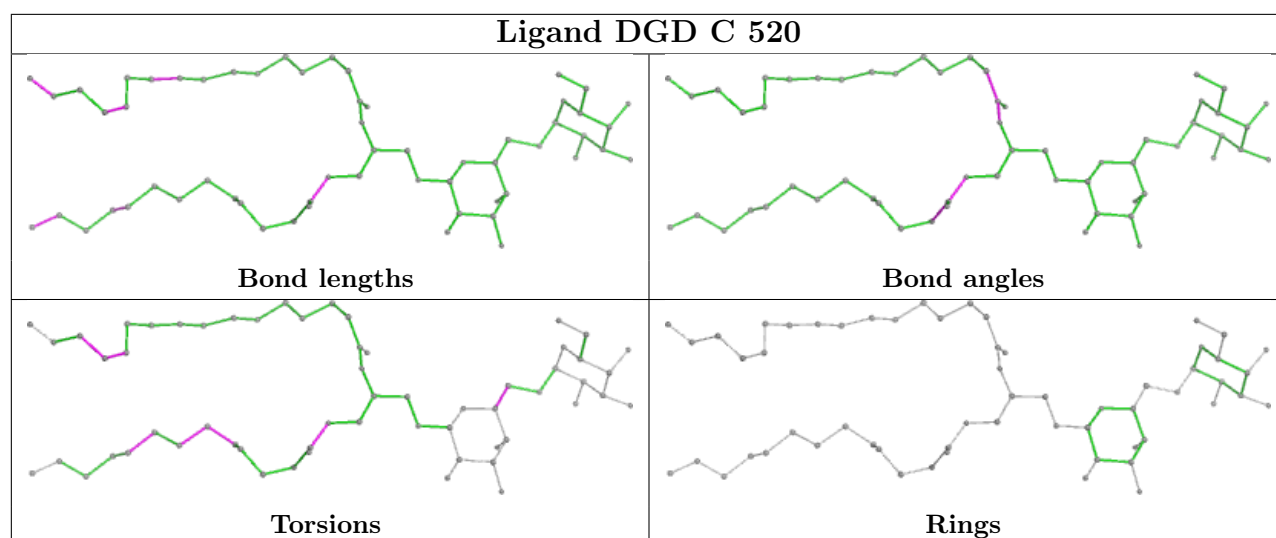


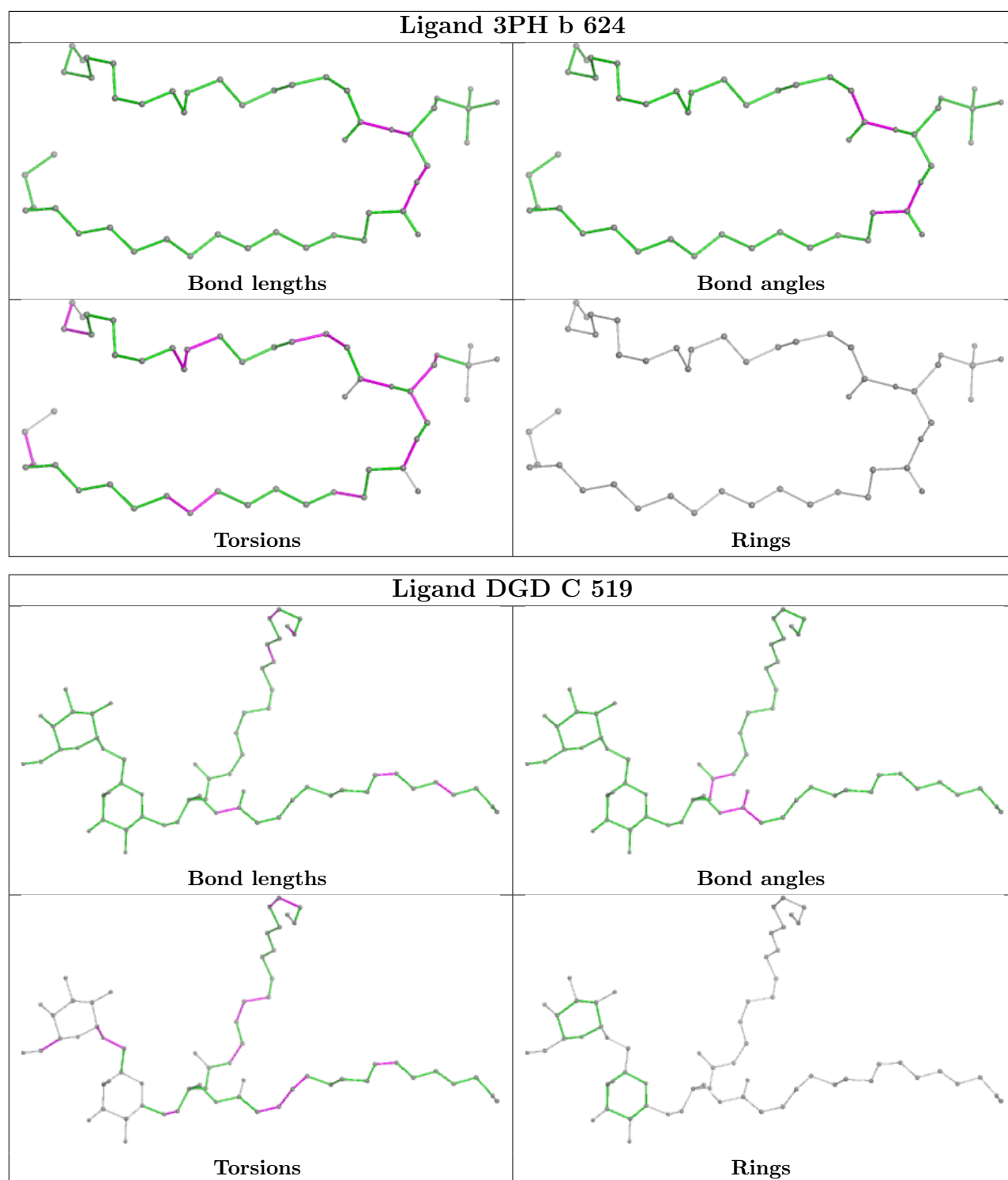
Rings



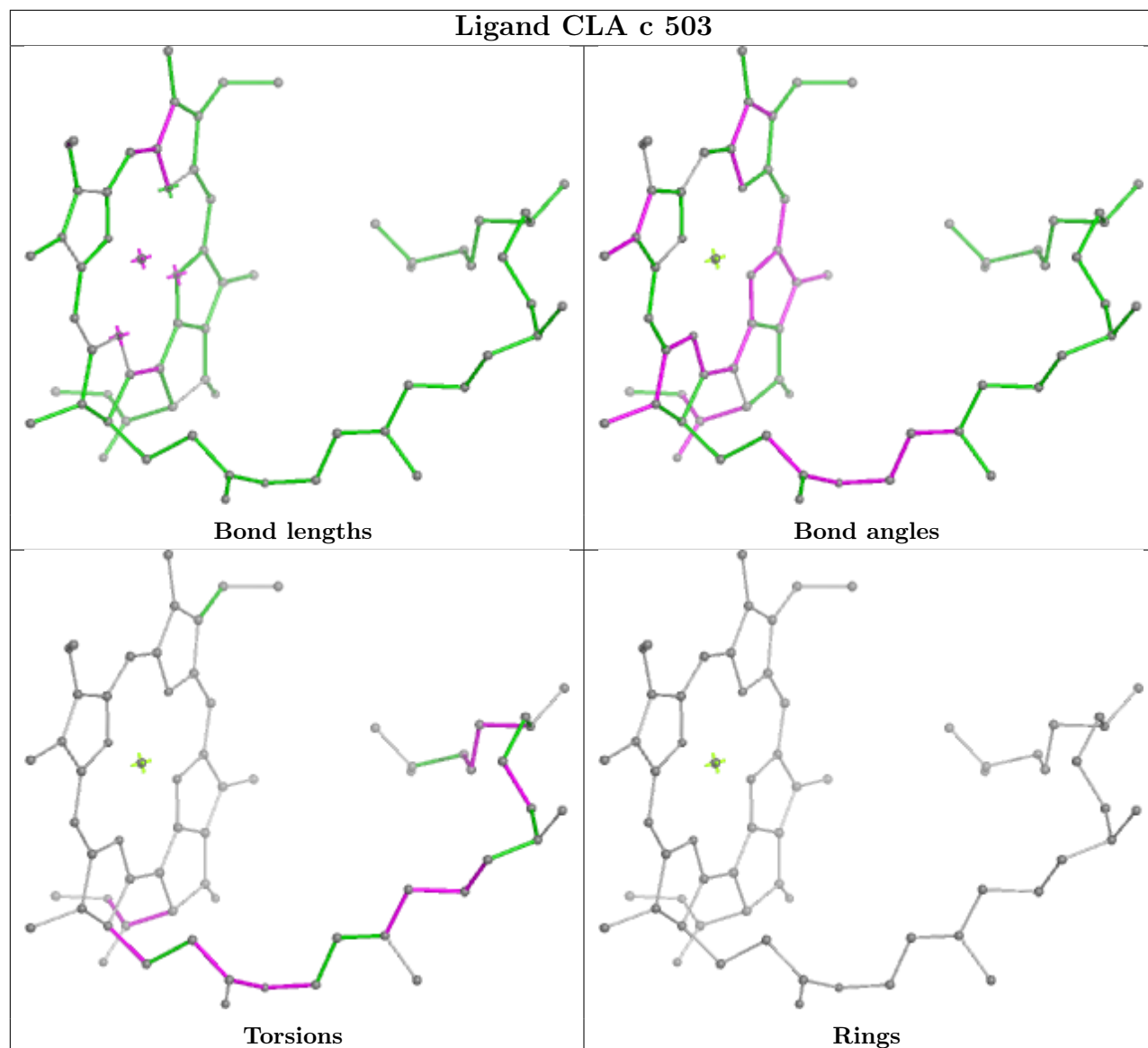




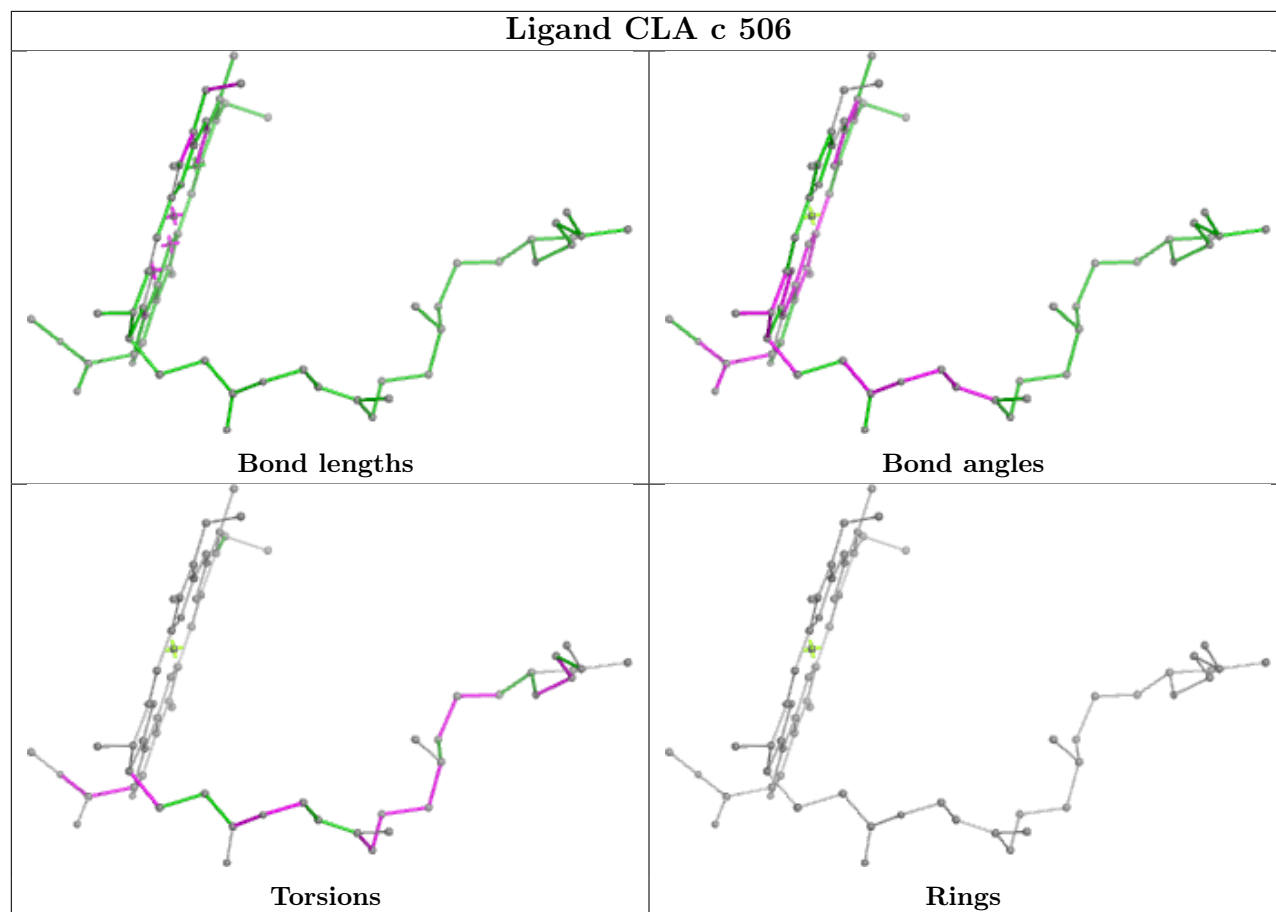




