



## wwPDB EM Validation Summary Report ⓘ

Jan 21, 2025 – 12:29 PM JST

PDB ID : 8Z82  
EMDB ID : EMD-39836  
Title : Photosynthetic LH1-RC-HiPIP complex from the purple bacterium *Halorhodospira halophila*  
Authors : Tani, K.; Kanno, R.; Nagashima, K.V.P.; 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 : 2.40 Å (reported)  
Based on initial models : 5Y5S, 5D8V

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

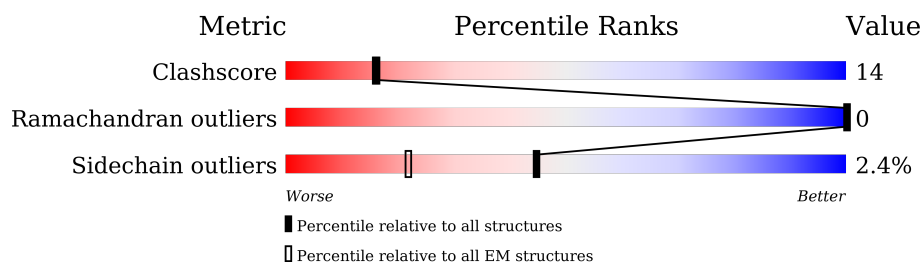
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415




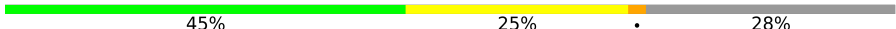


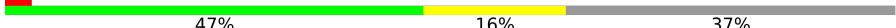









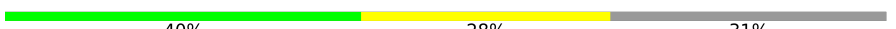
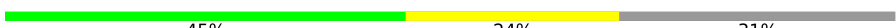

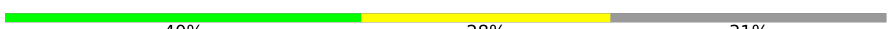
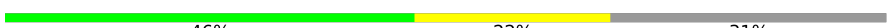
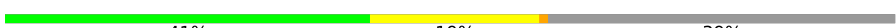



The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey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

Mol	Chain	Length	Quality of chain
1	C	362	73% 18% 7%
2	L	276	72% 28%
3	M	323	77% 21% ..
4	H	278	81% 17% .
5	3	64	52% 20% 28%
5	7	64	45% 27% 28%
5	A	64	53% 19% 28%

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Validation Pipeline (wwPDB-VP) : 2.40

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Mol	Chain	Length	Quality of chain
5	F	64	
5	K	64	
5	Q	64	
5	U	64	
5	Y	64	
6	4	75	
6	8	75	
6	B	75	
6	G	75	
6	N	75	
6	R	75	
6	V	75	
6	Z	75	
7	1	67	
7	5	67	
7	9	67	
7	D	67	
7	I	67	
7	O	67	
7	S	67	
7	W	67	
8	0	74	
8	2	74	
8	6	74	
8	E	74	

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Mol	Chain	Length	Quality of chain
8	J	74	 47% 14% 39%
8	P	74	 54% 7% 39%
8	T	74	 54% 7% 39%
8	X	74	 55% 5% 39%
9	a	142	 7% 63% 33%



## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 29018 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	336	Total	C	N	O	S	0	0
			2642	1616	453	549	24		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	33	THR	SER	conflict	UNP A1WXF5
C	47	ASN	THR	conflict	UNP A1WXF5
C	72	ARG	LYS	conflict	UNP A1WXF5
C	84	ASP	THR	conflict	UNP A1WXF5
C	103	SER	ALA	conflict	UNP A1WXF5
C	143	ASP	GLU	conflict	UNP A1WXF5
C	172	THR	GLU	conflict	UNP A1WXF5
C	173	PRO	LEU	conflict	UNP A1WXF5
C	175	VAL	PHE	conflict	UNP A1WXF5
C	177	MET	VAL	conflict	UNP A1WXF5
C	178	ALA	HIS	conflict	UNP A1WXF5
C	183	THR	ASP	conflict	UNP A1WXF5
C	184	MET	GLN	conflict	UNP A1WXF5
C	193	THR	VAL	conflict	UNP A1WXF5
C	194	GLU	GLY	conflict	UNP A1WXF5
C	195	TYR	PHE	conflict	UNP A1WXF5
C	202	ALA	VAL	conflict	UNP A1WXF5
C	223	HIS	ASN	conflict	UNP A1WXF5
C	239	SER	GLY	conflict	UNP A1WXF5
C	246	ALA	ASP	conflict	UNP A1WXF5
C	269	GLU	VAL	conflict	UNP A1WXF5
C	289	ILE	MET	conflict	UNP A1WXF5
C	298	GLU	ASP	conflict	UNP A1WXF5
C	341	ALA	GLU	conflict	UNP A1WXF5
C	354	ASP	GLU	conflict	UNP A1WXF5
C	360	ASN	ASP	conflict	UNP A1WXF5

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	274	Total	C	N	O	S	0	0
			2170	1461	348	353	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	99	THR	ALA	conflict	UNP A0A2L1K3P0
L	205	PRO	SER	conflict	UNP A0A2L1K3P0
L	220	ILE	VAL	conflict	UNP A0A2L1K3P0
L	241	GLY	ALA	conflict	UNP A0A2L1K3P0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	318	Total	C	N	O	S	0	0
			2518	1679	410	420	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	34	ALA	SER	conflict	UNP A0A2L1K3T5
M	65	ILE	LEU	conflict	UNP A0A2L1K3T5
M	66	VAL	LEU	conflict	UNP A0A2L1K3T5
M	84	LEU	ILE	conflict	UNP A0A2L1K3T5
M	86	PHE	TRP	conflict	UNP A0A2L1K3T5
M	126	VAL	ILE	conflict	UNP A0A2L1K3T5
M	130	PHE	TRP	conflict	UNP A0A2L1K3T5
M	131	ALA	VAL	conflict	UNP A0A2L1K3T5
M	236	GLU	ASP	conflict	UNP A0A2L1K3T5

- Molecule 4 is a protein called Photosynthetic reaction centre, H-chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	278	Total	C	N	O	S	0	0
			2174	1379	374	410	11		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	69	VAL	THR	conflict	UNP A1WXI3
H	97	GLU	ALA	conflict	UNP A1WXI3
H	118	LEU	VAL	conflict	UNP A1WXI3

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Chain	Residue	Modelled	Actual	Comment	Reference
H	135	GLY	ALA	conflict	UNP A1WXI3
H	137	LYS	ASN	conflict	UNP A1WXI3
H	141	CYS	ALA	conflict	UNP A1WXI3
H	158	ALA	ARG	conflict	UNP A1WXI3
H	163	GLU	GLN	conflict	UNP A1WXI3
H	164	ILE	LEU	conflict	UNP A1WXI3
H	171	TYR	ASP	conflict	UNP A1WXI3
H	179	LYS	THR	conflict	UNP A1WXI3
H	210	GLY	SER	conflict	UNP A1WXI3
H	226	SER	GLY	conflict	UNP A1WXI3
H	236	GLN	LYS	conflict	UNP A1WXI3
H	247	ALA	SER	conflict	UNP A1WXI3
H	262	PHE	TYR	conflict	UNP A1WXI3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	F	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	K	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	Q	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	U	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	Y	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	3	46	Total	C	N	O	S	0	0
			385	263	66	55	1		
5	7	46	Total	C	N	O	S	0	0
			385	263	66	55	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	48	Total	C	N	O	S	0	0
			386	259	60	66	1		
6	G	47	Total	C	N	O	S	0	0
			380	256	59	64	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	R	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	V	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	Z	48	Total	C	N	O	S	0	0
			386	259	60	66	1		
6	4	47	Total	C	N	O	S	0	0
			380	256	59	64	1		
6	8	47	Total	C	N	O	S	0	0
			380	256	59	64	1		

- Molecule 7 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	I	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	O	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	S	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	W	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	1	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	5	46	Total	C	N	O	S	0	0
			390	261	67	59	3		
7	9	46	Total	C	N	O	S	0	0
			390	261	67	59	3		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	37	ASN	SER	conflict	UNP A1WXF8
D	42	GLN	GLU	conflict	UNP A1WXF8
D	48	ASP	ASN	conflict	UNP A1WXF8
D	57	ASP	GLU	conflict	UNP A1WXF8
I	37	ASN	SER	conflict	UNP A1WXF8
I	42	GLN	GLU	conflict	UNP A1WXF8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	48	ASP	ASN	conflict	UNP A1WXF8
I	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 8 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	J	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	P	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	T	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	X	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	2	45	Total	C	N	O	S	0	0
			362	240	58	63	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	45	Total	C	N	O	S	0	0
			362	240	58	63	1		
8	0	45	Total	C	N	O	S	0	0
			362	240	58	63	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	30	ILE	VAL	conflict	UNP A1WXF9
J	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

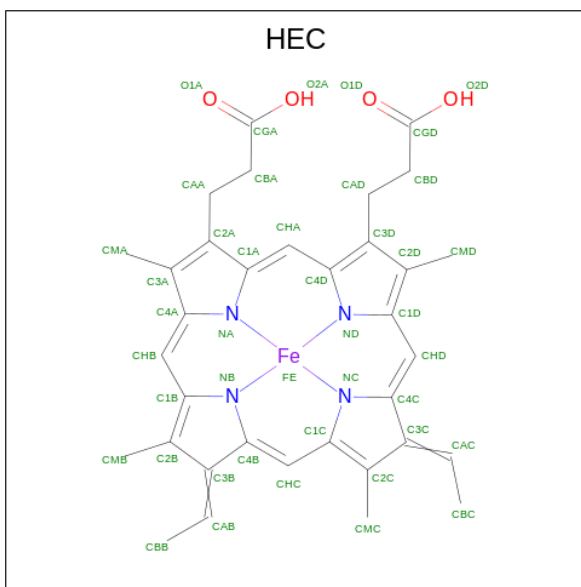
- Molecule 9 is a protein called High-potential iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	95	Total	C	N	O	S	0	0
			736	447	135	147	7		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	3	LYS	ASN	conflict	UNP A1WXH6
a	38	ASP	ASN	conflict	UNP A1WXH6
a	?	-	GLY	deletion	UNP A1WXH6
a	?	-	ASN	deletion	UNP A1WXH6
a	45	ARG	GLN	conflict	UNP A1WXH6
a	114	ASN	SER	conflict	UNP A1WXH6
a	129	VAL	ILE	conflict	UNP A1WXH6
a	136	ALA	GLU	conflict	UNP A1WXH6

- Molecule 10 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).

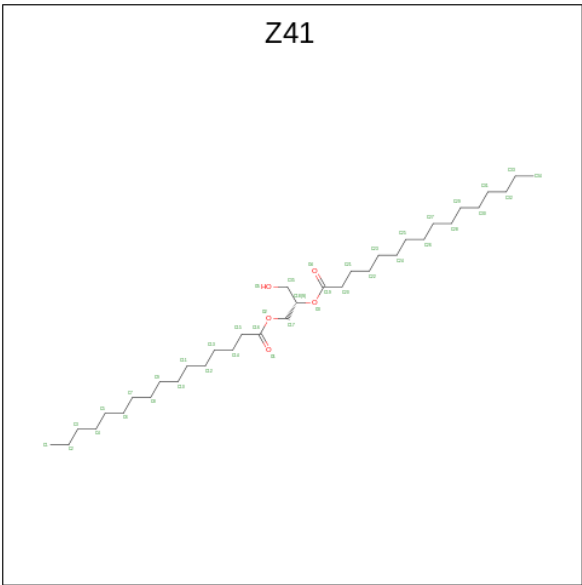


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

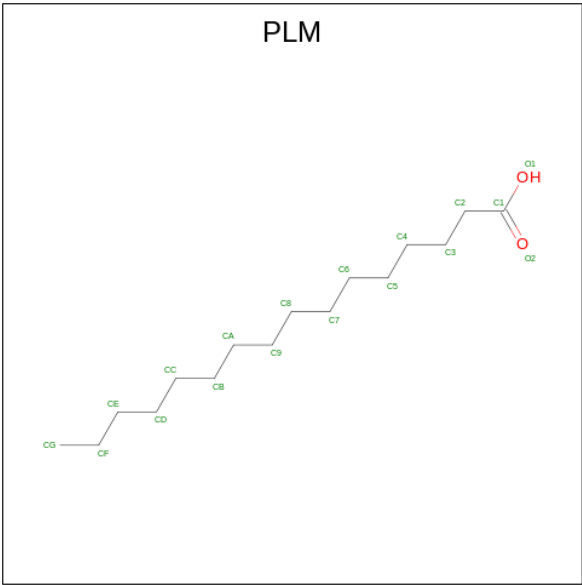
Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	

- Molecule 12 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (three-letter code: Z41) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			31	27	4	

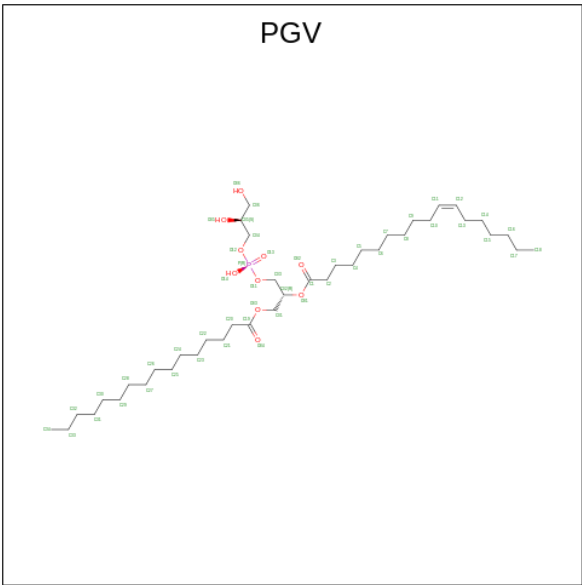
- Molecule 13 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			12	11	1	

- Molecule 14 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).





Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			32	21	10	1	
14	L	1	Total	C	O	P	0
			43	32	10	1	
14	H	1	Total	C	O	P	0
			36	25	10	1	
14	H	1	Total	C	O	P	0
			42	31	10	1	
14	B	1	Total	C	O	P	0
			44	33	10	1	
14	B	1	Total	C	O	P	0
			41	32	8	1	
14	E	1	Total	C	O	P	0
			38	27	10	1	
14	F	1	Total	C	O	P	0
			36	27	8	1	
14	G	1	Total	C	O	P	0
			49	38	10	1	
14	G	1	Total	C	O	P	0
			42	33	8	1	
14	I	1	Total	C	O	P	0
			50	39	10	1	
14	J	1	Total	C	O	P	0
			50	39	10	1	
14	J	1	Total	C	O	P	0
			33	24	8	1	
14	N	1	Total	C	O	P	0
			50	39	10	1	

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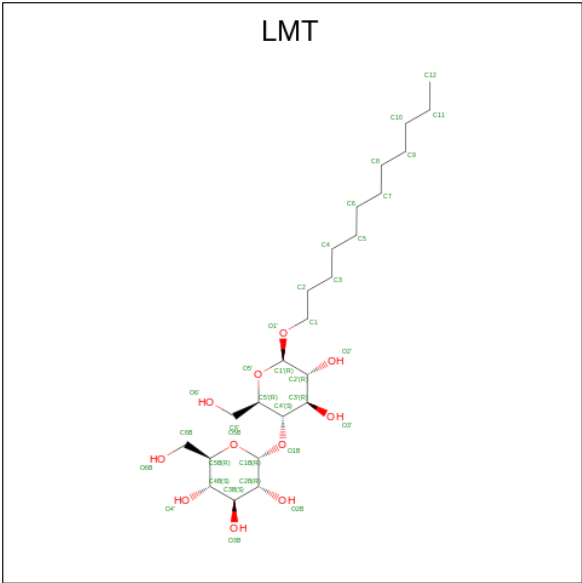
Mol	Chain	Residues	Atoms				AltConf
14	N	1	Total 47	C 36	O 10	P 1	0
14	N	1	Total 37	C 26	O 10	P 1	0
14	O	1	Total 51	C 40	O 10	P 1	0
14	P	1	Total 47	C 36	O 10	P 1	0
14	P	1	Total 40	C 31	O 8	P 1	0
14	R	1	Total 41	C 32	O 8	P 1	0
14	T	1	Total 43	C 32	O 10	P 1	0
14	T	1	Total 46	C 35	O 10	P 1	0
14	T	1	Total 47	C 36	O 10	P 1	0
14	V	1	Total 43	C 32	O 10	P 1	0
14	V	1	Total 44	C 33	O 10	P 1	0
14	X	1	Total 45	C 34	O 10	P 1	0
14	Z	1	Total 46	C 35	O 10	P 1	0
14	Z	1	Total 44	C 33	O 10	P 1	0
14	Z	1	Total 43	C 34	O 8	P 1	0
14	1	1	Total 45	C 34	O 10	P 1	0
14	1	1	Total 41	C 30	O 10	P 1	0
14	2	1	Total 46	C 36	O 9	P 1	0
14	2	1	Total 37	C 27	O 9	P 1	0
14	3	1	Total 30	C 21	O 8	P 1	0
14	4	1	Total 44	C 34	O 9	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
14	6	1	Total	C	O	P	0
			46	35	10	1	
14	6	1	Total	C	O	P	0
			44	34	9	1	
14	6	1	Total	C	O	P	0
			43	32	10	1	
14	8	1	Total	C	O	P	0
			43	32	10	1	
14	0	1	Total	C	O	P	0
			41	30	10	1	
14	0	1	Total	C	O	P	0
			44	33	10	1	
14	0	1	Total	C	O	P	0
			43	32	10	1	

- Molecule 15 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



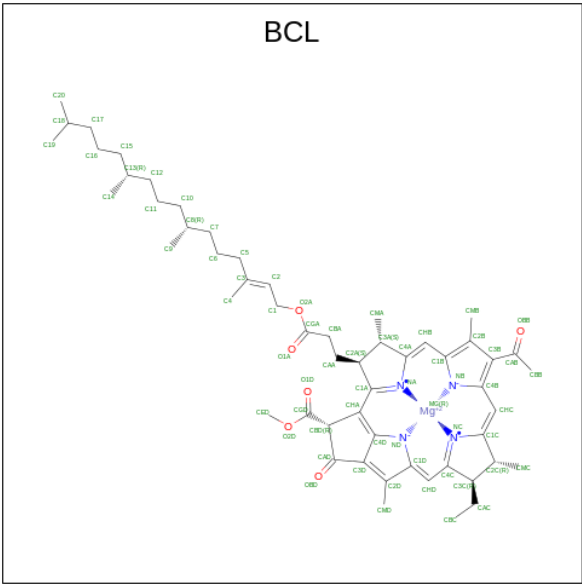
Mol	Chain	Residues	Atoms			AltConf
15	L	1	Total	C	O	0
			25	14	11	
15	M	1	Total	C	O	0
			35	24	11	
15	H	1	Total	C	O	0
			30	19	11	
15	H	1	Total	C	O	0
			26	15	11	

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Mol	Chain	Residues	Atoms			AltConf
15	F	1	Total	C	O	0
			33	22	11	
15	I	1	Total	C	O	0
			25	14	11	
15	O	1	Total	C	O	0
			29	18	11	
15	Q	1	Total	C	O	0
			32	21	11	
15	5	1	Total	C	O	0
			35	24	11	
15	5	1	Total	C	O	0
			24	13	11	
15	7	1	Total	C	O	0
			25	14	11	
15	7	1	Total	C	O	0
			35	24	11	
15	7	1	Total	C	O	0
			35	24	11	

- Molecule 16 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	L	1	Total 66	C 55	Mg 1	N 4	O 6	0

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

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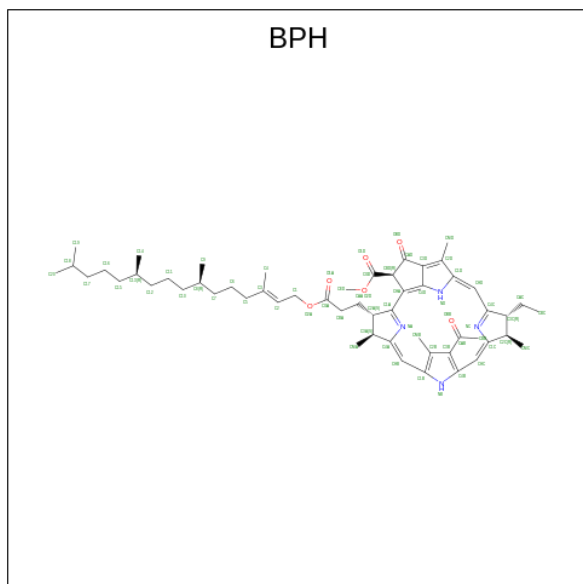
Mol	Chain	Residues	Atoms					AltConf
16	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
16	9	1	Total 66	C 55	Mg 1	N 4	O 6	0

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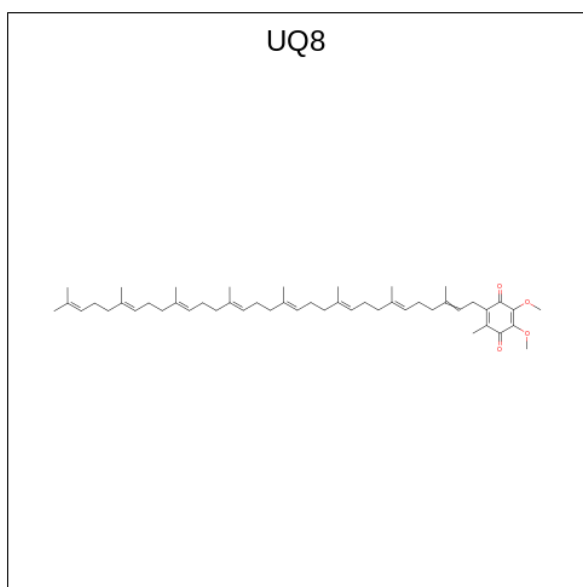
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	0	1	66	55	1	4	6	0

- Molecule 17 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



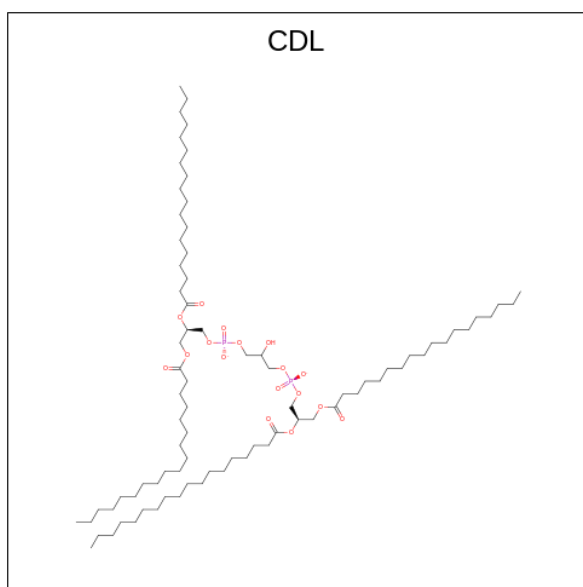
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
17	L	1	65	55	4	6	0
17	M	1	65	55	4	6	0

- Molecule 18 is Ubiquinone-8 (three-letter code: UQ8) (formula:  $C_{49}H_{74}O_4$ ).



Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total	C	O	0
			33	29	4	
18	L	1	Total	C	O	0
			38	34	4	
18	L	1	Total	C	O	0
			17	13	4	

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
19	L	1	Total	C	O	P	0
			75	56	17	2	

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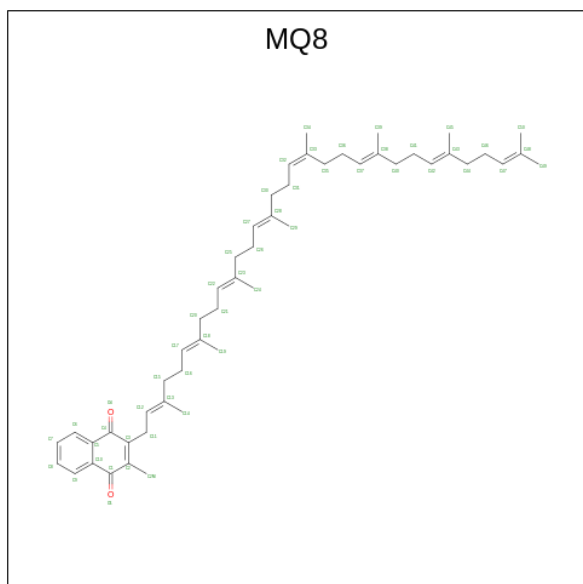
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Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			82	63	17	2	
19	M	1	Total	C	O	P	0
			80	61	17	2	
19	M	1	Total	C	O	P	0
			46	27	17	2	
19	M	1	Total	C	O	P	0
			56	37	17	2	
19	M	1	Total	C	O	P	0
			50	31	17	2	
19	H	1	Total	C	O	P	0
			64	45	17	2	
19	O	1	Total	C	O	P	0
			73	54	17	2	
19	S	1	Total	C	O	P	0
			51	32	17	2	

- Molecule 20 is FE (III) ION (three-letter code: FE) (formula: Fe).

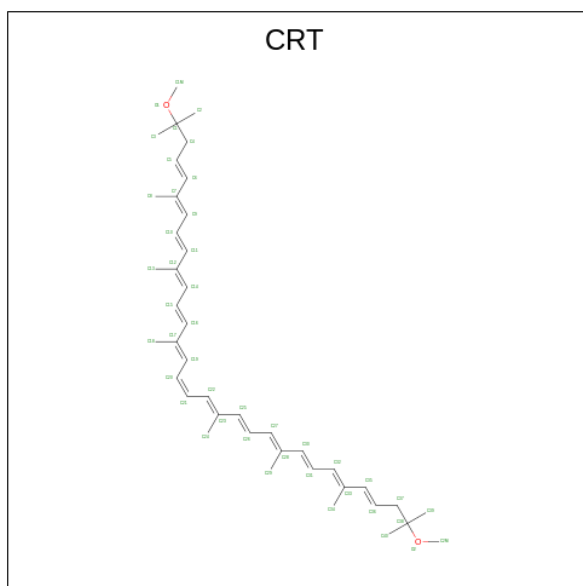
Mol	Chain	Residues	Atoms		AltConf
20	M	1	Total	Fe	0
			1	1	

- Molecule 21 is MENAQUINONE 8 (three-letter code: MQ8) (formula: C<sub>51</sub>H<sub>72</sub>O<sub>2</sub>).



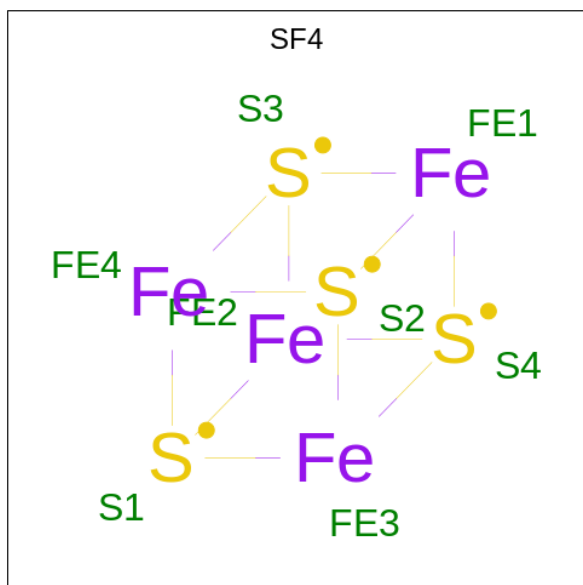
Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			53	51	2	

- Molecule 22 is SPIRILLOXANTHIN (three-letter code: CRT) (formula:  $C_{42}H_{60}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
22	M	1	Total	C	O	0
			44	42	2	
22	B	1	Total	C	O	0
			44	42	2	
22	G	1	Total	C	O	0
			44	42	2	
22	N	1	Total	C	O	0
			44	42	2	
22	R	1	Total	C	O	0
			44	42	2	
22	V	1	Total	C	O	0
			44	42	2	
22	Y	1	Total	C	O	0
			44	42	2	
22	4	1	Total	C	O	0
			44	42	2	
22	8	1	Total	C	O	0
			44	42	2	

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms			AltConf
23	a	1	Total	Fe	S	0
			8	4	4	

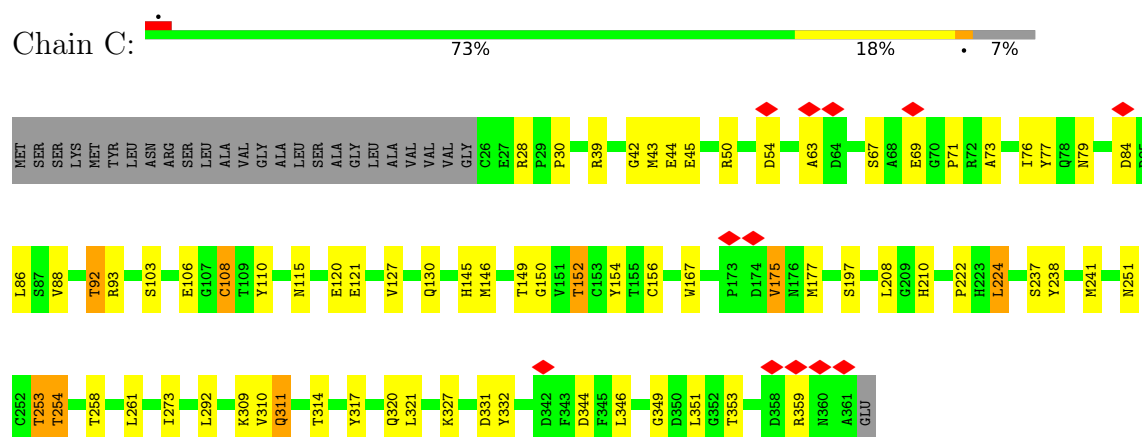
- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	C	4	Total	O	0
			4	4	
24	M	1	Total	O	0
			1	1	

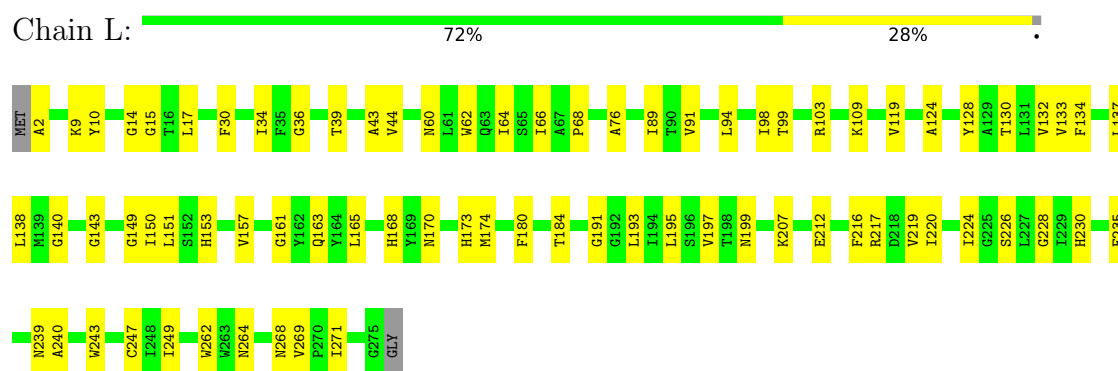
### 3 Residue-property plots

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.

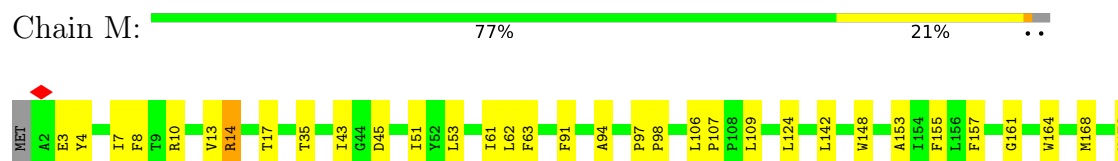
#### • Molecule 1: Photosynthetic reaction center cytochrome c subunit

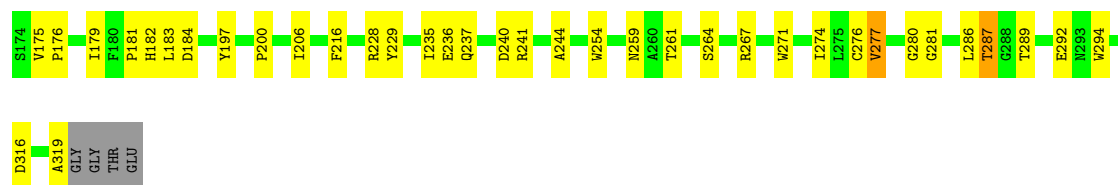


#### • Molecule 2: Reaction center protein L chain

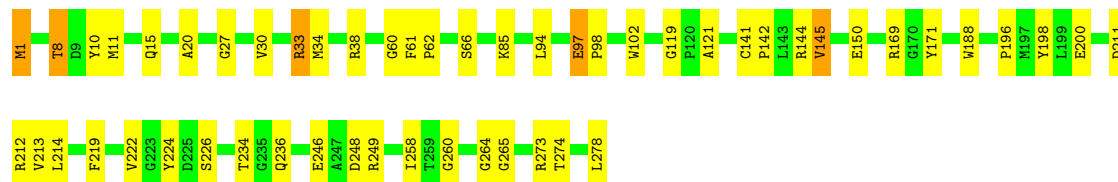
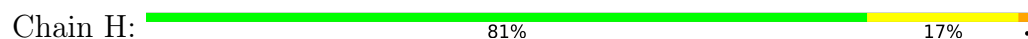


#### • Molecule 3: Reaction center protein M chain





- Molecule 4: Photosynthetic reaction centre, H-chain



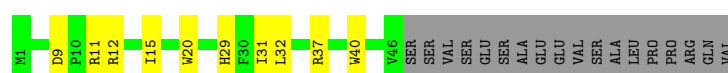
- Molecule 5: Antenna complex, alpha/beta subunit



- 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 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



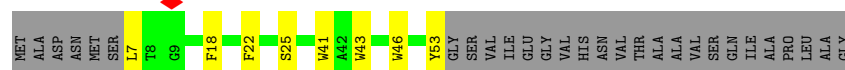
- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



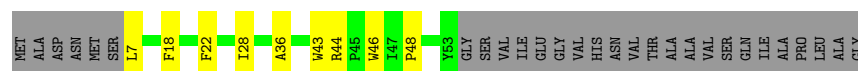
- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 6: Antenna complex, alpha/beta subunit



- Molecule 7: Antenna complex, alpha/beta subunit

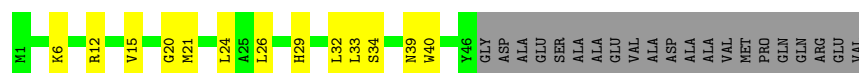


- Molecule 7: Antenna complex, alpha/beta subunit



- Molecule 7: Antenna complex, alpha/beta subunit

Chain O:  49% 19% 31%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain S:  40% 28% 31%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain W:  46% 22% 31%



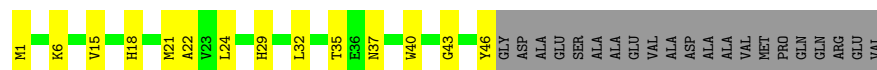
- Molecule 7: Antenna complex, alpha/beta subunit

Chain 1:  46% 22% 31%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain 5:  48% 21% 31%



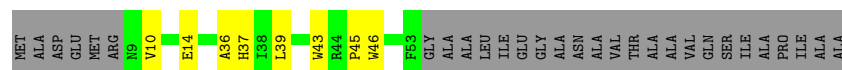
- Molecule 7: Antenna complex, alpha/beta subunit

Chain 9:  40% 28% 31%



- Molecule 8: Antenna complex, alpha/beta subunit

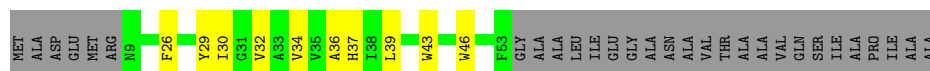
Chain E:  50% 11% 39%



- Molecule 8: Antenna complex, alpha/beta subunit

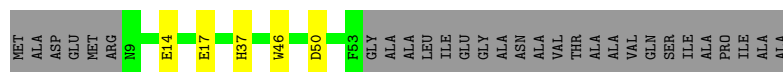


Chain J: 



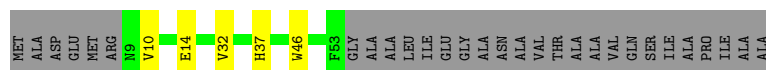
- Molecule 8: Antenna complex, alpha/beta subunit

Chain P: 



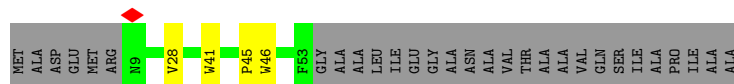
- Molecule 8: Antenna complex, alpha/beta subunit

Chain T: 



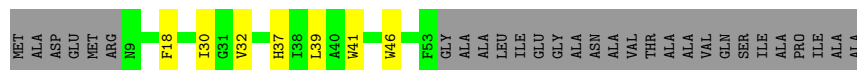
- Molecule 8: Antenna complex, alpha/beta subunit

Chain X: 



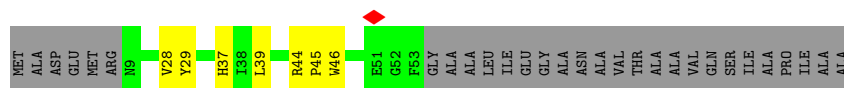
- Molecule 8: Antenna complex, alpha/beta subunit

Chain 2: 



- Molecule 8: Antenna complex, alpha/beta subunit

Chain 6: 

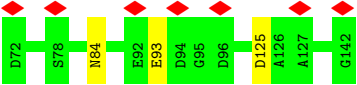
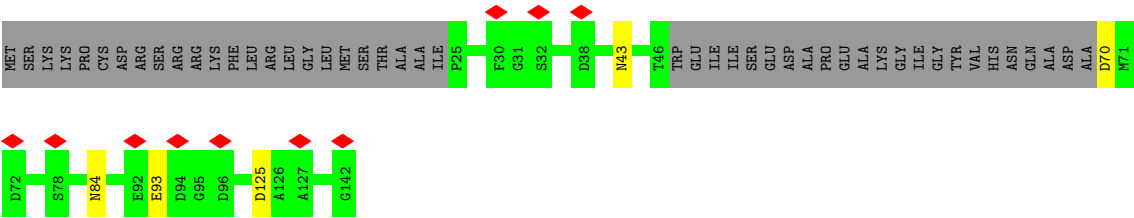


- Molecule 8: Antenna complex, alpha/beta subunit

Chain 0: 



- Molecule 9: High-potential iron-sulfur protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90126	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	0.213	Depositor
Minimum map value	-0.098	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, FE, PGV, PLM, LMT, Z41, HEC, UQ8, BPH, CRT, MG, BCL, SF4, MQ8

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	C	0.26	0/2702	0.50	0/3674
2	L	0.27	0/2252	0.43	0/3082
3	M	0.27	0/2613	0.44	0/3582
4	H	0.27	0/2229	0.49	0/3027
5	3	0.24	0/398	0.45	0/543
5	7	0.24	0/398	0.46	0/543
5	A	0.26	0/398	0.50	0/543
5	F	0.25	0/398	0.46	0/543
5	K	0.24	0/398	0.45	0/543
5	Q	0.24	0/398	0.45	0/543
5	U	0.25	0/398	0.44	0/543
5	Y	0.26	0/398	0.50	0/543
6	4	0.24	0/395	0.37	0/539
6	8	0.25	0/395	0.36	0/539
6	B	0.26	0/401	0.38	0/547
6	G	0.26	0/395	0.35	0/539
6	N	0.25	0/395	0.37	0/539
6	R	0.26	0/395	0.38	0/539
6	V	0.26	0/395	0.36	0/539
6	Z	0.24	0/401	0.38	0/547
7	1	0.25	0/402	0.43	0/547
7	5	0.24	0/402	0.43	0/547
7	9	0.26	0/402	0.42	0/547
7	D	0.26	0/402	0.45	0/547
7	I	0.25	0/402	0.42	0/547
7	O	0.24	0/402	0.43	0/547
7	S	0.25	0/402	0.45	0/547
7	W	0.25	0/402	0.45	0/547
8	0	0.25	0/376	0.35	0/514
8	2	0.26	0/376	0.37	0/514
8	6	0.25	0/376	0.35	0/514
8	E	0.26	0/376	0.36	0/514

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	J	0.25	0/376	0.37	0/514
8	P	0.25	0/376	0.36	0/514
8	T	0.25	0/376	0.35	0/514
8	X	0.25	0/376	0.36	0/514
9	a	0.25	0/755	0.49	0/1020
All	All	0.26	0/23131	0.44	0/31545

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 [i](#)

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	C	2642	0	2401	52	0
2	L	2170	0	2145	68	0
3	M	2518	0	2465	61	0
4	H	2174	0	2131	44	0
5	3	385	0	403	14	0
5	7	385	0	403	17	0
5	A	385	0	403	12	0
5	F	385	0	403	13	0
5	K	385	0	403	10	0
5	Q	385	0	403	15	0
5	U	385	0	403	18	0
5	Y	385	0	403	12	0
6	4	380	0	359	12	0
6	8	380	0	359	12	0
6	B	386	0	364	14	0
6	G	380	0	359	11	0
6	N	380	0	359	8	0
6	R	380	0	359	10	0
6	V	380	0	359	7	0
6	Z	386	0	364	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	390	0	401	18	0
7	5	390	0	401	18	0
7	9	390	0	401	21	0
7	D	390	0	401	22	0
7	I	390	0	401	17	0
7	O	390	0	401	15	0
7	S	390	0	401	20	0
7	W	390	0	401	14	0
8	0	362	0	333	13	0
8	2	362	0	333	10	0
8	6	362	0	333	9	0
8	E	362	0	333	8	0
8	J	362	0	333	16	0
8	P	362	0	333	3	0
8	T	362	0	333	5	0
8	X	362	0	333	5	0
9	a	736	0	641	0	0
10	C	172	0	121	16	0
11	C	1	0	0	0	0
12	C	31	0	0	0	0
13	C	12	0	18	1	0
14	0	128	0	161	10	0
14	1	86	0	108	10	0
14	2	83	0	106	6	0
14	3	30	0	31	3	0
14	4	44	0	59	3	0
14	6	133	0	173	8	0
14	8	43	0	54	7	0
14	B	85	0	107	13	0
14	C	32	0	34	6	0
14	E	38	0	44	2	0
14	F	36	0	41	2	0
14	G	91	0	122	9	0
14	H	78	0	99	6	0
14	I	50	0	71	5	0
14	J	83	0	108	9	0
14	L	43	0	59	6	0
14	N	134	0	178	6	0
14	O	51	0	76	7	0
14	P	87	0	116	6	0
14	R	41	0	53	5	0
14	T	136	0	182	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	V	87	0	110	5	0
14	X	45	0	62	2	0
14	Z	133	0	177	12	0
15	5	59	0	67	4	0
15	7	95	0	115	9	0
15	F	33	0	39	3	0
15	H	56	0	58	4	0
15	I	25	0	23	3	0
15	L	25	0	23	3	0
15	M	35	0	46	1	0
15	O	29	0	31	3	0
15	Q	32	0	37	2	0
16	0	66	0	74	8	0
16	1	132	0	148	15	0
16	2	66	0	74	10	0
16	3	66	0	74	6	0
16	4	66	0	74	9	0
16	5	132	0	148	18	0
16	6	66	0	74	8	0
16	7	66	0	74	3	0
16	8	66	0	74	10	0
16	9	132	0	148	15	0
16	A	66	0	74	5	0
16	B	66	0	74	8	0
16	D	132	0	148	15	0
16	E	66	0	74	9	0
16	F	66	0	74	5	0
16	G	66	0	74	11	0
16	I	132	0	148	19	0
16	J	66	0	74	10	0
16	K	66	0	74	8	0
16	L	198	0	222	16	0
16	M	66	0	74	6	0
16	N	66	0	74	5	0
16	O	132	0	148	13	0
16	P	66	0	74	9	0
16	Q	66	0	74	7	0
16	R	66	0	74	9	0
16	S	132	0	148	20	0
16	T	66	0	74	7	0
16	U	66	0	74	4	0
16	V	66	0	74	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	W	132	0	148	13	0
16	X	66	0	74	5	0
16	Y	132	0	148	9	0
16	Z	66	0	74	8	0
17	L	65	0	76	8	0
17	M	65	0	76	7	0
18	L	88	0	98	12	0
19	H	64	0	72	5	0
19	L	75	0	97	8	0
19	M	314	0	354	26	0
19	O	73	0	90	6	0
19	S	51	0	46	5	0
20	M	1	0	0	0	0
21	M	53	0	72	3	0
22	4	44	0	60	10	0
22	8	44	0	60	8	0
22	B	44	0	60	7	0
22	G	44	0	60	10	0
22	M	44	0	60	8	0
22	N	44	0	60	13	0
22	R	44	0	60	8	0
22	V	44	0	60	8	0
22	Y	44	0	60	8	0
23	a	8	0	0	0	0
24	C	4	0	0	0	0
24	M	1	0	0	0	0
All	All	29018	0	29521	811	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 14.

