



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 05:53 AM JST

PDB ID : 7VY2
EMDB ID : EMD-32192
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES DIMER
Authors : Tani, K.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Nagashima, K.V.P.; Hall, M.; Takahashi, A.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on : 2021-11-13
Resolution : 2.75 Å(reported)
Based on initial model : 7F0L

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:

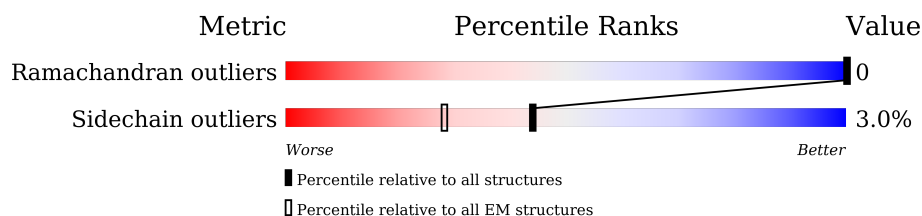
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

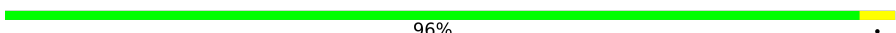
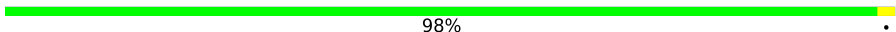
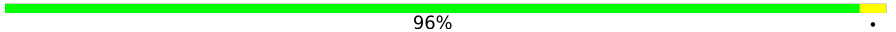
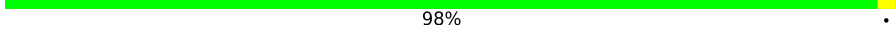
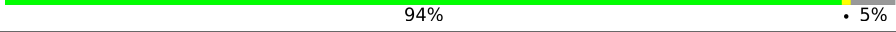
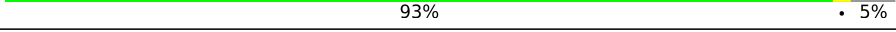
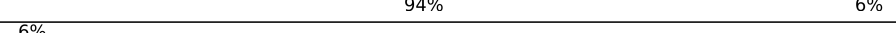
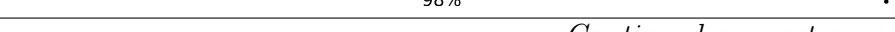
The reported resolution of this entry is 2.75 Å.

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	154571	4023
Sidechain outliers	154315	3826

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	L	281	 96% .
1	l	281	 98% .
2	M	307	 96% .
2	m	307	 98% .
3	H	260	 94% . 5%
3	h	260	 93% . 5%
4	01	54	 98% .
4	03	54	 94% 6%
4	05	54	 6% 98% .











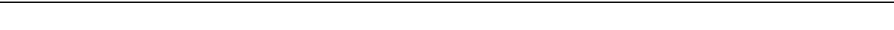

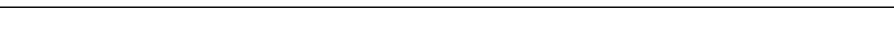
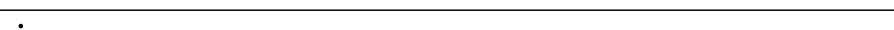







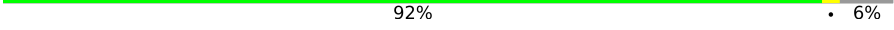



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	07	54	
4	1	54	
4	3	54	
4	5	54	
4	7	54	
4	A	54	
4	D	54	
4	F	54	
4	I	54	
4	K	54	
4	O	54	
4	Q	54	
4	S	54	
4	V	54	
4	Y	54	
4	a	54	
4	d	54	
4	f	54	
4	i	54	
4	k	54	
4	o	54	
4	q	54	
4	s	54	
4	v	54	
4	y	54	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	02	48	 88% 12%
5	04	48	 90% 10%
5	06	48	 12% 83% 12%
5	08	48	 19% 77% 21%
5	2	48	 85% 12%
5	4	48	 17% 88% 10%
5	6	48	 31% 88% 12%
5	8	48	 31% 79% 21%
5	B	48	 92% 8%
5	E	48	 81% 8% 10%
5	G	48	 88% 6% 6%
5	J	48	 88% 10%
5	N	48	 90% 10%
5	P	48	 83% 6% 10%
5	R	48	 88% 10%
5	T	48	 90% 10%
5	W	48	 88% 10%
5	Z	48	 88% 10%
5	b	48	 88% 10%
5	e	48	 85% 10%
5	g	48	 92% 6%
5	j	48	 88% 10%
5	n	48	 85% 10%
5	p	48	 88% 10%
5	r	48	 85% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	t	48	<div><div></div><div>88%</div><div></div><div>10%</div></div>
5	w	48	<div><div></div><div>90%</div><div></div><div>10%</div></div>
5	z	48	<div><div></div><div>83%</div><div>6%</div><div>10%</div></div>
6	X	81	<div><div></div><div>72%</div><div>5%</div><div>23%</div></div>
6	x	81	<div><div></div><div>70%</div><div></div><div>26%</div></div>
7	U	53	<div><div>40%</div><div>89%</div><div></div><div>9%</div></div>
7	u	53	<div><div>13%</div><div>25%</div><div>75%</div><div></div></div>

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 46292 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 Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		
1	l	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		
2	m	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		

- Molecule 3 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	248	Total	C	N	O	S	0	0
			1884	1209	320	345	10		
3	h	248	Total	C	N	O	S	0	0
			1884	1209	320	345	10		

- Molecule 4 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	45	Total	C	N	O	S	0	0
			386	266	59	58	3		
4	D	54	Total	C	N	O	S	0	0
			455	309	73	70	3		
4	F	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	I	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	O	54	Total 453	C 308	N 72	O 70	S 3	0	0
4	Q	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	S	54	Total 448	C 303	N 73	O 70	S 2	0	0
4	V	54	Total 451	C 308	N 70	O 70	S 3	0	0
4	Y	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	1	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	3	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	5	53	Total 447	C 305	N 72	O 68	S 2	0	0
4	7	51	Total 415	C 281	N 68	O 64	S 2	0	0
4	a	45	Total 386	C 266	N 59	O 58	S 3	0	0
4	d	54	Total 455	C 309	N 73	O 70	S 3	0	0
4	f	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	i	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	k	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	o	54	Total 453	C 308	N 72	O 70	S 3	0	0
4	q	54	Total 457	C 311	N 73	O 70	S 3	0	0
4	s	54	Total 454	C 309	N 73	O 70	S 2	0	0
4	v	54	Total 452	C 308	N 73	O 69	S 2	0	0
4	y	54	Total 452	C 308	N 73	O 69	S 2	0	0
4	01	54	Total 457	C 311	N 73	O 70	S 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	03	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	05	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	07	51	Total	C	N	O	S	0	0
			415	281	68	64	2		

- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	R	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	W	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	Z	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	2	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	4	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	6	42	Total	C	N	O	S	0	0
			332	222	54	55	1		
5	8	38	Total	C	N	O	S	0	0
			296	202	49	44	1		
5	b	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	e	43	Total	C	N	O	S	0	0
			351	236	55	59	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
5	j	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	n	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	p	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	r	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	t	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	w	43	Total	C	N	O	S	0	0
			347	234	55	57	1		
5	z	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	02	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
5	04	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	06	42	Total	C	N	O	S	0	0
			332	222	54	55	1		
5	08	38	Total	C	N	O	S	0	0
			296	202	49	44	1		

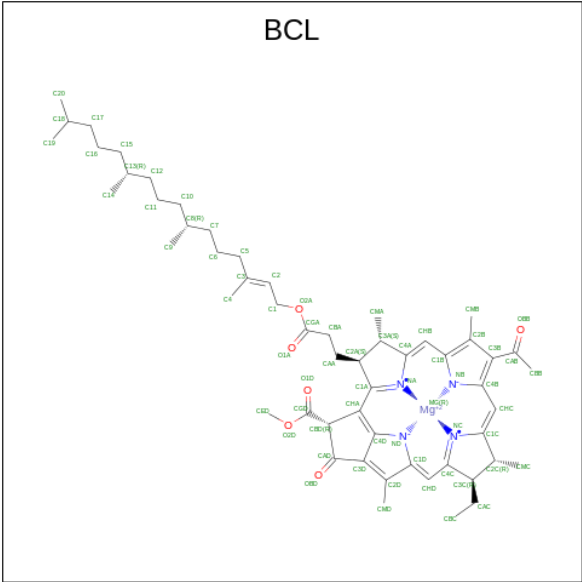
- Molecule 6 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	62	Total	C	N	O	S	0	0
			478	312	84	79	3		
6	x	60	Total	C	N	O	S	0	0
			456	301	78	74	3		

- Molecule 7 is a protein called protein-U.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	48	Total	C	N	O	S	0	0
			353	242	55	53	3		
7	u	13	Total	C	N	O		0	0
			71	45	13	13			

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	L	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	M	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	8	1	Total 60	C 49	Mg 1	N 4	O 6	0
8	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	m	1	Total 198	C 165	Mg 3	N 12	O 18	0
8	m	1	Total 198	C 165	Mg 3	N 12	O 18	0

Continued on next page...

Continued from previous page...

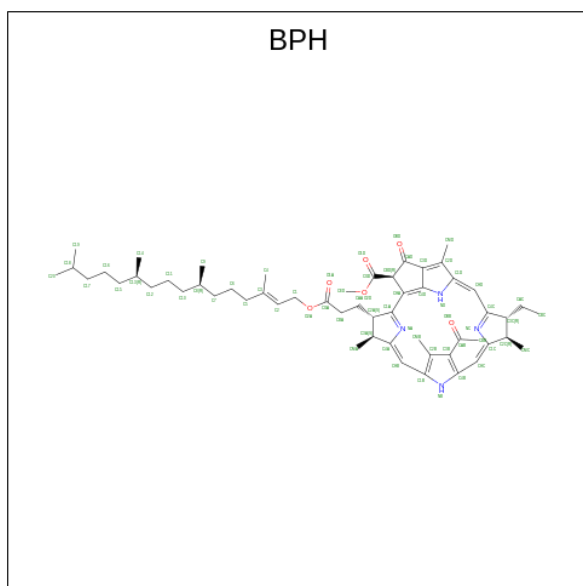
Mol	Chain	Residues	Atoms					AltConf
8	m	1	Total 198	C 165	Mg 3	N 12	O 18	0
8	a	1	Total 48	C 37	Mg 1	N 4	O 6	0
8	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	t	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	w	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	y	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	z	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	01	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	02	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	03	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	04	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	05	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	06	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	07	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	08	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



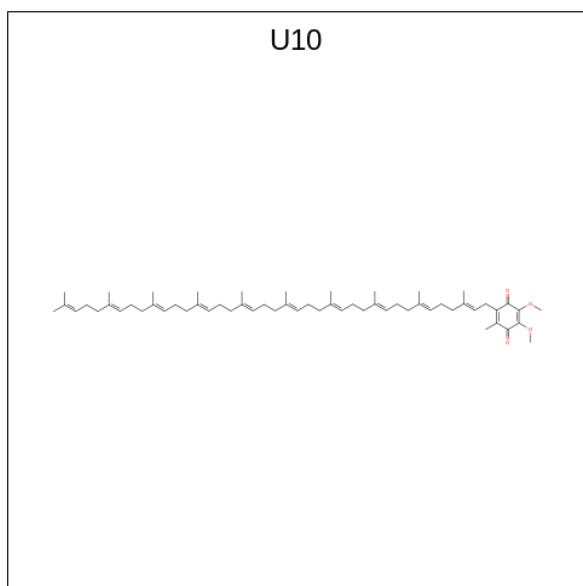
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			65	55	4	6	
9	l	1	Total	C	N	O	0
			65	55	4	6	

Continued on next page...

Continued from previous page...

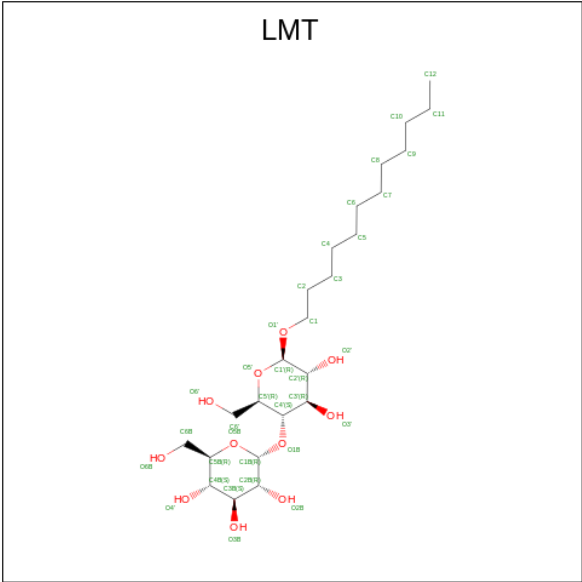
Mol	Chain	Residues	Atoms				AltConf
9	m	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	O		0
			70	62	8		
10	L	1	Total	C	O		0
			70	62	8		
10	M	1	Total	C	O		0
			63	59	4		
10	D	1	Total	C	O		0
			32	28	4		
10	l	1	Total	C	O		0
			70	62	8		
10	l	1	Total	C	O		0
			70	62	8		
10	m	1	Total	C	O		0
			59	55	4		
10	d	1	Total	C	O		0
			30	26	4		

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



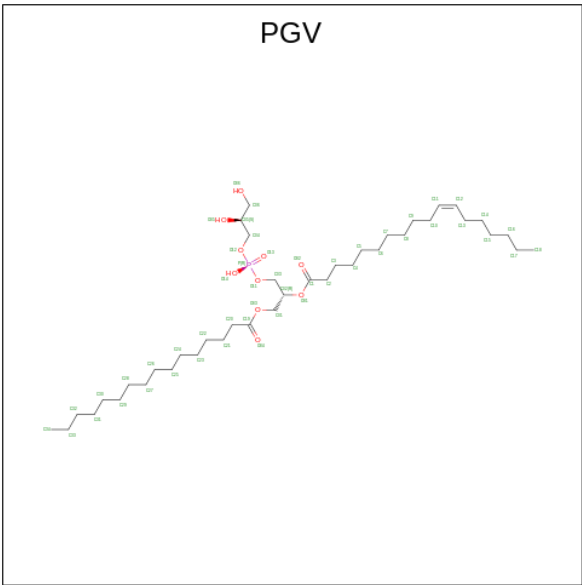
Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			53	32	21	
11	L	1	Total	C	O	0
			53	32	21	
11	M	1	Total	C	O	0
			115	80	35	
11	M	1	Total	C	O	0
			115	80	35	
11	M	1	Total	C	O	0
			115	80	35	
11	M	1	Total	C	O	0
			115	80	35	
11	H	1	Total	C	O	0
			35	24	11	
11	A	1	Total	C	O	0
			35	24	11	
11	I	1	Total	C	O	0
			35	24	11	
11	Q	1	Total	C	O	0
			24	18	6	
11	3	1	Total	C	O	0
			62	40	22	
11	3	1	Total	C	O	0
			62	40	22	
11	5	1	Total	C	O	0
			33	22	11	
11	U	1	Total	C	O	0
			102	69	33	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
11	U	1	Total	C	O	0
			102	69	33	
11	U	1	Total	C	O	0
			102	69	33	
11	m	1	Total	C	O	0
			68	46	22	
11	m	1	Total	C	O	0
			68	46	22	
11	h	1	Total	C	O	0
			62	44	18	
11	h	1	Total	C	O	0
			62	44	18	
11	i	1	Total	C	O	0
			61	40	21	
11	i	1	Total	C	O	0
			61	40	21	
11	q	1	Total	C	O	0
			24	18	6	
11	s	1	Total	C	O	0
			55	38	17	
11	s	1	Total	C	O	0
			55	38	17	
11	03	1	Total	C	O	0
			62	40	22	
11	03	1	Total	C	O	0
			62	40	22	

- Molecule 12 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
12	L	1	Total	C	O	P	0
			162	118	40	4	
12	L	1	Total	C	O	P	0
			162	118	40	4	
12	L	1	Total	C	O	P	0
			162	118	40	4	
12	L	1	Total	C	O	P	0
			162	118	40	4	
12	M	1	Total	C	O	P	0
			38	27	10	1	
12	H	1	Total	C	O	P	0
			113	82	28	3	
12	H	1	Total	C	O	P	0
			113	82	28	3	
12	H	1	Total	C	O	P	0
			113	82	28	3	
12	F	1	Total	C	O	P	0
			41	30	10	1	
12	K	1	Total	C	O	P	0
			41	34	6	1	
12	Q	1	Total	C	O	P	0
			29	18	10	1	
12	1	1	Total	C	O	P	0
			43	32	10	1	
12	l	1	Total	C	O	P	0
			144	100	40	4	
12	l	1	Total	C	O	P	0
			144	100	40	4	

Continued on next page...

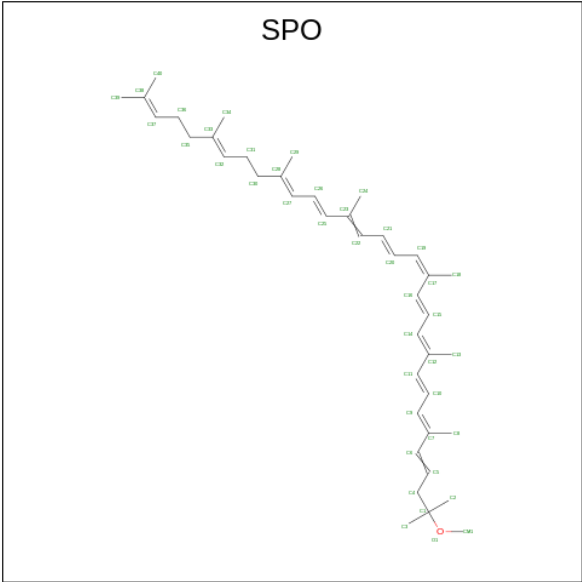
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
12	l	1	Total	C	O	P	0
			144	100	40	4	
12	l	1	Total	C	O	P	0
			144	100	40	4	
12	m	1	Total	C	O	P	0
			77	55	20	2	
12	m	1	Total	C	O	P	0
			77	55	20	2	
12	h	1	Total	C	O	P	0
			73	53	18	2	
12	h	1	Total	C	O	P	0
			73	53	18	2	
12	f	1	Total	C	O	P	0
			87	65	20	2	
12	f	1	Total	C	O	P	0
			87	65	20	2	
12	k	1	Total	C	O	P	0
			41	34	6	1	
12	q	1	Total	C	O	P	0
			34	23	10	1	
12	y	1	Total	C	O	P	0
			43	32	10	1	
12	x	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
13	M	1	Total	Fe	0
			1	1	
13	m	1	Total	Fe	0
			1	1	

- Molecule 14 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



Mol	Chain	Residues	Atoms			AltConf
14	M	1	Total	C	O	0
			42	41	1	
14	A	1	Total	C	O	0
			42	41	1	
14	B	1	Total	C	O	0
			84	82	2	
14	B	1	Total	C	O	0
			84	82	2	
14	E	1	Total	C	O	0
			42	41	1	
14	G	1	Total	C	O	0
			84	82	2	
14	G	1	Total	C	O	0
			84	82	2	
14	I	1	Total	C	O	0
			42	41	1	
14	J	1	Total	C	O	0
			42	41	1	
14	K	1	Total	C	O	0
			42	41	1	
14	N	1	Total	C	O	0
			42	41	1	
14	O	1	Total	C	O	0
			42	41	1	
14	P	1	Total	C	O	0
			42	41	1	
14	Q	1	Total	C	O	0
			42	41	1	

Continued on next page...

Continued from previous page...

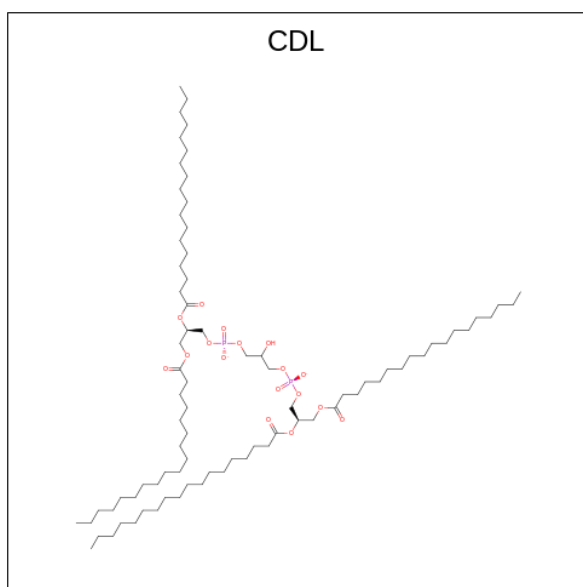
Mol	Chain	Residues	Atoms			AltConf
14	R	1	Total	C	O	0
			42	41	1	
14	S	1	Total	C	O	0
			84	82	2	
14	S	1	Total	C	O	0
			84	82	2	
14	T	1	Total	C	O	0
			42	41	1	
14	V	1	Total	C	O	0
			42	41	1	
14	Y	1	Total	C	O	0
			42	41	1	
14	2	1	Total	C	O	0
			126	123	3	
14	2	1	Total	C	O	0
			126	123	3	
14	2	1	Total	C	O	0
			126	123	3	
14	3	1	Total	C	O	0
			42	41	1	
14	4	1	Total	C	O	0
			42	41	1	
14	5	1	Total	C	O	0
			42	41	1	
14	6	1	Total	C	O	0
			42	41	1	
14	m	1	Total	C	O	0
			42	41	1	
14	a	1	Total	C	O	0
			42	41	1	
14	e	1	Total	C	O	0
			42	41	1	
14	f	1	Total	C	O	0
			84	82	2	
14	f	1	Total	C	O	0
			84	82	2	
14	g	1	Total	C	O	0
			84	82	2	
14	g	1	Total	C	O	0
			84	82	2	
14	j	1	Total	C	O	0
			42	41	1	

Continued on next page...

Continued from previous page...

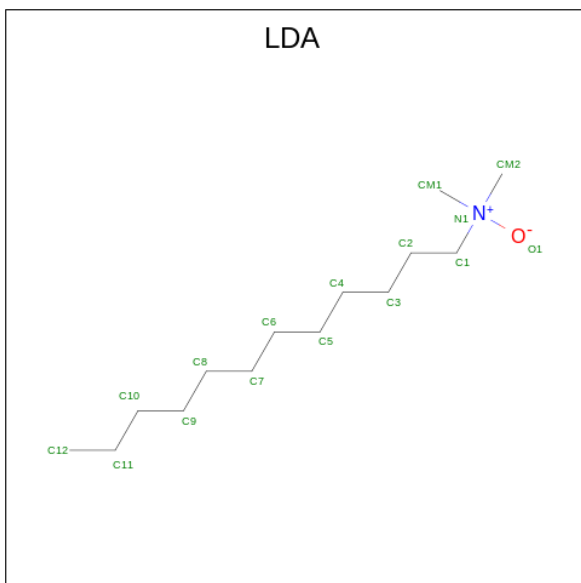
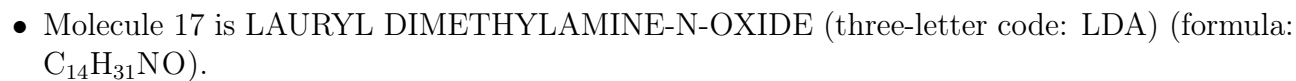
Mol	Chain	Residues	Atoms			AltConf
14	k	1	Total	C	O	0
			42	41	1	
14	n	1	Total	C	O	0
			84	82	2	
14	n	1	Total	C	O	0
			84	82	2	
14	p	1	Total	C	O	0
			42	41	1	
14	q	1	Total	C	O	0
			42	41	1	
14	r	1	Total	C	O	0
			84	82	2	
14	r	1	Total	C	O	0
			84	82	2	
14	s	1	Total	C	O	0
			84	82	2	
14	s	1	Total	C	O	0
			84	82	2	
14	v	1	Total	C	O	0
			42	41	1	
14	w	1	Total	C	O	0
			42	41	1	
14	y	1	Total	C	O	0
			42	41	1	
14	z	1	Total	C	O	0
			42	41	1	
14	01	1	Total	C	O	0
			84	82	2	
14	01	1	Total	C	O	0
			84	82	2	
14	02	1	Total	C	O	0
			42	41	1	
14	05	1	Total	C	O	0
			84	82	2	
14	05	1	Total	C	O	0
			84	82	2	
14	08	1	Total	C	O	0
			42	41	1	

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			79	60	17	2	
15	K	1	Total	C	O	P	0
			61	42	17	2	
15	Y	1	Total	C	O	P	0
			43	26	15	2	
15	X	1	Total	C	O	P	0
			151	98	47	6	
15	X	1	Total	C	O	P	0
			151	98	47	6	
15	X	1	Total	C	O	P	0
			151	98	47	6	
15	m	1	Total	C	O	P	0
			124	88	32	4	
15	m	1	Total	C	O	P	0
			124	88	32	4	
15	h	1	Total	C	O	P	0
			61	42	17	2	
15	y	1	Total	C	O	P	0
			48	30	16	2	
15	x	1	Total	C	O	P	0
			26	13	11	2	

- Molecule 16 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	y	1	12	10	1	1	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosynthetic reaction center L subunit

Chain L:  96%



- Molecule 1: Photosynthetic reaction center L subunit

Chain l:  98%



- Molecule 2: Reaction center protein M chain

Chain M:  96%



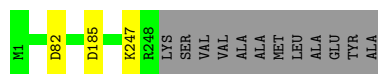
- Molecule 2: Reaction center protein M chain

Chain m:  98%



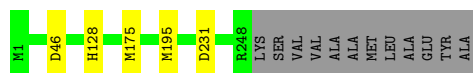
- Molecule 3: Photosynthetic reaction center subunit H

Chain H:  94% 5%




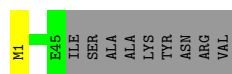
- Molecule 3: Photosynthetic reaction center subunit H

Chain h:  93% 5%



- Molecule 4: Antenna pigment protein alpha chain

Chain A:  81% 17%



- Molecule 4: Antenna pigment protein alpha chain

Chain D:  96%



- Molecule 4: Antenna pigment protein alpha chain

Chain F:  94% 6%



- Molecule 4: Antenna pigment protein alpha chain

Chain I:  96%



- Molecule 4: Antenna pigment protein alpha chain

Chain K:  98%



- Molecule 4: Antenna pigment protein alpha chain

Chain O:  98%



- Molecule 4: Antenna pigment protein alpha chain

Chain Q:  94% 6%



- Molecule 4: Antenna pigment protein alpha chain

Chain S:  93% 7%



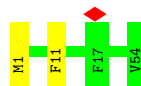
- Molecule 4: Antenna pigment protein alpha chain

Chain V:  98% .



- Molecule 4: Antenna pigment protein alpha chain

Chain Y:  96% .



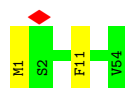
- Molecule 4: Antenna pigment protein alpha chain

Chain 1:  94% 6%



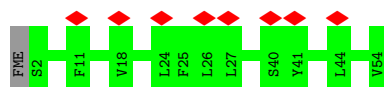
- Molecule 4: Antenna pigment protein alpha chain

Chain 3:  96% .

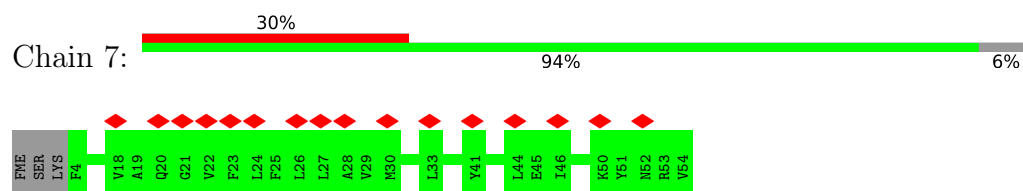


- Molecule 4: Antenna pigment protein alpha chain

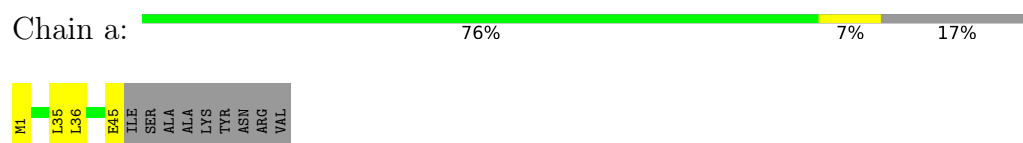
Chain 5:  15% 98% .



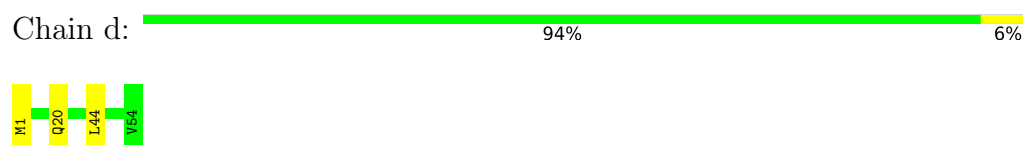
- Molecule 4: Antenna pigment protein alpha chain



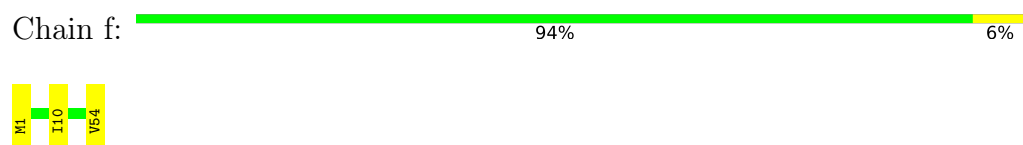
- Molecule 4: Antenna pigment protein alpha chain



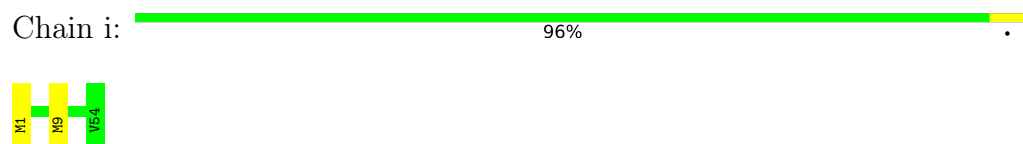
- Molecule 4: Antenna pigment protein alpha chain



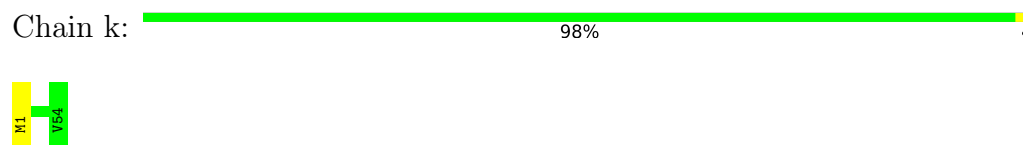
- Molecule 4: Antenna pigment protein alpha chain



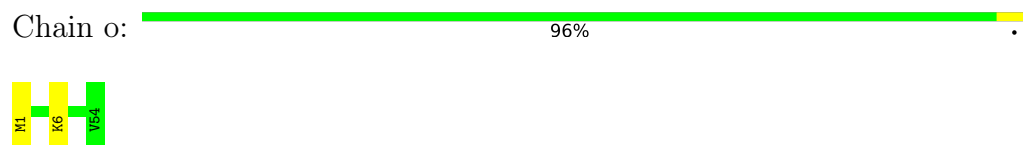
- Molecule 4: Antenna pigment protein alpha chain



- Molecule 4: Antenna pigment protein alpha chain



- Molecule 4: Antenna pigment protein alpha chain



- Molecule 4: Antenna pigment protein alpha chain

Chain q:  98% .



- Molecule 4: Antenna pigment protein alpha chain

Chain s:  96% .



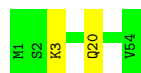
- Molecule 4: Antenna pigment protein alpha chain

Chain v:  98% .



- Molecule 4: Antenna pigment protein alpha chain

Chain y:  96% .



- Molecule 4: Antenna pigment protein alpha chain

Chain 01:  98% .



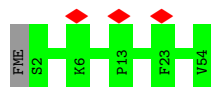
- Molecule 4: Antenna pigment protein alpha chain

Chain 03:  94% 6%

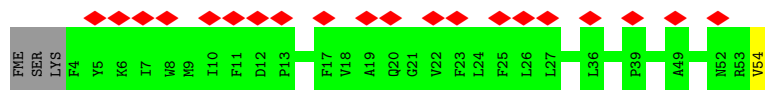
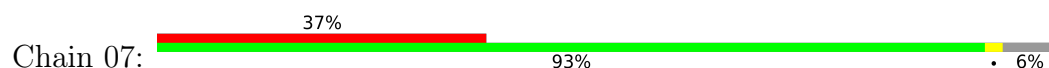


- Molecule 4: Antenna pigment protein alpha chain

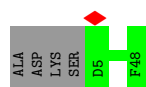
Chain 05:  98% .



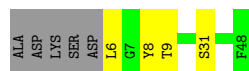
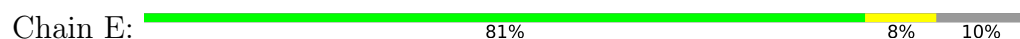
- Molecule 4: Antenna pigment protein alpha chain



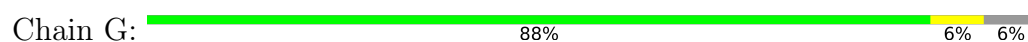
- Molecule 5: Antenna pigment protein beta chain



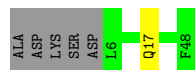
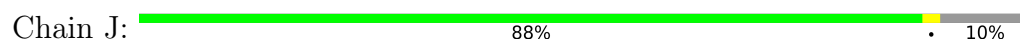
- Molecule 5: Antenna pigment protein beta chain



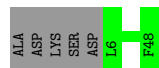
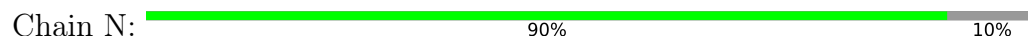
- Molecule 5: Antenna pigment protein beta chain



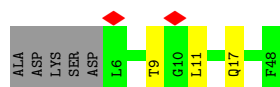
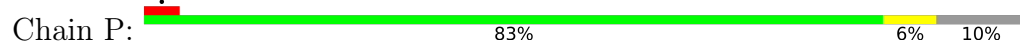
- Molecule 5: Antenna pigment protein beta chain



- Molecule 5: Antenna pigment protein beta chain

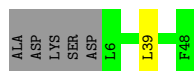


- Molecule 5: Antenna pigment protein beta chain




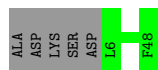
- Molecule 5: Antenna pigment protein beta chain

Chain R:  88% 10%



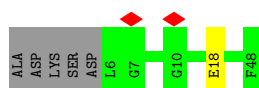
- Molecule 5: Antenna pigment protein beta chain

Chain T:  90% 10%




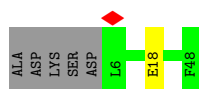
- Molecule 5: Antenna pigment protein beta chain

Chain W:  88% 10%



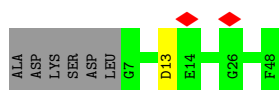
- Molecule 5: Antenna pigment protein beta chain

Chain Z:  88% 10%




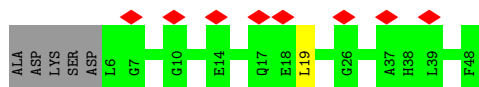
- Molecule 5: Antenna pigment protein beta chain

Chain 2:  85% 12%




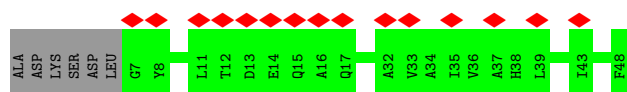
- Molecule 5: Antenna pigment protein beta chain

Chain 4:  17% 88% 10%

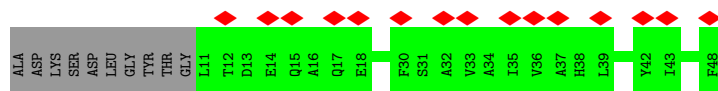
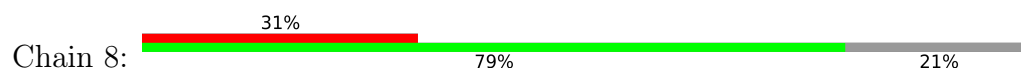


- Molecule 5: Antenna pigment protein beta chain

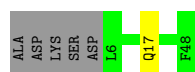
Chain 6:  31% 88% 12%



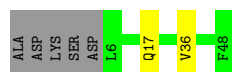
- Molecule 5: Antenna pigment protein beta chain



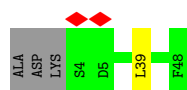
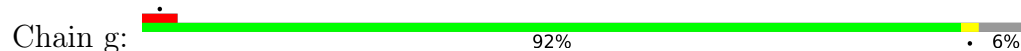
- Molecule 5: Antenna pigment protein beta chain



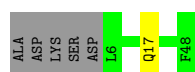
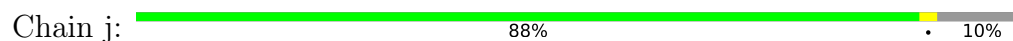
- Molecule 5: Antenna pigment protein beta chain



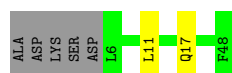
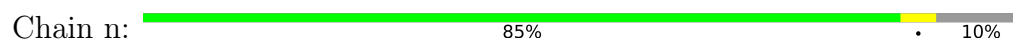
- Molecule 5: Antenna pigment protein beta chain



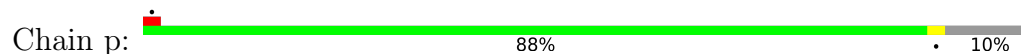
- Molecule 5: Antenna pigment protein beta chain

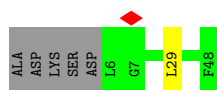


- Molecule 5: Antenna pigment protein beta chain

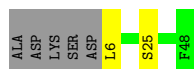
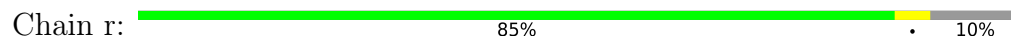


- Molecule 5: Antenna pigment protein beta chain

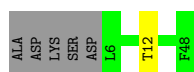
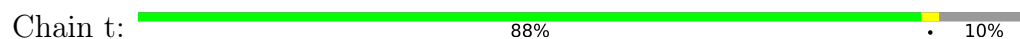




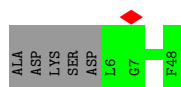
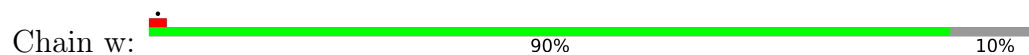
- Molecule 5: Antenna pigment protein beta chain



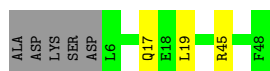
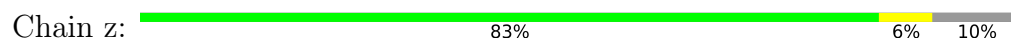
- Molecule 5: Antenna pigment protein beta chain



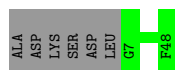
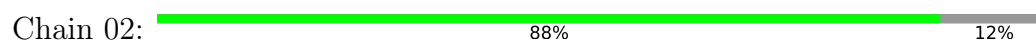
- Molecule 5: Antenna pigment protein beta chain



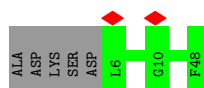
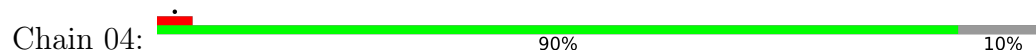
- Molecule 5: Antenna pigment protein beta chain



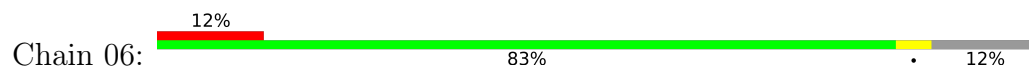
- Molecule 5: Antenna pigment protein beta chain



- Molecule 5: Antenna pigment protein beta chain

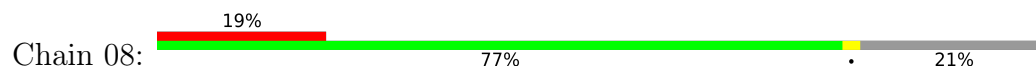


- Molecule 5: Antenna pigment protein beta chain





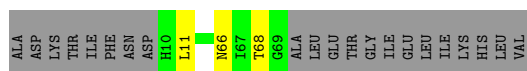
- Molecule 5: Antenna pigment protein beta chain



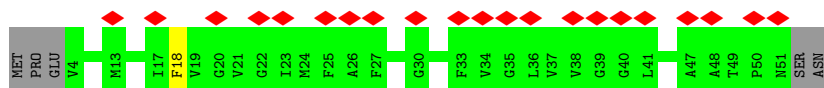
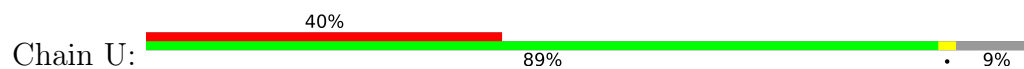
- Molecule 6: PufX



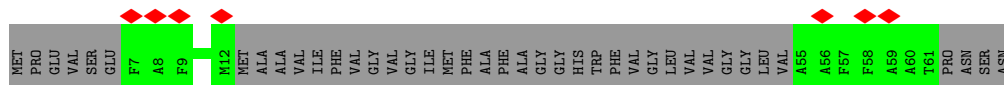
- Molecule 6: PufX



- Molecule 7: protein-U



- Molecule 7: protein-U



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	39.517	Depositor
Minimum map value	-18.203	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.2	Depositor
Map size (\AA)	369.0, 369.0, 369.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, LMT, FME, LDA, BPH, FE, PGV, CDL, U10, BCL, SPO

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	L	0.37	0/2321	0.47	0/3177
1	l	0.38	0/2321	0.46	0/3177
2	M	0.36	0/2530	0.48	0/3455
2	m	0.40	0/2530	0.47	0/3455
3	H	0.32	0/1934	0.49	0/2632
3	h	0.34	0/1934	0.50	0/2632
4	01	0.31	0/461	0.44	0/625
4	03	0.28	0/461	0.45	0/625
4	05	0.27	0/461	0.43	0/625
4	07	0.25	0/427	0.43	0/582
4	1	0.28	0/461	0.44	0/625
4	3	0.27	0/461	0.43	0/625
4	5	0.26	0/461	0.41	0/625
4	7	0.24	0/427	0.41	0/582
4	A	0.33	0/389	0.46	0/528
4	D	0.35	0/459	0.48	0/622
4	F	0.33	0/461	0.46	0/625
4	I	0.32	0/461	0.45	0/625
4	K	0.30	0/461	0.43	0/625
4	O	0.29	0/457	0.44	0/621
4	Q	0.29	0/461	0.44	0/625
4	S	0.29	0/454	0.44	0/616
4	V	0.29	0/455	0.44	0/618
4	Y	0.28	0/461	0.45	0/625
4	a	0.33	0/389	0.48	0/528
4	d	0.35	0/459	0.45	0/622
4	f	0.34	0/461	0.46	0/625
4	i	0.34	0/461	0.45	0/625
4	k	0.32	0/461	0.43	0/625
4	o	0.32	0/457	0.44	0/621
4	q	0.31	0/461	0.46	0/625
4	s	0.32	0/461	0.44	0/625

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	v	0.32	0/461	0.44	0/625
4	y	0.32	0/461	0.43	0/625
5	02	0.29	0/356	0.39	0/488
5	04	0.27	0/364	0.42	0/499
5	06	0.24	0/344	0.42	0/472
5	08	0.25	0/308	0.37	0/424
5	2	0.27	0/356	0.41	0/488
5	4	0.28	0/364	0.47	0/499
5	6	0.25	0/344	0.38	0/472
5	8	0.24	0/308	0.36	0/424
5	B	0.30	0/372	0.39	0/510
5	E	0.29	0/364	0.47	0/499
5	G	0.30	0/378	0.40	0/518
5	J	0.31	0/364	0.42	0/499
5	N	0.28	0/364	0.42	0/499
5	P	0.28	0/364	0.44	0/499
5	R	0.28	0/360	0.41	0/494
5	T	0.27	0/364	0.41	0/499
5	W	0.27	0/360	0.42	0/494
5	Z	0.26	0/364	0.40	0/499
5	b	0.30	0/364	0.42	0/499
5	e	0.33	0/364	0.43	0/499
5	g	0.31	0/378	0.41	0/518
5	j	0.33	0/364	0.43	0/499
5	n	0.28	0/364	0.41	0/499
5	p	0.29	0/364	0.41	0/499
5	r	0.29	0/360	0.41	0/494
5	t	0.28	0/364	0.42	0/499
5	w	0.29	0/360	0.44	0/494
5	z	0.31	0/364	0.44	0/499
6	X	0.28	0/492	0.49	0/669
6	x	0.28	0/470	0.48	0/640
7	U	0.28	0/364	0.40	0/493
7	u	0.25	0/70	0.33	0/94
All	All	0.32	0/37681	0.45	0/51389

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
1	l	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
2	M	304/307 (99%)	289 (95%)	15 (5%)	0	100	100
2	m	304/307 (99%)	292 (96%)	12 (4%)	0	100	100
3	H	246/260 (95%)	232 (94%)	14 (6%)	0	100	100
3	h	246/260 (95%)	236 (96%)	10 (4%)	0	100	100
4	01	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	03	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	05	51/54 (94%)	51 (100%)	0	0	100	100
4	07	49/54 (91%)	48 (98%)	1 (2%)	0	100	100
4	1	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	3	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	5	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
4	7	49/54 (91%)	49 (100%)	0	0	100	100
4	A	43/54 (80%)	41 (95%)	2 (5%)	0	100	100
4	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	F	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	I	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	K	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
4	O	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	Q	52/54 (96%)	50 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S	52/54 (96%)	52 (100%)	0	0	100	100
4	V	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	Y	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	a	43/54 (80%)	41 (95%)	2 (5%)	0	100	100
4	d	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	f	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	i	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	k	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	o	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	q	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	s	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
4	v	52/54 (96%)	52 (100%)	0	0	100	100
4	y	52/54 (96%)	52 (100%)	0	0	100	100
5	02	40/48 (83%)	39 (98%)	1 (2%)	0	100	100
5	04	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	06	40/48 (83%)	39 (98%)	1 (2%)	0	100	100
5	08	36/48 (75%)	36 (100%)	0	0	100	100
5	2	40/48 (83%)	40 (100%)	0	0	100	100
5	4	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	6	40/48 (83%)	40 (100%)	0	0	100	100
5	8	36/48 (75%)	36 (100%)	0	0	100	100
5	B	42/48 (88%)	42 (100%)	0	0	100	100
5	E	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	G	43/48 (90%)	41 (95%)	2 (5%)	0	100	100
5	J	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	N	41/48 (85%)	41 (100%)	0	0	100	100
5	P	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
5	R	41/48 (85%)	41 (100%)	0	0	100	100
5	T	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	W	41/48 (85%)	41 (100%)	0	0	100	100
5	Z	41/48 (85%)	41 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	b	41/48 (85%)	41 (100%)	0	0	100	100
5	e	41/48 (85%)	41 (100%)	0	0	100	100
5	g	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
5	j	41/48 (85%)	41 (100%)	0	0	100	100
5	n	41/48 (85%)	41 (100%)	0	0	100	100
5	p	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	r	41/48 (85%)	41 (100%)	0	0	100	100
5	t	41/48 (85%)	41 (100%)	0	0	100	100
5	w	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
5	z	41/48 (85%)	41 (100%)	0	0	100	100
6	X	60/81 (74%)	56 (93%)	4 (7%)	0	100	100
6	x	58/81 (72%)	54 (93%)	4 (7%)	0	100	100
7	U	46/53 (87%)	46 (100%)	0	0	100	100
7	u	9/53 (17%)	9 (100%)	0	0	100	100
All	All	4400/4820 (91%)	4266 (97%)	134 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	L	220/220 (100%)	209 (95%)	11 (5%)	24	42
1	l	220/220 (100%)	215 (98%)	5 (2%)	50	69
2	M	239/240 (100%)	229 (96%)	10 (4%)	30	49
2	m	239/240 (100%)	234 (98%)	5 (2%)	53	71
3	H	199/208 (96%)	196 (98%)	3 (2%)	65	78
3	h	199/208 (96%)	194 (98%)	5 (2%)	47	67
4	01	48/48 (100%)	48 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	03	48/48 (100%)	46 (96%)	2 (4%)	30	49
4	05	48/48 (100%)	48 (100%)	0	100	100
4	07	43/48 (90%)	42 (98%)	1 (2%)	50	69
4	1	48/48 (100%)	46 (96%)	2 (4%)	30	49
4	3	48/48 (100%)	47 (98%)	1 (2%)	53	71
4	5	48/48 (100%)	48 (100%)	0	100	100
4	7	43/48 (90%)	43 (100%)	0	100	100
4	A	41/48 (85%)	41 (100%)	0	100	100
4	D	47/48 (98%)	46 (98%)	1 (2%)	53	71
4	F	48/48 (100%)	46 (96%)	2 (4%)	30	49
4	I	48/48 (100%)	47 (98%)	1 (2%)	53	71
4	K	48/48 (100%)	48 (100%)	0	100	100
4	O	47/48 (98%)	47 (100%)	0	100	100
4	Q	48/48 (100%)	46 (96%)	2 (4%)	30	49
4	S	47/48 (98%)	43 (92%)	4 (8%)	10	19
4	V	47/48 (98%)	47 (100%)	0	100	100
4	Y	48/48 (100%)	47 (98%)	1 (2%)	53	71
4	a	41/48 (85%)	38 (93%)	3 (7%)	14	25
4	d	47/48 (98%)	45 (96%)	2 (4%)	29	48
4	f	48/48 (100%)	46 (96%)	2 (4%)	30	49
4	i	48/48 (100%)	47 (98%)	1 (2%)	53	71
4	k	48/48 (100%)	48 (100%)	0	100	100
4	o	47/48 (98%)	46 (98%)	1 (2%)	53	71
4	q	48/48 (100%)	48 (100%)	0	100	100
4	s	48/48 (100%)	46 (96%)	2 (4%)	30	49
4	v	48/48 (100%)	47 (98%)	1 (2%)	53	71
4	y	48/48 (100%)	46 (96%)	2 (4%)	30	49
5	02	34/39 (87%)	34 (100%)	0	100	100
5	04	35/39 (90%)	35 (100%)	0	100	100
5	06	32/39 (82%)	30 (94%)	2 (6%)	18	31
5	08	26/39 (67%)	25 (96%)	1 (4%)	33	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2	34/39 (87%)	33 (97%)	1 (3%)	42	62
5	4	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	6	32/39 (82%)	32 (100%)	0	100	100
5	8	26/39 (67%)	26 (100%)	0	100	100
5	B	36/39 (92%)	36 (100%)	0	100	100
5	E	35/39 (90%)	31 (89%)	4 (11%)	5	9
5	G	37/39 (95%)	34 (92%)	3 (8%)	11	21
5	J	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	N	35/39 (90%)	35 (100%)	0	100	100
5	P	35/39 (90%)	32 (91%)	3 (9%)	10	18
5	R	34/39 (87%)	33 (97%)	1 (3%)	42	62
5	T	35/39 (90%)	35 (100%)	0	100	100
5	W	34/39 (87%)	33 (97%)	1 (3%)	42	62
5	Z	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	b	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	e	35/39 (90%)	33 (94%)	2 (6%)	20	36
5	g	37/39 (95%)	36 (97%)	1 (3%)	44	65
5	j	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	n	35/39 (90%)	33 (94%)	2 (6%)	20	36
5	p	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	r	34/39 (87%)	32 (94%)	2 (6%)	19	34
5	t	35/39 (90%)	34 (97%)	1 (3%)	42	62
5	w	34/39 (87%)	34 (100%)	0	100	100
5	z	35/39 (90%)	32 (91%)	3 (9%)	10	18
6	X	49/65 (75%)	45 (92%)	4 (8%)	11	20
6	x	46/65 (71%)	43 (94%)	3 (6%)	17	30
7	U	32/37 (86%)	31 (97%)	1 (3%)	40	60
7	u	1/37 (3%)	1 (100%)	0	100	100
All	All	3713/3976 (93%)	3602 (97%)	111 (3%)	44	61

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	X	57	ILE
6	x	68	THR
3	h	175	MET
6	x	66	ASN
5	z	17	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	20	GLN
5	n	17	GLN
5	e	17	GLN
4	f	20	GLN
5	r	15	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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	$\# Z > 2$
4	FME	K	1	4	8,9,10	0.51	0	7,9,11	0.92	1 (14%)
4	FME	A	1	4	8,9,10	0.50	0	7,9,11	0.99	1 (14%)
4	FME	S	1	4	5,6,10	0.77	0	3,6,11	0.76	0
4	FME	o	1	4	8,9,10	0.52	0	7,9,11	1.09	1 (14%)
4	FME	O	1	4	8,9,10	0.52	0	7,9,11	1.01	1 (14%)
4	FME	V	1	4	8,9,10	0.53	0	7,9,11	0.87	1 (14%)
4	FME	d	1	4	8,9,10	0.51	0	7,9,11	0.92	1 (14%)
4	FME	k	1	4	8,9,10	0.49	0	7,9,11	1.01	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FME	q	1	4	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
4	FME	i	1	4	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
4	FME	Q	1	4	8,9,10	0.52	0	7,9,11	0.99	1 (14%)
4	FME	03	1	4	8,9,10	0.52	0	7,9,11	0.96	1 (14%)
4	FME	Y	1	4	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
4	FME	f	1	4	8,9,10	0.49	0	7,9,11	0.95	1 (14%)
4	FME	v	1	4	3,4,10	0.94	0	2,4,11	1.35	0
4	FME	s	1	4	5,6,10	0.78	0	3,6,11	0.64	0
4	FME	a	1	4	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
4	FME	01	1	4	8,9,10	0.52	0	7,9,11	1.01	1 (14%)
4	FME	F	1	4	8,9,10	0.50	0	7,9,11	0.97	1 (14%)
4	FME	I	1	4	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
4	FME	D	1	4	8,9,10	0.51	0	7,9,11	1.08	1 (14%)
4	FME	3	1	4	8,9,10	0.50	0	7,9,11	0.96	1 (14%)
4	FME	y	1	4	3,4,10	0.94	0	2,4,11	1.38	0
4	FME	1	1	4	8,9,10	0.51	0	7,9,11	1.01	1 (14%)

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
4	FME	K	1	4	-	1/7/9/11	-
4	FME	A	1	4	-	1/7/9/11	-
4	FME	S	1	4	-	1/2/5/11	-
4	FME	o	1	4	-	1/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	V	1	4	-	1/7/9/11	-
4	FME	d	1	4	-	1/7/9/11	-
4	FME	k	1	4	-	1/7/9/11	-
4	FME	q	1	4	-	0/7/9/11	-
4	FME	i	1	4	-	2/7/9/11	-
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	03	1	4	-	0/7/9/11	-
4	FME	Y	1	4	-	1/7/9/11	-
4	FME	f	1	4	-	1/7/9/11	-
4	FME	v	1	4	-	0/0/2/11	-
4	FME	s	1	4	-	1/2/5/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FME	a	1	4	-	0/7/9/11	-
4	FME	01	1	4	-	0/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	3	1	4	-	0/7/9/11	-
4	FME	y	1	4	-	0/0/2/11	-
4	FME	1	1	4	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	o	1	FME	O-C-CA	-2.63	117.89	124.78
4	D	1	FME	O-C-CA	-2.61	117.95	124.78
4	O	1	FME	O-C-CA	-2.53	118.14	124.78
4	a	1	FME	O-C-CA	-2.52	118.17	124.78
4	A	1	FME	O-C-CA	-2.52	118.17	124.78

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	F	1	FME	O1-CN-N-CA
4	K	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA
4	S	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 201 ligands modelled in this entry, 2 are monoatomic - leaving 199 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	$\# Z > 2$
15	CDL	K	401	-	60,60,99	1.20	4 (6%)	66,72,111	1.09	4 (6%)
11	LMT	L	305	-	28,28,36	0.53	0	39,39,47	1.35	6 (15%)
8	BCL	m	402	-	58,74,74	1.61	11 (18%)	69,115,115	1.67	13 (18%)
11	LMT	H	802	-	36,36,36	0.39	0	47,47,47	1.16	3 (6%)
11	LMT	h	802	-	27,27,36	0.48	0	32,33,47	0.69	0
12	PGV	L	307	-	38,38,50	1.03	2 (5%)	41,44,56	1.06	2 (4%)
14	SPO	01	103	-	40,41,41	0.64	0	47,50,50	1.83	15 (31%)
8	BCL	02	101	-	58,74,74	1.69	10 (17%)	69,115,115	1.63	12 (17%)
14	SPO	m	407	-	40,41,41	0.65	0	47,50,50	1.70	8 (17%)
12	PGV	L	310	-	38,38,50	1.00	2 (5%)	41,44,56	1.18	4 (9%)
14	SPO	R	101	-	40,41,41	0.66	0	47,50,50	2.09	13 (27%)
14	SPO	3	103	-	40,41,41	0.64	0	47,50,50	1.80	14 (29%)
9	BPH	l	302	-	51,70,70	0.66	2 (3%)	52,101,101	0.71	0
8	BCL	05	101	-	58,74,74	1.65	11 (18%)	69,115,115	1.66	16 (23%)
14	SPO	Q	104	-	40,41,41	0.63	0	47,50,50	1.70	11 (23%)
11	LMT	Q	101	-	24,24,36	0.43	0	29,29,47	0.56	0
8	BCL	2	103	-	58,74,74	1.68	9 (15%)	69,115,115	1.64	12 (17%)
12	PGV	f	103	-	39,39,50	1.03	2 (5%)	42,45,56	1.26	6 (14%)
14	SPO	I	103	-	40,41,41	0.62	0	47,50,50	1.78	14 (29%)
12	PGV	x	101	-	38,38,50	1.06	2 (5%)	41,44,56	1.03	2 (4%)
8	BCL	Z	101	-	58,74,74	1.62	9 (15%)	69,115,115	1.60	12 (17%)
8	BCL	O	101	-	58,74,74	1.66	9 (15%)	69,115,115	1.72	15 (21%)
11	LMT	s	104	-	31,31,36	0.40	0	42,42,47	0.63	0
16	PTY	f	105	-	36,36,49	0.34	0	39,41,54	0.40	0
8	BCL	f	102	-	58,74,74	1.59	8 (13%)	69,115,115	1.81	16 (23%)
14	SPO	05	103	-	40,41,41	0.63	0	47,50,50	2.04	13 (27%)
14	SPO	s	105	-	40,41,41	0.66	0	47,50,50	1.98	15 (31%)
15	CDL	y	102	-	47,47,99	1.18	3 (6%)	52,58,111	1.04	3 (5%)
14	SPO	E	102	-	40,41,41	0.65	0	47,50,50	1.78	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PGV	L	309	-	32,32,50	1.13	2 (6%)	35,38,56	1.22	3 (8%)
14	SPO	O	102	-	40,41,41	0.63	0	47,50,50	1.82	12 (25%)
15	CDL	X	101	-	58,58,99	1.21	4 (6%)	64,70,111	1.19	5 (7%)
14	SPO	A	703	-	40,41,41	0.65	0	47,50,50	2.05	19 (40%)
14	SPO	n	101	-	40,41,41	0.63	0	47,50,50	1.92	14 (29%)
8	BCL	b	101	-	58,74,74	1.61	8 (13%)	69,115,115	1.73	15 (21%)
11	LMT	M	407	-	27,27,36	0.46	0	32,33,47	0.70	0
14	SPO	G	101	-	40,41,41	0.63	0	47,50,50	1.64	10 (21%)
12	PGV	k	103	-	38,40,50	1.03	2 (5%)	40,42,56	1.08	3 (7%)
8	BCL	w	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.62	13 (18%)
12	PGV	l	308	-	23,23,50	1.32	2 (8%)	26,29,56	1.38	4 (15%)
12	PGV	l	306	-	50,50,50	0.90	2 (4%)	53,56,56	1.14	3 (5%)
8	BCL	F	502	-	58,74,74	1.62	8 (13%)	69,115,115	1.75	13 (18%)
14	SPO	n	103	-	40,41,41	0.66	0	47,50,50	1.70	13 (27%)
14	SPO	08	101	-	40,41,41	0.65	0	47,50,50	2.05	15 (31%)
14	SPO	2	104	-	40,41,41	0.62	0	47,50,50	2.00	15 (31%)
8	BCL	1	202	-	58,74,74	1.65	9 (15%)	69,115,115	1.73	16 (23%)
8	BCL	W	101	-	58,74,74	1.65	9 (15%)	69,115,115	1.60	13 (18%)
11	LMT	U	101	-	33,33,36	0.41	0	44,44,47	0.68	1 (2%)
14	SPO	z	101	-	40,41,41	0.68	0	47,50,50	1.77	13 (27%)
8	BCL	S	101	-	58,74,74	1.65	9 (15%)	69,115,115	1.72	17 (24%)
10	U10	L	303	-	35,35,63	0.83	2 (5%)	42,45,79	0.63	0
8	BCL	L	301	-	58,74,74	1.63	9 (15%)	69,115,115	1.70	15 (21%)
10	U10	M	405	-	63,63,63	0.66	2 (3%)	76,79,79	0.60	0
8	BCL	Q	103	-	58,74,74	1.65	9 (15%)	69,115,115	1.75	17 (24%)
14	SPO	f	106	-	40,41,41	0.61	0	47,50,50	1.69	10 (21%)
14	SPO	r	103	-	40,41,41	0.63	0	47,50,50	1.66	13 (27%)
8	BCL	m	403	-	58,74,74	1.66	10 (17%)	69,115,115	1.78	14 (20%)
15	CDL	Y	101	-	42,42,99	1.02	2 (4%)	46,52,111	0.92	2 (4%)
12	PGV	h	801	-	46,46,50	0.91	2 (4%)	49,52,56	1.10	4 (8%)
16	PTY	F	501	-	40,40,49	0.31	0	43,45,54	0.41	0
8	BCL	B	102	-	58,74,74	1.63	8 (13%)	69,115,115	1.75	13 (18%)
12	PGV	m	412	-	38,38,50	1.05	2 (5%)	41,44,56	1.09	3 (7%)
9	BPH	m	404	-	51,70,70	0.63	1 (1%)	52,101,101	0.83	4 (7%)
8	BCL	q	103	-	58,74,74	1.64	10 (17%)	69,115,115	1.76	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	LMT	U	102	-	36,36,36	0.38	0	47,47,47	0.83	2 (4%)
11	LMT	U	103	-	36,36,36	0.37	0	47,47,47	0.79	1 (2%)
8	BCL	P	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.63	13 (18%)
14	SPO	01	102	-	40,41,41	0.63	0	47,50,50	1.74	11 (23%)
14	SPO	G	103	-	40,41,41	0.65	0	47,50,50	2.16	14 (29%)
8	BCL	M	402	-	58,74,74	1.65	10 (17%)	69,115,115	1.82	15 (21%)
8	BCL	7	101	-	58,74,74	1.71	11 (18%)	69,115,115	1.68	12 (17%)
14	SPO	K	404	-	40,41,41	0.63	0	47,50,50	1.73	10 (21%)
17	LDA	y	101	-	8,11,15	2.60	1 (12%)	10,13,17	0.43	0
8	BCL	03	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.66	12 (17%)
8	BCL	Y	102	-	58,74,74	1.67	9 (15%)	69,115,115	1.80	18 (26%)
8	BCL	01	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.74	17 (24%)
11	LMT	M	408	-	25,25,36	0.38	0	30,30,47	0.63	0
8	BCL	p	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.73	15 (21%)
14	SPO	p	101	-	40,41,41	0.67	0	47,50,50	2.28	19 (40%)
11	LMT	q	101	-	24,24,36	0.39	0	29,29,47	0.65	0
10	U10	D	102	-	32,32,63	0.88	2 (6%)	38,41,79	0.67	0
11	LMT	L	306	-	27,27,36	0.49	0	38,38,47	0.92	1 (2%)
8	BCL	j	102	-	58,74,74	1.67	9 (15%)	69,115,115	1.65	13 (18%)
10	U10	d	102	-	30,30,63	0.88	2 (6%)	36,39,79	0.68	0
11	LMT	m	408	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
14	SPO	S	102	-	40,41,41	0.67	0	47,50,50	1.85	16 (34%)
8	BCL	6	101	-	58,74,74	1.74	11 (18%)	69,115,115	1.63	13 (18%)
8	BCL	d	101	-	58,74,74	1.61	9 (15%)	69,115,115	1.85	15 (21%)
8	BCL	t	101	-	58,74,74	1.64	9 (15%)	69,115,115	1.68	13 (18%)
8	BCL	8	101	-	52,68,74	1.83	11 (21%)	61,107,115	1.71	10 (16%)
14	SPO	4	102	-	40,41,41	0.65	0	47,50,50	2.03	13 (27%)
8	BCL	A	702	-	53,69,74	1.73	10 (18%)	63,109,115	1.77	14 (22%)
8	BCL	R	102	-	58,74,74	1.69	11 (18%)	69,115,115	1.61	14 (20%)
14	SPO	B	103	-	40,41,41	0.63	0	47,50,50	1.64	11 (23%)
8	BCL	L	311	-	58,74,74	1.59	8 (13%)	69,115,115	1.76	14 (20%)
11	LMT	I	101	-	36,36,36	0.42	0	47,47,47	0.73	1 (2%)
14	SPO	N	101	-	40,41,41	0.64	0	47,50,50	1.70	10 (21%)
14	SPO	r	101	-	40,41,41	0.64	0	47,50,50	1.79	12 (25%)
8	BCL	r	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.70	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	LMT	M	412	-	31,31,36	0.43	0	42,42,47	0.71	1 (2%)
8	BCL	J	102	-	58,74,74	1.64	8 (13%)	69,115,115	1.60	13 (18%)
14	SPO	5	103	-	40,41,41	0.65	0	47,50,50	1.88	14 (29%)
12	PGV	q	102	-	33,33,50	1.10	2 (6%)	36,39,56	1.15	3 (8%)
14	SPO	a	102	-	40,41,41	0.64	0	47,50,50	1.84	15 (31%)
12	PGV	L	308	-	50,50,50	0.91	2 (4%)	53,56,56	1.04	3 (5%)
16	PTY	H	803	-	36,36,49	0.32	0	39,41,54	0.41	0
8	BCL	N	102	-	58,74,74	1.66	8 (13%)	69,115,115	1.65	13 (18%)
11	LMT	3	104	-	28,28,36	0.45	0	39,39,47	0.71	0
11	LMT	03	101	-	36,36,36	0.38	0	47,47,47	0.71	1 (2%)
11	LMT	s	101	-	25,25,36	0.37	0	30,30,47	0.64	0
10	U10	L	304	-	35,35,63	0.77	2 (5%)	42,45,79	0.68	0
10	U10	l	303	-	35,35,63	0.87	2 (5%)	42,45,79	0.67	0
8	BCL	m	401	-	58,74,74	1.61	9 (15%)	69,115,115	1.78	14 (20%)
12	PGV	H	804	-	25,25,50	1.28	2 (8%)	28,30,56	1.33	3 (10%)
8	BCL	K	402	-	58,74,74	1.64	9 (15%)	69,115,115	1.72	17 (24%)
16	PTY	h	804	-	37,37,49	0.33	0	40,42,54	0.49	0
8	BCL	M	401	-	58,74,74	1.64	9 (15%)	69,115,115	1.67	15 (21%)
12	PGV	Q	102	-	28,28,50	1.22	2 (7%)	31,34,56	1.27	3 (9%)
14	SPO	6	102	-	40,41,41	0.63	0	47,50,50	2.12	14 (29%)
14	SPO	y	105	-	40,41,41	0.66	0	47,50,50	1.91	16 (34%)
8	BCL	5	102	-	58,74,74	1.68	11 (18%)	69,115,115	1.55	13 (18%)
14	SPO	02	102	-	40,41,41	0.64	0	47,50,50	1.94	13 (27%)
8	BCL	D	101	-	58,74,74	1.63	8 (13%)	69,115,115	1.74	14 (20%)
14	SPO	g	102	-	40,41,41	0.64	0	47,50,50	1.95	11 (23%)
8	BCL	l	301	-	58,74,74	1.62	10 (17%)	69,115,115	1.70	14 (20%)
14	SPO	M	406	-	40,41,41	0.64	0	47,50,50	1.70	10 (21%)
8	BCL	s	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.79	15 (21%)
10	U10	m	406	-	59,59,63	0.68	2 (3%)	71,74,79	0.60	0
15	CDL	m	413	-	44,44,99	1.09	3 (6%)	49,54,111	1.11	3 (6%)
14	SPO	T	102	-	40,41,41	0.62	0	47,50,50	1.85	11 (23%)
9	BPH	L	302	-	51,70,70	0.62	2 (3%)	52,101,101	0.72	1 (1%)
8	BCL	3	102	-	58,74,74	1.67	9 (15%)	69,115,115	1.66	15 (21%)
15	CDL	M	410	-	78,78,99	1.02	4 (5%)	84,90,111	1.20	7 (8%)
8	BCL	08	102	-	52,68,74	1.83	11 (21%)	61,107,115	1.67	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PGV	f	104	-	46,46,50	0.95	2 (4%)	49,52,56	1.03	2 (4%)
8	BCL	G	102	-	58,74,74	1.66	9 (15%)	69,115,115	1.67	15 (21%)
14	SPO	B	101	-	40,41,41	0.65	0	47,50,50	1.87	12 (25%)
8	BCL	g	103	-	58,74,74	1.64	10 (17%)	69,115,115	1.74	13 (18%)
8	BCL	i	103	-	58,74,74	1.64	10 (17%)	69,115,115	1.96	16 (23%)
8	BCL	07	101	-	58,74,74	1.69	11 (18%)	69,115,115	1.68	12 (17%)
12	PGV	h	806	-	25,25,50	1.29	2 (8%)	28,30,56	1.29	3 (10%)
11	LMT	3	101	-	36,36,36	0.39	0	47,47,47	0.69	0
14	SPO	j	101	-	40,41,41	0.64	0	47,50,50	1.99	12 (25%)
15	CDL	h	805	-	60,60,99	1.19	4 (6%)	66,72,111	1.14	5 (7%)
12	PGV	M	411	-	37,37,50	1.07	2 (5%)	40,43,56	1.17	3 (7%)
15	CDL	x	102	-	25,25,99	0.97	1 (4%)	28,32,111	0.87	1 (3%)
8	BCL	o	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.82	17 (24%)
12	PGV	y	104	-	42,42,50	1.00	2 (4%)	44,48,56	1.07	3 (6%)
14	SPO	q	104	-	40,41,41	0.64	0	47,50,50	1.81	12 (25%)
14	SPO	s	103	-	40,41,41	0.63	0	47,50,50	1.58	10 (21%)
11	LMT	i	101	-	27,27,36	0.53	0	38,38,47	0.93	1 (2%)
12	PGV	l	201	-	42,42,50	1.01	2 (4%)	44,48,56	1.06	3 (6%)
15	CDL	X	102	-	32,32,99	1.04	2 (6%)	34,40,111	1.16	2 (5%)
11	LMT	A	701	-	36,36,36	0.43	0	47,47,47	0.76	1 (2%)
10	U10	l	304	-	35,35,63	0.79	2 (5%)	42,45,79	0.68	0
8	BCL	k	101	-	58,74,74	1.65	8 (13%)	69,115,115	1.74	13 (18%)
12	PGV	H	805	-	39,39,50	1.03	2 (5%)	42,45,56	1.11	4 (9%)
14	SPO	Y	103	-	40,41,41	0.64	0	47,50,50	1.73	14 (29%)
9	BPH	M	403	-	51,70,70	0.61	2 (3%)	52,101,101	0.74	1 (1%)
12	PGV	K	403	-	38,40,50	1.03	2 (5%)	40,42,56	1.22	4 (10%)
14	SPO	w	101	-	40,41,41	0.67	0	47,50,50	1.77	12 (25%)
14	SPO	2	102	-	40,41,41	0.64	0	47,50,50	1.83	9 (19%)
8	BCL	n	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.67	15 (21%)
14	SPO	f	101	-	40,41,41	0.63	0	47,50,50	1.96	16 (34%)
11	LMT	m	409	-	34,34,36	0.50	0	45,45,47	1.02	4 (8%)
11	LMT	h	803	-	36,36,36	0.36	0	47,47,47	0.86	2 (4%)
12	PGV	l	307	-	29,29,50	1.19	2 (6%)	32,35,56	1.15	3 (9%)
14	SPO	05	102	-	40,41,41	0.64	0	47,50,50	1.76	11 (23%)
12	PGV	m	411	-	37,37,50	1.06	2 (5%)	40,43,56	1.17	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	4	101	-	58,74,74	1.76	11 (18%)	69,115,115	1.71	13 (18%)
8	BCL	v	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.79	17 (24%)
11	LMT	03	103	-	28,28,36	0.47	0	39,39,47	0.76	0
14	SPO	2	101	-	40,41,41	0.65	0	47,50,50	1.75	13 (27%)
14	SPO	J	101	-	40,41,41	0.63	0	47,50,50	1.77	13 (27%)
14	SPO	S	103	-	40,41,41	0.66	0	47,50,50	1.65	10 (21%)
8	BCL	04	101	-	58,74,74	1.74	11 (18%)	69,115,115	1.66	13 (18%)
8	BCL	y	103	-	58,74,74	1.63	9 (15%)	69,115,115	1.74	16 (23%)
14	SPO	V	102	-	40,41,41	0.64	0	47,50,50	1.73	12 (25%)
11	LMT	5	101	-	34,34,36	0.43	0	45,45,47	0.72	1 (2%)
11	LMT	i	102	-	36,36,36	0.36	0	47,47,47	0.79	1 (2%)
14	SPO	v	102	-	40,41,41	0.69	0	47,50,50	1.93	13 (27%)
8	BCL	e	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.71	15 (21%)
14	SPO	e	101	-	40,41,41	0.67	0	47,50,50	1.83	14 (29%)
8	BCL	E	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.71	16 (23%)
14	SPO	g	101	-	40,41,41	0.66	0	47,50,50	1.79	12 (25%)
14	SPO	P	101	-	40,41,41	0.63	0	47,50,50	1.76	10 (21%)
8	BCL	I	102	-	58,74,74	1.63	8 (13%)	69,115,115	1.78	17 (24%)
12	PGV	l	305	-	38,38,50	1.05	2 (5%)	41,44,56	1.16	3 (7%)
12	PGV	F	503	-	40,40,50	1.02	2 (5%)	43,46,56	1.13	3 (6%)
15	CDL	X	103	-	58,58,99	1.20	4 (6%)	64,70,111	1.35	8 (12%)
15	CDL	m	410	-	78,78,99	1.03	4 (5%)	84,90,111	1.19	6 (7%)
8	BCL	a	101	-	40,56,74	2.00	9 (22%)	47,93,115	1.83	13 (27%)
11	LMT	M	409	-	34,34,36	0.50	1 (2%)	45,45,47	1.02	4 (8%)
8	BCL	z	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.72	13 (18%)
8	BCL	V	101	-	58,74,74	1.64	8 (13%)	69,115,115	1.87	18 (26%)
8	BCL	06	101	-	58,74,74	1.73	11 (18%)	69,115,115	1.66	13 (18%)
12	PGV	H	801	-	46,46,50	0.92	2 (4%)	49,52,56	1.10	4 (8%)
14	SPO	k	102	-	40,41,41	0.63	0	47,50,50	1.64	13 (27%)
8	BCL	T	101	-	58,74,74	1.65	9 (15%)	69,115,115	1.60	13 (18%)

