



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 05:56 pm GMT

PDB ID : 7PI0
EMDB ID : EMD-13429
Title : Unstacked compact Dunaliella PSII
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on : 2021-08-19
Resolution : 2.43 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

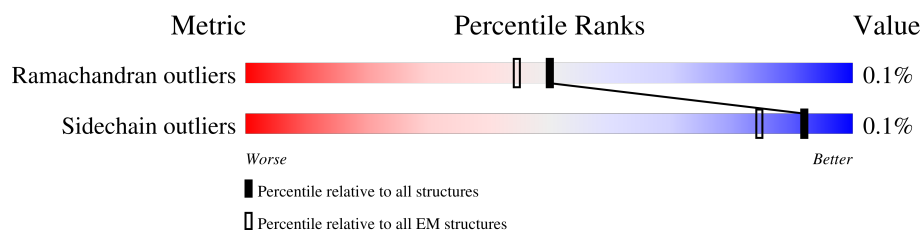
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 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.


















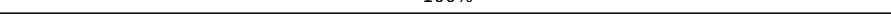
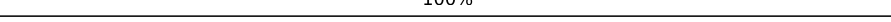
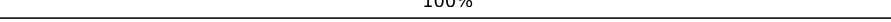

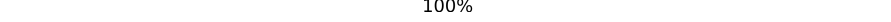
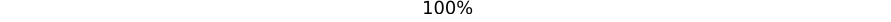
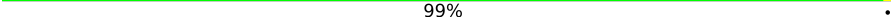
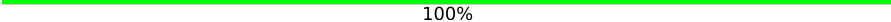


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	94% 5% •
1	a	336	100%
2	B	484	100%
2	b	484	100%
3	V	32	100%
3	v	32	100%
4	C	449	100%
4	c	449	100%
5	D	348	96% ••

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Mol	Chain	Length	Quality of chain
5	d	348	 100%
6	E	76	 100%
6	e	76	 100%
7	F	31	 100%
7	f	31	 100%
8	H	67	 100%
8	h	67	 100%
9	I	35	 100%
9	i	35	 100%
10	J	36	 100%
10	j	36	 100%
11	K	37	 100%
11	k	37	 100%
12	L	38	 100%
12	l	38	 100%
13	M	31	 100%
13	m	31	 100%
14	O	238	 100%
14	o	238	 100%
15	P	187	 21% 100%
15	p	187	 8% 99%
16	T	30	 100%
16	t	30	 100%
17	W	44	 100%
17	w	44	 100%

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Mol	Chain	Length	Quality of chain
18	X	30	 100%
18	x	30	 100%
19	Z	61	 100%
19	z	61	 100%
20	N	222	 100%
20	n	222	 100%
21	G	221	 100%
21	g	221	 100%
22	R	196	 99%
22	r	196	 99%
23	S	243	 100%
23	s	243	 100%
24	Y	222	 99%
24	y	222	 100%
25	U	27	 100%
25	u	27	 100%

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
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-
29	CLA	B	501	X	-	-	-
29	CLA	B	502	X	-	-	-
29	CLA	B	503	X	-	-	-
29	CLA	B	504	X	-	-	-
29	CLA	B	505	X	-	-	-
29	CLA	B	506	X	-	-	-
29	CLA	B	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	508	X	-	-	-
29	CLA	B	509	X	-	-	-
29	CLA	B	510	X	-	-	-
29	CLA	B	512	X	-	-	-
29	CLA	B	513	X	-	-	-
29	CLA	B	514	X	-	-	-
29	CLA	B	515	X	-	-	-
29	CLA	B	516	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	506	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	D	404	X	-	-	-
29	CLA	D	405	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	R	301	X	-	-	-
29	CLA	R	303	X	-	-	-
29	CLA	R	306	X	-	-	-
29	CLA	R	307	X	-	-	-
29	CLA	R	308	X	-	-	-
29	CLA	R	309	X	-	-	-
29	CLA	S	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	S	304	X	-	-	-
29	CLA	S	305	X	-	-	-
29	CLA	S	306	X	-	-	-
29	CLA	S	310	X	-	-	-
29	CLA	S	311	X	-	-	-
29	CLA	S	312	X	-	-	-
29	CLA	S	313	X	-	-	-
29	CLA	S	314	X	-	-	-
29	CLA	S	315	X	-	-	-
29	CLA	S	316	X	-	-	-
29	CLA	Y	303	X	-	-	-
29	CLA	Y	304	X	-	-	-
29	CLA	Y	305	X	-	-	-
29	CLA	Y	309	X	-	-	-
29	CLA	Y	311	X	-	-	-
29	CLA	Y	312	X	-	-	-
29	CLA	Y	313	X	-	-	-
29	CLA	Y	314	X	-	-	-
29	CLA	Y	315	X	-	-	-
29	CLA	a	404	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	b	501	X	-	-	-
29	CLA	b	502	X	-	-	-
29	CLA	b	503	X	-	-	-
29	CLA	b	504	X	-	-	-
29	CLA	b	505	X	-	-	-
29	CLA	b	506	X	-	-	-
29	CLA	b	507	X	-	-	-
29	CLA	b	509	X	-	-	-
29	CLA	b	510	X	-	-	-
29	CLA	b	512	X	-	-	-
29	CLA	b	513	X	-	-	-
29	CLA	b	514	X	-	-	-
29	CLA	b	515	X	-	-	-
29	CLA	b	516	X	-	-	-
29	CLA	c	502	X	-	-	-
29	CLA	c	504	X	-	-	-
29	CLA	c	505	X	-	-	-
29	CLA	c	507	X	-	-	-
29	CLA	c	508	X	-	-	-
29	CLA	c	509	X	-	-	-
29	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	c	512	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	d	404	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	609	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	r	302	X	-	-	-
29	CLA	r	304	X	-	-	-
29	CLA	r	307	X	-	-	-
29	CLA	r	308	X	-	-	-
29	CLA	r	309	X	-	-	-
29	CLA	r	310	X	-	-	-
29	CLA	s	303	X	-	-	-
29	CLA	s	305	X	-	-	-
29	CLA	s	310	X	-	-	-
29	CLA	s	311	X	-	-	-
29	CLA	s	312	X	-	-	-
29	CLA	s	313	X	-	-	-
29	CLA	s	314	X	-	-	-
29	CLA	s	315	X	-	-	-
29	CLA	s	316	X	-	-	-
29	CLA	y	304	X	-	-	-
29	CLA	y	305	X	-	-	-
29	CLA	y	306	X	-	-	-
29	CLA	y	310	X	-	-	-
29	CLA	y	312	X	-	-	-
29	CLA	y	313	X	-	-	-
29	CLA	y	314	X	-	-	-
29	CLA	y	316	X	-	-	-
34	C7Z	B	519	X	-	-	-
34	C7Z	b	519	X	-	-	-
45	RRX	H	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	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	R	304	X	-	-	-
46	CHL	R	305	X	-	-	-
46	CHL	S	302	X	-	-	-
46	CHL	S	307	X	-	-	-
46	CHL	S	308	X	-	-	-
46	CHL	S	309	X	-	-	-
46	CHL	Y	302	X	-	-	-
46	CHL	Y	306	X	-	-	-
46	CHL	Y	307	X	-	-	-
46	CHL	Y	308	X	-	-	-
46	CHL	Y	310	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	r	305	X	-	-	-
46	CHL	r	306	X	-	-	-
46	CHL	s	302	X	-	-	-
46	CHL	s	307	X	-	-	-
46	CHL	s	308	X	-	-	-
46	CHL	s	309	X	-	-	-
46	CHL	y	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	CHL	y	303	X	-	-	-
46	CHL	y	307	X	-	-	-
46	CHL	y	308	X	-	-	-
46	CHL	y	309	X	-	-	-
46	CHL	y	311	X	-	-	-
49	XAT	G	619	X	-	-	-
49	XAT	N	619	X	-	-	-
49	XAT	R	311	X	-	-	-
49	XAT	Y	301	X	-	-	-
49	XAT	g	619	X	-	-	-
49	XAT	n	618	X	-	-	-
49	XAT	r	312	X	-	-	-
49	XAT	y	302	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 77465 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	0	0
			2635	1719	432	468	16		
1	a	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

- 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	0	0
			266	183	40	43		

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

- 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		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

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 PSII 6.1 kDa protein.

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 Hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	30	Total	C	N	O	S	0	0
			201	132	32	37			
18	x	30	Total	C	N	O	S	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		
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 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total	C	N	O	S	0	0
			1703	1100	277	321	5		
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 of LHCII type 2, chloroplastic.

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

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		
22	r	196	Total	C	N	O	P S	0	0
			1490	943	251	292	1 3		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic, CP26.

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

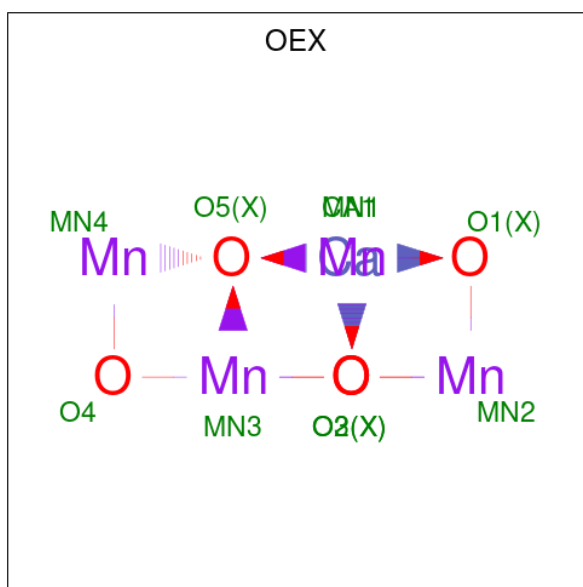
- Molecule 24 is a protein called Chlorophyll a-b binding protein of LHCII type 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called Photosystem II extrinsic protein U.

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

- Molecule 26 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

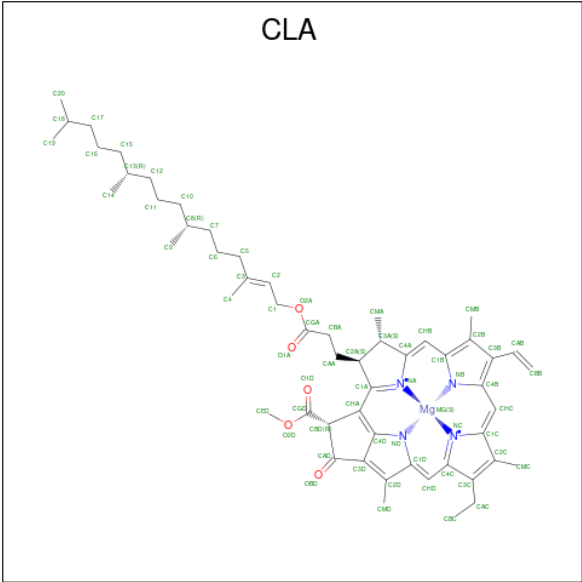
- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Fe	0
			1	1	
27	d	1	Total	Fe	0
			1	1	

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	C	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	D	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	N	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	R	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	n	1	Total 45	C 35	Mg 1	N 4	O 5	0

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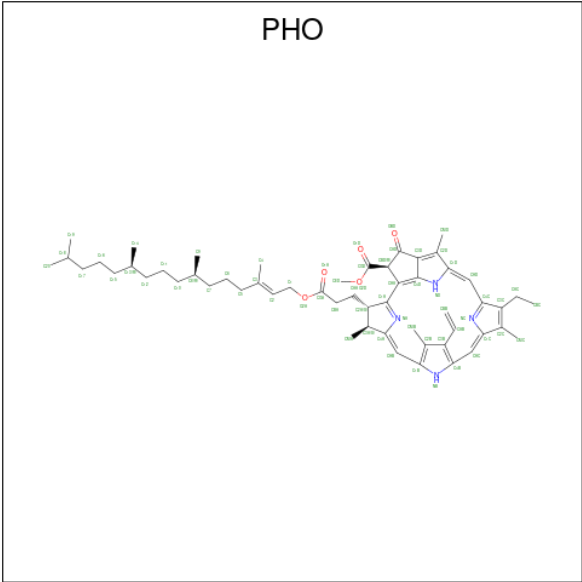
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	n	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 43	C 35	Mg 1	N 4	O 3	0
29	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	r	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 50	C 40	Mg 1	N 4	O 5	0

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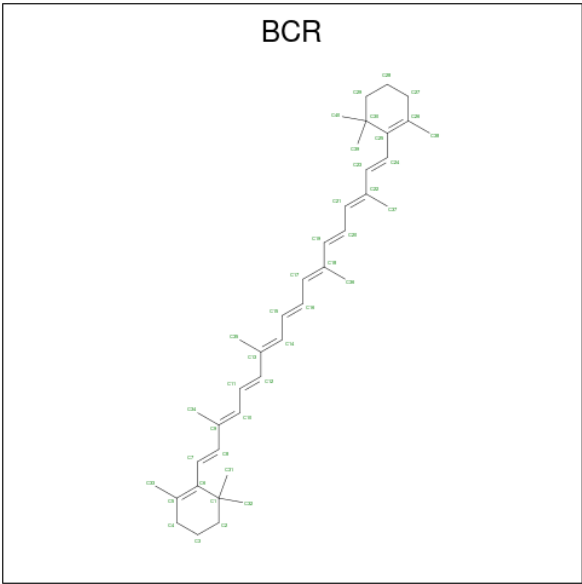
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).

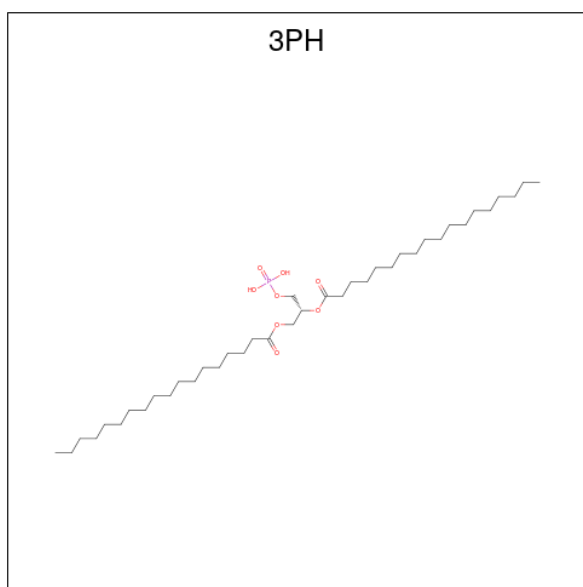


Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	F	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	v	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	f	1	Total C 40 40	0
31	z	1	Total C 40 40	0

- Molecule 32 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 33 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	P	0
			48	39	8	1	
33	B	1	Total	C	O	P	0
			48	39	8	1	
33	S	1	Total	C	O	P	0
			30	21	8	1	
33	a	1	Total	C	O	P	0
			48	39	8	1	
33	b	1	Total	C	O	P	0
			39	30	8	1	
33	s	1	Total	C	O	P	0
			48	39	8	1	

- 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: C₄₀H₅₆O₂).



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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



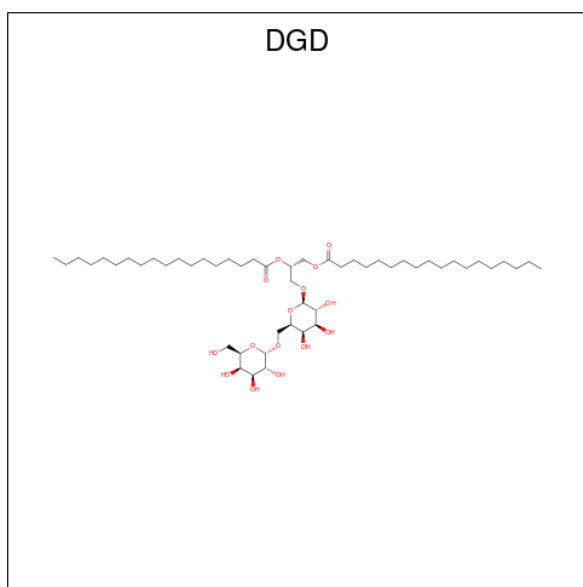
Mol	Chain	Residues	Atoms			AltCon
35	B	1	Total	C	O	0
			44	34	10	

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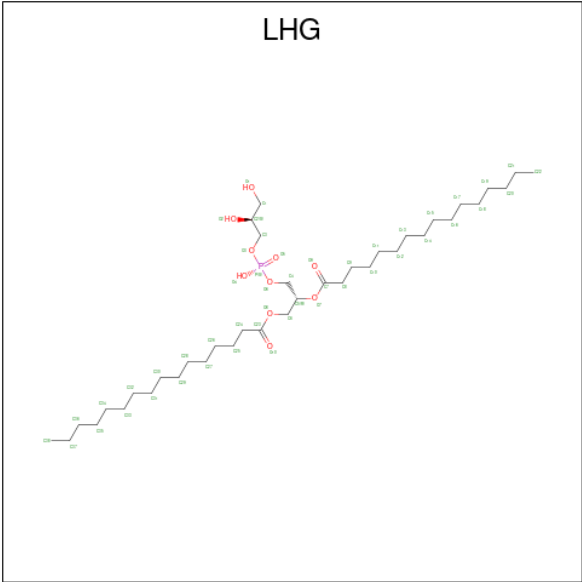
Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			47	37	10	
35	C	1	Total	C	O	0
			55	45	10	
35	C	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			42	32	10	
35	D	1	Total	C	O	0
			48	38	10	
35	W	1	Total	C	O	0
			40	30	10	
35	W	1	Total	C	O	0
			39	29	10	
35	b	1	Total	C	O	0
			44	34	10	
35	c	1	Total	C	O	0
			51	41	10	
35	c	1	Total	C	O	0
			55	45	10	
35	d	1	Total	C	O	0
			46	36	10	
35	d	1	Total	C	O	0
			48	38	10	
35	i	1	Total	C	O	0
			48	38	10	
35	w	1	Total	C	O	0
			39	29	10	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			43	28	15	
36	C	1	Total	C	O	0
			51	36	15	
36	C	1	Total	C	O	0
			53	38	15	
36	C	1	Total	C	O	0
			53	38	15	
36	c	1	Total	C	O	0
			55	40	15	
36	c	1	Total	C	O	0
			62	47	15	
36	c	1	Total	C	O	0
			59	44	15	
36	r	1	Total	C	O	0
			43	28	15	

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



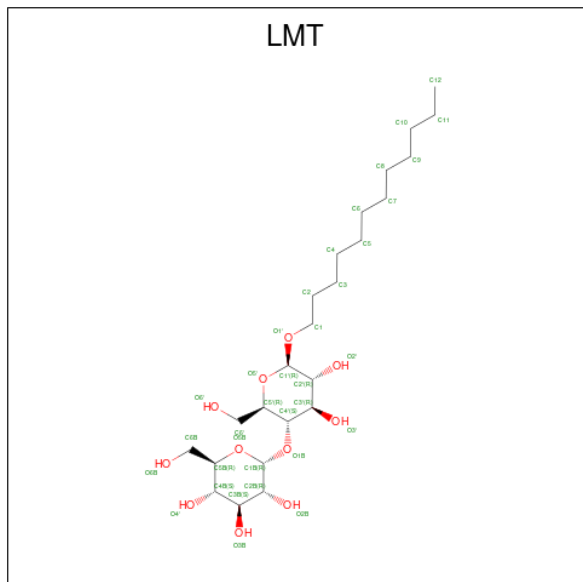
Mol	Chain	Residues	Atoms				AltConf
37	B	1	Total	C	O	P	0
			44	33	10	1	
37	D	1	Total	C	O	P	0
			49	38	10	1	
37	D	1	Total	C	O	P	0
			39	28	10	1	
37	L	1	Total	C	O	P	0
			49	38	10	1	
37	N	1	Total	C	O	P	0
			49	38	10	1	
37	G	1	Total	C	O	P	0
			49	38	10	1	
37	S	1	Total	C	O	P	0
			35	24	10	1	
37	S	1	Total	C	O	P	0
			45	34	10	1	
37	Y	1	Total	C	O	P	0
			49	38	10	1	
37	a	1	Total	C	O	P	0
			44	33	10	1	
37	a	1	Total	C	O	P	0
			39	28	10	1	
37	c	1	Total	C	O	P	0
			47	36	10	1	
37	d	1	Total	C	O	P	0
			49	38	10	1	
37	l	1	Total	C	O	P	0
			49	38	10	1	

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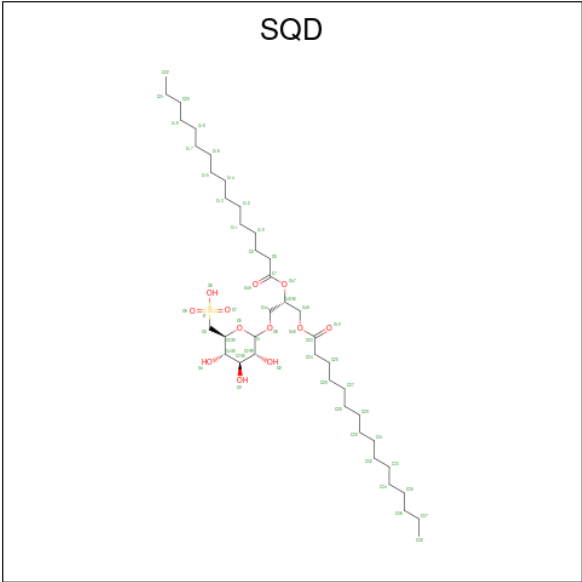
Mol	Chain	Residues	Atoms				AltConf
37	n	1	Total	C	O	P	0
			42	31	10	1	
37	g	1	Total	C	O	P	0
			49	38	10	1	
37	s	1	Total	C	O	P	0
			38	27	10	1	
37	s	1	Total	C	O	P	0
			45	34	10	1	
37	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 38 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



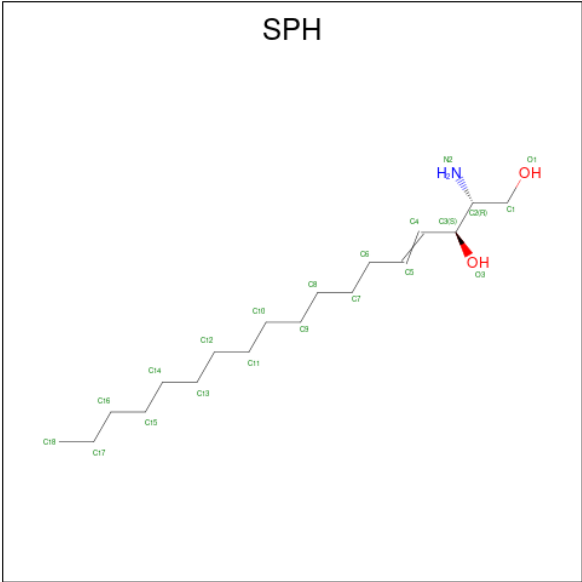
Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			35	24	11	
38	b	1	Total	C	O	0
			35	24	11	

- Molecule 39 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



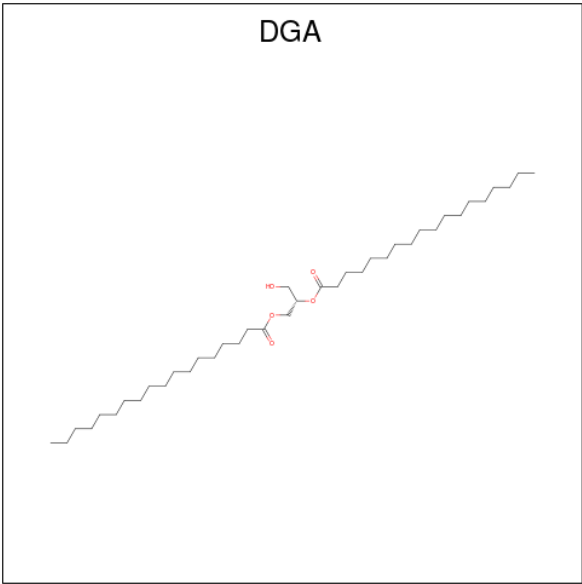
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	O	S	0
			42	29	12	1	
39	C	1	Total	C	O	S	0
			36	23	12	1	
39	L	1	Total	C	O	S	0
			42	29	12	1	
39	M	1	Total	C	O	S	0
			42	29	12	1	
39	a	1	Total	C	O	S	0
			51	38	12	1	
39	b	1	Total	C	O	S	0
			54	41	12	1	
39	c	1	Total	C	O	S	0
			54	41	12	1	
39	l	1	Total	C	O	S	0
			42	29	12	1	
39	m	1	Total	C	O	S	0
			42	29	12	1	
39	o	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 40 is SPHINGOSINE (three-letter code: SPH) (formula: C₁₈H₃₇NO₂).



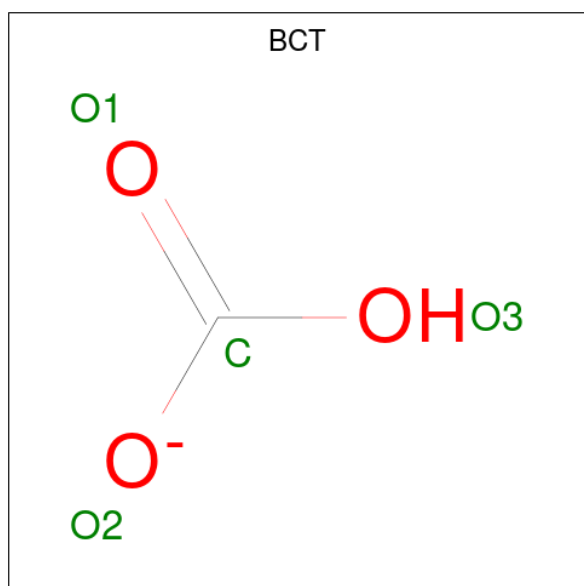
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	N	O	0
			21	18	1	2	
40	I	1	Total	C	N	O	0
			21	18	1	2	
40	c	1	Total	C	N	O	0
			21	18	1	2	
40	i	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 41 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



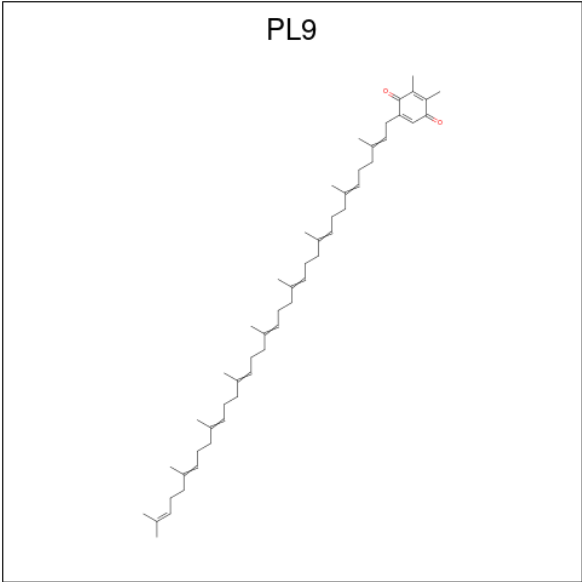
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			37	32	5	
41	J	1	Total	C	O	0
			29	24	5	
41	W	1	Total	C	O	0
			44	39	5	
41	b	1	Total	C	O	0
			44	39	5	
41	j	1	Total	C	O	0
			29	24	5	
41	w	1	Total	C	O	0
			44	39	5	

- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



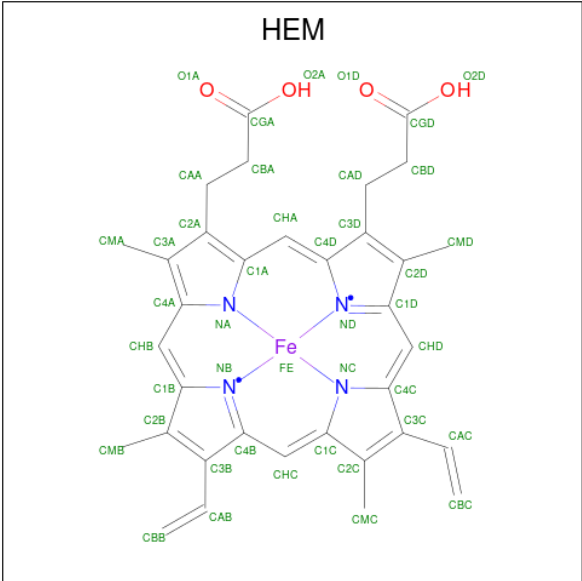
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	a	1	Total	C	O	0
			4	1	3	

- Molecule 43 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: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



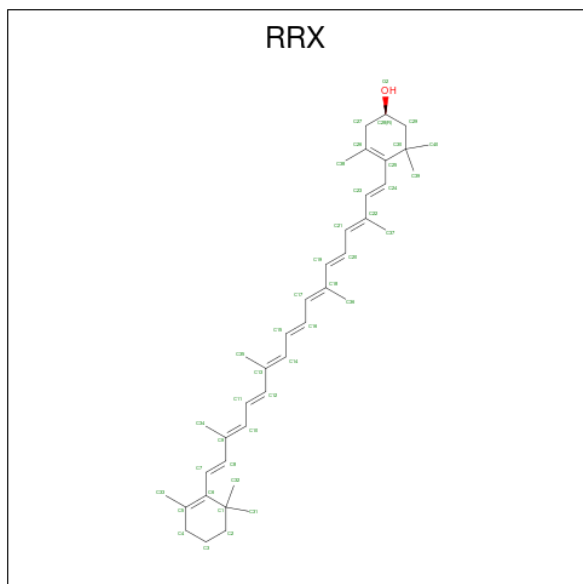
Mol	Chain	Residues	Atoms					AltConf
44	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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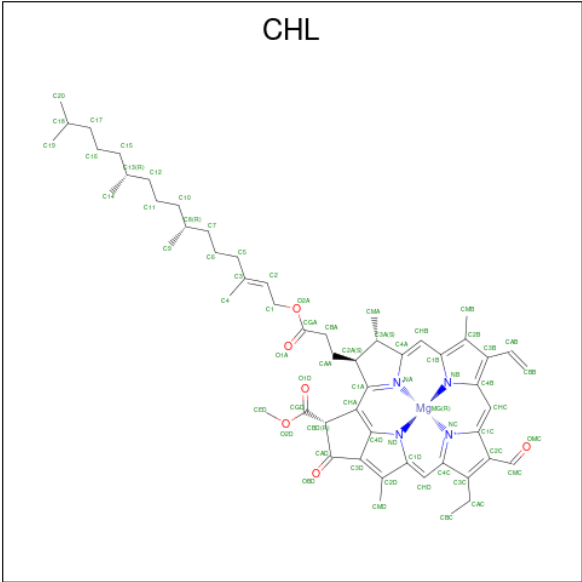
Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 45 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



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

- Molecule 46 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



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		
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	R	1	Total	C	Mg	N	O		0
			44	35	1	4	4		
46	R	1	Total	C	Mg	N	O		0
			50	39	1	4	6		

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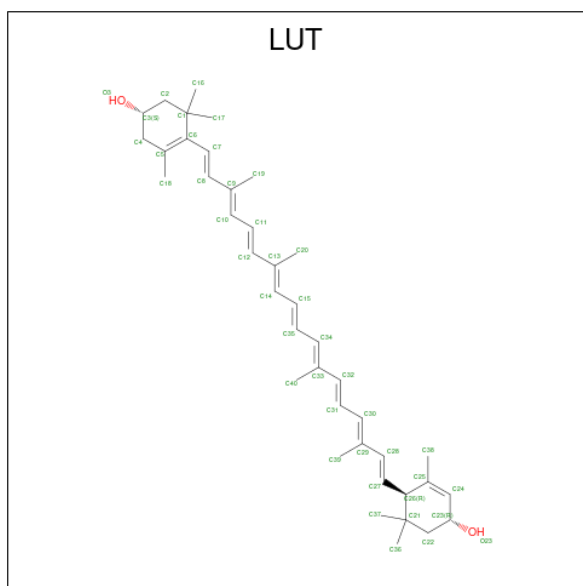
Mol	Chain	Residues	Atoms					AltConf
46	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
46	S	1	Total 61	C 50	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	n	1	Total 50	C 39	Mg 1	N 4	O 6	0
46	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	g	1	Total 48	C 37	Mg 1	N 4	O 6	0
46	g	1	Total 50	C 39	Mg 1	N 4	O 6	0
46	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	g	1	Total 44	C 35	Mg 1	N 4	O 4	0
46	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
46	r	1	Total 44	C 35	Mg 1	N 4	O 4	0

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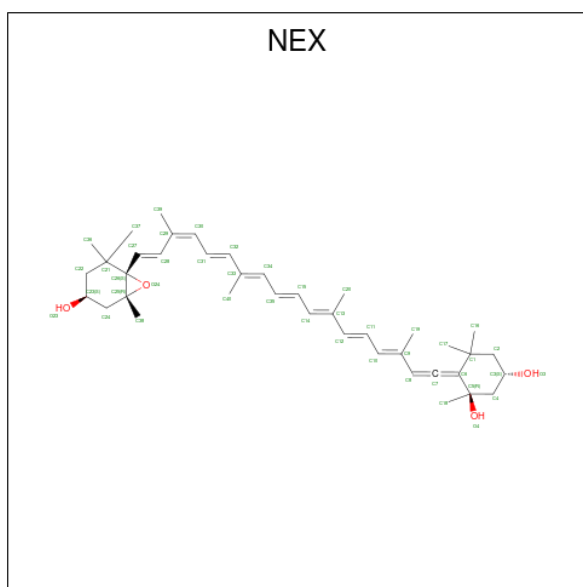
Mol	Chain	Residues	Atoms					AltConf
46	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
46	s	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	y	1	Total	C	Mg	N	O	0
			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
			51	40	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).



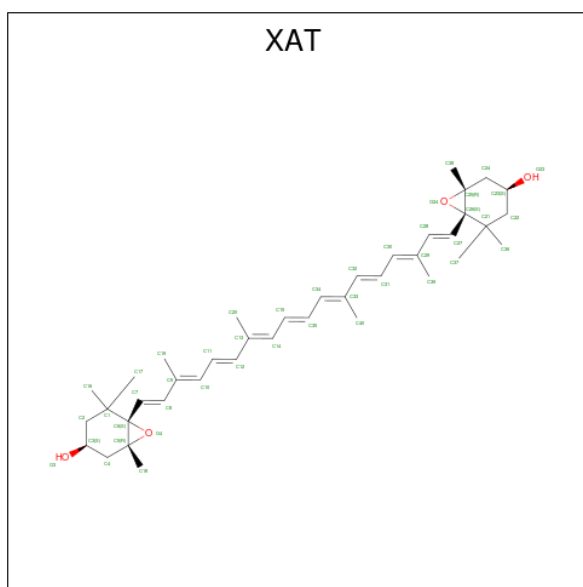
Mol	Chain	Residues	Atoms			AltConf
47	N	1	Total	C	O	0
			42	40	2	
47	N	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	G	1	Total	C	O	0
			42	40	2	
47	R	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	S	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
47	Y	1	Total	C	O	0
			42	40	2	
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	r	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 (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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



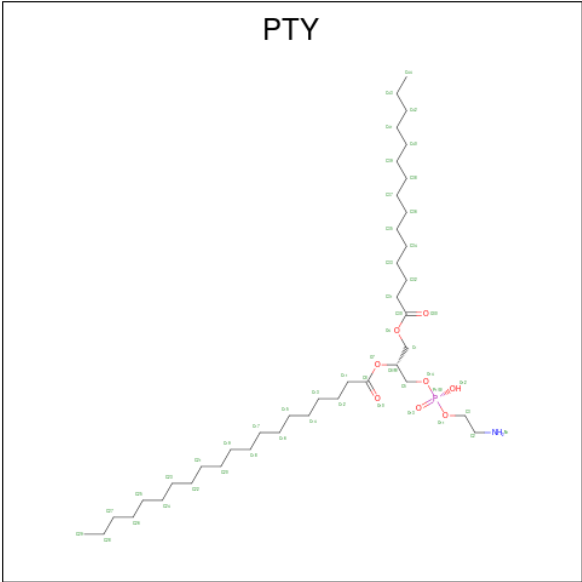
Mol	Chain	Residues	Atoms			AltConf
48	N	1	Total	C	O	0
			44	40	4	
48	G	1	Total	C	O	0
			44	40	4	
48	R	1	Total	C	O	0
			27	25	2	
48	S	1	Total	C	O	0
			44	40	4	
48	Y	1	Total	C	O	0
			44	40	4	
48	n	1	Total	C	O	0
			44	40	4	
48	g	1	Total	C	O	0
			44	40	4	
48	r	1	Total	C	O	0
			27	25	2	
48	s	1	Total	C	O	0
			44	40	4	
48	y	1	Total	C	O	0
			44	40	4	

- Molecule 49 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).



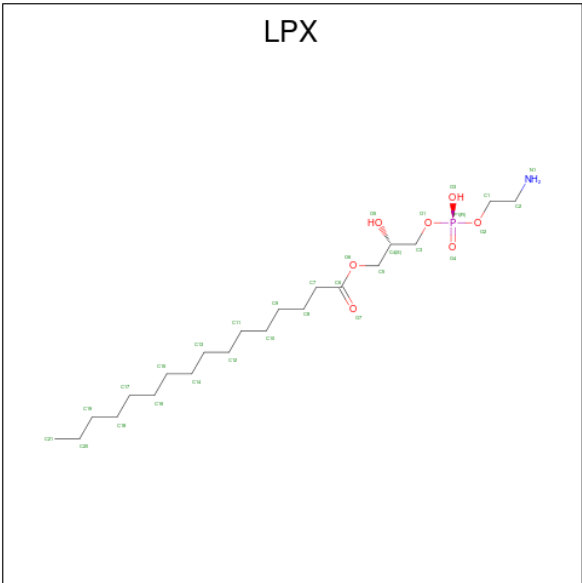
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	R	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	
49	n	1	Total	C	O	0
			44	40	4	
49	g	1	Total	C	O	0
			44	40	4	
49	r	1	Total	C	O	0
			44	40	4	
49	y	1	Total	C	O	0
			44	40	4	

- Molecule 50 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



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

- Molecule 51 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms					AltConf
51	S	1	Total	C	N	O	P	0
			20	11	1	7	1	
51	s	1	Total	C	N	O	P	0
			19	10	1	7	1	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	93	Total	O	0
			93	93	
52	B	144	Total	O	0
			144	144	
52	V	7	Total	O	0
			7	7	
52	C	110	Total	O	0
			110	110	
52	D	74	Total	O	0
			74	74	
52	E	15	Total	O	0
			15	15	
52	F	2	Total	O	0
			2	2	
52	H	13	Total	O	0
			13	13	
52	I	9	Total	O	0
			9	9	
52	J	5	Total	O	0
			5	5	
52	K	9	Total	O	0
			9	9	
52	L	14	Total	O	0
			14	14	
52	M	9	Total	O	0
			9	9	
52	O	75	Total	O	0
			75	75	
52	P	22	Total	O	0
			22	22	
52	T	5	Total	O	0
			5	5	
52	W	9	Total	O	0
			9	9	
52	X	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
52	Z	4	Total 4	O 4	0
52	N	63	Total 63	O 63	0
52	G	60	Total 60	O 60	0
52	R	36	Total 36	O 36	0
52	S	33	Total 33	O 33	0
52	Y	55	Total 55	O 55	0
52	U	8	Total 8	O 8	0
52	a	91	Total 91	O 91	0
52	b	123	Total 123	O 123	0
52	v	3	Total 3	O 3	0
52	c	102	Total 102	O 102	0
52	d	68	Total 68	O 68	0
52	e	23	Total 23	O 23	0
52	f	3	Total 3	O 3	0
52	h	18	Total 18	O 18	0
52	i	11	Total 11	O 11	0
52	j	3	Total 3	O 3	0
52	k	9	Total 9	O 9	0
52	l	8	Total 8	O 8	0
52	m	6	Total 6	O 6	0
52	o	78	Total 78	O 78	0

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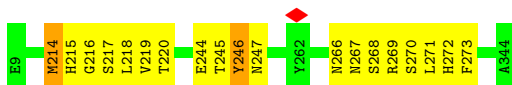
Mol	Chain	Residues	Atoms		AltConf
52	p	64	Total 64	O 64	0
52	t	2	Total 2	O 2	0
52	w	12	Total 12	O 12	0
52	x	9	Total 9	O 9	0
52	z	6	Total 6	O 6	0
52	n	36	Total 36	O 36	0
52	g	33	Total 33	O 33	0
52	r	33	Total 33	O 33	0
52	s	40	Total 40	O 40	0
52	y	61	Total 61	O 61	0
52	u	5	Total 5	O 5	0

3 Residue-property plots [i](#)

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

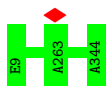
- Molecule 1: Photosystem II protein D1

Chain A:  94% 5%



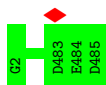
- Molecule 1: Photosystem II protein D1

Chain a:  100%



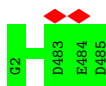
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  100%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  100%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  100%

There are no outlier residues recorded for this chain.

- 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%

There are no outlier residues recorded for this chain.

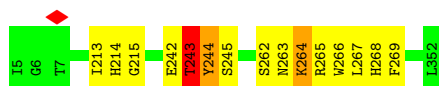
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Photosystem II D2 protein

Chain D:  96%



- Molecule 5: Photosystem II D2 protein

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit alpha

Chain E:  100%

There are no outlier residues recorded for this chain.

- 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:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein H

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein H

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein I

Chain I:  100%



- 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%

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 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:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: Photosystem II reaction center protein M

Chain M:  100%

There are no outlier residues recorded for this chain.

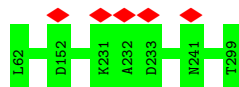
- Molecule 13: Photosystem II reaction center protein M

Chain m:  100%

There are no outlier residues recorded for this chain.

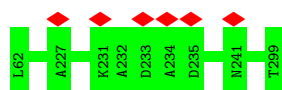
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O:  100%



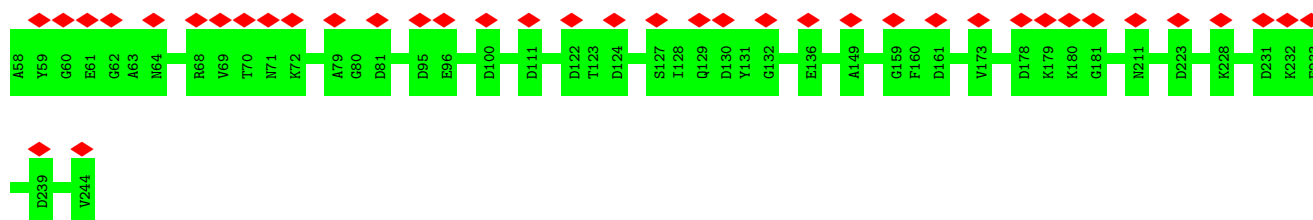
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o:  100%

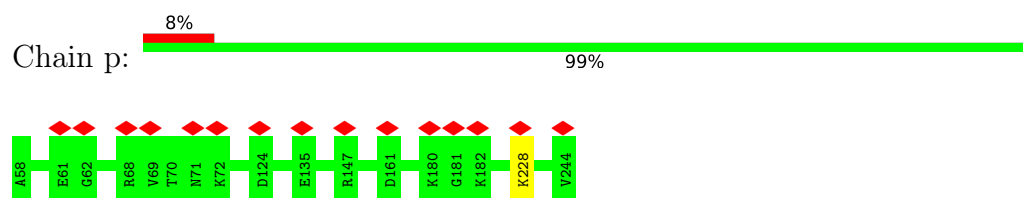


- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P:  21% 100%



- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic



- Molecule 16: Photosystem II reaction center protein T



There are no outlier residues recorded for this chain.

- Molecule 16: Photosystem II reaction center protein T



There are no outlier residues recorded for this chain.

- Molecule 17: PSII 6.1 kDa protein



There are no outlier residues recorded for this chain.

- Molecule 17: PSII 6.1 kDa protein



There are no outlier residues recorded for this chain.

- Molecule 18: Hypothetical protein



There are no outlier residues recorded for this chain.

- Molecule 18: Hypothetical protein



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.

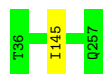
- Molecule 19: Photosystem II reaction center protein Z



There are no outlier residues recorded for this chain.

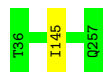
- Molecule 20: Chlorophyll a-b binding protein of LHCII type 3, chloroplastic

Chain N:  100%



- Molecule 20: Chlorophyll a-b binding protein of LHCII type 3, chloroplastic

Chain n:  100%



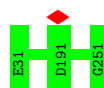
- Molecule 21: Chlorophyll a-b binding protein of LHCII type 2, chloroplastic

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 21: Chlorophyll a-b binding protein of LHCII type 2, chloroplastic

Chain g:  100%



- Molecule 22: Chlorophyll a-b binding protein, chloroplastic, CP29

Chain R:  99%



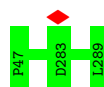
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic, CP29

Chain r:  99%



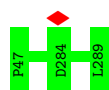
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

Chain S:  100%



- Molecule 23: Chlorophyll a-b binding protein, chloroplastic, CP26

Chain s:  100%



- Molecule 24: Chlorophyll a-b binding protein of LHCII type 1, chloroplastic

Chain Y:  99%



- Molecule 24: Chlorophyll a-b binding protein of LHCII type 1, chloroplastic

Chain y:  100%



- Molecule 25: Photosystem II extrinsic protein U

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: Photosystem II extrinsic protein U

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, C1	Depositor
Number of particles used	39357	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)	800	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	39.371	Depositor
Minimum map value	-16.255	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.5	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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.16	25/2717 (0.9%)	0.76	12/3707 (0.3%)
1	a	0.33	0/2717	0.50	0/3707
2	B	0.31	0/3906	0.50	0/5319
2	b	0.31	0/3906	0.50	0/5319
3	V	0.25	0/228	0.46	0/311
3	v	0.24	0/228	0.47	0/311
4	C	0.30	0/3602	0.49	0/4913
4	c	0.31	0/3602	0.49	0/4913
5	D	1.21	24/2860 (0.8%)	0.70	6/3899 (0.2%)
5	d	0.32	0/2860	0.49	0/3899
6	E	0.29	0/639	0.53	0/870
6	e	0.29	0/639	0.52	0/870
7	F	0.27	0/259	0.49	0/351
7	f	0.26	0/259	0.48	0/351
8	H	0.28	0/513	0.50	0/703
8	h	0.29	0/513	0.48	0/703
9	I	0.32	0/287	0.48	0/386
9	i	0.32	0/287	0.48	0/386
10	J	0.25	0/272	0.43	0/369
10	j	0.26	0/272	0.48	0/369
11	K	0.33	0/308	0.50	0/423
11	k	0.34	0/308	0.53	0/423
12	L	0.31	0/321	0.47	0/435
12	l	0.33	0/321	0.46	0/435
13	M	0.31	0/237	0.49	0/323
13	m	0.30	0/237	0.49	0/323
14	O	0.29	0/1855	0.54	0/2505
14	o	0.29	0/1855	0.55	0/2505
15	P	0.27	0/1473	0.53	0/1988
15	p	0.28	0/1473	0.52	0/1988
16	T	0.34	0/254	0.47	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	t	0.33	0/254	0.46	0/342
17	W	0.27	0/339	0.50	0/460
17	w	0.29	0/339	0.49	0/460
18	X	0.28	0/202	0.43	0/276
18	x	0.27	0/202	0.41	0/276
19	Z	0.26	0/469	0.40	0/641
19	z	0.26	0/469	0.42	0/641
20	N	0.29	0/1751	0.47	0/2386
20	n	0.29	0/1751	0.45	0/2386
21	G	0.27	0/1725	0.47	0/2348
21	g	0.28	0/1725	0.47	0/2348
22	R	0.27	0/1506	0.49	0/2035
22	r	0.27	0/1506	0.48	0/2035
23	S	0.28	0/1903	0.49	0/2590
23	s	0.29	0/1903	0.49	0/2590
24	Y	0.28	0/1715	0.48	1/2338 (0.0%)
24	y	0.29	0/1715	0.46	0/2338
25	U	0.27	0/224	0.58	0/298
25	u	0.35	0/224	0.75	0/298
All	All	0.46	49/59130 (0.1%)	0.52	19/80432 (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
5	D	0	2

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLY	C-O	-22.38	0.87	1.23
5	D	213	ILE	C-O	-18.58	0.88	1.23
5	D	264	LYS	C-O	-18.19	0.88	1.23
5	D	215	GLY	C-O	-18.02	0.94	1.23
5	D	268	HIS	C-O	-17.51	0.90	1.23

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	CB-CA-C	10.48	131.37	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	265	ARG	CB-CA-C	8.16	126.72	110.40
1	A	268	SER	N-CA-CB	-7.84	98.74	110.50
5	D	268	HIS	CB-CA-C	7.76	125.92	110.40
5	D	244	TYR	CA-CB-CG	6.80	126.31	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	243	THR	Mainchain
5	D	244	TYR	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
1	a	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	B	481/484 (99%)	470 (98%)	11 (2%)	0	100	100
2	b	481/484 (99%)	468 (97%)	13 (3%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
4	c	447/449 (100%)	434 (97%)	13 (3%)	0	100	100
5	D	346/348 (99%)	338 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	346/348 (99%)	340 (98%)	6 (2%)	0	100	100
6	E	74/76 (97%)	73 (99%)	1 (1%)	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%)	64 (98%)	1 (2%)	0	100	100
8	h	65/67 (97%)	65 (100%)	0	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	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
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	L	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
14	o	236/238 (99%)	218 (92%)	18 (8%)	0	100	100
15	P	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
16	T	28/30 (93%)	28 (100%)	0	0	100	100
16	t	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	28 (100%)	0	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%)	209 (95%)	10 (4%)	1 (0%)	25	30
20	n	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	25	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	G	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
21	g	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	R	191/196 (97%)	178 (93%)	13 (7%)	0	100	100
22	r	191/196 (97%)	174 (91%)	16 (8%)	1 (0%)	25	30
23	S	241/243 (99%)	228 (95%)	13 (5%)	0	100	100
23	s	241/243 (99%)	220 (91%)	21 (9%)	0	100	100
24	Y	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	25	30
24	y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	25	30
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
All	All	7334/7442 (98%)	7065 (96%)	264 (4%)	5 (0%)	50	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	r	176	LEU
24	y	146	ILE
24	Y	146	ILE
20	n	145	ILE
20	N	145	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	275/275 (100%)	273 (99%)	2 (1%)	81	89
1	a	275/275 (100%)	275 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	387 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	350 (100%)	0	100	100
5	D	279/279 (100%)	277 (99%)	2 (1%)	81	89
5	d	279/279 (100%)	279 (100%)	0	100	100
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
14	O	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
20	n	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
22	R	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
23	S	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
All	All	5934/5934 (100%)	5929 (100%)	5 (0%)	92	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	MET
1	A	246	TYR
5	D	243	THR
5	D	264	LYS
15	p	228	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
20	N	148	GLN
2	b	394	GLN
15	p	71	ASN
19	z	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	0.83	0	1,8,10	0.58	0
2	CSD	b	218	2	3,7,8	0.88	0	1,8,10	0.59	0
22	SEP	R	84	22	8,9,10	1.50	1 (12%)	8,12,14	1.64	2 (25%)
22	SEP	r	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.53	2 (25%)

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	-
22	SEP	R	84	22	-	1/5/8/10	-
22	SEP	r	84	22	-	4/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.35	1.61	1.50
22	r	84	SEP	P-O1P	3.33	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	84	SEP	P-OG-CB	-3.02	109.98	118.30
22	r	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	R	84	SEP	OG-CB-CA	2.94	111.00	108.14
22	r	84	SEP	P-OG-CB	-2.25	112.11	118.30

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	r	84	SEP	N-CA-CB-OG
22	r	84	SEP	CB-OG-P-O1P
22	r	84	SEP	CB-OG-P-O2P
22	r	84	SEP	CB-OG-P-O3P

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 354 ligands modelled in this entry, 8 are monoatomic - leaving 346 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
35	LMG	w	202	-	39,39,55	0.86	2 (5%)	47,47,63	1.05	2 (4%)
46	CHL	N	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.44	10 (19%)
29	CLA	B	505	-	65,73,73	1.00	3 (4%)	76,113,113	1.13	3 (3%)
29	CLA	S	304	-	65,73,73	1.03	4 (6%)	76,113,113	1.18	7 (9%)
48	NEX	G	617	-	38,46,46	3.31	9 (23%)	50,70,70	1.83	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	S	310	23	60,68,73	1.06	3 (5%)	70,107,113	1.08	3 (4%)
29	CLA	N	602	20	65,73,73	1.02	3 (4%)	76,113,113	1.00	5 (6%)
29	CLA	n	602	20	65,73,73	1.02	3 (4%)	76,113,113	1.07	5 (6%)
29	CLA	y	313	37	65,73,73	1.02	3 (4%)	76,113,113	0.96	3 (3%)
26	OEX	A	401	4,52,1	0,15,15	-	-	-		
29	CLA	g	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.09	4 (7%)
46	CHL	y	309	-	66,74,74	0.79	2 (3%)	73,114,114	1.27	11 (15%)
29	CLA	b	509	-	65,73,73	1.02	3 (4%)	76,113,113	1.07	4 (5%)
35	LMG	D	409	-	42,42,55	0.76	2 (4%)	50,50,63	0.97	2 (4%)
48	NEX	S	319	-	38,46,46	3.33	9 (23%)	50,70,70	1.80	13 (26%)
29	CLA	n	603	-	65,73,73	1.01	3 (4%)	76,113,113	1.00	4 (5%)
29	CLA	y	306	52	65,73,73	1.00	3 (4%)	76,113,113	1.11	5 (6%)
46	CHL	G	609	21	66,74,74	0.86	3 (4%)	73,114,114	1.24	12 (16%)
35	LMG	i	101	-	48,48,55	0.99	5 (10%)	56,56,63	1.07	3 (5%)
48	NEX	s	319	-	38,46,46	3.36	9 (23%)	50,70,70	1.67	10 (20%)
29	CLA	s	304	-	65,73,73	1.02	4 (6%)	76,113,113	1.17	5 (6%)
46	CHL	Y	310	24	66,74,74	0.84	3 (4%)	73,114,114	1.27	11 (15%)
47	LUT	g	616	-	42,43,43	2.37	1 (2%)	51,60,60	2.08	12 (23%)
29	CLA	S	312	37	65,73,73	1.02	3 (4%)	76,113,113	1.02	3 (3%)
37	LHG	s	320	29	44,44,48	0.41	0	47,50,54	1.03	3 (6%)
29	CLA	G	604	-	49,57,73	1.19	3 (6%)	55,93,113	1.07	4 (7%)
29	CLA	c	504	-	65,73,73	0.98	3 (4%)	76,113,113	1.05	3 (3%)
29	CLA	N	613	20	65,73,73	1.03	3 (4%)	76,113,113	0.96	2 (2%)
40	SPH	C	525	-	19,20,20	0.63	0	18,21,21	1.08	1 (5%)
26	OEX	a	401	4,52,1	0,15,15	-	-	-		
29	CLA	b	510	52	65,73,73	1.01	3 (4%)	76,113,113	0.92	1 (1%)
33	3PH	b	521	-	38,38,47	0.96	4 (10%)	42,43,52	1.17	2 (4%)
37	LHG	B	523	-	43,43,48	0.41	0	46,49,54	1.02	2 (4%)
29	CLA	a	405	52	65,73,73	1.01	3 (4%)	76,113,113	1.08	6 (7%)
47	LUT	s	317	-	42,43,43	2.36	1 (2%)	51,60,60	1.99	15 (29%)
46	CHL	y	301	-	66,74,74	0.81	2 (3%)	73,114,114	1.26	12 (16%)
36	DGD	C	518	-	52,52,67	1.02	4 (7%)	66,66,81	0.93	2 (3%)
46	CHL	N	606	-	66,74,74	0.92	4 (6%)	73,114,114	1.14	9 (12%)
35	LMG	W	203	-	39,39,55	0.85	2 (5%)	47,47,63	1.16	3 (6%)
46	CHL	n	605	20	66,74,74	0.91	4 (6%)	73,114,114	1.25	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	n	610	-	49,57,73	1.16	3 (6%)	55,93,113	1.04	3 (5%)
29	CLA	s	312	37	65,73,73	1.02	3 (4%)	76,113,113	1.06	4 (5%)
29	CLA	c	513	-	65,73,73	1.01	3 (4%)	76,113,113	1.04	3 (3%)
39	SQD	b	523	-	53,54,54	0.80	0	62,65,65	0.90	2 (3%)
29	CLA	G	611	-	65,73,73	1.02	3 (4%)	76,113,113	1.06	3 (3%)
29	CLA	r	308	22	60,68,73	1.08	3 (5%)	70,107,113	1.04	4 (5%)
29	CLA	b	508	-	65,73,73	0.99	3 (4%)	76,113,113	0.98	1 (1%)
33	3PH	a	415	-	47,47,47	0.85	4 (8%)	51,52,52	1.18	2 (3%)
47	LUT	r	311	-	42,43,43	2.42	2 (4%)	51,60,60	1.94	14 (27%)
29	CLA	y	315	24	65,73,73	1.00	3 (4%)	76,113,113	0.89	1 (1%)
51	LPX	S	321	-	19,19,29	1.20	2 (10%)	21,23,33	1.04	1 (4%)
29	CLA	S	311	23	65,73,73	1.02	3 (4%)	76,113,113	1.05	3 (3%)
51	LPX	s	321	-	18,18,29	1.23	2 (11%)	20,22,33	1.03	1 (5%)
46	CHL	Y	302	24	66,74,74	0.79	2 (3%)	73,114,114	1.22	10 (13%)
29	CLA	y	314	24	65,73,73	1.01	3 (4%)	76,113,113	1.02	3 (3%)
46	CHL	S	302	23	46,54,74	1.06	4 (8%)	49,90,114	1.41	7 (14%)
29	CLA	B	510	52	65,73,73	1.01	3 (4%)	76,113,113	0.93	2 (2%)
39	SQD	M	101	-	41,42,54	0.88	0	50,53,65	0.96	3 (6%)
46	CHL	r	306	-	50,58,74	1.02	3 (6%)	52,94,114	1.44	8 (15%)
49	XAT	N	619	-	39,47,47	0.70	1 (2%)	54,74,74	1.97	12 (22%)
29	CLA	b	507	52	65,73,73	0.99	3 (4%)	76,113,113	1.09	2 (2%)
29	CLA	B	514	-	65,73,73	1.04	3 (4%)	76,113,113	1.08	3 (3%)
46	CHL	y	307	24	46,54,74	1.03	3 (6%)	49,90,114	1.34	8 (16%)
29	CLA	a	406	52	49,57,73	1.15	3 (6%)	55,93,113	1.18	4 (7%)
29	CLA	y	305	-	65,73,73	1.00	3 (4%)	76,113,113	0.96	2 (2%)
29	CLA	B	502	-	65,73,73	1.00	3 (4%)	76,113,113	1.06	2 (2%)
29	CLA	b	506	-	57,65,73	1.07	3 (5%)	66,103,113	1.08	3 (4%)
29	CLA	B	504	-	65,73,73	1.01	3 (4%)	76,113,113	1.21	6 (7%)
29	CLA	s	313	23	45,53,73	1.23	3 (6%)	52,89,113	1.12	3 (5%)
29	CLA	b	514	-	65,73,73	1.03	3 (4%)	76,113,113	1.04	4 (5%)
29	CLA	r	309	22	60,68,73	1.07	3 (5%)	70,107,113	1.17	5 (7%)
29	CLA	S	303	23	60,68,73	1.06	3 (5%)	70,107,113	0.99	4 (5%)
29	CLA	r	304	-	49,57,73	1.15	3 (6%)	55,93,113	1.03	2 (3%)
29	CLA	y	312	24	65,73,73	1.00	4 (6%)	76,113,113	1.11	4 (5%)
29	CLA	s	316	23	50,58,73	1.16	3 (6%)	58,95,113	1.21	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LHG	c	521	-	46,46,48	0.40	0	49,52,54	1.03	2 (4%)
29	CLA	A	406	52	65,73,73	1.02	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	B	503	-	65,73,73	0.99	3 (4%)	76,113,113	1.12	5 (6%)
29	CLA	R	301	22	60,68,73	1.06	3 (5%)	70,107,113	1.09	4 (5%)
29	CLA	C	506	-	60,68,73	1.07	4 (6%)	70,107,113	1.04	2 (2%)
35	LMG	d	408	-	48,48,55	0.99	4 (8%)	56,56,63	1.11	2 (3%)
35	LMG	c	519	-	51,51,55	1.06	6 (11%)	59,59,63	1.11	3 (5%)
29	CLA	G	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.94	3 (3%)
37	LHG	N	618	29	48,48,48	0.39	0	51,54,54	1.05	4 (7%)
46	CHL	g	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.36	14 (19%)
49	XAT	y	302	-	39,47,47	0.73	1 (2%)	54,74,74	2.03	13 (24%)
31	BCR	f	101	-	41,41,41	1.82	4 (9%)	56,56,56	4.27	17 (30%)
46	CHL	N	601	20	66,74,74	0.82	3 (4%)	73,114,114	1.23	10 (13%)
36	DGD	c	518	-	60,60,67	1.06	6 (10%)	74,74,81	0.95	2 (2%)
48	NEX	y	319	-	38,46,46	3.31	11 (28%)	50,70,70	1.82	13 (26%)
29	CLA	r	310	-	51,59,73	1.17	3 (5%)	59,96,113	1.24	5 (8%)
36	DGD	c	516	-	56,56,67	0.98	4 (7%)	70,70,81	0.94	2 (2%)
29	CLA	s	303	23	60,68,73	1.05	3 (5%)	70,107,113	1.14	3 (4%)
29	CLA	G	612	21	43,51,73	1.22	3 (6%)	49,86,113	1.06	3 (6%)
46	CHL	y	311	24	66,74,74	0.86	3 (4%)	73,114,114	1.35	12 (16%)
48	NEX	N	617	-	38,46,46	3.33	9 (23%)	50,70,70	1.61	11 (22%)
29	CLA	g	603	-	65,73,73	1.01	3 (4%)	76,113,113	0.98	3 (3%)
29	CLA	C	505	52	55,63,73	1.08	3 (5%)	64,101,113	1.07	2 (3%)
47	LUT	Y	317	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
46	CHL	n	601	20	66,74,74	0.84	3 (4%)	73,114,114	1.25	9 (12%)
29	CLA	a	408	-	60,68,73	1.03	3 (5%)	70,107,113	1.11	5 (7%)
29	CLA	b	504	-	65,73,73	1.02	4 (6%)	76,113,113	1.22	5 (6%)
36	DGD	B	521	-	44,44,67	0.86	1 (2%)	58,58,81	1.15	5 (8%)
31	BCR	v	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	19 (33%)
39	SQD	m	101	-	41,42,54	0.89	0	50,53,65	0.96	3 (6%)
29	CLA	c	505	-	65,73,73	1.02	4 (6%)	76,113,113	1.08	3 (3%)
29	CLA	n	613	-	49,57,73	1.17	3 (6%)	55,93,113	1.20	3 (5%)
47	LUT	g	615	-	42,43,43	2.33	1 (2%)	51,60,60	1.96	13 (25%)
29	CLA	b	513	-	65,73,73	1.01	3 (4%)	76,113,113	0.97	2 (2%)
29	CLA	g	612	21	43,51,73	1.20	3 (6%)	49,86,113	1.11	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	513	-	65,73,73	1.01	3 (4%)	76,113,113	0.95	2 (2%)
46	CHL	n	607	-	50,58,74	0.93	2 (4%)	52,94,114	1.44	11 (21%)
48	NEX	R	312	-	24,28,46	3.24	6 (25%)	32,42,70	1.76	7 (21%)
29	CLA	B	506	-	65,73,73	1.02	3 (4%)	76,113,113	1.05	4 (5%)
46	CHL	s	308	-	43,51,74	1.09	3 (6%)	45,86,114	1.45	7 (15%)
29	CLA	g	611	37	65,73,73	1.02	3 (4%)	76,113,113	1.00	2 (2%)
31	BCR	b	517	-	41,41,41	1.85	4 (9%)	56,56,56	4.22	15 (26%)
31	BCR	z	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	13 (23%)
29	CLA	r	302	22	60,68,73	1.05	3 (5%)	70,107,113	1.11	4 (5%)
47	LUT	y	318	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	13 (25%)
29	CLA	B	516	-	55,63,73	1.10	4 (7%)	64,101,113	1.08	3 (4%)
31	BCR	B	517	-	41,41,41	1.86	5 (12%)	56,56,56	4.22	19 (33%)
39	SQD	L	102	-	41,42,54	0.87	0	50,53,65	0.96	3 (6%)
47	LUT	Y	316	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	15 (29%)
46	CHL	g	606	-	50,58,74	1.06	4 (8%)	52,94,114	1.38	10 (19%)
29	CLA	C	504	-	65,73,73	1.03	3 (4%)	76,113,113	0.91	3 (3%)
29	CLA	S	315	-	50,58,73	1.16	3 (6%)	58,95,113	1.11	3 (5%)
35	LMG	c	520	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
45	RRX	h	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.50	23 (40%)
29	CLA	D	405	-	60,68,73	1.07	3 (5%)	70,107,113	1.14	4 (5%)
43	PL9	d	405	-	55,55,55	1.28	5 (9%)	68,69,69	1.51	11 (16%)
31	BCR	C	515	-	41,41,41	1.82	4 (9%)	56,56,56	4.21	14 (25%)
35	LMG	C	522	-	55,55,55	1.12	6 (10%)	63,63,63	1.04	2 (3%)
39	SQD	c	522	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	d	403	-	65,73,73	1.01	4 (6%)	76,113,113	1.03	2 (2%)
29	CLA	C	503	-	65,73,73	1.01	3 (4%)	76,113,113	1.09	3 (3%)
29	CLA	n	604	-	65,73,73	1.00	3 (4%)	76,113,113	0.96	3 (3%)
37	LHG	S	301	-	34,34,48	0.44	0	37,40,54	1.17	2 (5%)
29	CLA	R	302	-	60,68,73	1.09	4 (6%)	70,107,113	1.11	5 (7%)
29	CLA	R	307	22	46,54,73	1.19	3 (6%)	53,90,113	1.19	4 (7%)
29	CLA	S	306	23	50,58,73	1.15	3 (6%)	58,95,113	1.32	3 (5%)
46	CHL	N	605	20	66,74,74	0.86	3 (4%)	73,114,114	1.21	7 (9%)
41	DGA	W	202	-	43,43,43	1.12	3 (6%)	45,45,45	1.49	3 (6%)
29	CLA	N	610	-	65,73,73	1.01	3 (4%)	76,113,113	1.11	3 (3%)
29	CLA	c	510	-	65,73,73	1.00	3 (4%)	76,113,113	0.99	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	g	602	21	65,73,73	1.03	3 (4%)	76,113,113	0.99	3 (3%)
29	CLA	C	513	-	65,73,73	1.02	3 (4%)	76,113,113	0.91	3 (3%)
29	CLA	s	310	-	60,68,73	1.05	3 (5%)	70,107,113	1.08	3 (4%)
29	CLA	N	614	-	49,57,73	1.16	3 (6%)	55,93,113	1.05	4 (7%)
46	CHL	S	308	-	43,51,74	1.03	3 (6%)	45,86,114	1.47	9 (20%)
29	CLA	y	310	-	50,58,73	1.16	3 (6%)	58,95,113	1.08	3 (5%)
29	CLA	b	512	-	65,73,73	1.00	3 (4%)	76,113,113	1.01	2 (2%)
29	CLA	S	313	23	45,53,73	1.23	3 (6%)	52,89,113	1.03	4 (7%)
29	CLA	r	303	-	60,68,73	1.09	4 (6%)	70,107,113	1.11	7 (10%)
47	LUT	n	614	-	42,43,43	2.36	1 (2%)	51,60,60	1.89	12 (23%)
46	CHL	R	305	-	50,58,74	1.02	3 (6%)	52,94,114	1.39	9 (17%)
35	LMG	B	520	-	44,44,55	0.86	3 (6%)	52,52,63	1.08	3 (5%)
48	NEX	n	616	-	38,46,46	3.36	9 (23%)	50,70,70	1.60	10 (20%)
29	CLA	Y	305	52	65,73,73	1.00	3 (4%)	76,113,113	0.99	5 (6%)
38	LMT	B	524	-	36,36,36	1.22	5 (13%)	47,47,47	1.18	5 (10%)
29	CLA	n	611	20	45,53,73	1.23	3 (6%)	52,89,113	1.10	4 (7%)
29	CLA	c	501	-	65,73,73	1.02	3 (4%)	76,113,113	1.02	5 (6%)
44	HEM	E	101	7,6	41,50,50	1.45	3 (7%)	45,82,82	1.36	5 (11%)
35	LMG	d	407	-	46,46,55	0.91	3 (6%)	54,54,63	1.05	2 (3%)
48	NEX	r	313	-	24,28,46	3.23	6 (25%)	32,42,70	1.83	7 (21%)
29	CLA	c	502	-	65,73,73	1.01	3 (4%)	76,113,113	1.09	4 (5%)
29	CLA	n	612	20	65,73,73	1.01	3 (4%)	76,113,113	0.96	2 (2%)
29	CLA	A	409	-	60,68,73	1.04	3 (5%)	70,107,113	1.10	4 (5%)
37	LHG	s	301	-	37,37,48	0.44	0	40,43,54	1.16	3 (7%)
29	CLA	R	309	-	50,58,73	1.17	3 (6%)	58,95,113	1.08	4 (6%)
29	CLA	R	303	-	49,57,73	1.16	3 (6%)	55,93,113	1.03	1 (1%)
29	CLA	N	612	20	45,53,73	1.22	3 (6%)	52,89,113	1.03	4 (7%)
33	3PH	B	522	-	47,47,47	0.86	4 (8%)	51,52,52	1.11	2 (3%)
31	BCR	C	516	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	14 (25%)
41	DGA	D	402	-	36,36,43	1.19	2 (5%)	38,38,45	1.30	3 (7%)
46	CHL	N	609	20	66,74,74	0.85	3 (4%)	73,114,114	1.24	11 (15%)
29	CLA	B	509	-	65,73,73	1.02	4 (6%)	76,113,113	1.05	3 (3%)
37	LHG	l	102	-	48,48,48	0.40	0	51,54,54	1.00	2 (3%)
46	CHL	Y	308	-	66,74,74	0.77	2 (3%)	73,114,114	1.23	10 (13%)
46	CHL	G	607	-	66,74,74	0.78	2 (3%)	73,114,114	1.26	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	CHL	y	303	24	66,74,74	0.89	3 (4%)	73,114,114	1.19	10 (13%)
29	CLA	C	502	-	65,73,73	1.02	3 (4%)	76,113,113	0.99	4 (5%)
29	CLA	N	603	-	65,73,73	1.03	3 (4%)	76,113,113	0.89	3 (3%)
46	CHL	g	608	-	44,52,74	1.06	3 (6%)	46,87,114	1.46	10 (21%)
46	CHL	g	609	21	66,74,74	0.90	3 (4%)	73,114,114	1.20	11 (15%)
29	CLA	c	507	52	65,73,73	1.03	4 (6%)	76,113,113	1.10	4 (5%)
29	CLA	B	512	-	65,73,73	1.00	3 (4%)	76,113,113	1.05	2 (2%)
46	CHL	G	605	21	48,56,74	0.98	3 (6%)	51,92,114	1.39	8 (15%)
29	CLA	a	404	-	65,73,73	1.03	3 (4%)	76,113,113	1.18	5 (6%)
46	CHL	G	606	-	50,58,74	1.03	4 (8%)	52,94,114	1.41	9 (17%)
36	DGD	C	519	-	54,54,67	1.00	4 (7%)	68,68,81	0.91	3 (4%)
41	DGA	b	522	-	43,43,43	1.11	2 (4%)	45,45,45	1.52	3 (6%)
42	BCT	D	403	27	2,3,3	1.29	0	2,3,3	1.23	0
46	CHL	y	308	52	51,59,74	0.97	3 (5%)	55,96,114	1.39	11 (20%)
47	LUT	n	615	-	42,43,43	2.32	1 (2%)	51,60,60	1.81	12 (23%)
49	XAT	R	311	-	39,47,47	0.67	1 (2%)	54,74,74	1.87	13 (24%)
46	CHL	Y	306	24	46,54,74	1.03	3 (6%)	49,90,114	1.34	9 (18%)
46	CHL	s	302	23	46,54,74	1.05	4 (8%)	49,90,114	1.41	9 (18%)
29	CLA	C	508	52	65,73,73	1.02	3 (4%)	76,113,113	1.10	3 (3%)
29	CLA	b	515	-	65,73,73	1.01	3 (4%)	76,113,113	0.91	2 (2%)
31	BCR	a	409	-	41,41,41	1.83	5 (12%)	56,56,56	4.25	15 (26%)
48	NEX	Y	318	-	38,46,46	3.31	9 (23%)	50,70,70	1.84	11 (22%)
29	CLA	c	508	-	65,73,73	1.02	3 (4%)	76,113,113	1.04	4 (5%)
46	CHL	g	601	21	66,74,74	0.85	3 (4%)	73,114,114	1.24	11 (15%)
29	CLA	b	511	-	65,73,73	1.03	3 (4%)	76,113,113	1.08	4 (5%)
47	LUT	R	310	-	42,43,43	2.38	1 (2%)	51,60,60	2.01	14 (27%)
29	CLA	Y	313	24	65,73,73	1.02	3 (4%)	76,113,113	0.95	3 (3%)
37	LHG	n	617	-	41,41,48	0.41	0	44,47,54	1.15	4 (9%)
29	CLA	d	404	-	65,73,73	1.02	3 (4%)	76,113,113	1.09	5 (6%)
29	CLA	c	506	-	60,68,73	1.05	3 (5%)	70,107,113	1.10	5 (7%)
37	LHG	G	618	-	48,48,48	0.38	0	51,54,54	1.07	3 (5%)
29	CLA	g	610	21	65,73,73	1.01	4 (6%)	76,113,113	1.25	5 (6%)
29	CLA	B	508	-	65,73,73	1.00	3 (4%)	76,113,113	0.95	2 (2%)
44	HEM	e	101	7,6	41,50,50	1.44	4 (9%)	45,82,82	1.30	4 (8%)
49	XAT	Y	301	-	39,47,47	0.71	1 (2%)	54,74,74	2.00	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	CHL	r	305	-	44,52,74	1.07	3 (6%)	46,87,114	1.35	8 (17%)
40	SPH	i	102	-	19,20,20	0.65	0	18,21,21	1.08	1 (5%)
41	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
29	CLA	n	609	20	65,73,73	1.03	4 (6%)	76,113,113	1.16	6 (7%)
29	CLA	c	509	-	65,73,73	1.03	3 (4%)	76,113,113	1.06	4 (5%)
29	CLA	C	512	4	65,73,73	1.04	3 (4%)	76,113,113	0.96	2 (2%)
29	CLA	S	314	23	55,63,73	1.12	3 (5%)	64,101,113	1.14	3 (4%)
37	LHG	S	320	29	44,44,48	0.41	0	47,50,54	1.04	3 (6%)
47	LUT	y	317	-	42,43,43	2.38	1 (2%)	51,60,60	1.87	13 (25%)
33	3PH	S	322	-	29,29,47	1.09	4 (13%)	33,34,52	1.24	2 (6%)
47	LUT	G	615	-	42,43,43	2.37	1 (2%)	51,60,60	1.92	13 (25%)
35	LMG	C	524	-	42,42,55	0.78	2 (4%)	50,50,63	1.17	4 (8%)
36	DGD	C	520	-	54,54,67	0.93	4 (7%)	68,68,81	0.90	2 (2%)
49	XAT	r	312	-	39,47,47	0.67	1 (2%)	54,74,74	1.89	11 (20%)
29	CLA	D	404	-	65,73,73	3.48	25 (38%)	76,113,113	3.77	31 (40%)
46	CHL	n	608	20	66,74,74	0.82	2 (3%)	73,114,114	1.31	12 (16%)
46	CHL	g	605	21	48,56,74	1.00	3 (6%)	51,92,114	1.31	9 (17%)
29	CLA	Y	309	52	50,58,73	1.15	3 (6%)	58,95,113	1.09	3 (5%)
29	CLA	C	509	-	65,73,73	1.01	3 (4%)	76,113,113	1.08	5 (6%)
29	CLA	b	503	-	65,73,73	1.00	3 (4%)	76,113,113	1.12	3 (3%)
29	CLA	G	613	21	65,73,73	1.01	3 (4%)	76,113,113	0.91	1 (1%)
34	C7Z	B	519	-	43,43,43	5.30	27 (62%)	58,60,60	2.46	23 (39%)
31	BCR	K	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	15 (26%)
29	CLA	R	308	22	60,68,73	1.06	3 (5%)	70,107,113	1.08	4 (5%)
29	CLA	y	316	-	65,73,73	1.03	3 (4%)	76,113,113	1.02	5 (6%)
47	LUT	S	317	-	42,43,43	2.25	1 (2%)	51,60,60	1.85	10 (19%)
35	LMG	b	520	-	44,44,55	0.86	2 (4%)	52,52,63	1.07	2 (3%)
41	DGA	J	101	-	28,28,43	1.29	3 (10%)	30,30,45	1.24	2 (6%)
29	CLA	N	604	-	65,73,73	1.01	3 (4%)	76,113,113	1.02	4 (5%)
29	CLA	c	503	-	65,73,73	1.03	3 (4%)	76,113,113	0.95	4 (5%)
37	LHG	Y	319	29	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
30	PHO	d	402	-	51,69,69	0.97	3 (5%)	47,99,99	1.25	5 (10%)
47	LUT	N	615	-	42,43,43	2.36	1 (2%)	51,60,60	1.88	13 (25%)
29	CLA	B	515	-	65,73,73	1.00	3 (4%)	76,113,113	0.89	2 (2%)
29	CLA	C	514	-	65,73,73	1.02	3 (4%)	76,113,113	1.03	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LHG	D	407	-	48,48,48	0.40	0	51,54,54	1.00	3 (5%)
29	CLA	Y	311	24	65,73,73	1.01	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	s	315	-	55,63,73	1.10	3 (5%)	64,101,113	1.03	3 (4%)
29	CLA	B	507	52	65,73,73	0.99	3 (4%)	76,113,113	1.01	3 (3%)
46	CHL	s	309	-	61,69,74	0.88	3 (4%)	67,108,114	1.26	10 (14%)
41	DGA	w	201	-	43,43,43	1.12	3 (6%)	45,45,45	1.50	3 (6%)
29	CLA	C	510	-	65,73,73	1.03	3 (4%)	76,113,113	1.04	4 (5%)
31	BCR	c	515	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	20 (35%)
39	SQD	C	501	-	41,42,54	0.87	0	50,53,65	0.99	2 (4%)
31	BCR	F	101	-	41,41,41	1.84	4 (9%)	56,56,56	4.13	14 (25%)
29	CLA	s	306	23	50,58,73	1.14	3 (6%)	58,95,113	1.24	6 (10%)
29	CLA	G	602	21	65,73,73	1.04	3 (4%)	76,113,113	0.96	3 (3%)
46	CHL	Y	307	-	66,74,74	0.94	4 (6%)	73,114,114	1.15	9 (12%)
29	CLA	Y	304	-	65,73,73	1.02	3 (4%)	76,113,113	0.93	2 (2%)
29	CLA	Y	315	-	65,73,73	1.02	3 (4%)	76,113,113	1.03	3 (3%)
36	DGD	c	517	-	63,63,67	1.11	7 (11%)	77,77,81	0.94	3 (3%)
46	CHL	N	607	-	66,74,74	0.89	3 (4%)	73,114,114	1.25	12 (16%)
29	CLA	b	505	-	65,73,73	1.01	3 (4%)	76,113,113	1.14	4 (5%)
43	PL9	D	406	-	55,55,55	1.34	6 (10%)	68,69,69	1.47	11 (16%)
29	CLA	c	512	-	65,73,73	1.02	3 (4%)	76,113,113	0.95	3 (3%)
29	CLA	b	501	-	65,73,73	1.01	3 (4%)	76,113,113	0.97	4 (5%)
46	CHL	n	606	-	66,74,74	0.95	3 (4%)	73,114,114	1.12	7 (9%)
34	C7Z	b	519	-	43,43,43	5.29	27 (62%)	58,60,60	2.41	24 (41%)
37	LHG	D	408	-	38,38,48	0.42	0	41,44,54	1.04	2 (4%)
47	LUT	S	318	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	12 (23%)
33	3PH	s	322	-	47,47,47	0.86	4 (8%)	51,52,52	1.10	2 (3%)
29	CLA	b	502	-	65,73,73	1.00	3 (4%)	76,113,113	1.01	3 (3%)
29	CLA	b	516	-	65,73,73	1.01	4 (6%)	76,113,113	0.98	3 (3%)
29	CLA	s	311	23	65,73,73	1.01	4 (6%)	76,113,113	1.12	5 (6%)
39	SQD	l	101	-	41,42,54	0.88	0	50,53,65	1.00	3 (6%)
29	CLA	S	316	23	50,58,73	1.18	3 (6%)	58,95,113	1.27	6 (10%)
46	CHL	S	307	-	44,52,74	1.08	3 (6%)	46,87,114	1.34	7 (15%)
30	PHO	a	407	-	51,69,69	0.99	4 (7%)	47,99,99	1.22	5 (10%)
42	BCT	a	412	27	2,3,3	0.31	0	2,3,3	5.05	2 (100%)
46	CHL	R	304	-	44,52,74	1.05	3 (6%)	46,87,114	1.34	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	CHL	s	307	-	44,52,74	0.98	2 (4%)	46,87,114	1.45	8 (17%)
39	SQD	o	301	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
29	CLA	B	511	-	65,73,73	1.02	3 (4%)	76,113,113	1.11	5 (6%)
37	LHG	g	618	29	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
48	NEX	g	617	-	38,46,46	3.29	9 (23%)	50,70,70	1.87	13 (26%)
39	SQD	a	410	-	50,51,54	0.81	0	59,62,65	0.93	2 (3%)
31	BCR	A	410	-	41,41,41	1.84	5 (12%)	56,56,56	4.27	15 (26%)
45	RRX	H	101	-	42,42,42	4.88	24 (57%)	57,58,58	2.58	22 (38%)
29	CLA	Y	312	37	65,73,73	1.01	3 (4%)	76,113,113	1.01	6 (7%)
29	CLA	C	507	-	65,73,73	1.01	3 (4%)	76,113,113	0.94	3 (3%)
29	CLA	Y	314	24	65,73,73	1.01	3 (4%)	76,113,113	0.88	1 (1%)
47	LUT	G	616	-	42,43,43	2.34	1 (2%)	51,60,60	1.93	11 (21%)
40	SPH	I	101	-	19,20,20	0.64	0	18,21,21	1.07	1 (5%)
31	BCR	B	518	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
46	CHL	G	608	-	44,52,74	1.08	3 (6%)	46,87,114	1.40	8 (17%)
38	LMT	b	524	-	36,36,36	1.24	6 (16%)	47,47,47	1.16	4 (8%)
49	XAT	G	619	-	39,47,47	0.68	1 (2%)	54,74,74	3.75	20 (37%)
29	CLA	Y	303	24	65,73,73	1.02	3 (4%)	76,113,113	1.04	4 (5%)
31	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	18 (32%)
29	CLA	y	304	24	65,73,73	1.02	3 (4%)	76,113,113	1.10	4 (5%)
29	CLA	B	501	-	65,73,73	1.02	3 (4%)	76,113,113	0.99	4 (5%)
37	LHG	L	101	-	48,48,48	0.38	0	51,54,54	1.23	3 (5%)
29	CLA	A	405	-	65,73,73	1.01	3 (4%)	76,113,113	1.05	4 (5%)
29	CLA	G	614	-	49,57,73	1.17	3 (6%)	55,93,113	1.02	2 (3%)
37	LHG	y	320	29	48,48,48	0.38	0	51,54,54	1.11	4 (7%)
50	PTY	N	620	-	49,49,49	0.87	4 (8%)	52,54,54	1.05	2 (3%)
50	PTY	Y	320	-	18,18,49	1.29	3 (16%)	21,23,54	1.45	2 (9%)
29	CLA	c	511	4	65,73,73	1.01	3 (4%)	76,113,113	1.09	3 (3%)
39	SQD	C	523	-	35,36,54	0.94	0	44,47,65	1.04	2 (4%)
29	CLA	G	610	21	65,73,73	1.02	3 (4%)	76,113,113	1.21	5 (6%)
29	CLA	g	613	21	65,73,73	1.01	3 (4%)	76,113,113	0.95	2 (2%)
29	CLA	R	306	-	60,68,73	1.06	4 (6%)	70,107,113	1.04	3 (4%)
37	LHG	d	406	-	48,48,48	0.39	0	51,54,54	1.00	3 (5%)
29	CLA	g	604	-	49,57,73	1.16	3 (6%)	55,93,113	1.11	3 (5%)
30	PHO	A	408	-	51,69,69	0.98	4 (7%)	47,99,99	1.20	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	LUT	s	318	-	42,43,43	2.29	1 (2%)	51,60,60	1.92	12 (23%)
35	LMG	W	201	-	40,40,55	0.76	2 (5%)	48,48,63	1.15	4 (8%)
33	3PH	A	412	-	47,47,47	0.84	3 (6%)	51,52,52	1.12	2 (3%)
47	LUT	N	616	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	12 (23%)
49	XAT	g	619	-	39,47,47	0.70	1 (2%)	54,74,74	3.73	17 (31%)
46	CHL	G	601	21	66,74,74	0.85	3 (4%)	73,114,114	1.26	10 (13%)
37	LHG	a	414	-	38,38,48	0.41	0	41,44,54	1.09	2 (4%)
36	DGD	r	301	-	44,44,67	0.86	1 (2%)	58,58,81	1.19	5 (8%)
37	LHG	a	413	-	43,43,48	0.41	0	46,49,54	1.05	2 (4%)
31	BCR	c	514	-	41,41,41	1.82	5 (12%)	56,56,56	4.17	19 (33%)
46	CHL	S	309	-	61,69,74	0.90	3 (4%)	67,108,114	1.36	12 (17%)
29	CLA	s	314	23	55,63,73	1.11	3 (5%)	64,101,113	1.10	3 (4%)
35	LMG	D	410	-	48,48,55	0.99	4 (8%)	56,56,63	1.08	2 (3%)
29	CLA	C	511	-	65,73,73	1.00	3 (4%)	76,113,113	0.95	3 (3%)
29	CLA	N	611	37	49,57,73	1.17	3 (6%)	55,93,113	1.09	3 (5%)
29	CLA	S	305	-	55,63,73	1.11	3 (5%)	64,101,113	1.07	2 (3%)
29	CLA	s	305	-	55,63,73	1.10	3 (5%)	64,101,113	1.20	3 (4%)
30	PHO	D	401	-	51,69,69	0.97	3 (5%)	47,99,99	1.20	4 (8%)
49	XAT	n	618	-	39,47,47	0.73	1 (2%)	54,74,74	1.99	13 (24%)
29	CLA	A	407	-	50,58,73	1.15	3 (6%)	58,95,113	1.09	4 (6%)
31	BCR	b	518	-	41,41,41	1.85	5 (12%)	56,56,56	4.12	15 (26%)
40	SPH	c	523	-	19,20,20	0.65	0	18,21,21	1.10	1 (5%)
29	CLA	r	307	-	60,68,73	1.06	4 (6%)	70,107,113	1.10	4 (5%)
35	LMG	C	521	-	47,47,55	0.96	4 (8%)	55,55,63	1.12	4 (7%)
50	PTY	y	321	-	18,18,49	1.30	3 (16%)	21,23,54	1.42	2 (9%)
50	PTY	n	619	-	49,49,49	0.88	4 (8%)	52,54,54	1.05	2 (3%)

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
35	LMG	w	202	-	-	17/34/54/70	0/1/1/1
46	CHL	N	608	-	3/3/16/26	5/20/118/137	-
29	CLA	B	505	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	S	304	-	1/1/15/20	17/37/115/115	-
48	NEX	G	617	-	-	4/27/83/83	0/3/3/3
29	CLA	S	310	23	1/1/14/20	9/31/109/115	-
29	CLA	N	602	20	1/1/15/20	14/37/115/115	-
29	CLA	n	602	20	1/1/15/20	11/37/115/115	-
29	CLA	y	313	37	1/1/15/20	6/37/115/115	-
29	CLA	g	614	-	1/1/11/20	9/18/96/115	-
46	CHL	y	309	-	4/4/20/26	12/39/137/137	-
29	CLA	b	509	-	1/1/15/20	5/37/115/115	-
35	LMG	D	409	-	-	3/37/57/70	0/1/1/1
48	NEX	S	319	-	-	2/27/83/83	0/3/3/3
29	CLA	n	603	-	1/1/15/20	12/37/115/115	-
29	CLA	y	306	52	1/1/15/20	15/37/115/115	-
46	CHL	G	609	21	4/4/20/26	11/39/137/137	-
35	LMG	i	101	-	-	18/43/63/70	0/1/1/1
48	NEX	s	319	-	-	2/27/83/83	0/3/3/3
29	CLA	s	304	-	-	14/37/115/115	-
46	CHL	Y	310	24	4/4/20/26	6/39/137/137	-
47	LUT	g	616	-	-	1/29/67/67	0/2/2/2
29	CLA	S	312	37	1/1/15/20	17/37/115/115	-
37	LHG	s	320	29	-	22/49/49/53	-
29	CLA	G	604	-	1/1/11/20	9/18/96/115	-
29	CLA	c	504	-	1/1/15/20	12/37/115/115	-
29	CLA	N	613	20	1/1/15/20	13/37/115/115	-
40	SPH	C	525	-	-	11/21/21/21	-
29	CLA	b	510	52	1/1/15/20	6/37/115/115	-
33	3PH	b	521	-	-	28/40/40/49	-
37	LHG	B	523	-	-	16/48/48/53	-
29	CLA	a	405	52	1/1/15/20	15/37/115/115	-
47	LUT	s	317	-	-	4/29/67/67	0/2/2/2
46	CHL	y	301	-	4/4/20/26	11/39/137/137	-
36	DGD	C	518	-	-	8/40/80/95	0/2/2/2
46	CHL	N	606	-	4/4/20/26	9/39/137/137	-
35	LMG	W	203	-	-	16/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CHL	n	605	20	4/4/20/26	11/39/137/137	-
29	CLA	n	610	-	1/1/11/20	5/18/96/115	-
29	CLA	s	312	37	1/1/15/20	14/37/115/115	-
29	CLA	c	513	-	-	12/37/115/115	-
39	SQD	b	523	-	-	19/49/69/69	0/1/1/1
29	CLA	G	611	-	1/1/15/20	11/37/115/115	-
29	CLA	r	308	22	1/1/14/20	13/31/109/115	-
29	CLA	b	508	-	-	4/37/115/115	-
33	3PH	a	415	-	-	25/49/49/49	-
47	LUT	r	311	-	-	5/29/67/67	0/2/2/2
29	CLA	y	315	24	-	8/37/115/115	-
51	LPX	S	321	-	-	7/21/21/31	-
29	CLA	S	311	23	1/1/15/20	10/37/115/115	-
51	LPX	s	321	-	-	10/20/20/31	-
46	CHL	Y	302	24	4/4/20/26	5/39/137/137	-
29	CLA	y	314	24	1/1/15/20	12/37/115/115	-
46	CHL	S	302	23	3/3/16/26	3/15/113/137	-
29	CLA	B	510	52	1/1/15/20	7/37/115/115	-
39	SQD	M	101	-	-	21/37/57/69	0/1/1/1
46	CHL	r	306	-	3/3/16/26	5/20/118/137	-
49	XAT	N	619	-	2/2/12/26	1/31/93/93	0/4/4/4
29	CLA	b	507	52	1/1/15/20	7/37/115/115	-
29	CLA	B	514	-	1/1/15/20	11/37/115/115	-
46	CHL	y	307	24	3/3/16/26	4/15/113/137	-
29	CLA	a	406	52	-	5/18/96/115	-
29	CLA	y	305	-	1/1/15/20	15/37/115/115	-
29	CLA	B	502	-	1/1/15/20	4/37/115/115	-
29	CLA	b	506	-	1/1/13/20	11/28/106/115	-
29	CLA	B	504	-	1/1/15/20	16/37/115/115	-
29	CLA	s	313	23	1/1/11/20	2/13/91/115	-
29	CLA	b	514	-	1/1/15/20	13/37/115/115	-
29	CLA	r	309	22	1/1/14/20	7/31/109/115	-
29	CLA	S	303	23	1/1/14/20	10/31/109/115	-
29	CLA	r	304	-	1/1/11/20	9/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	y	312	24	1/1/15/20	6/37/115/115	-
29	CLA	s	316	23	1/1/12/20	5/19/97/115	-
37	LHG	c	521	-	-	30/51/51/53	-
29	CLA	A	406	52	1/1/15/20	16/37/115/115	-
29	CLA	B	503	-	1/1/15/20	10/37/115/115	-
29	CLA	R	301	22	1/1/14/20	6/31/109/115	-
29	CLA	C	506	-	1/1/14/20	14/31/109/115	-
35	LMG	d	408	-	-	13/43/63/70	0/1/1/1
35	LMG	c	519	-	-	21/46/66/70	0/1/1/1
29	CLA	G	603	-	1/1/15/20	10/37/115/115	-
37	LHG	N	618	29	-	30/53/53/53	-
46	CHL	g	607	-	4/4/20/26	10/39/137/137	-
49	XAT	y	302	-	1/1/12/26	0/31/93/93	0/4/4/4
31	BCR	f	101	-	-	11/29/63/63	0/2/2/2
46	CHL	N	601	20	4/4/20/26	9/39/137/137	-
36	DGD	c	518	-	-	8/48/88/95	0/2/2/2
48	NEX	y	319	-	-	8/27/83/83	0/3/3/3
29	CLA	r	310	-	1/1/12/20	9/21/99/115	-
36	DGD	c	516	-	-	10/44/84/95	0/2/2/2
29	CLA	s	303	23	1/1/14/20	6/31/109/115	-
29	CLA	G	612	21	1/1/10/20	3/11/89/115	-
46	CHL	y	311	24	4/4/20/26	6/39/137/137	-
48	NEX	N	617	-	-	2/27/83/83	1/3/3/3
29	CLA	g	603	-	1/1/15/20	20/37/115/115	-
29	CLA	C	505	52	1/1/13/20	8/25/103/115	-
47	LUT	Y	317	-	-	2/29/67/67	0/2/2/2
46	CHL	n	601	20	4/4/20/26	12/39/137/137	-
29	CLA	a	408	-	-	8/31/109/115	-
29	CLA	b	504	-	1/1/15/20	12/37/115/115	-
36	DGD	B	521	-	-	13/32/72/95	0/2/2/2
31	BCR	v	101	-	-	12/29/63/63	0/2/2/2
39	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	c	505	-	1/1/15/20	18/37/115/115	-
29	CLA	n	613	-	1/1/11/20	3/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	LUT	g	615	-	-	2/29/67/67	0/2/2/2
29	CLA	b	513	-	1/1/15/20	11/37/115/115	-
29	CLA	g	612	21	-	2/11/89/115	-
29	CLA	B	513	-	1/1/15/20	11/37/115/115	-
46	CHL	n	607	-	3/3/16/26	3/20/118/137	-
48	NEX	R	312	-	-	9/19/50/83	0/2/2/3
29	CLA	B	506	-	1/1/15/20	14/37/115/115	-
46	CHL	s	308	-	3/3/15/26	0/12/110/137	-
29	CLA	g	611	37	1/1/15/20	8/37/115/115	-
31	BCR	b	517	-	-	11/29/63/63	0/2/2/2
31	BCR	z	101	-	-	13/29/63/63	0/2/2/2
29	CLA	r	302	22	1/1/14/20	7/31/109/115	-
47	LUT	y	318	-	-	1/29/67/67	0/2/2/2
29	CLA	B	516	-	1/1/13/20	11/25/103/115	-
31	BCR	B	517	-	-	8/29/63/63	0/2/2/2
39	SQD	L	102	-	-	13/37/57/69	0/1/1/1
47	LUT	Y	316	-	-	2/29/67/67	0/2/2/2
46	CHL	g	606	-	3/3/16/26	3/20/118/137	-
29	CLA	C	504	-	-	11/37/115/115	-
29	CLA	S	315	-	1/1/12/20	8/19/97/115	-
45	RRX	h	101	-	1/1/11/25	13/29/65/65	0/2/2/2
35	LMG	c	520	-	-	13/50/70/70	0/1/1/1
29	CLA	D	405	-	1/1/14/20	10/31/109/115	-
43	PL9	d	405	-	-	11/53/73/73	0/1/1/1
31	BCR	C	515	-	-	13/29/63/63	0/2/2/2
35	LMG	C	522	-	-	21/50/70/70	0/1/1/1
39	SQD	c	522	-	-	15/49/69/69	0/1/1/1
29	CLA	d	403	-	1/1/15/20	5/37/115/115	-
29	CLA	C	503	-	1/1/15/20	11/37/115/115	-
29	CLA	n	604	-	1/1/15/20	13/37/115/115	-
37	LHG	S	301	-	-	23/39/39/53	-
29	CLA	R	307	22	1/1/11/20	8/15/93/115	-
29	CLA	R	302	-	-	11/31/109/115	-
29	CLA	S	306	23	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CHL	N	605	20	4/4/20/26	15/39/137/137	-
41	DGA	W	202	-	-	23/45/45/45	-
29	CLA	N	610	-	1/1/15/20	13/37/115/115	-
29	CLA	c	510	-	1/1/15/20	9/37/115/115	-
29	CLA	g	602	21	1/1/15/20	16/37/115/115	-
29	CLA	C	513	-	1/1/15/20	17/37/115/115	-
29	CLA	s	310	-	1/1/14/20	17/31/109/115	-
29	CLA	N	614	-	1/1/11/20	8/18/96/115	-
46	CHL	S	308	-	3/3/15/26	0/12/110/137	-
29	CLA	y	310	-	1/1/12/20	8/19/97/115	-
29	CLA	b	512	-	1/1/15/20	10/37/115/115	-
29	CLA	S	313	23	1/1/11/20	3/13/91/115	-
29	CLA	r	303	-	-	12/31/109/115	-
47	LUT	n	614	-	-	4/29/67/67	0/2/2/2
46	CHL	R	305	-	3/3/16/26	6/20/118/137	-
35	LMG	B	520	-	-	13/39/59/70	0/1/1/1
48	NEX	n	616	-	-	2/27/83/83	1/3/3/3
29	CLA	Y	305	52	1/1/15/20	15/37/115/115	-
38	LMT	B	524	-	-	2/21/61/61	0/2/2/2
29	CLA	n	611	20	1/1/11/20	6/13/91/115	-
29	CLA	c	501	-	-	13/37/115/115	-
44	HEM	E	101	7,6	-	1/12/54/54	-
35	LMG	d	407	-	-	7/41/61/70	0/1/1/1
48	NEX	r	313	-	-	5/19/50/83	0/2/2/3
29	CLA	c	502	-	1/1/15/20	11/37/115/115	-
29	CLA	n	612	20	-	14/37/115/115	-
29	CLA	A	409	-	-	8/31/109/115	-
37	LHG	s	301	-	-	19/42/42/53	-
29	CLA	R	309	-	1/1/12/20	9/19/97/115	-
29	CLA	R	303	-	1/1/11/20	6/18/96/115	-
29	CLA	N	612	20	1/1/11/20	4/13/91/115	-
33	3PH	B	522	-	-	20/49/49/49	-
46	CHL	N	609	20	4/4/20/26	6/39/137/137	-
31	BCR	C	516	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	DGA	D	402	-	-	19/38/38/45	-
29	CLA	B	509	-	1/1/15/20	12/37/115/115	-
37	LHG	l	102	-	-	31/53/53/53	-
46	CHL	Y	308	-	4/4/20/26	11/39/137/137	-
46	CHL	G	607	-	4/4/20/26	13/39/137/137	-
46	CHL	y	303	24	4/4/20/26	8/39/137/137	-
29	CLA	C	502	-	-	13/37/115/115	-
29	CLA	N	603	-	1/1/15/20	21/37/115/115	-
46	CHL	g	608	-	3/3/15/26	0/13/111/137	-
46	CHL	g	609	21	4/4/20/26	8/39/137/137	-
29	CLA	c	507	52	1/1/15/20	13/37/115/115	-
29	CLA	B	512	-	1/1/15/20	9/37/115/115	-
46	CHL	G	605	21	3/3/16/26	6/18/116/137	-
29	CLA	a	404	-	1/1/15/20	12/37/115/115	-
46	CHL	G	606	-	3/3/16/26	5/20/118/137	-
36	DGD	C	519	-	-	11/42/82/95	0/2/2/2
41	DGA	b	522	-	-	19/45/45/45	-
46	CHL	y	308	52	3/3/17/26	2/21/119/137	-
47	LUT	n	615	-	-	2/29/67/67	0/2/2/2
49	XAT	R	311	-	2/2/12/26	0/31/93/93	0/4/4/4
46	CHL	Y	306	24	3/3/16/26	5/15/113/137	-
46	CHL	s	302	23	3/3/16/26	4/15/113/137	-
29	CLA	C	508	52	1/1/15/20	12/37/115/115	-
29	CLA	b	515	-	1/1/15/20	12/37/115/115	-
31	BCR	a	409	-	-	9/29/63/63	0/2/2/2
48	NEX	Y	318	-	-	8/27/83/83	0/3/3/3
29	CLA	c	508	-	1/1/15/20	6/37/115/115	-
46	CHL	g	601	21	4/4/20/26	10/39/137/137	-
29	CLA	b	511	-	-	12/37/115/115	-
47	LUT	R	310	-	-	5/29/67/67	0/2/2/2
29	CLA	Y	313	24	1/1/15/20	13/37/115/115	-
37	LHG	n	617	-	-	30/46/46/53	-
29	CLA	d	404	-	1/1/15/20	10/37/115/115	-
29	CLA	c	506	-	-	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	G	618	-	-	29/53/53/53	-
29	CLA	g	610	21	1/1/15/20	5/37/115/115	-
29	CLA	B	508	-	1/1/15/20	7/37/115/115	-
44	HEM	e	101	7,6	-	1/12/54/54	-
49	XAT	Y	301	-	1/1/12/26	0/31/93/93	0/4/4/4
46	CHL	r	305	-	3/3/15/26	4/13/111/137	-
40	SPH	i	102	-	-	11/21/21/21	-
41	DGA	j	101	-	-	16/30/30/45	-
29	CLA	n	609	20	1/1/15/20	11/37/115/115	-
29	CLA	c	509	-	1/1/15/20	14/37/115/115	-
29	CLA	C	512	4	1/1/15/20	5/37/115/115	-
29	CLA	S	314	23	1/1/13/20	11/25/103/115	-
37	LHG	S	320	29	-	15/49/49/53	-
47	LUT	y	317	-	-	2/29/67/67	0/2/2/2
33	3PH	S	322	-	-	7/31/31/49	-
47	LUT	G	615	-	-	0/29/67/67	0/2/2/2
35	LMG	C	524	-	-	19/37/57/70	0/1/1/1
36	DGD	C	520	-	-	5/42/82/95	0/2/2/2
49	XAT	r	312	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	D	404	-	1/1/15/20	11/37/115/115	-
46	CHL	n	608	20	4/4/20/26	7/39/137/137	-
46	CHL	g	605	21	3/3/16/26	4/18/116/137	-
29	CLA	Y	309	52	1/1/12/20	8/19/97/115	-
29	CLA	C	509	-	1/1/15/20	7/37/115/115	-
29	CLA	b	503	-	1/1/15/20	8/37/115/115	-
29	CLA	G	613	21	1/1/15/20	10/37/115/115	-
34	C7Z	B	519	-	1/1/12/26	9/29/67/67	0/2/2/2
31	BCR	K	101	-	-	11/29/63/63	0/2/2/2
29	CLA	R	308	22	1/1/14/20	11/31/109/115	-
29	CLA	y	316	-	1/1/15/20	14/37/115/115	-
47	LUT	S	317	-	-	3/29/67/67	0/2/2/2
35	LMG	b	520	-	-	12/39/59/70	0/1/1/1
41	DGA	J	101	-	-	14/30/30/45	-
29	CLA	N	604	-	1/1/15/20	8/37/115/115	-
29	CLA	c	503	-	-	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	Y	319	29	-	28/53/53/53	-
30	PHO	d	402	-	-	6/37/103/103	0/5/6/6
47	LUT	N	615	-	-	3/29/67/67	0/2/2/2
29	CLA	B	515	-	1/1/15/20	9/37/115/115	-
29	CLA	C	514	-	-	13/37/115/115	-
37	LHG	D	407	-	-	18/53/53/53	-
29	CLA	Y	311	24	1/1/15/20	4/37/115/115	-
29	CLA	s	315	-	1/1/13/20	6/25/103/115	-
29	CLA	B	507	52	1/1/15/20	23/37/115/115	-
46	CHL	s	309	-	4/4/19/26	5/33/131/137	-
41	DGA	w	201	-	-	27/45/45/45	-
29	CLA	C	510	-	1/1/15/20	16/37/115/115	-
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2
39	SQD	C	501	-	-	9/37/57/69	0/1/1/1
31	BCR	F	101	-	-	12/29/63/63	0/2/2/2
46	CHL	Y	307	-	4/4/20/26	16/39/137/137	-
29	CLA	G	602	21	1/1/15/20	14/37/115/115	-
29	CLA	s	306	23	-	6/19/97/115	-
29	CLA	Y	304	-	1/1/15/20	14/37/115/115	-
29	CLA	Y	315	-	1/1/15/20	13/37/115/115	-
36	DGD	c	517	-	-	17/51/91/95	0/2/2/2
46	CHL	N	607	-	4/4/20/26	12/39/137/137	-
29	CLA	b	505	-	1/1/15/20	9/37/115/115	-
43	PL9	D	406	-	-	10/53/73/73	0/1/1/1
29	CLA	c	512	-	1/1/15/20	15/37/115/115	-
29	CLA	b	501	-	1/1/15/20	22/37/115/115	-
46	CHL	n	606	-	4/4/20/26	9/39/137/137	-
34	C7Z	b	519	-	1/1/12/26	7/29/67/67	0/2/2/2
37	LHG	D	408	-	-	18/43/43/53	-
47	LUT	S	318	-	-	3/29/67/67	0/2/2/2
33	3PH	s	322	-	-	23/49/49/49	-
29	CLA	b	502	-	1/1/15/20	8/37/115/115	-
29	CLA	b	516	-	1/1/15/20	15/37/115/115	-
29	CLA	s	311	23	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CHL	S	307	-	3/3/15/26	1/13/111/137	-
29	CLA	S	316	23	1/1/12/20	6/19/97/115	-
39	SQD	l	101	-	-	14/37/57/69	0/1/1/1
30	PHO	a	407	-	-	7/37/103/103	0/5/6/6
46	CHL	R	304	-	3/3/15/26	4/13/111/137	-
46	CHL	s	307	-	3/3/15/26	1/13/111/137	-
39	SQD	o	301	-	-	14/49/69/69	0/1/1/1
29	CLA	B	511	-	-	11/37/115/115	-
37	LHG	g	618	29	-	30/53/53/53	-
48	NEX	g	617	-	-	5/27/83/83	0/3/3/3
45	RRX	H	101	-	1/1/11/25	8/29/65/65	0/2/2/2
31	BCR	A	410	-	-	9/29/63/63	0/2/2/2
39	SQD	a	410	-	-	17/46/66/69	0/1/1/1
29	CLA	Y	312	37	1/1/15/20	9/37/115/115	-
29	CLA	Y	314	24	1/1/15/20	18/37/115/115	-
29	CLA	C	507	-	-	8/37/115/115	-
47	LUT	G	616	-	-	2/29/67/67	0/2/2/2
40	SPH	I	101	-	-	10/21/21/21	-
31	BCR	B	518	-	-	13/29/63/63	0/2/2/2
46	CHL	G	608	-	3/3/15/26	1/13/111/137	-
38	LMT	b	524	-	-	13/21/61/61	0/2/2/2
49	XAT	G	619	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	Y	303	24	1/1/15/20	12/37/115/115	-
31	BCR	C	517	-	-	10/29/63/63	0/2/2/2
29	CLA	y	304	24	1/1/15/20	6/37/115/115	-
29	CLA	B	501	-	1/1/15/20	18/37/115/115	-
37	LHG	L	101	-	-	33/53/53/53	-
29	CLA	A	405	-	1/1/15/20	12/37/115/115	-
29	CLA	G	614	-	1/1/11/20	7/18/96/115	-
37	LHG	y	320	29	-	28/53/53/53	-
50	PTY	N	620	-	-	18/53/53/53	-
50	PTY	Y	320	-	-	12/20/20/53	-
29	CLA	c	511	4	-	12/37/115/115	-
39	SQD	C	523	-	-	12/31/51/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	610	21	1/1/15/20	5/37/115/115	-
29	CLA	g	613	21	-	21/37/115/115	-
29	CLA	R	306	-	1/1/14/20	11/31/109/115	-
37	LHG	d	406	-	-	22/53/53/53	-
29	CLA	g	604	-	1/1/11/20	8/18/96/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
47	LUT	s	318	-	-	1/29/67/67	0/2/2/2
35	LMG	W	201	-	-	10/35/55/70	0/1/1/1
33	3PH	A	412	-	-	27/49/49/49	-
47	LUT	N	616	-	-	3/29/67/67	0/2/2/2
49	XAT	g	619	-	1/1/12/26	1/31/93/93	0/4/4/4
46	CHL	G	601	21	4/4/20/26	11/39/137/137	-
37	LHG	a	414	-	-	21/43/43/53	-
36	DGD	r	301	-	-	8/32/72/95	0/2/2/2
37	LHG	a	413	-	-	22/48/48/53	-
31	BCR	c	514	-	-	13/29/63/63	0/2/2/2
46	CHL	S	309	-	4/4/19/26	7/33/131/137	-
29	CLA	s	314	23	1/1/13/20	11/25/103/115	-
35	LMG	D	410	-	-	17/43/63/70	0/1/1/1
29	CLA	C	511	-	1/1/15/20	14/37/115/115	-
29	CLA	N	611	37	1/1/11/20	4/18/96/115	-
29	CLA	S	305	-	1/1/13/20	7/25/103/115	-
29	CLA	s	305	-	1/1/13/20	11/25/103/115	-
30	PHO	D	401	-	-	4/37/103/103	0/5/6/6
49	XAT	n	618	-	2/2/12/26	1/31/93/93	0/4/4/4
29	CLA	A	407	-	1/1/12/20	8/19/97/115	-
31	BCR	b	518	-	-	12/29/63/63	0/2/2/2
40	SPH	c	523	-	-	3/21/21/21	-
29	CLA	r	307	-	1/1/14/20	13/31/109/115	-
35	LMG	C	521	-	-	9/42/62/70	0/1/1/1
50	PTY	y	321	-	-	14/20/20/53	-
50	PTY	n	619	-	-	28/53/53/53	-

The worst 5 of 1112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H	101	RRX	C26-C25	15.61	1.61	1.34
45	h	101	RRX	C26-C25	15.51	1.61	1.34
34	B	519	C7Z	C25-C26	15.39	1.61	1.34
34	b	519	C7Z	C25-C26	15.36	1.61	1.34
34	B	519	C7Z	C5-C6	14.83	1.60	1.34

The worst 5 of 2065 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	BCR	C10-C11-C12	17.66	178.32	123.22
31	C	517	BCR	C10-C11-C12	17.51	177.86	123.22
31	c	515	BCR	C10-C11-C12	17.44	177.64	123.22
31	b	517	BCR	C10-C11-C12	17.38	177.47	123.22
31	b	518	BCR	C10-C11-C12	17.35	177.38	123.22

5 of 311 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	B	501	CLA	ND
29	B	502	CLA	ND

5 of 3584 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA

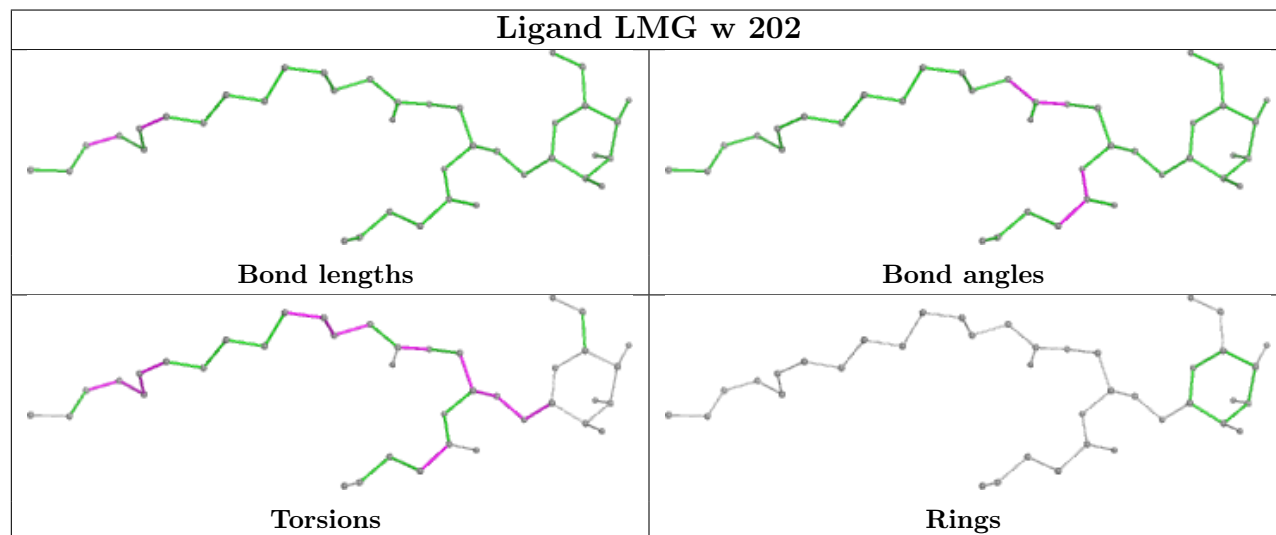
All (2) ring outliers are listed below:

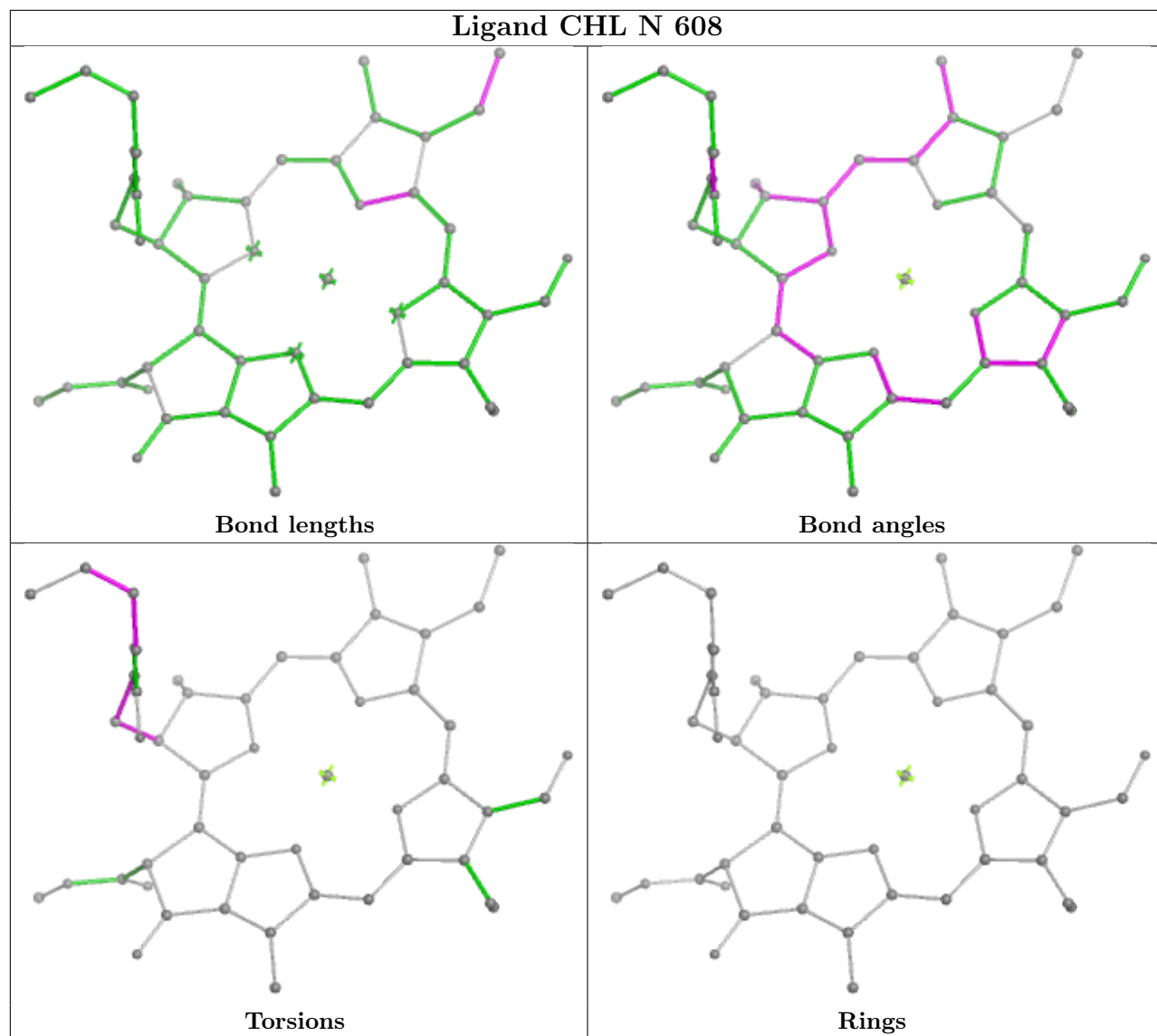
Mol	Chain	Res	Type	Atoms
48	n	616	NEX	C1-C2-C3-C4-C5-C6
48	N	617	NEX	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

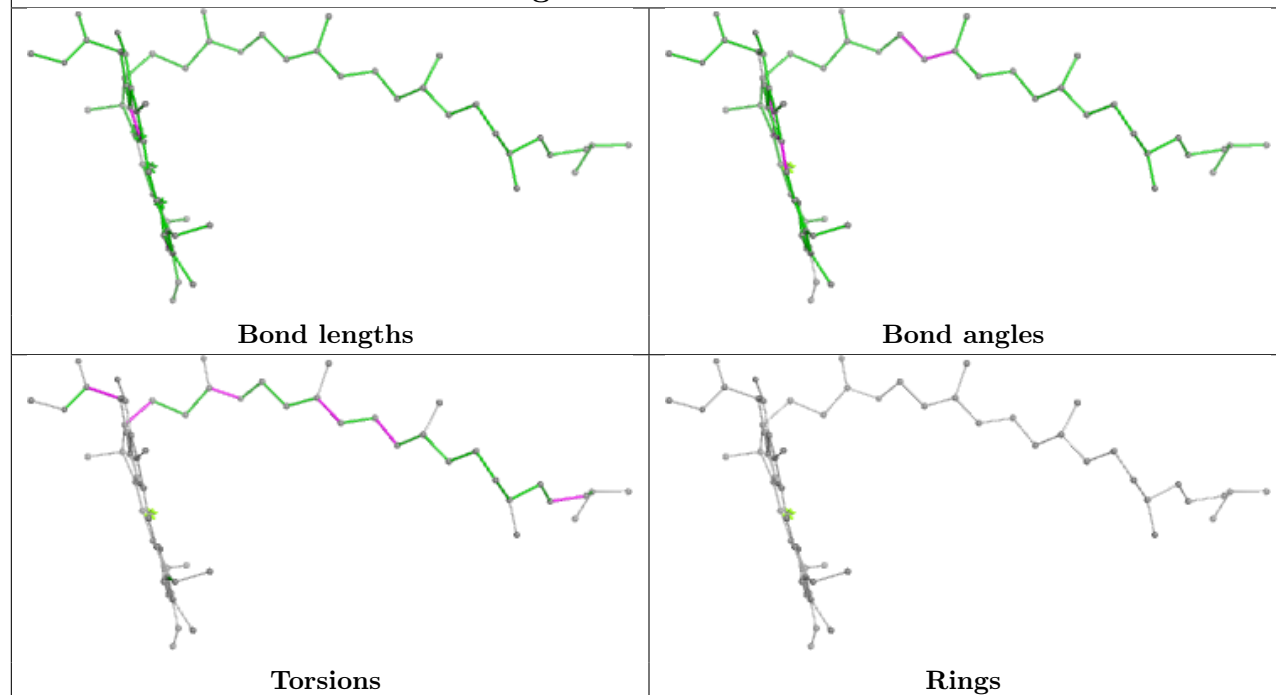
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

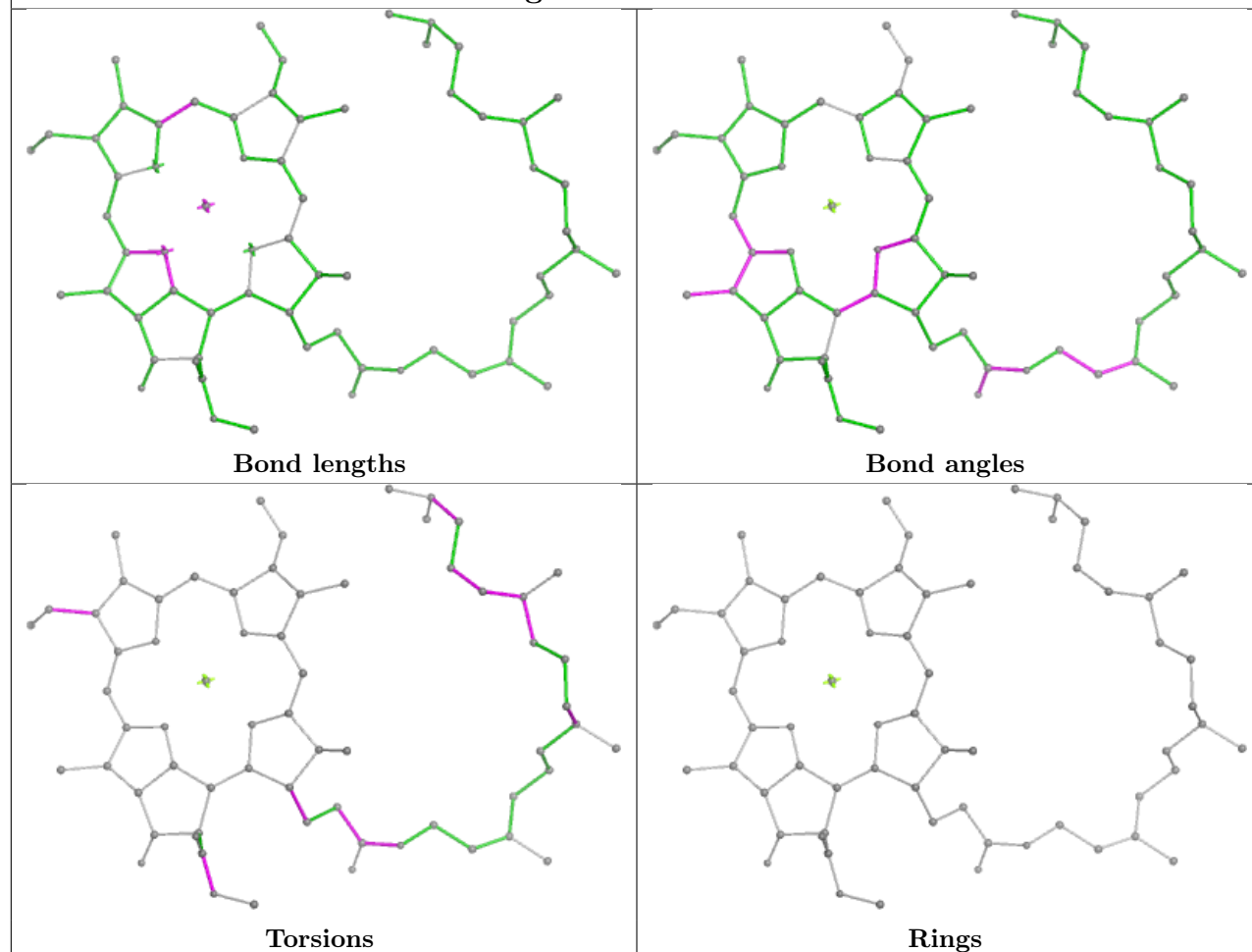


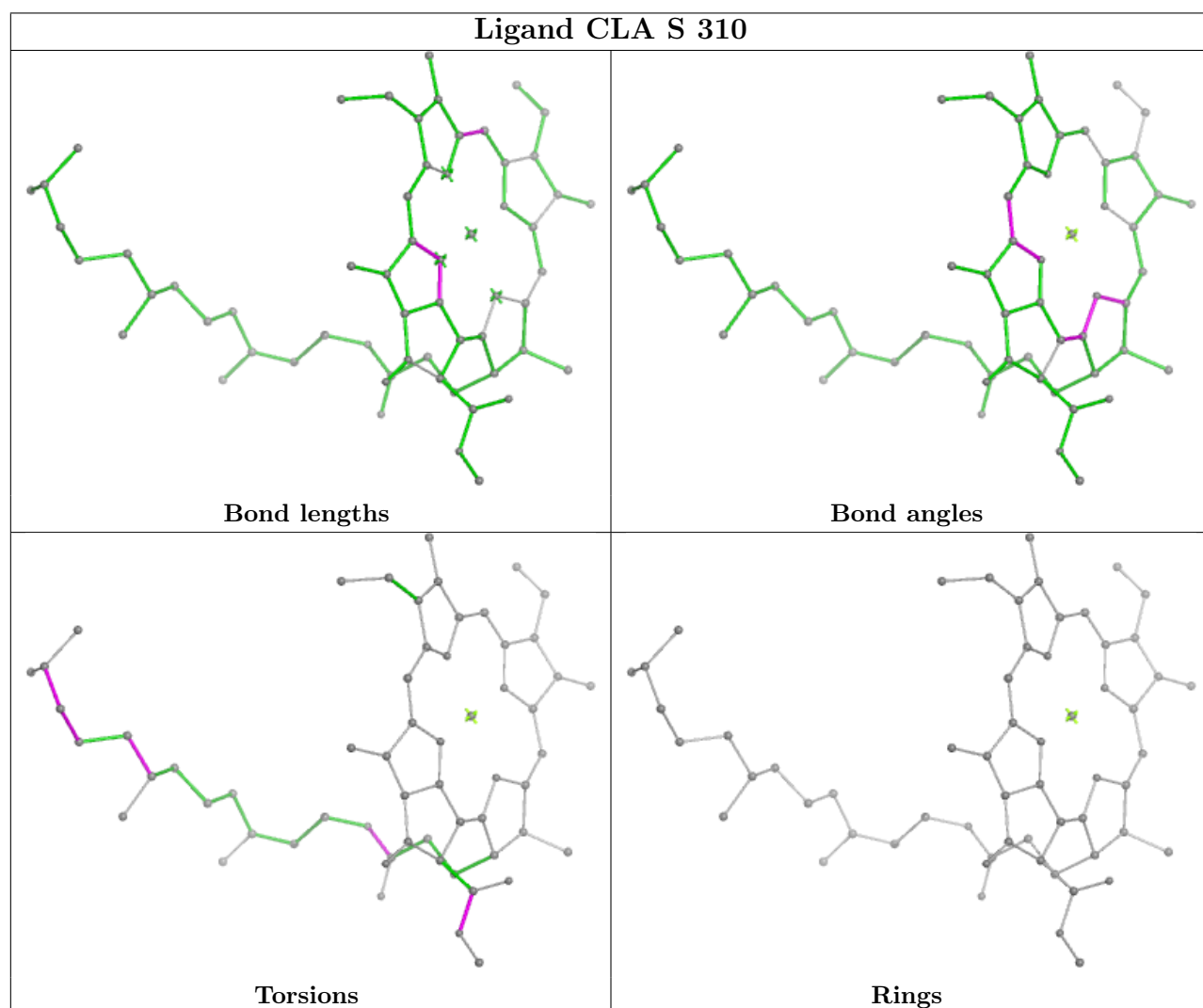
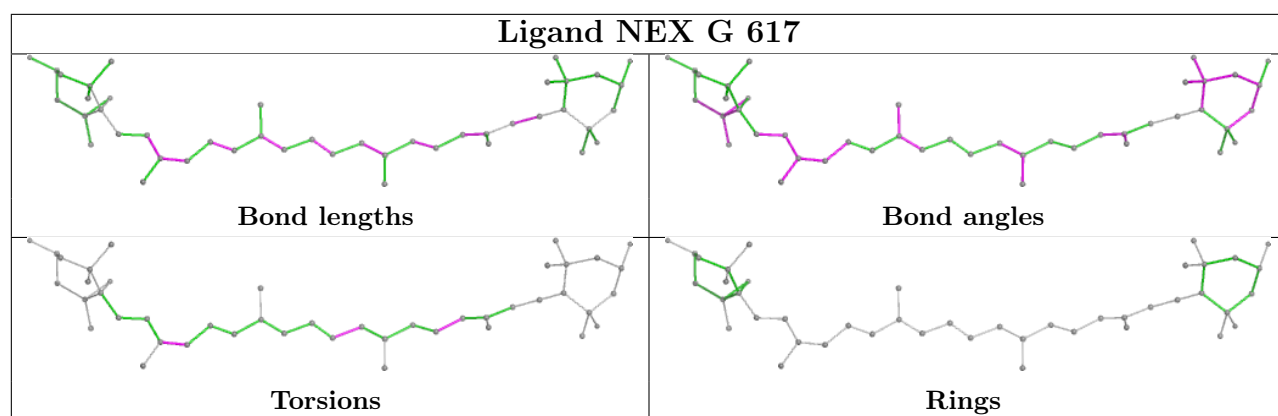


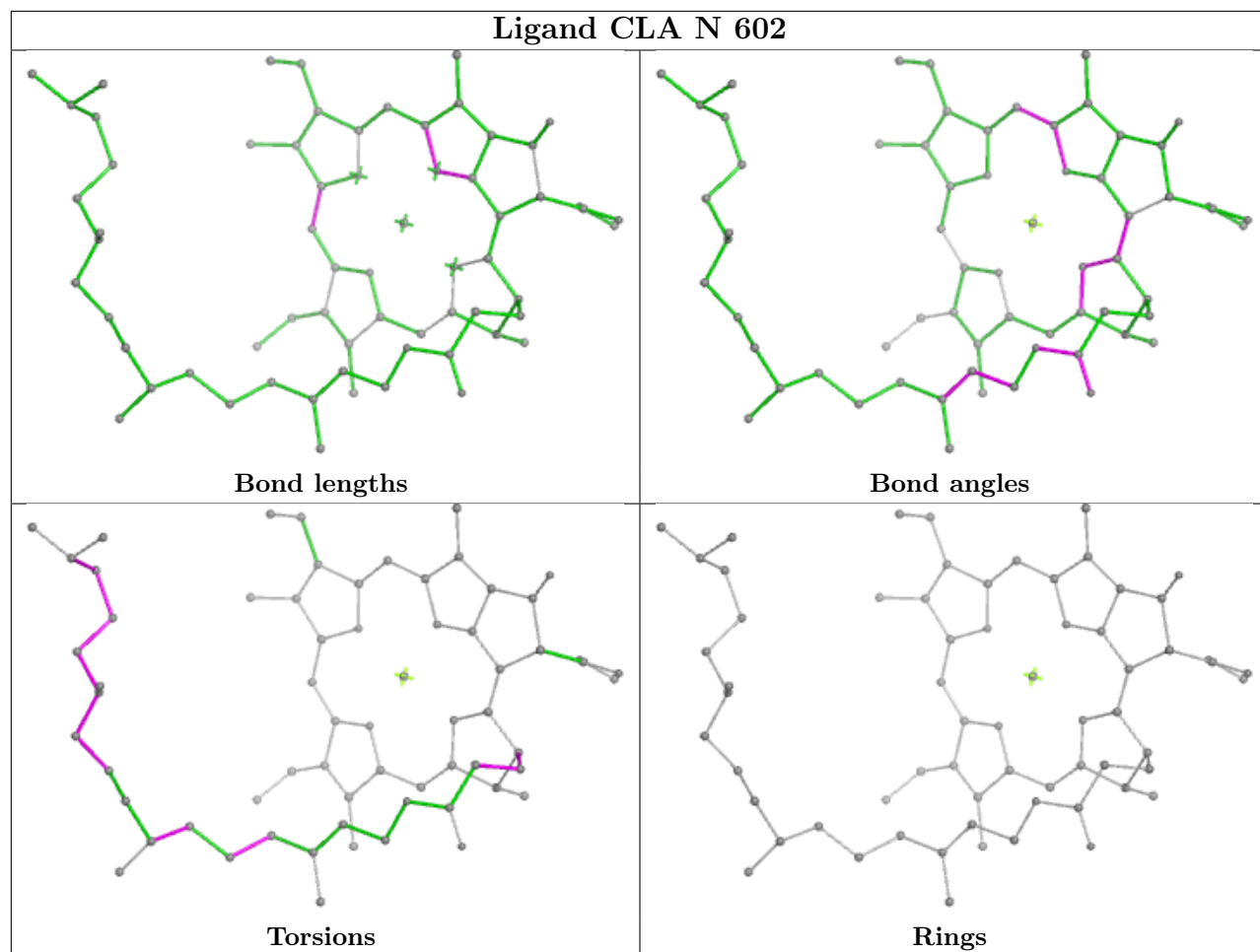
Ligand CLA B 505

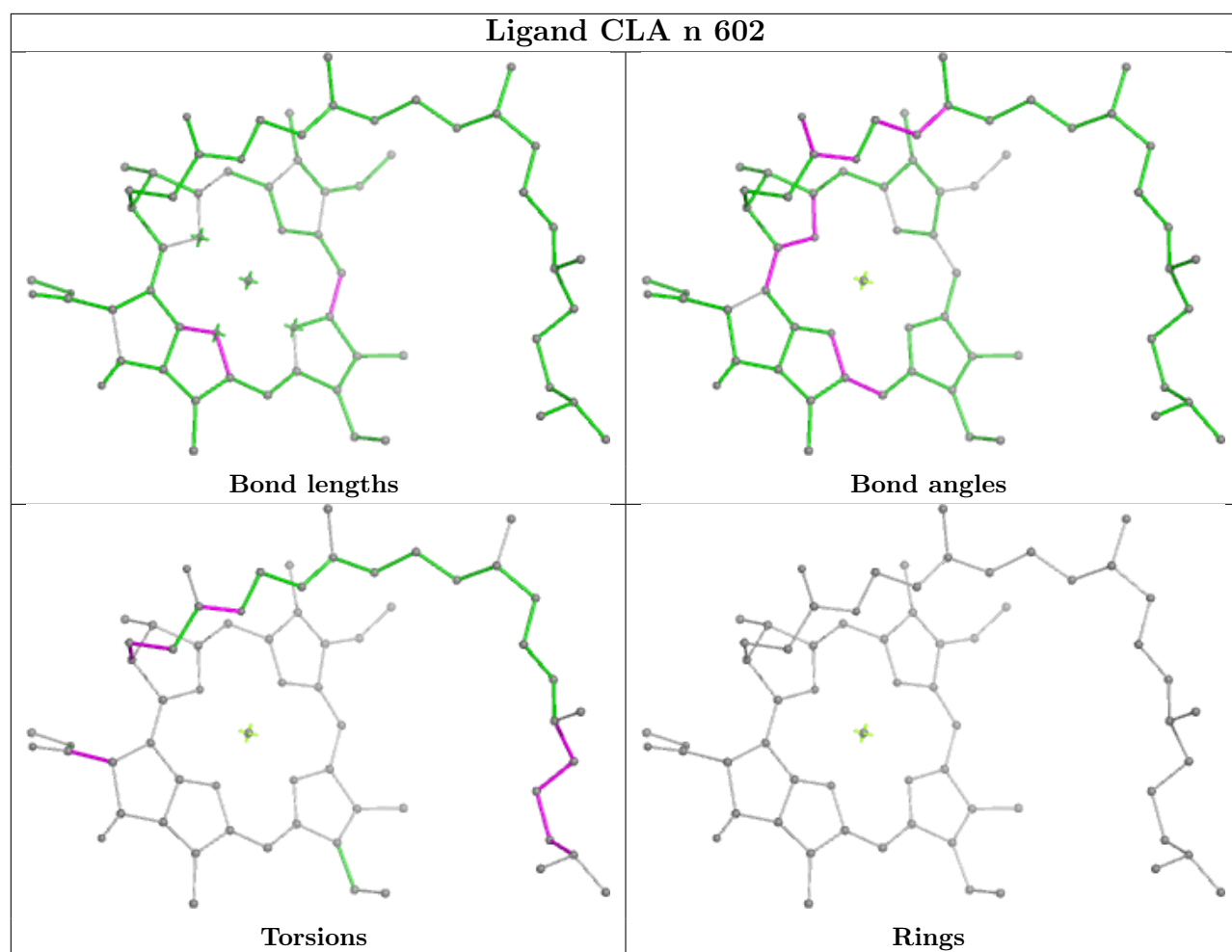


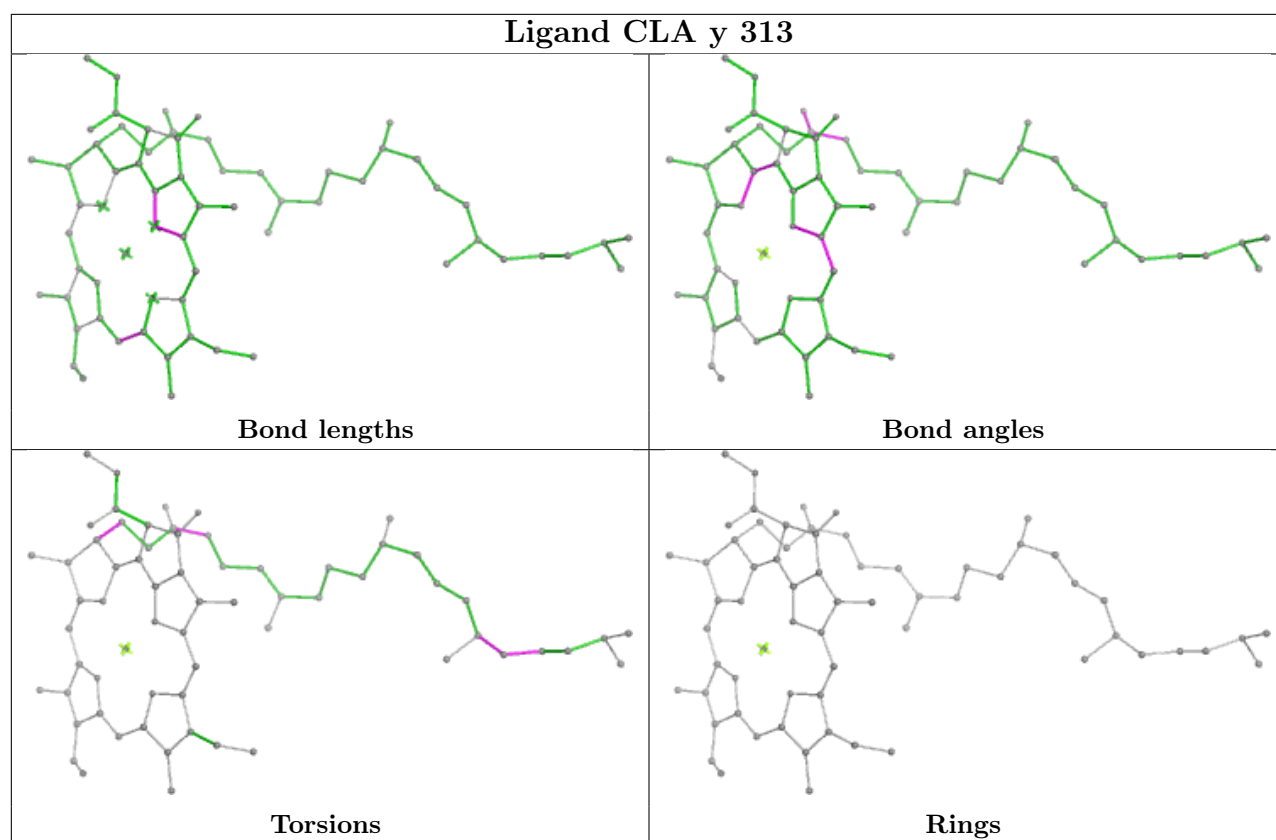
Ligand CLA S 304



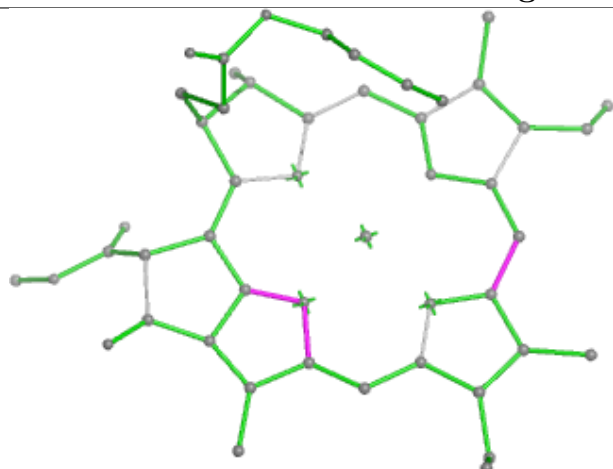




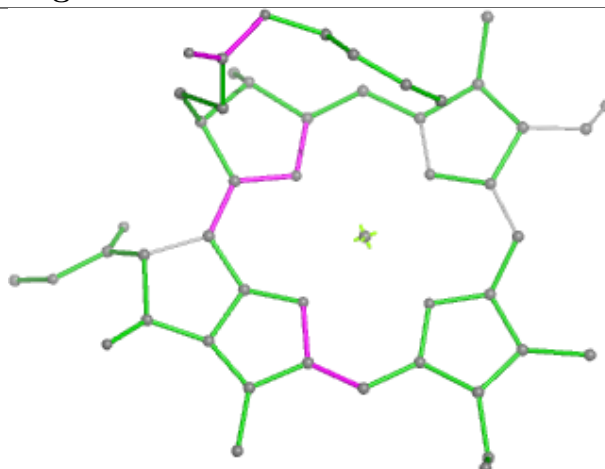




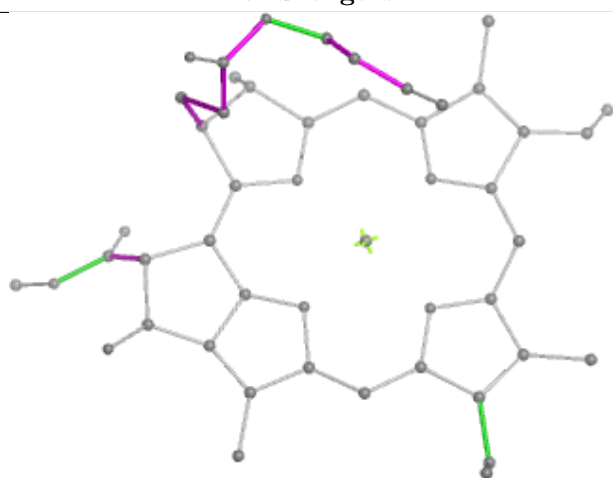
Ligand CLA g 614



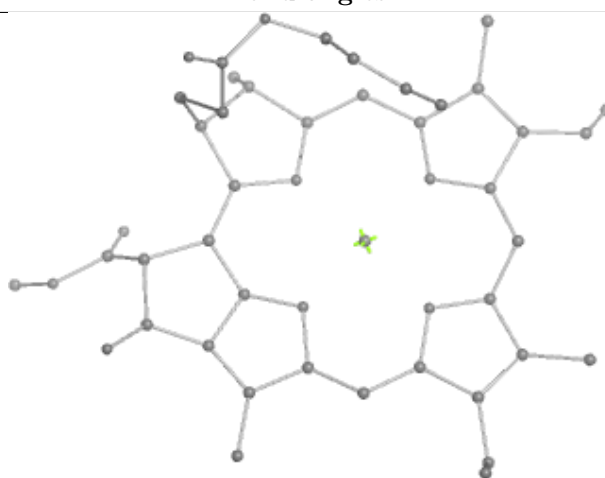
Bond lengths



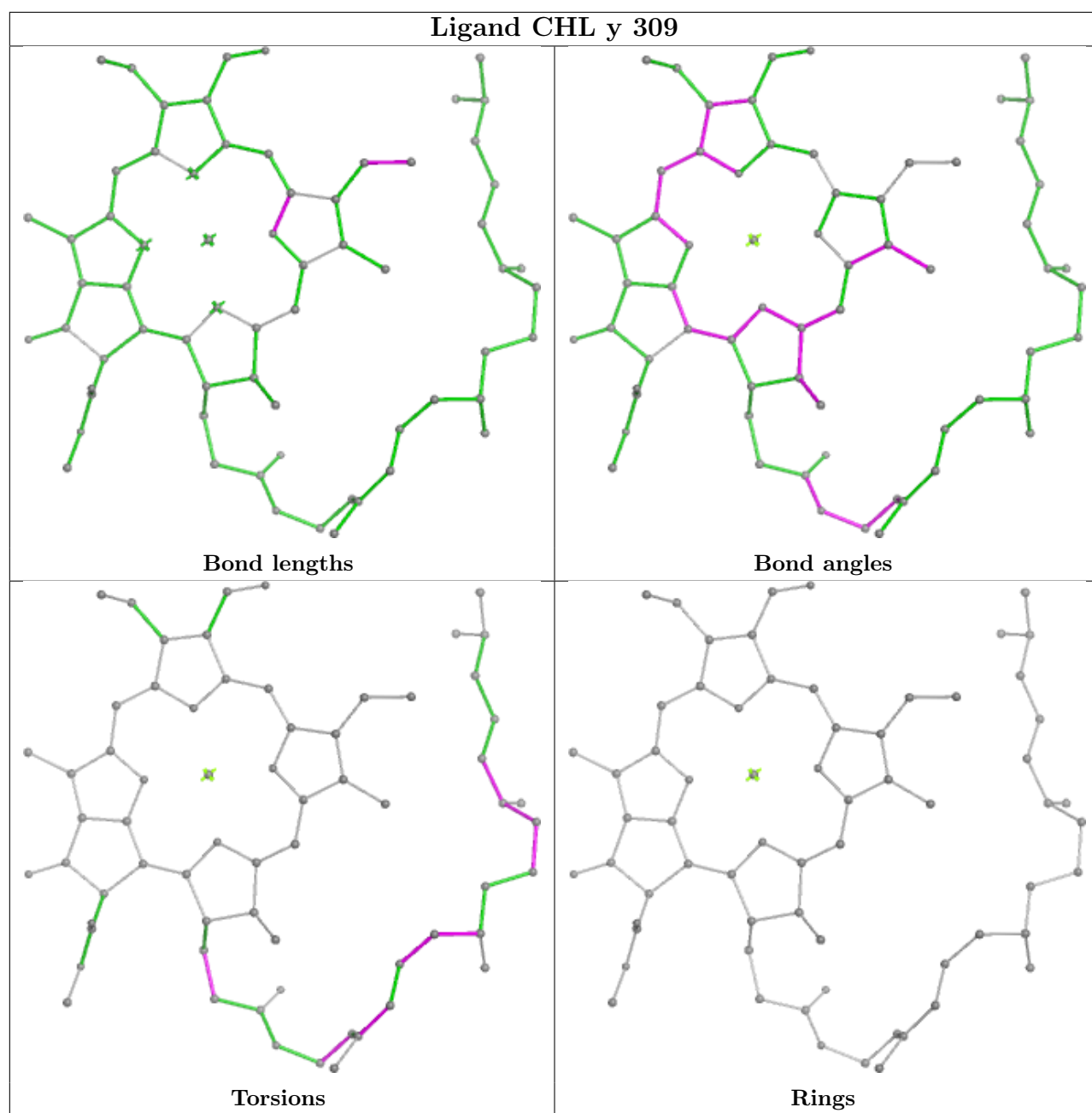
Bond angles

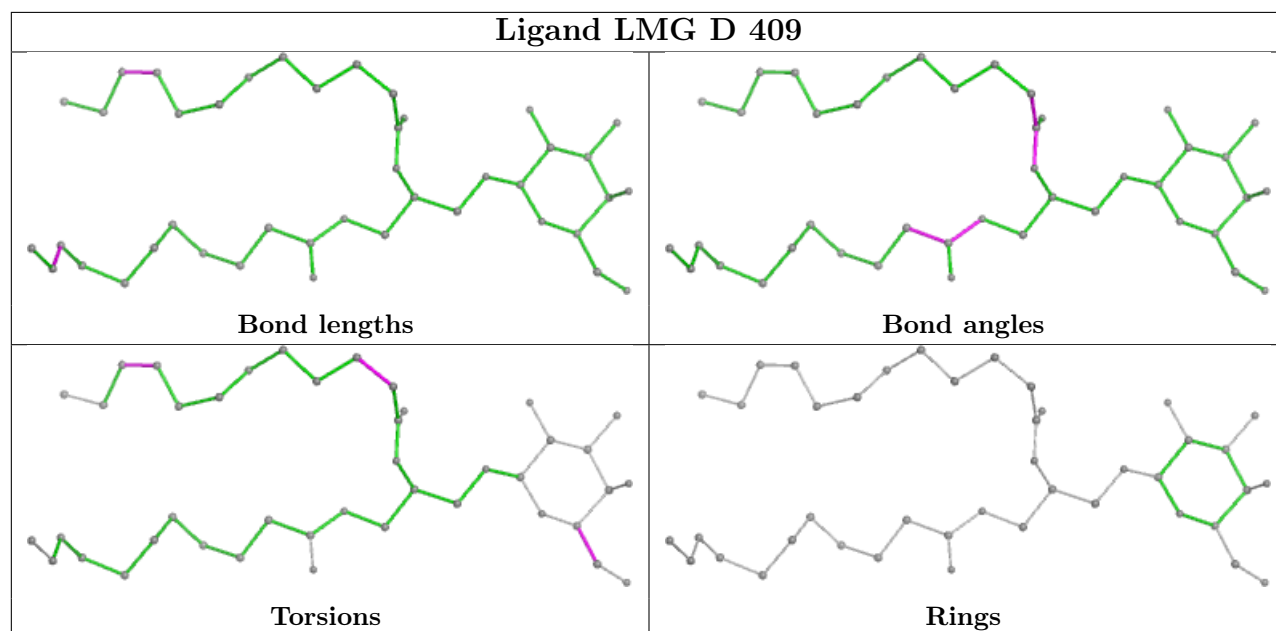
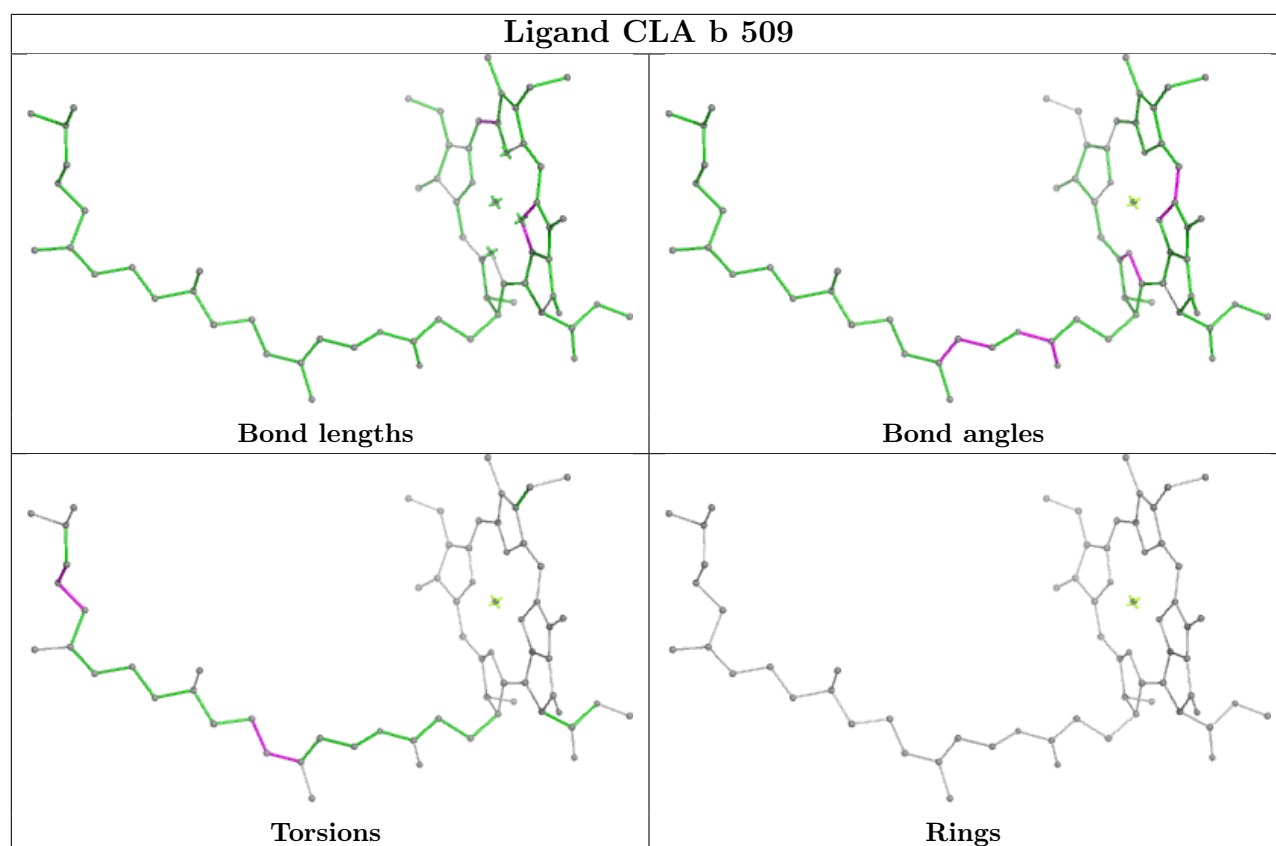