The worst 5 of 811 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)
1:C:108:CYS:SG	10:C:401:HEC:HAB	1.45	1.52
1:C:108:CYS:SG	10:C:401:HEC:CAB	2.12	1.37
1:C:108:CYS:CB	10:C:401:HEC:HAB	1.59	1.30
1:C:108:CYS:CB	10:C:401:HEC:CAB	2.37	1.02
1:C:108:CYS:HB3	10:C:401:HEC:C3B	2.00	0.90

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/362 (92%)	319 (96%)	15 (4%)	0	100	100
2	L	272/276 (99%)	263 (97%)	9 (3%)	0	100	100
3	M	316/323 (98%)	304 (96%)	12 (4%)	0	100	100
4	H	276/278 (99%)	273 (99%)	3 (1%)	0	100	100
5	3	44/64 (69%)	44 (100%)	0	0	100	100
5	7	44/64 (69%)	44 (100%)	0	0	100	100
5	A	44/64 (69%)	44 (100%)	0	0	100	100
5	F	44/64 (69%)	44 (100%)	0	0	100	100
5	K	44/64 (69%)	44 (100%)	0	0	100	100
5	Q	44/64 (69%)	44 (100%)	0	0	100	100
5	U	44/64 (69%)	44 (100%)	0	0	100	100
5	Y	44/64 (69%)	44 (100%)	0	0	100	100
6	4	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	8	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
6	B	46/75 (61%)	44 (96%)	2 (4%)	0	100	100
6	G	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
6	N	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	R	45/75 (60%)	43 (96%)	2 (4%)	0	100	100
6	V	45/75 (60%)	44 (98%)	1 (2%)	0	100	100
6	Z	46/75 (61%)	43 (94%)	3 (6%)	0	100	100
7	1	44/67 (66%)	44 (100%)	0	0	100	100
7	5	44/67 (66%)	44 (100%)	0	0	100	100
7	9	44/67 (66%)	43 (98%)	1 (2%)	0	100	100
7	D	44/67 (66%)	44 (100%)	0	0	100	100
7	I	44/67 (66%)	44 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	O	44/67 (66%)	44 (100%)	0	0	100	100
7	S	44/67 (66%)	44 (100%)	0	0	100	100
7	W	44/67 (66%)	44 (100%)	0	0	100	100
8	0	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	2	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	6	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
8	E	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	J	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	P	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
8	T	43/74 (58%)	41 (95%)	2 (5%)	0	100	100
8	X	43/74 (58%)	42 (98%)	1 (2%)	0	100	100
9	a	91/142 (64%)	84 (92%)	7 (8%)	0	100	100
All	All	2699/3621 (74%)	2628 (97%)	71 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	287/306 (94%)	271 (94%)	16 (6%)	17	30
2	L	218/219 (100%)	217 (100%)	1 (0%)	86	94
3	M	252/255 (99%)	243 (96%)	9 (4%)	30	49
4	H	228/228 (100%)	220 (96%)	8 (4%)	31	51
5	3	39/55 (71%)	39 (100%)	0	100	100
5	7	39/55 (71%)	38 (97%)	1 (3%)	41	62
5	A	39/55 (71%)	39 (100%)	0	100	100
5	F	39/55 (71%)	39 (100%)	0	100	100
5	K	39/55 (71%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	39/55 (71%)	38 (97%)	1 (3%)	41	62
5	U	39/55 (71%)	37 (95%)	2 (5%)	20	35
5	Y	39/55 (71%)	39 (100%)	0	100	100
6	4	37/57 (65%)	37 (100%)	0	100	100
6	8	37/57 (65%)	37 (100%)	0	100	100
6	B	38/57 (67%)	37 (97%)	1 (3%)	41	62
6	G	37/57 (65%)	37 (100%)	0	100	100
6	N	37/57 (65%)	37 (100%)	0	100	100
6	R	37/57 (65%)	37 (100%)	0	100	100
6	V	37/57 (65%)	37 (100%)	0	100	100
6	Z	38/57 (67%)	35 (92%)	3 (8%)	10	16
7	1	41/55 (74%)	41 (100%)	0	100	100
7	5	41/55 (74%)	41 (100%)	0	100	100
7	9	41/55 (74%)	41 (100%)	0	100	100
7	D	41/55 (74%)	41 (100%)	0	100	100
7	I	41/55 (74%)	40 (98%)	1 (2%)	44	64
7	O	41/55 (74%)	41 (100%)	0	100	100
7	S	41/55 (74%)	41 (100%)	0	100	100
7	W	41/55 (74%)	40 (98%)	1 (2%)	44	64
8	0	35/52 (67%)	32 (91%)	3 (9%)	8	14
8	2	35/52 (67%)	35 (100%)	0	100	100
8	6	35/52 (67%)	35 (100%)	0	100	100
8	E	35/52 (67%)	34 (97%)	1 (3%)	37	58
8	J	35/52 (67%)	35 (100%)	0	100	100
8	P	35/52 (67%)	34 (97%)	1 (3%)	37	58
8	T	35/52 (67%)	35 (100%)	0	100	100
8	X	35/52 (67%)	35 (100%)	0	100	100
9	a	73/111 (66%)	68 (93%)	5 (7%)	13	22
All	All	2276/2871 (79%)	2222 (98%)	54 (2%)	45	64

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	33	ARG
8	E	14	GLU
9	a	43	ASN
4	H	97	GLU
4	H	169	ARG

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

Mol	Chain	Res	Type
1	C	96	GLN
2	L	213	ASN
4	H	138	GLN
4	H	231	ASN
8	0	24	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 133 ligands modelled in this entry, 2 are monoatomic - leaving 131 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	PGV	P	102	-	46,46,50	0.95	2 (4%)	49,52,56	1.12	4 (8%)
14	PGV	I	101	-	49,49,50	0.93	2 (4%)	52,55,56	1.00	2 (3%)
14	PGV	Z	104	-	42,42,50	1.01	2 (4%)	45,47,56	1.09	3 (6%)
14	PGV	F	101	-	35,35,50	1.08	2 (5%)	38,40,56	1.09	2 (5%)
14	PGV	8	103	-	42,42,50	0.99	2 (4%)	45,48,56	1.01	3 (6%)
16	BCL	T	102	-	64,74,74	1.72	14 (21%)	78,115,115	2.14	21 (26%)
16	BCL	5	104	-	64,74,74	1.76	14 (21%)	78,115,115	2.18	22 (28%)
23	SF4	a	201	9	0,12,12	-	-	-	-	-
15	LMT	7	101	-	26,26,36	0.53	0	37,37,47	0.97	2 (5%)
18	UQ8	L	306	-	38,38,53	1.41	2 (5%)	46,49,67	1.58	9 (19%)
19	CDL	M	407	-	79,79,99	1.01	4 (5%)	85,91,111	1.05	5 (5%)
19	CDL	O	101	-	72,72,99	1.07	4 (5%)	78,84,111	1.14	6 (7%)
10	HEC	C	401	1	32,50,50	1.59	4 (12%)	24,82,82	1.38	2 (8%)
16	BCL	O	105	-	64,74,74	1.74	14 (21%)	78,115,115	2.19	21 (26%)
14	PGV	6	101	-	45,45,50	0.95	2 (4%)	48,51,56	1.10	3 (6%)
22	CRT	4	101	-	41,43,43	0.72	0	50,54,54	3.50	15 (30%)
16	BCL	7	104	-	64,74,74	1.69	12 (18%)	78,115,115	2.29	24 (30%)
14	PGV	0	103	-	43,43,50	0.98	2 (4%)	46,49,56	0.95	2 (4%)
19	CDL	M	402	-	81,81,99	1.04	4 (4%)	87,93,111	1.01	4 (4%)
14	PGV	T	101	-	42,42,50	0.99	2 (4%)	45,48,56	1.13	4 (8%)
18	UQ8	L	304	-	33,33,53	1.51	2 (6%)	40,43,67	1.59	8 (20%)
19	CDL	M	408	-	45,45,99	1.40	4 (8%)	51,57,111	1.41	6 (11%)
16	BCL	I	104	-	64,74,74	1.76	14 (21%)	78,115,115	2.21	23 (29%)
14	PGV	B	104	-	40,40,50	1.00	2 (5%)	42,45,56	1.14	3 (7%)
15	LMT	5	101	-	36,36,36	0.38	0	47,47,47	0.80	1 (2%)
22	CRT	R	101	-	41,43,43	0.72	0	50,54,54	3.51	18 (36%)
14	PGV	4	103	-	43,43,50	1.00	2 (4%)	46,48,56	1.12	3 (6%)
19	CDL	L	310	-	74,74,99	1.06	4 (5%)	80,86,111	1.11	6 (7%)
22	CRT	N	102	-	41,43,43	0.71	0	50,54,54	3.46	13 (26%)
14	PGV	P	103	-	39,39,50	1.07	2 (5%)	43,44,56	1.18	4 (9%)
14	PGV	2	102	-	45,45,50	0.98	2 (4%)	48,50,56	1.03	2 (4%)
15	LMT	5	102	-	25,25,36	0.46	0	36,36,47	0.70	1 (2%)
19	CDL	S	101	-	50,50,99	1.30	4 (8%)	56,62,111	1.29	6 (10%)
16	BCL	W	102	-	64,74,74	1.76	14 (21%)	78,115,115	2.23	20 (25%)
15	LMT	7	102	-	36,36,36	0.41	0	47,47,47	0.77	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	BCL	Z	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.20	19 (24%)
16	BCL	Y	401	19	64,74,74	1.71	13 (20%)	78,115,115	2.19	21 (26%)
14	PGV	0	101	-	40,40,50	1.02	2 (5%)	43,46,56	1.05	2 (4%)
16	BCL	X	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.20	20 (25%)
21	MQ8	M	405	-	54,54,54	1.32	2 (3%)	66,69,69	1.58	14 (21%)
14	PGV	R	103	-	40,40,50	1.04	2 (5%)	43,45,56	1.12	3 (6%)
22	CRT	M	406	-	41,43,43	0.71	0	50,54,54	1.85	14 (28%)
14	PGV	1	102	-	40,40,50	1.02	2 (5%)	42,46,56	1.10	3 (7%)
15	LMT	H	305	-	27,27,36	0.43	0	37,38,47	0.67	1 (2%)
15	LMT	O	103	-	30,30,36	0.42	0	41,41,47	0.92	2 (4%)
10	HEC	C	404	1	32,50,50	1.54	4 (12%)	24,82,82	1.41	2 (8%)
14	PGV	G	104	-	41,41,50	1.00	2 (4%)	44,46,56	1.11	3 (6%)
14	PGV	T	104	-	46,46,50	0.94	2 (4%)	48,52,56	0.96	3 (6%)
16	BCL	K	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.29	19 (24%)
14	PGV	H	302	-	35,35,50	1.08	2 (5%)	38,41,56	1.15	3 (7%)
14	PGV	6	103	-	42,43,50	0.98	2 (4%)	45,49,56	1.06	3 (6%)
14	PGV	C	408	-	31,31,50	1.15	2 (6%)	34,37,56	1.23	3 (8%)
16	BCL	N	103	-	64,74,74	1.71	14 (21%)	78,115,115	2.13	16 (20%)
14	PGV	O	102	-	50,50,50	0.92	2 (4%)	53,56,56	1.07	3 (5%)
18	UQ8	L	307	-	17,17,53	2.27	3 (17%)	19,23,67	2.04	6 (31%)
16	BCL	E	101	-	64,74,74	1.69	14 (21%)	78,115,115	2.20	19 (24%)
13	PLM	C	407	-	11,11,17	0.40	0	10,10,17	0.47	0
16	BCL	0	102	-	64,74,74	1.73	14 (21%)	78,115,115	2.18	18 (23%)
15	LMT	L	301	-	26,26,36	0.45	0	37,37,47	0.85	1 (2%)
14	PGV	V	103	-	42,42,50	1.00	2 (4%)	44,48,56	1.12	3 (6%)
16	BCL	R	102	-	64,74,74	1.68	14 (21%)	78,115,115	2.25	18 (23%)
16	BCL	8	102	-	64,74,74	1.68	14 (21%)	78,115,115	2.27	21 (26%)
16	BCL	I	103	-	64,74,74	1.72	14 (21%)	78,115,115	2.23	24 (30%)
14	PGV	6	104	-	42,42,50	1.00	2 (4%)	45,48,56	1.02	3 (6%)
10	HEC	C	403	1	32,50,50	1.57	4 (12%)	24,82,82	1.57	3 (12%)
22	CRT	B	101	-	41,43,43	0.74	0	50,54,54	3.42	13 (26%)
16	BCL	1	103	-	64,74,74	1.74	14 (21%)	78,115,115	2.25	24 (30%)
22	CRT	8	101	-	41,43,43	0.75	0	50,54,54	3.57	16 (32%)
14	PGV	E	102	-	37,37,50	1.06	2 (5%)	39,43,56	1.11	3 (7%)
16	BCL	5	103	-	64,74,74	1.69	14 (21%)	78,115,115	2.24	24 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	LMT	I	102	-	26,26,36	0.49	0	37,37,47	1.08	3 (8%)
16	BCL	M	403	-	64,74,74	1.71	13 (20%)	78,115,115	2.38	22 (28%)
14	PGV	3	101	-	29,29,50	1.19	2 (6%)	32,34,56	1.25	4 (12%)
16	BCL	G	103	-	64,74,74	1.70	13 (20%)	78,115,115	2.22	20 (25%)
14	PGV	2	103	-	36,36,50	1.08	2 (5%)	39,41,56	1.09	2 (5%)
16	BCL	Q	102	-	64,74,74	1.69	14 (21%)	78,115,115	2.32	20 (25%)
16	BCL	D	101	-	64,74,74	1.72	14 (21%)	78,115,115	2.31	23 (29%)
14	PGV	1	101	-	44,44,50	0.99	2 (4%)	47,50,56	1.04	3 (6%)
16	BCL	6	102	-	64,74,74	1.69	14 (21%)	78,115,115	2.17	20 (25%)
17	BPH	M	404	-	51,70,70	0.47	0	52,101,101	0.68	1 (1%)
16	BCL	S	103	-	64,74,74	1.76	14 (21%)	78,115,115	2.22	22 (28%)
22	CRT	G	102	-	41,43,43	0.76	0	50,54,54	3.51	16 (32%)
14	PGV	X	102	-	44,44,50	0.98	2 (4%)	47,50,56	1.09	3 (6%)
12	Z41	C	406	1	30,30,39	0.28	0	32,32,41	0.47	0
16	BCL	S	102	-	64,74,74	1.71	14 (21%)	78,115,115	2.26	25 (32%)
16	BCL	3	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.27	21 (26%)
16	BCL	9	101	-	64,74,74	1.72	14 (21%)	78,115,115	2.22	20 (25%)
16	BCL	V	102	-	64,74,74	1.68	14 (21%)	78,115,115	2.18	20 (25%)
14	PGV	L	305	-	42,42,50	0.98	2 (4%)	45,48,56	1.10	3 (6%)
19	CDL	M	409	-	55,55,99	1.24	4 (7%)	61,67,111	1.32	6 (9%)
15	LMT	Q	101	-	33,33,36	0.44	0	44,44,47	1.03	4 (9%)
14	PGV	J	103	-	32,32,50	1.20	2 (6%)	35,37,56	1.30	3 (8%)
16	BCL	L	302	-	64,74,74	1.68	14 (21%)	78,115,115	2.30	21 (26%)
22	CRT	V	101	-	41,43,43	0.73	0	50,54,54	3.57	18 (36%)
22	CRT	Y	403	-	41,43,43	0.72	0	50,54,54	3.53	15 (30%)
16	BCL	9	102	-	64,74,74	1.75	14 (21%)	78,115,115	2.18	22 (28%)
14	PGV	B	103	-	43,43,50	0.97	2 (4%)	46,49,56	1.04	2 (4%)
14	PGV	G	101	-	48,48,50	0.92	2 (4%)	51,54,56	0.94	3 (5%)
14	PGV	N	105	-	36,36,50	1.08	2 (5%)	38,42,56	1.13	3 (7%)
15	LMT	M	411	-	36,36,36	0.38	0	47,47,47	0.88	0
16	BCL	1	104	-	64,74,74	1.75	14 (21%)	78,115,115	2.30	24 (30%)
15	LMT	F	102	-	34,34,36	0.48	0	45,45,47	1.14	2 (4%)
16	BCL	F	103	-	64,74,74	1.69	14 (21%)	78,115,115	2.33	19 (24%)
16	BCL	D	102	-	64,74,74	1.76	14 (21%)	78,115,115	2.19	22 (28%)
16	BCL	L	309	-	64,74,74	1.71	14 (21%)	78,115,115	2.32	23 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	BCL	2	101	-	64,74,74	1.69	14 (21%)	78,115,115	2.22	20 (25%)
16	BCL	W	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.25	22 (28%)
14	PGV	N	104	-	46,46,50	0.96	2 (4%)	49,52,56	0.99	3 (6%)
10	HEC	C	402	1	32,50,50	1.55	4 (12%)	24,82,82	1.45	3 (12%)
14	PGV	J	101	-	49,49,50	0.92	2 (4%)	52,55,56	1.02	3 (5%)
19	CDL	H	301	-	63,63,99	1.06	4 (6%)	69,75,111	1.18	5 (7%)
16	BCL	B	102	-	64,74,74	1.71	14 (21%)	78,115,115	2.18	21 (26%)
15	LMT	7	103	-	36,36,36	0.40	0	47,47,47	0.84	1 (2%)
16	BCL	L	308	-	64,74,74	1.69	14 (21%)	78,115,115	2.24	22 (28%)
16	BCL	A	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.20	20 (25%)
14	PGV	V	104	-	43,43,50	0.99	2 (4%)	45,49,56	1.05	3 (6%)
16	BCL	4	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.27	19 (24%)
14	PGV	Z	103	-	43,43,50	0.99	2 (4%)	46,49,56	1.06	3 (6%)
16	BCL	P	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.21	18 (23%)
17	BPH	L	303	-	51,70,70	0.56	1 (1%)	52,101,101	0.76	2 (3%)
16	BCL	U	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.33	19 (24%)
16	BCL	J	102	-	64,74,74	1.72	14 (21%)	78,115,115	2.24	20 (25%)
14	PGV	T	103	-	45,45,50	0.96	2 (4%)	48,51,56	0.99	3 (6%)
16	BCL	Y	402	-	64,74,74	1.71	13 (20%)	78,115,115	2.23	17 (21%)
14	PGV	N	101	-	49,49,50	0.92	2 (4%)	52,55,56	1.01	2 (3%)
19	CDL	M	410	16	49,49,99	1.30	4 (8%)	55,61,111	1.22	5 (9%)
15	LMT	H	304	-	31,31,36	0.42	0	42,42,47	0.82	1 (2%)
14	PGV	H	303	-	41,41,50	1.00	2 (4%)	44,47,56	1.09	3 (6%)
14	PGV	O	104	-	42,42,50	0.99	2 (4%)	44,48,56	1.16	4 (9%)
14	PGV	Z	101	-	45,45,50	0.98	2 (4%)	48,51,56	1.09	4 (8%)
16	BCL	O	104	-	64,74,74	1.72	14 (21%)	78,115,115	2.33	19 (24%)

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
14	PGV	P	102	-	-	23/51/51/55	-
14	PGV	I	101	-	-	16/54/54/55	-
14	PGV	Z	104	-	-	21/46/46/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	F	101	-	-	18/39/39/55	-
14	PGV	8	103	-	-	21/47/47/55	-
16	BCL	T	102	-	-	14/37/137/137	-
16	BCL	5	104	-	-	20/37/137/137	-
23	SF4	a	201	9	-	-	0/6/5/5
15	LMT	7	101	-	-	4/11/51/61	0/2/2/2
18	UQ8	L	306	-	-	3/33/57/75	0/1/1/1
19	CDL	M	407	-	-	37/90/90/110	-
19	CDL	O	101	-	-	31/83/83/110	-
10	HEC	C	401	1	-	5/10/54/54	-
16	BCL	O	105	-	-	17/37/137/137	-
14	PGV	6	101	-	-	16/50/50/55	-
22	CRT	4	101	-	-	4/51/51/51	-
16	BCL	7	104	-	-	19/37/137/137	-
14	PGV	0	103	-	-	15/48/48/55	-
19	CDL	M	402	-	-	39/92/92/110	-
14	PGV	T	101	-	-	14/47/47/55	-
18	UQ8	L	304	-	-	6/27/51/75	0/1/1/1
19	CDL	M	408	-	-	23/55/55/110	-
16	BCL	I	104	-	-	19/37/137/137	-
14	PGV	B	104	-	-	15/44/44/55	-
15	LMT	5	101	-	-	10/21/61/61	0/2/2/2
22	CRT	R	101	-	-	8/51/51/51	-
14	PGV	4	103	-	-	16/47/47/55	-
19	CDL	L	310	-	-	32/85/85/110	-
22	CRT	N	102	-	-	4/51/51/51	-
14	PGV	P	103	-	-	8/41/41/55	-
14	PGV	2	102	-	-	18/49/49/55	-
15	LMT	5	102	-	-	0/10/50/61	0/2/2/2
19	CDL	S	101	-	-	26/61/61/110	-
16	BCL	W	102	-	-	14/37/137/137	-
15	LMT	7	102	-	-	3/21/61/61	0/2/2/2
16	BCL	Z	102	-	-	18/37/137/137	-
16	BCL	Y	401	19	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	0	101	-	-	20/45/45/55	-
16	BCL	X	101	-	-	14/37/137/137	-
21	MQ8	M	405	-	-	6/47/67/67	0/2/2/2
14	PGV	R	103	-	-	21/42/42/55	-
22	CRT	M	406	-	-	11/51/51/51	-
14	PGV	1	102	-	-	13/45/45/55	-
15	LMT	H	305	-	-	1/12/52/61	0/2/2/2
15	LMT	O	103	-	-	7/15/55/61	0/2/2/2
10	HEC	C	404	1	-	2/10/54/54	-
14	PGV	G	104	-	-	21/45/45/55	-
14	PGV	T	104	-	-	21/51/51/55	-
16	BCL	K	101	-	-	18/37/137/137	-
14	PGV	H	302	-	-	18/40/40/55	-
14	PGV	6	103	-	-	16/47/47/55	-
14	PGV	C	408	-	-	6/36/36/55	-
16	BCL	N	103	-	-	15/37/137/137	-
14	PGV	O	102	-	-	22/55/55/55	-
18	UQ8	L	307	-	-	1/8/32/75	0/1/1/1
16	BCL	E	101	-	-	9/37/137/137	-
13	PLM	C	407	-	-	0/8/9/15	-
16	BCL	0	102	-	-	5/37/137/137	-
15	LMT	L	301	-	-	1/11/51/61	0/2/2/2
14	PGV	V	103	-	-	18/47/47/55	-
16	BCL	R	102	-	-	18/37/137/137	-
16	BCL	8	102	-	-	9/37/137/137	-
16	BCL	I	103	-	-	13/37/137/137	-
14	PGV	6	104	-	-	10/47/47/55	-
10	HEC	C	403	1	-	3/10/54/54	-
22	CRT	B	101	-	-	6/51/51/51	-
16	BCL	1	103	-	-	16/37/137/137	-
22	CRT	8	101	-	-	4/51/51/51	-
14	PGV	E	102	-	-	9/42/42/55	-
16	BCL	5	103	-	-	15/37/137/137	-
15	LMT	I	102	-	-	8/11/51/61	0/2/2/2
16	BCL	M	403	-	-	17/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	3	101	-	-	13/33/33/55	-
16	BCL	G	103	-	-	16/37/137/137	-
14	PGV	2	103	-	-	15/40/40/55	-
16	BCL	Q	102	-	-	13/37/137/137	-
16	BCL	D	101	-	-	15/37/137/137	-
14	PGV	1	101	-	-	14/49/49/55	-
16	BCL	6	102	-	-	7/37/137/137	-
17	BPH	M	404	-	-	13/37/105/105	0/5/6/6
16	BCL	S	103	-	-	14/37/137/137	-
22	CRT	G	102	-	-	1/51/51/51	-
14	PGV	X	102	-	-	12/49/49/55	-
12	Z41	C	406	1	-	4/31/31/41	-
16	BCL	S	102	-	-	17/37/137/137	-
16	BCL	3	102	-	-	15/37/137/137	-
16	BCL	9	101	-	-	11/37/137/137	-
16	BCL	V	102	-	-	21/37/137/137	-
14	PGV	L	305	-	-	18/47/47/55	-
19	CDL	M	409	-	-	29/66/66/110	-
15	LMT	Q	101	-	-	7/18/58/61	0/2/2/2
14	PGV	J	103	-	-	8/34/34/55	-
16	BCL	L	302	-	-	11/37/137/137	-
22	CRT	V	101	-	-	6/51/51/51	-
22	CRT	Y	403	-	-	2/51/51/51	-
16	BCL	9	102	-	-	15/37/137/137	-
14	PGV	B	103	-	-	22/48/48/55	-
14	PGV	G	101	-	-	19/53/53/55	-
14	PGV	N	105	-	-	13/41/41/55	-
15	LMT	M	411	-	-	7/21/61/61	0/2/2/2
16	BCL	1	104	-	-	16/37/137/137	-
15	LMT	F	102	-	-	6/19/59/61	0/2/2/2
16	BCL	F	103	-	-	15/37/137/137	-
16	BCL	D	102	-	-	17/37/137/137	-
16	BCL	L	309	-	-	16/37/137/137	-
16	BCL	2	101	-	-	11/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCL	W	101	-	-	16/37/137/137	-
14	PGV	N	104	-	-	22/51/51/55	-
10	HEC	C	402	1	-	2/10/54/54	-
14	PGV	J	101	-	-	23/54/54/55	-
19	CDL	H	301	-	-	28/73/73/110	-
16	BCL	B	102	-	-	13/37/137/137	-
15	LMT	7	103	-	-	4/21/61/61	0/2/2/2
16	BCL	L	308	-	-	13/37/137/137	-
16	BCL	A	101	-	-	17/37/137/137	-
14	PGV	V	104	-	-	9/48/48/55	-
16	BCL	4	102	-	-	10/37/137/137	-
14	PGV	Z	103	-	-	23/48/48/55	-
16	BCL	P	101	-	-	13/37/137/137	-
17	BPH	L	303	-	-	8/37/105/105	0/5/6/6
16	BCL	U	101	-	-	14/37/137/137	-
16	BCL	J	102	-	-	13/37/137/137	-
14	PGV	T	103	-	-	19/50/50/55	-
16	BCL	Y	402	-	-	13/37/137/137	-
14	PGV	N	101	-	-	18/54/54/55	-
19	CDL	M	410	16	-	21/60/60/110	-
15	LMT	H	304	-	-	6/16/56/61	0/2/2/2
14	PGV	H	303	-	-	17/46/46/55	-
14	PGV	0	104	-	-	17/47/47/55	-
14	PGV	Z	101	-	-	20/50/50/55	-
16	BCL	O	104	-	-	19/37/137/137	-

The worst 5 of 765 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	M	405	MQ8	C3-C2	7.84	1.49	1.35
18	L	304	UQ8	C6-C1	7.70	1.49	1.35
18	L	307	UQ8	C6-C1	7.68	1.49	1.35
18	L	306	UQ8	C6-C1	7.55	1.49	1.35
16	Y	402	BCL	O2D-CGD	5.21	1.45	1.33

The worst 5 of 1316 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	101	CRT	C2-C1-C4	-16.52	85.50	110.86
22	4	101	CRT	C2-C1-C4	-16.06	86.20	110.86
22	N	102	CRT	C2-C1-C4	-15.95	86.37	110.86
22	8	101	CRT	C2-C1-C4	-15.86	86.50	110.86
22	G	102	CRT	C3-C1-C4	-15.59	86.92	110.86

There are no chirality outliers.

5 of 1783 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	408	PGV	C04-O12-P-O13
14	L	305	PGV	C03-O11-P-O13
14	H	302	PGV	C03-O11-P-O13
14	H	302	PGV	C04-O12-P-O11
14	H	302	PGV	C04-O12-P-O13

There are no ring outliers.

127 monomers are involved in 616 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	P	102	PGV	5	0
14	I	101	PGV	5	0
14	Z	104	PGV	7	0
14	F	101	PGV	2	0
14	8	103	PGV	7	0
16	T	102	BCL	7	0
16	5	104	BCL	6	0
15	7	101	LMT	5	0
18	L	306	UQ8	6	0
19	M	407	CDL	4	0
19	O	101	CDL	6	0
10	C	401	HEC	10	0
16	O	105	BCL	6	0
14	6	101	PGV	3	0
22	4	101	CRT	10	0
16	7	104	BCL	3	0
14	0	103	PGV	4	0
19	M	402	CDL	9	0
14	T	101	PGV	2	0
18	L	304	UQ8	3	0
19	M	408	CDL	2	0
16	I	104	BCL	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	104	PGV	9	0
15	5	101	LMT	3	0
22	R	101	CRT	8	0
14	4	103	PGV	3	0
19	L	310	CDL	8	0
22	N	102	CRT	13	0
14	P	103	PGV	3	0
14	2	102	PGV	4	0
15	5	102	LMT	1	0
19	S	101	CDL	5	0
16	W	102	BCL	2	0
15	7	102	LMT	2	0
16	Z	102	BCL	8	0
16	Y	401	BCL	6	0
14	0	101	PGV	4	0
16	X	101	BCL	5	0
21	M	405	MQ8	3	0
14	R	103	PGV	5	0
22	M	406	CRT	8	0
14	1	102	PGV	5	0
15	O	103	LMT	3	0
10	C	404	HEC	2	0
14	G	104	PGV	2	0
14	T	104	PGV	4	0
16	K	101	BCL	8	0
14	H	302	PGV	1	0
14	6	103	PGV	2	0
14	C	408	PGV	6	0
16	N	103	BCL	5	0
14	O	102	PGV	7	0
18	L	307	UQ8	3	0
16	E	101	BCL	9	0
13	C	407	PLM	1	0
16	0	102	BCL	8	0
15	L	301	LMT	3	0
14	V	103	PGV	3	0
16	R	102	BCL	9	0
16	8	102	BCL	10	0
16	I	103	BCL	6	0
14	6	104	PGV	3	0
10	C	403	HEC	3	0
22	B	101	CRT	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	103	BCL	10	0
22	8	101	CRT	8	0
14	E	102	PGV	2	0
16	5	103	BCL	13	0
15	I	102	LMT	3	0
16	M	403	BCL	6	0
14	3	101	PGV	3	0
16	G	103	BCL	11	0
14	2	103	PGV	2	0
16	Q	102	BCL	7	0
16	D	101	BCL	9	0
14	1	101	PGV	9	0
16	6	102	BCL	8	0
17	M	404	BPH	7	0
16	S	103	BCL	8	0
22	G	102	CRT	10	0
14	X	102	PGV	2	0
16	S	102	BCL	12	0
16	3	102	BCL	6	0
16	9	101	BCL	11	0
16	V	102	BCL	8	0
14	L	305	PGV	6	0
19	M	409	CDL	7	0
15	Q	101	LMT	2	0
14	J	103	PGV	2	0
16	L	302	BCL	4	0
22	V	101	CRT	8	0
22	Y	403	CRT	8	0
16	9	102	BCL	4	0
14	B	103	PGV	5	0
14	G	101	PGV	7	0
15	M	411	LMT	1	0
16	1	104	BCL	5	0
15	F	102	LMT	3	0
16	F	103	BCL	5	0
16	D	102	BCL	7	0
16	L	309	BCL	7	0
16	2	101	BCL	10	0
16	W	101	BCL	12	0
14	N	104	PGV	4	0
10	C	402	HEC	1	0
14	J	101	PGV	7	0

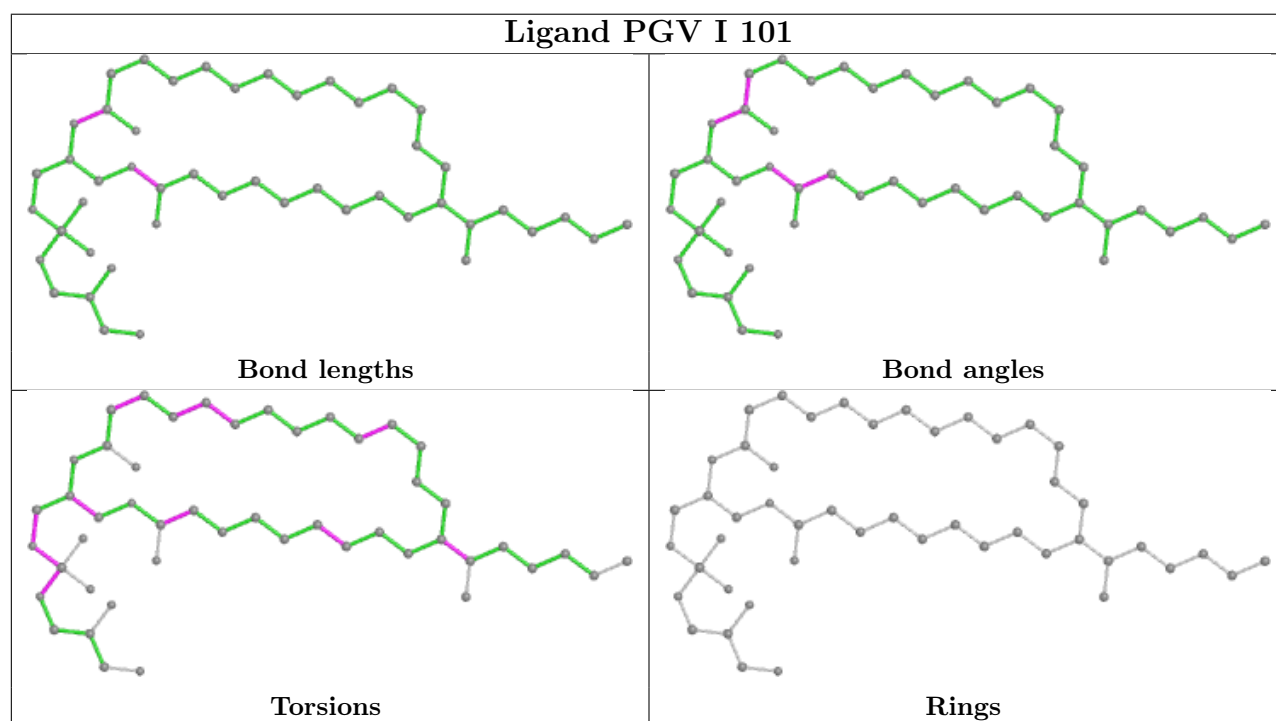
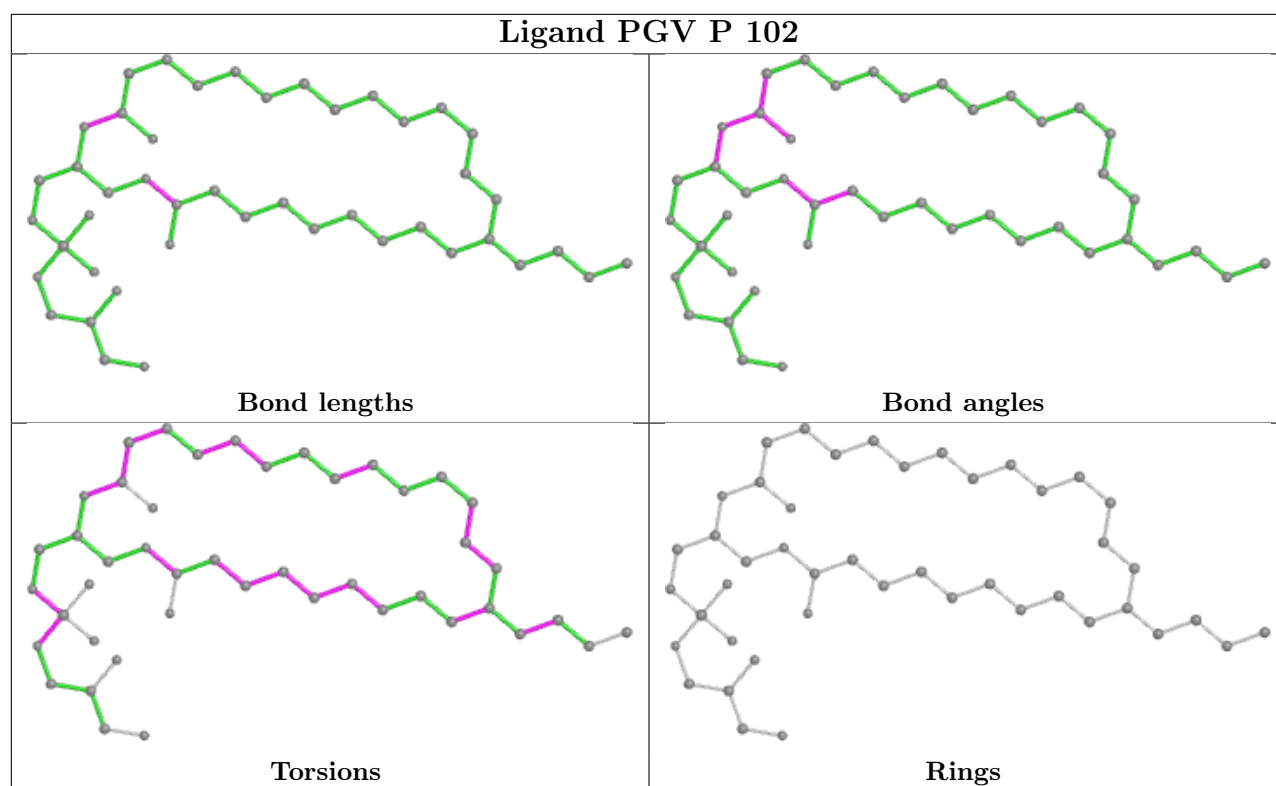
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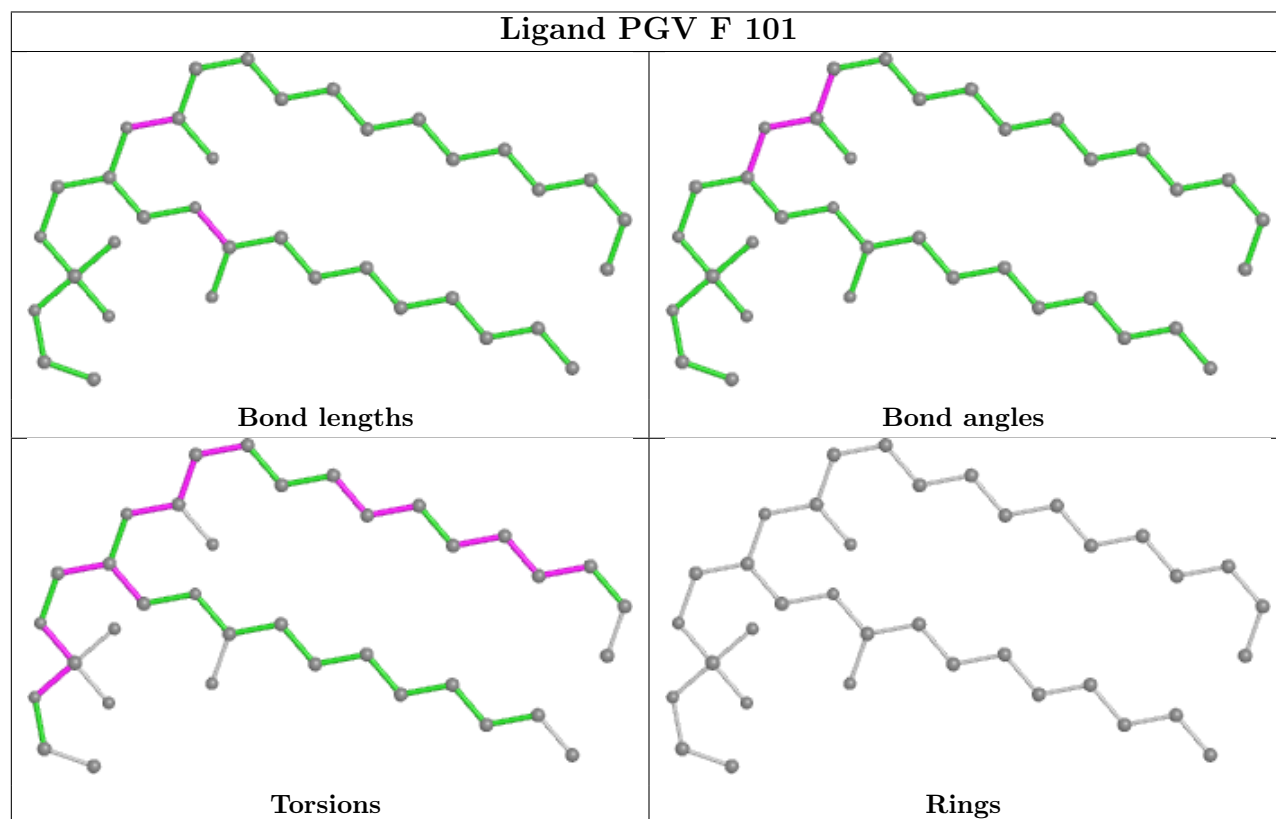
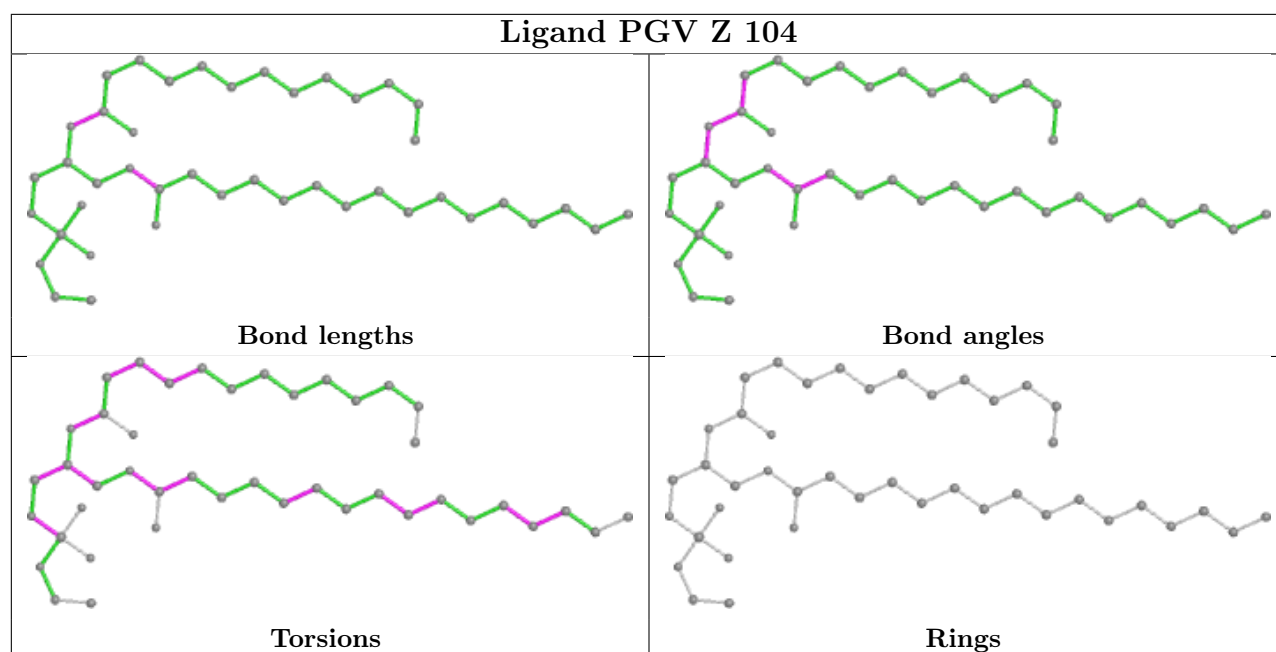
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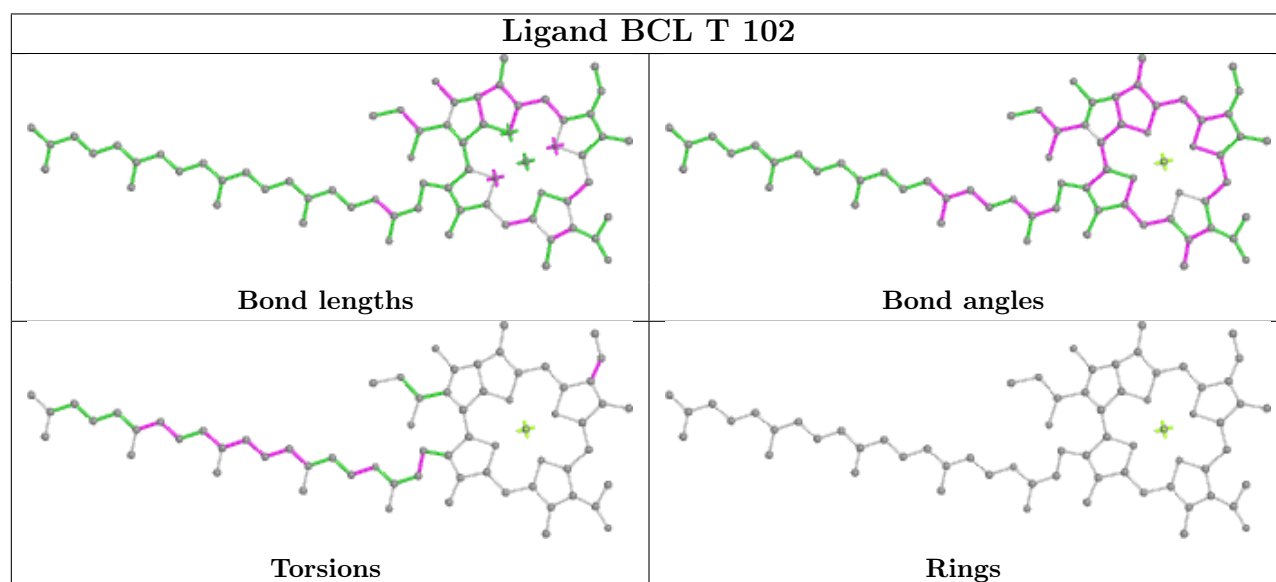
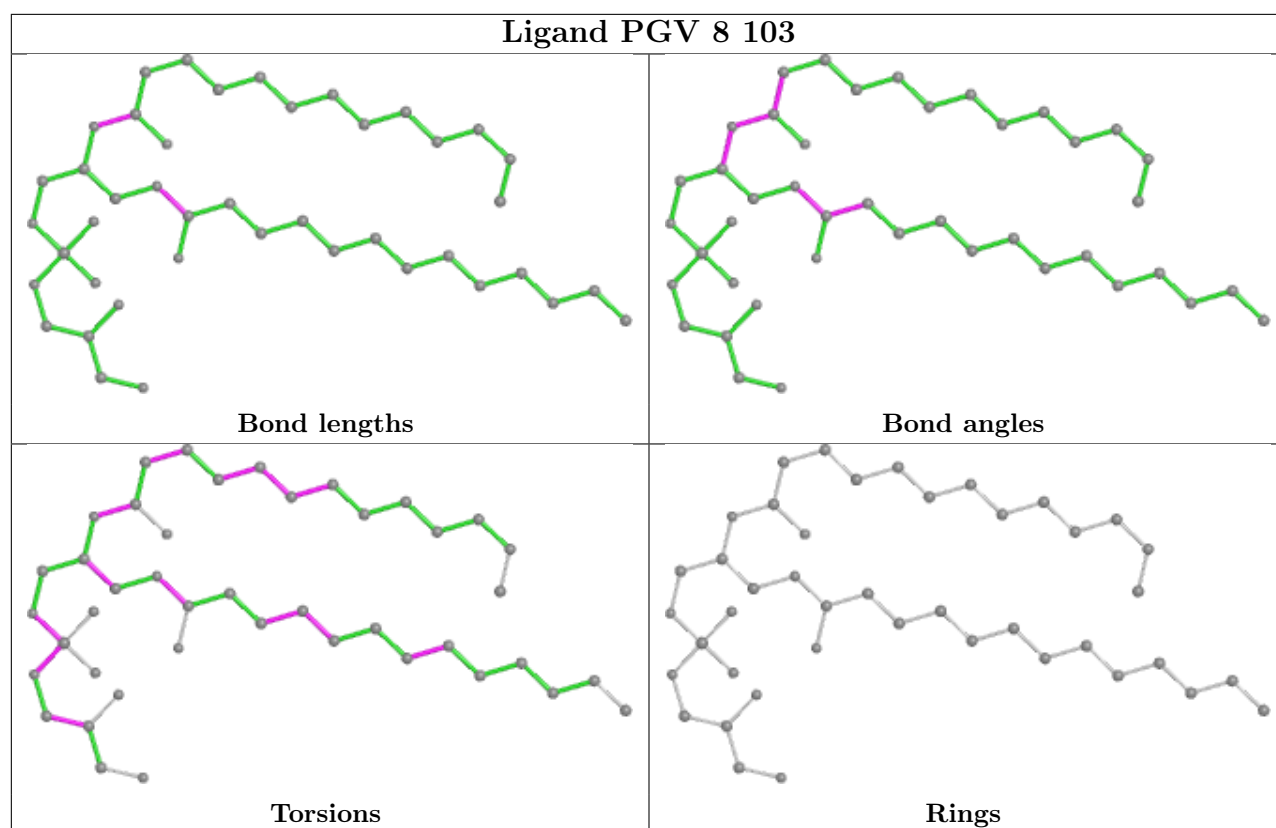
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	301	CDL	5	0
16	B	102	BCL	8	0
15	7	103	LMT	2	0
16	L	308	BCL	5	0
16	A	101	BCL	5	0
14	V	104	PGV	2	0
16	4	102	BCL	9	0
14	Z	103	PGV	3	0
16	P	101	BCL	9	0
17	L	303	BPH	8	0
16	U	101	BCL	4	0
16	J	102	BCL	10	0
14	T	103	PGV	3	0
16	Y	402	BCL	3	0
14	N	101	PGV	2	0
19	M	410	CDL	5	0
15	H	304	LMT	4	0
14	H	303	PGV	5	0
14	O	104	PGV	2	0
14	Z	101	PGV	2	0
16	O	104	BCL	7	0

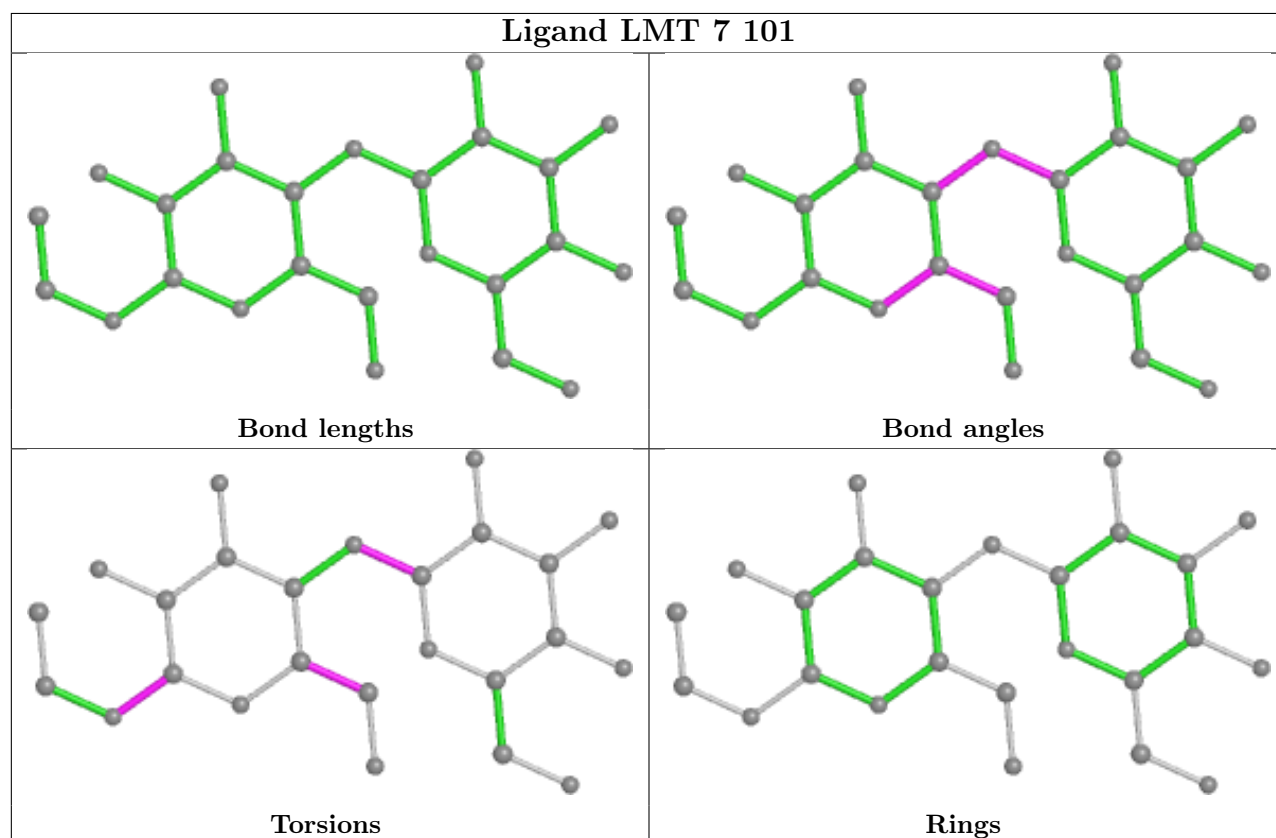
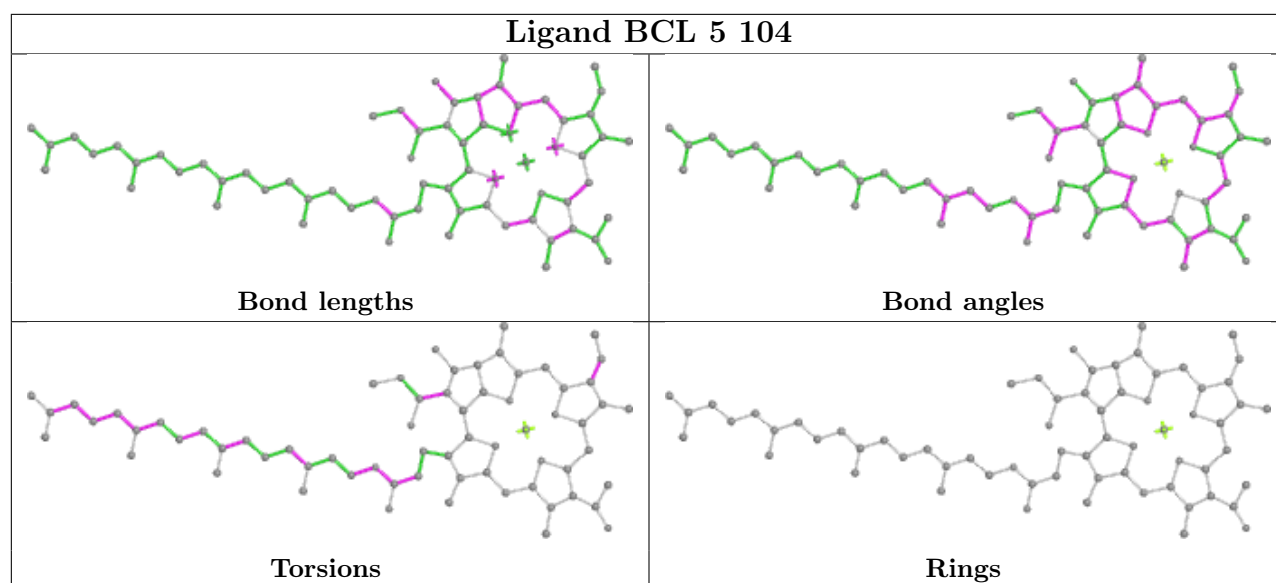
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