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
15	CDL	K	401	-	-	24/71/71/110	-
11	LMT	L	305	-	-	4/13/53/61	0/2/2/2
8	BCL	m	402	-	-	18/37/137/137	-
11	LMT	H	802	-	-	7/21/61/61	0/2/2/2
11	LMT	h	802	-	-	3/19/39/61	0/1/1/2
12	PGV	L	307	-	-	15/43/43/55	-
14	SPO	01	103	-	-	5/47/47/47	-
8	BCL	02	101	-	-	17/37/137/137	-
14	SPO	m	407	-	-	7/47/47/47	-
12	PGV	L	310	-	-	10/43/43/55	-
14	SPO	R	101	-	-	3/47/47/47	-
14	SPO	3	103	-	-	6/47/47/47	-
9	BPH	l	302	-	-	4/37/105/105	0/5/6/6
8	BCL	05	101	-	-	14/37/137/137	-
14	SPO	Q	104	-	-	6/47/47/47	-
11	LMT	Q	101	-	-	4/15/35/61	0/1/1/2
8	BCL	2	103	-	-	22/37/137/137	-
12	PGV	f	103	-	-	15/44/44/55	-
14	SPO	I	103	-	-	4/47/47/47	-
12	PGV	x	101	-	-	12/43/43/55	-
8	BCL	Z	101	-	-	13/37/137/137	-
8	BCL	O	101	-	-	14/37/137/137	-
11	LMT	s	104	-	-	3/16/56/61	0/2/2/2
16	PTY	f	105	-	-	7/40/40/53	-
8	BCL	f	102	-	-	11/37/137/137	-
14	SPO	05	103	-	-	8/47/47/47	-
14	SPO	s	105	-	-	5/47/47/47	-
15	CDL	y	102	-	-	10/56/56/110	-
14	SPO	E	102	-	-	5/47/47/47	-
12	PGV	L	309	-	-	11/37/37/55	-
14	SPO	O	102	-	-	2/47/47/47	-
15	CDL	X	101	-	-	19/69/69/110	-
14	SPO	A	703	-	-	8/47/47/47	-
14	SPO	n	101	-	-	12/47/47/47	-
8	BCL	b	101	-	-	16/37/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LMT	M	407	-	-	3/19/39/61	0/1/1/2
14	SPO	G	101	-	-	6/47/47/47	-
12	PGV	k	103	-	-	9/40/42/55	-
8	BCL	w	102	-	-	16/37/137/137	-
12	PGV	l	308	-	-	12/28/28/55	-
12	PGV	l	306	-	-	14/55/55/55	-
8	BCL	F	502	-	-	16/37/137/137	-
14	SPO	n	103	-	-	5/47/47/47	-
14	SPO	08	101	-	-	8/47/47/47	-
14	SPO	2	104	-	-	1/47/47/47	-
8	BCL	1	202	-	-	15/37/137/137	-
8	BCL	W	101	-	-	16/37/137/137	-
11	LMT	U	101	-	-	8/18/58/61	0/2/2/2
14	SPO	z	101	-	-	9/47/47/47	-
8	BCL	S	101	-	-	15/37/137/137	-
10	U10	L	303	-	-	8/30/54/87	0/1/1/1
8	BCL	L	301	-	-	14/37/137/137	-
10	U10	M	405	-	-	15/63/87/87	0/1/1/1
8	BCL	Q	103	-	-	18/37/137/137	-
14	SPO	f	106	-	-	3/47/47/47	-
14	SPO	r	103	-	-	11/47/47/47	-
8	BCL	m	403	-	-	10/37/137/137	-
15	CDL	Y	101	-	-	17/49/49/110	-
12	PGV	h	801	-	-	7/51/51/55	-
16	PTY	F	501	-	-	6/44/44/53	-
8	BCL	B	102	-	-	16/37/137/137	-
12	PGV	m	412	-	-	12/43/43/55	-
9	BPH	m	404	-	-	7/37/105/105	0/5/6/6
8	BCL	q	103	-	-	12/37/137/137	-
11	LMT	U	102	-	-	7/21/61/61	0/2/2/2
11	LMT	U	103	-	-	6/21/61/61	0/2/2/2
8	BCL	P	102	-	-	20/37/137/137	-
14	SPO	01	102	-	-	10/47/47/47	-
14	SPO	G	103	-	-	10/47/47/47	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	M	402	-	-	17/37/137/137	-
8	BCL	7	101	-	-	9/37/137/137	-
14	SPO	K	404	-	-	2/47/47/47	-
17	LDA	y	101	-	-	0/9/9/13	-
8	BCL	03	102	-	-	9/37/137/137	-
8	BCL	Y	102	-	-	16/37/137/137	-
8	BCL	01	101	-	-	17/37/137/137	-
11	LMT	M	408	-	-	4/17/37/61	0/1/1/2
8	BCL	p	102	-	-	15/37/137/137	-
14	SPO	p	101	-	-	6/47/47/47	-
11	LMT	q	101	-	-	3/15/35/61	0/1/1/2
10	U10	D	102	-	-	10/26/50/87	0/1/1/1
11	LMT	L	306	-	-	4/11/51/61	0/2/2/2
8	BCL	j	102	-	-	19/37/137/137	-
10	U10	d	102	-	-	7/24/48/87	0/1/1/1
11	LMT	m	408	-	-	7/21/61/61	0/2/2/2
14	SPO	S	102	-	-	4/47/47/47	-
8	BCL	6	101	-	-	17/37/137/137	-
8	BCL	d	101	-	-	14/37/137/137	-
8	BCL	t	101	-	-	20/37/137/137	-
8	BCL	8	101	-	-	15/29/129/137	-
14	SPO	4	102	-	-	5/47/47/47	-
8	BCL	A	702	-	-	14/31/131/137	-
8	BCL	R	102	-	-	21/37/137/137	-
14	SPO	B	103	-	-	8/47/47/47	-
8	BCL	L	311	-	-	8/37/137/137	-
11	LMT	I	101	-	-	9/21/61/61	0/2/2/2
14	SPO	N	101	-	-	4/47/47/47	-
14	SPO	r	101	-	-	6/47/47/47	-
8	BCL	r	102	-	-	21/37/137/137	-
11	LMT	M	412	-	-	3/16/56/61	0/2/2/2
8	BCL	J	102	-	-	12/37/137/137	-
14	SPO	5	103	-	-	6/47/47/47	-
12	PGV	q	102	-	-	11/38/38/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SPO	a	102	-	-	4/47/47/47	-
12	PGV	L	308	-	-	7/55/55/55	-
16	PTY	H	803	-	-	9/40/40/53	-
8	BCL	N	102	-	-	15/37/137/137	-
11	LMT	3	104	-	-	3/13/53/61	0/2/2/2
11	LMT	03	101	-	-	8/21/61/61	0/2/2/2
11	LMT	s	101	-	-	7/17/37/61	0/1/1/2
10	U10	L	304	-	-	5/30/54/87	0/1/1/1
10	U10	l	303	-	-	11/30/54/87	0/1/1/1
8	BCL	m	401	-	-	11/37/137/137	-
12	PGV	H	804	-	-	11/29/29/55	-
8	BCL	K	402	-	-	9/37/137/137	-
16	PTY	h	804	-	-	8/41/41/53	-
8	BCL	M	401	-	-	13/37/137/137	-
12	PGV	Q	102	-	-	14/33/33/55	-
14	SPO	6	102	-	-	8/47/47/47	-
14	SPO	y	105	-	-	9/47/47/47	-
8	BCL	5	102	-	-	16/37/137/137	-
14	SPO	02	102	-	-	2/47/47/47	-
8	BCL	D	101	-	-	13/37/137/137	-
14	SPO	g	102	-	-	8/47/47/47	-
8	BCL	l	301	-	-	12/37/137/137	-
14	SPO	M	406	-	-	9/47/47/47	-
8	BCL	s	102	-	-	9/37/137/137	-
10	U10	m	406	-	-	16/59/83/87	0/1/1/1
15	CDL	m	413	-	-	17/51/51/110	-
14	SPO	T	102	-	-	6/47/47/47	-
9	BPH	L	302	-	-	5/37/105/105	0/5/6/6
8	BCL	3	102	-	-	8/37/137/137	-
15	CDL	M	410	-	-	29/89/89/110	-
8	BCL	08	102	-	-	13/29/129/137	-
12	PGV	f	104	-	-	11/51/51/55	-
8	BCL	G	102	-	-	17/37/137/137	-
14	SPO	B	101	-	-	8/47/47/47	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	g	103	-	-	16/37/137/137	-
8	BCL	i	103	-	-	11/37/137/137	-
8	BCL	07	101	-	-	14/37/137/137	-
12	PGV	h	806	-	-	13/29/29/55	-
11	LMT	3	101	-	-	5/21/61/61	0/2/2/2
14	SPO	j	101	-	-	10/47/47/47	-
15	CDL	h	805	-	-	27/71/71/110	-
12	PGV	M	411	-	-	22/42/42/55	-
15	CDL	x	102	-	-	7/29/29/110	-
8	BCL	o	101	-	-	11/37/137/137	-
12	PGV	y	104	-	-	5/47/47/55	-
14	SPO	q	104	-	-	6/47/47/47	-
14	SPO	s	103	-	-	2/47/47/47	-
11	LMT	i	101	-	-	3/11/51/61	0/2/2/2
12	PGV	l	201	-	-	9/47/47/55	-
15	CDL	X	102	-	-	19/38/38/110	-
11	LMT	A	701	-	-	5/21/61/61	0/2/2/2
10	U10	l	304	-	-	1/30/54/87	0/1/1/1
8	BCL	k	101	-	-	14/37/137/137	-
12	PGV	H	805	-	-	16/44/44/55	-
14	SPO	Y	103	-	-	5/47/47/47	-
9	BPH	M	403	-	-	2/37/105/105	0/5/6/6
12	PGV	K	403	-	-	8/40/42/55	-
14	SPO	w	101	-	-	5/47/47/47	-
14	SPO	2	102	-	-	6/47/47/47	-
8	BCL	n	102	-	-	14/37/137/137	-
14	SPO	f	101	-	-	9/47/47/47	-
11	LMT	m	409	-	-	5/19/59/61	0/2/2/2
11	LMT	h	803	-	-	5/21/61/61	0/2/2/2
12	PGV	l	307	-	-	12/34/34/55	-
14	SPO	05	102	-	-	6/47/47/47	-
12	PGV	m	411	-	-	18/42/42/55	-
8	BCL	4	101	-	-	12/37/137/137	-
8	BCL	v	101	-	-	17/37/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LMT	03	103	-	-	5/13/53/61	0/2/2/2
14	SPO	2	101	-	-	9/47/47/47	-
14	SPO	J	101	-	-	4/47/47/47	-
14	SPO	S	103	-	-	1/47/47/47	-
8	BCL	04	101	-	-	11/37/137/137	-
8	BCL	y	103	-	-	10/37/137/137	-
14	SPO	V	102	-	-	4/47/47/47	-
11	LMT	5	101	-	-	4/19/59/61	0/2/2/2
11	LMT	i	102	-	-	2/21/61/61	0/2/2/2
14	SPO	v	102	-	-	8/47/47/47	-
8	BCL	e	102	-	-	11/37/137/137	-
14	SPO	e	101	-	-	8/47/47/47	-
8	BCL	E	101	-	-	20/37/137/137	-
14	SPO	g	101	-	-	4/47/47/47	-
14	SPO	P	101	-	-	5/47/47/47	-
8	BCL	I	102	-	-	11/37/137/137	-
12	PGV	l	305	-	-	13/43/43/55	-
12	PGV	F	503	-	-	14/45/45/55	-
15	CDL	X	103	-	-	21/69/69/110	-
15	CDL	m	410	-	-	30/89/89/110	-
8	BCL	a	101	-	-	8/16/116/137	-
11	LMT	M	409	-	-	8/19/59/61	0/2/2/2
8	BCL	z	102	-	-	14/37/137/137	-
8	BCL	V	101	-	-	15/37/137/137	-
8	BCL	06	101	-	-	14/37/137/137	-
12	PGV	H	801	-	-	12/51/51/55	-
14	SPO	k	102	-	-	4/47/47/47	-
8	BCL	T	101	-	-	17/37/137/137	-

The worst 5 of 707 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	y	101	LDA	O1-N1	-7.34	1.25	1.42
8	8	101	BCL	C3B-C2B	5.24	1.48	1.39
8	4	101	BCL	C3B-C2B	5.24	1.48	1.39
8	3	102	BCL	O2D-CGD	5.22	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	101	BCL	O2D-CGD	5.18	1.45	1.33

The worst 5 of 1766 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	p	101	SPO	C21-C22-C23	-8.43	115.28	127.31
14	G	103	SPO	C20-C19-C17	-6.52	118.00	127.31
14	R	101	SPO	C21-C22-C23	-6.39	118.19	127.31
8	V	101	BCL	O2D-CGD-CBD	6.36	122.56	111.27
14	s	105	SPO	C21-C22-C23	-6.25	118.39	127.31

There are no chirality outliers.

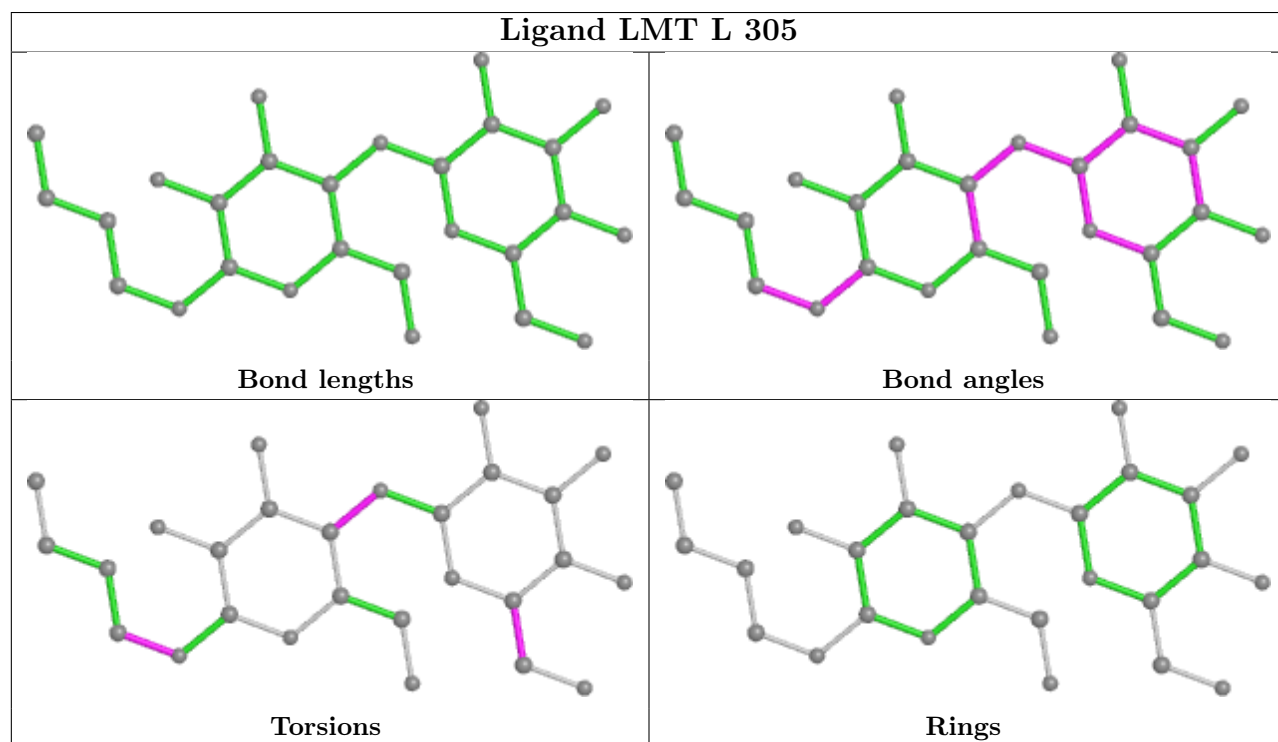
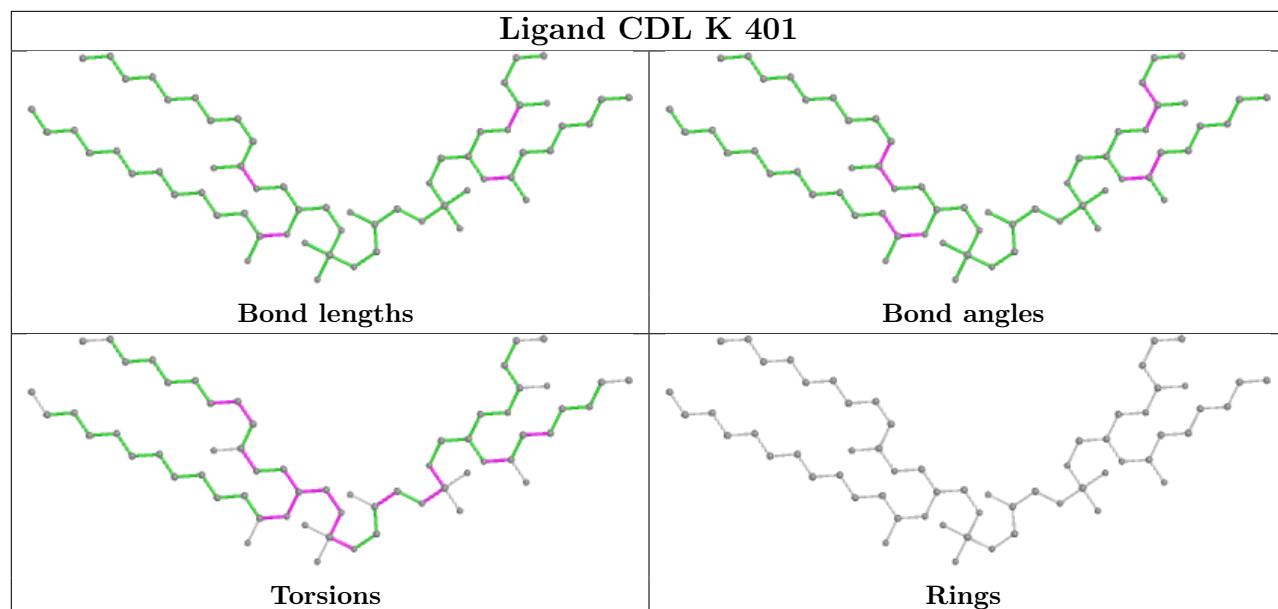
5 of 2027 torsion outliers are listed below:

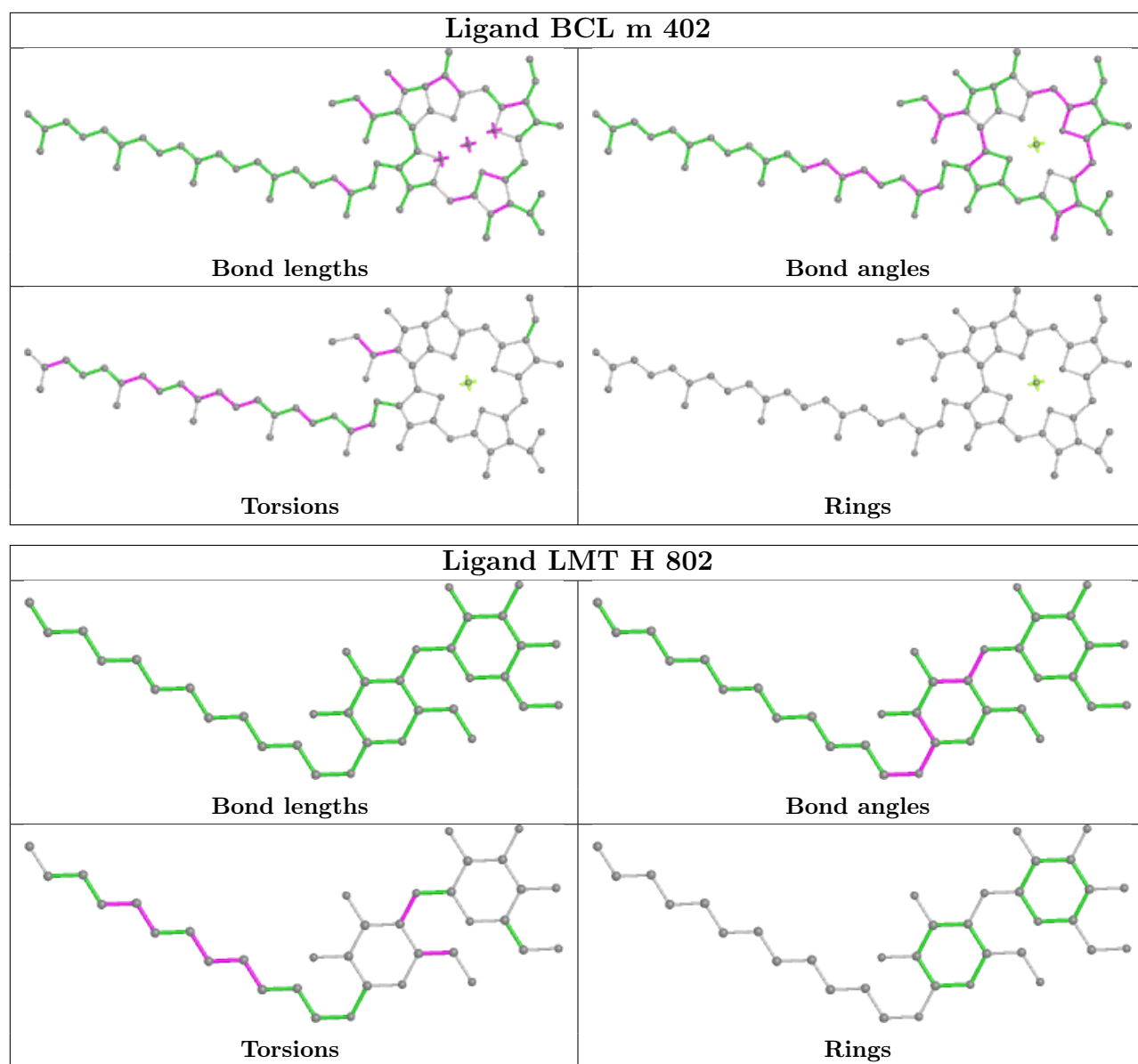
Mol	Chain	Res	Type	Atoms
8	M	401	BCL	CHA-CBD-CGD-O1D
8	M	401	BCL	CHA-CBD-CGD-O2D
8	B	102	BCL	C1A-C2A-CAA-CBA
8	B	102	BCL	C3A-C2A-CAA-CBA
8	B	102	BCL	CBD-CGD-O2D-CED

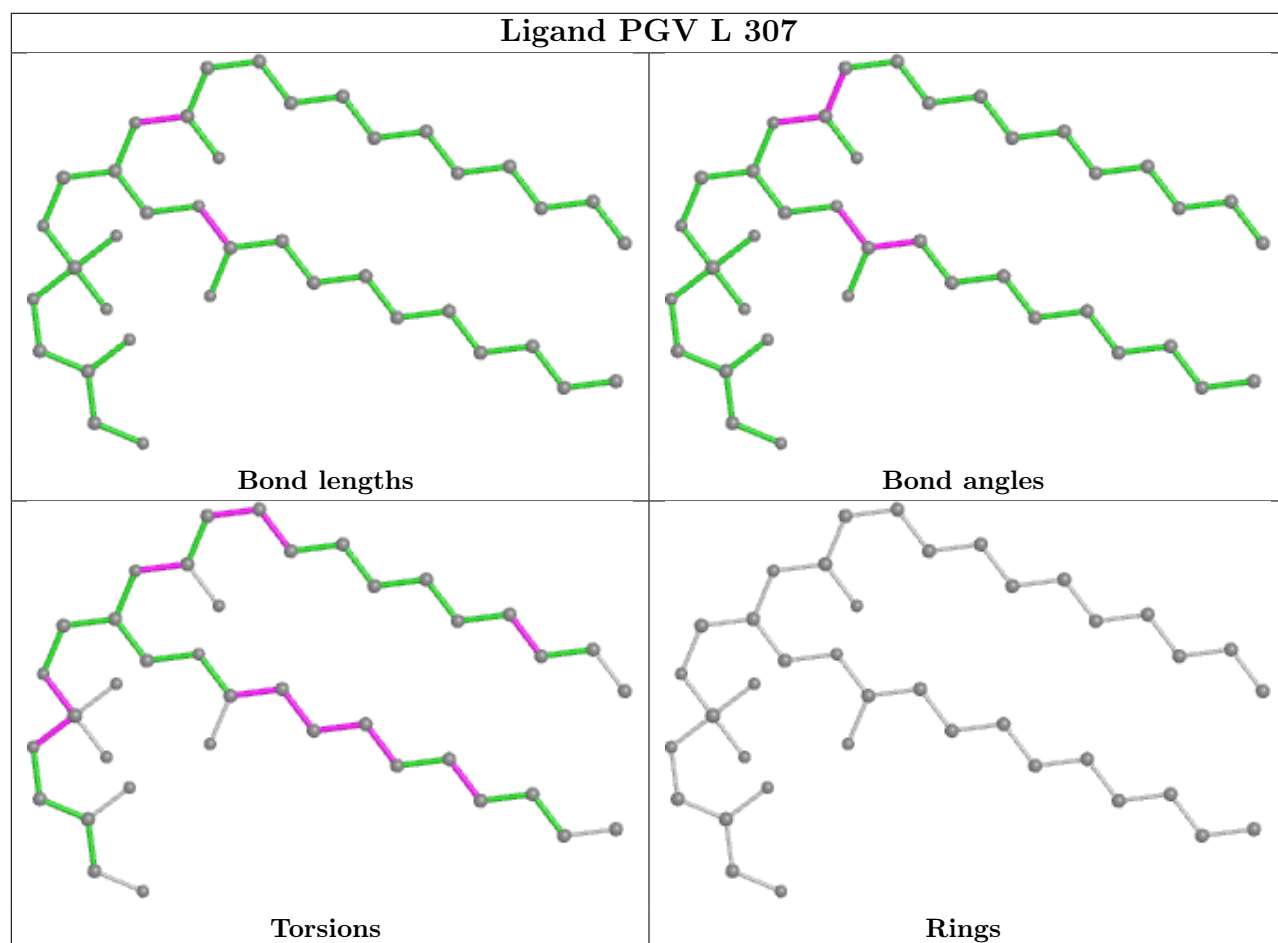
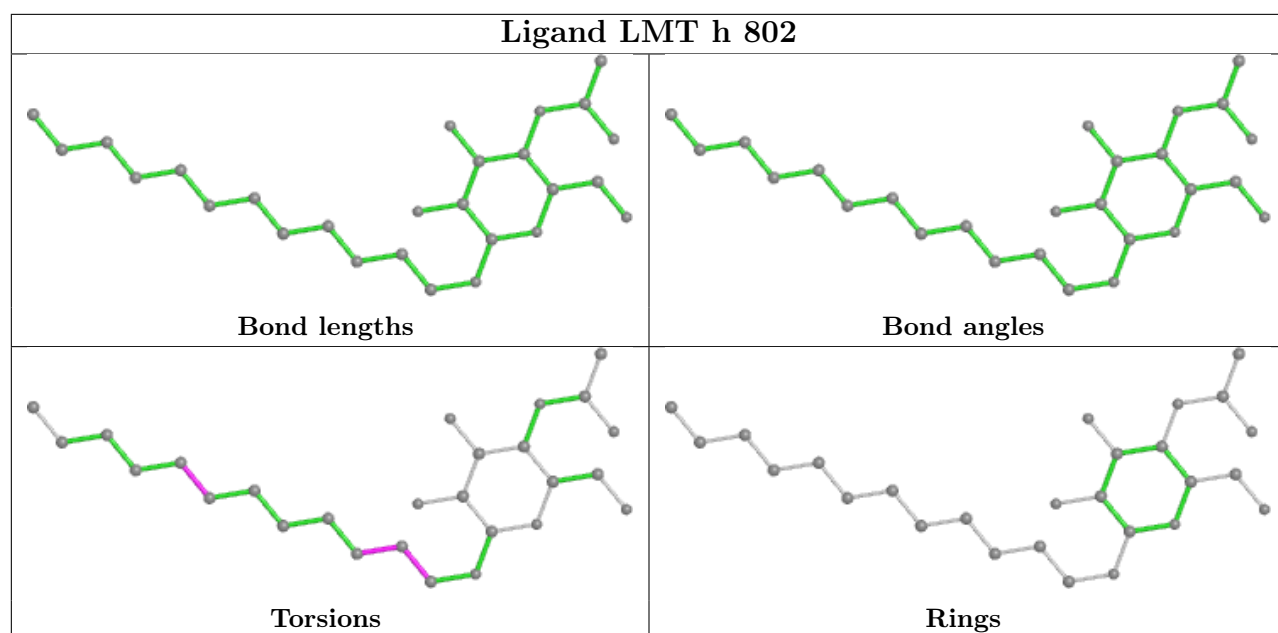
There are no ring outliers.

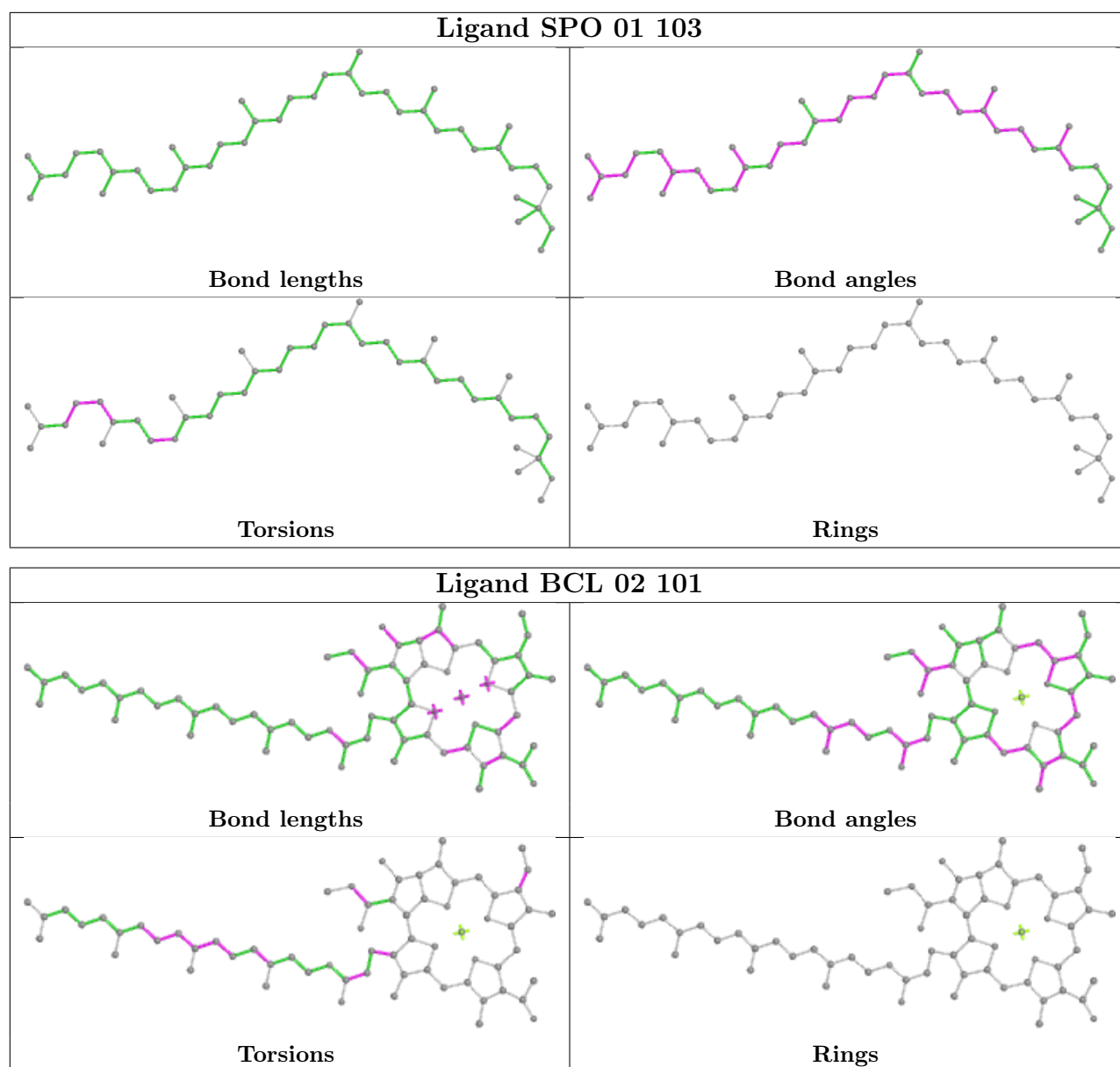
No monomer is involved in short contacts.

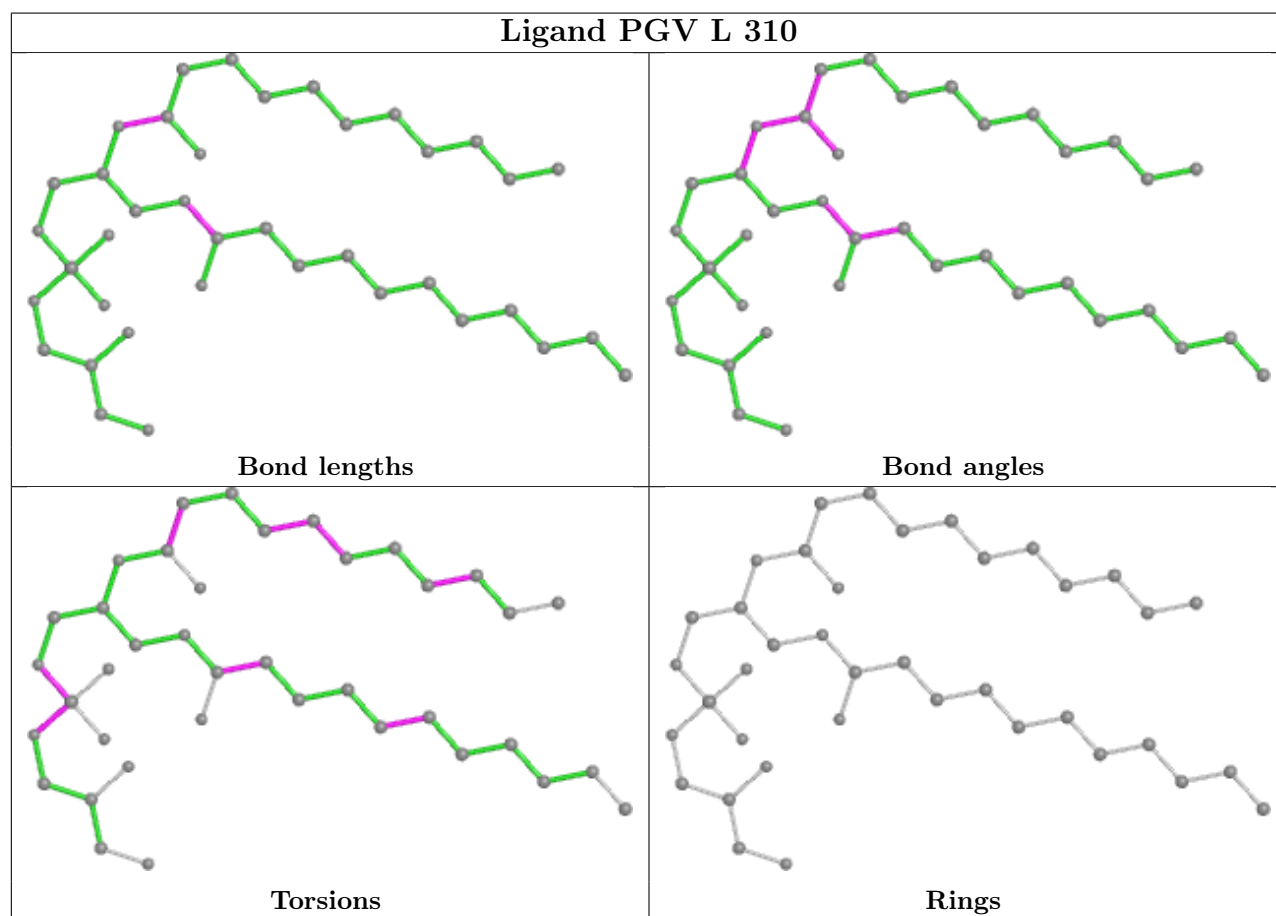
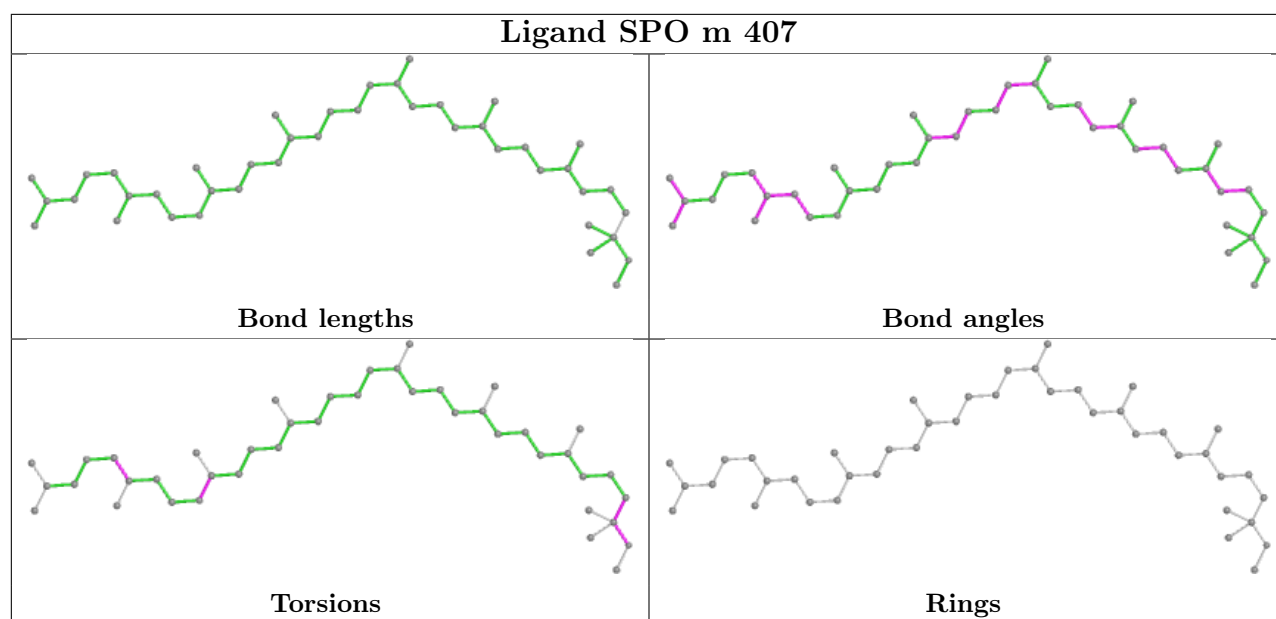
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

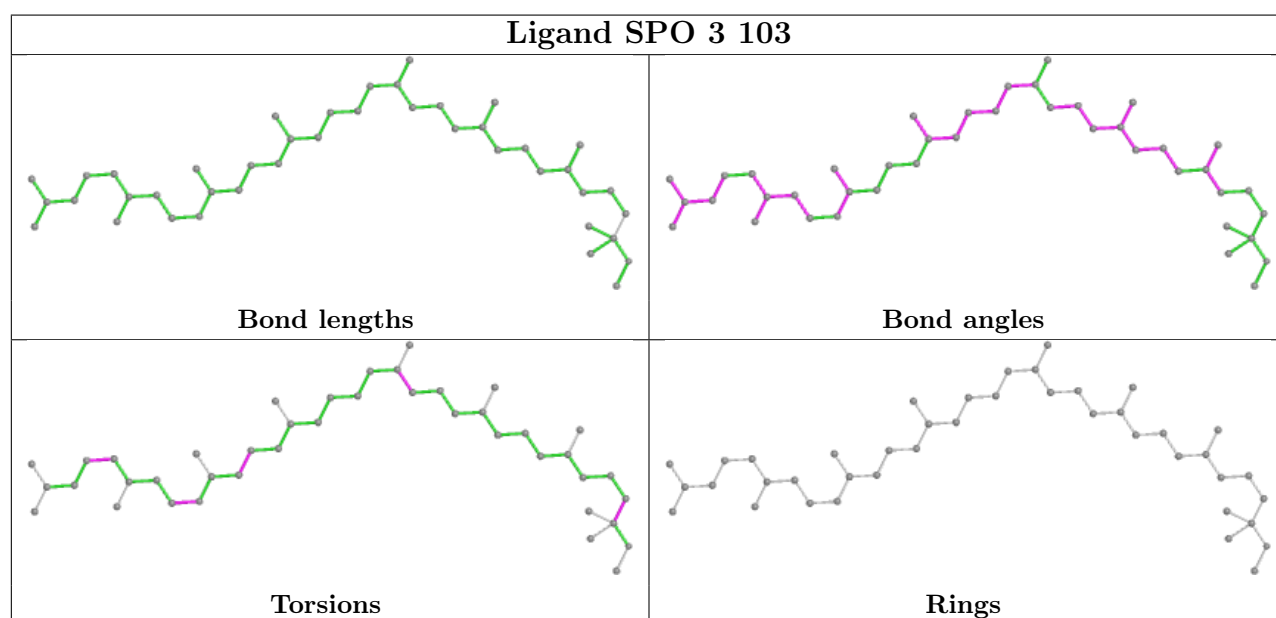
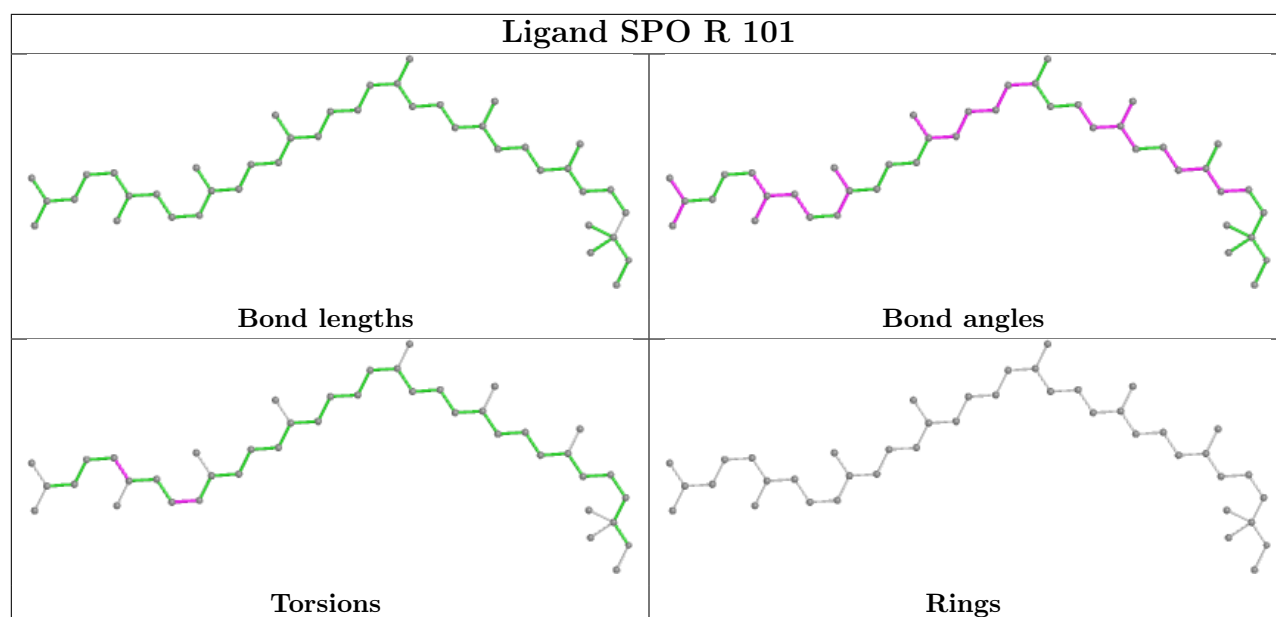


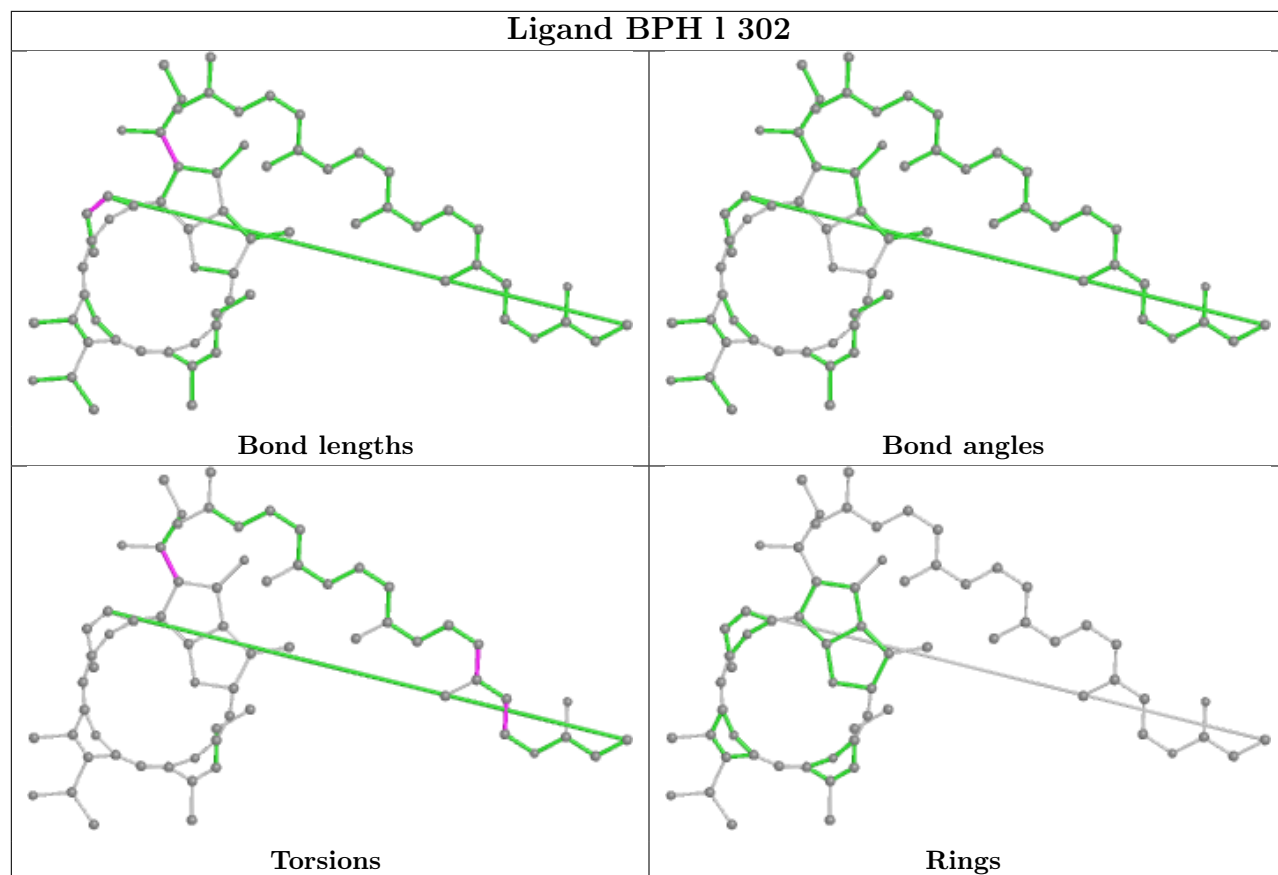
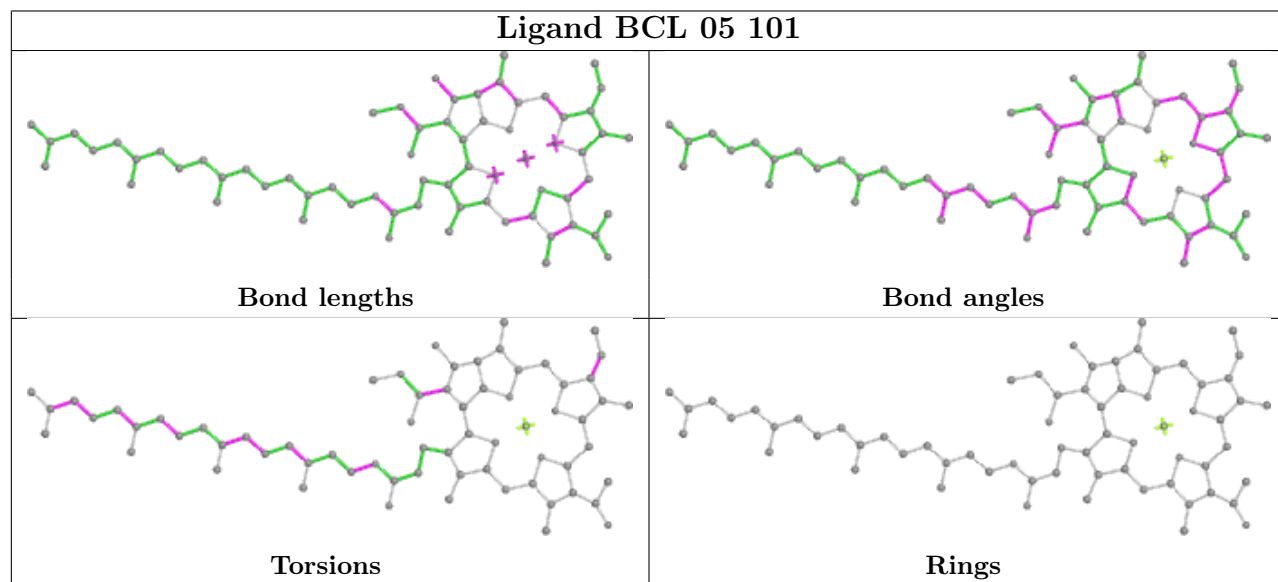


