



## wwPDB EM Validation Summary Report ⓘ

Jun 12, 2024 – 06:29 PM JST

PDB ID : 7VOR  
EMDB ID : EMD-32058  
Title : The structure of dimeric photosynthetic RC-LH1 supercomplex in Class-1  
Authors : Cao, P.; Li, M.; Liu, L.N.  
Deposited on : 2021-10-14  
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev92
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	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

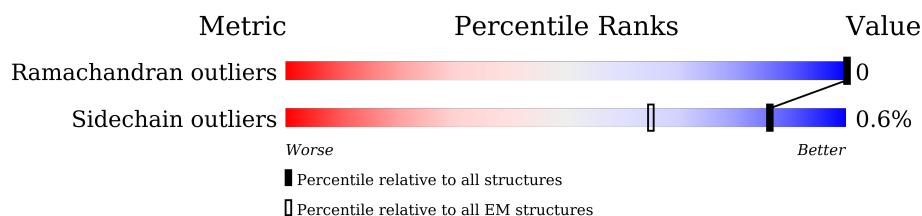
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

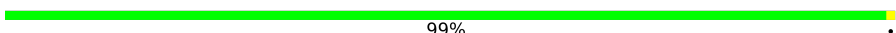
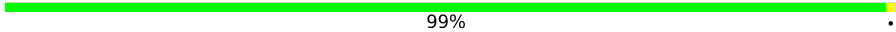
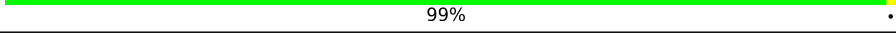
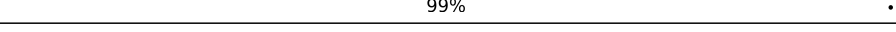
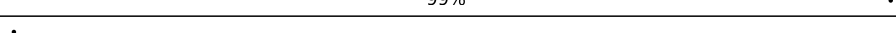




The reported resolution of this entry is 2.74 Å.

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.





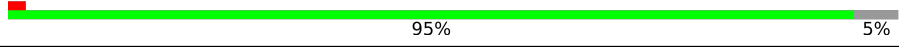
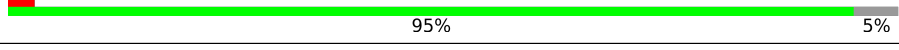
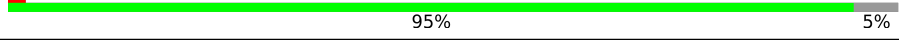
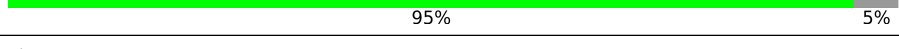
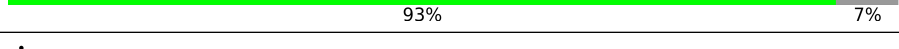
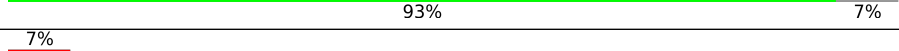
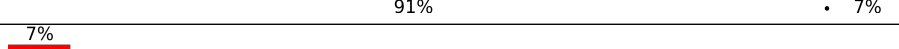
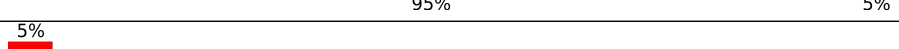
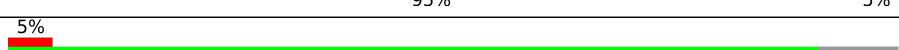
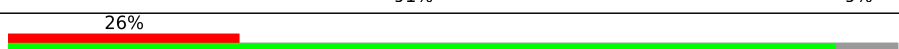
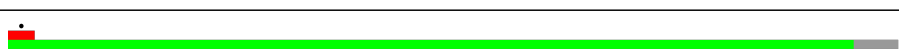

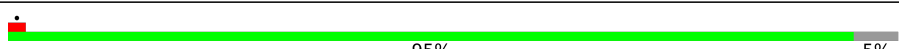
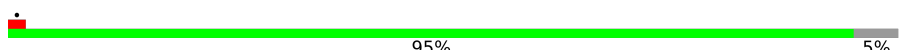
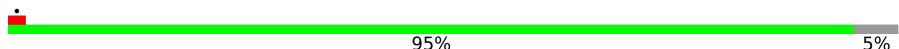
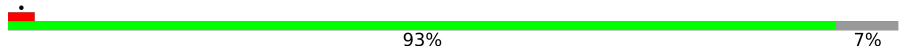
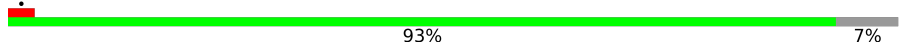

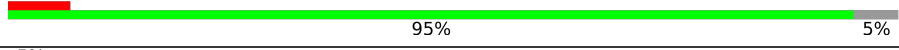
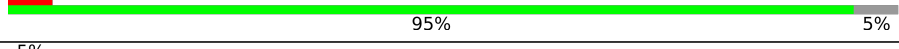
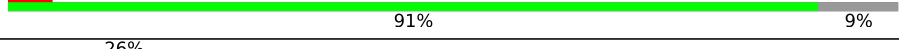
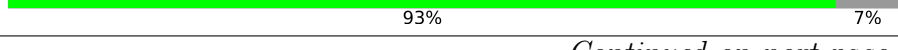

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	L	282	 99% .
1	l	282	 99% .
2	M	308	 99% .
2	m	308	 99% .
3	H	260	 99% .
3	h	260	 99% .
4	1	58	 66% 81% 19%
4	3	58	 55% 88% . 10%
4	5	58	 55% 88% . 10%

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Mol	Chain	Length	Quality of chain
4	6	58	
4	7	58	
4	9	58	
4	A	58	
4	D	58	
4	F	58	
4	I	58	
4	K	58	
4	O	58	
4	Q	58	
4	S	58	
4	U	58	
4	W	58	
4	a	58	
4	b1	58	
4	b9	58	
4	d	58	
4	f	58	
4	i	58	
4	k	58	
4	o	58	
4	q	58	
4	s	58	
4	u	58	
4	w	58	

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Mol	Chain	Length	Quality of chain
5	0	49	
5	2	49	
5	4	49	
5	8	49	
5	B	49	
5	C	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	V	49	
5	Z	49	
5	b	49	
5	b0	49	
5	b8	49	
5	c	49	
5	e	49	
5	g	49	
5	j	49	
5	n	49	
5	p	49	
5	r	49	

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Mol	Chain	Length	Quality of chain
5	t	49	<div><div></div><div>84%</div><div>14%</div></div>
5	v	49	<div><div>16%</div><div>86%</div><div>14%</div></div>
5	z	49	<div><div>73%</div><div>84%</div><div>14%</div></div>
6	X	82	<div><div>6%</div><div>83%</div><div>17%</div></div>
6	x	82	<div><div>6%</div><div>83%</div><div>17%</div></div>
7	Y	53	<div><div></div><div>92%</div><div>8%</div></div>
7	y	53	<div><div>83%</div><div>92%</div><div>8%</div></div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 44980 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		
1	l	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		
2	m	307	Total	C	N	O	S	0	0
			2445	1630	400	404	11		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	260	Total	C	N	O	S	0	0
			1973	1264	335	363	11		
3	h	260	Total	C	N	O	S	0	0
			1973	1264	335	363	11		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	D	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	F	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	O	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	Q	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	S	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	U	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	W	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	3	52	Total	C	N	O	S	0	0
			437	299	70	66	2		
4	1	47	Total	C	N	O	S	0	0
			392	266	64	60	2		
4	7	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	9	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	a	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	d	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	f	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	i	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	k	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	o	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	q	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	s	55	Total	C	N	O	S	0	0
			460	313	74	70	3		
4	u	53	Total	C	N	O	S	0	0
			447	305	72	68	2		
4	w	54	Total	C	N	O	S	0	0
			452	308	73	69	2		
4	5	52	Total	C	N	O	S	0	0
			437	299	70	66	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	b1	47	Total	C	N	O	S	0	0
			392	266	64	60	2		
4	6	48	Total	C	N	O	S	0	0
			403	277	62	61	3		
4	b9	55	Total	C	N	O	S	0	0
			460	313	74	70	3		

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	E	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	G	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	J	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	N	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	P	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	R	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	T	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	V	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	C	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	Z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	2	38	Total	C	N	O	S	0	0
			309	206	50	52	1		
5	8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	0	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	b	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	e	43	Total	C	N	O	S	0	0
			352	236	55	60	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	j	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	n	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	p	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	r	43	Total	C	N	O	S	0	0
			352	236	55	60	1		
5	t	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	v	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	c	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	z	42	Total	C	N	O	S	0	0
			344	230	54	59	1		
5	4	38	Total	C	N	O	S	0	0
			309	206	50	52	1		
5	b8	44	Total	C	N	O	S	0	0
			360	240	56	63	1		
5	b0	44	Total	C	N	O	S	0	0
			360	240	56	63	1		

- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	68	Total	C	N	O	S	0	0
			529	345	93	88	3		
6	x	68	Total	C	N	O	S	0	0
			529	345	93	88	3		

- Molecule 7 is a protein called Rsp\_7571 Protein-Y PufY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	49	Total	C	N	O	S	0	0
			361	248	55	55	3		
7	y	49	Total	C	N	O	S	0	0
			361	248	55	55	3		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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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	U	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	C	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
8	Z	1	Total 56	C 45	Mg 1	N 4	O 6	0
8	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
8	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
8	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	0	1	Total 61	C 50	Mg 1	N 4	O 6	0
8	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	l	1	Total 63	C 52	Mg 1	N 4	O 6	0
8	m	1	Total 66	C 55	Mg 1	N 4	O 6	0

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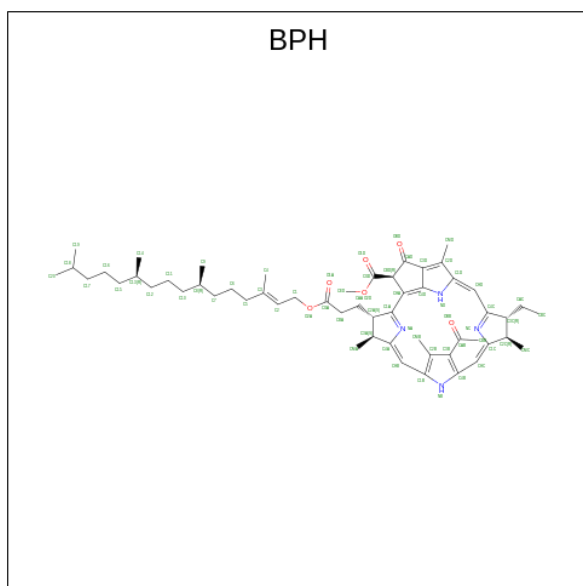
Mol	Chain	Residues	Atoms					AltConf
8	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	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	u	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	c	1	Total 61	C 50	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
8	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
8	z	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	b1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	b9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	b0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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



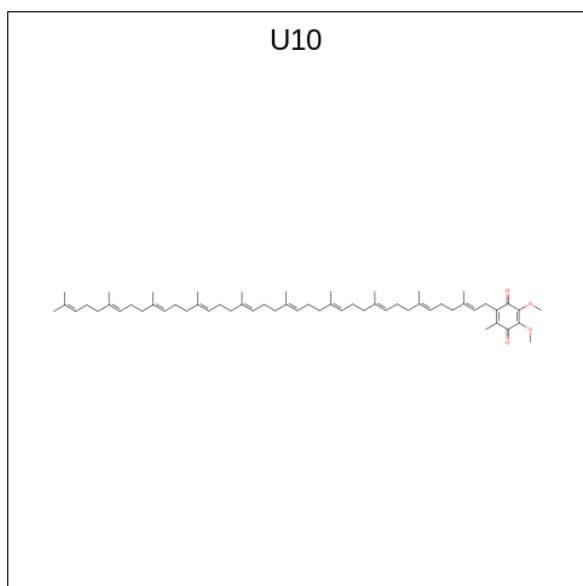
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			65	55	4	6	
9	M	1	Total	C	N	O	0
			55	45	4	6	
9	l	1	Total	C	N	O	0
			65	55	4	6	

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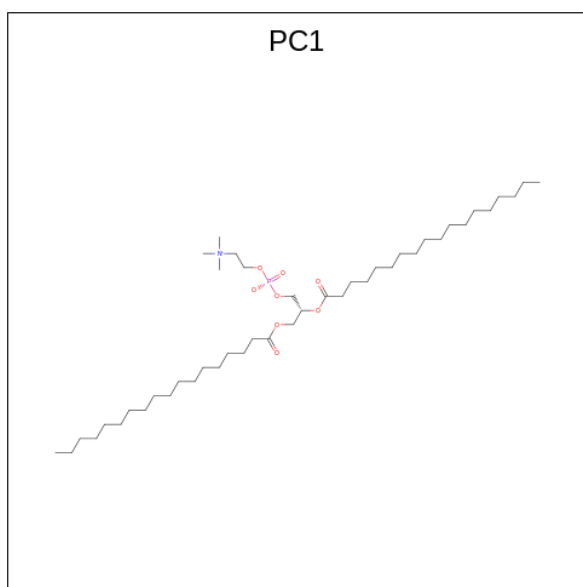
Mol	Chain	Residues	Atoms				AltConf
9	m	1	Total	C	N	O	0
			55	45	4	6	

- 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
			38	34	4		
10	L	1	Total	C	O		0
			43	39	4		
10	M	1	Total	C	O		0
			48	44	4		
10	l	1	Total	C	O		0
			38	34	4		
10	l	1	Total	C	O		0
			43	39	4		
10	m	1	Total	C	O		0
			48	44	4		

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
11	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	H	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	H	1	Total	C	N	O	P	0
			34	24	1	8	1	
11	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
11	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
11	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
11	D	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	l	1	Total	C	N	O	P	0
			39	29	1	8	1	
11	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
11	h	1	Total	C	N	O	P	0
			43	33	1	8	1	
11	h	1	Total	C	N	O	P	0
			34	24	1	8	1	
11	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
11	a	1	Total	C	N	O	P	0
			31	21	1	8	1	

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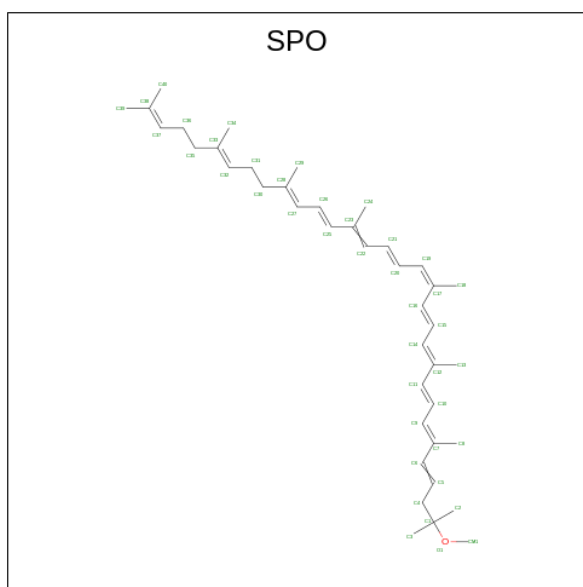
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Mol	Chain	Residues	Atoms					AltConf
11	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
11	d	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).



Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			42	41	1	
13	A	1	Total	C	O	0
			42	41	1	
13	B	1	Total	C	O	0
			42	41	1	
13	D	1	Total	C	O	0
			42	41	1	
13	E	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
13	E	1	Total 42	C 41	O 1	0
13	G	1	Total 42	C 41	O 1	0
13	G	1	Total 42	C 41	O 1	0
13	I	1	Total 42	C 41	O 1	0
13	J	1	Total 42	C 41	O 1	0
13	N	1	Total 42	C 41	O 1	0
13	O	1	Total 42	C 41	O 1	0
13	P	1	Total 42	C 41	O 1	0
13	Q	1	Total 42	C 41	O 1	0
13	Q	1	Total 42	C 41	O 1	0
13	Q	1	Total 42	C 41	O 1	0
13	S	1	Total 42	C 41	O 1	0
13	S	1	Total 42	C 41	O 1	0
13	U	1	Total 42	C 41	O 1	0
13	U	1	Total 42	C 41	O 1	0
13	C	1	Total 42	C 41	O 1	0
13	3	1	Total 42	C 41	O 1	0
13	3	1	Total 42	C 41	O 1	0
13	9	1	Total 42	C 41	O 1	0
13	0	1	Total 42	C 41	O 1	0
13	X	1	Total 42	C 41	O 1	0

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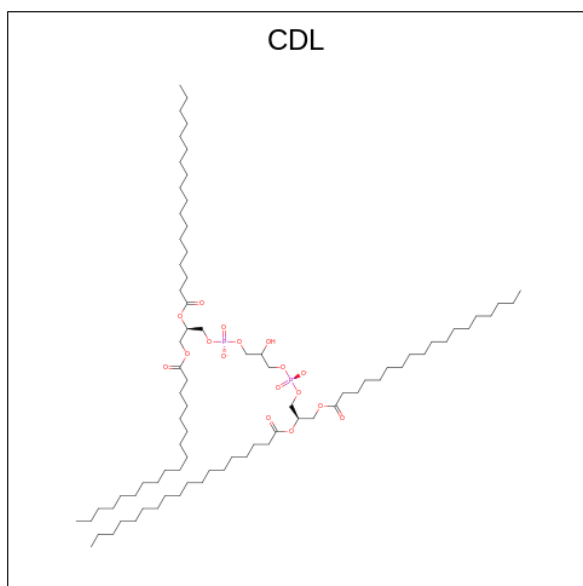
Mol	Chain	Residues	Atoms			AltConf
13	m	1	Total 42	C 41	O 1	0
13	a	1	Total 42	C 41	O 1	0
13	b	1	Total 42	C 41	O 1	0
13	d	1	Total 42	C 41	O 1	0
13	e	1	Total 42	C 41	O 1	0
13	e	1	Total 42	C 41	O 1	0
13	g	1	Total 42	C 41	O 1	0
13	g	1	Total 42	C 41	O 1	0
13	i	1	Total 42	C 41	O 1	0
13	j	1	Total 42	C 41	O 1	0
13	n	1	Total 42	C 41	O 1	0
13	o	1	Total 42	C 41	O 1	0
13	p	1	Total 42	C 41	O 1	0
13	q	1	Total 42	C 41	O 1	0
13	q	1	Total 42	C 41	O 1	0
13	q	1	Total 42	C 41	O 1	0
13	s	1	Total 42	C 41	O 1	0
13	s	1	Total 42	C 41	O 1	0
13	u	1	Total 42	C 41	O 1	0
13	u	1	Total 42	C 41	O 1	0
13	c	1	Total 42	C 41	O 1	0

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Mol	Chain	Residues	Atoms			AltConf
13	5	1	Total	C	O	0
			42	41	1	
13	5	1	Total	C	O	0
			42	41	1	
13	b9	1	Total	C	O	0
			42	41	1	
13	b0	1	Total	C	O	0
			42	41	1	
13	x	1	Total	C	O	0
			42	41	1	

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			82	63	17	2	
14	F	1	Total	C	O	P	0
			63	44	17	2	
14	m	1	Total	C	O	P	0
			82	63	17	2	
14	f	1	Total	C	O	P	0
			63	44	17	2	

### 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.

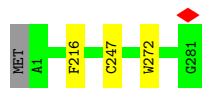
- Molecule 1: Reaction center protein L chain

Chain L:  99%



- Molecule 1: Reaction center protein L chain

Chain l:  99%



- Molecule 2: Reaction center protein M chain

Chain M:  99%



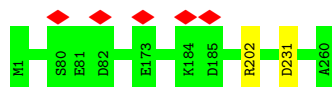
- Molecule 2: Reaction center protein M chain

Chain m:  99%



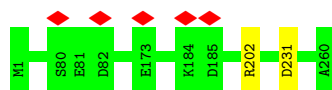
- Molecule 3: Reaction center protein H chain

Chain H:  99%



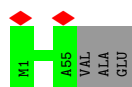
- Molecule 3: Reaction center protein H chain

Chain h:  99%



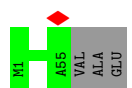
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain A:  95%



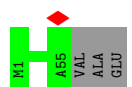
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain D:  95%



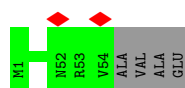
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain F:  95%



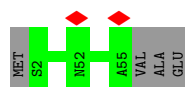
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain I:  93%



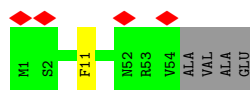
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain K:  93%

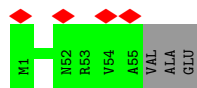


- Molecule 4: Light-harvesting protein B-875 alpha chain

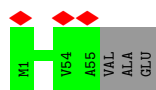
Chain O:  91%



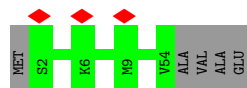
- Molecule 4: Light-harvesting protein B-875 alpha chain



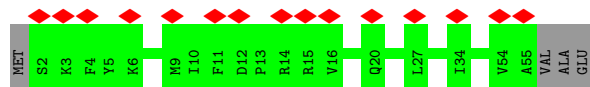
- Molecule 4: Light-harvesting protein B-875 alpha chain



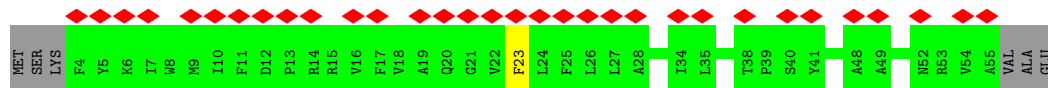
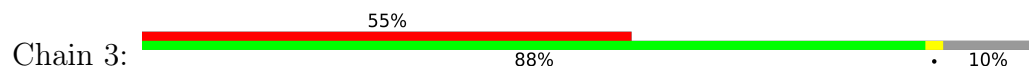
- Molecule 4: Light-harvesting protein B-875 alpha chain



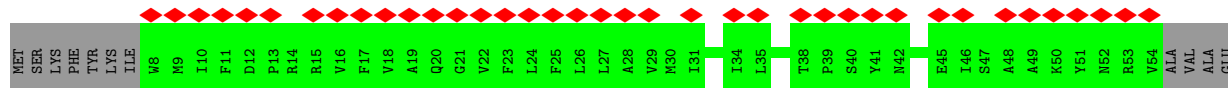
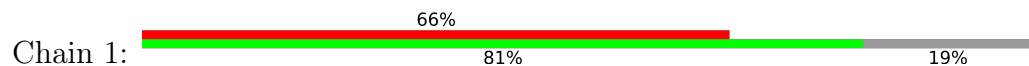
- Molecule 4: Light-harvesting protein B-875 alpha chain



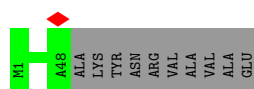
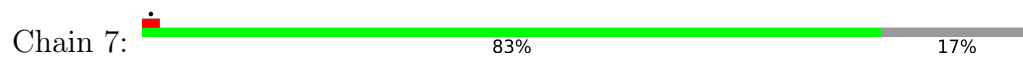
- Molecule 4: Light-harvesting protein B-875 alpha chain



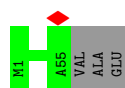
- Molecule 4: Light-harvesting protein B-875 alpha chain



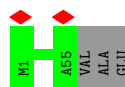
- Molecule 4: Light-harvesting protein B-875 alpha chain



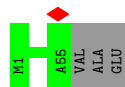
- Molecule 4: Light-harvesting protein B-875 alpha chain



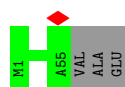
- Molecule 4: Light-harvesting protein B-875 alpha chain



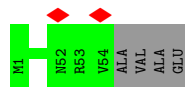
- Molecule 4: Light-harvesting protein B-875 alpha chain



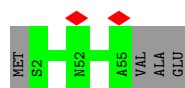
- Molecule 4: Light-harvesting protein B-875 alpha chain



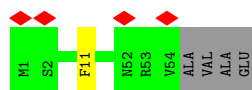
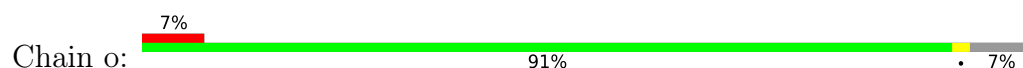
- Molecule 4: Light-harvesting protein B-875 alpha chain



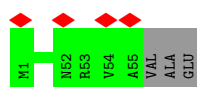
- Molecule 4: Light-harvesting protein B-875 alpha chain



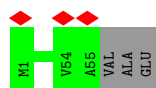
- Molecule 4: Light-harvesting protein B-875 alpha chain



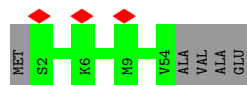
- Molecule 4: Light-harvesting protein B-875 alpha chain



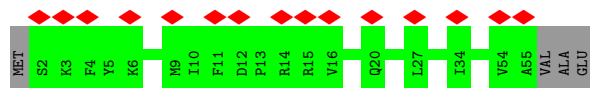
- Molecule 4: Light-harvesting protein B-875 alpha chain



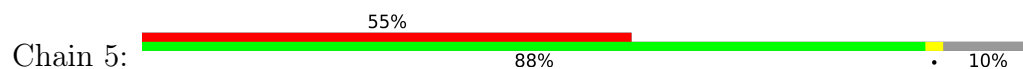
- Molecule 4: Light-harvesting protein B-875 alpha chain



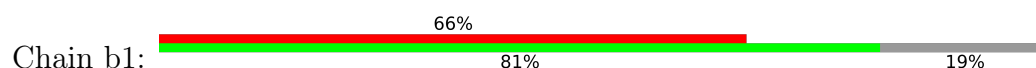
- Molecule 4: Light-harvesting protein B-875 alpha chain



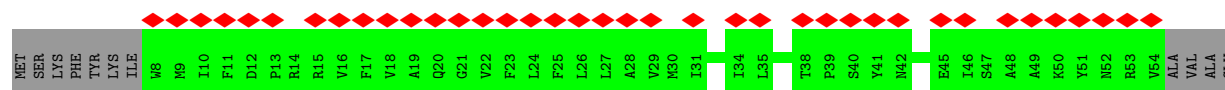
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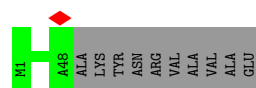
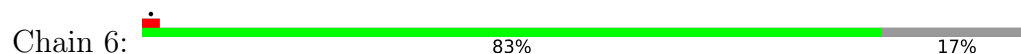
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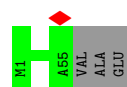




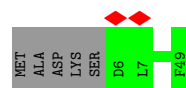
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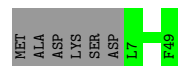
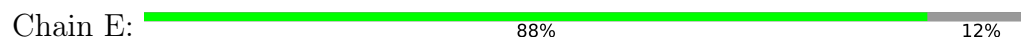
- Molecule 4: Light-harvesting protein B-875 alpha chain



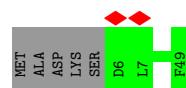
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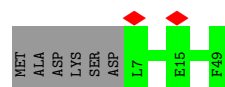
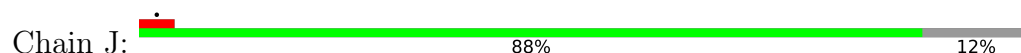
- Molecule 5: Light-harvesting protein B-875 beta chain



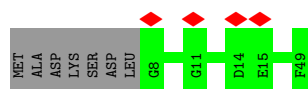
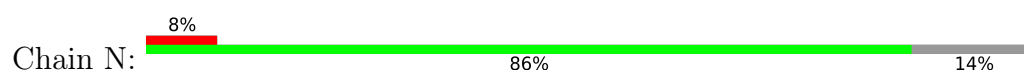
- Molecule 5: Light-harvesting protein B-875 beta chain



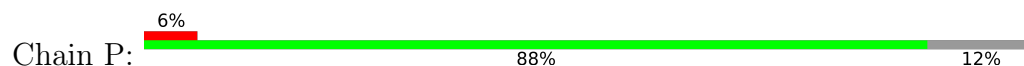
- Molecule 5: Light-harvesting protein B-875 beta chain



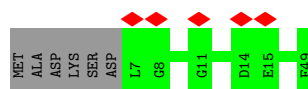
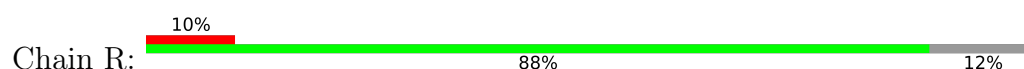
- Molecule 5: Light-harvesting protein B-875 beta chain



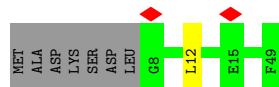
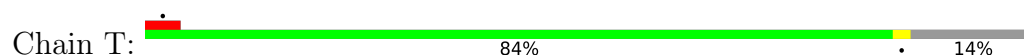
- Molecule 5: Light-harvesting protein B-875 beta chain



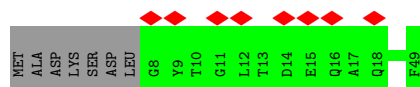
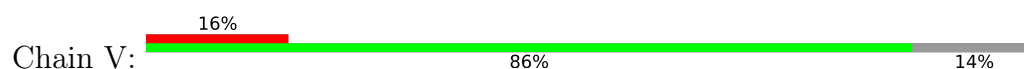
- Molecule 5: Light-harvesting protein B-875 beta chain



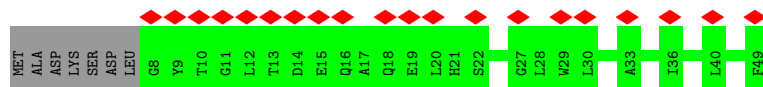
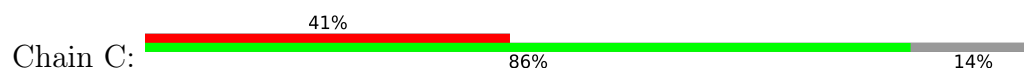
- Molecule 5: Light-harvesting protein B-875 beta chain



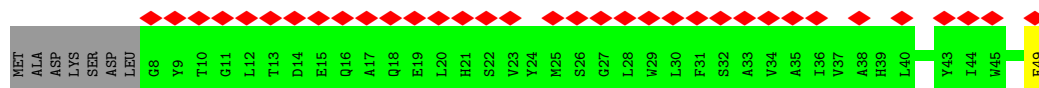
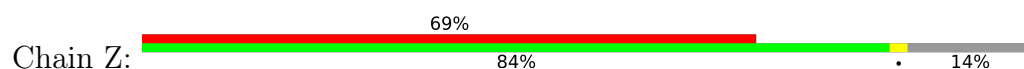
- Molecule 5: Light-harvesting protein B-875 beta chain



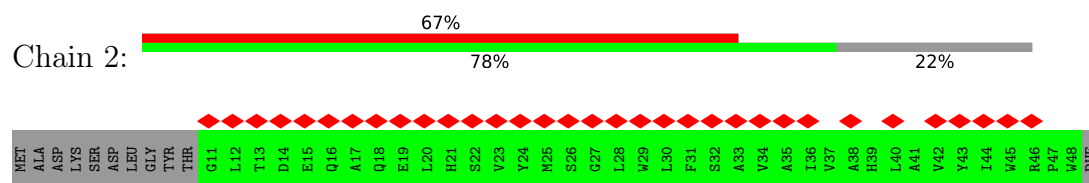
- Molecule 5: Light-harvesting protein B-875 beta chain



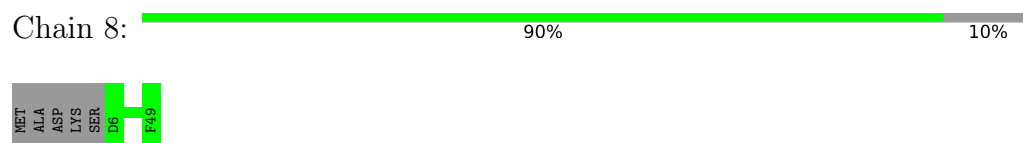
- Molecule 5: Light-harvesting protein B-875 beta chain



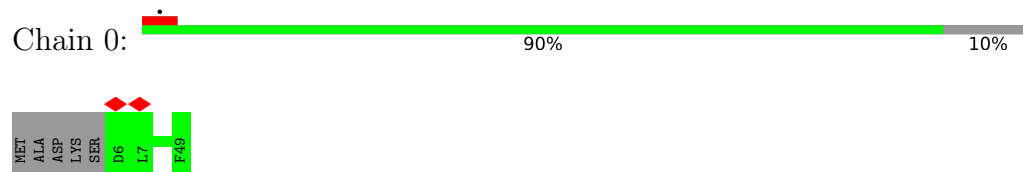
- Molecule 5: Light-harvesting protein B-875 beta chain



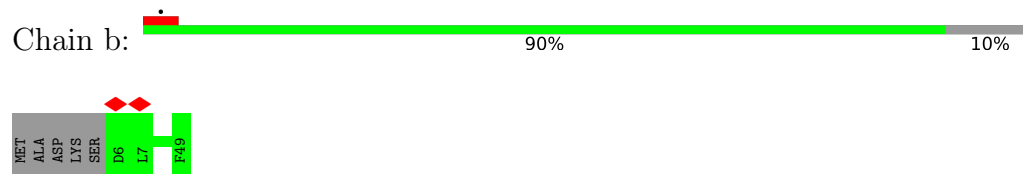
- Molecule 5: Light-harvesting protein B-875 beta chain



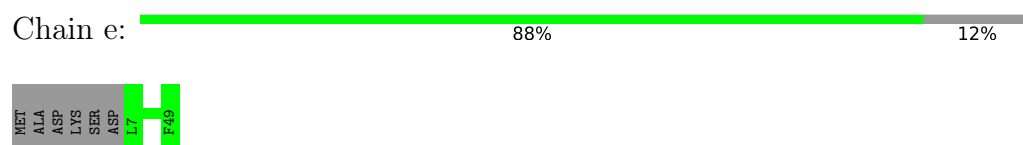
- Molecule 5: Light-harvesting protein B-875 beta chain



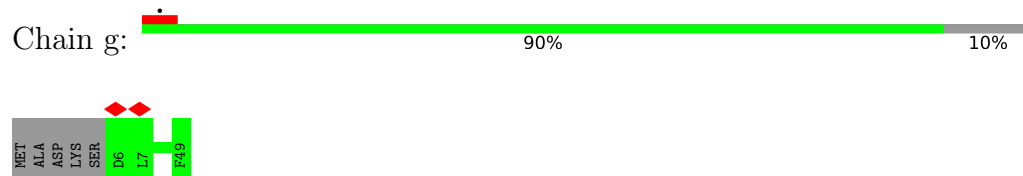
- Molecule 5: Light-harvesting protein B-875 beta chain



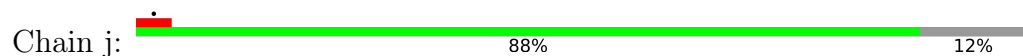
- Molecule 5: Light-harvesting protein B-875 beta chain

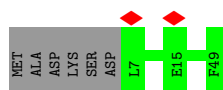


- Molecule 5: Light-harvesting protein B-875 beta chain

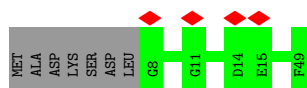
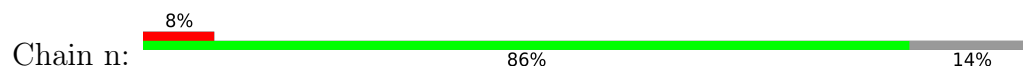


- Molecule 5: Light-harvesting protein B-875 beta chain

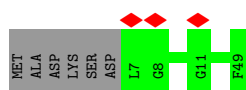
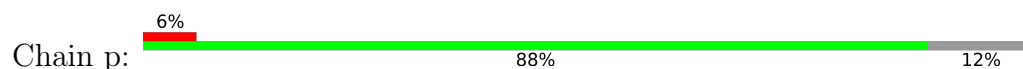




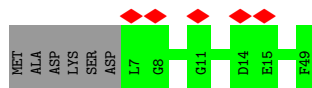
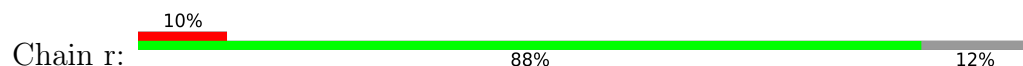
- Molecule 5: Light-harvesting protein B-875 beta chain



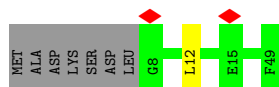
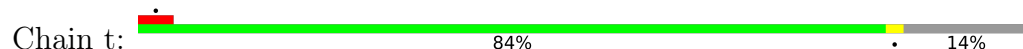
- Molecule 5: Light-harvesting protein B-875 beta chain



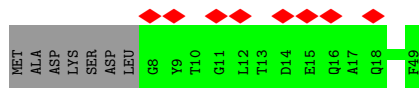
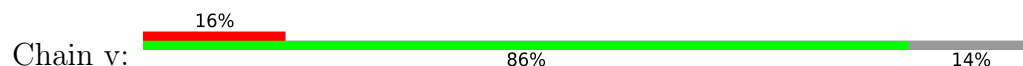
- Molecule 5: Light-harvesting protein B-875 beta chain



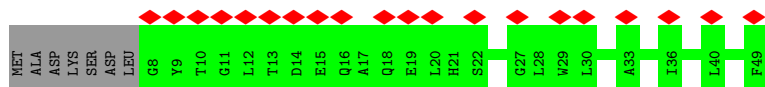
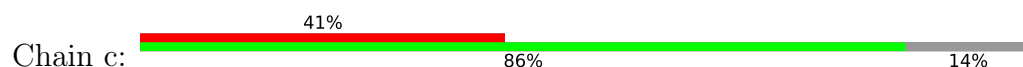
- Molecule 5: Light-harvesting protein B-875 beta chain



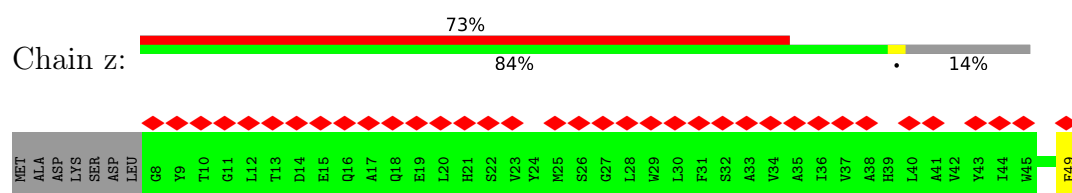
- Molecule 5: Light-harvesting protein B-875 beta chain



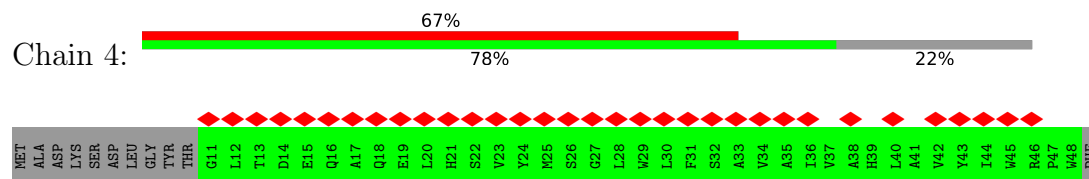
- Molecule 5: Light-harvesting protein B-875 beta chain



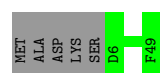
- Molecule 5: Light-harvesting protein B-875 beta chain



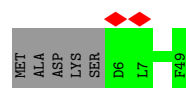
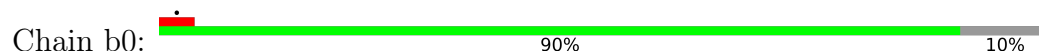
- Molecule 5: Light-harvesting protein B-875 beta chain



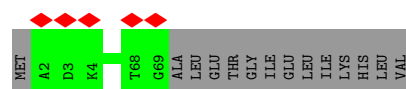
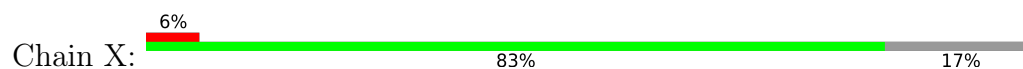
- Molecule 5: Light-harvesting protein B-875 beta chain



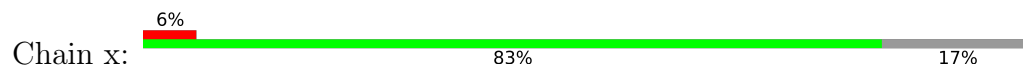
- Molecule 5: Light-harvesting protein B-875 beta chain



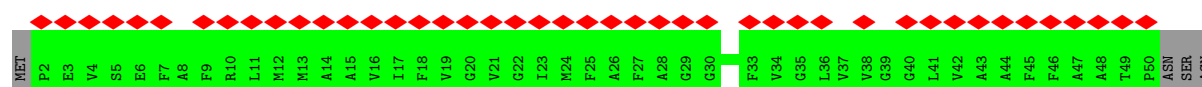
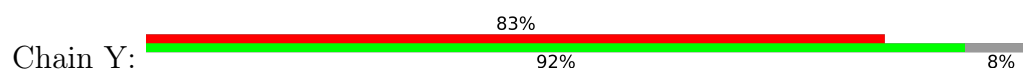
- Molecule 6: Intrinsic membrane protein PufX



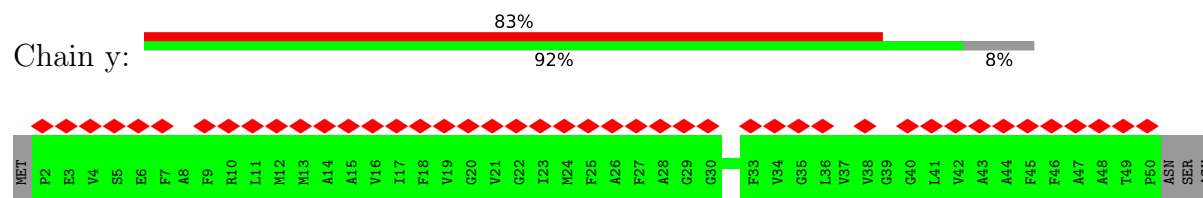
- Molecule 6: Intrinsic membrane protein PufX



- Molecule 7: Rsp\_7571 Protein-Y PufY



Chain y:



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	145392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	432.63998, 432.63998, 432.63998	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U10, BPH, PC1, FE2, SPO, CDL, BCL

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	0.38	0/2320	0.45	0/3175
1	l	0.38	0/2320	0.45	0/3175
2	M	0.38	0/2538	0.45	0/3464
2	m	0.38	0/2538	0.45	0/3464
3	H	0.28	0/2024	0.46	0/2752
3	h	0.28	0/2024	0.46	0/2752
4	1	0.24	0/404	0.40	0/550
4	3	0.24	0/451	0.42	0/613
4	5	0.24	0/451	0.42	0/613
4	6	0.36	0/416	0.42	0/564
4	7	0.36	0/416	0.42	0/564
4	9	0.36	0/474	0.44	0/642
4	A	0.35	0/474	0.45	0/642
4	D	0.36	0/474	0.45	0/642
4	F	0.34	0/474	0.43	0/642
4	I	0.33	0/469	0.44	0/635
4	K	0.32	0/466	0.42	0/632
4	O	0.31	0/469	0.42	0/635
4	Q	0.31	0/474	0.43	0/642
4	S	0.32	0/474	0.43	0/642
4	U	0.27	0/461	0.42	0/625
4	W	0.26	0/466	0.40	0/632
4	a	0.35	0/474	0.45	0/642
4	b1	0.24	0/404	0.40	0/550
4	b9	0.36	0/474	0.44	0/642
4	d	0.36	0/474	0.45	0/642
4	f	0.35	0/474	0.43	0/642
4	i	0.33	0/469	0.44	0/635
4	k	0.32	0/466	0.42	0/632
4	o	0.31	0/469	0.42	0/635
4	q	0.31	0/474	0.43	0/642
4	s	0.32	0/474	0.43	0/642



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	u	0.27	0/461	0.42	0/625
4	w	0.26	0/466	0.40	0/632
5	0	0.34	0/373	0.40	0/510
5	2	0.23	0/320	0.34	0/439
5	4	0.23	0/320	0.34	0/439
5	8	0.33	0/373	0.39	0/510
5	B	0.33	0/373	0.39	0/510
5	C	0.26	0/357	0.38	0/488
5	E	0.32	0/365	0.43	0/499
5	G	0.31	0/373	0.39	0/510
5	J	0.27	0/365	0.39	0/499
5	N	0.29	0/357	0.37	0/488
5	P	0.35	0/365	0.39	0/499
5	R	0.30	0/365	0.38	0/499
5	T	0.28	0/357	0.40	0/488
5	V	0.27	0/357	0.39	0/488
5	Z	0.24	0/357	0.36	0/488
5	b	0.33	0/373	0.39	0/510
5	b0	0.34	0/373	0.40	0/510
5	b8	0.33	0/373	0.39	0/510
5	c	0.26	0/357	0.38	0/488
5	e	0.32	0/365	0.43	0/499
5	g	0.31	0/373	0.39	0/510
5	j	0.27	0/365	0.39	0/499
5	n	0.29	0/357	0.37	0/488
5	p	0.35	0/365	0.39	0/499
5	r	0.30	0/365	0.38	0/499
5	t	0.28	0/357	0.40	0/488
5	v	0.27	0/357	0.39	0/488
5	z	0.24	0/357	0.36	0/488
6	X	0.27	0/543	0.42	0/736
6	x	0.27	0/543	0.42	0/736
7	Y	0.27	0/373	0.39	0/505
7	y	0.27	0/373	0.38	0/505
All	All	0.32	0/38602	0.43	0/52570

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	279/282 (99%)	272 (98%)	7 (2%)	0	100	100
1	l	279/282 (99%)	272 (98%)	7 (2%)	0	100	100
2	M	305/308 (99%)	299 (98%)	6 (2%)	0	100	100
2	m	305/308 (99%)	299 (98%)	6 (2%)	0	100	100
3	H	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
3	h	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
4	1	45/58 (78%)	45 (100%)	0	0	100	100
4	3	50/58 (86%)	49 (98%)	1 (2%)	0	100	100
4	5	50/58 (86%)	49 (98%)	1 (2%)	0	100	100
4	6	46/58 (79%)	44 (96%)	2 (4%)	0	100	100
4	7	46/58 (79%)	44 (96%)	2 (4%)	0	100	100
4	9	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	A	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	D	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	F	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	I	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	K	52/58 (90%)	52 (100%)	0	0	100	100
4	O	52/58 (90%)	52 (100%)	0	0	100	100
4	Q	53/58 (91%)	50 (94%)	3 (6%)	0	100	100
4	S	53/58 (91%)	53 (100%)	0	0	100	100
4	U	51/58 (88%)	50 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	W	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	a	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	b1	45/58 (78%)	45 (100%)	0	0	100	100
4	b9	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	d	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	f	53/58 (91%)	51 (96%)	2 (4%)	0	100	100
4	i	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	k	52/58 (90%)	52 (100%)	0	0	100	100
4	o	52/58 (90%)	52 (100%)	0	0	100	100
4	q	53/58 (91%)	50 (94%)	3 (6%)	0	100	100
4	s	53/58 (91%)	53 (100%)	0	0	100	100
4	u	51/58 (88%)	50 (98%)	1 (2%)	0	100	100
4	w	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
5	0	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	2	36/49 (74%)	36 (100%)	0	0	100	100
5	4	36/49 (74%)	36 (100%)	0	0	100	100
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	C	40/49 (82%)	40 (100%)	0	0	100	100
5	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	G	42/49 (86%)	42 (100%)	0	0	100	100
5	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	N	40/49 (82%)	40 (100%)	0	0	100	100
5	P	41/49 (84%)	41 (100%)	0	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	40/49 (82%)	40 (100%)	0	0	100	100
5	V	40/49 (82%)	40 (100%)	0	0	100	100
5	Z	40/49 (82%)	40 (100%)	0	0	100	100
5	b	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	b0	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	b8	42/49 (86%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	c	40/49 (82%)	40 (100%)	0	0	100	100
5	e	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	42/49 (86%)	42 (100%)	0	0	100	100
5	j	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	n	40/49 (82%)	40 (100%)	0	0	100	100
5	p	41/49 (84%)	41 (100%)	0	0	100	100
5	r	41/49 (84%)	41 (100%)	0	0	100	100
5	t	40/49 (82%)	40 (100%)	0	0	100	100
5	v	40/49 (82%)	40 (100%)	0	0	100	100
5	z	40/49 (82%)	40 (100%)	0	0	100	100
6	X	66/82 (80%)	64 (97%)	2 (3%)	0	100	100
6	x	66/82 (80%)	64 (97%)	2 (3%)	0	100	100
7	Y	47/53 (89%)	47 (100%)	0	0	100	100
7	y	47/53 (89%)	47 (100%)	0	0	100	100
All	All	4482/4966 (90%)	4402 (98%)	80 (2%)	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	220/221 (100%)	217 (99%)	3 (1%)	67	80
1	l	220/221 (100%)	217 (99%)	3 (1%)	67	80
2	M	240/241 (100%)	237 (99%)	3 (1%)	69	82
2	m	240/241 (100%)	237 (99%)	3 (1%)	69	82
3	H	208/208 (100%)	206 (99%)	2 (1%)	76	85
3	h	208/208 (100%)	206 (99%)	2 (1%)	76	85
4	1	42/51 (82%)	42 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	46/51 (90%)	45 (98%)	1 (2%)	52	71
4	5	46/51 (90%)	45 (98%)	1 (2%)	52	71
4	6	44/51 (86%)	44 (100%)	0	100	100
4	7	44/51 (86%)	44 (100%)	0	100	100
4	9	49/51 (96%)	49 (100%)	0	100	100
4	A	49/51 (96%)	49 (100%)	0	100	100
4	D	49/51 (96%)	49 (100%)	0	100	100
4	F	49/51 (96%)	49 (100%)	0	100	100
4	I	49/51 (96%)	49 (100%)	0	100	100
4	K	48/51 (94%)	48 (100%)	0	100	100
4	O	49/51 (96%)	48 (98%)	1 (2%)	55	72
4	Q	49/51 (96%)	49 (100%)	0	100	100
4	S	49/51 (96%)	49 (100%)	0	100	100
4	U	48/51 (94%)	48 (100%)	0	100	100
4	W	48/51 (94%)	48 (100%)	0	100	100
4	a	49/51 (96%)	49 (100%)	0	100	100
4	b1	42/51 (82%)	42 (100%)	0	100	100
4	b9	49/51 (96%)	49 (100%)	0	100	100
4	d	49/51 (96%)	49 (100%)	0	100	100
4	f	49/51 (96%)	49 (100%)	0	100	100
4	i	49/51 (96%)	49 (100%)	0	100	100
4	k	48/51 (94%)	48 (100%)	0	100	100
4	o	49/51 (96%)	48 (98%)	1 (2%)	55	72
4	q	49/51 (96%)	49 (100%)	0	100	100
4	s	49/51 (96%)	49 (100%)	0	100	100
4	u	48/51 (94%)	48 (100%)	0	100	100
4	w	48/51 (94%)	48 (100%)	0	100	100
5	0	36/40 (90%)	36 (100%)	0	100	100
5	2	31/40 (78%)	31 (100%)	0	100	100
5	4	31/40 (78%)	31 (100%)	0	100	100
5	8	36/40 (90%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	B	36/40 (90%)	36 (100%)	0	100	100
5	C	34/40 (85%)	34 (100%)	0	100	100
5	E	35/40 (88%)	35 (100%)	0	100	100
5	G	36/40 (90%)	36 (100%)	0	100	100
5	J	35/40 (88%)	35 (100%)	0	100	100
5	N	34/40 (85%)	34 (100%)	0	100	100
5	P	35/40 (88%)	35 (100%)	0	100	100
5	R	35/40 (88%)	35 (100%)	0	100	100
5	T	34/40 (85%)	33 (97%)	1 (3%)	42	62
5	V	34/40 (85%)	34 (100%)	0	100	100
5	Z	34/40 (85%)	33 (97%)	1 (3%)	42	62
5	b	36/40 (90%)	36 (100%)	0	100	100
5	b0	36/40 (90%)	36 (100%)	0	100	100
5	b8	36/40 (90%)	36 (100%)	0	100	100
5	c	34/40 (85%)	34 (100%)	0	100	100
5	e	35/40 (88%)	35 (100%)	0	100	100
5	g	36/40 (90%)	36 (100%)	0	100	100
5	j	35/40 (88%)	35 (100%)	0	100	100
5	n	34/40 (85%)	34 (100%)	0	100	100
5	p	35/40 (88%)	35 (100%)	0	100	100
5	r	35/40 (88%)	35 (100%)	0	100	100
5	t	34/40 (85%)	33 (97%)	1 (3%)	42	62
5	v	34/40 (85%)	34 (100%)	0	100	100
5	z	34/40 (85%)	33 (97%)	1 (3%)	42	62
6	X	54/66 (82%)	54 (100%)	0	100	100
6	x	54/66 (82%)	54 (100%)	0	100	100
7	Y	33/37 (89%)	33 (100%)	0	100	100
7	y	33/37 (89%)	33 (100%)	0	100	100
All	All	3816/4094 (93%)	3792 (99%)	24 (1%)	86	91