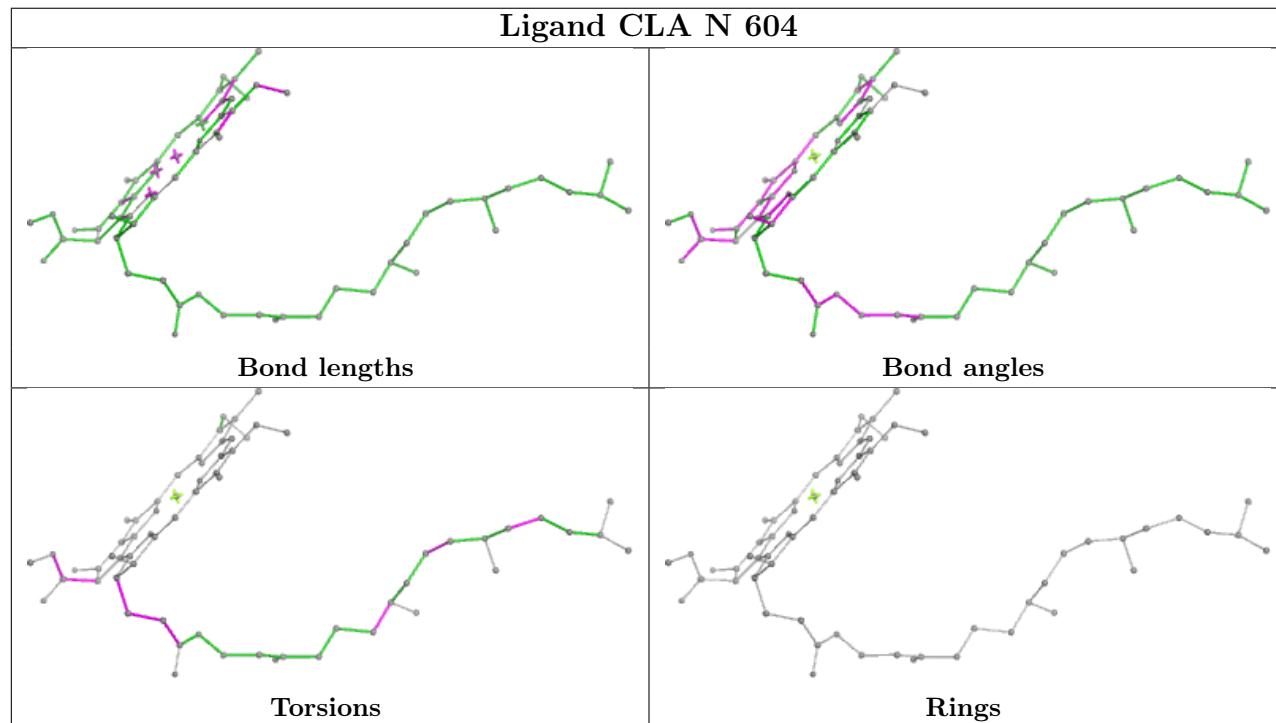
Ligand CLA c 503

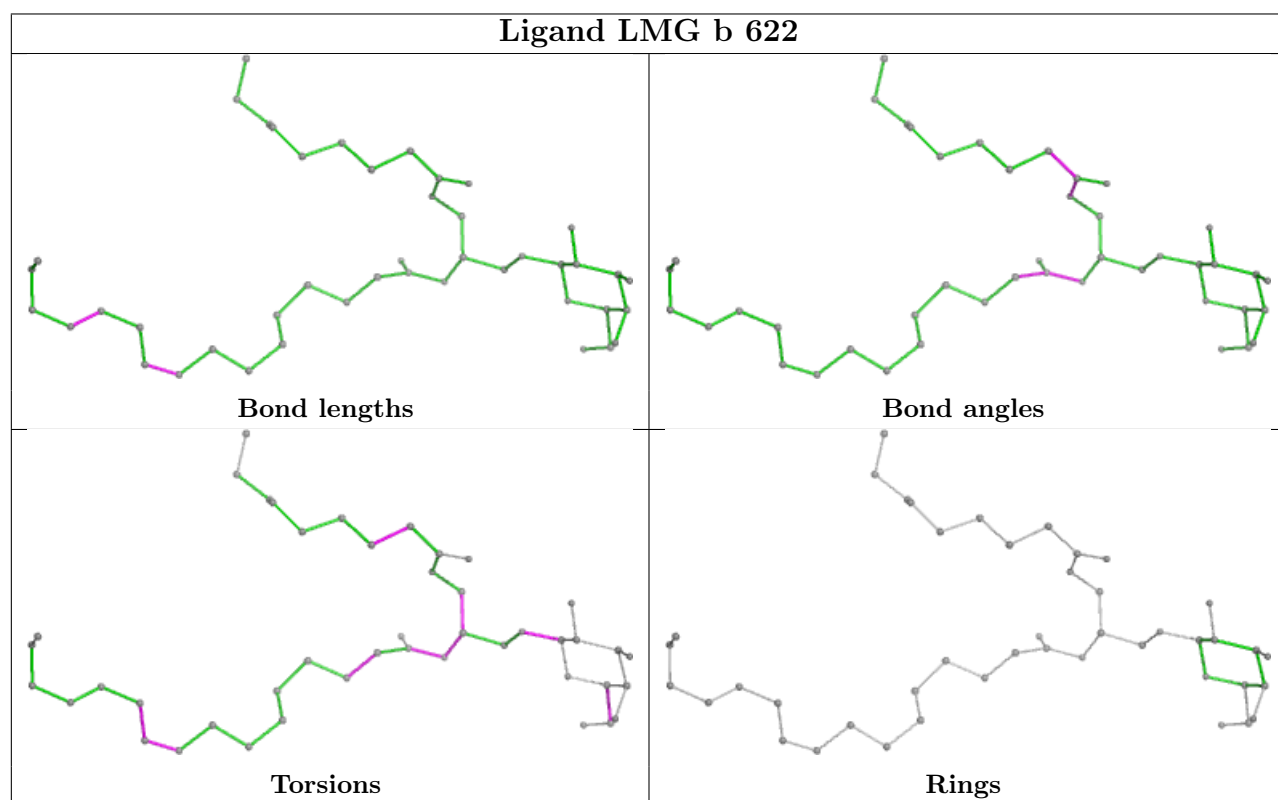
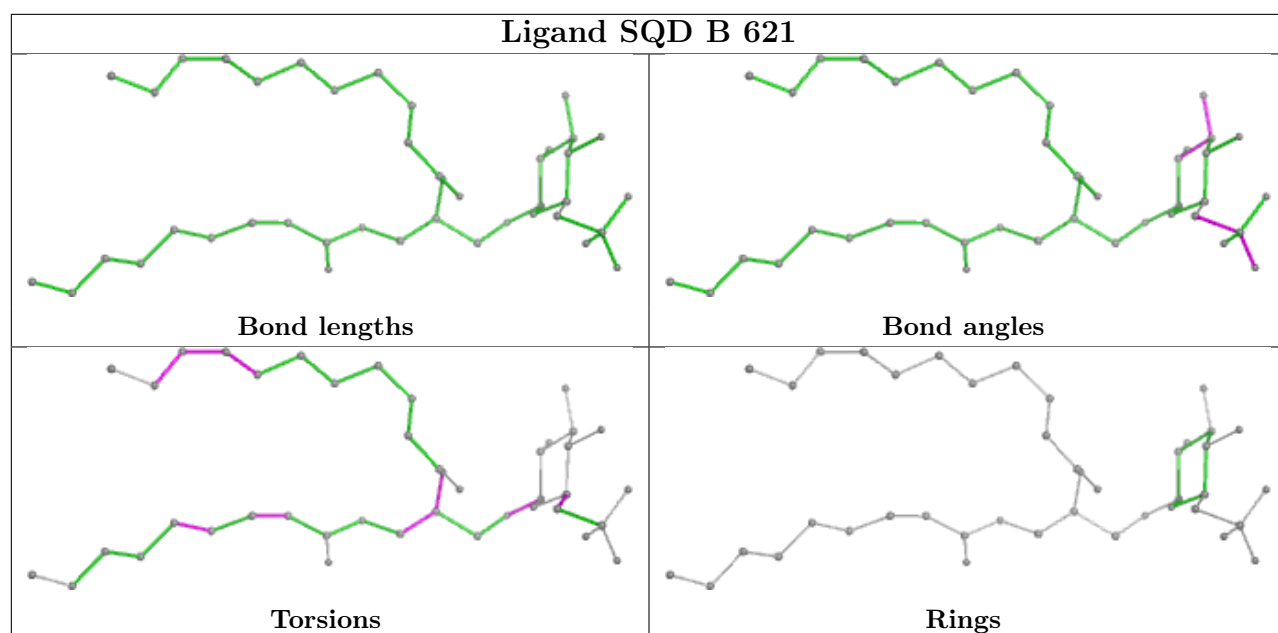