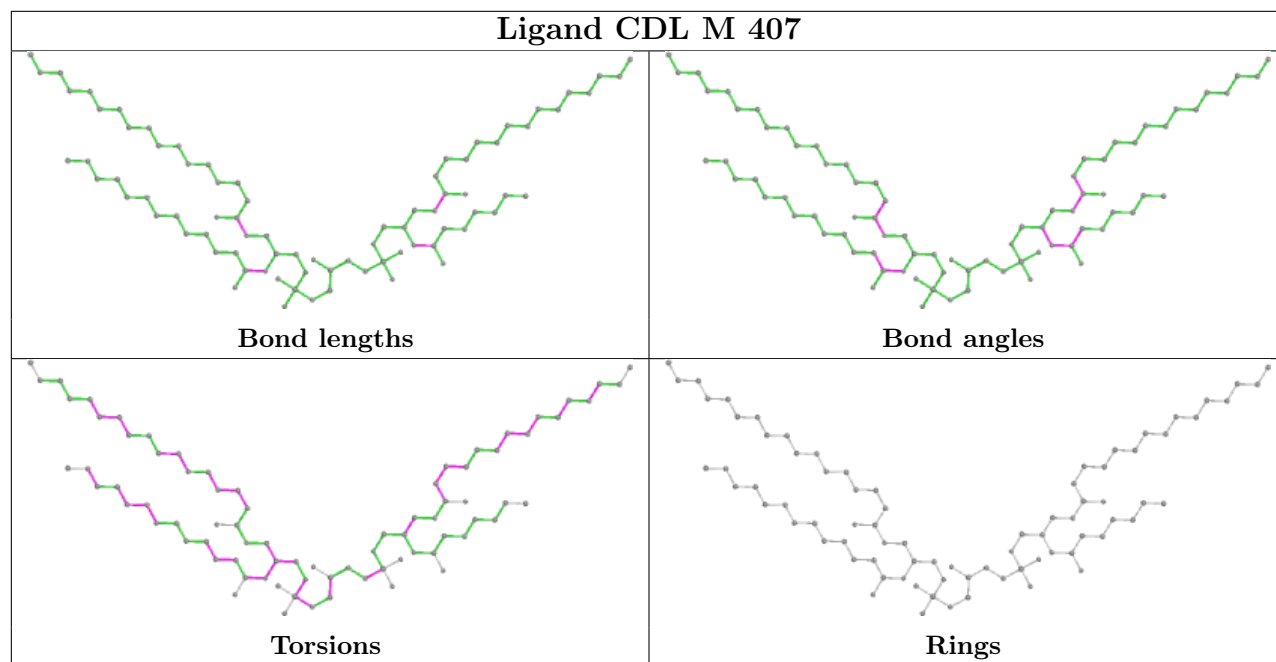
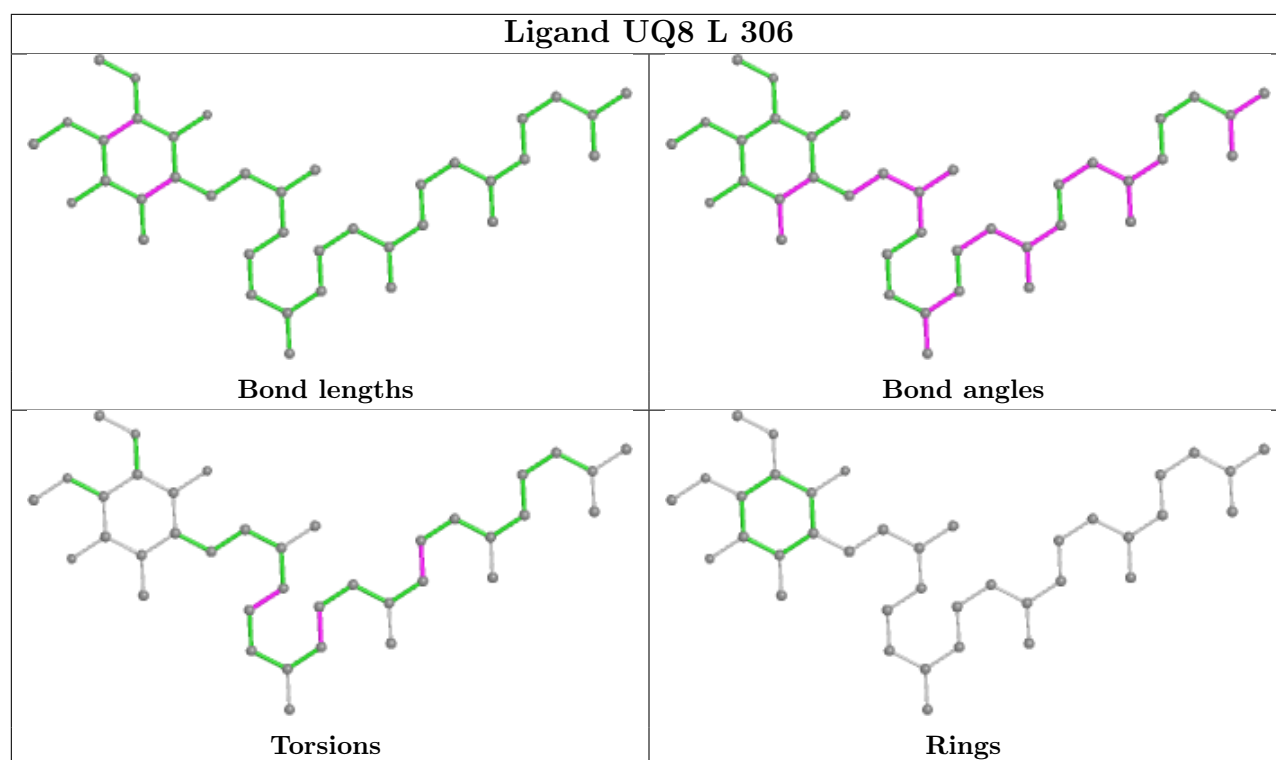


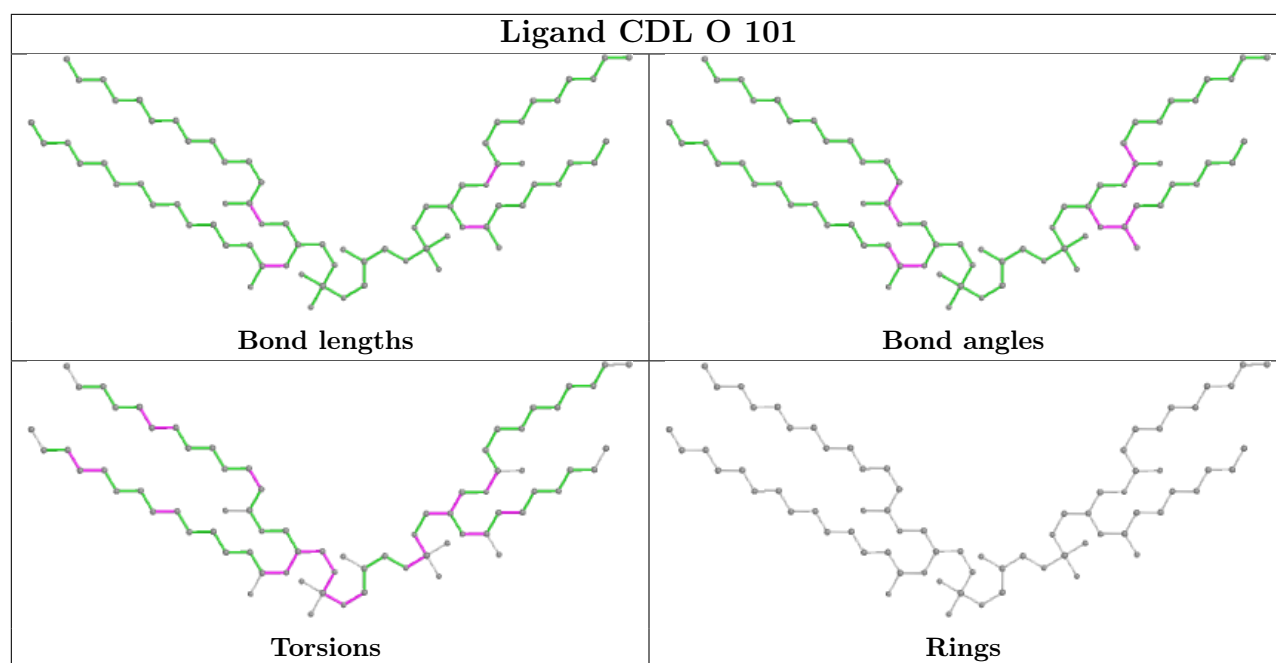


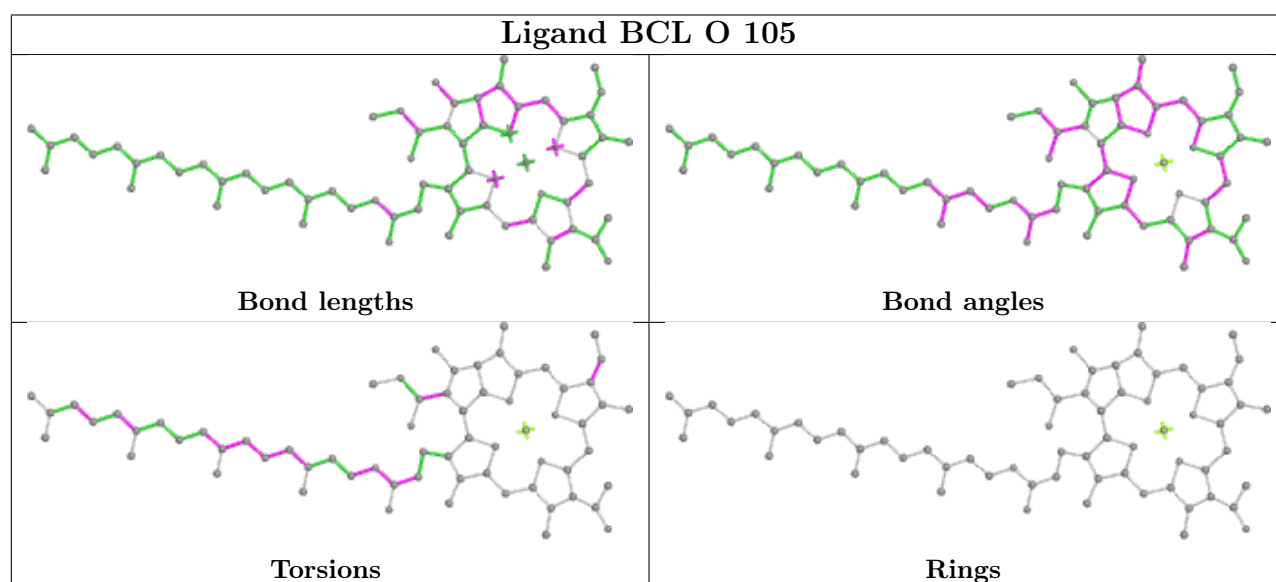
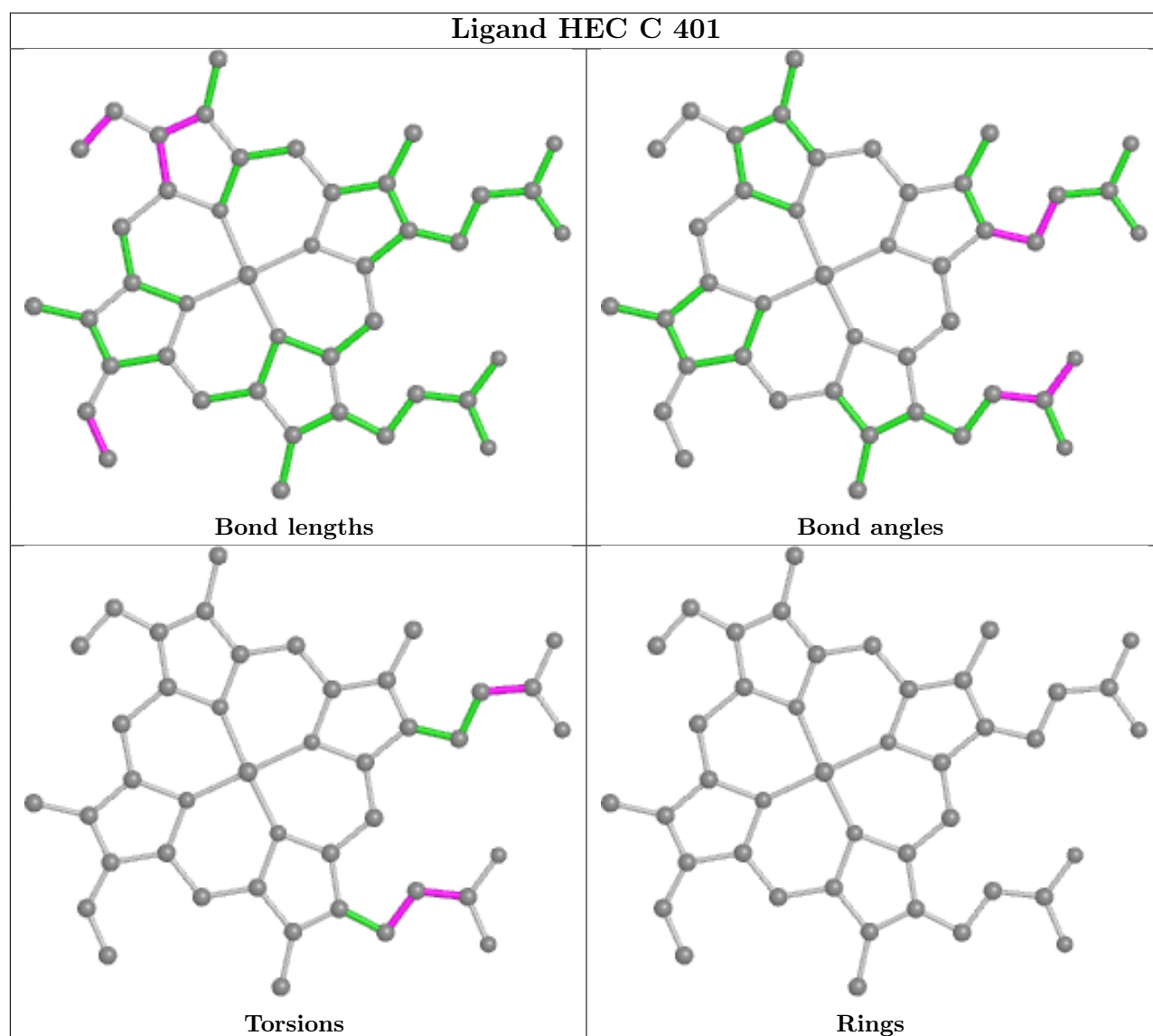




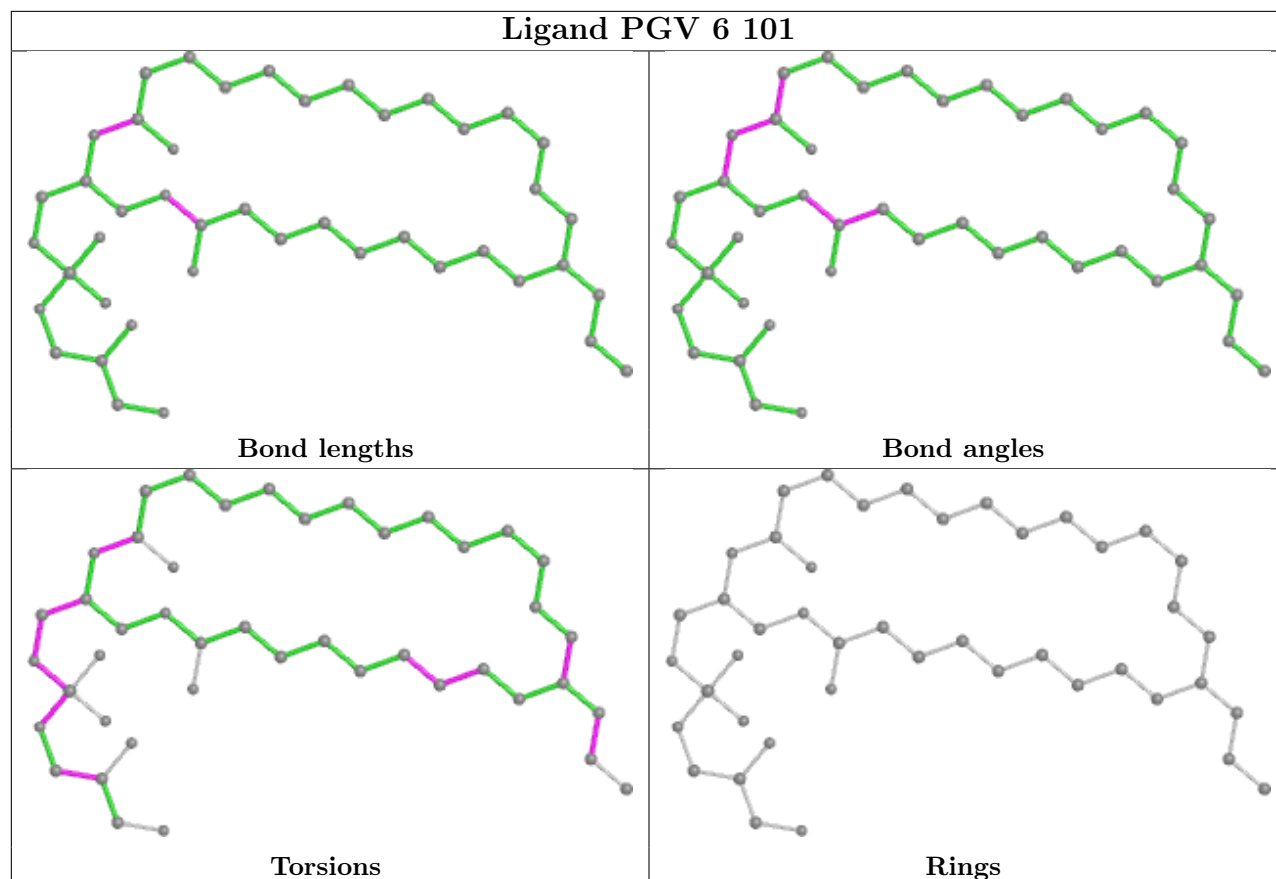




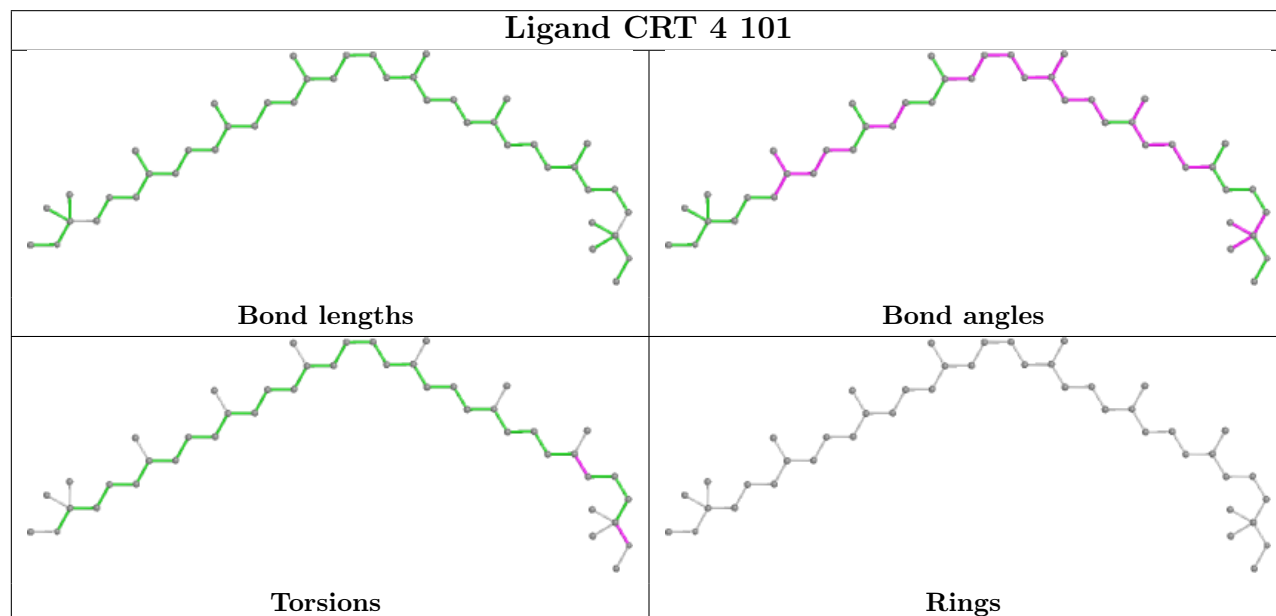




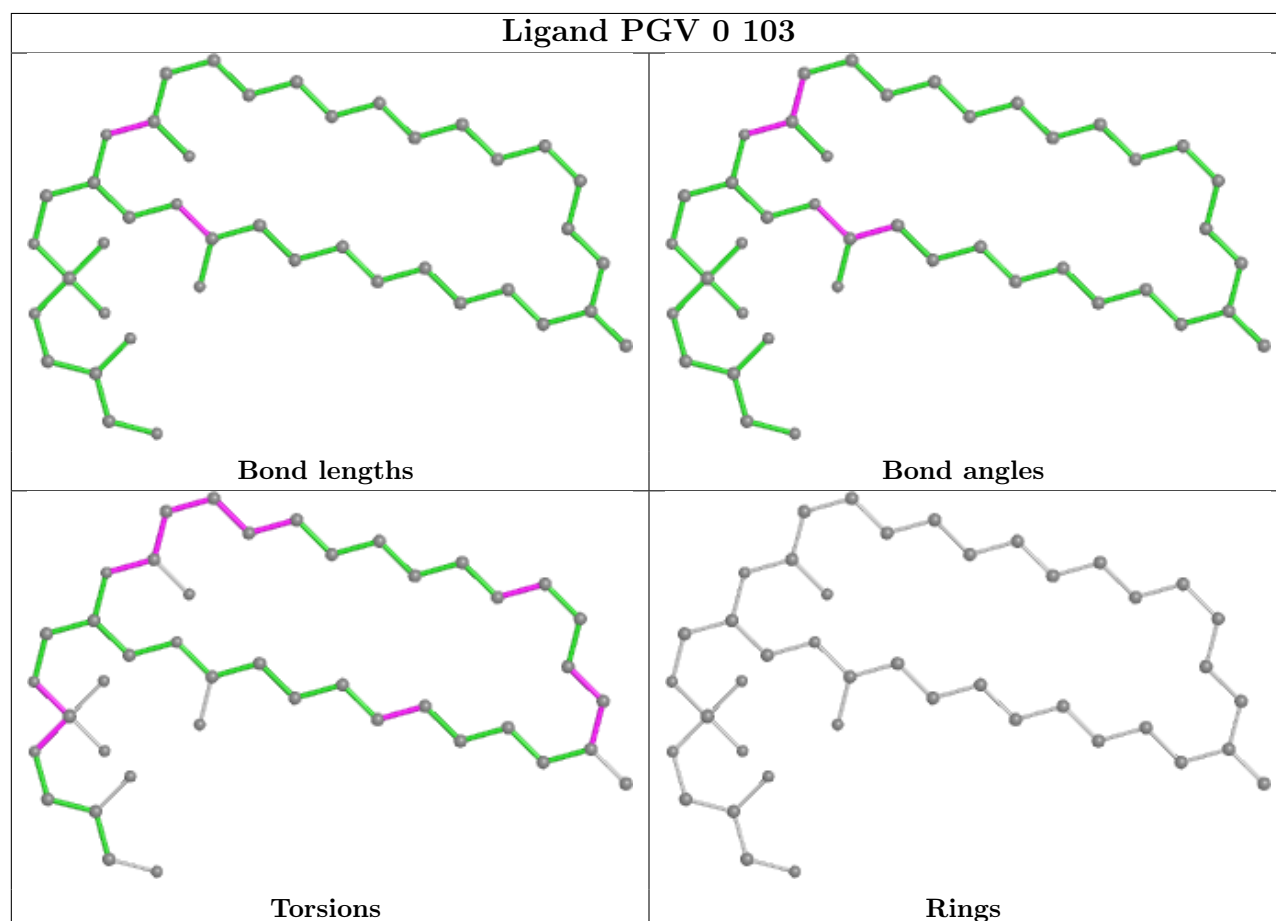
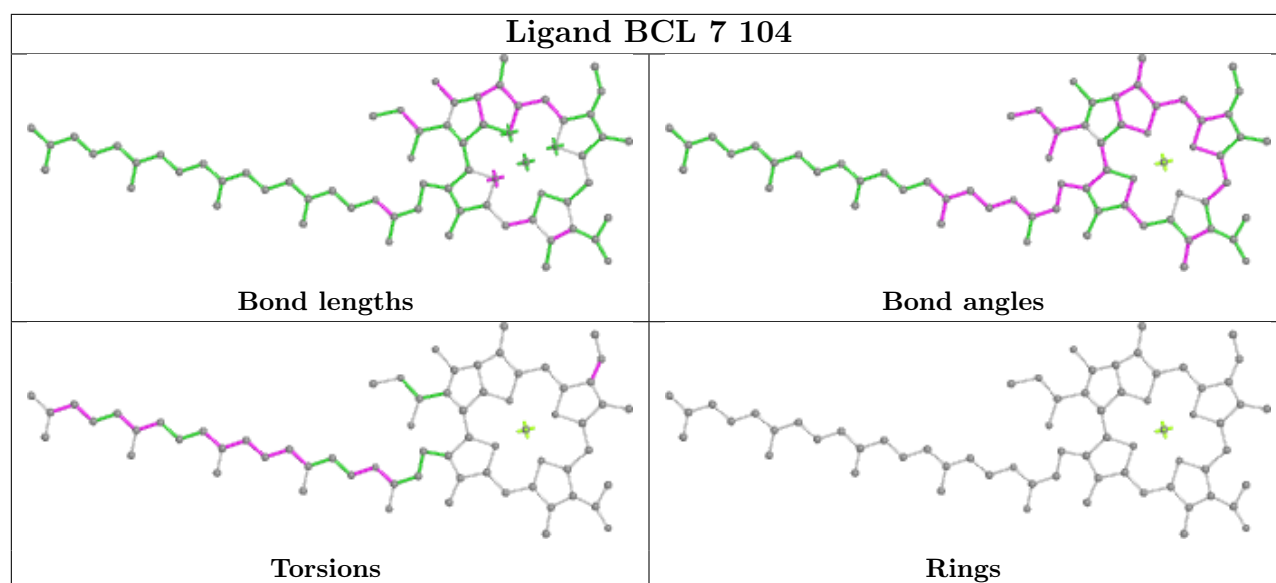
## Ligand PGV 6 101

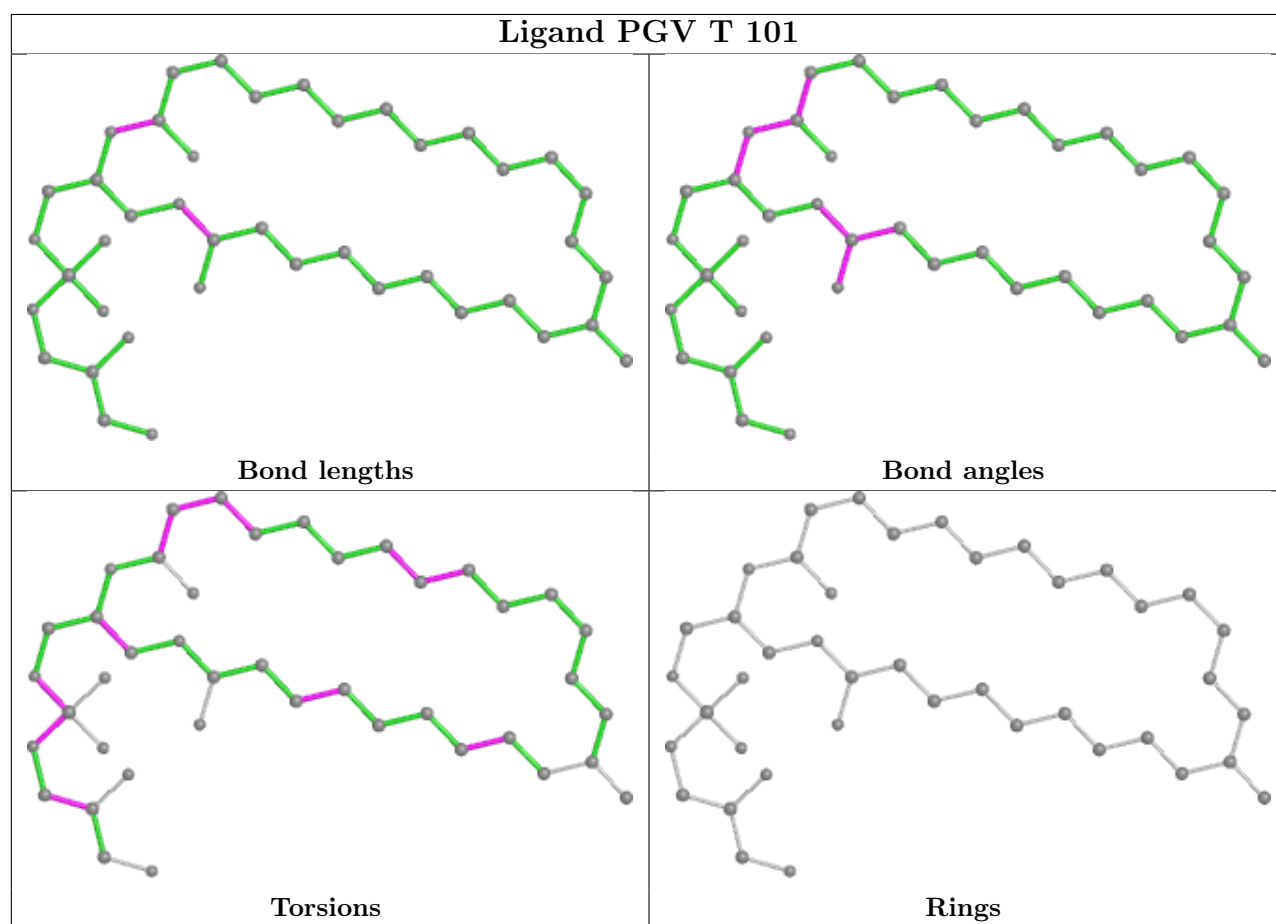
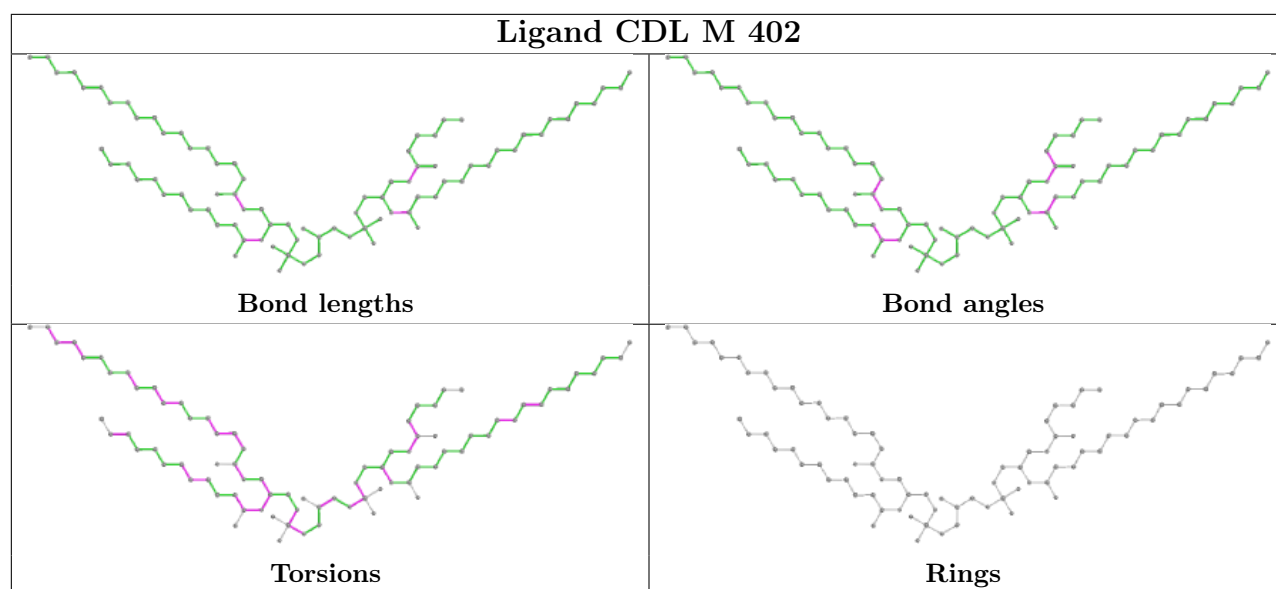


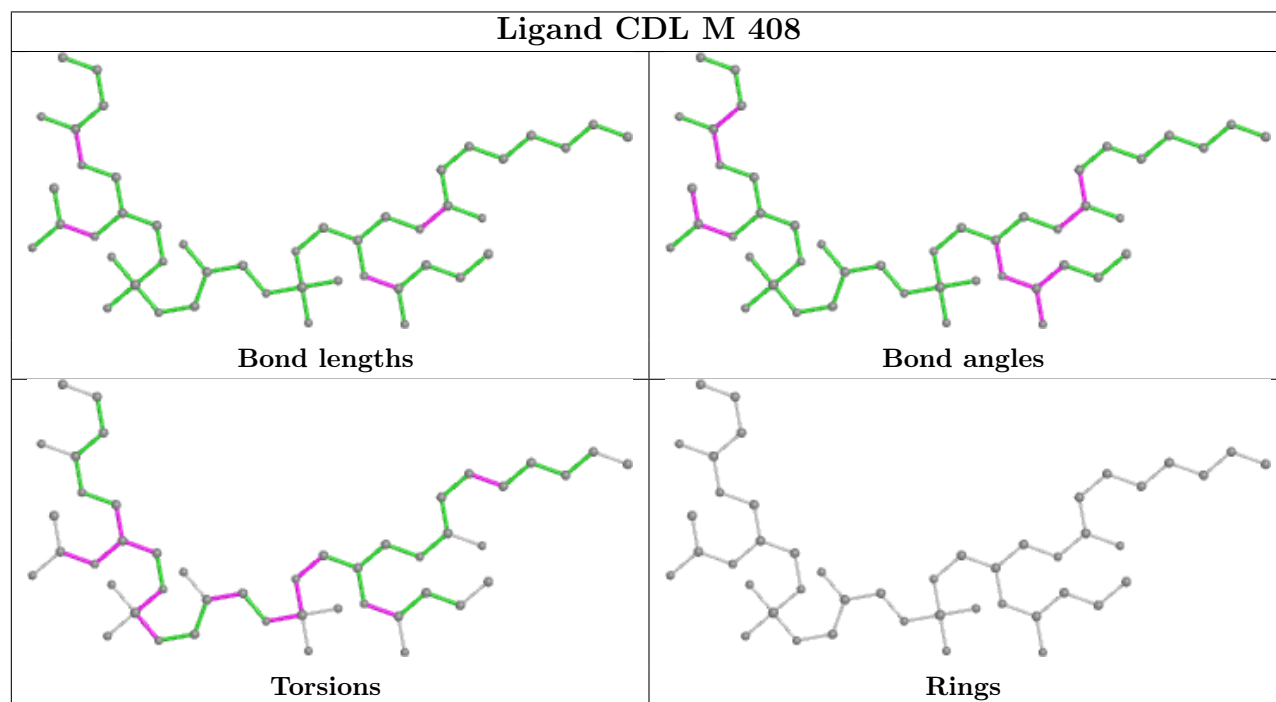
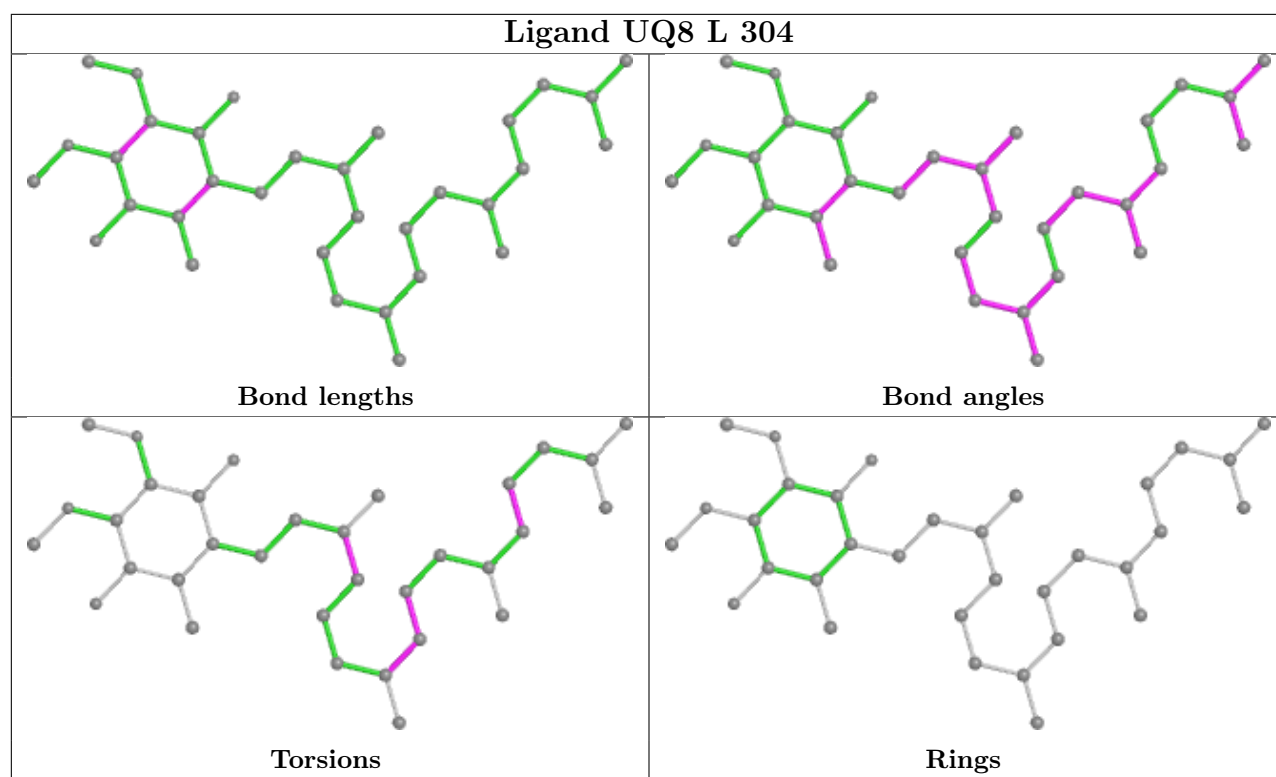
## Ligand CRT 4 101

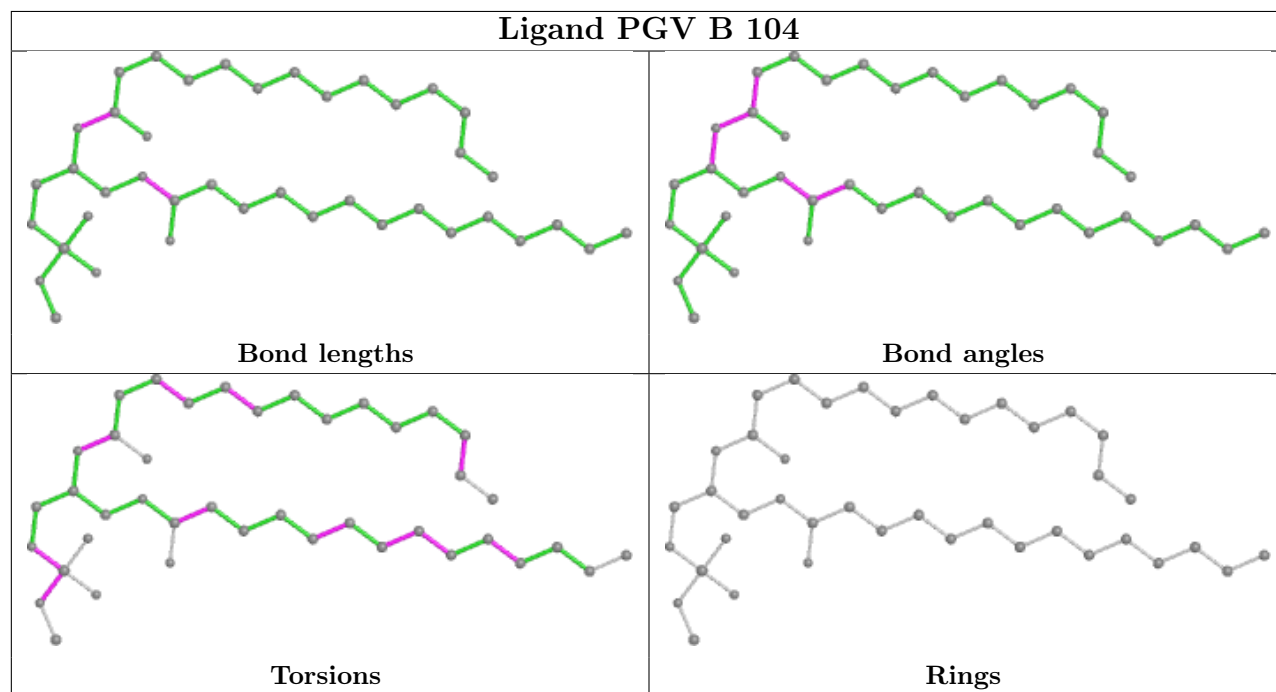
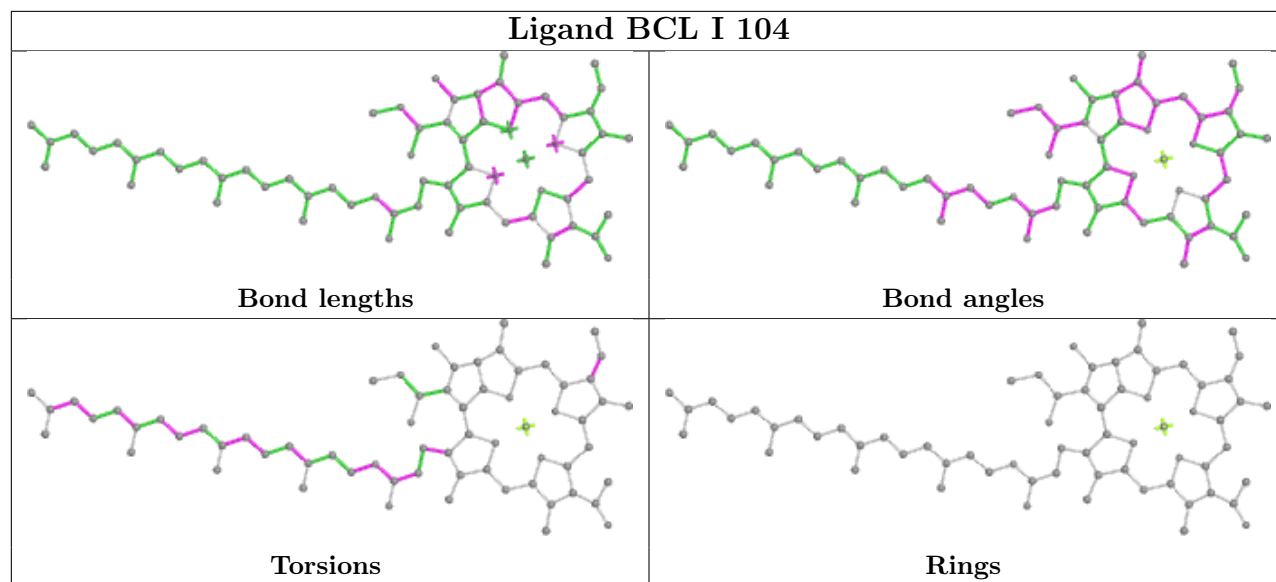


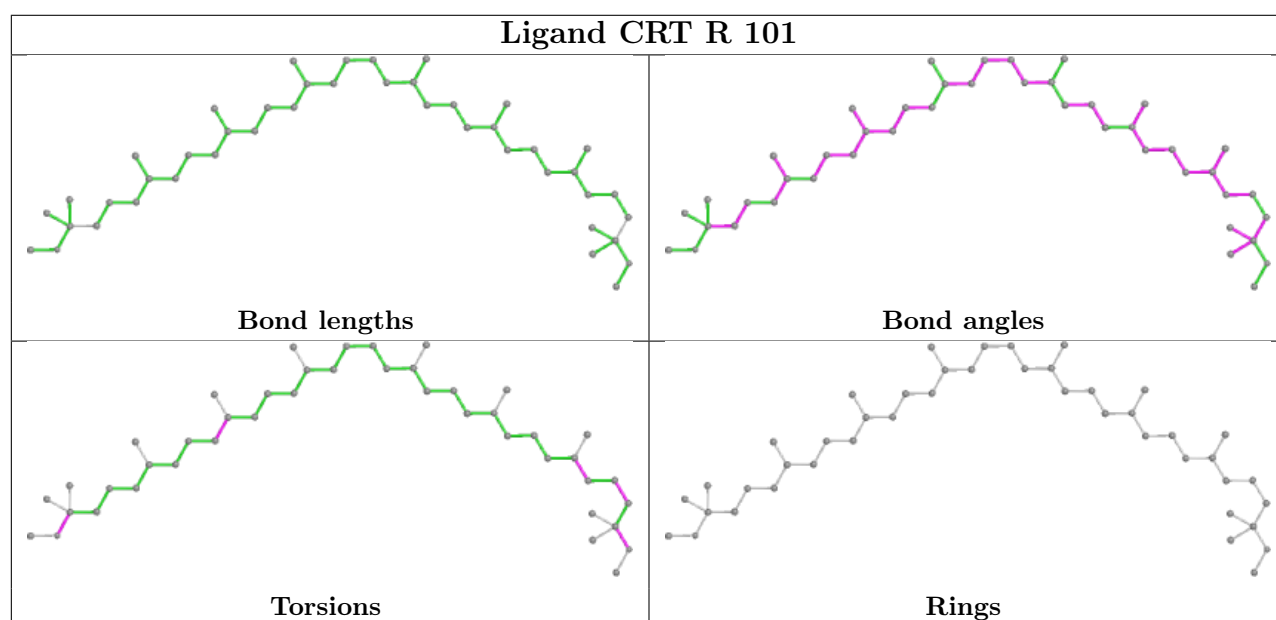
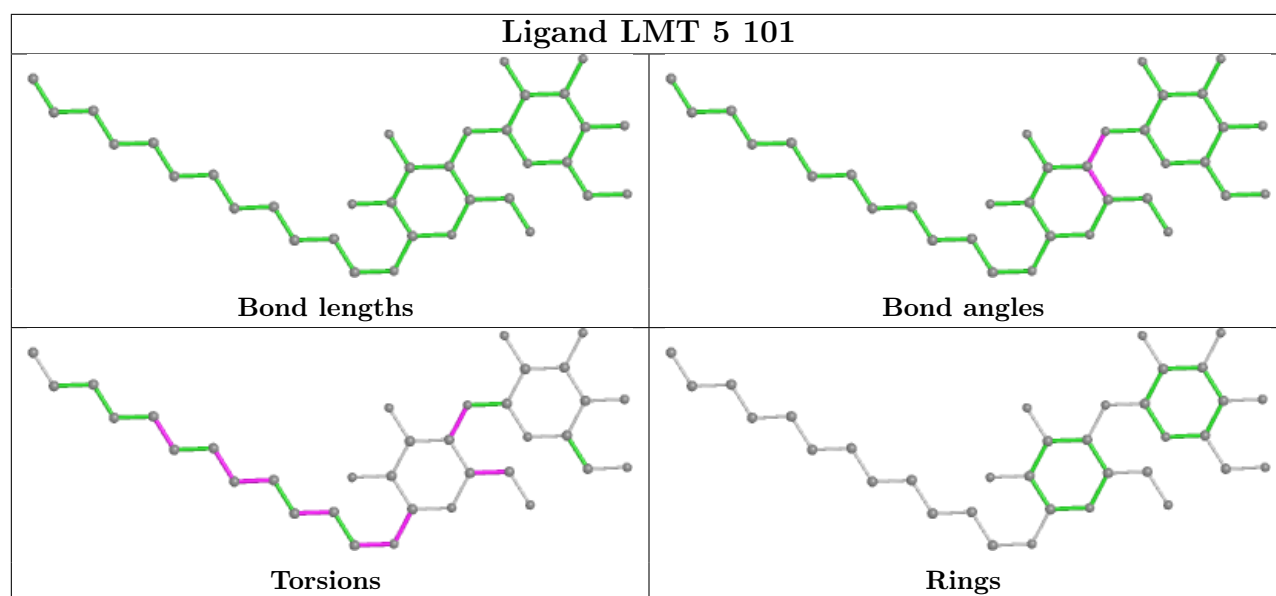




