



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:47 PM UTC

PDB ID : 8Z81 / pdb_00008z81
EMDB ID : EMD-39835
Title : Photosynthetic LH2-LH1 complex from the purple bacterium *Halorhodospira halophila*
Authors : Tani, K.; Nagashima, K.V.P.; Kanno, R.; Hiwatashi, N.; Kawakami, M.; Nakata, K.; Nagashima, S.; Inoue, K.; Takaichi, S.; Purba, E.R.; Hall, M.; Yu, L.-J.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.
Deposited on : 2024-04-21
Resolution : 2.20 Å (reported)
Based on initial models : 5Y5S, 1NKZ

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)

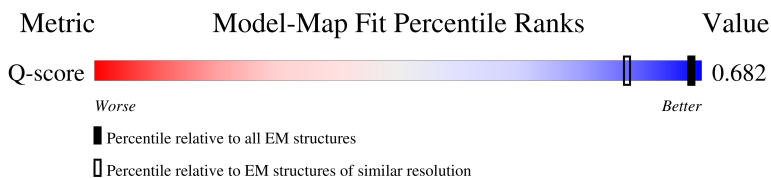
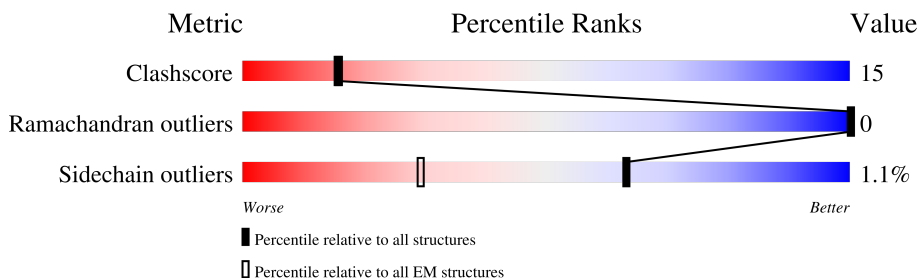
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3184 (1.71 - 2.70)

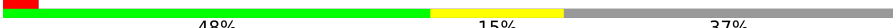
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	64	 61% 11% 28%
1	7	64	 59% 12% 28%

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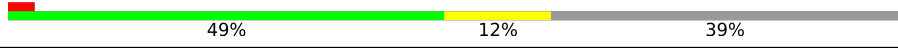
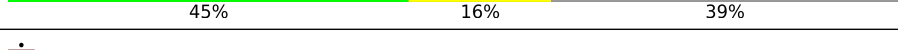
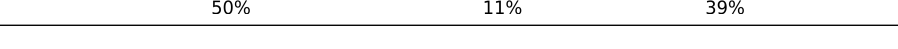
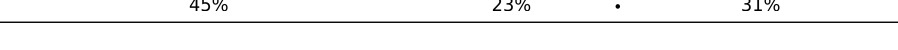
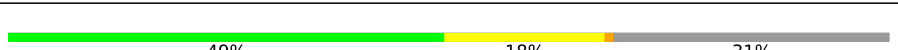
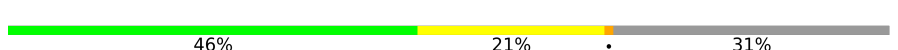
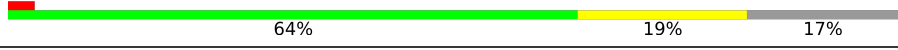
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	A	64	
1	E	64	
1	I	64	
1	M	64	
1	Q	64	
1	U	64	
1	Y	64	
2	4	75	
2	8	75	
2	B	75	
2	F	75	
2	J	75	
2	N	75	
2	R	75	
2	V	75	
2	Z	75	
3	1	67	
3	5	67	
3	9	67	
3	C	67	
3	G	67	
3	K	67	
3	O	67	
3	S	67	
3	W	67	

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Mol	Chain	Length	Quality of chain
4	0	74	
4	2	74	
4	6	74	
4	D	74	
4	H	74	
4	L	74	
4	P	74	
4	T	74	
4	X	74	
5	a	71	
5	c	71	
5	e	71	
5	g	71	
5	i	71	
5	k	71	
5	m	71	
5	o	71	
5	q	71	
6	b	59	
6	d	59	
6	f	59	
6	h	59	
6	j	59	
6	l	59	
6	n	59	

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Mol	Chain	Length	Quality of chain
6	p	59	
6	r	59	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 29349 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 Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	E	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	I	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	M	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	Q	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	U	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	Y	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	3	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
1	7	46	Total	C	N	O	S	0	0
			385	263	66	55	1		

- Molecule 2 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
2	F	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
2	J	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
2	N	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
2	R	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
2	V	47	Total	C	N	O	S	0	0
			380	256	59	64	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
2	4	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
2	8	47	Total	C	N	O	S	0	0
			380	256	59	64	1		

- Molecule 3 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	G	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	K	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	O	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	S	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	W	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	1	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	5	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
3	9	46	Total	C	N	O	S	0	0
			390	261	67	59	3		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	ASN	SER	conflict	UNP A1WXF8
C	42	GLN	GLU	conflict	UNP A1WXF8
C	48	ASP	ASN	conflict	UNP A1WXF8
C	57	ASP	GLU	conflict	UNP A1WXF8
G	37	ASN	SER	conflict	UNP A1WXF8
G	42	GLN	GLU	conflict	UNP A1WXF8
G	48	ASP	ASN	conflict	UNP A1WXF8
G	57	ASP	GLU	conflict	UNP A1WXF8
K	37	ASN	SER	conflict	UNP A1WXF8
K	42	GLN	GLU	conflict	UNP A1WXF8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	48	ASP	ASN	conflict	UNP A1WXF8
K	57	ASP	GLU	conflict	UNP A1WXF8
O	37	ASN	SER	conflict	UNP A1WXF8
O	42	GLN	GLU	conflict	UNP A1WXF8
O	48	ASP	ASN	conflict	UNP A1WXF8
O	57	ASP	GLU	conflict	UNP A1WXF8
S	37	ASN	SER	conflict	UNP A1WXF8
S	42	GLN	GLU	conflict	UNP A1WXF8
S	48	ASP	ASN	conflict	UNP A1WXF8
S	57	ASP	GLU	conflict	UNP A1WXF8
W	37	ASN	SER	conflict	UNP A1WXF8
W	42	GLN	GLU	conflict	UNP A1WXF8
W	48	ASP	ASN	conflict	UNP A1WXF8
W	57	ASP	GLU	conflict	UNP A1WXF8
1	37	ASN	SER	conflict	UNP A1WXF8
1	42	GLN	GLU	conflict	UNP A1WXF8
1	48	ASP	ASN	conflict	UNP A1WXF8
1	57	ASP	GLU	conflict	UNP A1WXF8
5	37	ASN	SER	conflict	UNP A1WXF8
5	42	GLN	GLU	conflict	UNP A1WXF8
5	48	ASP	ASN	conflict	UNP A1WXF8
5	57	ASP	GLU	conflict	UNP A1WXF8
9	37	ASN	SER	conflict	UNP A1WXF8
9	42	GLN	GLU	conflict	UNP A1WXF8
9	48	ASP	ASN	conflict	UNP A1WXF8
9	57	ASP	GLU	conflict	UNP A1WXF8

- Molecule 4 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
4	H	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
4	L	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
4	P	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
4	T	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
4	X	45	Total	C	N	O	S	0	0
			362	240	58	63	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
4	6	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
4	0	45	Total	C	N	O	S	0	0
			362	240	58	63	1		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	ILE	VAL	conflict	UNP A1WXF9
H	30	ILE	VAL	conflict	UNP A1WXF9
L	30	ILE	VAL	conflict	UNP A1WXF9
P	30	ILE	VAL	conflict	UNP A1WXF9
T	30	ILE	VAL	conflict	UNP A1WXF9
X	30	ILE	VAL	conflict	UNP A1WXF9
2	30	ILE	VAL	conflict	UNP A1WXF9
6	30	ILE	VAL	conflict	UNP A1WXF9
0	30	ILE	VAL	conflict	UNP A1WXF9

- Molecule 5 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	c	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	e	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	g	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	i	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	k	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	m	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	o	49	Total	C	N	O	S	0	0
			383	258	61	63	1		
5	q	49	Total	C	N	O	S	0	0
			383	258	61	63	1		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	19	PHE	LEU	conflict	UNP A1WWW3
a	27	SER	ALA	conflict	UNP A1WWW3
a	43	ALA	SER	conflict	UNP A1WWW3
a	44	PHE	TYR	conflict	UNP A1WWW3
a	61	SER	GLY	conflict	UNP A1WWW3
c	19	PHE	LEU	conflict	UNP A1WWW3
c	27	SER	ALA	conflict	UNP A1WWW3
c	43	ALA	SER	conflict	UNP A1WWW3
c	44	PHE	TYR	conflict	UNP A1WWW3
c	61	SER	GLY	conflict	UNP A1WWW3
e	19	PHE	LEU	conflict	UNP A1WWW3
e	27	SER	ALA	conflict	UNP A1WWW3
e	43	ALA	SER	conflict	UNP A1WWW3
e	44	PHE	TYR	conflict	UNP A1WWW3
e	61	SER	GLY	conflict	UNP A1WWW3
g	19	PHE	LEU	conflict	UNP A1WWW3
g	27	SER	ALA	conflict	UNP A1WWW3
g	43	ALA	SER	conflict	UNP A1WWW3
g	44	PHE	TYR	conflict	UNP A1WWW3
g	61	SER	GLY	conflict	UNP A1WWW3
i	19	PHE	LEU	conflict	UNP A1WWW3
i	27	SER	ALA	conflict	UNP A1WWW3
i	43	ALA	SER	conflict	UNP A1WWW3
i	44	PHE	TYR	conflict	UNP A1WWW3
i	61	SER	GLY	conflict	UNP A1WWW3
k	19	PHE	LEU	conflict	UNP A1WWW3
k	27	SER	ALA	conflict	UNP A1WWW3
k	43	ALA	SER	conflict	UNP A1WWW3
k	44	PHE	TYR	conflict	UNP A1WWW3
k	61	SER	GLY	conflict	UNP A1WWW3
m	19	PHE	LEU	conflict	UNP A1WWW3
m	27	SER	ALA	conflict	UNP A1WWW3
m	43	ALA	SER	conflict	UNP A1WWW3
m	44	PHE	TYR	conflict	UNP A1WWW3
m	61	SER	GLY	conflict	UNP A1WWW3
o	19	PHE	LEU	conflict	UNP A1WWW3
o	27	SER	ALA	conflict	UNP A1WWW3
o	43	ALA	SER	conflict	UNP A1WWW3
o	44	PHE	TYR	conflict	UNP A1WWW3
o	61	SER	GLY	conflict	UNP A1WWW3
q	19	PHE	LEU	conflict	UNP A1WWW3
q	27	SER	ALA	conflict	UNP A1WWW3

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Chain	Residue	Modelled	Actual	Comment	Reference
q	43	ALA	SER	conflict	UNP A1WWW3
q	44	PHE	TYR	conflict	UNP A1WWW3
q	61	SER	GLY	conflict	UNP A1WWW3

- Molecule 6 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	b	49	Total	C	N	O	0	0
			391	261	62	68		
6	d	49	Total	C	N	O	0	0
			391	261	62	68		
6	f	49	Total	C	N	O	0	0
			391	261	62	68		
6	h	49	Total	C	N	O	0	0
			391	261	62	68		
6	j	49	Total	C	N	O	0	0
			391	261	62	68		
6	l	49	Total	C	N	O	0	0
			391	261	62	68		
6	n	49	Total	C	N	O	0	0
			391	261	62	68		
6	p	49	Total	C	N	O	0	0
			391	261	62	68		
6	r	49	Total	C	N	O	0	0
			391	261	62	68		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
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	N	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	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 66	C 55	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	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	2	1	Total 66	C 55	Mg 1	N 4	O 6	0

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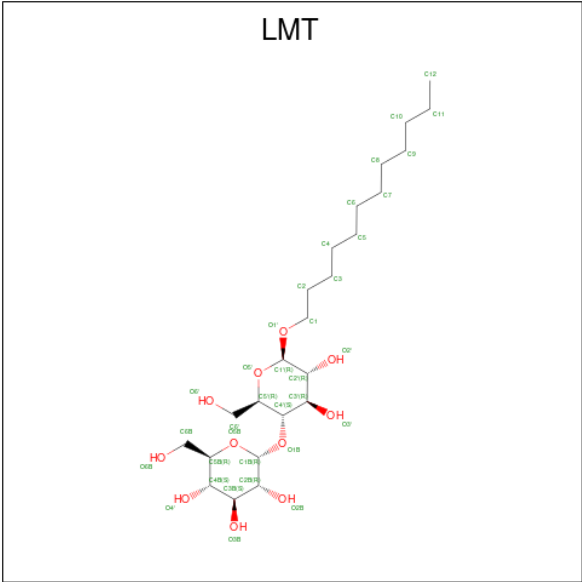
Mol	Chain	Residues	Atoms					AltConf
7	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	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	a	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	c	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	c	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	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	g	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
7	h	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	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	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	n	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	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	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

- Molecule 8 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	24	11	
8	C	1	Total	C	O	0
			35	24	11	
8	C	1	Total	C	O	0
			35	24	11	
8	C	1	Total	C	O	0
			32	21	11	
8	E	1	Total	C	O	0
			35	24	11	
8	G	1	Total	C	O	0
			35	24	11	
8	G	1	Total	C	O	0
			35	24	11	
8	G	1	Total	C	O	0
			32	21	11	
8	I	1	Total	C	O	0
			35	24	11	
8	K	1	Total	C	O	0
			35	24	11	
8	K	1	Total	C	O	0
			35	24	11	
8	K	1	Total	C	O	0
			32	21	11	
8	M	1	Total	C	O	0
			35	24	11	
8	O	1	Total	C	O	0
			35	24	11	

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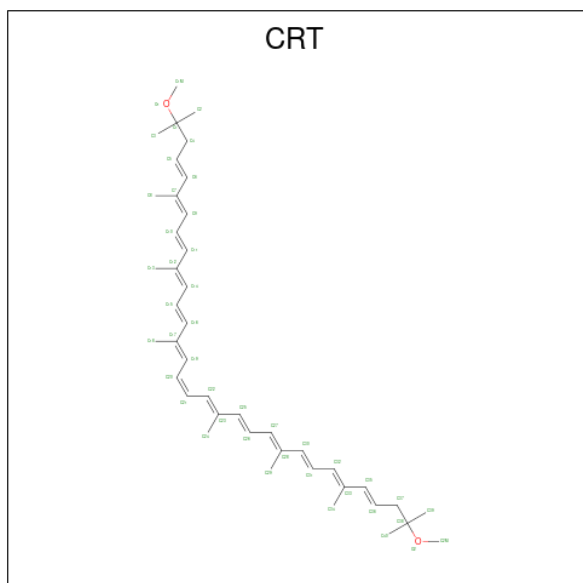
Mol	Chain	Residues	Atoms			AltConf
8	O	1	Total	C	O	0
			35	24	11	
8	O	1	Total	C	O	0
			32	21	11	
8	Q	1	Total	C	O	0
			35	24	11	
8	S	1	Total	C	O	0
			35	24	11	
8	S	1	Total	C	O	0
			35	24	11	
8	S	1	Total	C	O	0
			32	21	11	
8	U	1	Total	C	O	0
			35	24	11	
8	W	1	Total	C	O	0
			35	24	11	
8	W	1	Total	C	O	0
			35	24	11	
8	W	1	Total	C	O	0
			32	21	11	
8	Y	1	Total	C	O	0
			35	24	11	
8	1	1	Total	C	O	0
			35	24	11	
8	1	1	Total	C	O	0
			35	24	11	
8	1	1	Total	C	O	0
			32	21	11	
8	3	1	Total	C	O	0
			35	24	11	
8	5	1	Total	C	O	0
			35	24	11	
8	5	1	Total	C	O	0
			35	24	11	
8	5	1	Total	C	O	0
			32	21	11	
8	7	1	Total	C	O	0
			35	24	11	
8	9	1	Total	C	O	0
			35	24	11	
8	9	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
8	9	1	Total	C	O	0
			32	21	11	
8	b	1	Total	C	O	0
			35	24	11	
8	d	1	Total	C	O	0
			35	24	11	
8	f	1	Total	C	O	0
			35	24	11	
8	h	1	Total	C	O	0
			35	24	11	
8	j	1	Total	C	O	0
			35	24	11	
8	l	1	Total	C	O	0
			35	24	11	
8	n	1	Total	C	O	0
			35	24	11	
8	p	1	Total	C	O	0
			35	24	11	
8	r	1	Total	C	O	0
			35	24	11	

- Molecule 9 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: $C_{42}H_{60}O_2$).



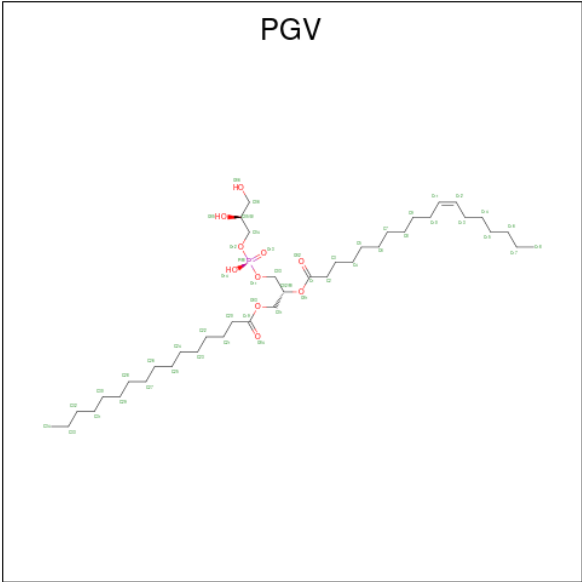
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
9	F	1	Total	C	O	0
			44	42	2	
9	J	1	Total	C	O	0
			44	42	2	
9	N	1	Total	C	O	0
			44	42	2	
9	R	1	Total	C	O	0
			44	42	2	
9	V	1	Total	C	O	0
			44	42	2	
9	Z	1	Total	C	O	0
			44	42	2	
9	4	1	Total	C	O	0
			44	42	2	
9	8	1	Total	C	O	0
			44	42	2	
9	a	1	Total	C	O	0
			44	42	2	
9	b	1	Total	C	O	0
			44	42	2	
9	e	1	Total	C	O	0
			44	42	2	
9	f	1	Total	C	O	0
			44	42	2	
9	h	1	Total	C	O	0
			44	42	2	
9	k	1	Total	C	O	0
			44	42	2	
9	m	1	Total	C	O	0
			44	42	2	
9	o	1	Total	C	O	0
			44	42	2	
9	q	1	Total	C	O	0
			44	42	2	

- Molecule 10 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total	C	O	P	0
			45	36	8	1	
10	D	1	Total	C	O	P	0
			44	35	8	1	
10	F	1	Total	C	O	P	0
			45	36	8	1	
10	H	1	Total	C	O	P	0
			44	35	8	1	
10	J	1	Total	C	O	P	0
			45	36	8	1	
10	L	1	Total	C	O	P	0
			44	35	8	1	
10	N	1	Total	C	O	P	0
			45	36	8	1	
10	P	1	Total	C	O	P	0
			44	35	8	1	
10	R	1	Total	C	O	P	0
			45	36	8	1	
10	T	1	Total	C	O	P	0
			44	35	8	1	
10	V	1	Total	C	O	P	0
			45	36	8	1	
10	X	1	Total	C	O	P	0
			44	35	8	1	
10	2	1	Total	C	O	P	0
			45	36	8	1	
10	2	1	Total	C	O	P	0
			44	35	8	1	

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Mol	Chain	Residues	Atoms				AltConf
10	4	1	Total	C	O	P	0
			45	36	8	1	
10	6	1	Total	C	O	P	0
			44	35	8	1	
10	8	1	Total	C	O	P	0
			45	36	8	1	
10	0	1	Total	C	O	P	0
			44	35	8	1	
10	a	1	Total	C	O	P	0
			42	33	8	1	
10	a	1	Total	C	O	P	0
			51	40	10	1	
10	c	1	Total	C	O	P	0
			42	33	8	1	
10	c	1	Total	C	O	P	0
			51	40	10	1	
10	e	1	Total	C	O	P	0
			42	33	8	1	
10	e	1	Total	C	O	P	0
			51	40	10	1	
10	g	1	Total	C	O	P	0
			42	33	8	1	
10	g	1	Total	C	O	P	0
			51	40	10	1	
10	i	1	Total	C	O	P	0
			42	33	8	1	
10	i	1	Total	C	O	P	0
			51	40	10	1	
10	k	1	Total	C	O	P	0
			42	33	8	1	
10	k	1	Total	C	O	P	0
			51	40	10	1	
10	m	1	Total	C	O	P	0
			42	33	8	1	
10	m	1	Total	C	O	P	0
			51	40	10	1	
10	o	1	Total	C	O	P	0
			42	33	8	1	
10	o	1	Total	C	O	P	0
			51	40	10	1	
10	q	1	Total	C	O	P	0
			42	33	8	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	q	1	51	40	10	1	0

3 Residue-property plots

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.

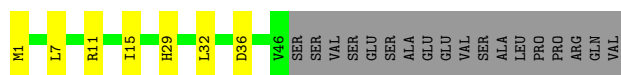
- Molecule 1: Antenna complex, alpha/beta subunit

Chain A: 



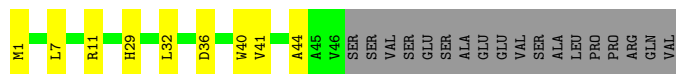
- Molecule 1: Antenna complex, alpha/beta subunit

Chain E: 



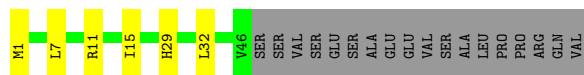
- Molecule 1: Antenna complex, alpha/beta subunit

Chain I: 



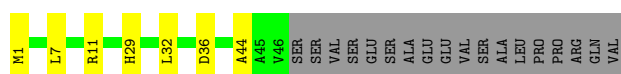
- Molecule 1: Antenna complex, alpha/beta subunit

Chain M: 



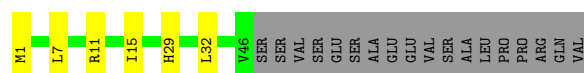
- Molecule 1: Antenna complex, alpha/beta subunit

Chain Q: 



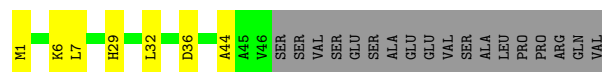
- Molecule 1: Antenna complex, alpha/beta subunit

Chain U:  62% 9% 28%



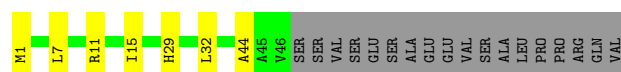
- Molecule 1: Antenna complex, alpha/beta subunit

Chain Y:  61% 11% 28%



- Molecule 1: Antenna complex, alpha/beta subunit

Chain 3:  61% 11% 28%



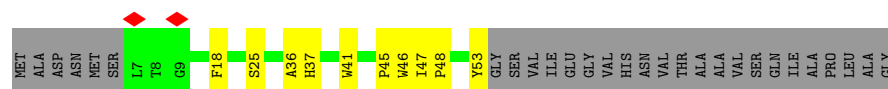
- Molecule 1: Antenna complex, alpha/beta subunit

Chain 7:  59% 12% 28%

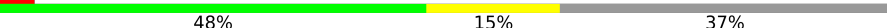


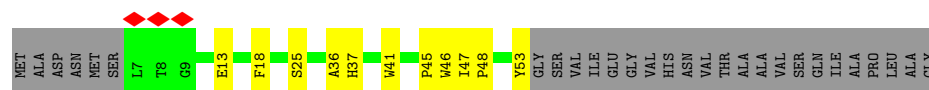
- Molecule 2: Antenna complex, alpha/beta subunit

Chain B:  49% 13% 37%

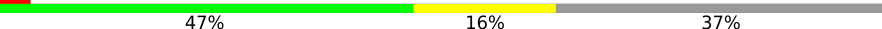


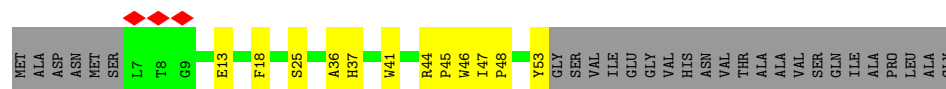
- Molecule 2: Antenna complex, alpha/beta subunit

Chain F:  48% 15% 37%

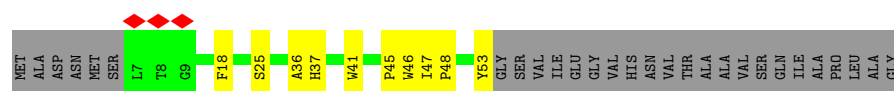


- Molecule 2: Antenna complex, alpha/beta subunit

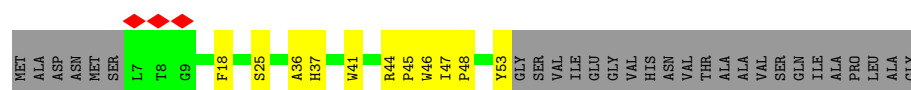
Chain J:  47% 16% 37%



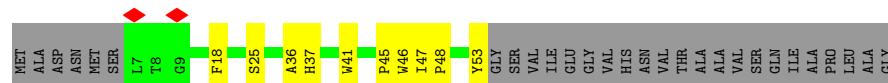
- Molecule 2: Antenna complex, alpha/beta subunit



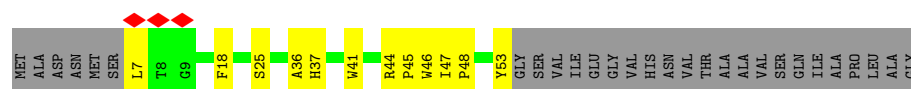
- Molecule 2: Antenna complex, alpha/beta subunit



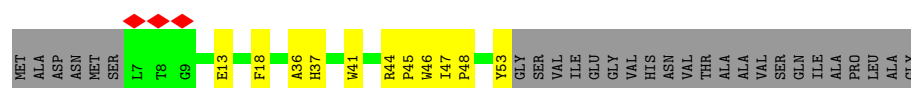
- Molecule 2: Antenna complex, alpha/beta subunit



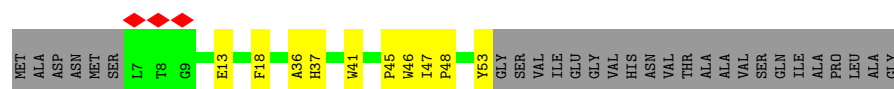
- Molecule 2: Antenna complex, alpha/beta subunit



- Molecule 2: Antenna complex, alpha/beta subunit



- Molecule 2: Antenna complex, alpha/beta subunit

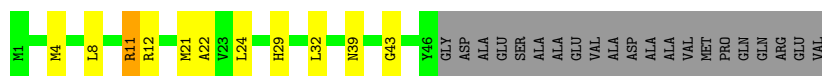


- Molecule 3: Antenna complex, alpha/beta subunit



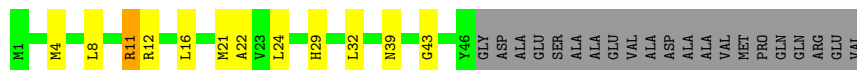
- Molecule 3: Antenna complex, alpha/beta subunit

Chain G:  52% 15% 31%



- Molecule 3: Antenna complex, alpha/beta subunit

Chain K:  51% 16% 31%



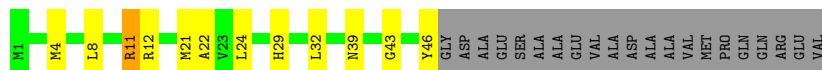
- Molecule 3: Antenna complex, alpha/beta subunit

Chain O:  52% 15% 31%



- Molecule 3: Antenna complex, alpha/beta subunit

Chain S:  51% 16% 31%



- Molecule 3: Antenna complex, alpha/beta subunit

Chain W:  52% 15% 31%



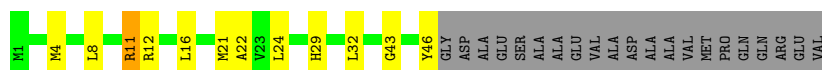
- Molecule 3: Antenna complex, alpha/beta subunit

Chain 1:  54% 13% 31%



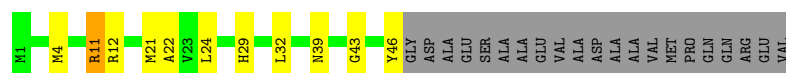
- Molecule 3: Antenna complex, alpha/beta subunit

Chain 5:  51% 16% 31%



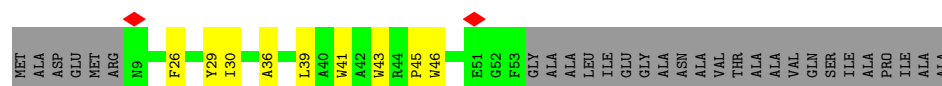
- Molecule 3: Antenna complex, alpha/beta subunit

Chain 9:  52% 15% 31%



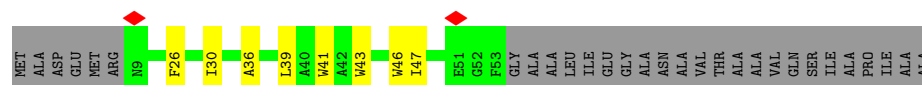
- Molecule 4: Antenna complex, alpha/beta subunit

Chain D:  49% 12% 39%



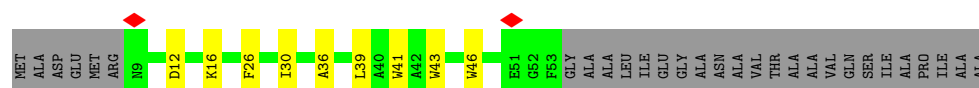
- Molecule 4: Antenna complex, alpha/beta subunit

Chain H:  50% 11% 39%



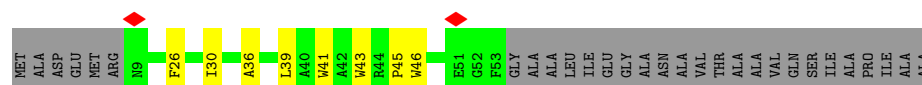
- Molecule 4: Antenna complex, alpha/beta subunit

Chain L:  49% 12% 39%

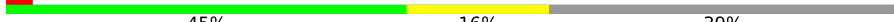


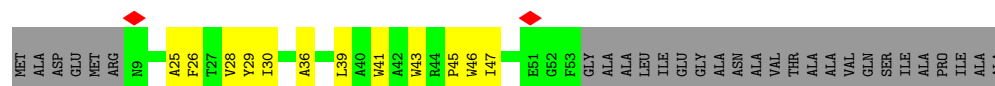
- Molecule 4: Antenna complex, alpha/beta subunit

Chain P:  50% 11% 39%



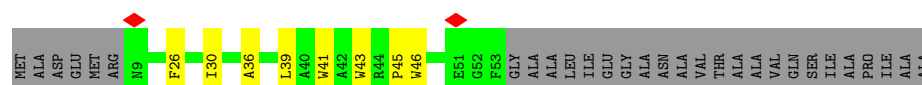
- Molecule 4: Antenna complex, alpha/beta subunit

Chain T:  45% 16% 39%



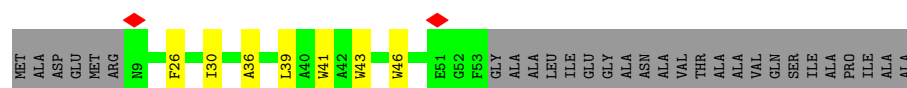
- Molecule 4: Antenna complex, alpha/beta subunit

Chain X:  50% 11% 39%



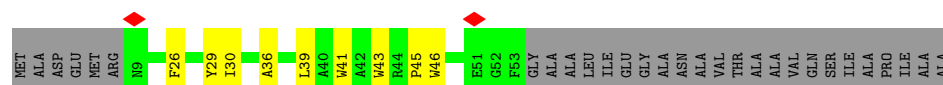
- Molecule 4: Antenna complex, alpha/beta subunit

Chain 2:  51% 9% 39%



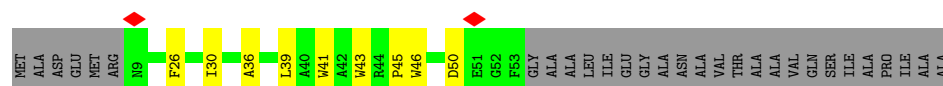
- Molecule 4: Antenna complex, alpha/beta subunit

Chain 6:  49% 12% 39%



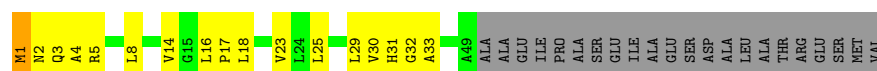
- Molecule 4: Antenna complex, alpha/beta subunit

Chain 0:  49% 12% 39%



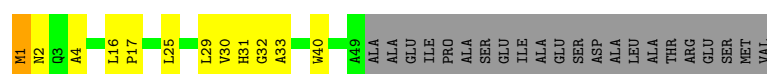
- Molecule 5: Antenna complex, alpha/beta subunit

Chain a:  45% 23% 31%



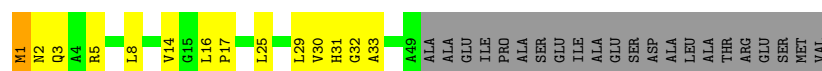
- Molecule 5: Antenna complex, alpha/beta subunit

Chain c:  52% 15% 31%



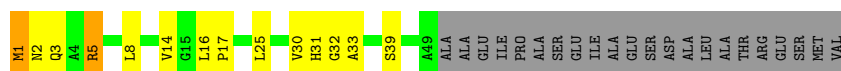
- Molecule 5: Antenna complex, alpha/beta subunit

Chain e:  49% 18% 31%

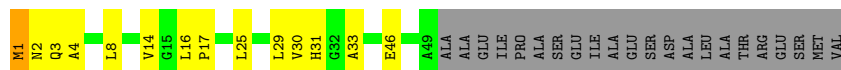


- Molecule 5: Antenna complex, alpha/beta subunit

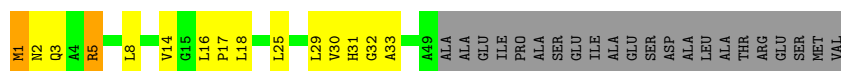
Chain g:  49% 17% 31%



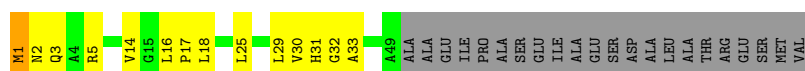
- Molecule 5: Antenna complex, alpha/beta subunit



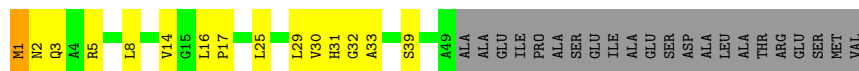
- Molecule 5: Antenna complex, alpha/beta subunit



- Molecule 5: Antenna complex, alpha/beta subunit



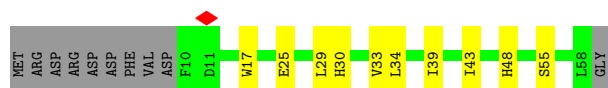
- Molecule 5: Antenna complex, alpha/beta subunit



- Molecule 5: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit

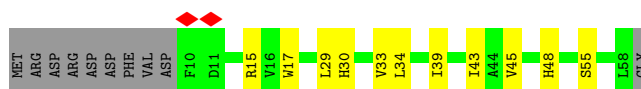




- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



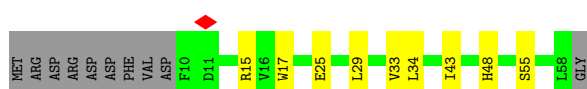
- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size ($\text{\AA}$)	328.0, 328.0, 328.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRT, CXM, PGV, BCL, LMT

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	3	0.15	0/398	0.23	0/543
1	7	0.14	0/398	0.22	0/543
1	A	0.14	0/398	0.22	0/543
1	E	0.14	0/398	0.24	0/543
1	I	0.14	0/398	0.22	0/543
1	M	0.14	0/398	0.23	0/543
1	Q	0.14	0/398	0.24	0/543
1	U	0.14	0/398	0.23	0/543
1	Y	0.14	0/398	0.23	0/543
2	4	0.13	0/395	0.20	0/539
2	8	0.13	0/395	0.20	0/539
2	B	0.13	0/395	0.20	0/539
2	F	0.13	0/395	0.19	0/539
2	J	0.14	0/395	0.20	0/539
2	N	0.13	0/395	0.20	0/539
2	R	0.13	0/395	0.20	0/539
2	V	0.13	0/395	0.20	0/539
2	Z	0.13	0/395	0.20	0/539
3	1	0.15	0/402	0.29	0/547
3	5	0.14	0/402	0.26	0/547
3	9	0.14	0/402	0.26	0/547
3	C	0.15	0/402	0.29	0/547
3	G	0.14	0/402	0.26	0/547
3	K	0.14	0/402	0.25	0/547
3	O	0.14	0/402	0.25	0/547
3	S	0.14	0/402	0.25	0/547
3	W	0.15	0/402	0.26	0/547
4	0	0.13	0/376	0.18	0/514
4	2	0.14	0/376	0.18	0/514
4	6	0.13	0/376	0.17	0/514
4	D	0.13	0/376	0.18	0/514
4	H	0.13	0/376	0.18	0/514

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	L	0.13	0/376	0.18	0/514
4	P	0.13	0/376	0.19	0/514
4	T	0.13	0/376	0.18	0/514
4	X	0.13	0/376	0.18	0/514
5	a	0.18	0/383	0.32	0/526
5	c	0.18	0/383	0.32	0/526
5	e	0.18	0/383	0.32	0/526
5	g	0.18	0/383	0.31	0/526
5	i	0.18	0/383	0.32	0/526
5	k	0.18	0/383	0.32	0/526
5	m	0.18	0/383	0.32	0/526
5	o	0.18	0/383	0.32	0/526
5	q	0.18	0/383	0.32	0/526
6	b	0.15	0/406	0.27	0/558
6	d	0.15	0/406	0.27	0/558
6	f	0.15	0/406	0.28	0/558
6	h	0.15	0/406	0.27	0/558
6	j	0.15	0/406	0.27	0/558
6	l	0.15	0/406	0.27	0/558
6	n	0.15	0/406	0.27	0/558
6	p	0.15	0/406	0.28	0/558
6	r	0.15	0/406	0.27	0/558
All	All	0.15	0/21240	0.25	0/29043

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	385	0	403	7	0
1	7	385	0	403	9	0
1	A	385	0	403	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	385	0	403	7	0
1	I	385	0	403	8	0
1	M	385	0	403	7	0
1	Q	385	0	403	8	0
1	U	385	0	403	6	0
1	Y	385	0	403	8	0
2	4	380	0	359	9	0
2	8	380	0	359	9	0
2	B	380	0	359	10	0
2	F	380	0	359	10	0
2	J	380	0	359	11	0
2	N	380	0	359	9	0
2	R	380	0	359	11	0
2	V	380	0	359	9	0
2	Z	380	0	359	11	0
3	1	390	0	401	14	0
3	5	390	0	401	15	0
3	9	390	0	401	14	0
3	C	390	0	401	14	0
3	G	390	0	401	15	0
3	K	390	0	401	15	0
3	O	390	0	401	13	0
3	S	390	0	401	16	0
3	W	390	0	401	13	0
4	0	362	0	333	9	0
4	2	362	0	333	7	0
4	6	362	0	333	10	0
4	D	362	0	333	8	0
4	H	362	0	333	8	0
4	L	362	0	333	8	0
4	P	362	0	333	8	0
4	T	362	0	333	12	0
4	X	362	0	333	8	0
5	a	383	0	398	20	0
5	c	383	0	398	15	0
5	e	383	0	398	17	0
5	g	383	0	398	17	0
5	i	383	0	398	15	0
5	k	383	0	398	17	0
5	m	383	0	398	17	0
5	o	383	0	398	17	0
5	q	383	0	398	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	b	391	0	371	12	0
6	d	391	0	371	14	0
6	f	391	0	371	12	0
6	h	391	0	371	13	0
6	j	391	0	371	10	0
6	l	391	0	371	9	0
6	n	391	0	371	14	0
6	p	391	0	371	10	0
6	r	391	0	371	12	0
7	0	66	0	74	6	0
7	1	132	0	148	10	0
7	2	66	0	74	6	0
7	3	66	0	74	1	0
7	4	66	0	74	6	0
7	5	132	0	148	8	0
7	6	66	0	74	7	0
7	7	66	0	74	3	0
7	8	66	0	74	8	0
7	9	132	0	148	12	0
7	A	66	0	74	1	0
7	B	66	0	74	6	0
7	C	132	0	148	10	0
7	D	66	0	74	3	0
7	E	66	0	74	3	0
7	F	66	0	74	6	0
7	G	132	0	148	10	0
7	H	66	0	74	6	0
7	I	66	0	74	4	0
7	J	66	0	74	6	0
7	K	132	0	148	9	0
7	L	66	0	74	6	0
7	M	66	0	74	2	0
7	N	66	0	74	6	0
7	O	132	0	148	9	0
7	P	66	0	74	4	0
7	Q	66	0	74	2	0
7	R	66	0	74	9	0
7	S	132	0	148	10	0
7	T	66	0	74	6	0
7	U	66	0	74	3	0
7	V	66	0	74	4	0
7	W	132	0	148	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	66	0	74	5	0
7	Y	66	0	74	2	0
7	Z	66	0	74	7	0
7	a	132	0	148	9	0
7	b	66	0	74	8	0
7	c	132	0	148	8	0
7	d	66	0	74	6	0
7	e	132	0	148	11	0
7	f	66	0	74	7	0
7	g	132	0	148	8	0
7	h	66	0	74	7	0
7	i	132	0	148	13	0
7	j	66	0	74	5	0
7	k	132	0	148	14	0
7	l	66	0	74	7	0
7	m	132	0	148	12	0
7	n	66	0	74	6	0
7	o	132	0	148	13	0
7	p	66	0	74	4	0
7	q	132	0	148	12	0
7	r	66	0	74	4	0
8	1	102	0	129	12	0
8	3	35	0	46	1	0
8	5	102	0	129	8	0
8	7	35	0	46	1	0
8	9	102	0	129	9	0
8	A	35	0	46	1	0
8	C	102	0	129	10	0
8	E	35	0	46	2	0
8	G	102	0	129	13	0
8	I	35	0	46	0	0
8	K	102	0	129	15	0
8	M	35	0	46	1	0
8	O	102	0	129	9	0
8	Q	35	0	46	1	0
8	S	102	0	129	12	0
8	U	35	0	46	1	0
8	W	102	0	129	7	0
8	Y	35	0	46	0	0
8	b	35	0	46	3	0
8	d	35	0	46	2	0
8	f	35	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	h	35	0	46	3	0
8	j	35	0	46	2	0
8	l	35	0	46	2	0
8	n	35	0	46	4	0
8	p	35	0	46	3	0
8	r	35	0	46	2	0
9	4	44	0	60	5	0
9	8	44	0	60	5	0
9	B	44	0	60	5	0
9	F	44	0	60	5	0
9	J	44	0	60	6	0
9	N	44	0	60	6	0
9	R	44	0	60	5	0
9	V	44	0	60	6	0
9	Z	44	0	60	5	0
9	a	44	0	60	7	0
9	b	44	0	60	7	0
9	e	44	0	60	8	0
9	f	44	0	60	8	0
9	h	44	0	60	9	0
9	k	44	0	60	10	0
9	m	44	0	60	8	0
9	o	44	0	60	9	0
9	q	44	0	60	8	0
10	0	44	0	60	2	0
10	2	89	0	122	10	0
10	4	45	0	62	9	0
10	6	44	0	60	5	0
10	8	45	0	62	11	0
10	B	45	0	62	7	0
10	D	44	0	60	5	0
10	F	45	0	62	9	0
10	H	44	0	60	5	0
10	J	45	0	62	7	0
10	L	44	0	60	3	0
10	N	45	0	62	9	0
10	P	44	0	60	3	0
10	R	45	0	62	7	0
10	T	44	0	60	3	0
10	V	45	0	62	6	0
10	X	44	0	60	4	0
10	a	93	0	132	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	c	93	0	132	16	0
10	e	93	0	132	16	0
10	g	93	0	132	17	0
10	i	93	0	132	15	0
10	k	93	0	132	17	0
10	m	93	0	132	18	0
10	o	93	0	132	17	0
10	q	93	0	132	14	0
All	All	29349	0	31068	877	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 877 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:103:LMT:H2O1	8:O:105:LMT:H3O2	1.21	0.85
8:9:103:LMT:H2O1	8:9:105:LMT:H3O2	1.19	0.85
10:c:103:PGV:H201	10:e:104:PGV:H82	1.65	0.77
10:e:104:PGV:H201	10:g:103:PGV:H82	1.64	0.77
3:S:4:MET:HE1	9:V:101:CRT:H132	1.68	0.75

There are no symmetry-related clashes.

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	3	44/64 (69%)	44 (100%)	0	0	100	100
1	7	44/64 (69%)	44 (100%)	0	0	100	100
1	A	44/64 (69%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	44/64 (69%)	44 (100%)	0	0	100	100
1	I	44/64 (69%)	44 (100%)	0	0	100	100
1	M	44/64 (69%)	44 (100%)	0	0	100	100
1	Q	44/64 (69%)	44 (100%)	0	0	100	100
1	U	44/64 (69%)	44 (100%)	0	0	100	100
1	Y	44/64 (69%)	44 (100%)	0	0	100	100
2	4	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	8	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	B	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	F	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	J	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	N	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	R	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	V	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
2	Z	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
3	1	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
3	5	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
3	9	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
3	C	44/67 (66%)	44 (100%)	0	0	100	100
3	G	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
3	K	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
3	O	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
3	S	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
3	W	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
4	0	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
4	2	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
4	6	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
4	D	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
4	H	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
4	L	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
4	P	43/74 (58%)	42 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	T	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
4	X	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
5	a	47/71 (66%)	47 (100%)	0	0	100	100
5	c	47/71 (66%)	47 (100%)	0	0	100	100
5	e	47/71 (66%)	47 (100%)	0	0	100	100
5	g	47/71 (66%)	47 (100%)	0	0	100	100
5	i	47/71 (66%)	47 (100%)	0	0	100	100
5	k	47/71 (66%)	47 (100%)	0	0	100	100
5	m	47/71 (66%)	47 (100%)	0	0	100	100
5	o	47/71 (66%)	47 (100%)	0	0	100	100
5	q	47/71 (66%)	47 (100%)	0	0	100	100
6	b	47/59 (80%)	47 (100%)	0	0	100	100
6	d	47/59 (80%)	47 (100%)	0	0	100	100
6	f	47/59 (80%)	47 (100%)	0	0	100	100
6	h	47/59 (80%)	47 (100%)	0	0	100	100
6	j	47/59 (80%)	47 (100%)	0	0	100	100
6	l	47/59 (80%)	47 (100%)	0	0	100	100
6	n	47/59 (80%)	47 (100%)	0	0	100	100
6	p	47/59 (80%)	47 (100%)	0	0	100	100
6	r	47/59 (80%)	47 (100%)	0	0	100	100
All	All	2430/3690 (66%)	2395 (99%)	35 (1%)	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	3	39/55 (71%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	39/55 (71%)	39 (100%)	0	100	100
1	A	39/55 (71%)	39 (100%)	0	100	100
1	E	39/55 (71%)	39 (100%)	0	100	100
1	I	39/55 (71%)	39 (100%)	0	100	100
1	M	39/55 (71%)	39 (100%)	0	100	100
1	Q	39/55 (71%)	39 (100%)	0	100	100
1	U	39/55 (71%)	39 (100%)	0	100	100
1	Y	39/55 (71%)	39 (100%)	0	100	100
2	4	37/57 (65%)	36 (97%)	1 (3%)	39	53
2	8	37/57 (65%)	36 (97%)	1 (3%)	39	53
2	B	37/57 (65%)	37 (100%)	0	100	100
2	F	37/57 (65%)	36 (97%)	1 (3%)	39	53
2	J	37/57 (65%)	36 (97%)	1 (3%)	39	53
2	N	37/57 (65%)	37 (100%)	0	100	100
2	R	37/57 (65%)	37 (100%)	0	100	100
2	V	37/57 (65%)	37 (100%)	0	100	100
2	Z	37/57 (65%)	37 (100%)	0	100	100
3	1	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	5	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	9	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	C	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	G	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	K	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	O	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	S	41/55 (74%)	40 (98%)	1 (2%)	43	58
3	W	41/55 (74%)	40 (98%)	1 (2%)	43	58
4	0	35/52 (67%)	35 (100%)	0	100	100
4	2	35/52 (67%)	35 (100%)	0	100	100
4	6	35/52 (67%)	35 (100%)	0	100	100
4	D	35/52 (67%)	35 (100%)	0	100	100
4	H	35/52 (67%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	35/52 (67%)	35 (100%)	0	100	100
4	P	35/52 (67%)	35 (100%)	0	100	100
4	T	35/52 (67%)	35 (100%)	0	100	100
4	X	35/52 (67%)	35 (100%)	0	100	100
5	a	40/56 (71%)	39 (98%)	1 (2%)	42	56
5	c	40/56 (71%)	40 (100%)	0	100	100
5	e	40/56 (71%)	40 (100%)	0	100	100
5	g	40/56 (71%)	38 (95%)	2 (5%)	22	28
5	i	40/56 (71%)	39 (98%)	1 (2%)	42	56
5	k	40/56 (71%)	38 (95%)	2 (5%)	22	28
5	m	40/56 (71%)	39 (98%)	1 (2%)	42	56
5	o	40/56 (71%)	39 (98%)	1 (2%)	42	56
5	q	40/56 (71%)	39 (98%)	1 (2%)	42	56
6	b	40/49 (82%)	40 (100%)	0	100	100
6	d	40/49 (82%)	40 (100%)	0	100	100
6	f	40/49 (82%)	40 (100%)	0	100	100
6	h	40/49 (82%)	40 (100%)	0	100	100
6	j	40/49 (82%)	40 (100%)	0	100	100
6	l	40/49 (82%)	40 (100%)	0	100	100
6	n	40/49 (82%)	40 (100%)	0	100	100
6	p	40/49 (82%)	40 (100%)	0	100	100
6	r	40/49 (82%)	40 (100%)	0	100	100
All	All	2088/2916 (72%)	2066 (99%)	22 (1%)	63	79

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	g	3	GLN
5	k	3	GLN
5	i	3	GLN
5	k	5	ARG
3	S	11	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
3	5	39	ASN
5	a	2	ASN
5	o	2	ASN
3	9	39	ASN
5	c	2	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CXM	e	1	5,7	9,10,11	0.51	0	9,11,13	1.05	1 (11%)
5	CXM	i	1	5,7	9,10,11	0.53	0	9,11,13	1.04	1 (11%)
5	CXM	q	1	5,7	9,10,11	0.51	0	9,11,13	1.02	1 (11%)
5	CXM	o	1	5,7	9,10,11	0.52	0	9,11,13	1.05	1 (11%)
5	CXM	m	1	5,7	9,10,11	0.51	0	9,11,13	1.01	1 (11%)
5	CXM	k	1	5,7	9,10,11	0.51	0	9,11,13	1.01	1 (11%)
5	CXM	g	1	5,7	9,10,11	0.52	0	9,11,13	1.01	1 (11%)
5	CXM	a	1	5,7	9,10,11	0.53	0	9,11,13	1.04	1 (11%)
5	CXM	c	1	5,7	9,10,11	0.53	0	9,11,13	1.01	1 (11%)

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
5	CXM	e	1	5,7	-	2/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CXM	i	1	5,7	-	2/9/10/12	-
5	CXM	q	1	5,7	-	2/9/10/12	-
5	CXM	o	1	5,7	-	2/9/10/12	-
5	CXM	m	1	5,7	-	2/9/10/12	-
5	CXM	k	1	5,7	-	2/9/10/12	-
5	CXM	g	1	5,7	-	2/9/10/12	-
5	CXM	a	1	5,7	-	2/9/10/12	-
5	CXM	c	1	5,7	-	2/9/10/12	-

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	i	1	CXM	O-C-CA	-2.66	117.94	124.77
5	e	1	CXM	O-C-CA	-2.65	117.96	124.77
5	a	1	CXM	O-C-CA	-2.65	117.97	124.77
5	o	1	CXM	O-C-CA	-2.65	117.97	124.77
5	q	1	CXM	O-C-CA	-2.64	117.97	124.77

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	1	CXM	C-CA-N-CN
5	c	1	CXM	C-CA-N-CN
5	g	1	CXM	C-CA-N-CN
5	i	1	CXM	C-CA-N-CN
5	o	1	CXM	C-CA-N-CN

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	e	1	CXM	1	0
5	i	1	CXM	1	0
5	q	1	CXM	1	0
5	o	1	CXM	2	0
5	m	1	CXM	3	0
5	k	1	CXM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	g	1	CXM	2	0
5	a	1	CXM	2	0
5	c	1	CXM	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