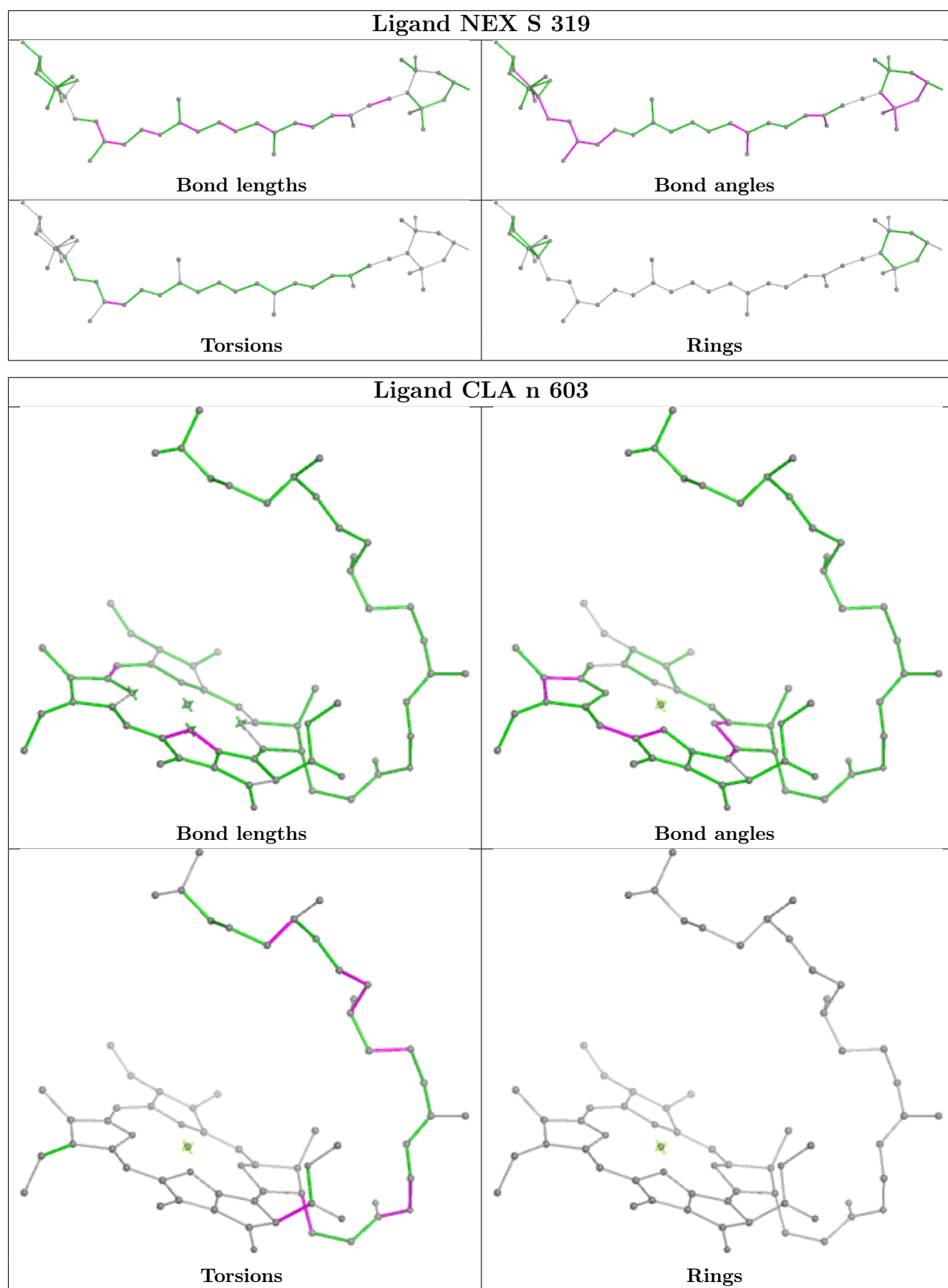
Torsions



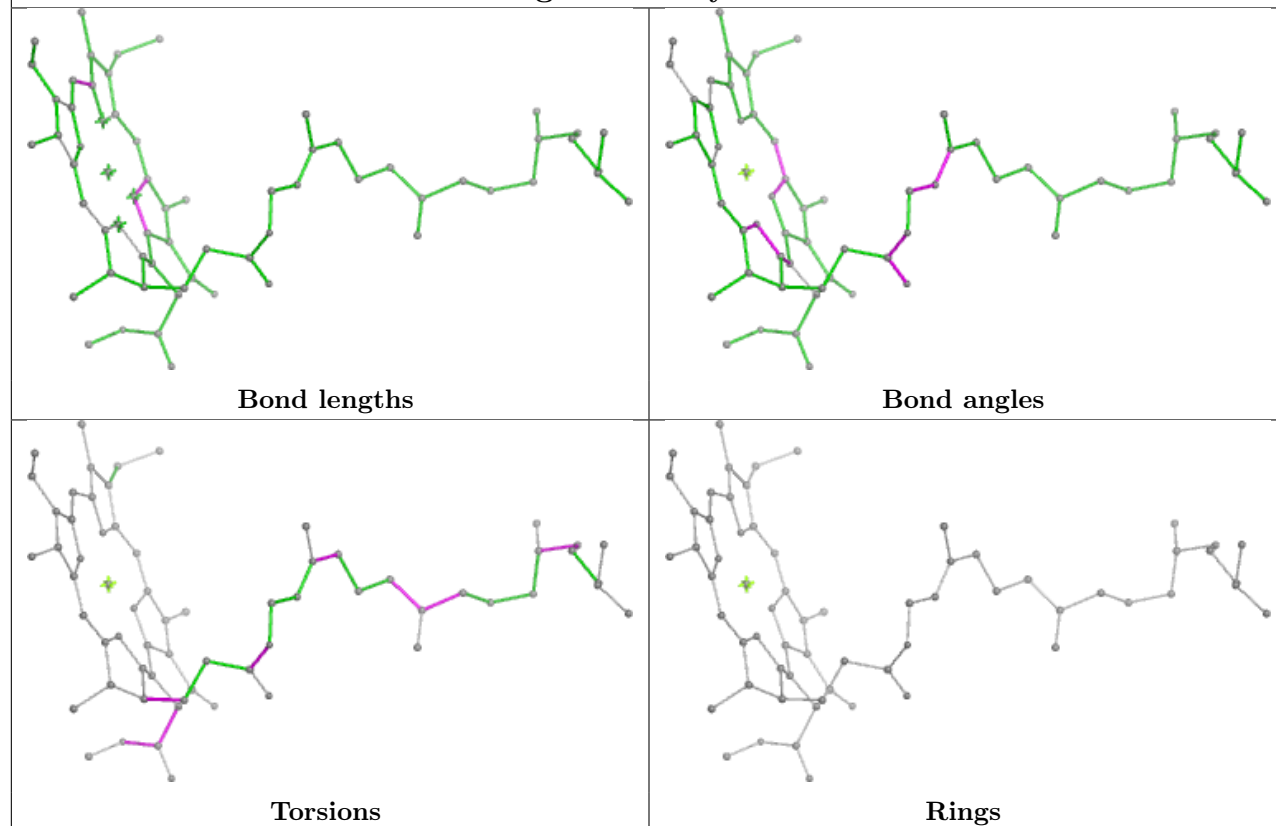
Rings



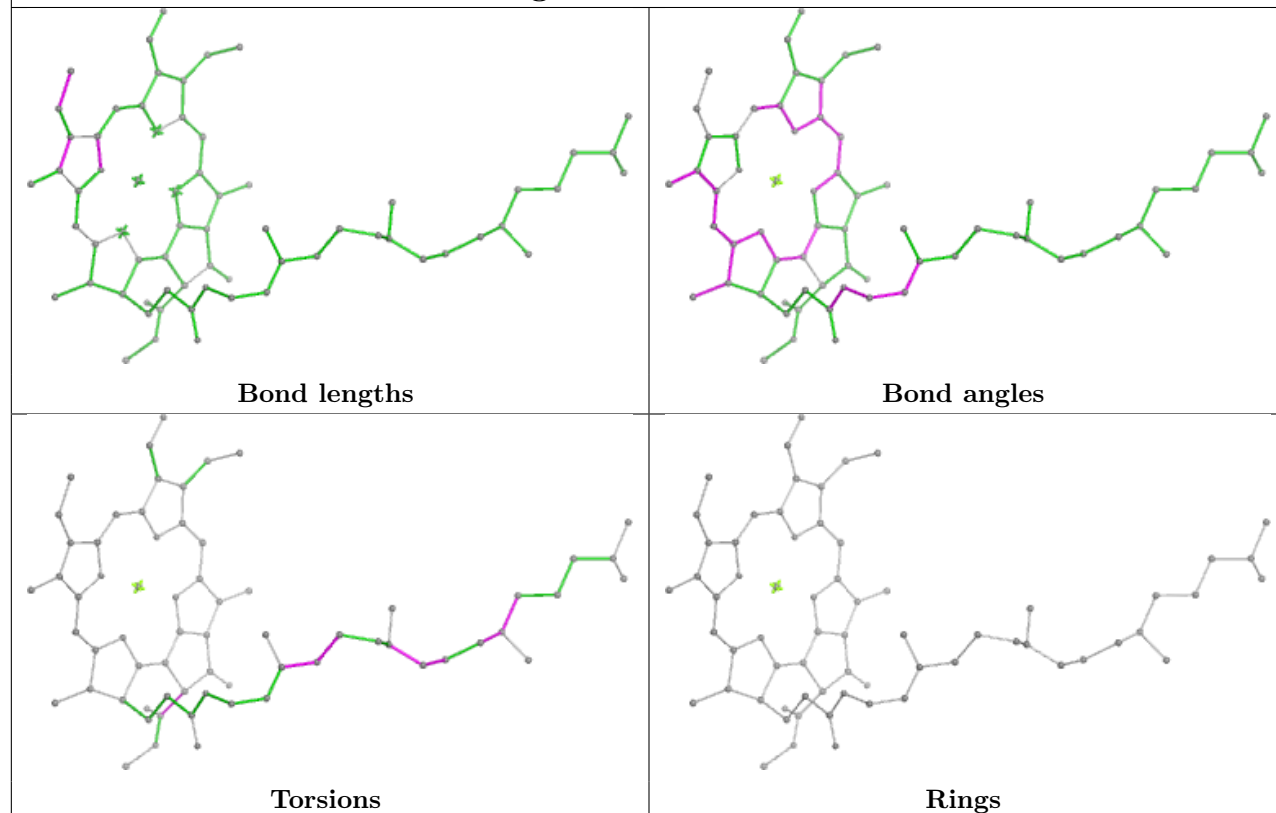


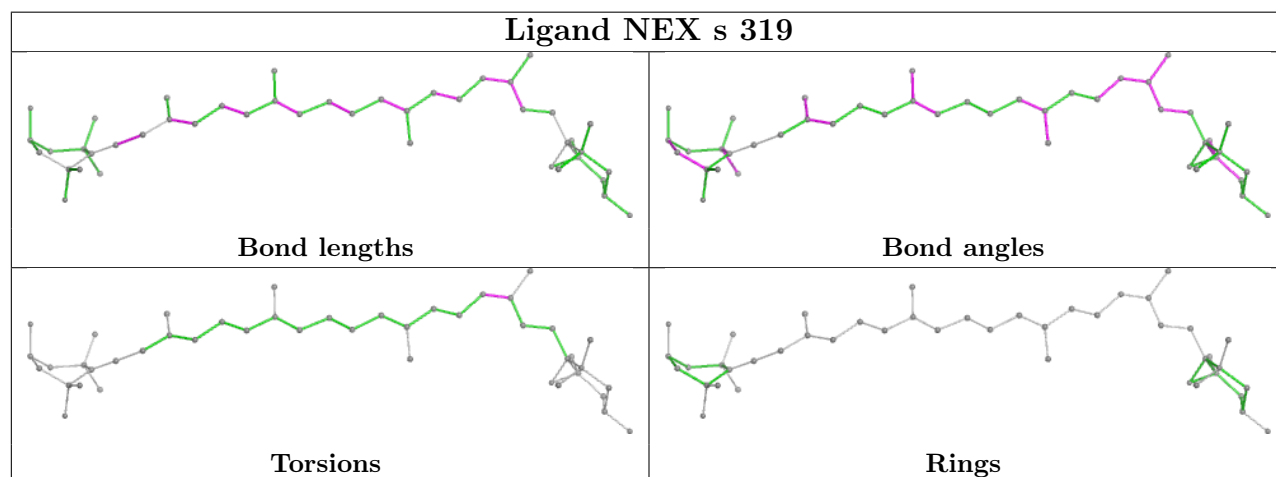
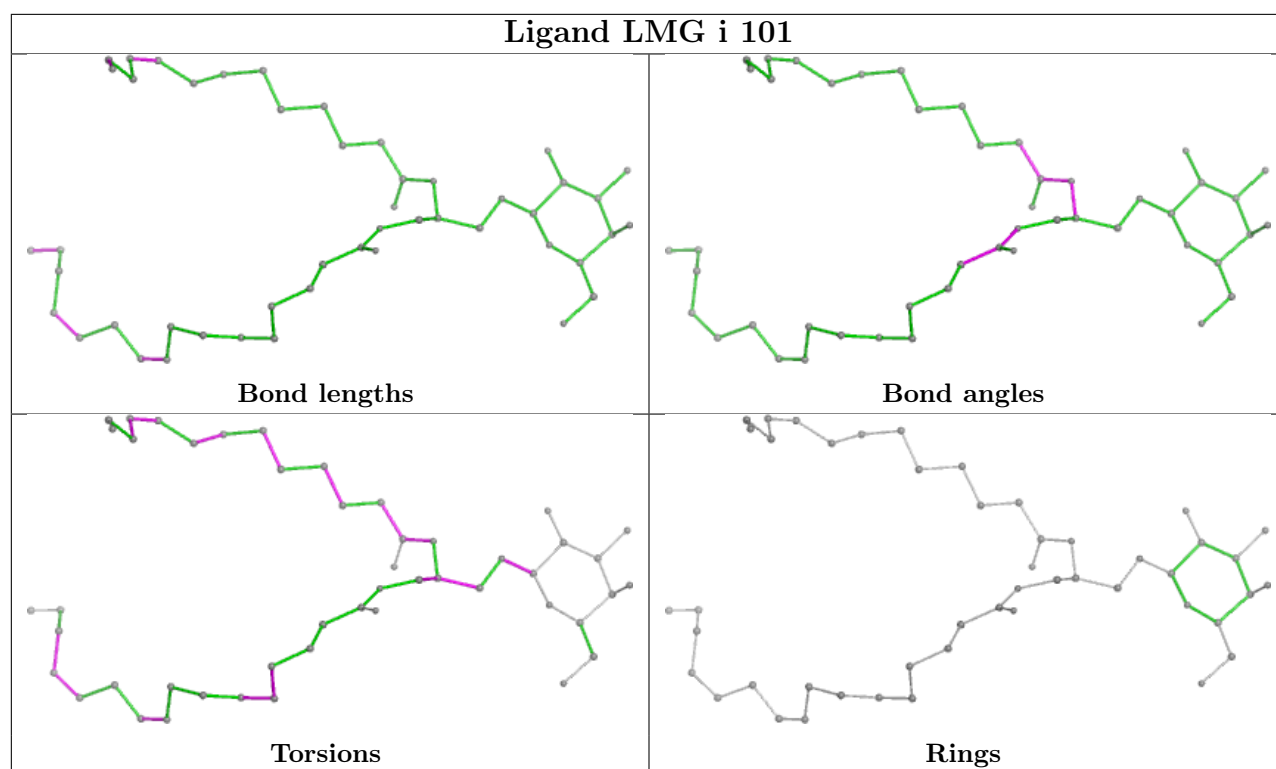


Ligand CLA y 306

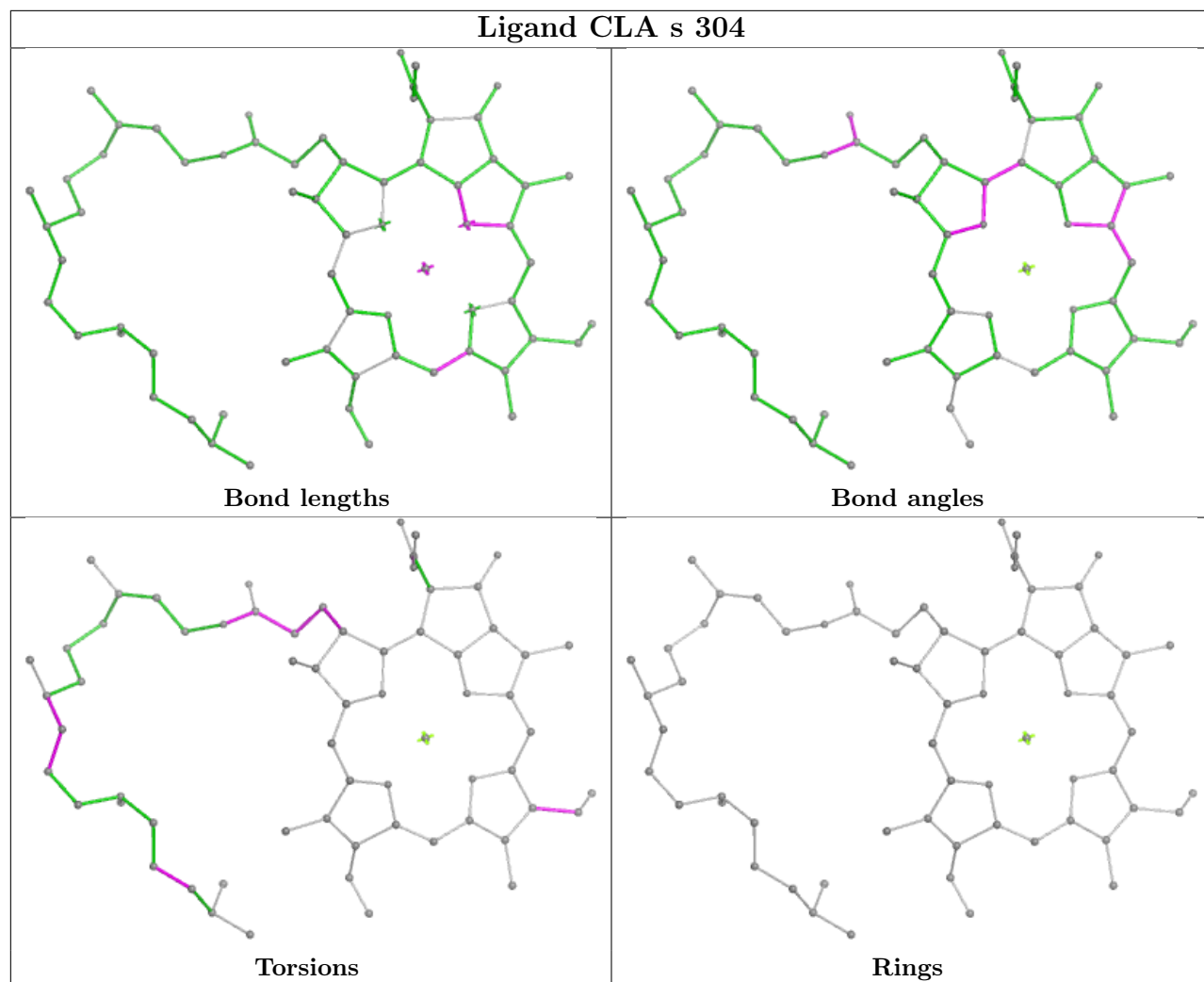


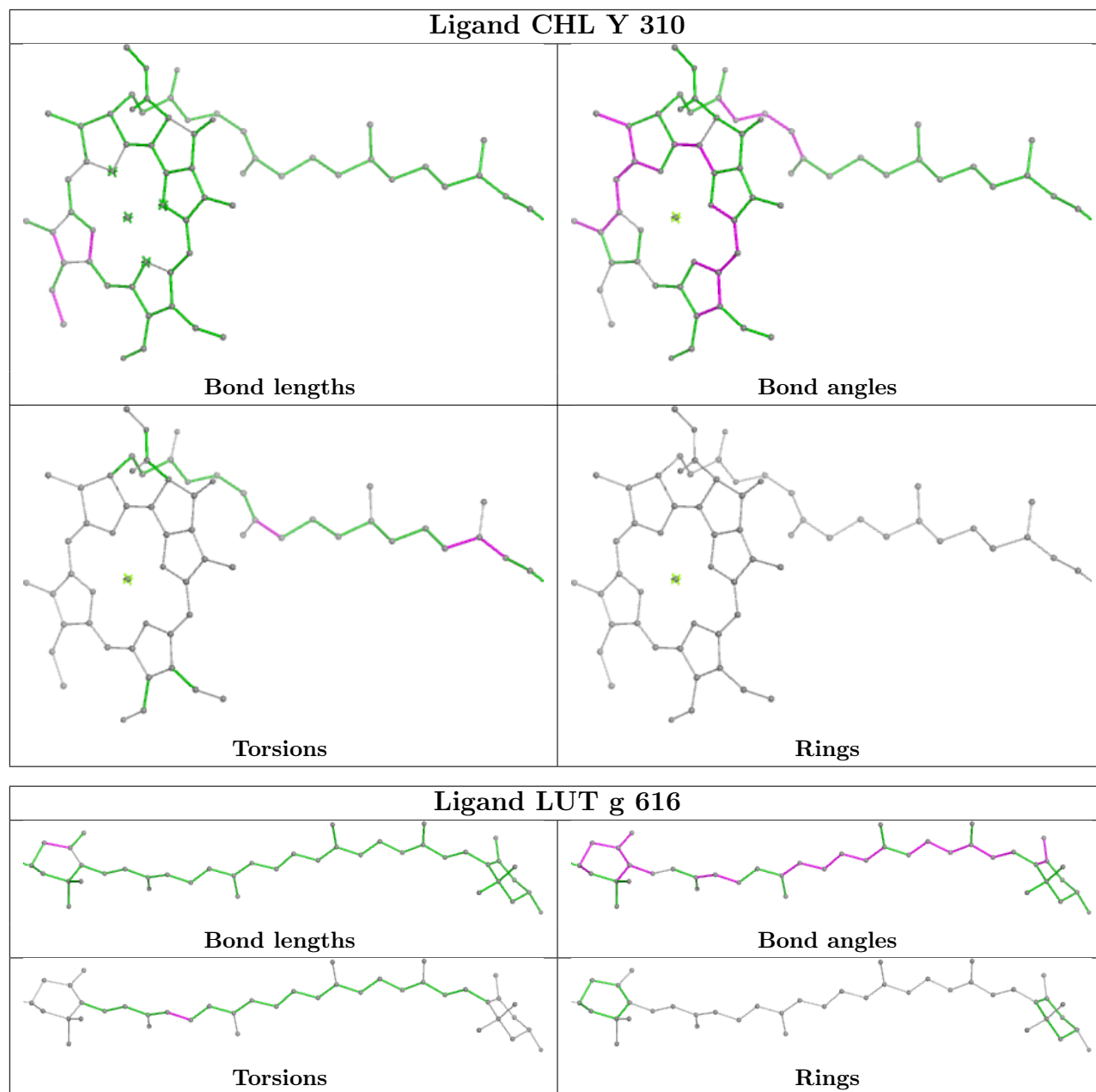
Ligand CHL G 609

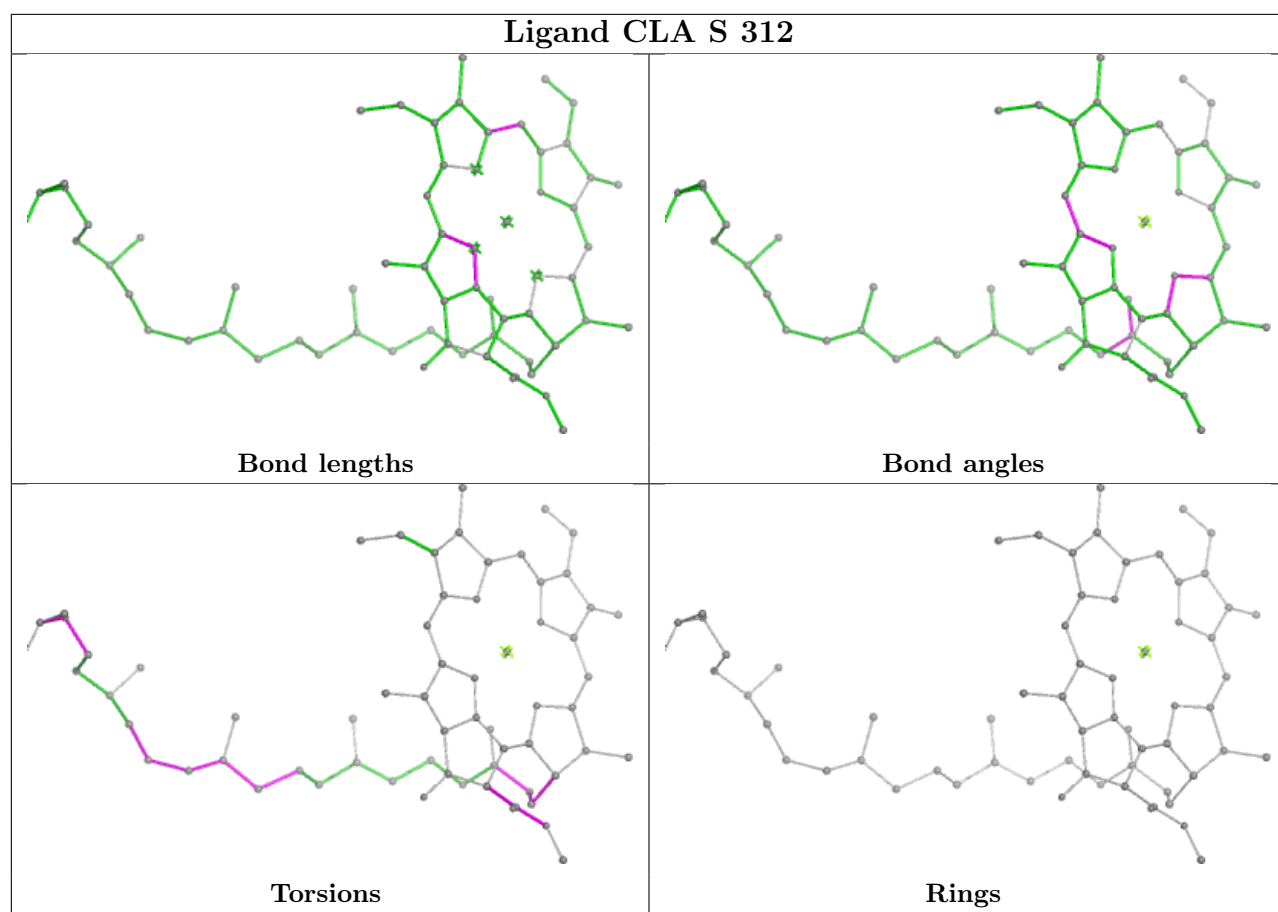


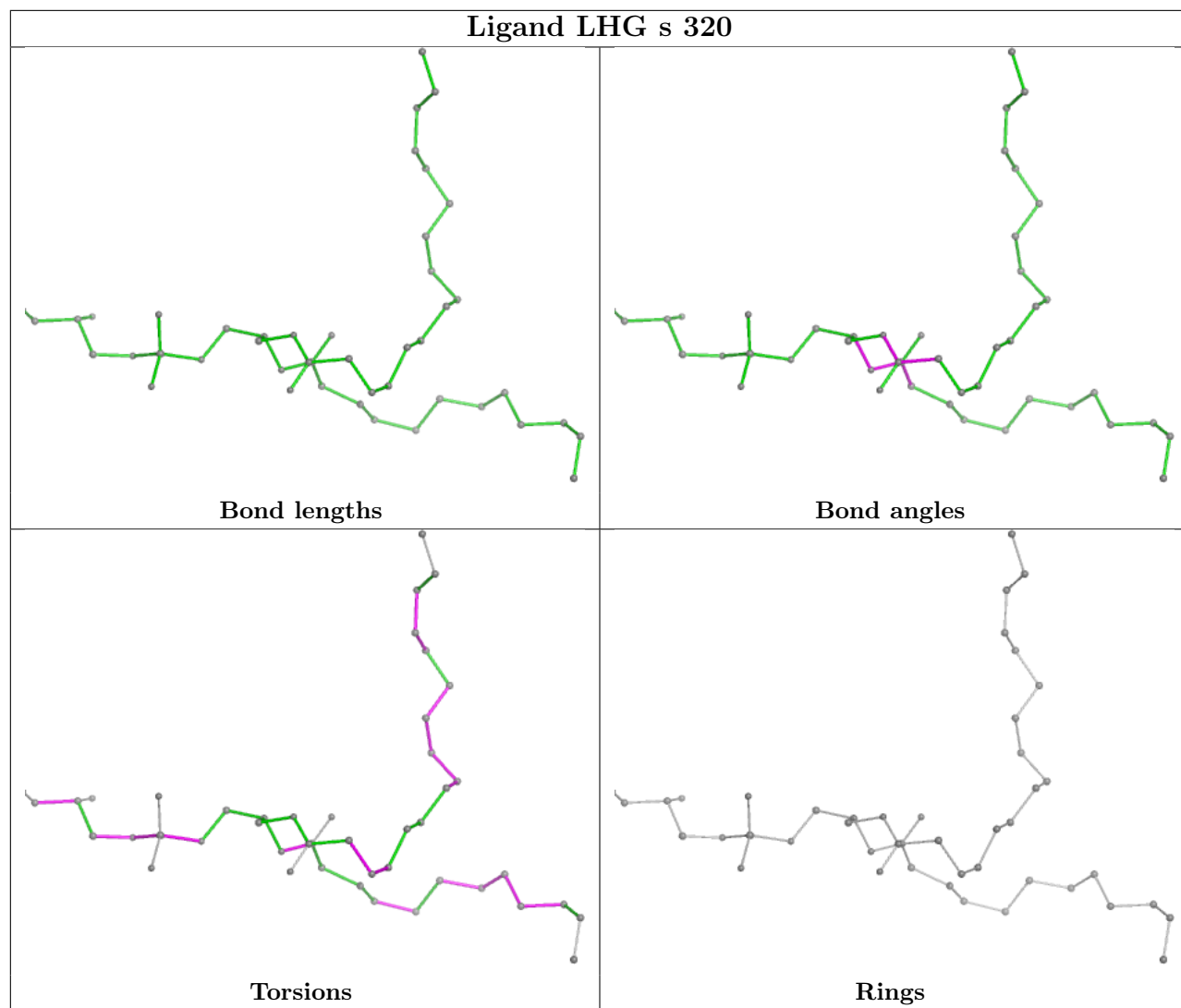


Ligand CLA s 304

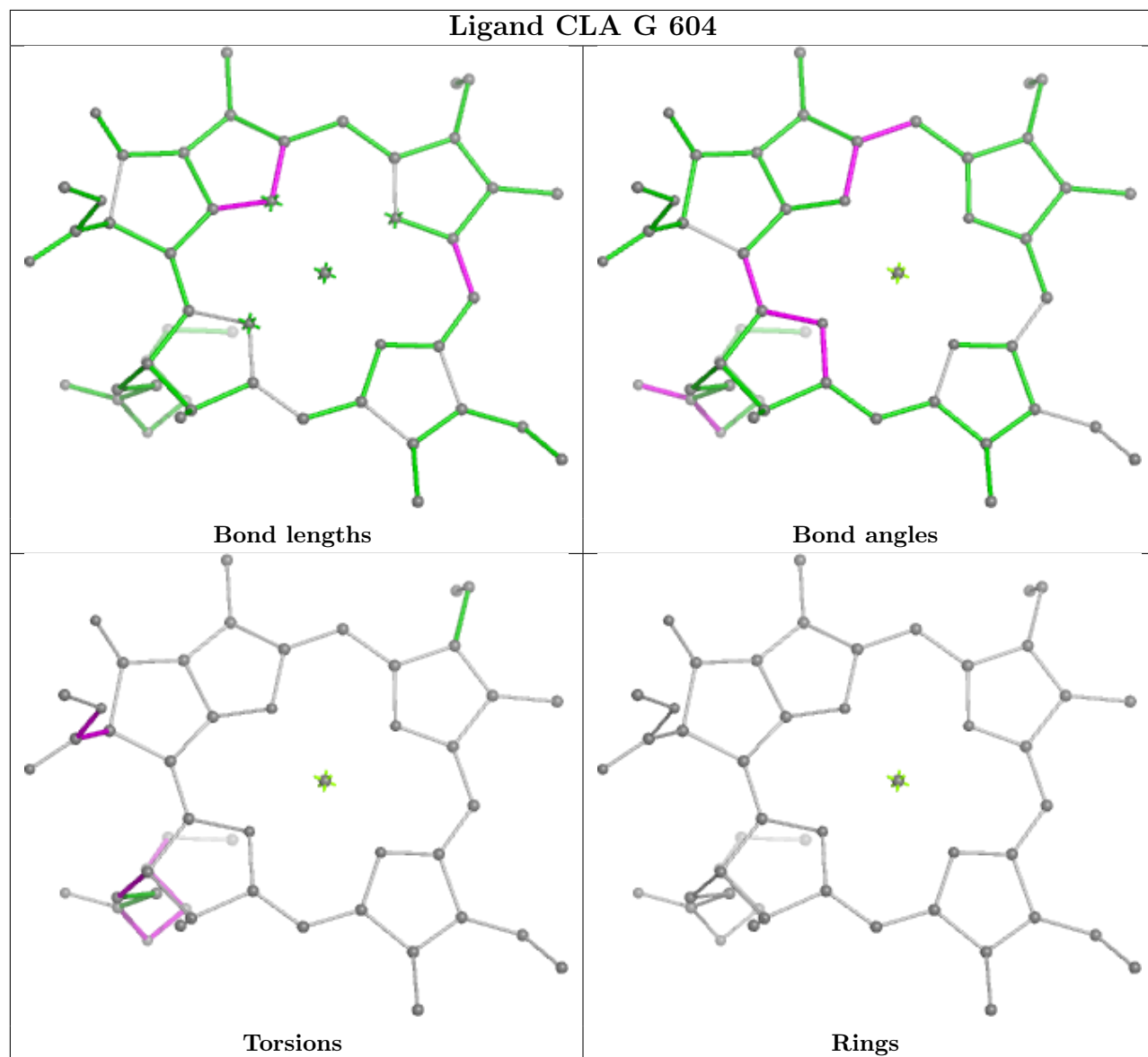


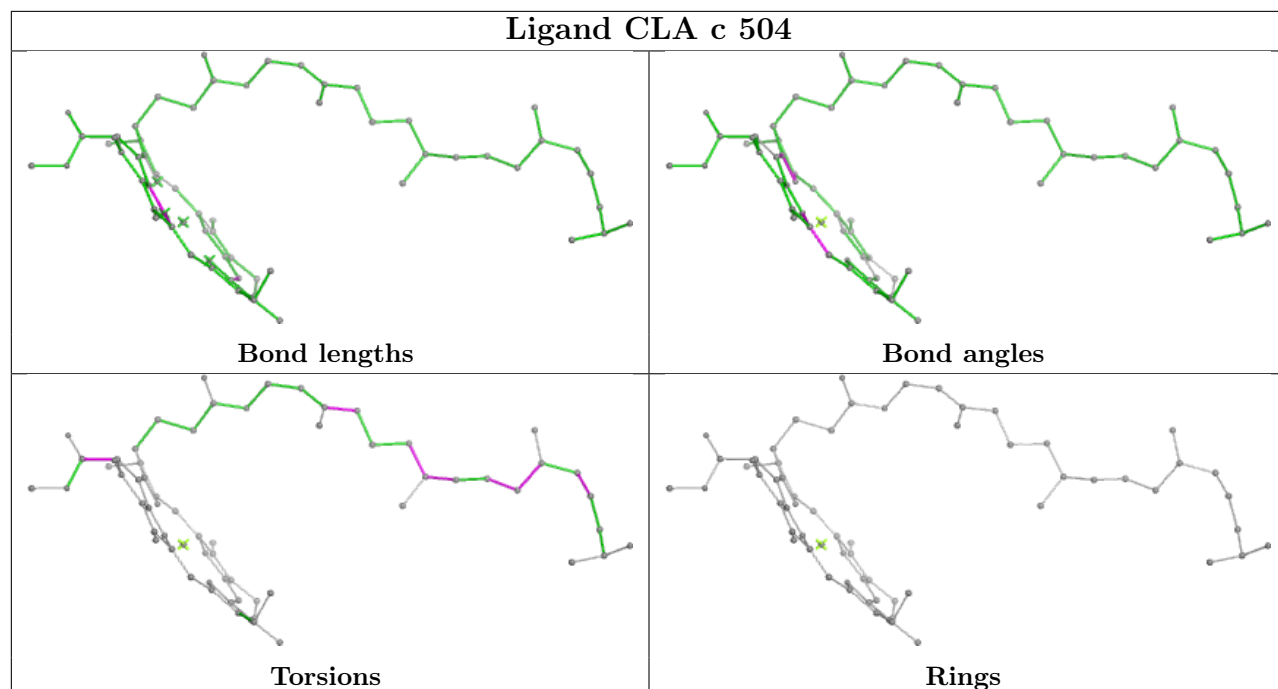
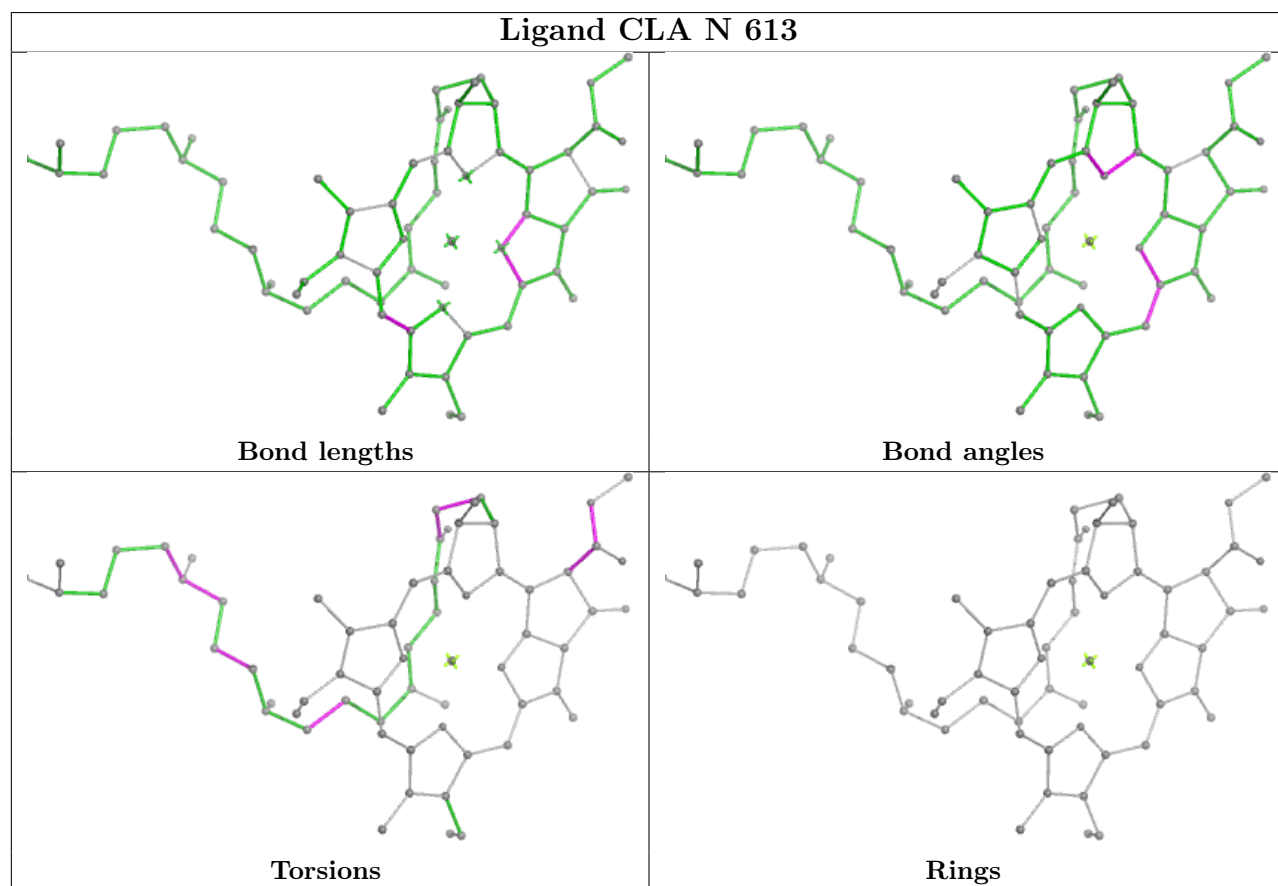


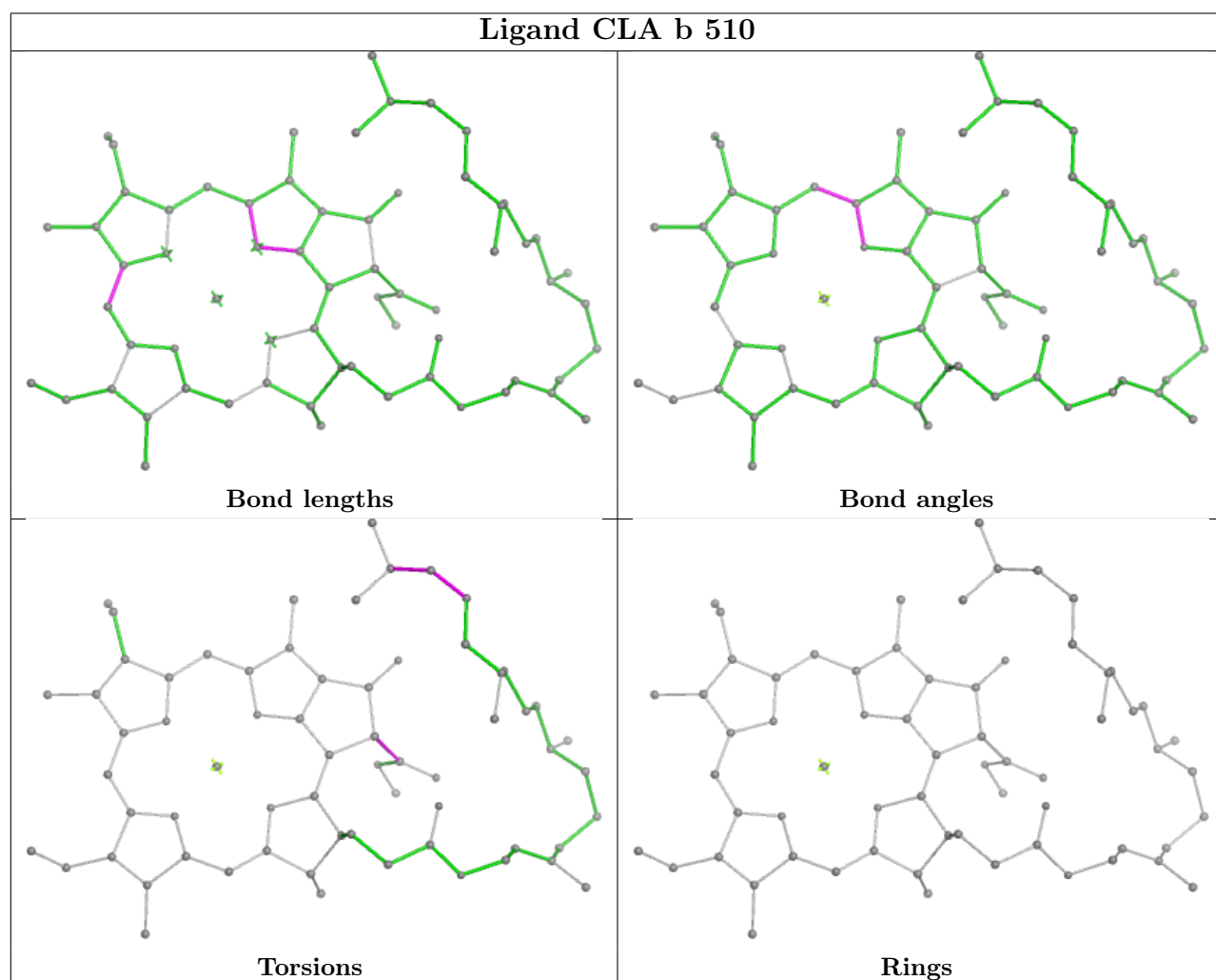
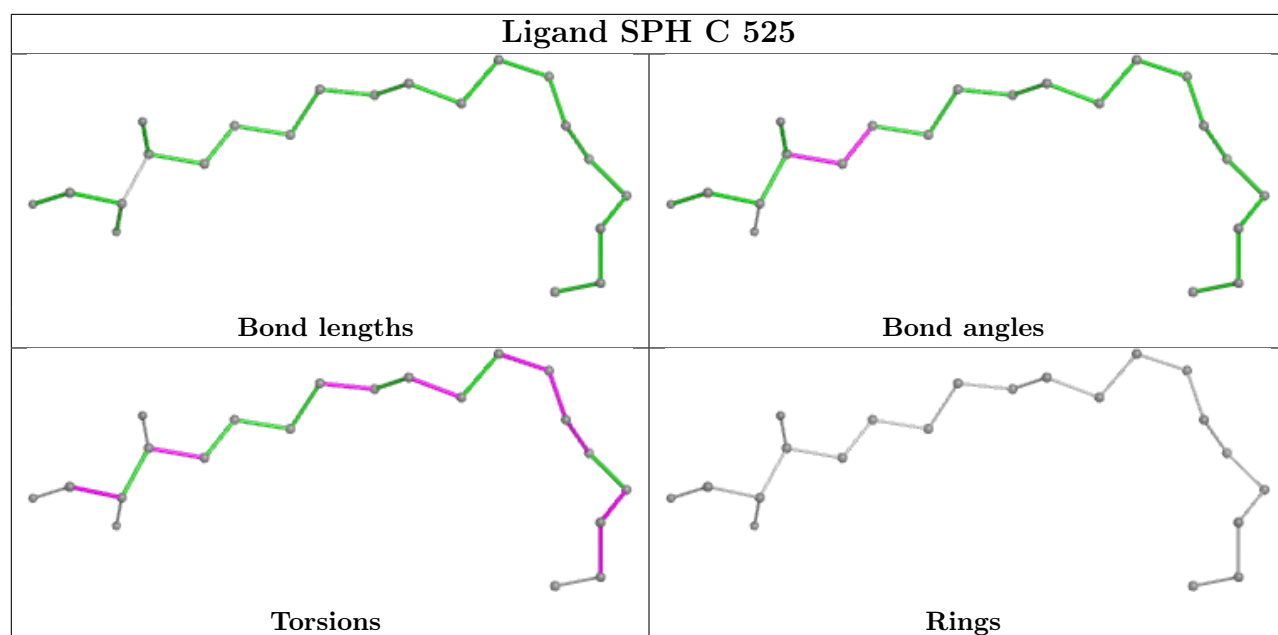


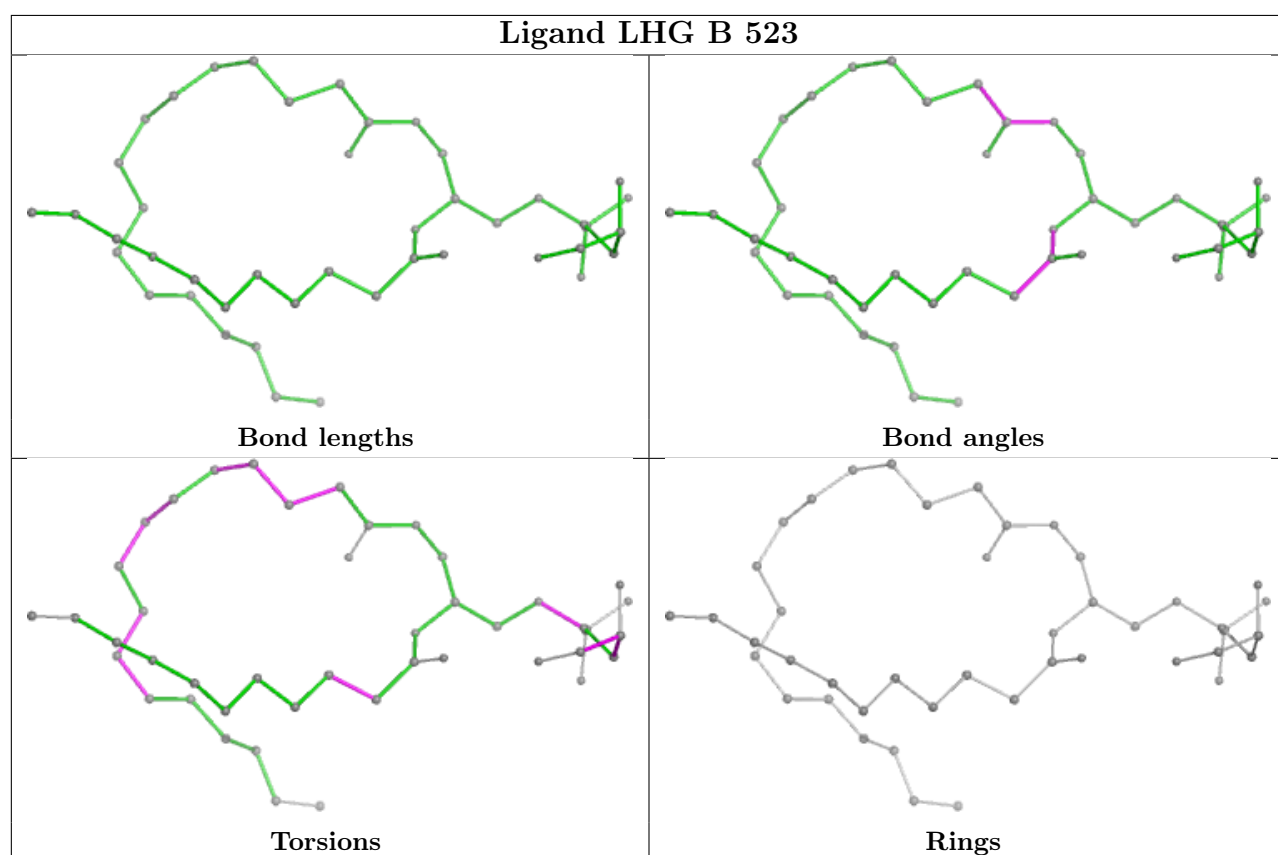
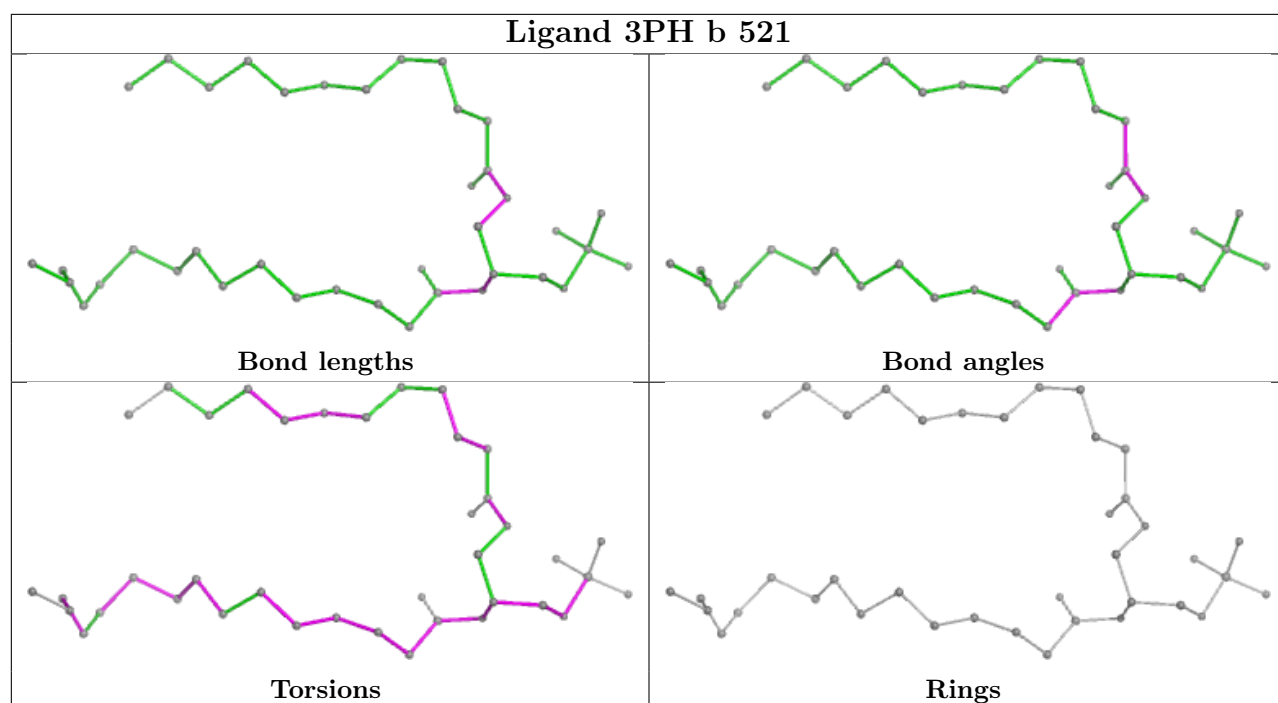


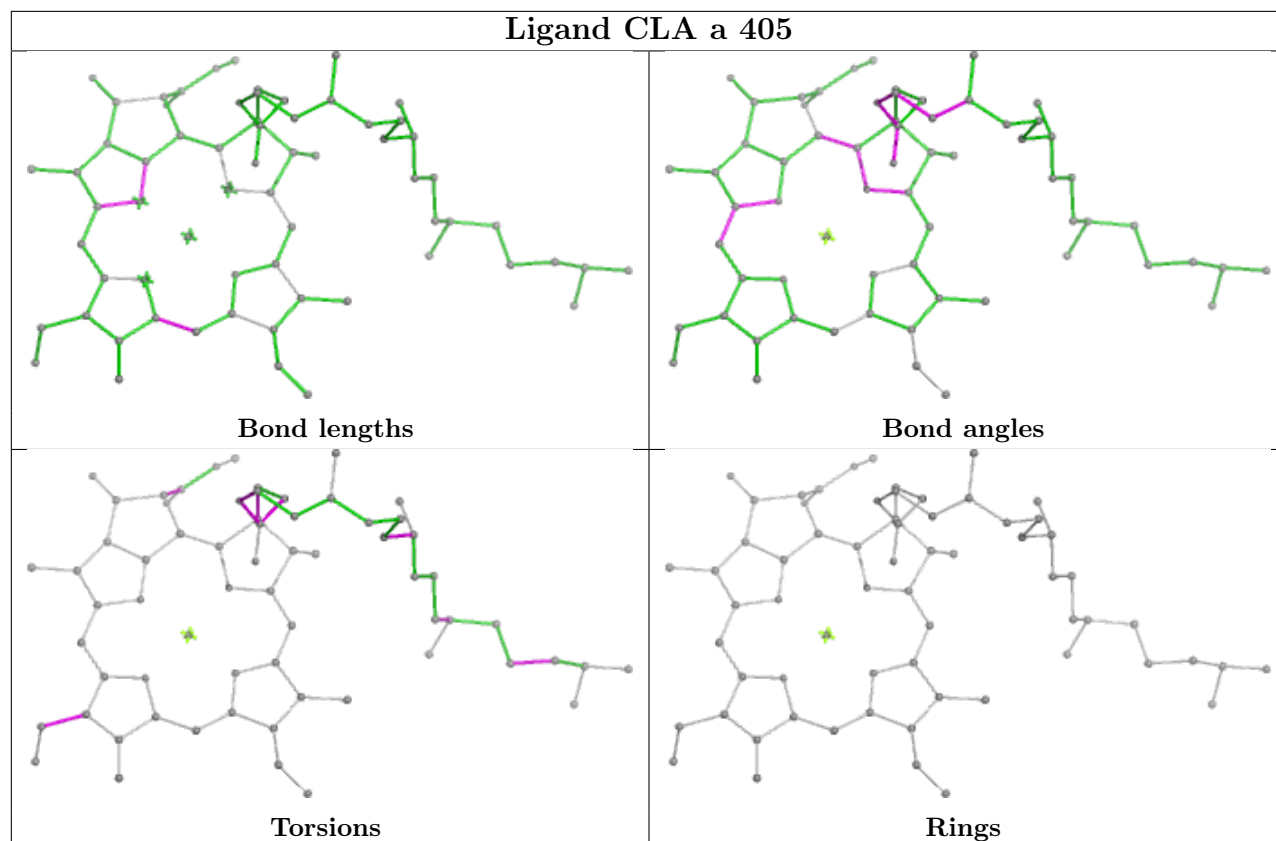
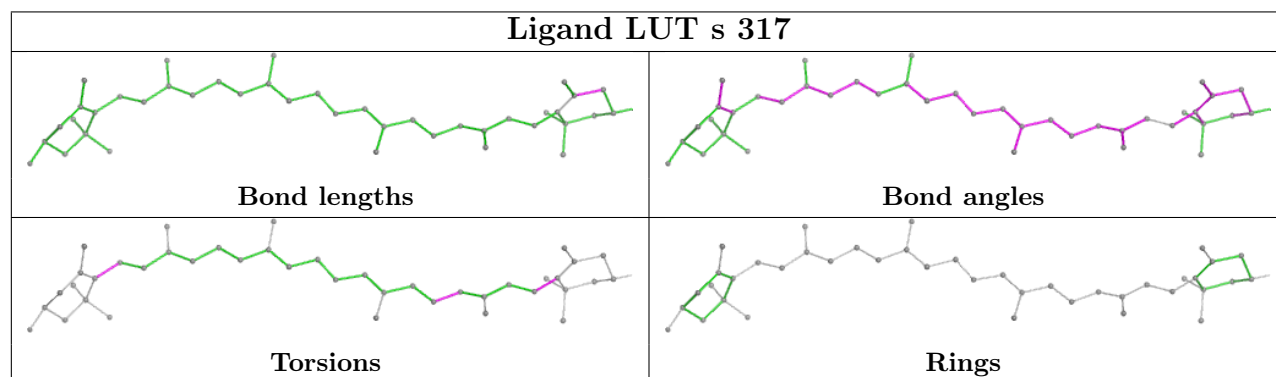
Ligand CLA G 604

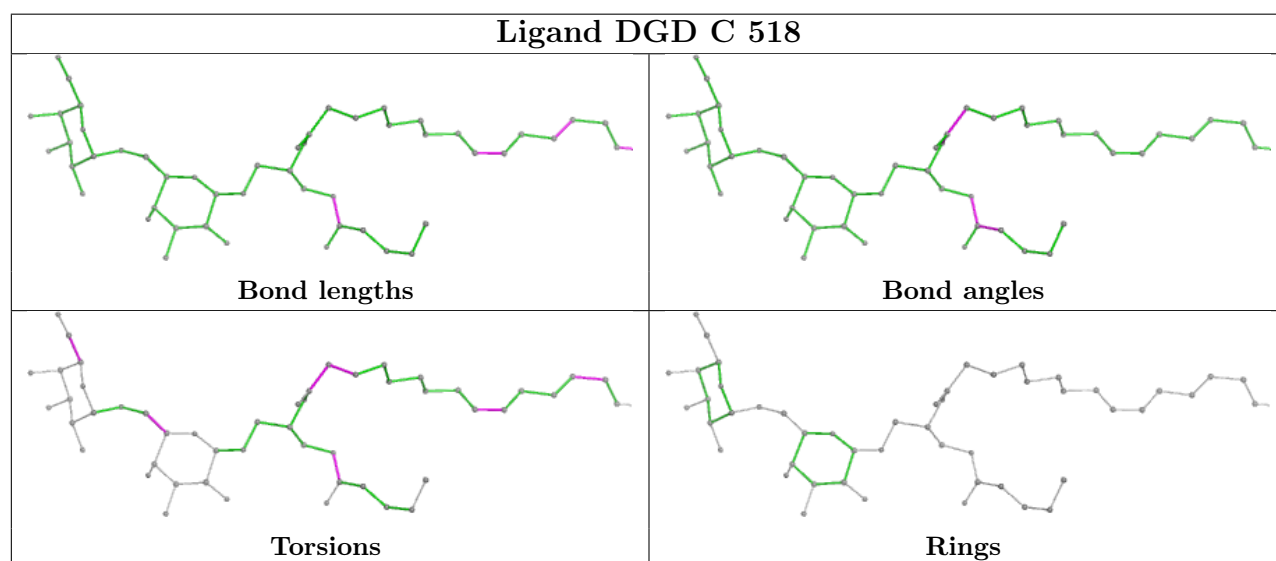
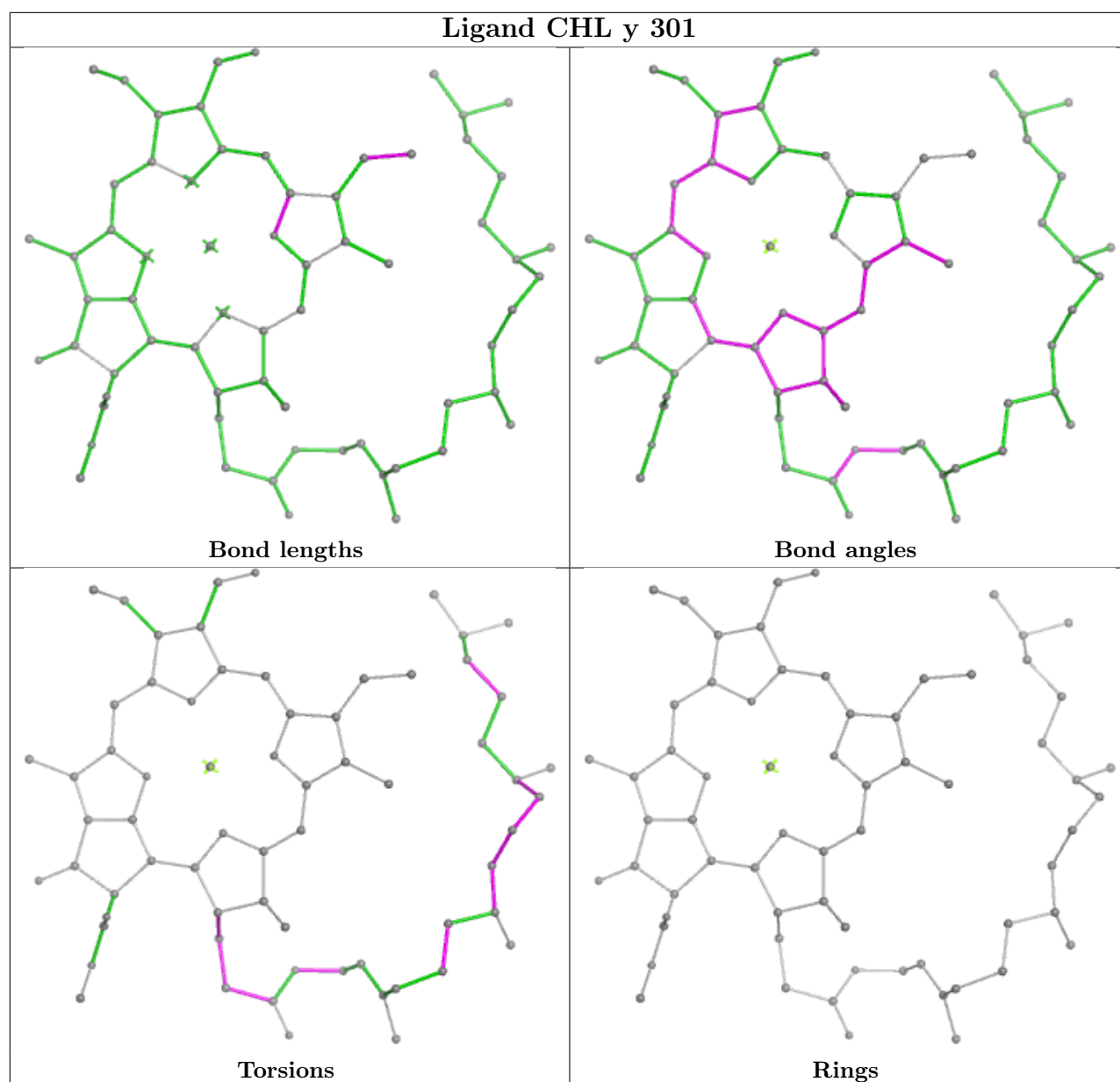


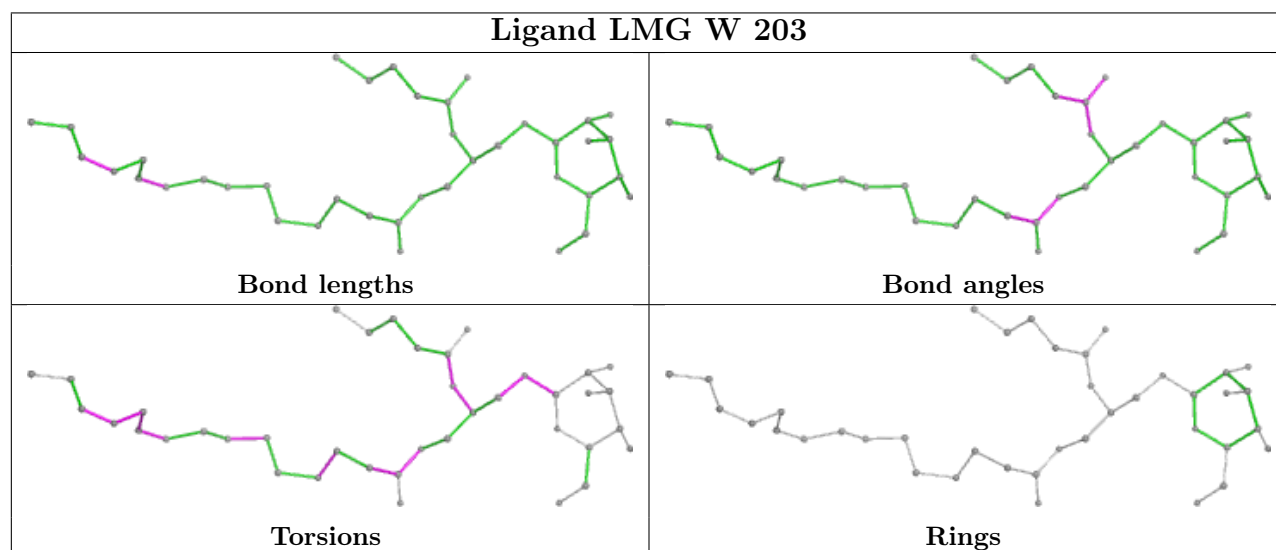
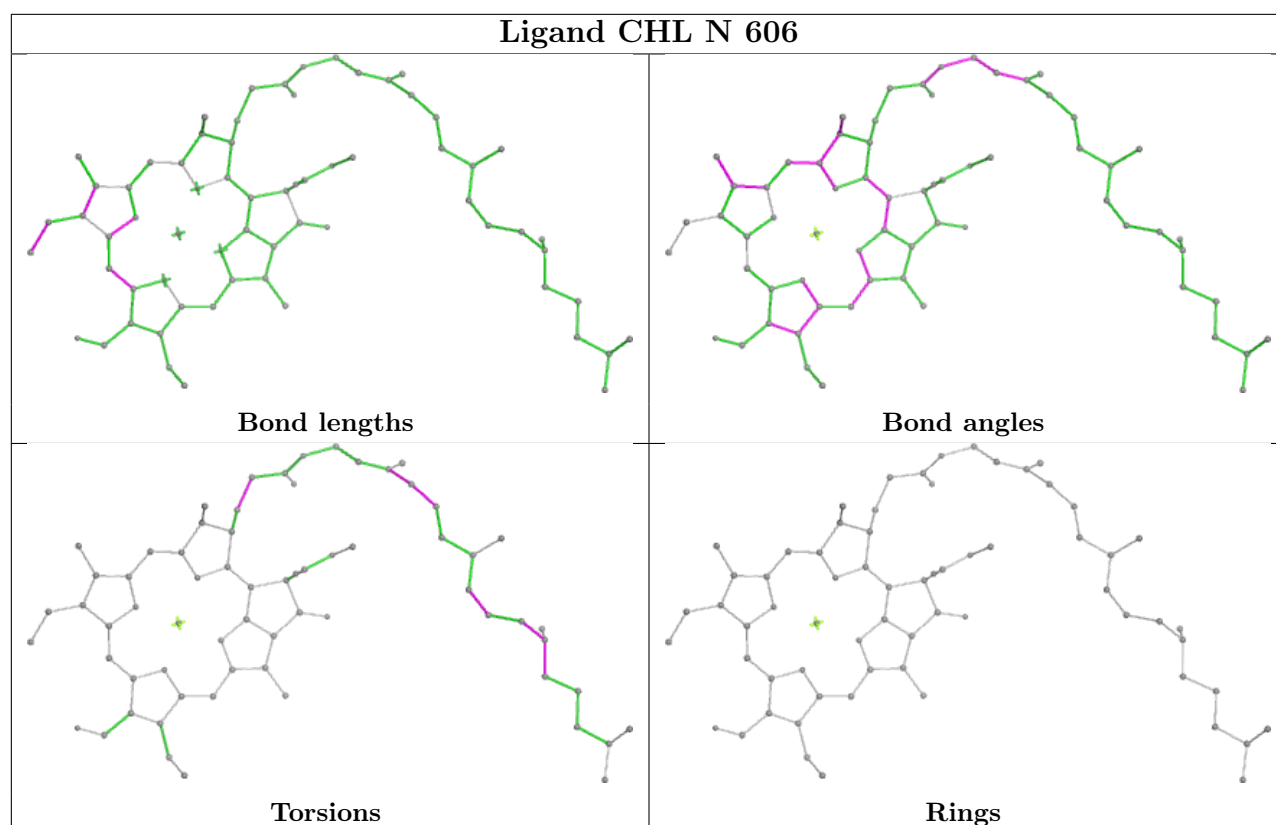
Ligand CLA c 504**Ligand CLA N 613**

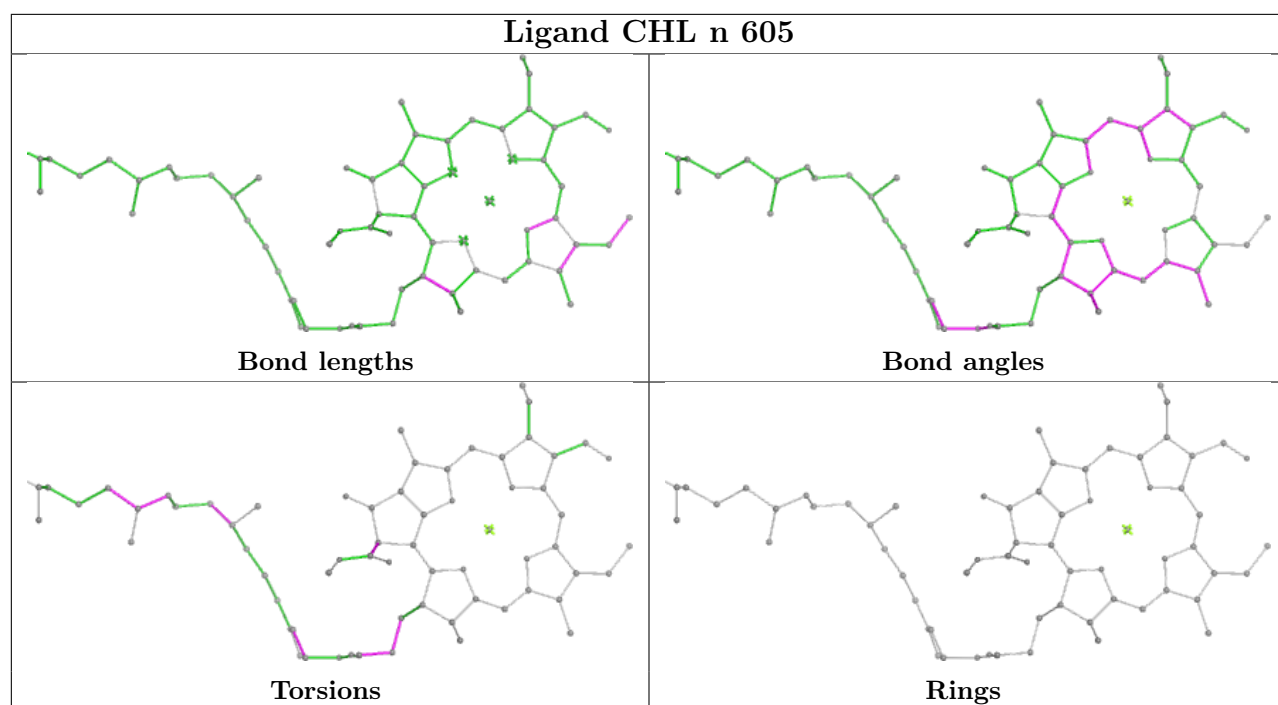




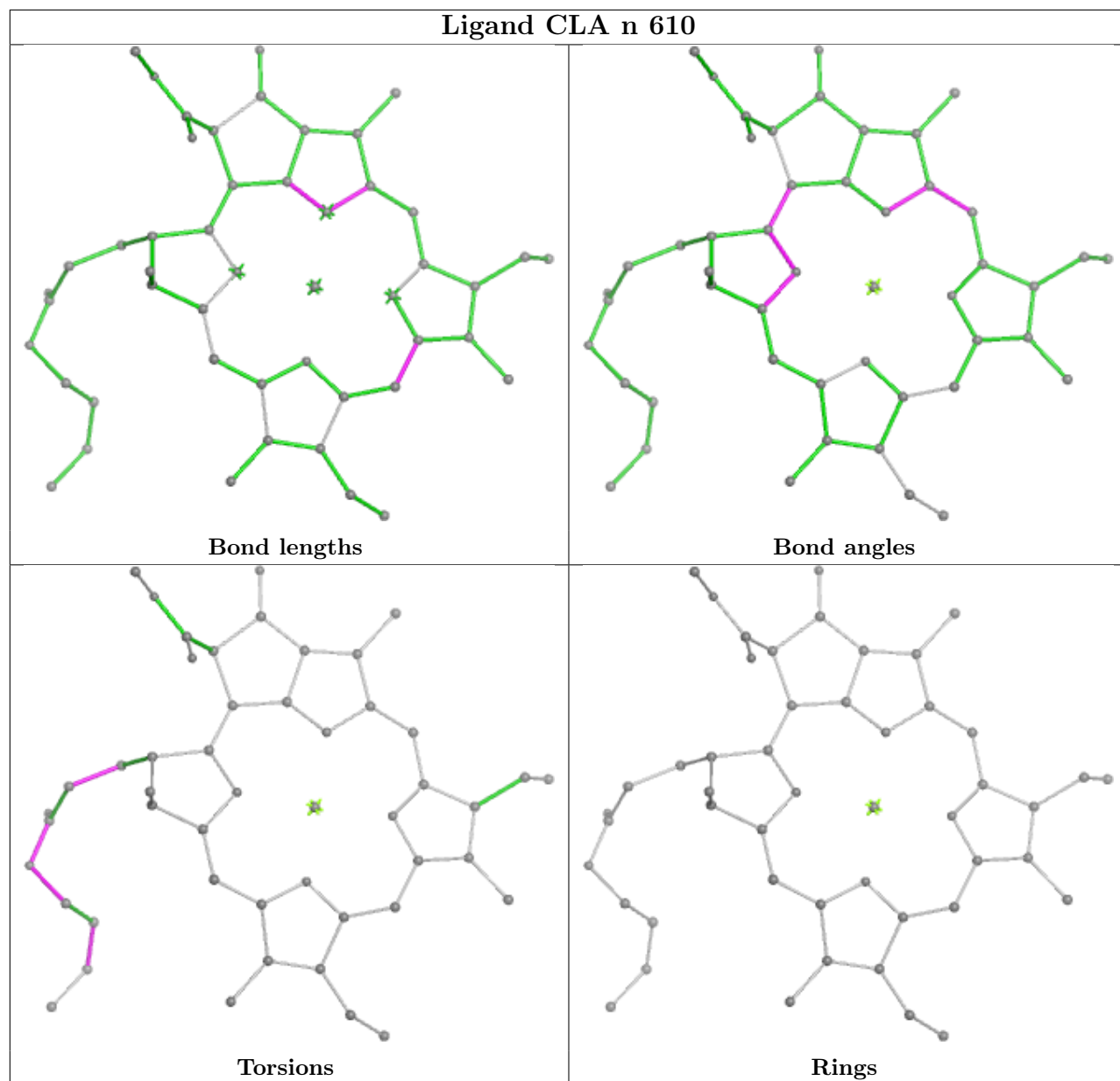
Ligand CLA a 405**Ligand LUT s 317**

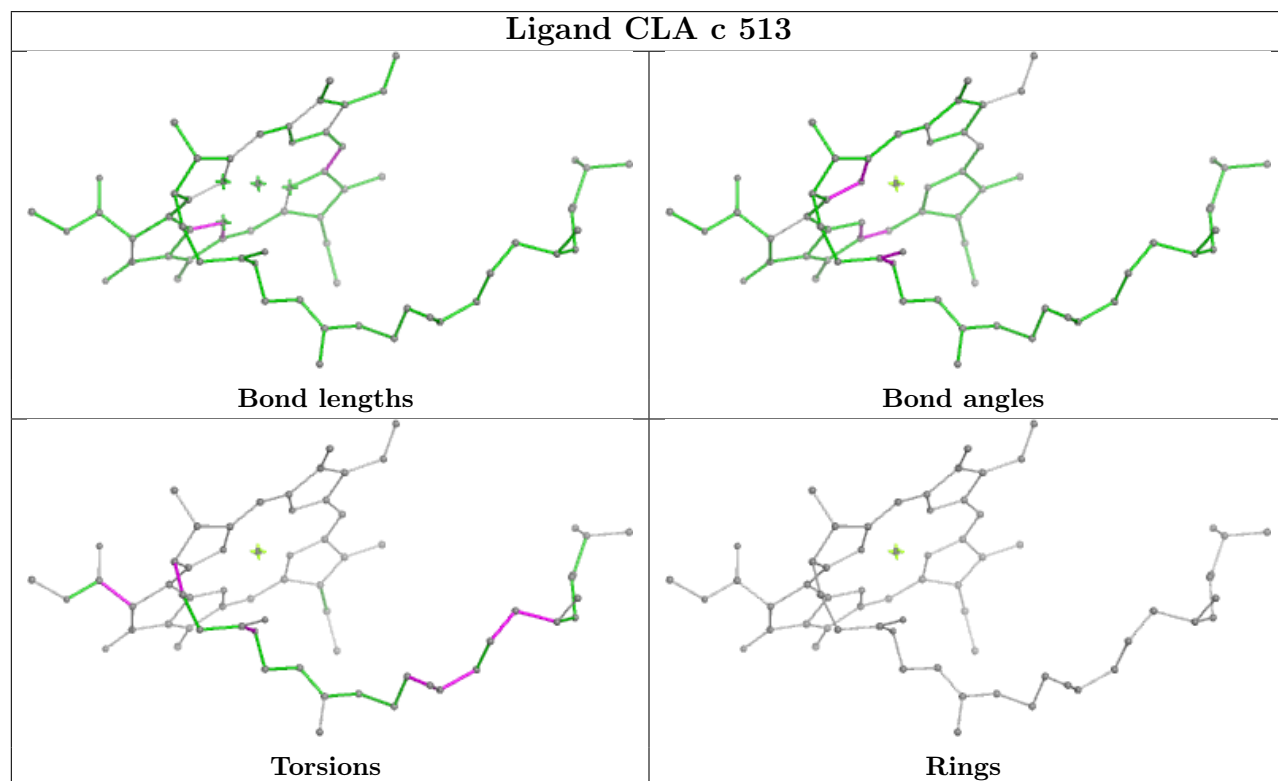
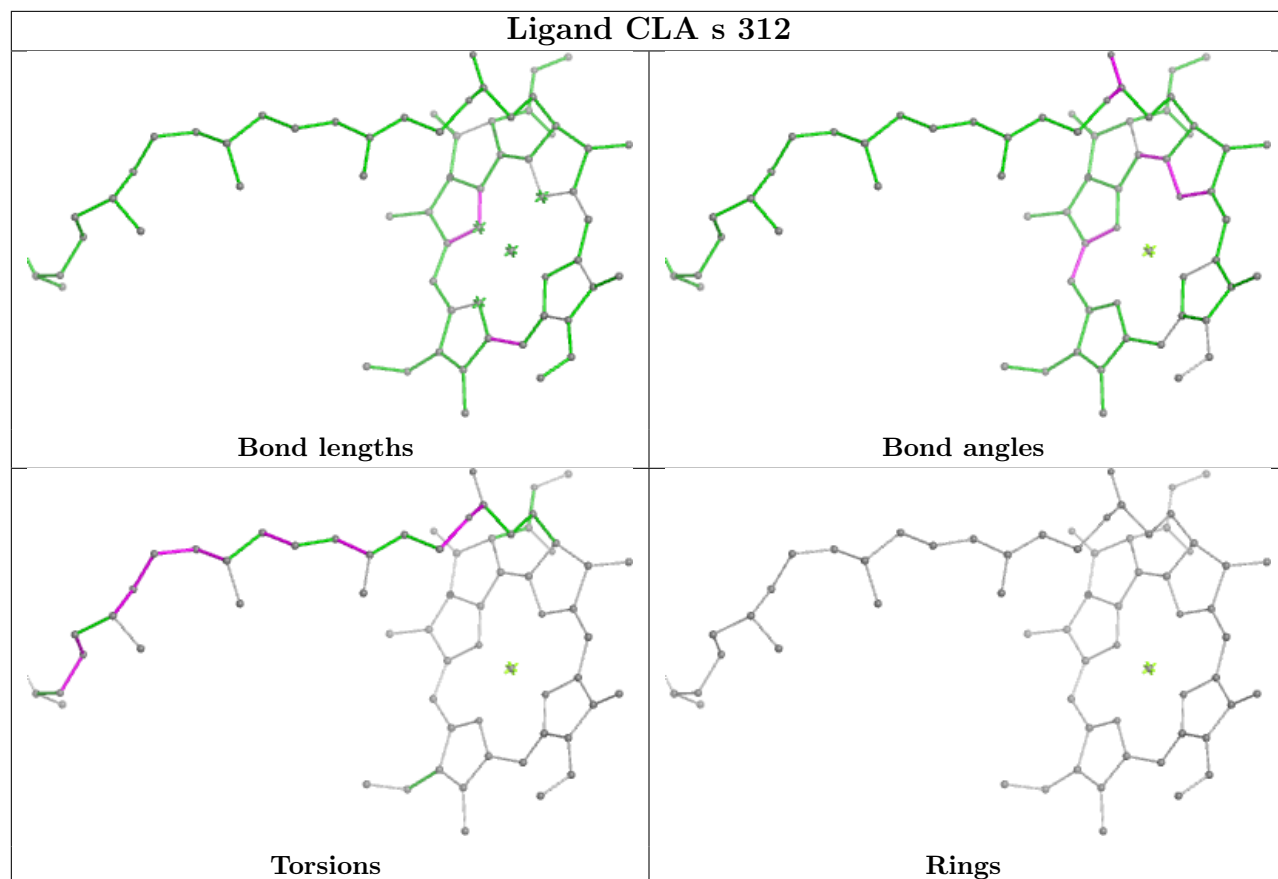




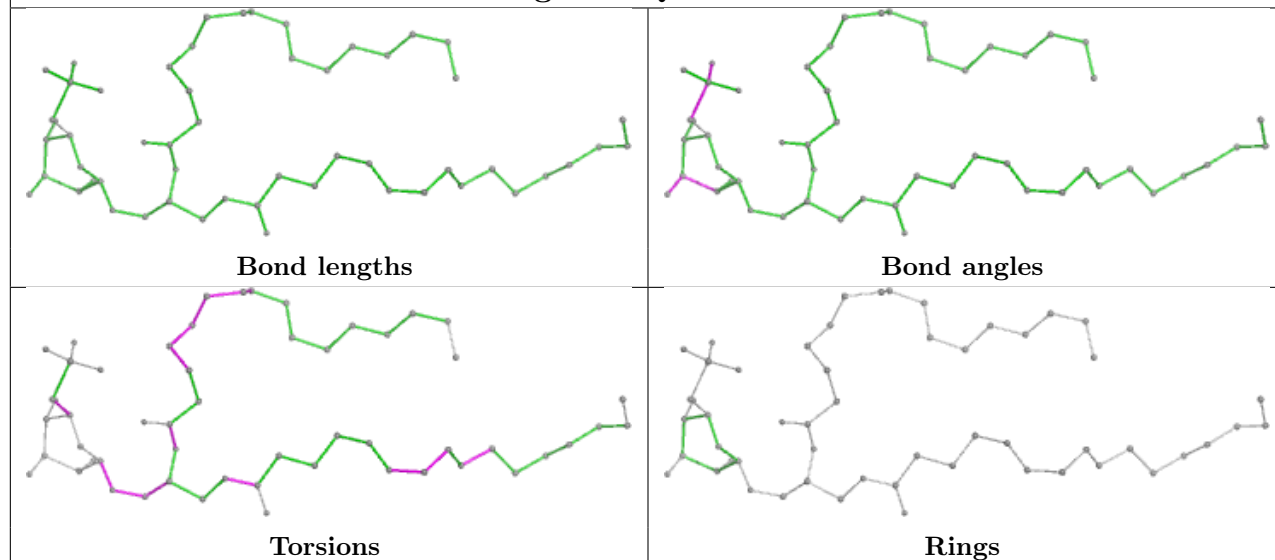


Ligand CLA n 610

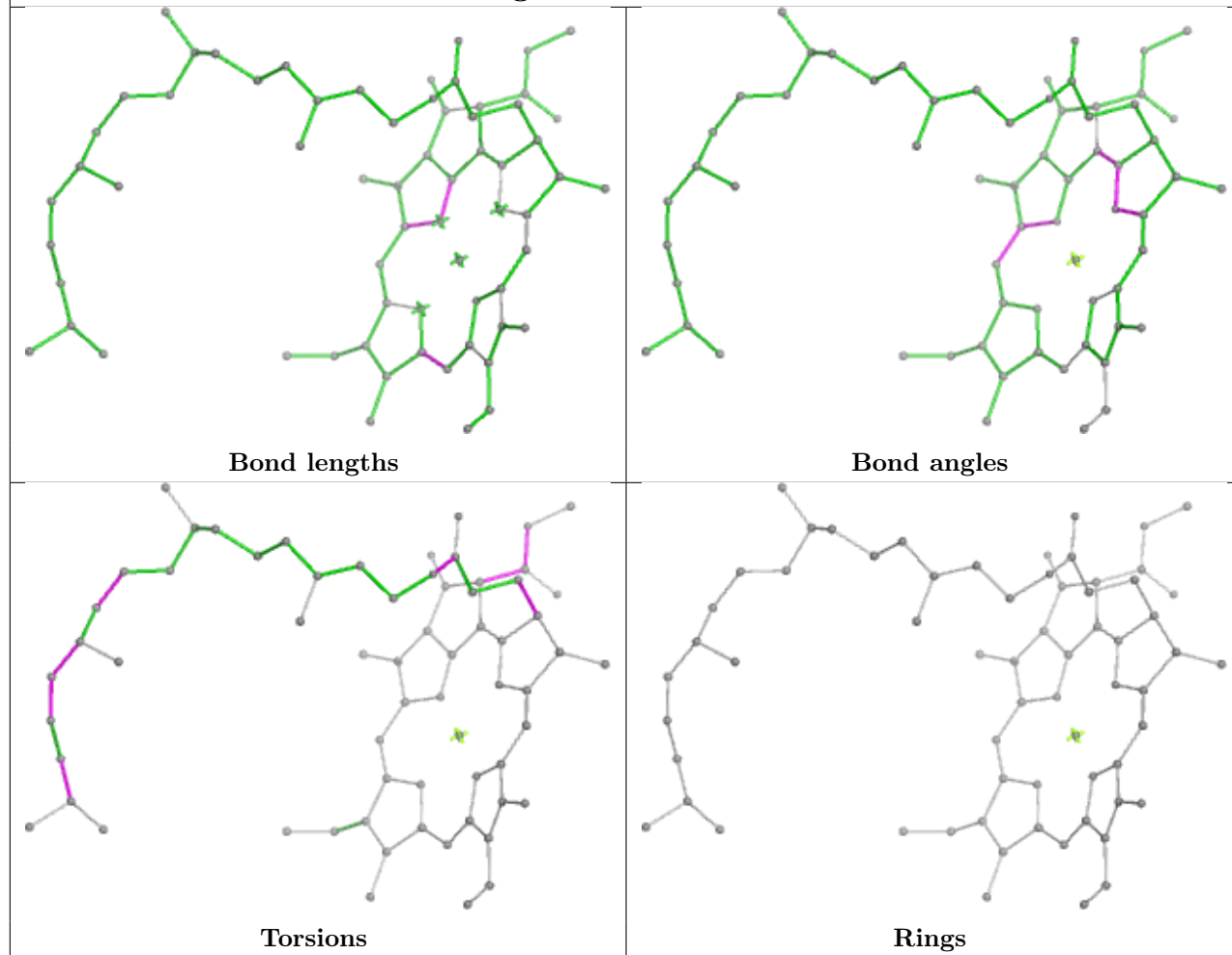




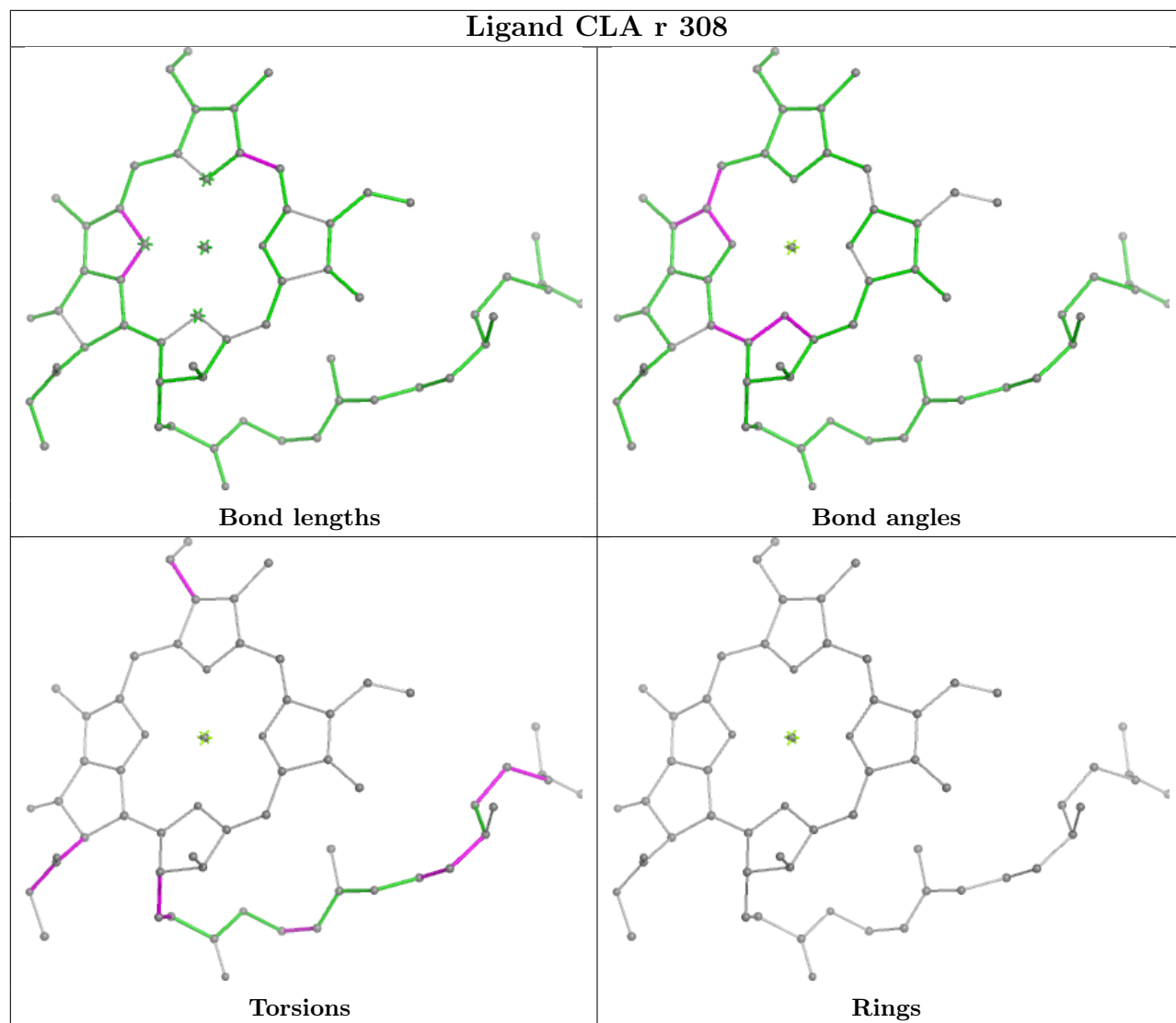
Ligand SQD b 523

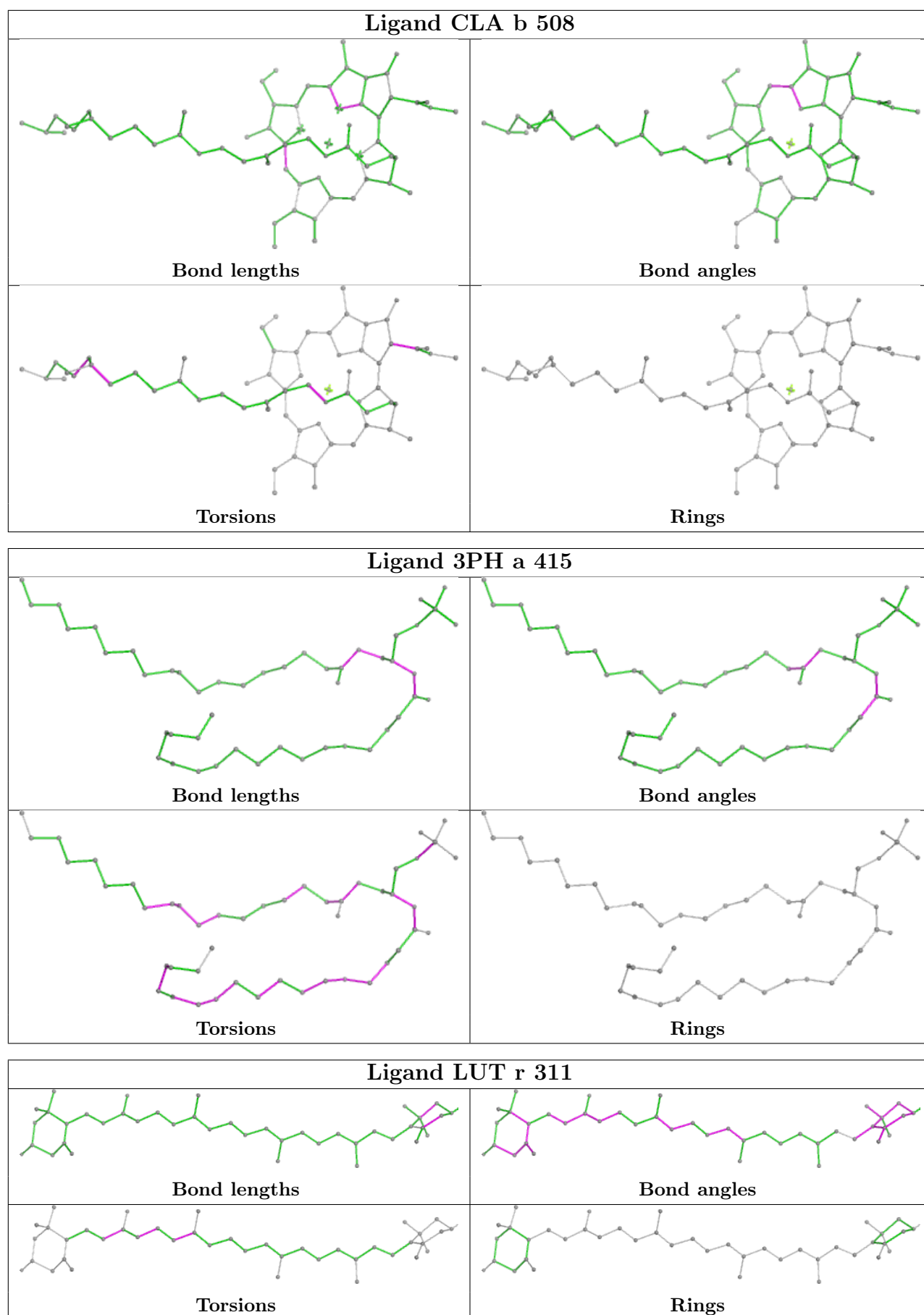


Ligand CLA G 611

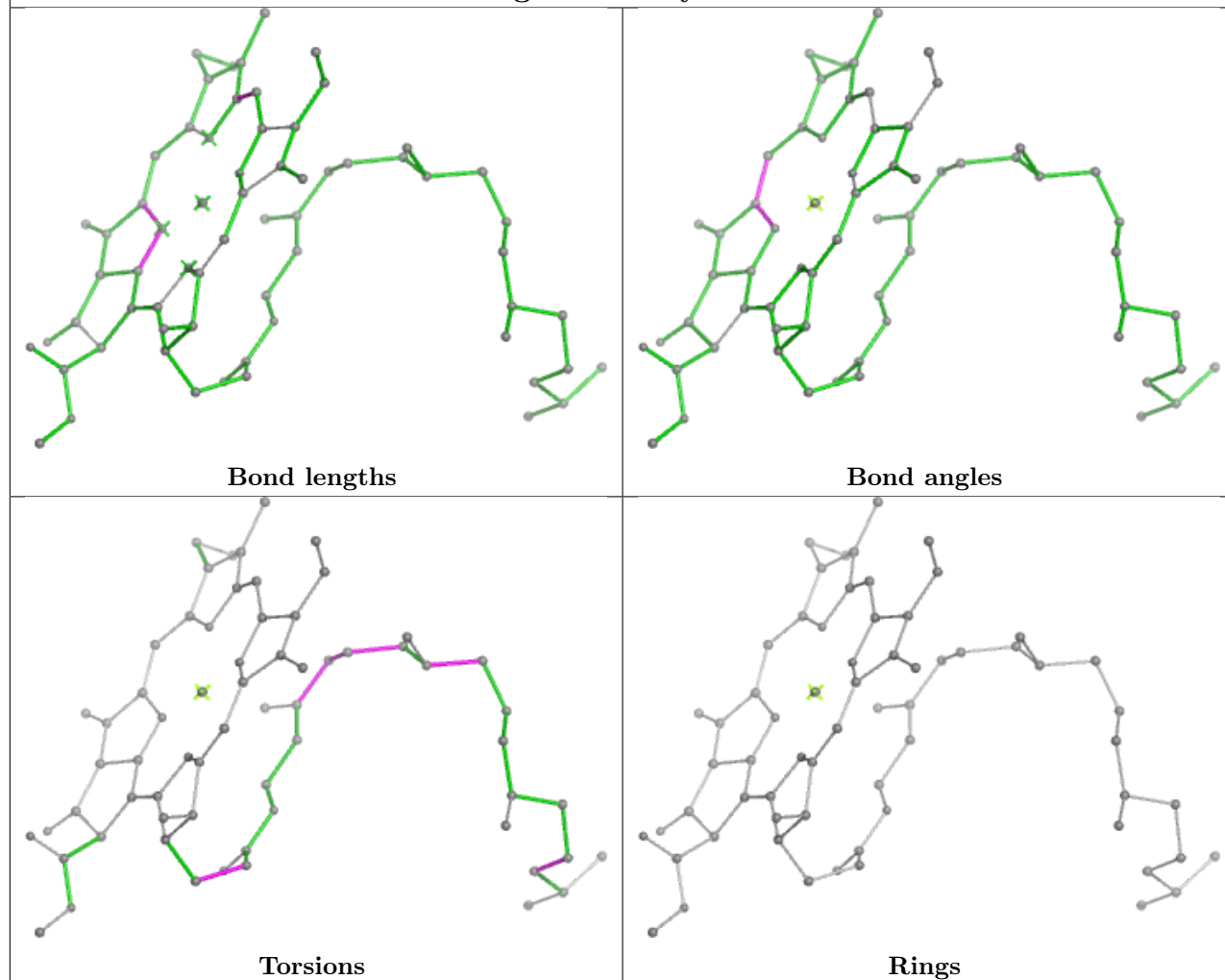


Ligand CLA r 308

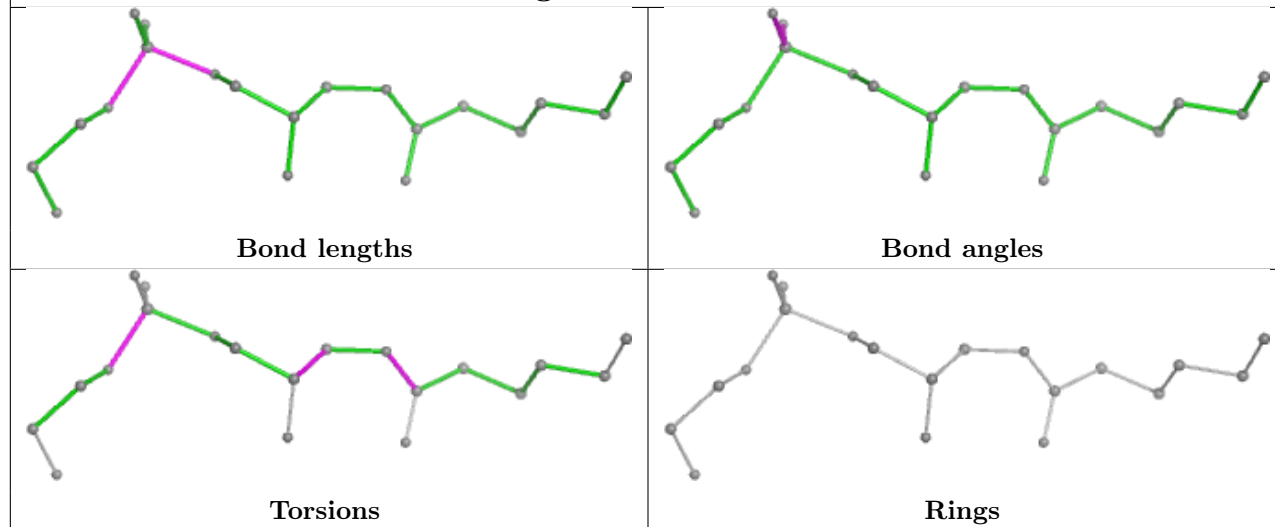


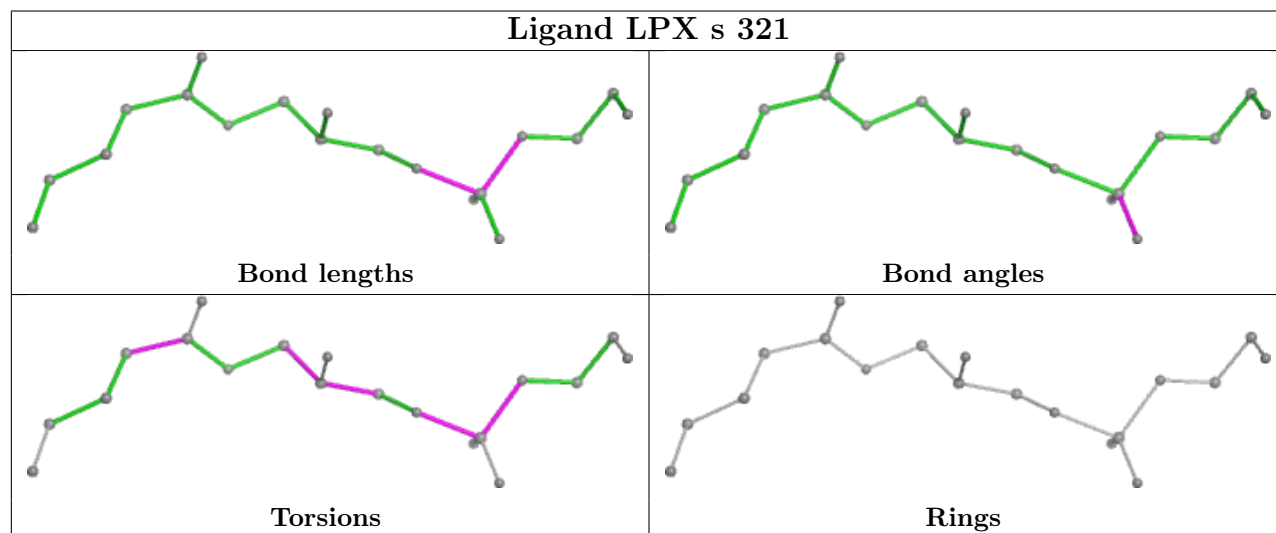
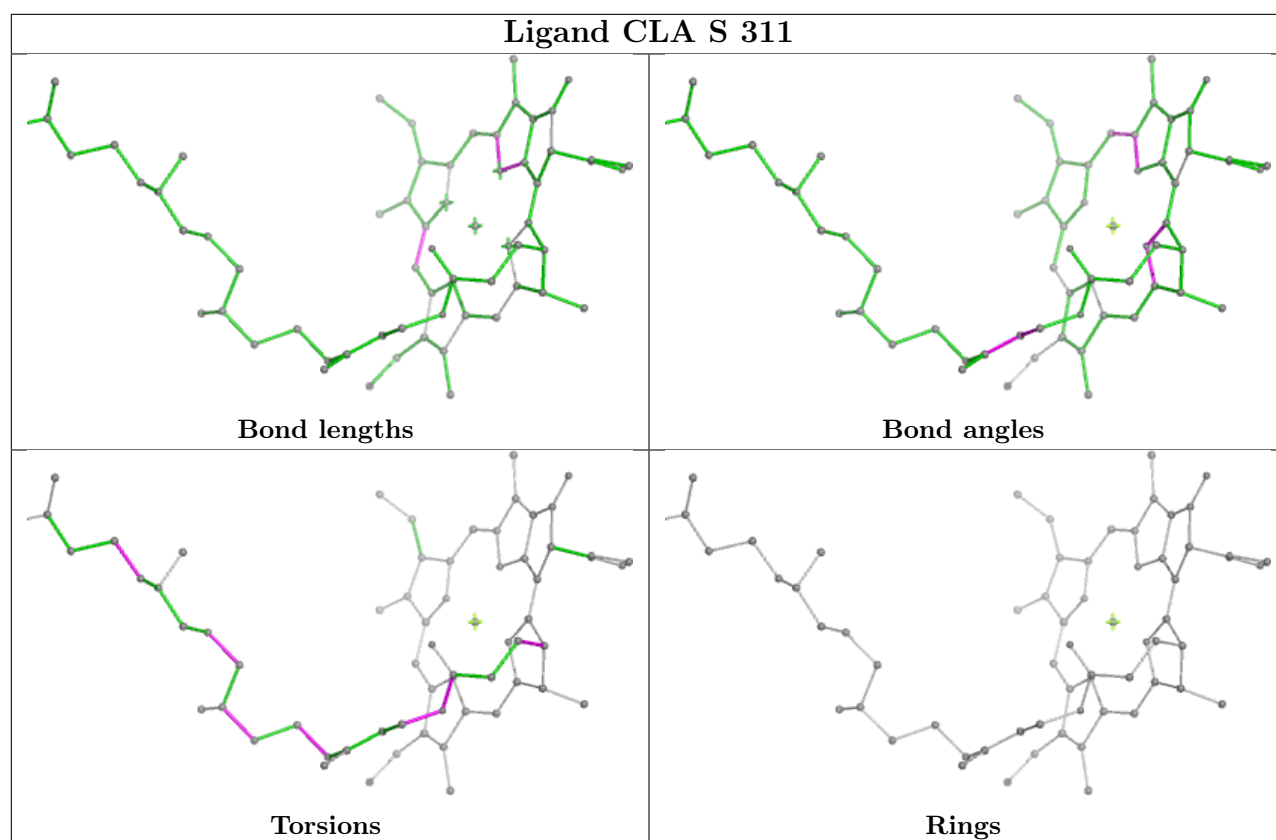


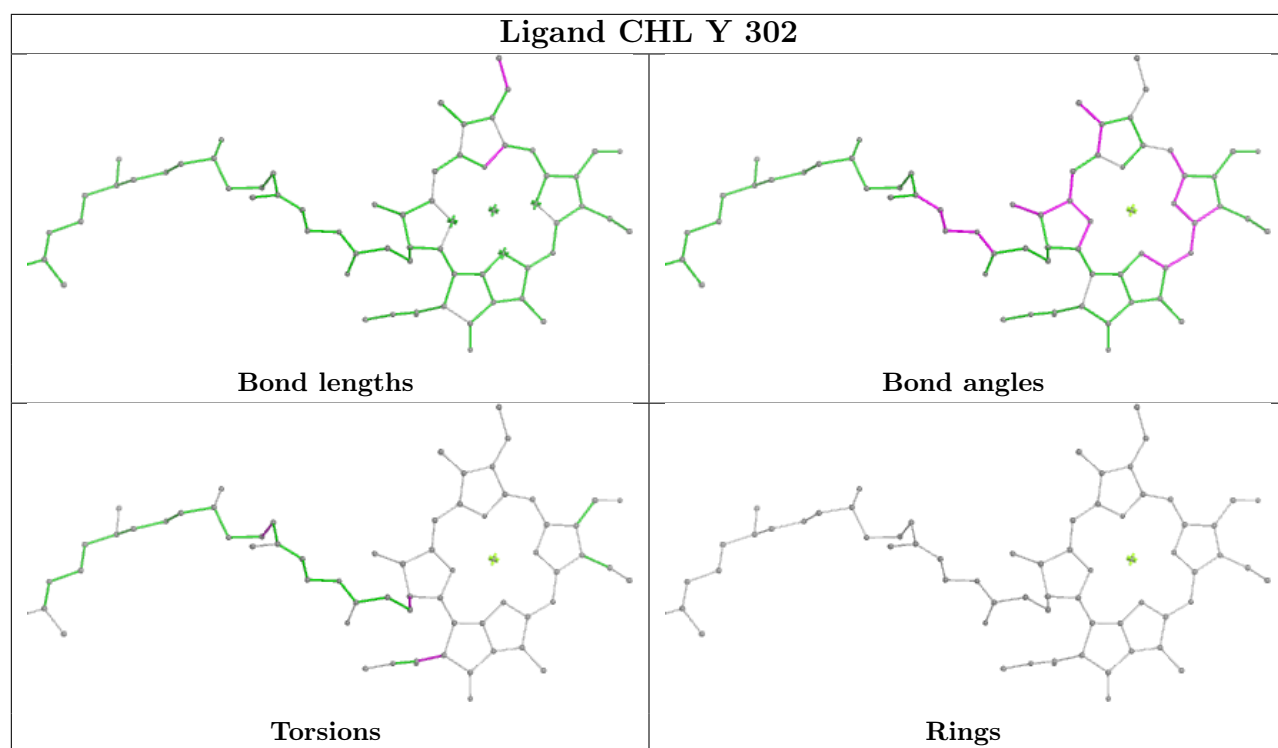
Ligand CLA y 315



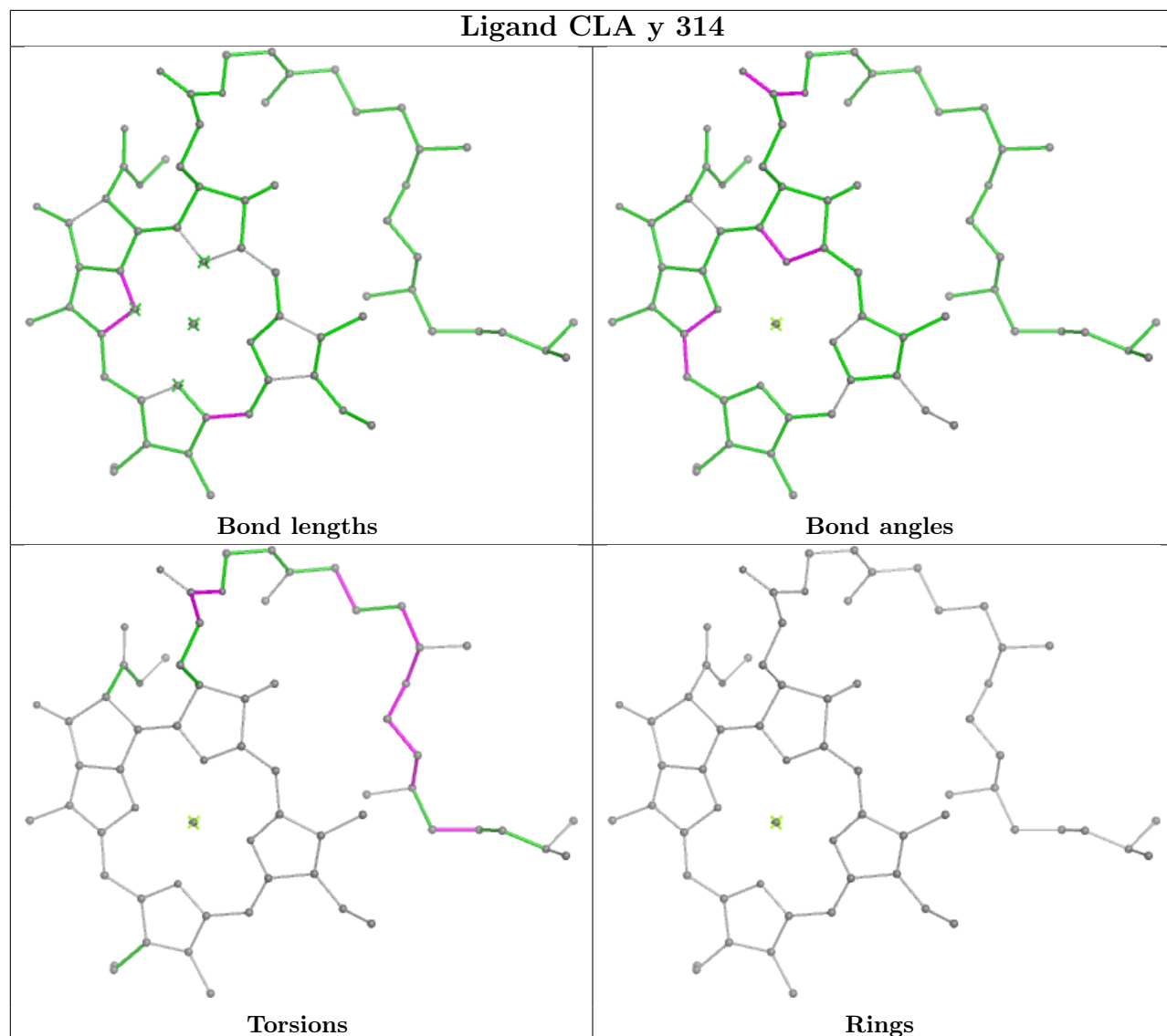
Ligand LPX S 321



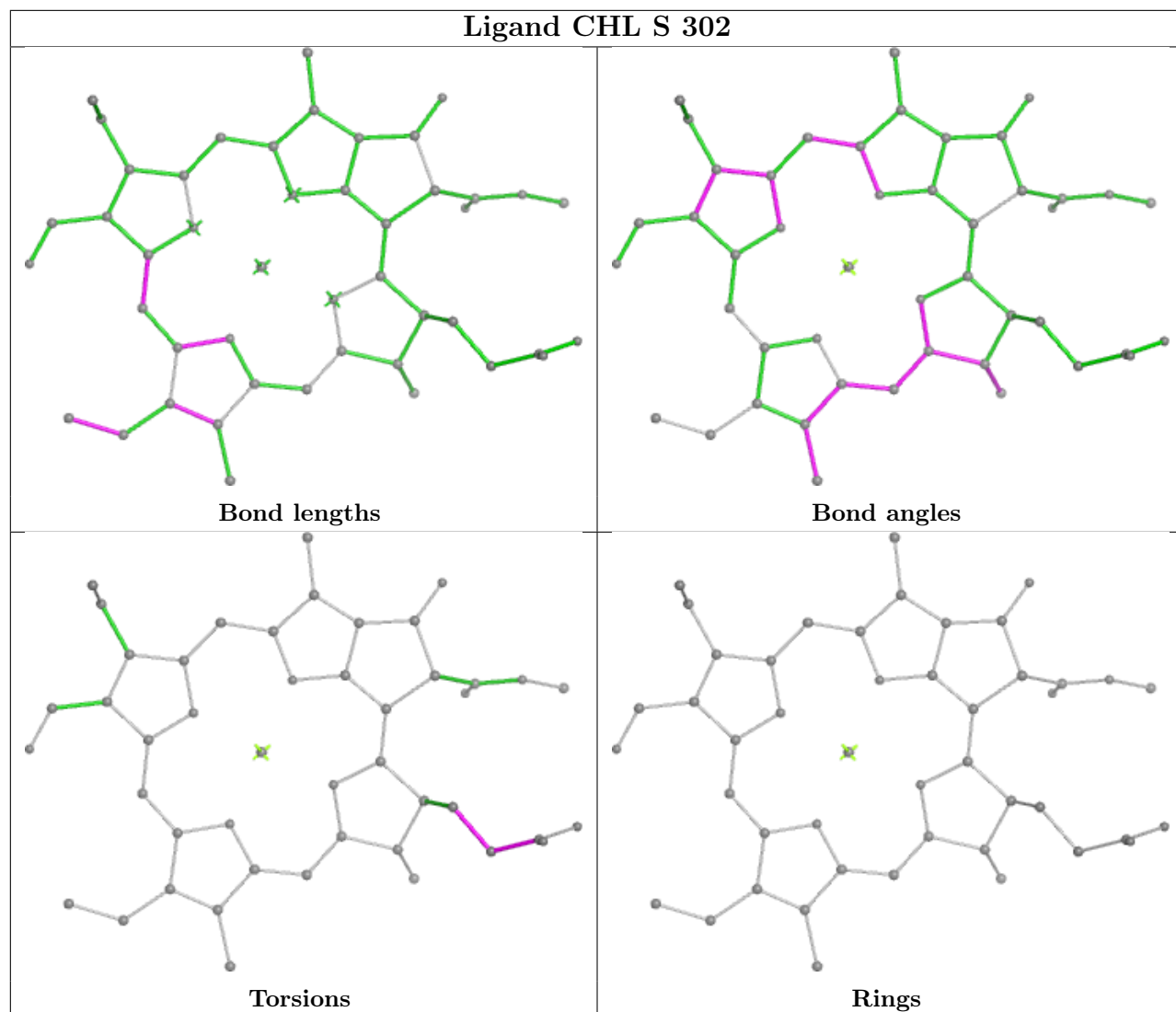




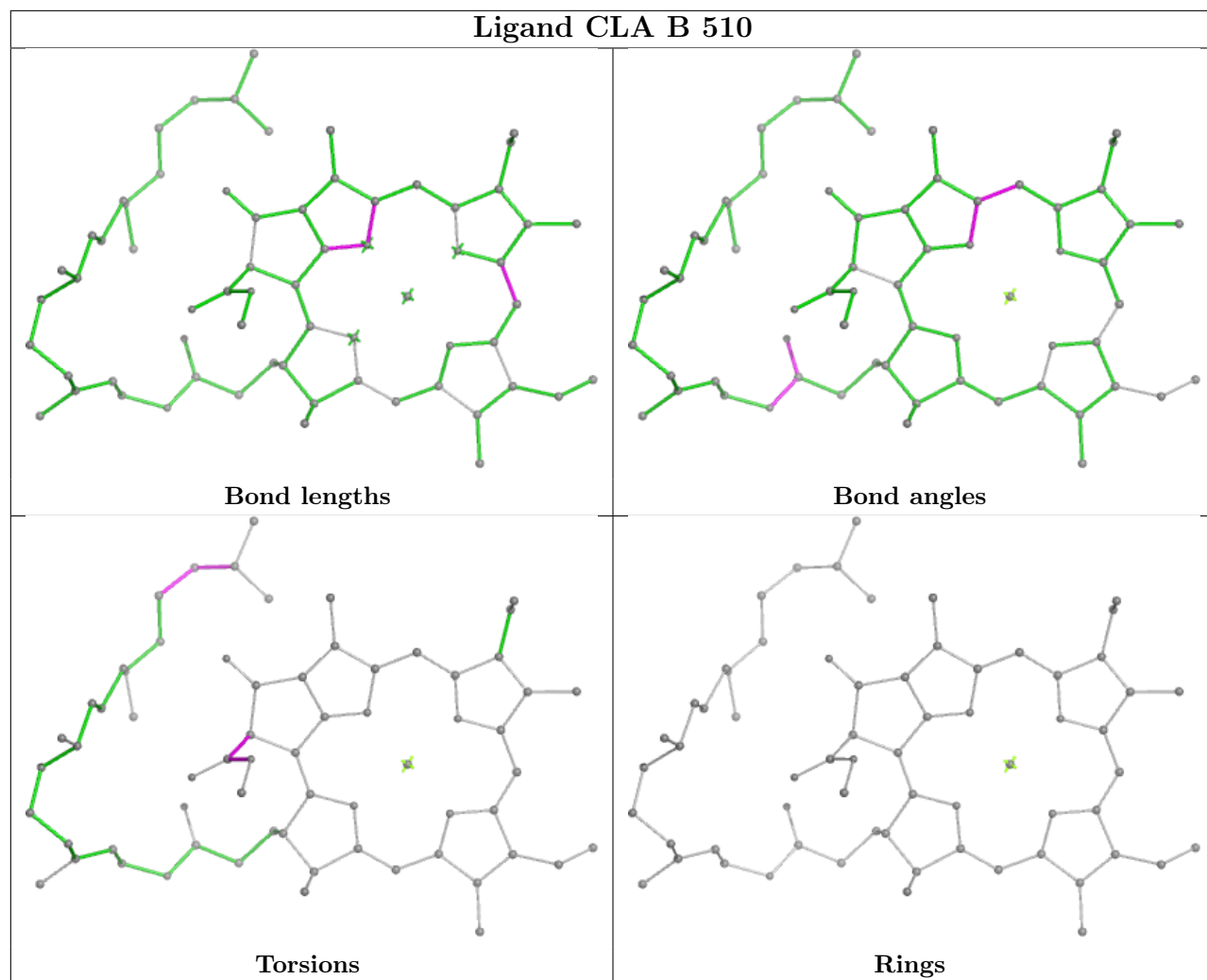
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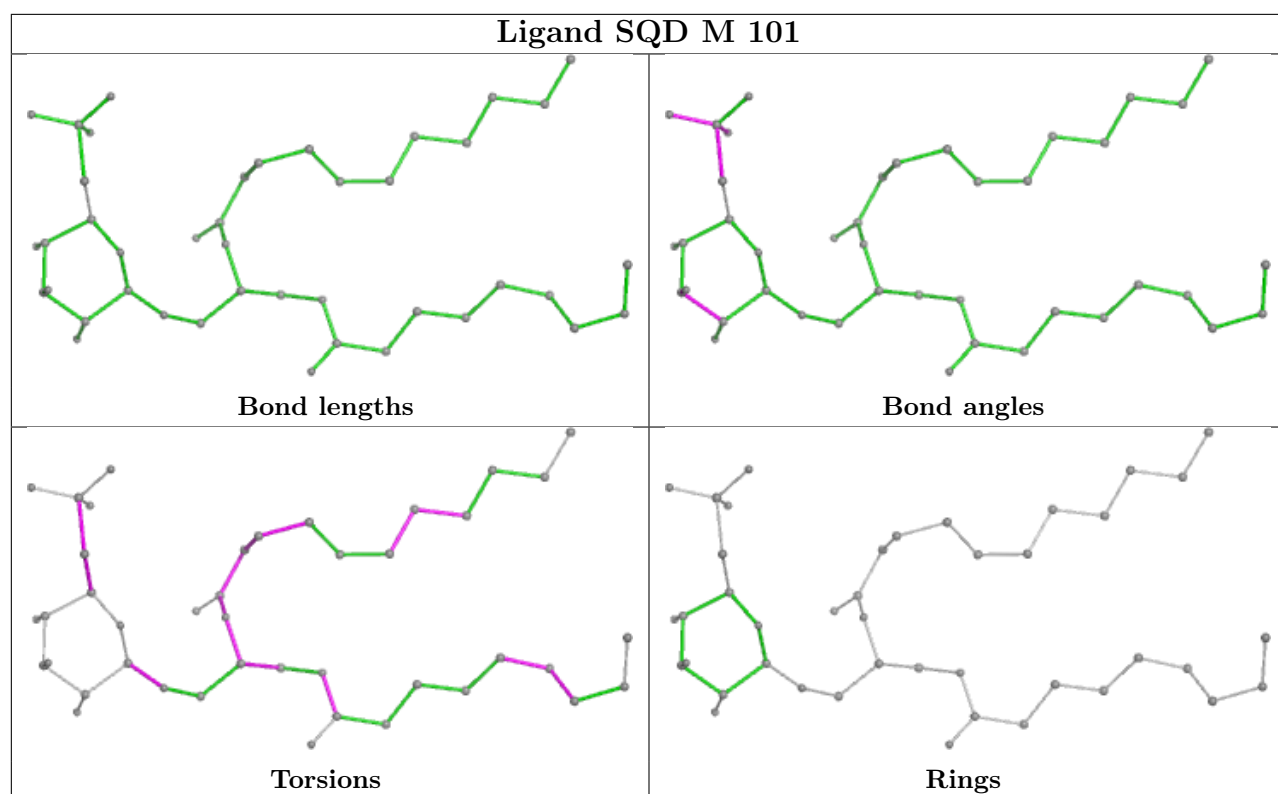


Ligand CHL S 302

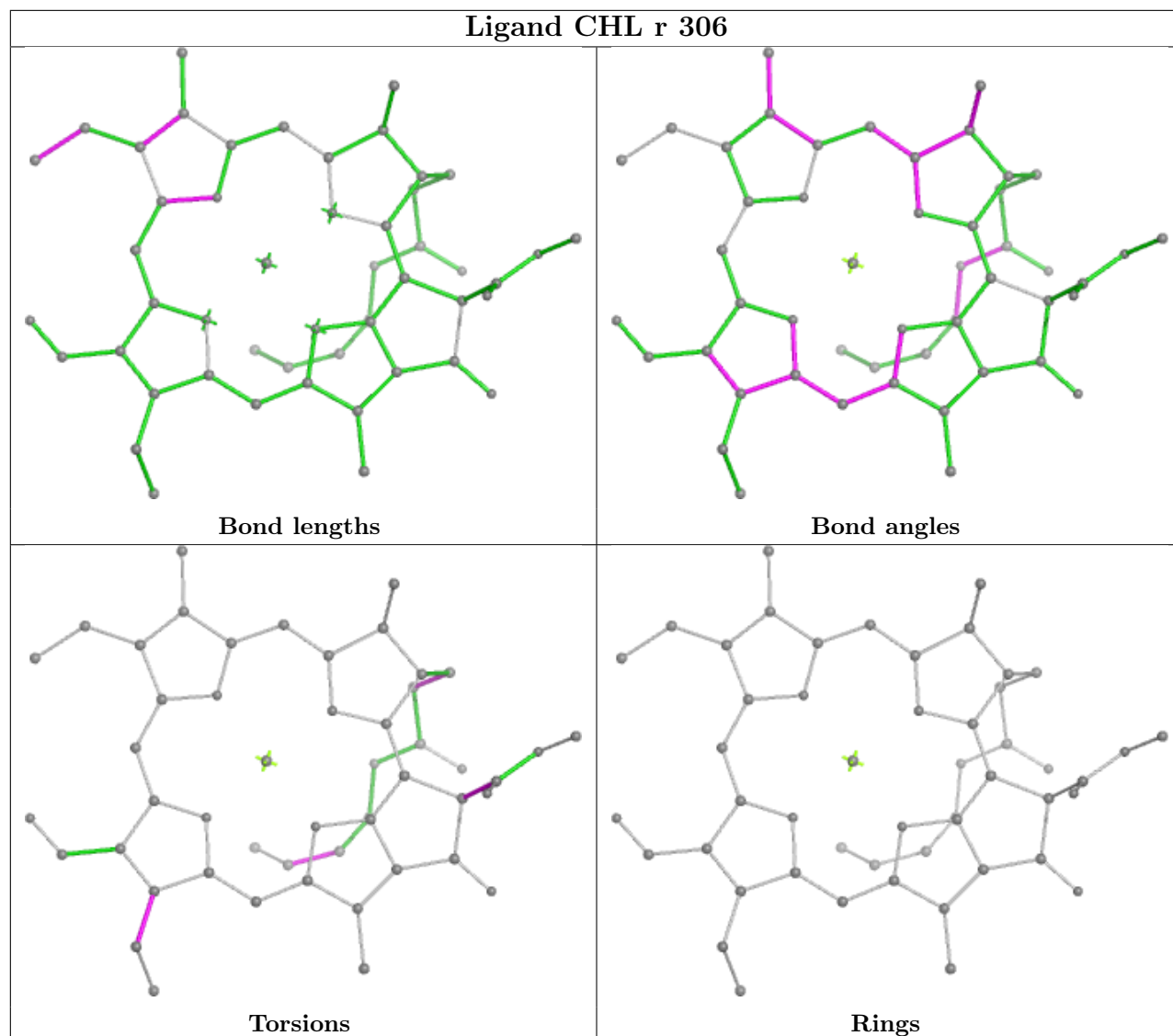


Ligand CLA B 510

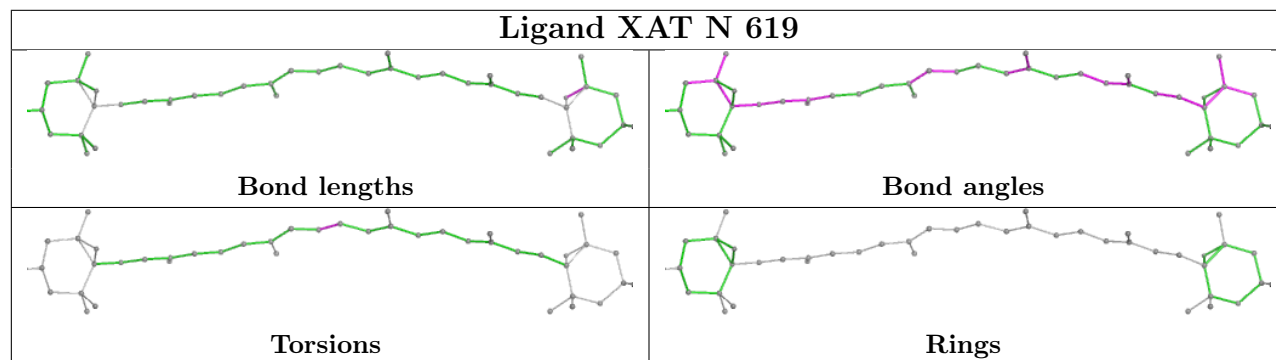


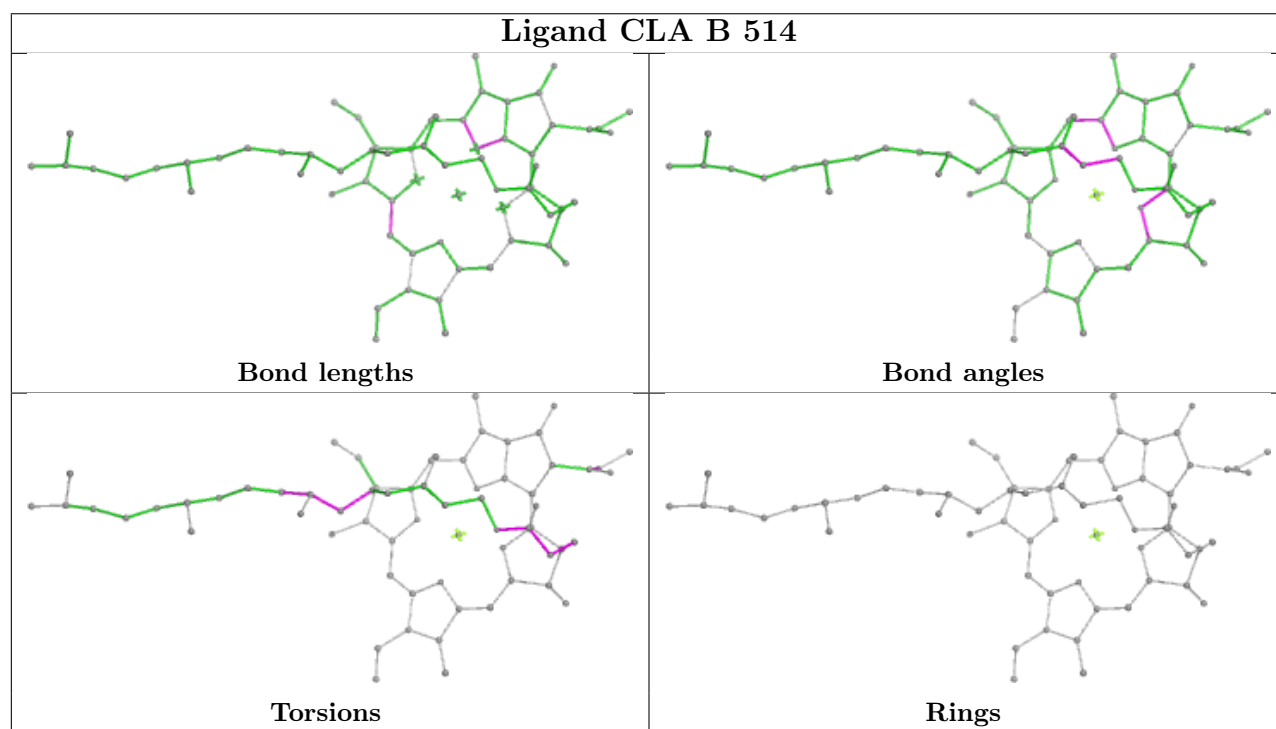
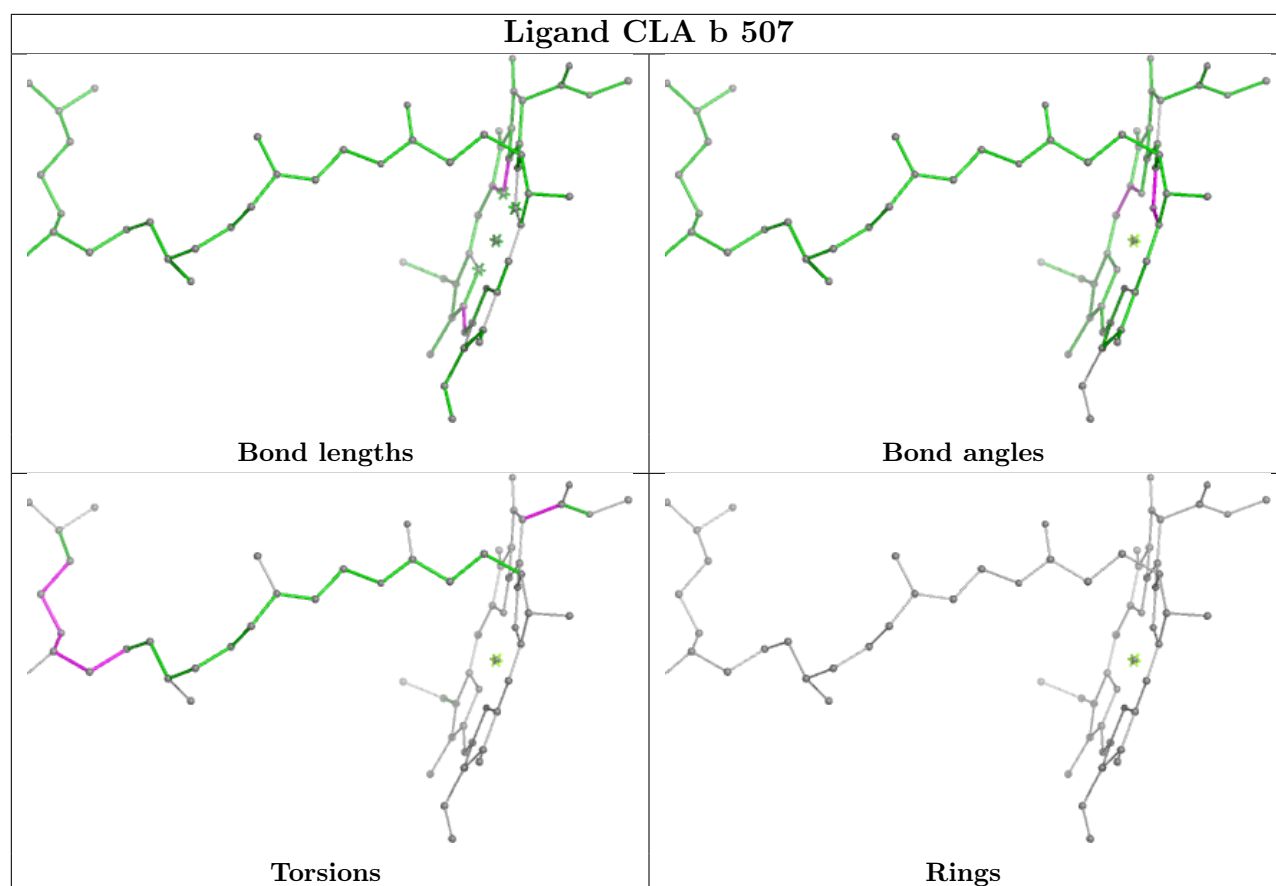