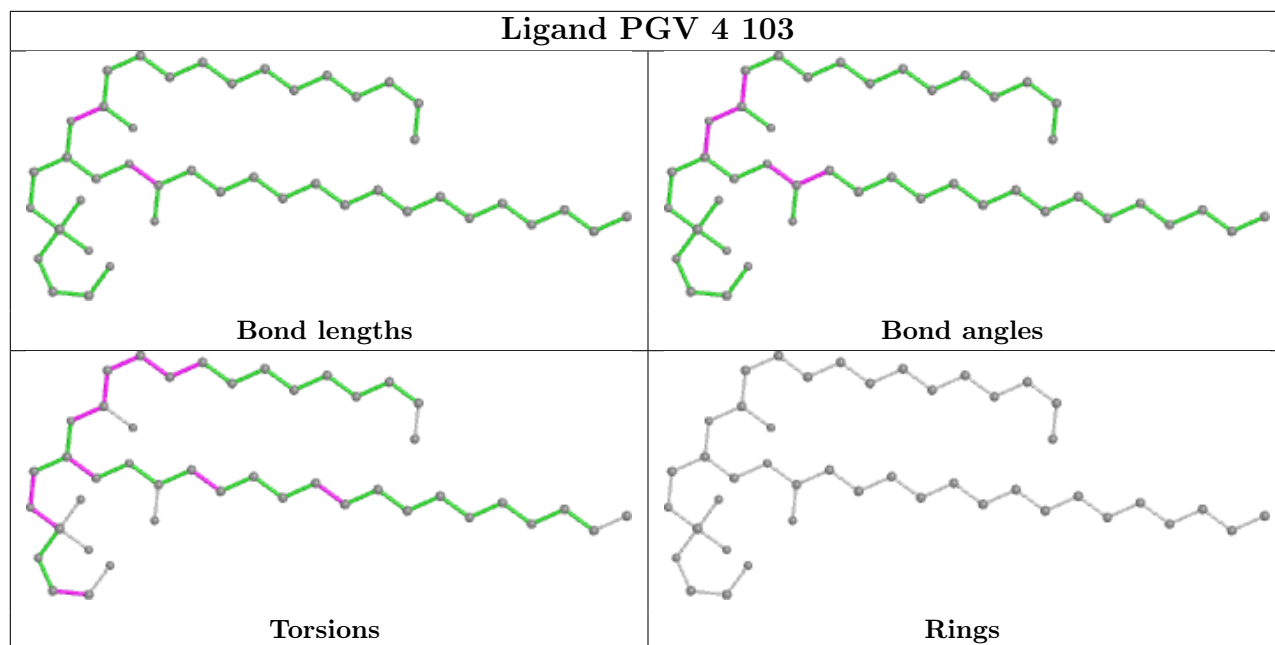




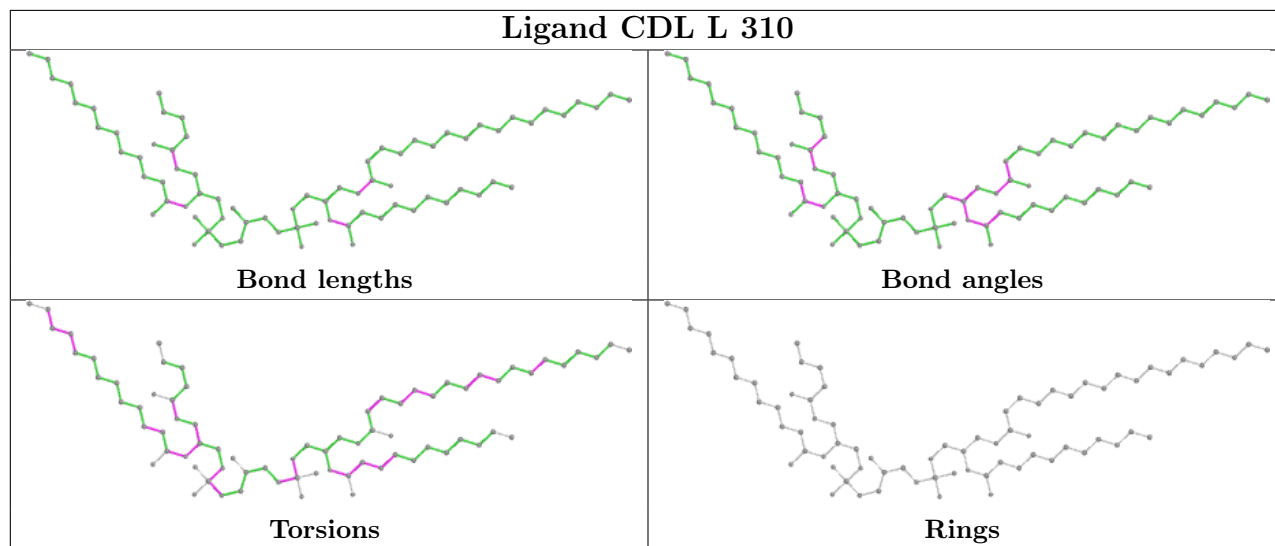


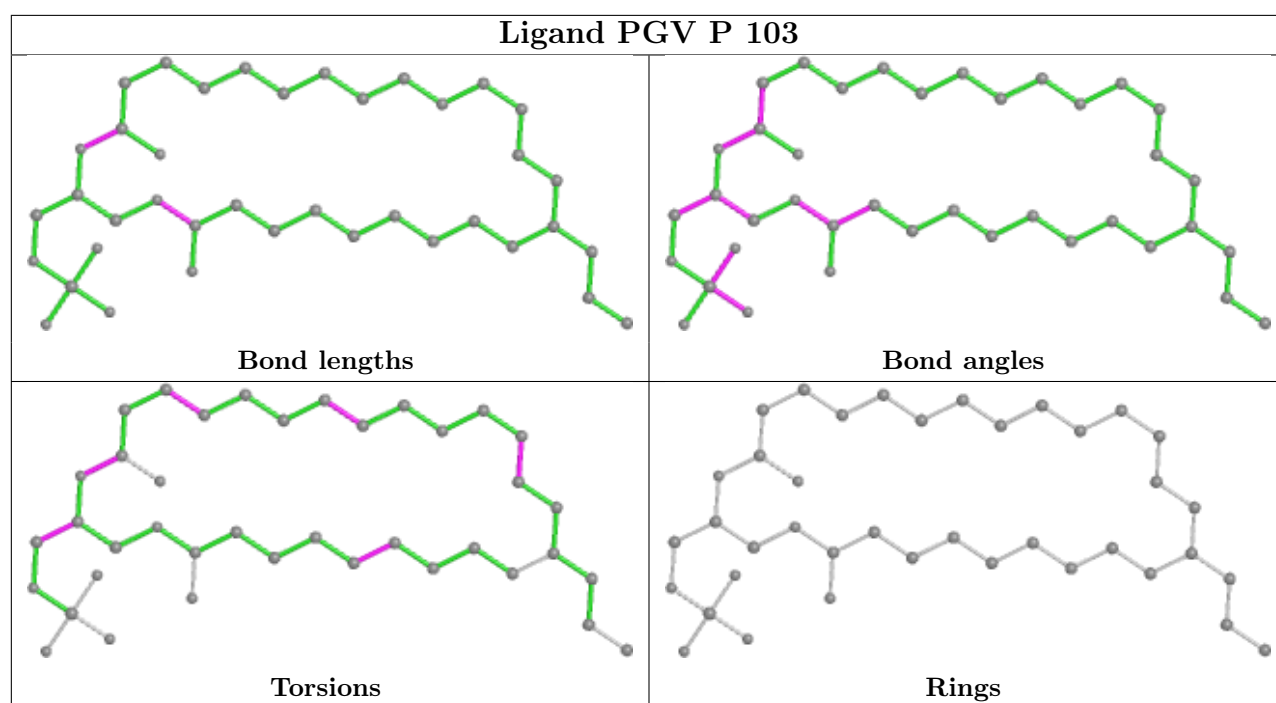
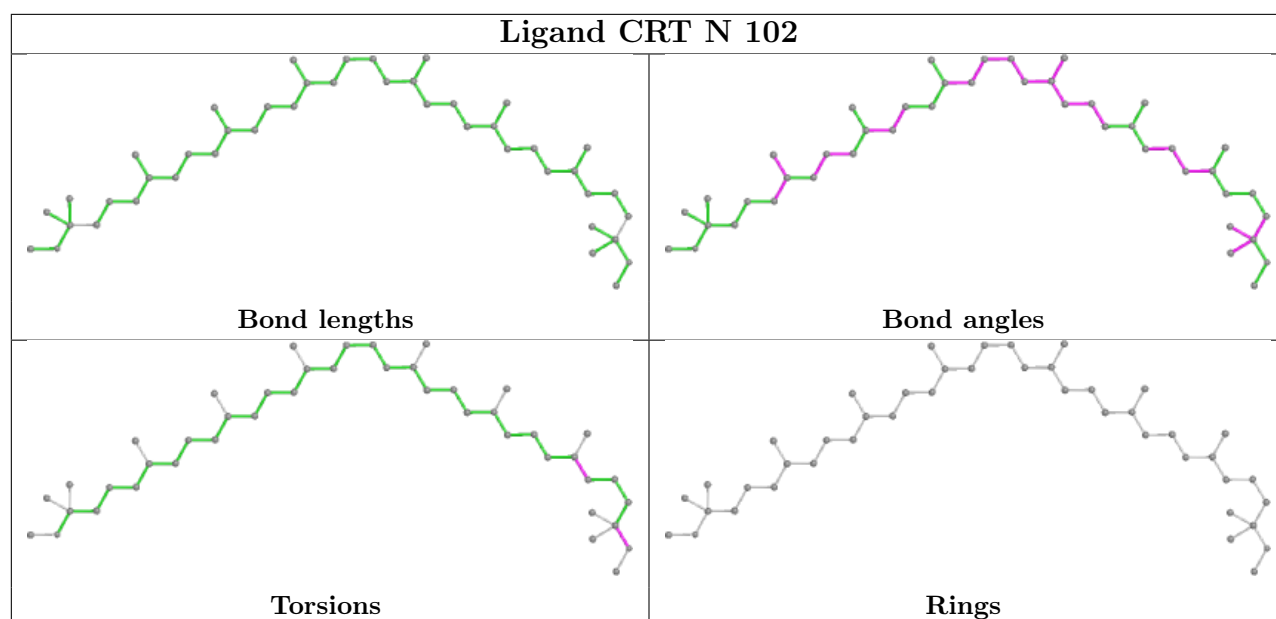


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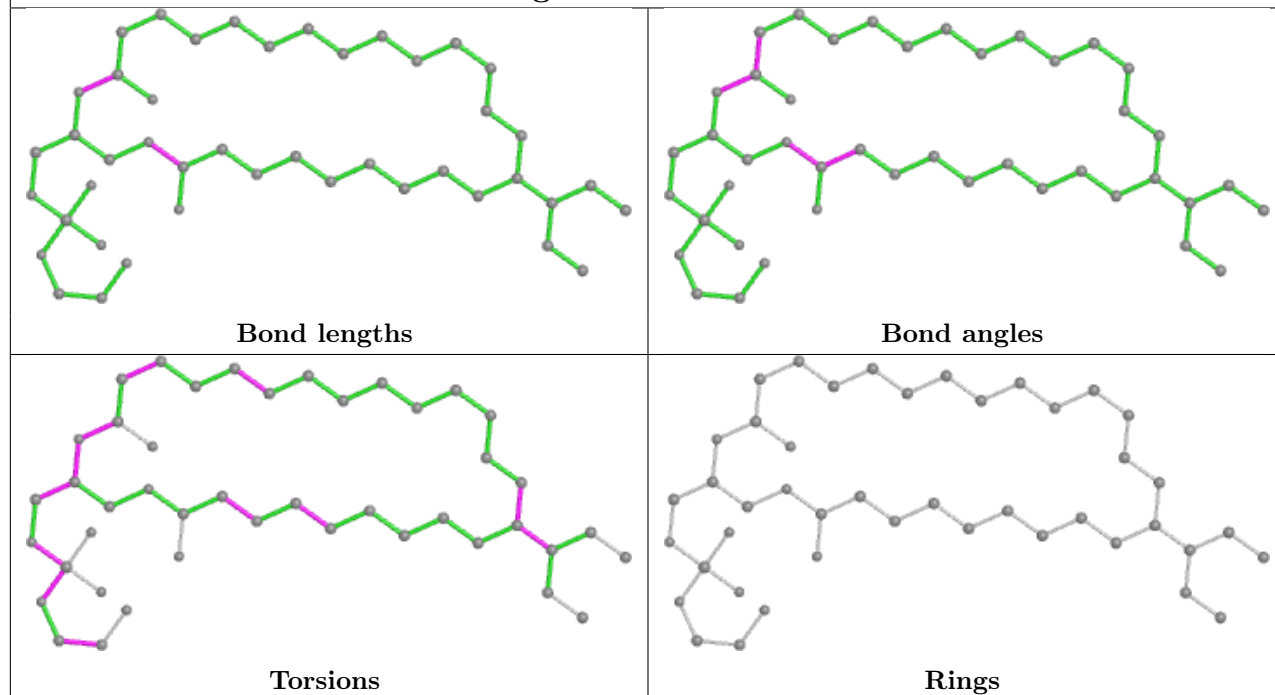


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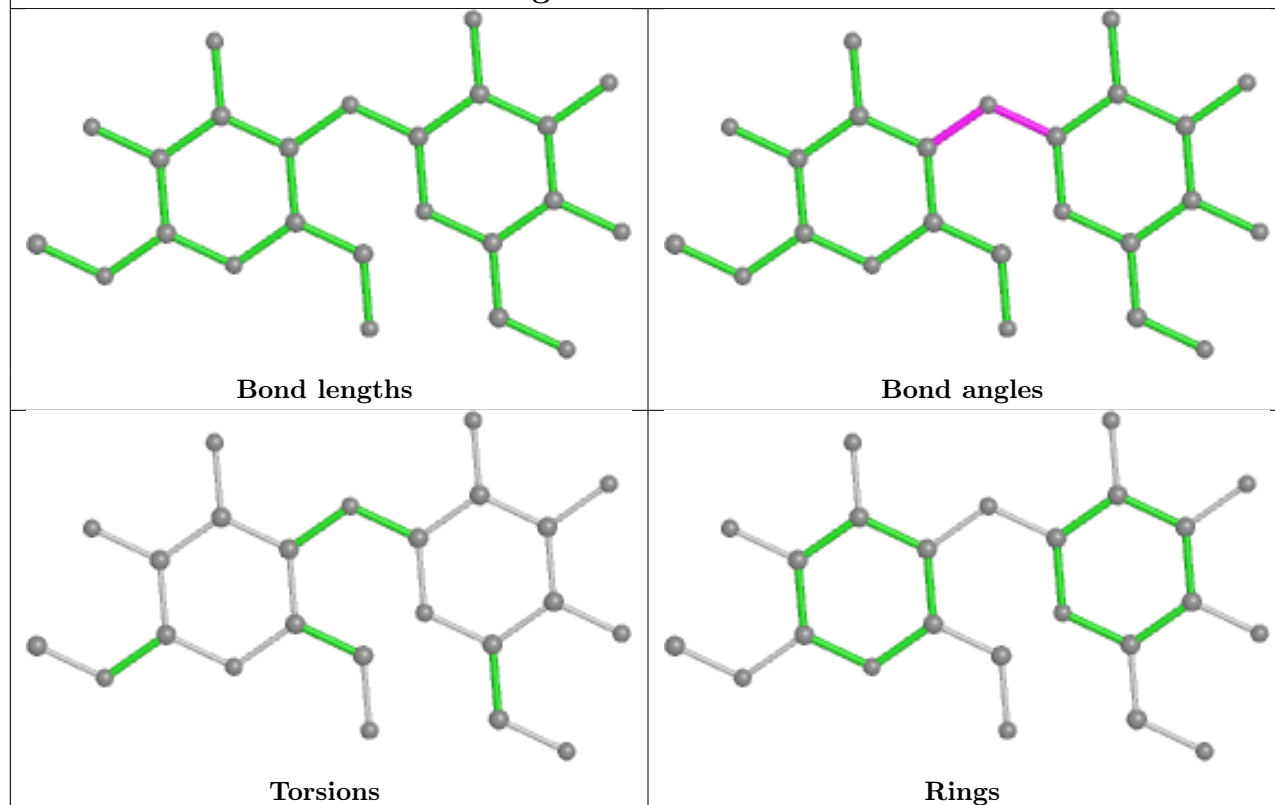




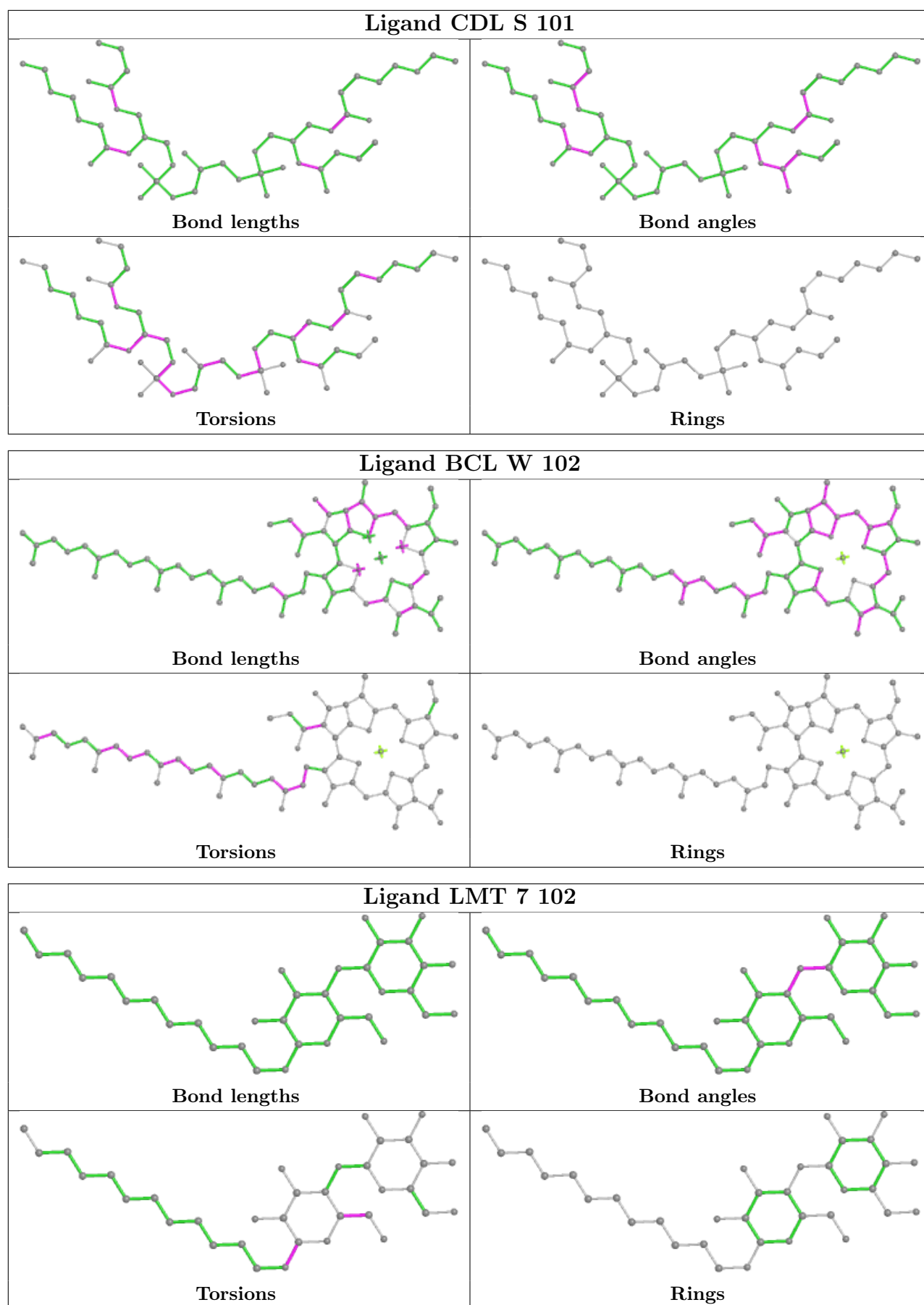
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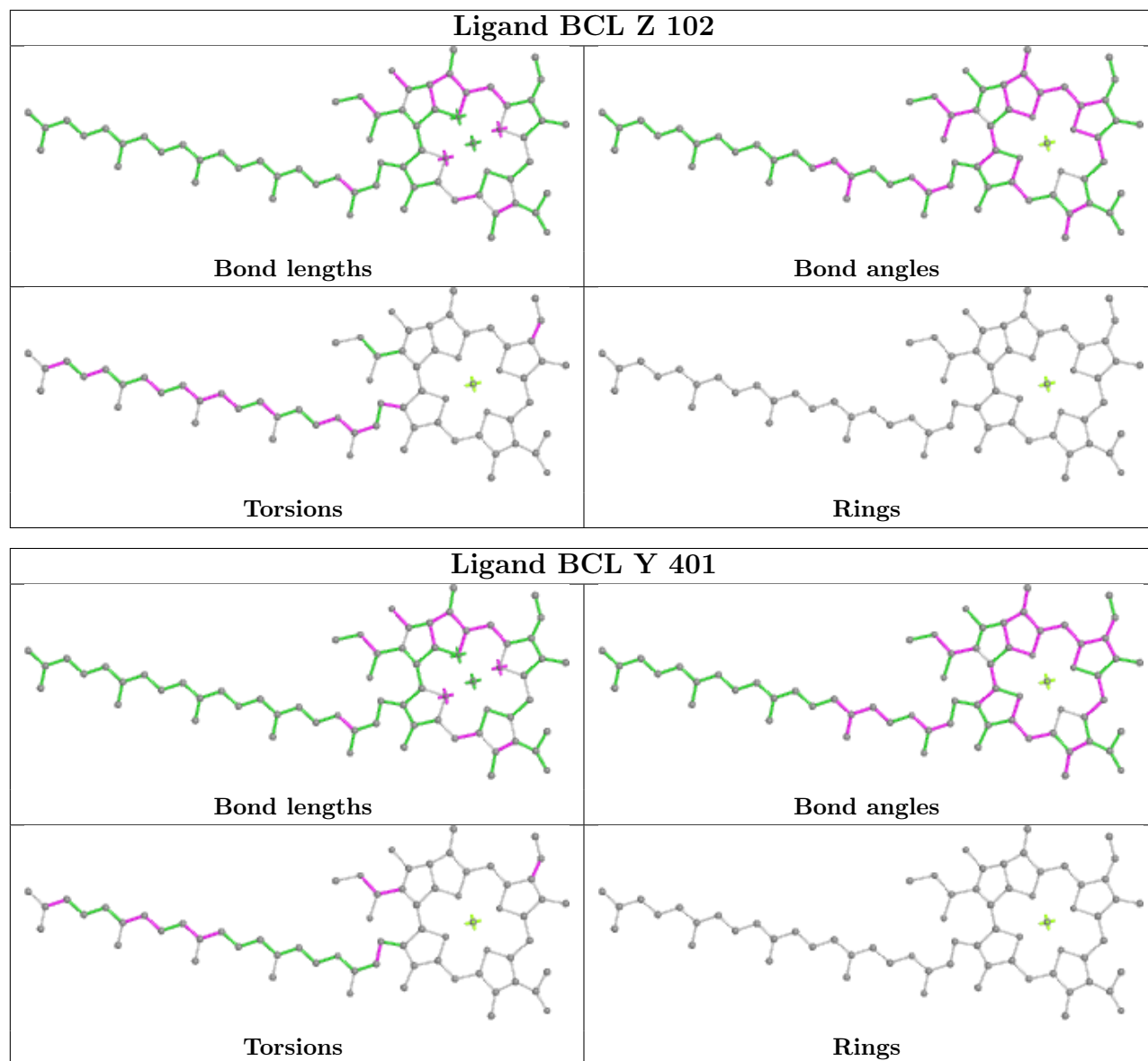


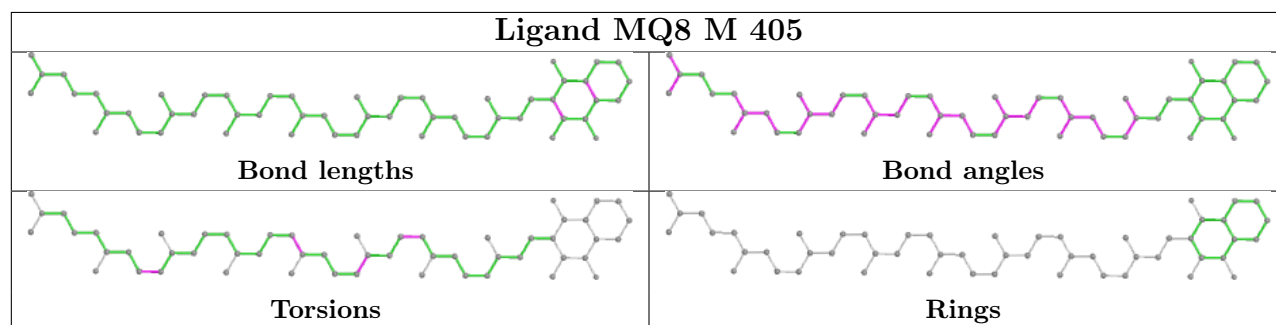
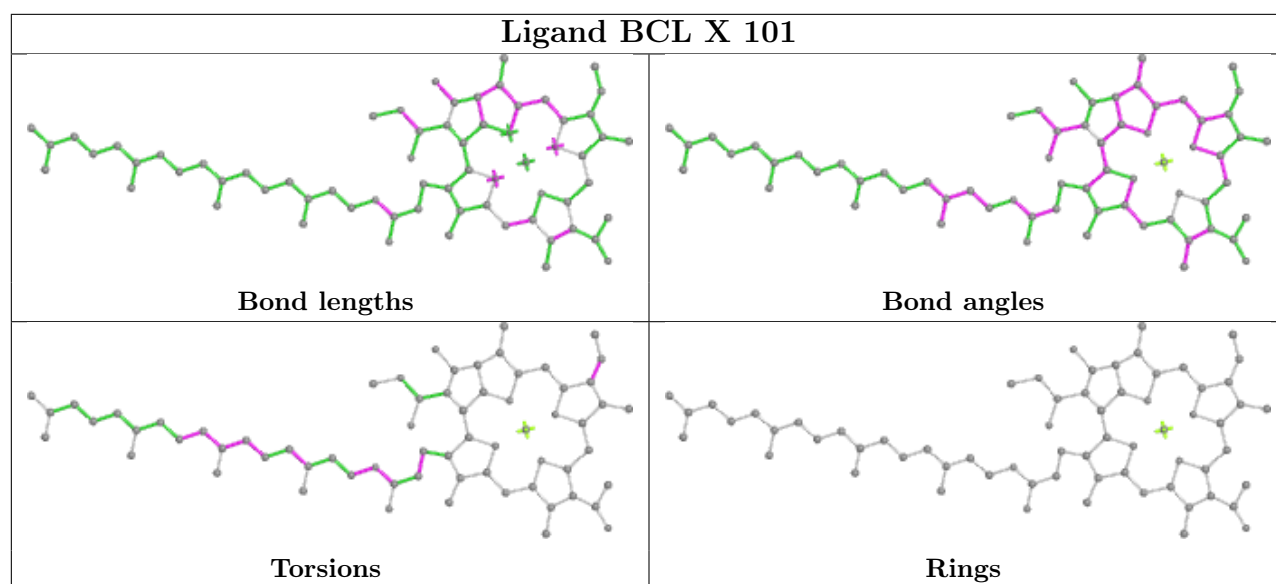
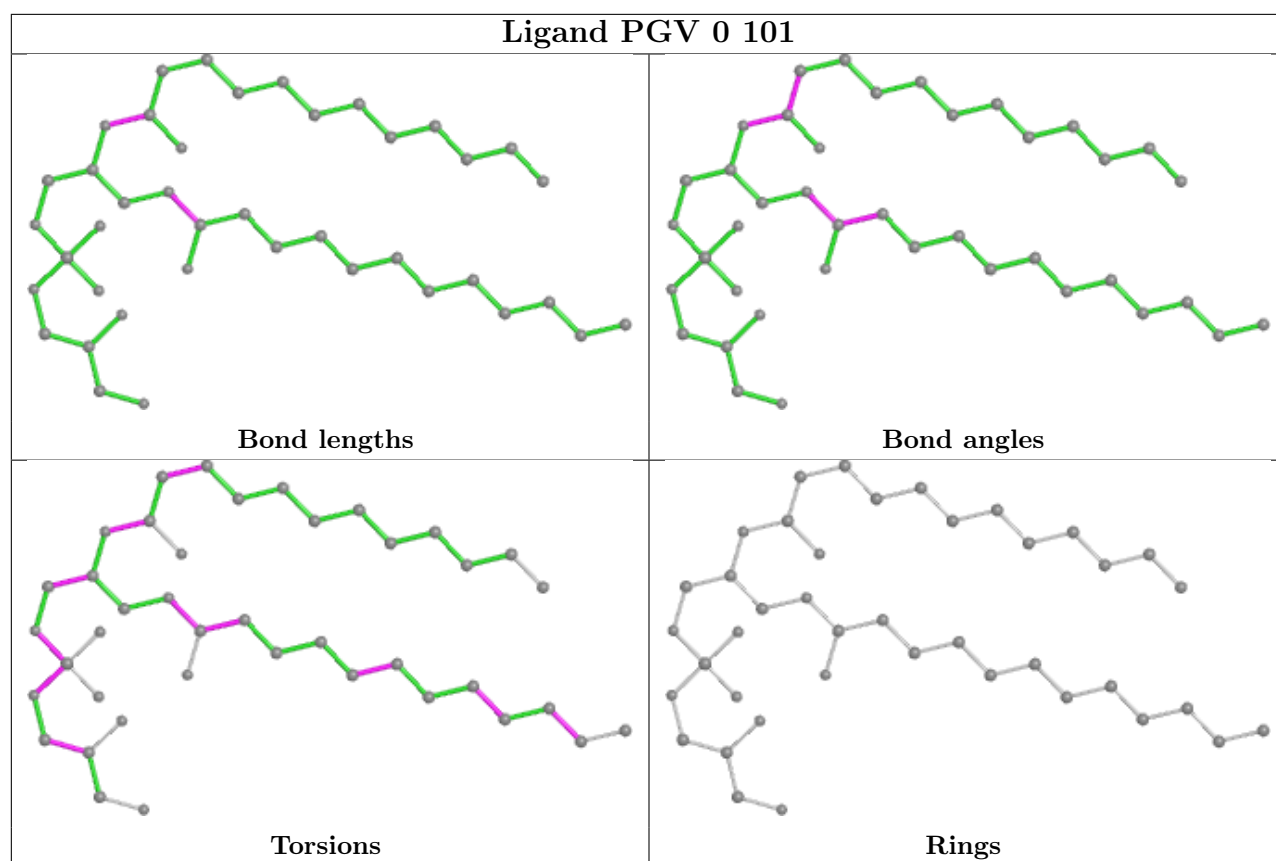
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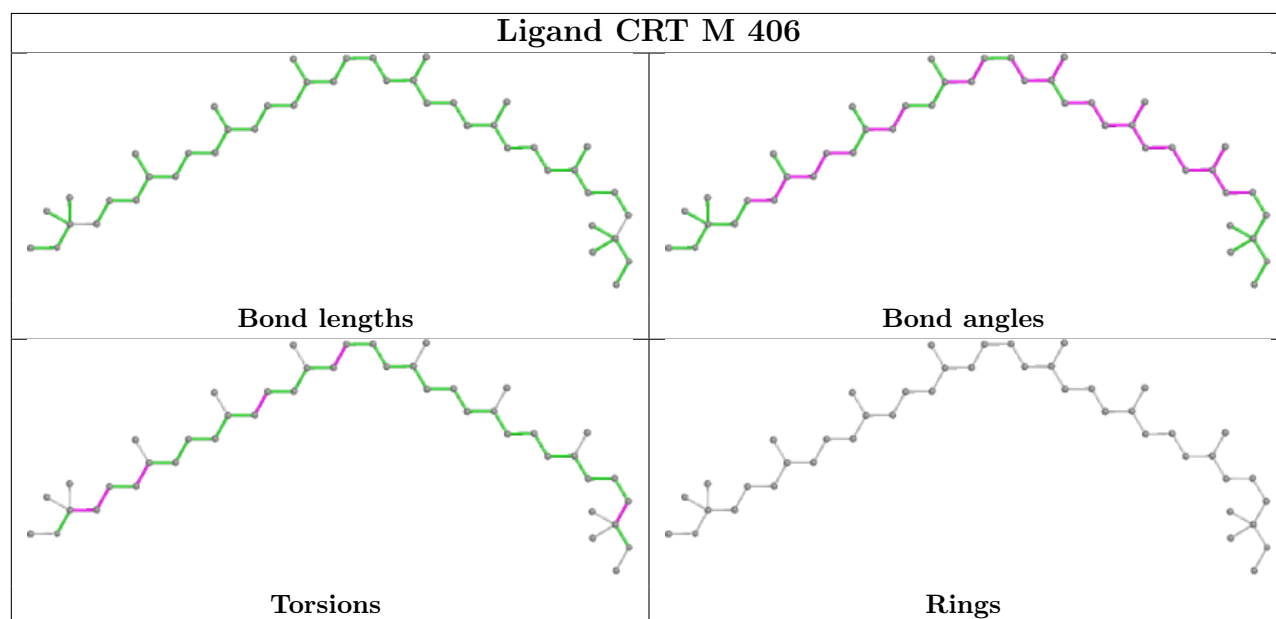
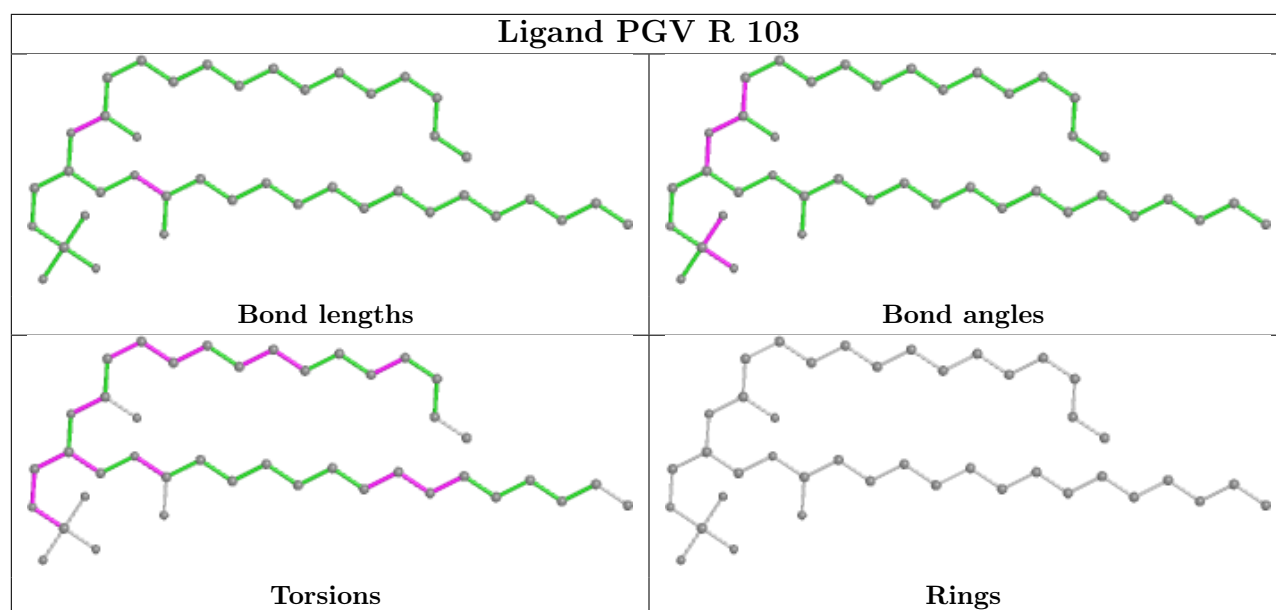




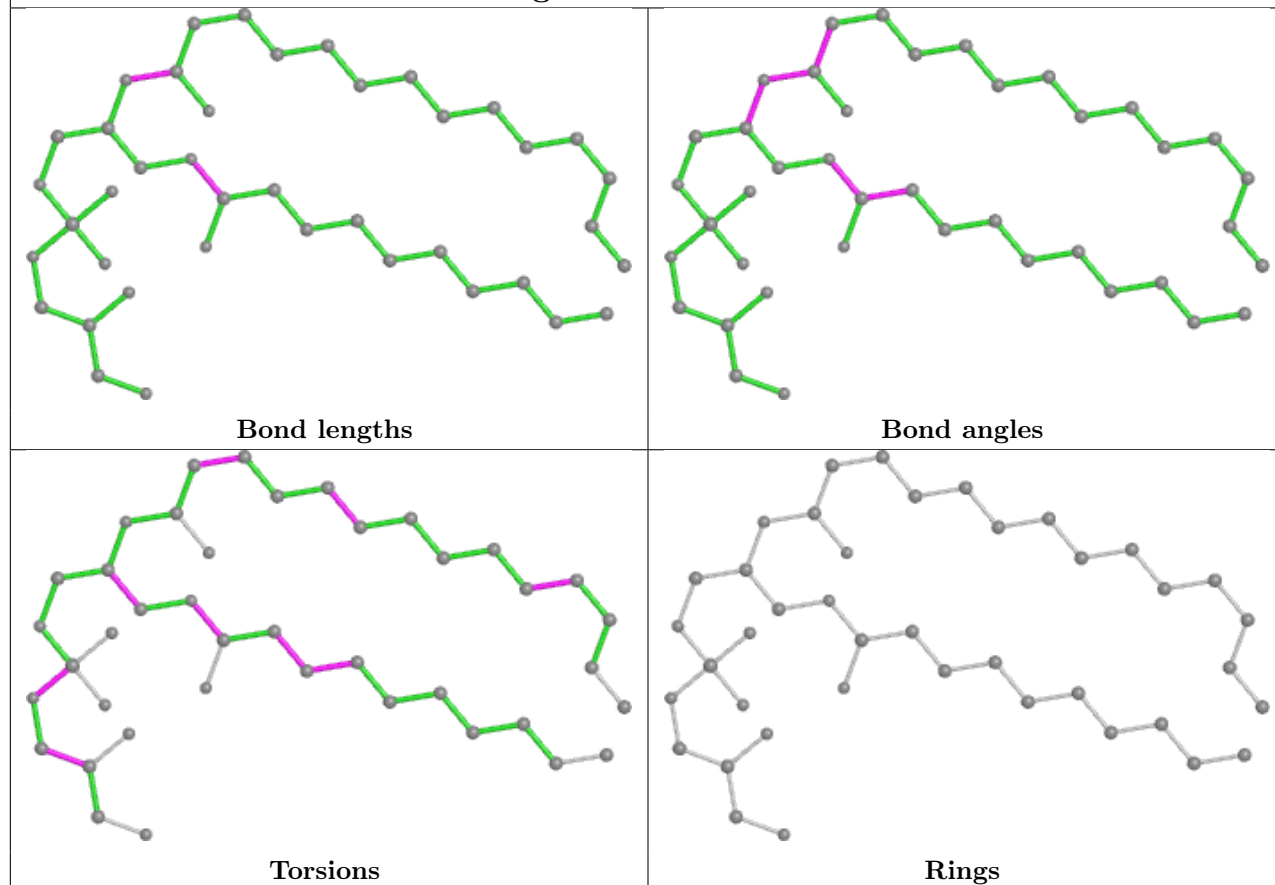




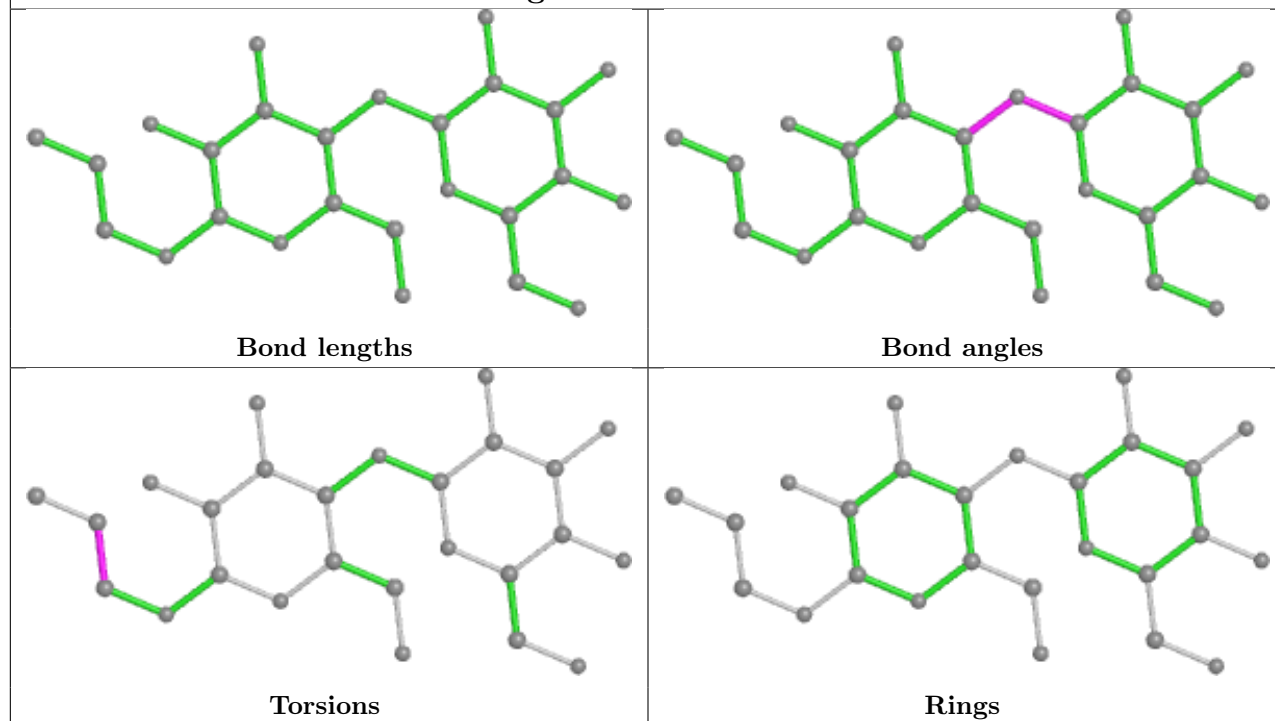


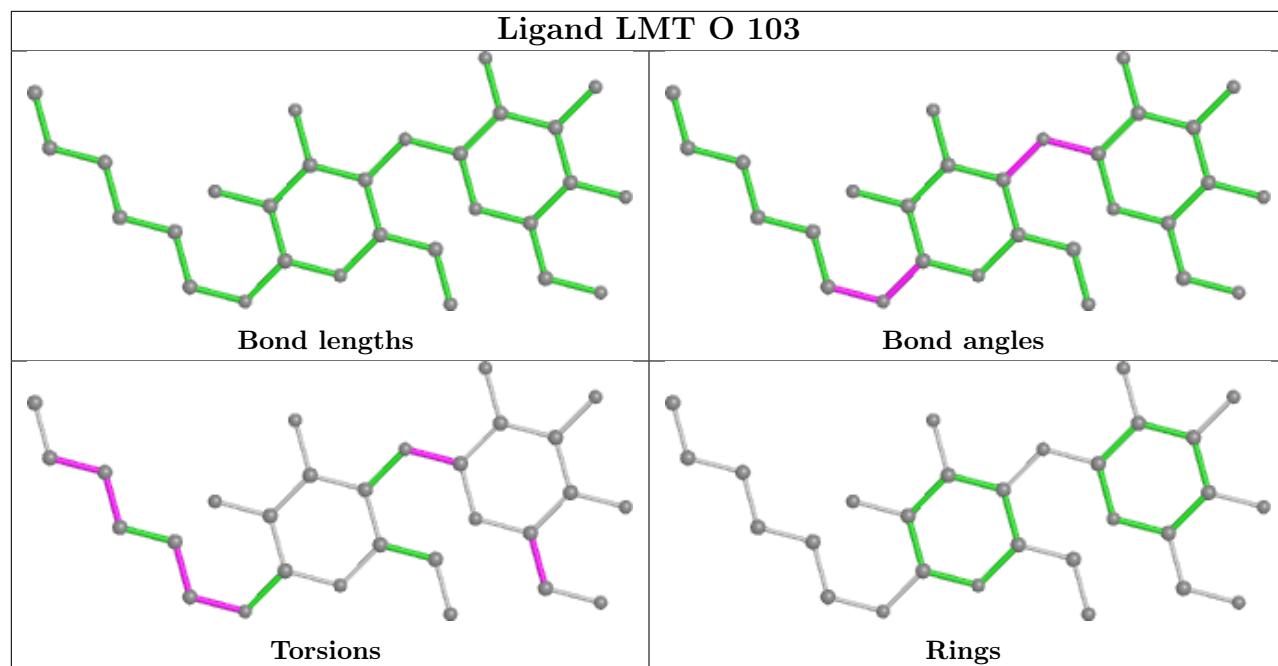


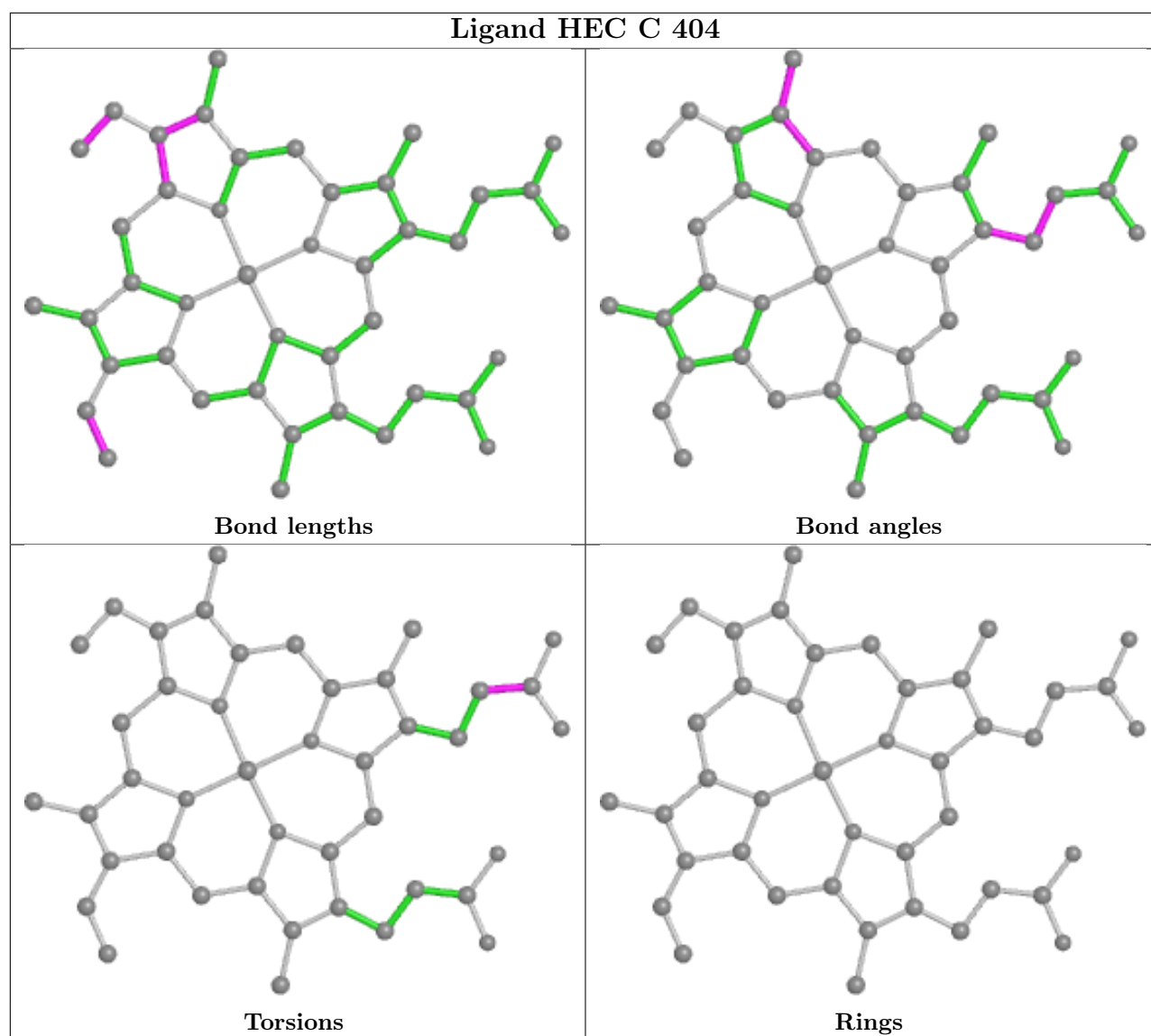
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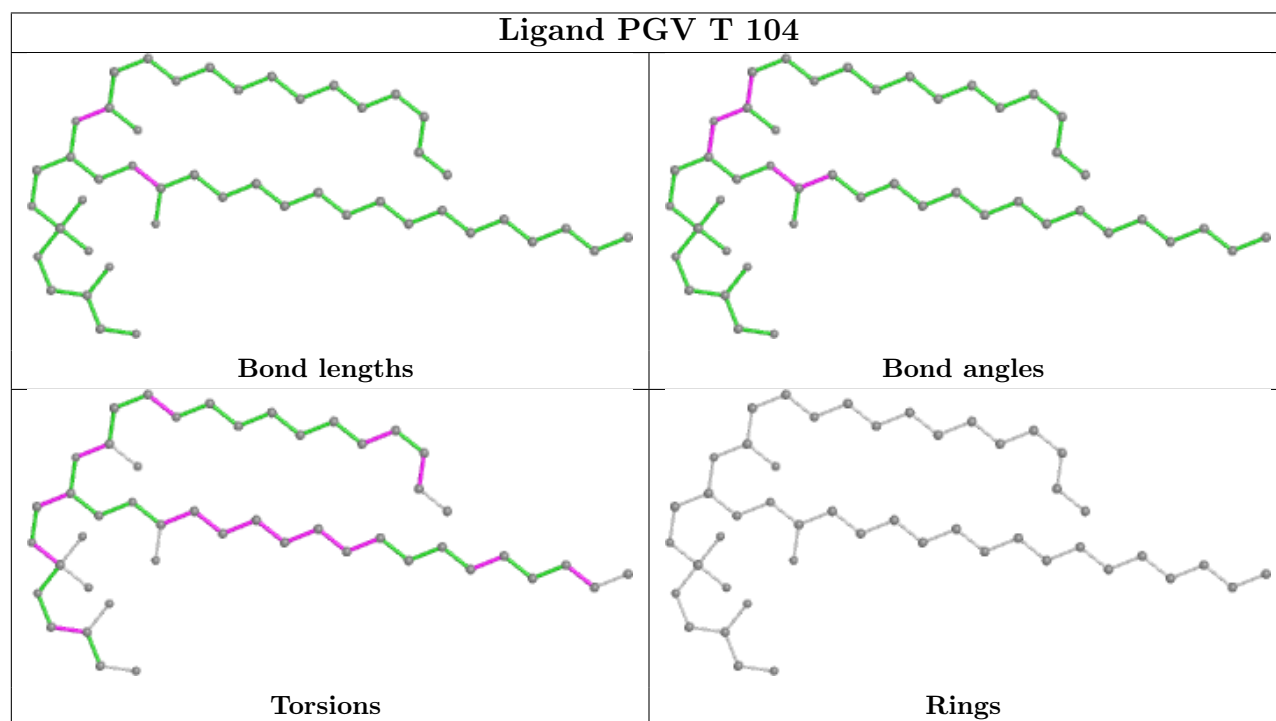
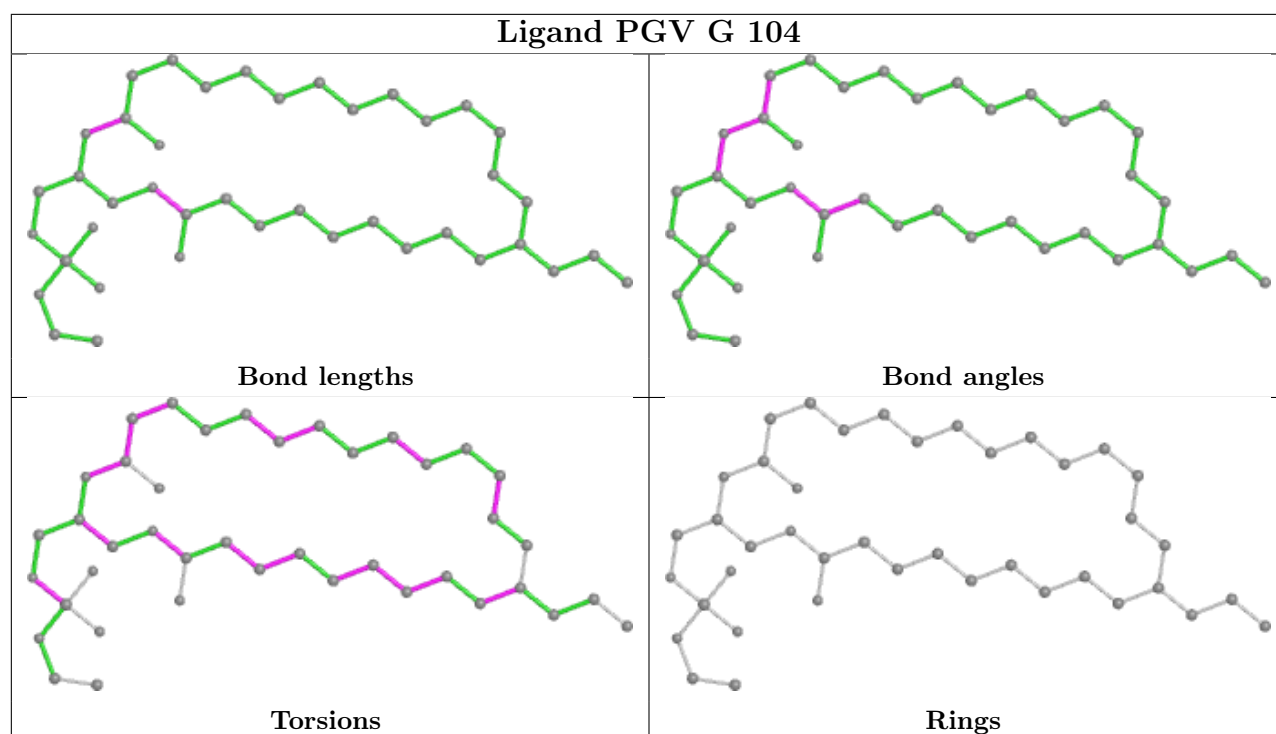