171 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	BCL	g	102	5	69,74,74	1.77	17 (24%)	79,115,115	2.25	24 (30%)
10	PGV	T	102	-	43,43,50	0.98	2 (4%)	46,48,56	1.12	3 (6%)
7	BCL	i	102	5	69,74,74	1.76	17 (24%)	79,115,115	2.25	25 (31%)
10	PGV	a	104	-	50,50,50	0.92	2 (4%)	53,56,56	0.98	3 (5%)
8	LMT	O	103	-	36,36,36	0.39	0	47,47,47	0.90	2 (4%)
7	BCL	T	101	-	69,74,74	1.76	15 (21%)	79,115,115	2.14	21 (26%)
8	LMT	S	105	-	33,33,36	0.43	0	44,44,47	0.98	4 (9%)
8	LMT	S	103	-	36,36,36	0.38	0	47,47,47	0.96	2 (4%)
10	PGV	6	102	-	43,43,50	0.97	2 (4%)	46,48,56	1.11	3 (6%)
8	LMT	K	103	-	36,36,36	0.39	0	47,47,47	1.03	3 (6%)
9	CRT	m	101	-	43,43,43	0.62	0	48,54,54	2.29	16 (33%)
10	PGV	V	103	-	44,44,50	0.98	2 (4%)	47,49,56	1.00	2 (4%)
7	BCL	f	103	-	69,74,74	1.76	17 (24%)	79,115,115	2.11	19 (24%)
9	CRT	h	101	-	43,43,43	0.62	0	48,54,54	2.26	14 (29%)
7	BCL	l	101	-	69,74,74	1.80	17 (24%)	79,115,115	2.24	25 (31%)
10	PGV	g	104	-	50,50,50	0.91	2 (4%)	53,56,56	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	LMT	S	104	-	36,36,36	0.41	0	47,47,47	0.84	1 (2%)
7	BCL	9	101	-	69,74,74	1.79	16 (23%)	79,115,115	2.22	27 (34%)
8	LMT	b	102	-	36,36,36	0.38	0	47,47,47	0.81	1 (2%)
7	BCL	J	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.13	21 (26%)
7	BCL	R	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.13	21 (26%)
7	BCL	K	102	-	69,74,74	1.77	16 (23%)	79,115,115	2.23	24 (30%)
7	BCL	B	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.12	21 (26%)
8	LMT	I	102	-	36,36,36	0.40	0	47,47,47	0.64	1 (2%)
10	PGV	N	103	-	44,44,50	0.98	2 (4%)	47,49,56	1.01	2 (4%)
7	BCL	a	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.16	22 (27%)
7	BCL	b	103	-	69,74,74	1.76	17 (24%)	79,115,115	2.13	19 (24%)
9	CRT	k	101	-	43,43,43	0.62	0	48,54,54	2.33	15 (31%)
7	BCL	n	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.10	19 (24%)
8	LMT	f	102	-	36,36,36	0.38	0	47,47,47	0.79	1 (2%)
9	CRT	J	101	-	43,43,43	0.68	0	48,54,54	2.19	19 (39%)
8	LMT	A	102	-	36,36,36	0.38	0	47,47,47	0.66	1 (2%)
10	PGV	e	104	-	41,41,50	1.01	2 (4%)	44,46,56	1.06	2 (4%)
9	CRT	N	101	-	43,43,43	0.68	0	48,54,54	2.16	17 (35%)
8	LMT	C	104	-	36,36,36	0.41	0	47,47,47	0.83	1 (2%)
8	LMT	n	101	-	36,36,36	0.38	0	47,47,47	0.82	1 (2%)
9	CRT	4	101	-	43,43,43	0.67	0	48,54,54	2.12	18 (37%)
10	PGV	R	103	-	44,44,50	0.98	2 (4%)	47,49,56	1.01	2 (4%)
7	BCL	k	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.17	22 (27%)
7	BCL	G	101	-	69,74,74	1.80	17 (24%)	79,115,115	2.23	26 (32%)
9	CRT	e	101	-	43,43,43	0.63	0	48,54,54	2.28	15 (31%)
8	LMT	E	102	-	36,36,36	0.39	0	47,47,47	0.64	1 (2%)
8	LMT	9	104	-	36,36,36	0.41	0	47,47,47	0.82	1 (2%)
7	BCL	8	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.12	21 (26%)
10	PGV	k	105	-	50,50,50	0.91	2 (4%)	53,56,56	0.97	2 (3%)
7	BCL	K	101	-	69,74,74	1.79	16 (23%)	79,115,115	2.26	27 (34%)
7	BCL	3	101	-	69,74,74	1.78	17 (24%)	79,115,115	2.18	23 (29%)
7	BCL	e	103	5	69,74,74	1.77	17 (24%)	79,115,115	2.24	24 (30%)
10	PGV	2	101	-	44,44,50	0.98	2 (4%)	47,49,56	1.01	2 (4%)
10	PGV	B	103	-	44,44,50	0.98	2 (4%)	47,49,56	1.01	2 (4%)
8	LMT	5	105	-	33,33,36	0.43	0	44,44,47	0.95	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	LMT	5	103	-	36,36,36	0.40	0	47,47,47	0.91	2 (4%)
10	PGV	q	104	-	41,41,50	1.01	2 (4%)	44,46,56	1.13	3 (6%)
7	BCL	V	102	-	69,74,74	1.75	15 (21%)	79,115,115	2.12	21 (26%)
8	LMT	G	104	-	36,36,36	0.39	0	47,47,47	0.85	1 (2%)
7	BCL	M	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.17	23 (29%)
7	BCL	7	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.17	23 (29%)
8	LMT	5	104	-	36,36,36	0.39	0	47,47,47	0.84	1 (2%)
10	PGV	P	102	-	43,43,50	0.98	2 (4%)	46,48,56	1.11	3 (6%)
9	CRT	o	101	-	43,43,43	0.62	0	48,54,54	2.31	15 (31%)
8	LMT	7	102	-	36,36,36	0.39	0	47,47,47	0.66	1 (2%)
7	BCL	O	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.22	26 (32%)
10	PGV	o	105	-	50,50,50	0.92	2 (4%)	53,56,56	0.95	2 (3%)
7	BCL	5	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.27	26 (32%)
7	BCL	0	101	-	69,74,74	1.76	16 (23%)	79,115,115	2.14	21 (26%)
7	BCL	W	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.24	25 (31%)
8	LMT	1	103	-	36,36,36	0.37	0	47,47,47	0.90	1 (2%)
8	LMT	j	101	-	36,36,36	0.39	0	47,47,47	0.78	1 (2%)
7	BCL	C	101	-	69,74,74	1.79	17 (24%)	79,115,115	2.27	28 (35%)
7	BCL	m	103	5	69,74,74	1.76	17 (24%)	79,115,115	2.27	24 (30%)
7	BCL	h	103	-	69,74,74	1.76	16 (23%)	79,115,115	2.11	19 (24%)
10	PGV	a	103	-	41,41,50	1.02	2 (4%)	44,46,56	1.08	3 (6%)
8	LMT	G	103	-	36,36,36	0.40	0	47,47,47	0.88	2 (4%)
8	LMT	O	105	-	33,33,36	0.43	0	44,44,47	1.00	3 (6%)
7	BCL	W	102	-	69,74,74	1.79	17 (24%)	79,115,115	2.21	25 (31%)
8	LMT	1	105	-	33,33,36	0.42	0	44,44,47	1.01	2 (4%)
7	BCL	j	102	-	69,74,74	1.77	18 (26%)	79,115,115	2.12	20 (25%)
10	PGV	0	102	-	43,43,50	0.98	2 (4%)	46,48,56	1.12	3 (6%)
10	PGV	c	103	-	41,41,50	1.02	2 (4%)	44,46,56	1.08	3 (6%)
10	PGV	i	103	-	41,41,50	1.02	2 (4%)	44,46,56	1.11	3 (6%)
10	PGV	m	104	-	41,41,50	1.02	2 (4%)	44,46,56	1.16	4 (9%)
10	PGV	4	103	-	44,44,50	0.98	2 (4%)	47,49,56	1.01	2 (4%)
8	LMT	h	102	-	36,36,36	0.38	0	47,47,47	0.81	1 (2%)
10	PGV	X	102	-	43,43,50	0.97	2 (4%)	46,48,56	1.12	3 (6%)
8	LMT	G	105	-	33,33,36	0.43	0	44,44,47	1.02	3 (6%)
7	BCL	S	101	-	69,74,74	1.80	17 (24%)	79,115,115	2.25	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	9	102	-	69,74,74	1.79	18 (26%)	79,115,115	2.24	24 (30%)
7	BCL	O	102	-	69,74,74	1.78	16 (23%)	79,115,115	2.26	23 (29%)
7	BCL	5	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.19	22 (27%)
8	LMT	U	102	-	36,36,36	0.39	0	47,47,47	0.65	1 (2%)
8	LMT	d	101	-	36,36,36	0.38	0	47,47,47	0.82	1 (2%)
9	CRT	Z	101	-	43,43,43	0.68	0	48,54,54	2.19	19 (39%)
10	PGV	k	104	-	41,41,50	1.02	2 (4%)	44,46,56	1.11	3 (6%)
8	LMT	K	105	-	33,33,36	0.44	0	44,44,47	0.97	3 (6%)
10	PGV	g	103	-	41,41,50	1.02	2 (4%)	44,46,56	1.10	3 (6%)
8	LMT	C	103	-	36,36,36	0.39	0	47,47,47	0.84	1 (2%)
7	BCL	D	101	-	69,74,74	1.76	15 (21%)	79,115,115	2.15	22 (27%)
7	BCL	i	101	-	69,74,74	1.77	16 (23%)	79,115,115	2.17	20 (25%)
7	BCL	F	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.12	21 (26%)
7	BCL	o	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.18	20 (25%)
7	BCL	Z	102	-	69,74,74	1.76	17 (24%)	79,115,115	2.16	21 (26%)
7	BCL	4	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.12	21 (26%)
7	BCL	q	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.14	22 (27%)
7	BCL	d	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.12	19 (24%)
9	CRT	V	101	-	43,43,43	0.68	0	48,54,54	2.16	20 (41%)
10	PGV	q	105	-	50,50,50	0.91	2 (4%)	53,56,56	0.96	3 (5%)
10	PGV	8	103	-	44,44,50	0.98	2 (4%)	47,49,56	1.00	2 (4%)
10	PGV	o	104	-	41,41,50	1.02	2 (4%)	44,46,56	1.11	3 (6%)
7	BCL	L	101	-	69,74,74	1.76	14 (20%)	79,115,115	2.15	23 (29%)
7	BCL	I	101	-	69,74,74	1.77	16 (23%)	79,115,115	2.21	24 (30%)
8	LMT	Y	102	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
8	LMT	r	101	-	36,36,36	0.38	0	47,47,47	0.81	1 (2%)
10	PGV	D	102	-	43,43,50	0.98	2 (4%)	46,48,56	1.11	3 (6%)
8	LMT	9	105	-	33,33,36	0.43	0	44,44,47	1.02	2 (4%)
7	BCL	X	101	-	69,74,74	1.77	14 (20%)	79,115,115	2.12	21 (26%)
9	CRT	q	101	-	43,43,43	0.62	0	48,54,54	2.29	14 (29%)
7	BCL	Q	101	-	69,74,74	1.76	17 (24%)	79,115,115	2.19	23 (29%)
7	BCL	G	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.19	22 (27%)
7	BCL	o	103	5	69,74,74	1.77	17 (24%)	79,115,115	2.25	25 (31%)
8	LMT	W	105	-	33,33,36	0.43	0	44,44,47	0.97	4 (9%)
8	LMT	C	105	-	33,33,36	0.43	0	44,44,47	0.94	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	q	103	5	69,74,74	1.77	17 (24%)	79,115,115	2.24	24 (30%)
8	LMT	l	104	-	36,36,36	0.40	0	47,47,47	0.85	1 (2%)
8	LMT	p	101	-	36,36,36	0.38	0	47,47,47	0.78	1 (2%)
7	BCL	r	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.11	20 (25%)
7	BCL	m	102	-	69,74,74	1.78	18 (26%)	79,115,115	2.15	21 (26%)
7	BCL	g	101	-	69,74,74	1.77	16 (23%)	79,115,115	2.17	23 (29%)
7	BCL	2	102	-	69,74,74	1.76	15 (21%)	79,115,115	2.15	22 (27%)
7	BCL	N	102	-	69,74,74	1.76	17 (24%)	79,115,115	2.15	20 (25%)
7	BCL	U	101	-	69,74,74	1.76	17 (24%)	79,115,115	2.21	22 (27%)
7	BCL	e	102	-	69,74,74	1.77	17 (24%)	79,115,115	2.15	22 (27%)
9	CRT	a	105	-	43,43,43	0.63	0	48,54,54	2.24	14 (29%)
7	BCL	6	101	-	69,74,74	1.76	15 (21%)	79,115,115	2.13	23 (29%)
9	CRT	8	101	-	43,43,43	0.68	0	48,54,54	2.16	18 (37%)
9	CRT	R	101	-	43,43,43	0.67	0	48,54,54	2.18	18 (37%)
7	BCL	p	102	-	69,74,74	1.75	16 (23%)	79,115,115	2.13	19 (24%)
8	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.68	1 (2%)
9	CRT	f	101	-	43,43,43	0.63	0	48,54,54	2.31	15 (31%)
7	BCL	C	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.22	23 (29%)
9	CRT	B	101	-	43,43,43	0.68	0	48,54,54	2.15	17 (35%)
7	BCL	Y	101	-	69,74,74	1.76	16 (23%)	79,115,115	2.18	22 (27%)
8	LMT	W	103	-	36,36,36	0.40	0	47,47,47	0.96	3 (6%)
7	BCL	P	101	-	69,74,74	1.76	14 (20%)	79,115,115	2.14	23 (29%)
10	PGV	m	105	-	50,50,50	0.91	2 (4%)	53,56,56	0.99	2 (3%)
7	BCL	H	101	-	69,74,74	1.76	16 (23%)	79,115,115	2.14	21 (26%)
7	BCL	l	102	-	69,74,74	1.78	17 (24%)	79,115,115	2.20	24 (30%)
8	LMT	O	104	-	36,36,36	0.38	0	47,47,47	0.84	1 (2%)
10	PGV	F	103	-	44,44,50	0.97	2 (4%)	47,49,56	1.01	2 (4%)
7	BCL	S	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.23	23 (29%)
8	LMT	l	101	-	36,36,36	0.38	0	47,47,47	0.81	1 (2%)
10	PGV	J	103	-	44,44,50	0.97	2 (4%)	47,49,56	1.01	2 (4%)
8	LMT	Q	102	-	36,36,36	0.39	0	47,47,47	0.67	1 (2%)
7	BCL	c	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.16	21 (26%)
10	PGV	e	105	-	50,50,50	0.91	2 (4%)	53,56,56	0.97	2 (3%)
10	PGV	2	103	-	43,43,50	0.97	2 (4%)	46,48,56	1.11	3 (6%)
9	CRT	F	101	-	43,43,43	0.68	0	48,54,54	2.19	18 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	LMT	W	104	-	36,36,36	0.40	0	47,47,47	0.82	1 (2%)
10	PGV	c	104	-	50,50,50	0.91	2 (4%)	53,56,56	0.96	3 (5%)
7	BCL	A	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.22	24 (30%)
10	PGV	H	102	-	43,43,50	0.98	2 (4%)	46,48,56	1.12	3 (6%)
10	PGV	i	104	-	50,50,50	0.91	2 (4%)	53,56,56	0.95	2 (3%)
7	BCL	l	102	-	69,74,74	1.76	16 (23%)	79,115,115	2.10	20 (25%)
7	BCL	c	102	5	69,74,74	1.75	17 (24%)	79,115,115	2.28	23 (29%)
8	LMT	9	103	-	36,36,36	0.41	0	47,47,47	0.89	1 (2%)
7	BCL	a	102	5	69,74,74	1.77	17 (24%)	79,115,115	2.25	25 (31%)
7	BCL	k	103	5	69,74,74	1.76	17 (24%)	79,115,115	2.27	25 (31%)
8	LMT	3	102	-	36,36,36	0.40	0	47,47,47	0.71	1 (2%)
10	PGV	L	102	-	43,43,50	0.96	2 (4%)	46,48,56	1.11	3 (6%)
9	CRT	b	101	-	43,43,43	0.61	0	48,54,54	2.30	14 (29%)
8	LMT	K	104	-	36,36,36	0.40	0	47,47,47	0.83	1 (2%)
7	BCL	E	101	-	69,74,74	1.77	17 (24%)	79,115,115	2.21	25 (31%)

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
7	BCL	g	102	5	-	22/41/137/137	-
10	PGV	T	102	-	-	18/47/47/55	-
7	BCL	i	102	5	-	21/41/137/137	-
10	PGV	a	104	-	-	14/55/55/55	-
8	LMT	O	103	-	-	9/21/61/61	0/2/2/2
7	BCL	T	101	-	-	7/41/137/137	-
8	LMT	S	105	-	-	9/18/58/61	0/2/2/2
8	LMT	S	103	-	-	10/21/61/61	0/2/2/2
10	PGV	6	102	-	-	16/47/47/55	-
8	LMT	K	103	-	-	8/21/61/61	0/2/2/2
9	CRT	m	101	-	-	13/51/51/51	-
10	PGV	V	103	-	-	9/48/48/55	-
7	BCL	f	103	-	-	17/41/137/137	-
9	CRT	h	101	-	-	13/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	1	101	-	-	14/41/137/137	-
10	PGV	g	104	-	-	15/55/55/55	-
8	LMT	S	104	-	-	3/21/61/61	0/2/2/2
7	BCL	9	101	-	-	14/41/137/137	-
8	LMT	b	102	-	-	5/21/61/61	0/2/2/2
7	BCL	J	102	-	-	15/41/137/137	-
7	BCL	R	102	-	-	11/41/137/137	-
7	BCL	K	102	-	-	15/41/137/137	-
7	BCL	B	102	-	-	14/41/137/137	-
8	LMT	I	102	-	-	5/21/61/61	0/2/2/2
10	PGV	N	103	-	-	12/48/48/55	-
7	BCL	a	101	-	-	14/41/137/137	-
7	BCL	b	103	-	-	17/41/137/137	-
9	CRT	k	101	-	-	13/51/51/51	-
7	BCL	n	102	-	-	15/41/137/137	-
8	LMT	f	102	-	-	6/21/61/61	0/2/2/2
9	CRT	J	101	-	-	5/51/51/51	-
8	LMT	A	102	-	-	5/21/61/61	0/2/2/2
10	PGV	e	104	-	-	15/45/45/55	-
9	CRT	N	101	-	-	6/51/51/51	-
8	LMT	C	104	-	-	4/21/61/61	0/2/2/2
8	LMT	n	101	-	-	7/21/61/61	0/2/2/2
9	CRT	4	101	-	-	5/51/51/51	-
10	PGV	R	103	-	-	11/48/48/55	-
7	BCL	k	102	-	-	15/41/137/137	-
7	BCL	G	101	-	-	15/41/137/137	-
9	CRT	e	101	-	-	13/51/51/51	-
8	LMT	E	102	-	-	5/21/61/61	0/2/2/2
8	LMT	9	104	-	-	5/21/61/61	0/2/2/2
7	BCL	8	102	-	-	15/41/137/137	-
10	PGV	k	105	-	-	15/55/55/55	-
7	BCL	K	101	-	-	14/41/137/137	-
7	BCL	3	101	-	-	19/41/137/137	-
7	BCL	e	103	5	-	21/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PGV	2	101	-	-	10/48/48/55	-
10	PGV	B	103	-	-	11/48/48/55	-
8	LMT	5	105	-	-	8/18/58/61	0/2/2/2
8	LMT	5	103	-	-	9/21/61/61	0/2/2/2
10	PGV	q	104	-	-	13/45/45/55	-
7	BCL	V	102	-	-	15/41/137/137	-
8	LMT	G	104	-	-	5/21/61/61	0/2/2/2
7	BCL	M	101	-	-	17/41/137/137	-
7	BCL	7	101	-	-	19/41/137/137	-
8	LMT	5	104	-	-	5/21/61/61	0/2/2/2
10	PGV	P	102	-	-	17/47/47/55	-
9	CRT	o	101	-	-	12/51/51/51	-
8	LMT	7	102	-	-	4/21/61/61	0/2/2/2
7	BCL	O	101	-	-	14/41/137/137	-
10	PGV	o	105	-	-	16/55/55/55	-
7	BCL	5	101	-	-	15/41/137/137	-
7	BCL	0	101	-	-	6/41/137/137	-
7	BCL	W	101	-	-	14/41/137/137	-
8	LMT	1	103	-	-	8/21/61/61	0/2/2/2
8	LMT	j	101	-	-	7/21/61/61	0/2/2/2
7	BCL	C	101	-	-	15/41/137/137	-
7	BCL	m	103	5	-	19/41/137/137	-
7	BCL	h	103	-	-	15/41/137/137	-
10	PGV	a	103	-	-	15/45/45/55	-
8	LMT	G	103	-	-	9/21/61/61	0/2/2/2
8	LMT	O	105	-	-	8/18/58/61	0/2/2/2
7	BCL	W	102	-	-	13/41/137/137	-
8	LMT	1	105	-	-	9/18/58/61	0/2/2/2
7	BCL	j	102	-	-	17/41/137/137	-
10	PGV	0	102	-	-	19/47/47/55	-
10	PGV	c	103	-	-	15/45/45/55	-
10	PGV	i	103	-	-	12/45/45/55	-
10	PGV	m	104	-	-	10/45/45/55	-
10	PGV	4	103	-	-	9/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LMT	h	102	-	-	6/21/61/61	0/2/2/2
10	PGV	X	102	-	-	18/47/47/55	-
8	LMT	G	105	-	-	9/18/58/61	0/2/2/2
7	BCL	S	101	-	-	14/41/137/137	-
7	BCL	9	102	-	-	14/41/137/137	-
7	BCL	O	102	-	-	14/41/137/137	-
7	BCL	5	102	-	-	14/41/137/137	-
8	LMT	U	102	-	-	6/21/61/61	0/2/2/2
8	LMT	d	101	-	-	6/21/61/61	0/2/2/2
9	CRT	Z	101	-	-	6/51/51/51	-
10	PGV	k	104	-	-	12/45/45/55	-
8	LMT	K	105	-	-	8/18/58/61	0/2/2/2
10	PGV	g	103	-	-	13/45/45/55	-
8	LMT	C	103	-	-	7/21/61/61	0/2/2/2
7	BCL	D	101	-	-	7/41/137/137	-
7	BCL	i	101	-	-	15/41/137/137	-
7	BCL	F	102	-	-	13/41/137/137	-
7	BCL	o	102	-	-	13/41/137/137	-
7	BCL	Z	102	-	-	16/41/137/137	-
7	BCL	4	102	-	-	13/41/137/137	-
7	BCL	q	102	-	-	12/41/137/137	-
7	BCL	d	102	-	-	15/41/137/137	-
9	CRT	V	101	-	-	4/51/51/51	-
10	PGV	q	105	-	-	21/55/55/55	-
10	PGV	8	103	-	-	8/48/48/55	-
10	PGV	o	104	-	-	13/45/45/55	-
7	BCL	L	101	-	-	10/41/137/137	-
7	BCL	I	101	-	-	18/41/137/137	-
8	LMT	Y	102	-	-	7/21/61/61	0/2/2/2
8	LMT	r	101	-	-	5/21/61/61	0/2/2/2
10	PGV	D	102	-	-	18/47/47/55	-
8	LMT	9	105	-	-	7/18/58/61	0/2/2/2
7	BCL	X	101	-	-	6/41/137/137	-
9	CRT	q	101	-	-	13/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	Q	101	-	-	18/41/137/137	-
7	BCL	G	102	-	-	14/41/137/137	-
7	BCL	o	103	5	-	22/41/137/137	-
8	LMT	W	105	-	-	8/18/58/61	0/2/2/2
8	LMT	C	105	-	-	8/18/58/61	0/2/2/2
7	BCL	q	103	5	-	20/41/137/137	-
8	LMT	l	104	-	-	4/21/61/61	0/2/2/2
8	LMT	p	101	-	-	6/21/61/61	0/2/2/2
7	BCL	r	102	-	-	20/41/137/137	-
7	BCL	m	102	-	-	14/41/137/137	-
7	BCL	g	101	-	-	13/41/137/137	-
7	BCL	2	102	-	-	7/41/137/137	-
7	BCL	N	102	-	-	13/41/137/137	-
7	BCL	U	101	-	-	17/41/137/137	-
7	BCL	e	102	-	-	13/41/137/137	-
9	CRT	a	105	-	-	13/51/51/51	-
7	BCL	6	101	-	-	6/41/137/137	-
9	CRT	8	101	-	-	5/51/51/51	-
9	CRT	R	101	-	-	6/51/51/51	-
7	BCL	p	102	-	-	16/41/137/137	-
8	LMT	M	102	-	-	5/21/61/61	0/2/2/2
9	CRT	f	101	-	-	13/51/51/51	-
7	BCL	C	102	-	-	13/41/137/137	-
9	CRT	B	101	-	-	4/51/51/51	-
7	BCL	Y	101	-	-	18/41/137/137	-
8	LMT	W	103	-	-	11/21/61/61	0/2/2/2
7	BCL	P	101	-	-	7/41/137/137	-
10	PGV	m	105	-	-	15/55/55/55	-
7	BCL	H	101	-	-	8/41/137/137	-
7	BCL	l	102	-	-	13/41/137/137	-
8	LMT	O	104	-	-	5/21/61/61	0/2/2/2
10	PGV	F	103	-	-	10/48/48/55	-
7	BCL	S	102	-	-	14/41/137/137	-
8	LMT	l	101	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PGV	J	103	-	-	10/48/48/55	-
8	LMT	Q	102	-	-	6/21/61/61	0/2/2/2
7	BCL	c	101	-	-	12/41/137/137	-
10	PGV	e	105	-	-	16/55/55/55	-
10	PGV	2	103	-	-	18/47/47/55	-
9	CRT	F	101	-	-	7/51/51/51	-
8	LMT	W	104	-	-	3/21/61/61	0/2/2/2
10	PGV	c	104	-	-	21/55/55/55	-
7	BCL	A	101	-	-	18/41/137/137	-
10	PGV	H	102	-	-	16/47/47/55	-
10	PGV	i	104	-	-	15/55/55/55	-
7	BCL	l	102	-	-	15/41/137/137	-
7	BCL	c	102	5	-	23/41/137/137	-
8	LMT	9	103	-	-	8/21/61/61	0/2/2/2
7	BCL	a	102	5	-	22/41/137/137	-
7	BCL	k	103	5	-	22/41/137/137	-
8	LMT	3	102	-	-	4/21/61/61	0/2/2/2
10	PGV	L	102	-	-	16/47/47/55	-
9	CRT	b	101	-	-	13/51/51/51	-
8	LMT	K	104	-	-	5/21/61/61	0/2/2/2
7	BCL	E	101	-	-	18/41/137/137	-

The worst 5 of 1257 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	k	102	BCL	O2D-CGD	5.17	1.45	1.33
7	m	102	BCL	O2D-CGD	5.15	1.45	1.33
7	g	101	BCL	O2D-CGD	5.15	1.45	1.33
7	q	102	BCL	O2D-CGD	5.15	1.45	1.33
7	e	102	BCL	O2D-CGD	5.14	1.45	1.33

The worst 5 of 2085 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	102	BCL	CMD-C2D-C1D	8.38	139.49	124.73
7	q	103	BCL	CMD-C2D-C1D	8.16	139.10	124.73
7	c	102	BCL	CMD-C2D-C1D	8.12	139.03	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	k	103	BCL	CMD-C2D-C1D	8.11	139.01	124.73
7	S	102	BCL	CMD-C2D-C1D	8.10	138.99	124.73

There are no chirality outliers.

5 of 2033 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	101	BCL	C4C-C3C-CAC-CBC
7	B	102	BCL	C1A-C2A-CAA-CBA
7	B	102	BCL	C3A-C2A-CAA-CBA
7	C	101	BCL	C6-C7-C8-C9
7	E	101	BCL	C2C-C3C-CAC-CBC

There are no ring outliers.

169 monomers are involved in 738 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	g	102	BCL	3	0
10	T	102	PGV	3	0
7	i	102	BCL	7	0
10	a	104	PGV	11	0
8	O	103	LMT	4	0
7	T	101	BCL	6	0
8	S	105	LMT	5	0
8	S	103	LMT	4	0
10	6	102	PGV	5	0
8	K	103	LMT	7	0
9	m	101	CRT	8	0
10	V	103	PGV	6	0
7	f	103	BCL	7	0
9	h	101	CRT	9	0
7	l	101	BCL	5	0
10	g	104	PGV	11	0
8	S	104	LMT	6	0
7	9	101	BCL	6	0
8	b	102	LMT	3	0
7	J	102	BCL	6	0
7	R	102	BCL	9	0
7	K	102	BCL	5	0
7	B	102	BCL	6	0
10	N	103	PGV	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	a	101	BCL	6	0
7	b	103	BCL	8	0
9	k	101	CRT	10	0
7	n	102	BCL	6	0
8	f	102	LMT	3	0
9	J	101	CRT	6	0
8	A	102	LMT	1	0
10	e	104	PGV	6	0
9	N	101	CRT	6	0
8	C	104	LMT	4	0
8	n	101	LMT	4	0
9	4	101	CRT	5	0
10	R	103	PGV	7	0
7	k	102	BCL	9	0
7	G	101	BCL	8	0
9	e	101	CRT	8	0
8	E	102	LMT	2	0
8	9	104	LMT	5	0
7	8	102	BCL	8	0
10	k	105	PGV	9	0
7	K	101	BCL	5	0
7	3	101	BCL	1	0
7	e	103	BCL	5	0
10	2	101	PGV	8	0
10	B	103	PGV	7	0
8	5	105	LMT	4	0
8	5	103	LMT	5	0
10	q	104	PGV	6	0
7	V	102	BCL	4	0
8	G	104	LMT	5	0
7	M	101	BCL	2	0
7	7	101	BCL	3	0
8	5	104	LMT	2	0
10	P	102	PGV	3	0
9	o	101	CRT	9	0
8	7	102	LMT	1	0
7	O	101	BCL	5	0
10	o	105	PGV	10	0
7	5	101	BCL	5	0
7	0	101	BCL	6	0
7	W	101	BCL	6	0
8	1	103	LMT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	j	101	LMT	2	0
7	C	101	BCL	6	0
7	m	103	BCL	6	0
7	h	103	BCL	7	0
10	a	103	PGV	6	0
8	G	103	LMT	5	0
8	O	105	LMT	4	0
7	W	102	BCL	4	0
8	l	105	LMT	6	0
7	j	102	BCL	5	0
10	0	102	PGV	2	0
10	c	103	PGV	5	0
10	i	103	PGV	5	0
10	m	104	PGV	8	0
10	4	103	PGV	9	0
8	h	102	LMT	3	0
10	X	102	PGV	4	0
8	G	105	LMT	6	0
7	S	101	BCL	6	0
7	9	102	BCL	7	0
7	O	102	BCL	5	0
7	5	102	BCL	4	0
8	U	102	LMT	1	0
8	d	101	LMT	2	0
9	Z	101	CRT	5	0
10	k	104	PGV	8	0
8	K	105	LMT	6	0
10	g	103	PGV	6	0
8	C	103	LMT	4	0
7	D	101	BCL	3	0
7	i	101	BCL	6	0
7	F	102	BCL	6	0
7	o	102	BCL	8	0
7	Z	102	BCL	7	0
7	4	102	BCL	6	0
7	q	102	BCL	8	0
7	d	102	BCL	6	0
9	V	101	CRT	6	0
10	q	105	PGV	8	0
10	8	103	PGV	11	0
10	o	104	PGV	7	0
7	L	101	BCL	6	0

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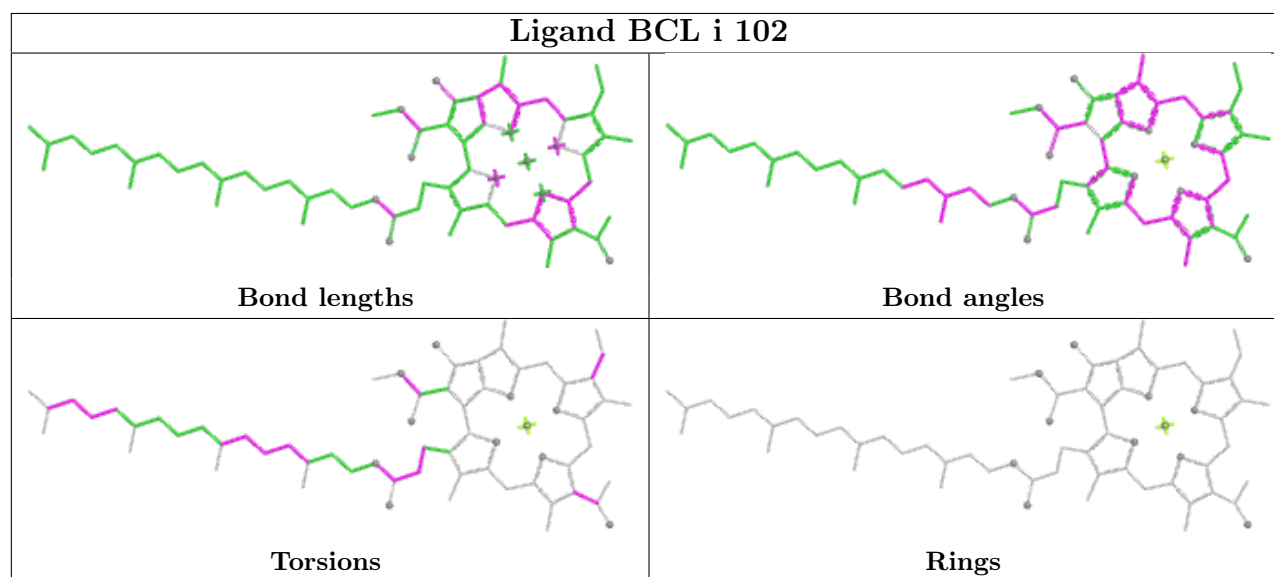
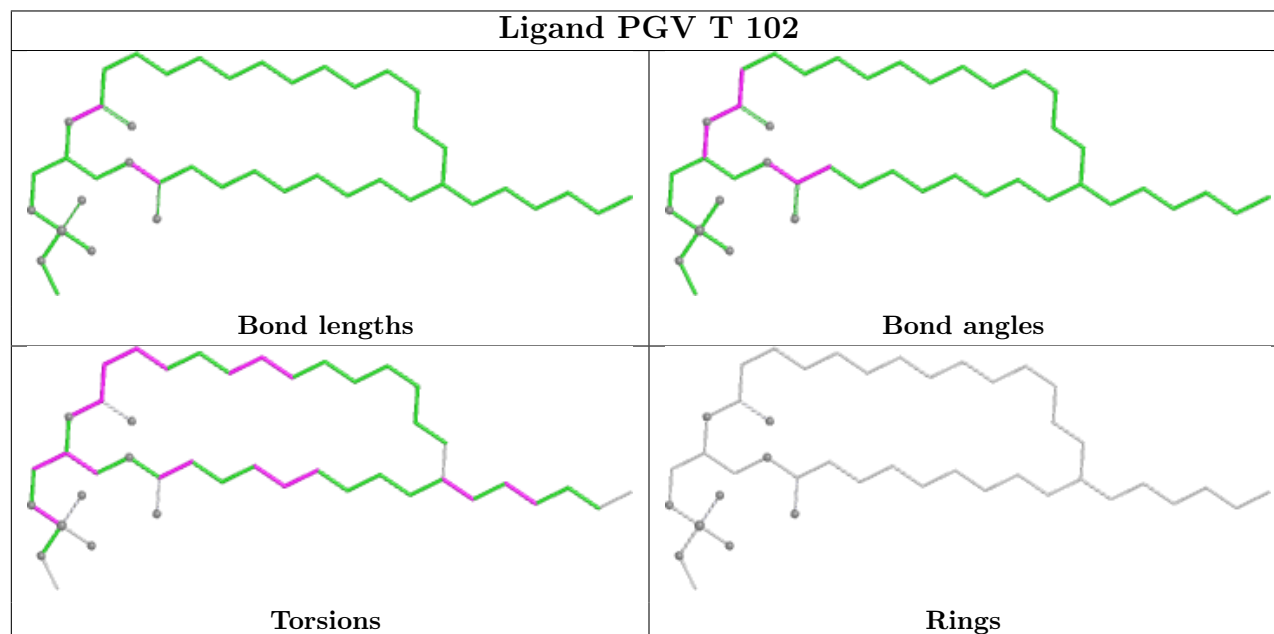
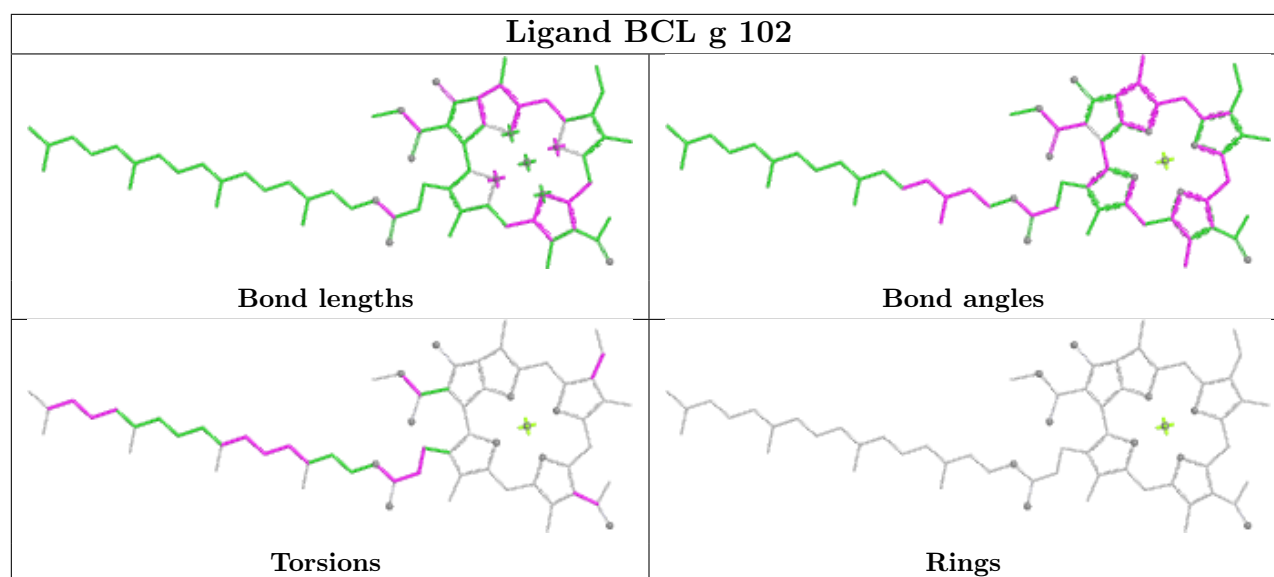
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	101	BCL	4	0
8	r	101	LMT	2	0
10	D	102	PGV	5	0
8	9	105	LMT	5	0
7	X	101	BCL	5	0
9	q	101	CRT	8	0
7	Q	101	BCL	2	0
7	G	102	BCL	4	0
7	o	103	BCL	5	0
8	W	105	LMT	2	0
8	C	105	LMT	5	0
7	q	103	BCL	4	0
8	l	104	LMT	4	0
8	p	101	LMT	3	0
7	r	102	BCL	4	0
7	m	102	BCL	6	0
7	g	101	BCL	5	0
7	2	102	BCL	6	0
7	N	102	BCL	6	0
7	U	101	BCL	3	0
7	e	102	BCL	6	0
9	a	105	CRT	7	0
7	6	101	BCL	7	0
9	8	101	CRT	5	0
9	R	101	CRT	5	0
7	p	102	BCL	4	0
8	M	102	LMT	1	0
9	f	101	CRT	8	0
7	C	102	BCL	5	0
9	B	101	CRT	5	0
7	Y	101	BCL	2	0
8	W	103	LMT	3	0
7	P	101	BCL	4	0
10	m	105	PGV	10	0
7	H	101	BCL	6	0
7	l	102	BCL	6	0
8	O	104	LMT	3	0
10	F	103	PGV	9	0
7	S	102	BCL	4	0
8	l	101	LMT	2	0
10	J	103	PGV	7	0
8	Q	102	LMT	1	0

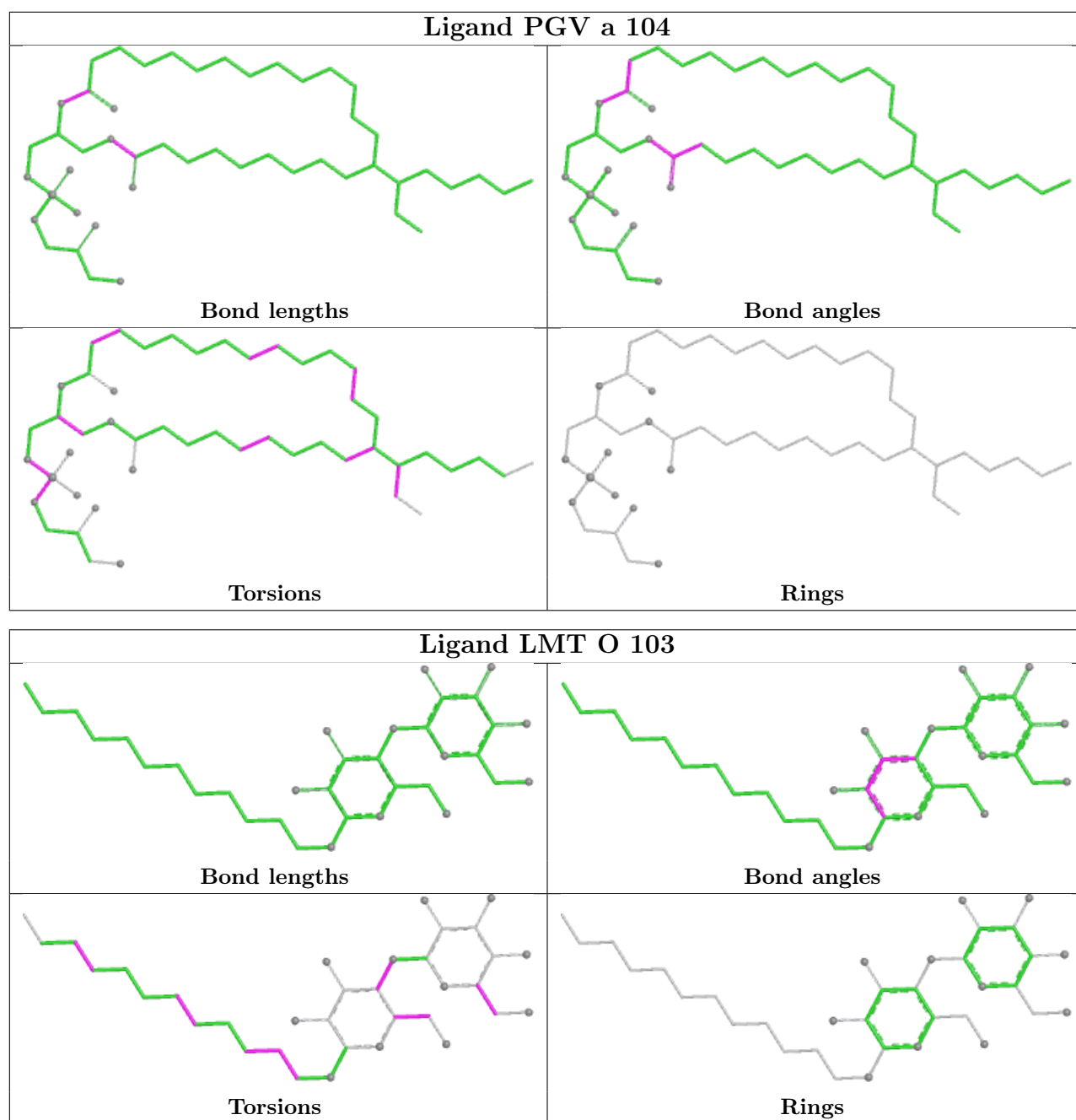
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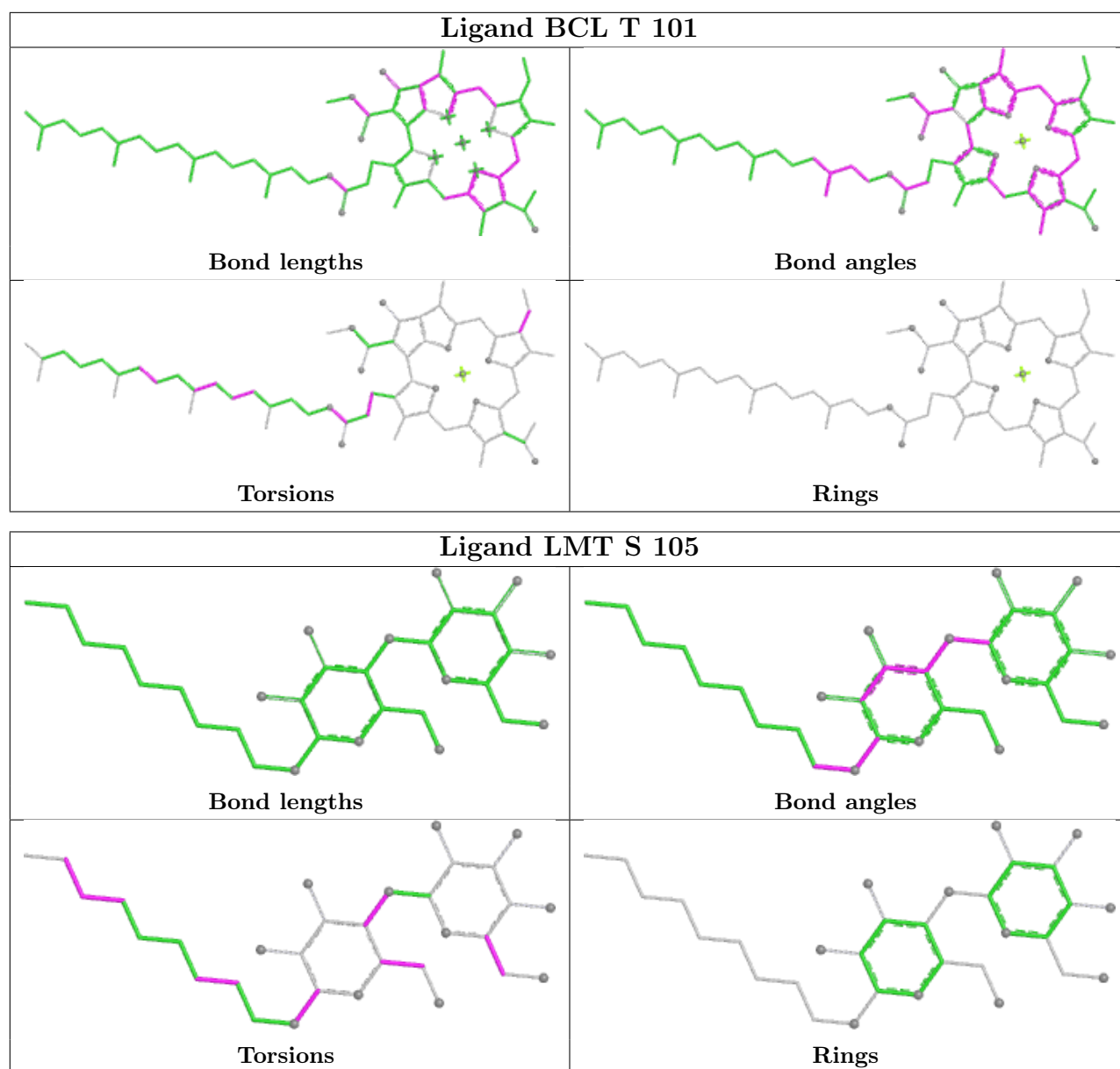
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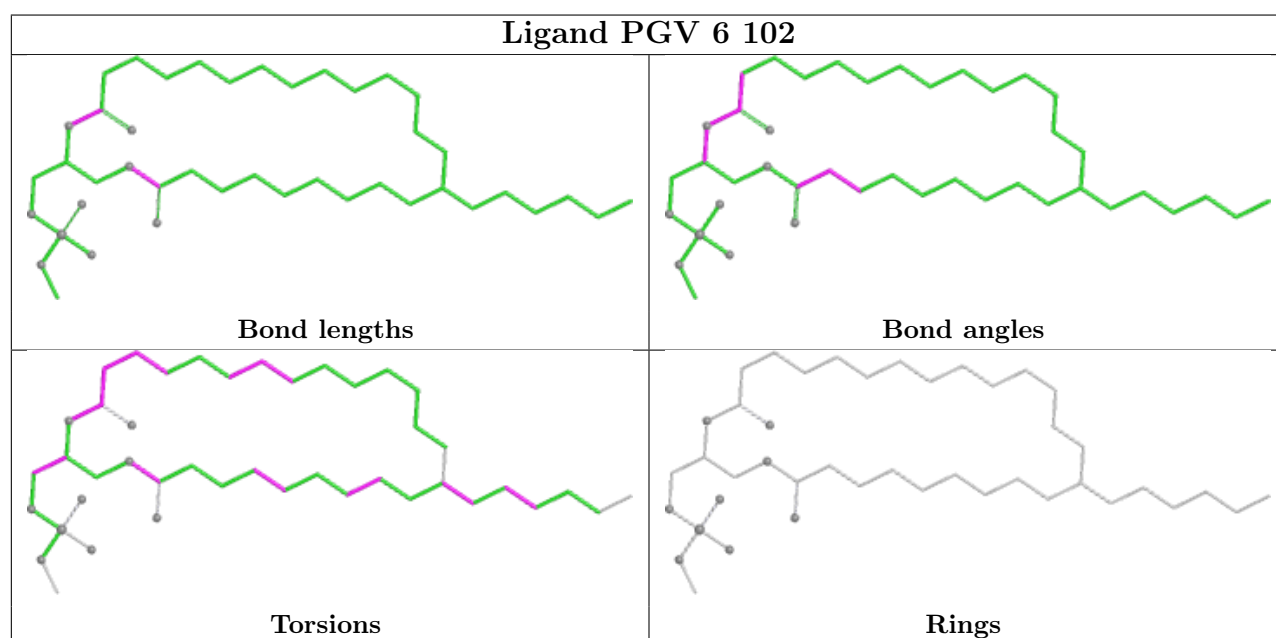
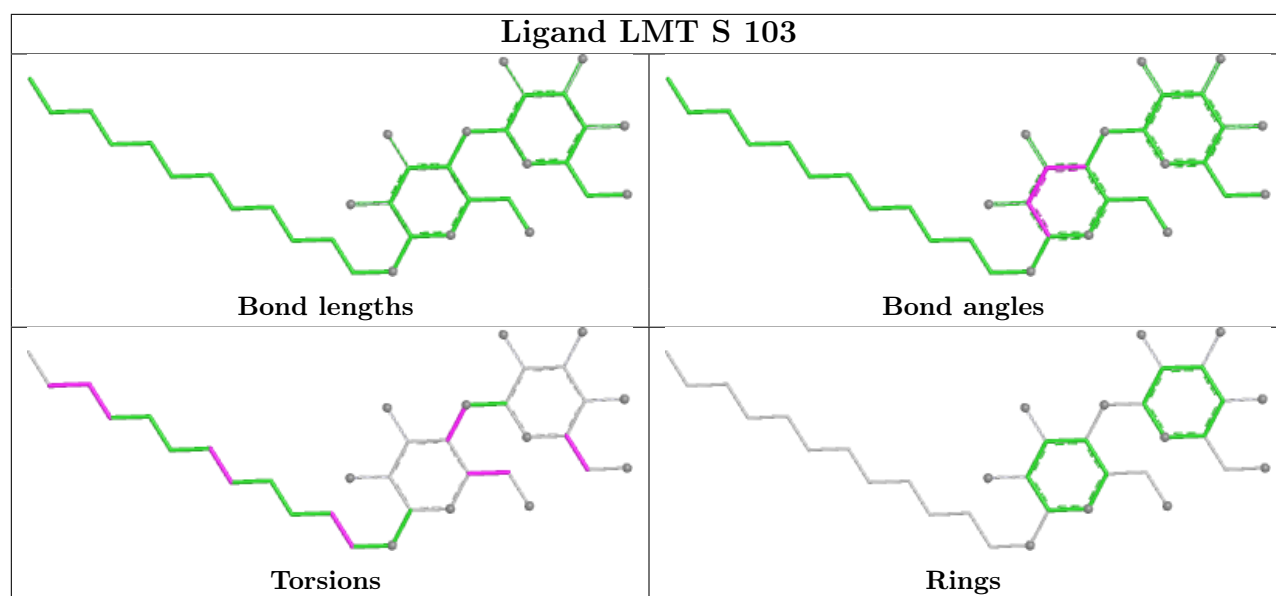
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	c	101	BCL	5	0
10	e	105	PGV	10	0
10	2	103	PGV	2	0
9	F	101	CRT	5	0
8	W	104	LMT	3	0
10	c	104	PGV	11	0
7	A	101	BCL	1	0
10	H	102	PGV	5	0
10	i	104	PGV	10	0
7	l	102	BCL	7	0
7	c	102	BCL	3	0
8	9	103	LMT	3	0
7	a	102	BCL	3	0
7	k	103	BCL	5	0
8	3	102	LMT	1	0
10	L	102	PGV	3	0
9	b	101	CRT	7	0
8	K	104	LMT	6	0
7	E	101	BCL	3	0

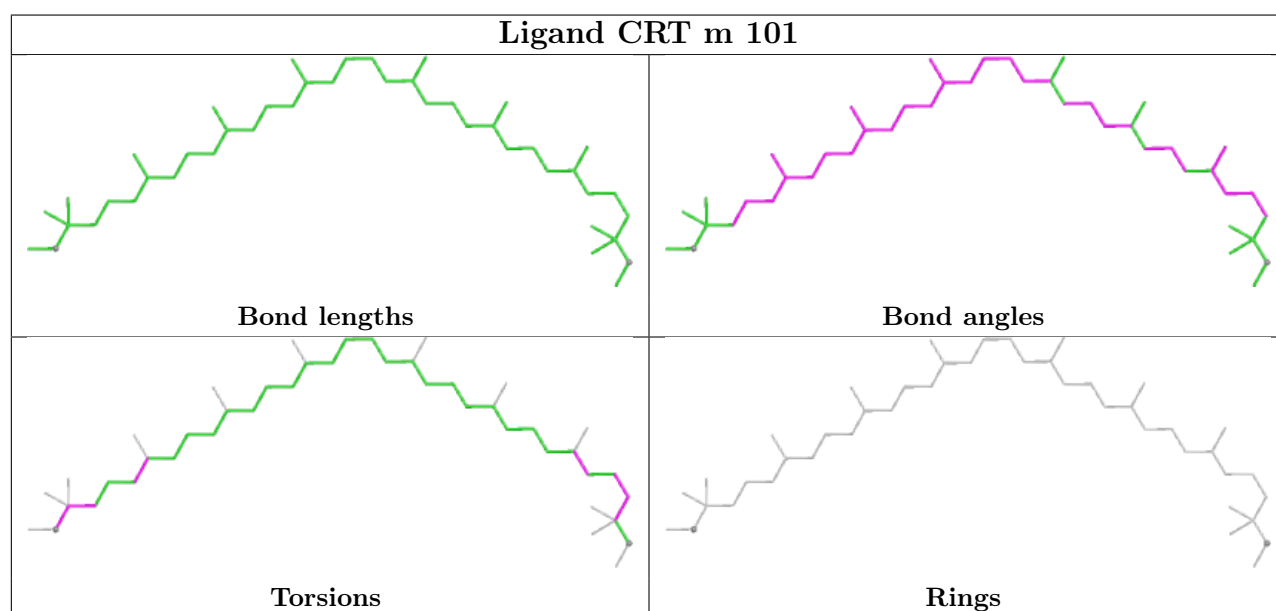
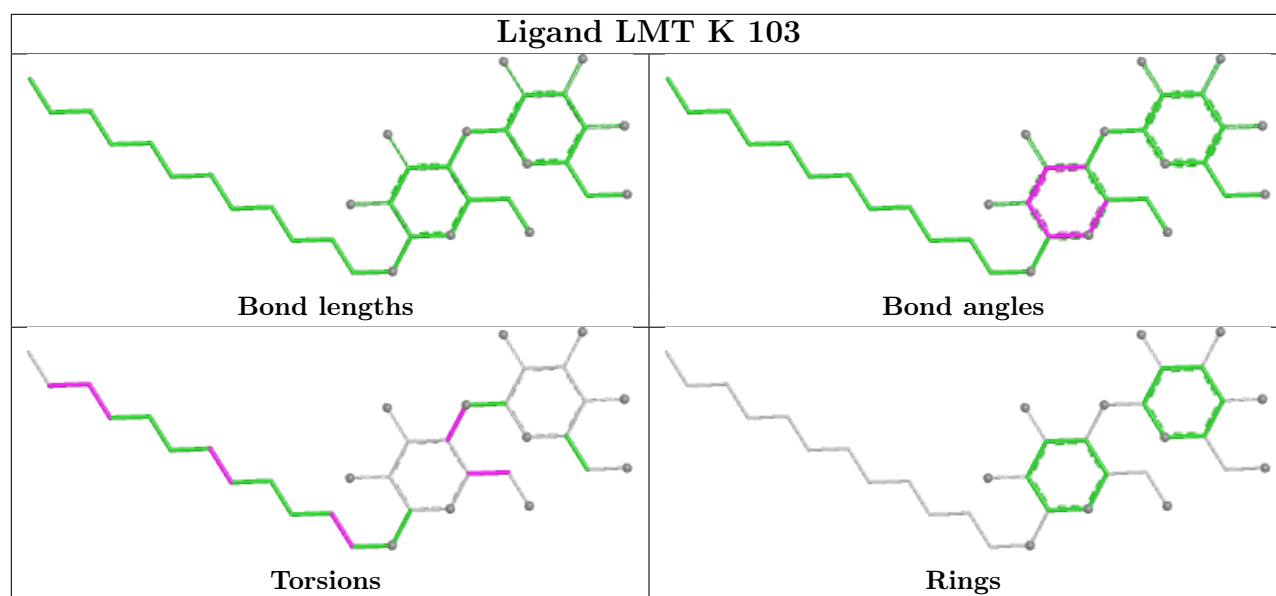
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

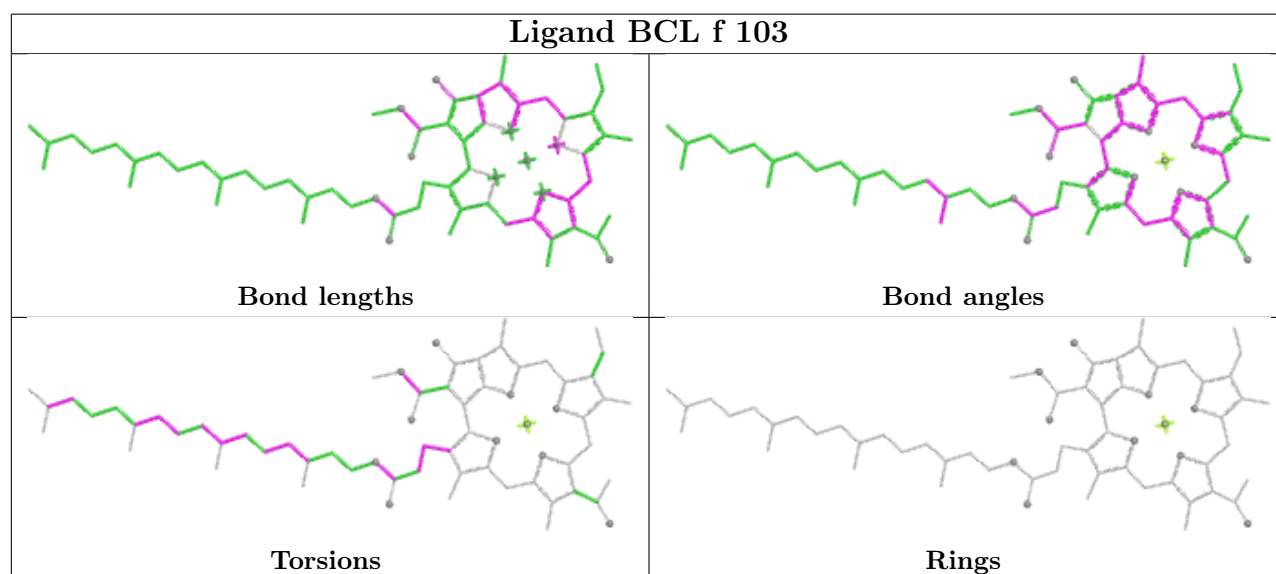
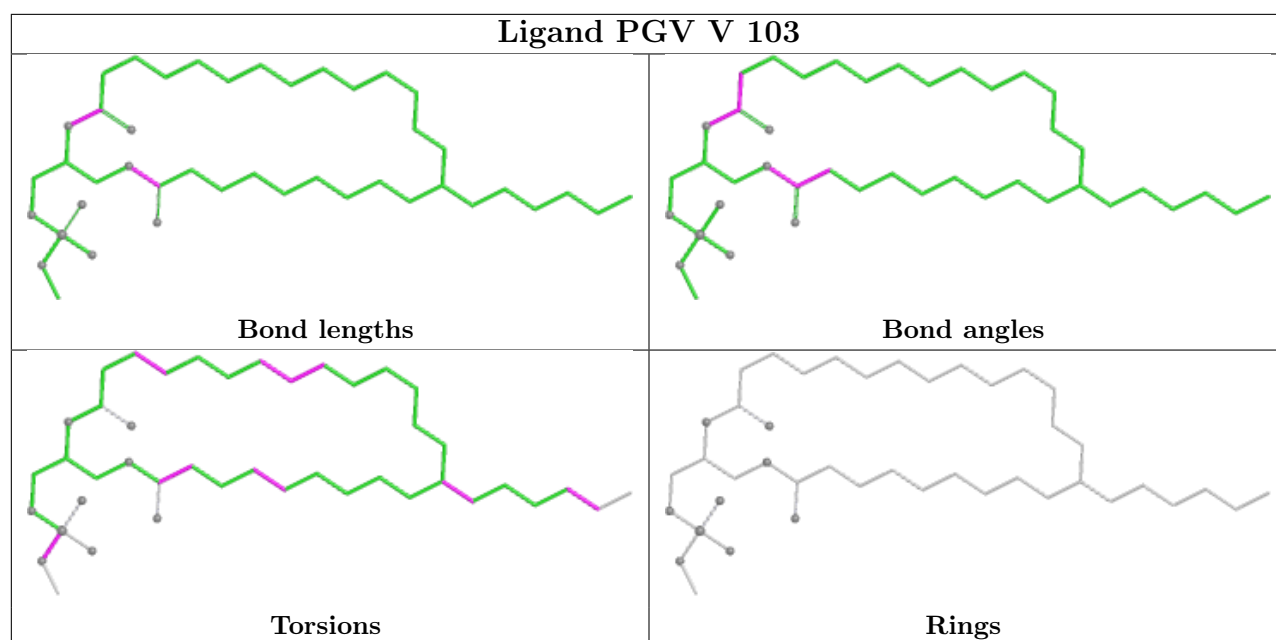


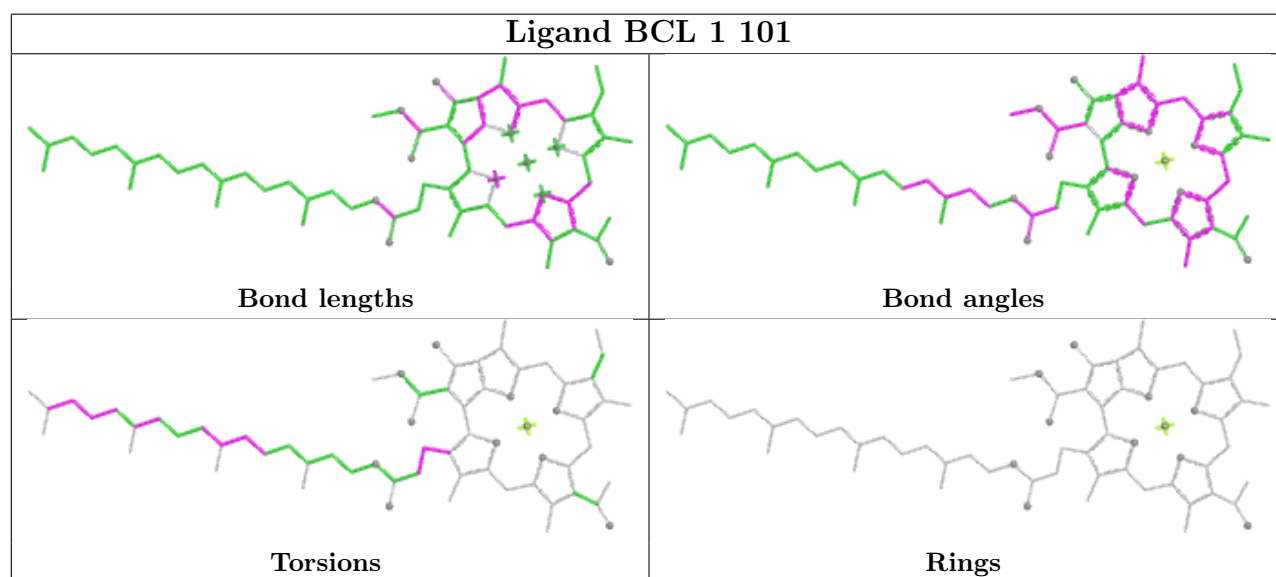
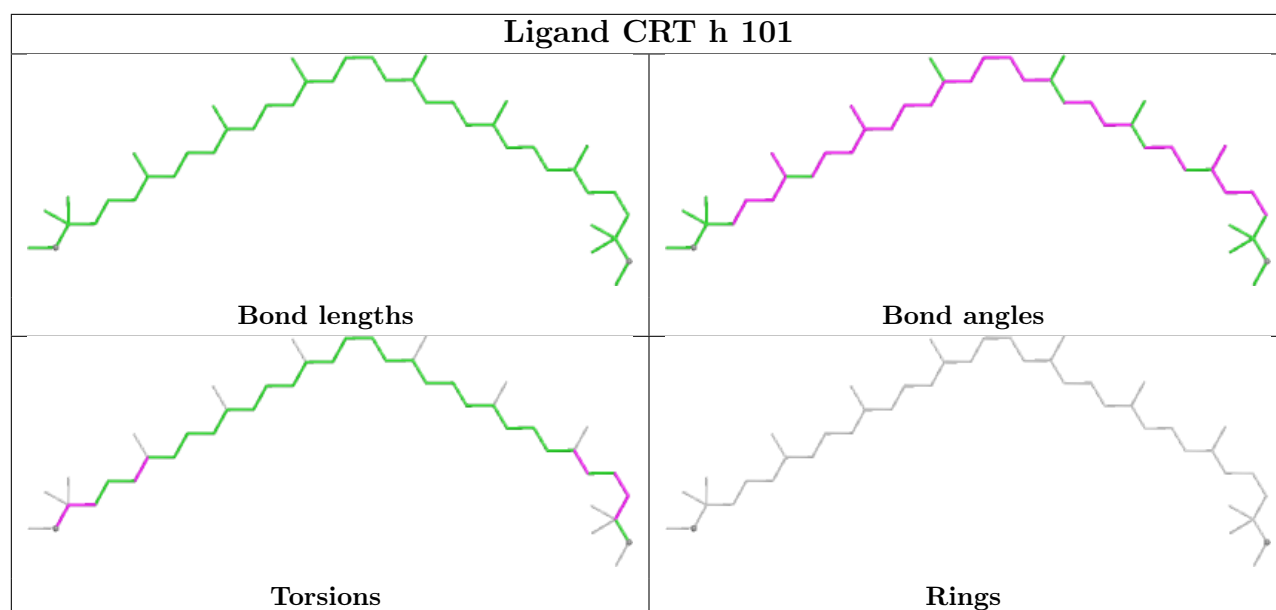