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	272	TRP
2	m	216	PHE
2	m	214	LEU
3	h	202	ARG
3	H	202	ARG

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

Mol	Chain	Res	Type
2	M	307	ASN
3	H	35	ASN
2	m	299	GLN
2	m	307	ASN
3	h	35	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 148 ligands modelled in this entry, 2 are monoatomic - leaving 146 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
8	BCL	S	101	-	64,74,74	1.24	7 (10%)	78,115,115	1.58	12 (15%)
13	SPO	C	102	-	40,41,41	0.22	0	47,50,50	0.44	0
13	SPO	O	102	-	40,41,41	0.27	0	47,50,50	0.43	0
8	BCL	K	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.56	12 (15%)
8	BCL	l	302	-	61,71,74	1.25	7 (11%)	74,111,115	1.54	11 (14%)
13	SPO	U	103	-	40,41,41	0.17	0	47,50,50	0.39	0
8	BCL	L	302	-	61,71,74	1.25	7 (11%)	74,111,115	1.54	11 (14%)
8	BCL	R	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.46	10 (12%)
8	BCL	6	102	-	59,69,74	1.23	5 (8%)	72,109,115	1.63	12 (16%)
13	SPO	a	102	-	40,41,41	0.30	0	47,50,50	0.34	0
10	U10	M	405	-	48,48,63	2.65	14 (29%)	58,61,79	1.73	15 (25%)
8	BCL	J	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.50	10 (12%)
8	BCL	N	102	-	64,74,74	1.22	5 (7%)	78,115,115	1.51	11 (14%)
8	BCL	L	301	-	64,74,74	1.23	7 (10%)	78,115,115	1.51	11 (14%)
13	SPO	p	101	-	40,41,41	0.19	0	47,50,50	0.33	0
13	SPO	G	101	-	40,41,41	0.22	0	47,50,50	0.29	0
11	PC1	A	105	-	37,37,53	0.57	0	43,45,61	0.60	1 (2%)
8	BCL	z	101	-	54,64,74	1.35	4 (7%)	66,103,115	1.54	8 (12%)
8	BCL	a	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.59	12 (15%)
8	BCL	C	101	-	59,69,74	1.28	6 (10%)	72,109,115	1.51	10 (13%)
8	BCL	9	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.60	11 (14%)
13	SPO	g	101	-	40,41,41	0.22	0	47,50,50	0.29	0
13	SPO	E	103	-	40,41,41	0.22	0	47,50,50	0.38	0
11	PC1	H	301	-	42,42,53	1.12	5 (11%)	48,50,61	1.16	3 (6%)
13	SPO	B	102	-	40,41,41	0.27	0	47,50,50	0.30	0
13	SPO	b9	102	-	40,41,41	0.31	0	47,50,50	0.35	0
9	BPH	L	303	-	51,70,70	0.95	1 (1%)	52,101,101	1.28	6 (11%)
8	BCL	g	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.54	11 (14%)
8	BCL	p	102	-	64,74,74	1.22	5 (7%)	78,115,115	1.50	11 (14%)
11	PC1	h	301	-	42,42,53	1.12	5 (11%)	48,50,61	1.16	3 (6%)
13	SPO	b	102	-	40,41,41	0.27	0	47,50,50	0.30	0
8	BCL	r	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.46	10 (12%)
13	SPO	u	102	-	40,41,41	0.20	0	47,50,50	0.42	0
10	U10	m	405	-	48,48,63	2.65	14 (29%)	58,61,79	1.73	15 (25%)
13	SPO	c	102	-	40,41,41	0.22	0	47,50,50	0.44	0
13	SPO	s	103	-	40,41,41	0.26	0	47,50,50	0.35	0
13	SPO	D	103	-	40,41,41	0.20	0	47,50,50	0.32	0
13	SPO	N	101	-	40,41,41	0.20	0	47,50,50	0.32	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	SPO	e	103	-	40,41,41	0.22	0	47,50,50	0.38	0
11	PC1	L	307	-	39,39,53	1.13	4 (10%)	45,47,61	1.12	3 (6%)
8	BCL	j	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.50	10 (12%)
14	CDL	m	407	-	81,81,99	1.02	9 (11%)	87,93,111	1.19	6 (6%)
13	SPO	J	102	-	40,41,41	0.16	0	47,50,50	0.30	0
11	PC1	l	306	-	38,38,53	1.15	4 (10%)	44,46,61	1.19	3 (6%)
13	SPO	j	102	-	40,41,41	0.16	0	47,50,50	0.30	0
13	SPO	q	103	-	40,41,41	0.20	0	47,50,50	0.50	1 (2%)
13	SPO	Q	103	-	40,41,41	0.20	0	47,50,50	0.50	1 (2%)
8	BCL	G	102	-	64,74,74	1.24	5 (7%)	78,115,115	1.54	12 (15%)
11	PC1	a	105	-	37,37,53	0.57	0	43,45,61	0.60	1 (2%)
8	BCL	s	101	-	64,74,74	1.24	7 (10%)	78,115,115	1.58	12 (15%)
8	BCL	d	102	-	64,74,74	1.24	6 (9%)	78,115,115	1.58	11 (14%)
11	PC1	H	302	-	33,33,53	1.26	4 (12%)	39,41,61	1.09	3 (7%)
8	BCL	c	101	-	59,69,74	1.28	5 (8%)	72,109,115	1.51	10 (13%)
8	BCL	T	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.48	12 (15%)
8	BCL	Z	101	-	54,64,74	1.35	4 (7%)	66,103,115	1.53	8 (12%)
11	PC1	A	104	-	30,30,53	1.31	4 (13%)	36,38,61	1.19	3 (8%)
8	BCL	b9	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.60	11 (14%)
8	BCL	M	402	-	64,74,74	1.21	6 (9%)	78,115,115	1.57	10 (12%)
11	PC1	D	101	-	38,38,53	1.18	4 (10%)	44,46,61	1.19	3 (6%)
10	U10	L	304	-	38,38,63	2.63	12 (31%)	46,49,79	1.74	12 (26%)
13	SPO	Q	102	-	40,41,41	0.22	0	47,50,50	0.31	0
11	PC1	h	302	-	33,33,53	1.26	4 (12%)	39,41,61	1.09	3 (7%)
13	SPO	5	103	-	40,41,41	0.17	0	47,50,50	0.32	0
13	SPO	n	101	-	40,41,41	0.20	0	47,50,50	0.32	0
8	BCL	7	101	-	59,69,74	1.24	4 (6%)	72,109,115	1.63	13 (18%)
8	BCL	b1	101	-	44,54,74	1.47	4 (9%)	54,91,115	1.72	9 (16%)
8	BCL	q	101	-	64,74,74	1.23	6 (9%)	78,115,115	1.61	13 (16%)
13	SPO	q	104	-	40,41,41	0.20	0	47,50,50	0.31	0
11	PC1	A	103	-	44,44,53	1.09	4 (9%)	50,52,61	1.20	3 (6%)
11	PC1	d	101	-	38,38,53	1.18	4 (10%)	44,46,61	1.19	3 (6%)
8	BCL	I	101	-	64,74,74	1.22	7 (10%)	78,115,115	1.59	11 (14%)
9	BPH	l	303	-	51,70,70	0.95	1 (1%)	52,101,101	1.28	6 (11%)
13	SPO	u	103	-	40,41,41	0.17	0	47,50,50	0.39	0
8	BCL	n	102	-	64,74,74	1.22	5 (7%)	78,115,115	1.51	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	F	101	-	64,74,74	1.24	5 (7%)	78,115,115	1.58	11 (14%)
13	SPO	9	102	-	40,41,41	0.31	0	47,50,50	0.35	0
8	BCL	W	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.55	11 (14%)
8	BCL	4	101	-	44,54,74	1.47	4 (9%)	54,91,115	1.66	8 (14%)
8	BCL	o	101	-	64,74,74	1.21	6 (9%)	78,115,115	1.56	12 (15%)
8	BCL	5	101	-	49,59,74	1.46	5 (10%)	60,97,115	1.72	11 (18%)
13	SPO	3	102	-	40,41,41	0.17	0	47,50,50	0.37	0
14	CDL	f	102	-	62,62,99	1.14	8 (12%)	68,74,111	1.25	6 (8%)
13	SPO	G	103	-	40,41,41	0.18	0	47,50,50	0.39	0
13	SPO	M	406	-	40,41,41	0.29	0	47,50,50	0.48	1 (2%)
13	SPO	i	102	-	40,41,41	0.22	0	47,50,50	0.33	0
8	BCL	6	101	-	59,69,74	1.24	4 (6%)	72,109,115	1.63	13 (18%)
8	BCL	w	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.55	11 (14%)
13	SPO	m	406	-	40,41,41	0.29	0	47,50,50	0.48	1 (2%)
8	BCL	u	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.55	11 (14%)
8	BCL	b	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.62	12 (15%)
8	BCL	A	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.59	12 (15%)
8	BCL	m	402	-	64,74,74	1.21	6 (9%)	78,115,115	1.57	10 (12%)
13	SPO	g	103	-	40,41,41	0.18	0	47,50,50	0.39	0
8	BCL	D	102	-	64,74,74	1.24	6 (9%)	78,115,115	1.58	11 (14%)
13	SPO	x	101	-	40,41,41	0.28	0	47,50,50	0.44	0
13	SPO	P	101	-	40,41,41	0.19	0	47,50,50	0.32	0
8	BCL	2	101	-	44,54,74	1.47	4 (9%)	54,91,115	1.66	8 (14%)
8	BCL	k	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.56	12 (15%)
8	BCL	0	101	-	59,69,74	1.26	5 (8%)	72,109,115	1.69	13 (18%)
8	BCL	M	403	-	64,74,74	1.25	7 (10%)	78,115,115	1.58	10 (12%)
13	SPO	Q	104	-	40,41,41	0.20	0	47,50,50	0.31	0
8	BCL	O	101	-	64,74,74	1.21	6 (9%)	78,115,115	1.56	12 (15%)
8	BCL	v	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.50	12 (15%)
8	BCL	e	102	-	64,74,74	1.22	5 (7%)	78,115,115	1.52	13 (16%)
8	BCL	P	102	-	64,74,74	1.22	5 (7%)	78,115,115	1.51	11 (14%)
13	SPO	U	102	-	40,41,41	0.20	0	47,50,50	0.42	0
13	SPO	5	102	-	40,41,41	0.17	0	47,50,50	0.37	0
14	CDL	F	102	-	62,62,99	1.14	8 (12%)	68,74,111	1.26	6 (8%)
13	SPO	0	102	-	40,41,41	0.25	0	47,50,50	0.33	0
11	PC1	a	104	-	30,30,53	1.32	4 (13%)	36,38,61	1.19	3 (8%)
9	BPH	m	404	-	41,60,70	1.08	3 (7%)	40,89,101	1.16	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	SPO	s	102	-	40,41,41	0.23	0	47,50,50	0.30	0
13	SPO	E	101	-	40,41,41	0.29	0	47,50,50	0.28	0
8	BCL	V	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.50	12 (15%)
8	BCL	i	101	-	64,74,74	1.22	7 (10%)	78,115,115	1.59	11 (14%)
13	SPO	b0	102	-	40,41,41	0.25	0	47,50,50	0.33	0
13	SPO	3	103	-	40,41,41	0.17	0	47,50,50	0.32	0
11	PC1	a	103	-	44,44,53	1.09	4 (9%)	50,52,61	1.20	3 (6%)
13	SPO	X	101	-	40,41,41	0.28	0	47,50,50	0.44	0
8	BCL	Q	101	-	64,74,74	1.23	6 (9%)	78,115,115	1.62	13 (16%)
10	U10	L	305	-	43,43,63	2.68	13 (30%)	52,55,79	1.76	13 (25%)
8	BCL	l	101	-	44,54,74	1.47	4 (9%)	54,91,115	1.72	9 (16%)
13	SPO	S	102	-	40,41,41	0.23	0	47,50,50	0.30	0
13	SPO	o	102	-	40,41,41	0.27	0	47,50,50	0.43	0
8	BCL	E	102	-	64,74,74	1.22	5 (7%)	78,115,115	1.52	13 (16%)
9	BPH	M	404	-	41,60,70	1.08	3 (7%)	40,89,101	1.16	4 (10%)
13	SPO	S	103	-	40,41,41	0.26	0	47,50,50	0.35	0
8	BCL	l	301	-	64,74,74	1.23	7 (10%)	78,115,115	1.51	11 (14%)
8	BCL	f	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.59	11 (14%)
13	SPO	d	103	-	40,41,41	0.20	0	47,50,50	0.32	0
11	PC1	l	307	-	39,39,53	1.14	4 (10%)	45,47,61	1.12	3 (6%)
8	BCL	b0	101	-	59,69,74	1.26	5 (8%)	72,109,115	1.69	13 (18%)
11	PC1	L	306	-	38,38,53	1.15	4 (10%)	44,46,61	1.19	3 (6%)
10	U10	l	305	-	43,43,63	2.68	13 (30%)	52,55,79	1.76	13 (25%)
13	SPO	A	102	-	40,41,41	0.30	0	47,50,50	0.34	0
13	SPO	e	101	-	40,41,41	0.29	0	47,50,50	0.28	0
10	U10	l	304	-	38,38,63	2.63	12 (31%)	46,49,79	1.74	12 (26%)
8	BCL	3	101	-	49,59,74	1.45	5 (10%)	60,97,115	1.72	11 (18%)
8	BCL	B	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.62	12 (15%)
14	CDL	M	407	-	81,81,99	1.02	9 (11%)	87,93,111	1.19	6 (6%)
8	BCL	t	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.48	12 (15%)
8	BCL	U	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.55	11 (14%)
8	BCL	m	403	-	64,74,74	1.25	7 (10%)	78,115,115	1.59	10 (12%)
8	BCL	7	102	-	59,69,74	1.23	5 (8%)	72,109,115	1.63	12 (16%)
13	SPO	q	102	-	40,41,41	0.22	0	47,50,50	0.31	0
13	SPO	I	102	-	40,41,41	0.22	0	47,50,50	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	S	101	-	-	0/37/137/137	-
13	SPO	C	102	-	-	16/47/47/47	-
13	SPO	O	102	-	-	15/47/47/47	-
8	BCL	K	101	-	-	1/37/137/137	-
8	BCL	l	302	-	-	0/34/134/137	-
13	SPO	U	103	-	-	9/47/47/47	-
8	BCL	L	302	-	-	0/34/134/137	-
8	BCL	R	101	-	-	4/37/137/137	-
8	BCL	6	102	-	-	7/31/131/137	-
13	SPO	a	102	-	-	12/47/47/47	-
10	U10	M	405	-	-	10/45/69/87	0/1/1/1
8	BCL	J	101	-	-	5/37/137/137	-
8	BCL	N	102	-	-	5/37/137/137	-
8	BCL	L	301	-	-	0/37/137/137	-
13	SPO	p	101	-	-	12/47/47/47	-
13	SPO	G	101	-	-	12/47/47/47	-
11	PC1	A	105	-	-	18/41/41/57	-
8	BCL	z	101	-	-	4/25/125/137	-
8	BCL	a	101	-	-	3/37/137/137	-
8	BCL	C	101	-	-	4/31/131/137	-
8	BCL	9	101	-	-	3/37/137/137	-
13	SPO	g	101	-	-	12/47/47/47	-
13	SPO	E	103	-	-	16/47/47/47	-
11	PC1	H	301	-	-	12/46/46/57	-
13	SPO	B	102	-	-	14/47/47/47	-
13	SPO	b9	102	-	-	14/47/47/47	-
9	BPH	L	303	-	-	2/37/105/105	0/5/6/6
8	BCL	g	102	-	-	1/37/137/137	-
8	BCL	p	102	-	-	4/37/137/137	-
11	PC1	h	301	-	-	12/46/46/57	-
13	SPO	b	102	-	-	14/47/47/47	-
8	BCL	r	101	-	-	5/37/137/137	-
13	SPO	u	102	-	-	7/47/47/47	-
10	U10	m	405	-	-	10/45/69/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SPO	c	102	-	-	16/47/47/47	-
13	SPO	s	103	-	-	9/47/47/47	-
13	SPO	D	103	-	-	15/47/47/47	-
13	SPO	N	101	-	-	10/47/47/47	-
13	SPO	e	103	-	-	16/47/47/47	-
11	PC1	L	307	-	-	19/43/43/57	-
8	BCL	j	101	-	-	5/37/137/137	-
14	CDL	m	407	-	-	27/92/92/110	-
13	SPO	J	102	-	-	13/47/47/47	-
11	PC1	l	306	-	-	12/42/42/57	-
13	SPO	j	102	-	-	13/47/47/47	-
13	SPO	q	103	-	-	12/47/47/47	-
13	SPO	Q	103	-	-	12/47/47/47	-
8	BCL	G	102	-	-	1/37/137/137	-
11	PC1	a	105	-	-	18/41/41/57	-
8	BCL	s	101	-	-	0/37/137/137	-
8	BCL	d	102	-	-	3/37/137/137	-
11	PC1	H	302	-	-	13/37/37/57	-
8	BCL	c	101	-	-	4/31/131/137	-
8	BCL	T	101	-	-	4/37/137/137	-
8	BCL	Z	101	-	-	4/25/125/137	-
11	PC1	A	104	-	-	17/34/34/57	-
8	BCL	b9	101	-	-	3/37/137/137	-
8	BCL	M	402	-	-	4/37/137/137	-
11	PC1	D	101	-	-	13/42/42/57	-
10	U10	L	304	-	-	14/33/57/87	0/1/1/1
13	SPO	Q	102	-	-	8/47/47/47	-
11	PC1	h	302	-	-	13/37/37/57	-
13	SPO	5	103	-	-	13/47/47/47	-
13	SPO	n	101	-	-	10/47/47/47	-
8	BCL	7	101	-	-	6/31/131/137	-
8	BCL	b1	101	-	-	2/13/113/137	-
8	BCL	q	101	-	-	4/37/137/137	-
13	SPO	q	104	-	-	12/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PC1	A	103	-	-	17/48/48/57	-
11	PC1	d	101	-	-	13/42/42/57	-
8	BCL	I	101	-	-	2/37/137/137	-
9	BPH	l	303	-	-	2/37/105/105	0/5/6/6
13	SPO	u	103	-	-	9/47/47/47	-
8	BCL	n	102	-	-	5/37/137/137	-
8	BCL	F	101	-	-	2/37/137/137	-
13	SPO	9	102	-	-	14/47/47/47	-
8	BCL	W	101	-	-	0/37/137/137	-
8	BCL	4	101	-	-	2/13/113/137	-
8	BCL	o	101	-	-	0/37/137/137	-
8	BCL	5	101	-	-	0/19/119/137	-
13	SPO	3	102	-	-	13/47/47/47	-
14	CDL	f	102	-	-	29/73/73/110	-
13	SPO	G	103	-	-	11/47/47/47	-
13	SPO	M	406	-	-	9/47/47/47	-
13	SPO	i	102	-	-	13/47/47/47	-
8	BCL	6	101	-	-	6/31/131/137	-
8	BCL	w	101	-	-	0/37/137/137	-
13	SPO	m	406	-	-	9/47/47/47	-
8	BCL	u	101	-	-	0/37/137/137	-
8	BCL	b	101	-	-	5/37/137/137	-
8	BCL	A	101	-	-	3/37/137/137	-
8	BCL	m	402	-	-	4/37/137/137	-
13	SPO	g	103	-	-	11/47/47/47	-
8	BCL	D	102	-	-	3/37/137/137	-
13	SPO	x	101	-	-	9/47/47/47	-
13	SPO	P	101	-	-	12/47/47/47	-
8	BCL	2	101	-	-	2/13/113/137	-
8	BCL	k	101	-	-	1/37/137/137	-
8	BCL	0	101	-	-	3/31/131/137	-
8	BCL	M	403	-	-	1/37/137/137	-
13	SPO	Q	104	-	-	12/47/47/47	-
8	BCL	O	101	-	-	0/37/137/137	-
8	BCL	v	101	-	-	4/37/137/137	-
8	BCL	e	102	-	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	P	102	-	-	4/37/137/137	-
13	SPO	U	102	-	-	7/47/47/47	-
13	SPO	5	102	-	-	13/47/47/47	-
14	CDL	F	102	-	-	29/73/73/110	-
13	SPO	0	102	-	-	14/47/47/47	-
11	PC1	a	104	-	-	17/34/34/57	-
9	BPH	m	404	-	-	4/25/93/105	0/5/6/6
13	SPO	s	102	-	-	14/47/47/47	-
13	SPO	E	101	-	-	11/47/47/47	-
8	BCL	V	101	-	-	4/37/137/137	-
8	BCL	i	101	-	-	2/37/137/137	-
13	SPO	b0	102	-	-	14/47/47/47	-
13	SPO	3	103	-	-	13/47/47/47	-
11	PC1	a	103	-	-	17/48/48/57	-
13	SPO	X	101	-	-	9/47/47/47	-
8	BCL	Q	101	-	-	4/37/137/137	-
10	U10	L	305	-	-	10/39/63/87	0/1/1/1
8	BCL	1	101	-	-	2/13/113/137	-
13	SPO	S	102	-	-	14/47/47/47	-
13	SPO	o	102	-	-	15/47/47/47	-
8	BCL	E	102	-	-	6/37/137/137	-
9	BPH	M	404	-	-	4/25/93/105	0/5/6/6
13	SPO	S	103	-	-	9/47/47/47	-
8	BCL	l	301	-	-	0/37/137/137	-
8	BCL	f	101	-	-	2/37/137/137	-
13	SPO	d	103	-	-	15/47/47/47	-
11	PC1	l	307	-	-	19/43/43/57	-
8	BCL	b0	101	-	-	3/31/131/137	-
11	PC1	L	306	-	-	12/42/42/57	-
10	U10	l	305	-	-	10/39/63/87	0/1/1/1
13	SPO	A	102	-	-	12/47/47/47	-
13	SPO	e	101	-	-	11/47/47/47	-
10	U10	l	304	-	-	14/33/57/87	0/1/1/1
8	BCL	3	101	-	-	0/19/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	B	101	-	-	5/37/137/137	-
14	CDL	M	407	-	-	27/92/92/110	-
8	BCL	t	101	-	-	4/37/137/137	-
8	BCL	U	101	-	-	0/37/137/137	-
8	BCL	m	403	-	-	1/37/137/137	-
8	BCL	7	102	-	-	7/31/131/137	-
13	SPO	q	102	-	-	8/47/47/47	-
13	SPO	I	102	-	-	13/47/47/47	-

The worst 5 of 526 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	305	U10	C13-C14	6.05	1.47	1.33
10	l	305	U10	C13-C14	6.05	1.47	1.33
10	L	305	U10	C8-C9	6.00	1.47	1.33
10	l	305	U10	C8-C9	5.98	1.47	1.33
10	L	305	U10	C28-C29	5.97	1.47	1.33

The worst 5 of 883 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	402	BCL	CHD-C1D-ND	-5.61	119.30	124.45
8	m	402	BCL	CHD-C1D-ND	-5.61	119.30	124.45
8	I	101	BCL	CHD-C1D-ND	-5.55	119.36	124.45
8	i	101	BCL	CHD-C1D-ND	-5.55	119.36	124.45
8	m	403	BCL	C4D-CHA-C1A	5.46	127.89	121.25

There are no chirality outliers.

5 of 1239 torsion outliers are listed below:

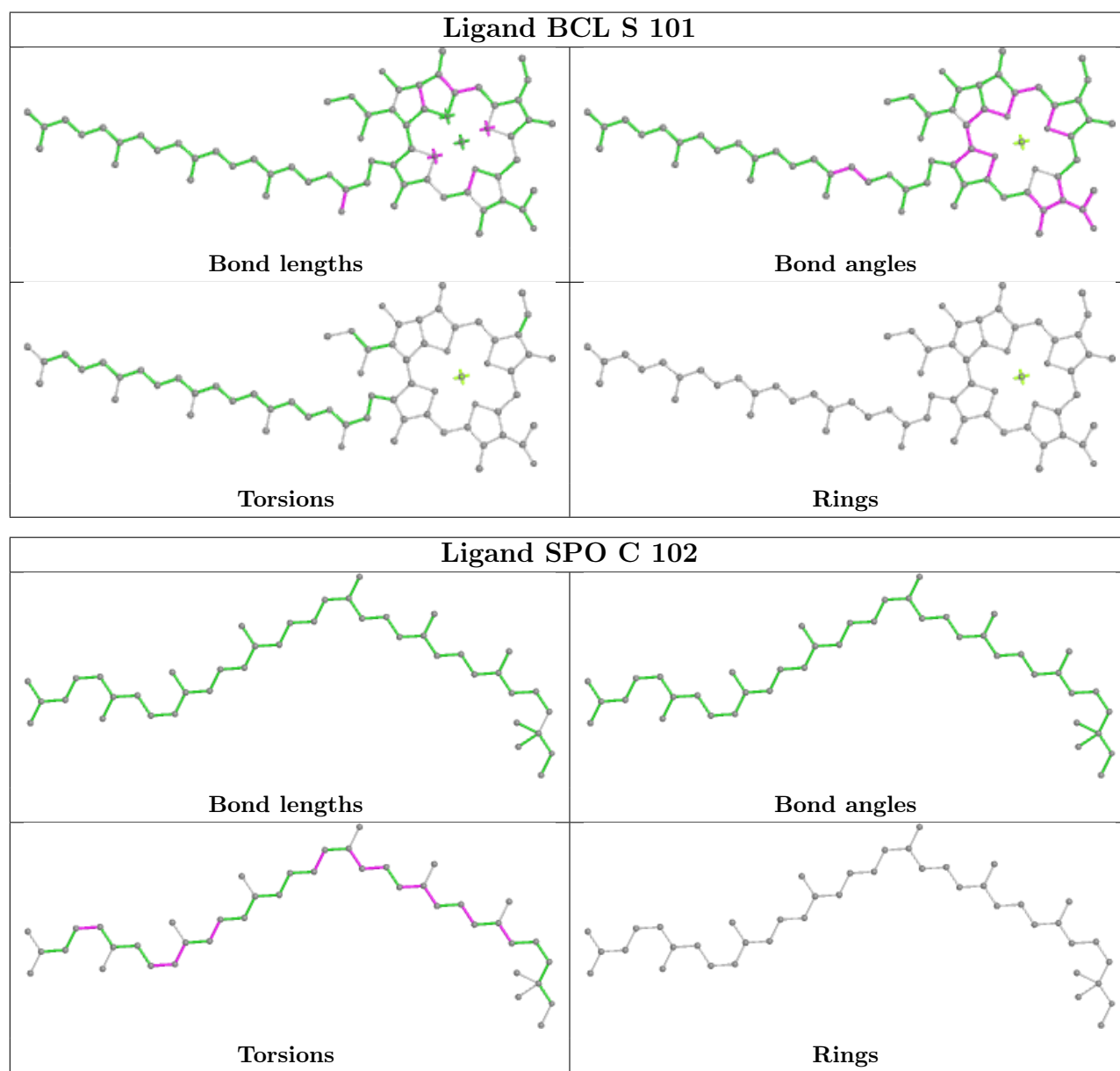
Mol	Chain	Res	Type	Atoms
8	J	101	BCL	C2A-CAA-CBA-CGA
8	7	101	BCL	C2-C3-C5-C6
8	7	101	BCL	C4-C3-C5-C6
8	7	102	BCL	C4-C3-C5-C6
8	0	101	BCL	C2A-CAA-CBA-CGA

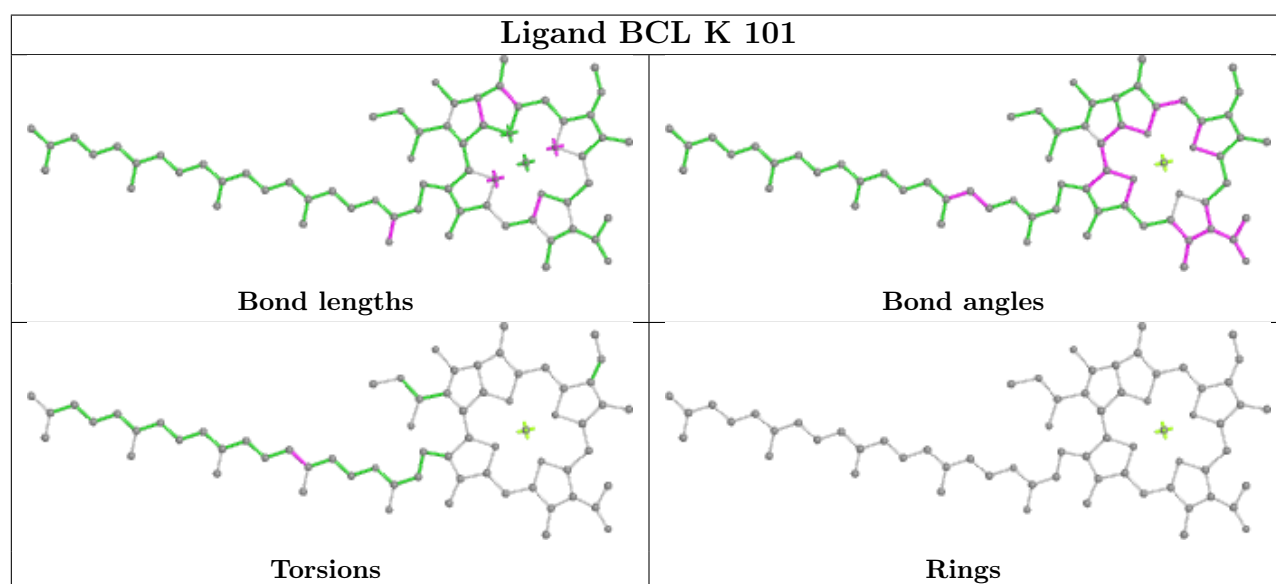
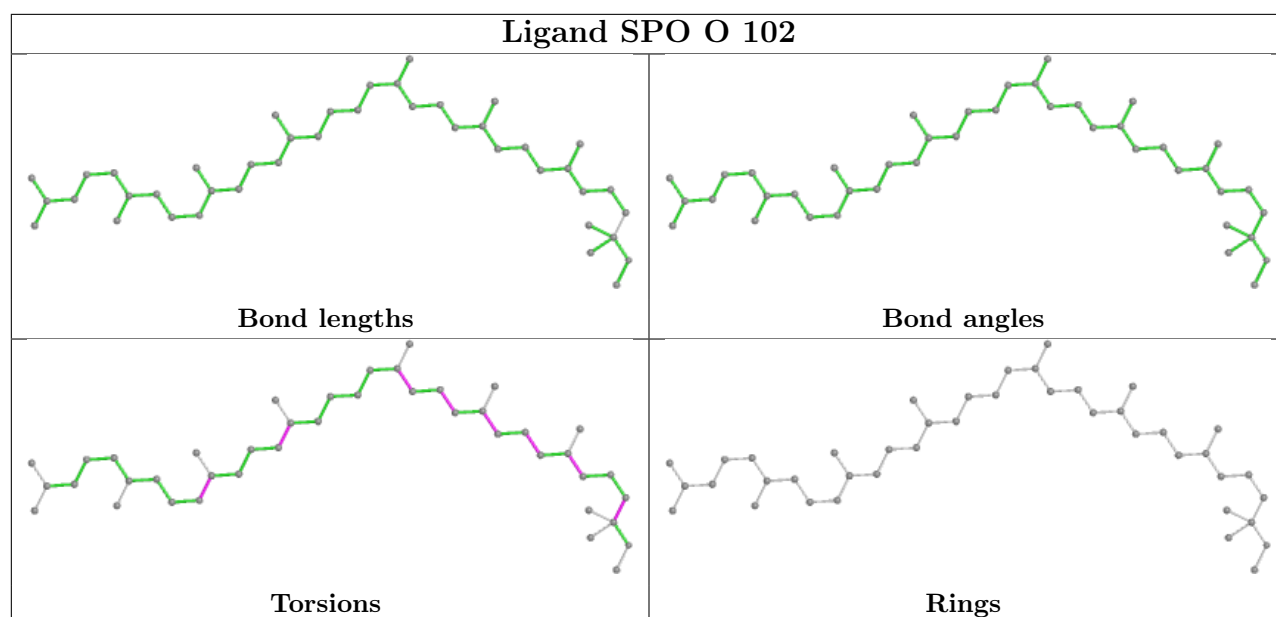
There are no ring outliers.

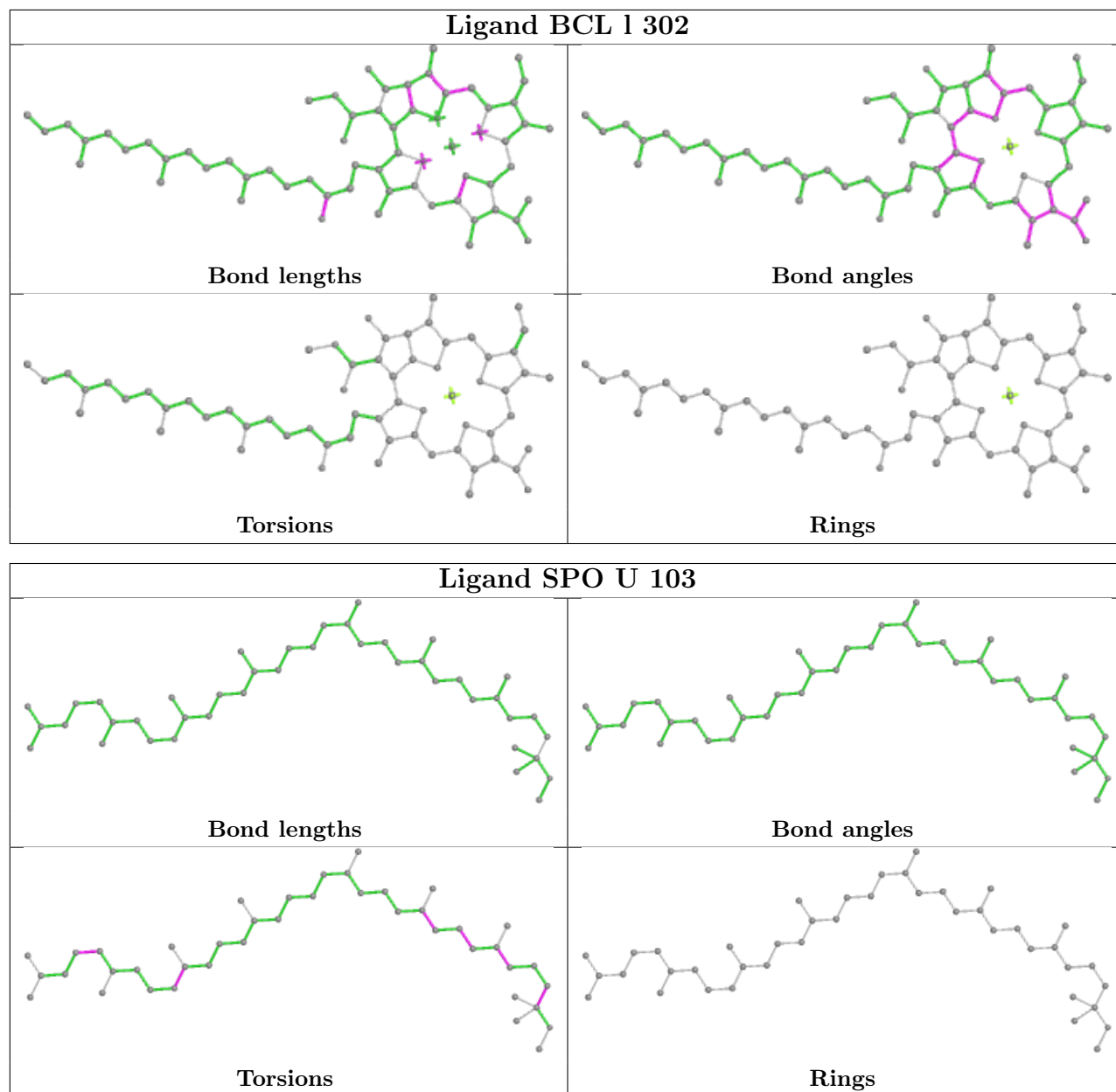
No monomer is involved in short contacts.

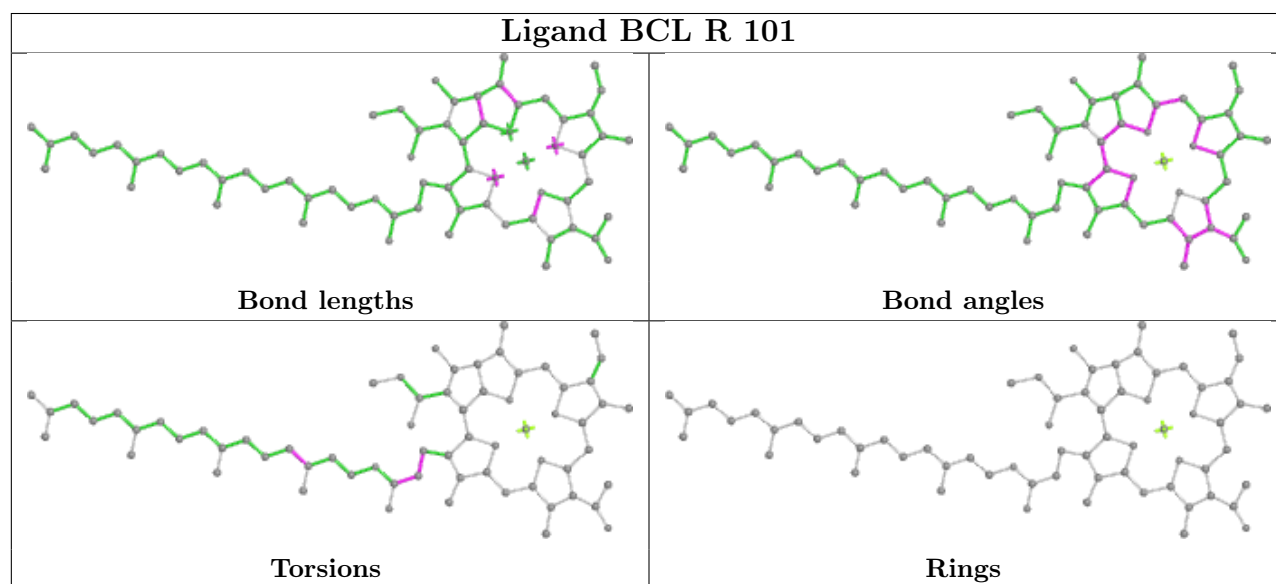
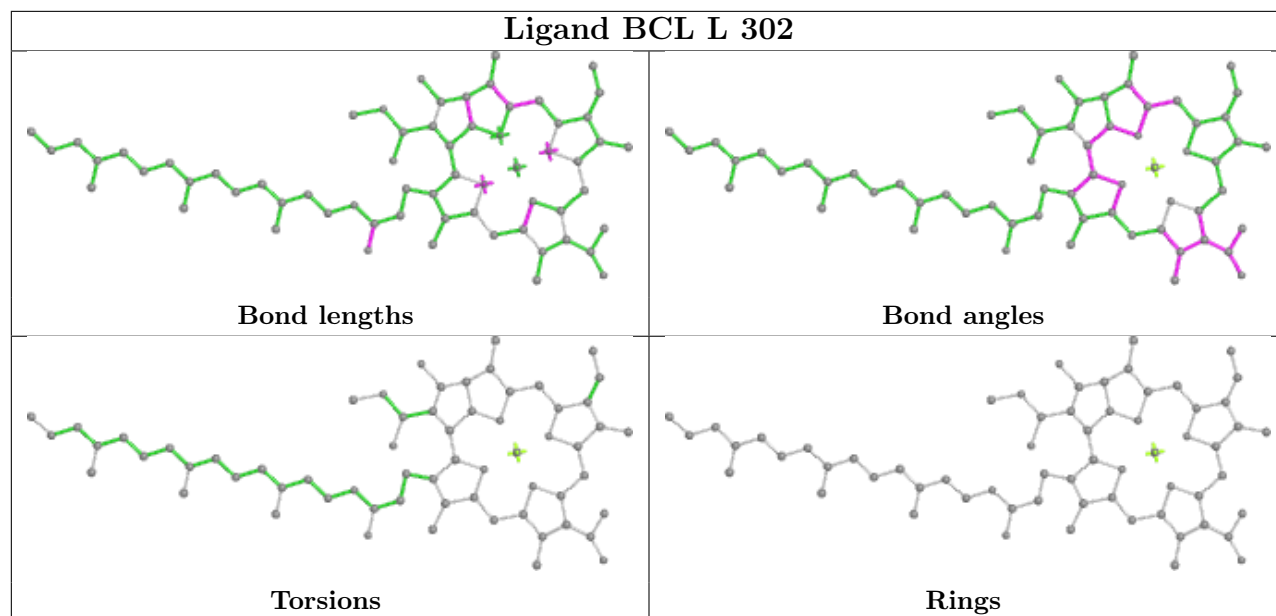


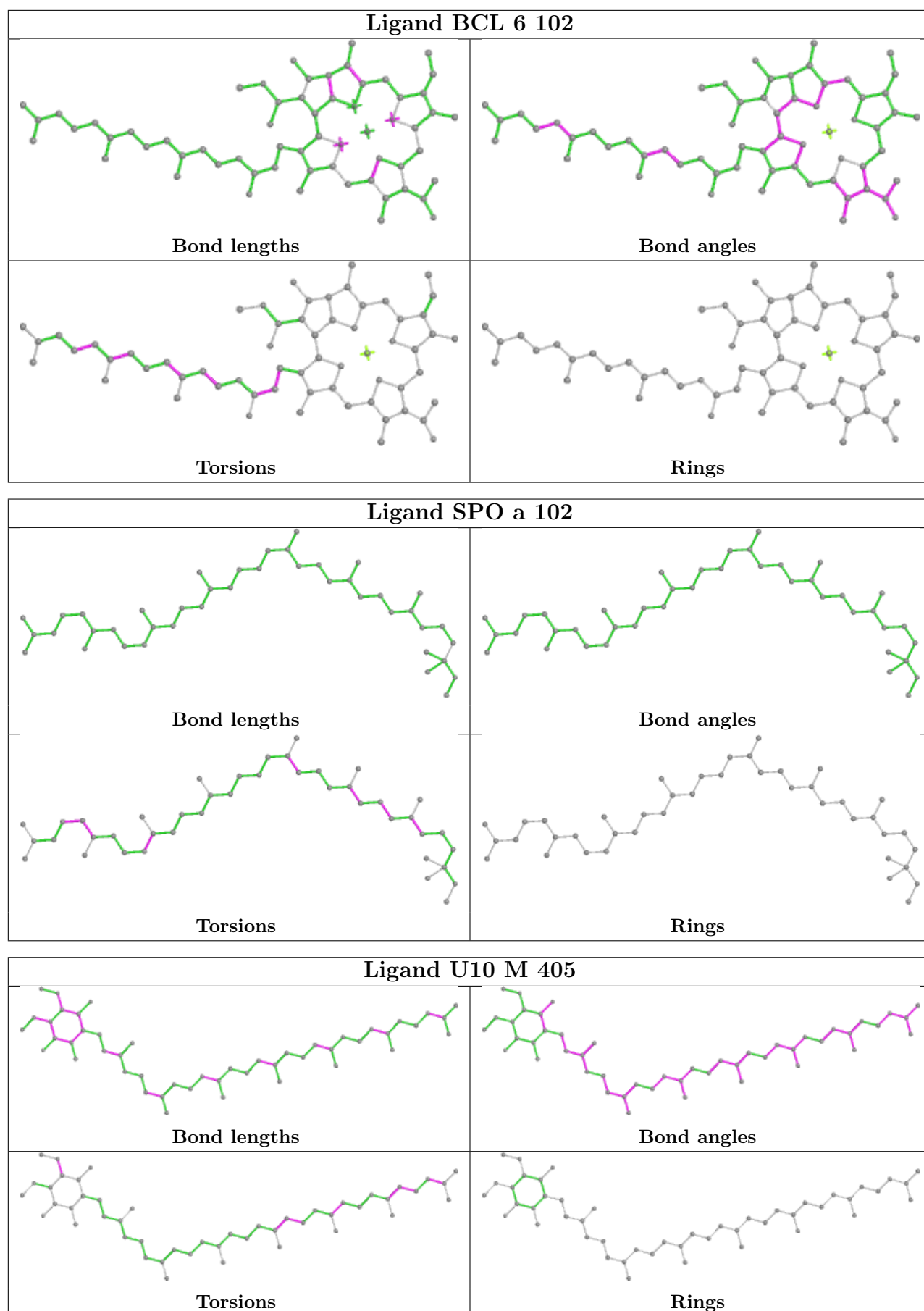
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

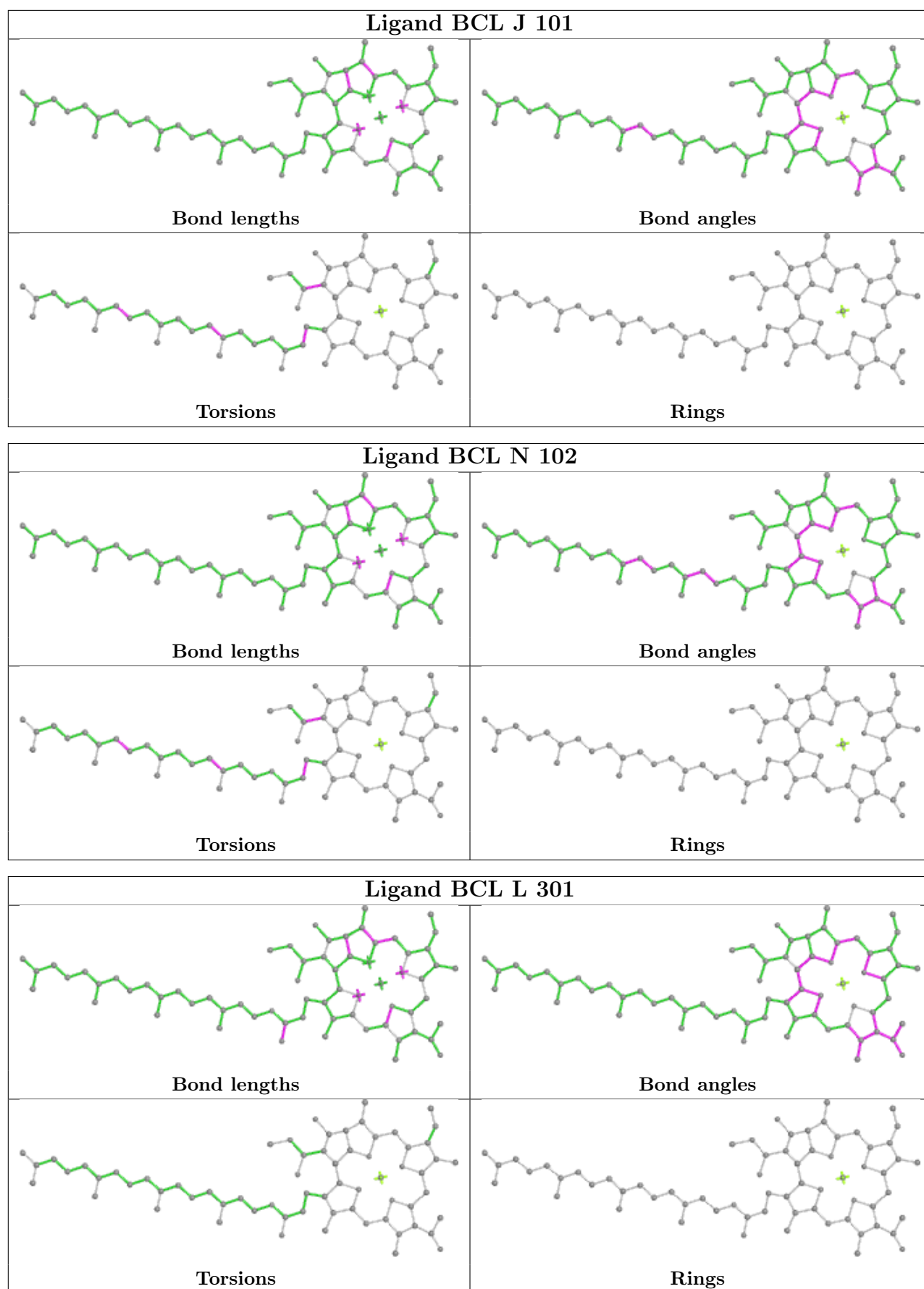


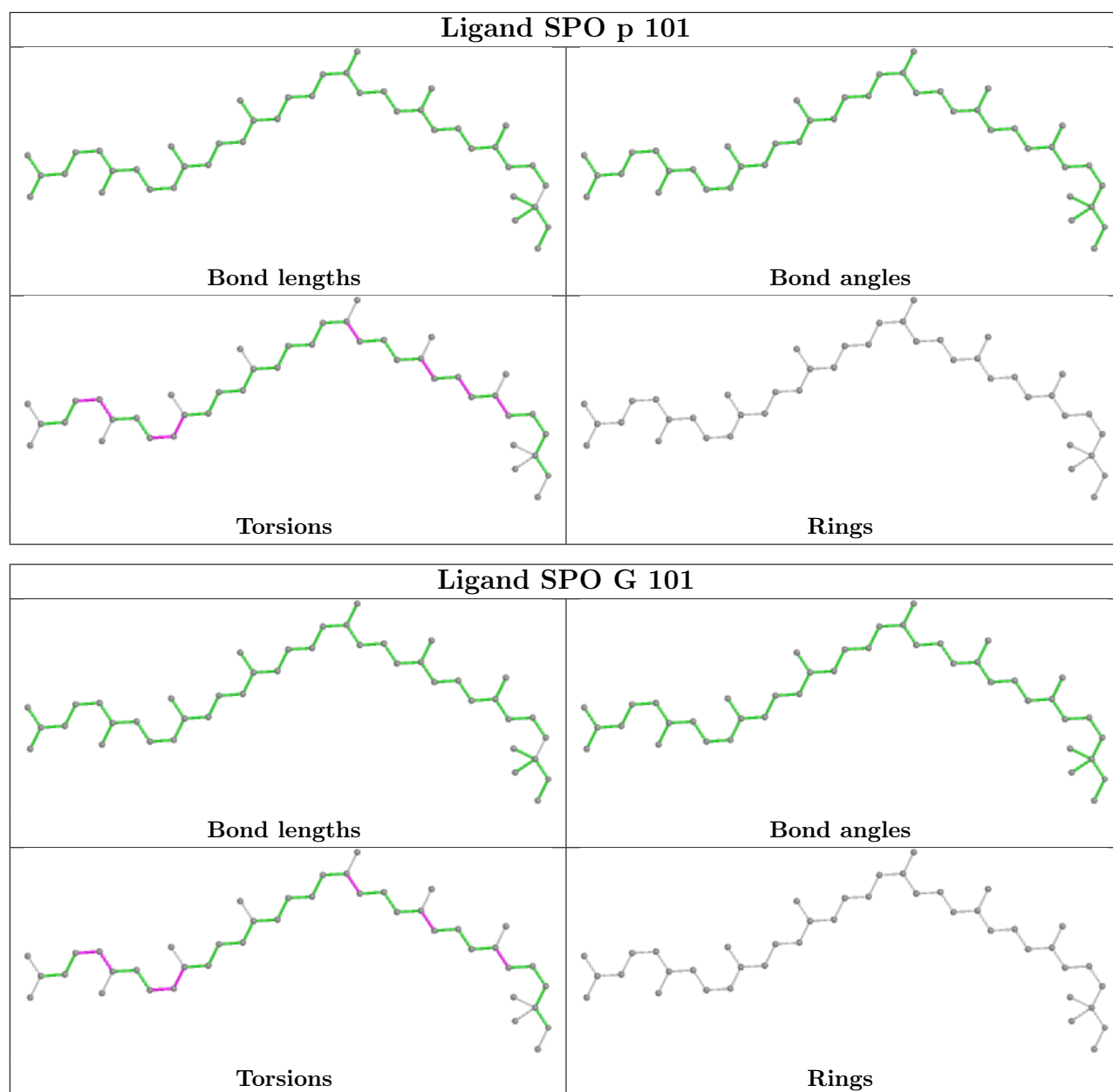


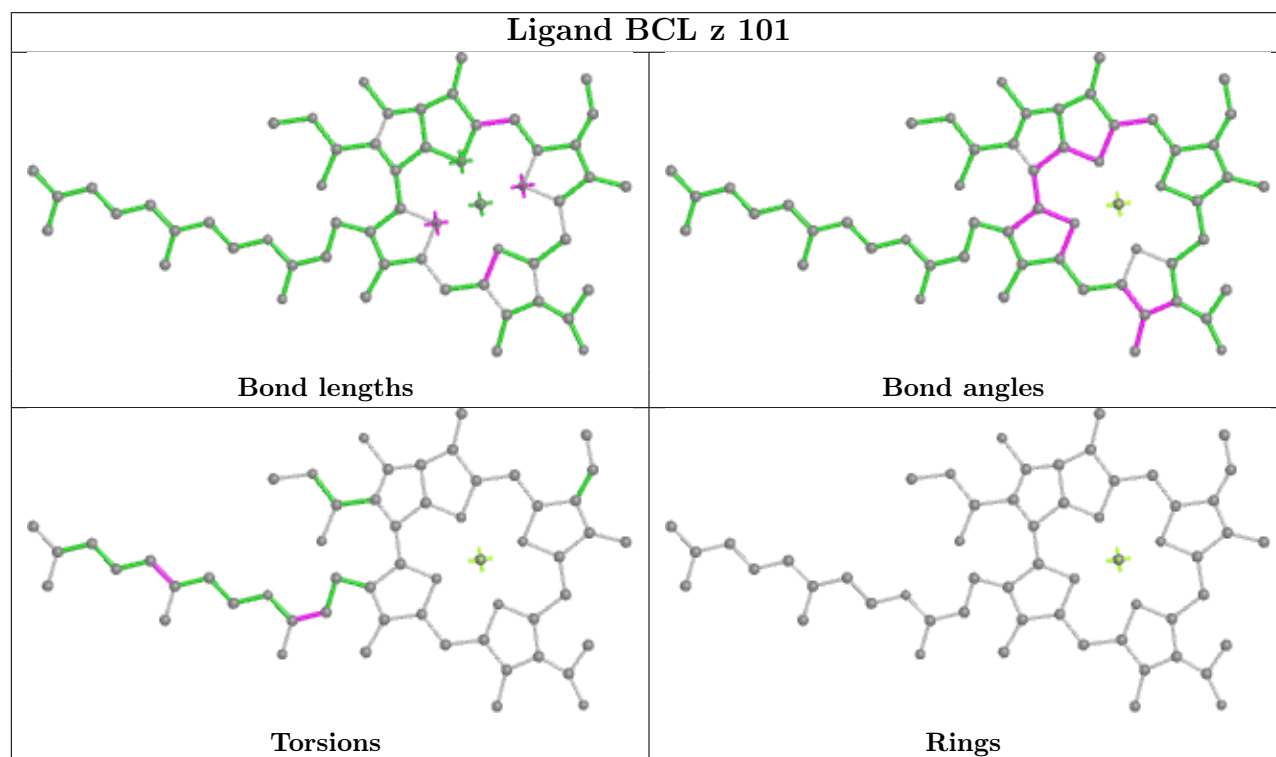
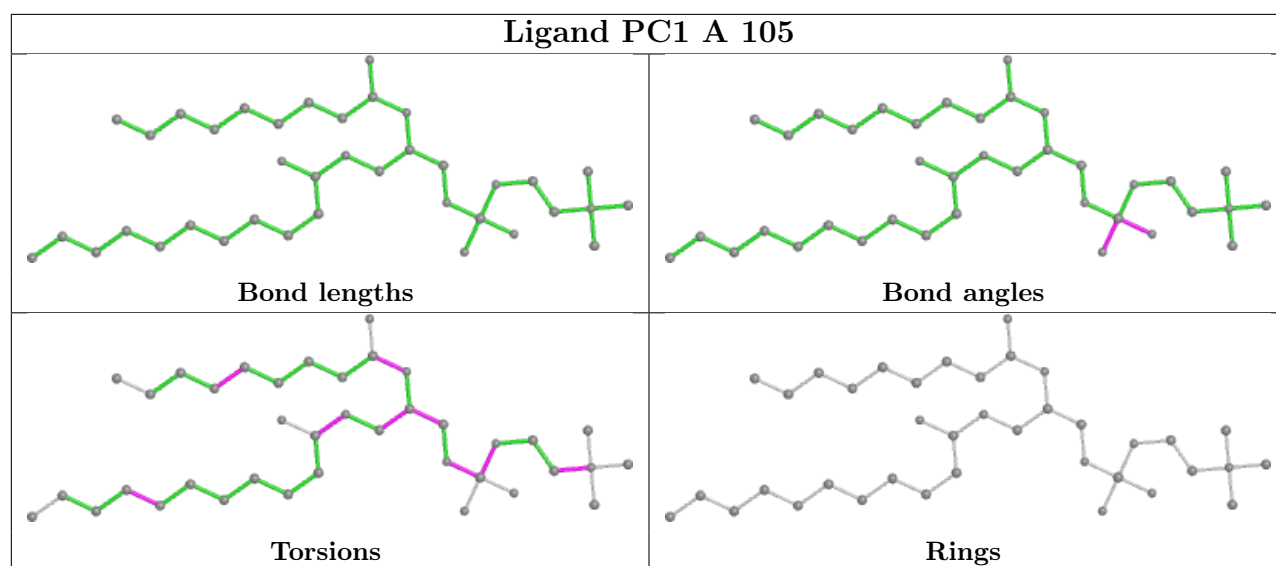