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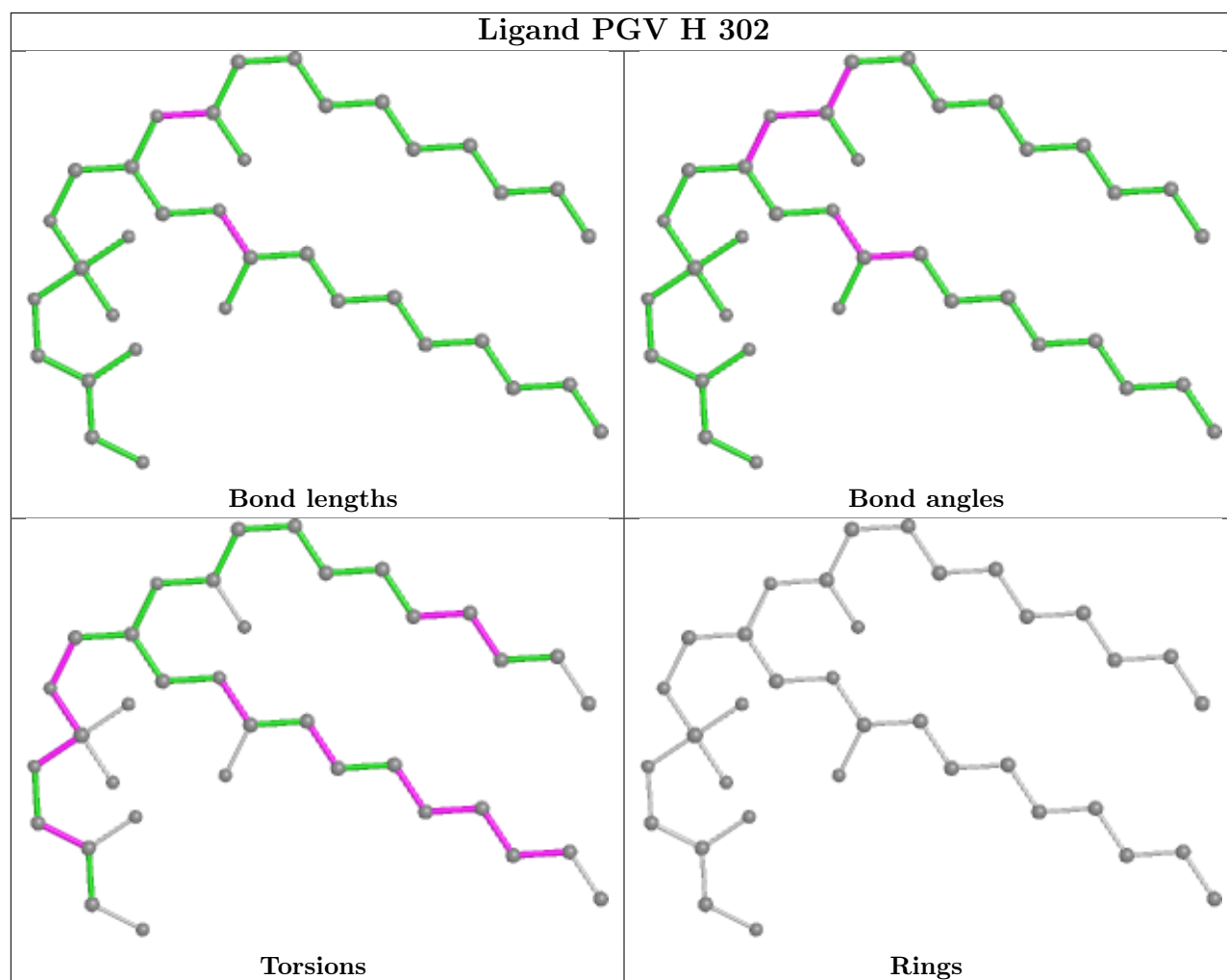
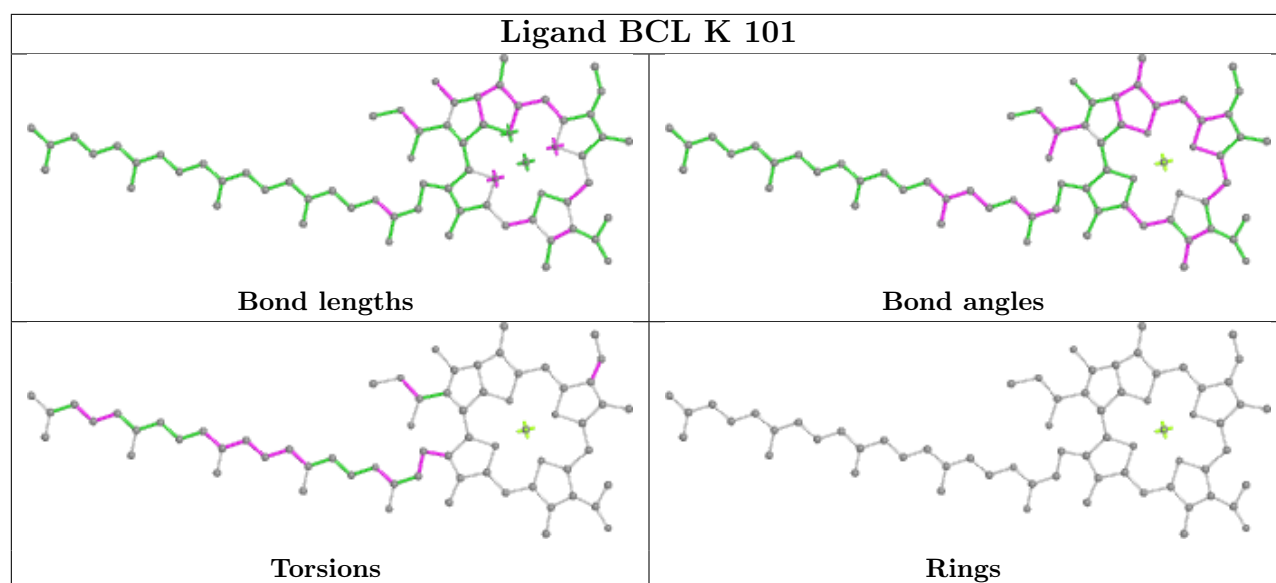




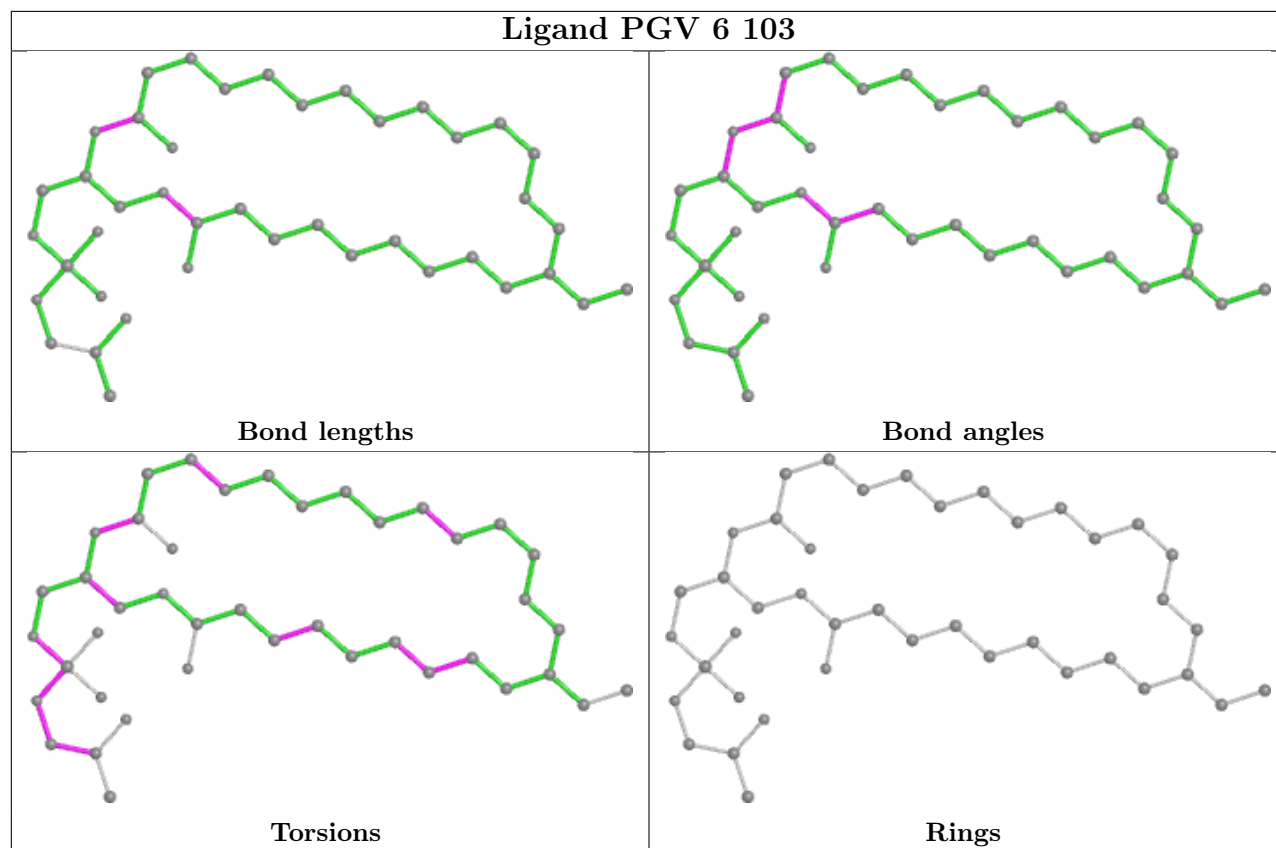




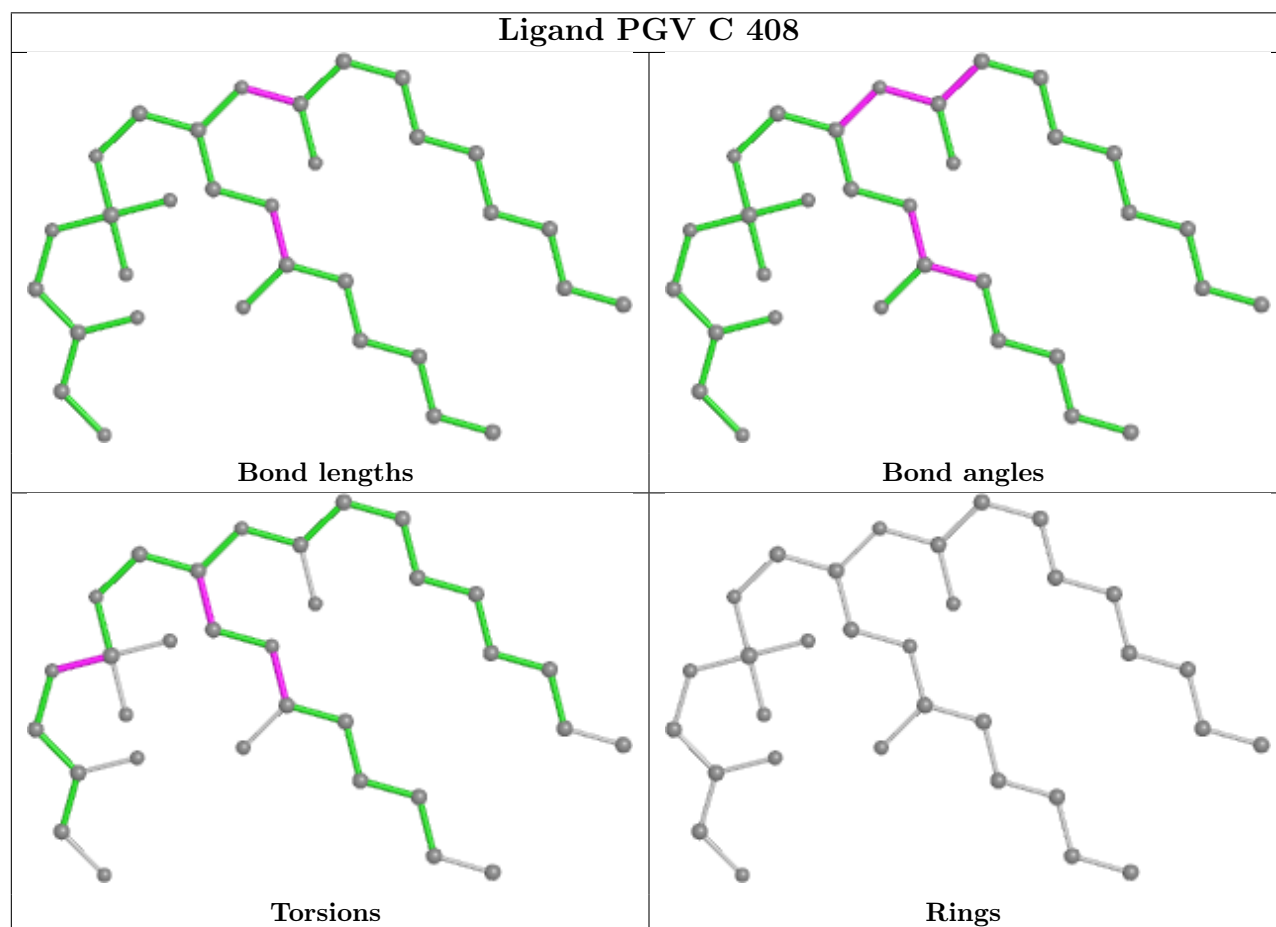


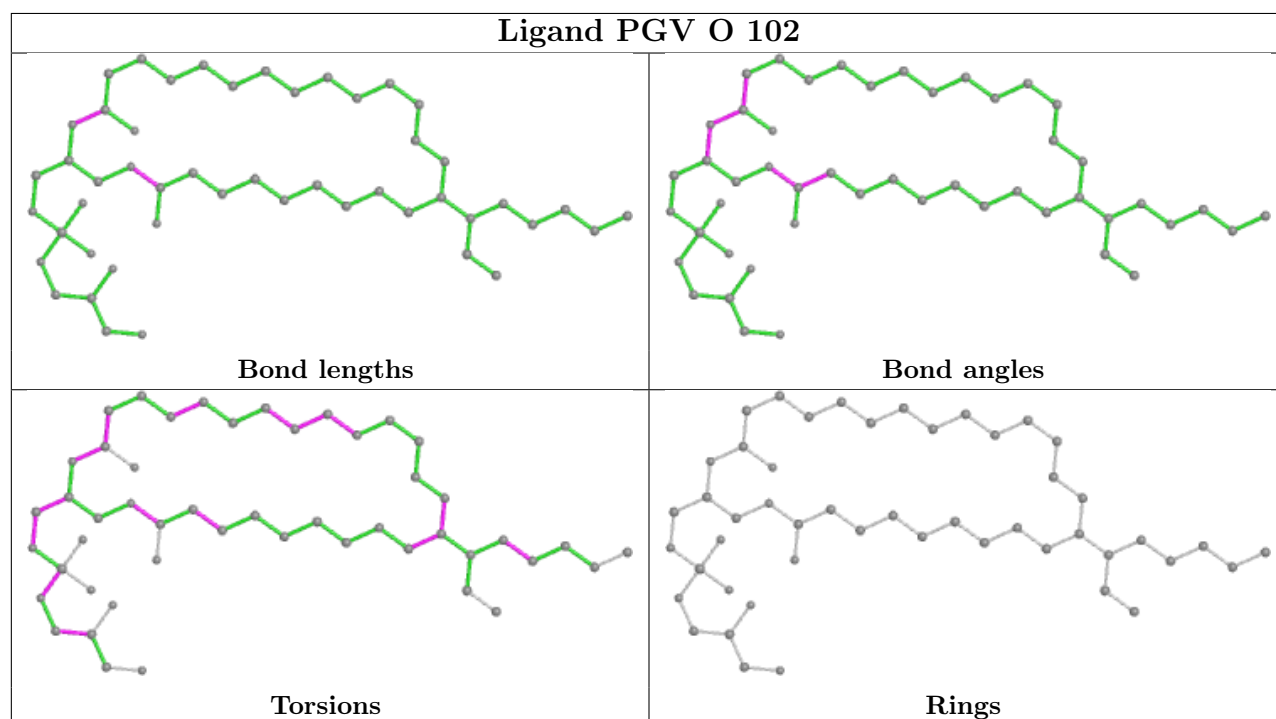
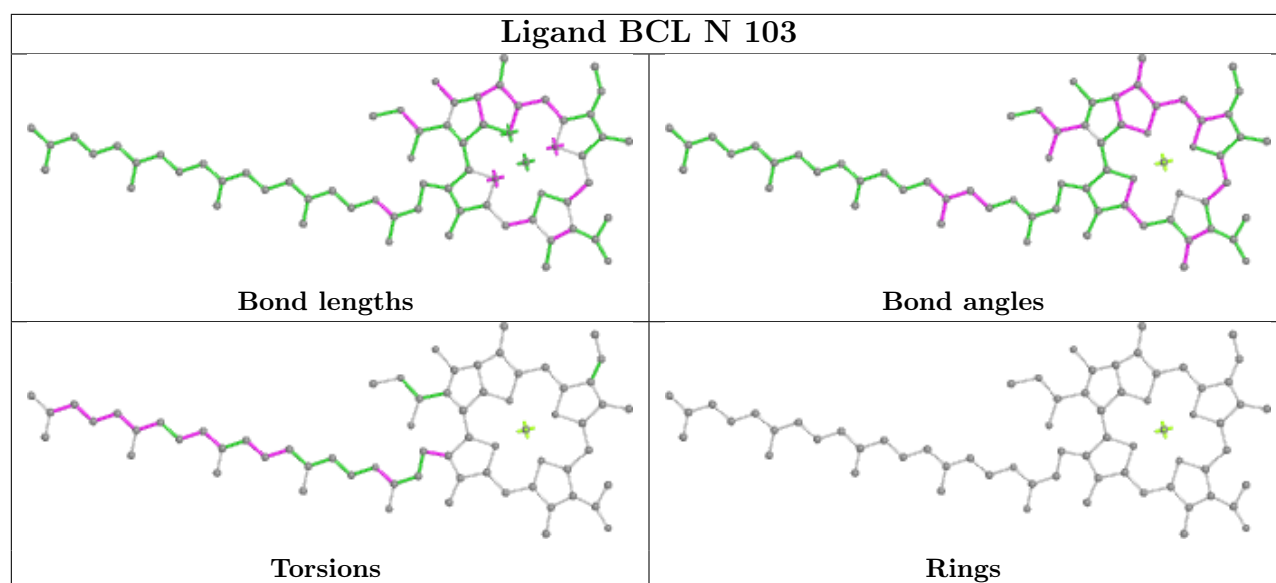


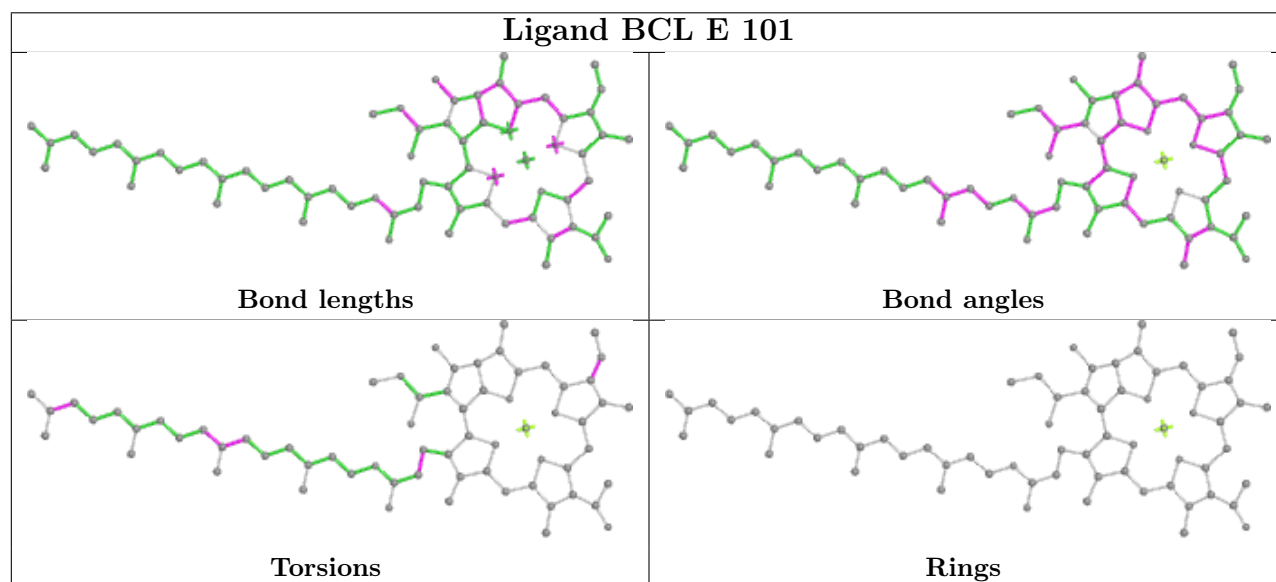
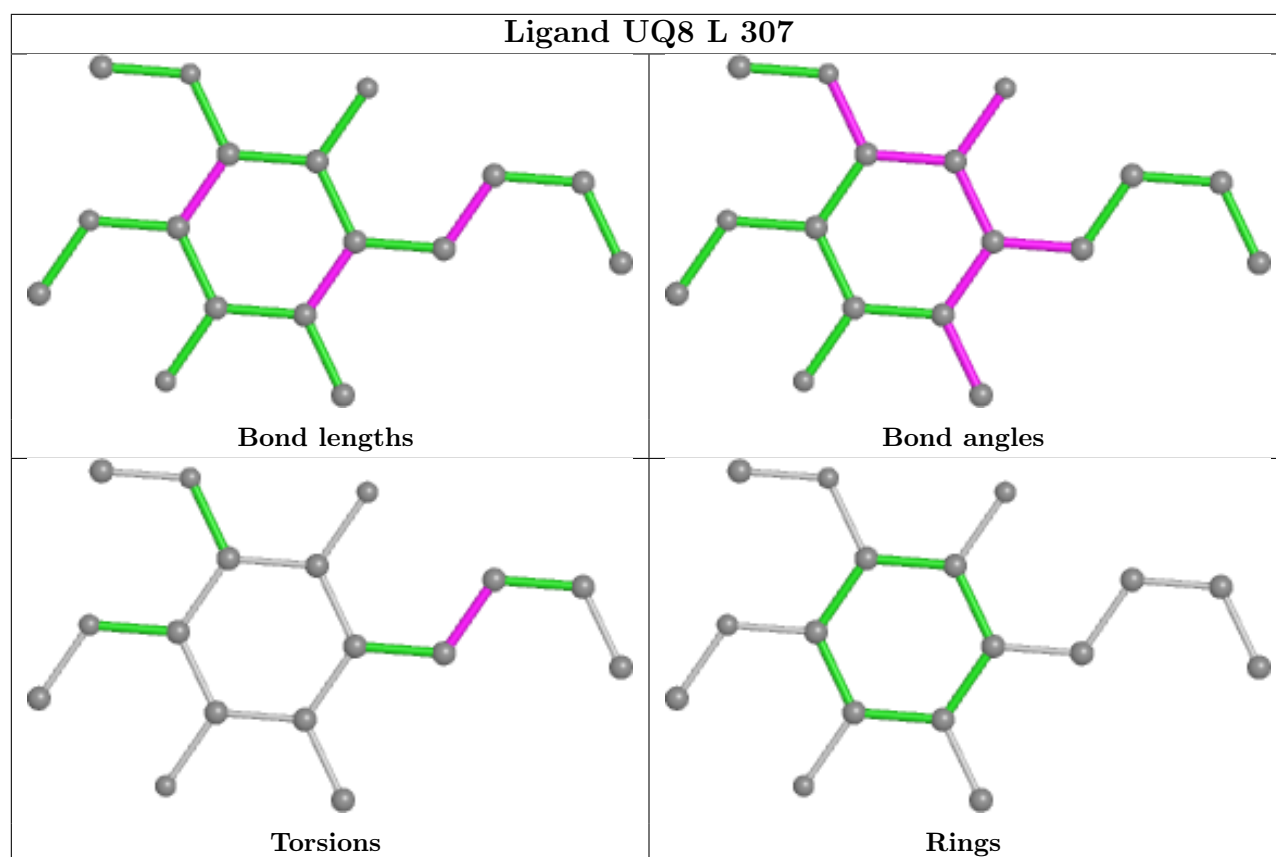
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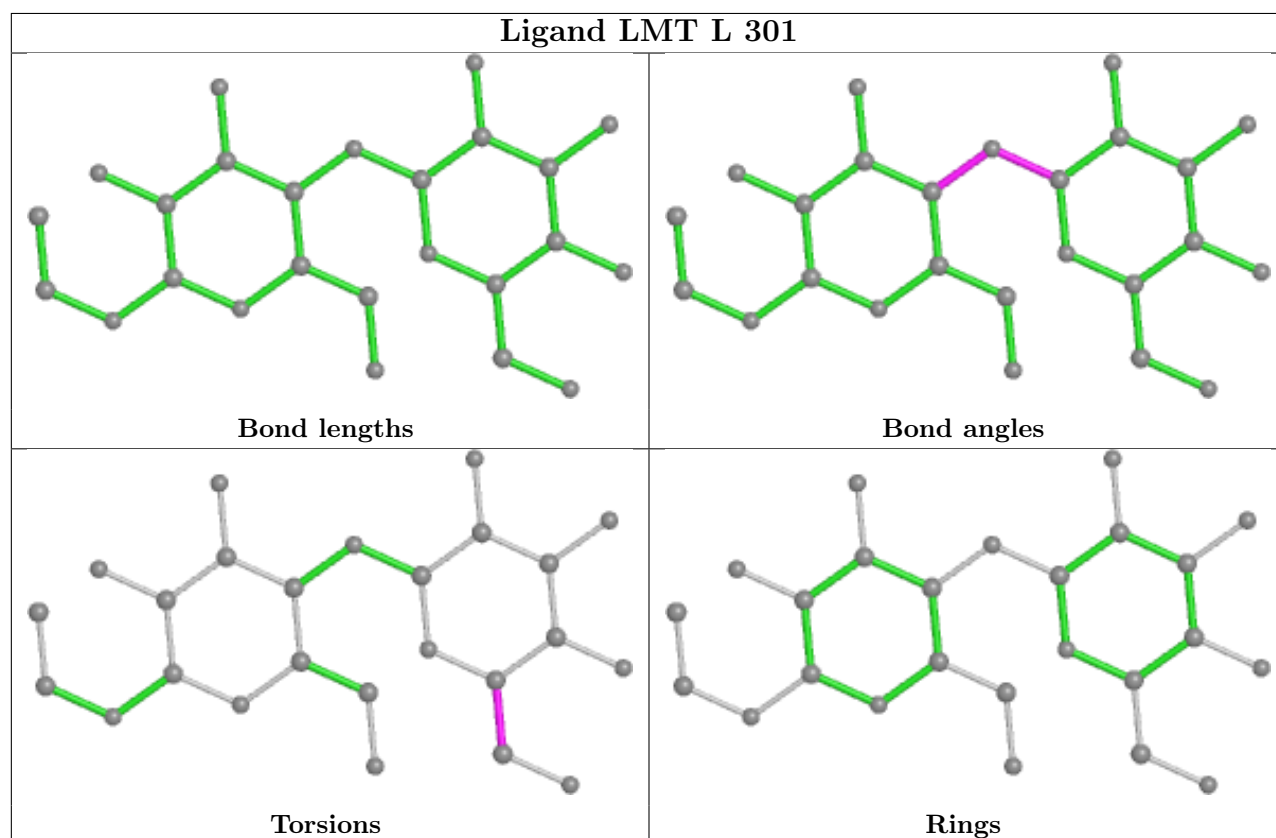
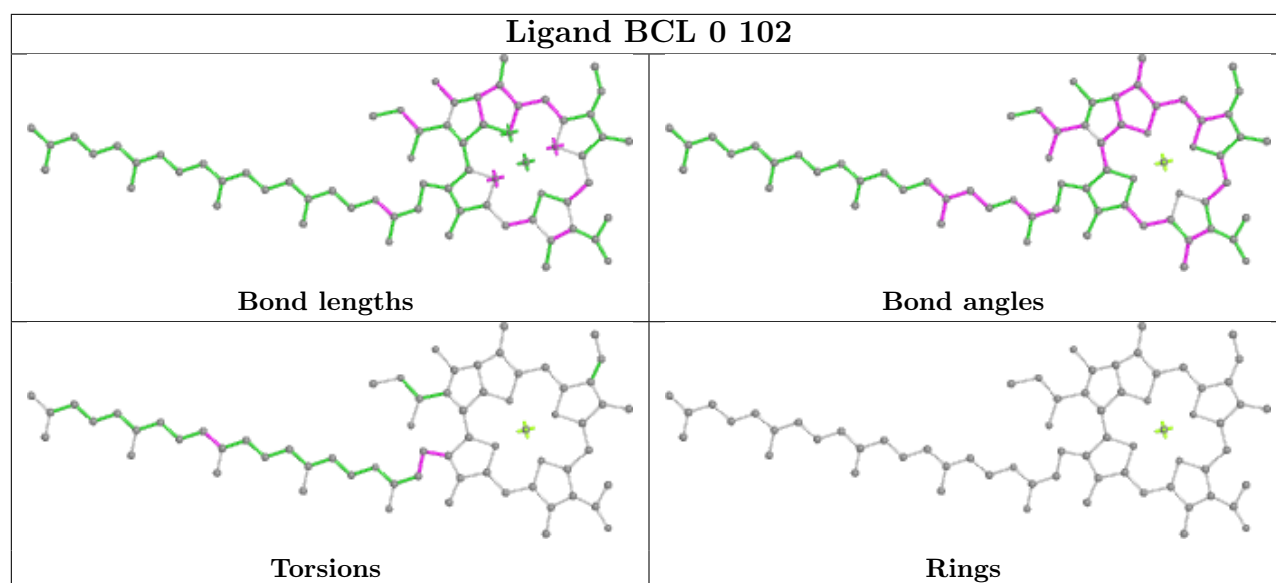


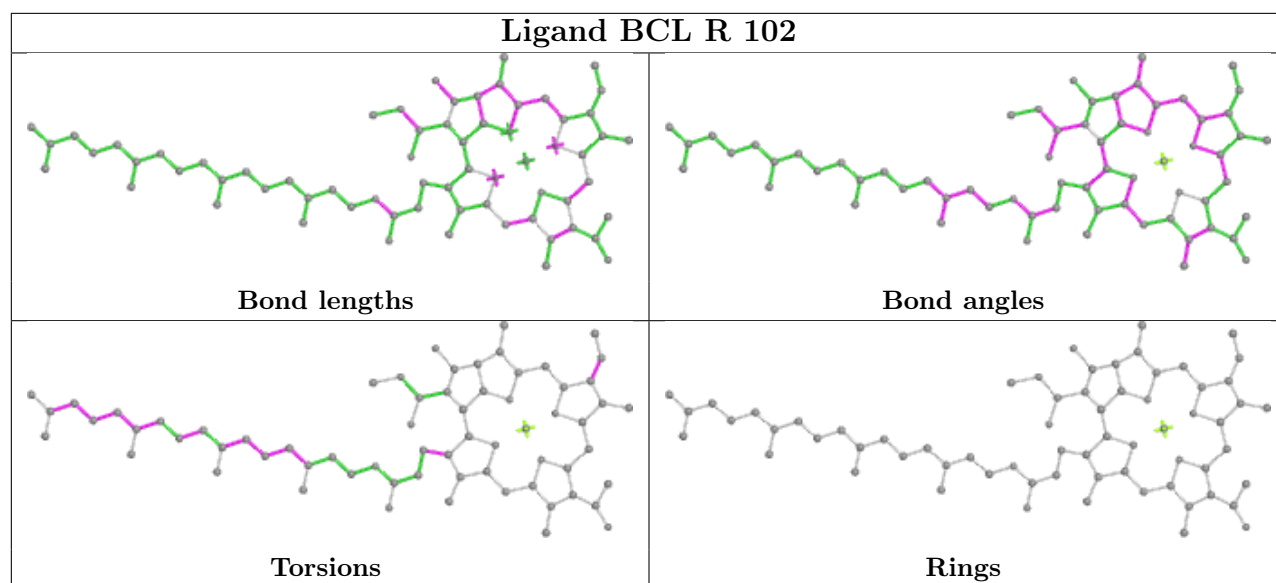
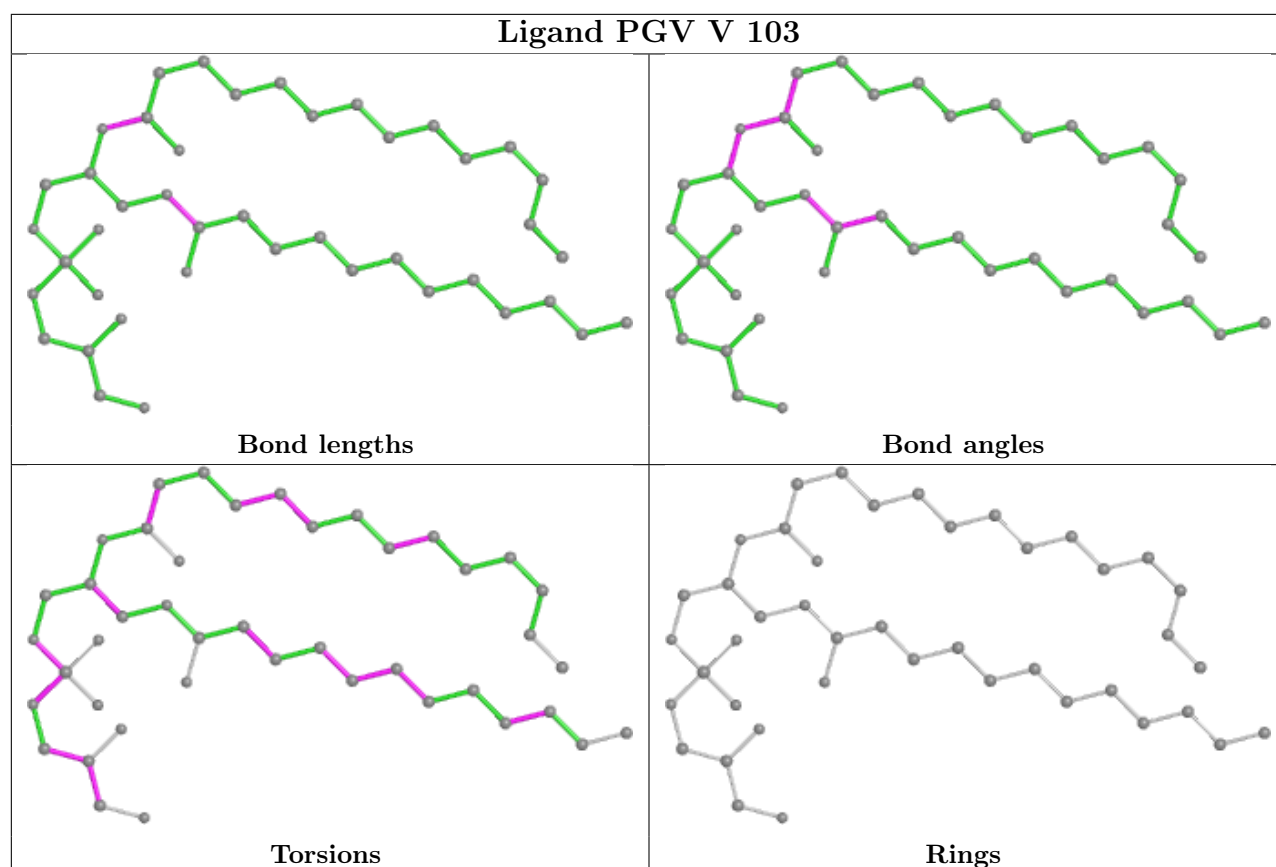
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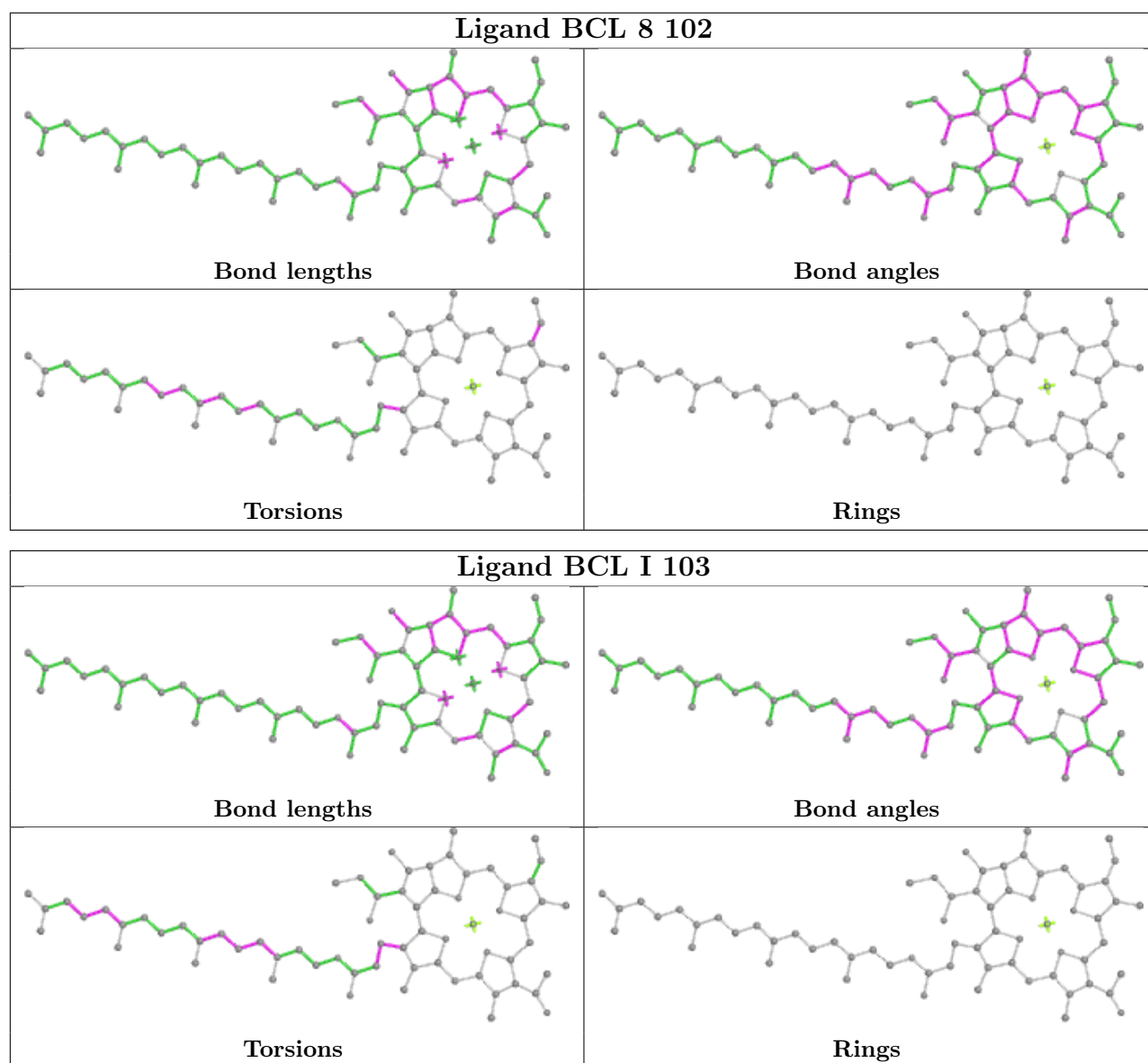


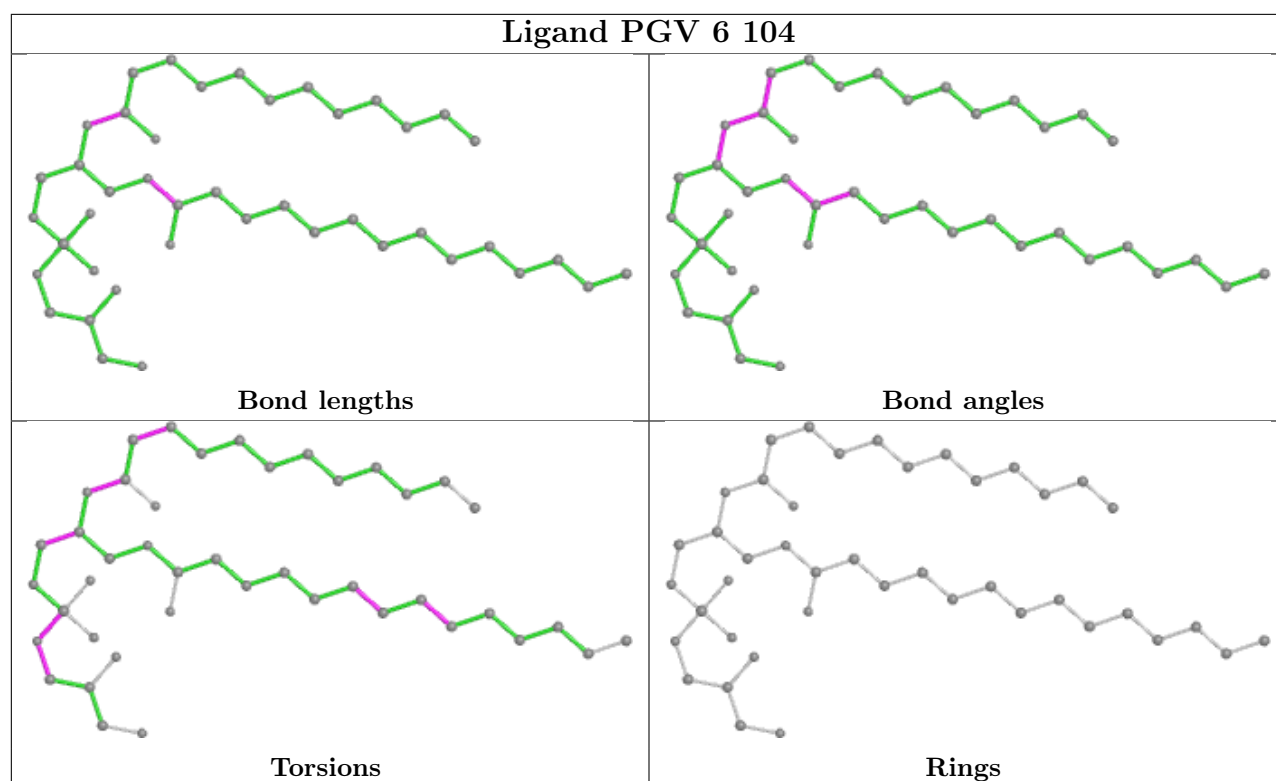




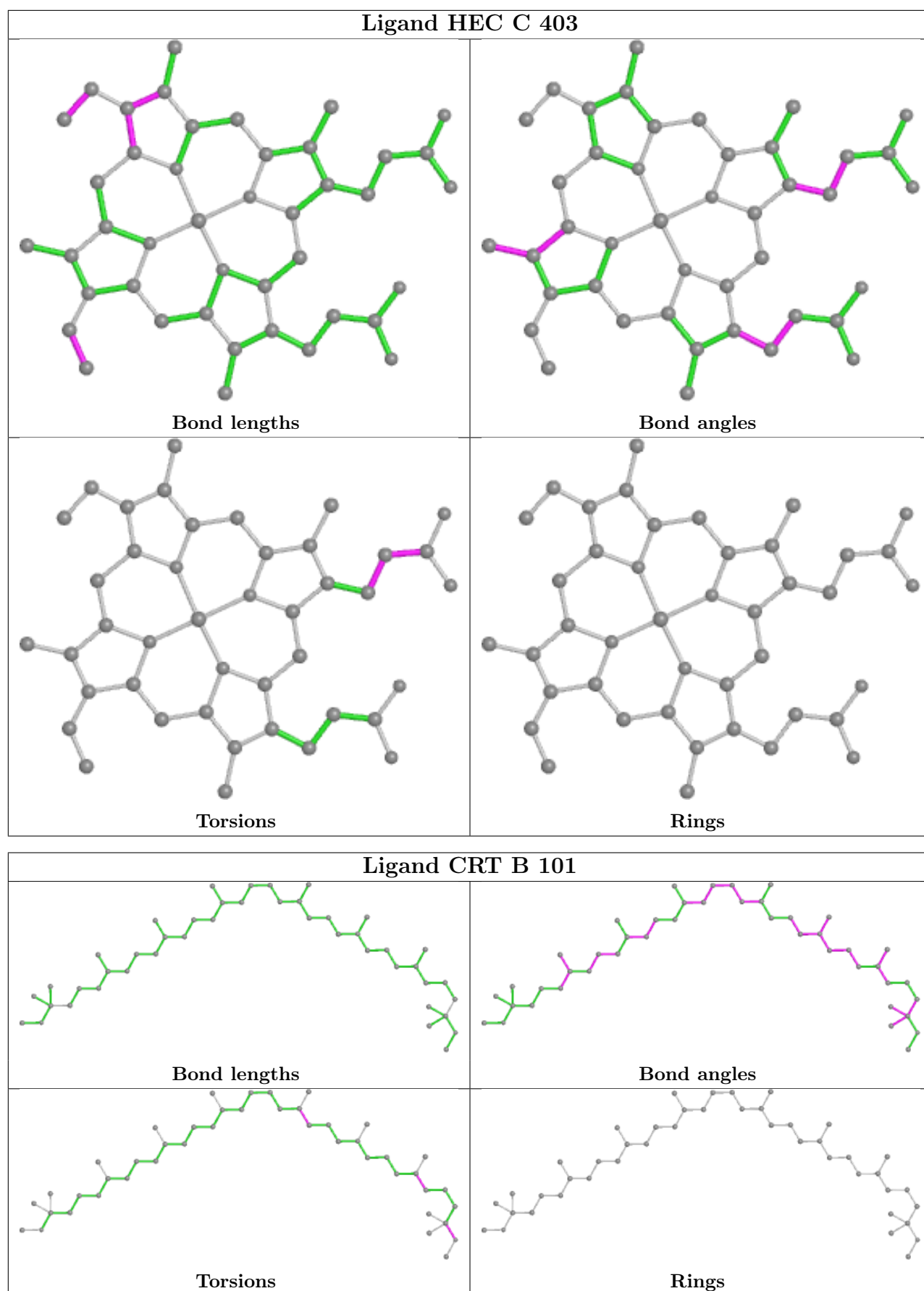


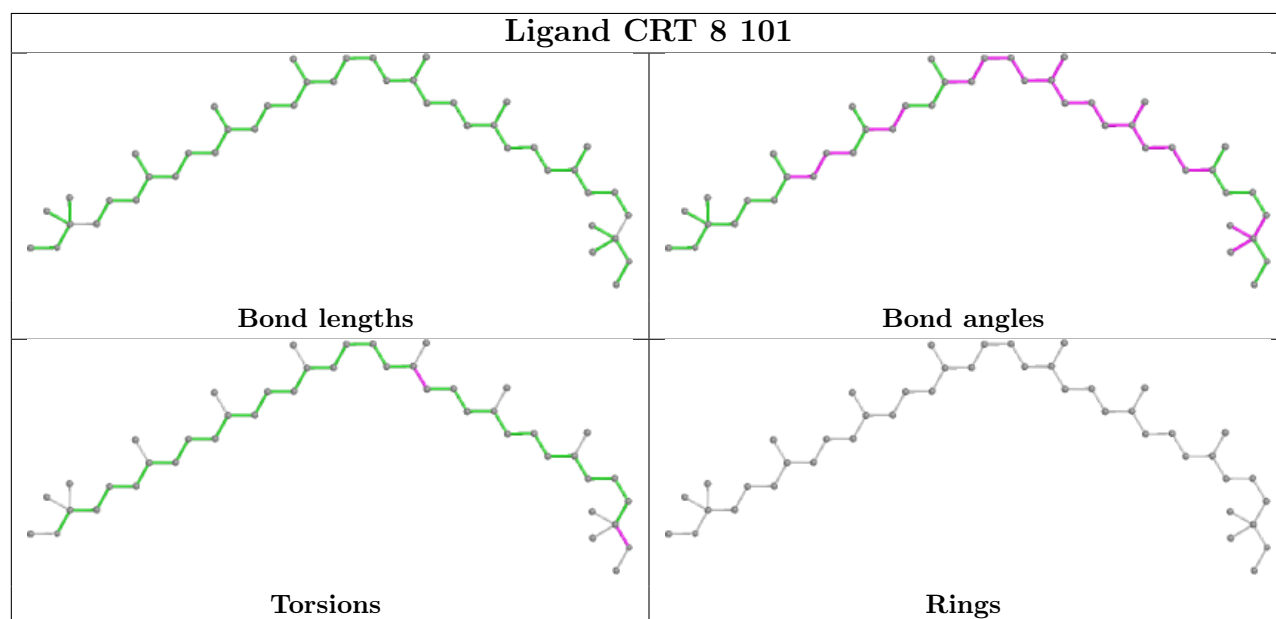
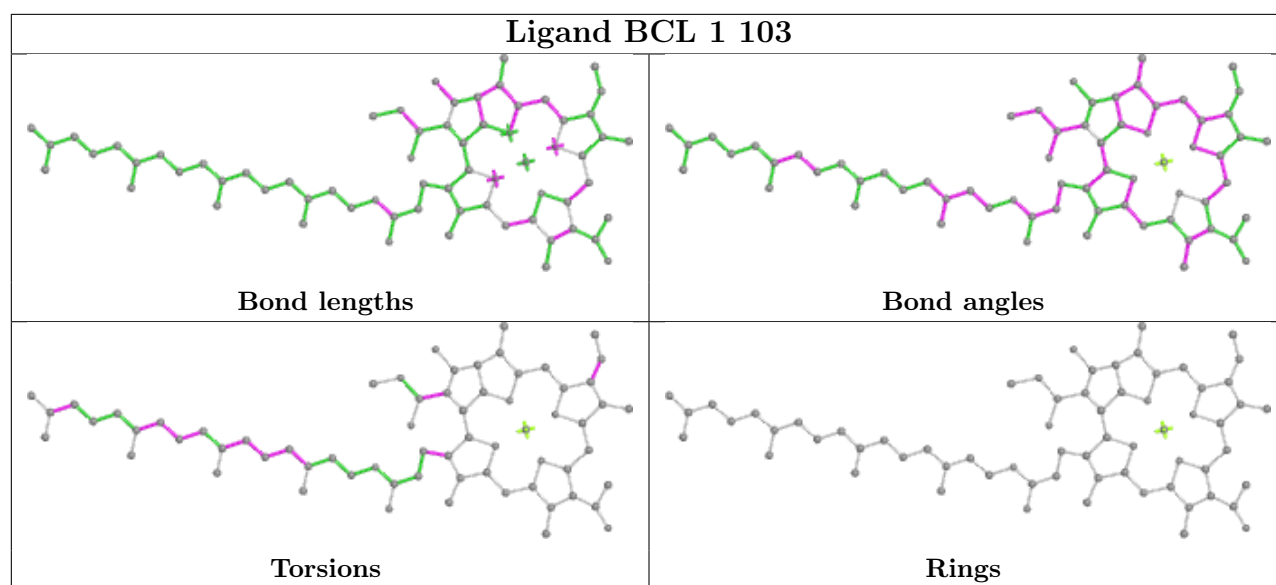