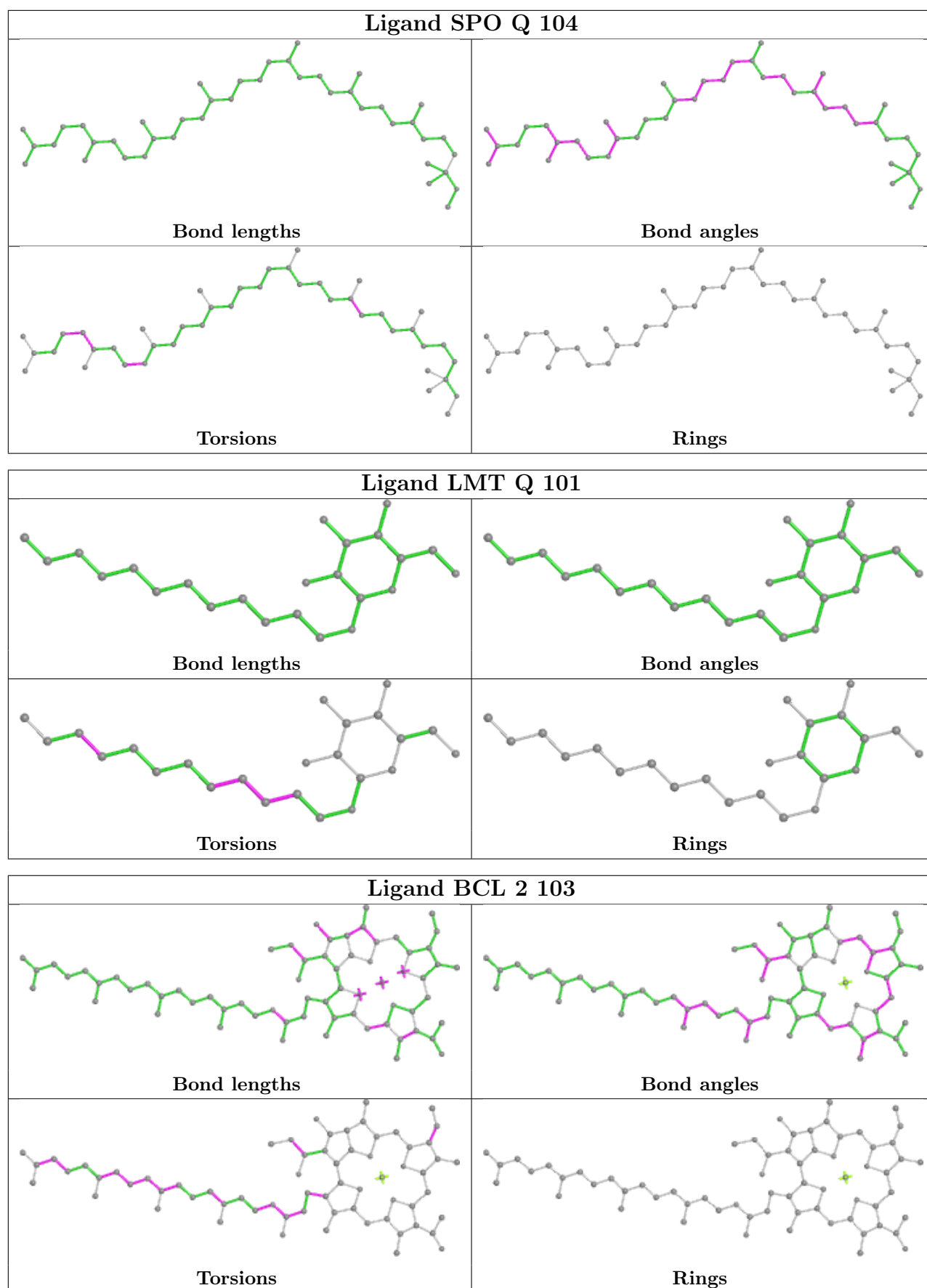




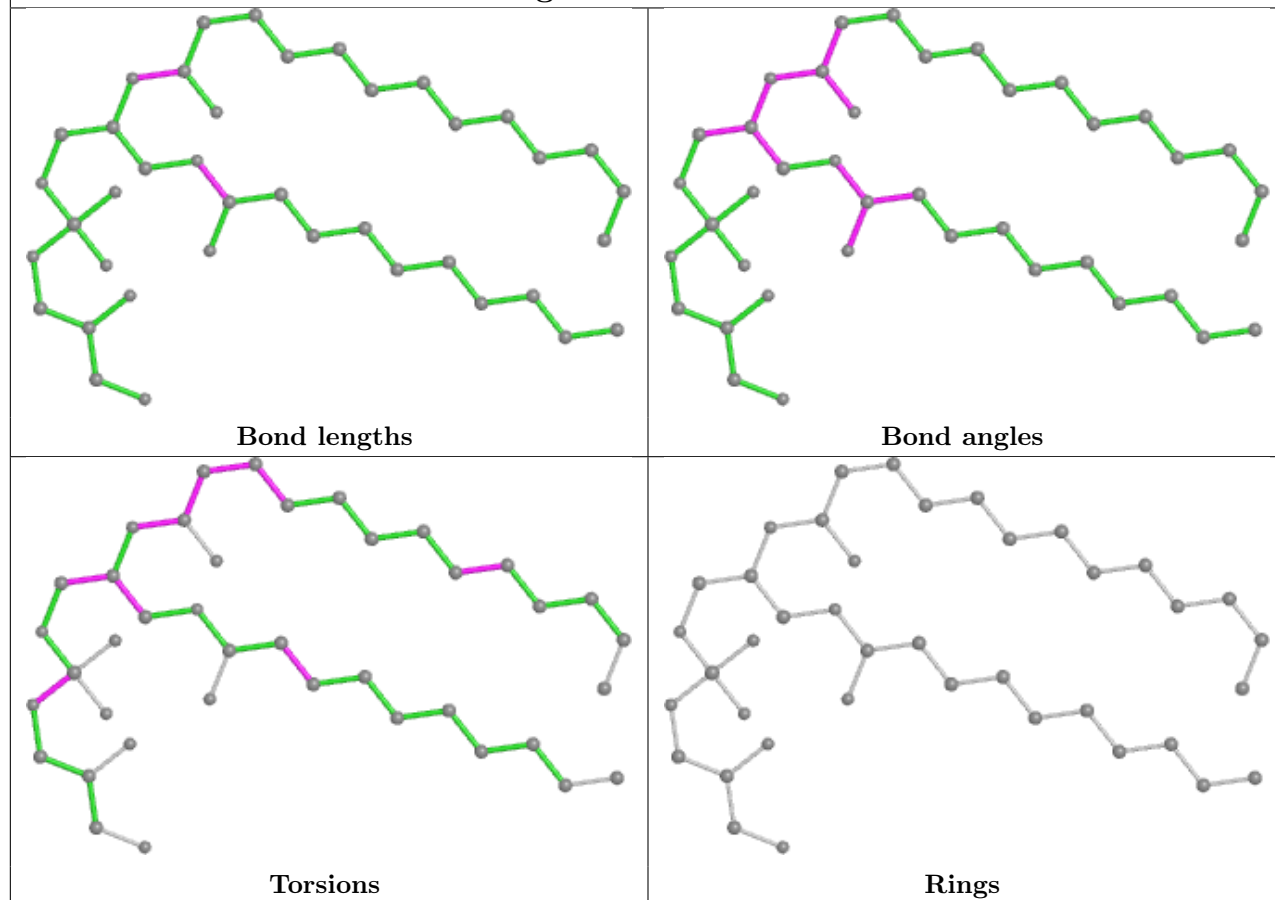




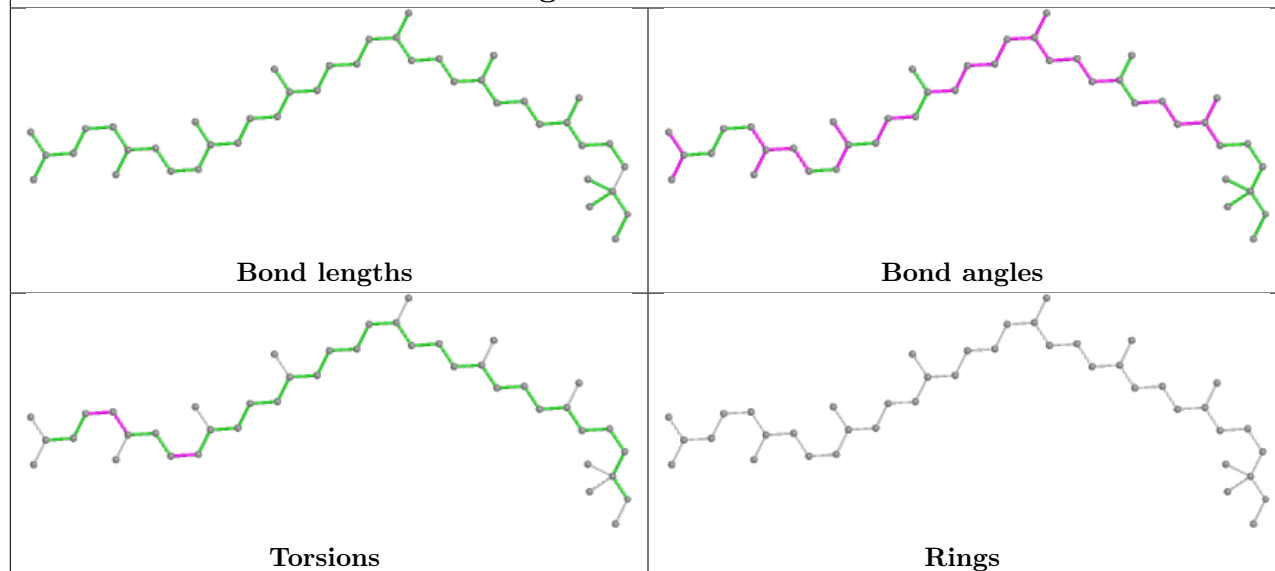
Ligand BPH 1 302**Ligand BCL 05 101**

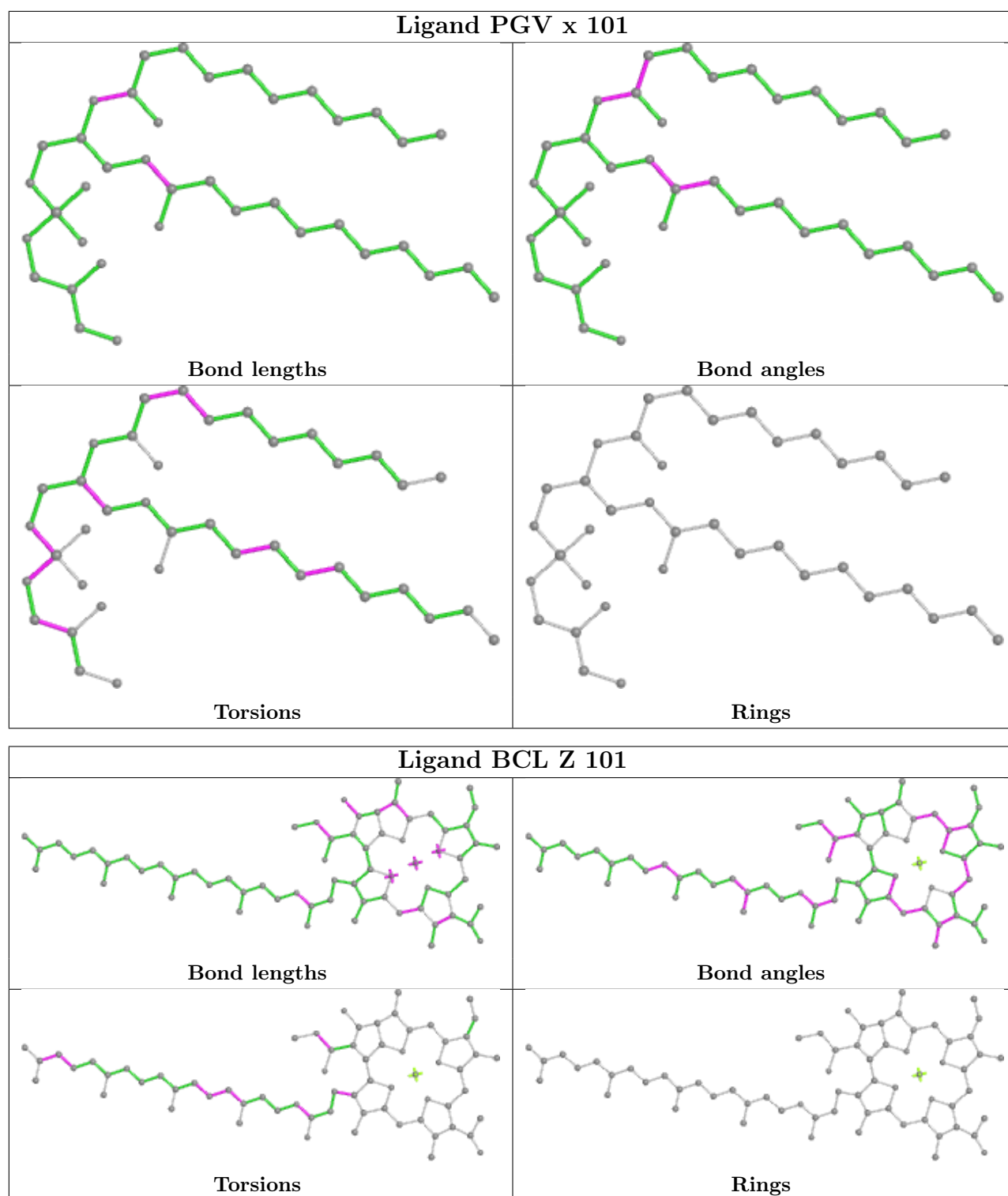


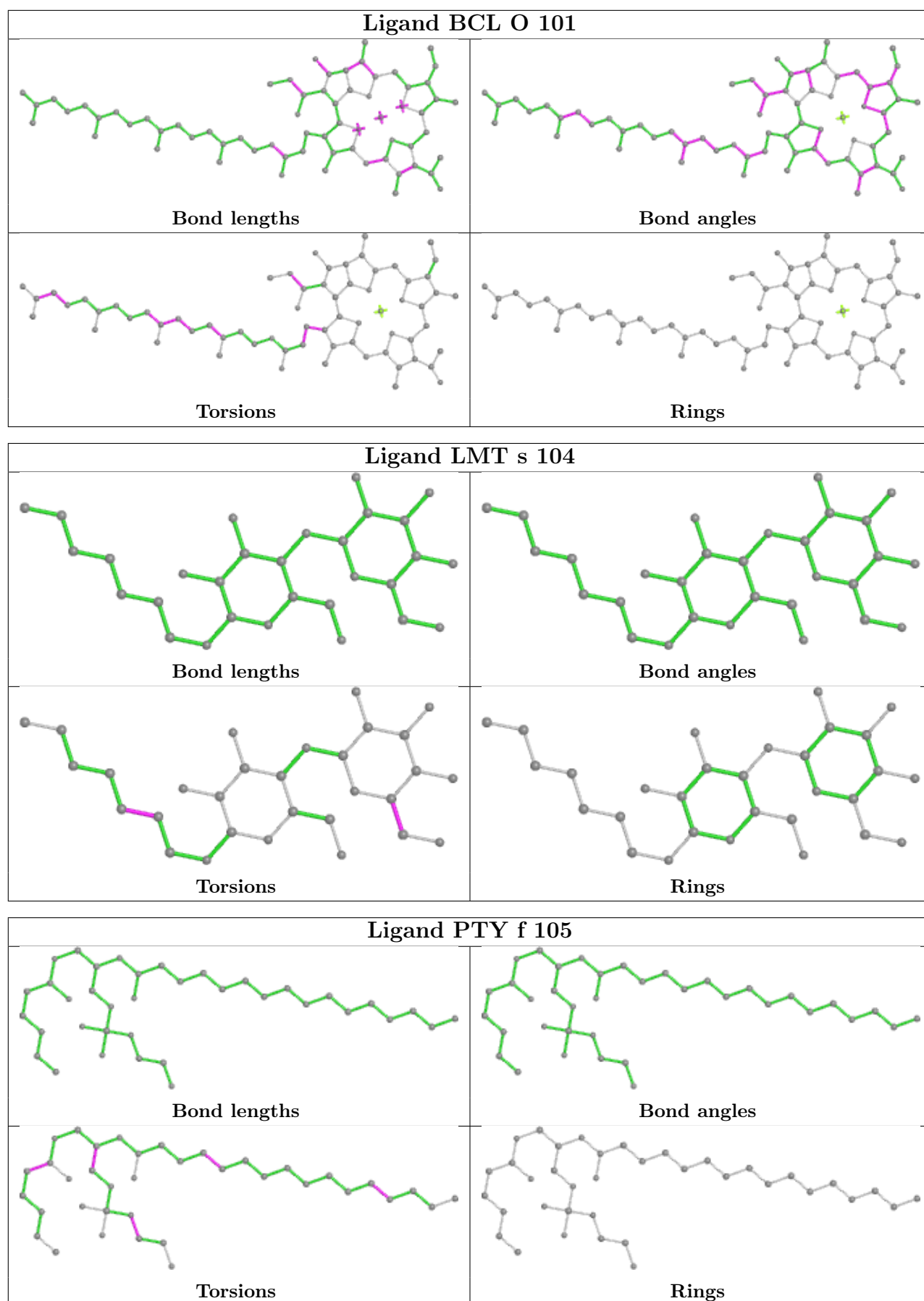
Ligand PGV f 103

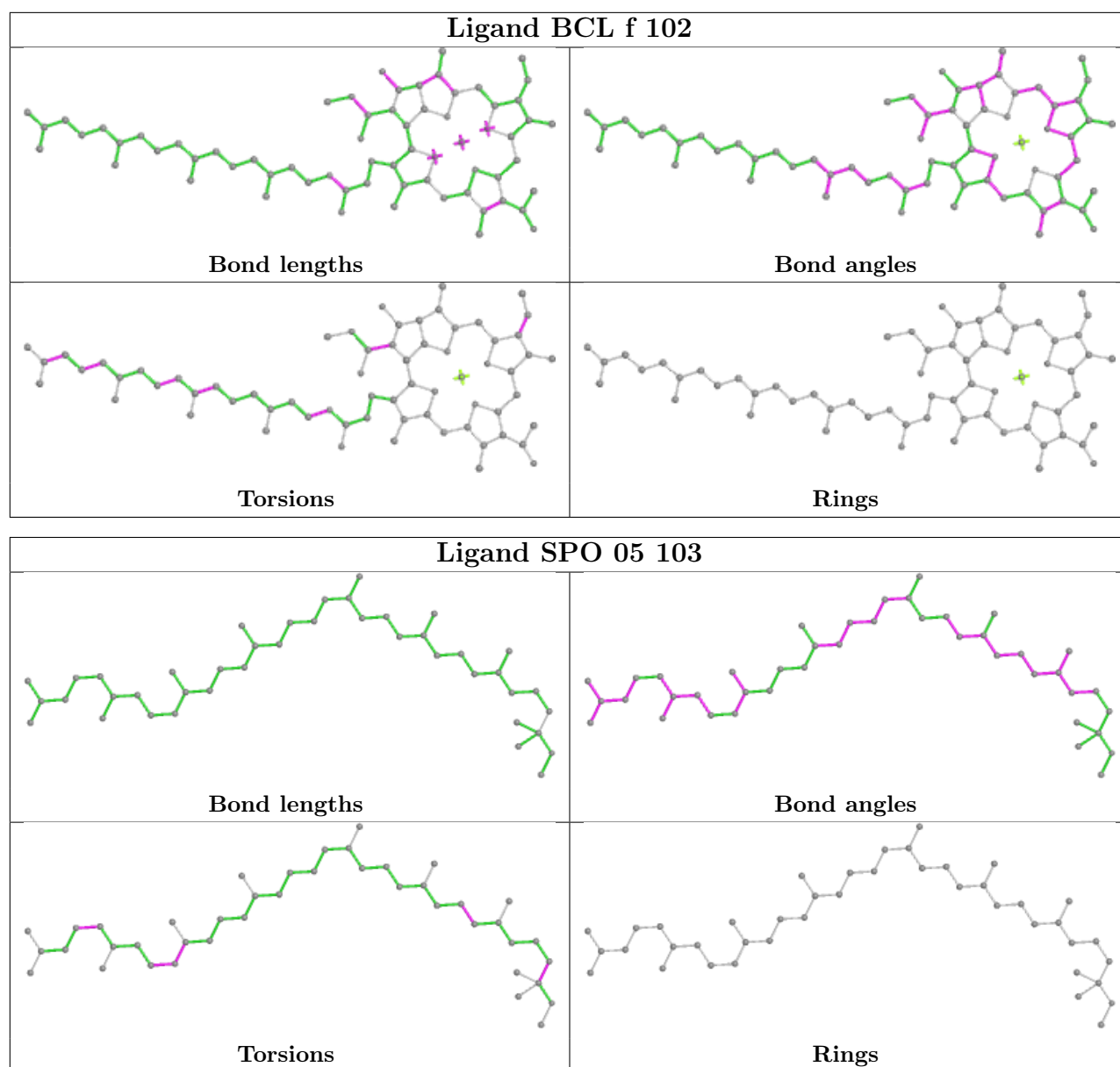


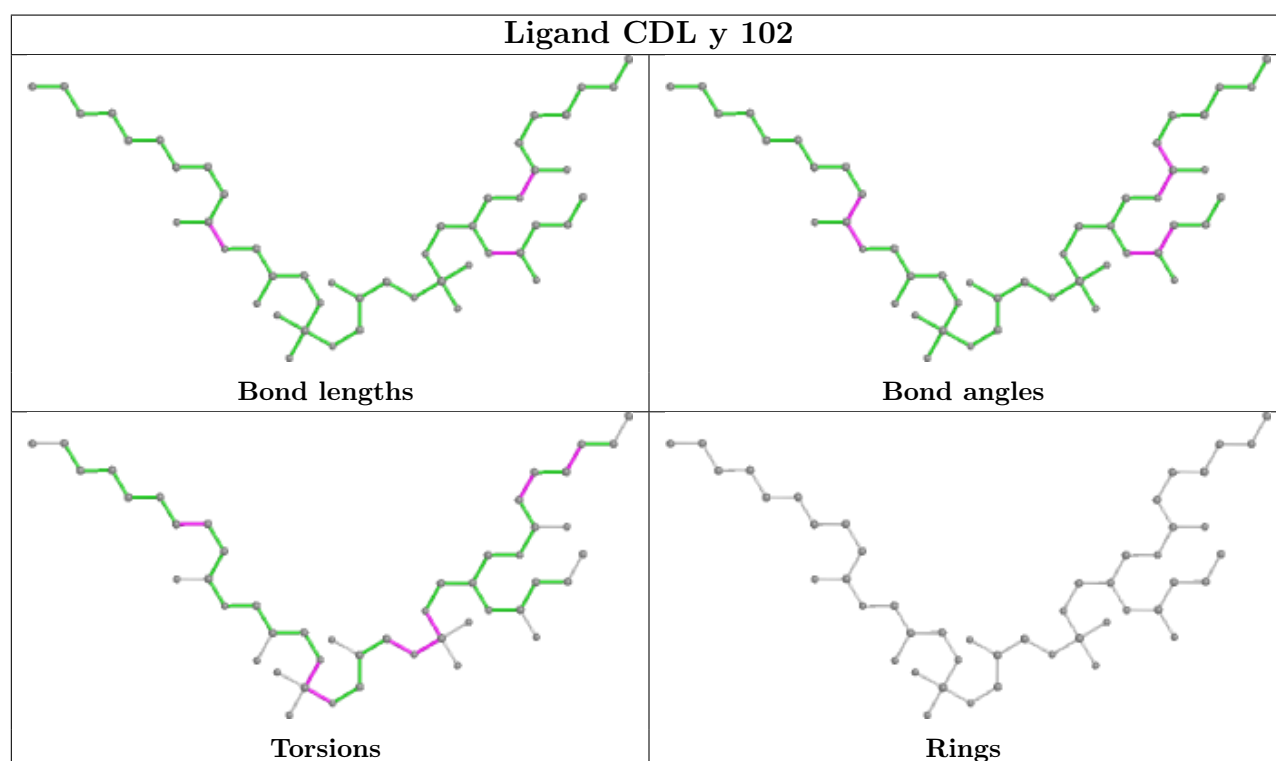
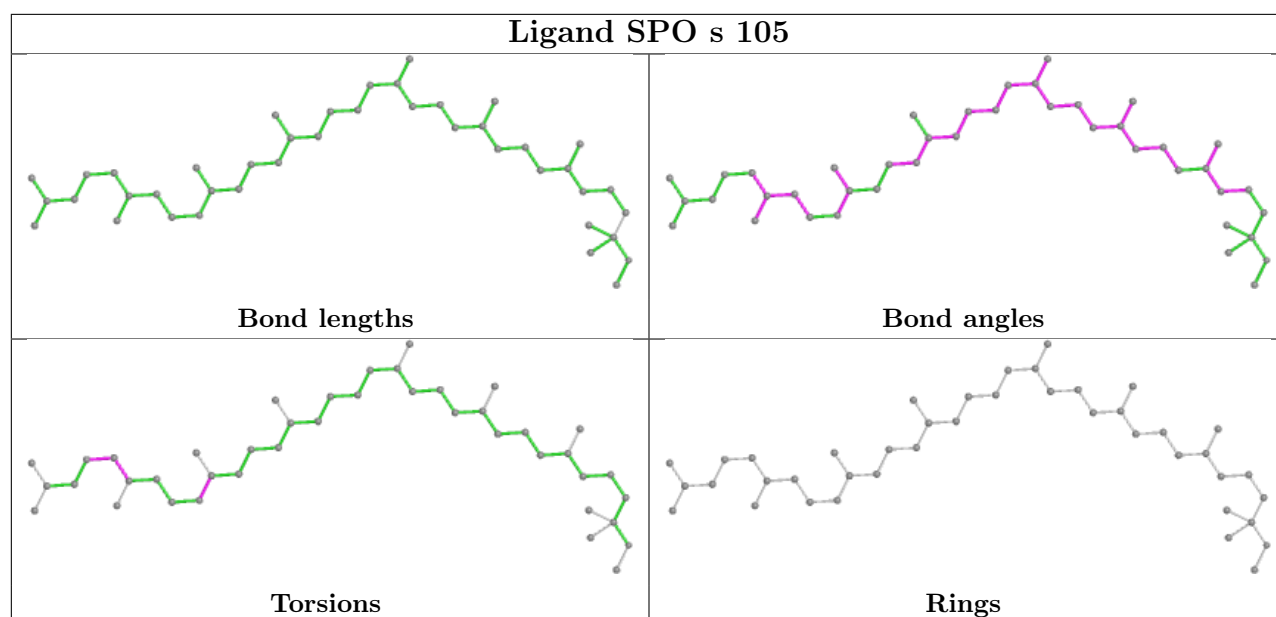
Ligand SPO I 103

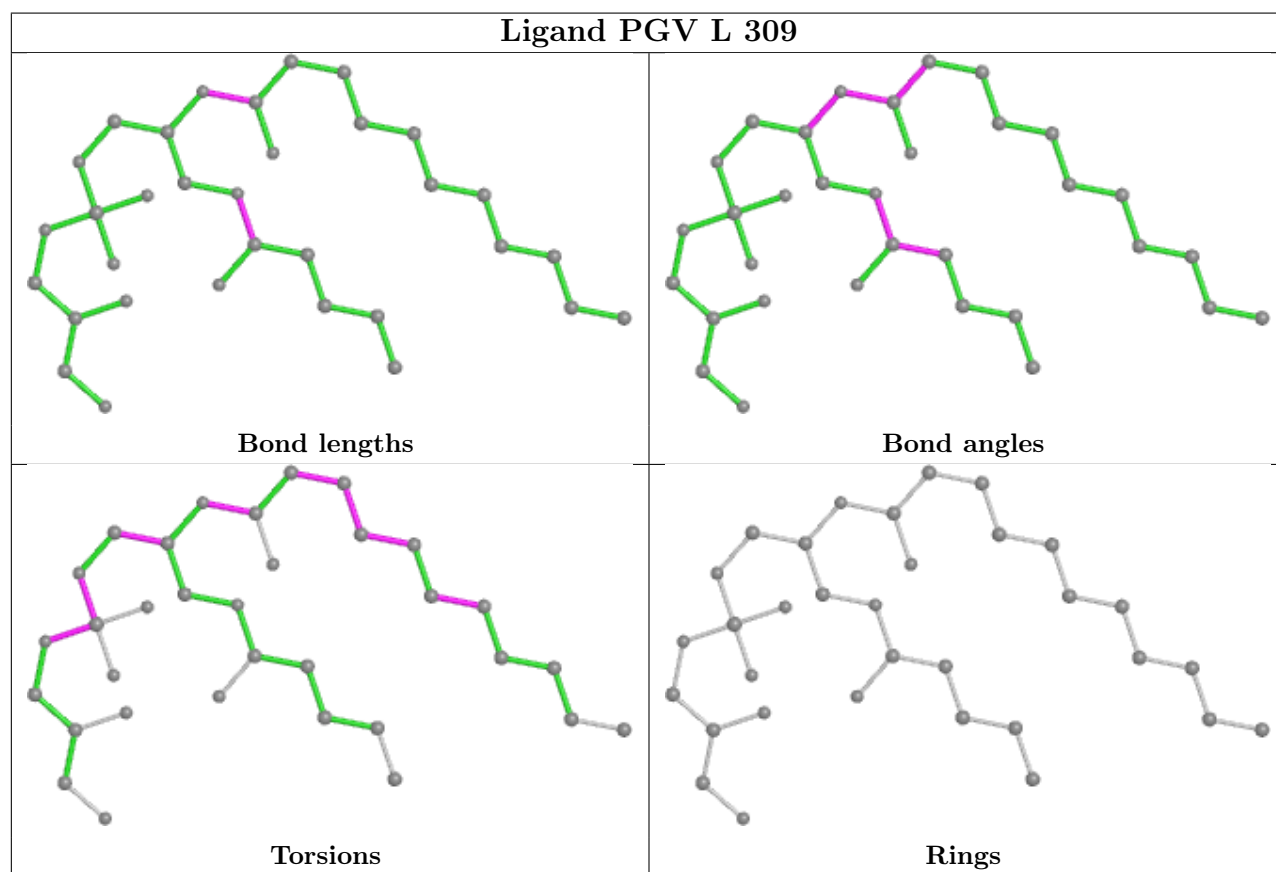
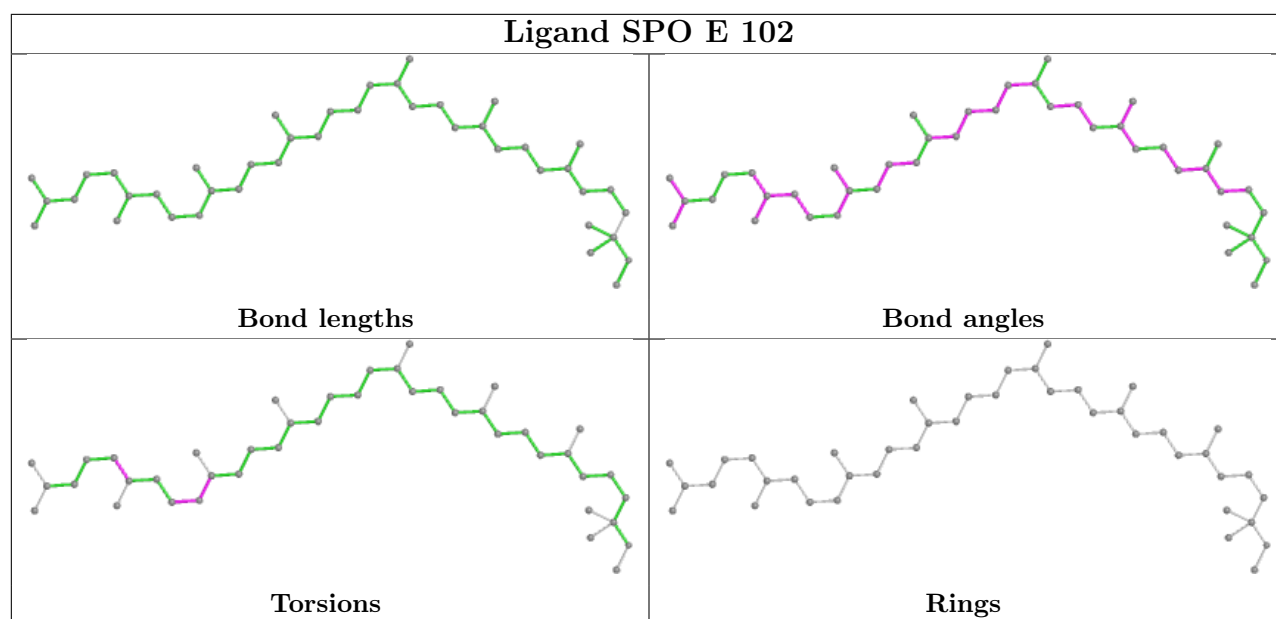


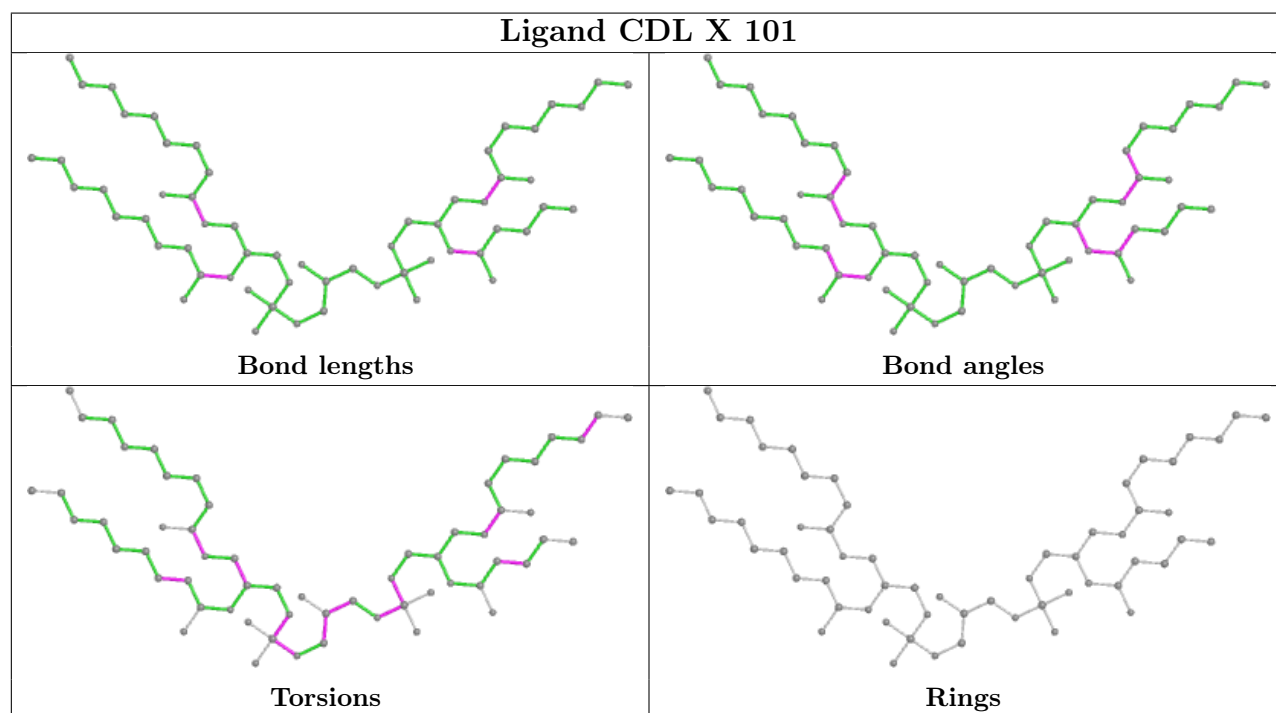
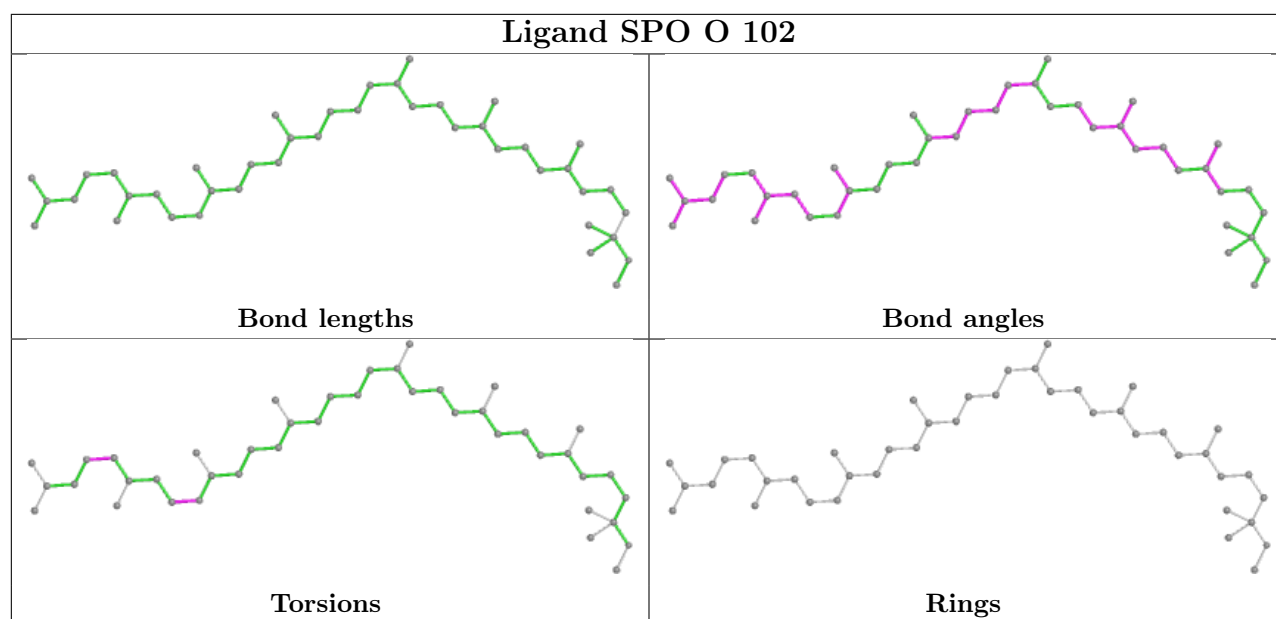


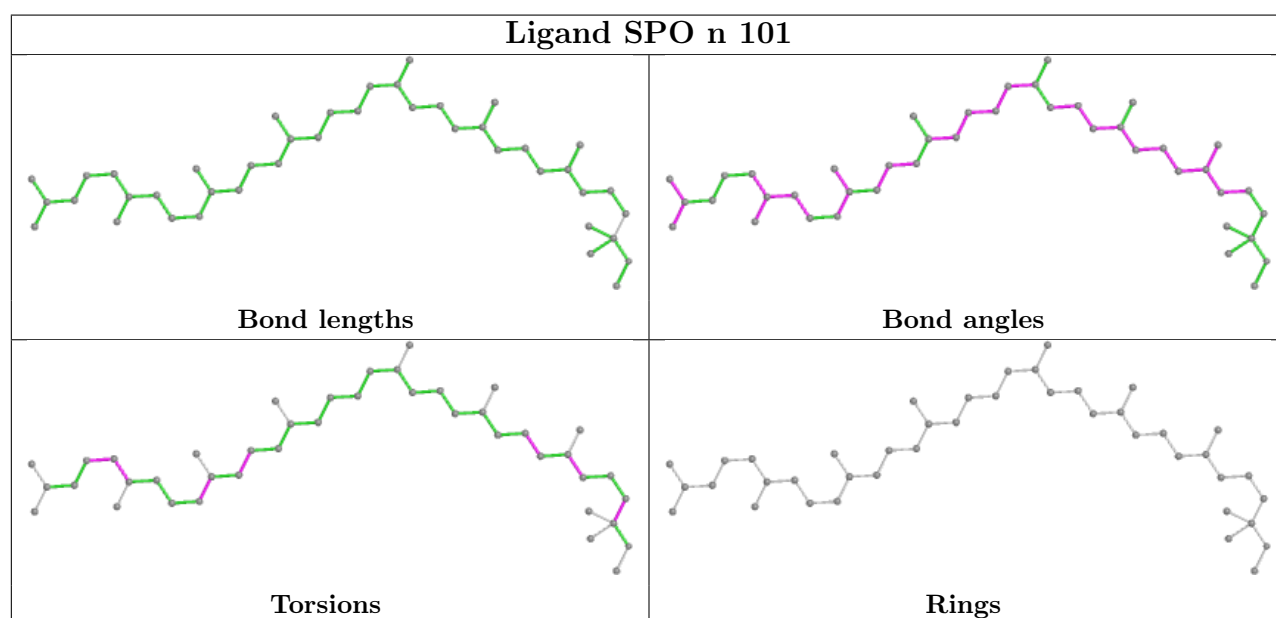
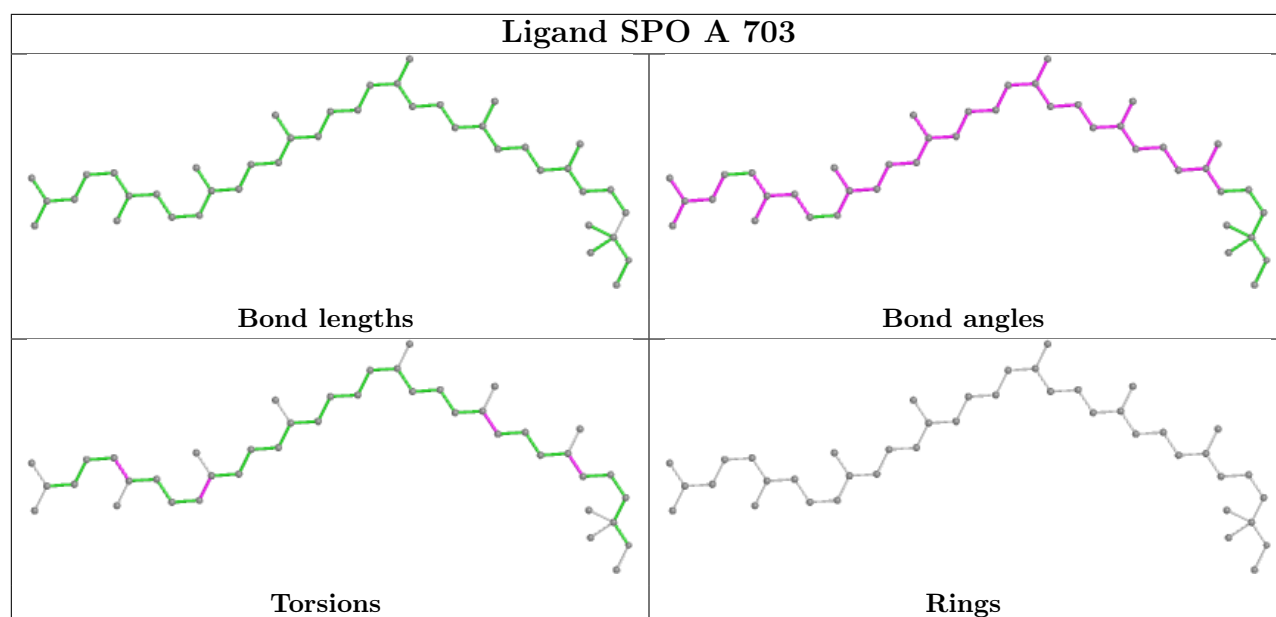


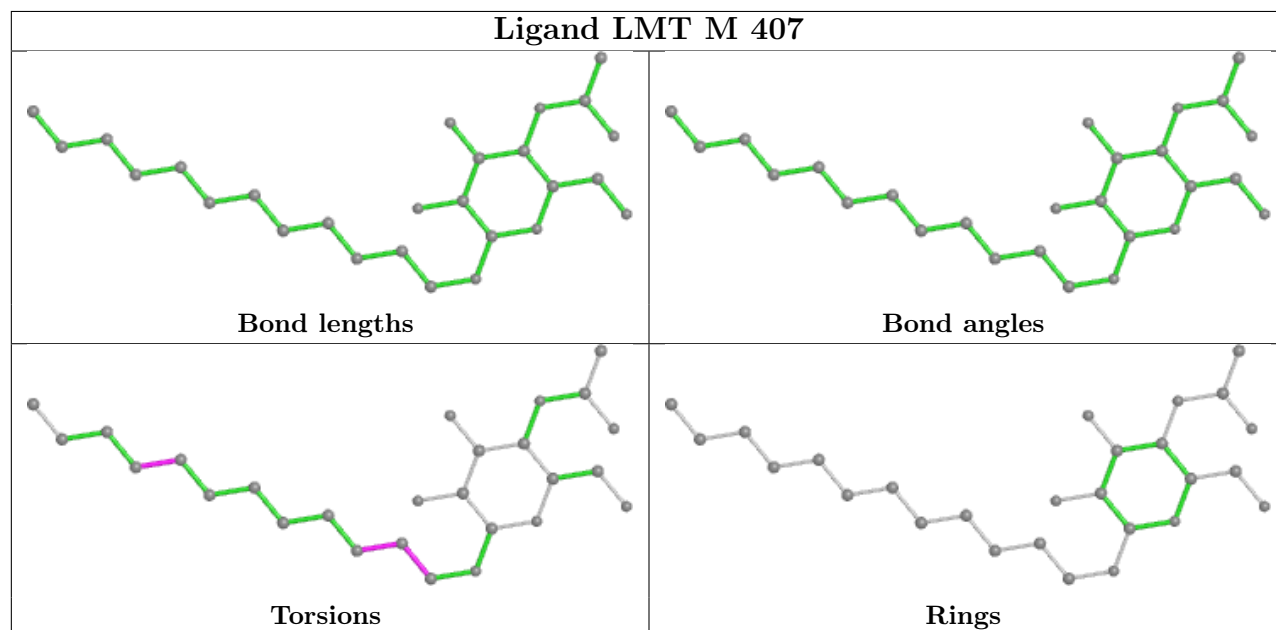
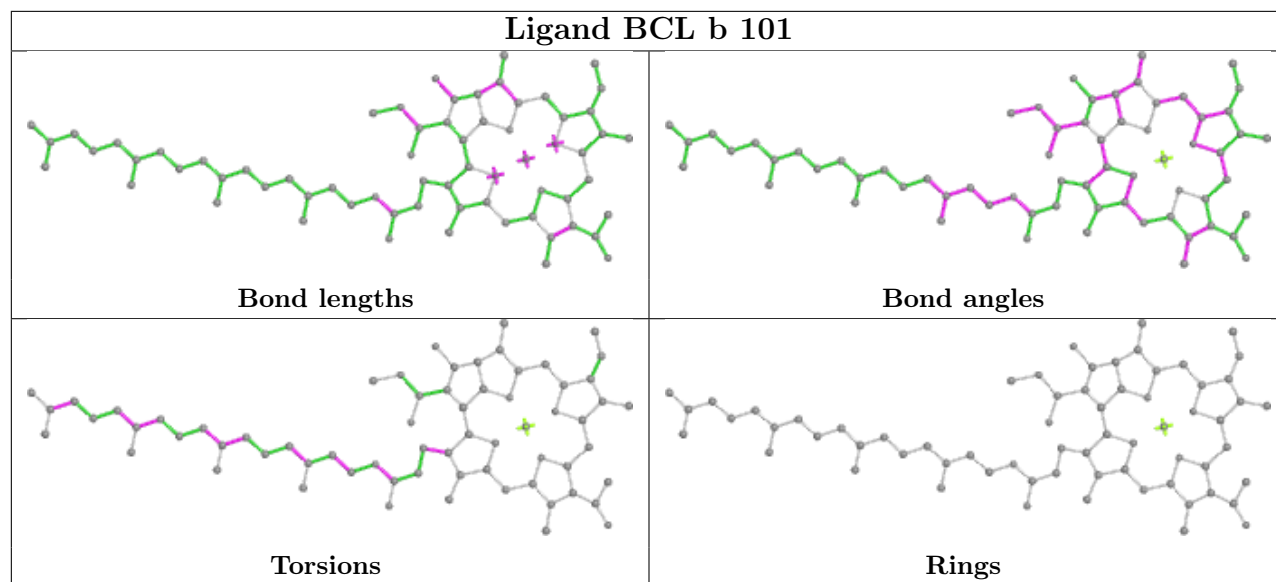


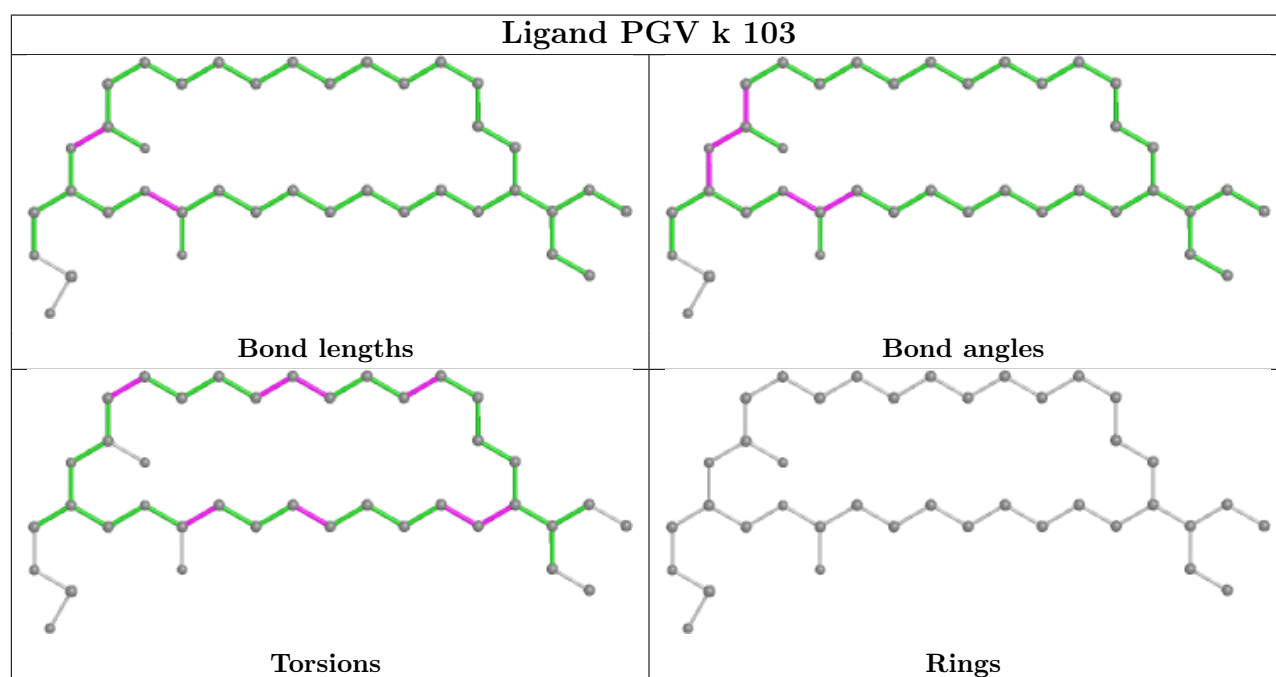
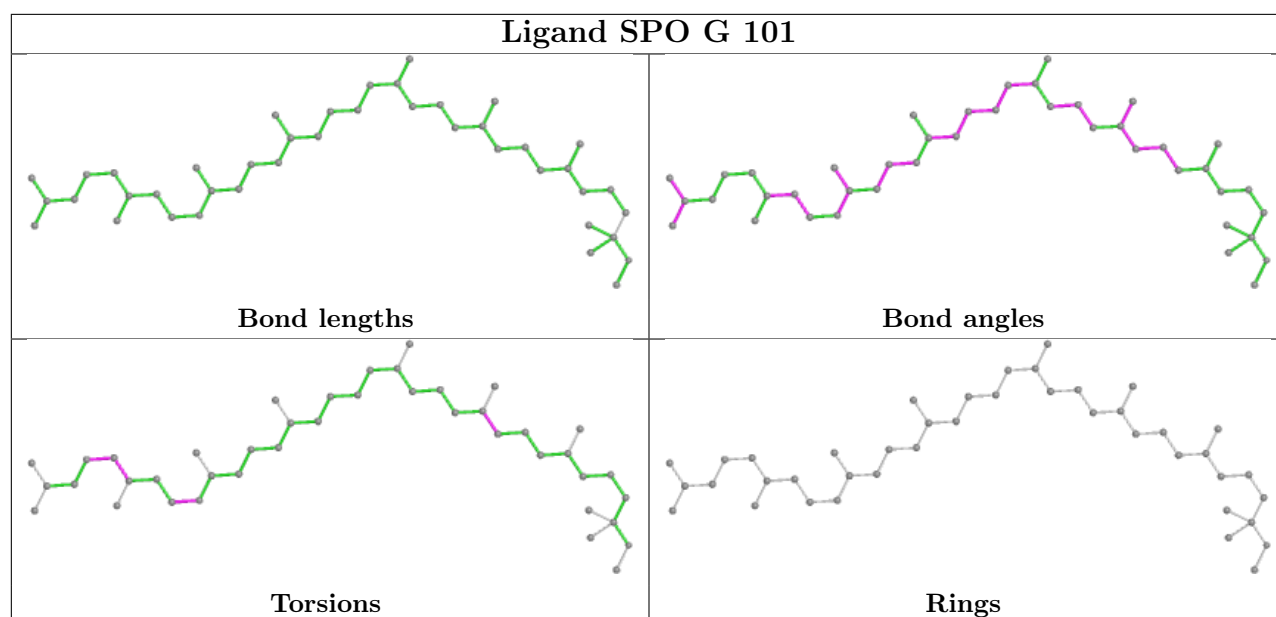


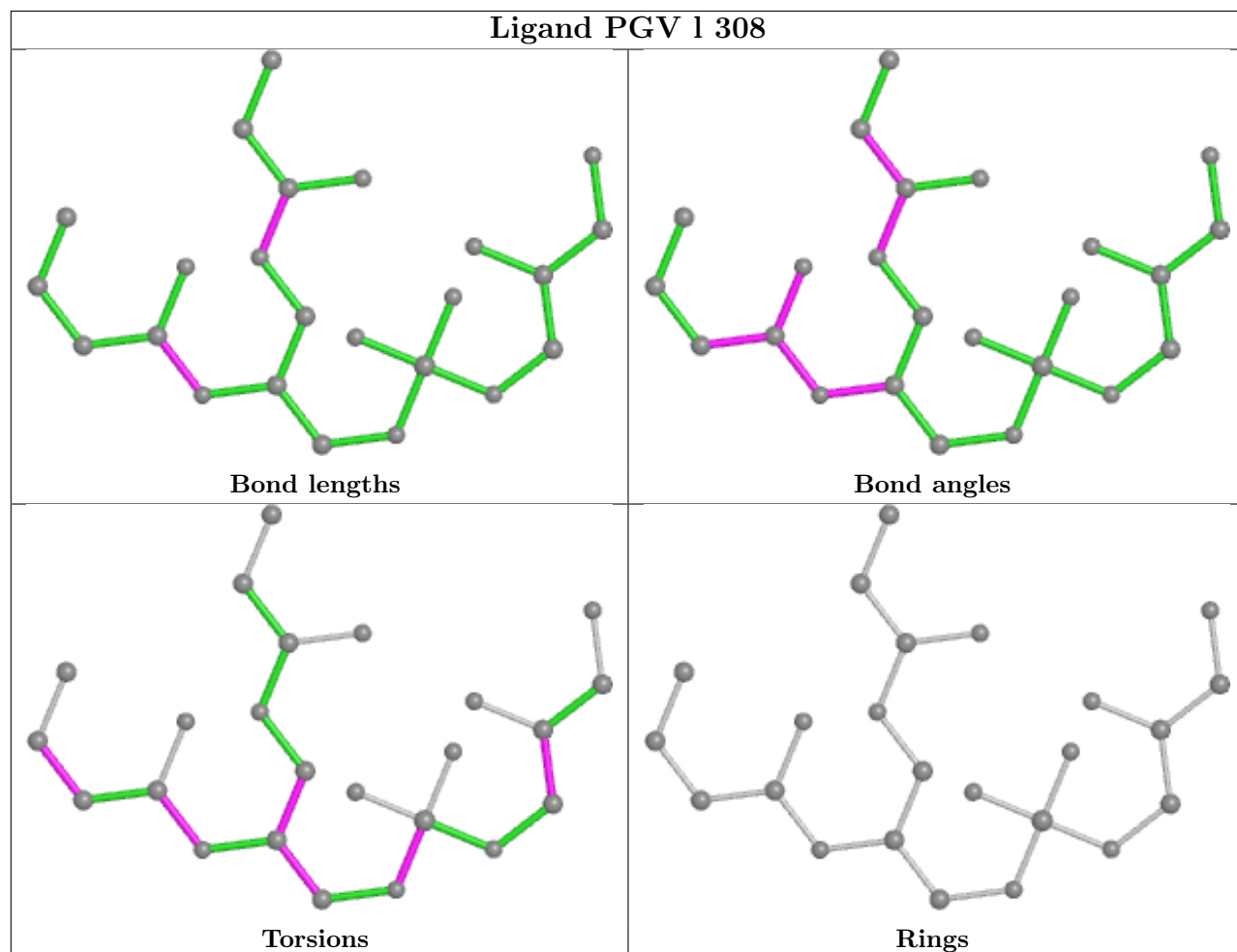
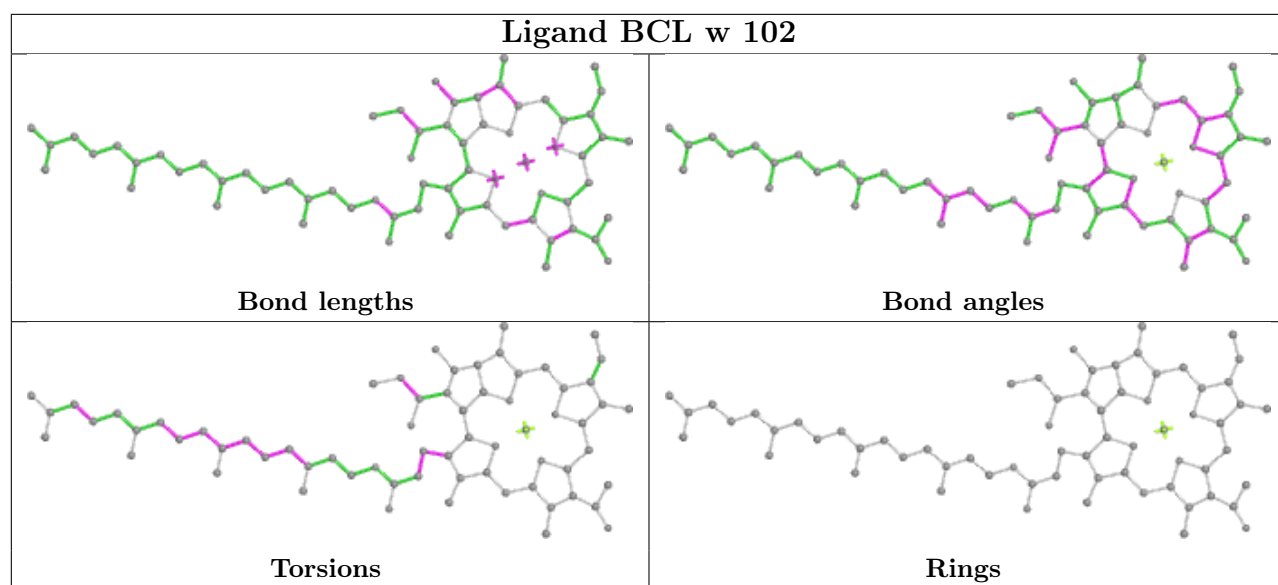


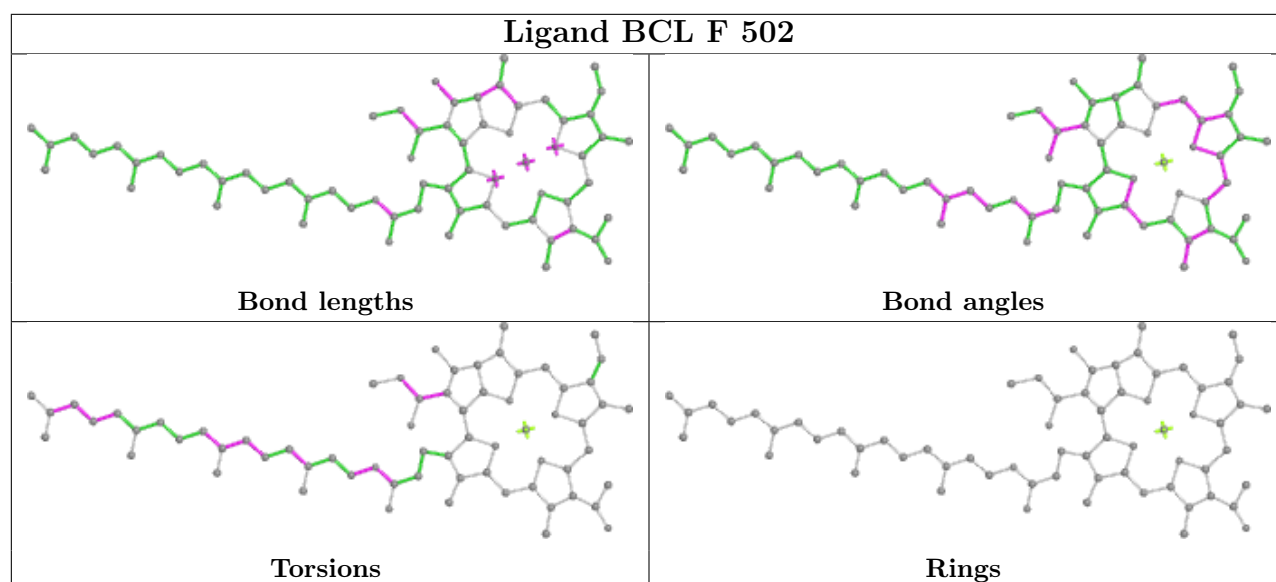
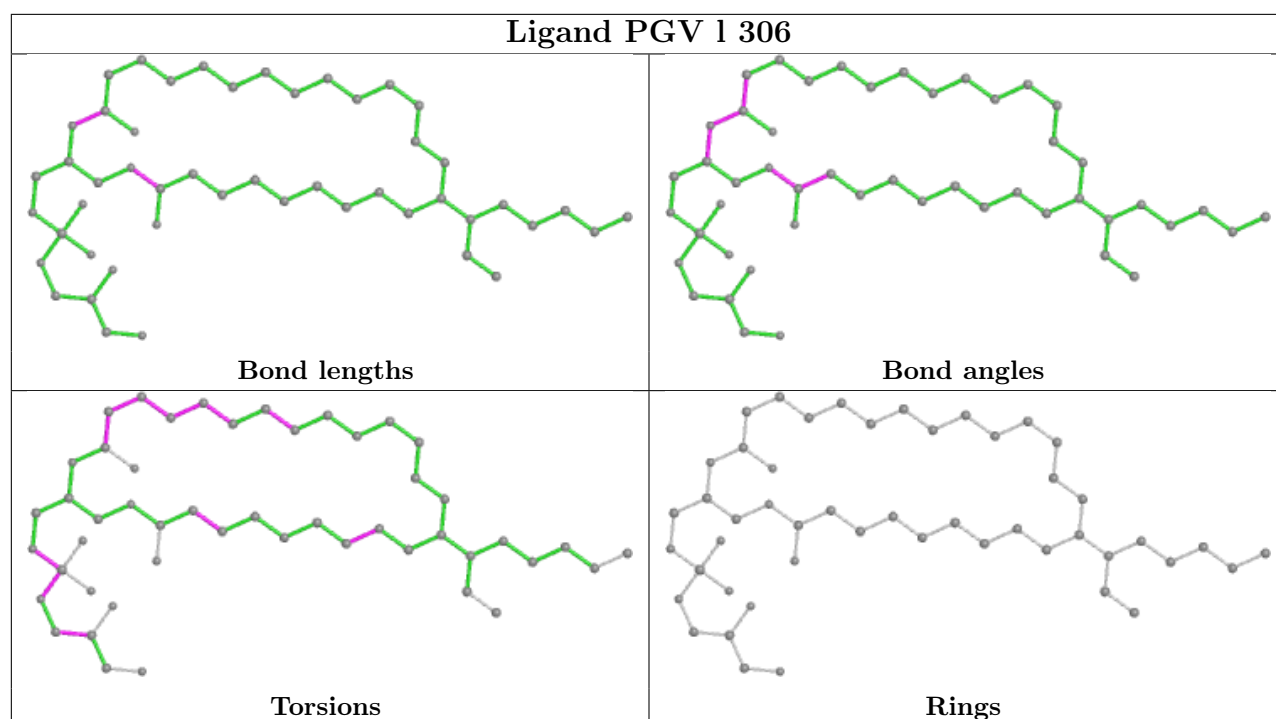


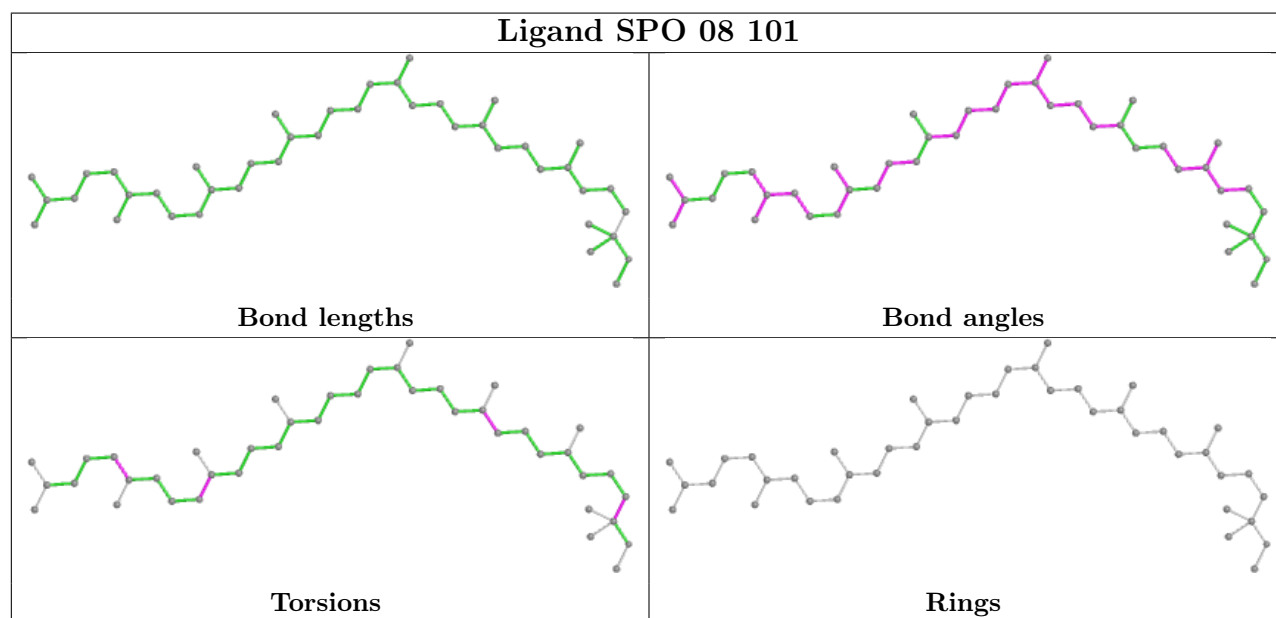
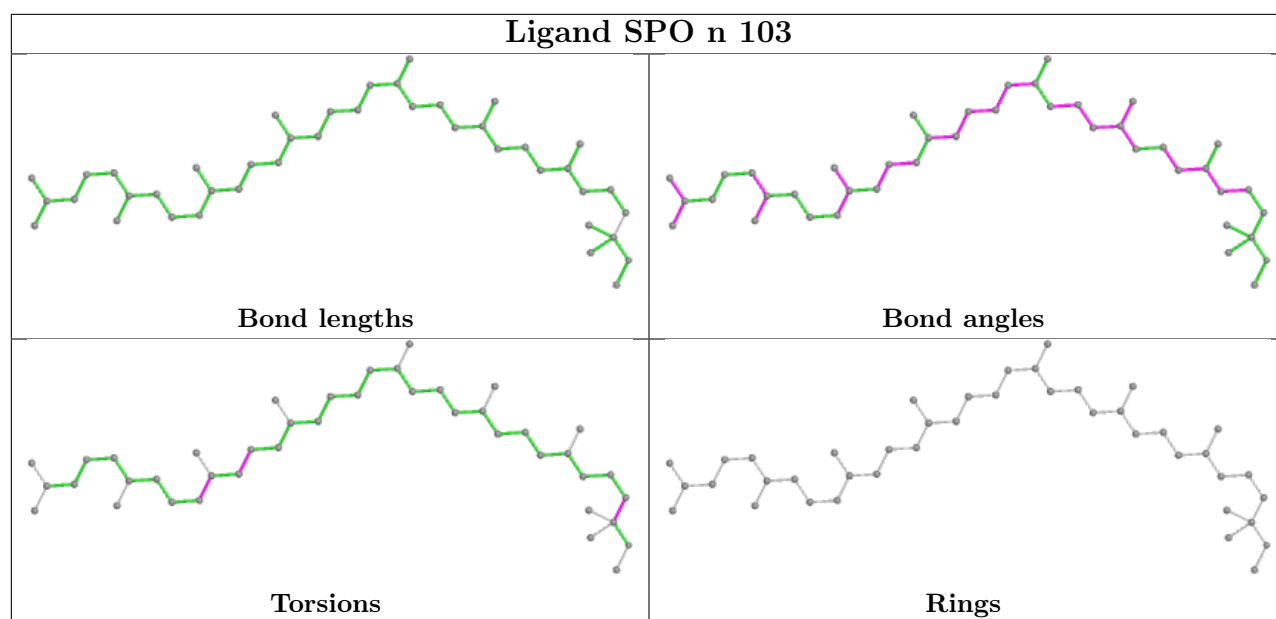


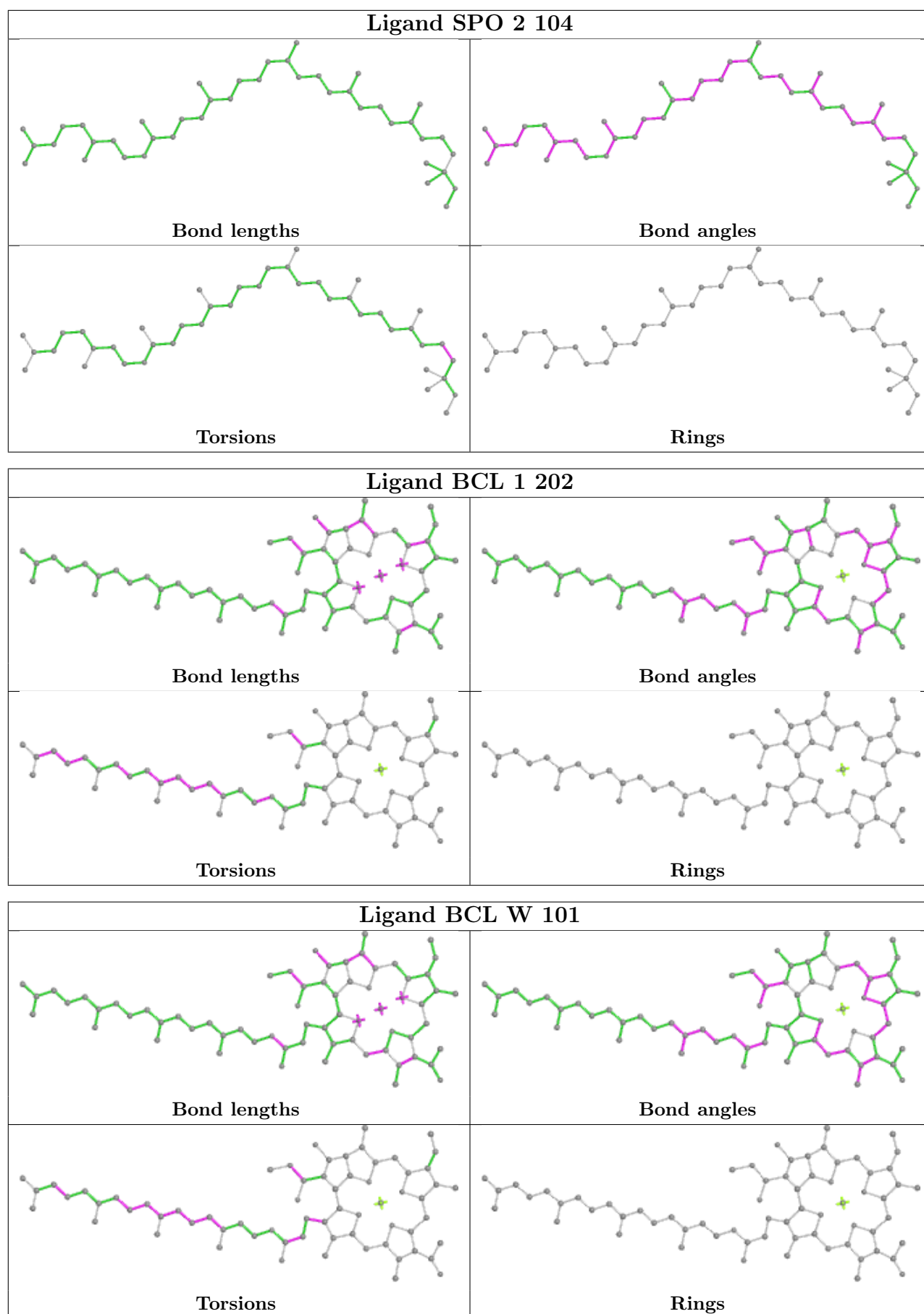


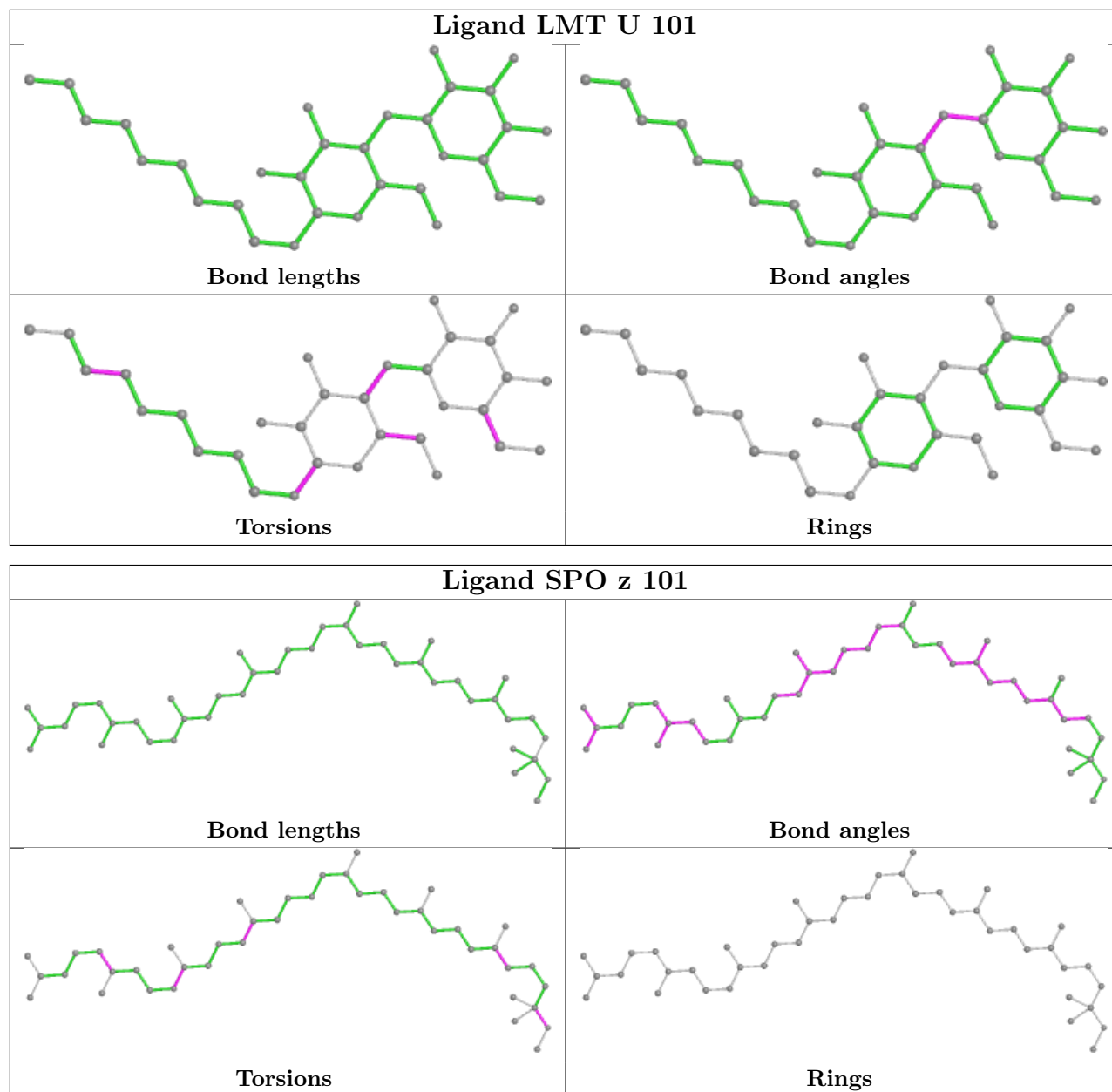


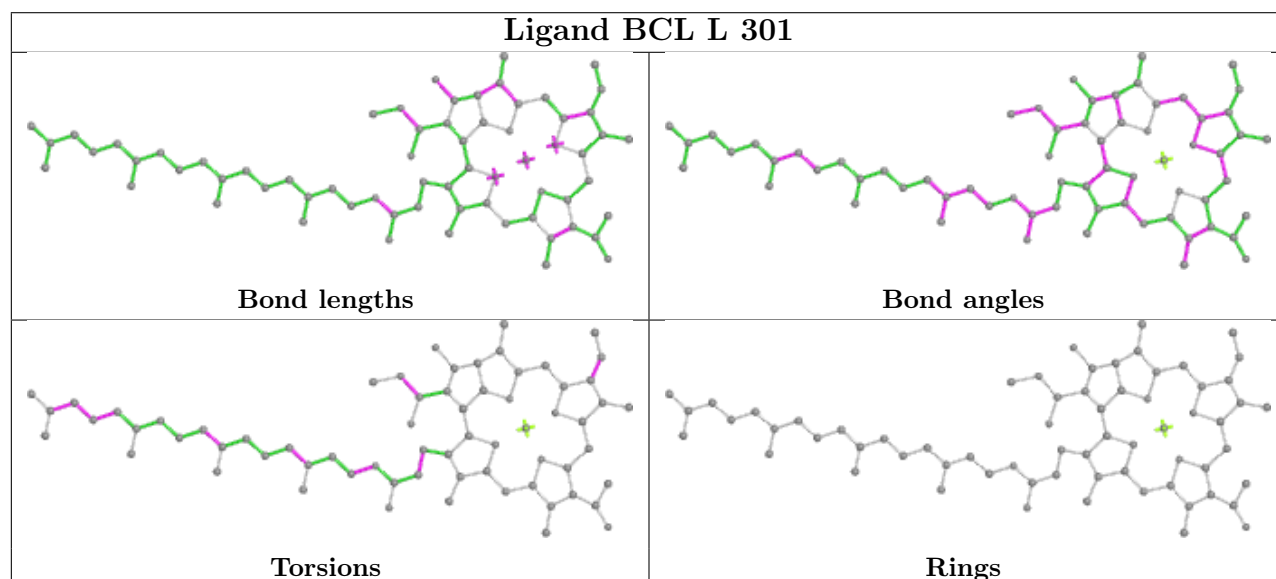
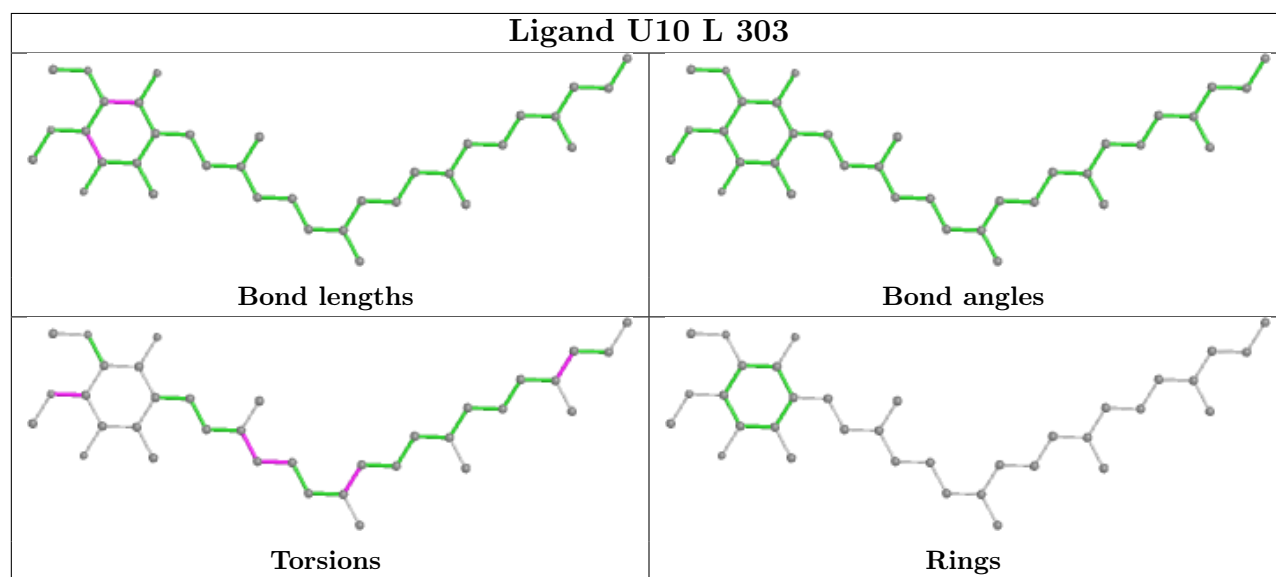
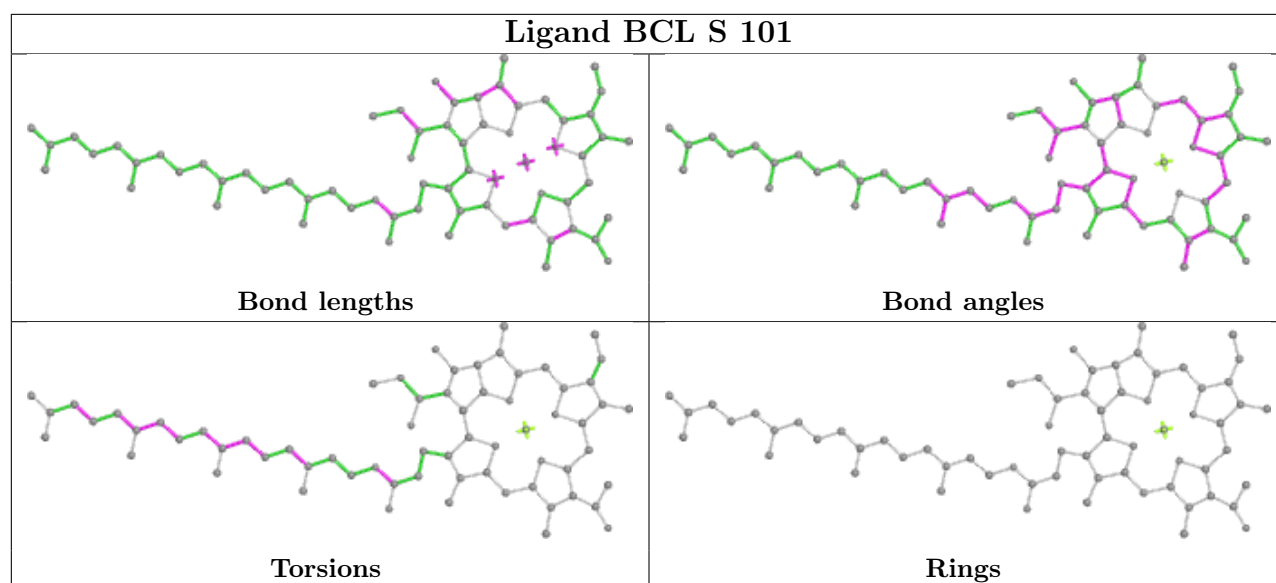