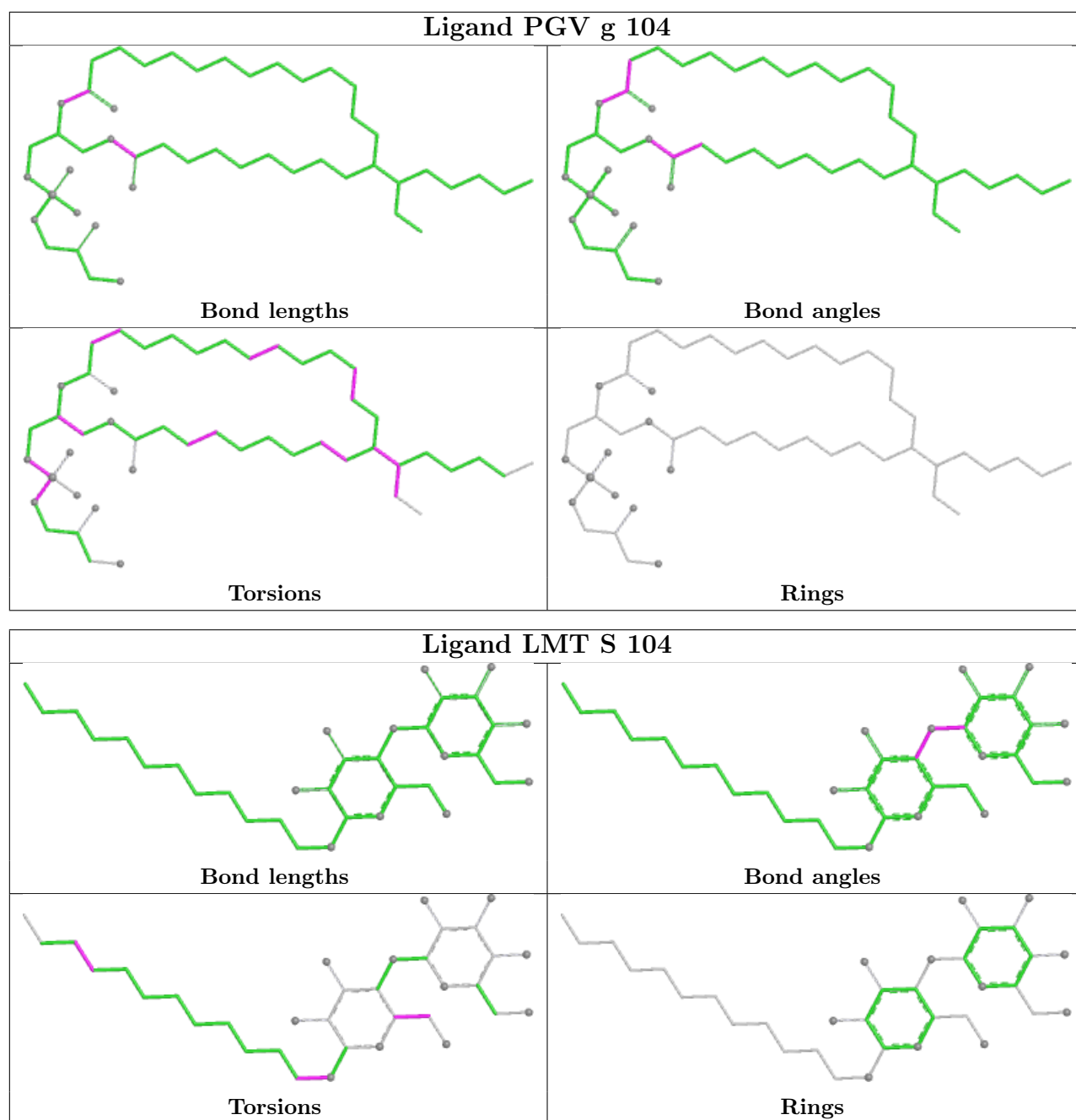


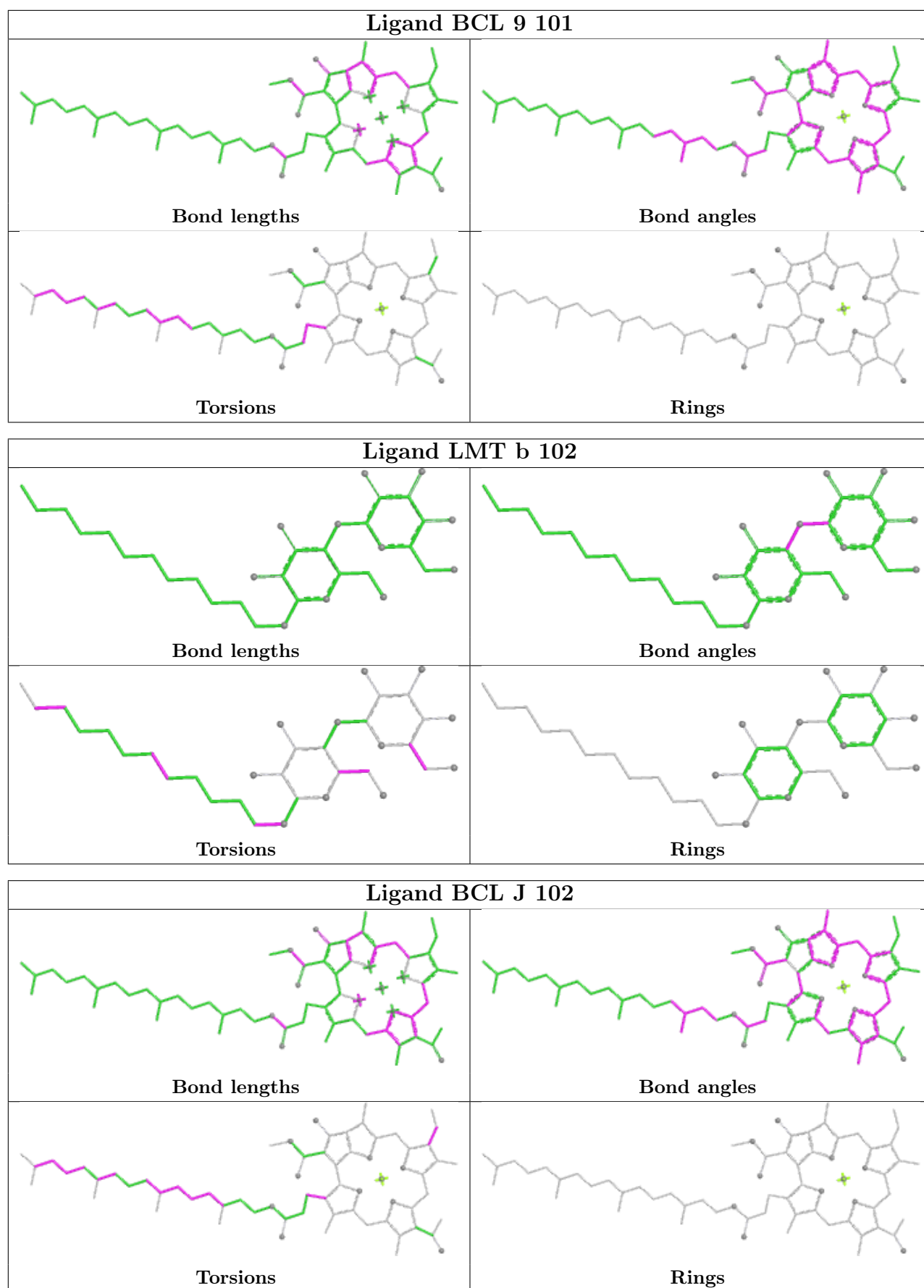


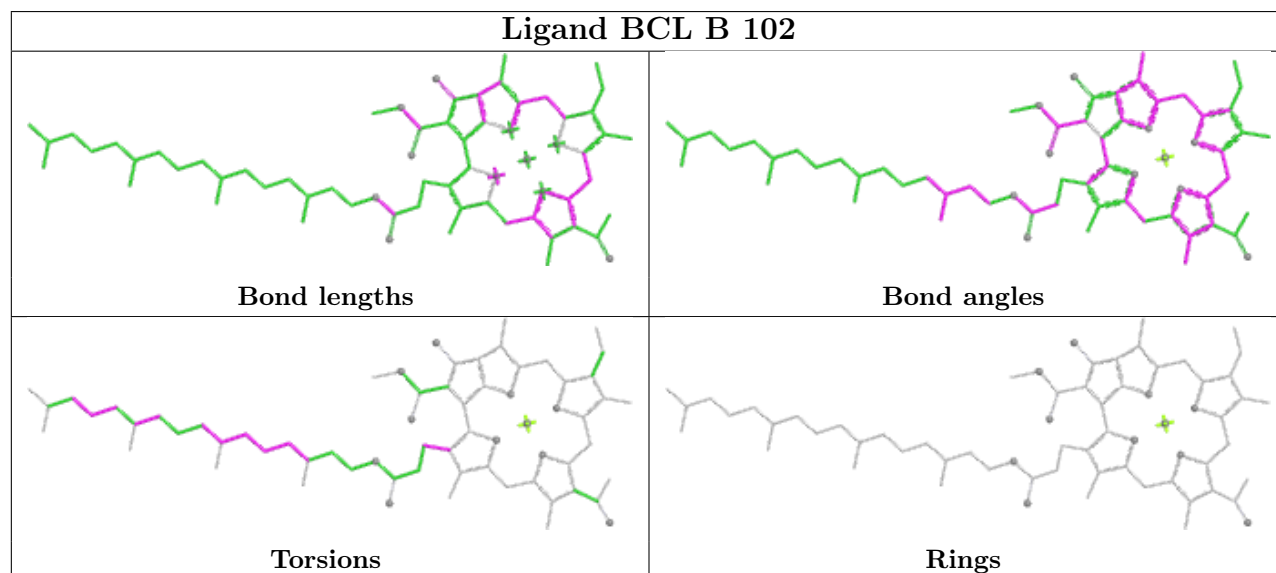
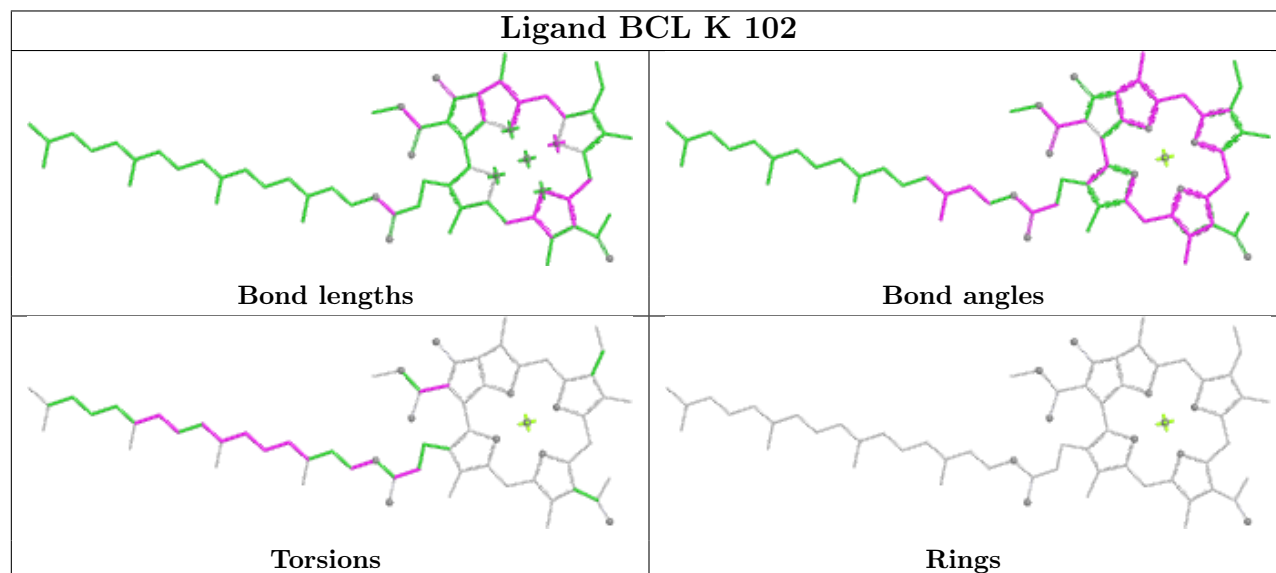
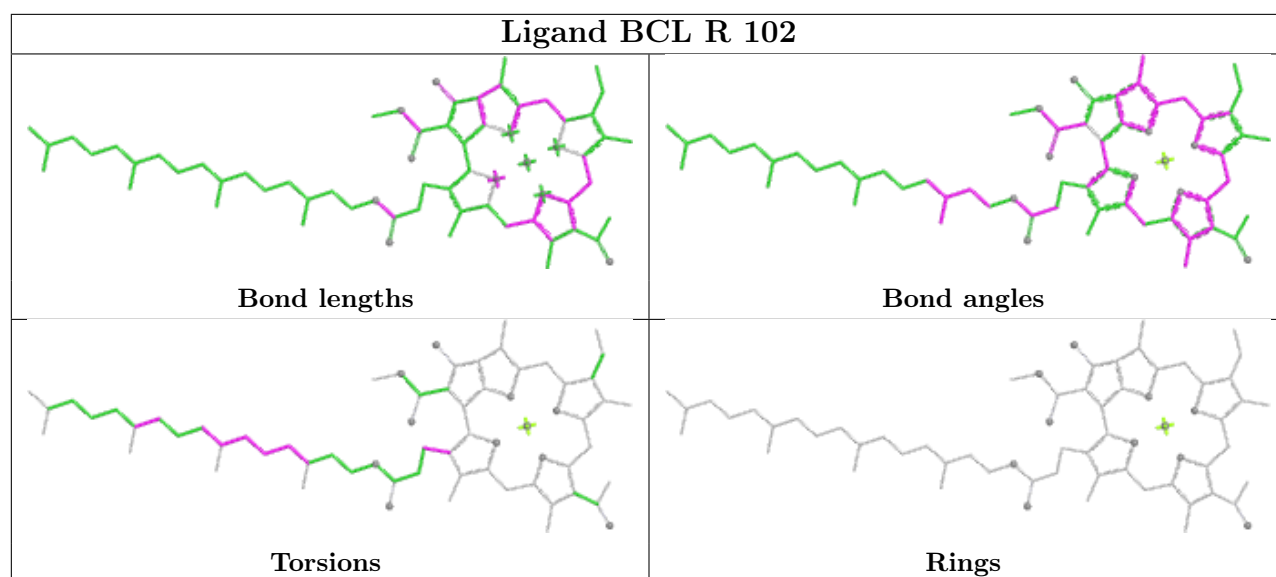


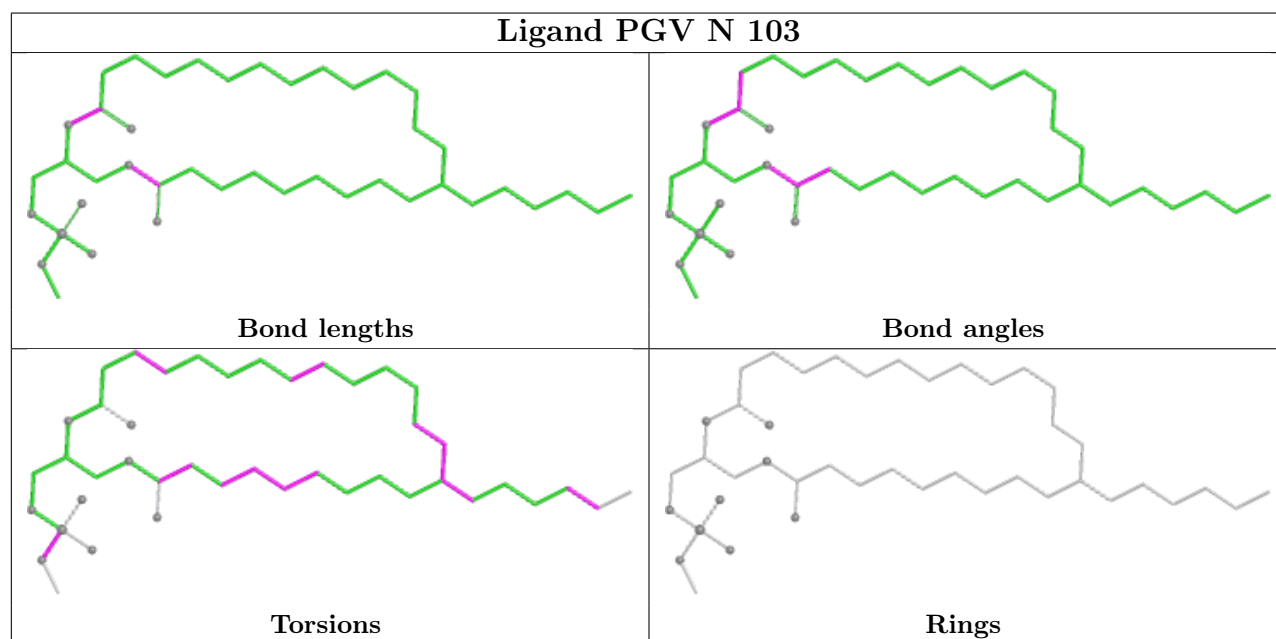
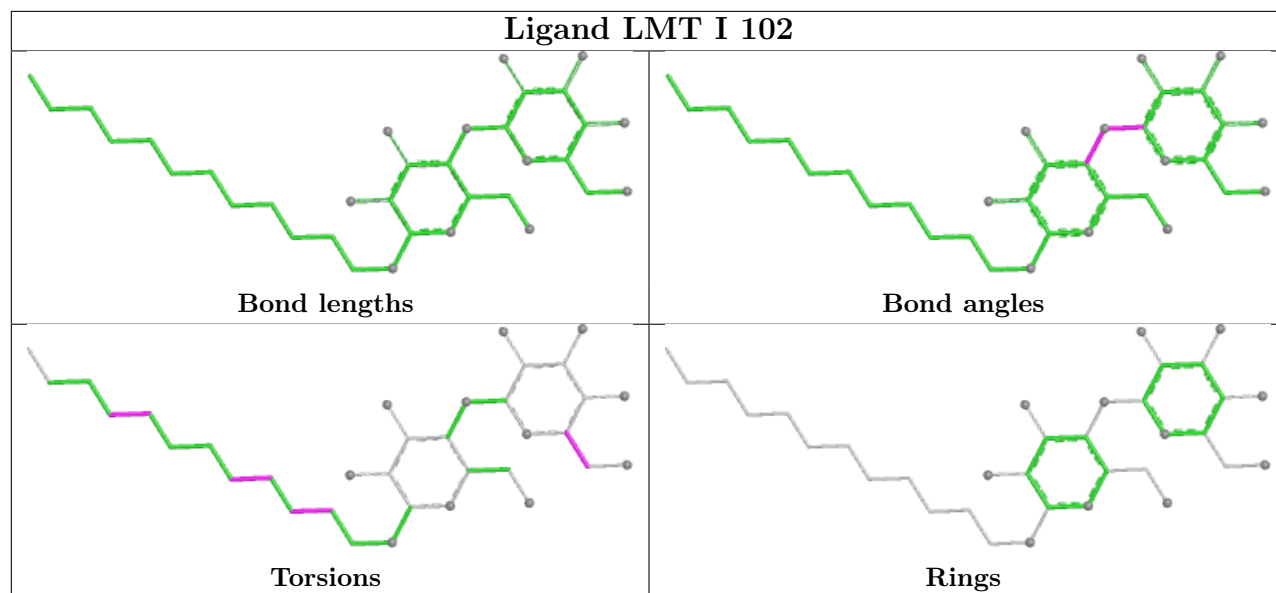


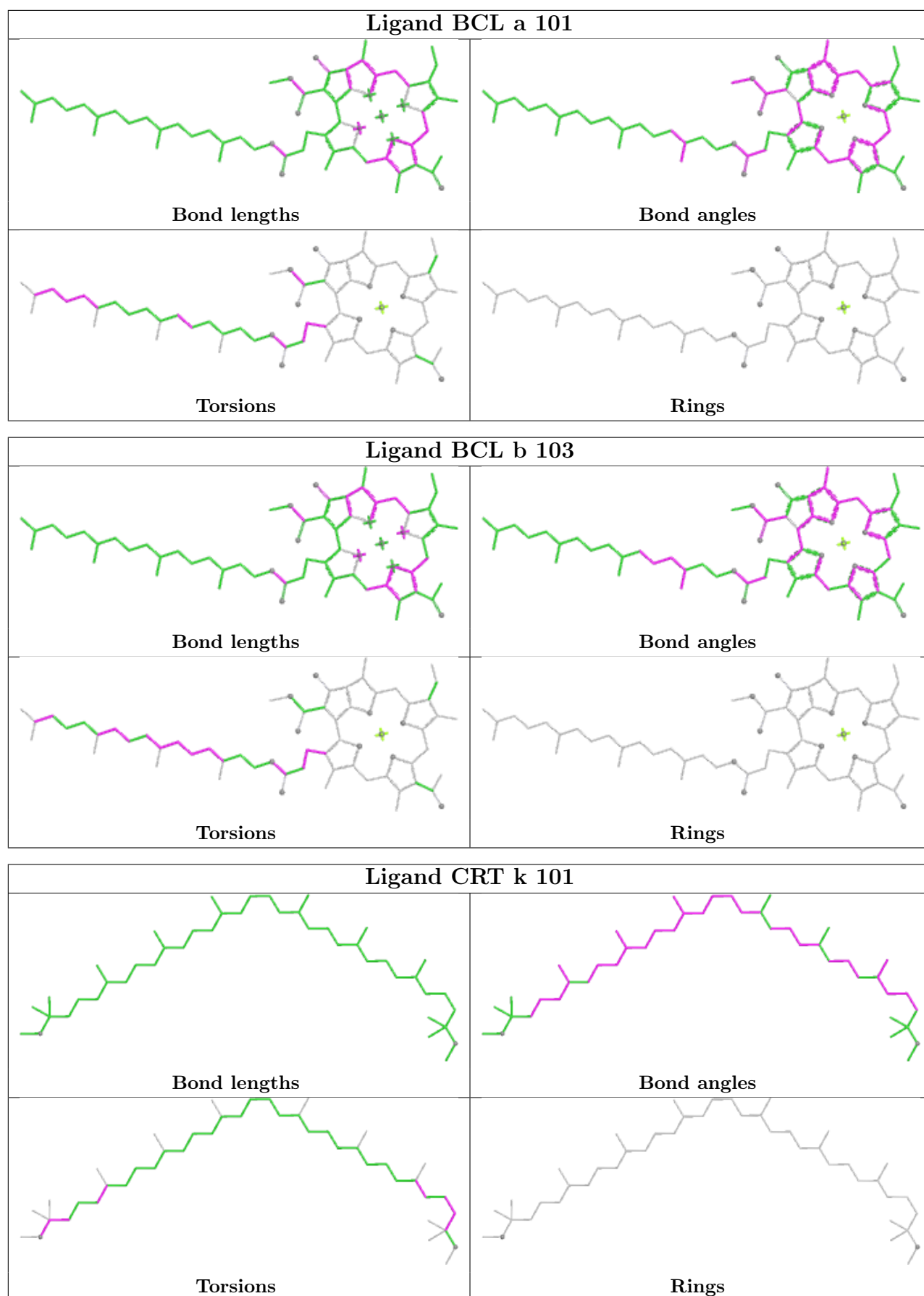


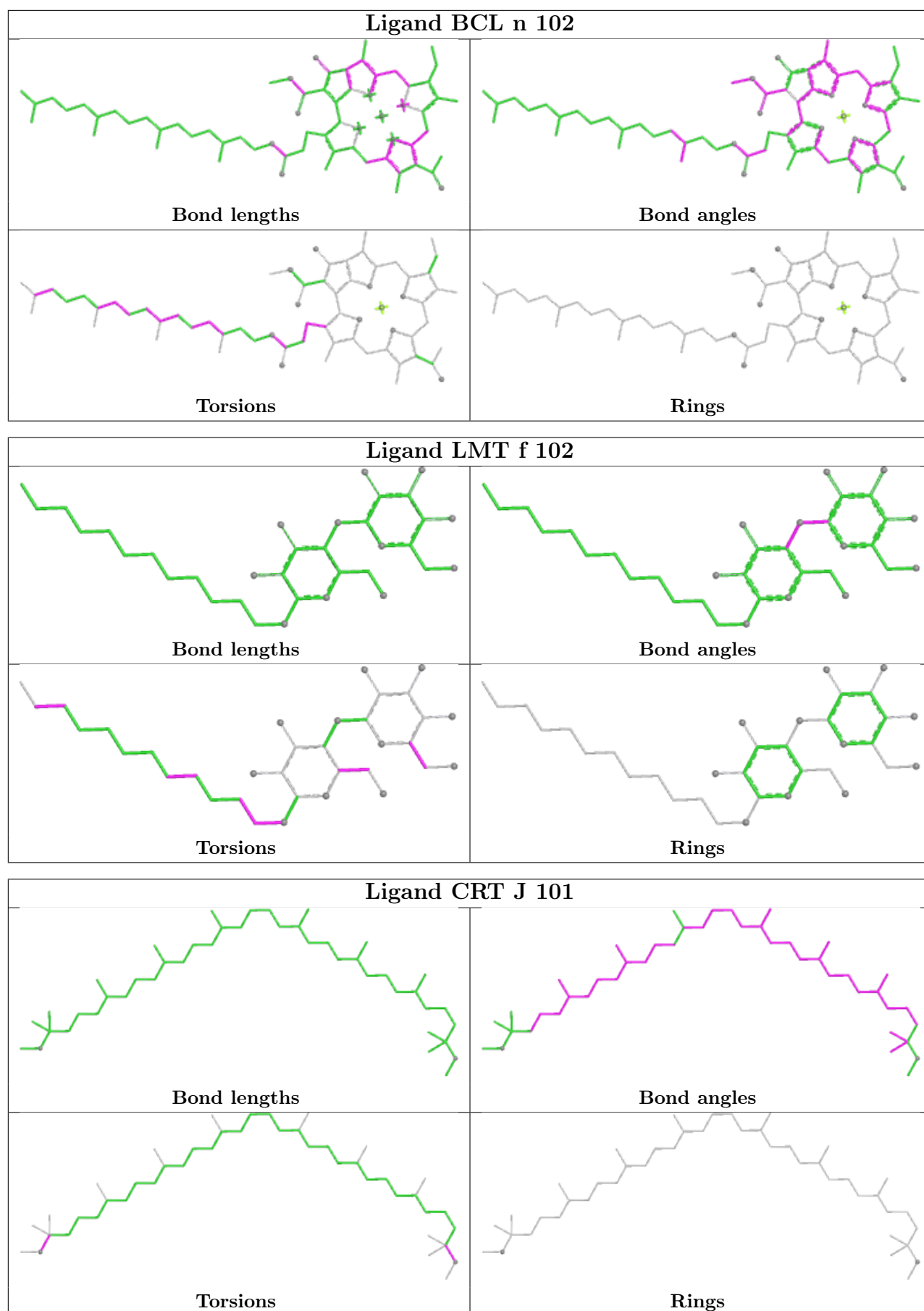


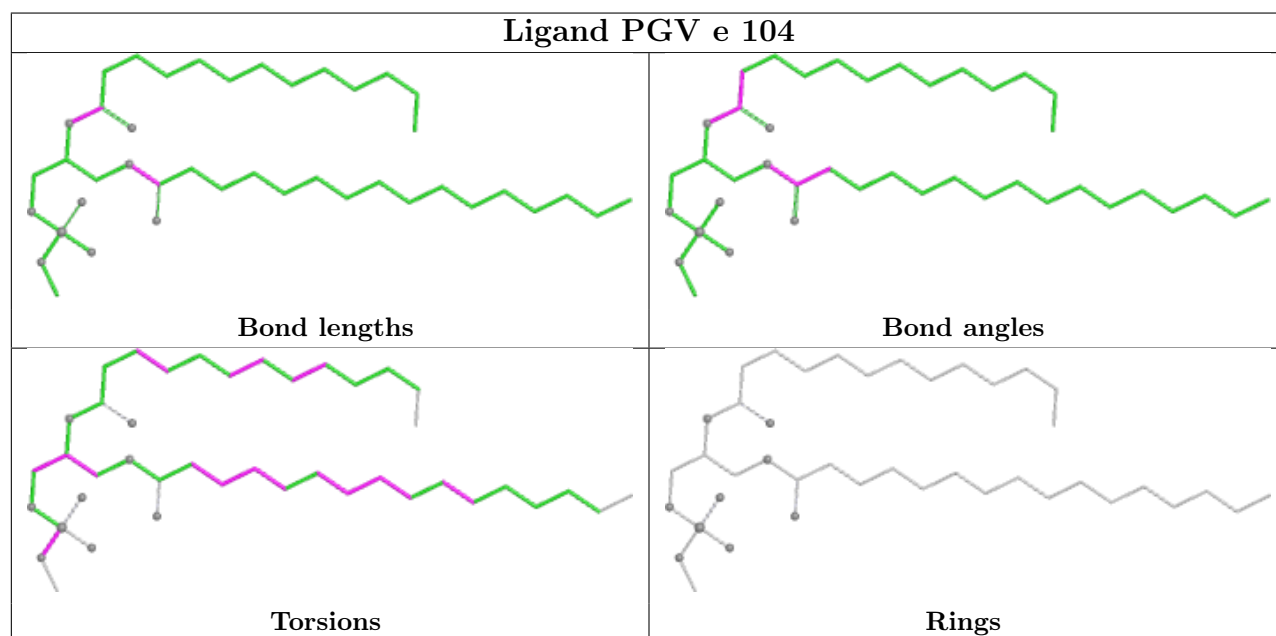
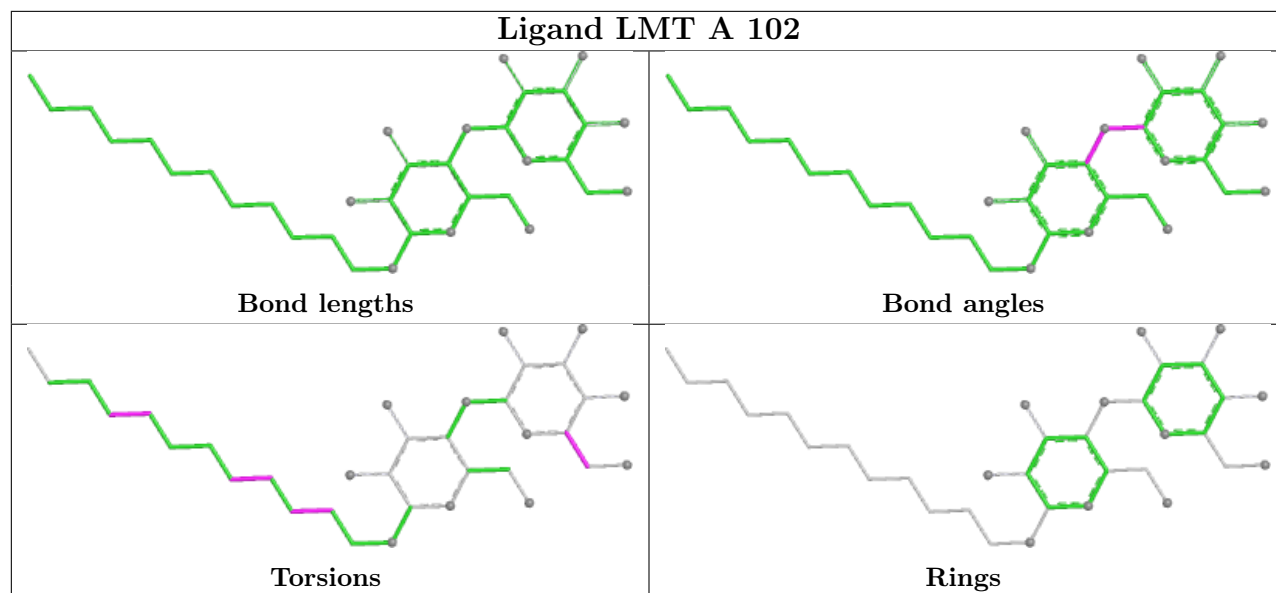


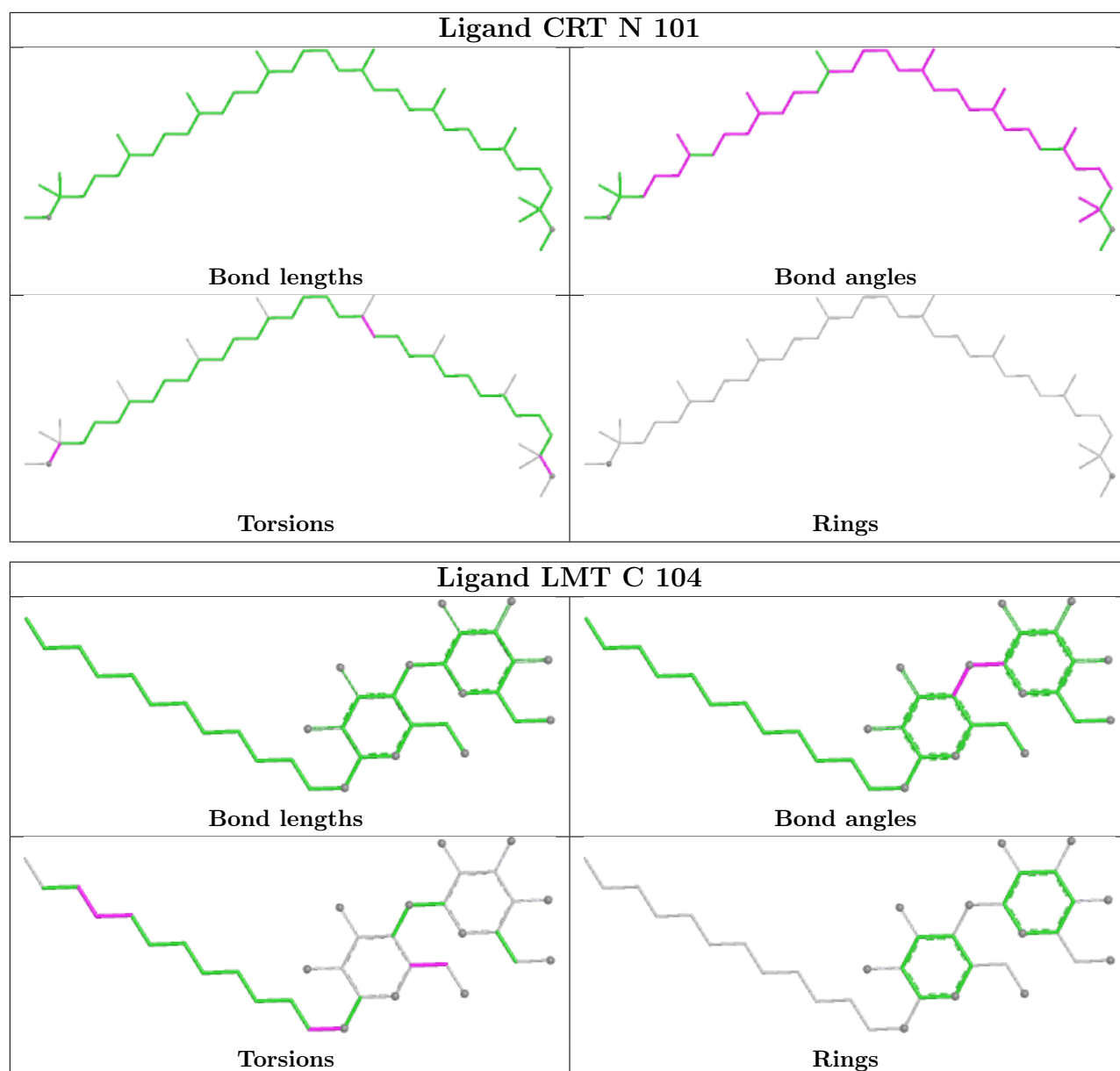


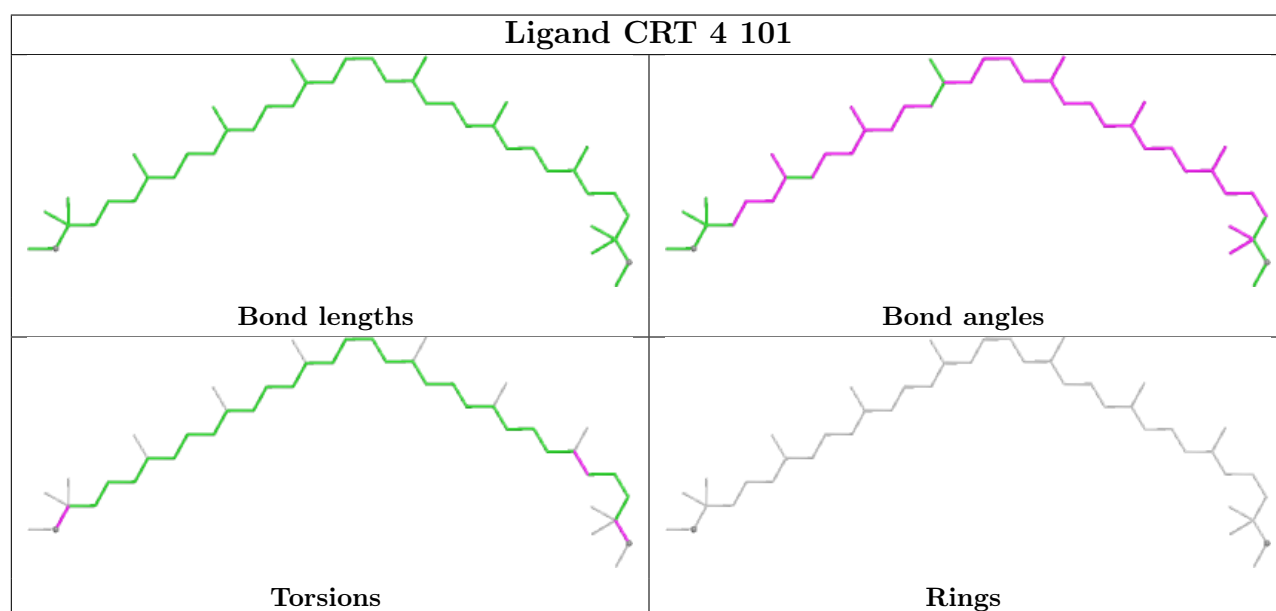
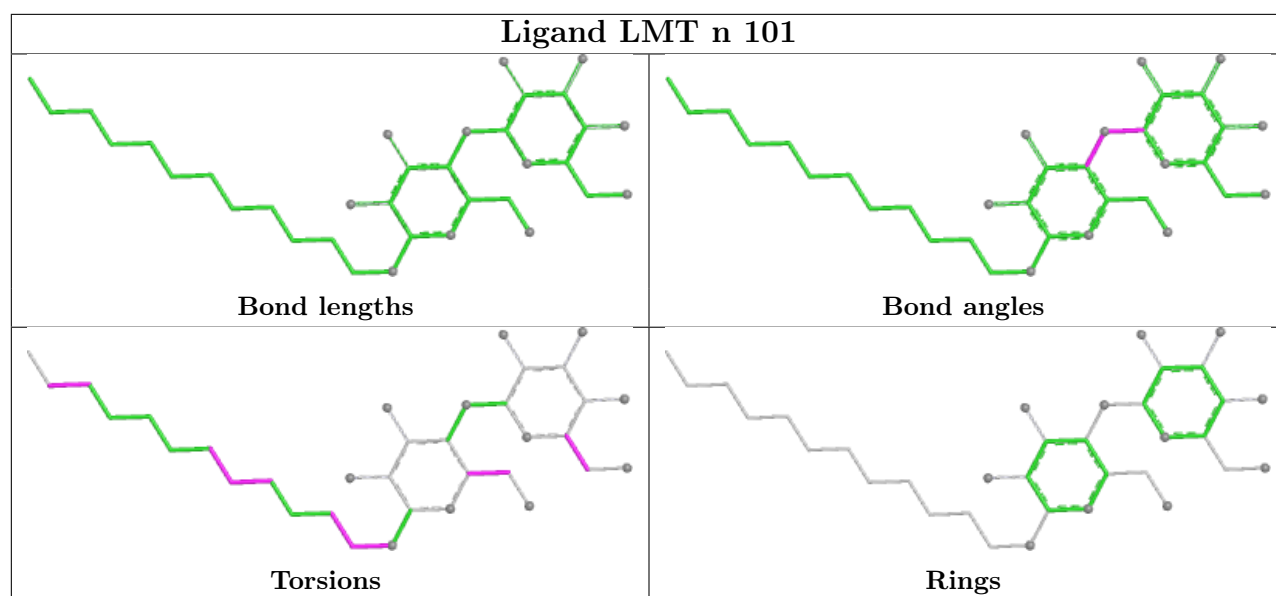


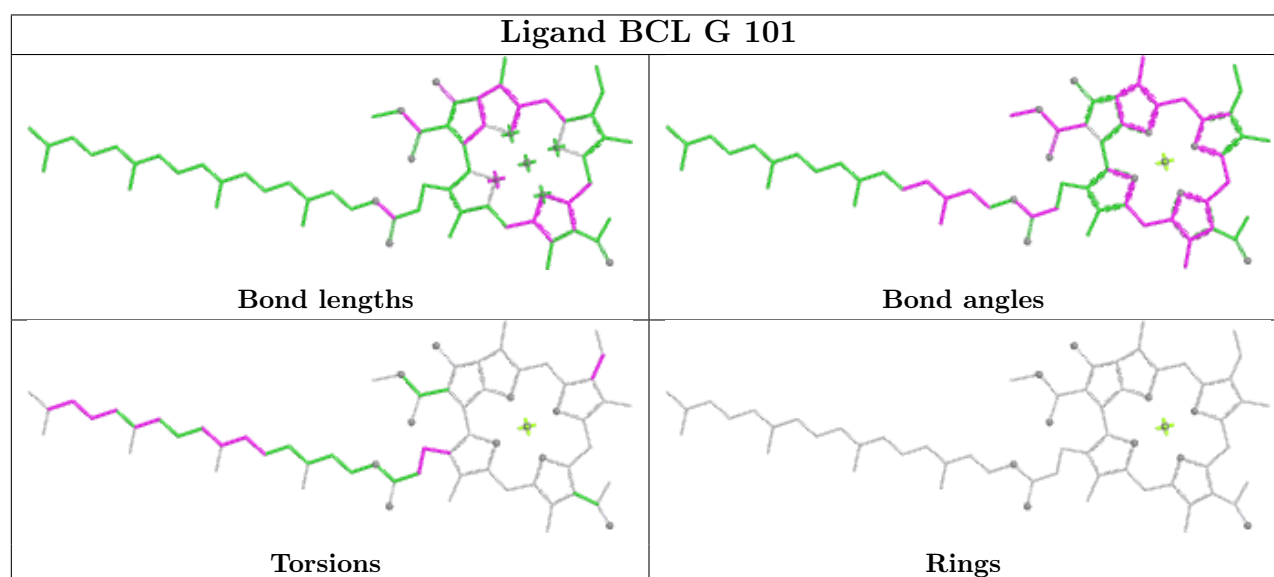
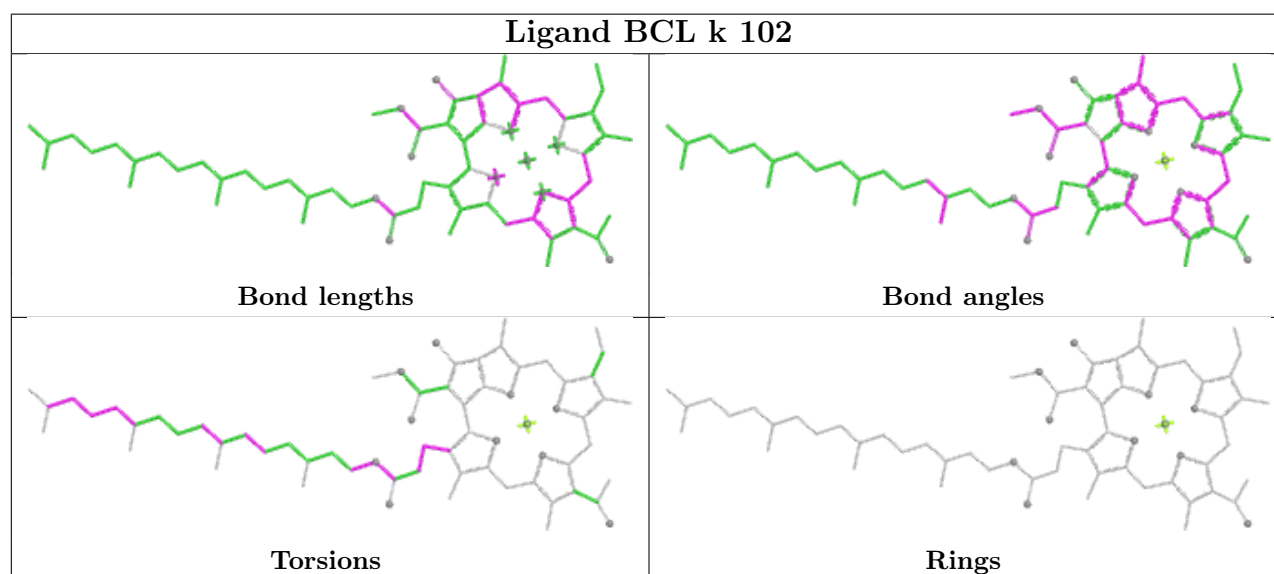
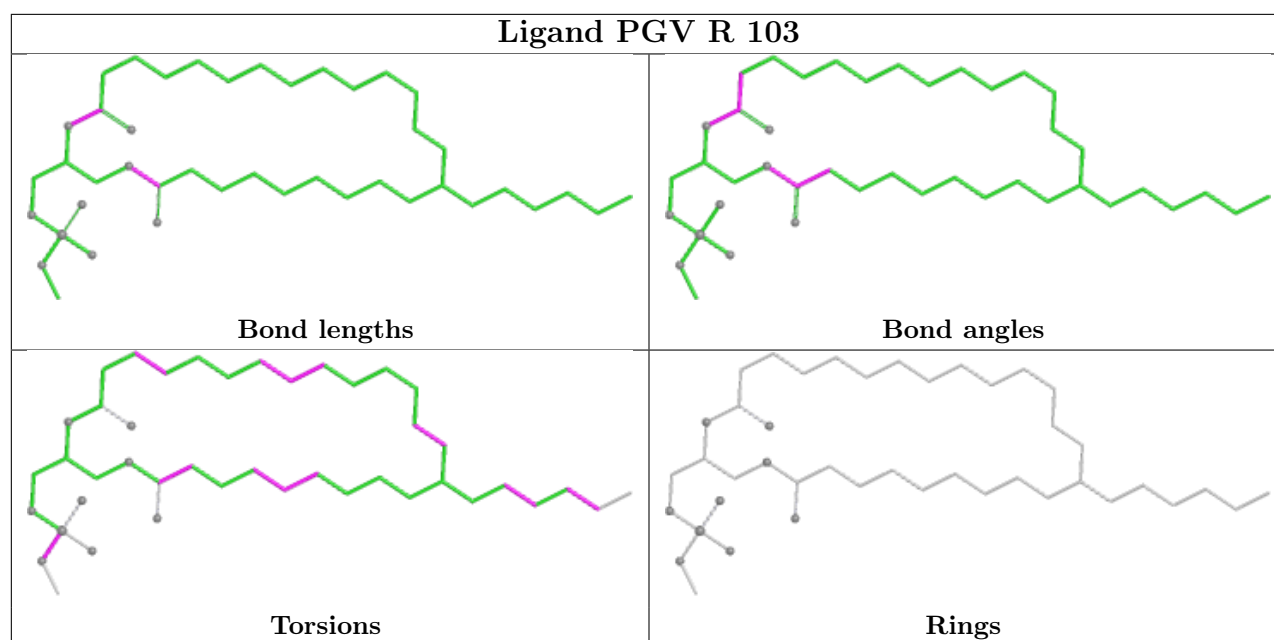


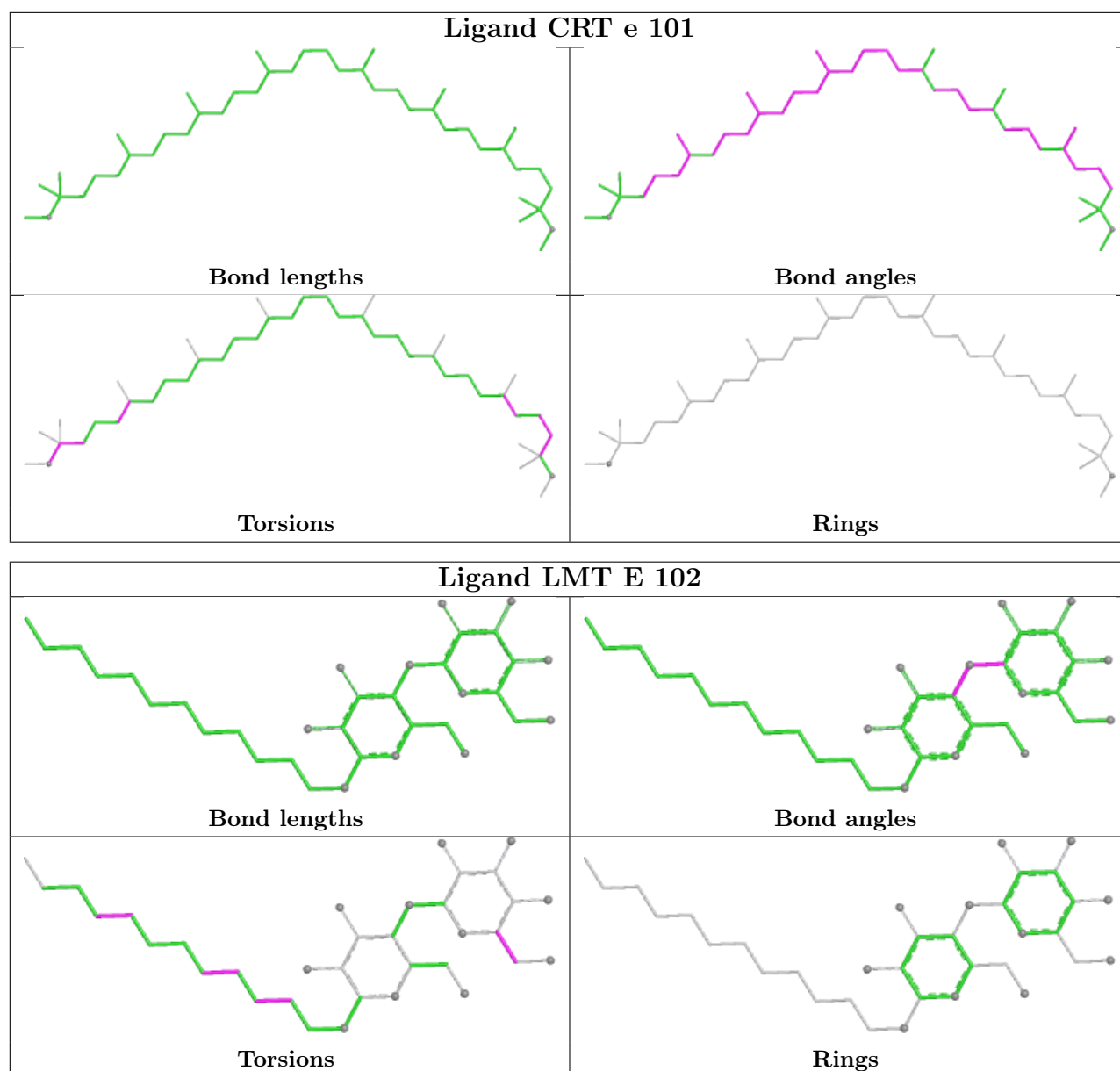


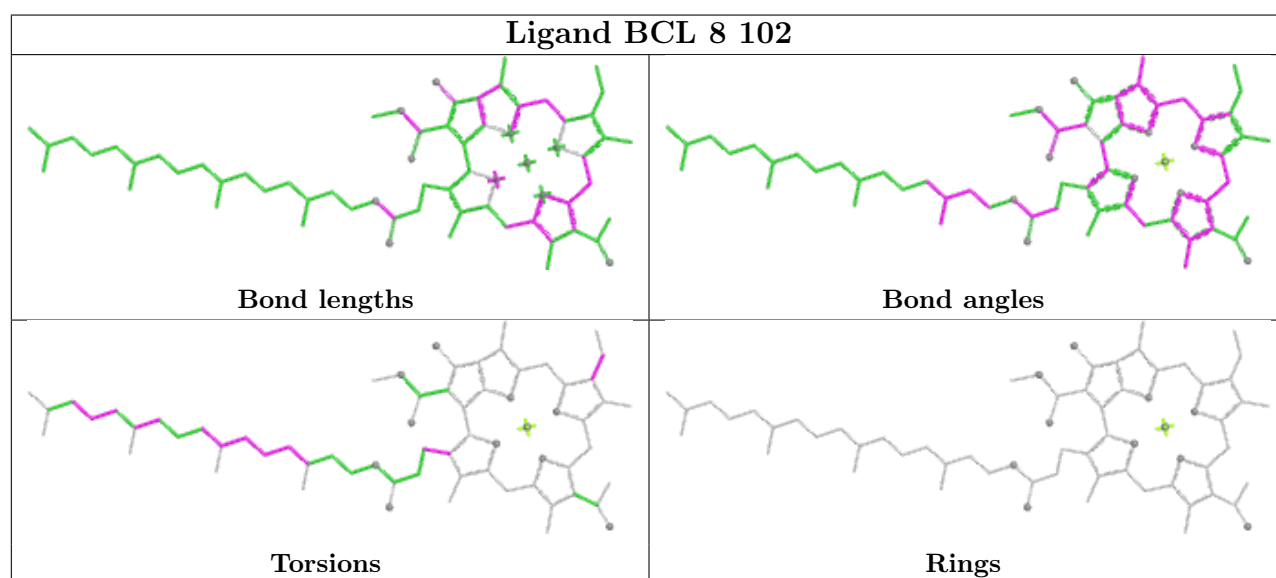
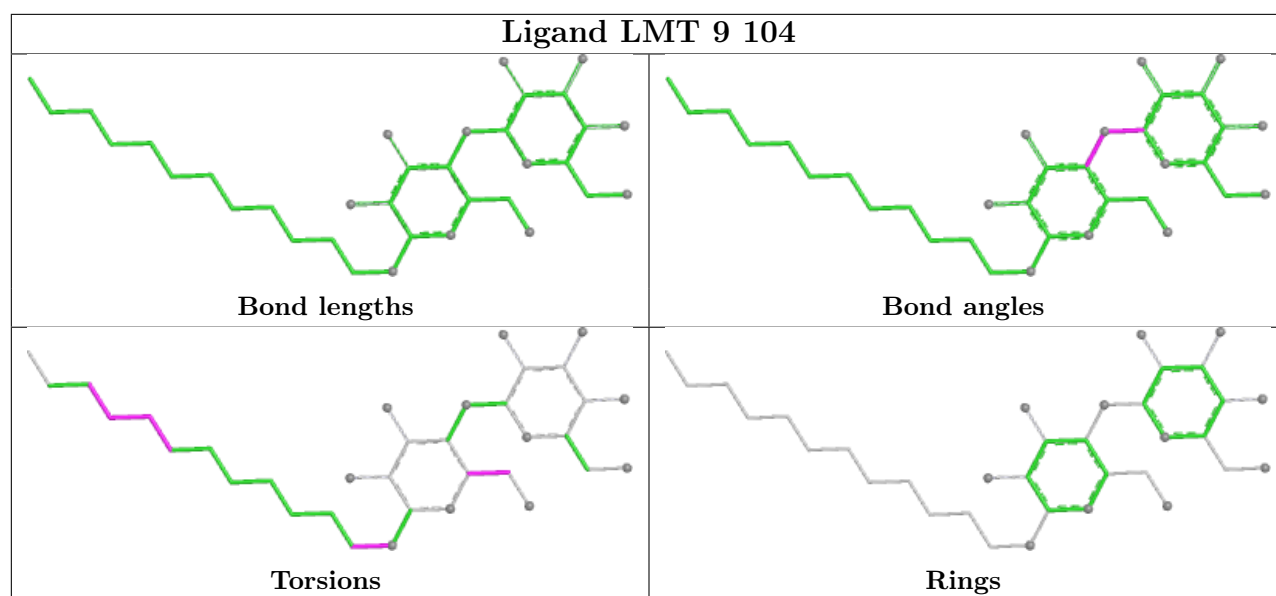


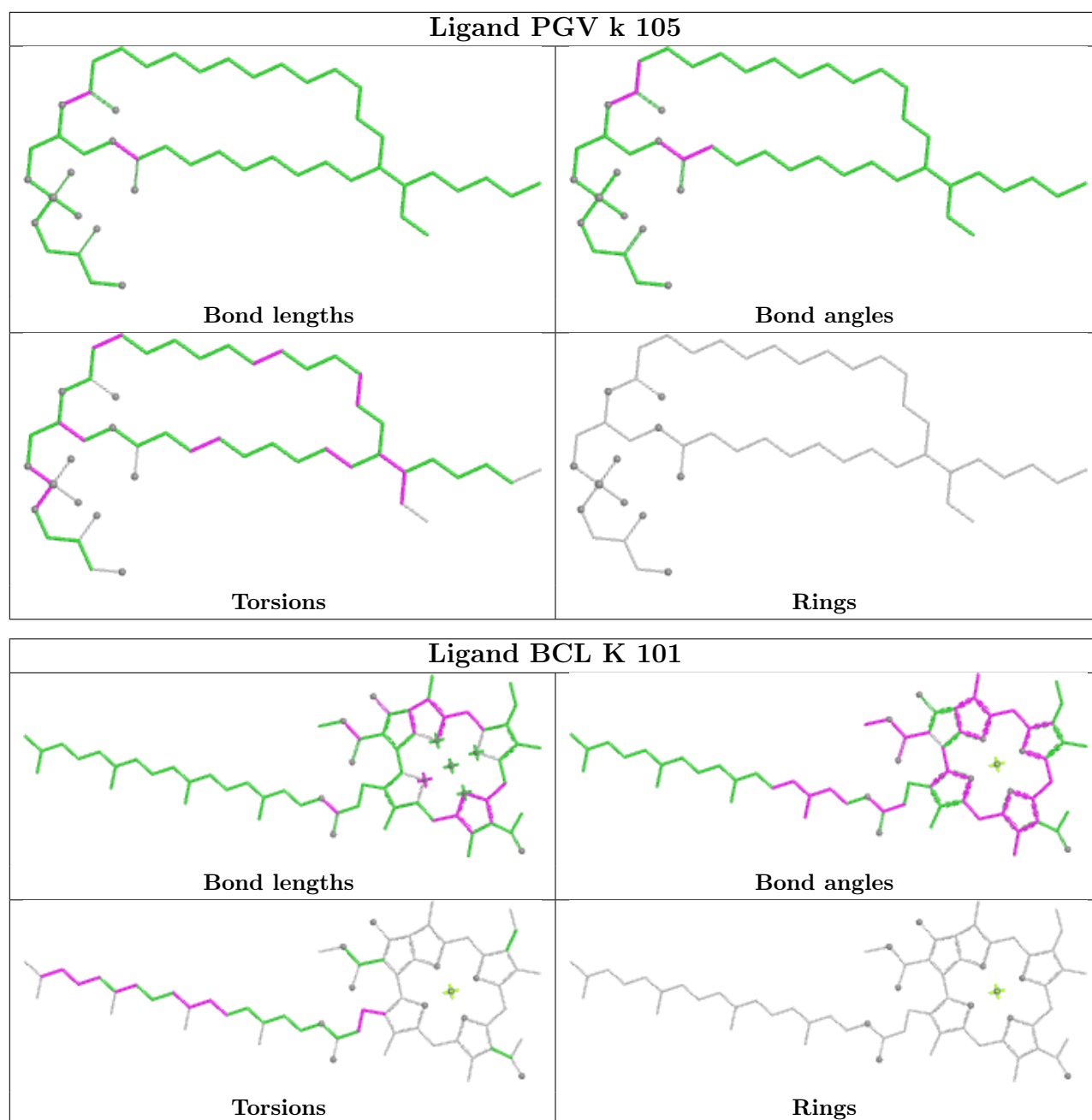


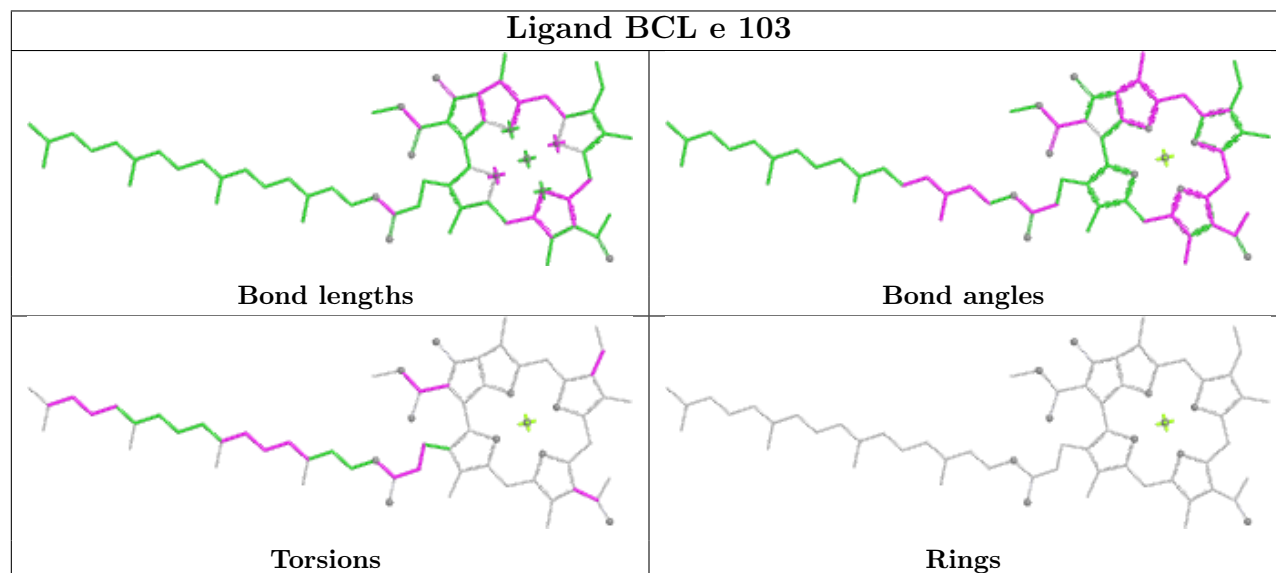
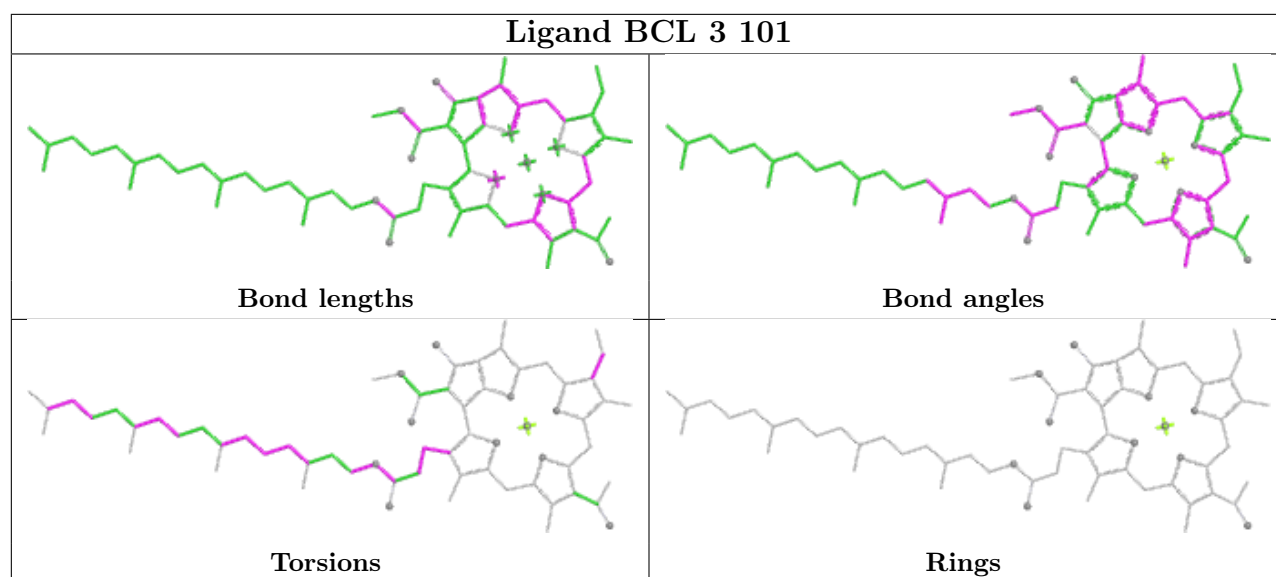


