



## wwPDB EM Validation Summary Report ⓘ

Jun 11, 2024 – 04:10 PM JST

PDB ID : 7VA9  
EMDB ID : EMD-31835  
Title : Rba sphaeroides PufY-KO RC-LH1 dimer type-1  
Authors : Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.  
Deposited on : 2021-08-27  
Resolution : 3.08 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:

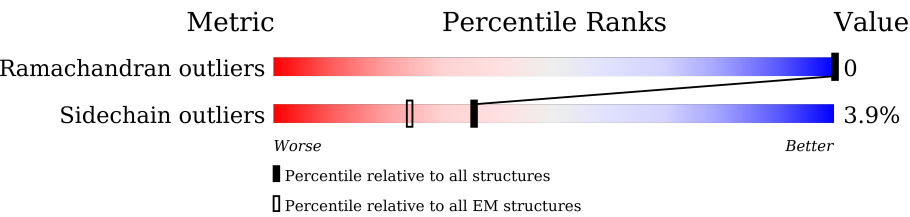
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.08 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.





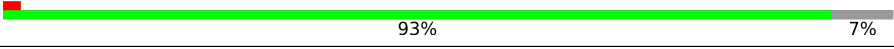
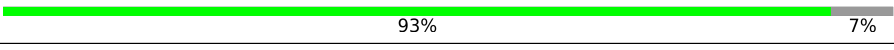
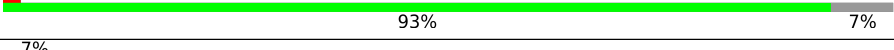
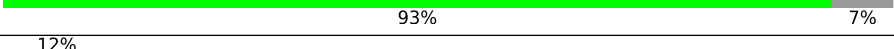
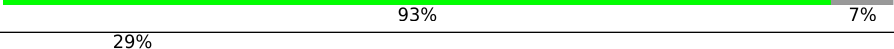
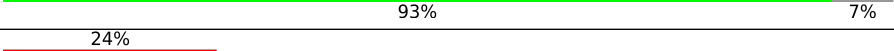
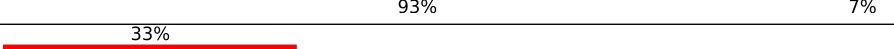
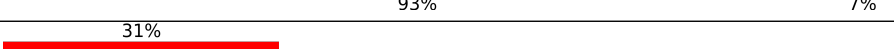
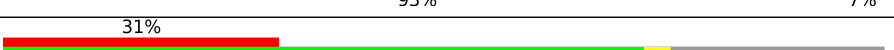


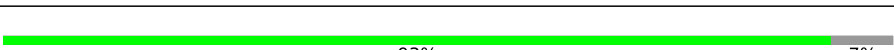
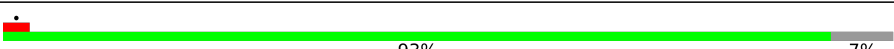
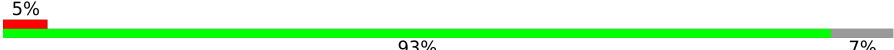

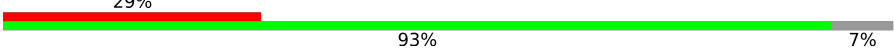
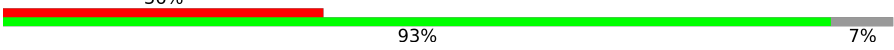

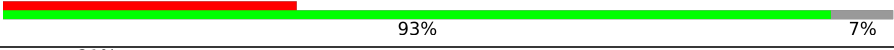
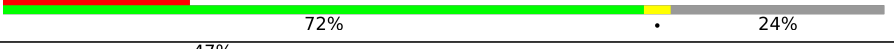



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	<div><div></div><div>98%</div><div></div></div>
1	l	282	<div><div></div><div>98%</div><div></div></div>
2	M	308	<div><div></div><div>97%</div><div></div></div>
2	m	308	<div><div></div><div>97%</div><div></div></div>
3	H	260	<div><div>8%</div><div>92%</div><div>6%</div></div>
3	h	260	<div><div>9%</div><div>92%</div><div>6%</div></div>
4	1	58	<div><div>74%</div><div>71%</div><div>26%</div></div>
4	3	58	<div><div></div><div>91%</div><div>7%</div></div>
4	5	58	<div><div>72%</div><div>71%</div><div>26%</div></div>

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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	Y	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	y	58	

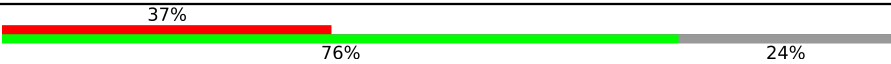

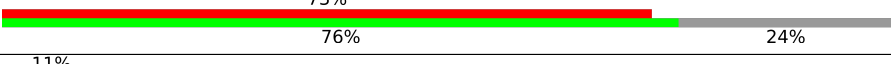
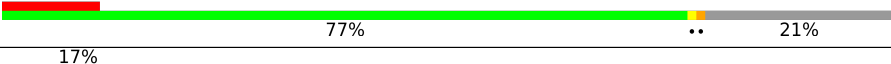

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Mol	Chain	Length	Quality of chain
5	0	49	
5	2	49	
5	4	49	
5	8	49	
5	B	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	
5	V	49	
5	X	49	
5	Z	49	
5	aa	49	
5	ab	49	
5	b	49	
5	e	49	
5	g	49	
5	j	49	
5	n	49	
5	p	49	
5	r	49	
5	t	49	

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Mol	Chain	Length	Quality of chain
5	v	49	
5	x	49	
5	z	49	
6	C	82	
6	c	82	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SPO	0	102	-	X	-	-
12	SPO	3	101	-	X	-	-
12	SPO	3	103	-	X	-	-
12	SPO	8	101	-	X	-	-
12	SPO	9	102	-	X	-	-
12	SPO	A	102	-	X	-	-
12	SPO	B	102	-	X	-	-
12	SPO	B	103	-	X	-	-
12	SPO	D	102	-	X	-	-
12	SPO	F	102	-	X	-	-
12	SPO	G	102	-	X	-	-
12	SPO	G	103	-	X	-	-
12	SPO	I	102	-	X	-	-
12	SPO	K	102	-	X	-	-
12	SPO	M	1305	-	X	-	-
12	SPO	N	101	-	X	-	-
12	SPO	N	103	-	X	-	-
12	SPO	O	102	-	X	-	-
12	SPO	O	103	-	X	-	-
12	SPO	Q	102	-	X	-	-
12	SPO	R	102	-	X	-	-
12	SPO	S	102	-	X	-	-
12	SPO	T	102	-	X	-	-
12	SPO	U	102	-	X	-	-
12	SPO	a	104	-	X	-	-
12	SPO	aa	101	-	X	-	-
12	SPO	ab	102	-	X	-	-
12	SPO	d	103	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	SPO	e	101	-	X	-	-
12	SPO	e	103	-	X	-	-
12	SPO	g	102	-	X	-	-
12	SPO	i	102	-	X	-	-
12	SPO	j	101	-	X	-	-
12	SPO	j	103	-	X	-	-
12	SPO	k	102	-	X	-	-
12	SPO	m	1305	-	X	-	-
12	SPO	n	101	-	X	-	-
12	SPO	o	102	-	X	-	-
12	SPO	q	102	-	X	-	-
12	SPO	r	102	-	X	-	-
12	SPO	s	102	-	X	-	-
12	SPO	s	104	-	X	-	-
12	SPO	s	105	-	X	-	-
12	SPO	t	101	-	X	-	-

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 42176 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	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		
2	m	305	Total	C	N	O	S	0	0
			2431	1623	397	400	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
			1972	1264	335	362	11		
3	h	260	Total	C	N	O	S	0	0
			1972	1264	335	362	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	D	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	F	54	Total	C	N	O	S	0	0
			455	310	73	69	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 455	C 310	N 73	O 69	S 3	0	0
4	O	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	Q	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	S	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	U	44	Total 362	C 244	N 60	O 57	S 1	0	0
4	W	43	Total 351	C 235	N 59	O 56	S 1	0	0
4	Y	43	Total 351	C 235	N 59	O 56	S 1	0	0
4	1	43	Total 351	C 235	N 59	O 56	S 1	0	0
4	7	46	Total 392	C 271	N 60	O 58	S 3	0	0
4	9	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	a	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	d	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	f	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	i	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	k	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	o	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	q	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	s	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	u	44	Total 362	C 244	N 60	O 57	S 1	0	0
4	w	43	Total 351	C 235	N 59	O 56	S 1	0	0
4	y	43	Total 351	C 235	N 59	O 56	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	43	Total	C	N	O	S	0	0
			351	235	59	56	1		
4	6	46	Total	C	N	O	S	0	0
			392	271	60	58	3		
4	3	54	Total	C	N	O	S	0	0
			455	310	73	69	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
			359	240	56	62	1		
5	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	G	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	N	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	P	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	R	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	T	38	Total	C	N	O	S	0	0
			316	213	50	52	1		
5	V	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	X	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	Z	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	2	36	Total	C	N	O	S	0	0
			297	198	48	50	1		
5	8	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	0	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	b	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	e	43	Total	C	N	O	S	0	0
			351	236	55	59	1		

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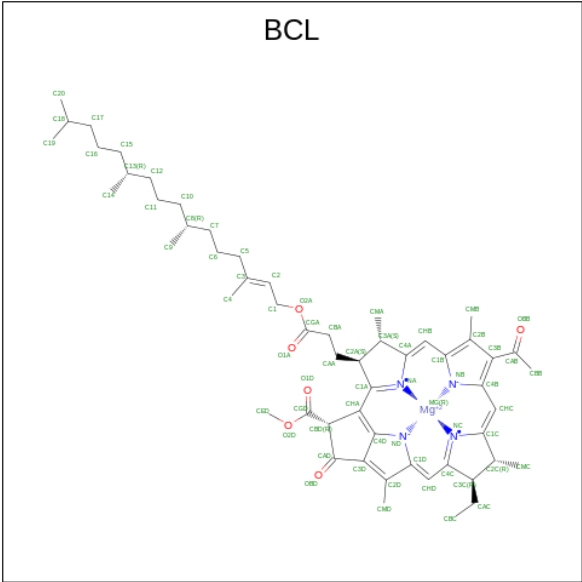
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	j	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
5	n	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	p	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	r	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	t	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	v	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	x	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	z	37	Total	C	N	O	S	0	0
			308	207	49	51	1		
5	4	36	Total	C	N	O	S	0	0
			297	198	48	50	1		
5	aa	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	ab	44	Total	C	N	O	S	0	0
			359	240	56	62	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	65	Total	C	N	O	S	0	0
			507	332	89	83	3		
6	c	65	Total	C	N	O	S	0	0
			507	332	89	83	3		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
7	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	S	1	Total 56	C 45	Mg 1	N 4	O 6	0
7	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	W	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	1	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	7	1	Total 61	C 50	Mg 1	N 4	O 6	0
7	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	0	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	l	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	m	1	Total 66	C 55	Mg 1	N 4	O 6	0

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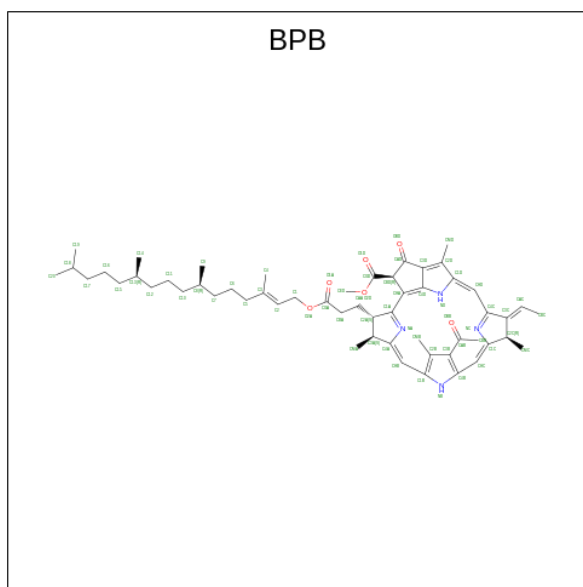
Mol	Chain	Residues	Atoms					AltConf
7	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	f	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	g	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	o	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	p	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	s	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	u	1	Total 51	C 40	Mg 1	N 4	O 6	0
7	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	w	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	x	1	Total 46	C 35	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
7	y	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	z	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
7	aa	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	ab	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	c	1	Total 61	C 50	Mg 1	N 4	O 6	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



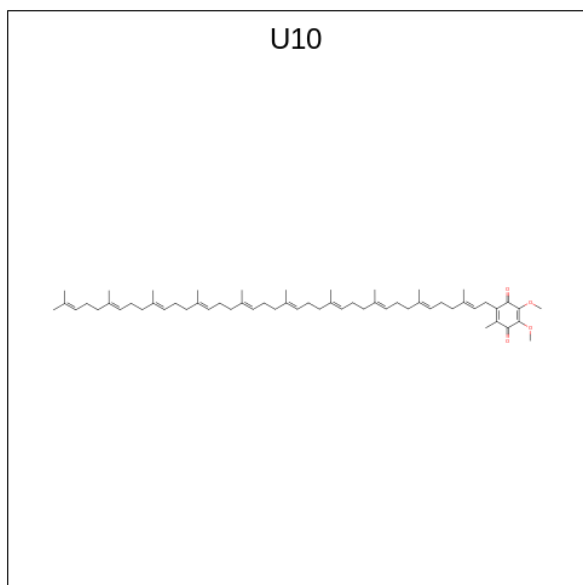
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total	C	N	O	0
			62	52	4	6	
8	L	1	Total	C	N	O	0
			55	45	4	6	
8	1	1	Total	C	N	O	0
			62	52	4	6	

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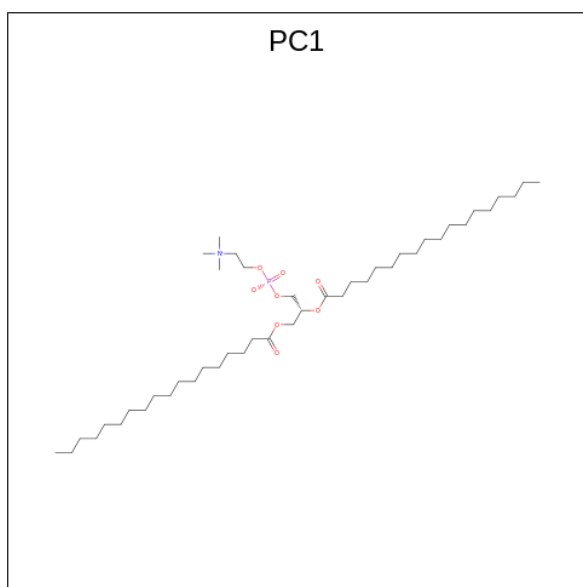
Mol	Chain	Residues	Atoms				AltConf
8	1	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			43	39	4	
9	M	1	Total	C	O	0
			48	44	4	
9	l	1	Total	C	O	0
			63	59	4	
9	m	1	Total	C	O	0
			48	44	4	

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).

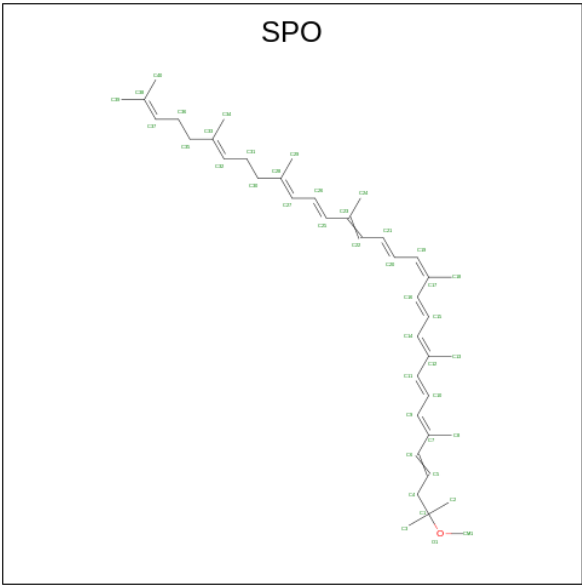


Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total	C	N	O	P	0
			43	33	1	8	1	
10	M	1	Total	C	N	O	P	0
			53	43	1	8	1	
10	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
10	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
10	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
10	l	1	Total	C	N	O	P	0
			48	38	1	8	1	
10	h	1	Total	C	N	O	P	0
			48	38	1	8	1	
10	h	1	Total	C	N	O	P	0
			29	19	1	8	1	
10	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
10	a	1	Total	C	N	O	P	0
			49	39	1	8	1	
10	d	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 11 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	M	1	Total	C	O	0
			42	41	1	
12	A	1	Total	C	O	0
			42	41	1	
12	B	1	Total	C	O	0
			42	41	1	
12	B	1	Total	C	O	0
			42	41	1	
12	D	1	Total	C	O	0
			42	41	1	
12	F	1	Total	C	O	0
			42	41	1	
12	G	1	Total	C	O	0
			42	41	1	
12	G	1	Total	C	O	0
			42	41	1	
12	I	1	Total	C	O	0
			42	41	1	

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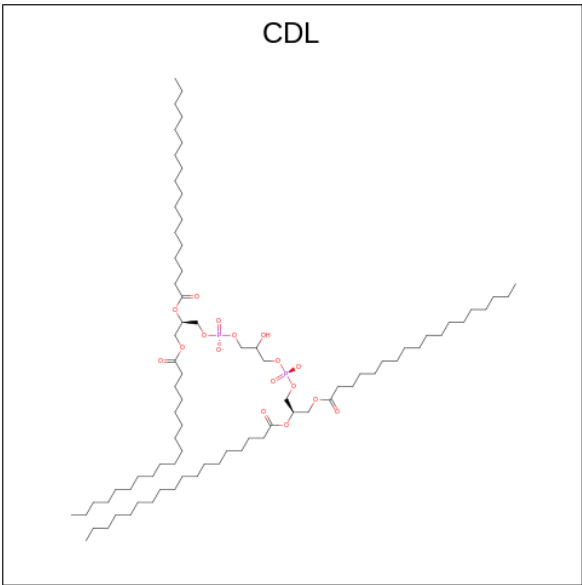
Mol	Chain	Residues	Atoms			AltConf
12	K	1	Total	C	O	0
			42	41	1	
12	N	1	Total	C	O	0
			42	41	1	
12	N	1	Total	C	O	0
			42	41	1	
12	O	1	Total	C	O	0
			42	41	1	
12	O	1	Total	C	O	0
			42	41	1	
12	Q	1	Total	C	O	0
			38	37	1	
12	R	1	Total	C	O	0
			42	41	1	
12	S	1	Total	C	O	0
			38	37	1	
12	T	1	Total	C	O	0
			42	41	1	
12	U	1	Total	C	O	0
			42	41	1	
12	8	1	Total	C	O	0
			42	41	1	
12	9	1	Total	C	O	0
			42	41	1	
12	0	1	Total	C	O	0
			42	41	1	
12	m	1	Total	C	O	0
			42	41	1	
12	a	1	Total	C	O	0
			42	41	1	
12	d	1	Total	C	O	0
			42	41	1	
12	e	1	Total	C	O	0
			42	41	1	
12	e	1	Total	C	O	0
			37	36	1	
12	g	1	Total	C	O	0
			42	41	1	
12	i	1	Total	C	O	0
			42	41	1	
12	j	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
12	j	1	Total	C	O	0
			42	41	1	
12	k	1	Total	C	O	0
			32	31	1	
12	n	1	Total	C	O	0
			42	41	1	
12	o	1	Total	C	O	0
			42	41	1	
12	q	1	Total	C	O	0
			42	41	1	
12	r	1	Total	C	O	0
			42	41	1	
12	s	1	Total	C	O	0
			42	41	1	
12	s	1	Total	C	O	0
			42	41	1	
12	s	1	Total	C	O	0
			42	41	1	
12	t	1	Total	C	O	0
			42	41	1	
12	aa	1	Total	C	O	0
			42	41	1	
12	3	1	Total	C	O	0
			42	41	1	
12	3	1	Total	C	O	0
			42	41	1	
12	ab	1	Total	C	O	0
			42	41	1	

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).

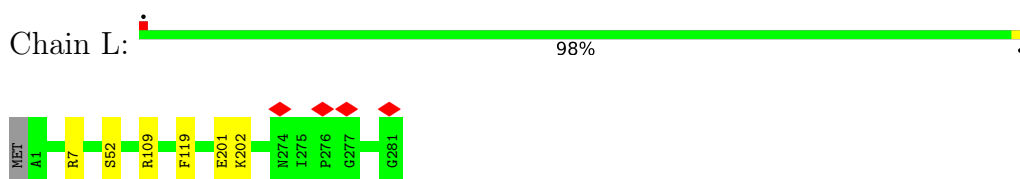


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	M	1	100	81	17	2	0
13	m	1	100	81	17	2	0

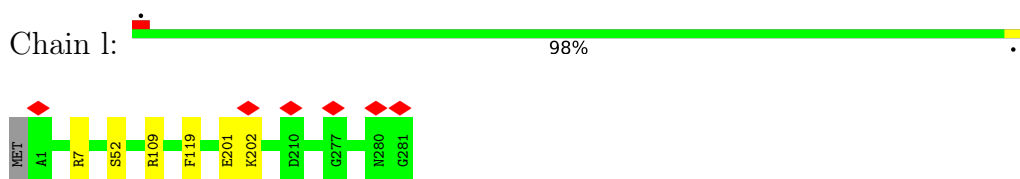
### 3 Residue-property plots [i](#)

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

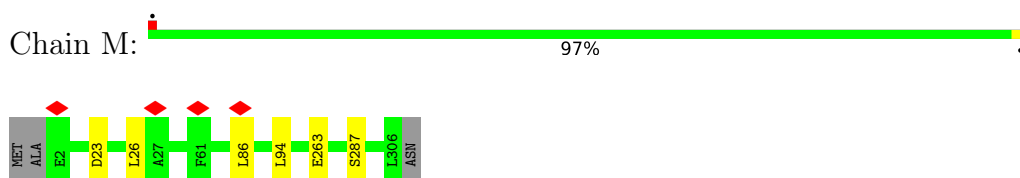
- Molecule 1: Reaction center protein L chain



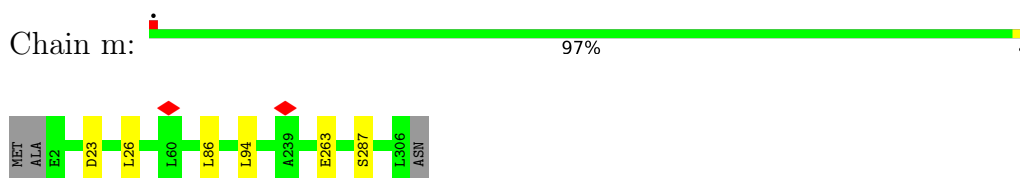
- Molecule 1: Reaction center protein L chain



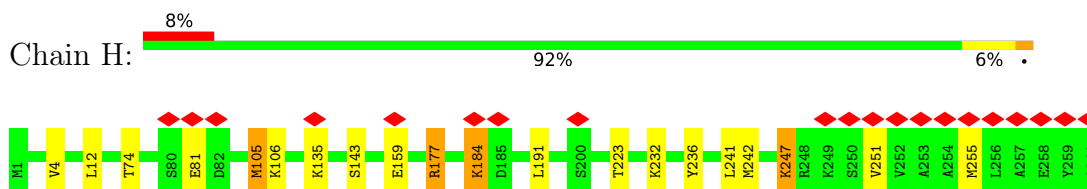
- Molecule 2: Reaction center protein M chain



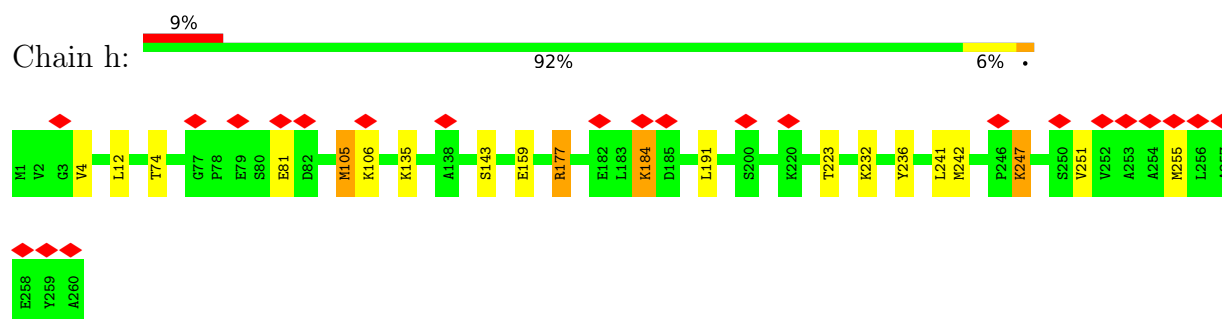
- Molecule 2: Reaction center protein M chain



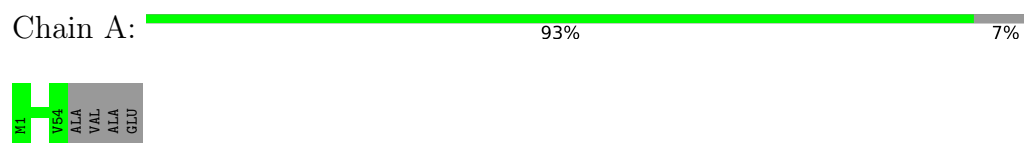
- Molecule 3: Reaction center protein H chain



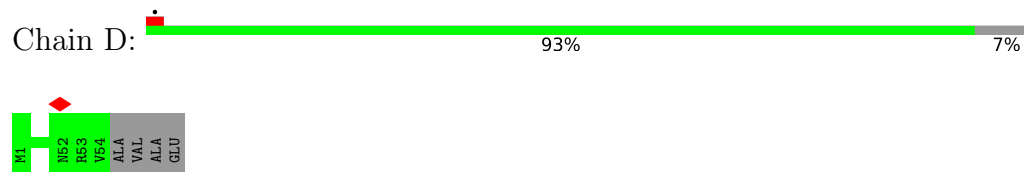
- Molecule 3: Reaction center protein H chain



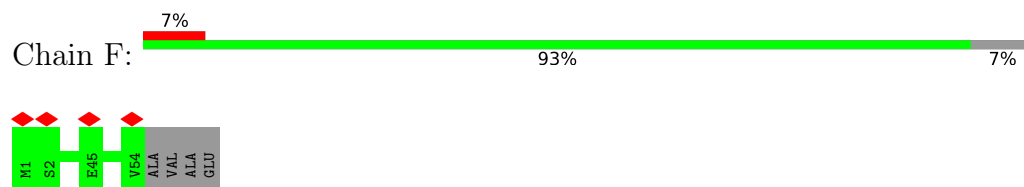
- Molecule 4: Light-harvesting protein B-875 alpha chain



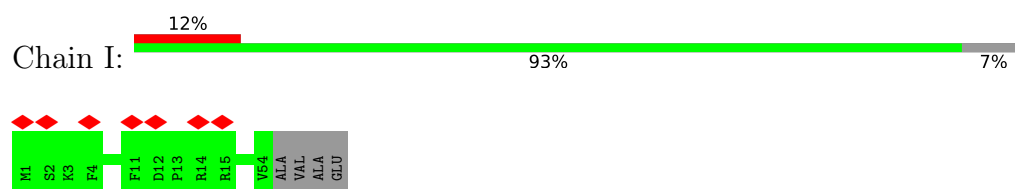
- Molecule 4: Light-harvesting protein B-875 alpha chain



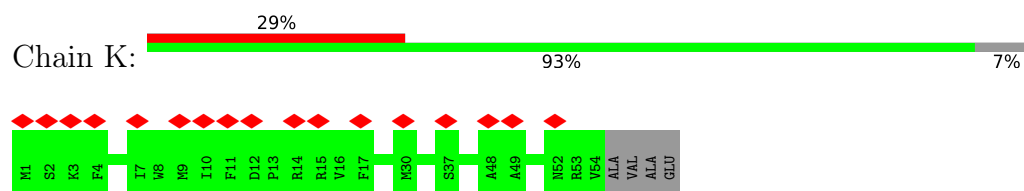
- Molecule 4: Light-harvesting protein B-875 alpha chain



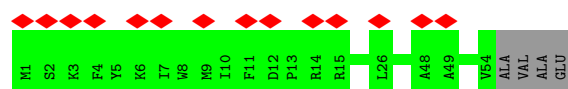
- Molecule 4: Light-harvesting protein B-875 alpha chain



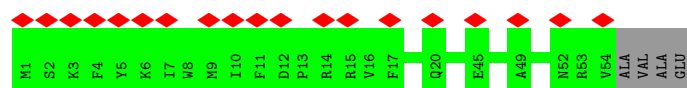
- Molecule 4: Light-harvesting protein B-875 alpha chain



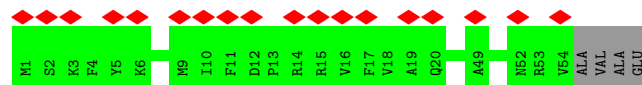
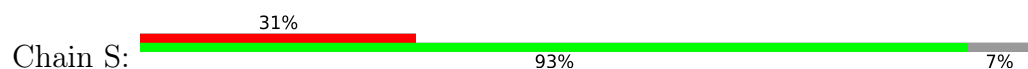
- Molecule 4: Light-harvesting protein B-875 alpha chain



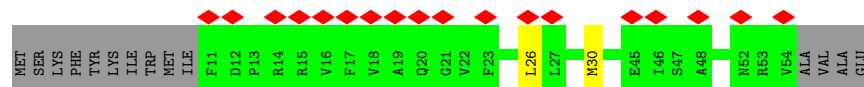
- Molecule 4: Light-harvesting protein B-875 alpha chain



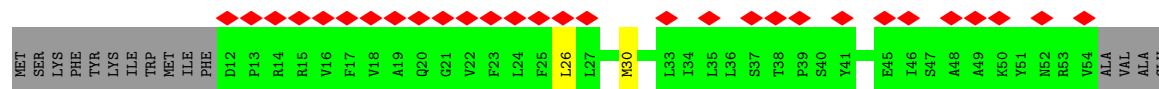
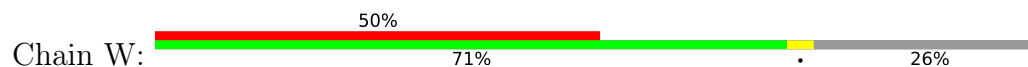
- Molecule 4: Light-harvesting protein B-875 alpha chain



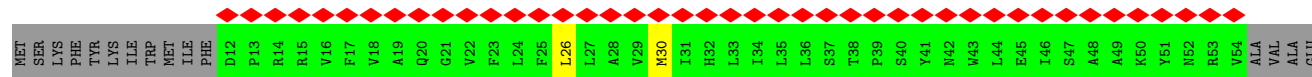
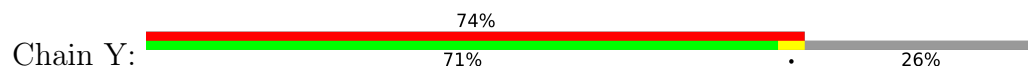
- Molecule 4: Light-harvesting protein B-875 alpha chain



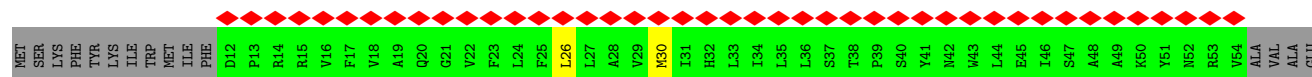
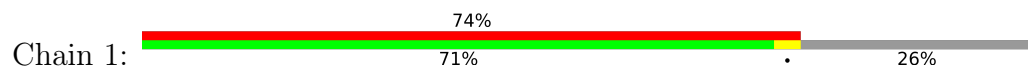
- Molecule 4: Light-harvesting protein B-875 alpha chain




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

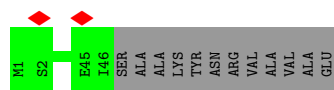


- Molecule 4: Light-harvesting protein B-875 alpha chain



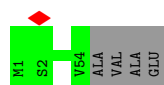
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 7:  79% 21%



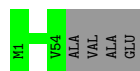
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain 9:  93% 7%



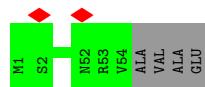
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain a:  93% 7%



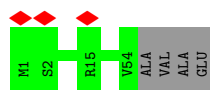
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain d:  93% 7%

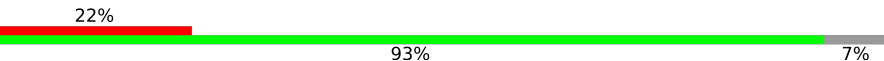


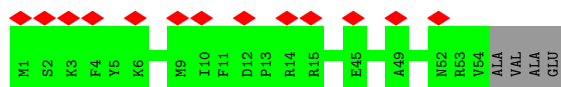
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain f:  5% 93% 7%

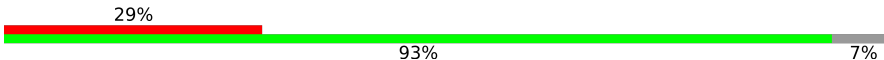


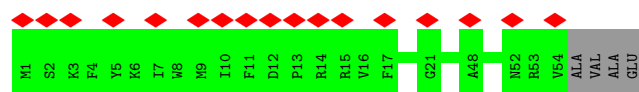
- Molecule 4: Light-harvesting protein B-875 alpha chain

Chain i:  22% 93% 7%

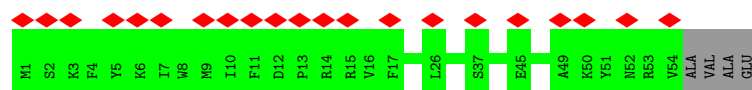


- Molecule 4: Light-harvesting protein B-875 alpha chain

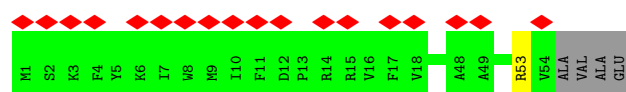
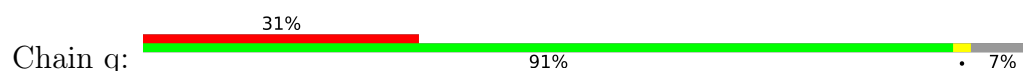
Chain k:  29% 93% 7%



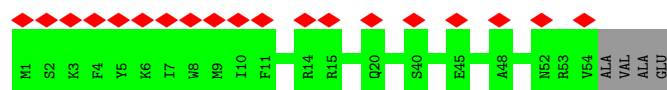
- Molecule 4: Light-harvesting protein B-875 alpha chain



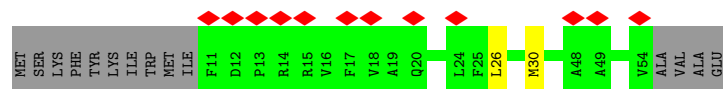
- Molecule 4: Light-harvesting protein B-875 alpha chain



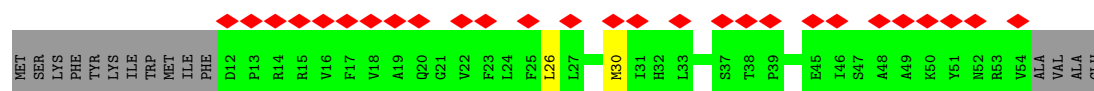
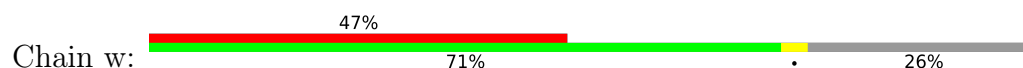
- Molecule 4: Light-harvesting protein B-875 alpha chain



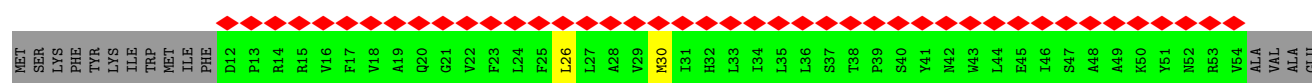
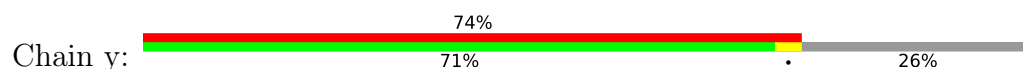
- Molecule 4: Light-harvesting protein B-875 alpha chain



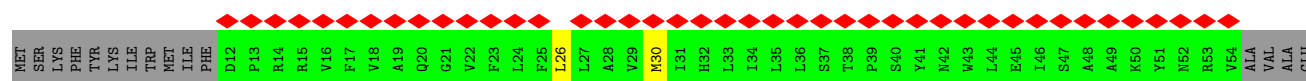
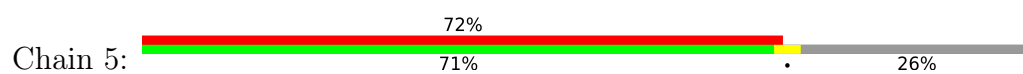
- Molecule 4: Light-harvesting protein B-875 alpha chain



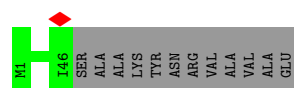
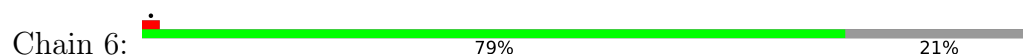
- Molecule 4: Light-harvesting protein B-875 alpha chain



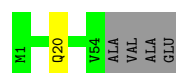
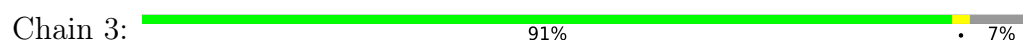
- Molecule 4: Light-harvesting protein B-875 alpha chain



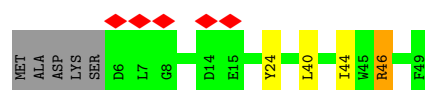
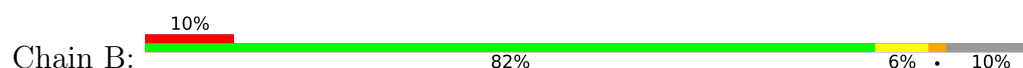
- Molecule 4: Light-harvesting protein B-875 alpha chain



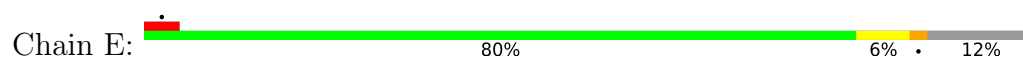
- Molecule 4: Light-harvesting protein B-875 alpha chain



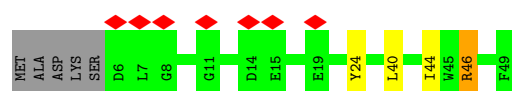
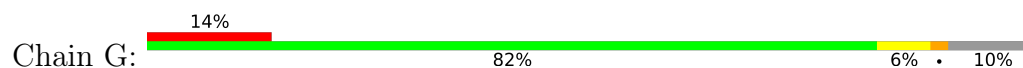
- Molecule 5: Light-harvesting protein B-875 beta chain



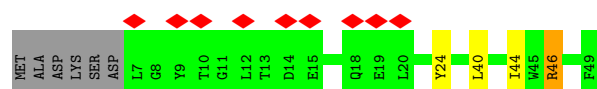
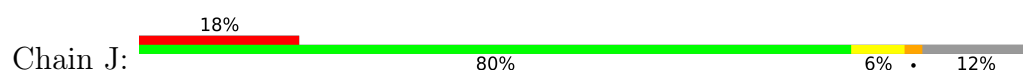
- Molecule 5: Light-harvesting protein B-875 beta chain



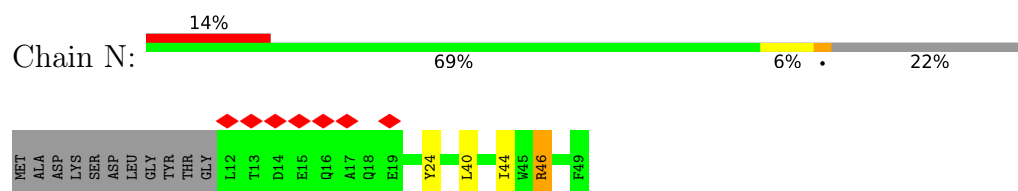
- Molecule 5: Light-harvesting protein B-875 beta chain



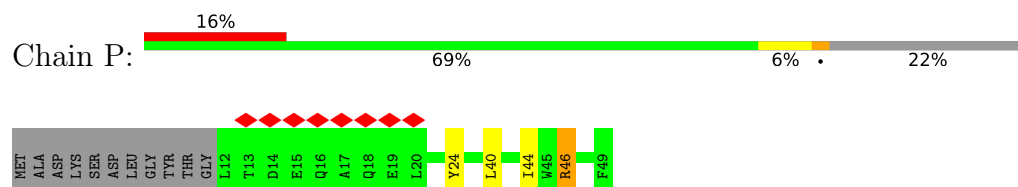
- Molecule 5: Light-harvesting protein B-875 beta chain



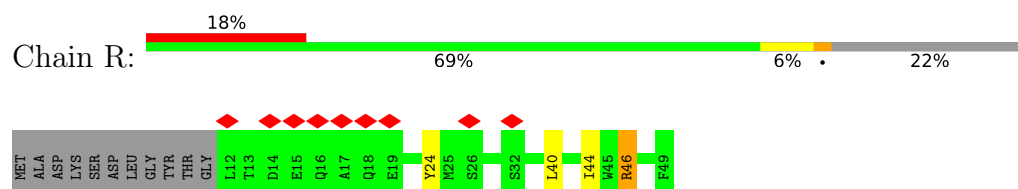
- Molecule 5: Light-harvesting protein B-875 beta chain



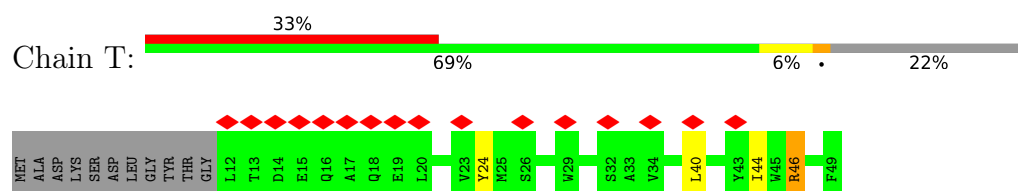
- Molecule 5: Light-harvesting protein B-875 beta chain



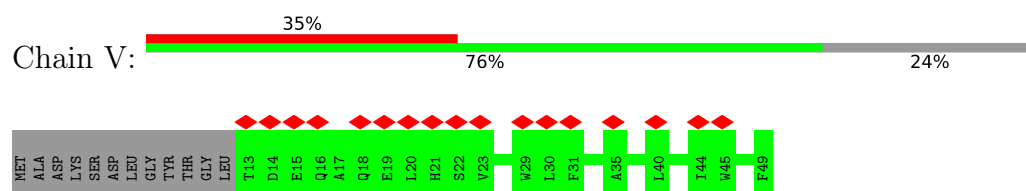
- Molecule 5: Light-harvesting protein B-875 beta chain



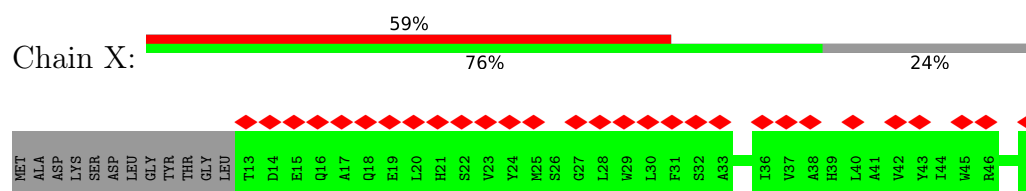
- Molecule 5: Light-harvesting protein B-875 beta chain



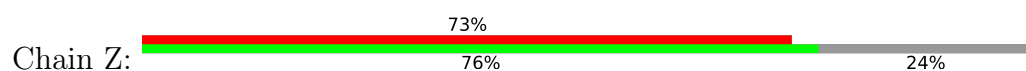
- Molecule 5: Light-harvesting protein B-875 beta chain

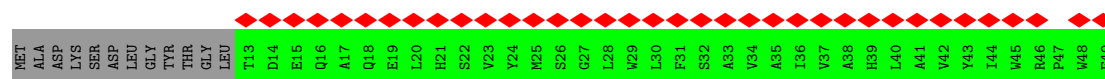


- Molecule 5: Light-harvesting protein B-875 beta chain

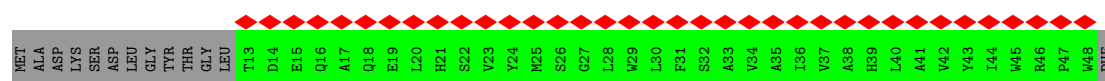


- Molecule 5: Light-harvesting protein B-875 beta chain

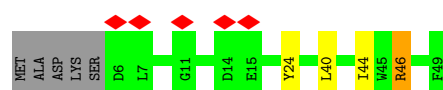
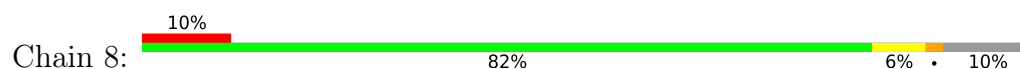




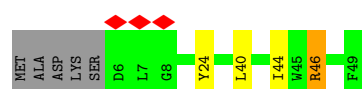
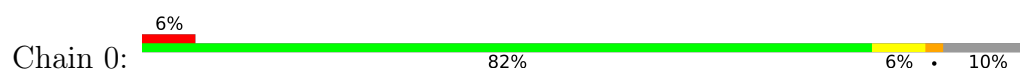
- Molecule 5: Light-harvesting protein B-875 beta chain



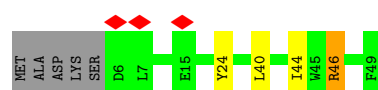
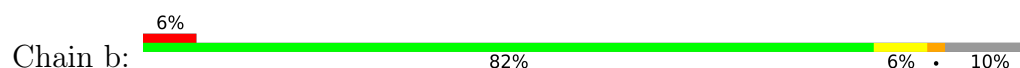
- Molecule 5: Light-harvesting protein B-875 beta chain



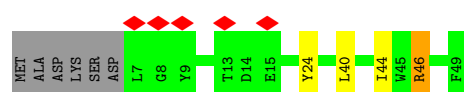
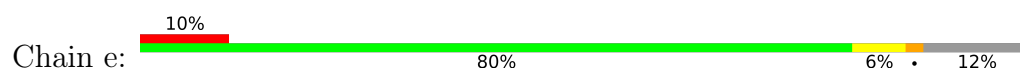
- Molecule 5: Light-harvesting protein B-875 beta chain



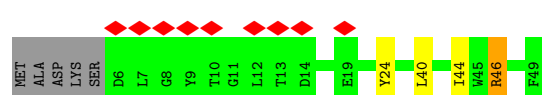
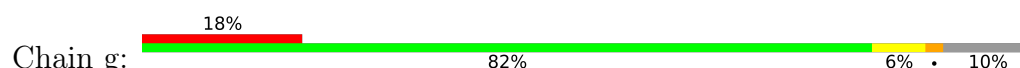
- Molecule 5: Light-harvesting protein B-875 beta chain



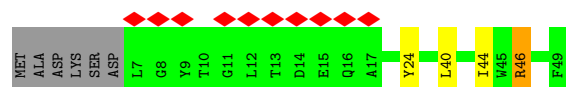
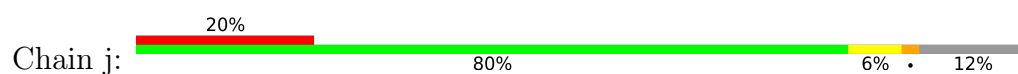
- Molecule 5: Light-harvesting protein B-875 beta chain



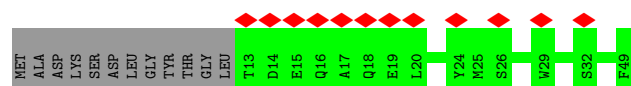
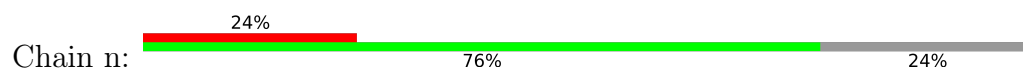
- Molecule 5: Light-harvesting protein B-875 beta chain



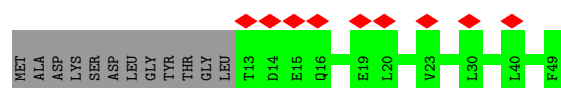
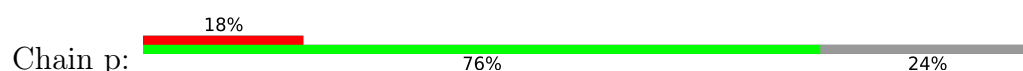
- Molecule 5: Light-harvesting protein B-875 beta chain



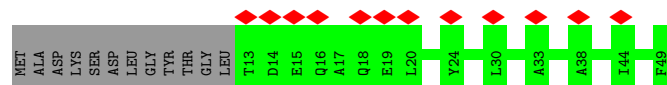
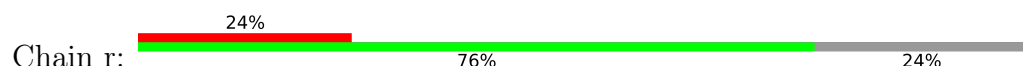
- Molecule 5: Light-harvesting protein B-875 beta chain