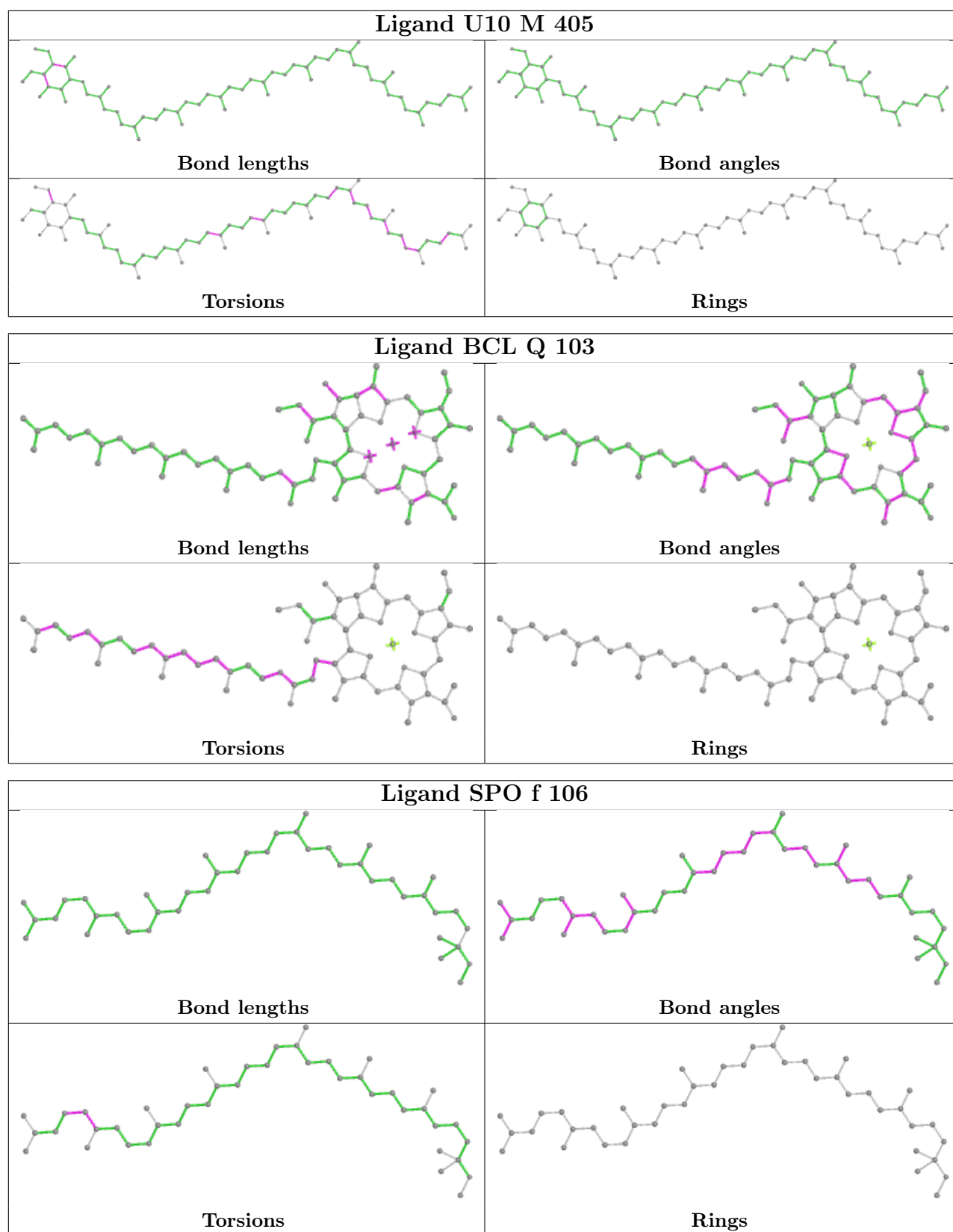


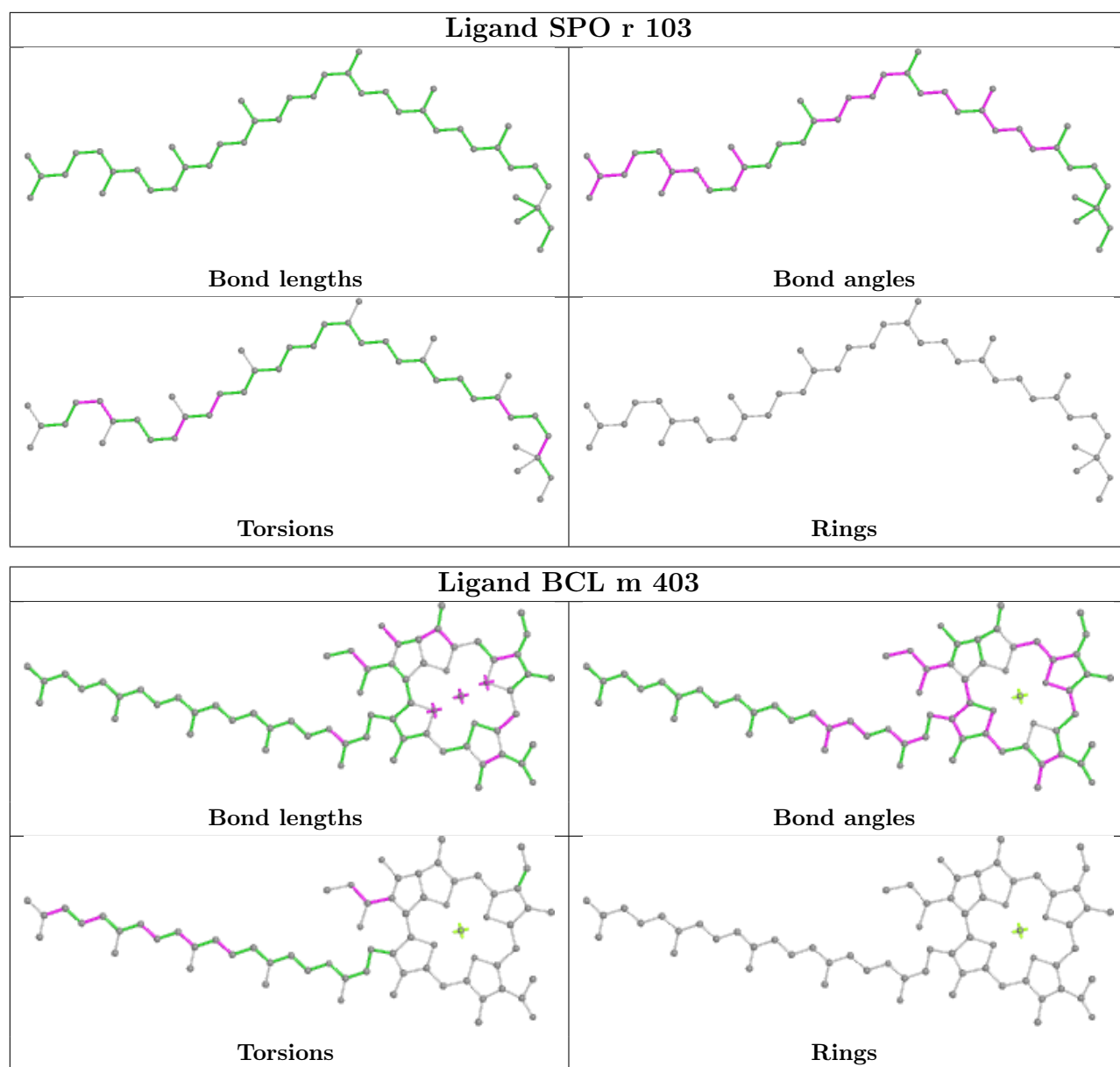


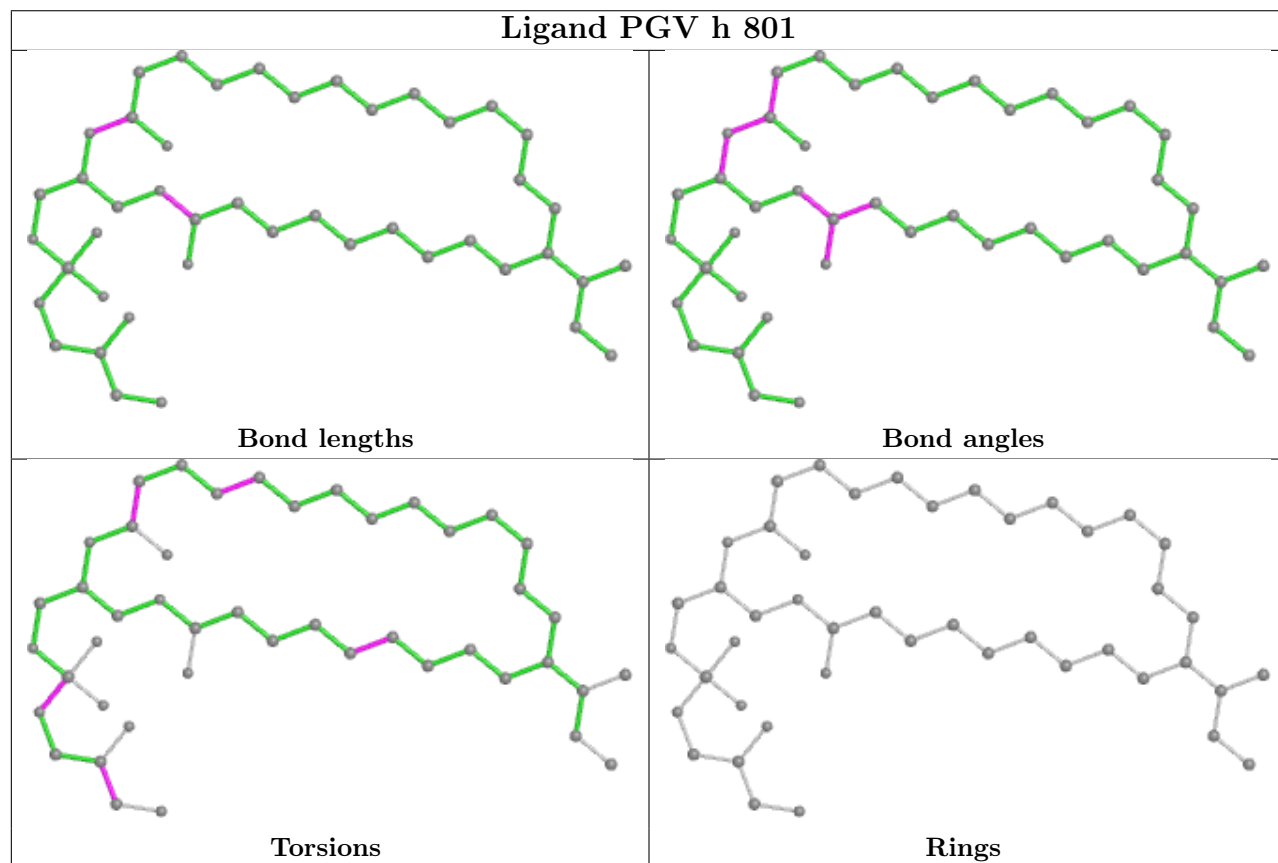
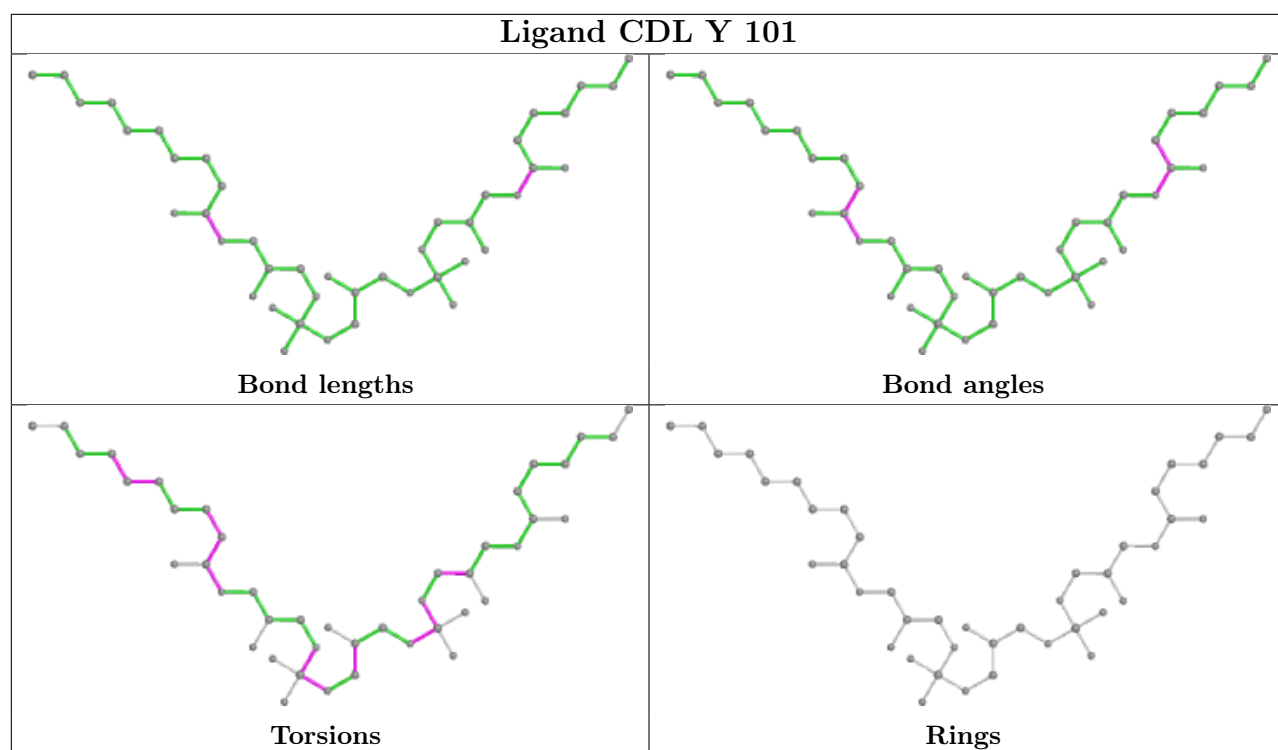


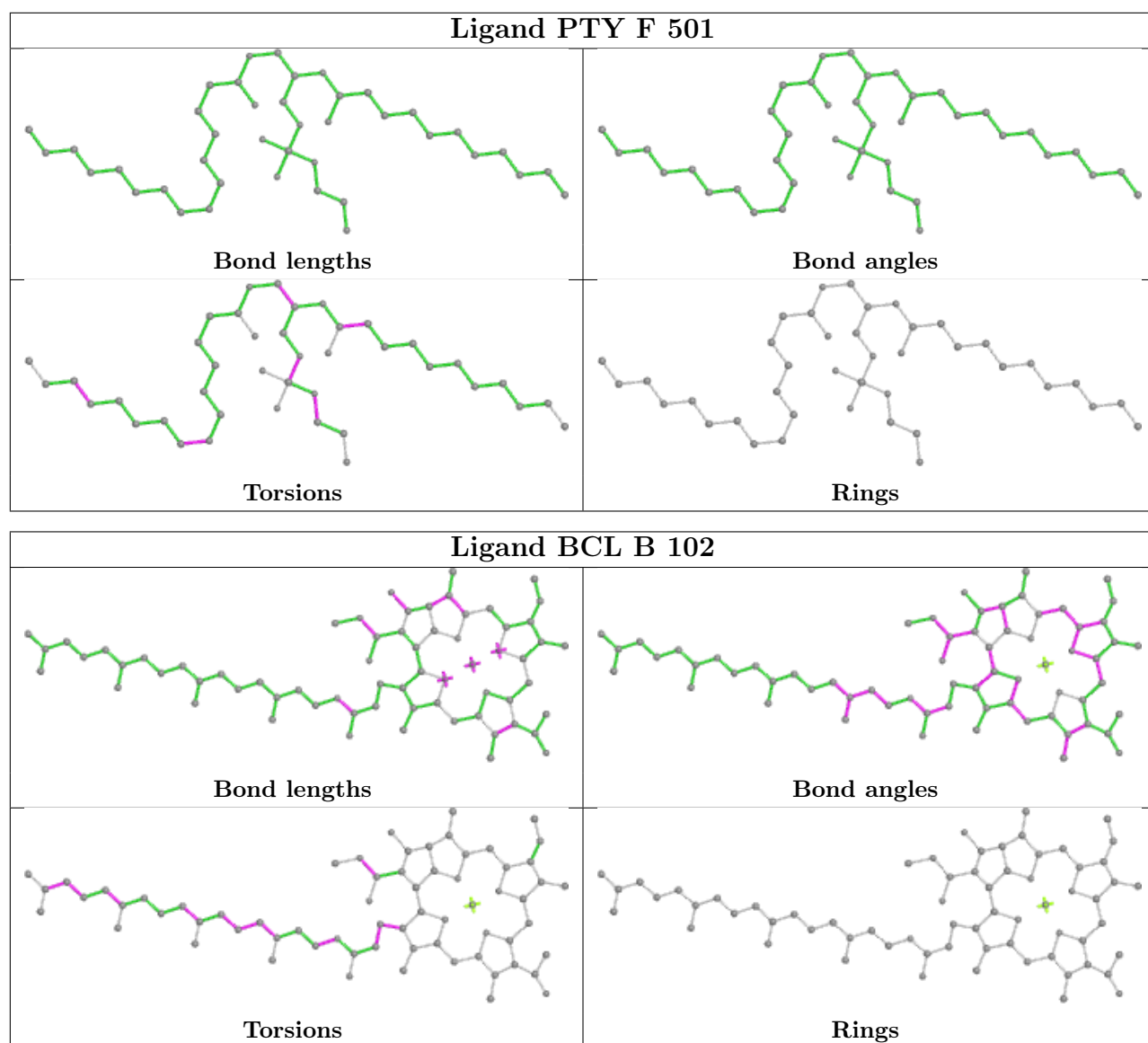


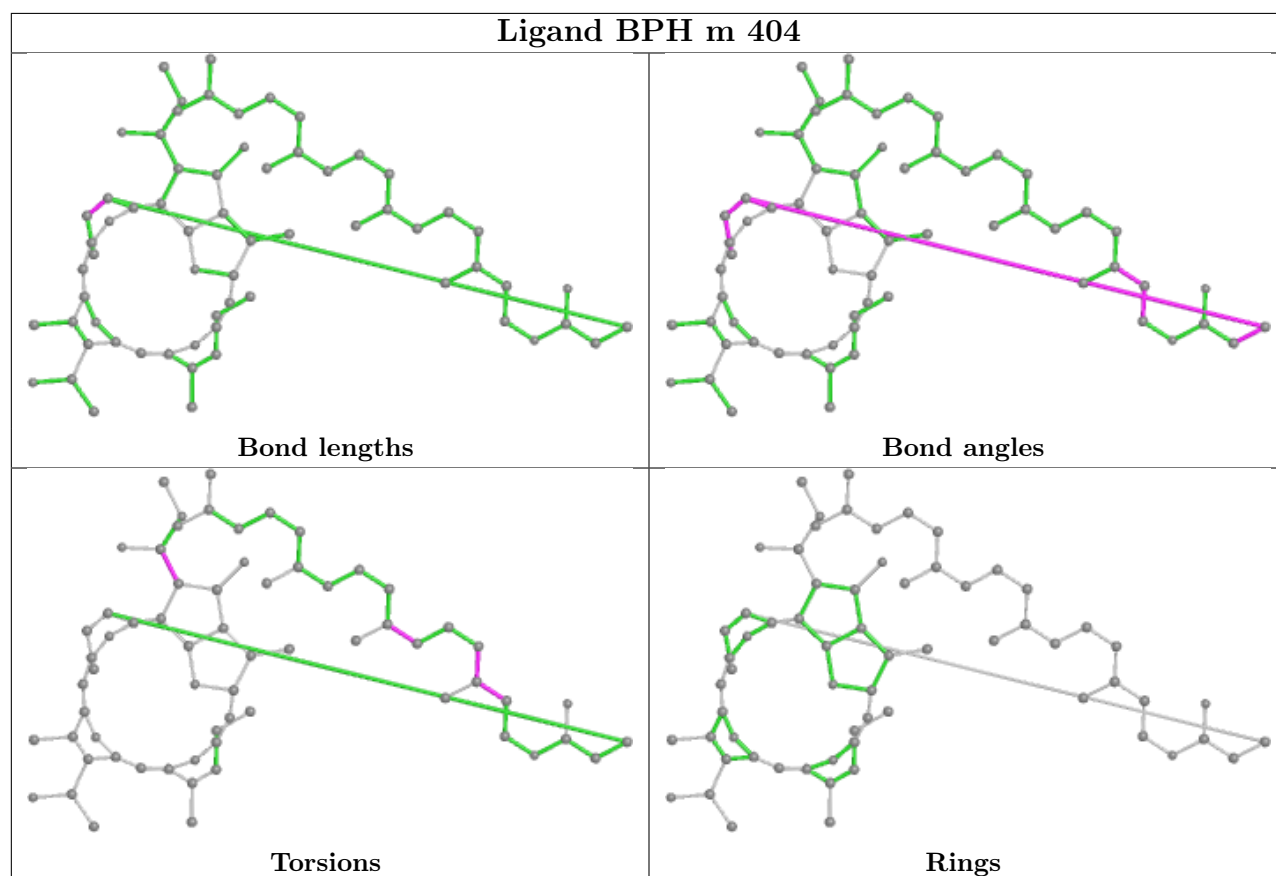
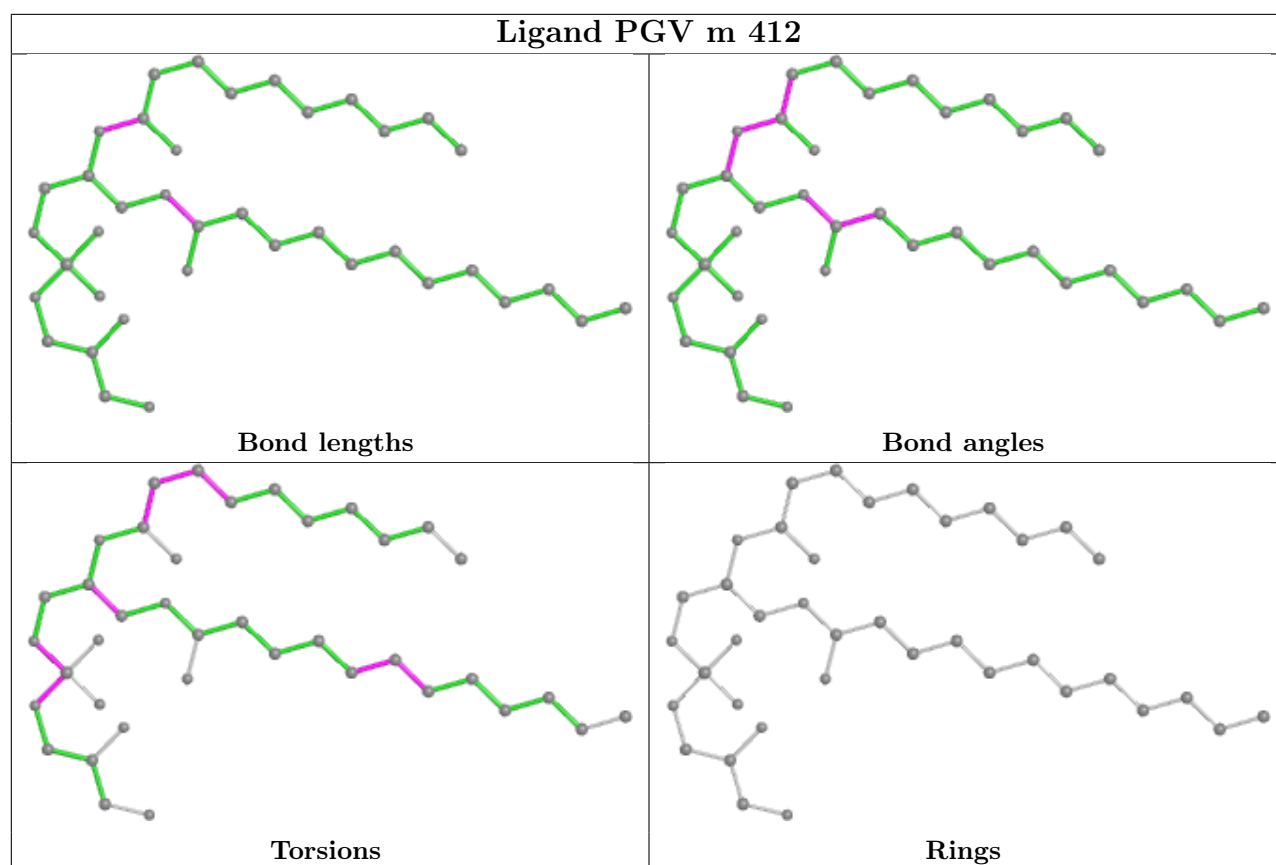


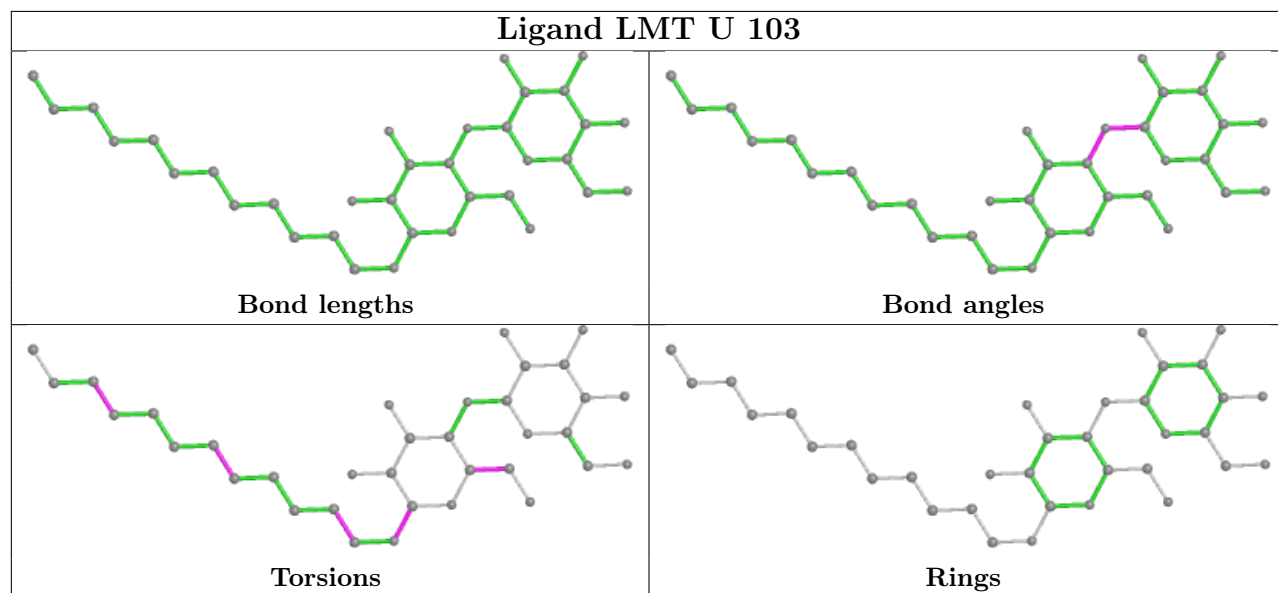
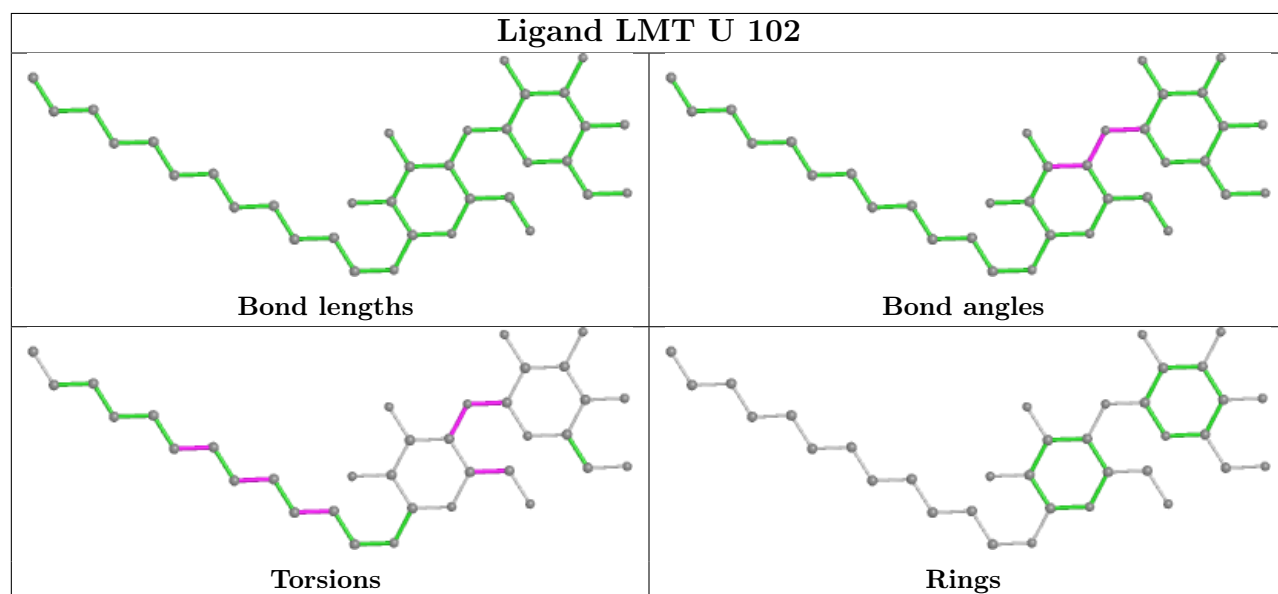
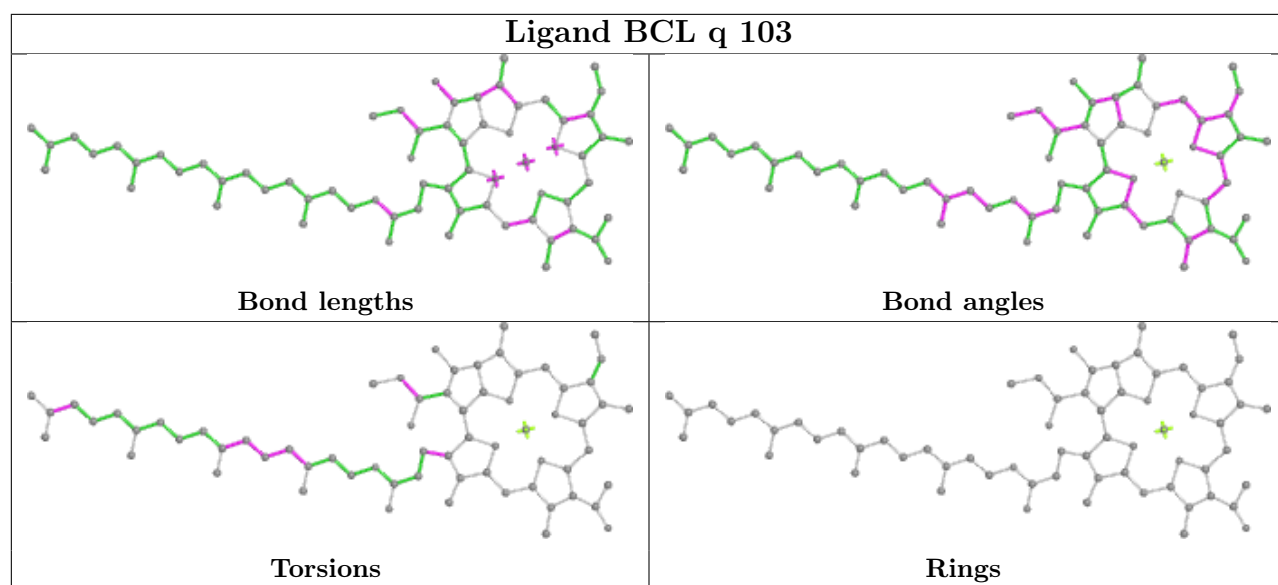


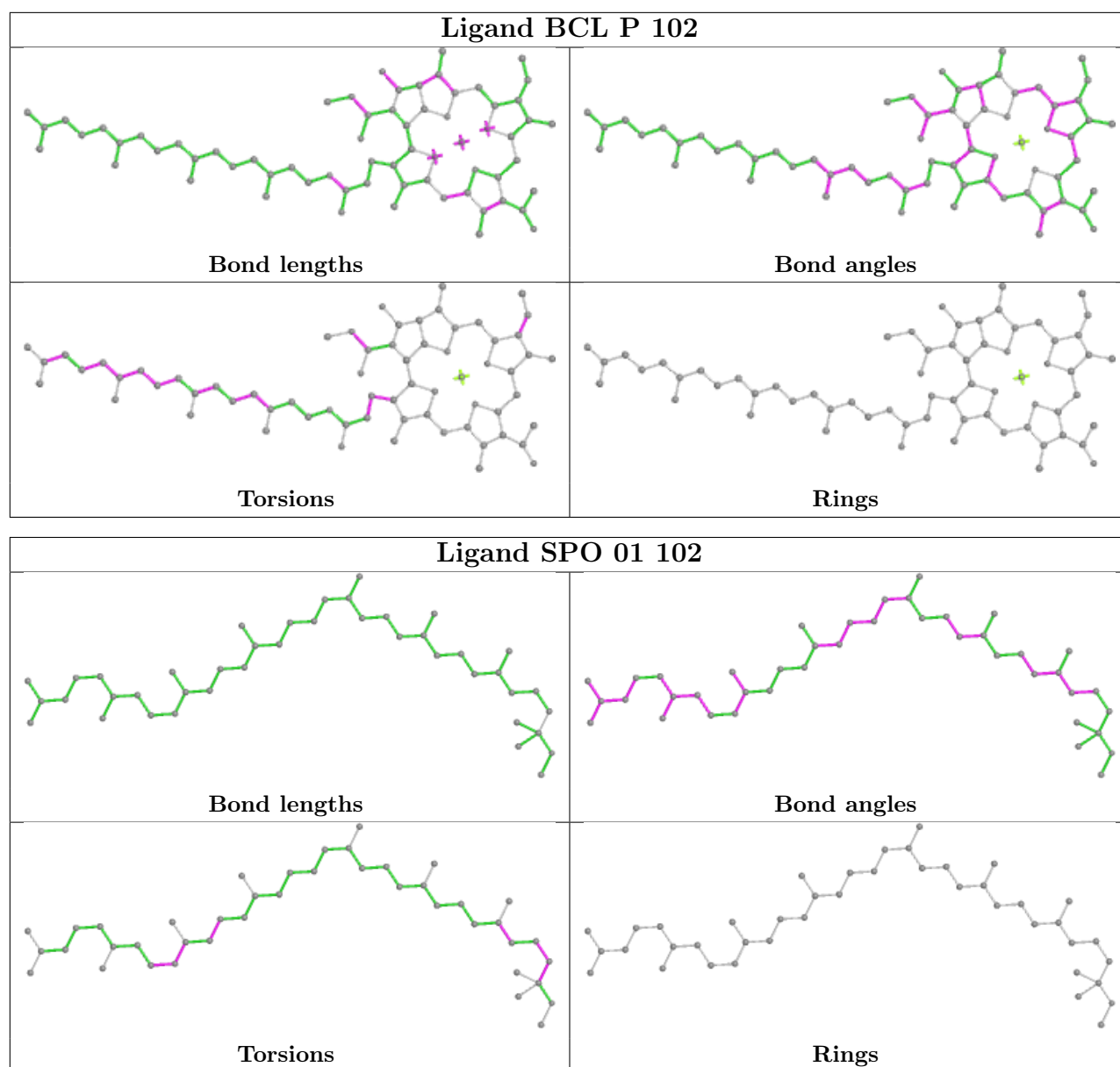


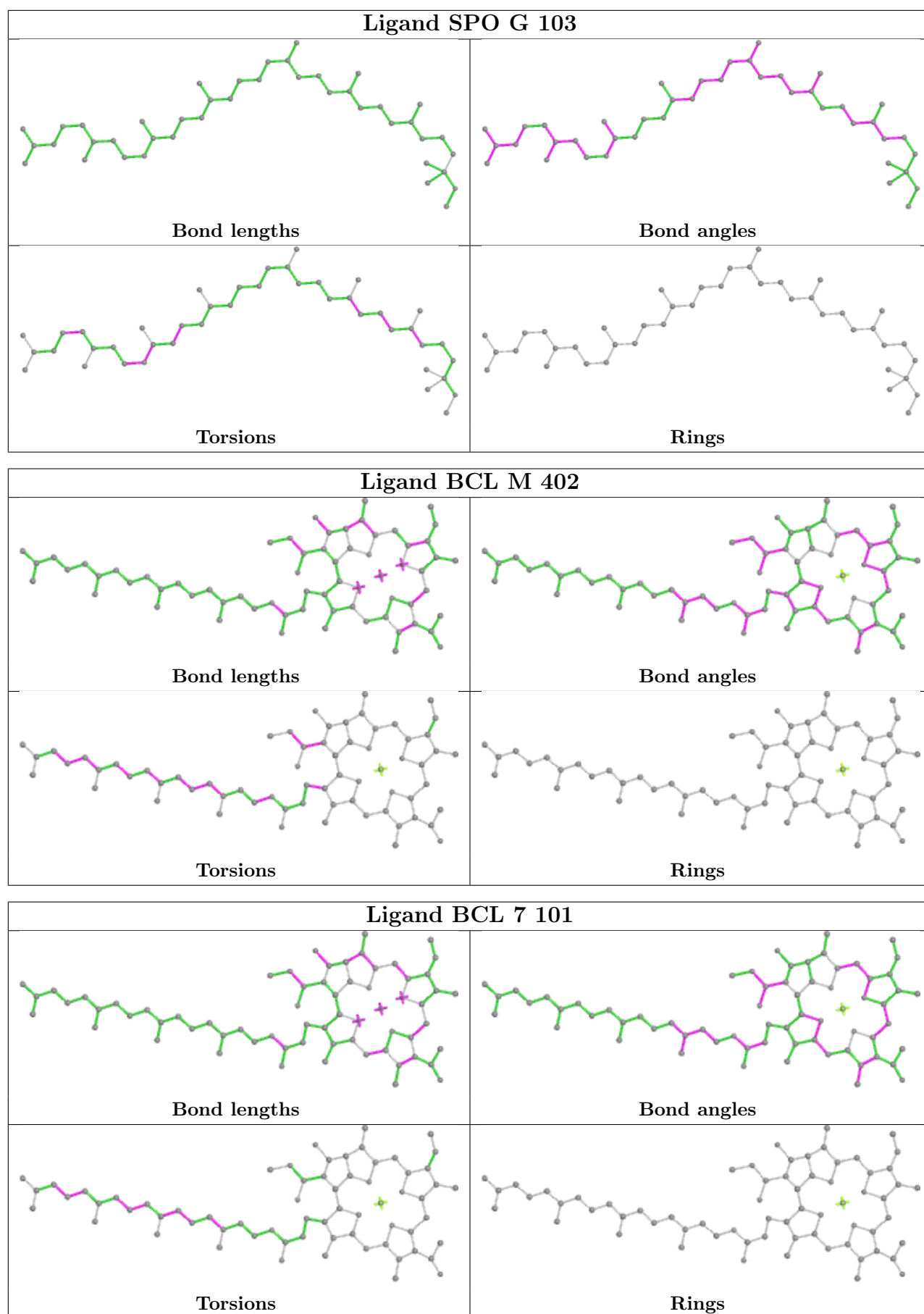


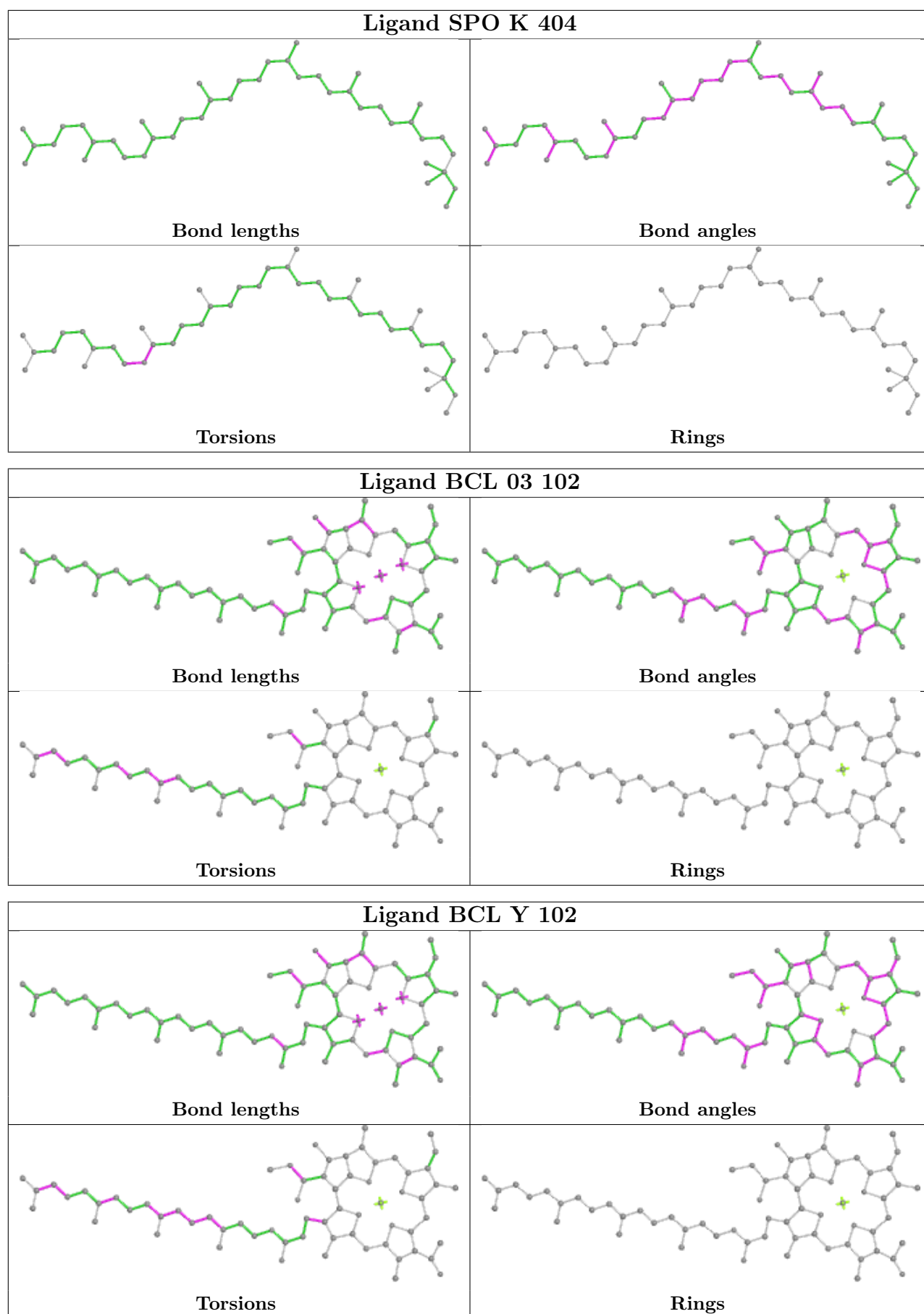


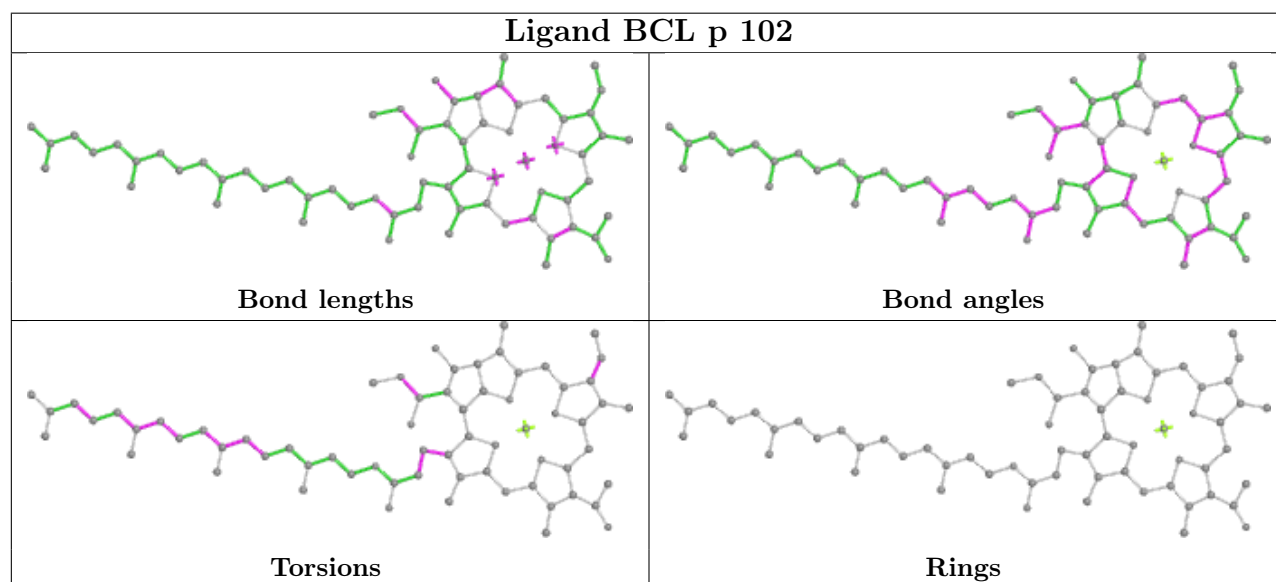
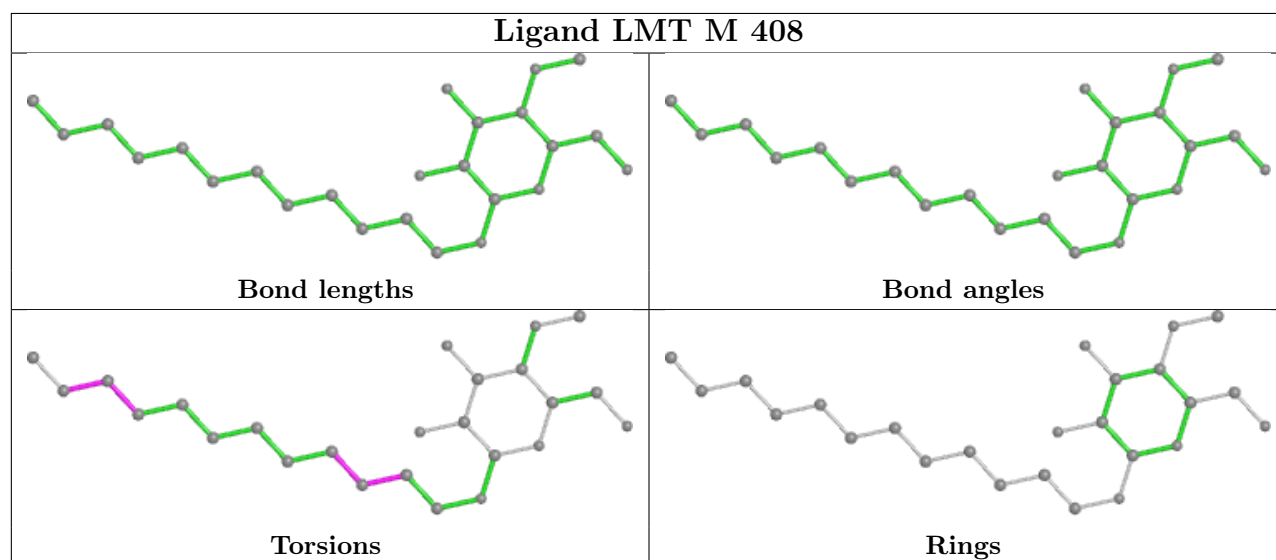
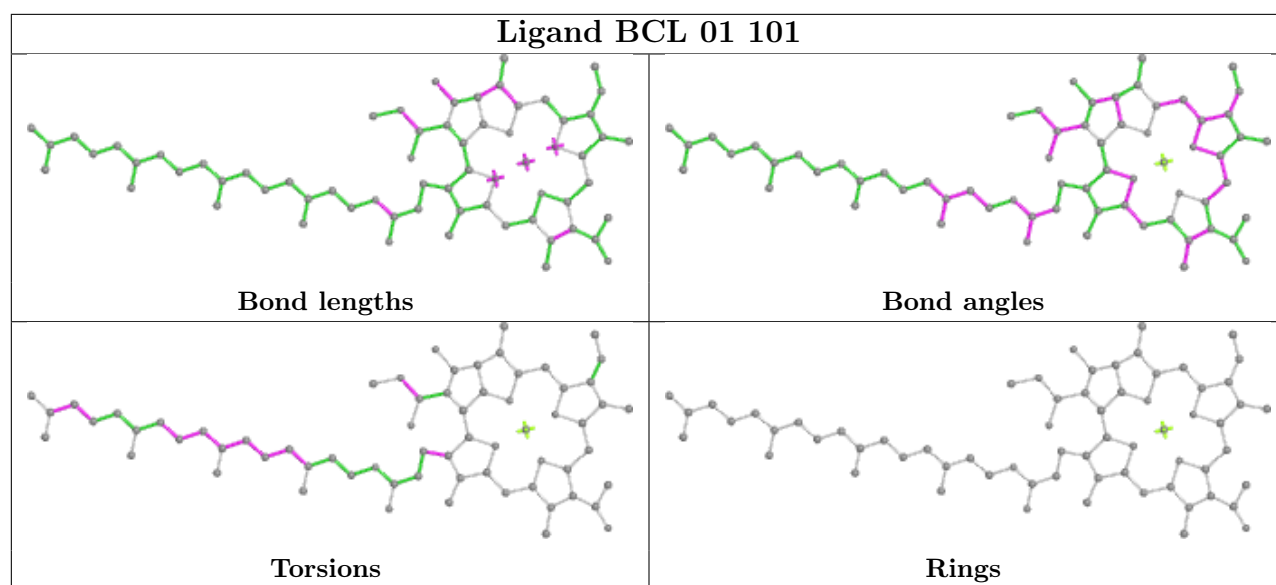


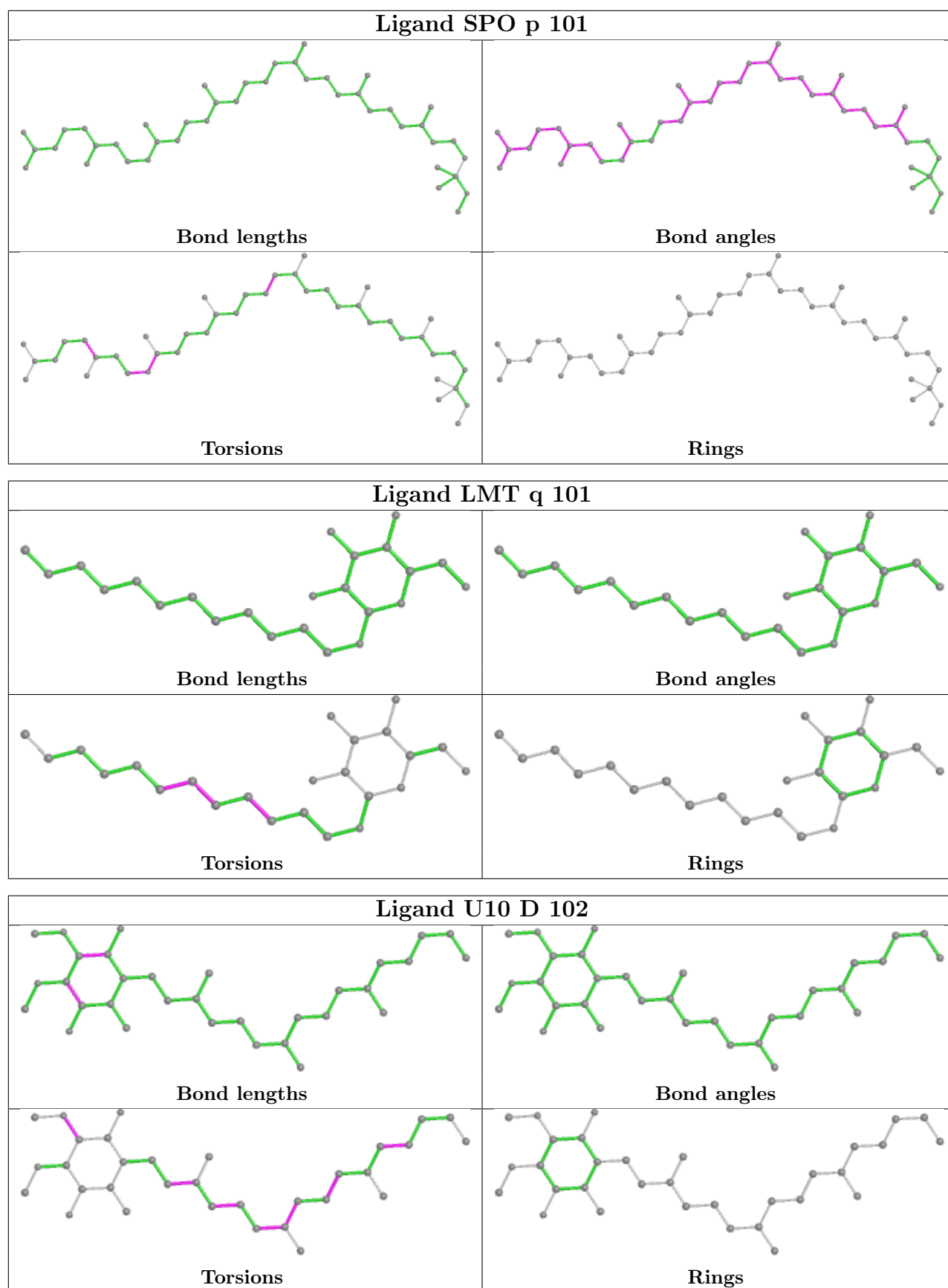


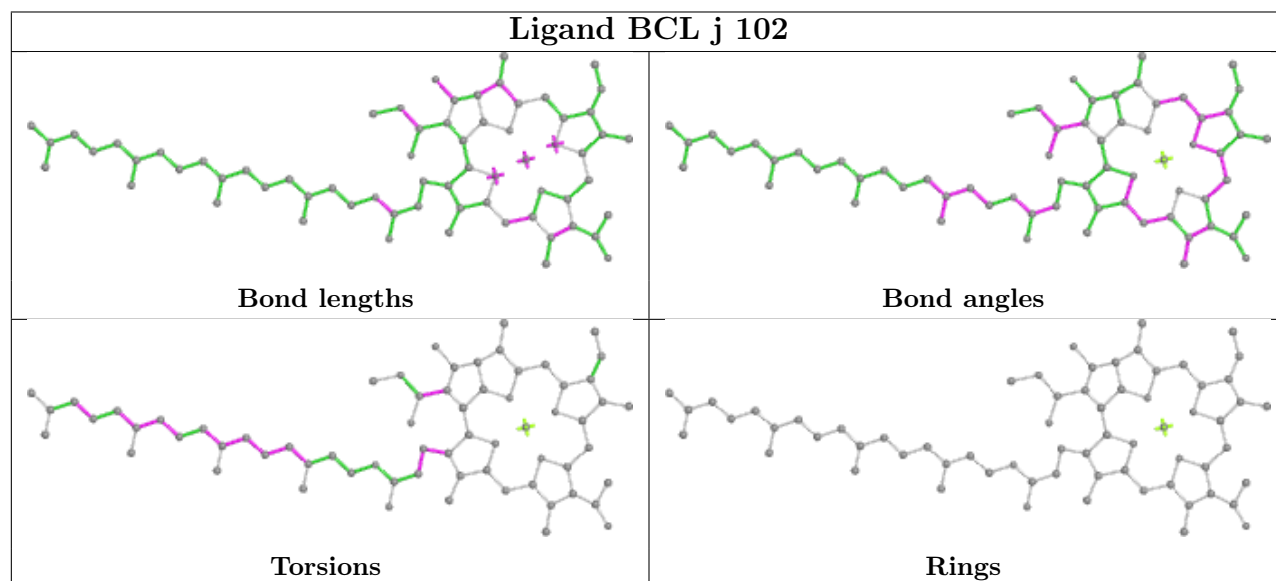
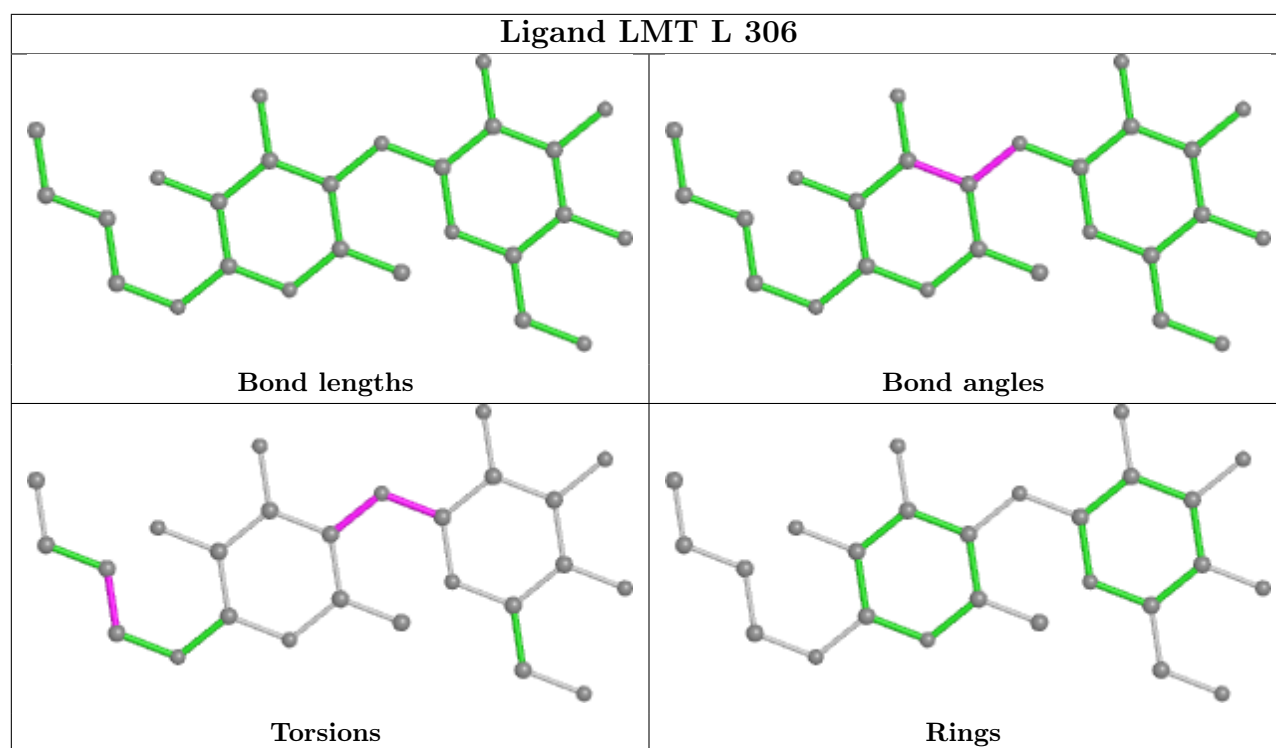


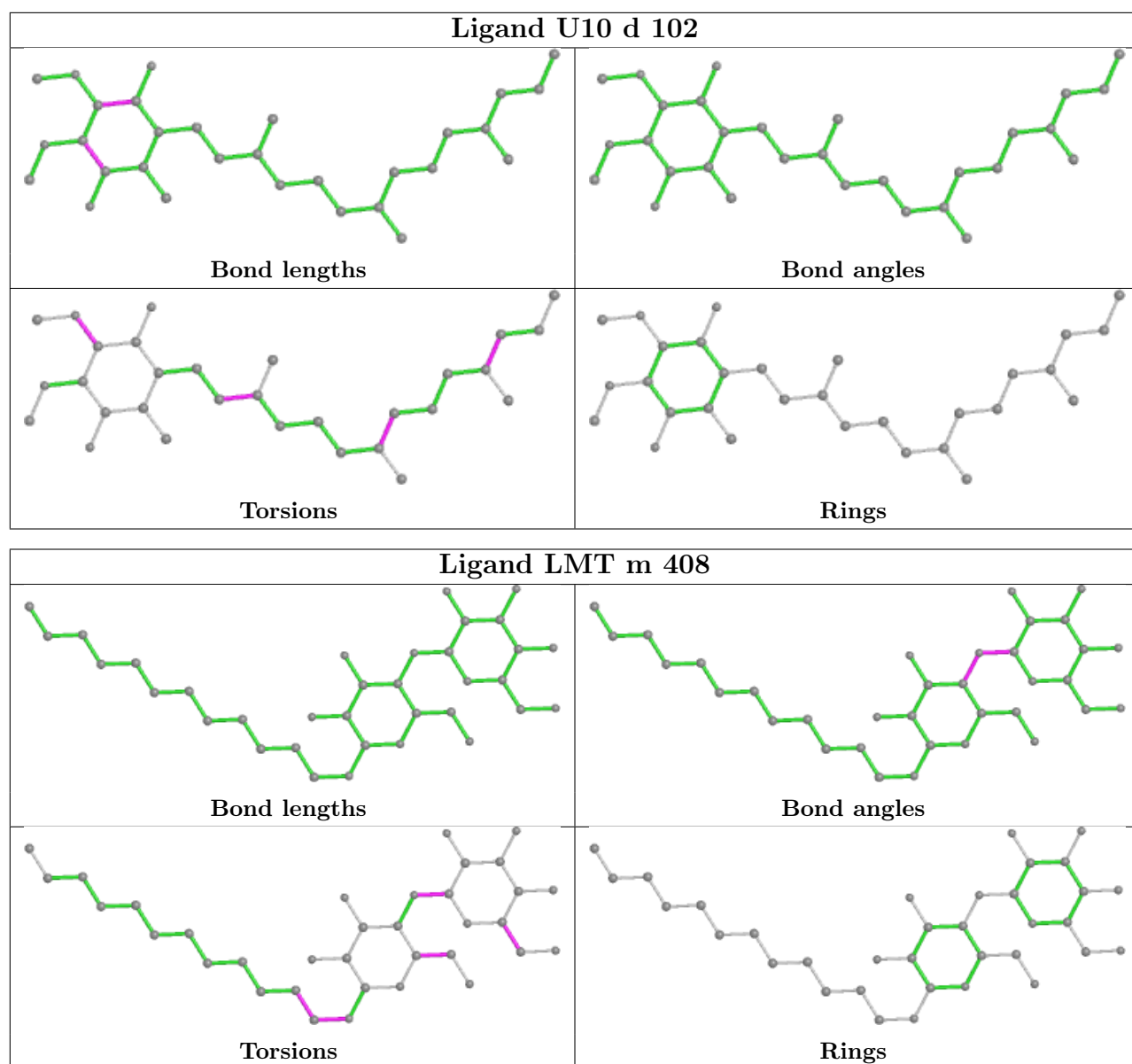


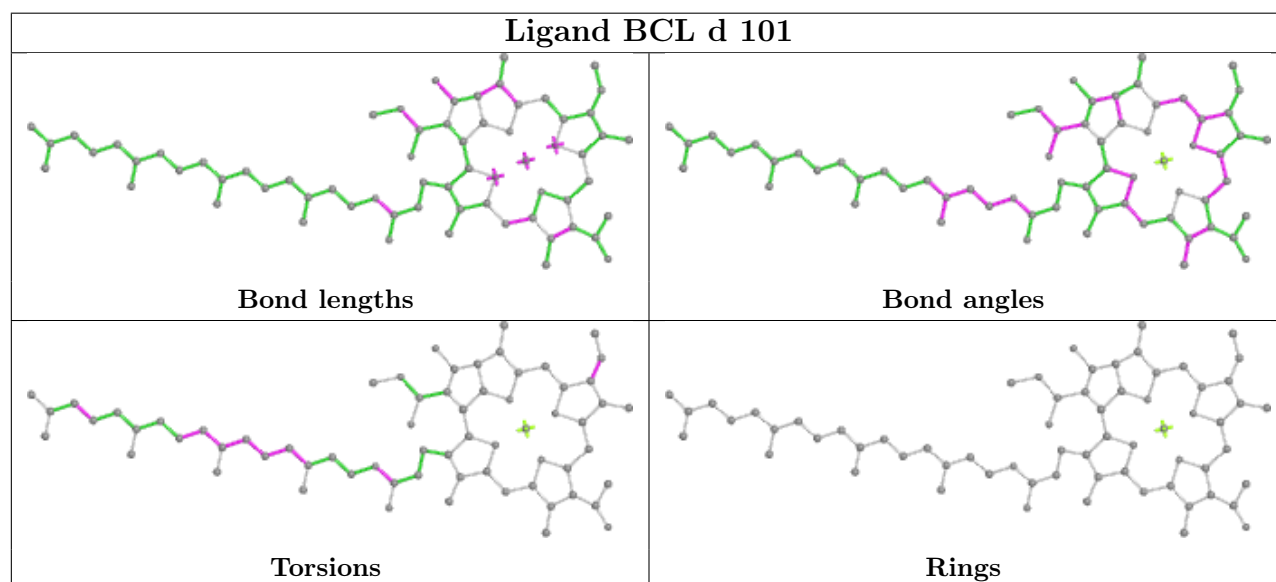
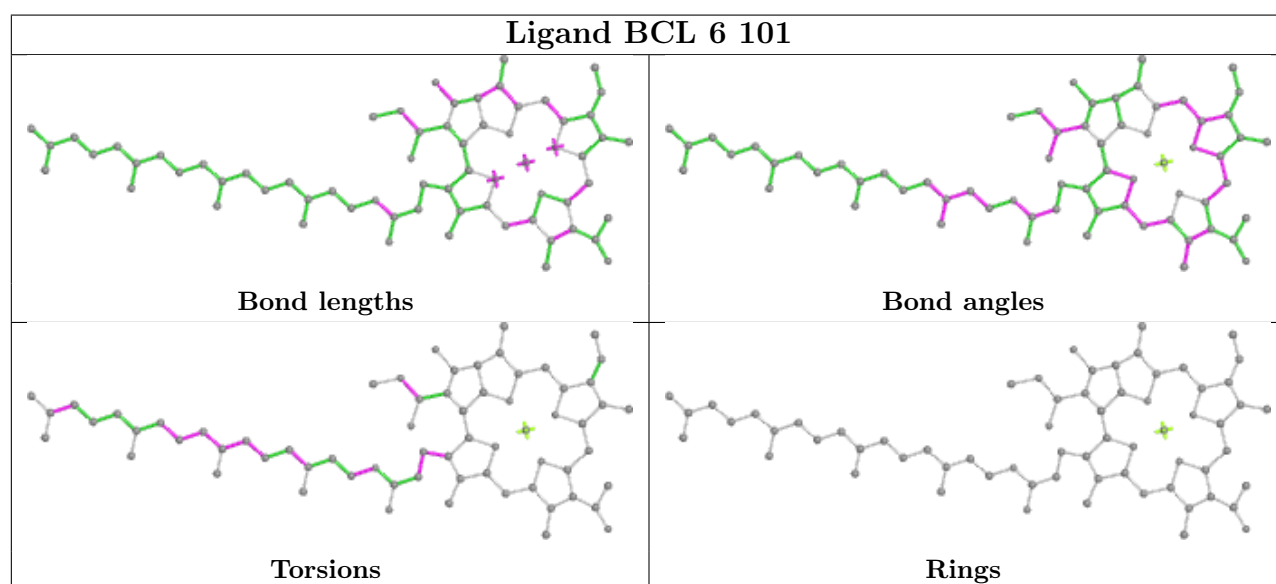
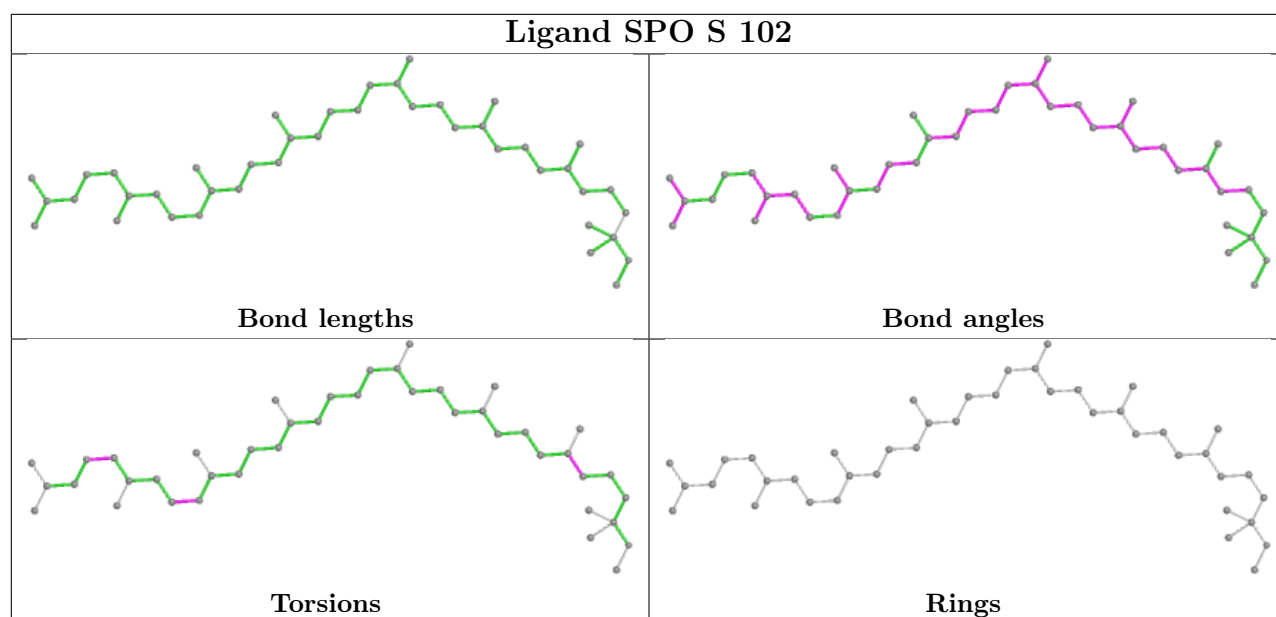