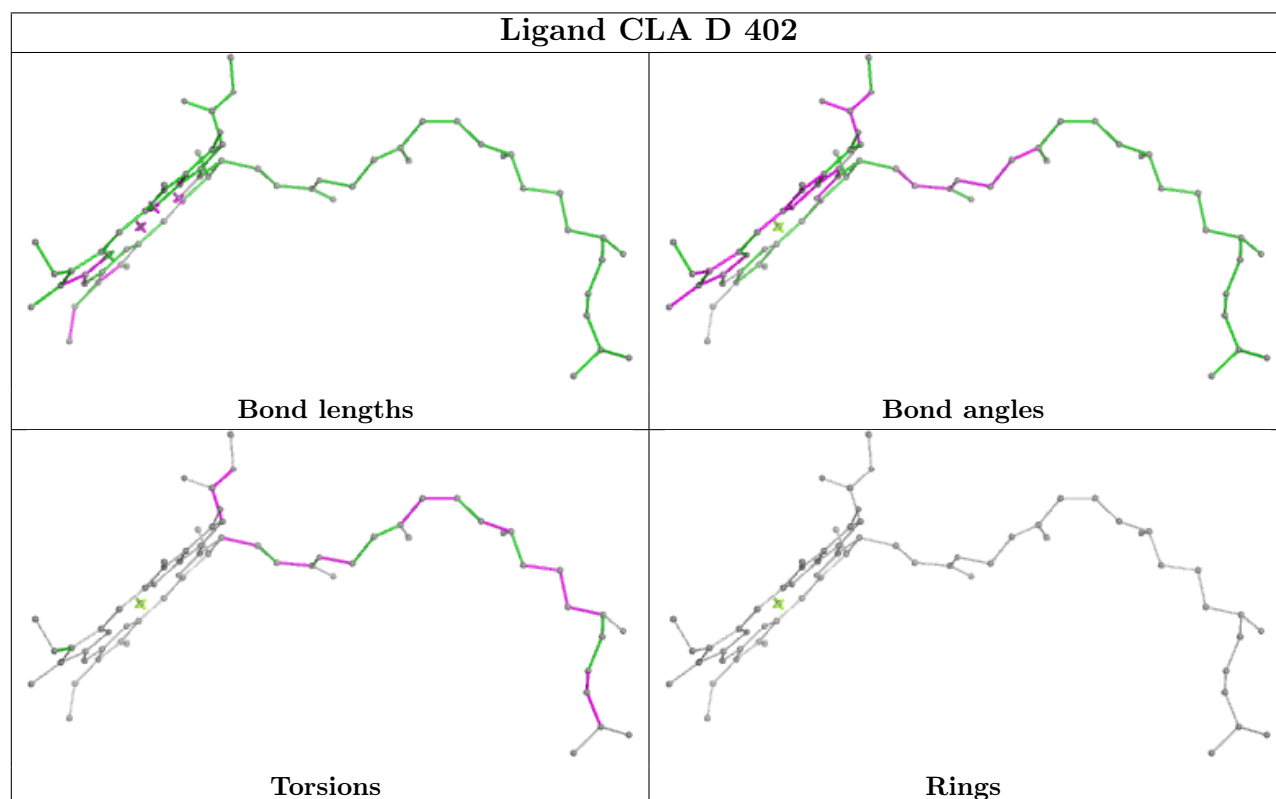
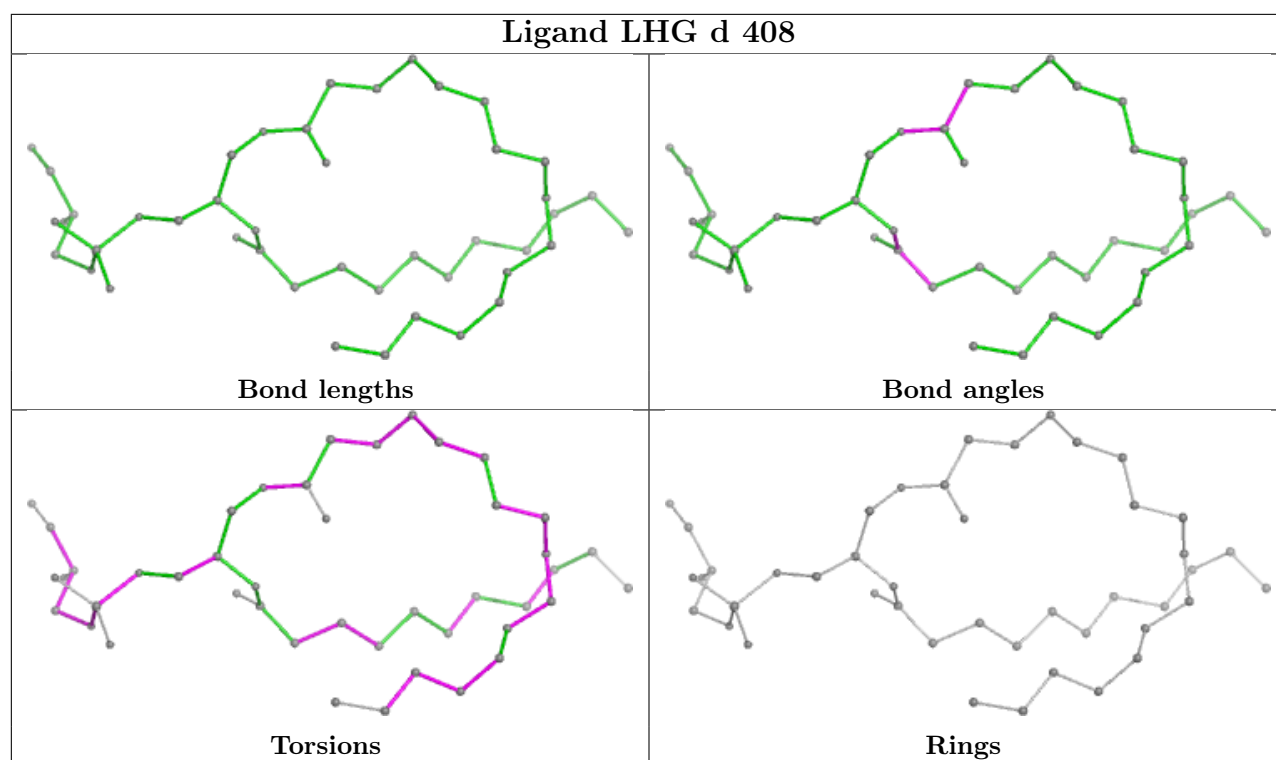
Ligand CLA c 506