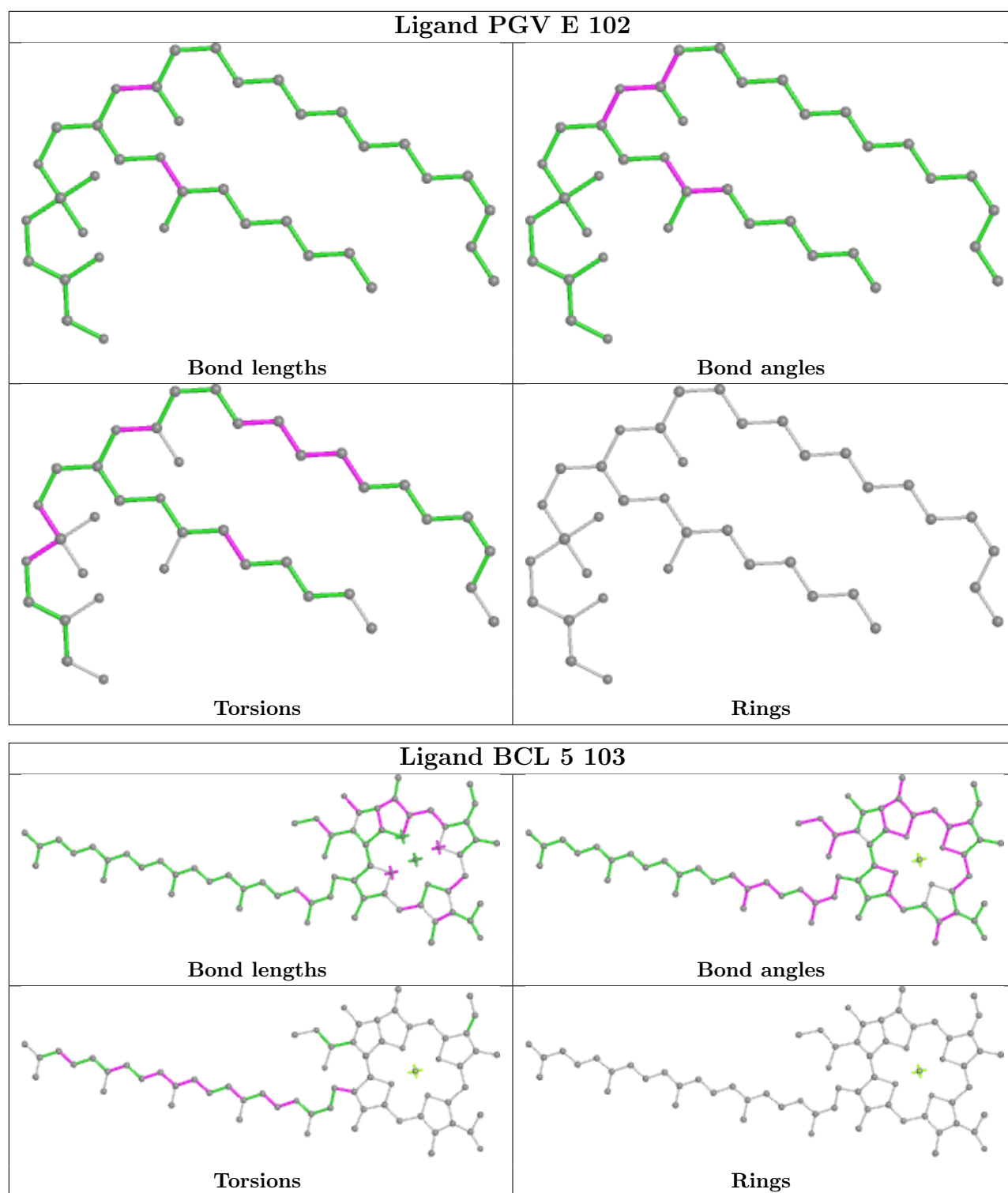




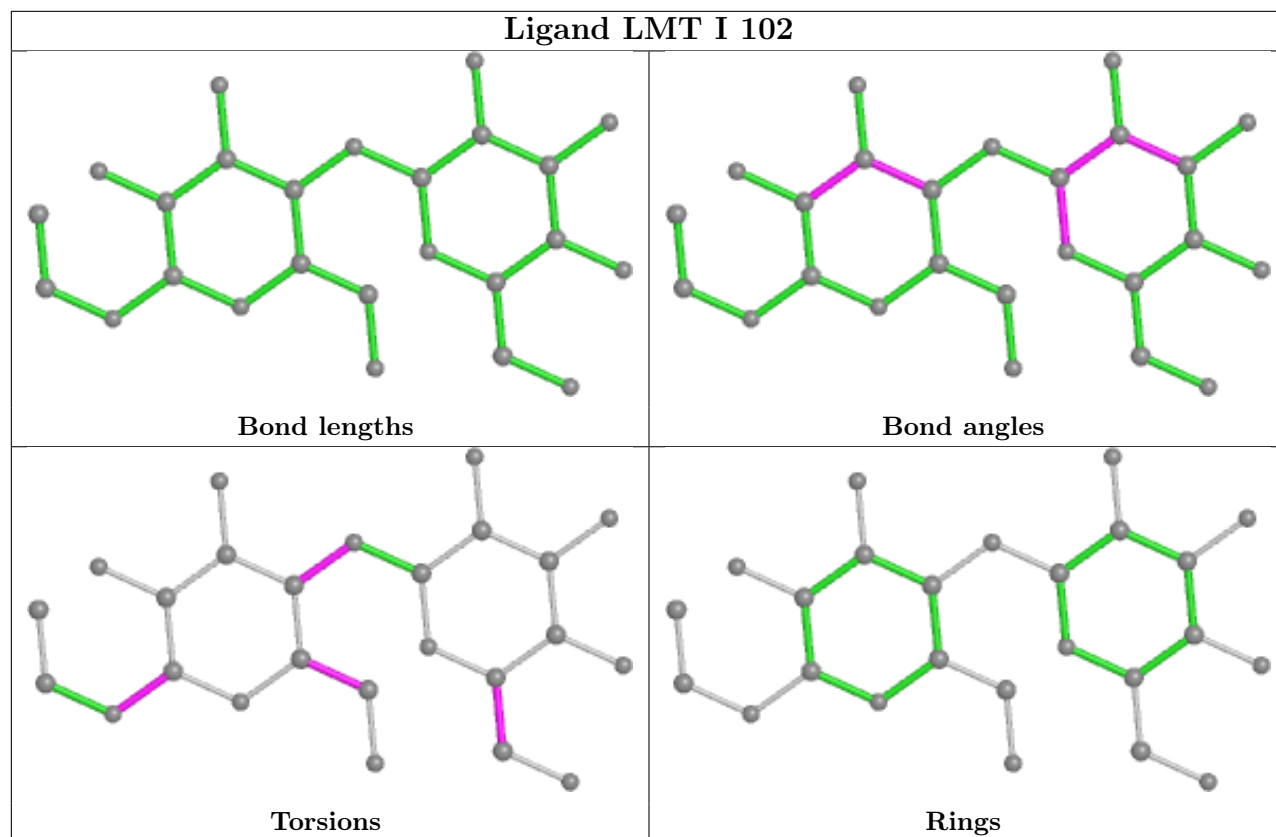




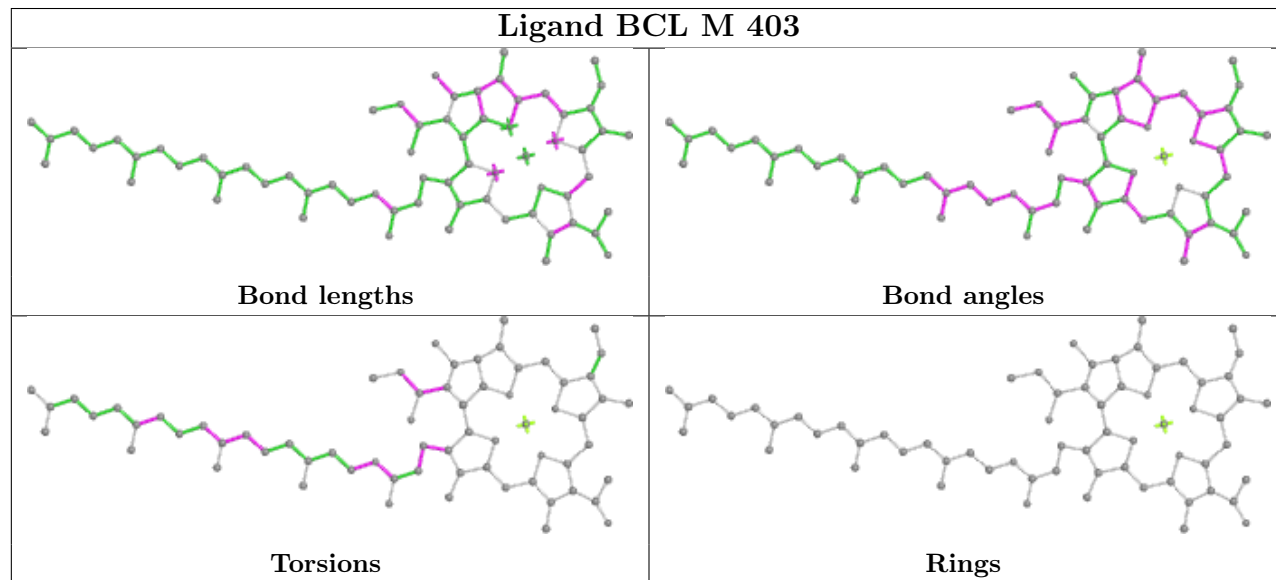


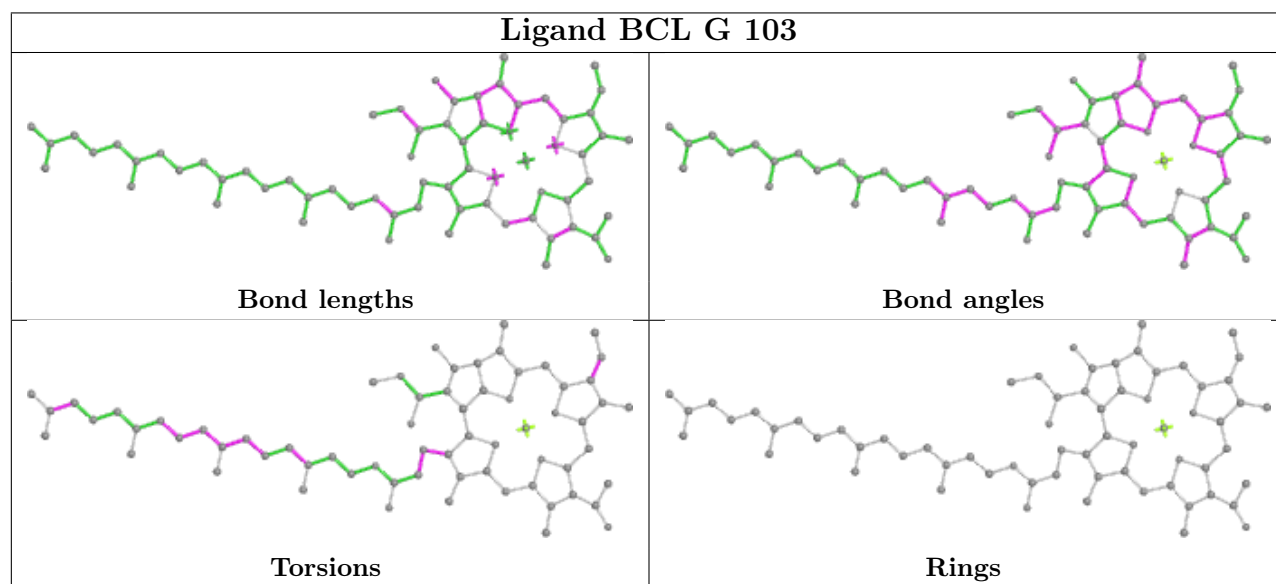
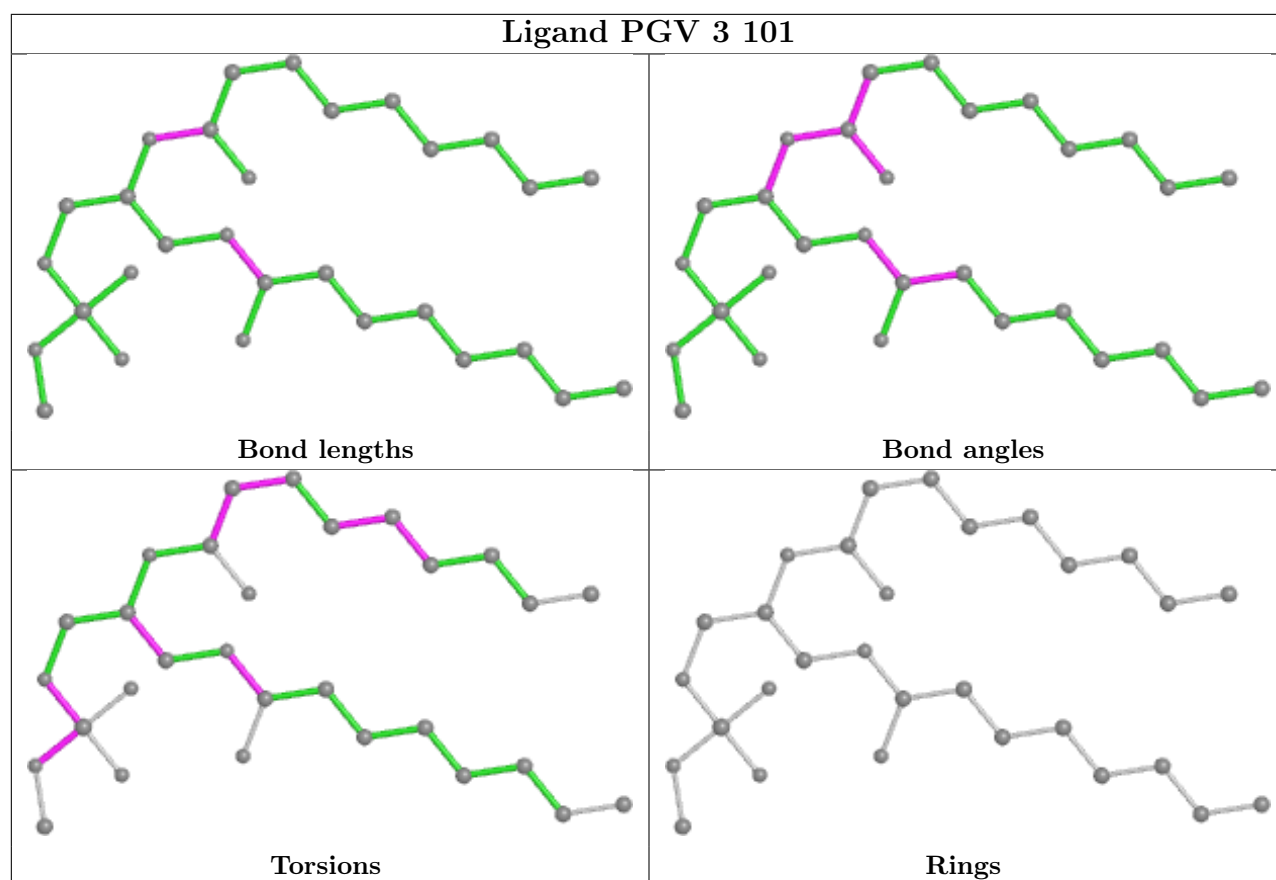


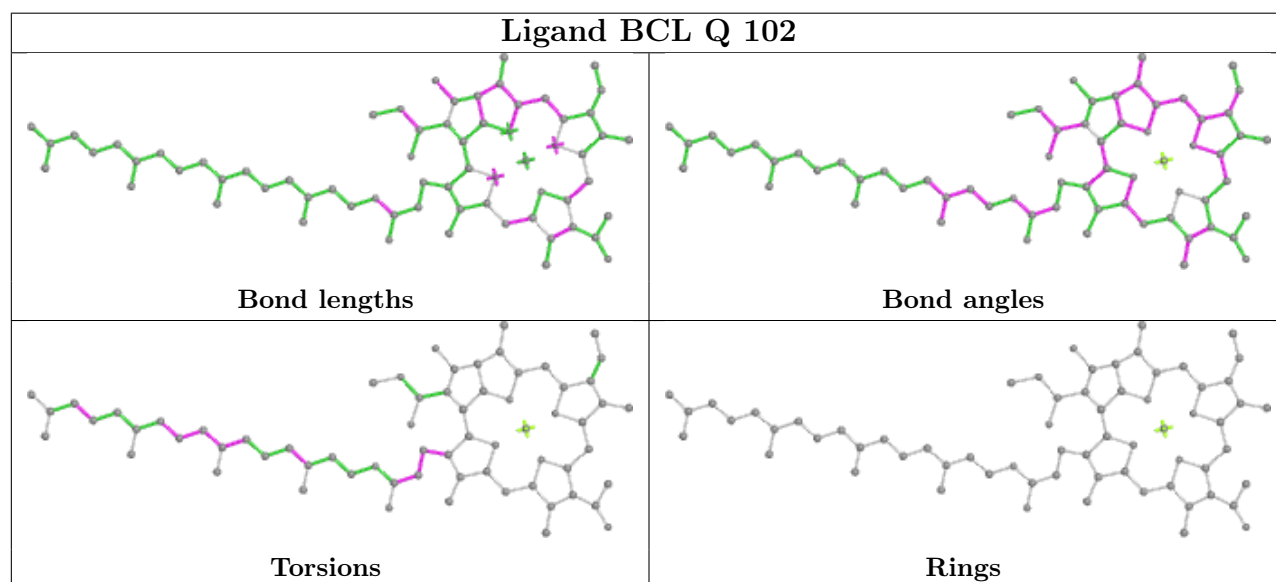
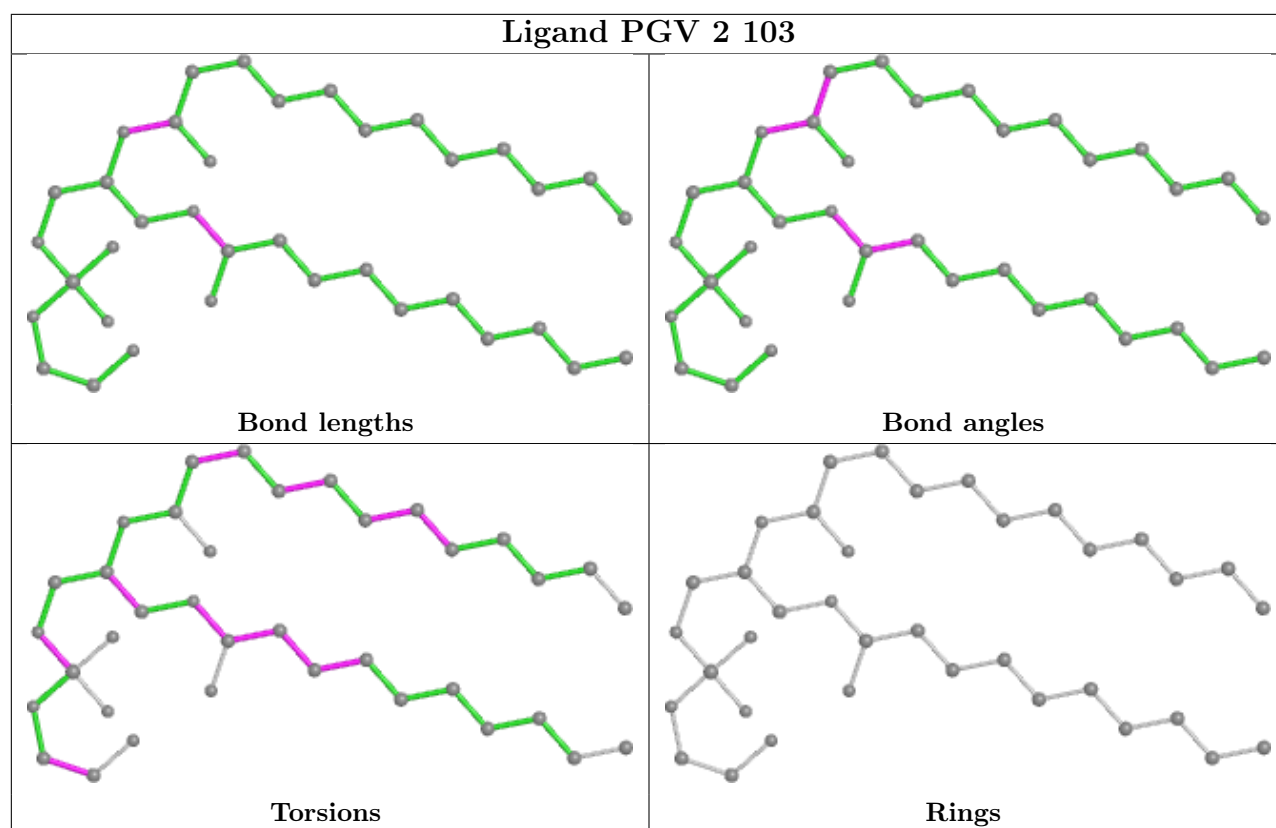
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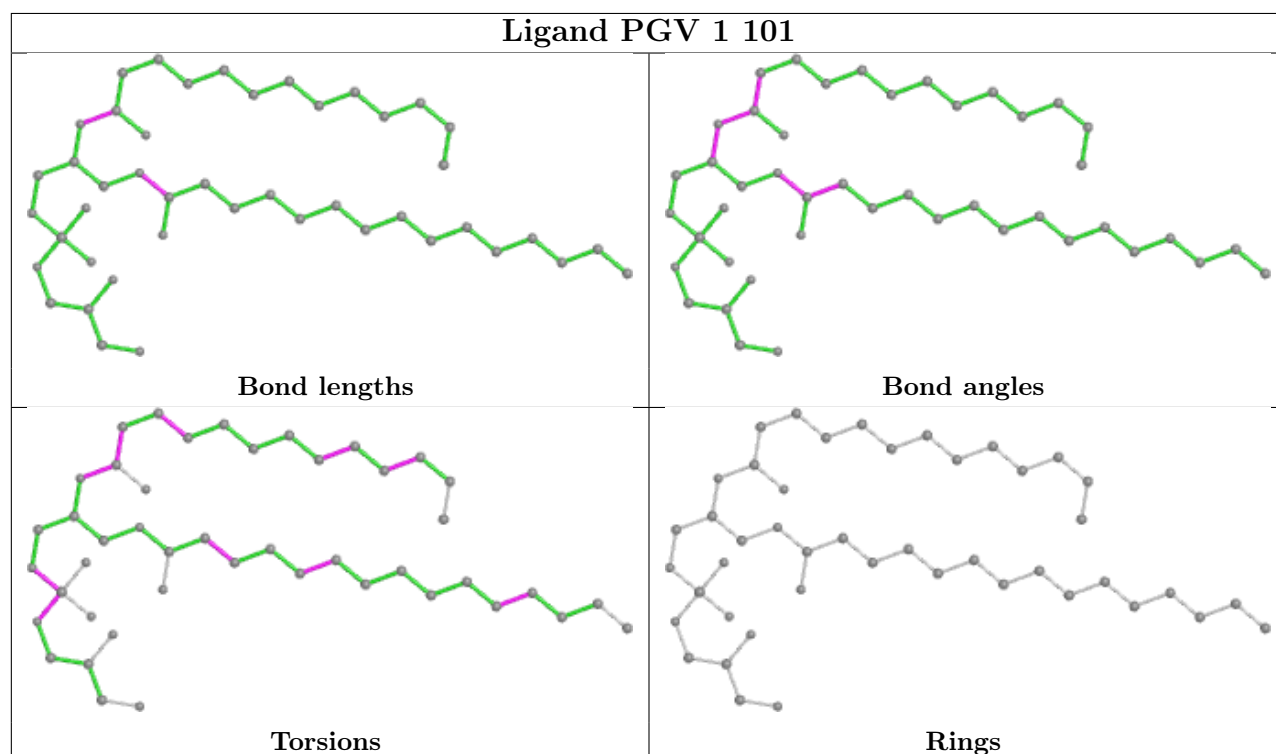
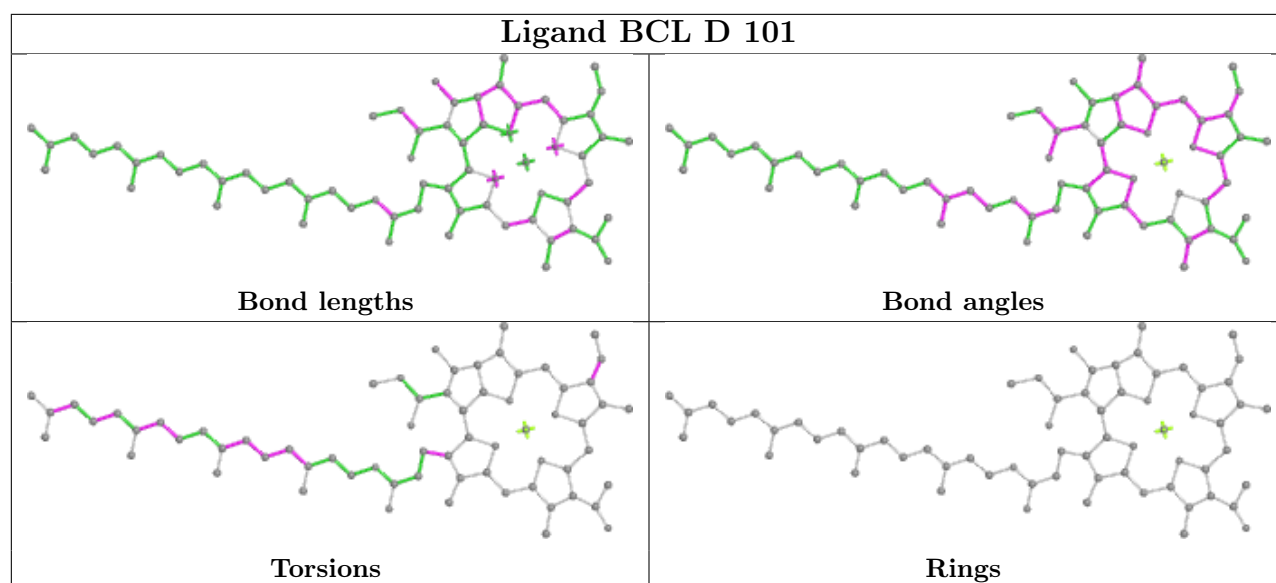


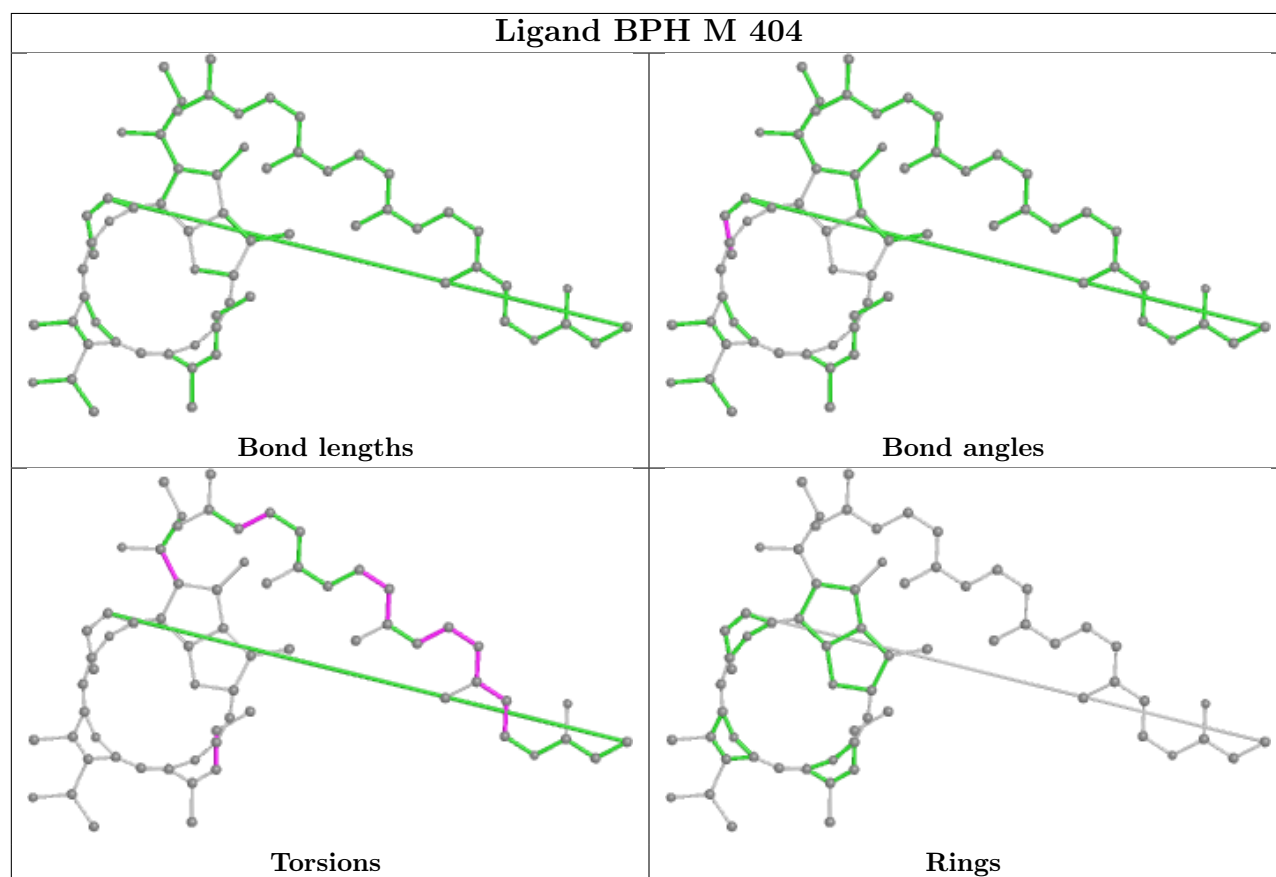
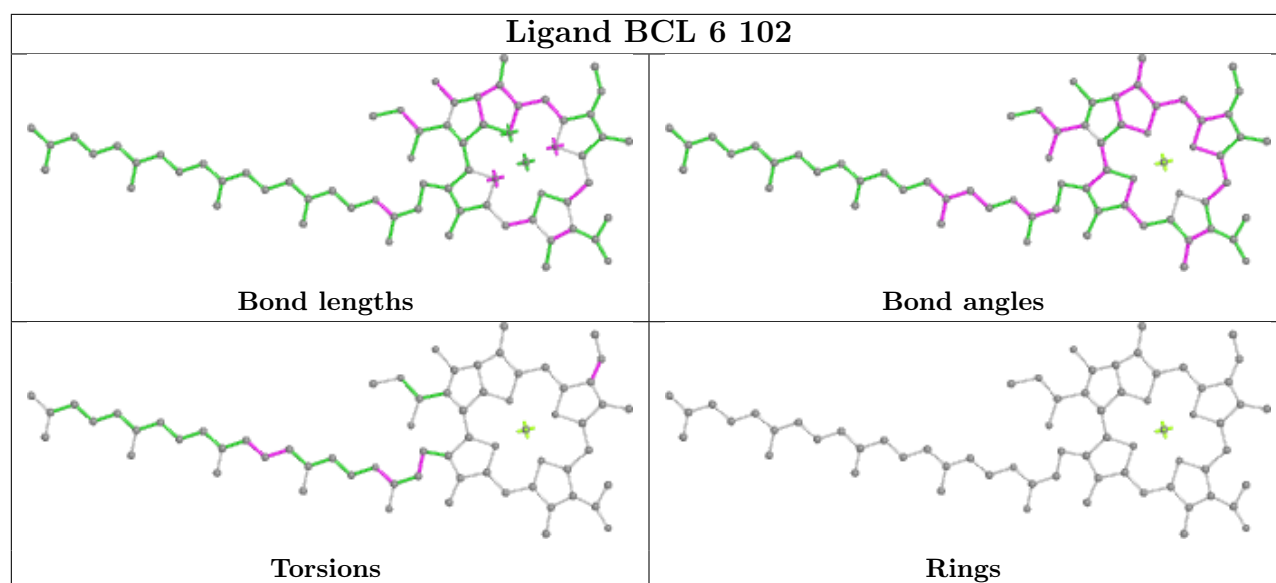
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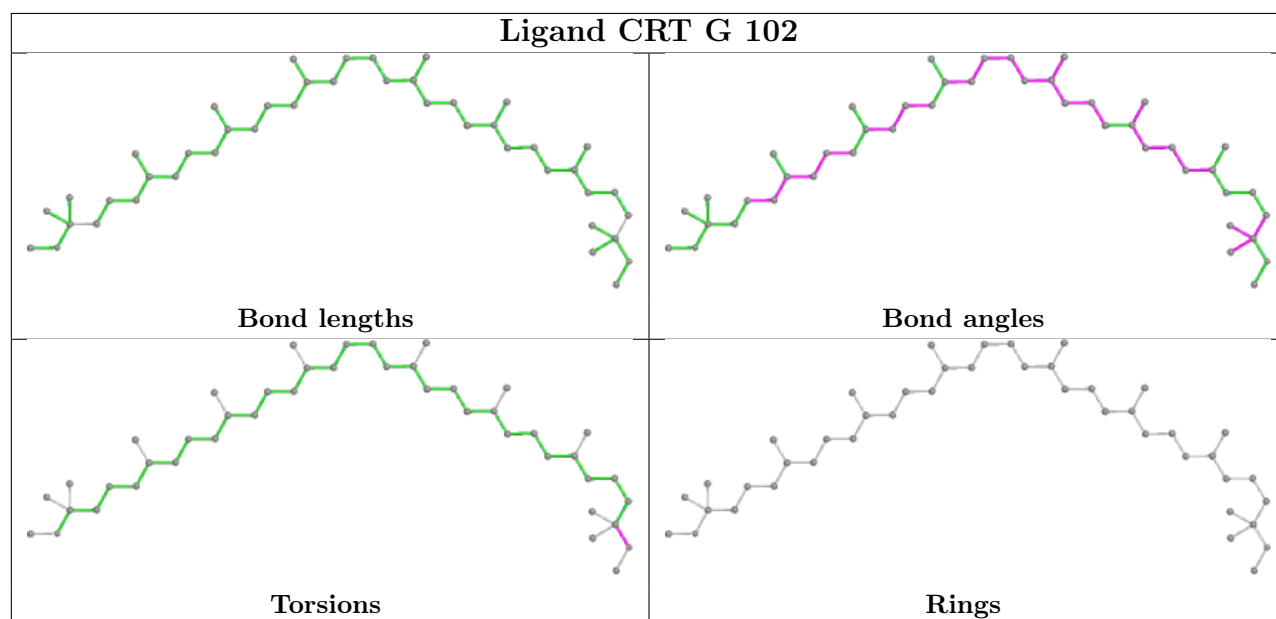
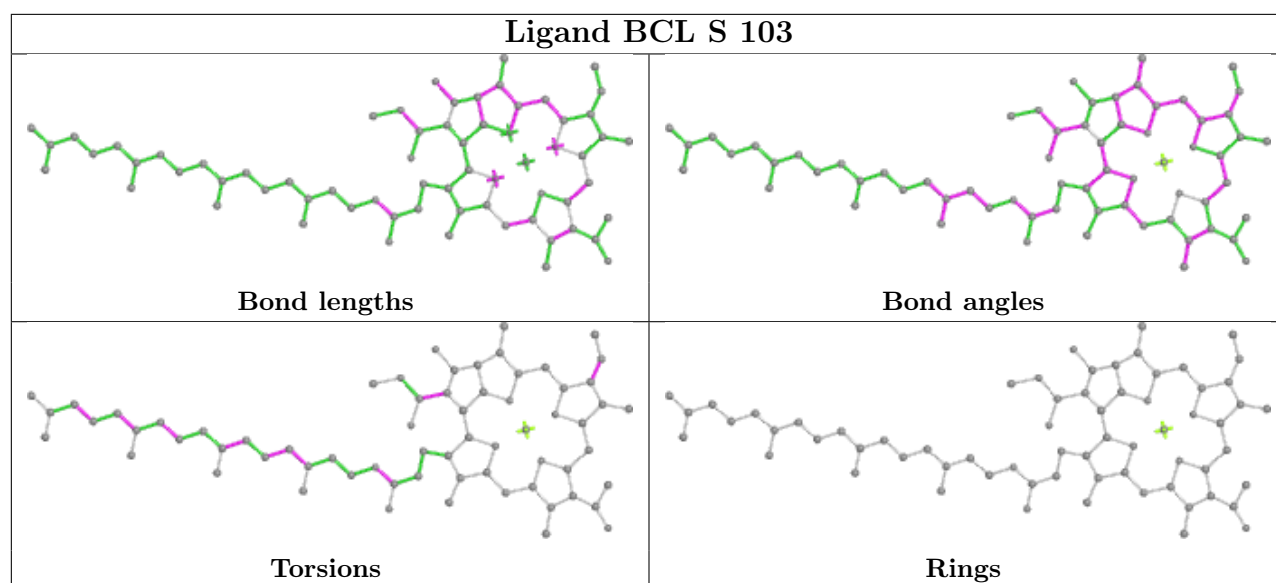


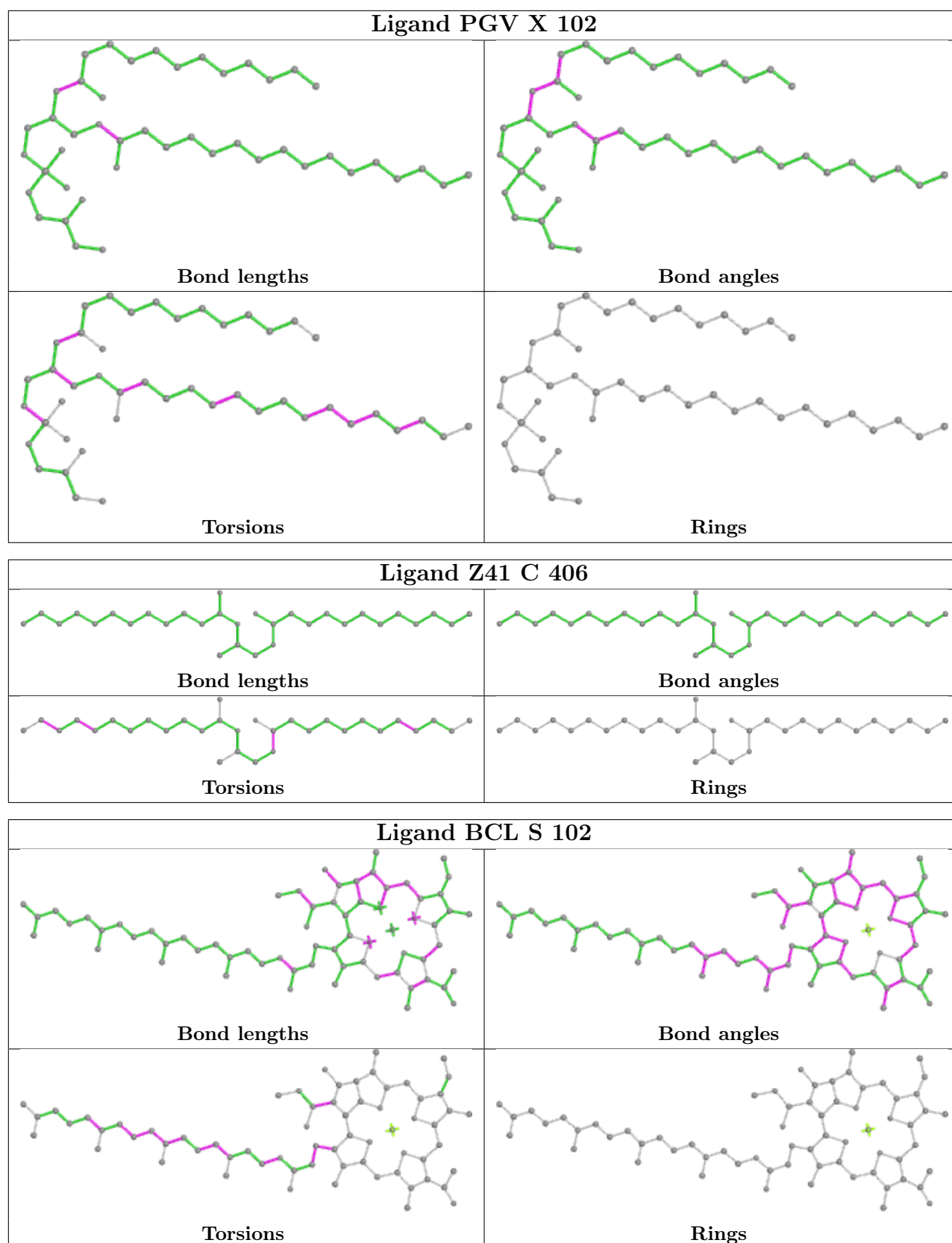


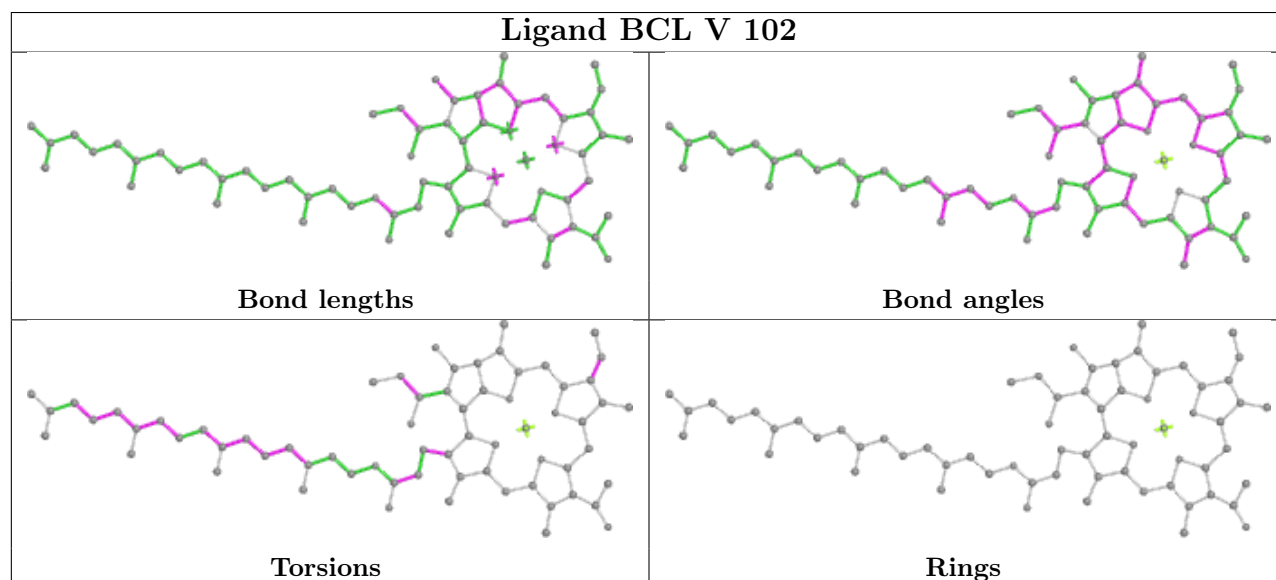
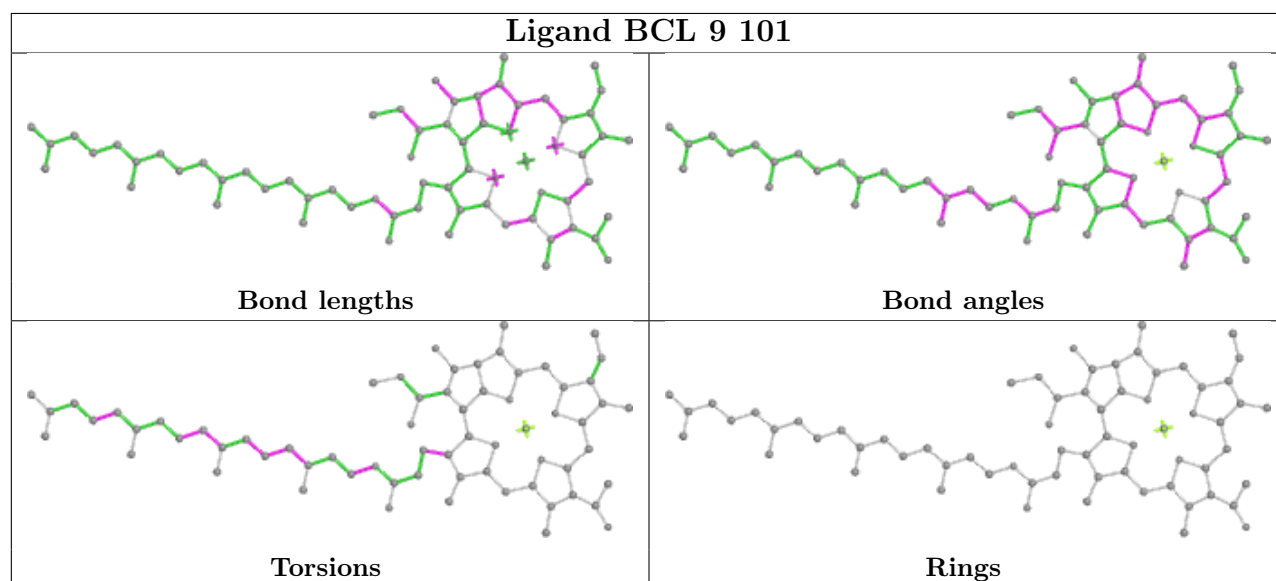
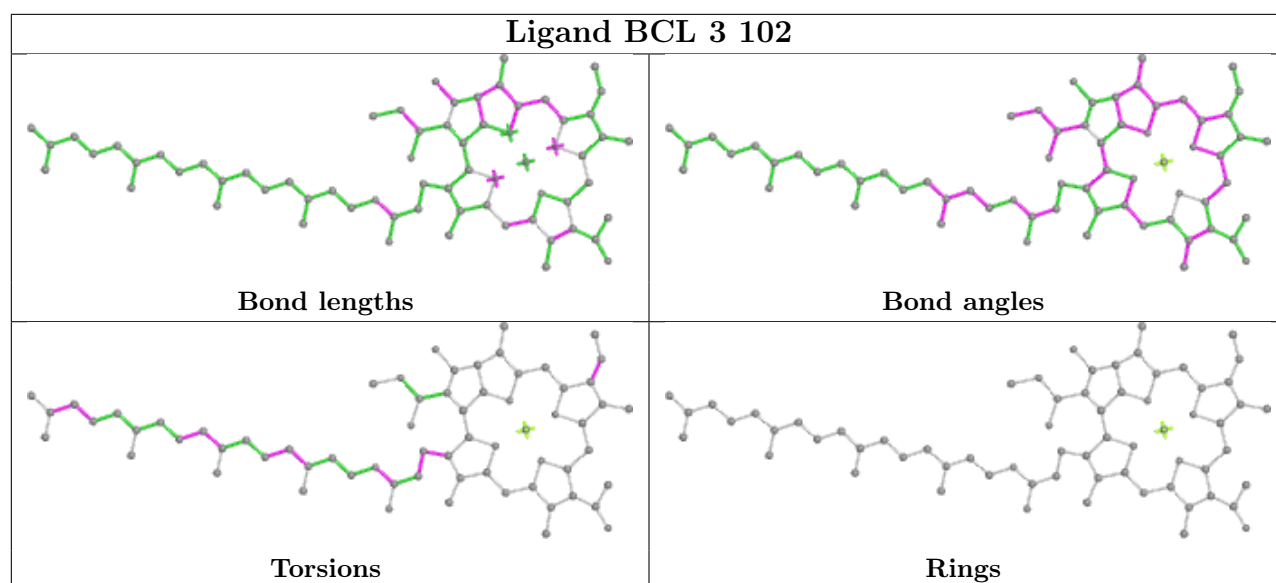