Ligand CHL r 306

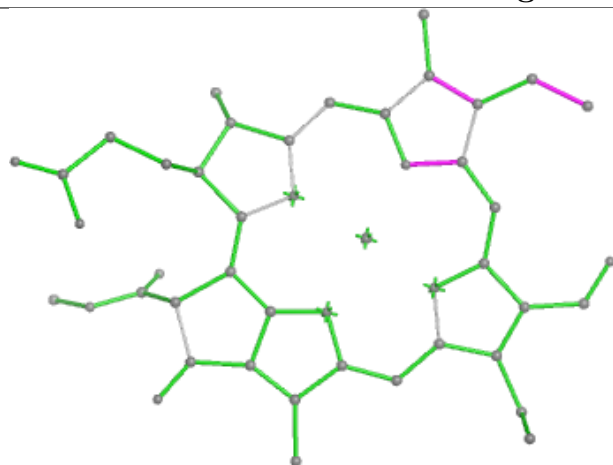


Ligand XAT N 619

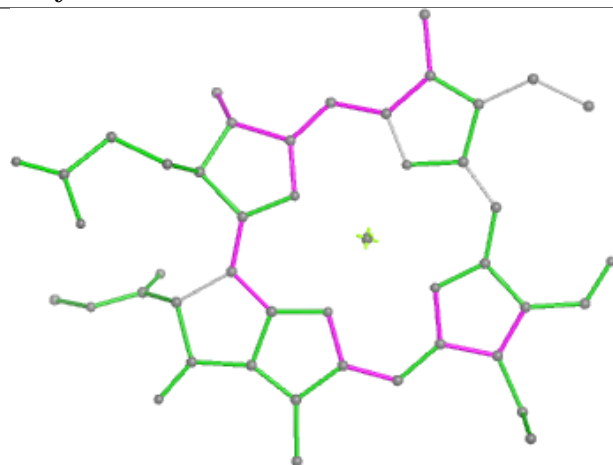




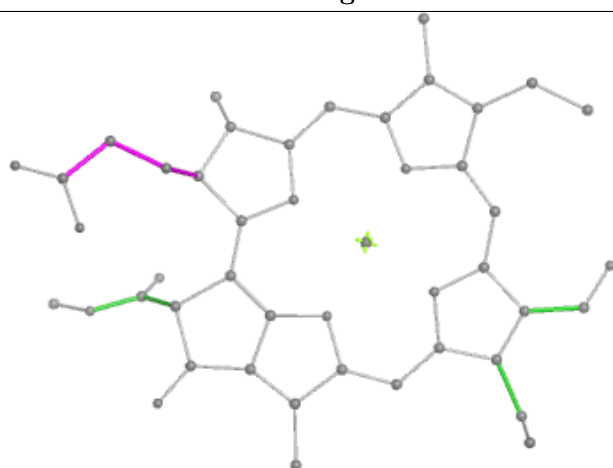
Ligand CHL y 307



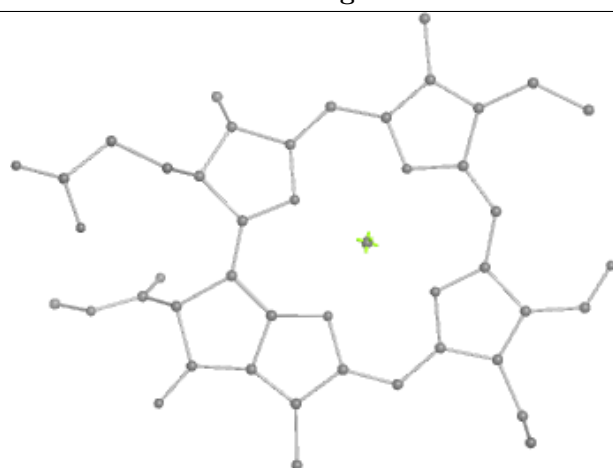
Bond lengths



Bond angles

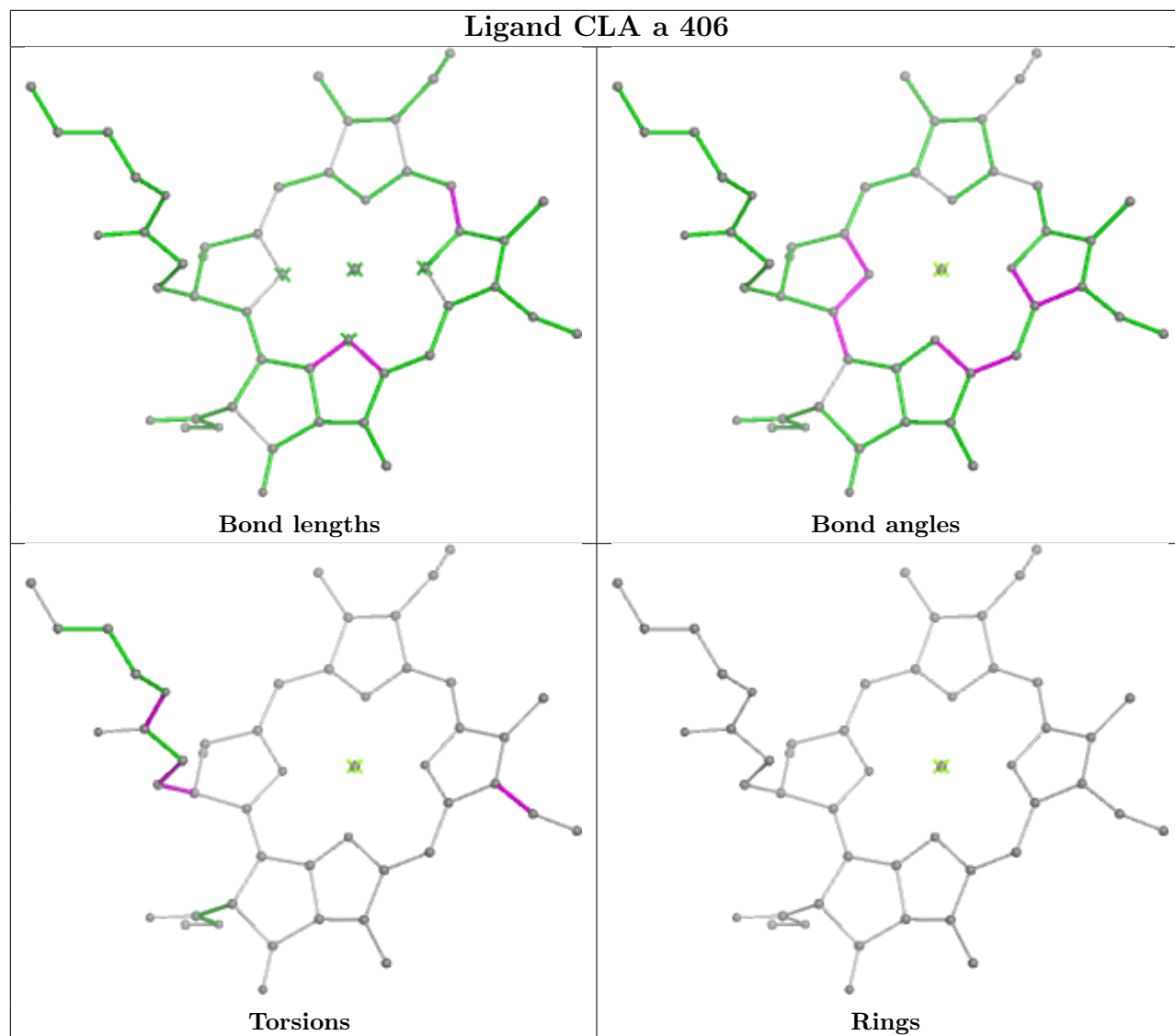


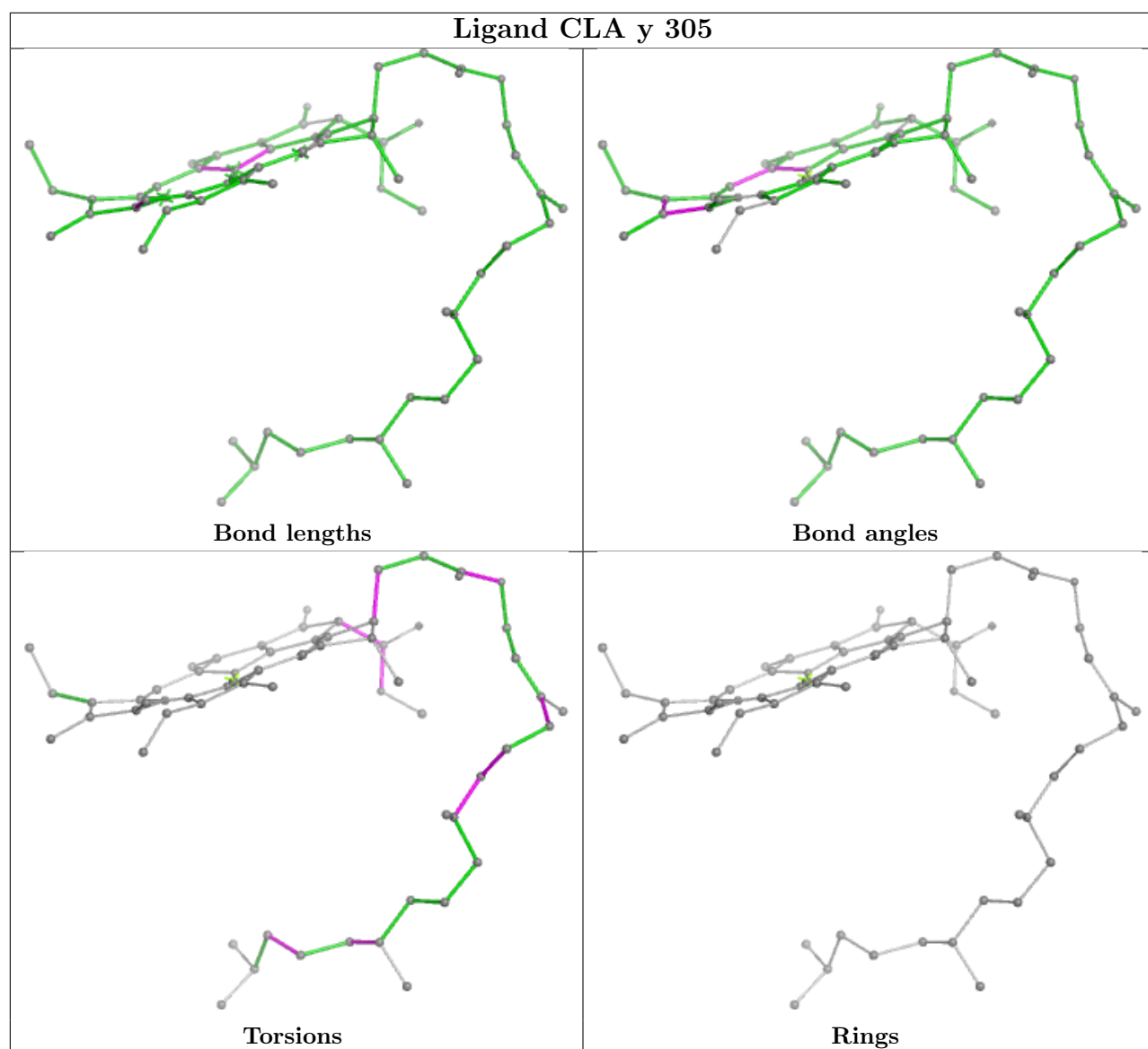
Torsions

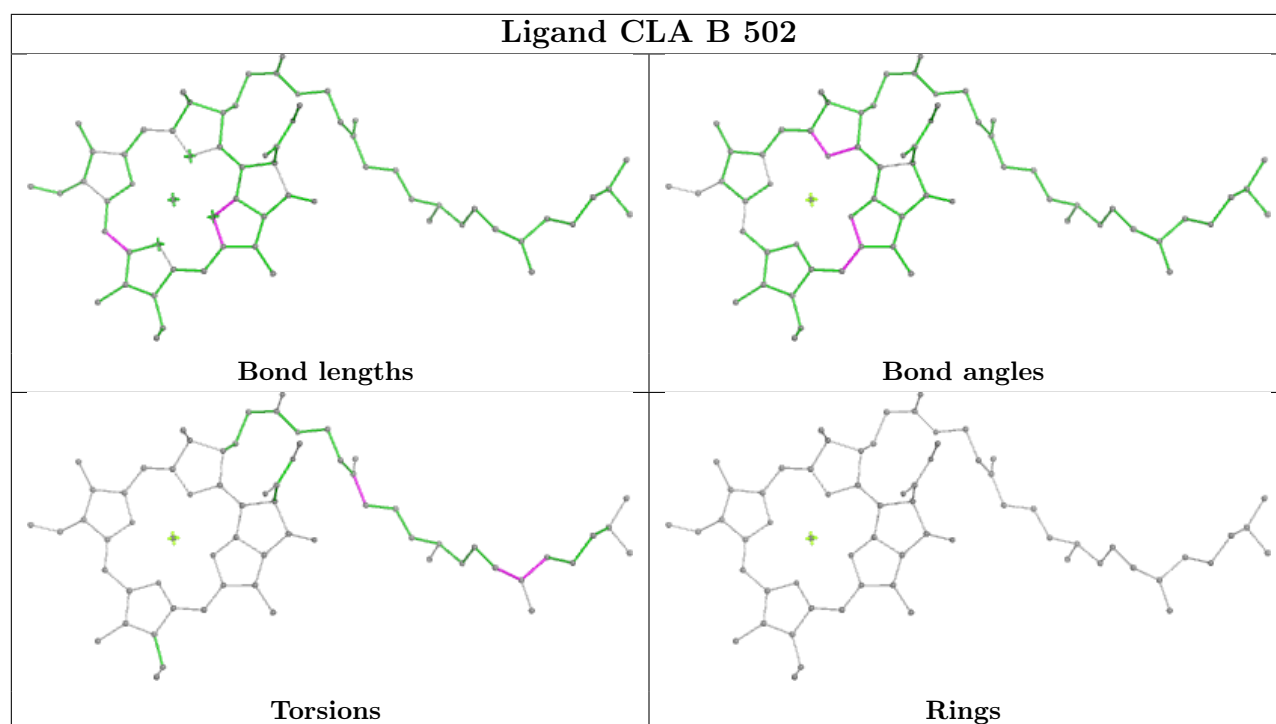


Rings

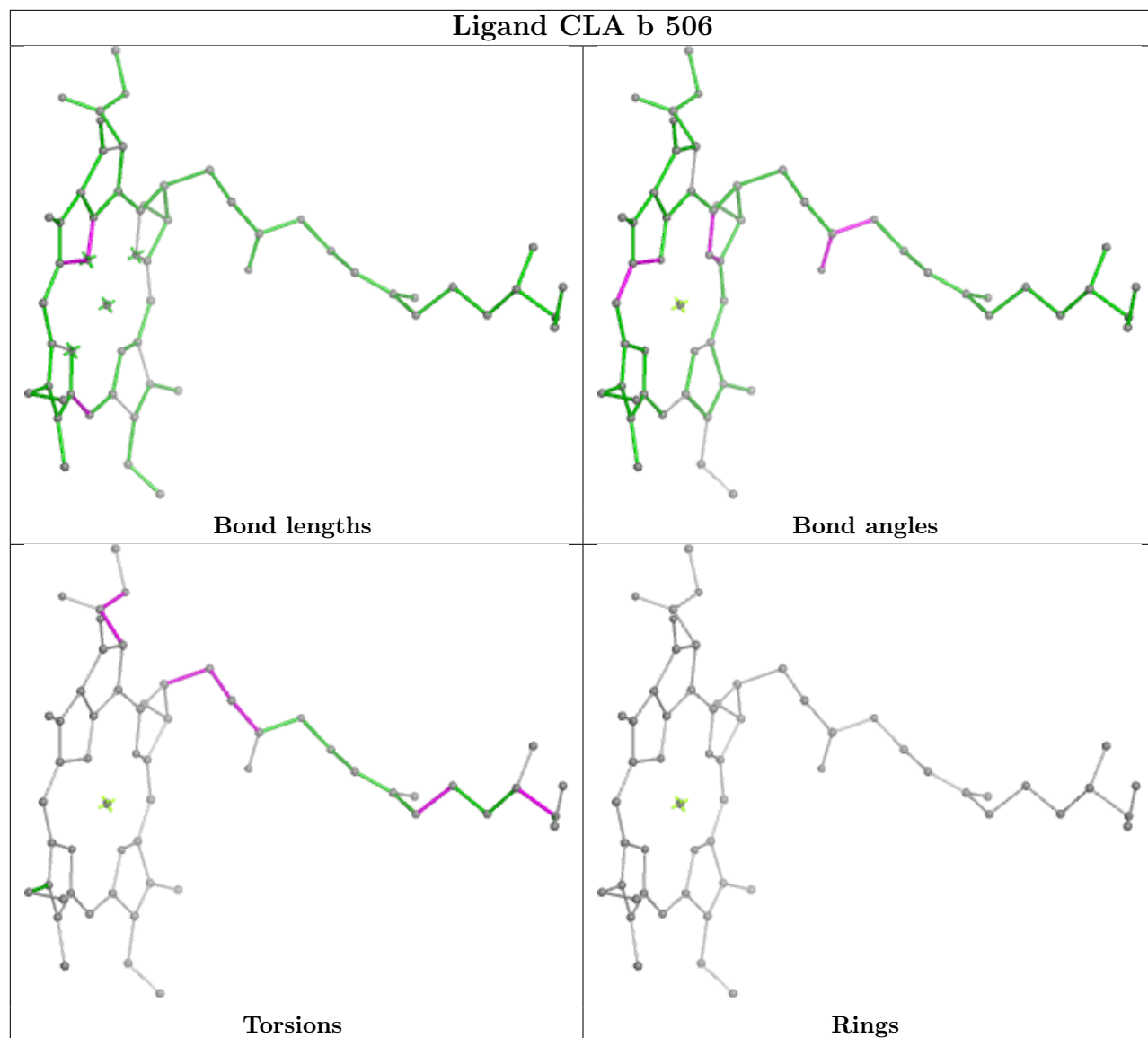
Ligand CLA a 406

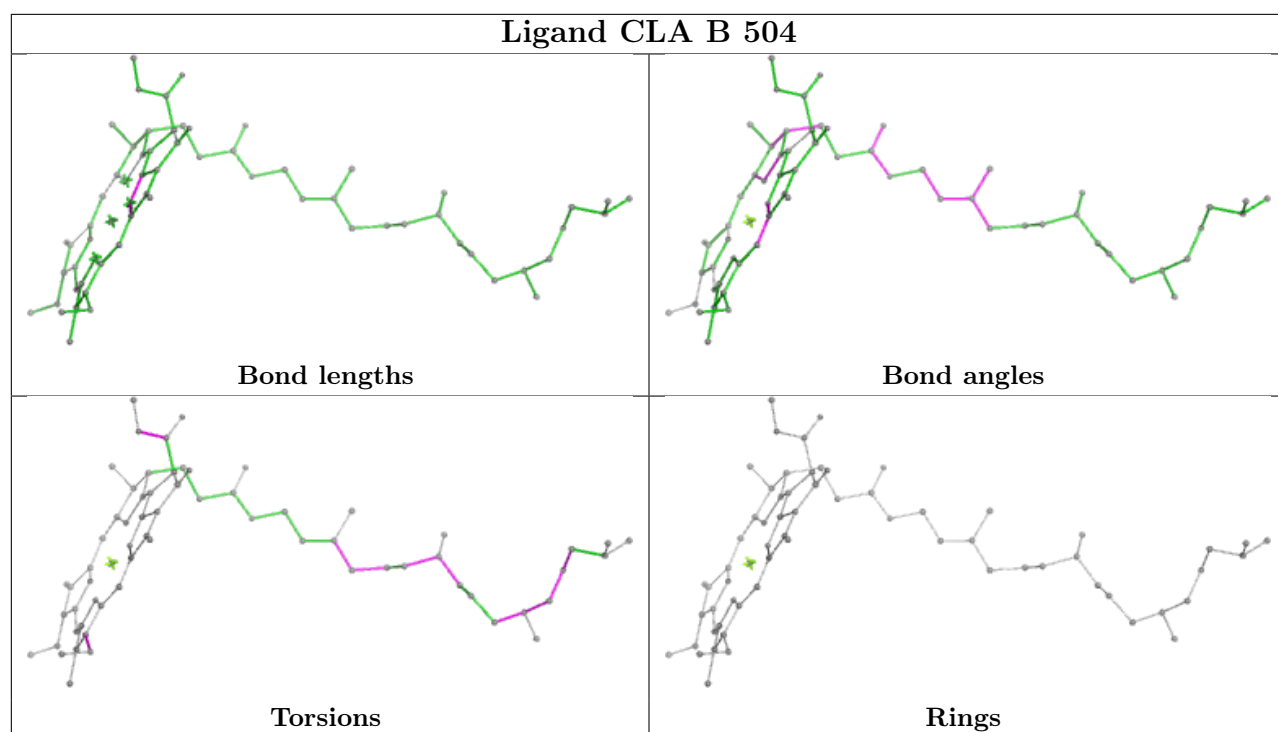




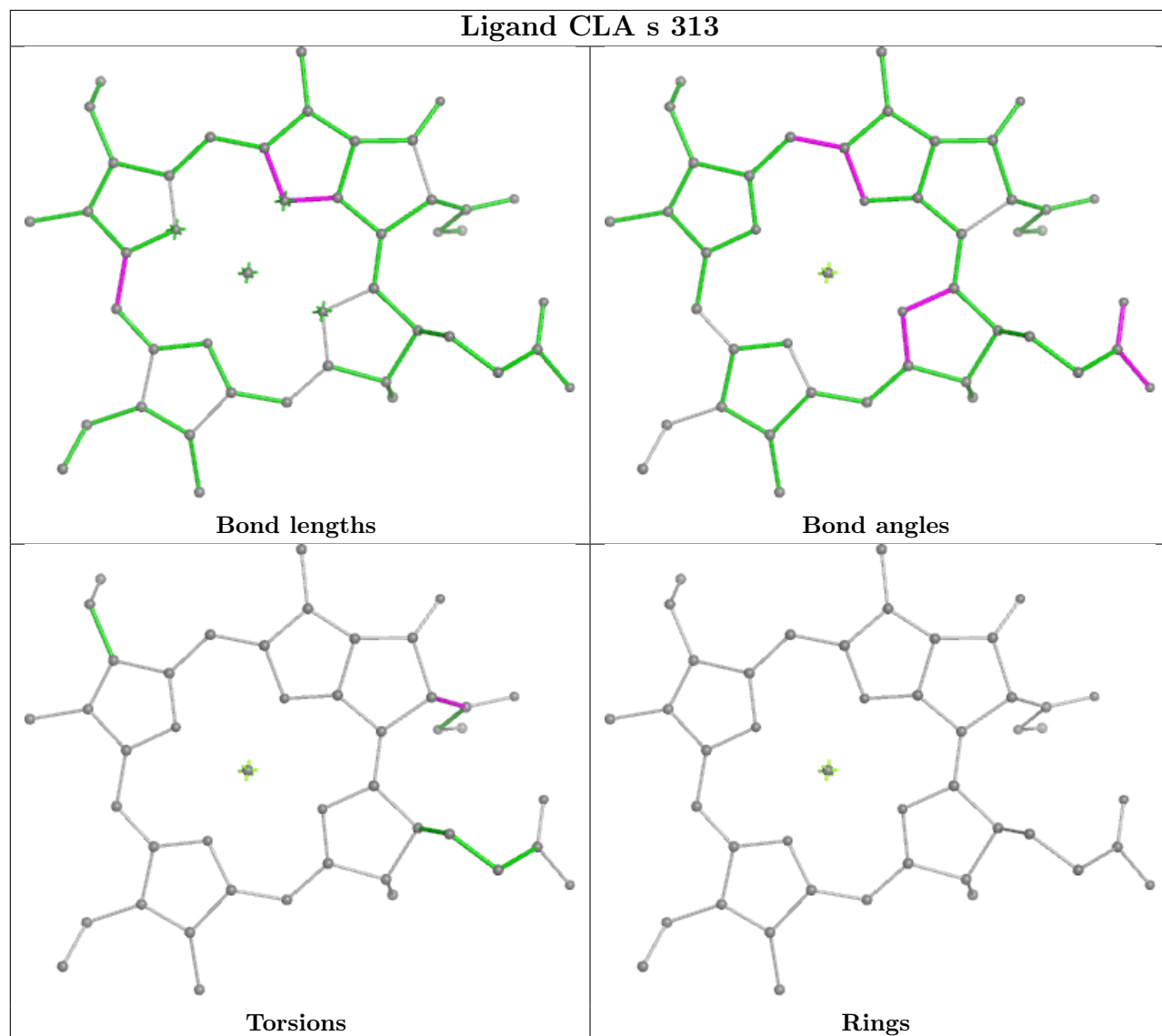


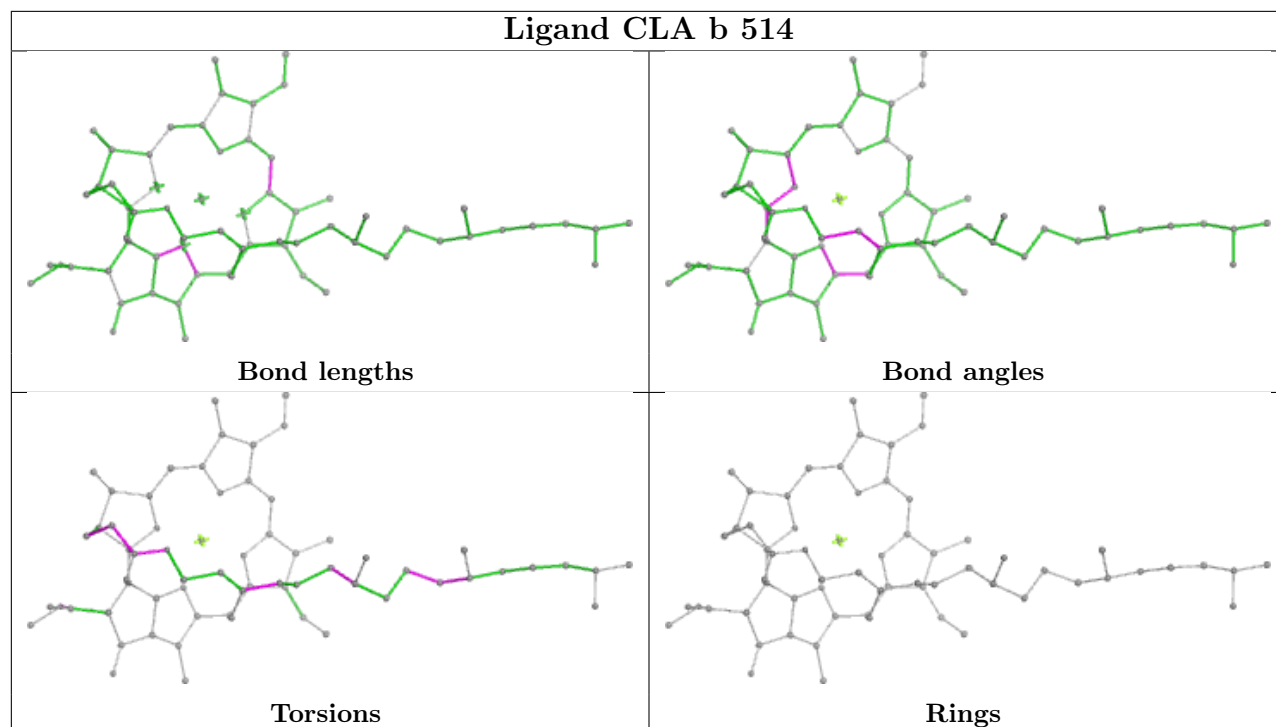
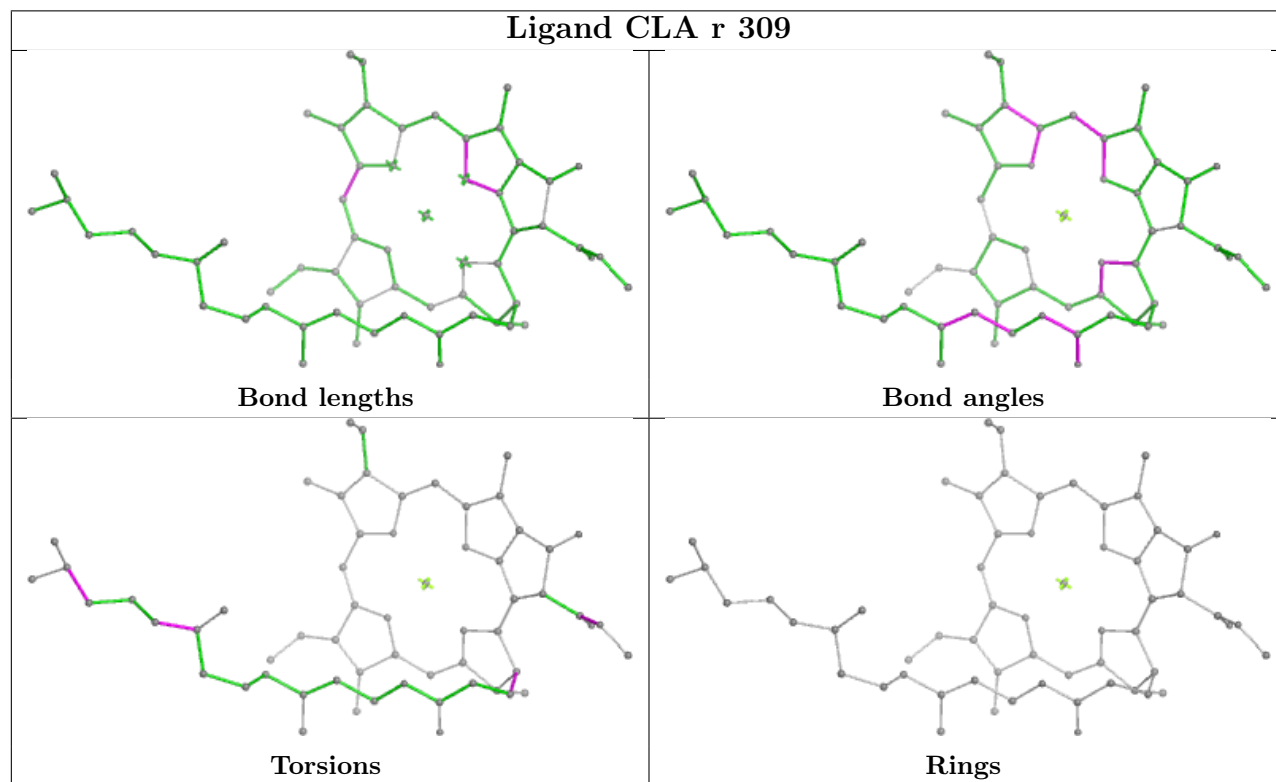
Ligand CLA b 506



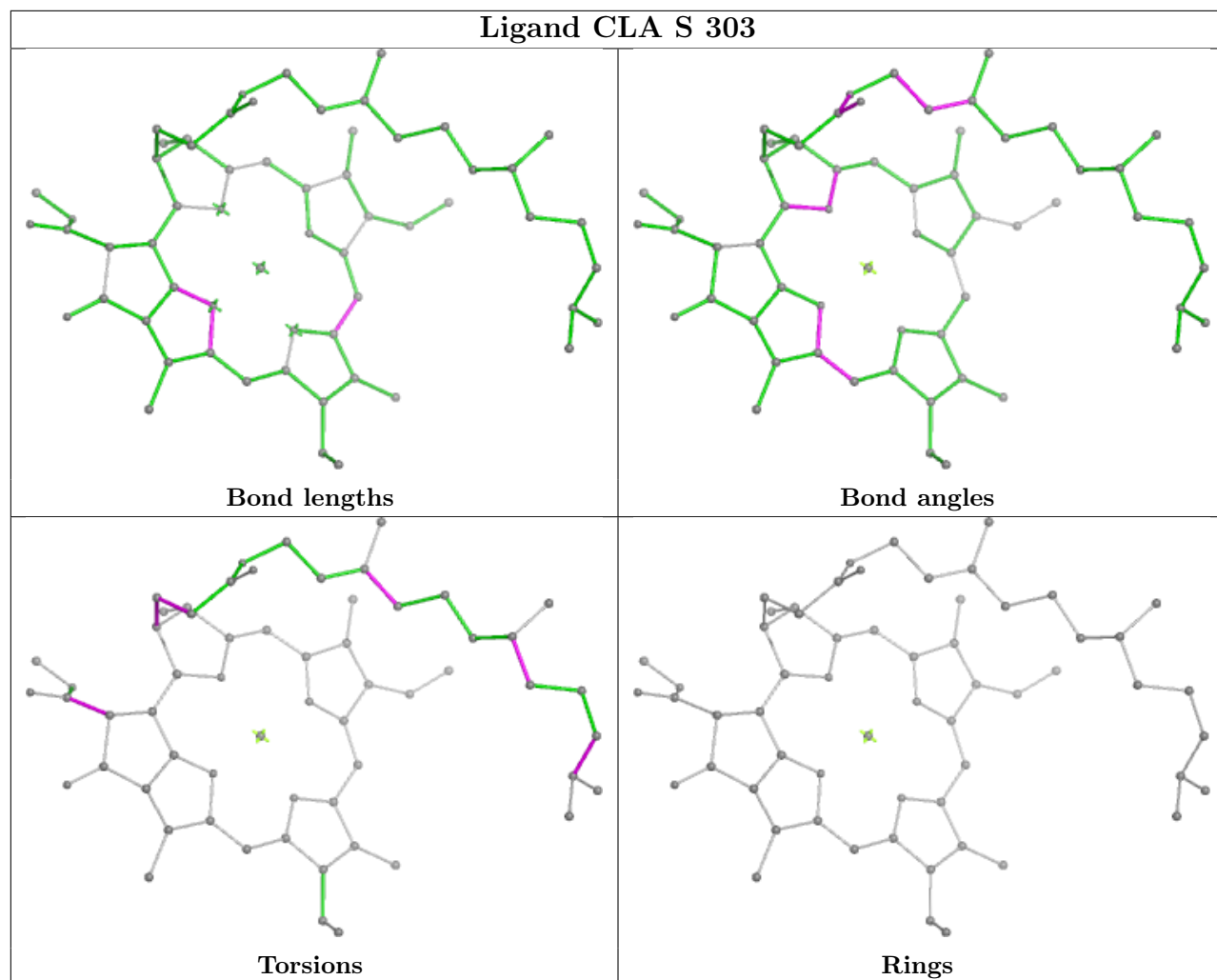


Ligand CLA s 313

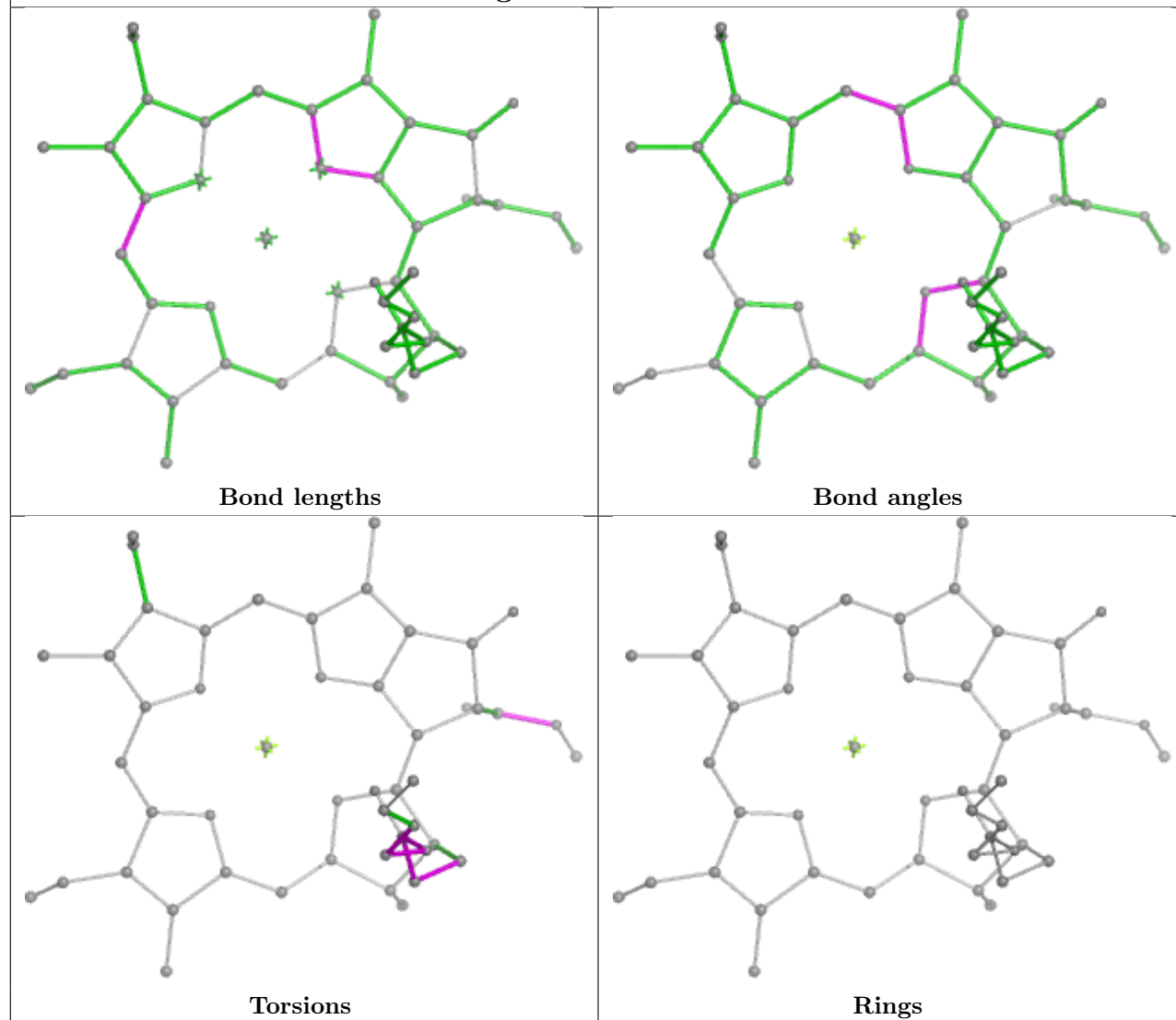


Ligand CLA b 514**Ligand CLA r 309**

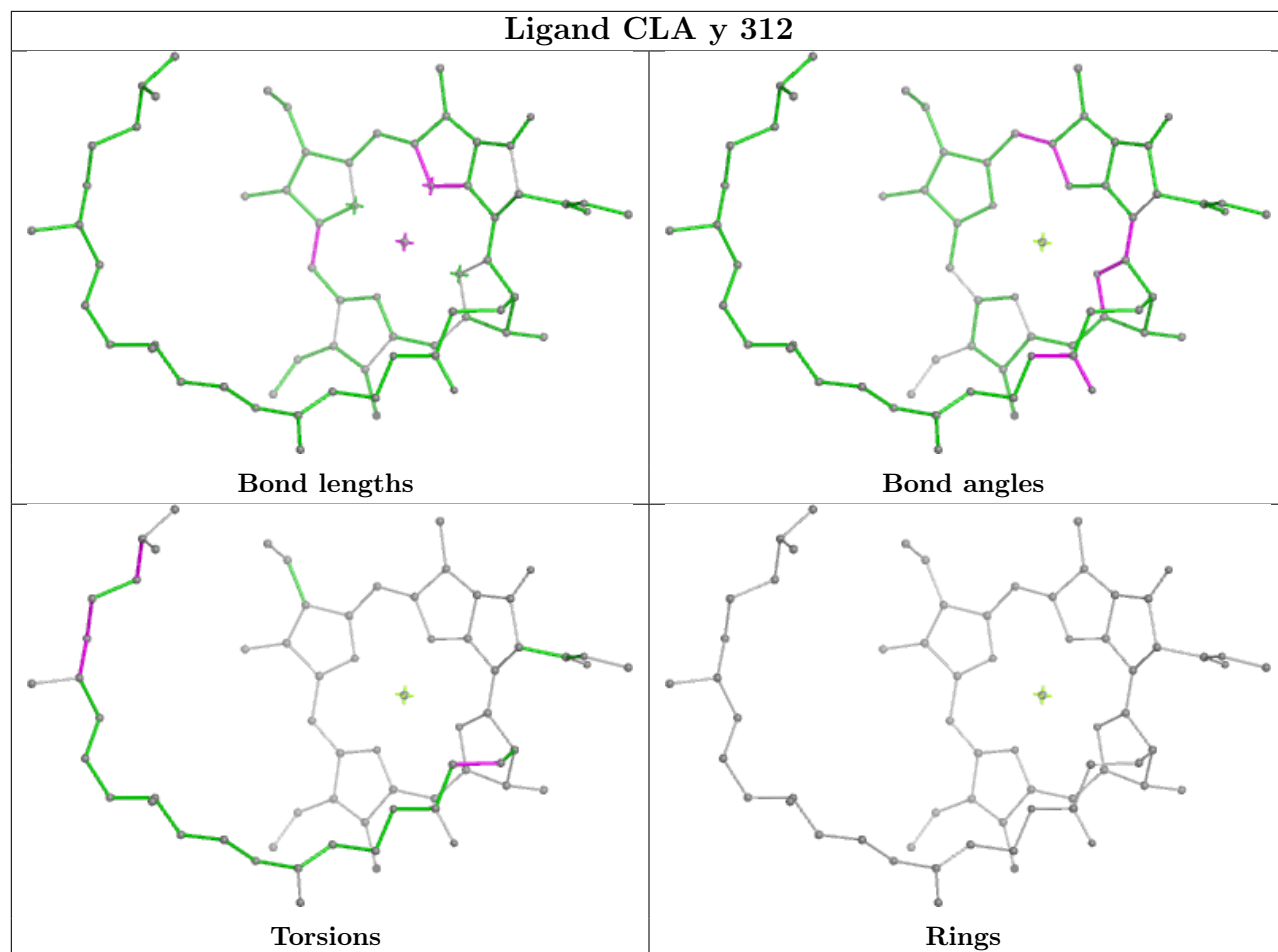
Ligand CLA S 303



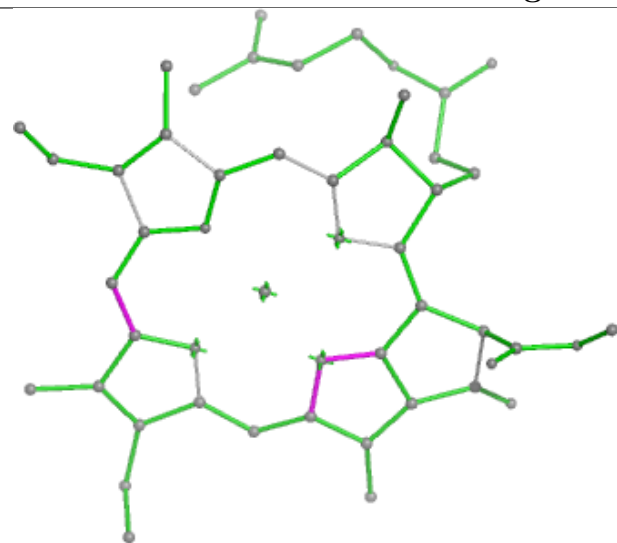
Ligand CLA r 304



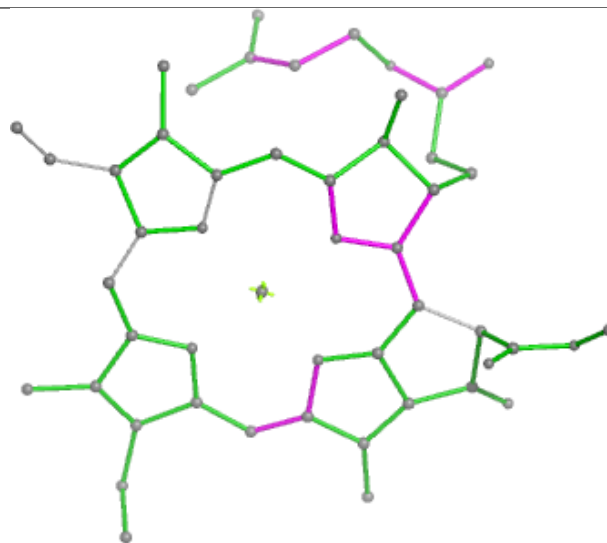
Ligand CLA y 312



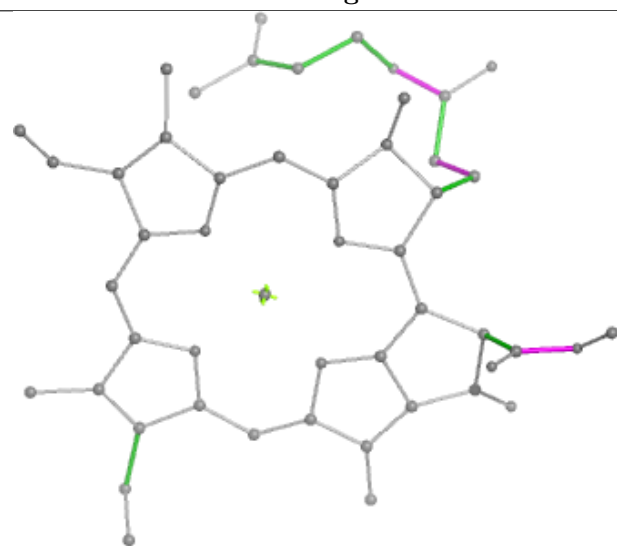
Ligand CLA s 316



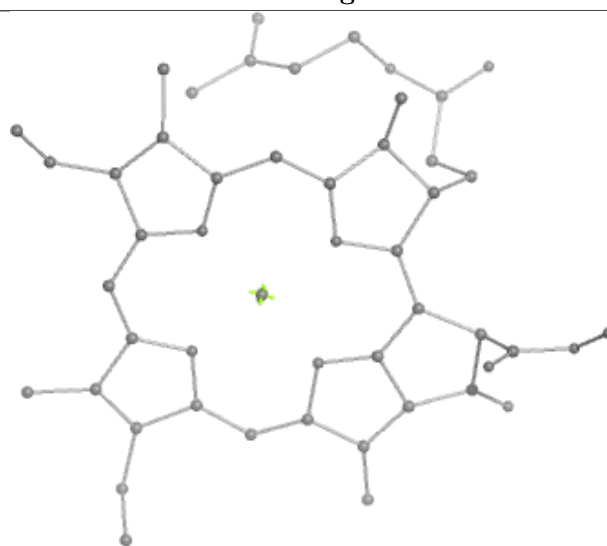
Bond lengths



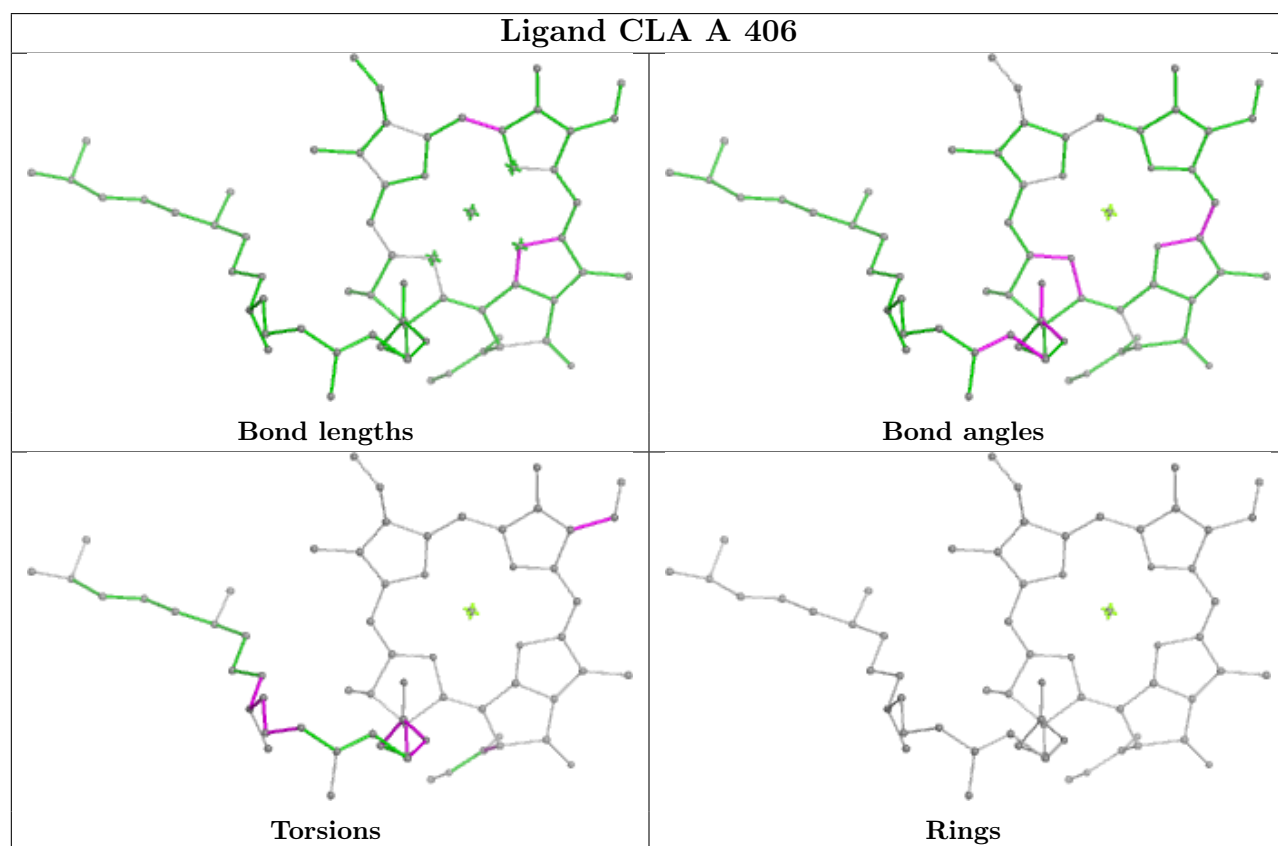
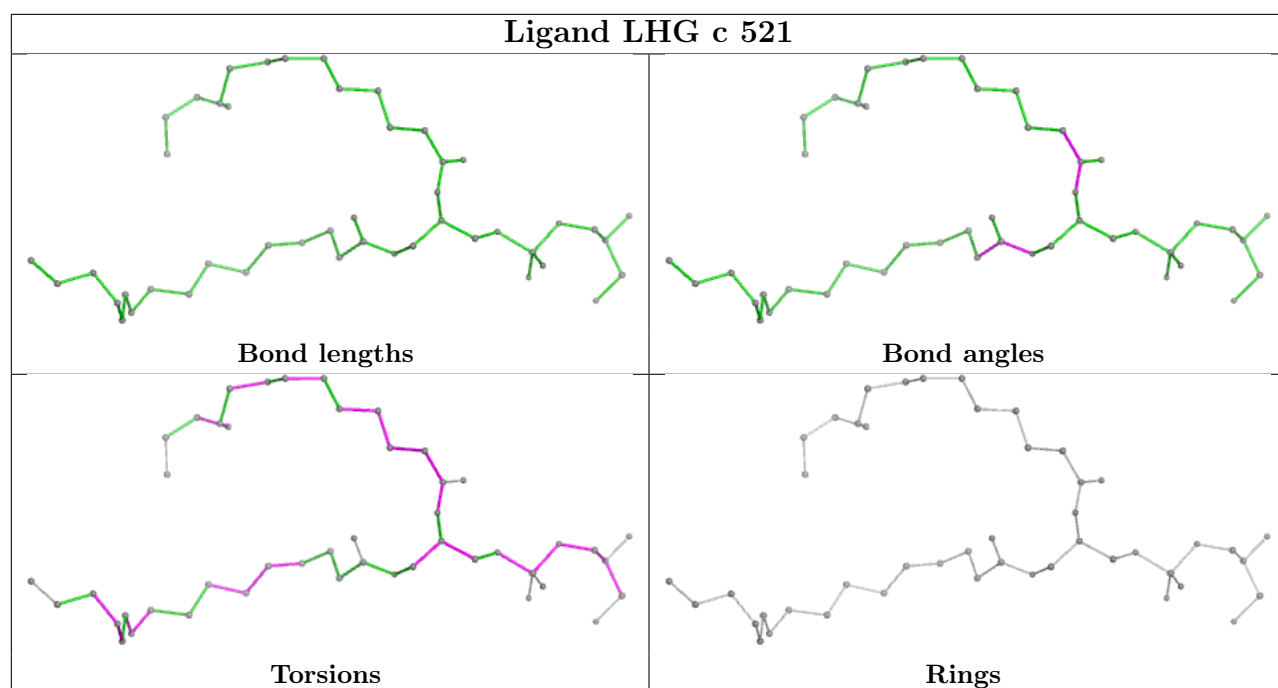
Bond angles

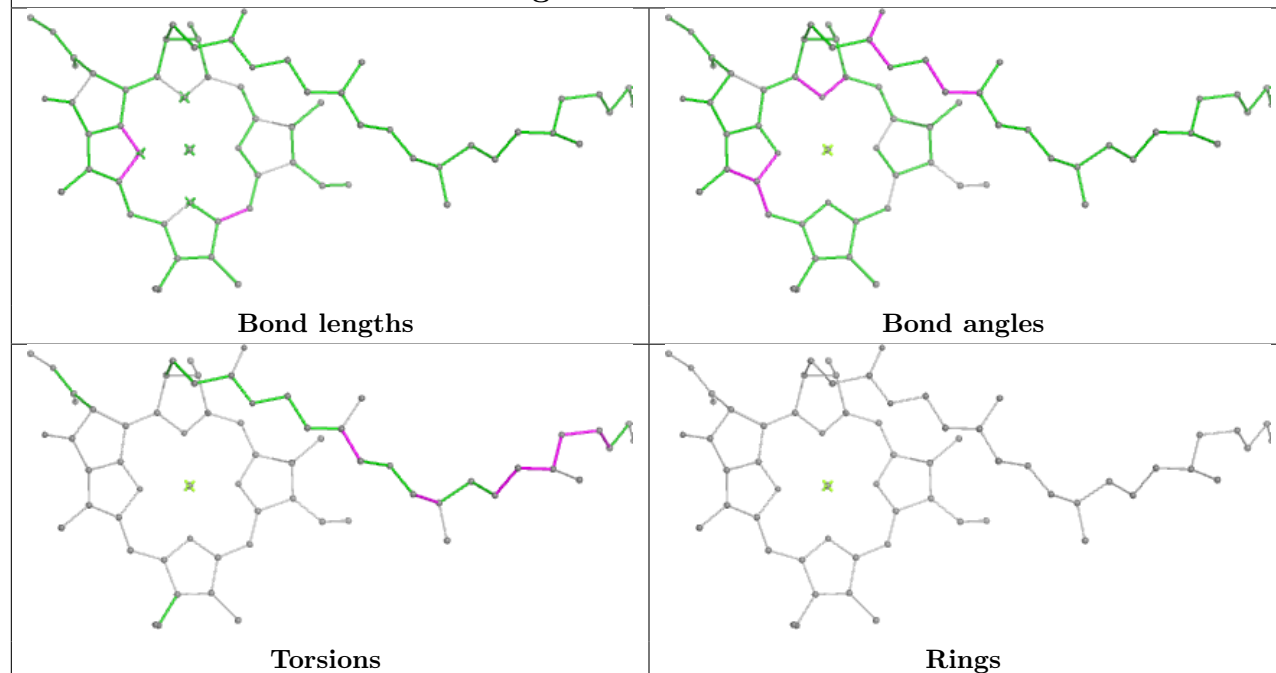
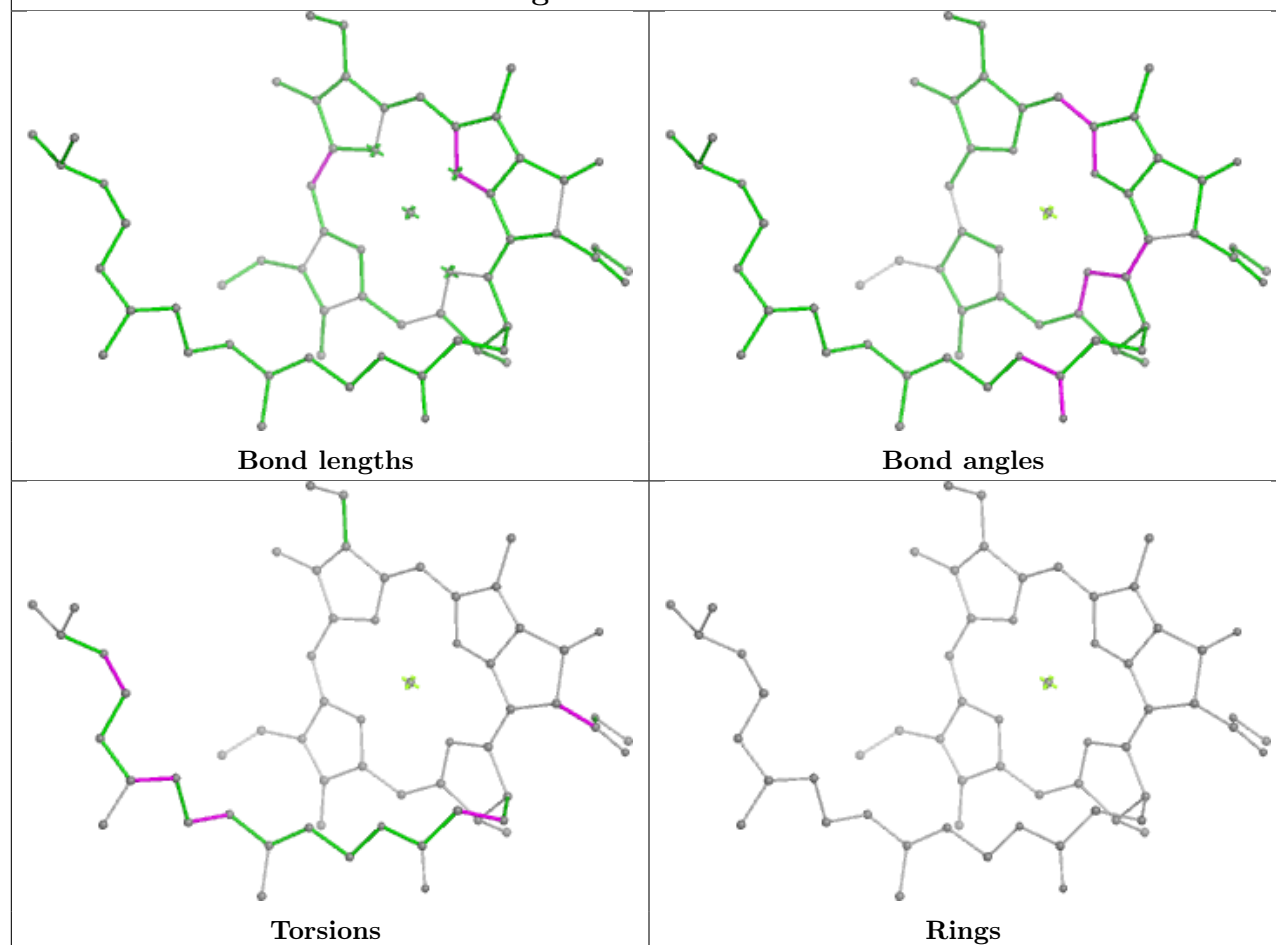


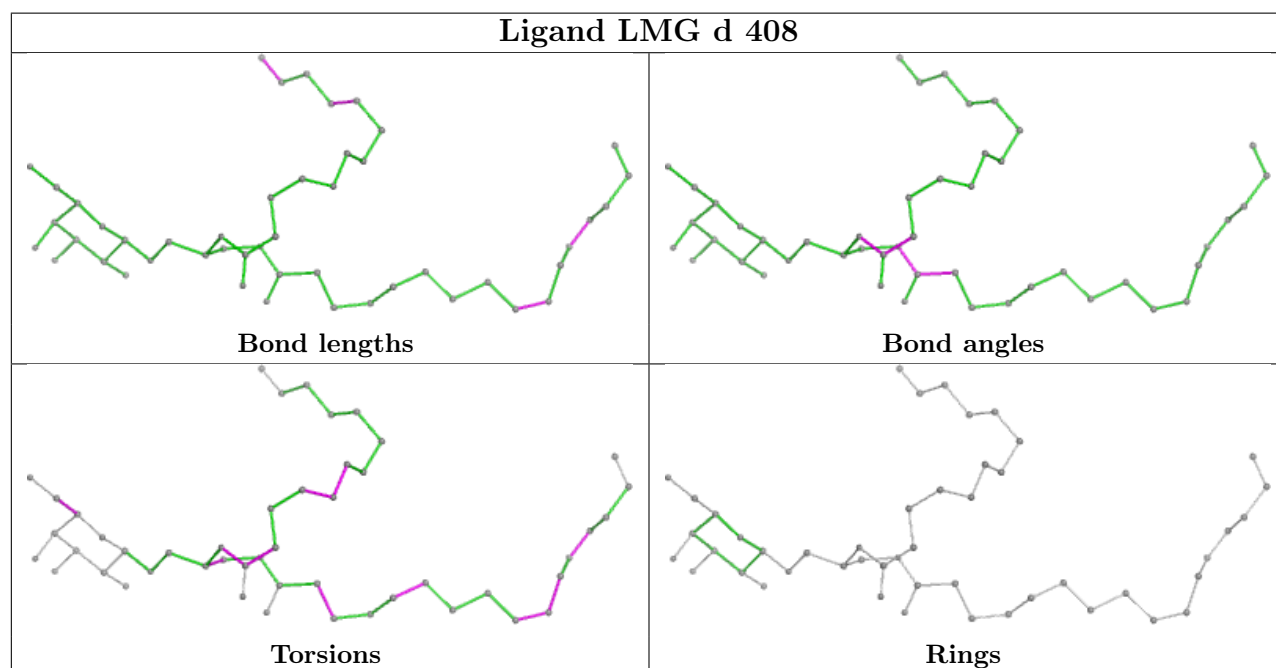
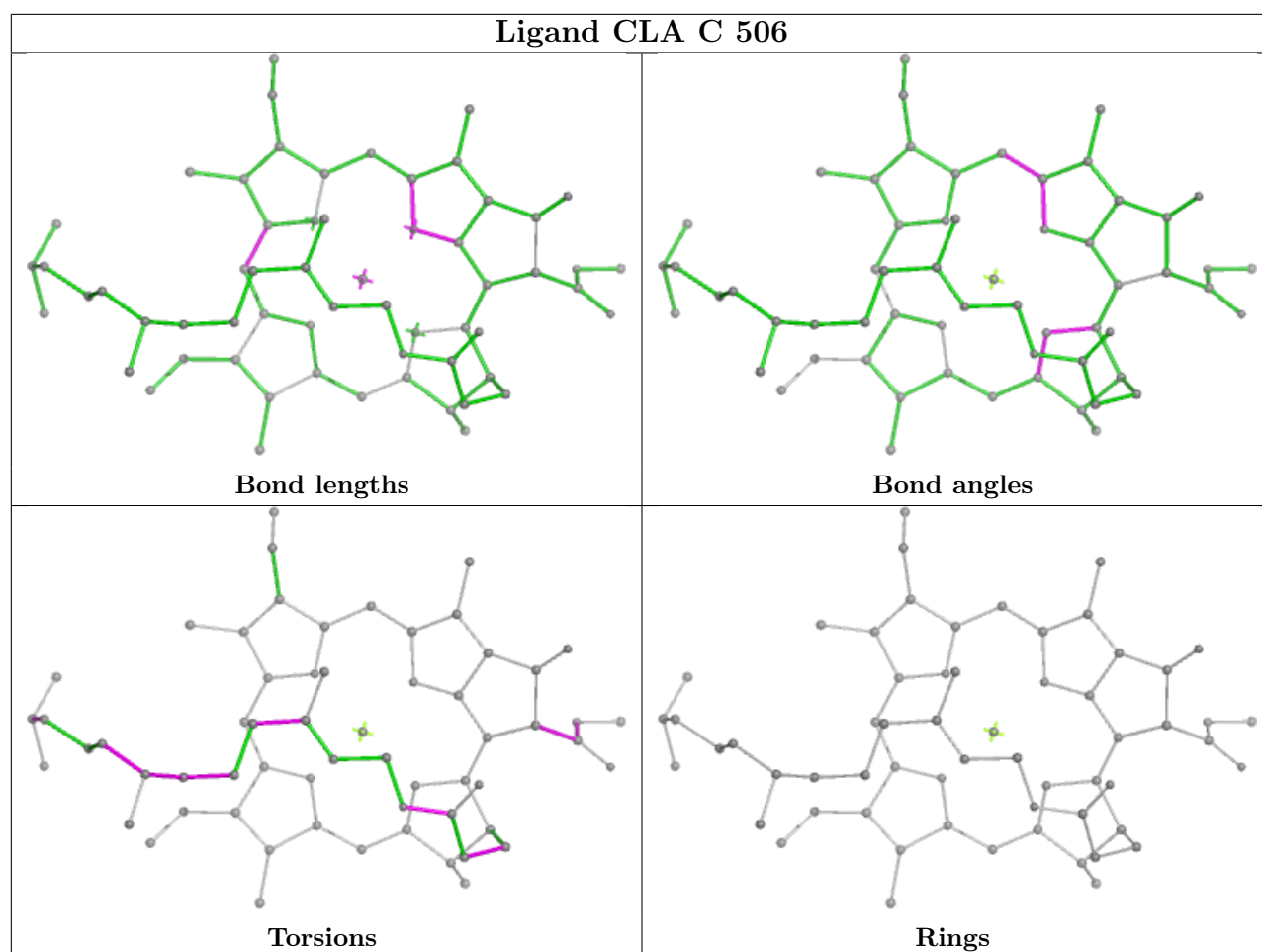
Torsions

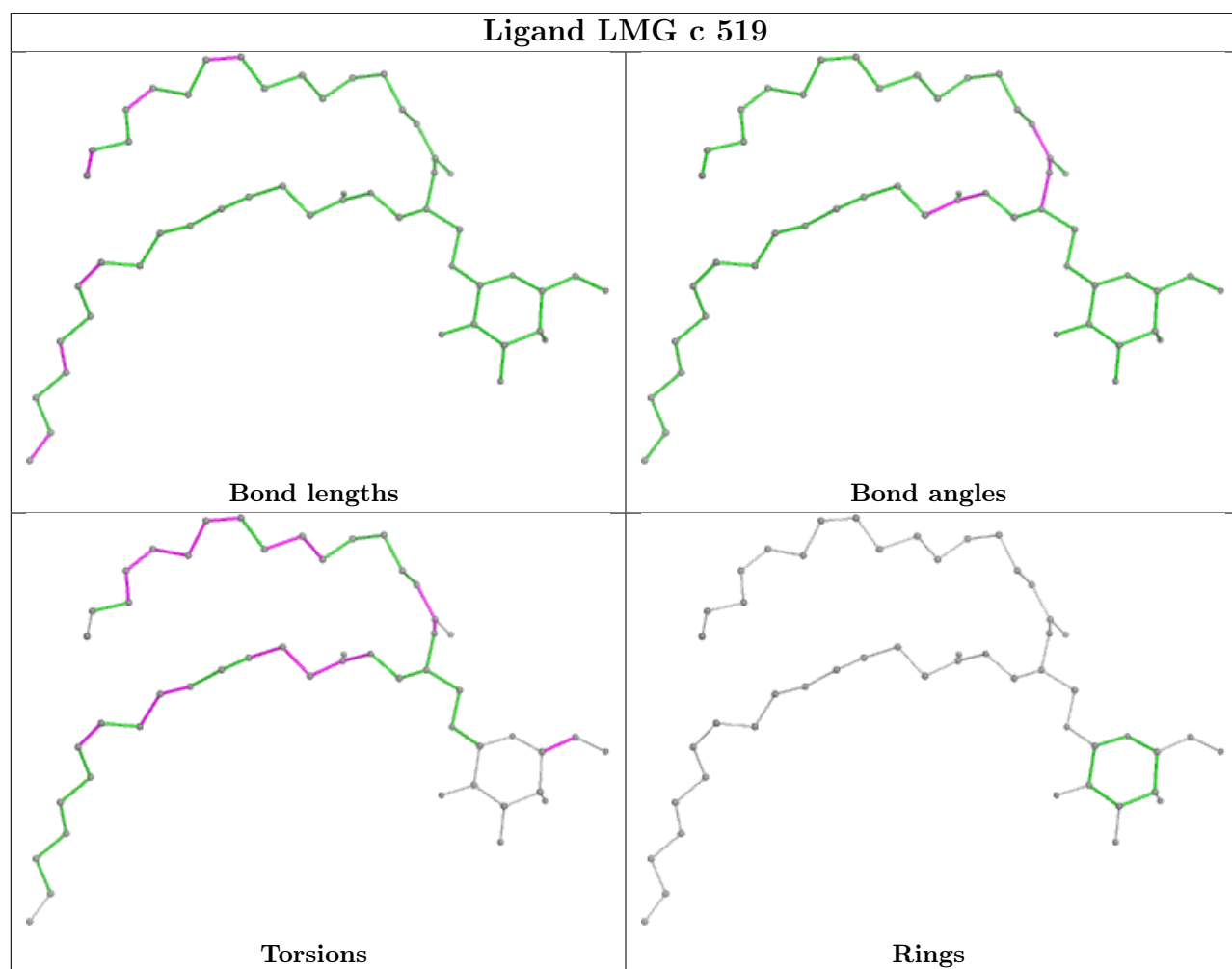


Rings

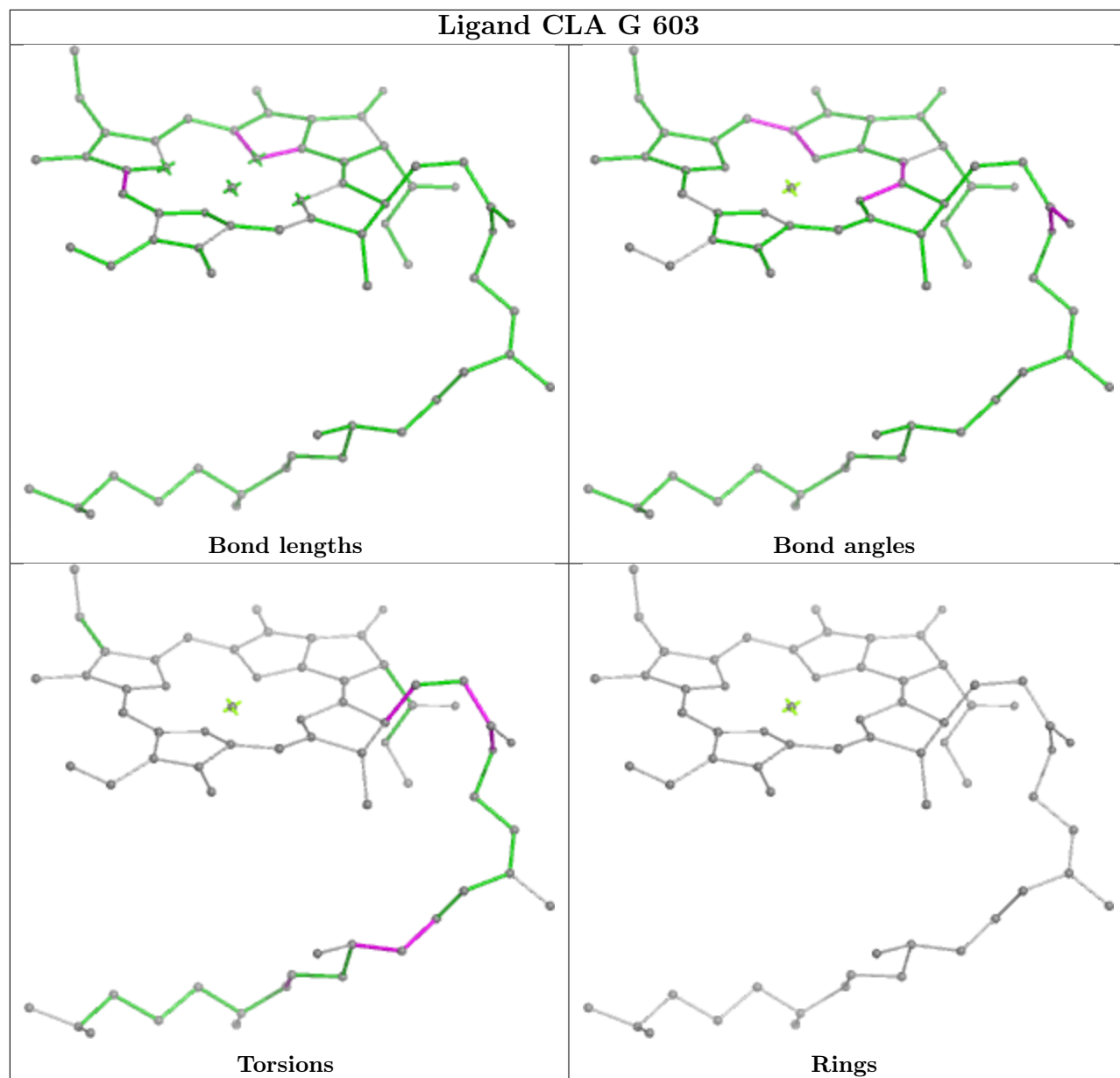


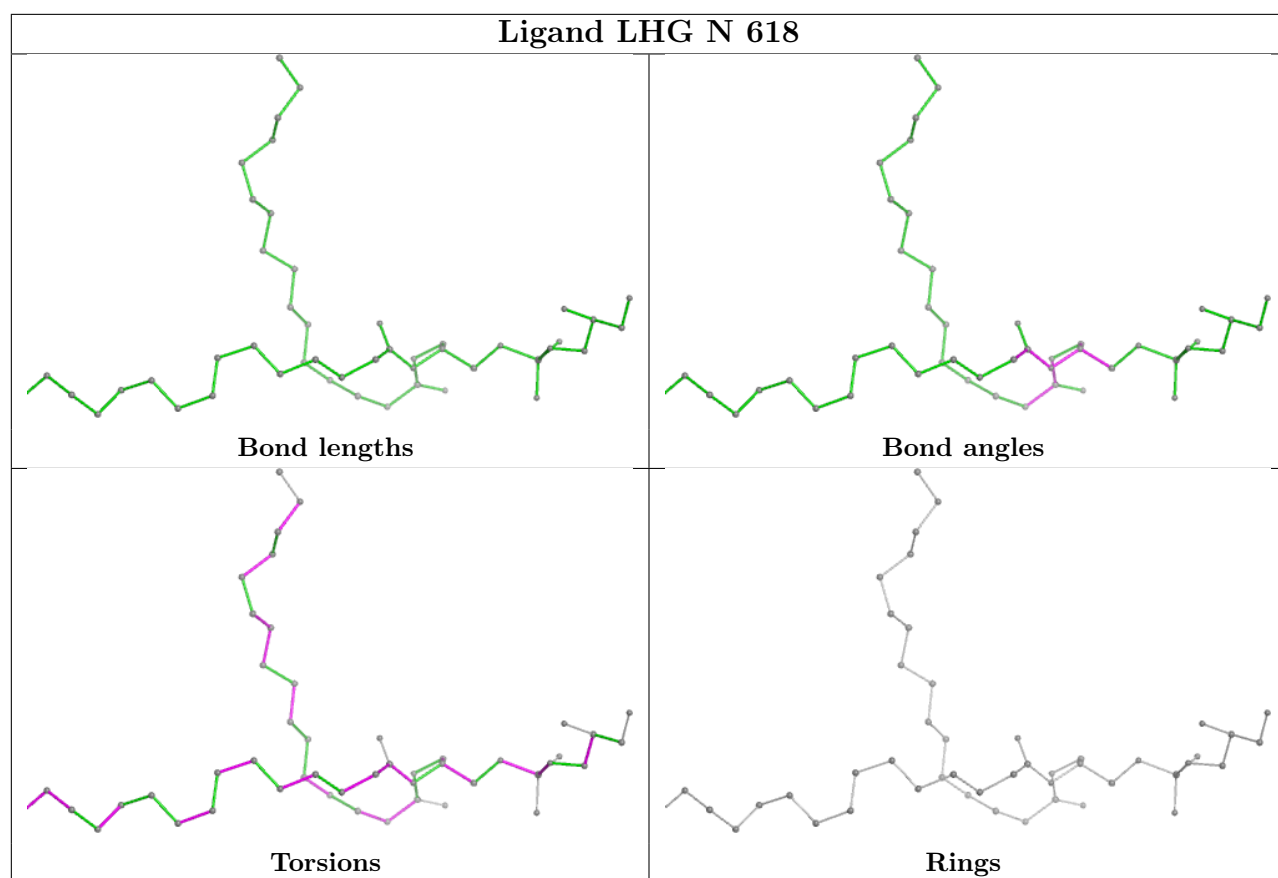
Ligand CLA B 503**Ligand CLA R 301**

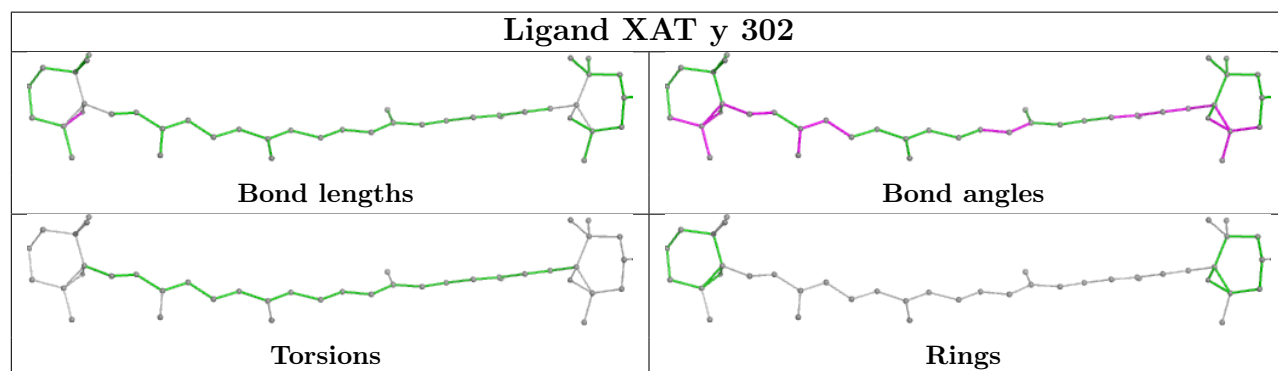
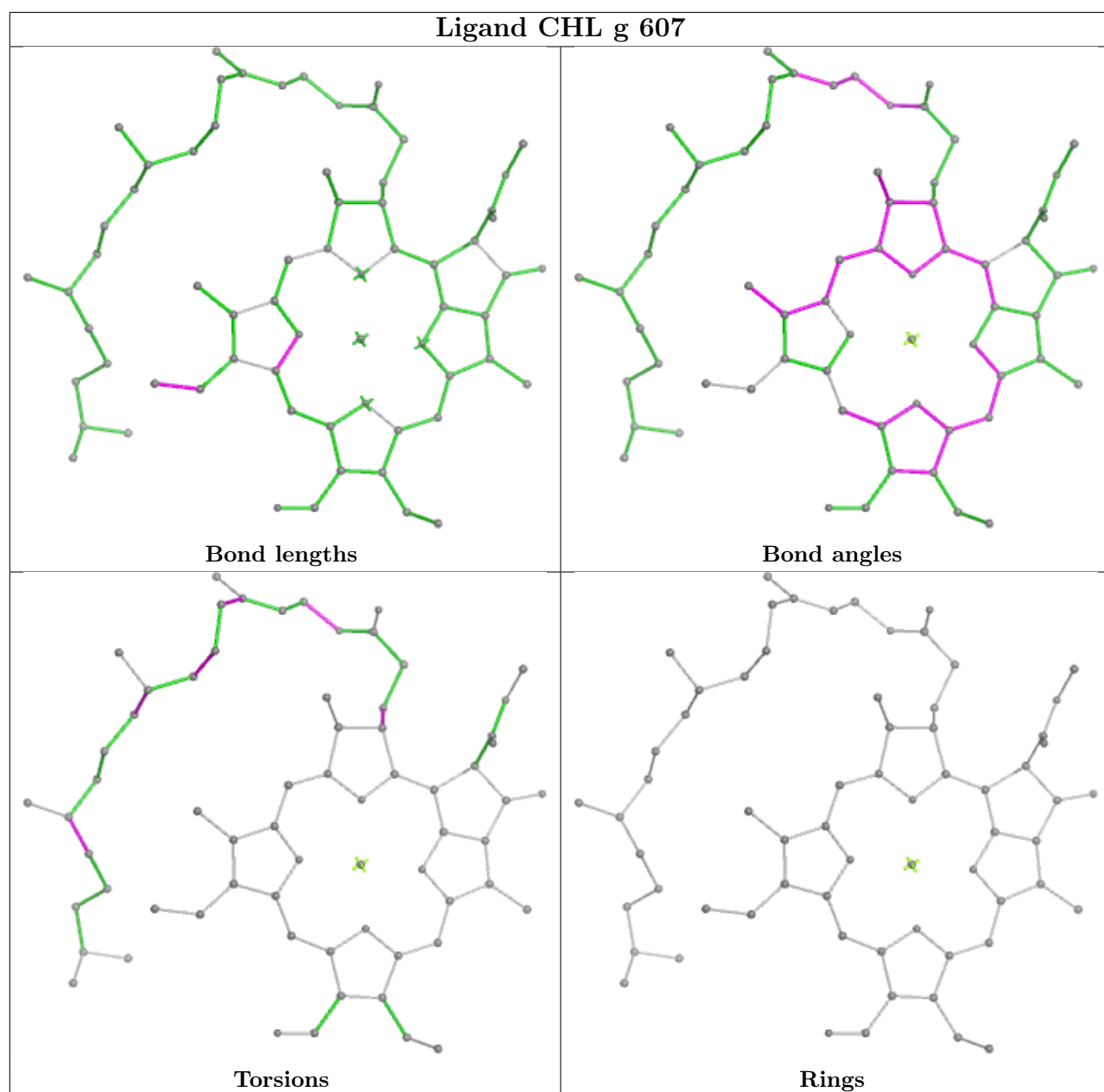


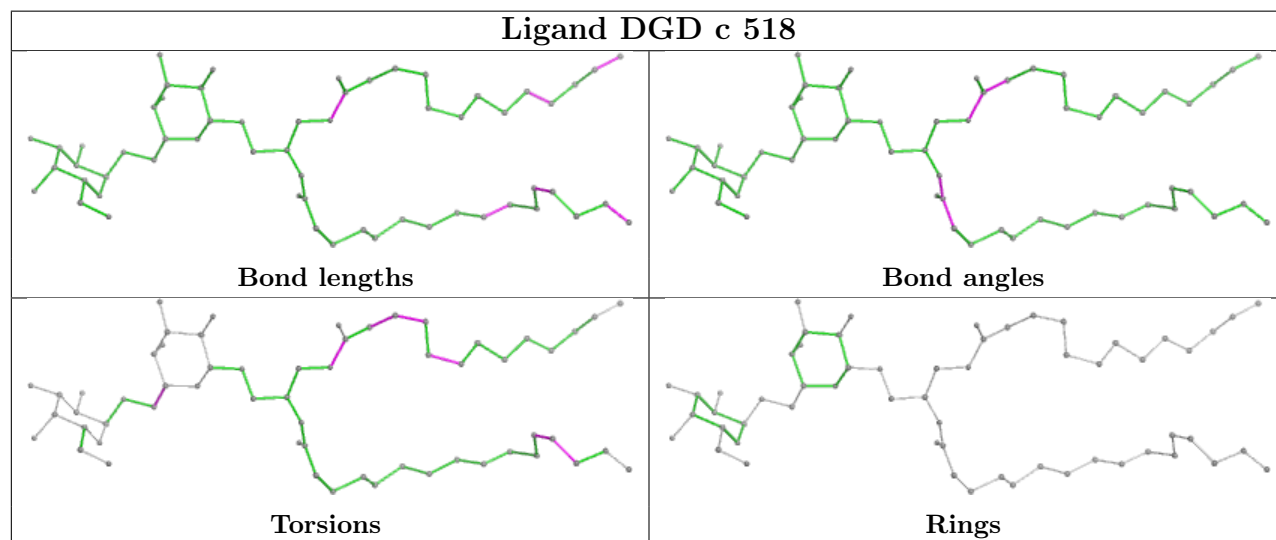
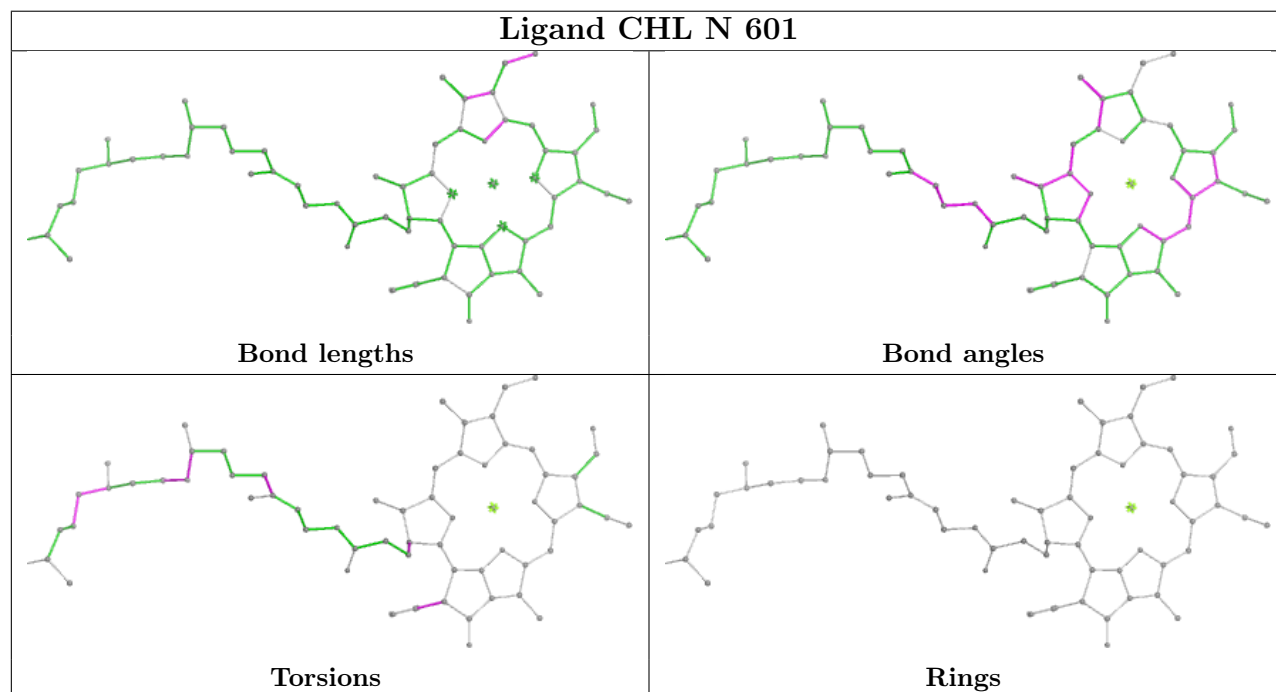
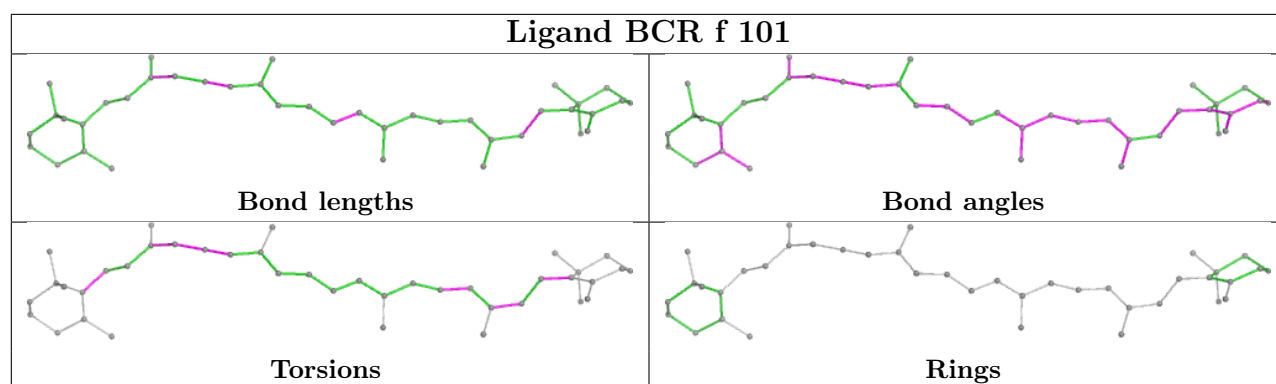


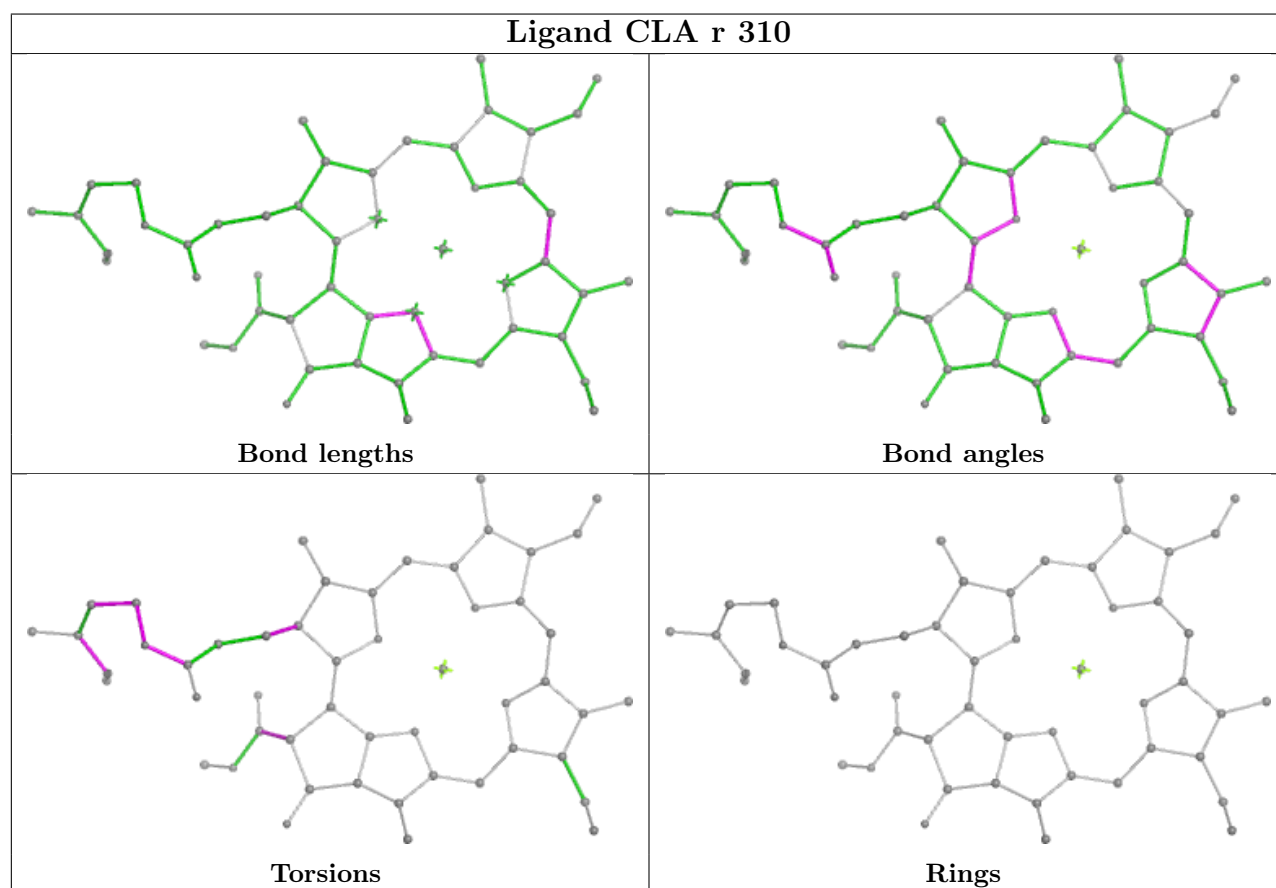
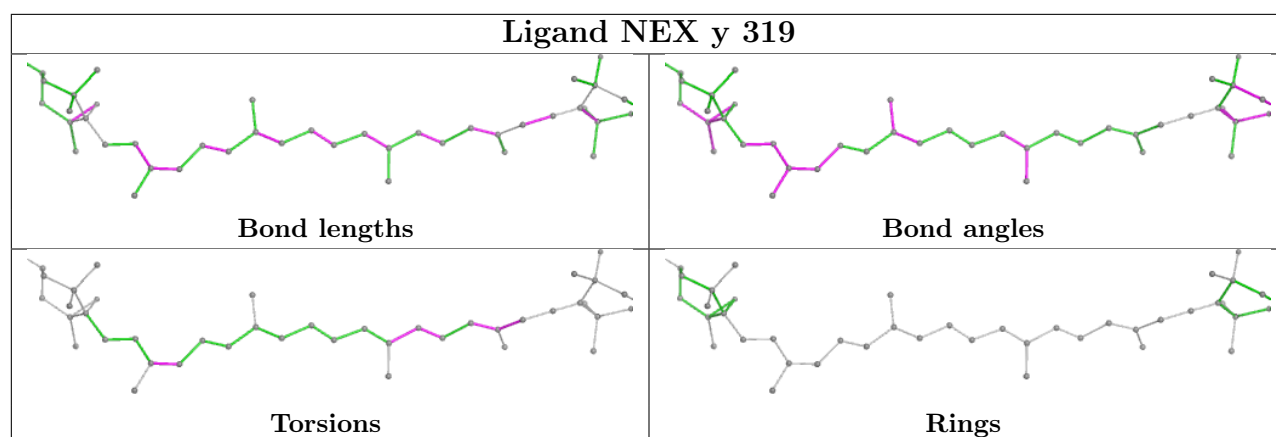
Ligand CLA G 603

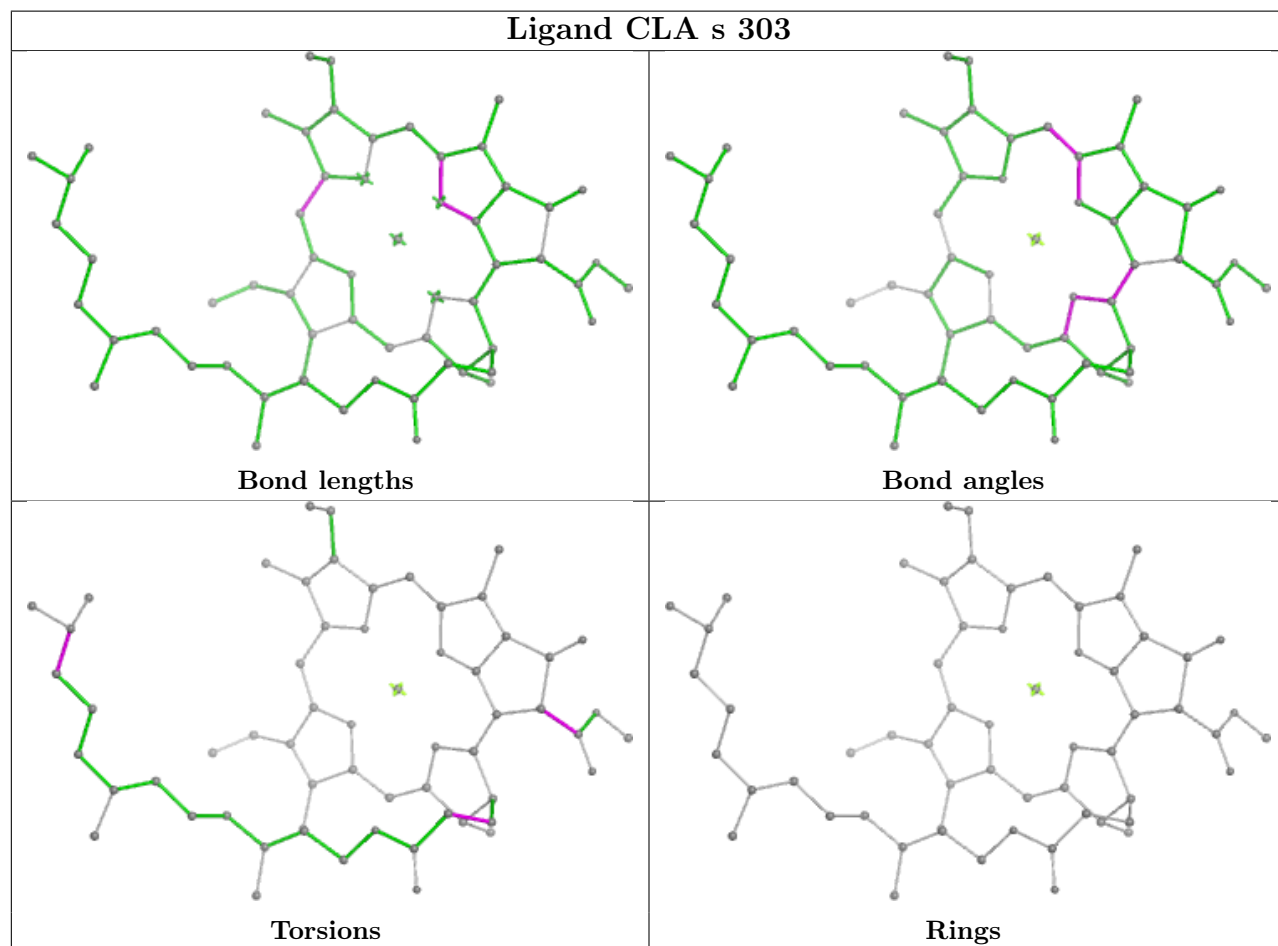
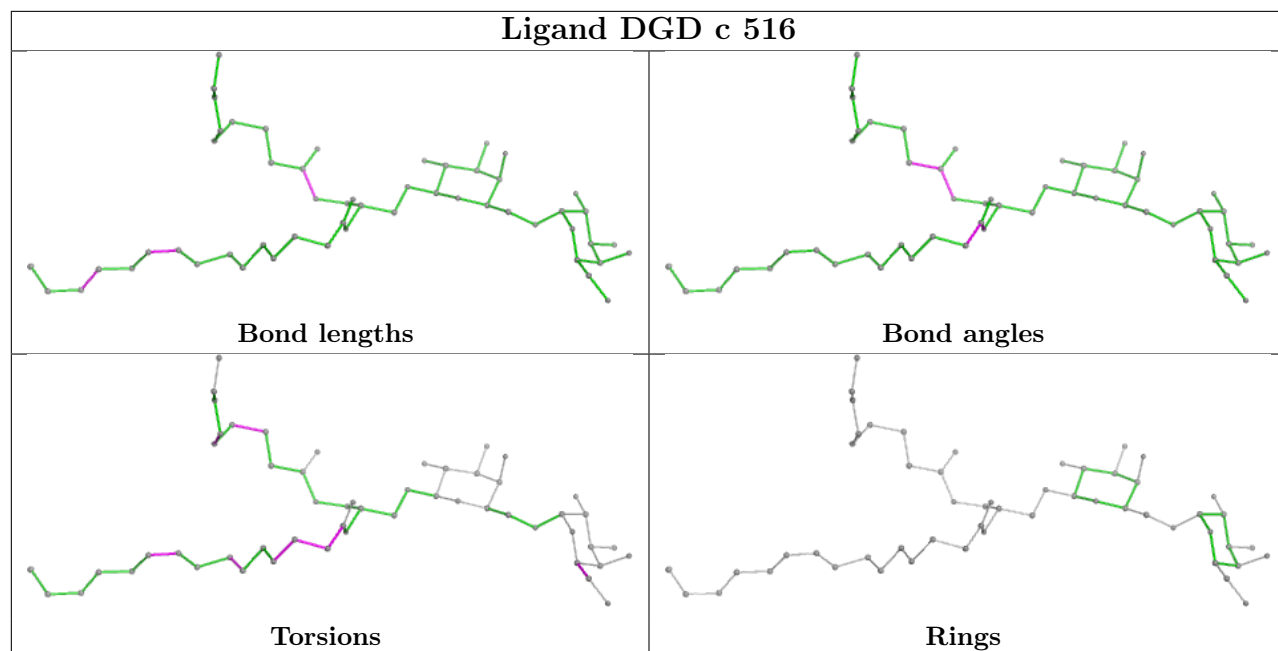


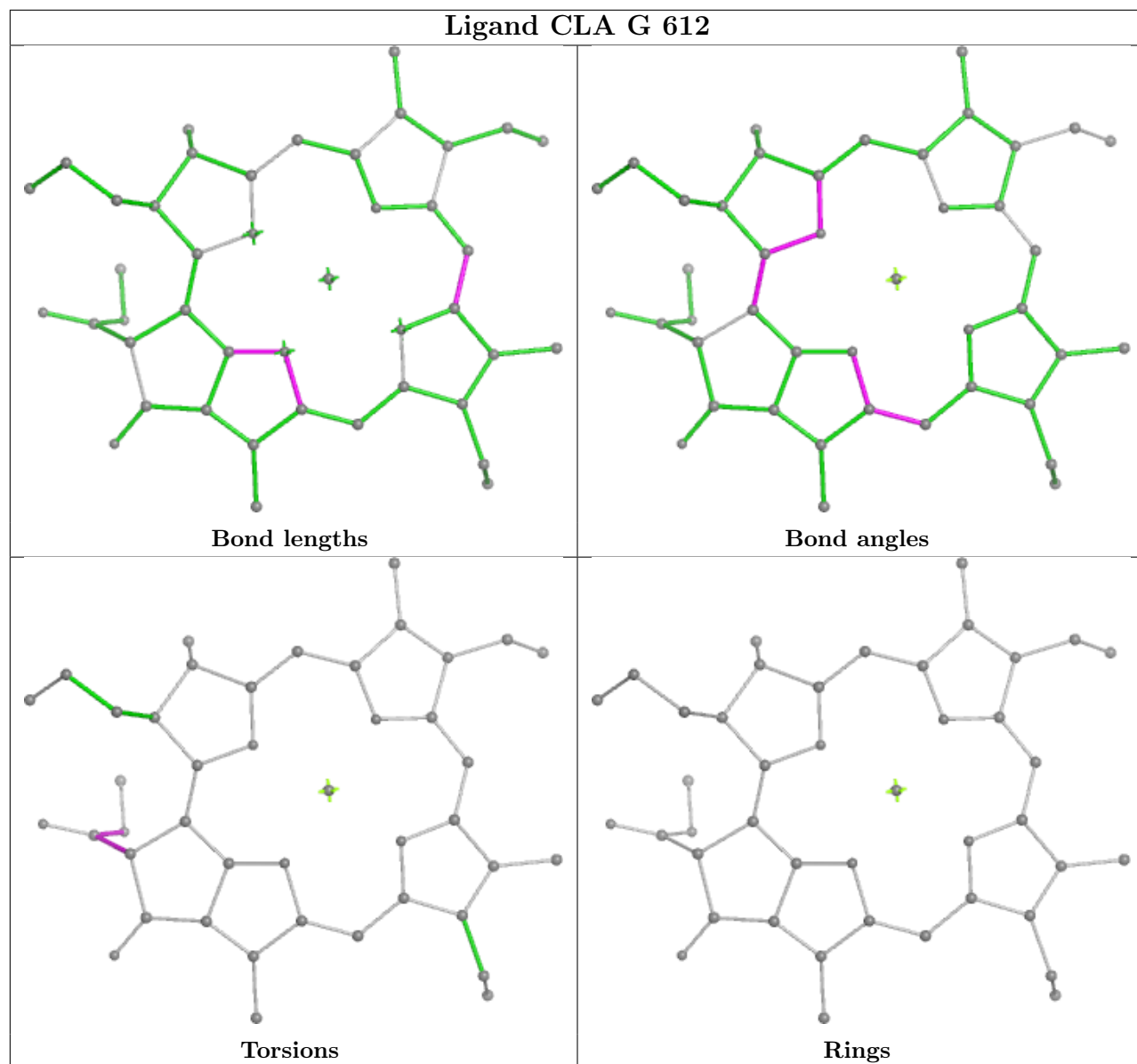


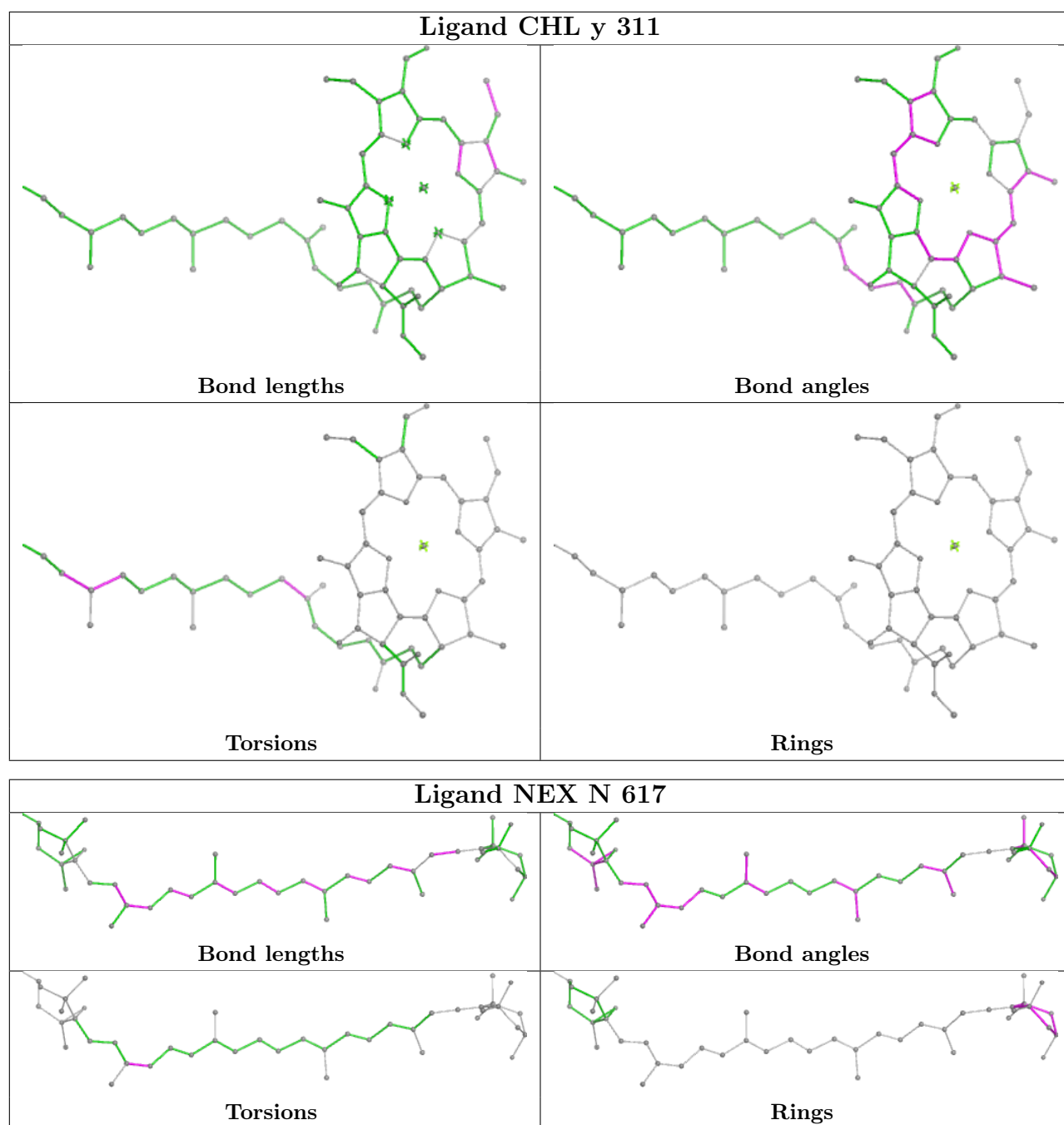




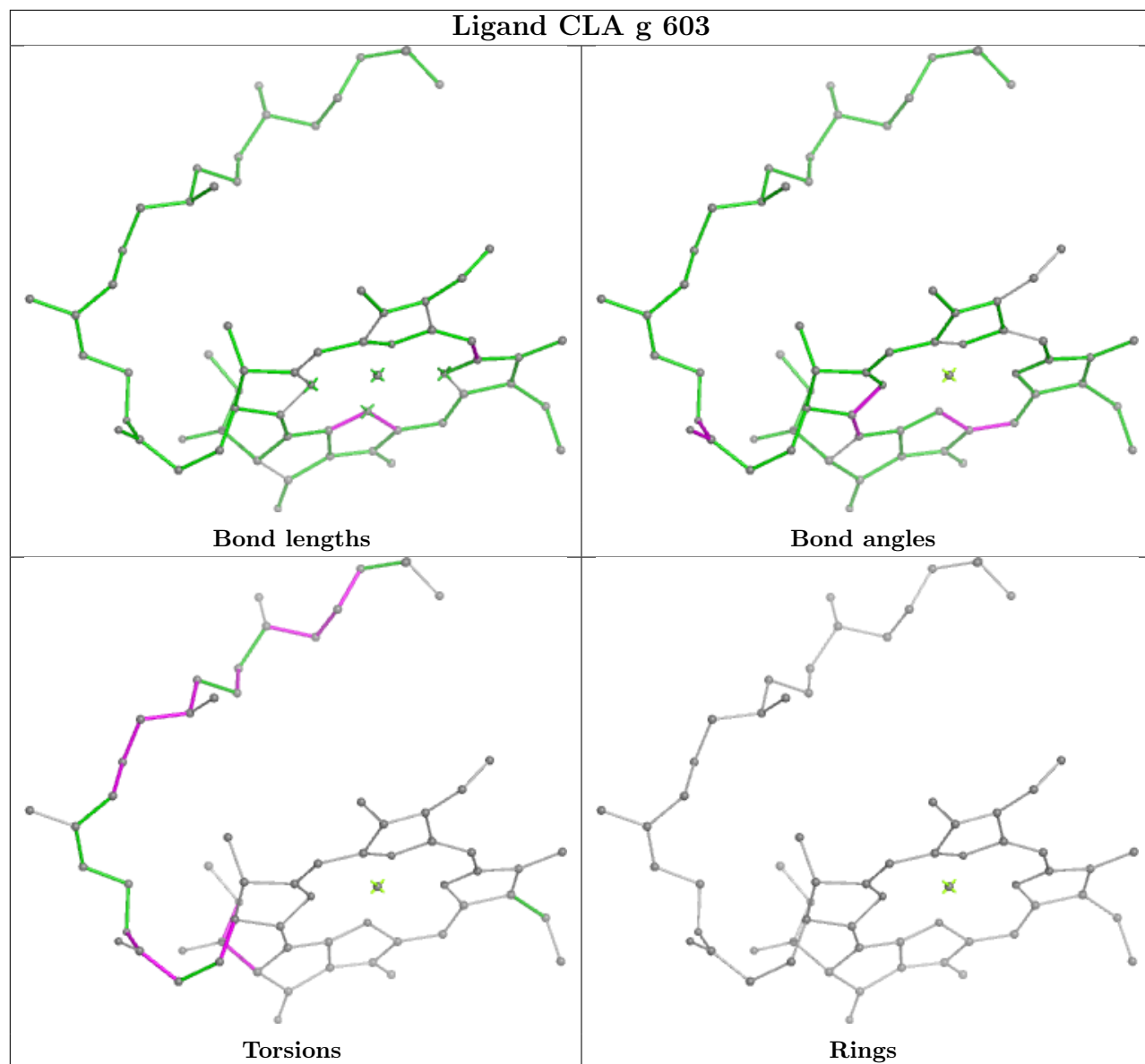


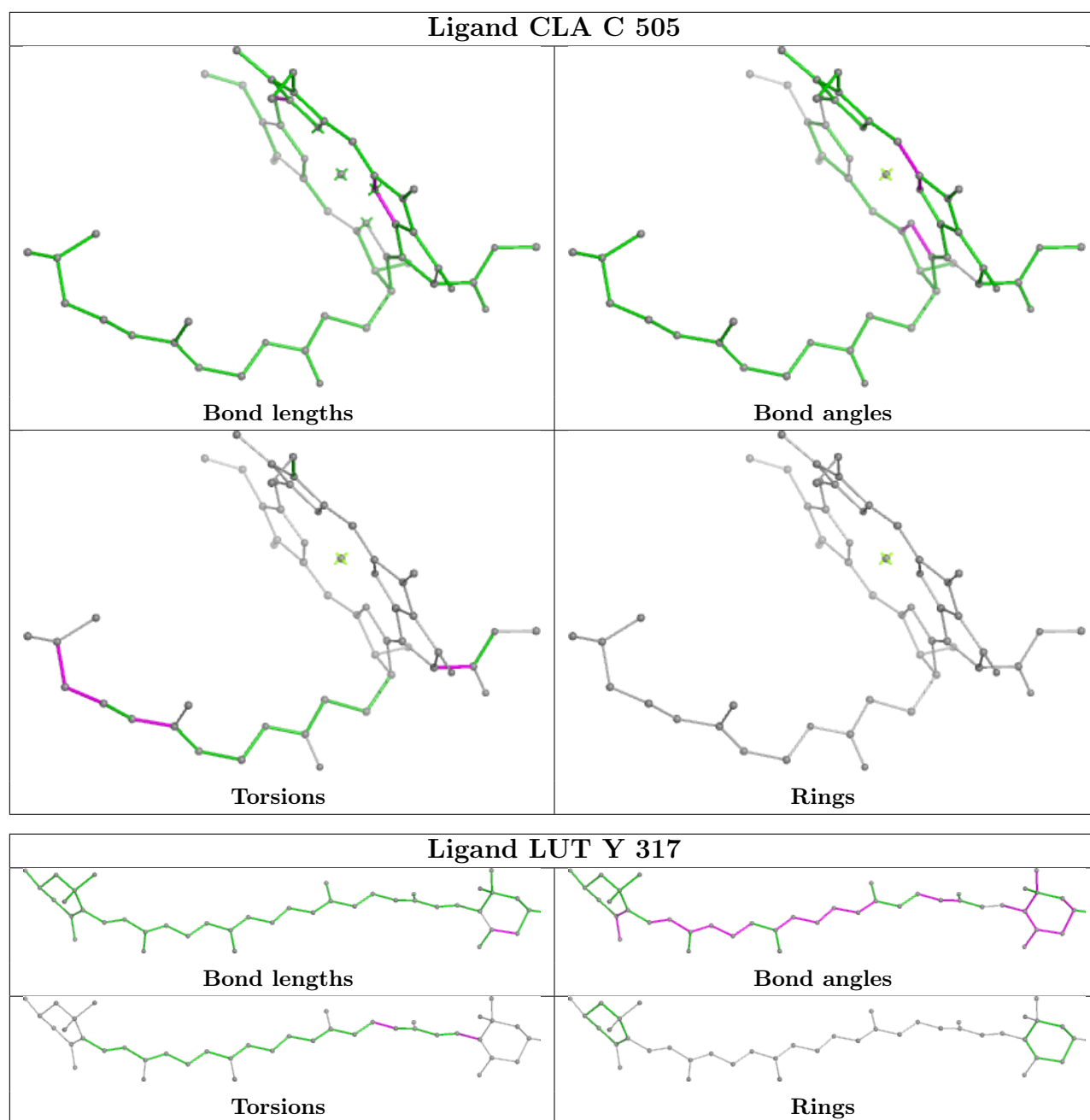


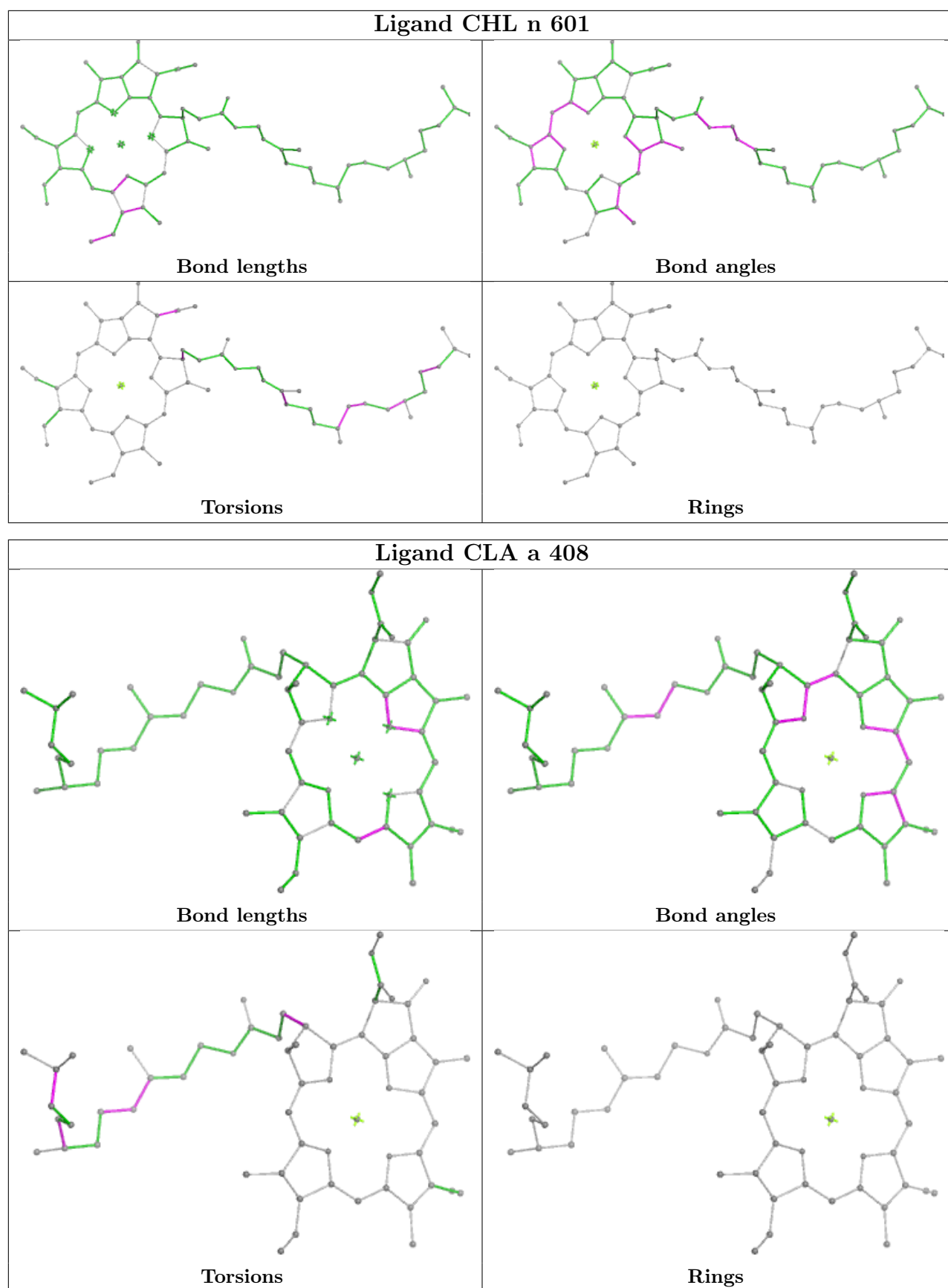


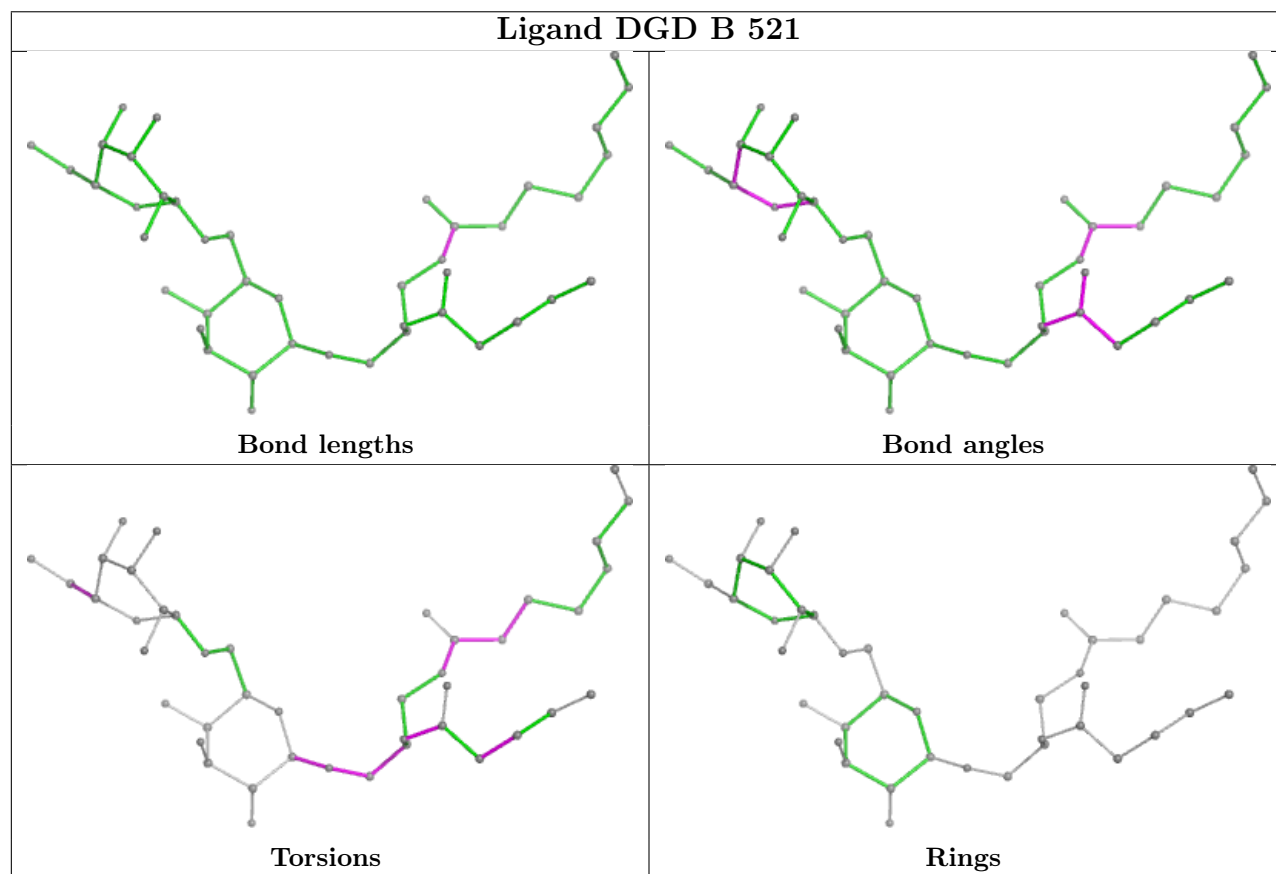
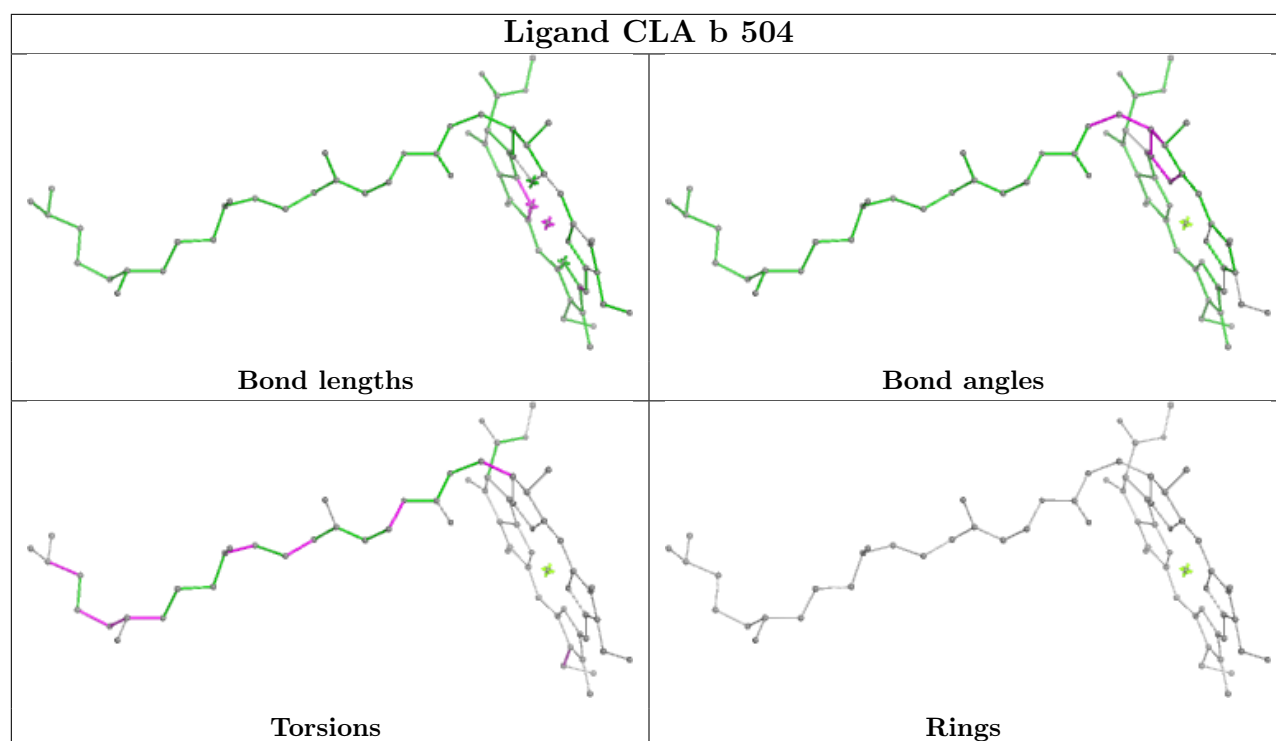


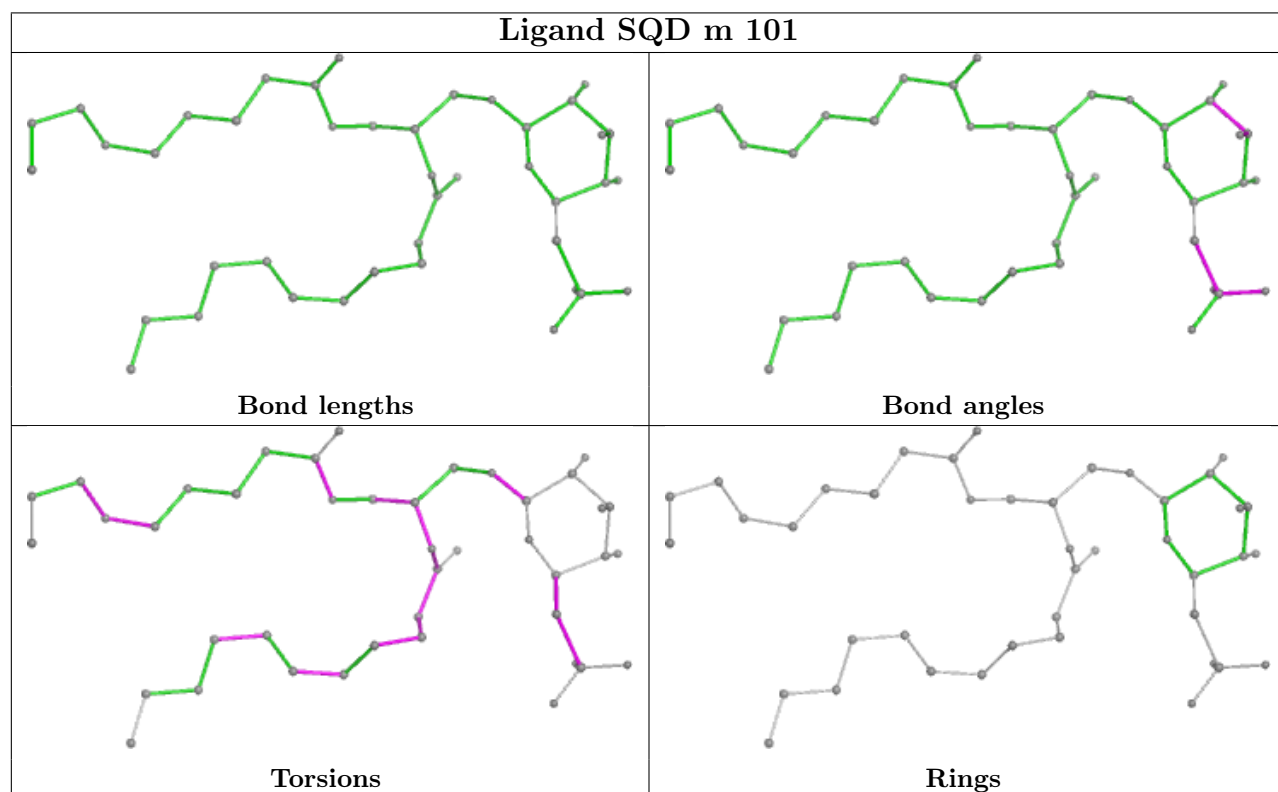
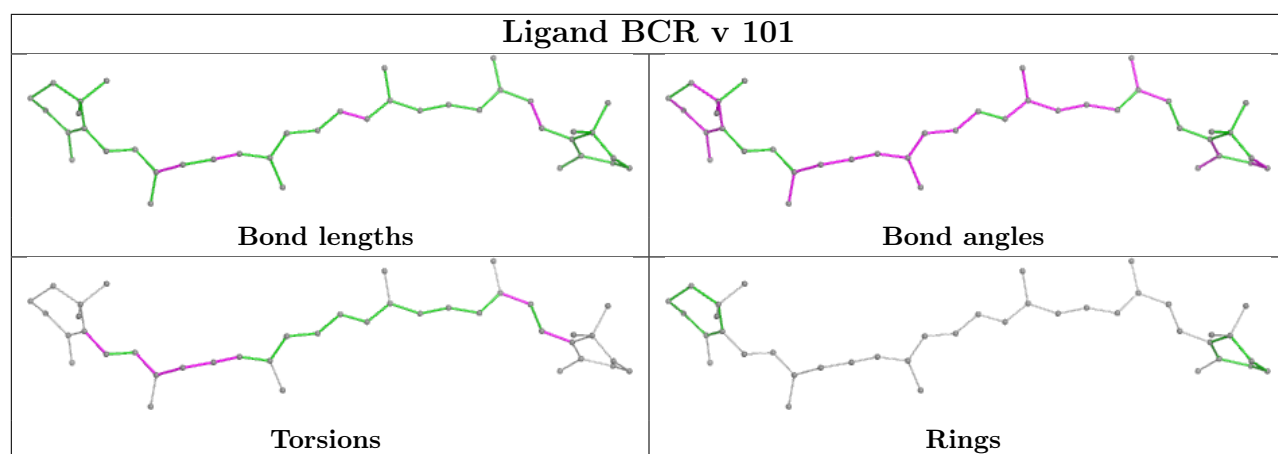
Ligand CLA g 603