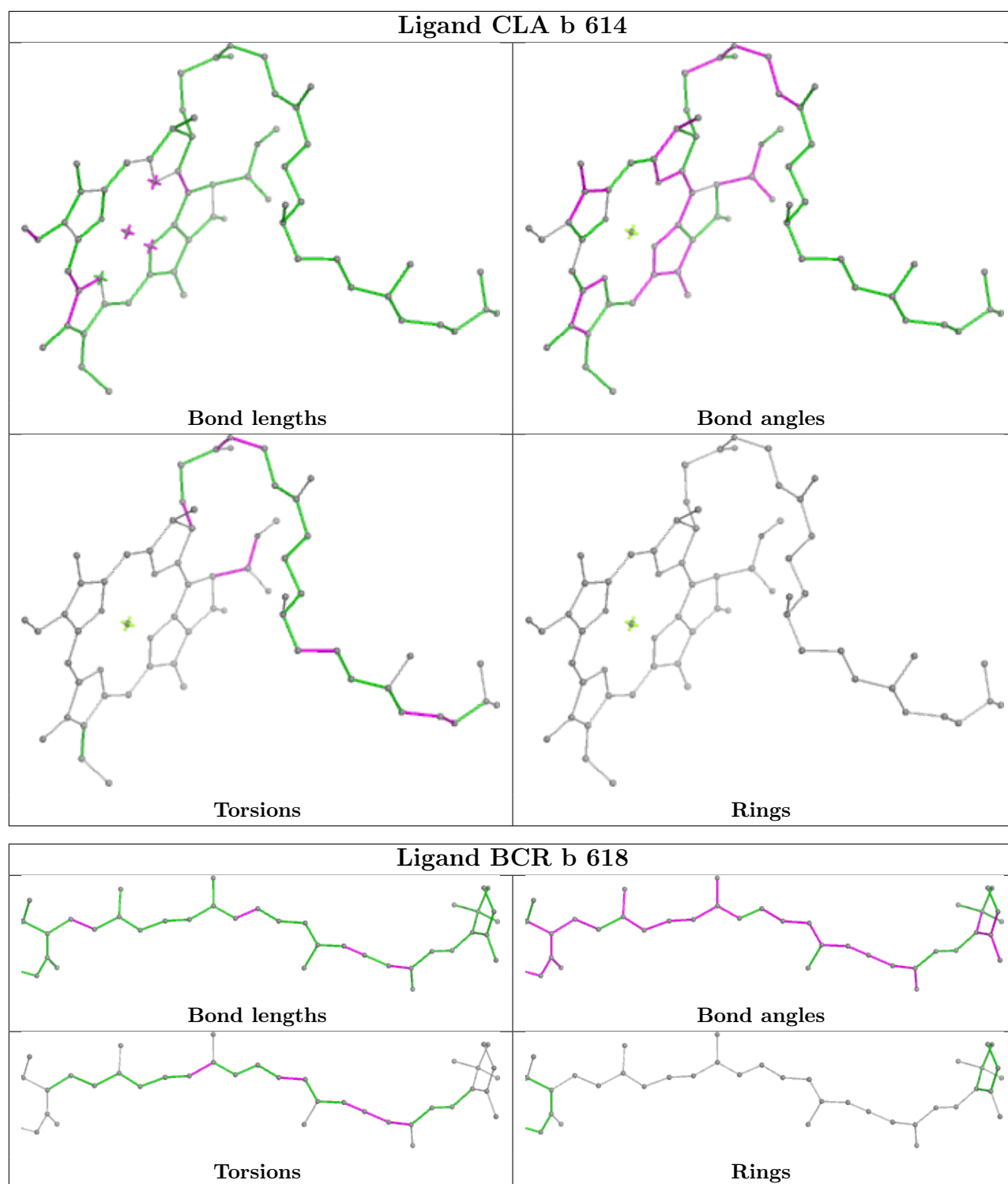


Ligand CLA N 604

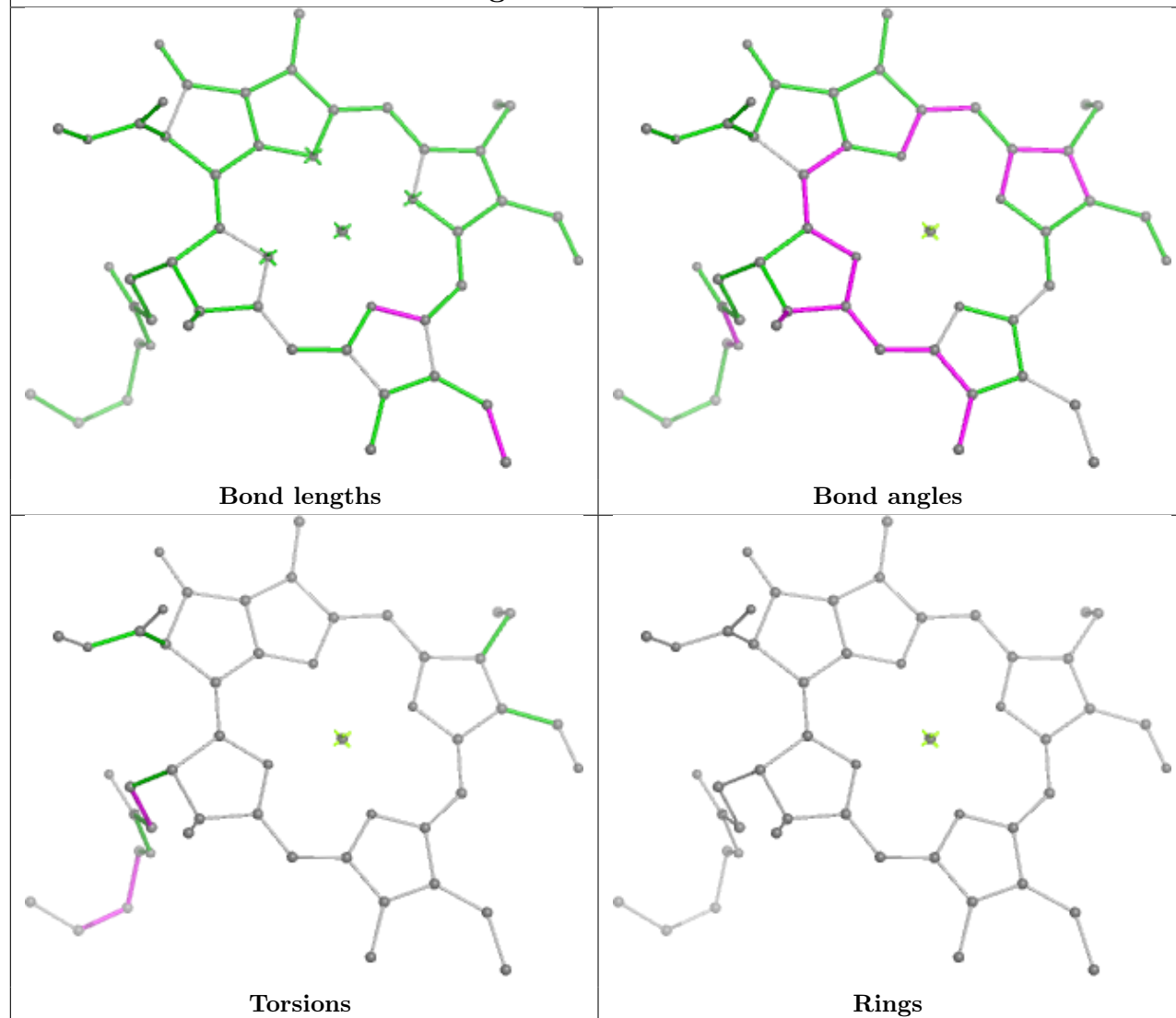




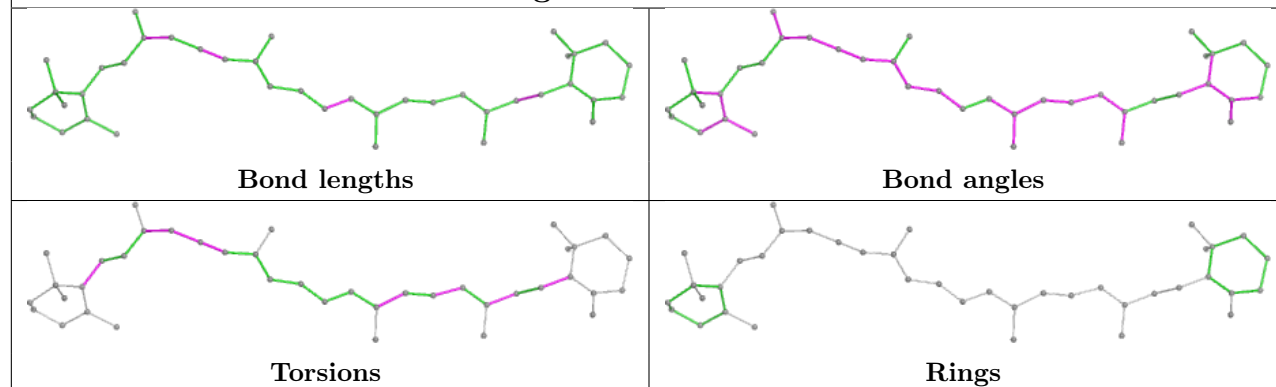




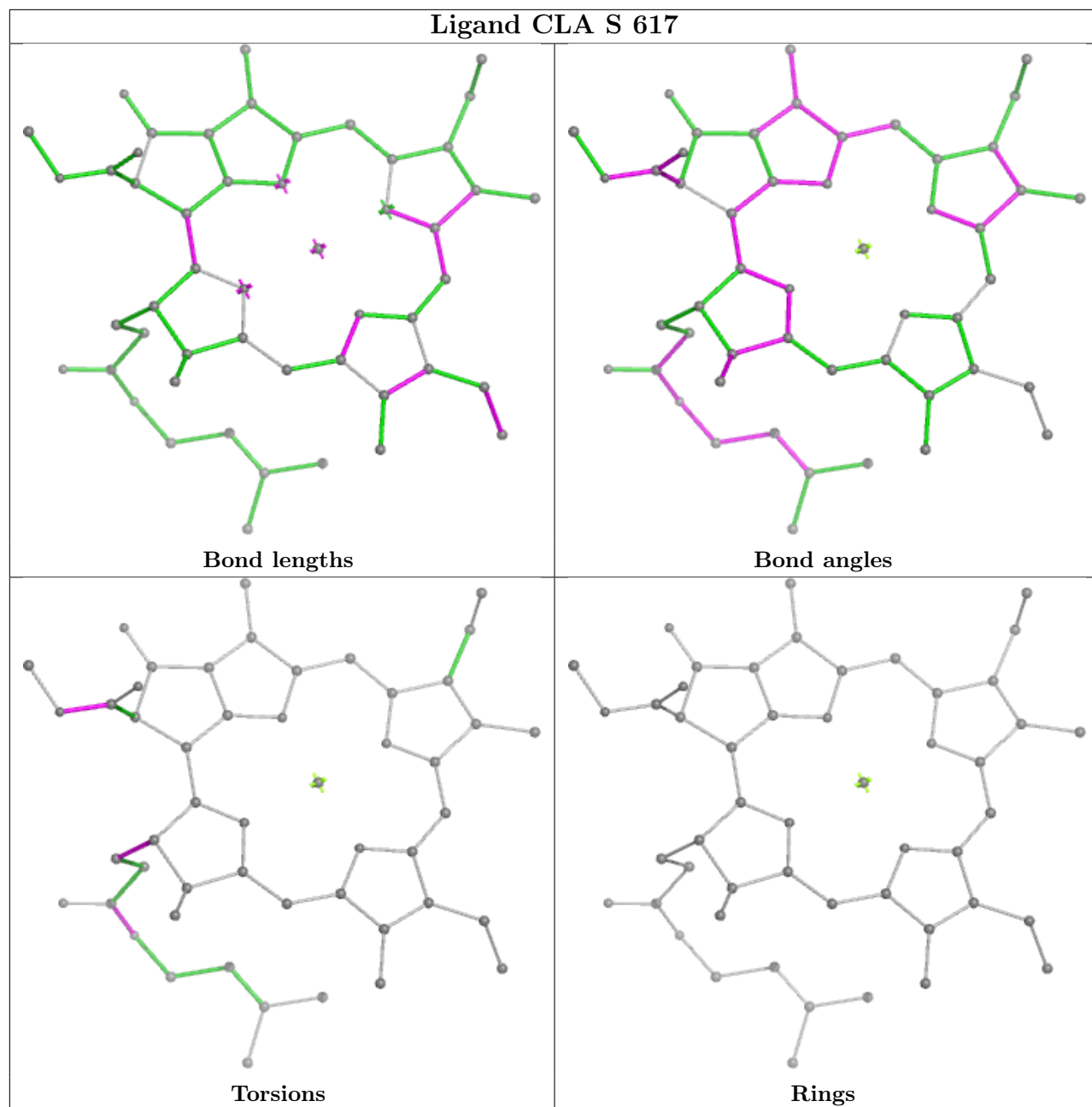
Ligand CHL N 608



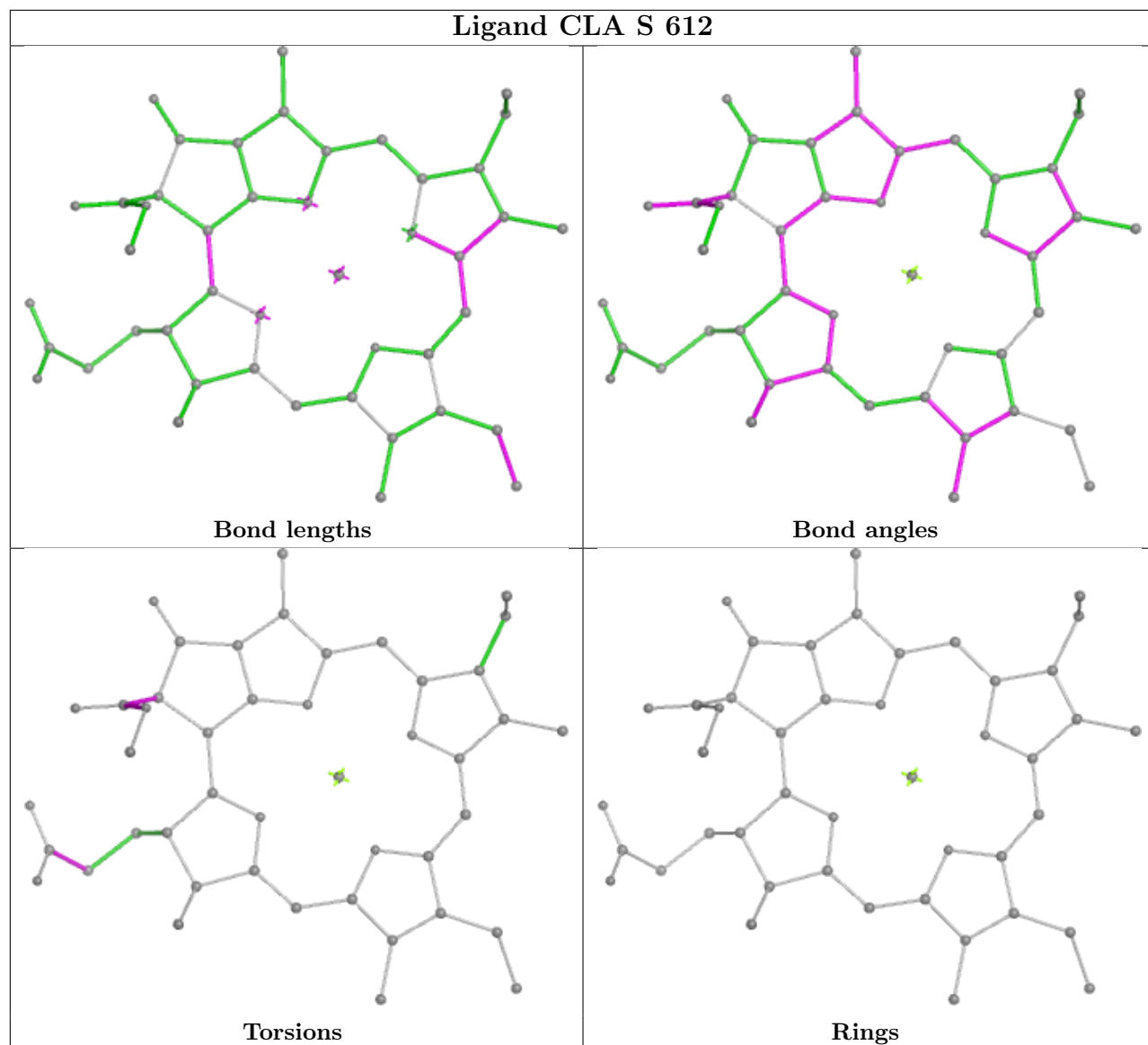
Ligand BCR d 404

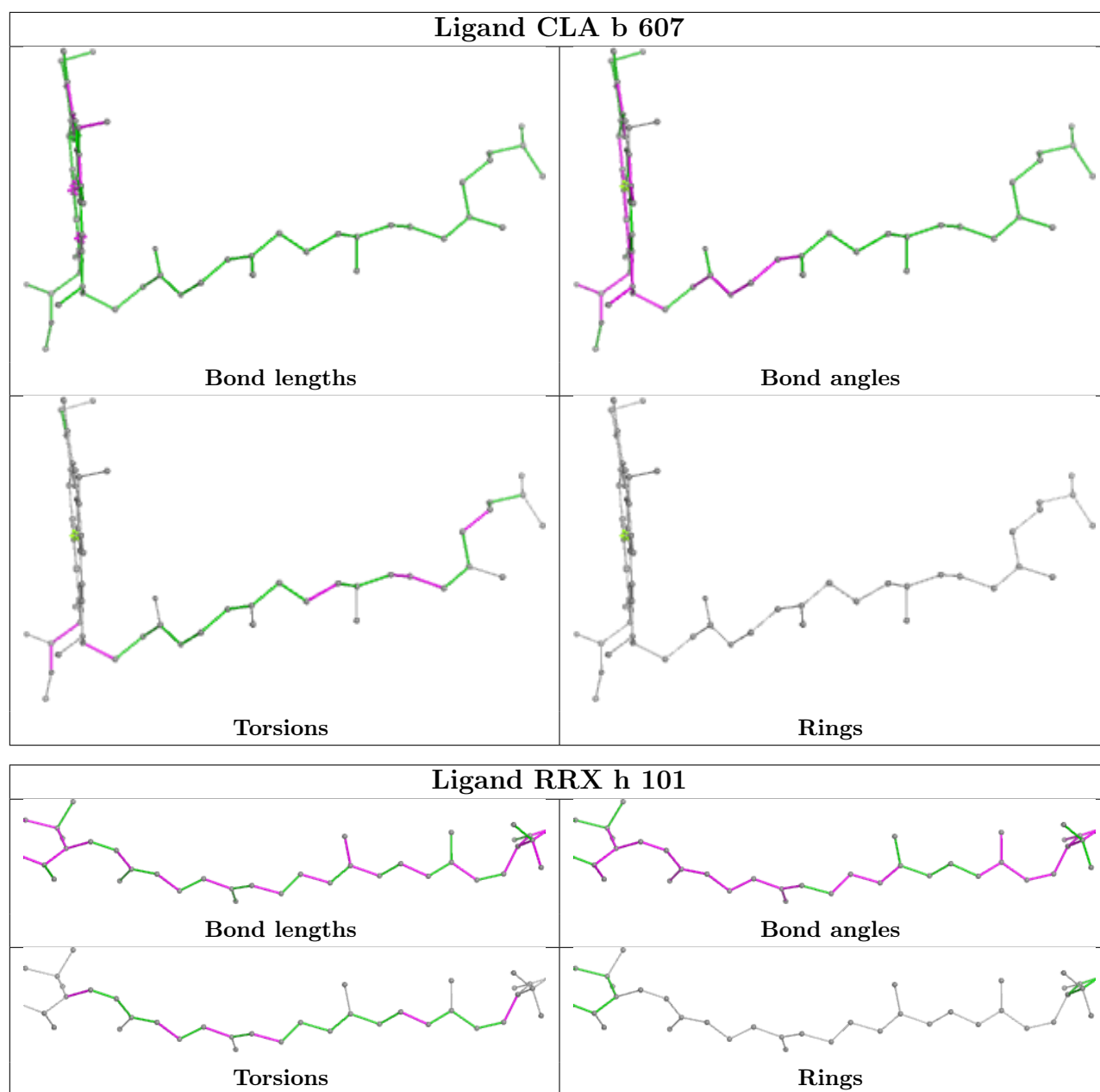


Ligand CLA S 617



Ligand CLA S 612





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.

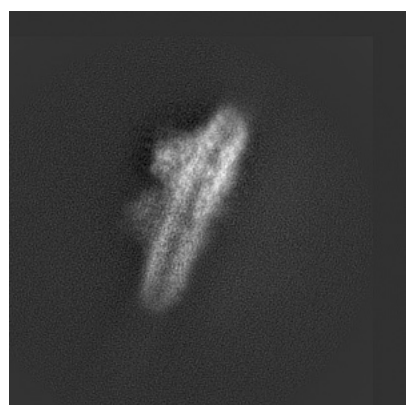