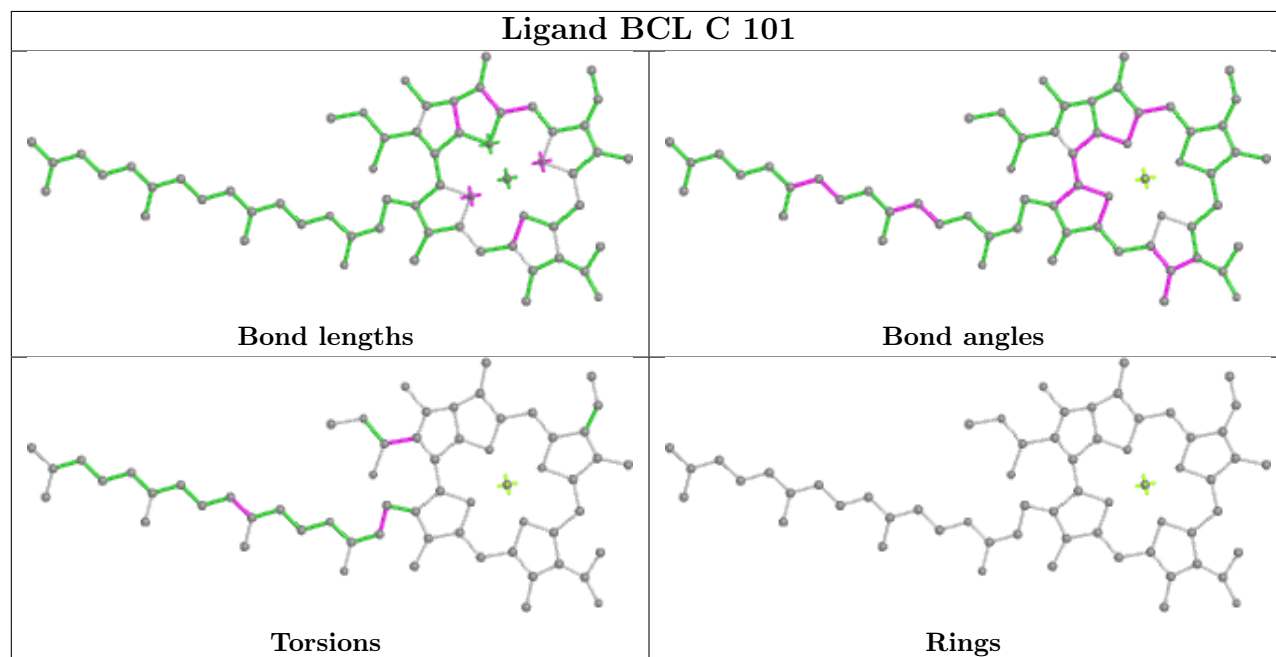
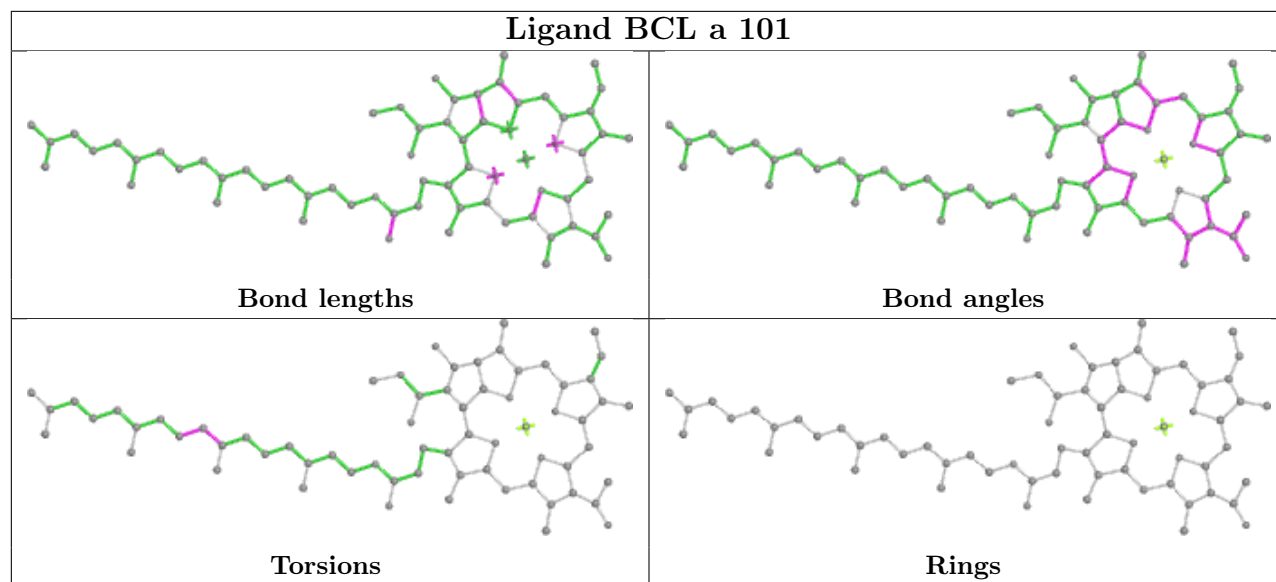


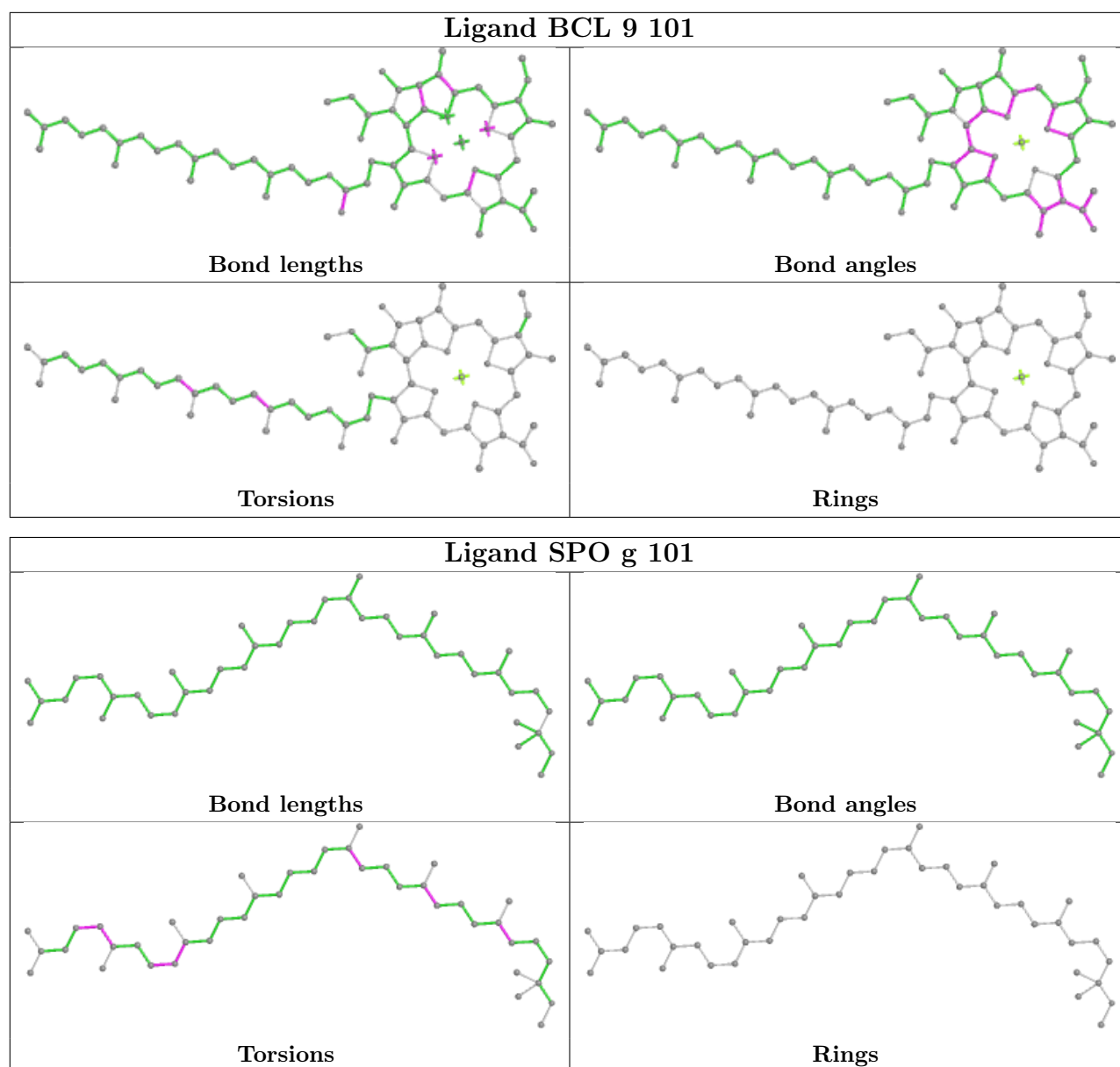


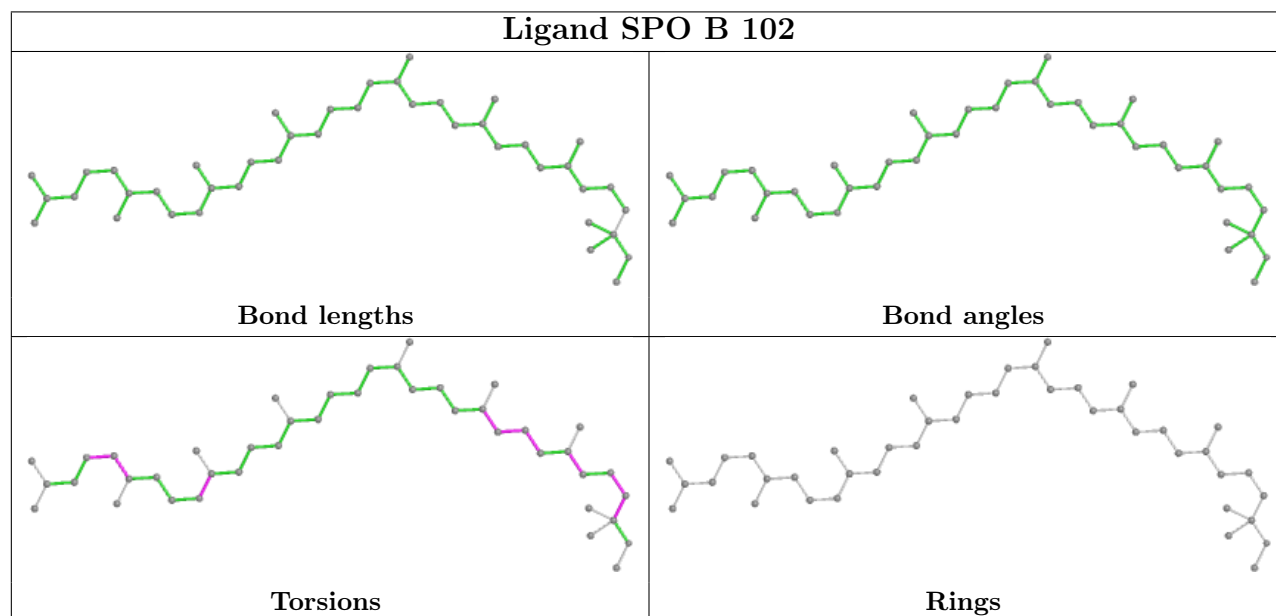
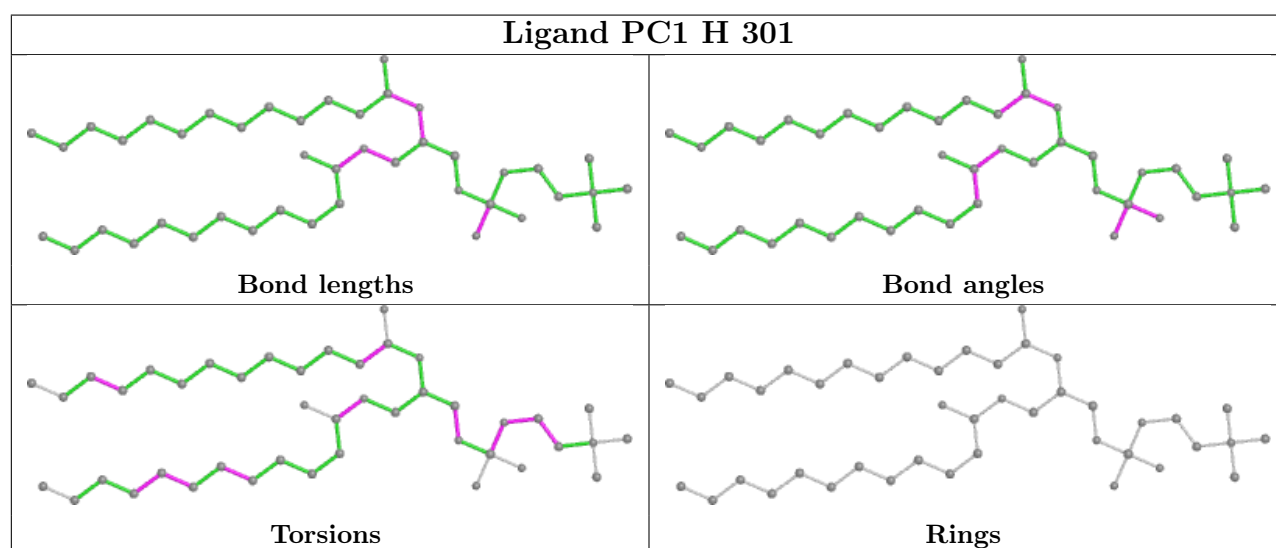
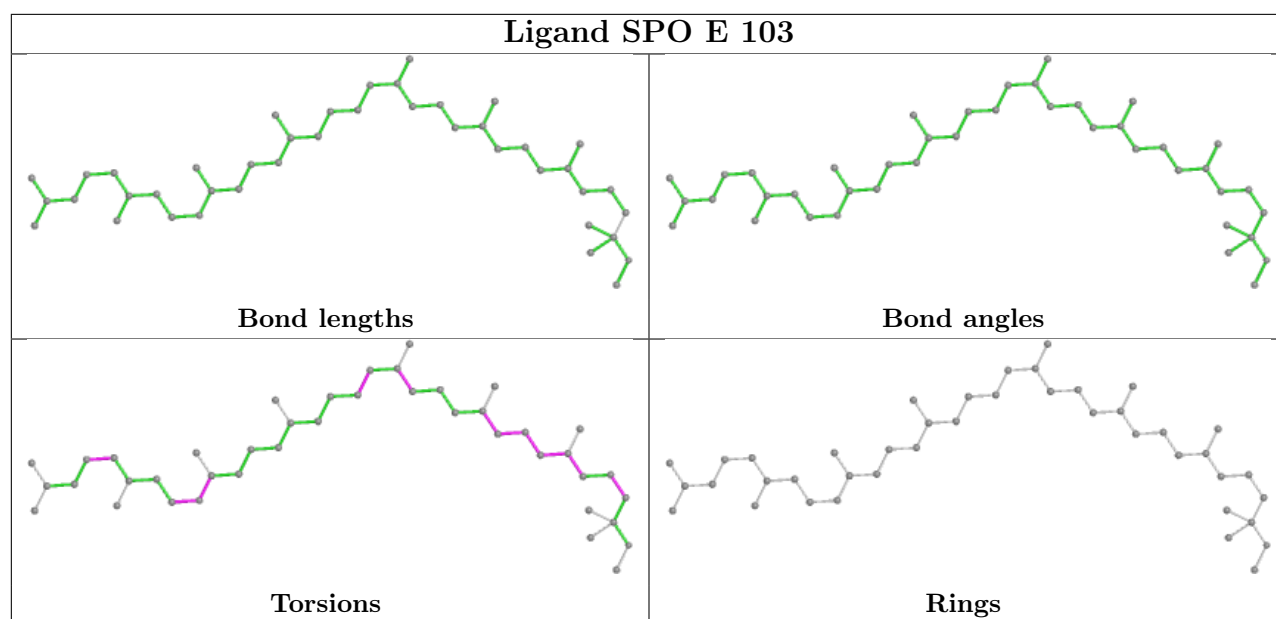


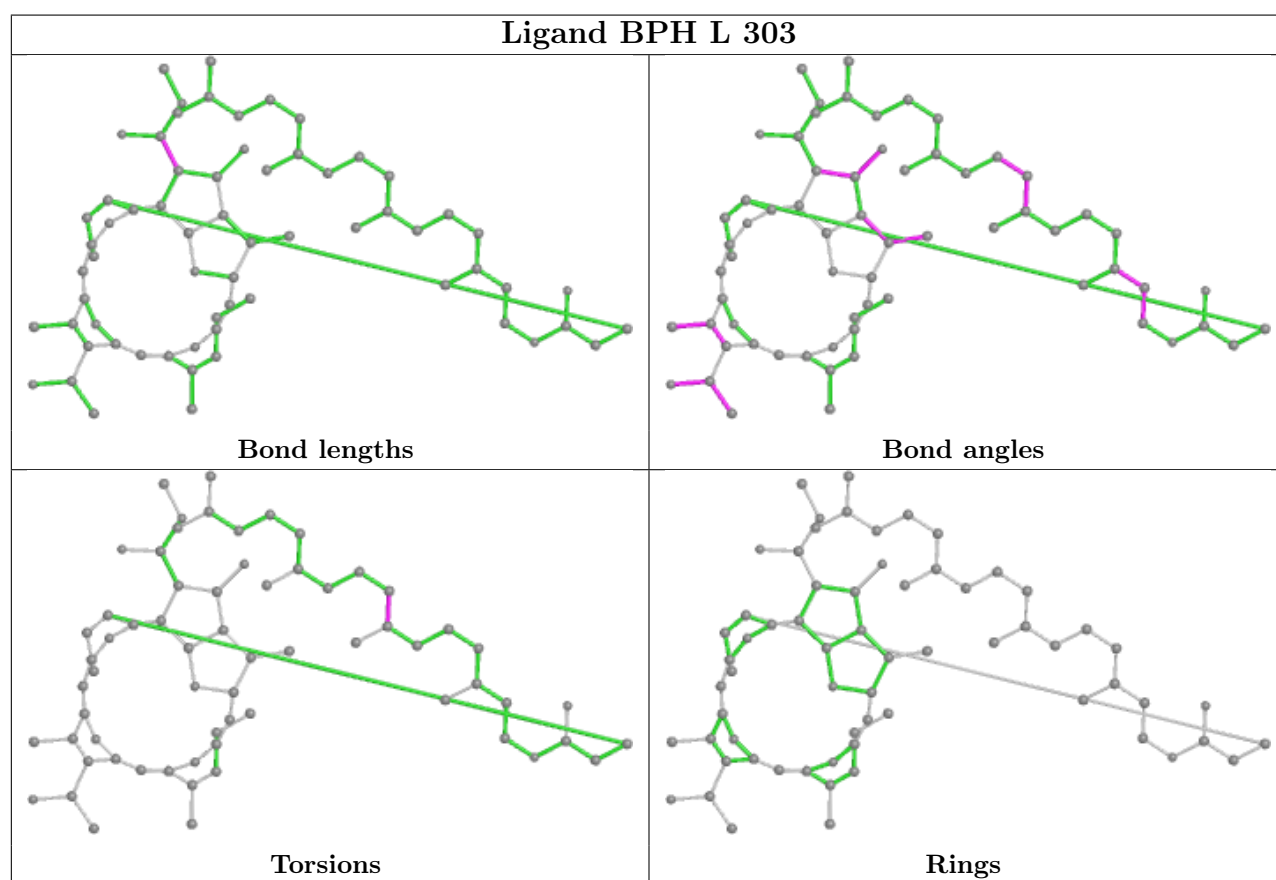
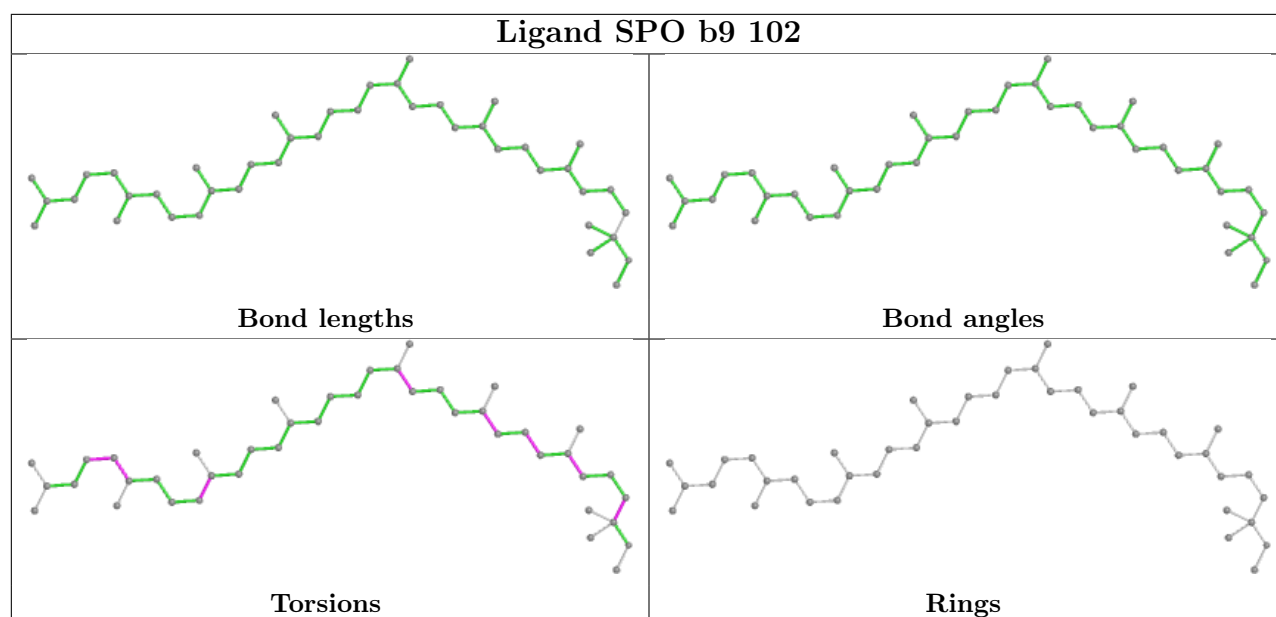


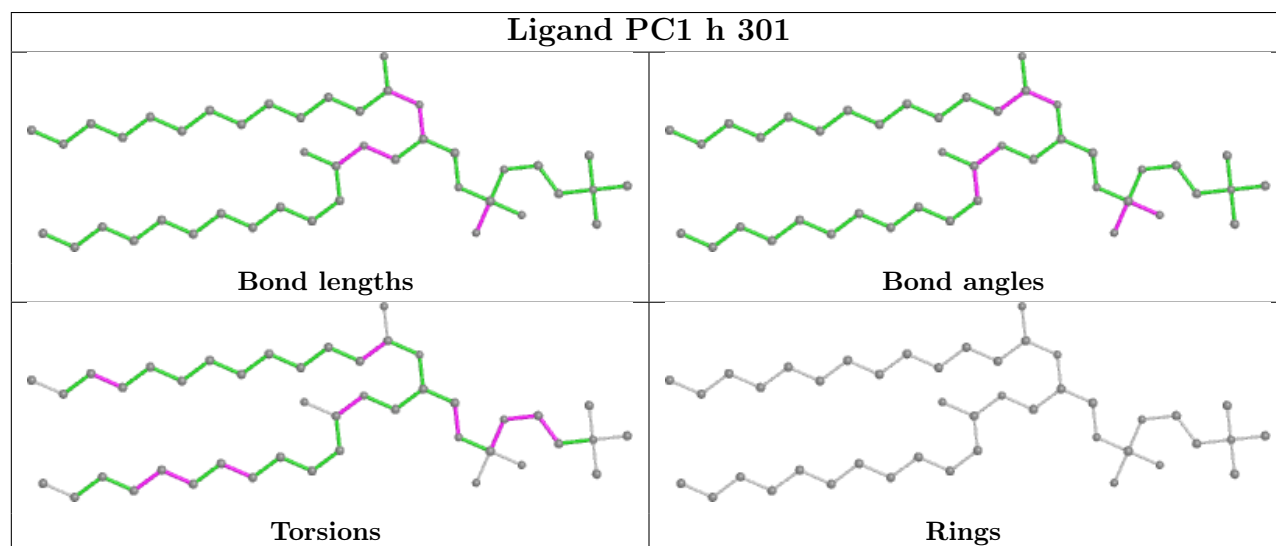
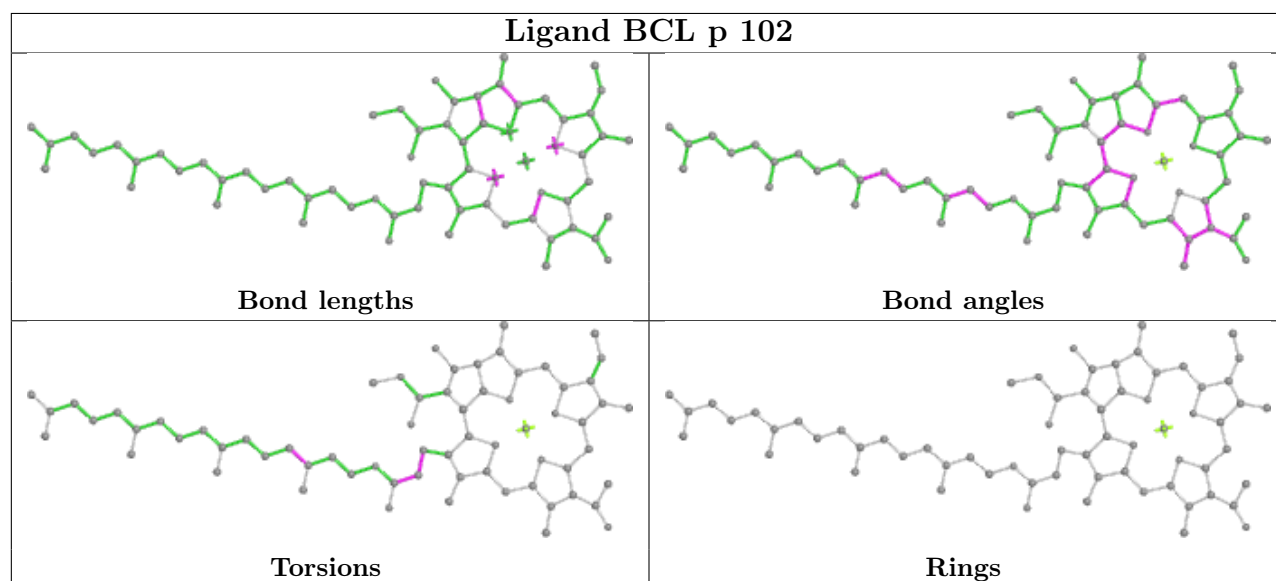
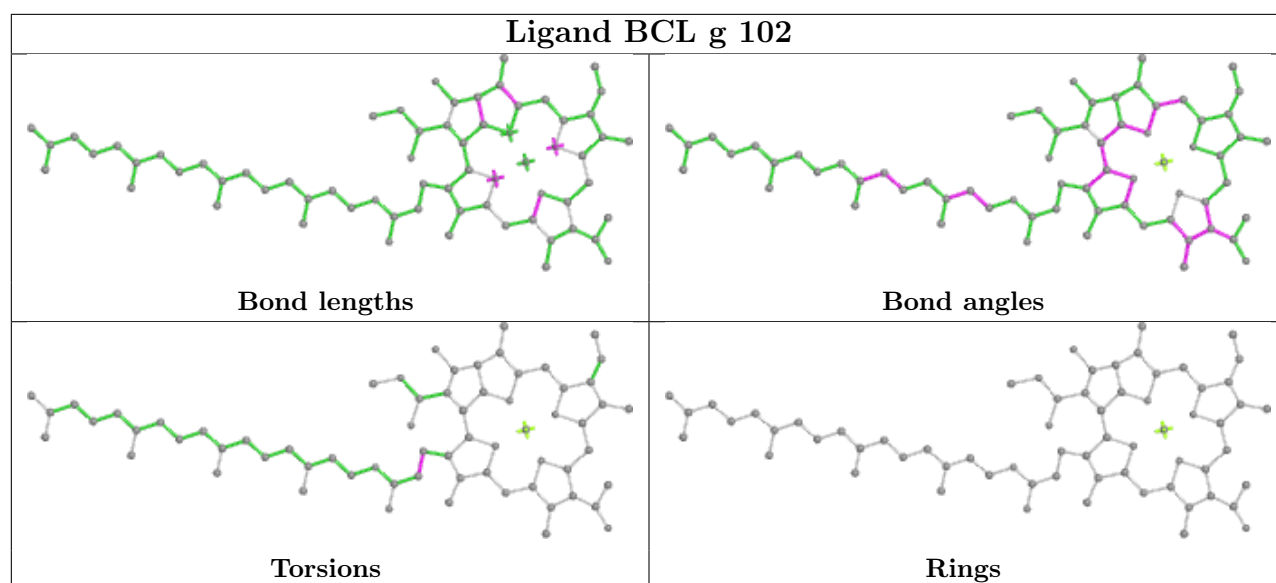


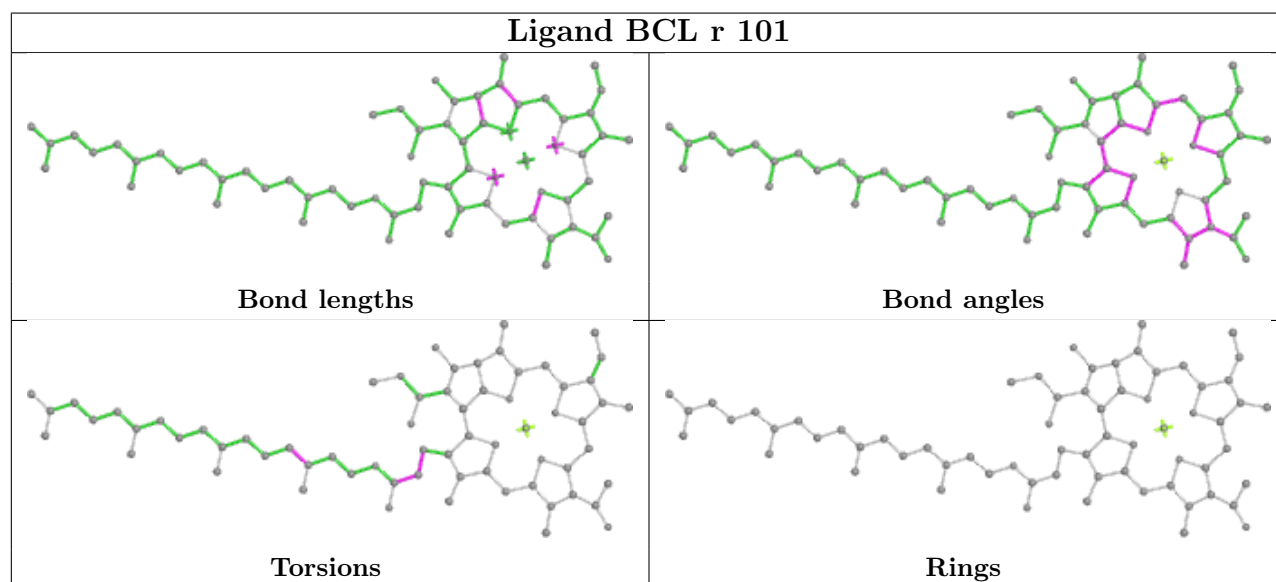
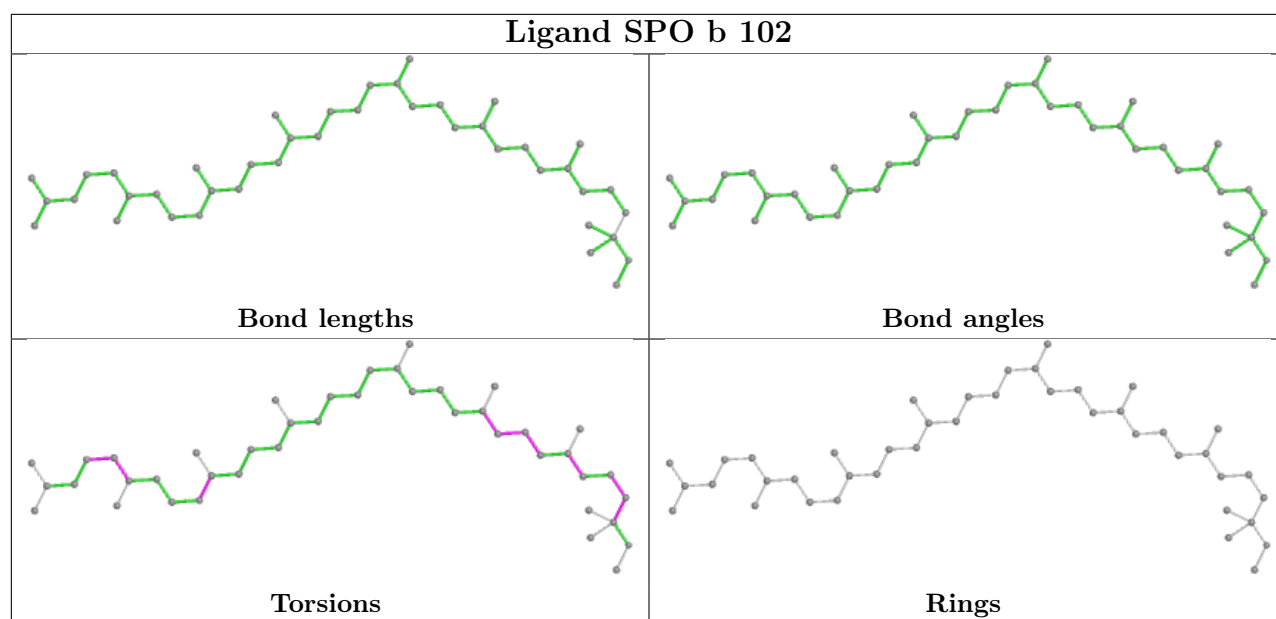


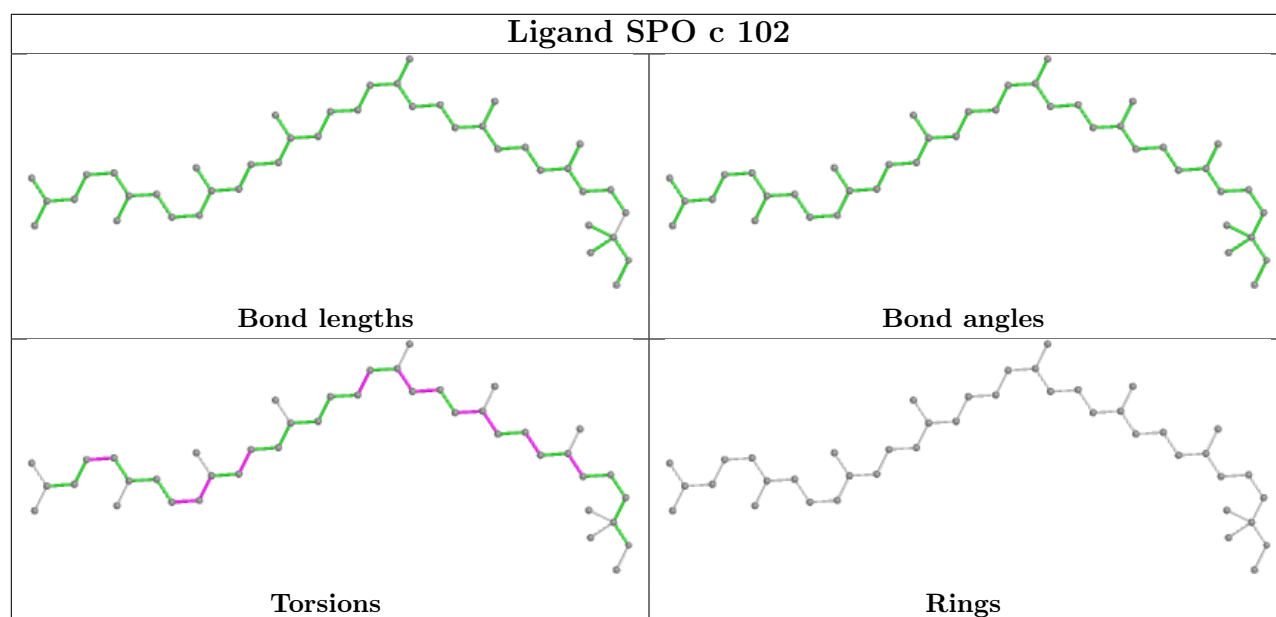
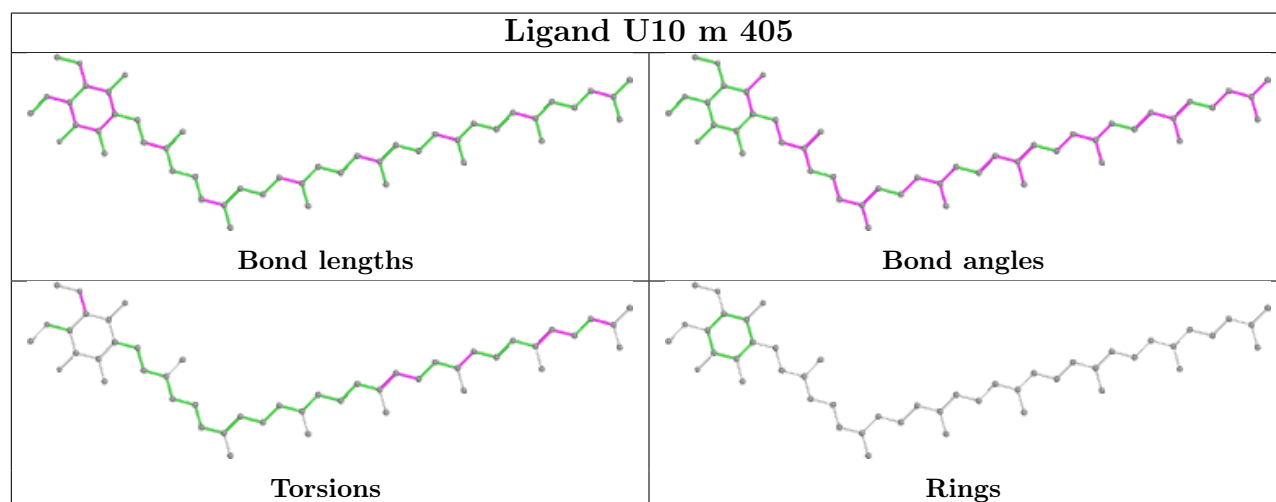
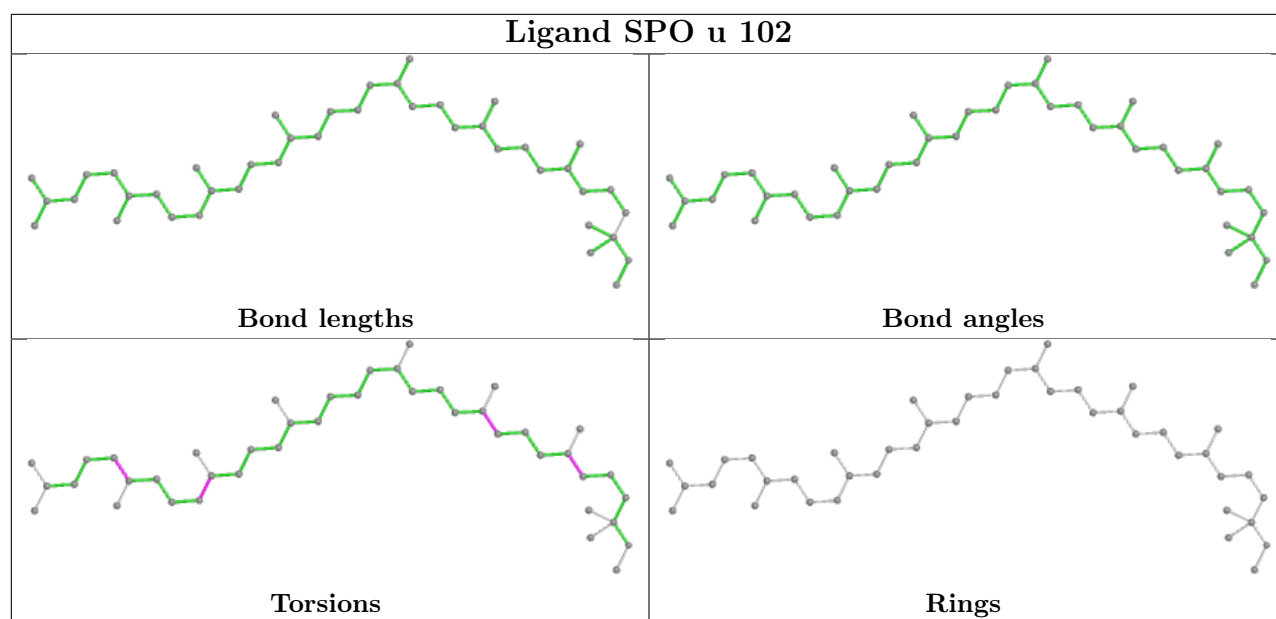