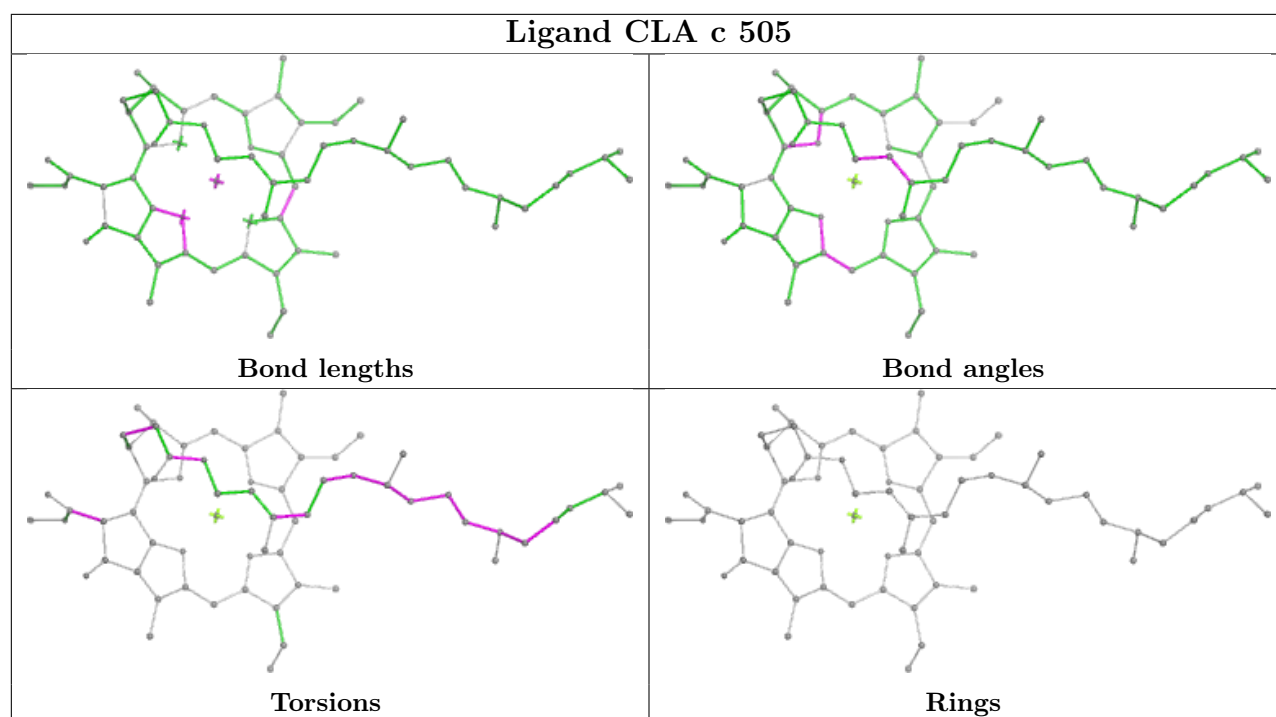




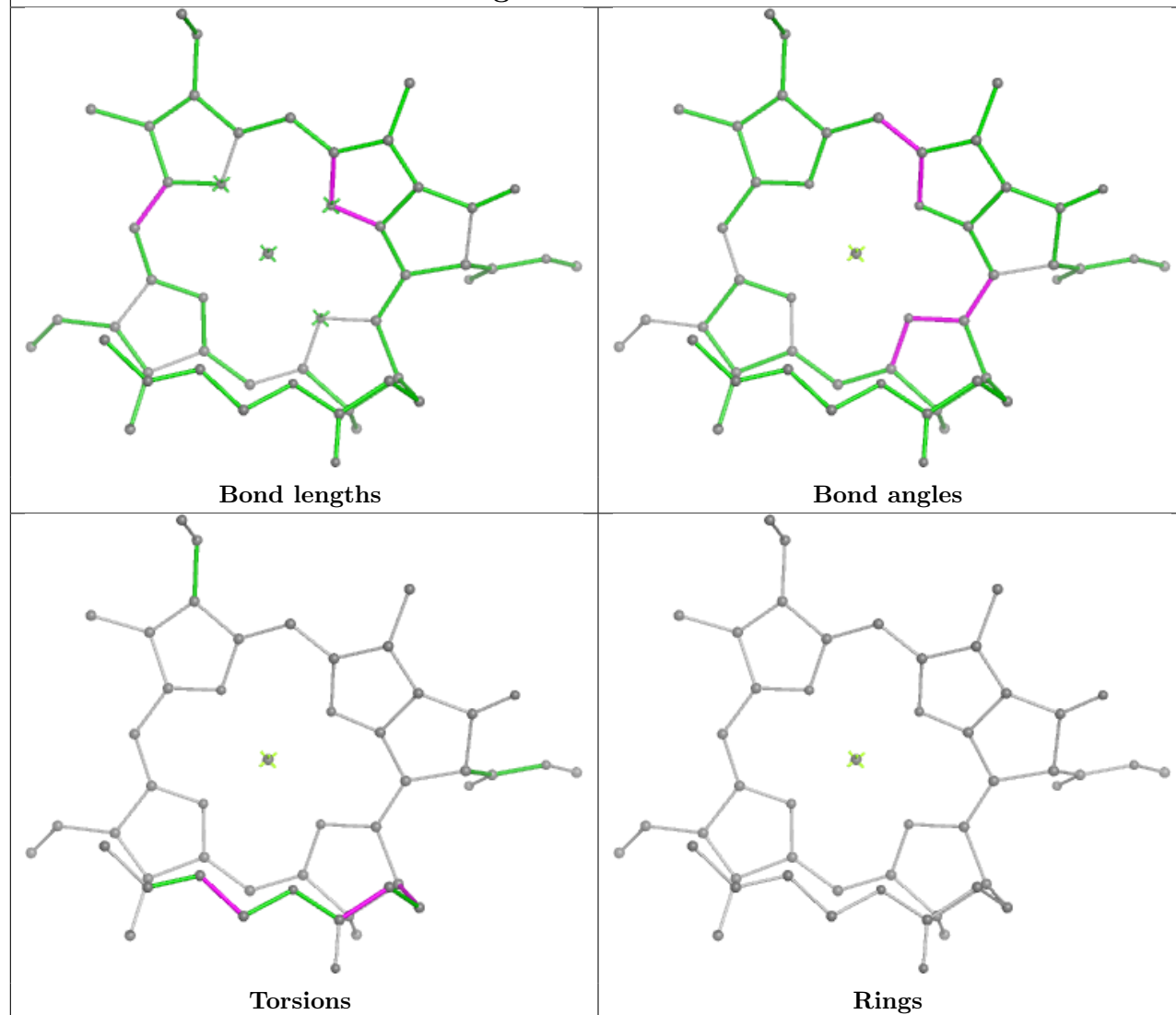




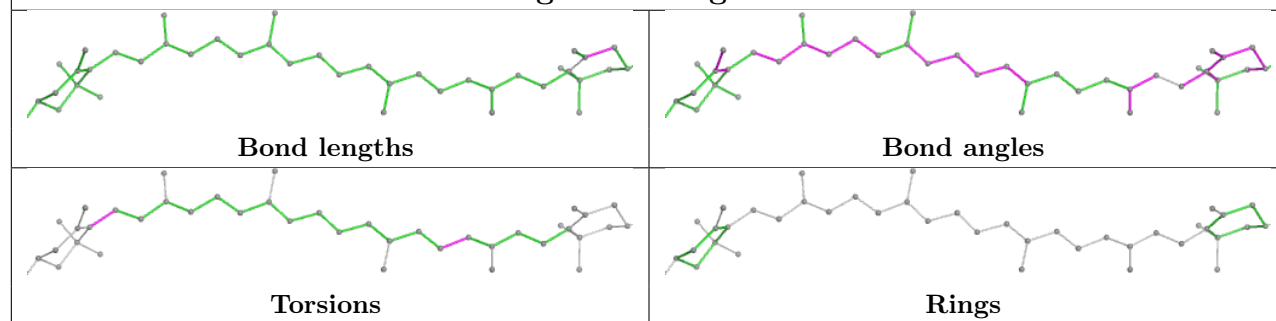


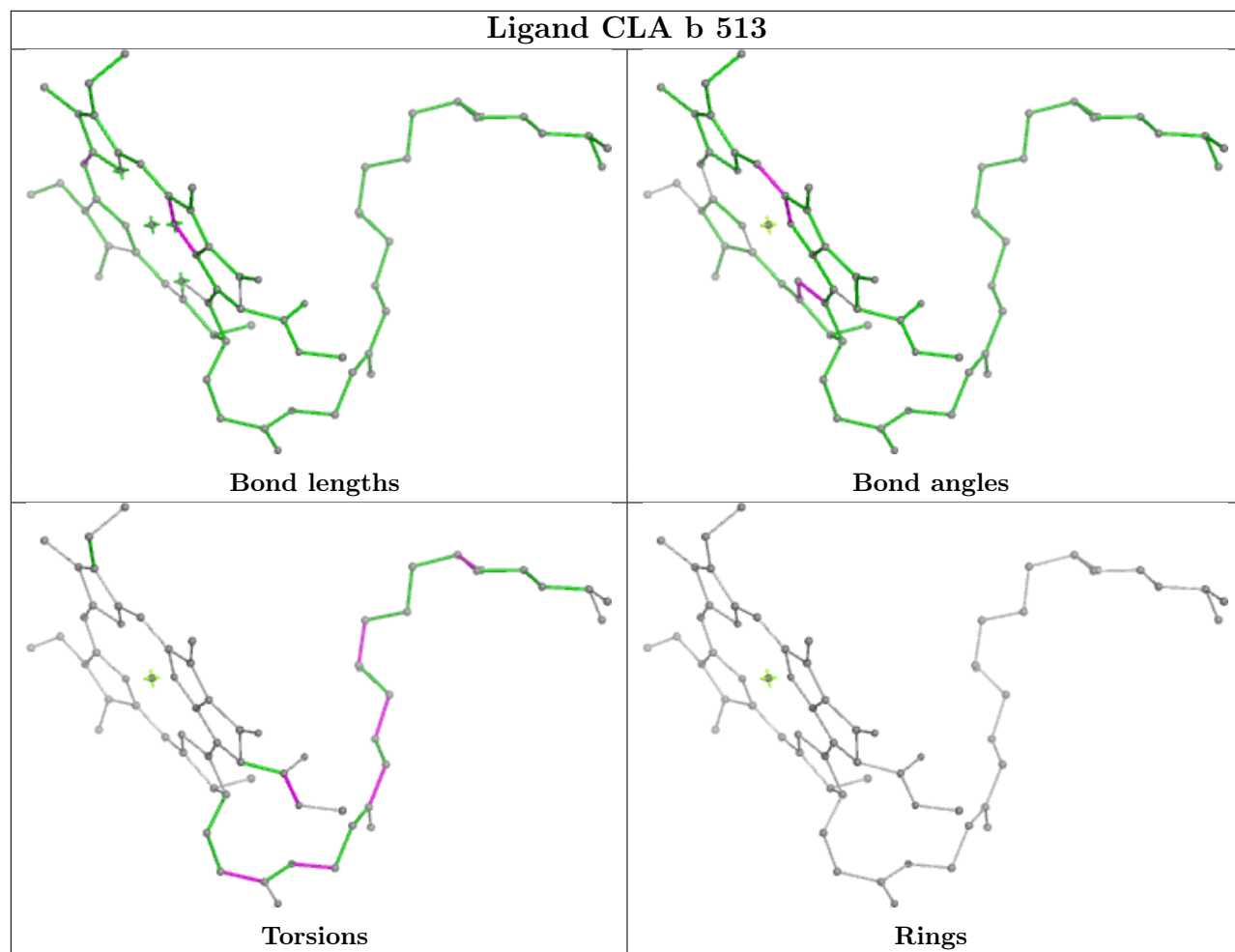


Ligand CLA n 613

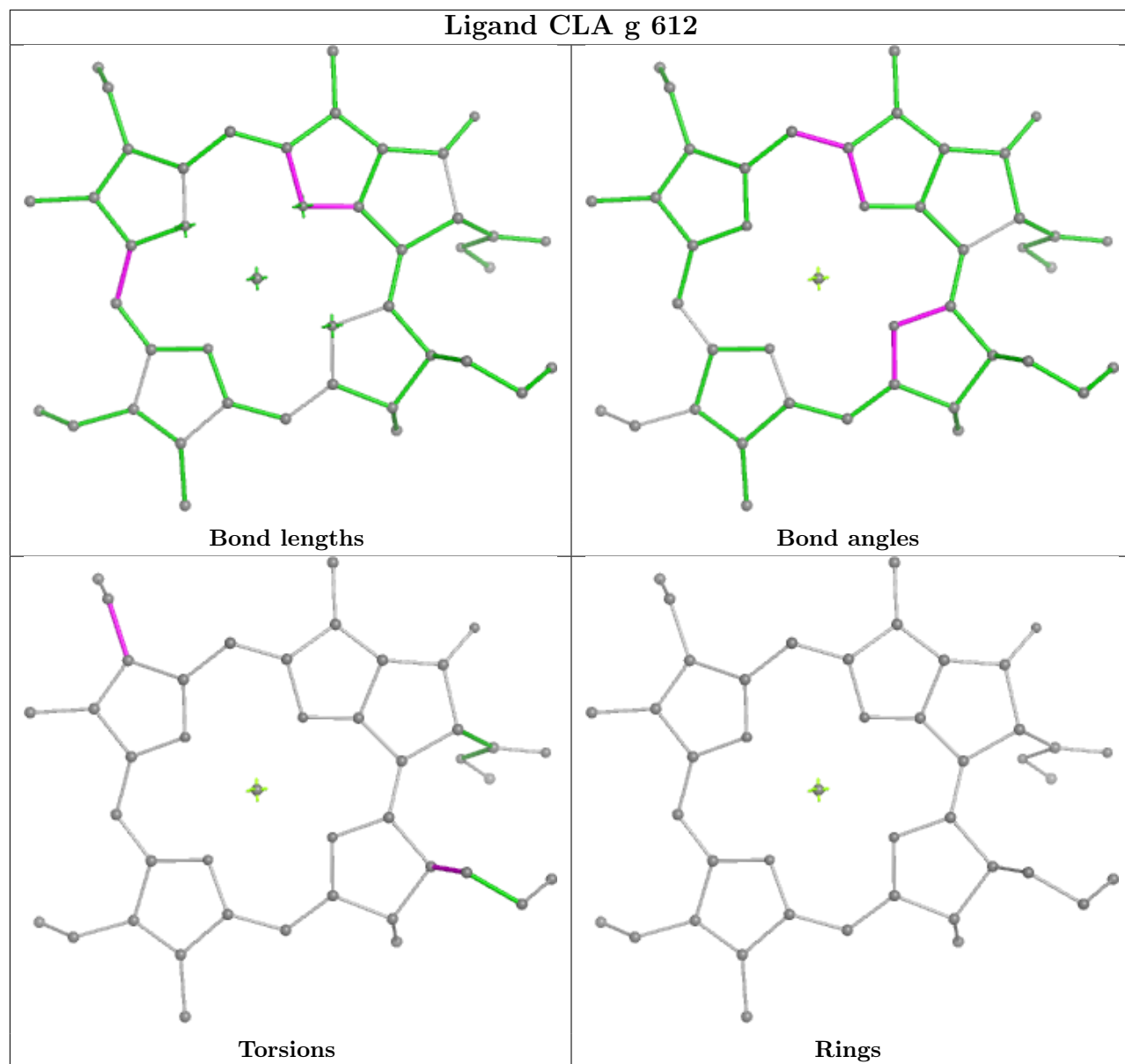


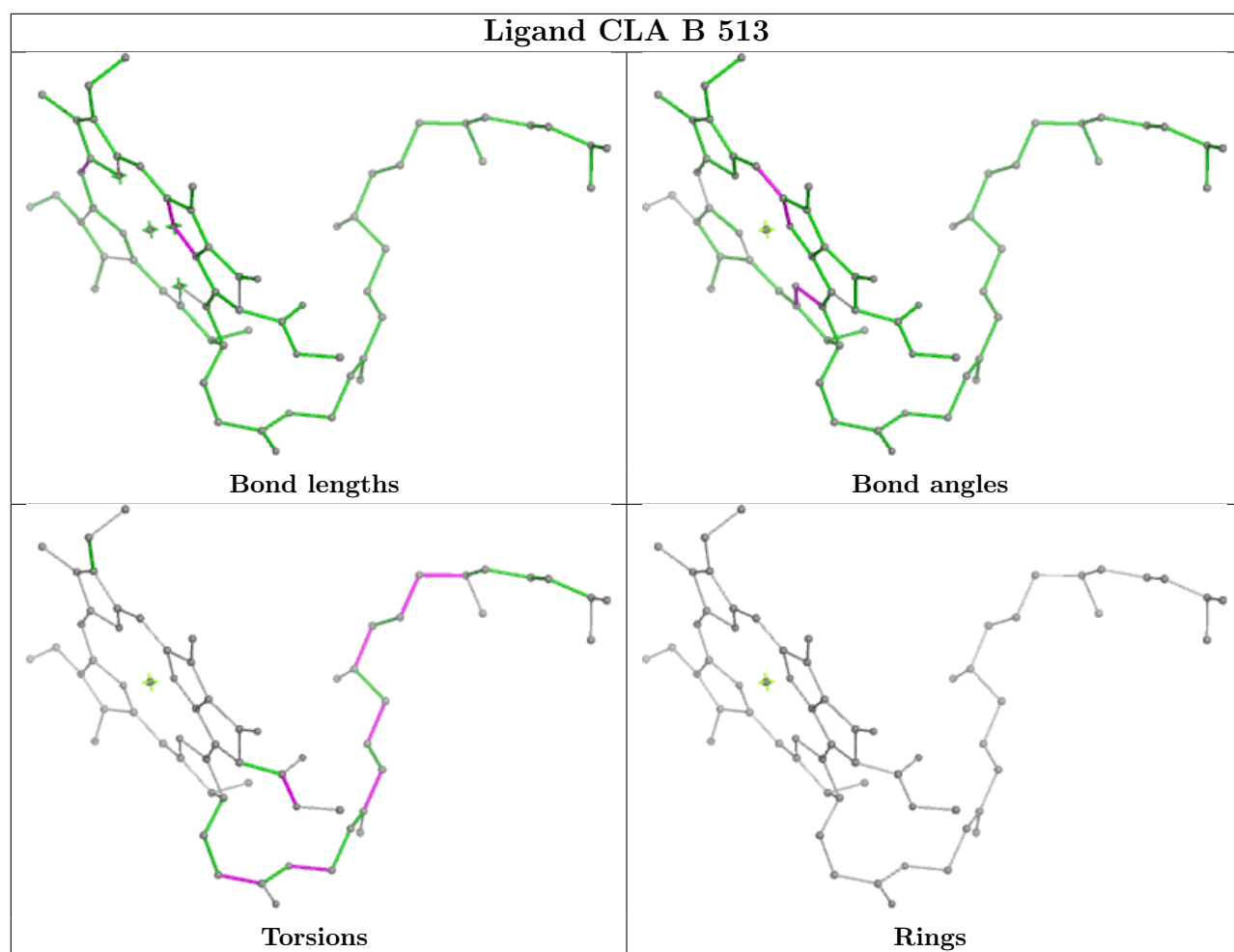
Ligand LUT g 615



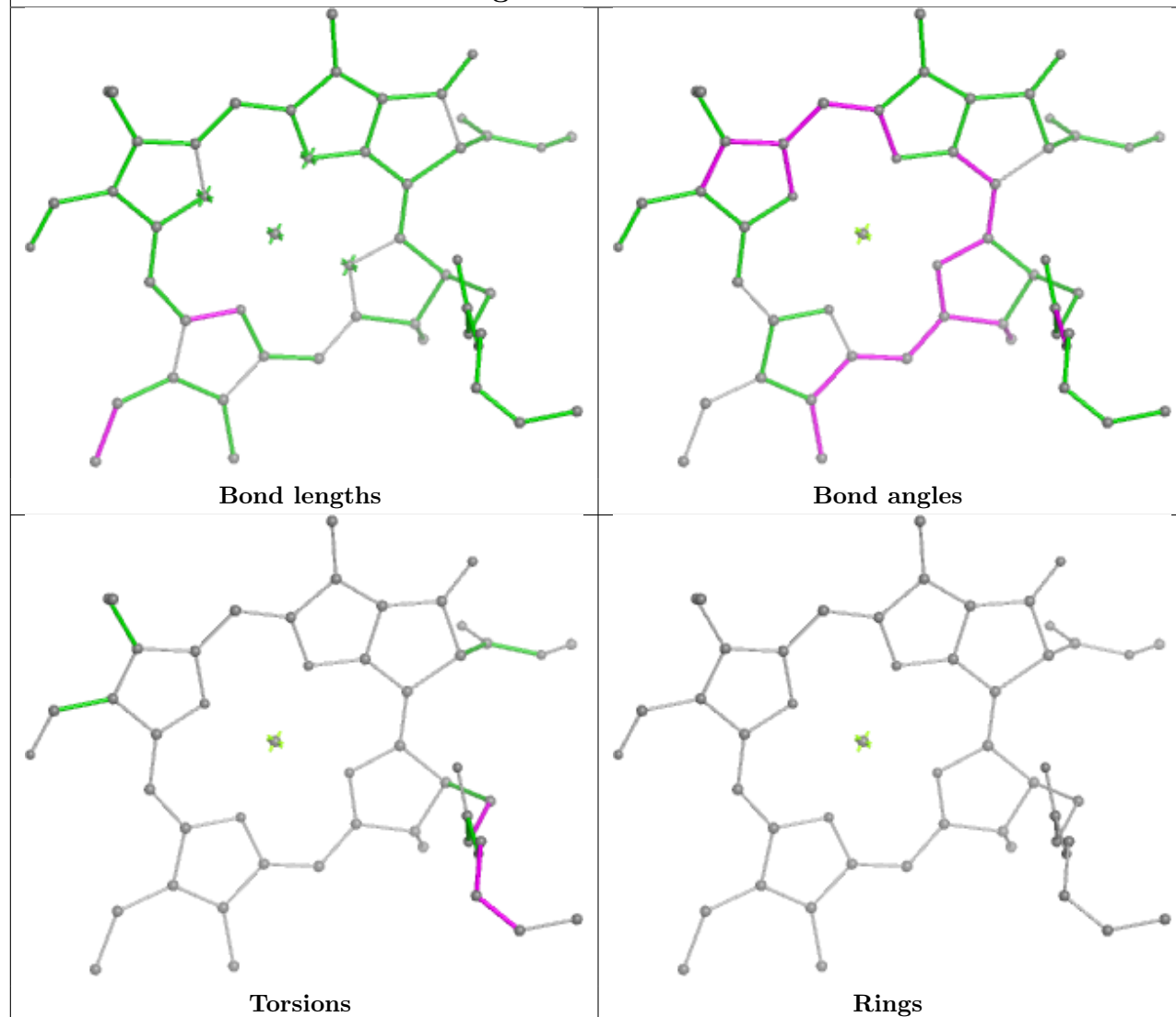


Ligand CLA g 612

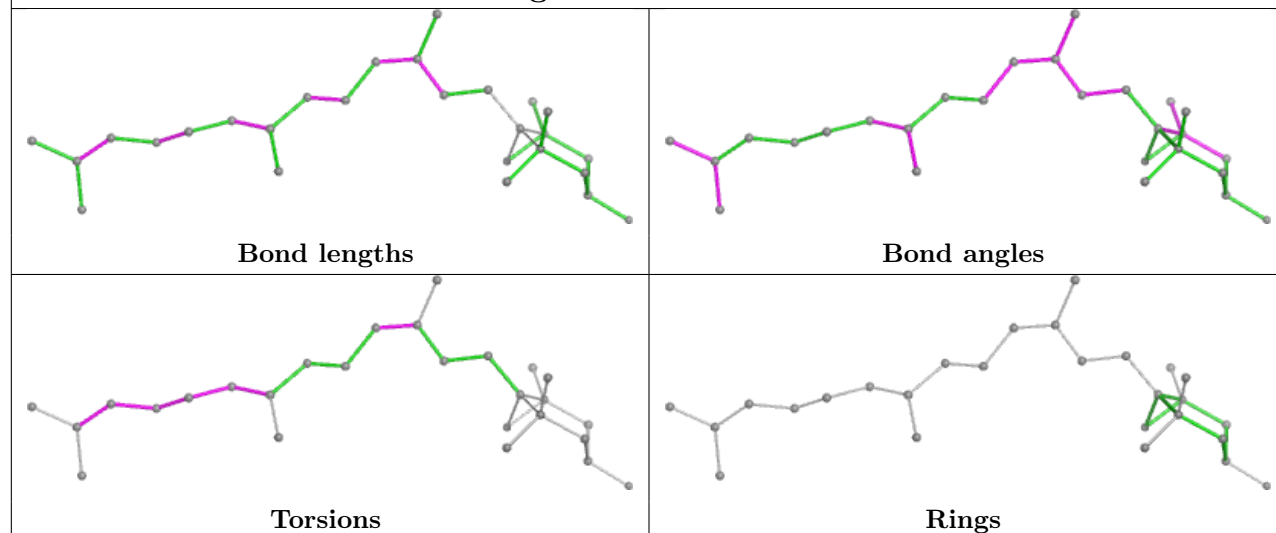


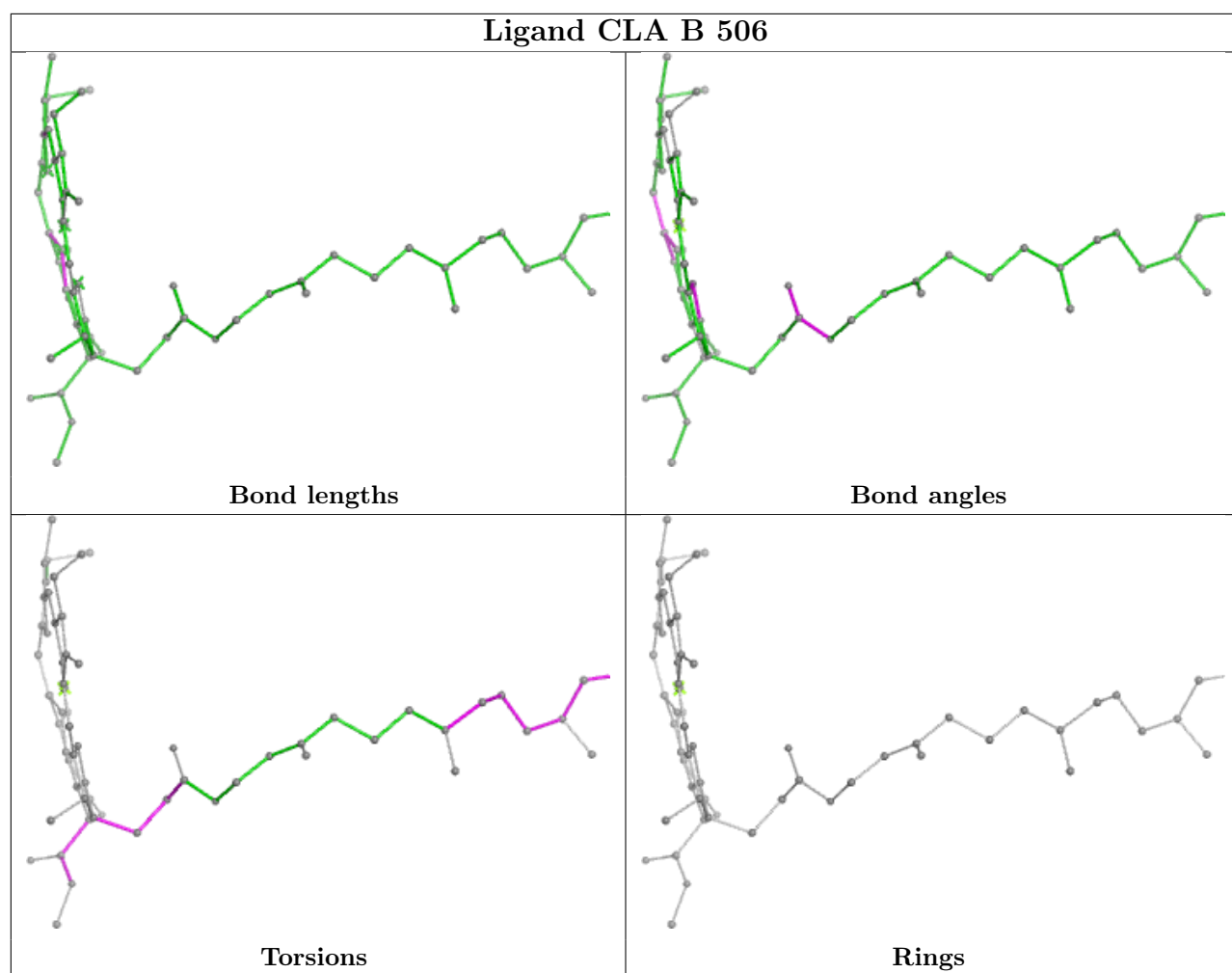


Ligand CHL n 607

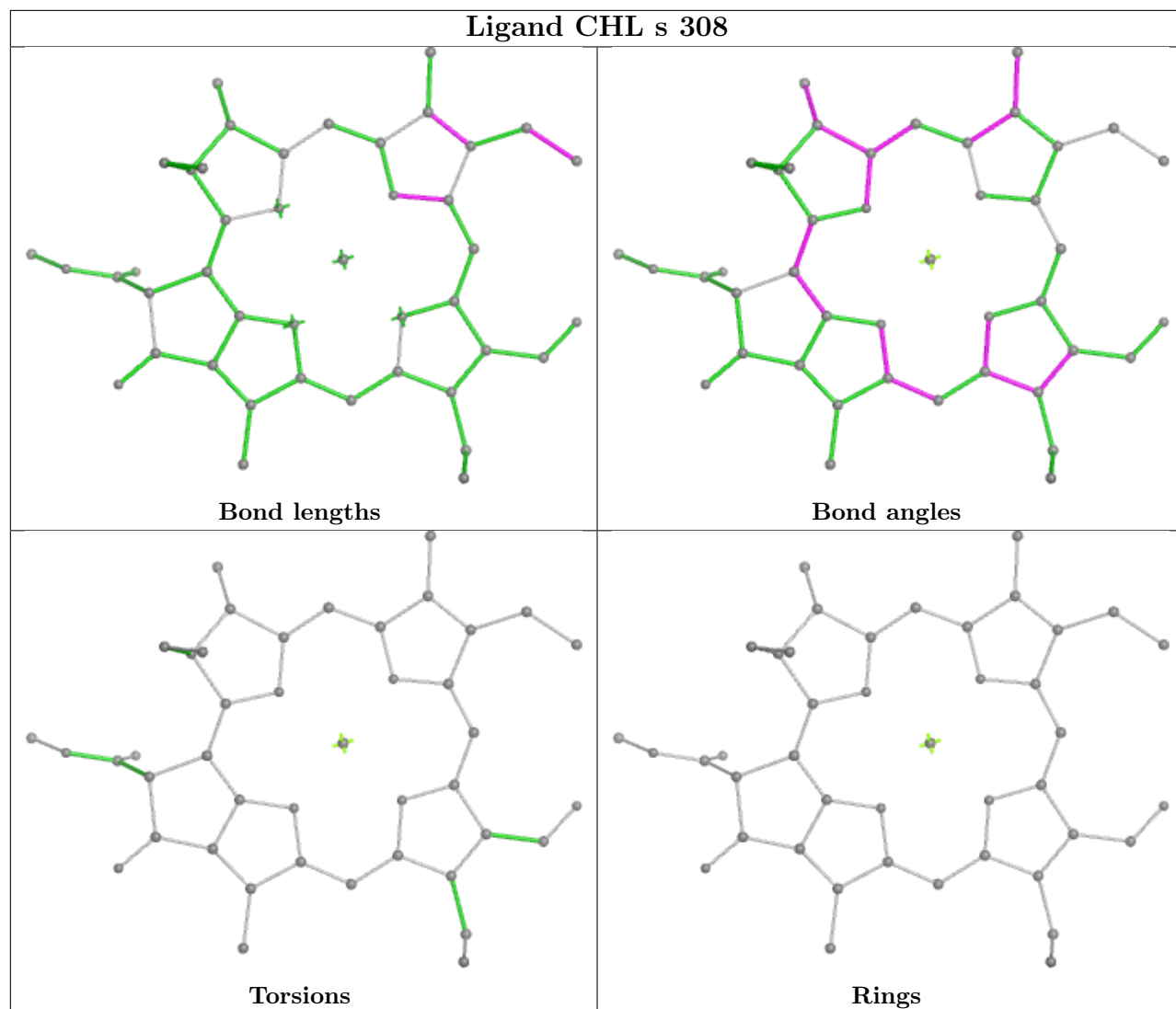


Ligand NEX R 312

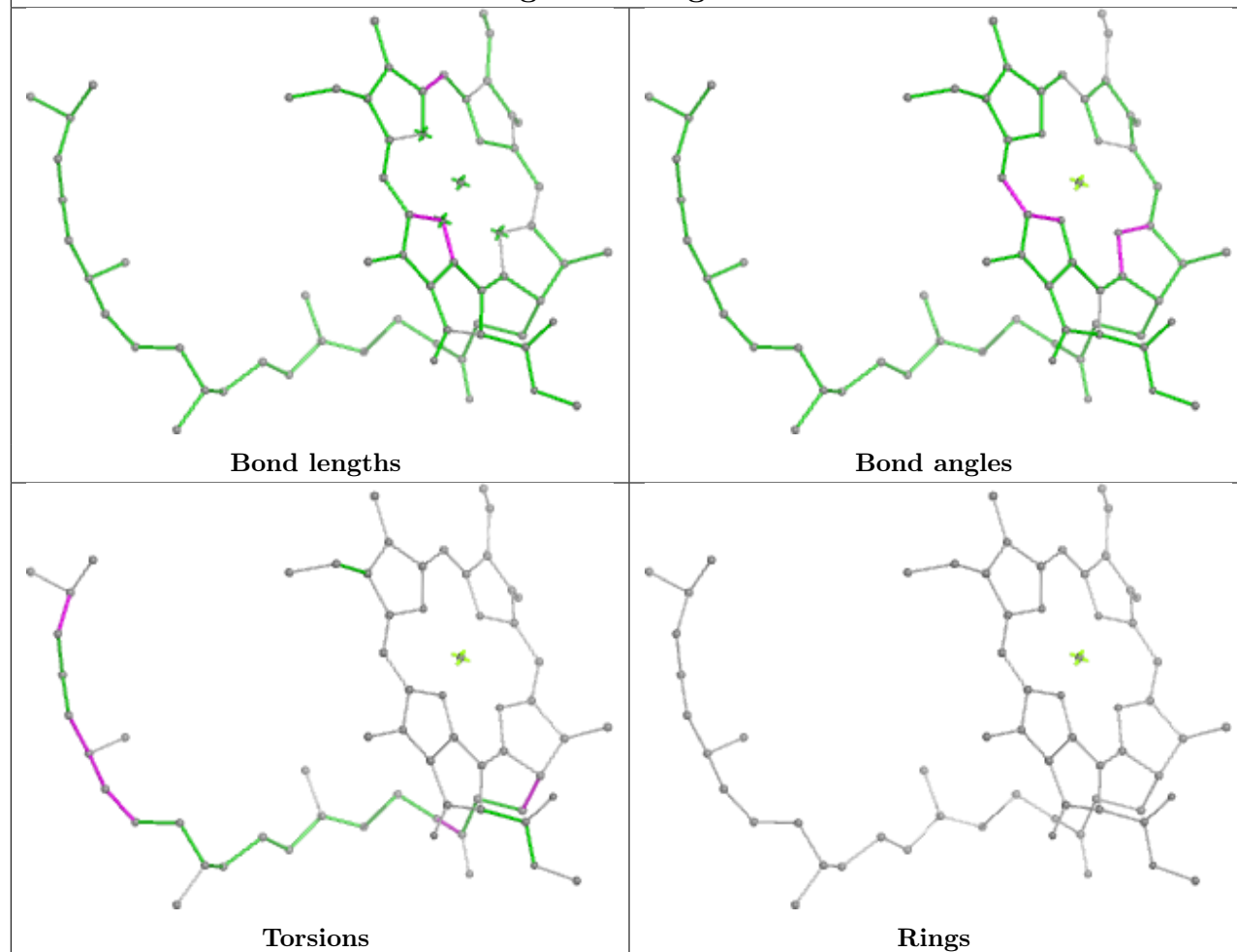




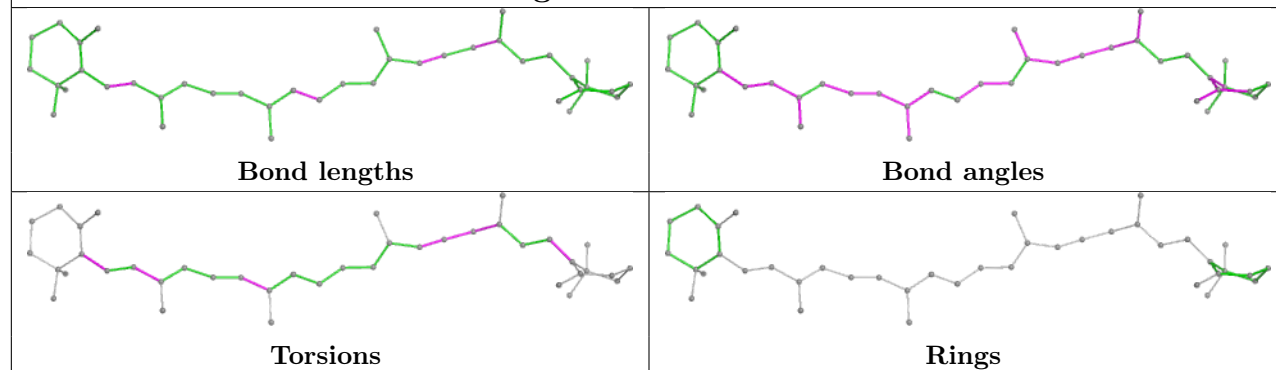
Ligand CHL s 308

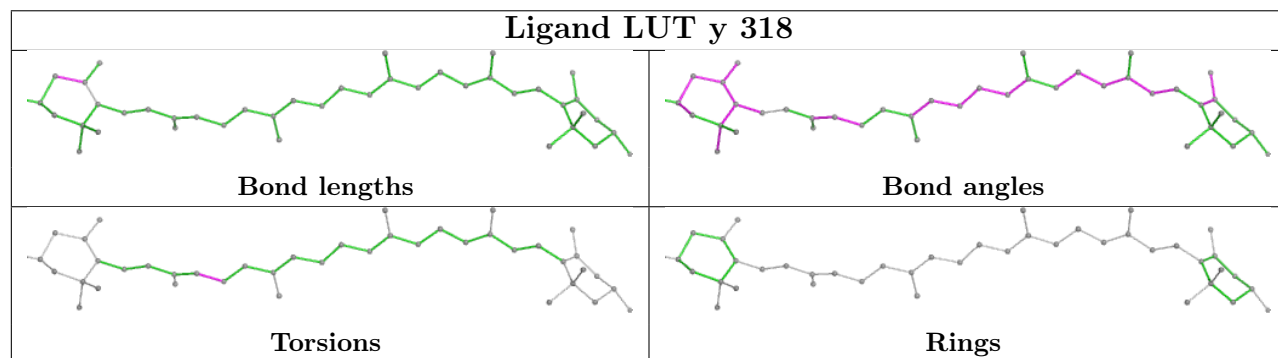
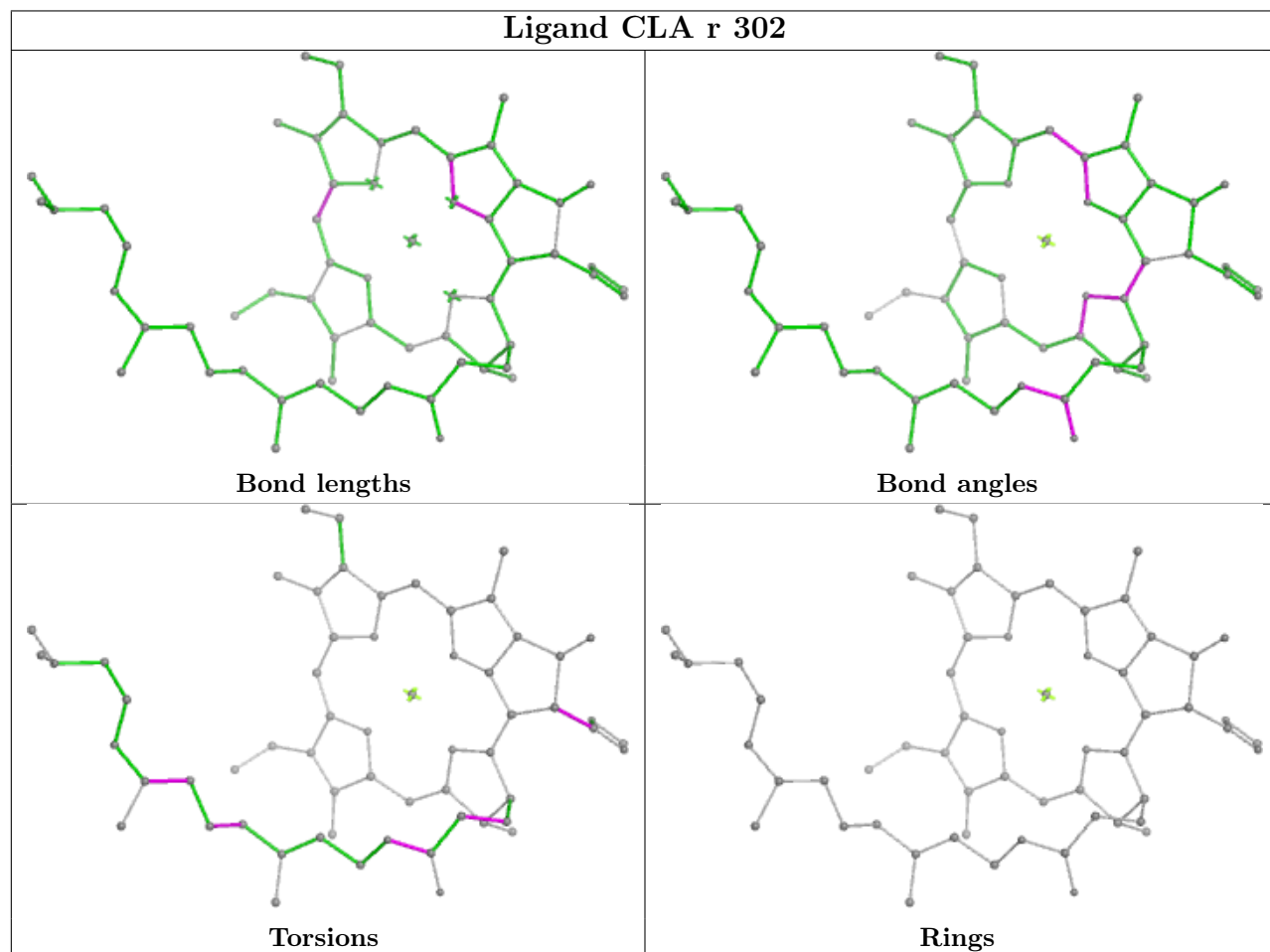
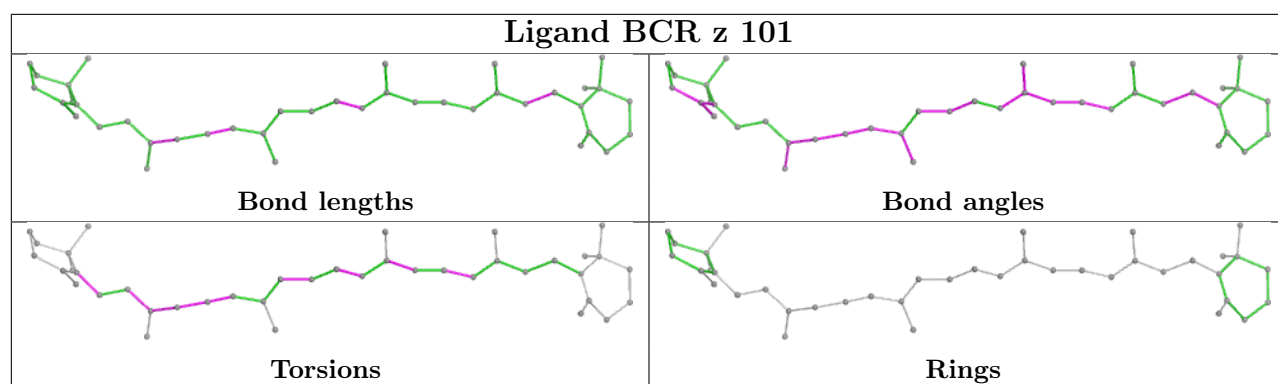


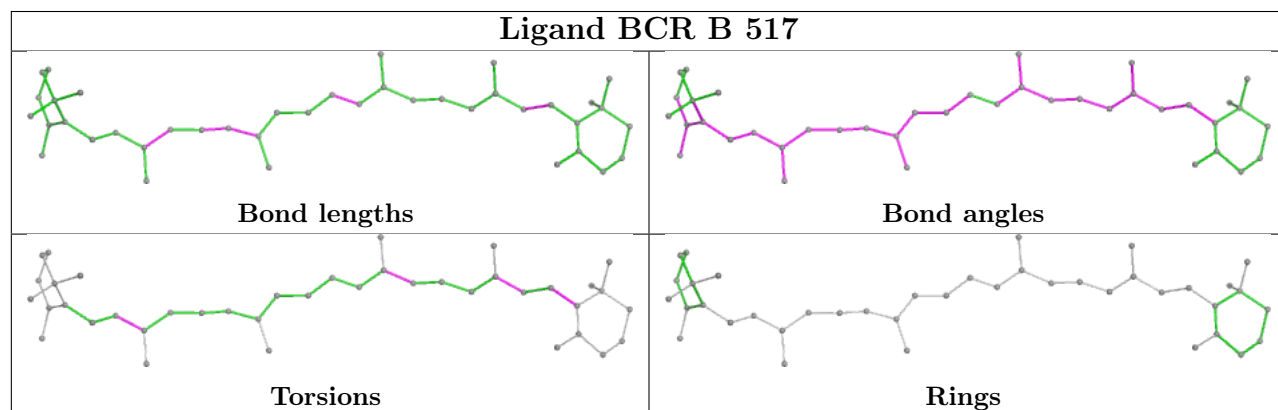
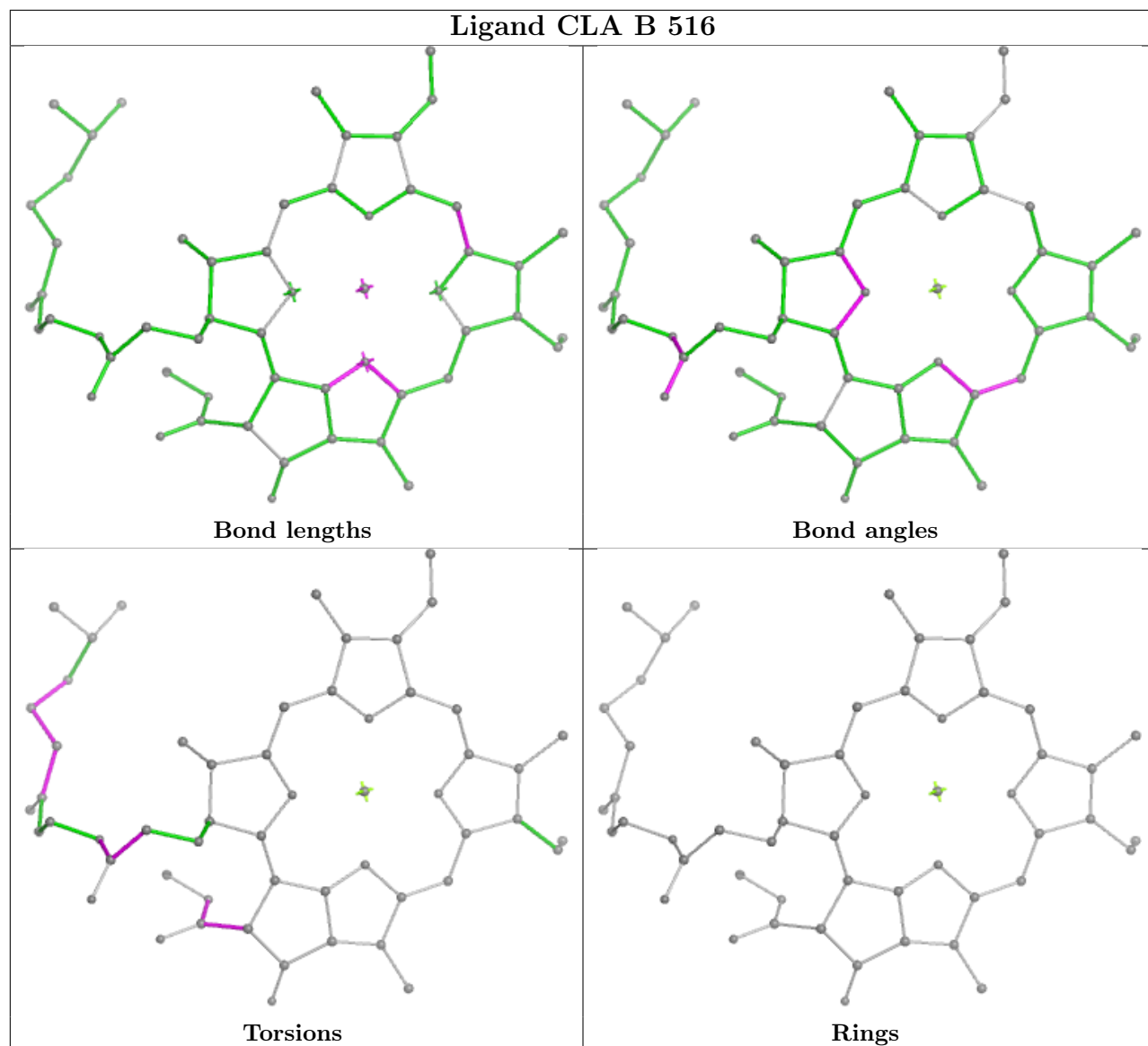
Ligand CLA g 611

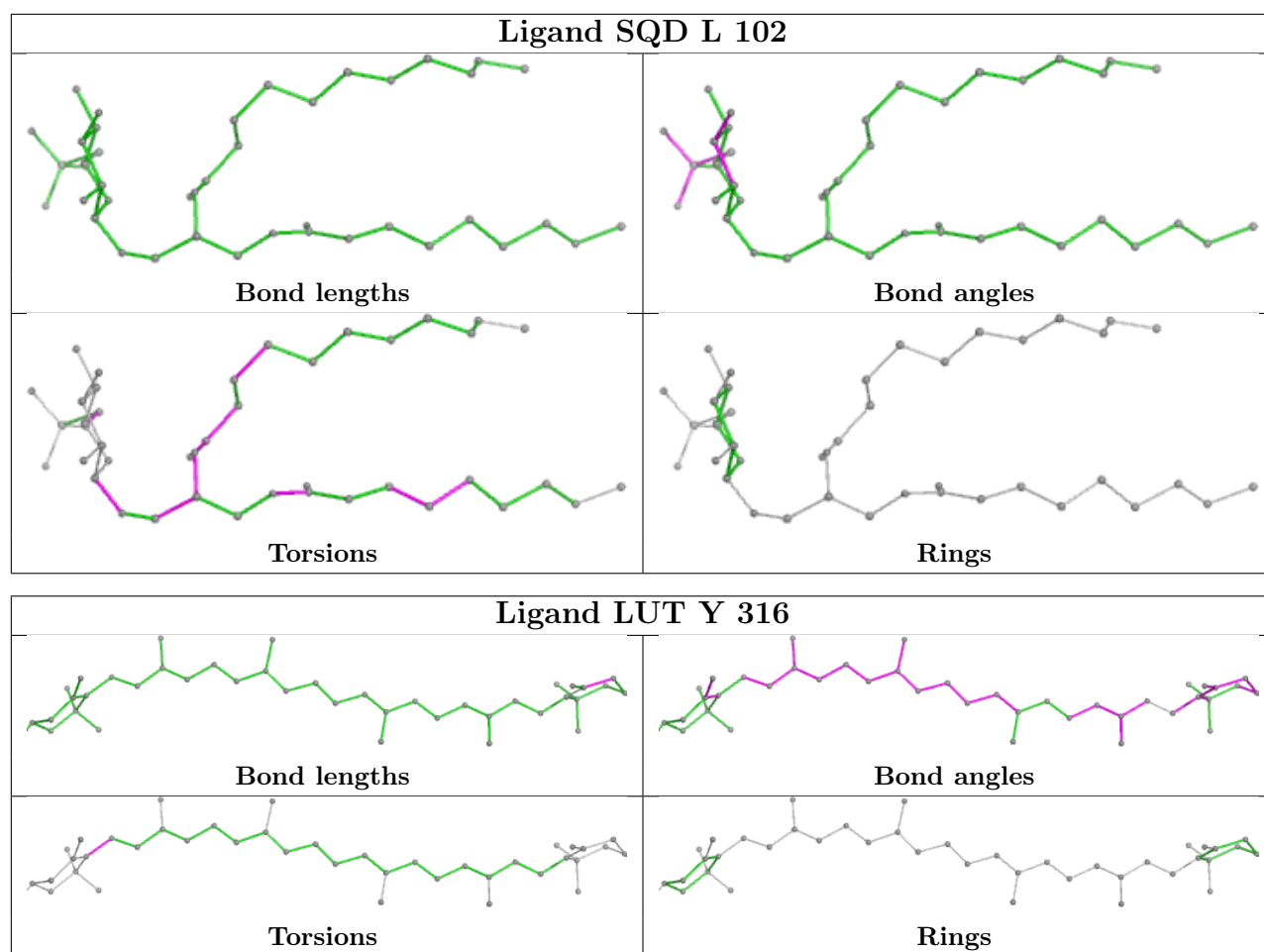


Ligand BCR b 517

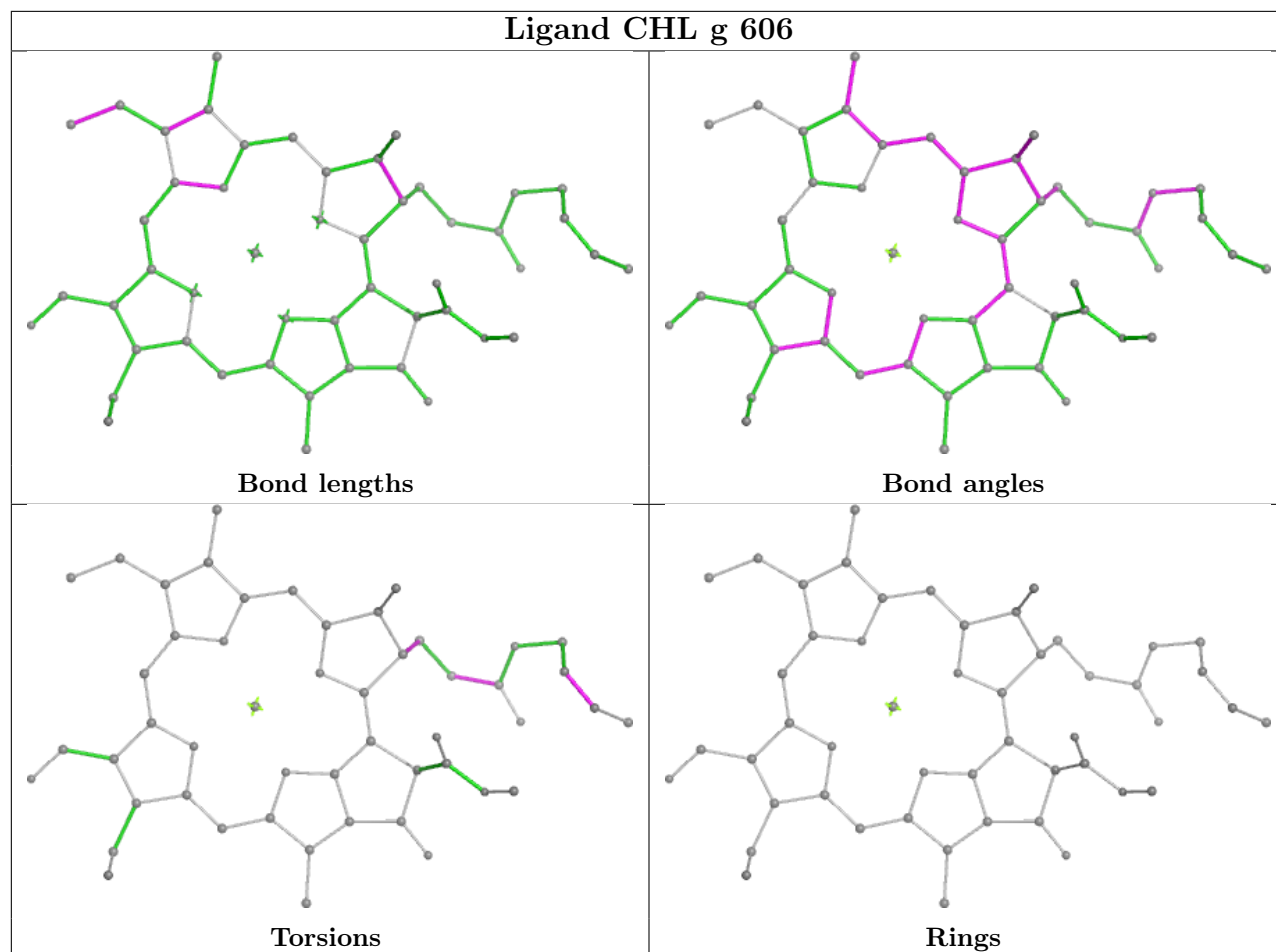




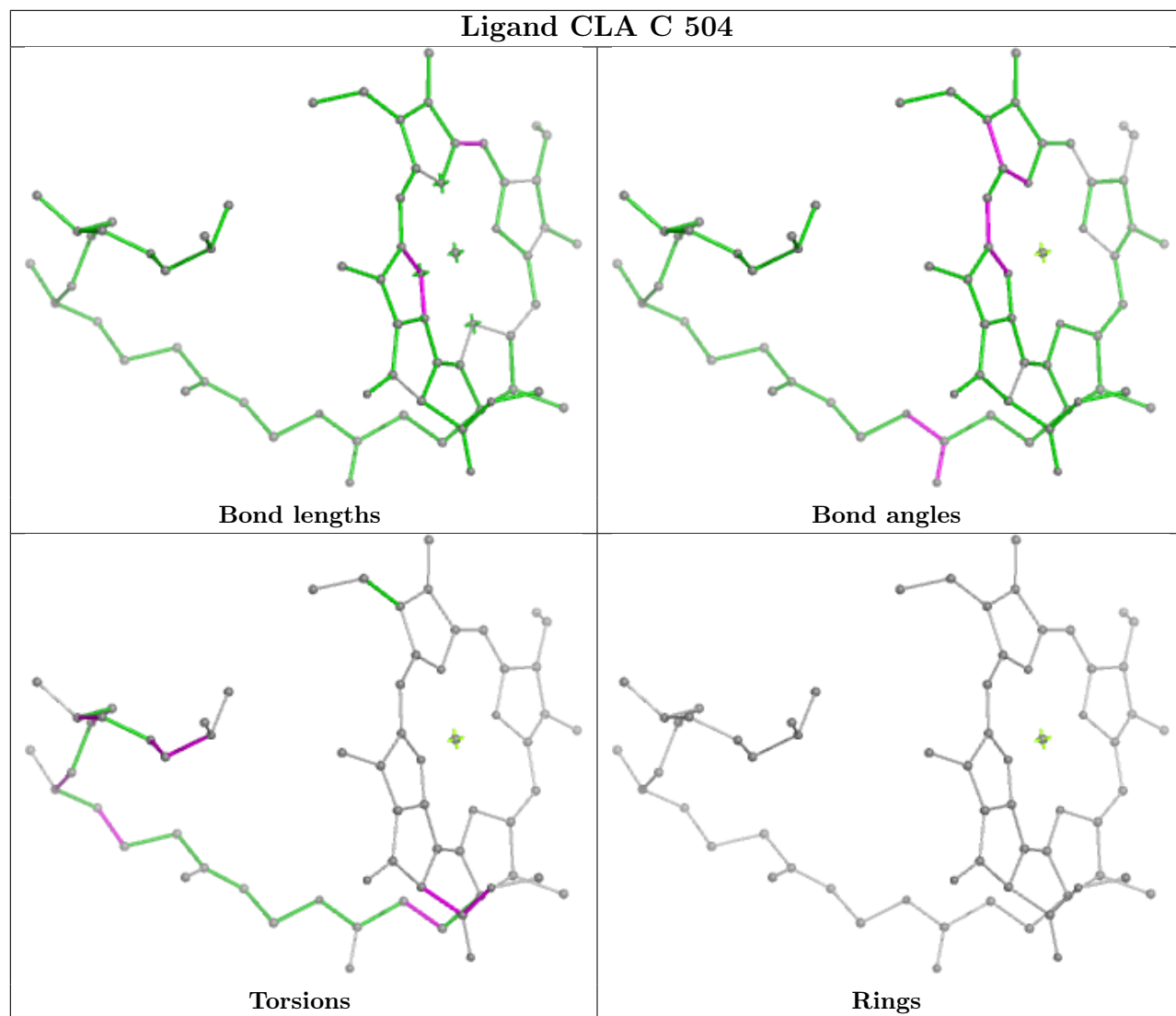




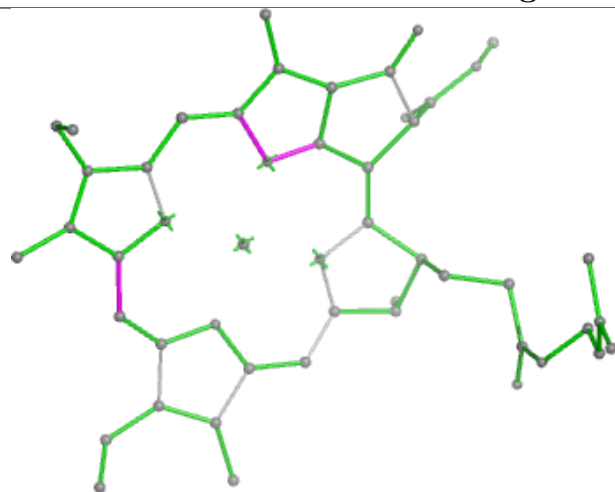
Ligand CHL g 606



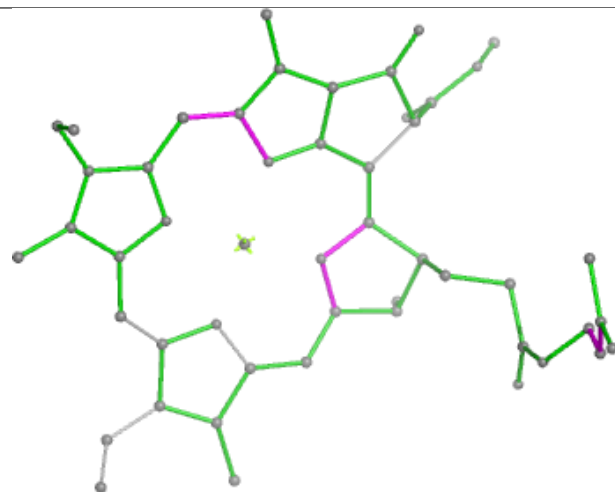
Ligand CLA C 504



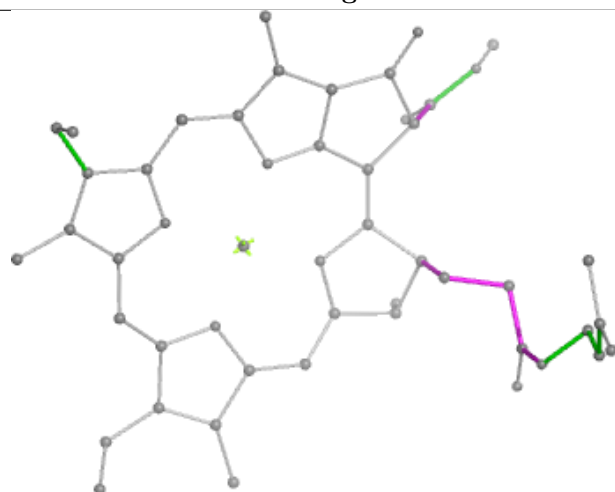
Ligand CLA S 315



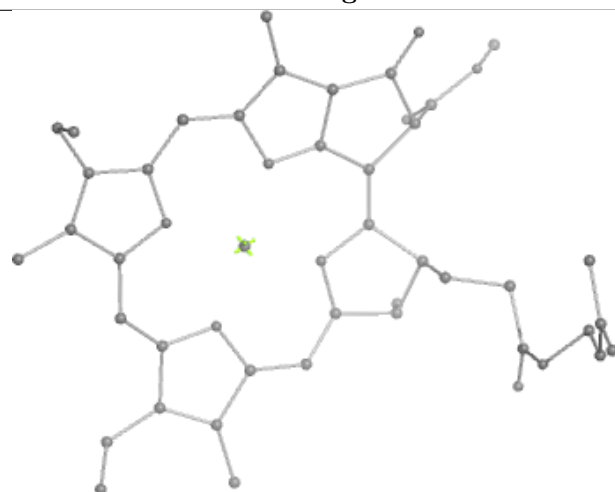
Bond lengths



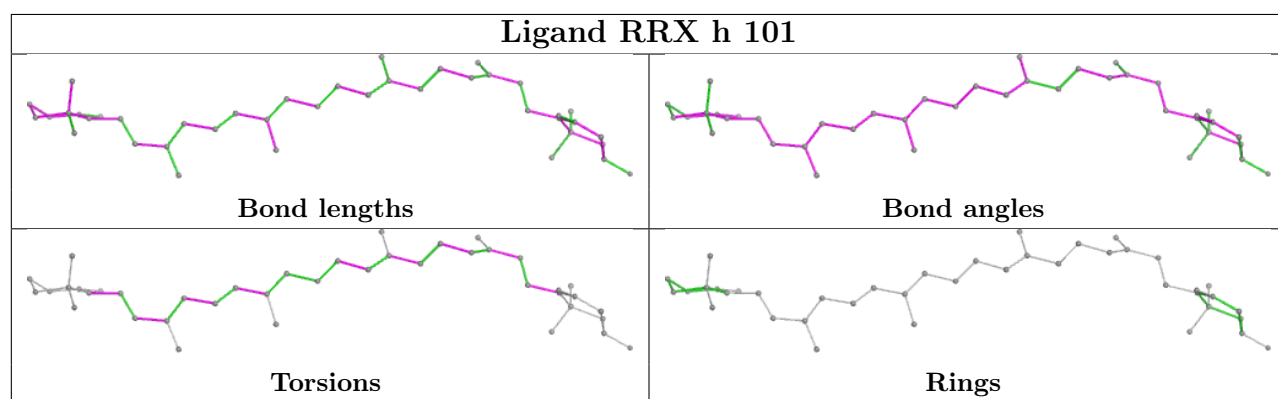
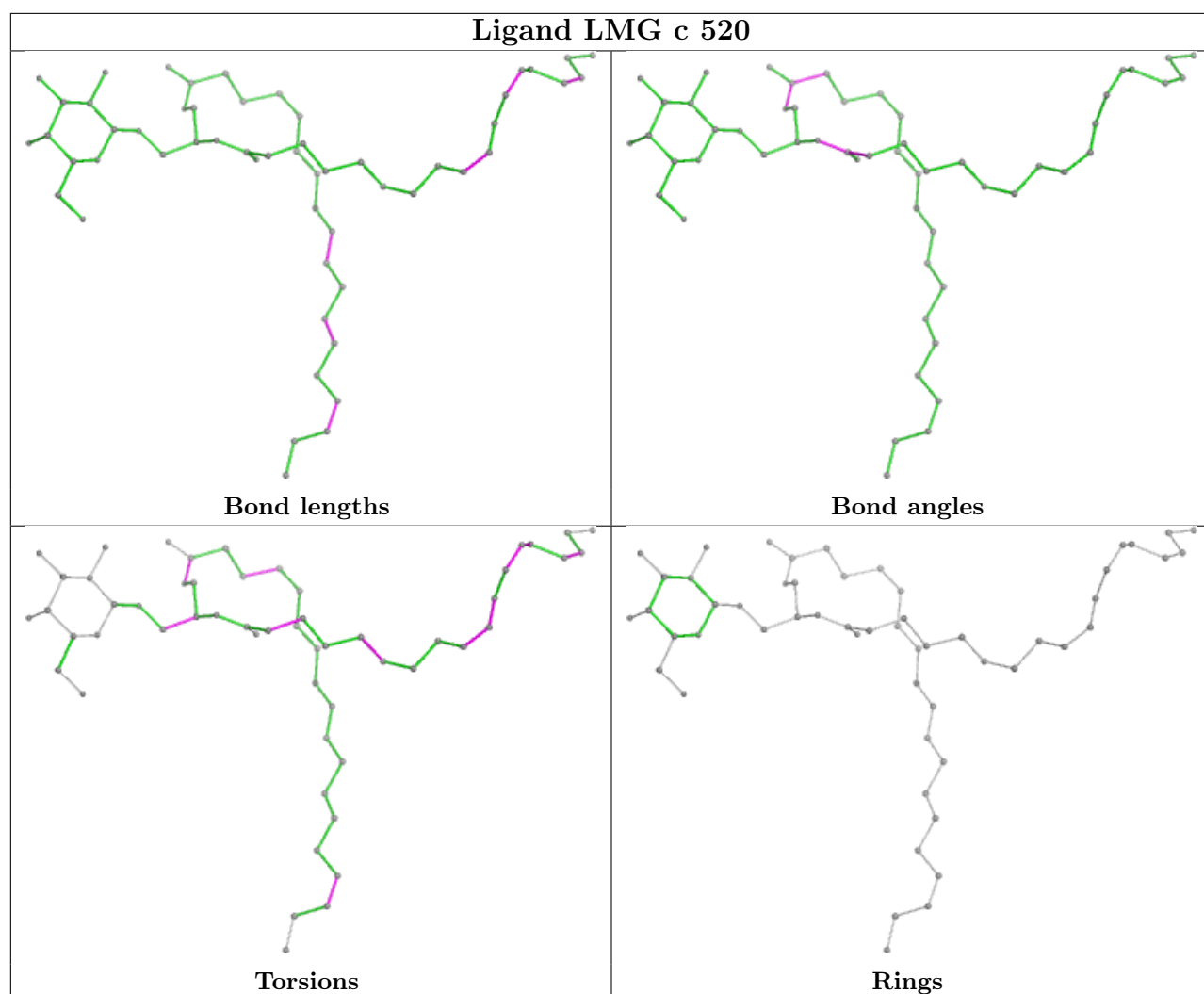
Bond angles



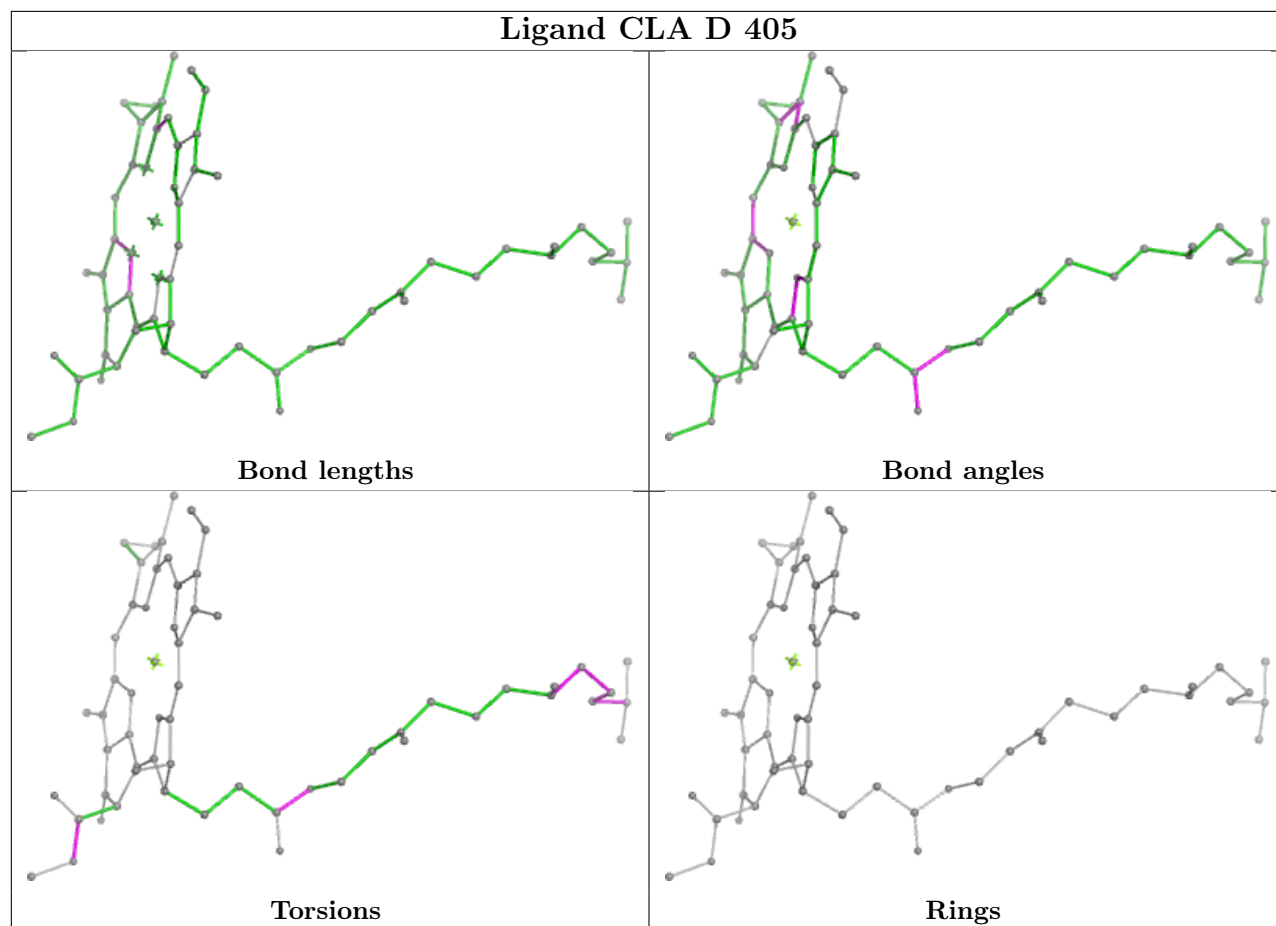
Torsions



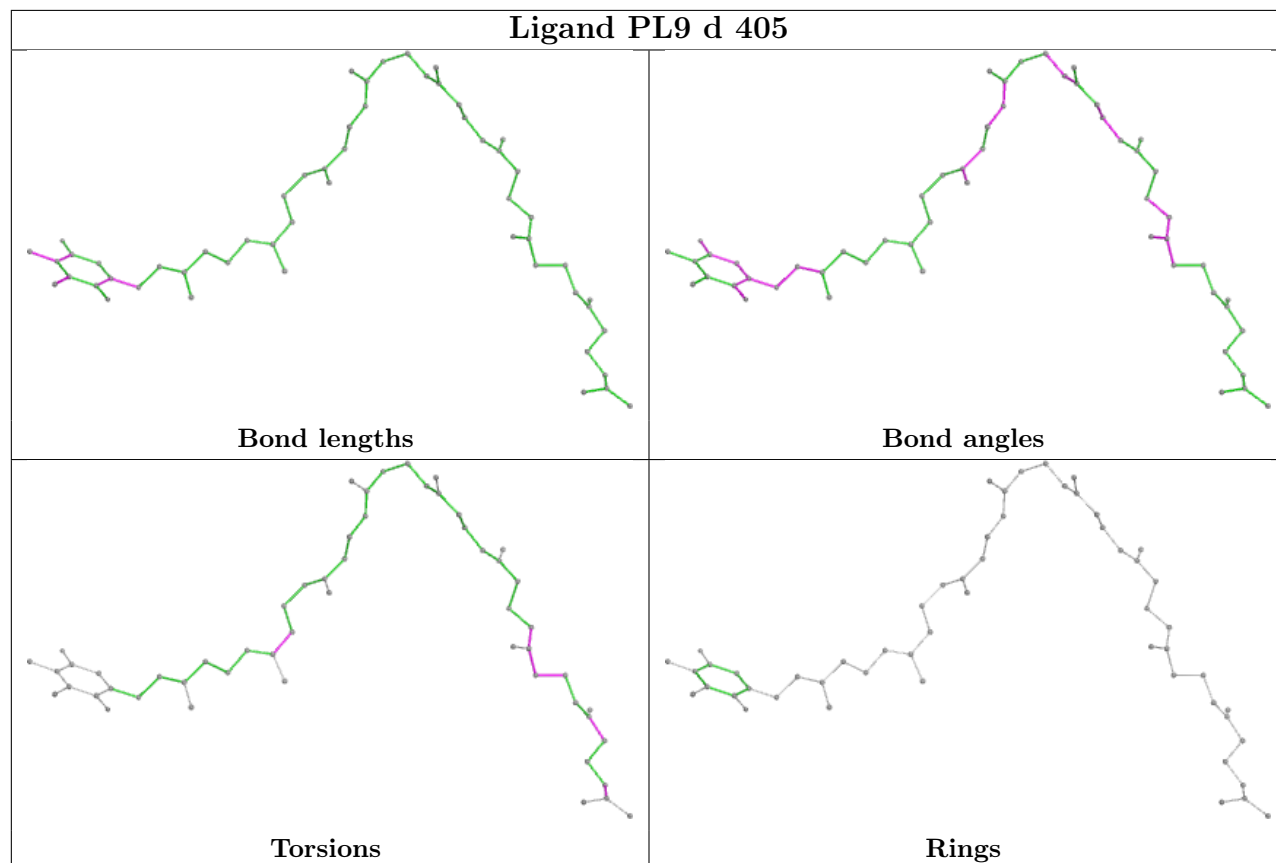
Rings

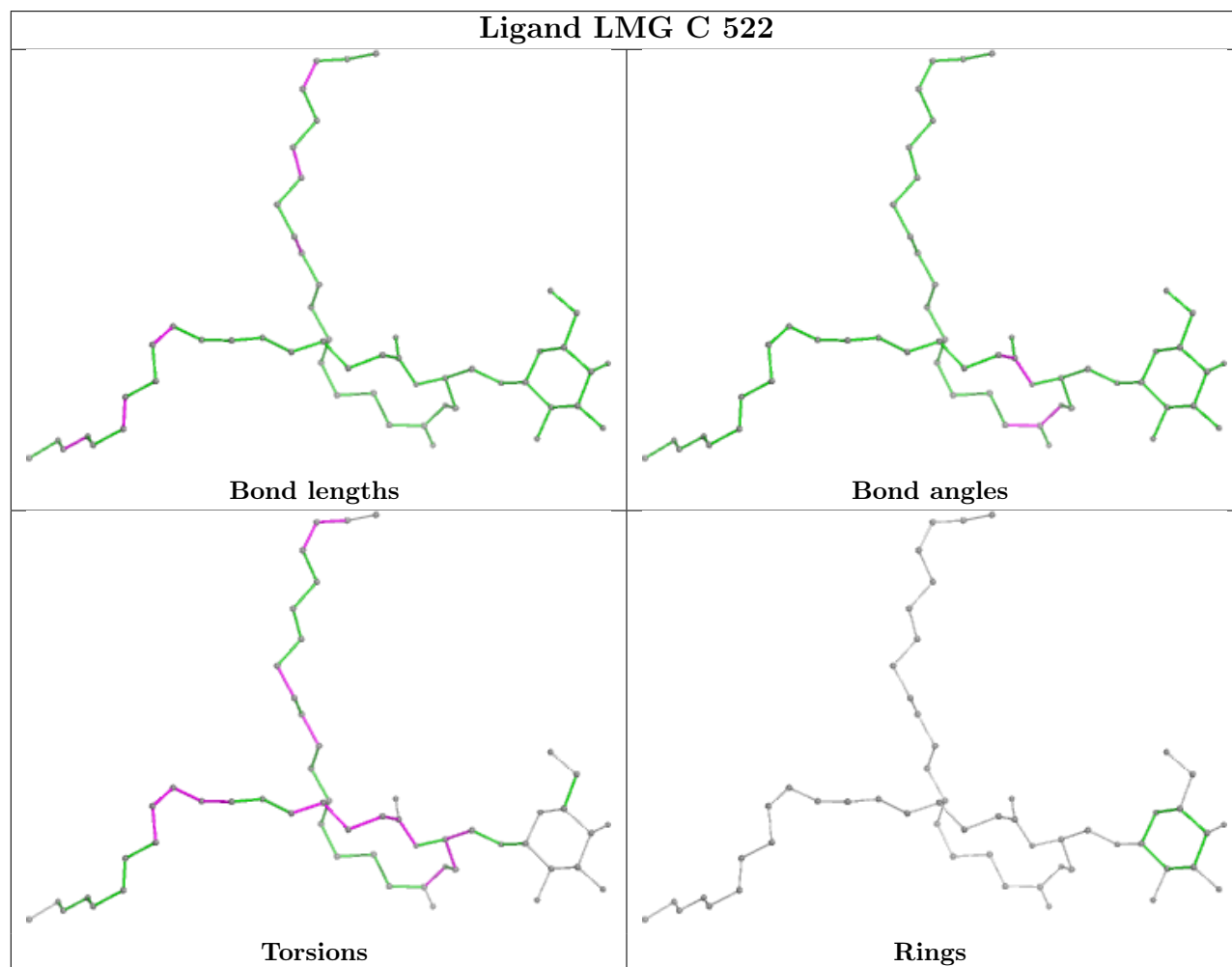
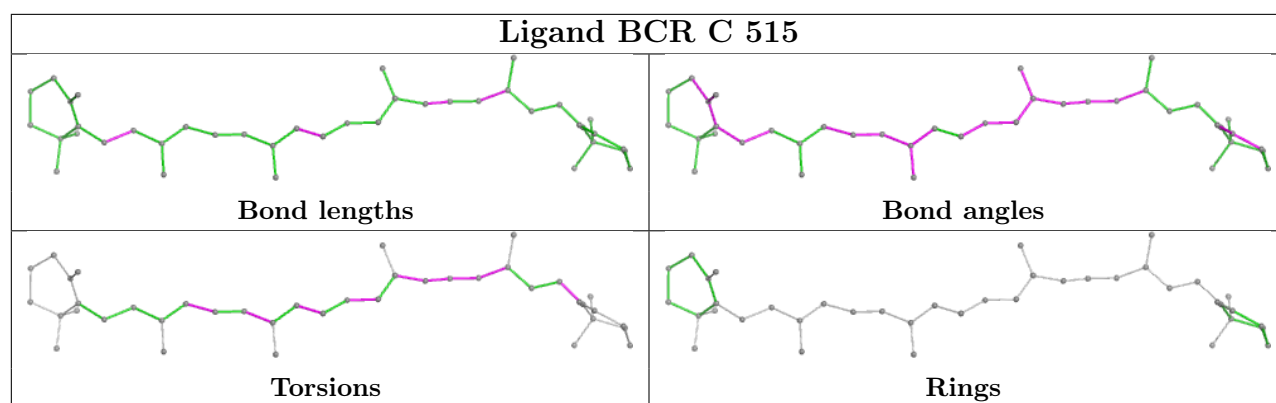


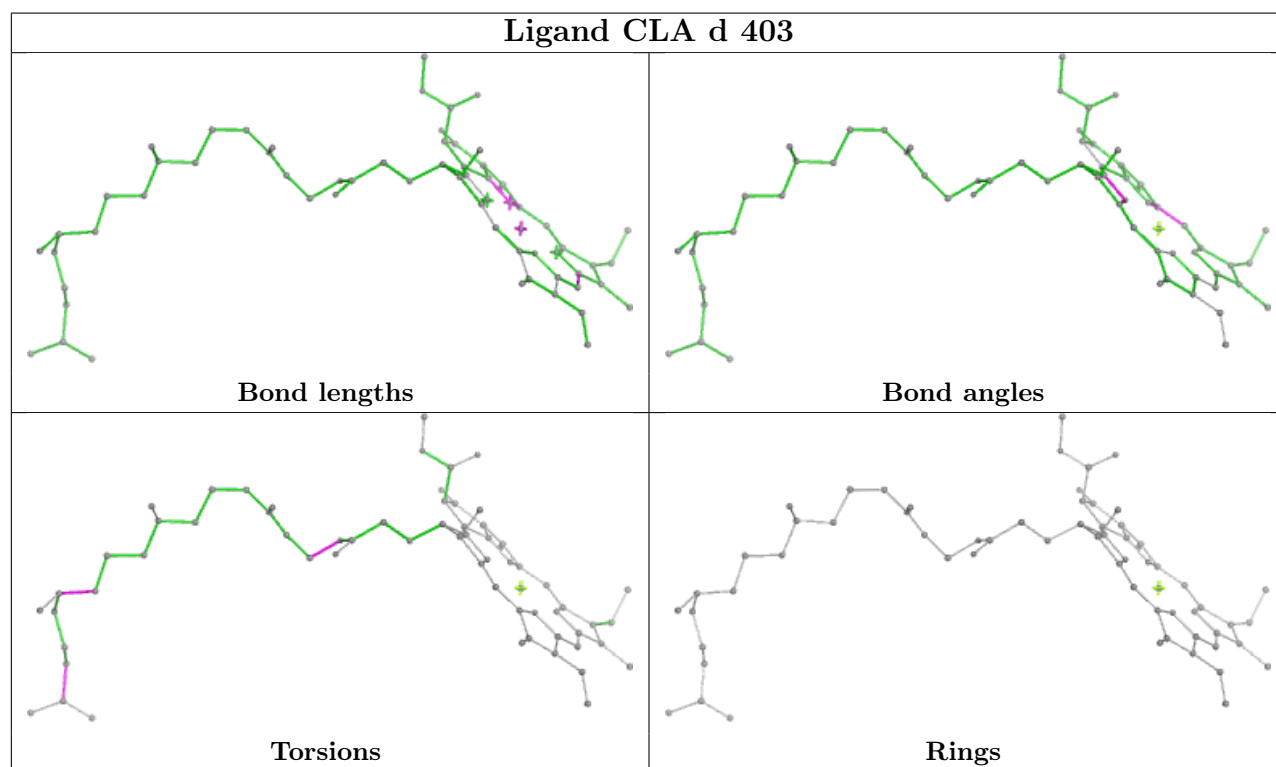
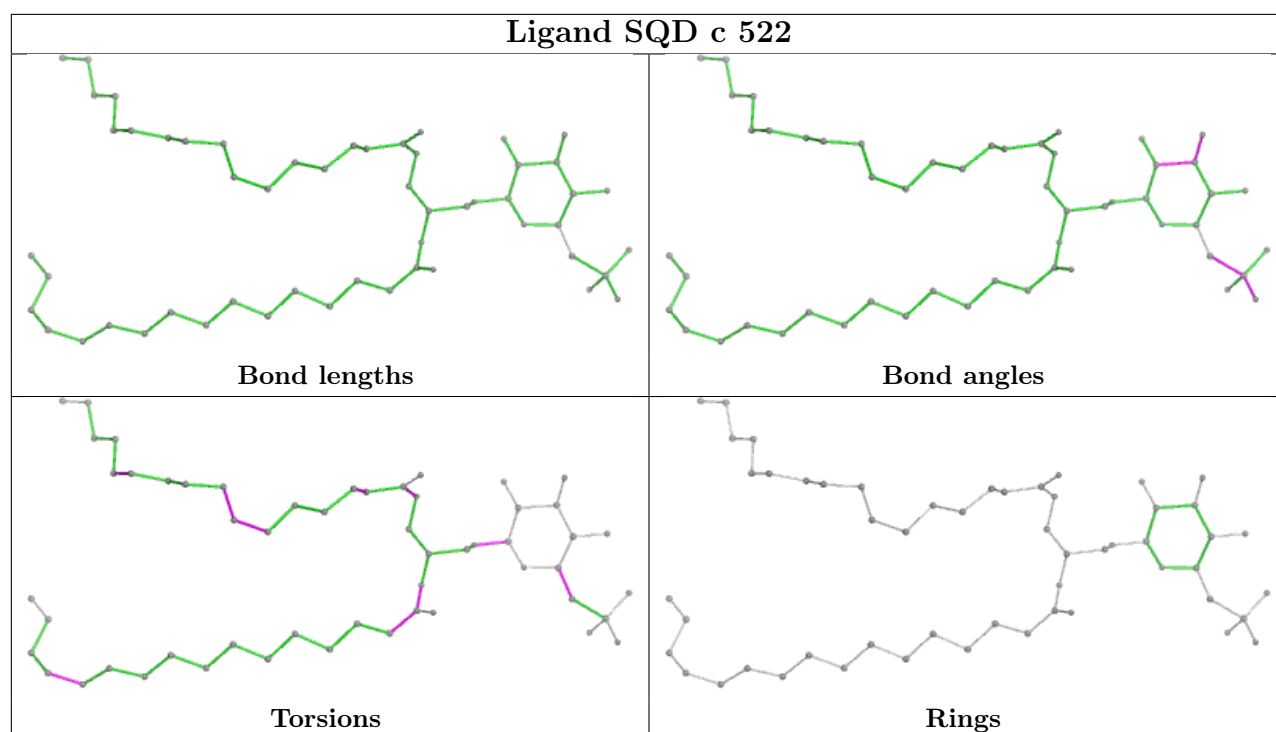
Ligand CLA D 405

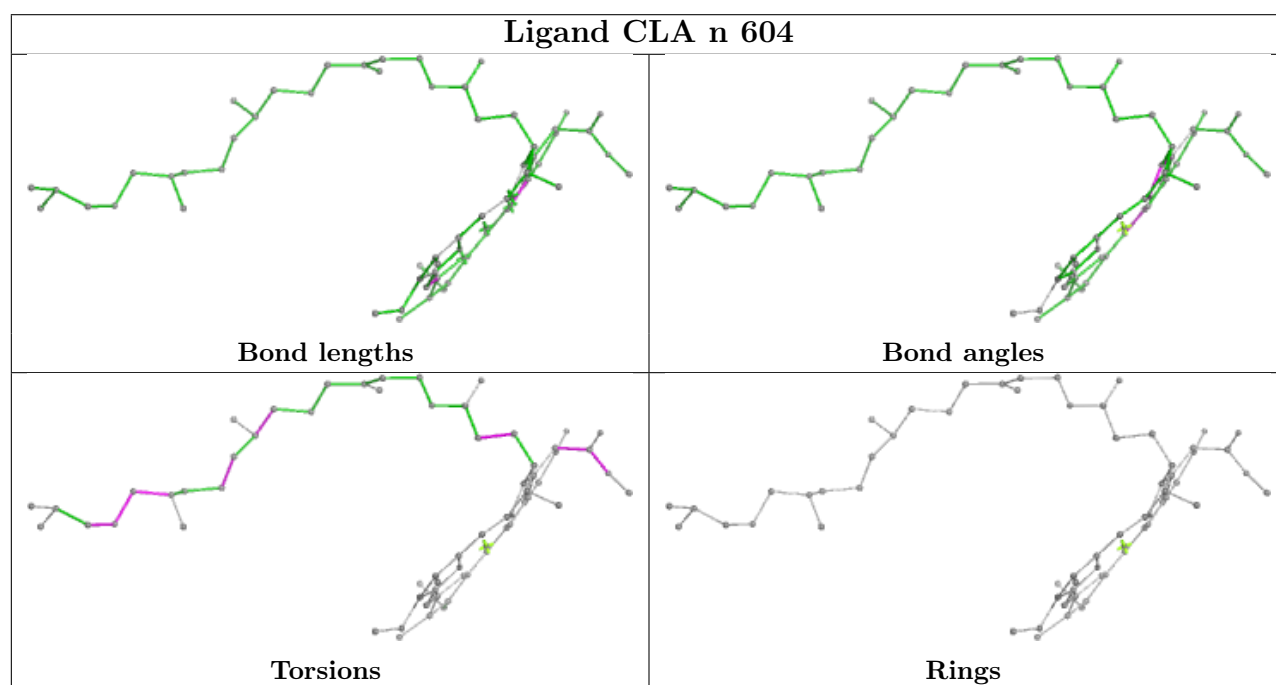
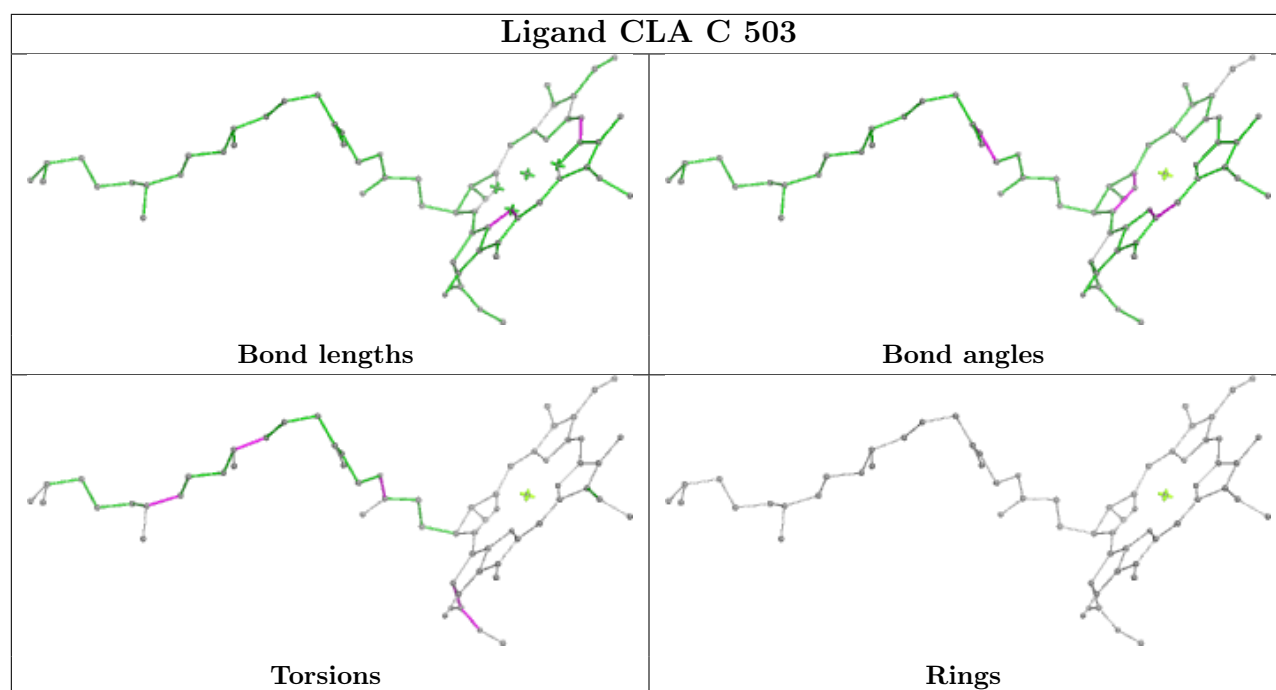


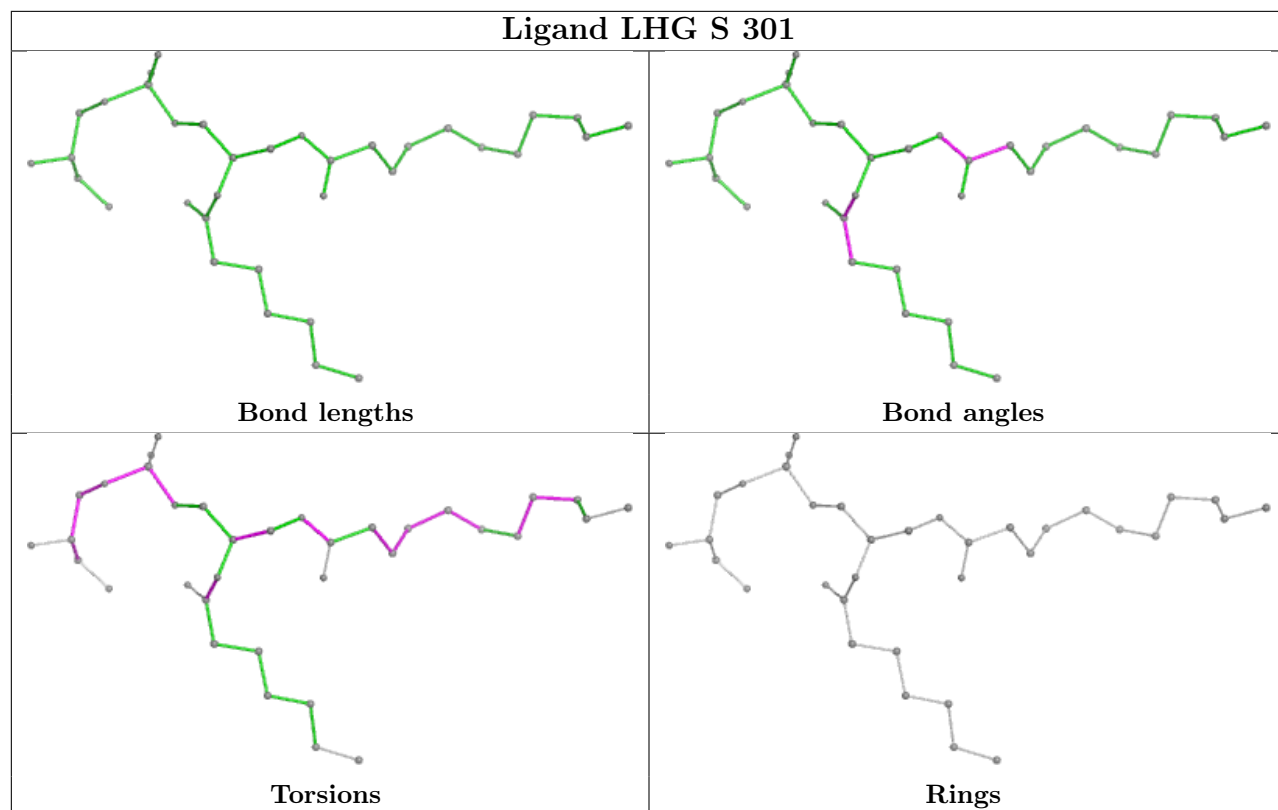
Ligand PL9 d 405

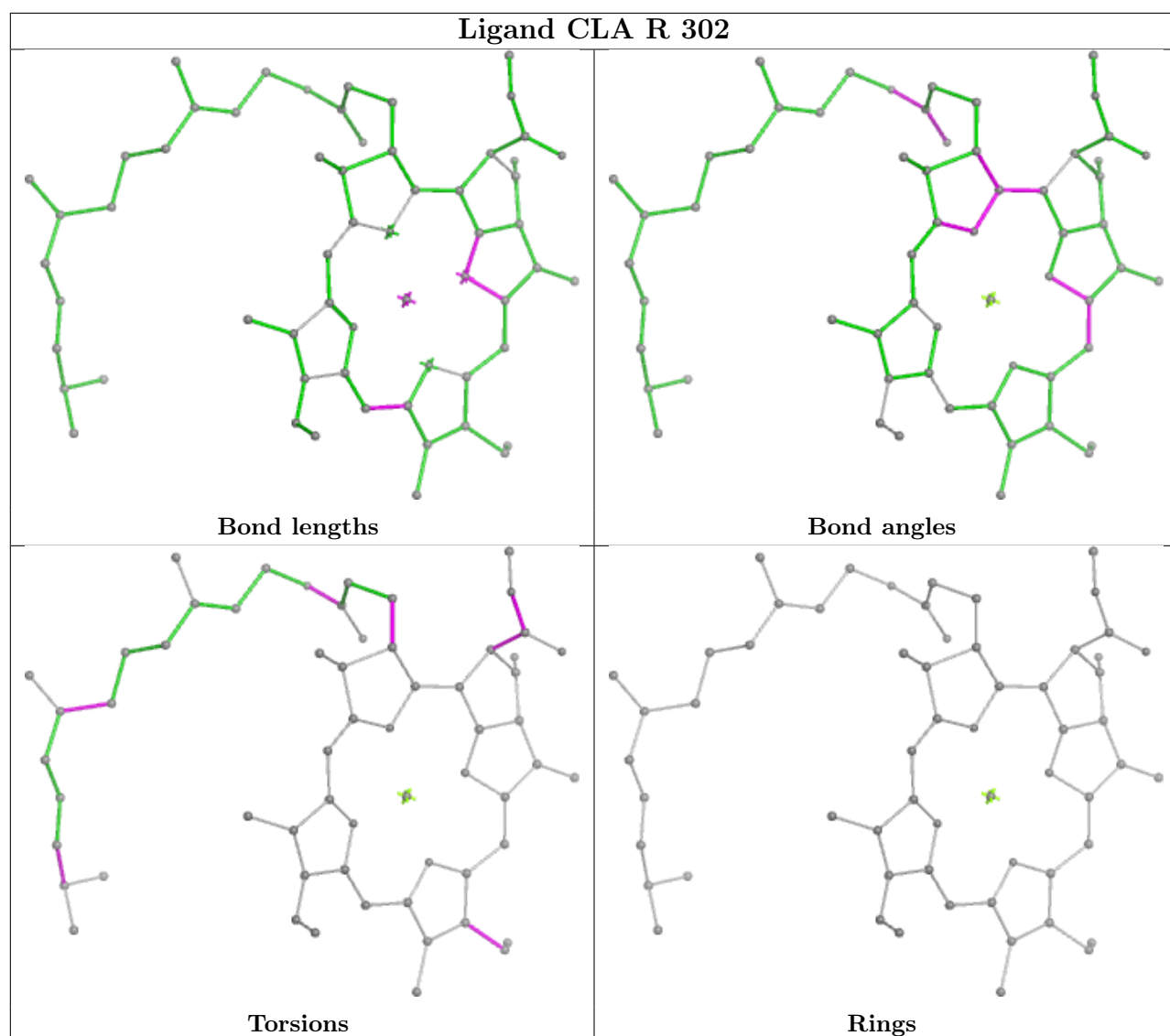




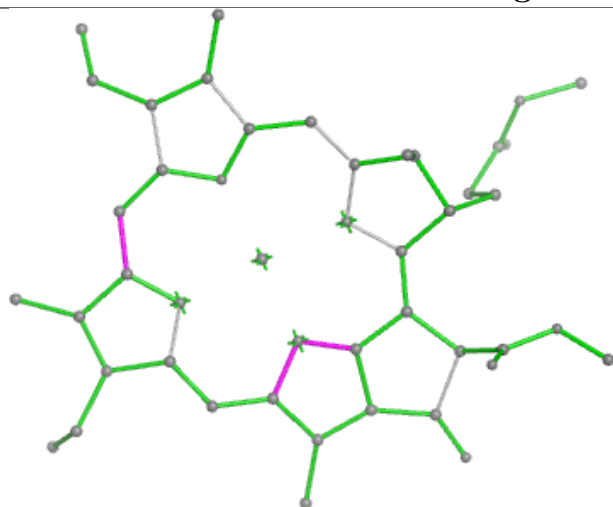




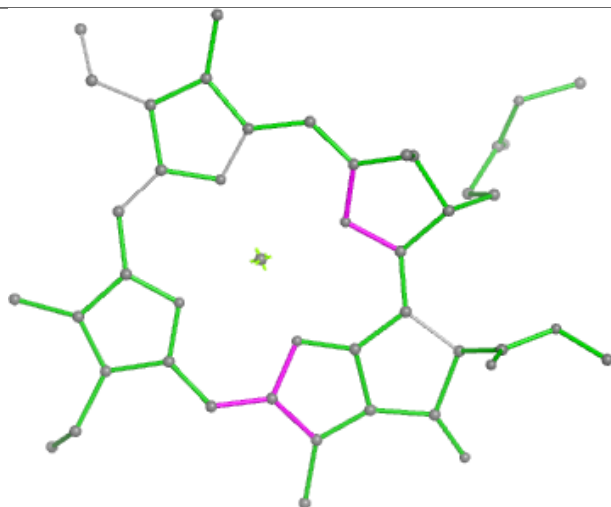




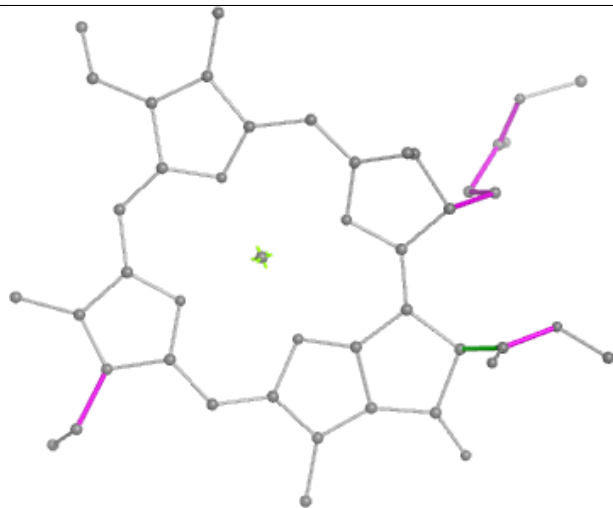
Ligand CLA R 307



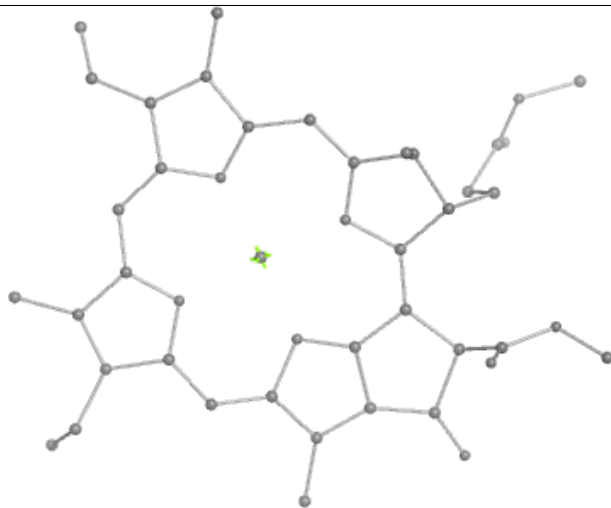
Bond lengths



Bond angles

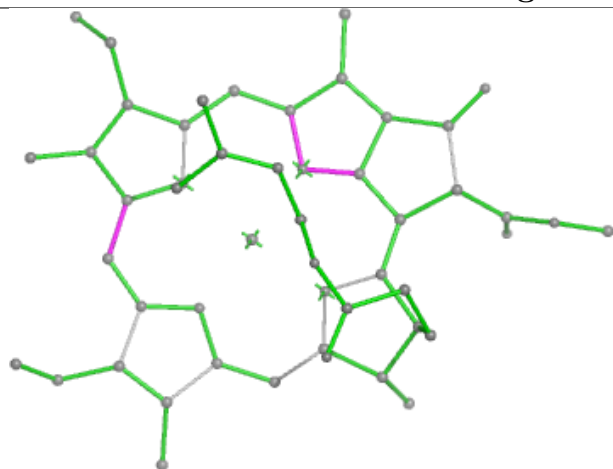


Torsions

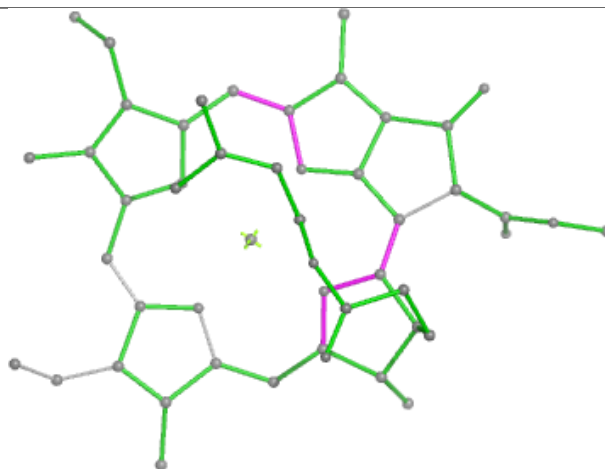


Rings

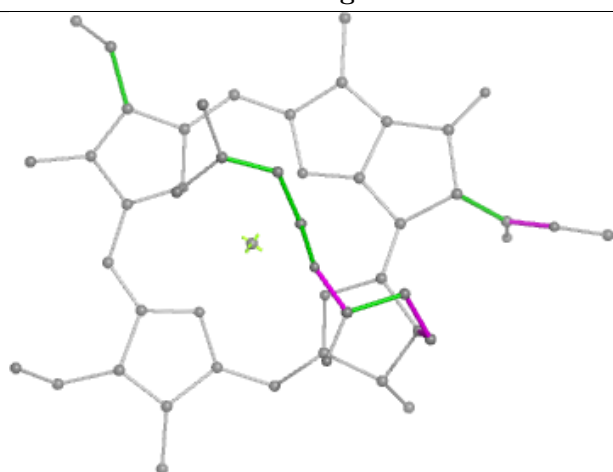
Ligand CLA S 306



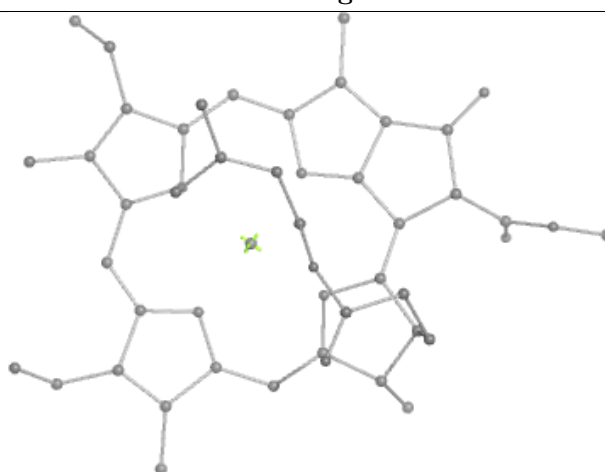
Bond lengths



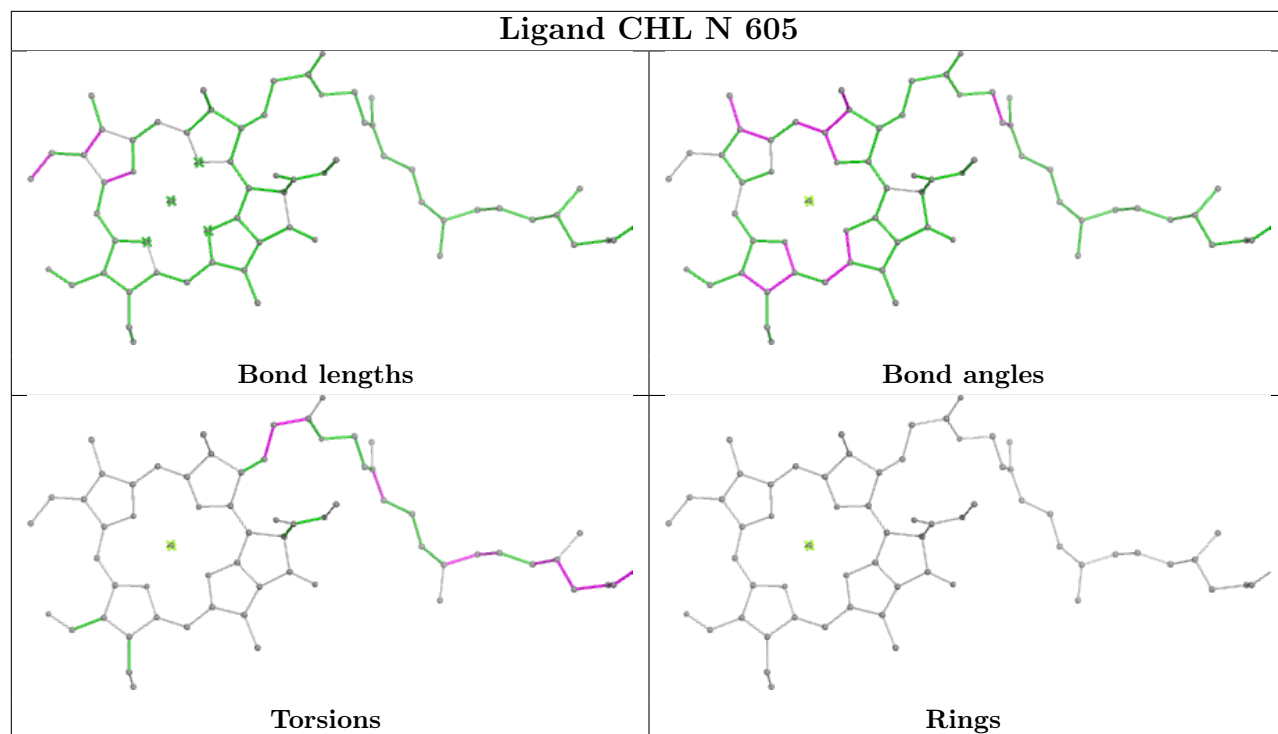
Bond angles

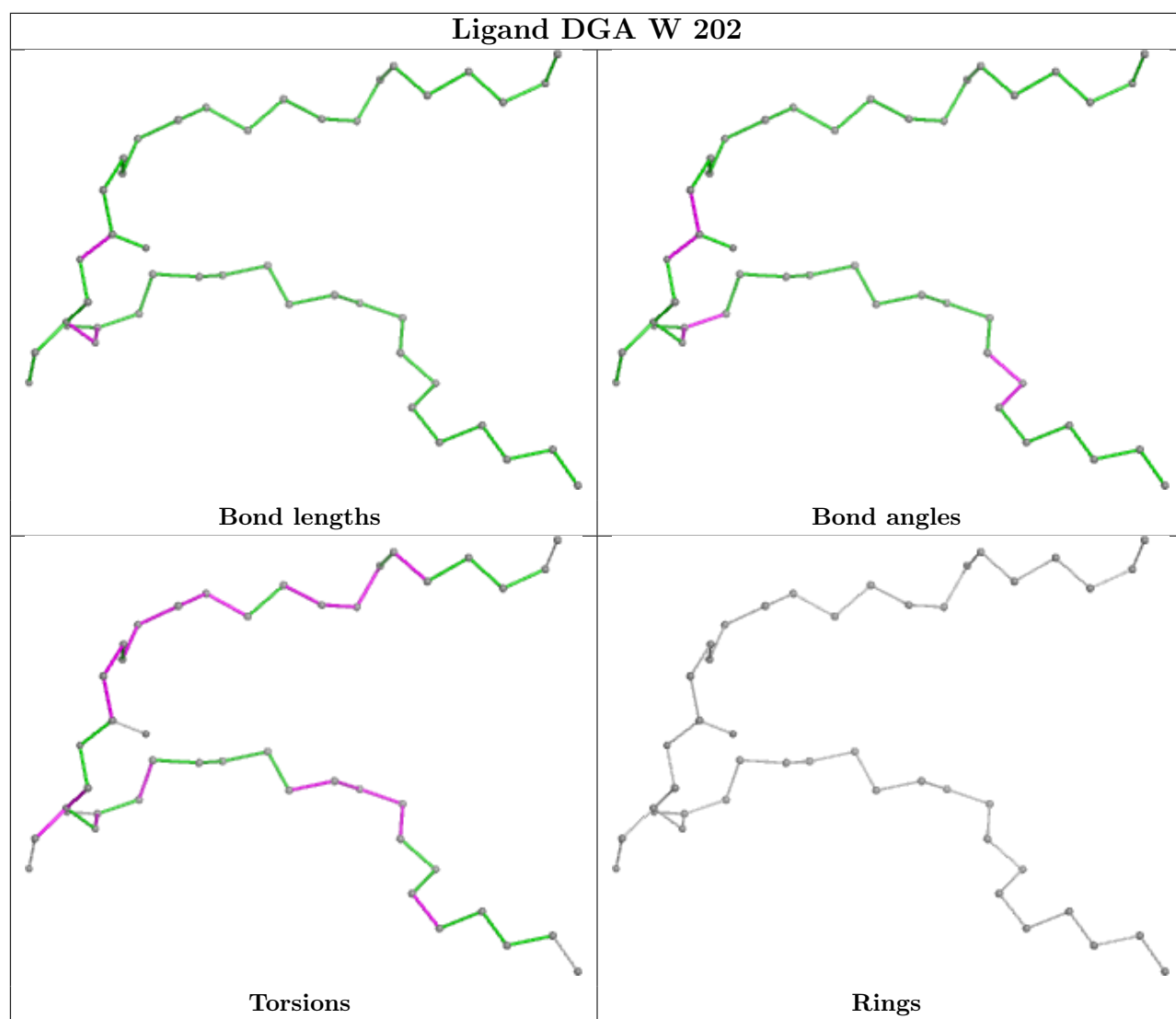


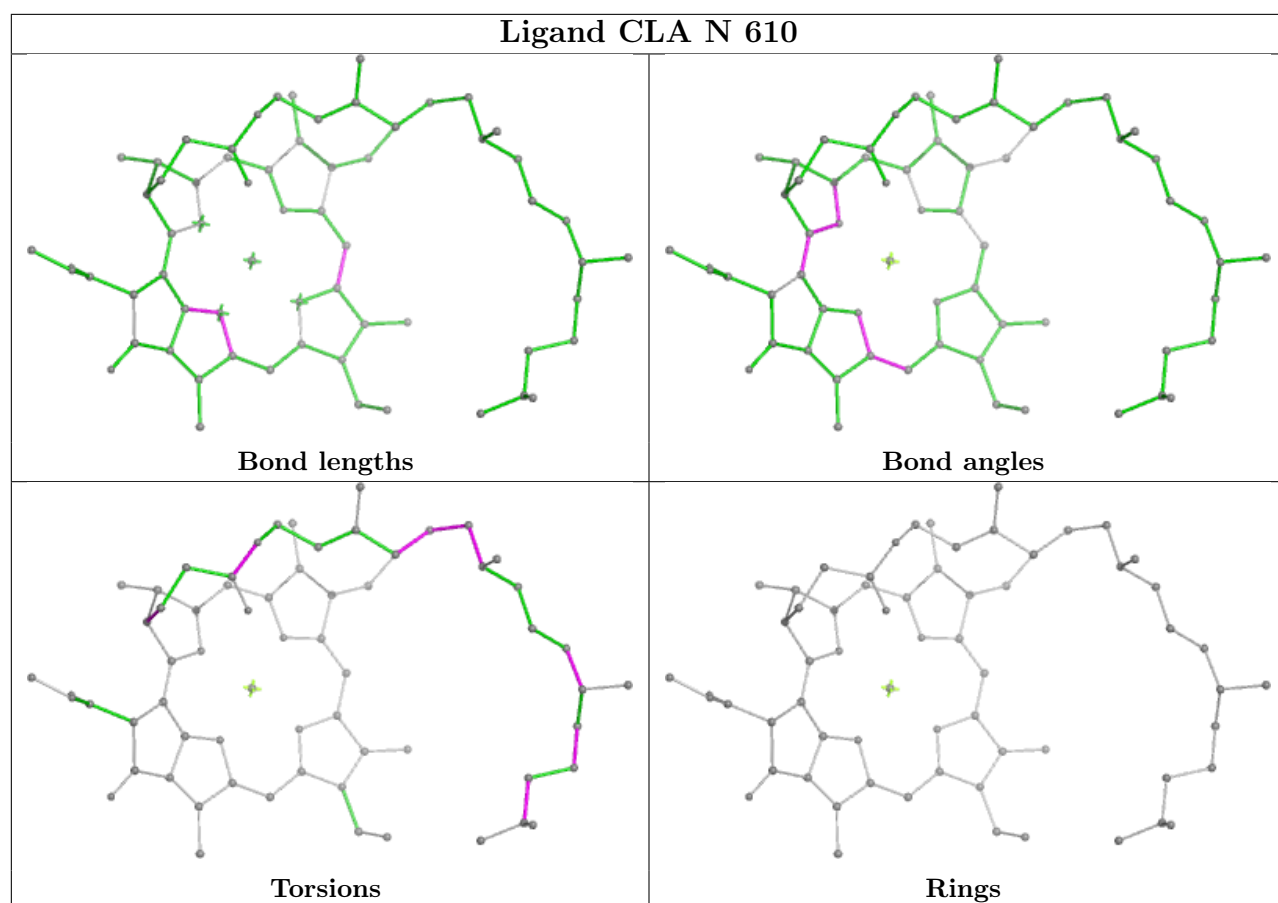
Torsions



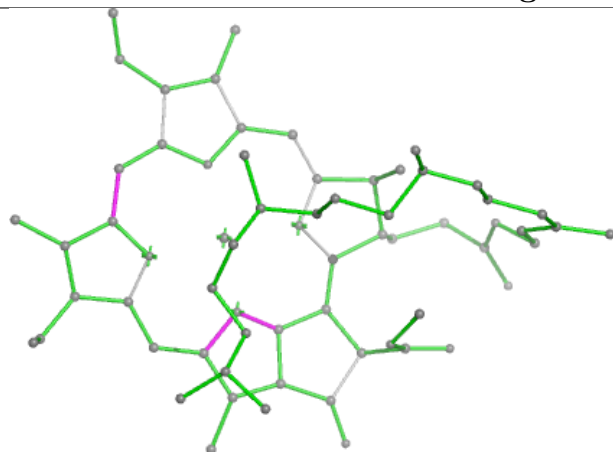
Rings



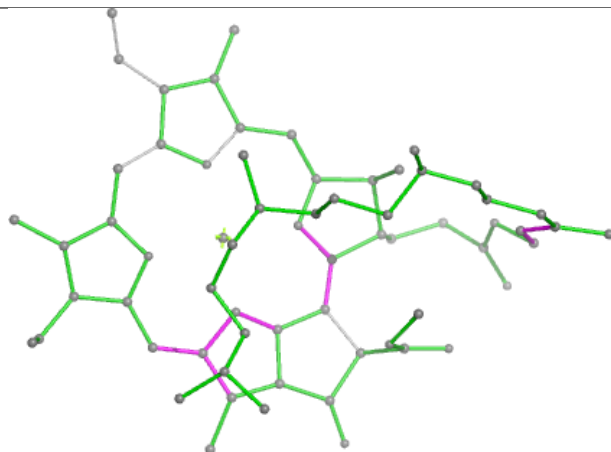




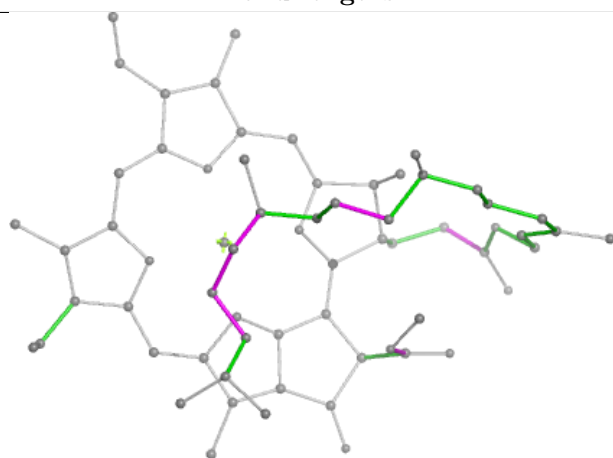
Ligand CLA c 510



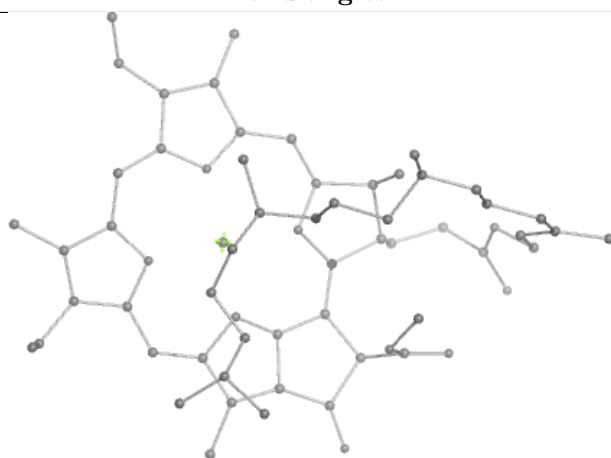
Bond lengths



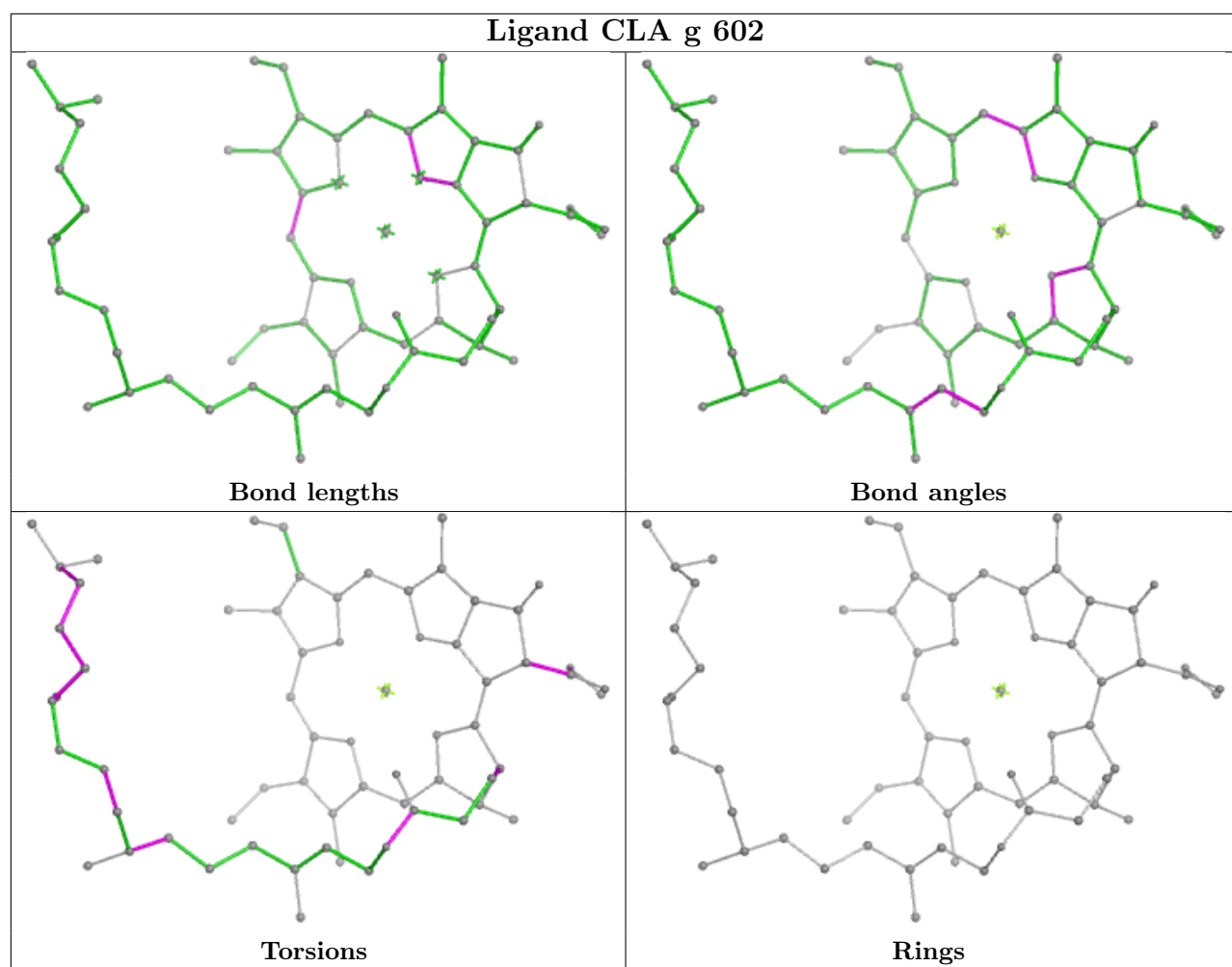
Bond angles



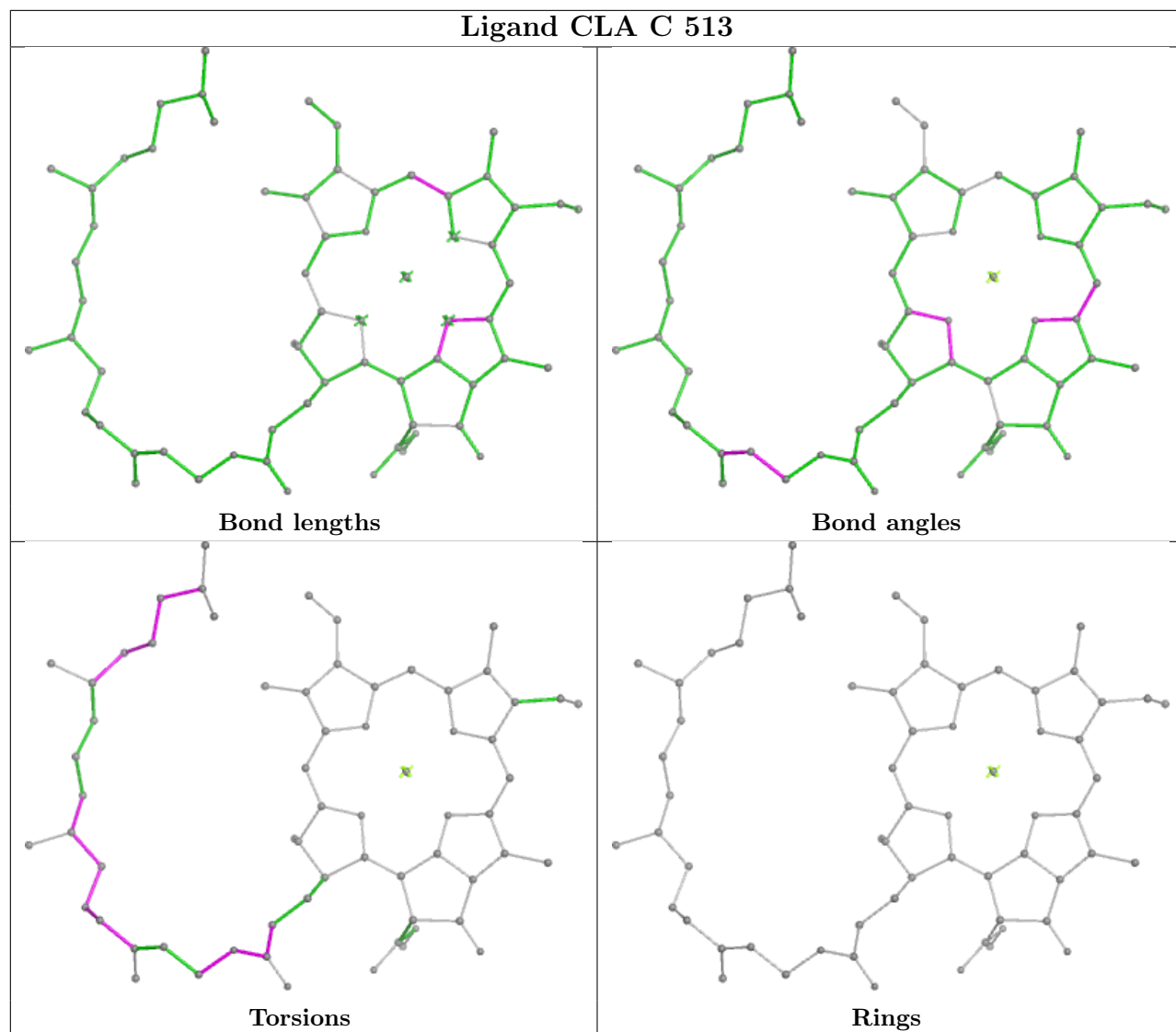
Torsions



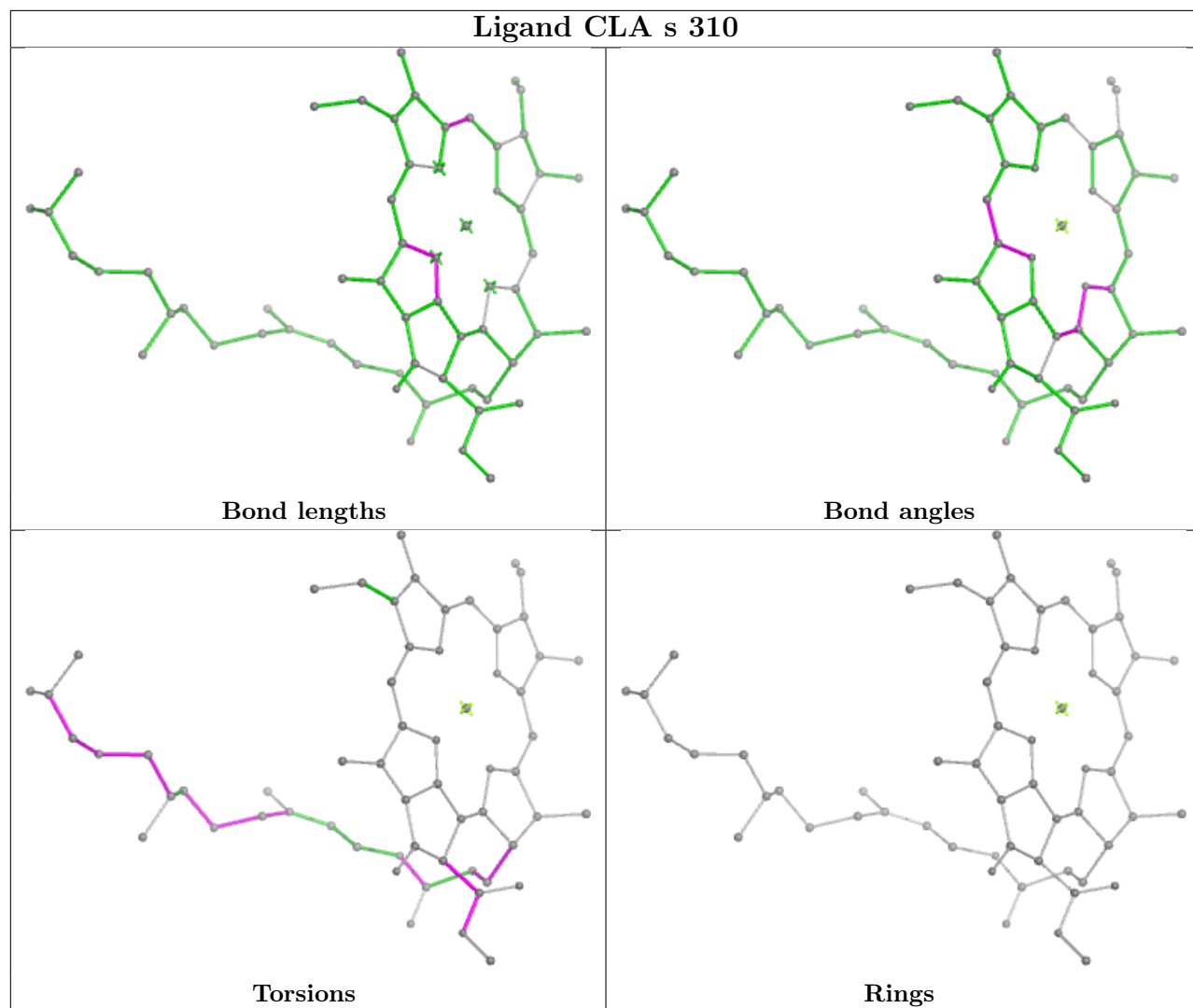
Rings



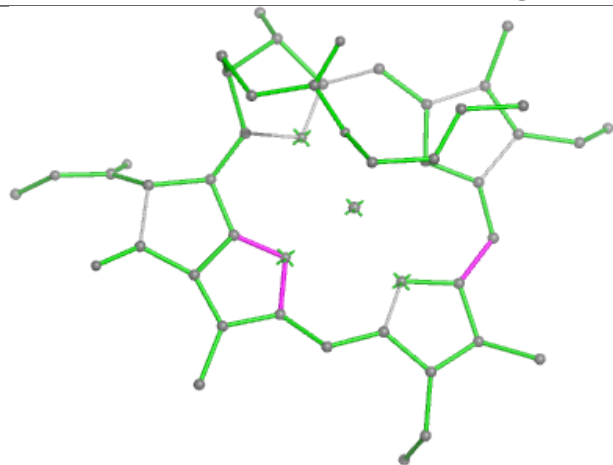
Ligand CLA C 513



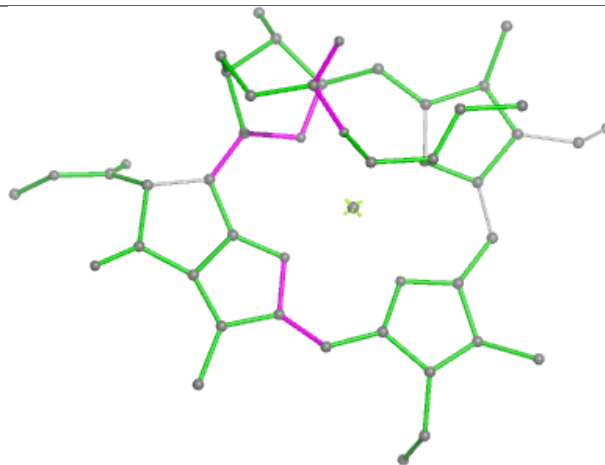
Ligand CLA s 310



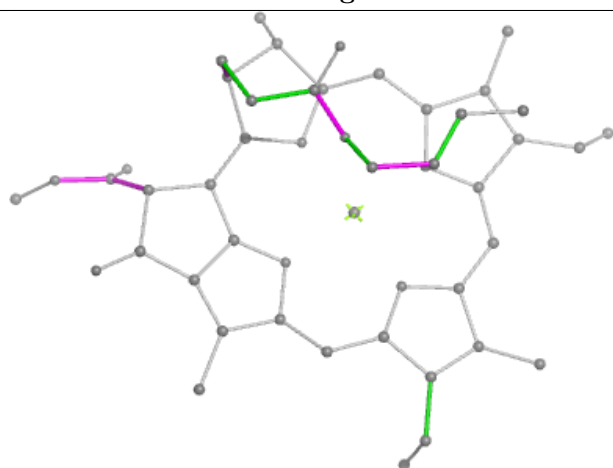
Ligand CLA N 614



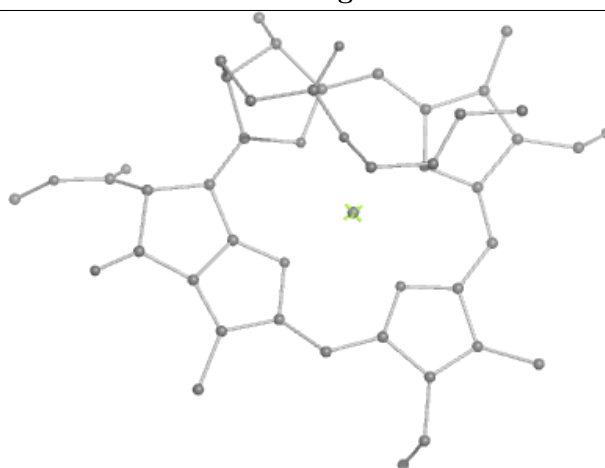
Bond lengths



Bond angles

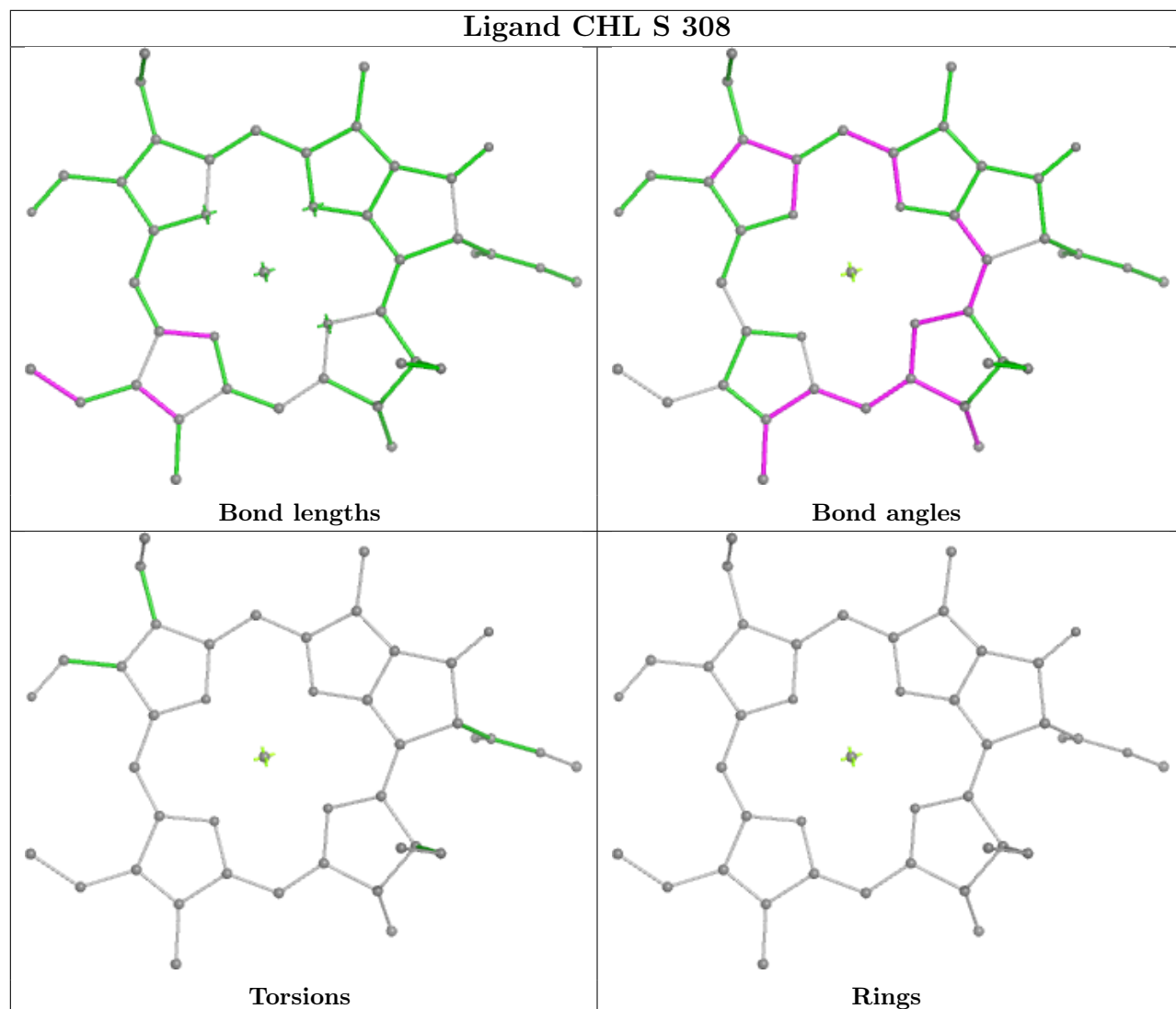


Torsions

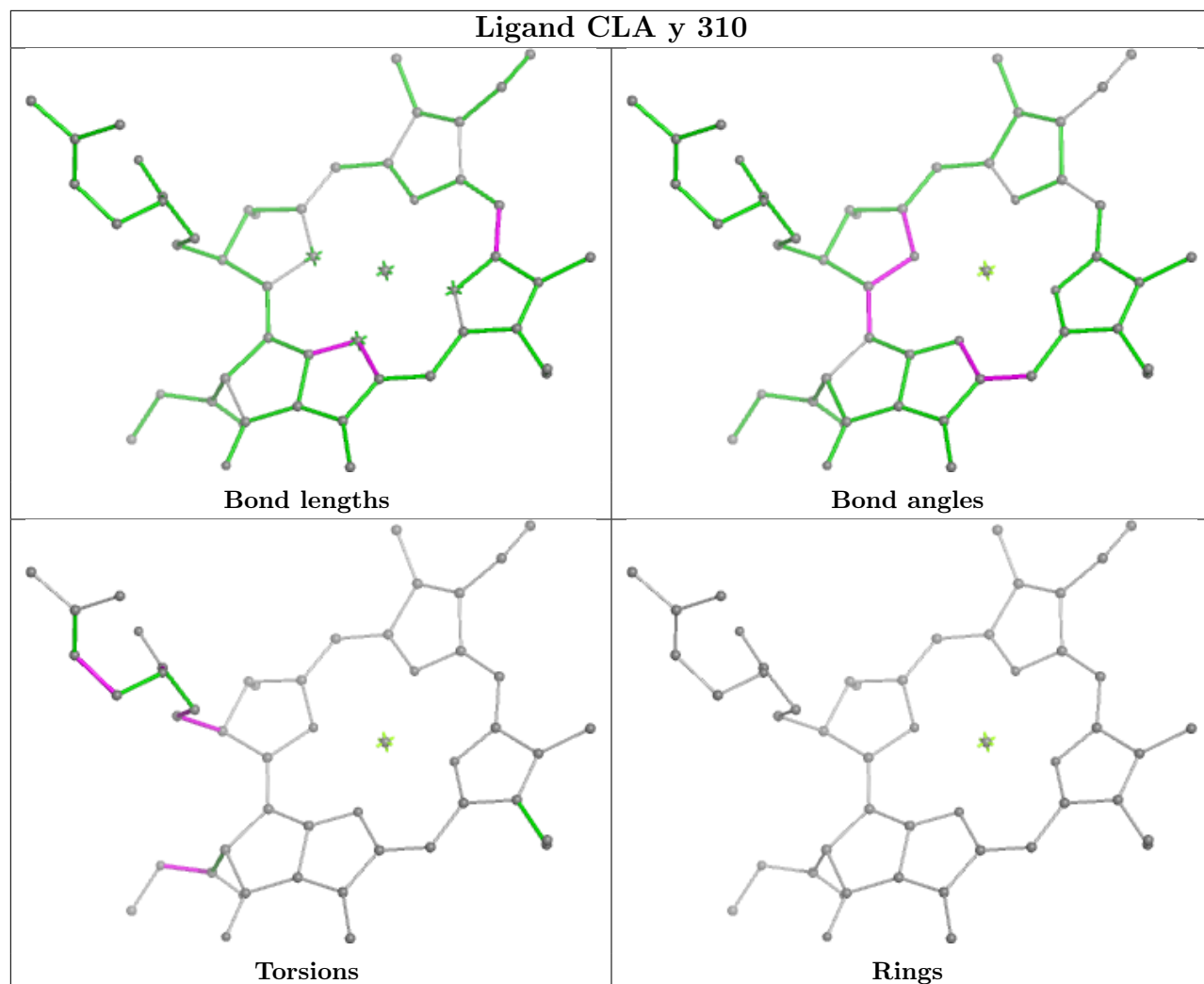


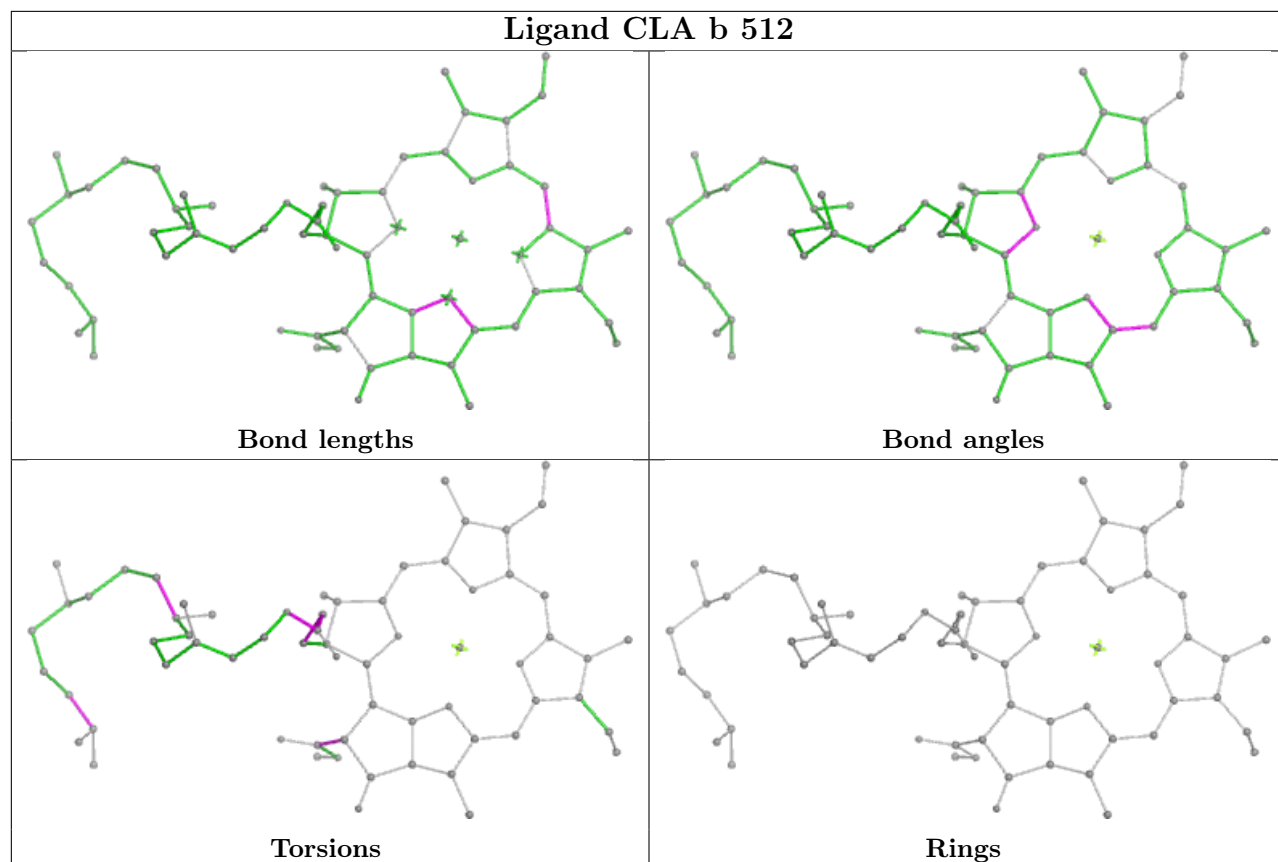
Rings

Ligand CHL S 308

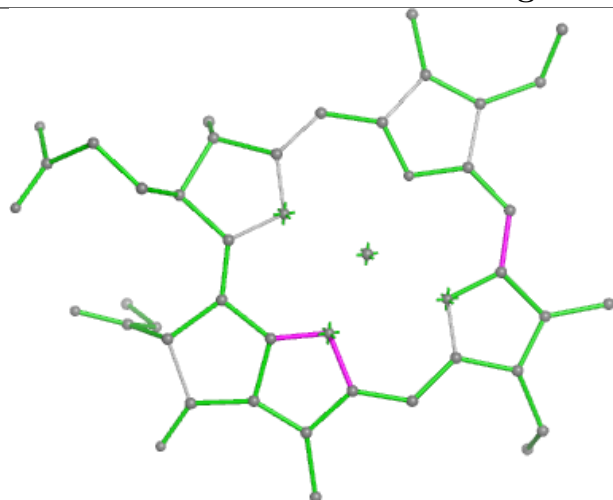


Ligand CLA y 310

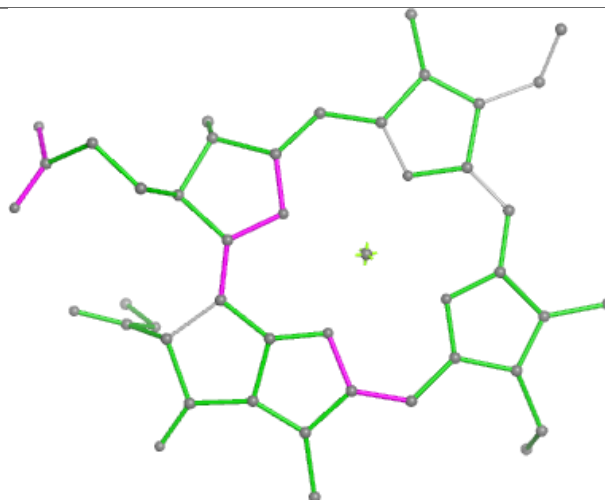




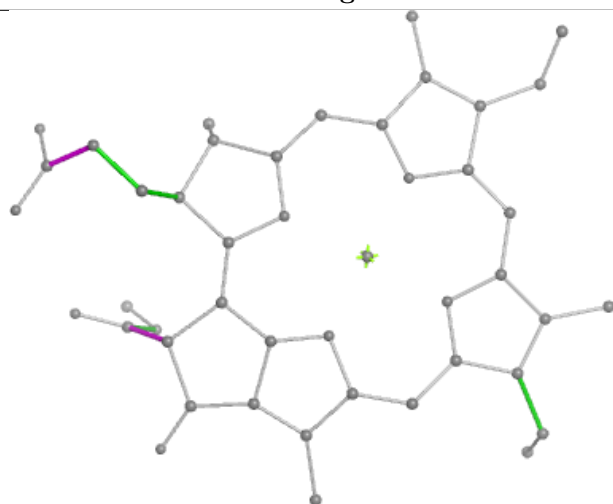
Ligand CLA S 313



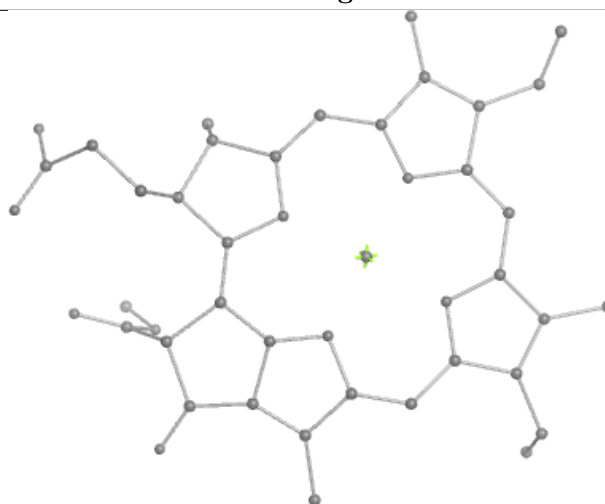
Bond lengths



Bond angles

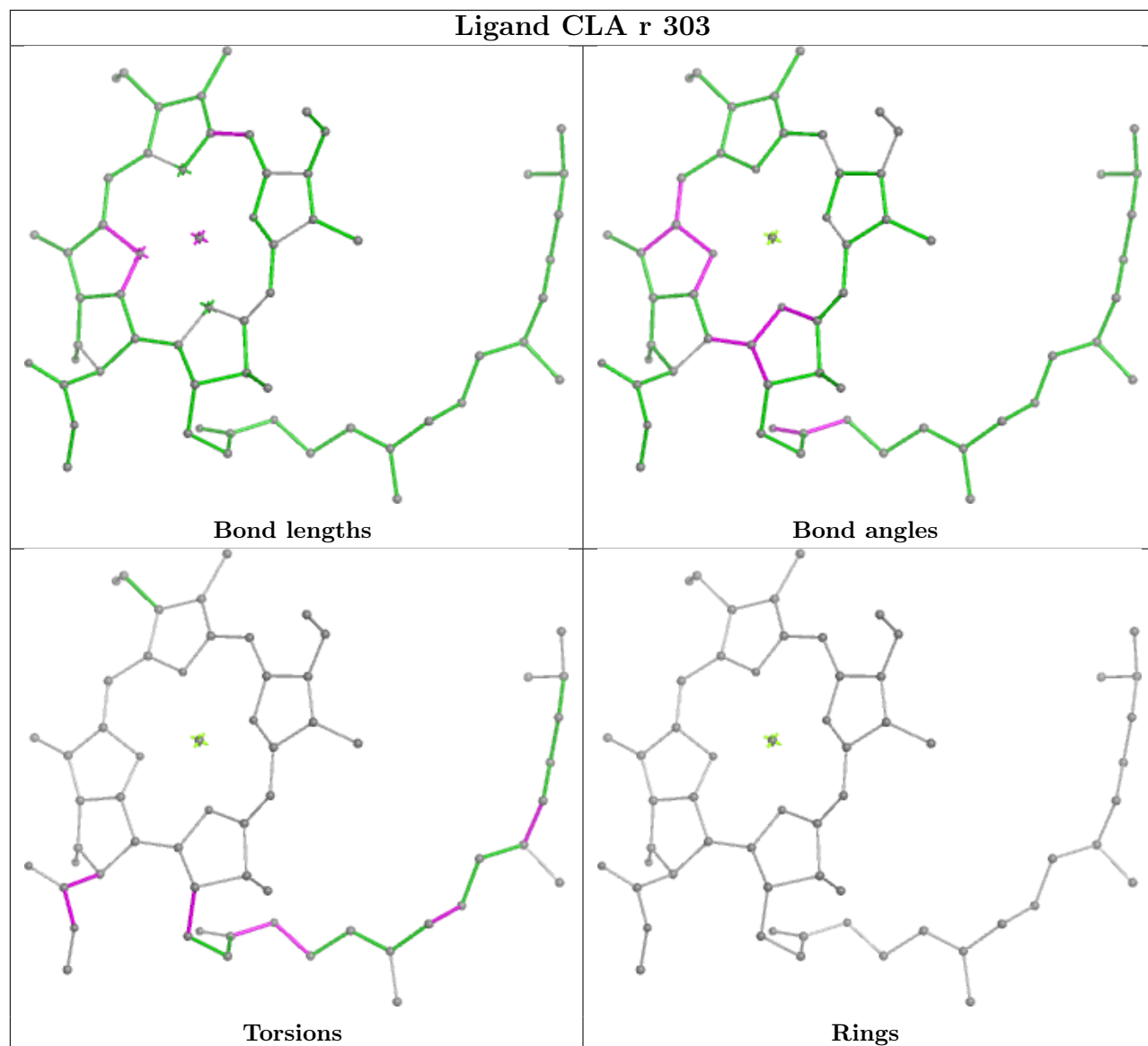


Torsions

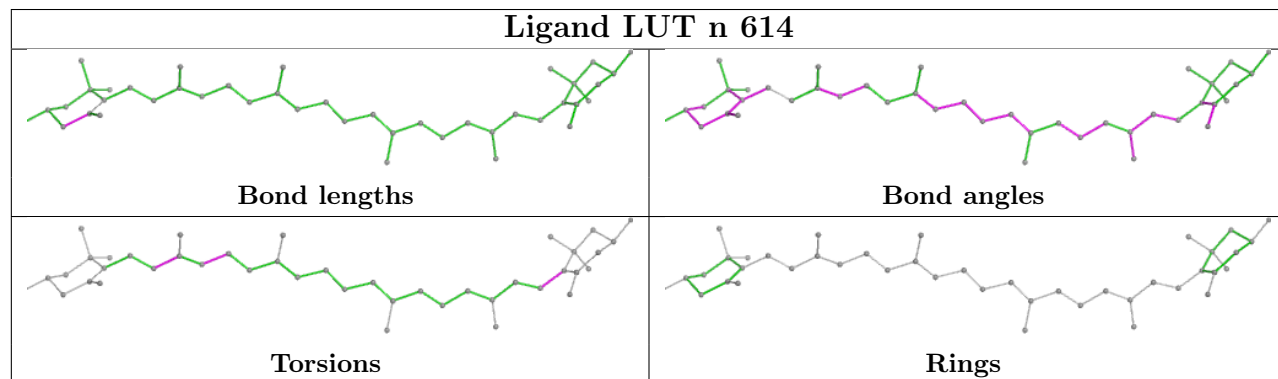


Rings

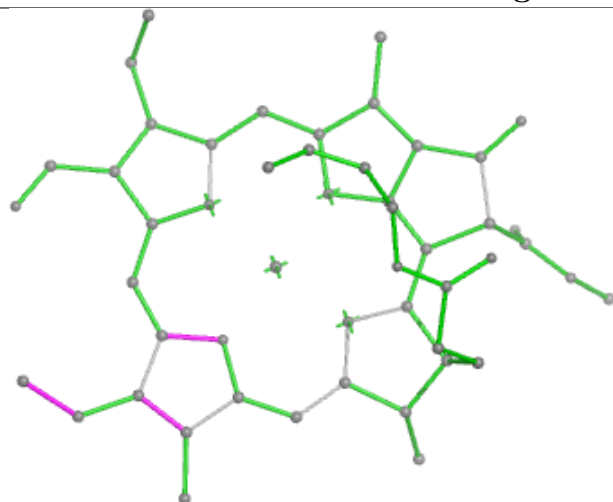
Ligand CLA r 303



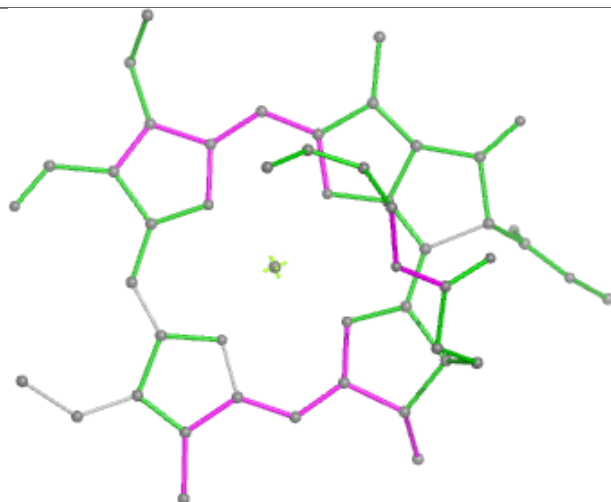
Ligand LUT n 614



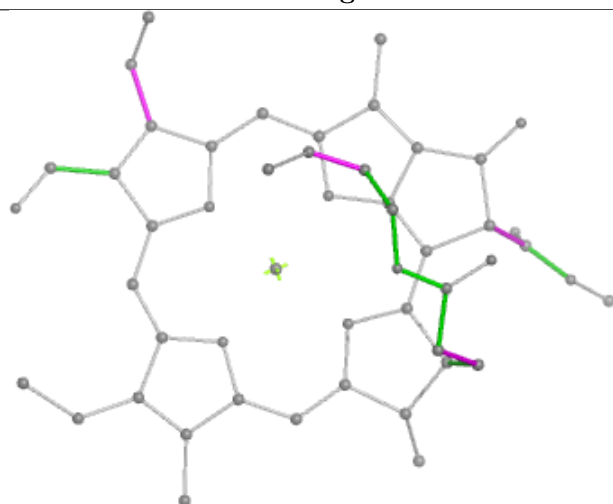
Ligand CHL R 305



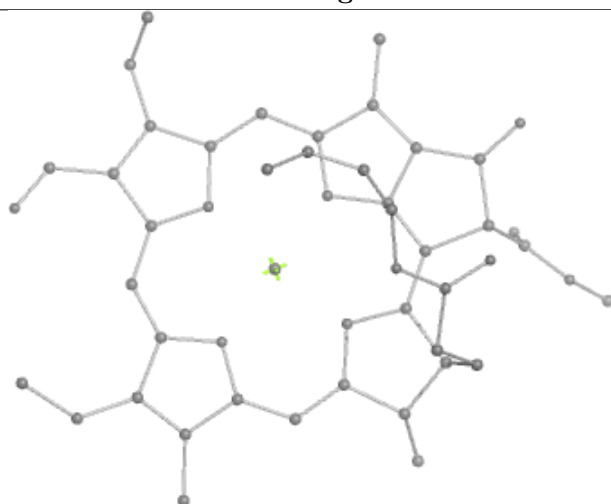
Bond lengths



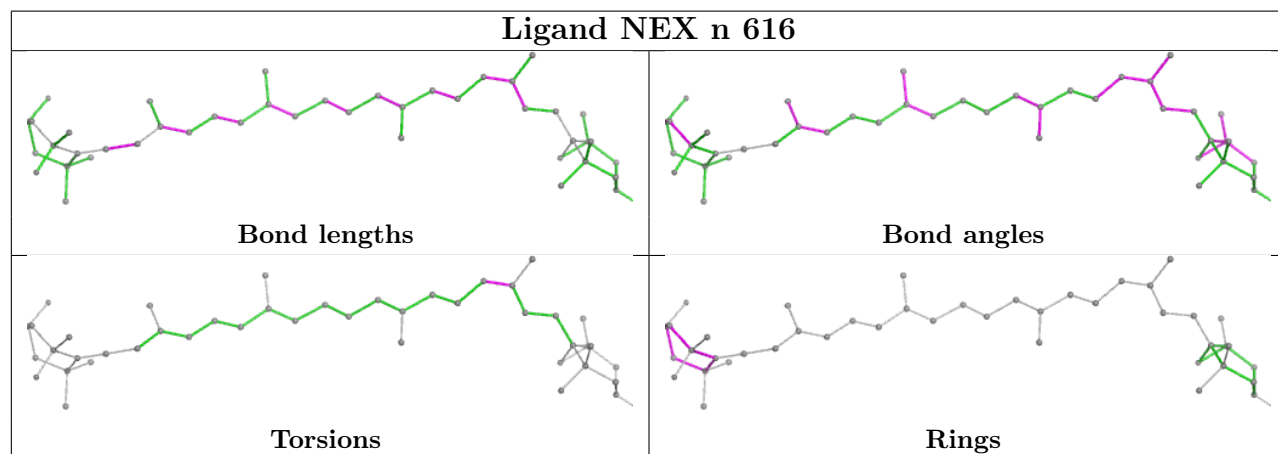
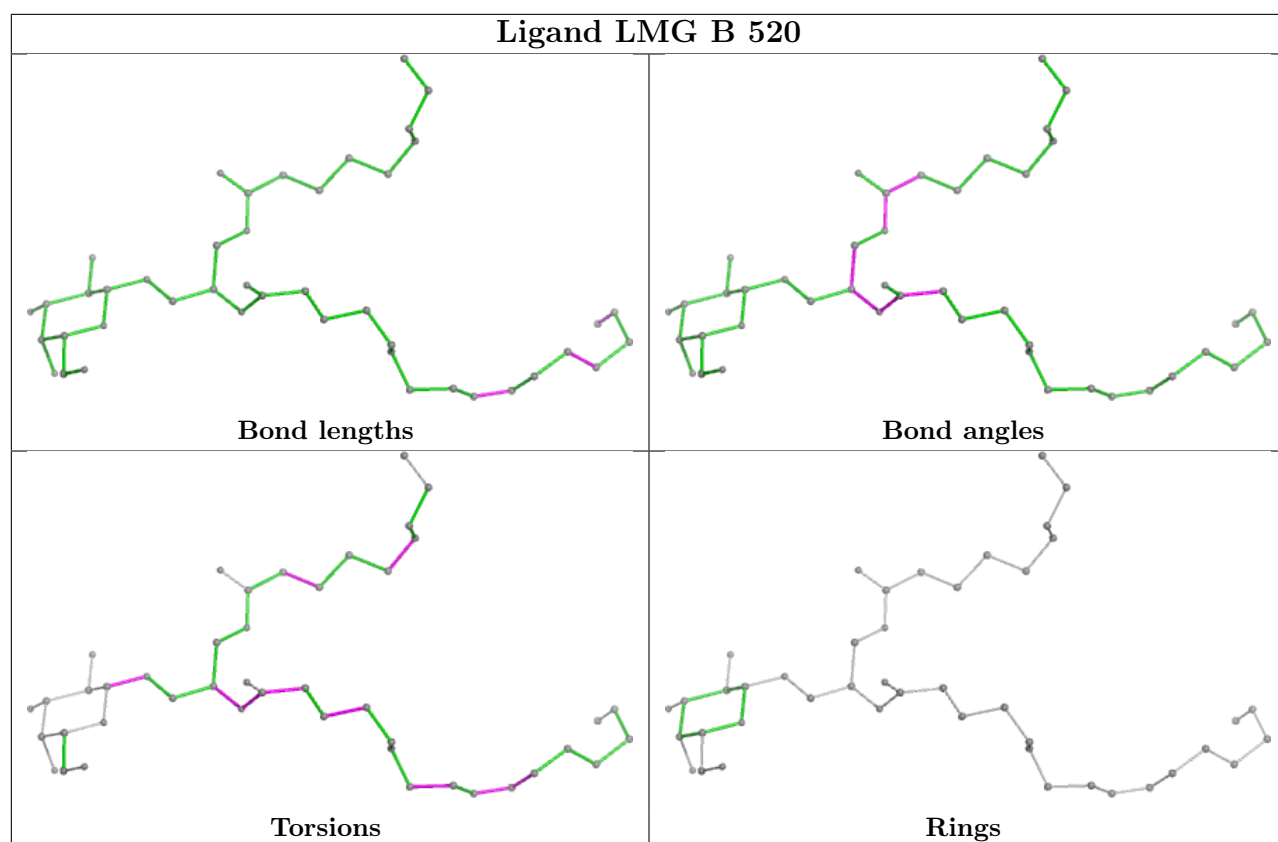
Bond angles