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13548. These allow visual inspection of the internal detail of the map and identification of artifacts.

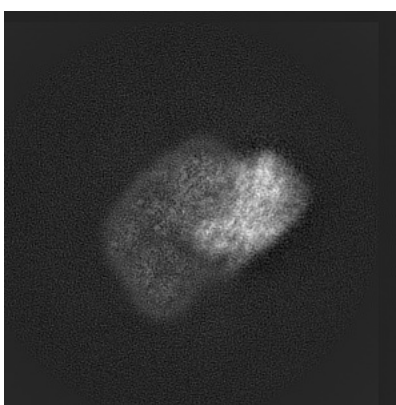
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

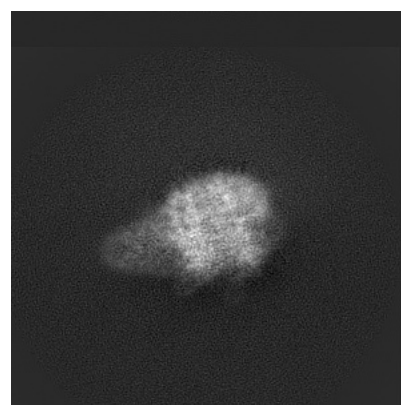
6.1.1 Primary map



X



Y

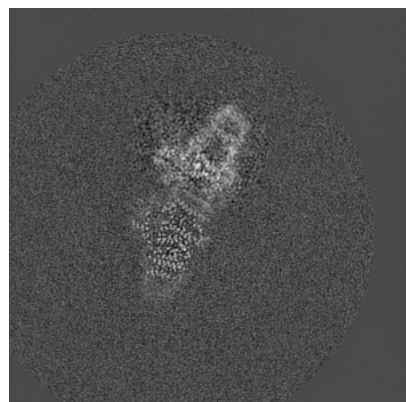


Z

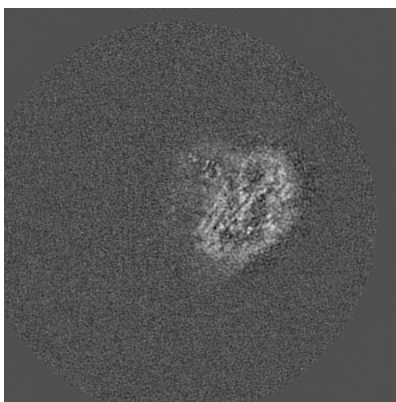
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