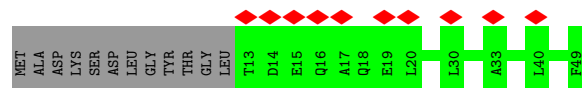
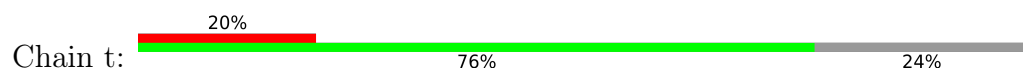
- Molecule 5: Light-harvesting protein B-875 beta chain



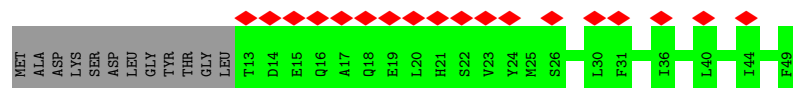
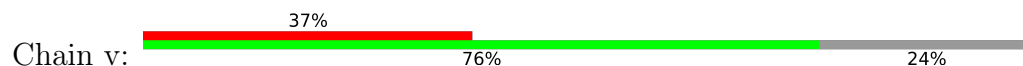
- Molecule 5: Light-harvesting protein B-875 beta chain



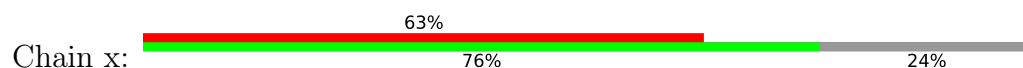
- Molecule 5: Light-harvesting protein B-875 beta chain

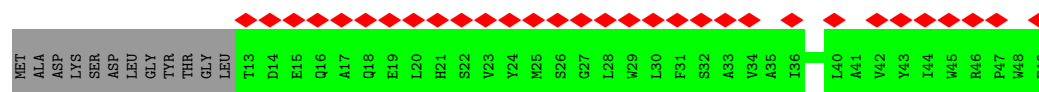


- Molecule 5: Light-harvesting protein B-875 beta chain

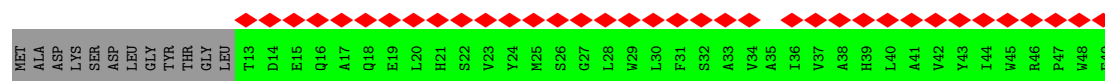
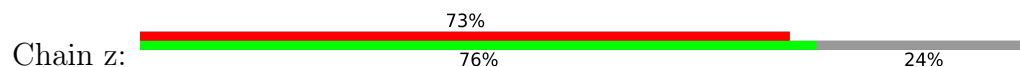


- Molecule 5: Light-harvesting protein B-875 beta chain

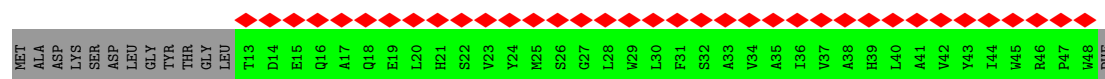




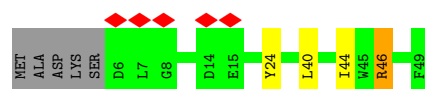
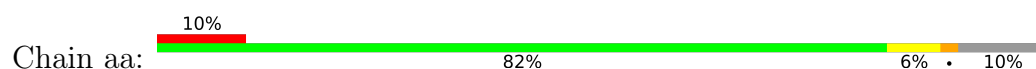
- Molecule 5: Light-harvesting protein B-875 beta chain



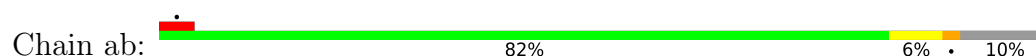
- Molecule 5: Light-harvesting protein B-875 beta chain



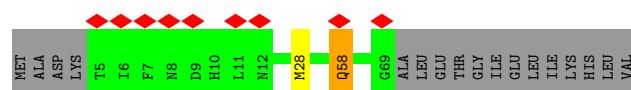
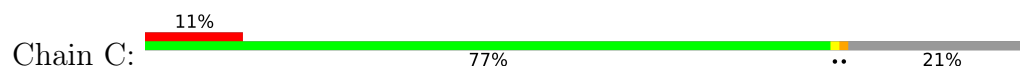
- Molecule 5: Light-harvesting protein B-875 beta chain



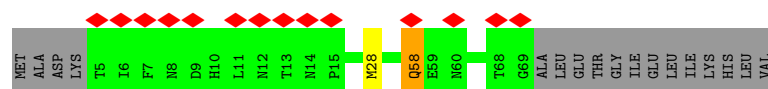
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 6: Intrinsic membrane protein PufX



- Molecule 6: Intrinsic membrane protein PufX



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71027	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.868	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0245	Depositor
Map size (Å)	289.97498, 289.97498, 289.97498	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8284999, 0.8284999, 0.8284999	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, SPO, FE2, U10, PC1, BPB, 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	0.40	0/2320	0.52	0/3175
1	l	0.40	0/2320	0.52	0/3175
2	M	0.37	0/2524	0.50	1/3446 (0.0%)
2	m	0.37	0/2524	0.50	1/3446 (0.0%)
3	H	0.41	0/2023	0.69	3/2752 (0.1%)
3	h	0.41	0/2023	0.69	3/2752 (0.1%)
4	1	0.31	0/360	0.48	0/490
4	3	0.41	0/469	0.48	0/635
4	5	0.32	0/360	0.48	0/490
4	6	0.38	0/405	0.47	0/549
4	7	0.47	0/405	0.57	0/549
4	9	0.40	0/469	0.49	0/635
4	A	0.36	0/469	0.44	0/635
4	D	0.35	0/469	0.47	0/635
4	F	0.36	0/469	0.46	0/635
4	I	0.36	0/469	0.50	0/635
4	K	0.36	0/469	0.48	0/635
4	O	0.37	0/469	0.47	0/635
4	Q	0.35	0/469	0.49	0/635
4	S	0.35	0/469	0.49	0/635
4	U	0.32	0/372	0.48	0/506
4	W	0.31	0/360	0.48	0/490
4	Y	0.32	0/360	0.48	0/490
4	a	0.42	0/469	0.50	0/635
4	d	0.37	0/469	0.48	0/635
4	f	0.36	0/469	0.49	0/635
4	i	0.35	0/469	0.48	0/635
4	k	0.38	0/469	0.50	0/635
4	o	0.37	0/469	0.51	0/635
4	q	0.37	0/469	0.48	0/635
4	s	0.39	0/469	0.49	0/635
4	u	0.32	0/372	0.48	0/506

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	w	0.32	0/360	0.48	0/490
4	y	0.32	0/360	0.48	0/490
5	0	0.38	0/372	0.65	1/510 (0.2%)
5	2	0.28	0/308	0.40	0/423
5	4	0.26	0/308	0.41	0/423
5	8	0.37	0/372	0.64	1/510 (0.2%)
5	B	0.37	0/372	0.62	1/510 (0.2%)
5	E	0.37	0/364	0.61	1/499 (0.2%)
5	G	0.36	0/372	0.60	1/510 (0.2%)
5	J	0.36	0/364	0.65	1/499 (0.2%)
5	N	0.37	0/328	0.61	1/450 (0.2%)
5	P	0.37	0/328	0.61	1/450 (0.2%)
5	R	0.37	0/328	0.62	1/450 (0.2%)
5	T	0.36	0/328	0.61	1/450 (0.2%)
5	V	0.27	0/320	0.36	0/439
5	X	0.25	0/320	0.36	0/439
5	Z	0.27	0/320	0.48	0/439
5	aa	0.37	0/372	0.61	1/510 (0.2%)
5	ab	0.37	0/372	0.61	1/510 (0.2%)
5	b	0.37	0/372	0.61	1/510 (0.2%)
5	e	0.37	0/364	0.61	1/499 (0.2%)
5	g	0.36	0/372	0.62	1/510 (0.2%)
5	j	0.36	0/364	0.63	1/499 (0.2%)
5	n	0.34	0/320	0.42	0/439
5	p	0.36	0/320	0.46	0/439
5	r	0.27	0/320	0.39	0/439
5	t	0.38	0/320	0.45	0/439
5	v	0.27	0/320	0.40	0/439
5	x	0.25	0/320	0.37	0/439
5	z	0.28	0/320	0.42	0/439
6	C	0.38	0/521	0.64	1/707 (0.1%)
6	c	0.38	0/521	0.64	1/707 (0.1%)
All	All	0.37	0/36492	0.54	26/49752 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	l	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	3
3	h	0	3
All	All	0	8

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	247	LYS	CD-CE-NZ	8.38	130.98	111.70
3	h	247	LYS	CD-CE-NZ	8.35	130.91	111.70
5	R	46	ARG	NE-CZ-NH1	-6.53	117.03	120.30
5	ab	46	ARG	NE-CZ-NH1	-6.53	117.03	120.30
5	G	46	ARG	NE-CZ-NH1	-6.50	117.05	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	105	MET	Peptide
3	H	106	LYS	Peptide
3	H	184	LYS	Peptide
1	L	201	GLU	Peptide
1	l	201	GLU	Peptide

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/282 (99%)	271 (97%)	8 (3%)	0	100	100
1	l	279/282 (99%)	271 (97%)	8 (3%)	0	100	100
2	M	303/308 (98%)	298 (98%)	5 (2%)	0	100	100
2	m	303/308 (98%)	298 (98%)	5 (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	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	3	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	5	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	6	44/58 (76%)	44 (100%)	0	0	100	100
4	7	44/58 (76%)	44 (100%)	0	0	100	100
4	9	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	A	52/58 (90%)	52 (100%)	0	0	100	100
4	D	52/58 (90%)	52 (100%)	0	0	100	100
4	F	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	I	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	K	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	O	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	Q	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	S	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	U	42/58 (72%)	41 (98%)	1 (2%)	0	100	100
4	W	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	Y	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	a	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	d	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	f	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	i	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	k	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	o	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	q	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	s	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
4	u	42/58 (72%)	41 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	w	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
4	y	41/58 (71%)	40 (98%)	1 (2%)	0	100	100
5	0	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	2	34/49 (69%)	34 (100%)	0	0	100	100
5	4	34/49 (69%)	34 (100%)	0	0	100	100
5	8	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	B	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	G	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	J	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	N	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	P	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	R	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	T	36/49 (74%)	35 (97%)	1 (3%)	0	100	100
5	V	35/49 (71%)	35 (100%)	0	0	100	100
5	X	35/49 (71%)	35 (100%)	0	0	100	100
5	Z	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	aa	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	ab	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	b	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
5	e	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	g	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
5	j	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	n	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	p	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	r	35/49 (71%)	35 (100%)	0	0	100	100
5	t	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
5	v	35/49 (71%)	35 (100%)	0	0	100	100
5	x	35/49 (71%)	35 (100%)	0	0	100	100
5	z	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
6	C	63/82 (77%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
All	All	4222/4860 (87%)	4126 (98%)	96 (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%)	215 (98%)	5 (2%)	50	75
1	l	220/221 (100%)	215 (98%)	5 (2%)	50	75
2	M	239/241 (99%)	234 (98%)	5 (2%)	53	77
2	m	239/241 (99%)	234 (98%)	5 (2%)	53	77
3	H	208/208 (100%)	190 (91%)	18 (9%)	10	35
3	h	208/208 (100%)	190 (91%)	18 (9%)	10	35
4	1	38/51 (74%)	36 (95%)	2 (5%)	22	53
4	3	49/51 (96%)	48 (98%)	1 (2%)	55	78
4	5	38/51 (74%)	36 (95%)	2 (5%)	22	53
4	6	43/51 (84%)	43 (100%)	0	100	100
4	7	43/51 (84%)	43 (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	49/51 (96%)	49 (100%)	0	100	100
4	O	49/51 (96%)	49 (100%)	0	100	100
4	Q	49/51 (96%)	49 (100%)	0	100	100
4	S	49/51 (96%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	U	39/51 (76%)	37 (95%)	2 (5%)	24	54
4	W	38/51 (74%)	36 (95%)	2 (5%)	22	53
4	Y	38/51 (74%)	36 (95%)	2 (5%)	22	53
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	49/51 (96%)	49 (100%)	0	100	100
4	o	49/51 (96%)	49 (100%)	0	100	100
4	q	49/51 (96%)	48 (98%)	1 (2%)	55	78
4	s	49/51 (96%)	49 (100%)	0	100	100
4	u	39/51 (76%)	37 (95%)	2 (5%)	24	54
4	w	38/51 (74%)	36 (95%)	2 (5%)	22	53
4	y	38/51 (74%)	36 (95%)	2 (5%)	22	53
5	0	36/40 (90%)	32 (89%)	4 (11%)	6	23
5	2	30/40 (75%)	30 (100%)	0	100	100
5	4	30/40 (75%)	30 (100%)	0	100	100
5	8	36/40 (90%)	32 (89%)	4 (11%)	6	23
5	B	36/40 (90%)	32 (89%)	4 (11%)	6	23
5	E	35/40 (88%)	31 (89%)	4 (11%)	5	22
5	G	36/40 (90%)	32 (89%)	4 (11%)	6	23
5	J	35/40 (88%)	31 (89%)	4 (11%)	5	22
5	N	32/40 (80%)	28 (88%)	4 (12%)	4	17
5	P	32/40 (80%)	28 (88%)	4 (12%)	4	17
5	R	32/40 (80%)	28 (88%)	4 (12%)	4	17
5	T	32/40 (80%)	28 (88%)	4 (12%)	4	17
5	V	31/40 (78%)	31 (100%)	0	100	100
5	X	31/40 (78%)	31 (100%)	0	100	100
5	Z	31/40 (78%)	31 (100%)	0	100	100
5	aa	36/40 (90%)	32 (89%)	4 (11%)	6	23
5	ab	36/40 (90%)	32 (89%)	4 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	b	36/40 (90%)	32 (89%)	4 (11%)	6	23
5	e	35/40 (88%)	31 (89%)	4 (11%)	5	22
5	g	36/40 (90%)	32 (89%)	4 (11%)	6	23
5	j	35/40 (88%)	31 (89%)	4 (11%)	5	22
5	n	31/40 (78%)	31 (100%)	0	100	100
5	p	31/40 (78%)	31 (100%)	0	100	100
5	r	31/40 (78%)	31 (100%)	0	100	100
5	t	31/40 (78%)	31 (100%)	0	100	100
5	v	31/40 (78%)	31 (100%)	0	100	100
5	x	31/40 (78%)	31 (100%)	0	100	100
5	z	31/40 (78%)	31 (100%)	0	100	100
6	C	52/66 (79%)	50 (96%)	2 (4%)	33	64
6	c	52/66 (79%)	50 (96%)	2 (4%)	33	64
All	All	3638/4020 (90%)	3496 (96%)	142 (4%)	36	64

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	g	40	LEU
5	j	40	LEU
4	5	30	MET
5	P	24	TYR
5	N	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
6	c	66	ASN
6	c	58	GLN
5	b	21	HIS
1	l	280	ASN
5	t	18	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 131 ligands modelled in this entry, 2 are monoatomic - leaving 129 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$
12	SPO	aa	101	-	40,41,41	5.16	17 (42%)	47,50,50	6.05	34 (72%)
12	SPO	g	102	-	40,41,41	5.62	17 (42%)	47,50,50	5.61	29 (61%)
7	BCL	R	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.59	12 (15%)
7	BCL	ab	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	13 (16%)
10	PC1	h	301	-	47,47,53	1.13	3 (6%)	53,55,61	1.10	4 (7%)
7	BCL	D	101	-	64,74,74	1.24	7 (10%)	78,115,115	1.58	11 (14%)
12	SPO	I	102	-	40,41,41	5.74	17 (42%)	47,50,50	5.27	28 (59%)
9	U10	M	1304	-	48,48,63	2.67	14 (29%)	58,61,79	1.65	13 (22%)
7	BCL	s	101	-	64,74,74	1.23	5 (7%)	78,115,115	1.58	11 (14%)
10	PC1	C	1201	-	53,53,53	1.12	3 (5%)	59,61,61	0.94	3 (5%)
7	BCL	O	101	-	64,74,74	1.25	7 (10%)	78,115,115	1.56	11 (14%)
7	BCL	x	101	-	44,54,74	1.45	4 (9%)	54,91,115	1.58	8 (14%)
7	BCL	8	102	-	64,74,74	1.21	5 (7%)	78,115,115	1.59	12 (15%)
12	SPO	0	102	-	40,41,41	5.47	17 (42%)	47,50,50	5.63	31 (65%)
12	SPO	i	102	-	40,41,41	5.41	17 (42%)	47,50,50	6.23	27 (57%)
7	BCL	5	102	-	44,54,74	1.41	5 (11%)	54,91,115	1.66	12 (22%)
7	BCL	o	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.54	10 (12%)
7	BCL	y	101	-	44,54,74	1.44	5 (11%)	54,91,115	1.81	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	SPO	d	103	-	40,41,41	5.24	15 (37%)	47,50,50	6.17	31 (65%)
7	BCL	d	101	-	64,74,74	1.26	7 (10%)	78,115,115	1.60	11 (14%)
7	BCL	E	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	13 (16%)
8	BPB	L	305	-	39,60,70	1.74	4 (10%)	35,89,101	1.41	6 (17%)
7	BCL	s	103	-	44,54,74	1.45	5 (11%)	54,91,115	1.77	10 (18%)
12	SPO	3	101	-	40,41,41	5.70	17 (42%)	47,50,50	5.26	30 (63%)
7	BCL	U	103	-	44,54,74	1.40	5 (11%)	54,91,115	1.85	11 (20%)
12	SPO	e	103	-	35,36,41	5.52	16 (45%)	41,44,50	6.71	29 (70%)
7	BCL	u	101	-	49,59,74	1.40	5 (10%)	60,97,115	1.86	12 (20%)
7	BCL	l	101	-	44,54,74	1.36	5 (11%)	54,91,115	2.11	14 (25%)
10	PC1	h	302	-	28,28,53	1.55	5 (17%)	34,36,61	1.30	3 (8%)
7	BCL	e	102	-	64,74,74	1.21	5 (7%)	78,115,115	1.59	12 (15%)
7	BCL	5	101	-	44,54,74	1.45	5 (11%)	54,91,115	1.80	10 (18%)
12	SPO	B	103	-	40,41,41	5.56	17 (42%)	47,50,50	5.45	30 (63%)
7	BCL	7	101	-	59,69,74	1.26	6 (10%)	72,109,115	1.76	11 (15%)
12	SPO	S	102	-	36,37,41	5.85	16 (44%)	42,45,50	5.60	26 (61%)
12	SPO	q	102	-	40,41,41	5.72	17 (42%)	47,50,50	5.26	29 (61%)
12	SPO	k	102	-	30,31,41	5.01	15 (50%)	36,38,50	6.44	28 (77%)
7	BCL	I	101	-	64,74,74	1.23	7 (10%)	78,115,115	1.58	11 (14%)
12	SPO	r	102	-	40,41,41	5.61	17 (42%)	47,50,50	5.59	32 (68%)
13	CDL	M	1306	-	99,99,99	1.07	7 (7%)	105,111,111	0.95	5 (4%)
9	U10	m	1304	-	48,48,63	2.67	14 (29%)	58,61,79	1.65	13 (22%)
12	SPO	8	101	-	40,41,41	5.16	16 (40%)	47,50,50	5.96	34 (72%)
12	SPO	O	103	-	40,41,41	5.72	17 (42%)	47,50,50	5.46	31 (65%)
7	BCL	a	101	-	64,74,74	1.25	8 (12%)	78,115,115	1.57	11 (14%)
12	SPO	R	102	-	40,41,41	5.69	17 (42%)	47,50,50	5.24	32 (68%)
7	BCL	w	101	-	44,54,74	1.44	4 (9%)	54,91,115	1.80	11 (20%)
12	SPO	ab	102	-	40,41,41	5.56	17 (42%)	47,50,50	5.93	32 (68%)
10	PC1	a	103	-	48,48,53	1.14	3 (6%)	54,56,61	1.12	5 (9%)
7	BCL	G	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	12 (15%)
12	SPO	D	102	-	40,41,41	5.70	17 (42%)	47,50,50	5.25	29 (61%)
12	SPO	Q	102	-	36,37,41	5.84	16 (44%)	42,45,50	5.53	26 (61%)
7	BCL	B	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	12 (15%)
7	BCL	U	101	-	64,74,74	1.24	5 (7%)	78,115,115	1.63	13 (16%)
12	SPO	U	102	-	40,41,41	5.54	17 (42%)	47,50,50	5.53	31 (65%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCL	L	304	-	64,74,74	1.26	7 (10%)	78,115,115	1.59	12 (15%)
7	BCL	P	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	12 (15%)
10	PC1	l	304	-	47,47,53	1.17	3 (6%)	53,55,61	0.96	3 (5%)
7	BCL	k	103	-	64,74,74	1.23	5 (7%)	78,115,115	1.74	16 (20%)
12	SPO	T	102	-	40,41,41	5.66	17 (42%)	47,50,50	5.52	31 (65%)
7	BCL	m	1303	-	64,74,74	1.24	7 (10%)	78,115,115	1.58	10 (12%)
12	SPO	9	102	-	40,41,41	5.69	17 (42%)	47,50,50	5.19	27 (57%)
12	SPO	G	103	-	40,41,41	5.61	17 (42%)	47,50,50	5.53	32 (68%)
7	BCL	K	101	-	64,74,74	1.22	7 (10%)	78,115,115	1.56	11 (14%)
7	BCL	M	1301	-	64,74,74	1.25	7 (10%)	78,115,115	1.76	14 (17%)
12	SPO	t	101	-	40,41,41	5.26	17 (42%)	47,50,50	5.96	31 (65%)
7	BCL	Y	201	-	44,54,74	1.44	5 (11%)	54,91,115	1.80	11 (20%)
7	BCL	T	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.58	12 (15%)
10	PC1	a	102	-	39,39,53	1.23	3 (7%)	45,47,61	1.03	3 (6%)
9	U10	L	303	-	43,43,63	2.70	13 (30%)	52,55,79	1.66	13 (25%)
7	BCL	S	101	-	54,64,74	1.36	7 (12%)	66,103,115	1.65	10 (15%)
12	SPO	o	102	-	40,41,41	5.72	17 (42%)	47,50,50	5.30	28 (59%)
7	BCL	Z	101	-	44,54,74	1.43	5 (11%)	54,91,115	1.56	7 (12%)
12	SPO	F	102	-	40,41,41	5.67	17 (42%)	47,50,50	5.21	29 (61%)
12	SPO	K	102	-	40,41,41	5.74	17 (42%)	47,50,50	5.26	28 (59%)
7	BCL	W	101	-	44,54,74	1.45	5 (11%)	54,91,115	1.80	11 (20%)
7	BCL	c	101	-	59,69,74	1.32	7 (11%)	72,109,115	1.81	14 (19%)
12	SPO	j	103	-	40,41,41	5.60	17 (42%)	47,50,50	5.68	32 (68%)
12	SPO	m	1305	-	40,41,41	5.60	17 (42%)	47,50,50	5.30	31 (65%)
7	BCL	F	101	-	64,74,74	1.23	7 (10%)	78,115,115	1.61	14 (17%)
12	SPO	O	102	-	40,41,41	5.53	17 (42%)	47,50,50	5.69	33 (70%)
7	BCL	N	102	-	64,74,74	1.21	5 (7%)	78,115,115	1.59	13 (16%)
7	BCL	2	101	-	44,54,74	1.44	5 (11%)	54,91,115	1.81	11 (20%)
8	BPB	L	302	-	46,67,70	1.54	3 (6%)	43,97,101	1.68	8 (18%)
7	BCL	Q	101	-	64,74,74	1.26	7 (10%)	78,115,115	1.58	12 (15%)
7	BCL	q	101	-	64,74,74	1.18	5 (7%)	78,115,115	1.63	11 (14%)
12	SPO	n	101	-	40,41,41	5.72	17 (42%)	47,50,50	5.53	30 (63%)
7	BCL	aa	102	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	12 (15%)
7	BCL	3	102	-	64,74,74	1.23	7 (10%)	78,115,115	1.62	10 (12%)
8	BPB	l	302	-	46,67,70	1.54	3 (6%)	43,97,101	1.68	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	SPO	e	101	-	40,41,41	5.69	17 (42%)	47,50,50	5.24	29 (61%)
12	SPO	s	105	-	40,41,41	5.76	17 (42%)	47,50,50	5.41	30 (63%)
7	BCL	v	101	-	64,74,74	1.23	4 (6%)	78,115,115	1.58	14 (17%)
12	SPO	a	104	-	40,41,41	5.51	17 (42%)	47,50,50	5.69	31 (65%)
7	BCL	X	101	-	44,54,74	1.42	5 (11%)	54,91,115	1.72	9 (16%)
12	SPO	s	104	-	40,41,41	5.69	17 (42%)	47,50,50	5.30	29 (61%)
12	SPO	N	103	-	40,41,41	5.63	17 (42%)	47,50,50	5.86	30 (63%)
12	SPO	G	102	-	40,41,41	5.57	17 (42%)	47,50,50	5.91	31 (65%)
7	BCL	r	101	-	64,74,74	1.20	6 (9%)	78,115,115	1.51	11 (14%)
7	BCL	j	102	-	64,74,74	1.21	5 (7%)	78,115,115	1.59	13 (16%)
7	BCL	J	101	-	64,74,74	1.22	5 (7%)	78,115,115	1.59	12 (15%)
12	SPO	3	103	-	40,41,41	5.60	17 (42%)	47,50,50	5.46	31 (65%)
7	BCL	A	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.55	11 (14%)
12	SPO	j	101	-	40,41,41	5.70	17 (42%)	47,50,50	5.18	28 (59%)
12	SPO	M	1305	-	40,41,41	5.60	17 (42%)	47,50,50	5.30	31 (65%)
10	PC1	A	103	-	50,50,53	1.09	3 (6%)	56,58,61	0.97	3 (5%)
7	BCL	i	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.63	10 (12%)
12	SPO	s	102	-	40,41,41	5.72	17 (42%)	47,50,50	5.24	29 (61%)
7	BCL	z	101	-	44,54,74	1.52	5 (11%)	54,91,115	1.75	11 (20%)
10	PC1	d	102	-	40,40,53	1.17	3 (7%)	46,48,61	1.14	4 (8%)
7	BCL	9	101	-	64,74,74	1.26	8 (12%)	78,115,115	1.67	12 (15%)
7	BCL	b	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.59	13 (16%)
7	BCL	p	101	-	64,74,74	1.21	6 (9%)	78,115,115	1.66	14 (17%)
12	SPO	A	102	-	40,41,41	5.68	17 (42%)	47,50,50	5.26	29 (61%)
8	BPB	l	306	-	39,60,70	1.74	4 (10%)	35,89,101	1.41	6 (17%)
7	BCL	M	1303	-	64,74,74	1.23	7 (10%)	78,115,115	1.58	10 (12%)
12	SPO	N	101	-	40,41,41	5.74	17 (42%)	47,50,50	5.24	28 (59%)
7	BCL	f	101	-	64,74,74	1.26	7 (10%)	78,115,115	1.57	11 (14%)
7	BCL	l	305	-	64,74,74	1.26	7 (10%)	78,115,115	1.59	11 (14%)
10	PC1	L	306	-	42,42,53	1.14	2 (4%)	48,50,61	1.01	2 (4%)
12	SPO	B	102	-	40,41,41	5.60	17 (42%)	47,50,50	5.60	32 (68%)
7	BCL	l	301	-	64,74,74	1.24	7 (10%)	78,115,115	1.53	10 (12%)
7	BCL	g	101	-	64,74,74	1.22	6 (9%)	78,115,115	1.59	12 (15%)
9	U10	l	303	-	63,63,63	2.71	17 (26%)	76,79,79	1.73	21 (27%)
7	BCL	0	101	-	64,74,74	1.21	5 (7%)	78,115,115	1.59	13 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCL	m	1301	-	64,74,74	1.25	7 (10%)	78,115,115	1.75	14 (17%)
10	PC1	M	1307	-	52,52,53	1.08	3 (5%)	58,60,61	1.12	4 (6%)
10	PC1	A	104	-	45,45,53	1.10	3 (6%)	51,53,61	1.03	4 (7%)
7	BCL	k	101	-	64,74,74	1.24	6 (9%)	78,115,115	1.65	11 (14%)
13	CDL	m	1306	-	99,99,99	1.07	7 (7%)	105,111,111	0.95	5 (4%)
7	BCL	L	301	-	64,74,74	1.24	7 (10%)	78,115,115	1.54	10 (12%)

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
12	SPO	aa	101	-	-	16/47/47/47	-
12	SPO	g	102	-	-	27/47/47/47	-
7	BCL	R	101	-	-	4/37/137/137	-
7	BCL	ab	101	-	-	4/37/137/137	-
10	PC1	h	301	-	-	23/51/51/57	-
7	BCL	D	101	-	-	7/37/137/137	-
12	SPO	I	102	-	-	23/47/47/47	-
9	U10	M	1304	-	-	5/45/69/87	0/1/1/1
7	BCL	s	101	-	-	4/37/137/137	-
10	PC1	C	1201	-	-	25/57/57/57	-
7	BCL	O	101	-	-	6/37/137/137	-
7	BCL	x	101	-	-	4/13/113/137	-
7	BCL	8	102	-	-	4/37/137/137	-
12	SPO	0	102	-	-	16/47/47/47	-
12	SPO	i	102	-	-	18/47/47/47	-
7	BCL	5	102	-	-	8/13/113/137	-
7	BCL	o	101	-	-	9/37/137/137	-
7	BCL	y	101	-	-	0/13/113/137	-
12	SPO	d	103	-	-	22/47/47/47	-
7	BCL	d	101	-	-	8/37/137/137	-
7	BCL	E	101	-	-	4/37/137/137	-
8	BPB	L	305	-	-	7/25/93/105	0/5/6/6
7	BCL	s	103	-	-	3/13/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SPO	3	101	-	-	25/47/47/47	-
7	BCL	U	103	-	-	5/13/113/137	-
12	SPO	e	103	-	-	18/41/41/47	-
7	BCL	u	101	-	-	1/19/119/137	-
7	BCL	l	101	-	-	6/13/113/137	-
10	PC1	h	302	-	-	14/32/32/57	-
7	BCL	e	102	-	-	4/37/137/137	-
7	BCL	5	101	-	-	0/13/113/137	-
12	SPO	B	103	-	-	23/47/47/47	-
7	BCL	7	101	-	-	6/31/131/137	-
12	SPO	S	102	-	-	21/43/43/47	-
12	SPO	q	102	-	-	23/47/47/47	-
12	SPO	k	102	-	-	18/35/35/47	-
7	BCL	I	101	-	-	3/37/137/137	-
12	SPO	r	102	-	-	20/47/47/47	-
13	CDL	M	1306	-	-	44/110/110/110	-
9	U10	m	1304	-	-	5/45/69/87	0/1/1/1
12	SPO	8	101	-	-	18/47/47/47	-
12	SPO	O	103	-	-	26/47/47/47	-
7	BCL	a	101	-	-	7/37/137/137	-
12	SPO	R	102	-	-	21/47/47/47	-
7	BCL	w	101	-	-	0/13/113/137	-
12	SPO	ab	102	-	-	22/47/47/47	-
10	PC1	a	103	-	-	26/52/52/57	-
7	BCL	G	101	-	-	4/37/137/137	-
12	SPO	D	102	-	-	23/47/47/47	-
12	SPO	Q	102	-	-	21/43/43/47	-
7	BCL	B	101	-	-	4/37/137/137	-
7	BCL	U	101	-	-	2/37/137/137	-
12	SPO	U	102	-	-	20/47/47/47	-
7	BCL	L	304	-	-	6/37/137/137	-
7	BCL	P	101	-	-	4/37/137/137	-
10	PC1	l	304	-	-	23/51/51/57	-
7	BCL	k	103	-	-	5/37/137/137	-
12	SPO	T	102	-	-	19/47/47/47	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	m	1303	-	-	1/37/137/137	-
12	SPO	9	102	-	-	24/47/47/47	-
12	SPO	G	103	-	-	21/47/47/47	-
7	BCL	K	101	-	-	6/37/137/137	-
7	BCL	M	1301	-	-	11/37/137/137	-
12	SPO	t	101	-	-	18/47/47/47	-
7	BCL	Y	201	-	-	0/13/113/137	-
7	BCL	T	101	-	-	4/37/137/137	-
10	PC1	a	102	-	-	20/43/43/57	-
9	U10	L	303	-	-	16/39/63/87	0/1/1/1
7	BCL	S	101	-	-	3/25/125/137	-
12	SPO	o	102	-	-	24/47/47/47	-
7	BCL	Z	101	-	-	2/13/113/137	-
12	SPO	F	102	-	-	24/47/47/47	-
12	SPO	K	102	-	-	25/47/47/47	-
7	BCL	W	101	-	-	0/13/113/137	-
7	BCL	c	101	-	-	9/31/131/137	-
12	SPO	j	103	-	-	26/47/47/47	-
12	SPO	m	1305	-	-	25/47/47/47	-
7	BCL	F	101	-	-	6/37/137/137	-
12	SPO	O	102	-	-	19/47/47/47	-
7	BCL	N	102	-	-	4/37/137/137	-
7	BCL	2	101	-	-	0/13/113/137	-
8	BPB	L	302	-	-	8/34/102/105	0/5/6/6
7	BCL	Q	101	-	-	3/37/137/137	-
7	BCL	q	101	-	-	12/37/137/137	-
12	SPO	n	101	-	-	28/47/47/47	-
7	BCL	aa	102	-	-	4/37/137/137	-
7	BCL	3	102	-	-	8/37/137/137	-
8	BPB	l	302	-	-	9/34/102/105	0/5/6/6
12	SPO	e	101	-	-	24/47/47/47	-
12	SPO	s	105	-	-	25/47/47/47	-
7	BCL	v	101	-	-	15/37/137/137	-
12	SPO	a	104	-	-	22/47/47/47	-
7	BCL	X	101	-	-	3/13/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SPO	s	104	-	-	20/47/47/47	-
12	SPO	N	103	-	-	25/47/47/47	-
12	SPO	G	102	-	-	22/47/47/47	-
7	BCL	r	101	-	-	15/37/137/137	-
7	BCL	j	102	-	-	4/37/137/137	-
7	BCL	J	101	-	-	4/37/137/137	-
12	SPO	3	103	-	-	24/47/47/47	-
7	BCL	A	101	-	-	6/37/137/137	-
12	SPO	j	101	-	-	25/47/47/47	-
12	SPO	M	1305	-	-	25/47/47/47	-
10	PC1	A	103	-	-	13/54/54/57	-
7	BCL	i	101	-	-	11/37/137/137	-
12	SPO	s	102	-	-	23/47/47/47	-
7	BCL	z	101	-	-	6/13/113/137	-
10	PC1	d	102	-	-	5/44/44/57	-
7	BCL	9	101	-	-	7/37/137/137	-
7	BCL	b	101	-	-	4/37/137/137	-
7	BCL	p	101	-	-	6/37/137/137	-
12	SPO	A	102	-	-	23/47/47/47	-
8	BPB	l	306	-	-	7/25/93/105	0/5/6/6
7	BCL	M	1303	-	-	2/37/137/137	-
12	SPO	N	101	-	-	24/47/47/47	-
7	BCL	f	101	-	-	5/37/137/137	-
7	BCL	l	305	-	-	6/37/137/137	-
10	PC1	L	306	-	-	11/46/46/57	-
12	SPO	B	102	-	-	19/47/47/47	-
7	BCL	l	301	-	-	5/37/137/137	-
7	BCL	g	101	-	-	4/37/137/137	-
9	U10	l	303	-	-	24/63/87/87	0/1/1/1
7	BCL	0	101	-	-	4/37/137/137	-
7	BCL	m	1301	-	-	11/37/137/137	-
10	PC1	M	1307	-	-	25/56/56/57	-
10	PC1	A	104	-	-	16/49/49/57	-
7	BCL	k	101	-	-	6/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	m	1306	-	-	44/110/110/110	-
7	BCL	L	301	-	-	5/37/137/137	-

The worst 5 of 1228 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	103	SPO	C27-C28	19.02	1.53	1.34
12	s	105	SPO	C27-C28	18.77	1.53	1.34
12	K	102	SPO	C27-C28	18.75	1.53	1.34
12	3	101	SPO	C27-C28	18.71	1.53	1.34
12	q	102	SPO	C27-C28	18.71	1.53	1.34

The worst 5 of 2194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	e	103	SPO	C15-C14-C12	-16.95	103.12	127.31
12	i	102	SPO	C10-C9-C7	-16.86	103.25	127.31
12	e	103	SPO	C10-C9-C7	-16.00	104.48	127.31
12	ab	102	SPO	C15-C14-C12	-14.99	105.91	127.31
12	N	103	SPO	C10-C9-C7	-14.36	106.82	127.31

There are no chirality outliers.

5 of 1669 torsion outliers are listed below:

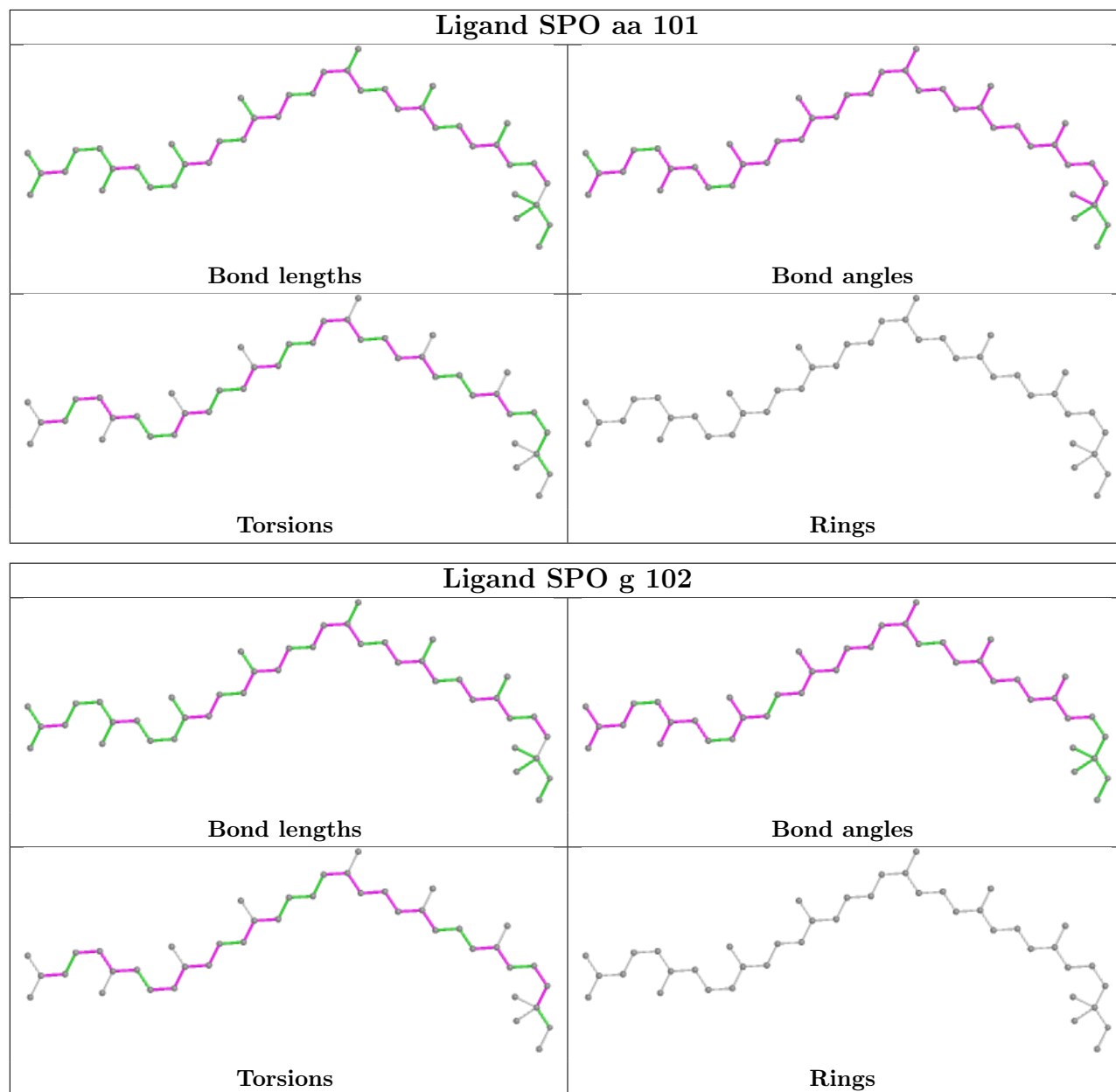
Mol	Chain	Res	Type	Atoms
7	M	1301	BCL	C1A-C2A-CAA-CBA
7	M	1301	BCL	C2A-CAA-CBA-CGA
7	M	1301	BCL	O2A-C1-C2-C3
7	B	101	BCL	O2A-C1-C2-C3
7	E	101	BCL	O2A-C1-C2-C3

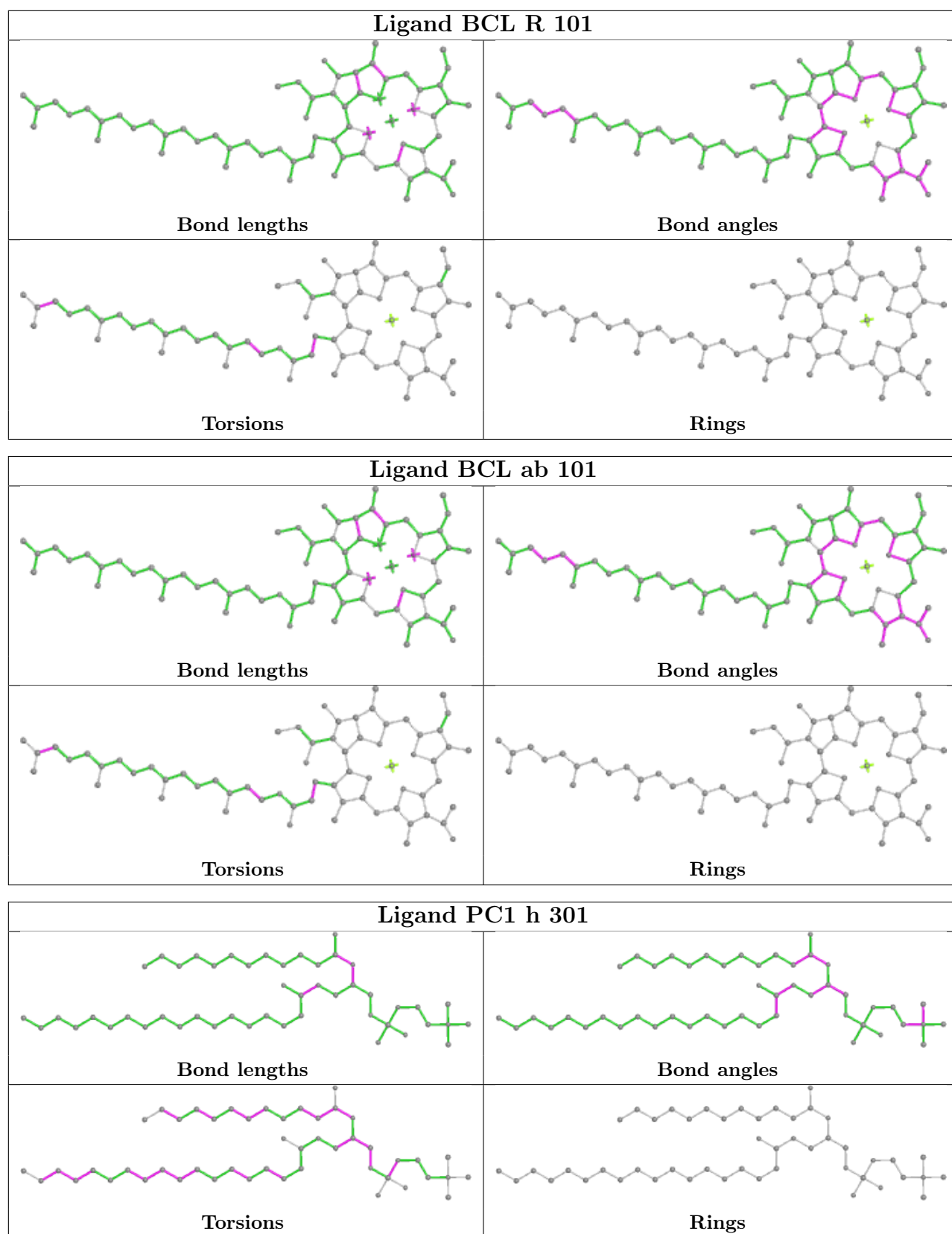
There are no ring outliers.

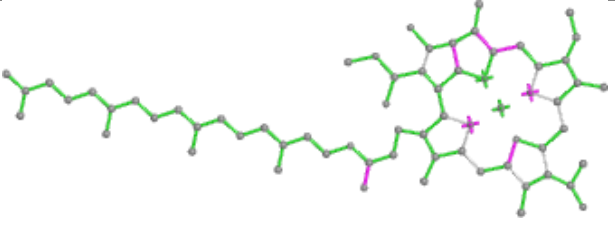
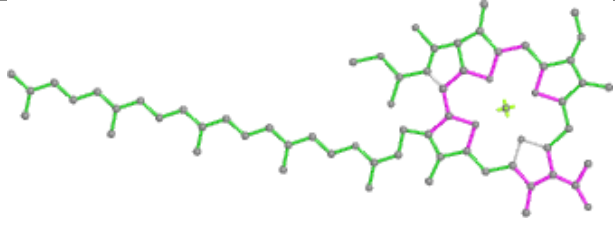
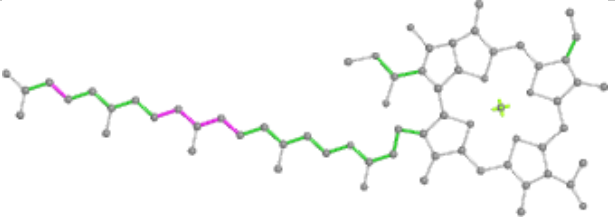
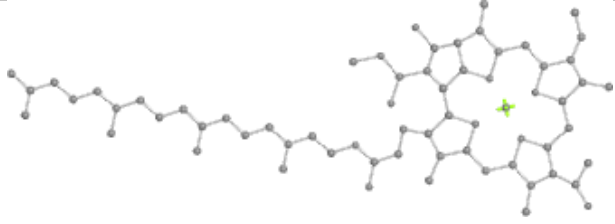
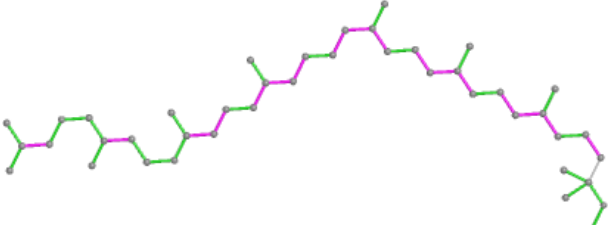
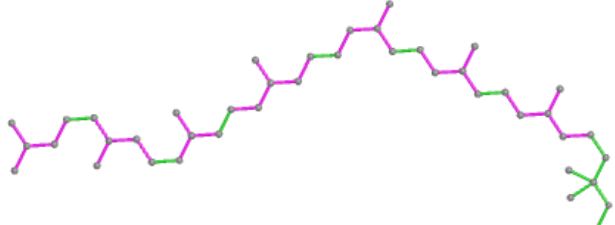
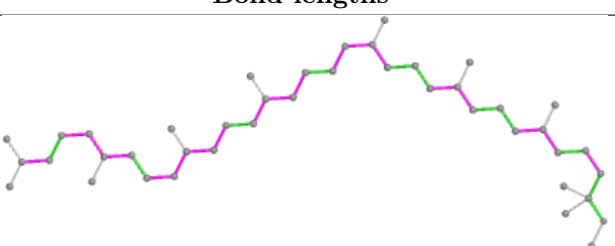
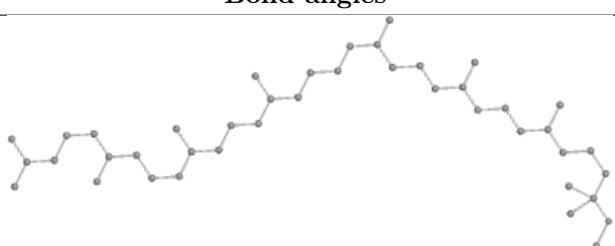
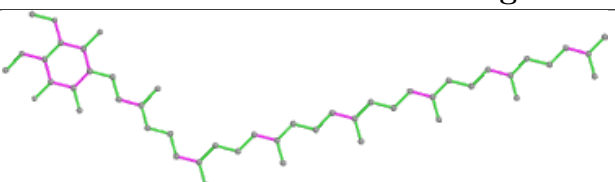
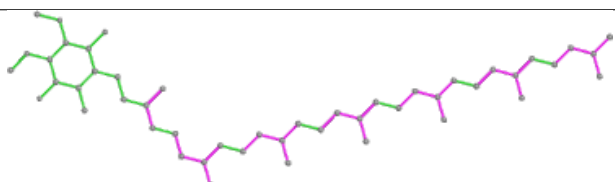

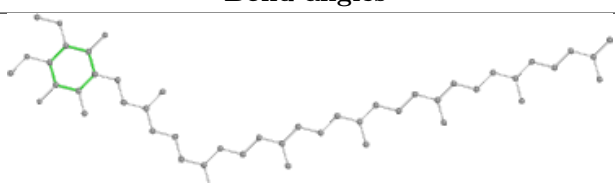
No monomer is involved in short contacts.