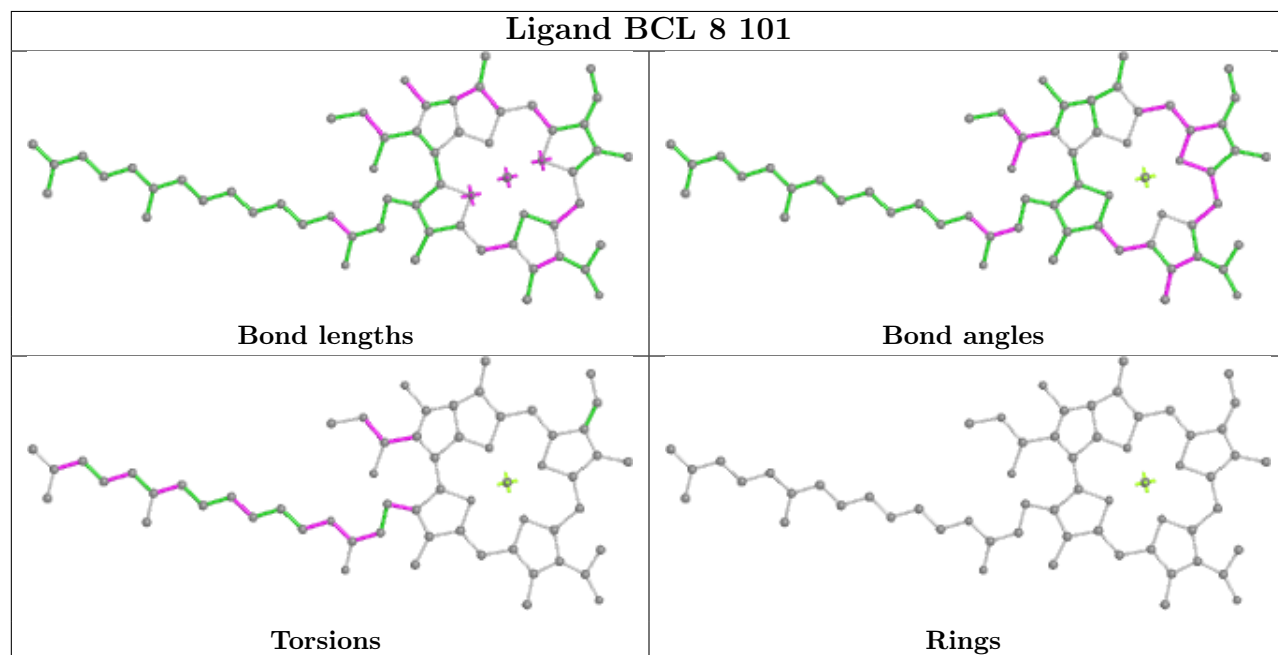
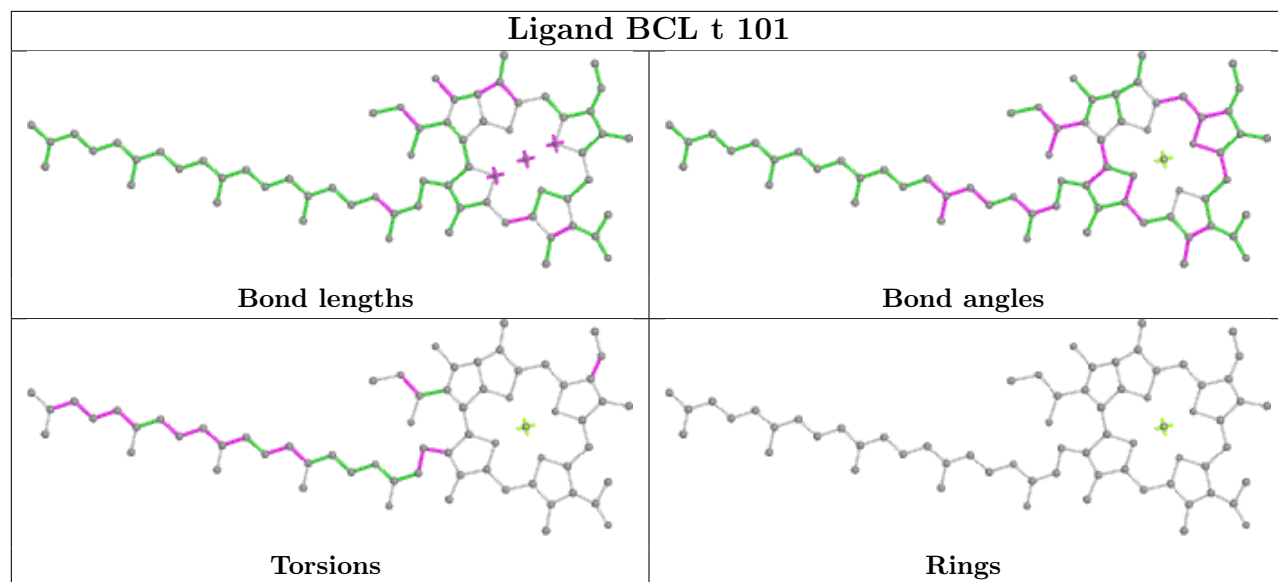


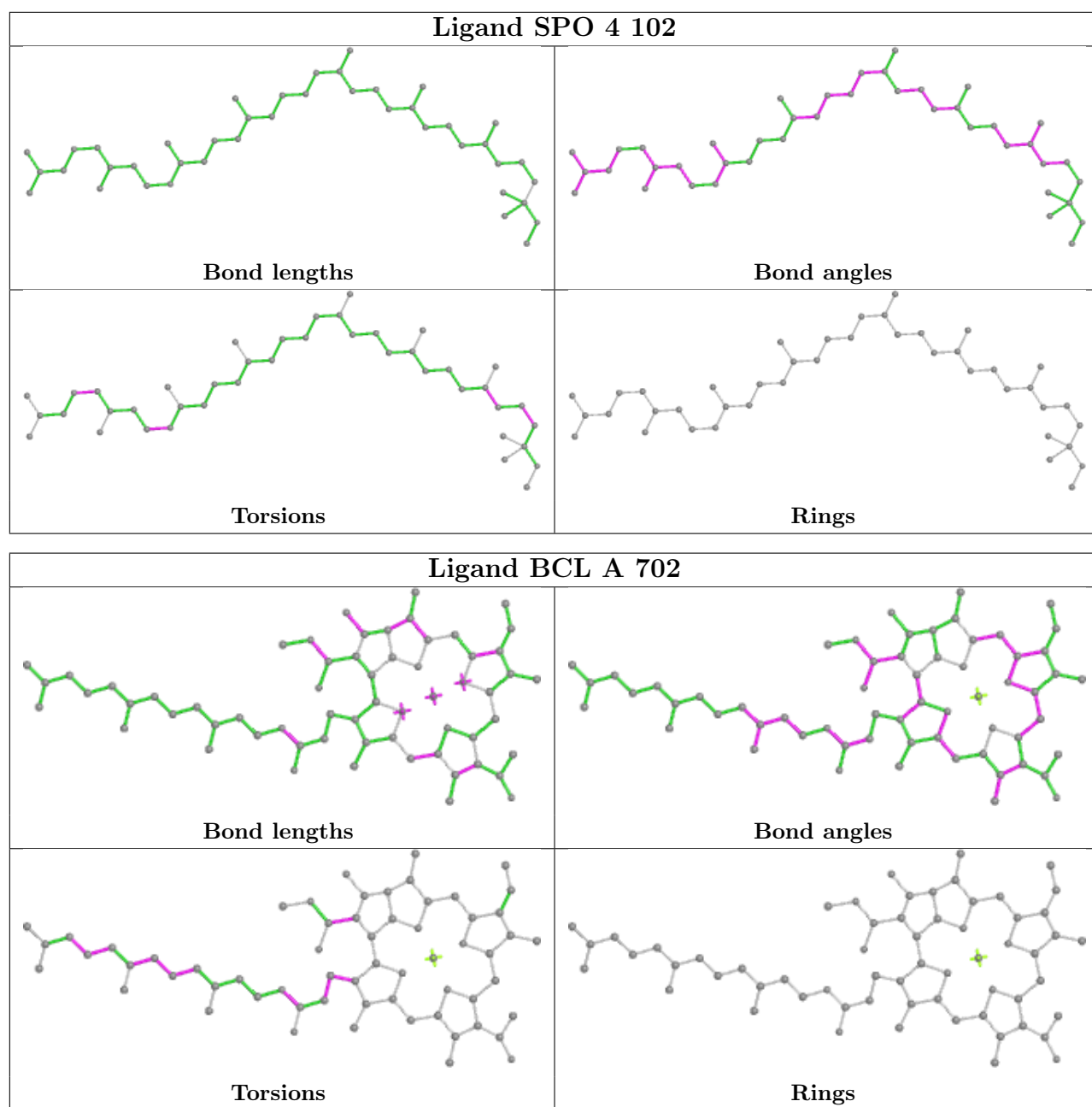


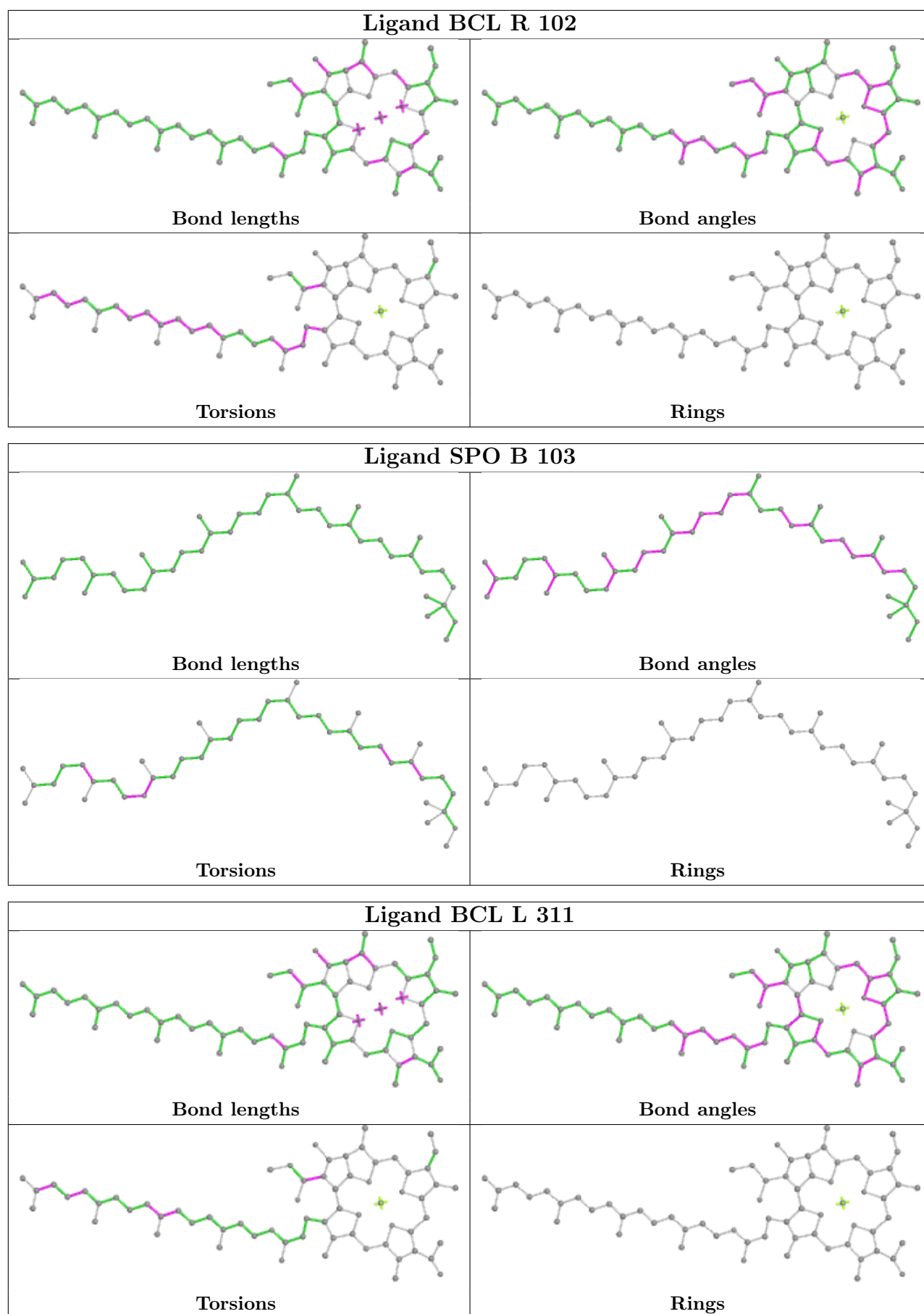


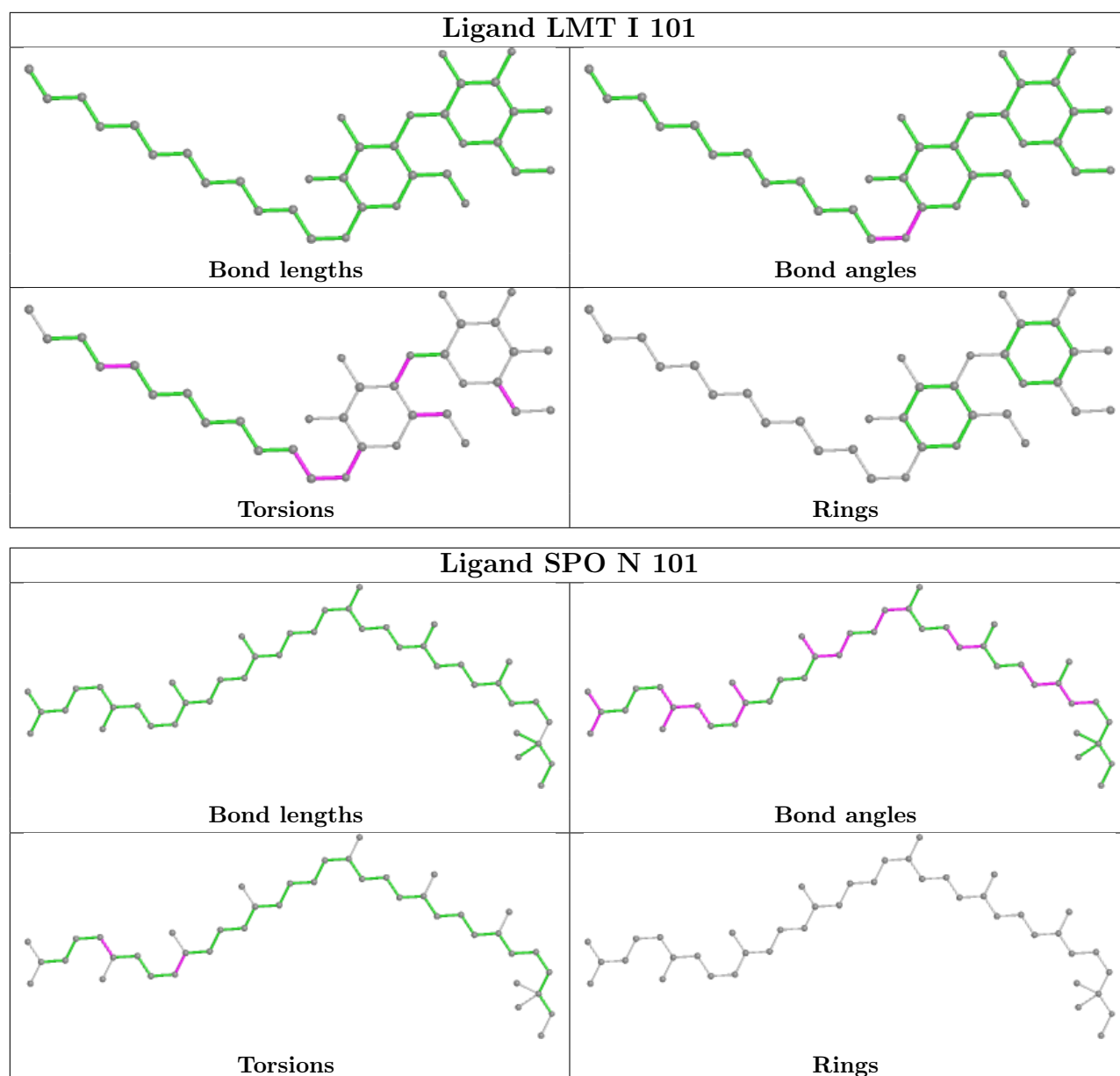


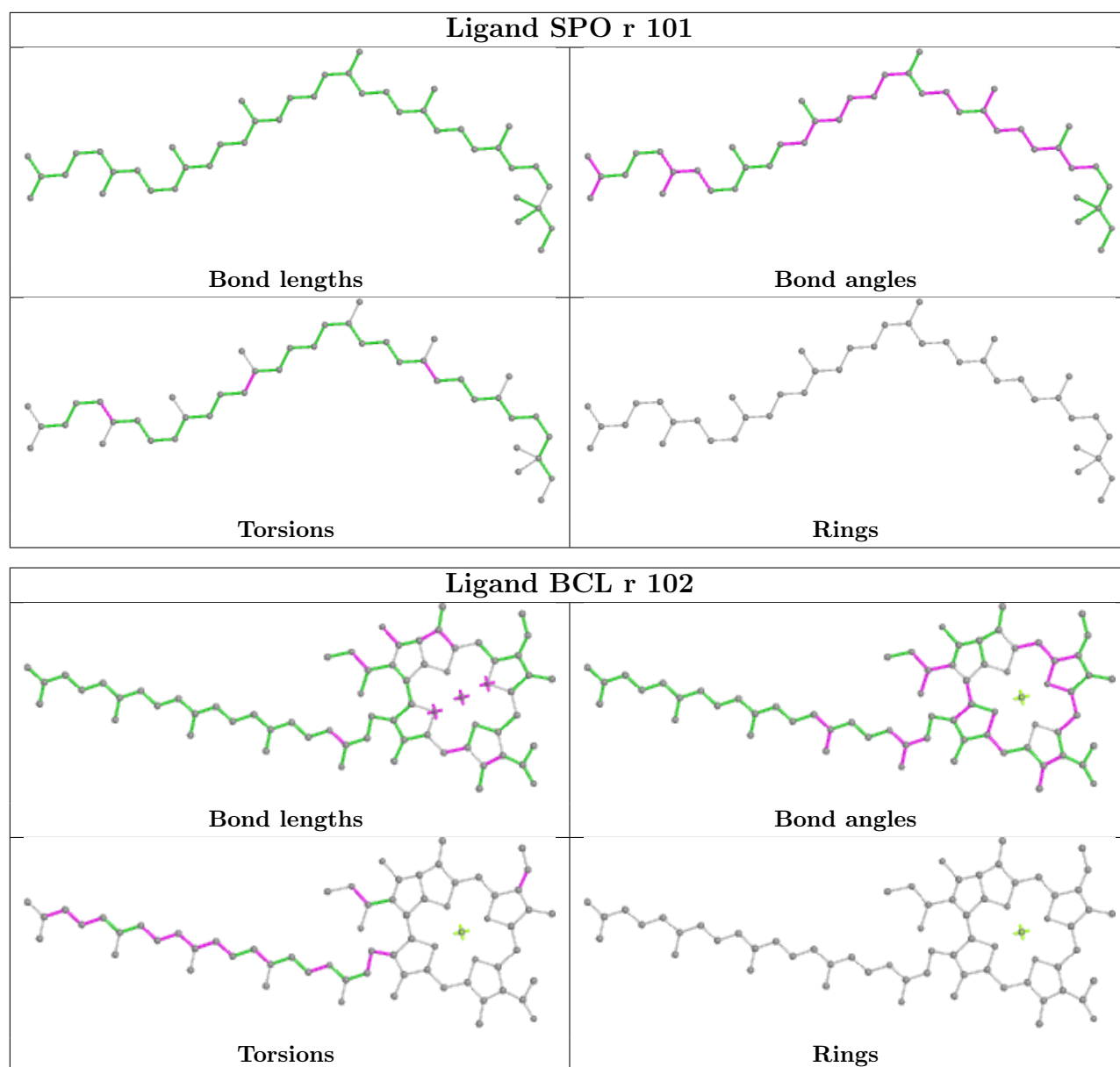


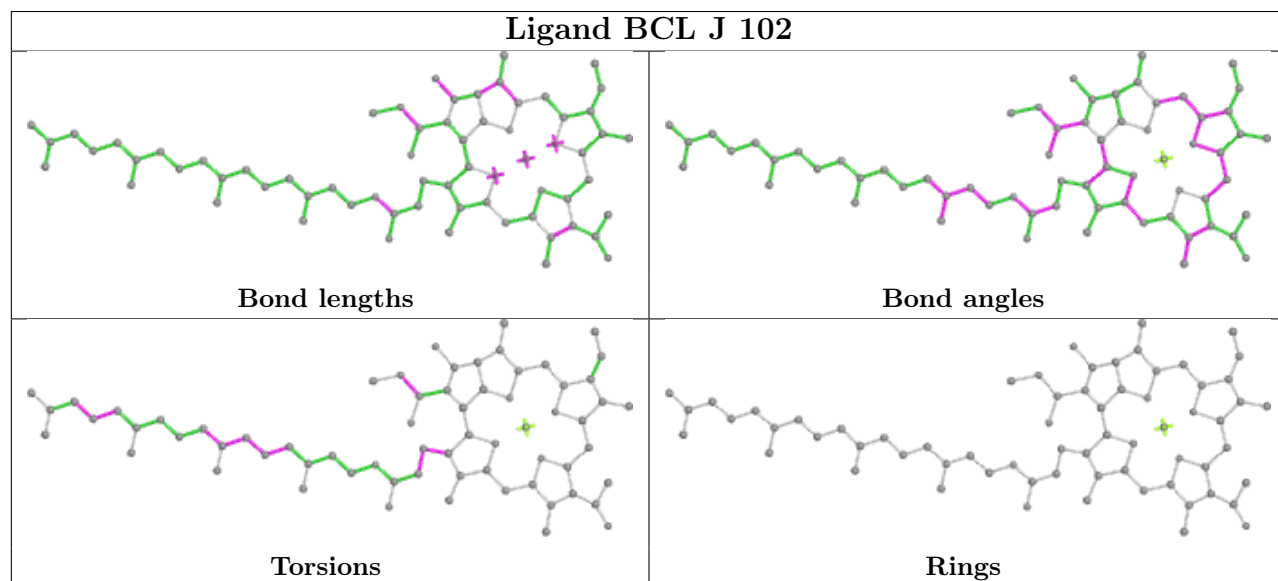
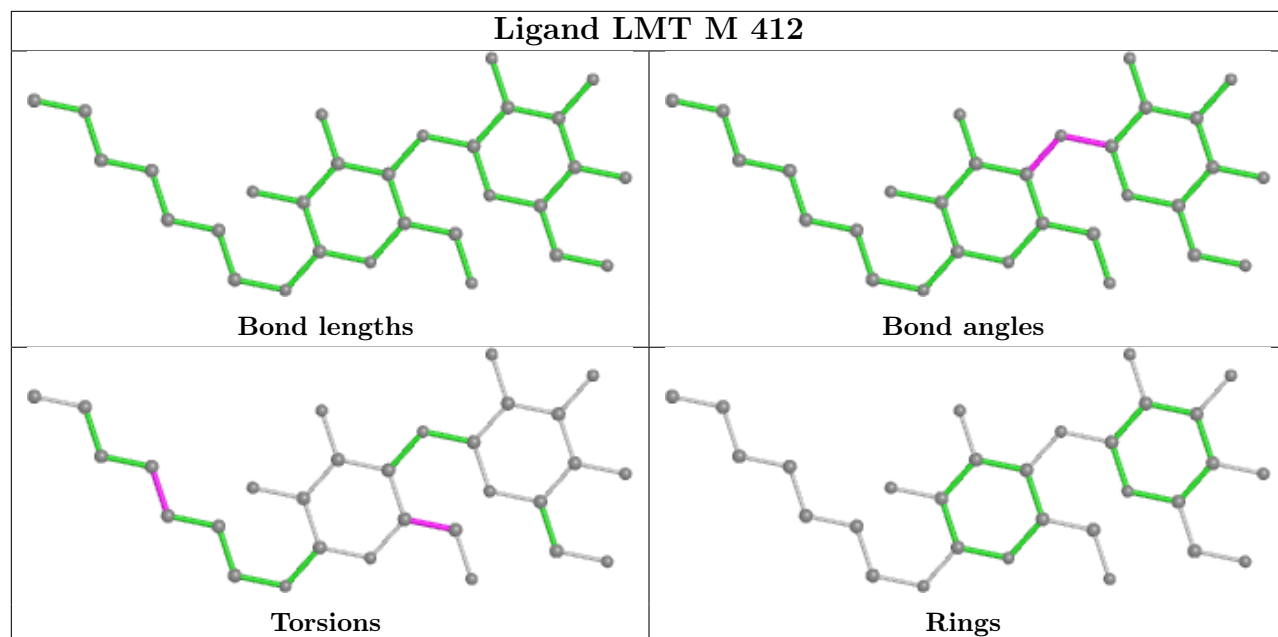


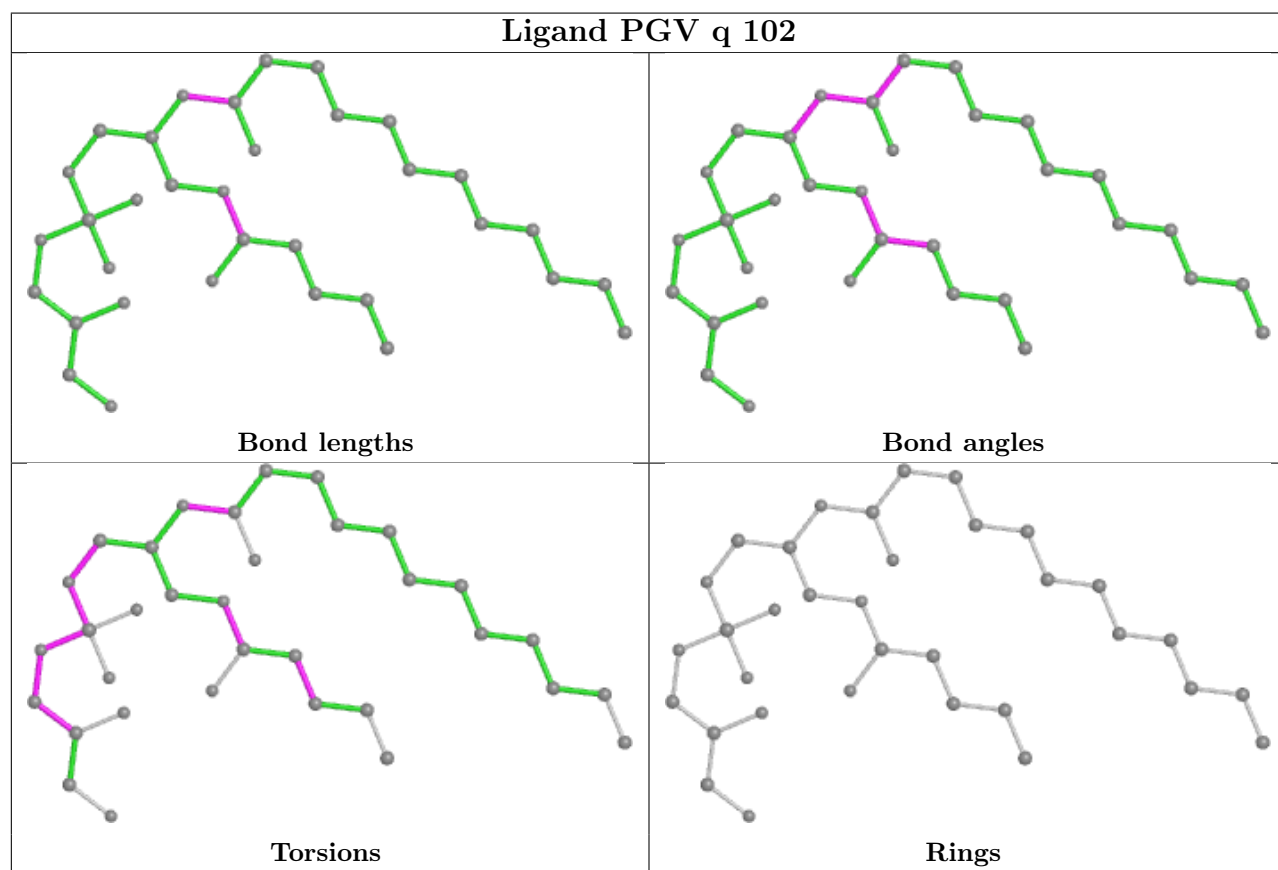
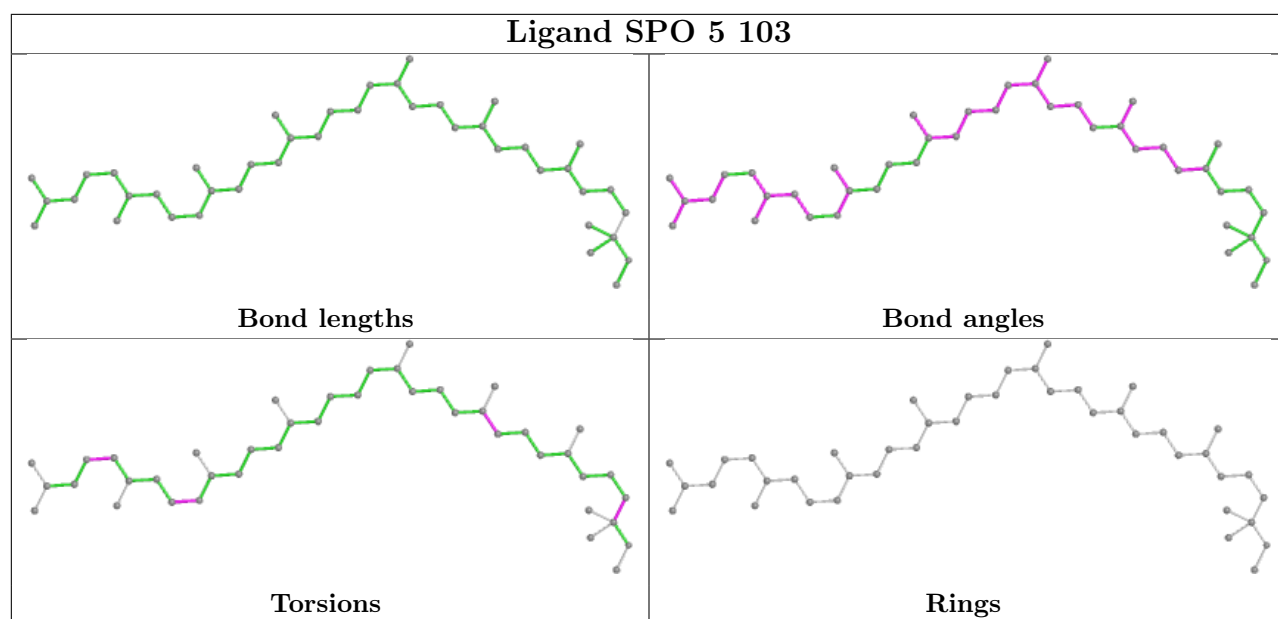


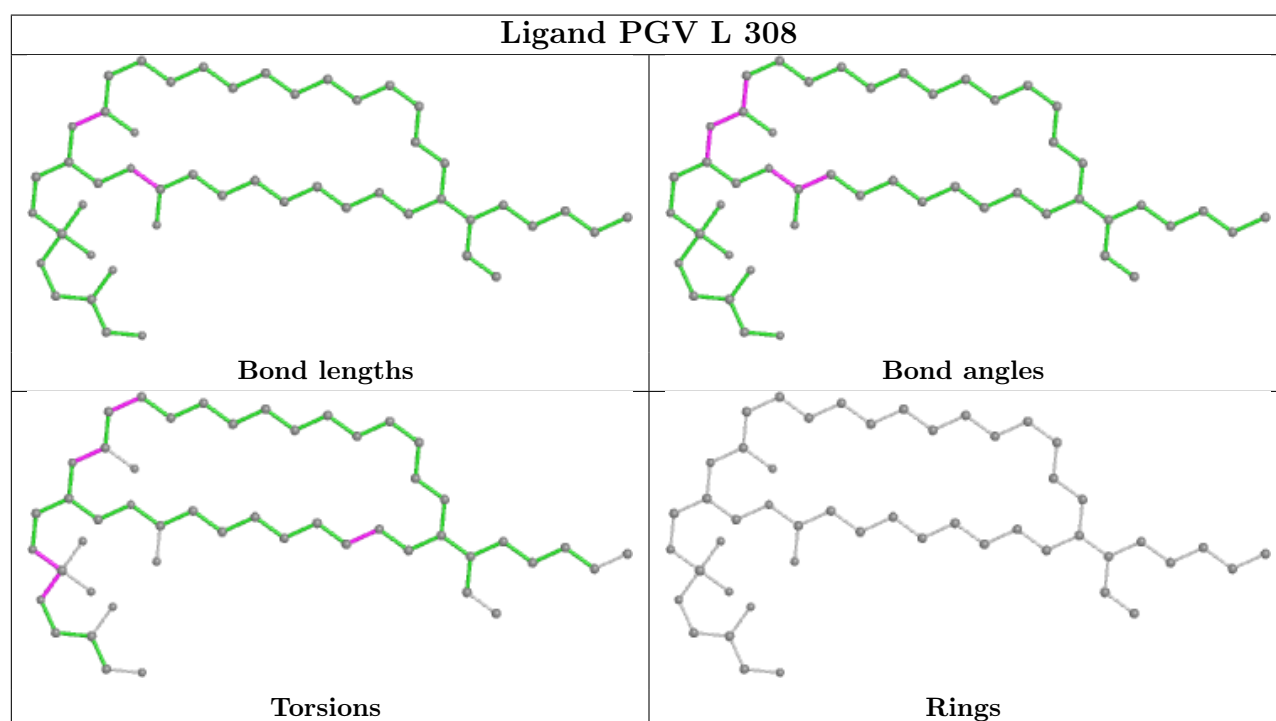
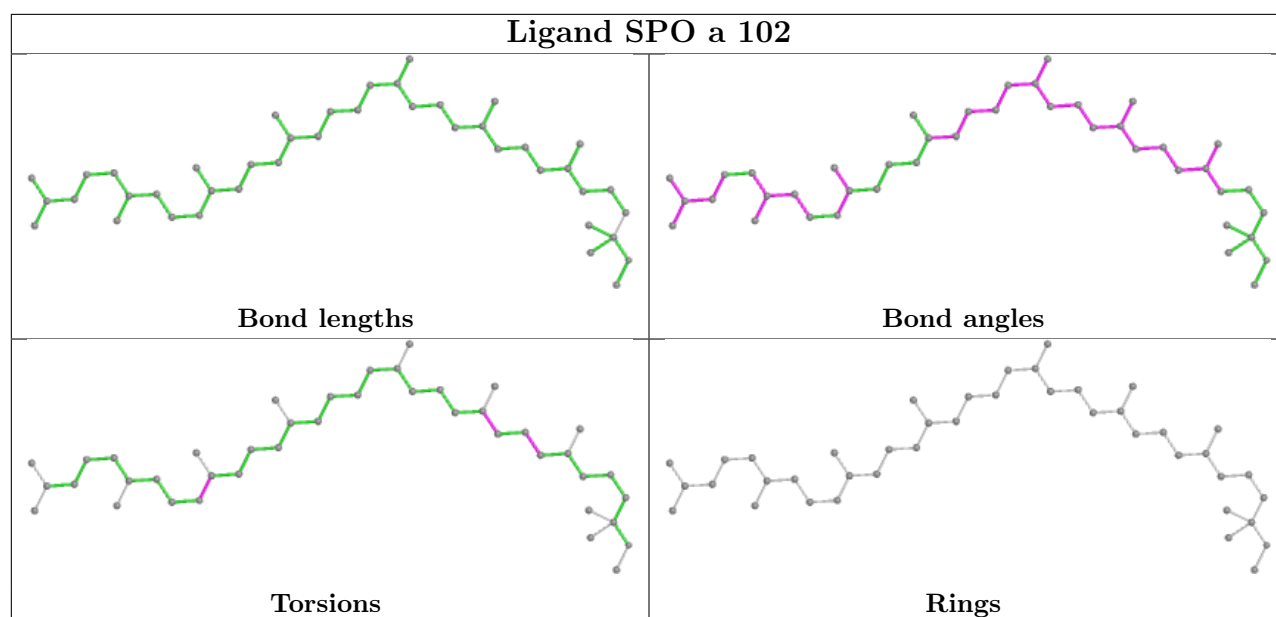


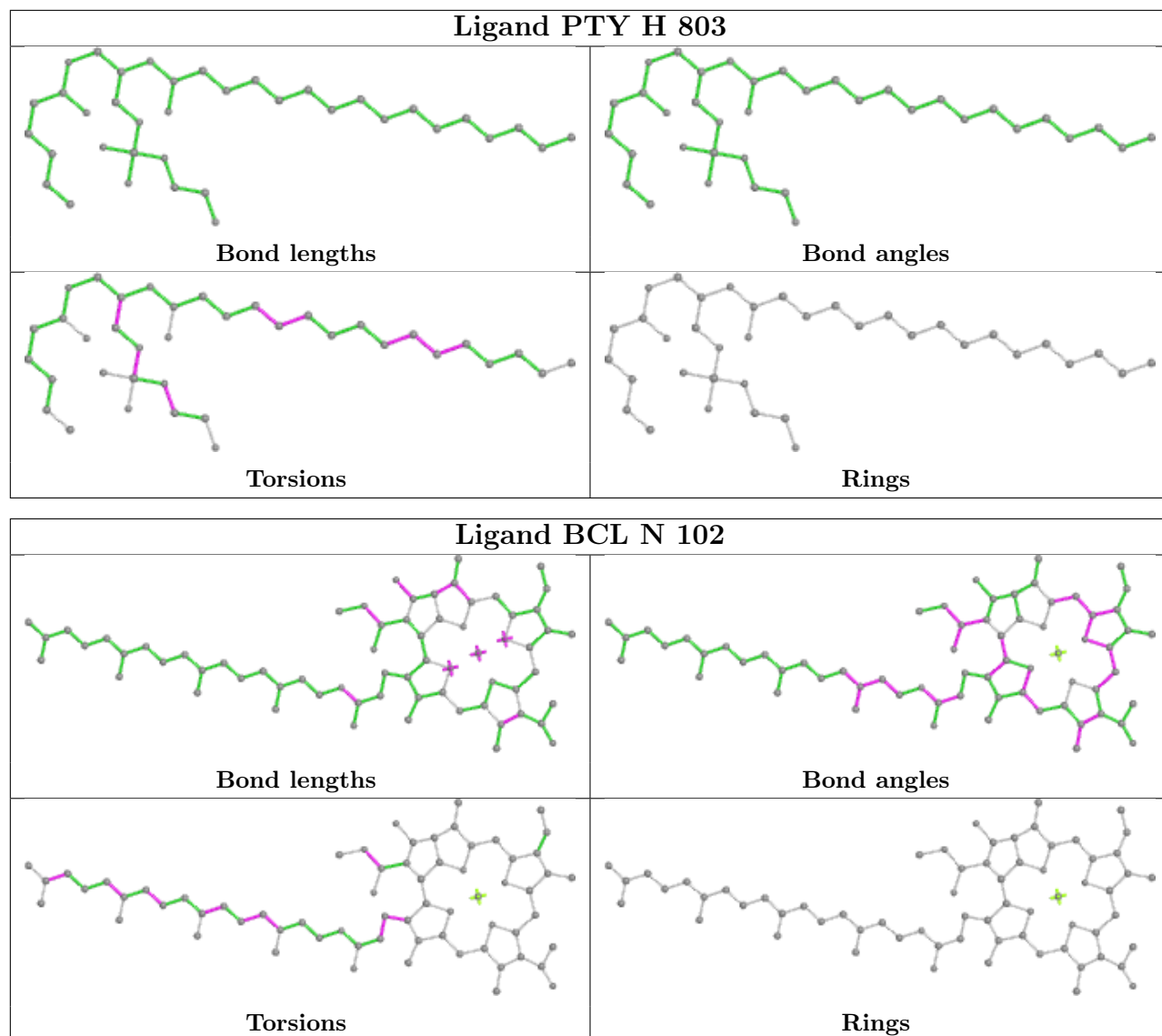


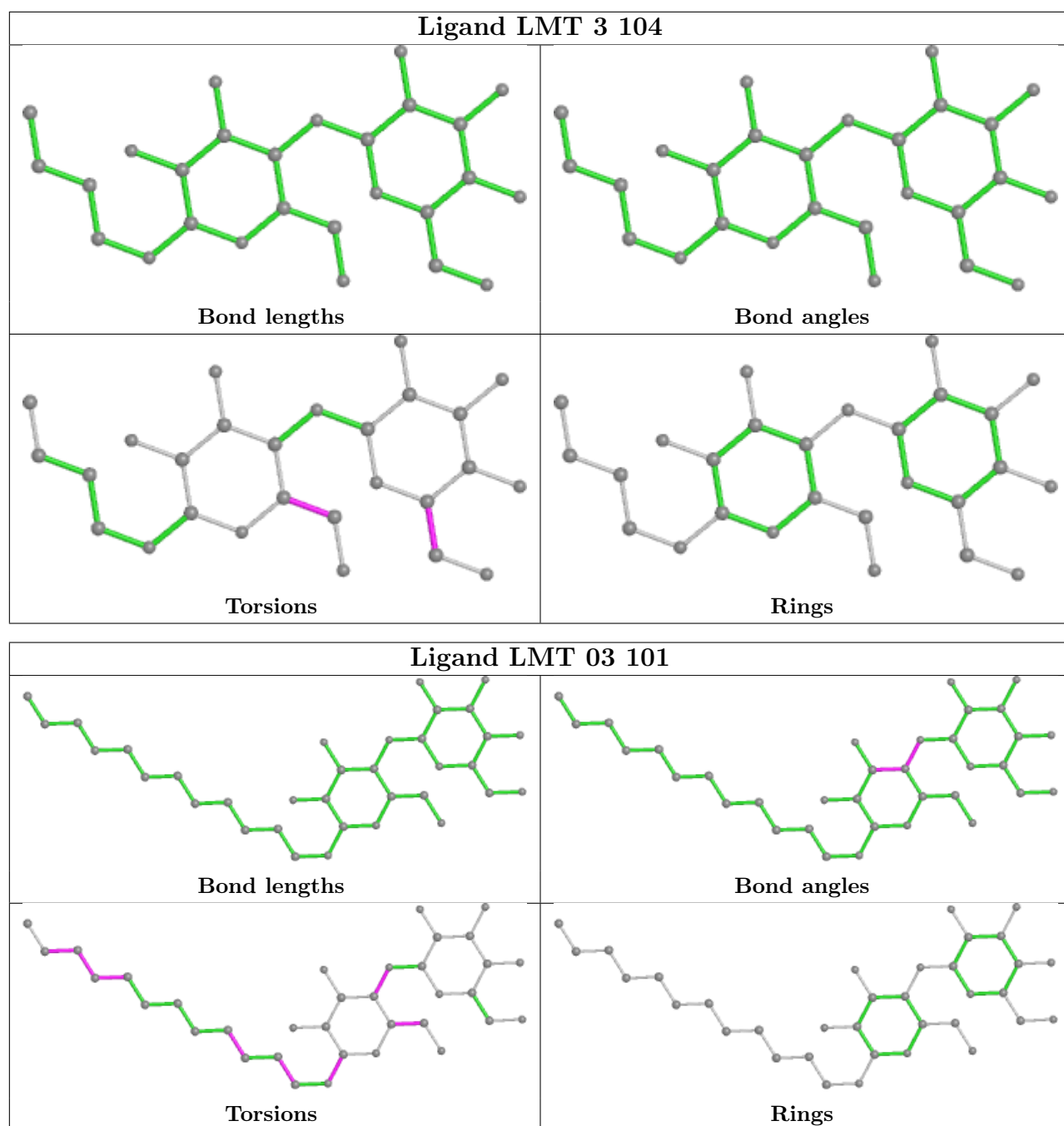


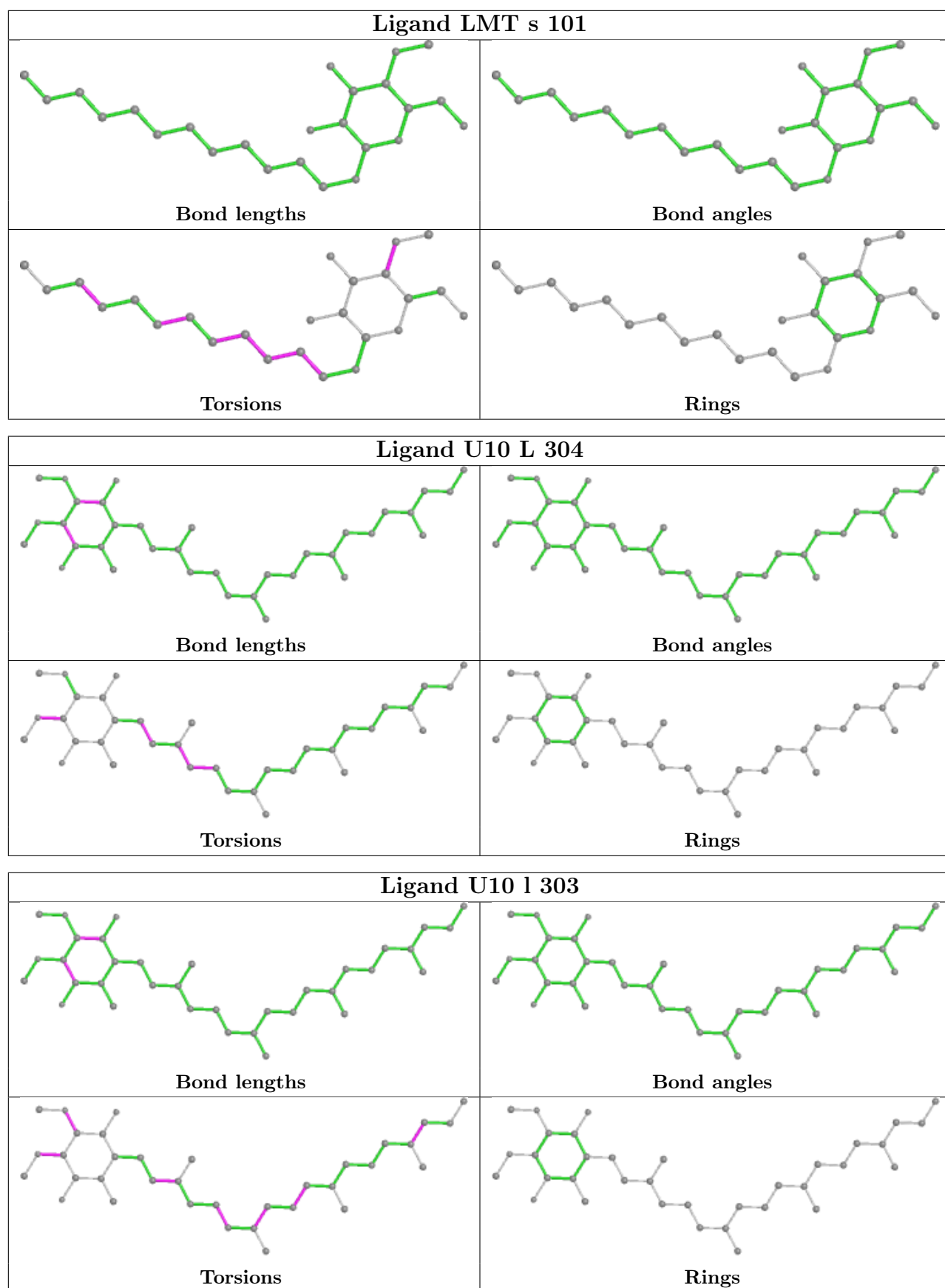


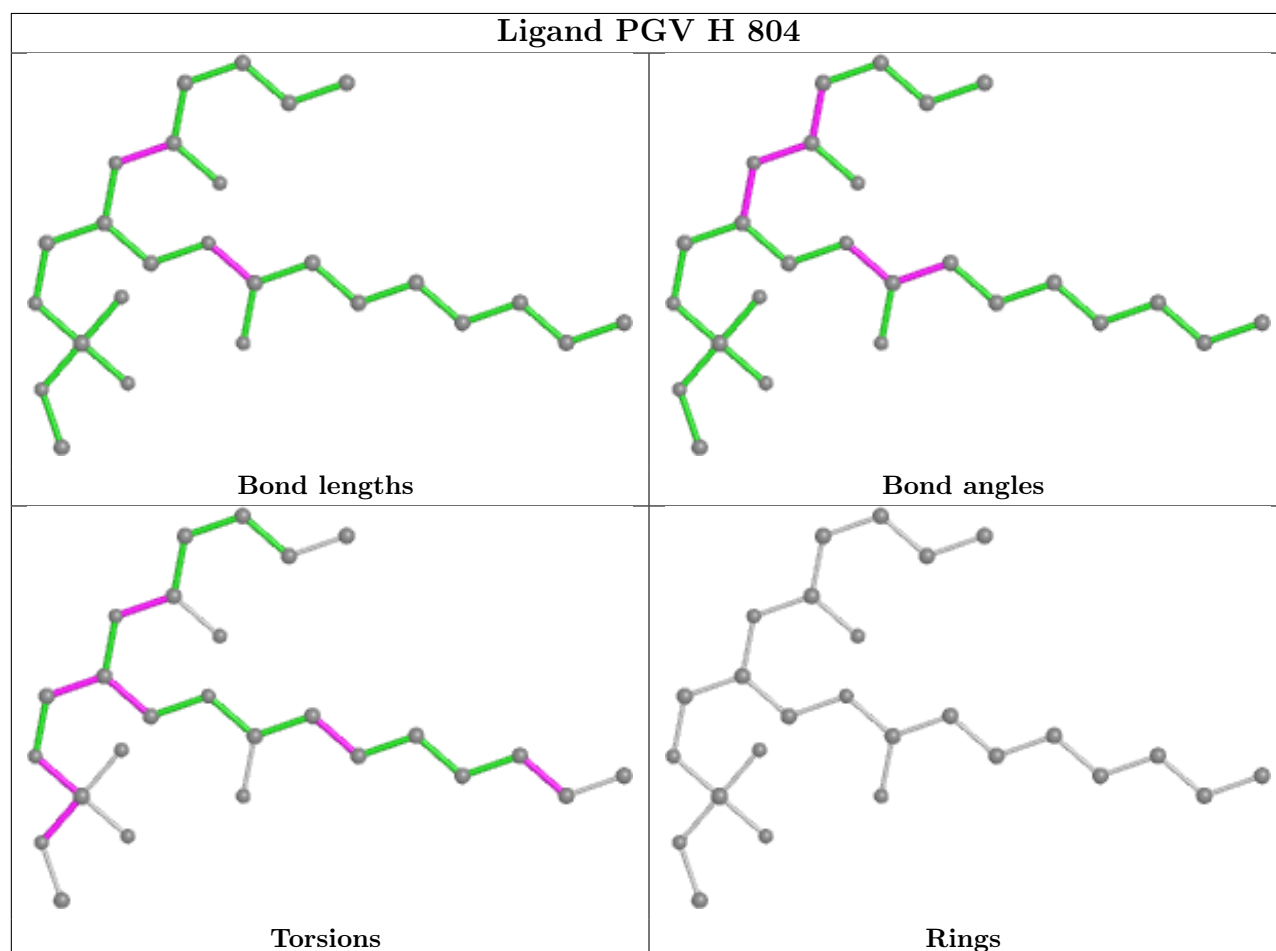
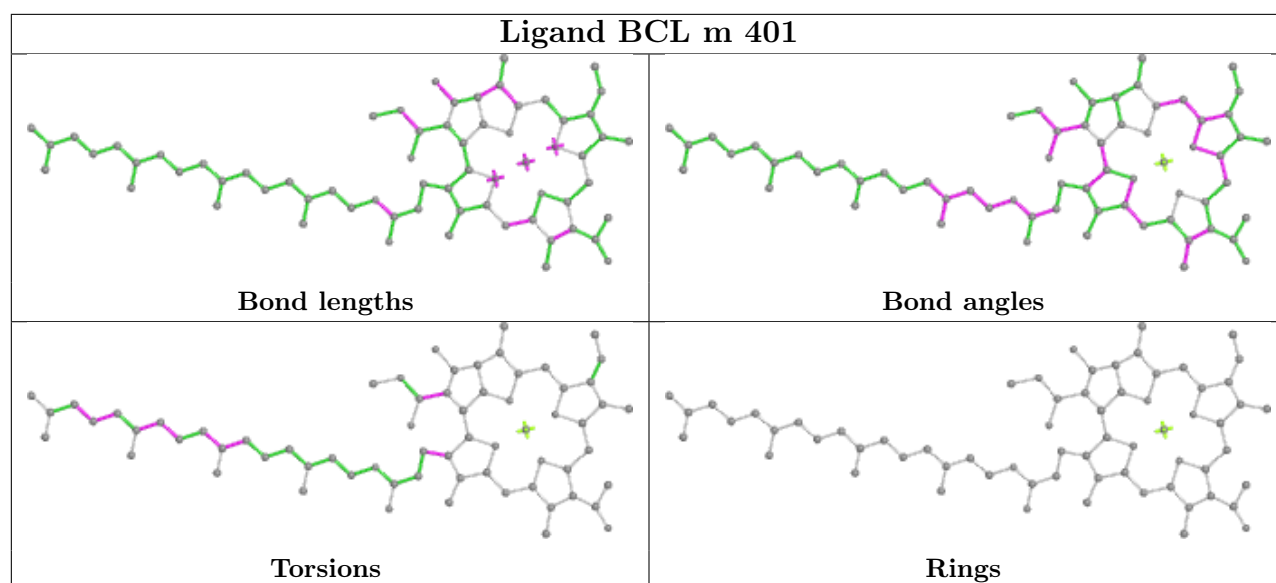


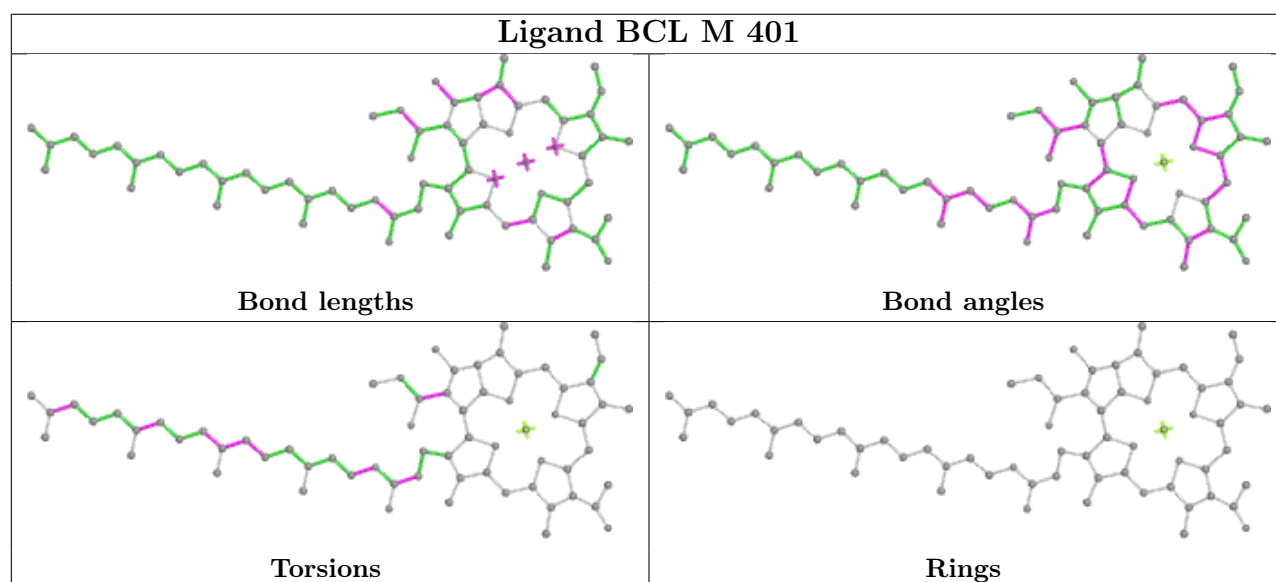
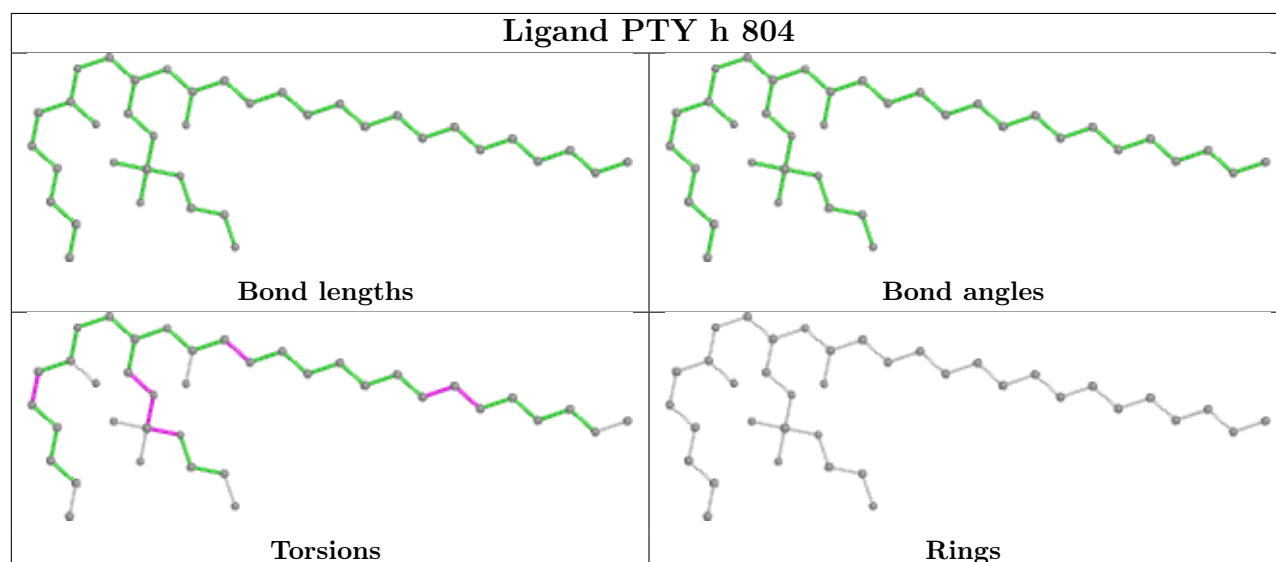
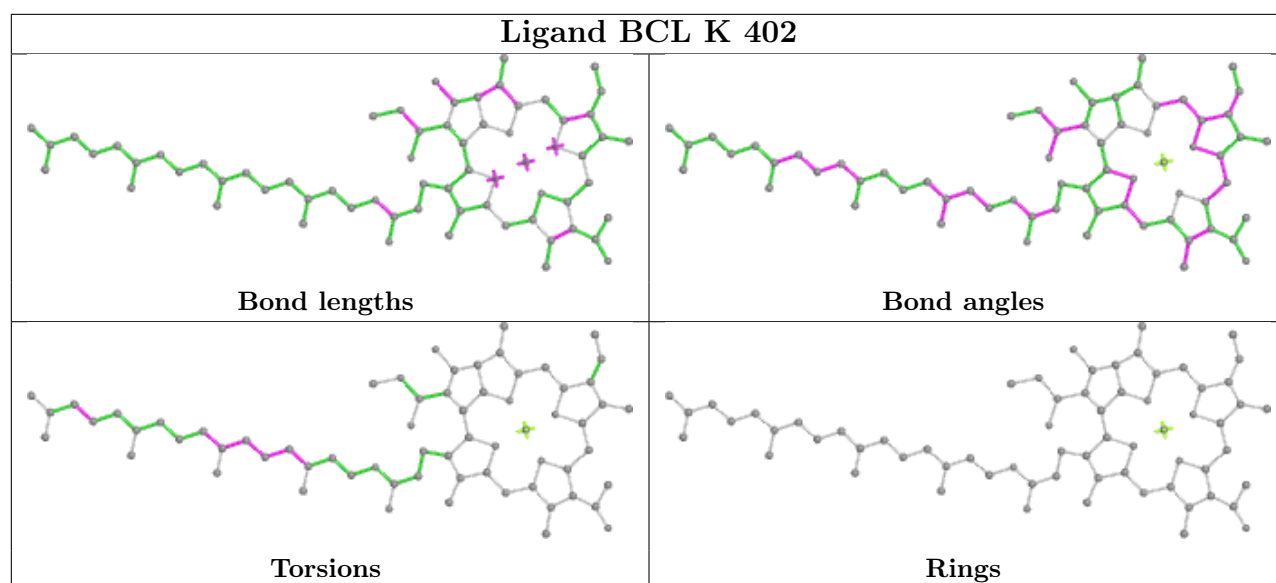


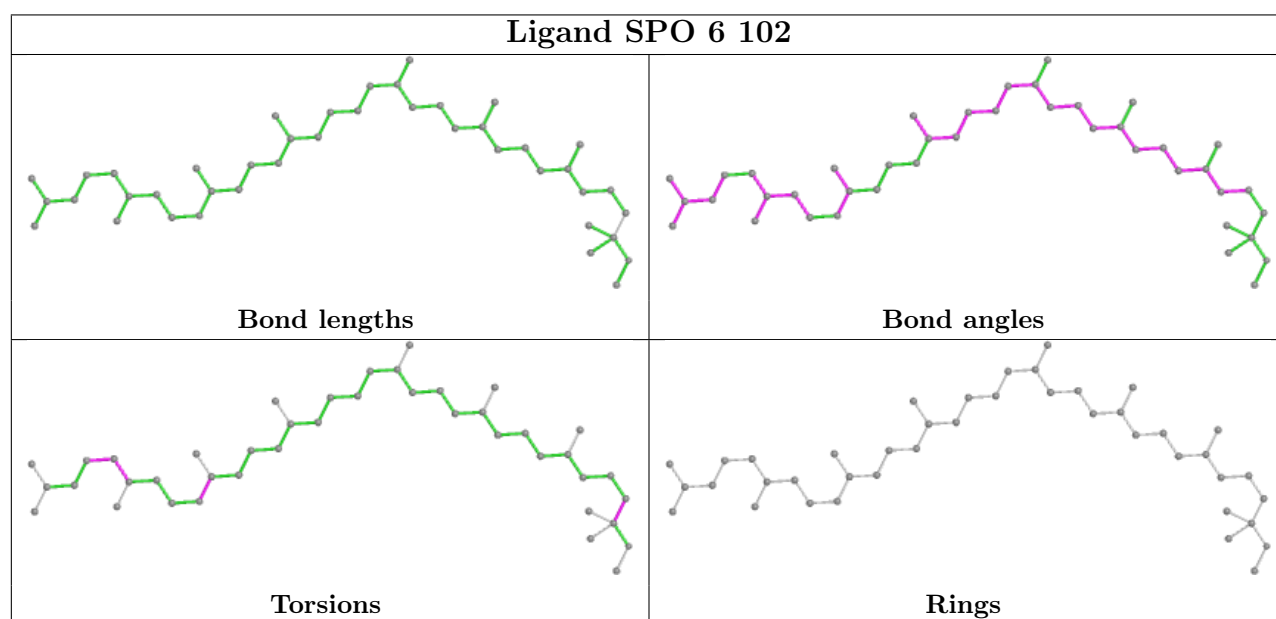
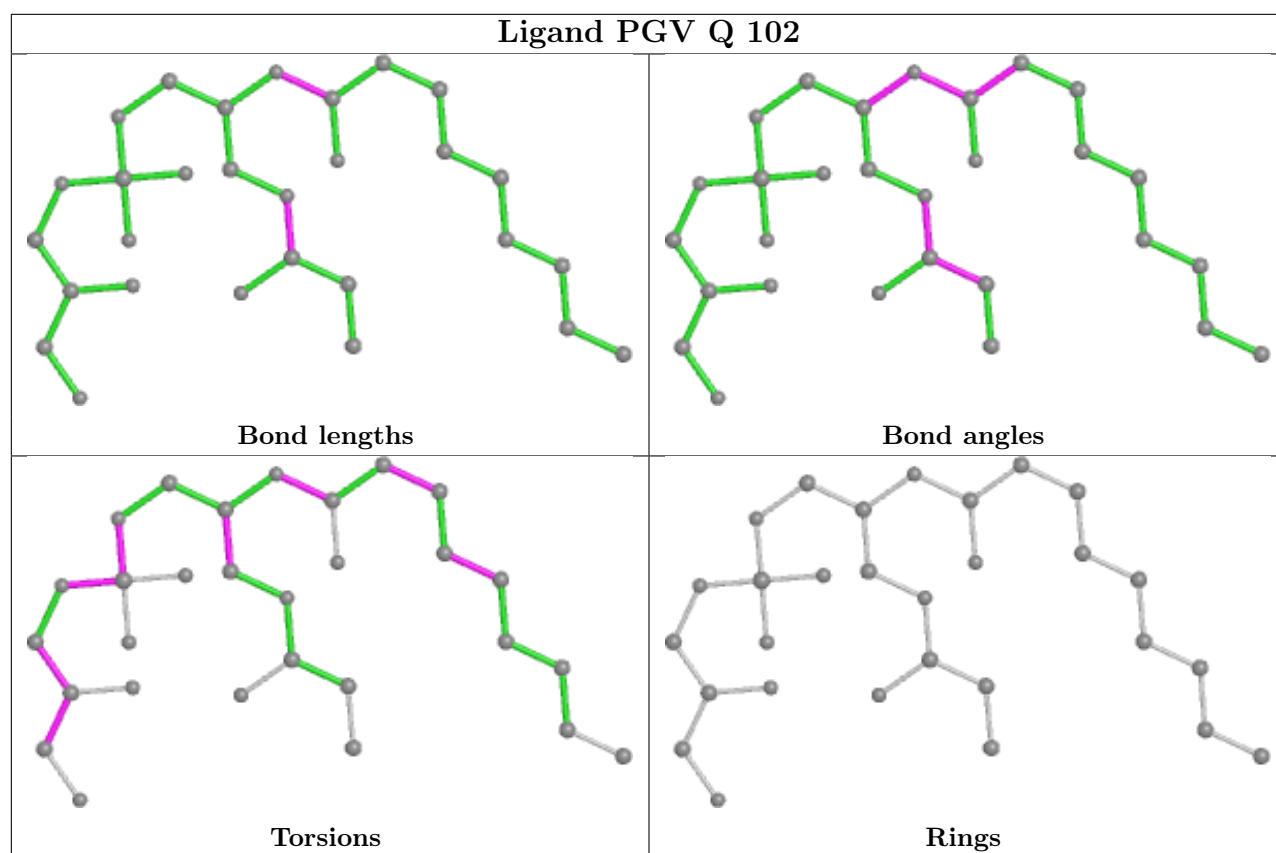


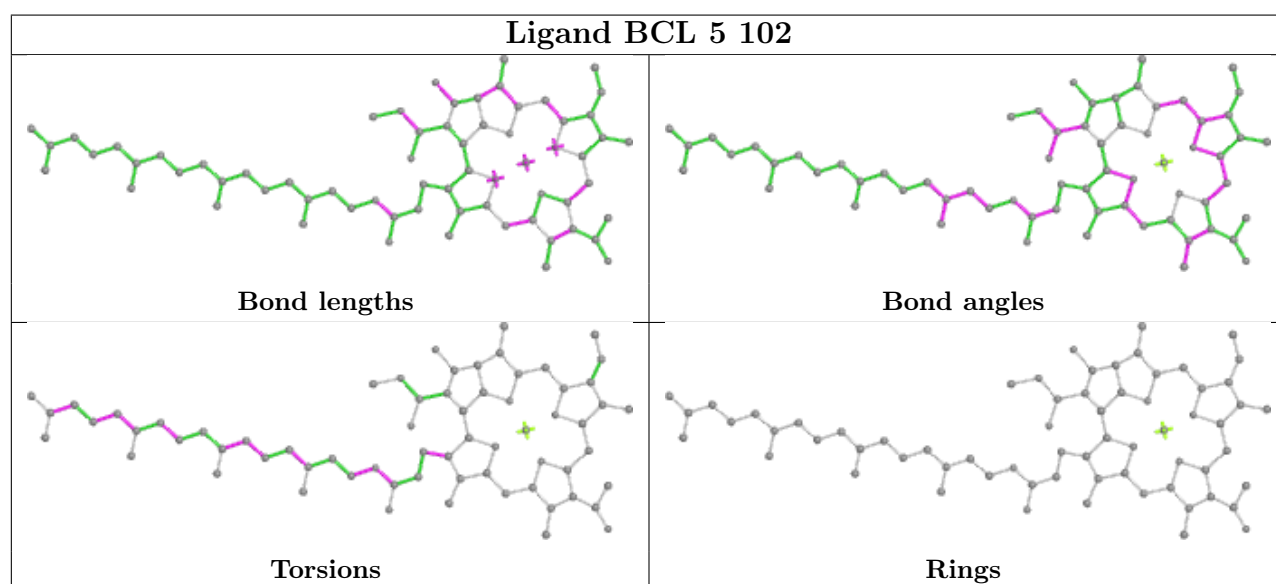
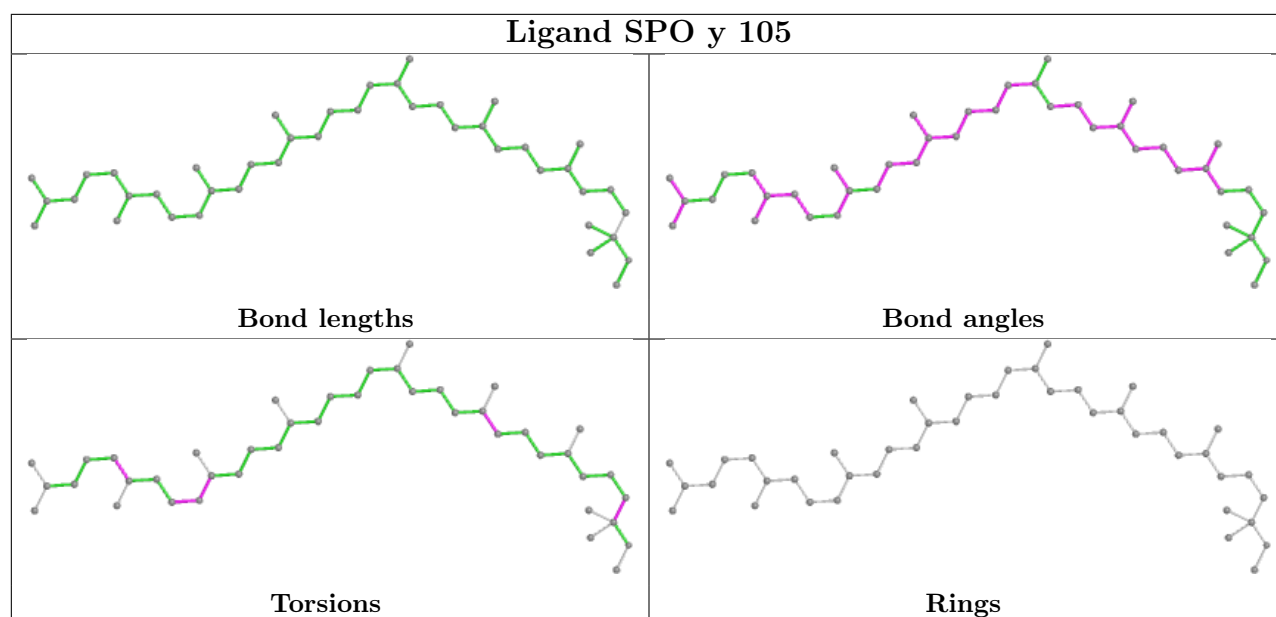