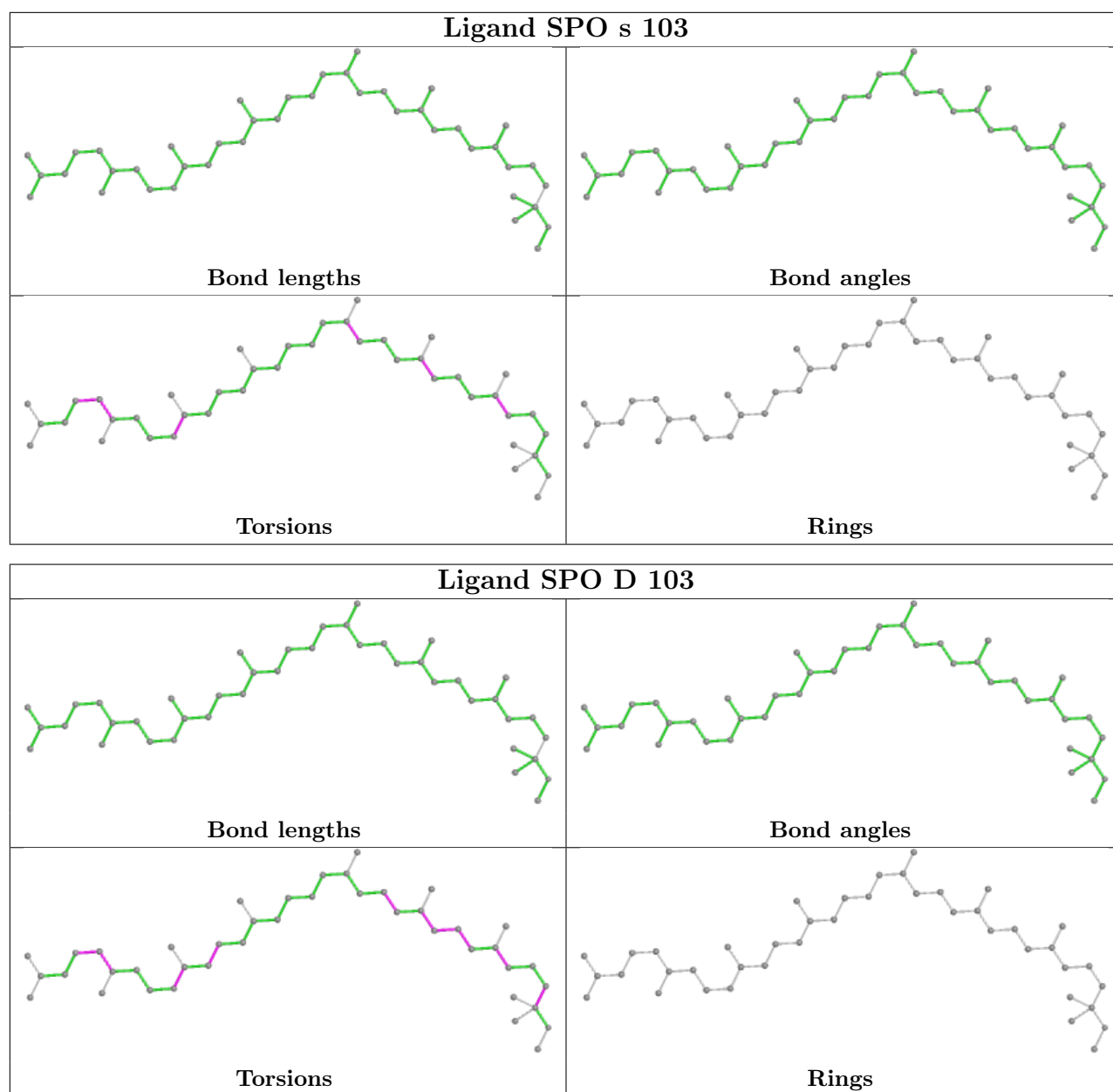




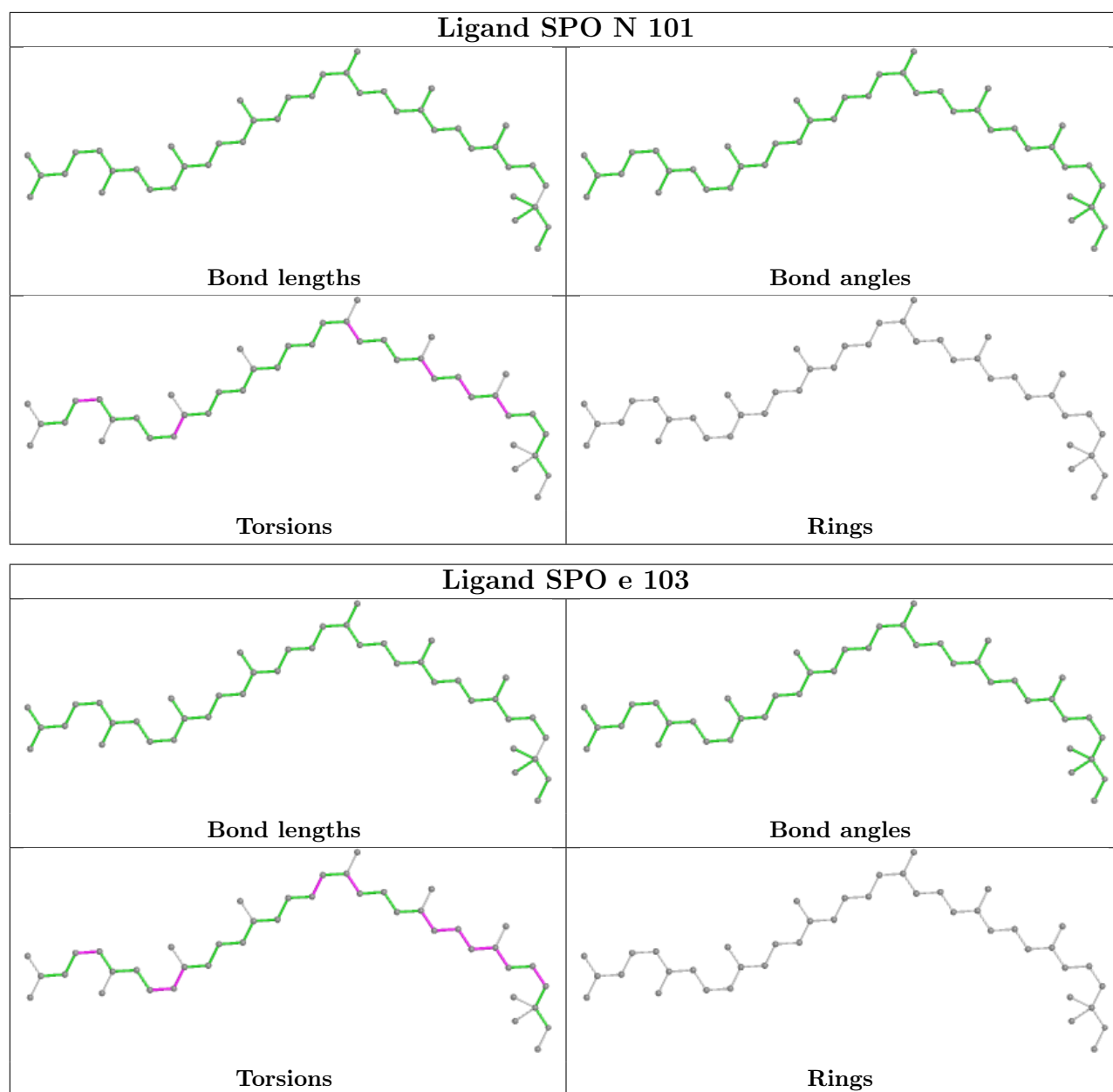


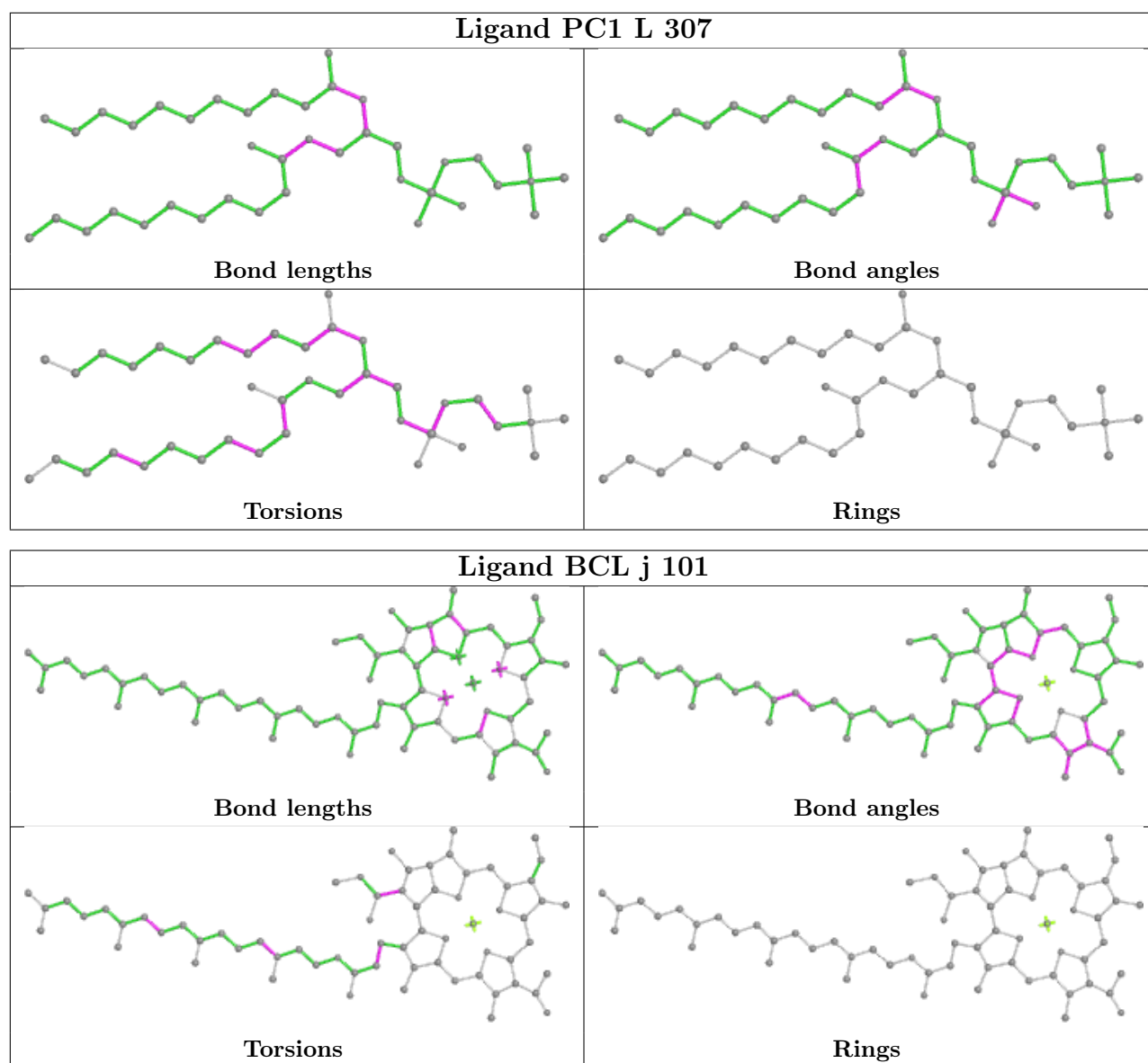


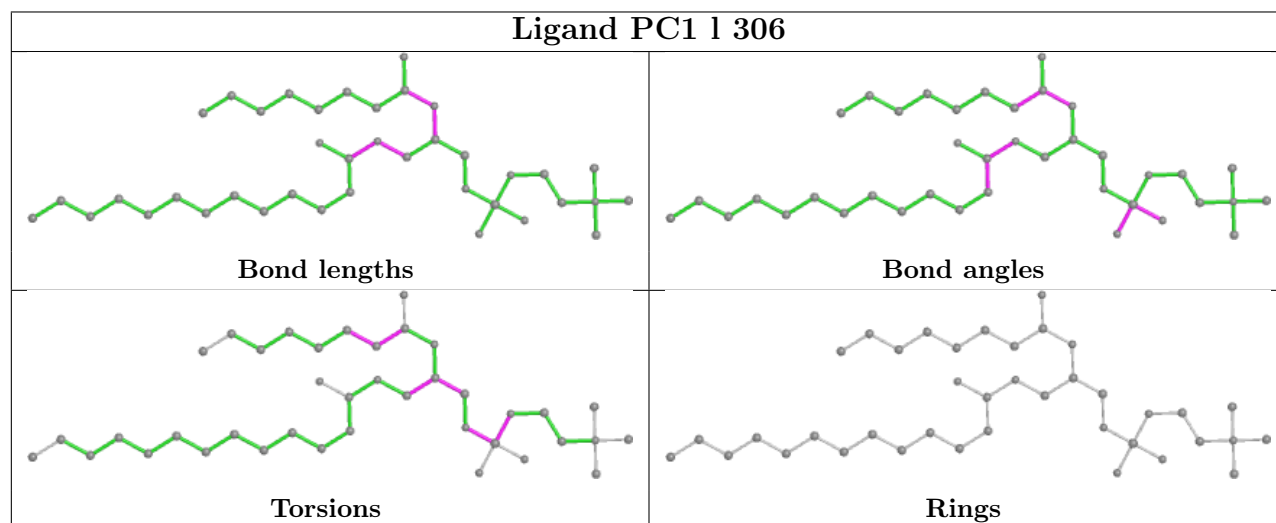
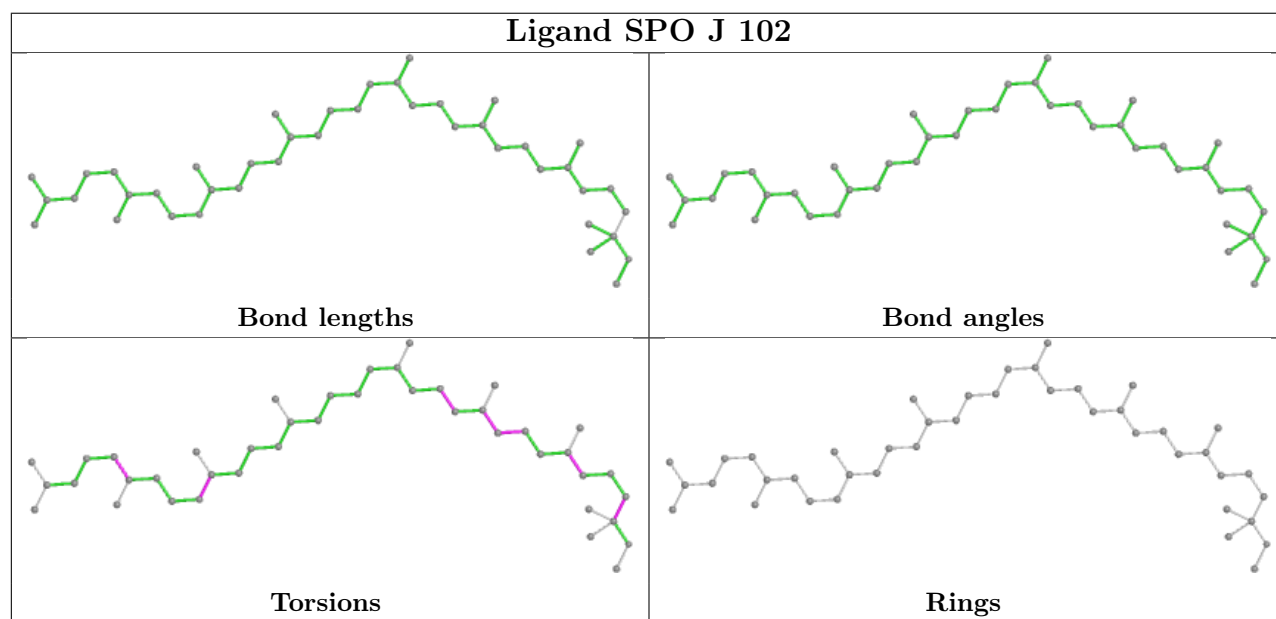
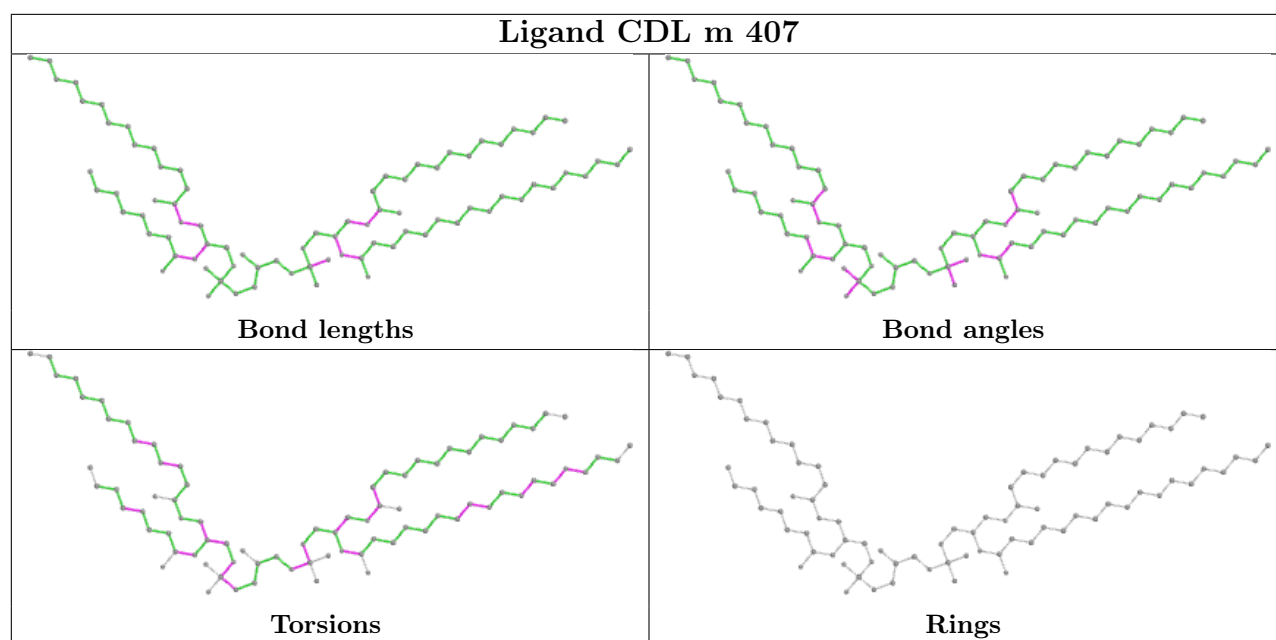


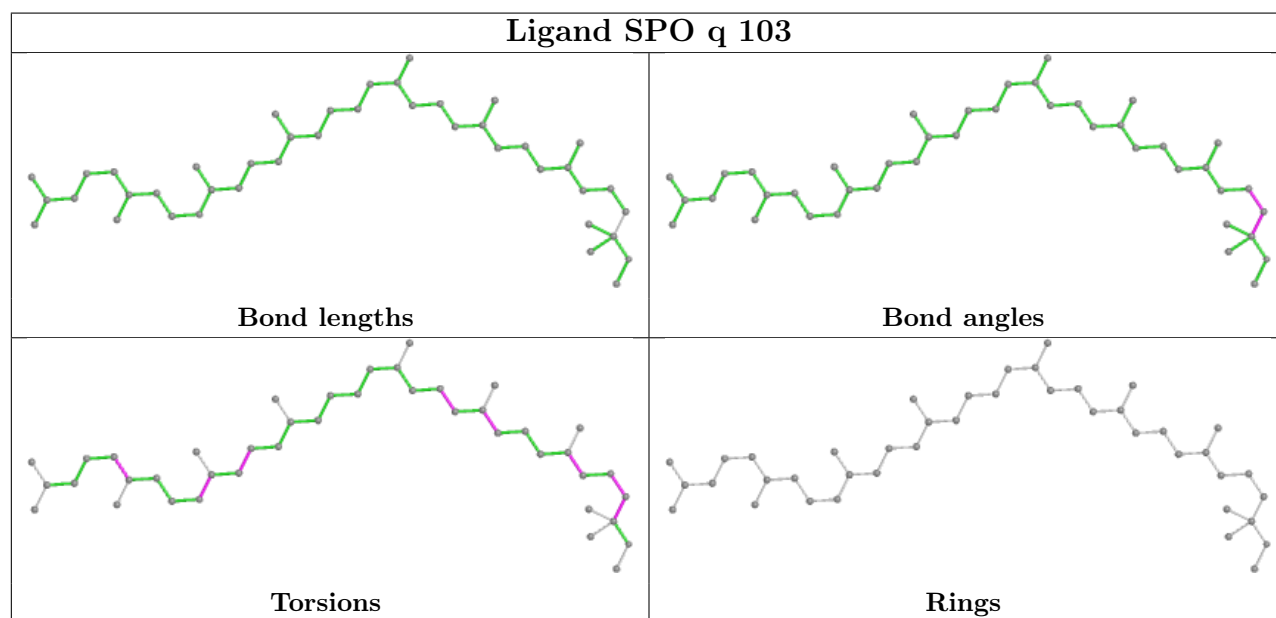
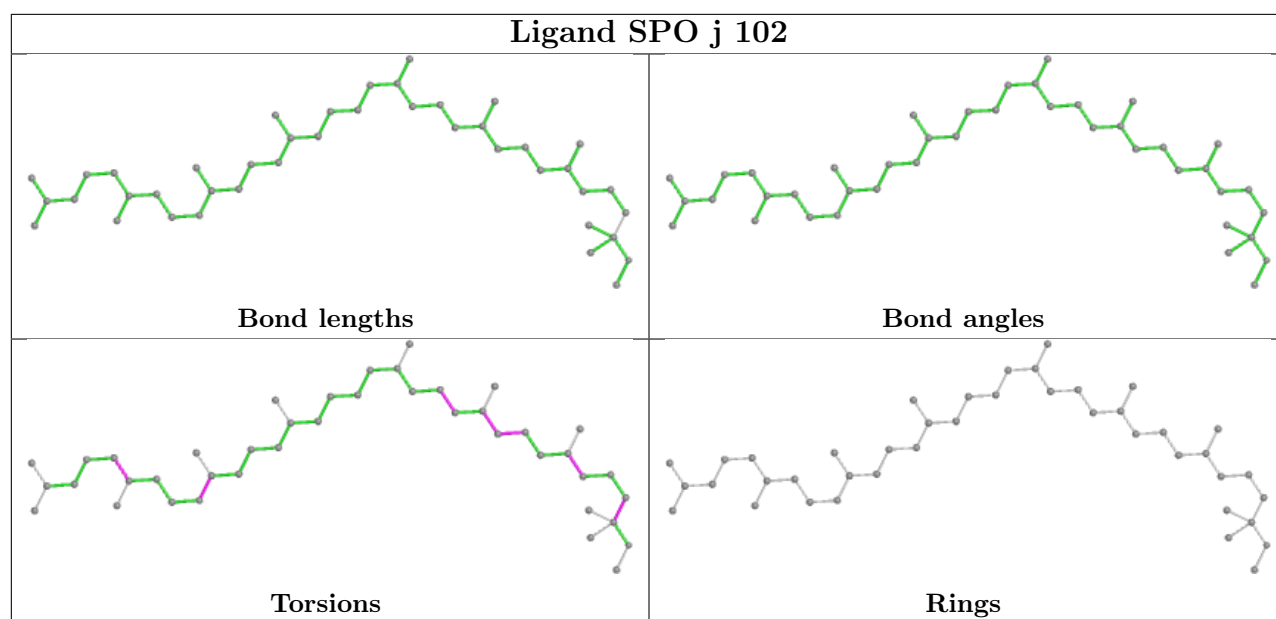


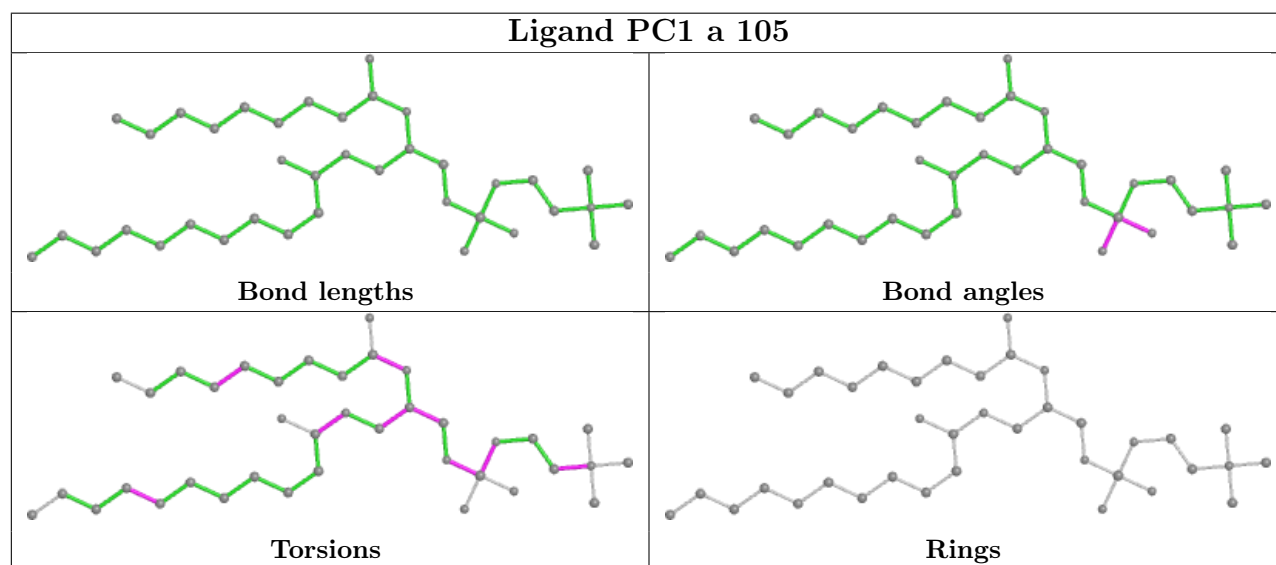
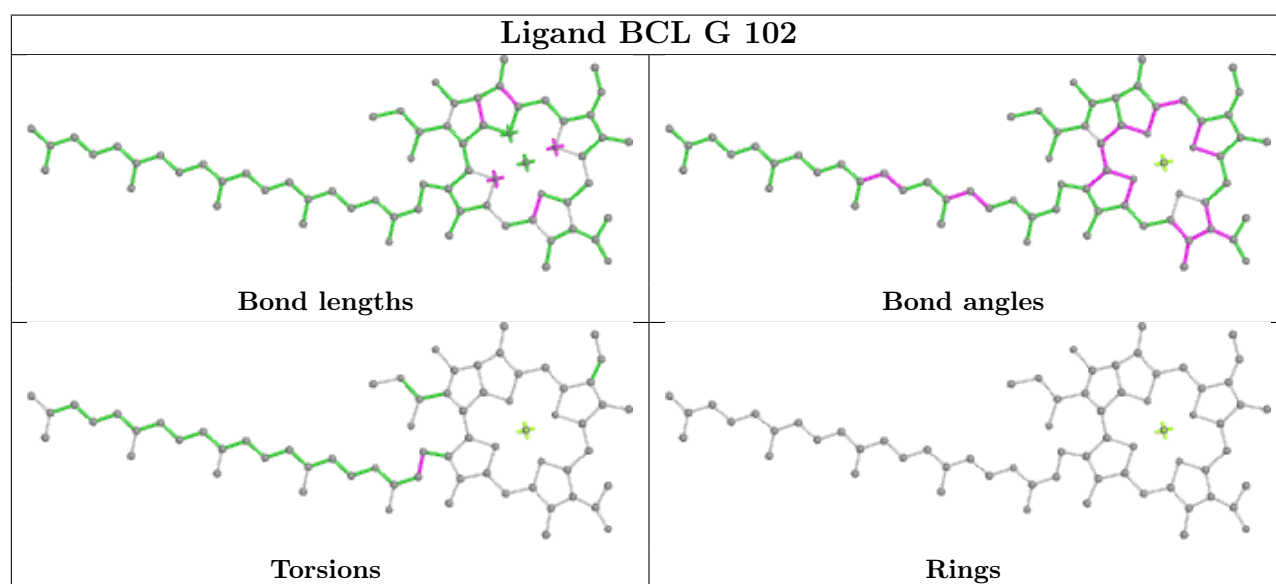
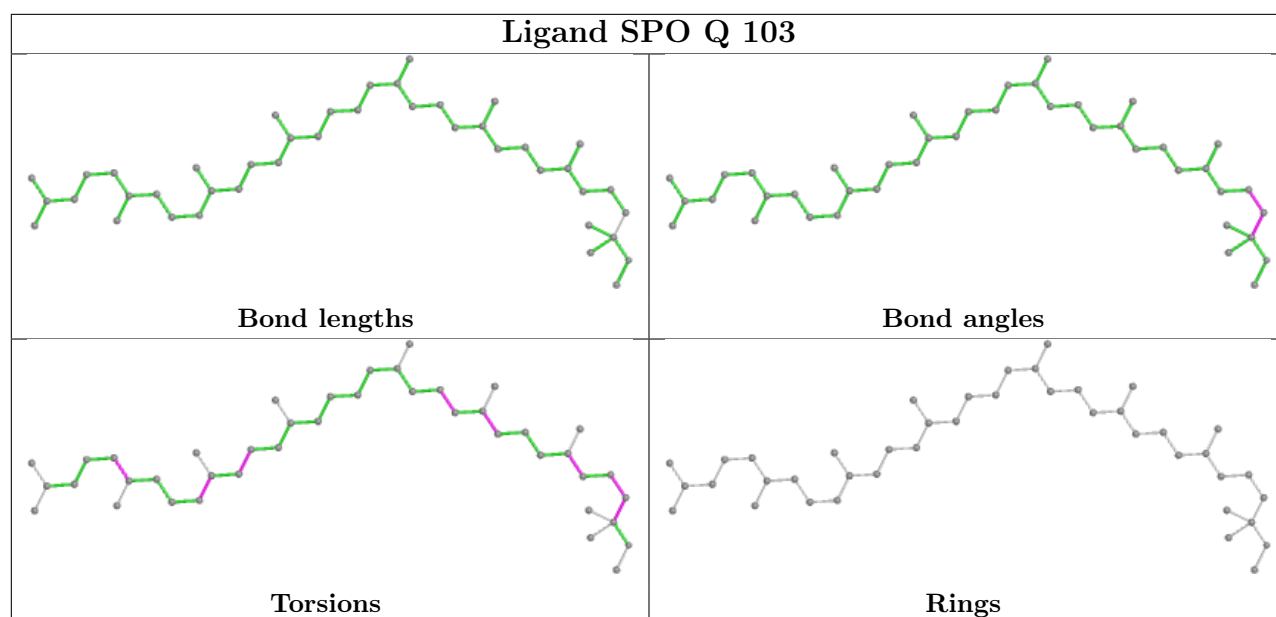


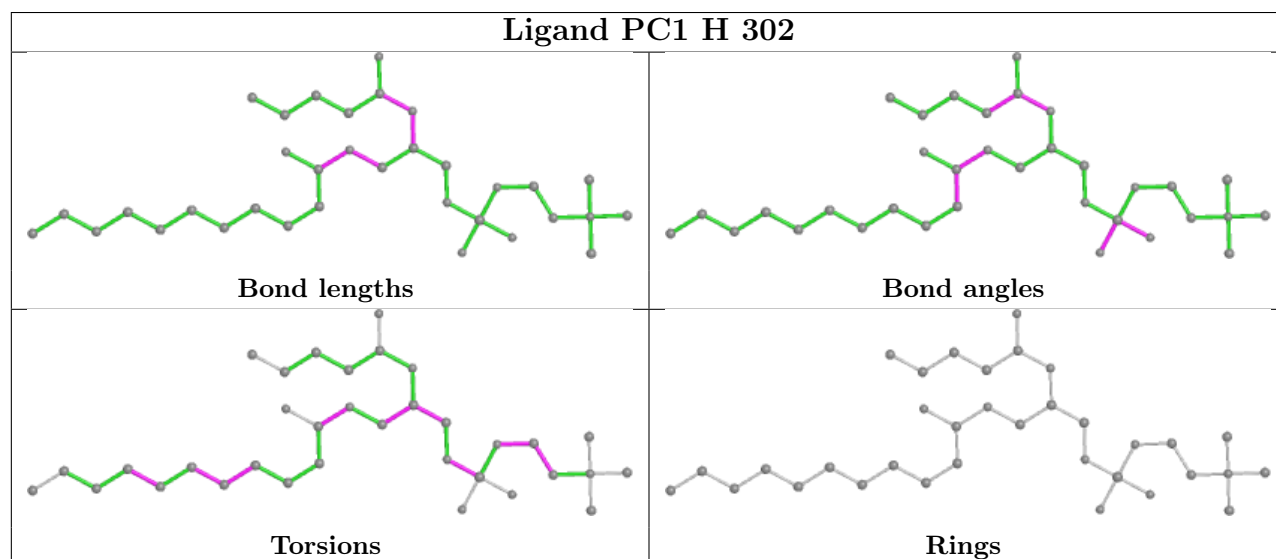
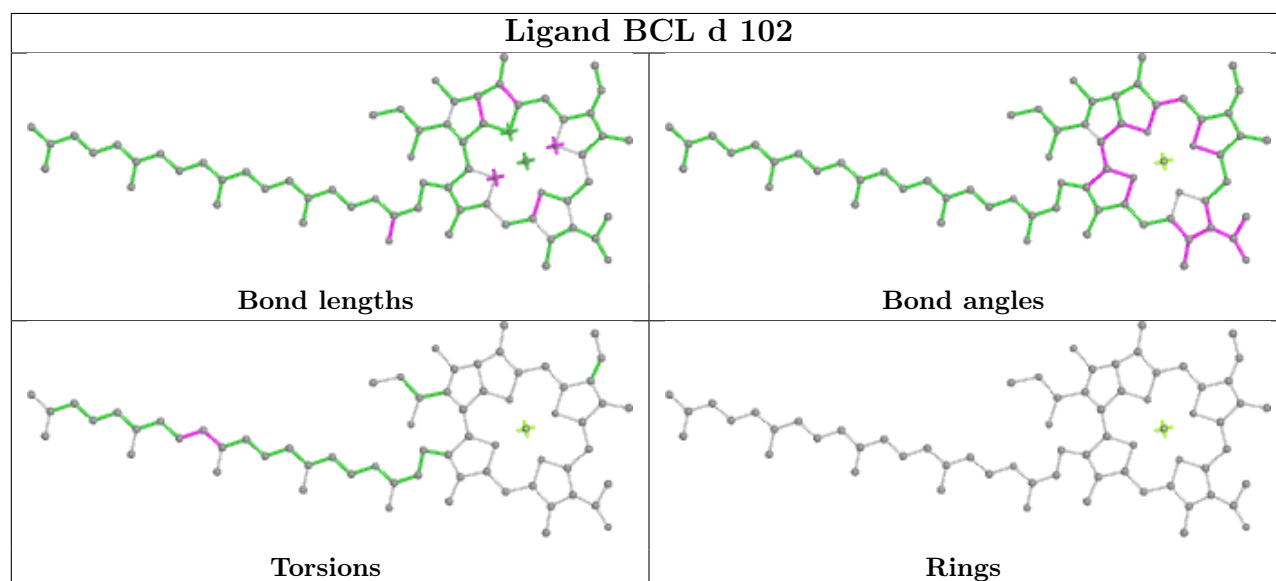
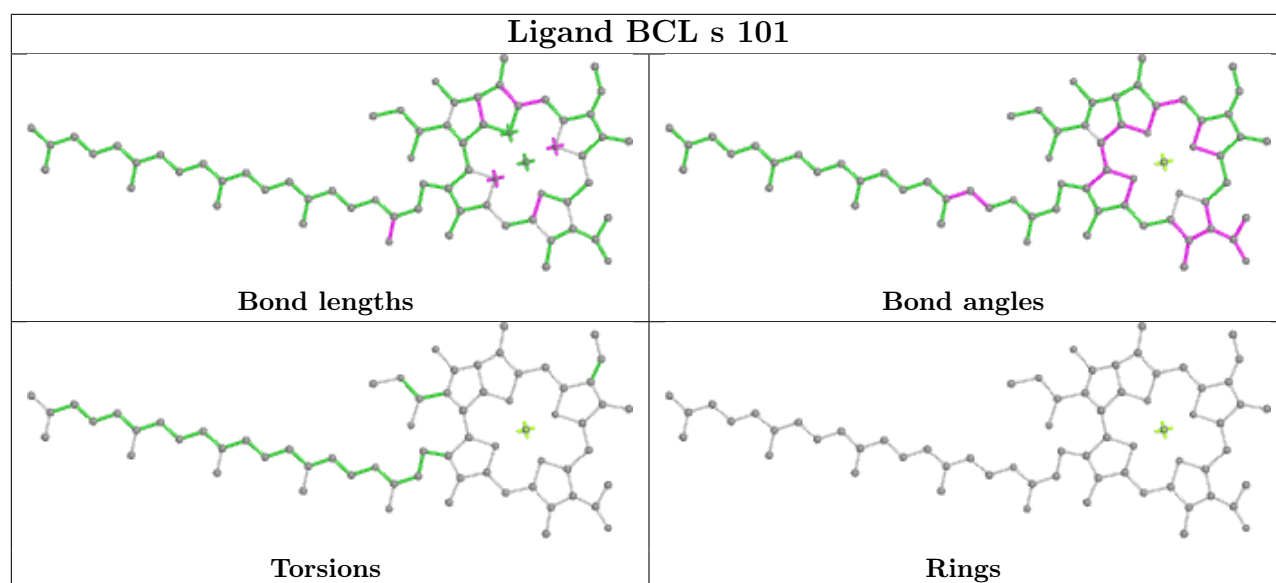


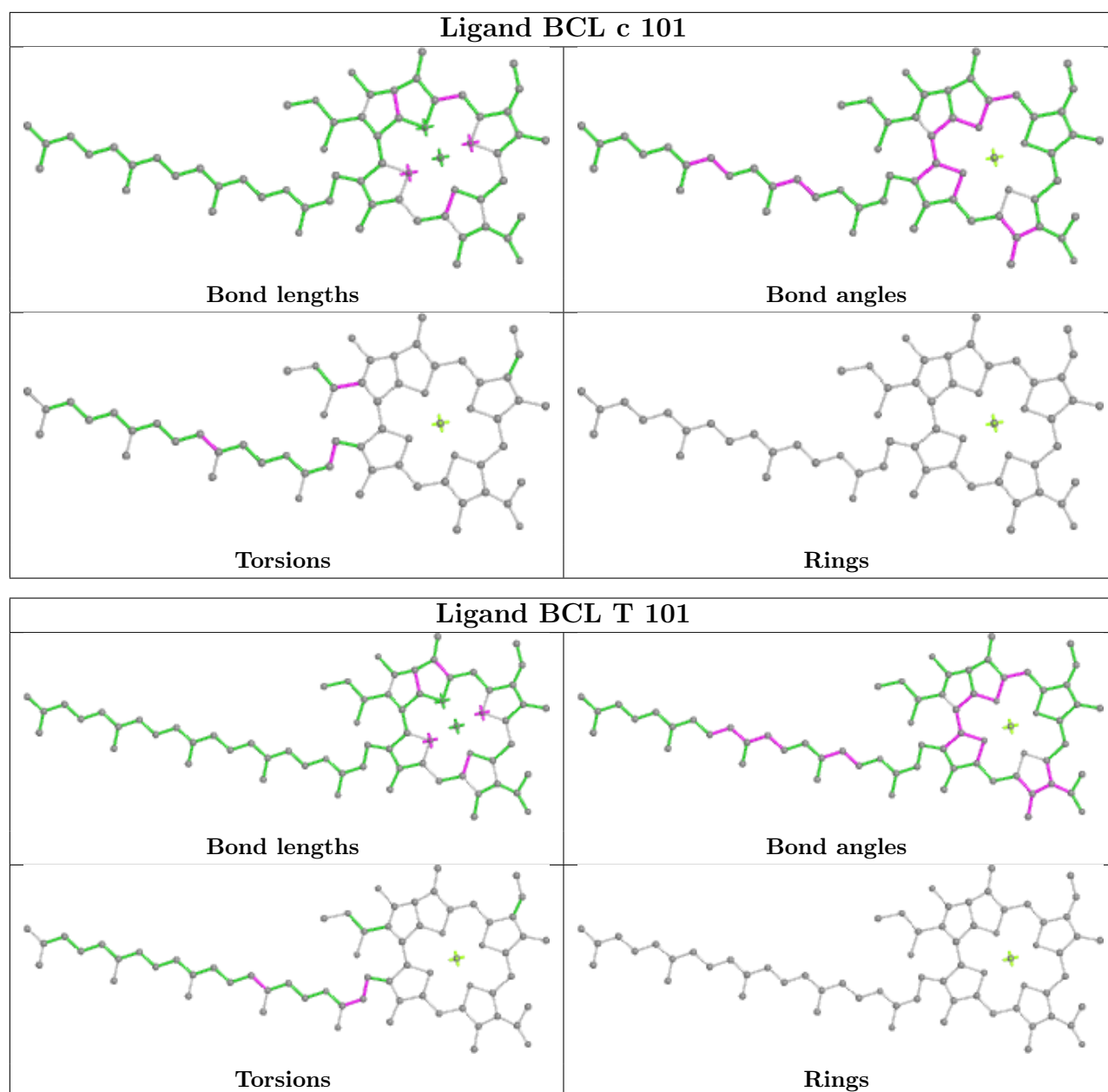


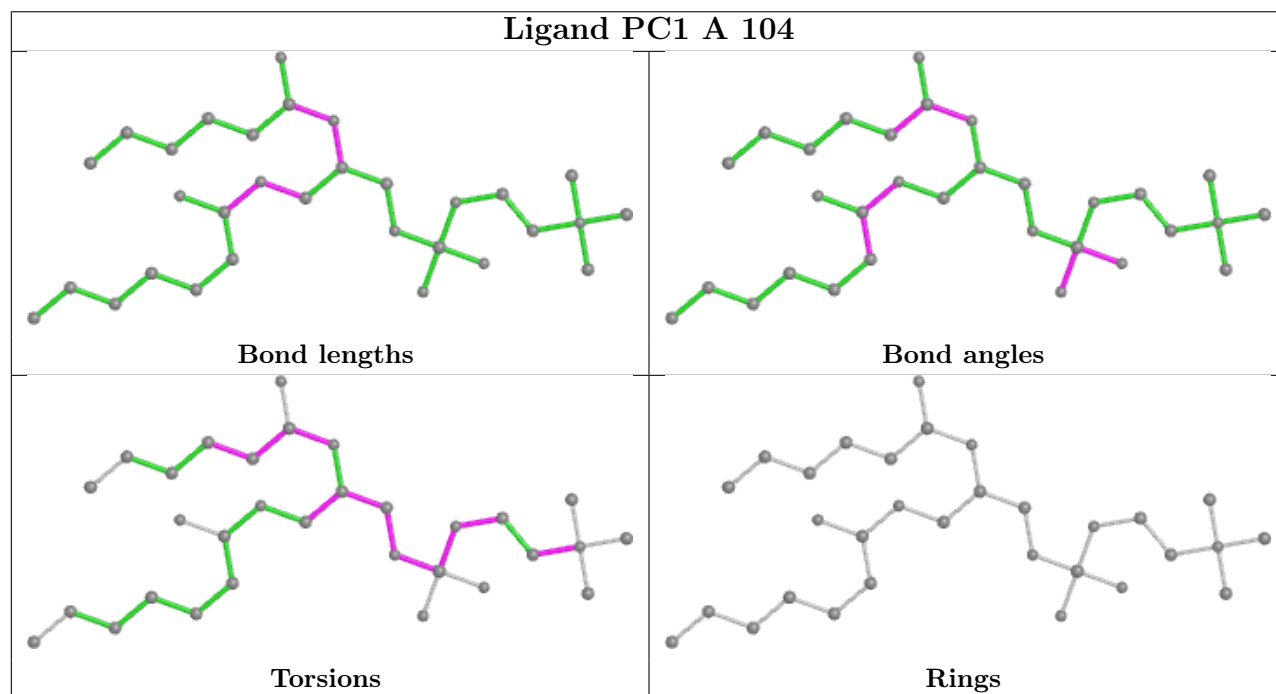
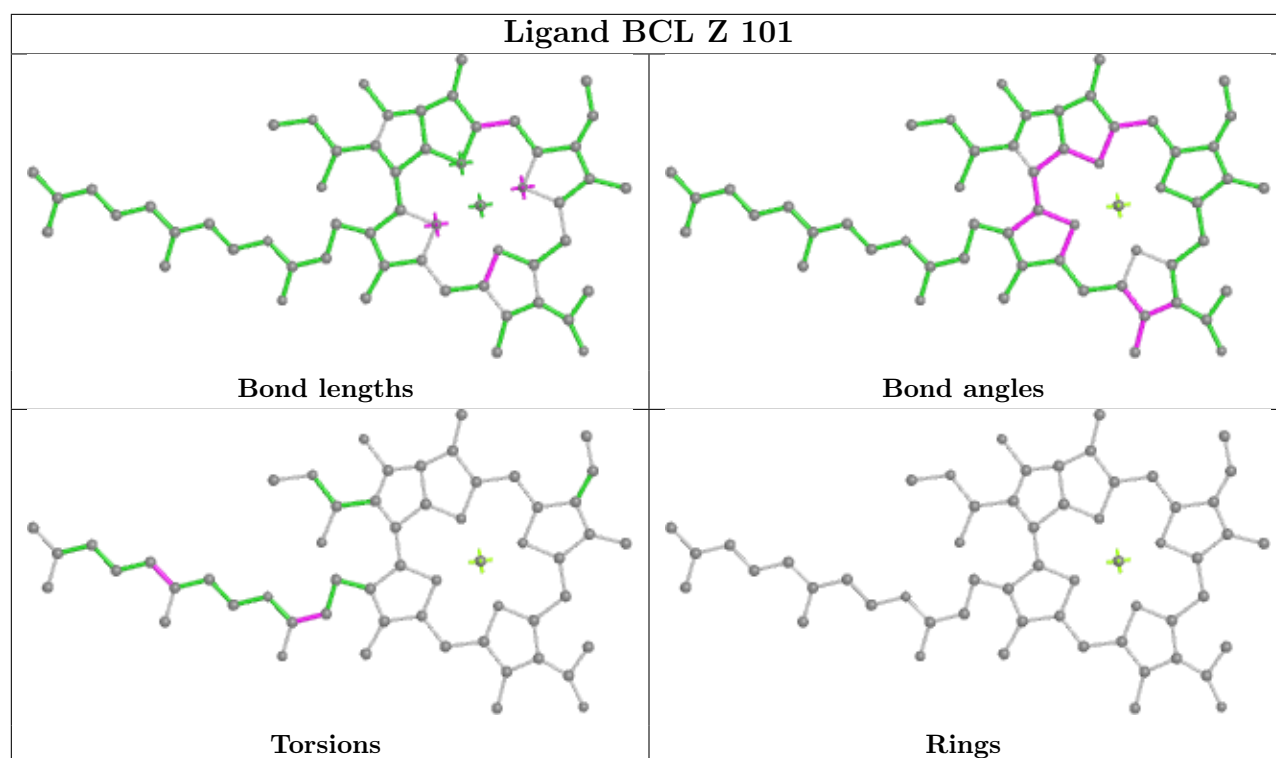




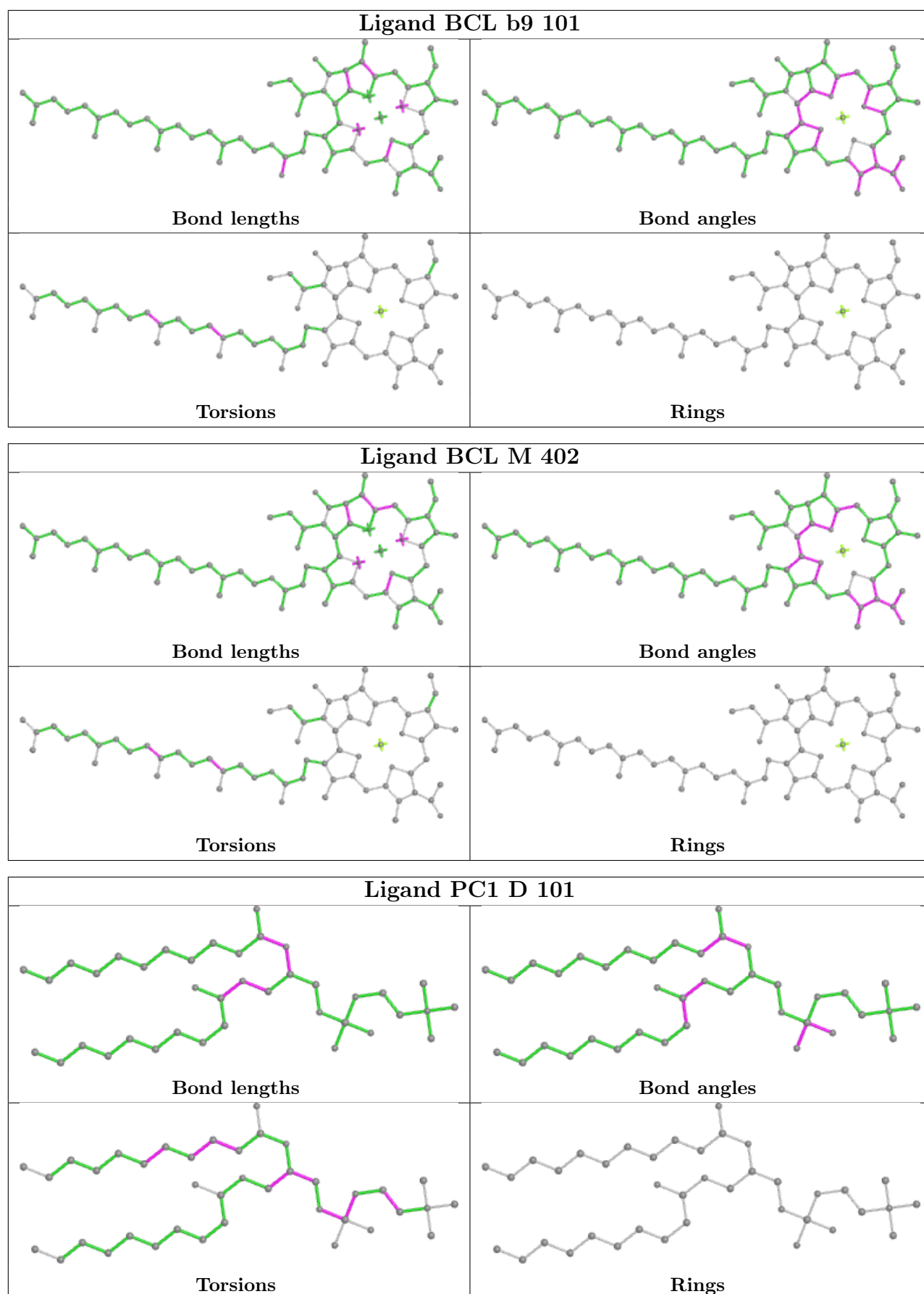


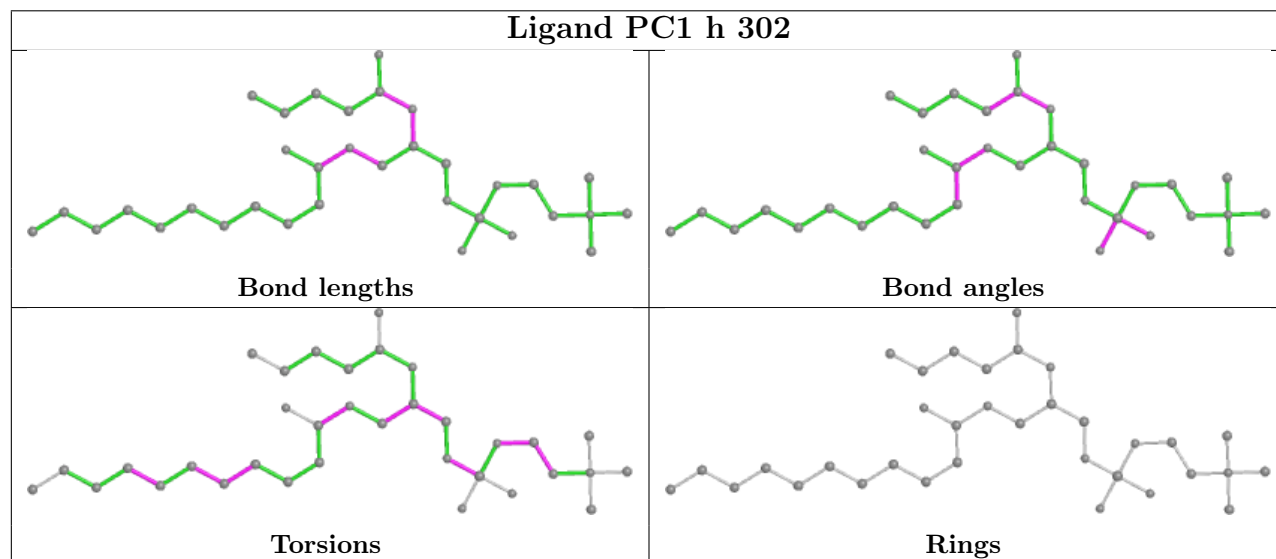
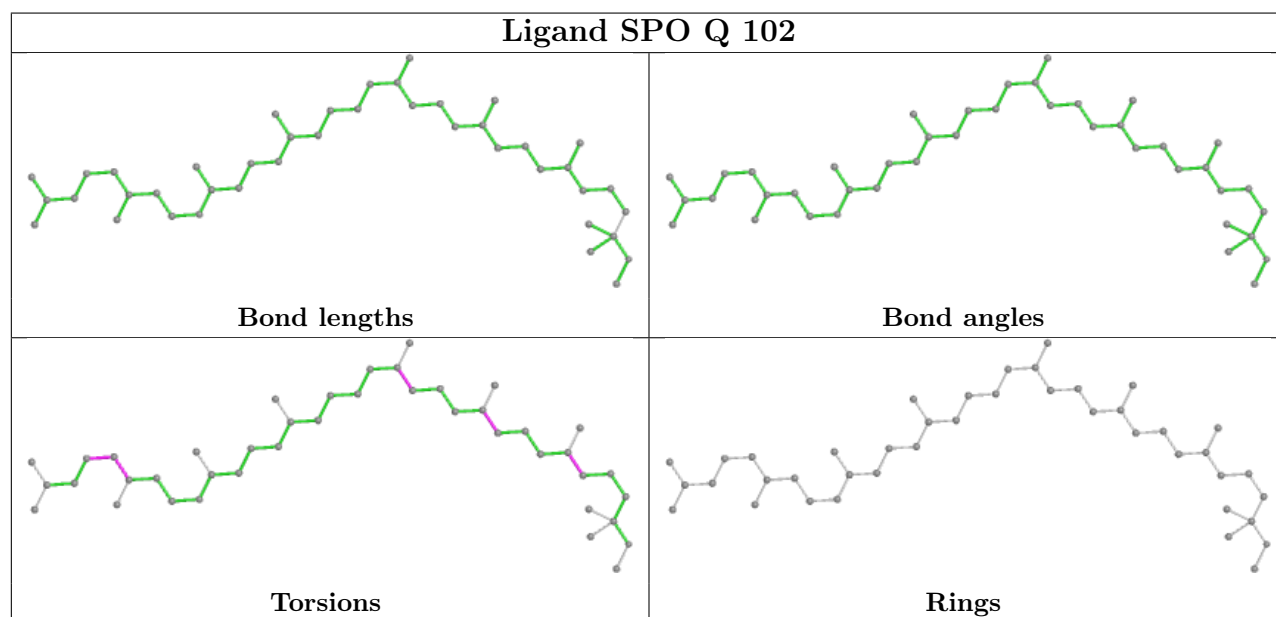
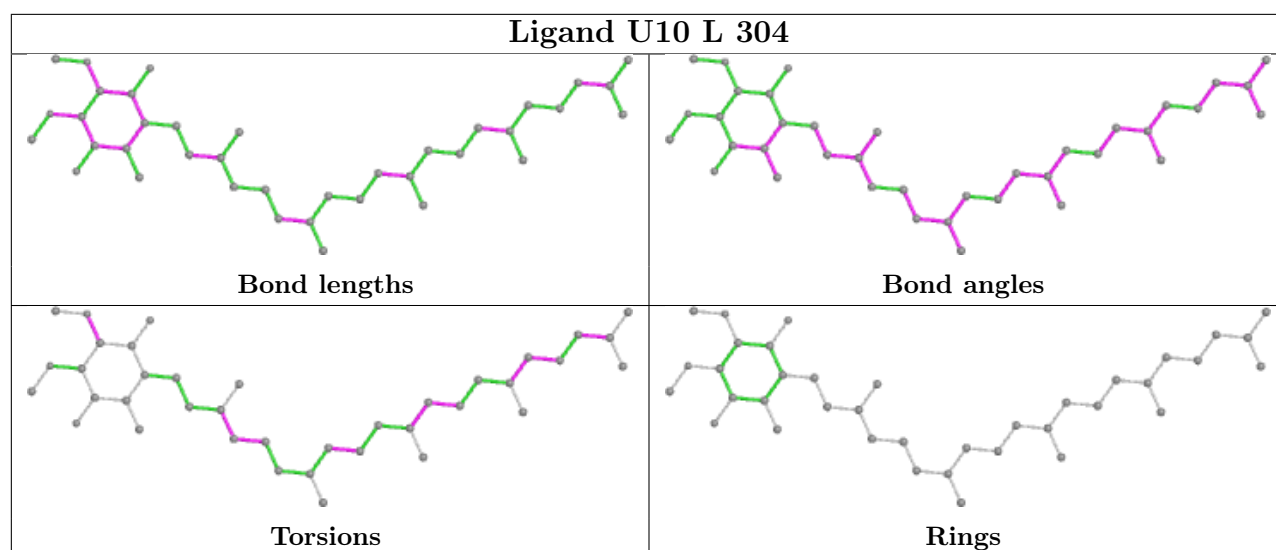