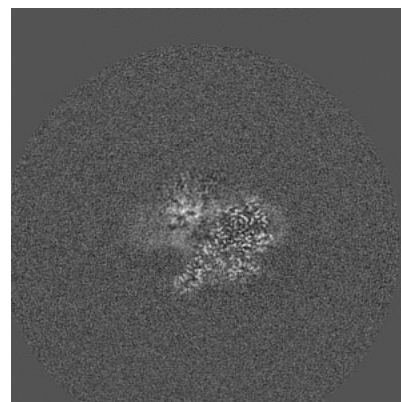
6.2.1 Primary map



X Index: 250



Y Index: 250

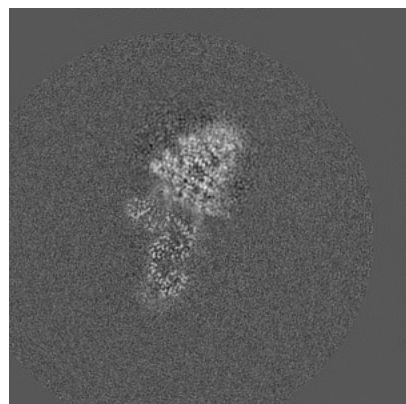


Z Index: 250

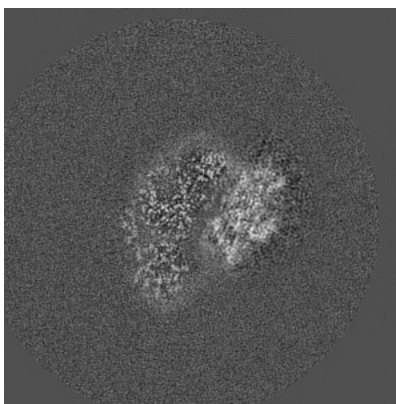
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

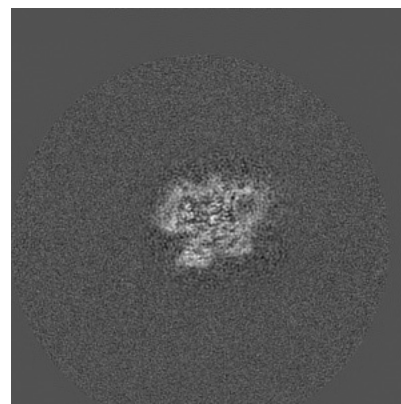
6.3.1 Primary map



X Index: 225



Y Index: 219

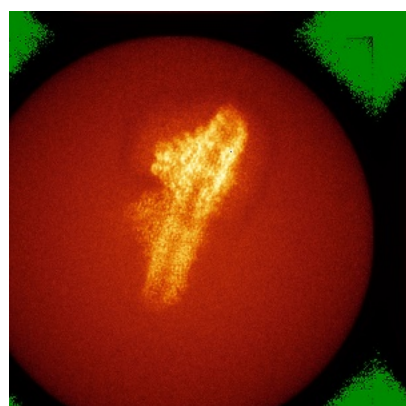


Z Index: 304

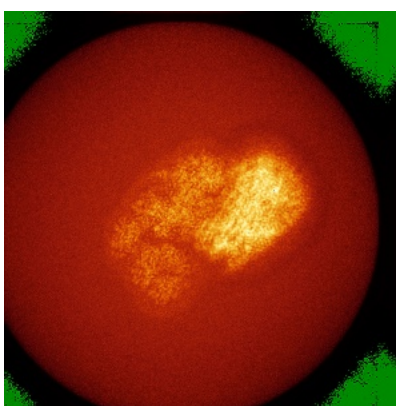
The images above show the largest variance slices of the map in three orthogonal directions.

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

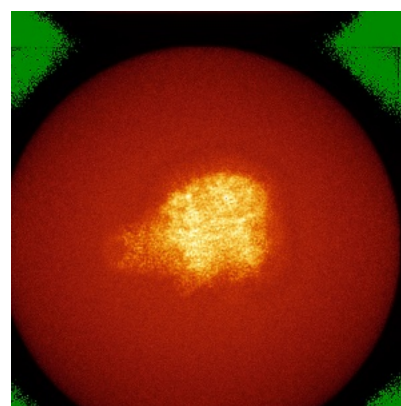
6.4.1 Primary map



X



Y

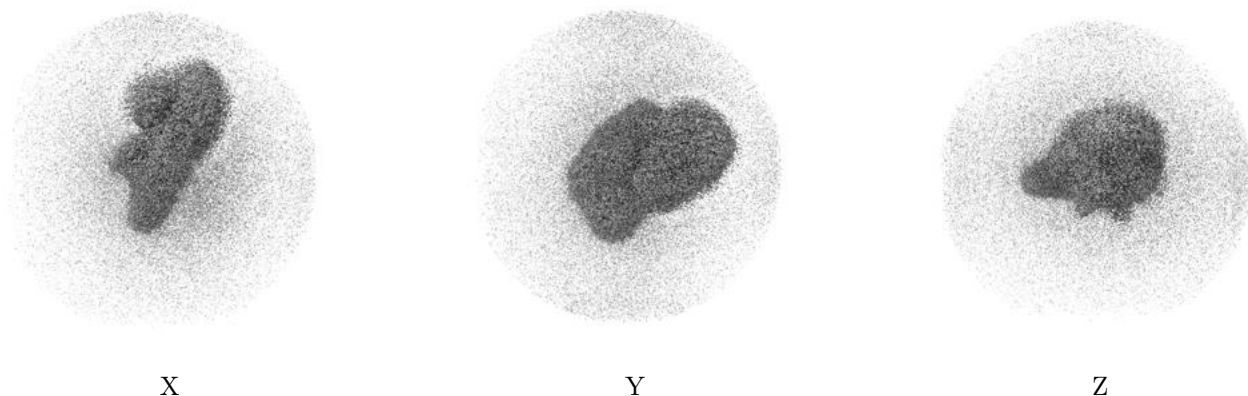


Z

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 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

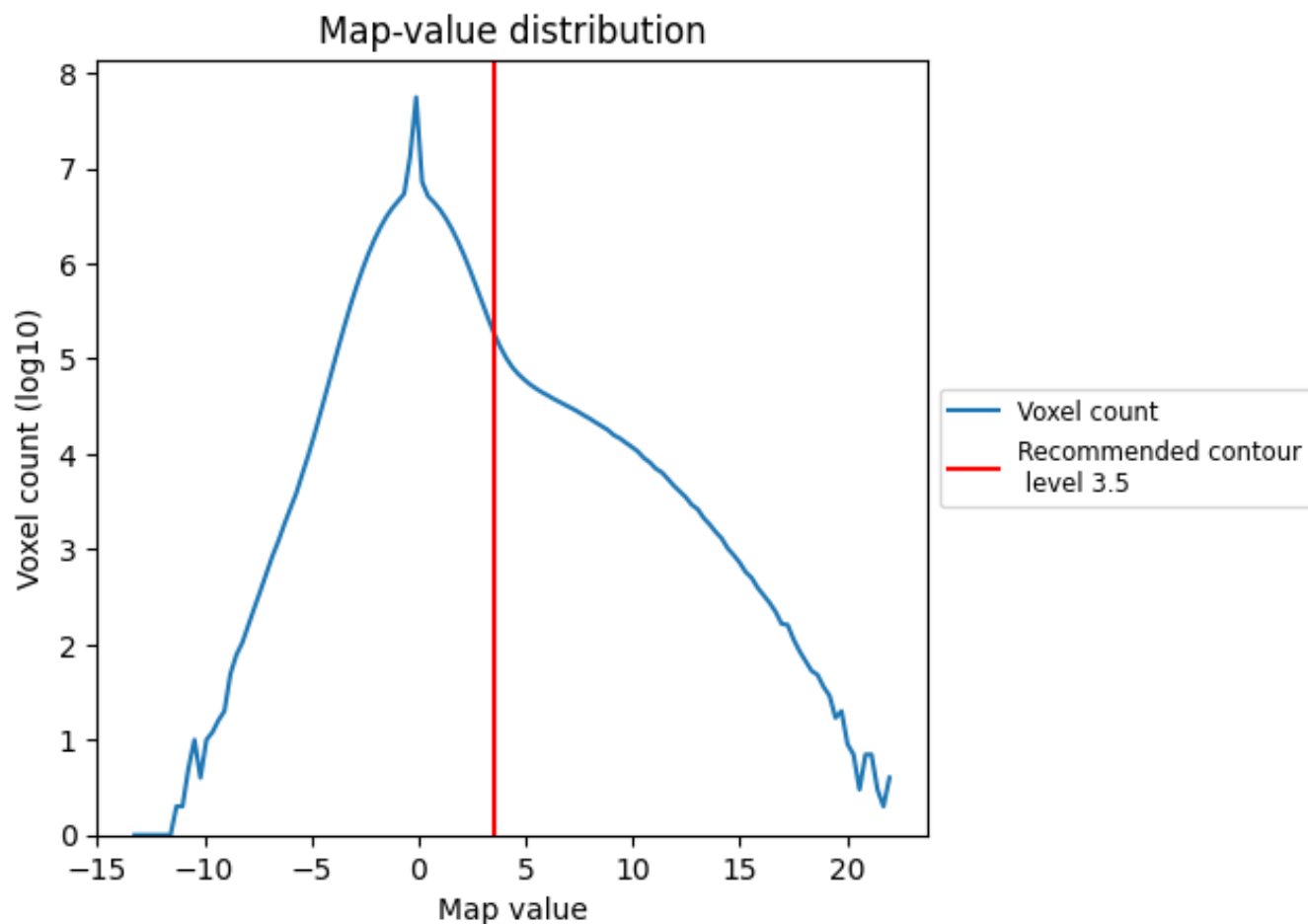
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