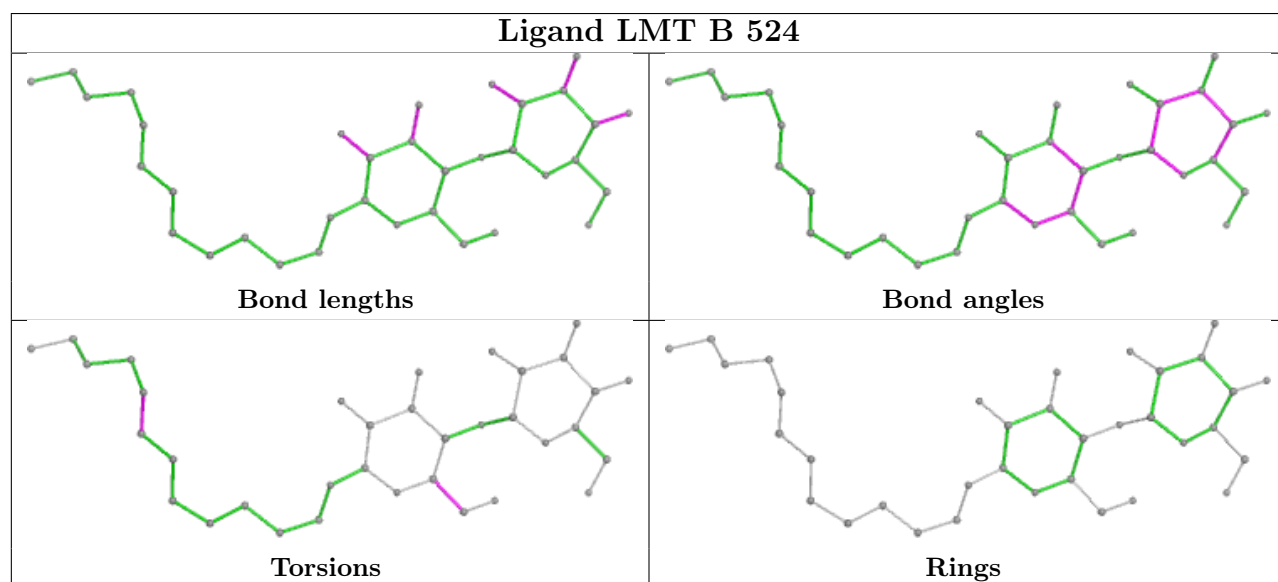
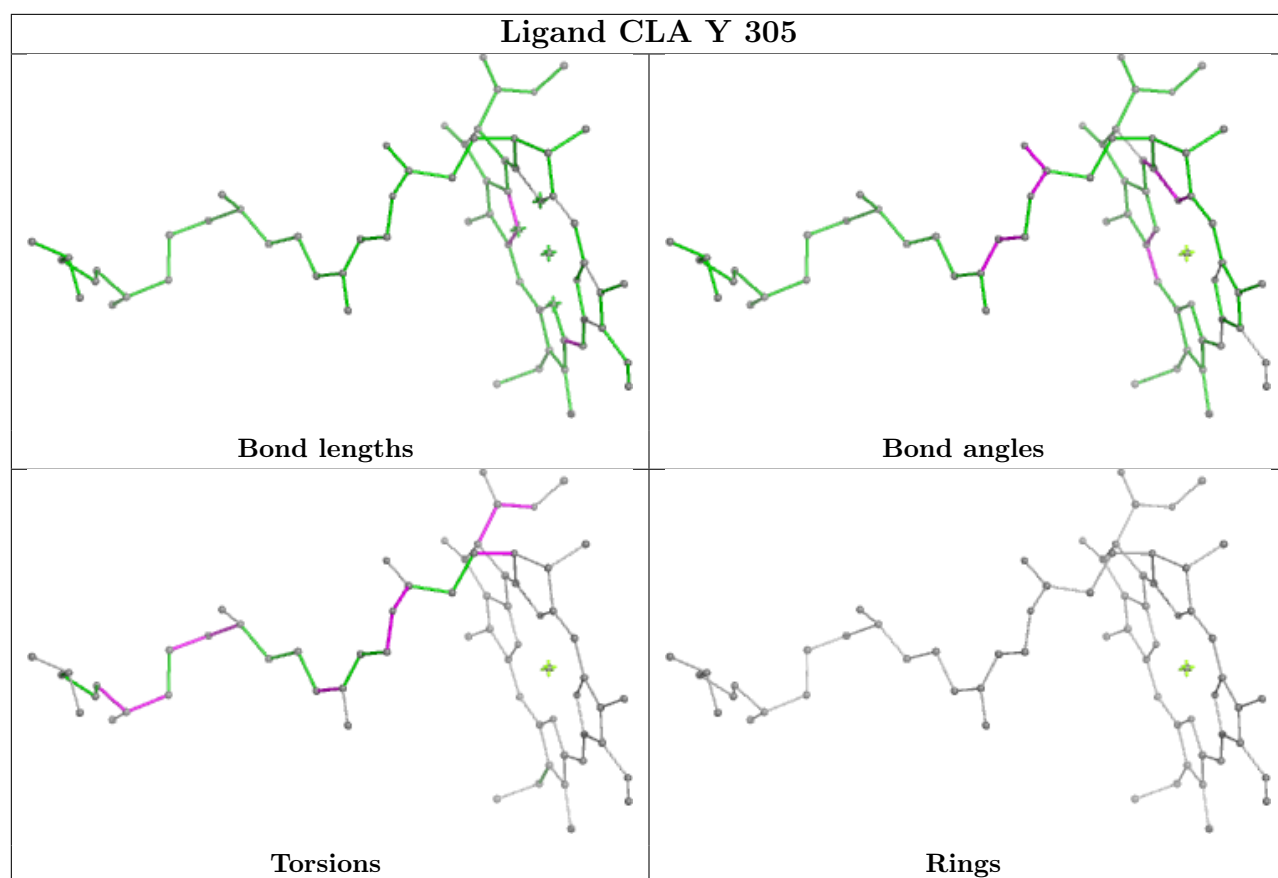


Torsions

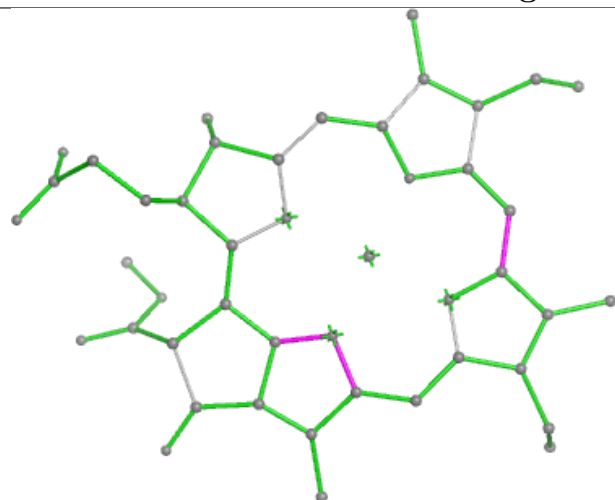


Rings

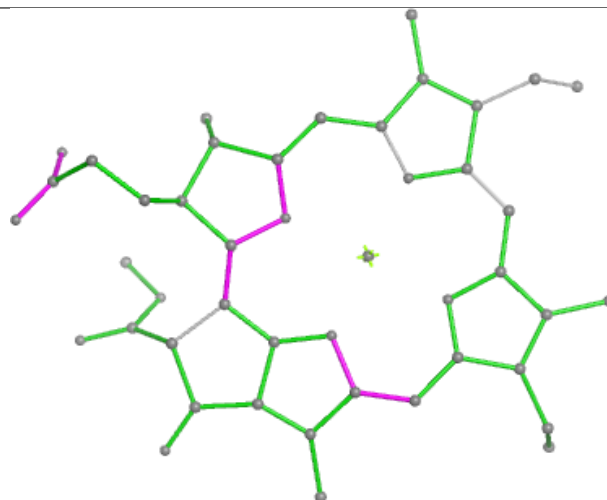




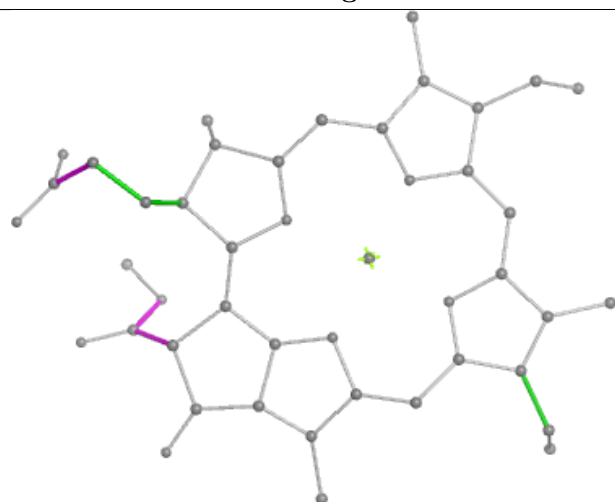
Ligand CLA n 611



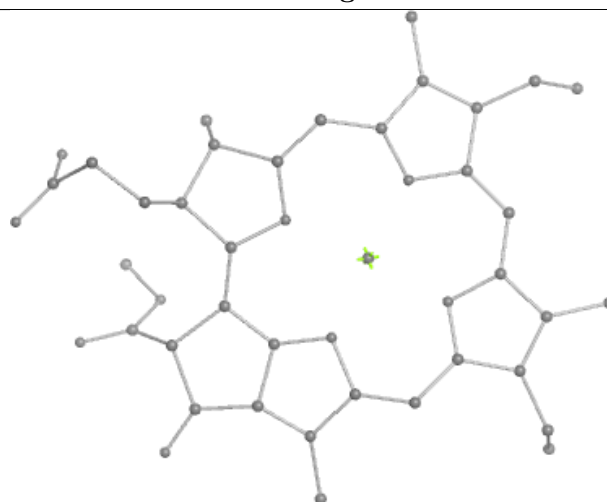
Bond lengths



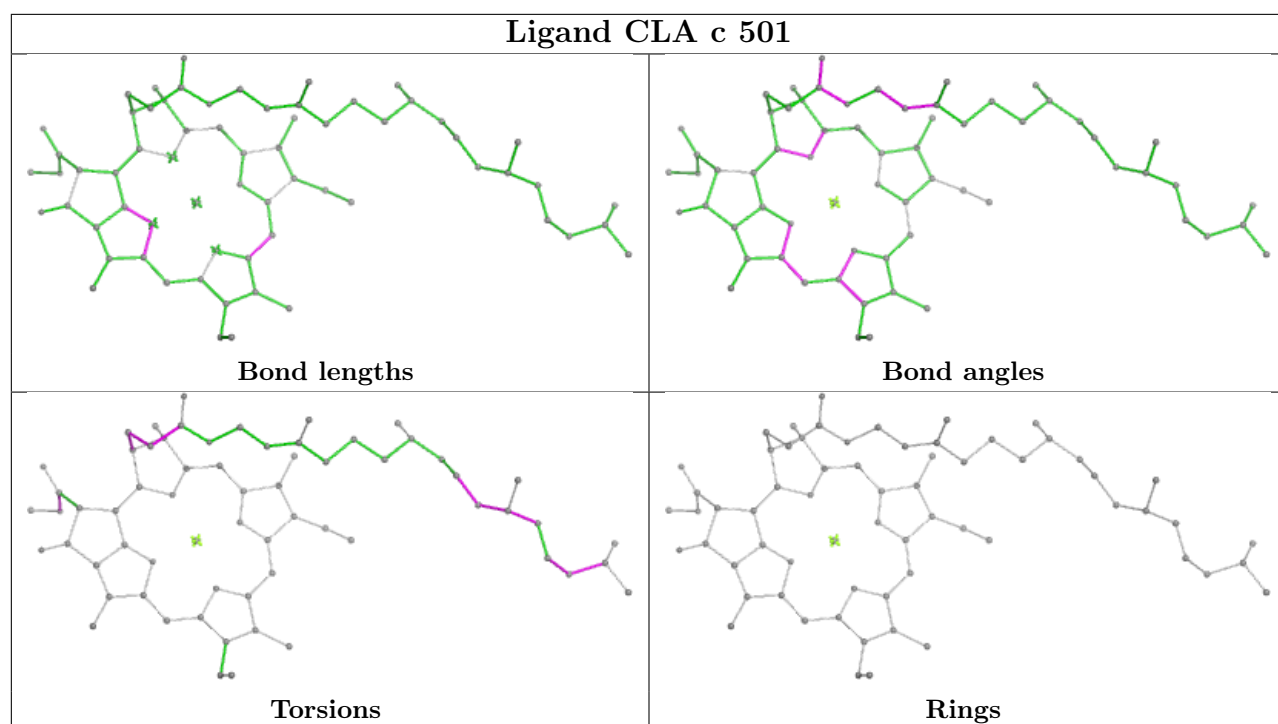
Bond angles

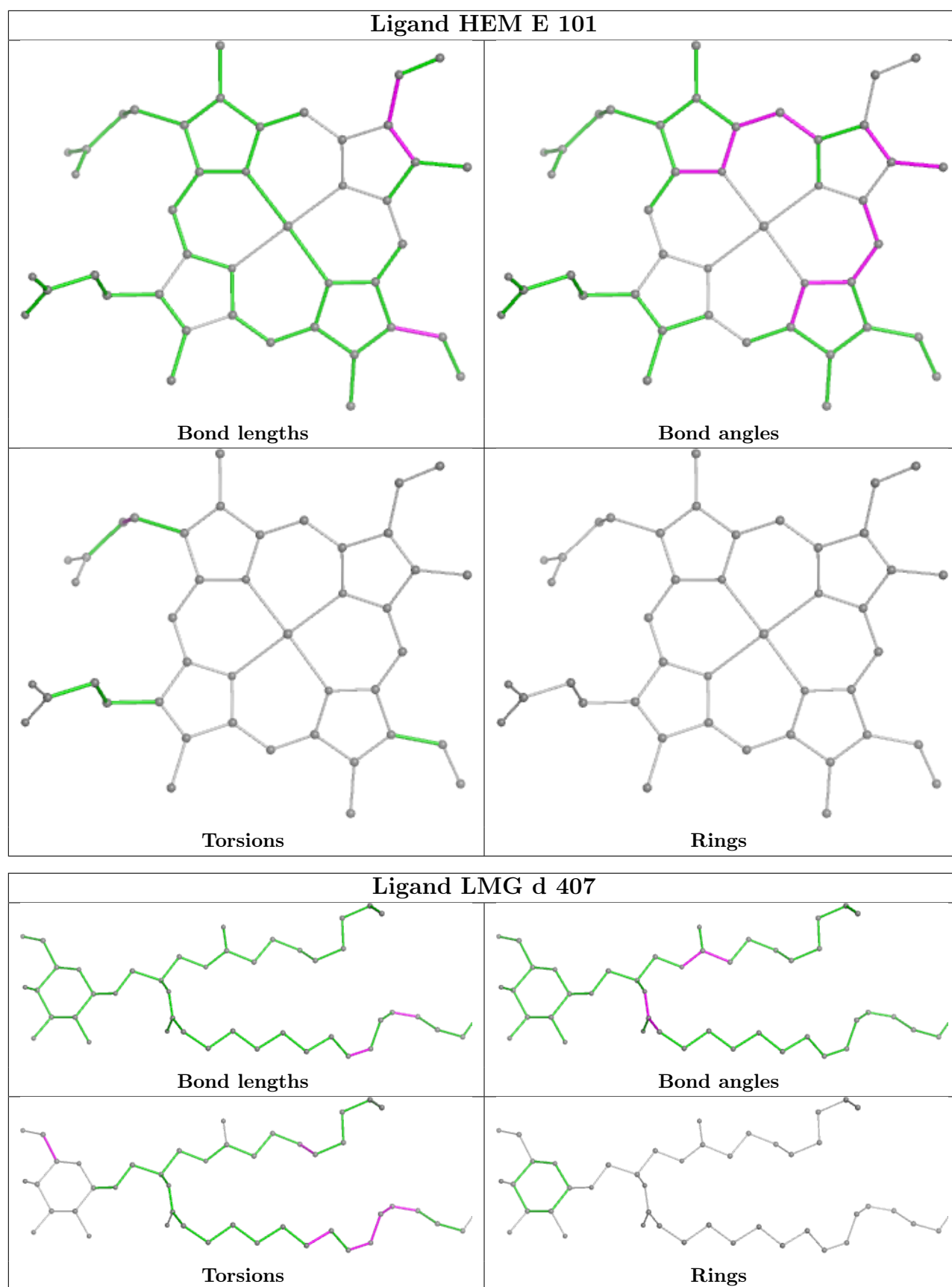


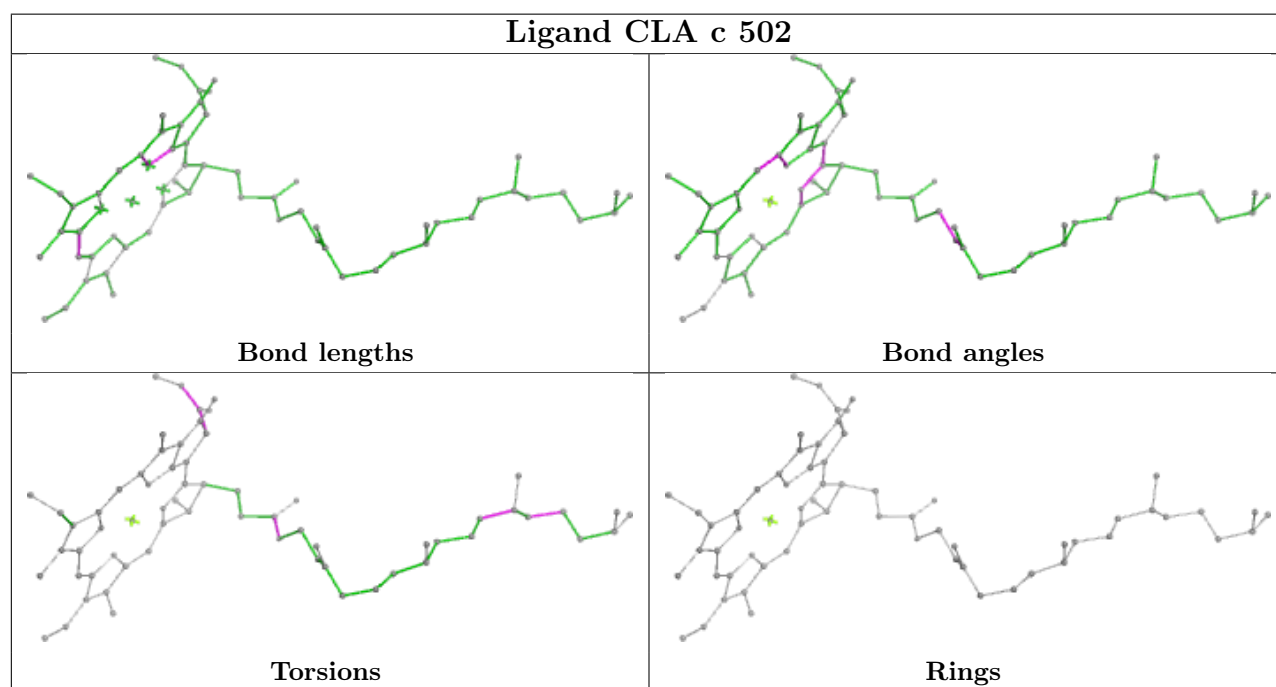
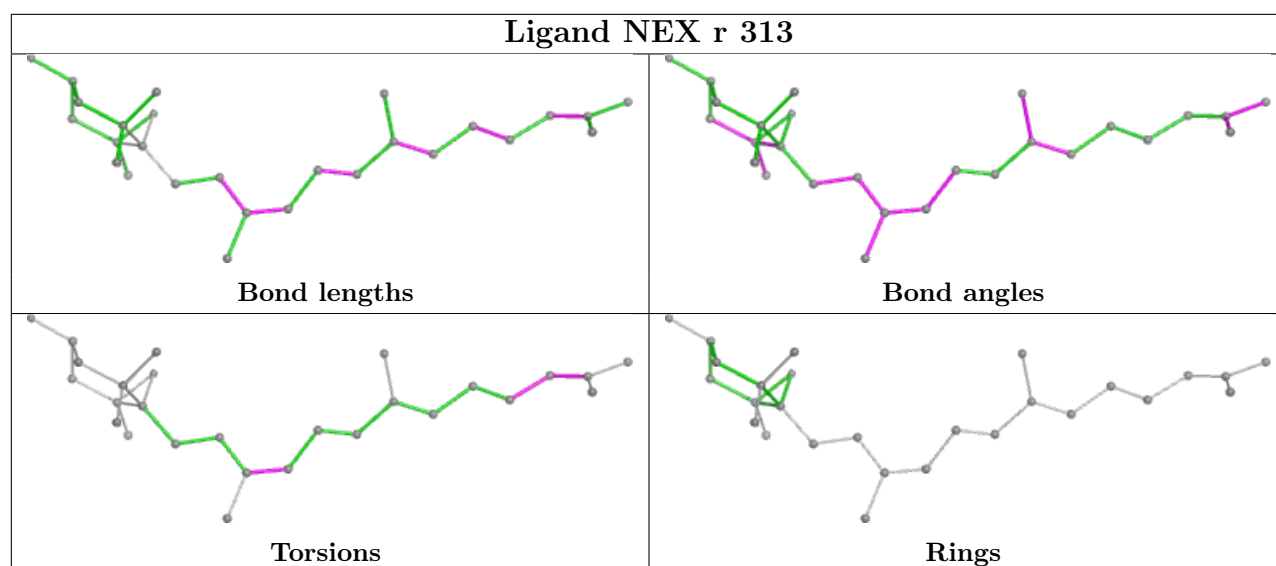
Torsions



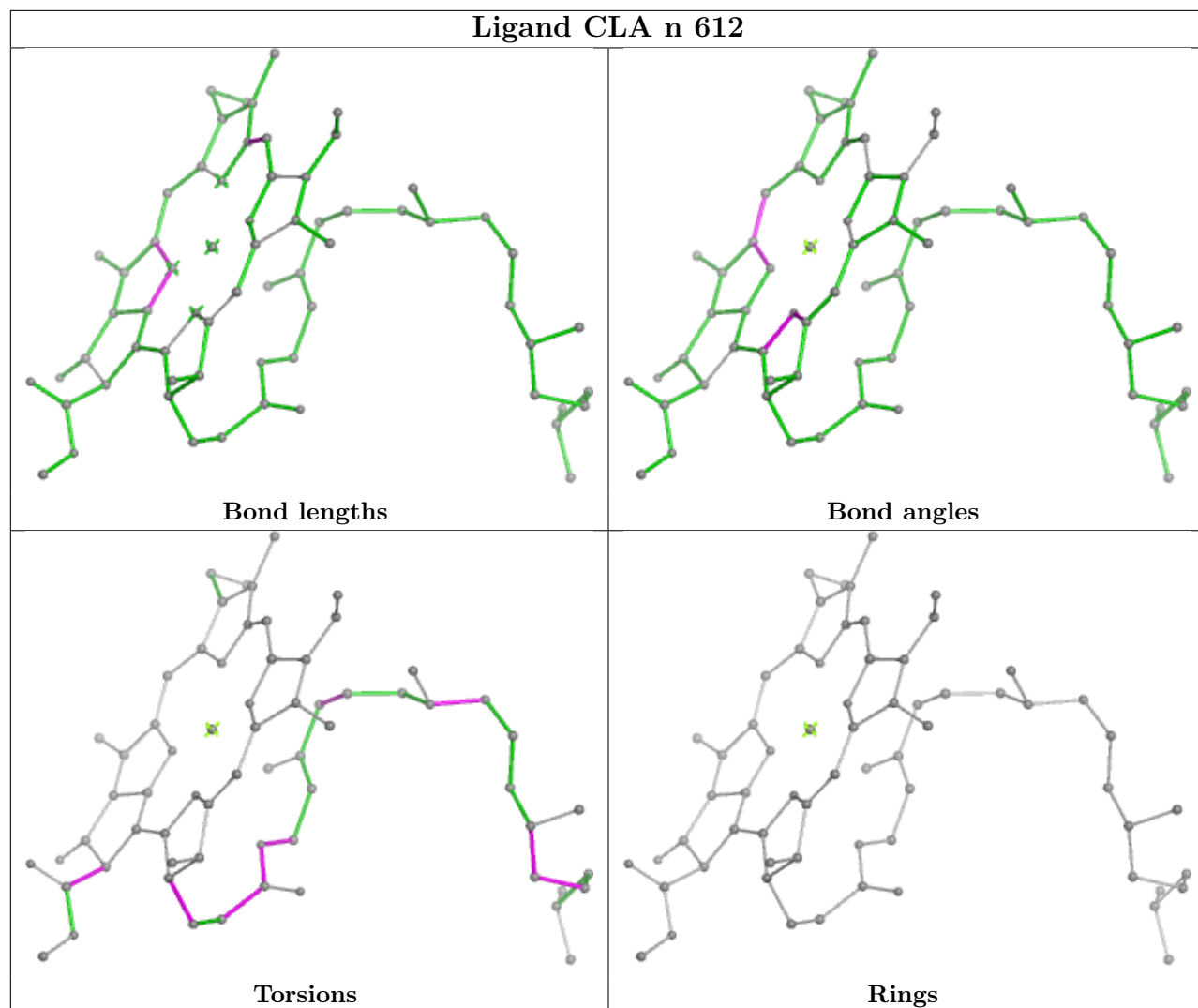
Rings

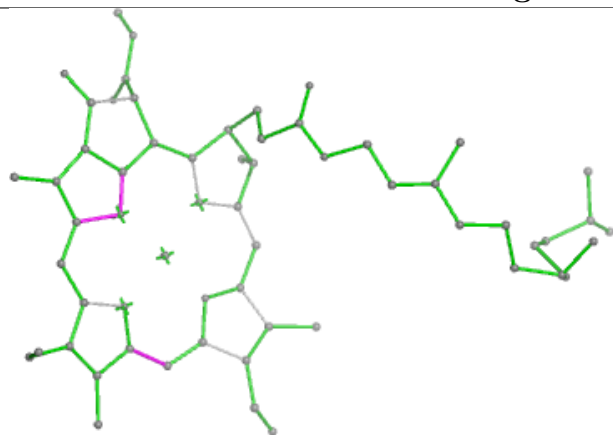
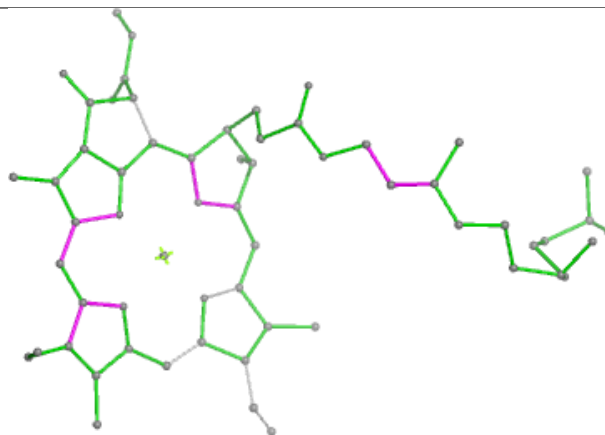
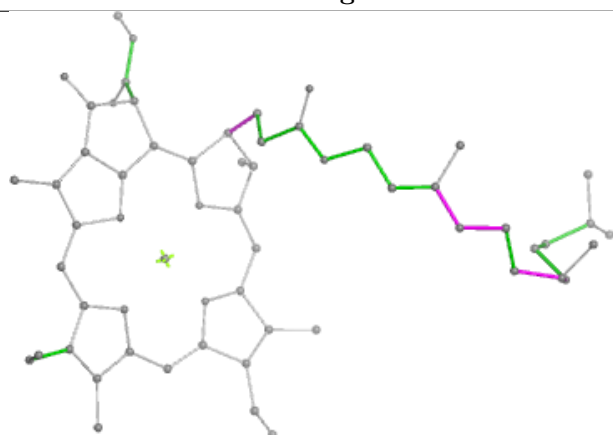
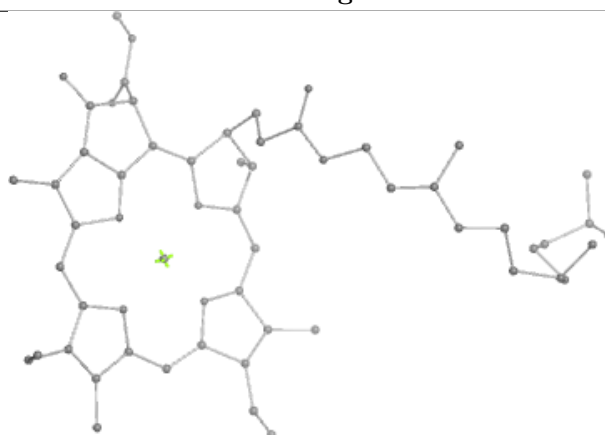
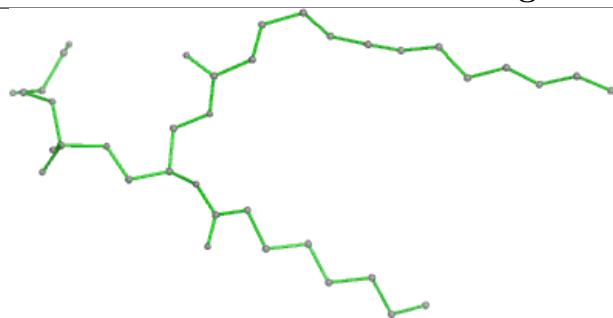
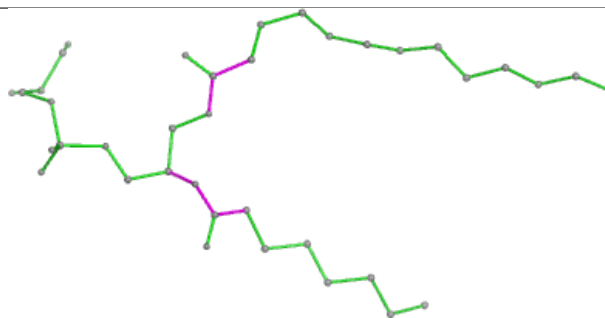
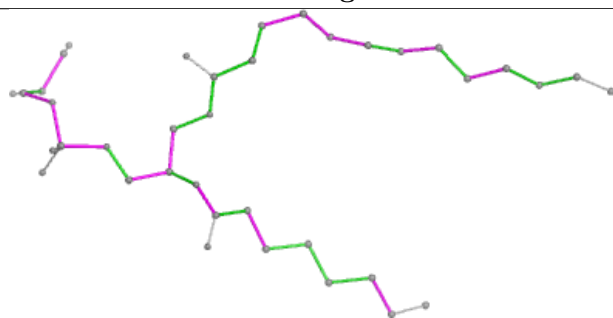
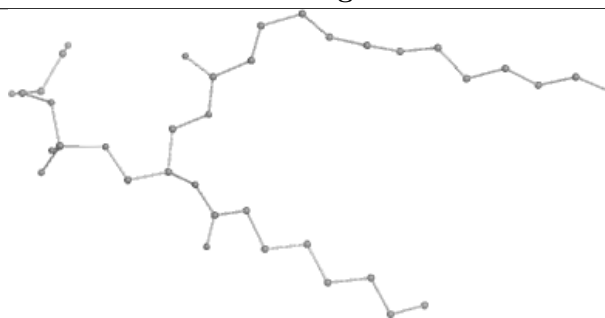




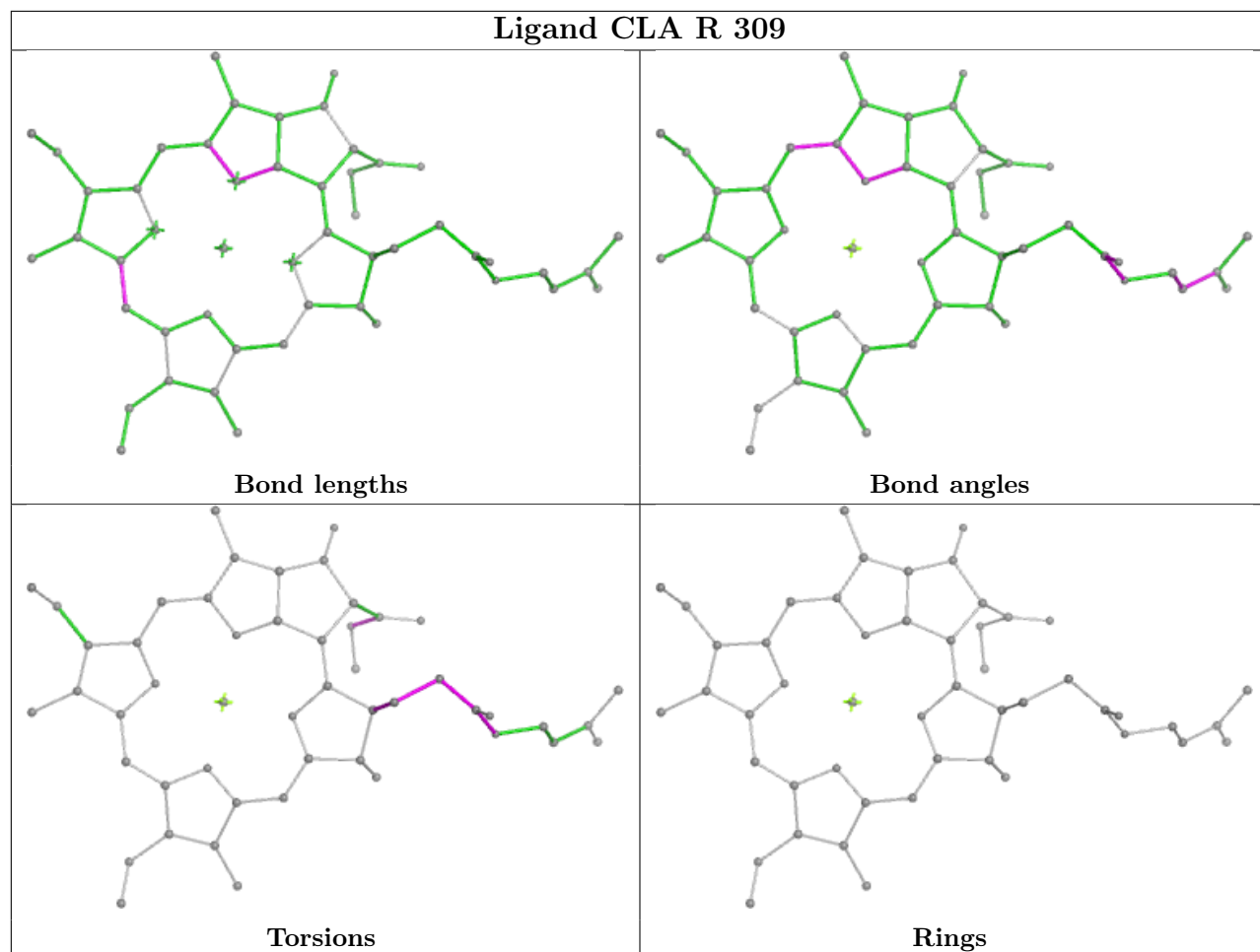


Ligand CLA n 612

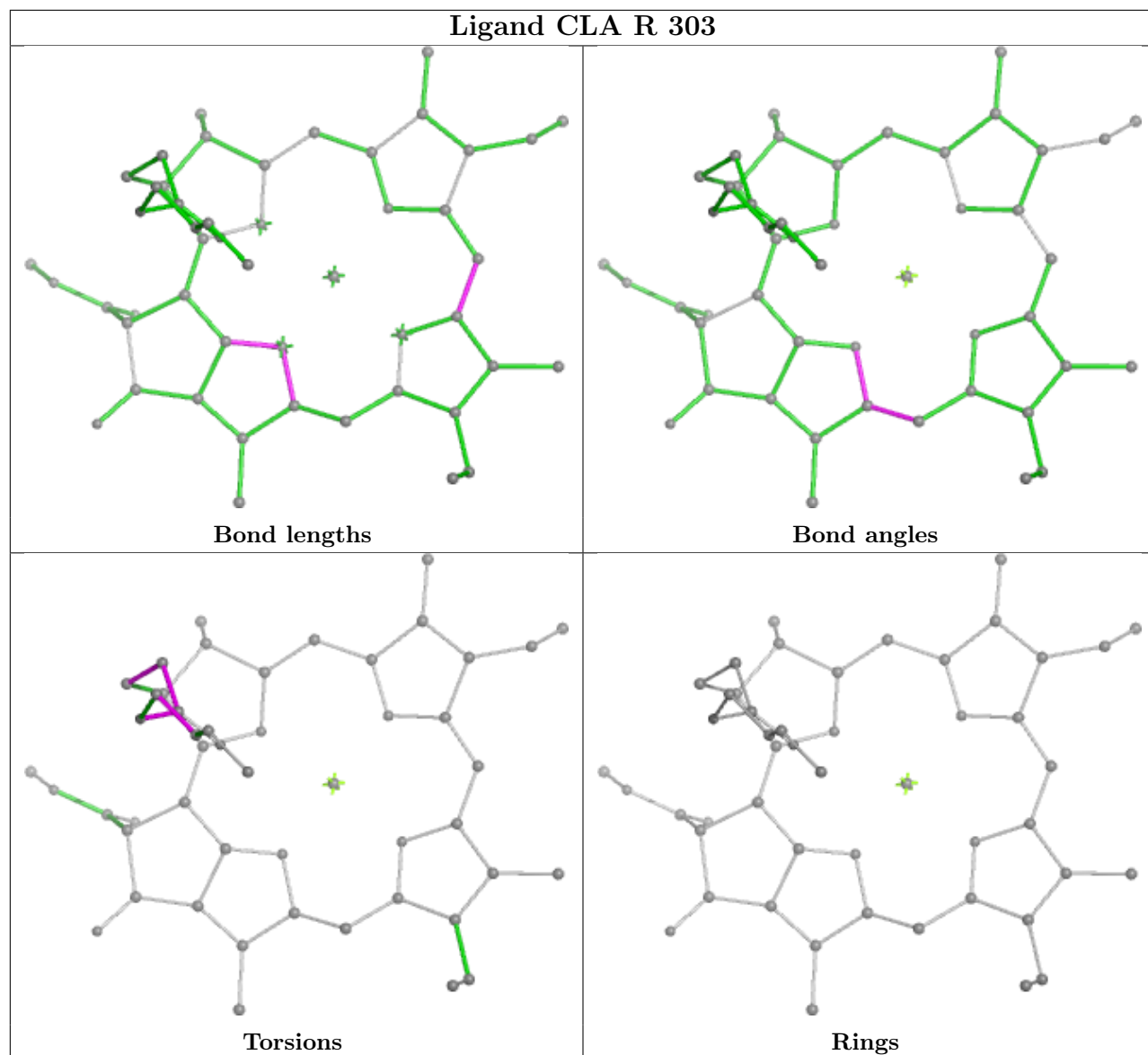


Ligand CLA A 409**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG s 301****Bond lengths****Bond angles****Torsions****Rings**

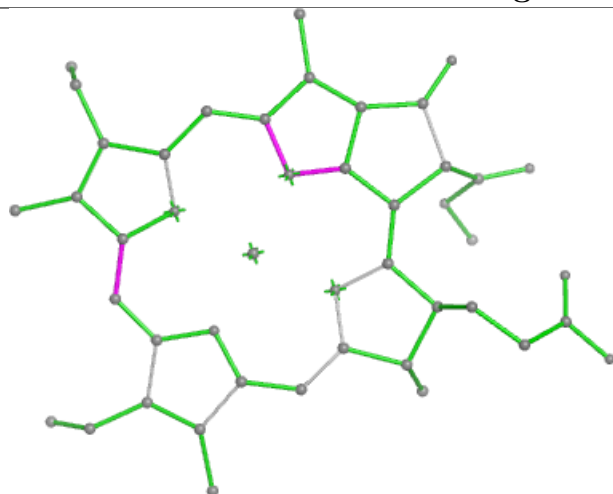
Ligand CLA R 309



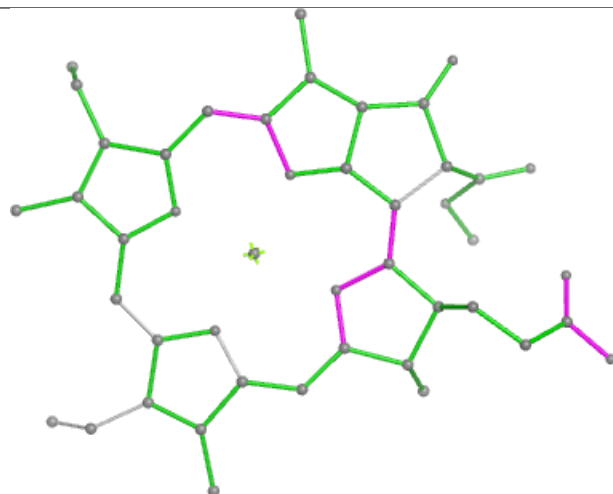
Ligand CLA R 303



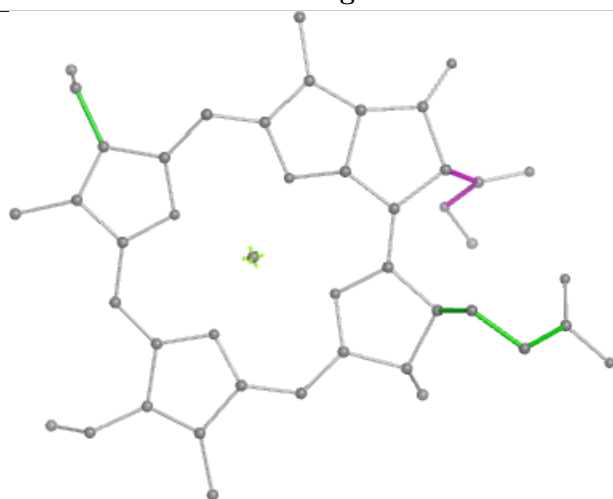
Ligand CLA N 612



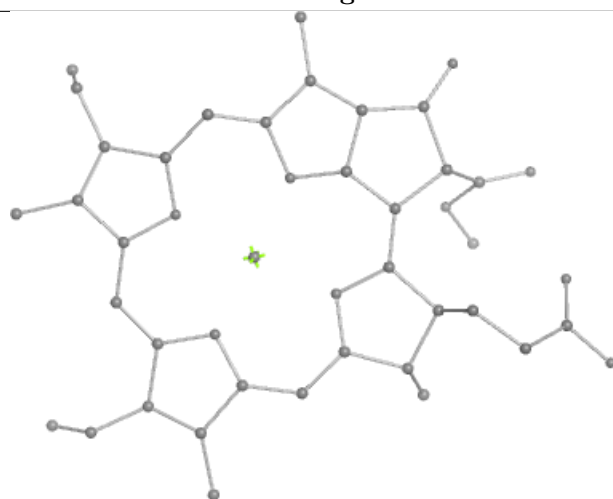
Bond lengths



Bond angles

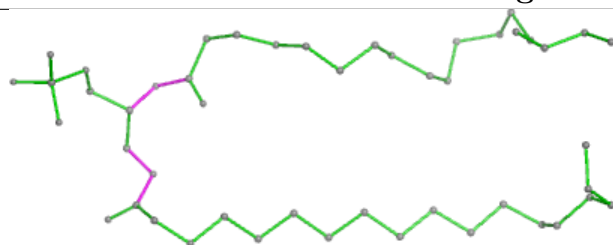


Torsions

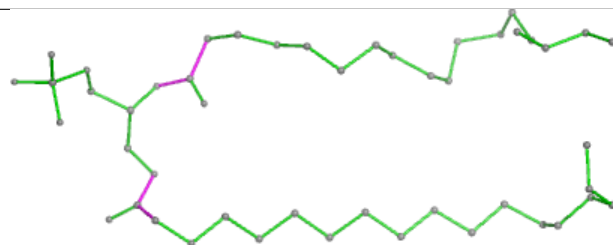


Rings

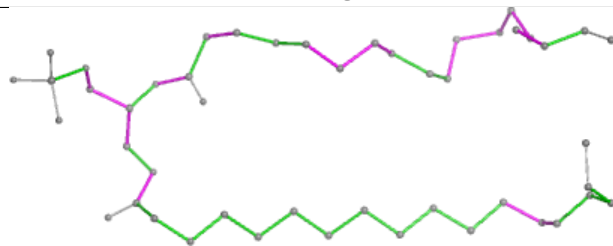
Ligand 3PH B 522



Bond lengths



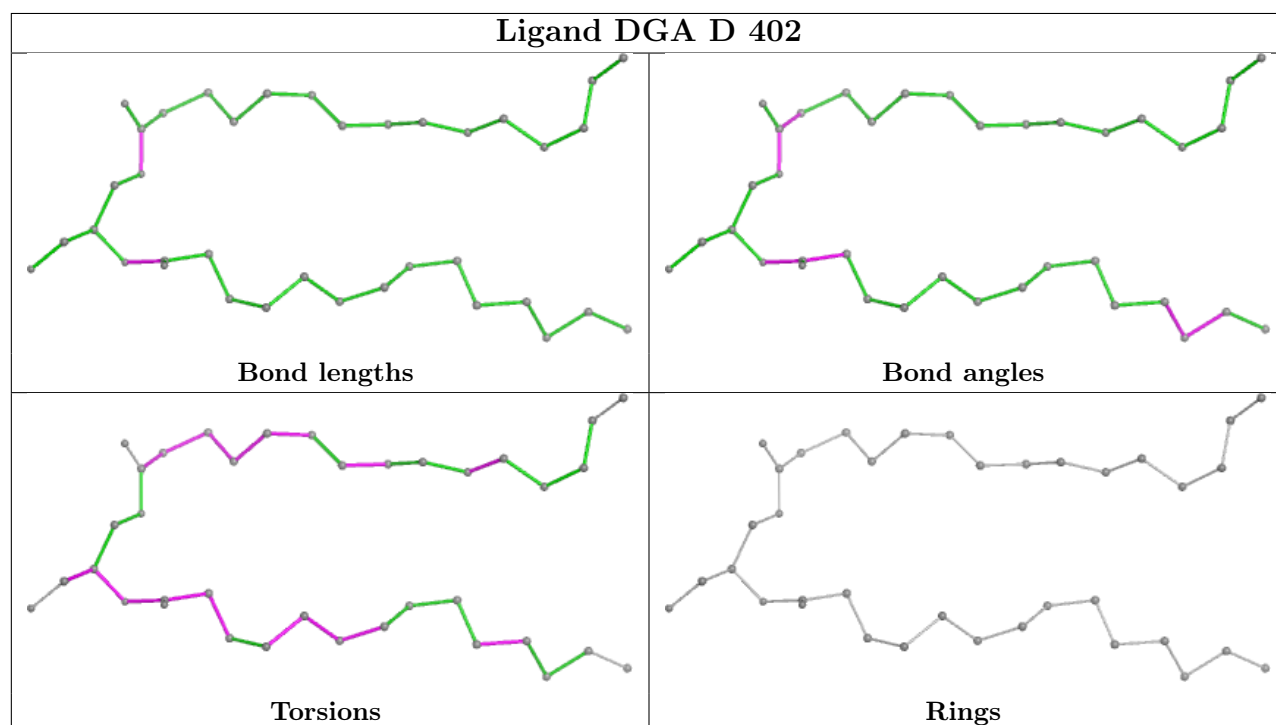
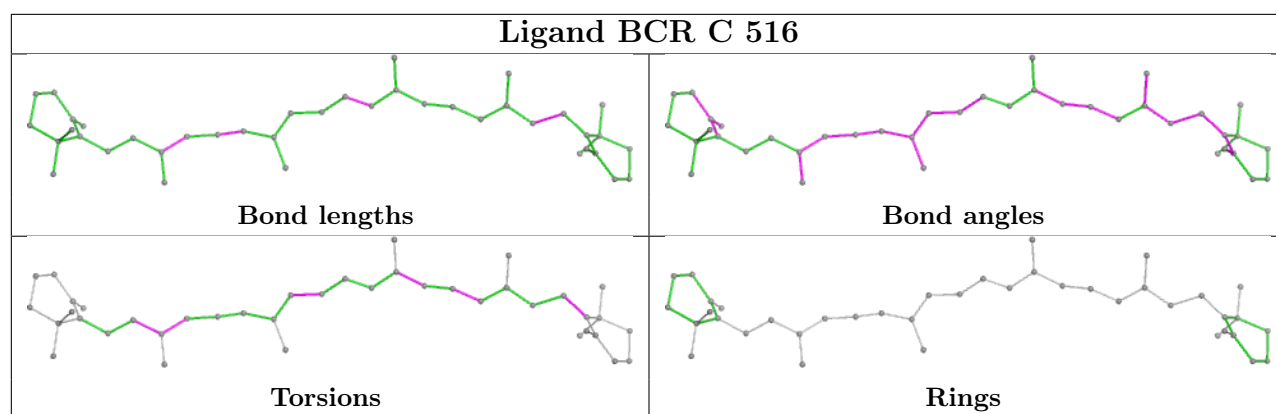
Bond angles

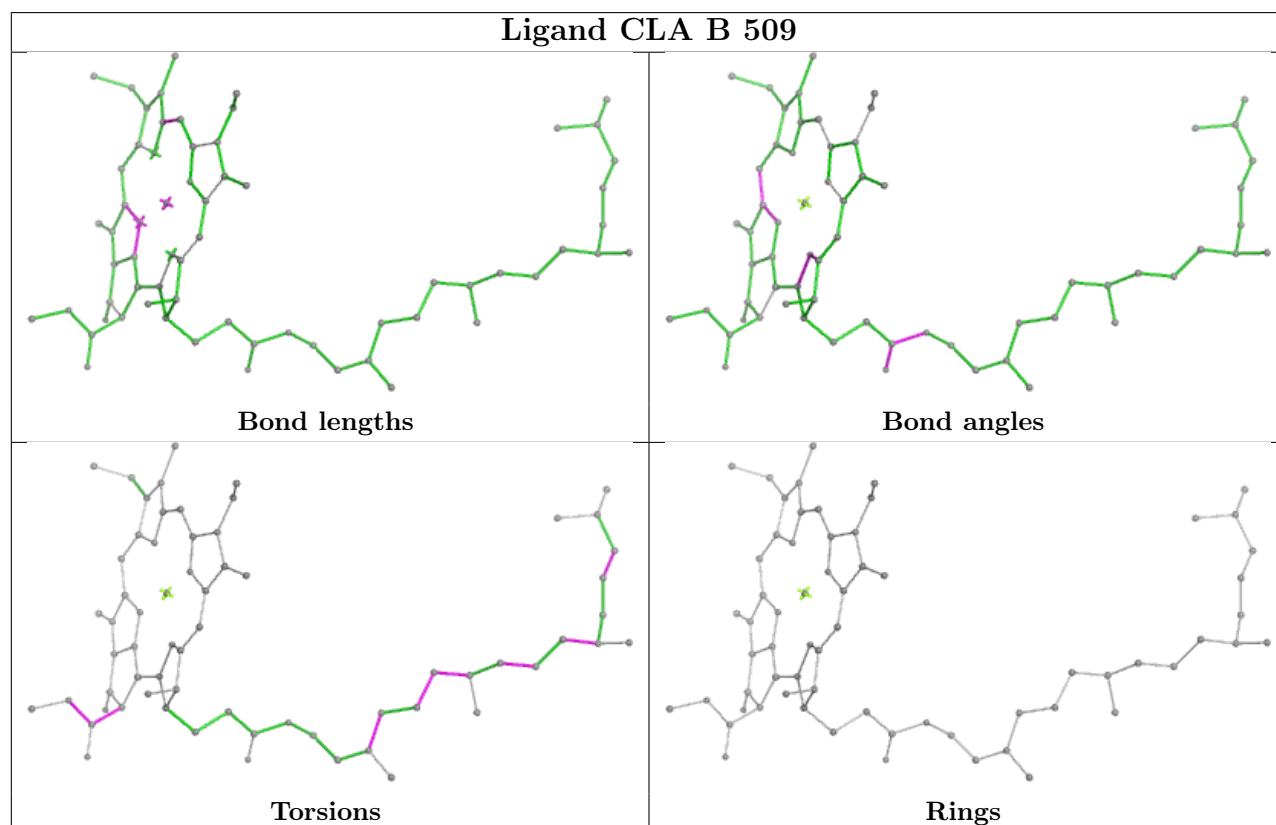
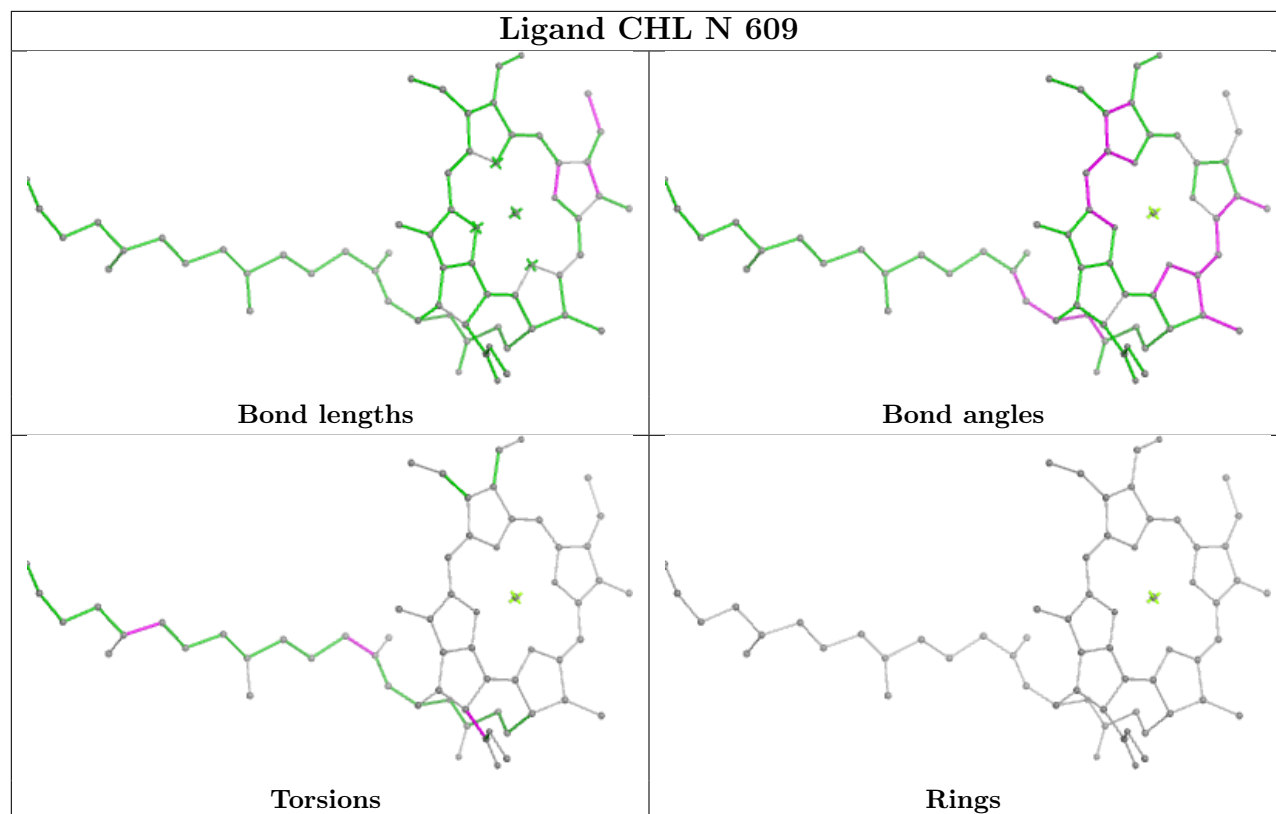


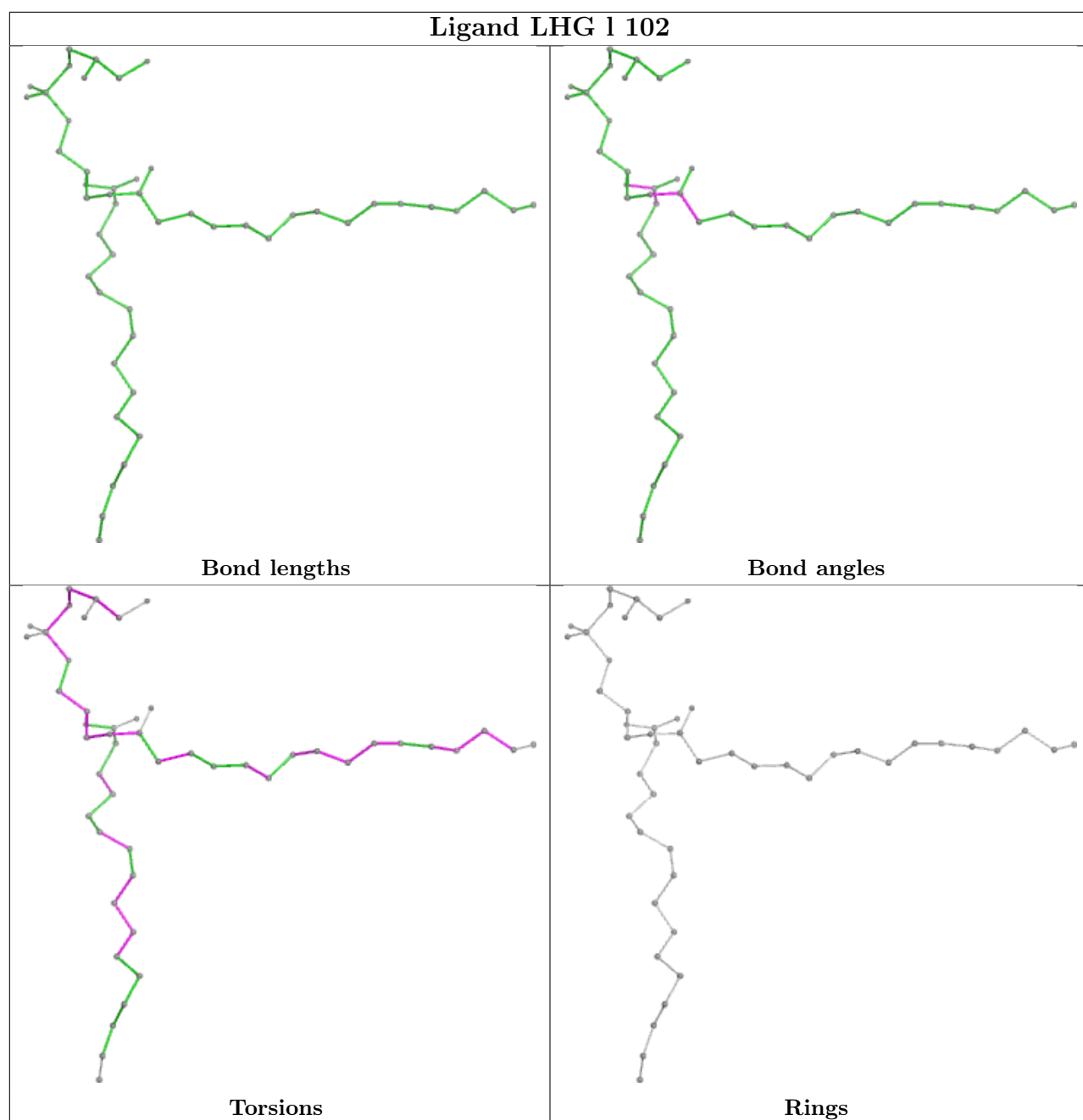
Torsions

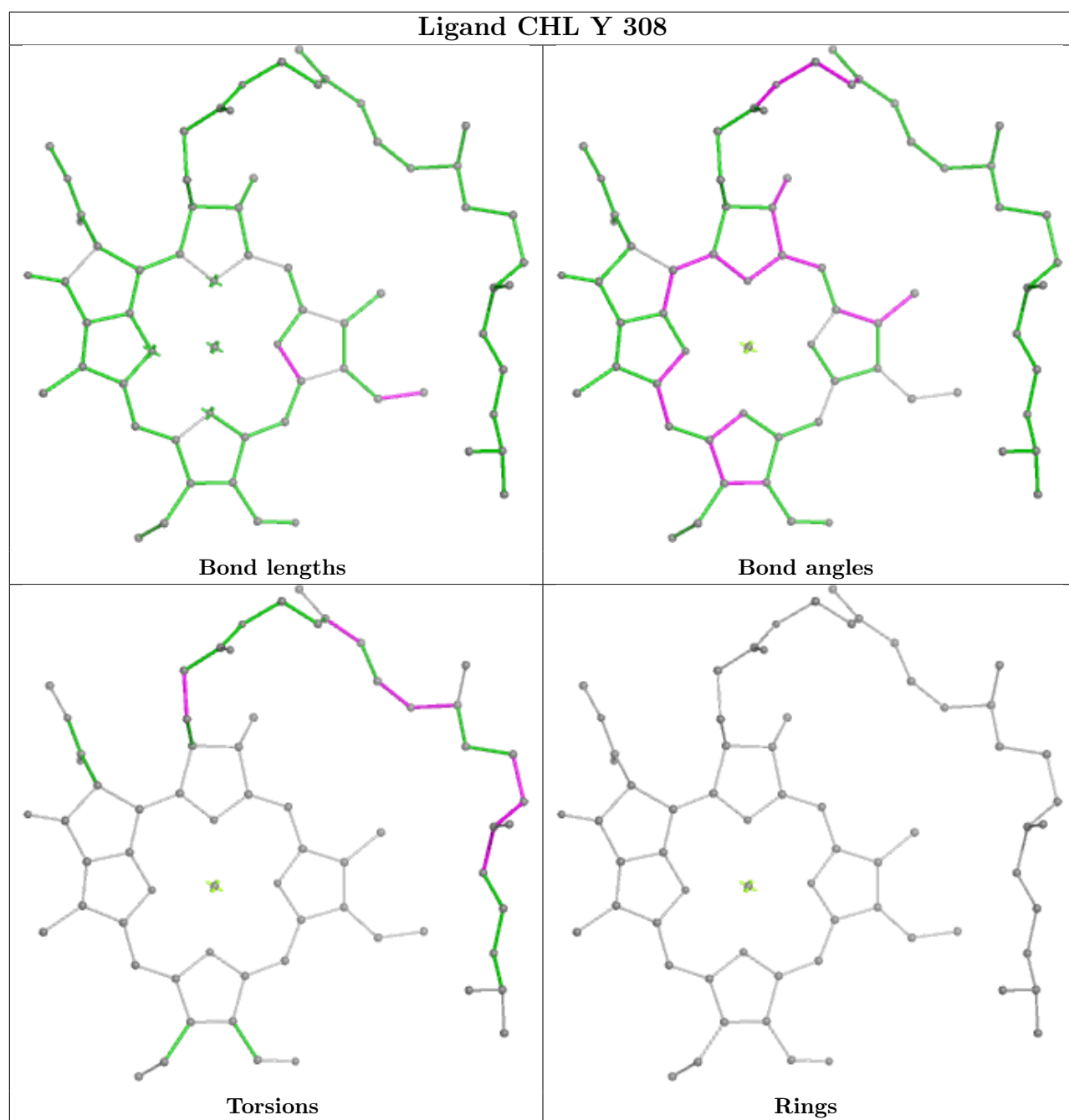


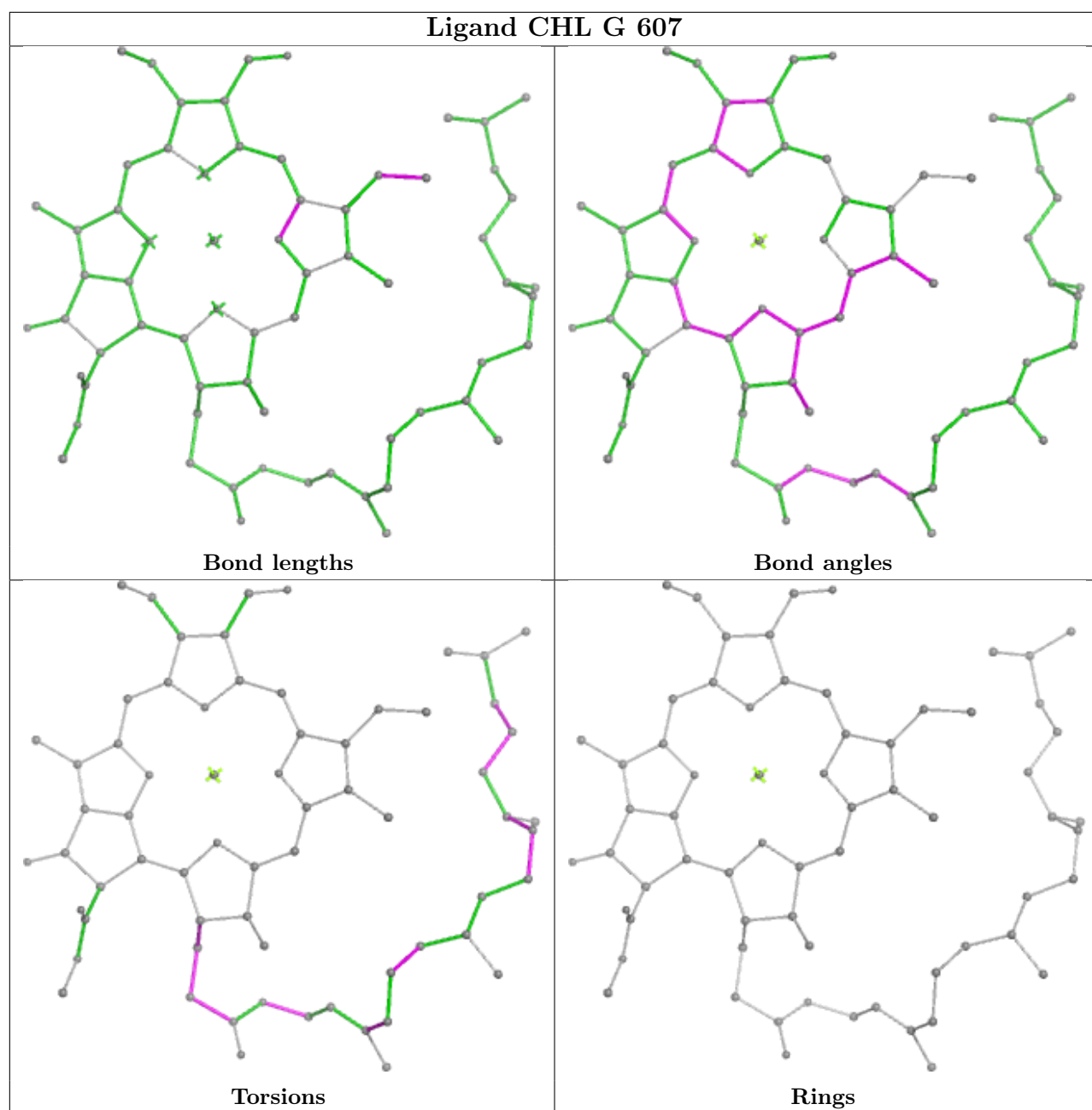
Rings

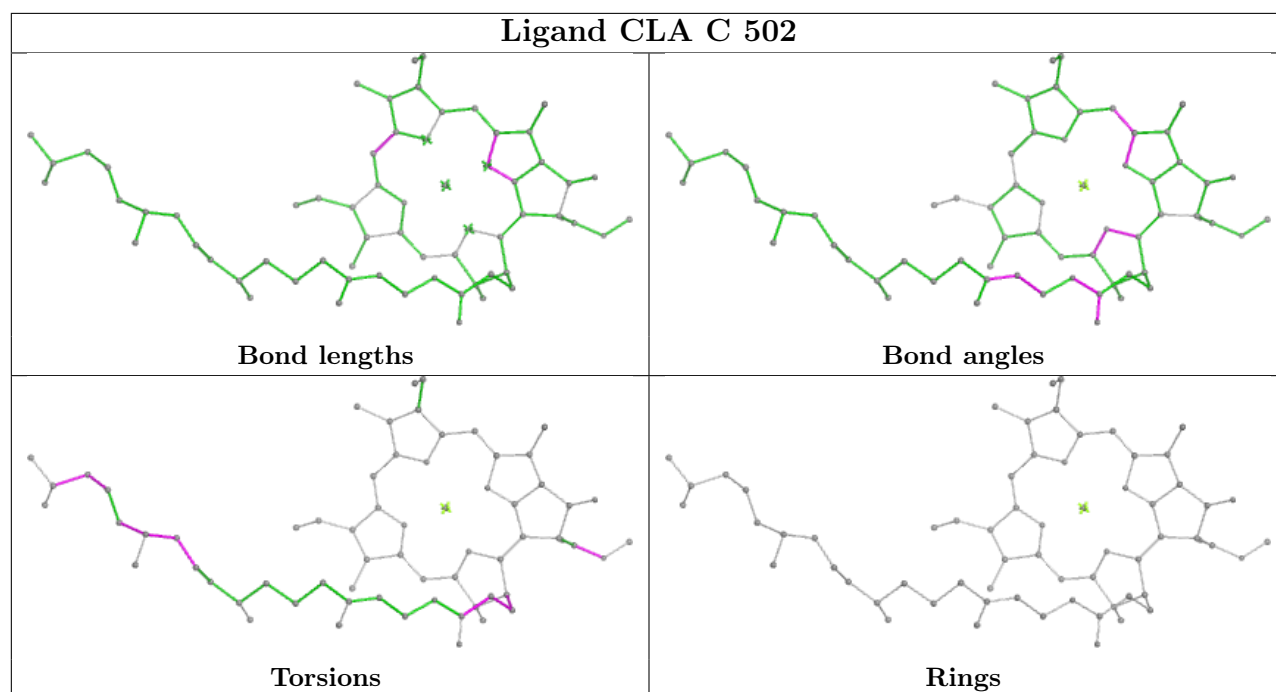
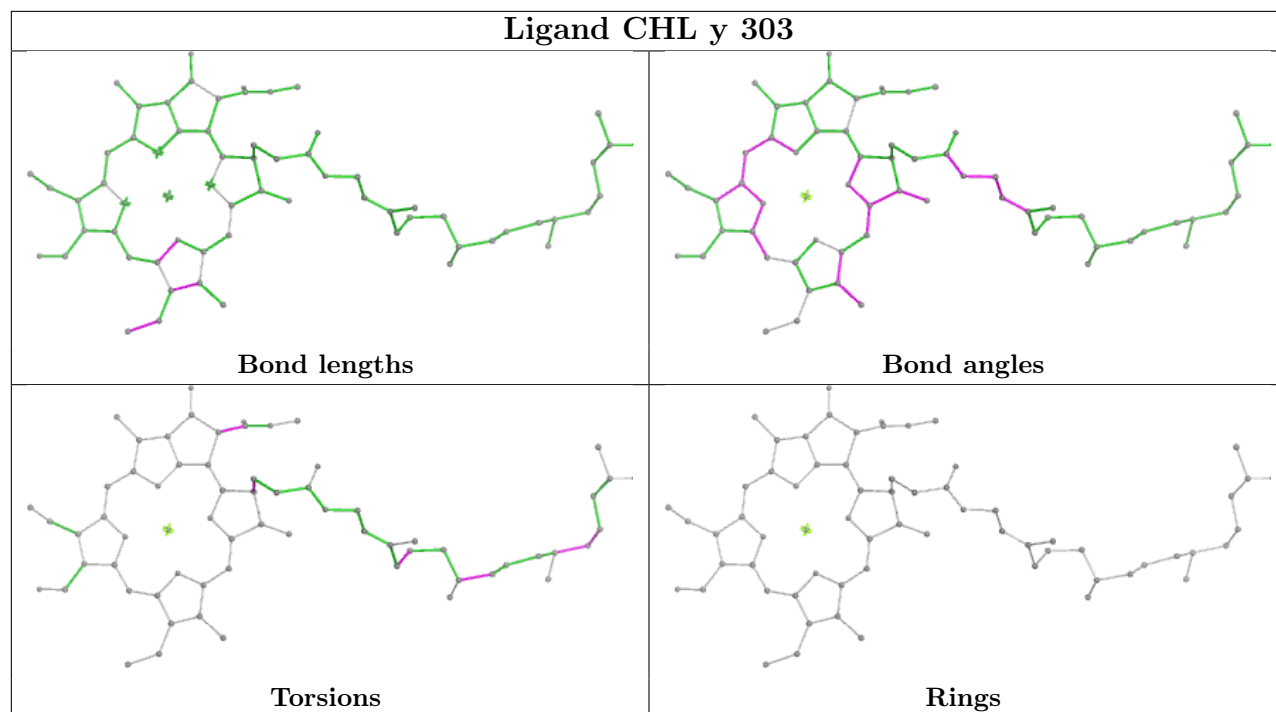


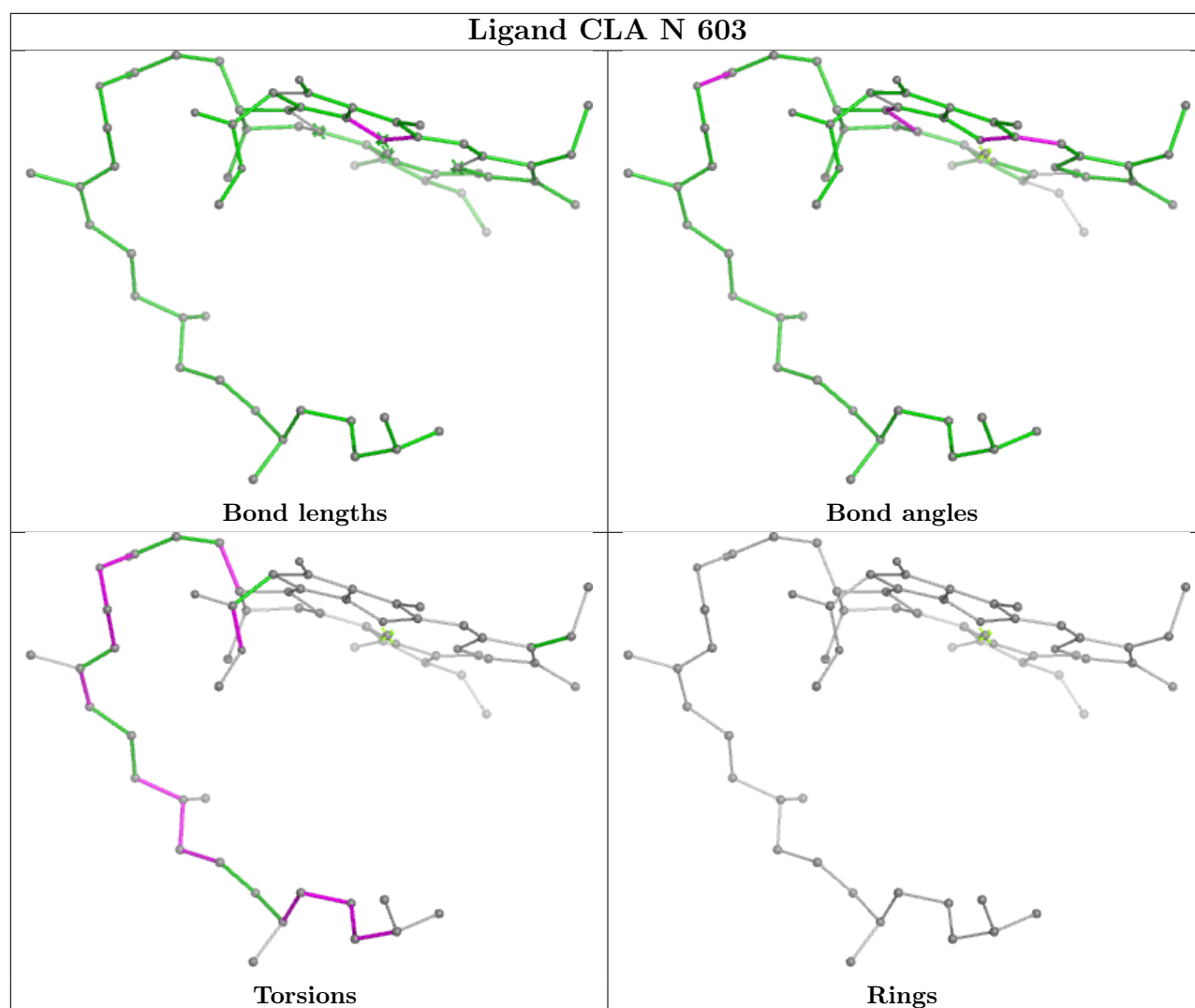




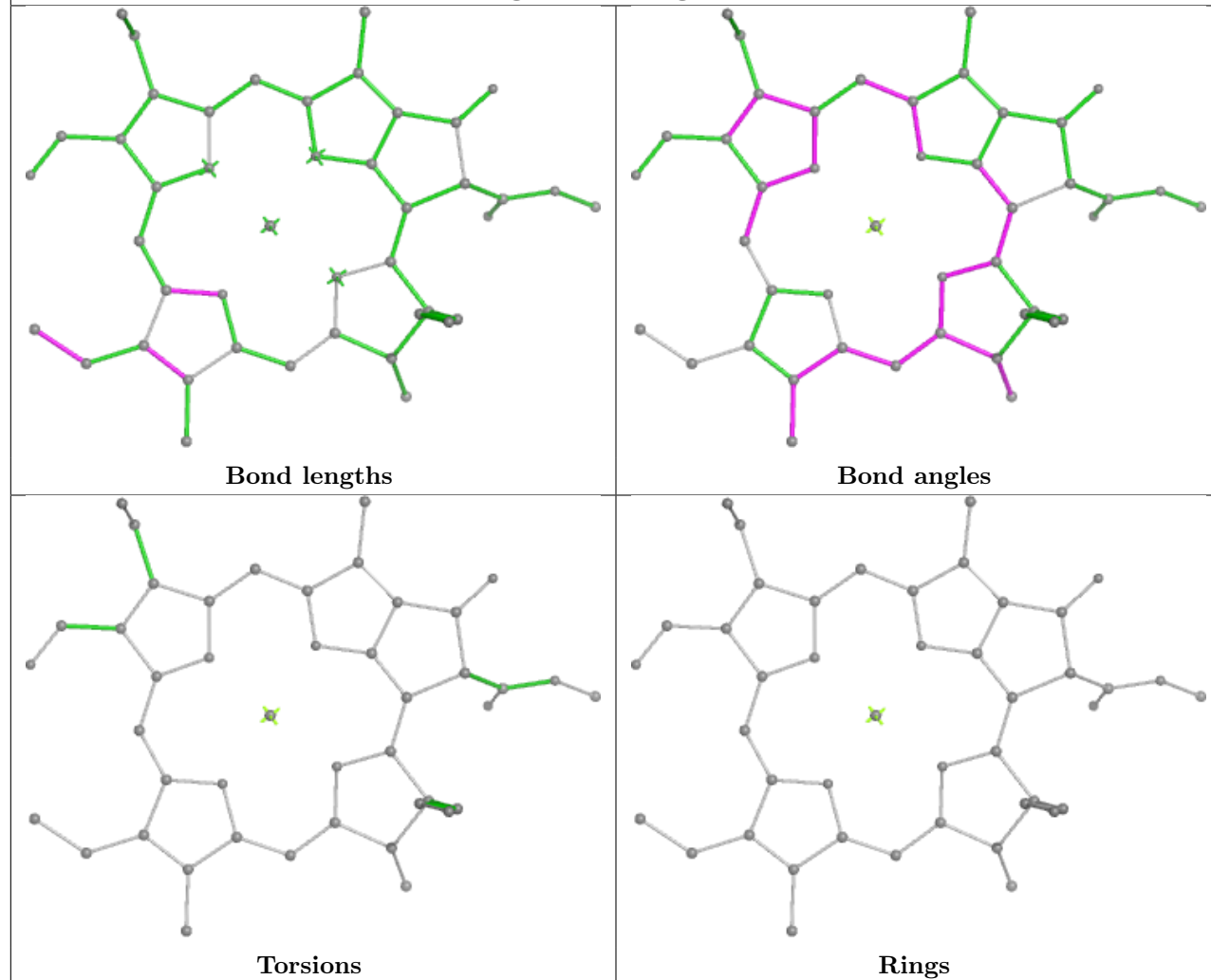


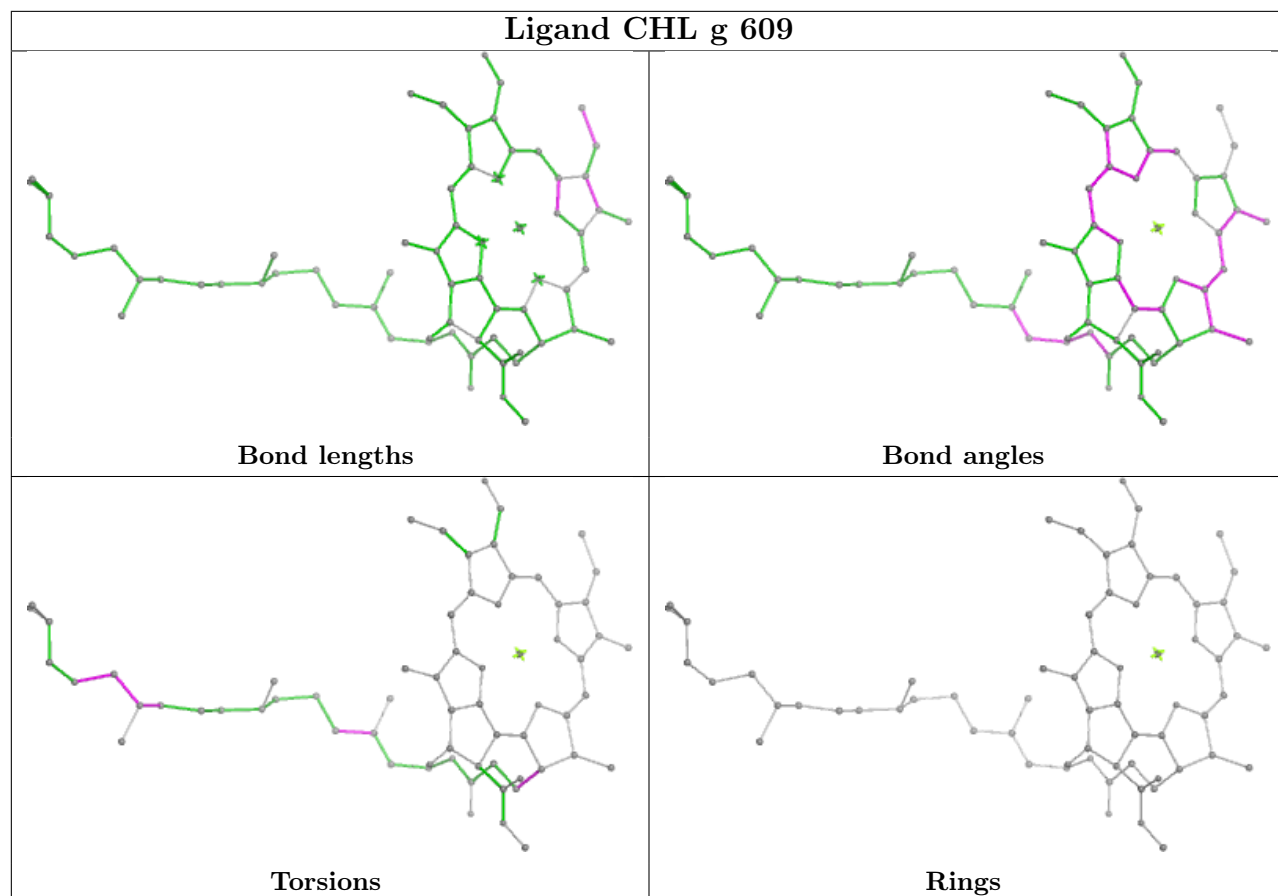




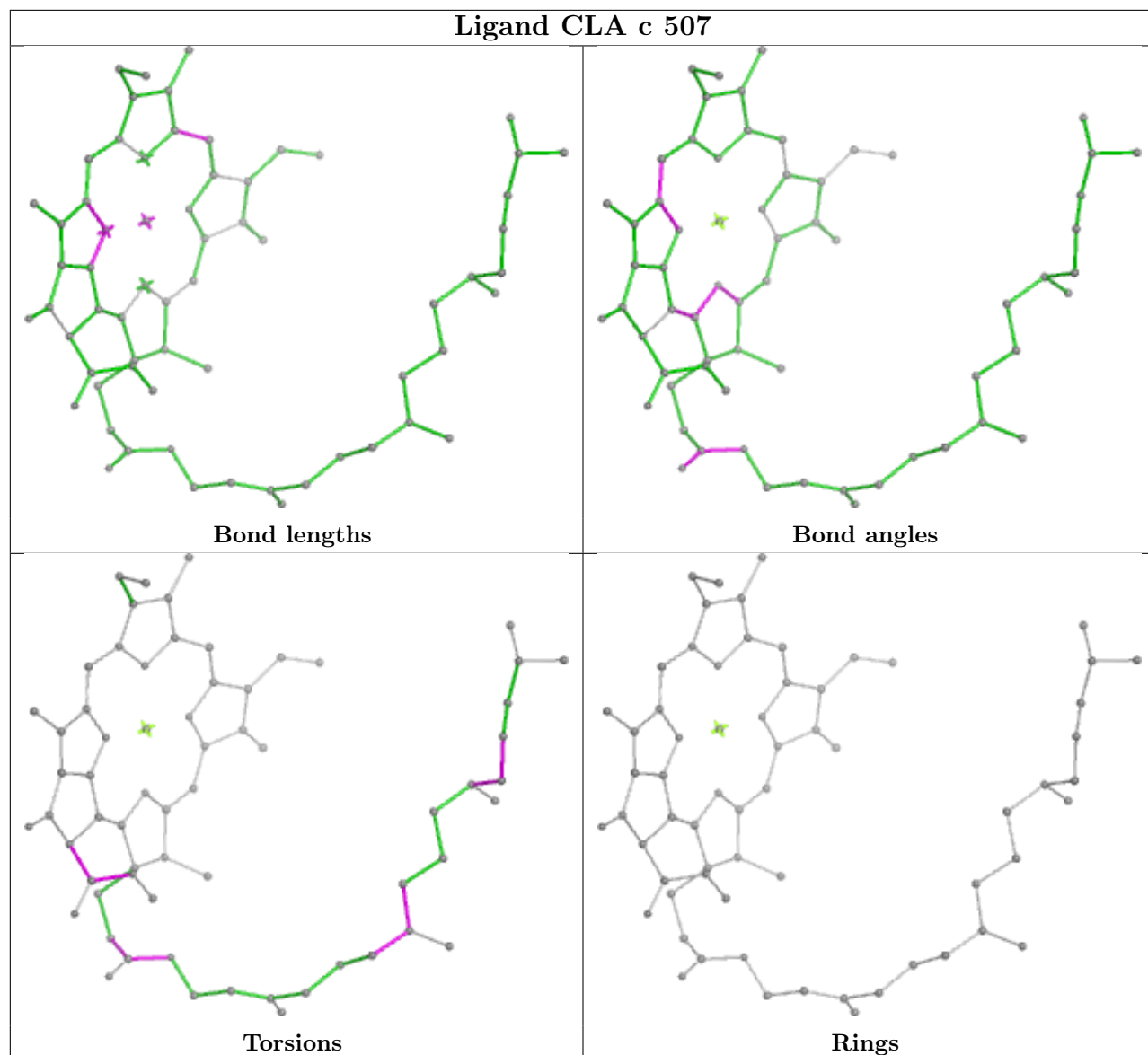


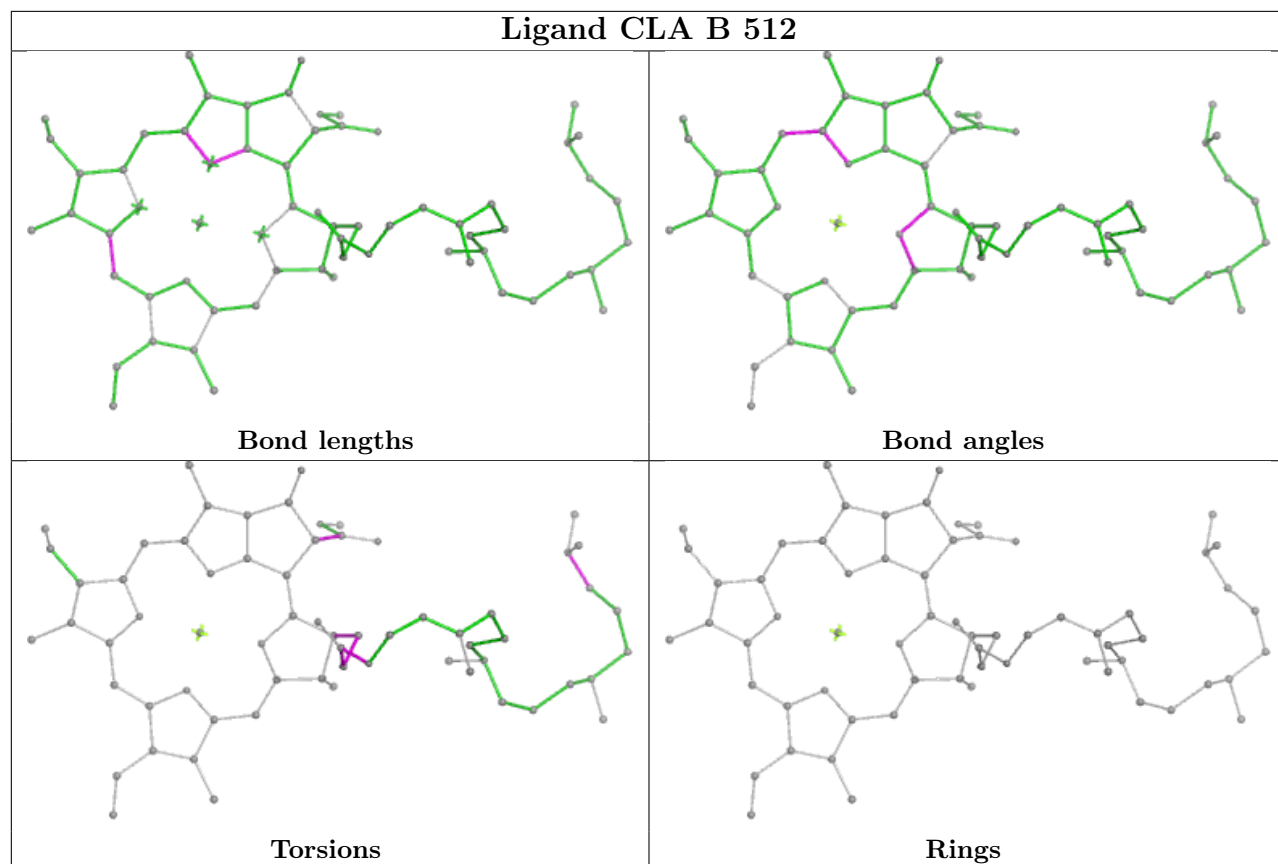
Ligand CHL g 608

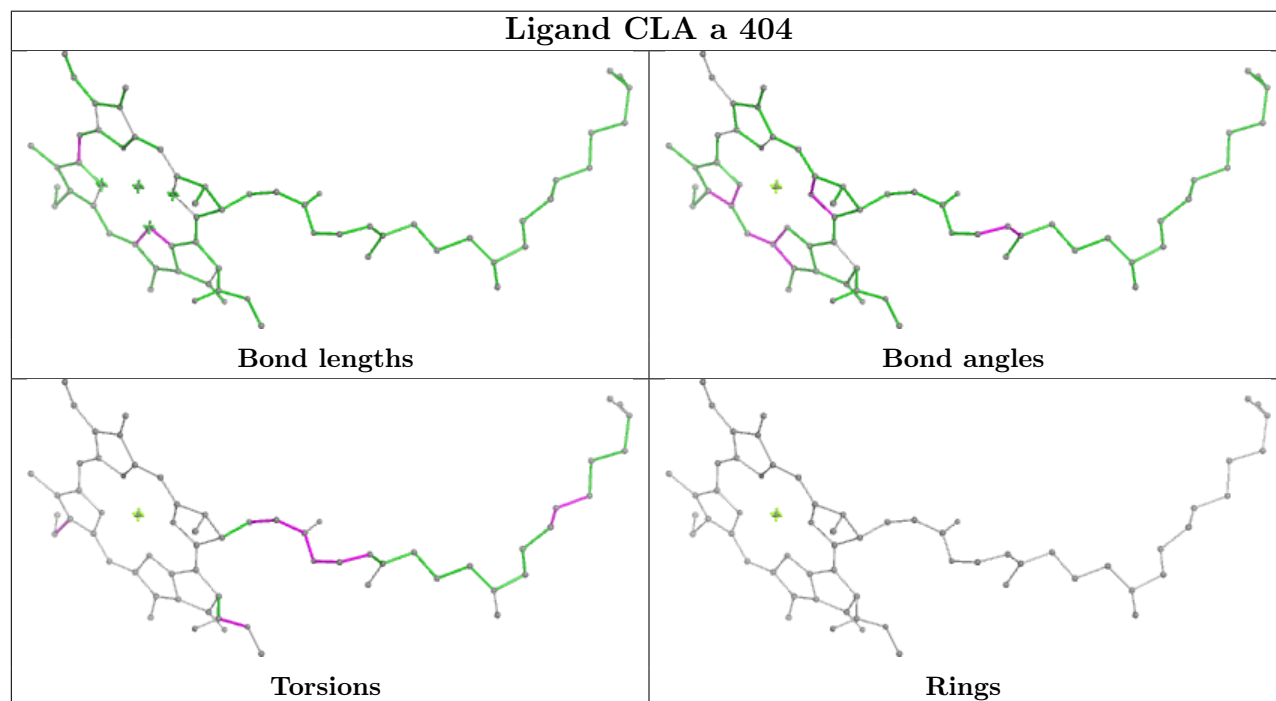
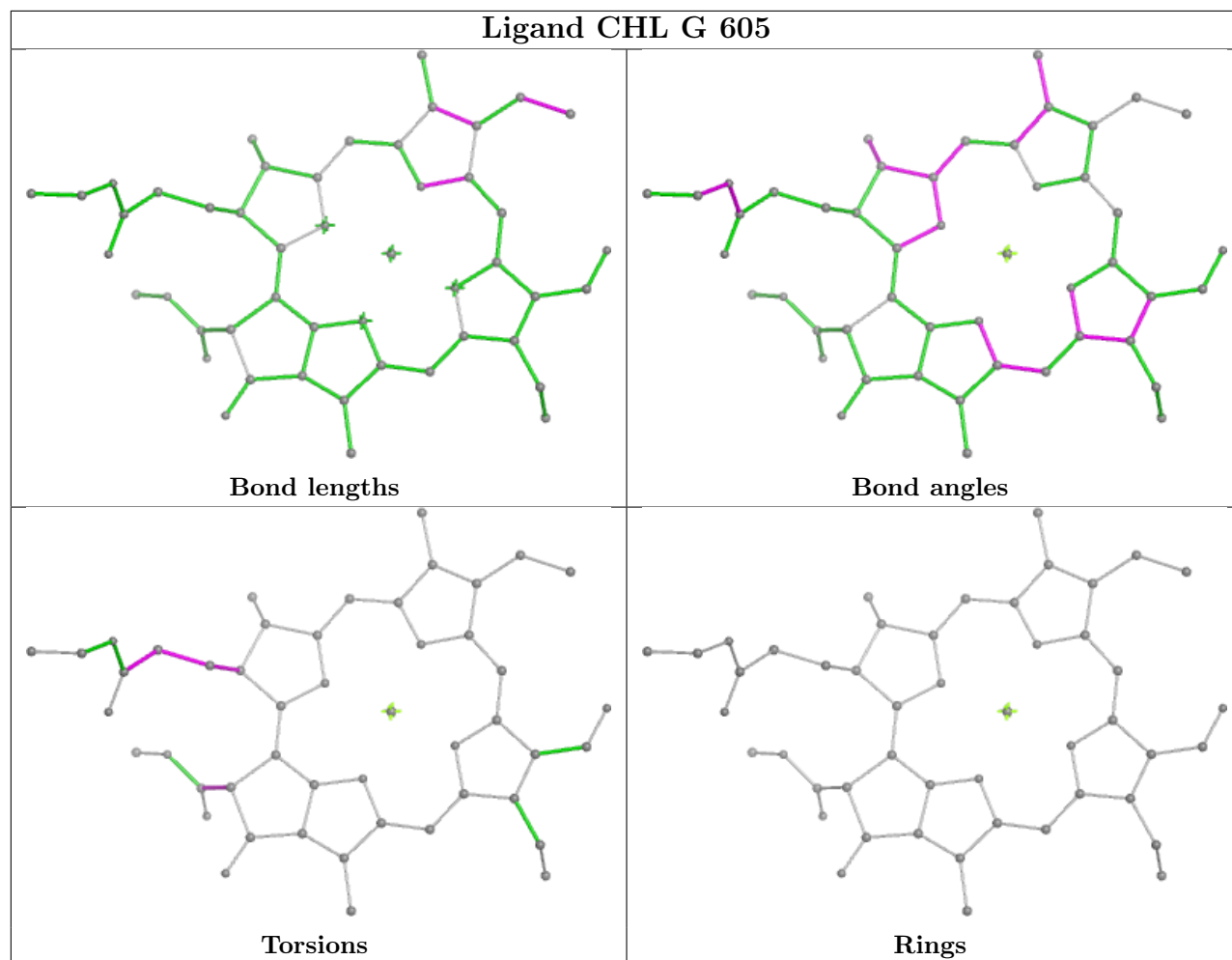


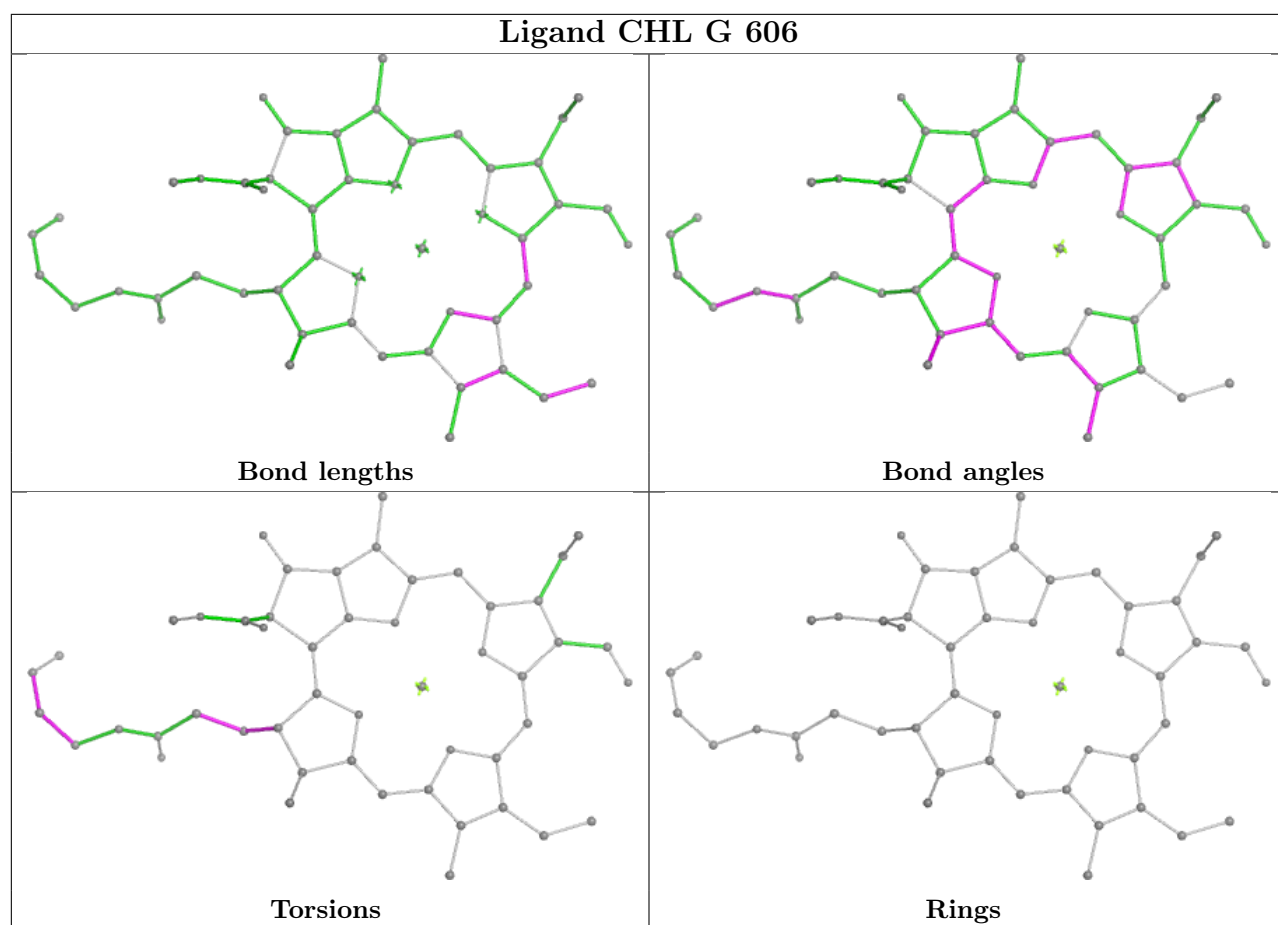


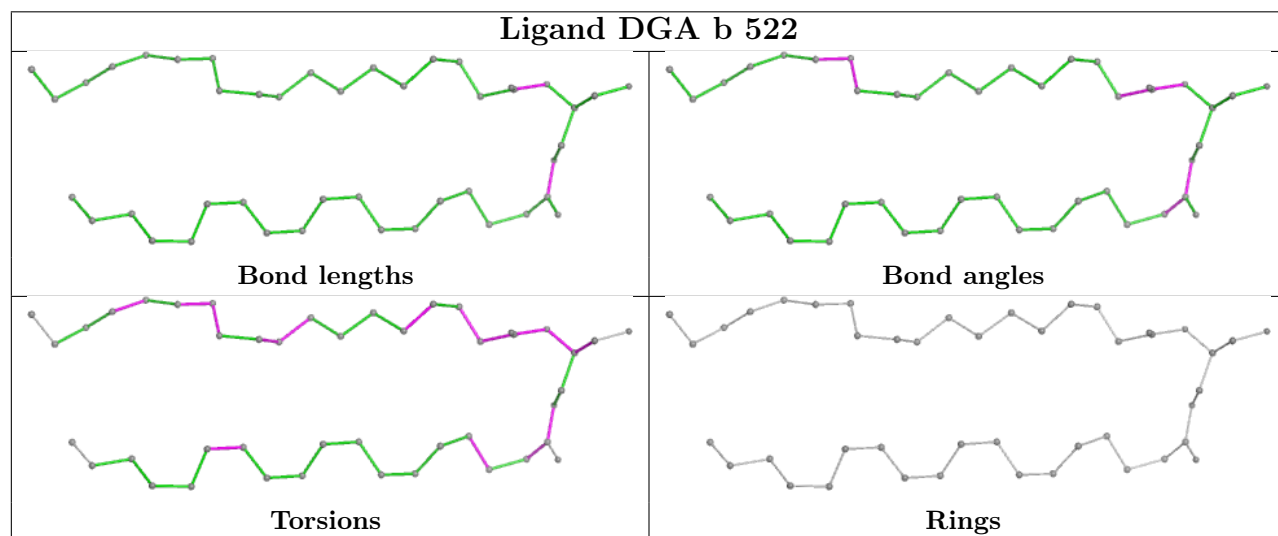
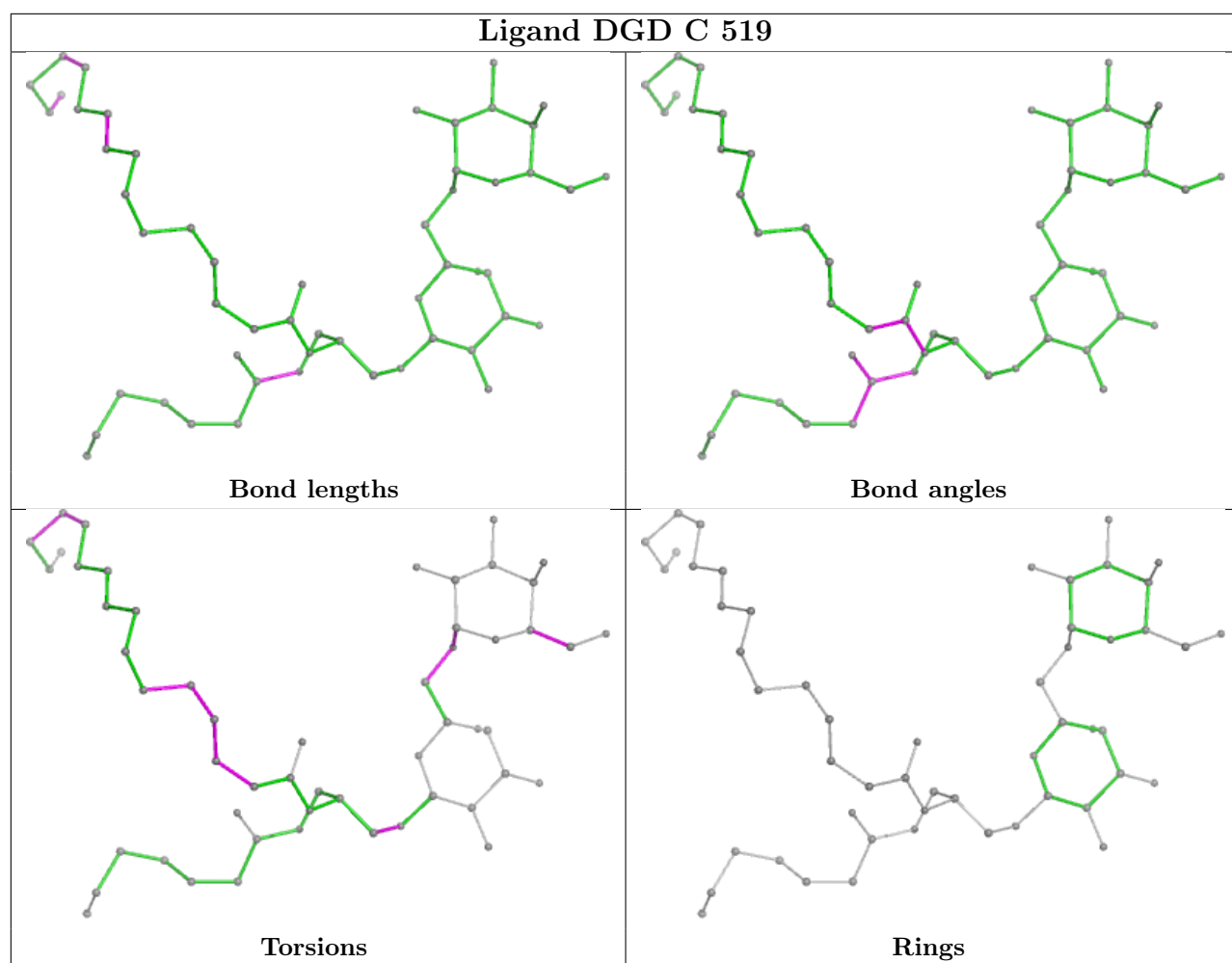
Ligand CLA c 507

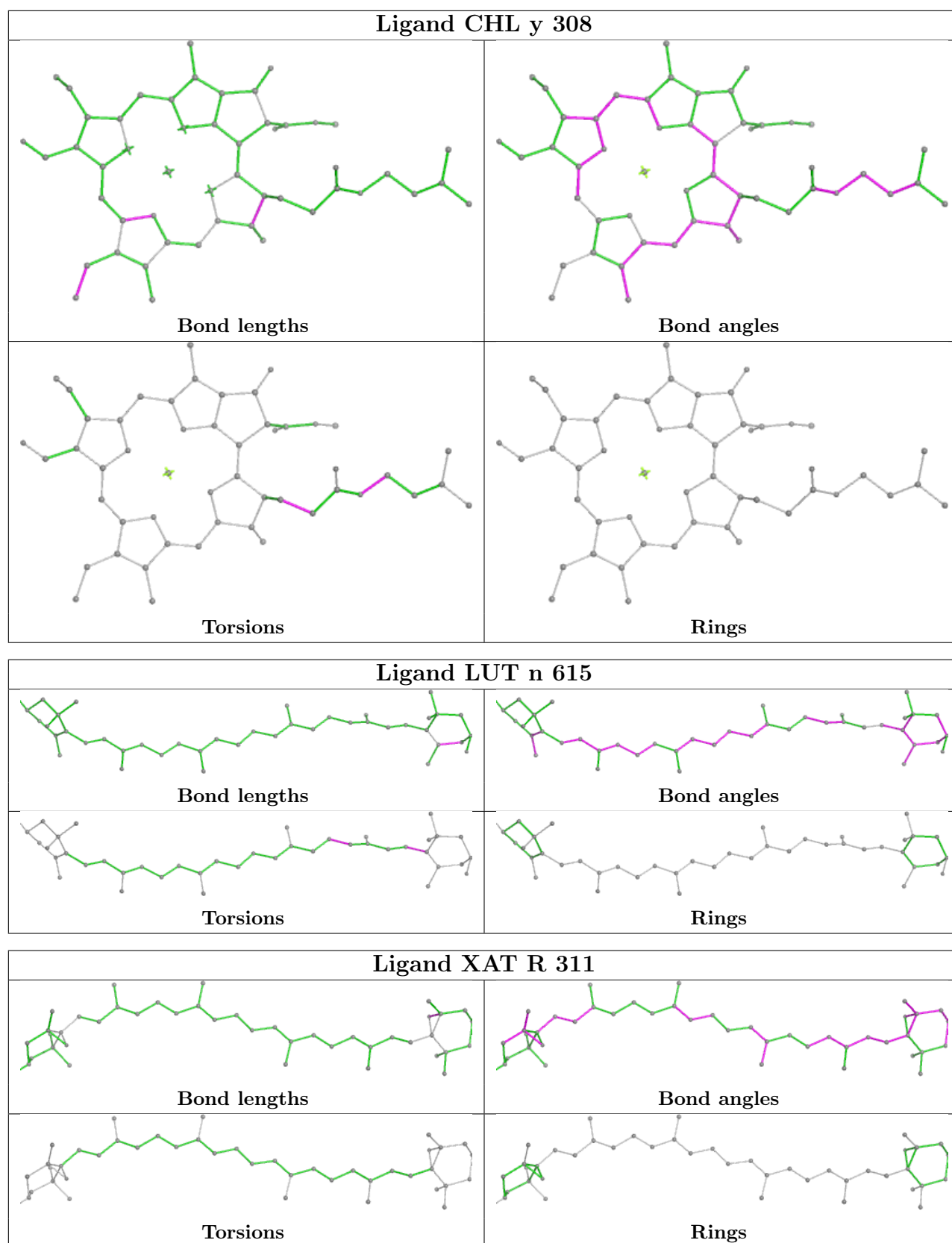




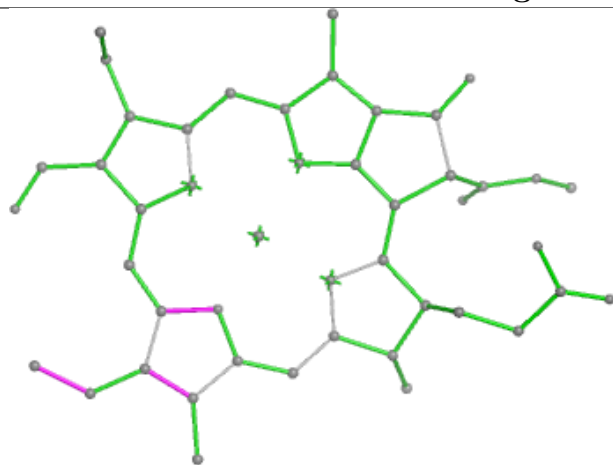




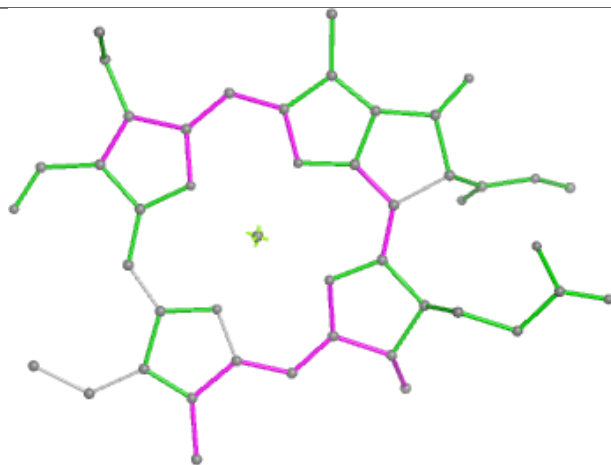




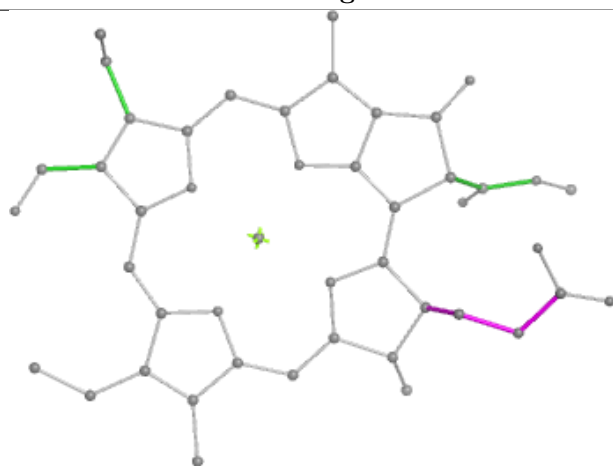
Ligand CHL Y 306



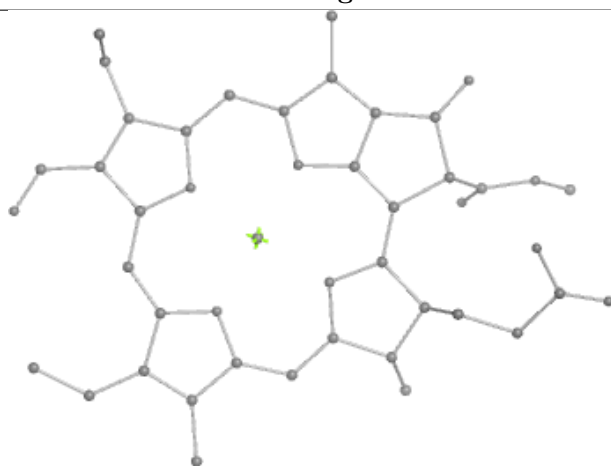
Bond lengths



Bond angles

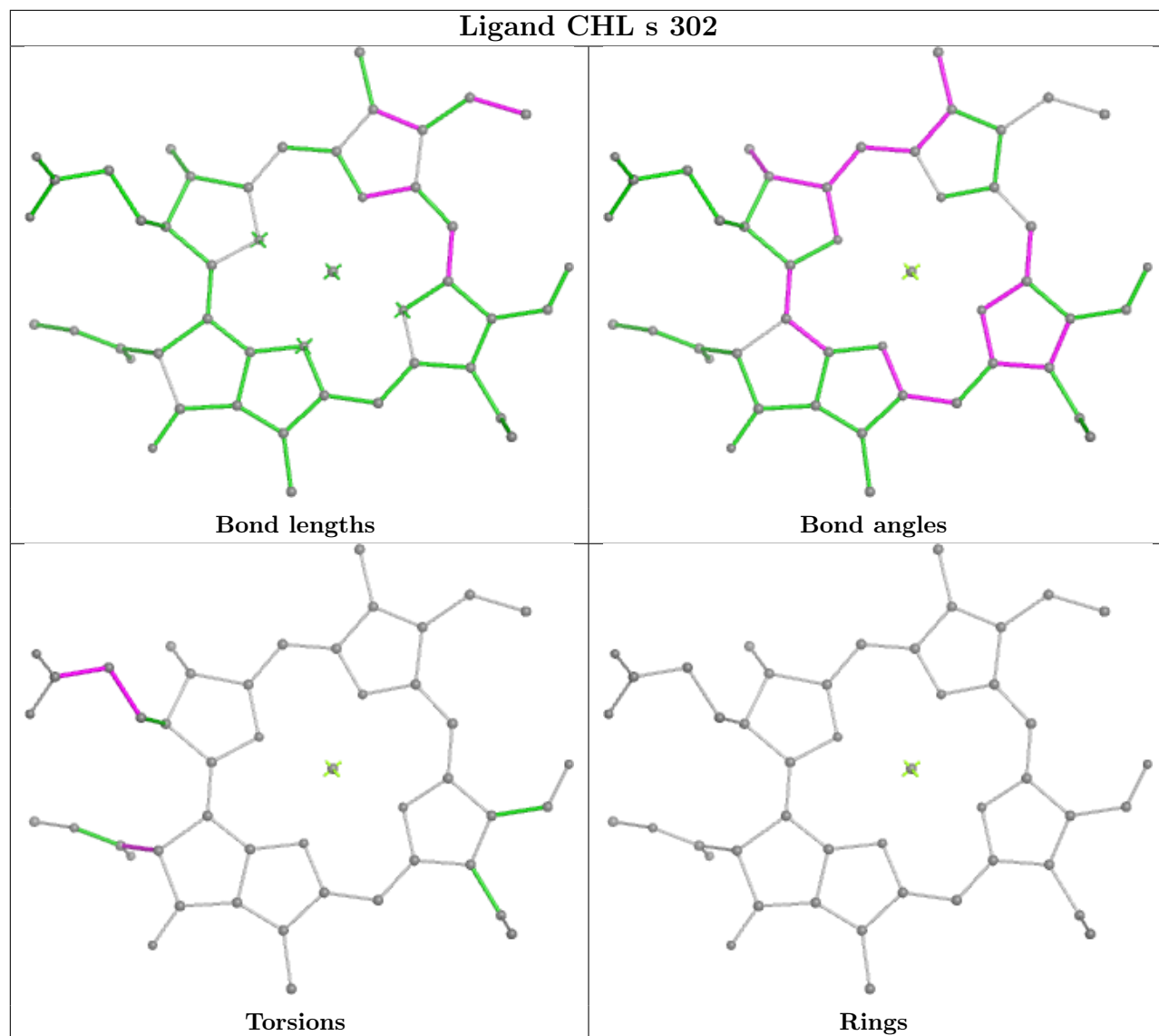


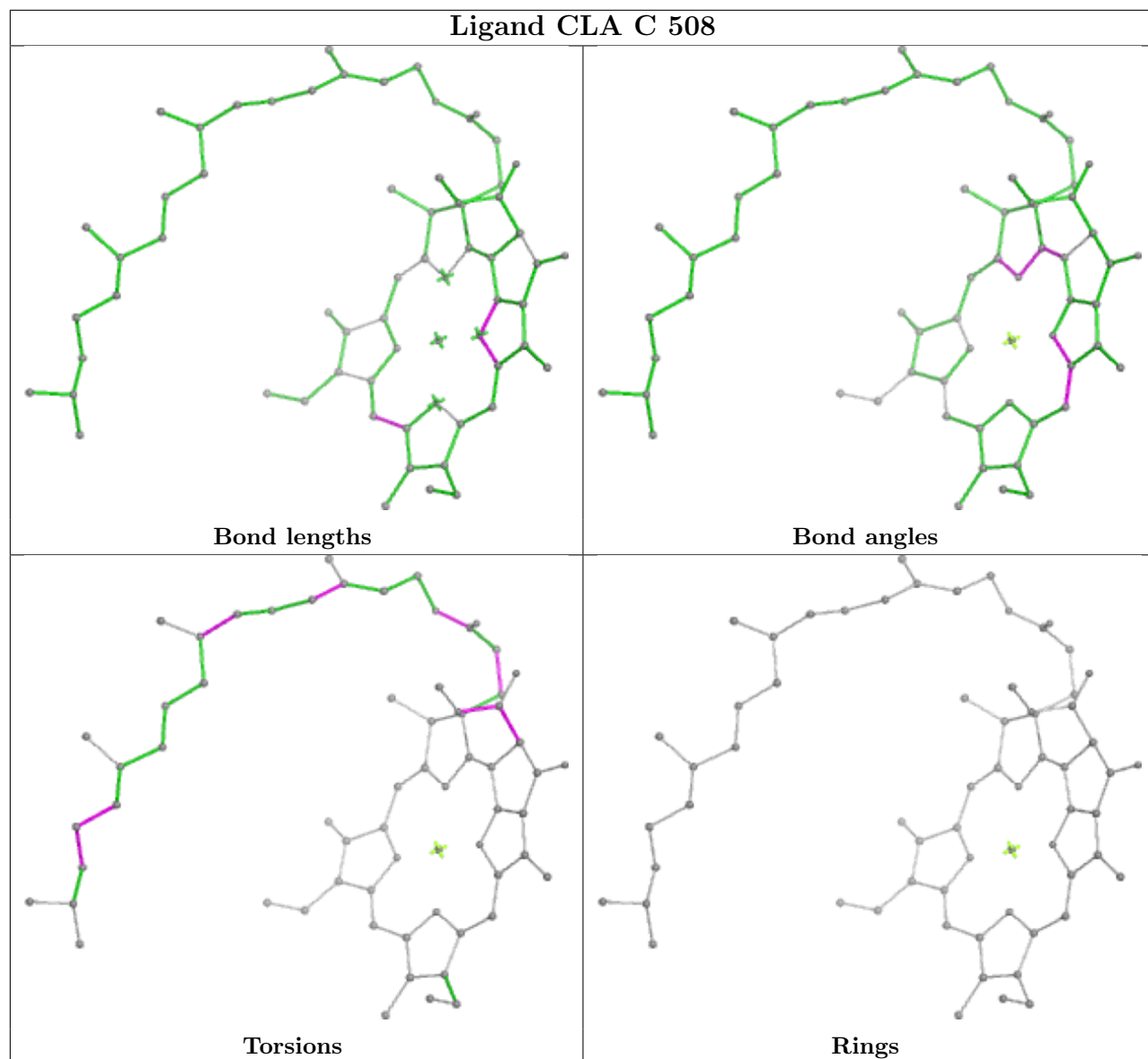
Torsions



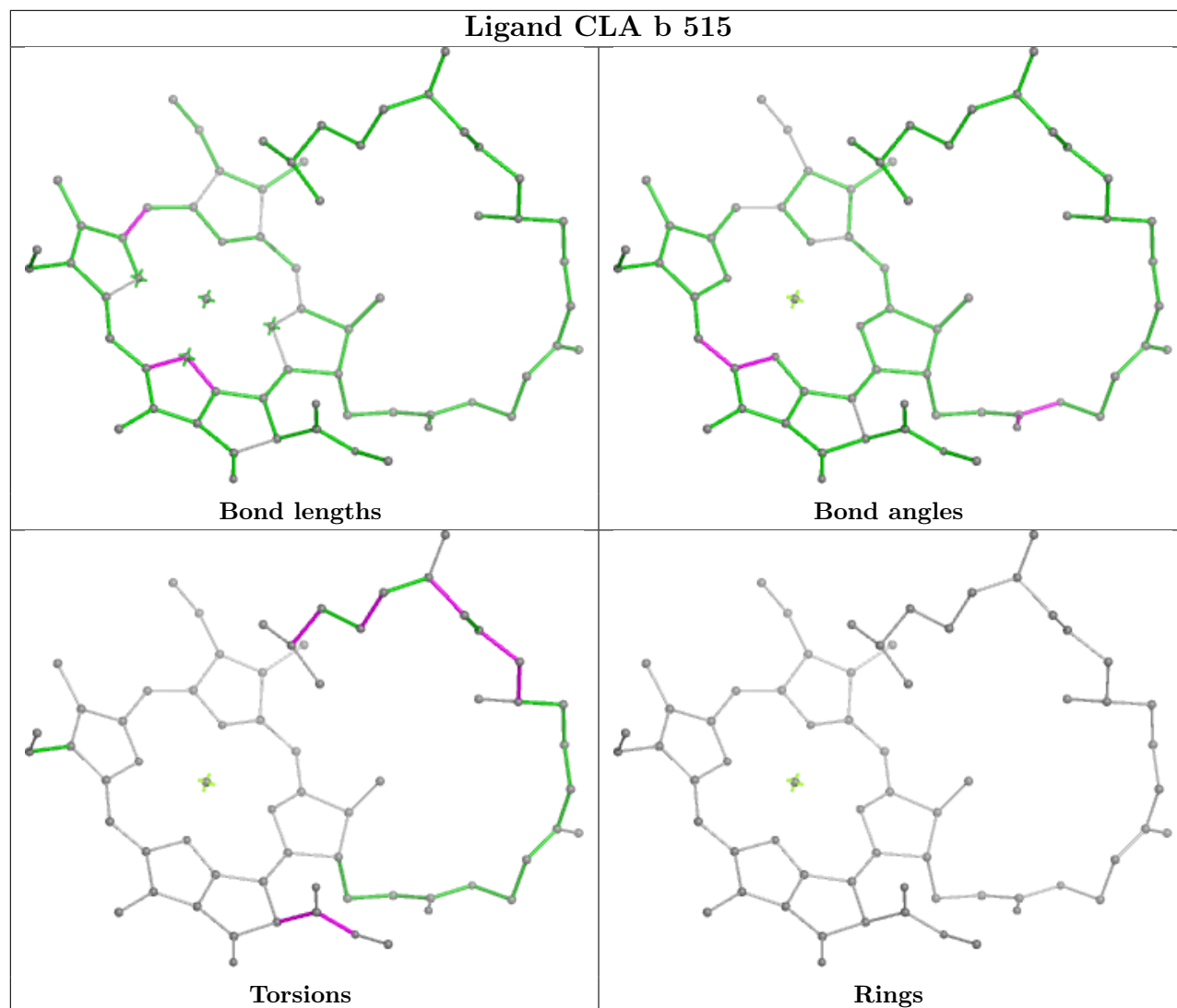
Rings

Ligand CHL s 302

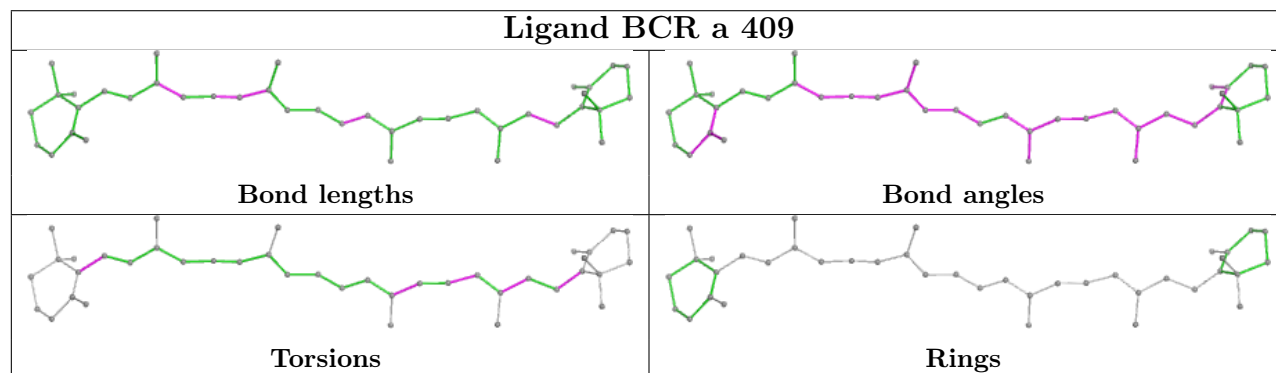


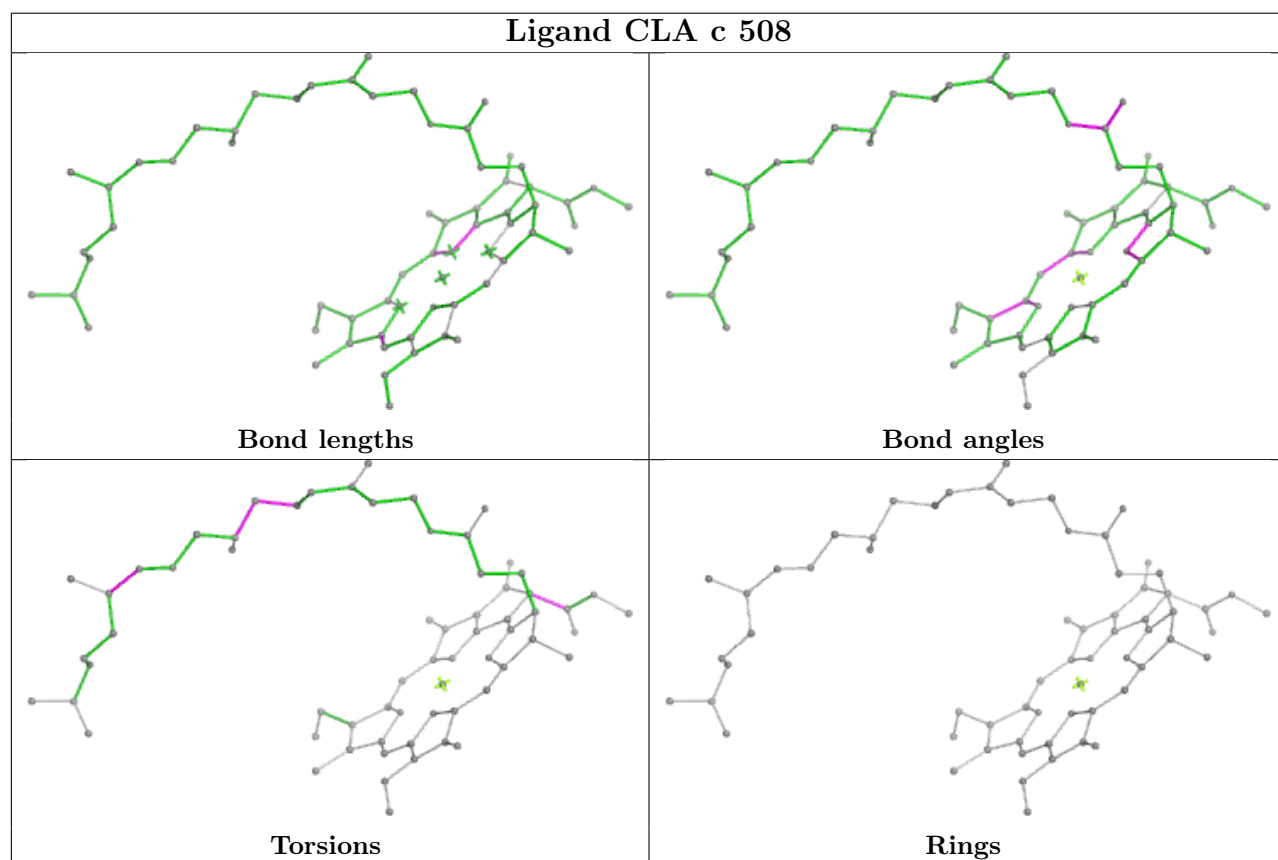
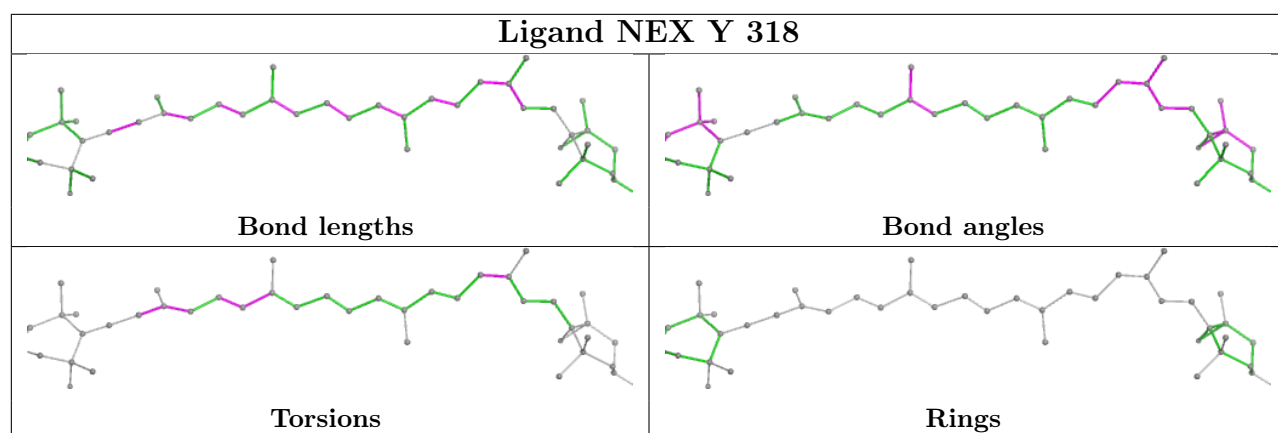


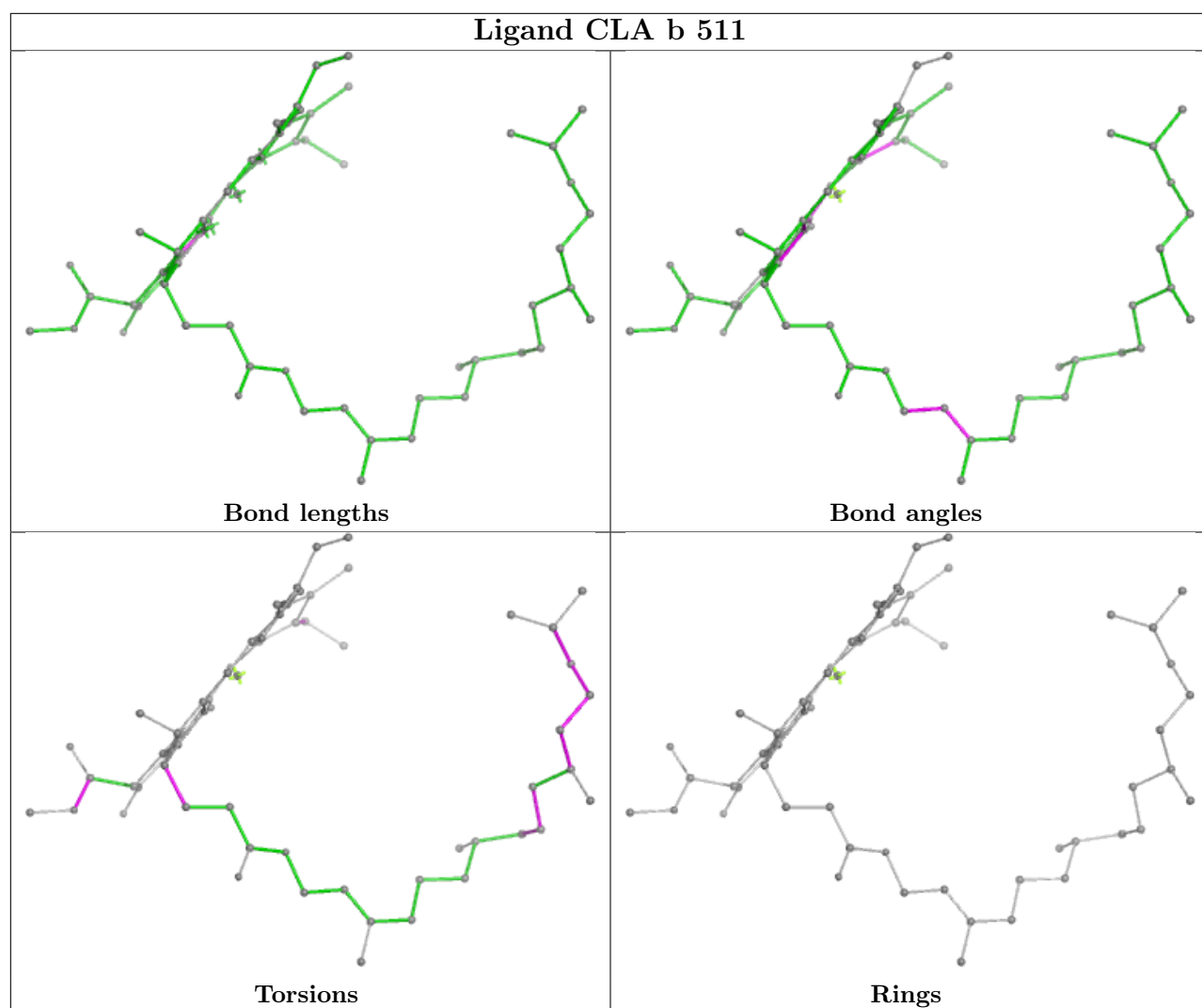
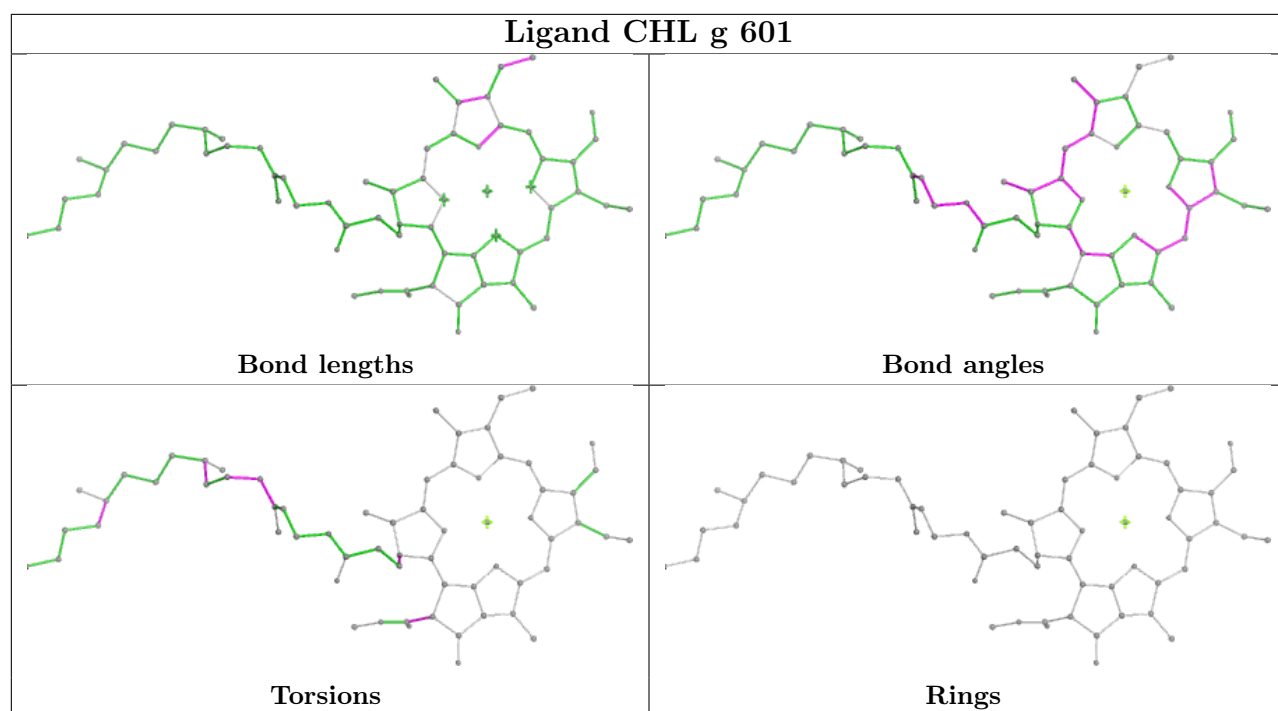
Ligand CLA b 515