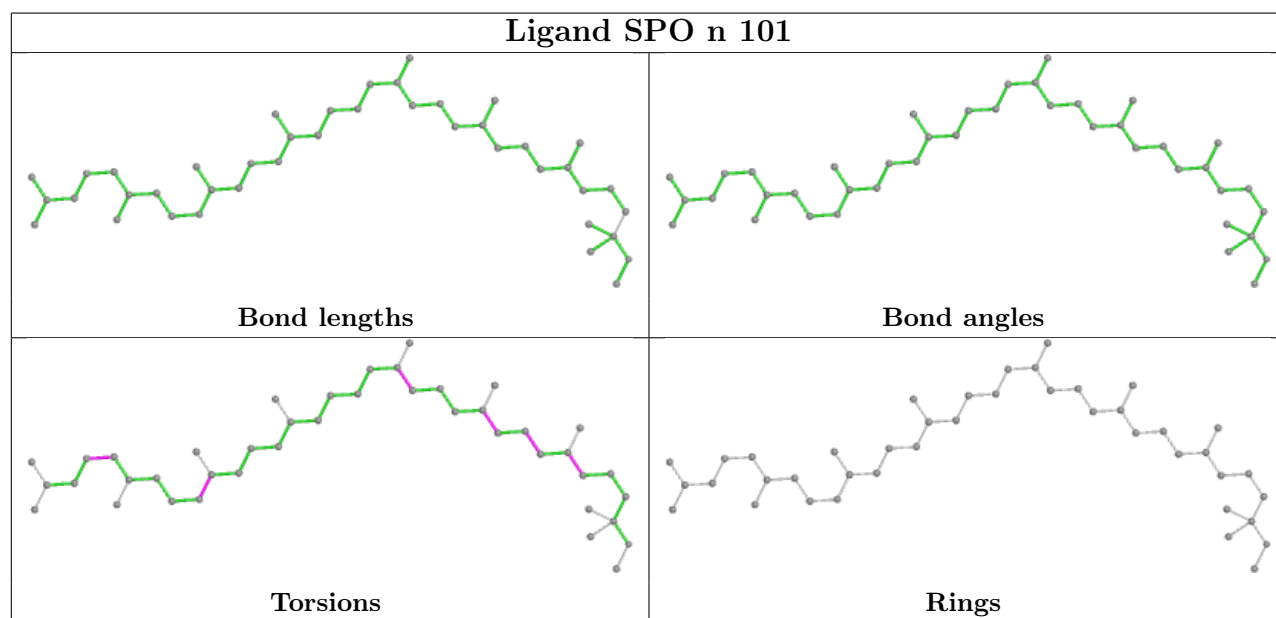
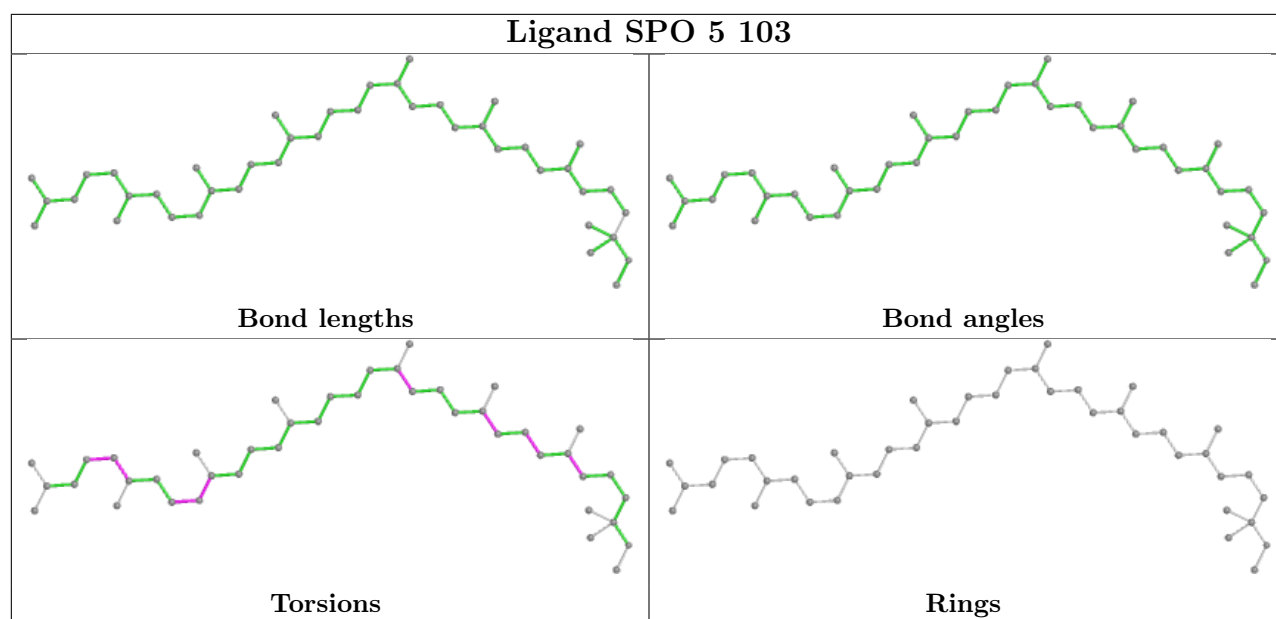


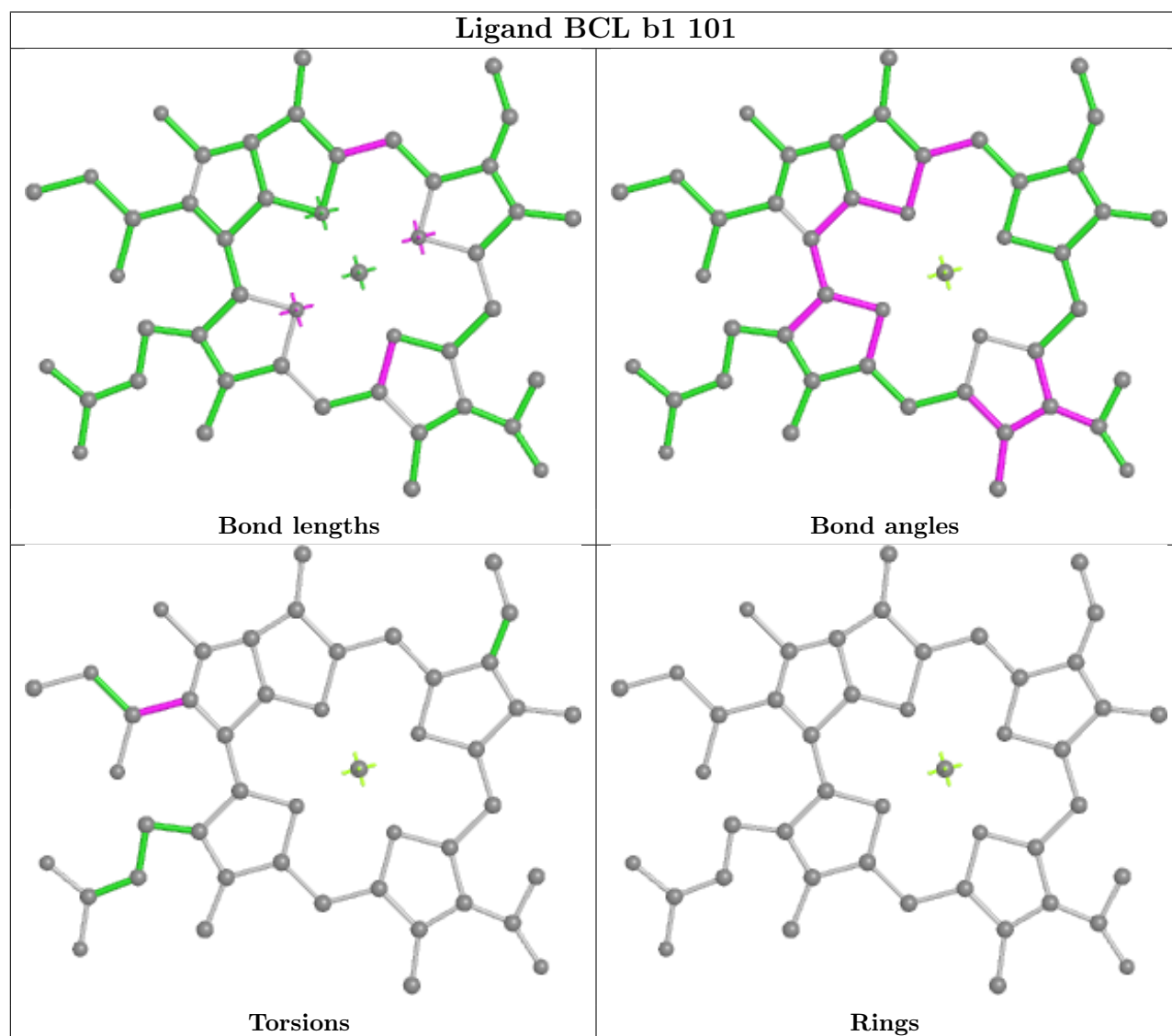
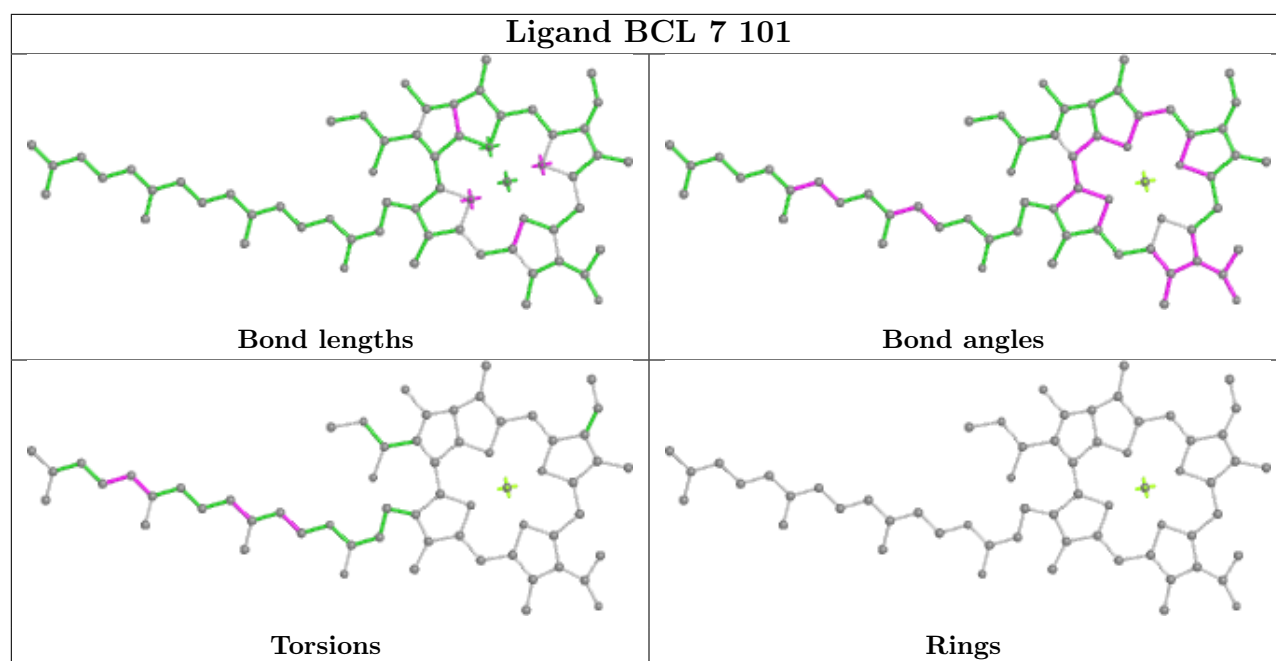


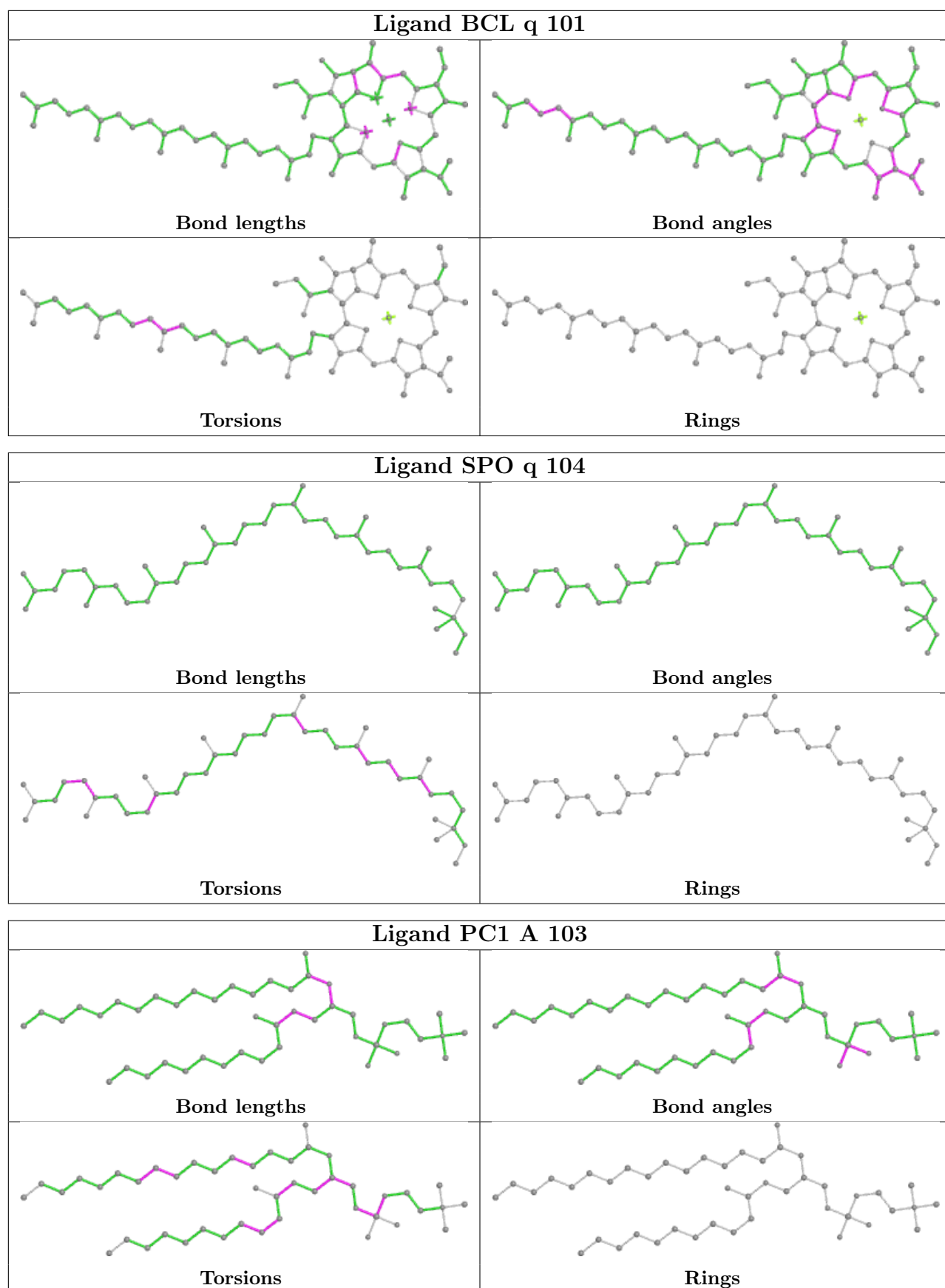


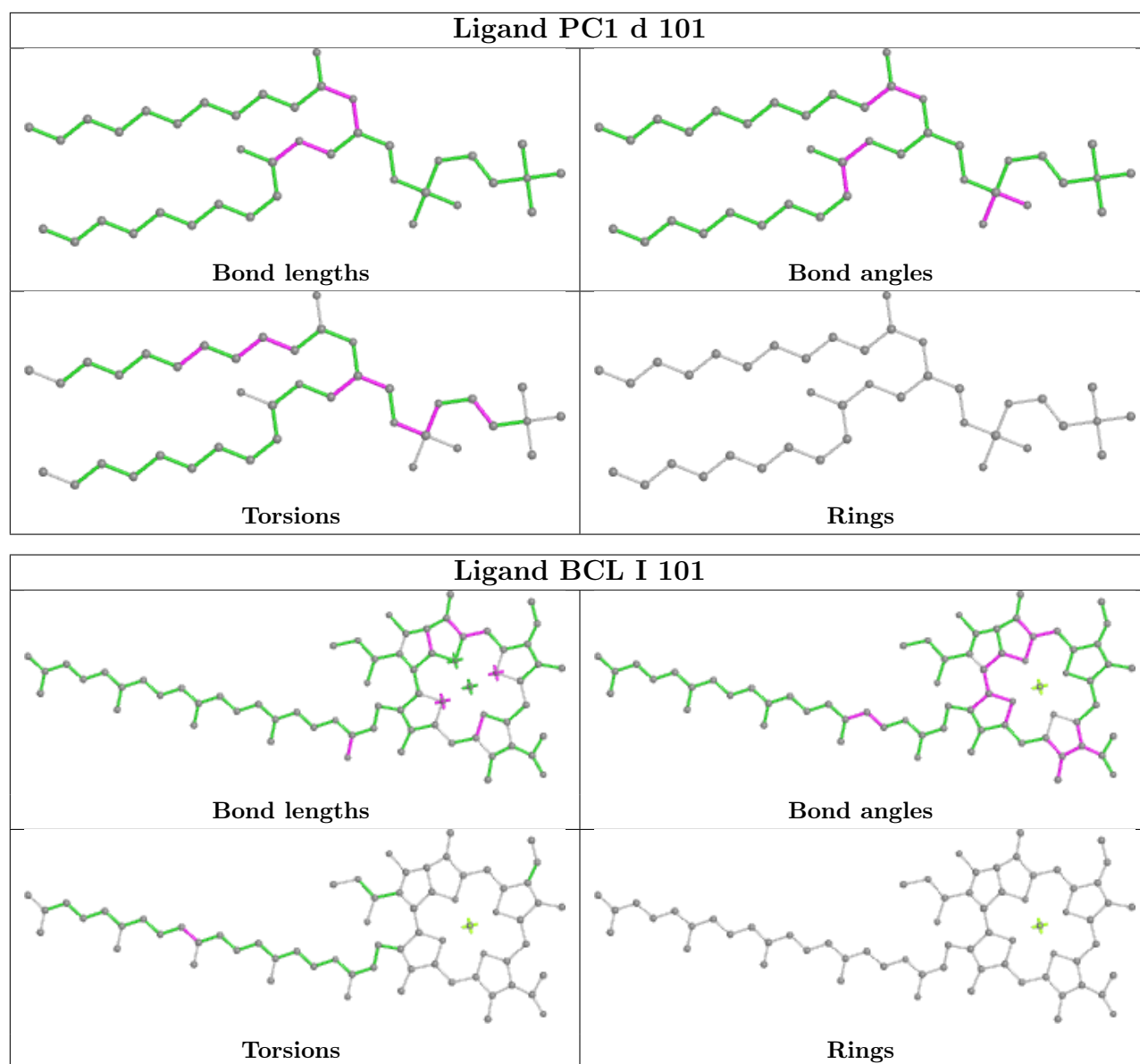


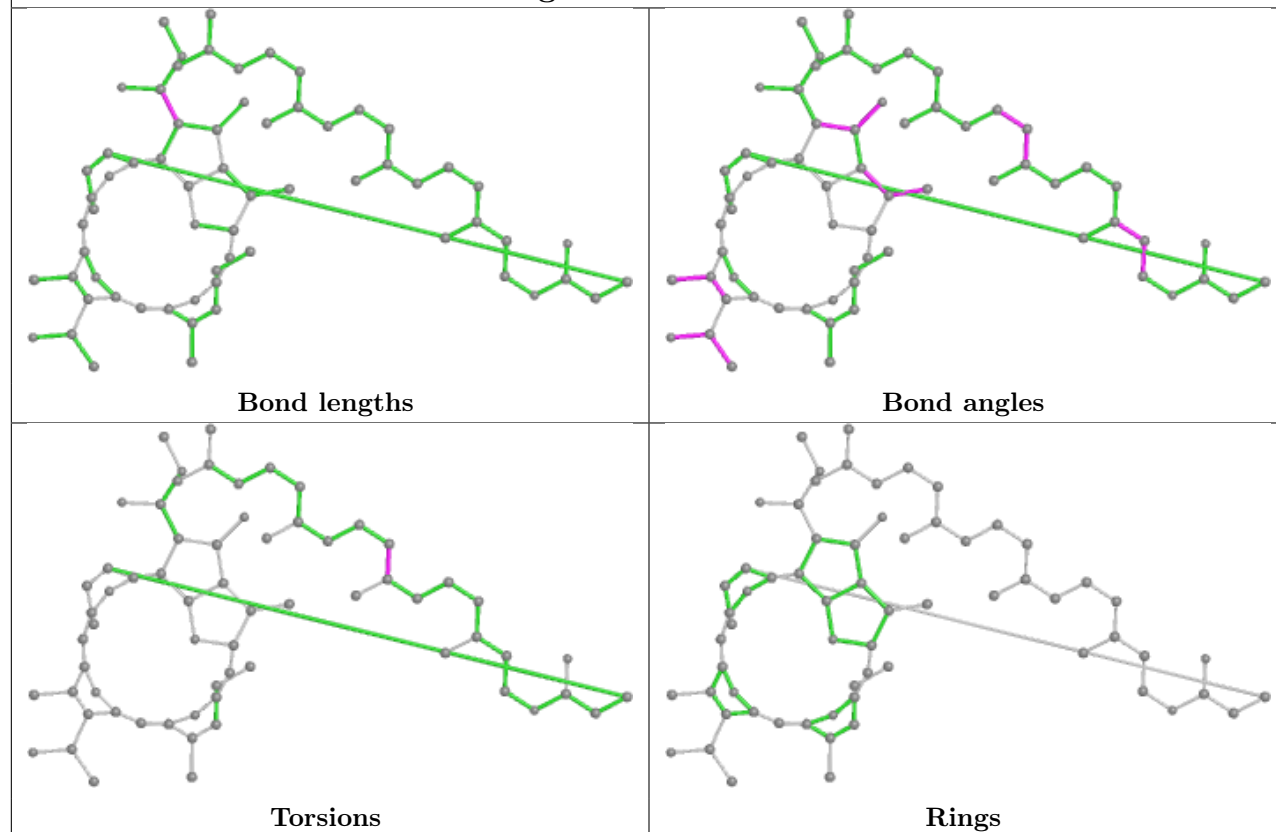
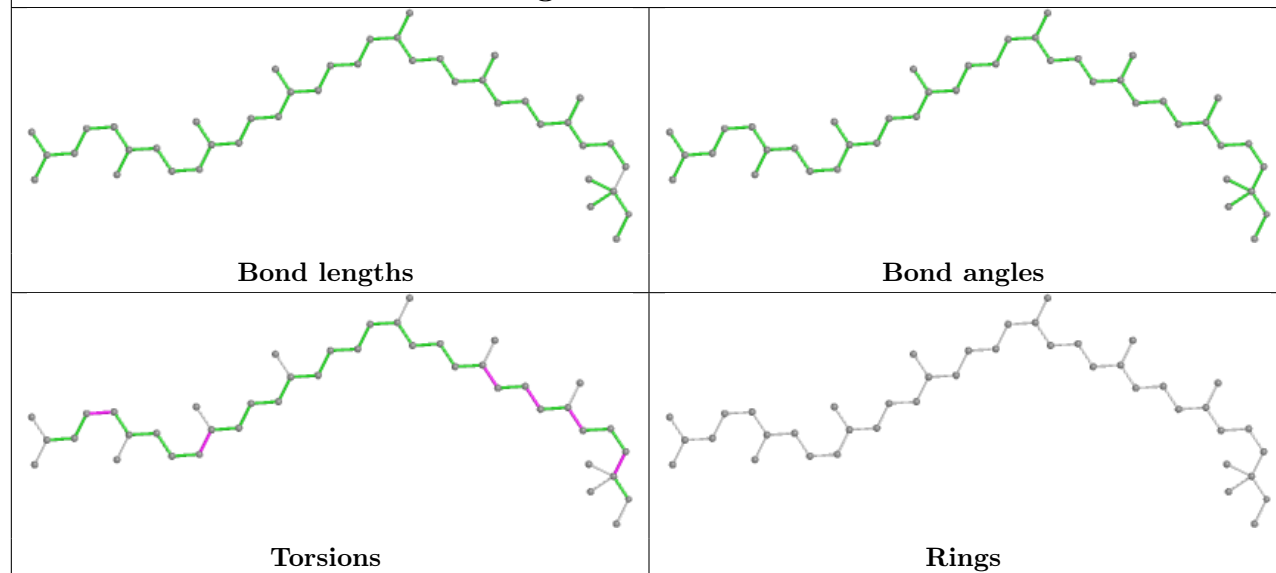


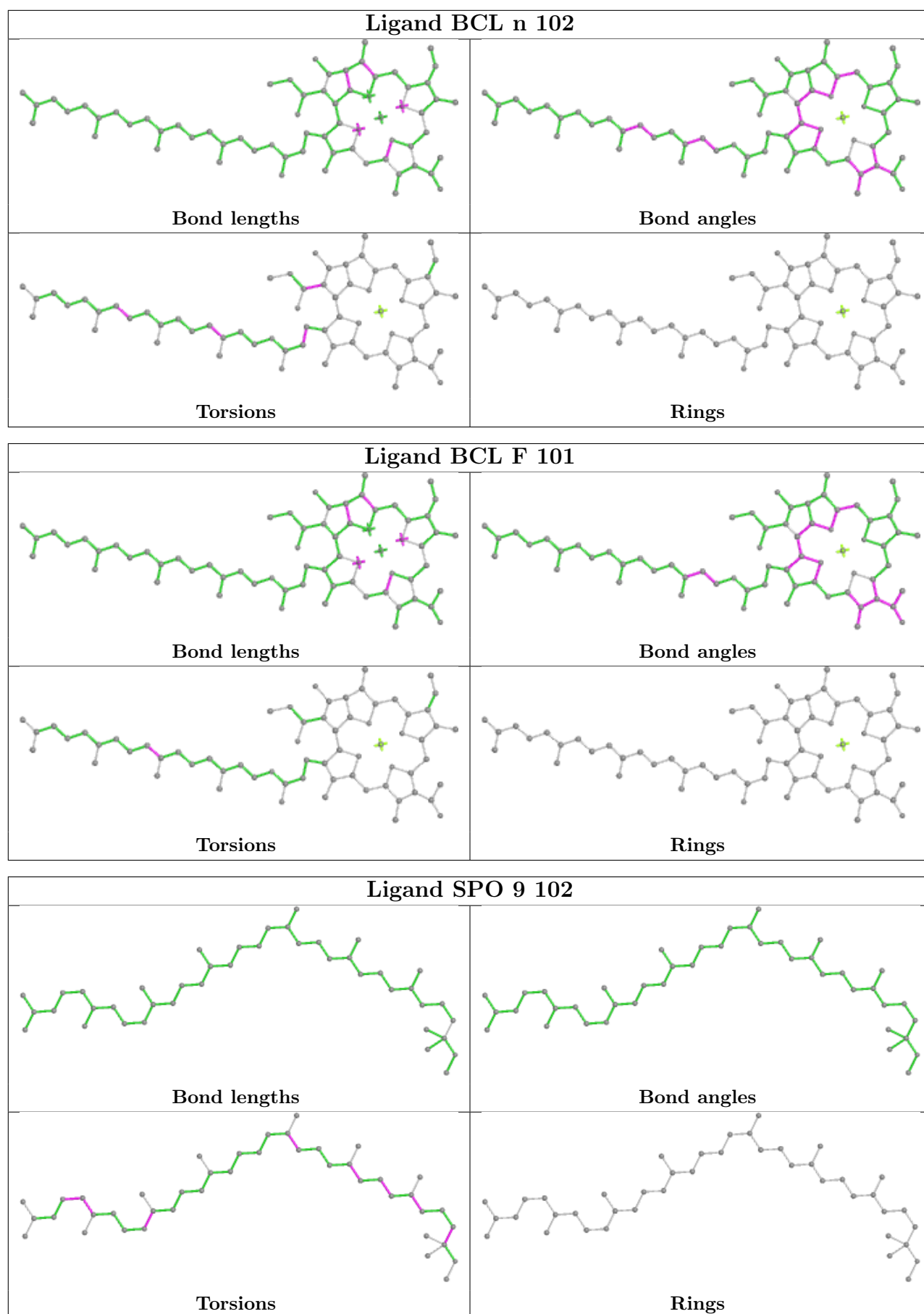




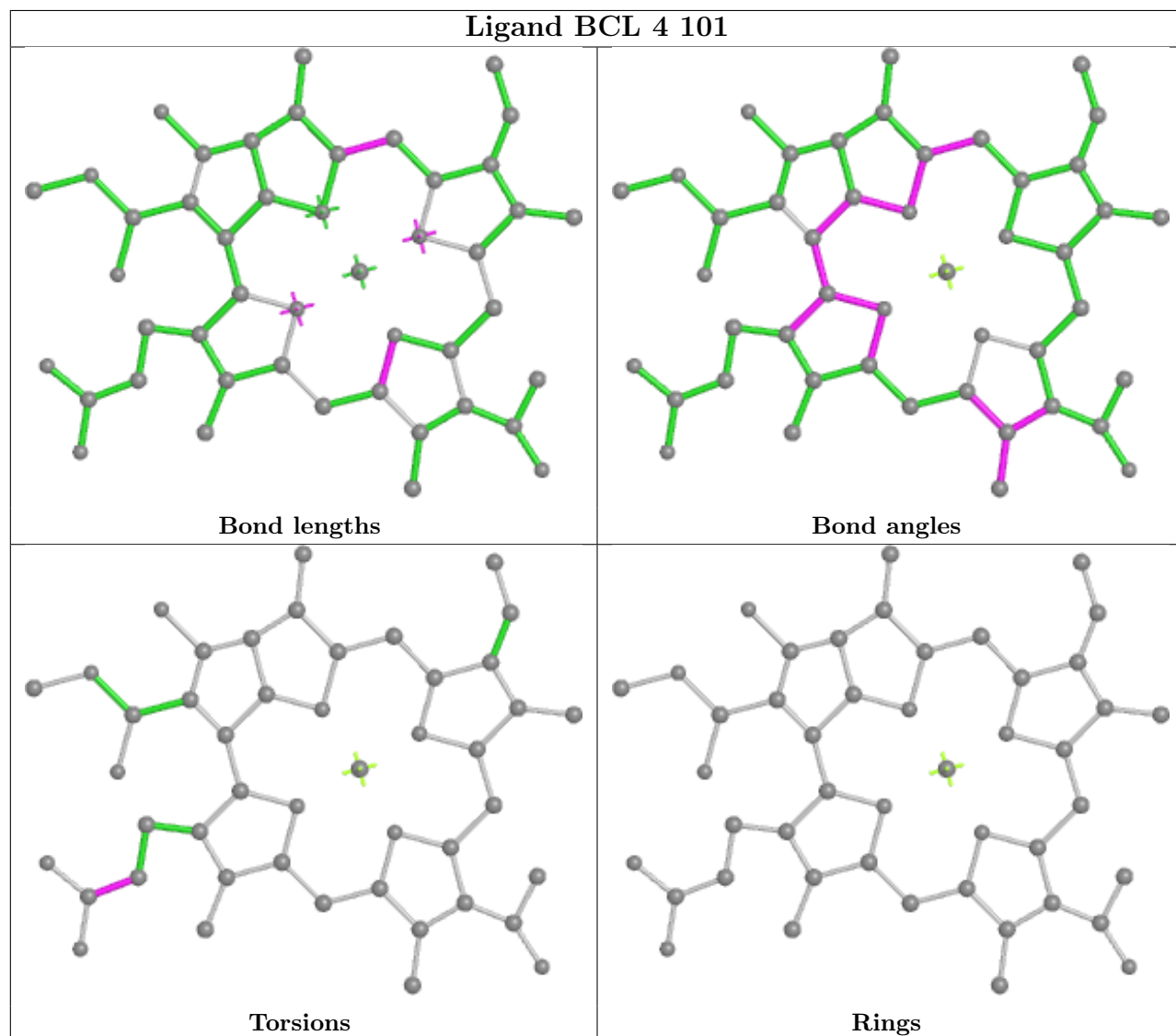
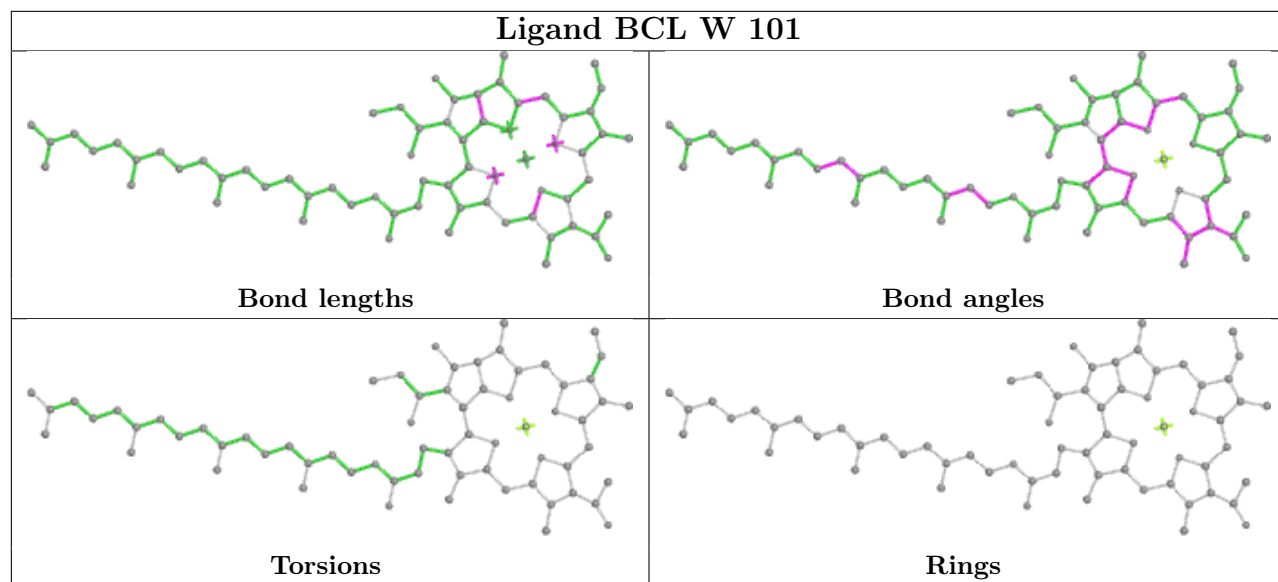


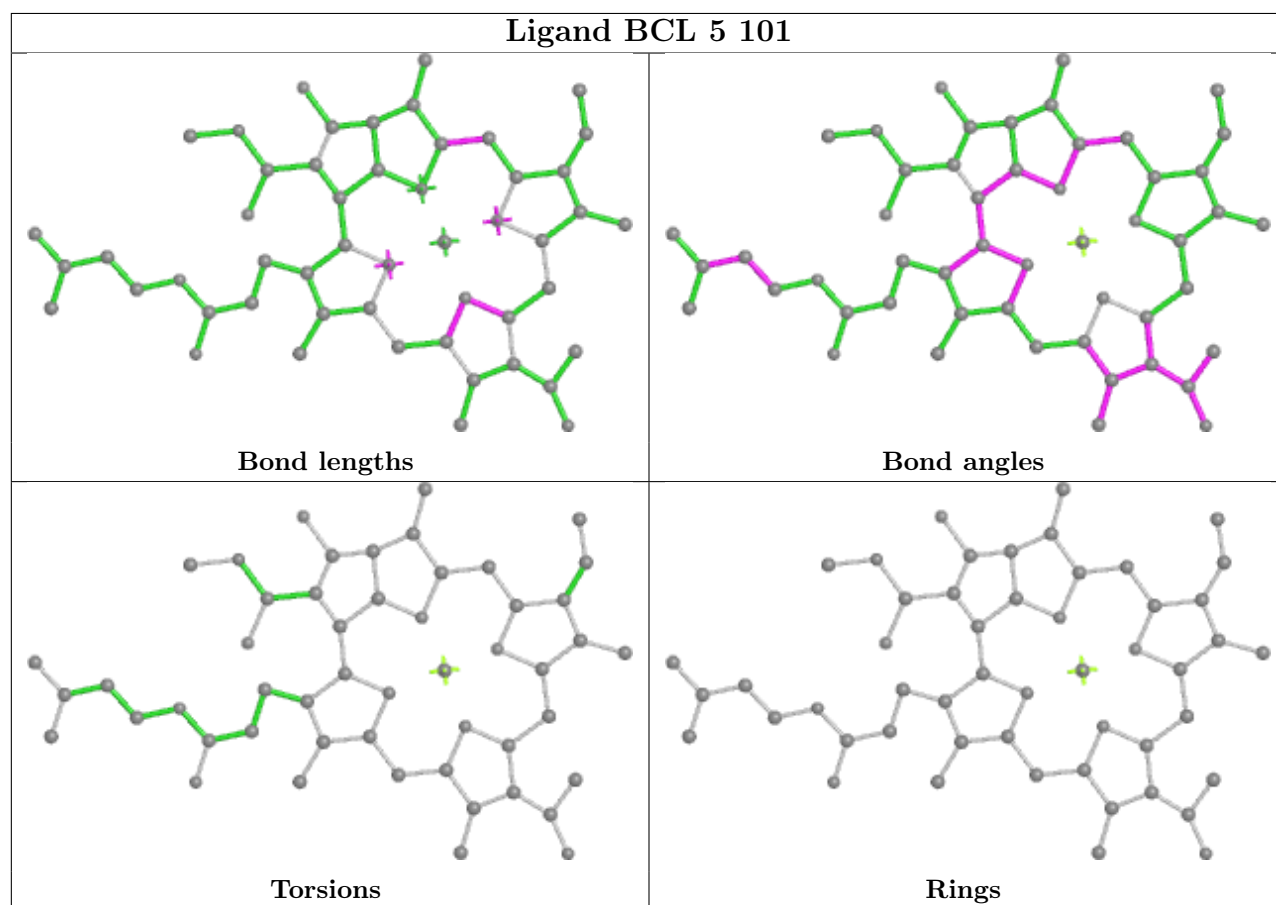
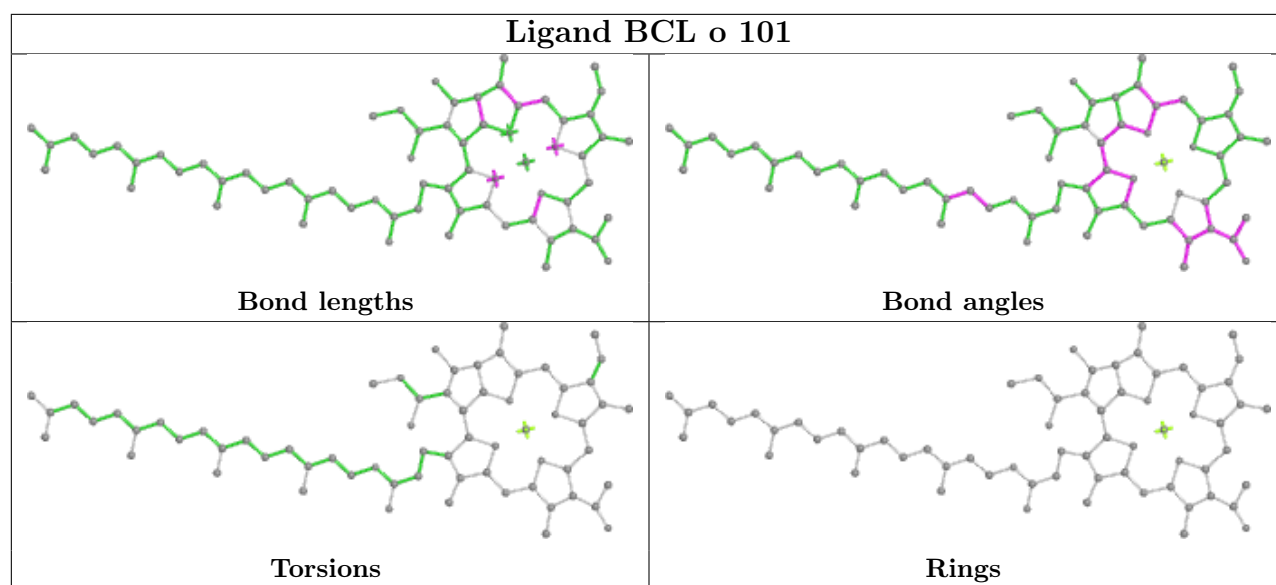


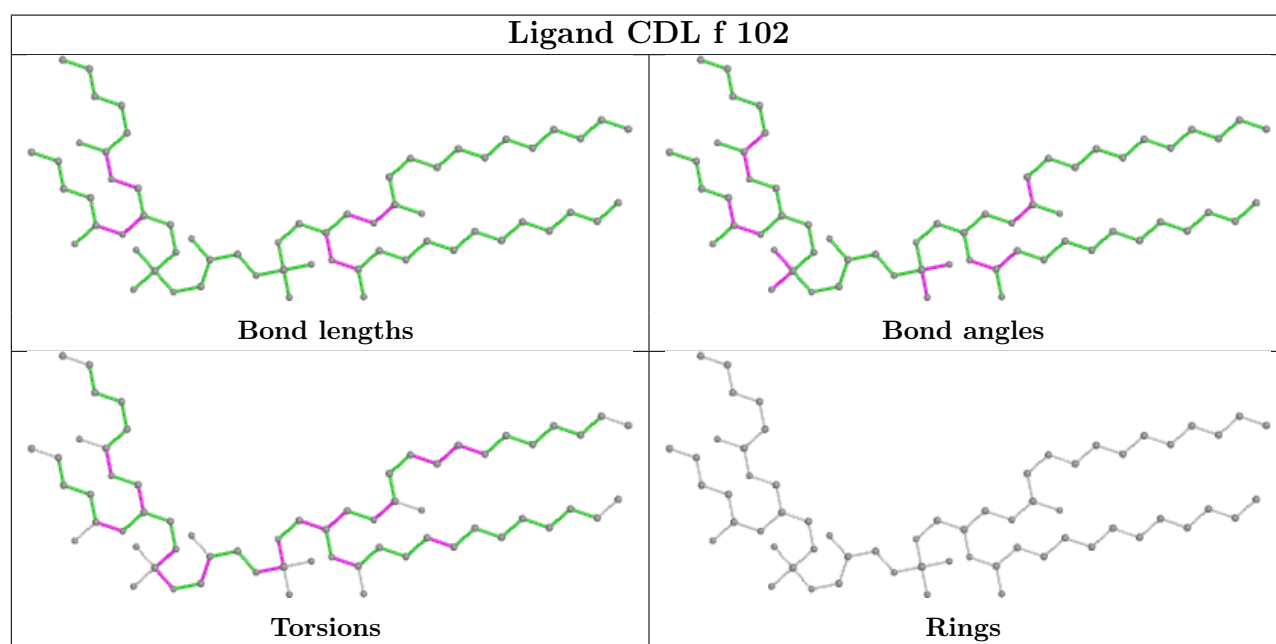
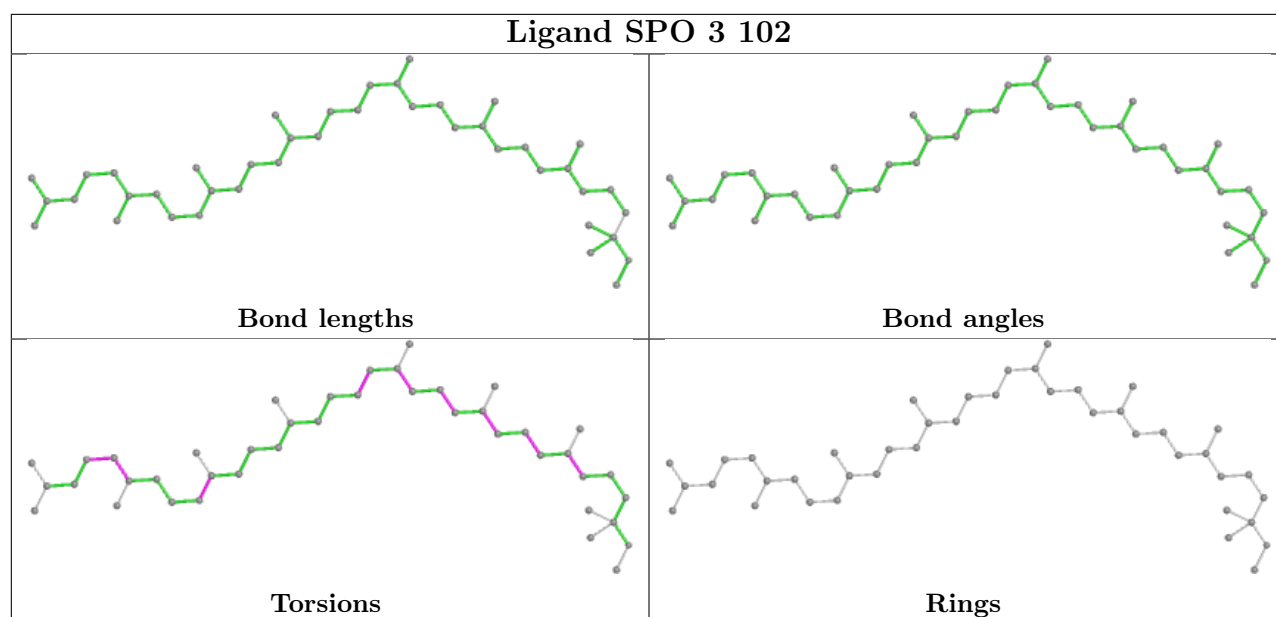
**Ligand BPH 1 303****Ligand SPO u 103**