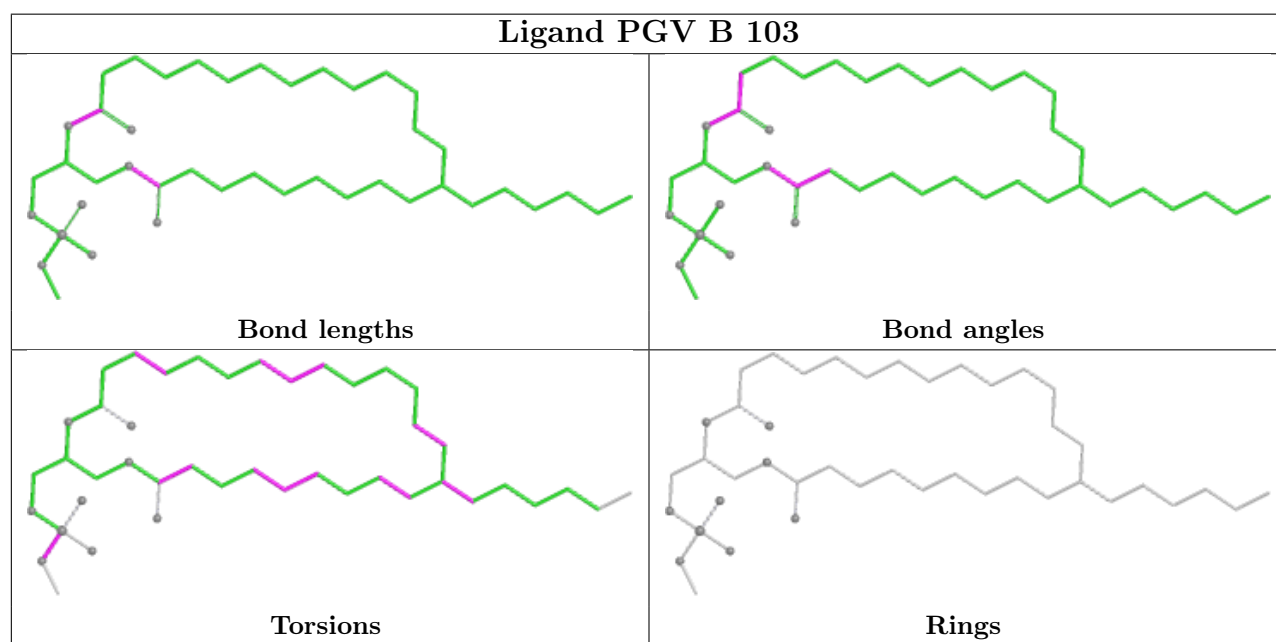
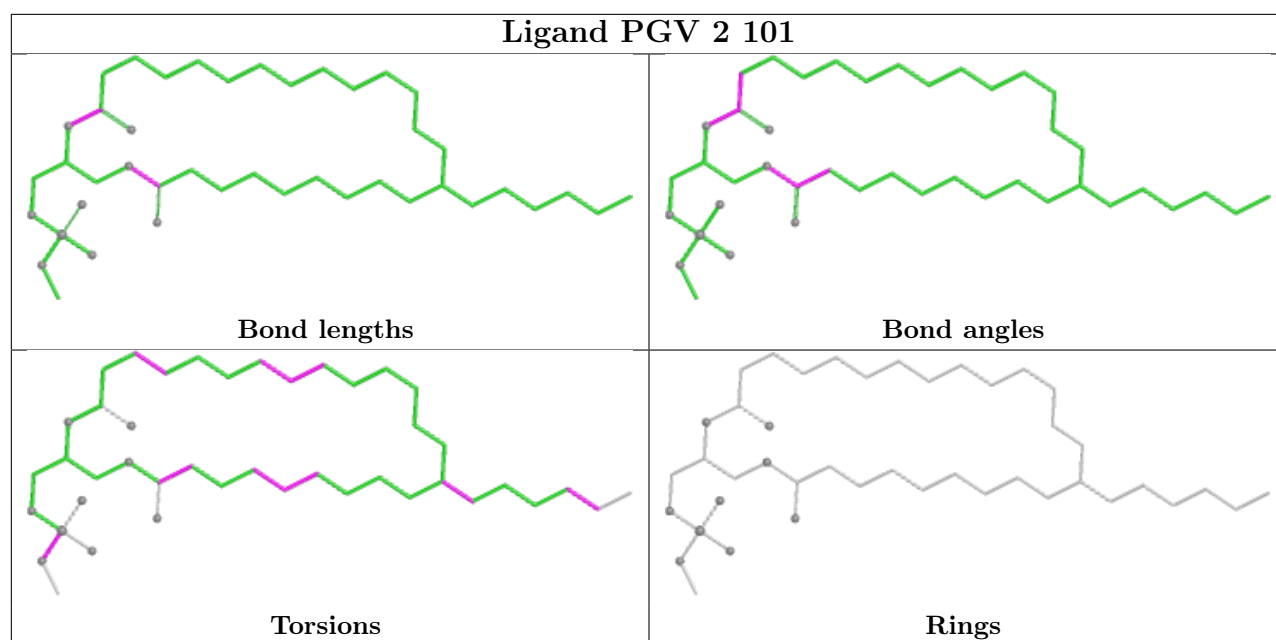


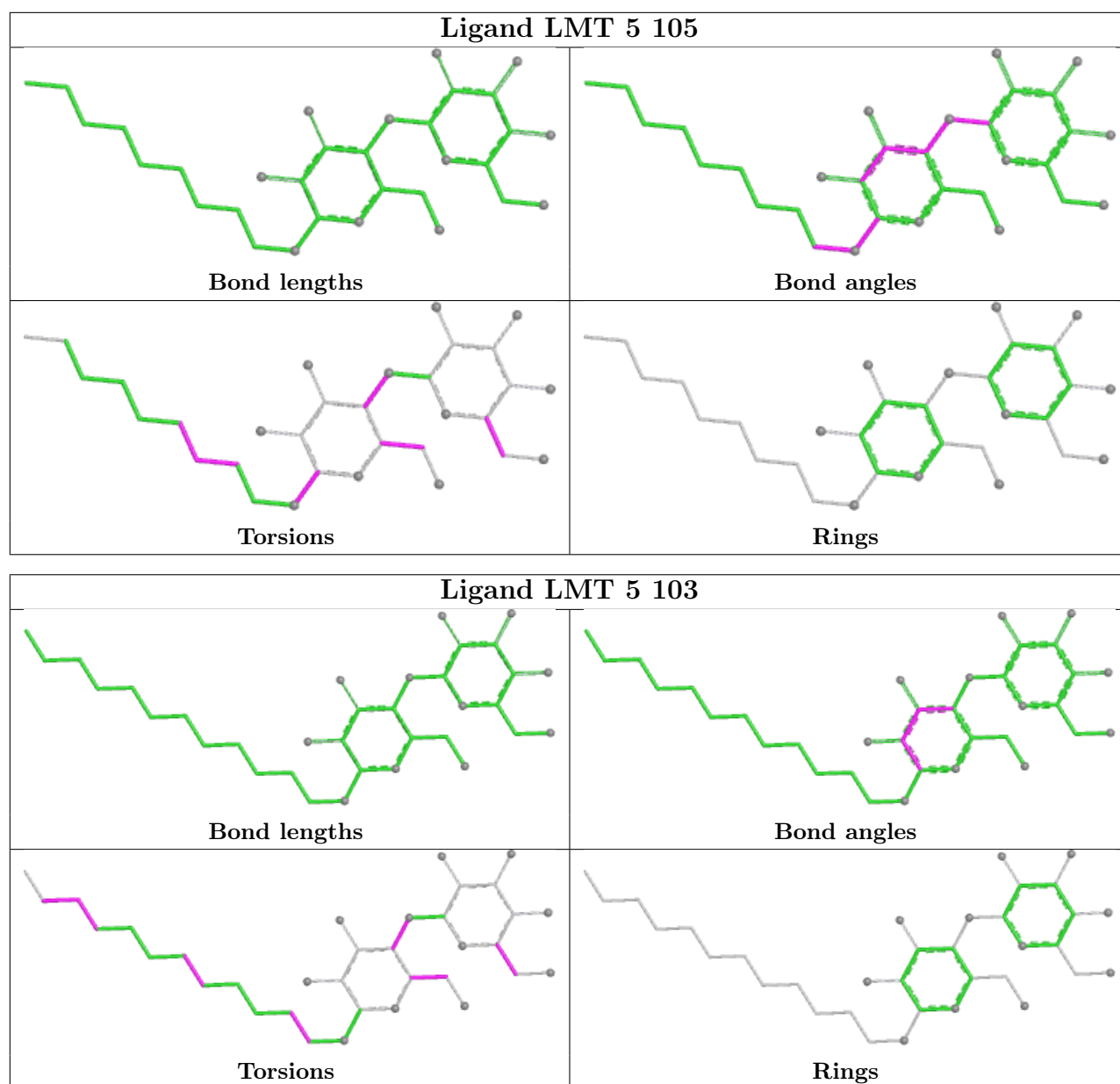


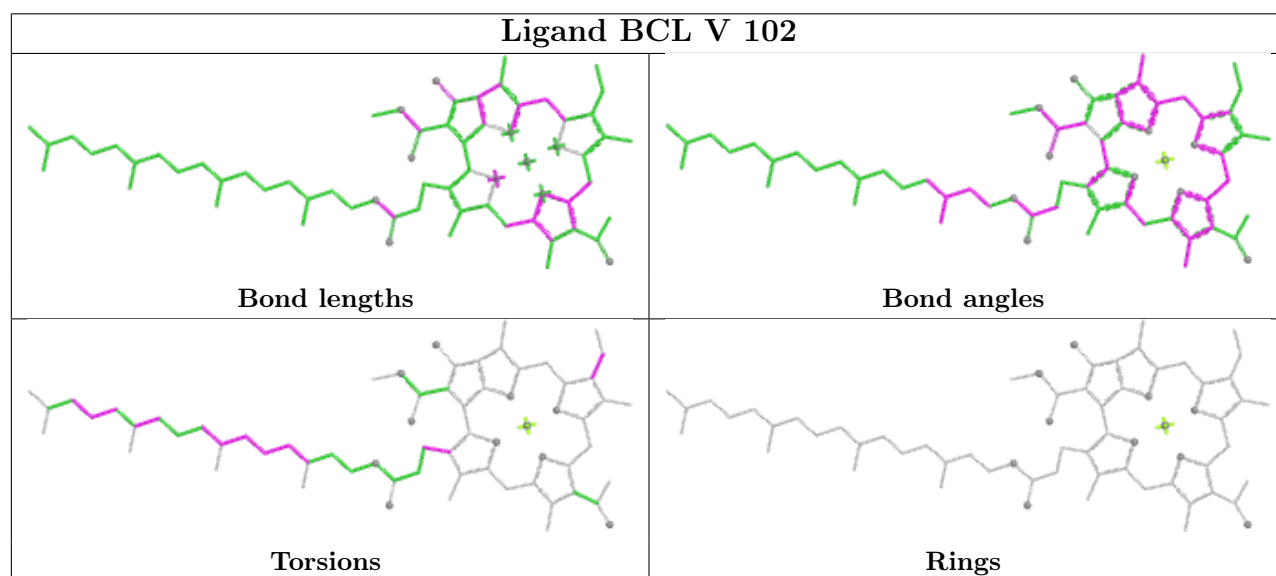
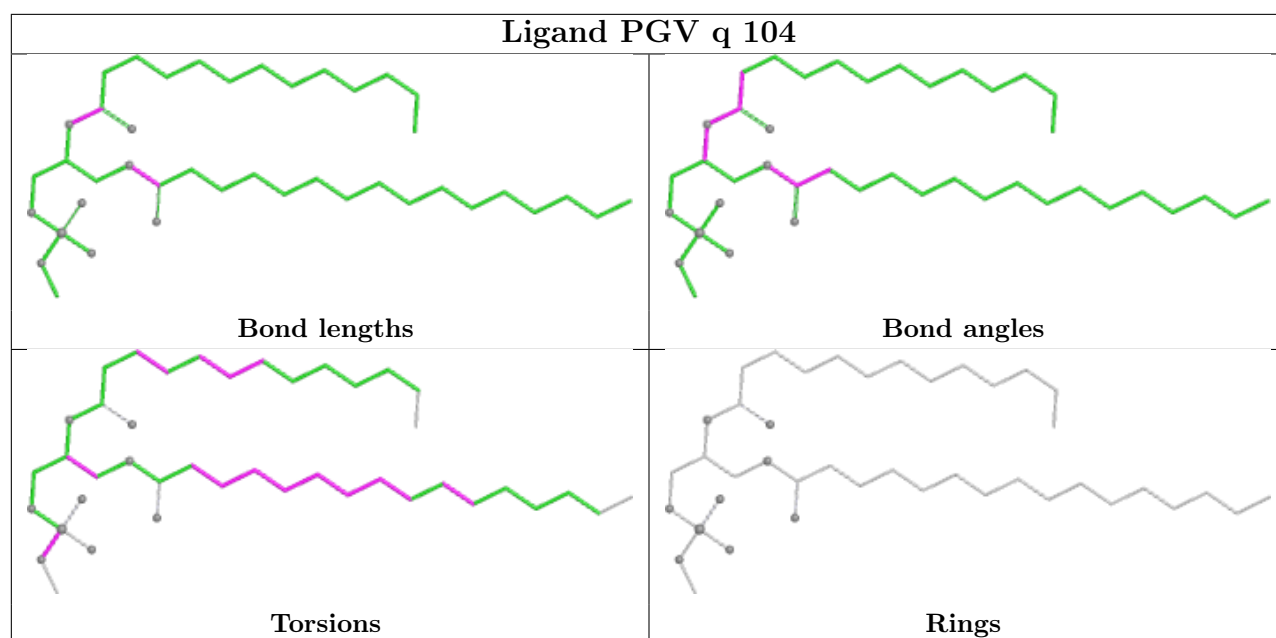


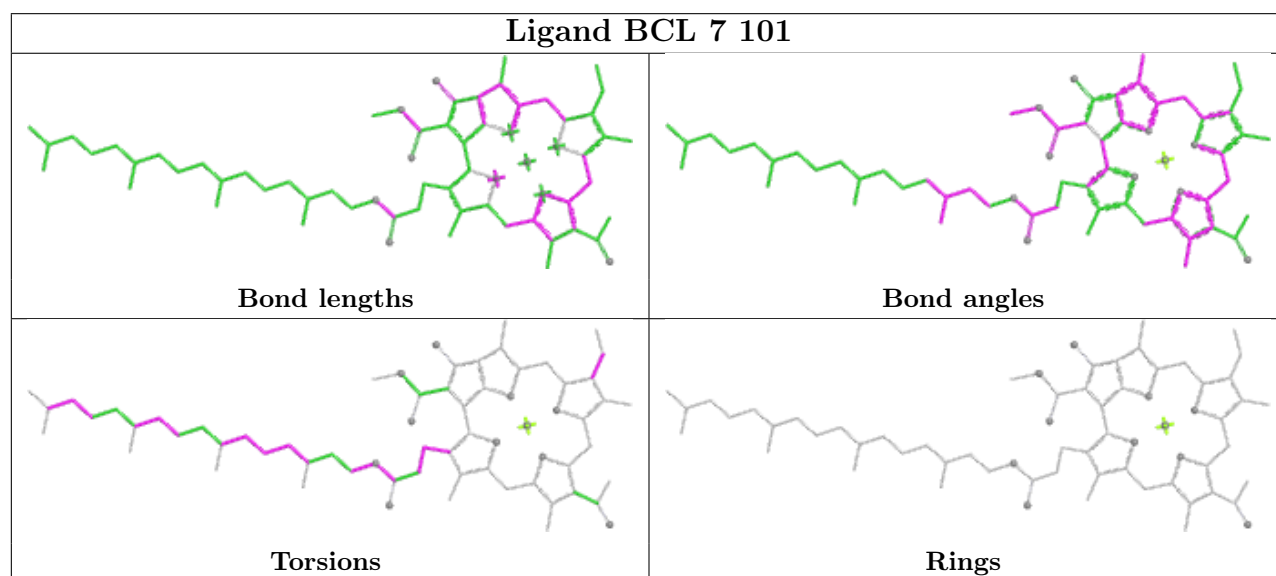
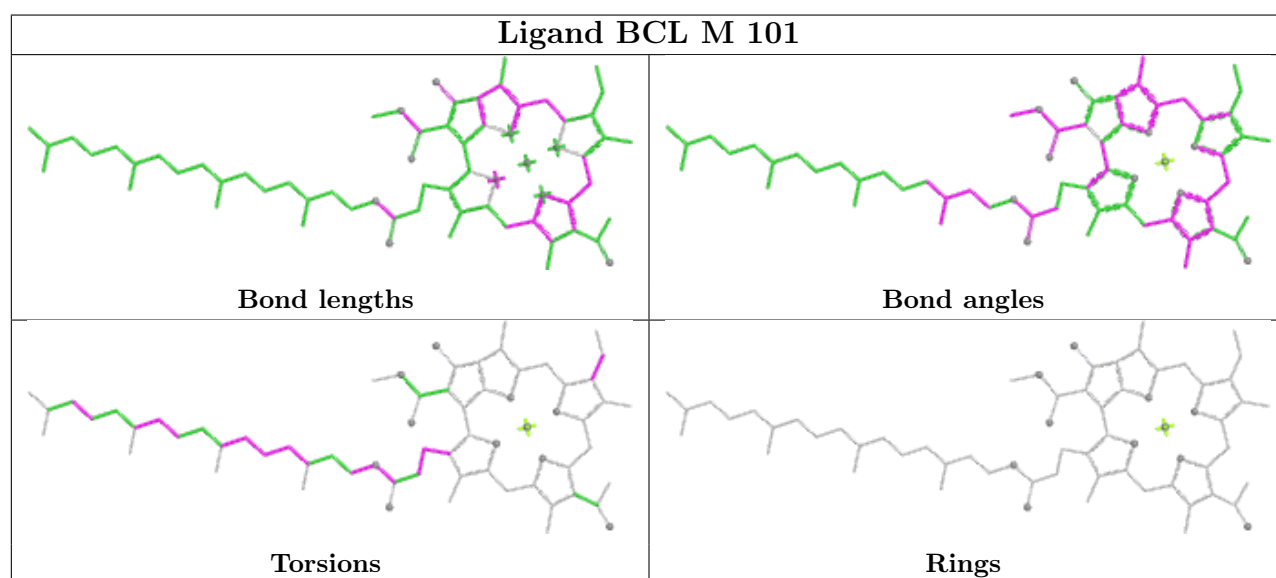
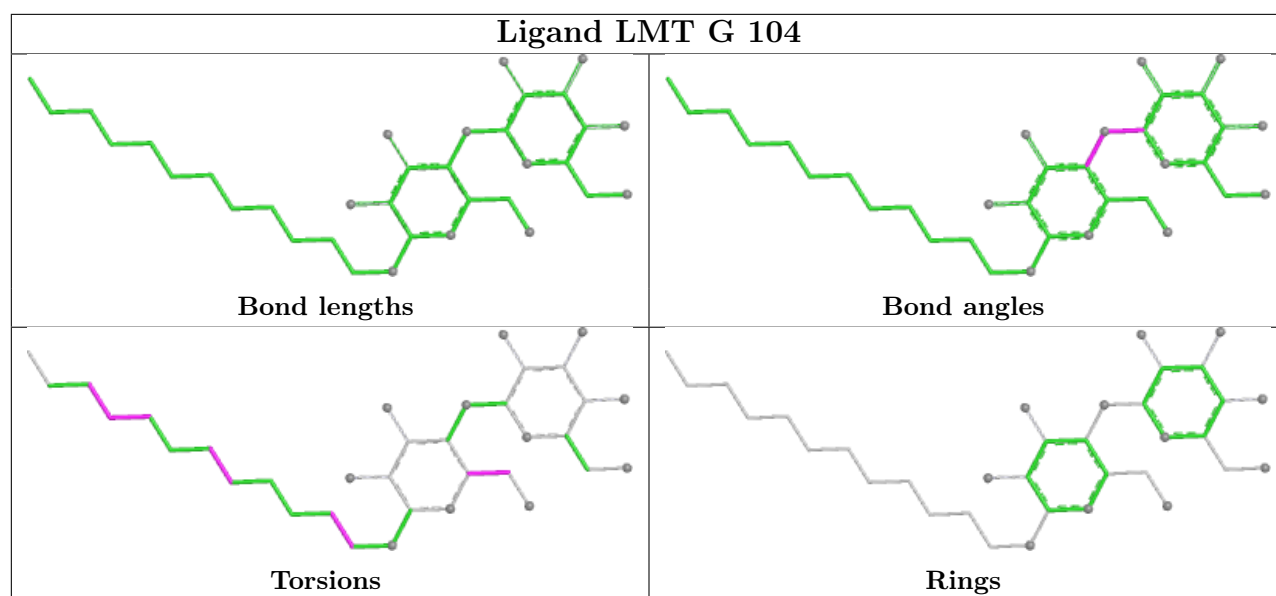


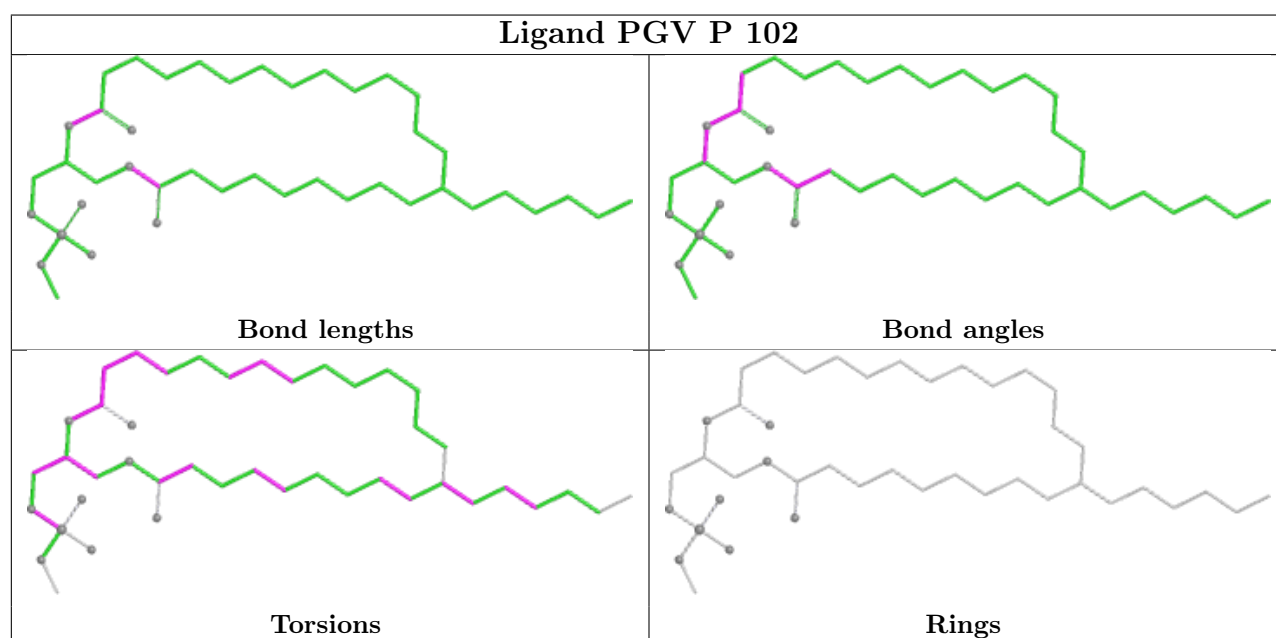
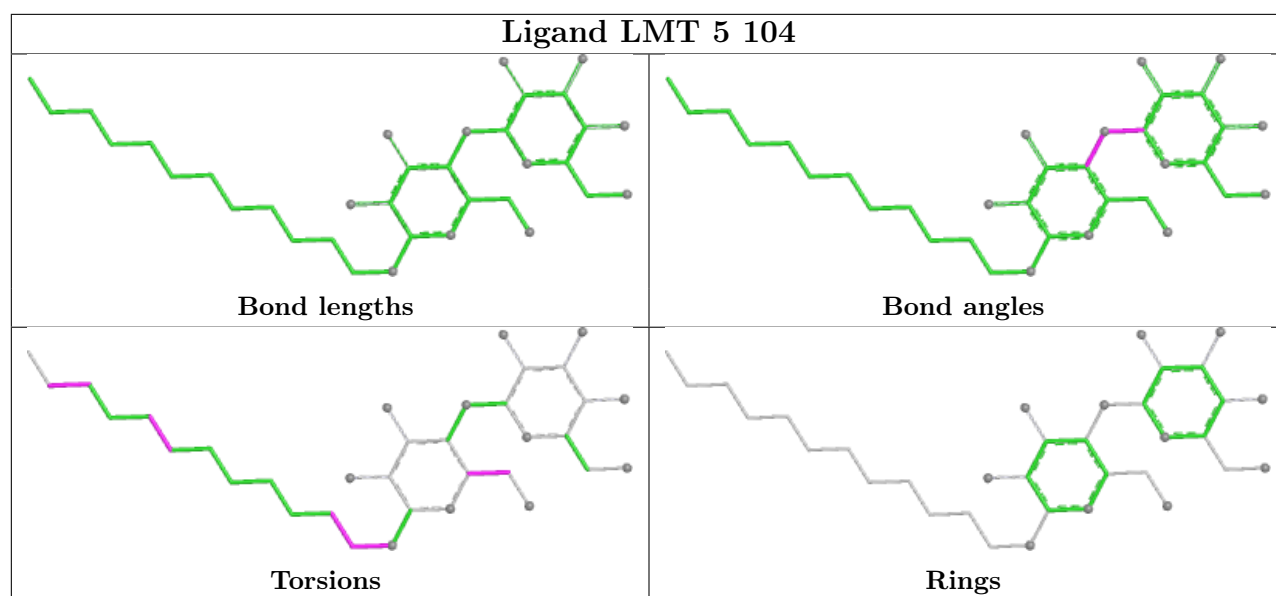


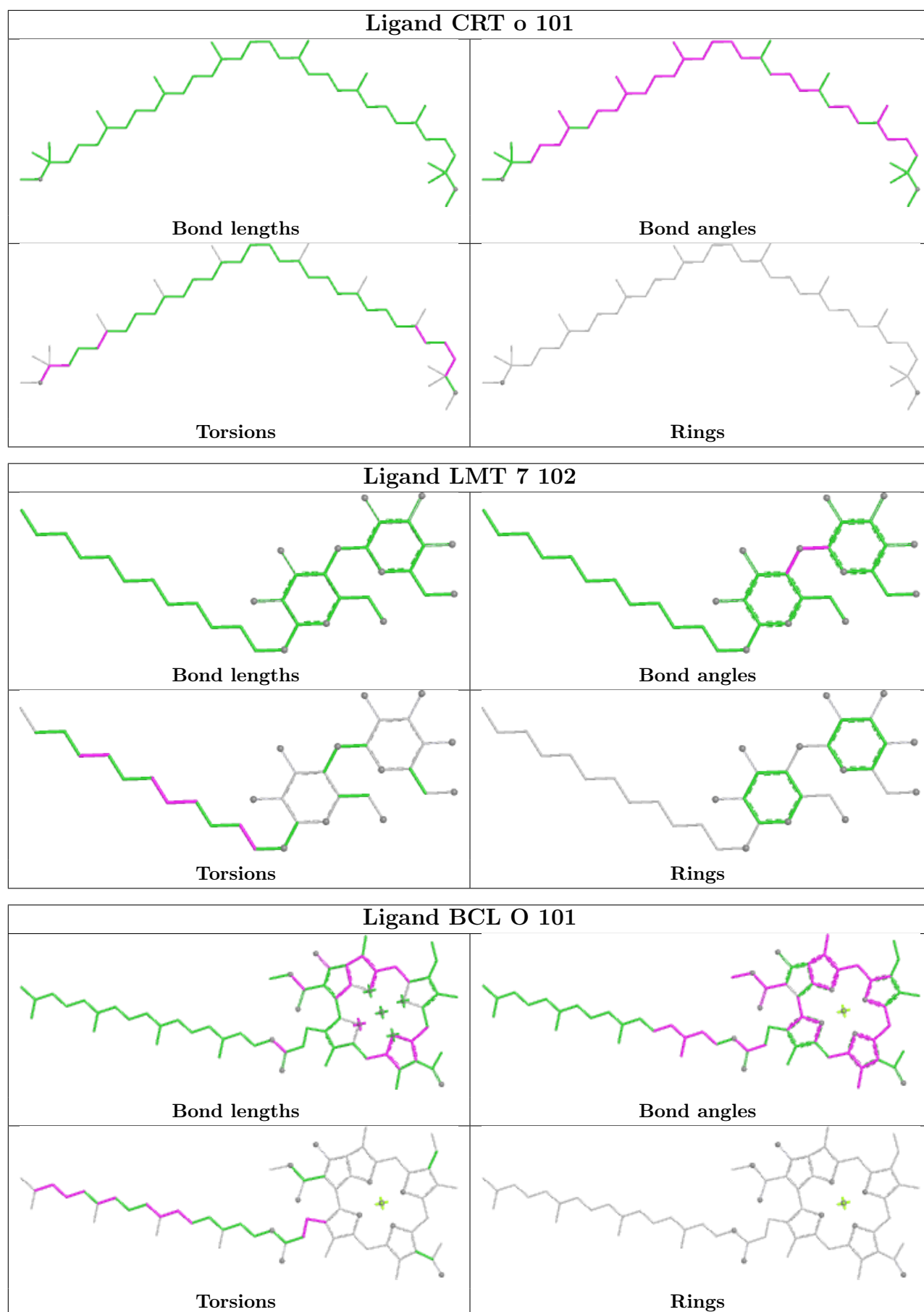


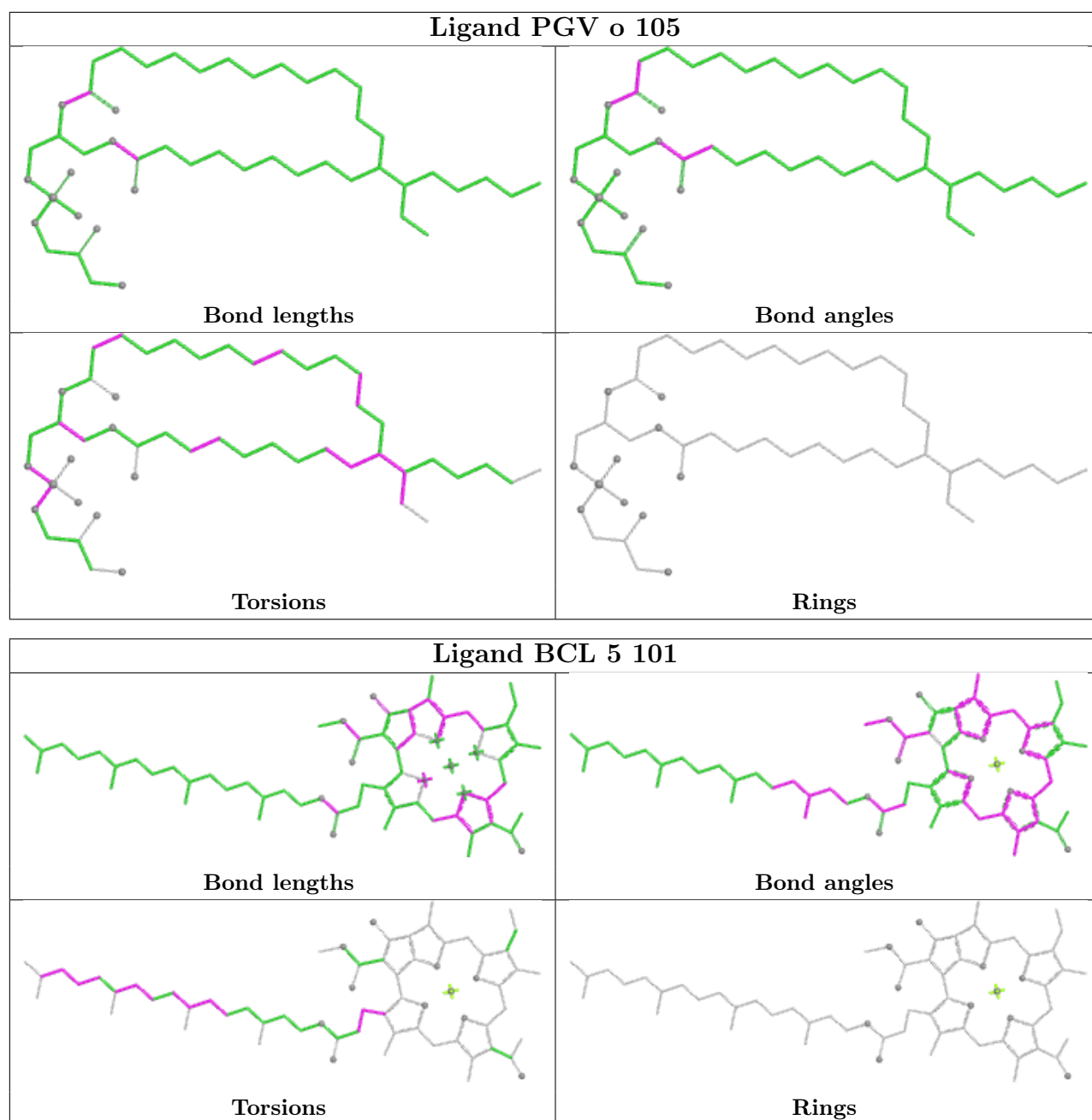


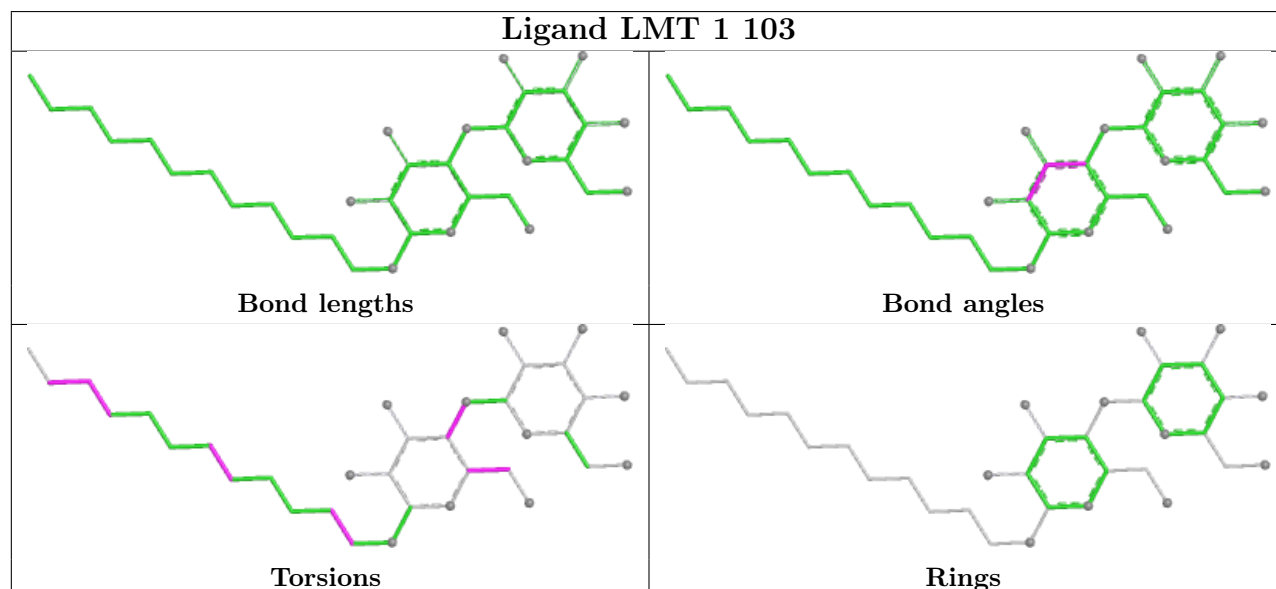
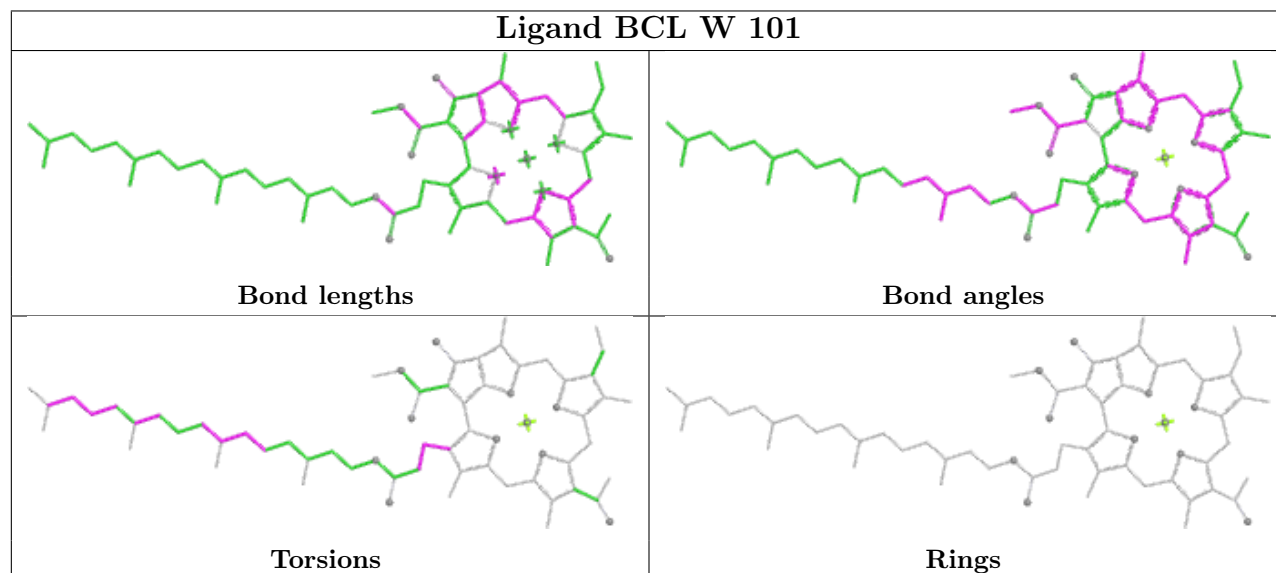
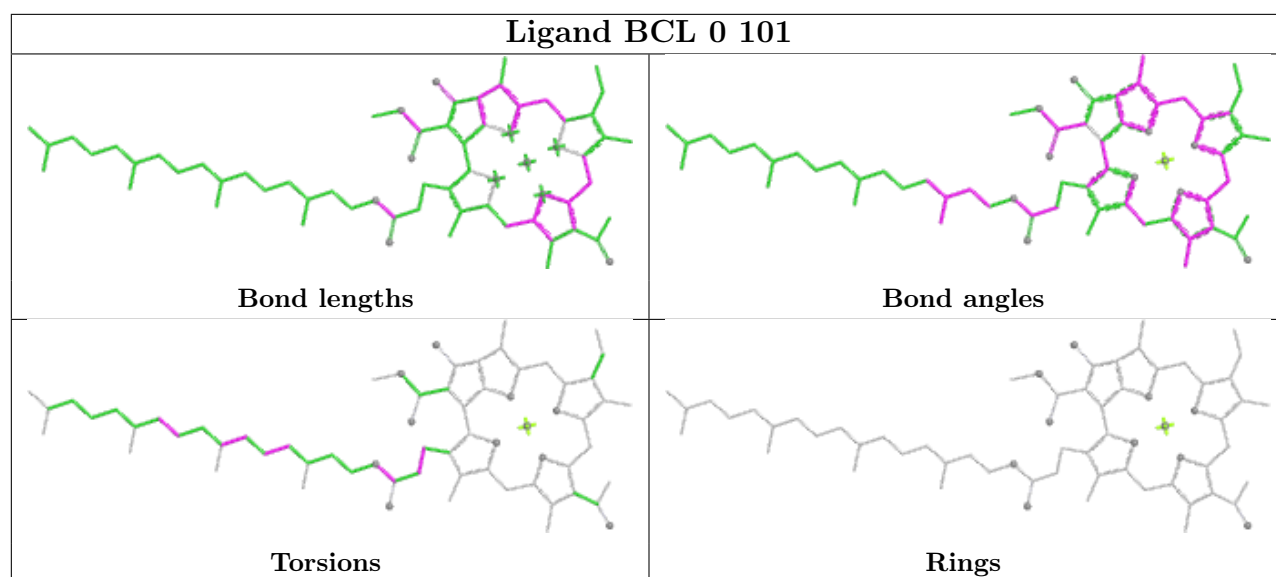


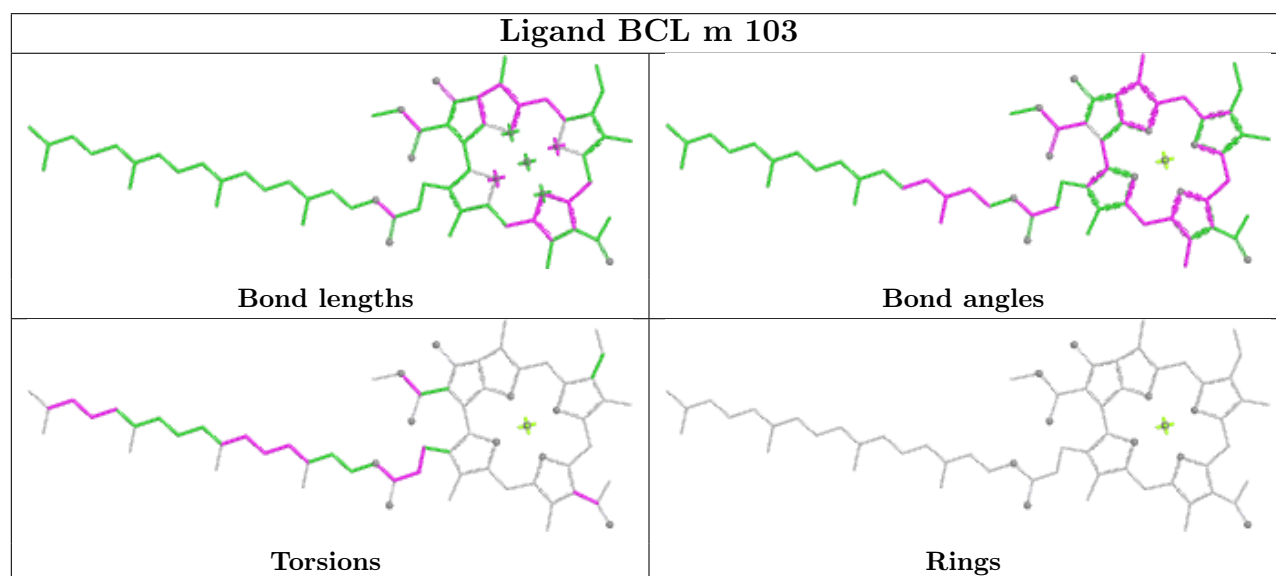
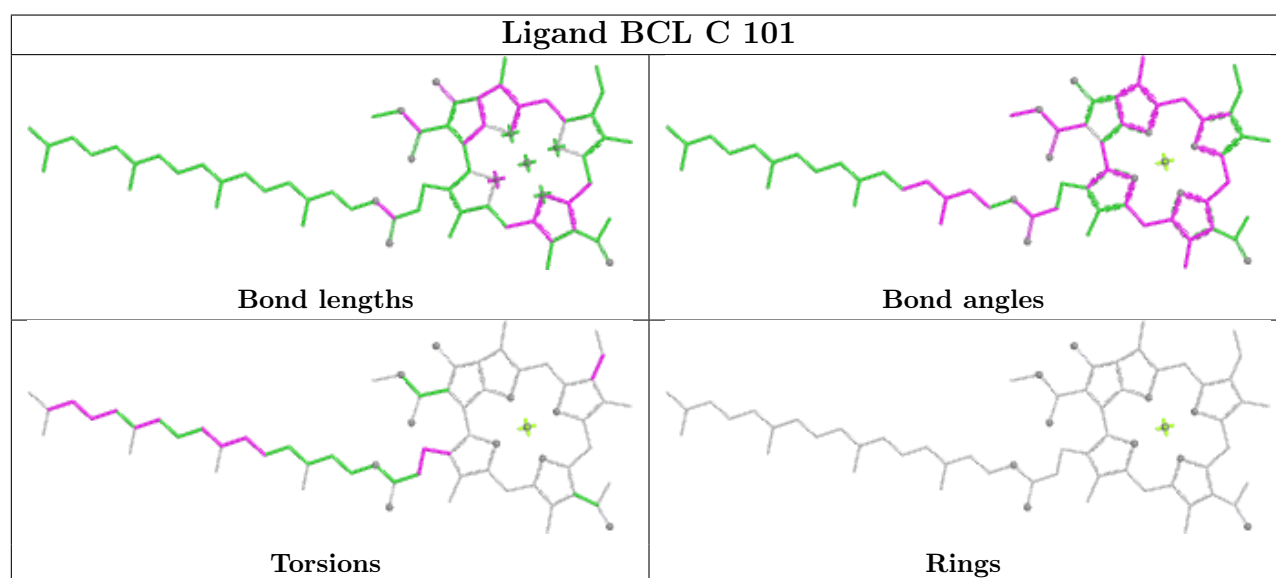
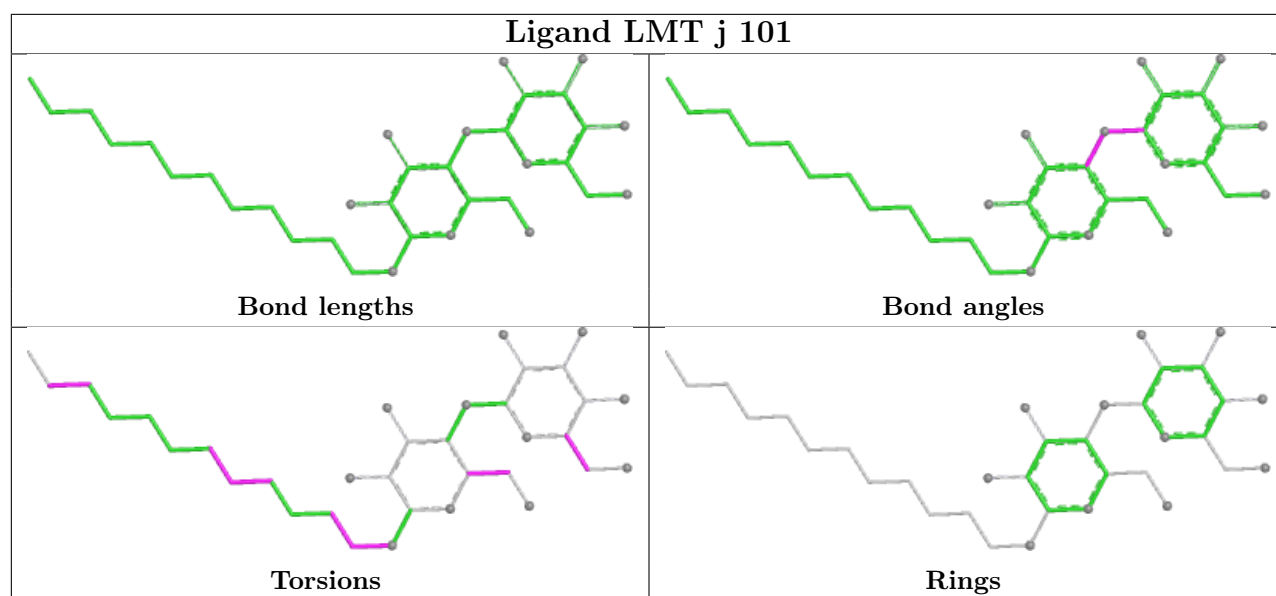


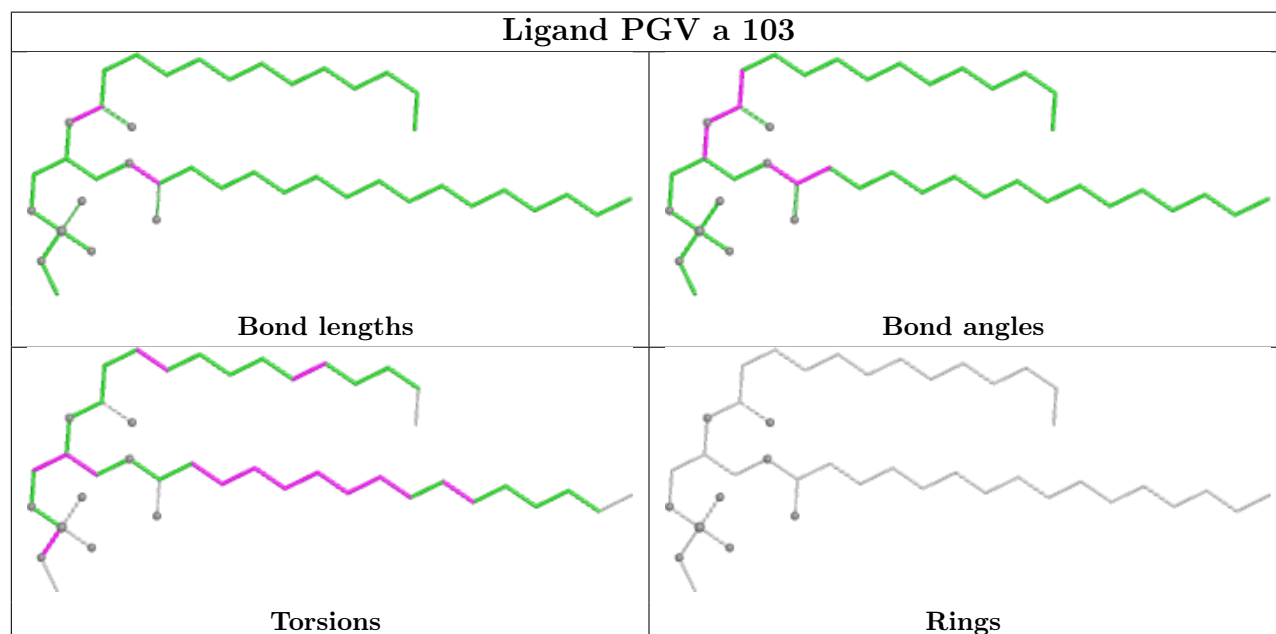
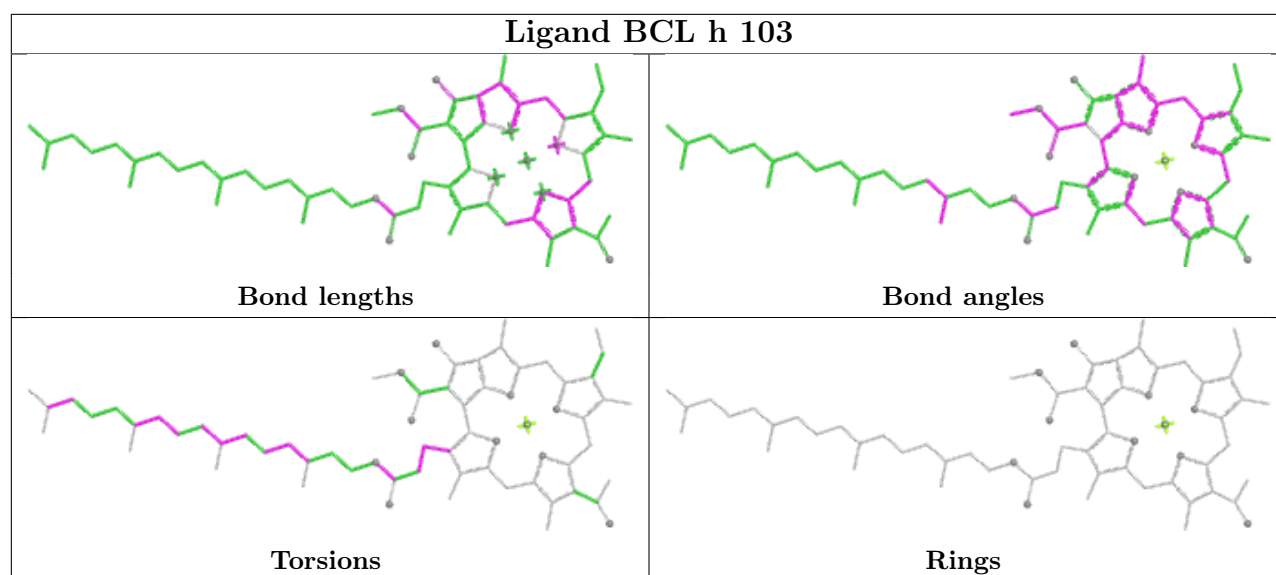


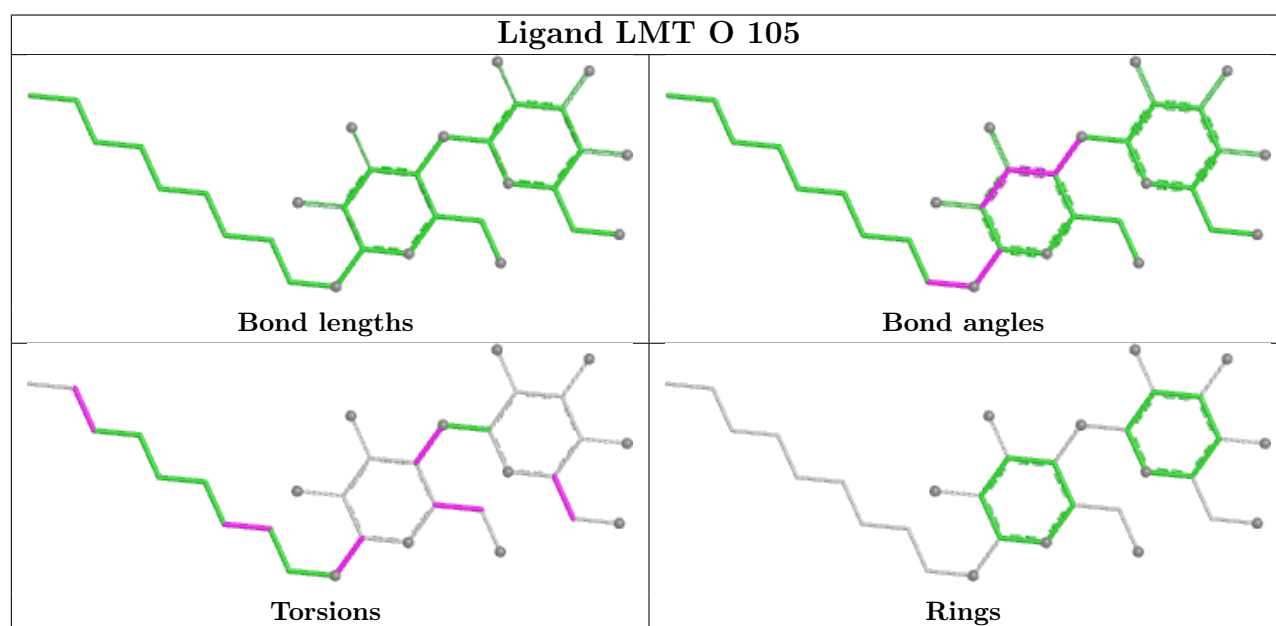
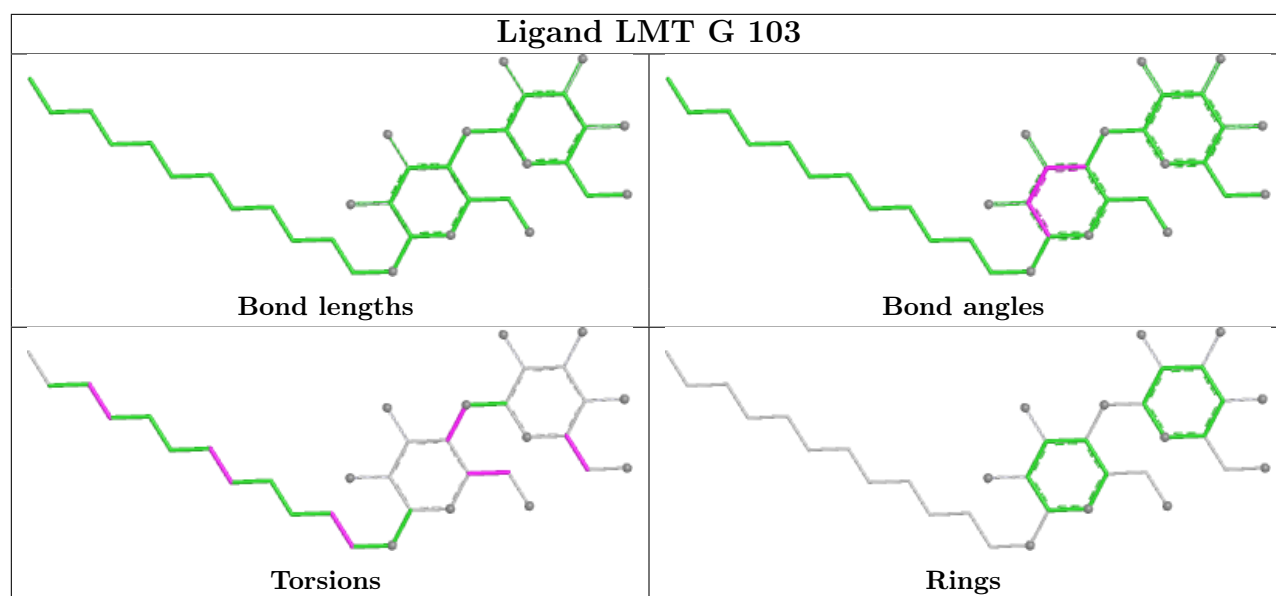