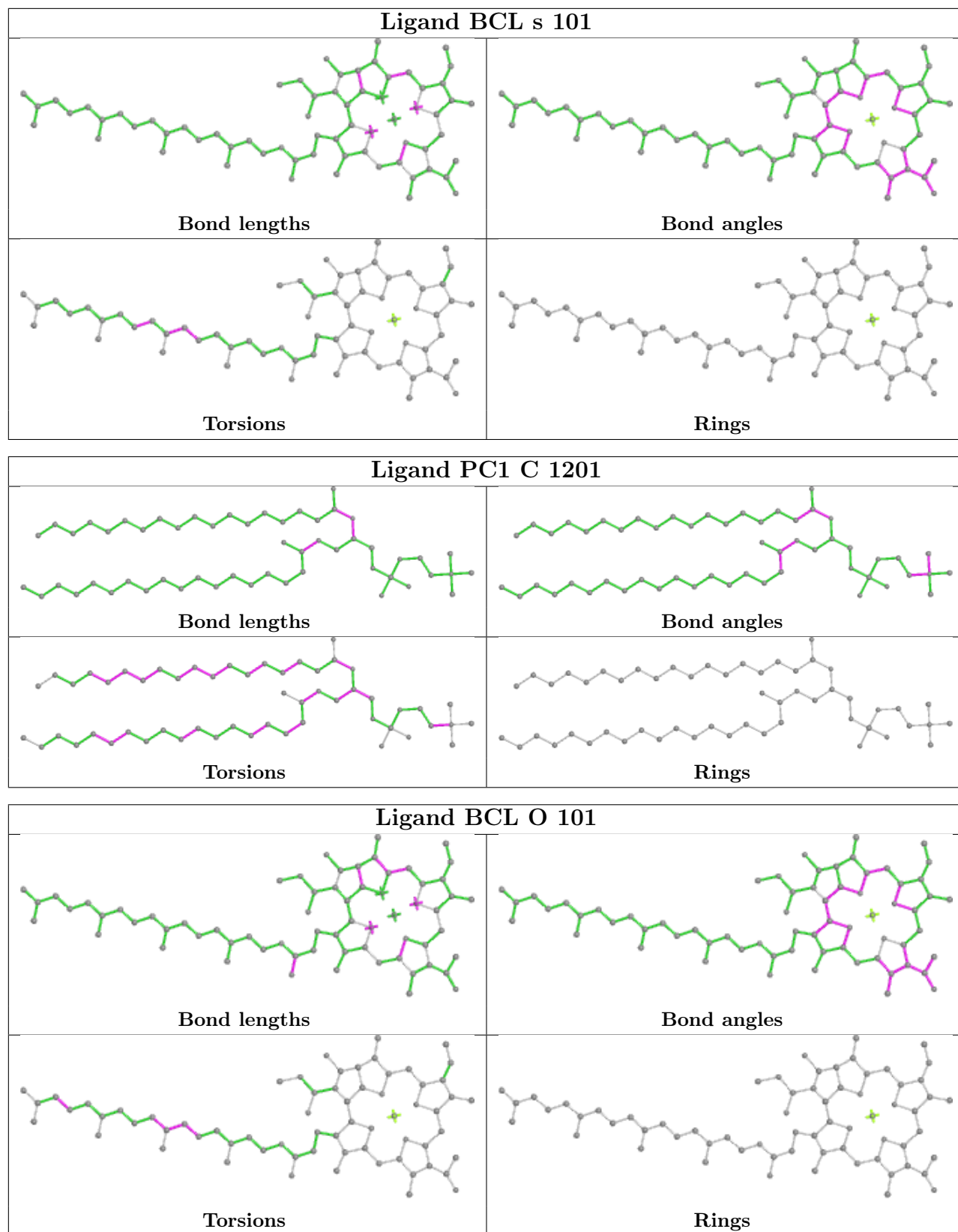
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

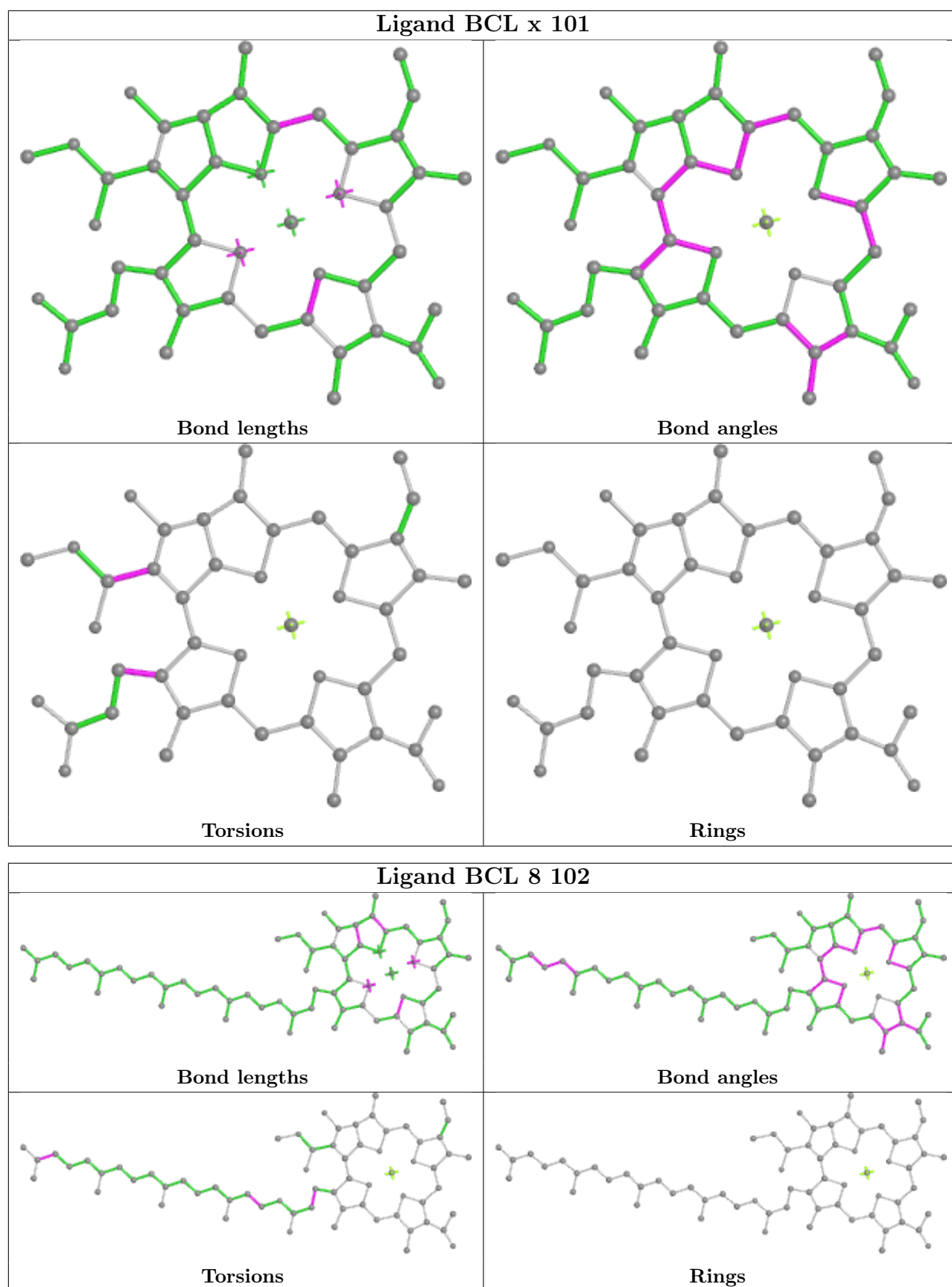
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

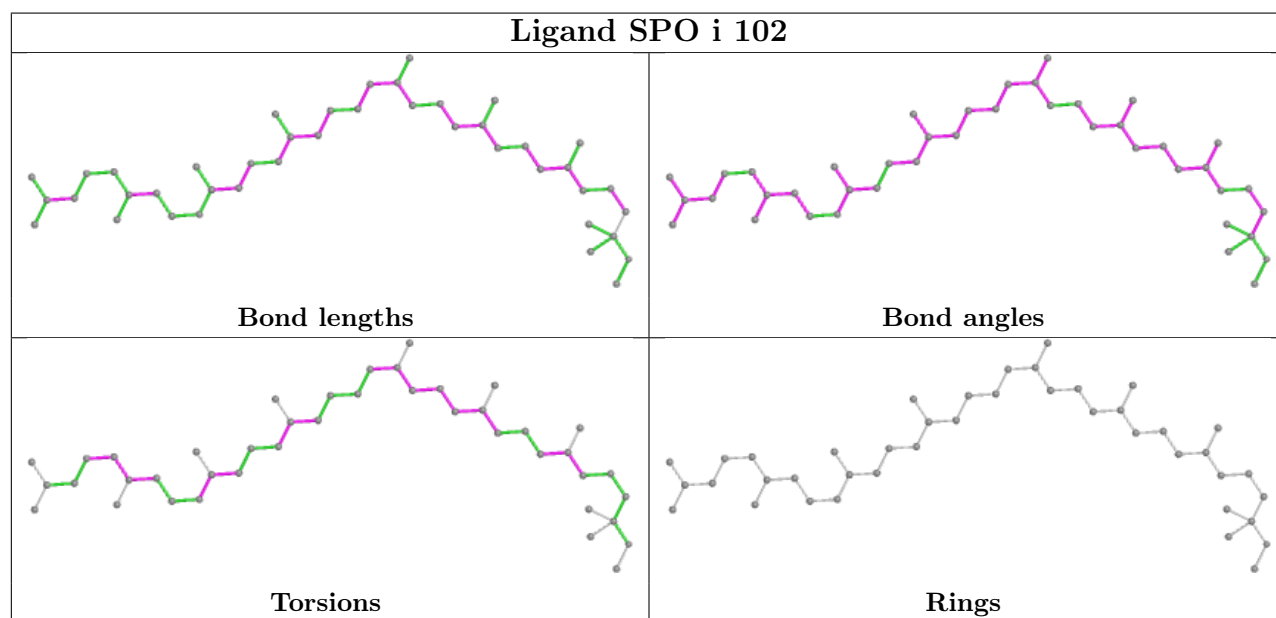
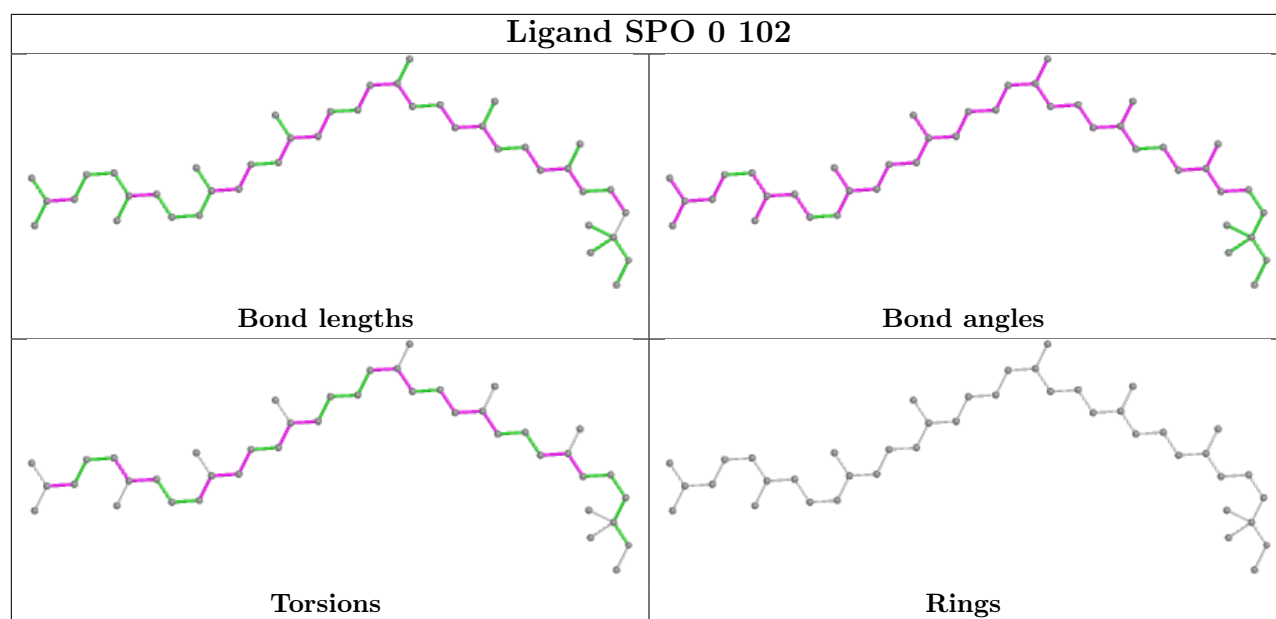




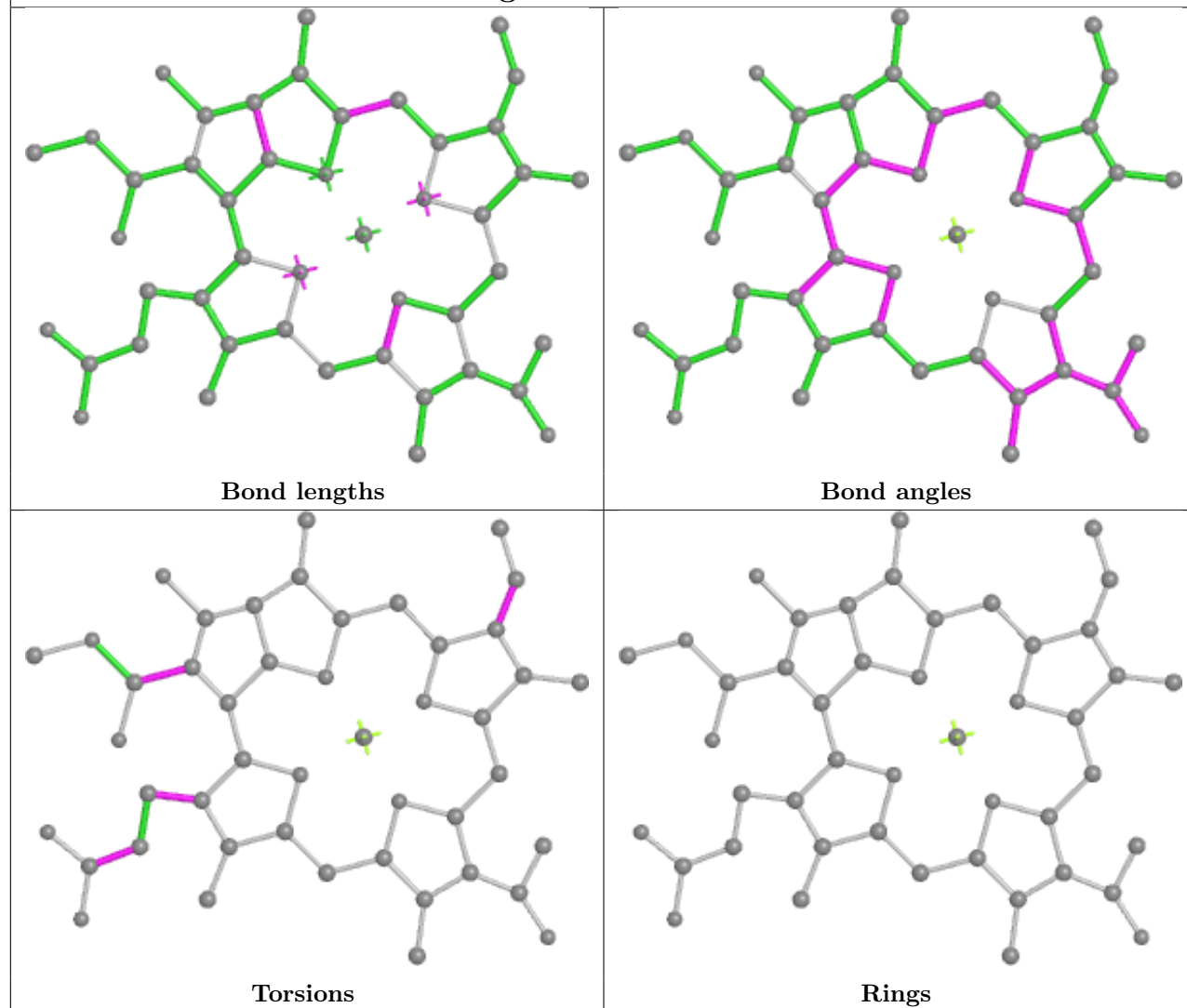
Ligand BCL D 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand SPO I 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand U10 M 1304	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