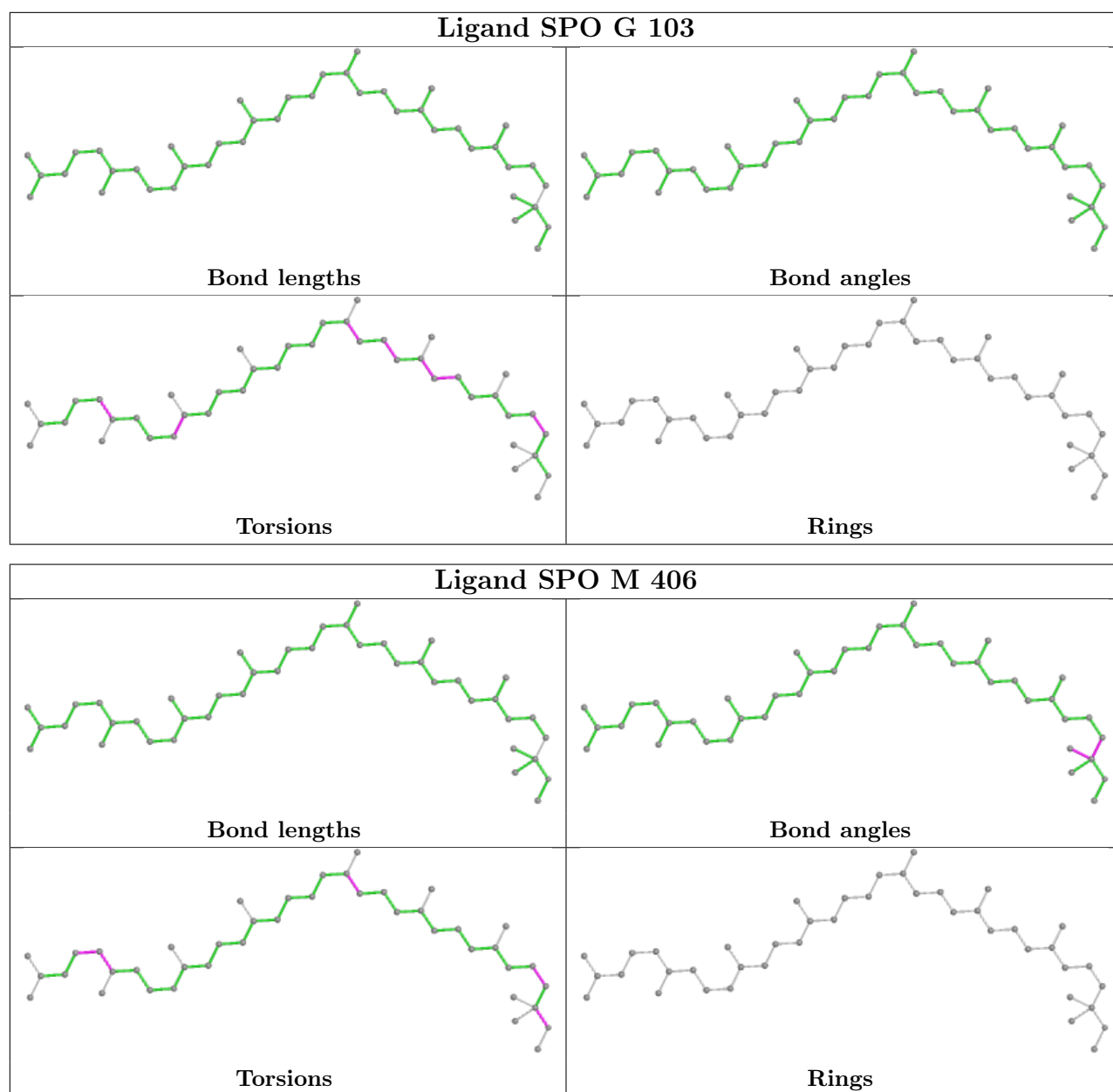


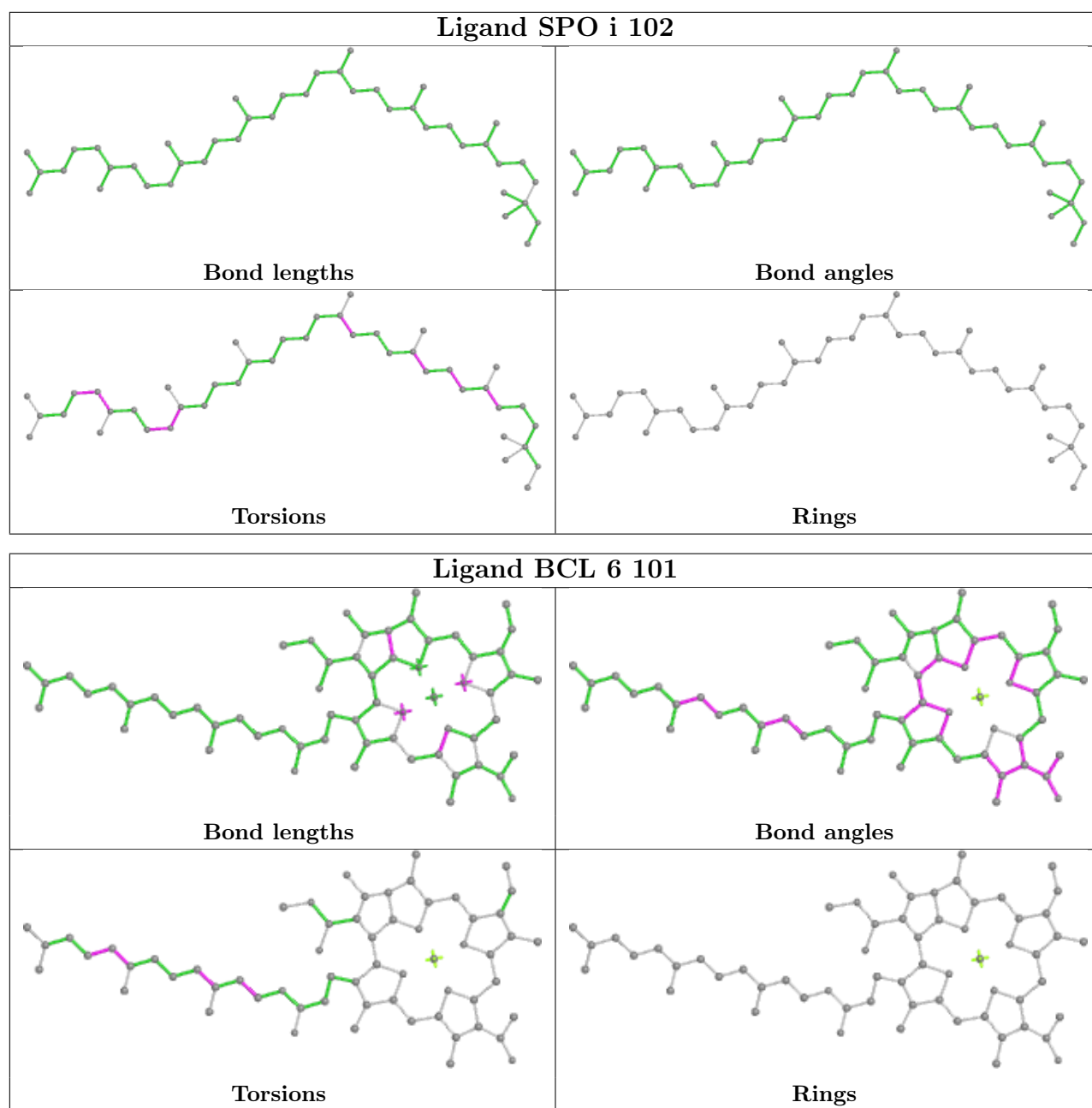


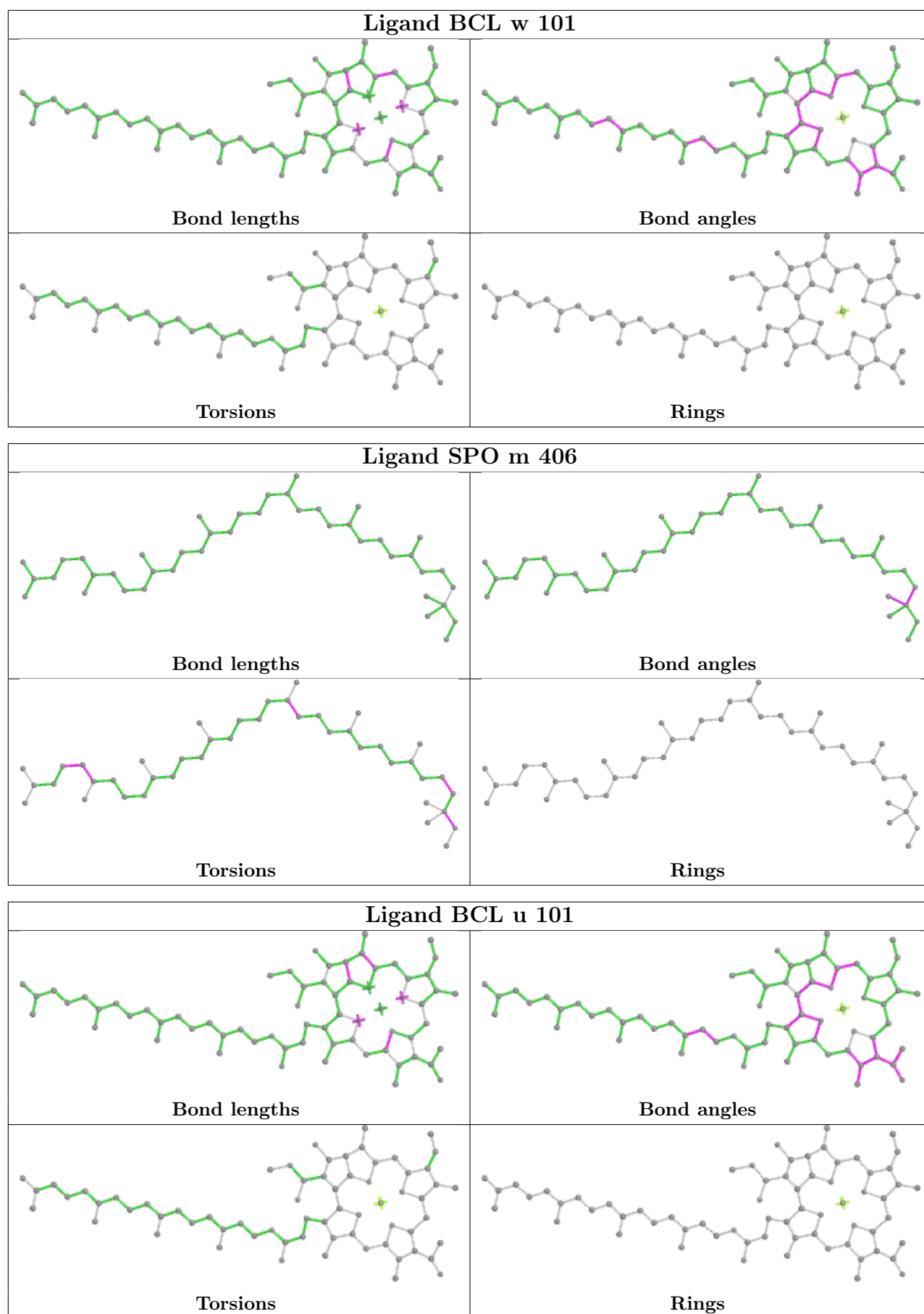


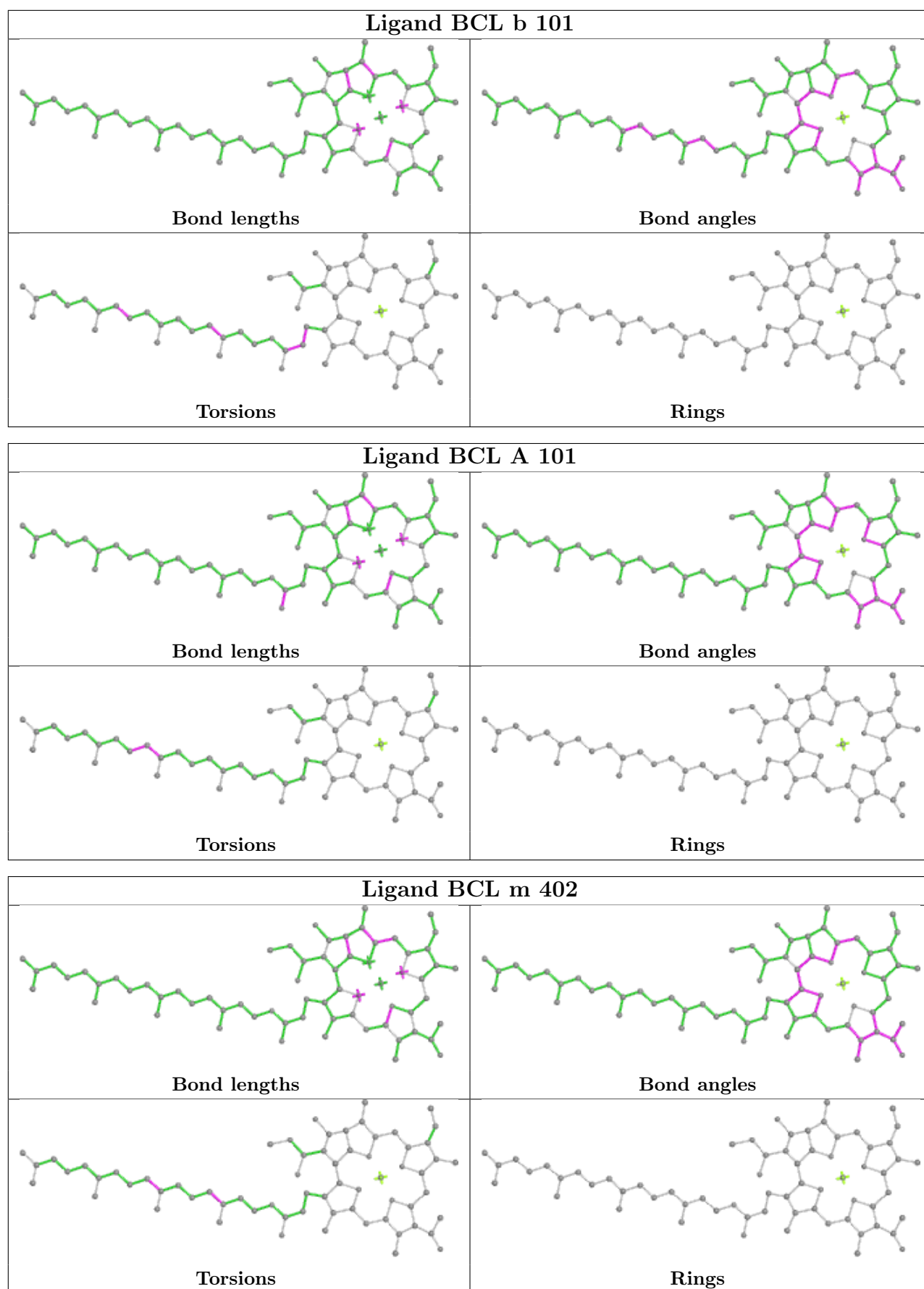


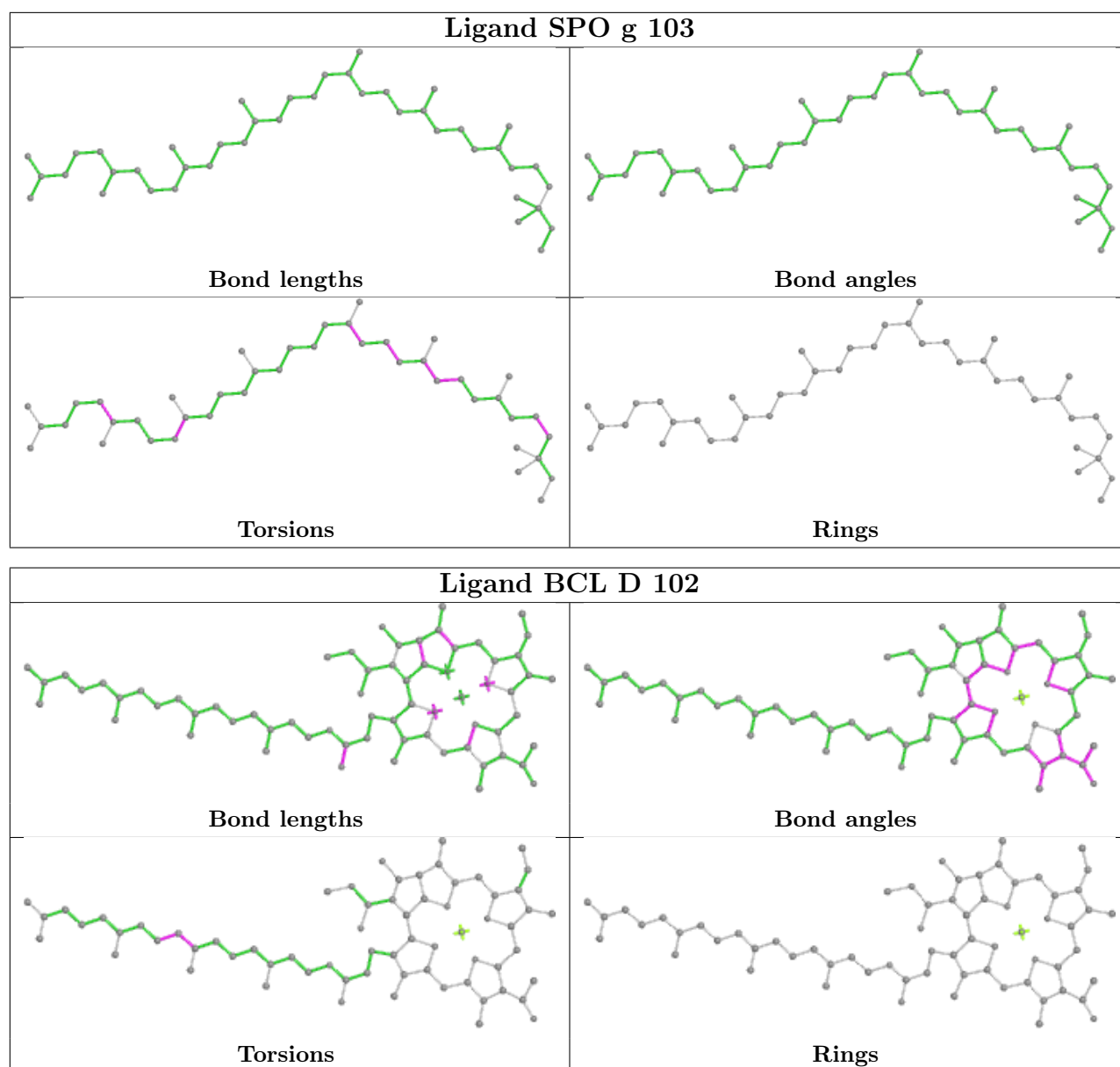




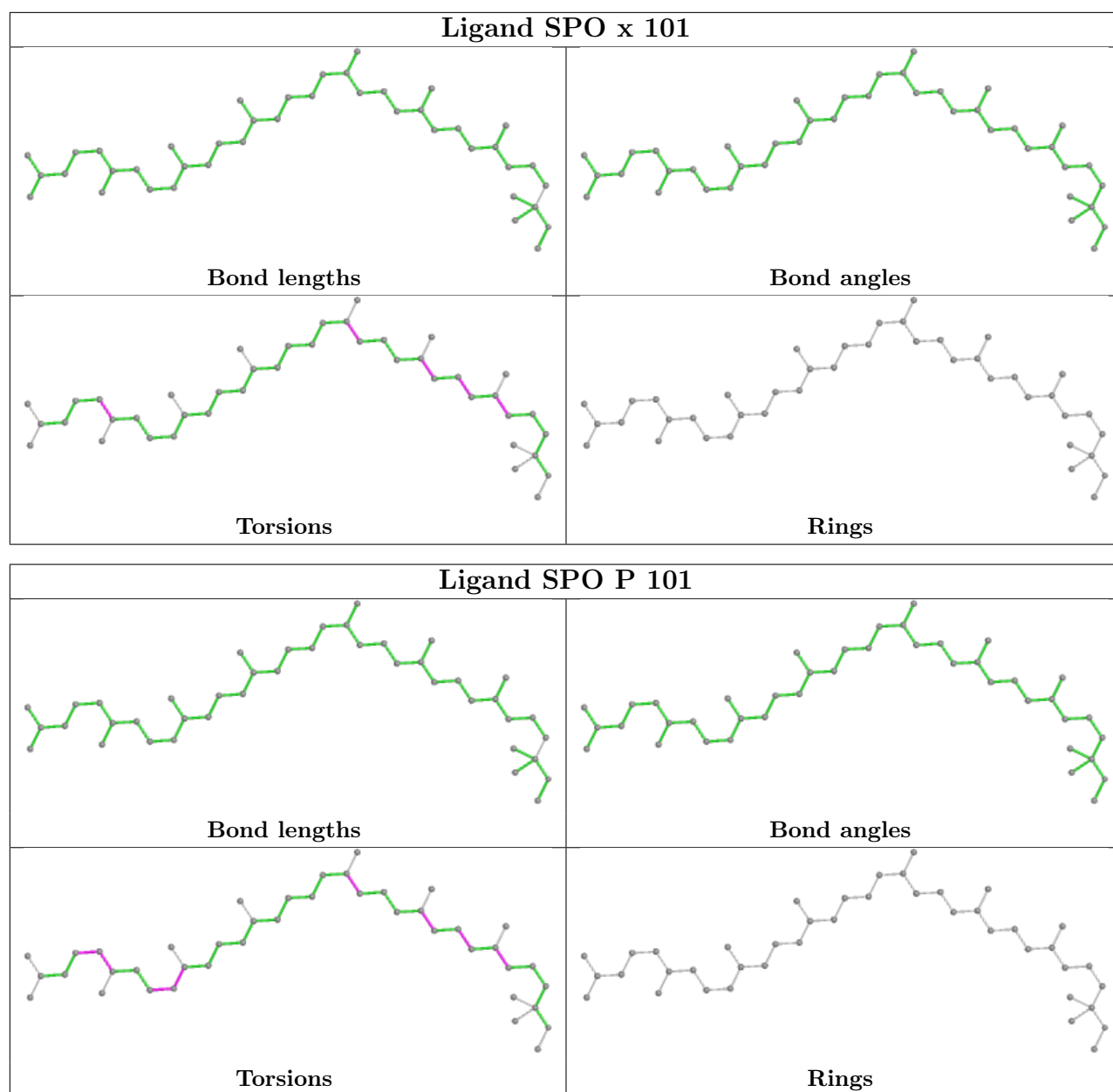


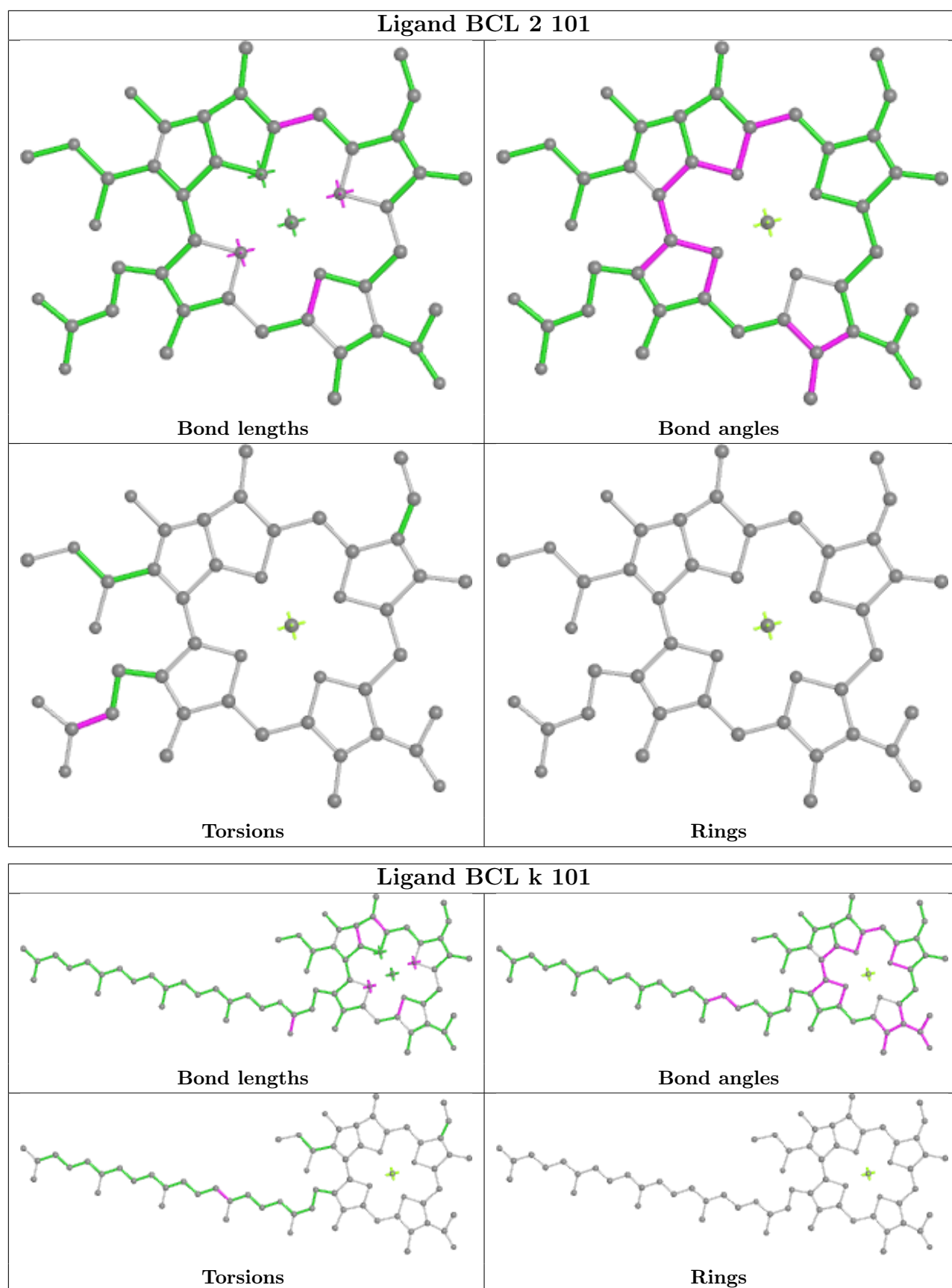


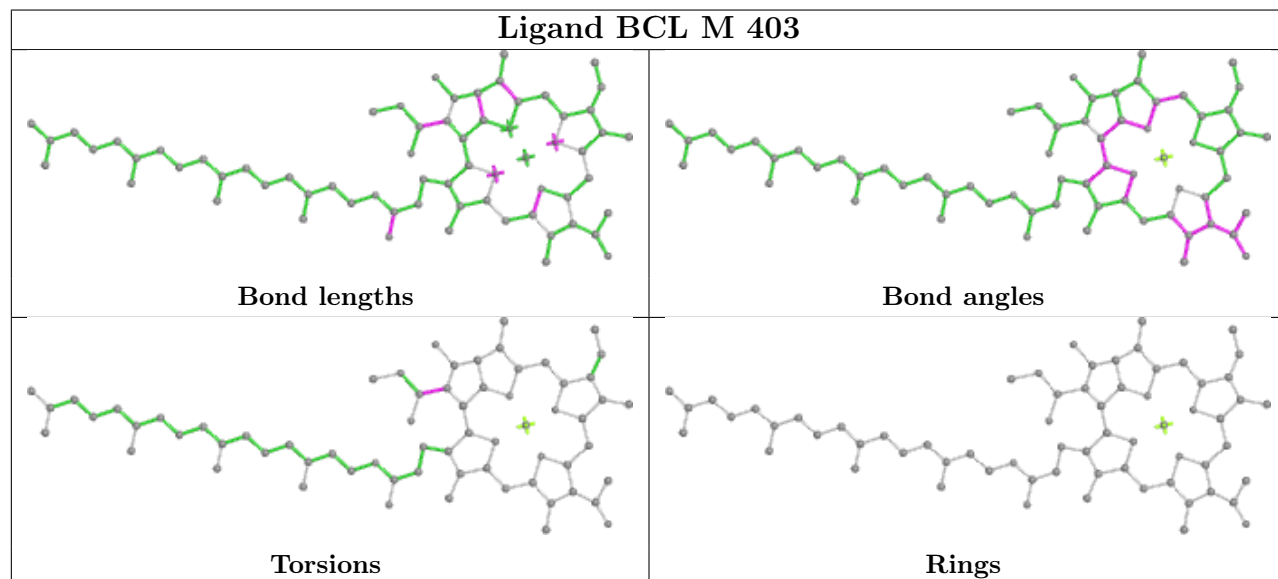
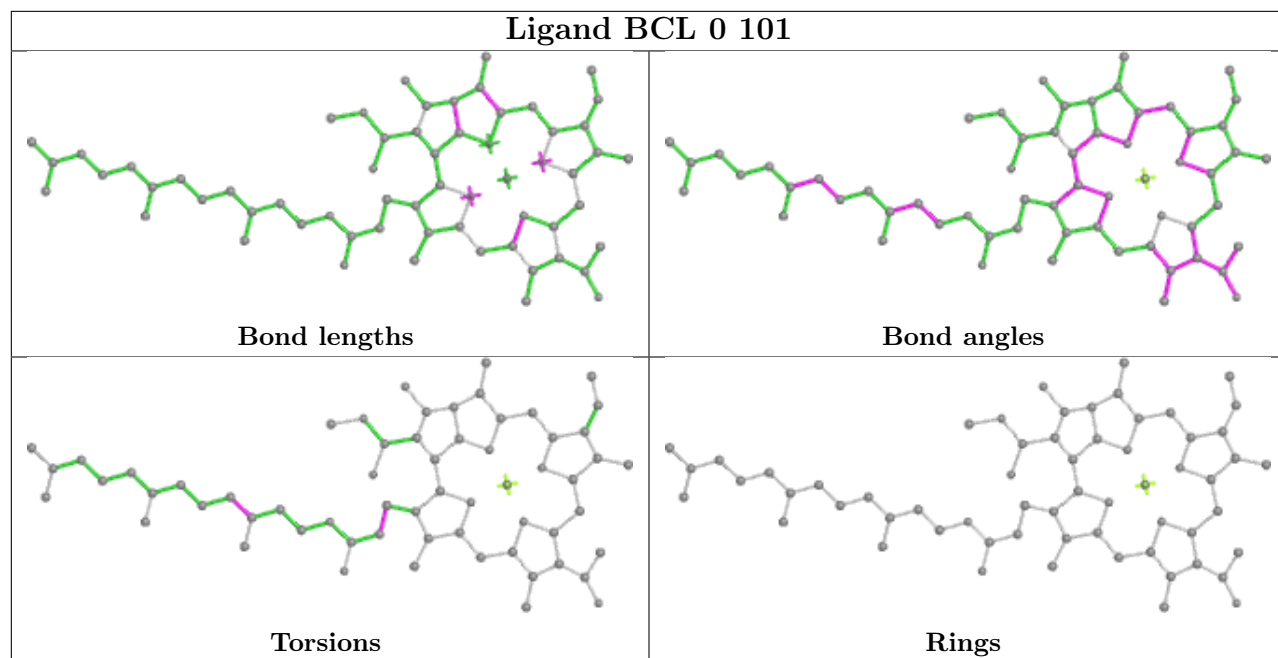


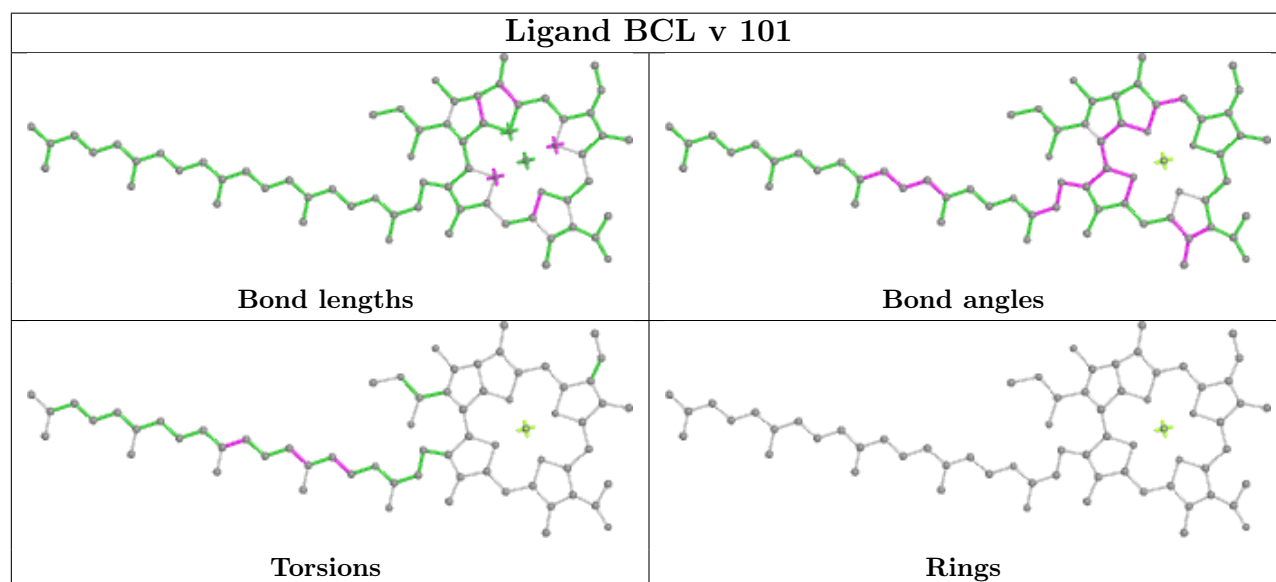
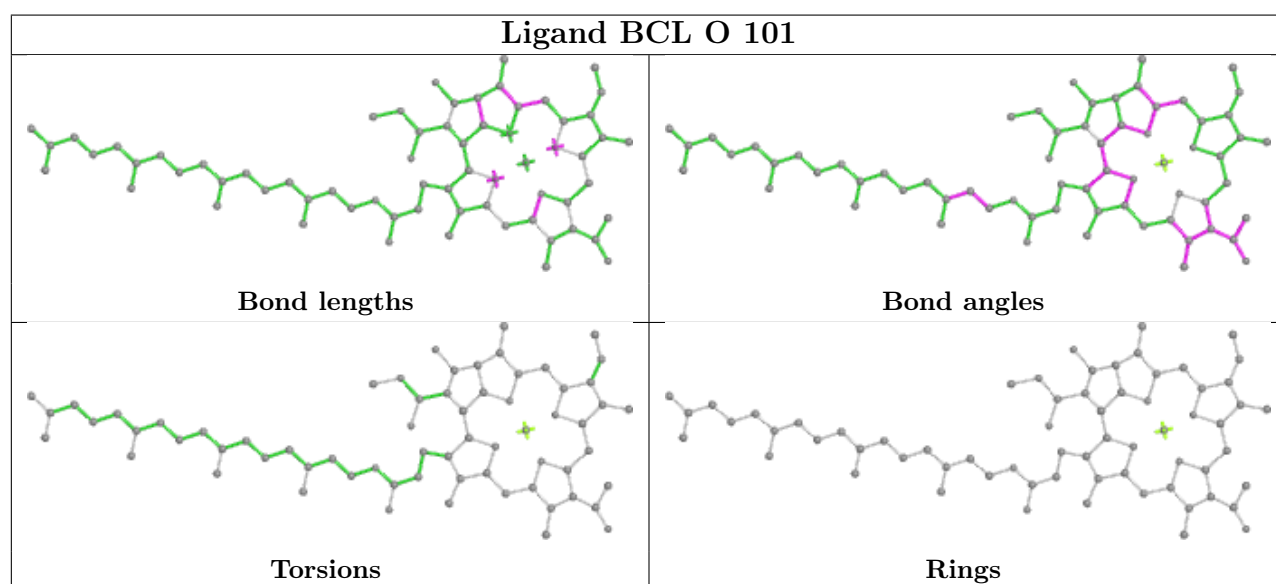
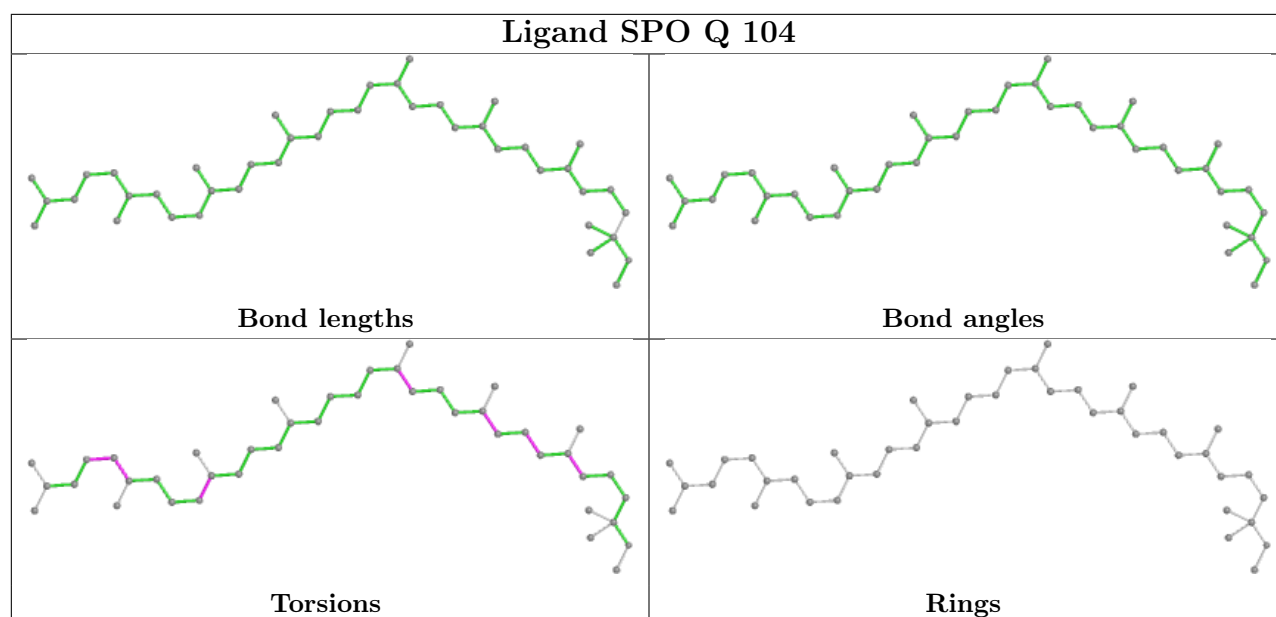


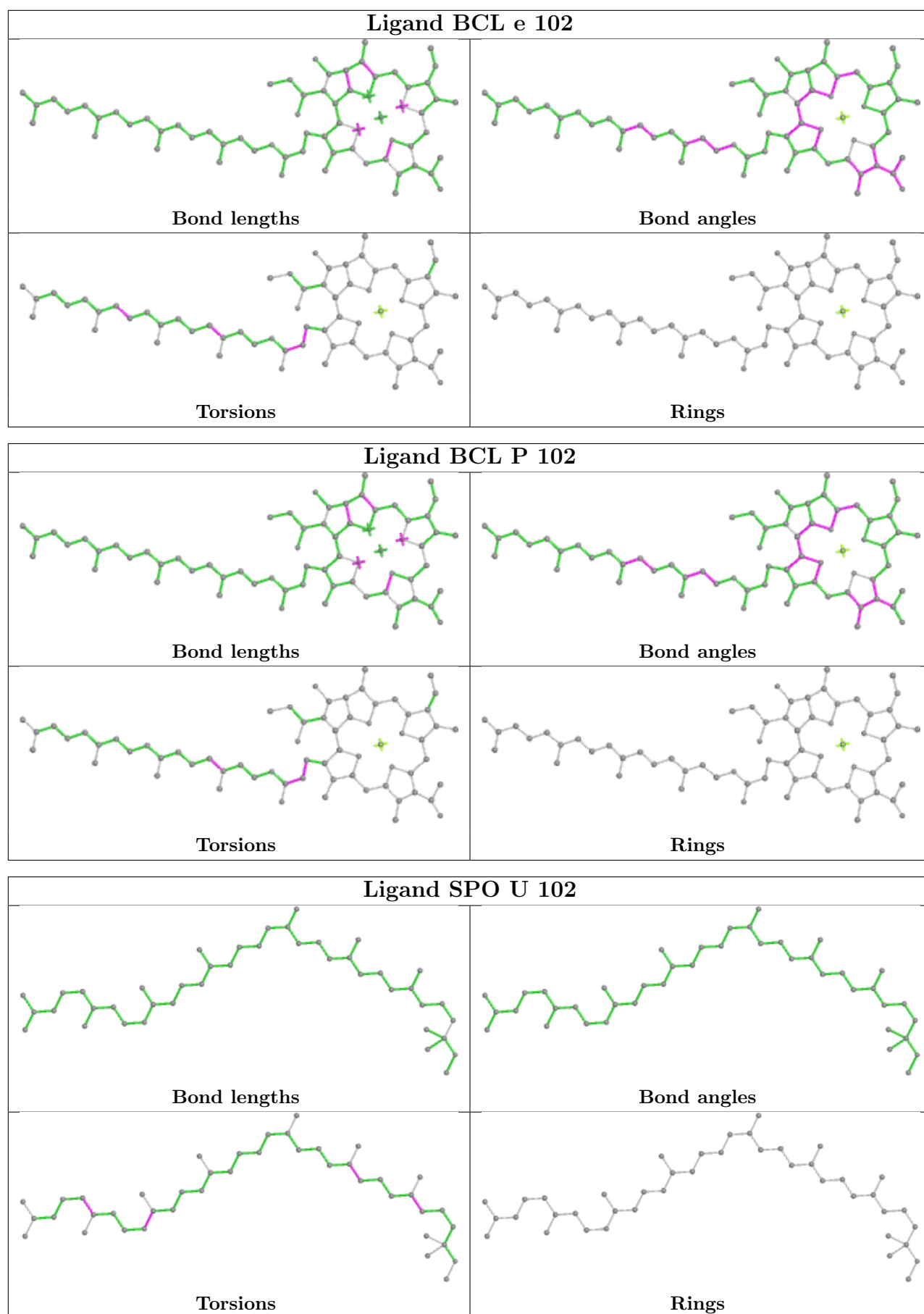


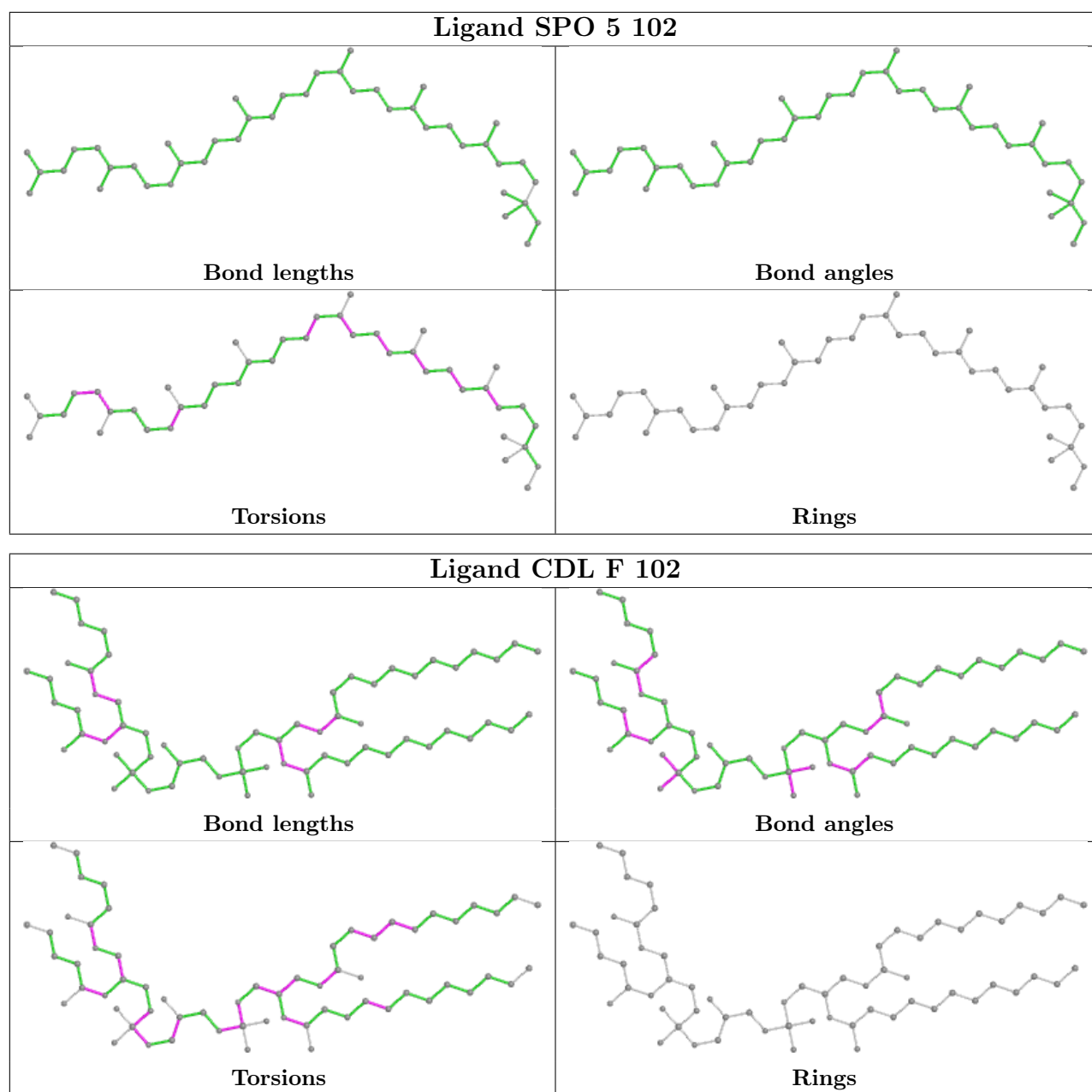


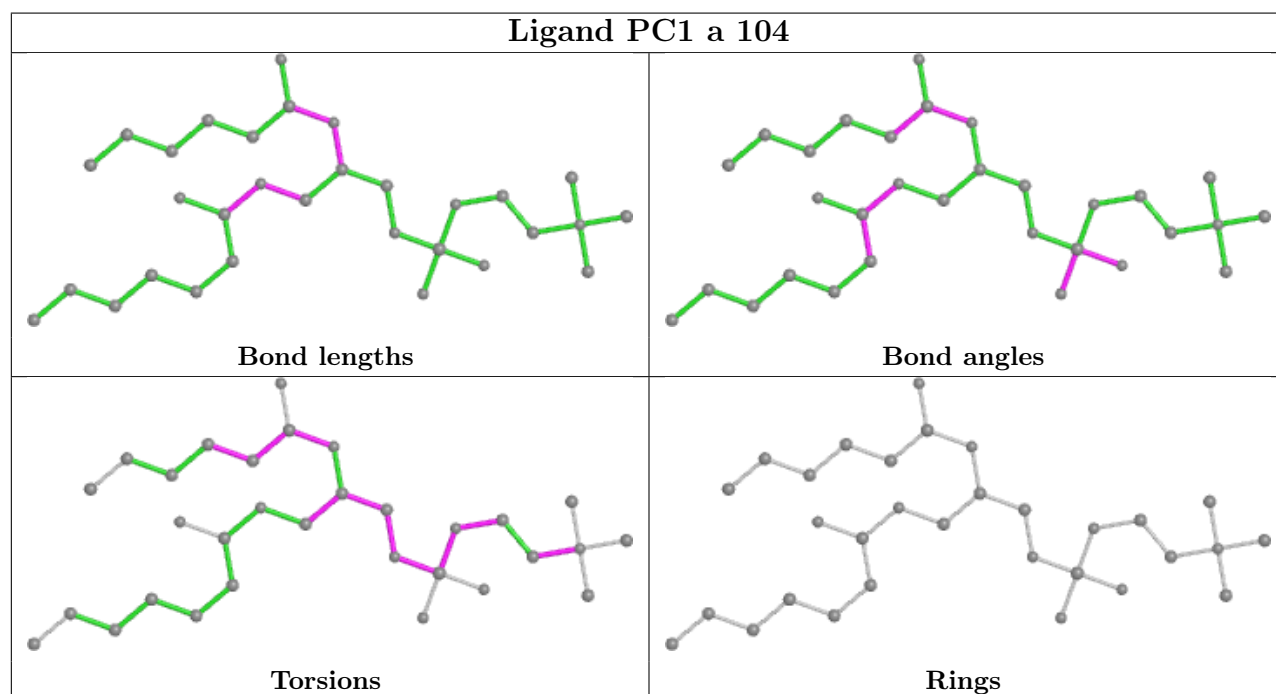
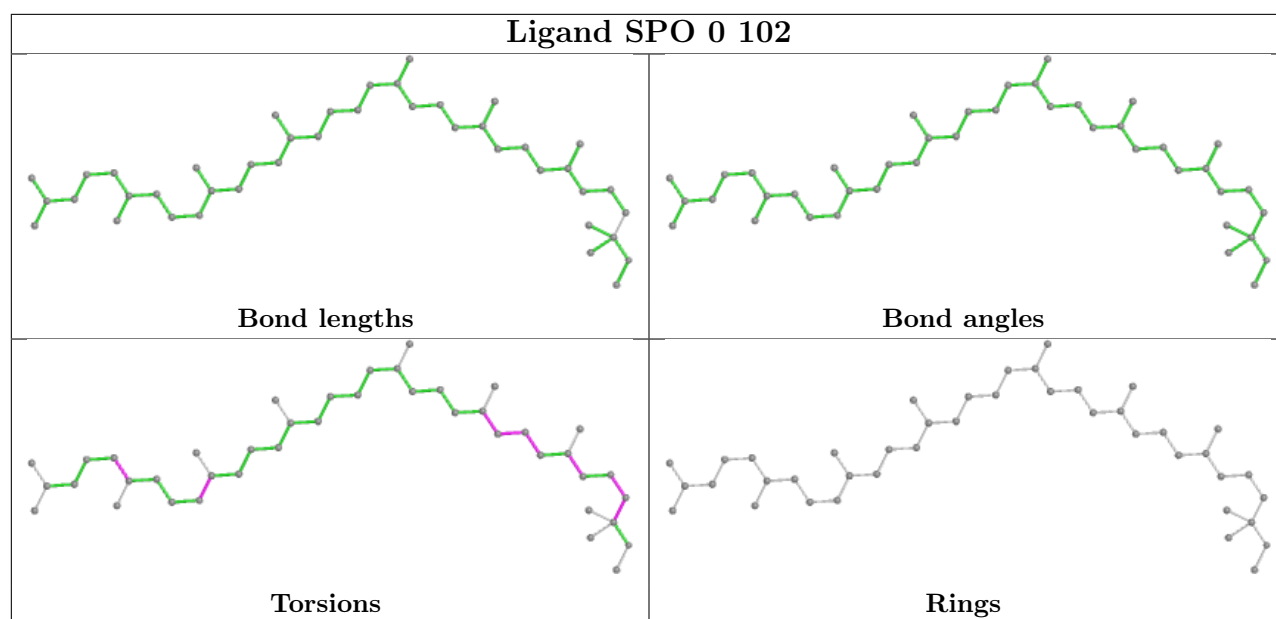


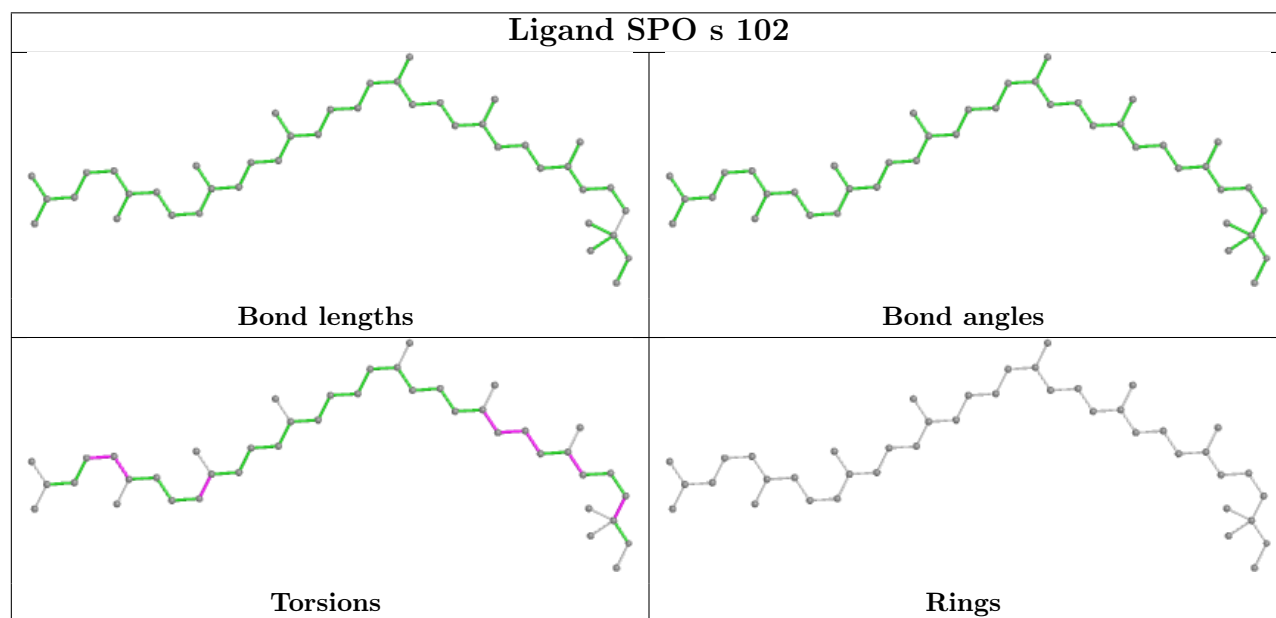
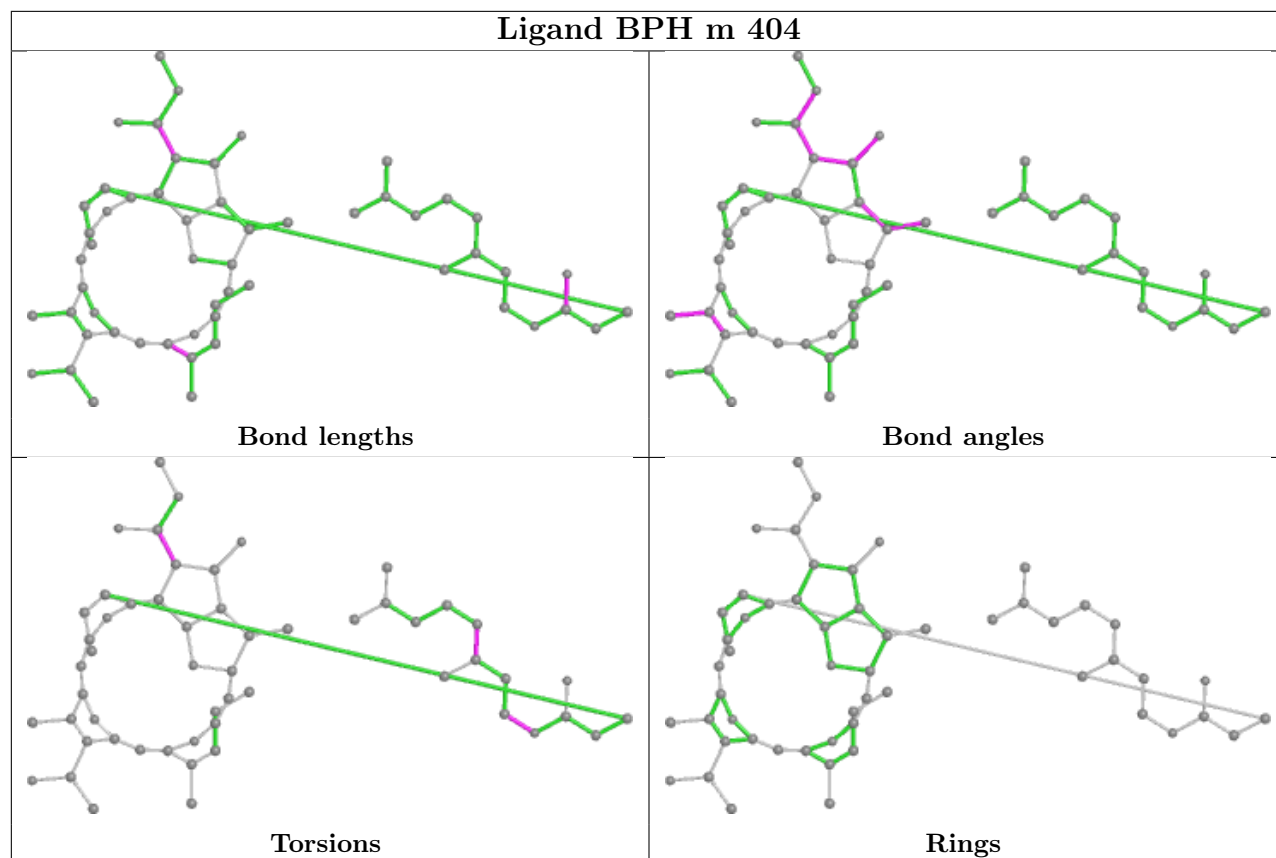




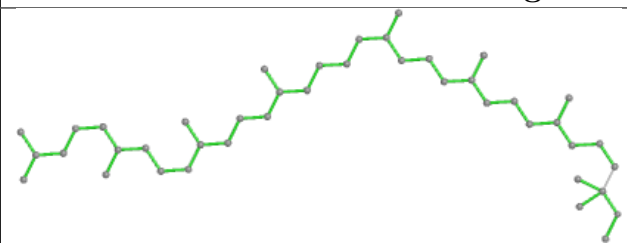
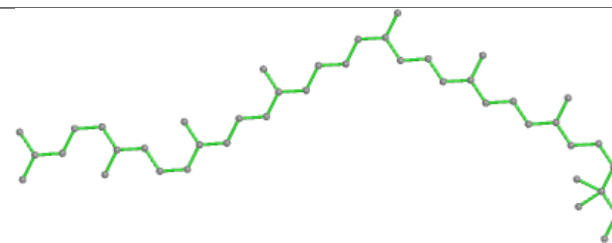
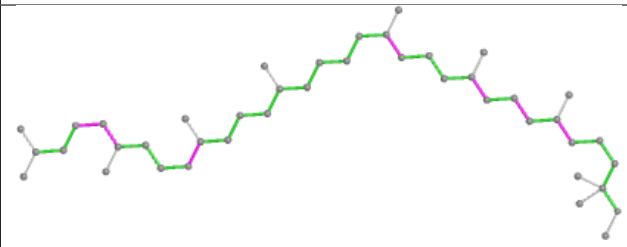
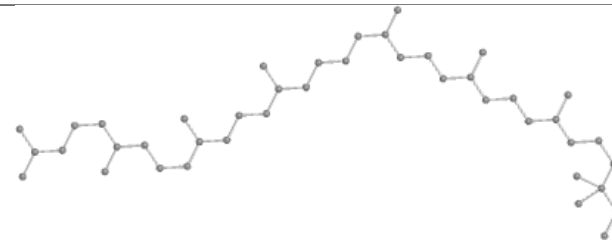