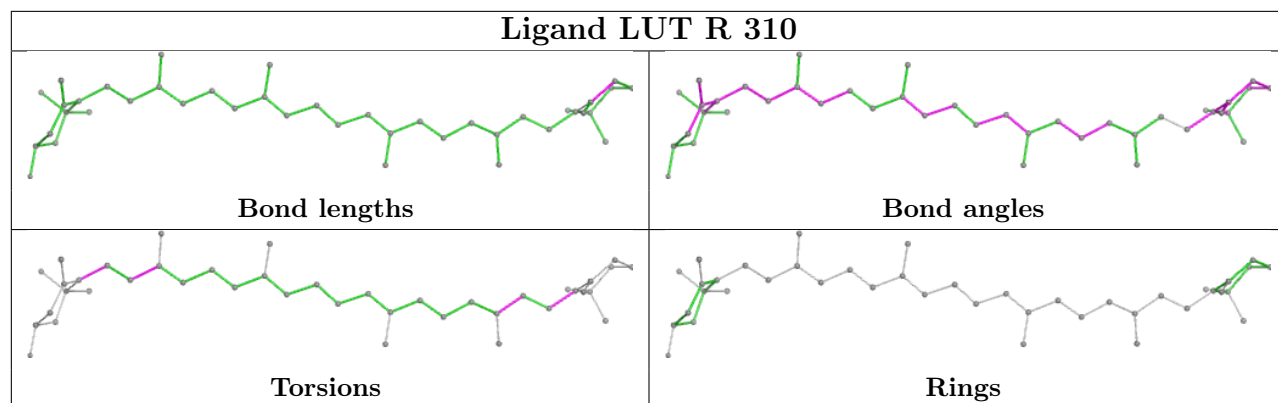
Ligand BCR a 409



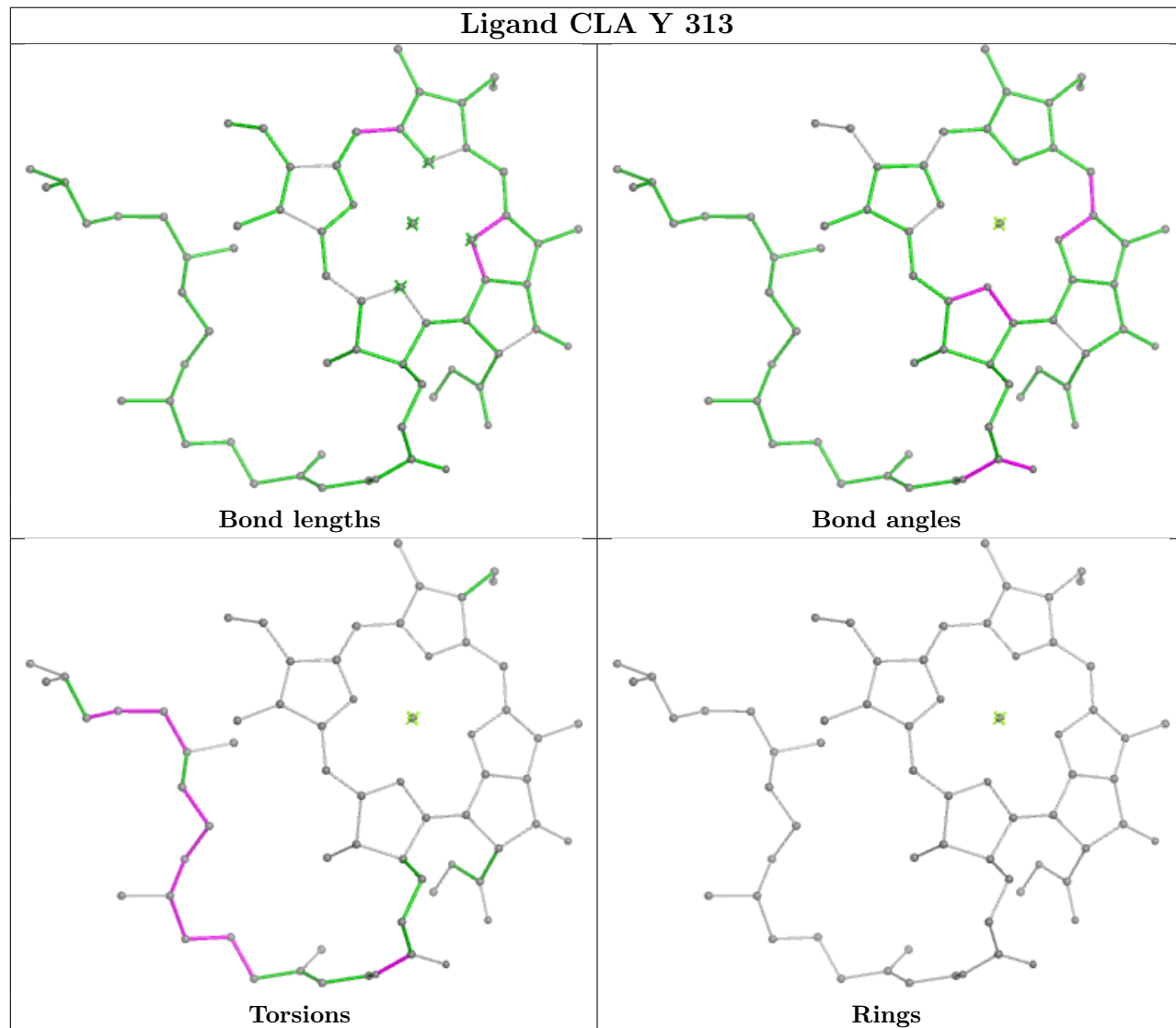


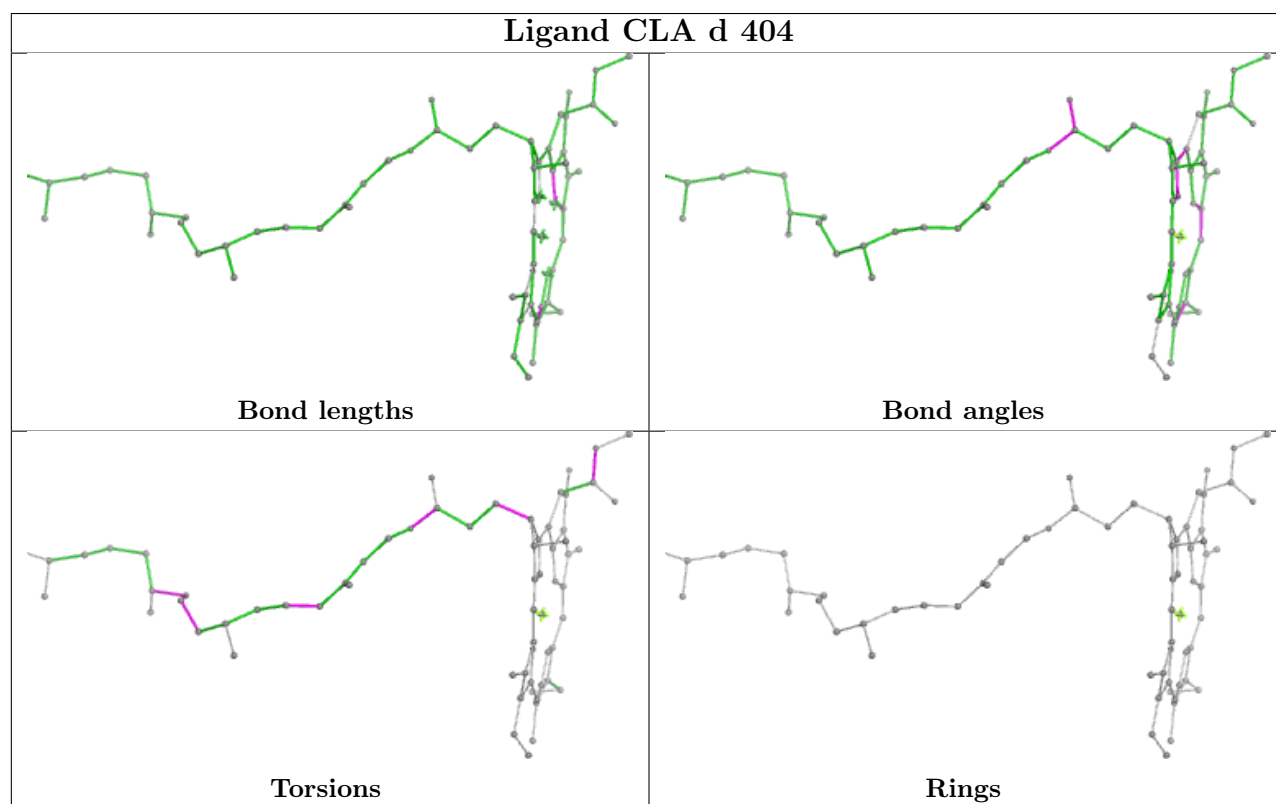
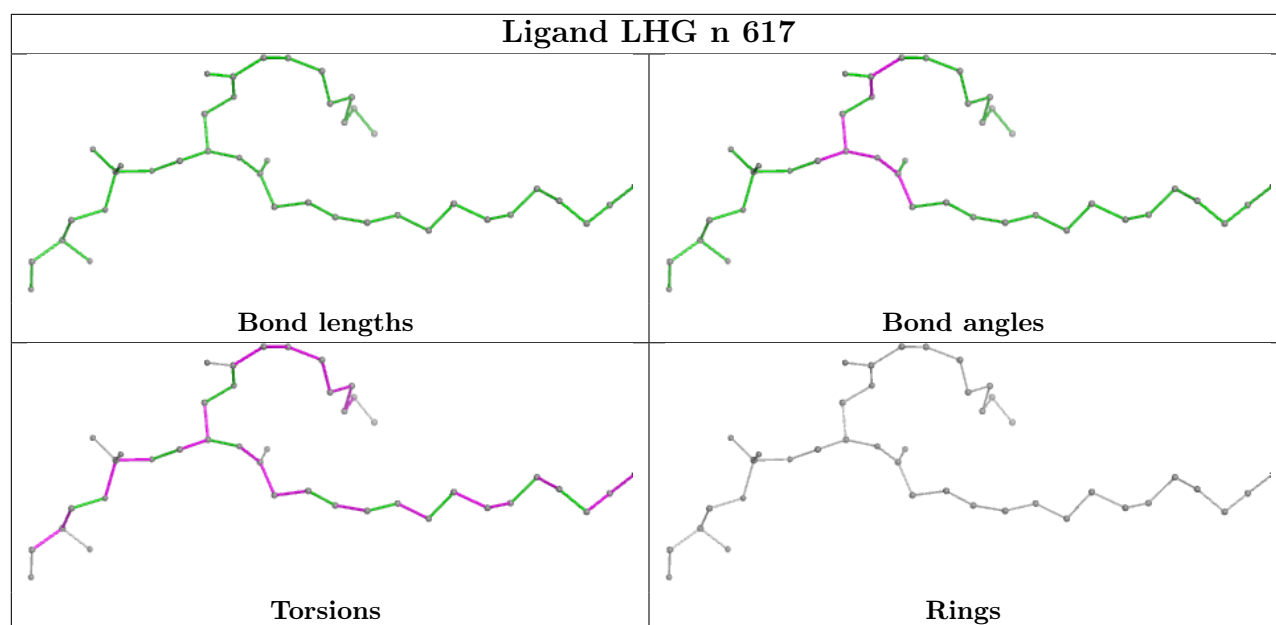


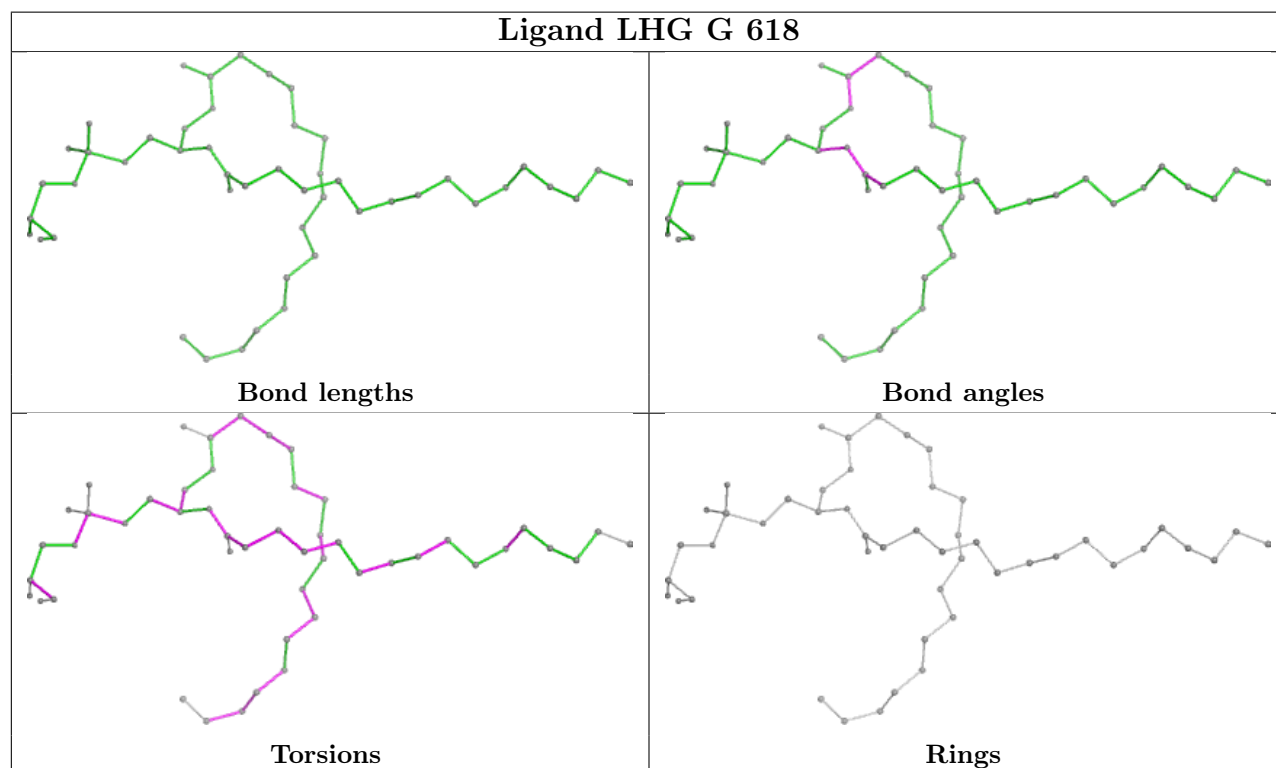
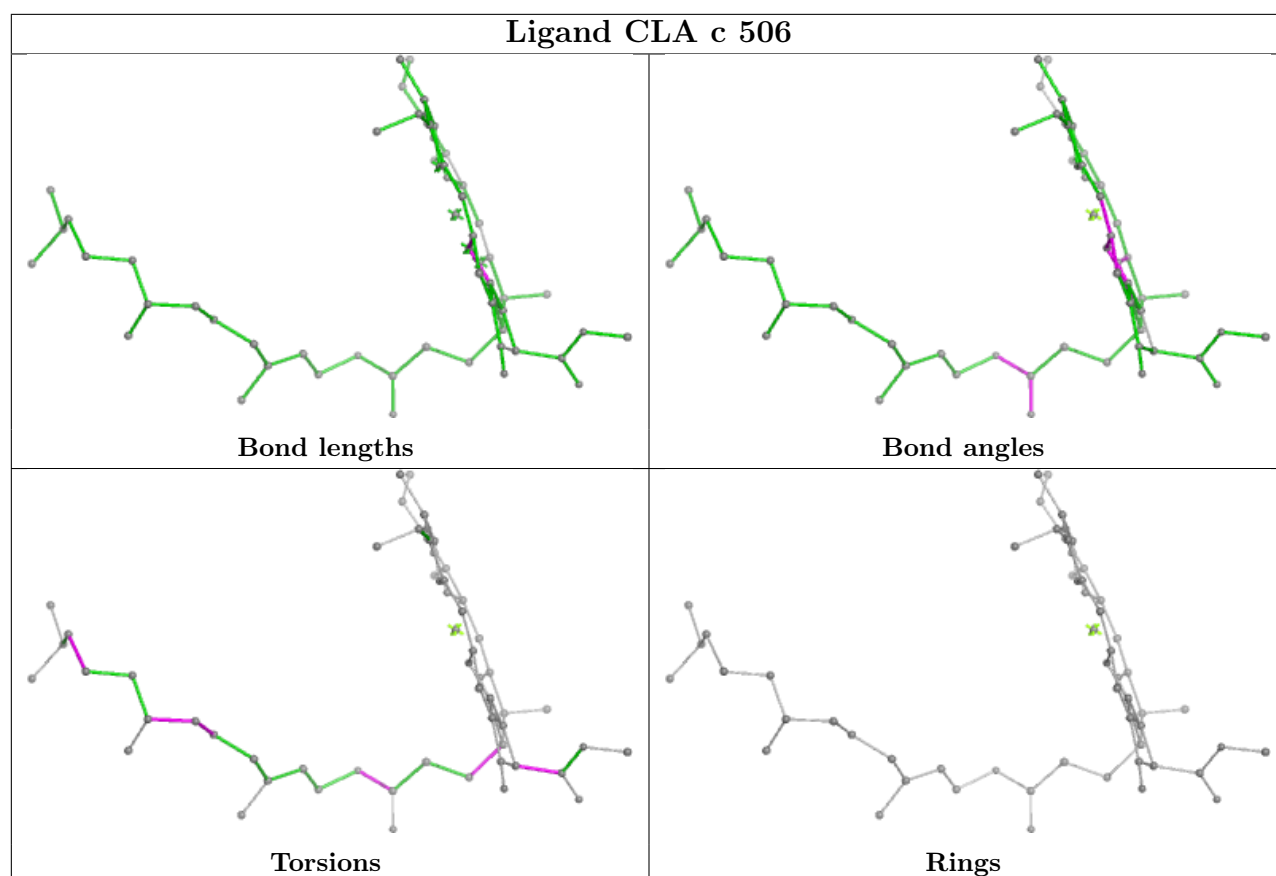
Ligand LUT R 310



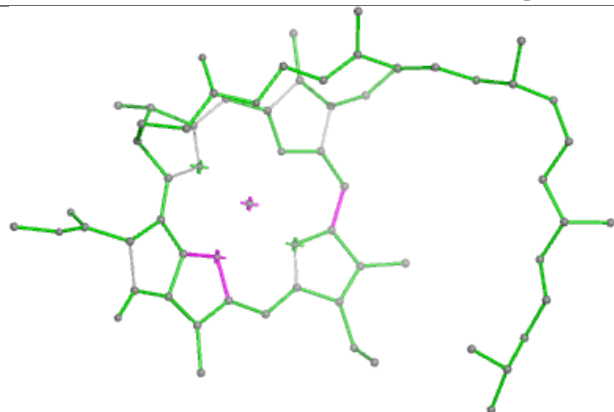
Ligand CLA Y 313



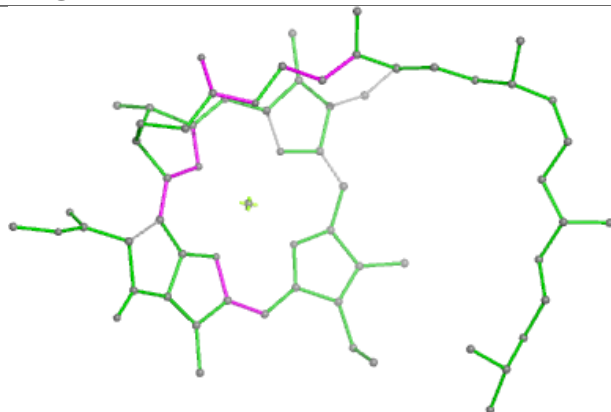




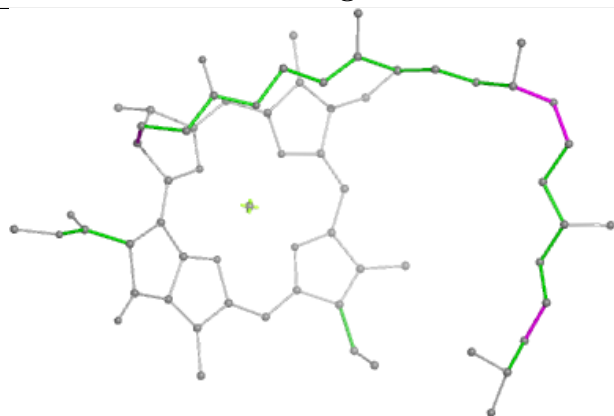
Ligand CLA g 610



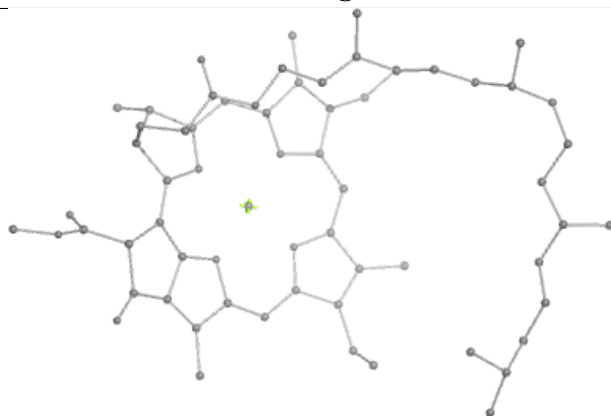
Bond lengths



Bond angles

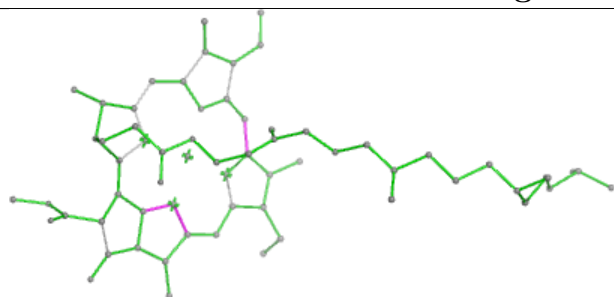


Torsions

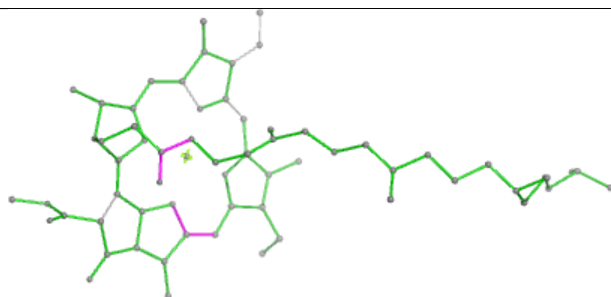


Rings

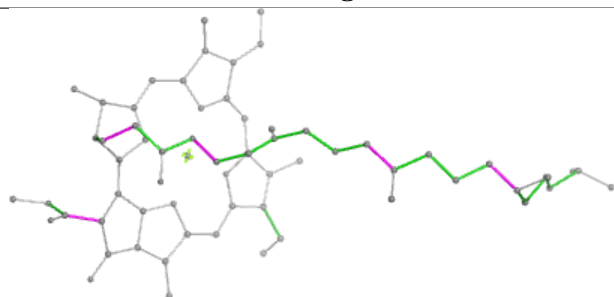
Ligand CLA B 508



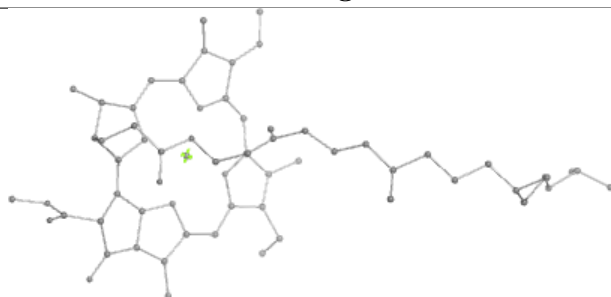
Bond lengths



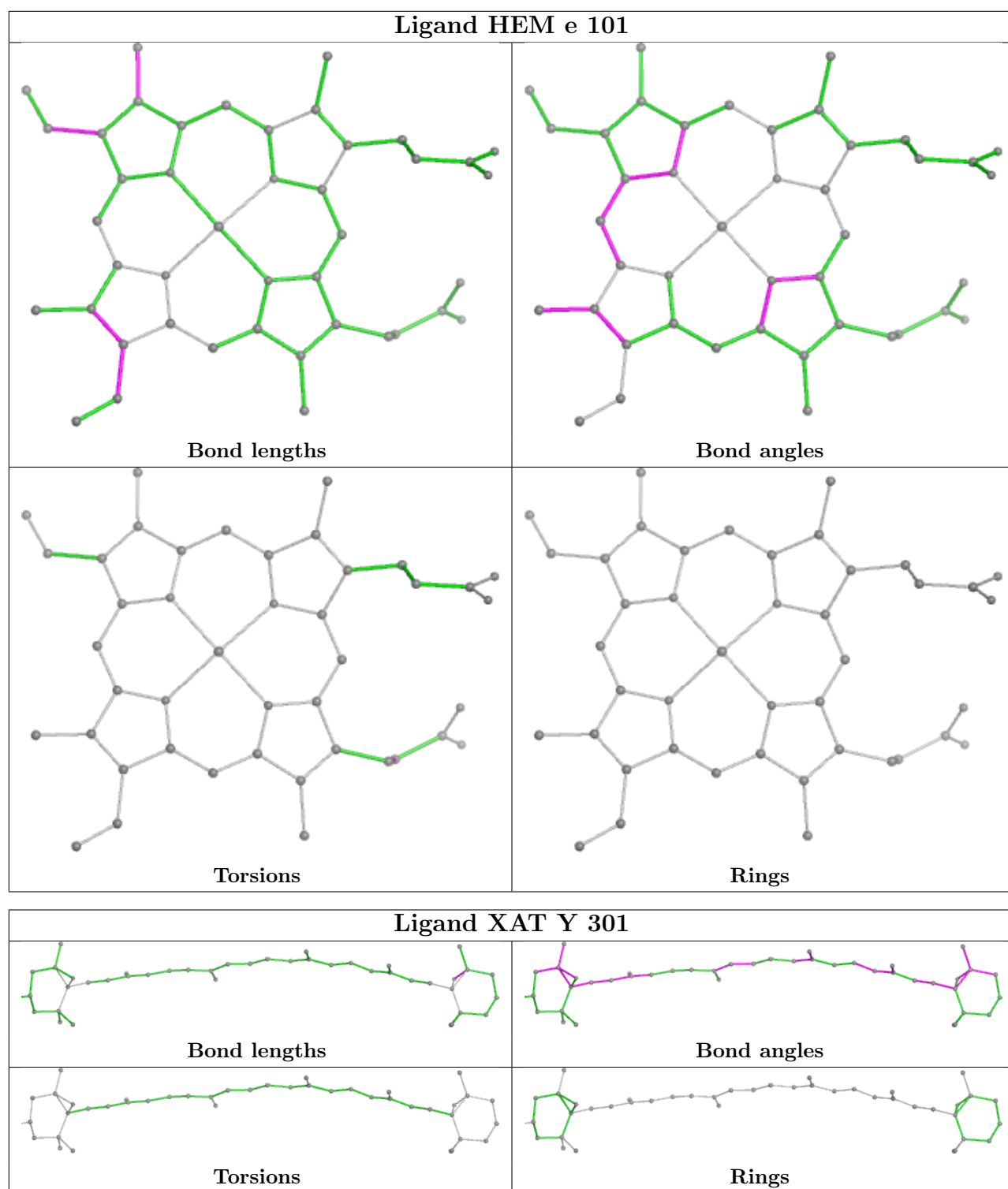
Bond angles



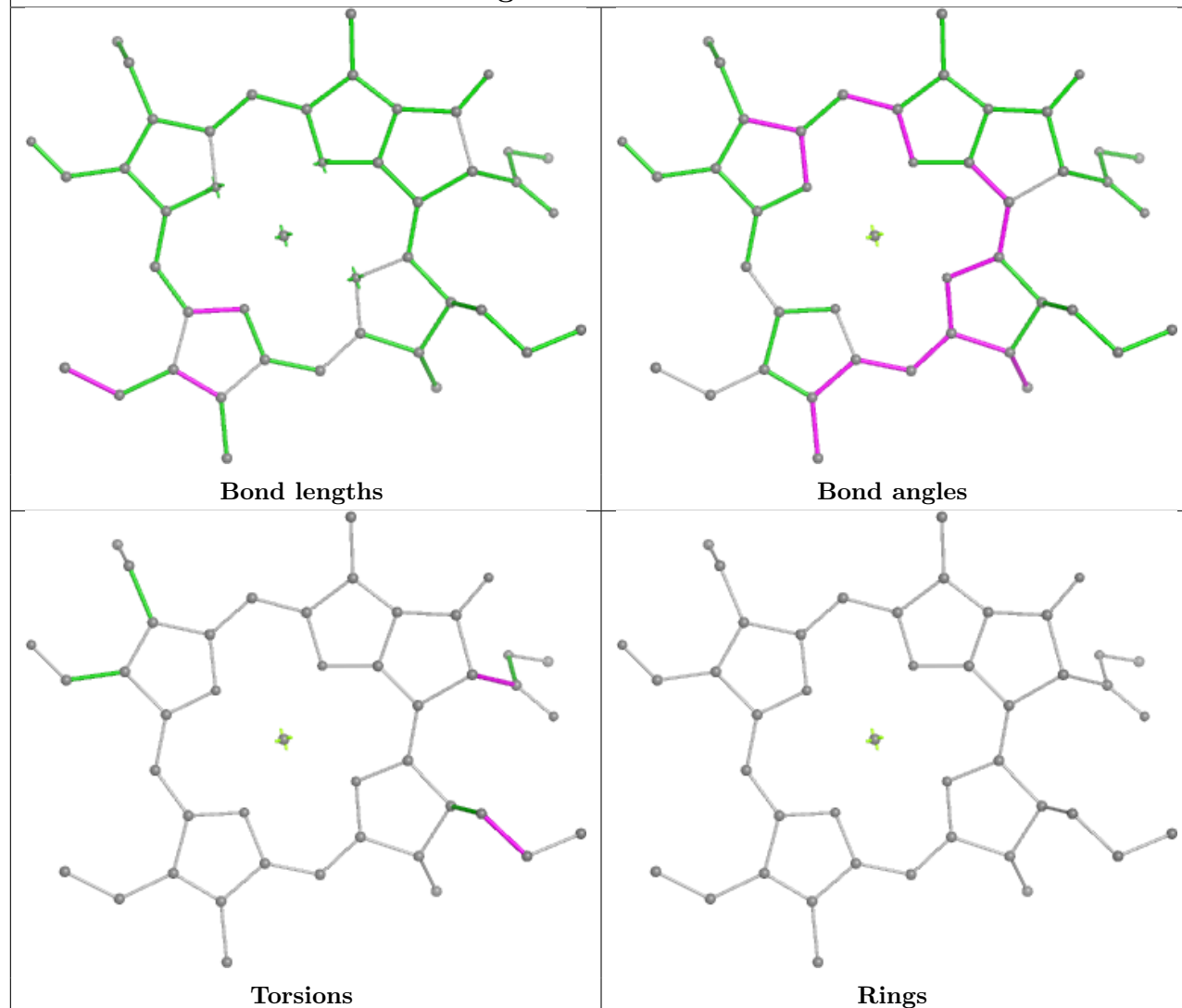
Torsions



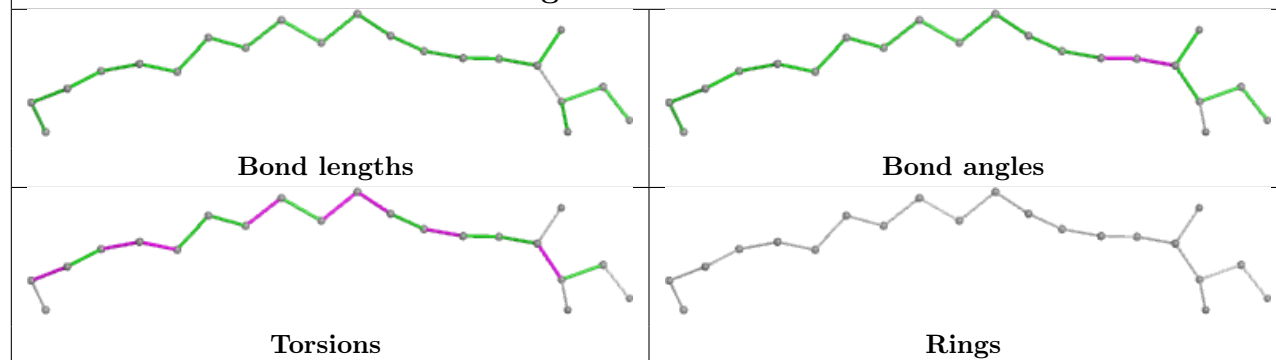
Rings

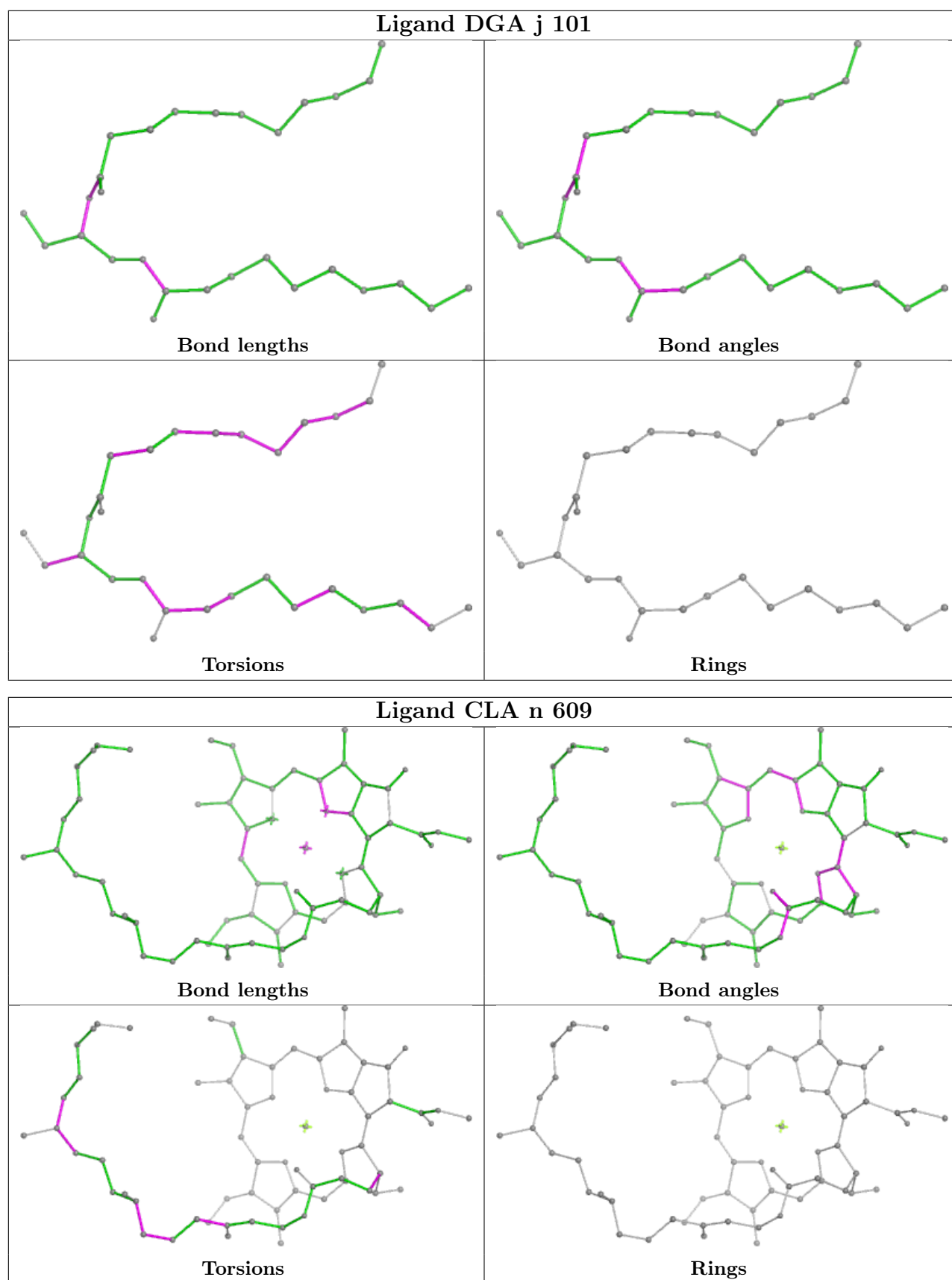


Ligand CHL r 305

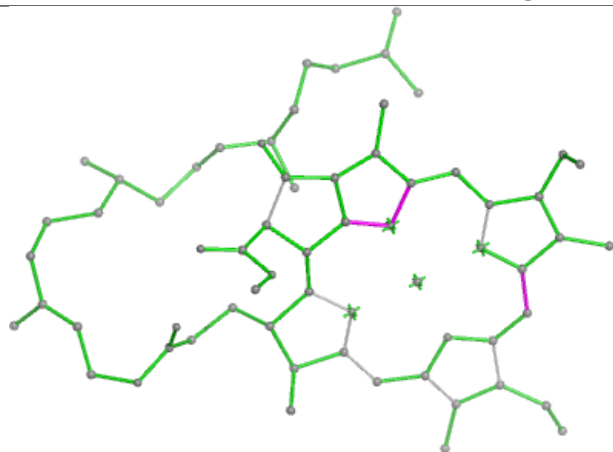


Ligand SPH i 102

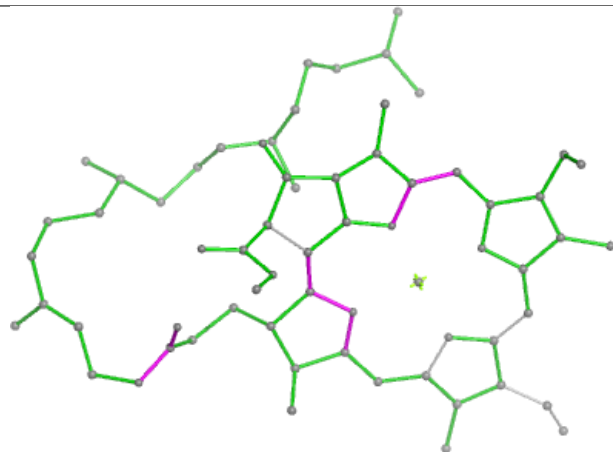




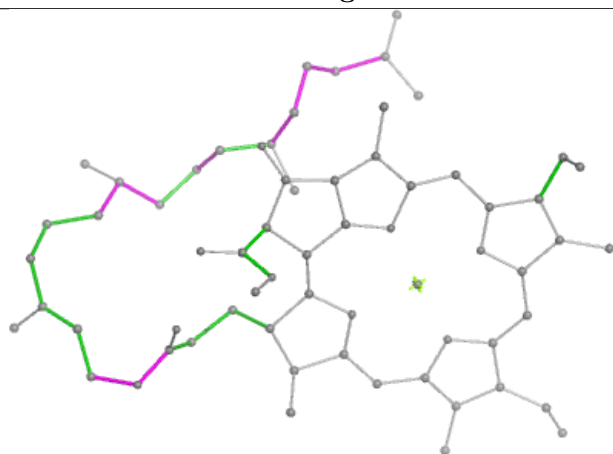
Ligand CLA c 509



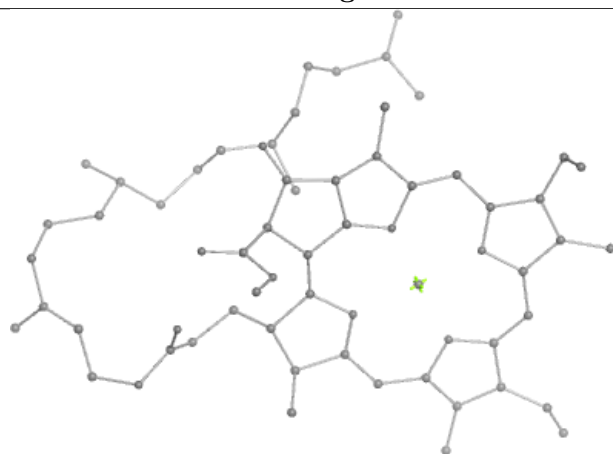
Bond lengths



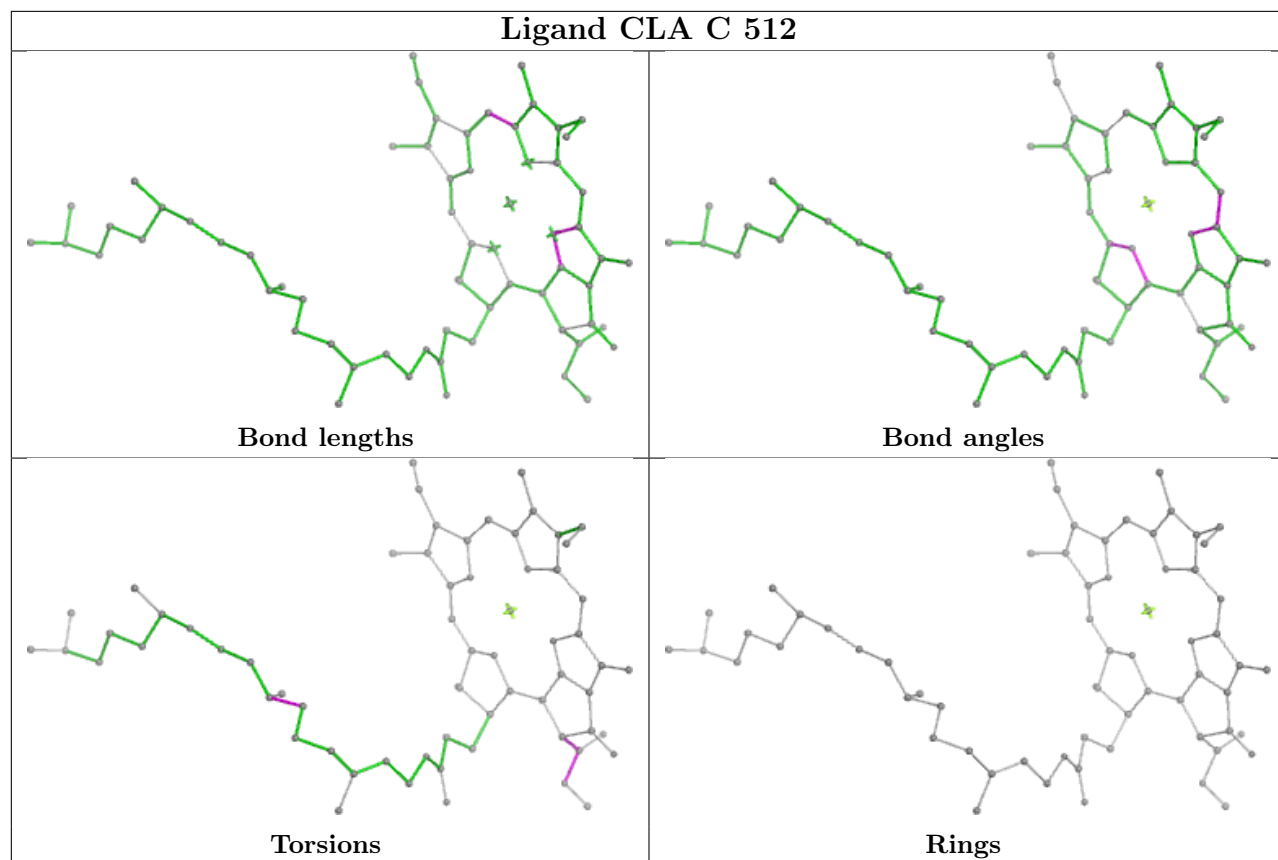
Bond angles



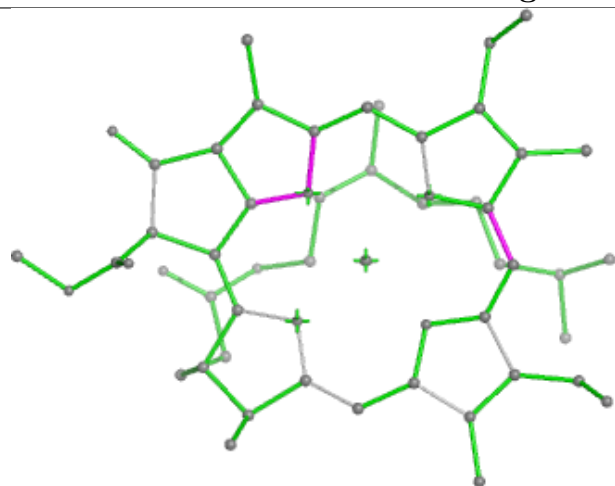
Torsions



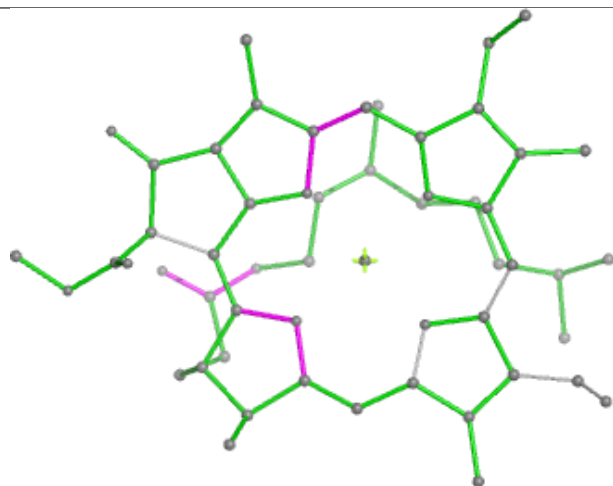
Rings



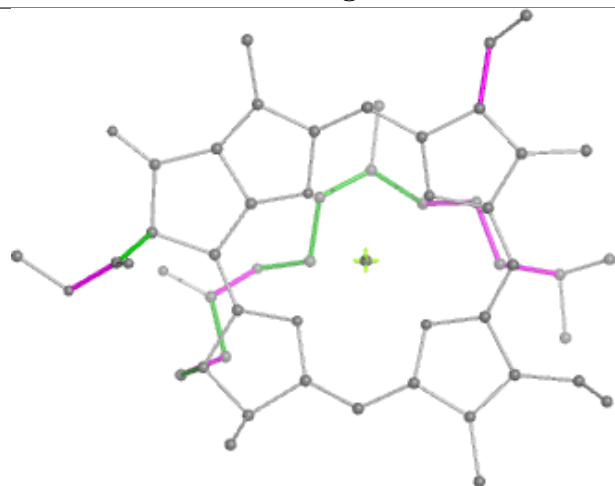
Ligand CLA S 314



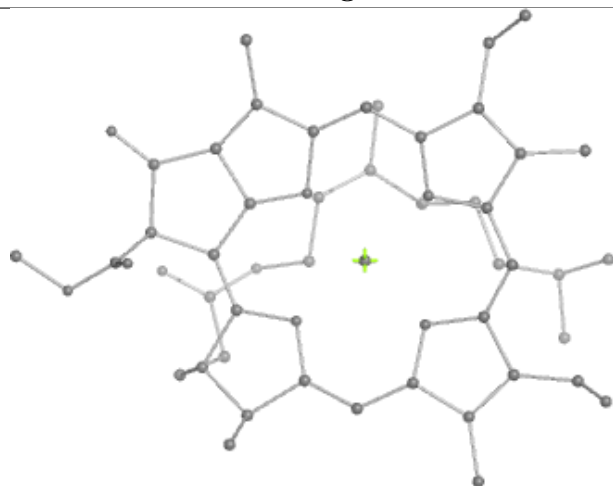
Bond lengths



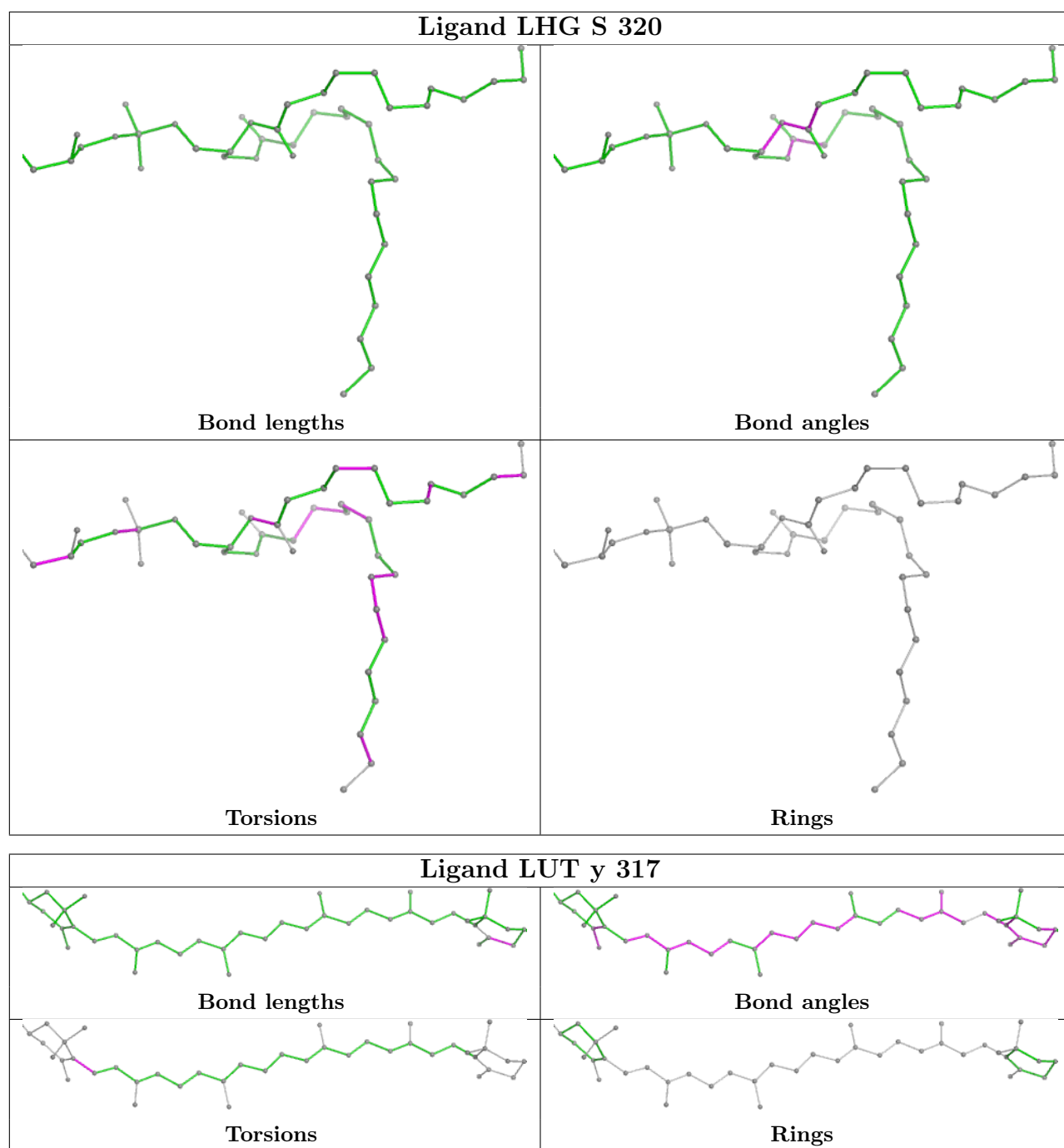
Bond angles



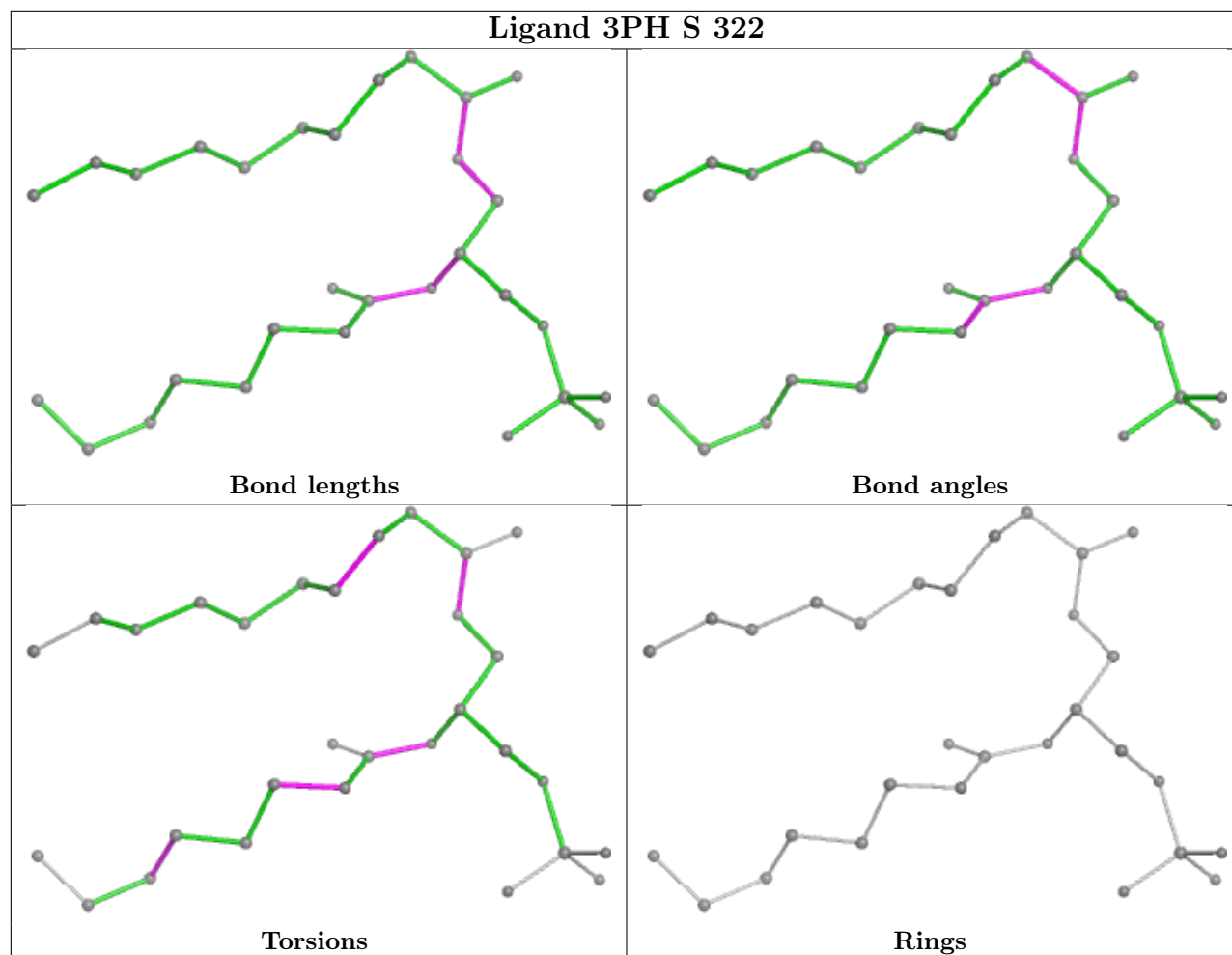
Torsions



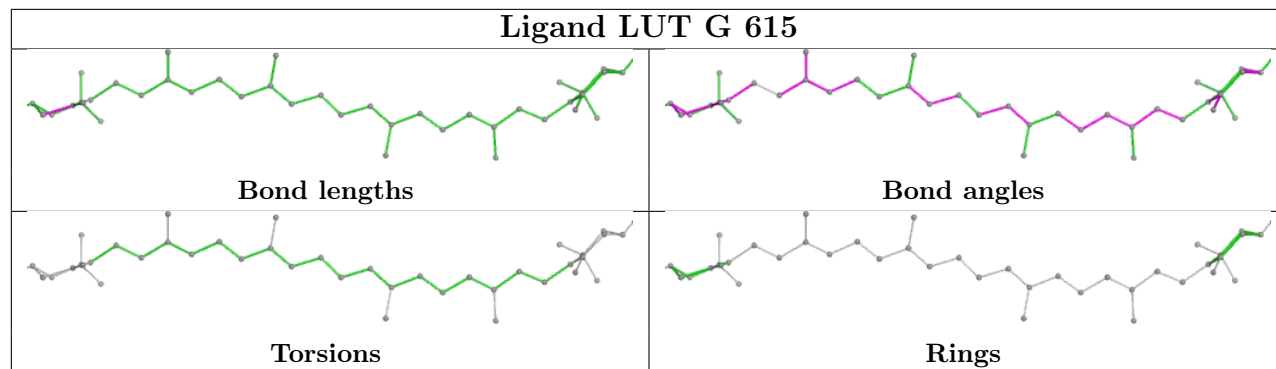
Rings

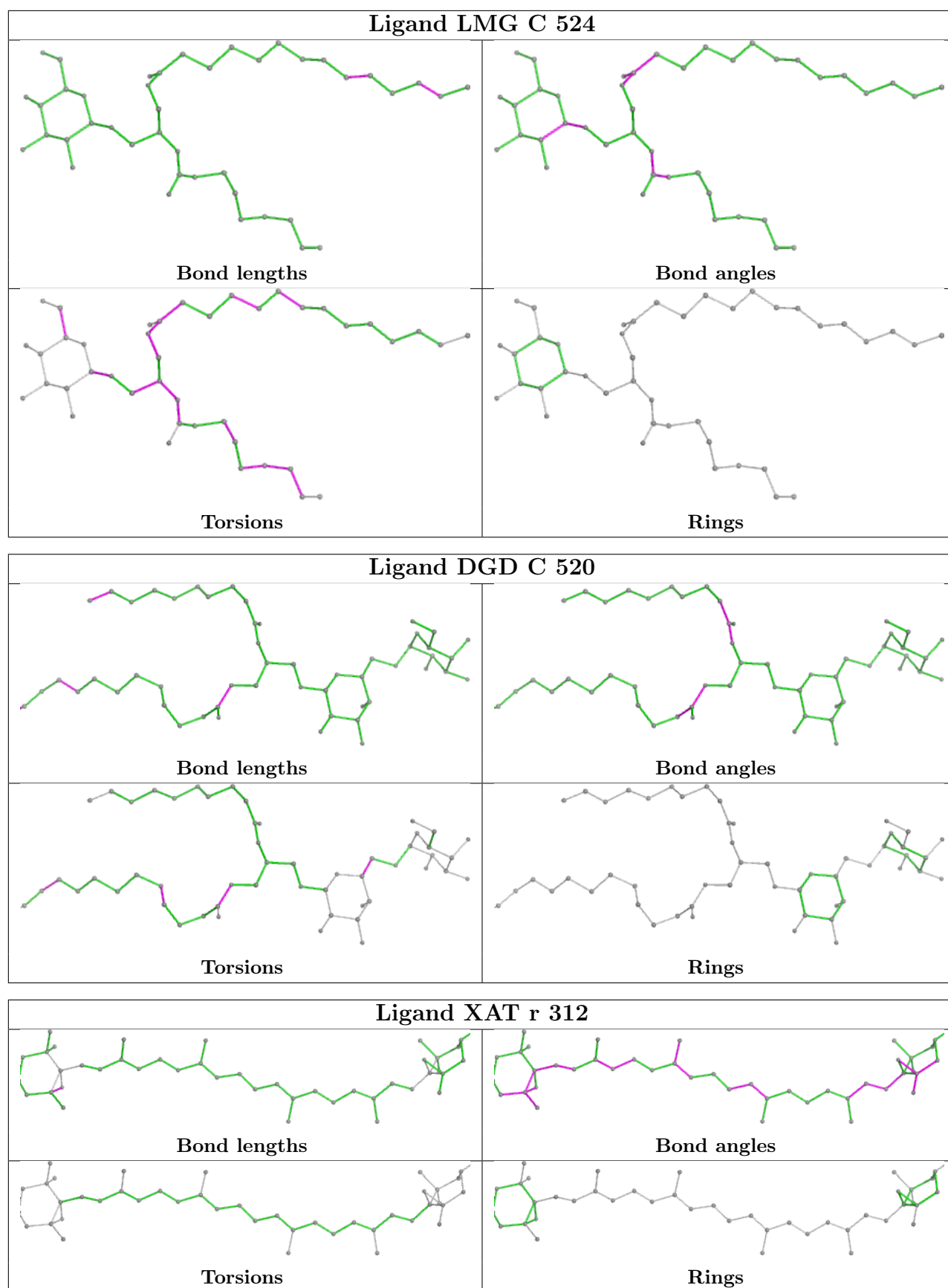


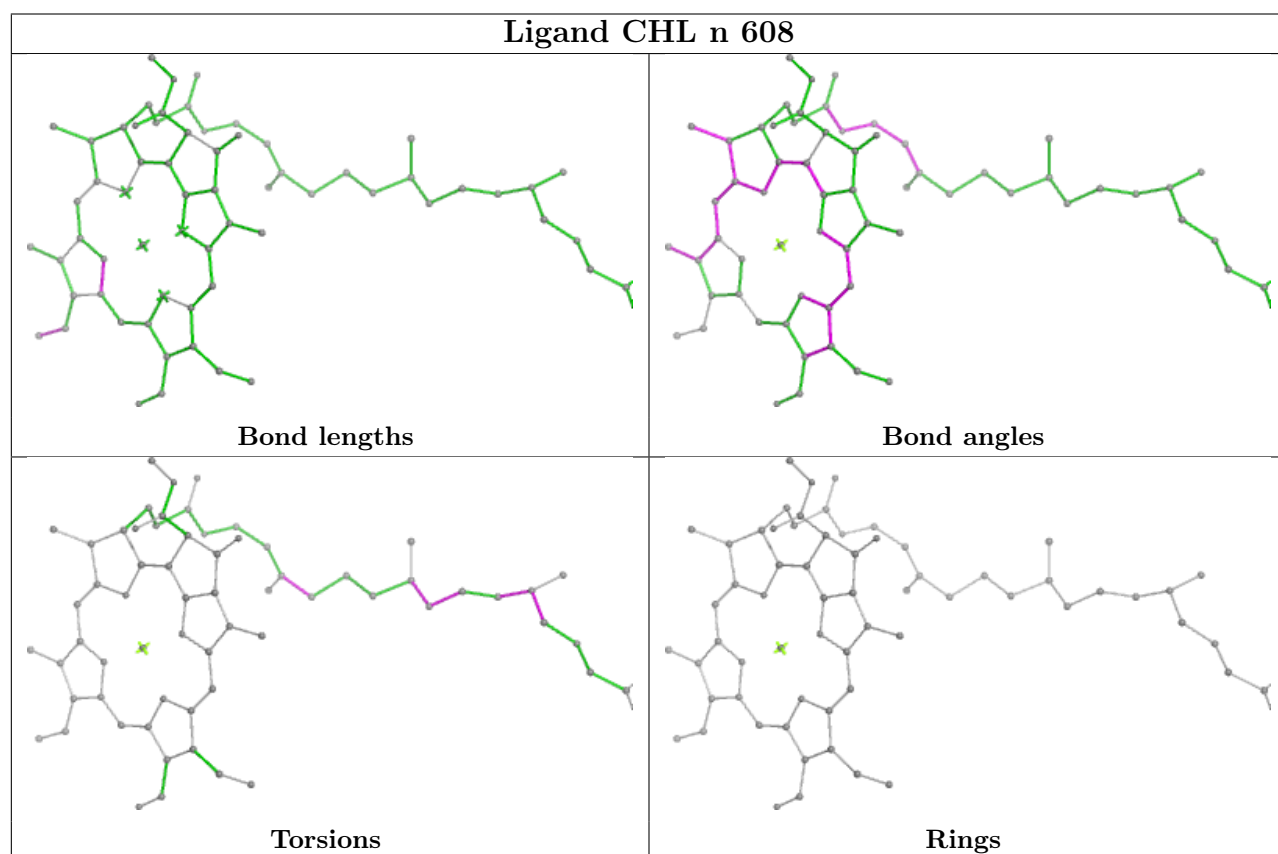
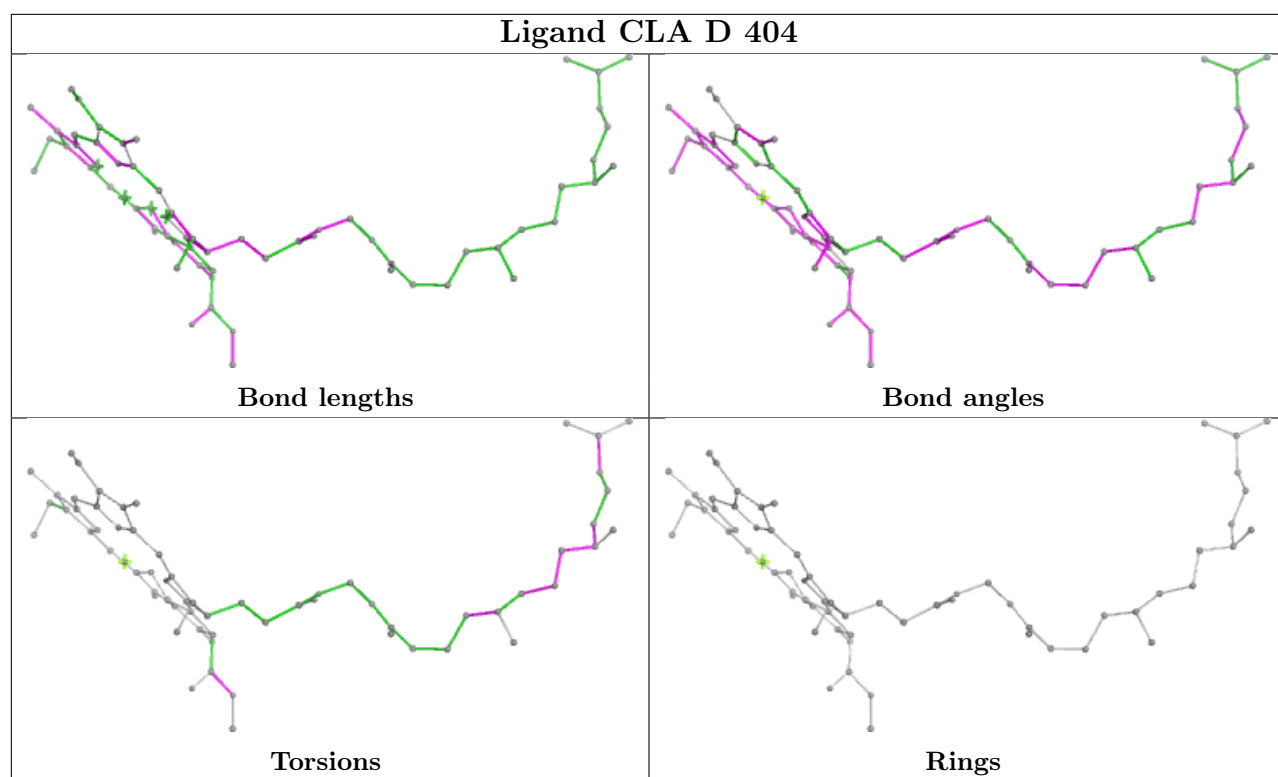
Ligand 3PH S 322



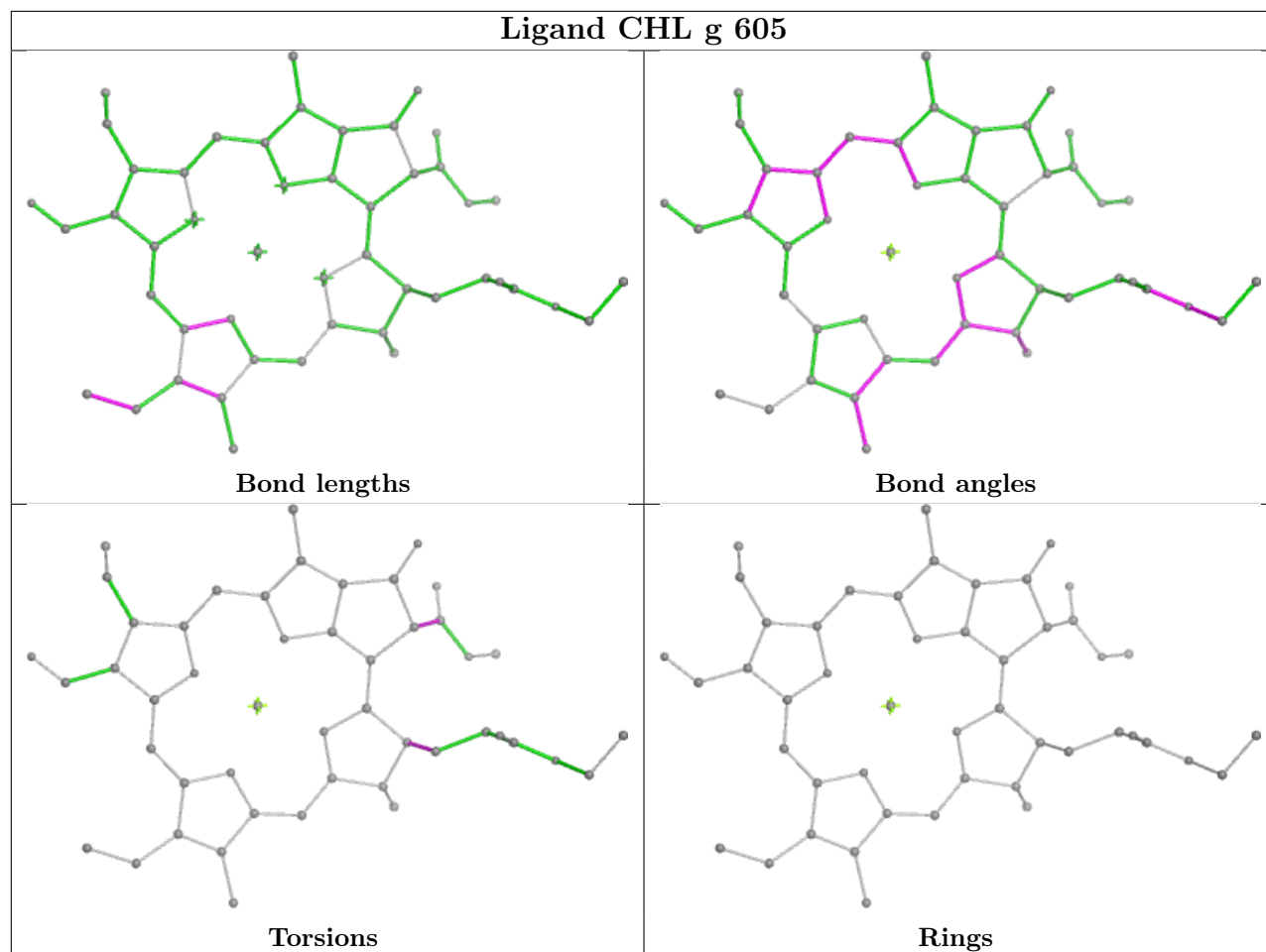
Ligand LUT G 615



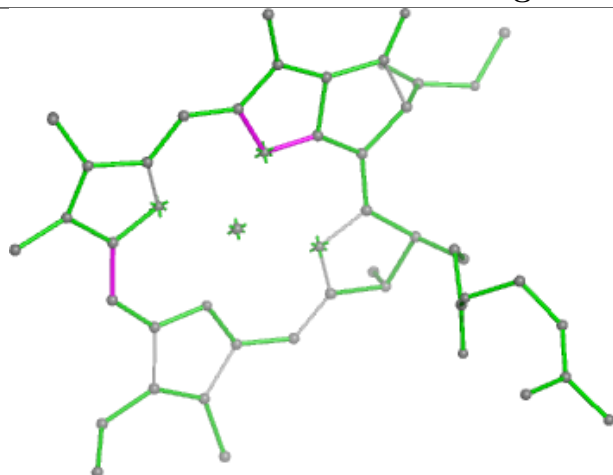




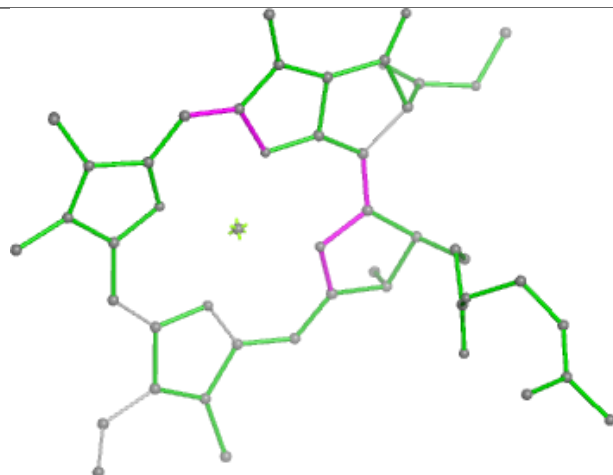
Ligand CHL g 605



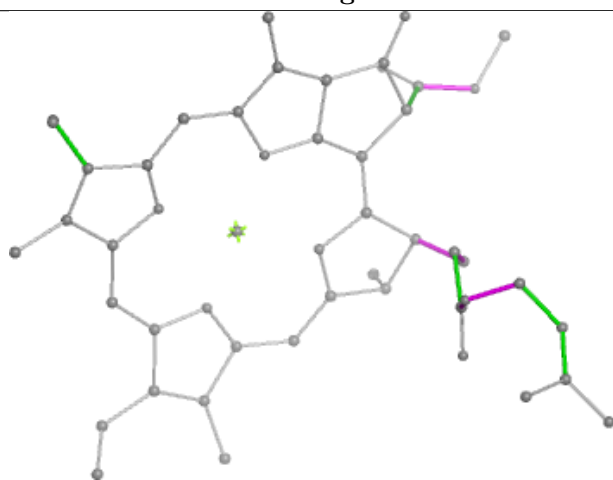
Ligand CLA Y 309



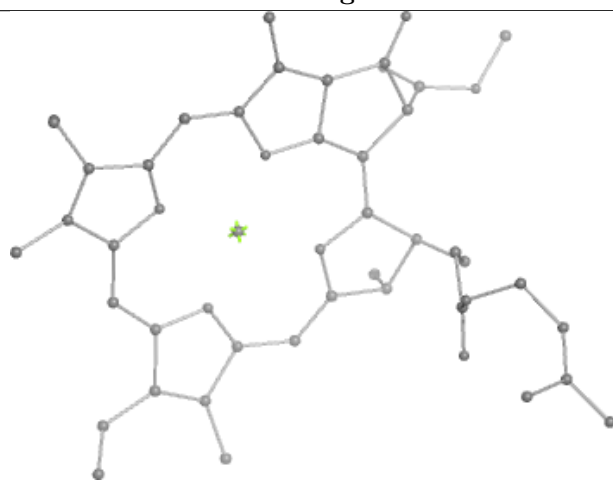
Bond lengths



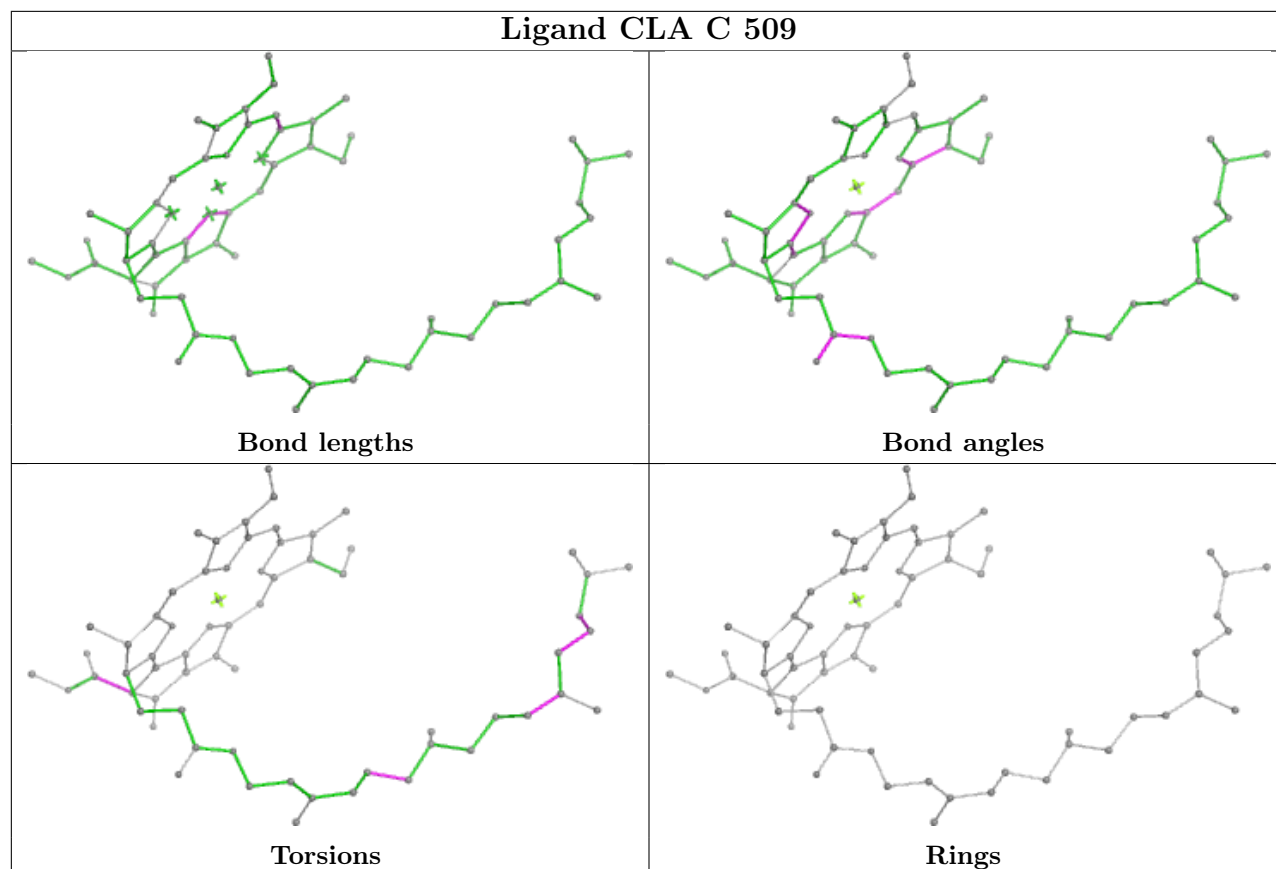
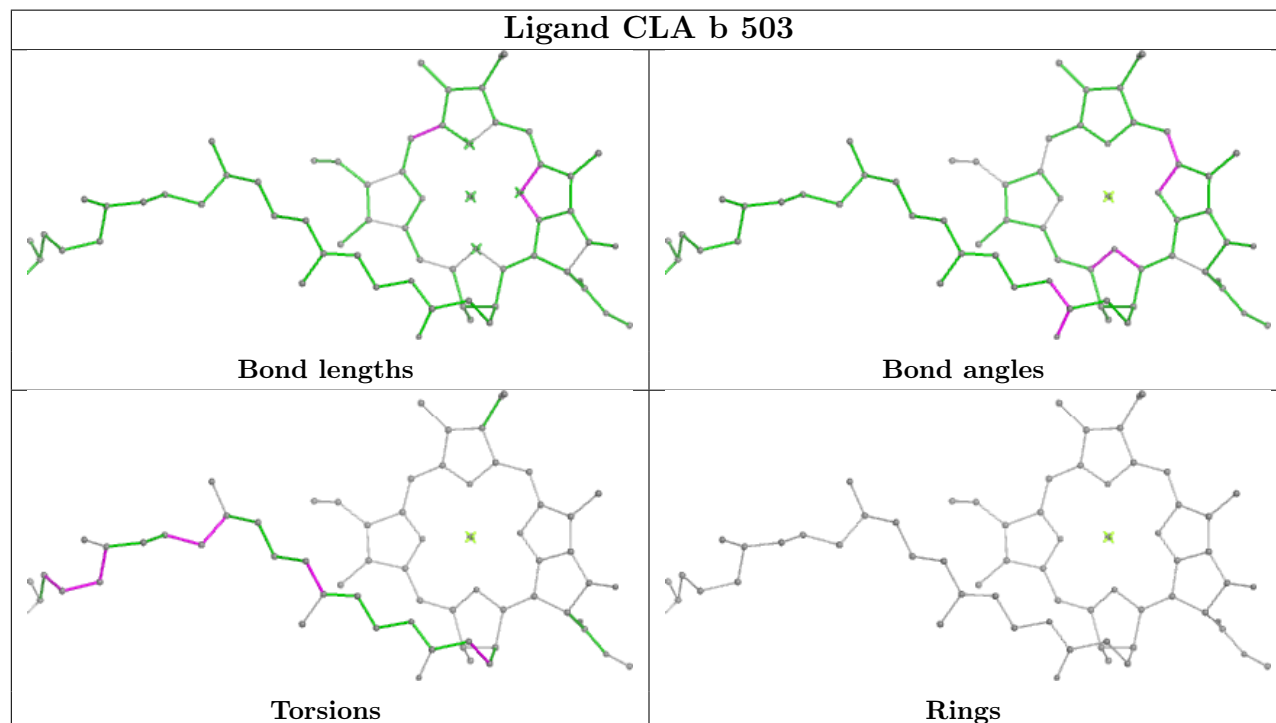
Bond angles

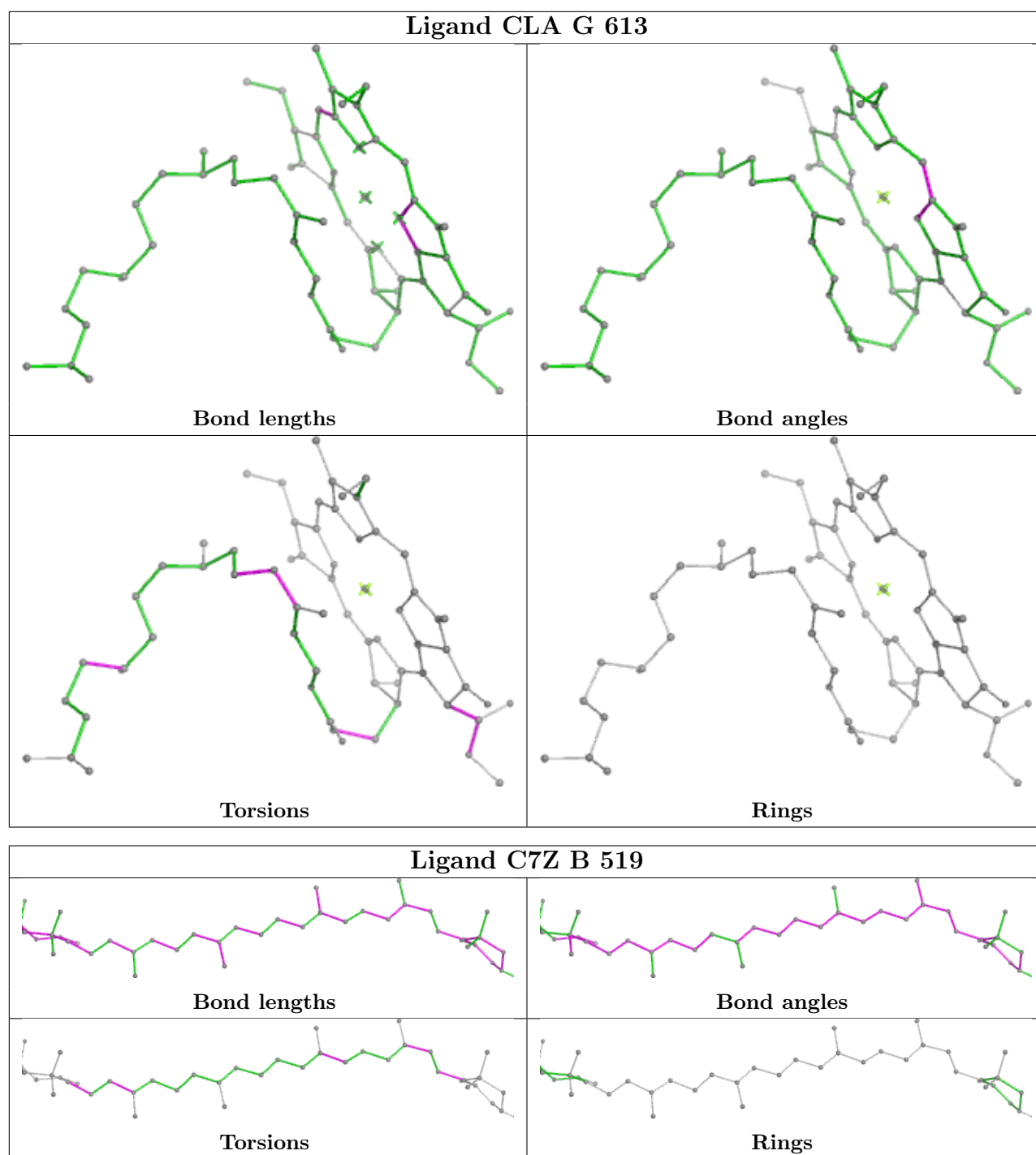


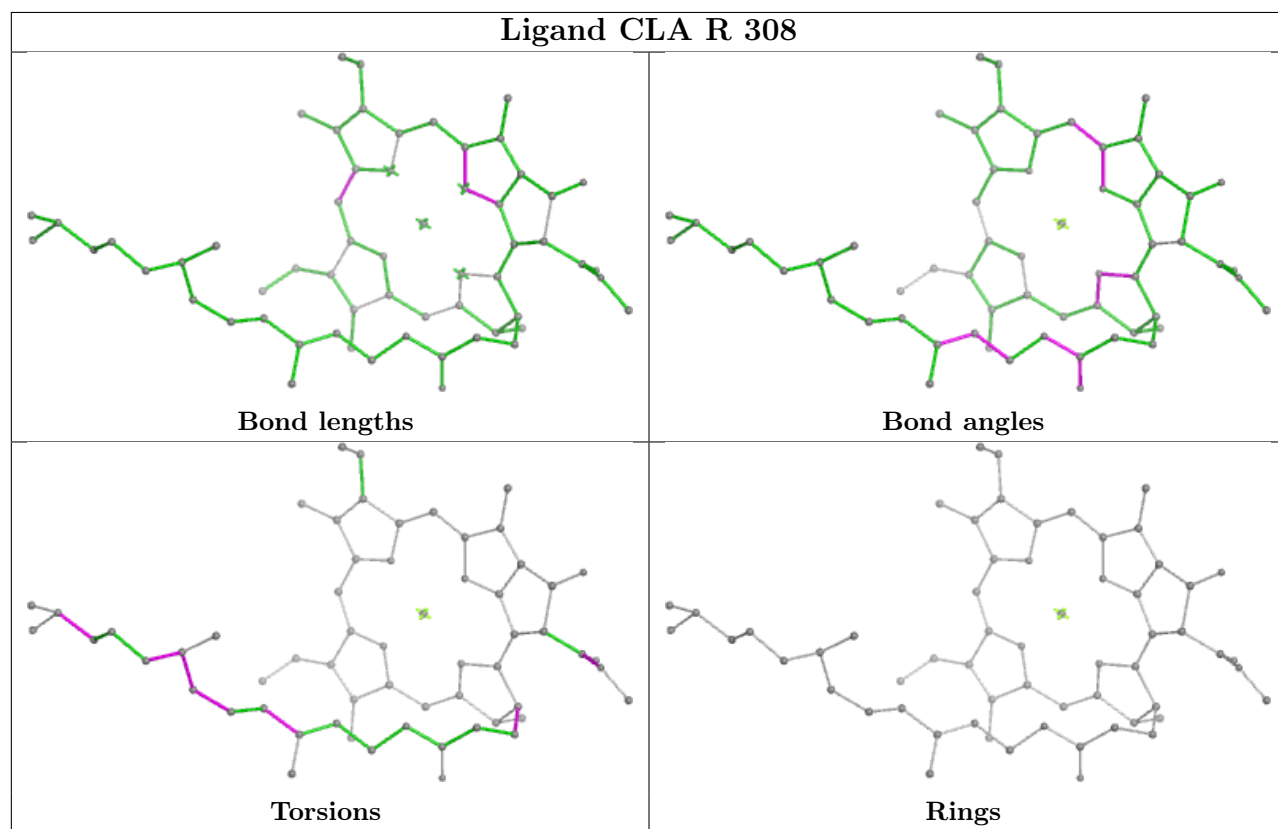
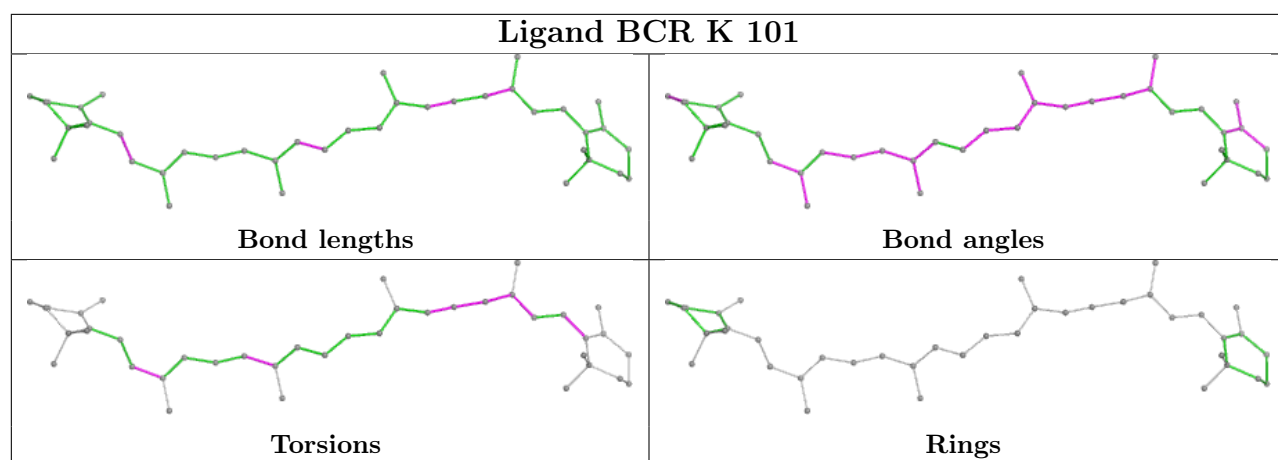
Torsions

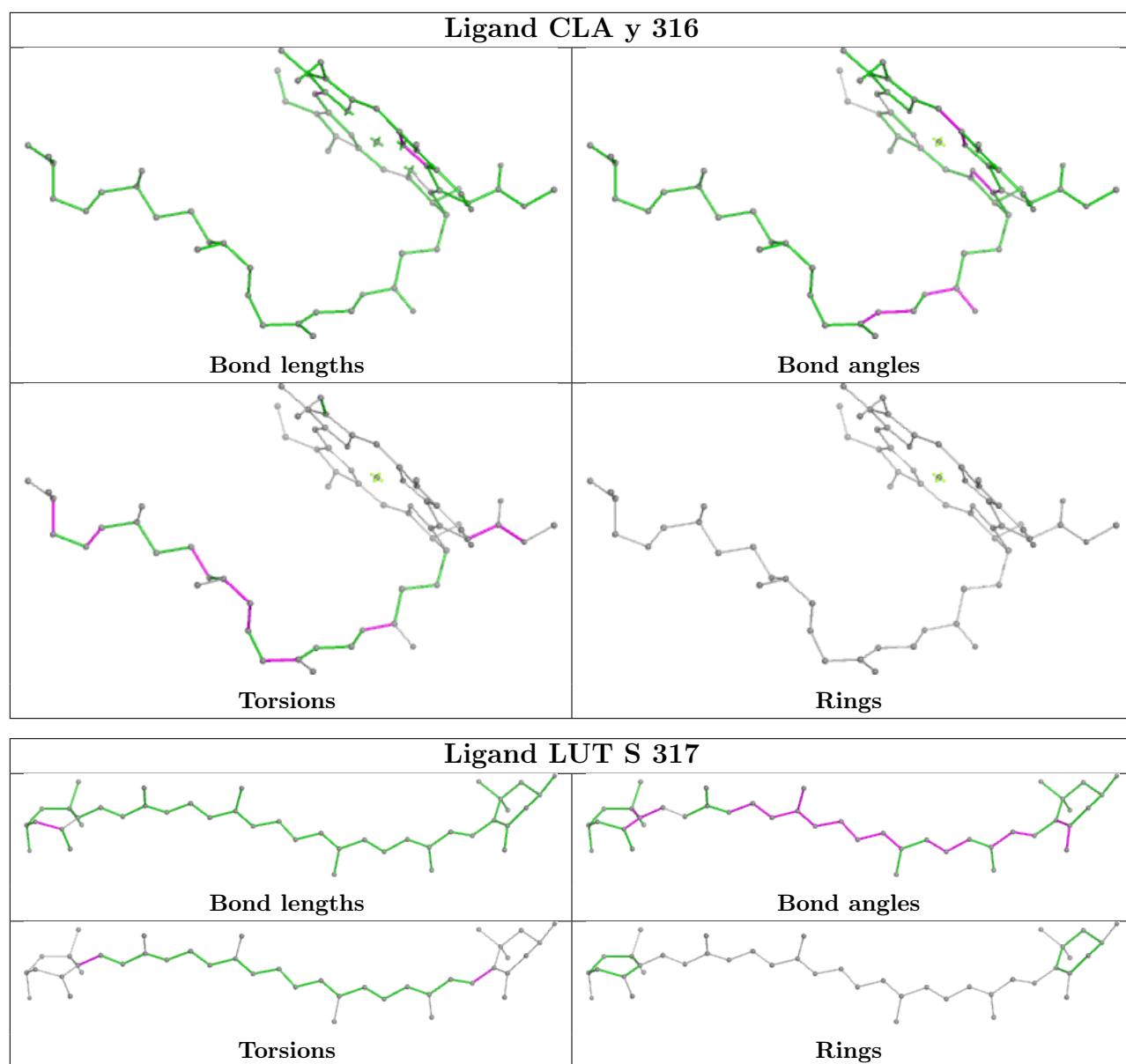


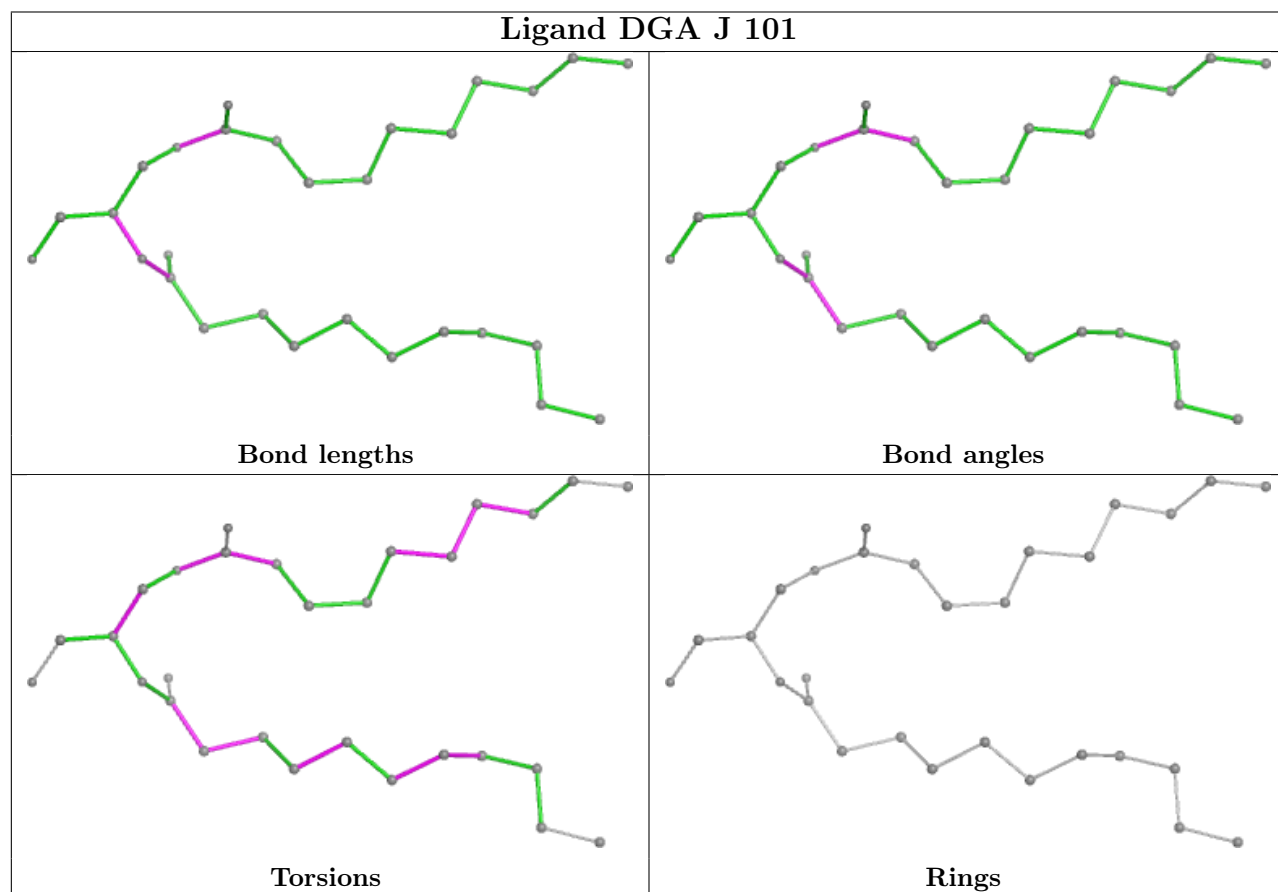
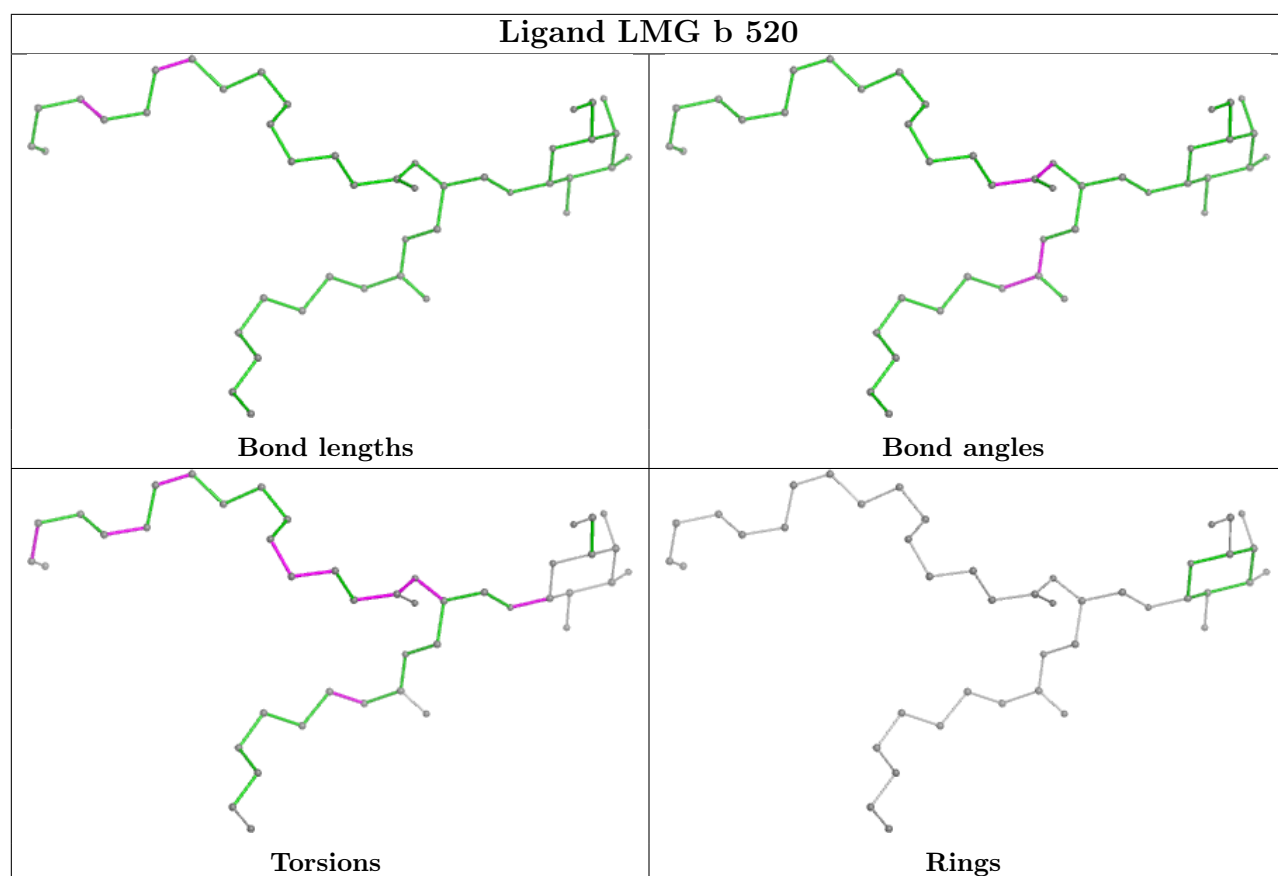
Rings

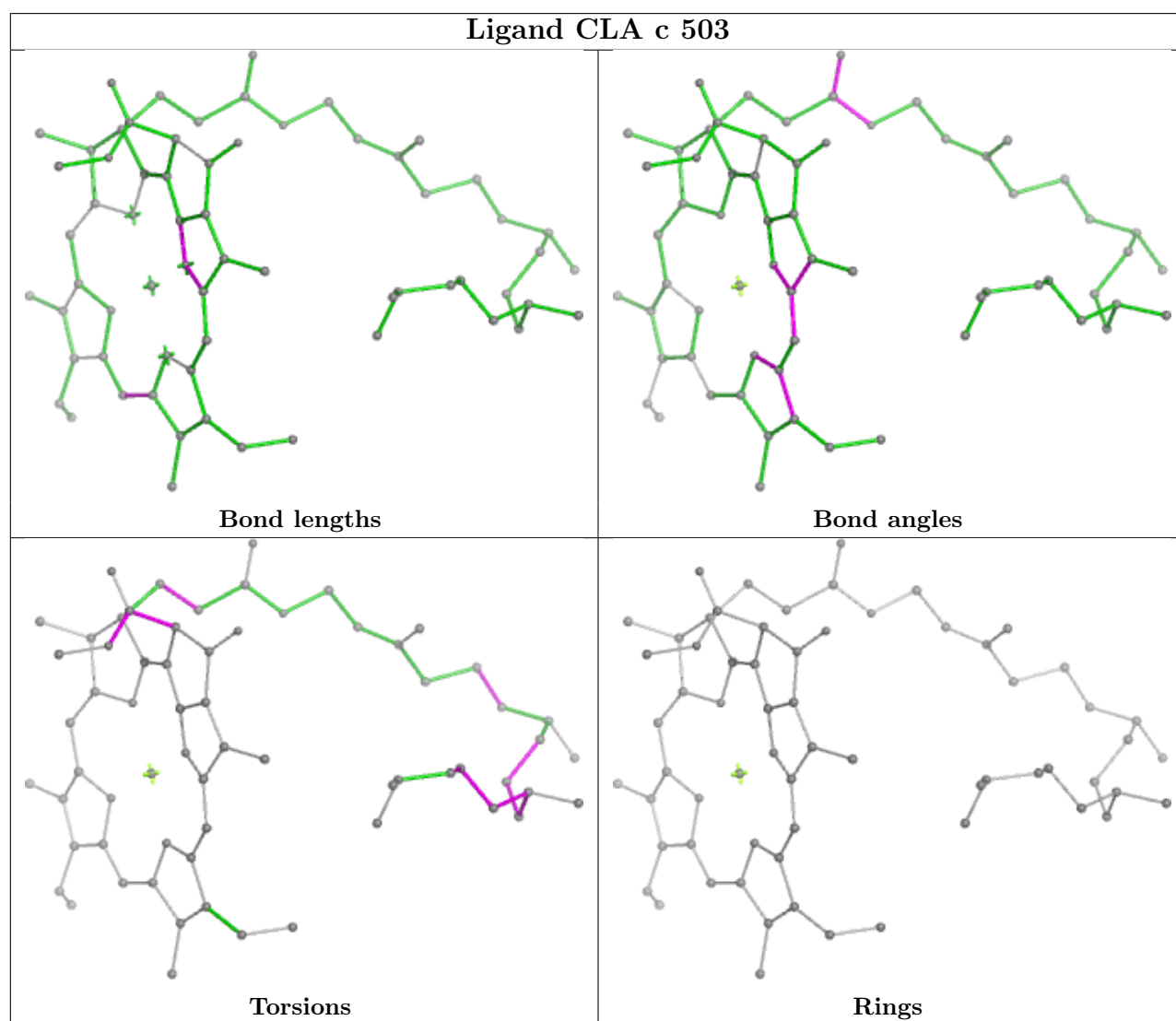
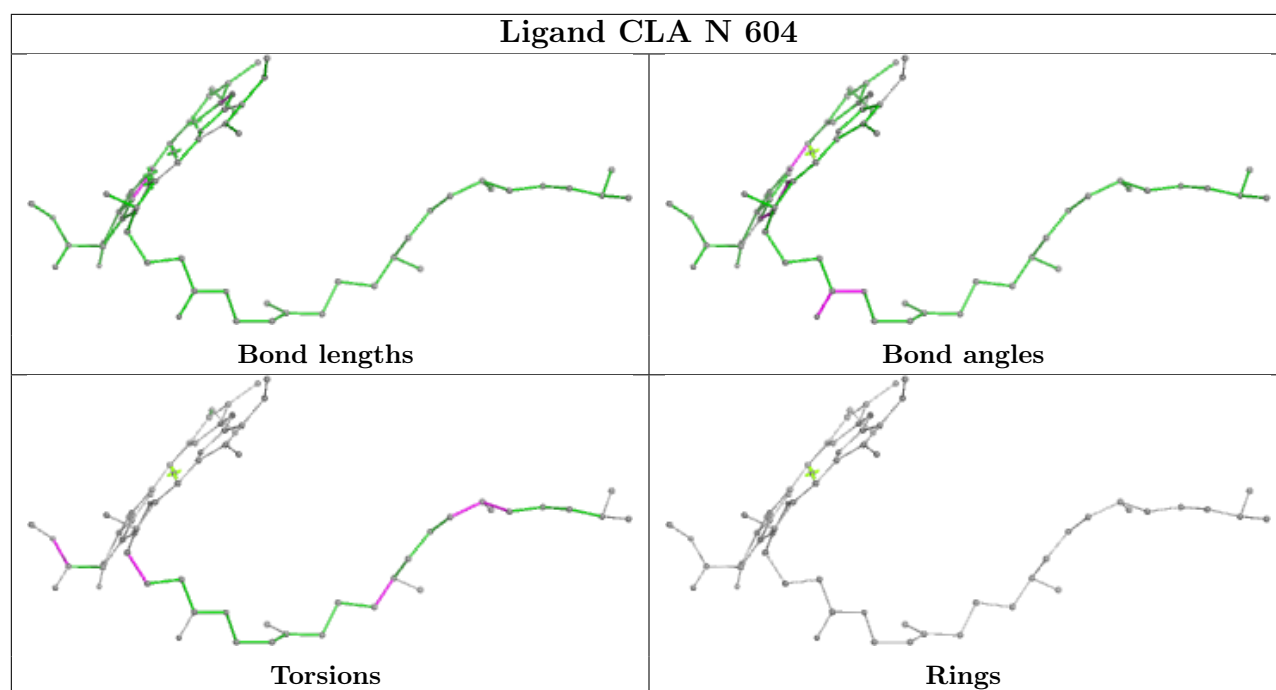
Ligand CLA C 509**Ligand CLA b 503**

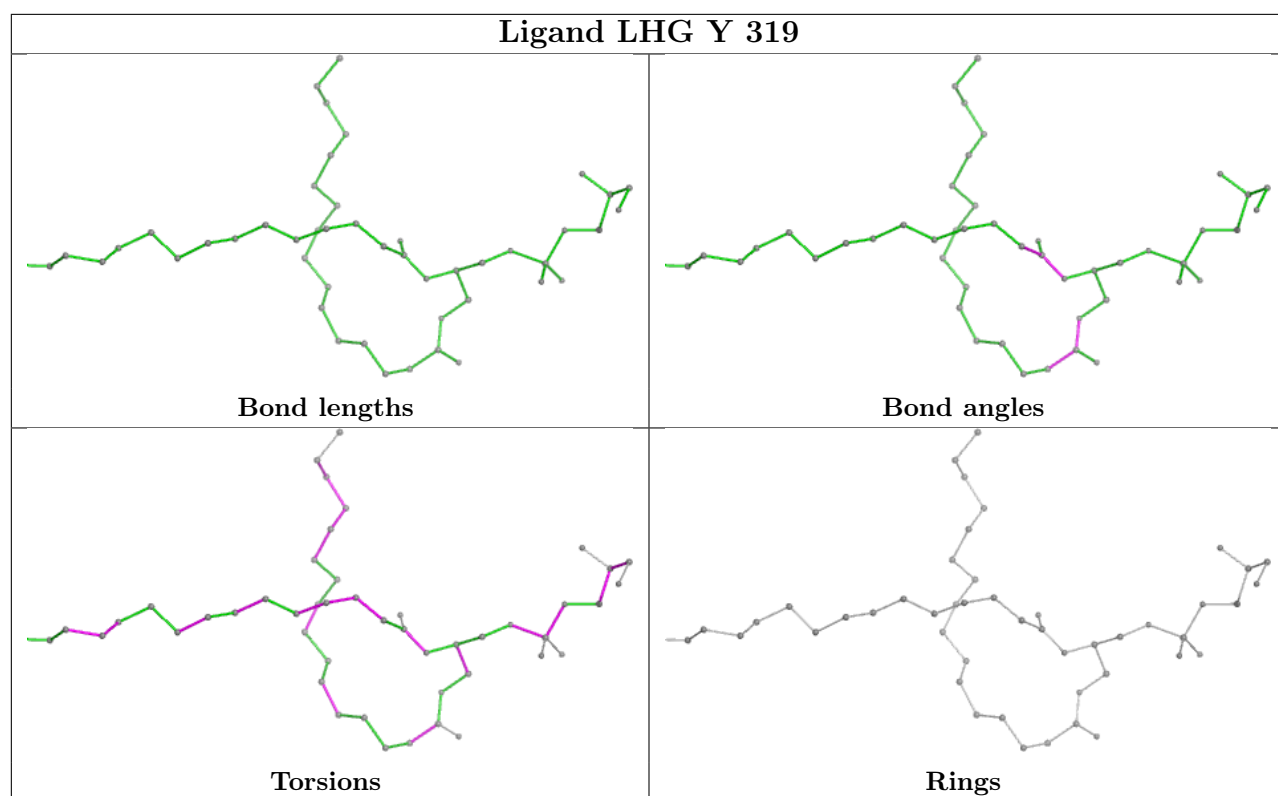




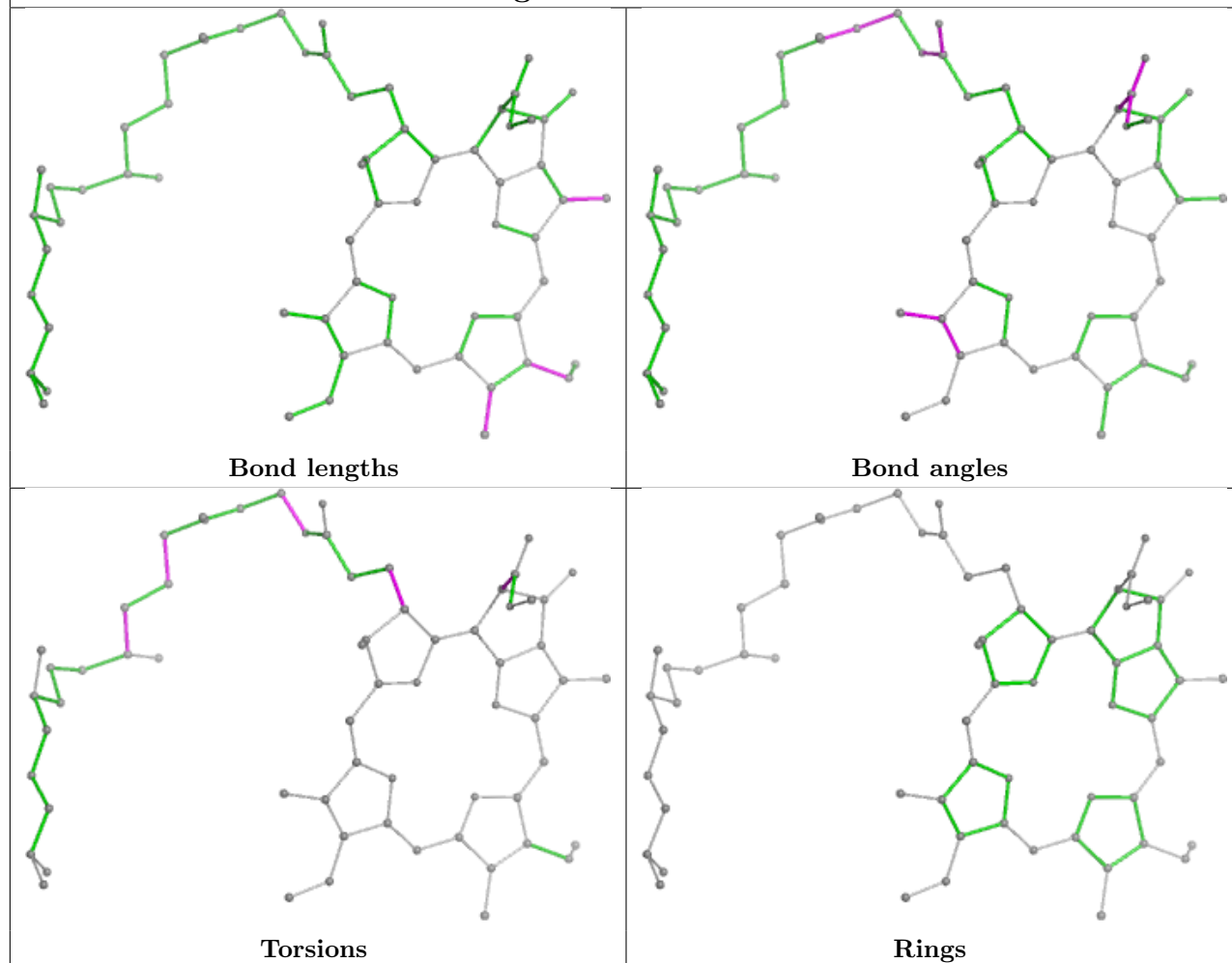




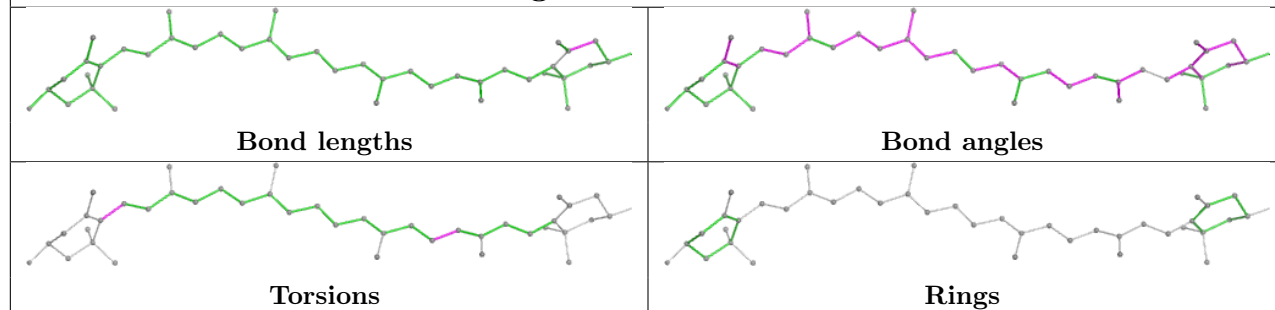




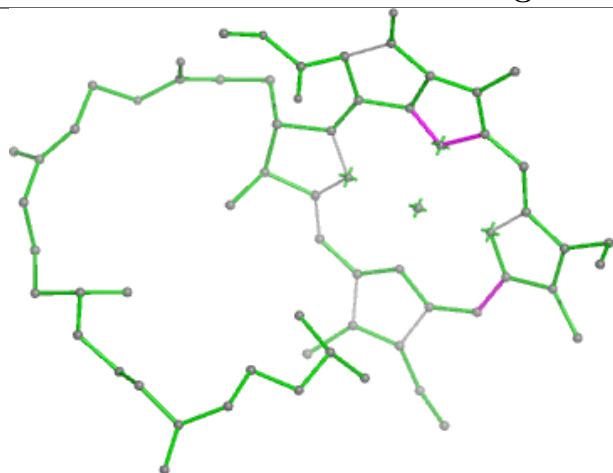
Ligand PHO d 402



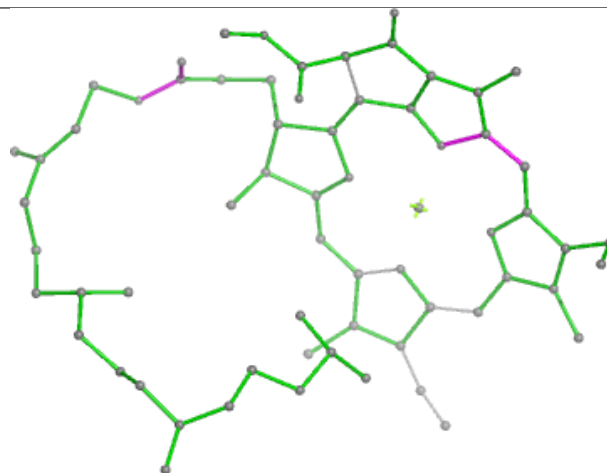
Ligand LUT N 615



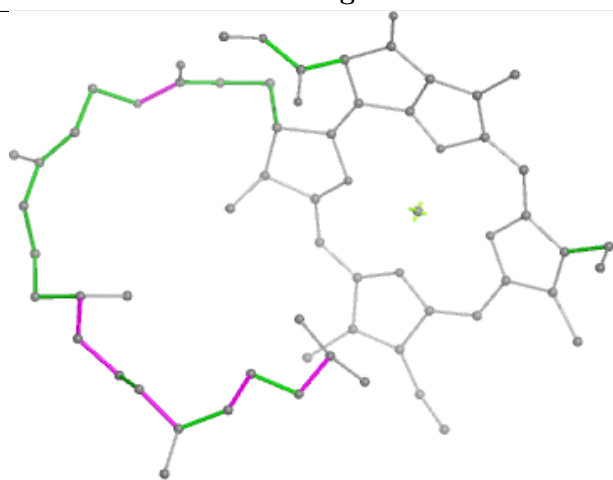
Ligand CLA B 515



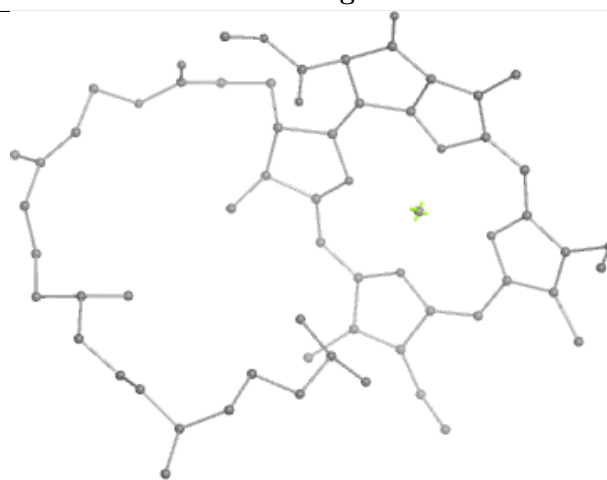
Bond lengths



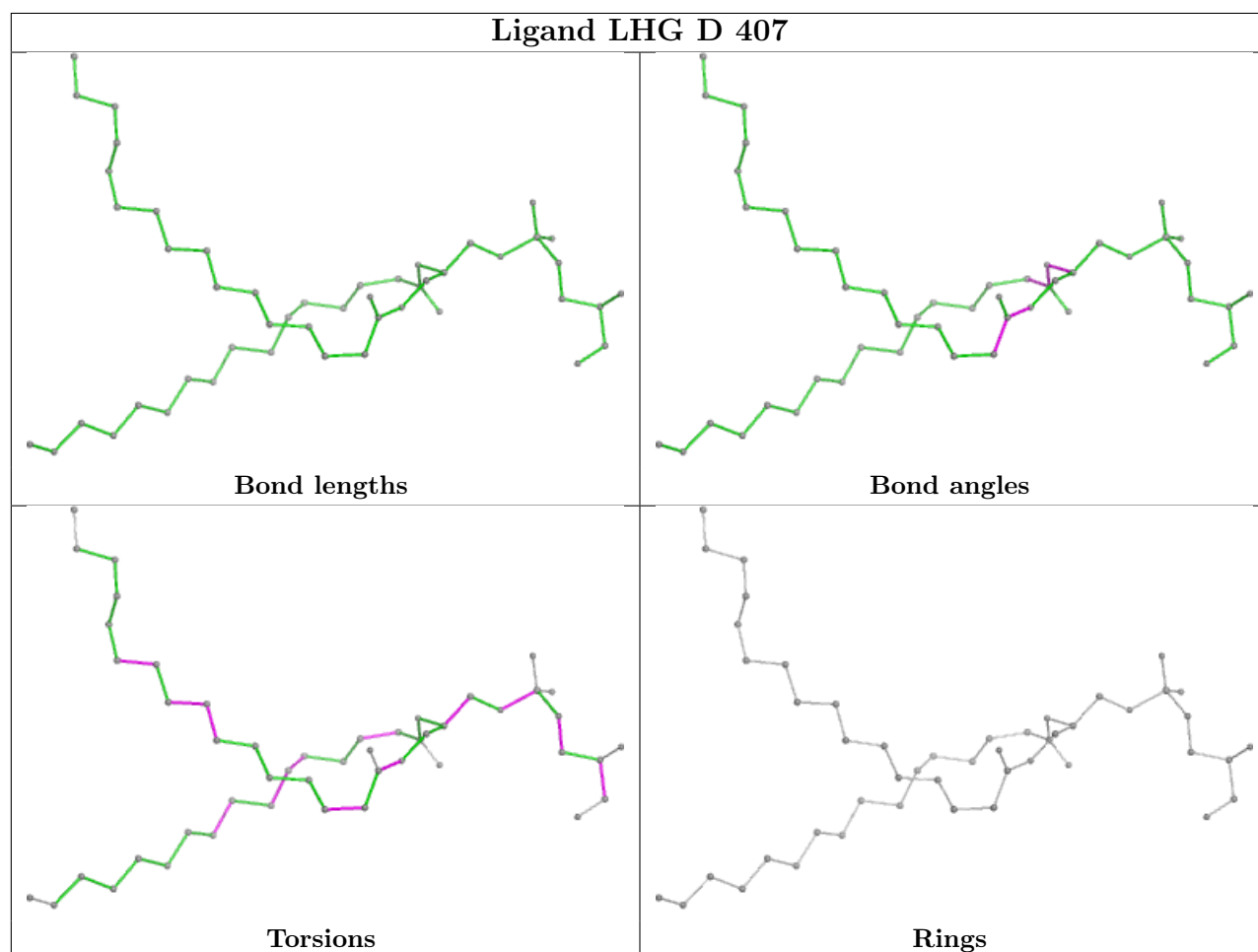
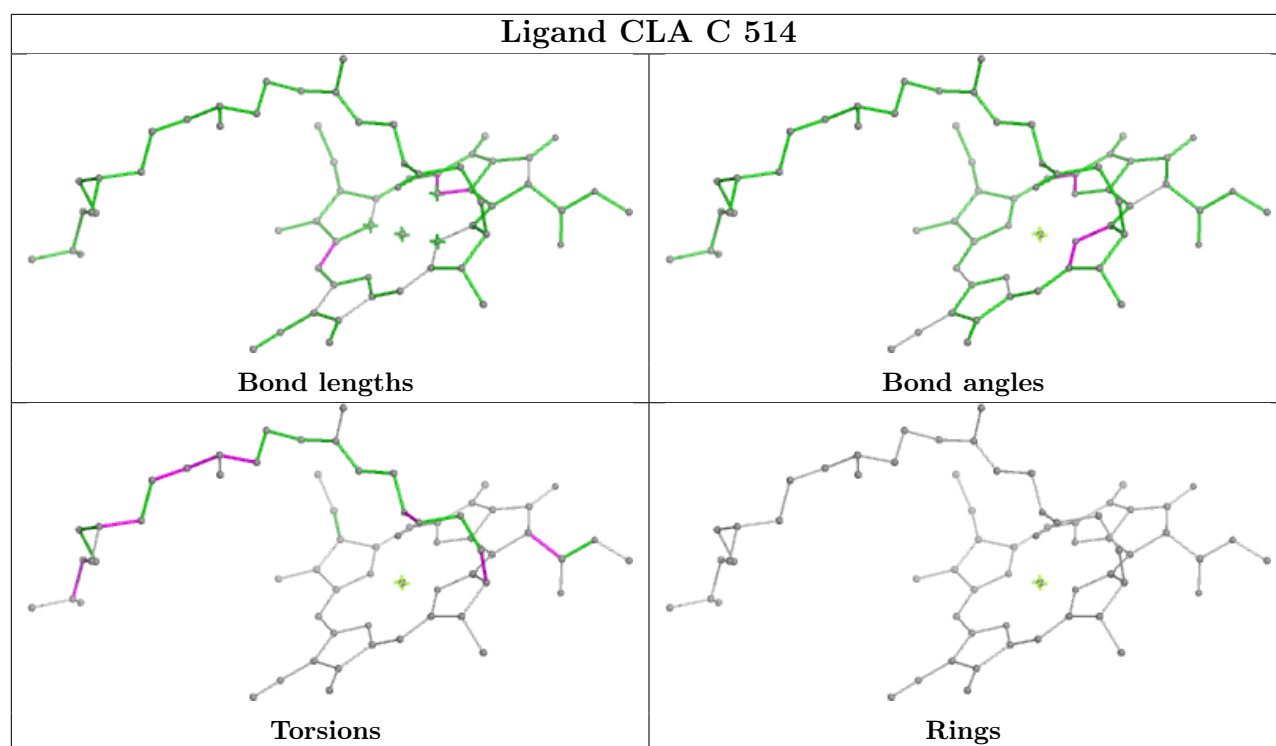
Bond angles



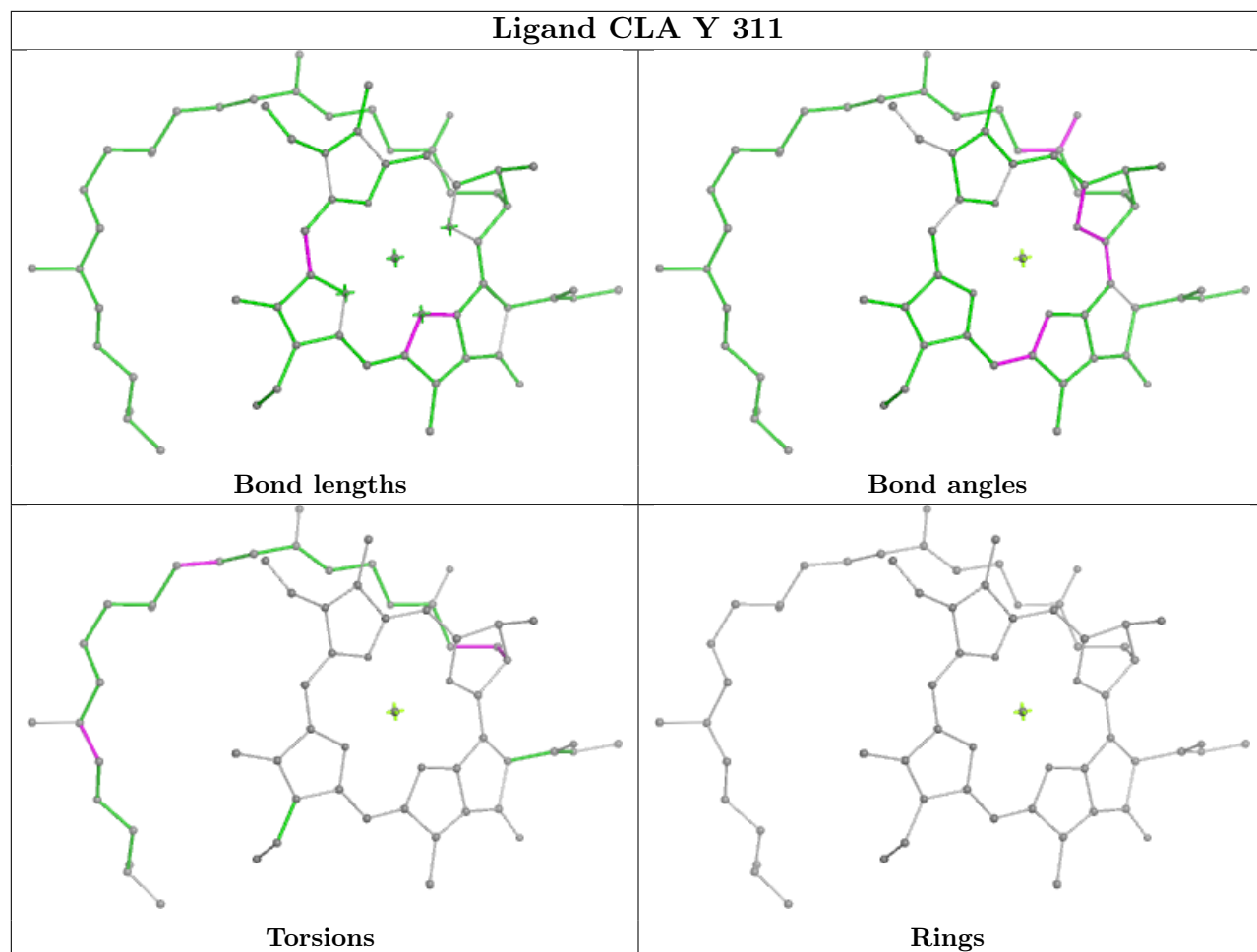
Torsions



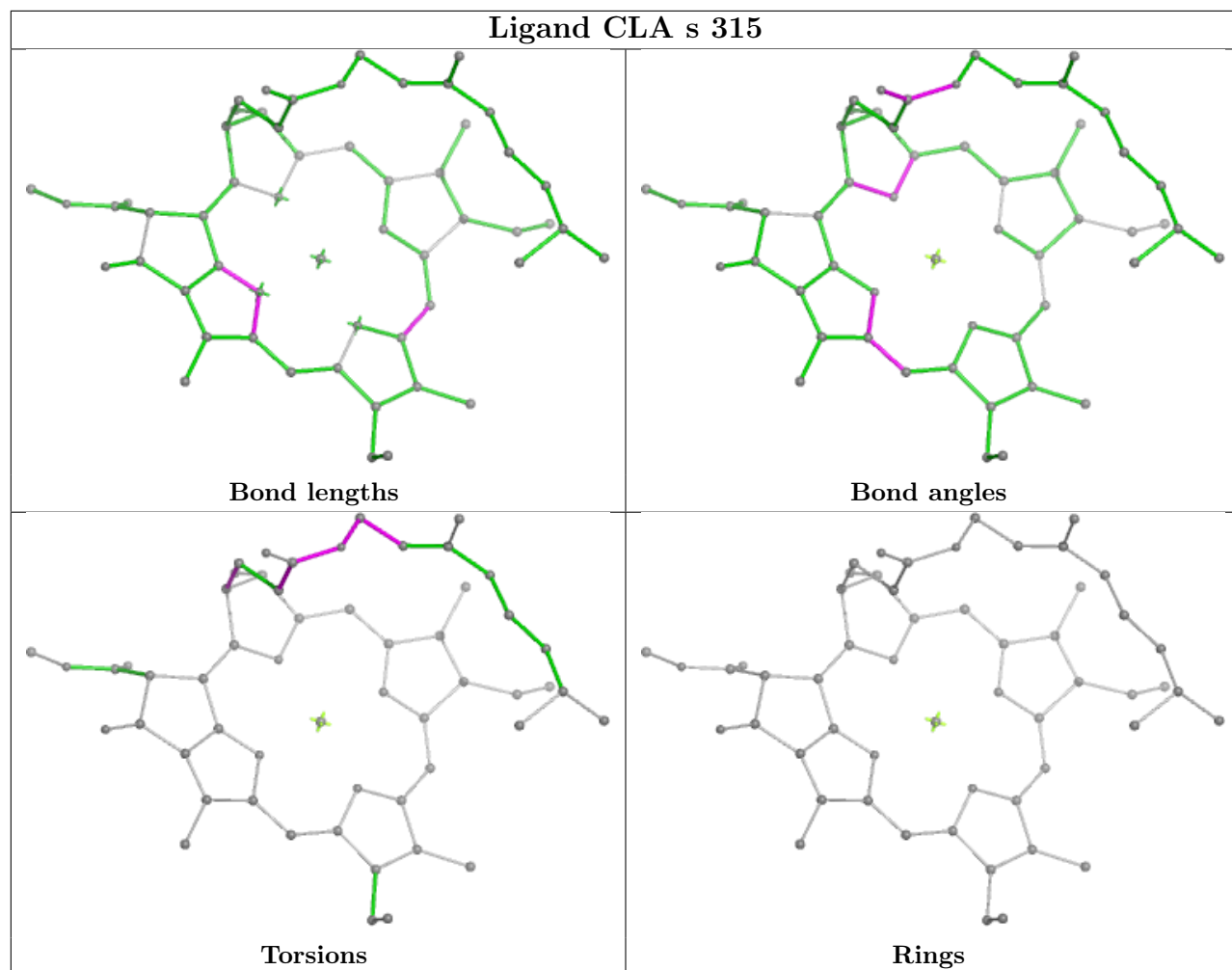
Rings



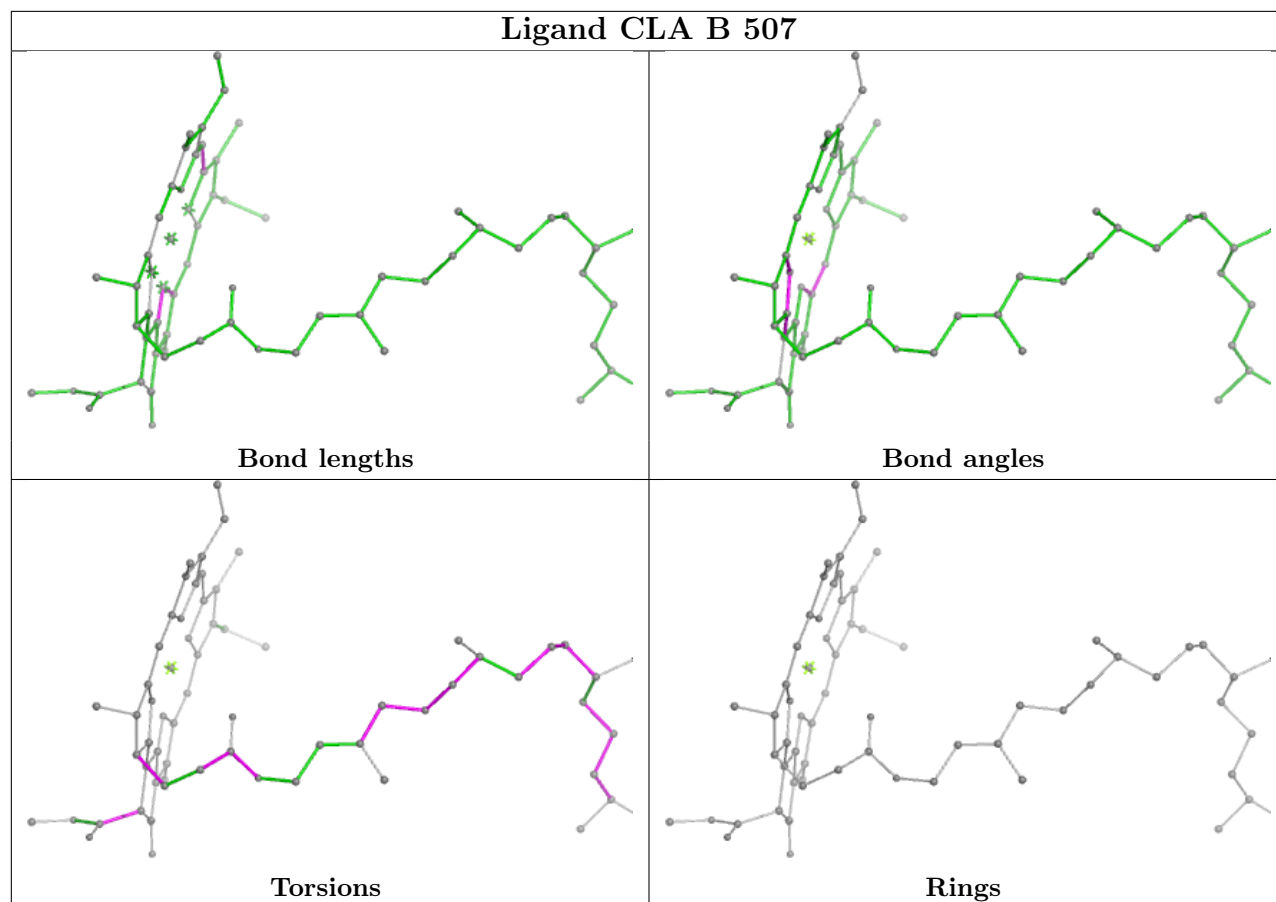
Ligand CLA Y 311



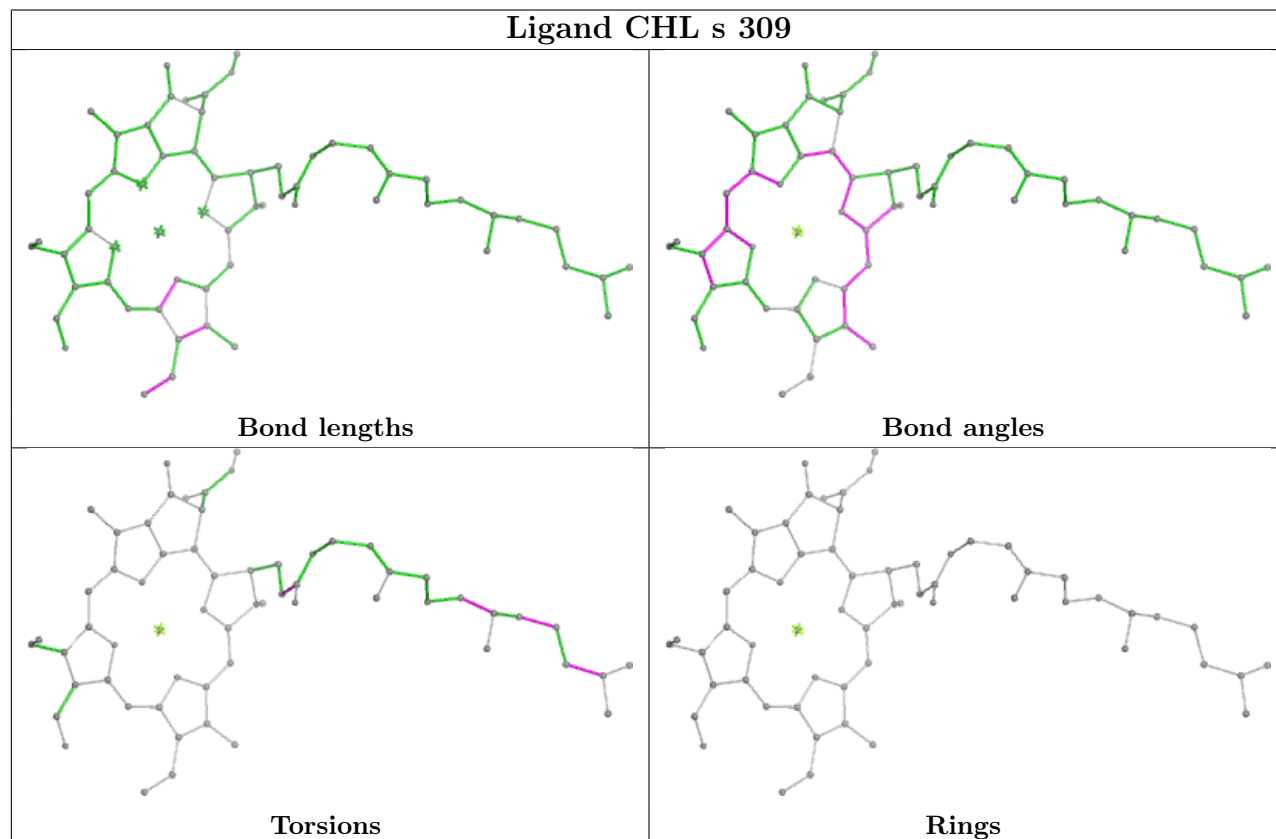
Ligand CLA s 315

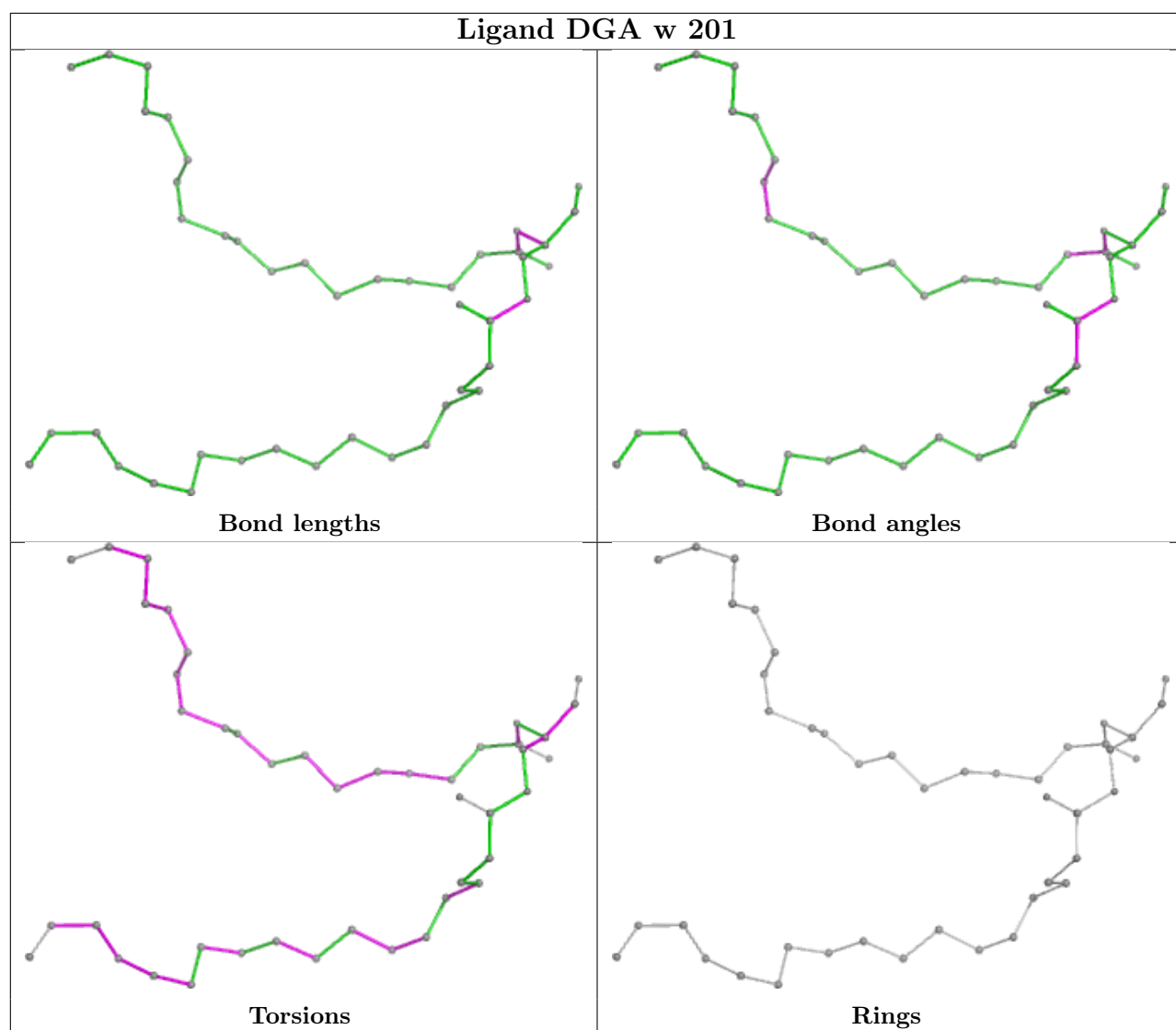


Ligand CLA B 507

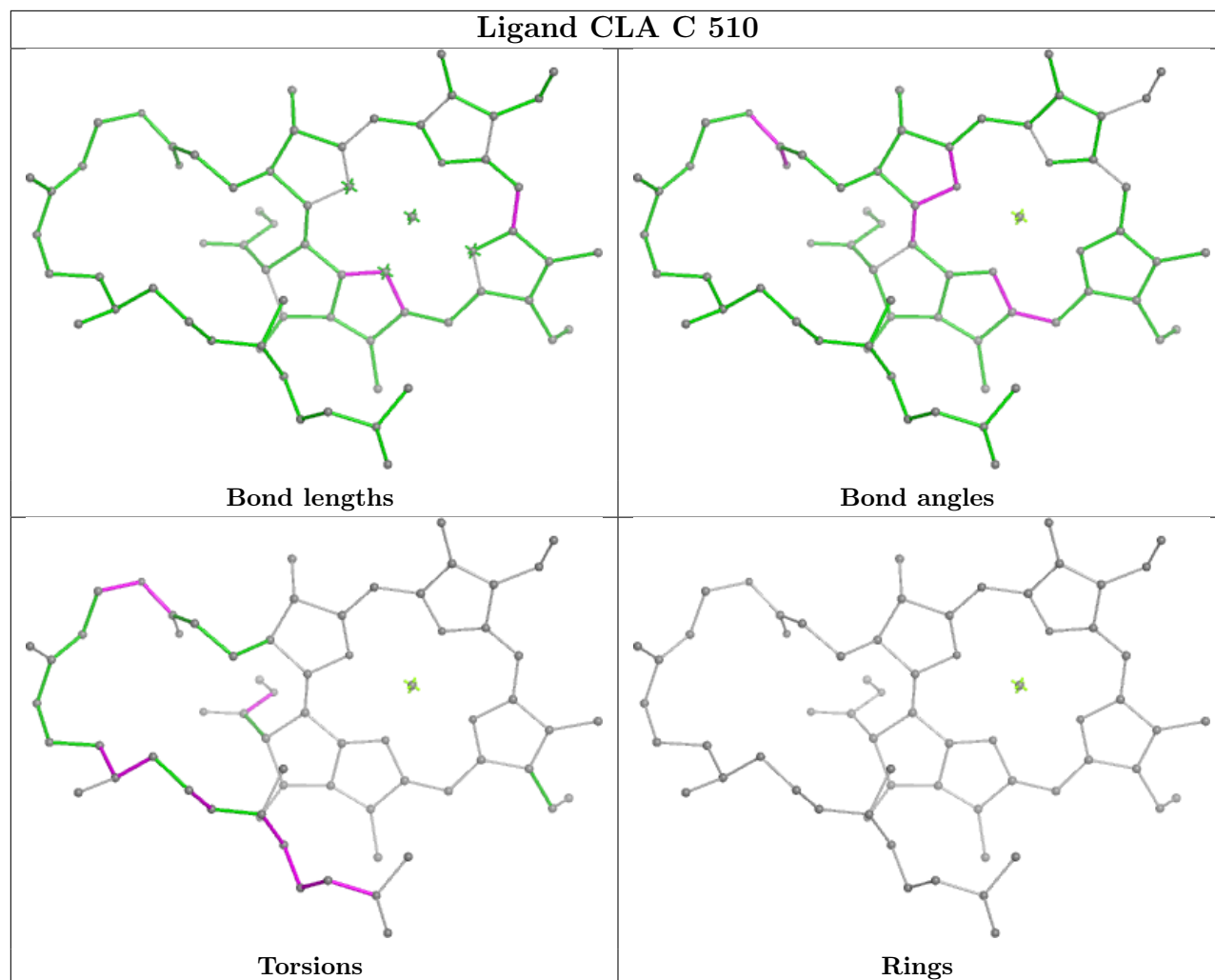


Ligand CHL s 309

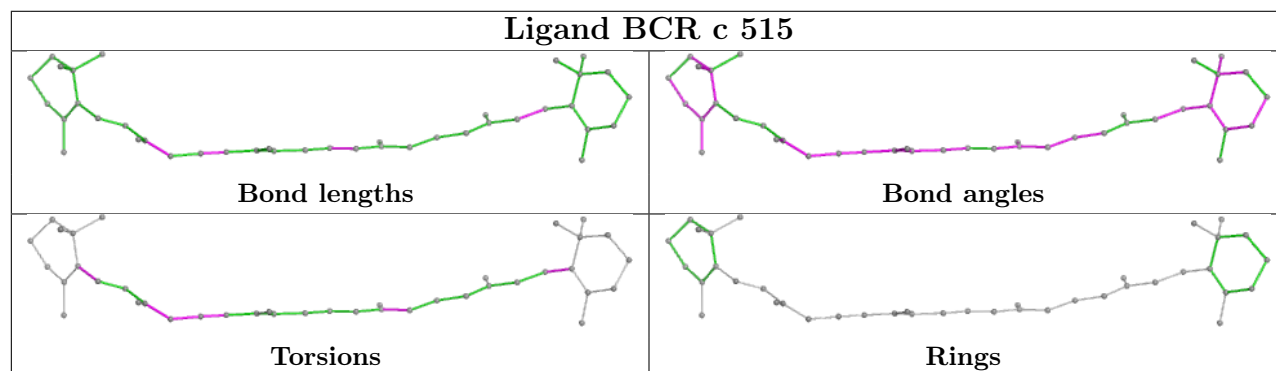


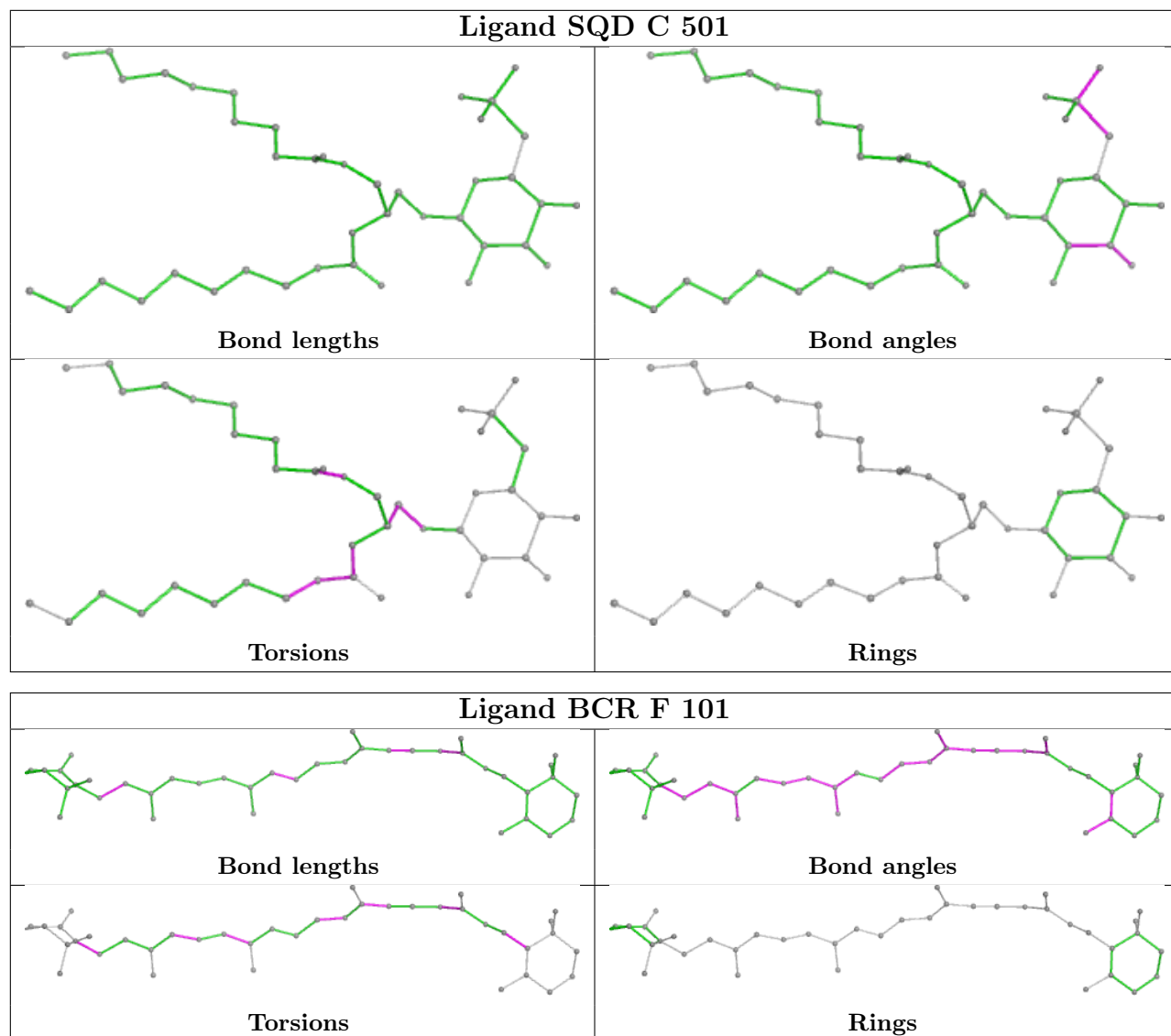


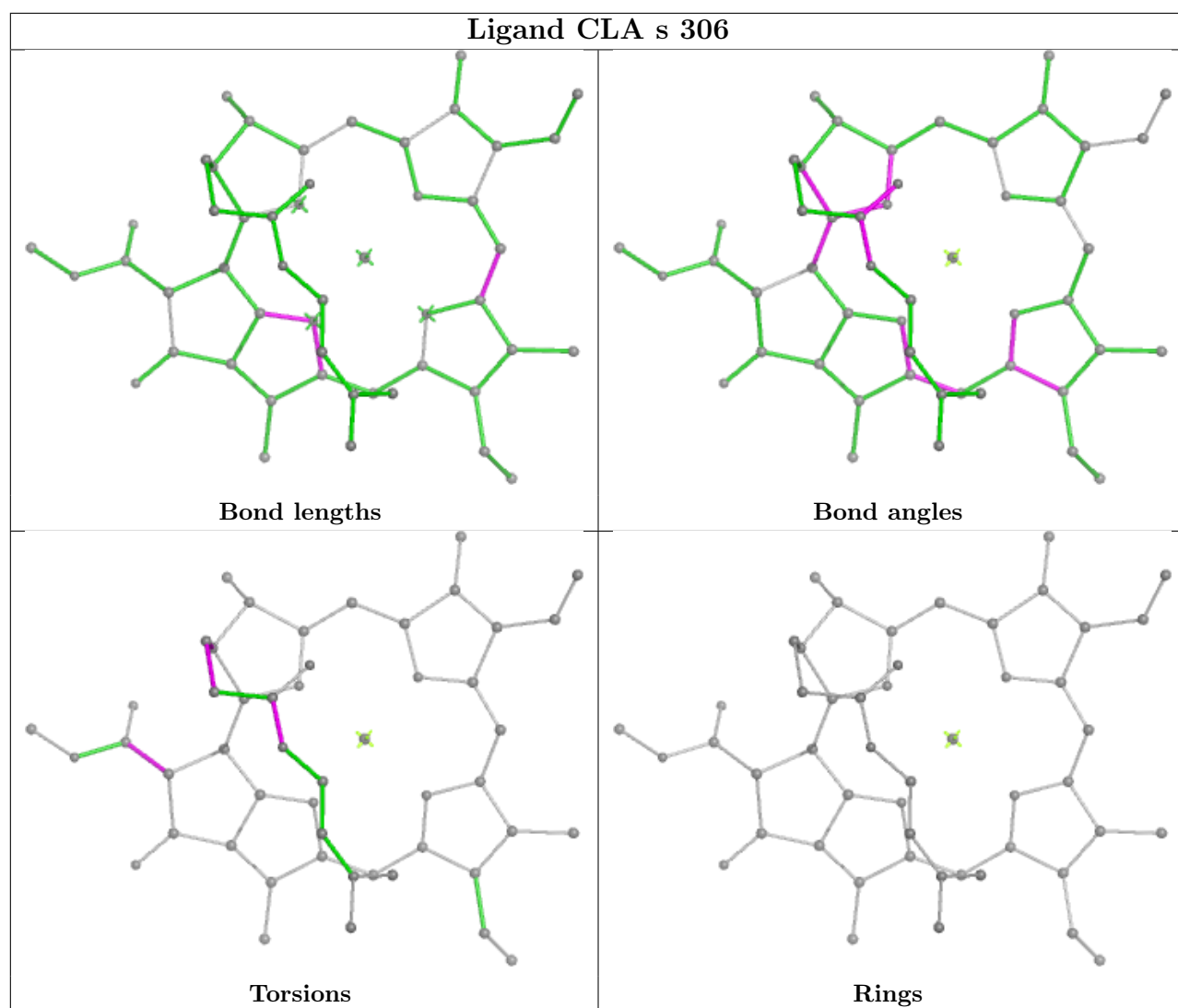
Ligand CLA C 510

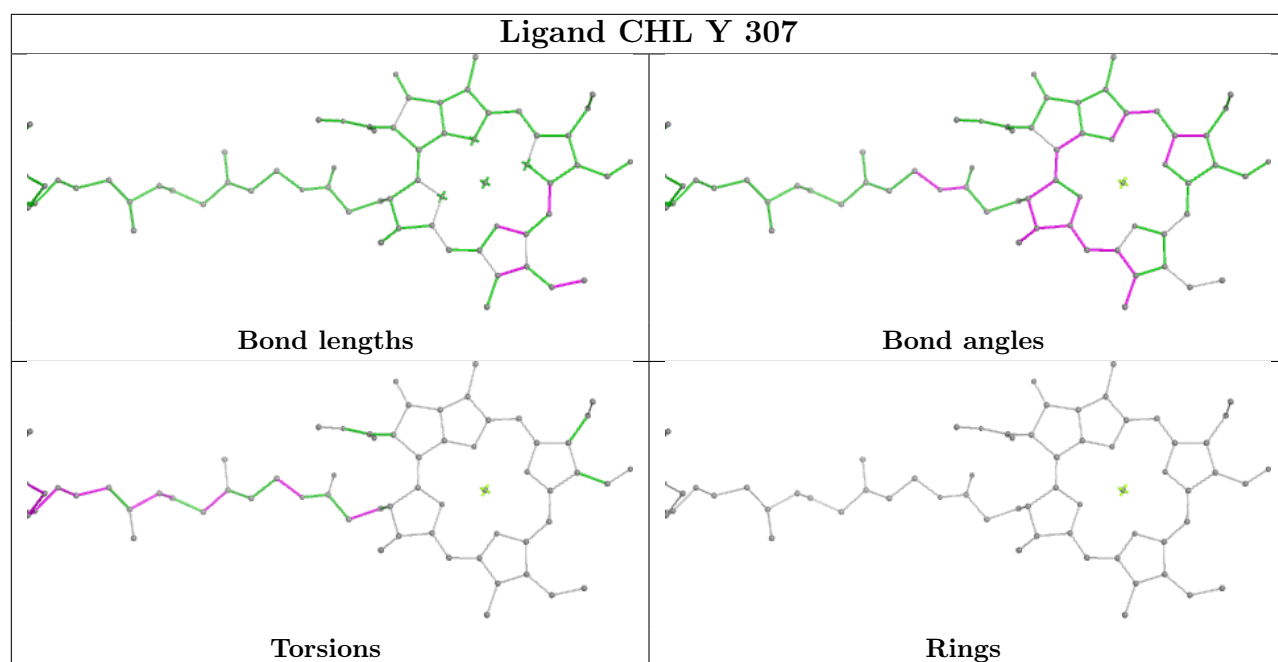
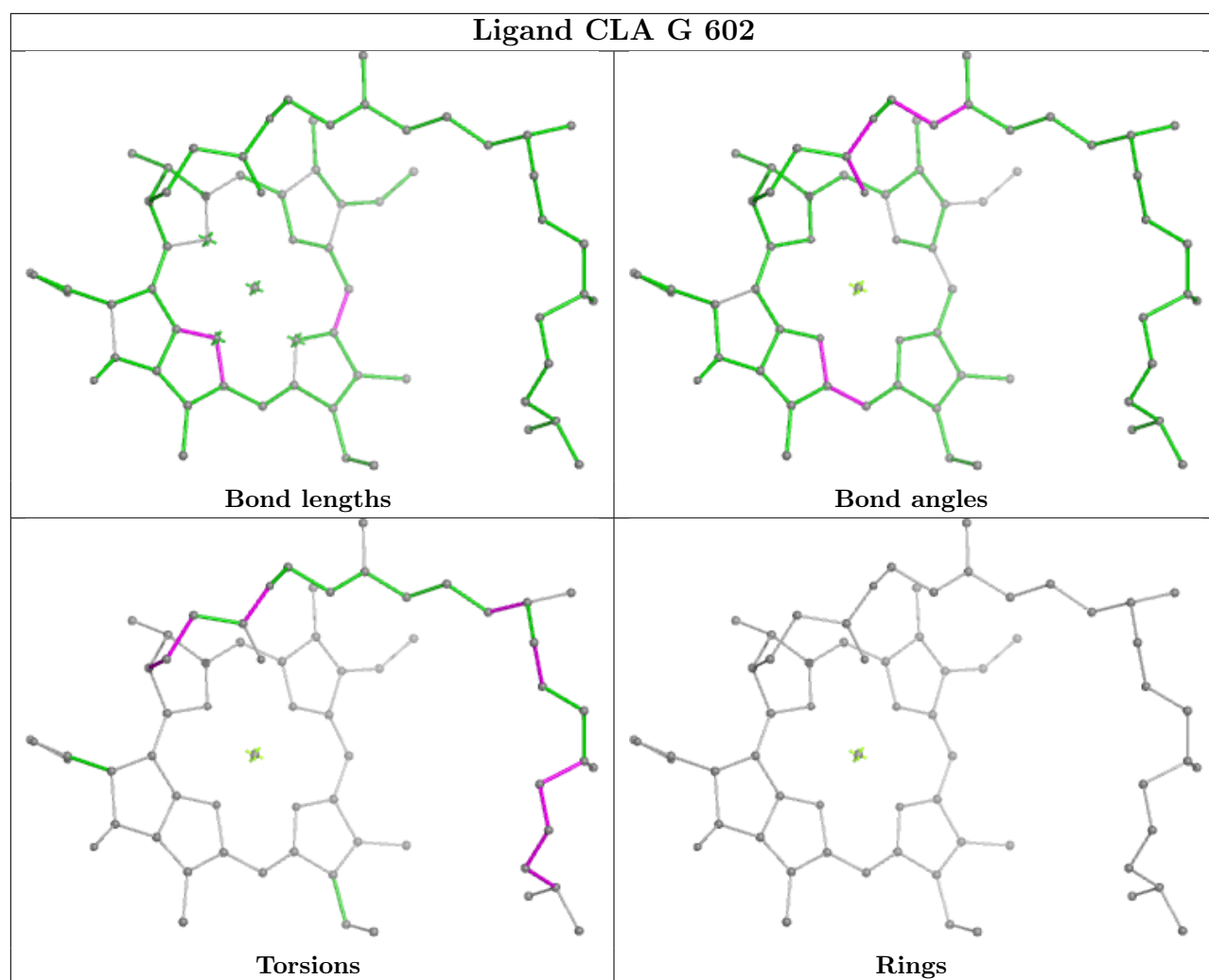