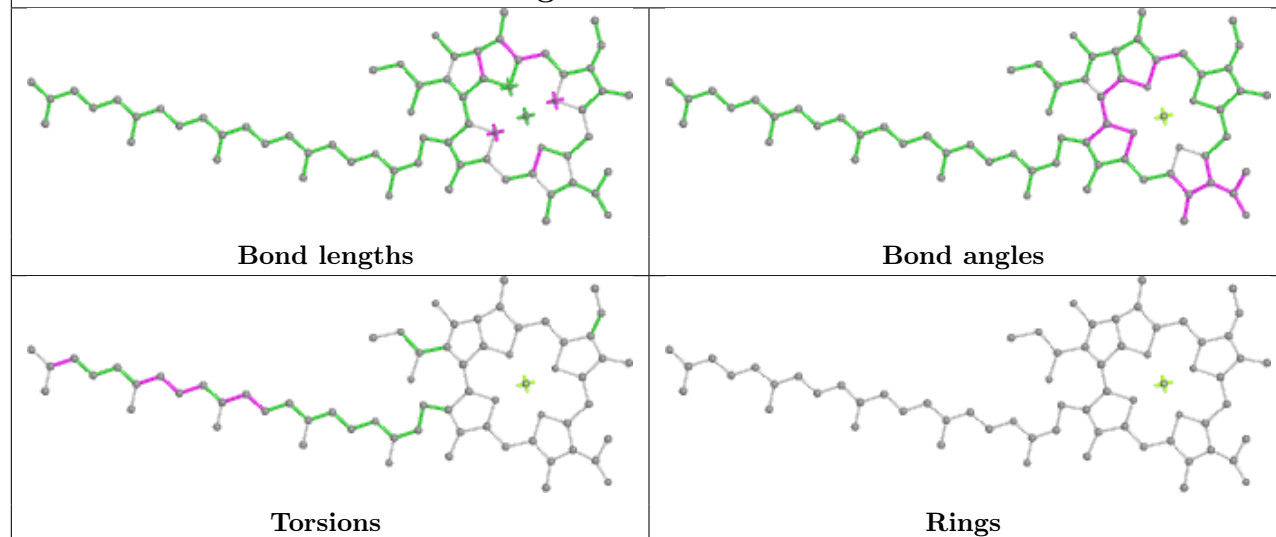




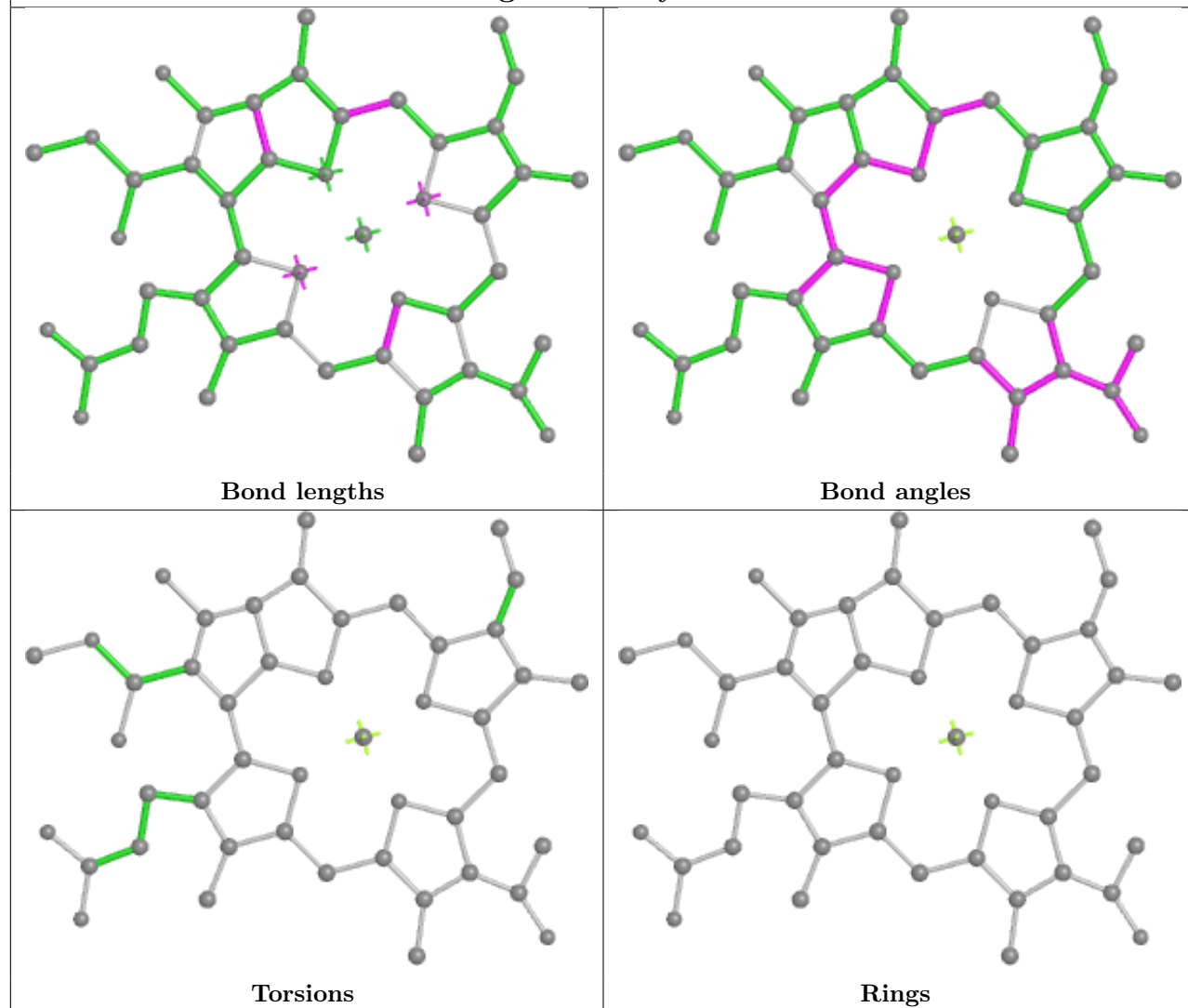
## Ligand BCL 5 102



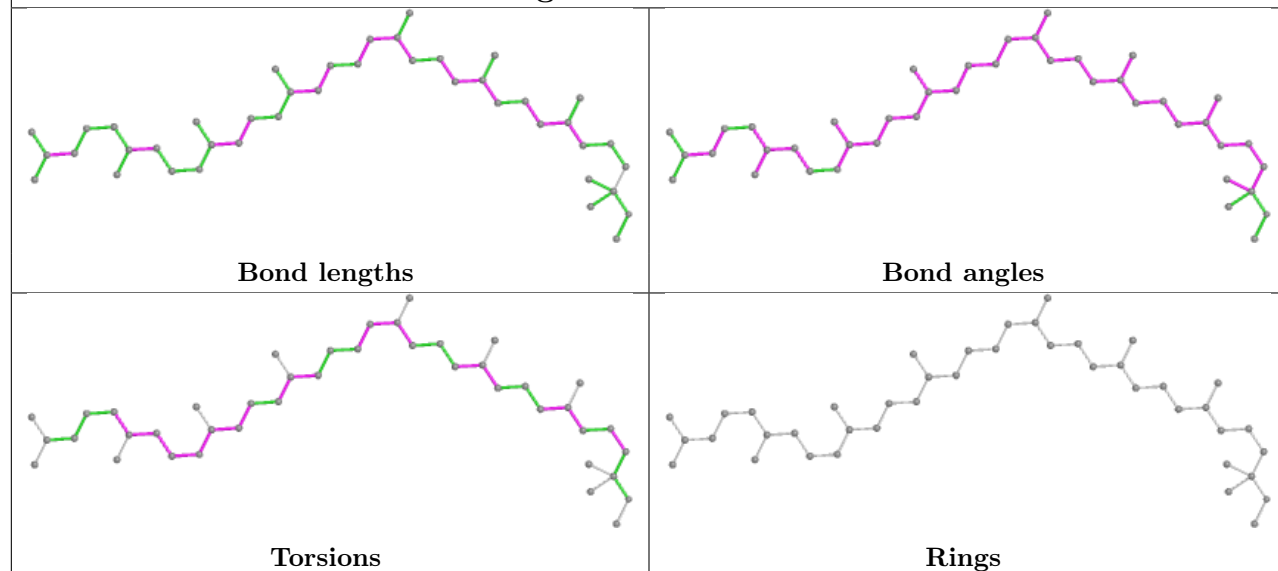
## Ligand BCL o 101

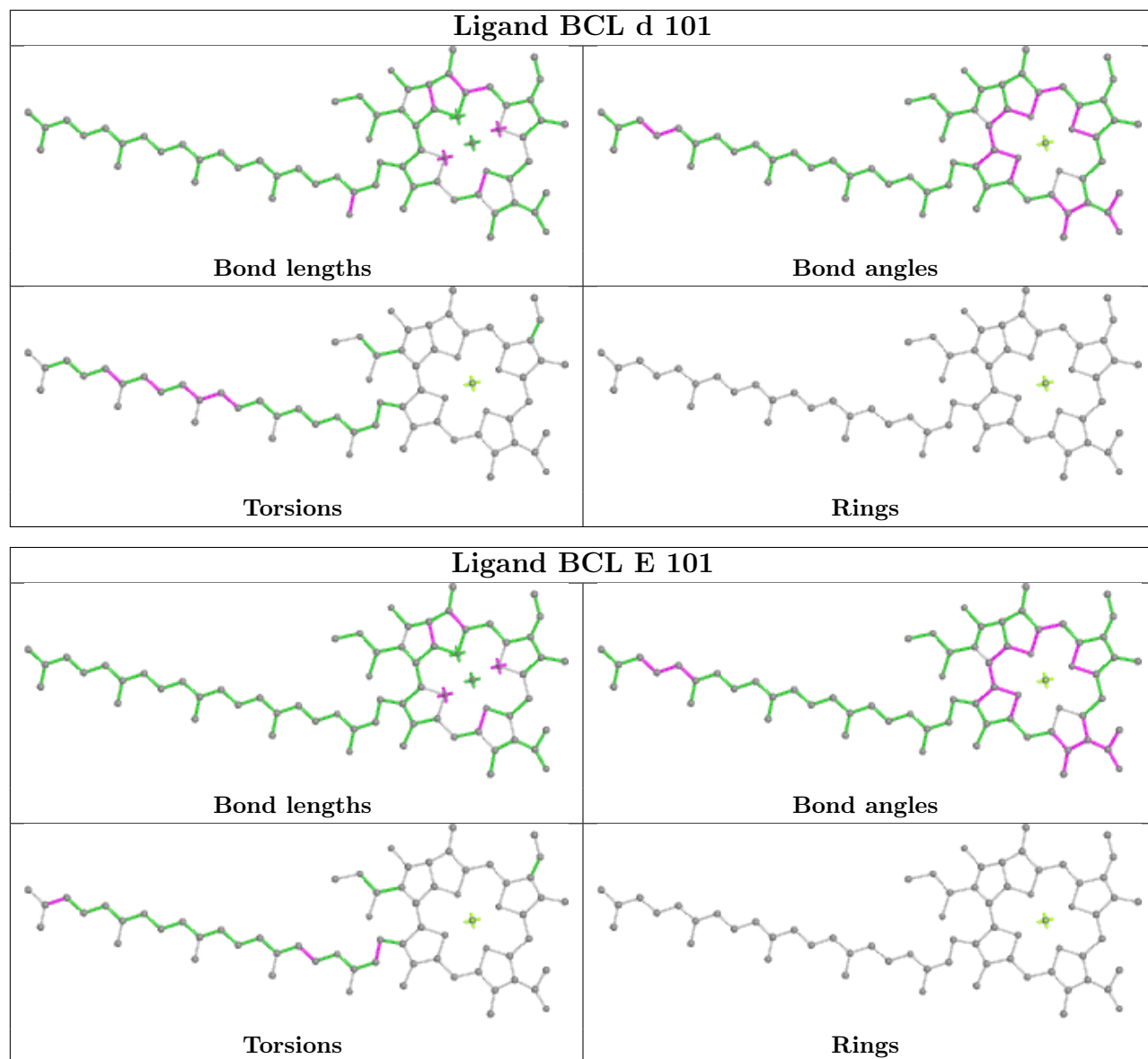


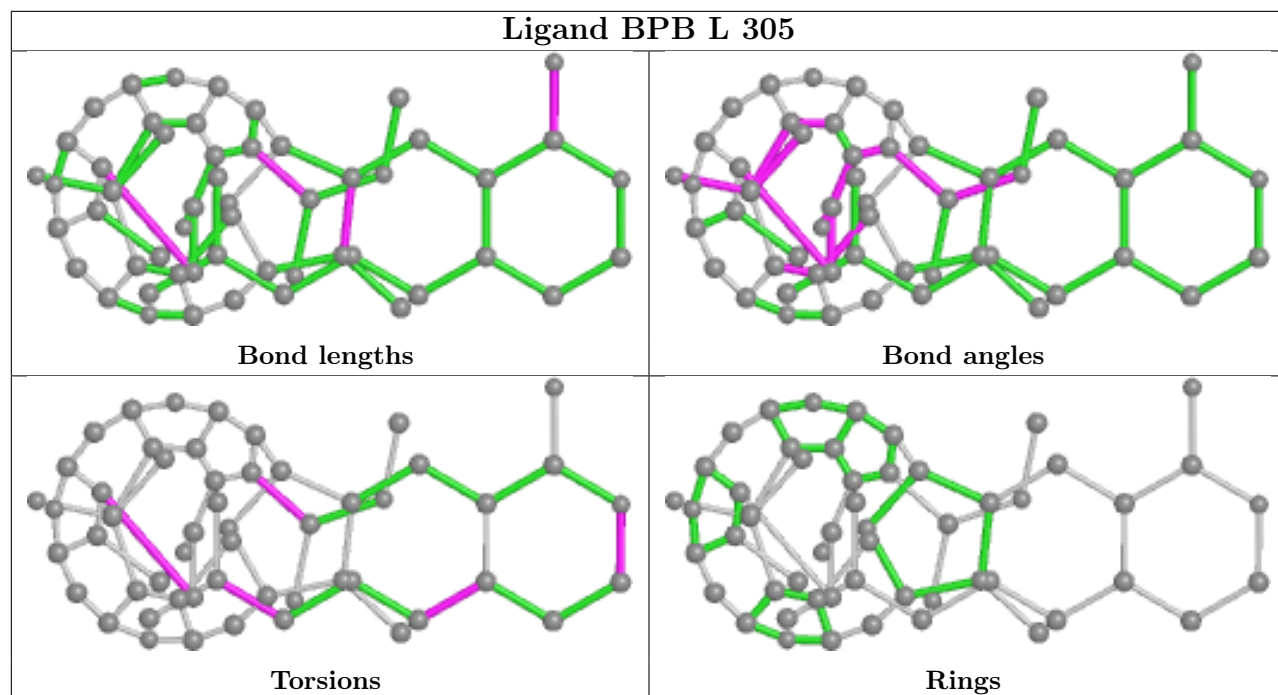
## Ligand BCL y 101



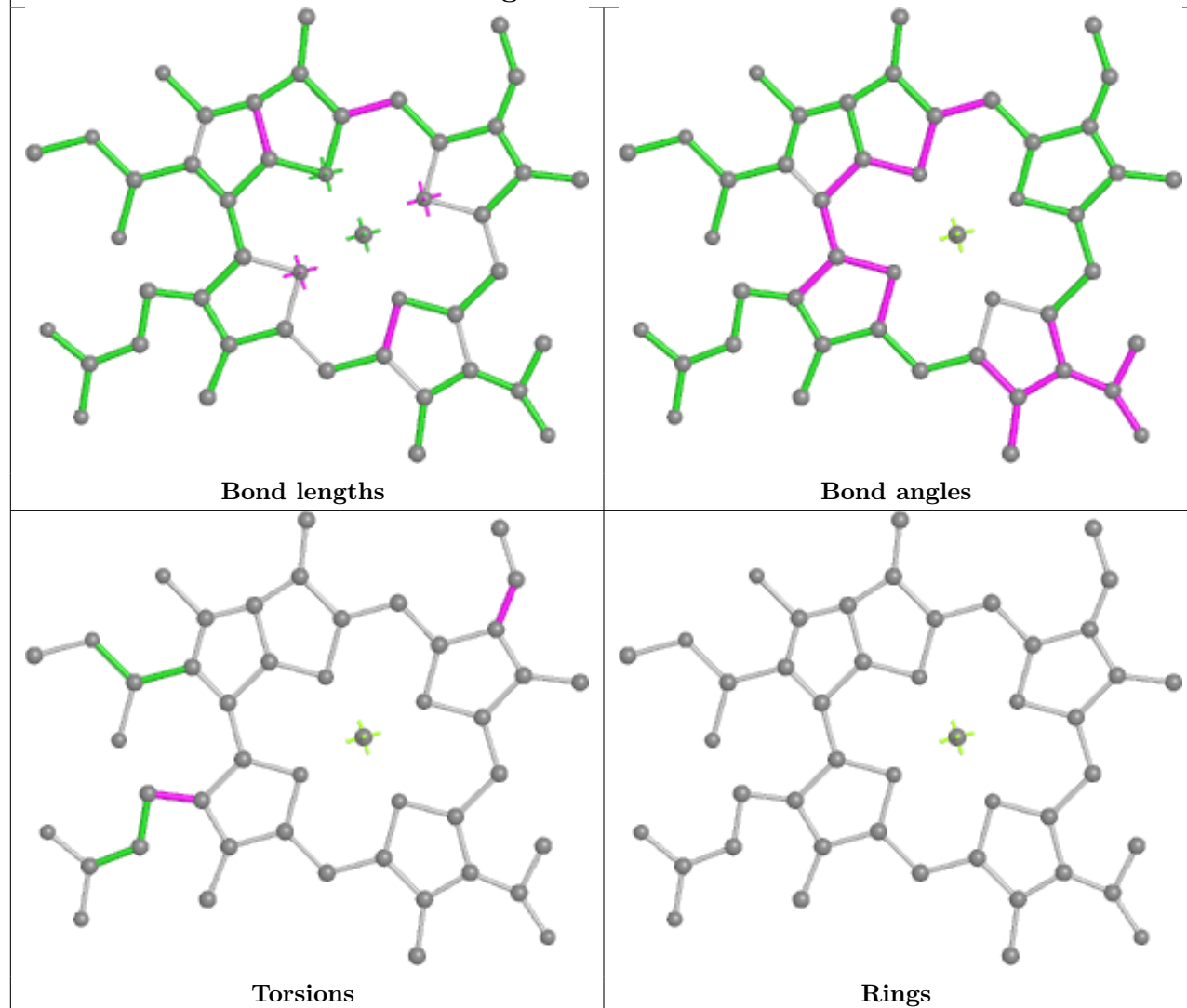
## Ligand SPO d 103



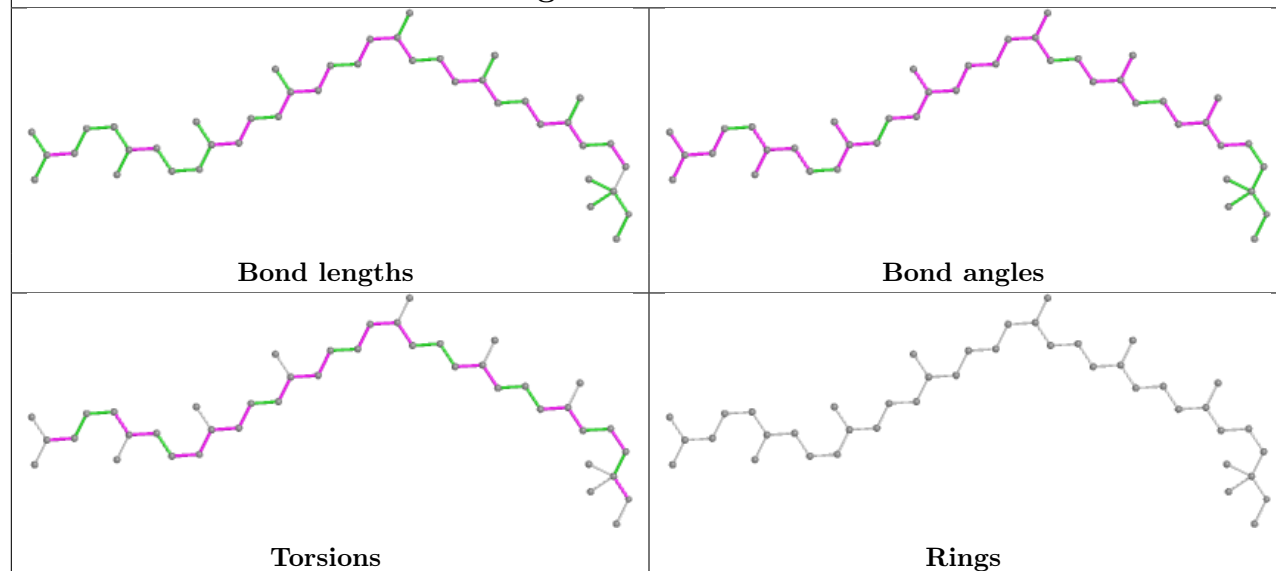


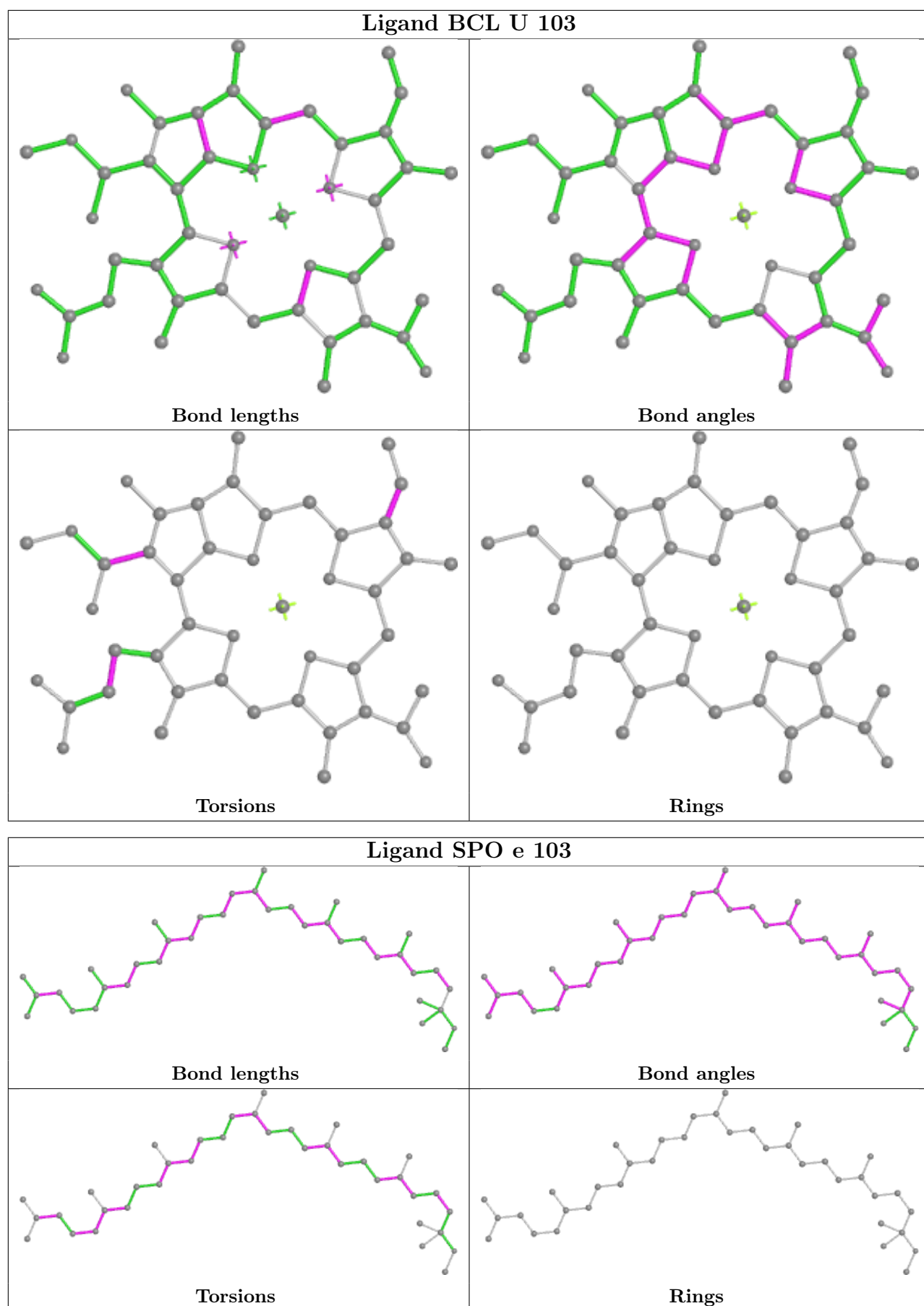


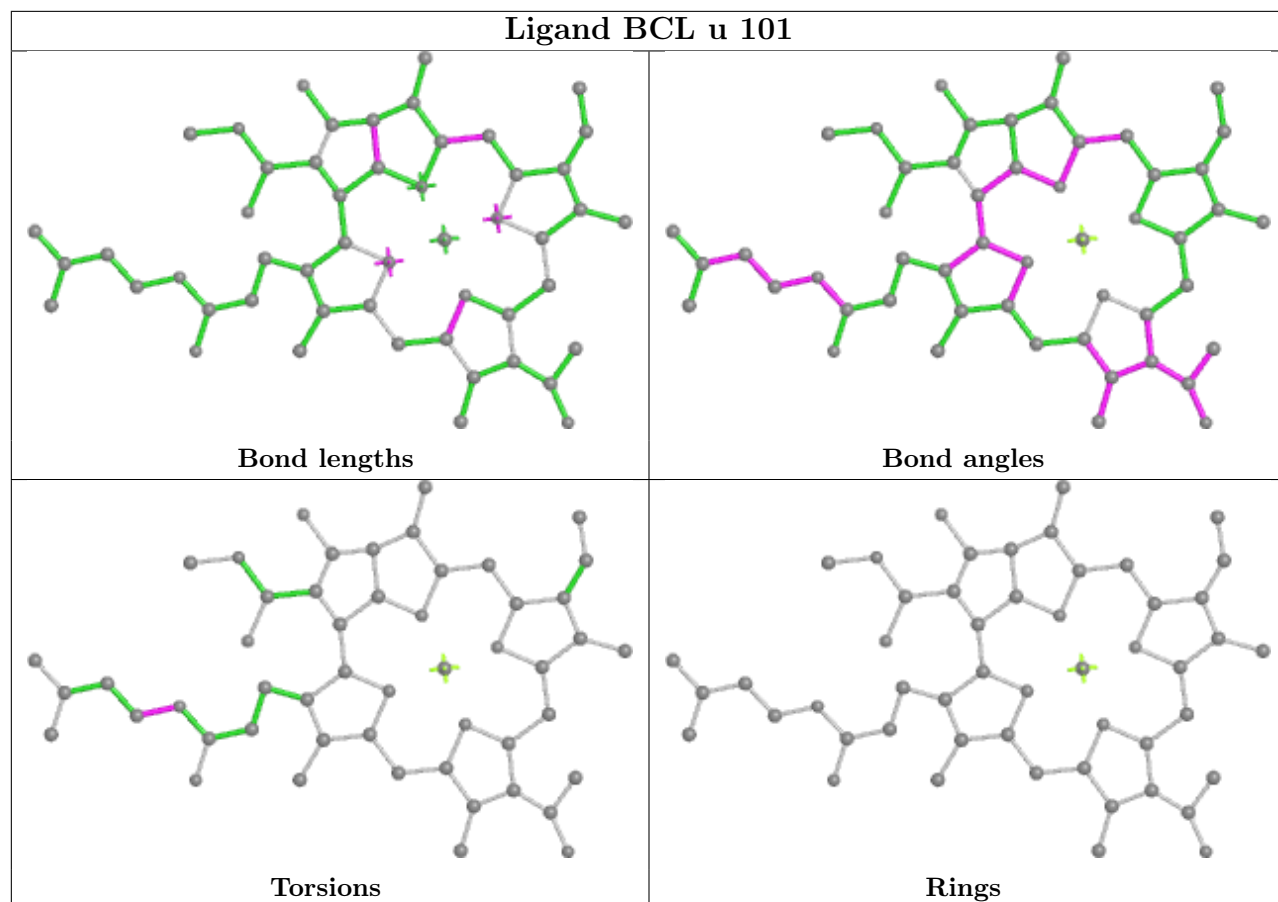
## Ligand BCL s 103



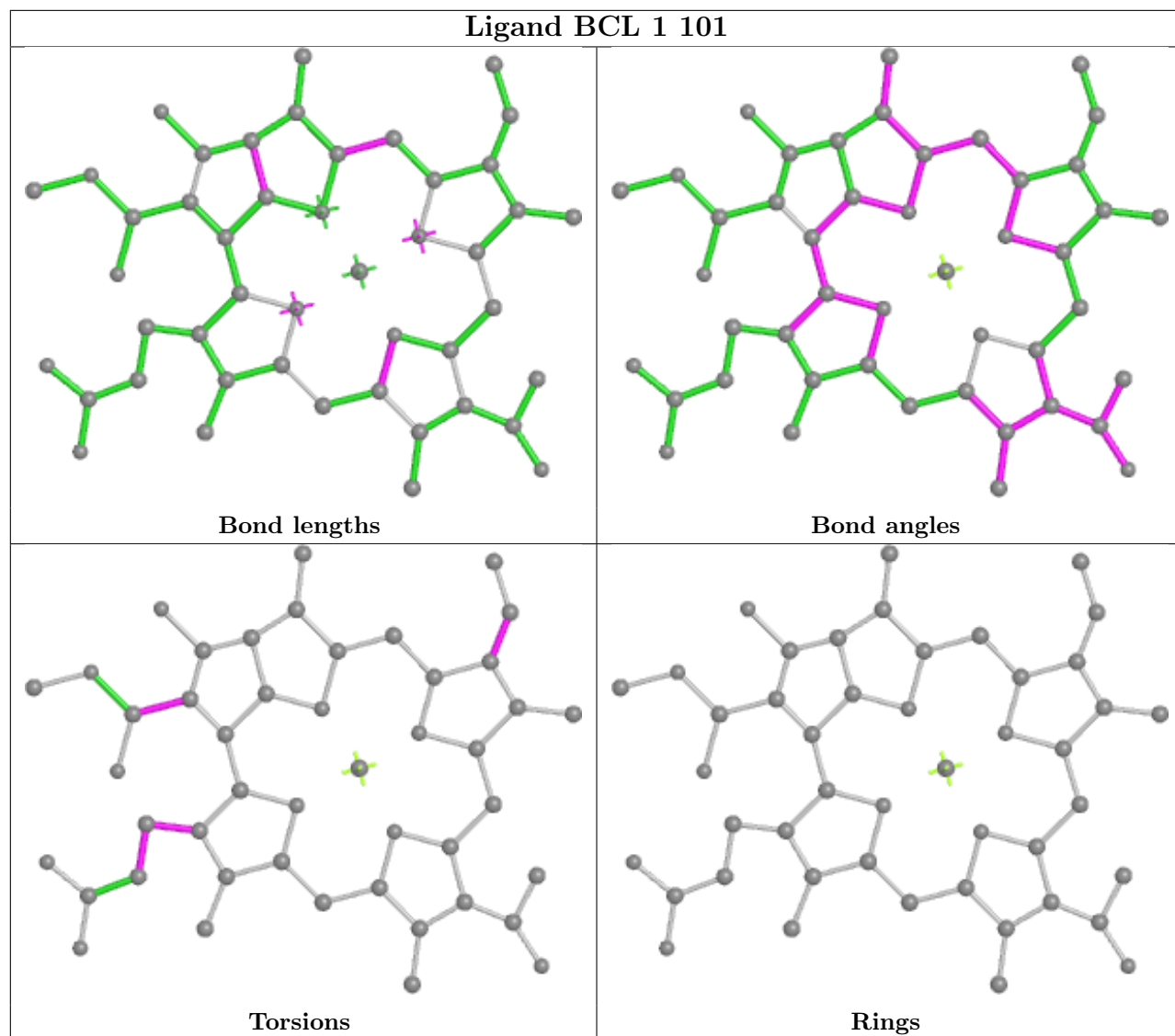
## Ligand SPO 3 101

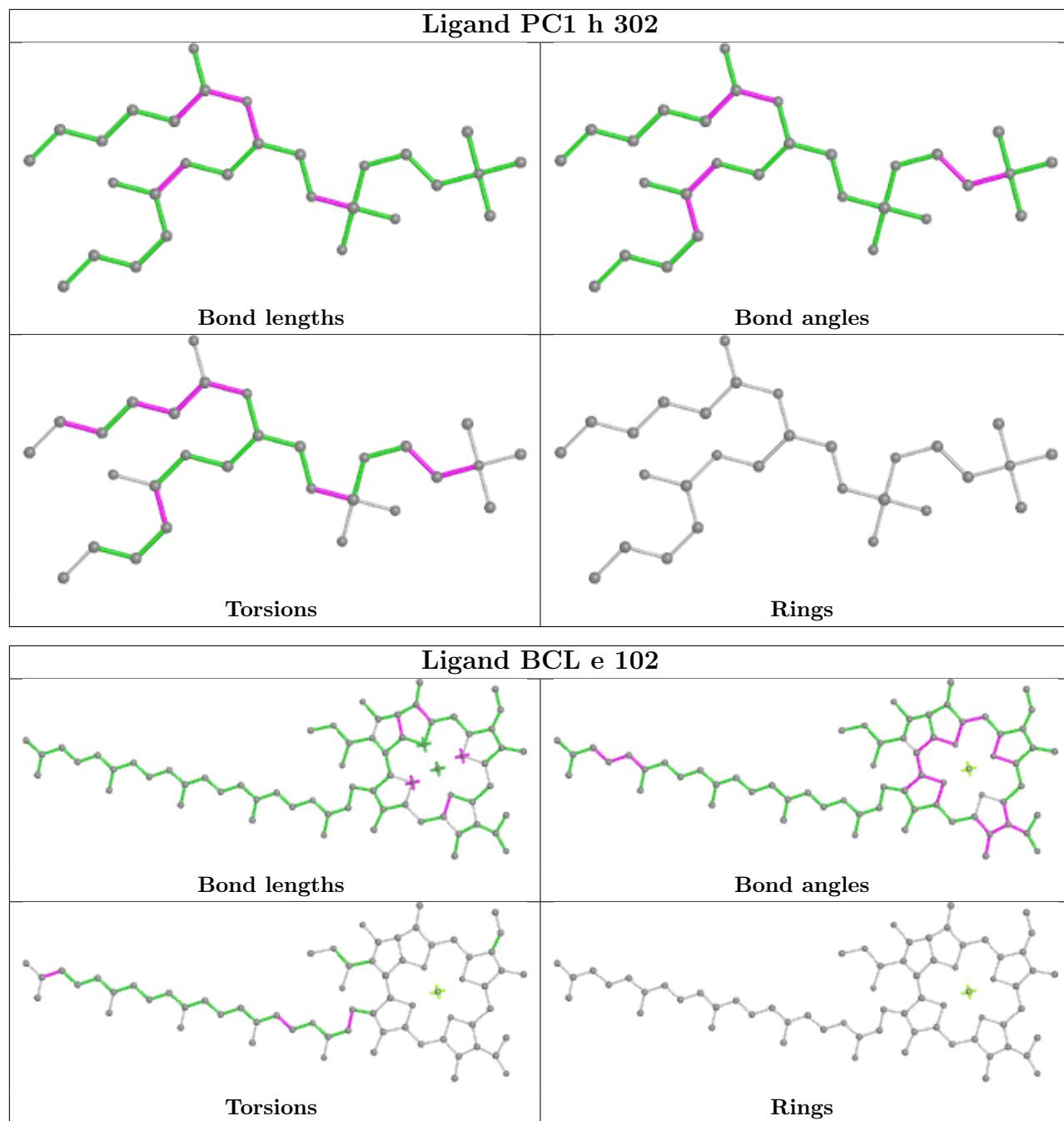




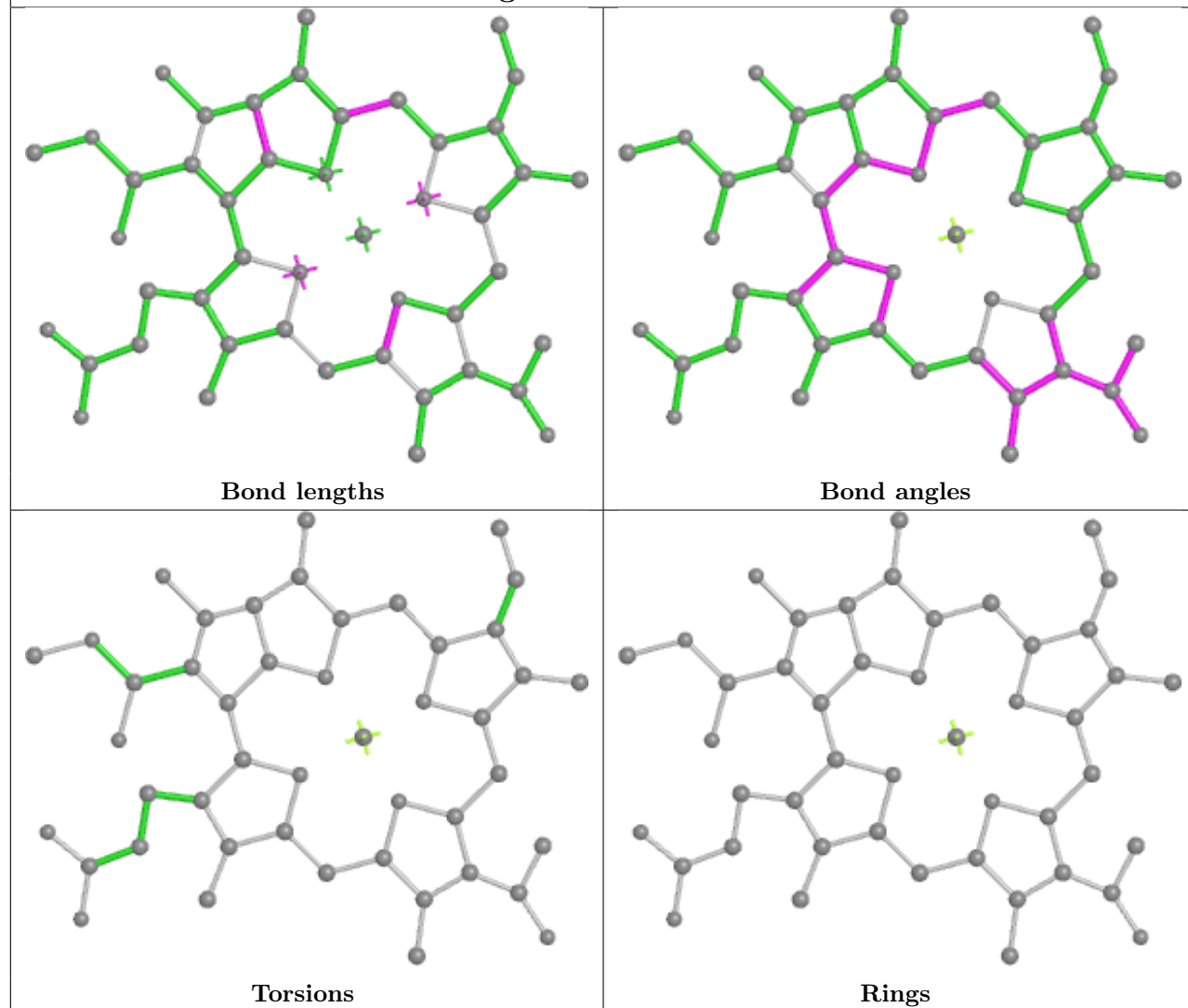


## Ligand BCL 1 101

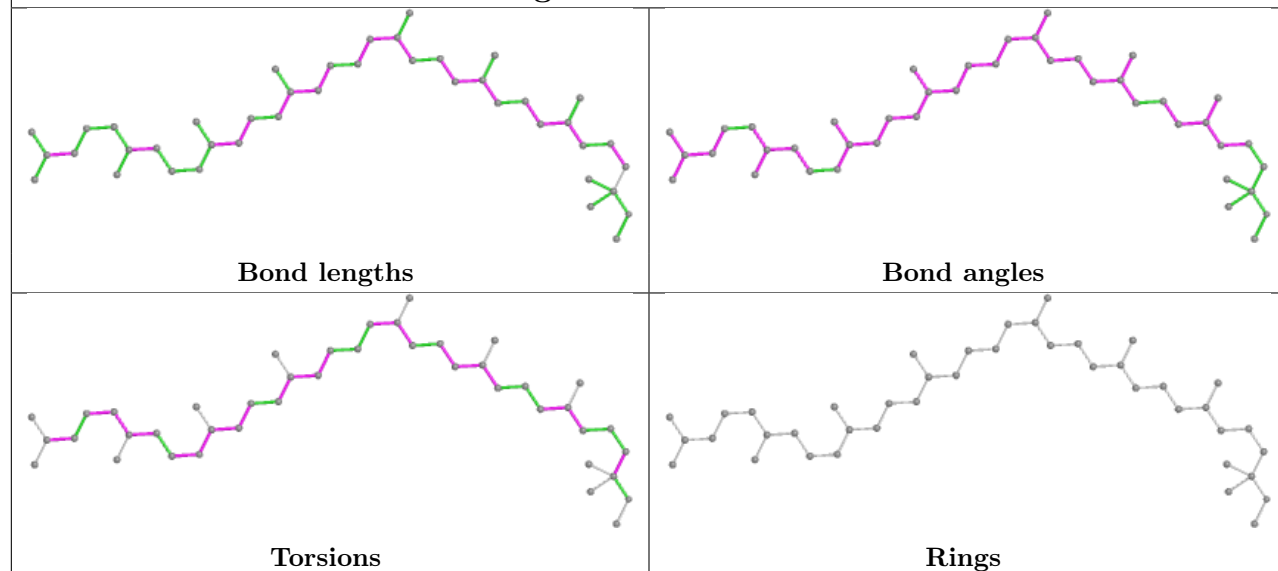


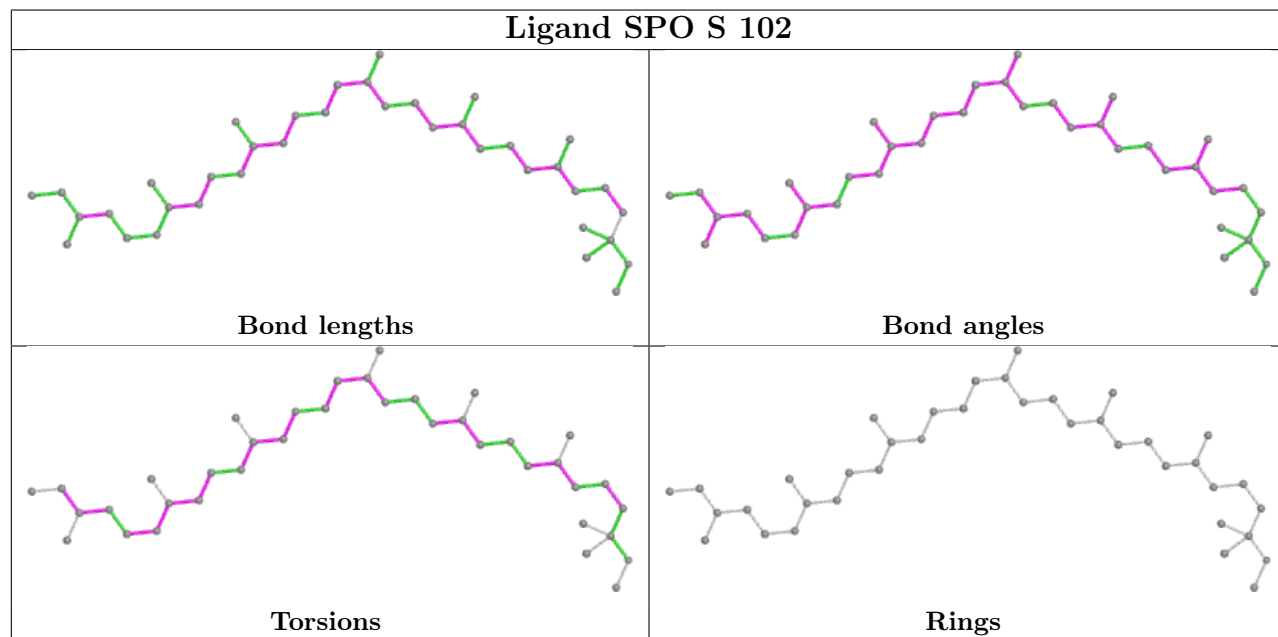
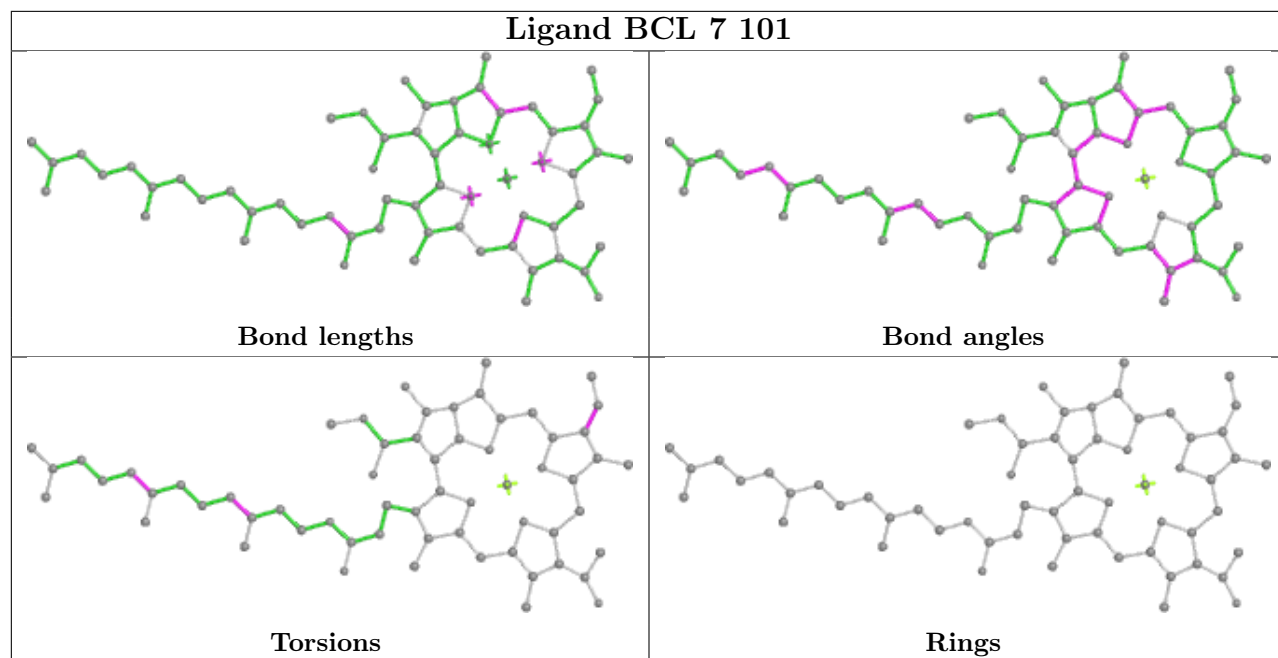


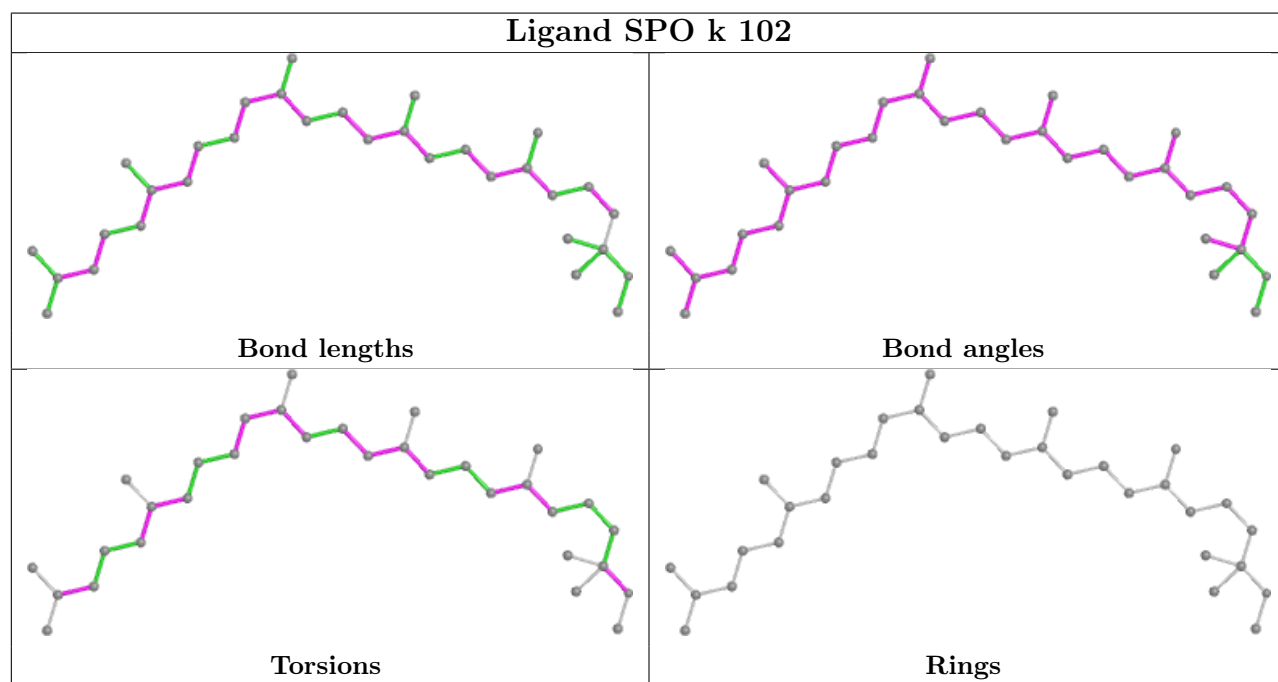
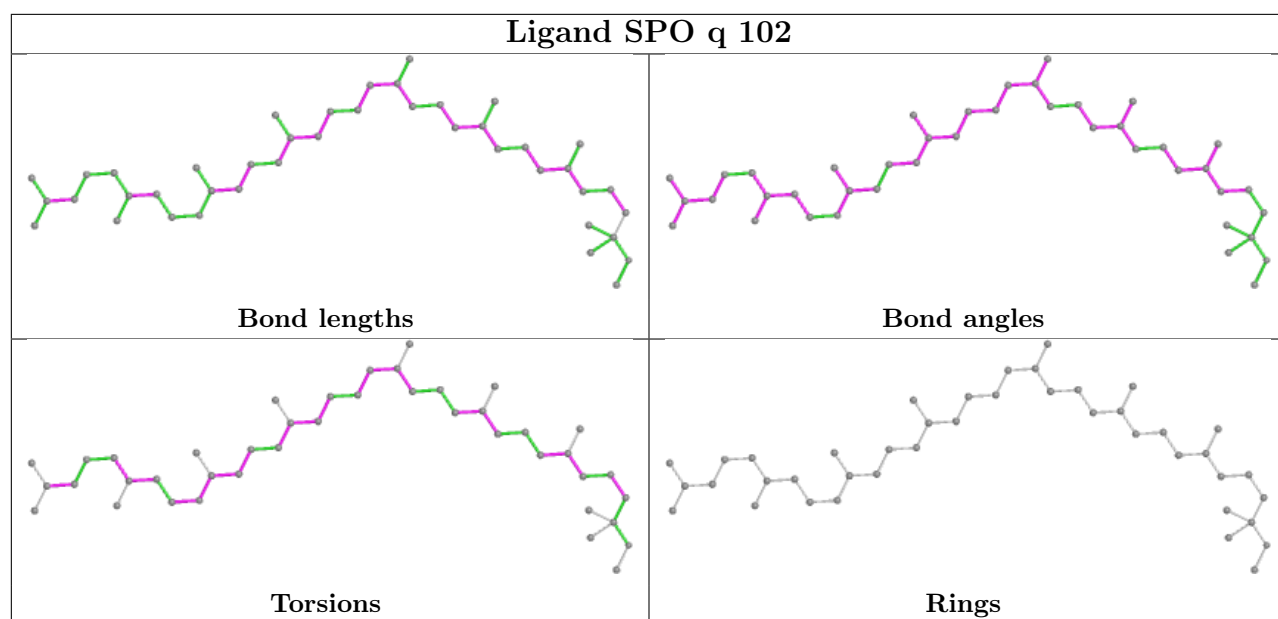
## Ligand BCL 5 101

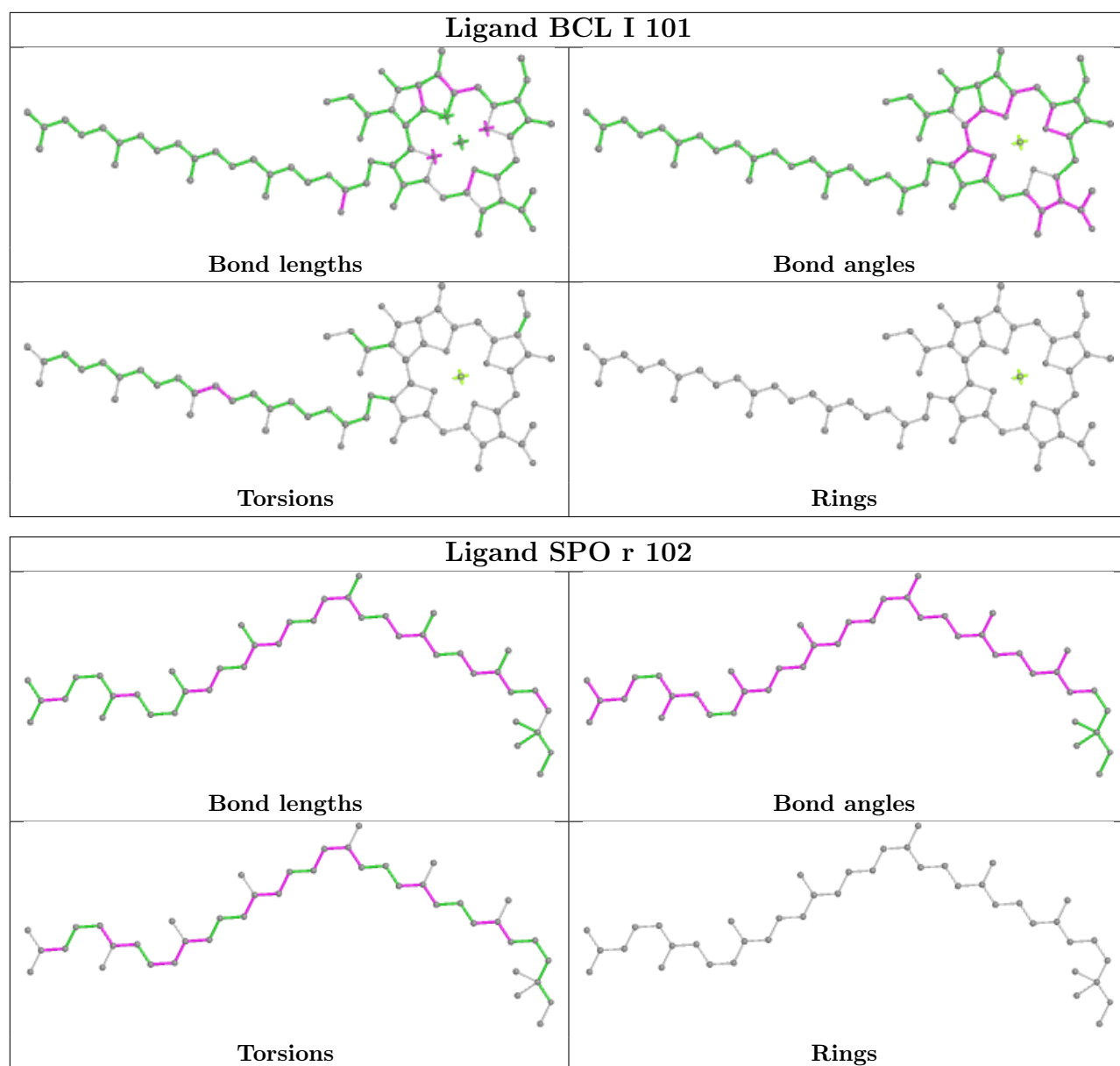


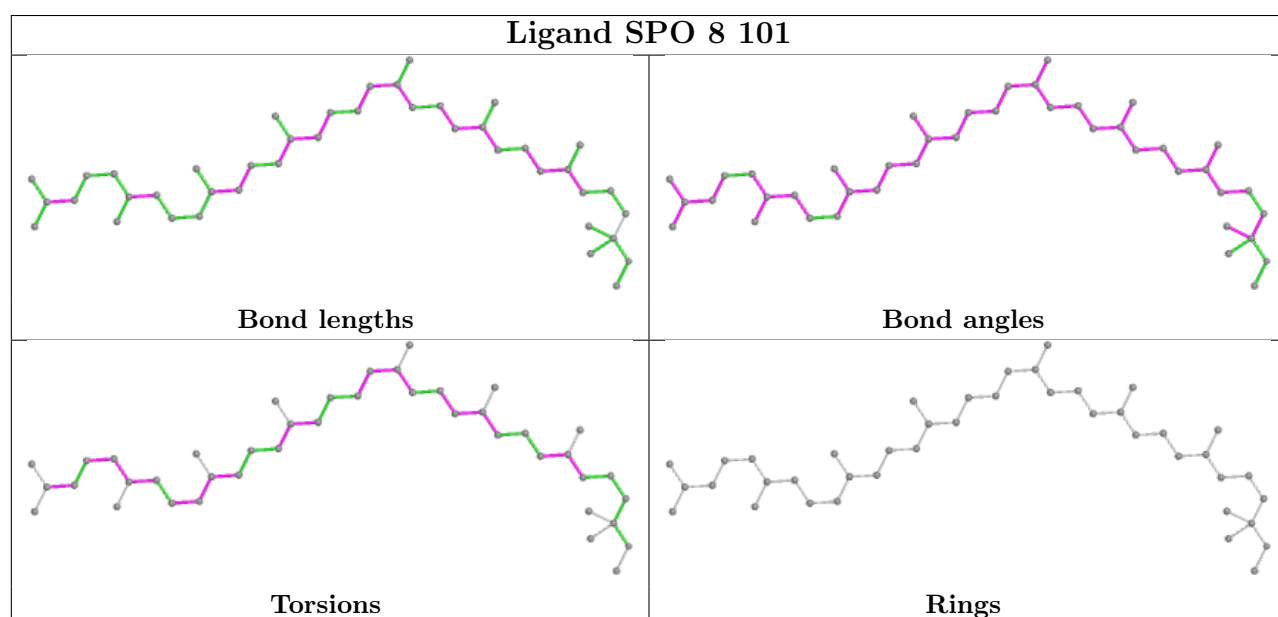
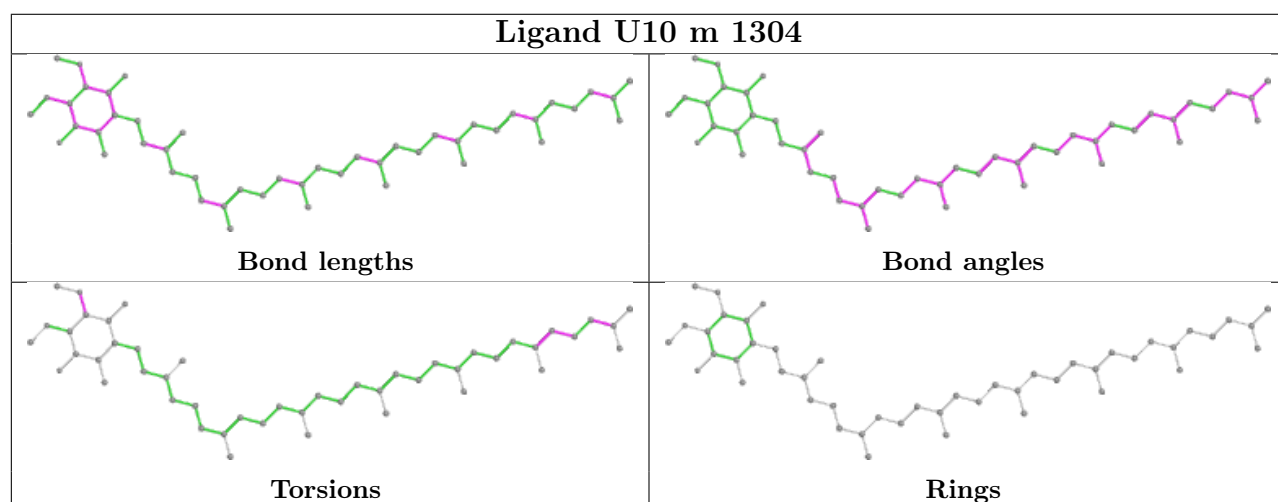
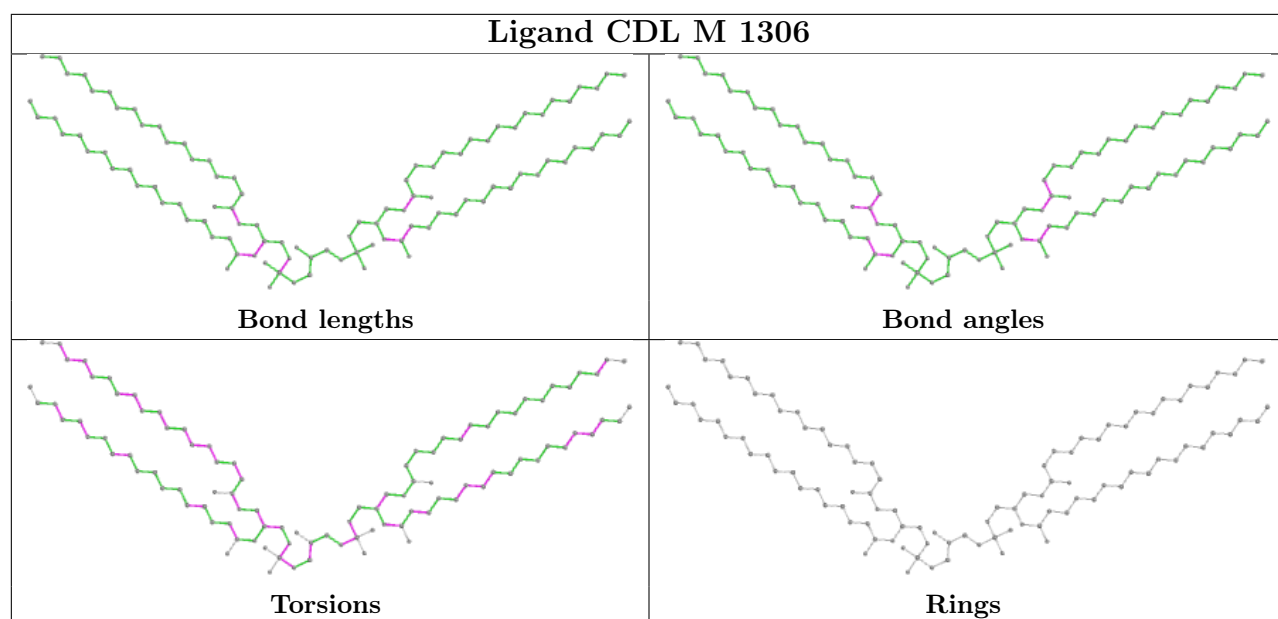
## Ligand SPO B 103

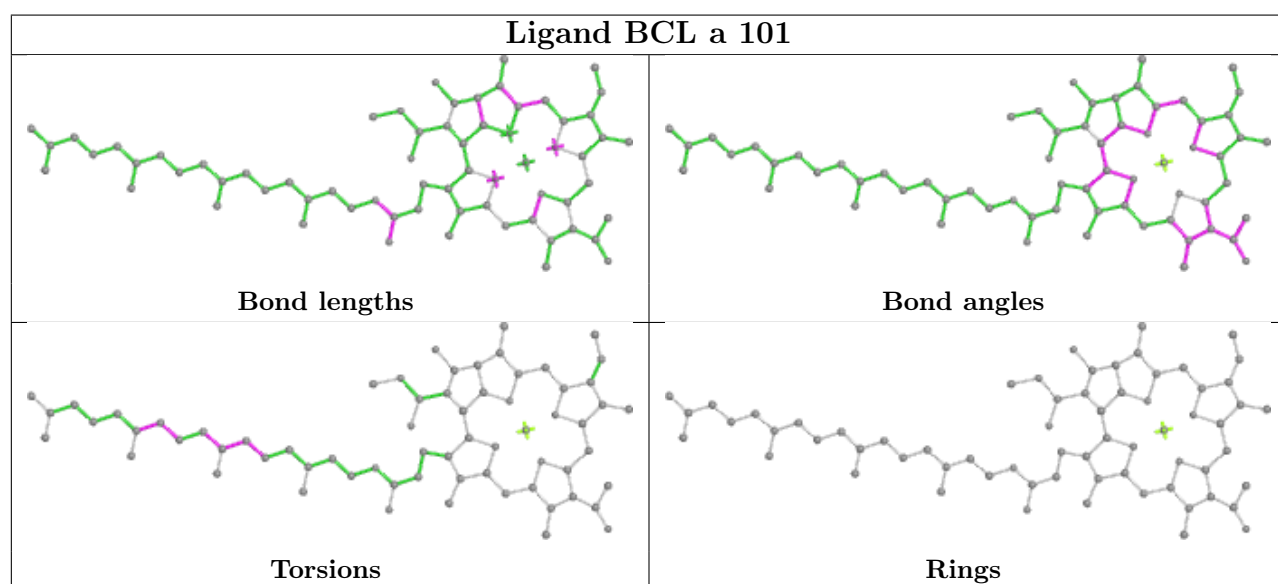
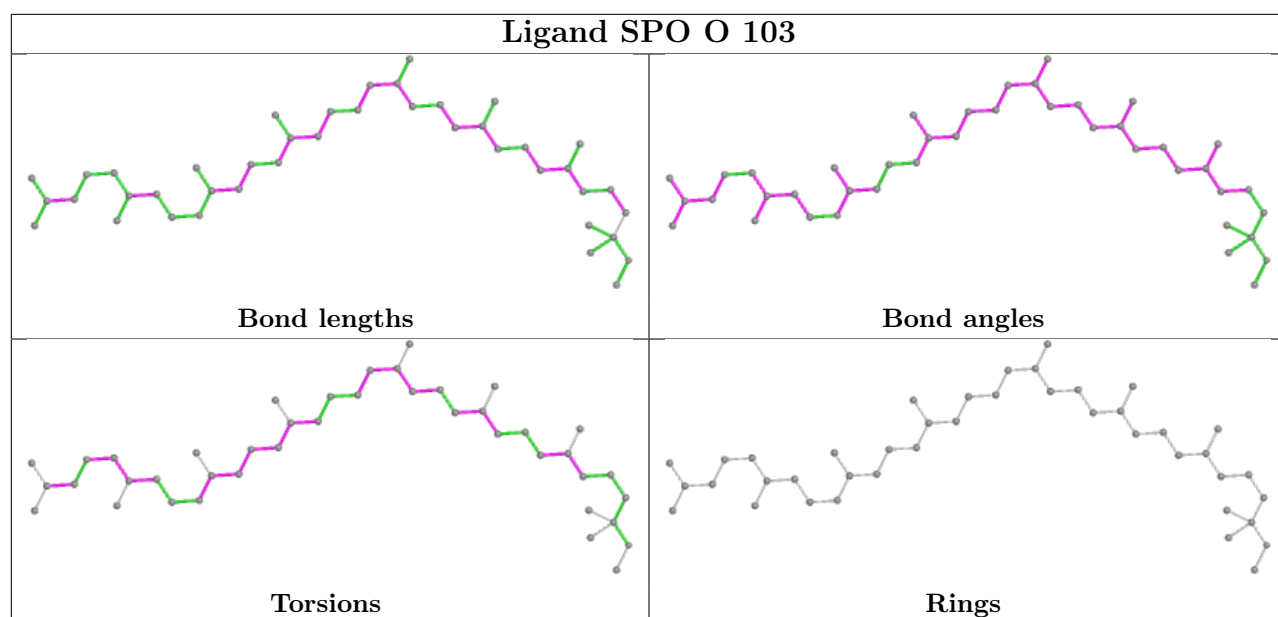


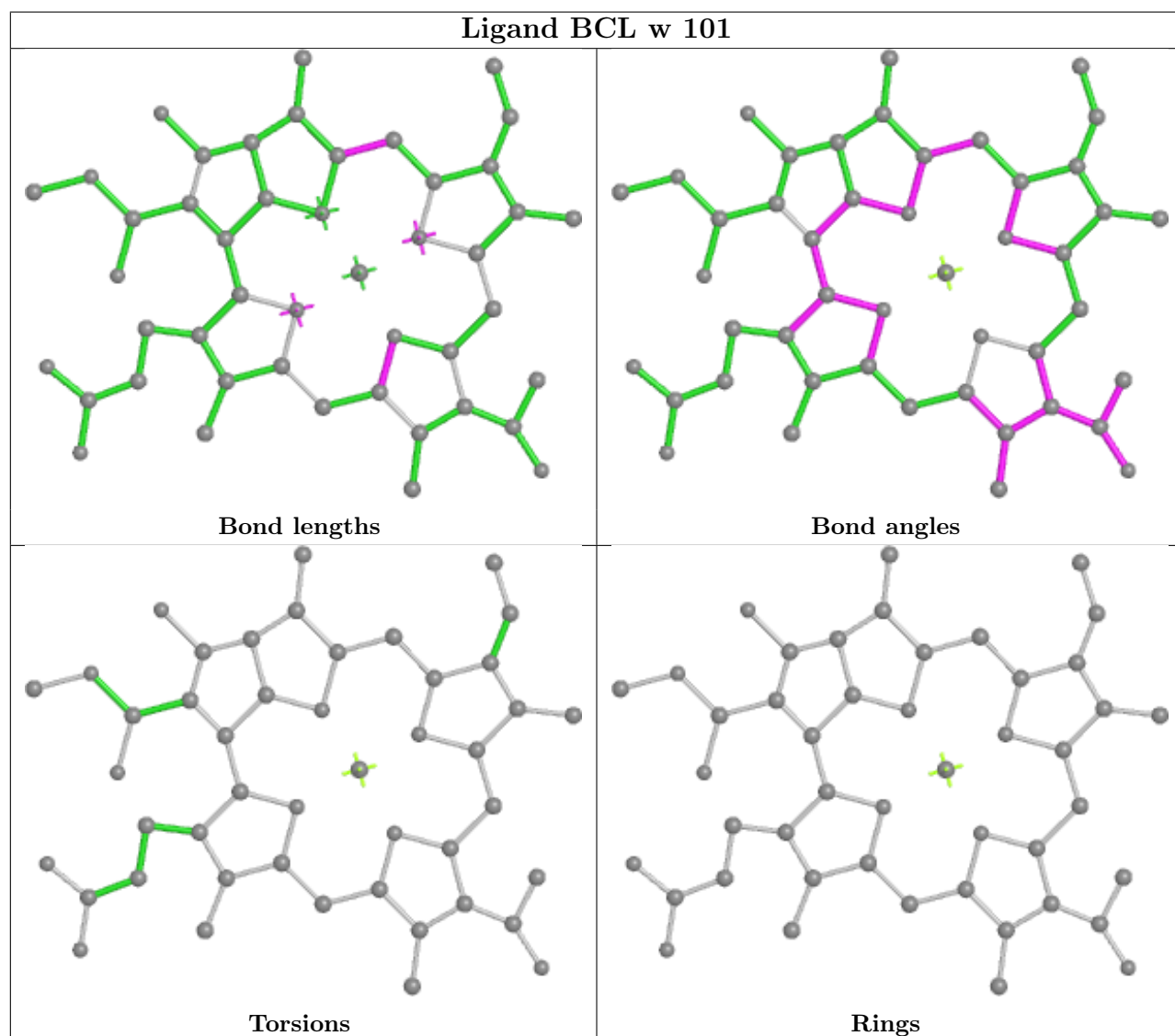
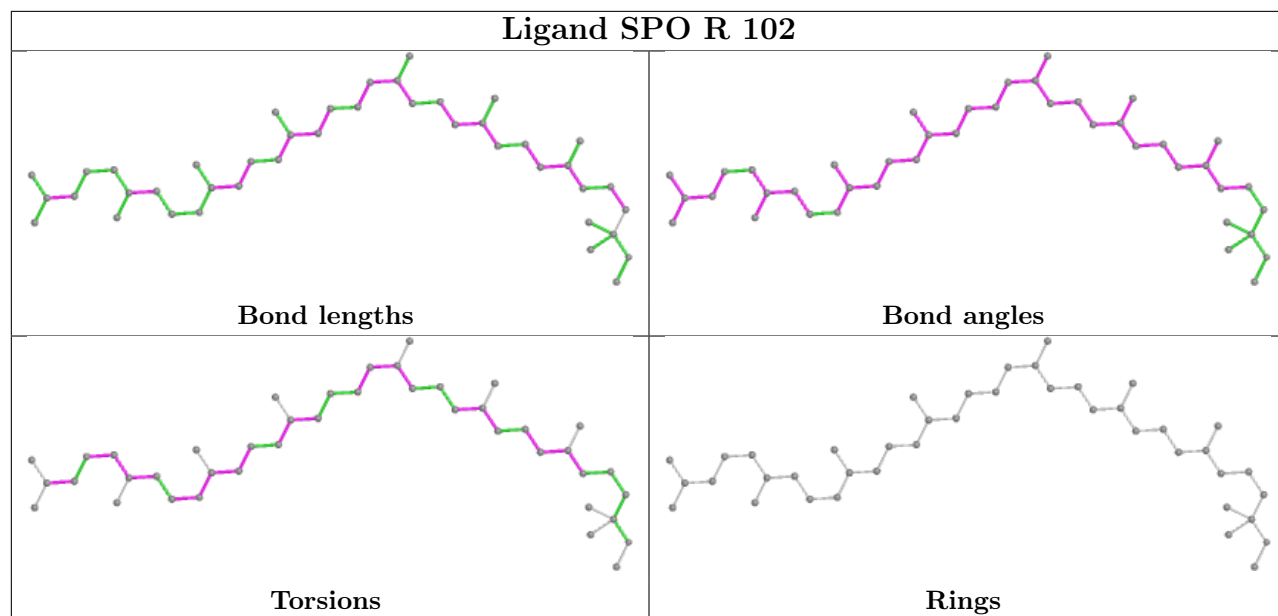


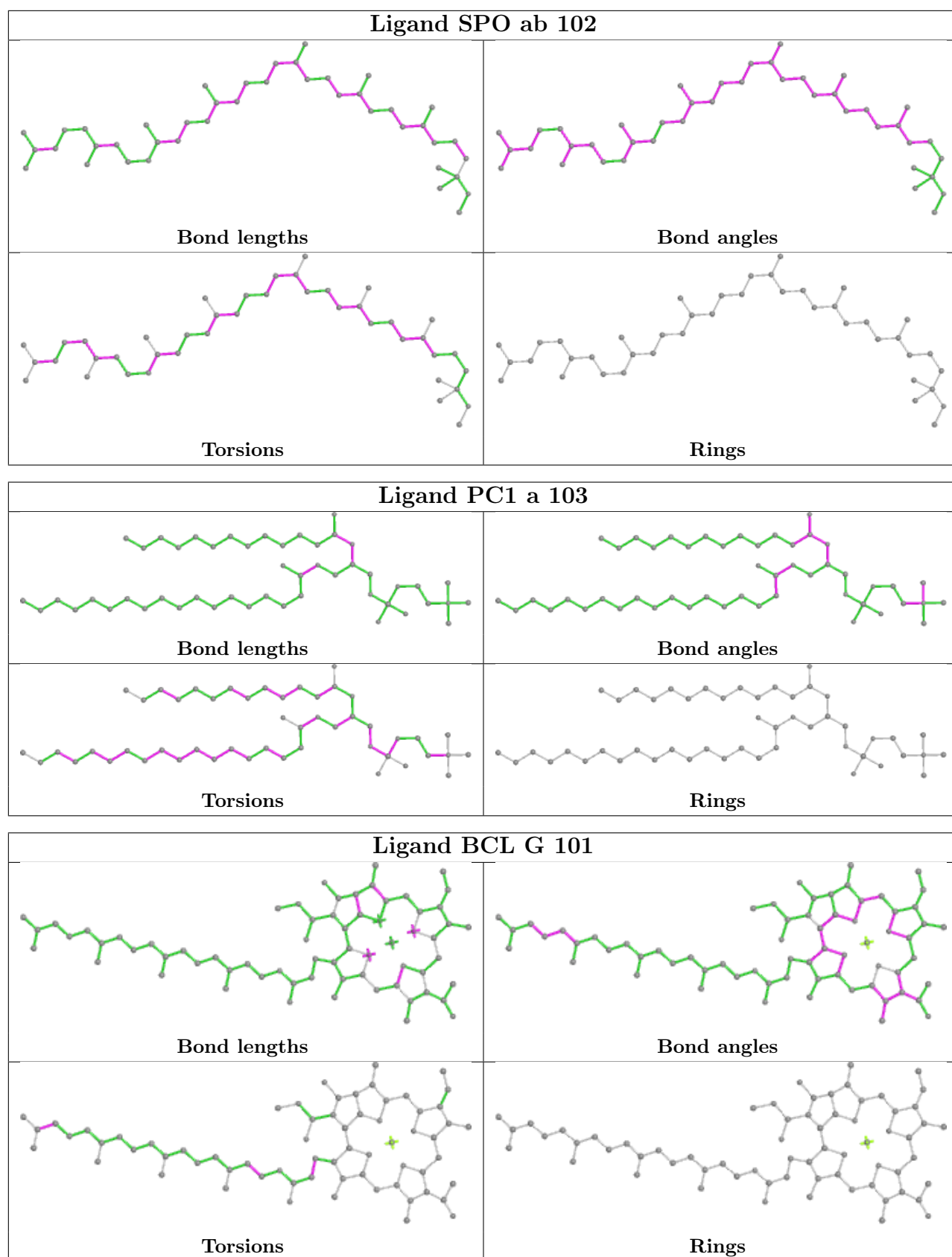


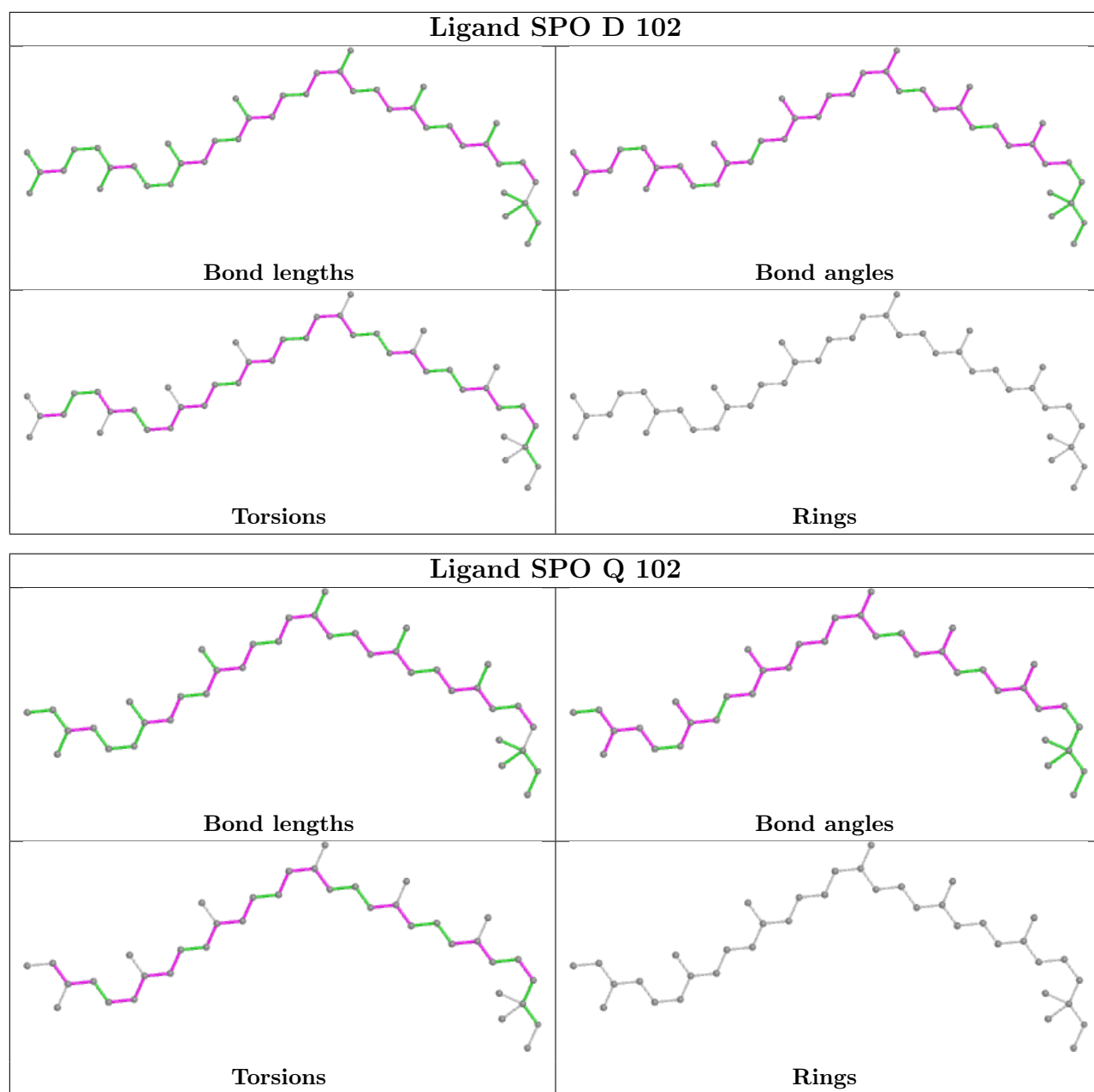


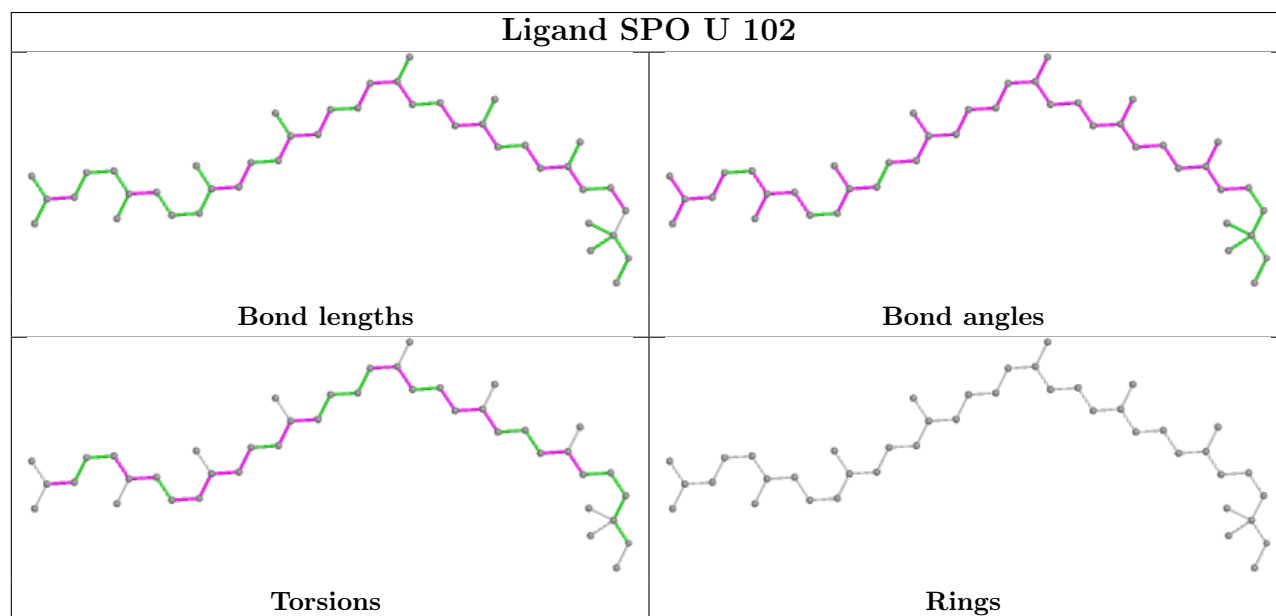
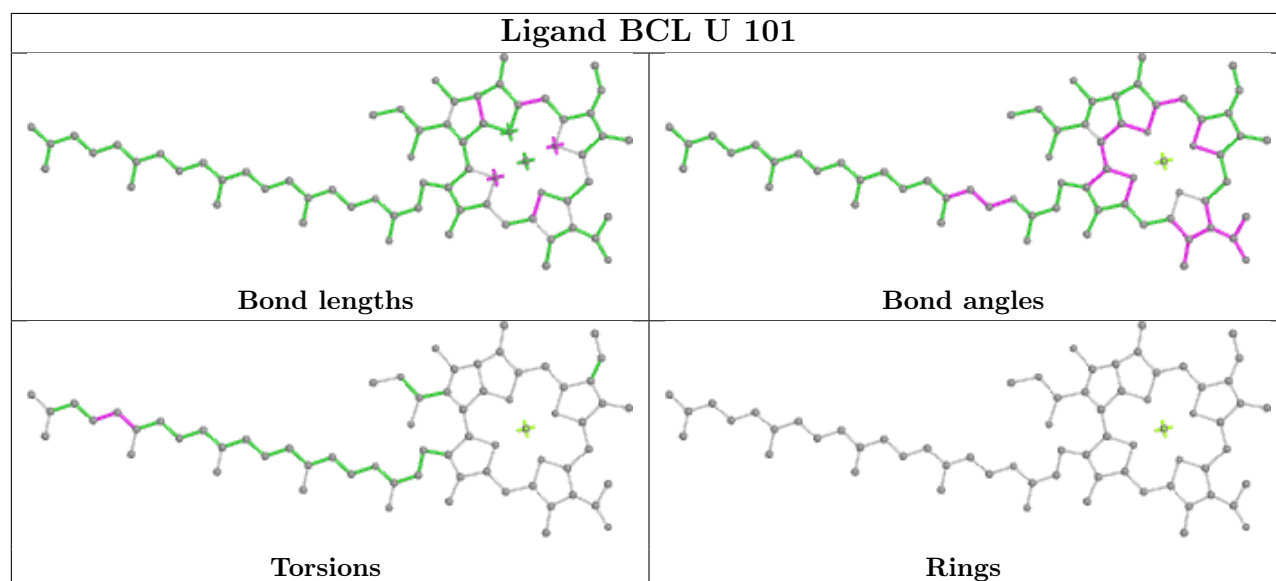
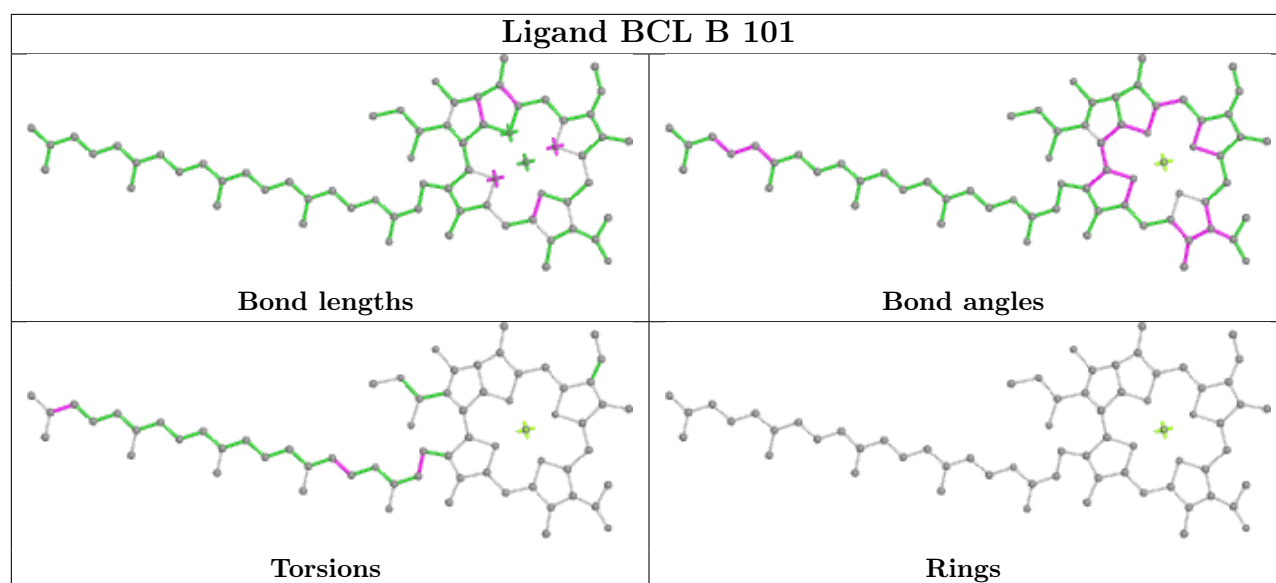