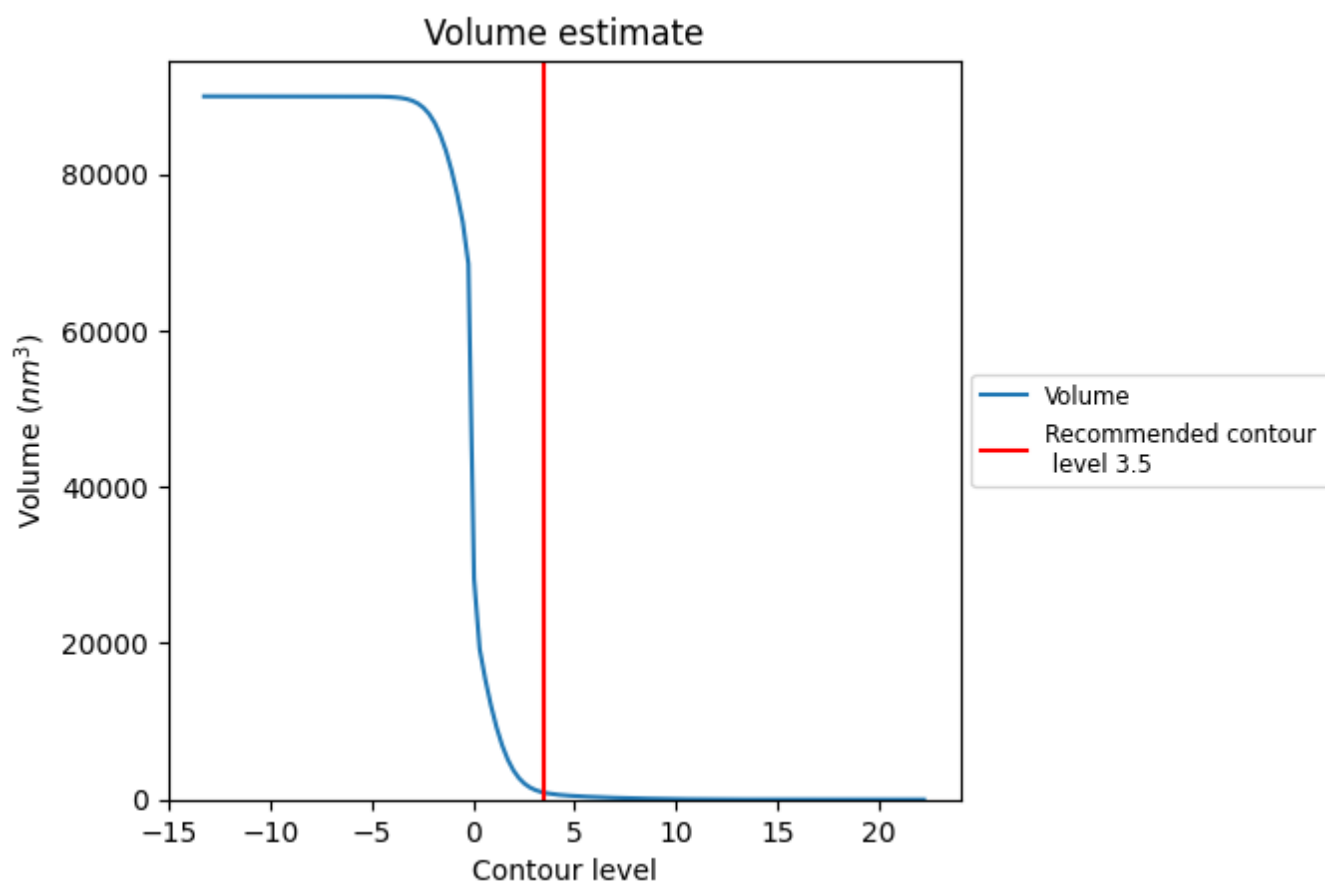
This section contains the results of statistical analysis of the map.

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.

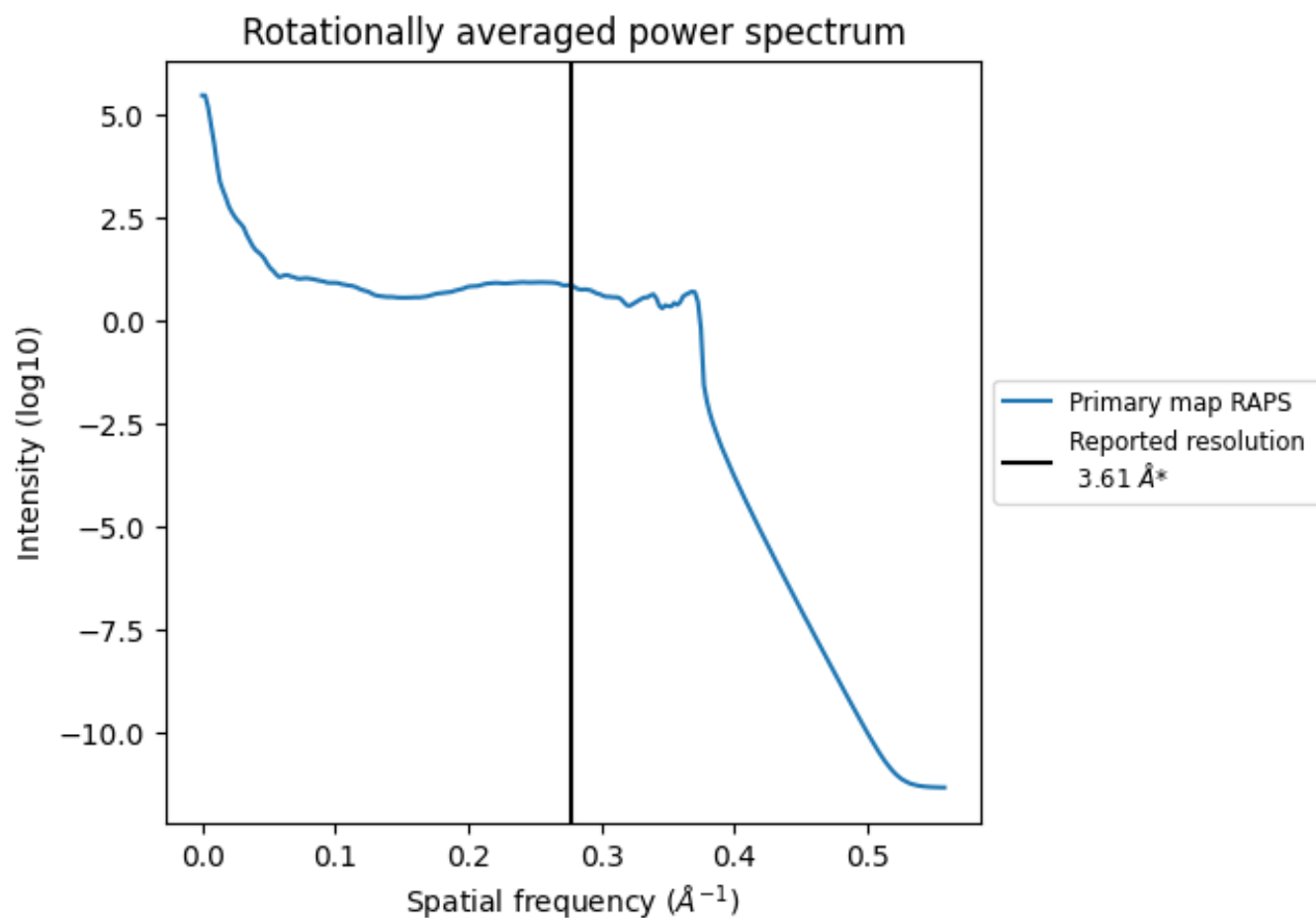
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 898 nm³; this corresponds to an approximate mass of 811 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 ⓘ