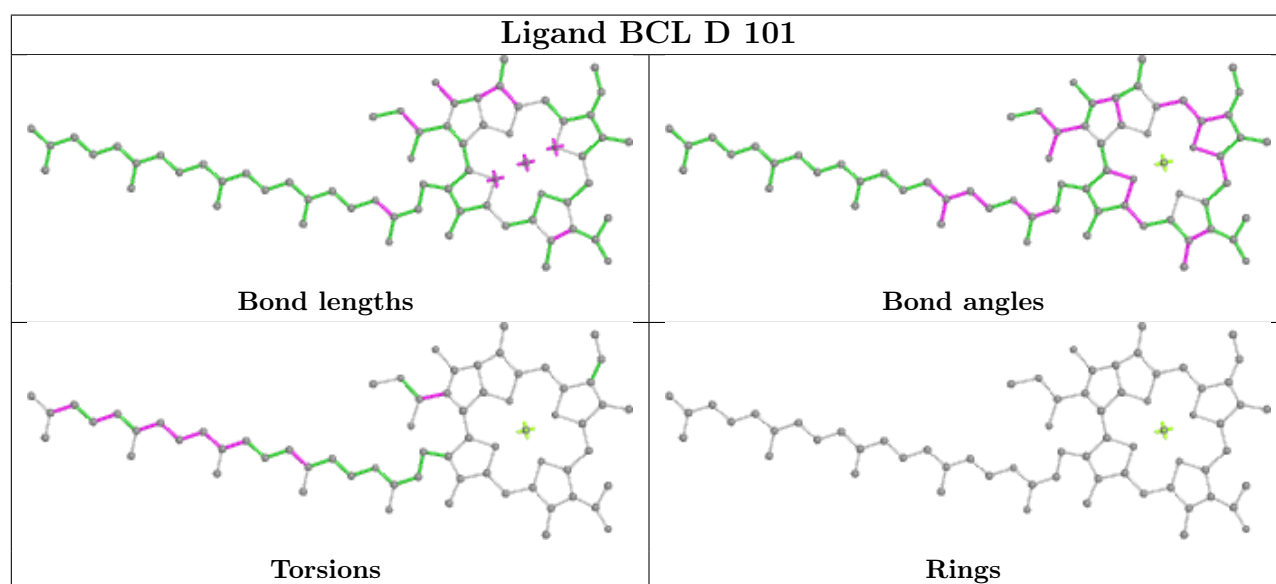
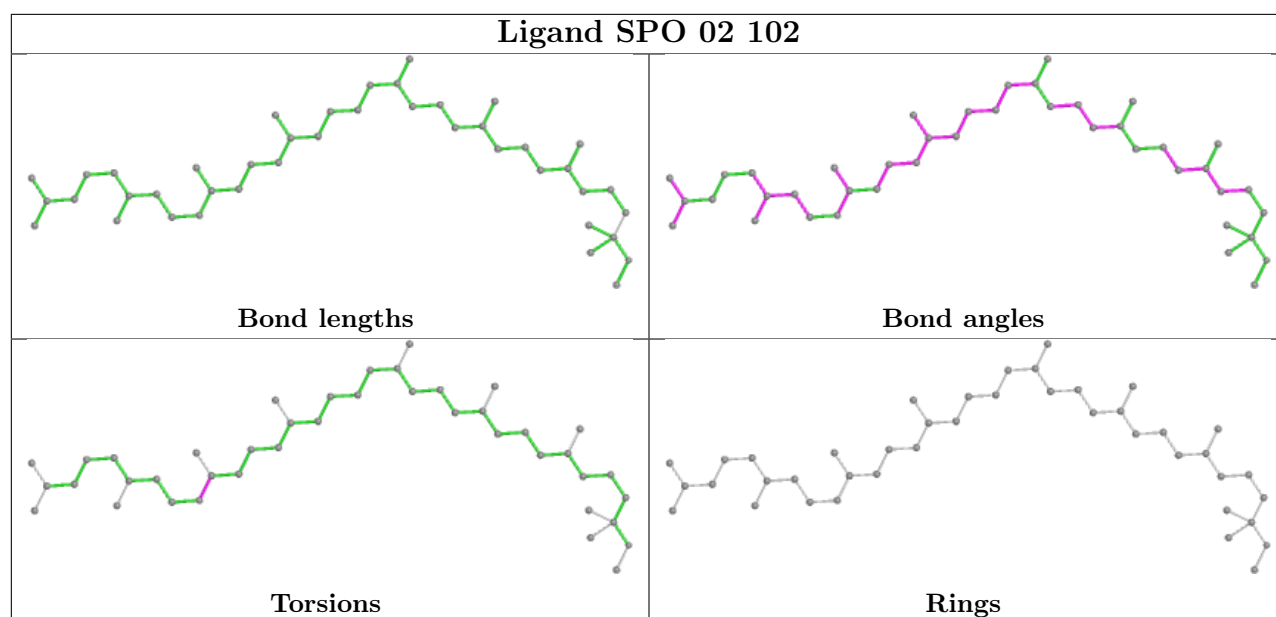


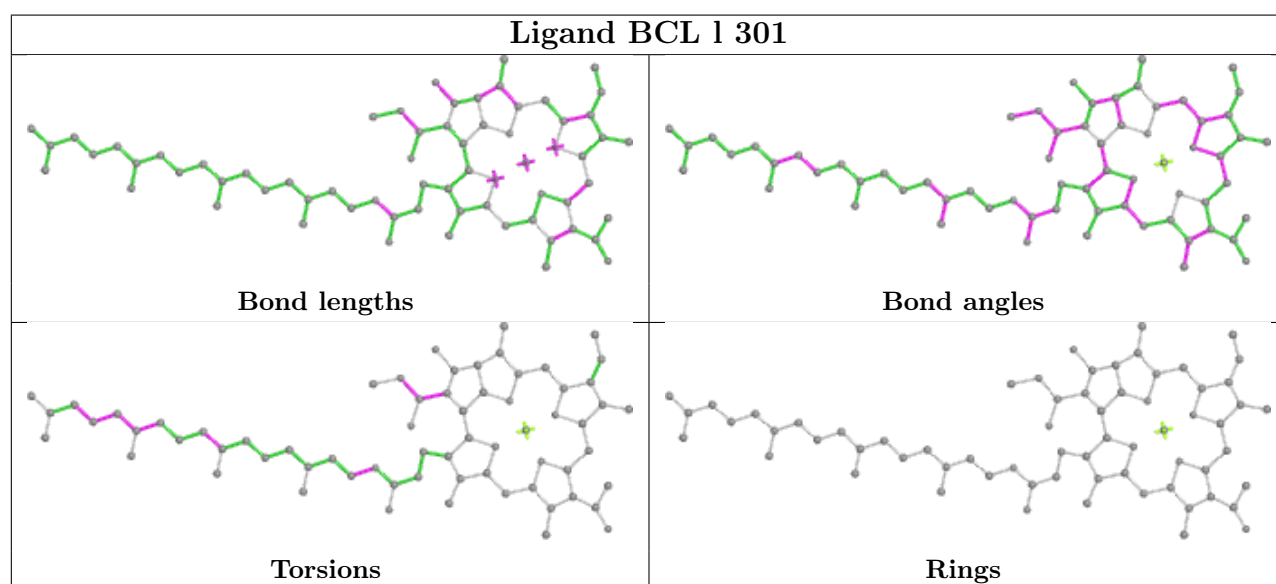
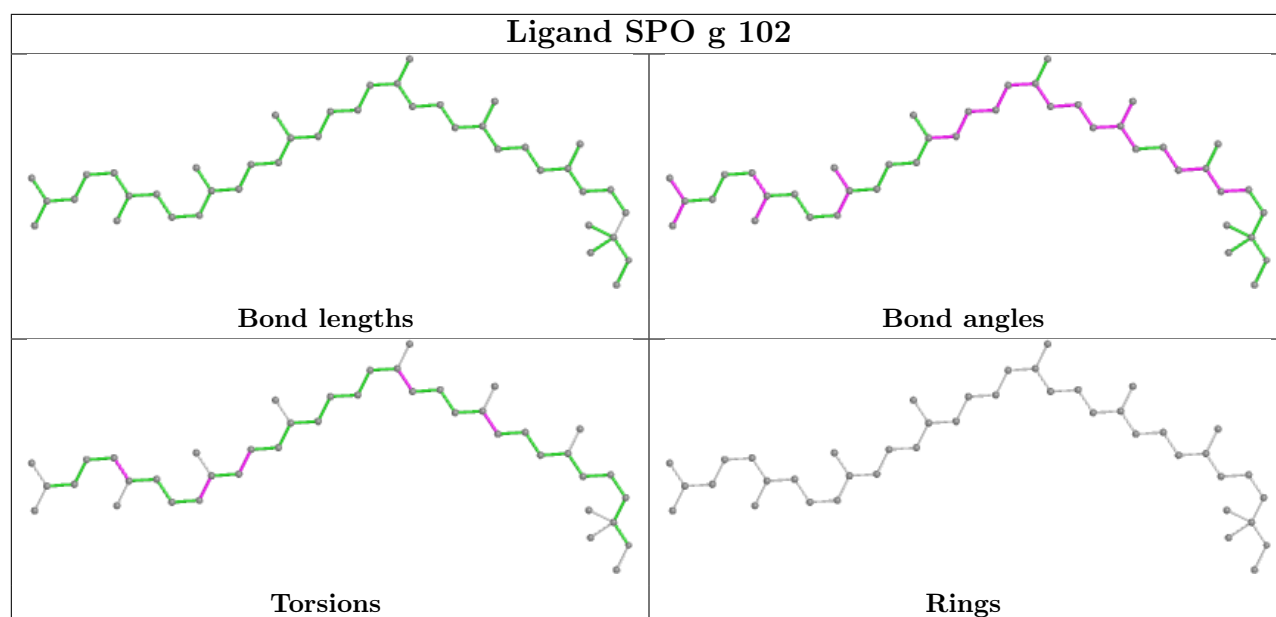


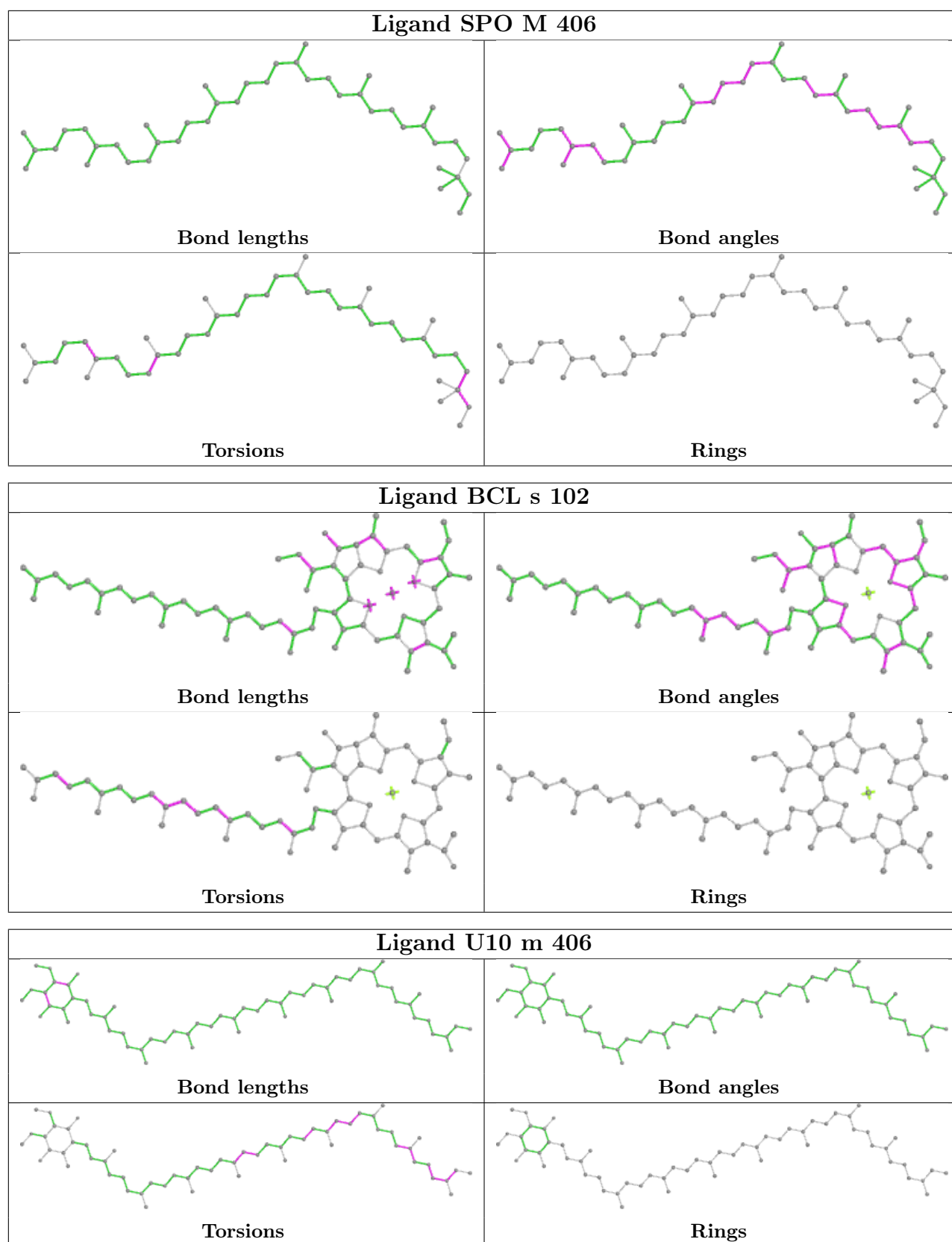


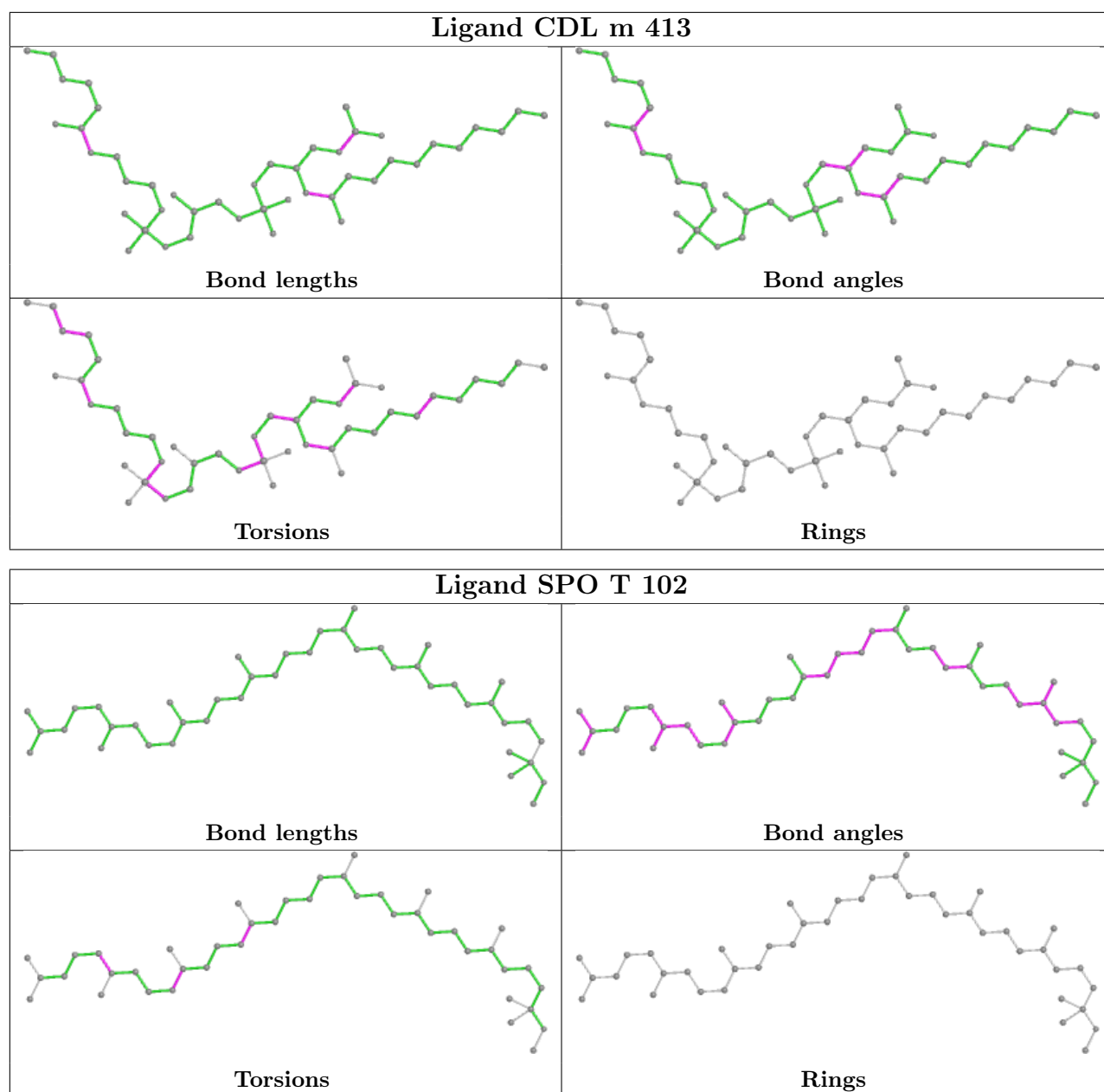




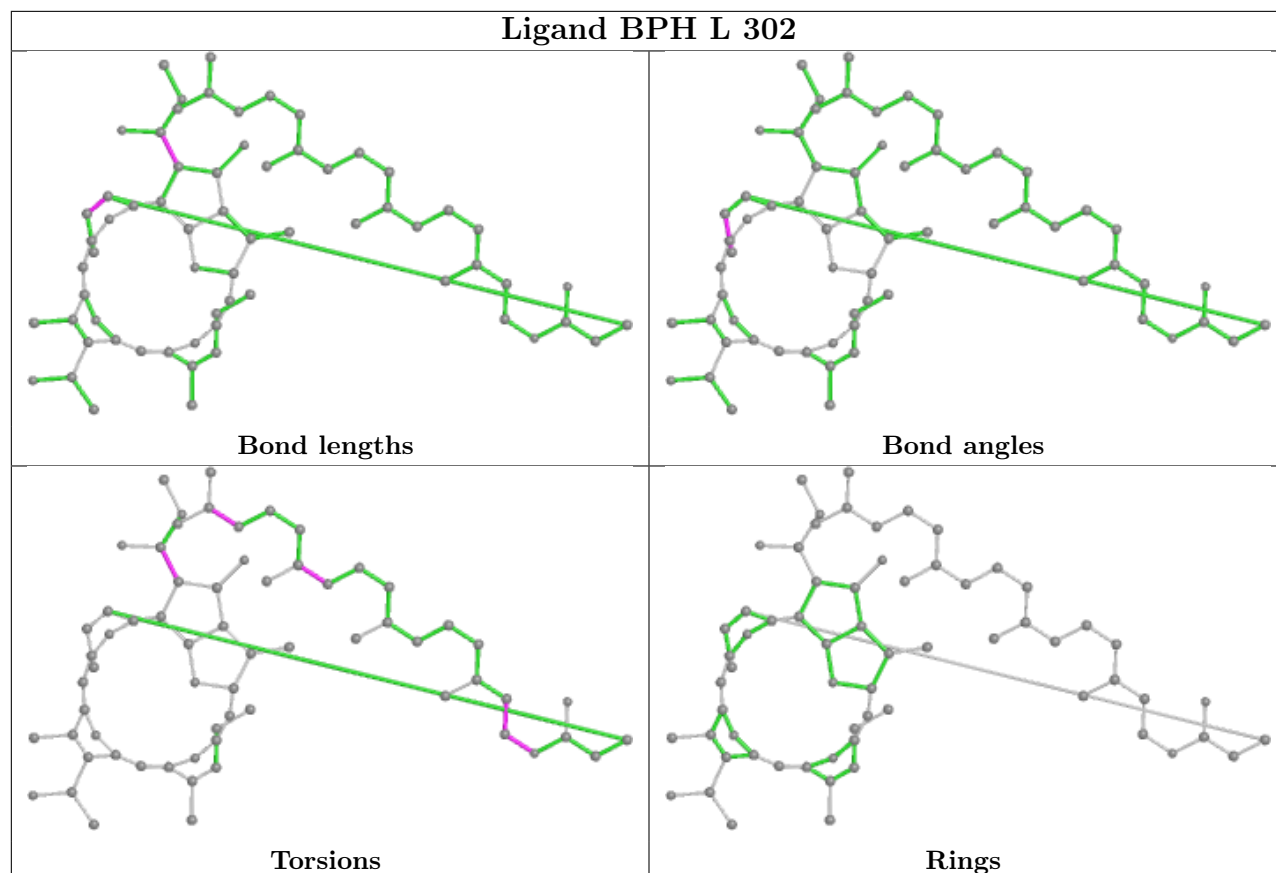




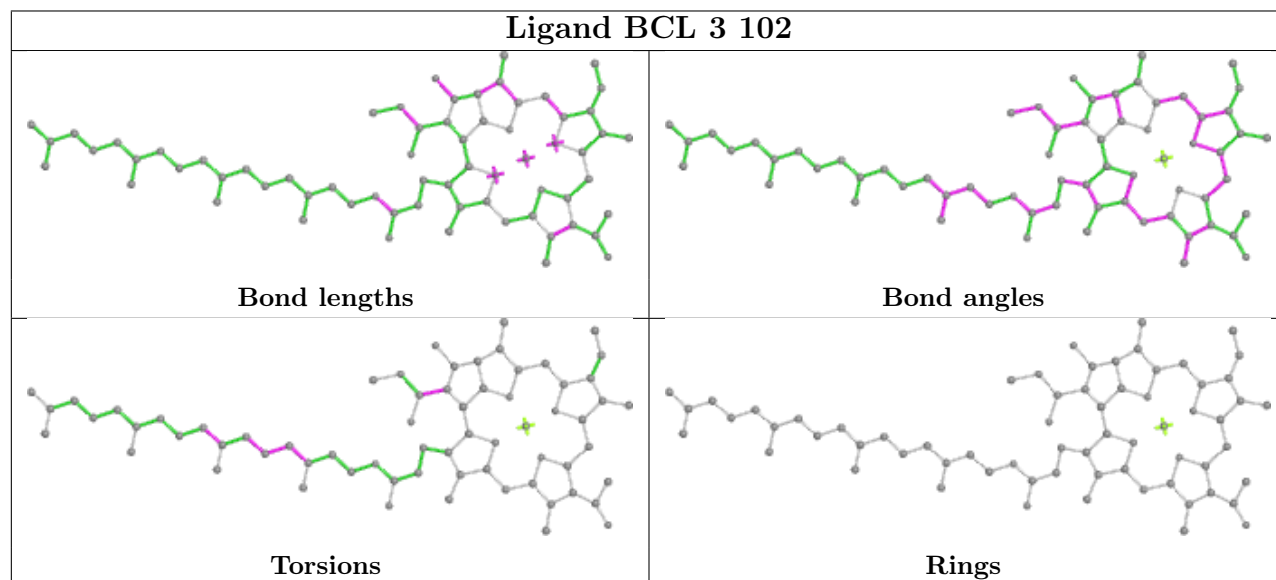


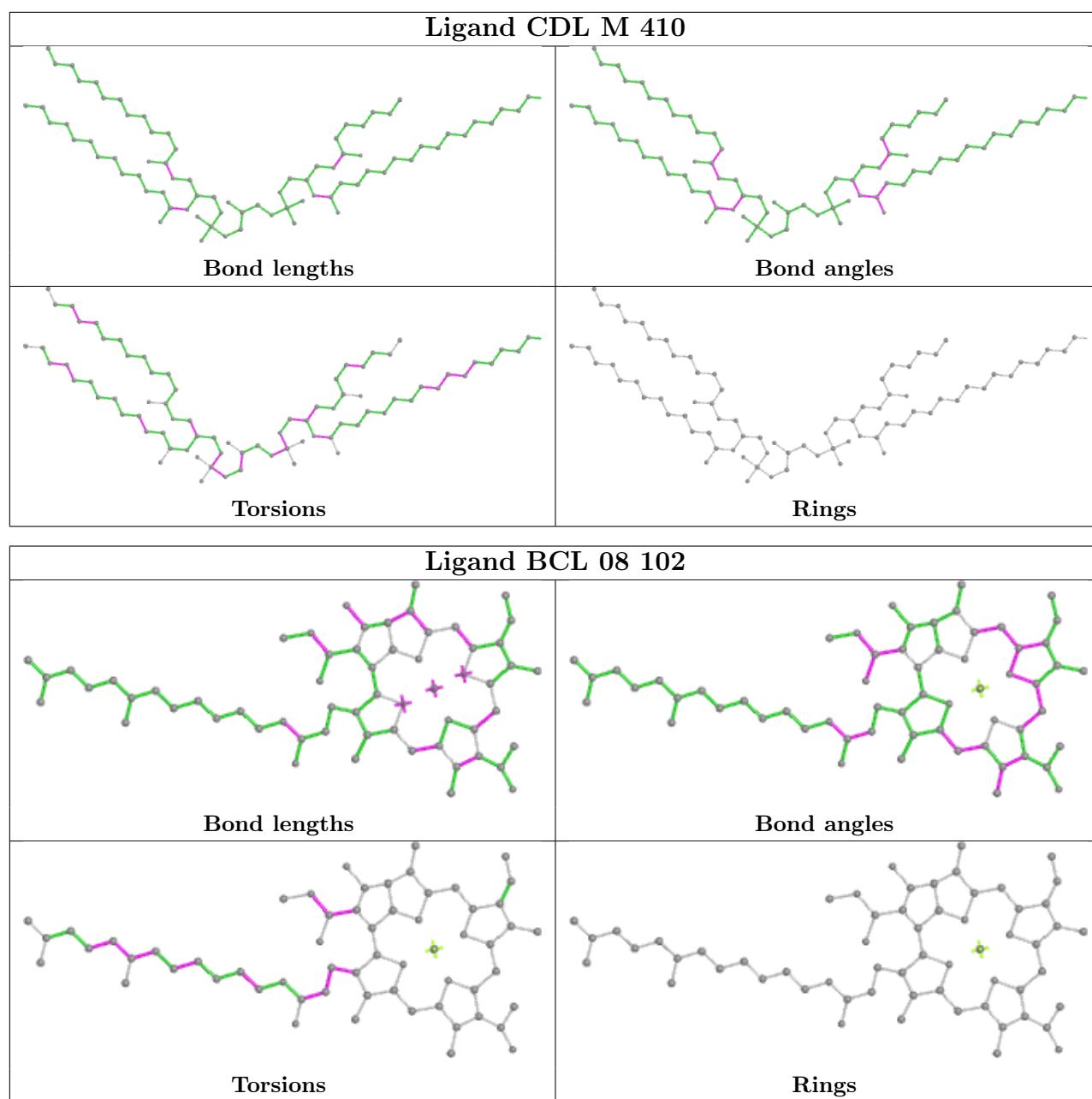


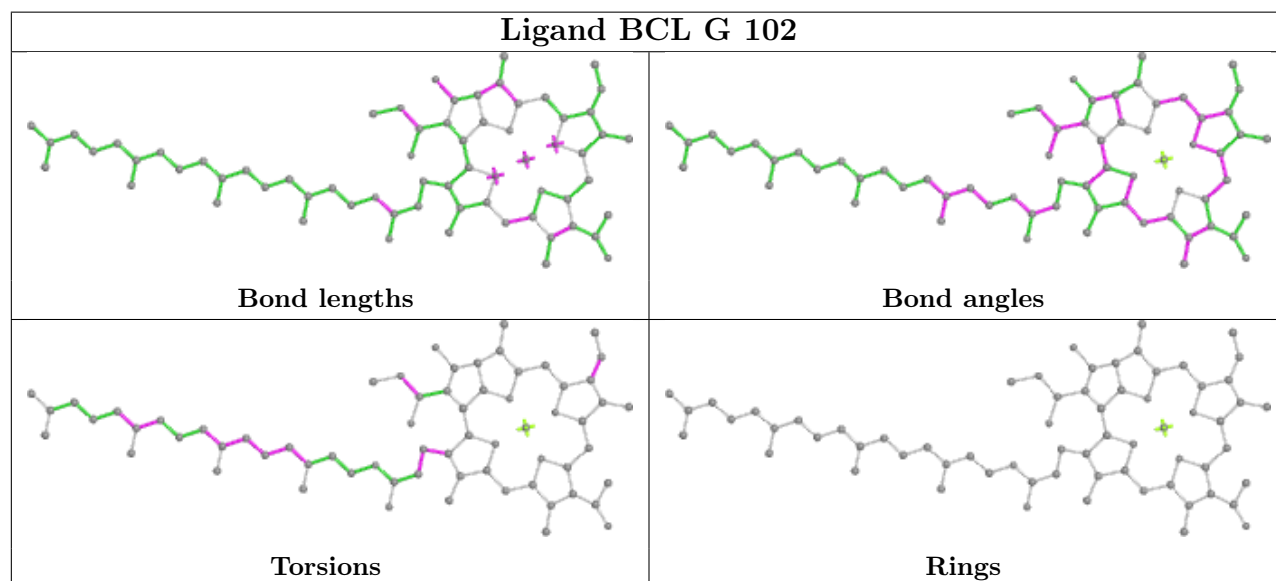
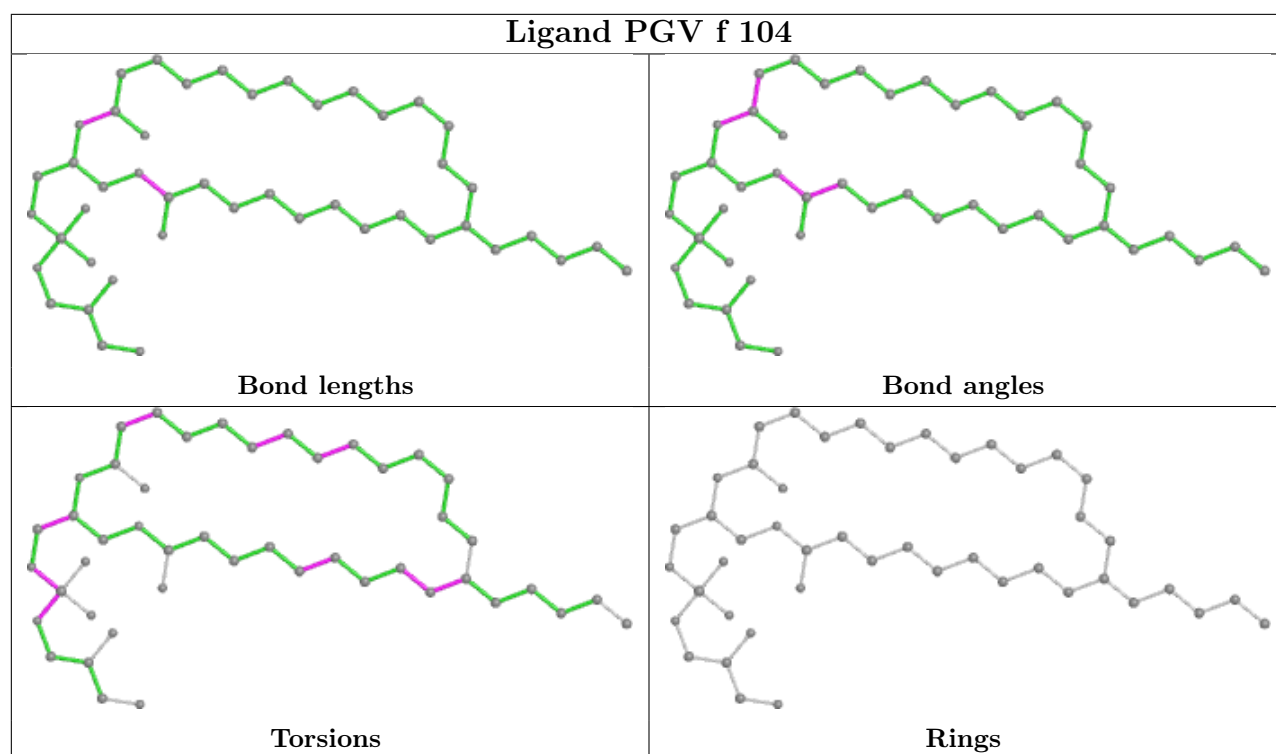
Ligand BPH L 302

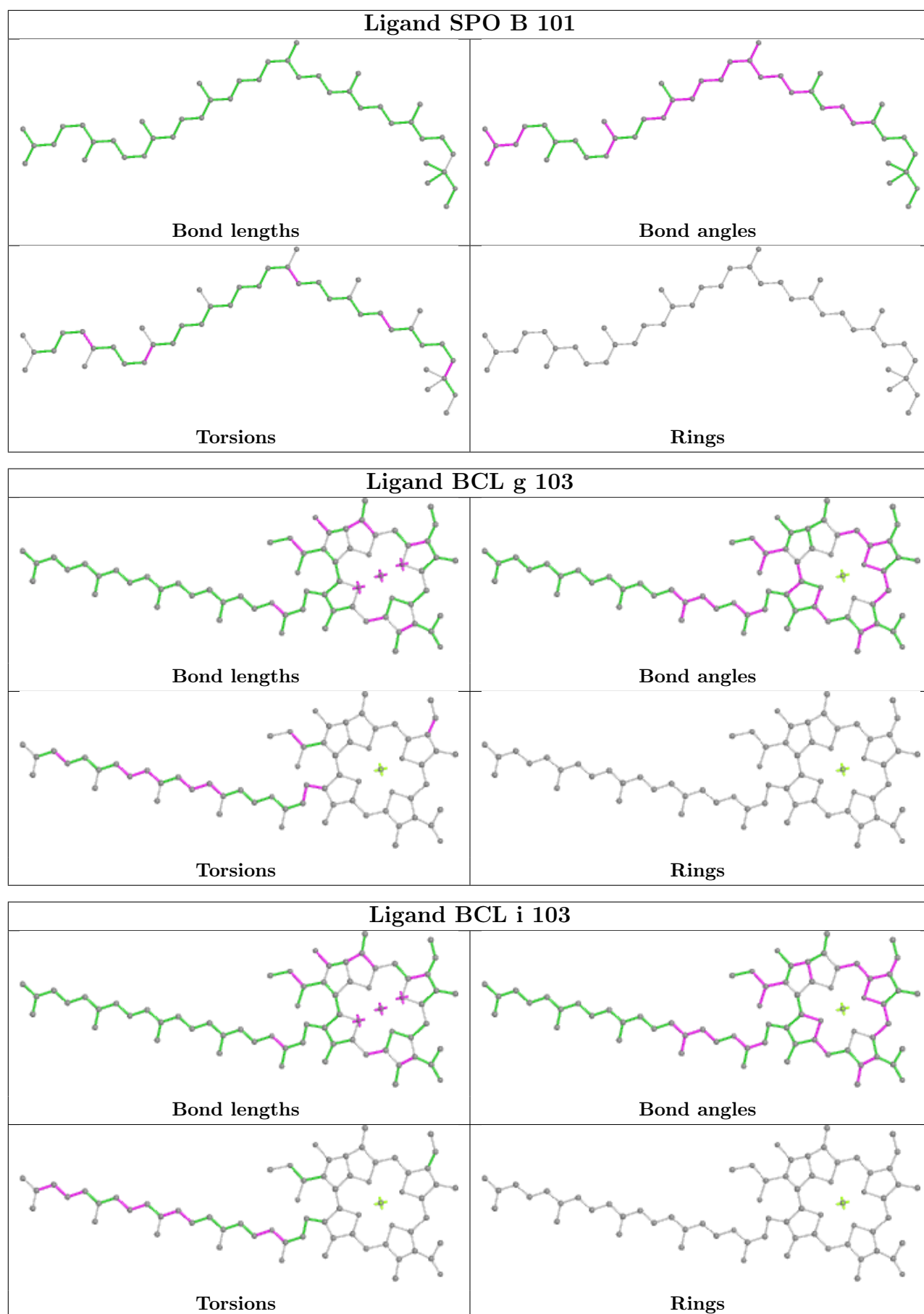


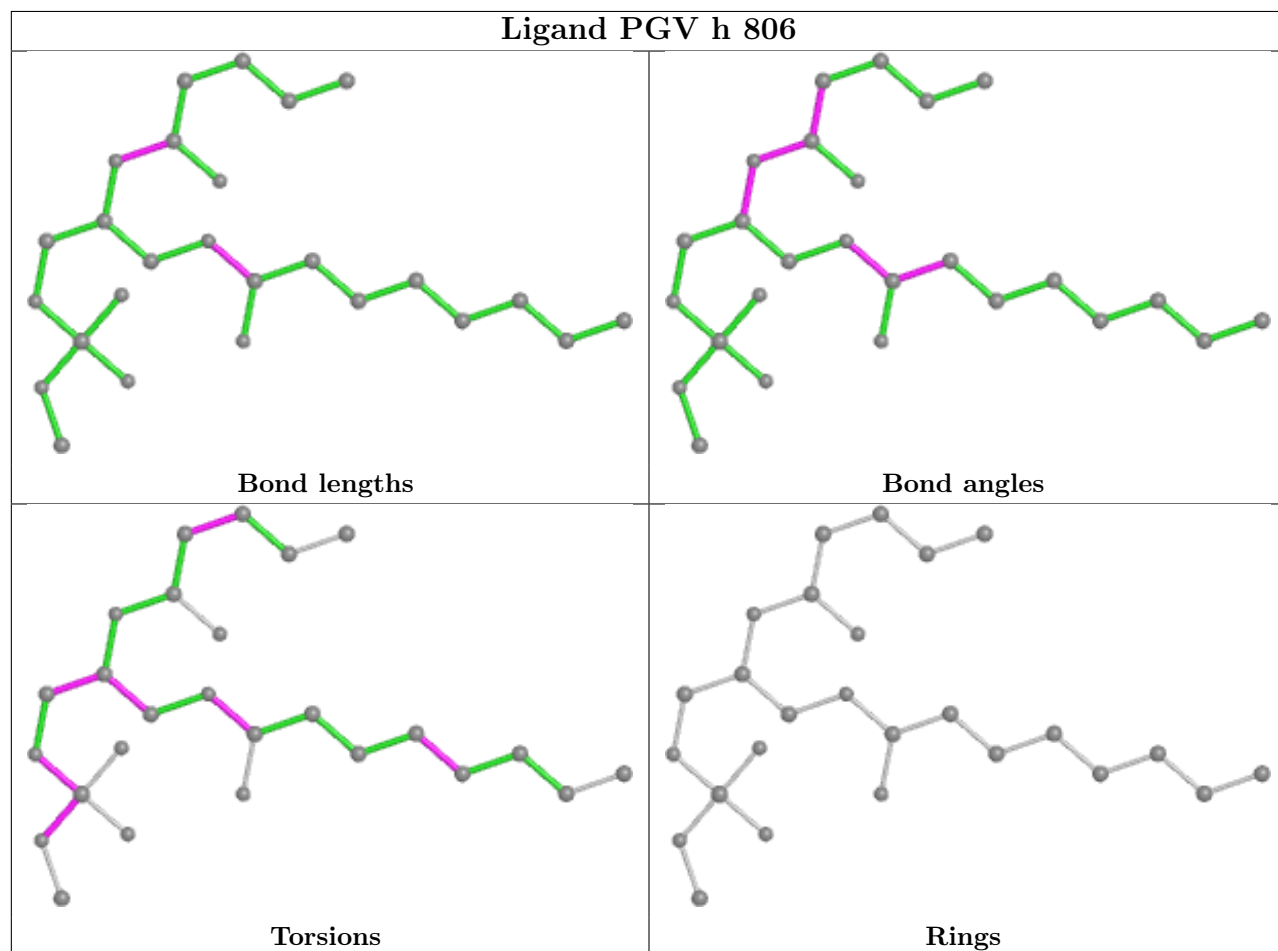
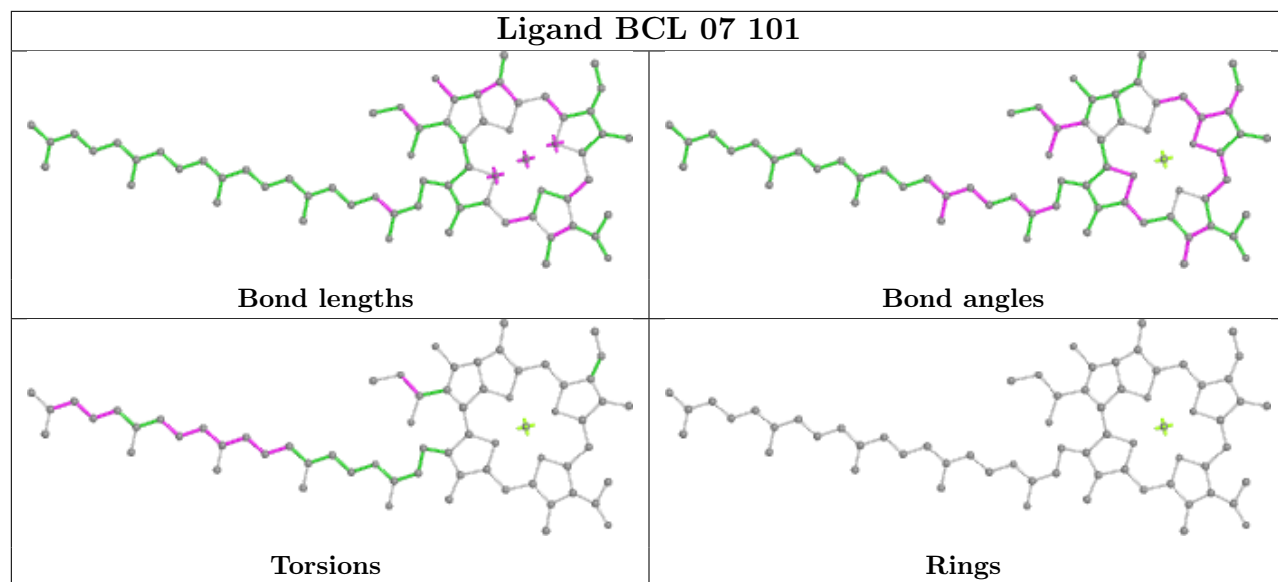
Ligand BCL 3 102

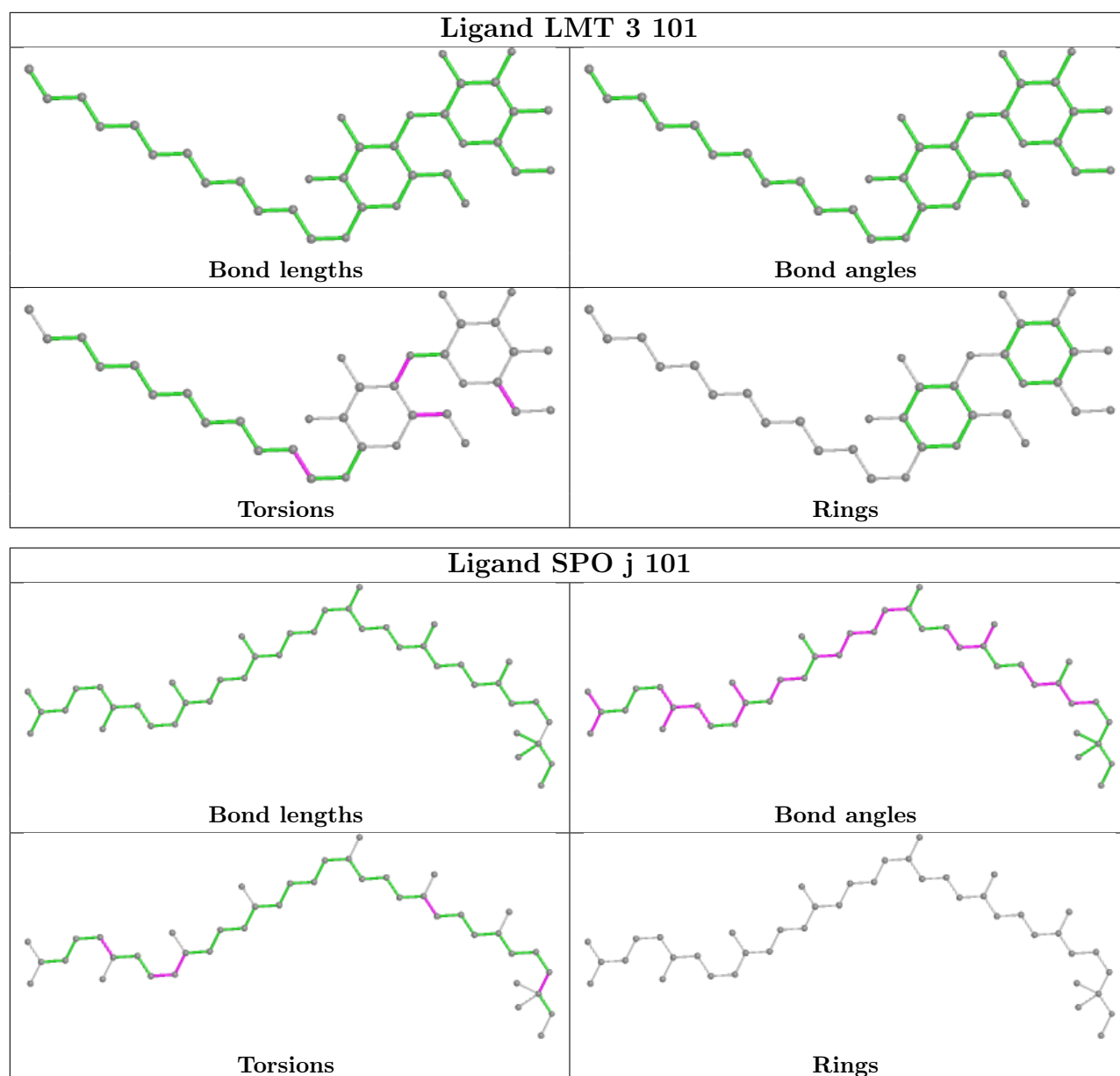


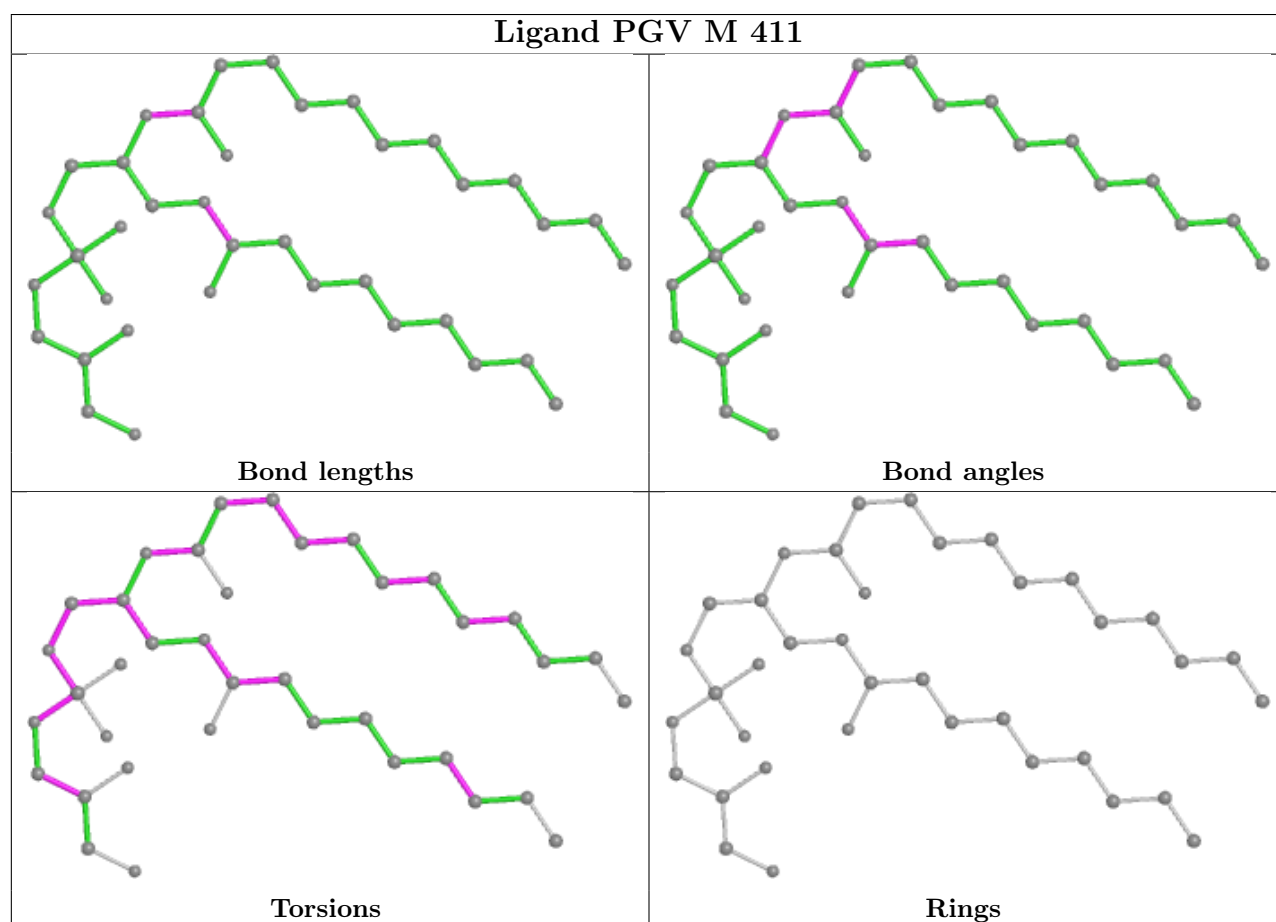
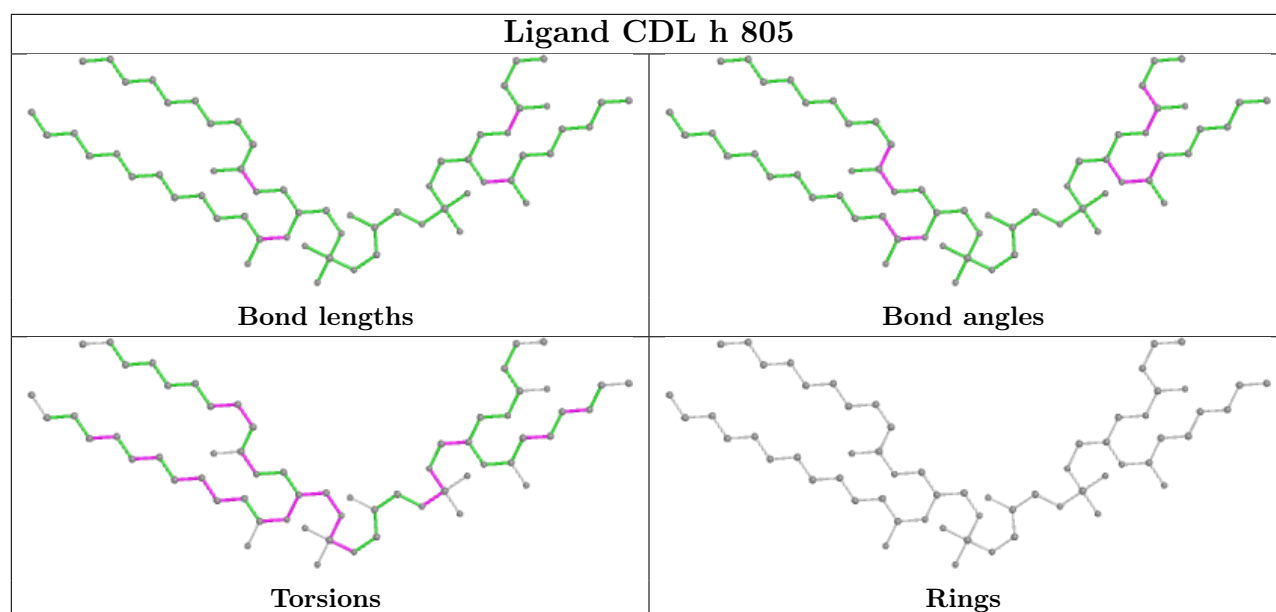


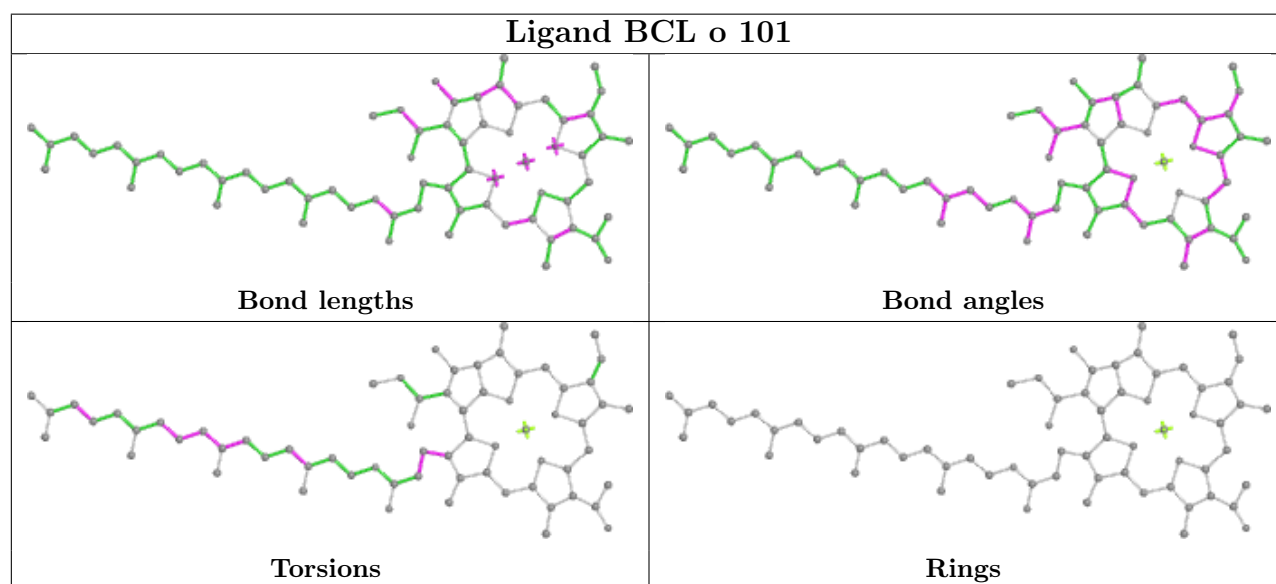
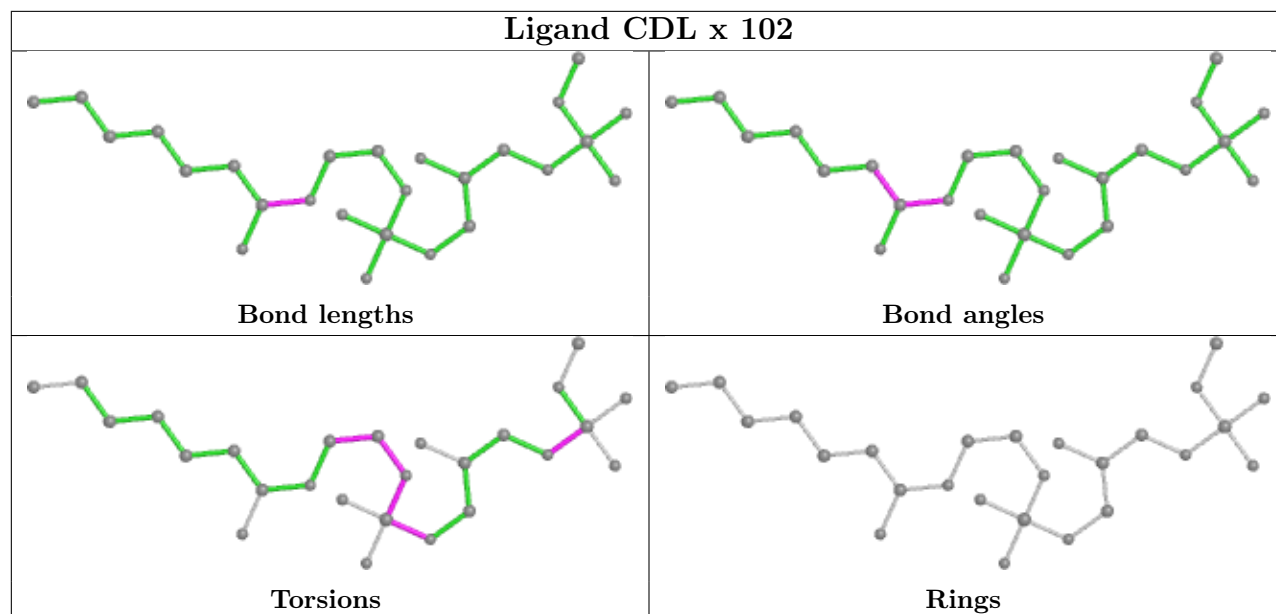


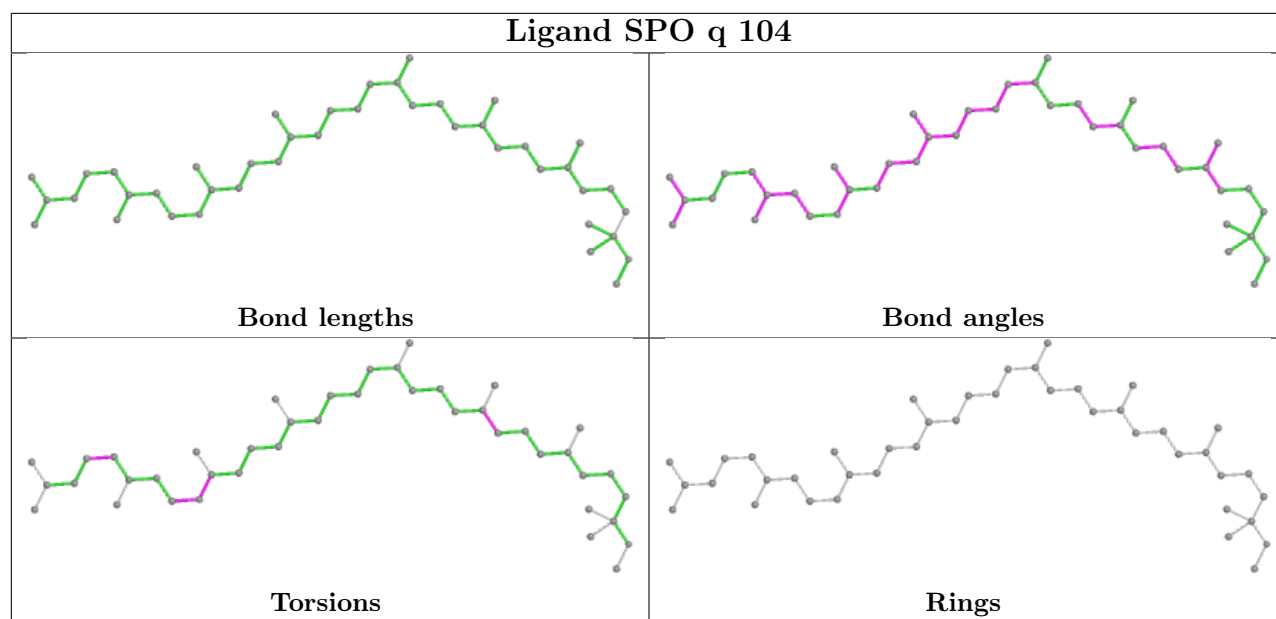
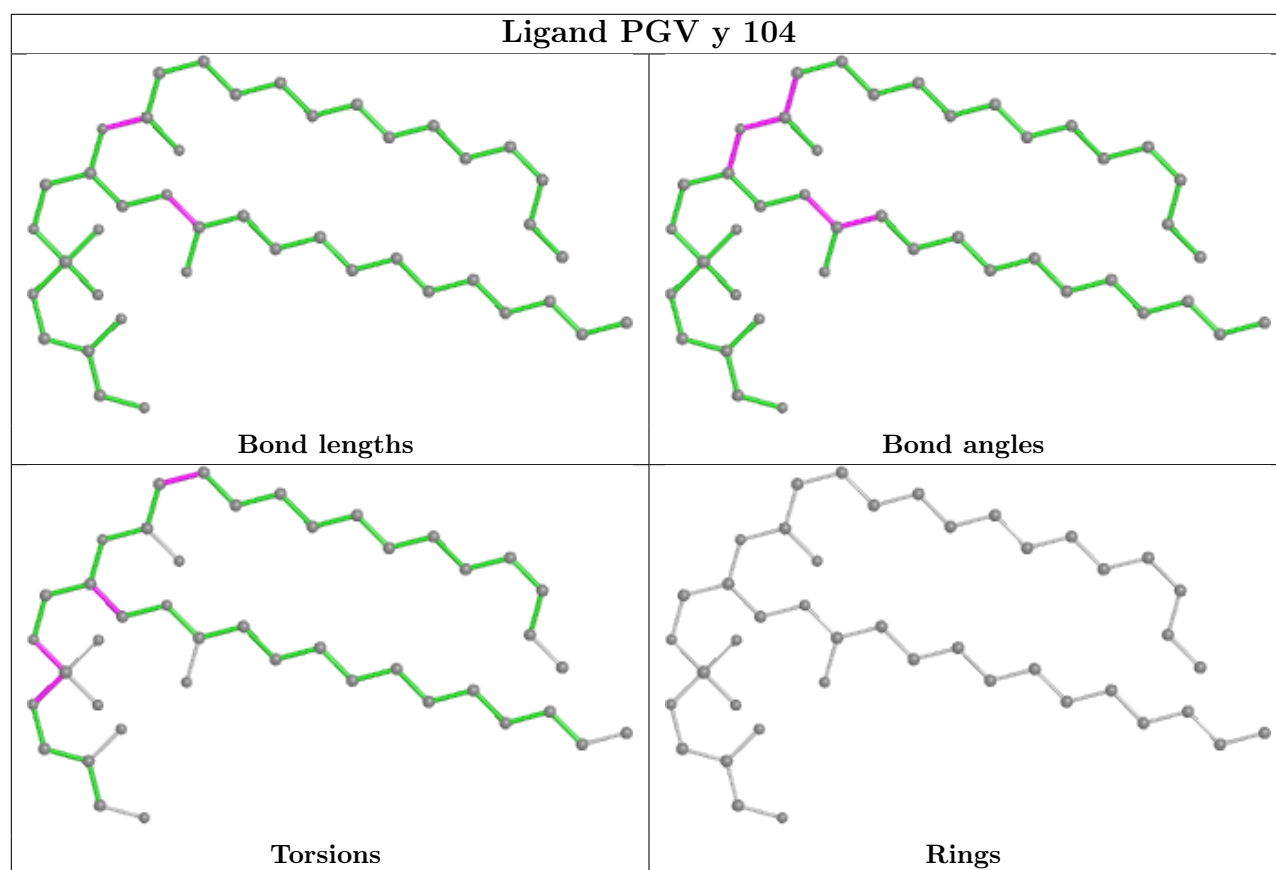


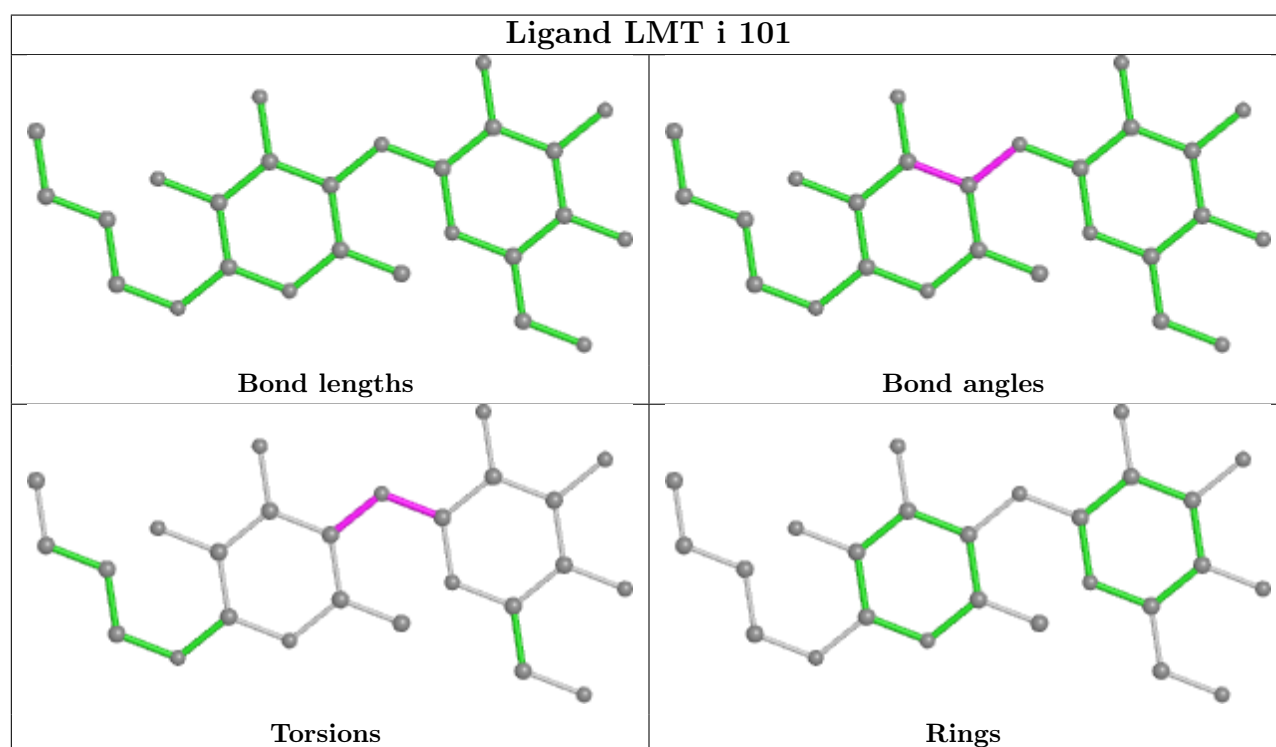
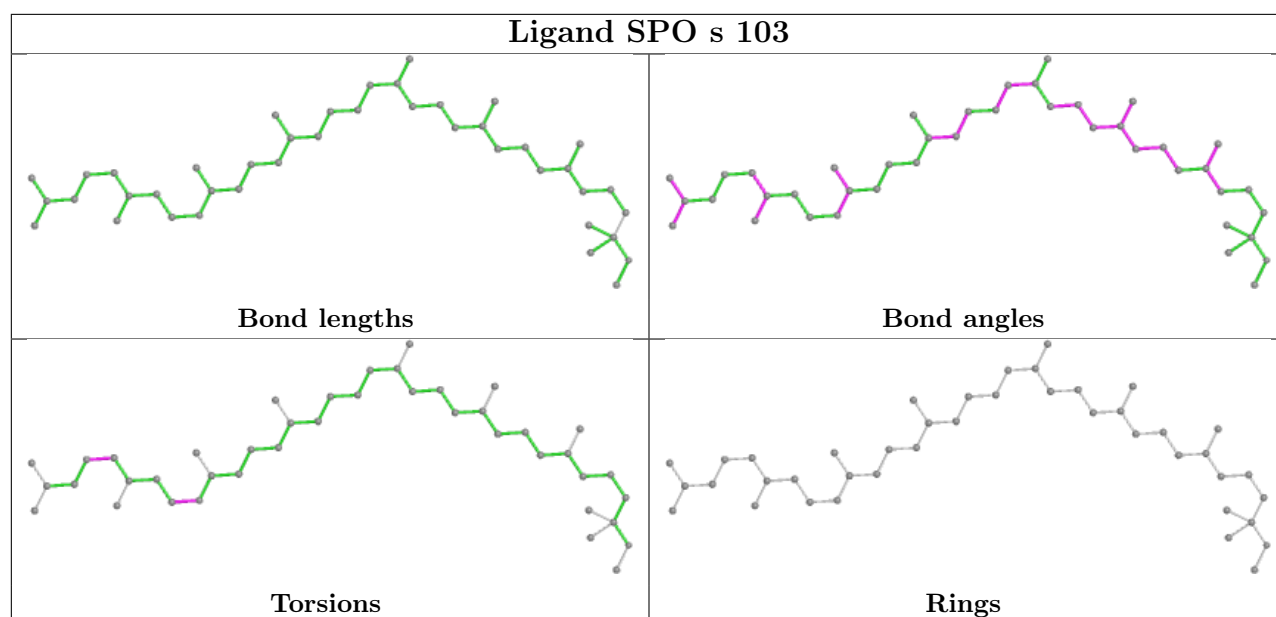