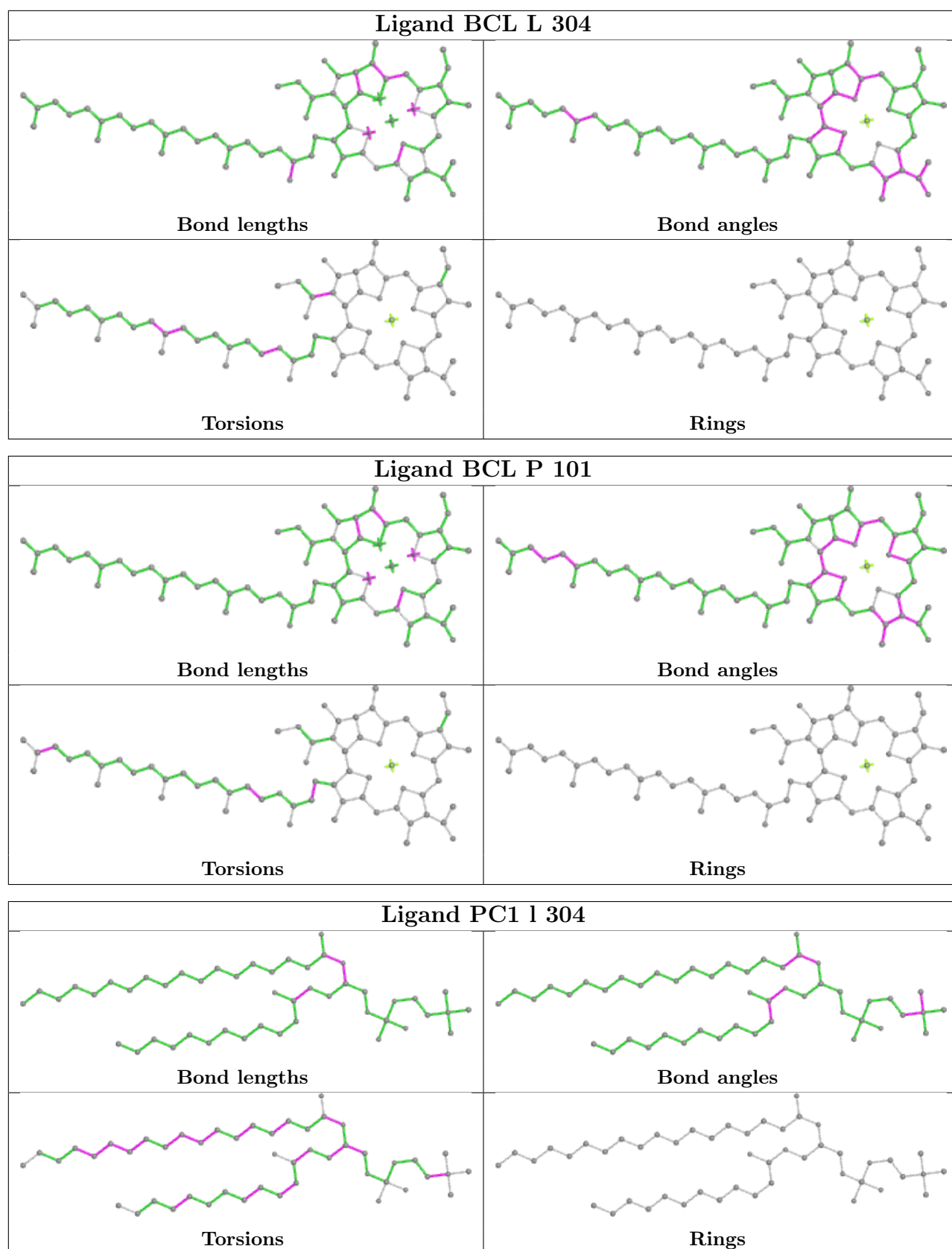


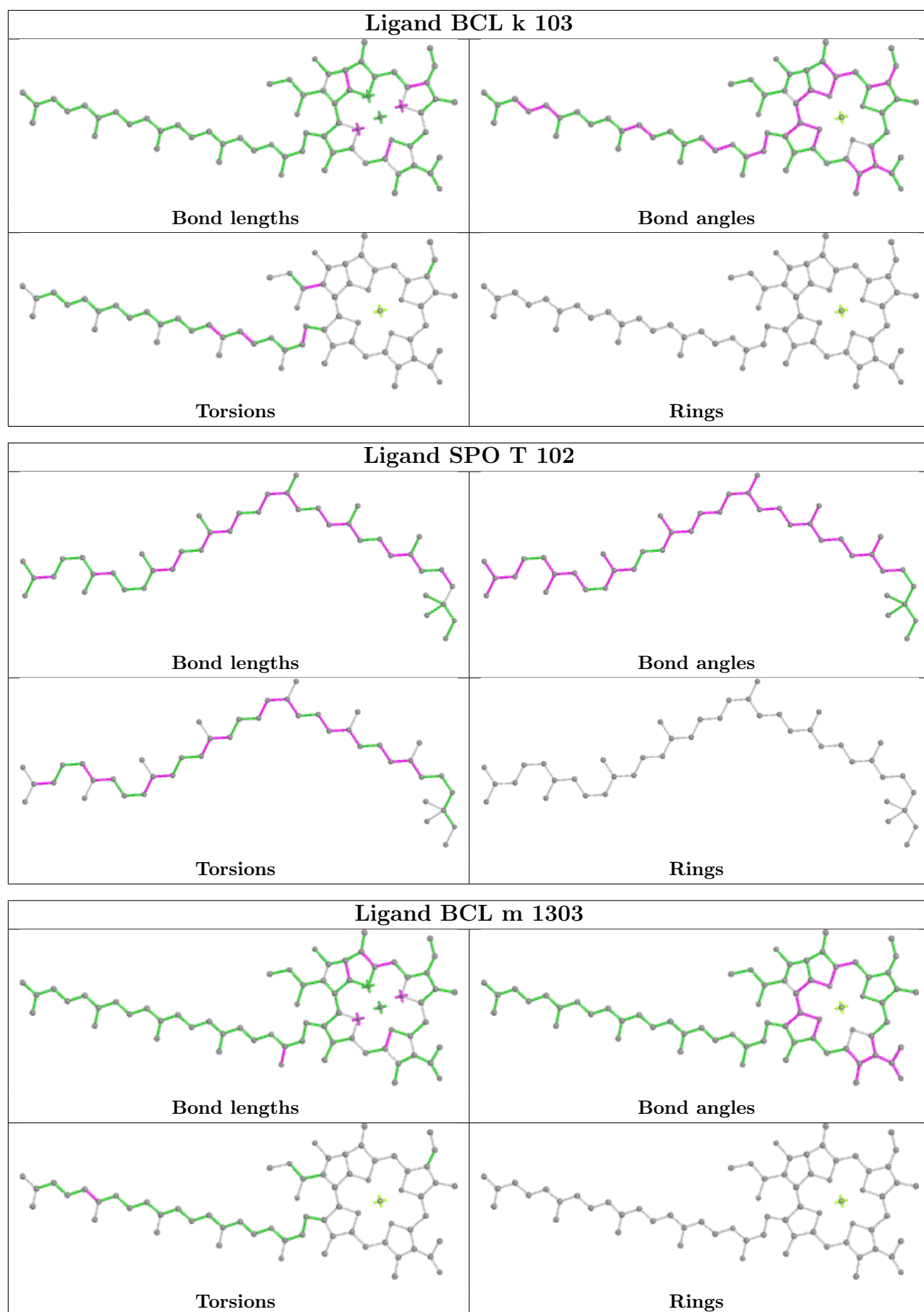


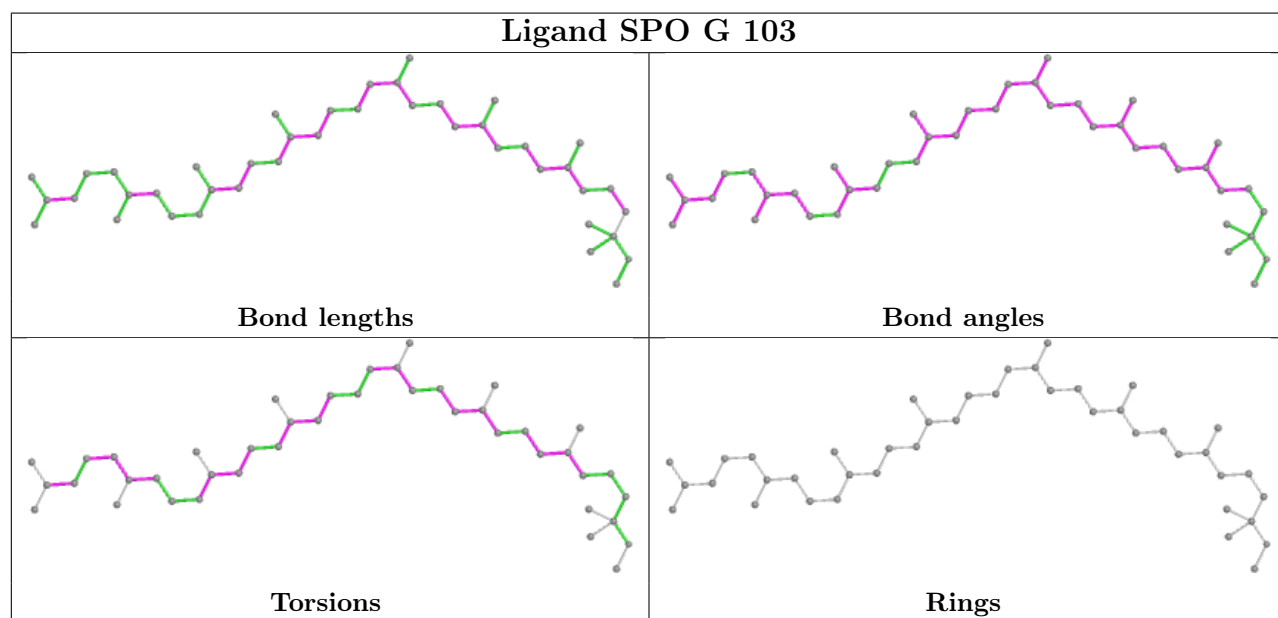
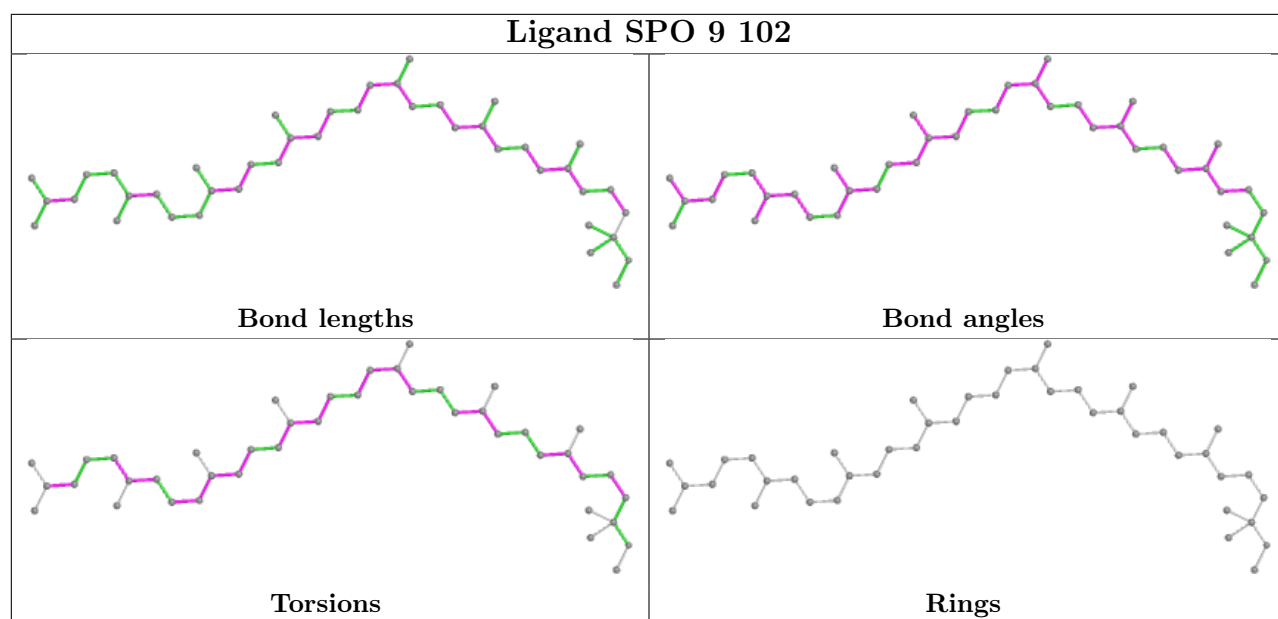


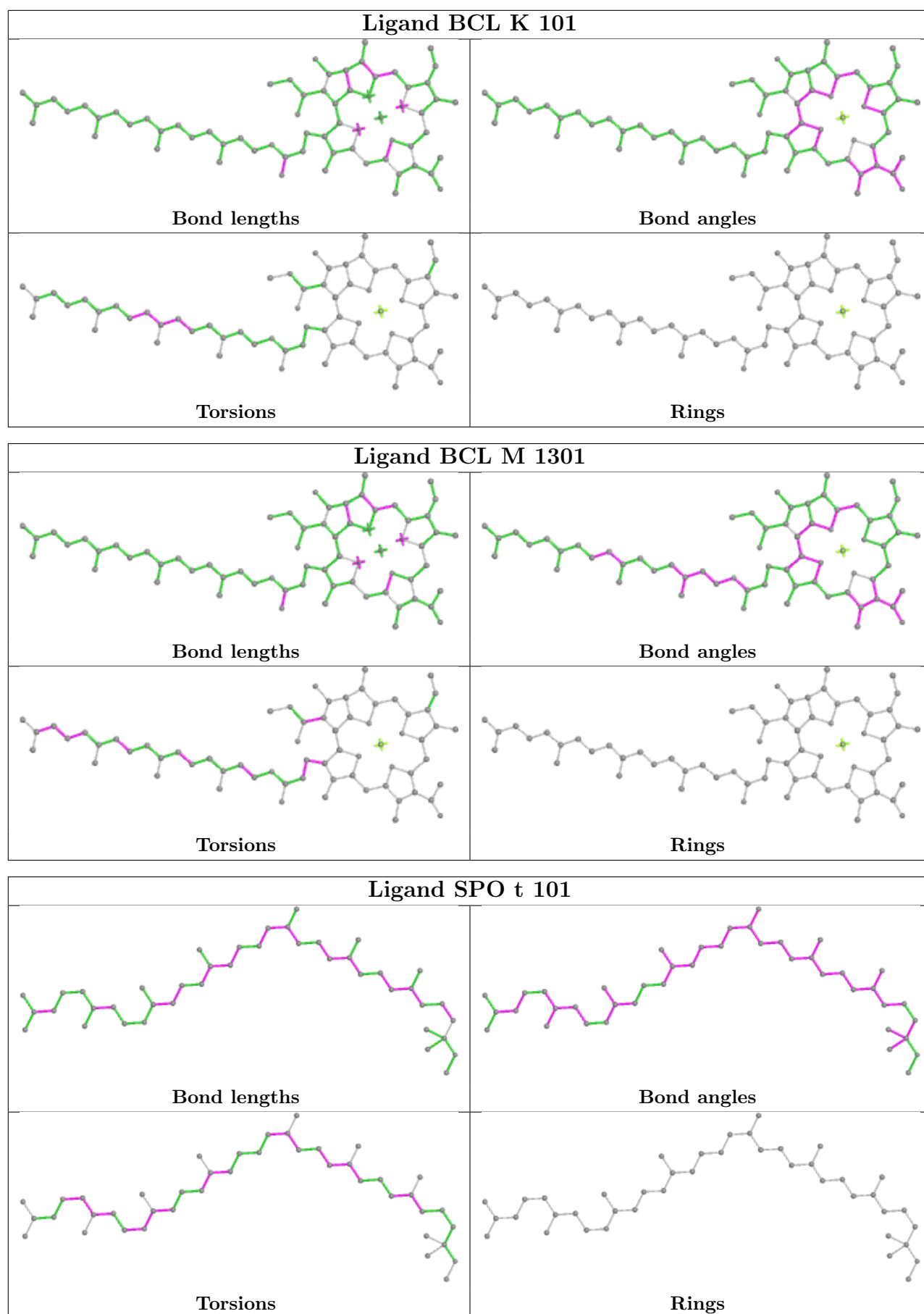




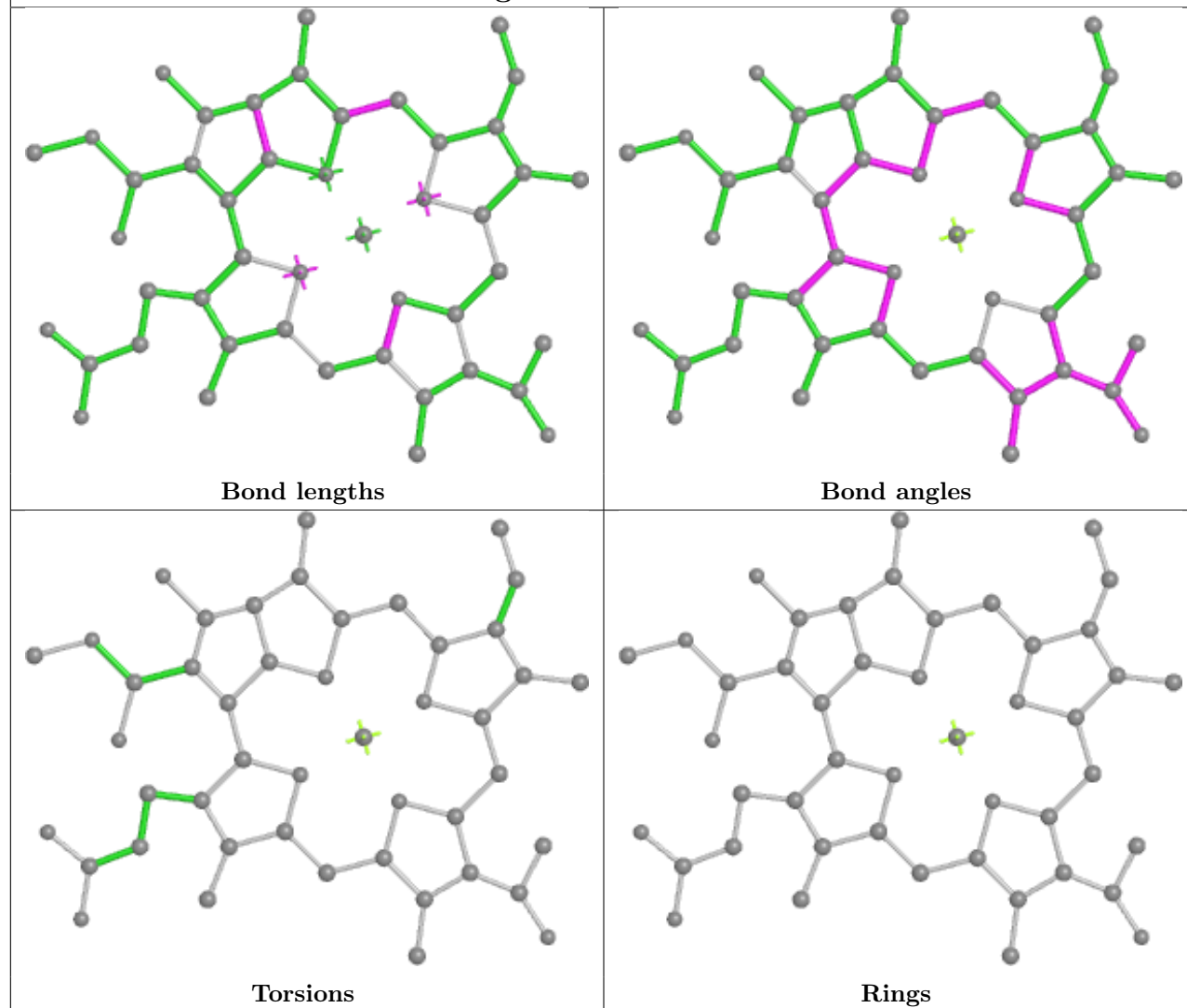




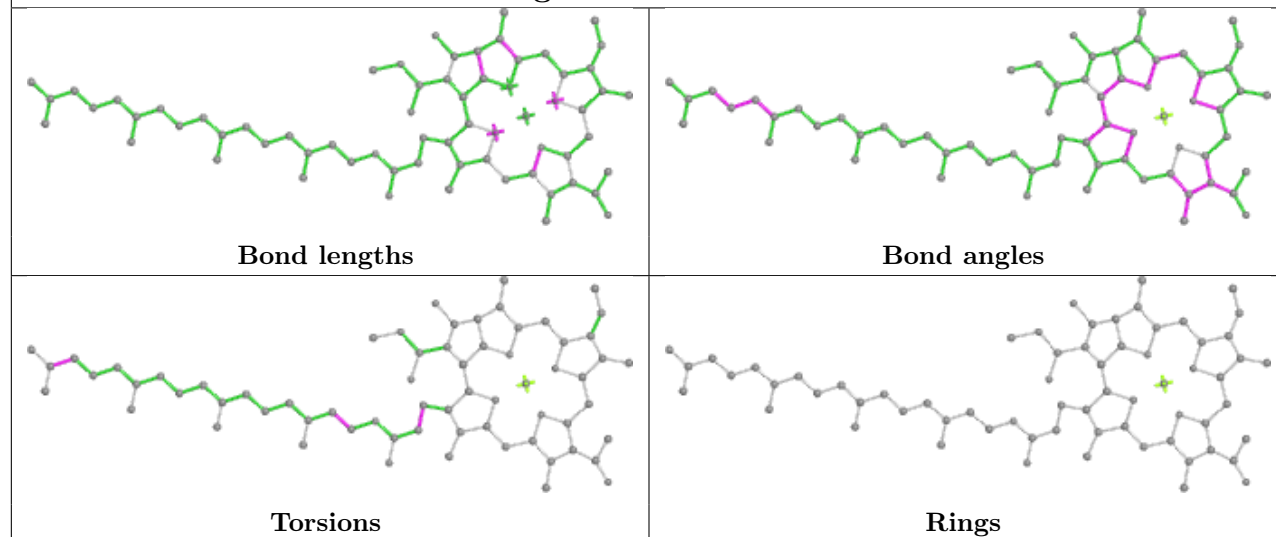


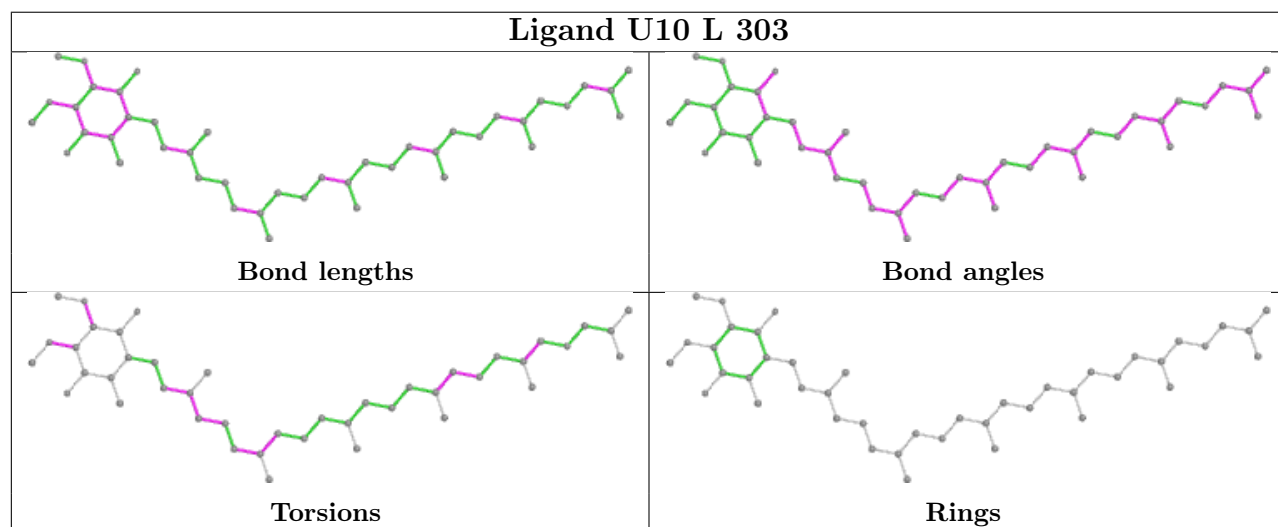
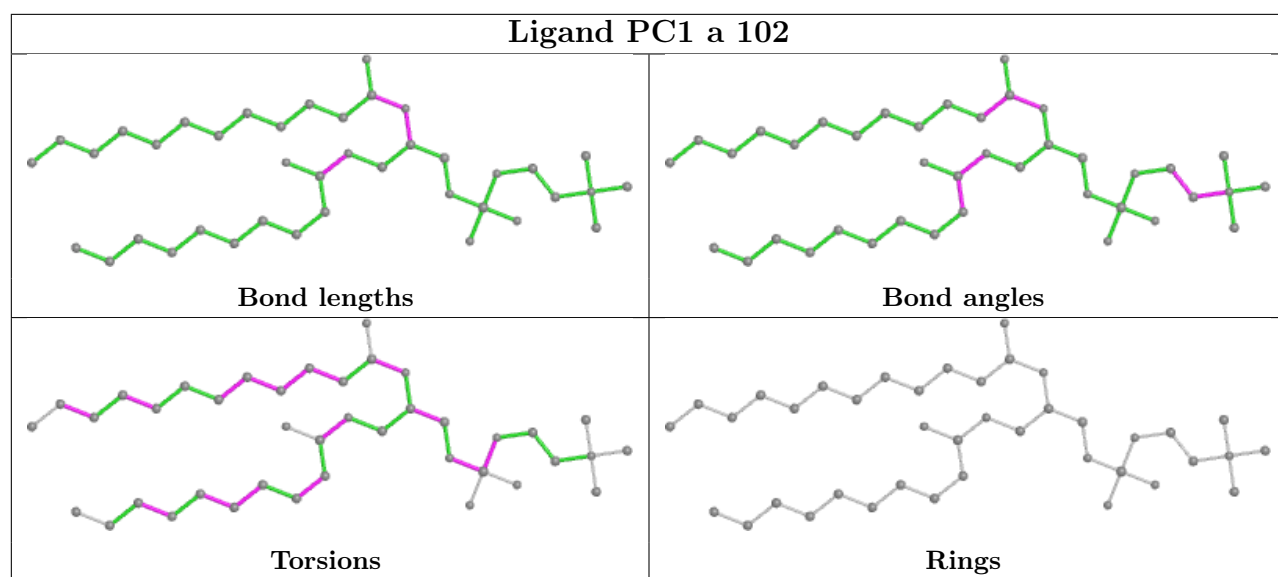


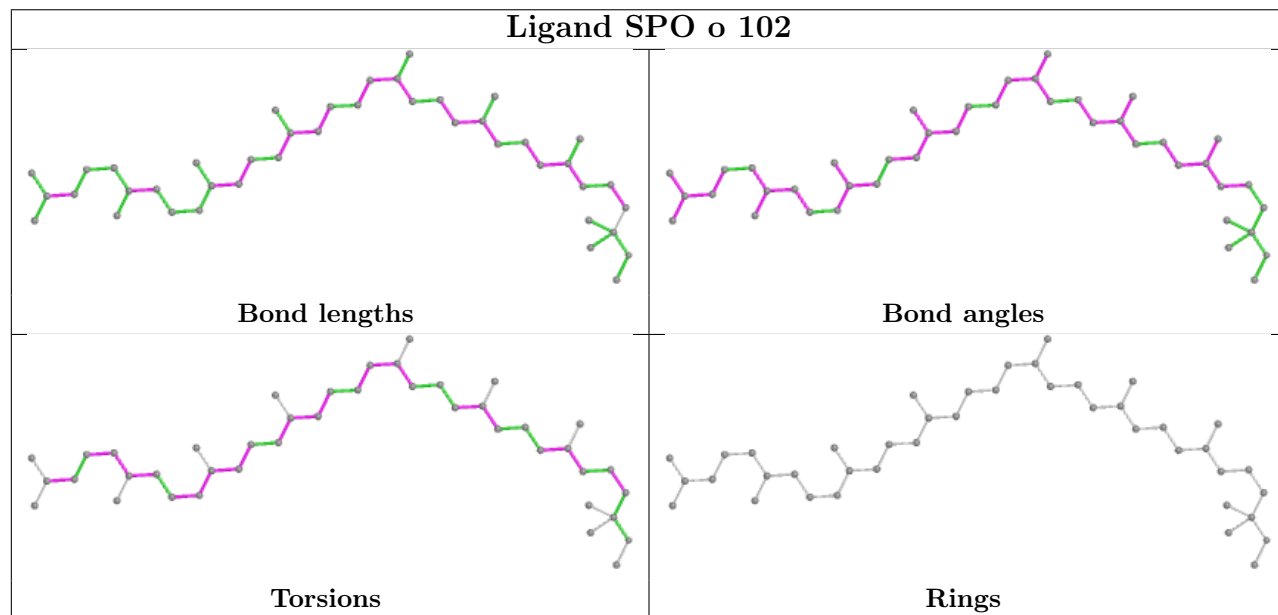
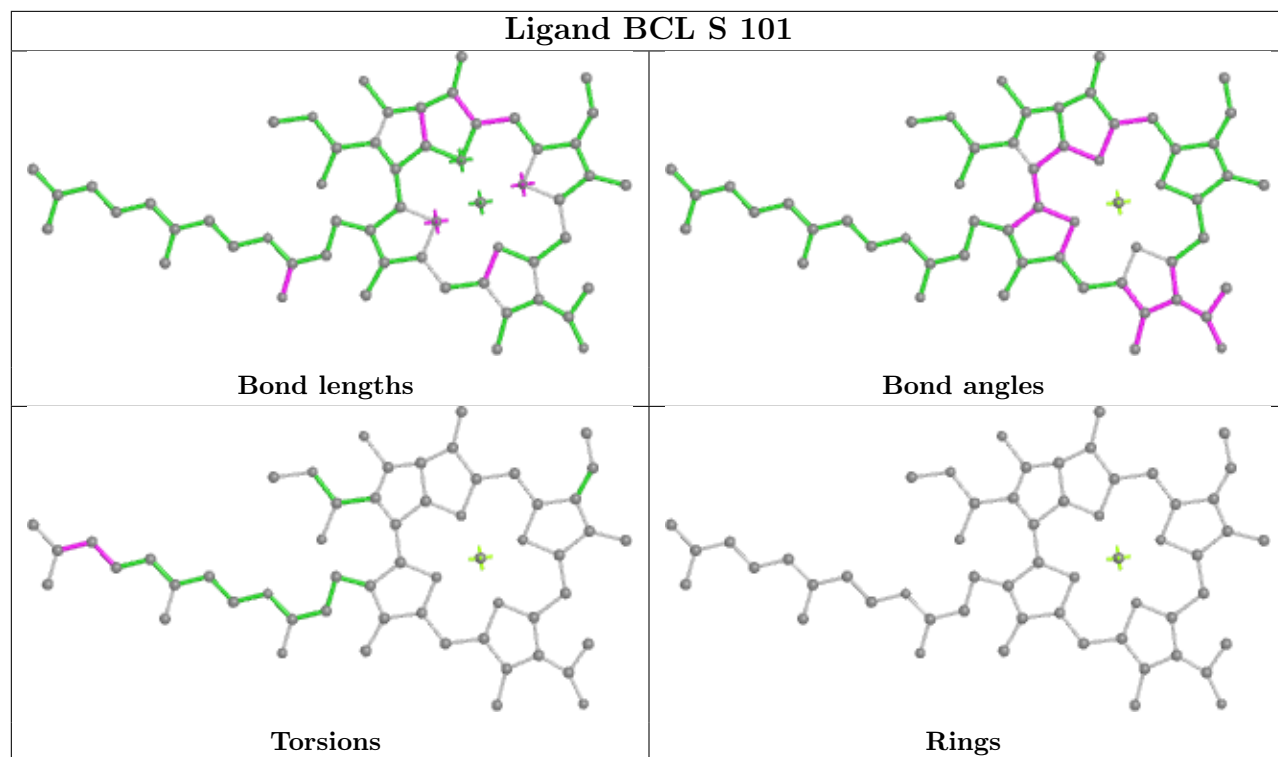
## Ligand BCL Y 201



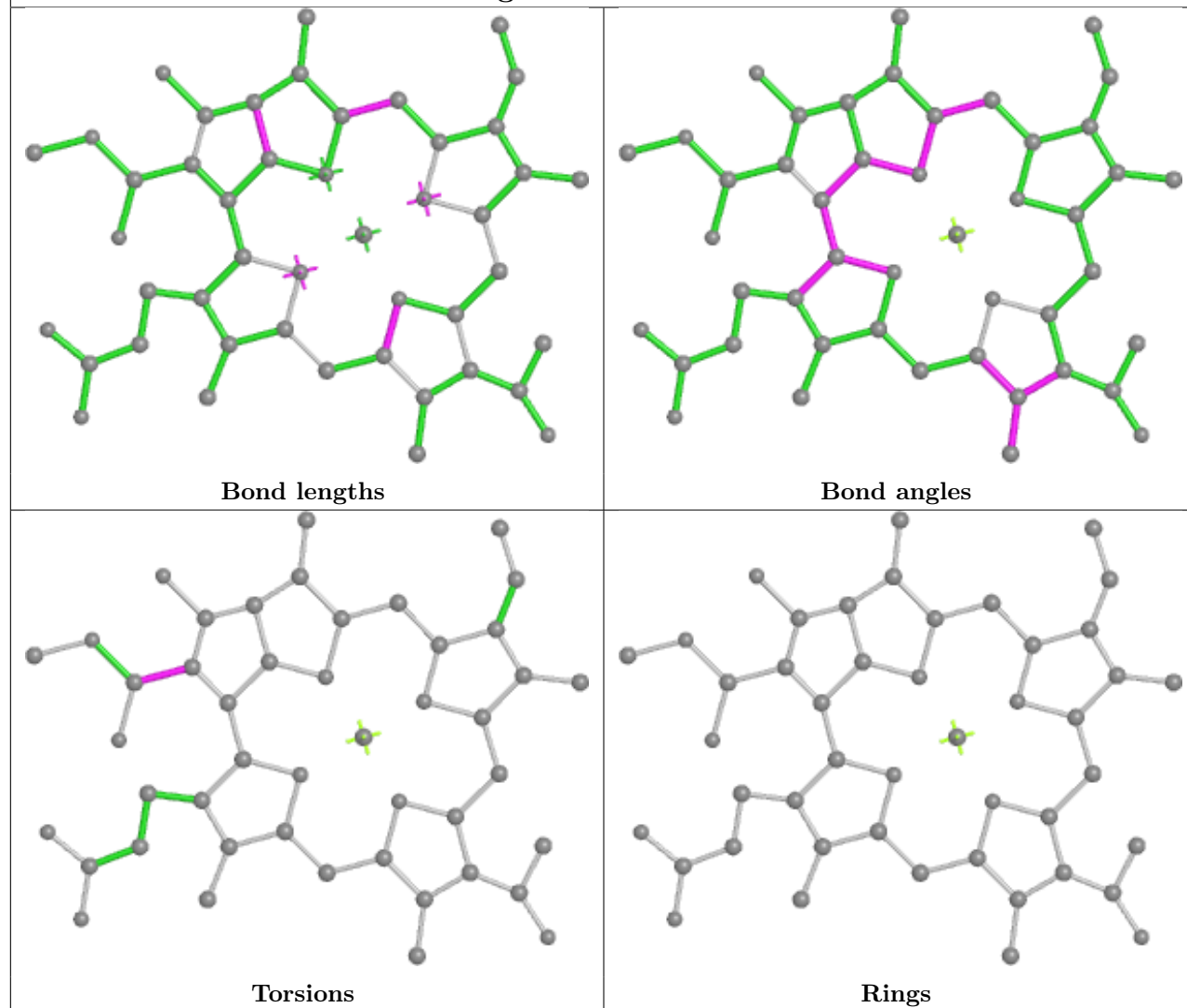
## Ligand BCL T 101



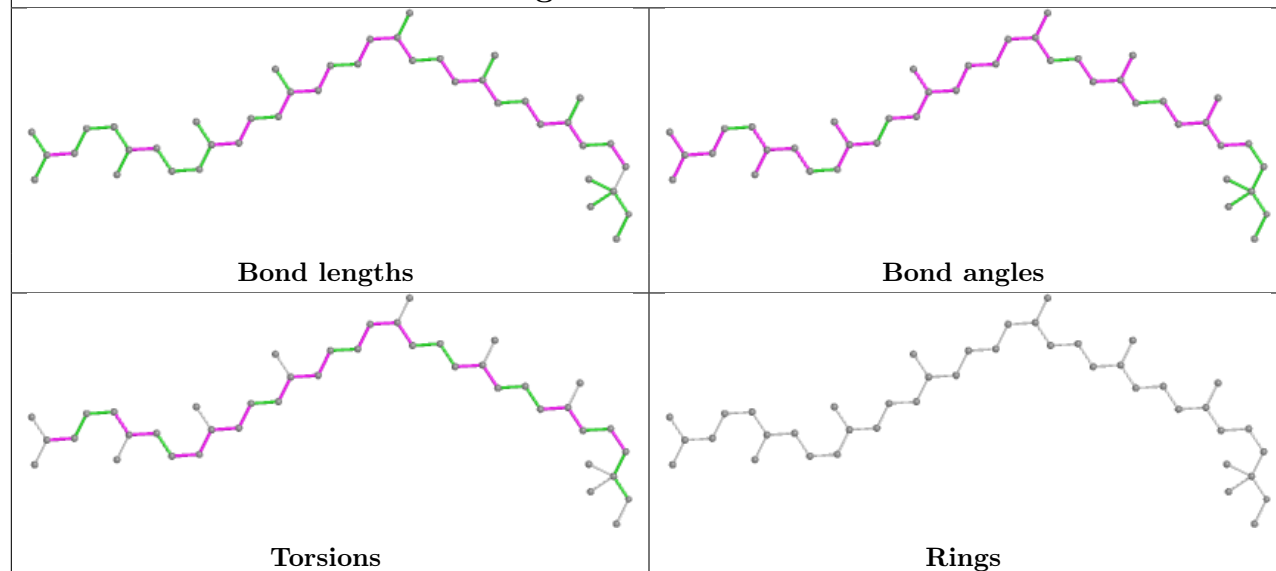


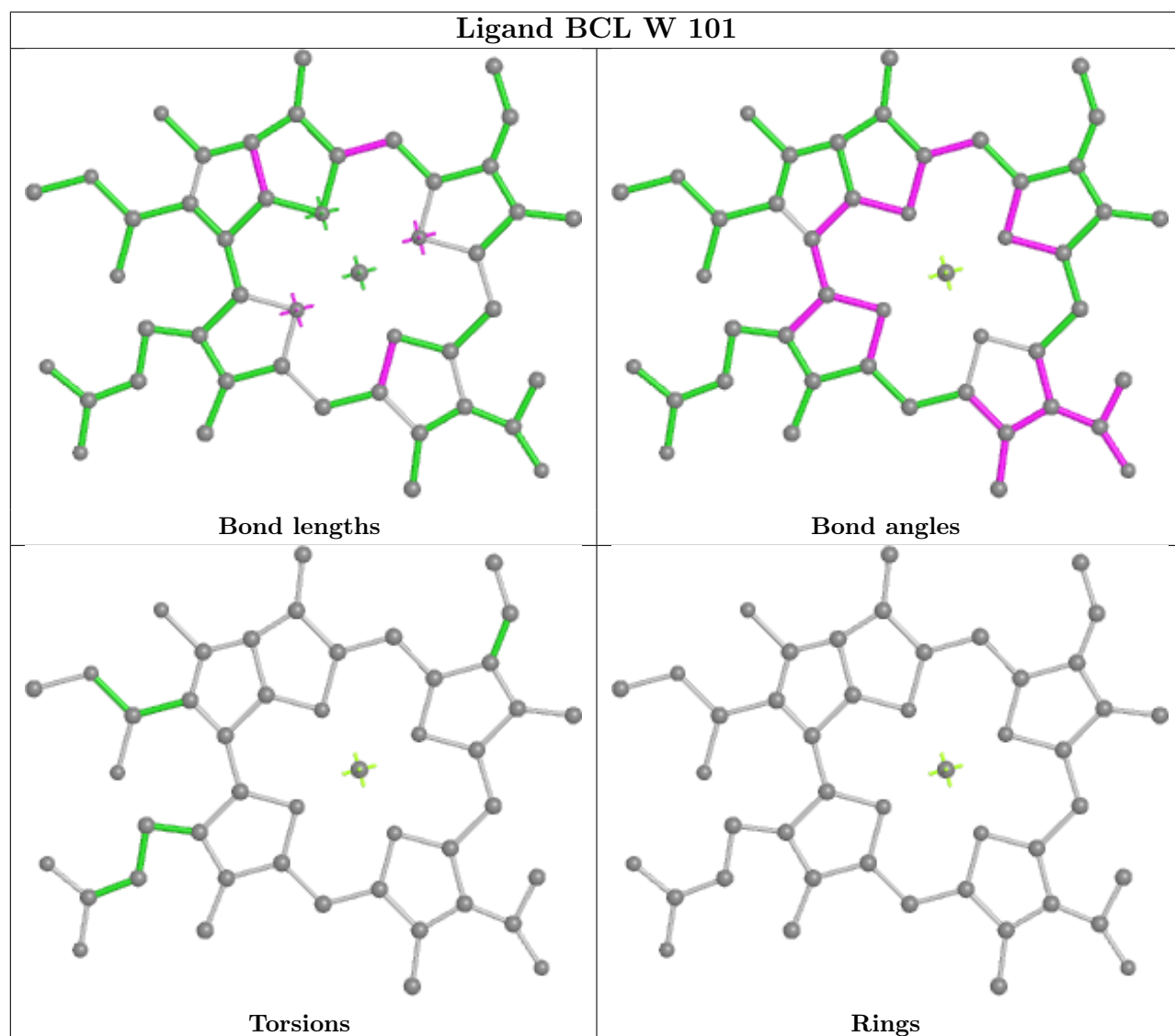
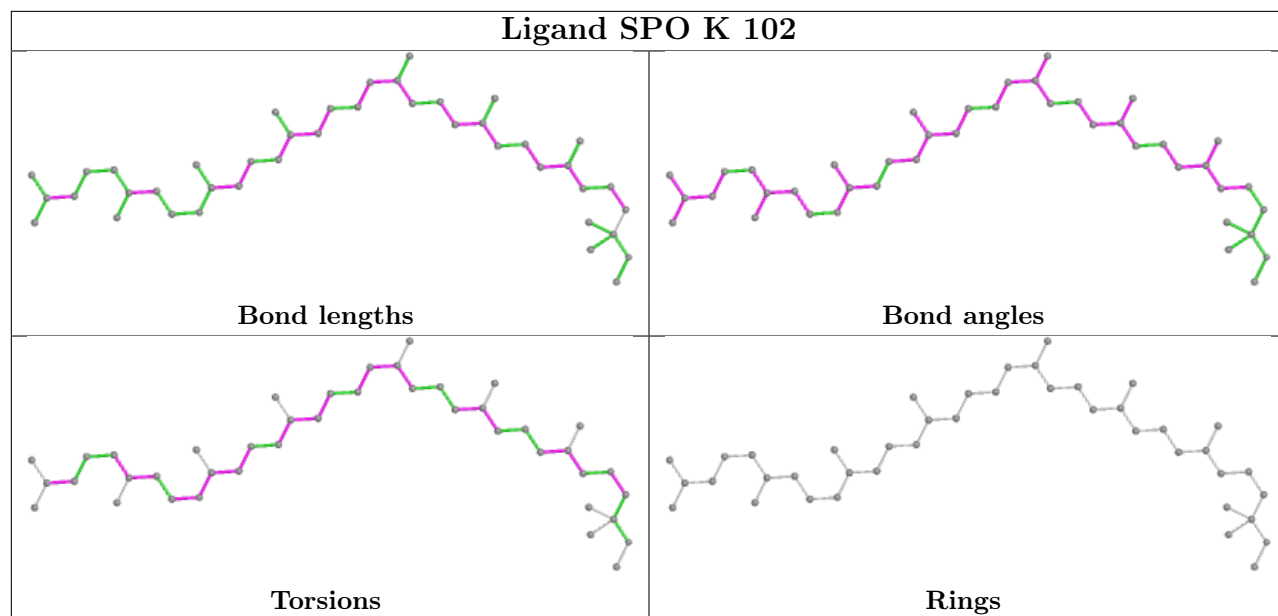