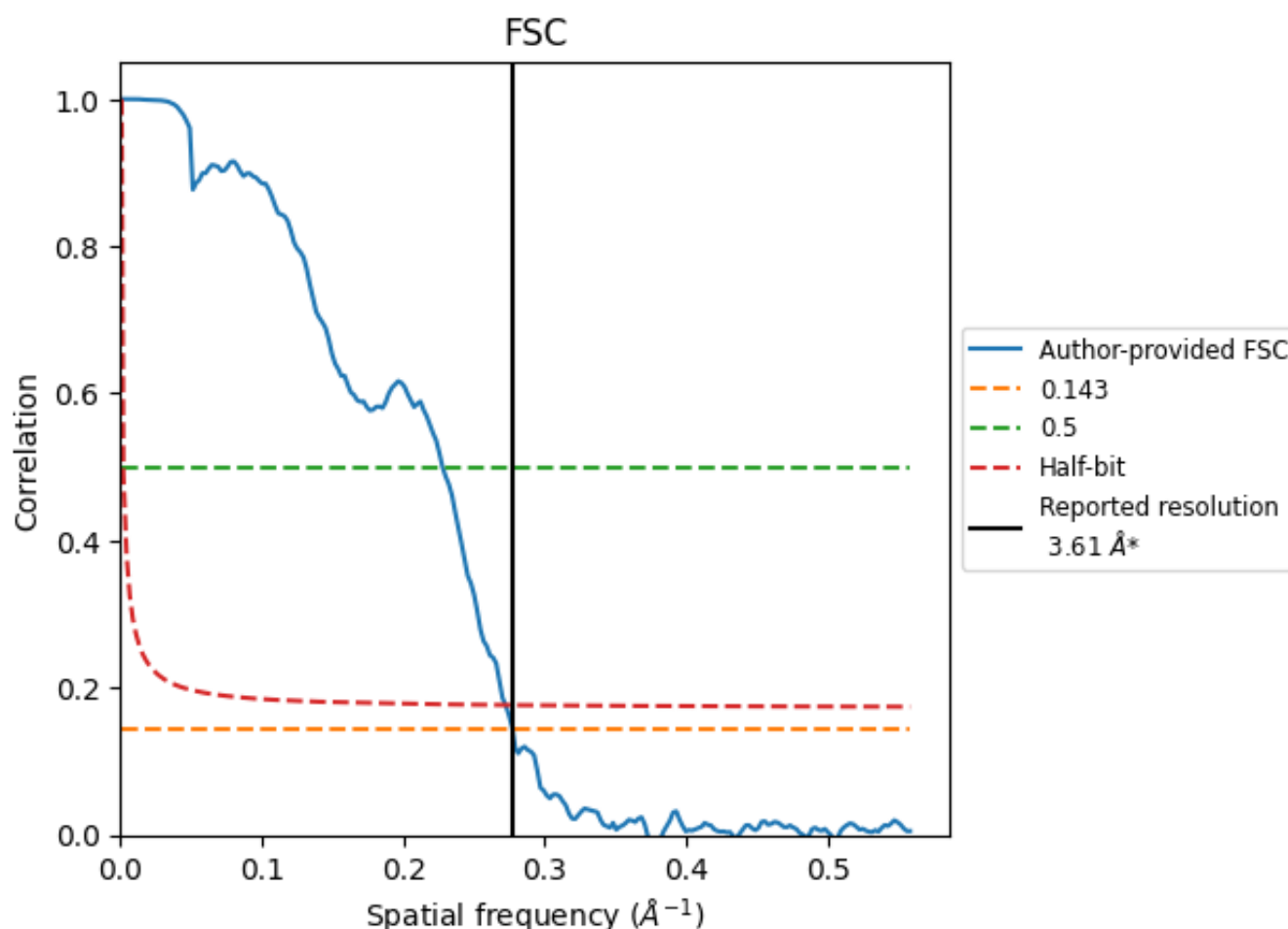


*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

8.2 Resolution estimates [i](#)

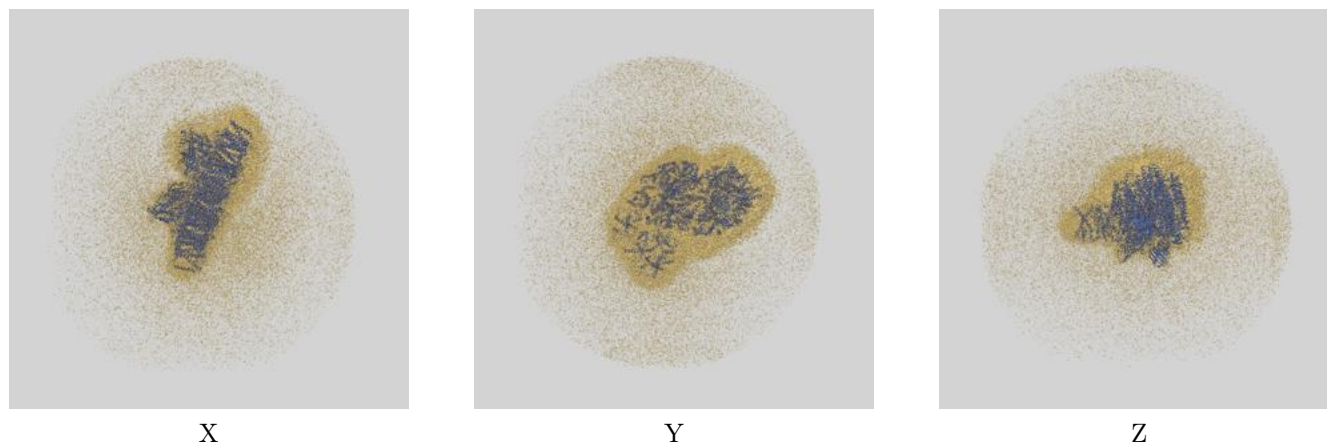
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	3.61	4.39	3.67
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

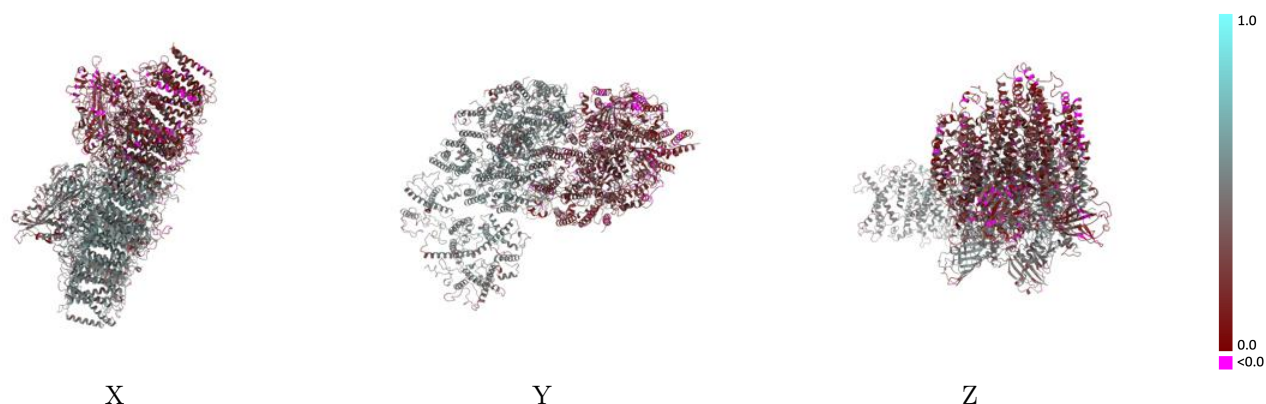
This section contains information regarding the fit between EMDB map EMD-13548 and PDB model 7PNK. Per-residue inclusion information can be found in section [3](#) on page [37](#).

9.1 Map-model overlay [i](#)



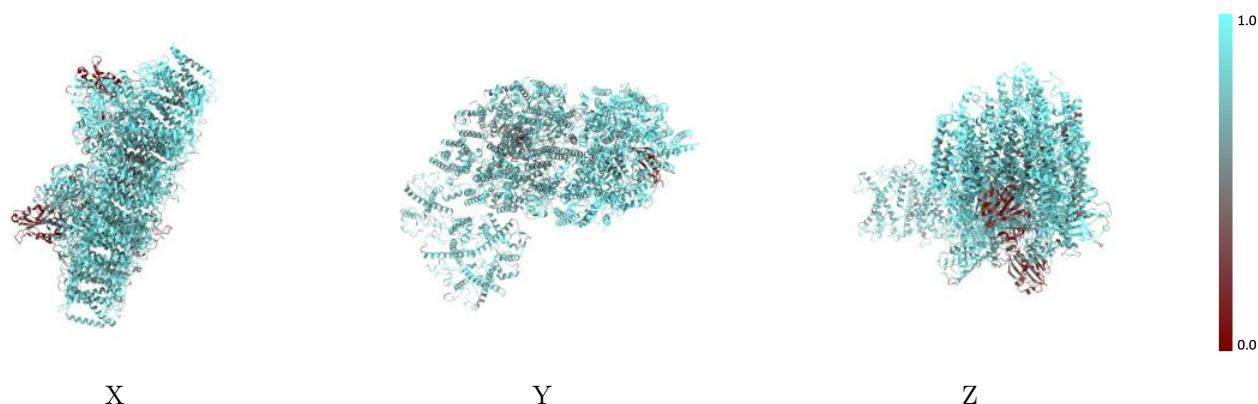
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



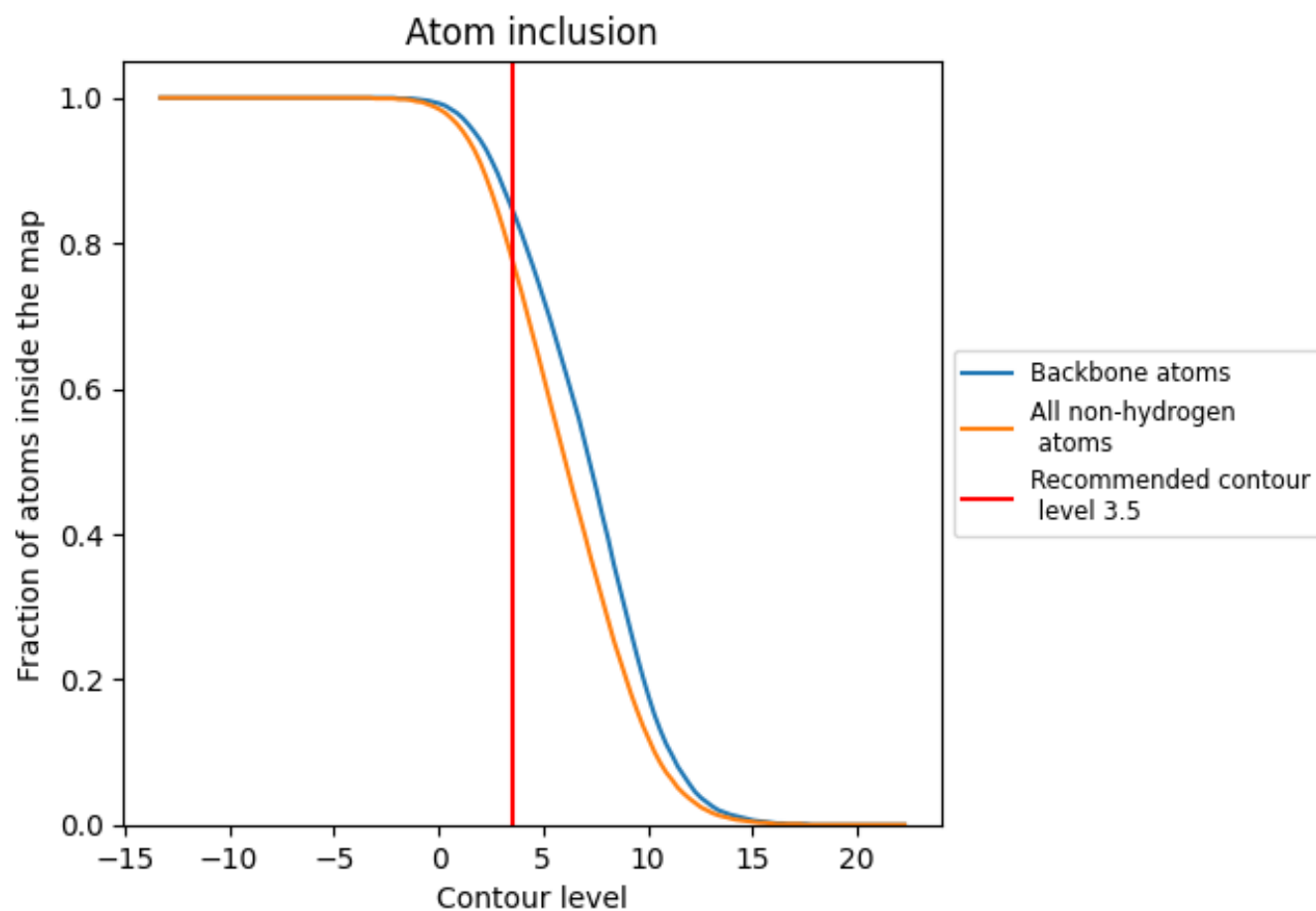
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 78% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3810
A	 0.7720	 0.5100
B	 0.8000	 0.4910
C	 0.8120	 0.5310
D	 0.8180	 0.5240
E	 0.8140	 0.4740
F	 0.8080	 0.4820
G	 0.7440	 0.4420
H	 0.7960	 0.4790
I	 0.6840	 0.4500
J	 0.7280	 0.4740
K	 0.7340	 0.4710
L	 0.7490	 0.4910
M	 0.6470	 0.3770
N	 0.7750	 0.4800
O	 0.7230	 0.4310
P	 0.2770	 0.3450
S	 0.7710	 0.4780
T	 0.5970	 0.4100
U	 0.6330	 0.3920
V	 0.7600	 0.4840
W	 0.6560	 0.4540
X	 0.7510	 0.4430
Y	 0.7500	 0.4910
Z	 0.7910	 0.4930
a	 0.8530	 0.2340
b	 0.8320	 0.2570
c	 0.8620	 0.2170
d	 0.8790	 0.2770
e	 0.9490	 0.2380
f	 0.8950	 0.2490
h	 0.8330	 0.2430
i	 0.7810	 0.2010
j	 0.8760	 0.2850
k	 0.8860	 0.2450



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.6840	 0.1810
m	 0.6650	 0.2260
o	 0.8250	 0.2010
p	 0.3550	 0.1570
t	 0.6010	 0.2440
u	 0.9400	 0.2420
v	 0.8980	 0.2180
w	 0.7950	 0.1740
x	 0.8660	 0.1970
z	 0.8970	 0.1980