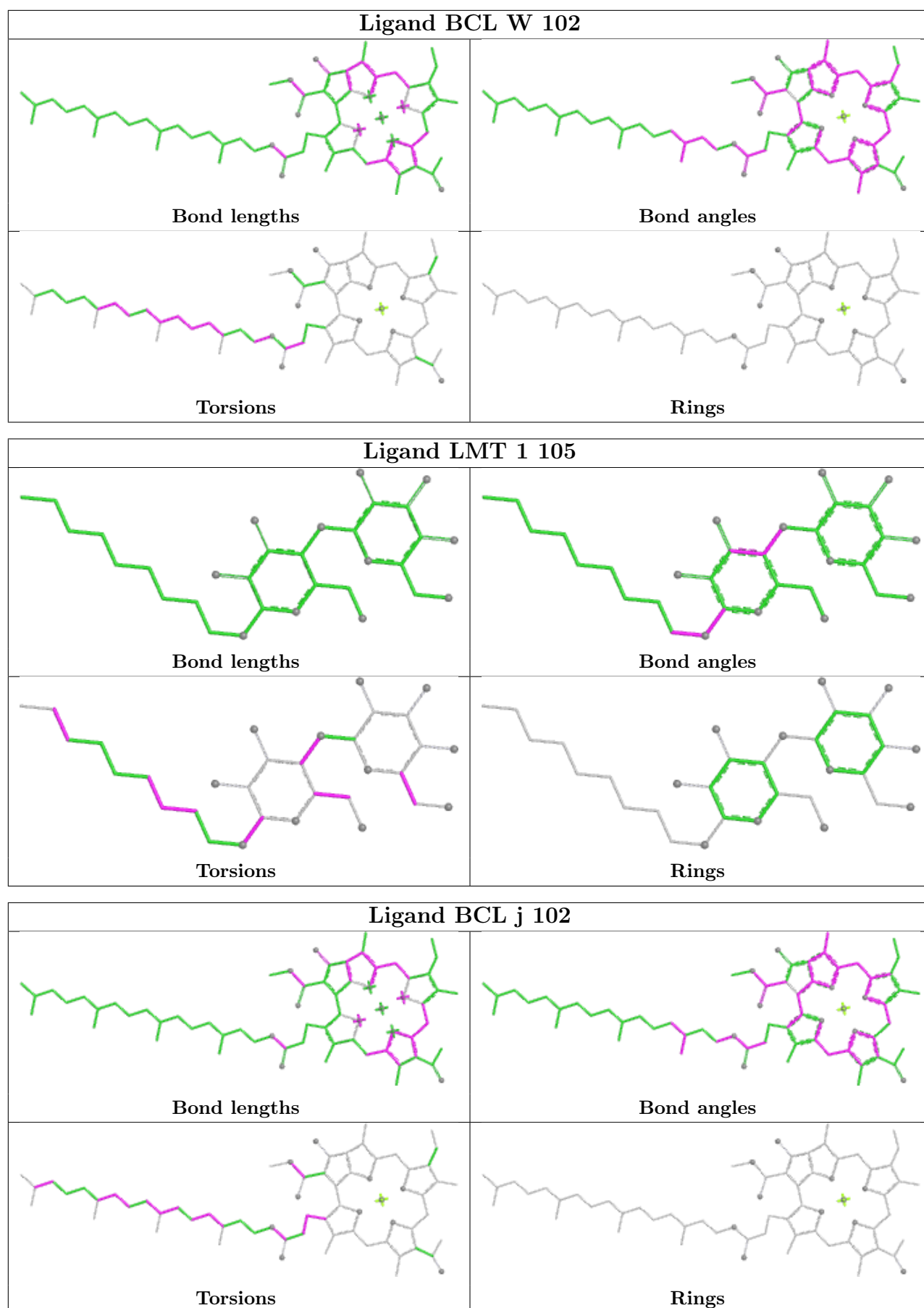


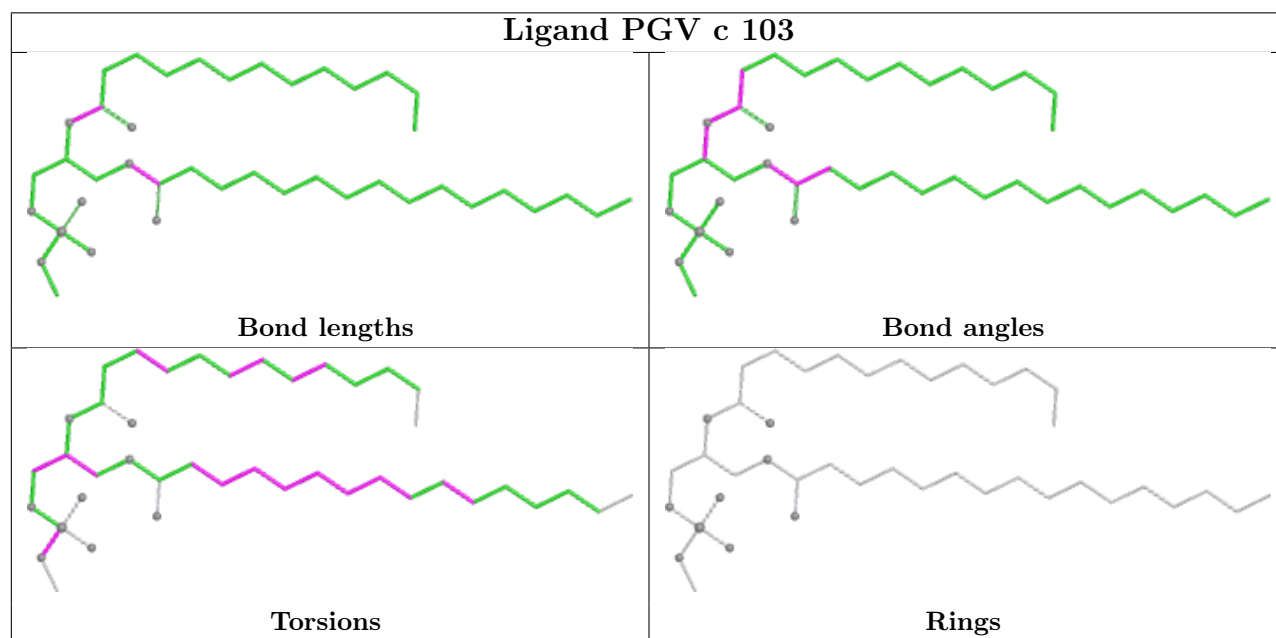
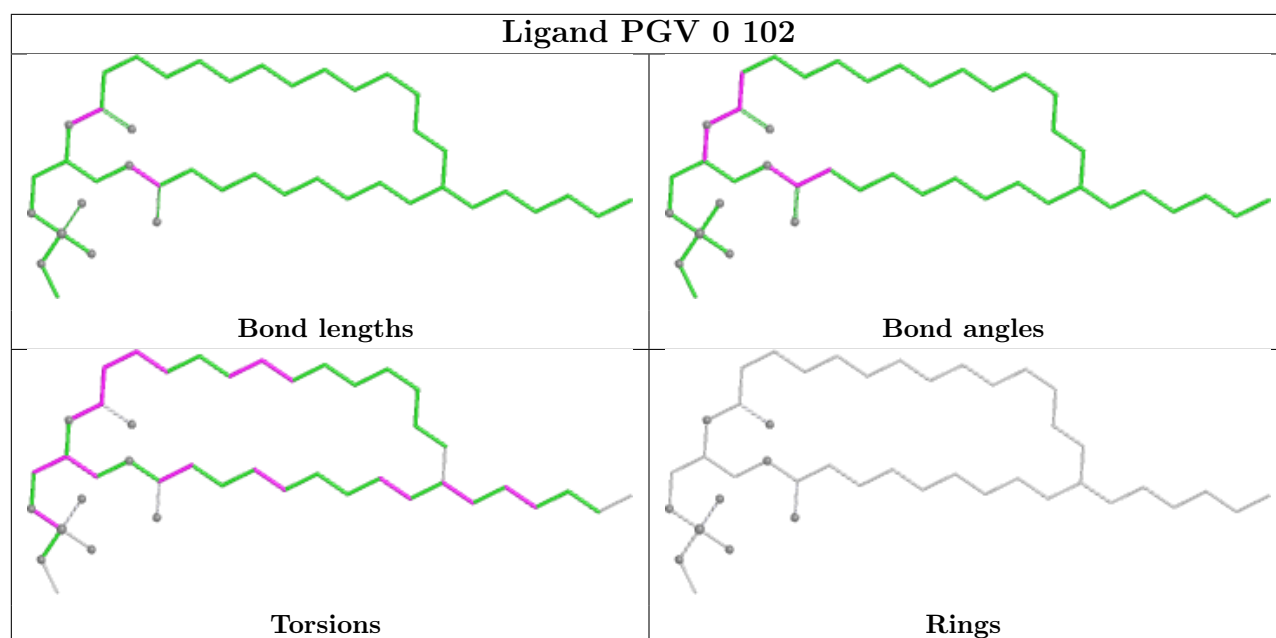


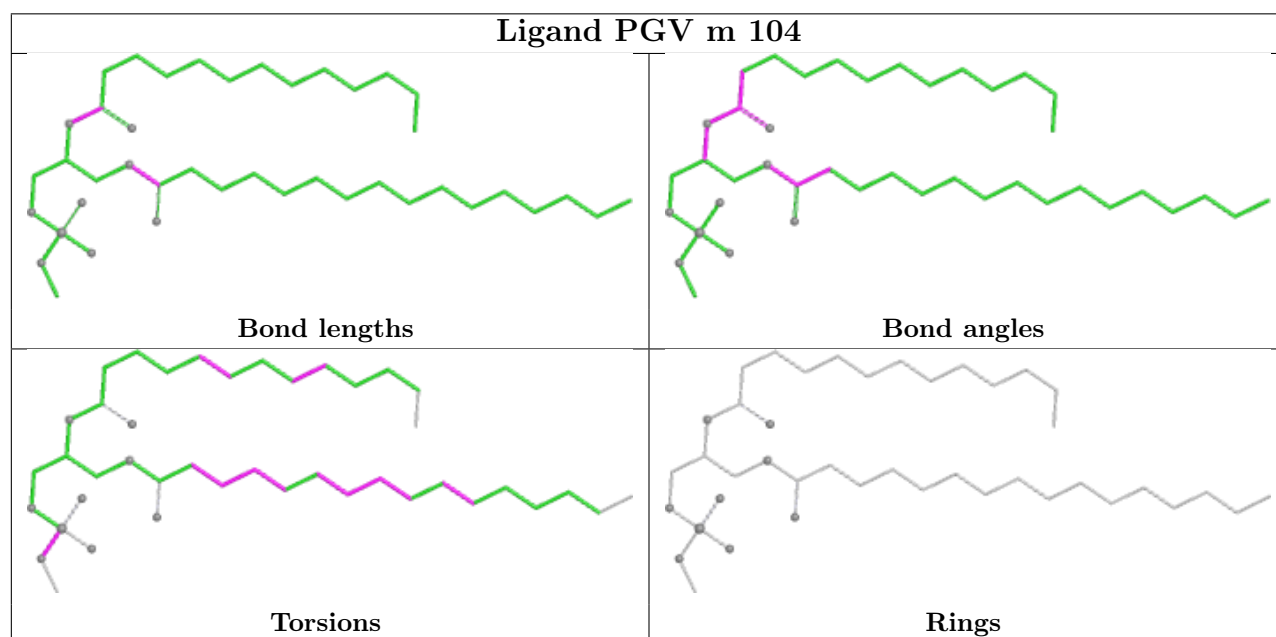
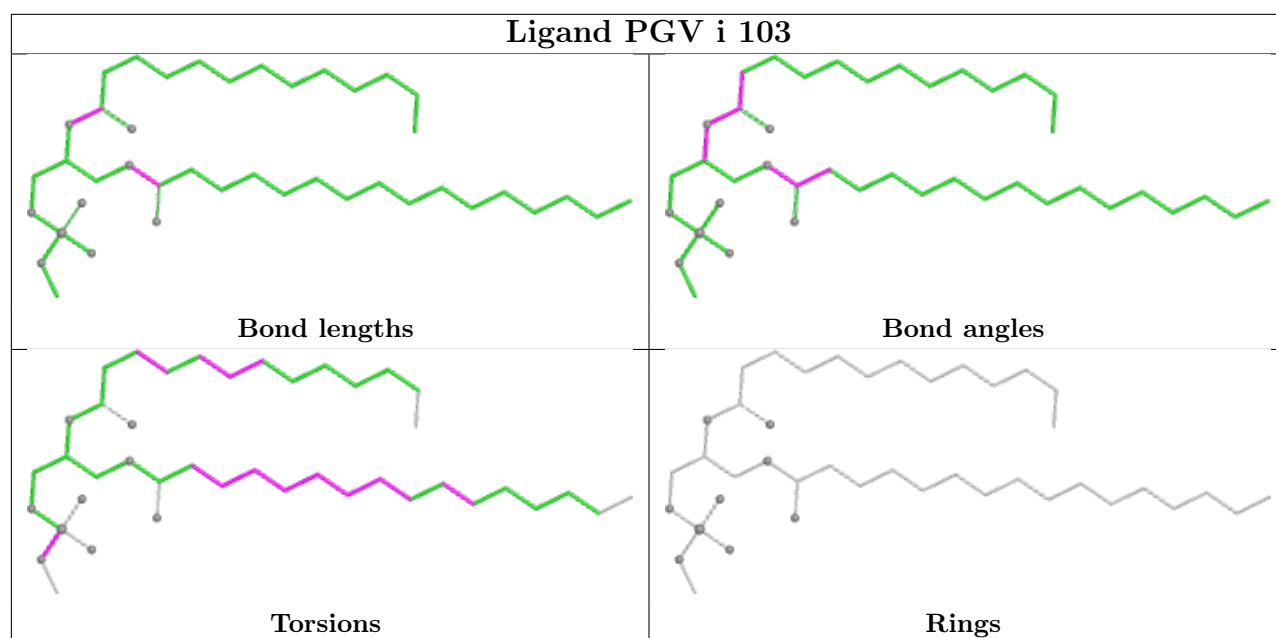


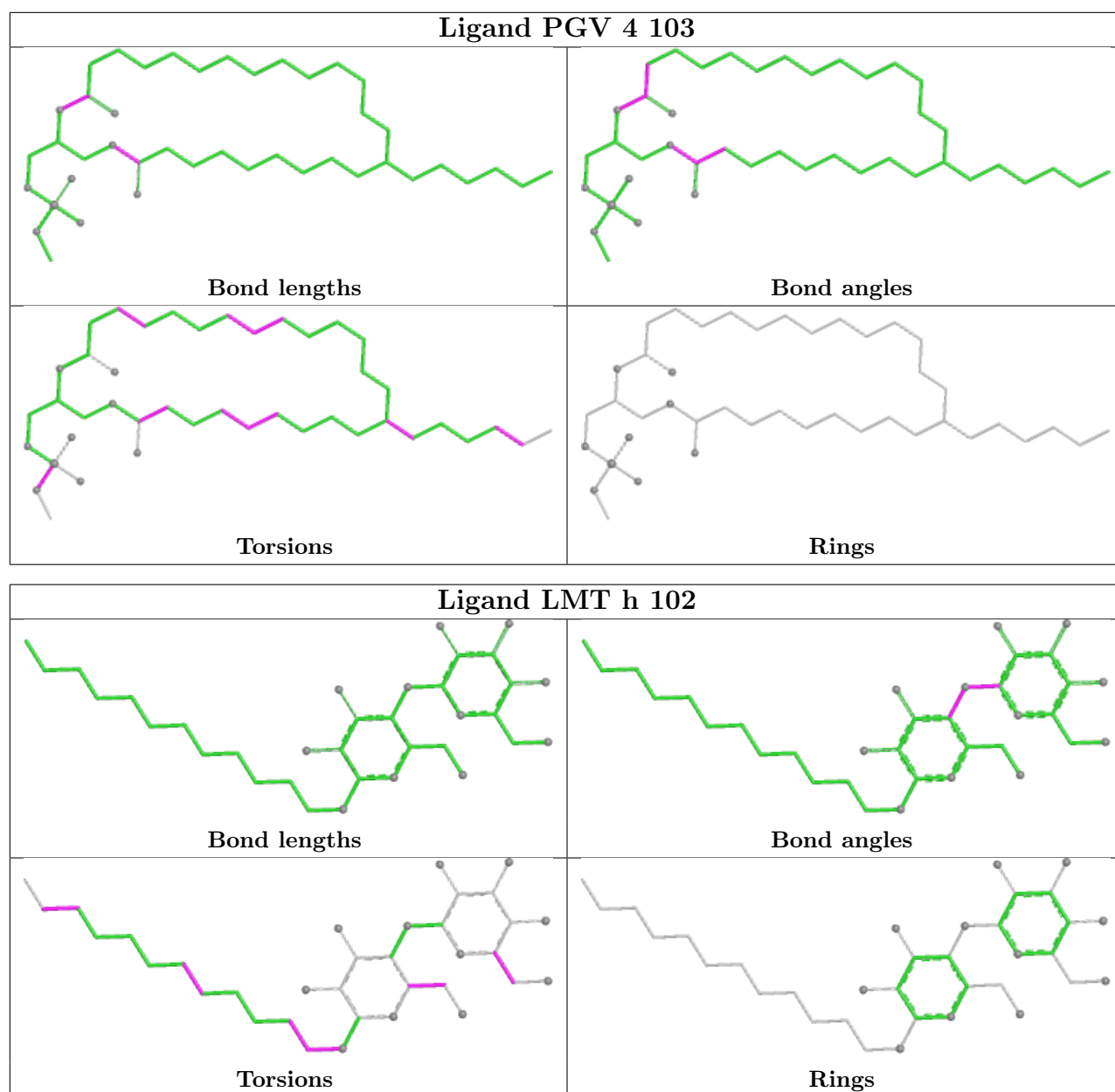


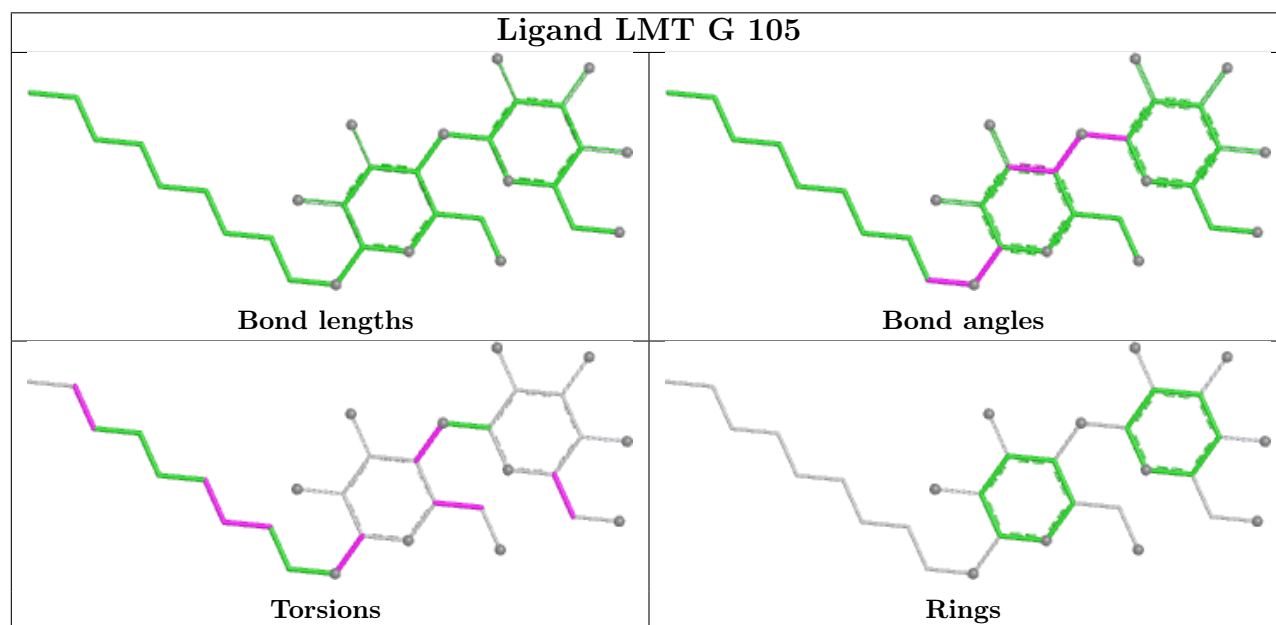
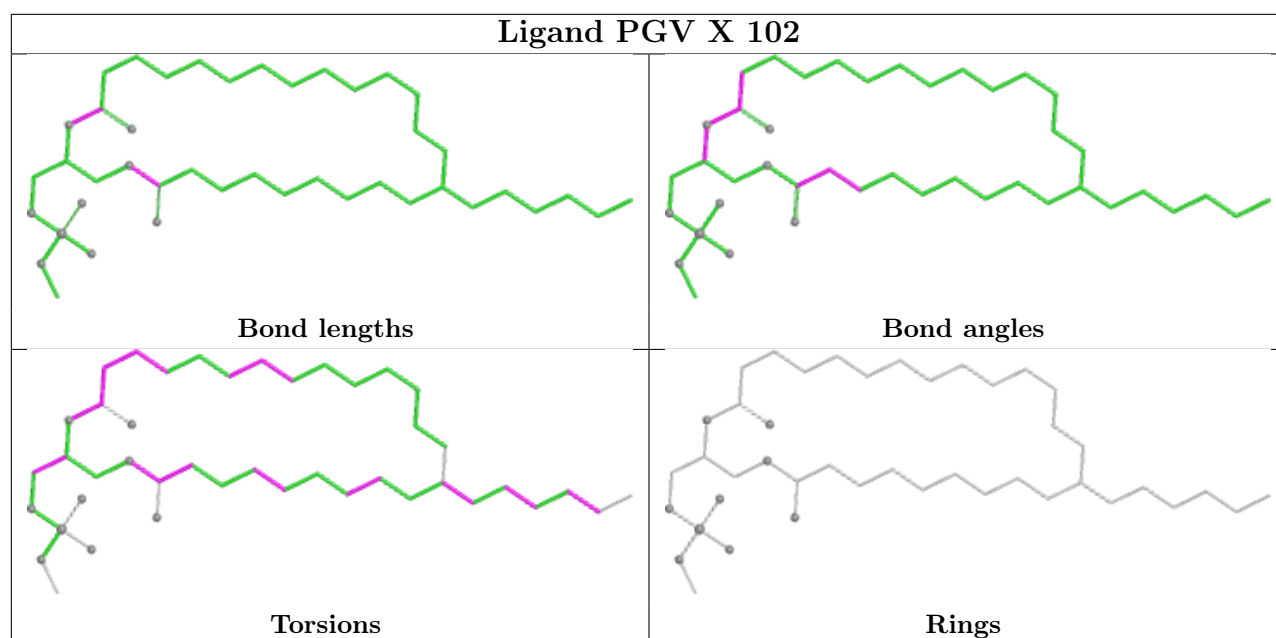


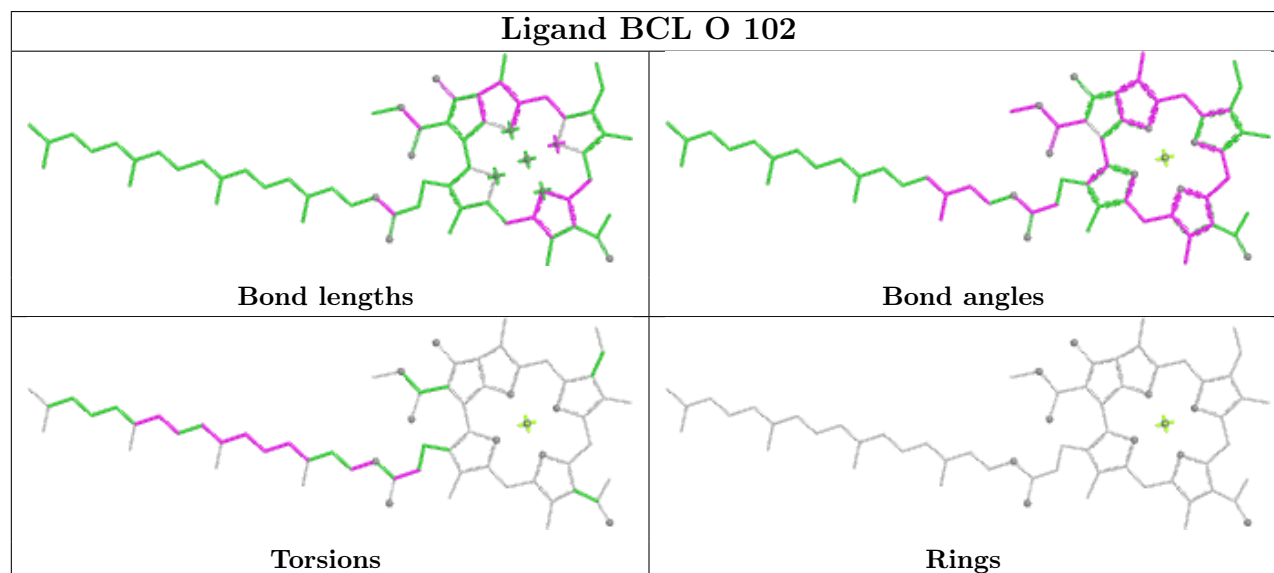
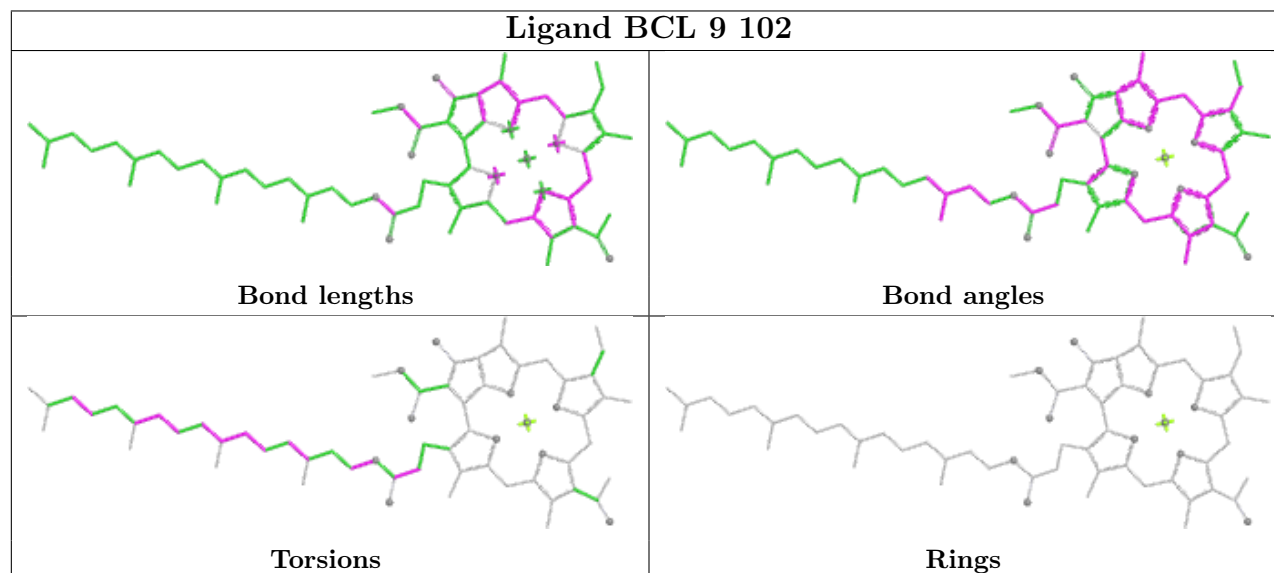
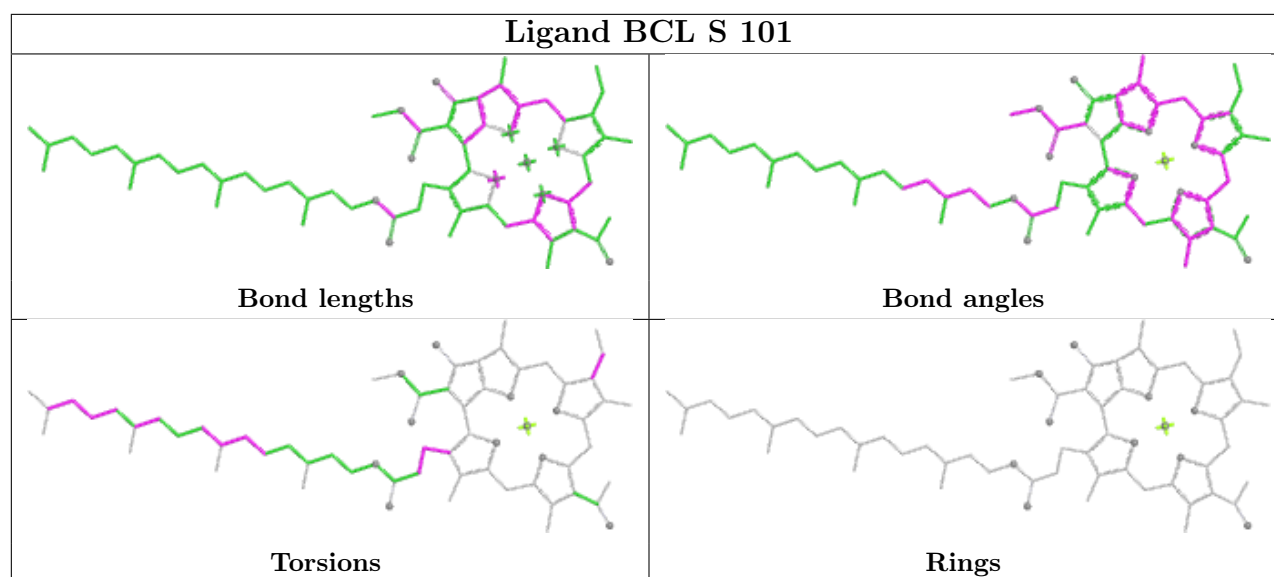


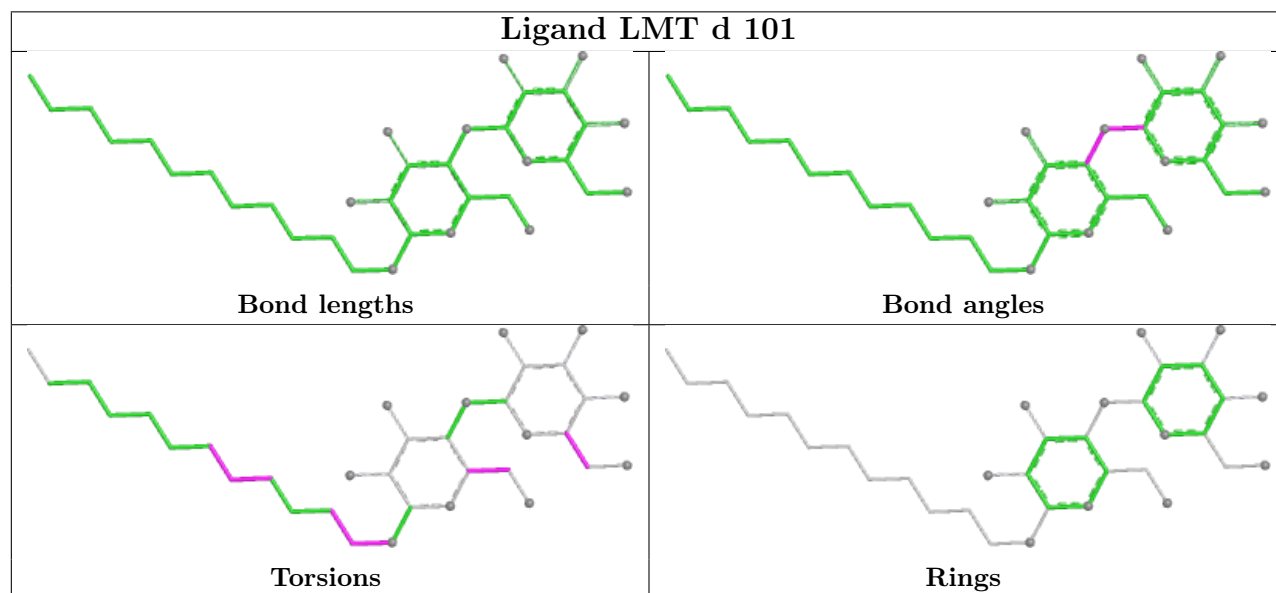
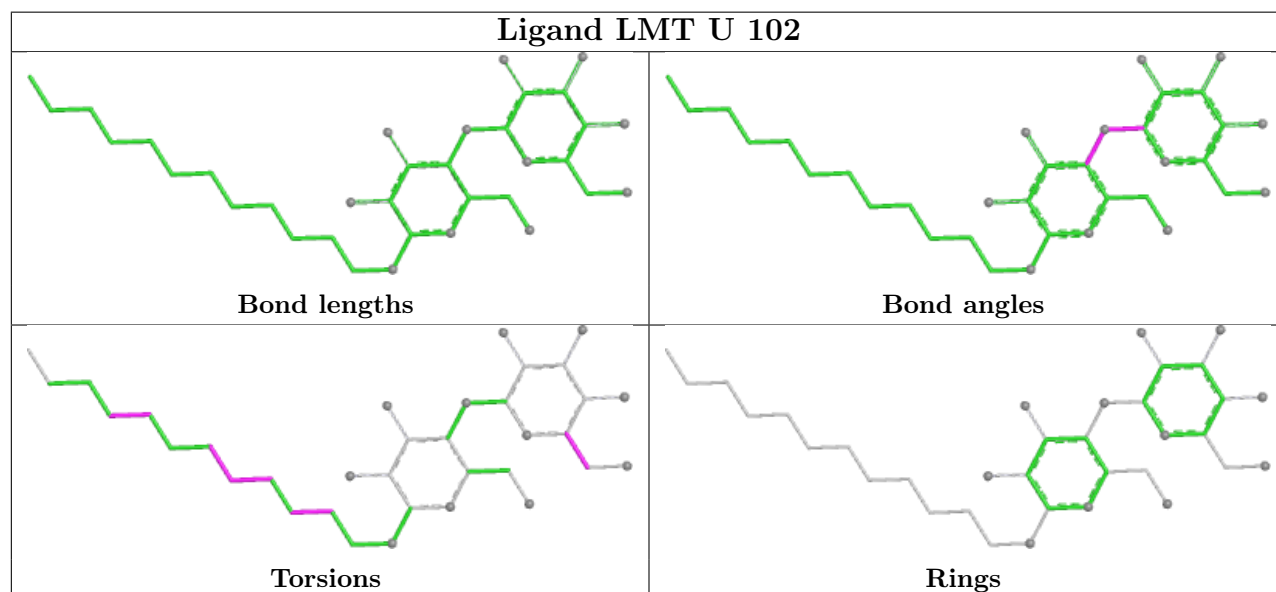
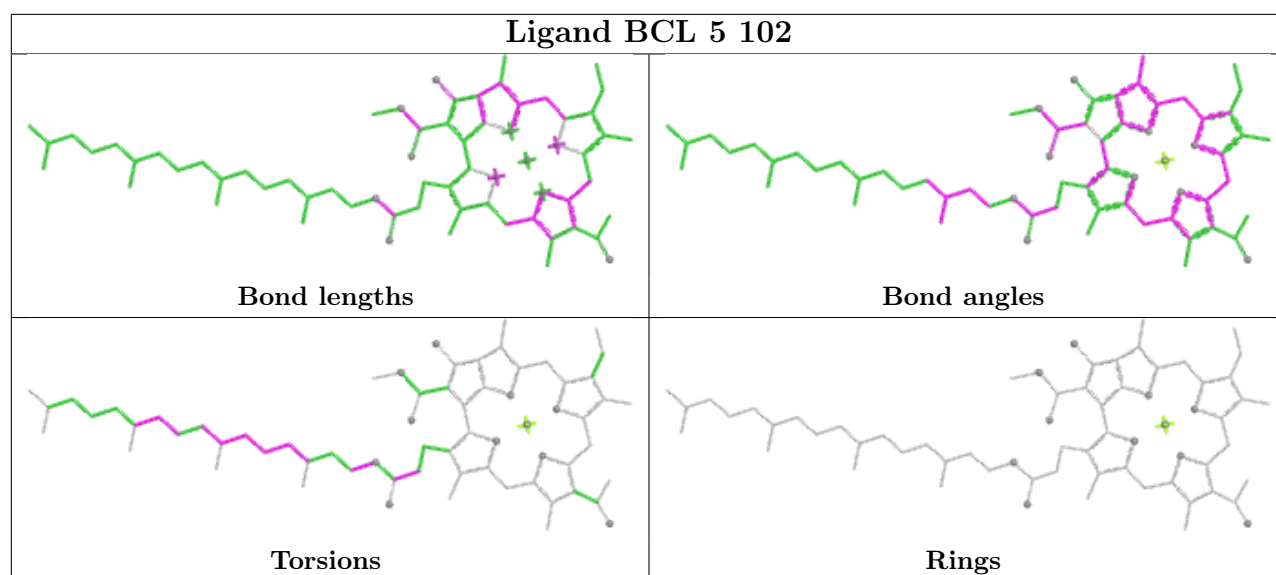


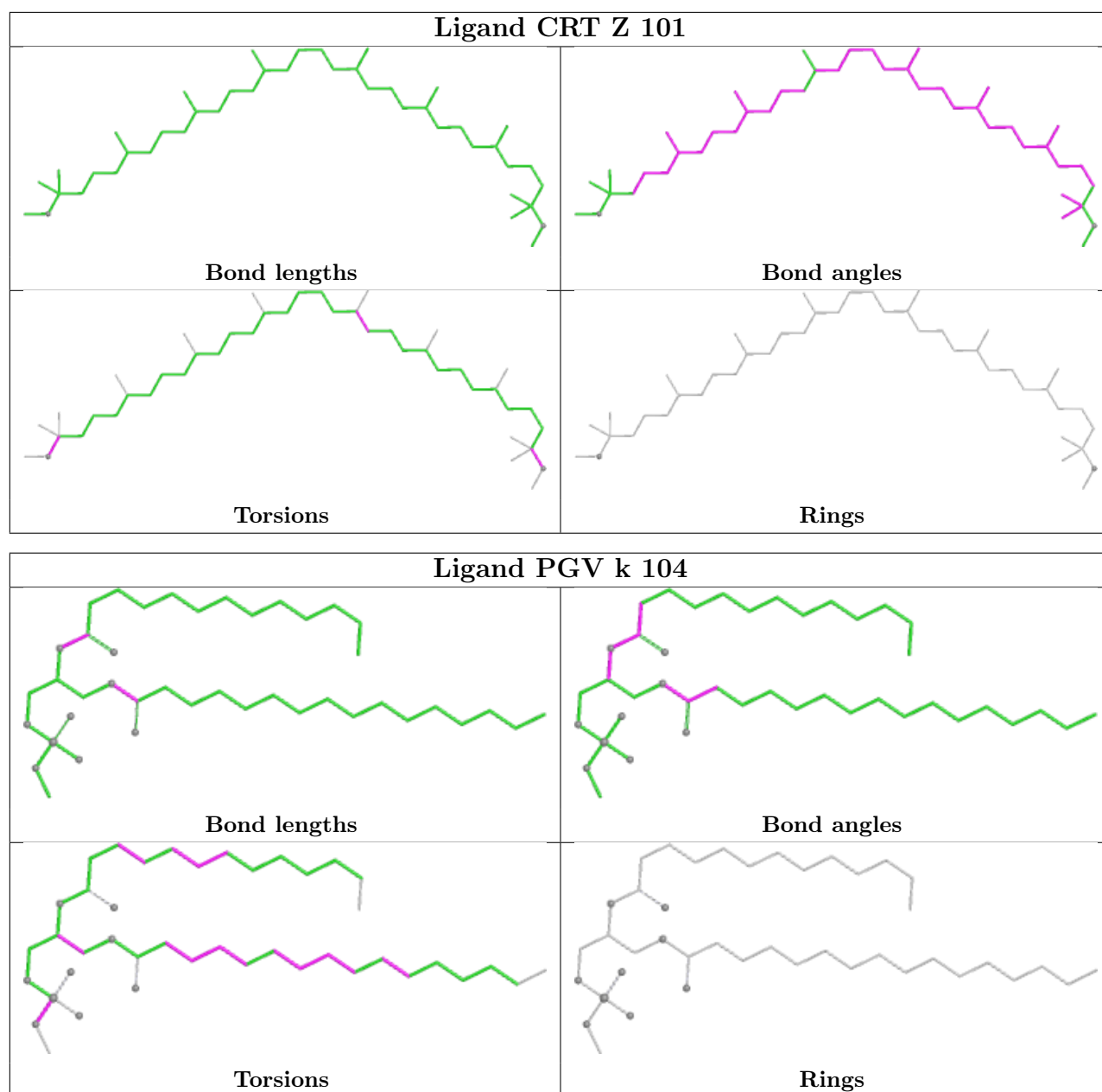


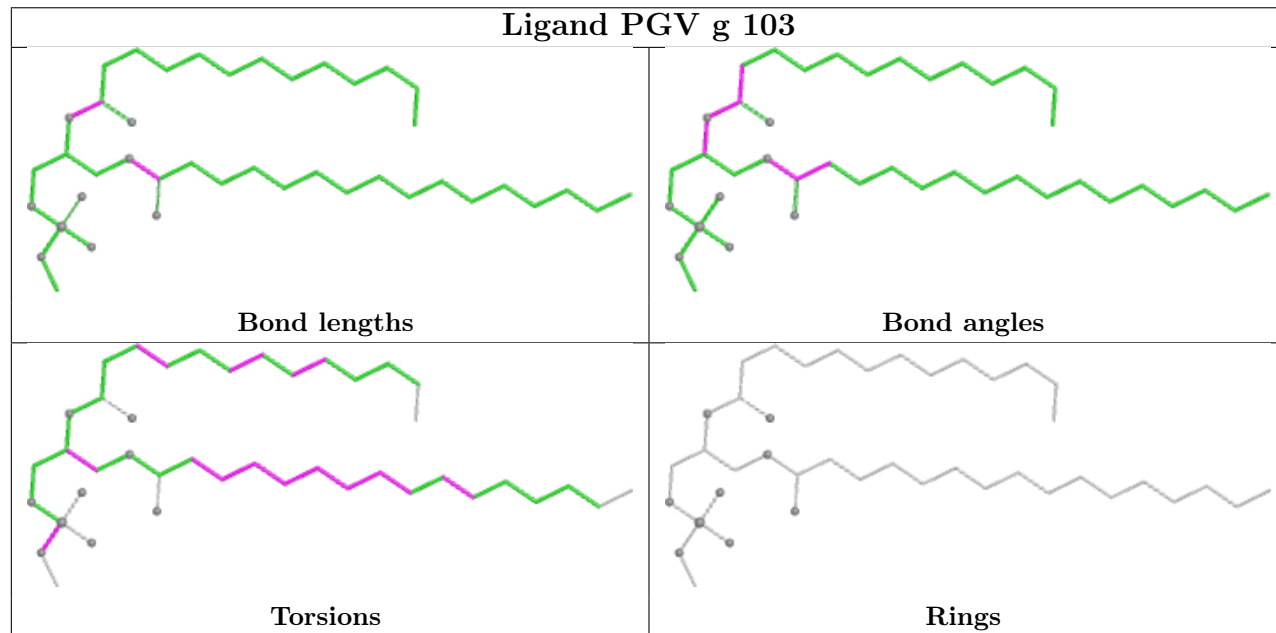
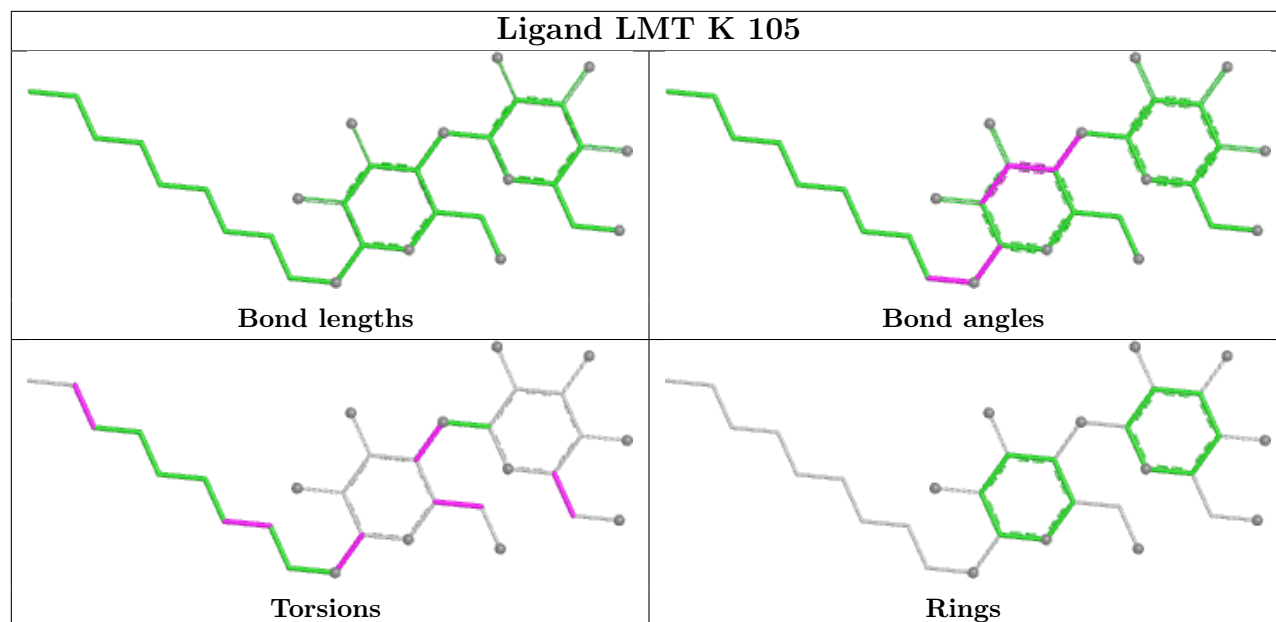


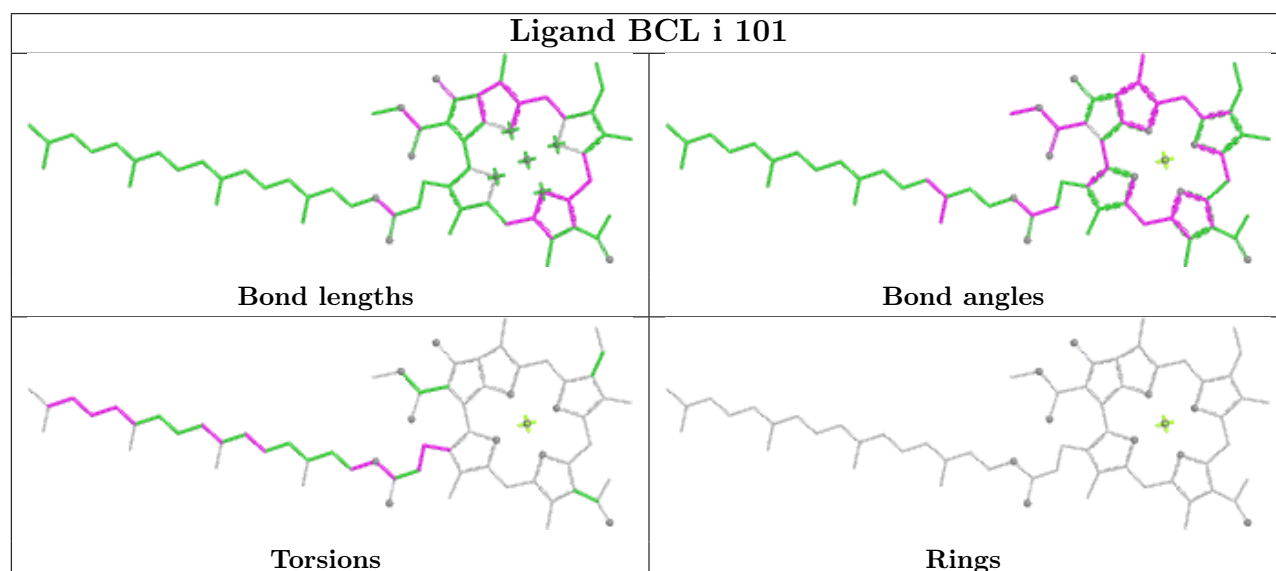
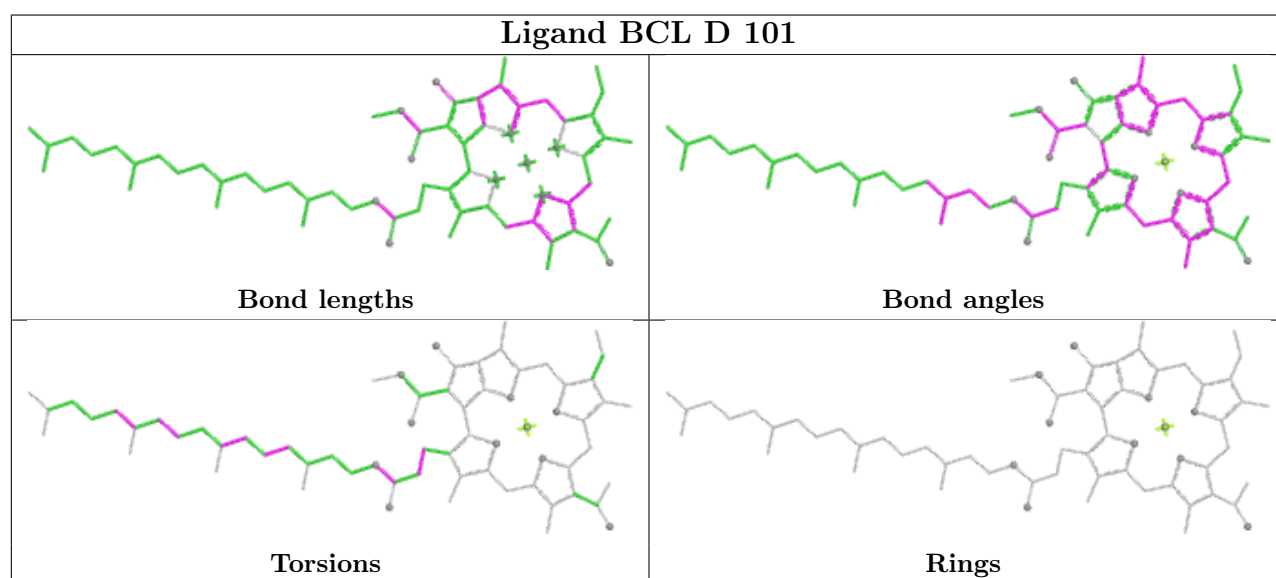
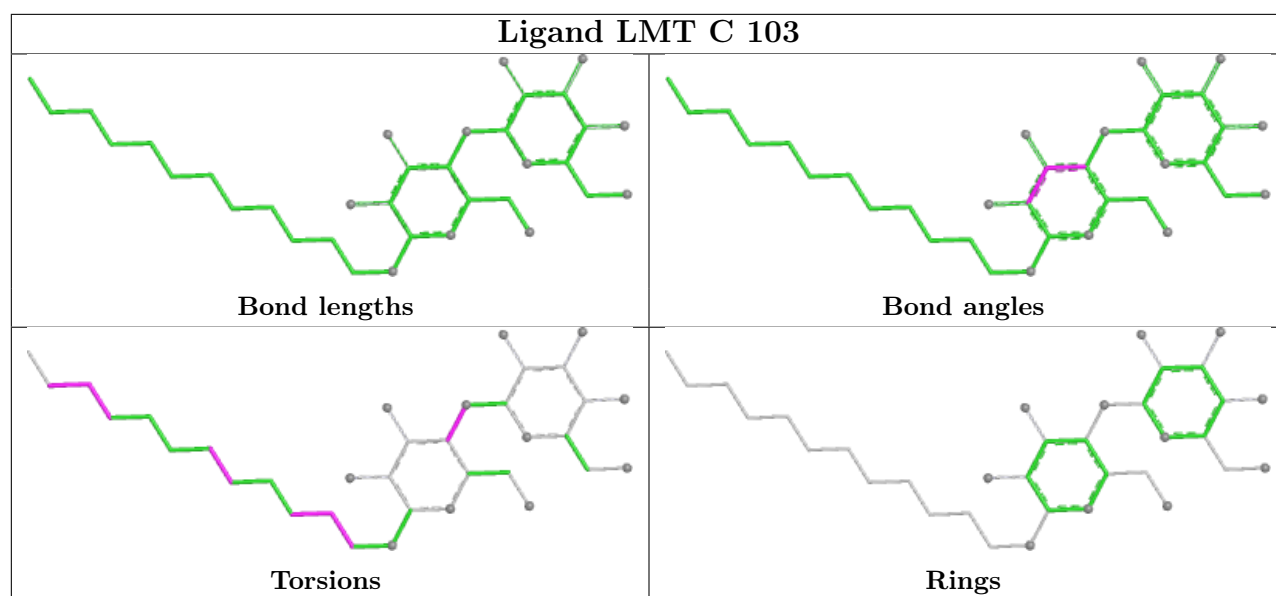


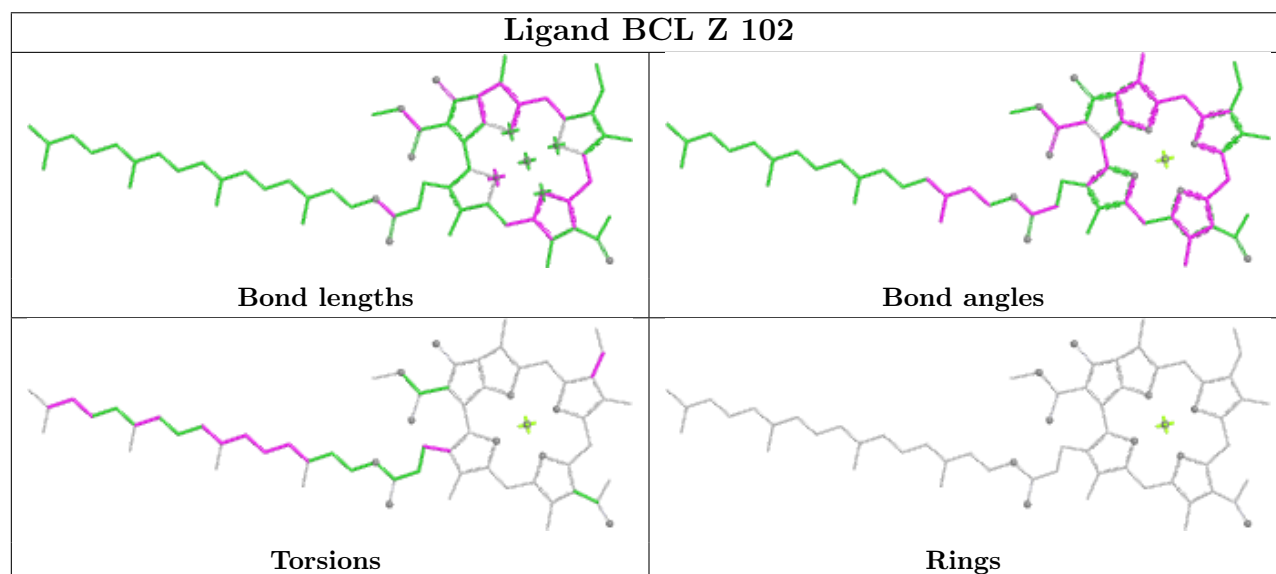
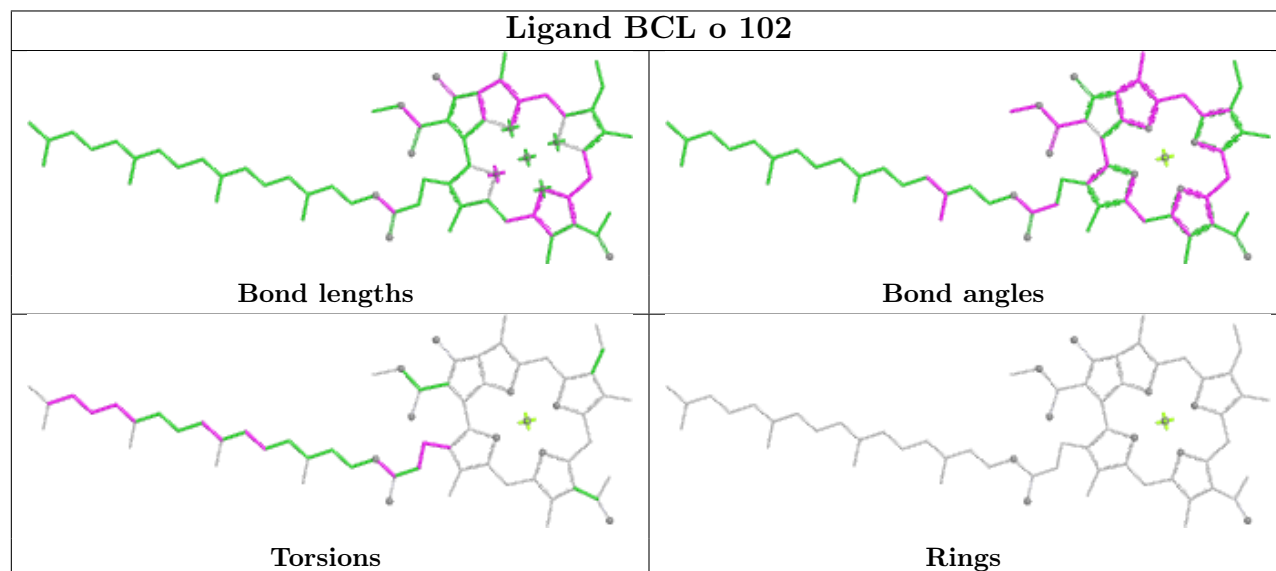
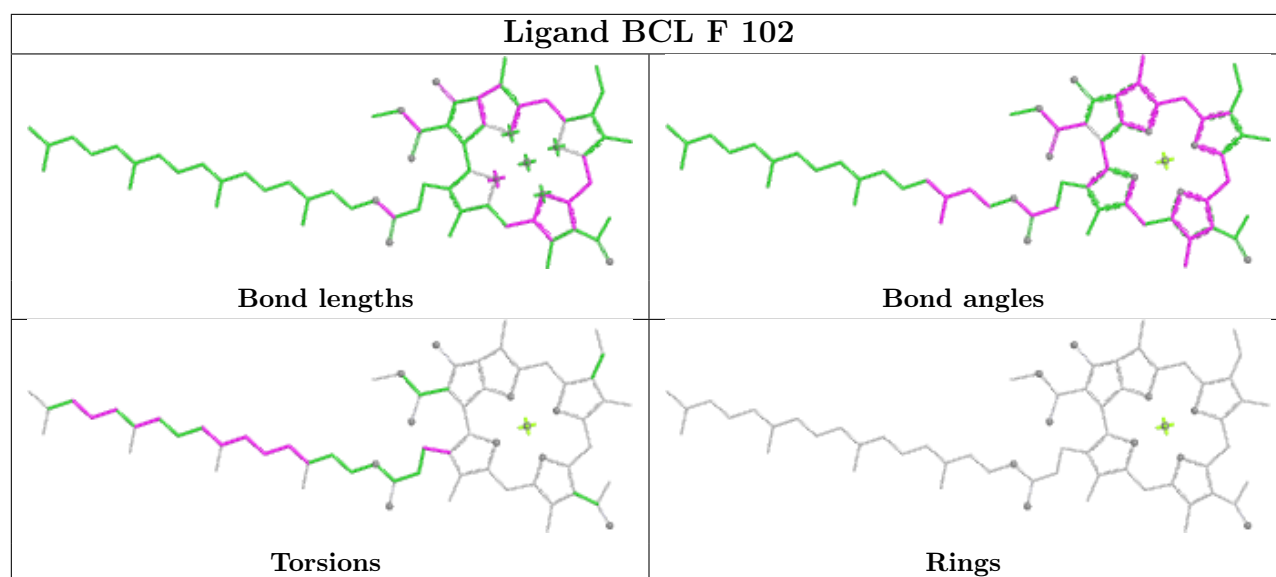