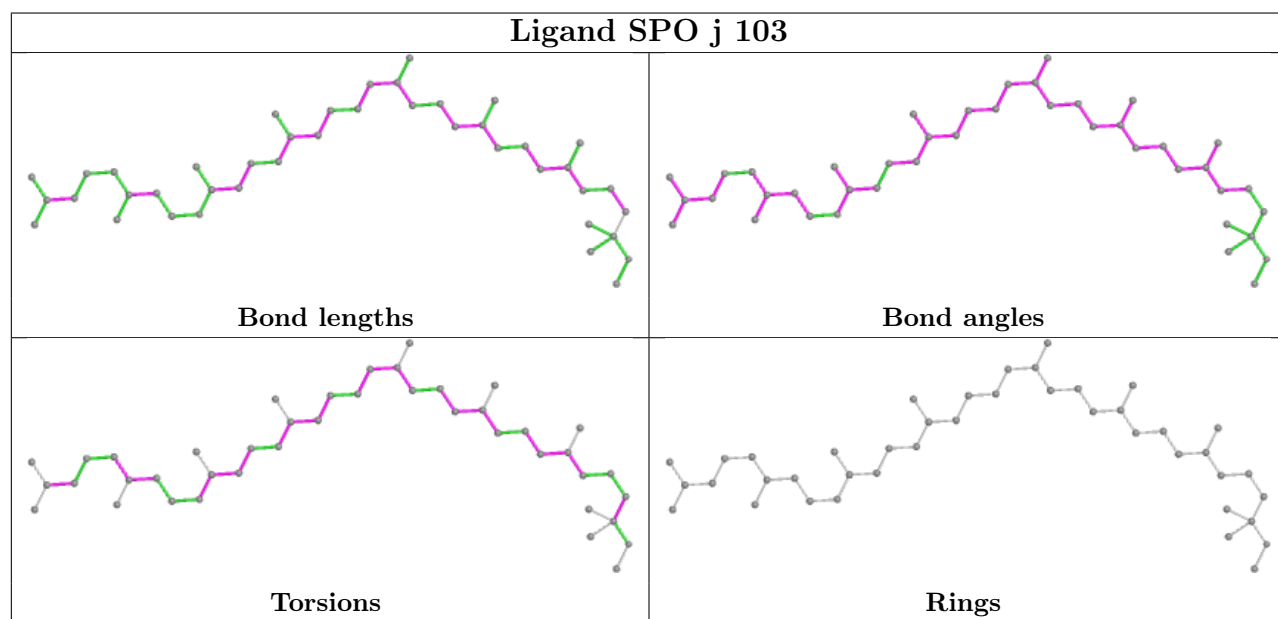
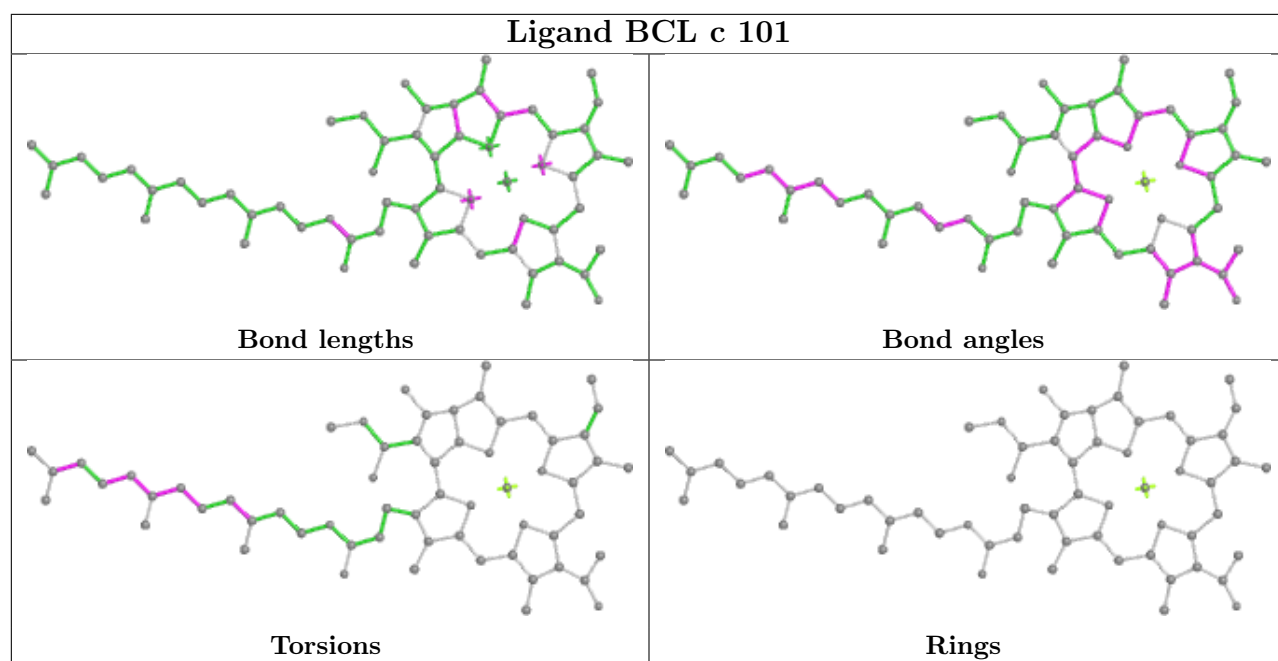
## Ligand BCL Z 101

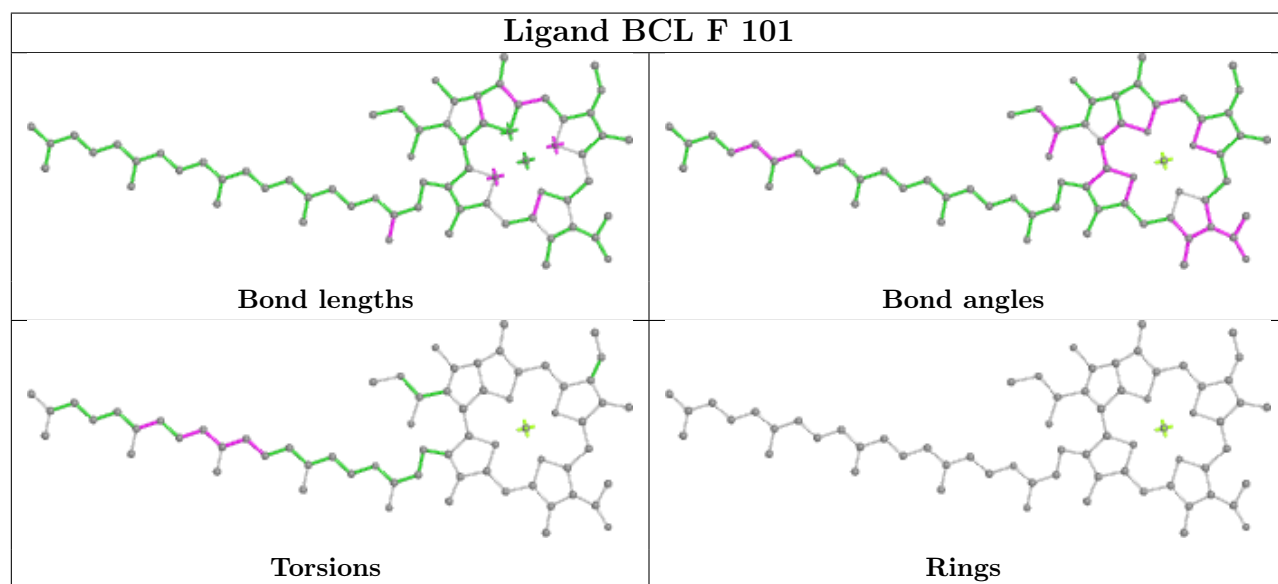
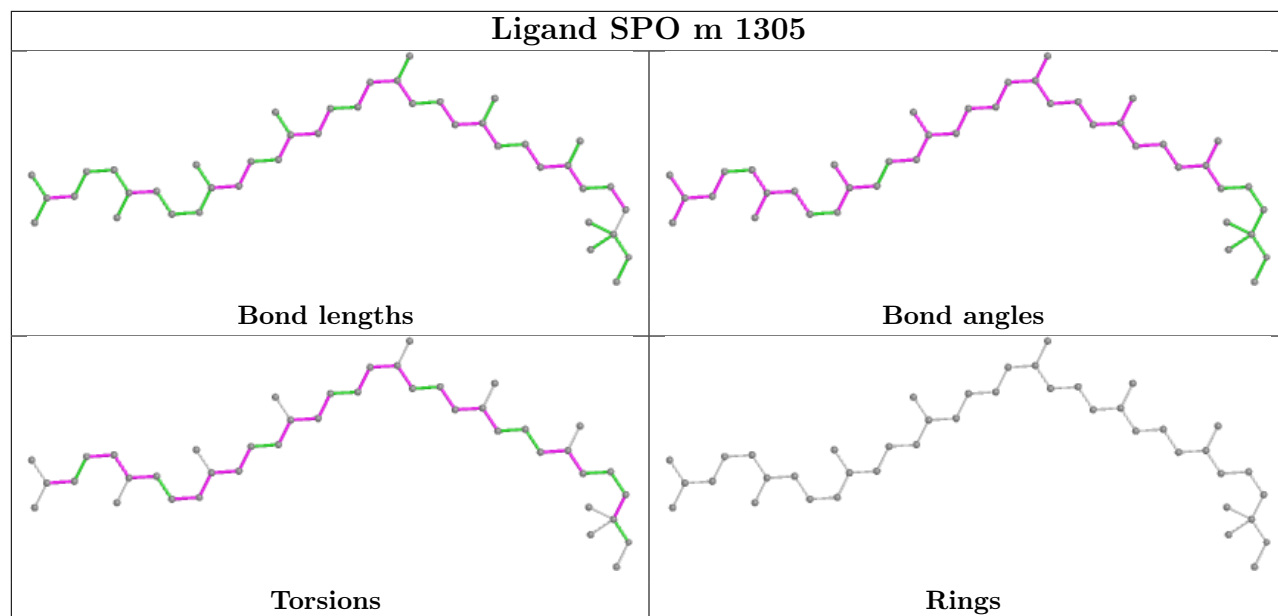


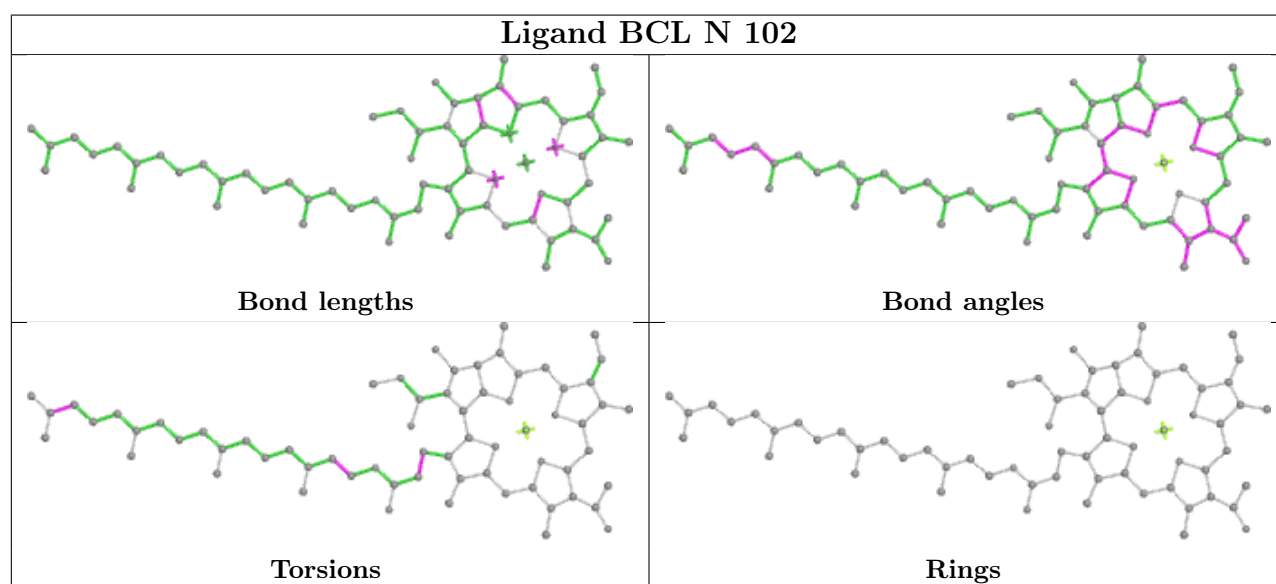
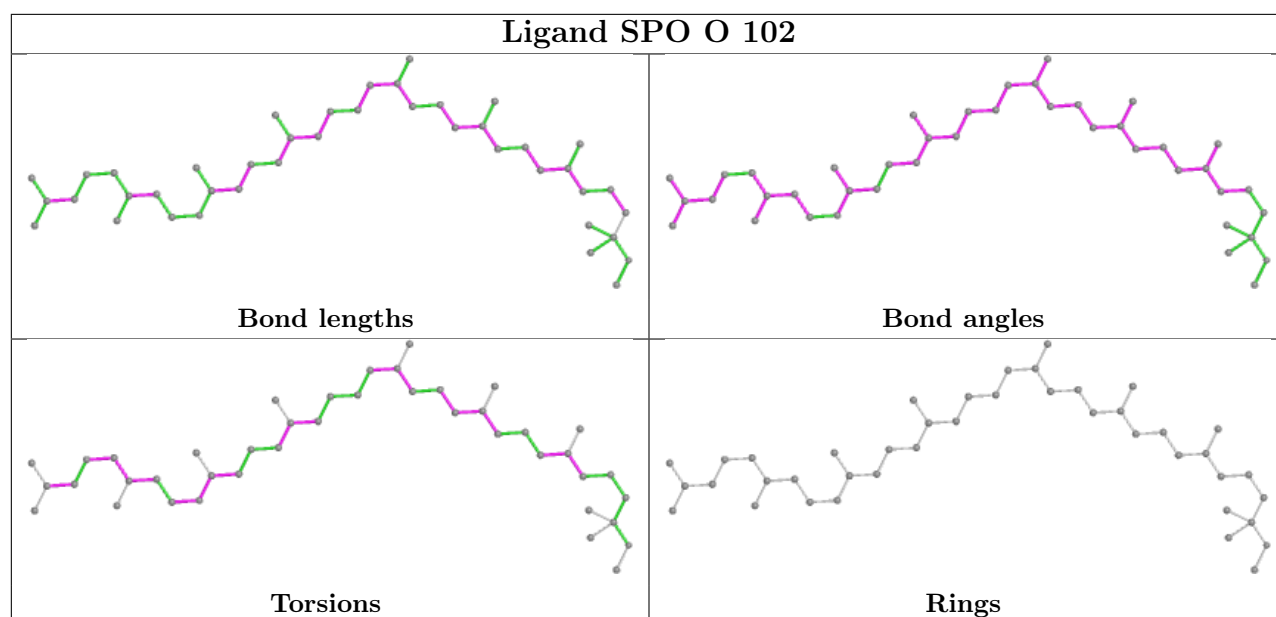
## Ligand SPO F 102



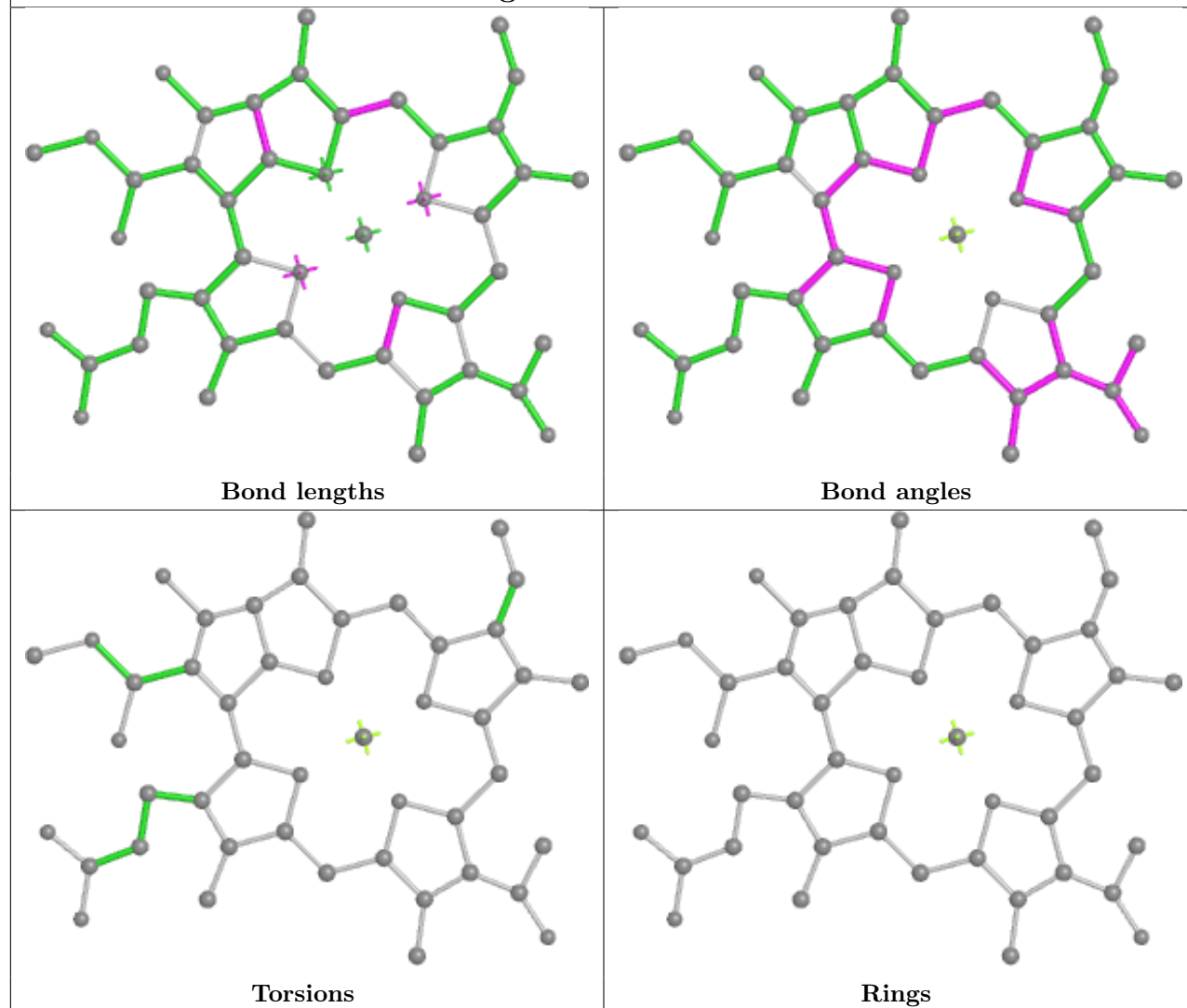




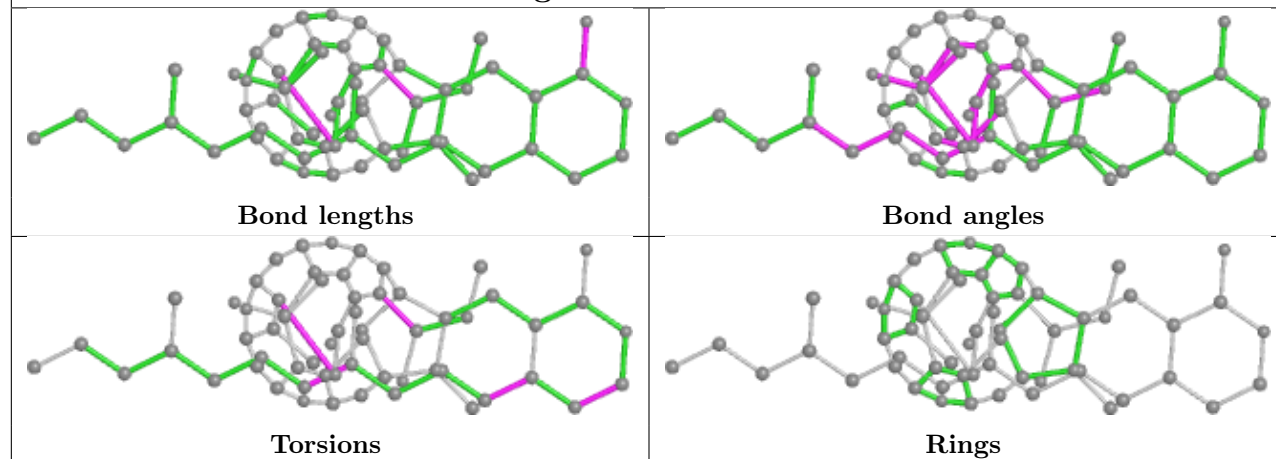


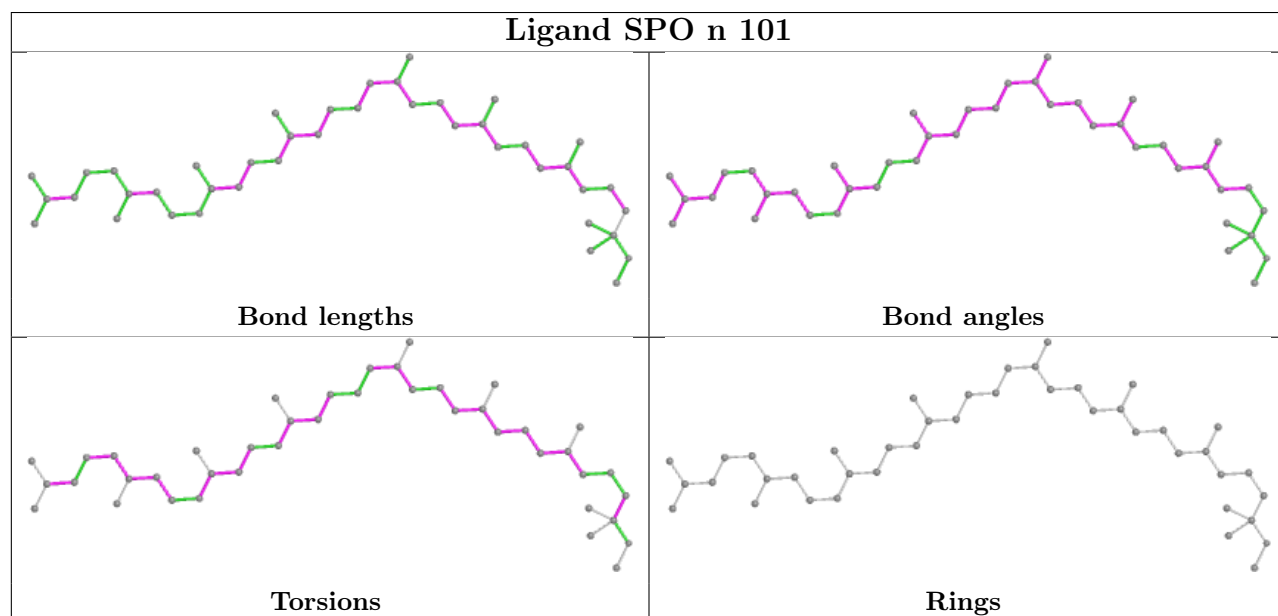
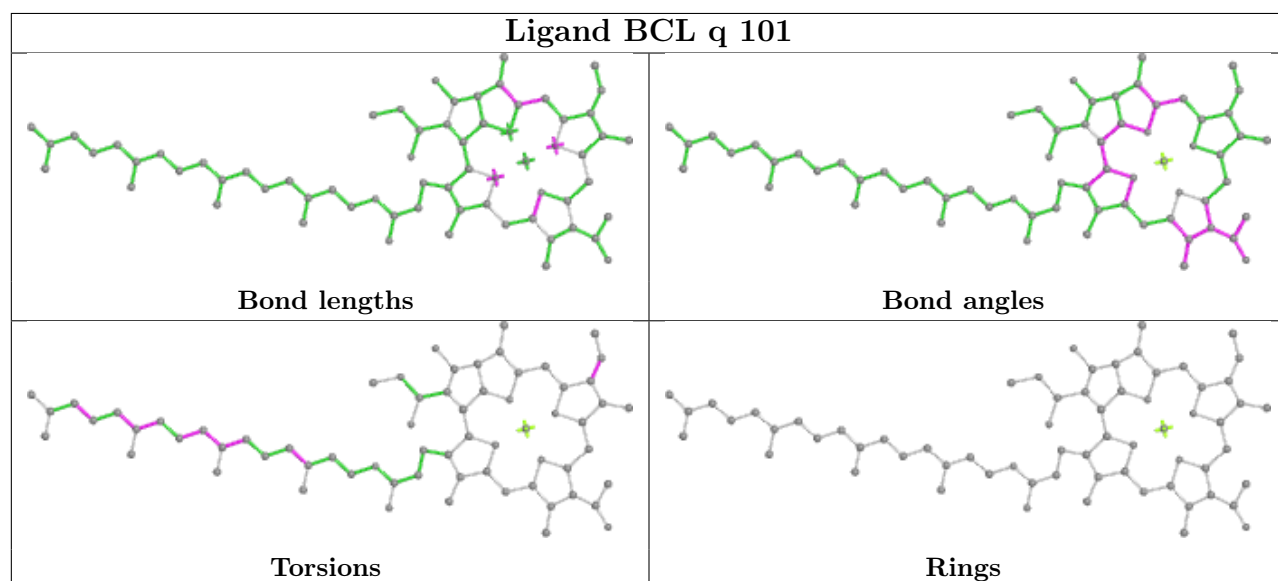
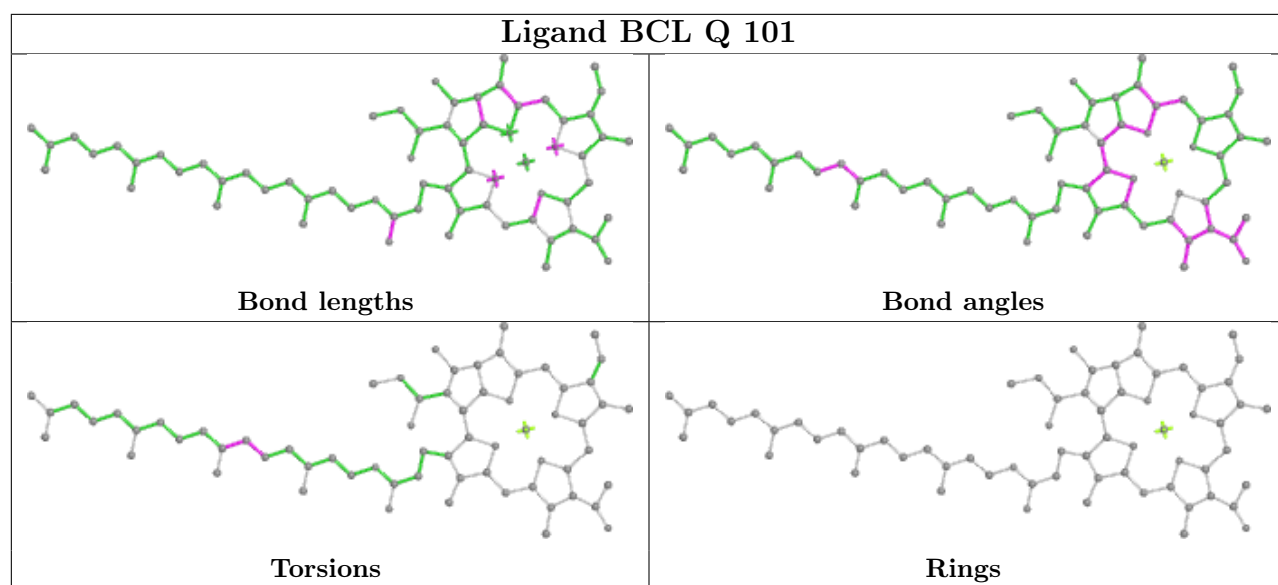


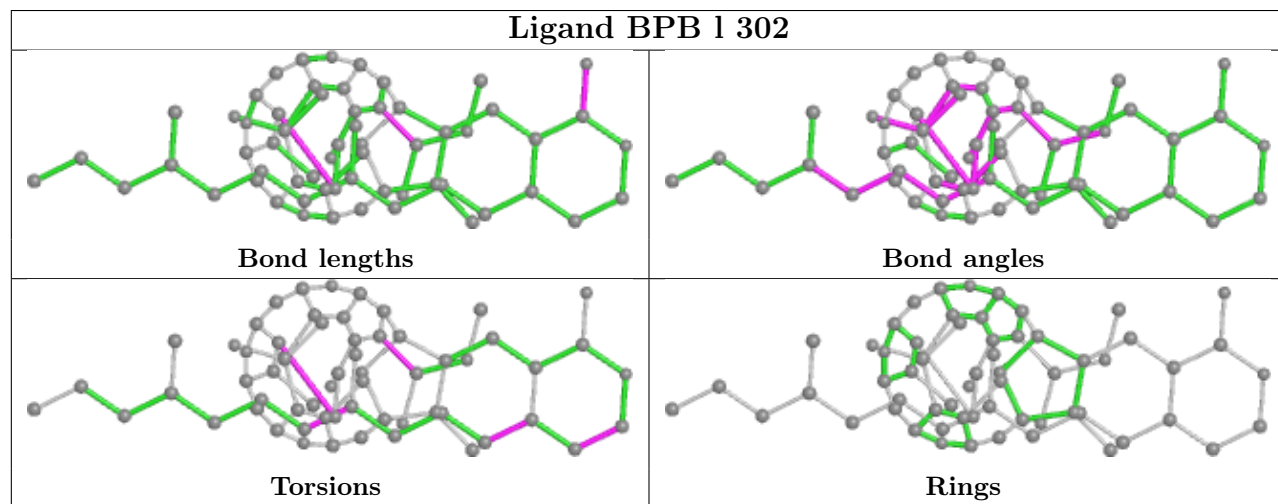
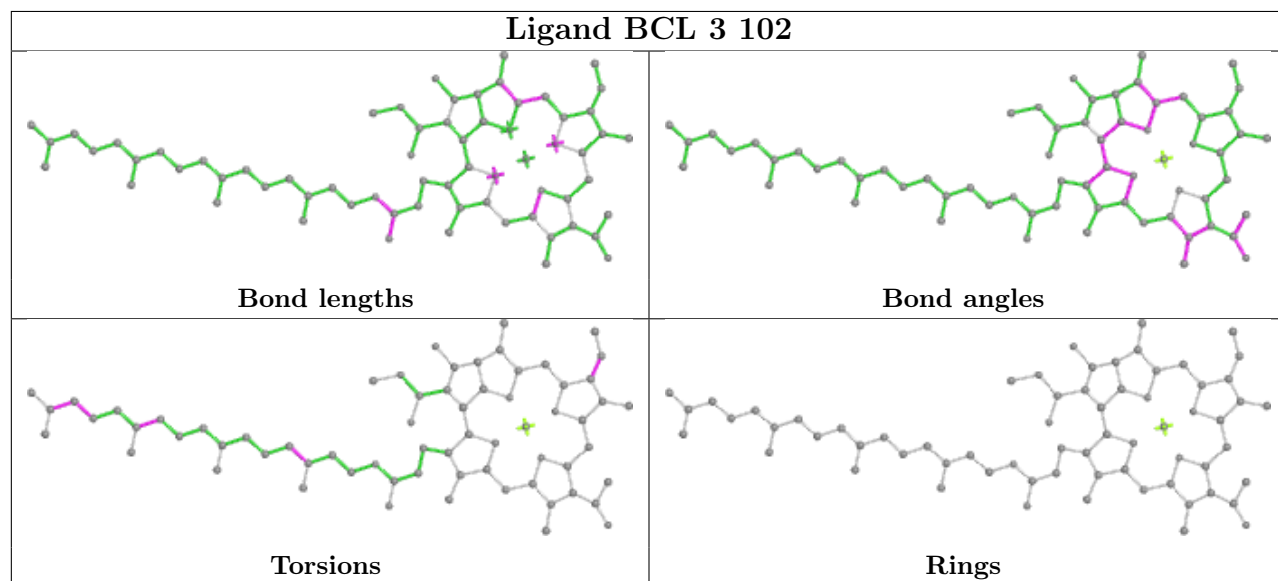
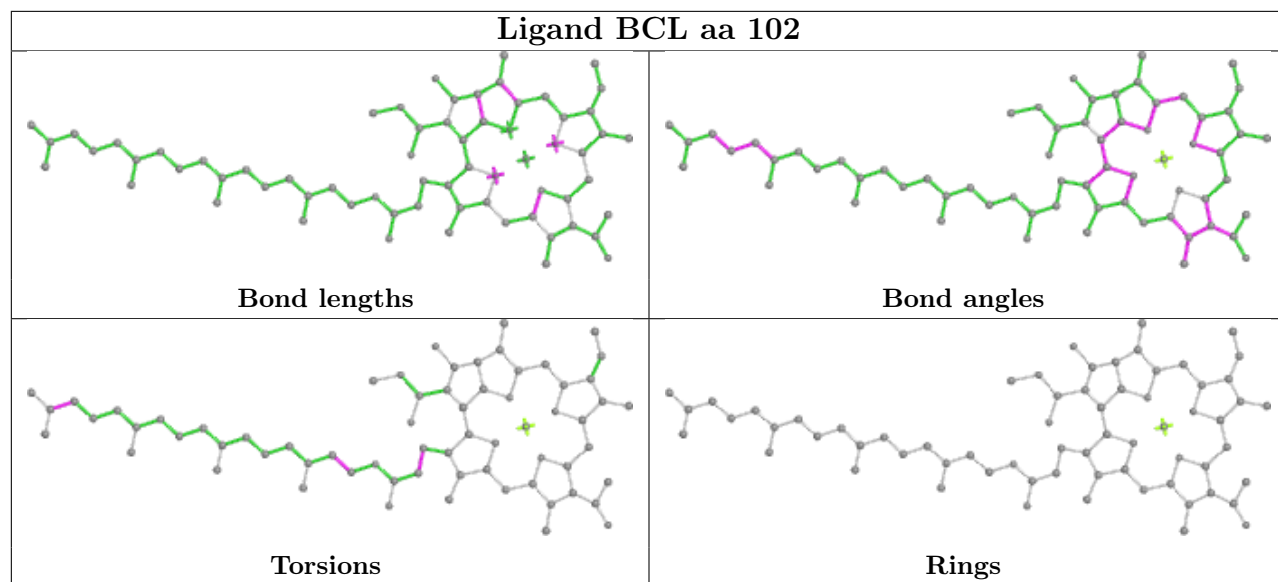
## Ligand BCL 2 101

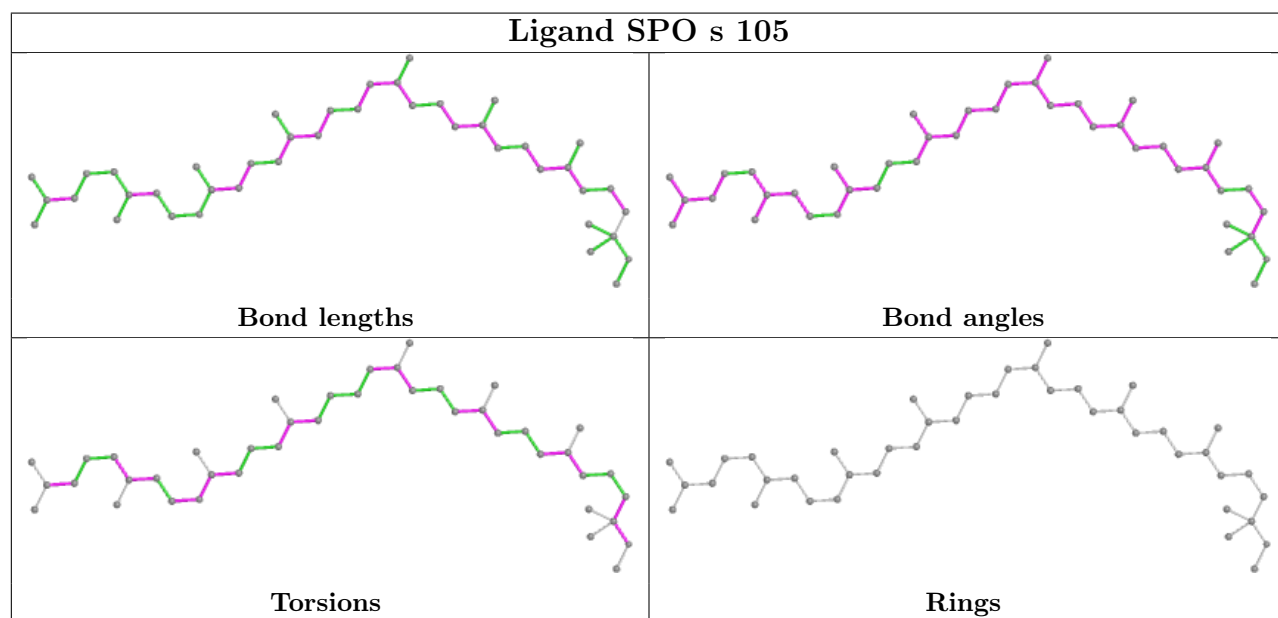
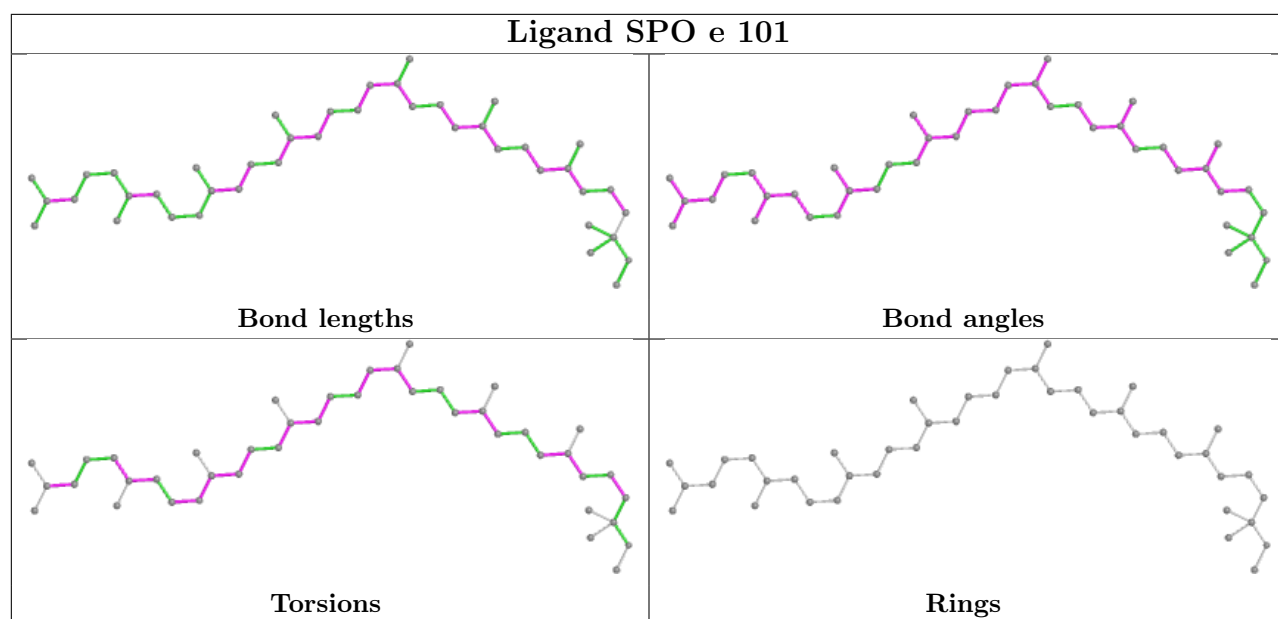


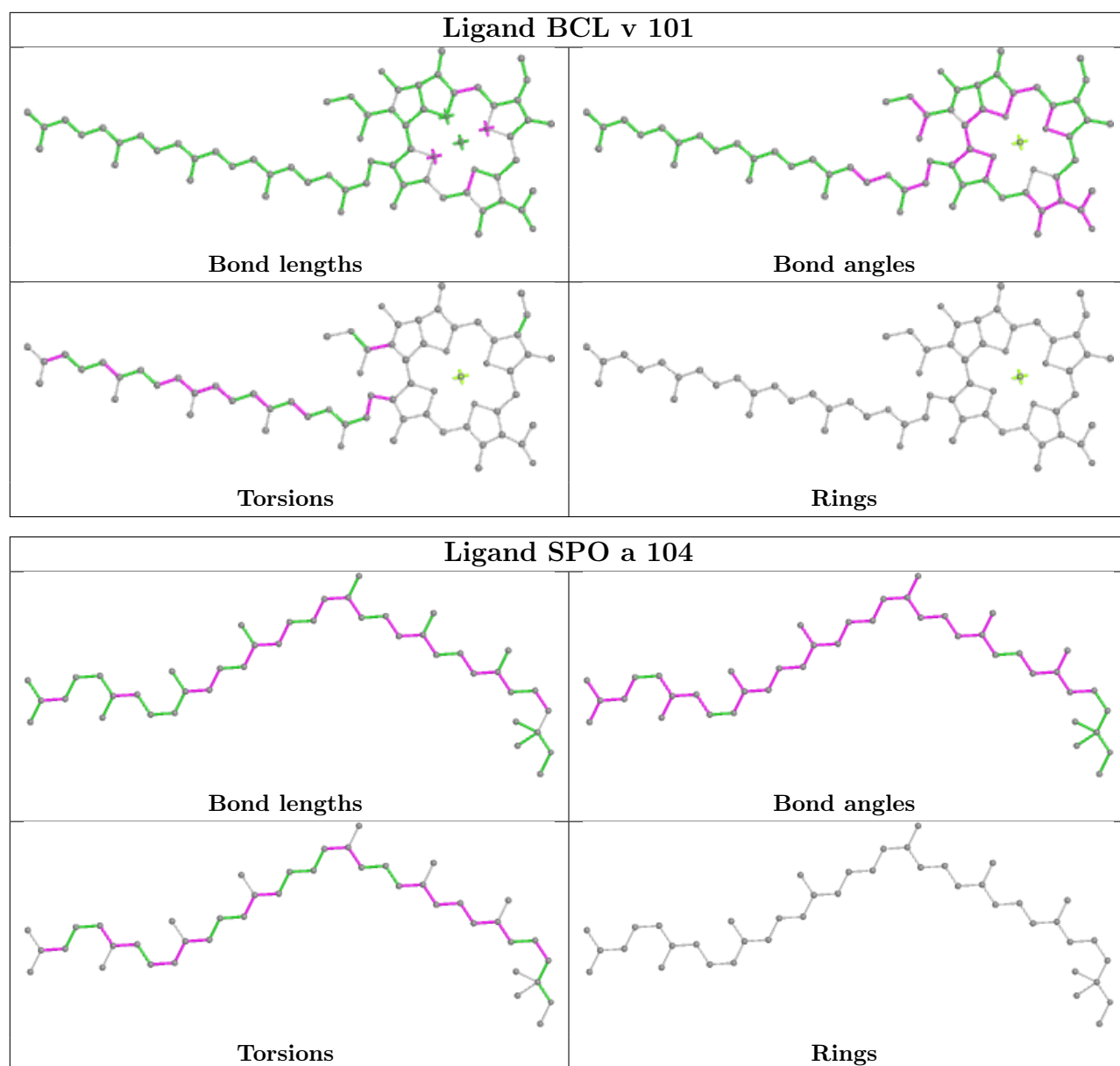
## Ligand BPB L 302

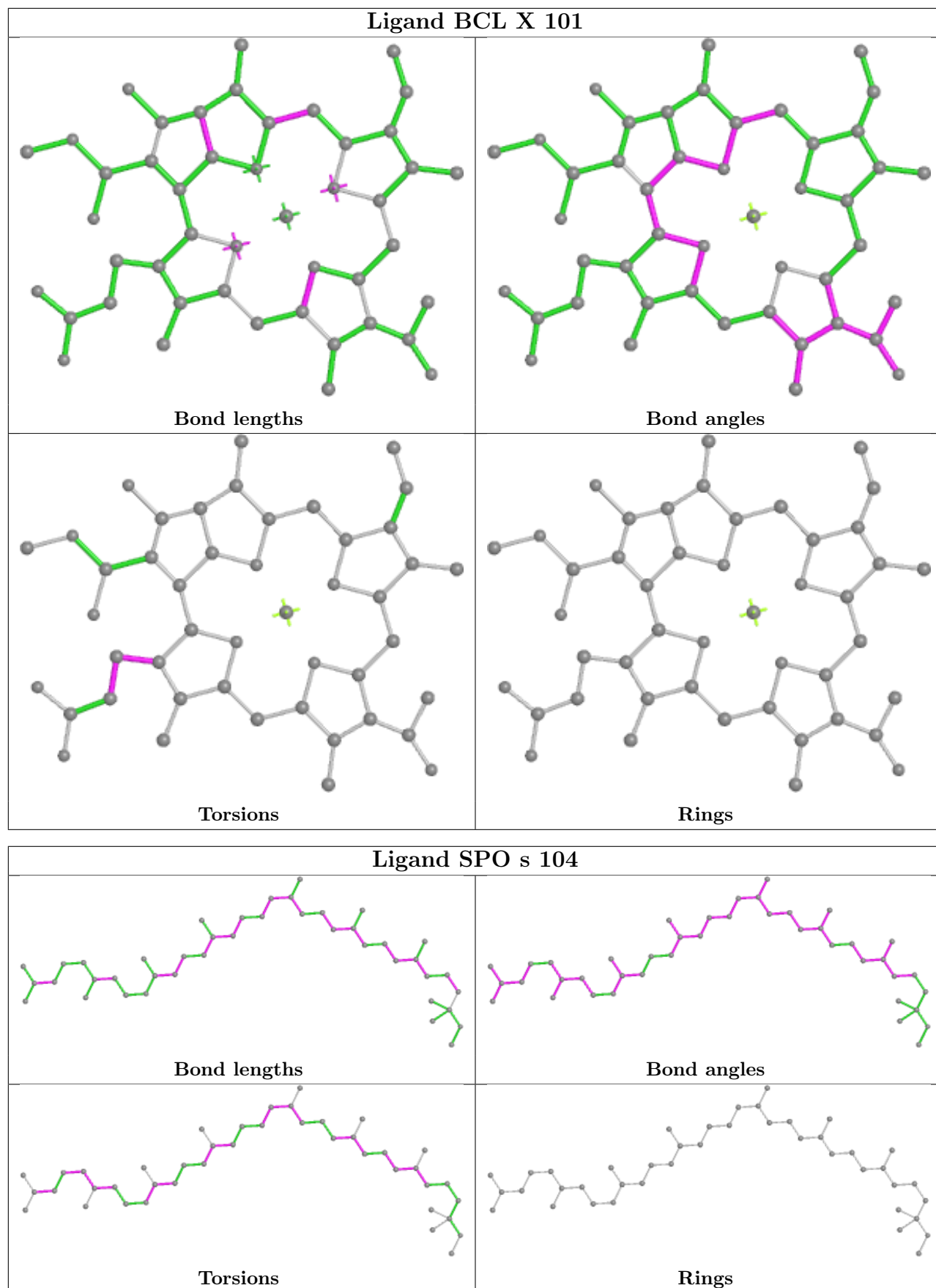


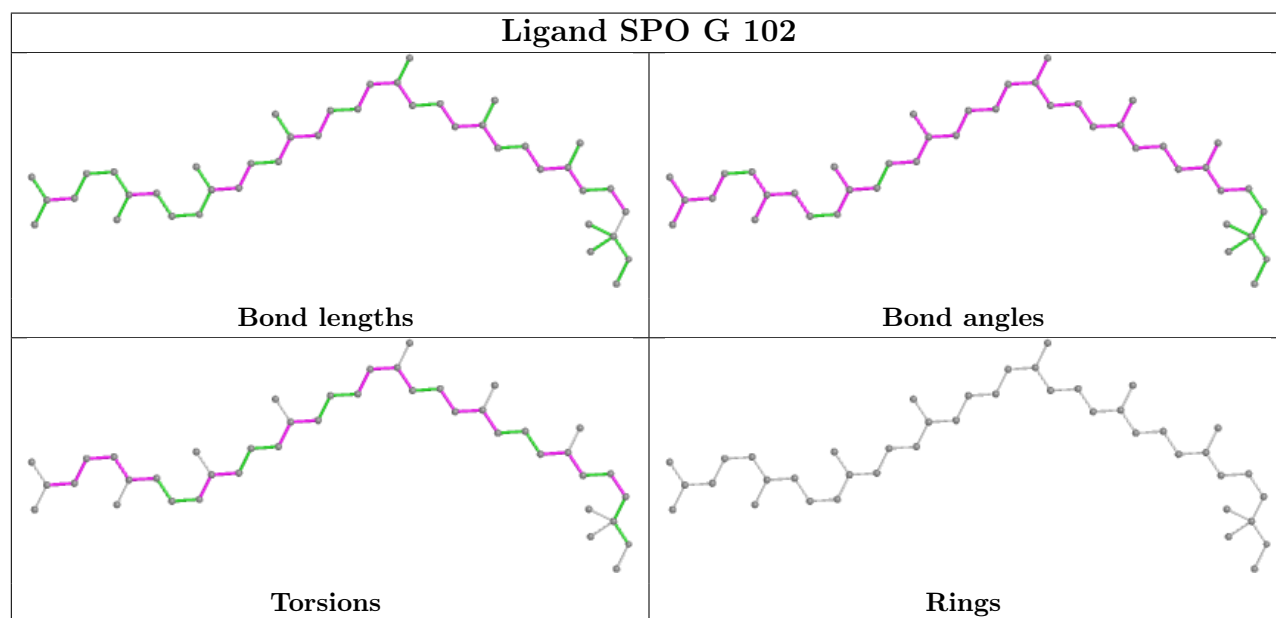
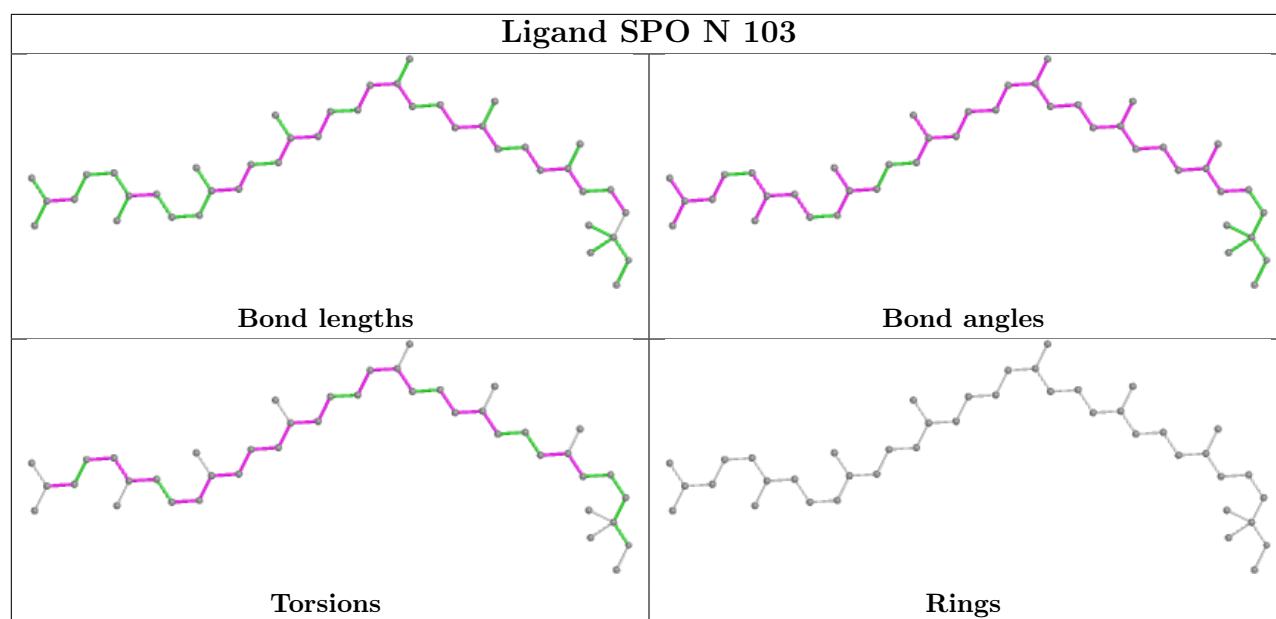