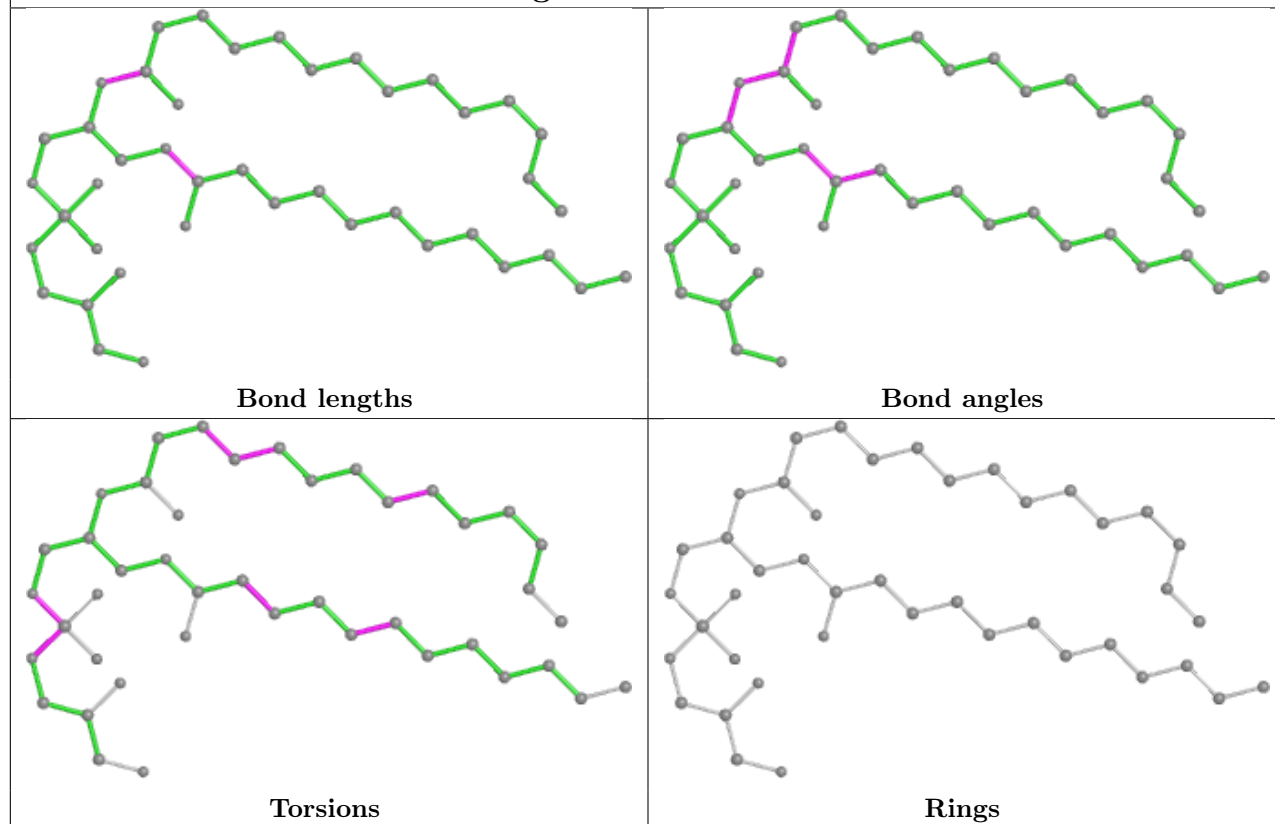




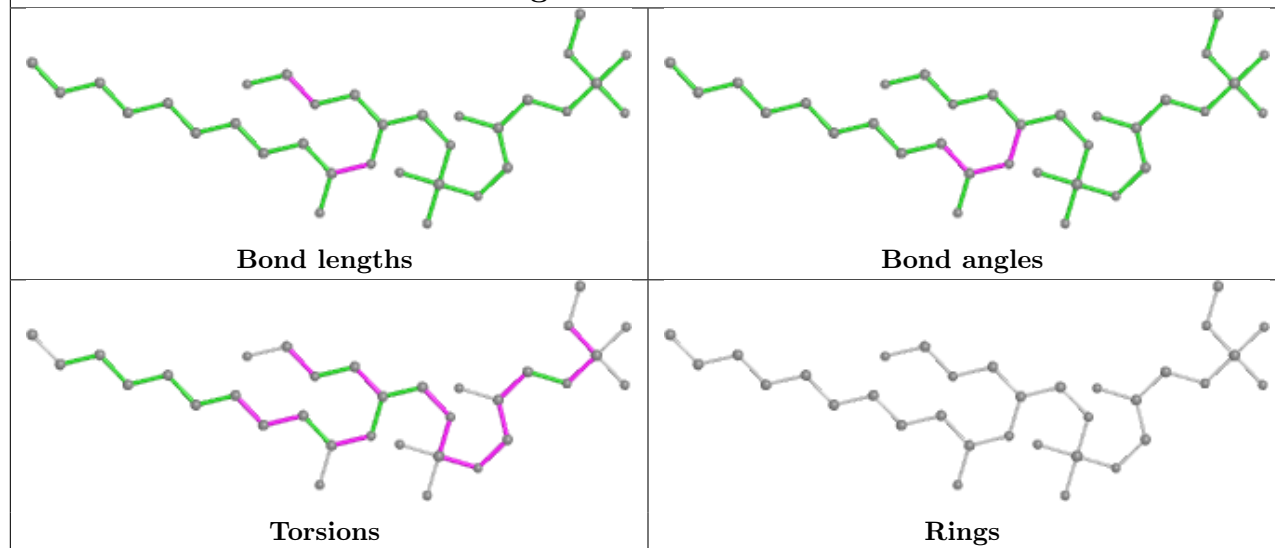


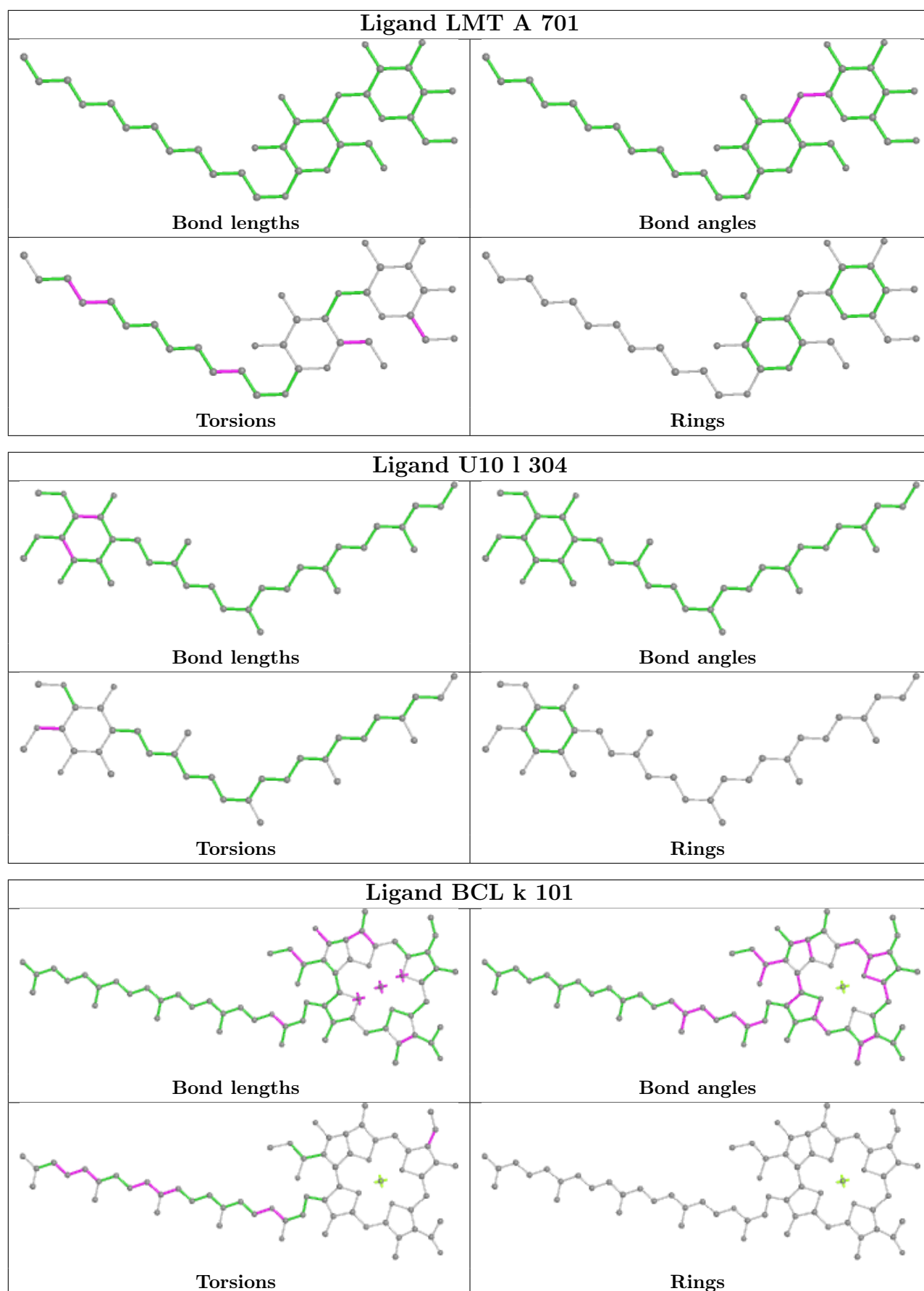


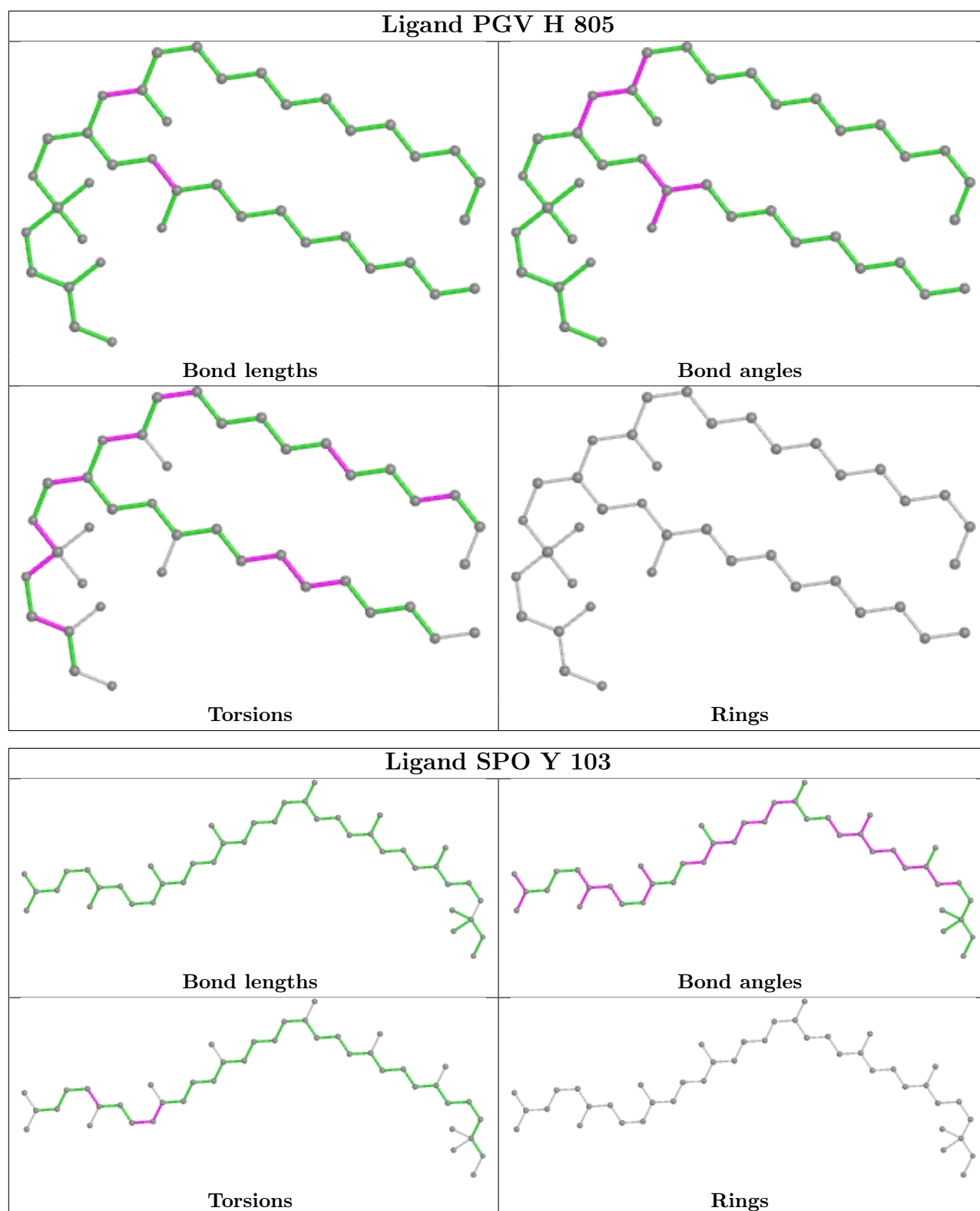
Ligand PGV 1 201

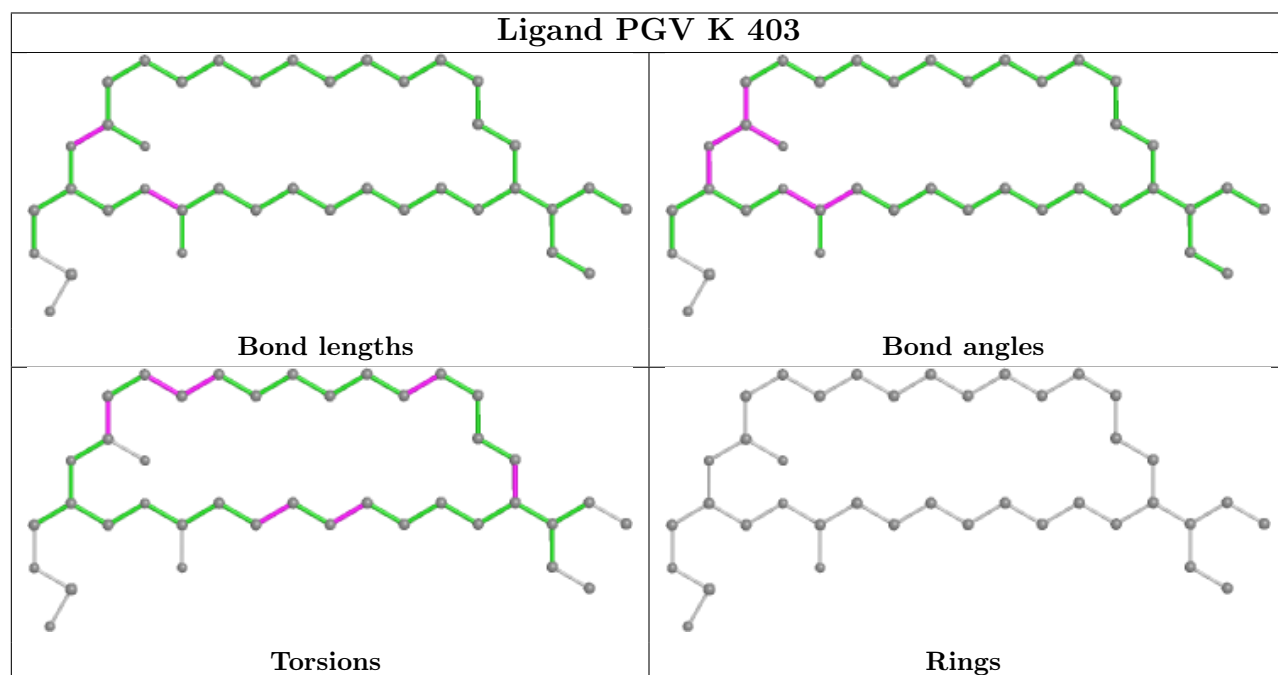
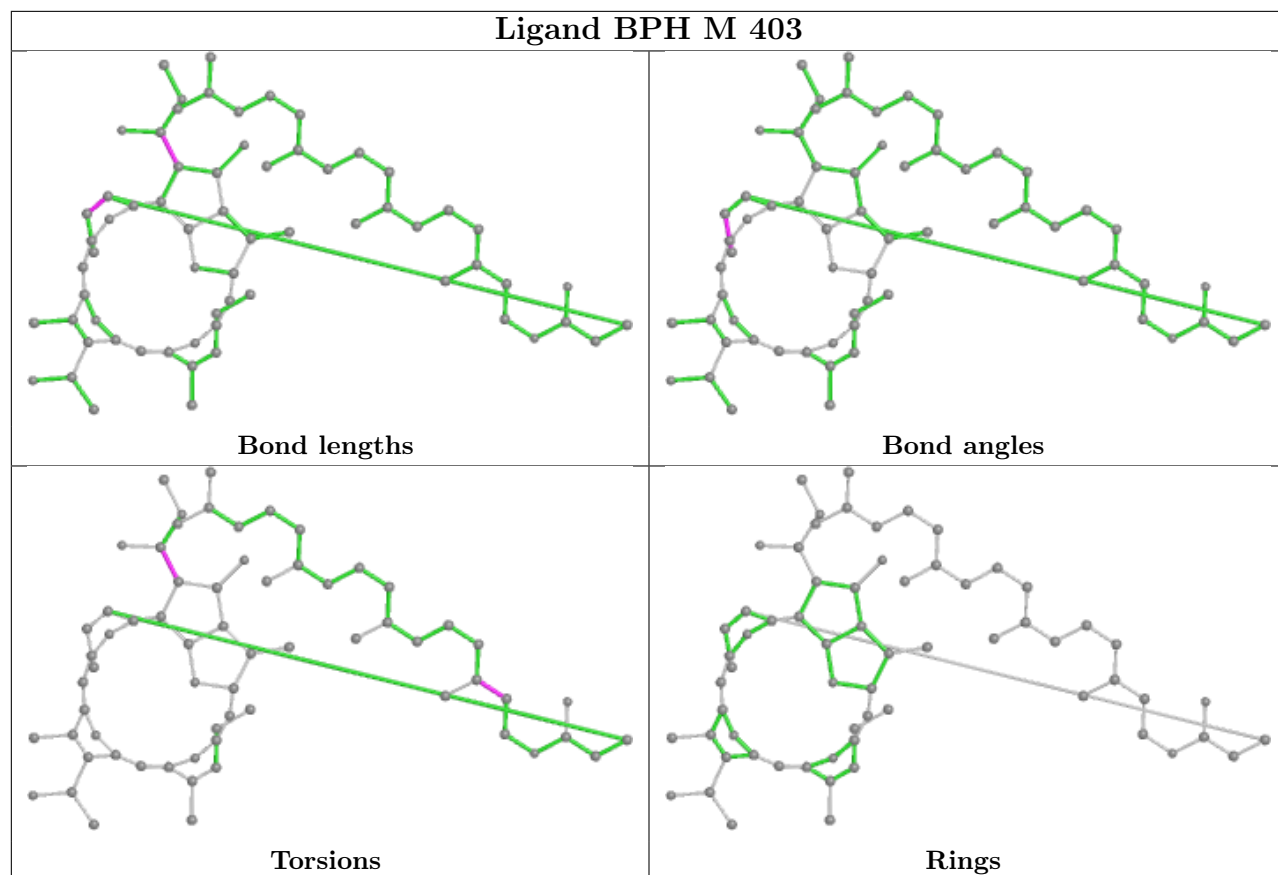


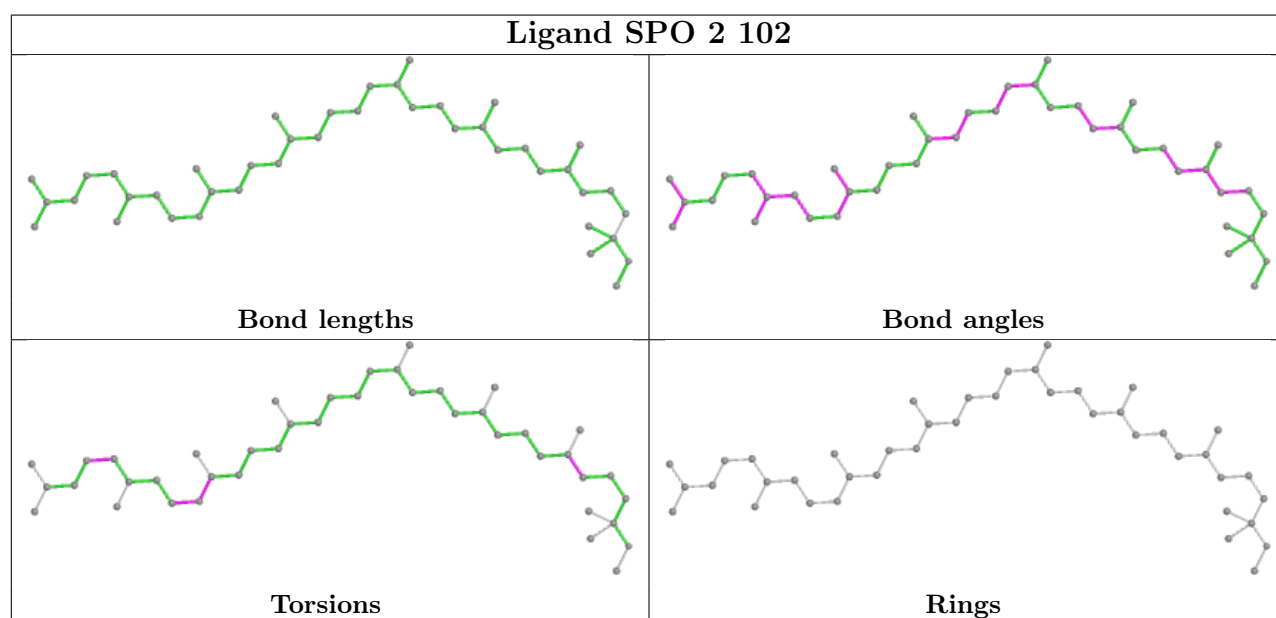
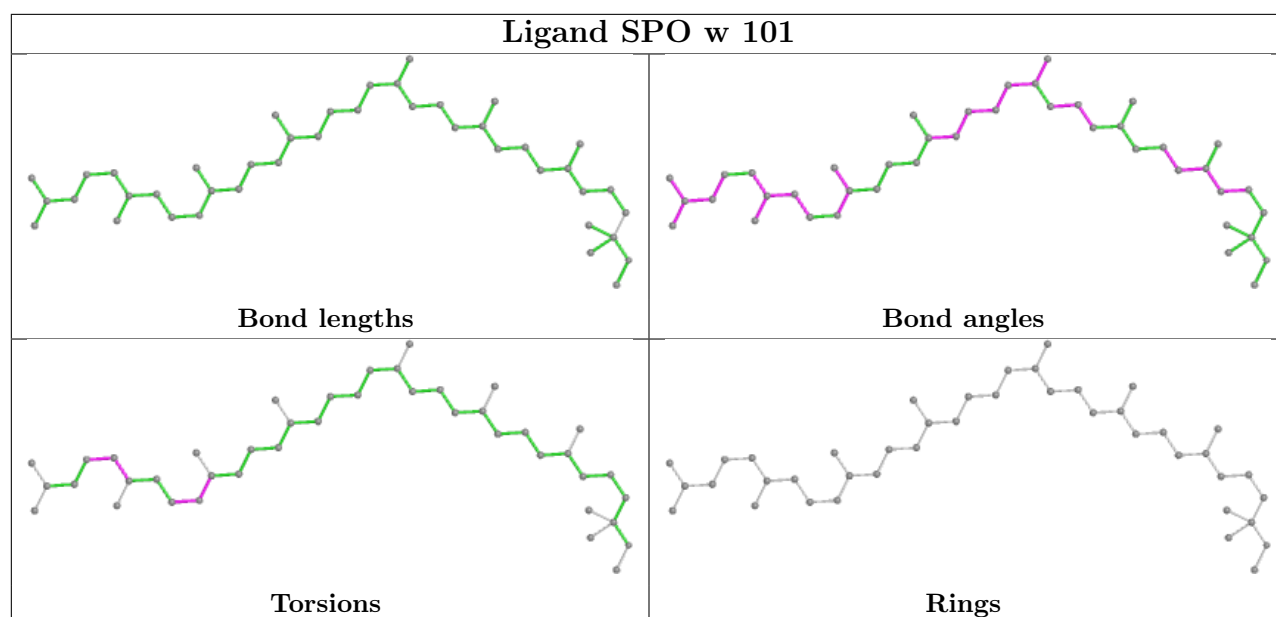
Ligand CDL X 102

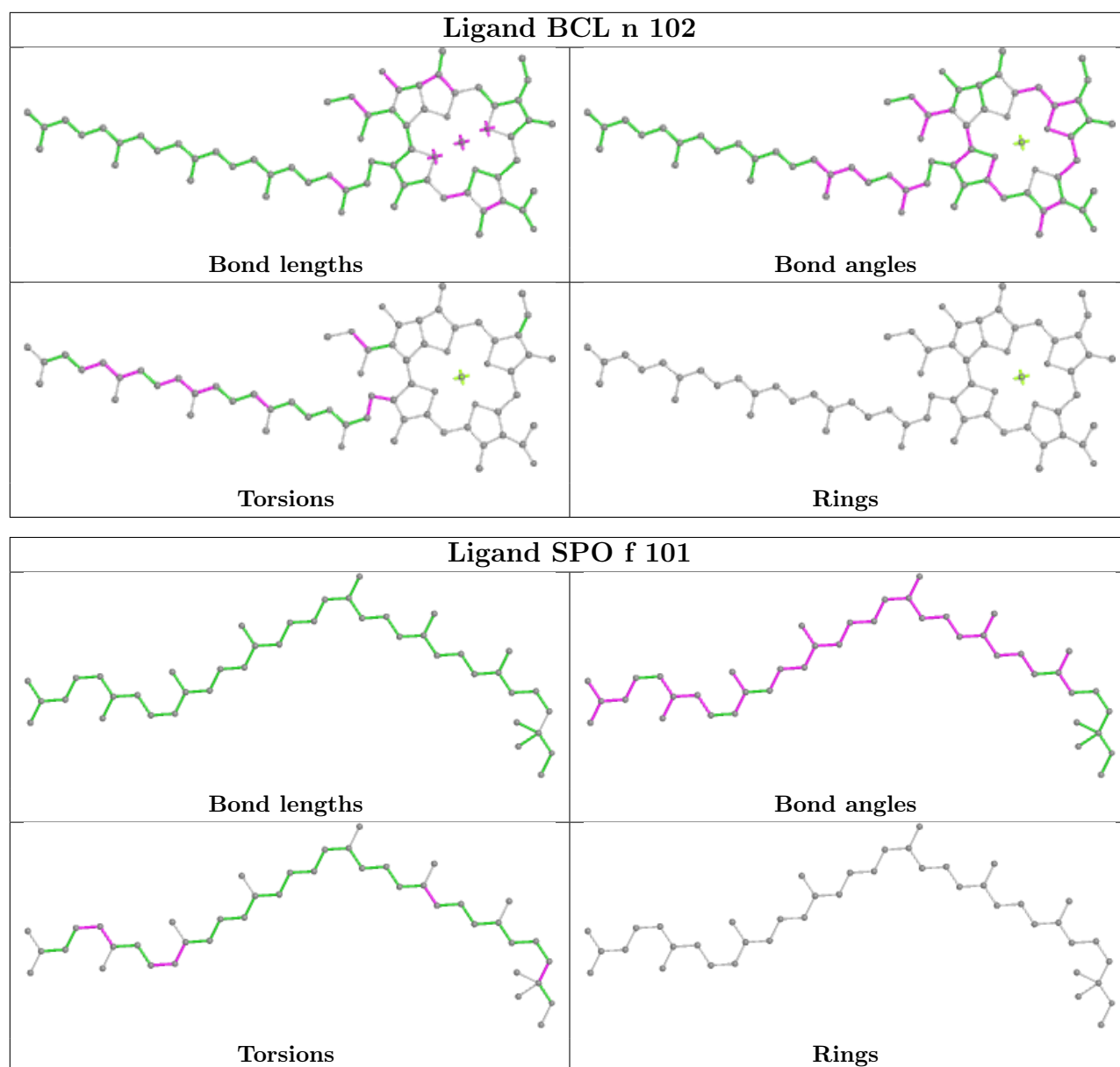


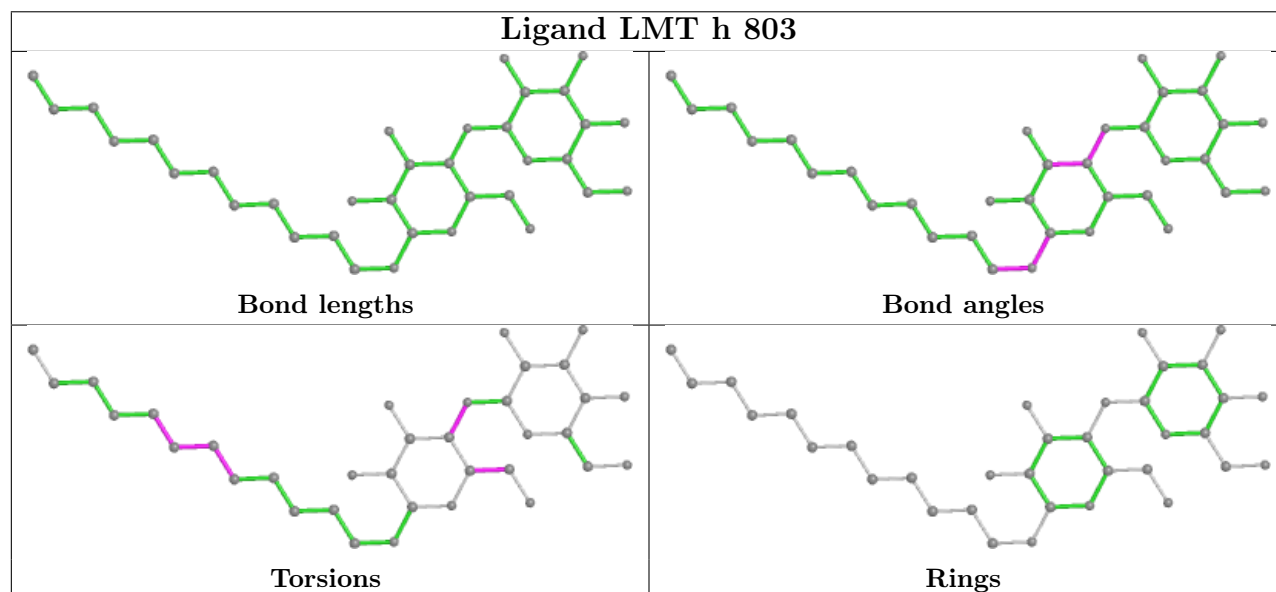
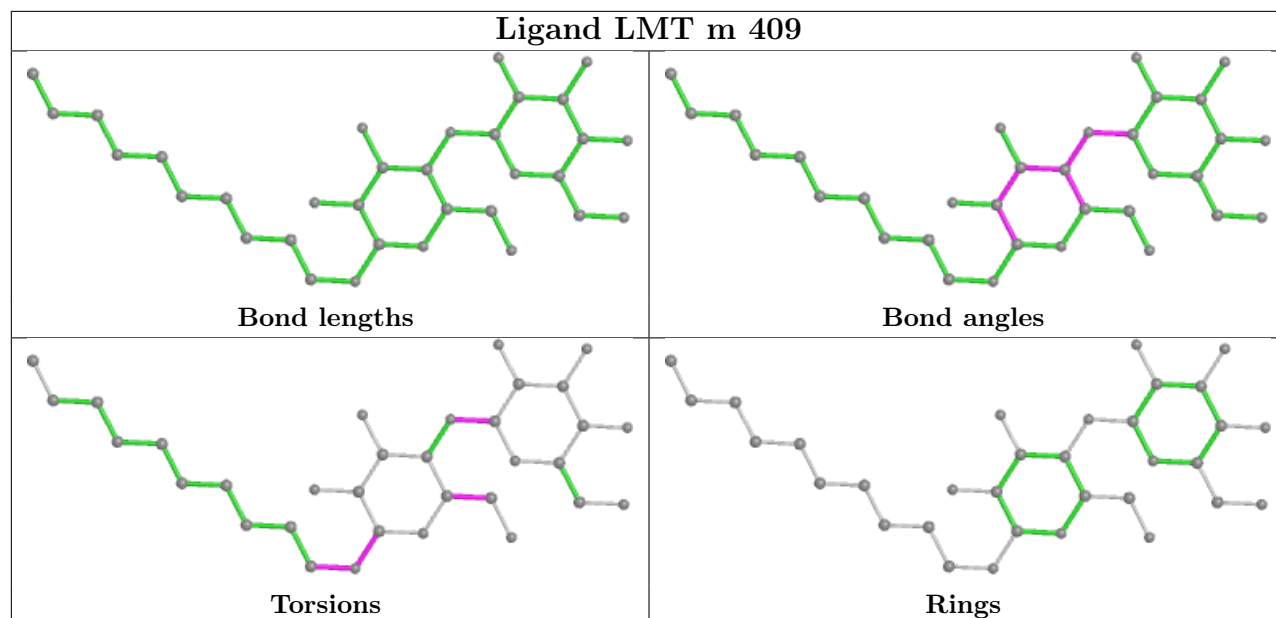




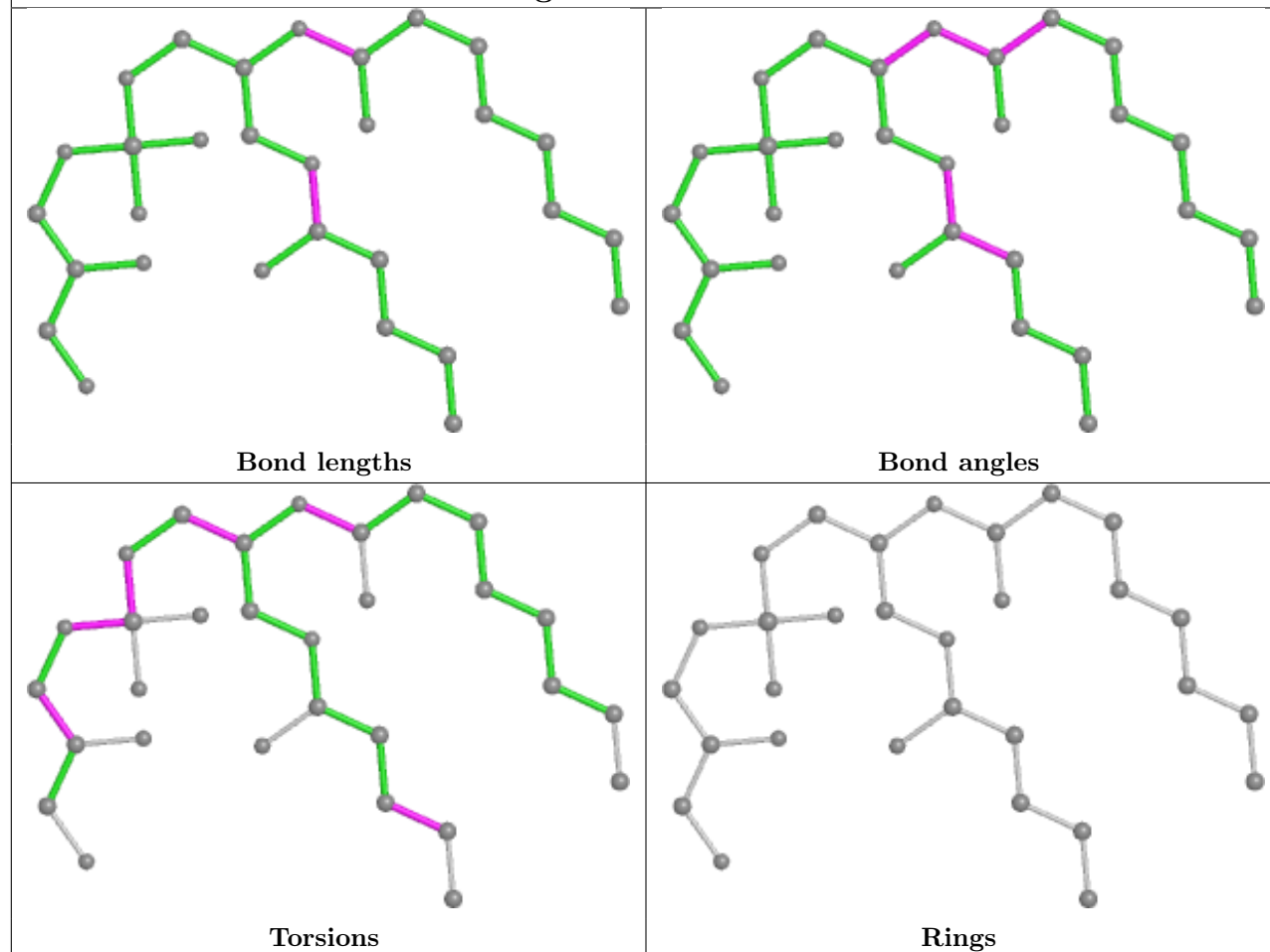




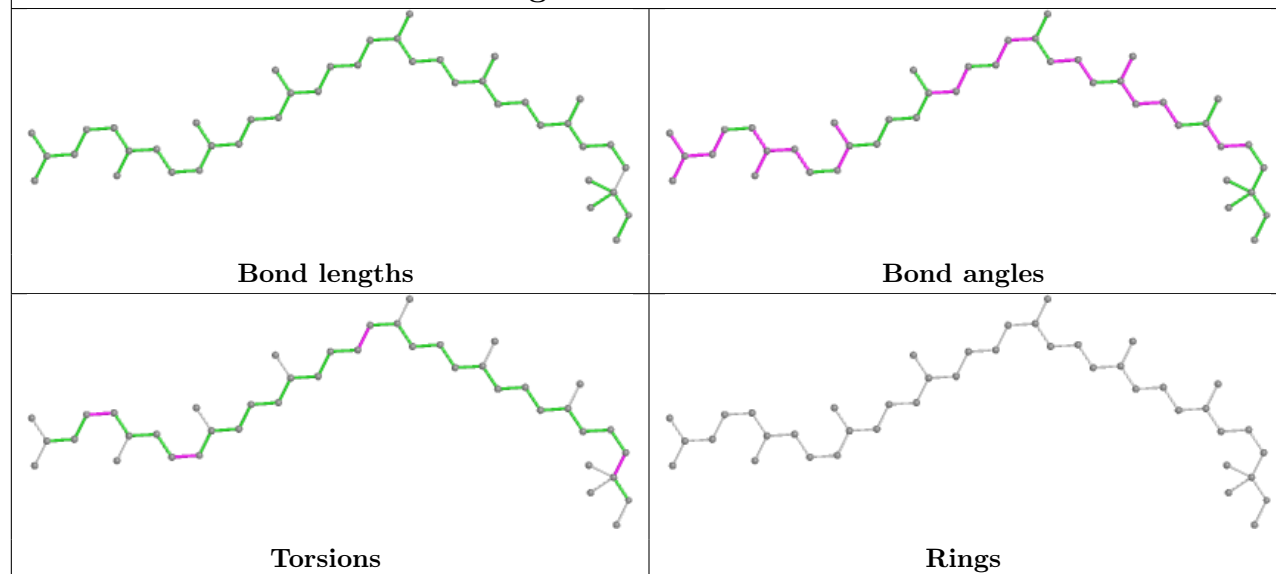


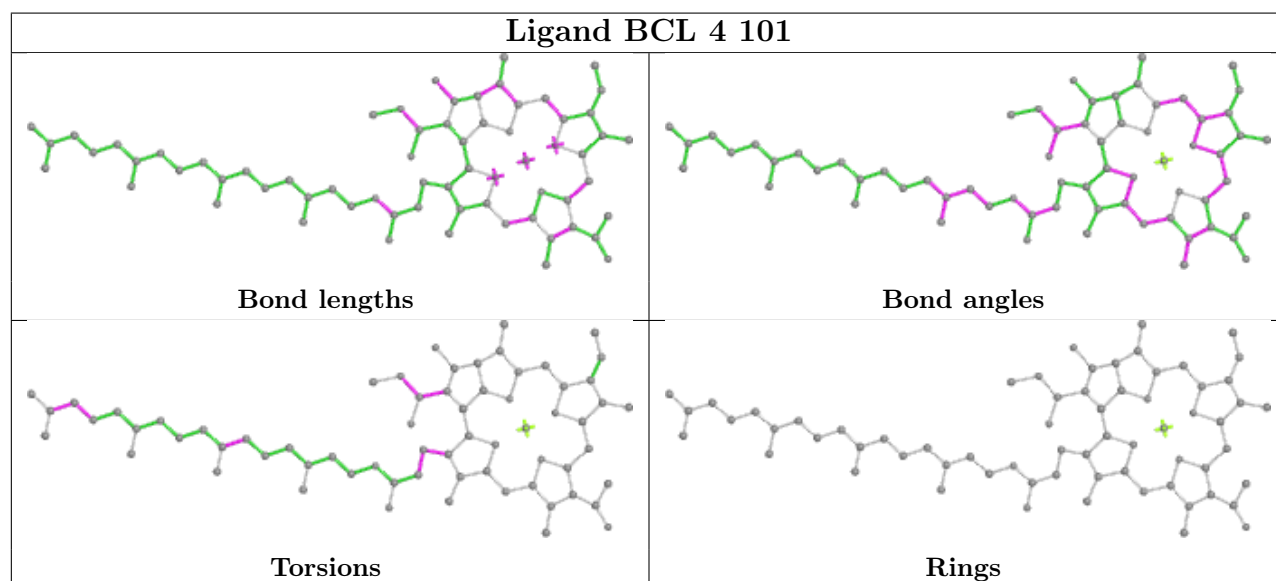
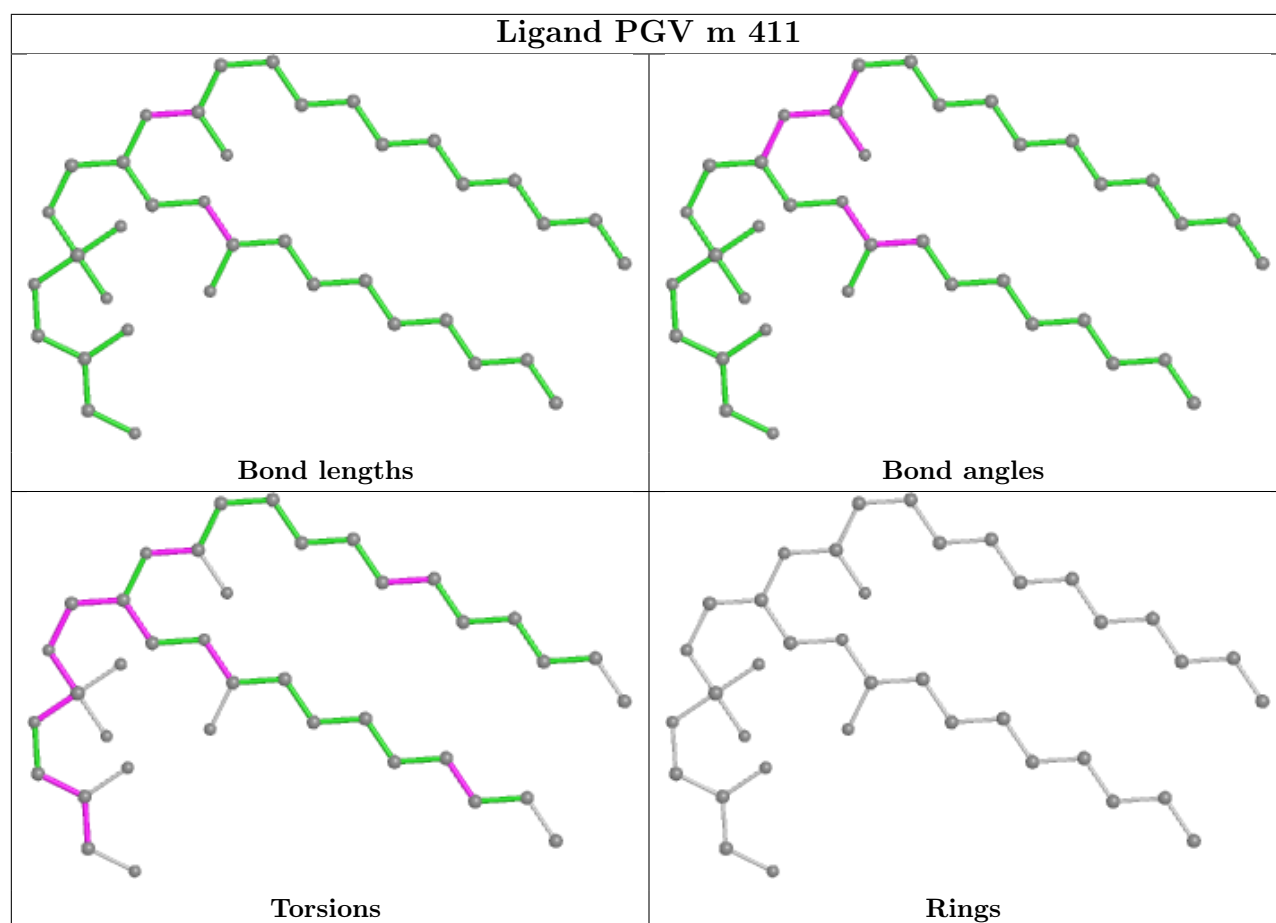


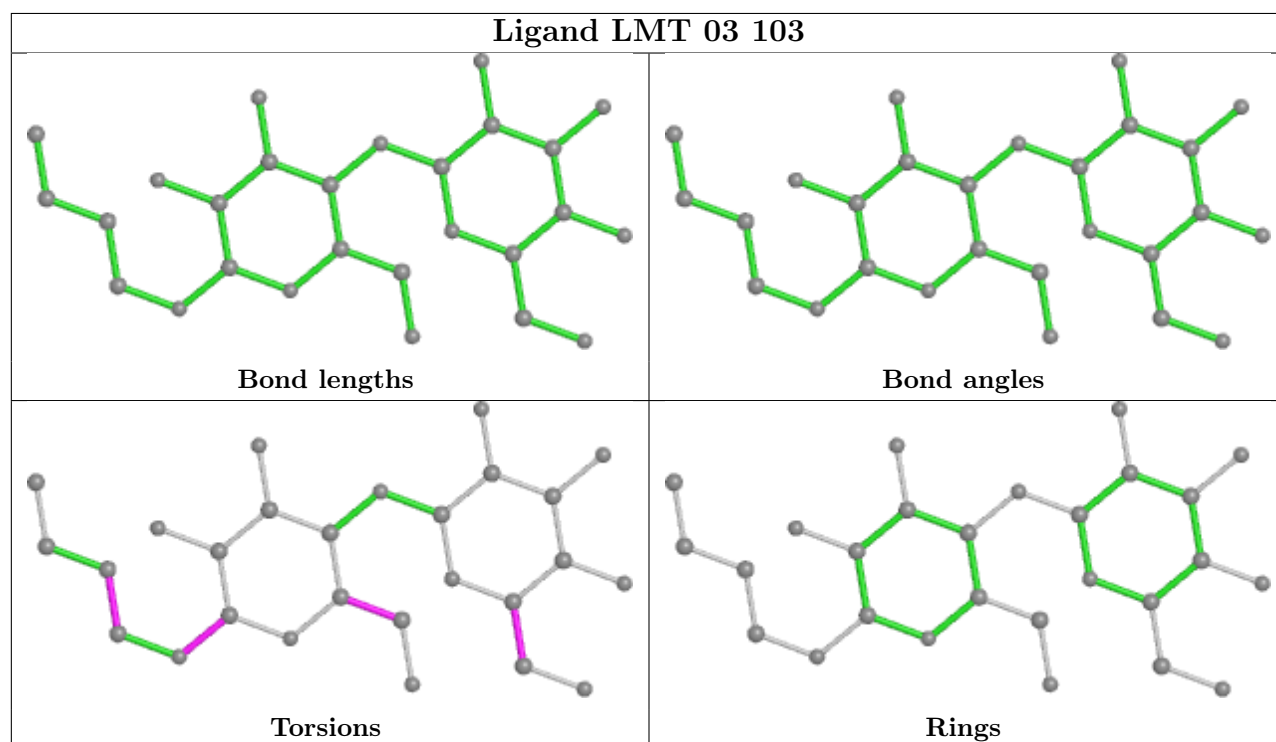
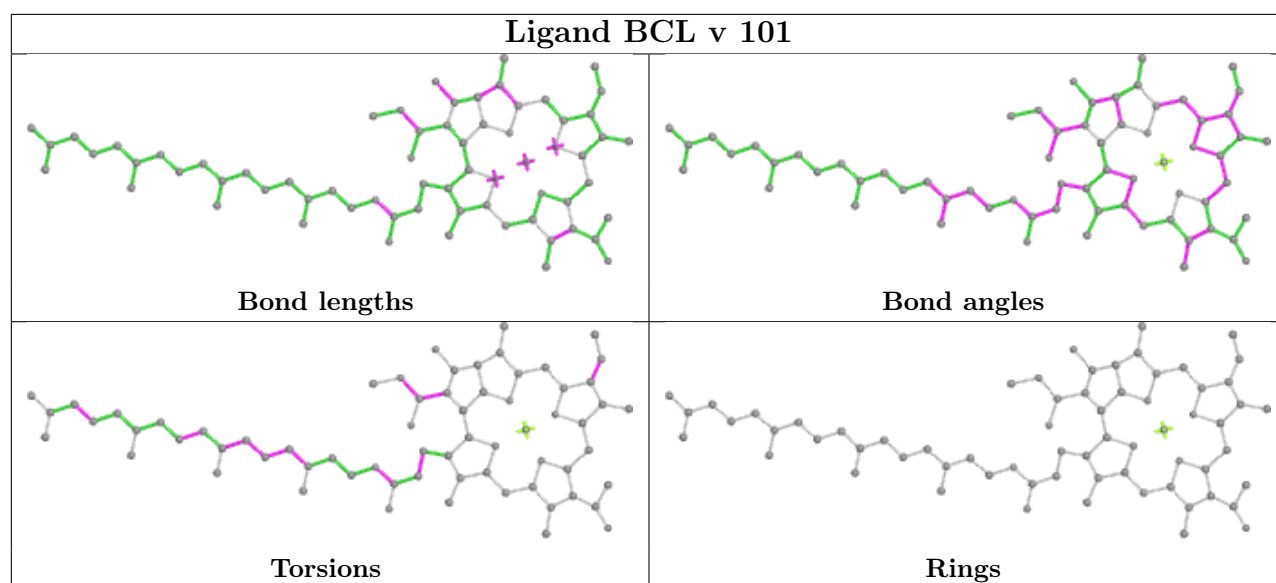
Ligand PGV 1 307

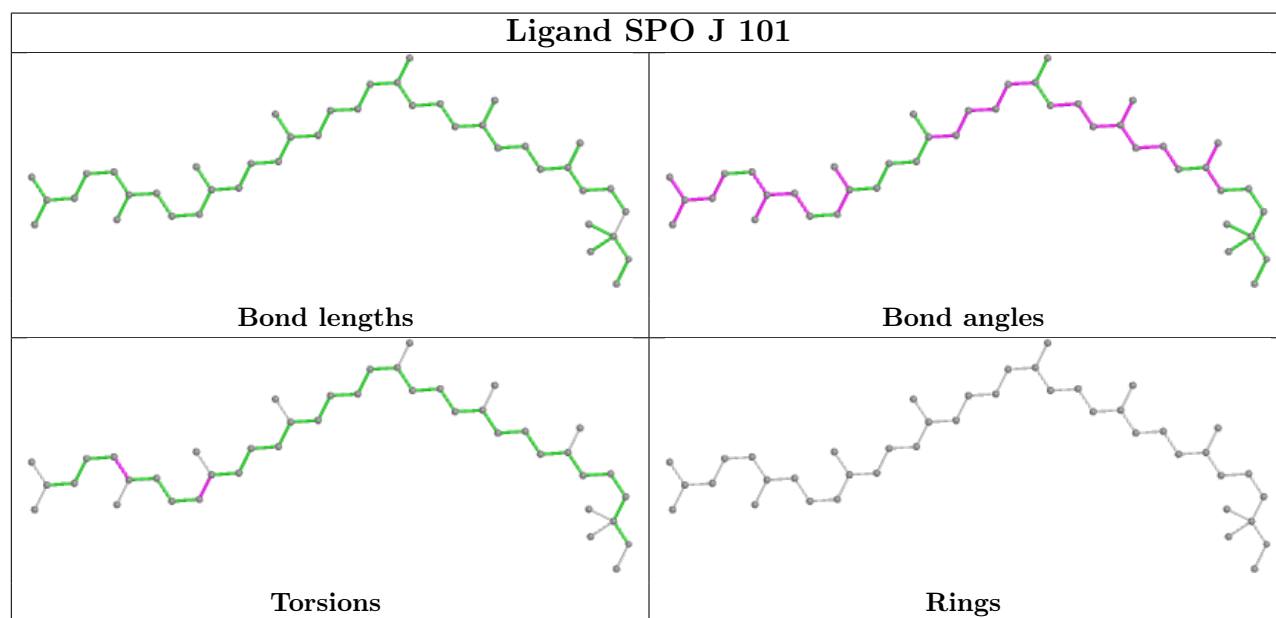
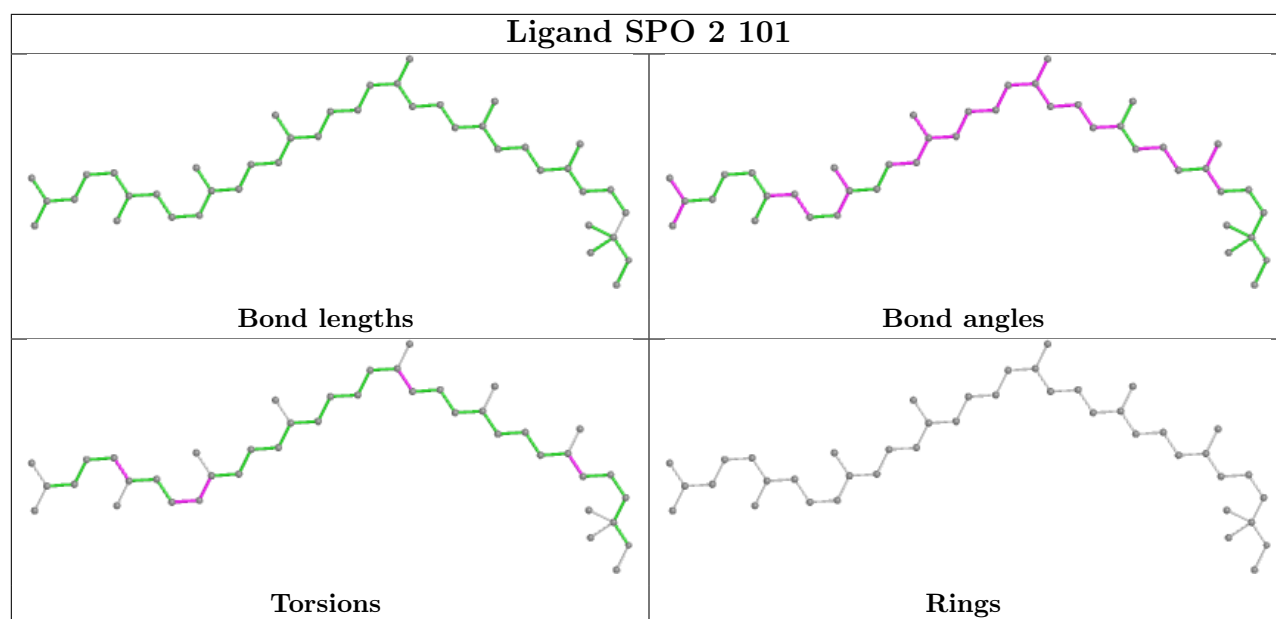


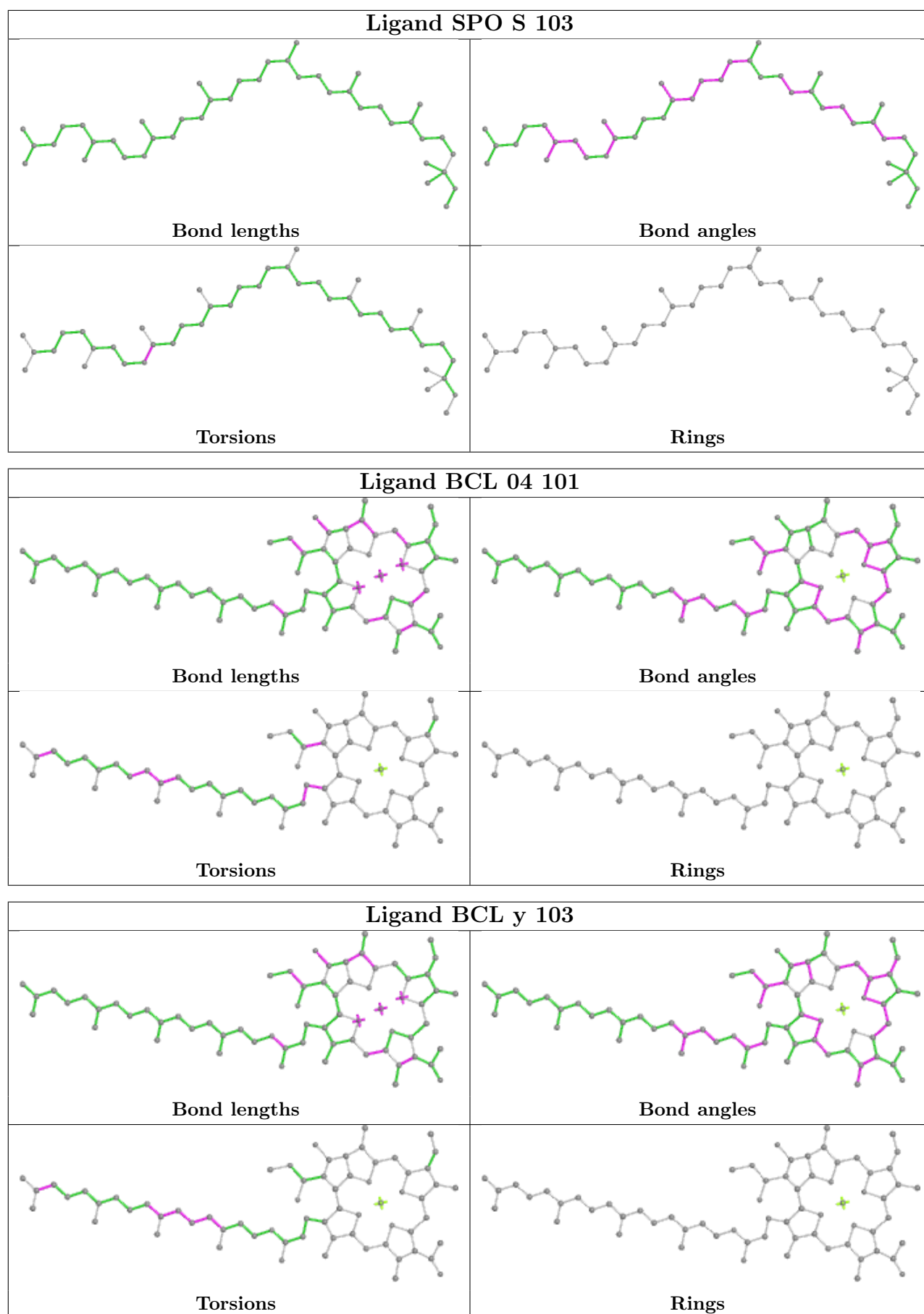
Ligand SPO 05 102

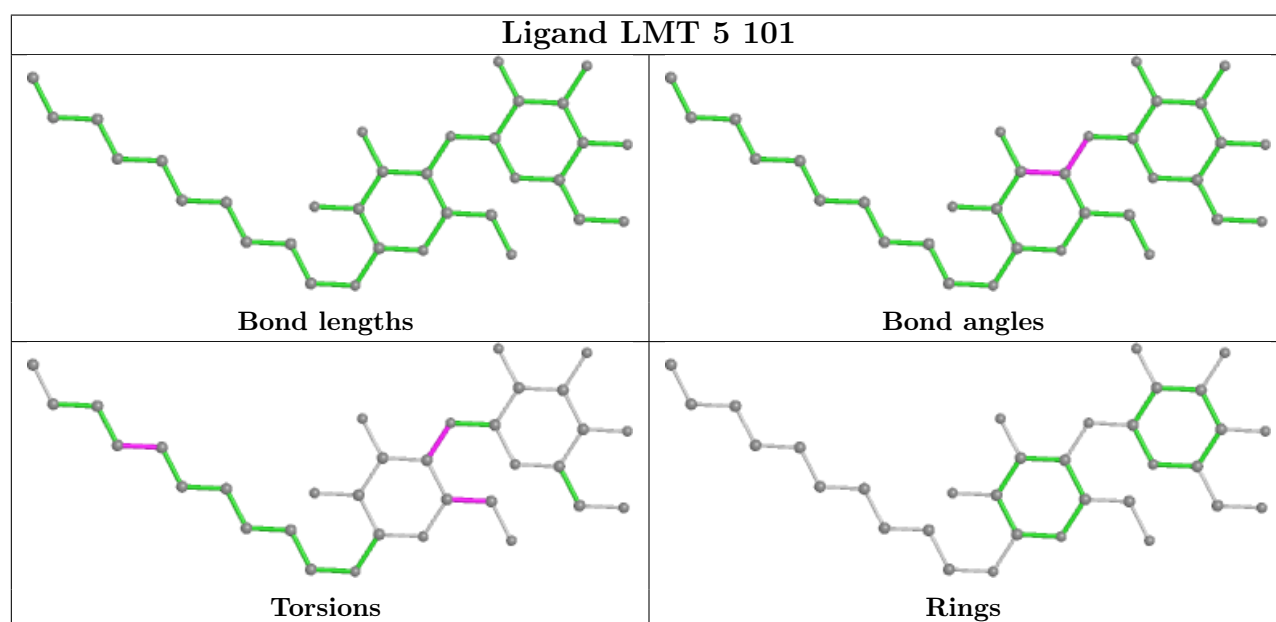
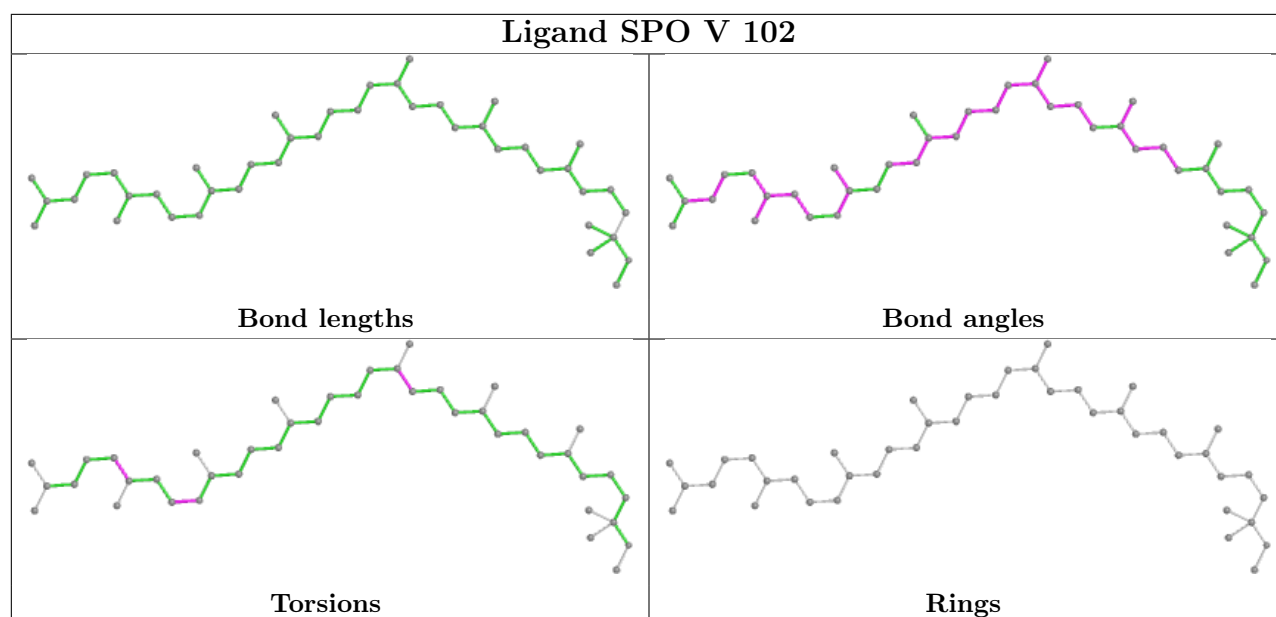


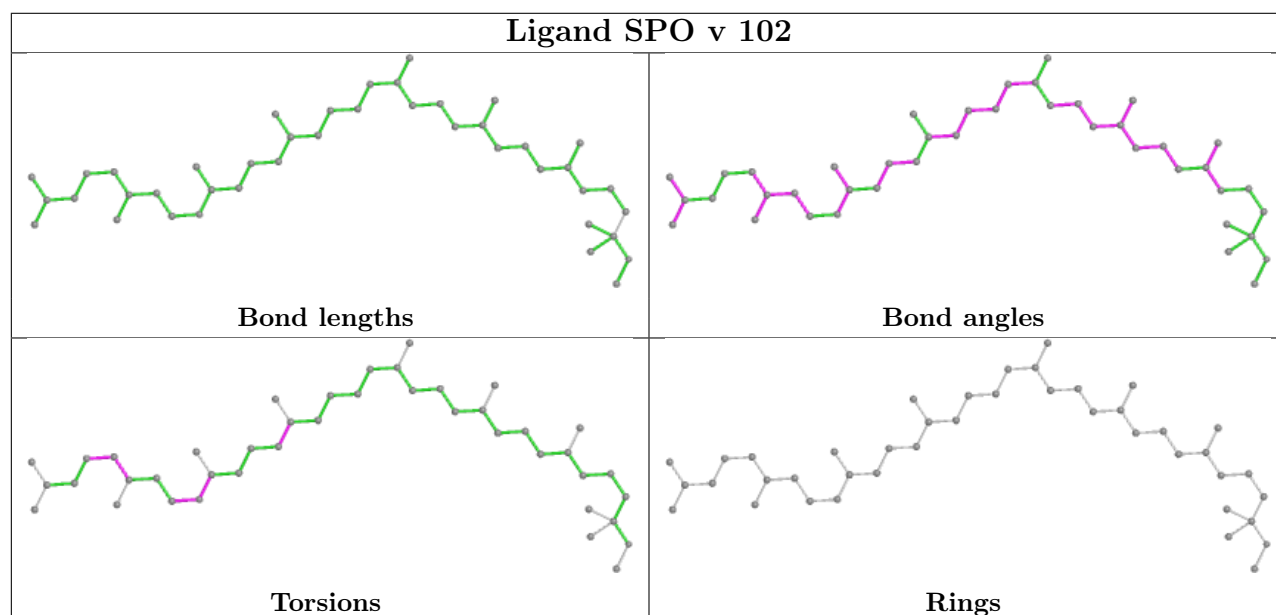
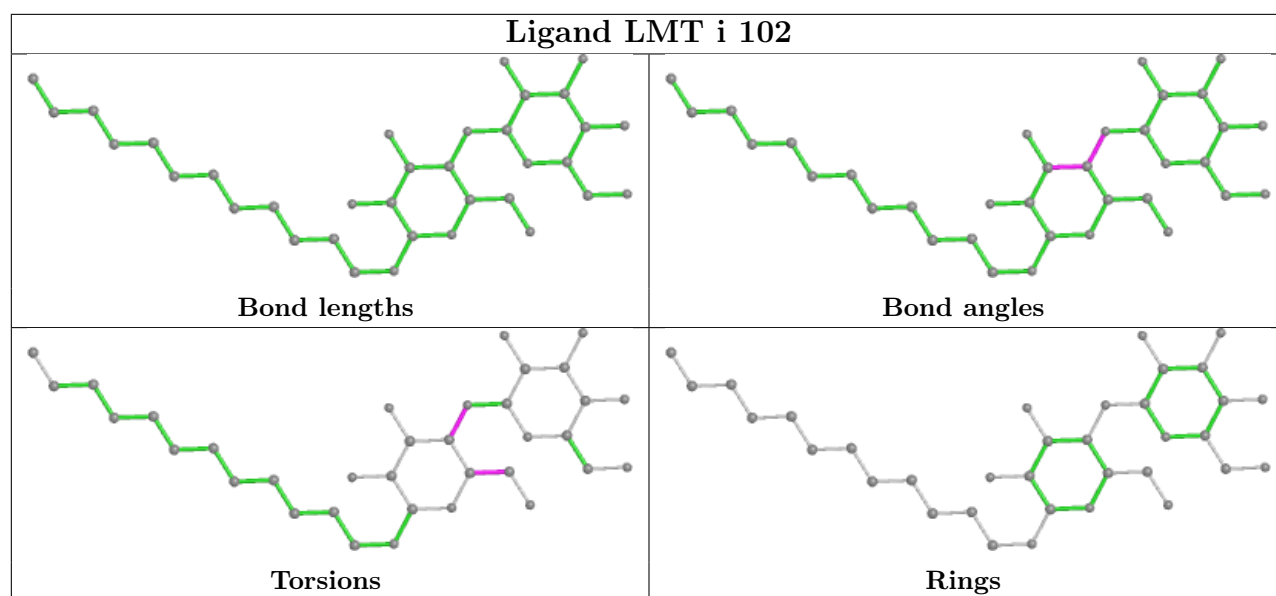