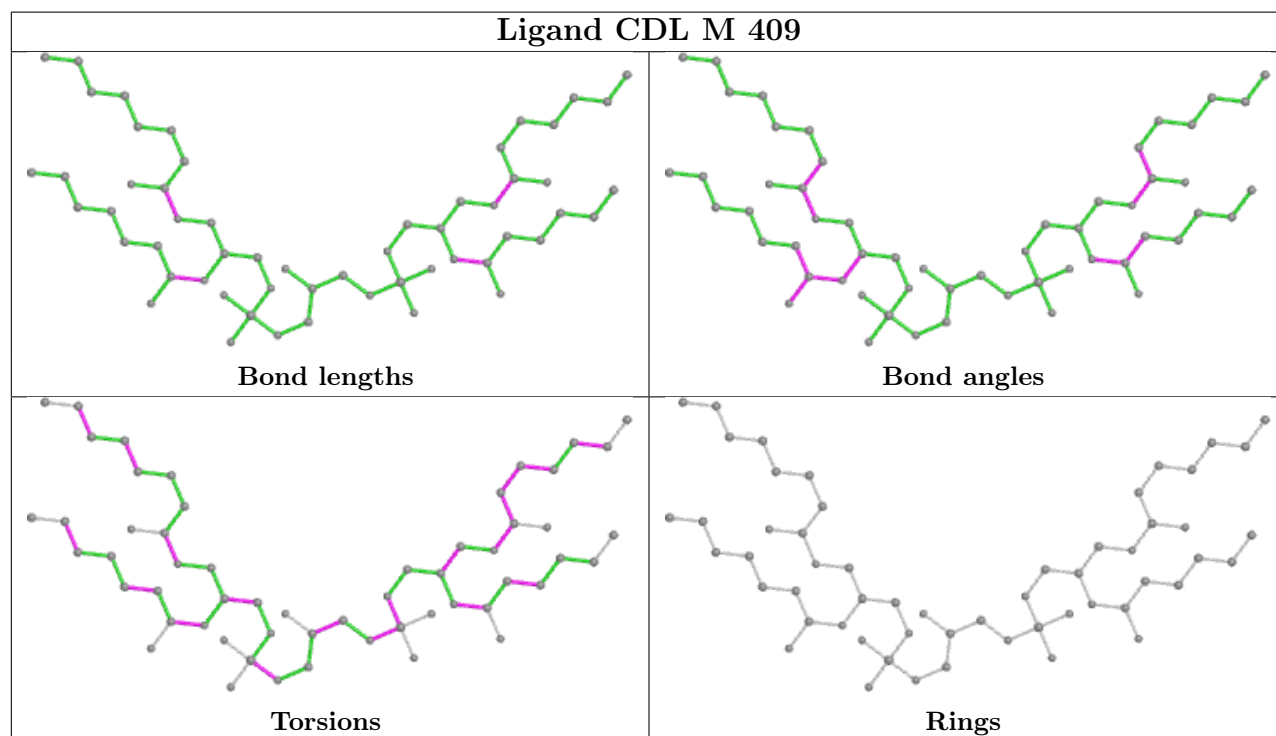
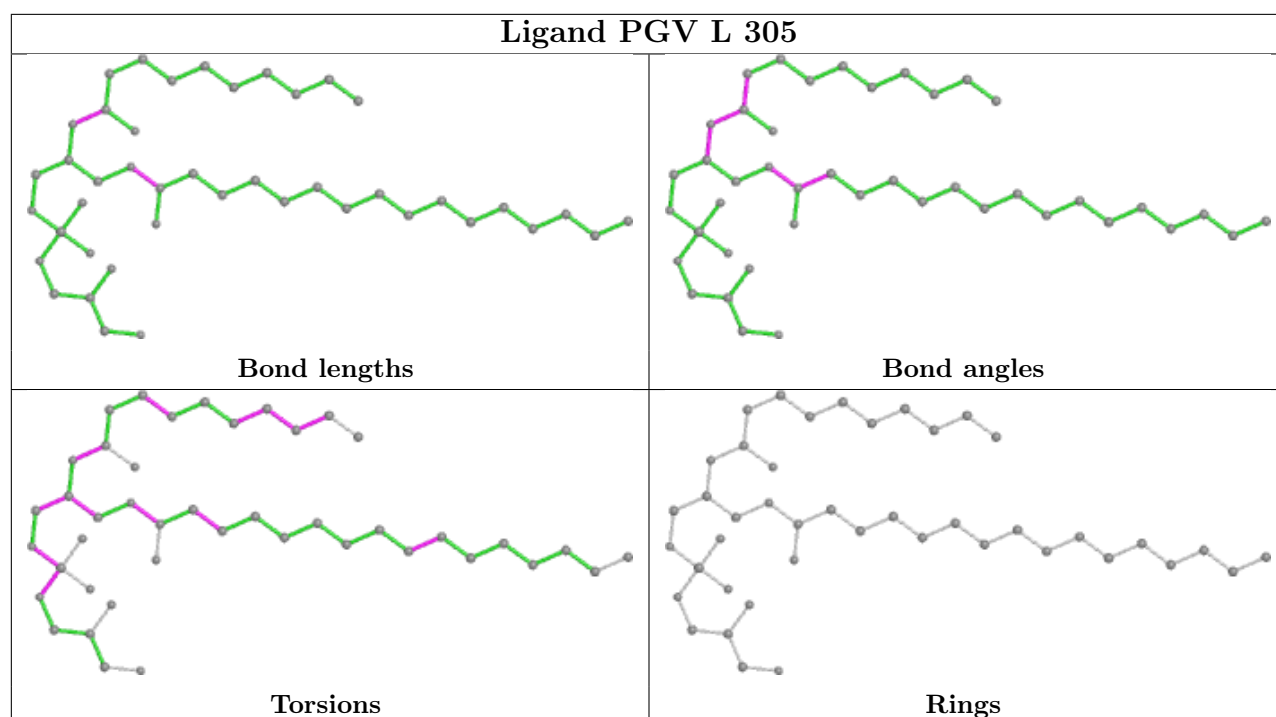


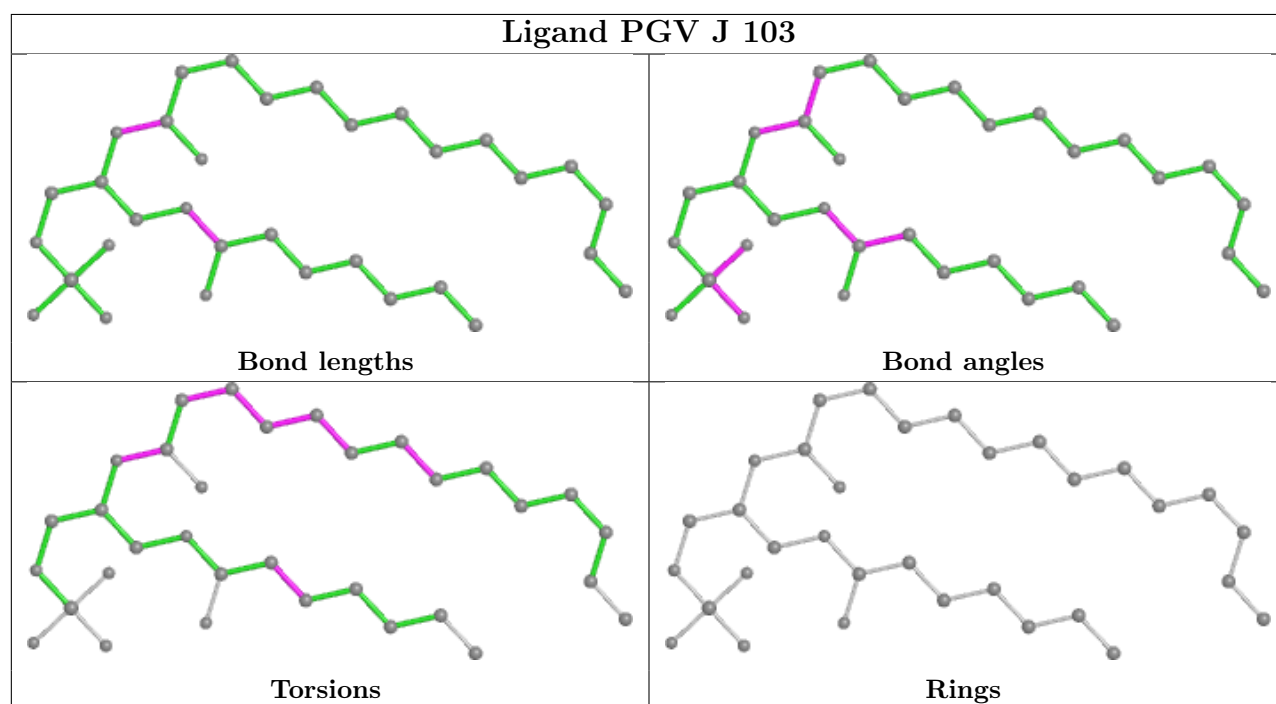
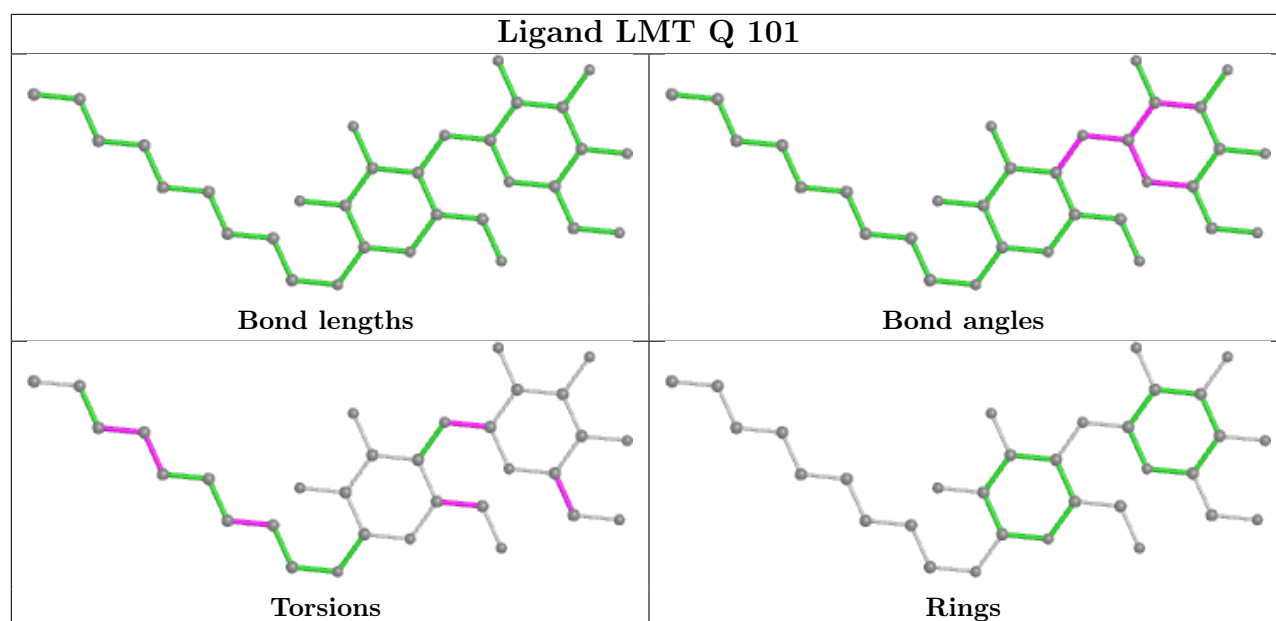


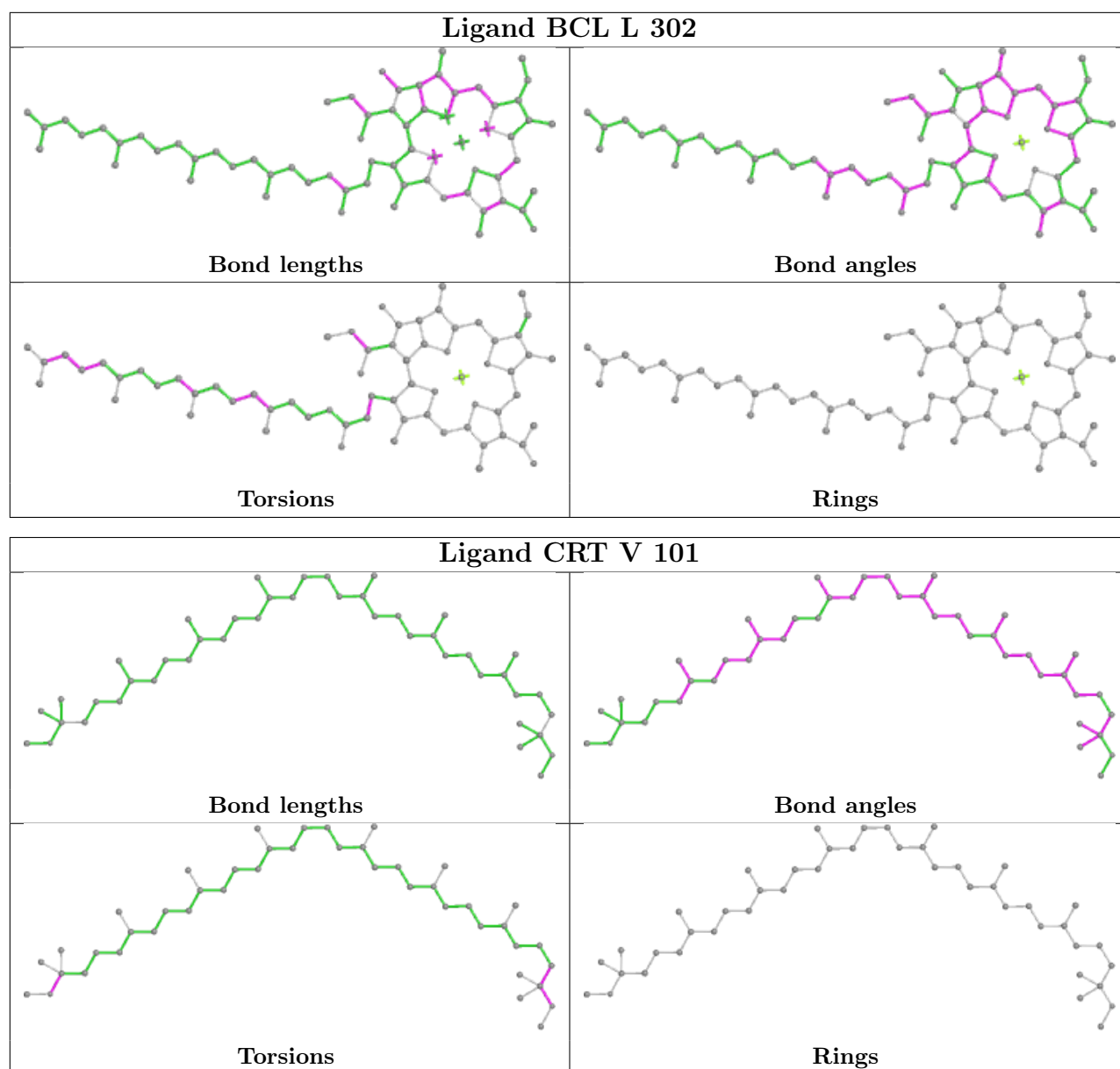


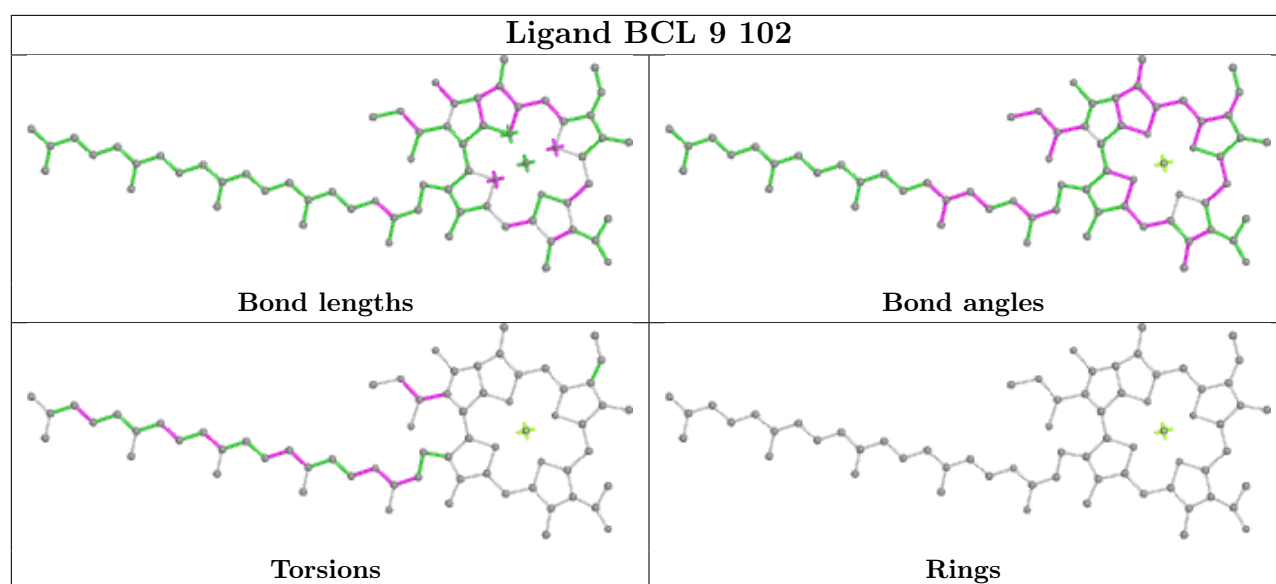
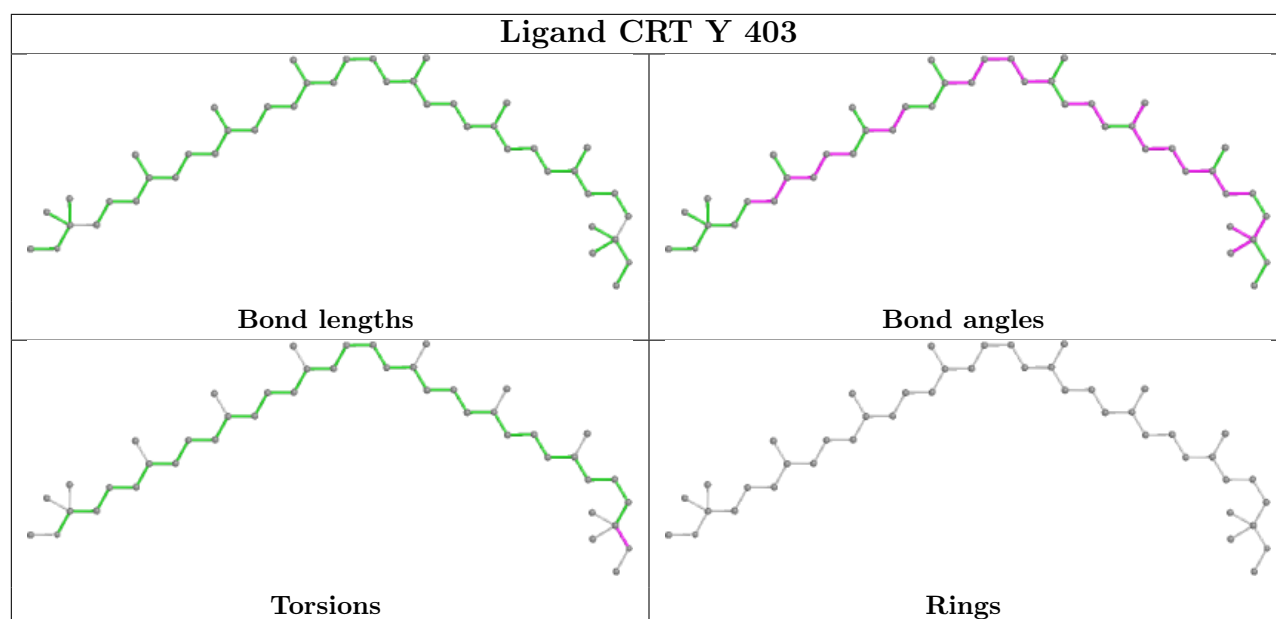


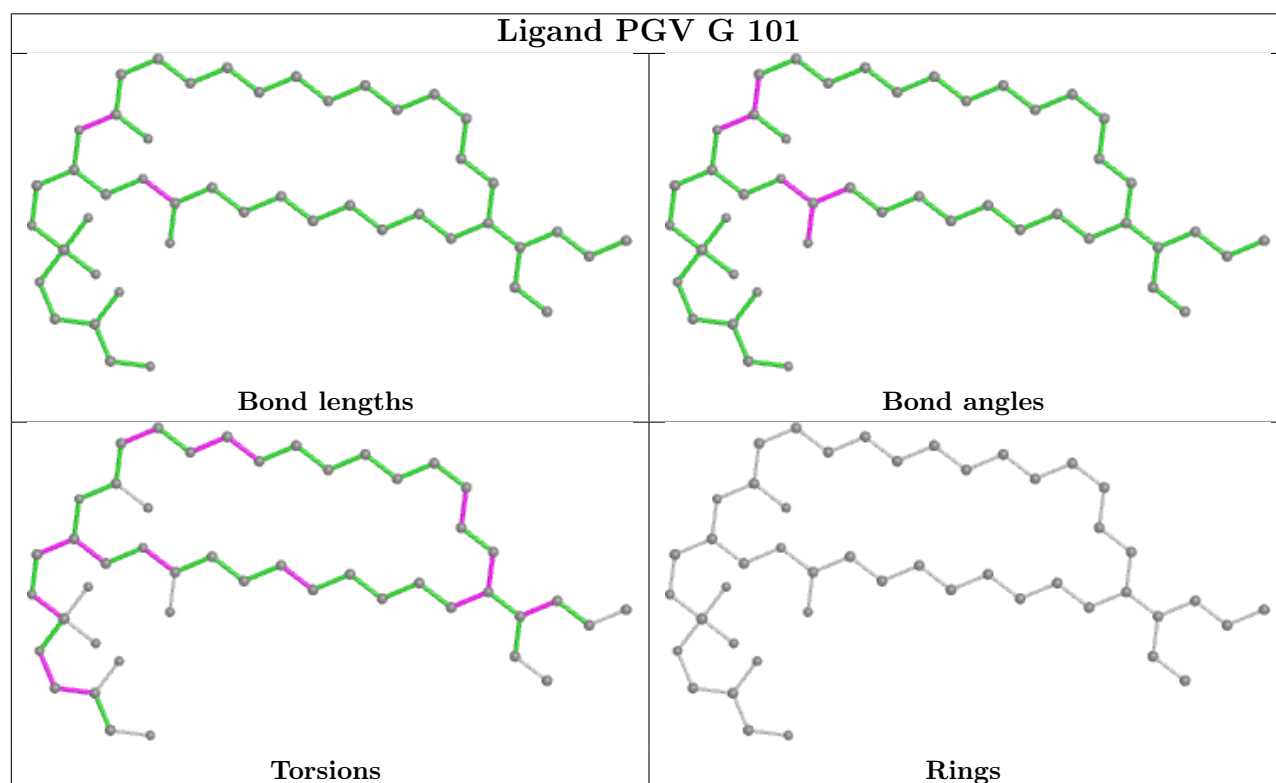
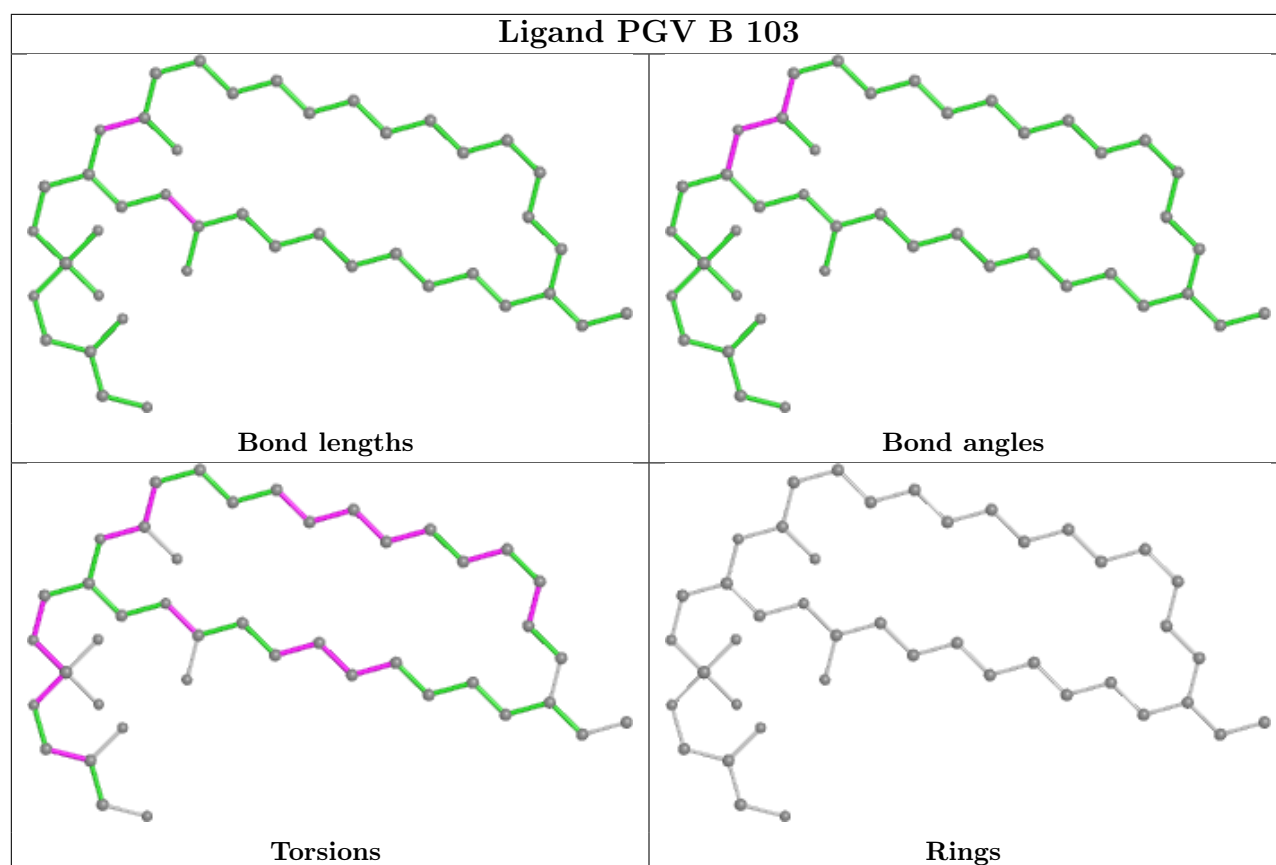




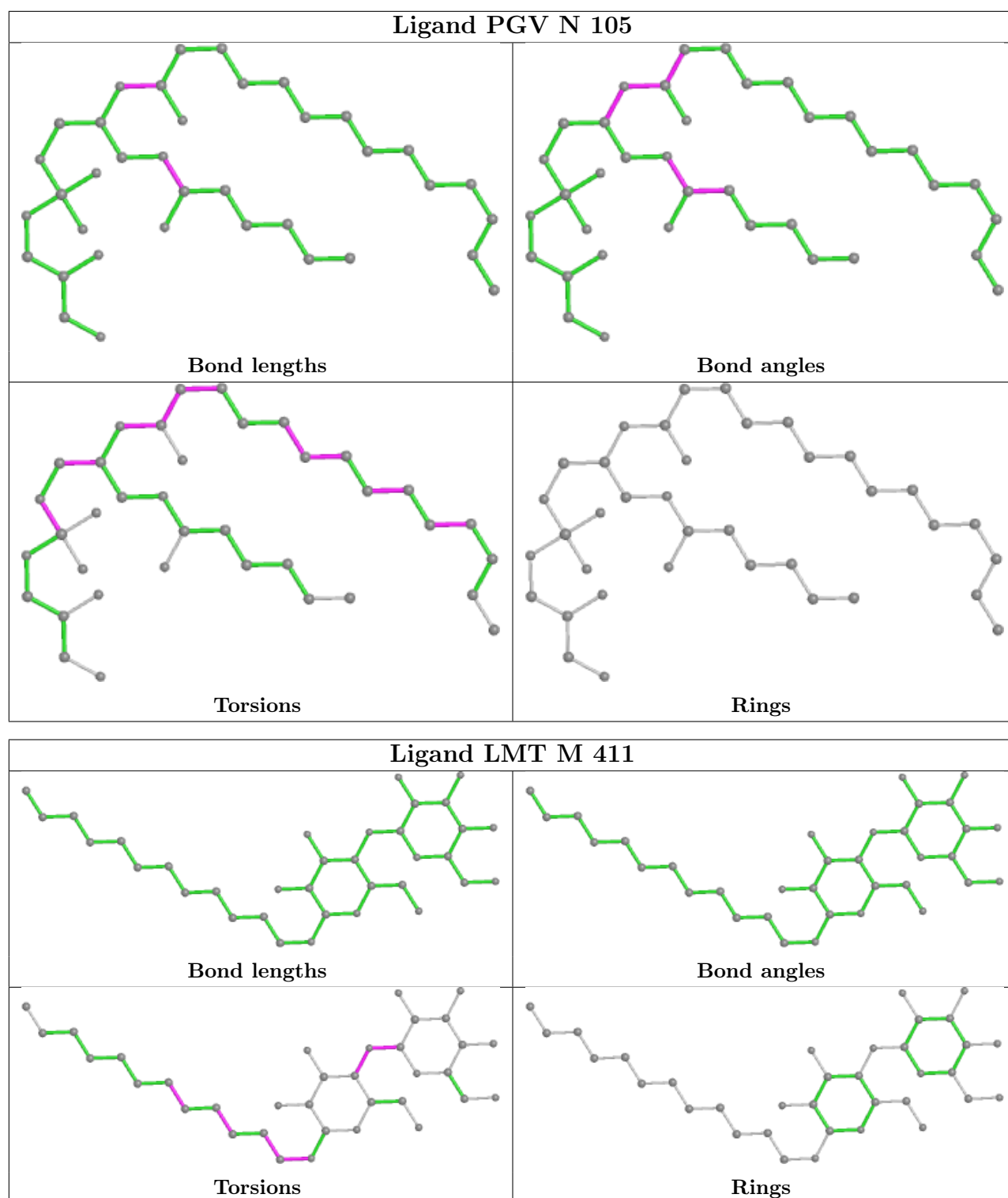


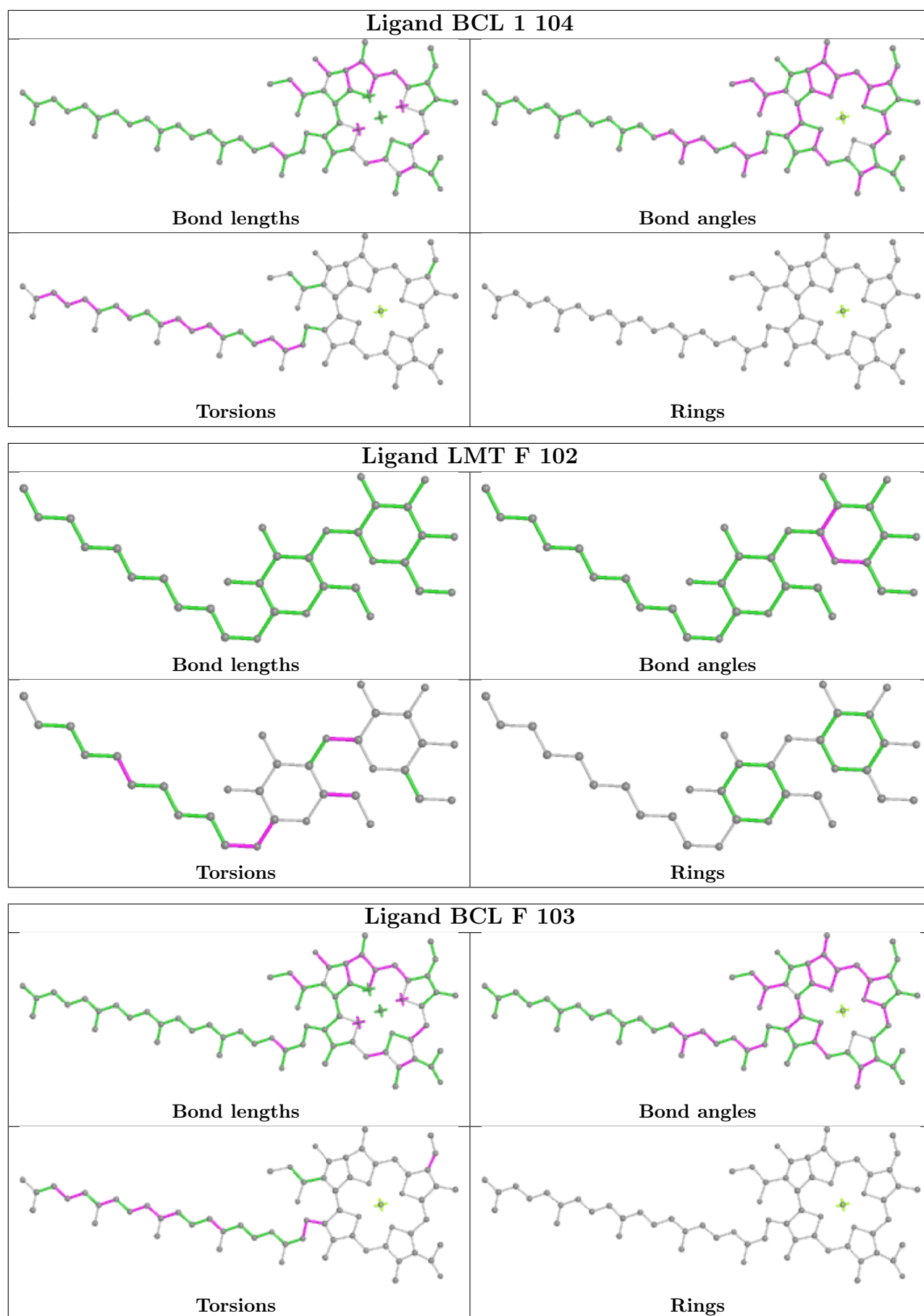


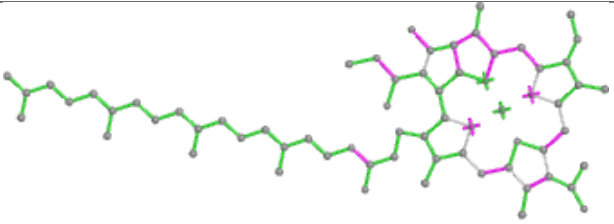
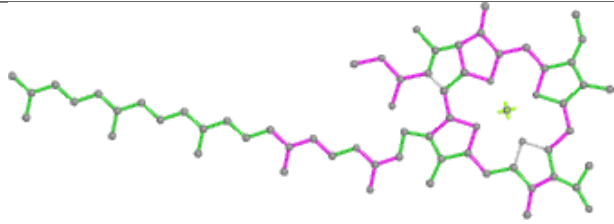
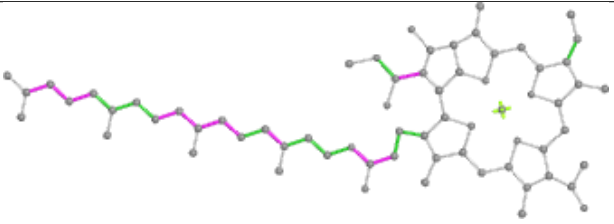
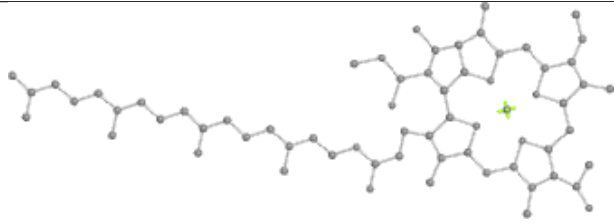
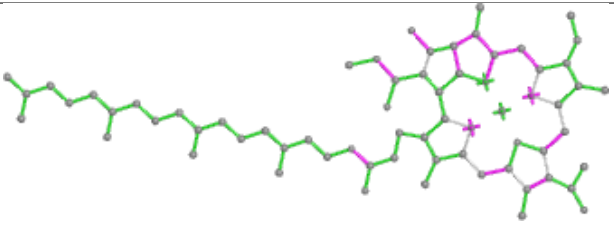
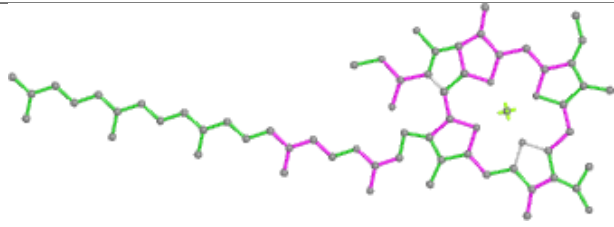
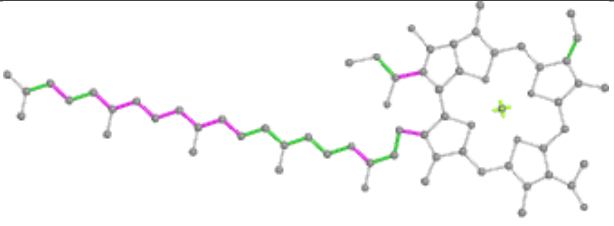
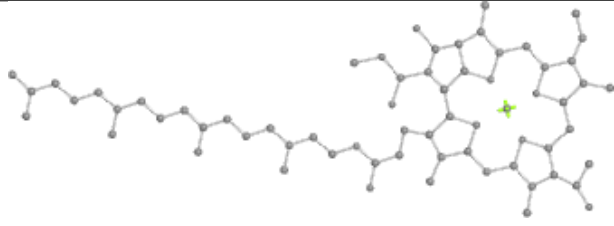
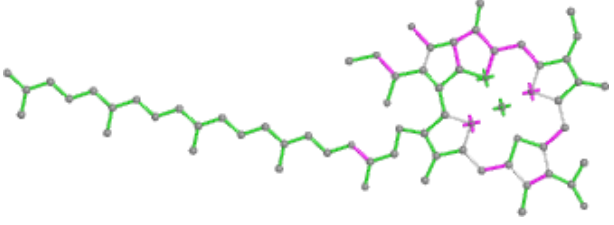
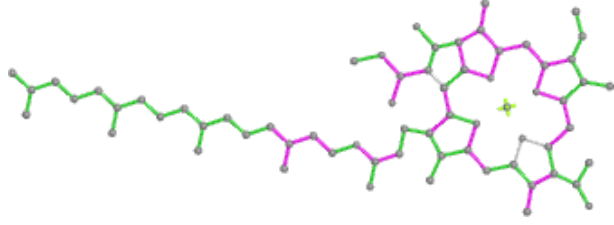
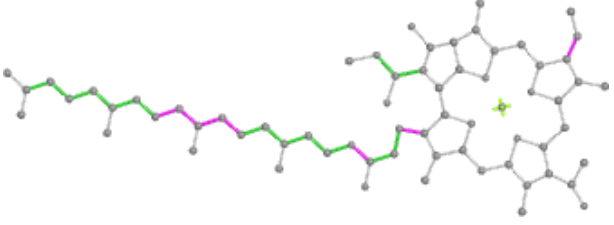
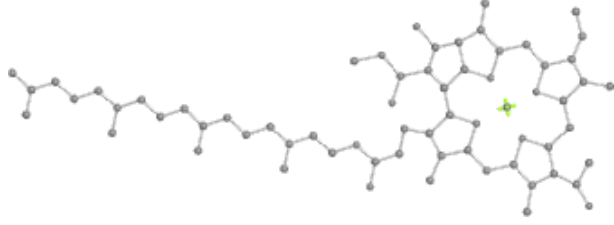


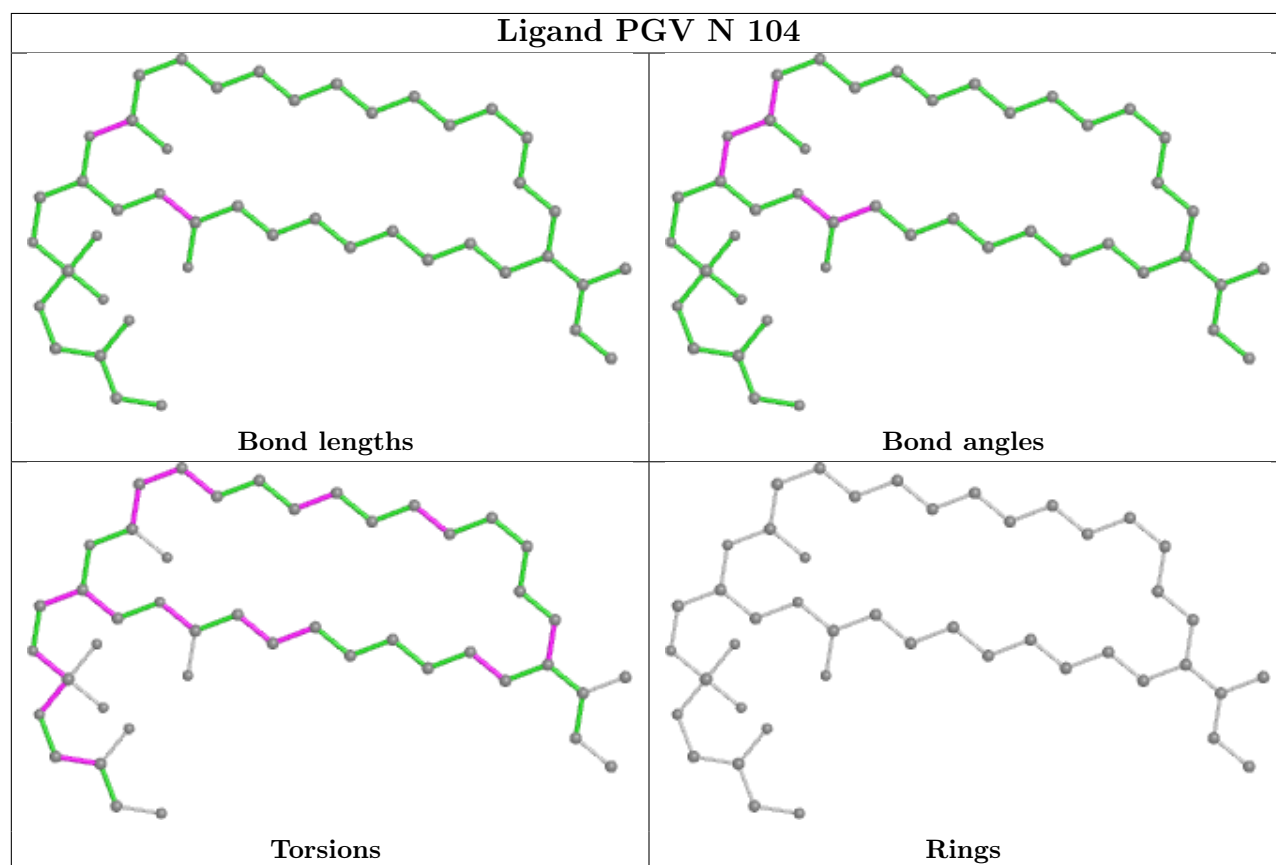
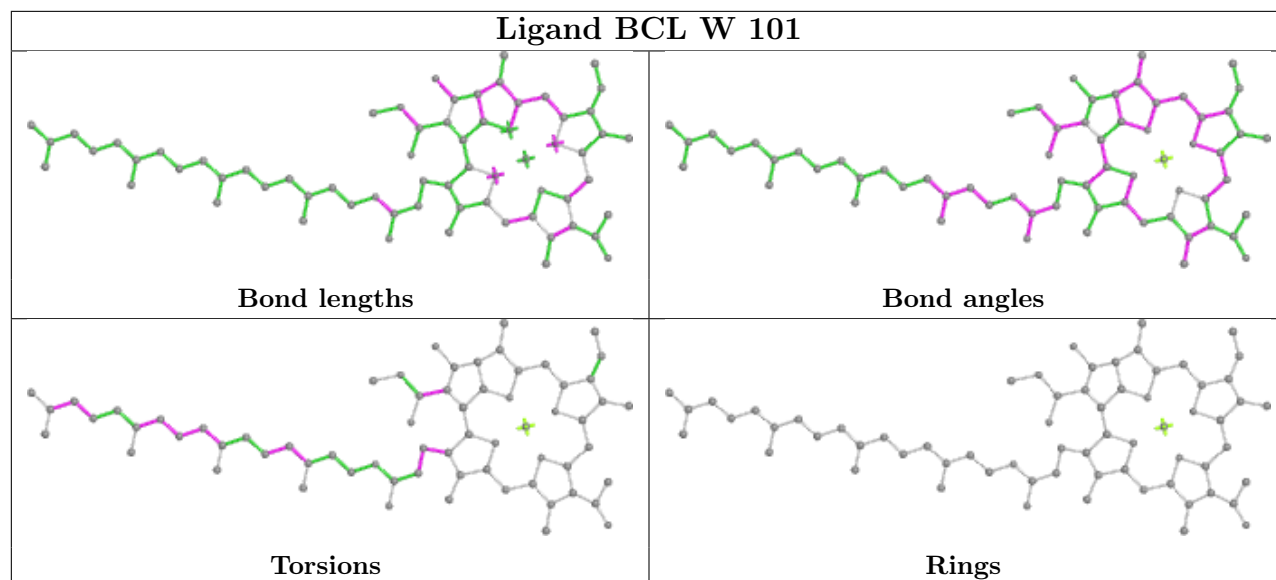