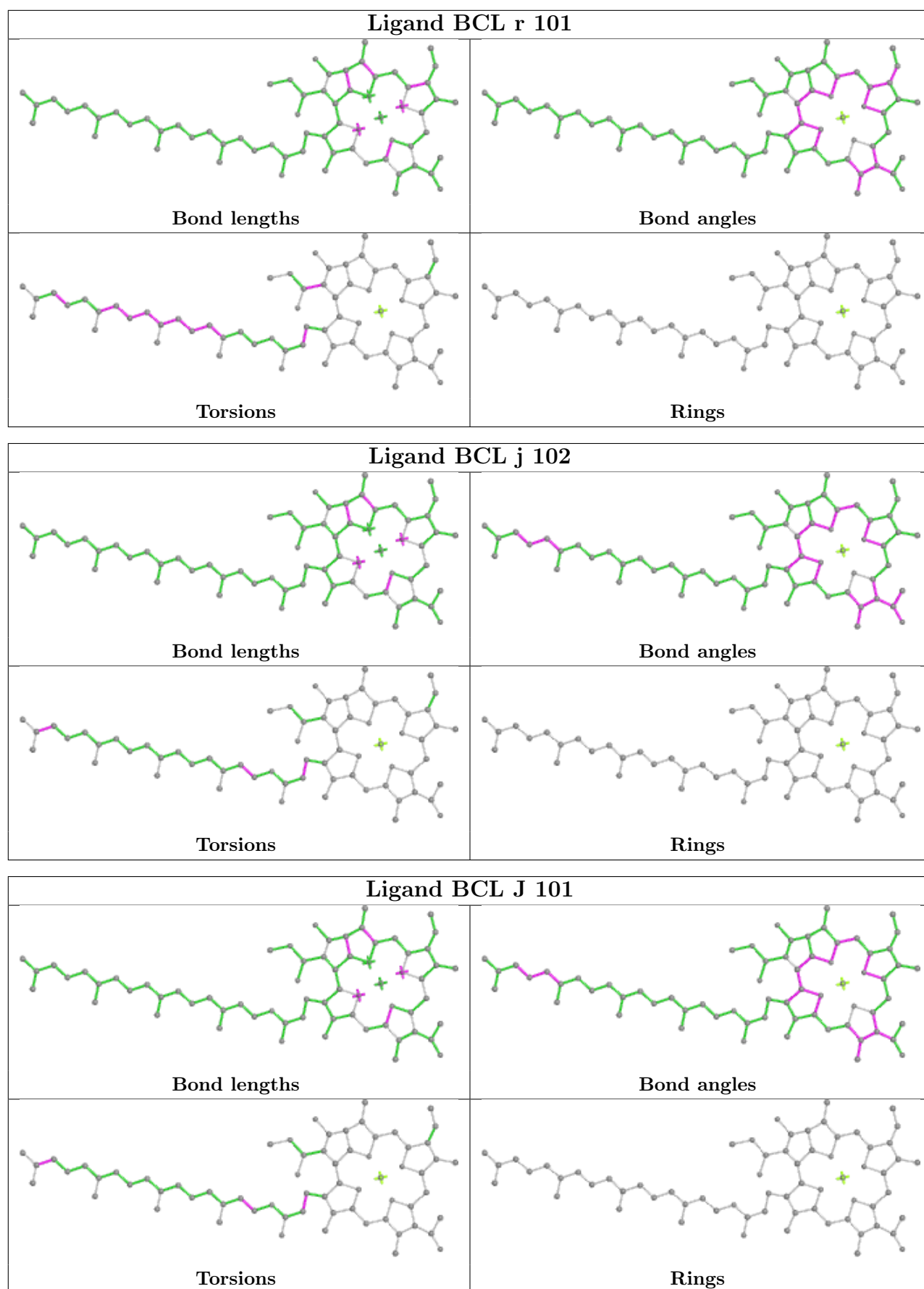


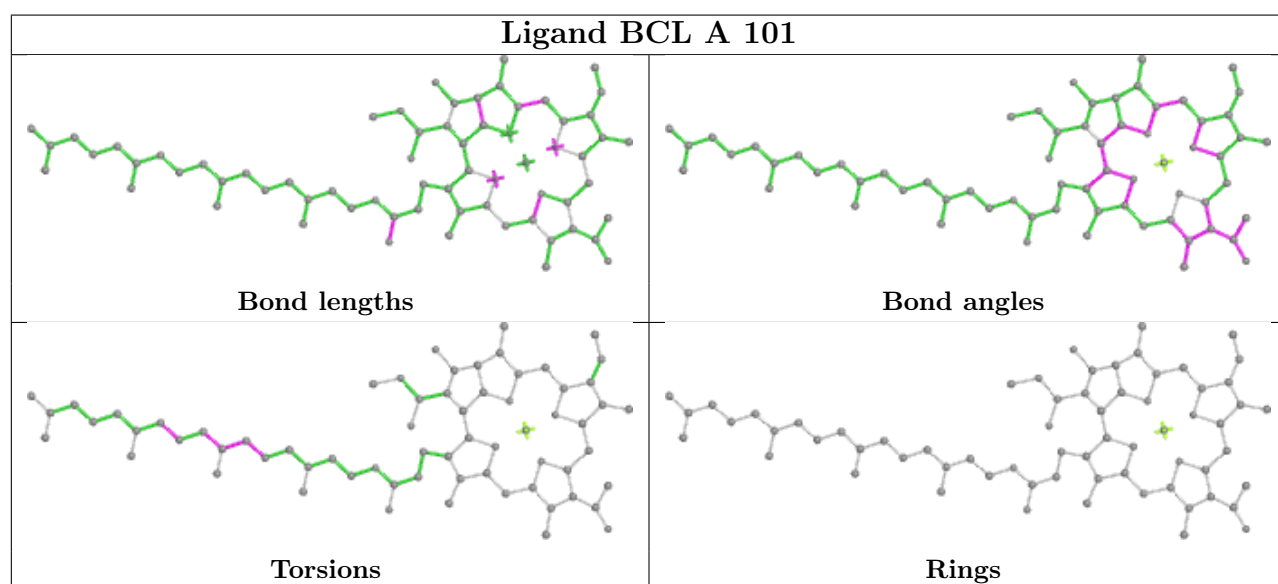
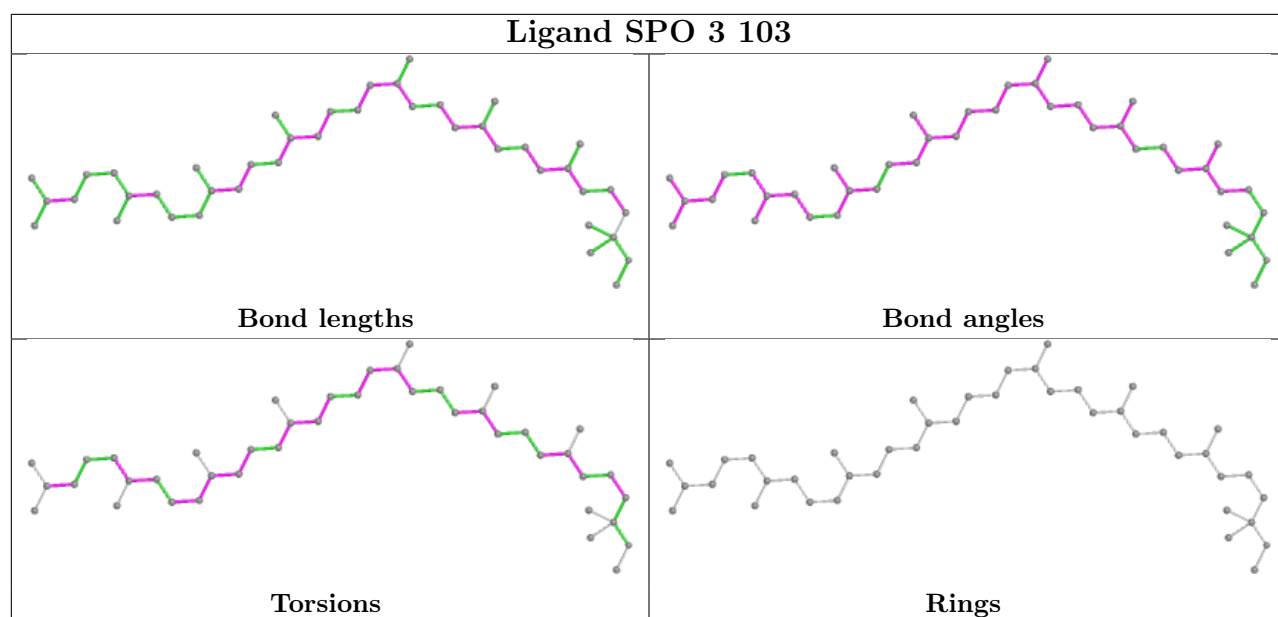


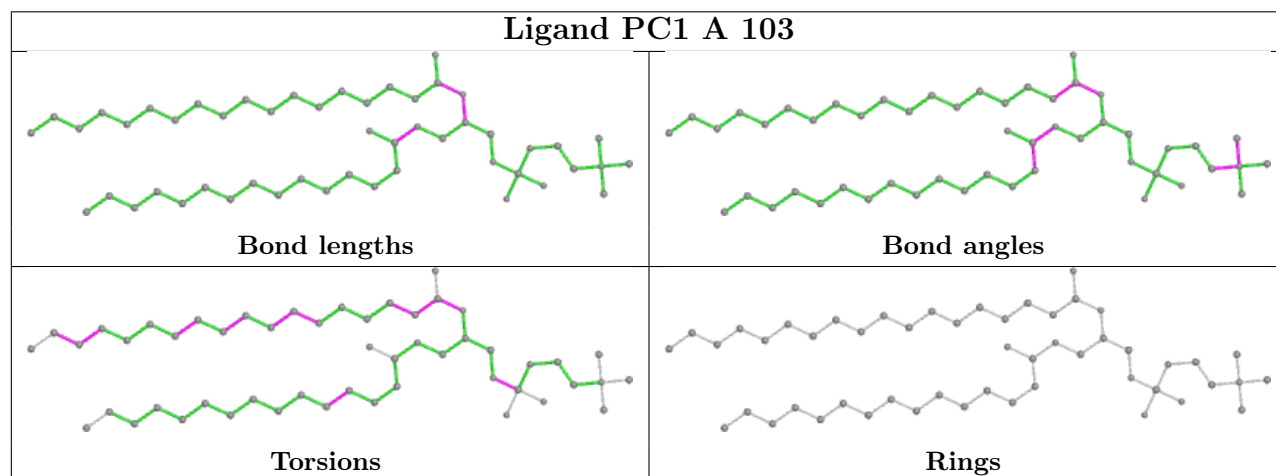
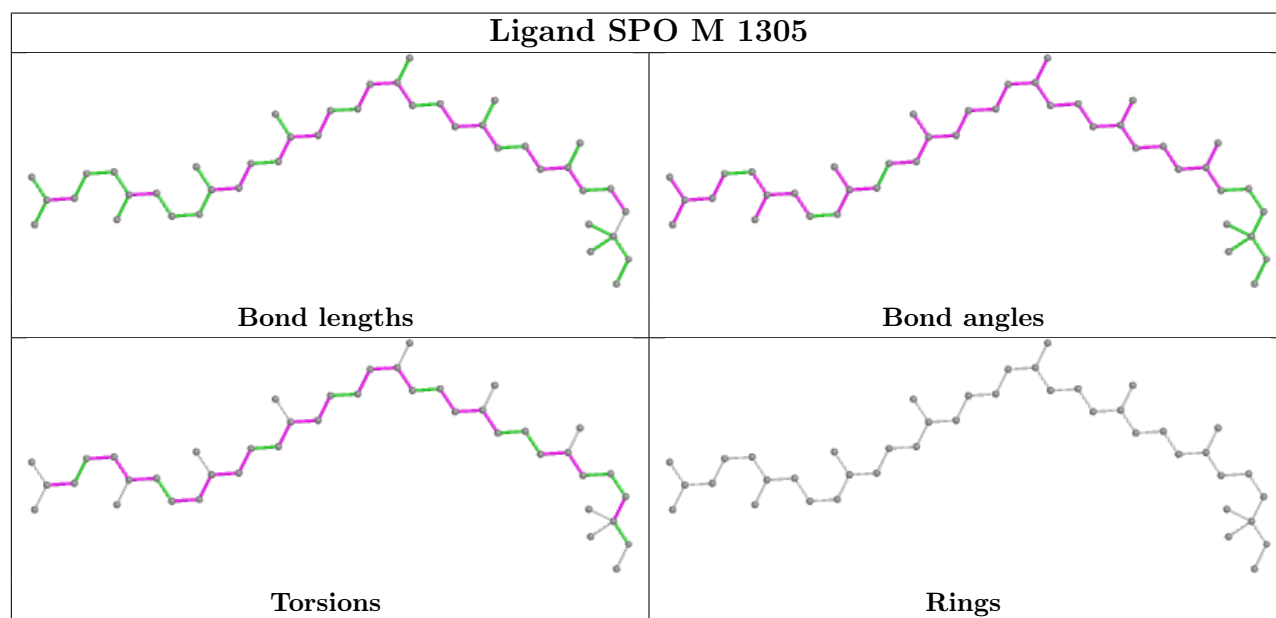
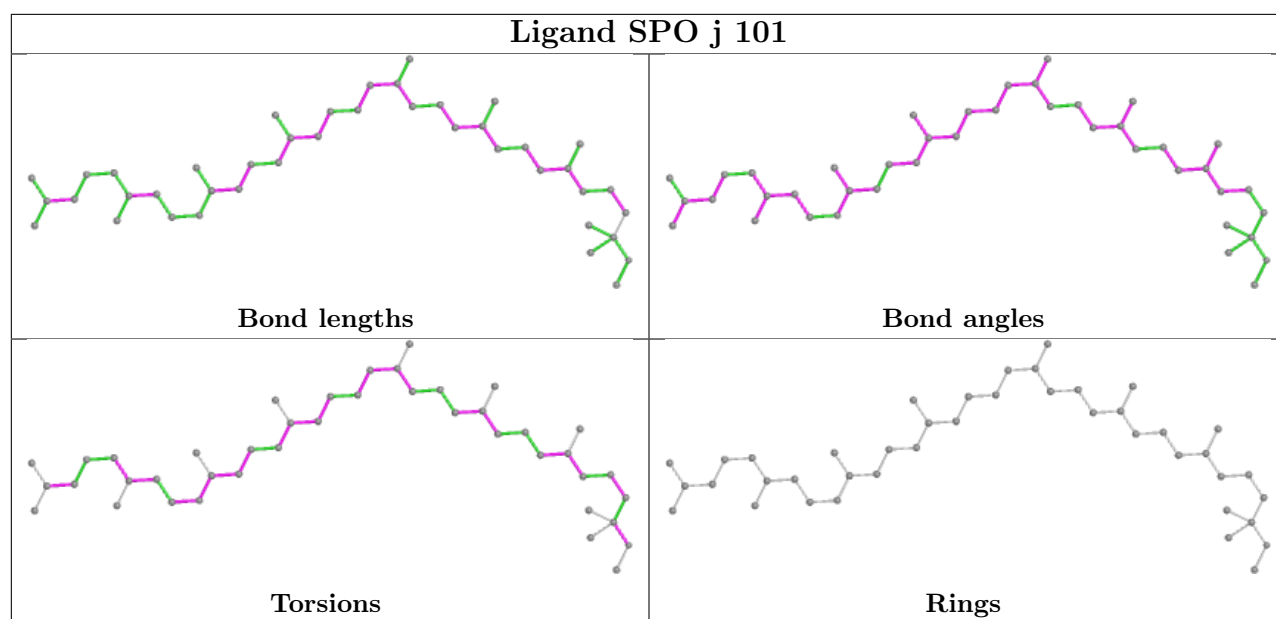


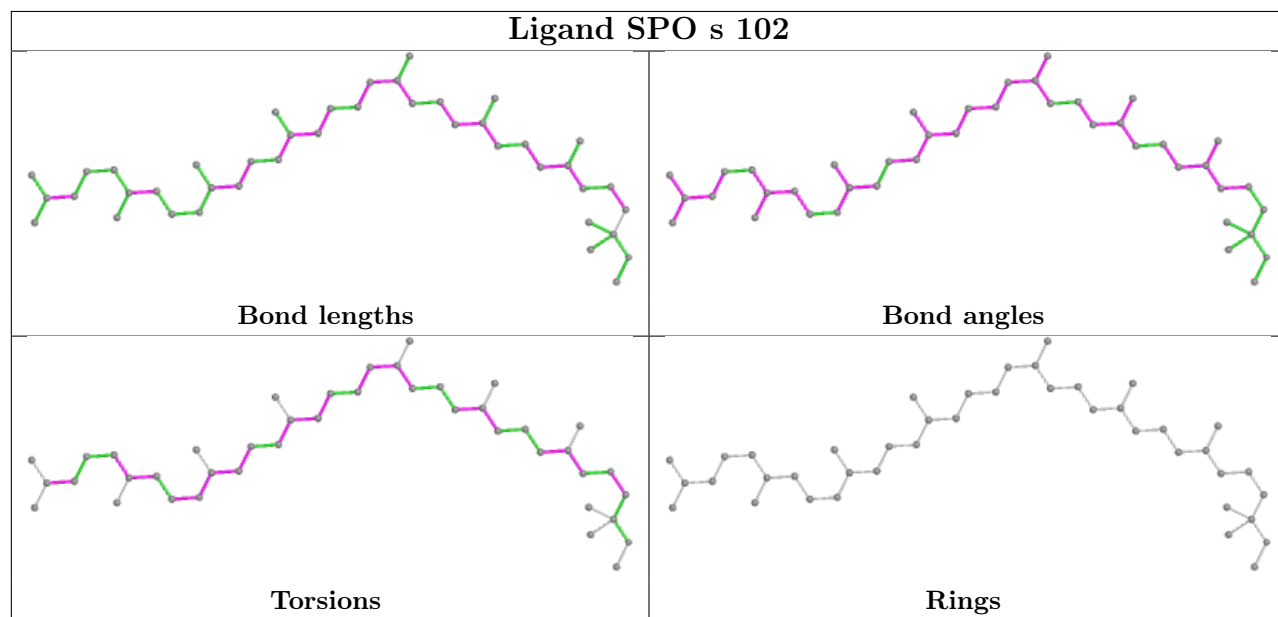
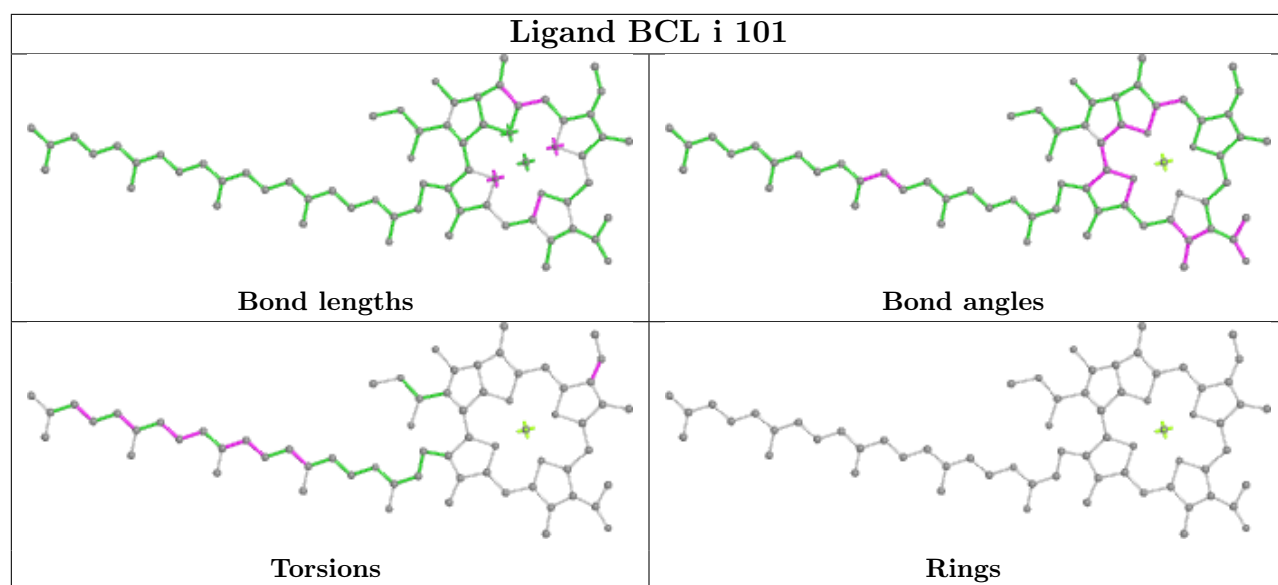




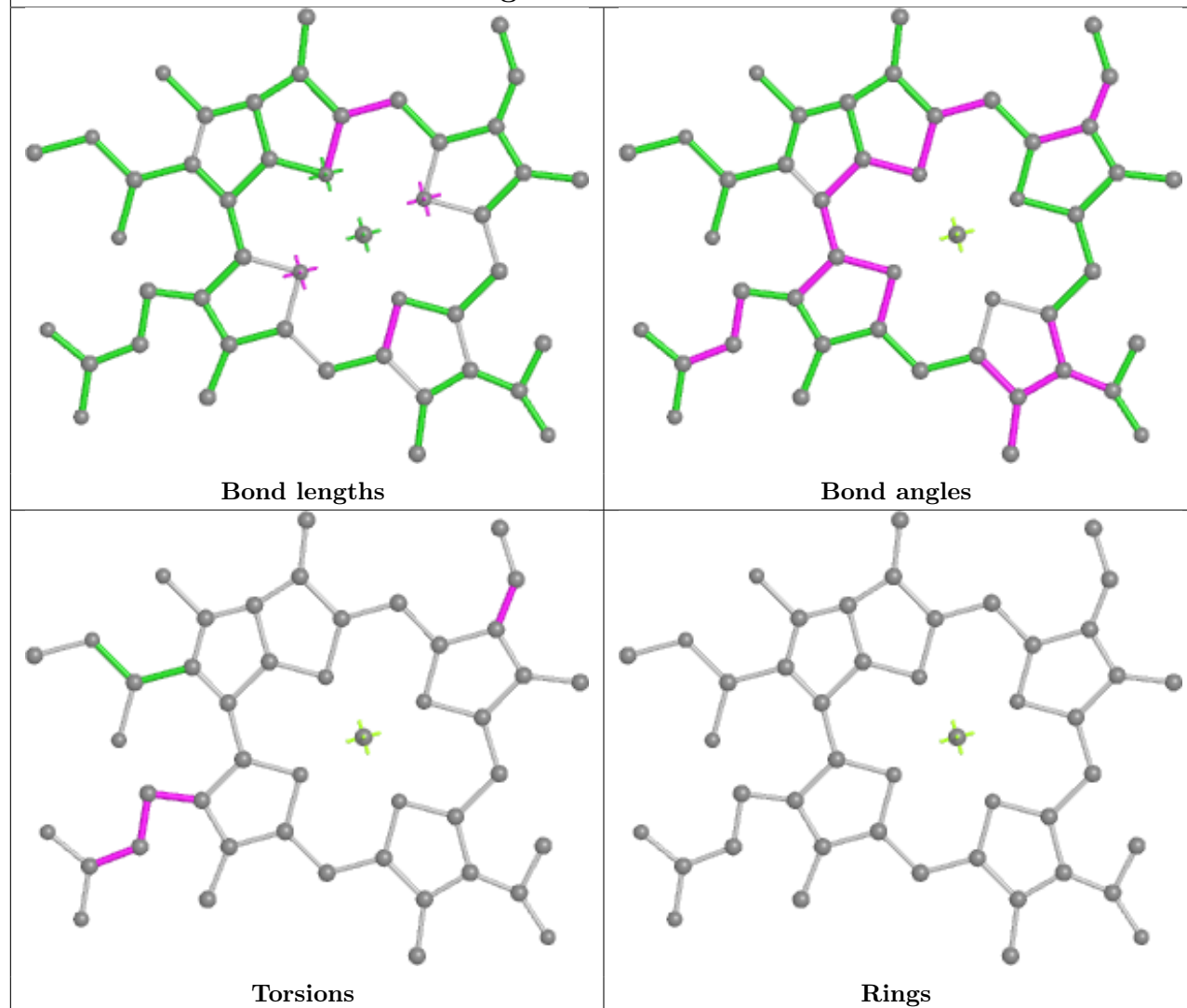




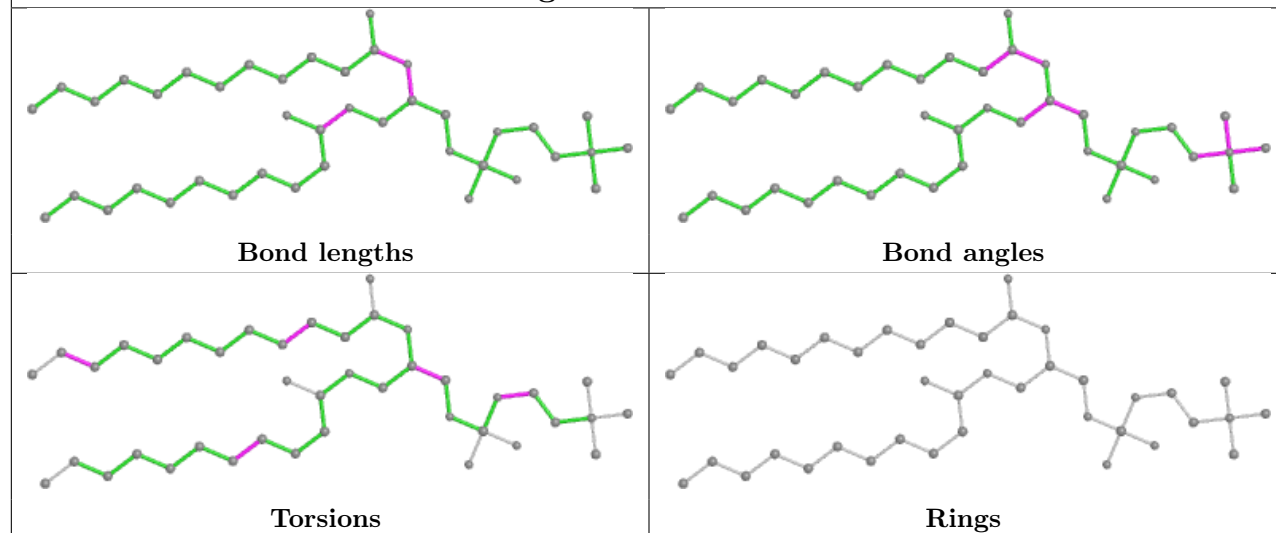


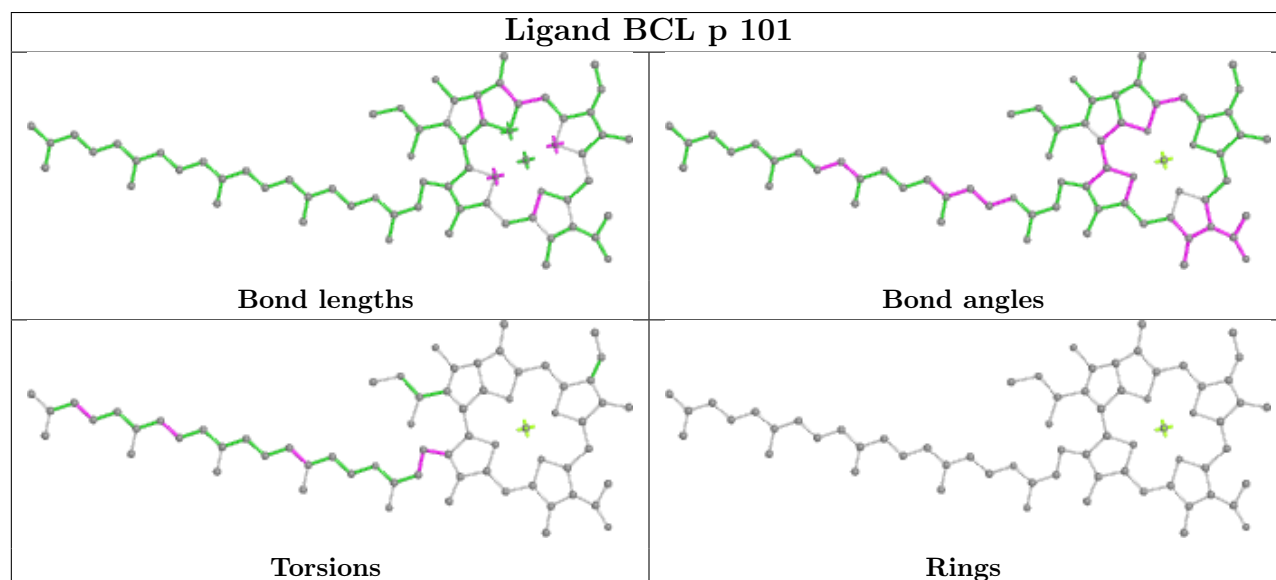
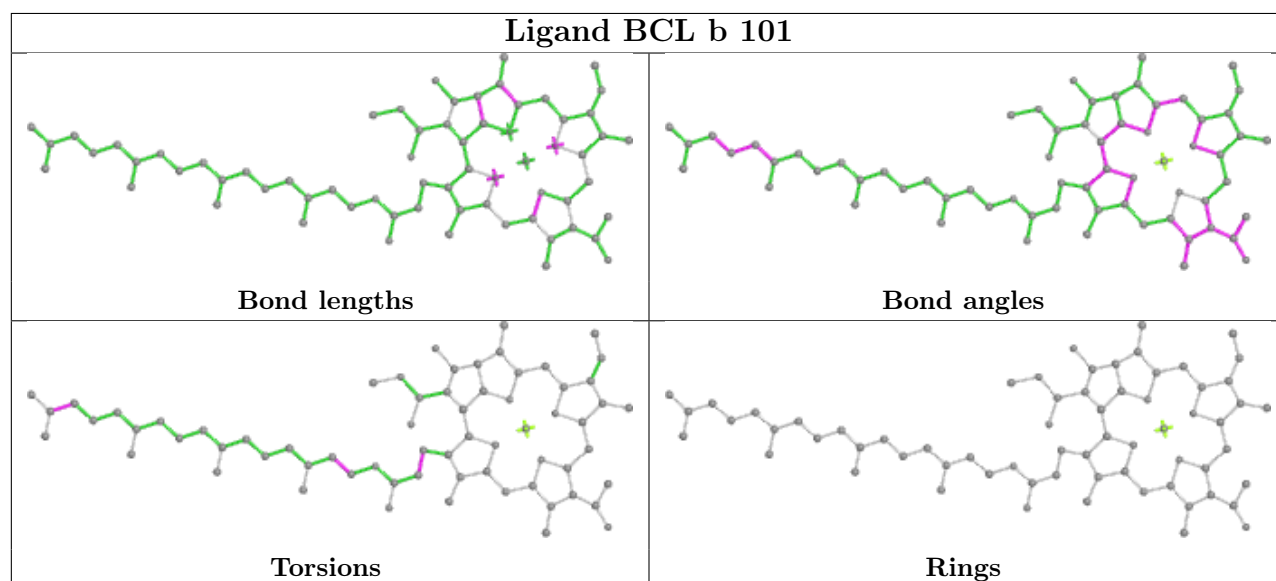
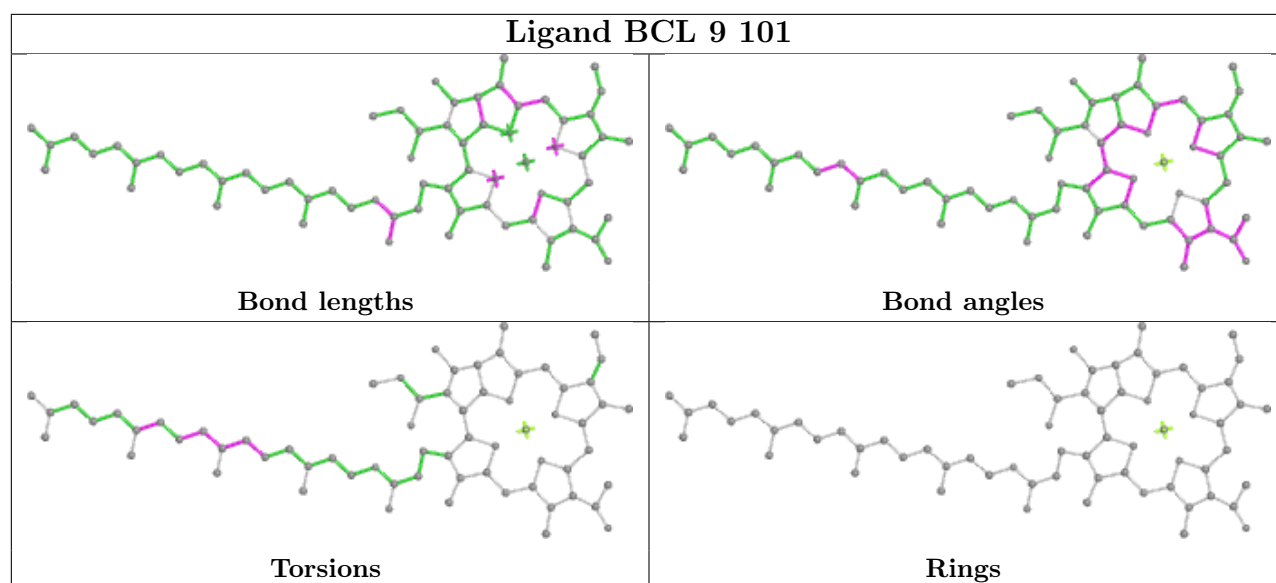


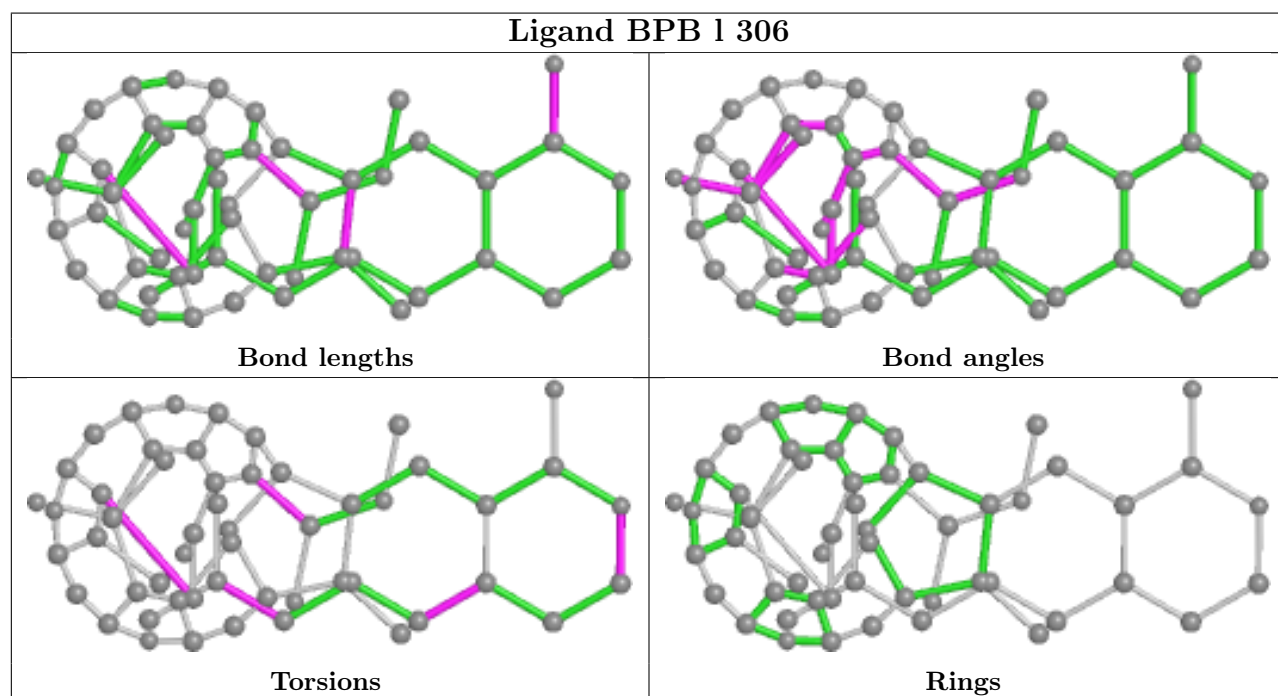
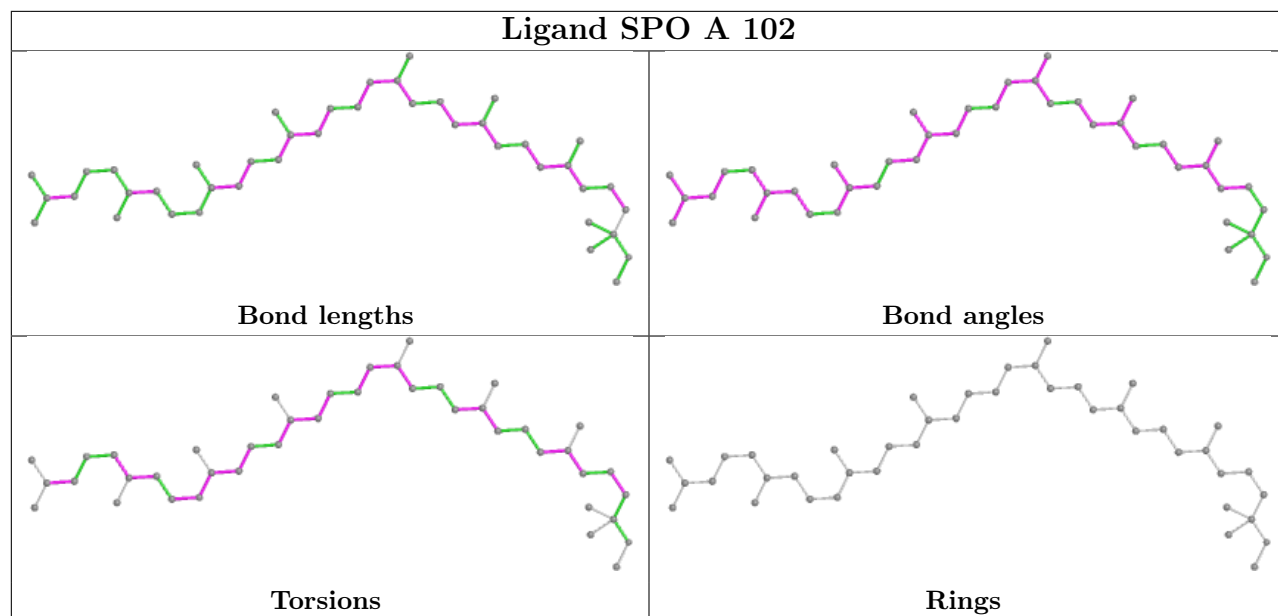
## Ligand BCL z 101