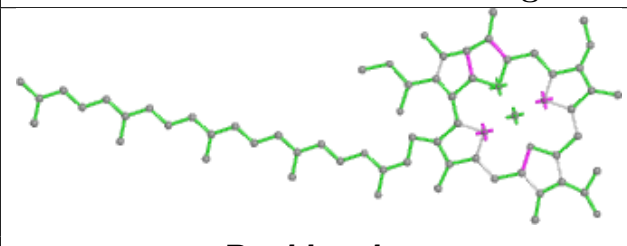
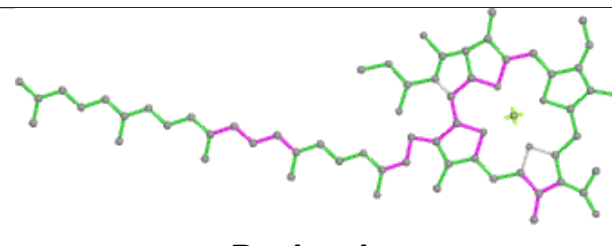
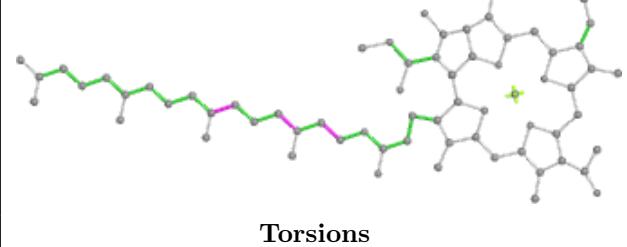
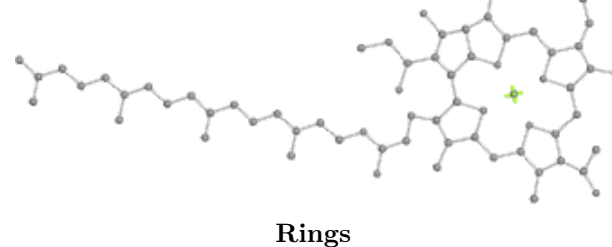


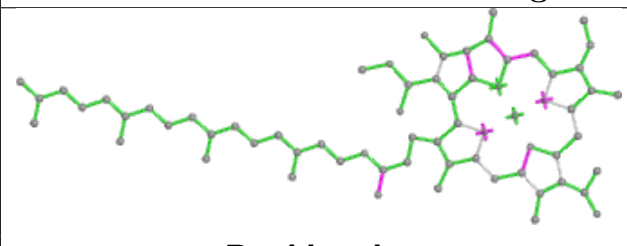
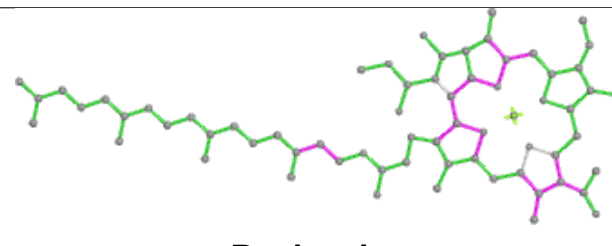
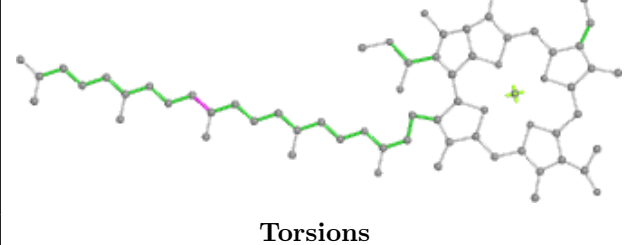
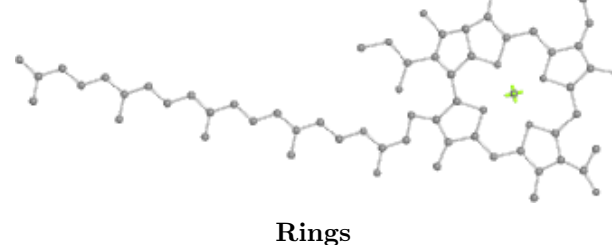


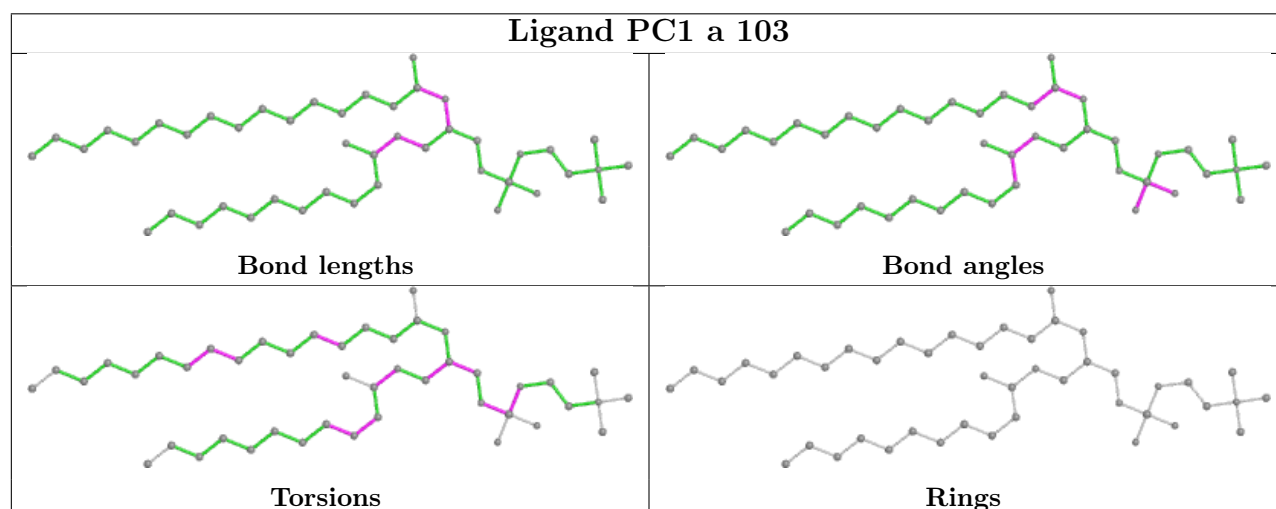
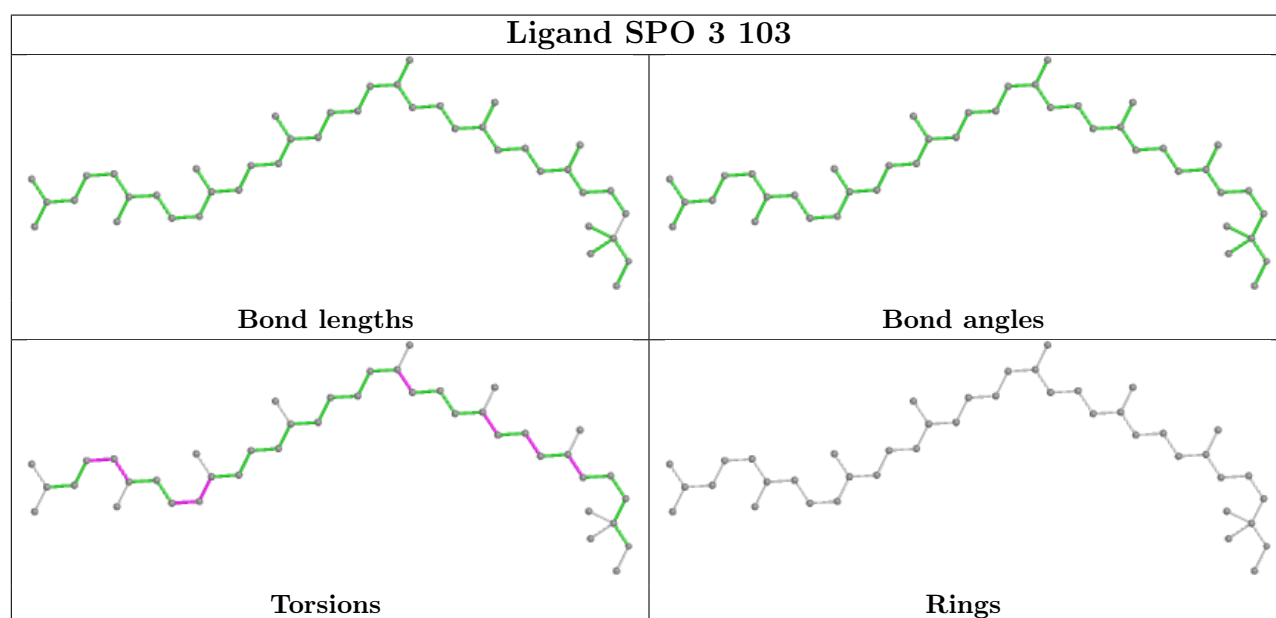
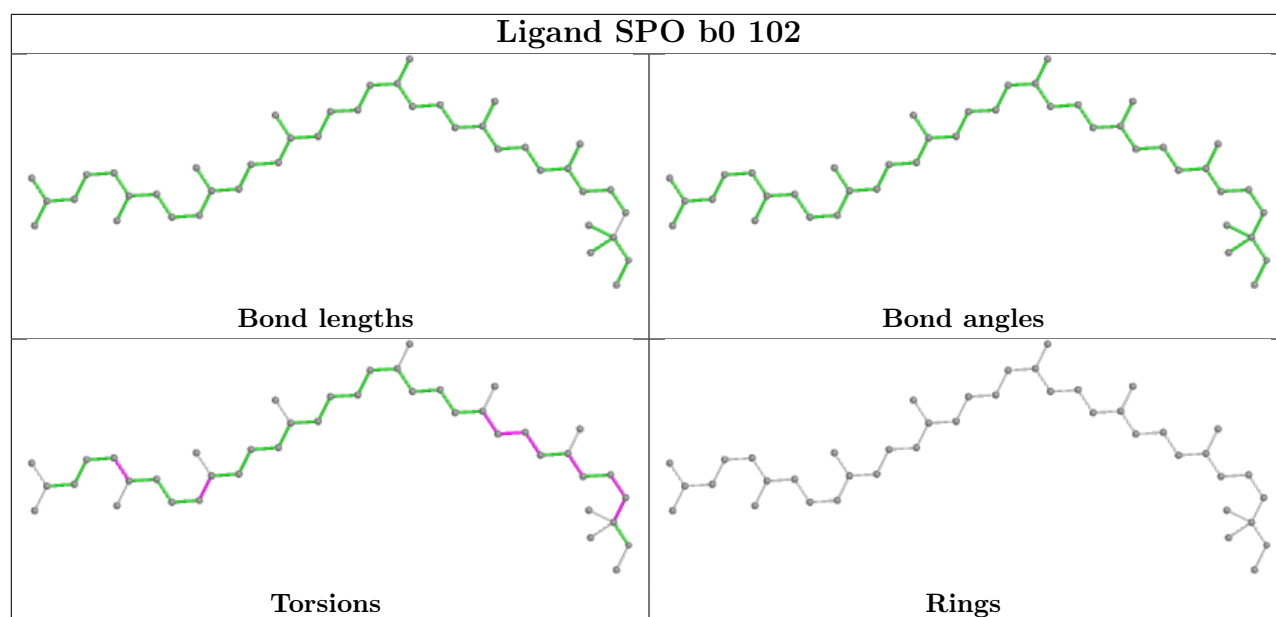


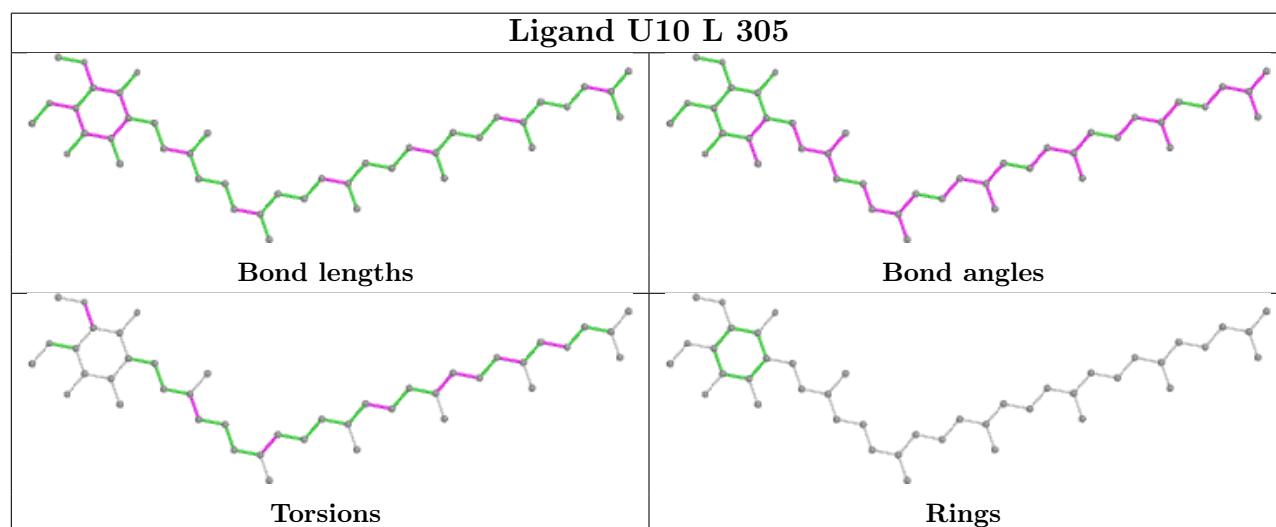
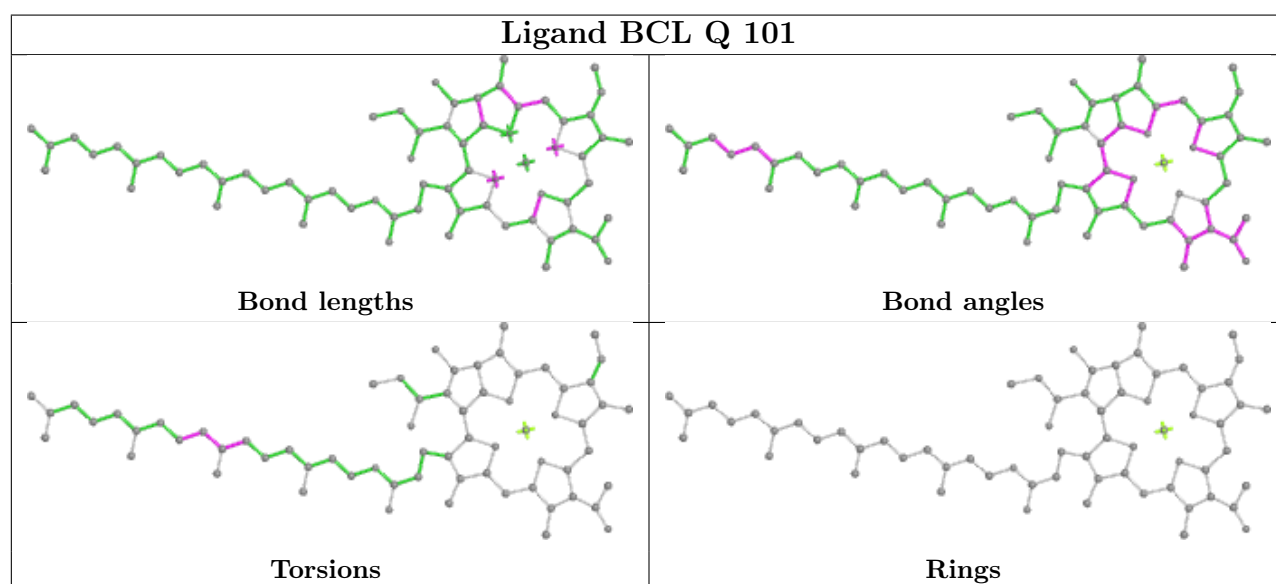
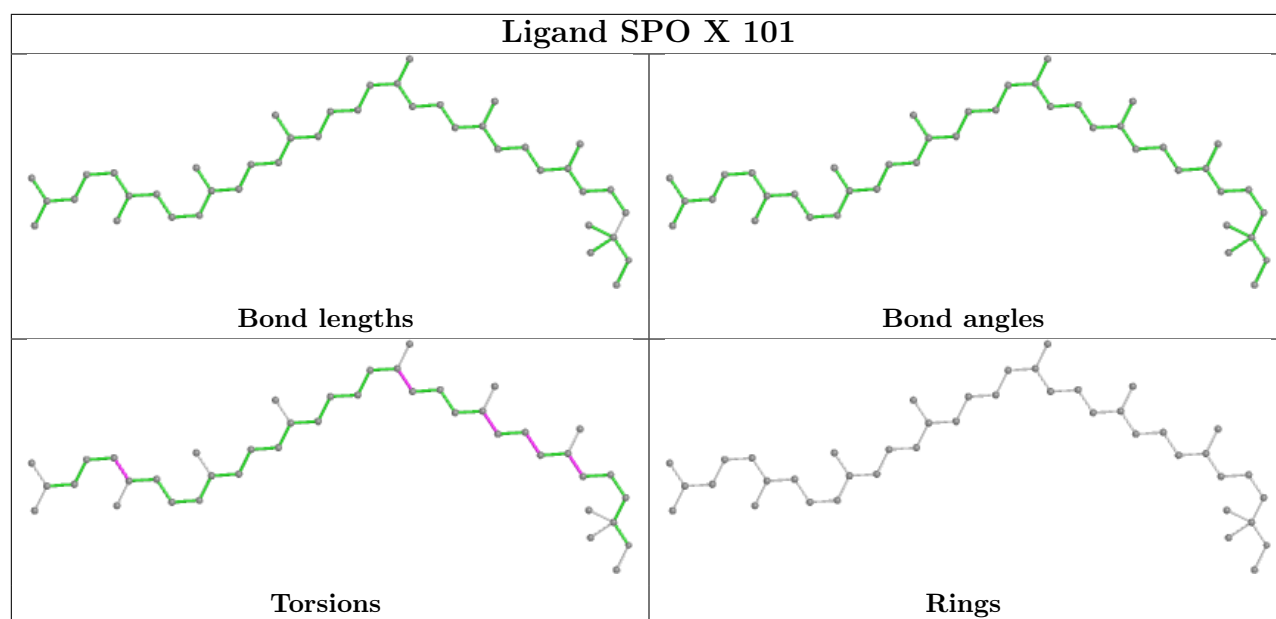


Ligand SPO E 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

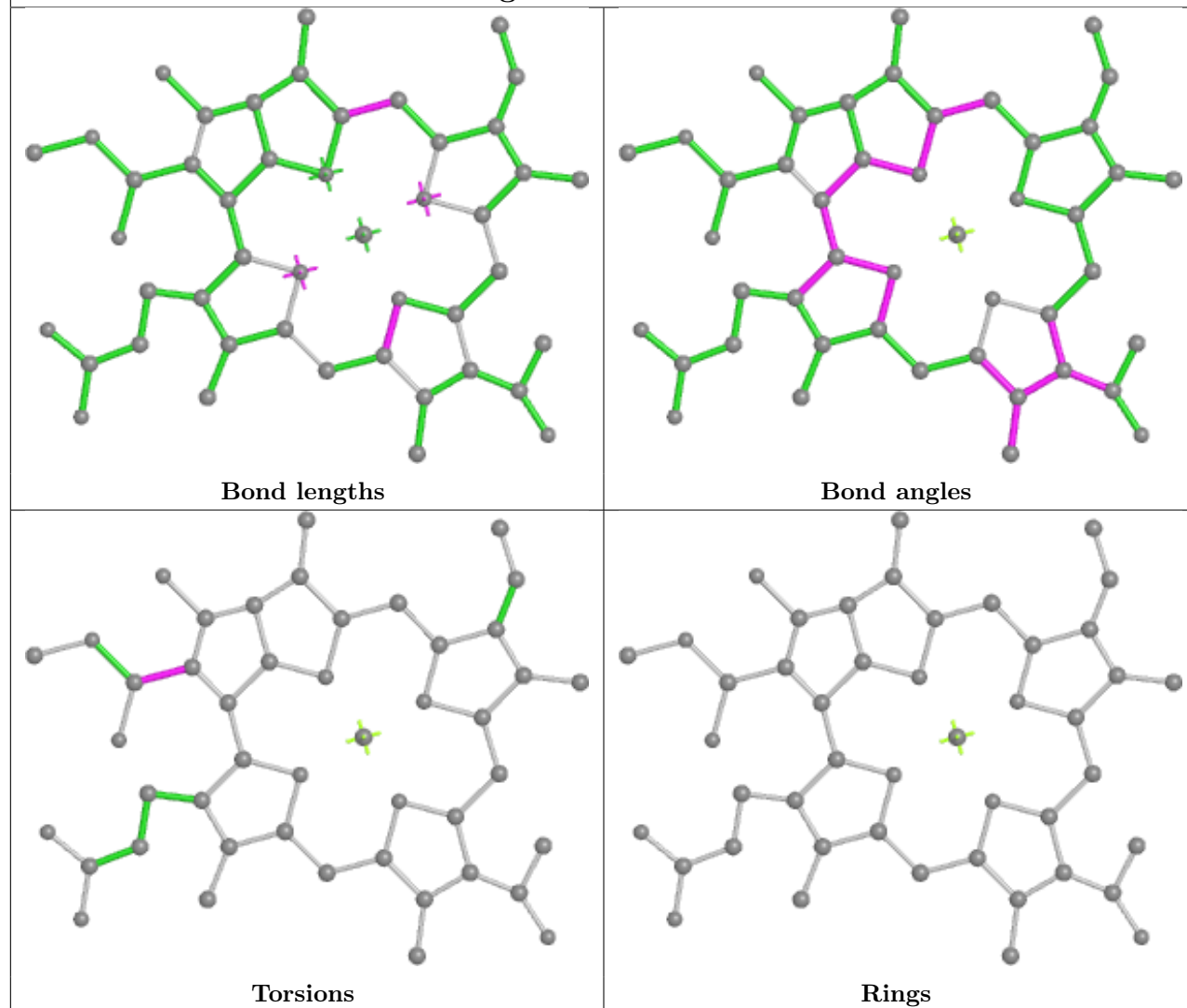
Ligand BCL V 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL i 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

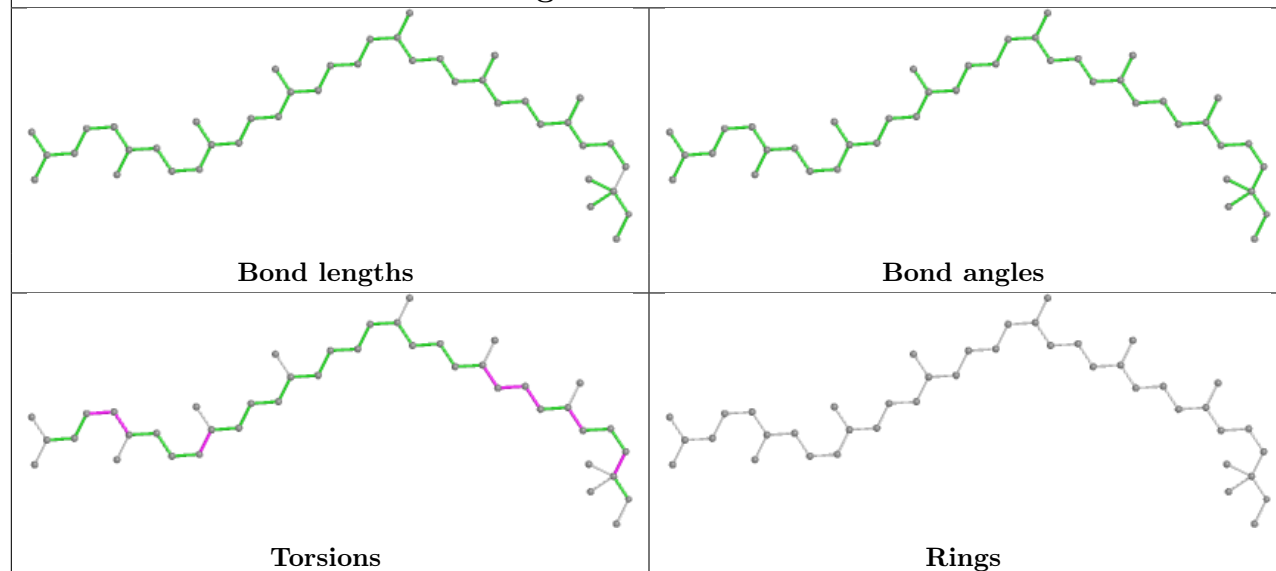


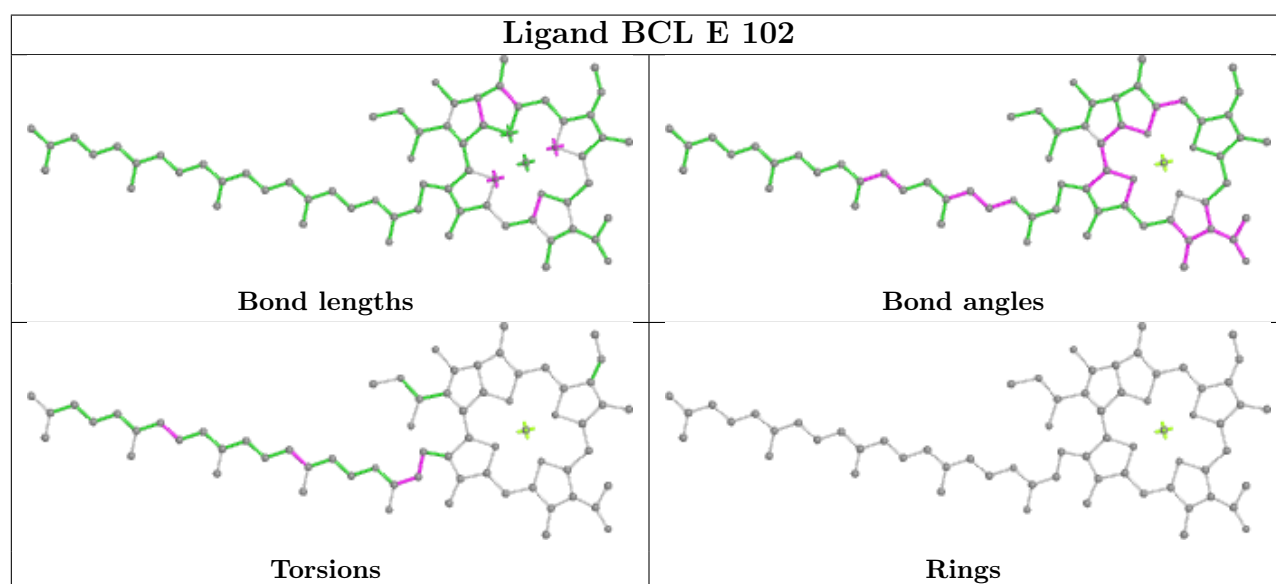
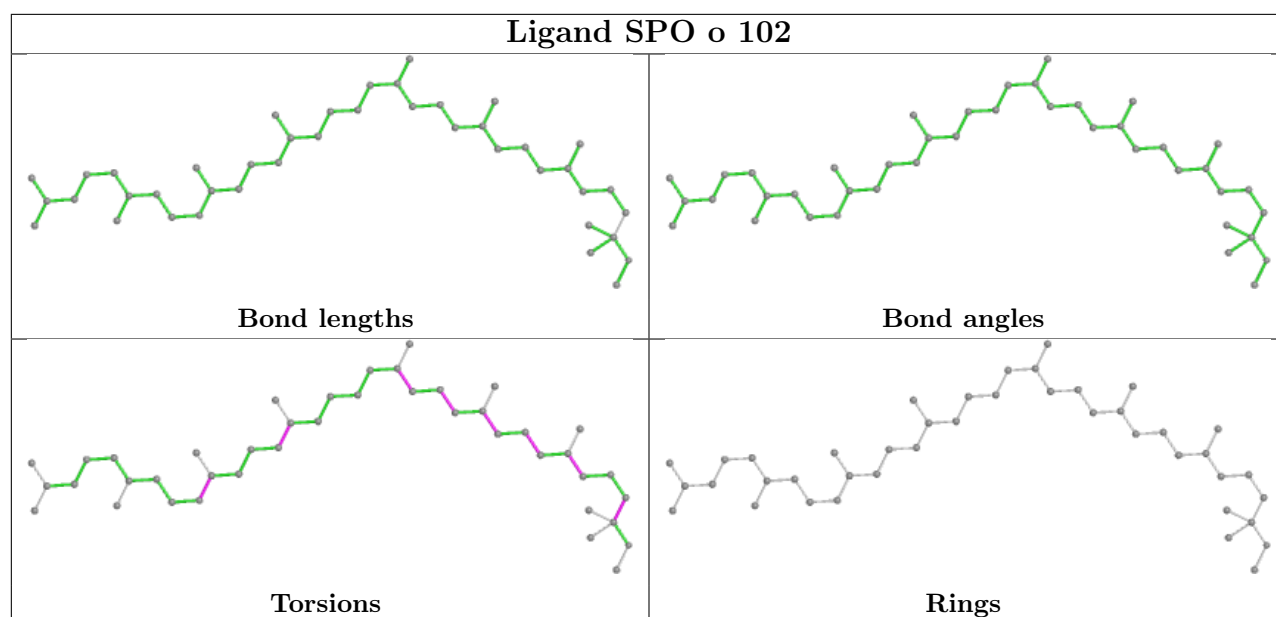


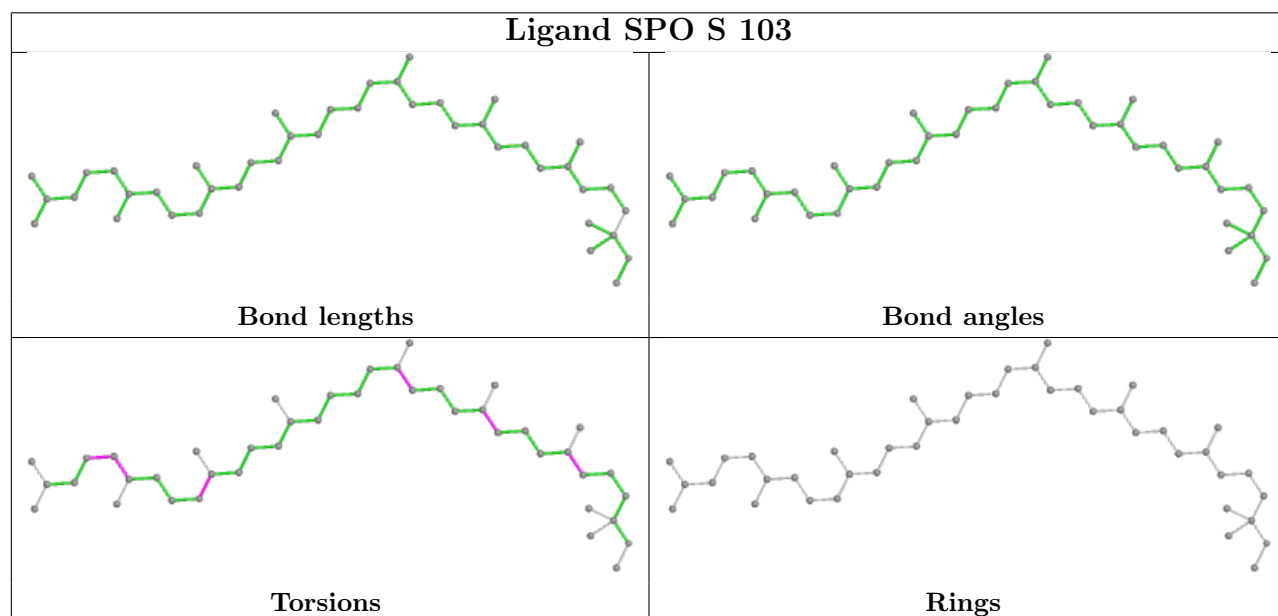
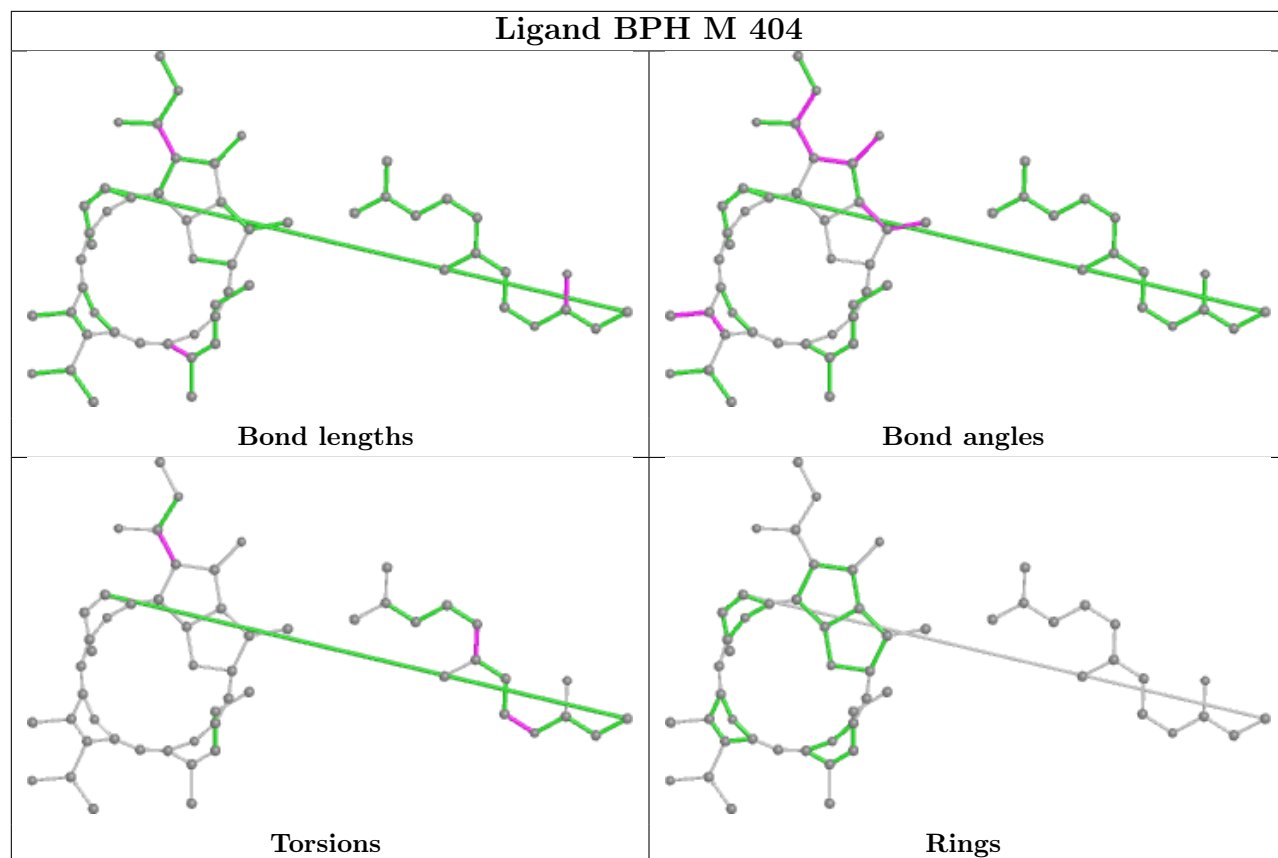
## Ligand BCL 1 101

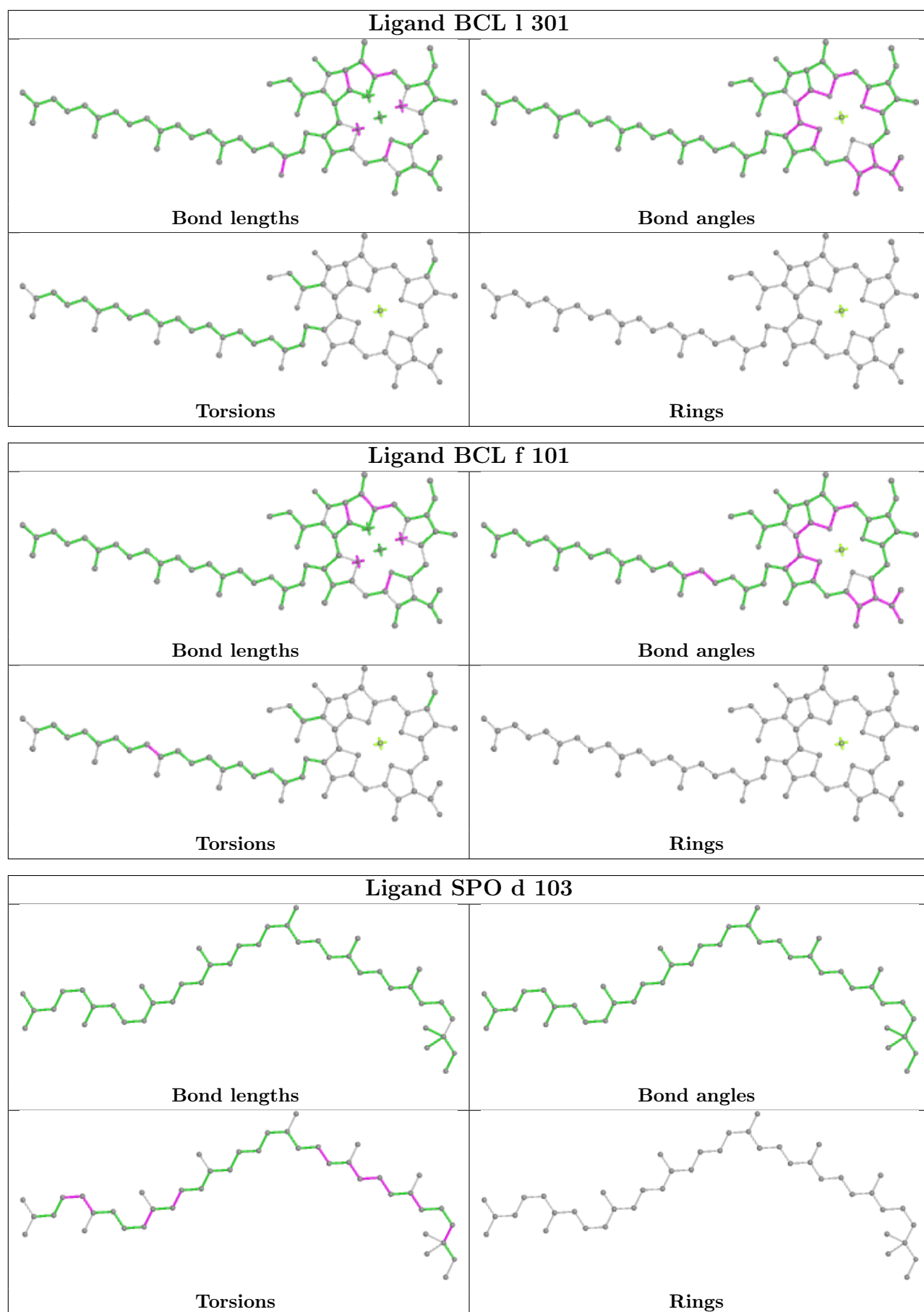


## Ligand SPO S 102

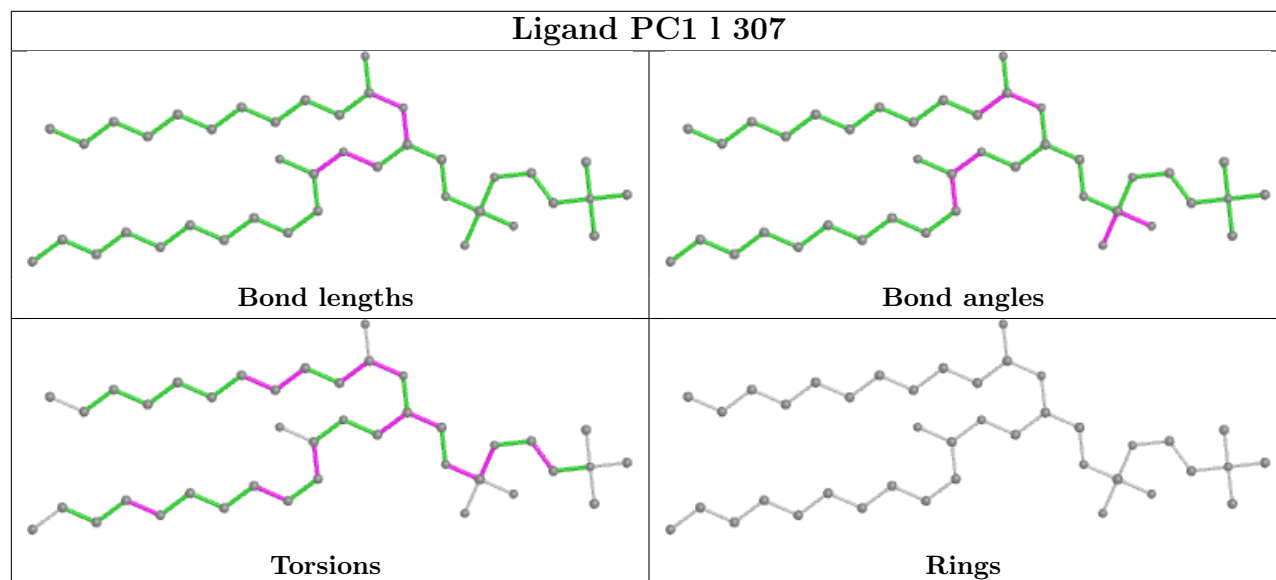




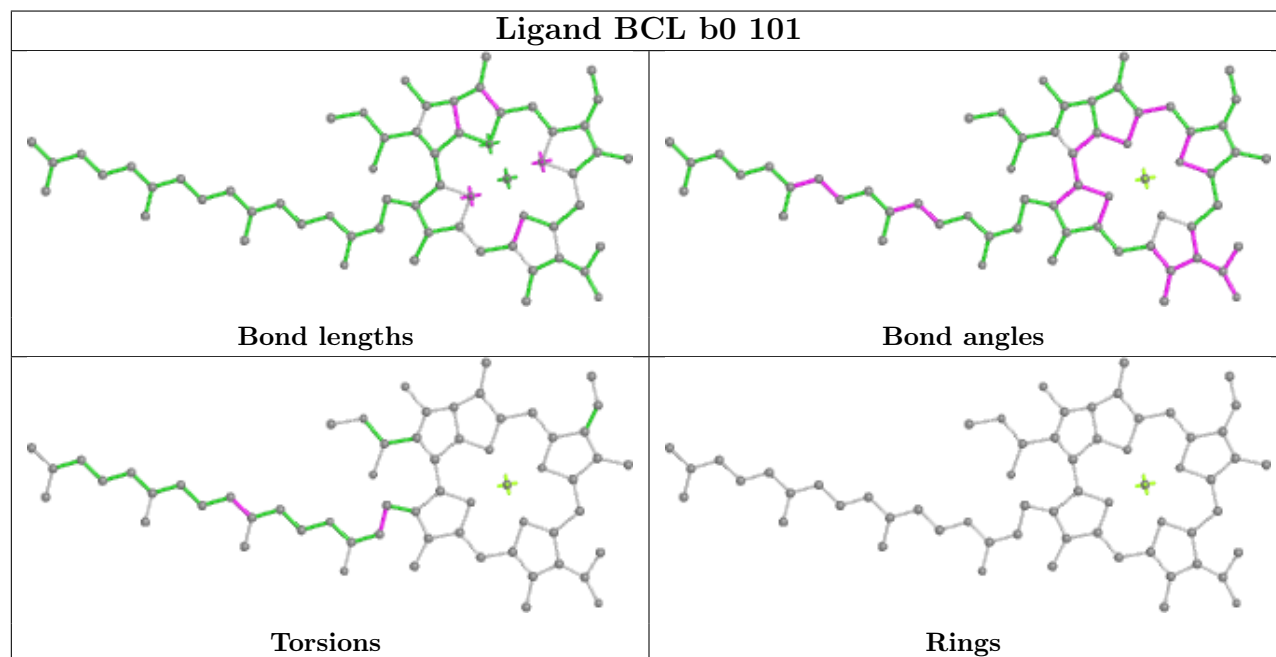




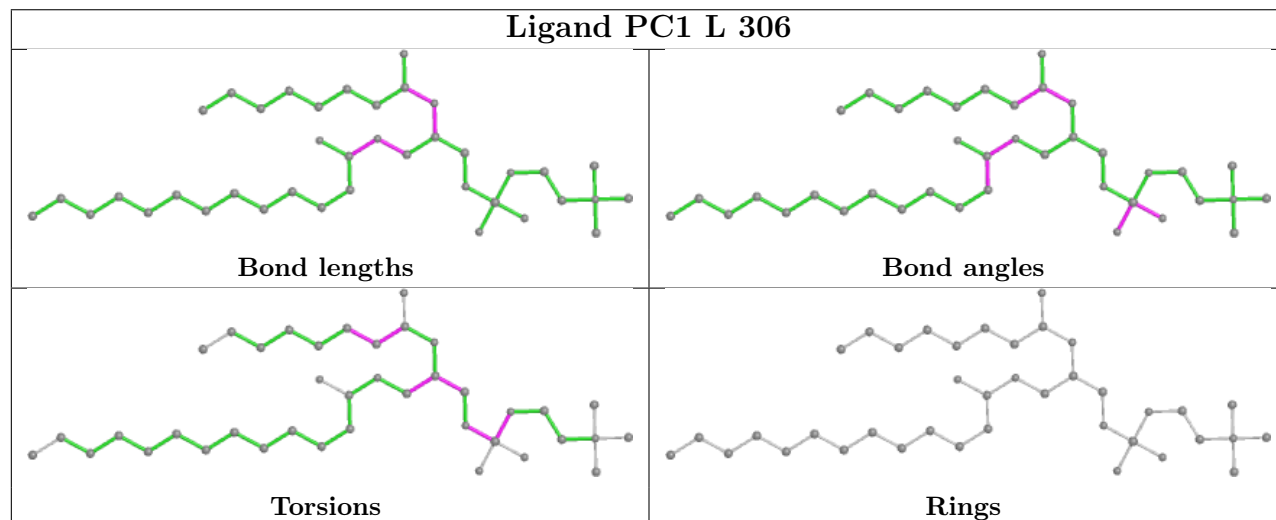
## Ligand PC1 I 307



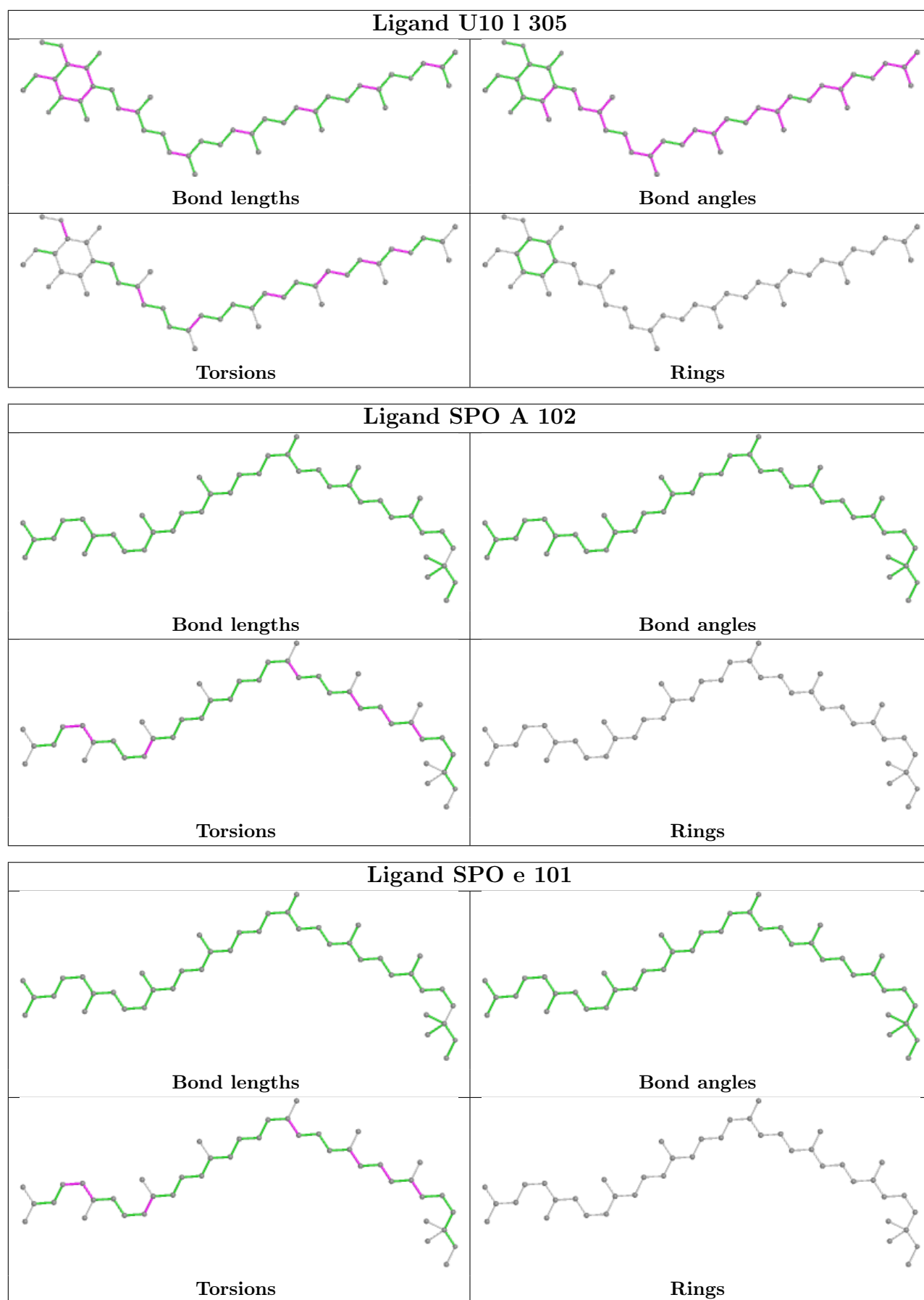
## Ligand BCL b0 101

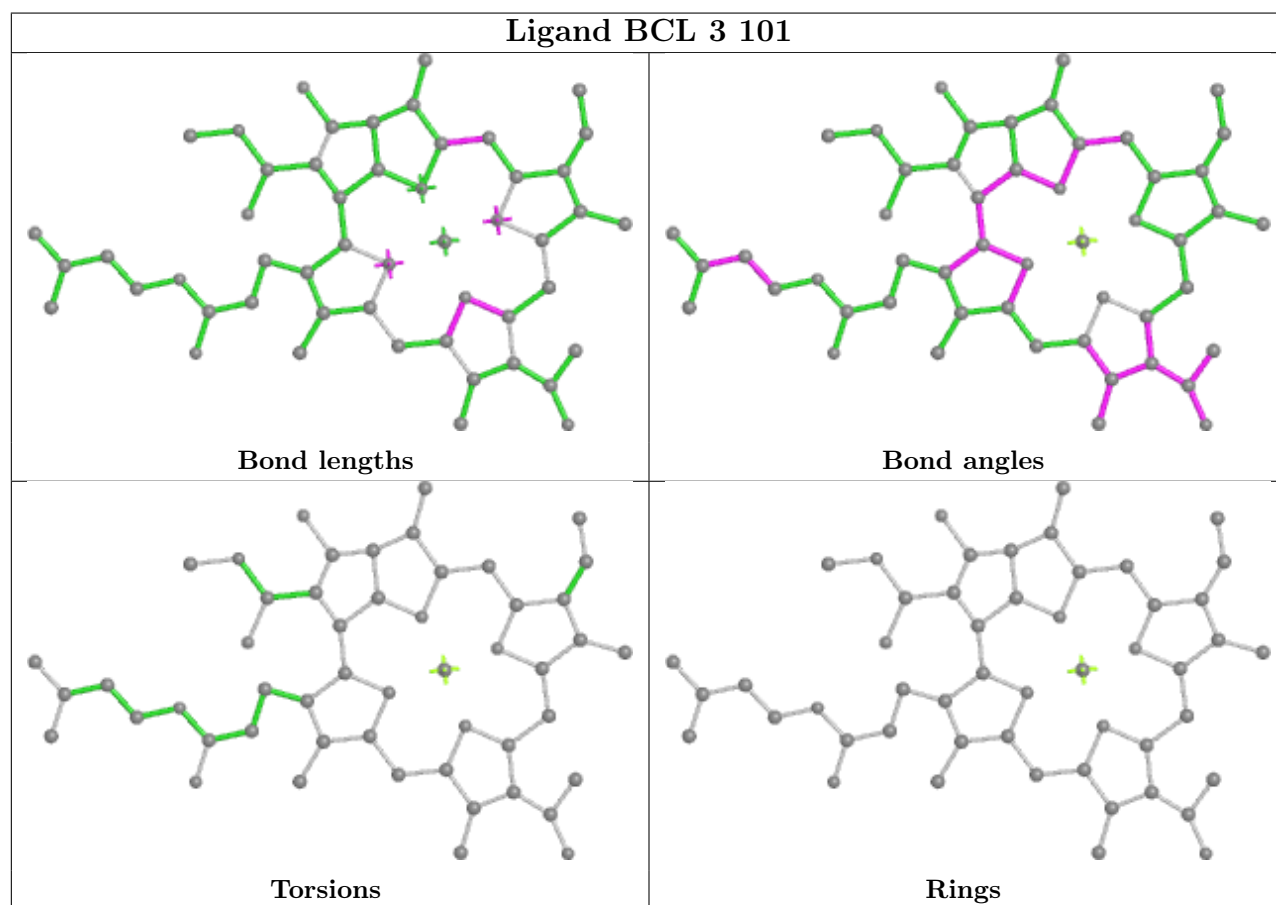
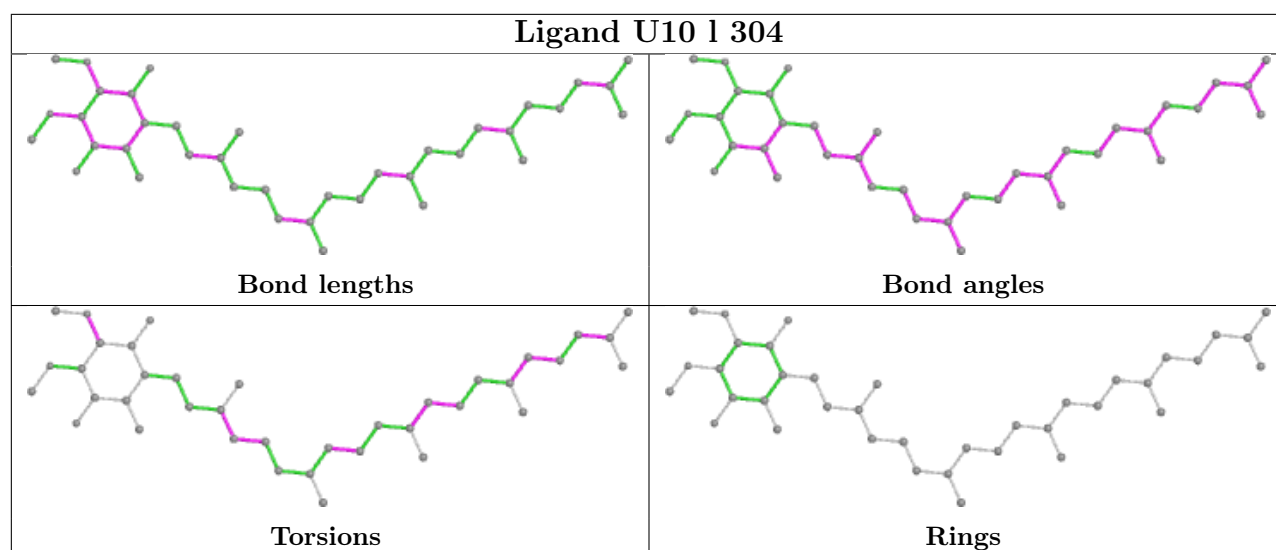