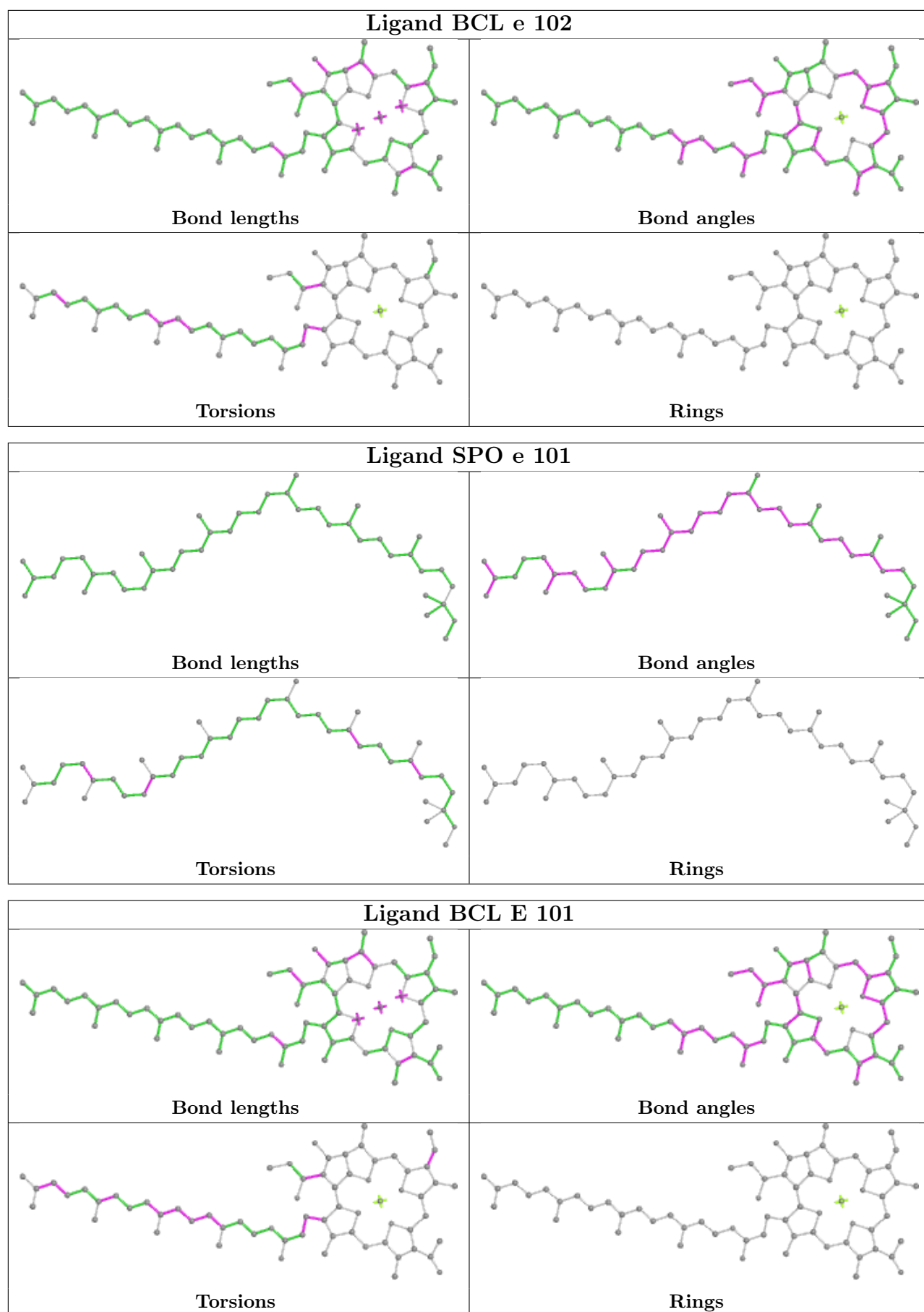


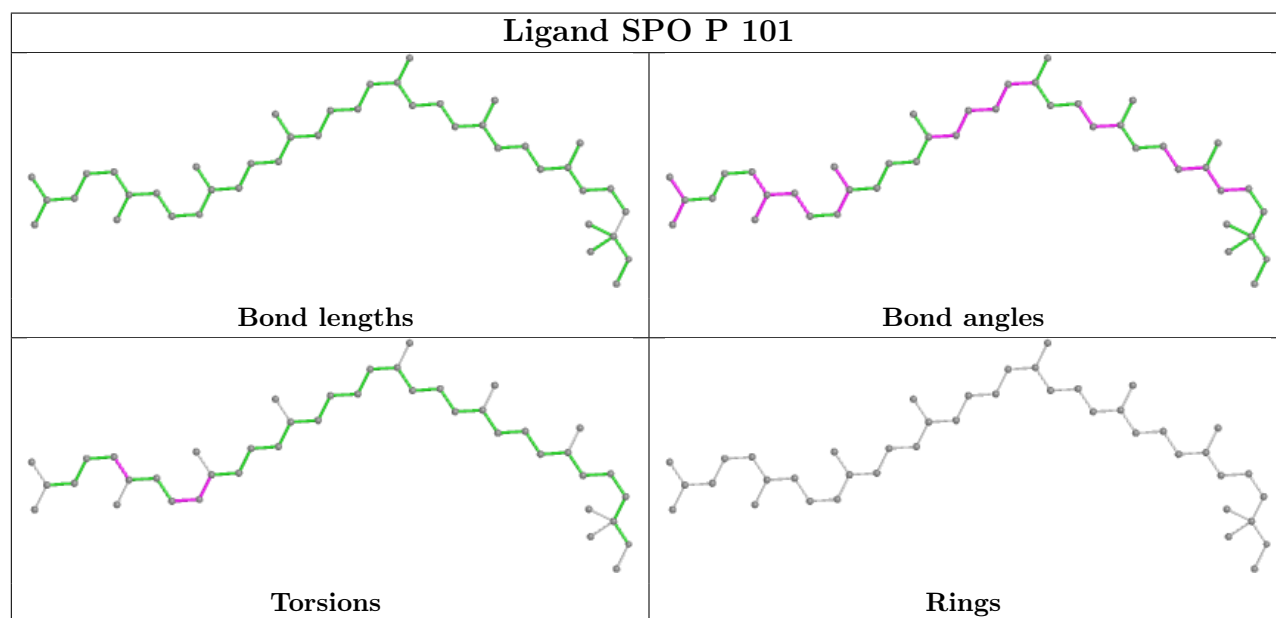
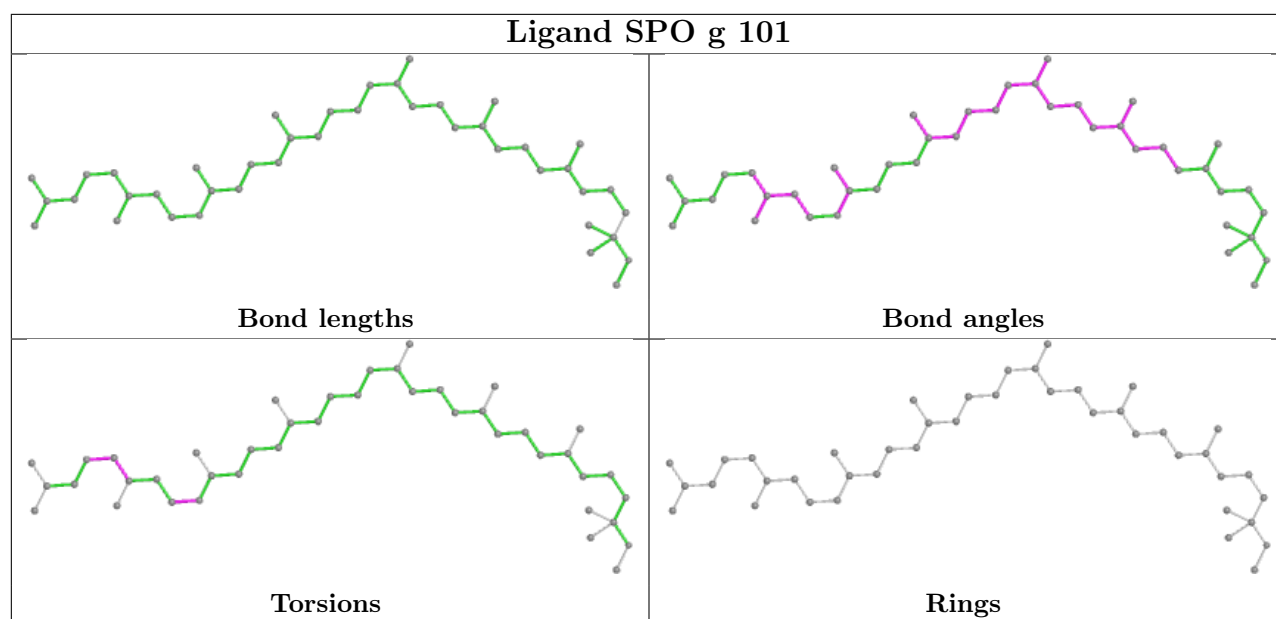


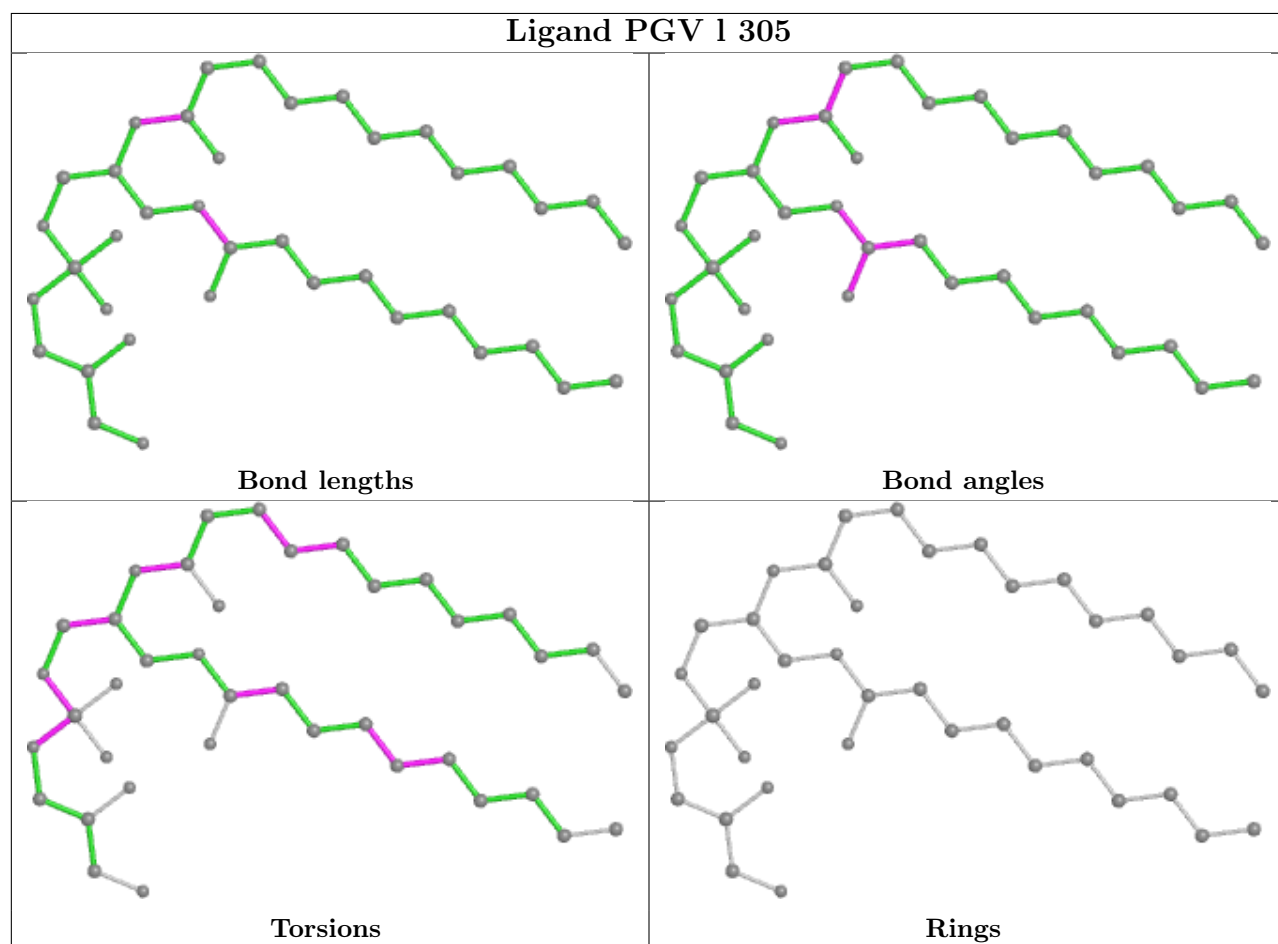
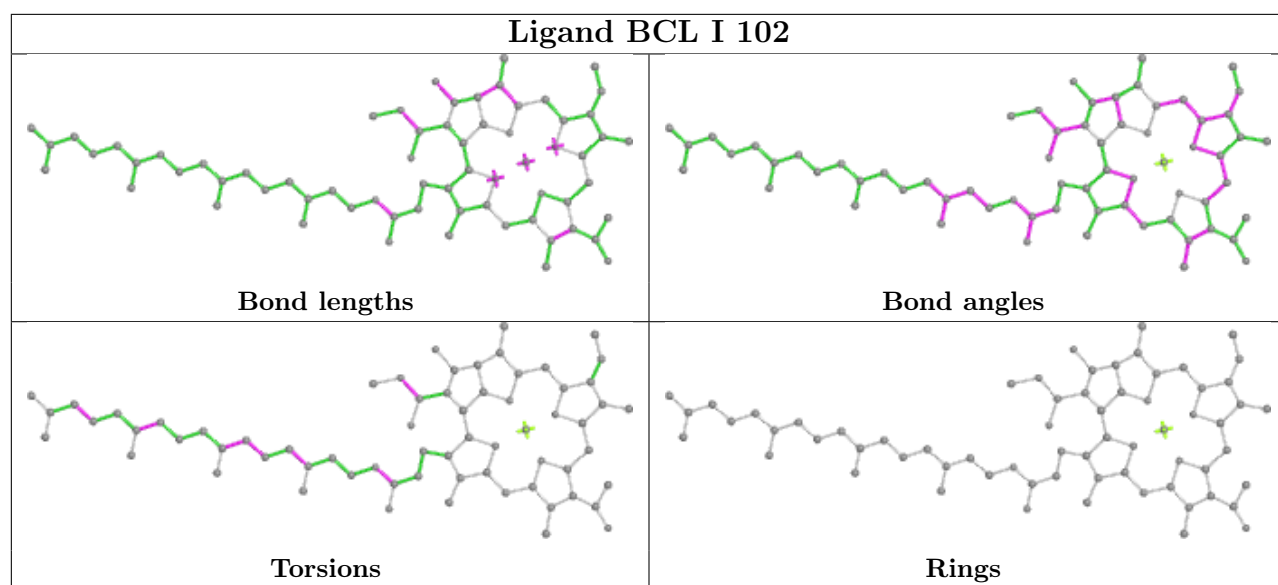


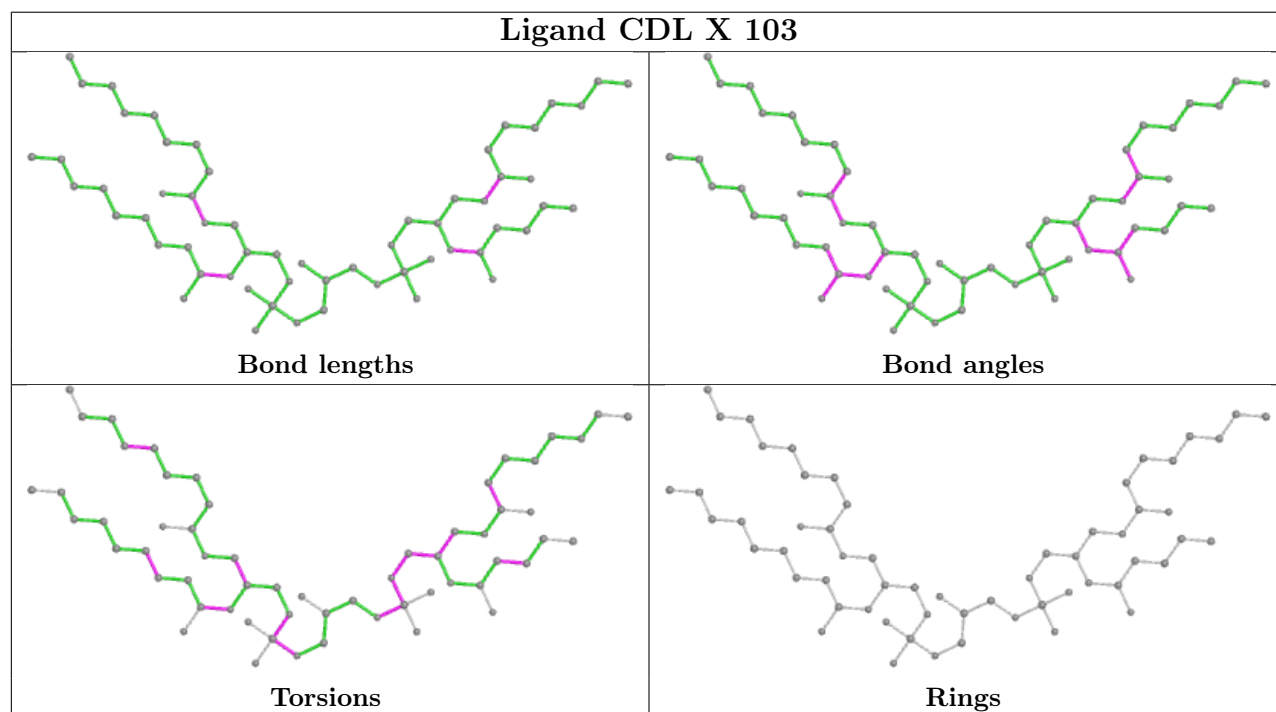
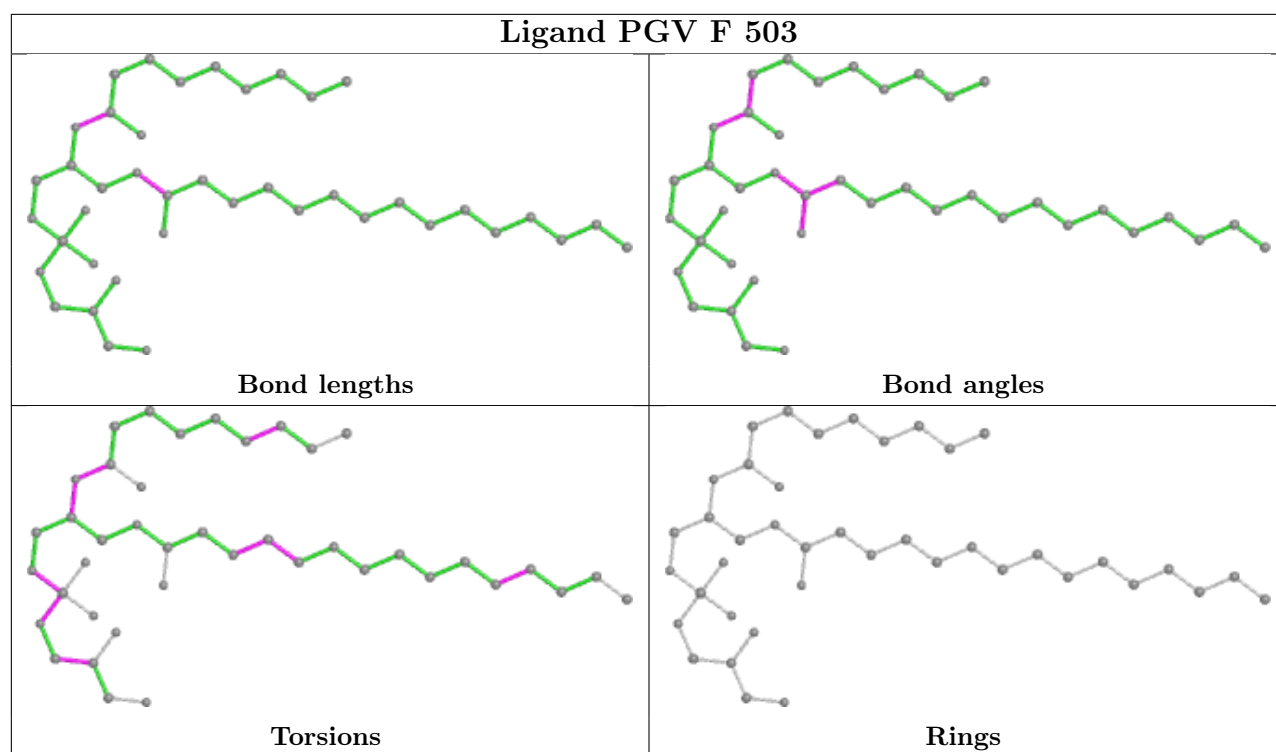


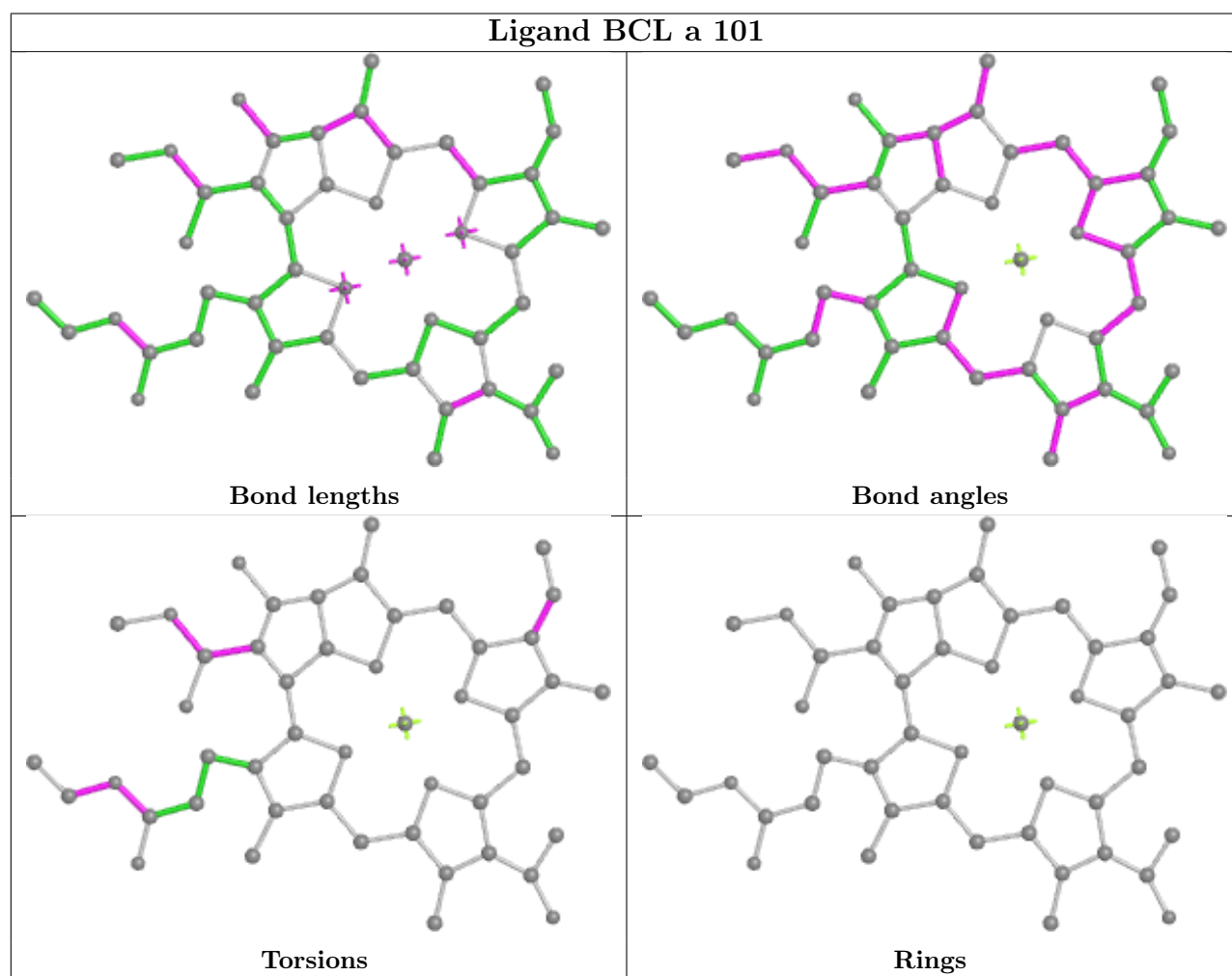
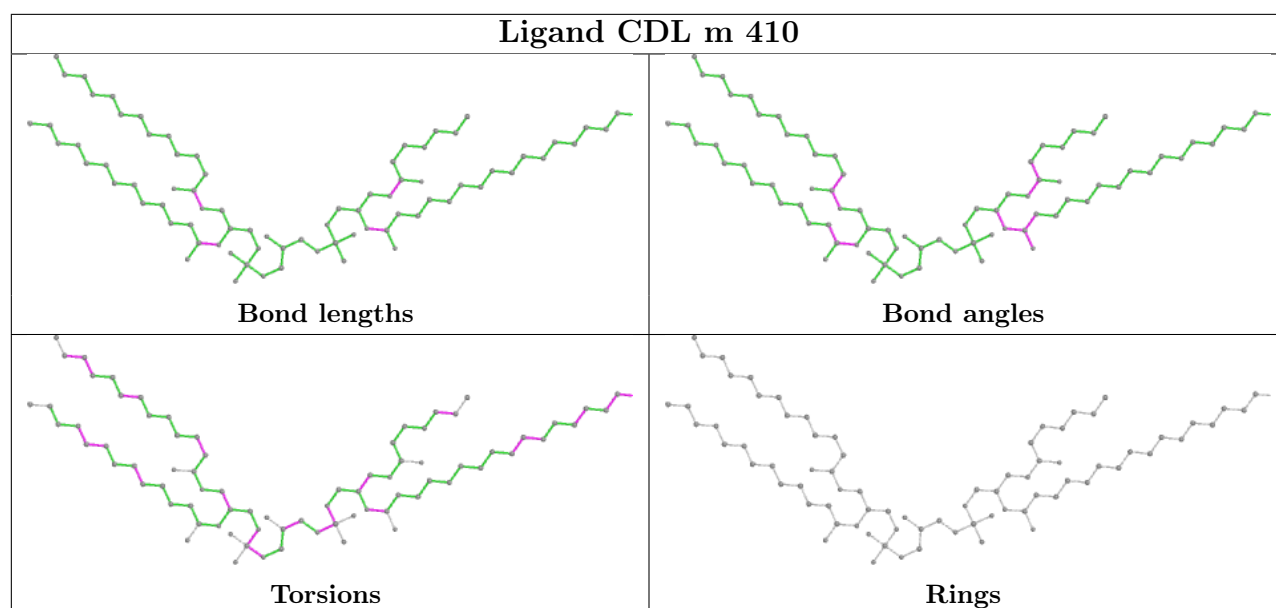


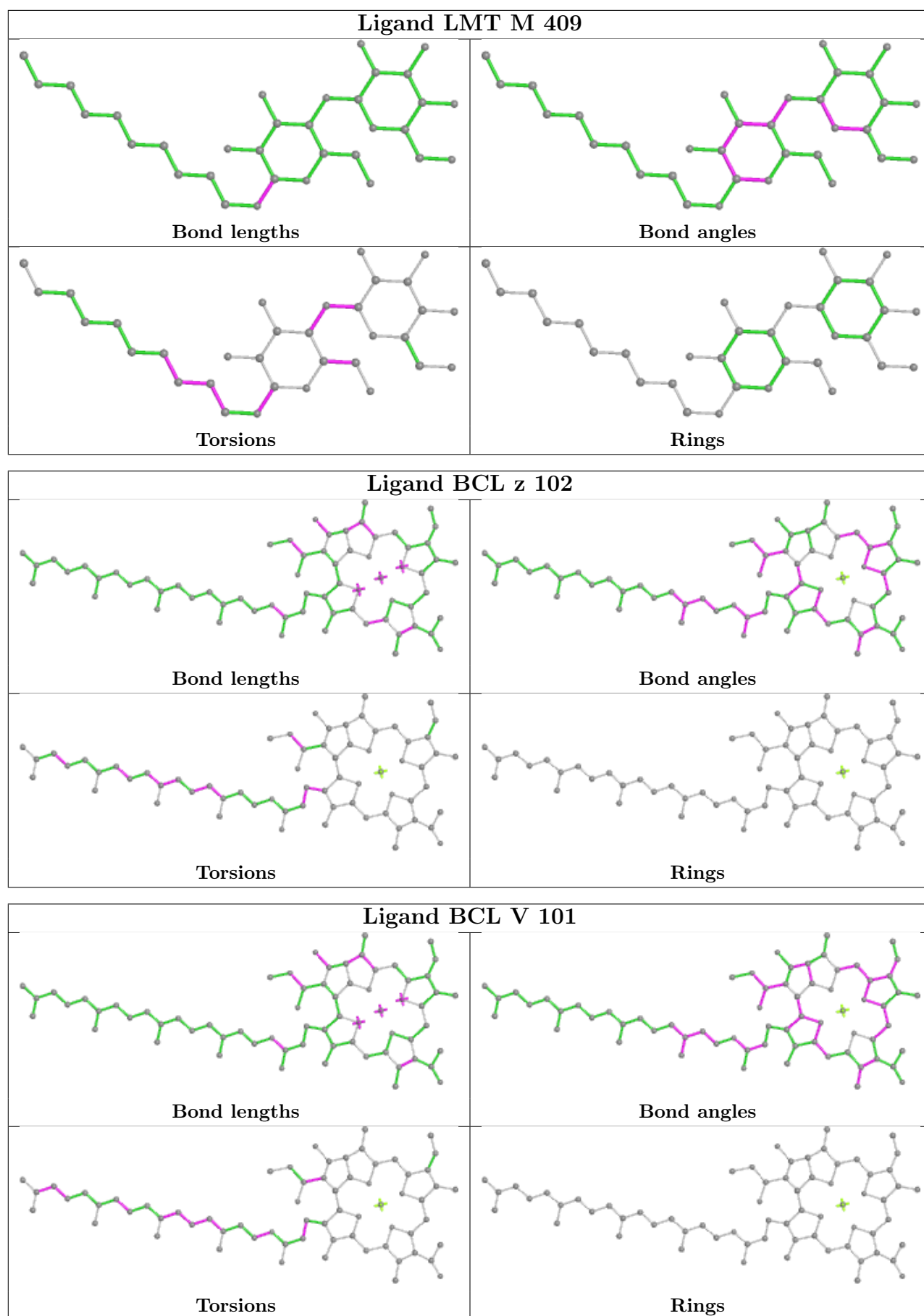


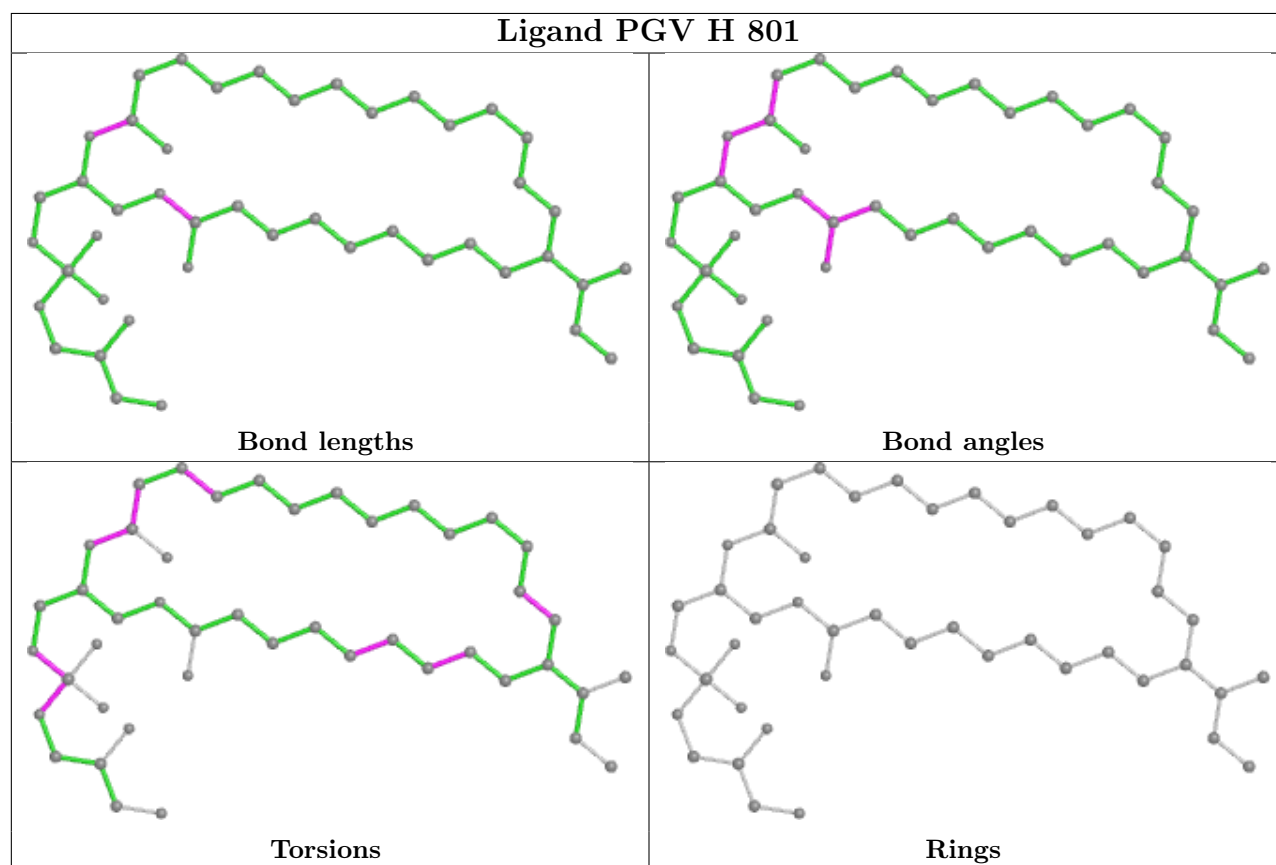
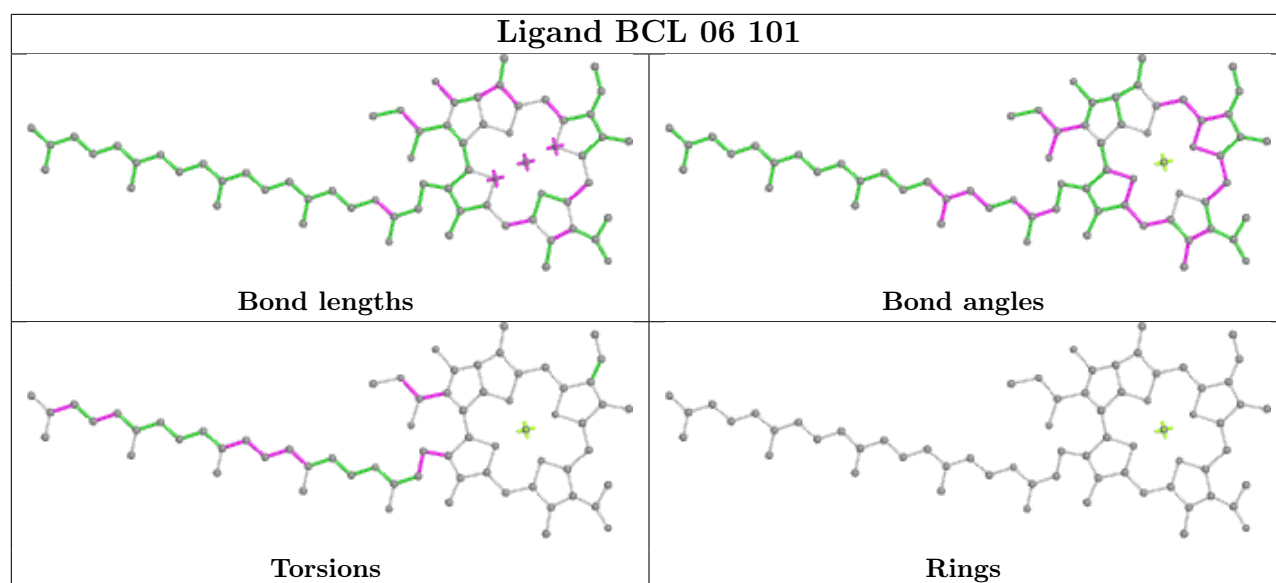


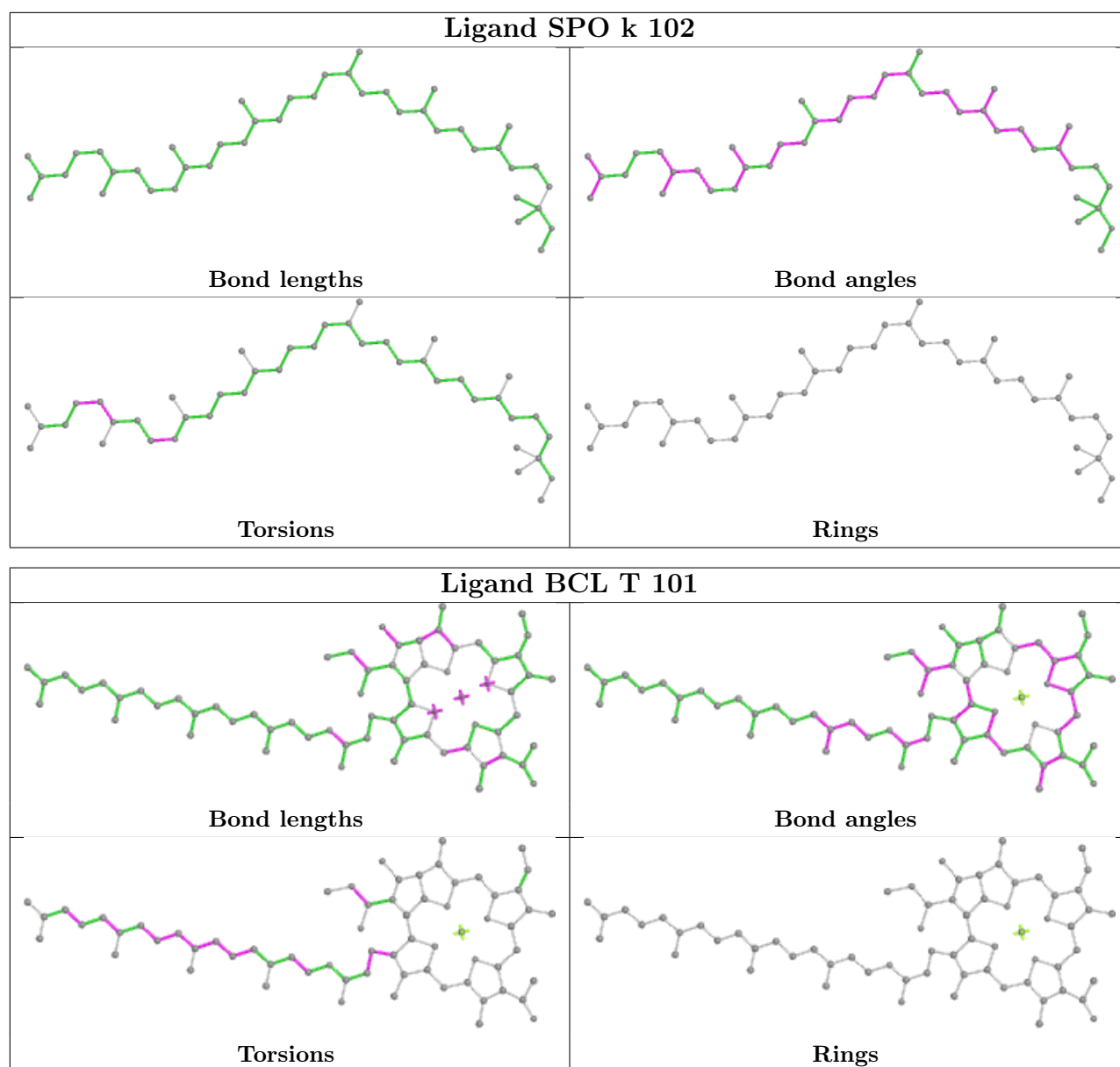












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

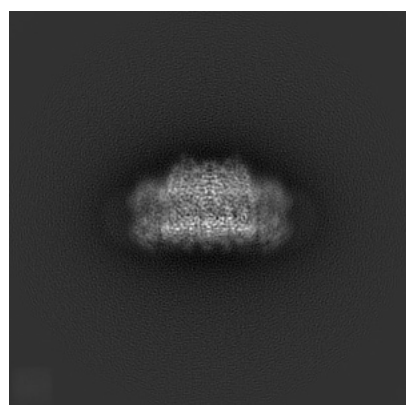
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32192. These allow visual inspection of the internal detail of the map and identification of artifacts.

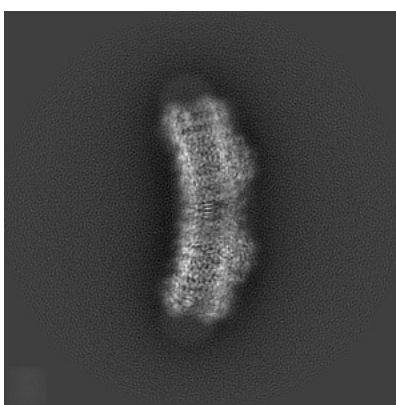
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

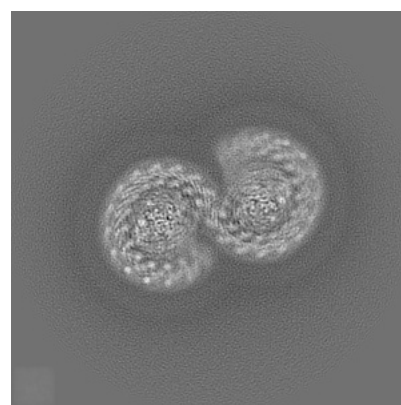
6.1.1 Primary map



X



Y

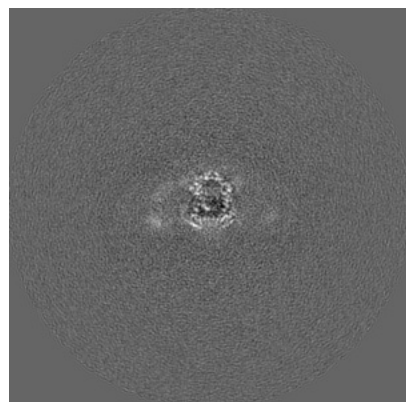


Z

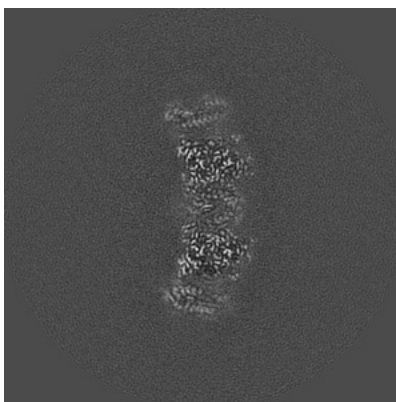
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

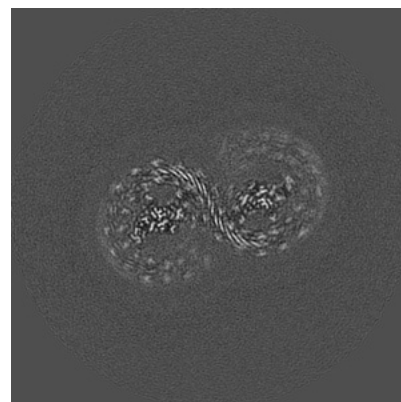
6.2.1 Primary map



X Index: 225



Y Index: 225

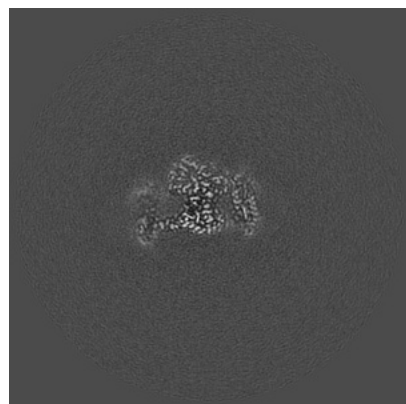


Z Index: 225

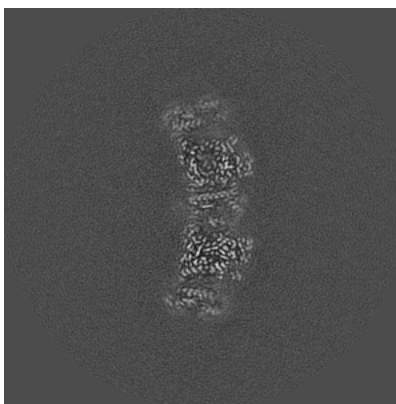
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

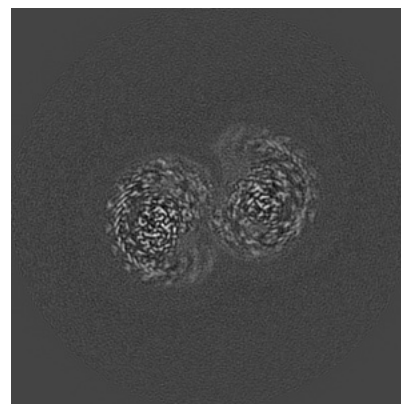
6.3.1 Primary map



X Index: 163



Y Index: 221



Z Index: 209

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

6.4 Orthogonal surface views [i](#)

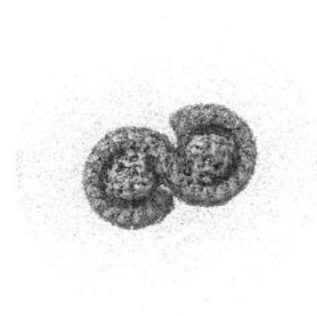
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

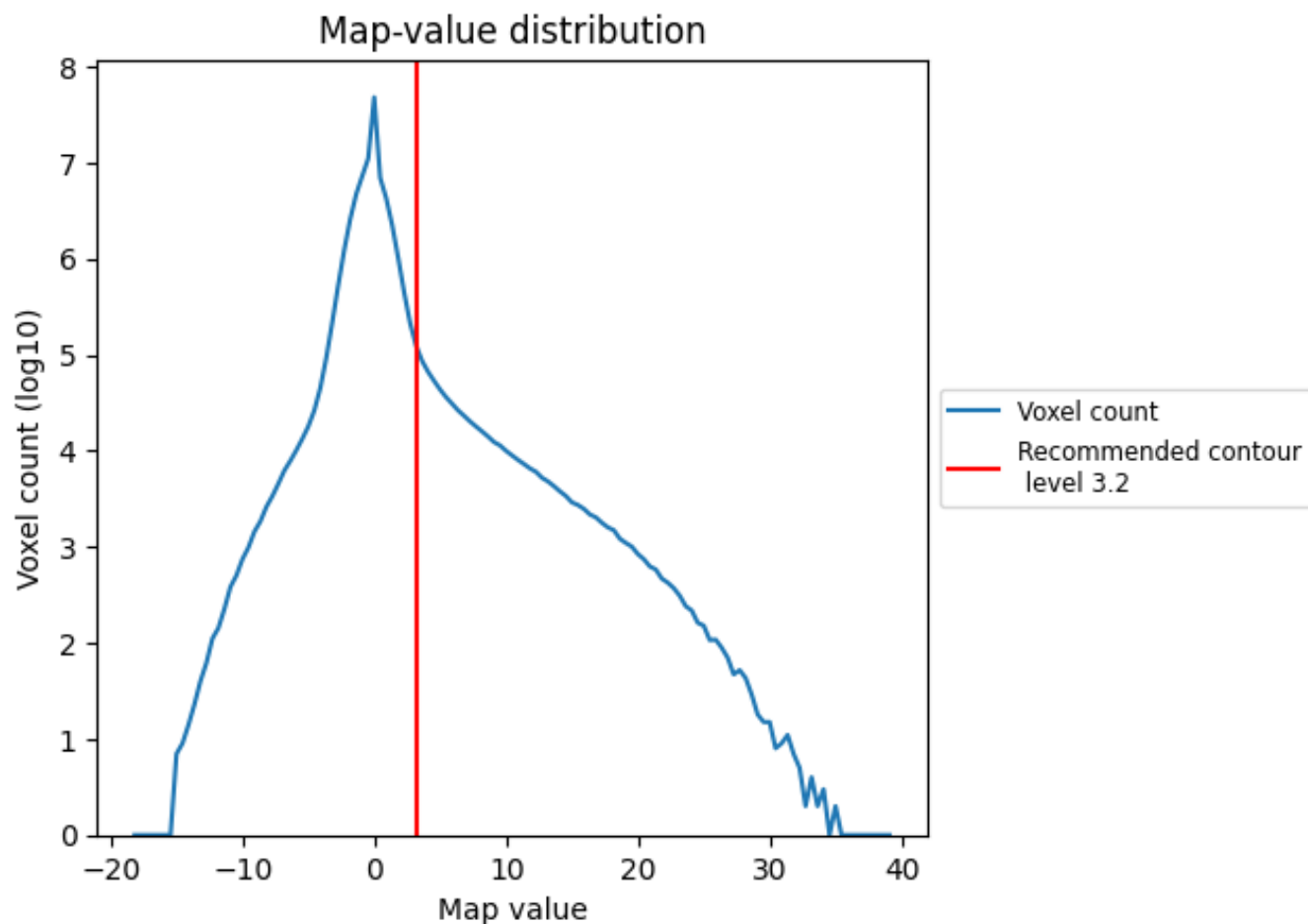
6.5 Mask visualisation

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

7 Map analysis [i](#)

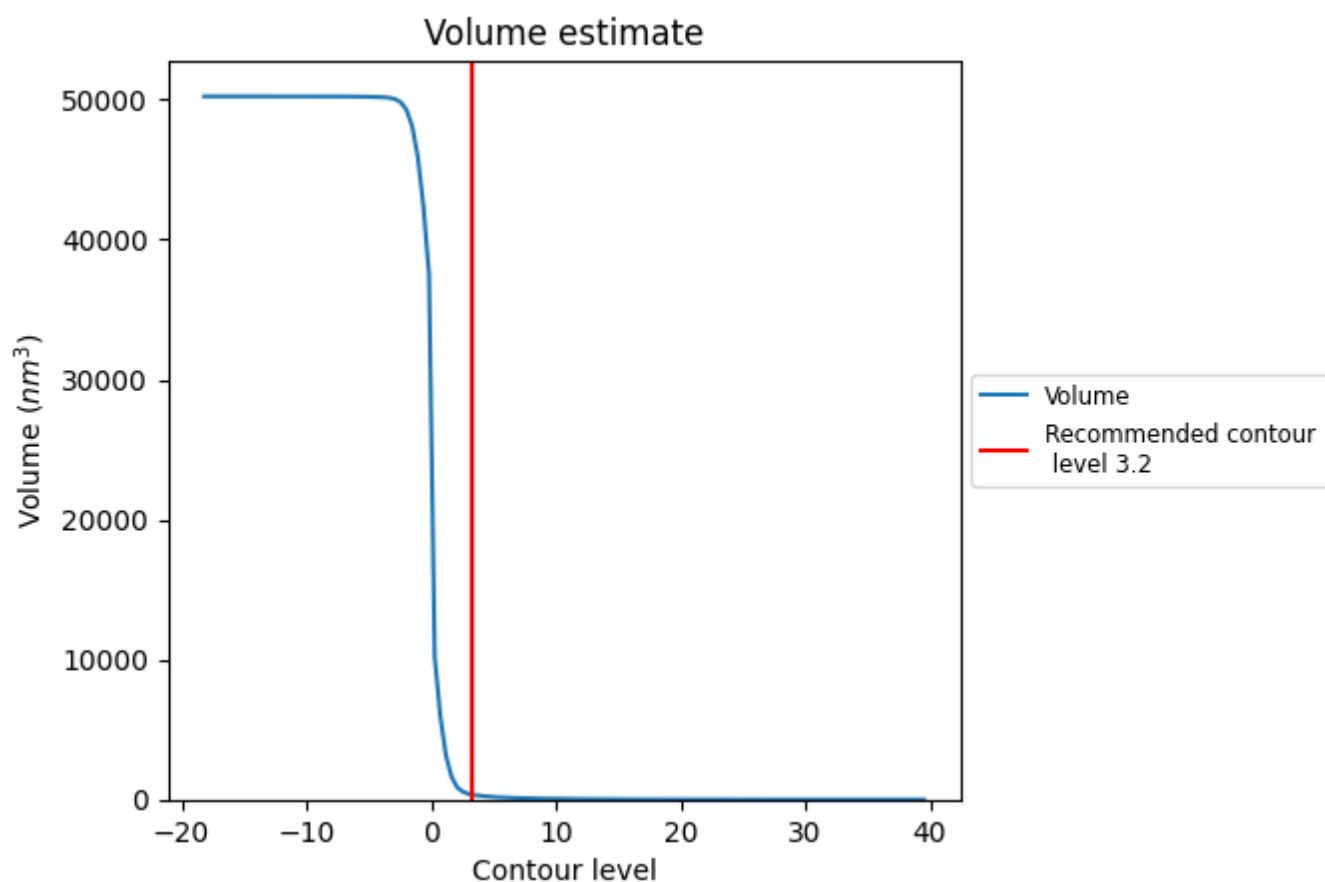
This section contains the results of statistical analysis of the map.

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.

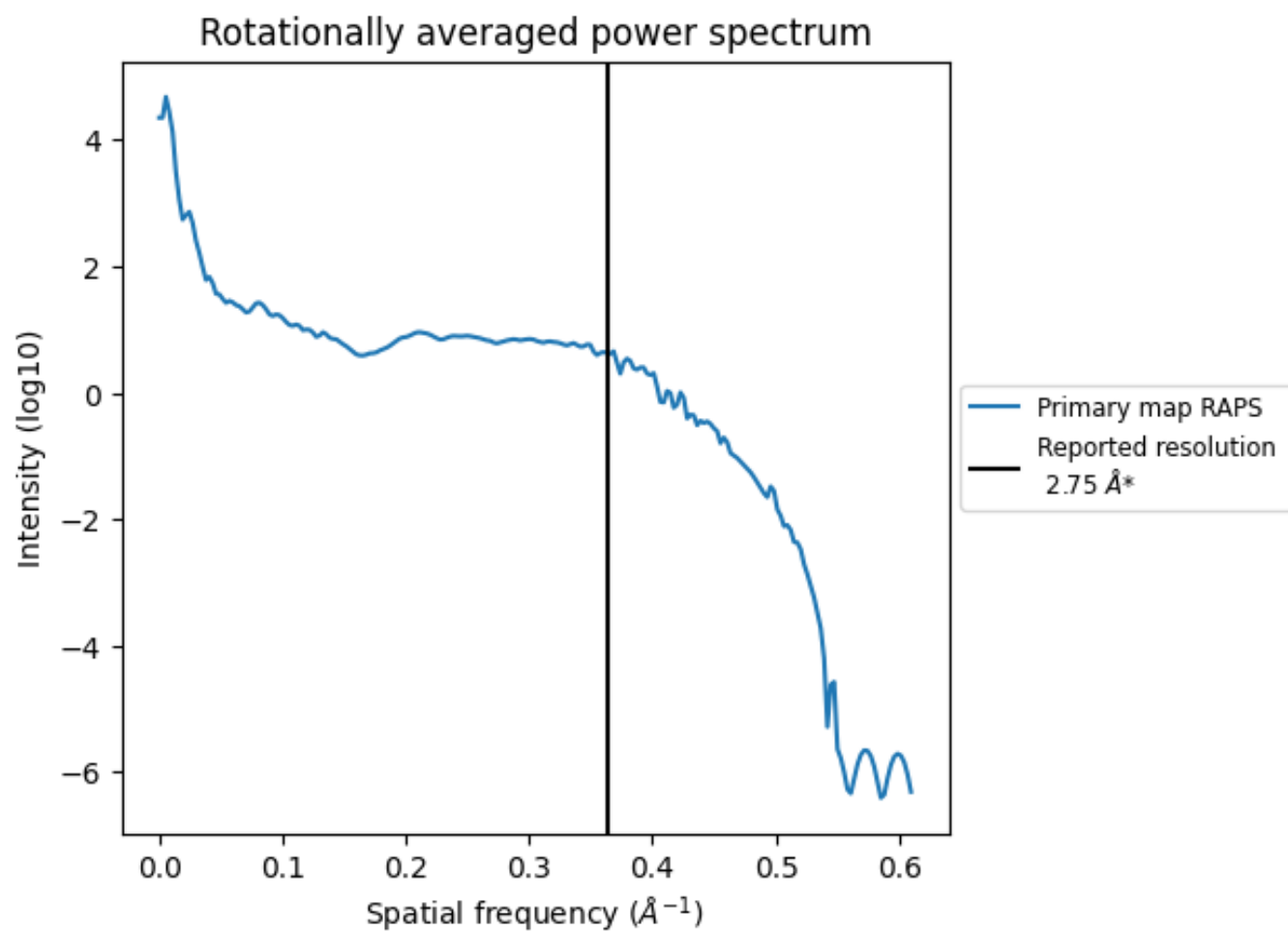
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 369 nm^3 ; this corresponds to an approximate mass of 334 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

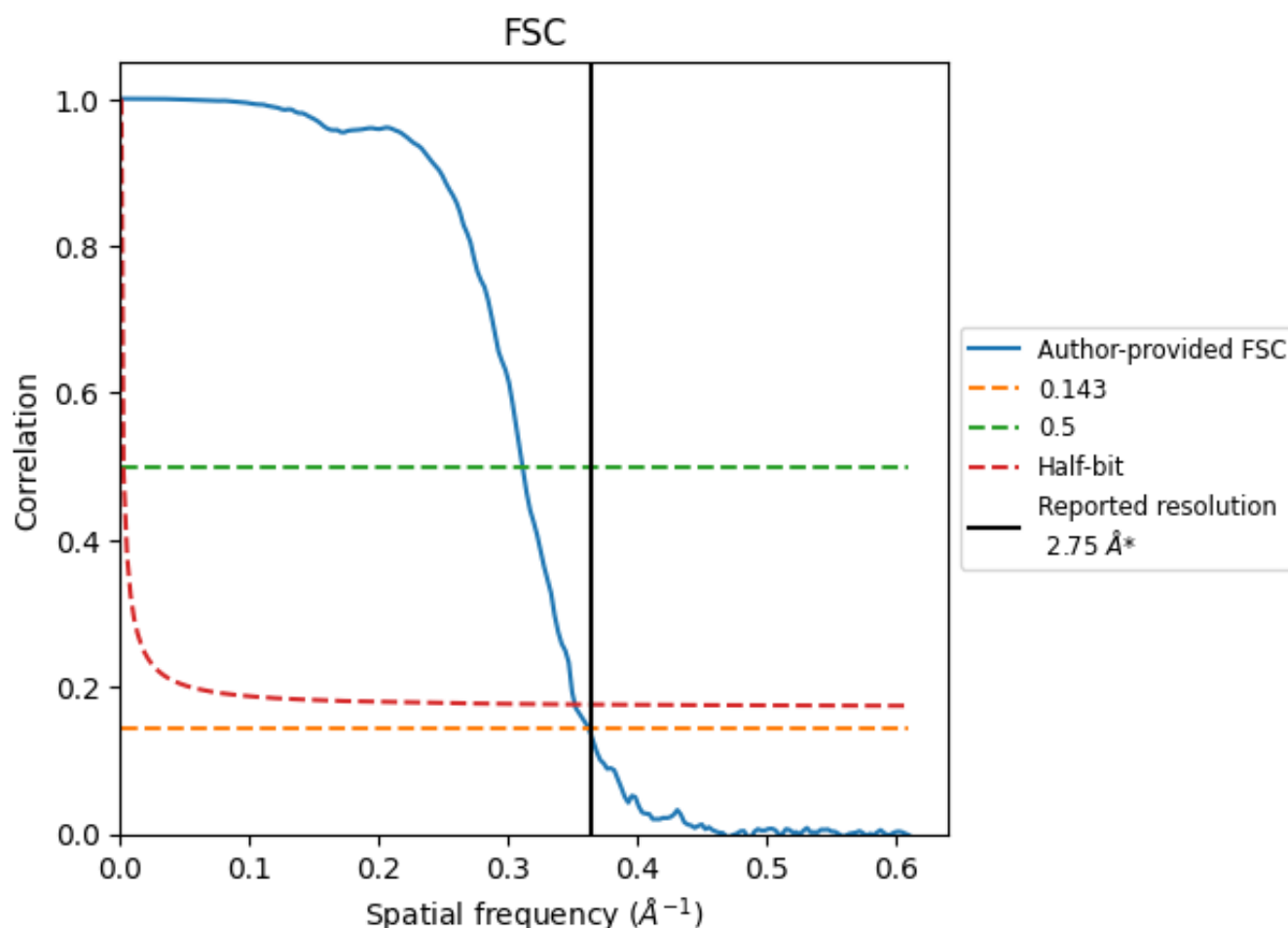


*Reported resolution corresponds to spatial frequency of 0.364 Å⁻¹

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 0.364 Å⁻¹

8.2 Resolution estimates [i](#)

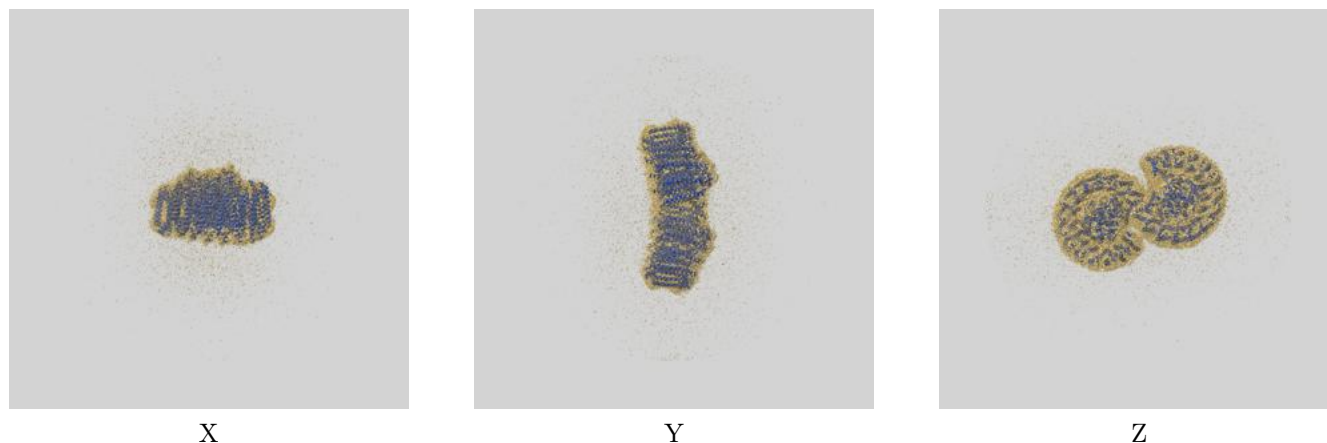
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.76	3.22	2.84
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

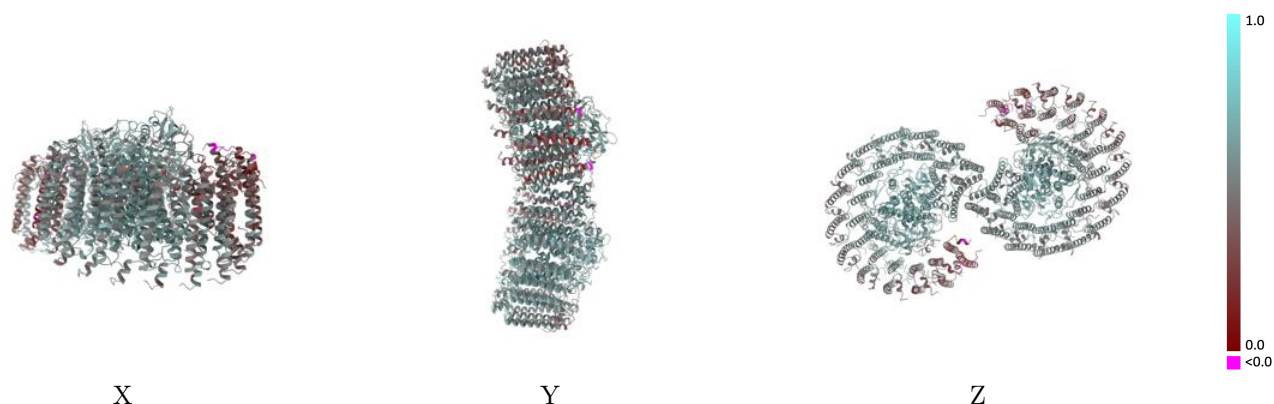
This section contains information regarding the fit between EMDB map EMD-32192 and PDB model 7VY2. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



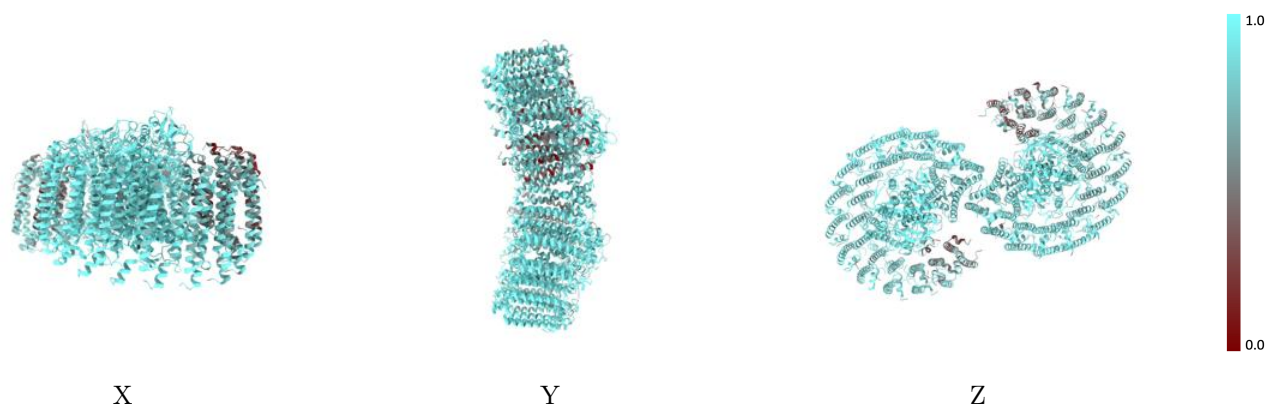
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



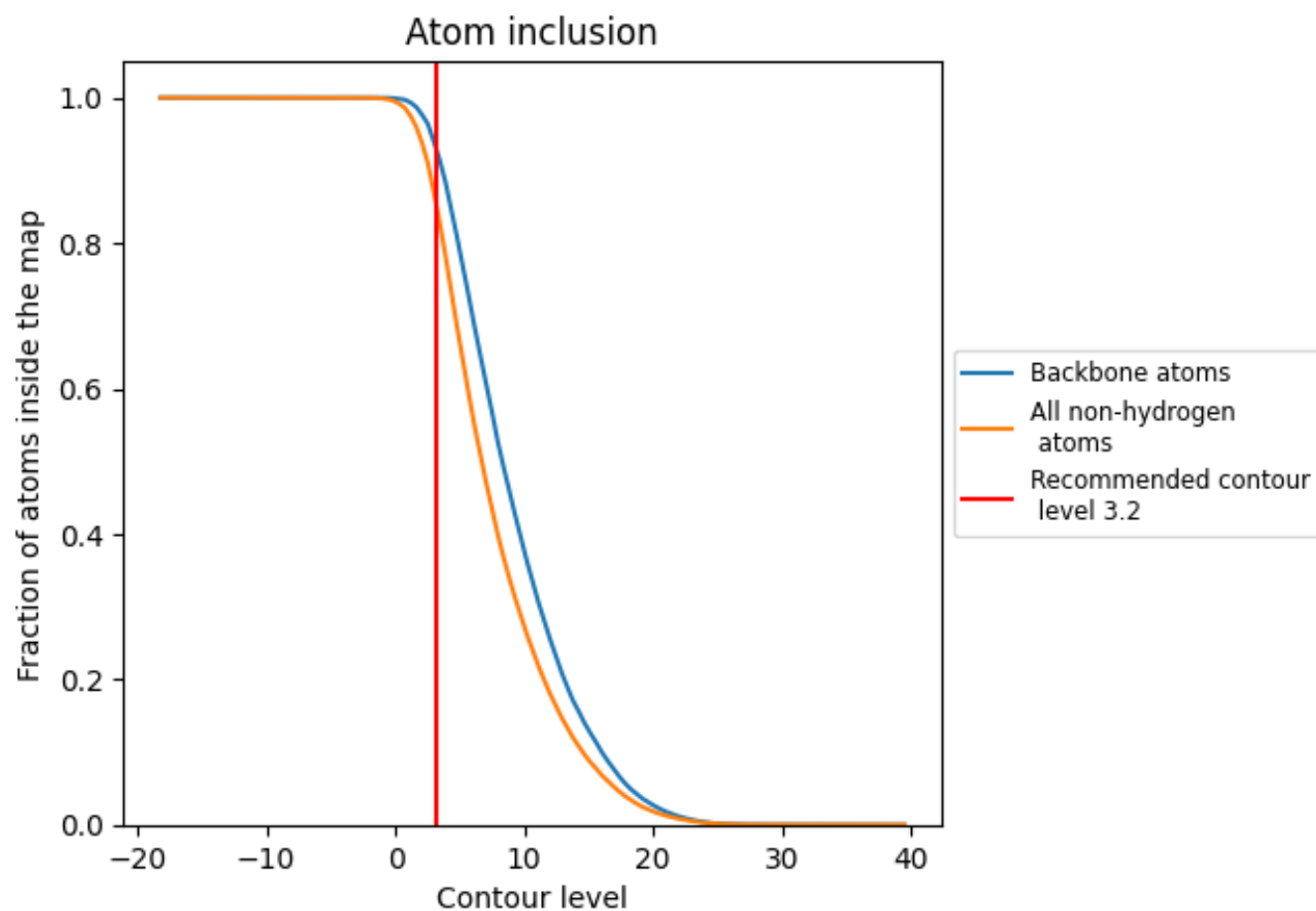
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

































































The table lists the average atom inclusion at the recommended contour level (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8524	 0.5340
01	 0.8581	 0.5400
02	 0.8497	 0.5040
03	 0.7877	 0.4750
04	 0.7407	 0.3920
05	 0.6289	 0.3950
06	 0.6848	 0.3400
07	 0.5332	 0.2820
08	 0.5090	 0.2570
1	 0.7768	 0.4610
2	 0.6864	 0.4350
3	 0.6225	 0.3840
4	 0.6174	 0.3640
5	 0.5951	 0.3770
6	 0.4848	 0.2950
7	 0.5418	 0.3420
8	 0.4841	 0.3260
A	 0.9082	 0.5620
B	 0.8652	 0.5340
D	 0.9275	 0.5610
E	 0.8546	 0.5180
F	 0.9034	 0.5560
G	 0.8270	 0.5140
H	 0.9313	 0.5860
I	 0.8906	 0.5410
J	 0.8635	 0.5020
K	 0.8466	 0.5330
L	 0.9372	 0.6060
M	 0.9212	 0.6020
N	 0.8523	 0.5060
O	 0.8590	 0.5110
P	 0.8143	 0.4950
Q	 0.8093	 0.5000
R	 0.8172	 0.4950
S	 0.8010	 0.5010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	 0.8054	 0.4800
U	 0.5022	 0.4050
V	 0.8095	 0.4950
W	 0.8030	 0.4440
X	 0.8422	 0.5170
Y	 0.7504	 0.4640
Z	 0.7951	 0.4490
a	 0.9353	 0.5570
b	 0.9111	 0.5610
d	 0.9366	 0.5730
e	 0.9217	 0.5580
f	 0.9092	 0.5780
g	 0.8867	 0.5620
h	 0.9453	 0.6110
i	 0.8981	 0.5510
j	 0.8837	 0.5490
k	 0.9019	 0.5630
l	 0.9541	 0.6310
m	 0.9624	 0.6480
n	 0.8569	 0.5310
o	 0.9206	 0.5640
p	 0.8725	 0.5250
q	 0.9178	 0.5630
r	 0.8557	 0.5010
s	 0.8960	 0.5680
t	 0.8889	 0.5250
u	 0.4085	 0.3190
v	 0.9211	 0.5720
w	 0.8668	 0.5080
x	 0.8660	 0.5180
y	 0.8596	 0.5560
z	 0.8568	 0.5040