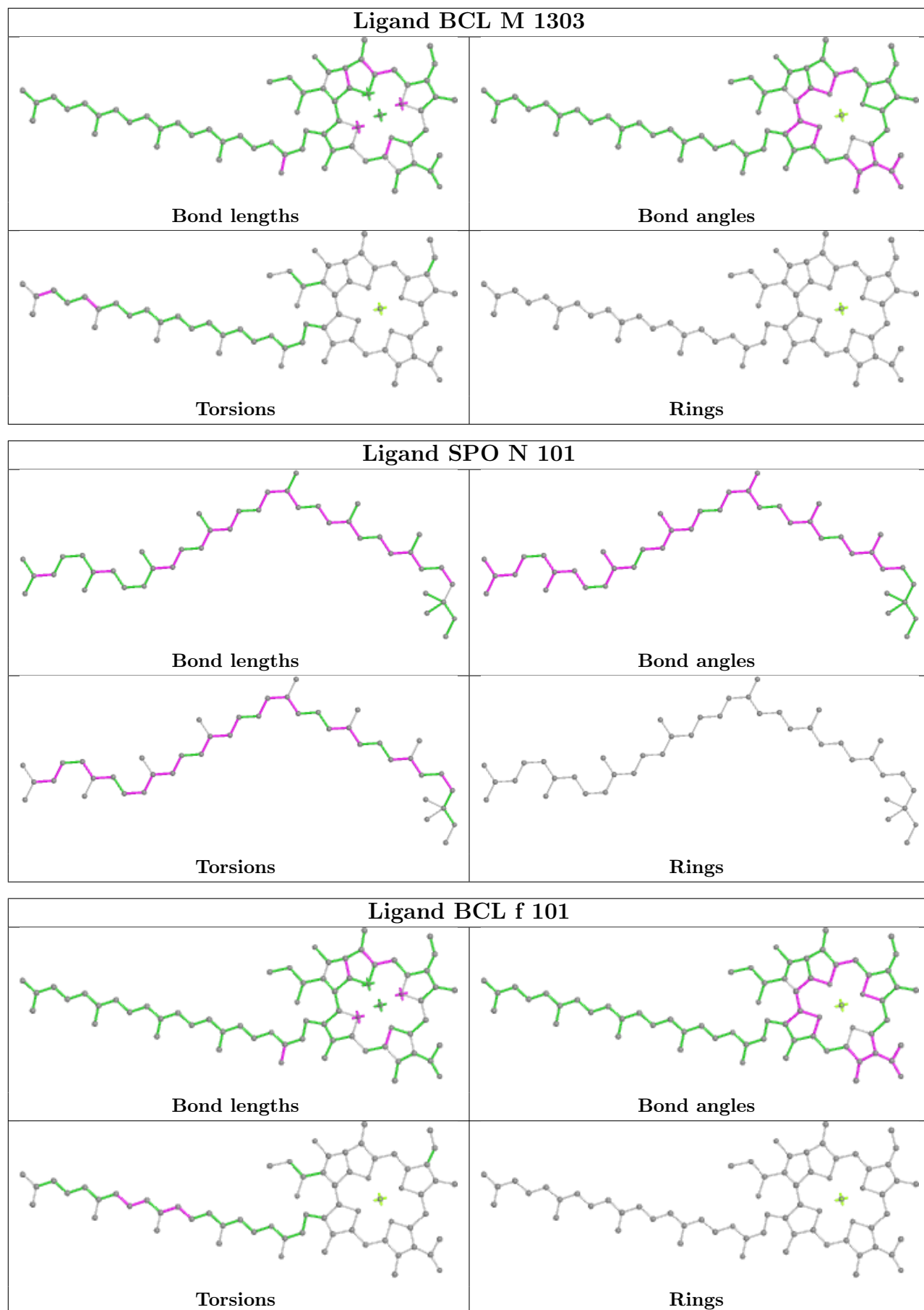


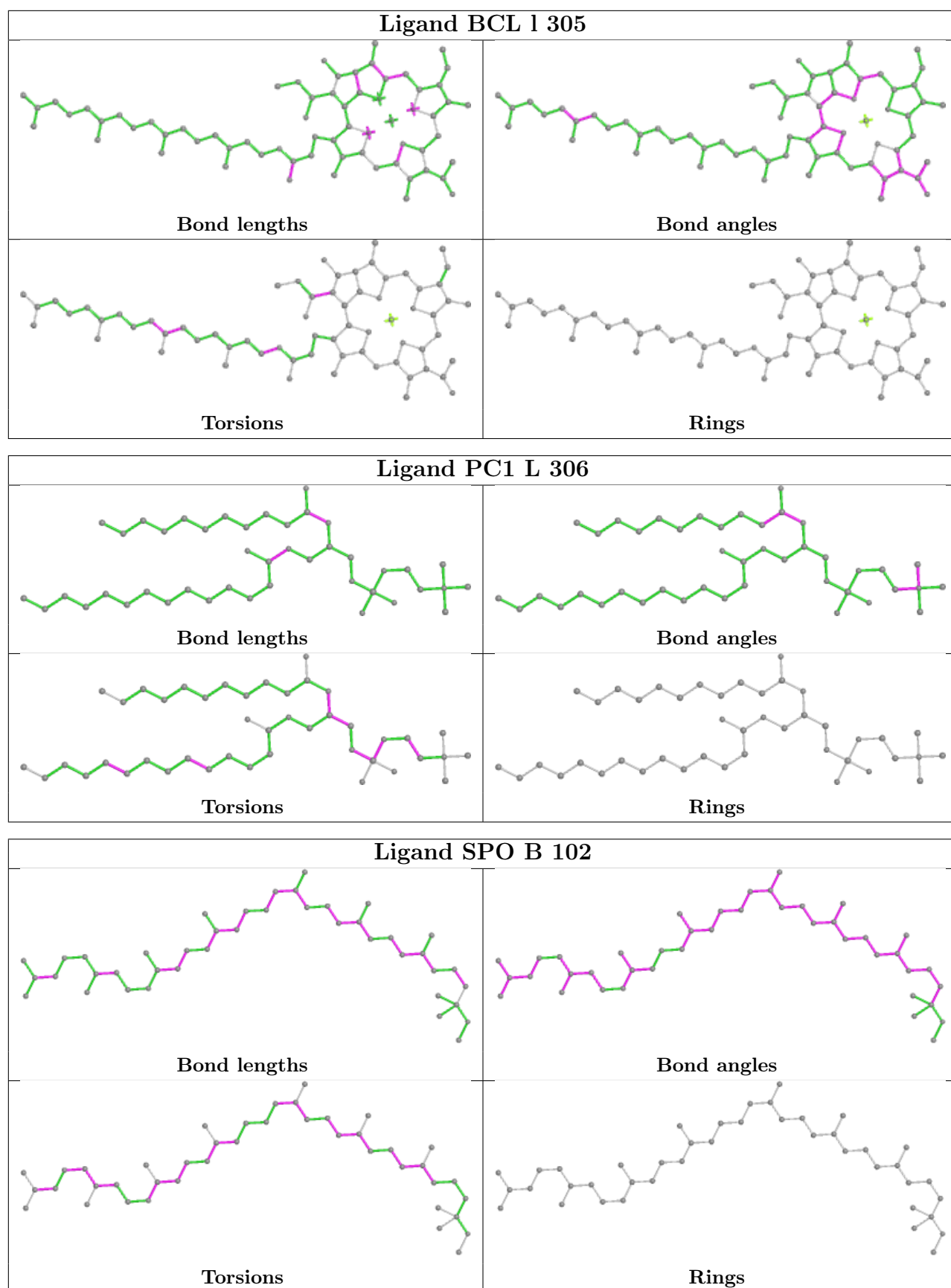
## Ligand PC1 d 102

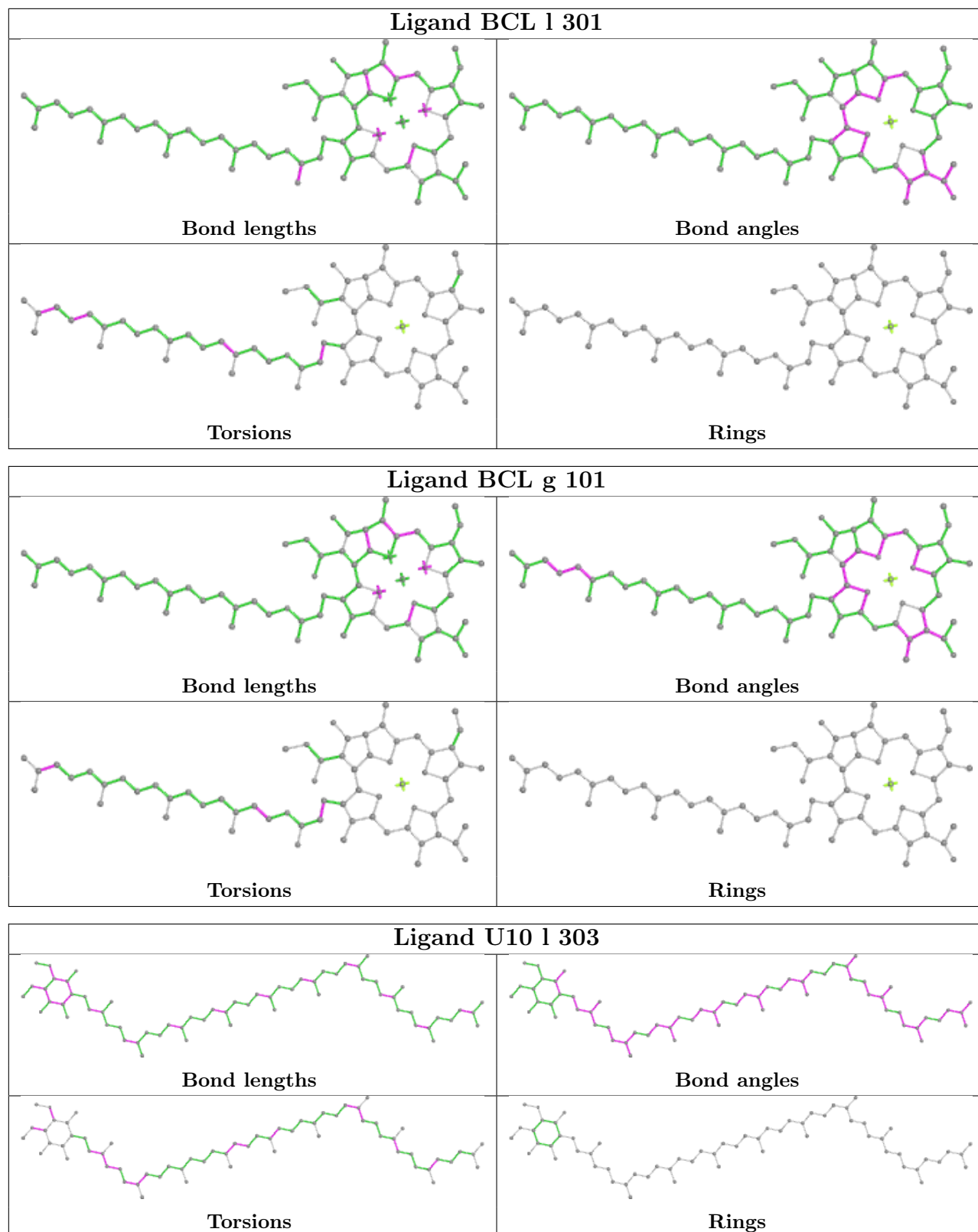


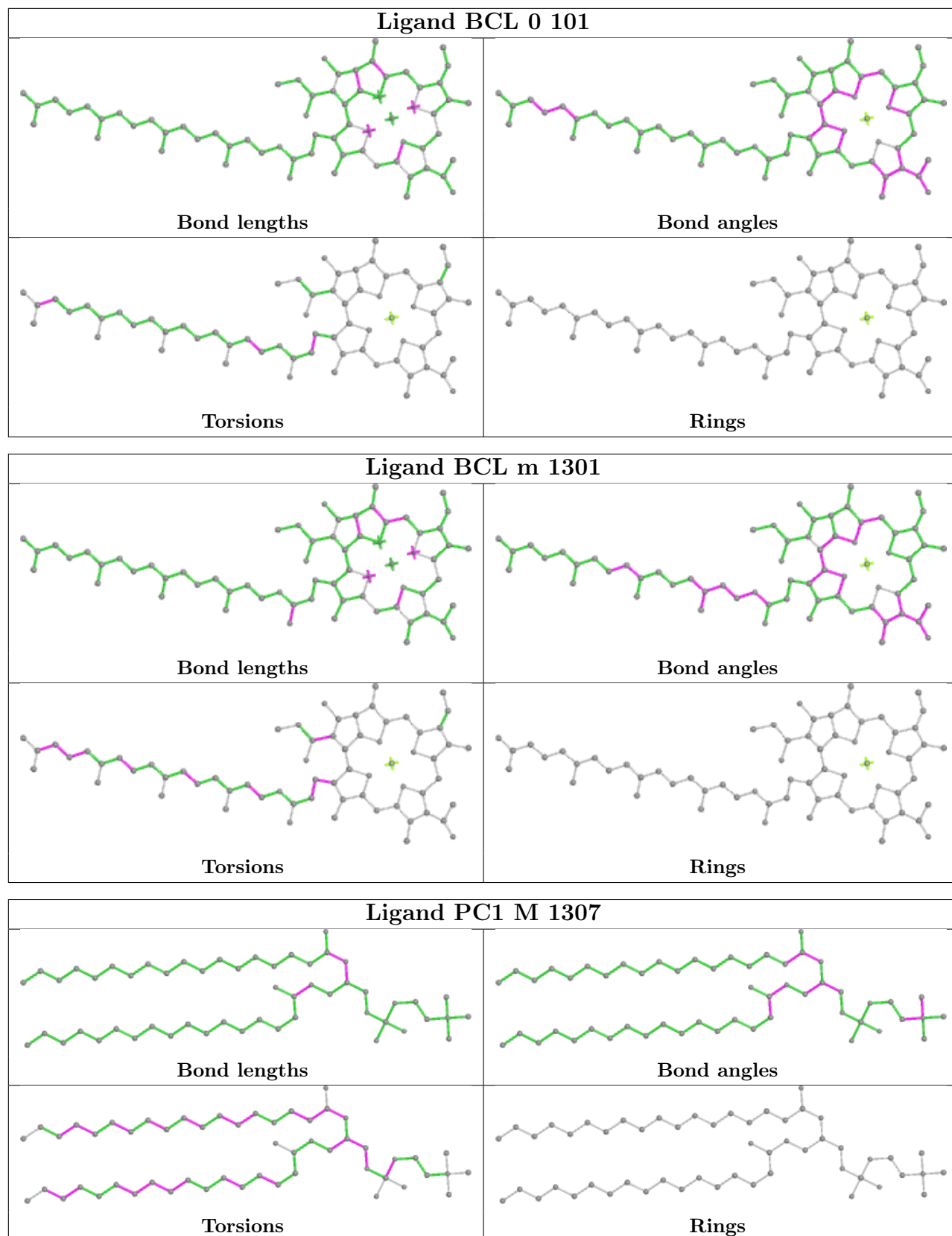


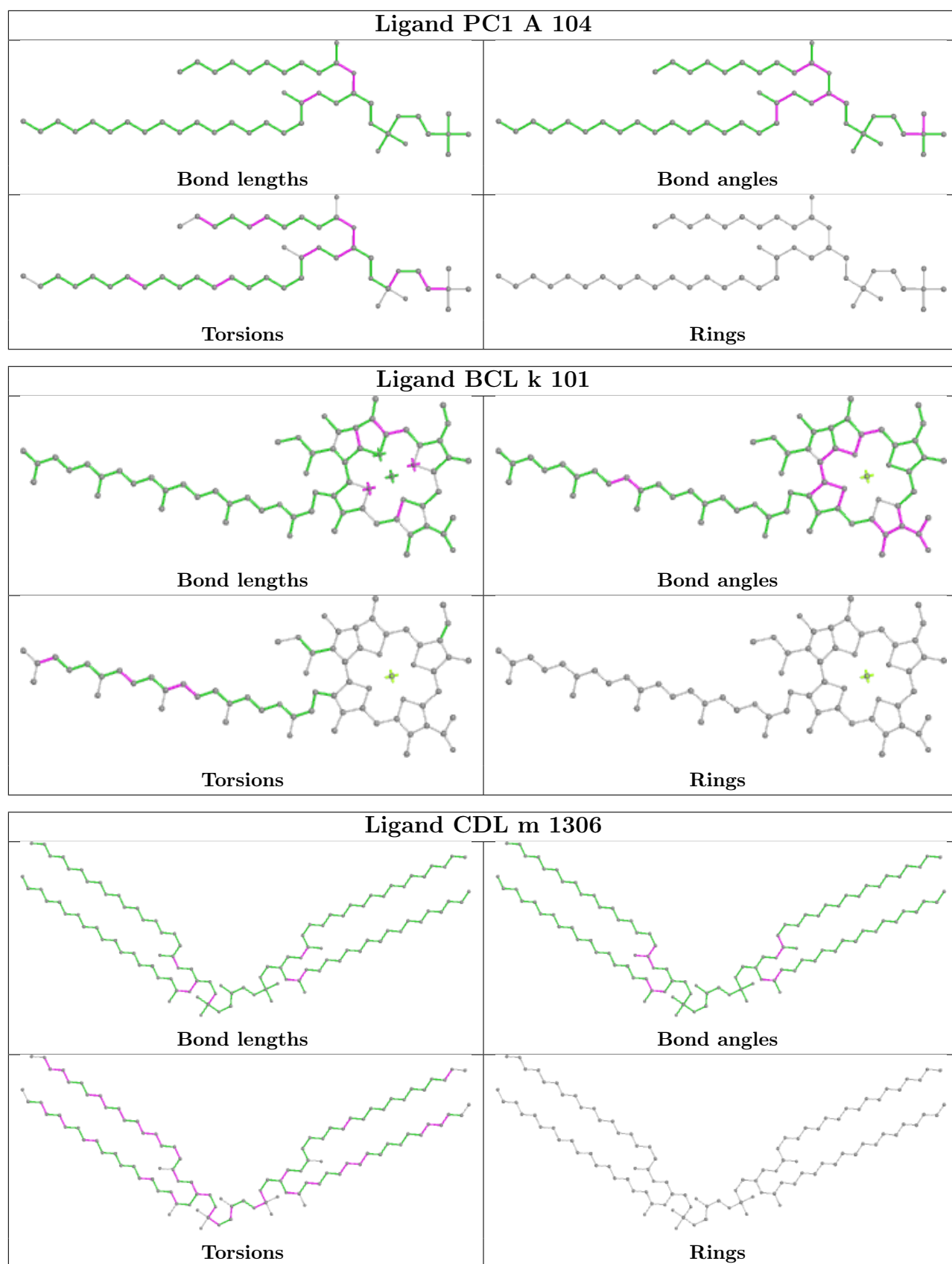


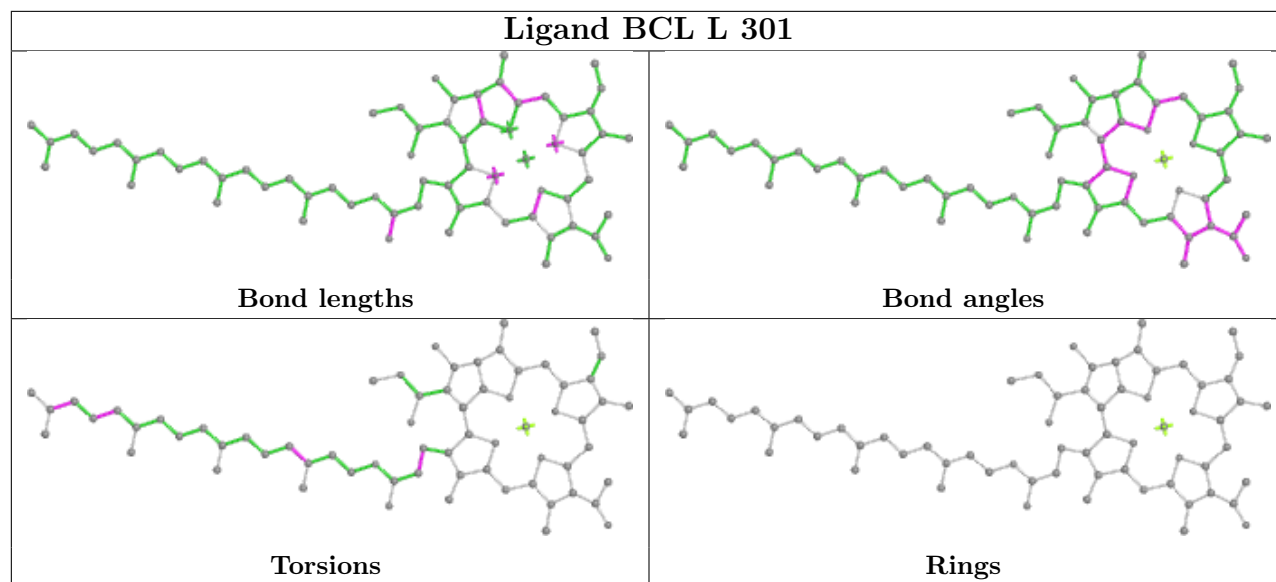












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

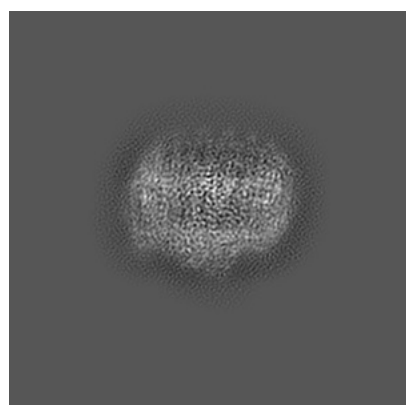
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31835. These allow visual inspection of the internal detail of the map and identification of artifacts.

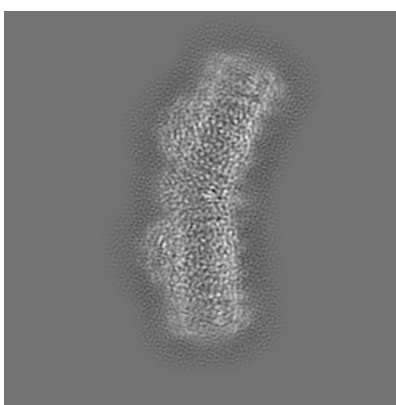
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

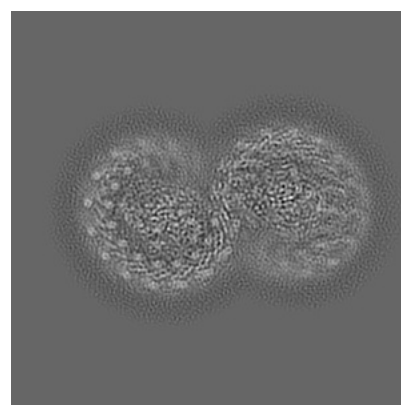
#### 6.1.1 Primary map



X



Y

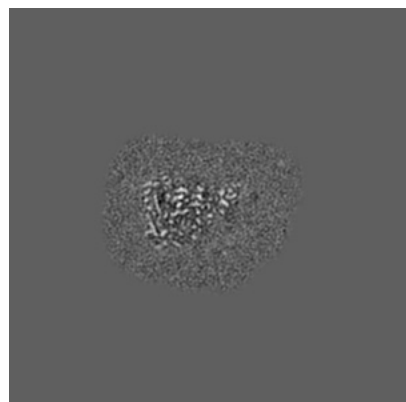


Z

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

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

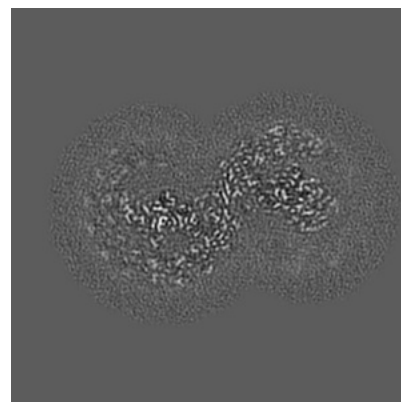
#### 6.2.1 Primary map



X Index: 175



Y Index: 175

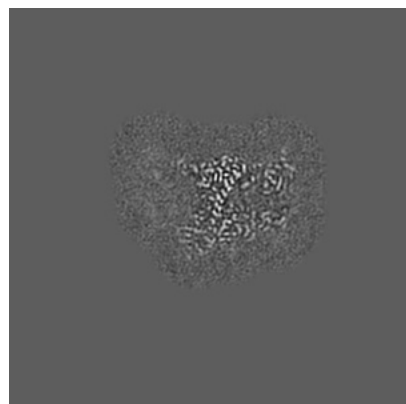


Z Index: 175

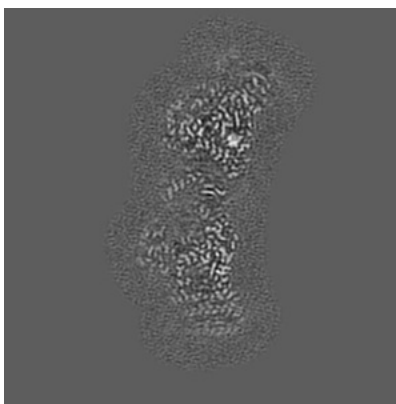
The images above show central slices of the map in three orthogonal directions.

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

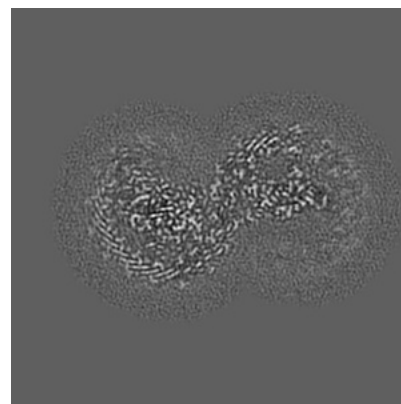
### 6.3.1 Primary map



X Index: 240



Y Index: 179

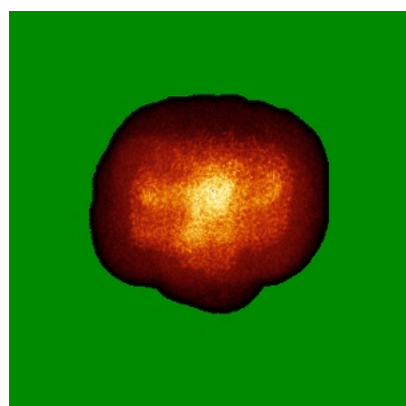


Z Index: 189

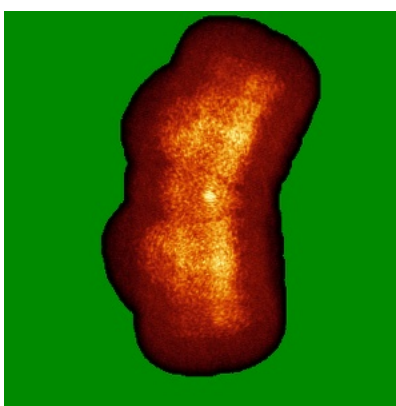
The images above show the largest variance slices of the map in three orthogonal directions.

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

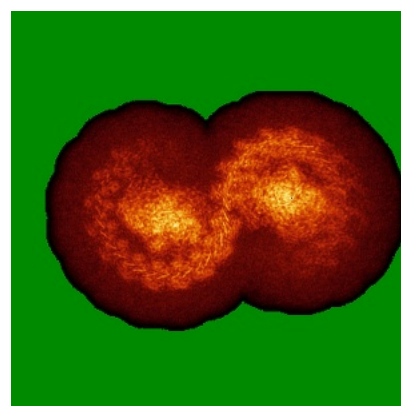
### 6.4.1 Primary map



X



Y

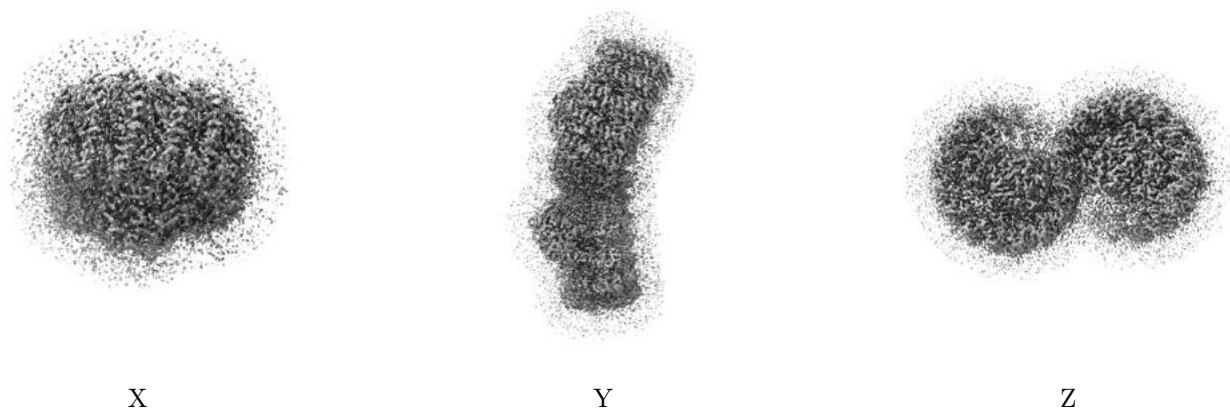


Z

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 0.0245. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

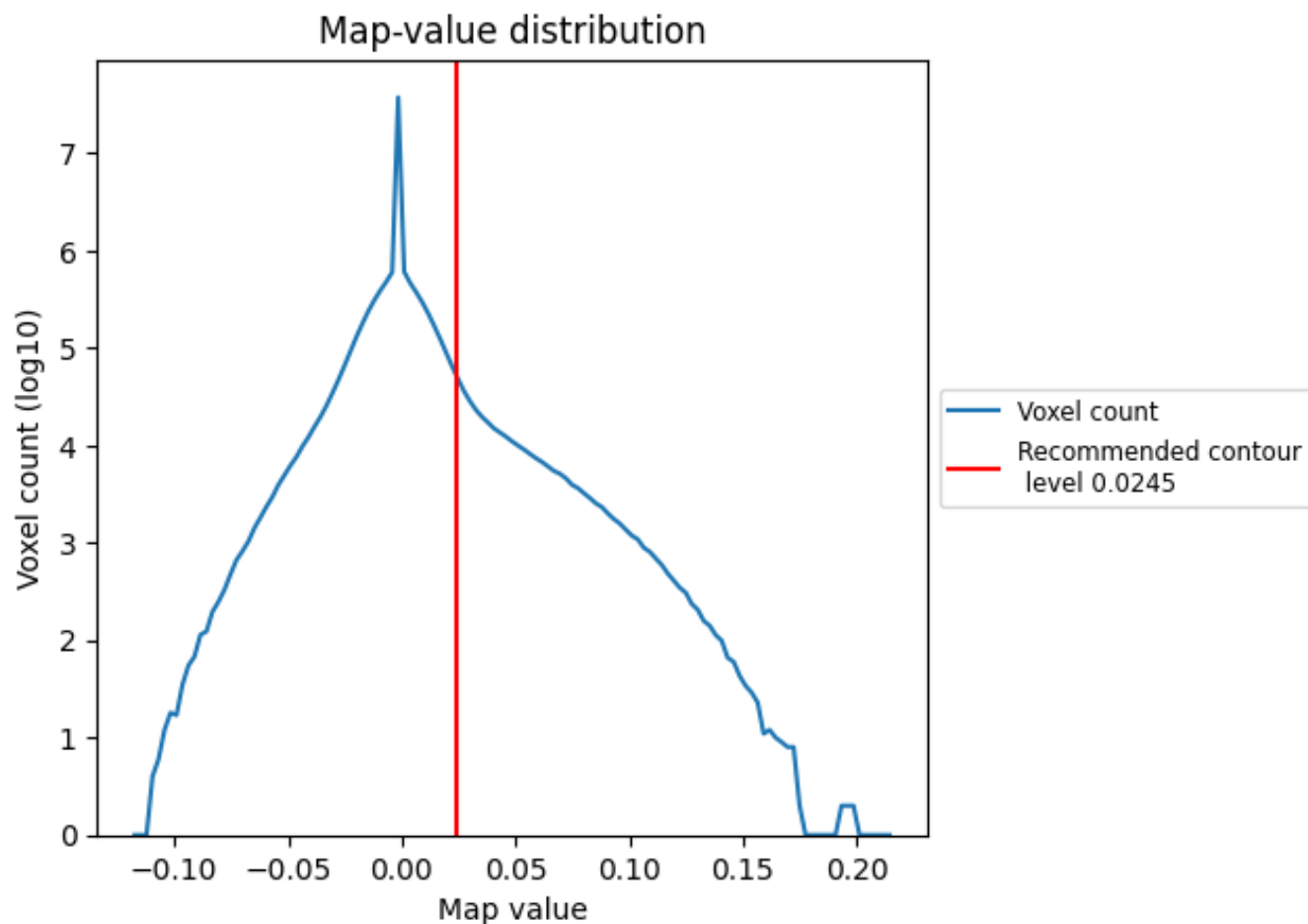
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

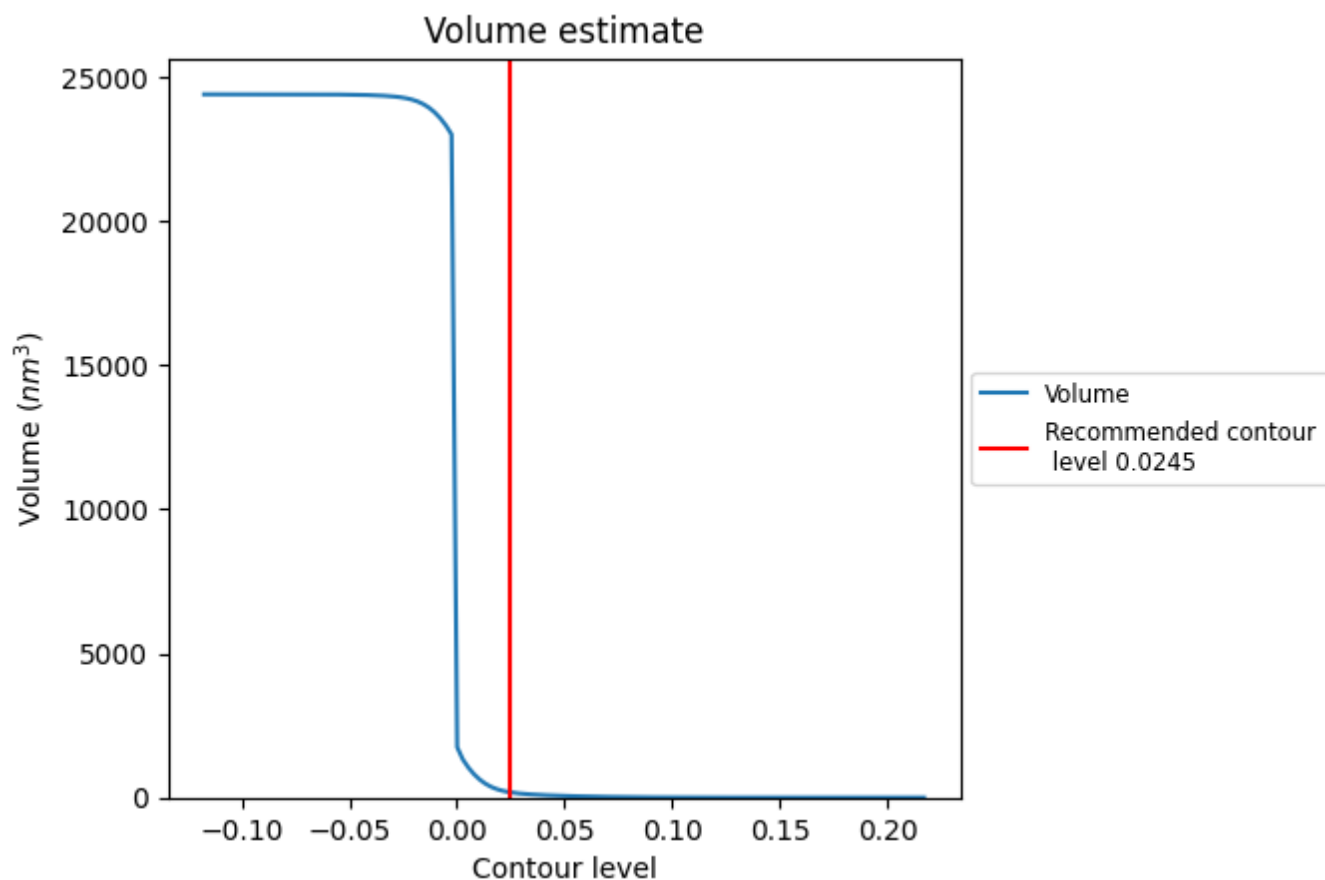
This section contains the results of statistical analysis of the map.

### 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.

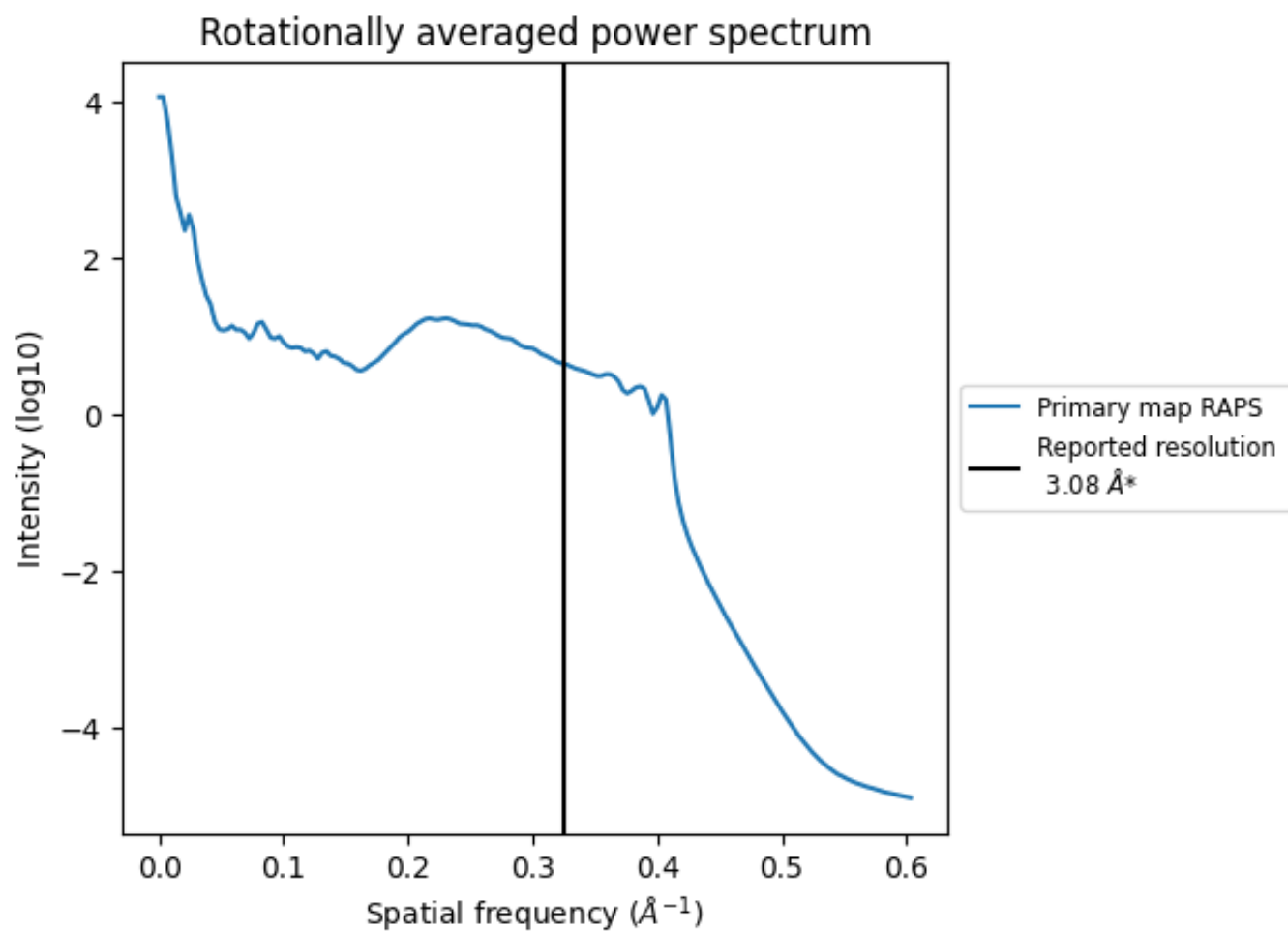
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm<sup>3</sup>; this corresponds to an approximate mass of 168 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 ⓘ

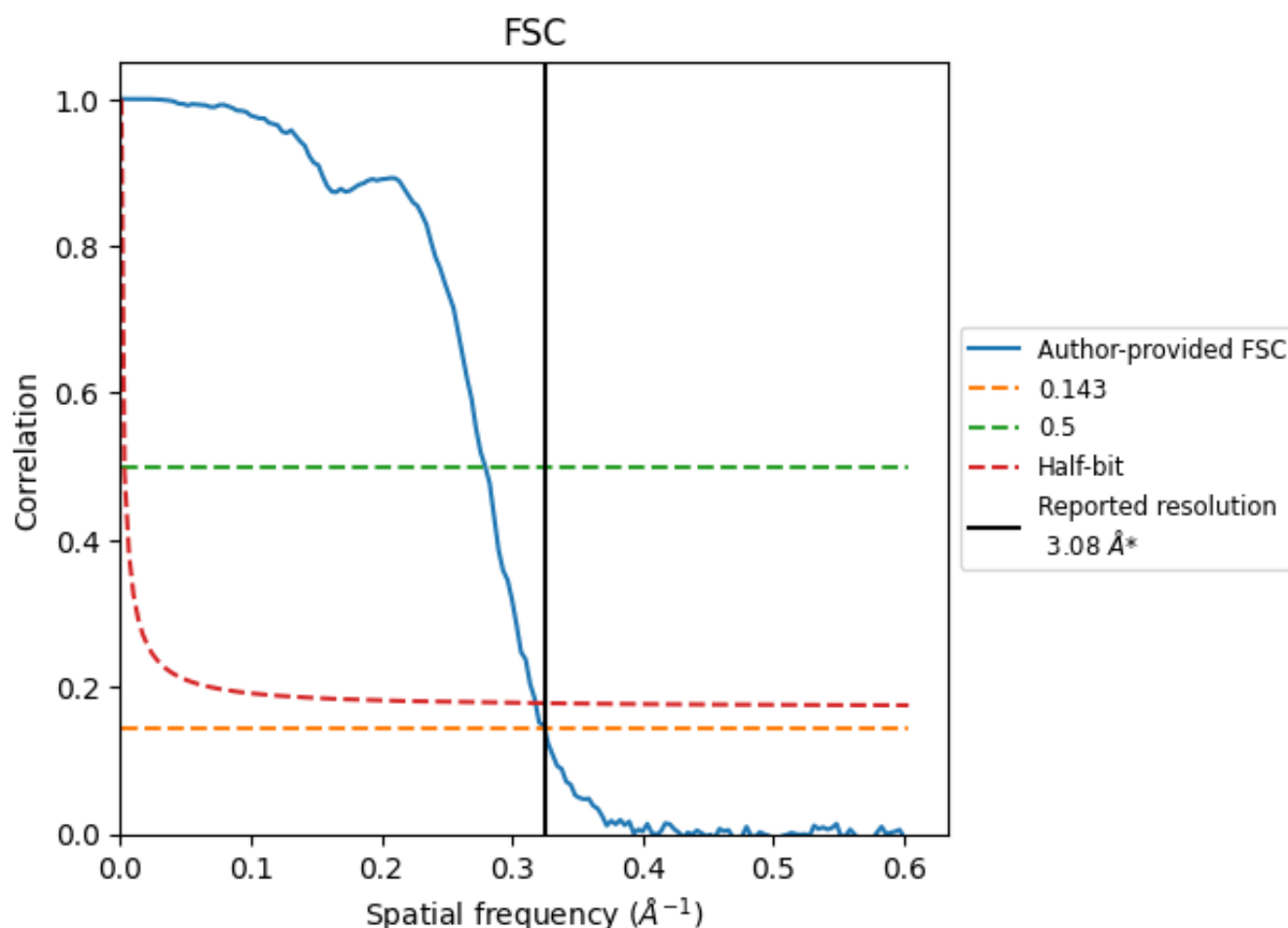


\*Reported resolution corresponds to spatial frequency of 0.325 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.325 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

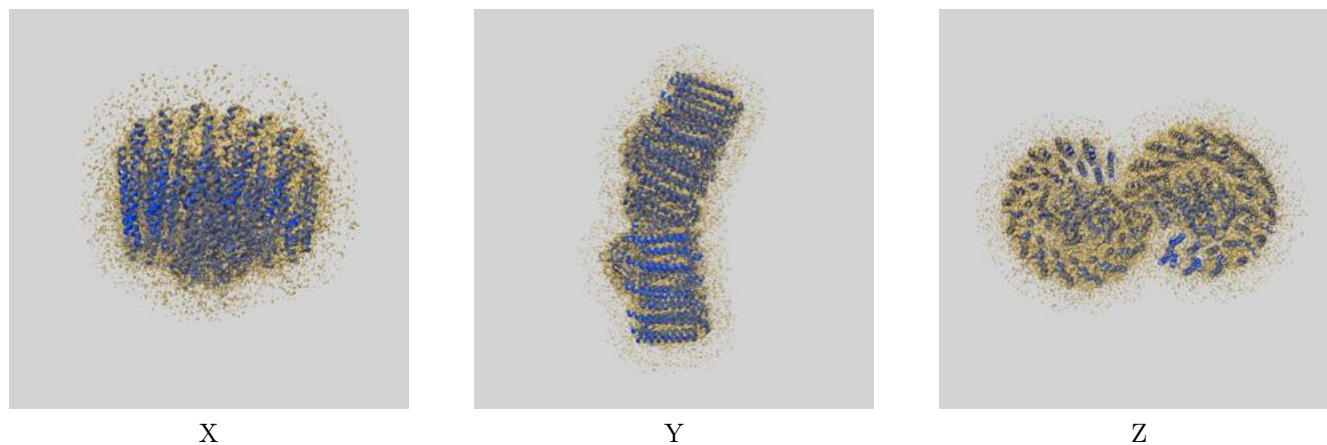
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.58	3.15
Unmasked-calculated*	-	-	-

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

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

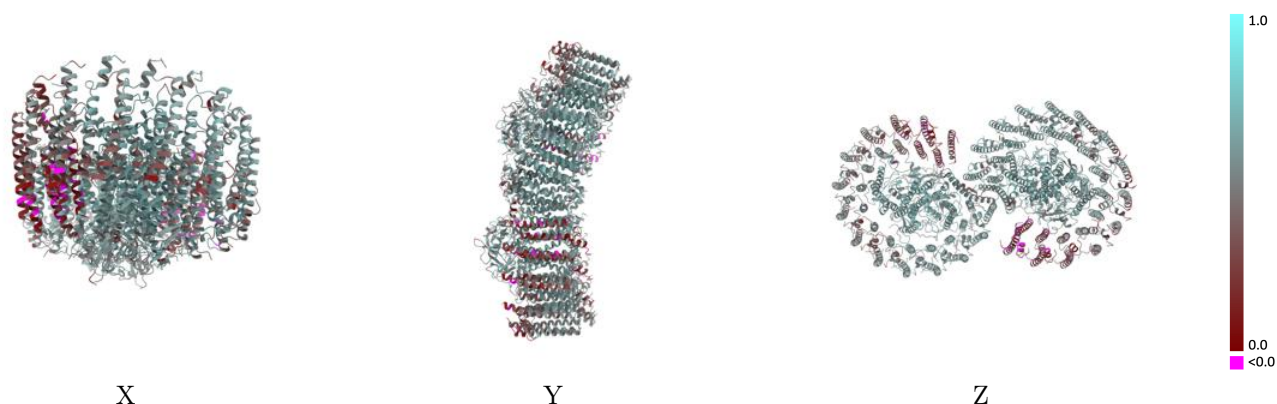
This section contains information regarding the fit between EMDB map EMD-31835 and PDB model 7VA9. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



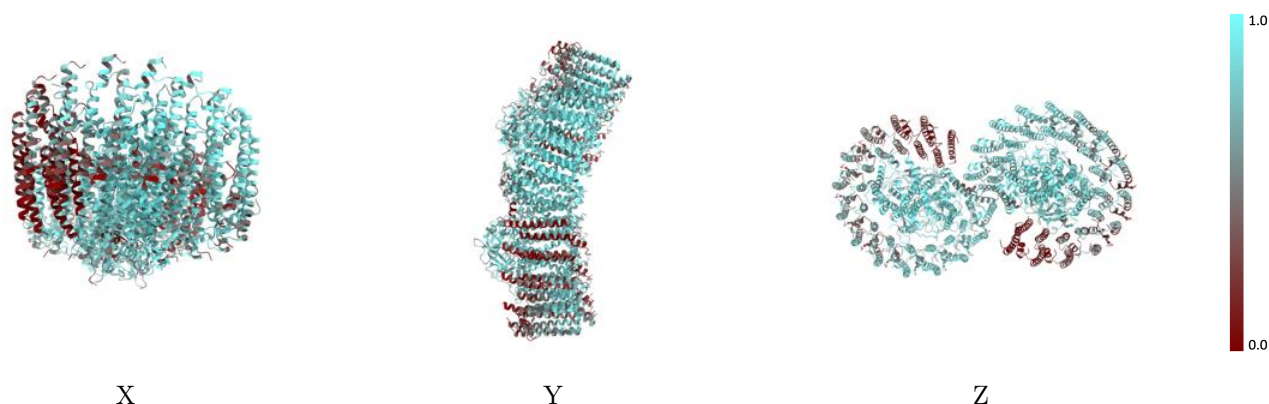
The images above show the 3D surface view of the map at the recommended contour level 0.0245 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



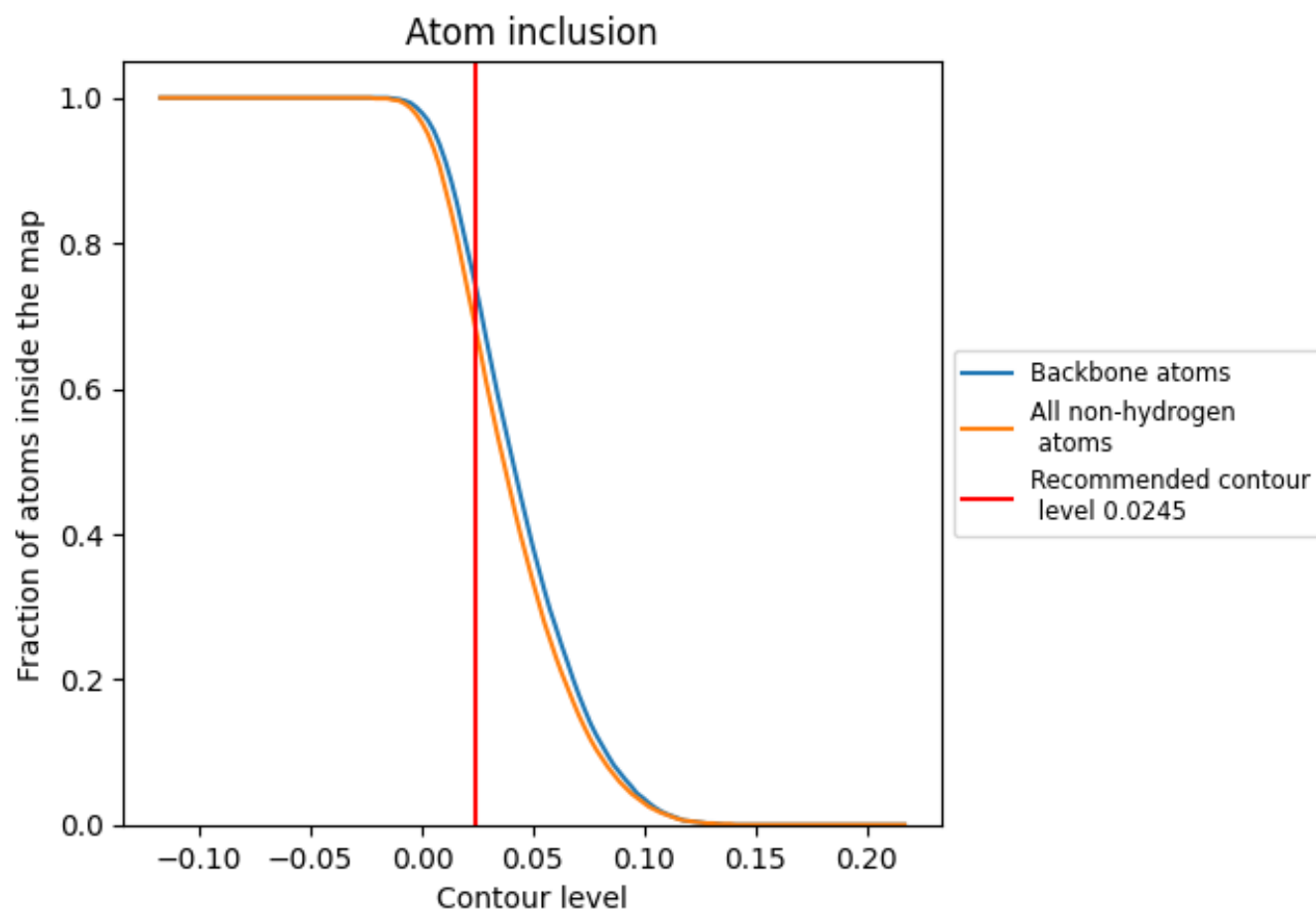
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0245).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.0245) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.5170
0	 0.7980	 0.5760
1	 0.0340	 0.1340
2	 0.0630	 0.1850
3	 0.8800	 0.6020
4	 0.0790	 0.2420
5	 0.0630	 0.1710
6	 0.8460	 0.5700
7	 0.7980	 0.5400
8	 0.7910	 0.5620
9	 0.8800	 0.5950
A	 0.8270	 0.5800
B	 0.7770	 0.5520
C	 0.7150	 0.5470
D	 0.8470	 0.5910
E	 0.7780	 0.5630
F	 0.7960	 0.5760
G	 0.6820	 0.5150
H	 0.7330	 0.5370
I	 0.6920	 0.5420
J	 0.6520	 0.4930
K	 0.6220	 0.4960
L	 0.8980	 0.6320
M	 0.8800	 0.6260
N	 0.5960	 0.4830
O	 0.5610	 0.4750
P	 0.6010	 0.4650
Q	 0.5850	 0.4960
R	 0.5400	 0.4580
S	 0.5600	 0.4770
T	 0.4650	 0.4200
U	 0.5070	 0.4630
V	 0.4090	 0.3920
W	 0.3390	 0.3590
X	 0.2390	 0.3080



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Chain	Atom inclusion	Q-score
Y	 0.1540	 0.2220
Z	 0.1020	 0.2080
a	 0.8220	 0.5790
aa	 0.7800	 0.5530
ab	 0.7540	 0.5440
b	 0.7840	 0.5470
c	 0.6910	 0.5260
d	 0.7720	 0.5810
e	 0.7500	 0.5430
f	 0.7490	 0.5570
g	 0.6750	 0.5100
h	 0.7220	 0.5370
i	 0.6310	 0.4930
j	 0.5580	 0.4710
k	 0.5870	 0.4830
l	 0.9040	 0.6310
m	 0.8800	 0.6220
n	 0.4980	 0.4250
o	 0.5550	 0.4640
p	 0.5760	 0.4730
q	 0.5530	 0.4770
r	 0.5090	 0.4710
s	 0.5210	 0.4810
t	 0.4810	 0.4400
u	 0.5370	 0.4730
v	 0.4240	 0.3990
w	 0.3850	 0.3830
x	 0.2160	 0.2590
y	 0.1380	 0.2310
z	 0.1460	 0.1940