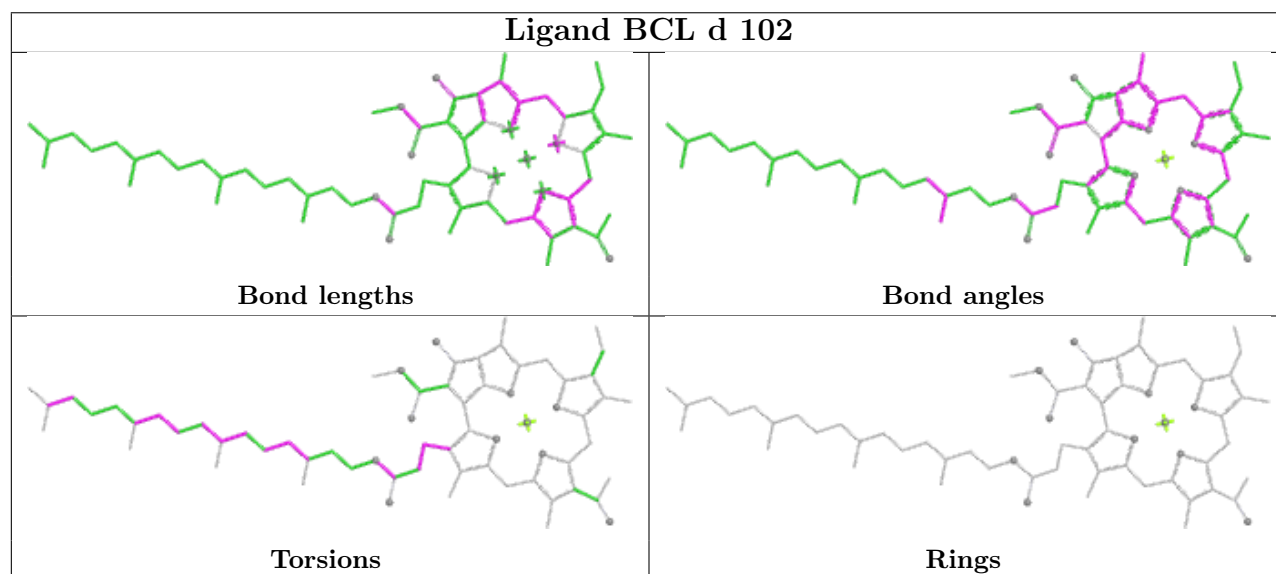
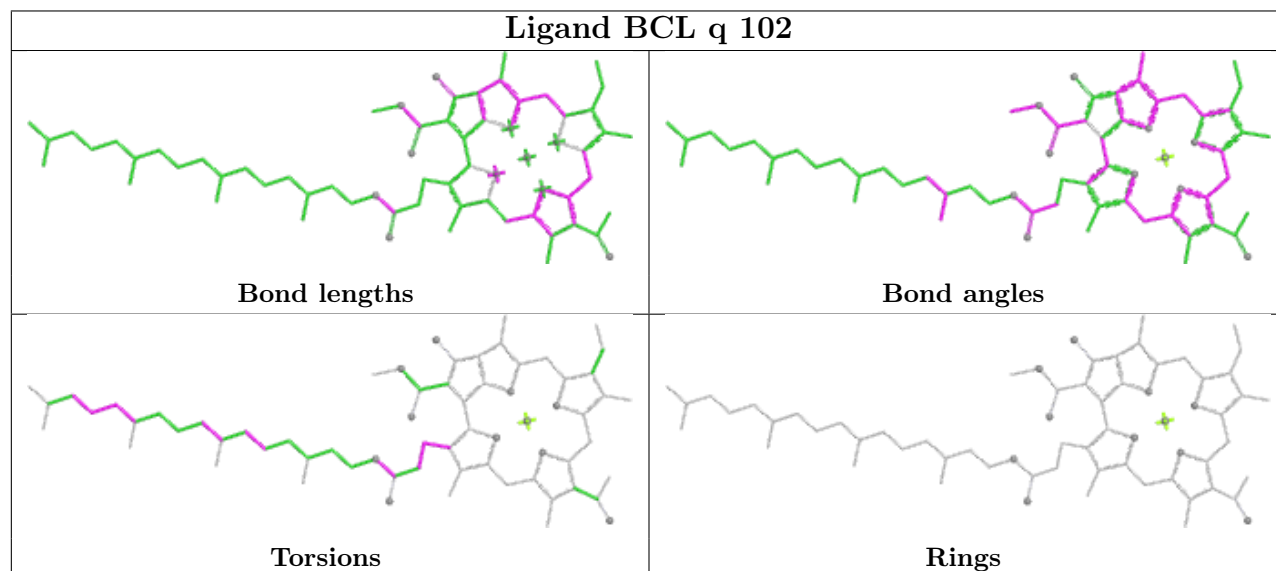
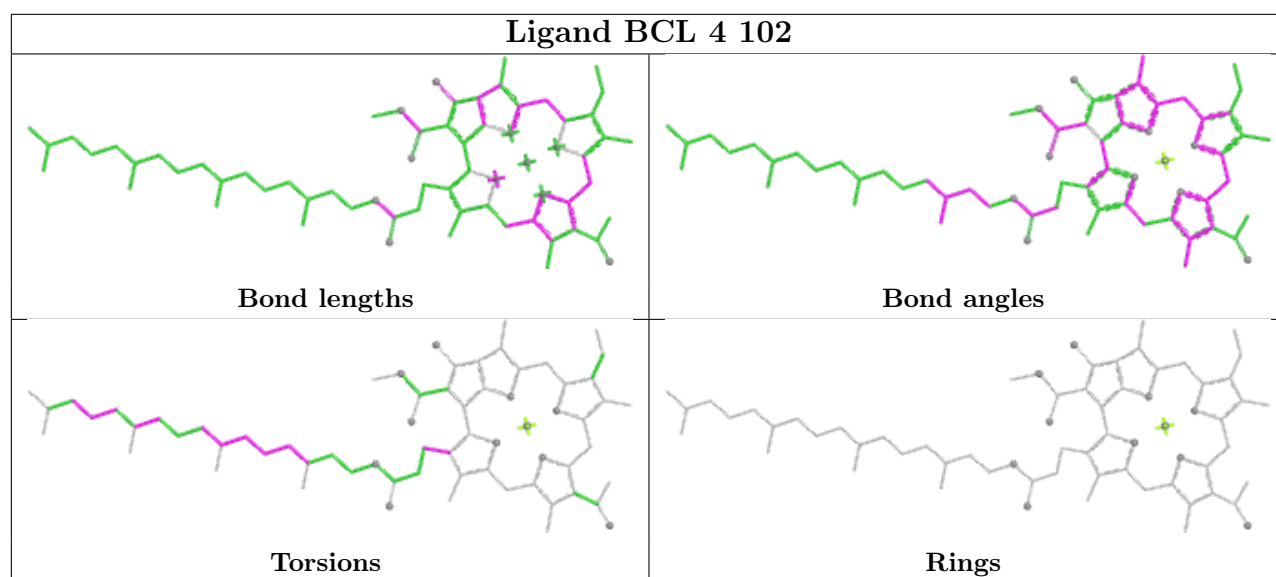


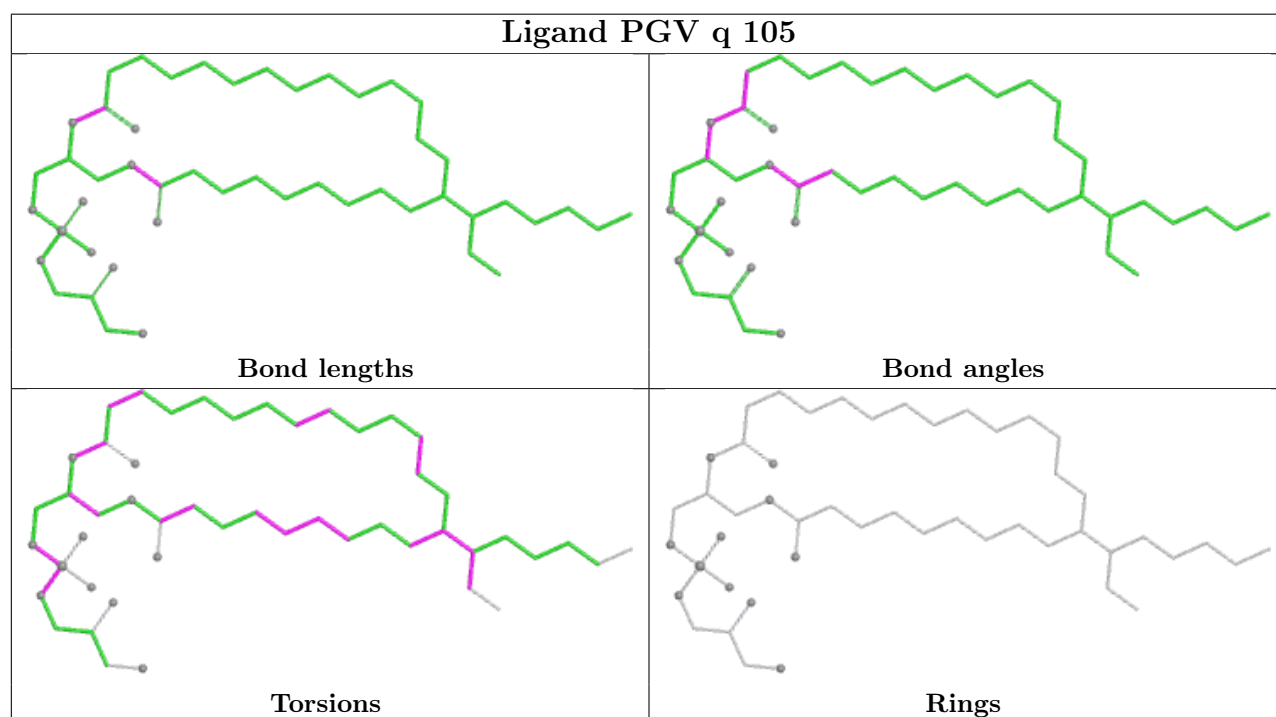
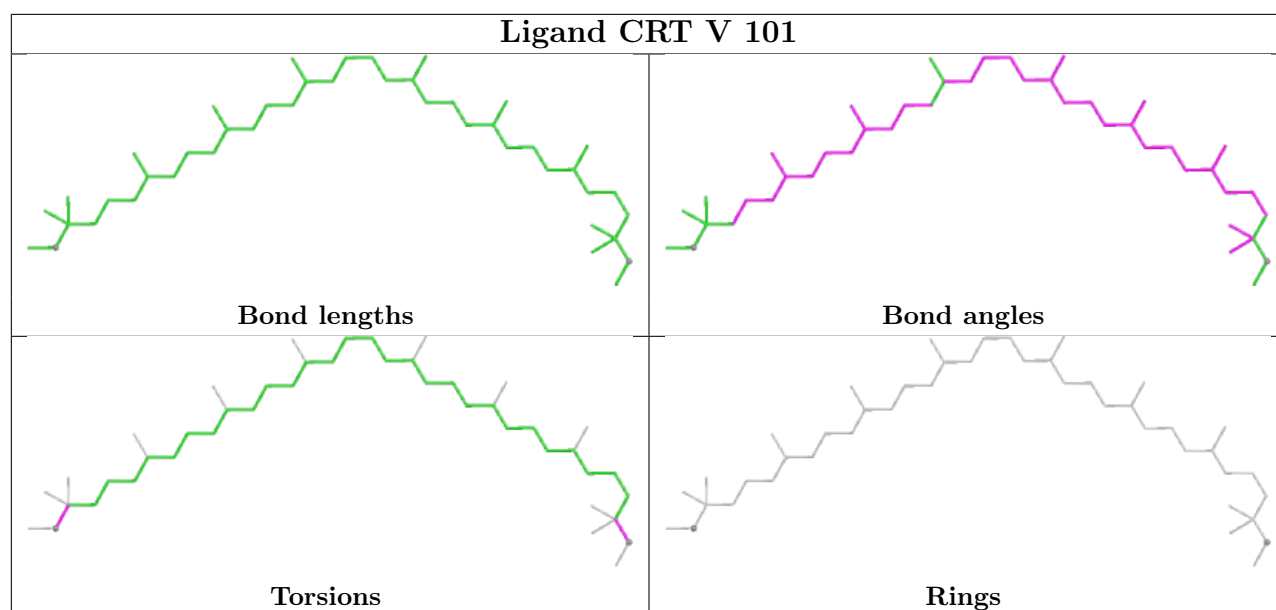


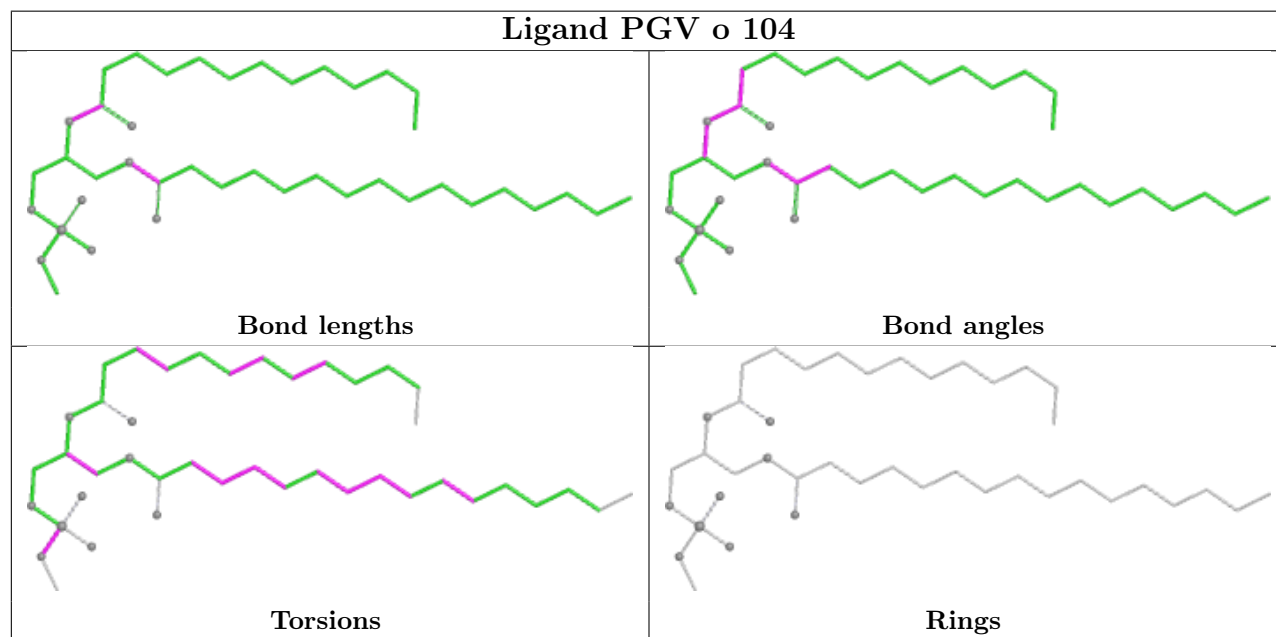
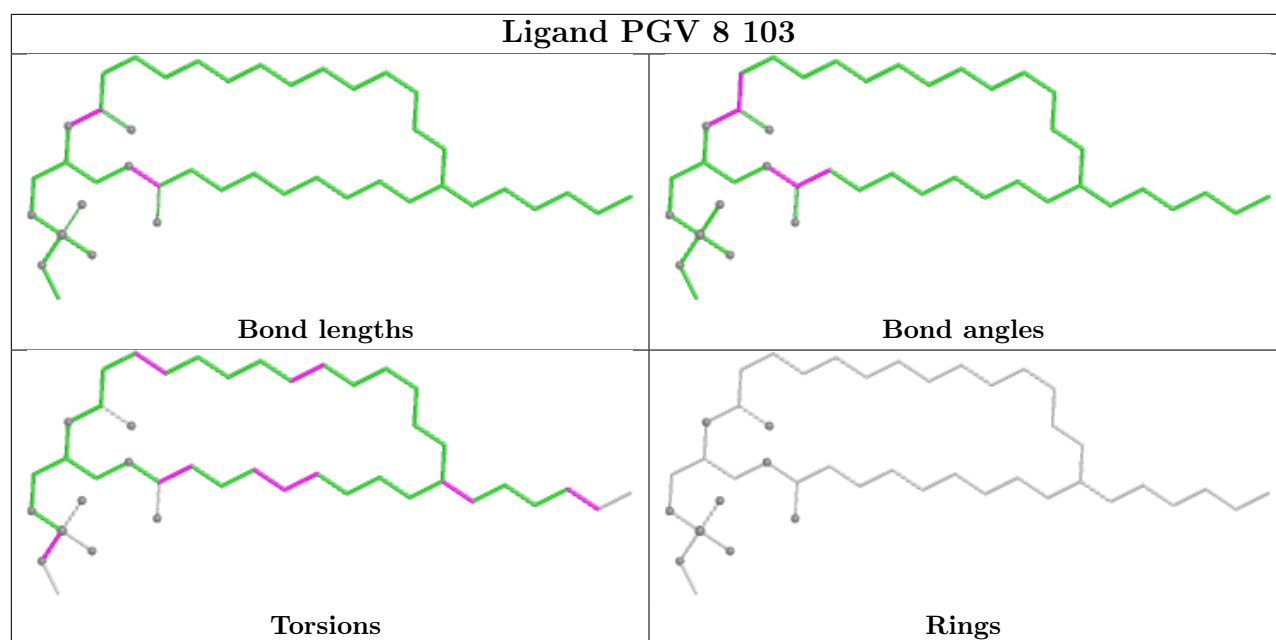


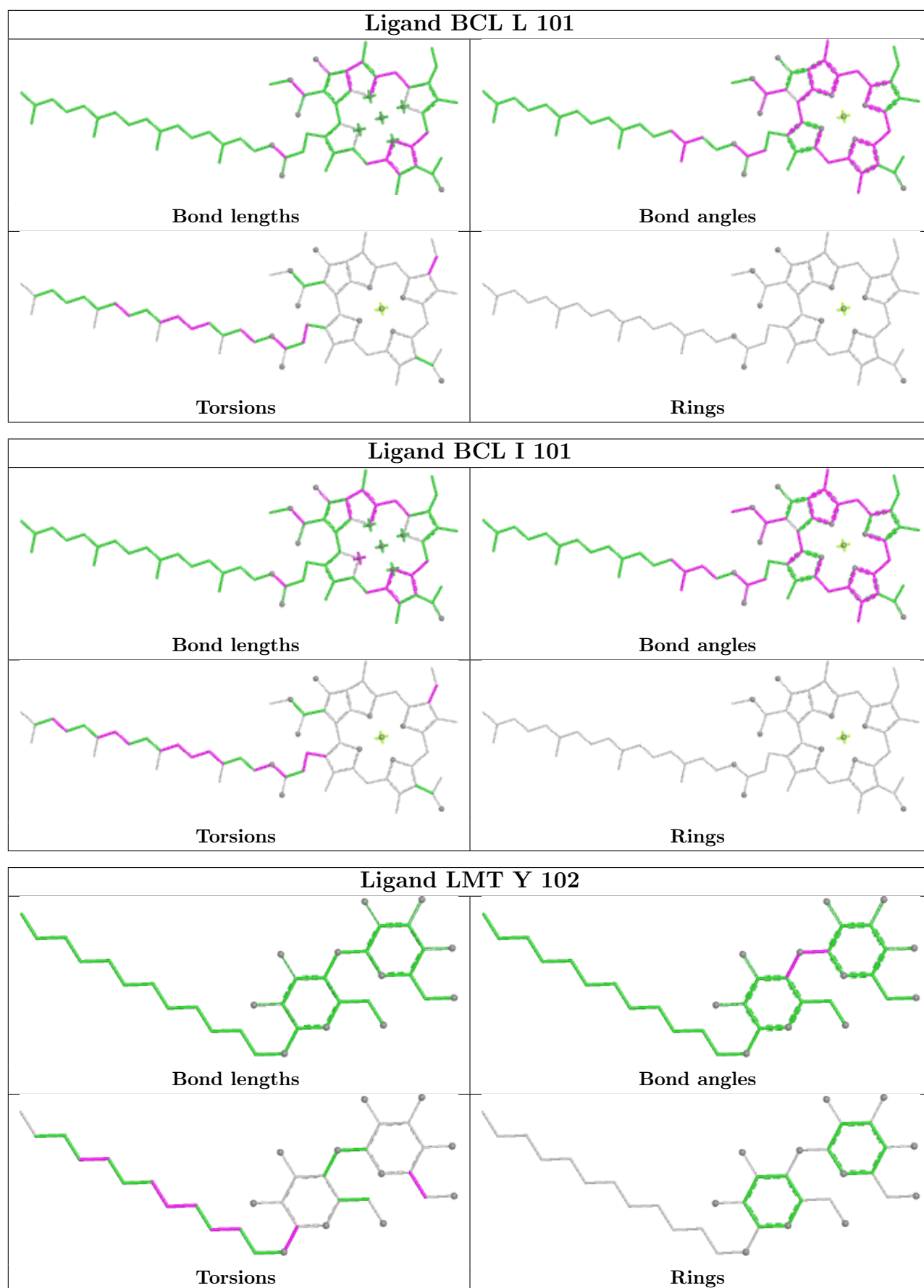


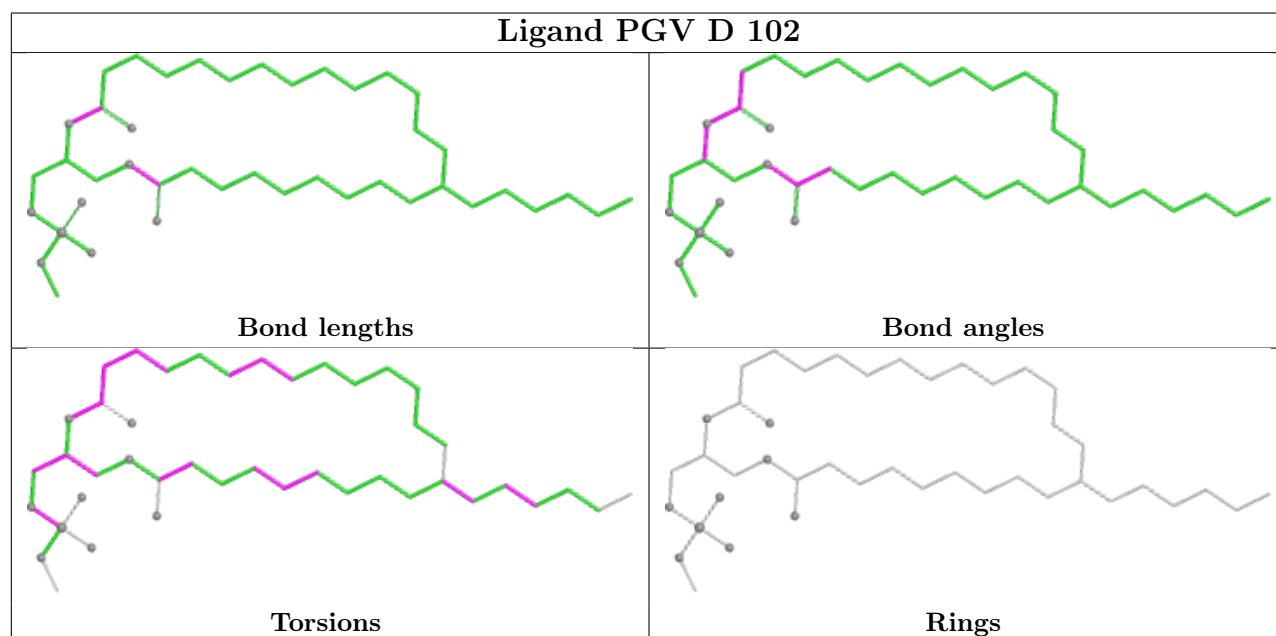
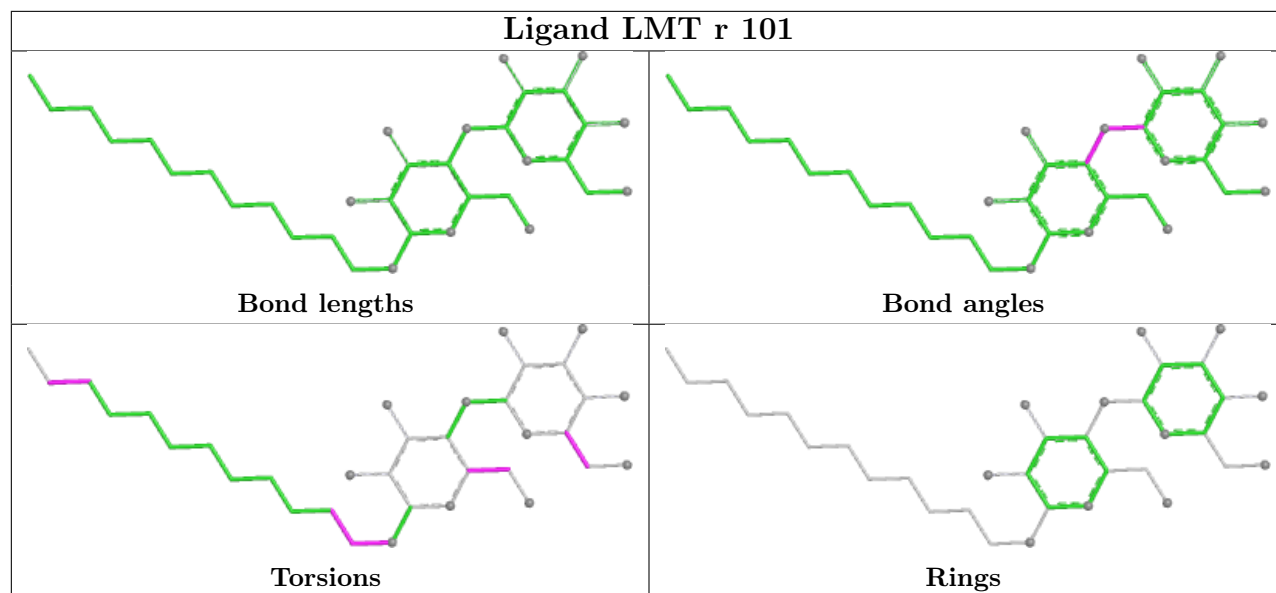


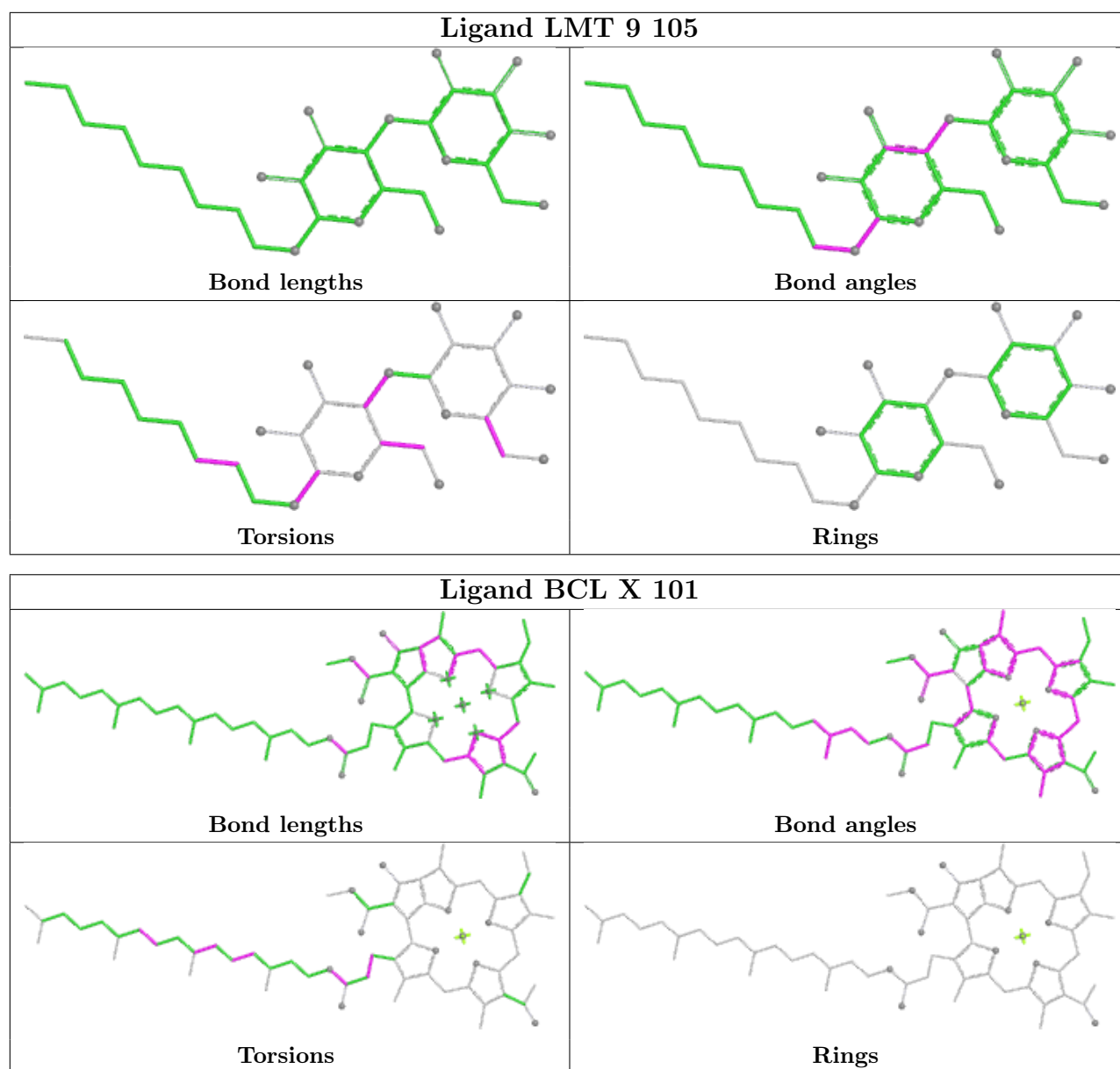


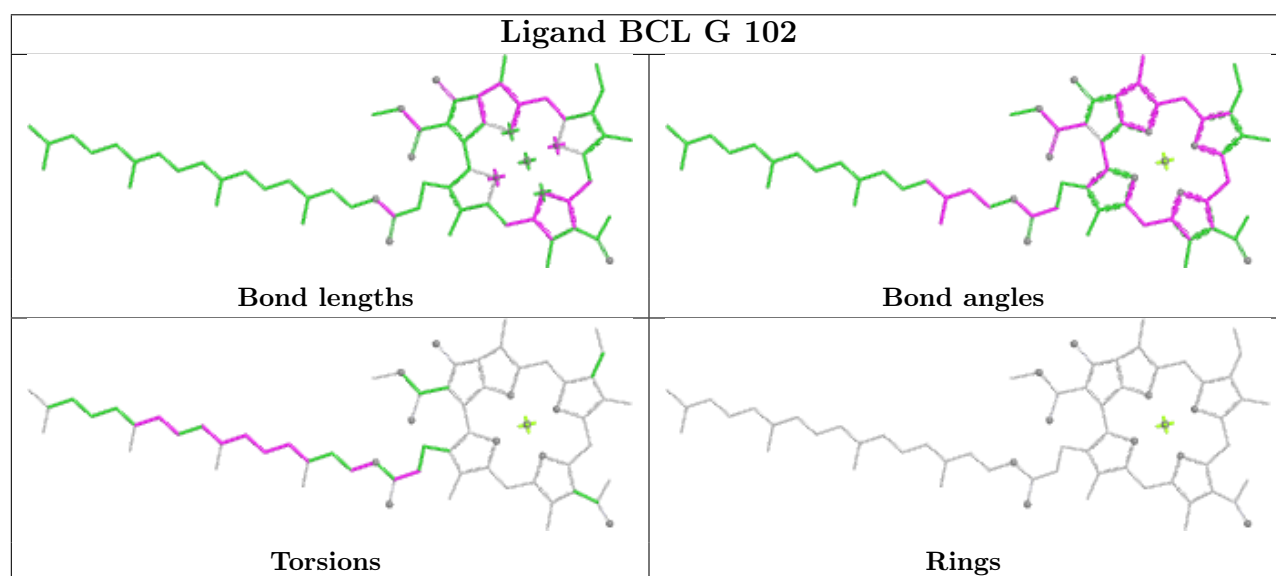
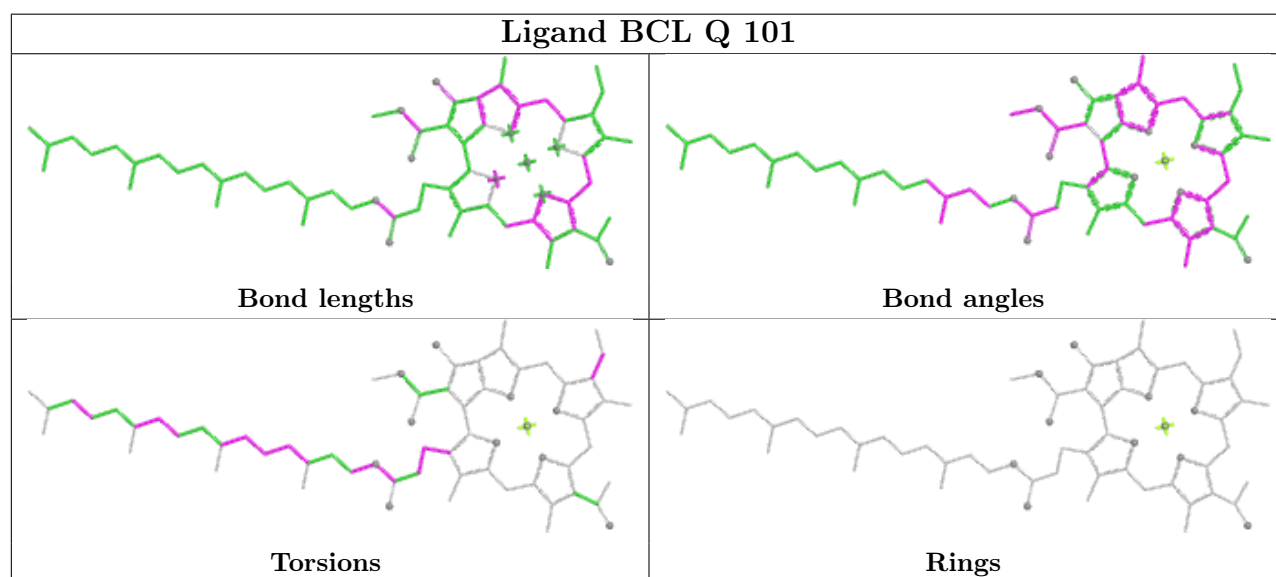
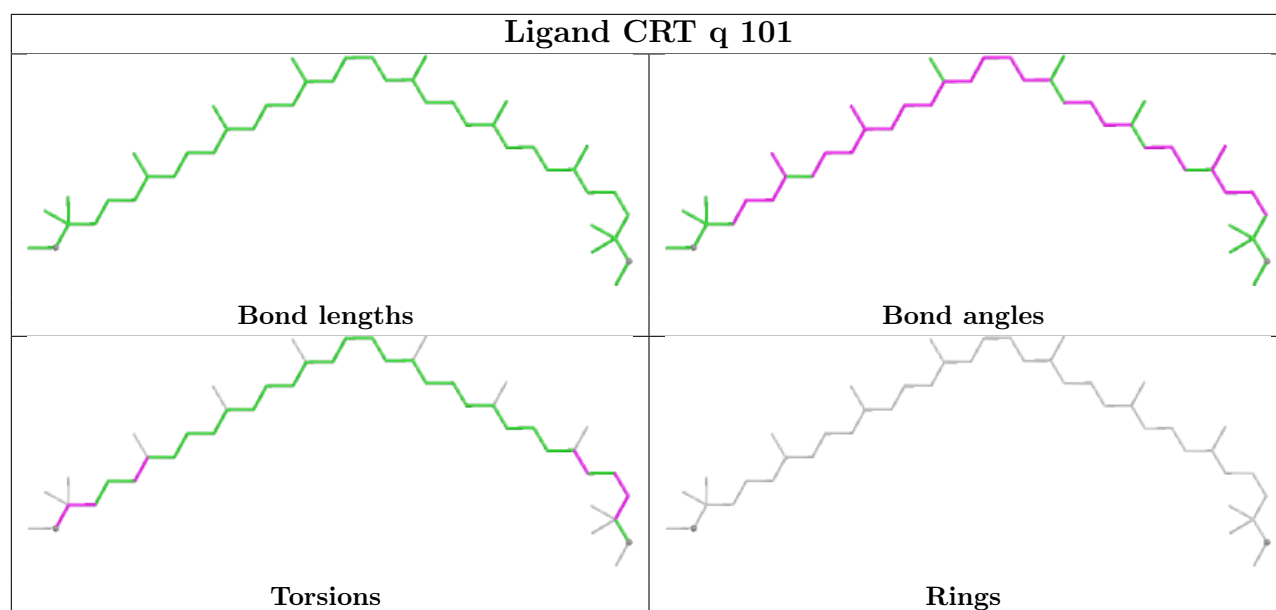


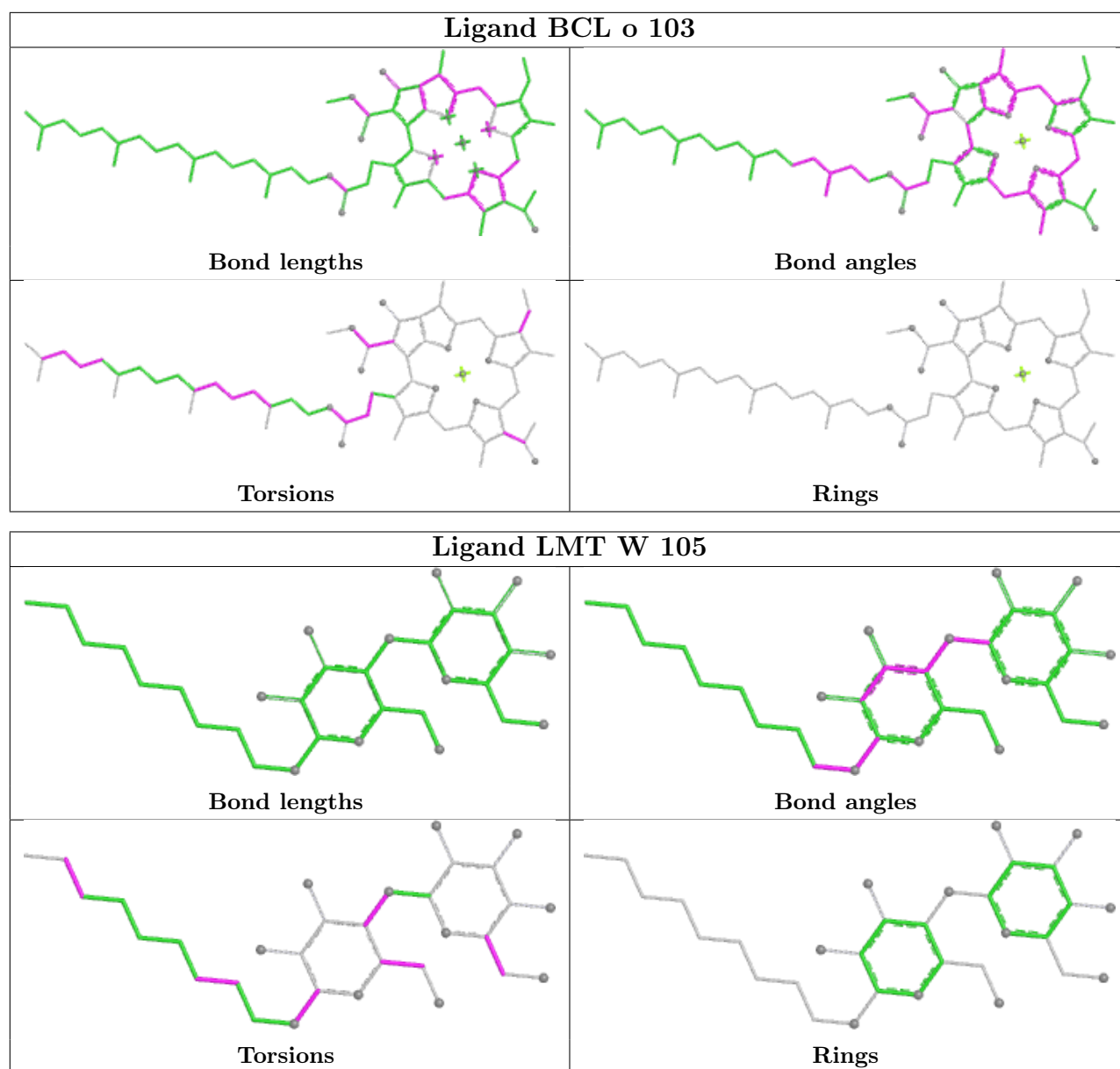


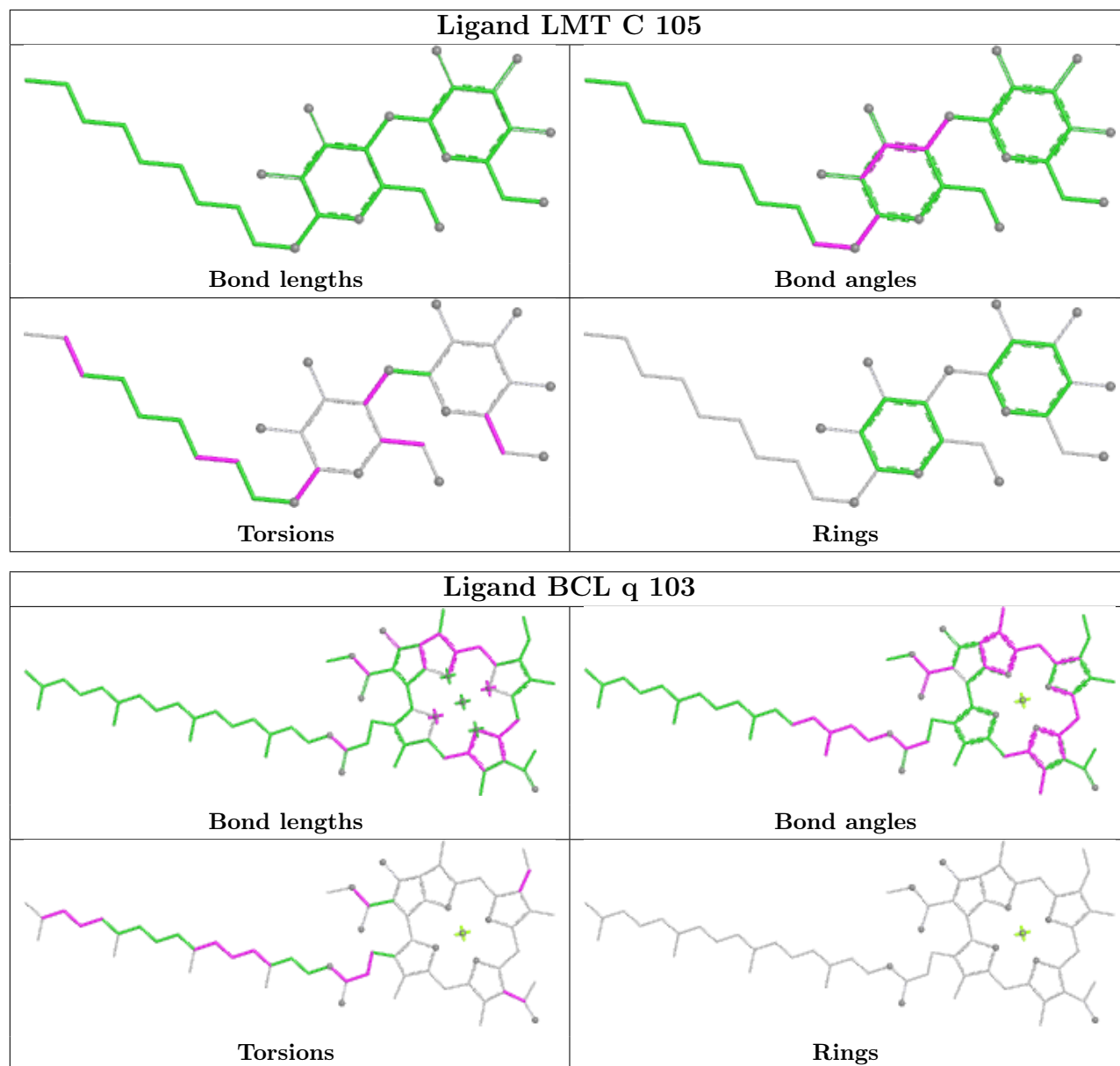


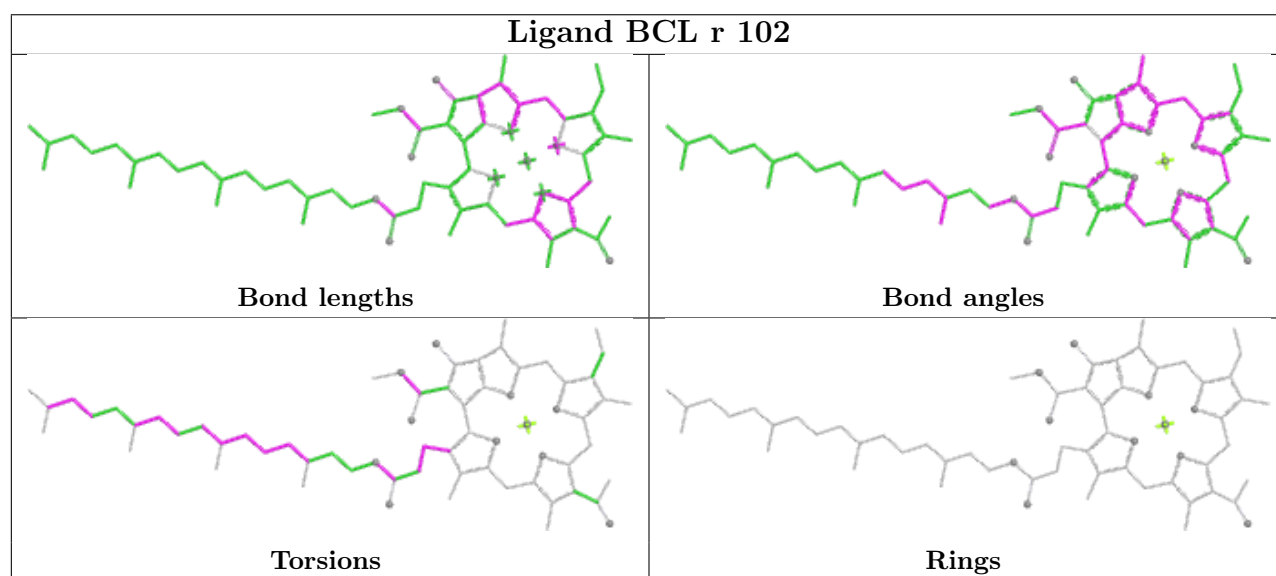
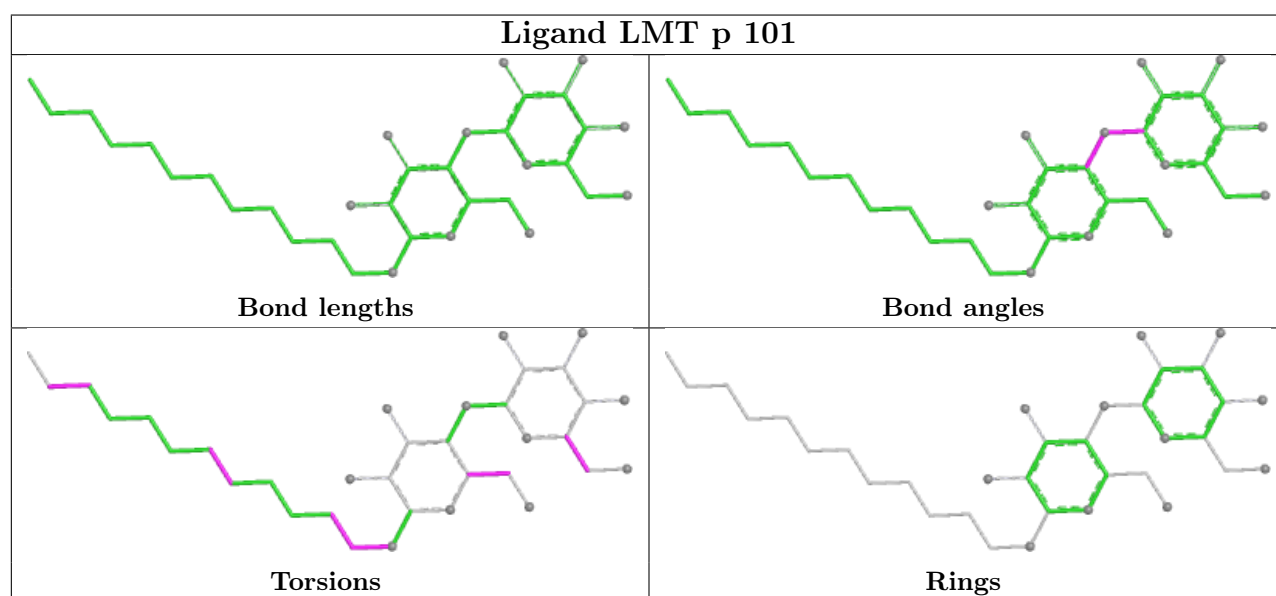
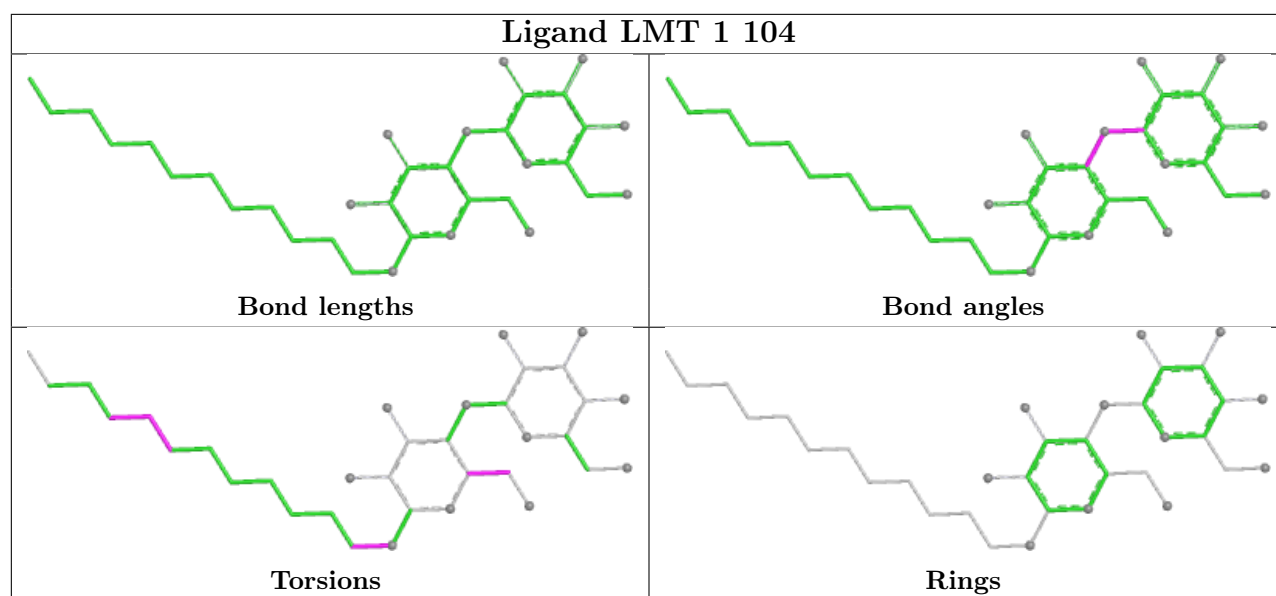


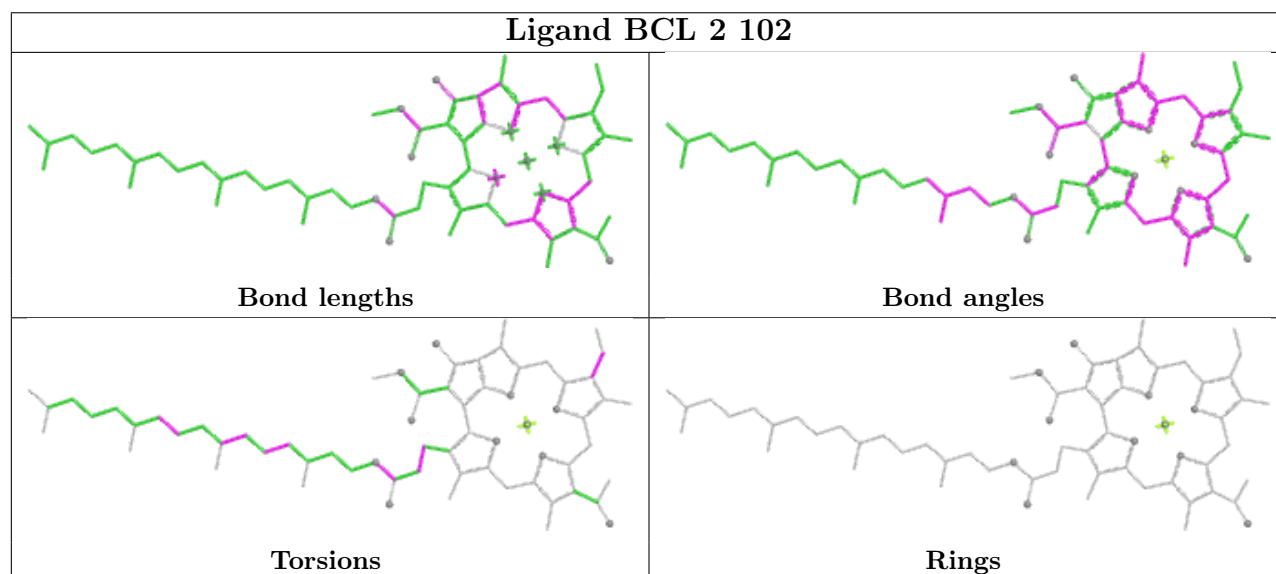
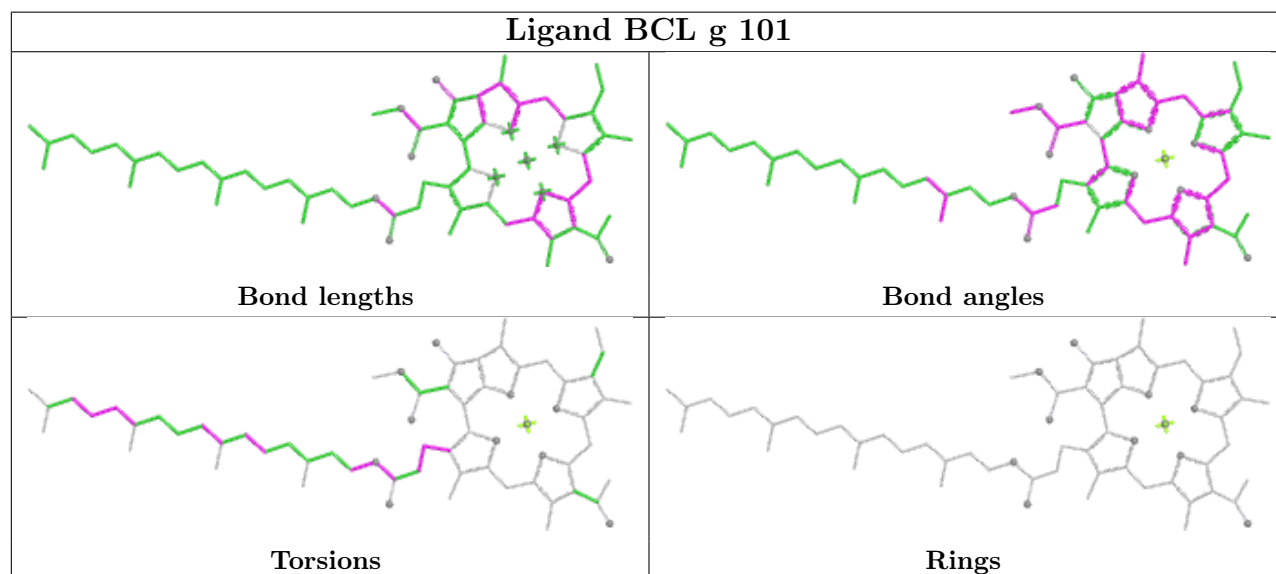
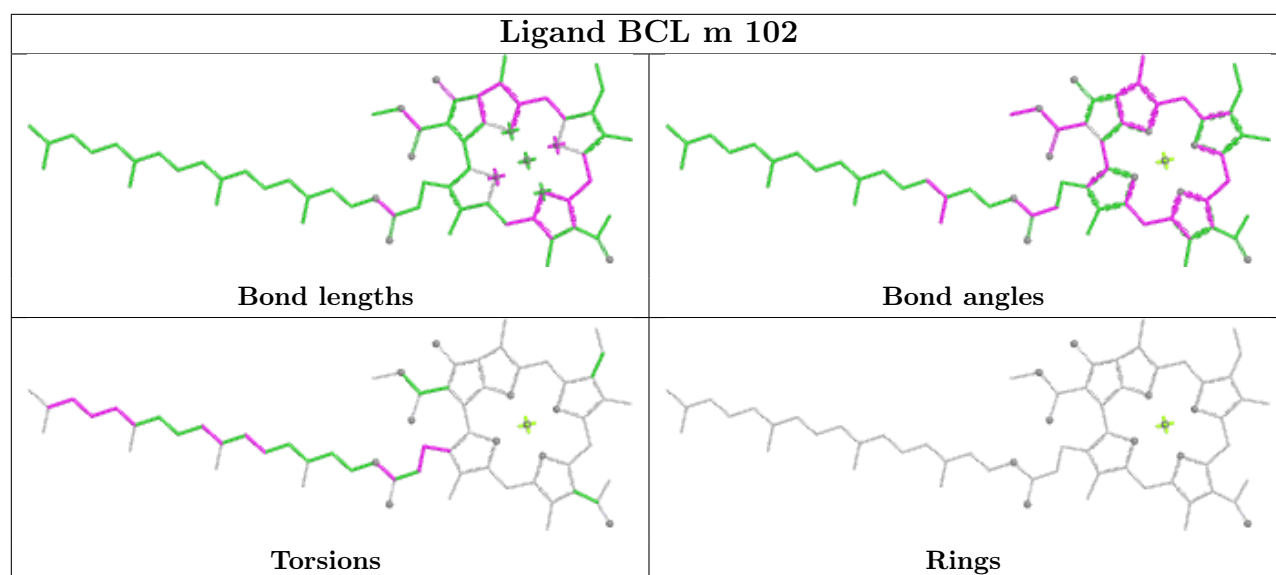


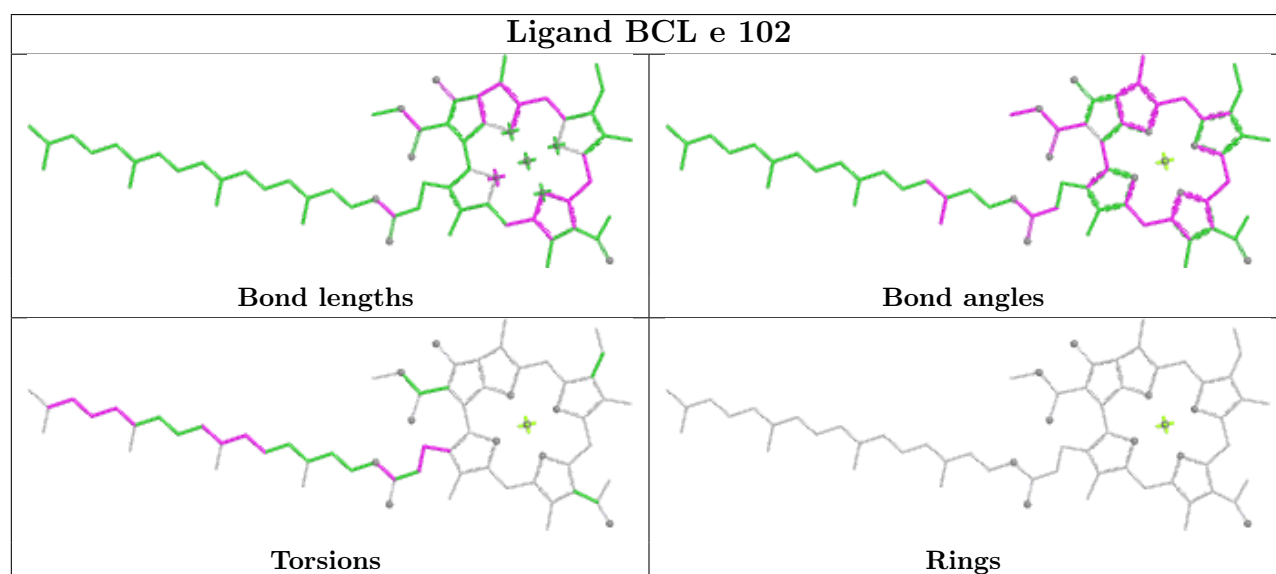
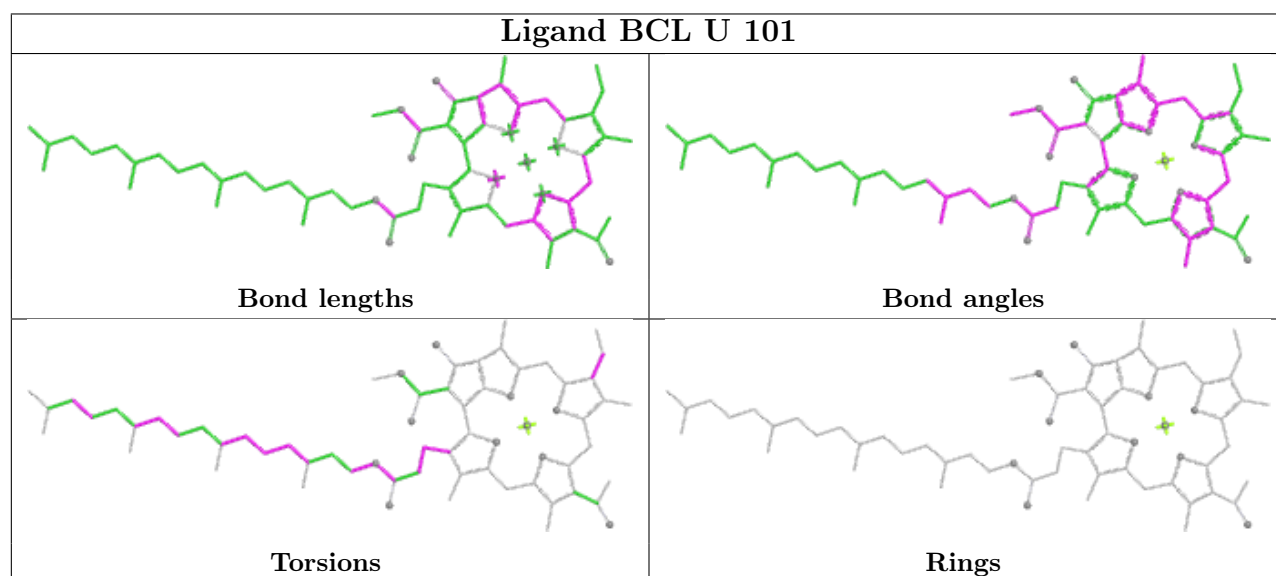
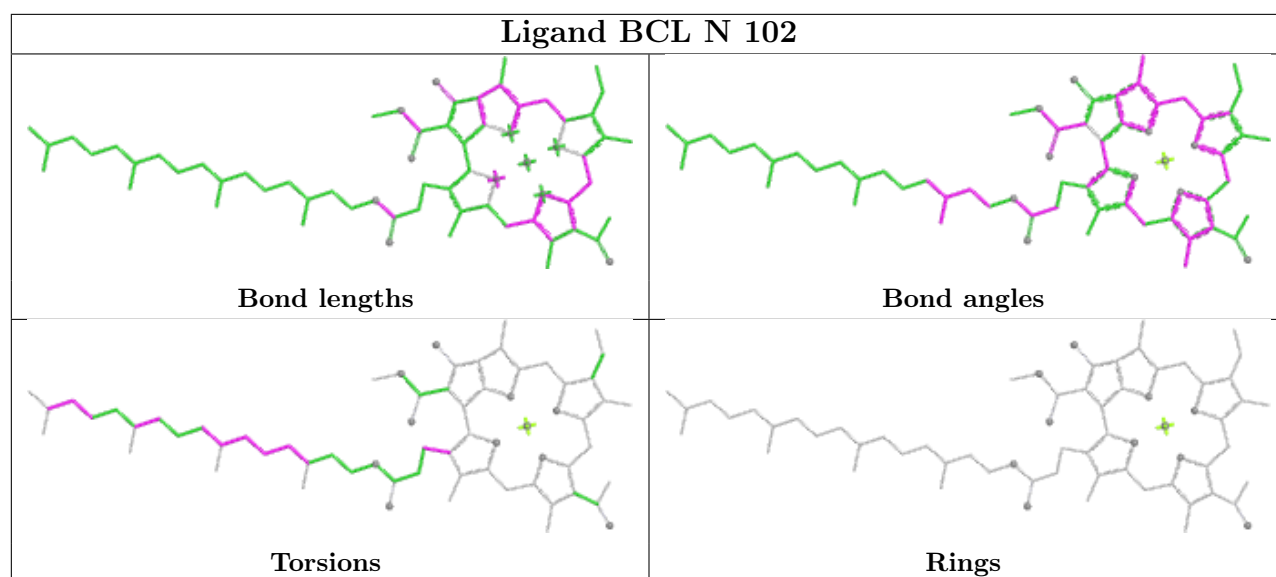