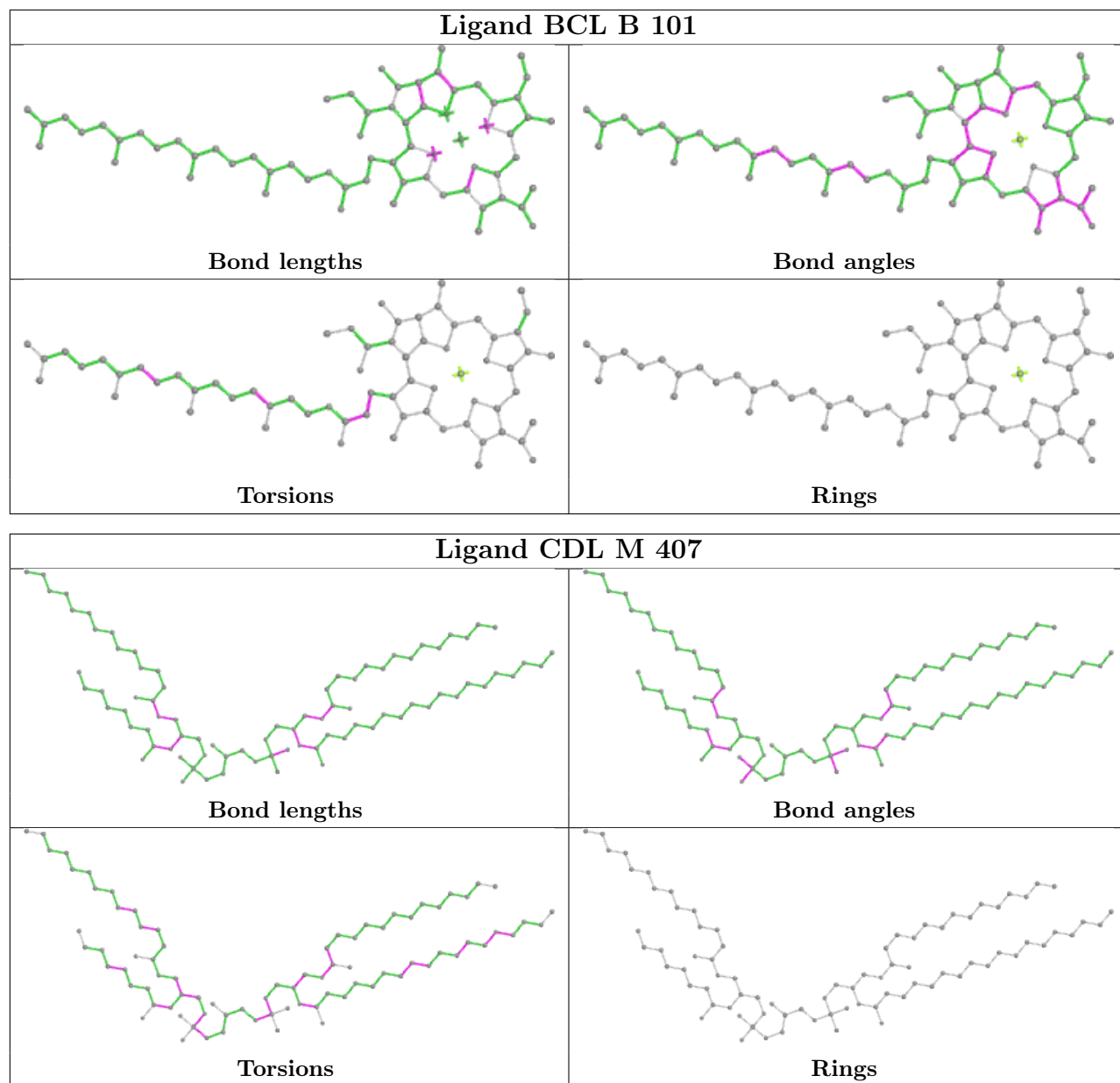
## Ligand PC1 L 306

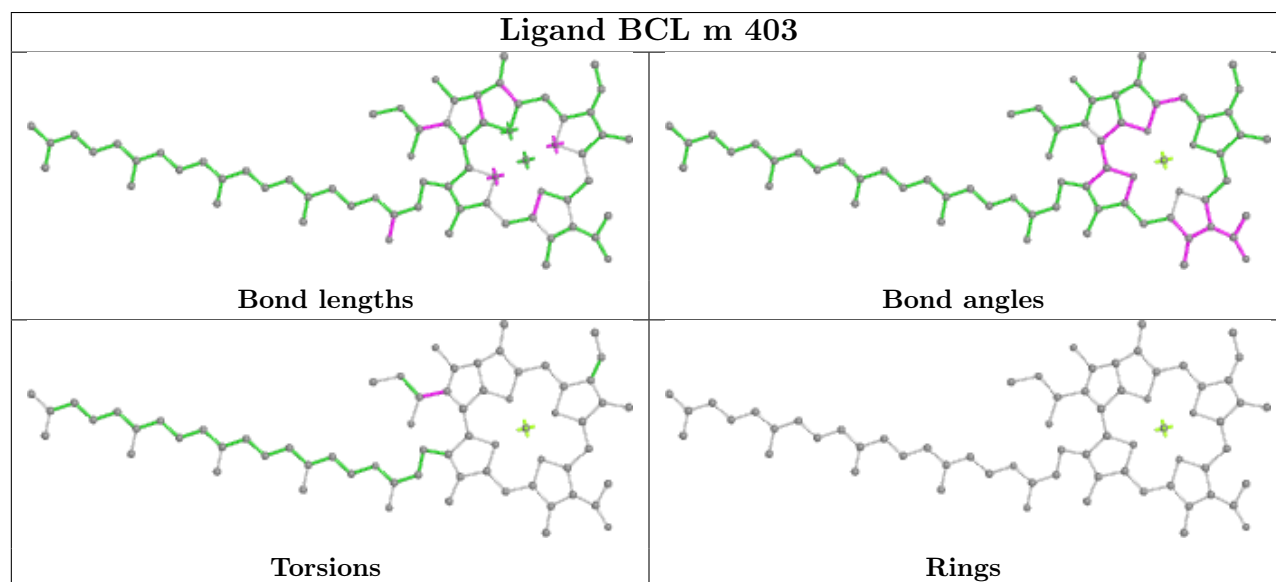
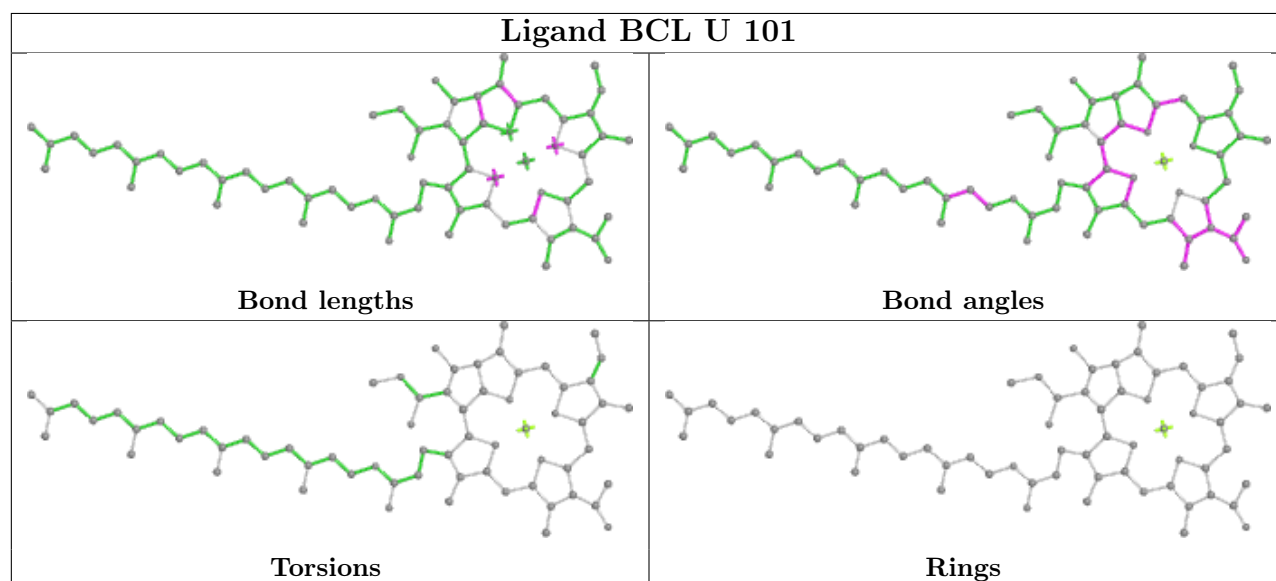
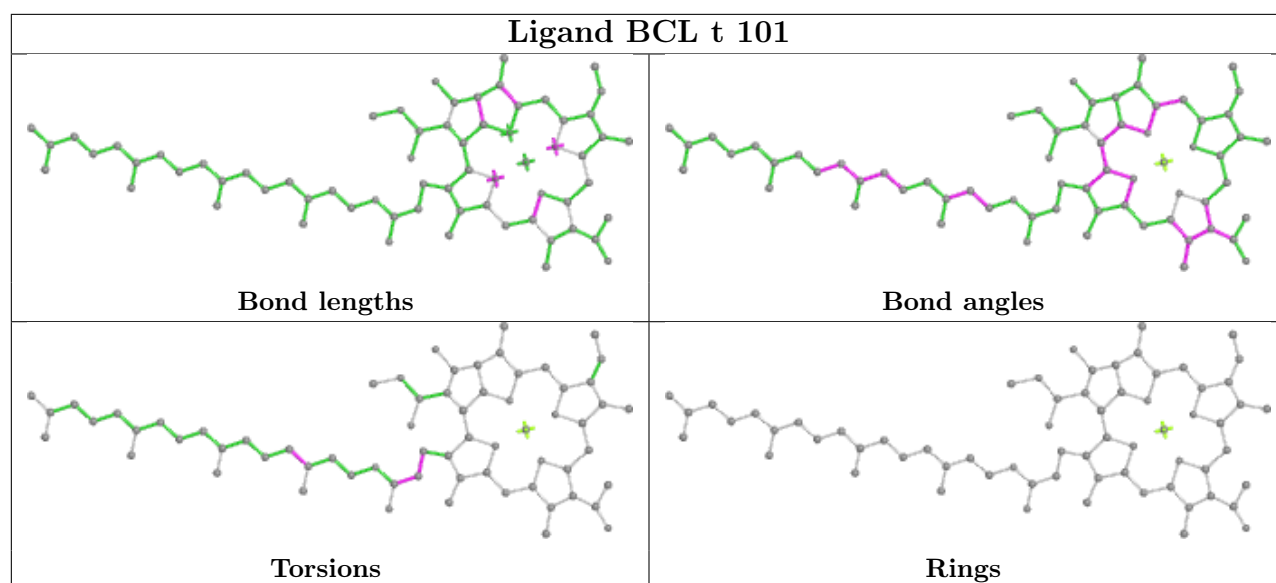


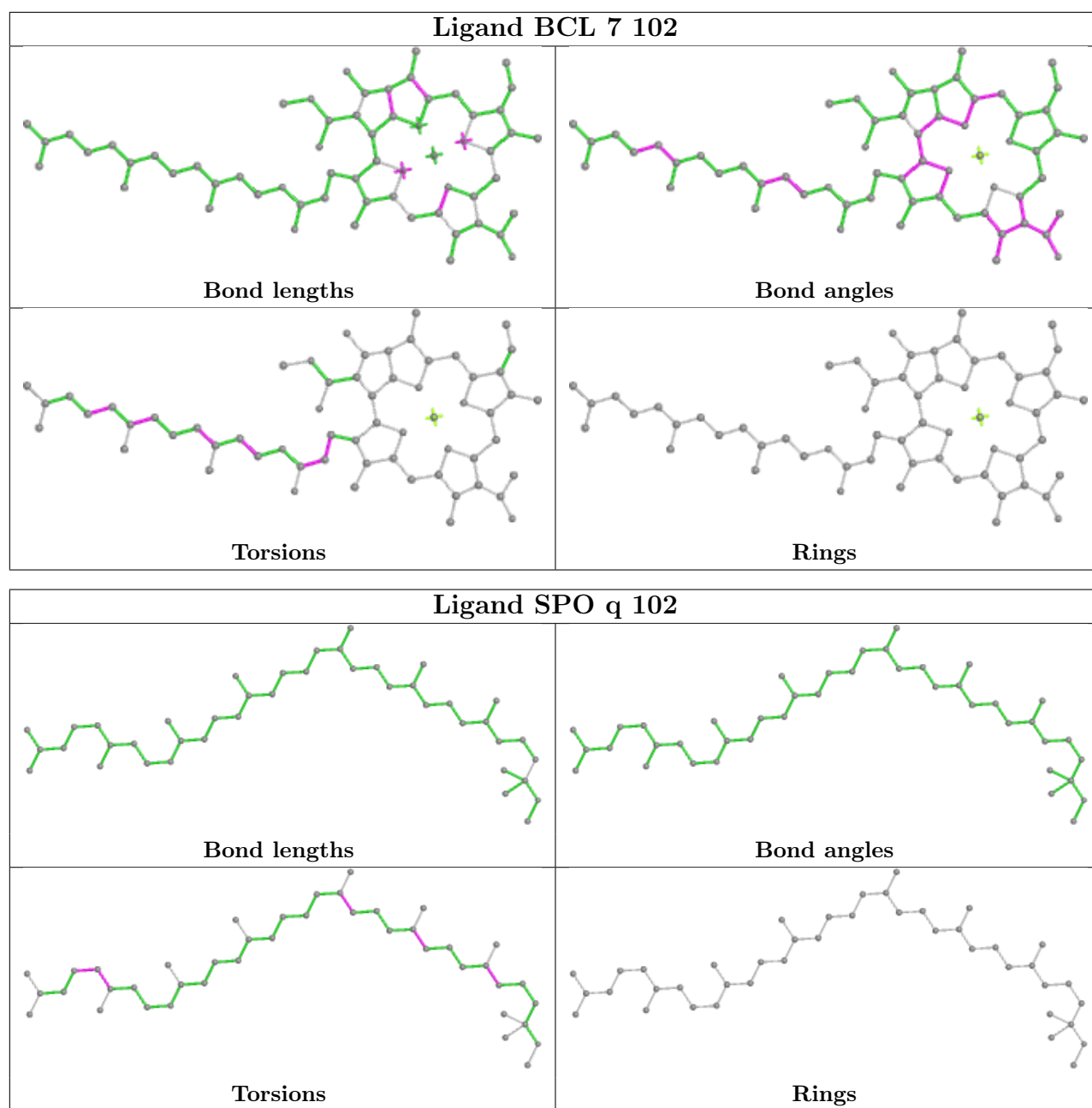


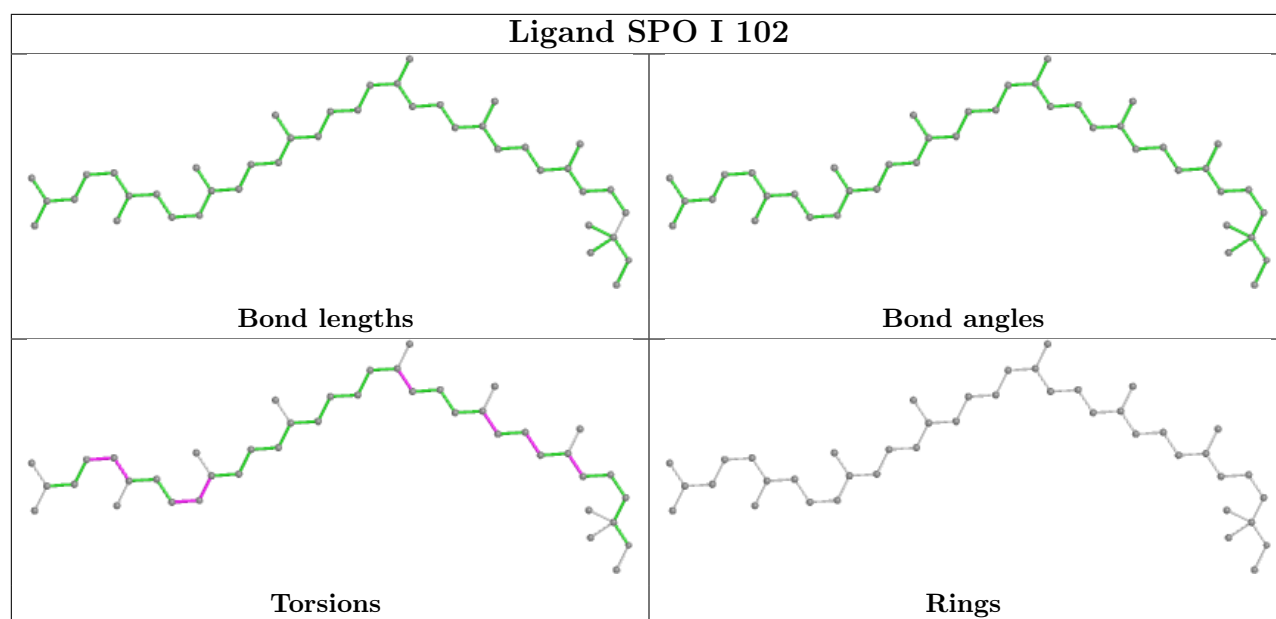












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

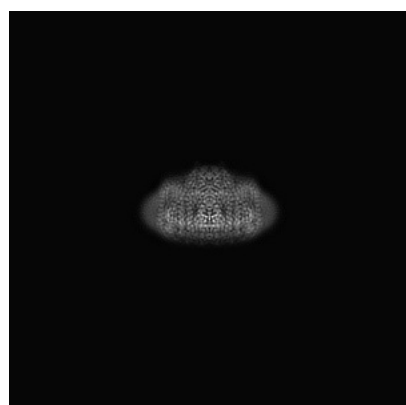
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32058. These allow visual inspection of the internal detail of the map and identification of artifacts.

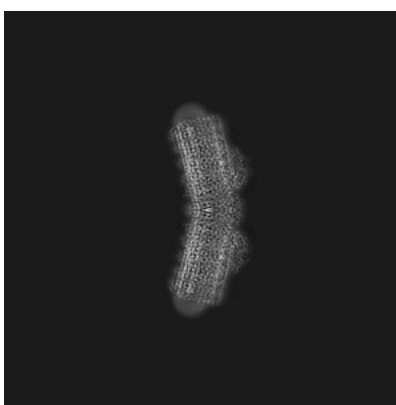
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

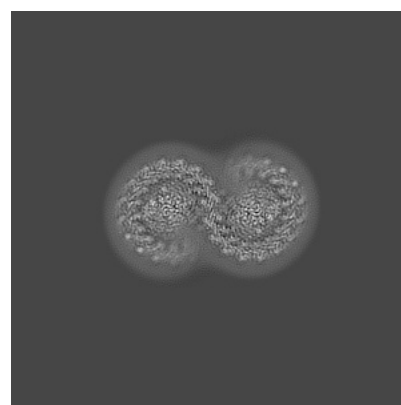
#### 6.1.1 Primary map



X



Y

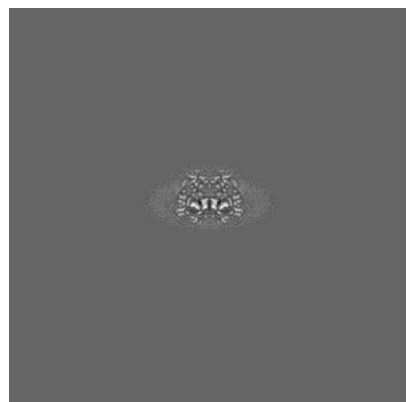


Z

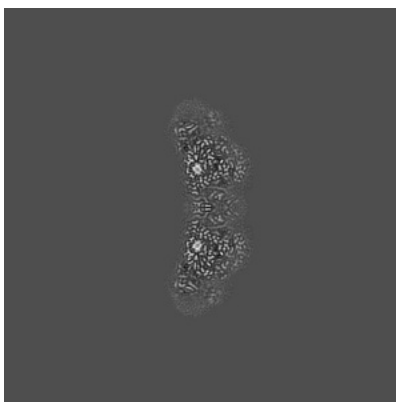
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

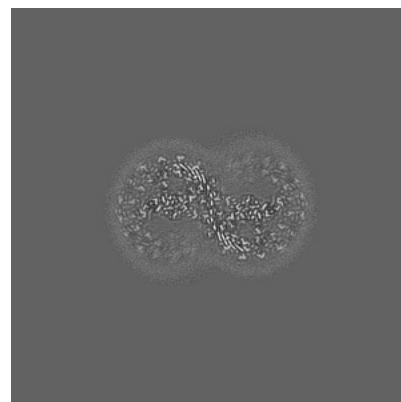
#### 6.2.1 Primary map



X Index: 208



Y Index: 208

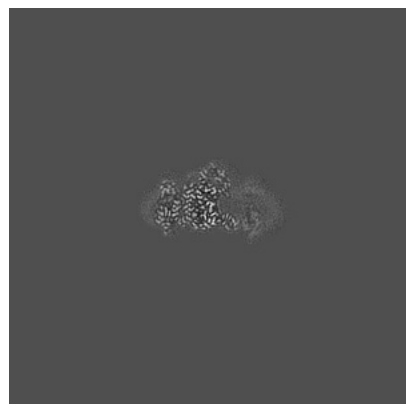


Z Index: 208

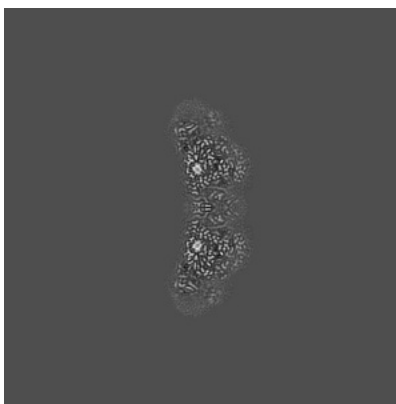
The images above show central slices of the map in three orthogonal directions.

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

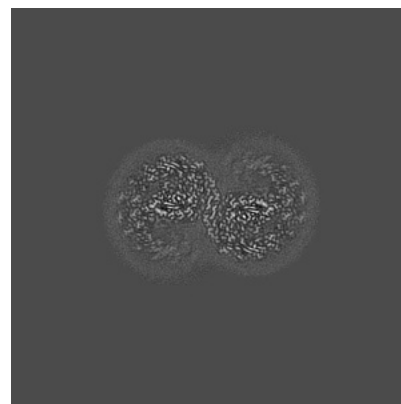
### 6.3.1 Primary map



X Index: 257



Y Index: 208

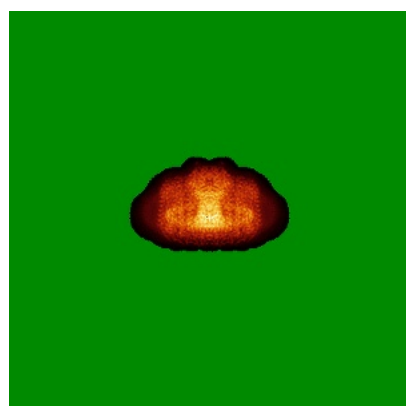


Z Index: 202

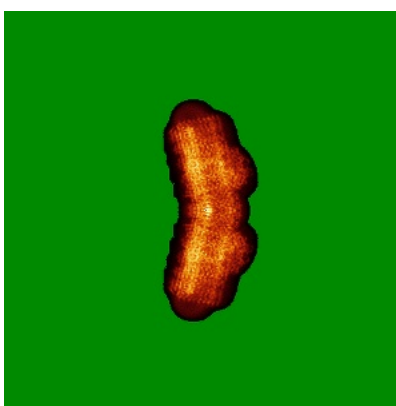
The images above show the largest variance slices of the map in three orthogonal directions.

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

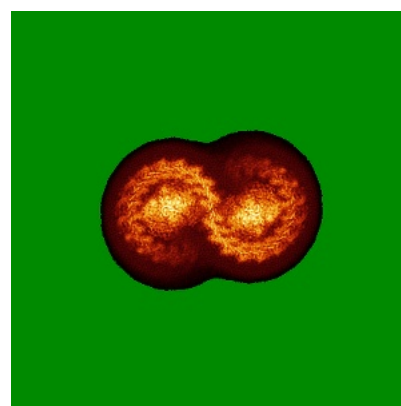
### 6.4.1 Primary map



X



Y



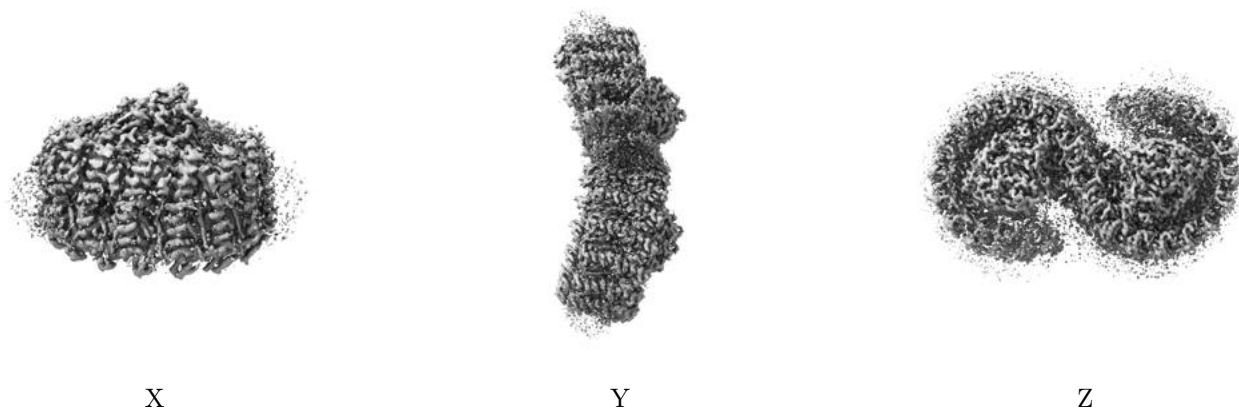
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

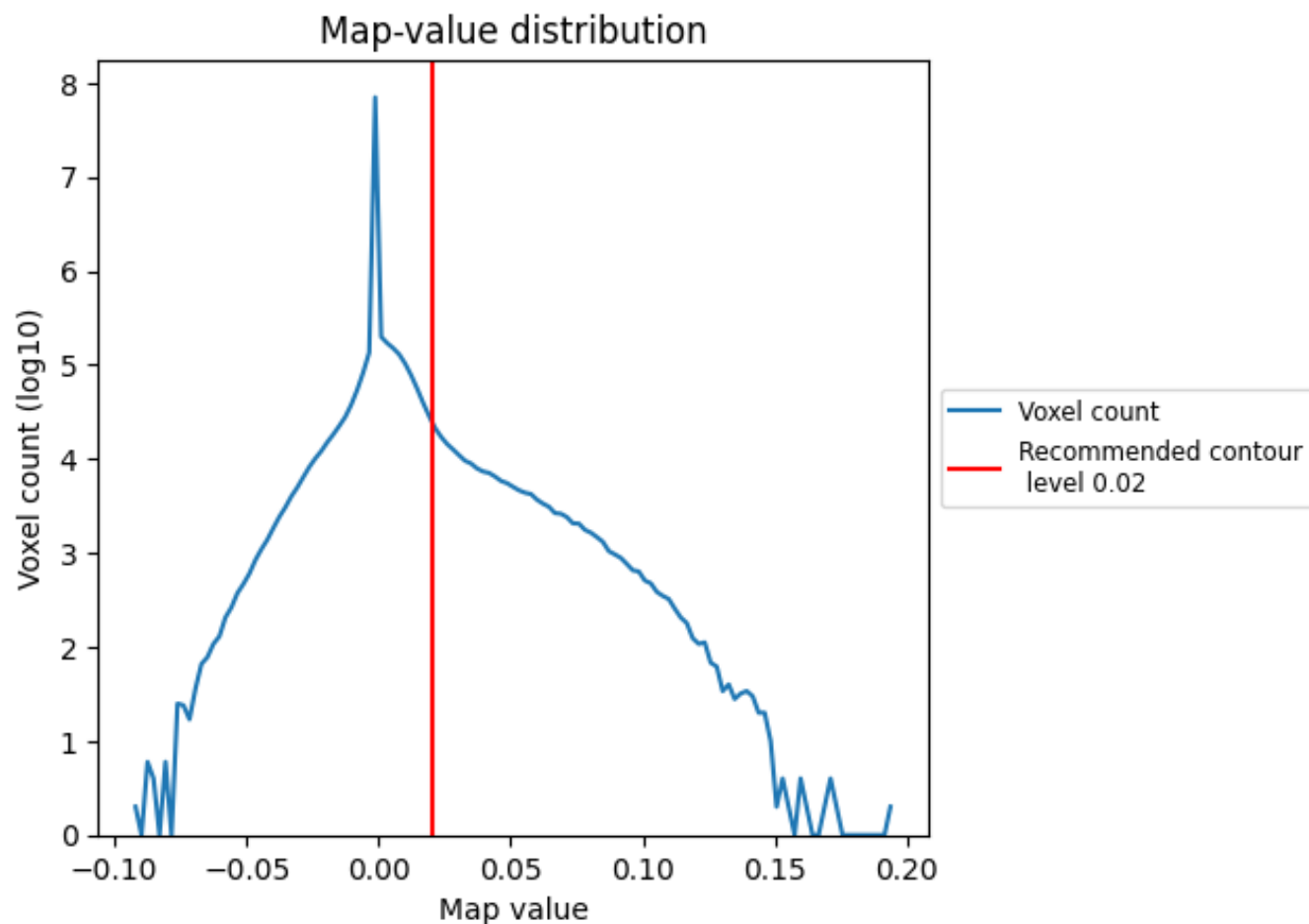
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

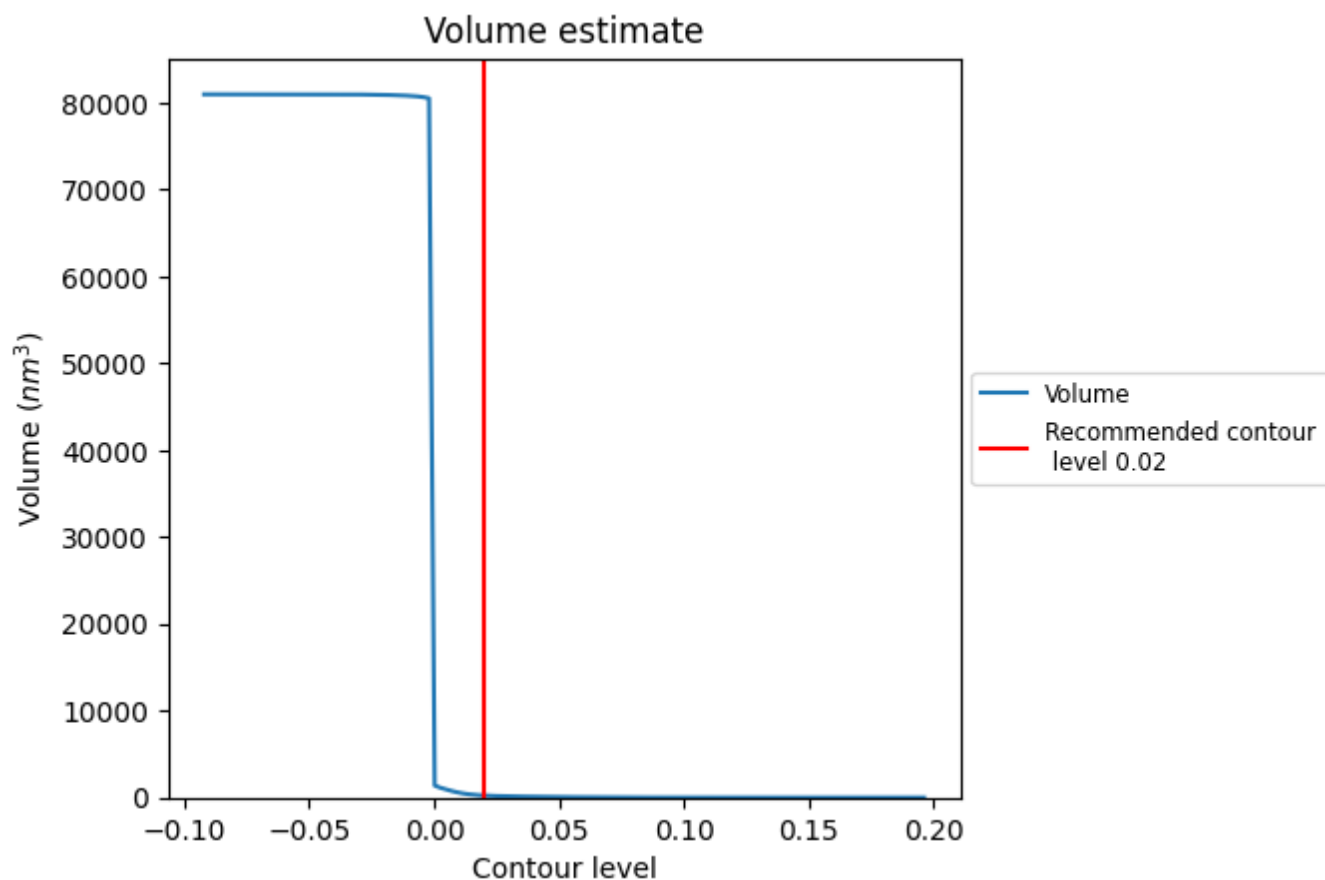
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

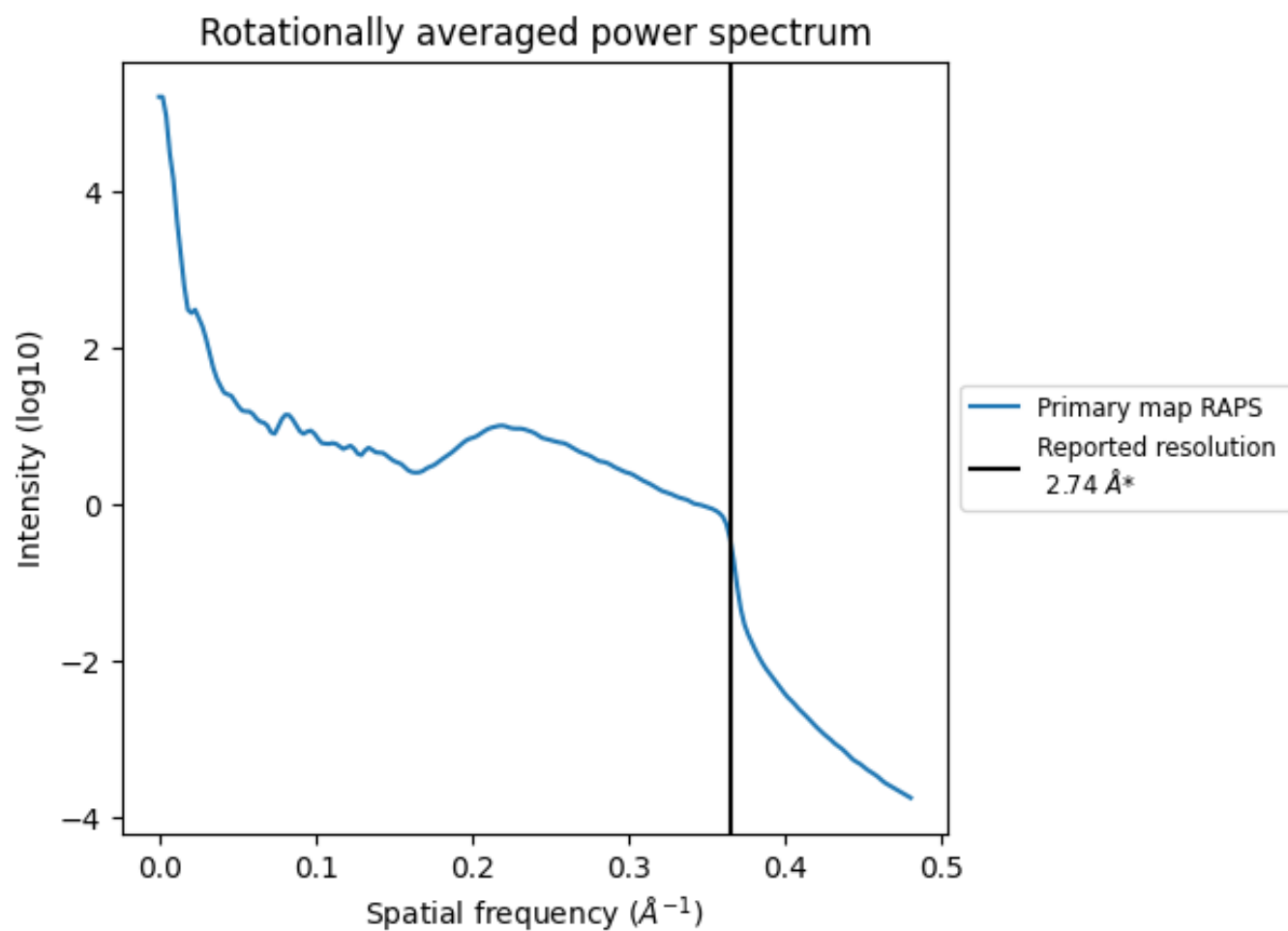
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234  $\text{nm}^3$ ; this corresponds to an approximate mass of 211 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 0.365 Å<sup>-1</sup>

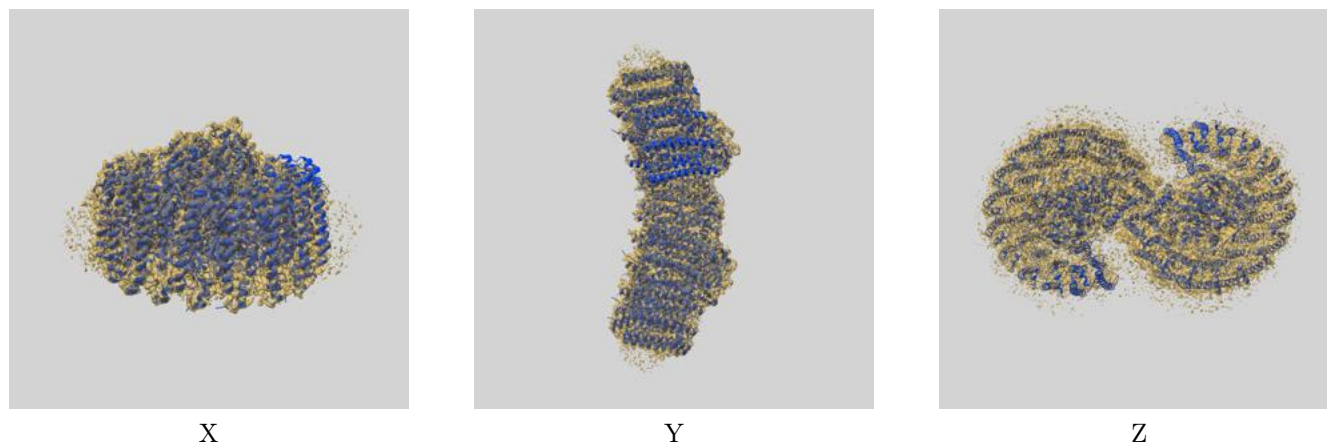
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

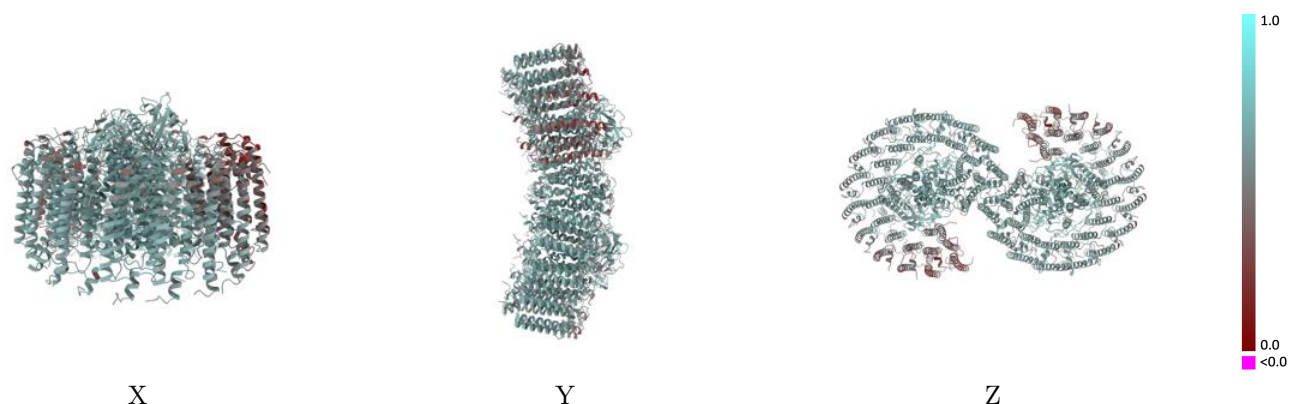
This section contains information regarding the fit between EMDB map EMD-32058 and PDB model 7VOR. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

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



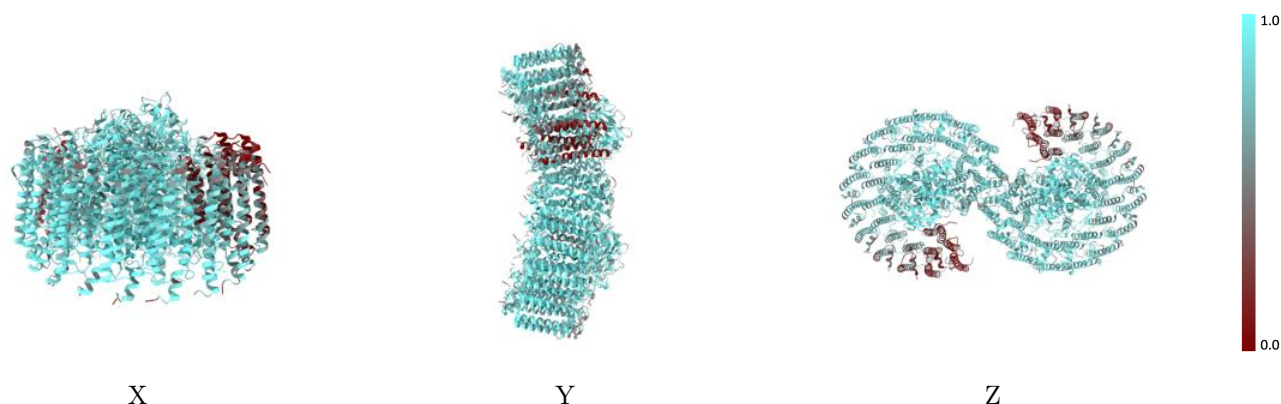
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



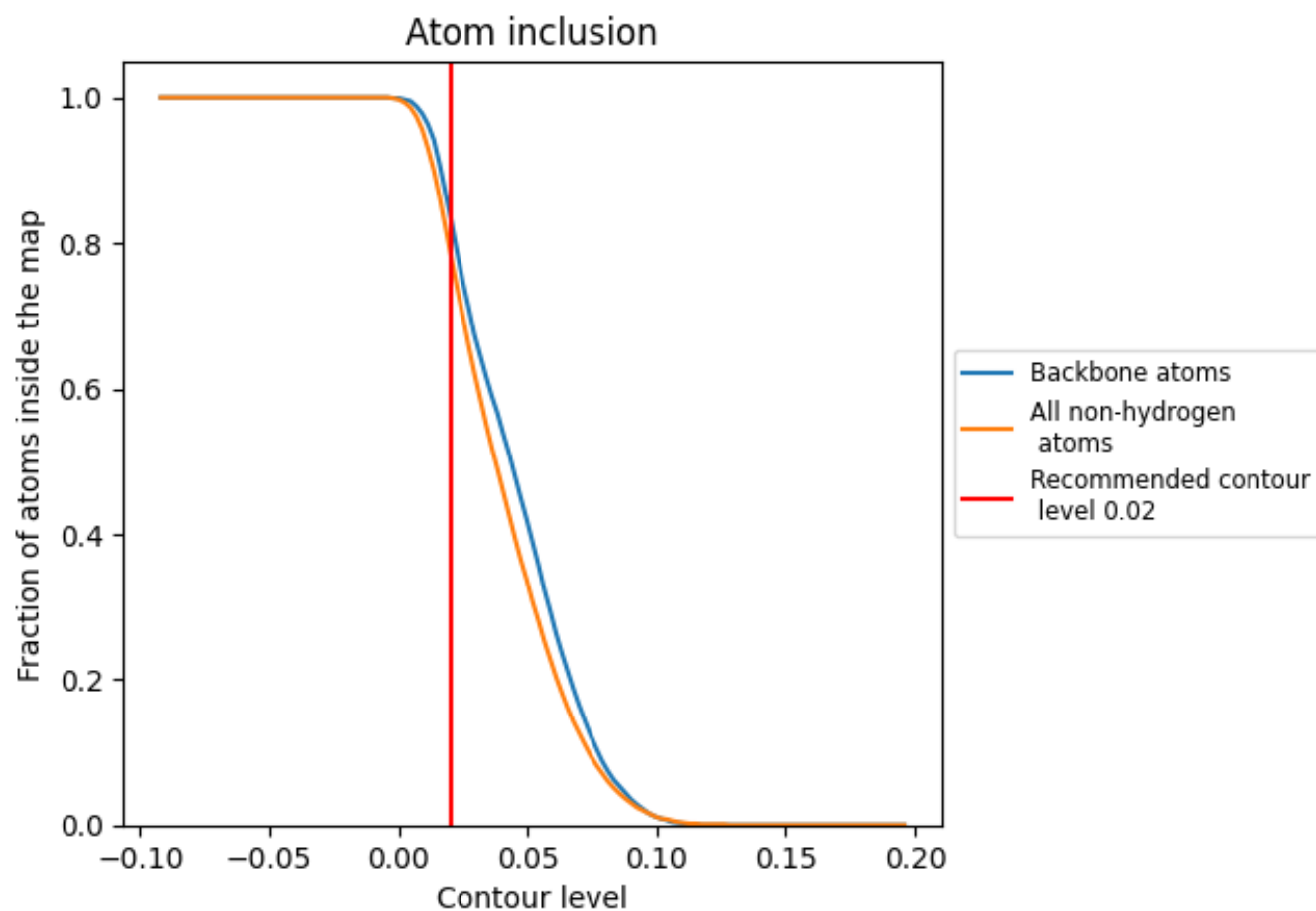
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 84% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

































































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7890	 0.5730
0	 0.8740	 0.6040
1	 0.2550	 0.3540
2	 0.1720	 0.3220
3	 0.3640	 0.4140
4	 0.1720	 0.3260
5	 0.3660	 0.4140
6	 0.9060	 0.6190
7	 0.9060	 0.6190
8	 0.8950	 0.6040
9	 0.9290	 0.6210
A	 0.8980	 0.6140
B	 0.8680	 0.6040
C	 0.4600	 0.4220
D	 0.8870	 0.6130
E	 0.8650	 0.5910
F	 0.8470	 0.5930
G	 0.8050	 0.5790
H	 0.8450	 0.5980
I	 0.8630	 0.5960
J	 0.8080	 0.5760
K	 0.8250	 0.5830
L	 0.9390	 0.6410
M	 0.9360	 0.6360
N	 0.7930	 0.5680
O	 0.8140	 0.5780
P	 0.7860	 0.5730
Q	 0.8130	 0.5830
R	 0.7860	 0.5580
S	 0.7800	 0.5730
T	 0.7690	 0.5450
U	 0.7100	 0.5370
V	 0.6580	 0.4820
W	 0.5610	 0.4640
X	 0.8080	 0.5830



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Chain	Atom inclusion	Q-score
Y	 0.2150	 0.4160
Z	 0.2860	 0.3440
a	 0.8980	 0.6160
b	 0.8660	 0.6110
b0	 0.8710	 0.6100
b1	 0.2570	 0.3580
b8	 0.8950	 0.6080
b9	 0.9260	 0.6240
c	 0.4580	 0.4240
d	 0.8830	 0.6170
e	 0.8610	 0.5960
f	 0.8480	 0.5950
g	 0.8070	 0.5860
h	 0.8420	 0.5980
i	 0.8650	 0.6010
j	 0.8080	 0.5790
k	 0.8250	 0.5850
l	 0.9380	 0.6400
m	 0.9350	 0.6370
n	 0.7950	 0.5730
o	 0.8140	 0.5800
p	 0.7860	 0.5750
q	 0.8160	 0.5850
r	 0.7830	 0.5610
s	 0.7810	 0.5760
t	 0.7710	 0.5460
u	 0.7080	 0.5420
v	 0.6610	 0.4840
w	 0.5590	 0.4640
x	 0.8080	 0.5800
y	 0.2150	 0.4180
z	 0.2830	 0.3490