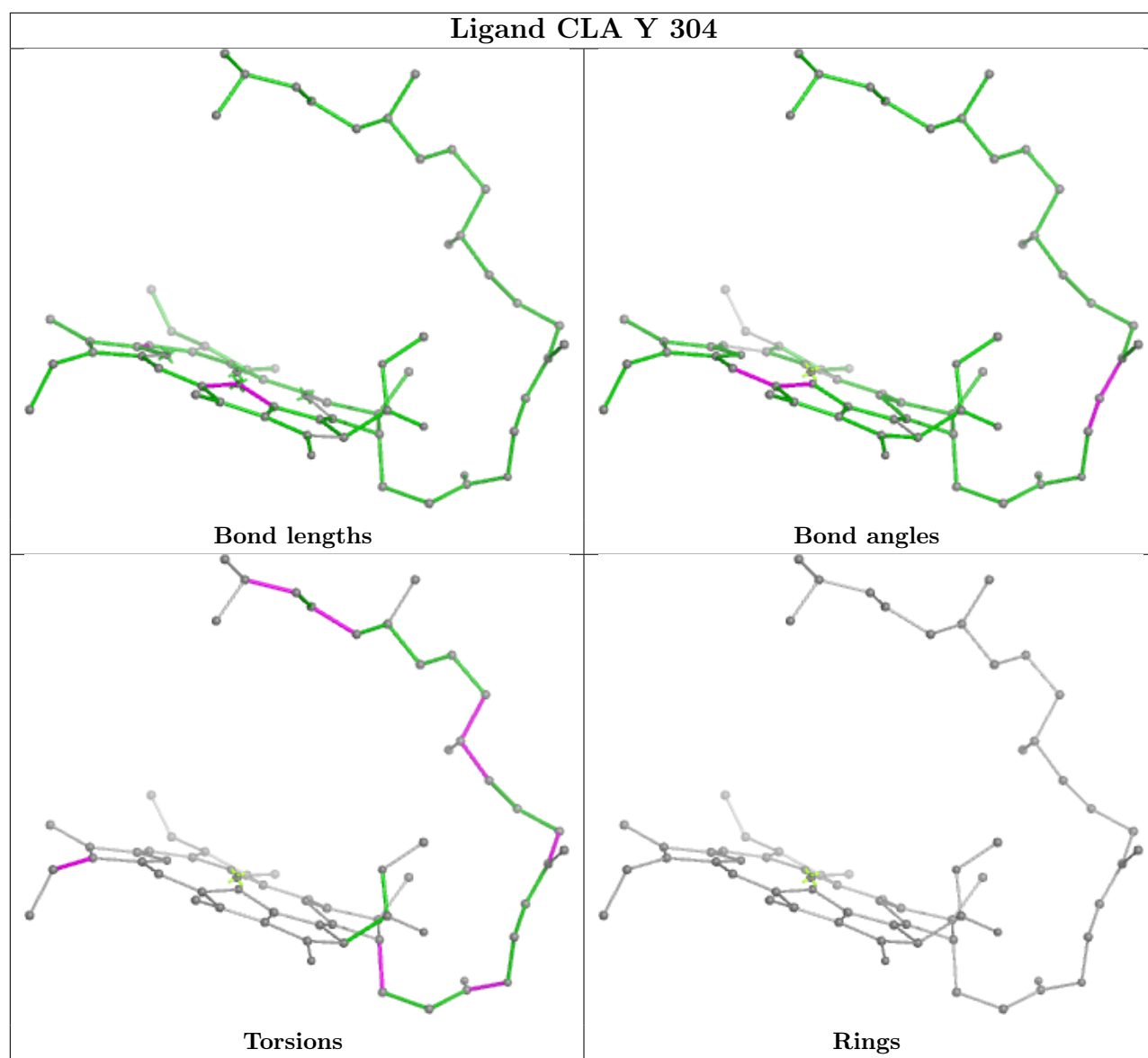
Ligand BCR c 515

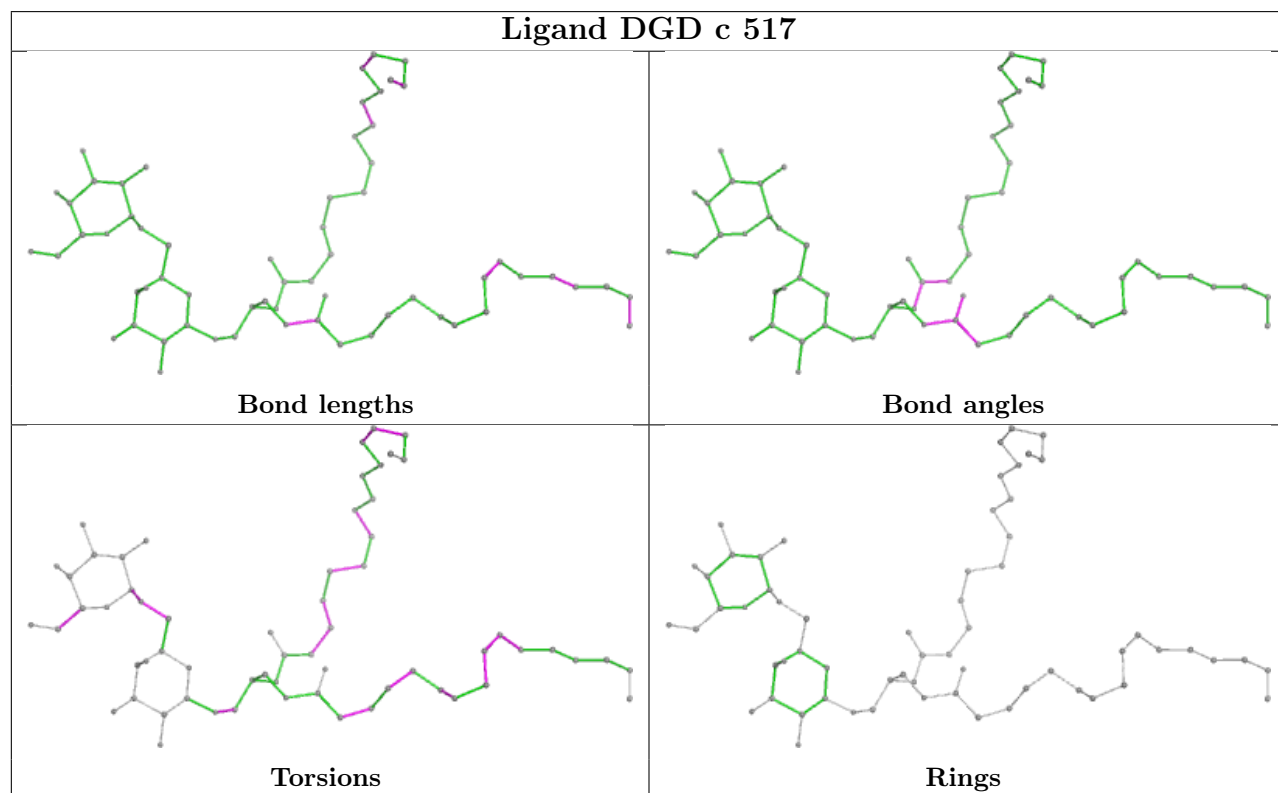
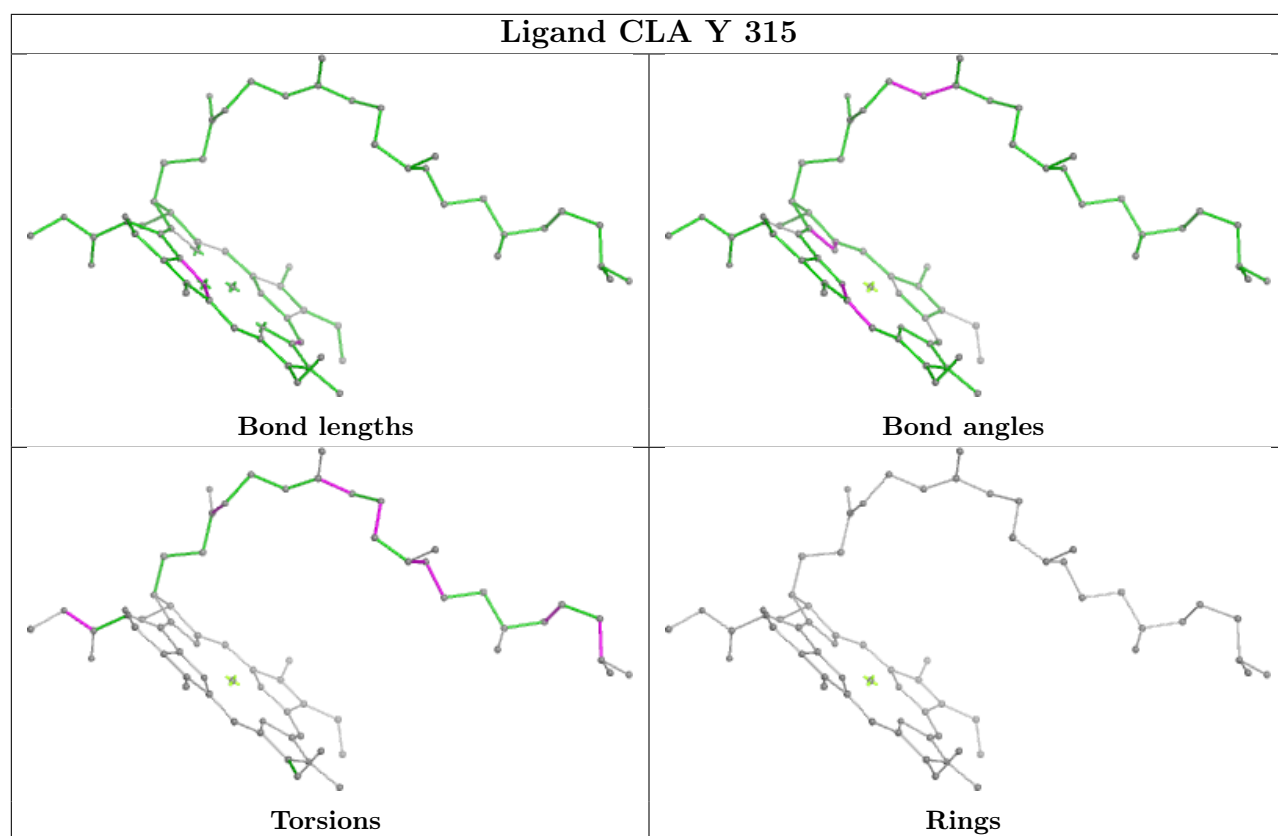


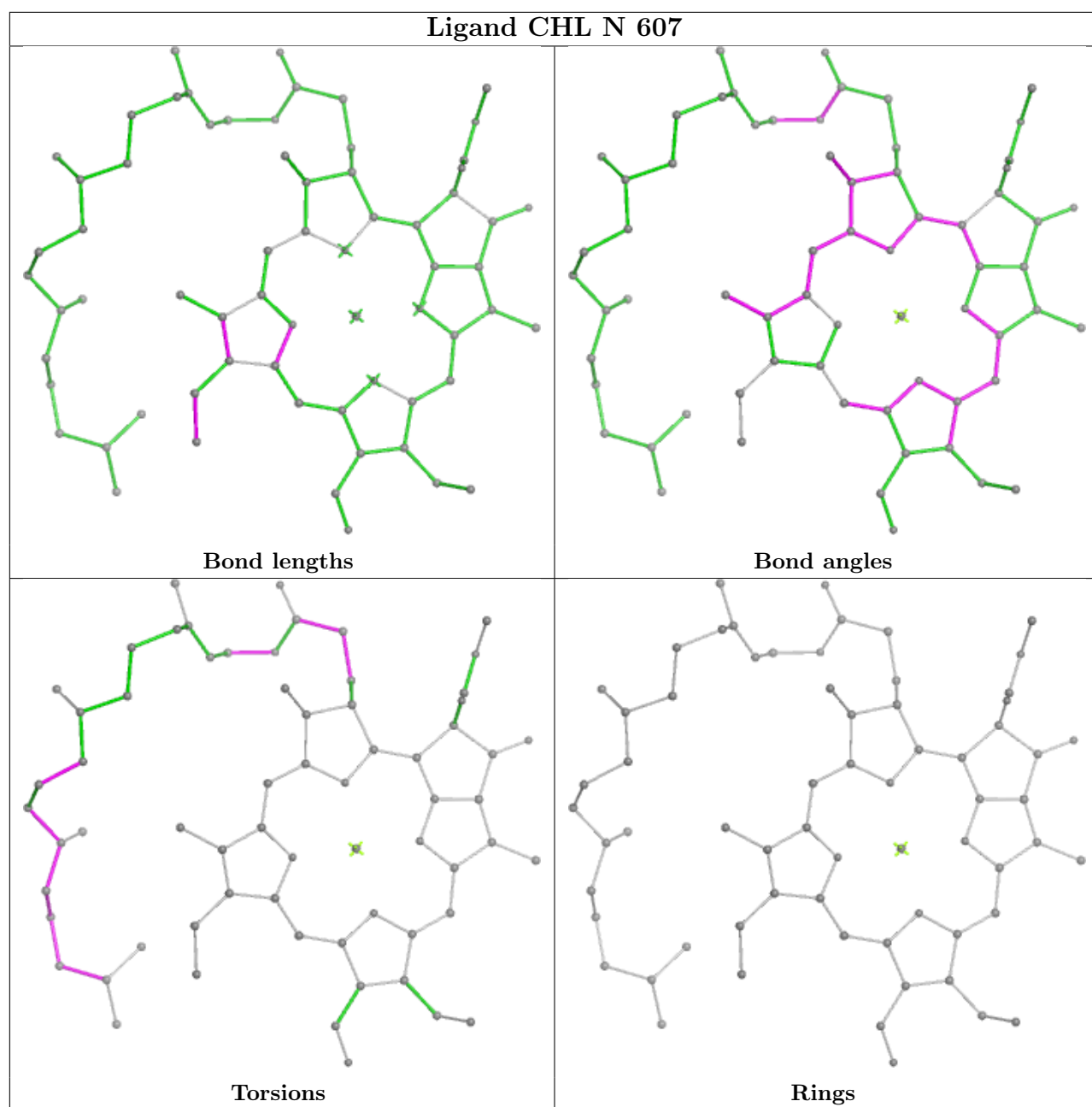


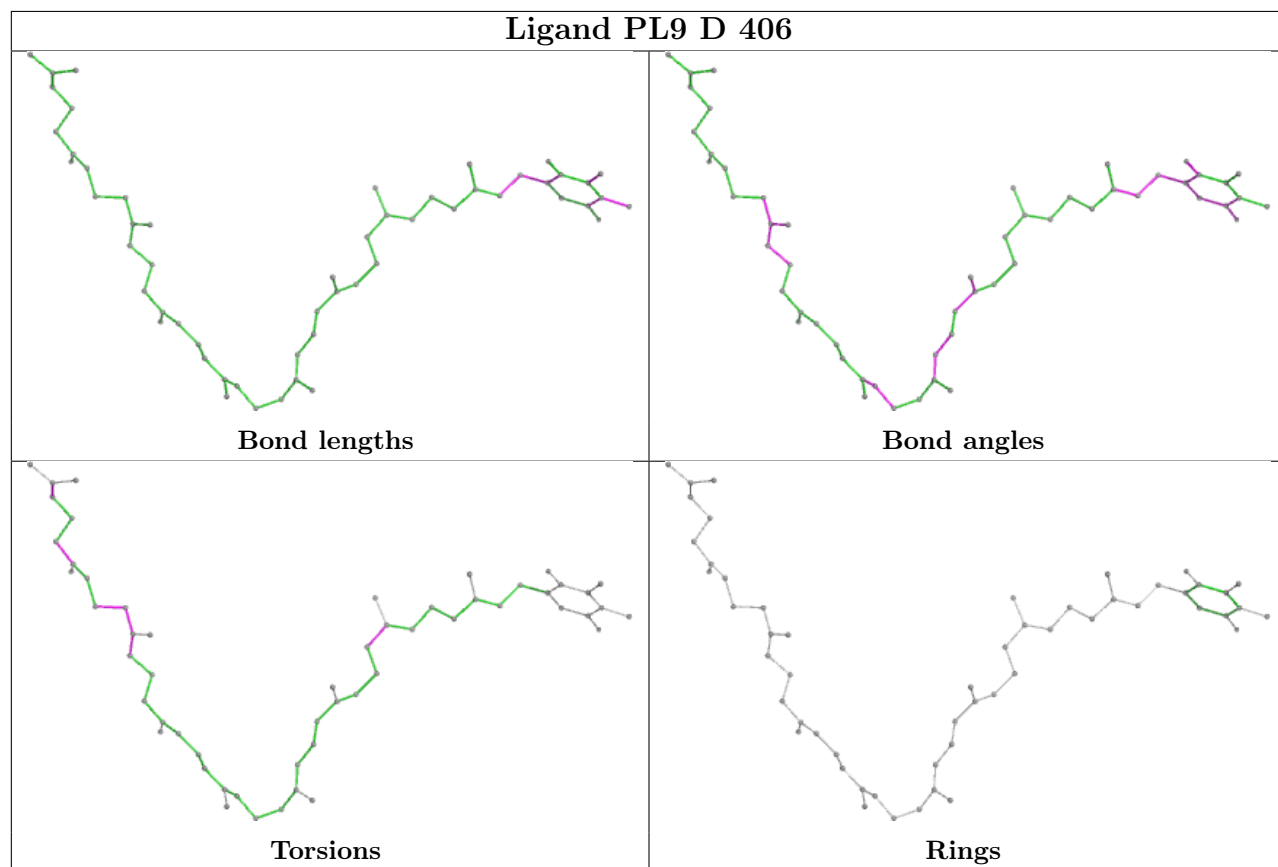
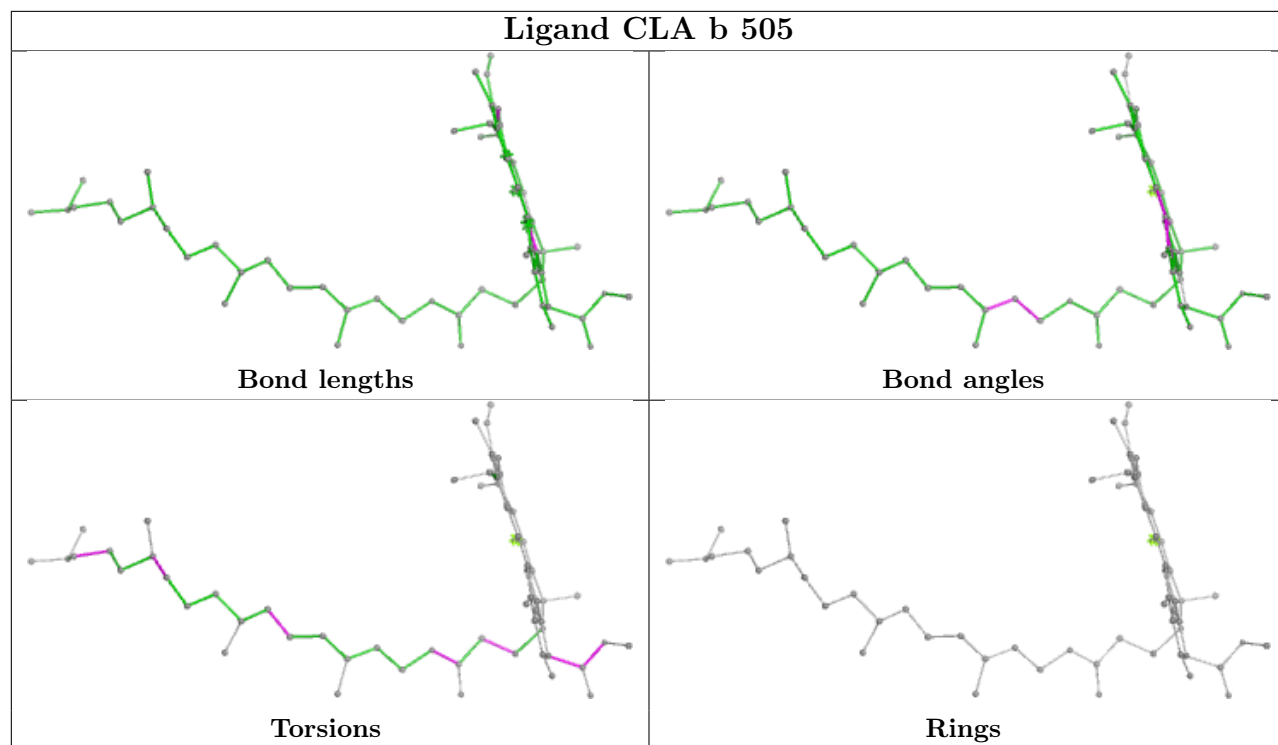




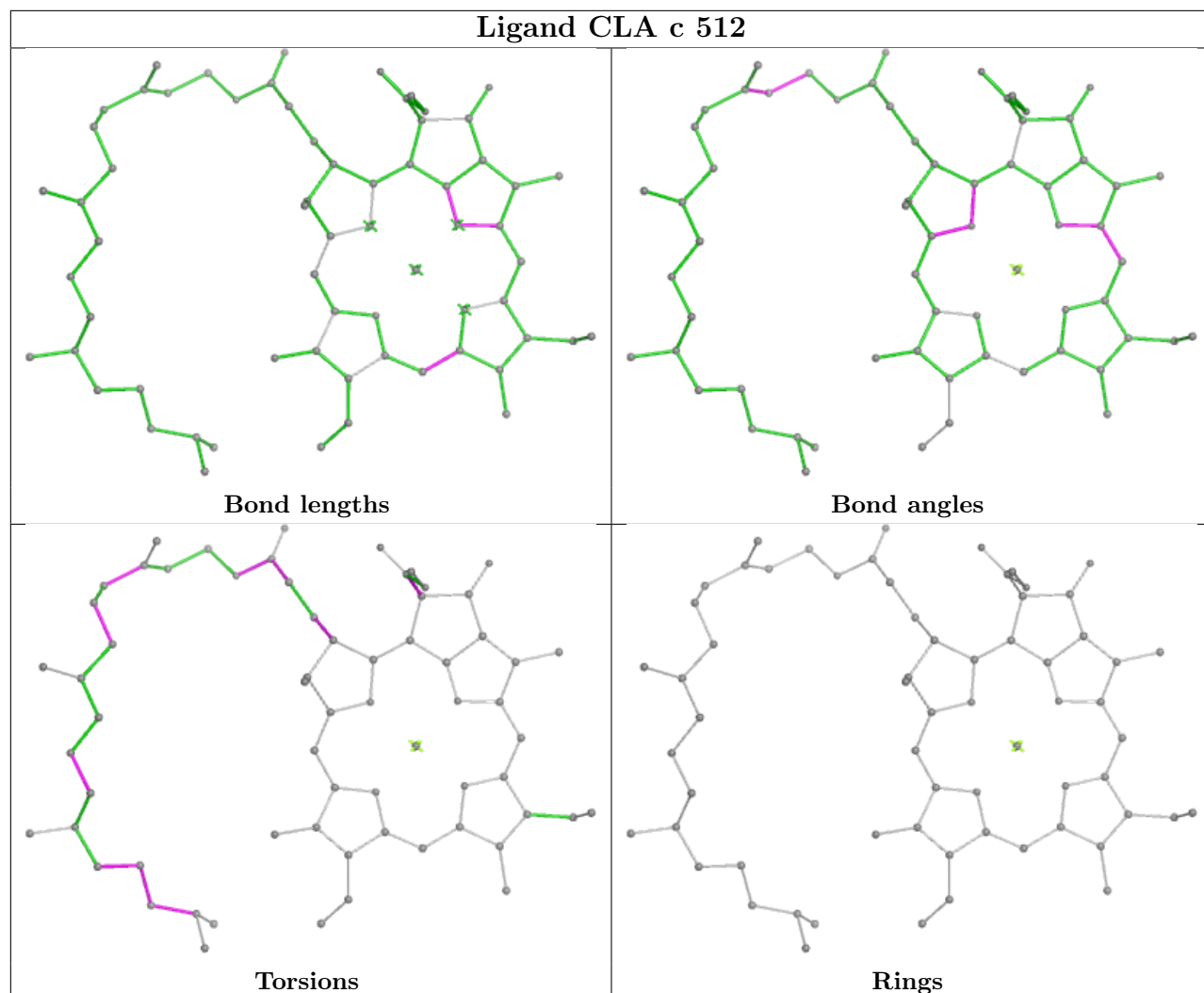




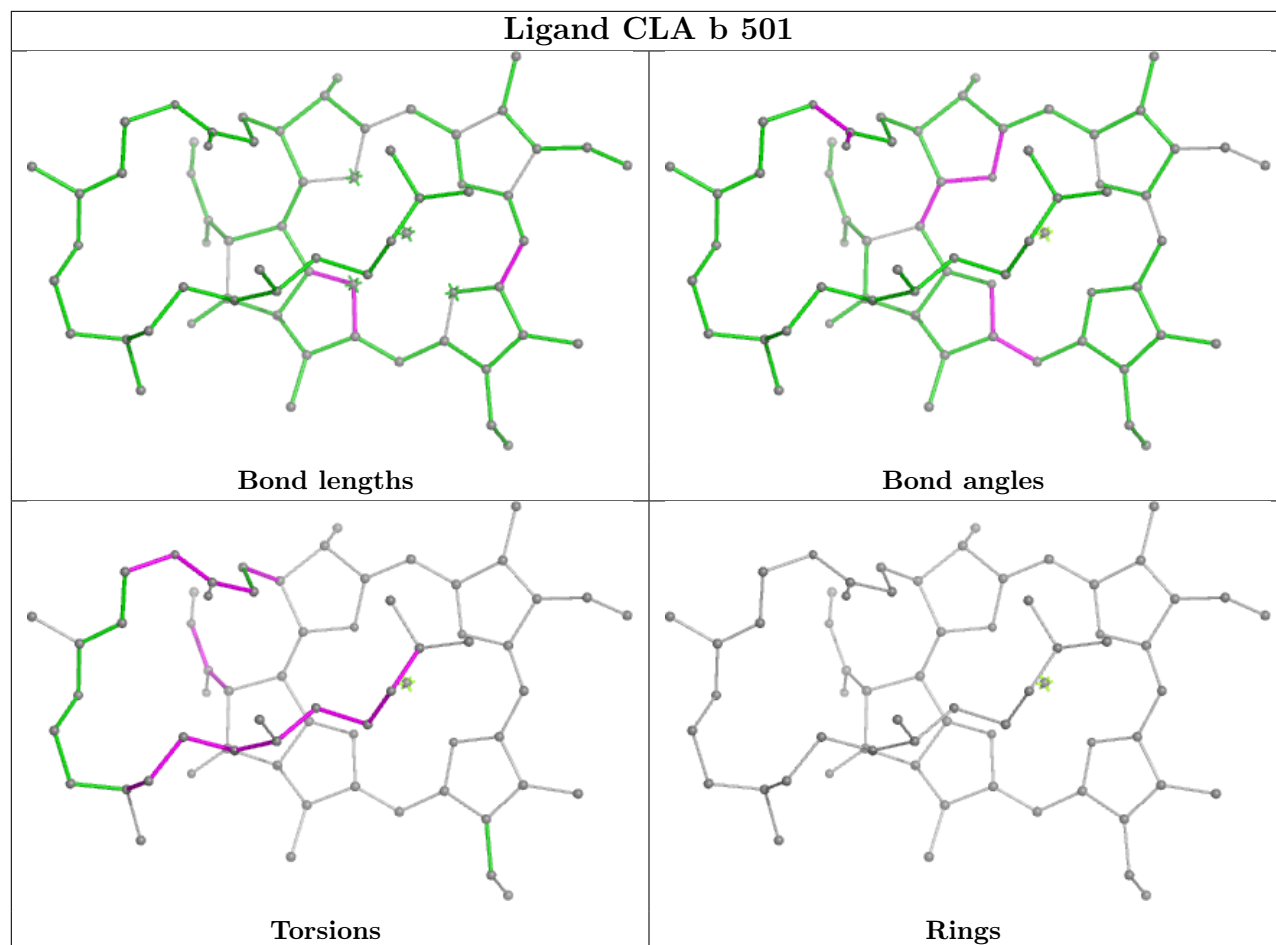


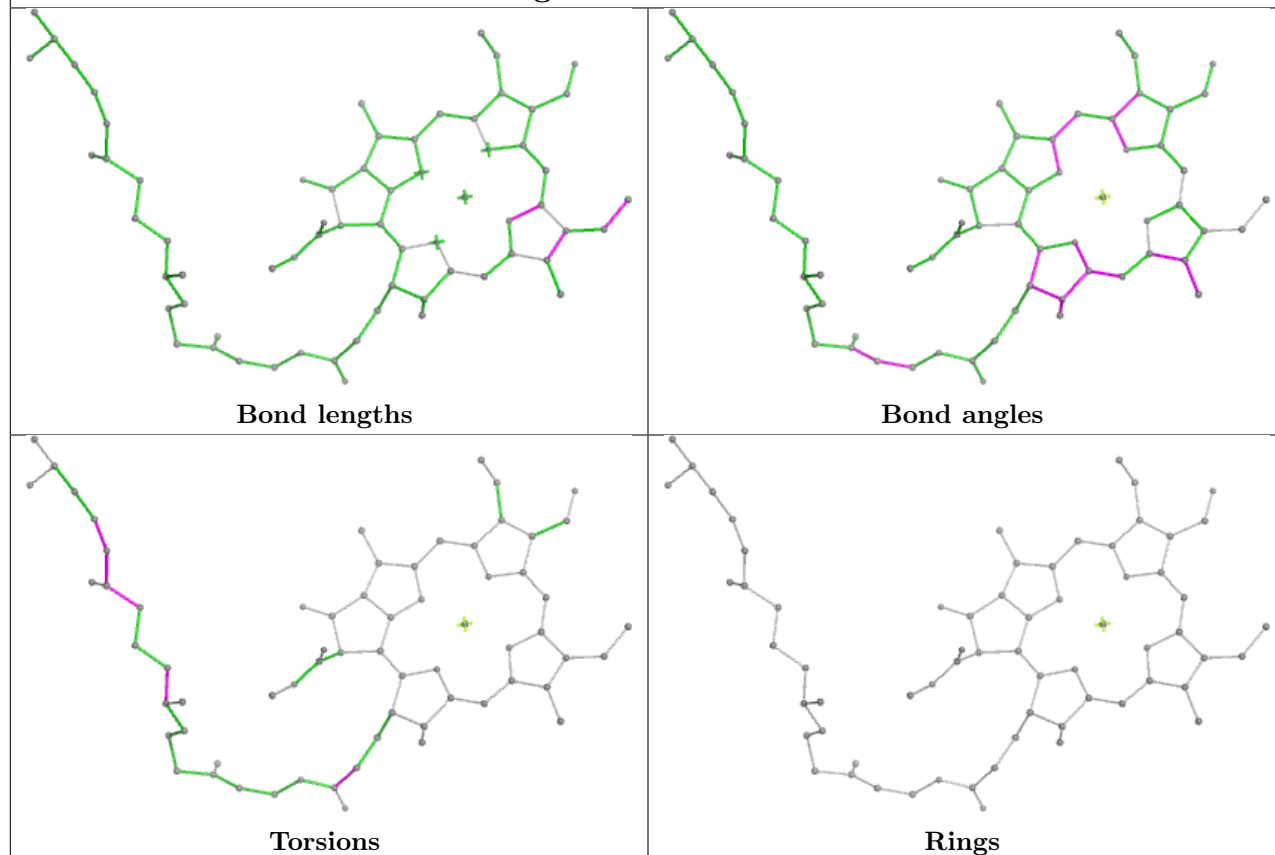
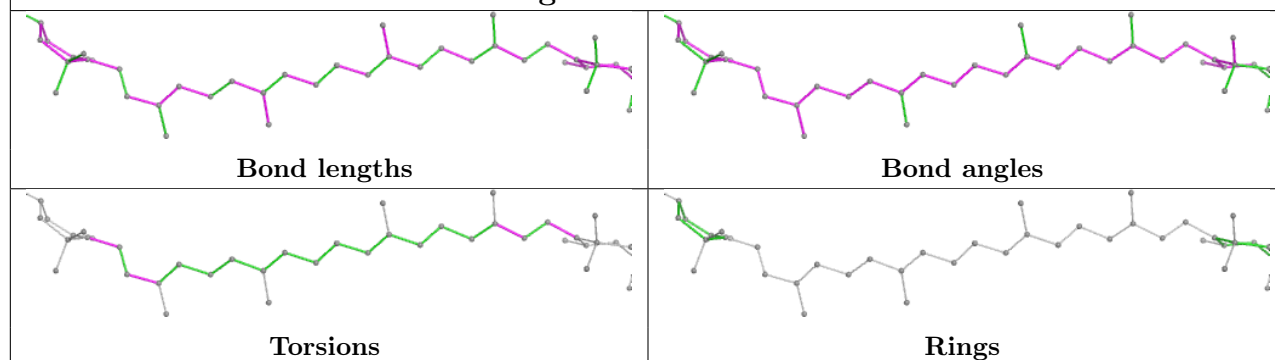


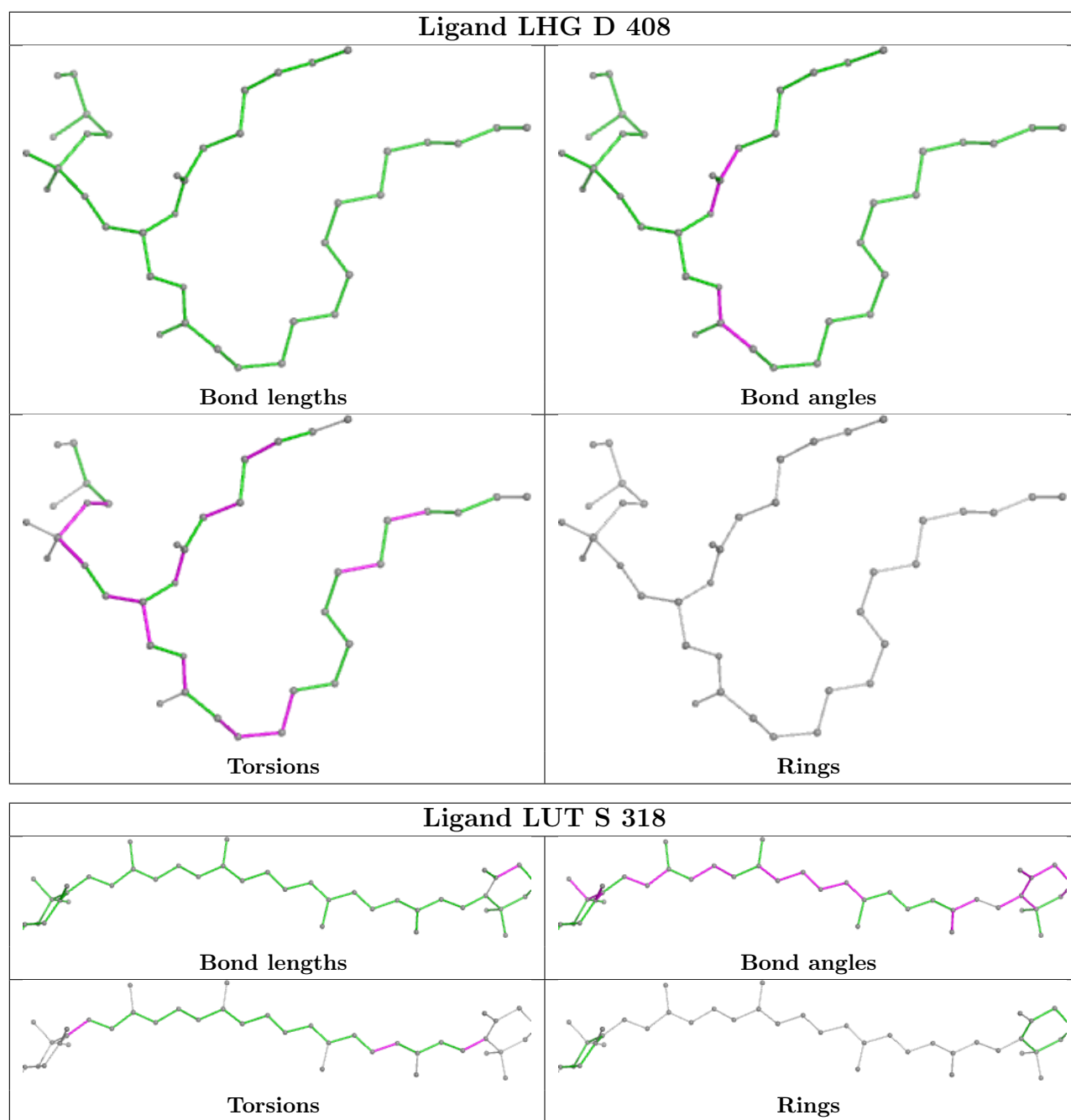
Ligand CLA c 512

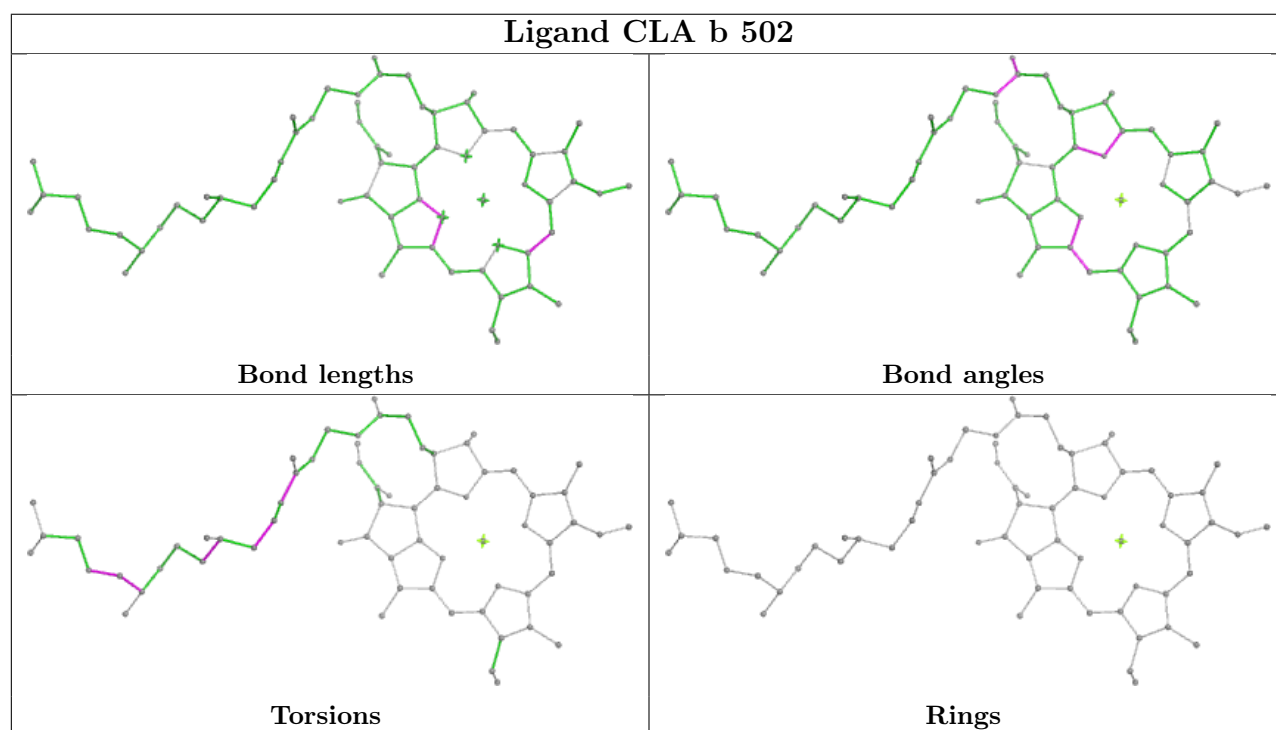
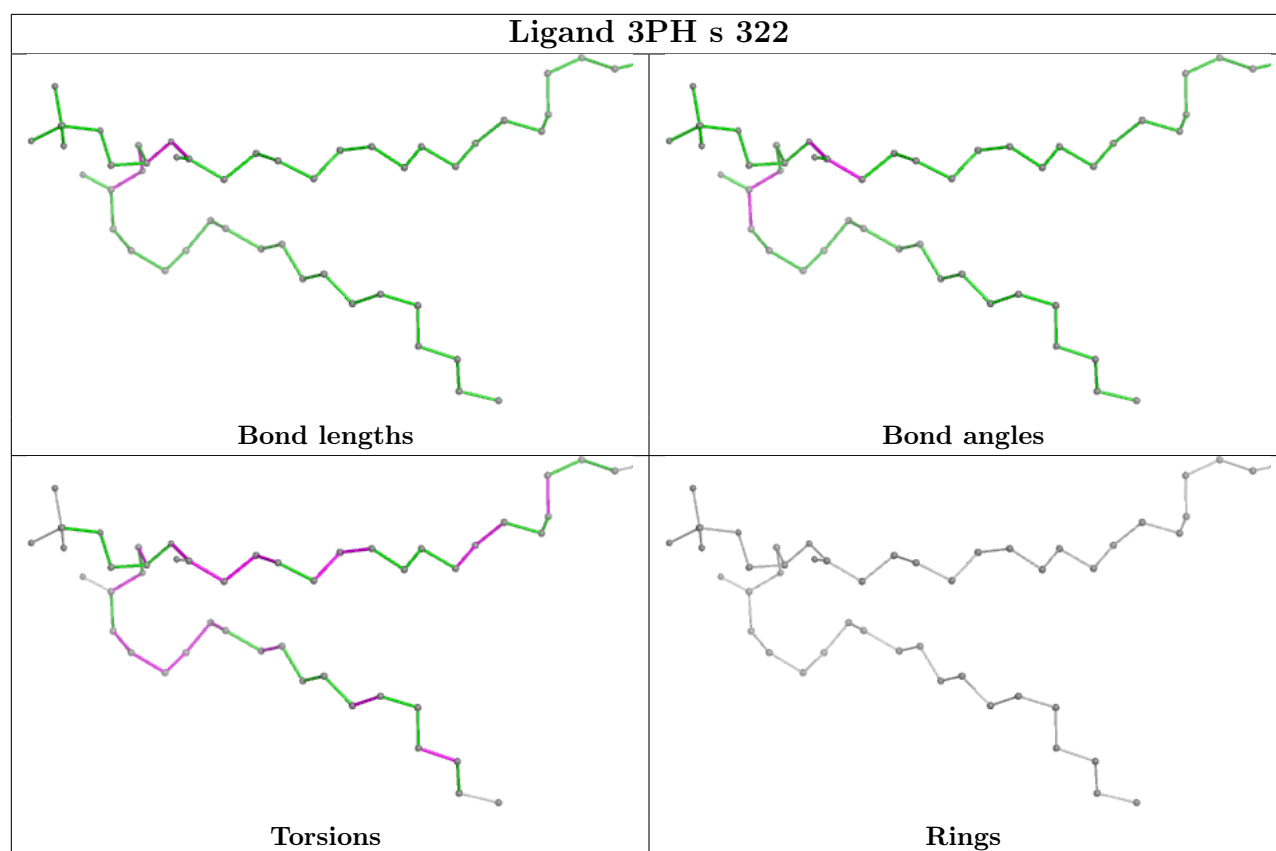


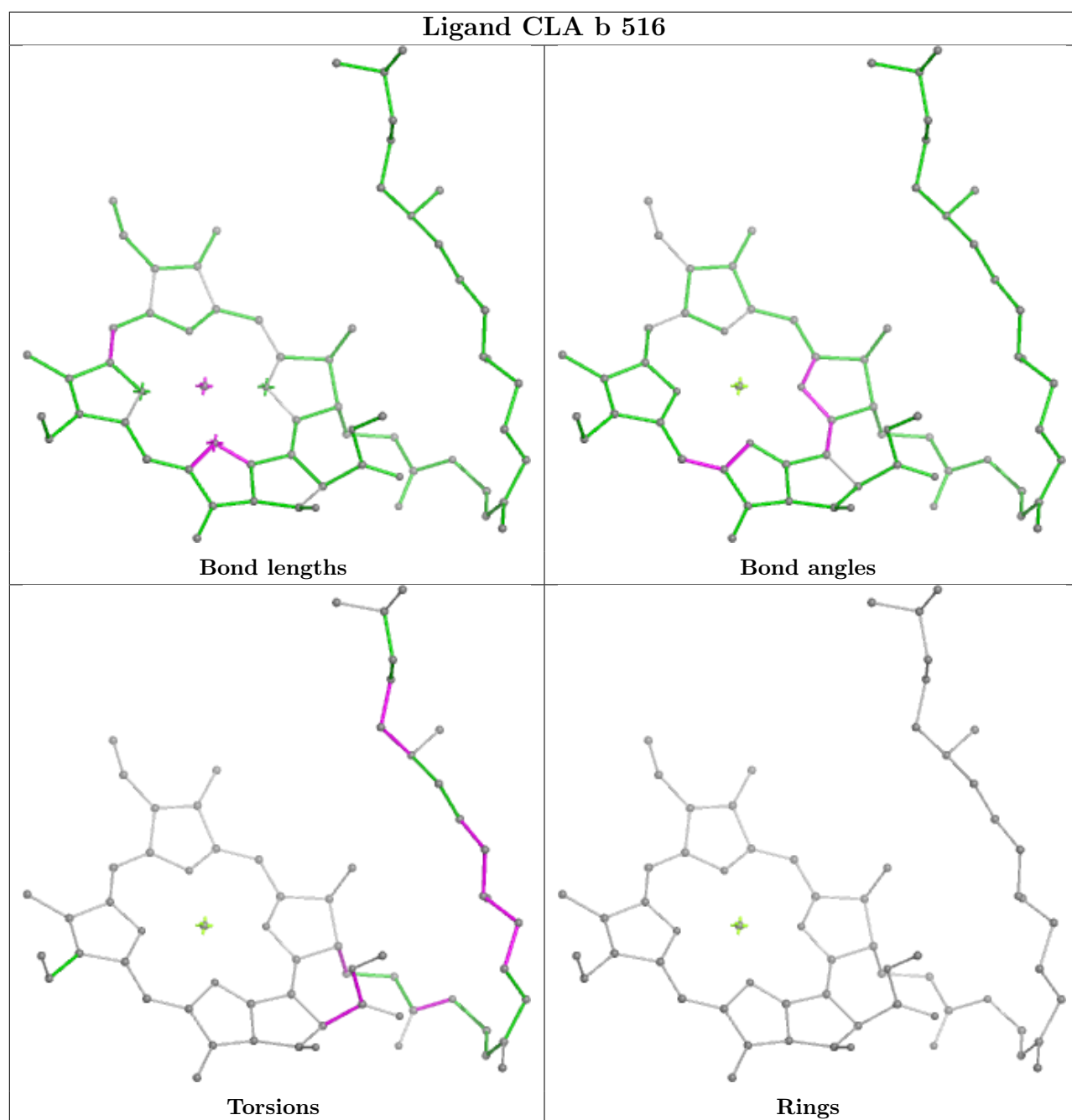
Ligand CLA b 501

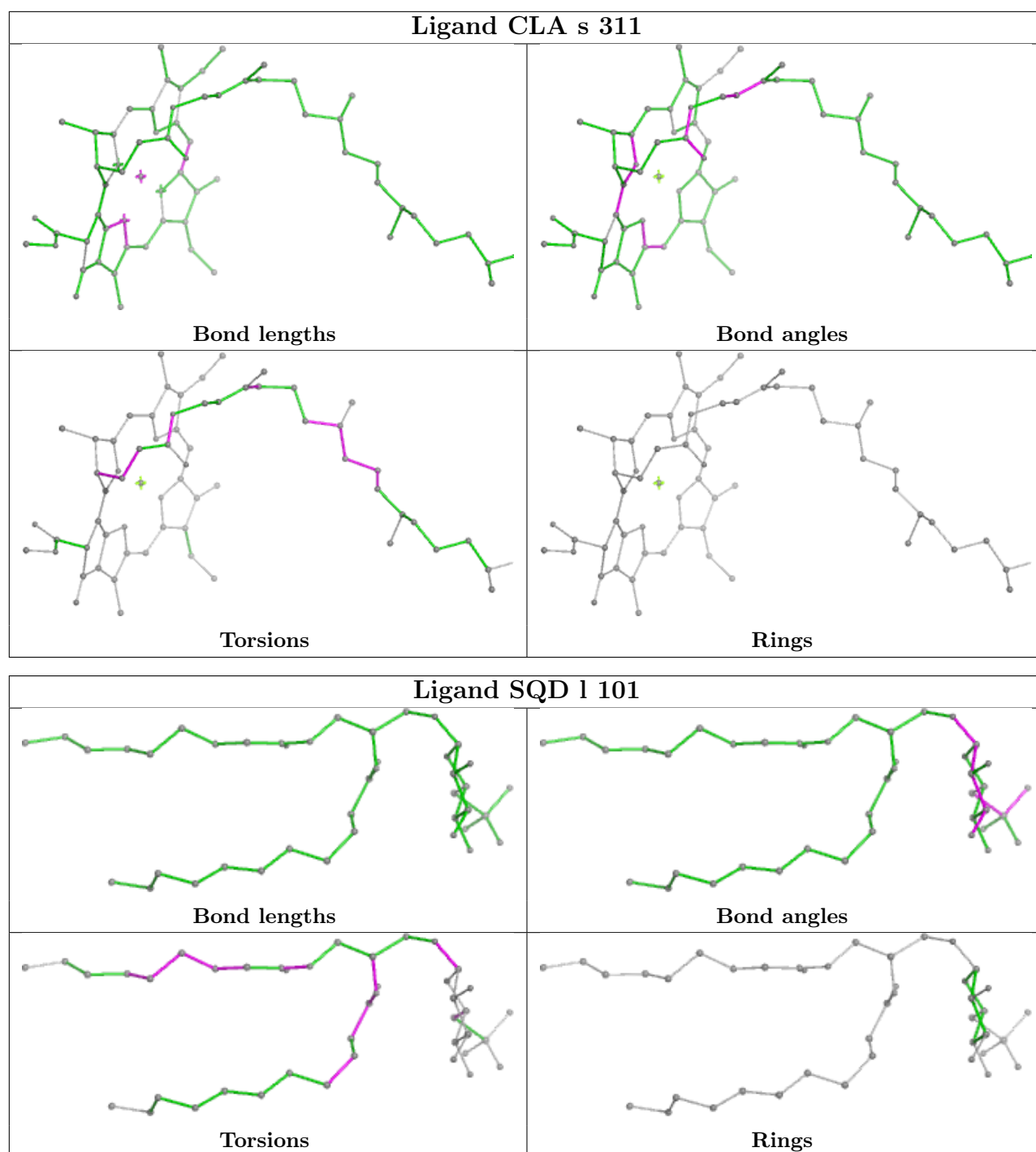


Ligand CHL n 606**Ligand C7Z b 519**

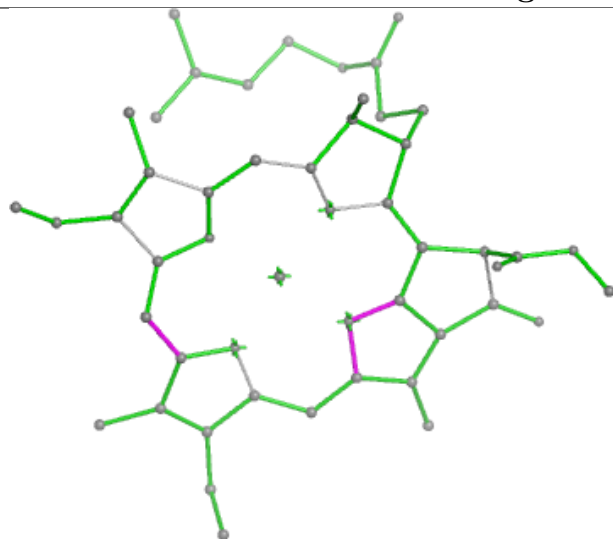




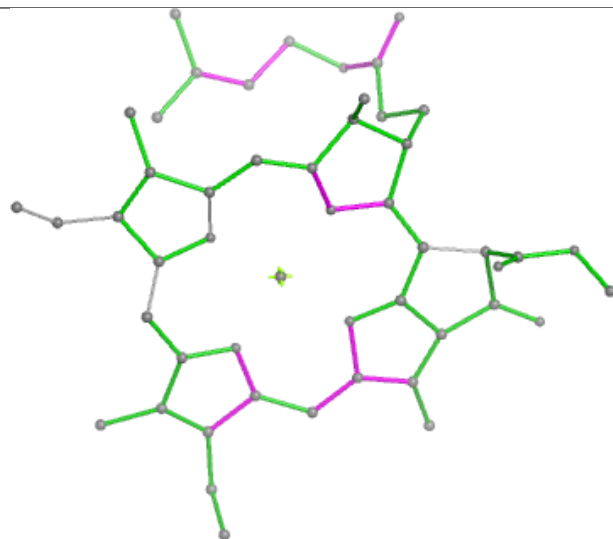




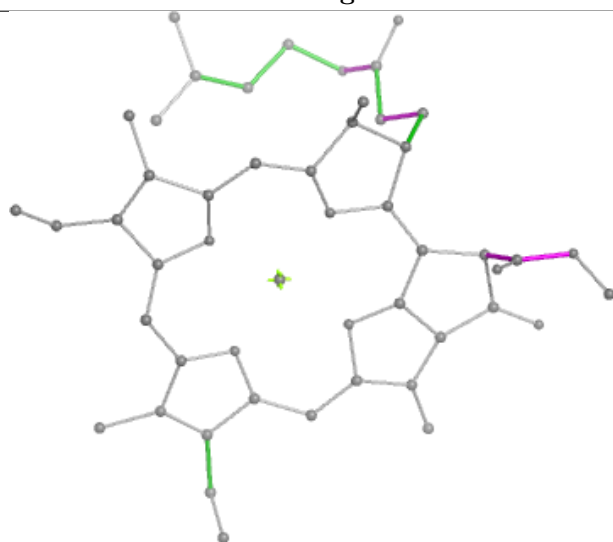
Ligand CLA S 316



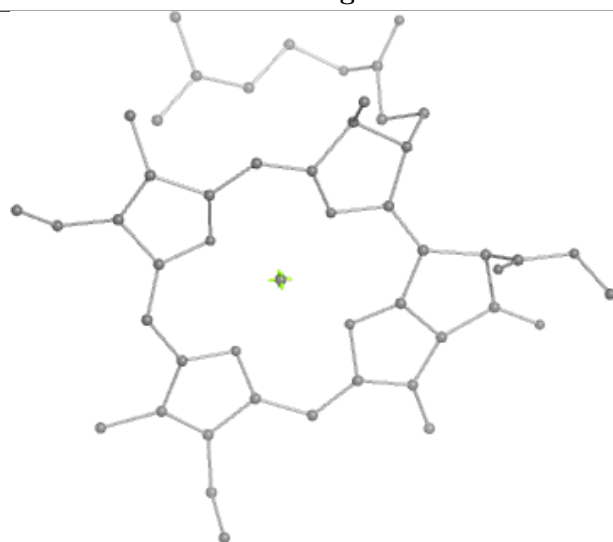
Bond lengths



Bond angles

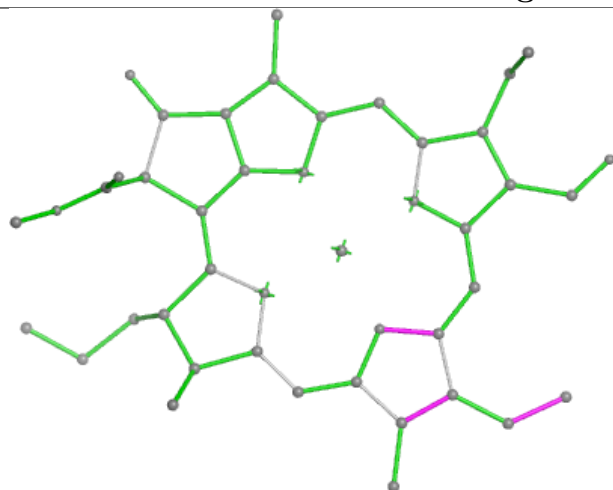


Torsions

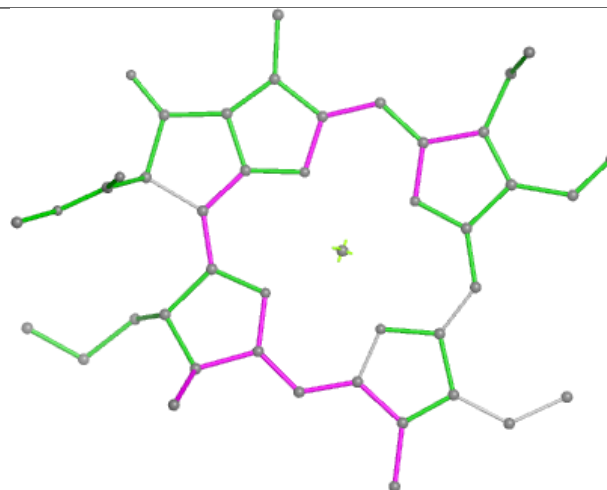


Rings

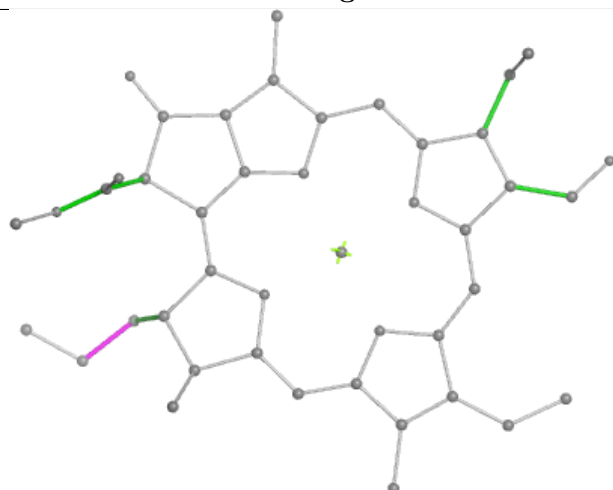
Ligand CHL S 307



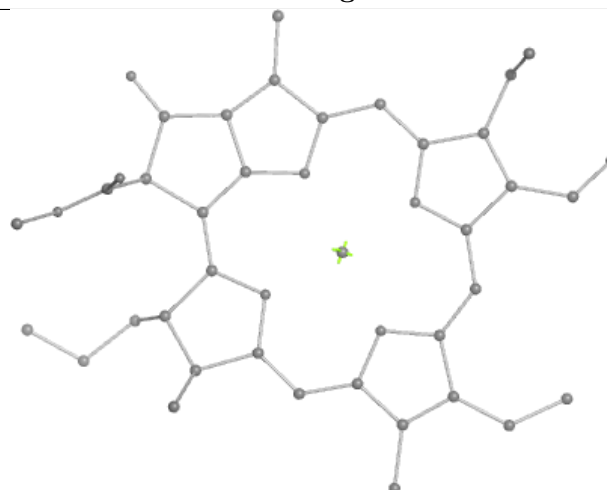
Bond lengths



Bond angles

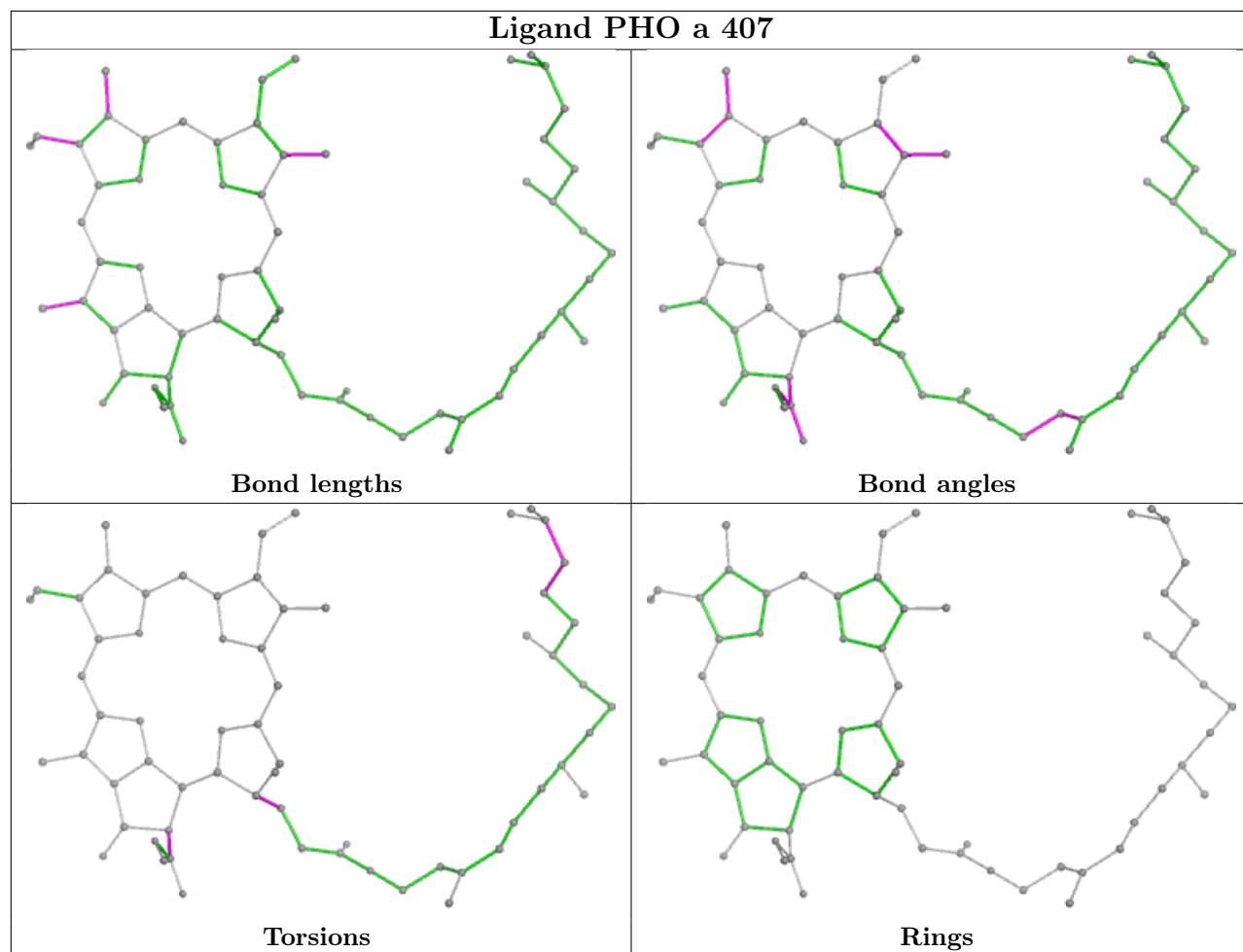


Torsions

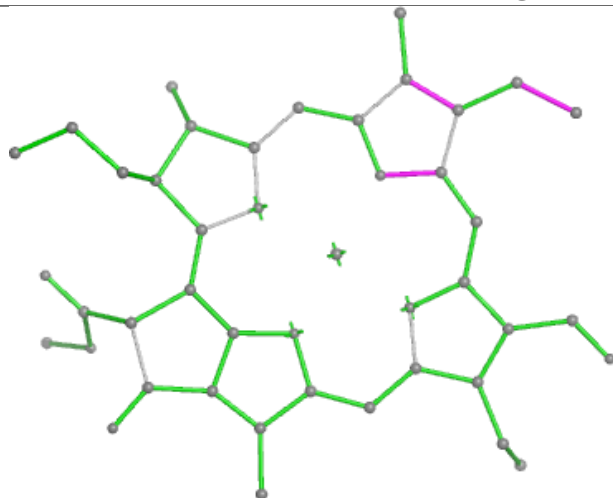


Rings

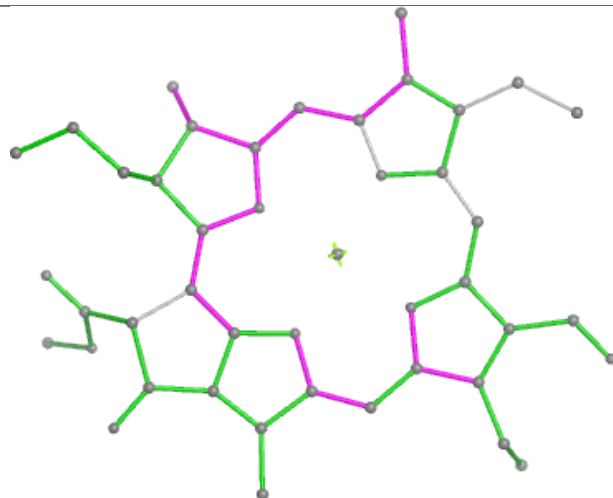
Ligand PHO a 407



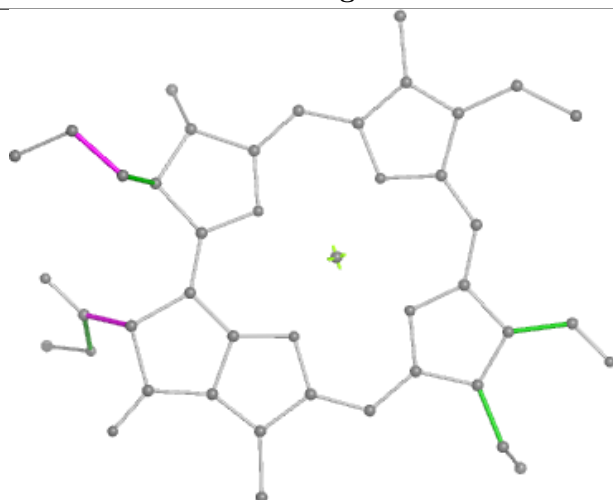
Ligand CHL R 304



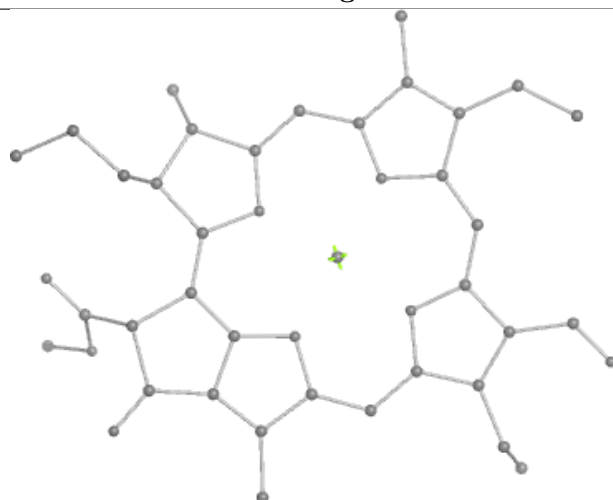
Bond lengths



Bond angles

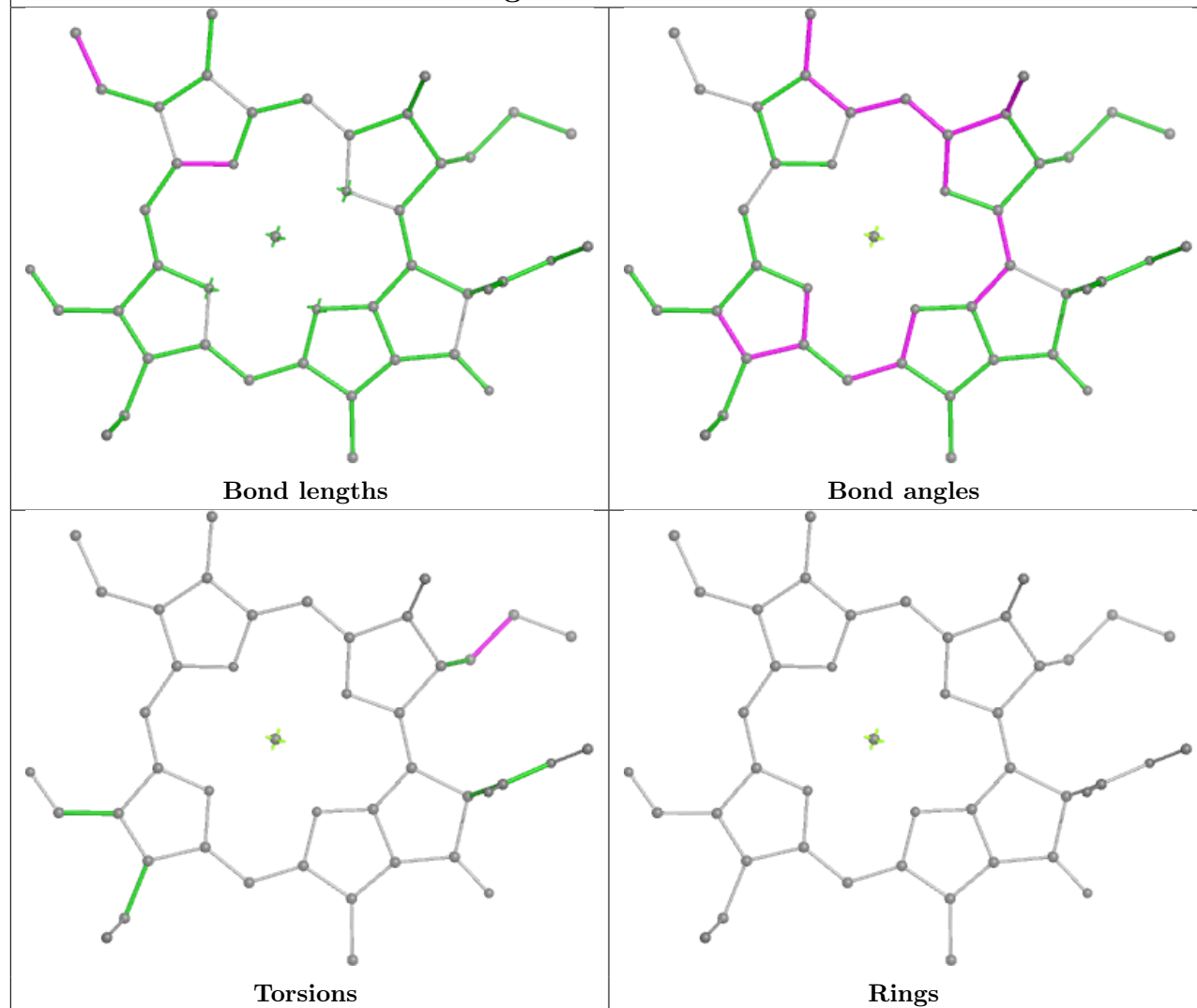


Torsions

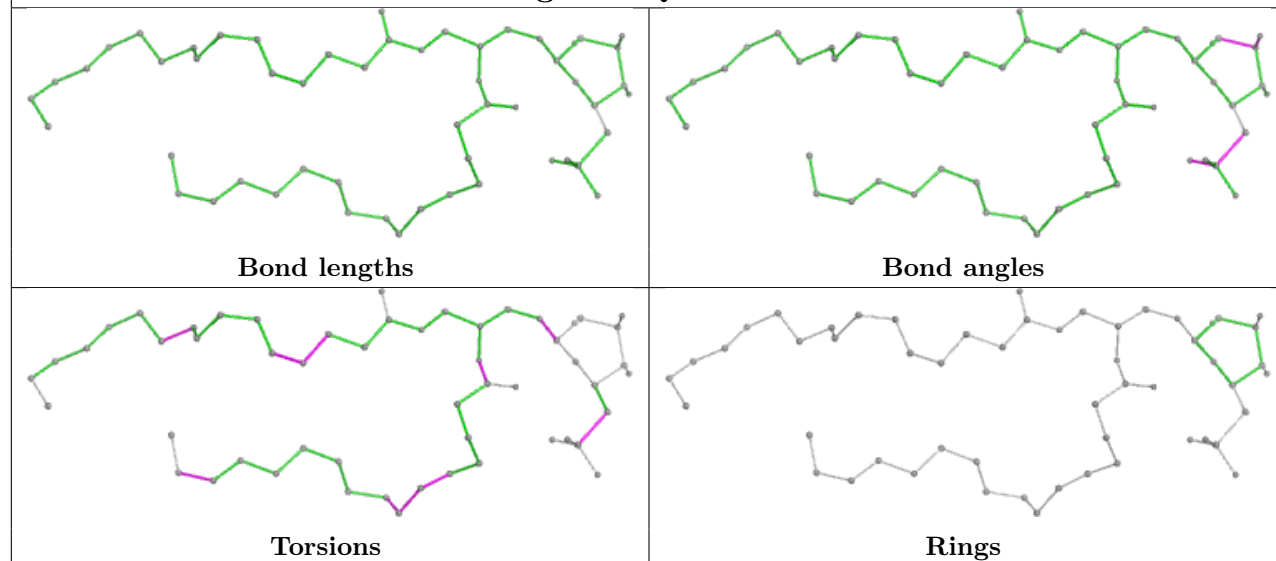


Rings

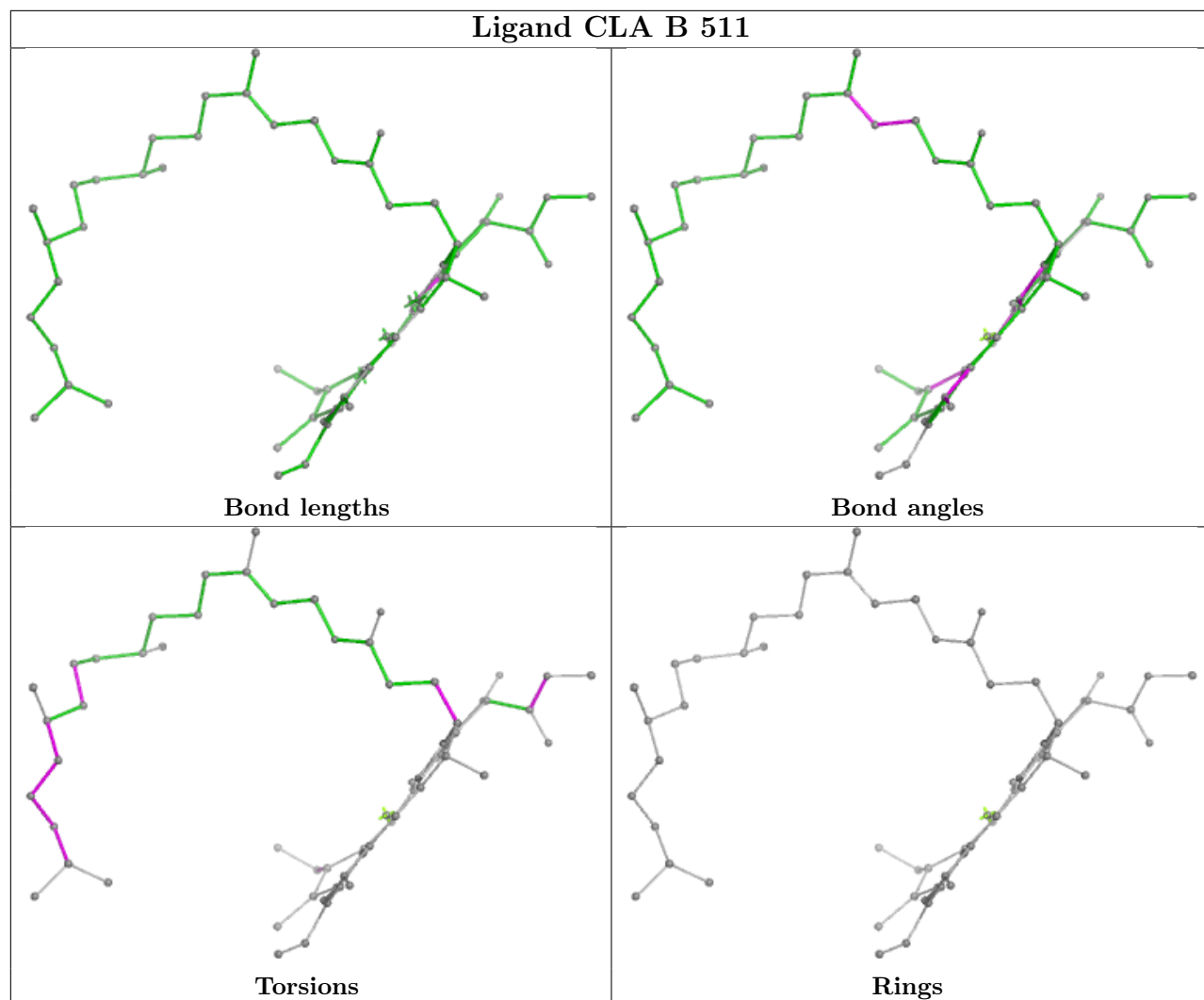
Ligand CHL s 307



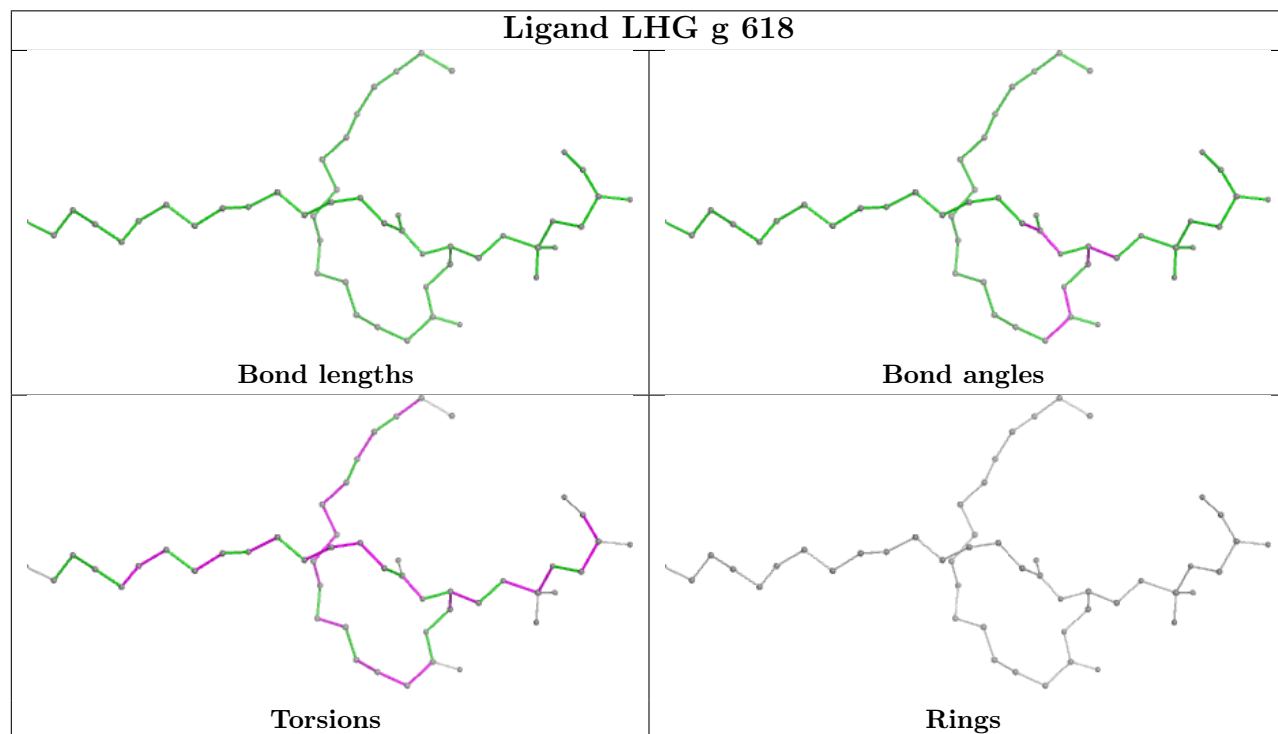
Ligand SQD o 301

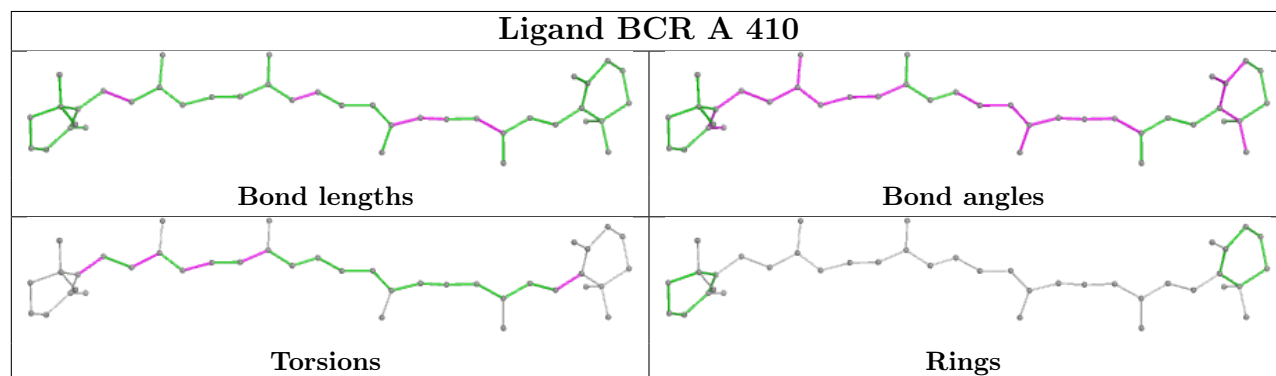
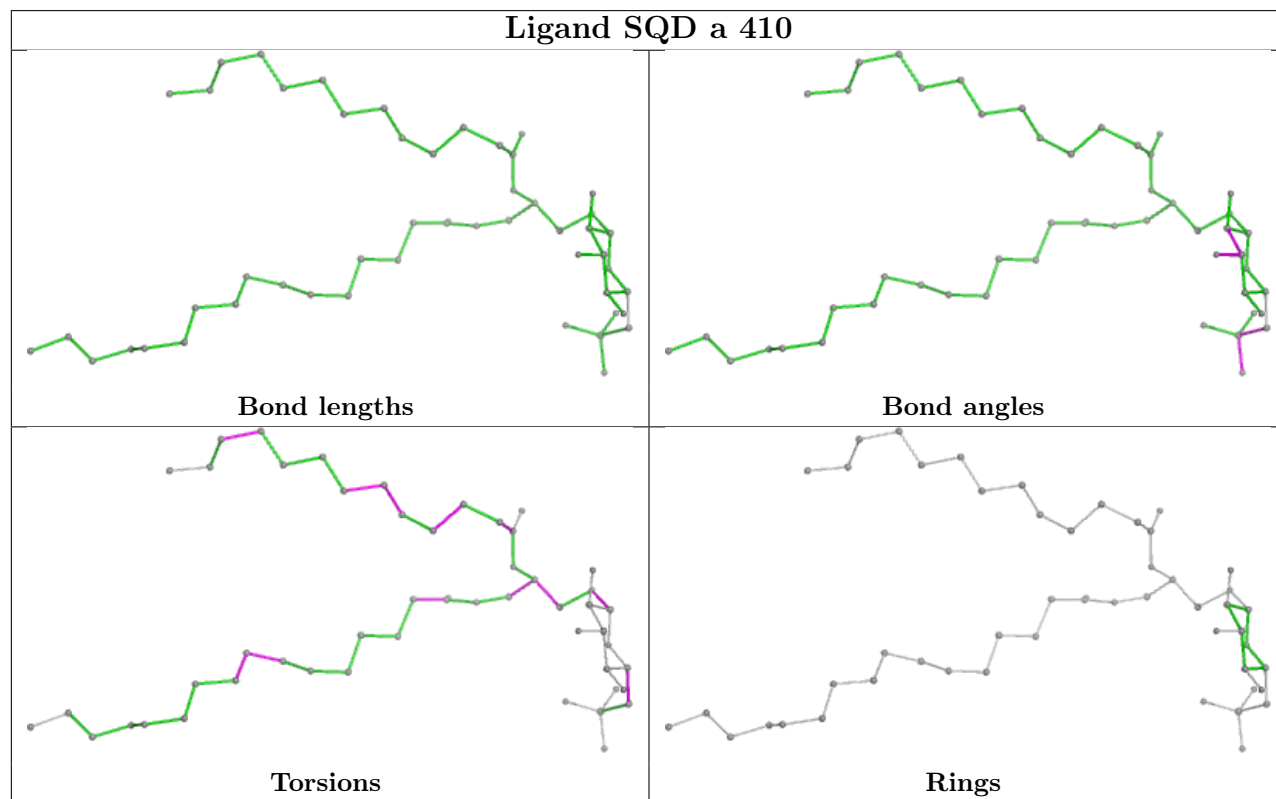
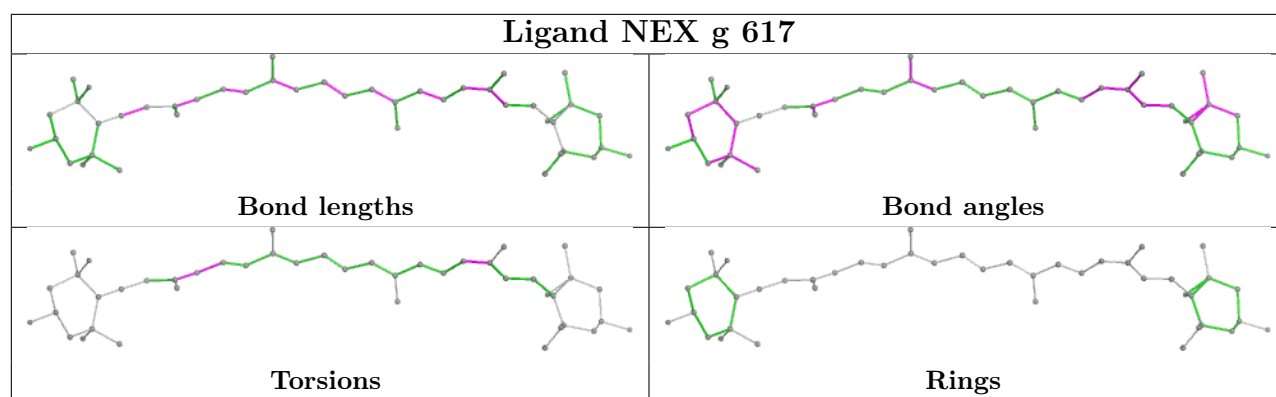


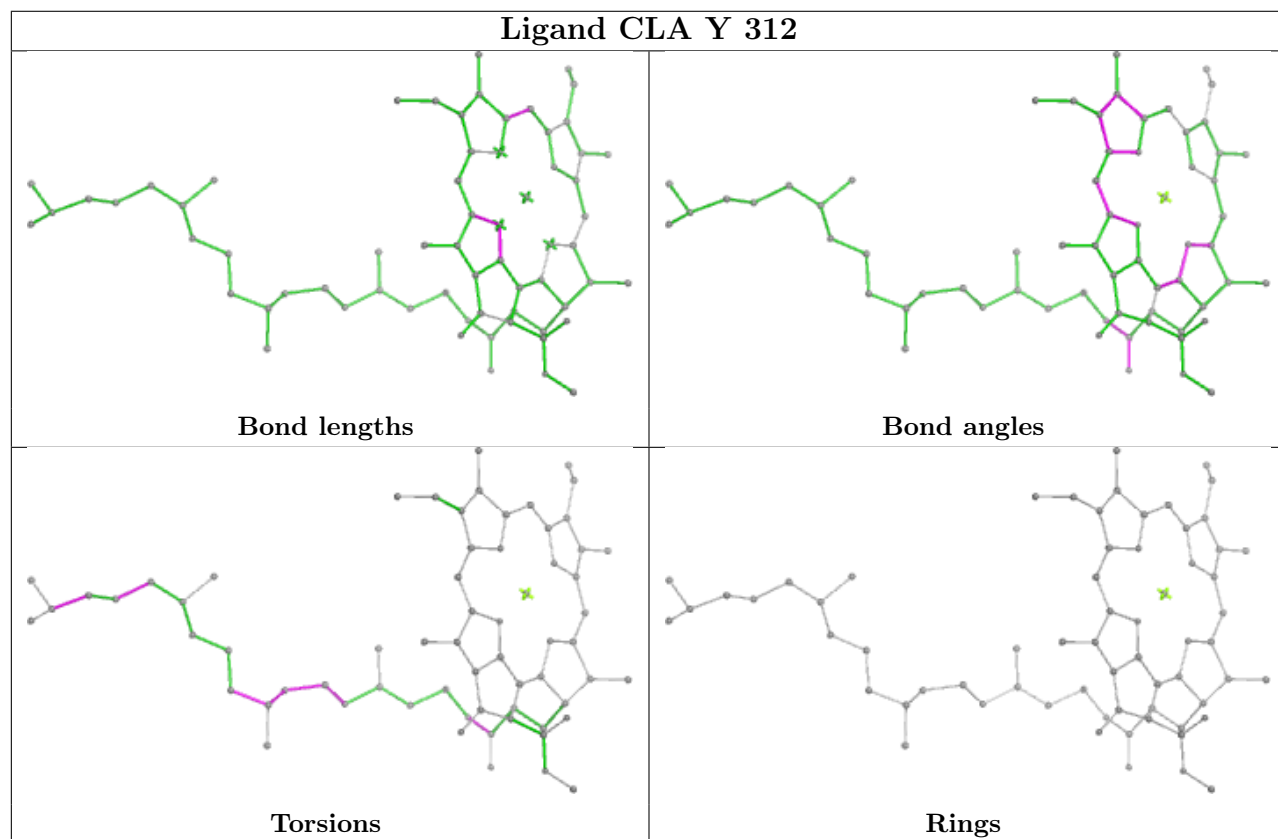
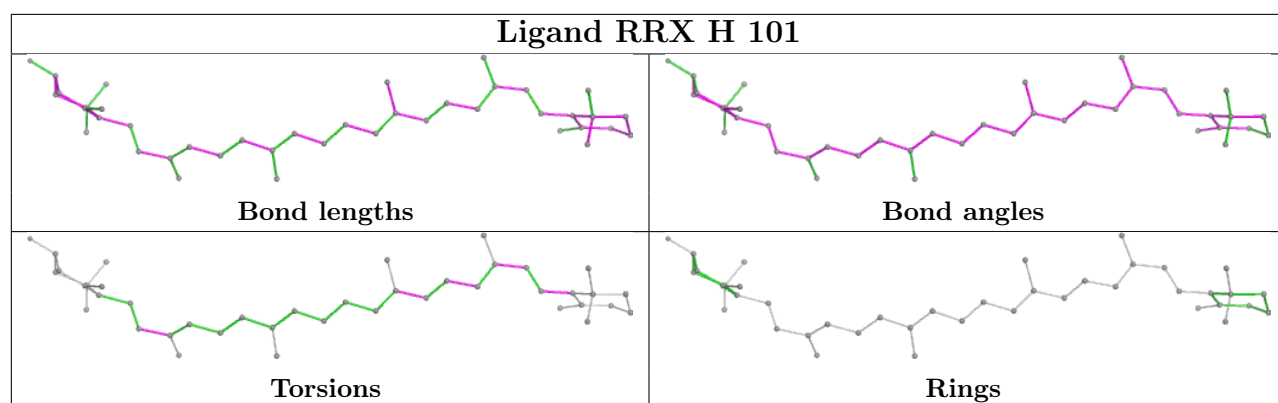
Ligand CLA B 511

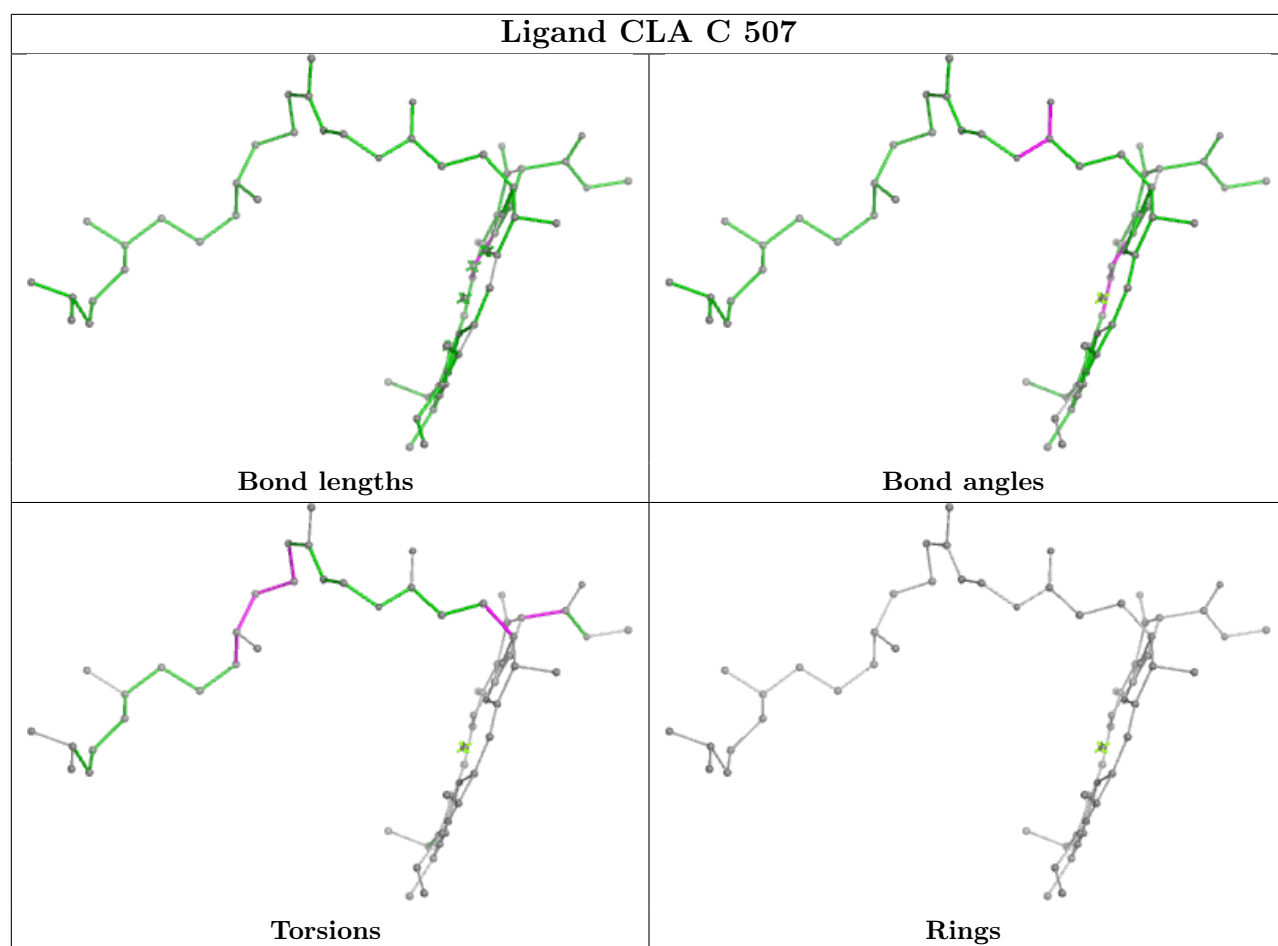


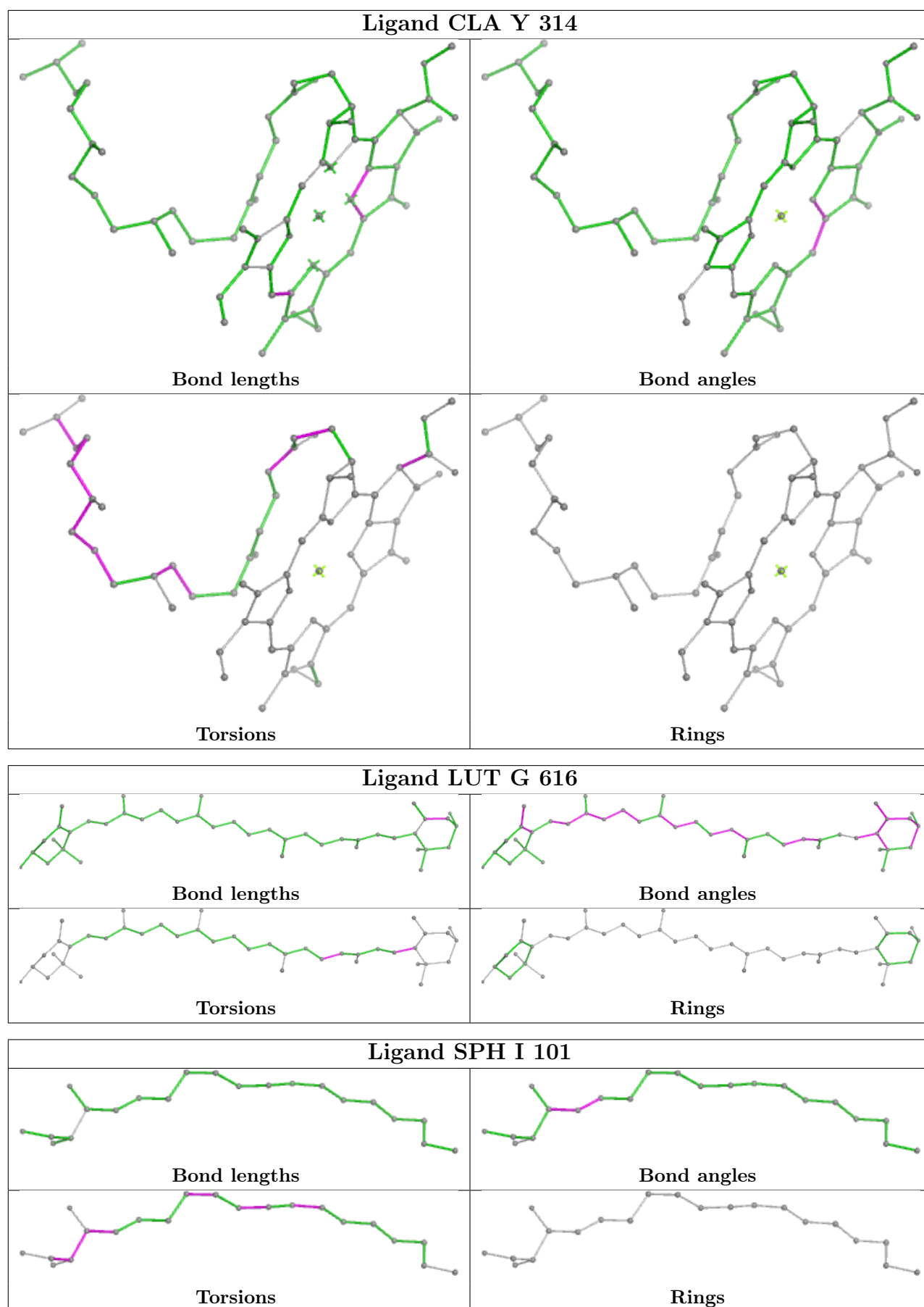
Ligand LHG g 618

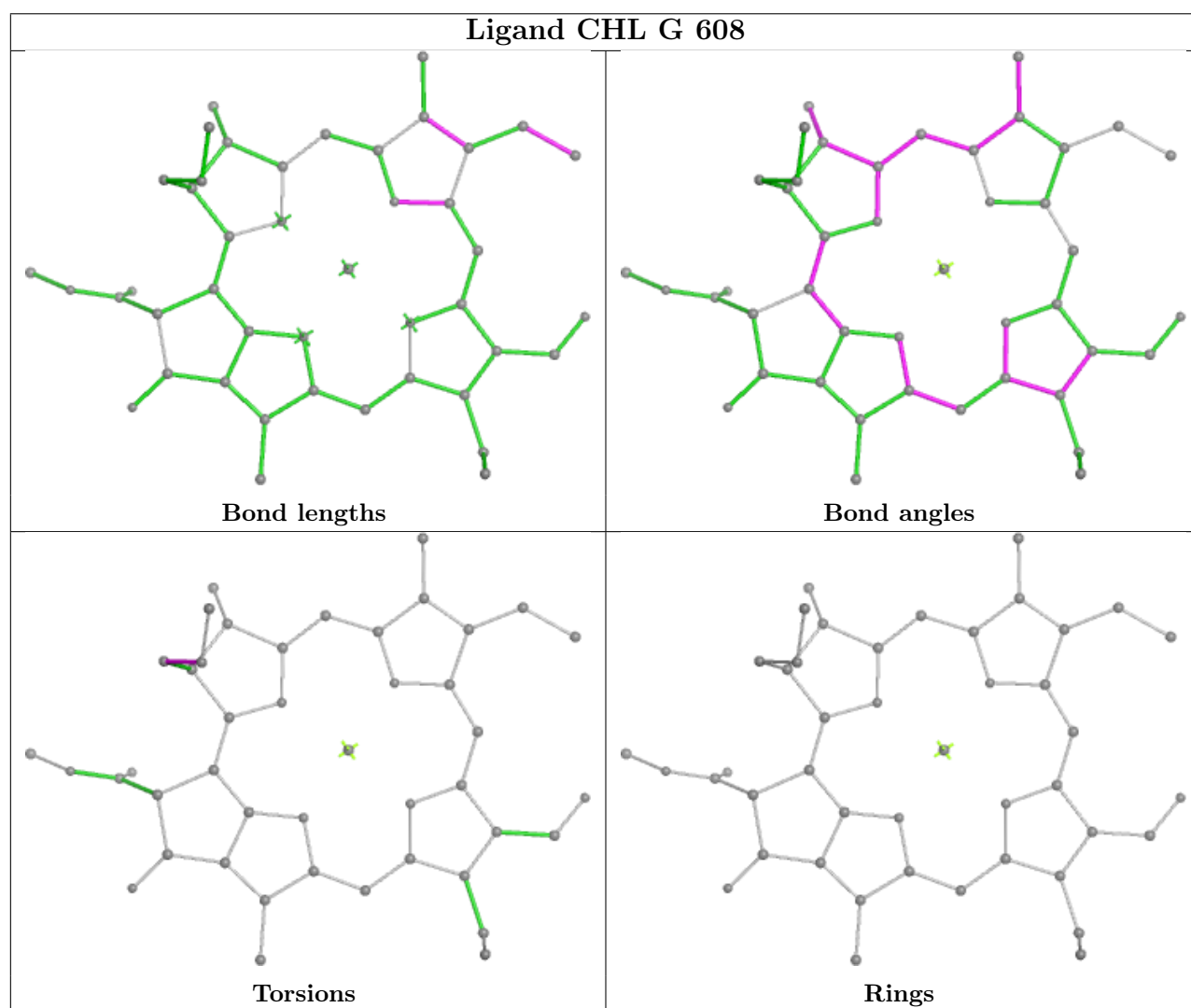
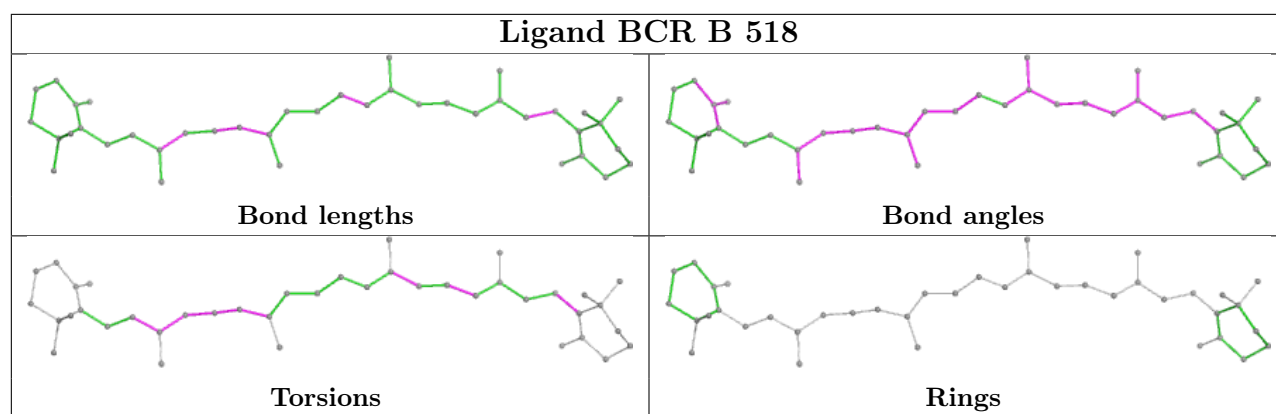


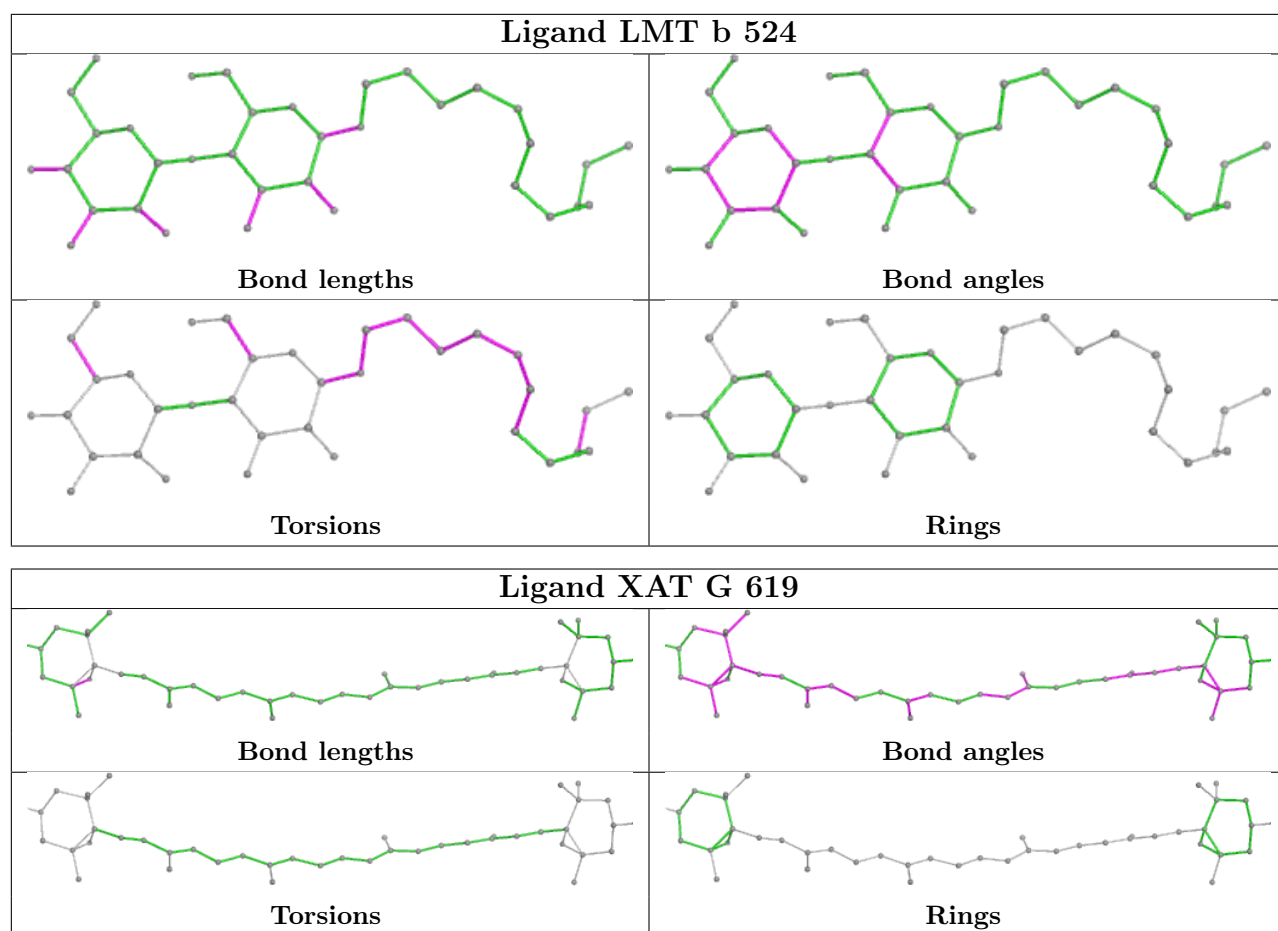




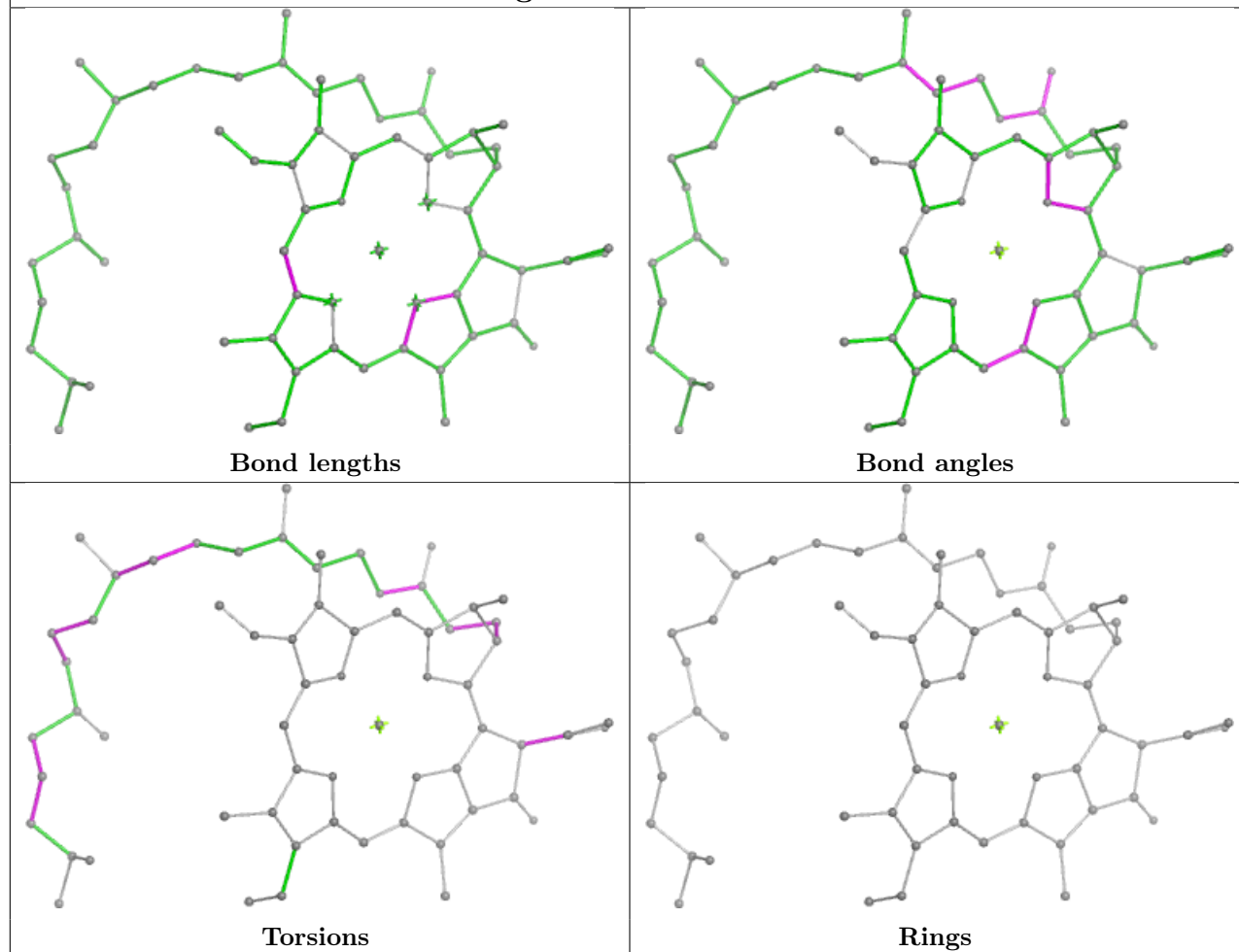




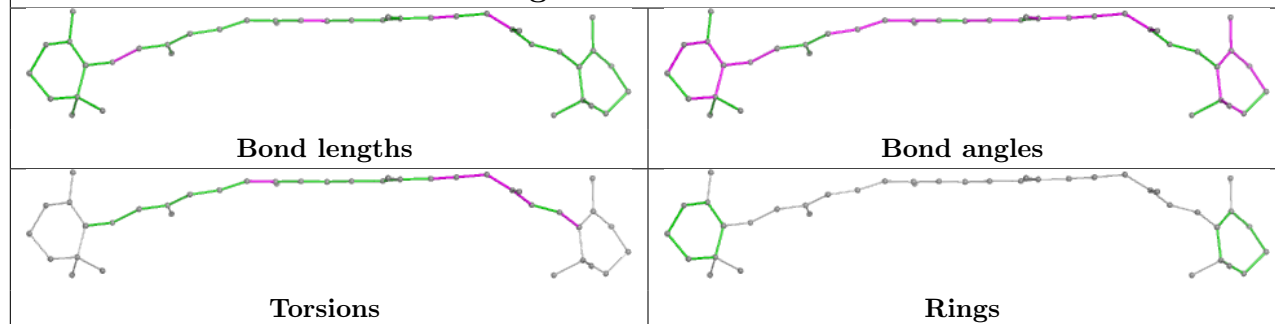




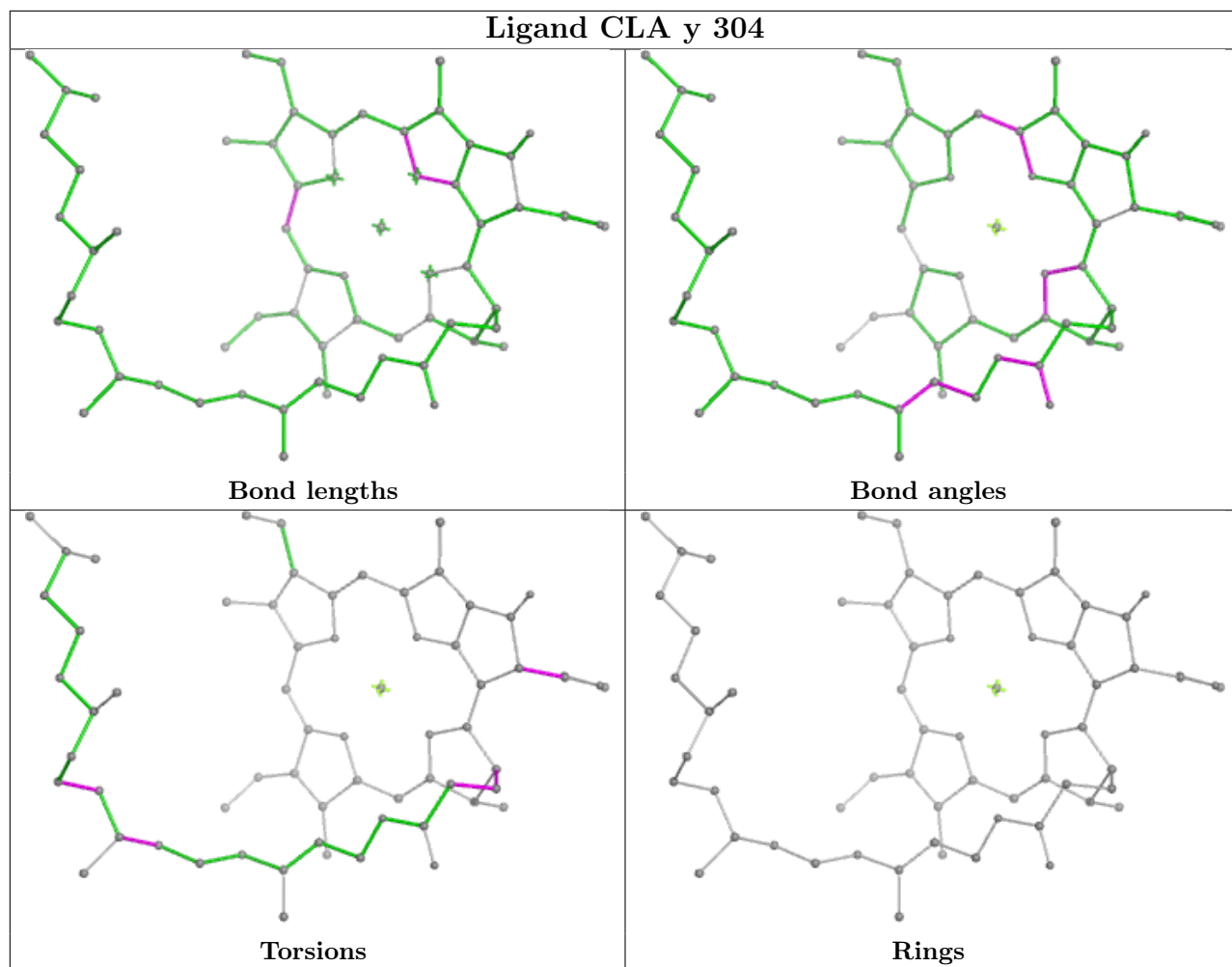
Ligand CLA Y 303



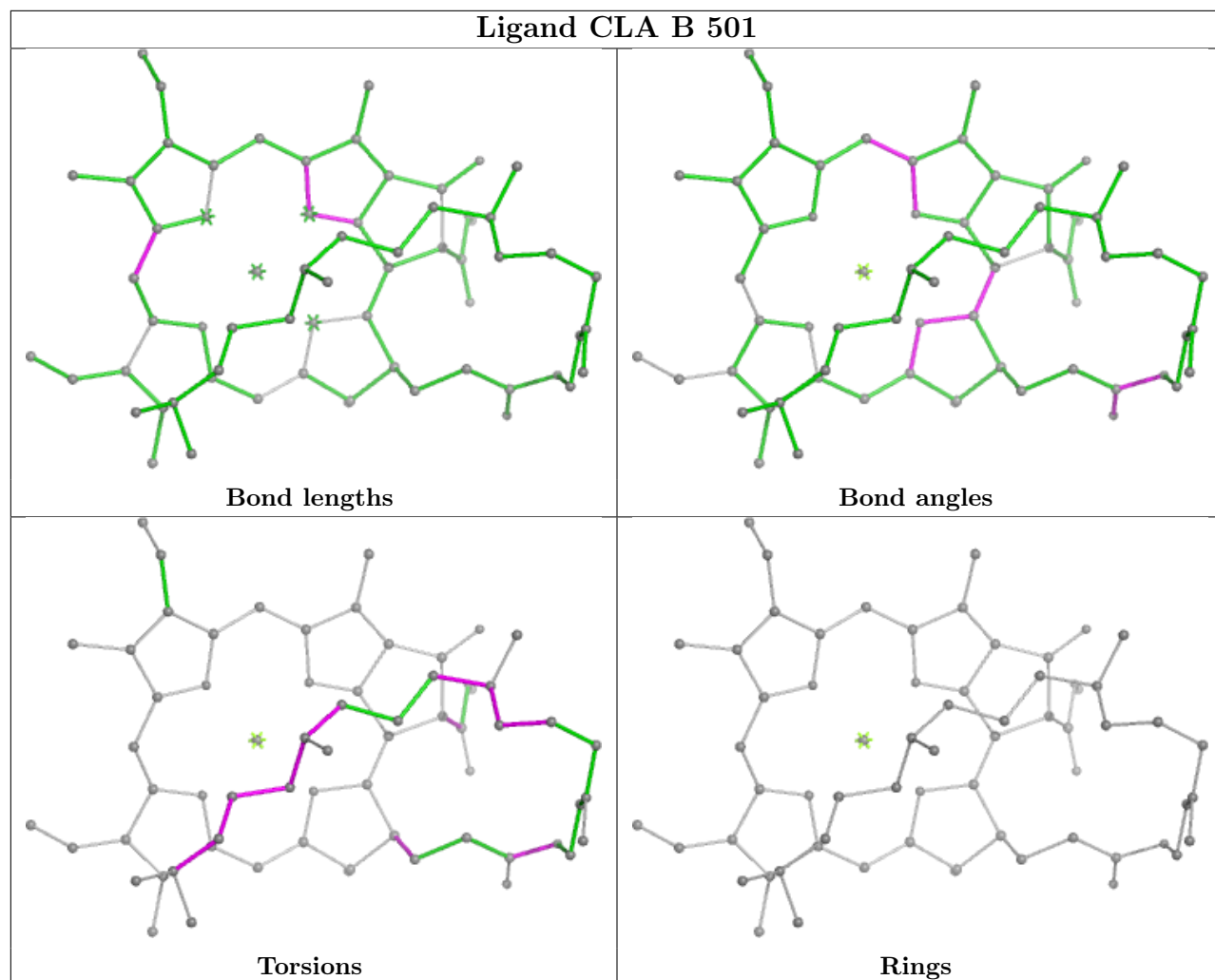
Ligand BCR C 517

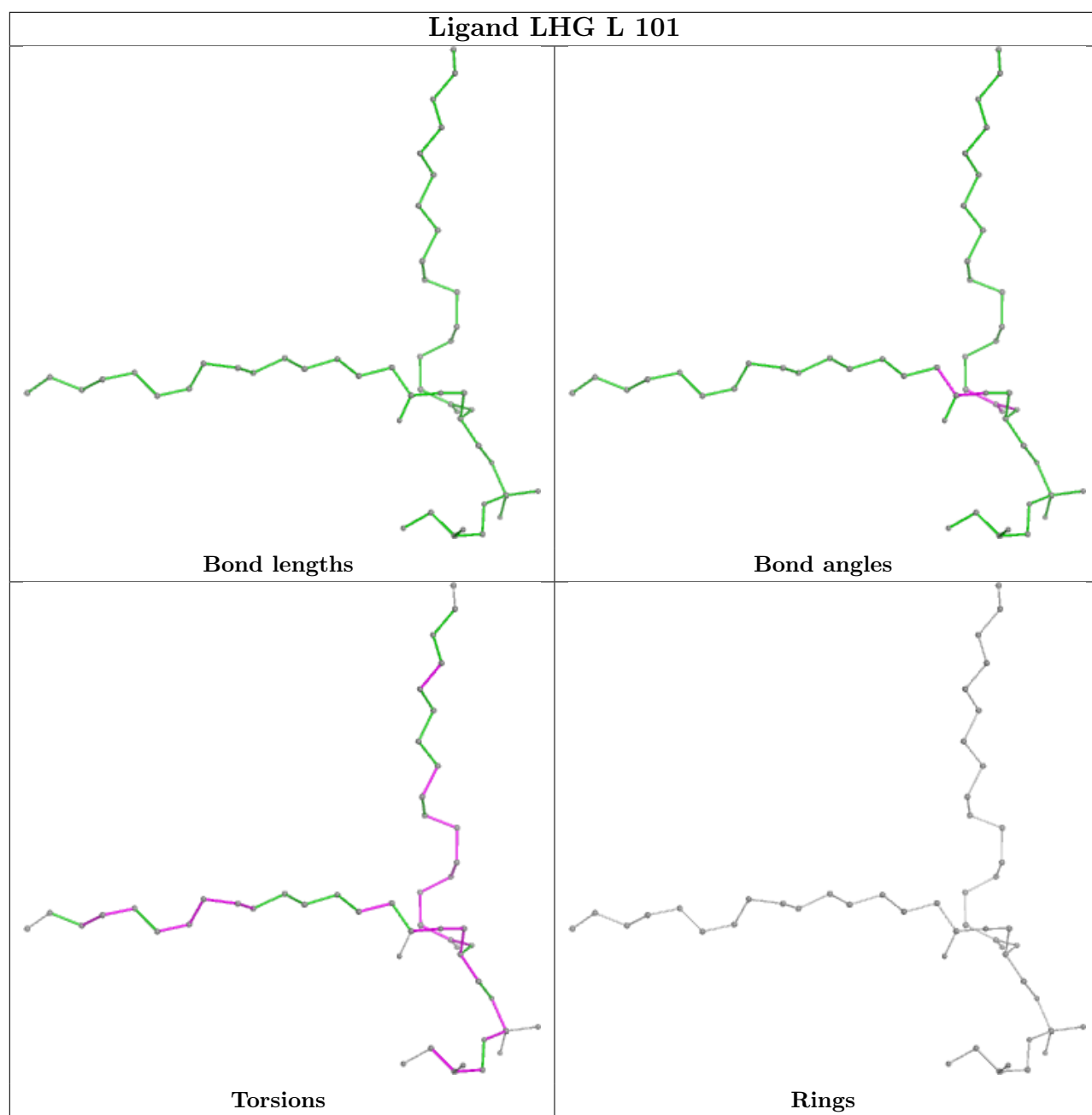


Ligand CLA y 304

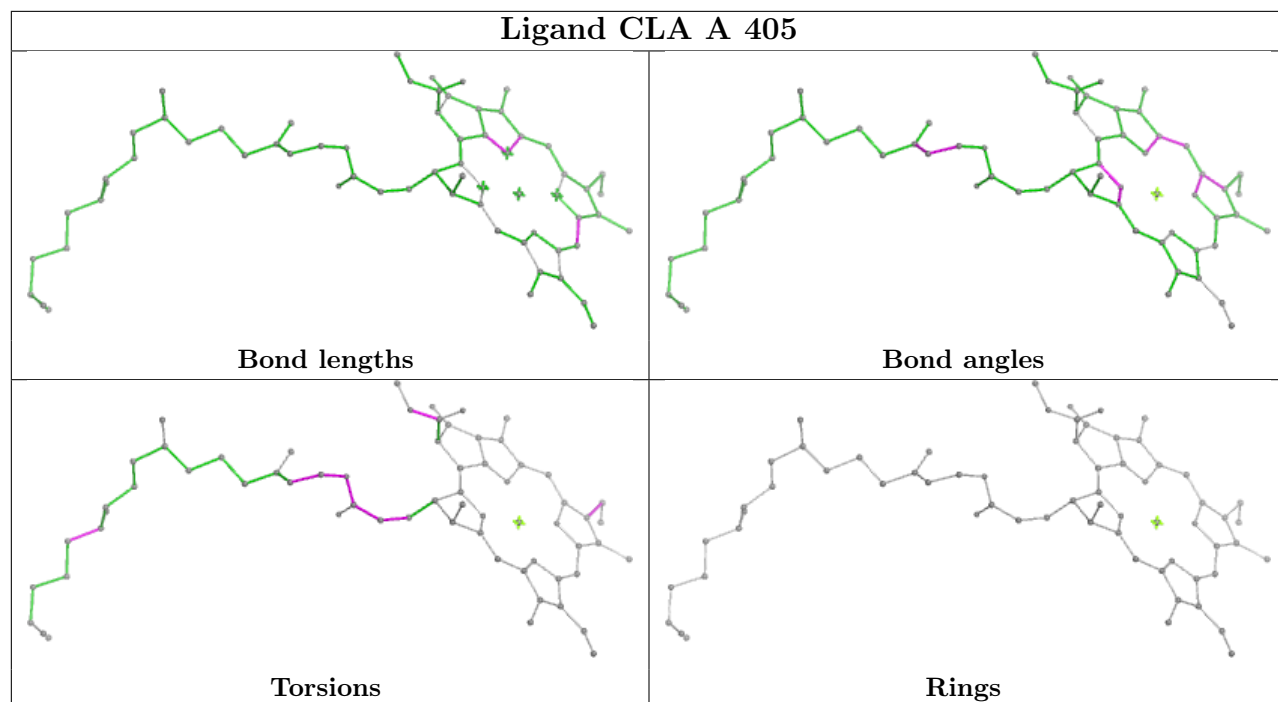


Ligand CLA B 501

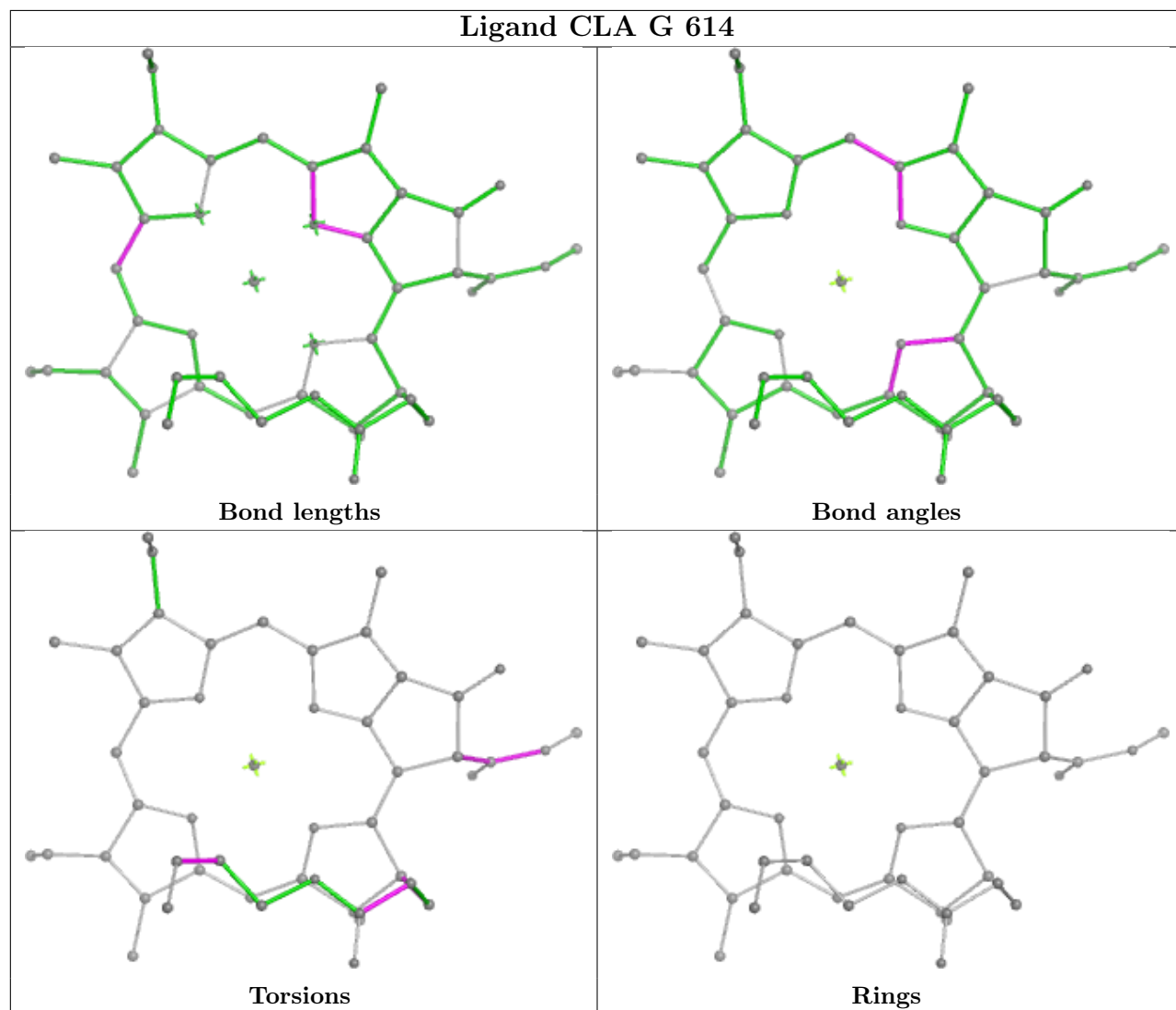


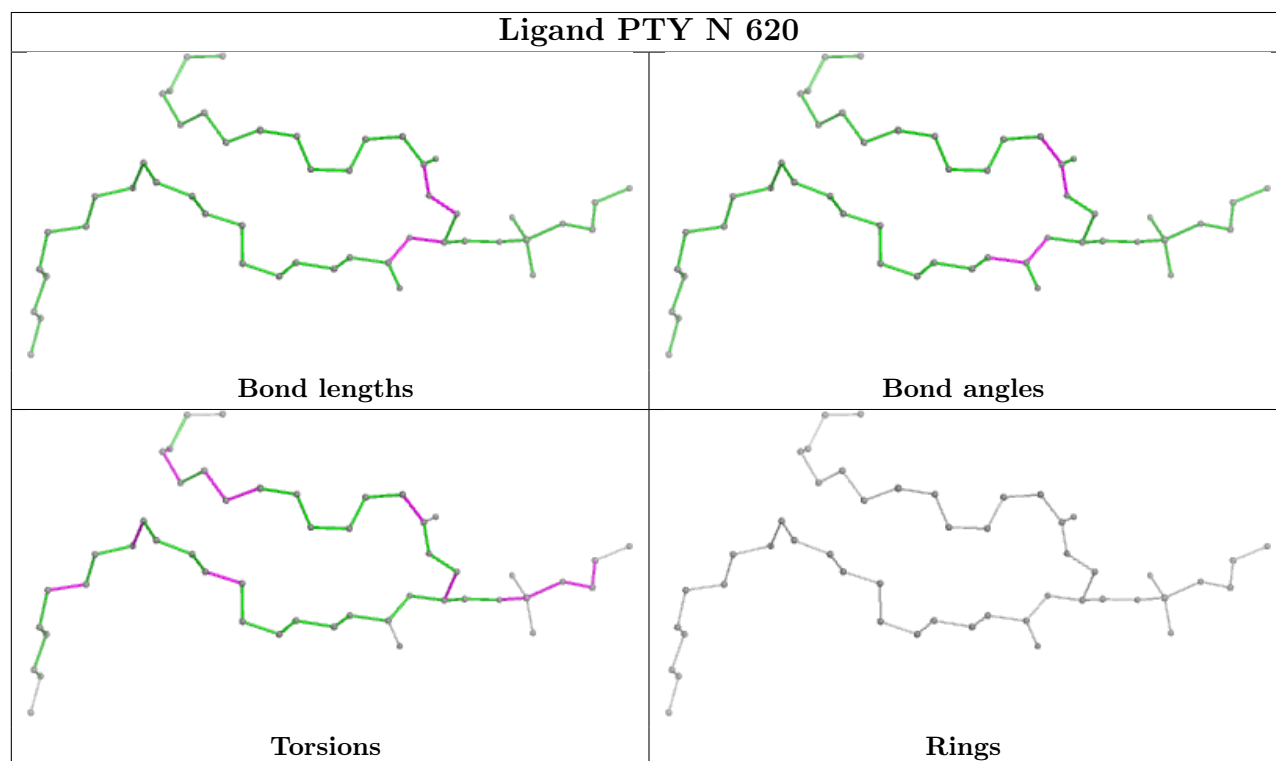
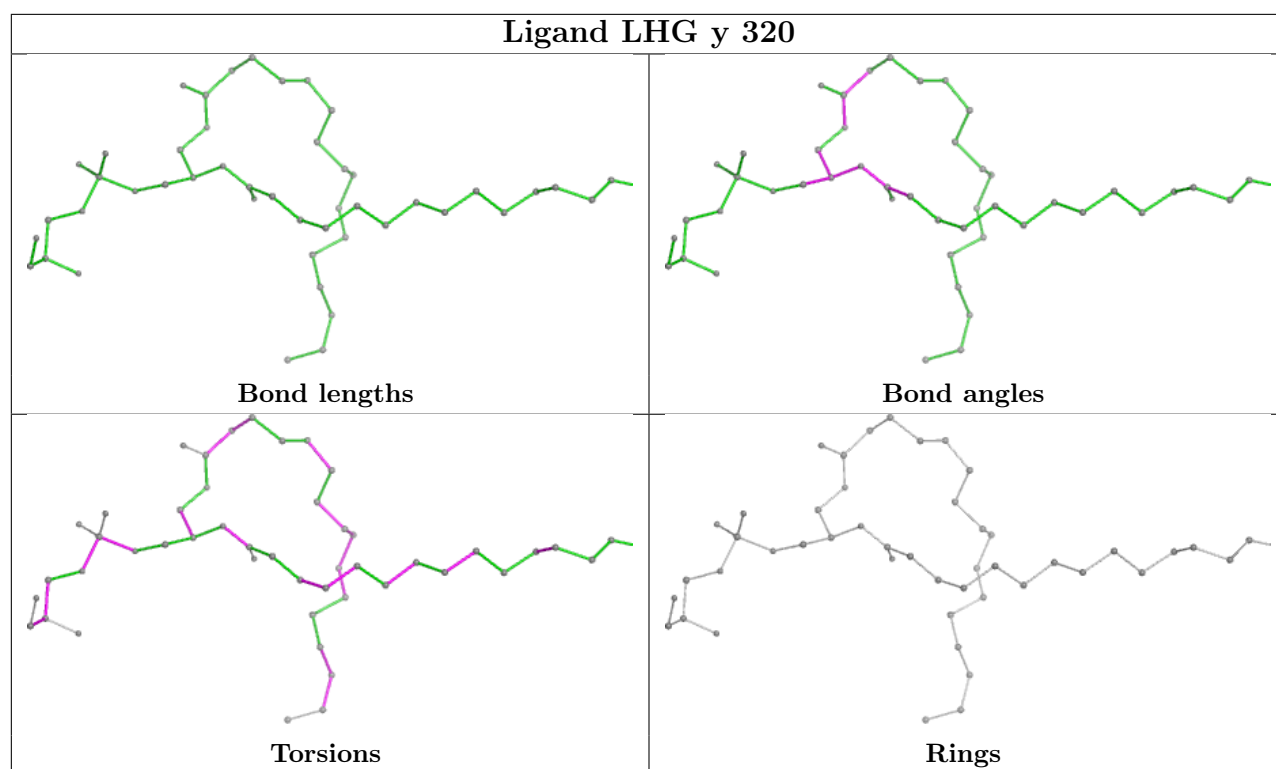