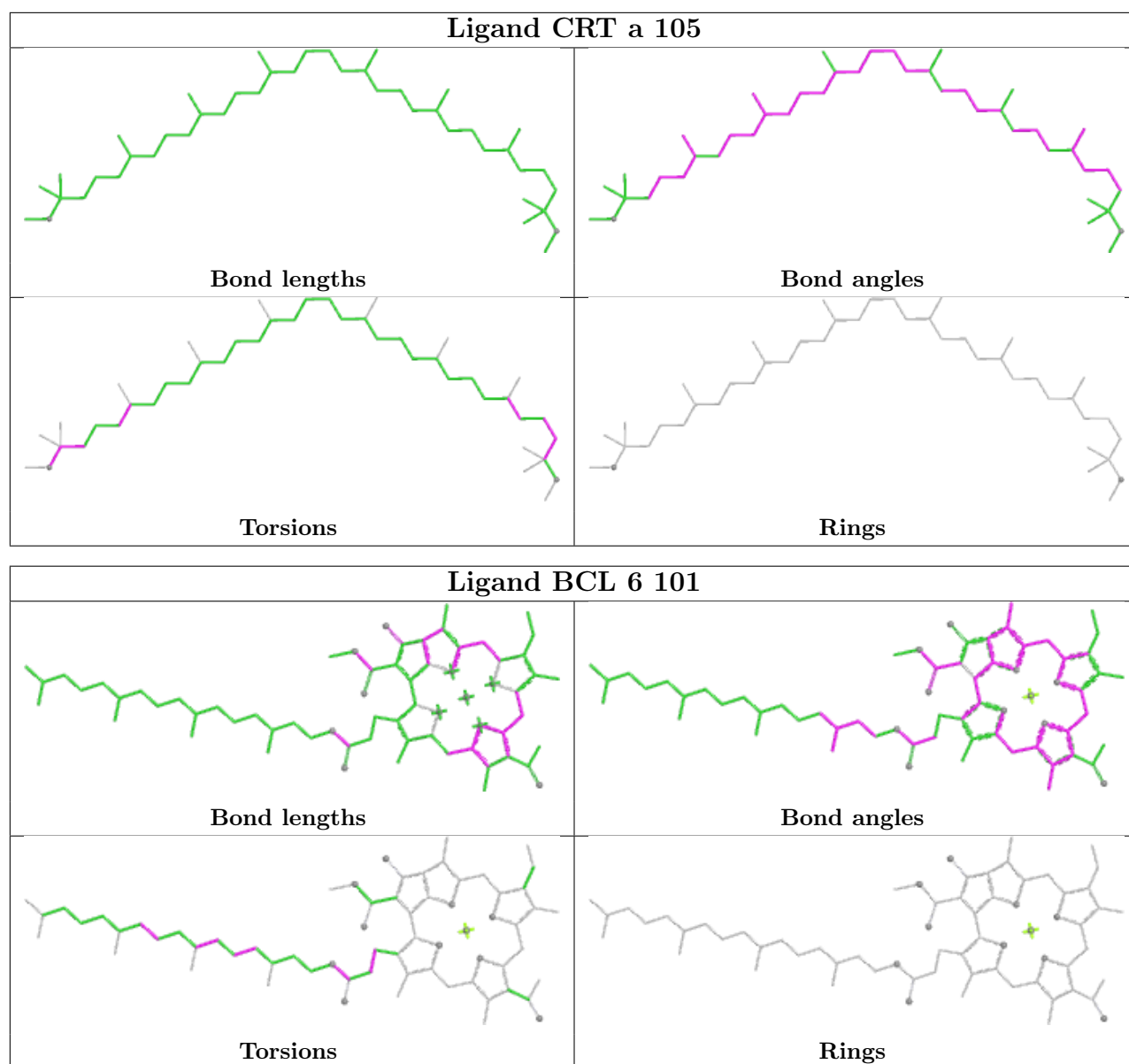


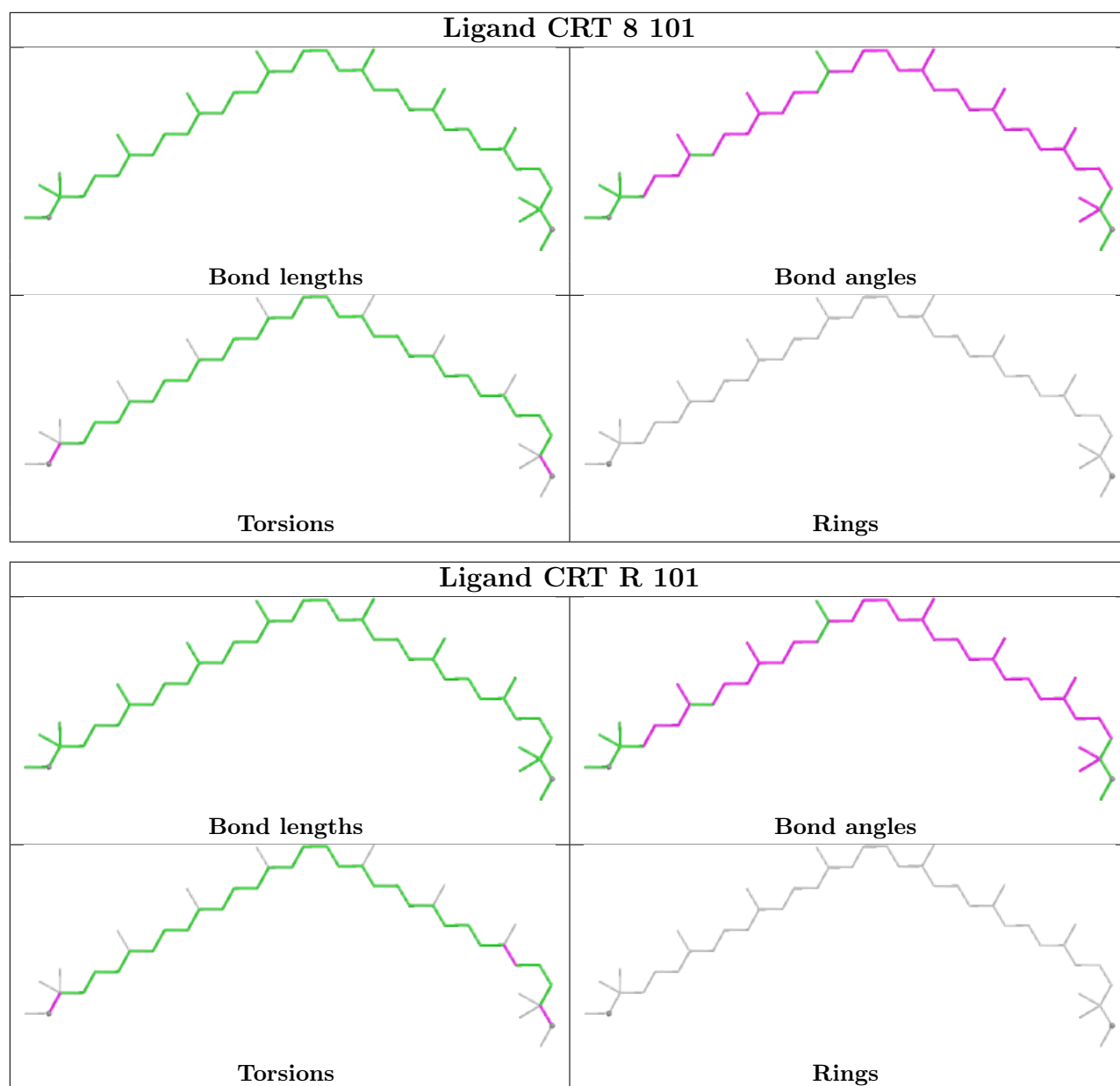


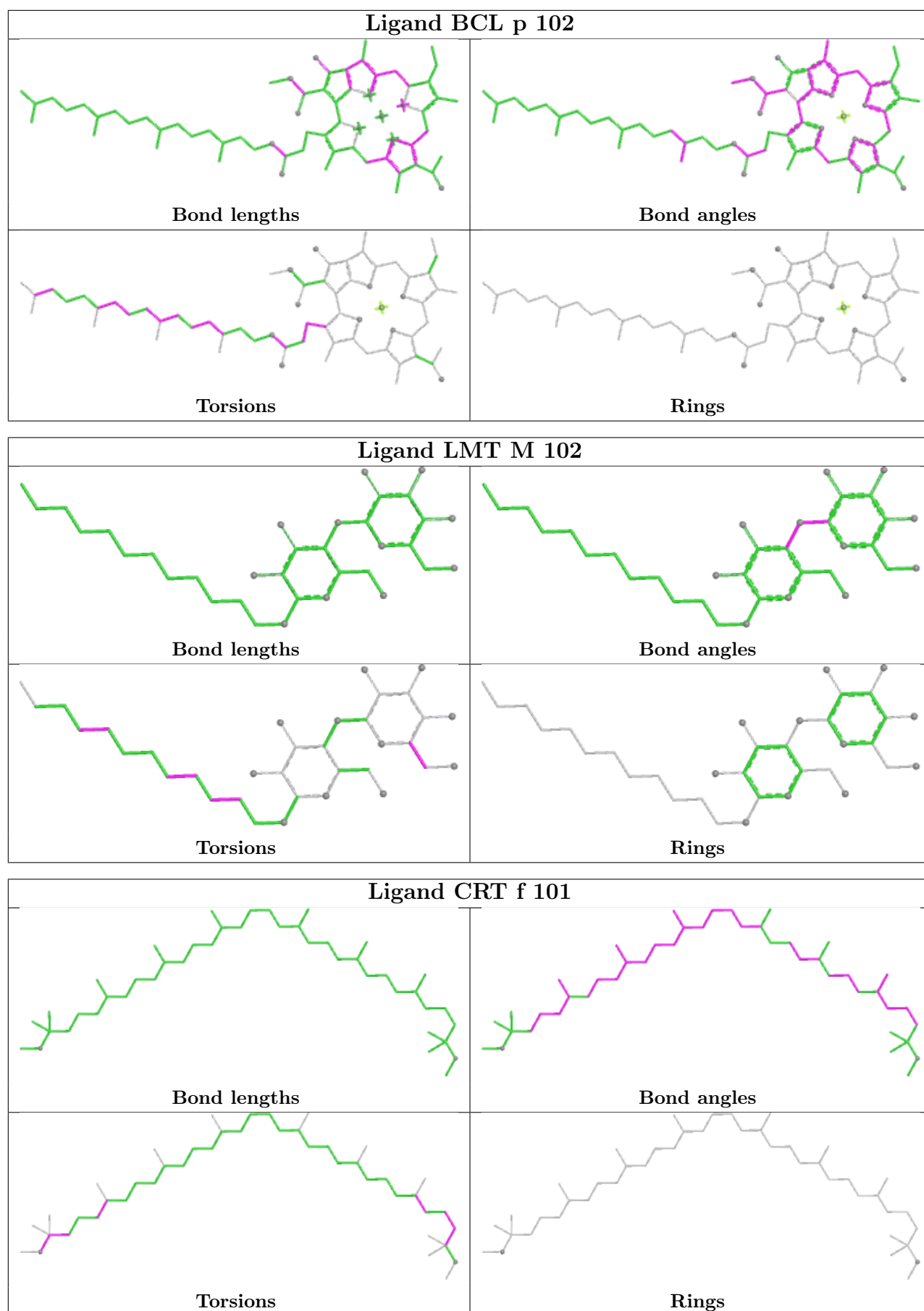


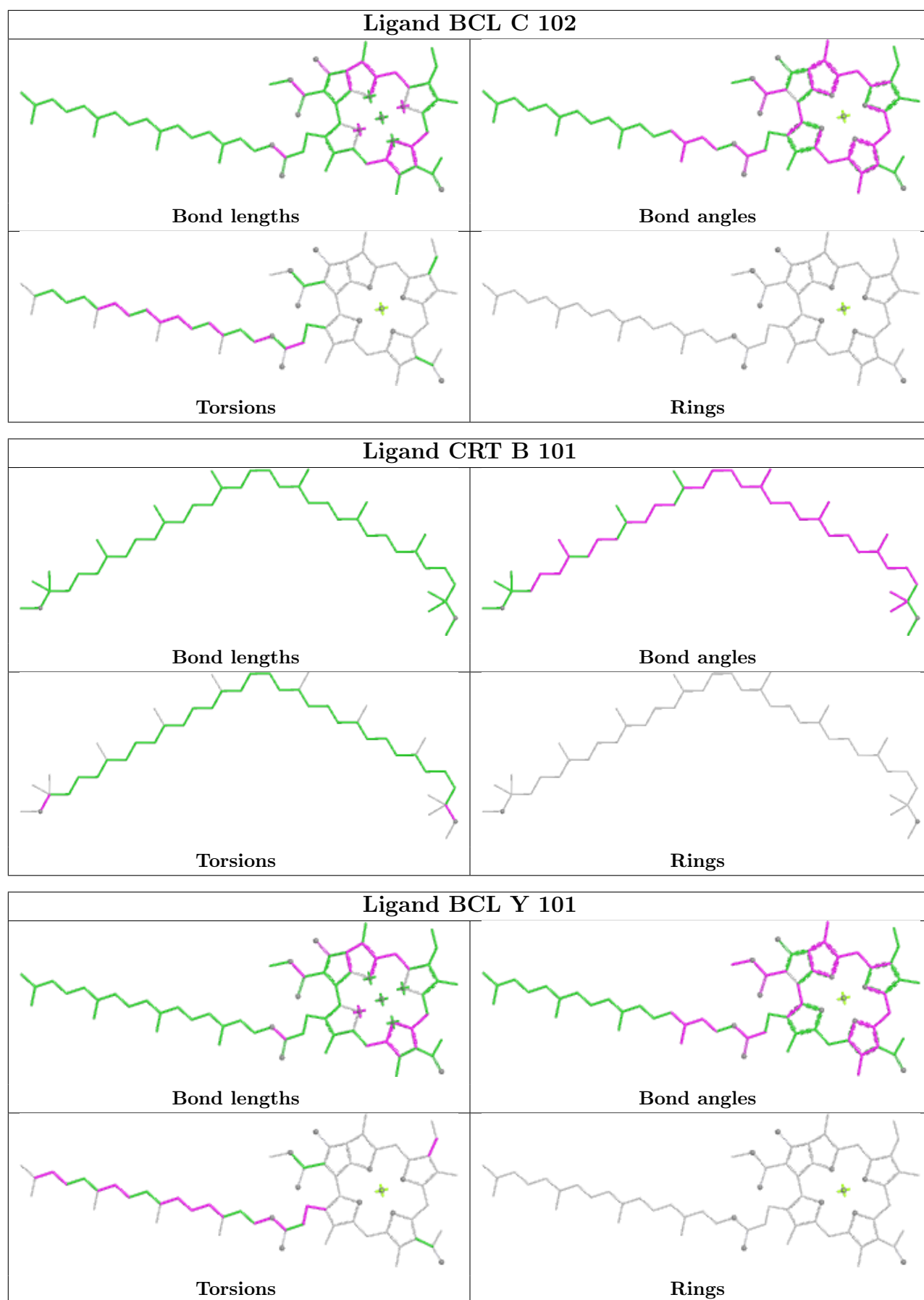


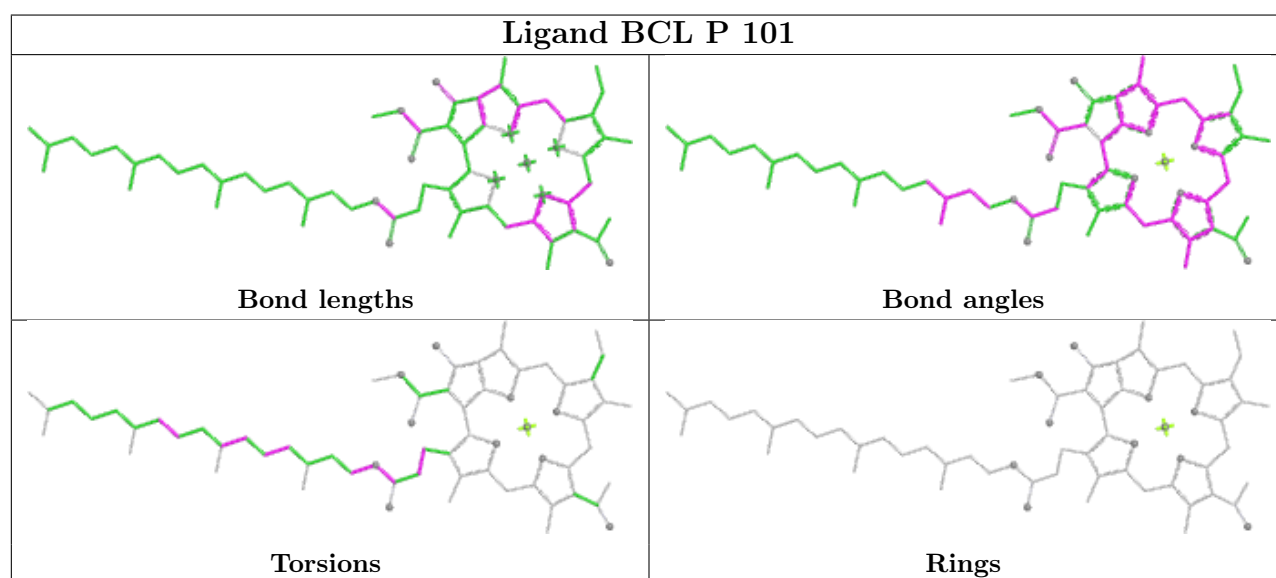
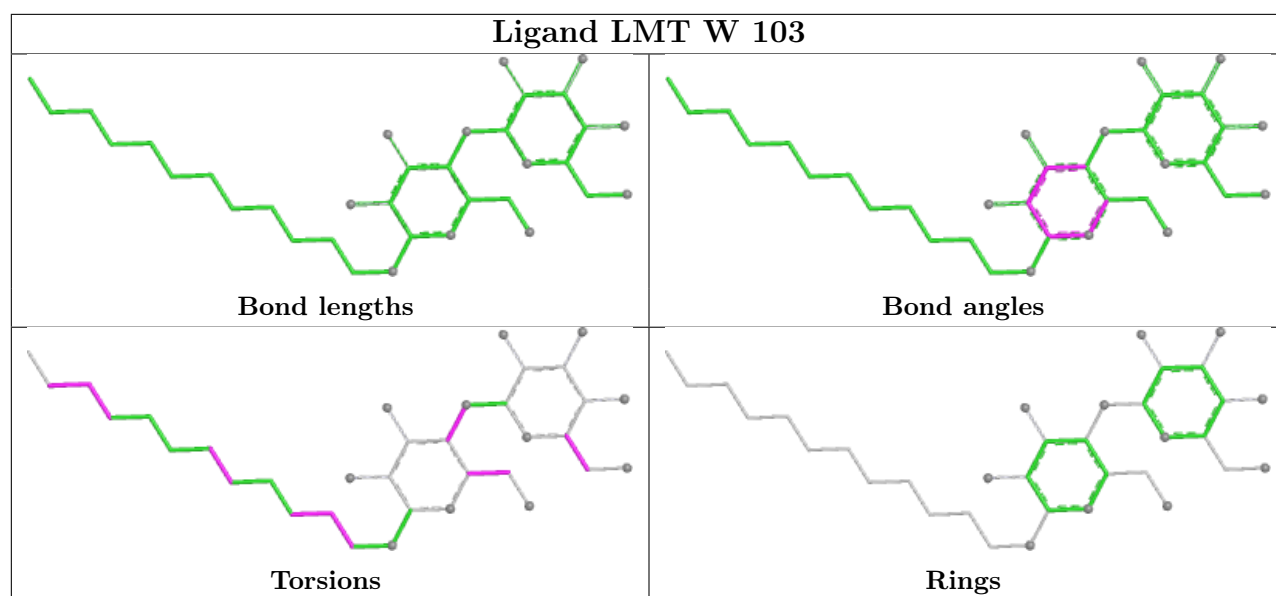


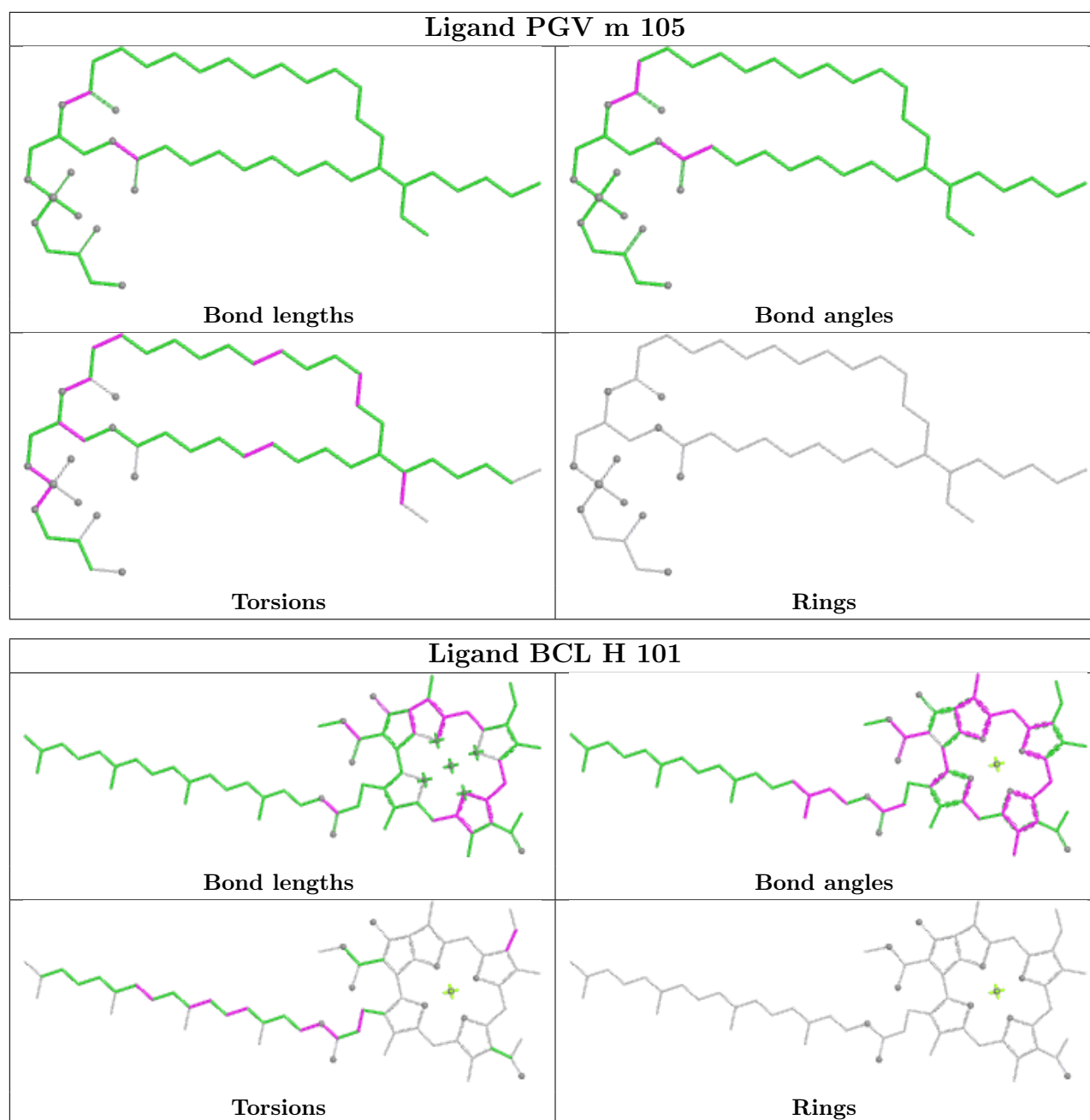


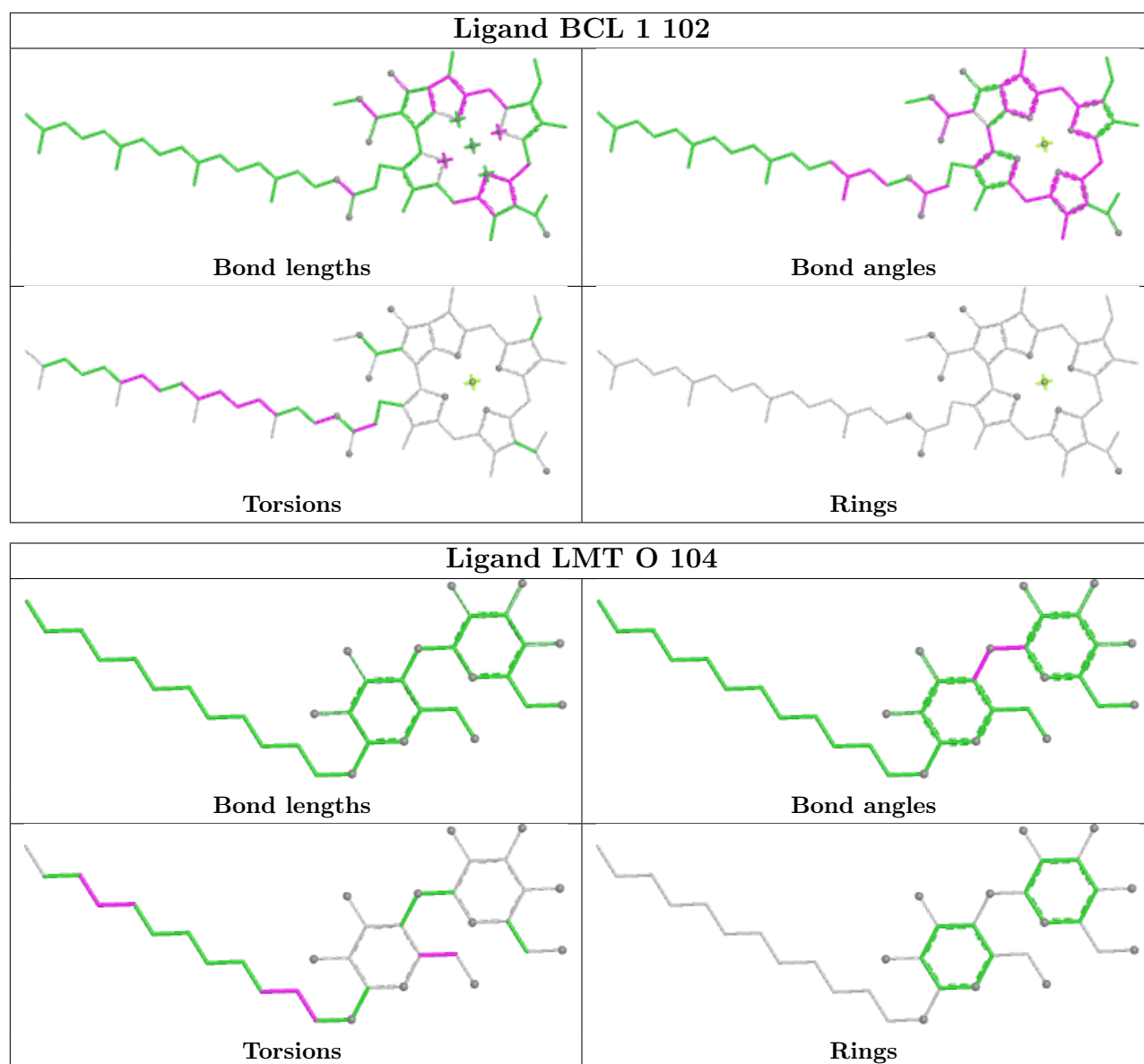


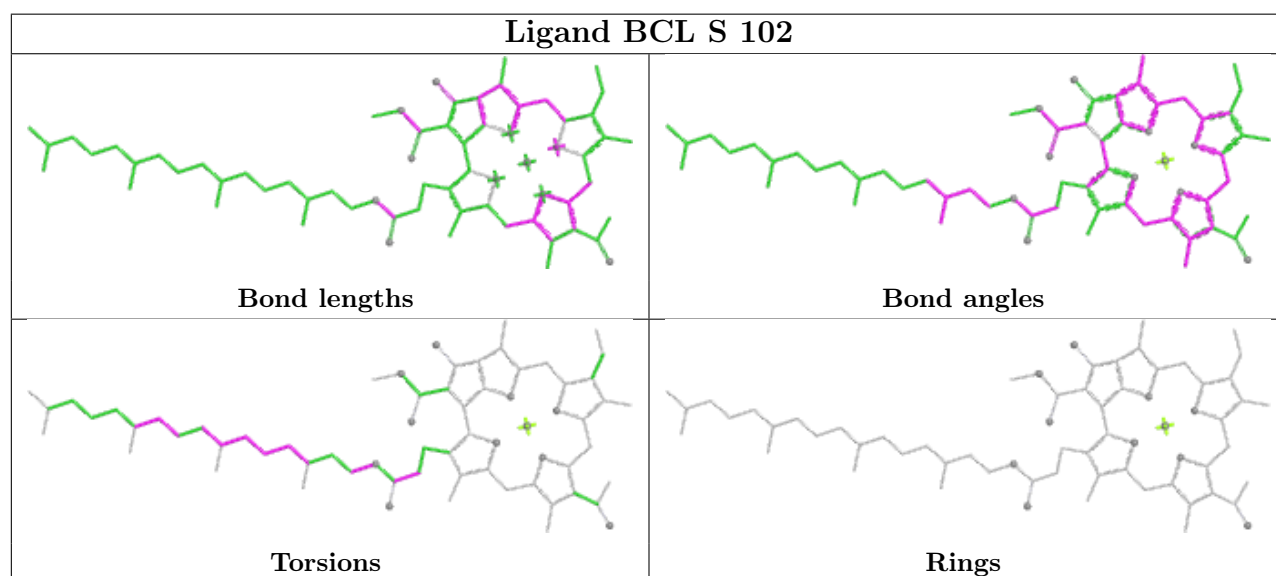
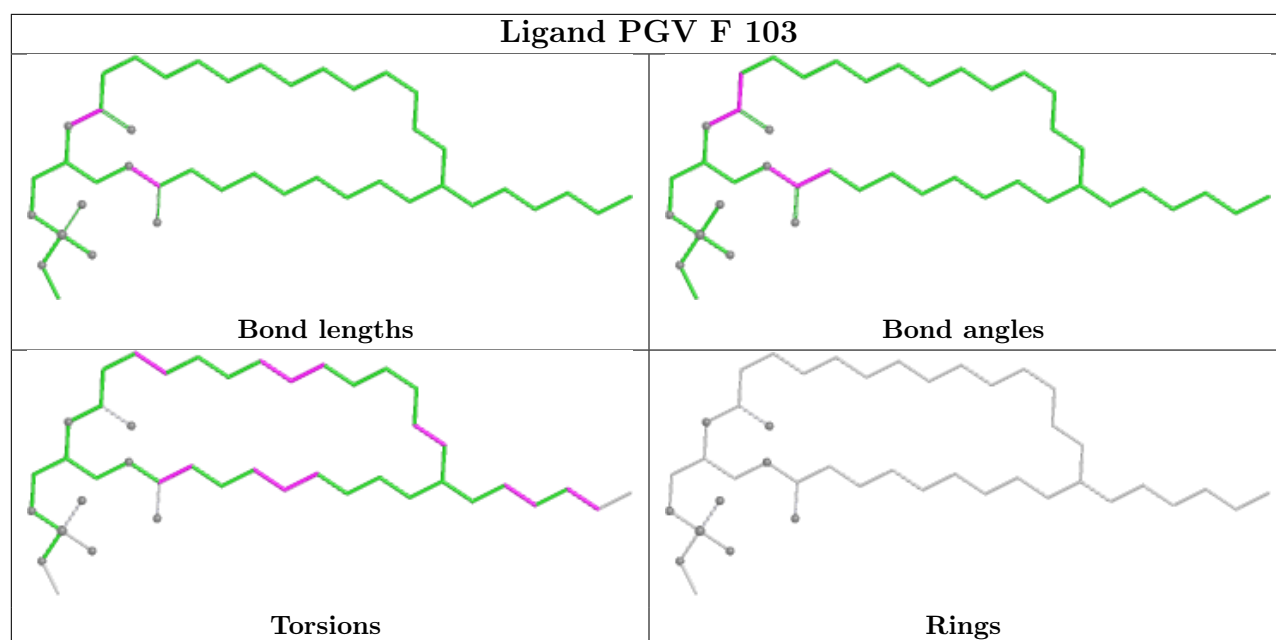


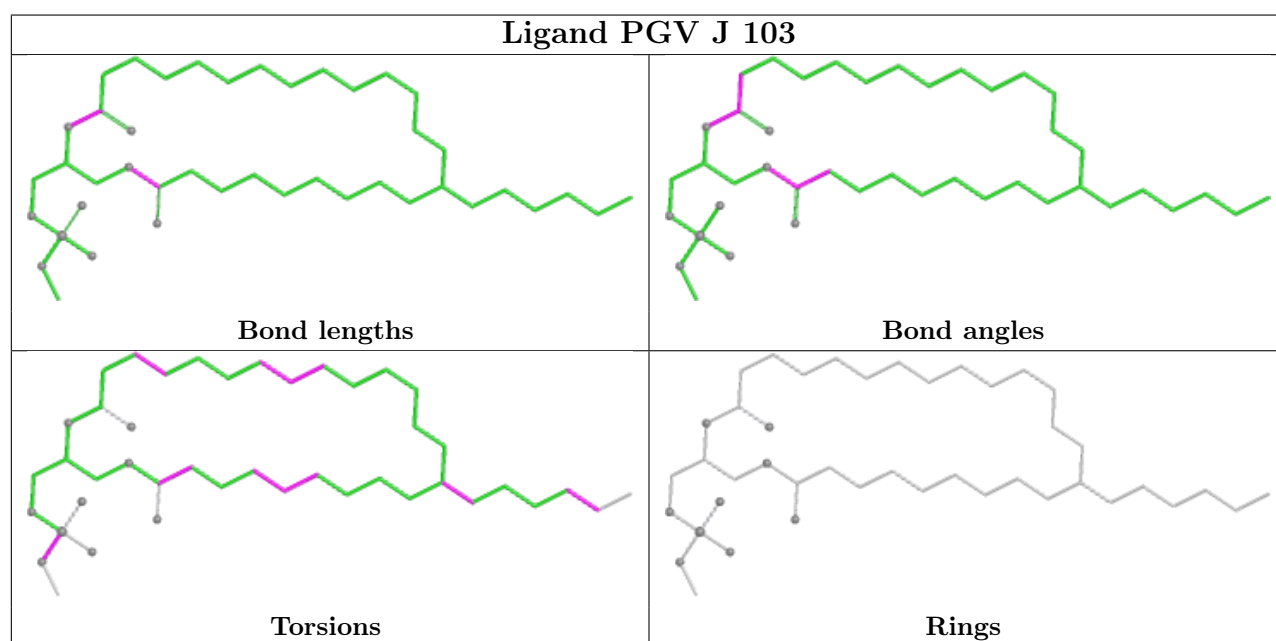
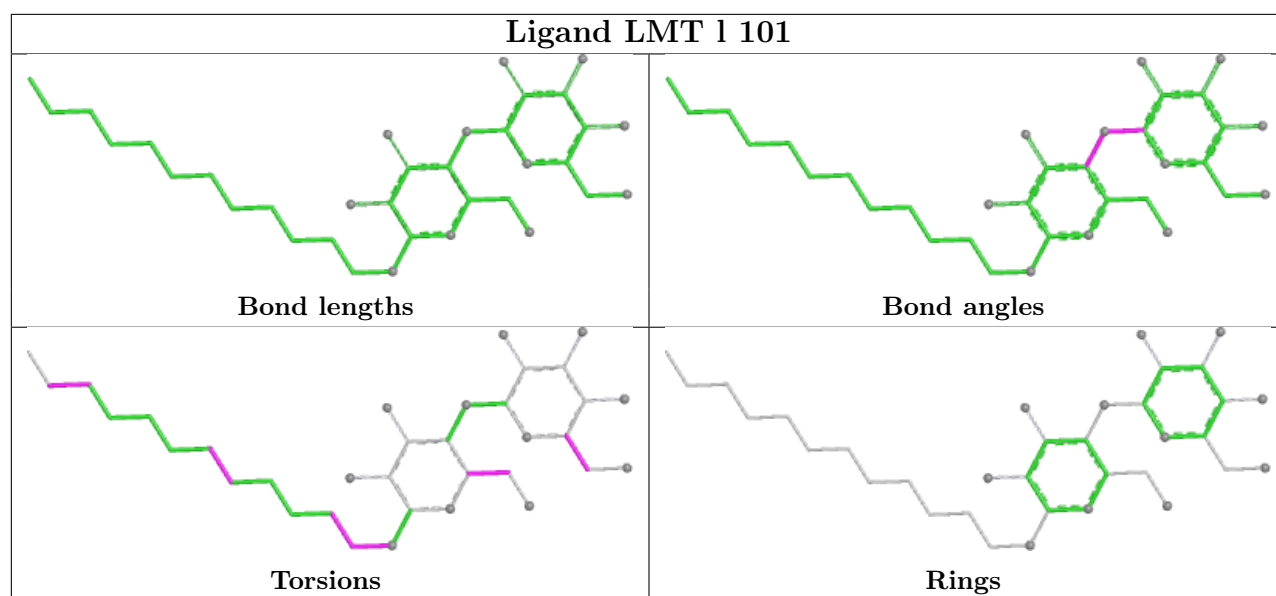


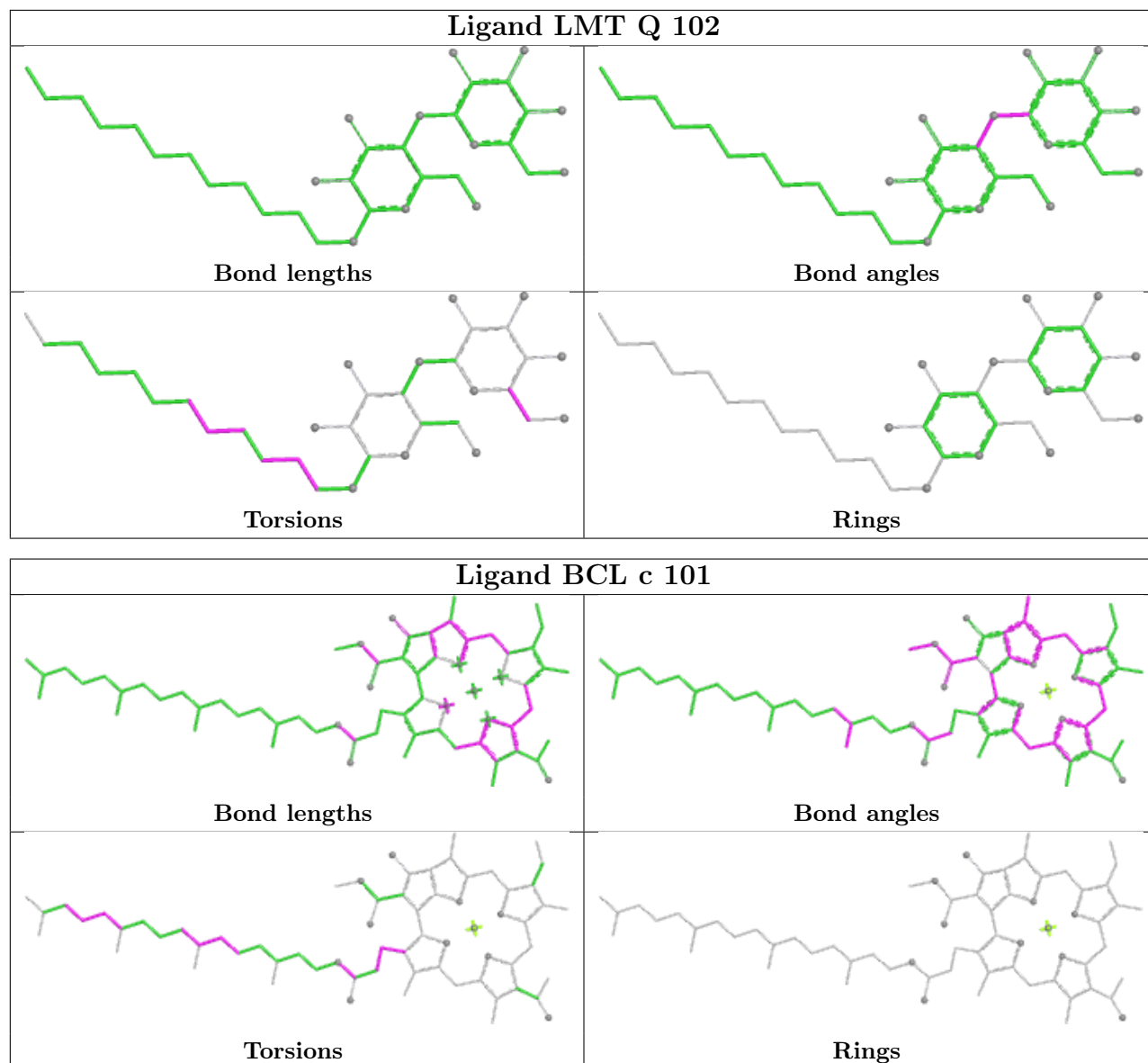


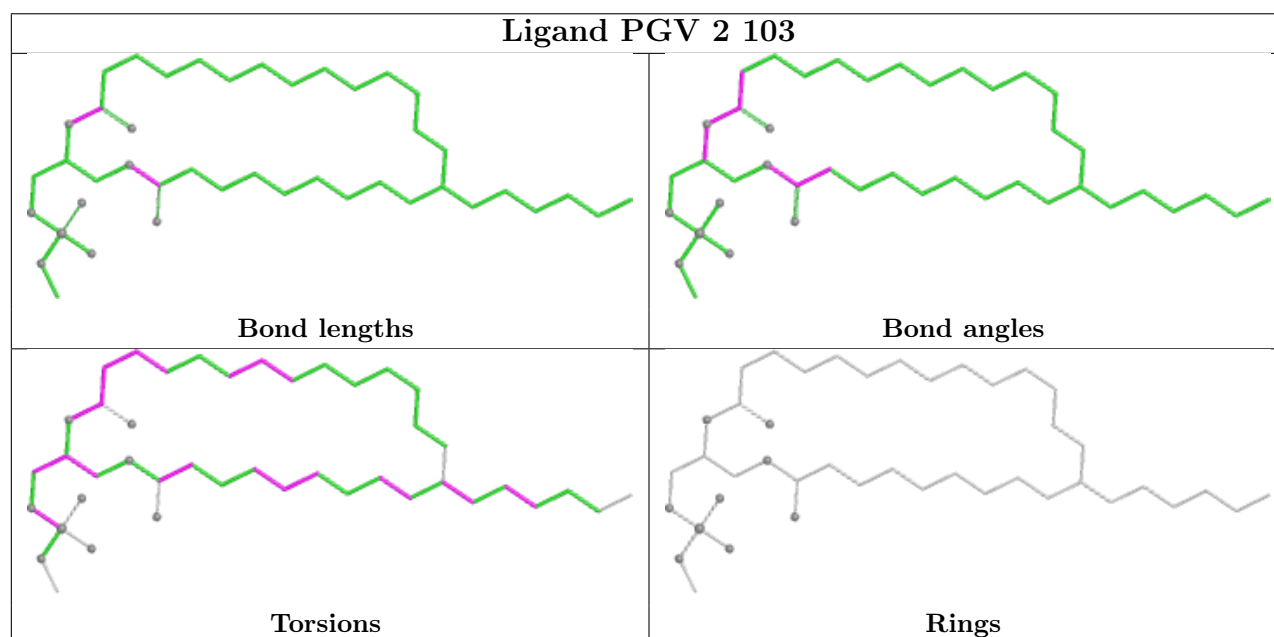
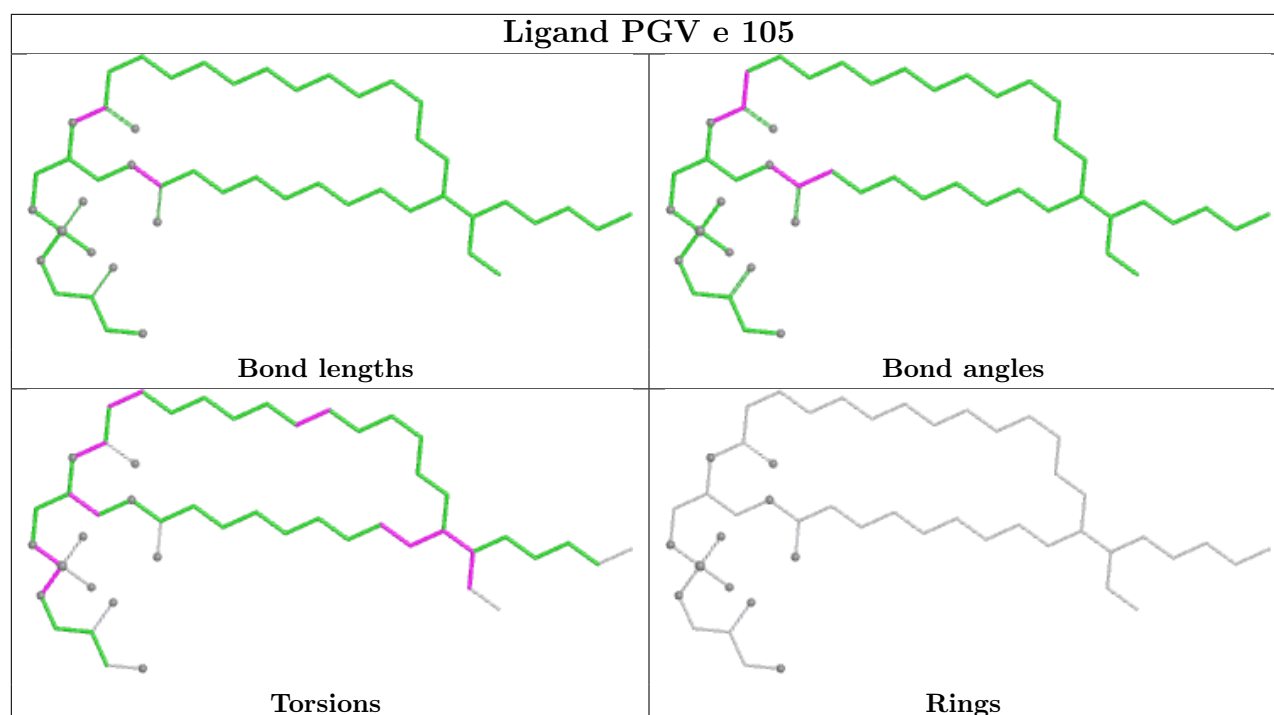


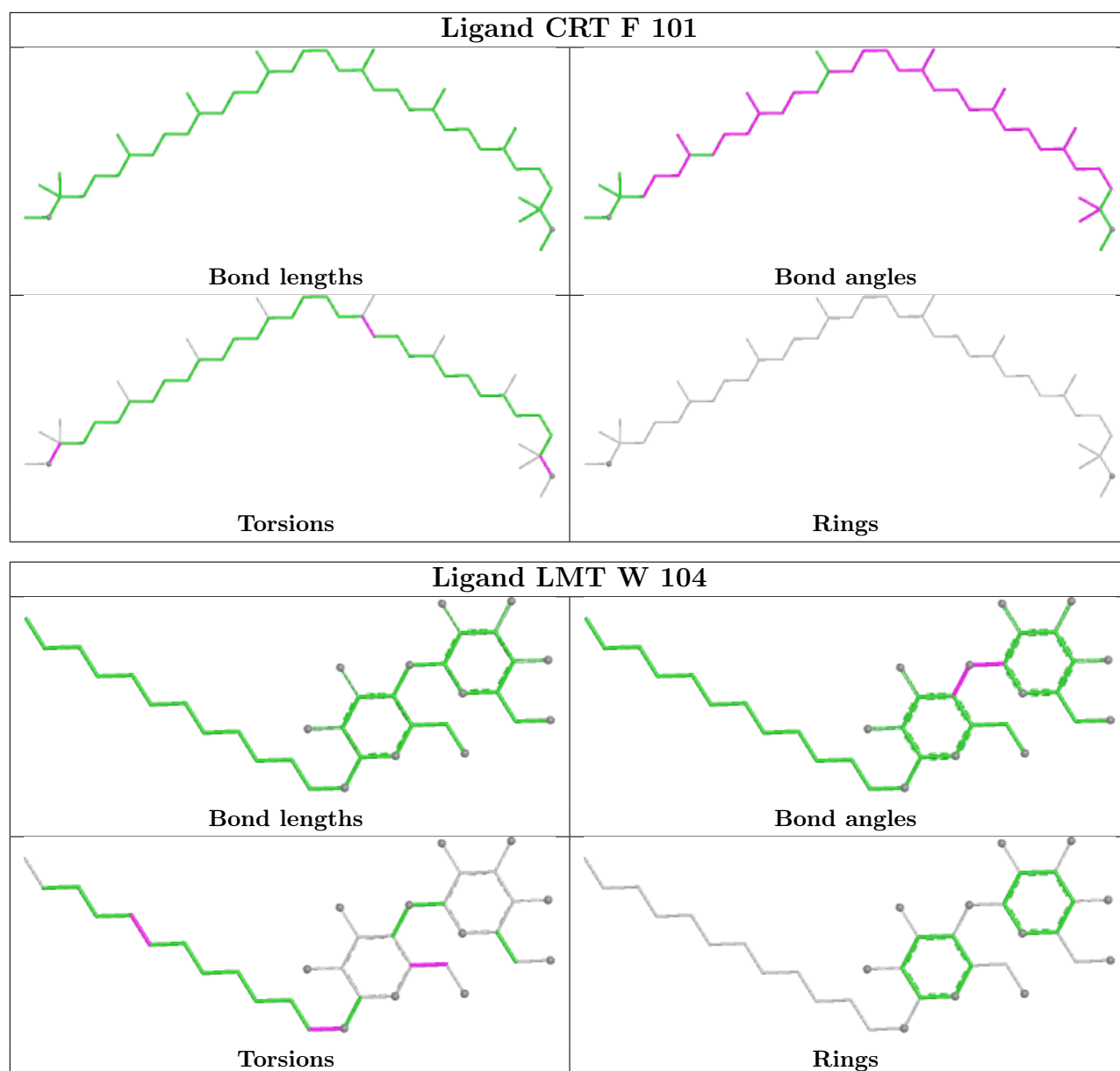


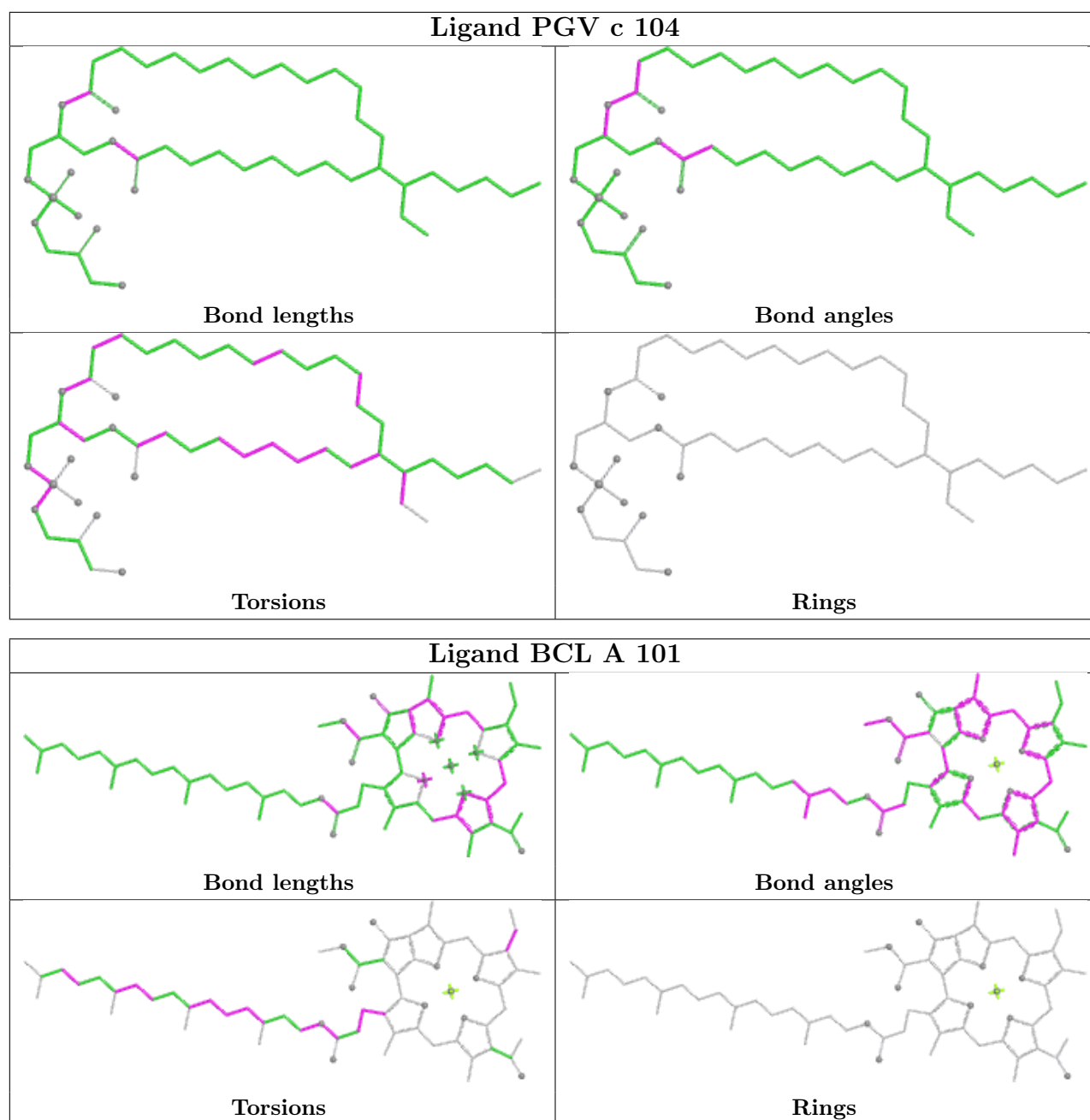


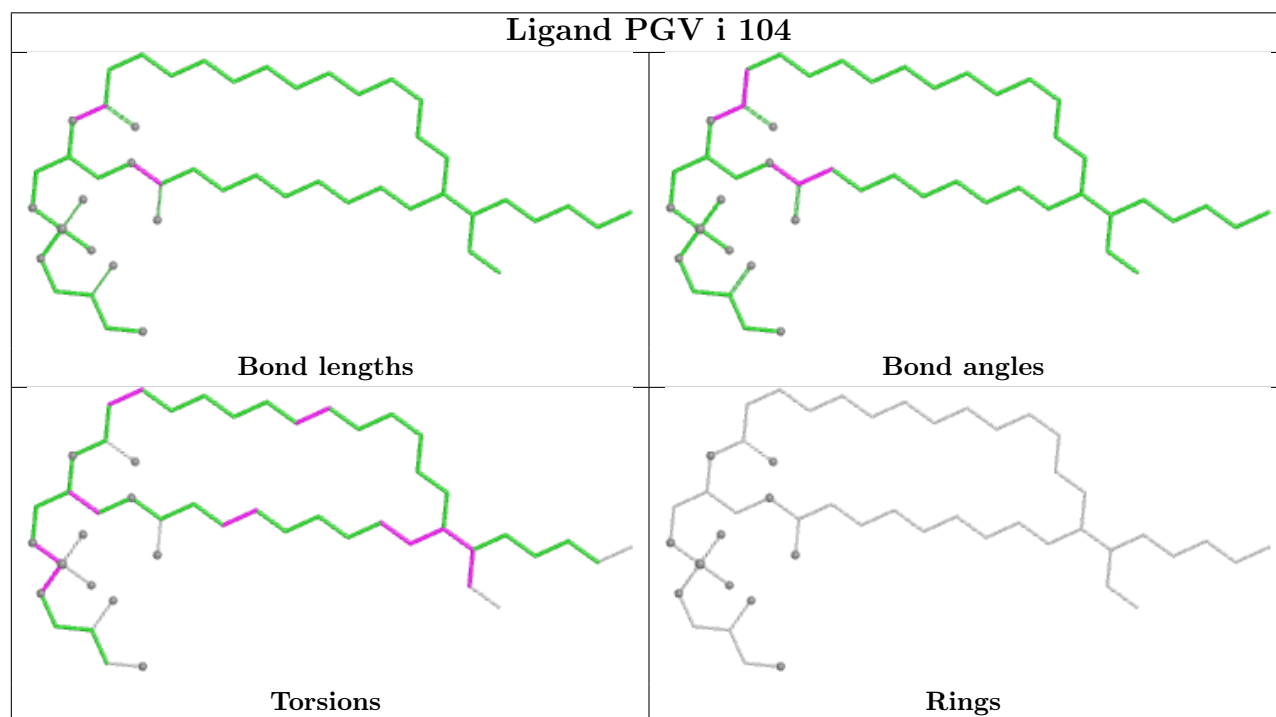
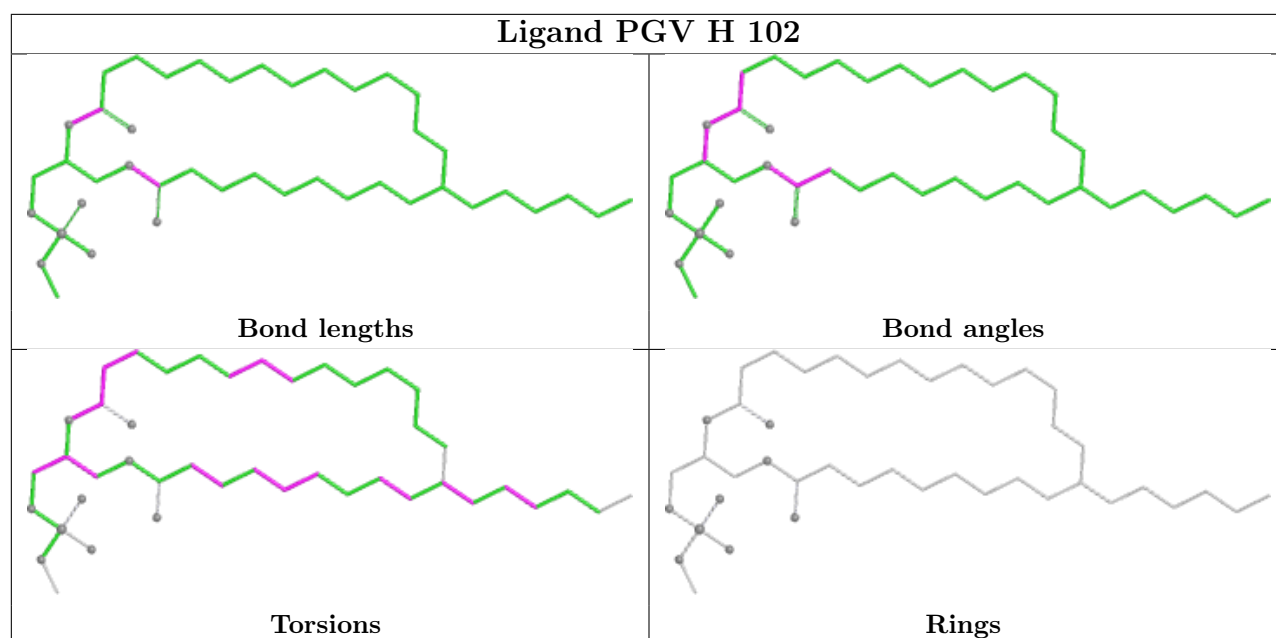