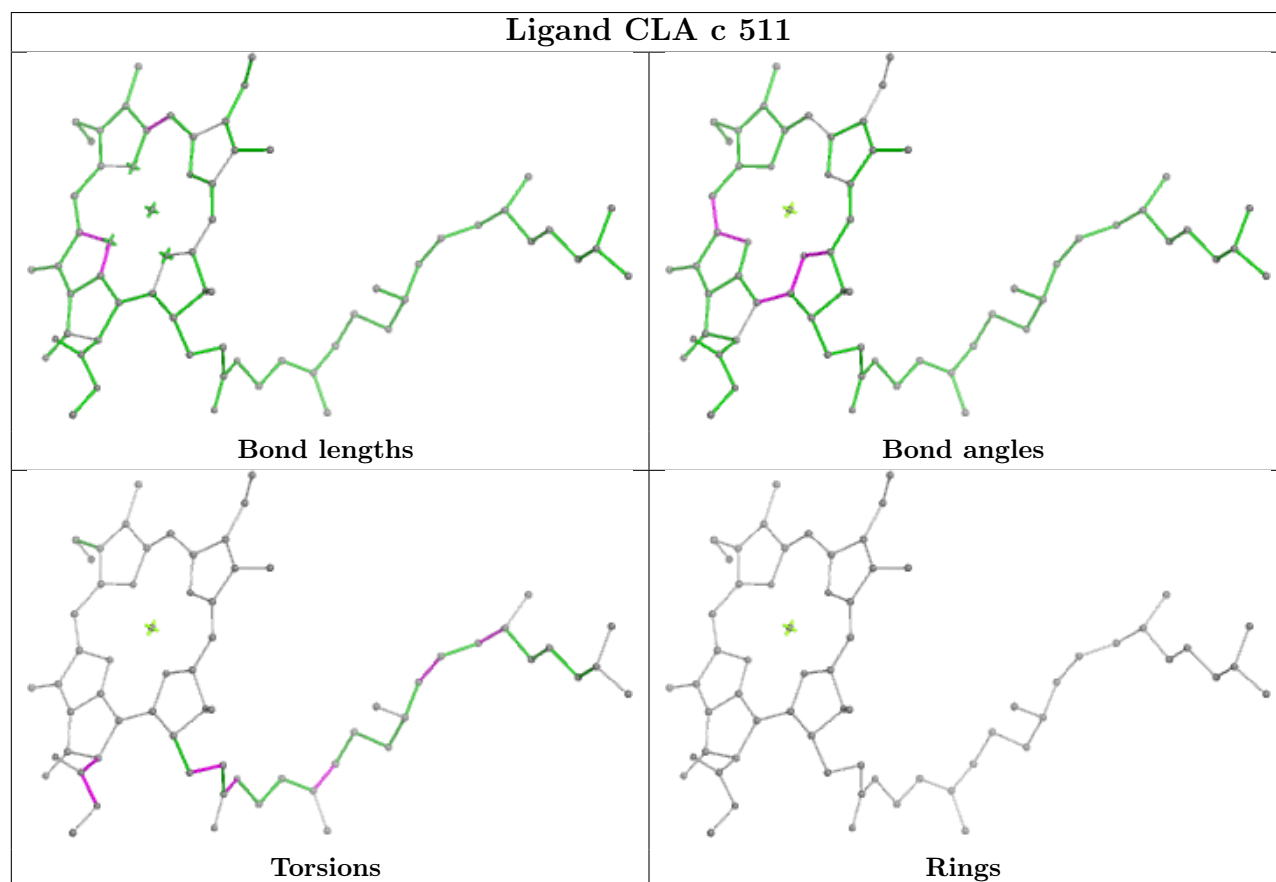
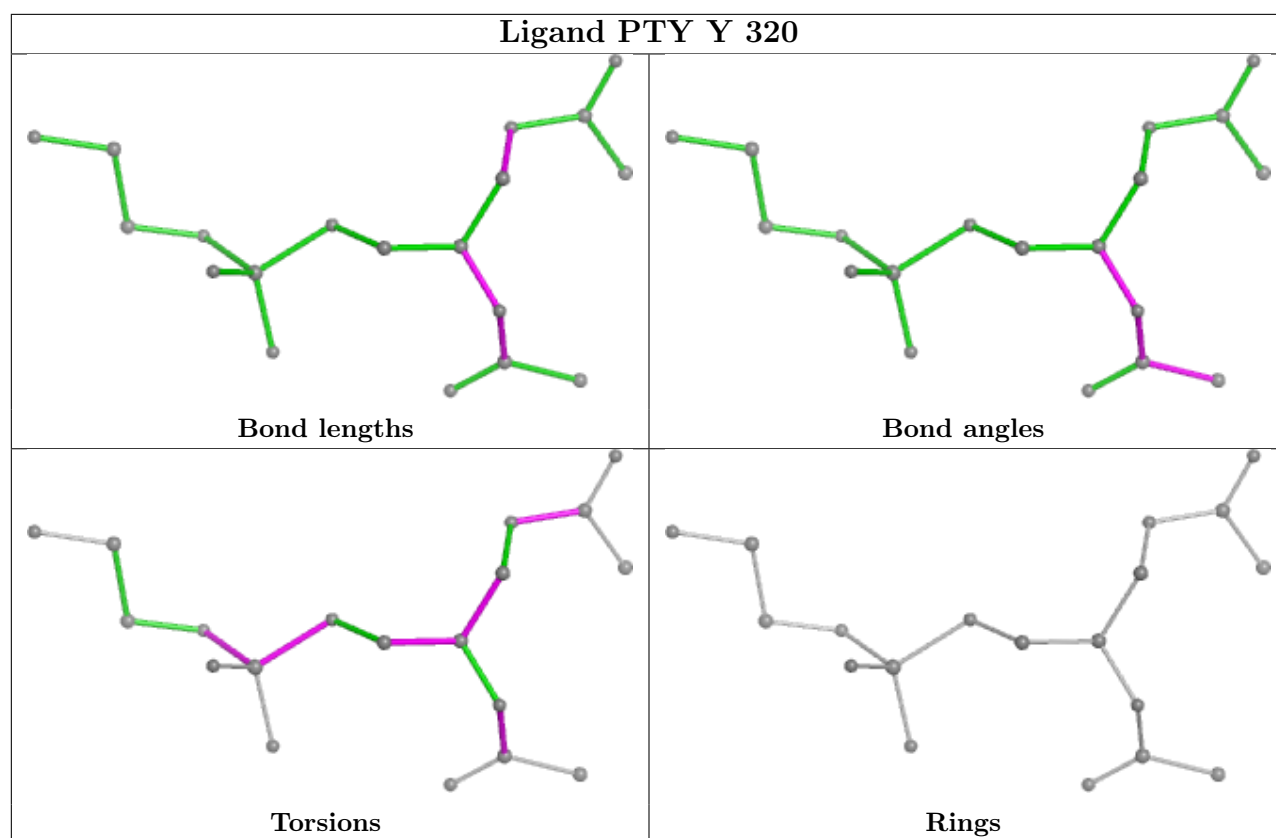
Ligand CLA A 405



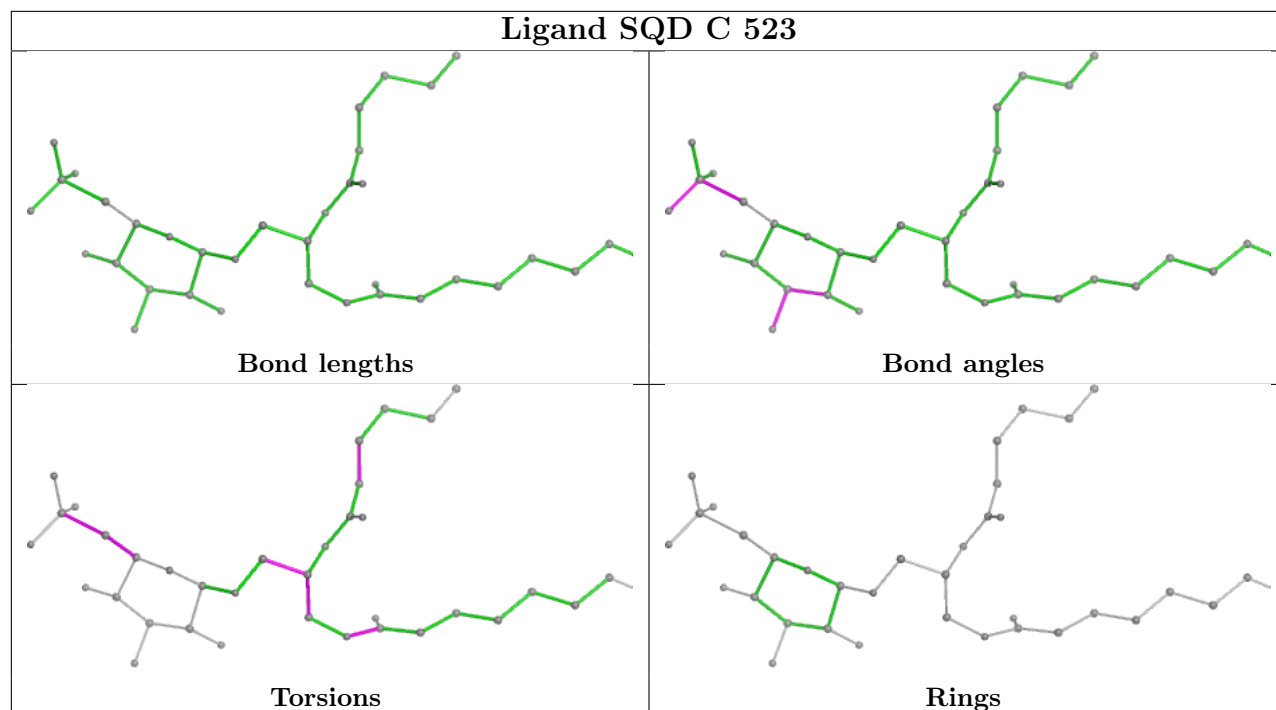
Ligand CLA G 614



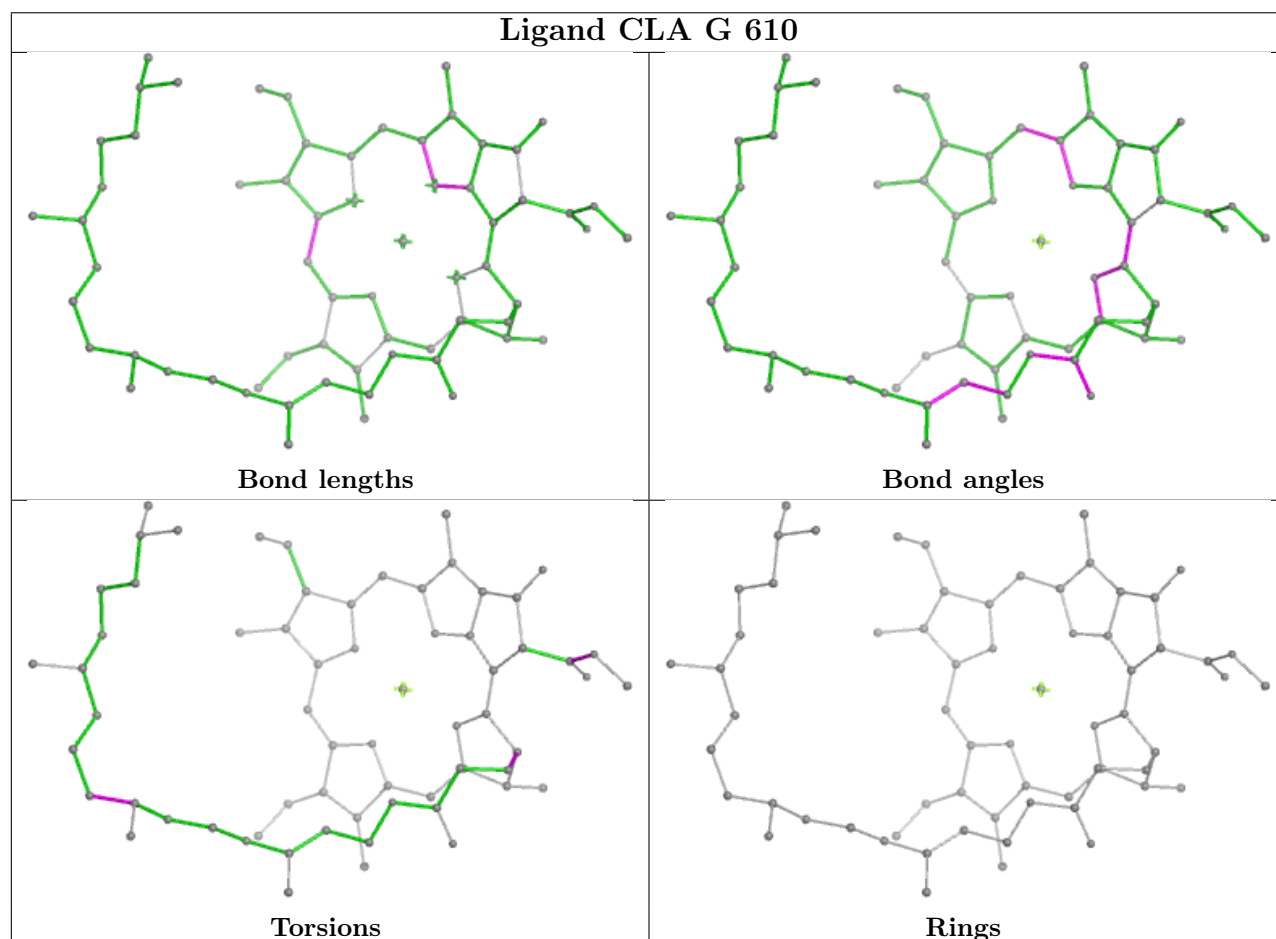


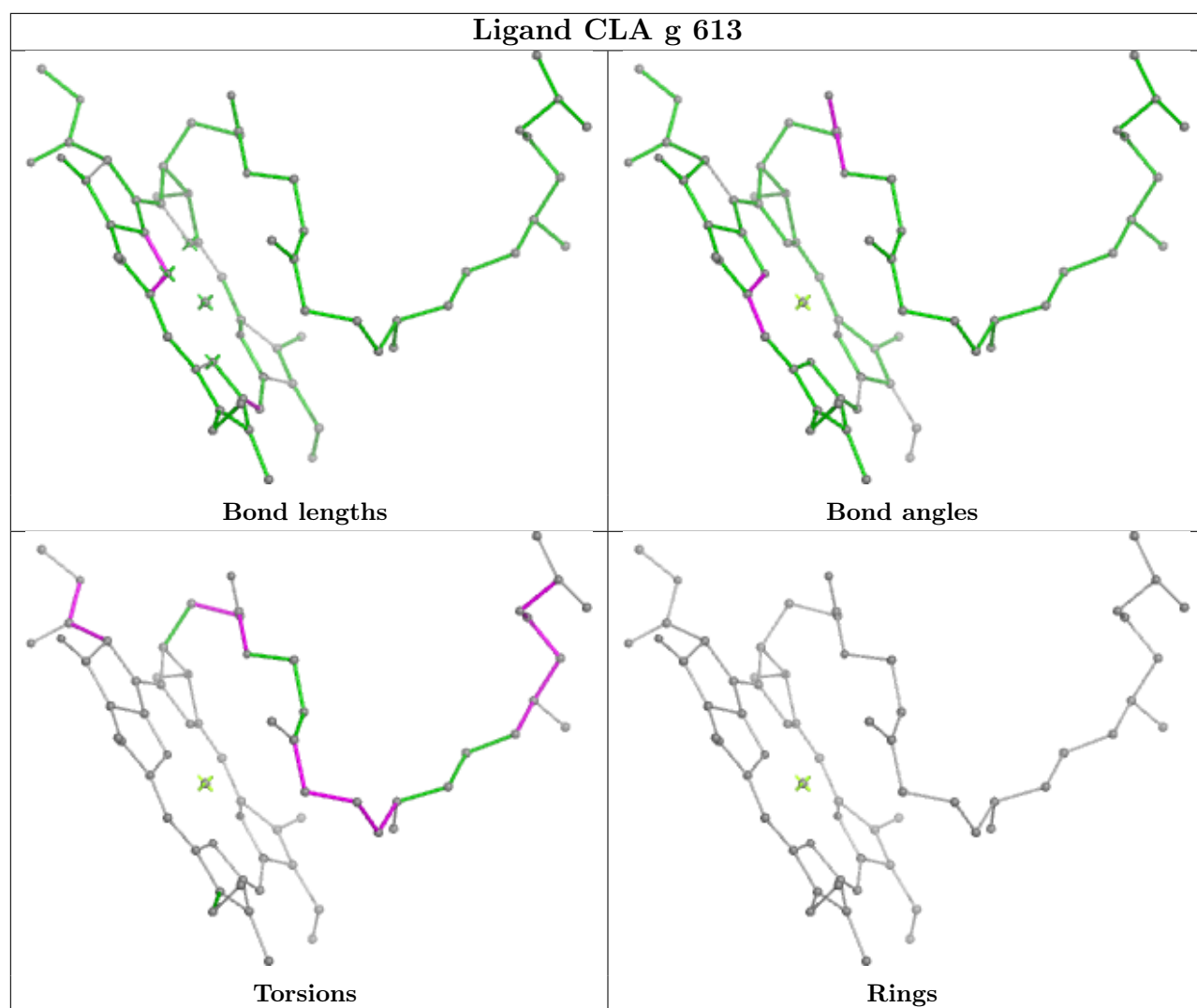


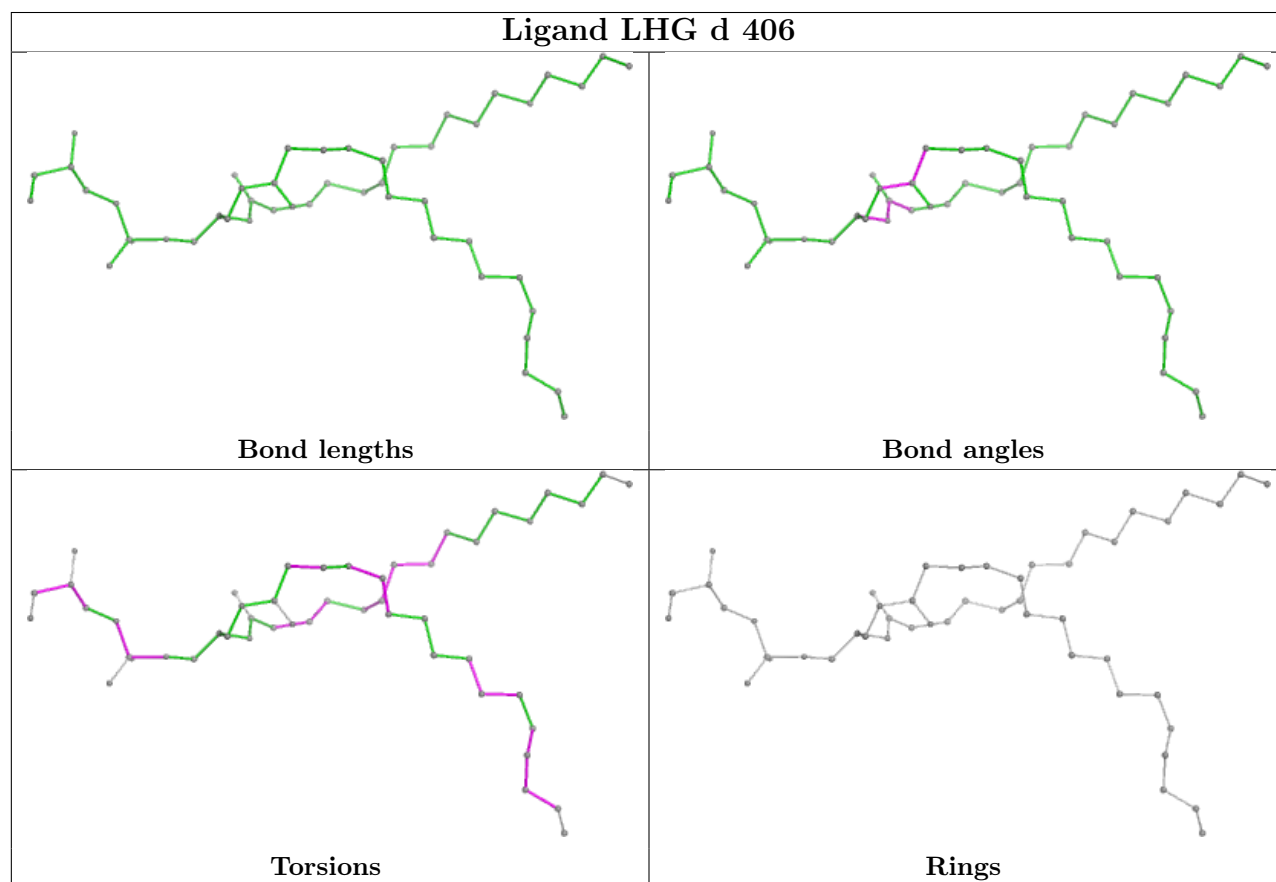
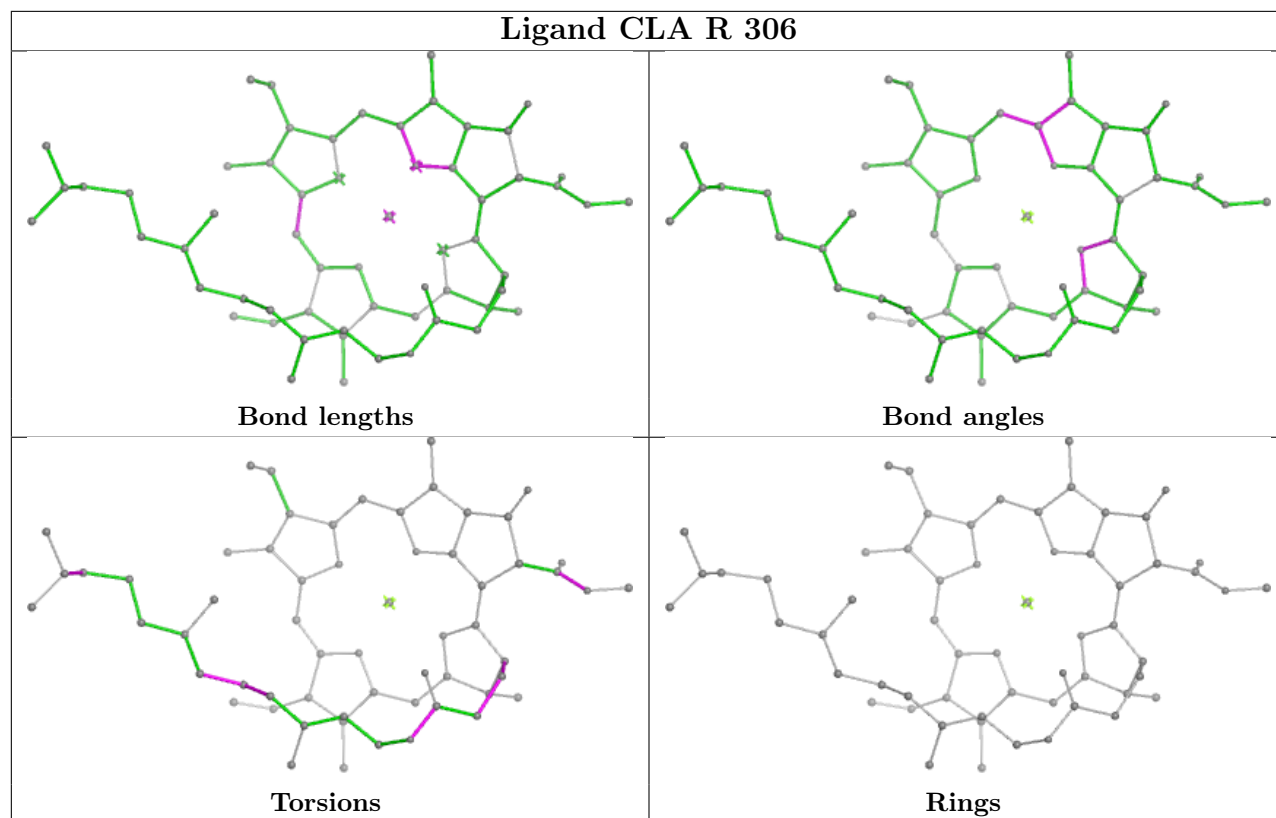
Ligand SQD C 523



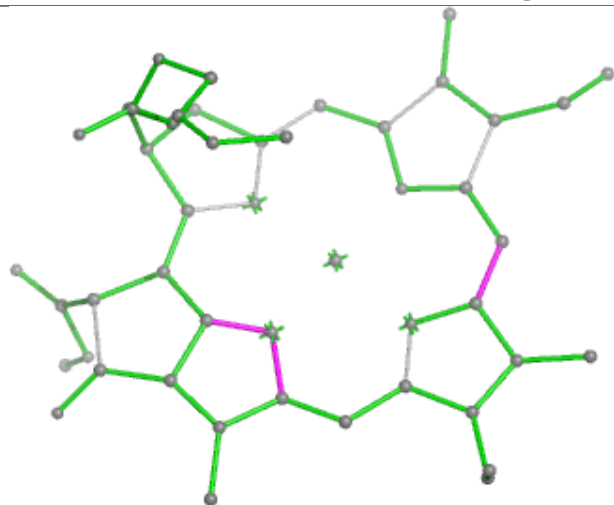
Ligand CLA G 610



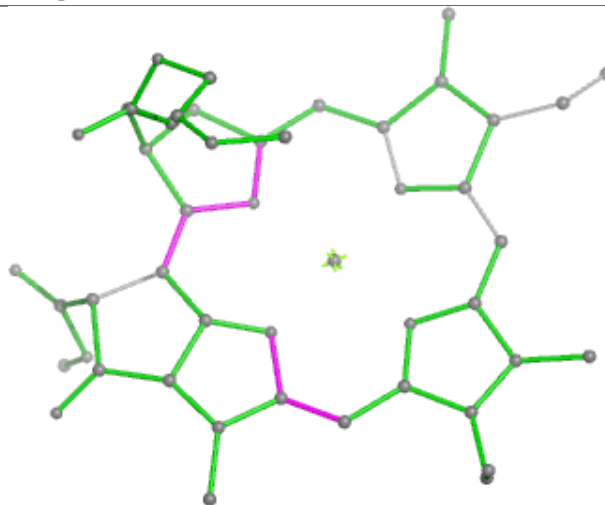




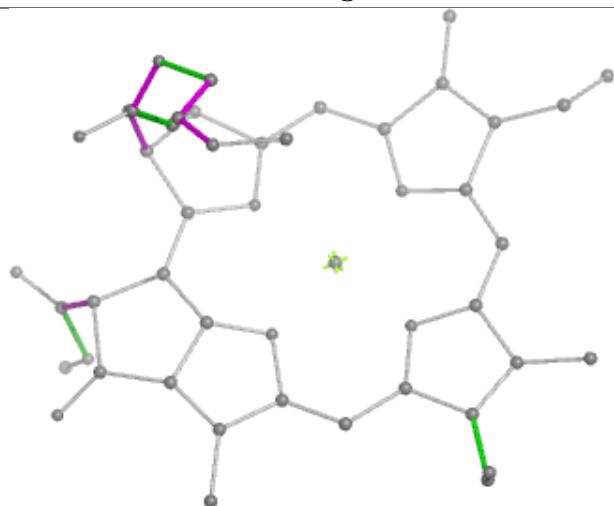
Ligand CLA g 604



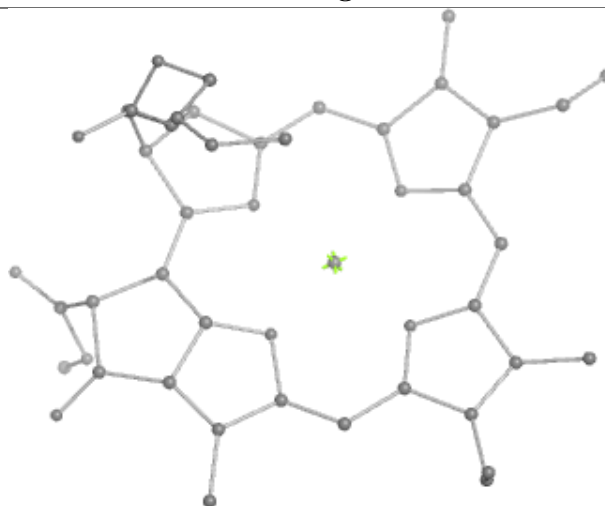
Bond lengths



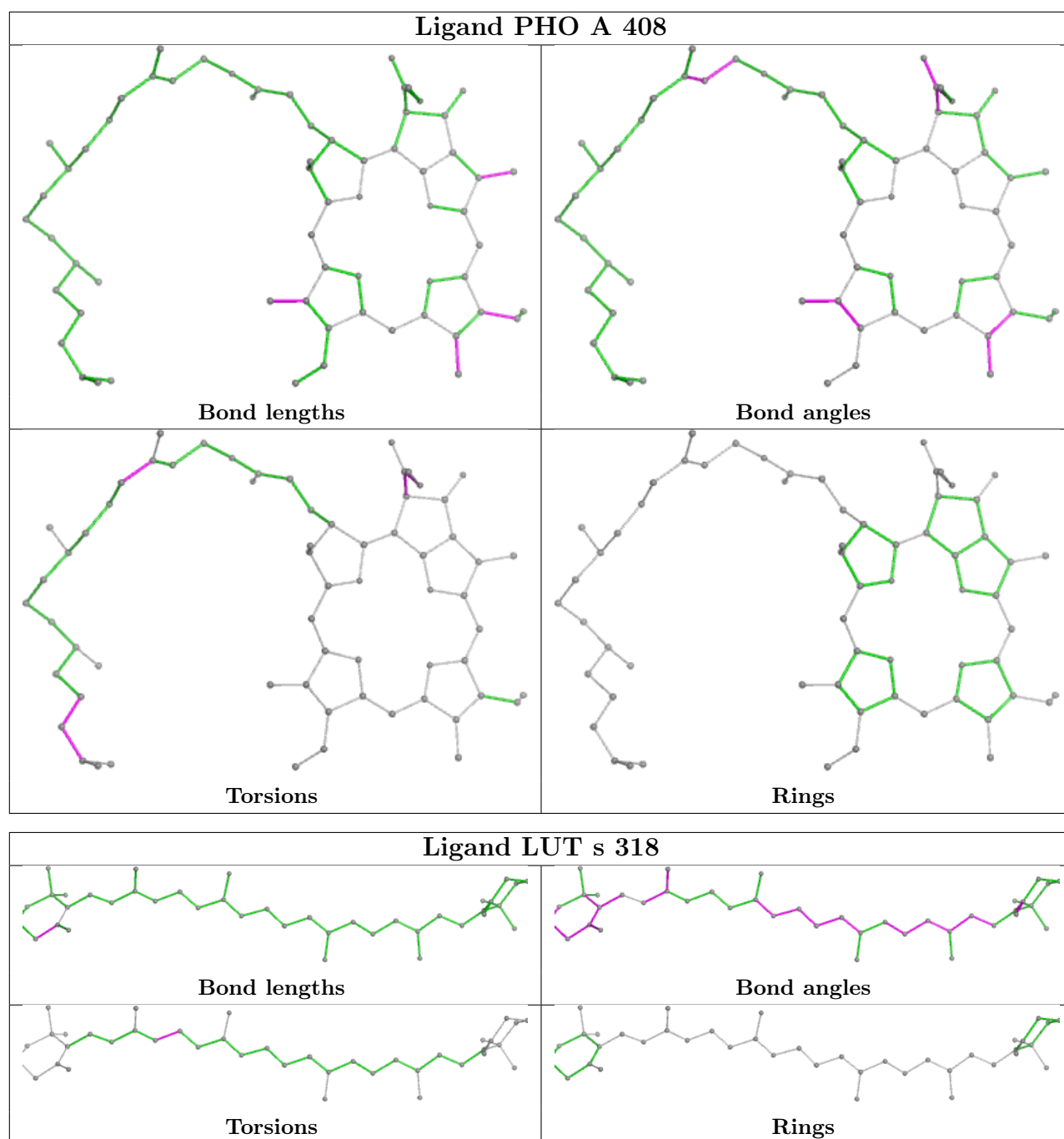
Bond angles

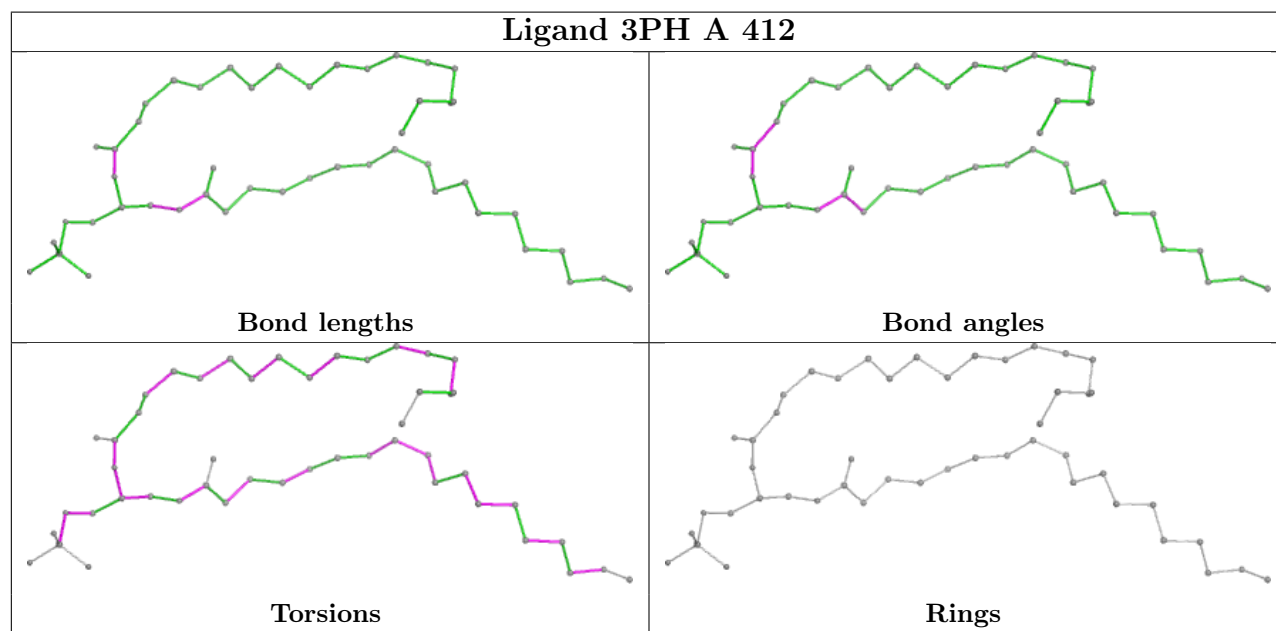
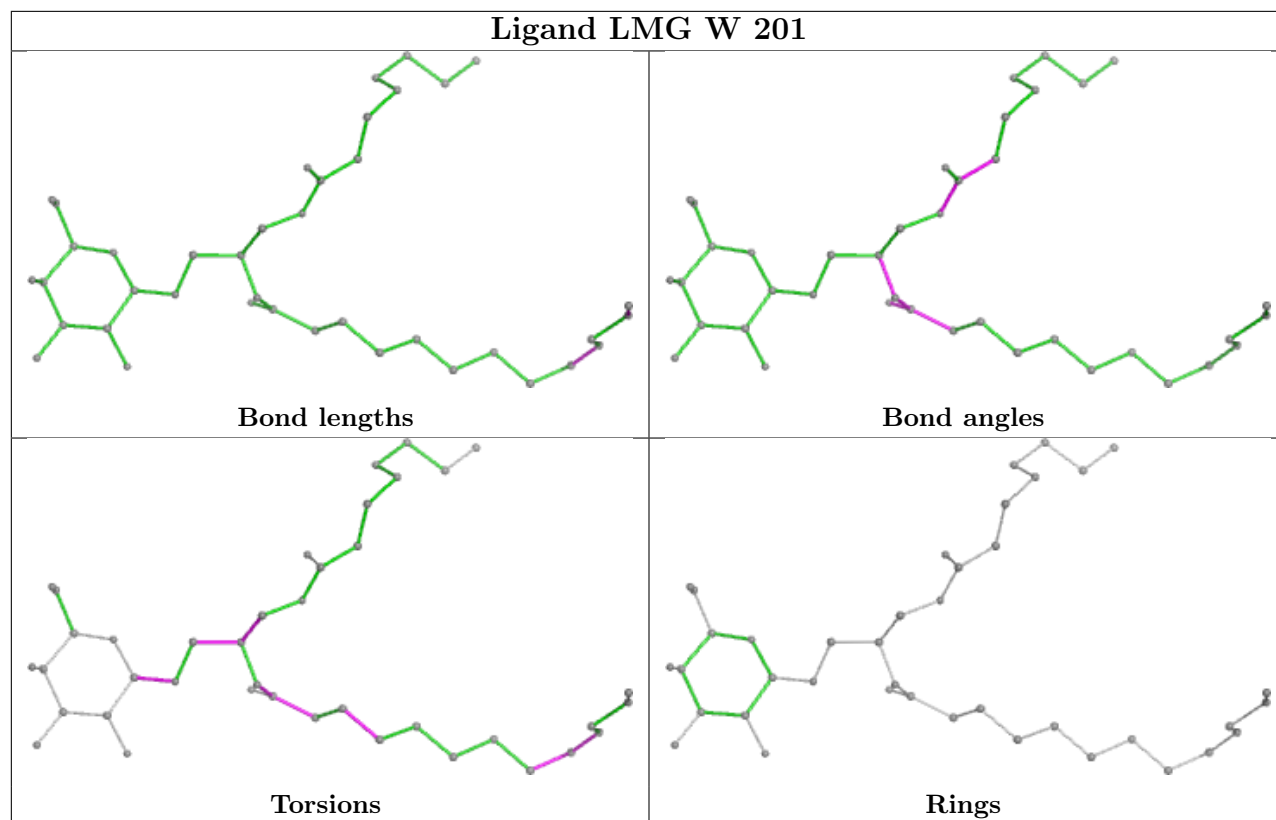


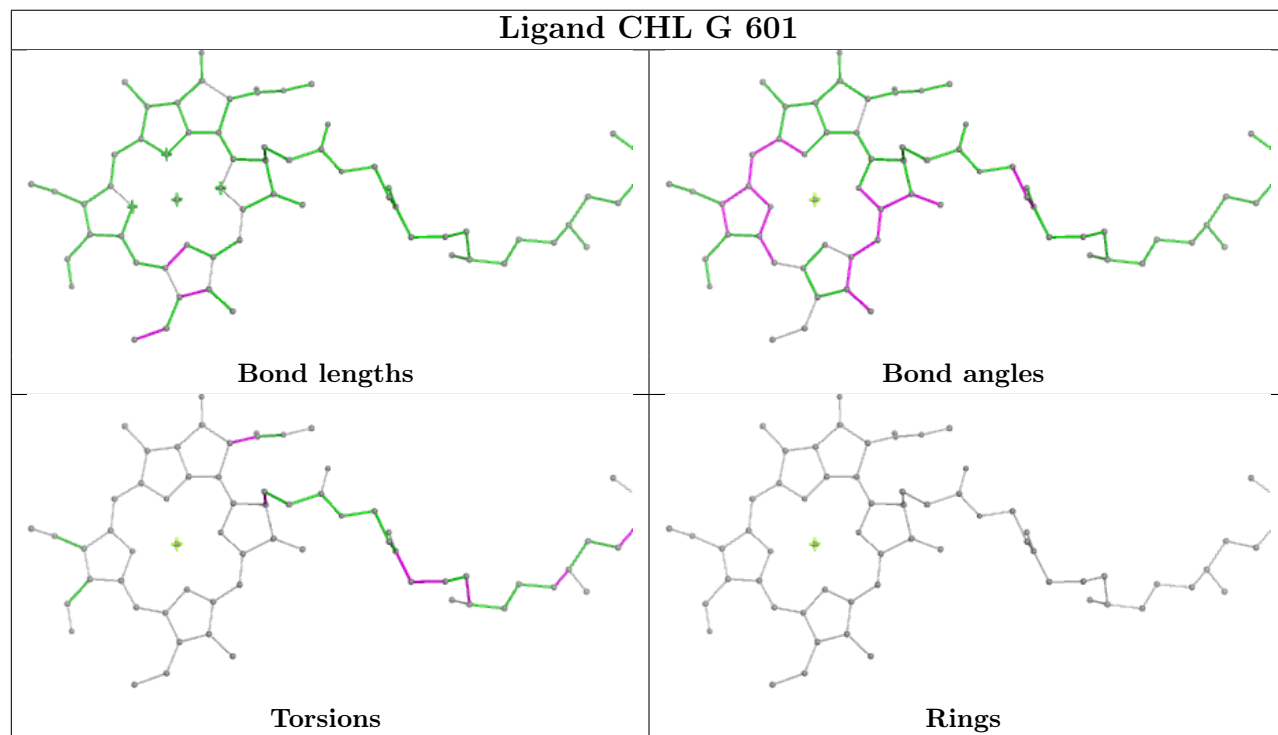
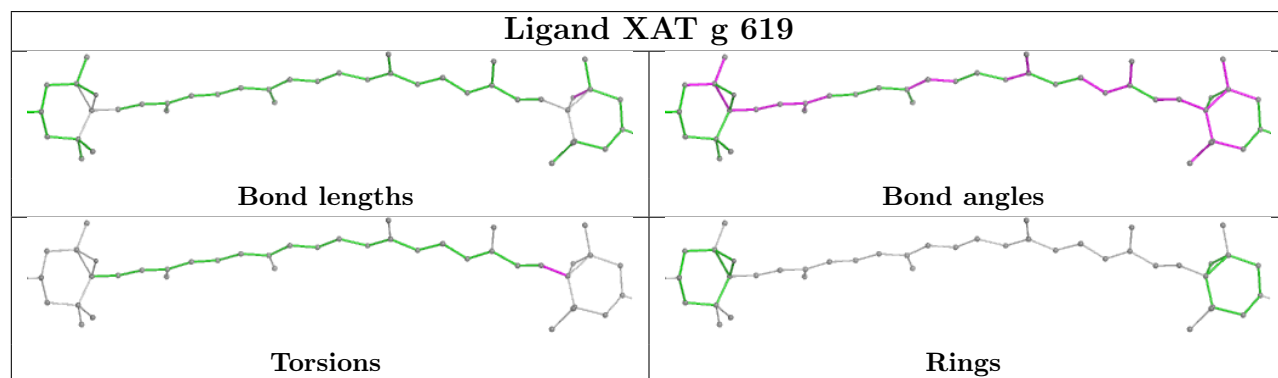
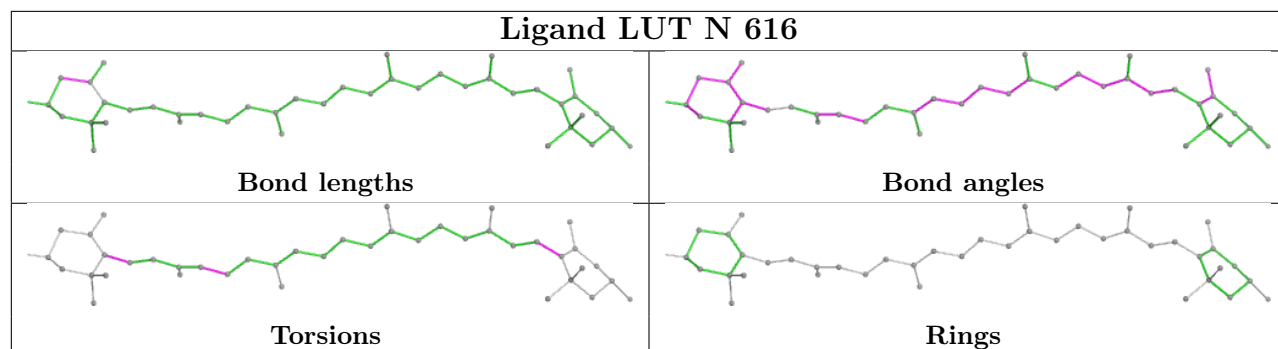
Torsions



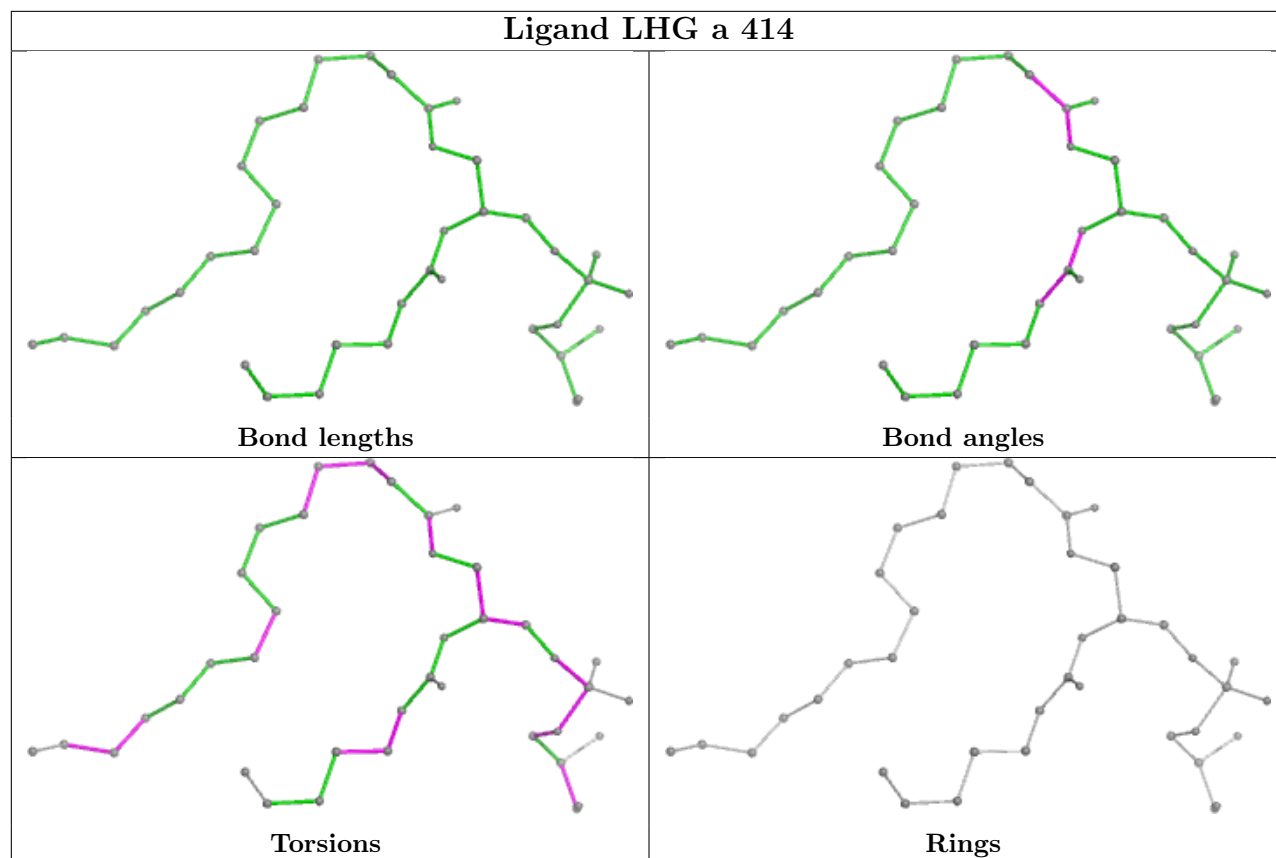
Rings



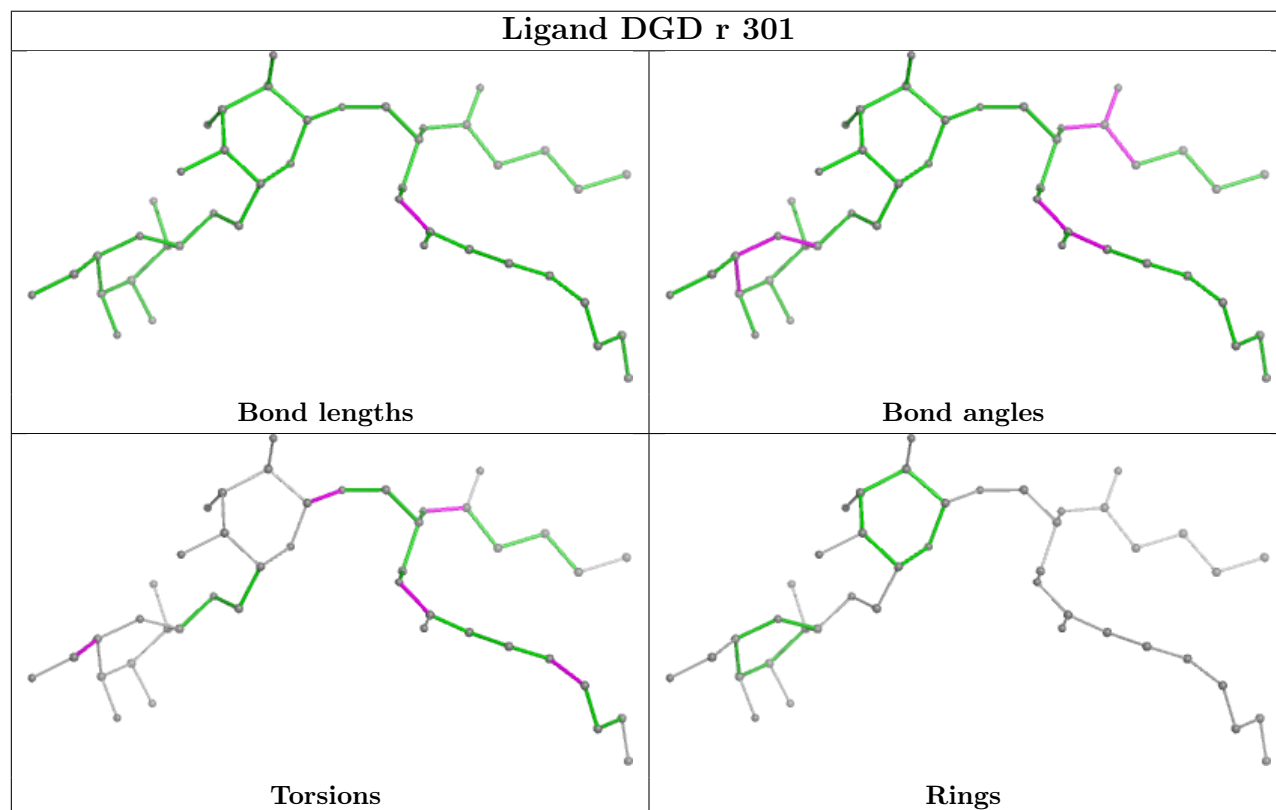


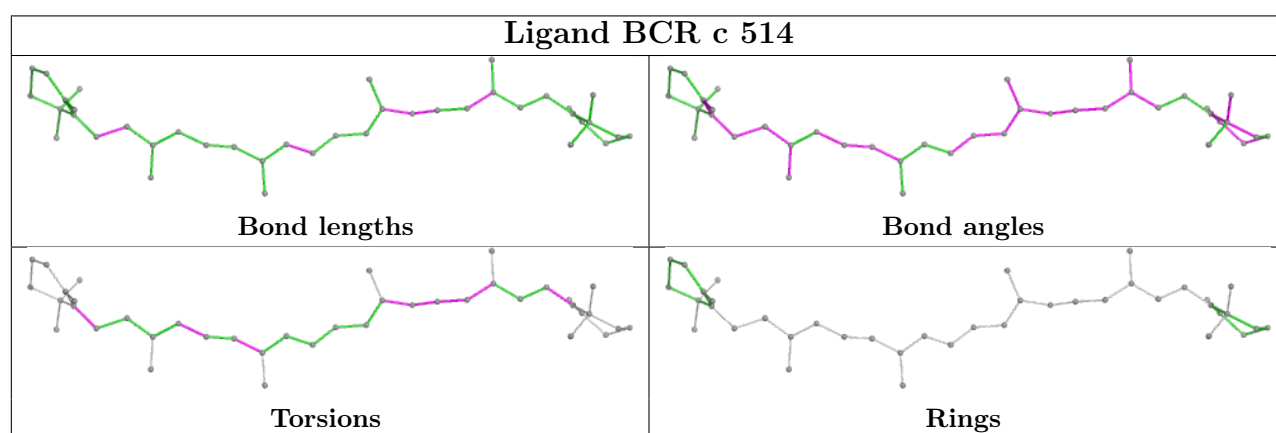
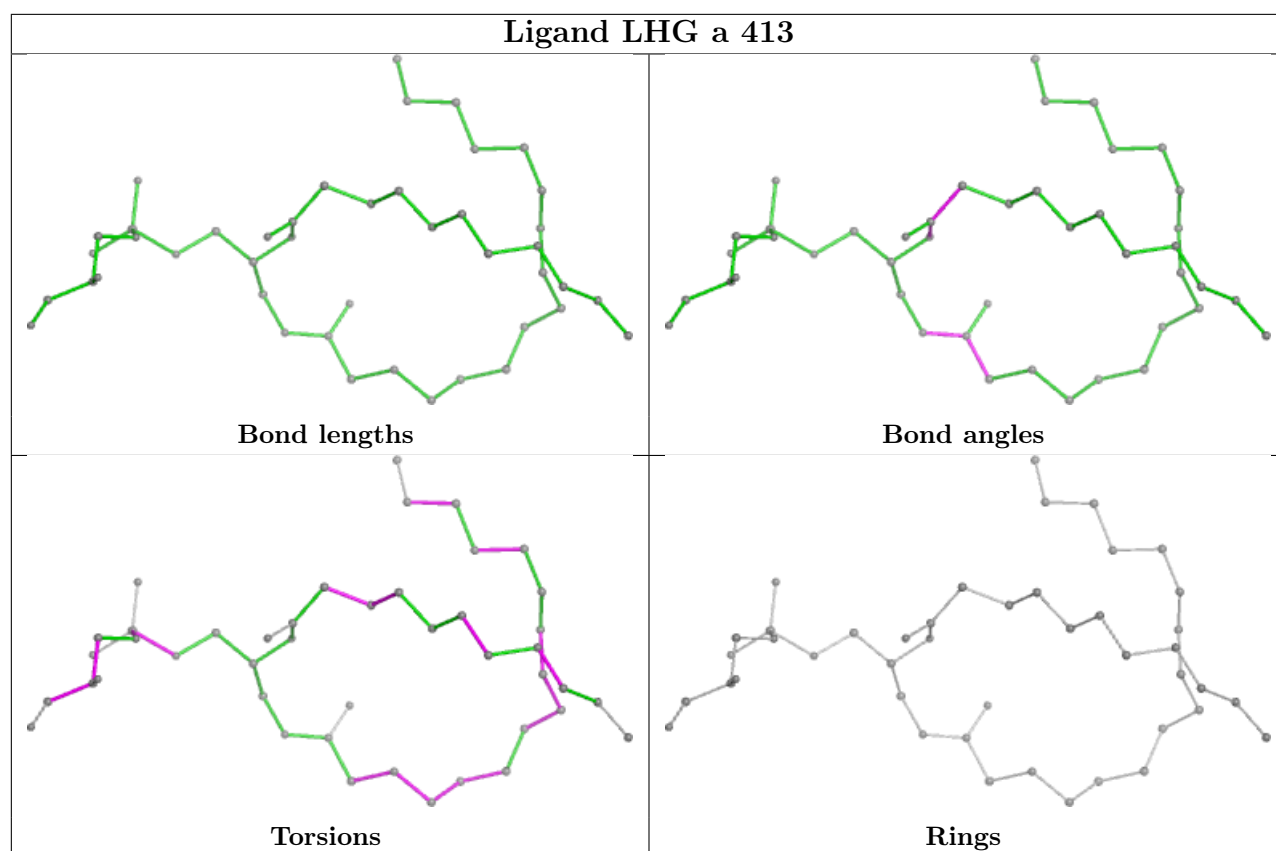


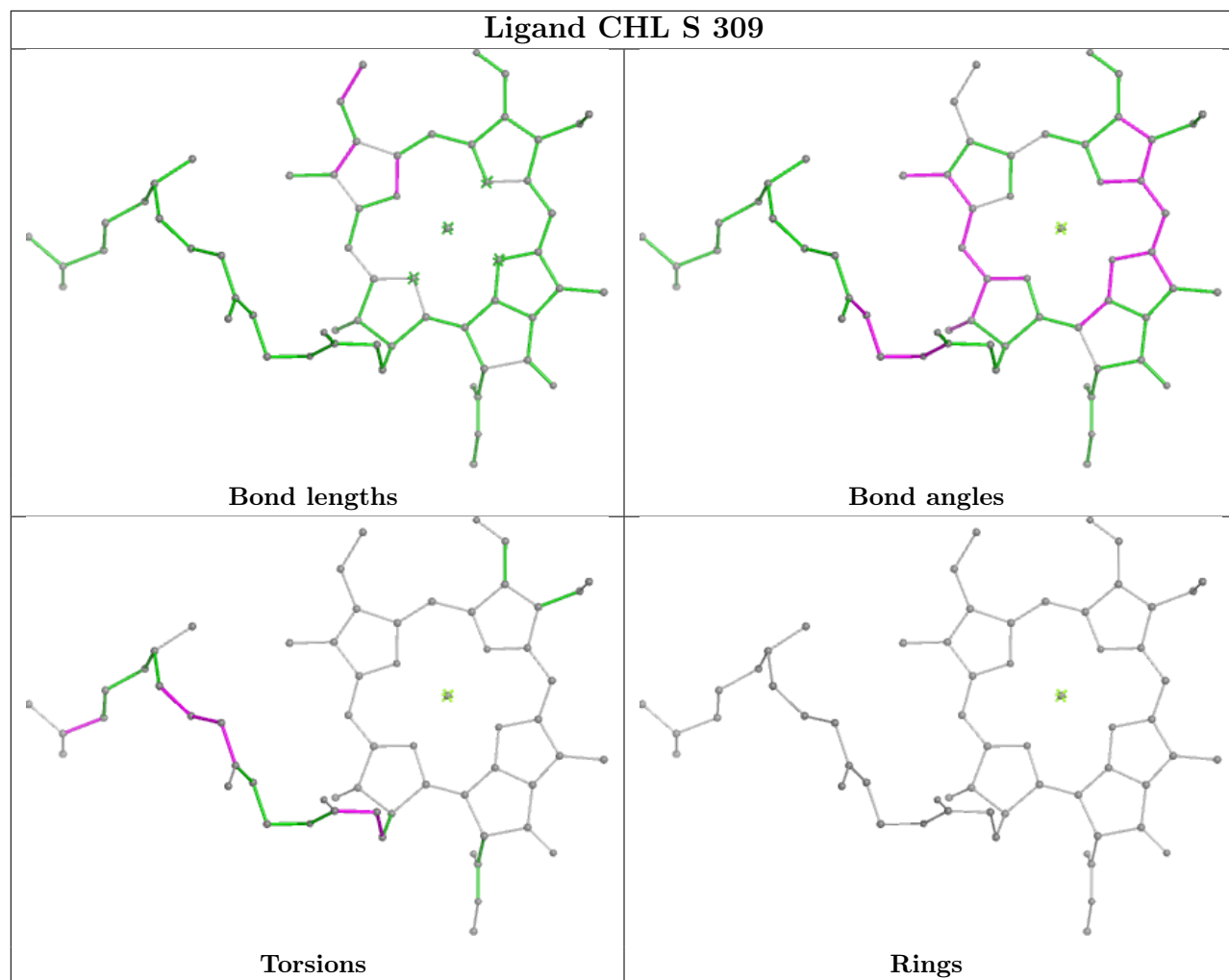
Ligand LHG a 414



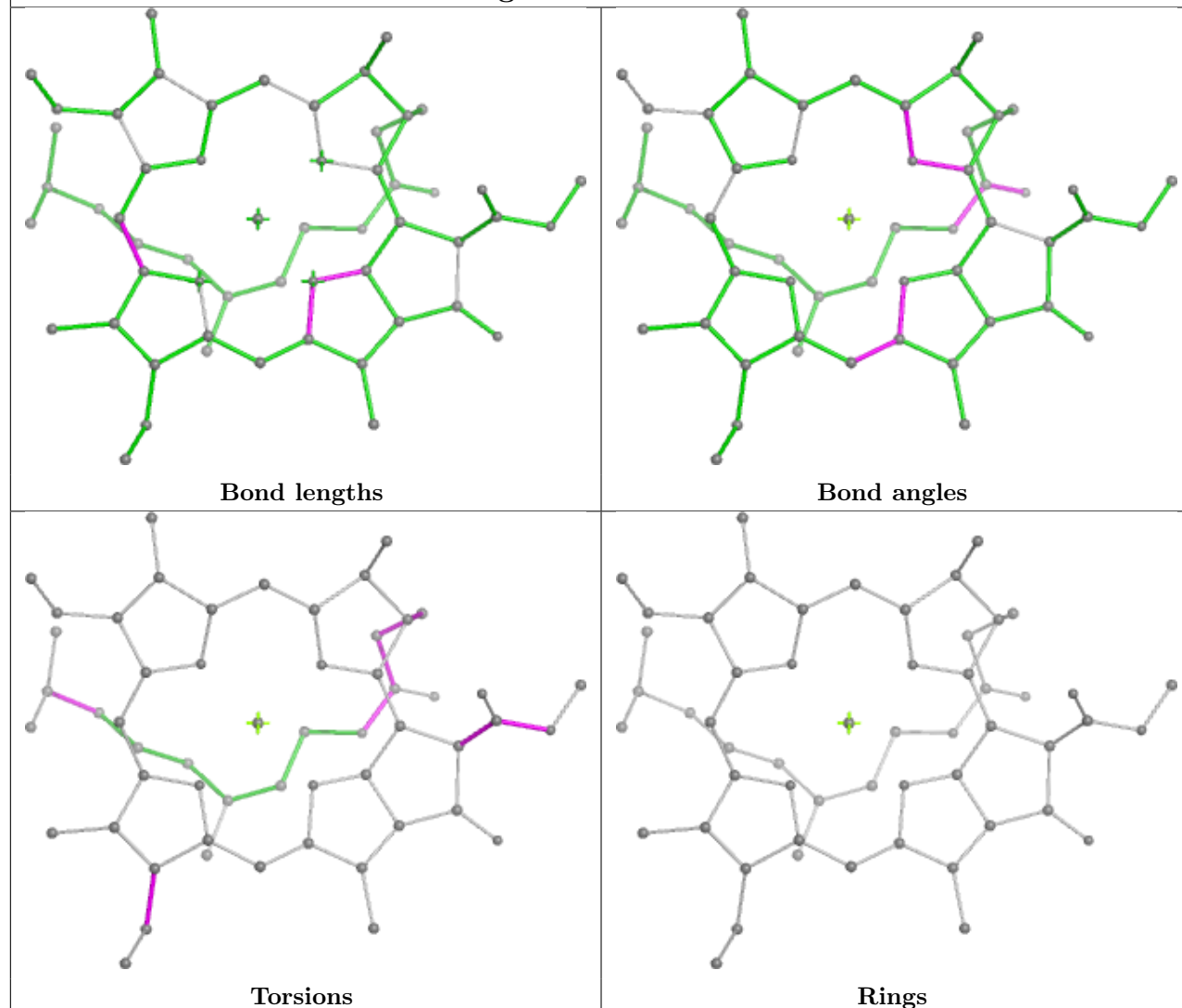
Ligand DGD r 301



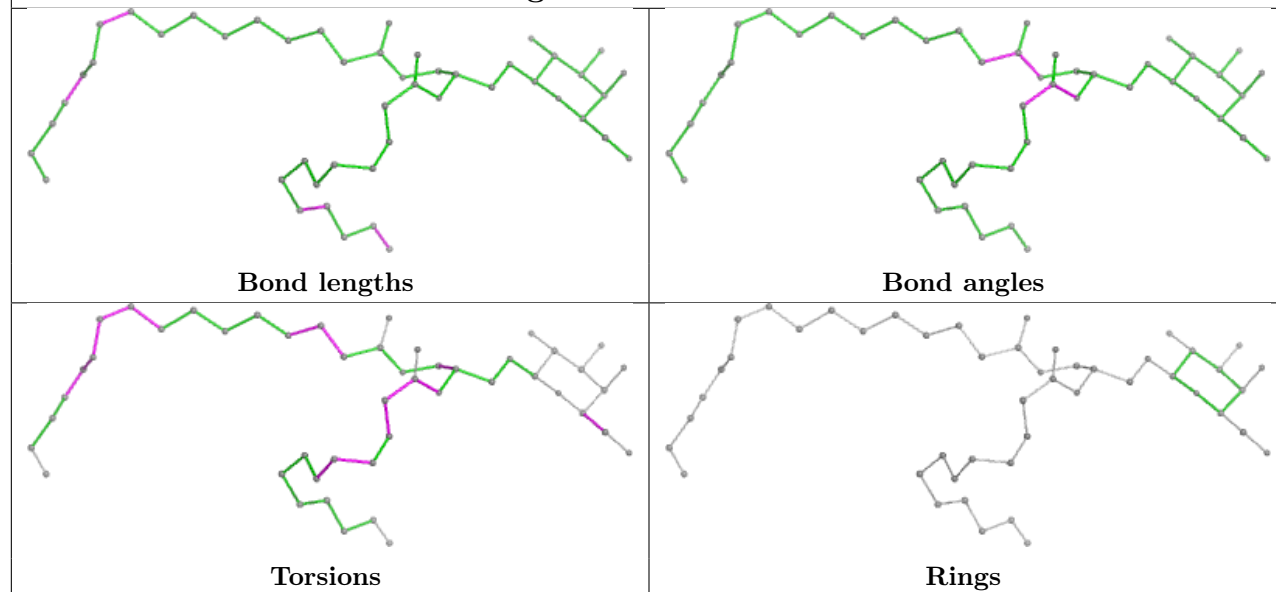




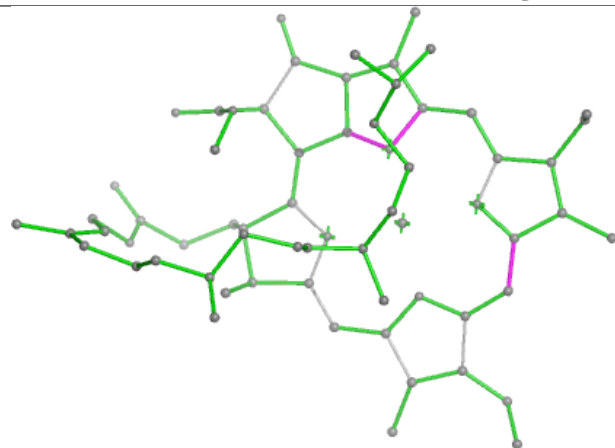
Ligand CLA s 314



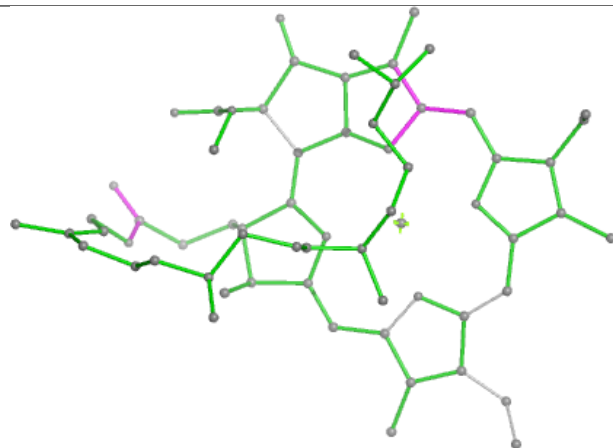
Ligand LMG D 410



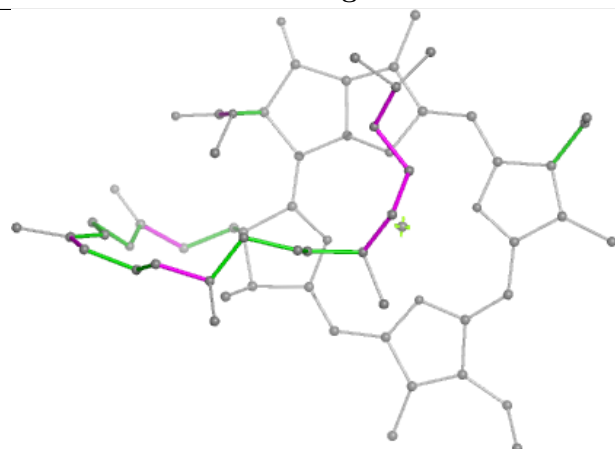
Ligand CLA C 511



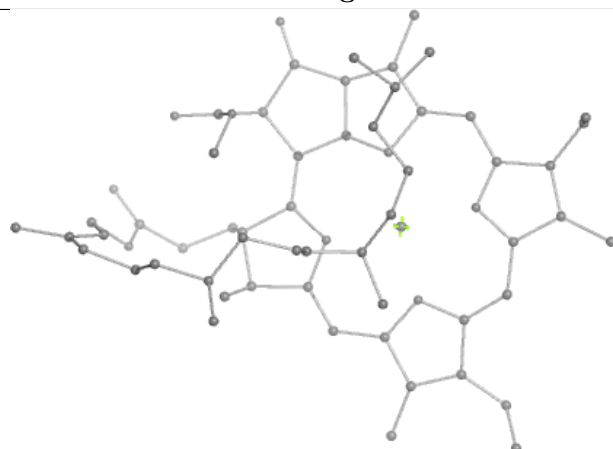
Bond lengths



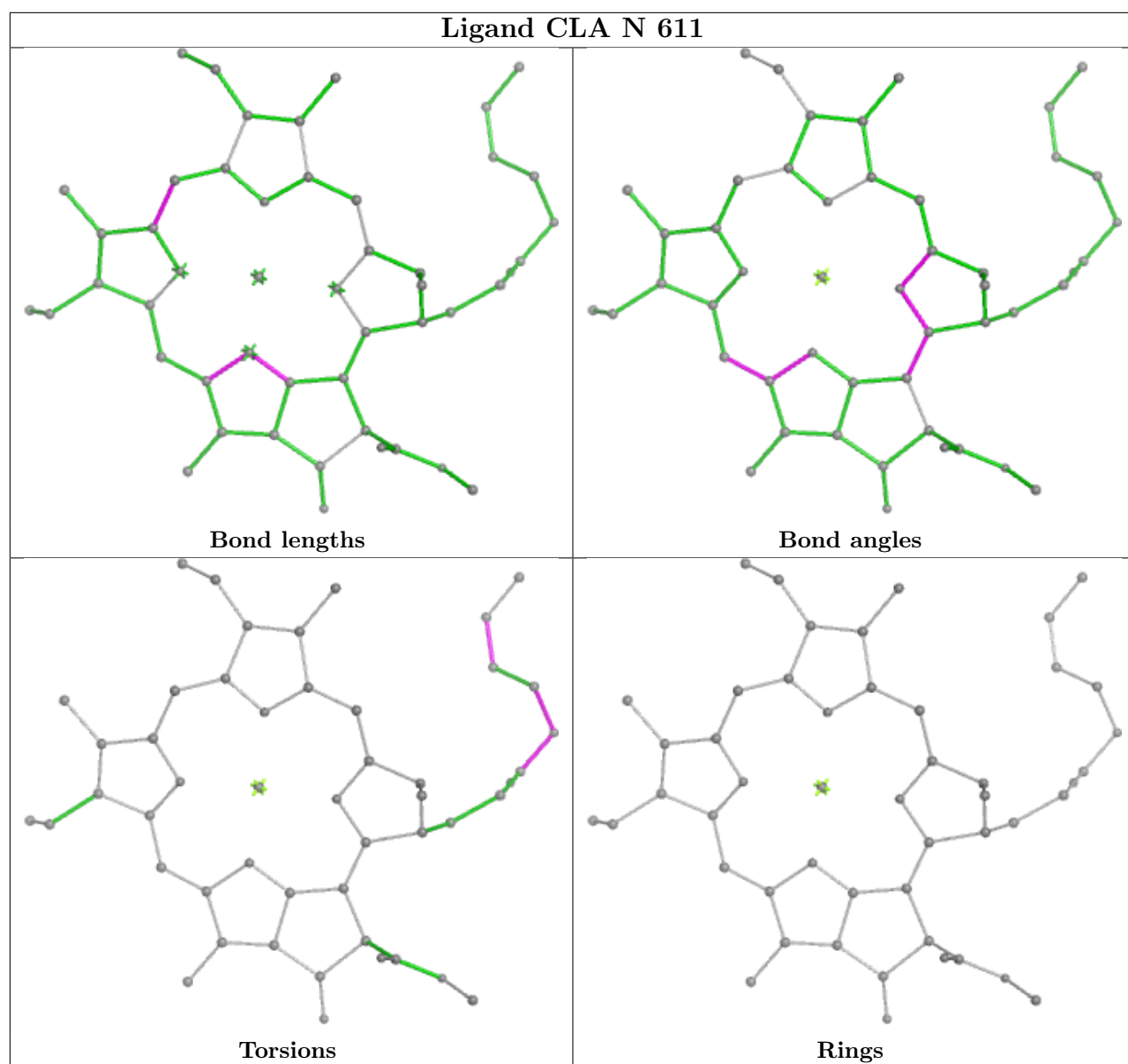
Bond angles

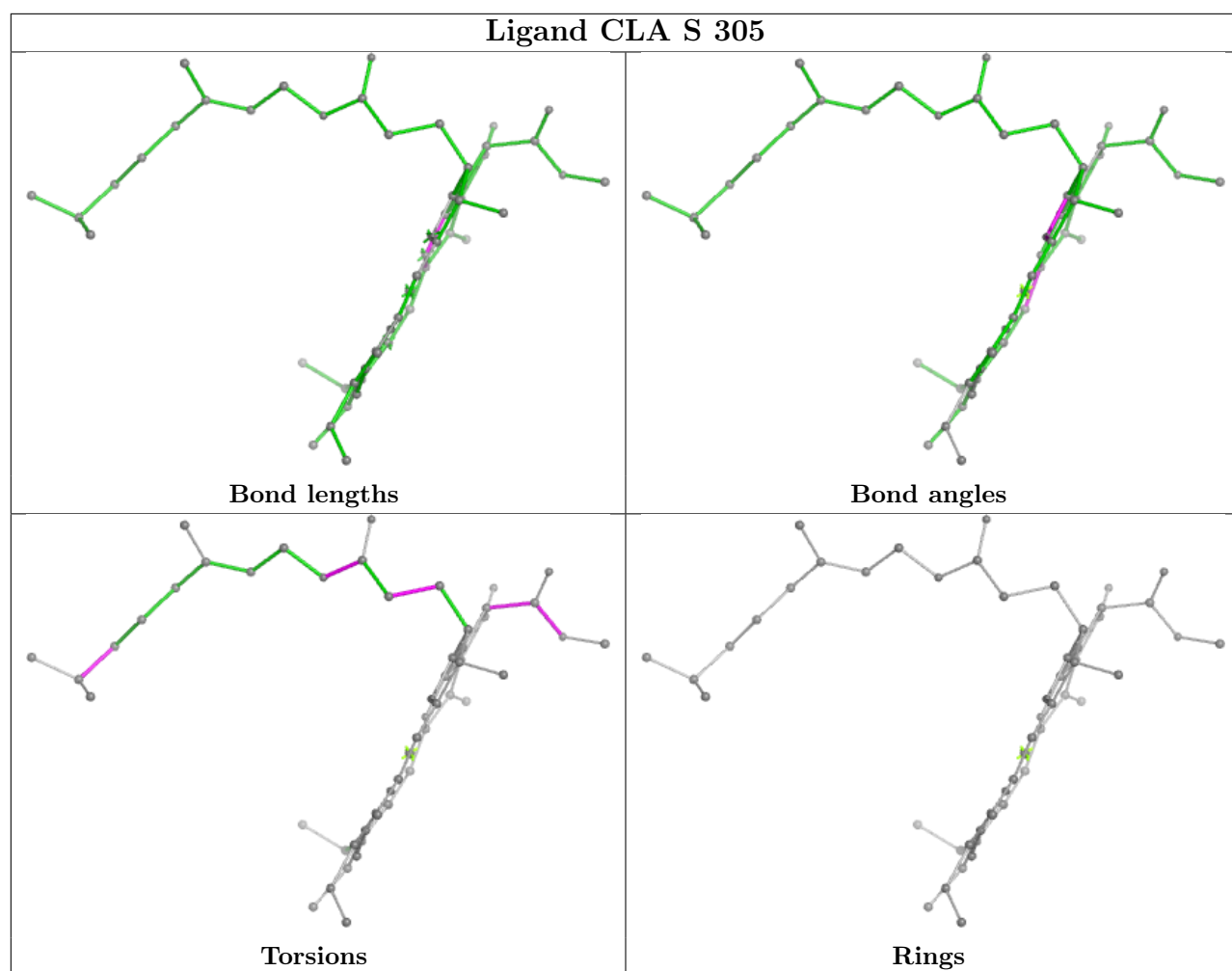


Torsions

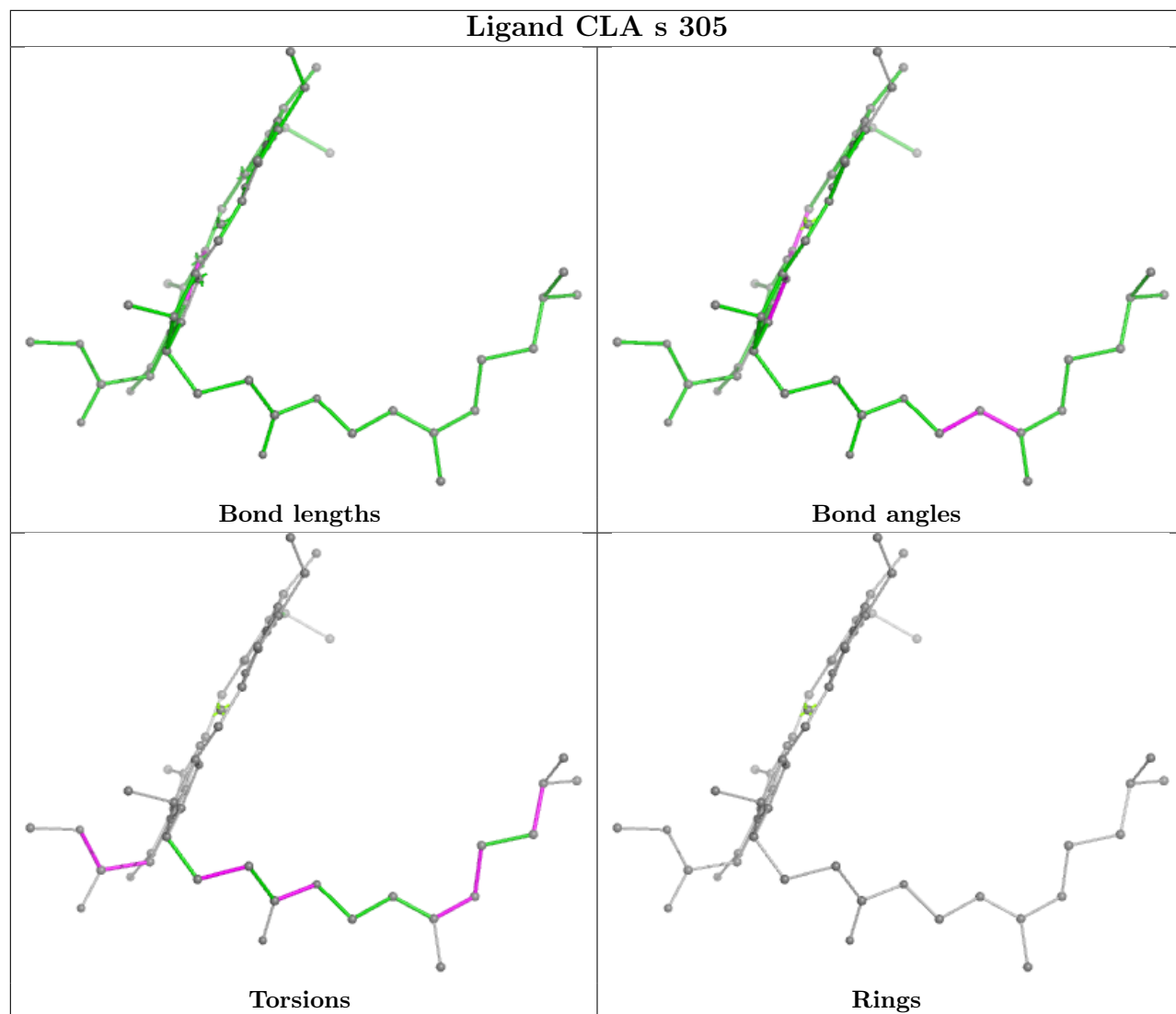


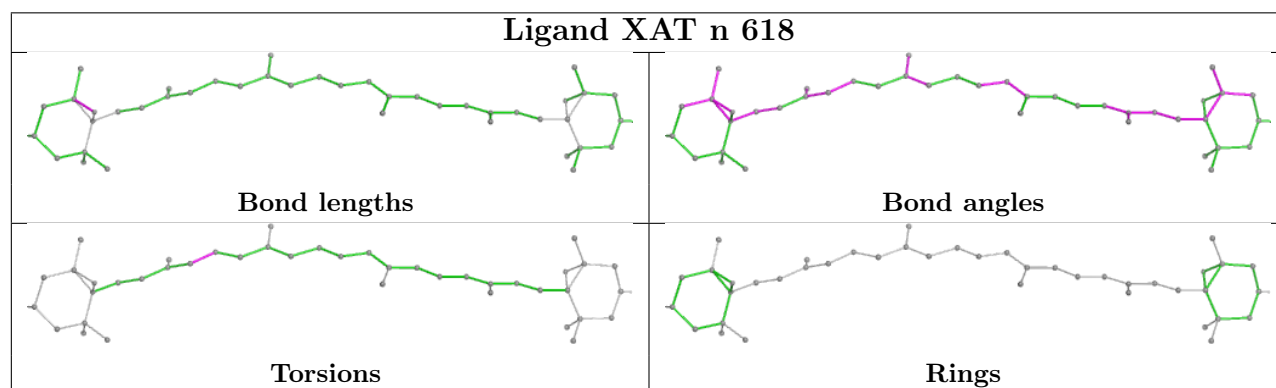
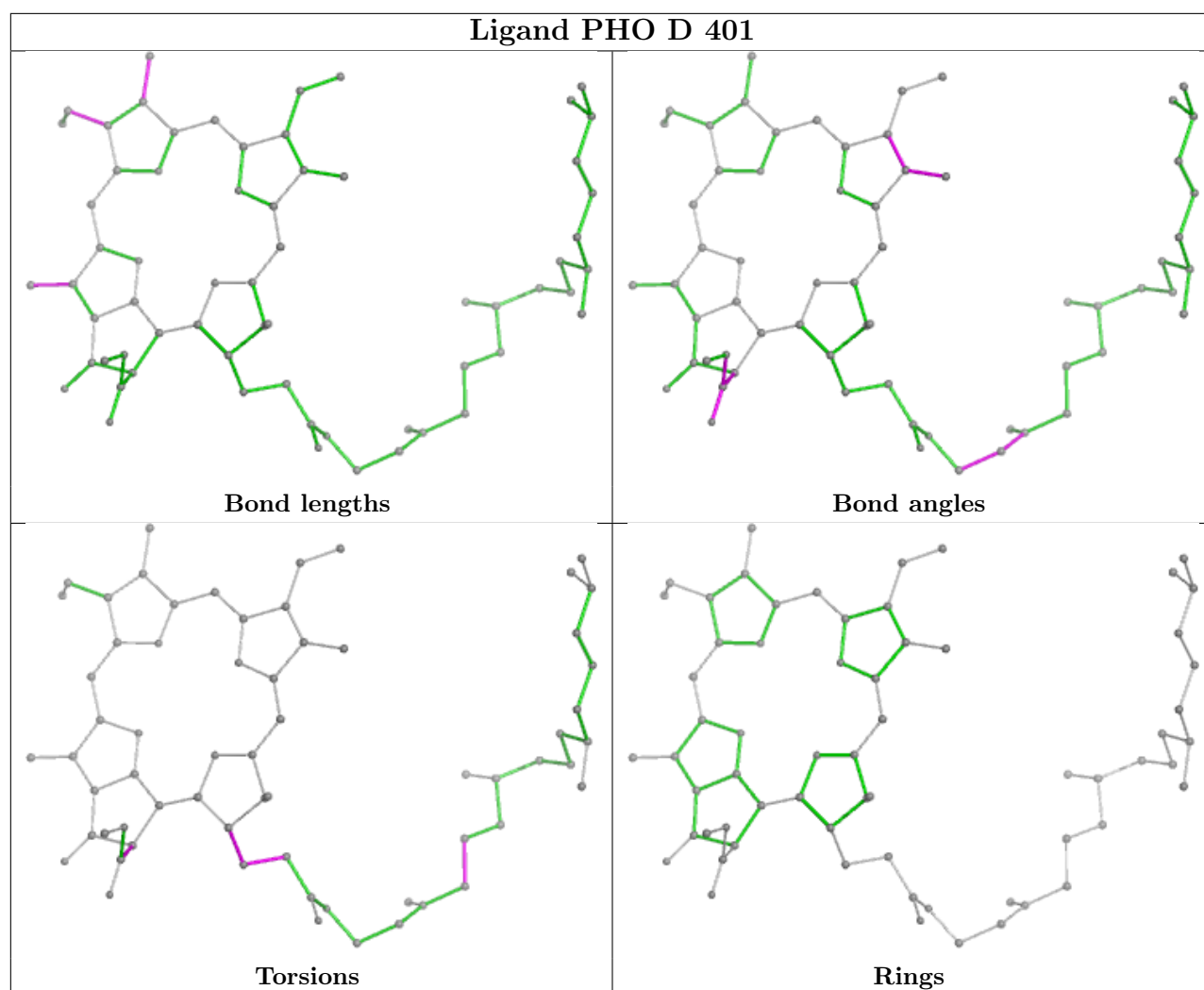
Rings



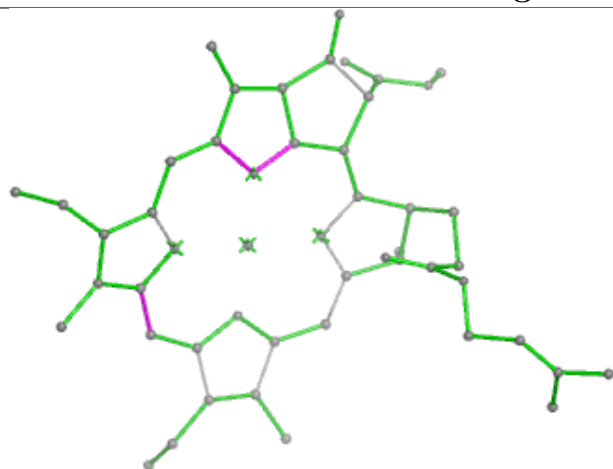


Ligand CLA s 305

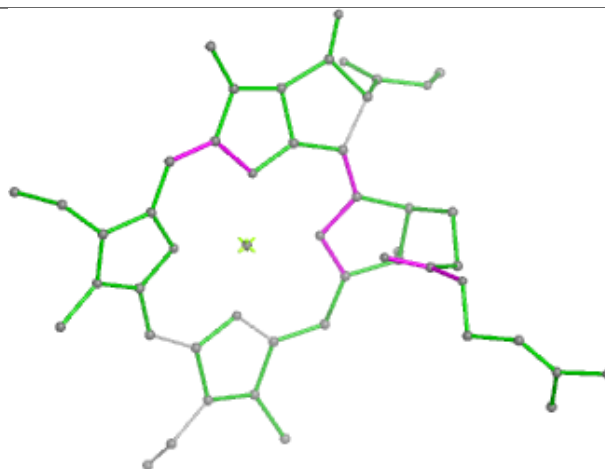




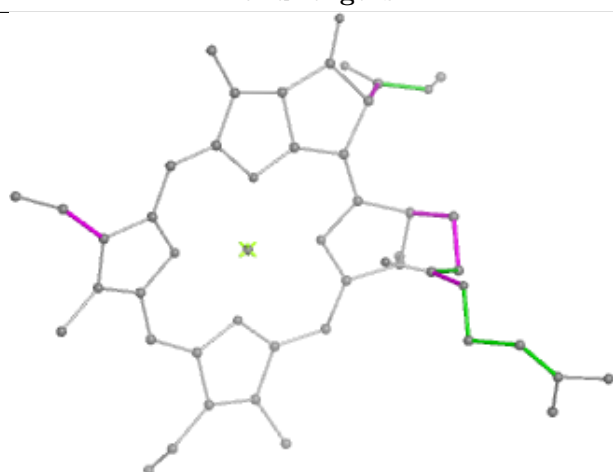
Ligand CLA A 407



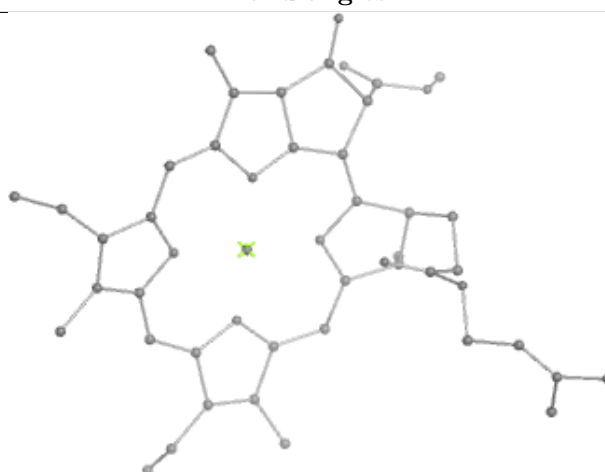
Bond lengths



Bond angles

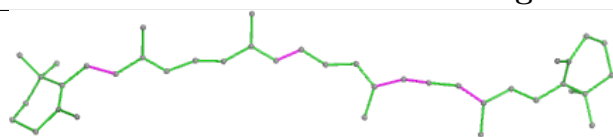


Torsions

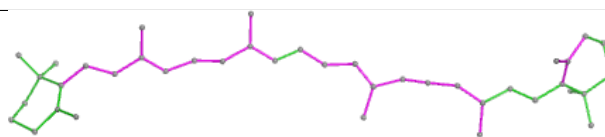


Rings

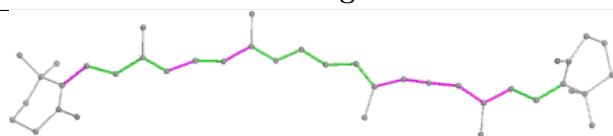
Ligand BCR b 518



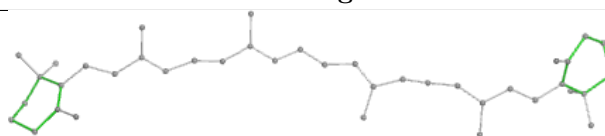
Bond lengths



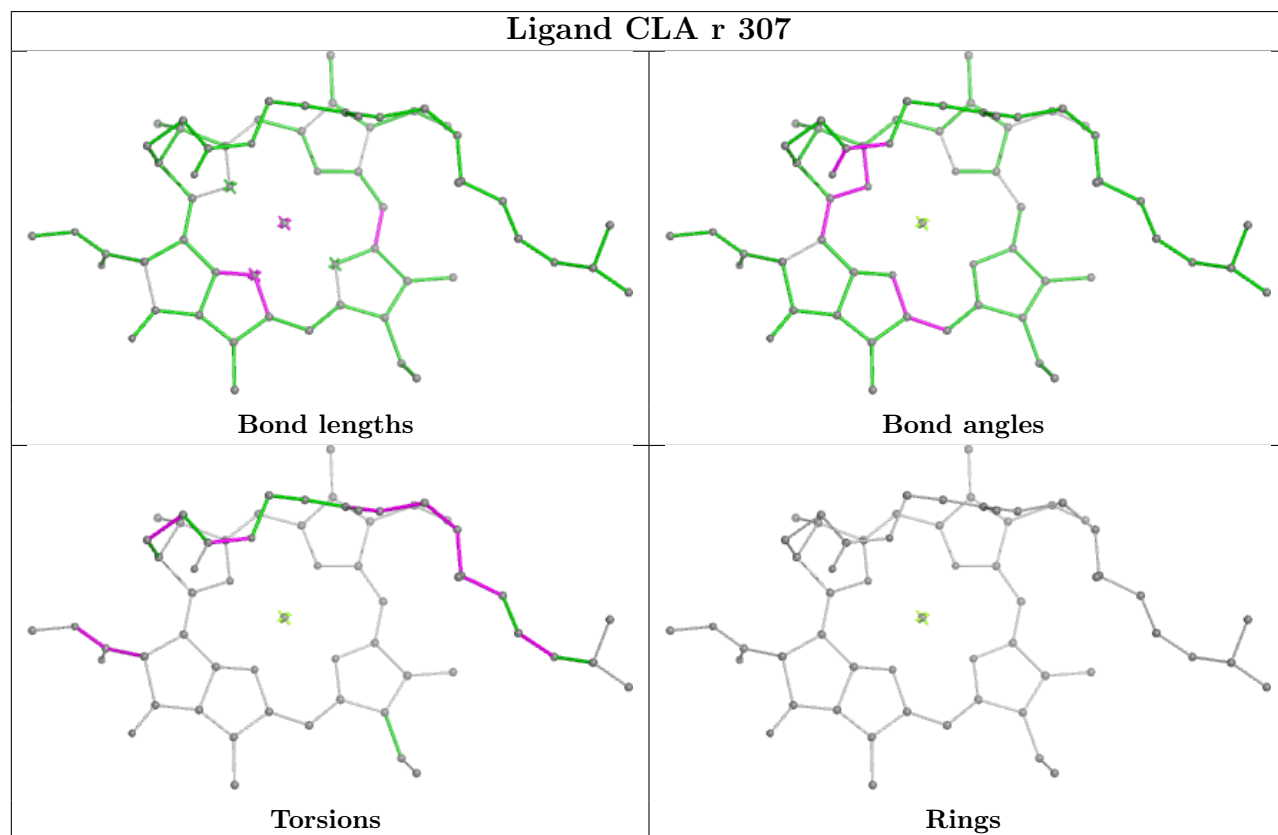
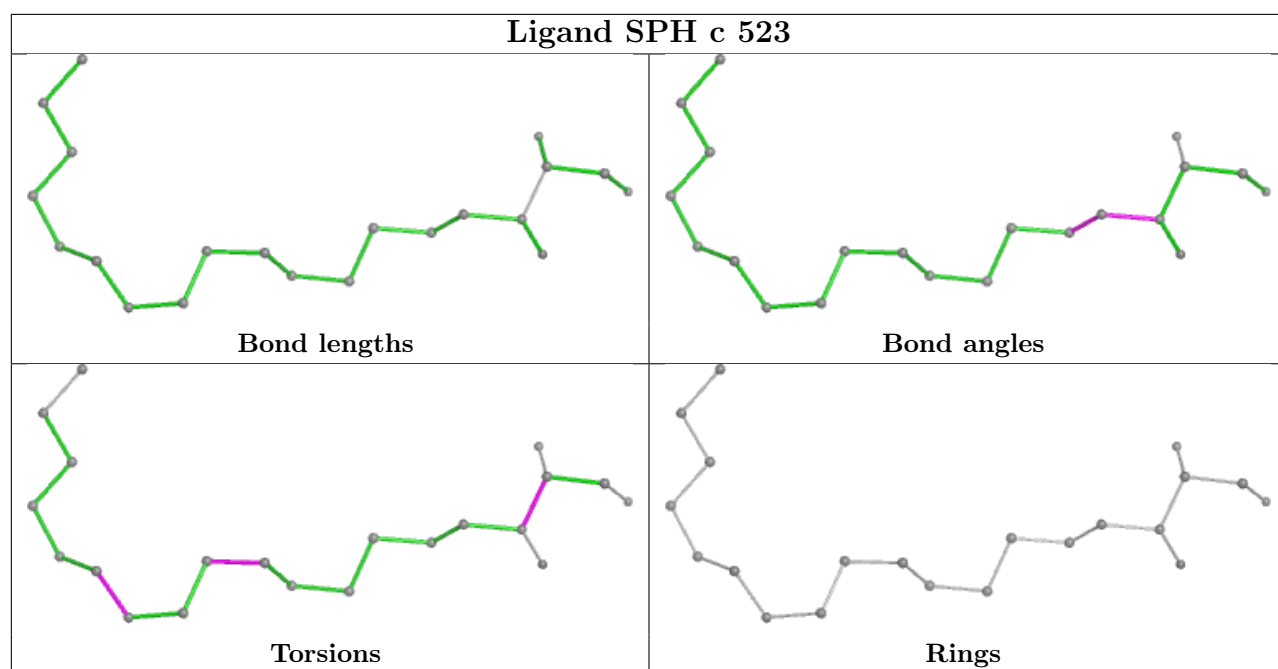
Bond angles

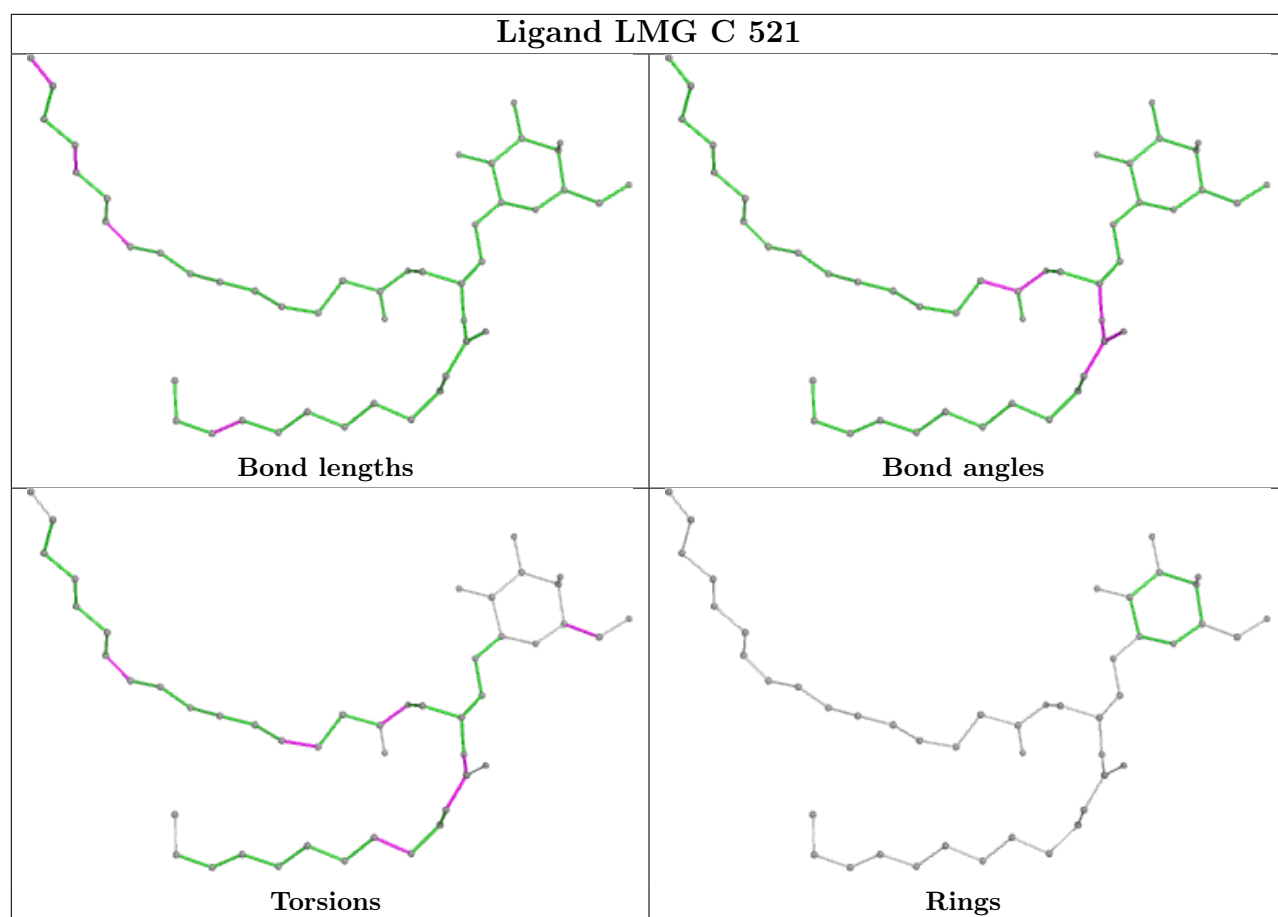


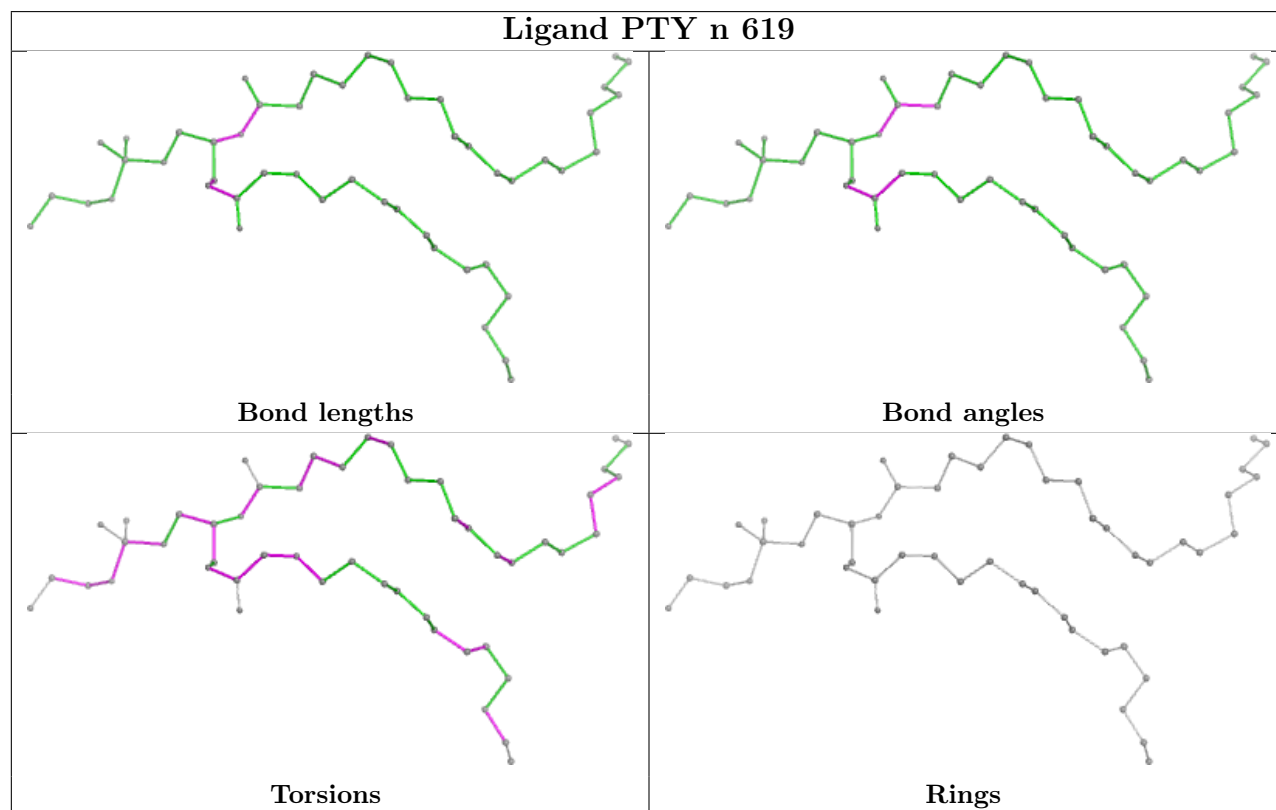
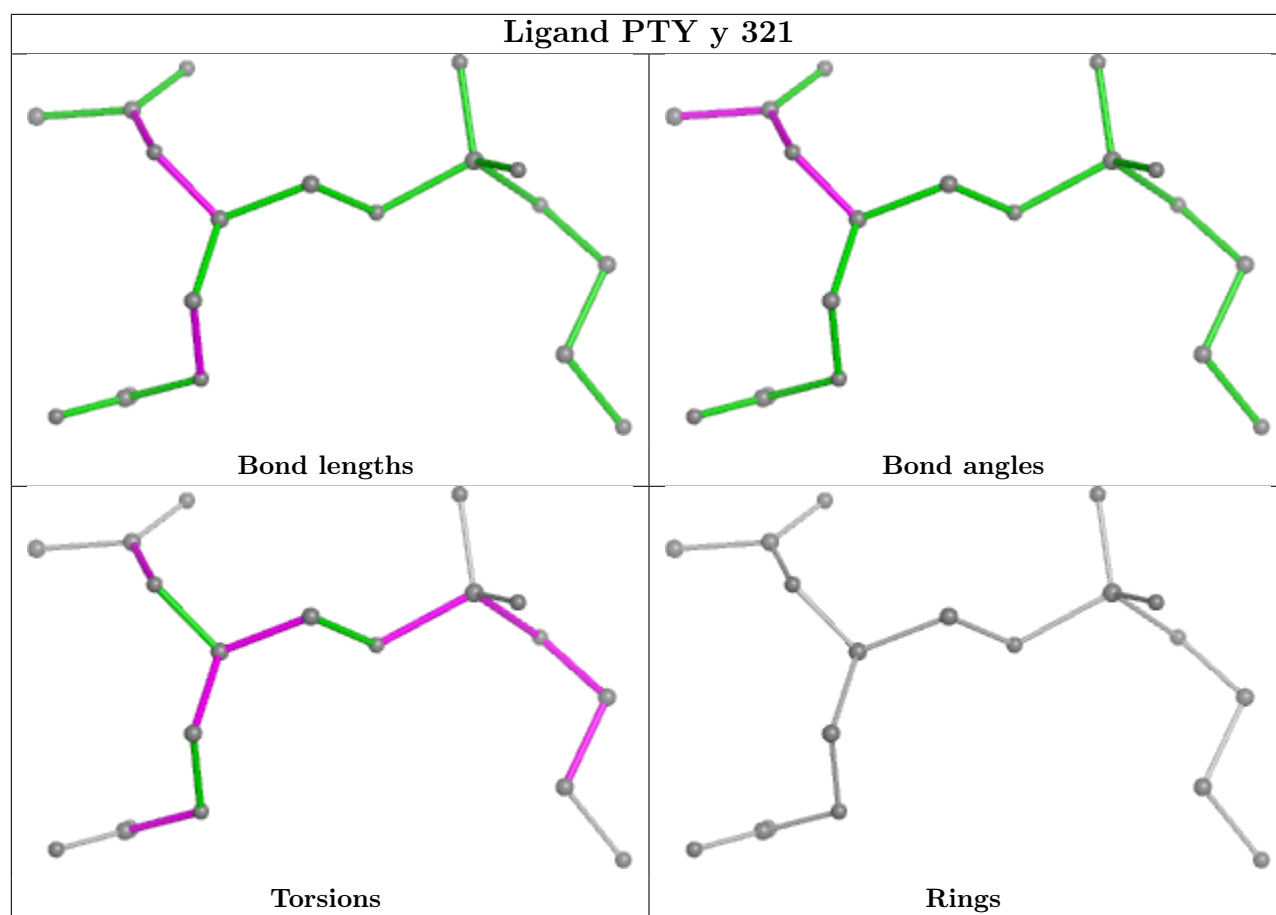
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	D	6
1	A	3
22	r	1
22	R	1

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	13.60
1	R	110:PRO	C	126:GLU	N	12.92
1	A	269:ARG	C	270:SER	N	1.20
1	D	243:THR	C	244:TYR	N	1.20
1	D	213:ILE	C	214:HIS	N	1.19

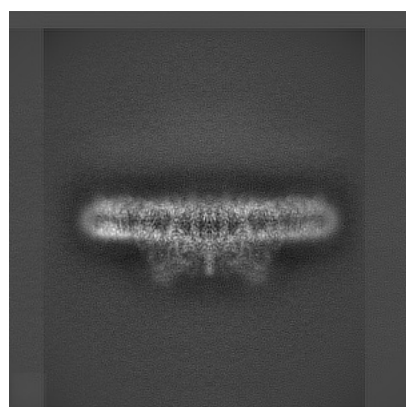
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13429. These allow visual inspection of the internal detail of the map and identification of artifacts.

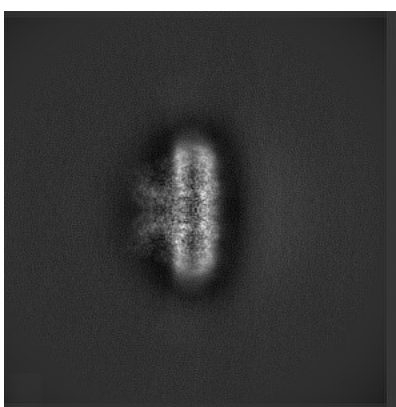
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

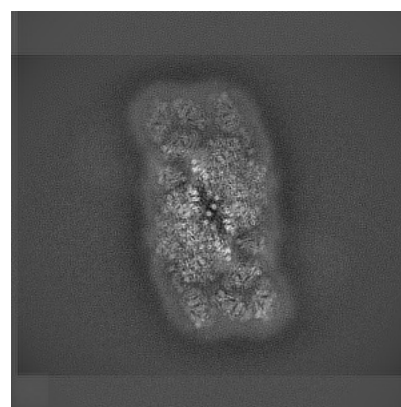
6.1.1 Primary map



X



Y

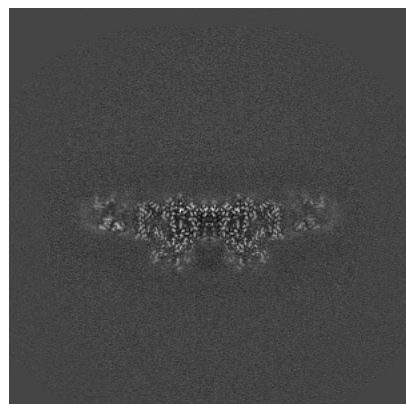


Z

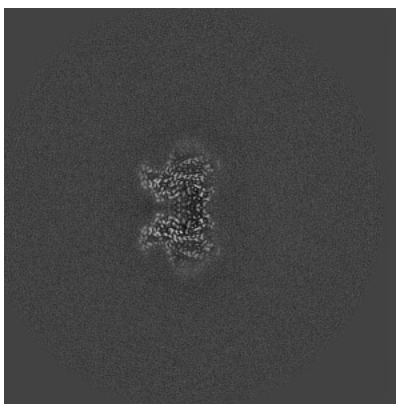
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

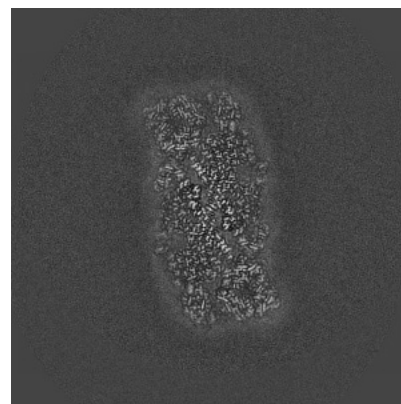
6.2.1 Primary map



X Index: 250



Y Index: 250

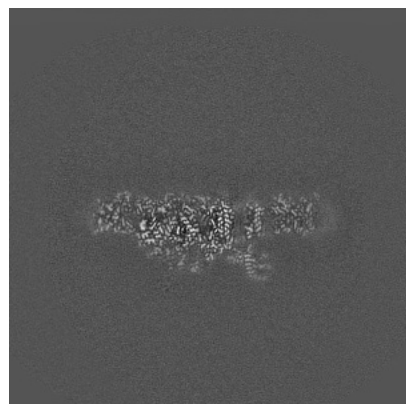


Z Index: 250

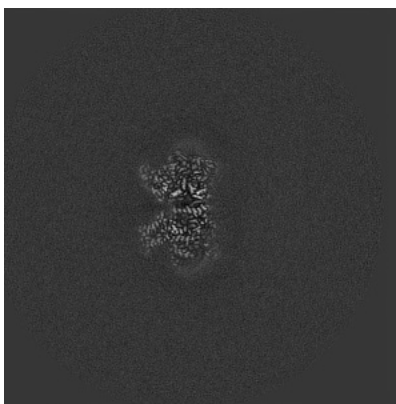
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

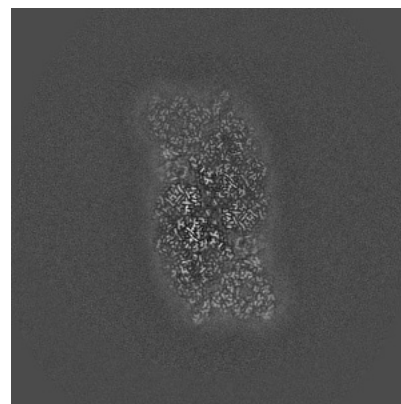
6.3.1 Primary map



X Index: 229



Y Index: 247

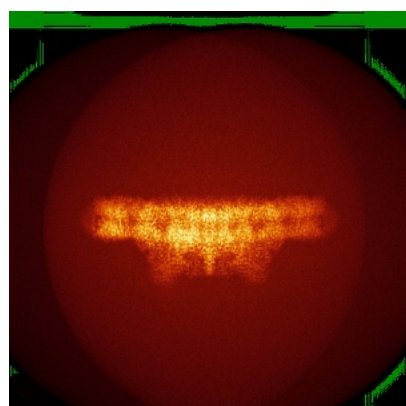


Z Index: 221

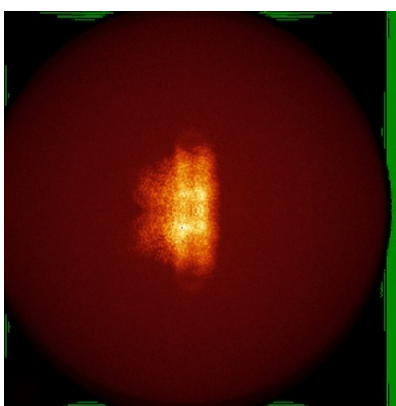
The images above show the largest variance slices of the map in three orthogonal directions.

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

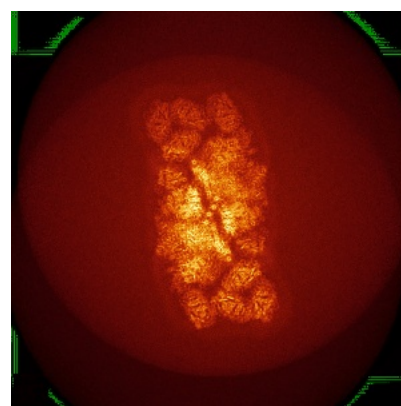
6.4.1 Primary map



X



Y

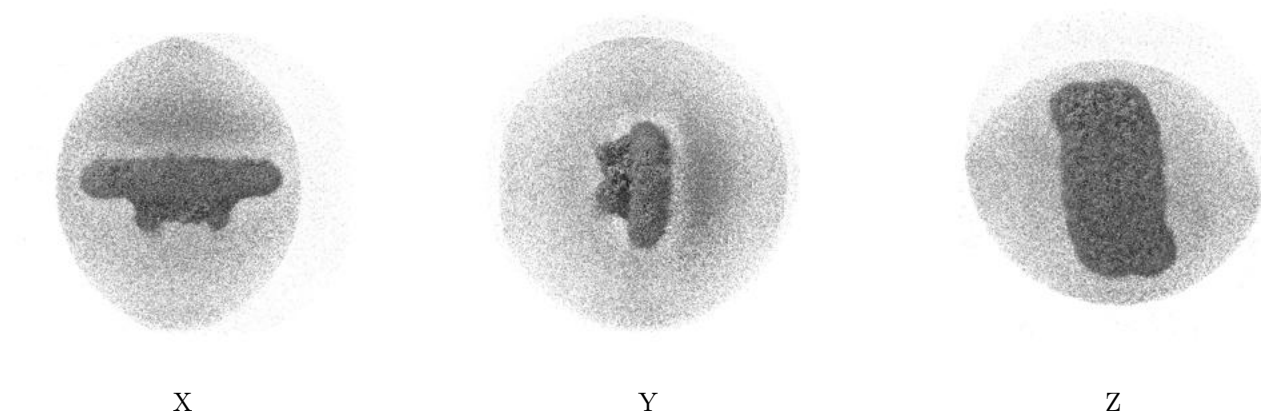


Z

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

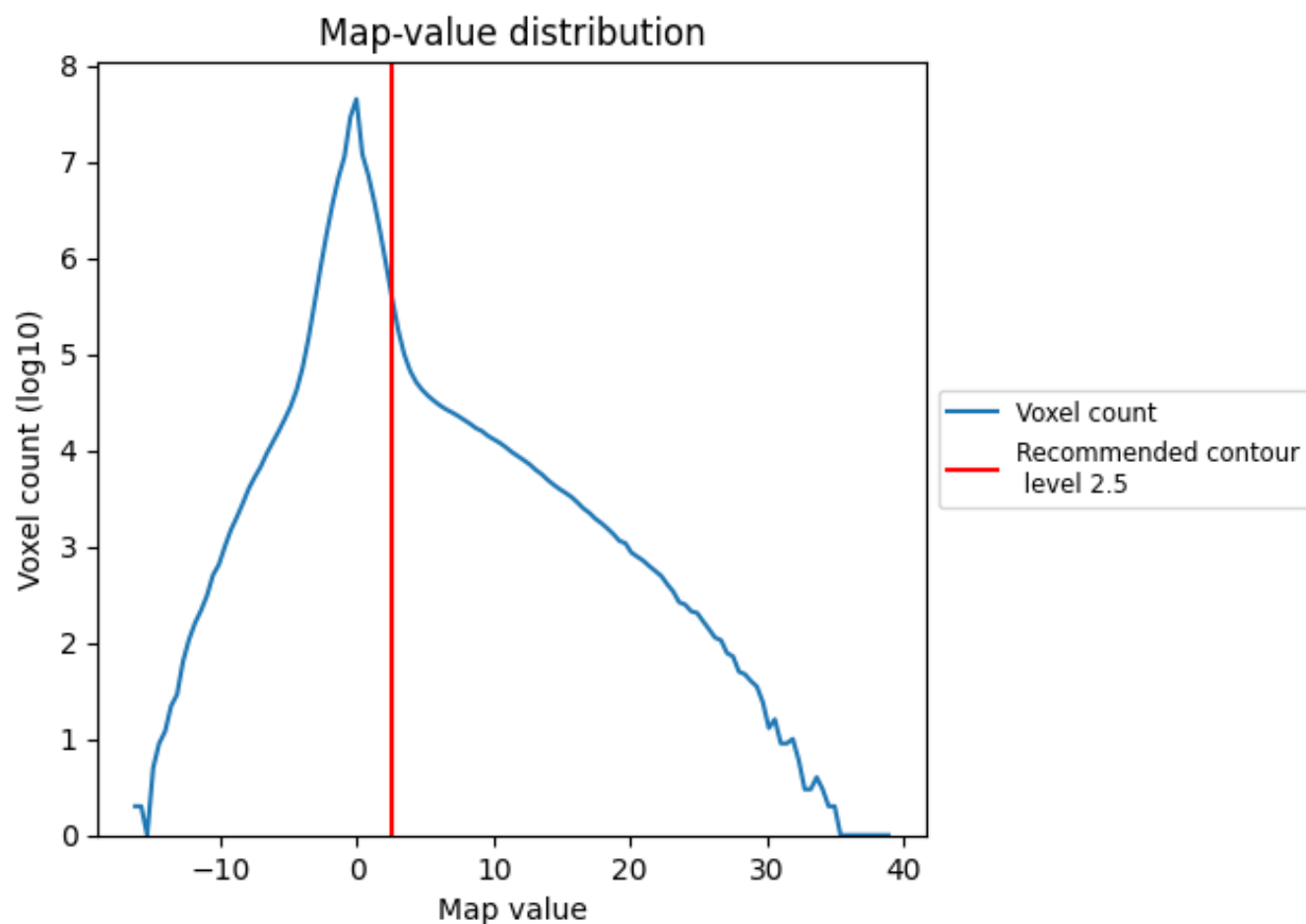
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

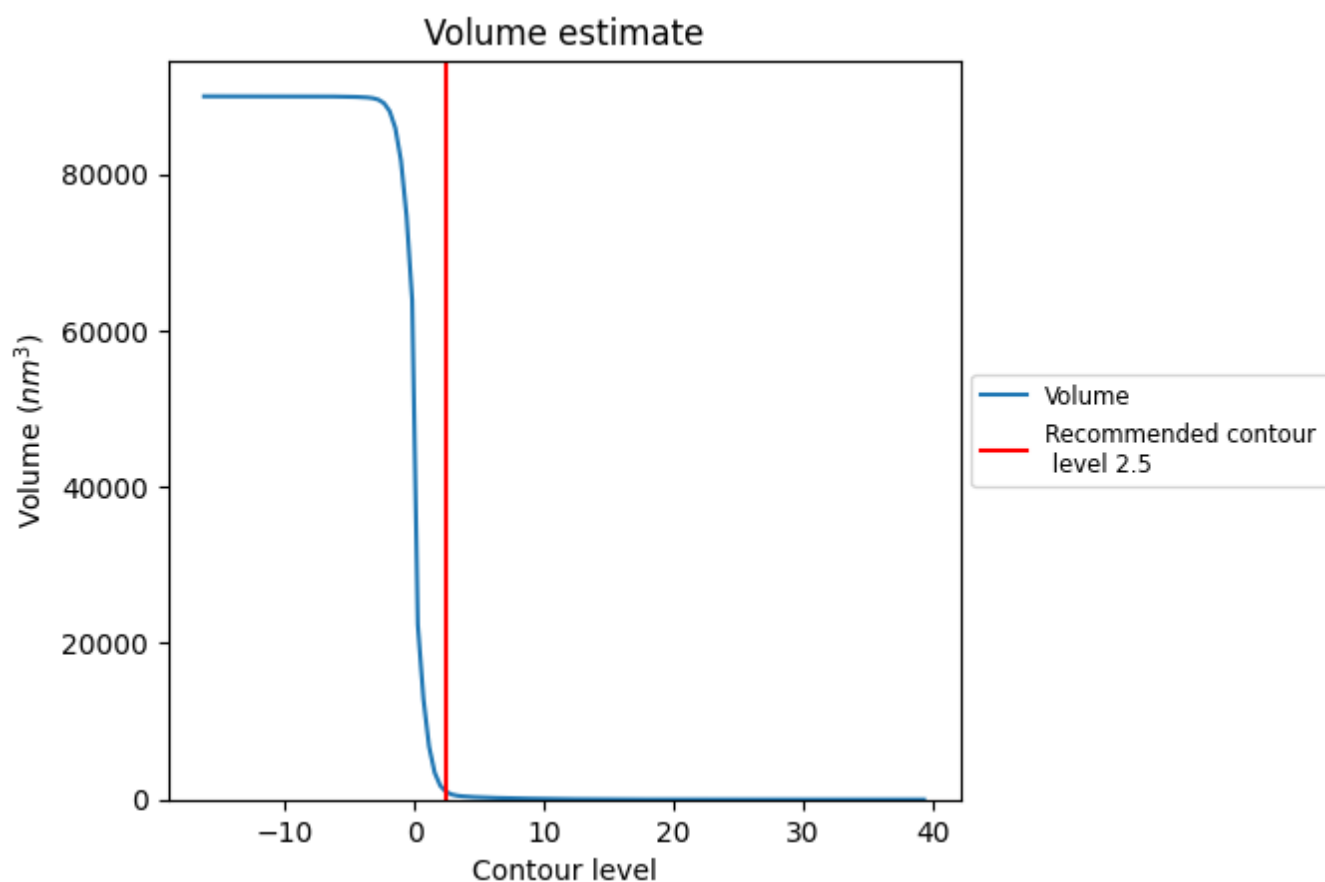
This section contains the results of statistical analysis of the map.

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.

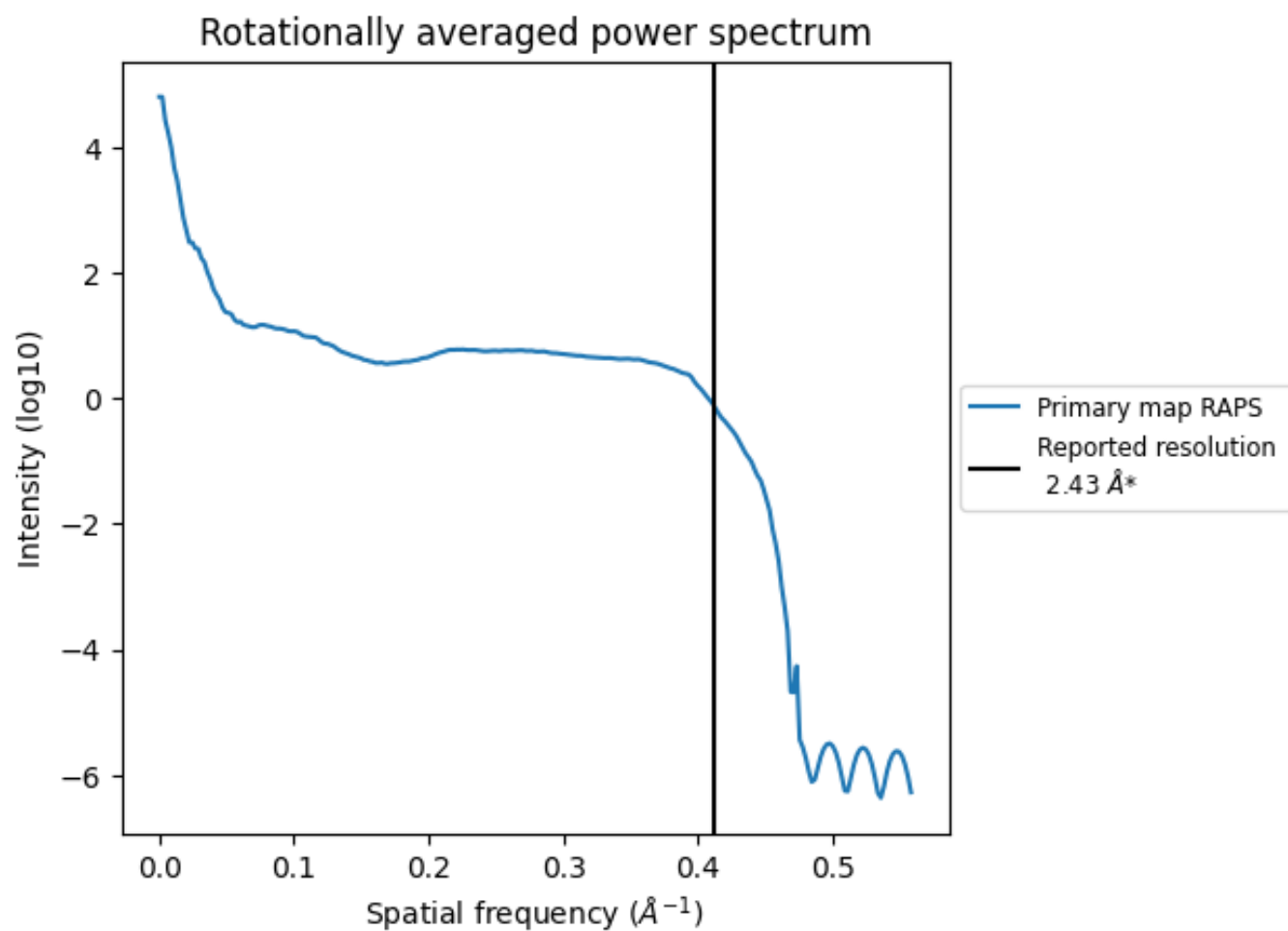
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 948 nm^3 ; this corresponds to an approximate mass of 856 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

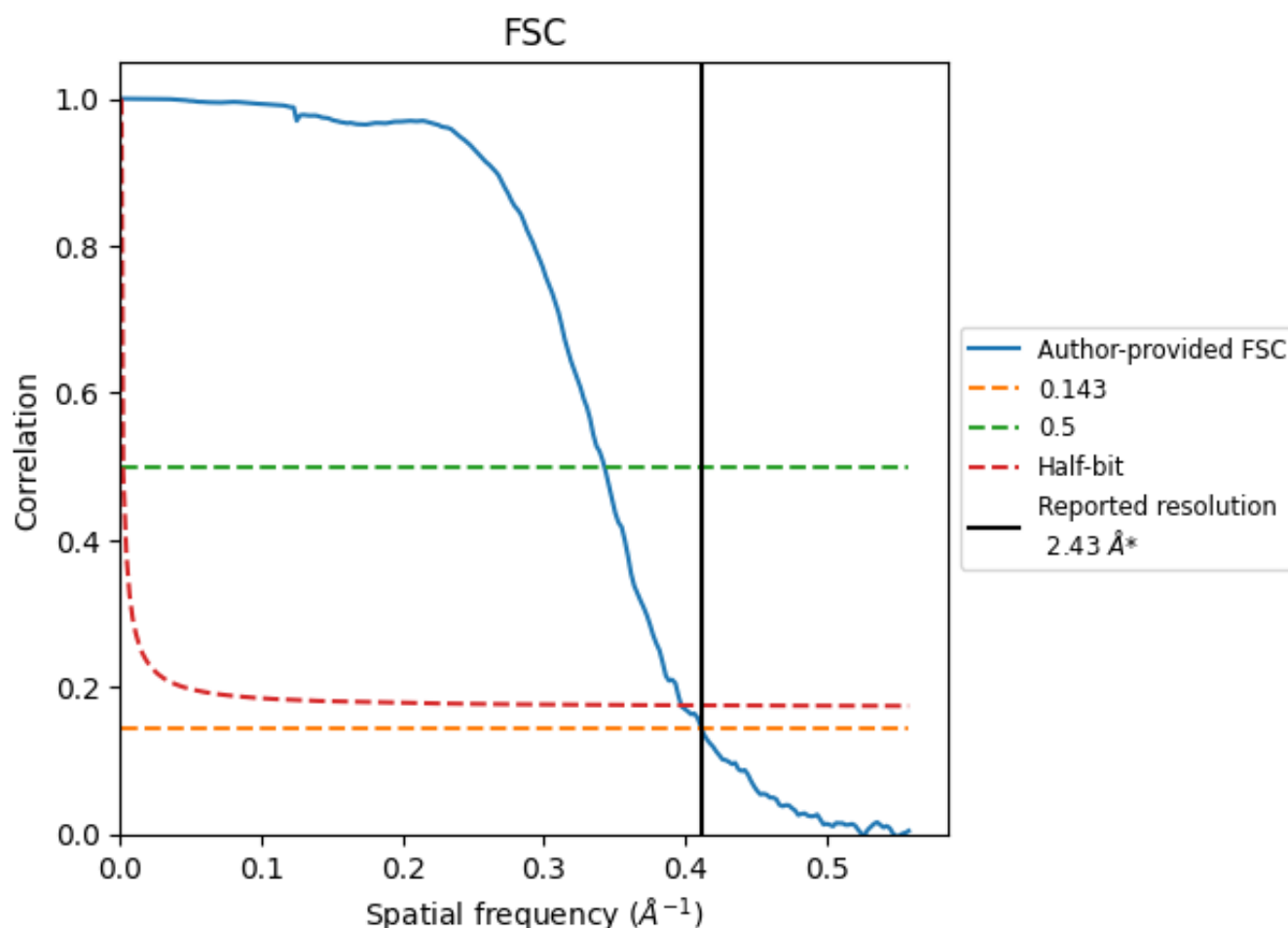


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

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 0.412 Å⁻¹

8.2 Resolution estimates [i](#)

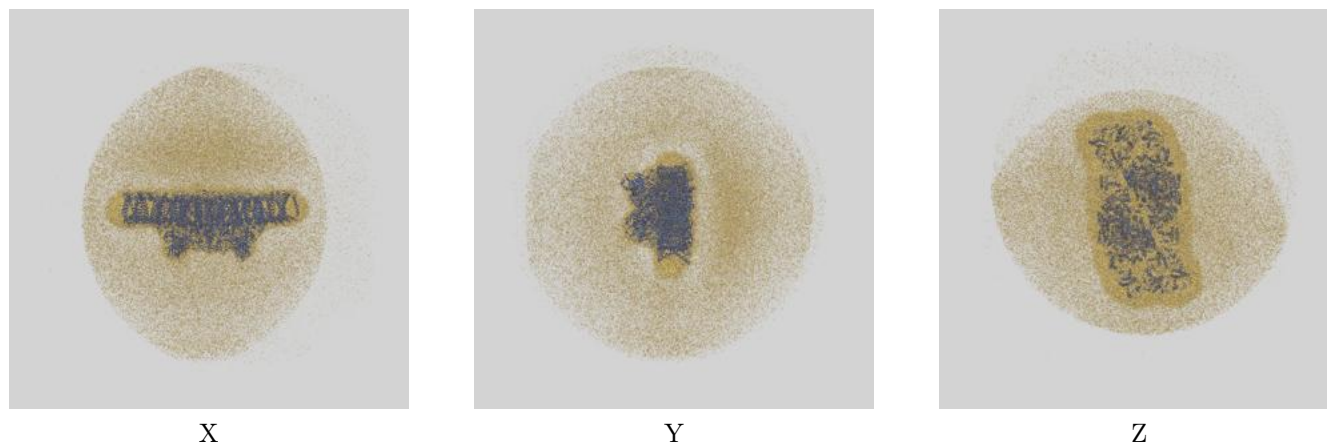
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.43	2.92	2.52
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

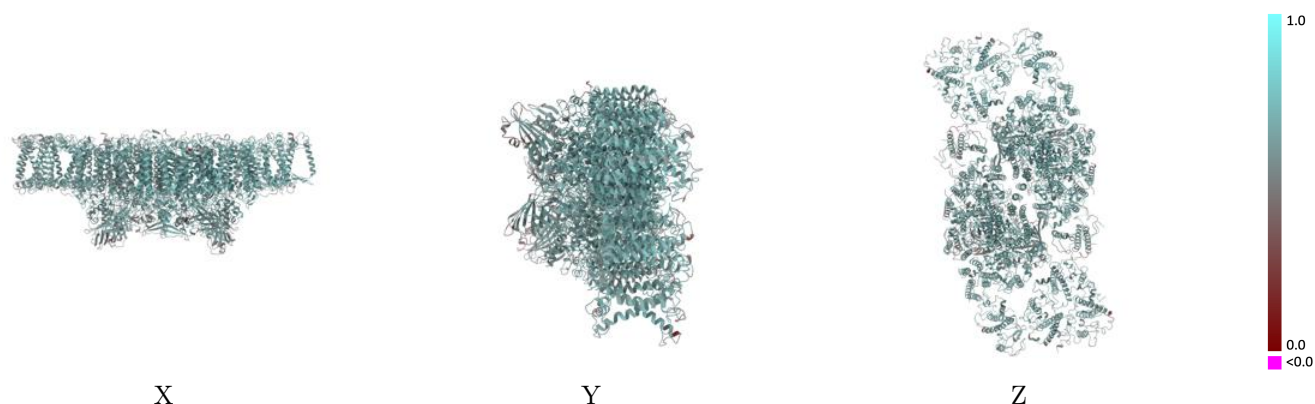
This section contains information regarding the fit between EMDB map EMD-13429 and PDB model 7PI0. Per-residue inclusion information can be found in section 3 on page 47.

9.1 Map-model overlay [i](#)



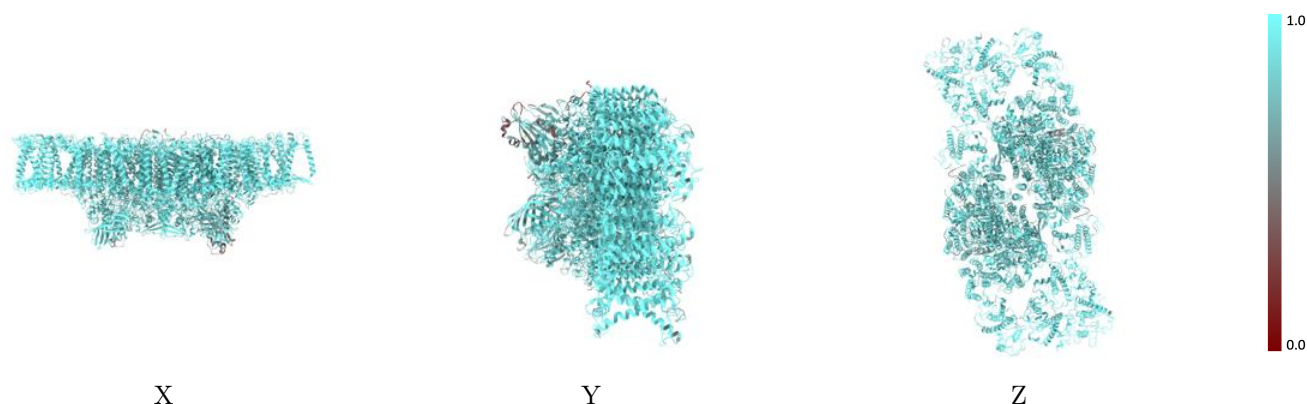
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



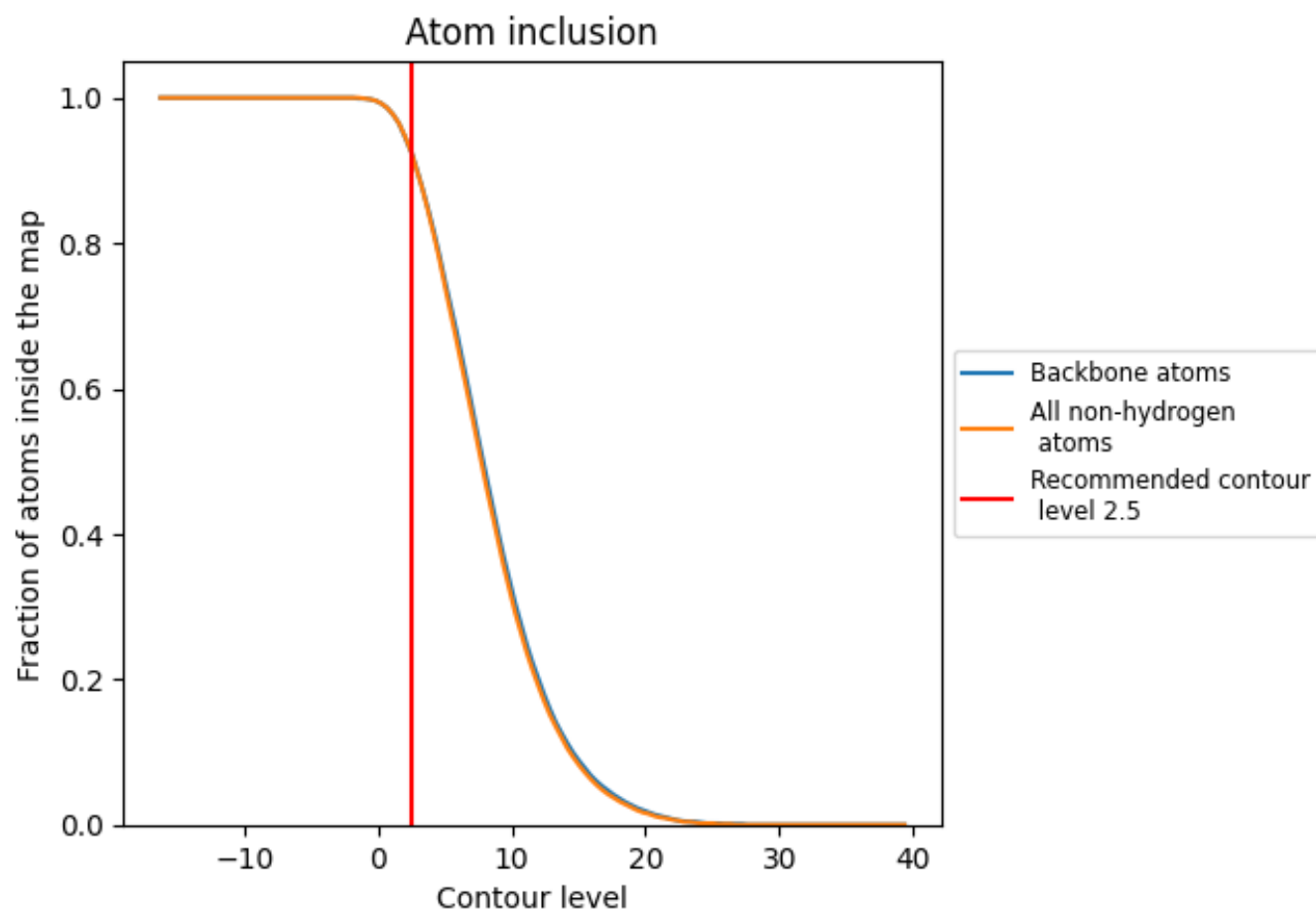
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6230
A	 0.9700	 0.6740
B	 0.9620	 0.6610
C	 0.9500	 0.6650
D	 0.9640	 0.6760
E	 0.9400	 0.6310
F	 0.9510	 0.6330
G	 0.9000	 0.6040
H	 0.9590	 0.6480
I	 0.9530	 0.6540
J	 0.9210	 0.6230
K	 0.9490	 0.6590
L	 0.9470	 0.6280
M	 0.9380	 0.6120
N	 0.9070	 0.6180
O	 0.8920	 0.5830
P	 0.6080	 0.5280
R	 0.8970	 0.5670
S	 0.9130	 0.6180
T	 0.9340	 0.6320
U	 0.8300	 0.5380
V	 0.9290	 0.6250
W	 0.8820	 0.5940
X	 0.8950	 0.5910
Y	 0.9250	 0.6340
Z	 0.9580	 0.6380
a	 0.9590	 0.6550
b	 0.9560	 0.6450
c	 0.9430	 0.6440
d	 0.9590	 0.6520
e	 0.9330	 0.5960
f	 0.9160	 0.6000
g	 0.9360	 0.5770
h	 0.9610	 0.6250
i	 0.9360	 0.6510



Continued on next page...

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Chain	Atom inclusion	Q-score
j	 0.9070	 0.6080
k	 0.9560	 0.6300
l	 0.9570	 0.6330
m	 0.9490	 0.6100
n	 0.9410	 0.6030
o	 0.8940	 0.5620
p	 0.7120	 0.5100
r	 0.9090	 0.5520
s	 0.9200	 0.5880
t	 0.9300	 0.6340
u	 0.7940	 0.5130
v	 0.9170	 0.6030
w	 0.8730	 0.5780
x	 0.8860	 0.5720
y	 0.9390	 0.6210
z	 0.9540	 0.6120