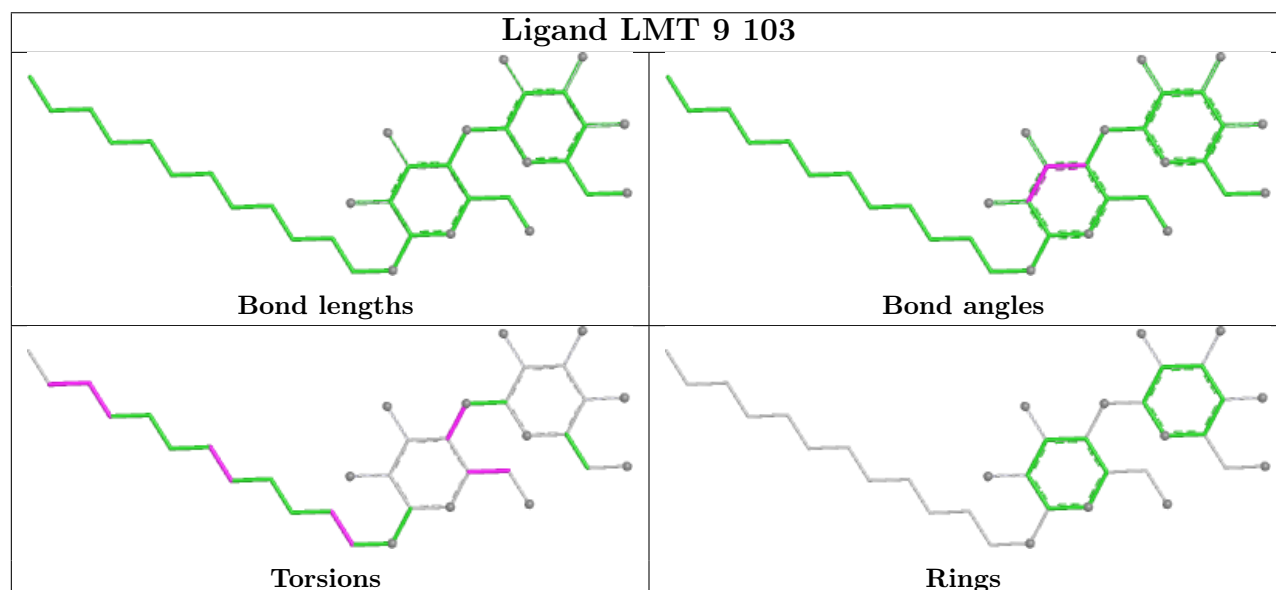
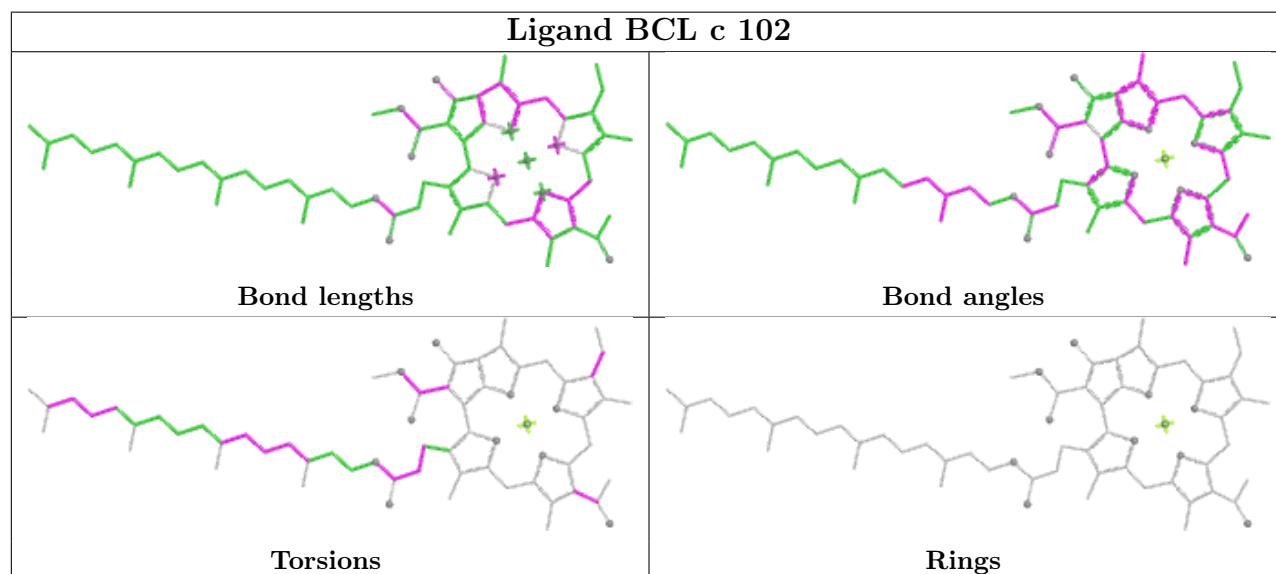
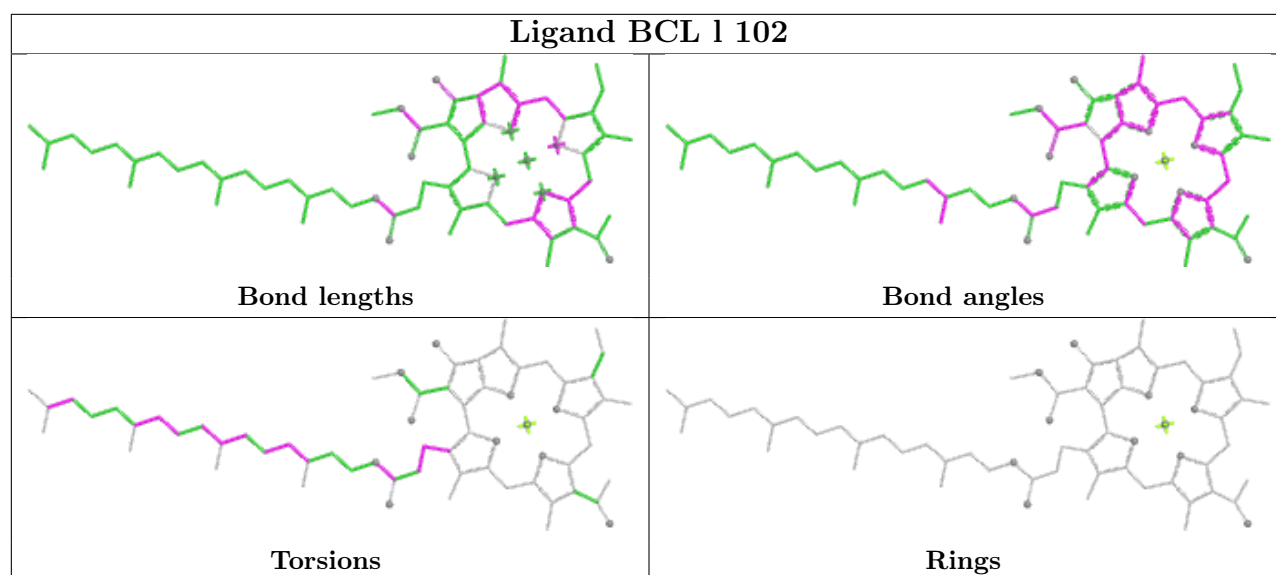


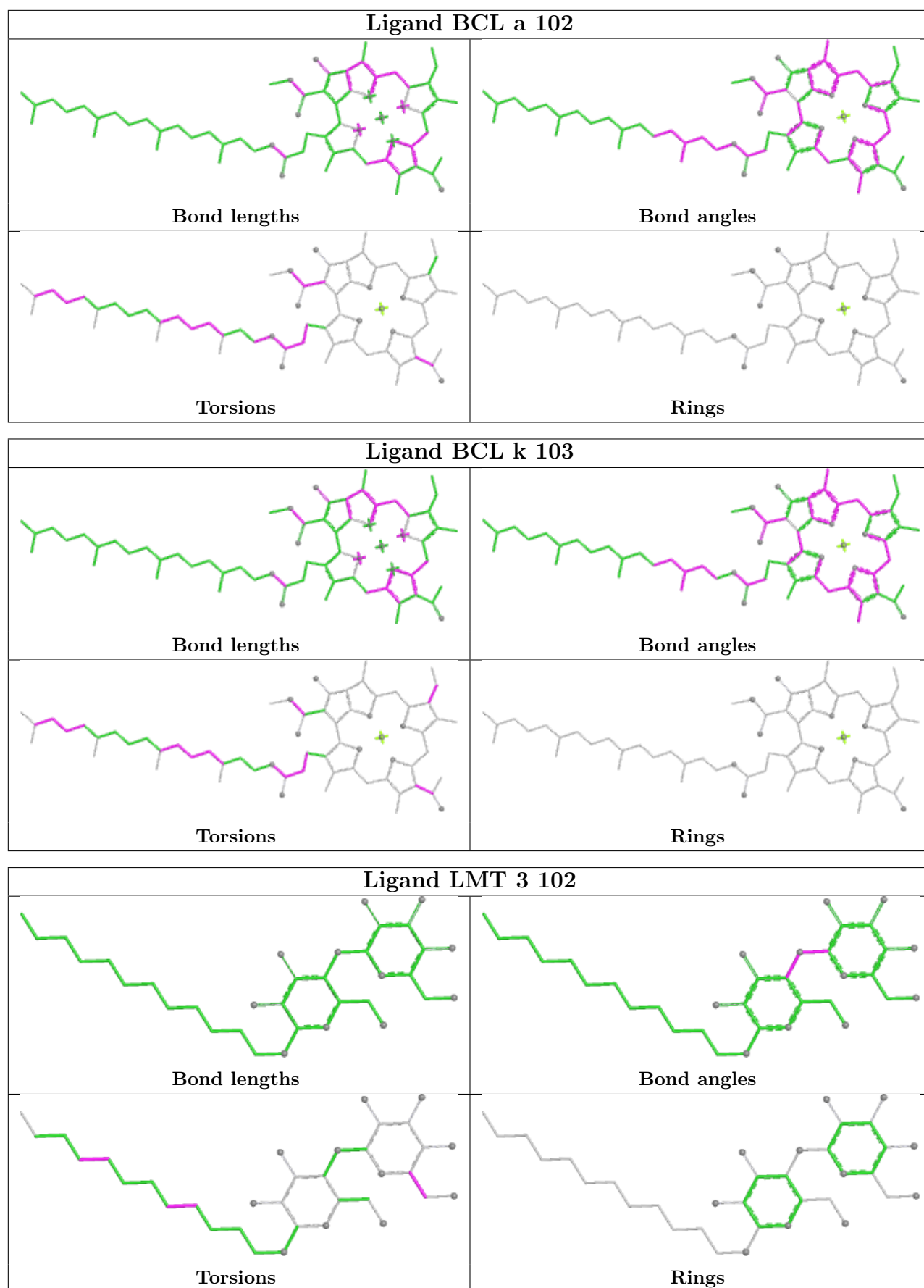


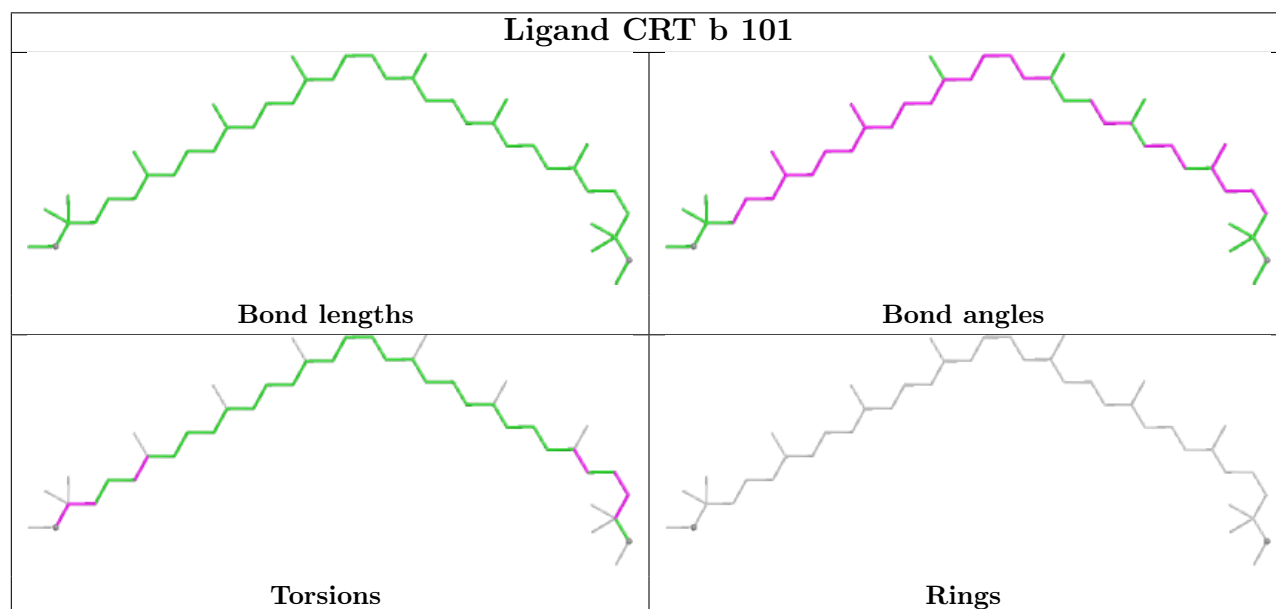
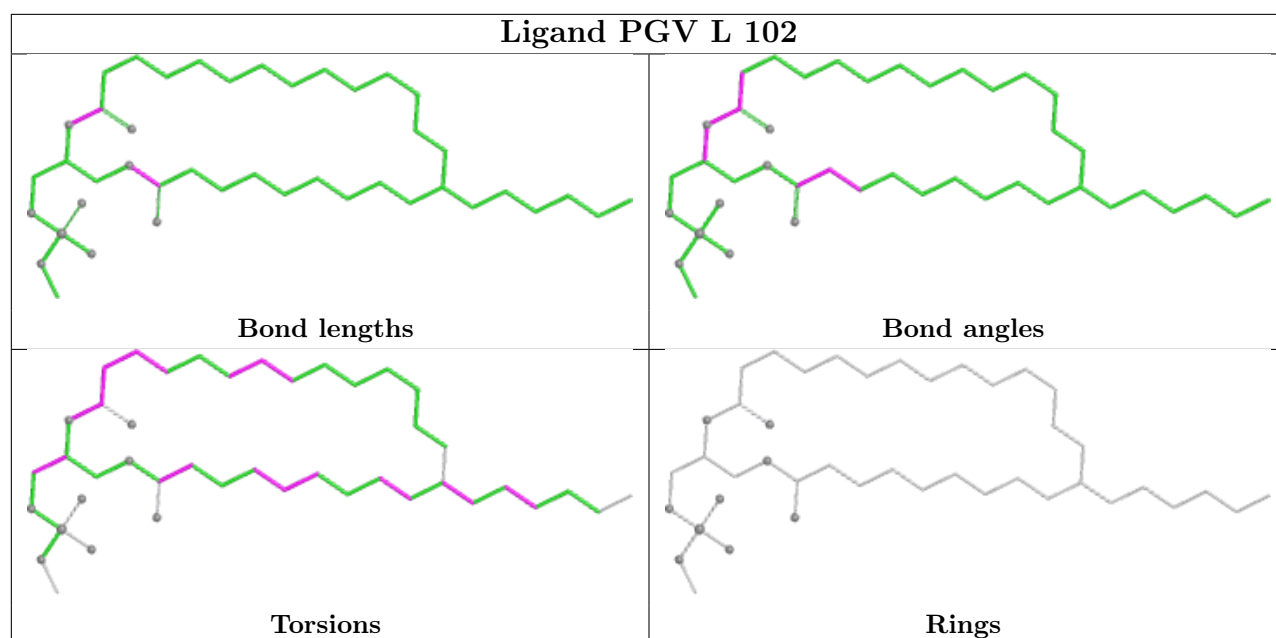


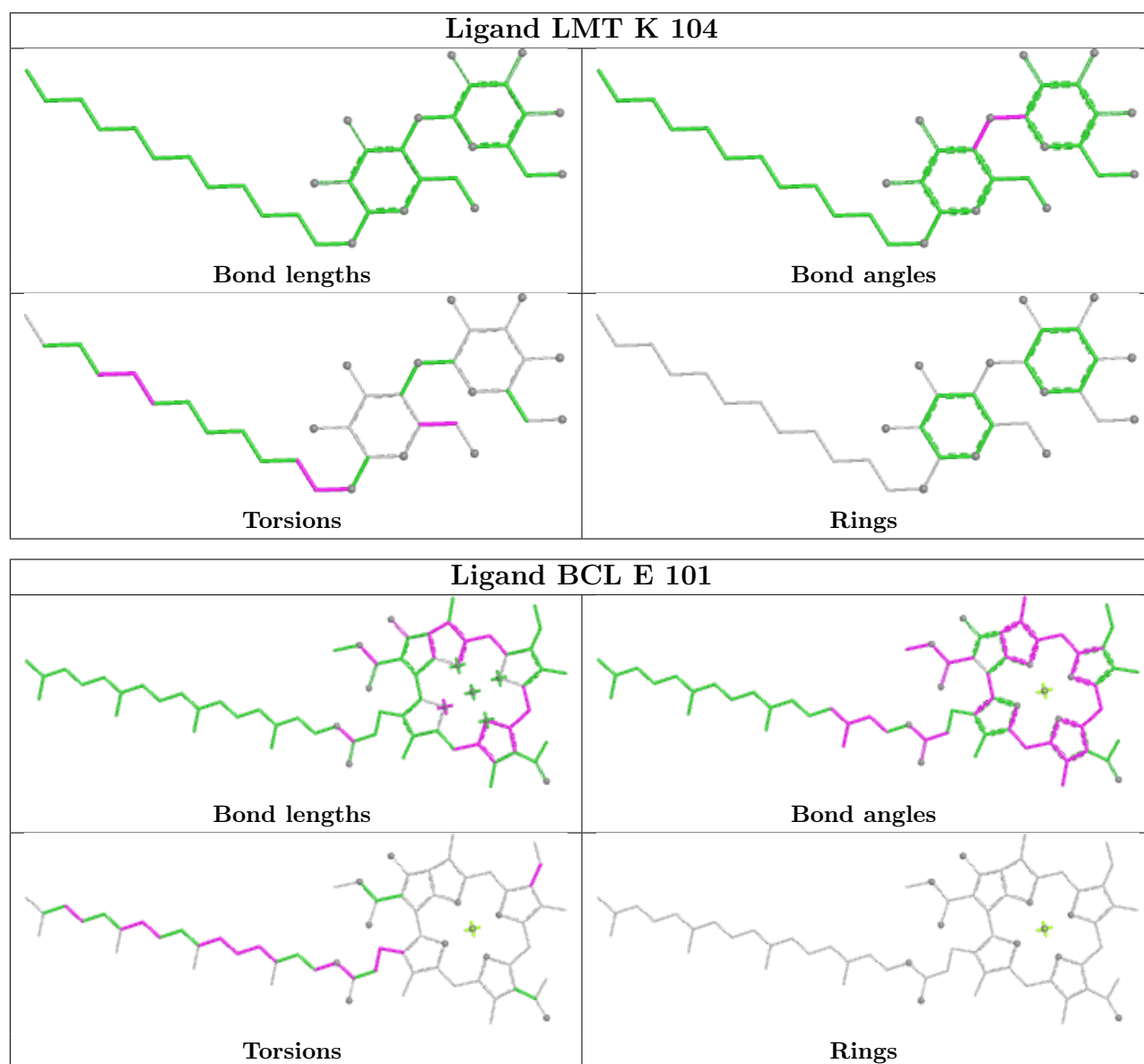












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

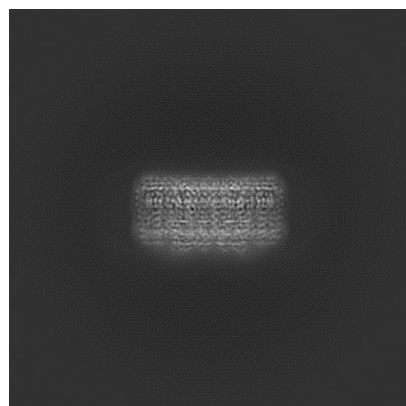
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39835. These allow visual inspection of the internal detail of the map and identification of artifacts.

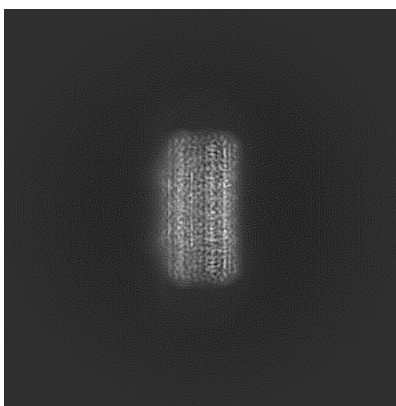
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

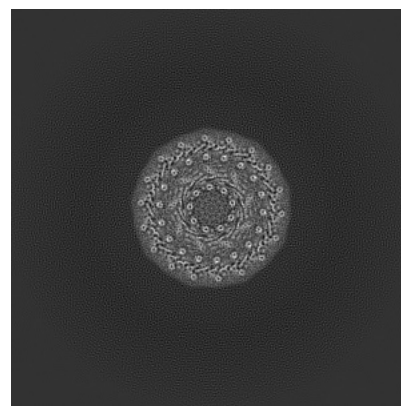
6.1.1 Primary map



X

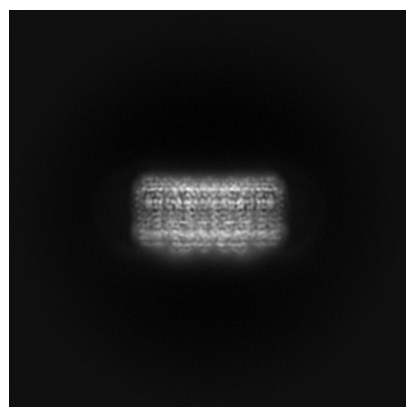


Y

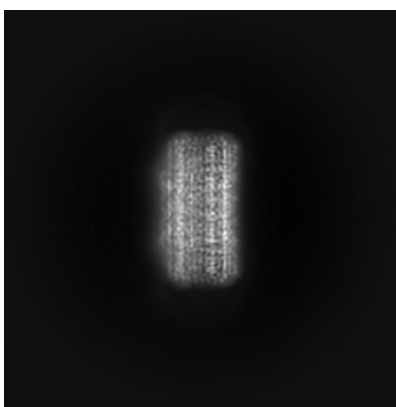


Z

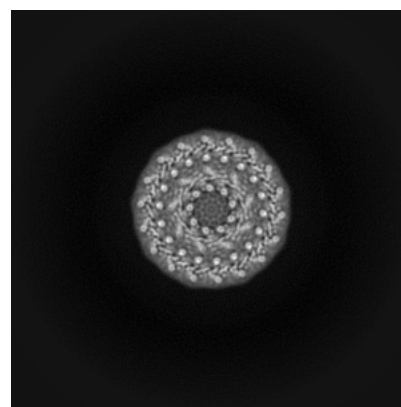
6.1.2 Raw map



X



Y

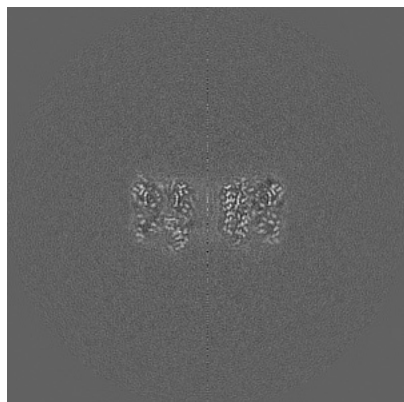


Z

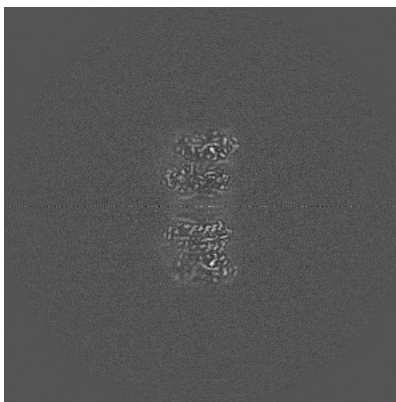
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

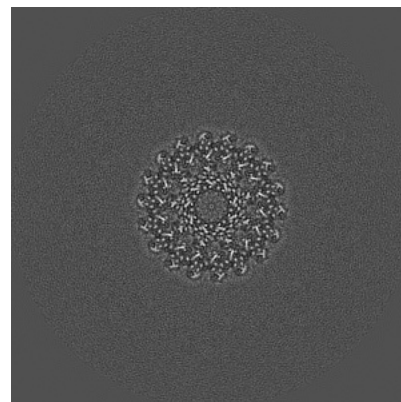
6.2.1 Primary map



X Index: 200

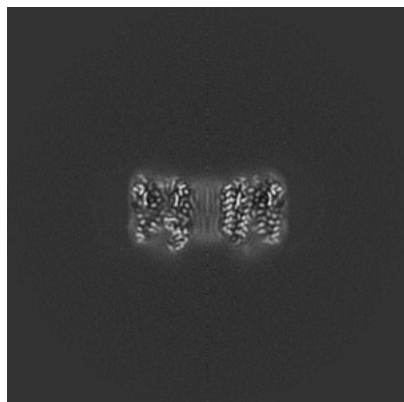


Y Index: 200

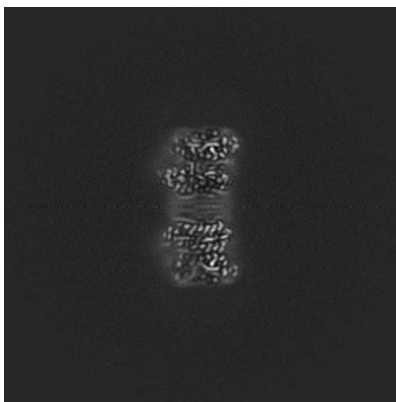


Z Index: 200

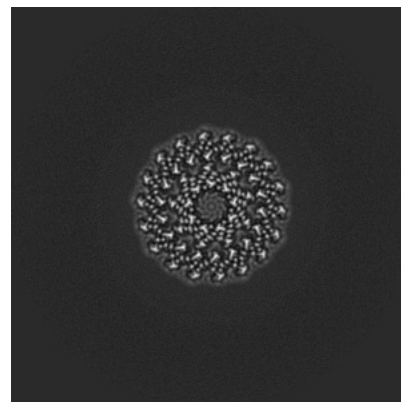
6.2.2 Raw map



X Index: 200



Y Index: 200

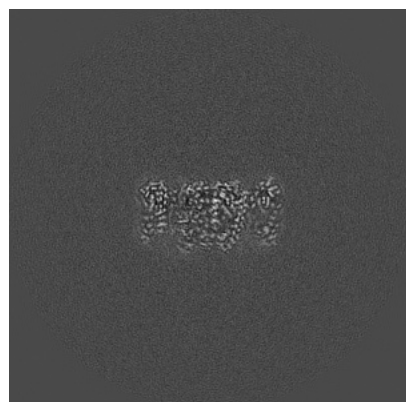


Z Index: 200

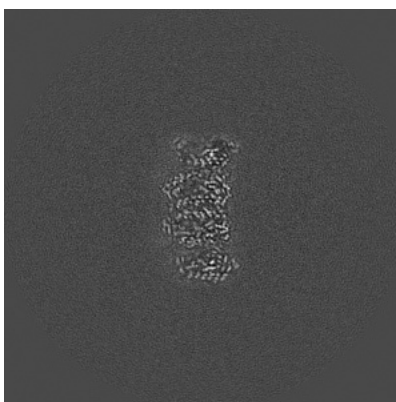
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

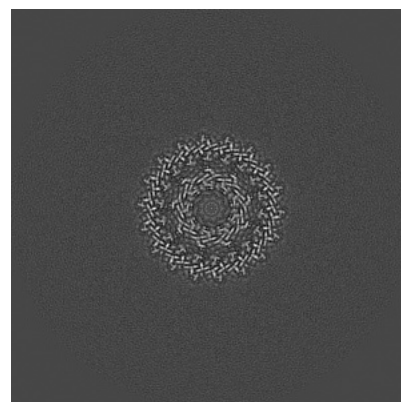
6.3.1 Primary map



X Index: 223

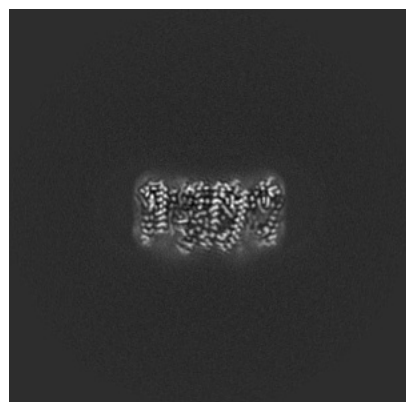


Y Index: 180

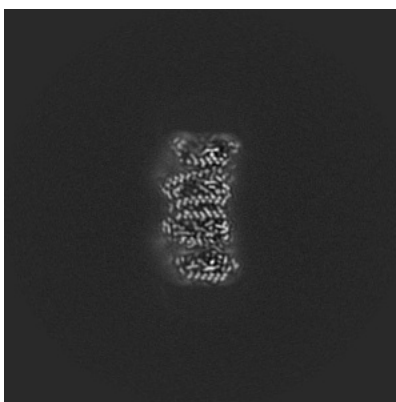


Z Index: 207

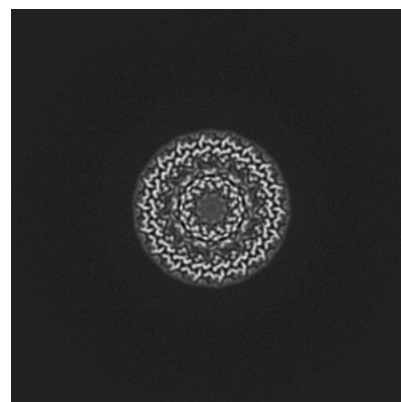
6.3.2 Raw map



X Index: 223



Y Index: 180

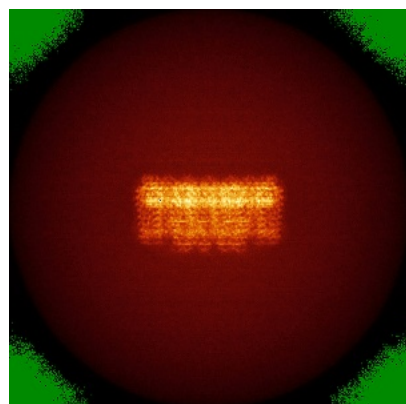


Z Index: 220

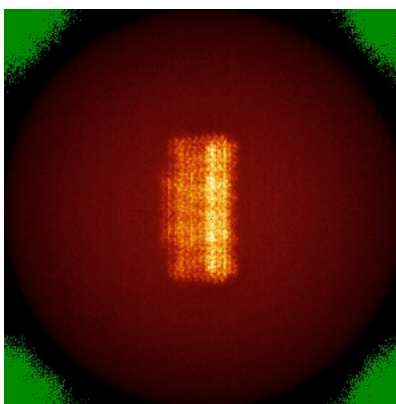
The images above show the largest variance slices of the map in three orthogonal directions.

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

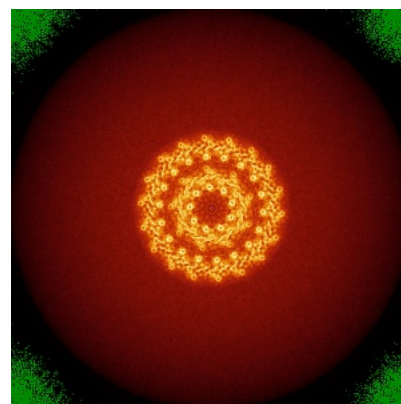
6.4.1 Primary map



X

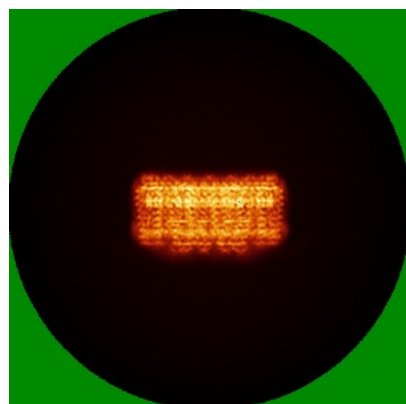


Y

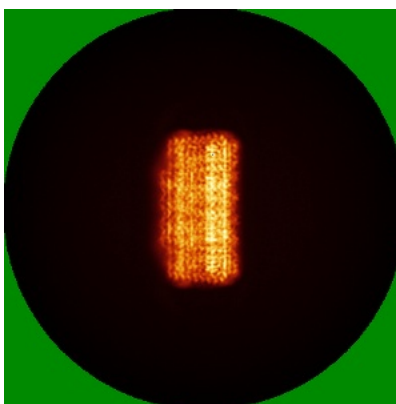


Z

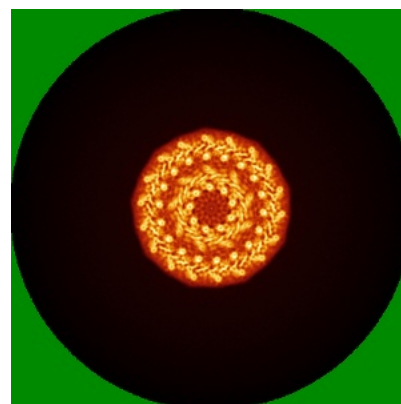
6.4.2 Raw map



X



Y

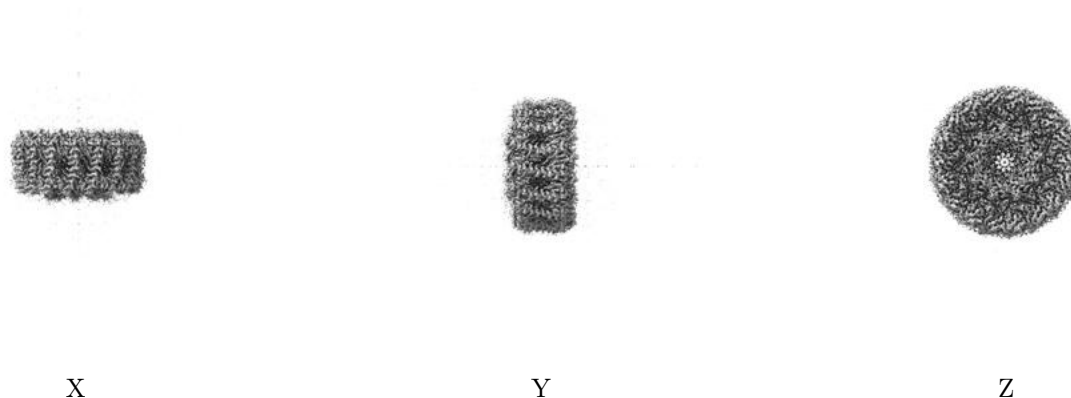


Z

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

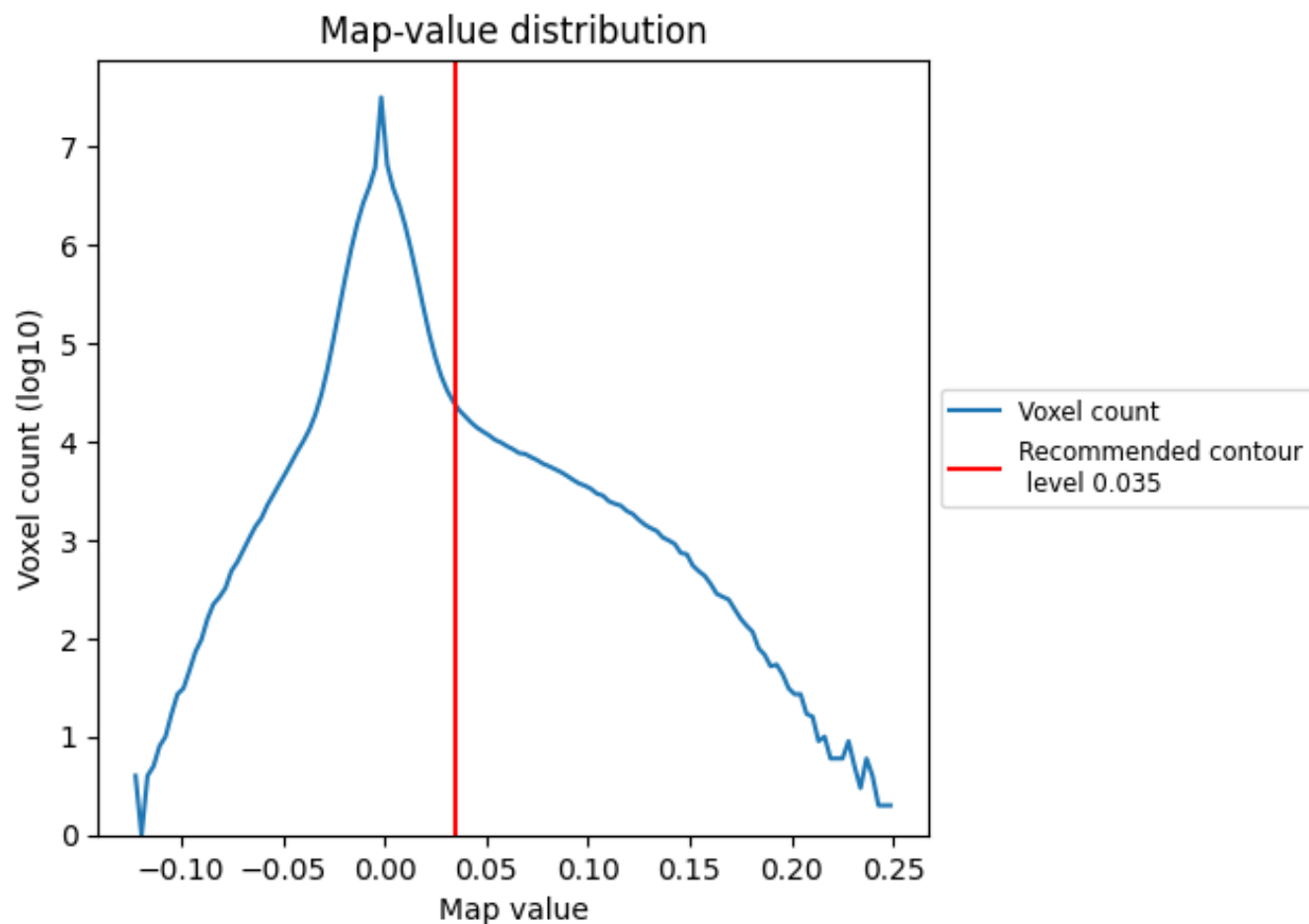
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

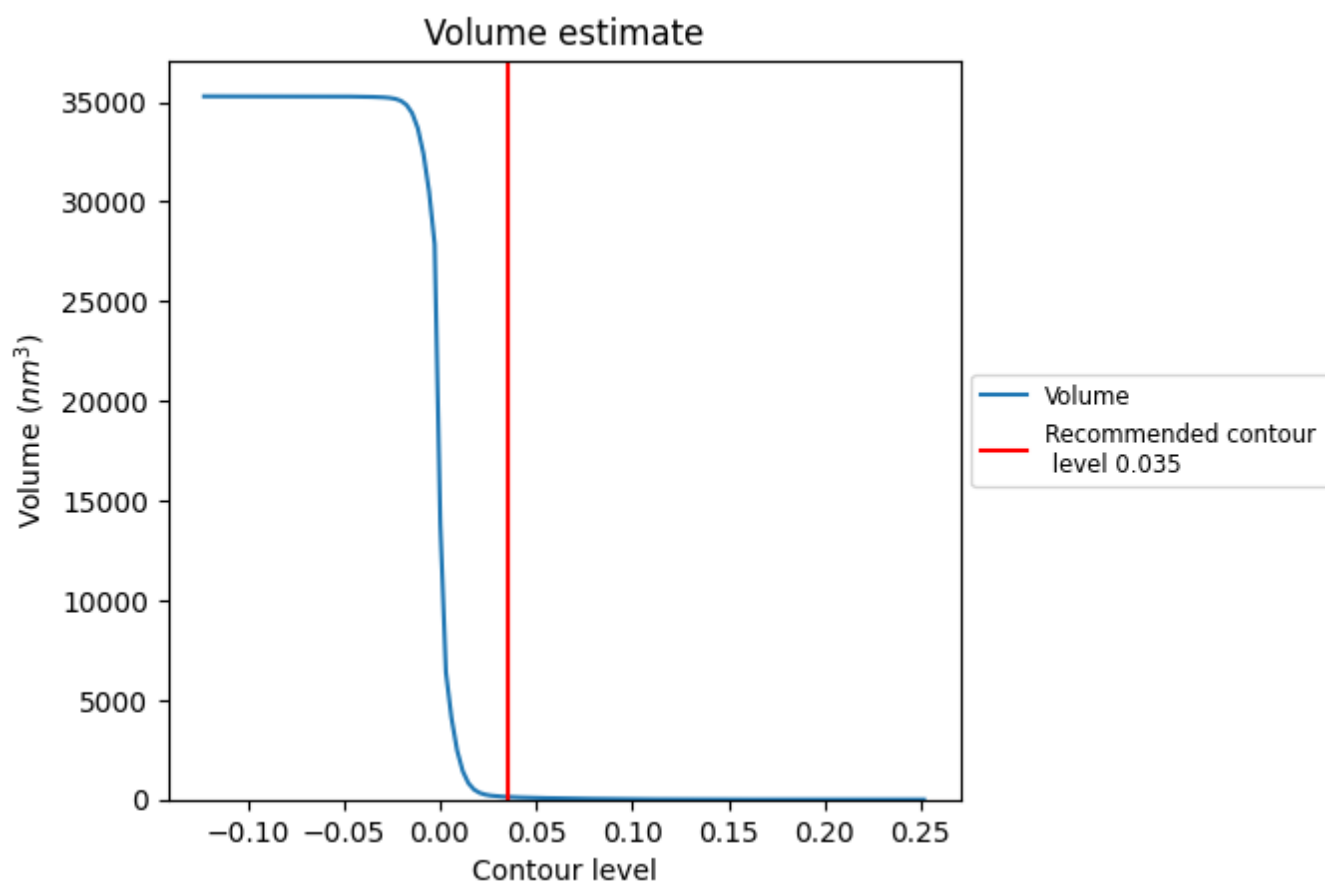
This section contains the results of statistical analysis of the map.

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.

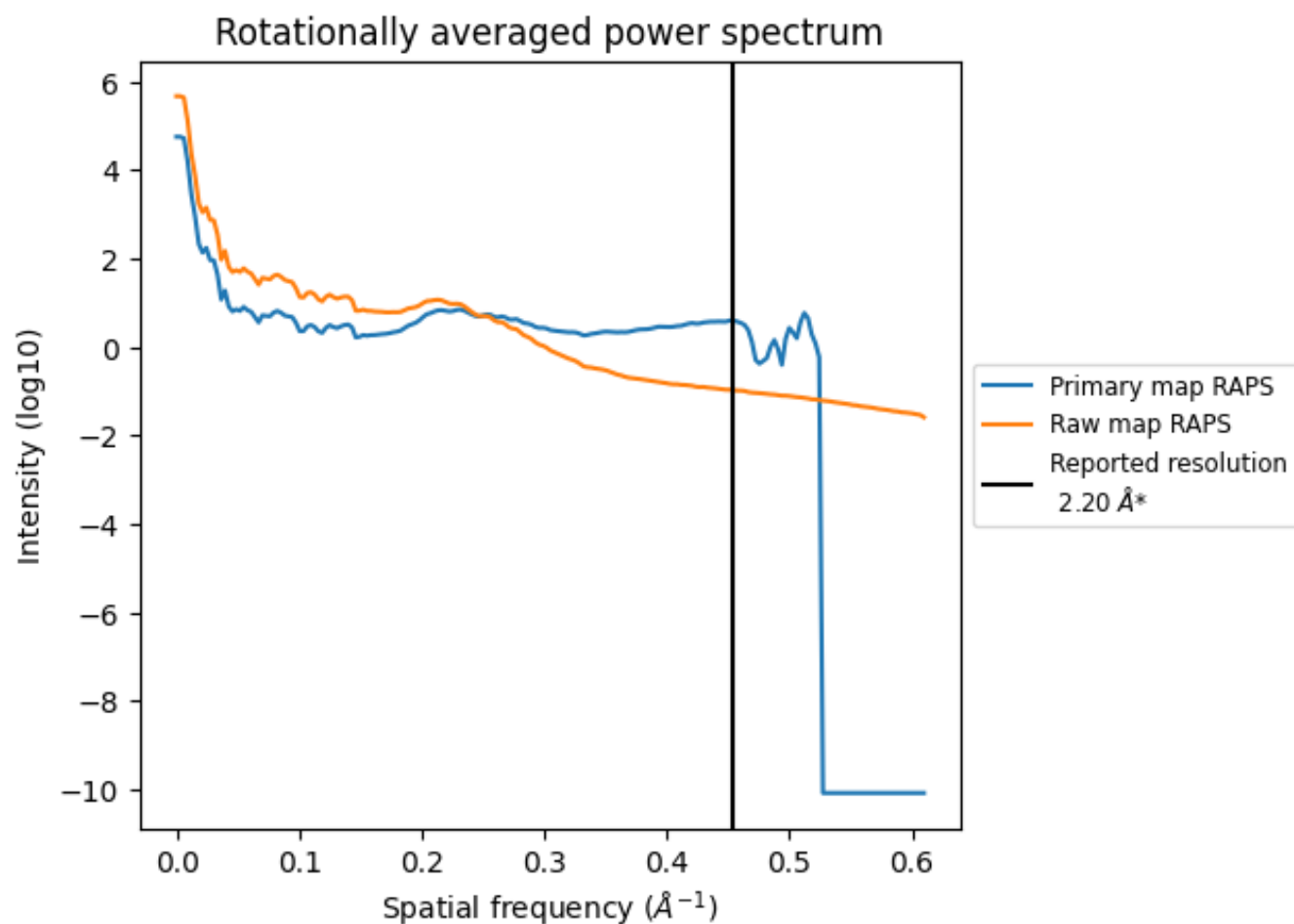
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 134 nm³; this corresponds to an approximate mass of 121 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 ⓘ

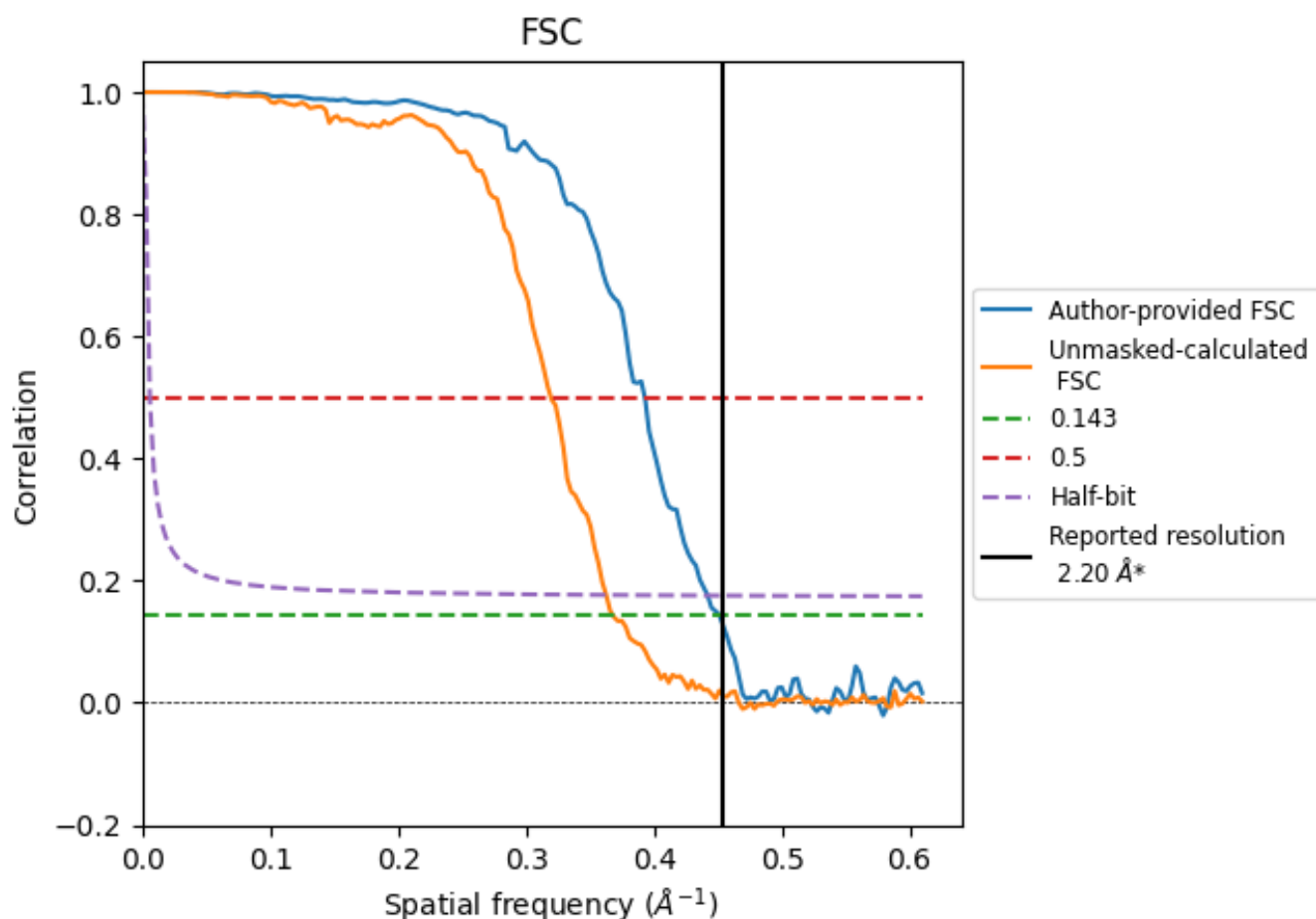


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

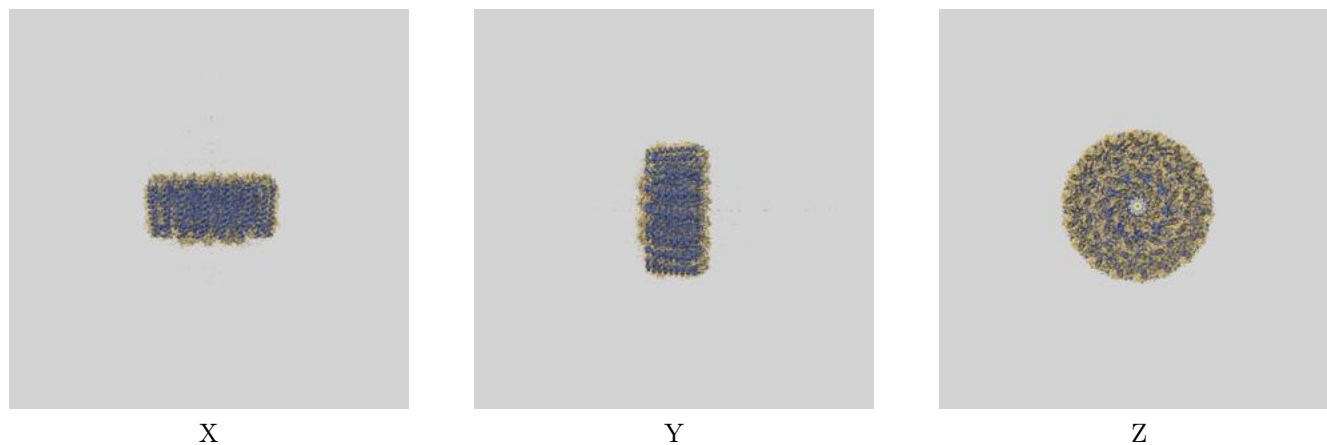
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.22	2.54	2.26
Unmasked-calculated*	2.72	3.13	2.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.72 differs from the reported value 2.2 by more than 10 %

9 Map-model fit [i](#)

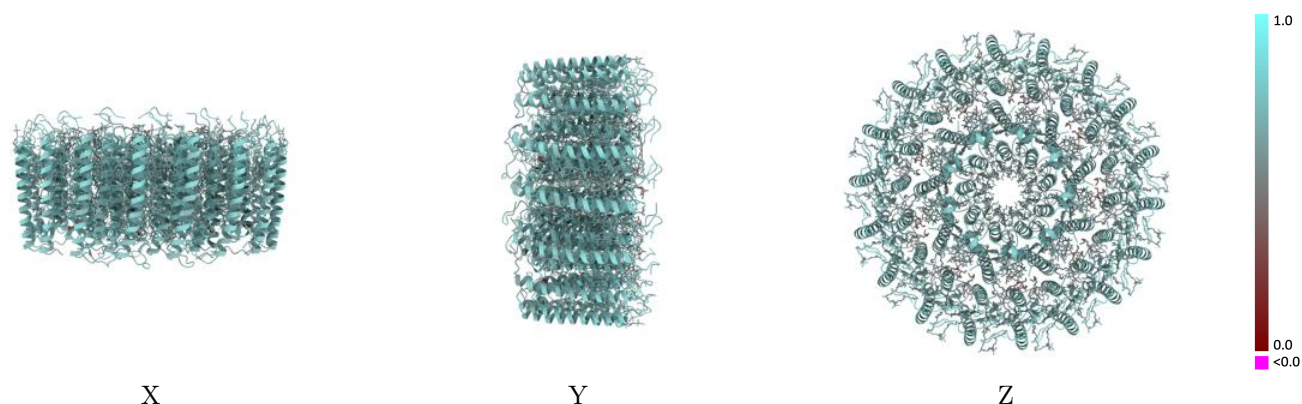
This section contains information regarding the fit between EMDB map EMD-39835 and PDB model 8Z81. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



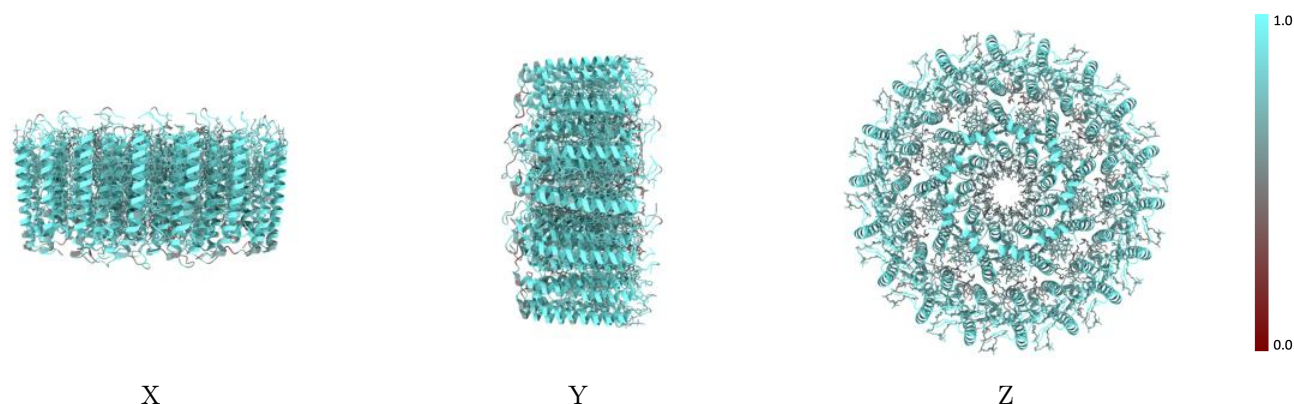
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



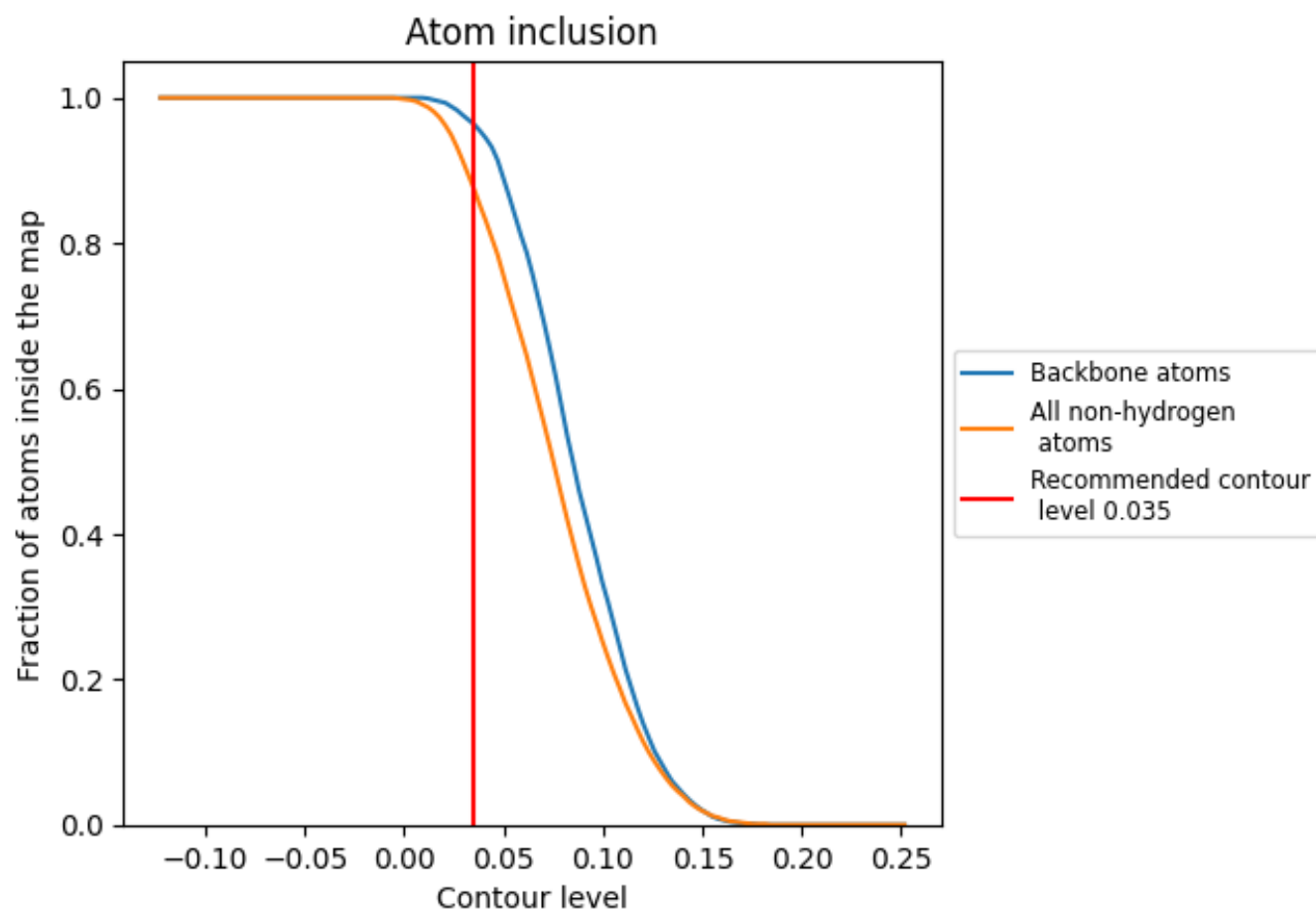
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8750	 0.6820
0	 0.8680	 0.6800
1	 0.8510	 0.6550
2	 0.8620	 0.6750
3	 0.8980	 0.7030
4	 0.8590	 0.6870
5	 0.8460	 0.6530
6	 0.8770	 0.6850
7	 0.9060	 0.7040
8	 0.8610	 0.6870
9	 0.8410	 0.6550
A	 0.9020	 0.7050
B	 0.8650	 0.6870
C	 0.8510	 0.6540
D	 0.8770	 0.6850
E	 0.9060	 0.7070
F	 0.8610	 0.6910
G	 0.8500	 0.6550
H	 0.8850	 0.6850
I	 0.9040	 0.7070
J	 0.8630	 0.6880
K	 0.8530	 0.6550
L	 0.8660	 0.6830
M	 0.8950	 0.7050
N	 0.8630	 0.6900
O	 0.8430	 0.6560
P	 0.8750	 0.6810
Q	 0.9060	 0.7080
R	 0.8630	 0.6900
S	 0.8450	 0.6560
T	 0.8790	 0.6830
U	 0.9020	 0.7040
V	 0.8590	 0.6890
W	 0.8480	 0.6570
X	 0.8770	 0.6820



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Chain	Atom inclusion	Q-score
Y	 0.9020	 0.7040
Z	 0.8830	 0.6940
a	 0.8920	 0.6860
b	 0.8910	 0.6800
c	 0.8870	 0.6880
d	 0.8810	 0.6840
e	 0.8810	 0.6890
f	 0.8870	 0.6830
g	 0.8820	 0.6900
h	 0.8870	 0.6820
i	 0.8810	 0.6890
j	 0.8790	 0.6820
k	 0.8810	 0.6870
l	 0.8850	 0.6800
m	 0.8840	 0.6840
n	 0.8830	 0.6800
o	 0.8760	 0.6840
p	 0.8790	 0.6790
q	 0.8830	 0.6870
r	 0.8900	 0.6810