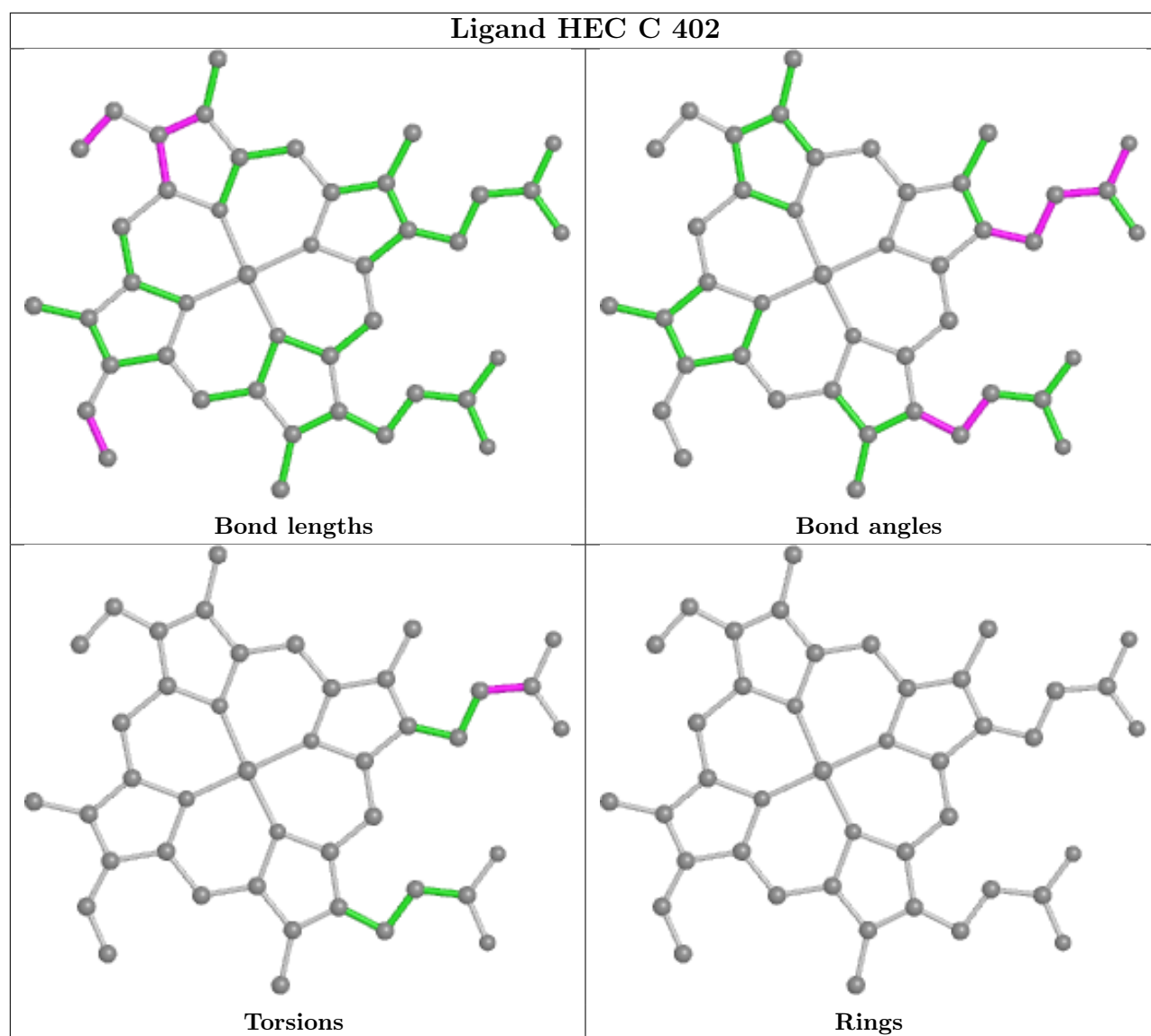


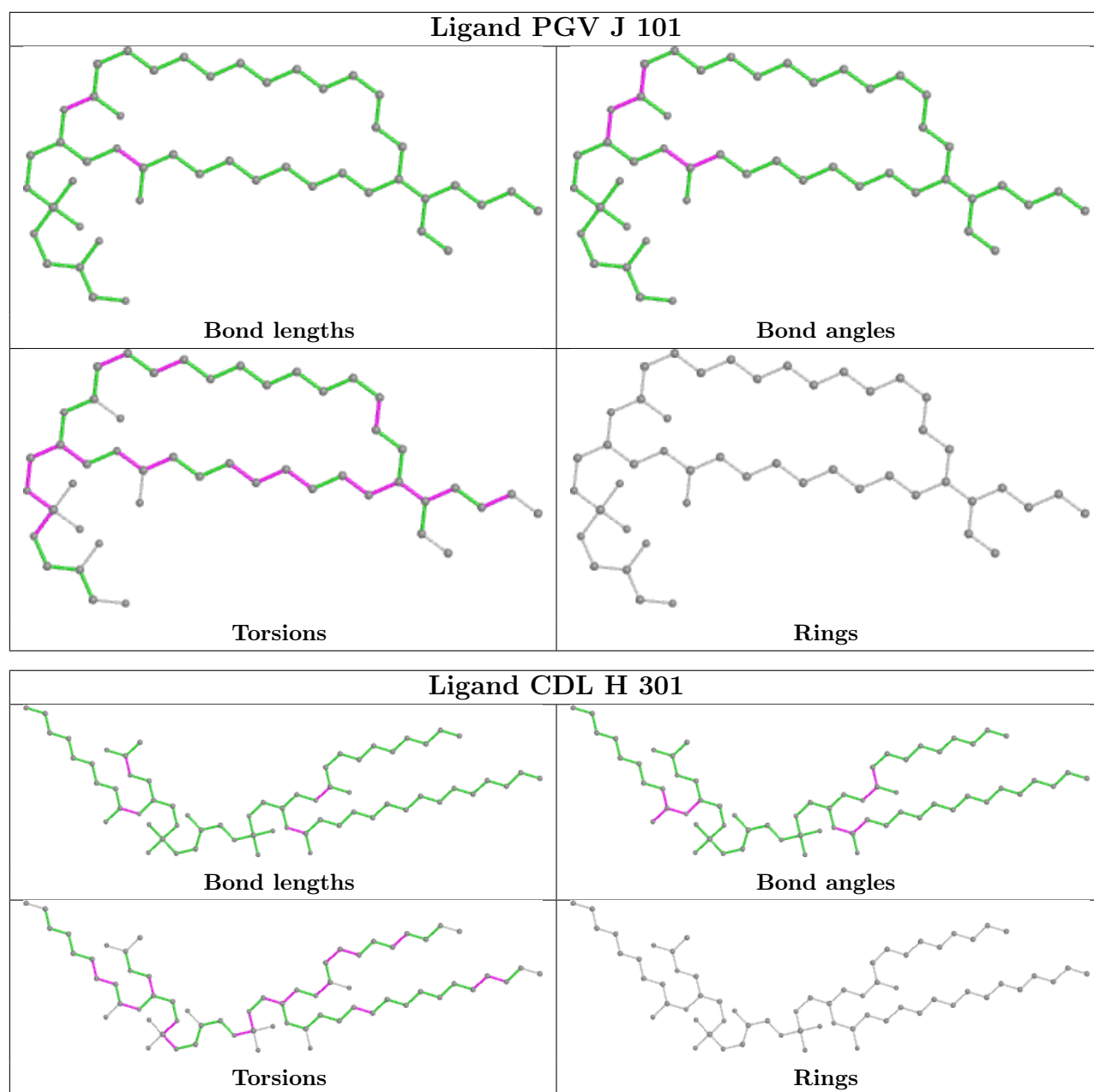


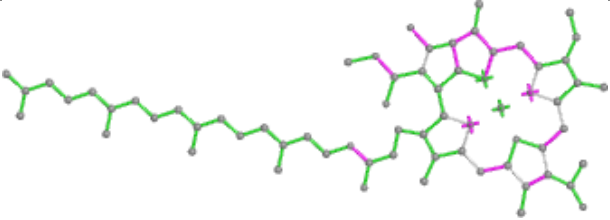
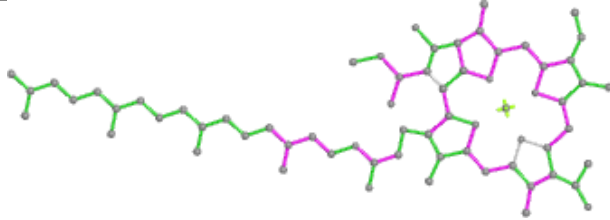
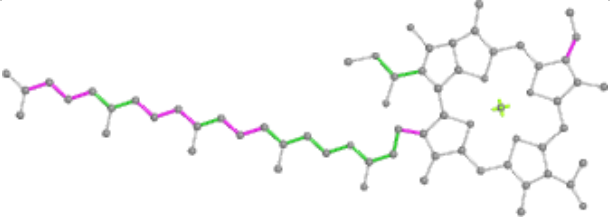
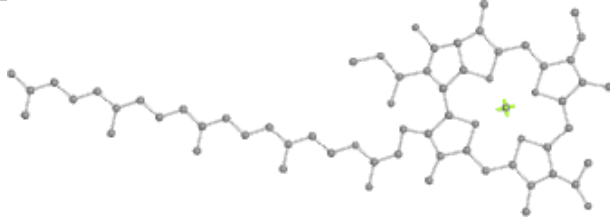
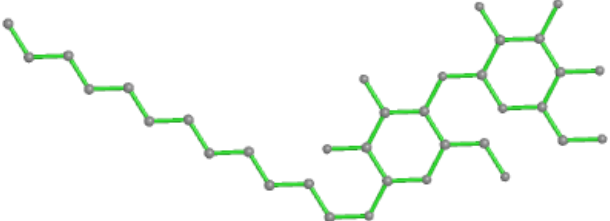
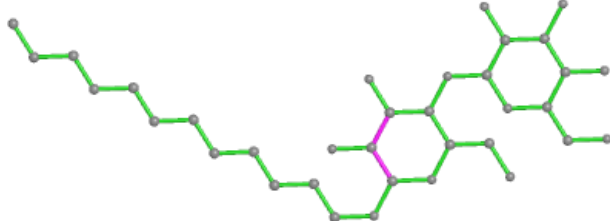
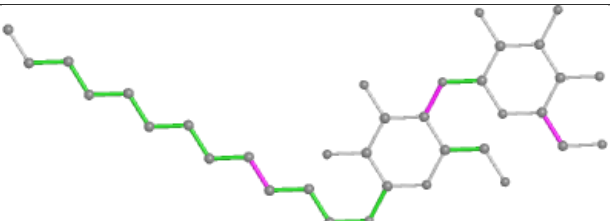
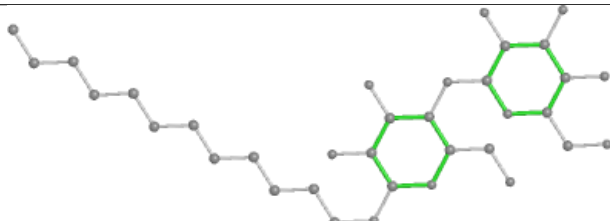
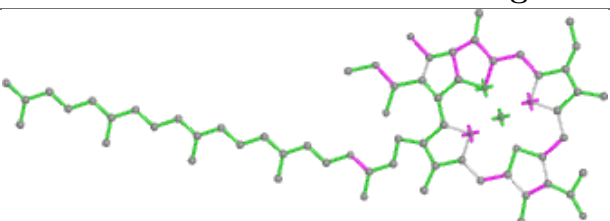
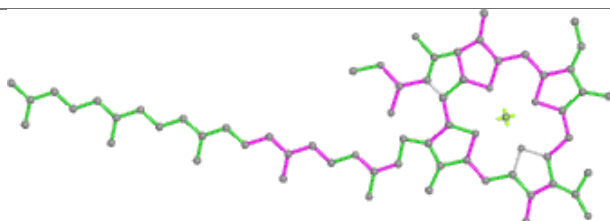
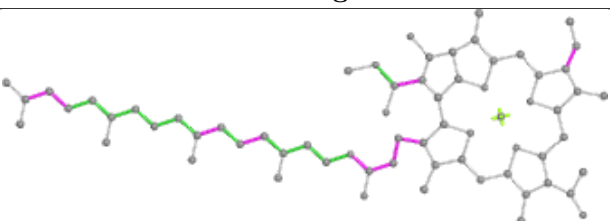
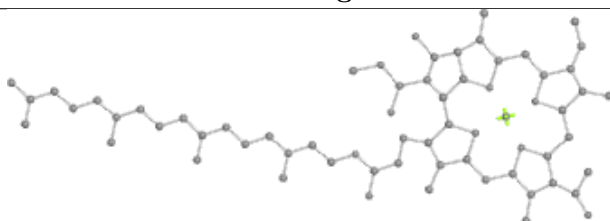


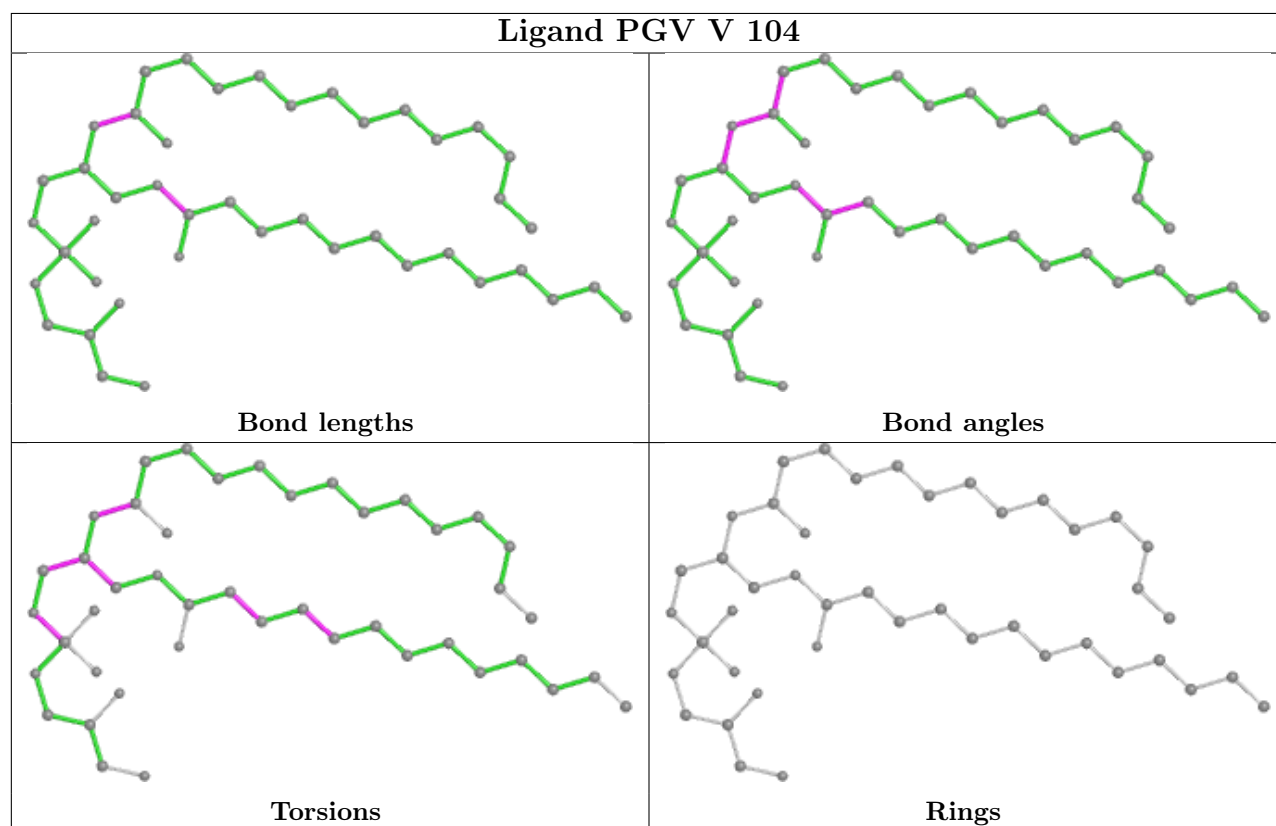
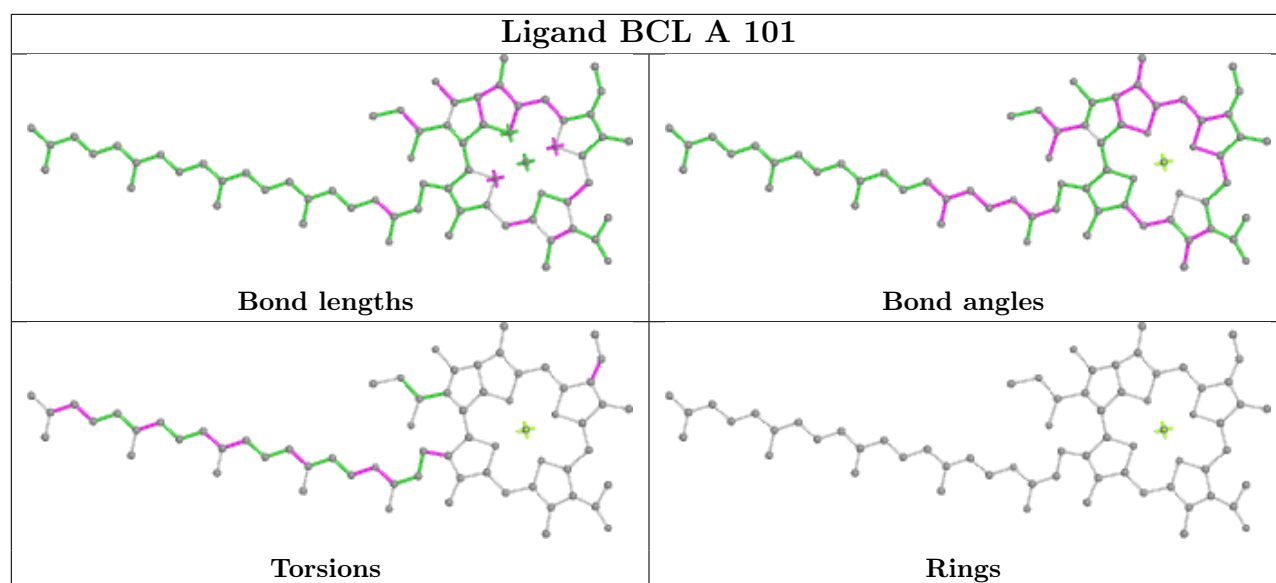
Ligand BCL D 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL L 309	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL 2 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



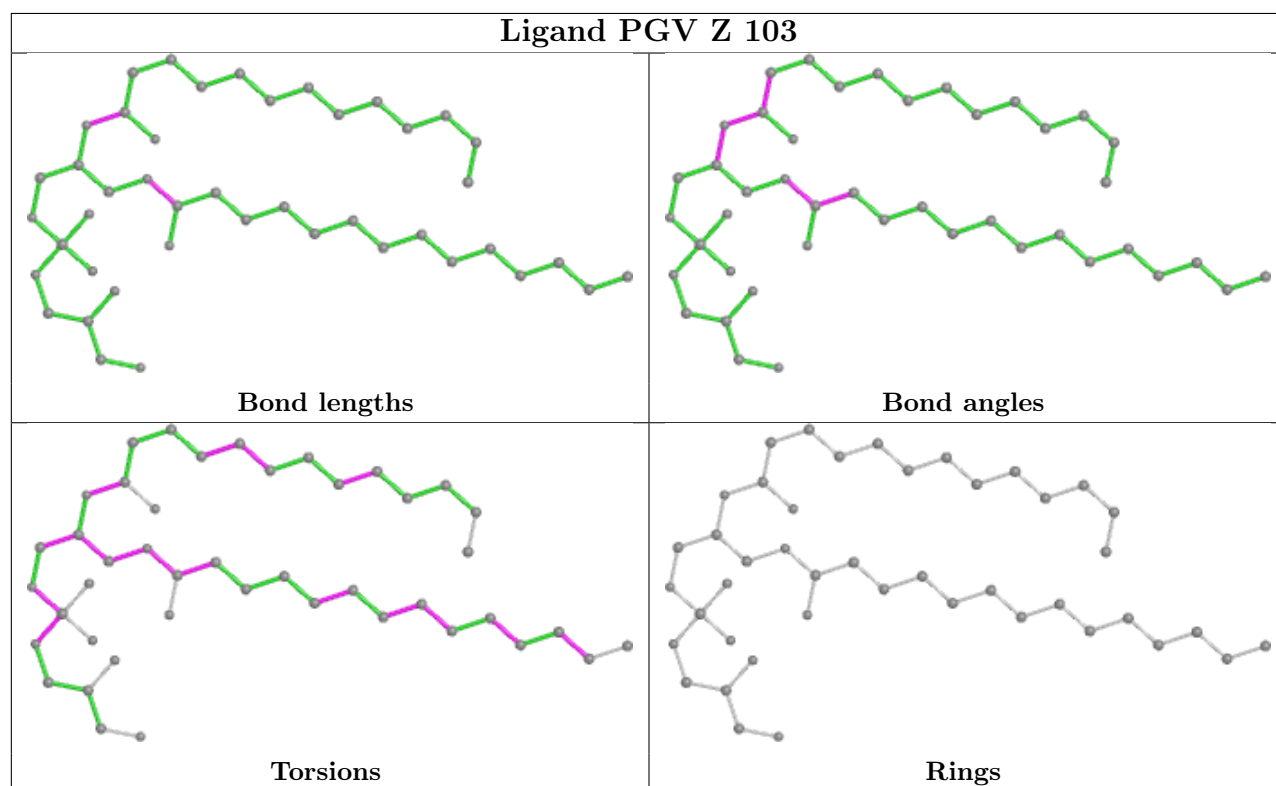
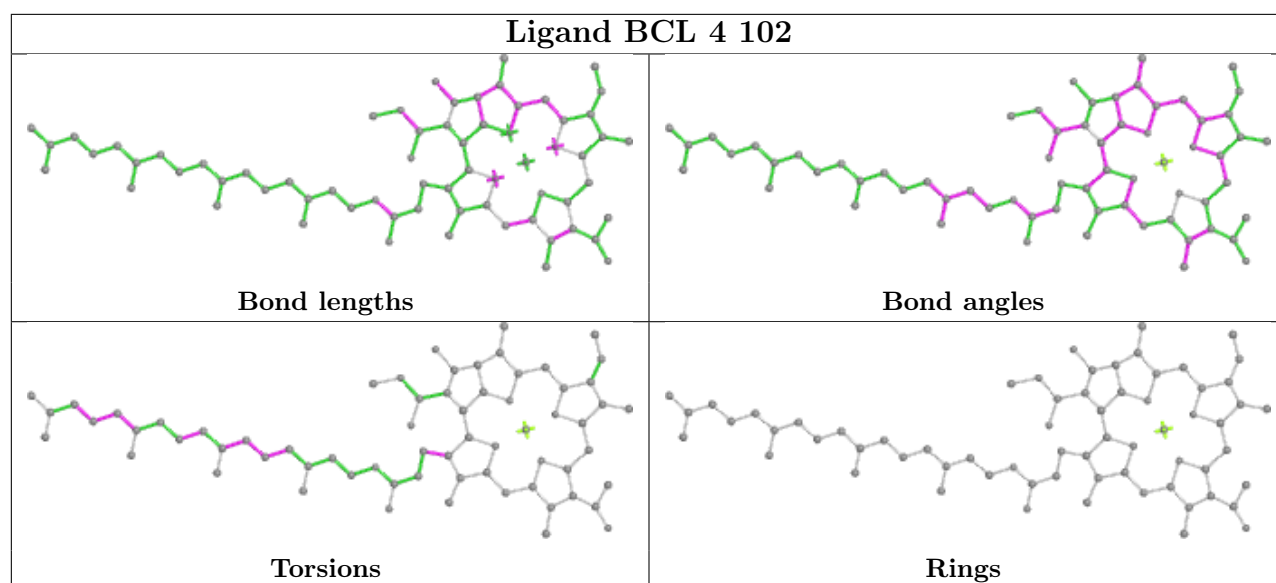


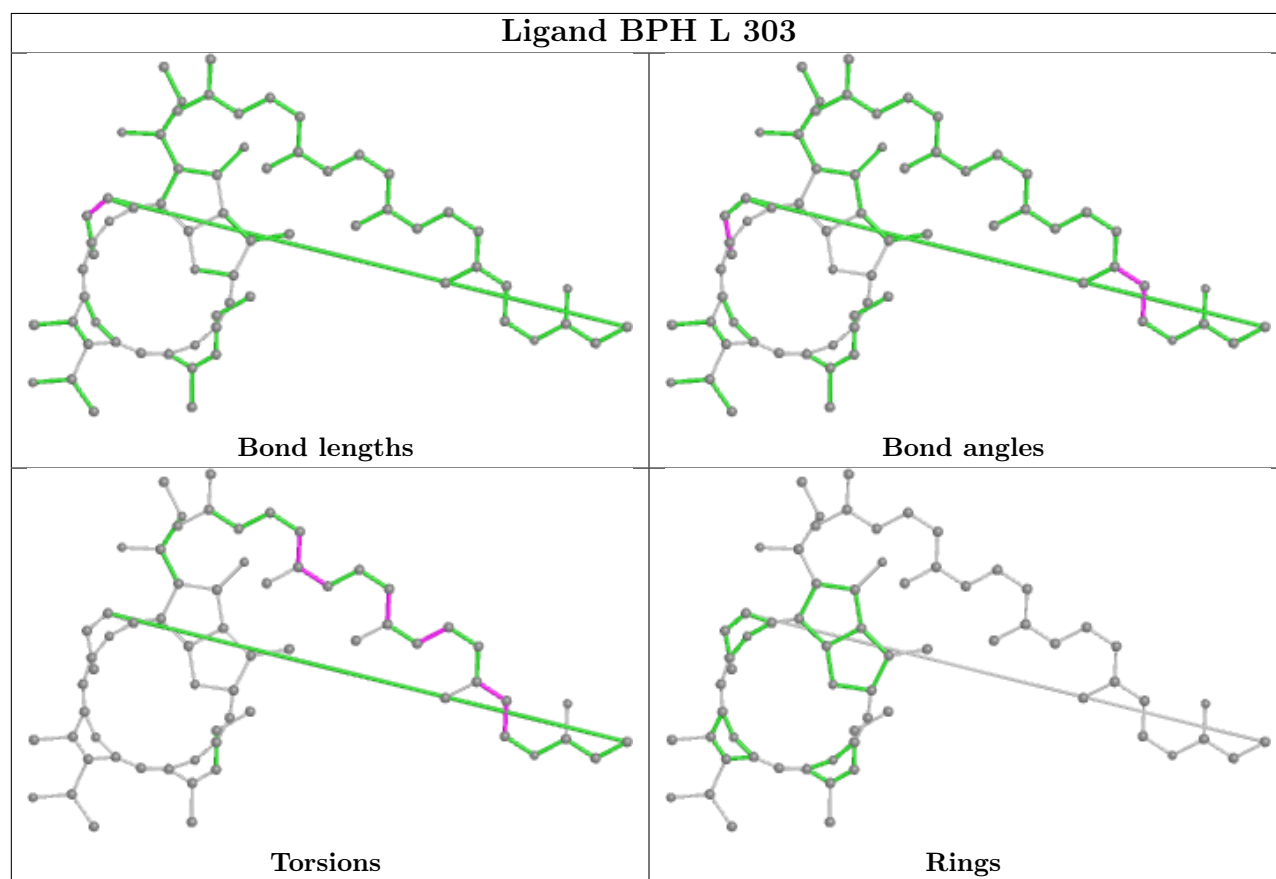
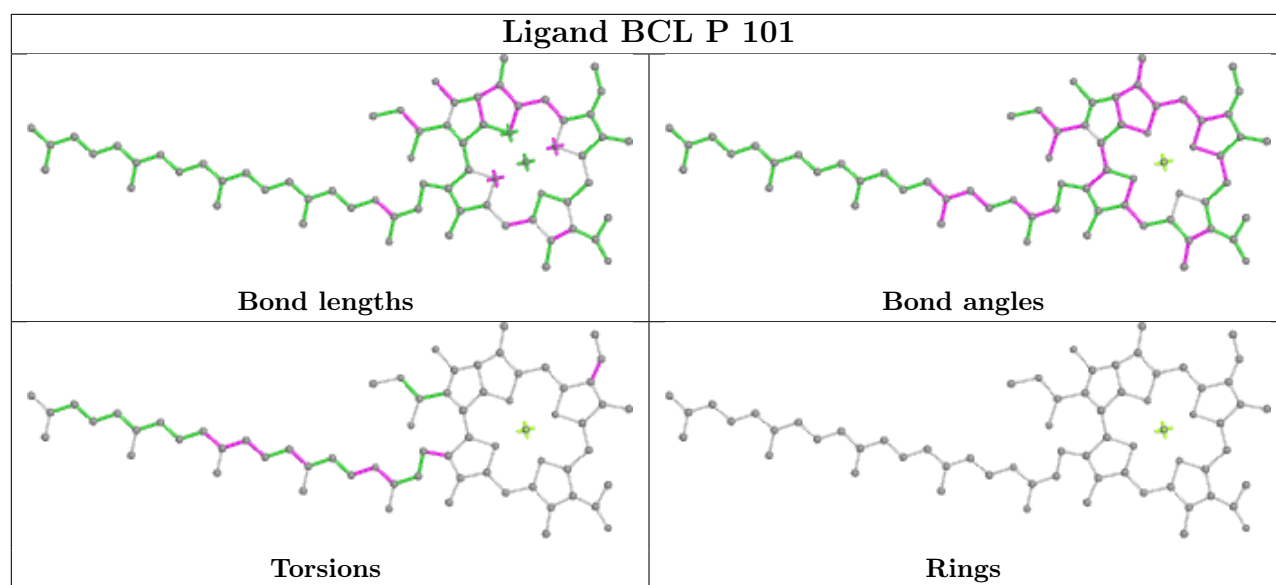


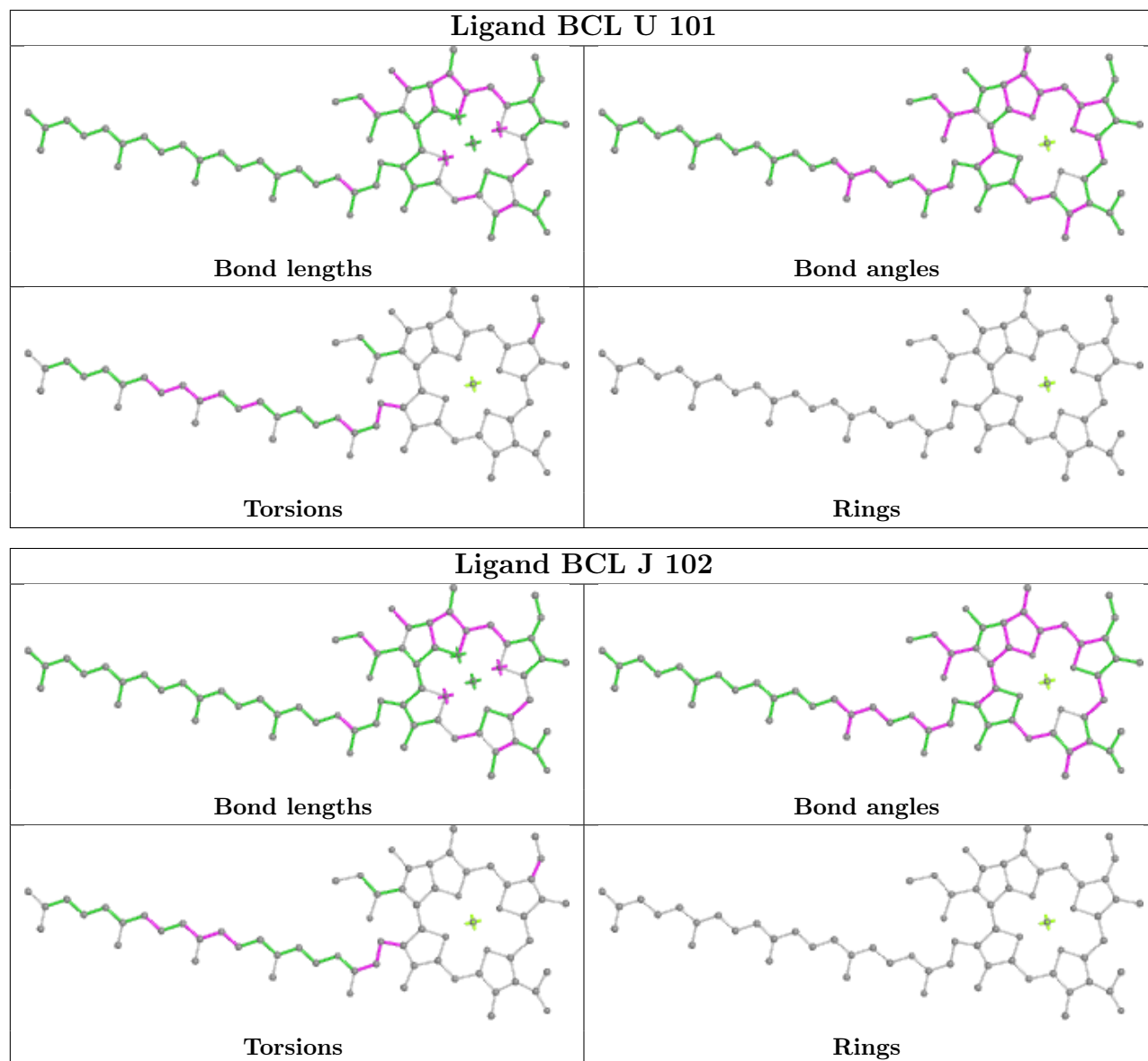
Ligand BCL B 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMT 7 103	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL L 308	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

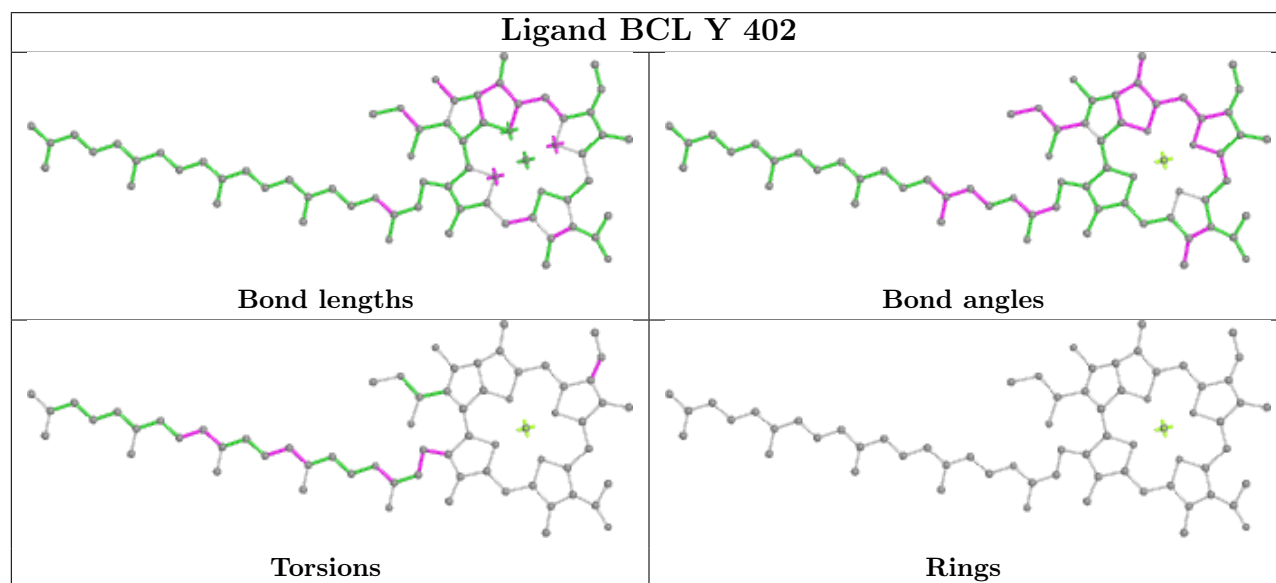
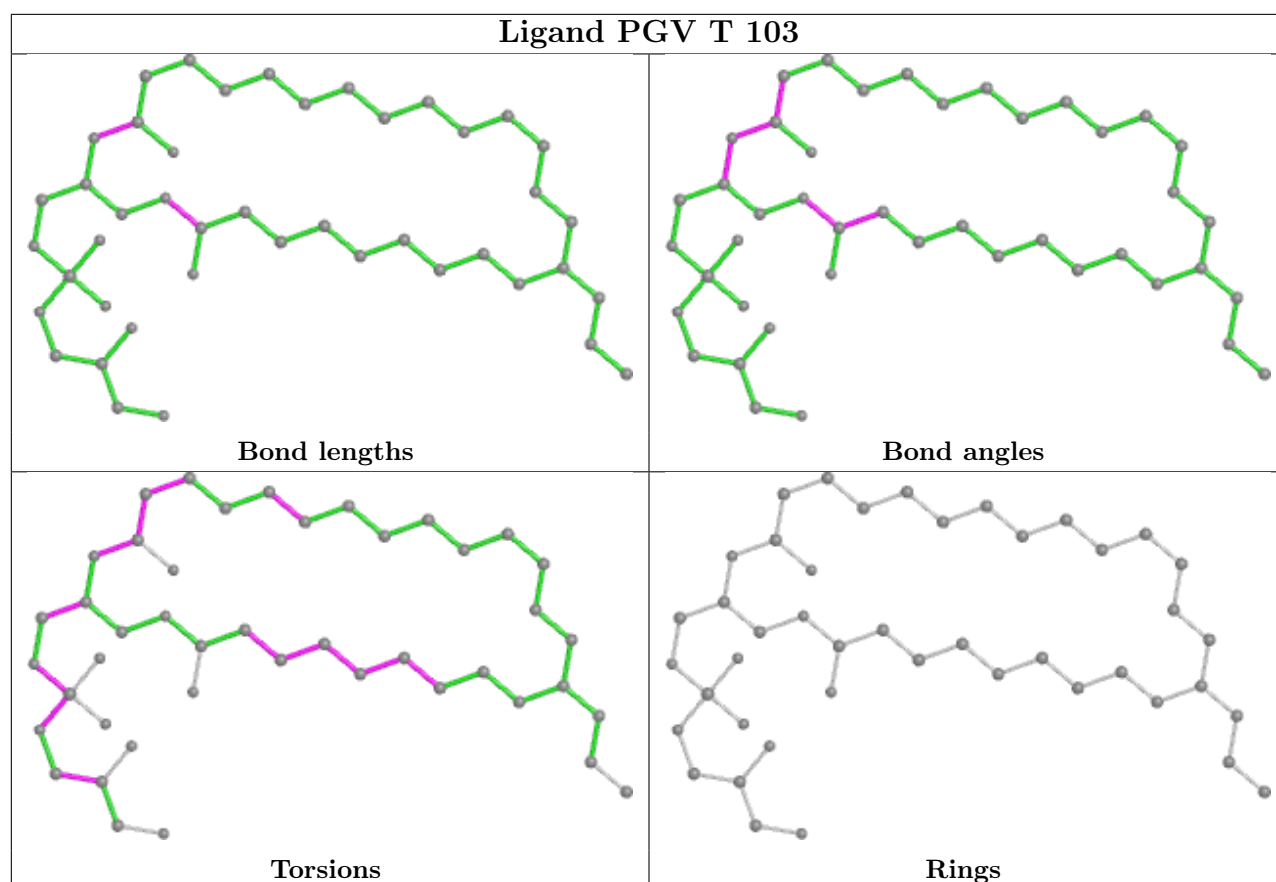


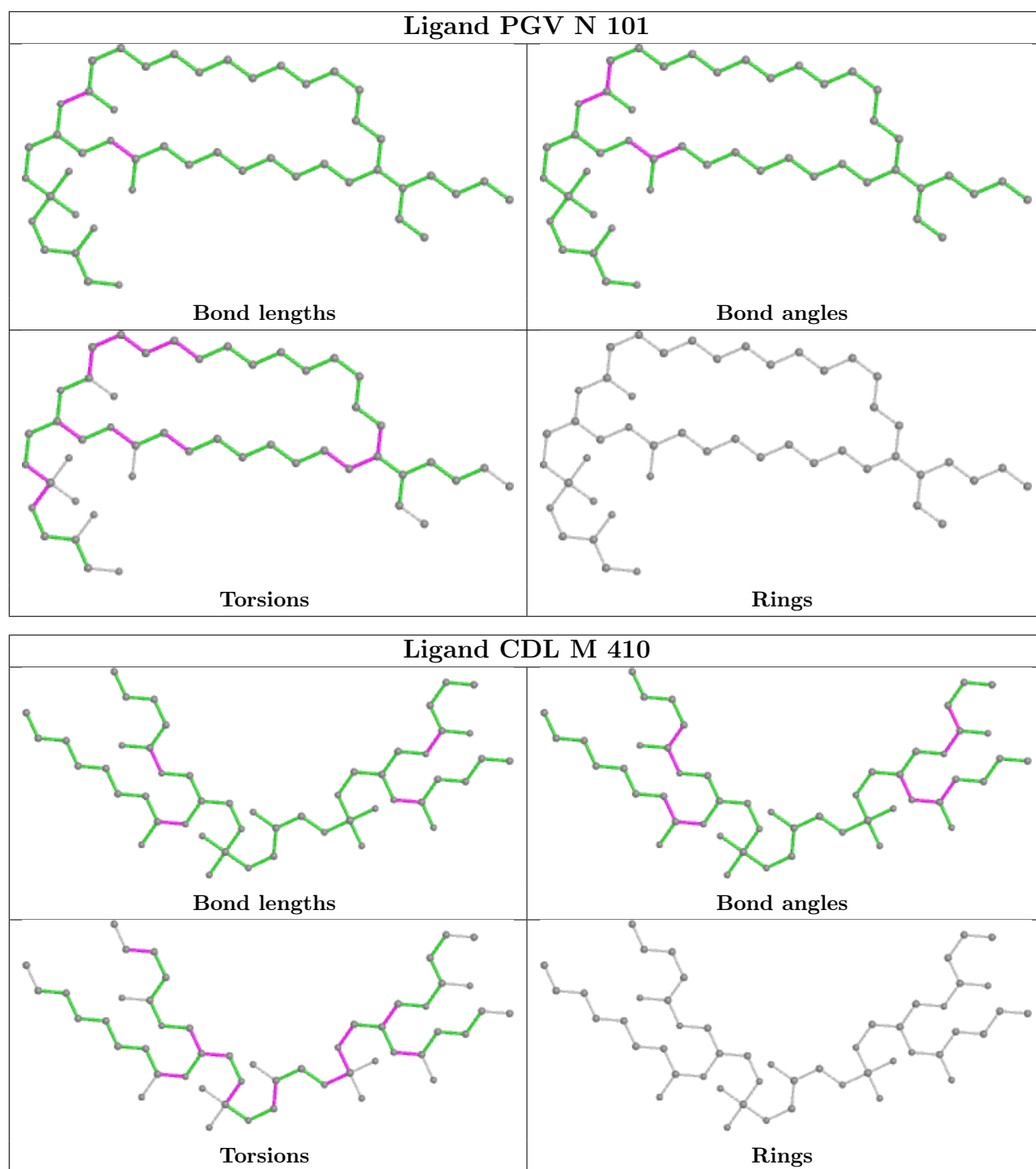


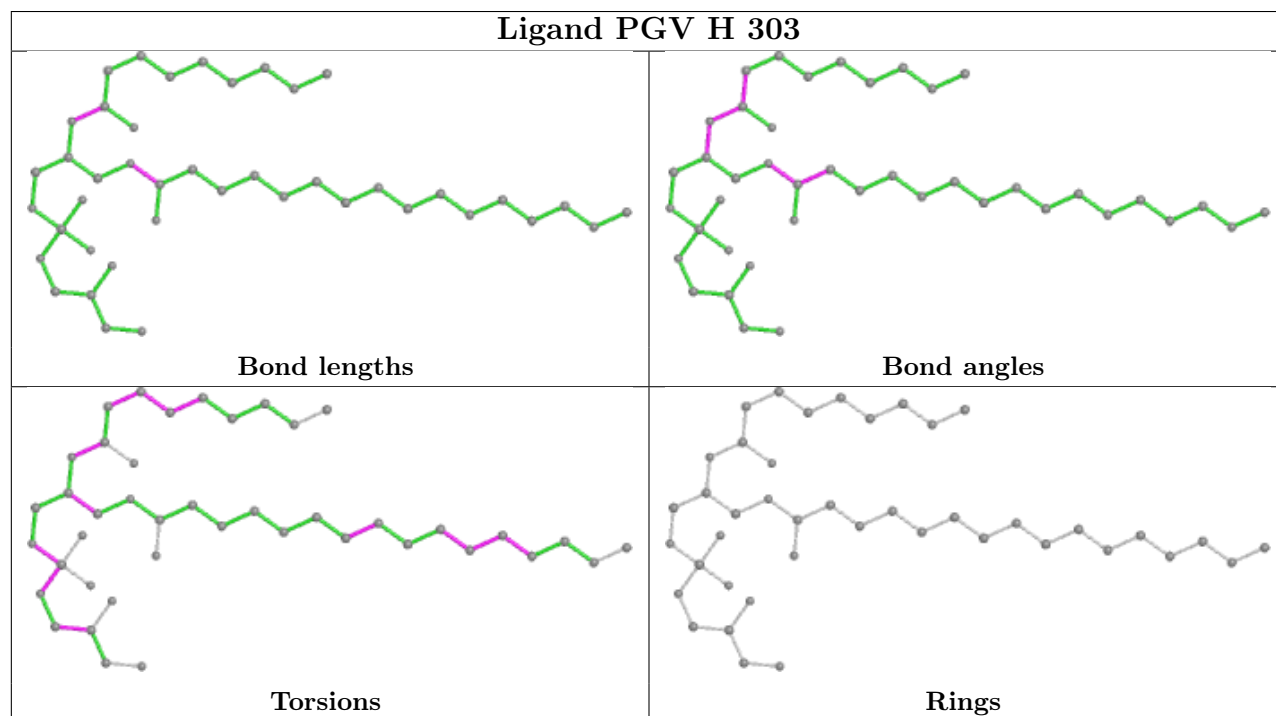
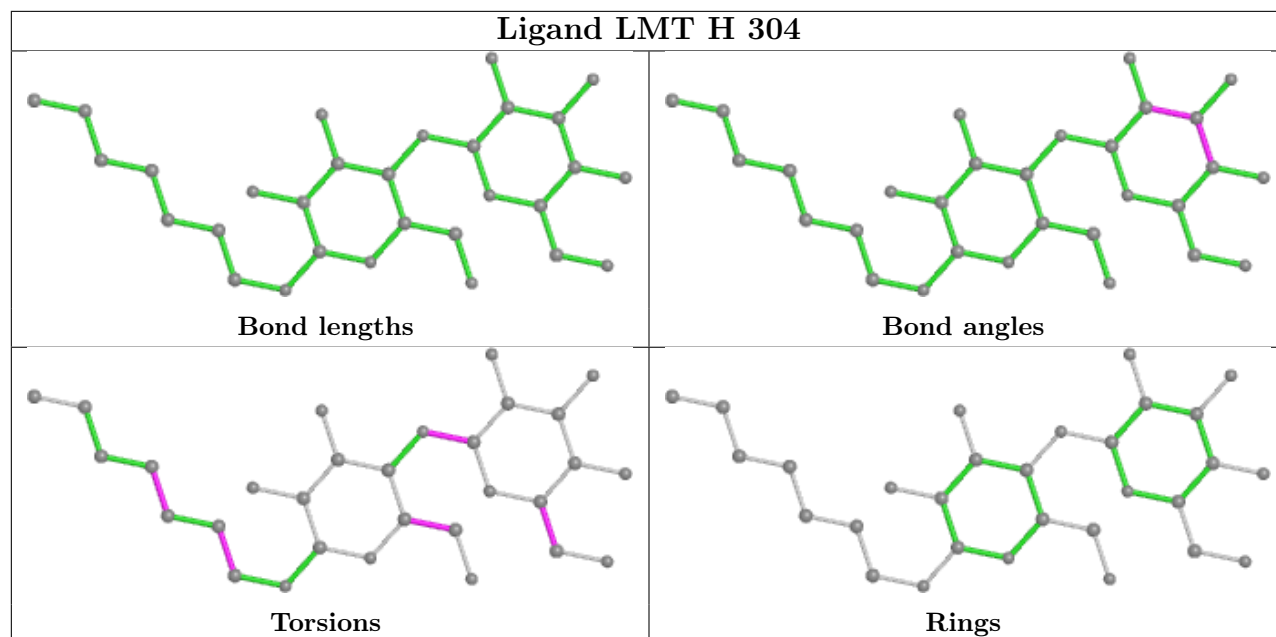




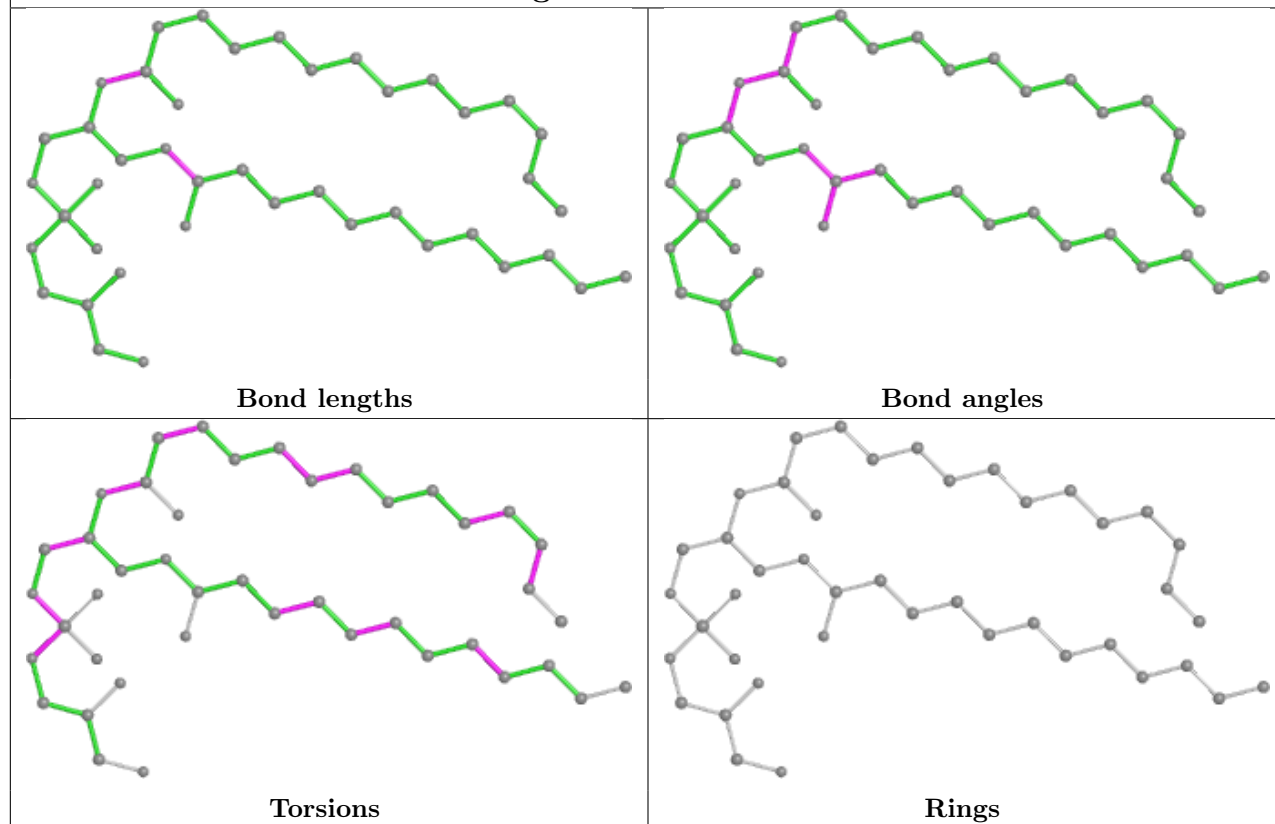




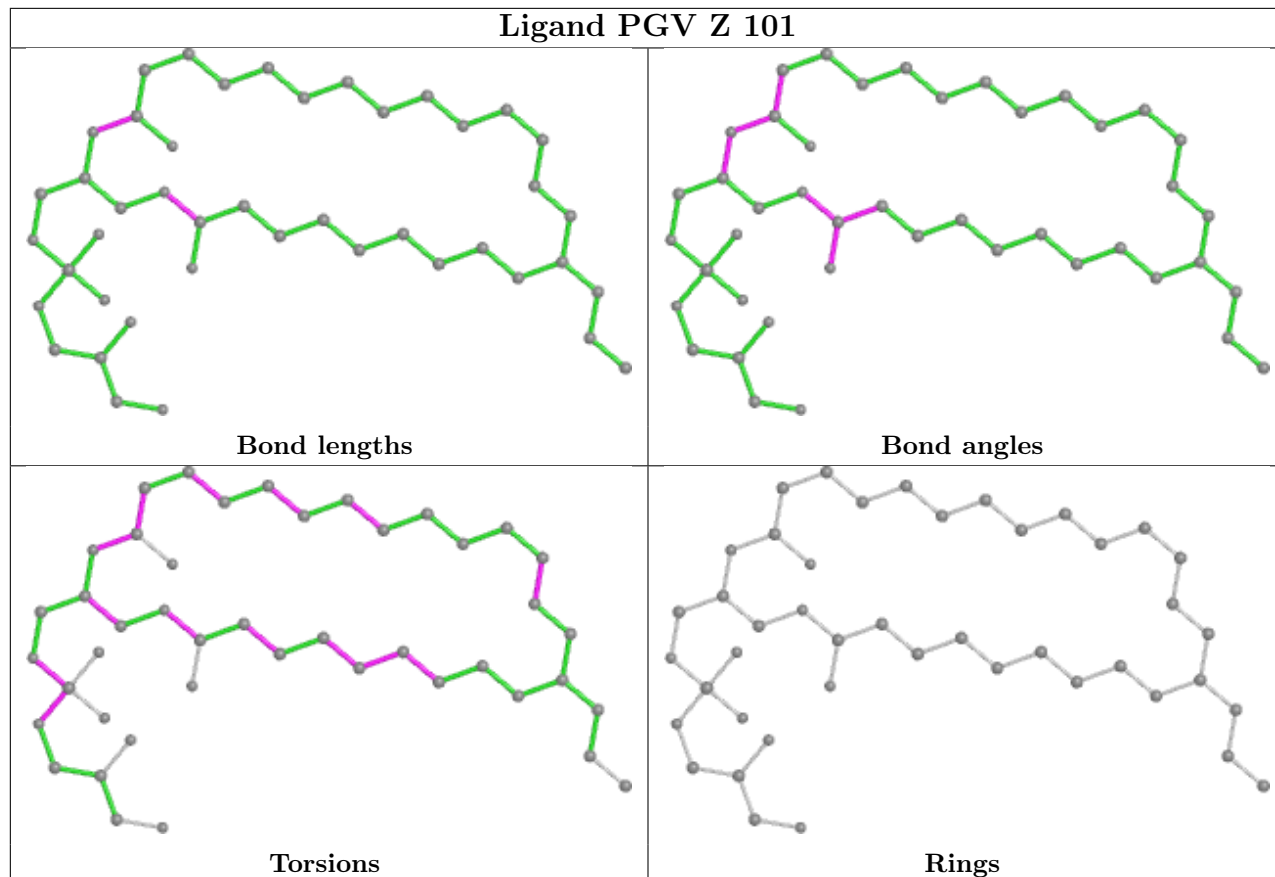


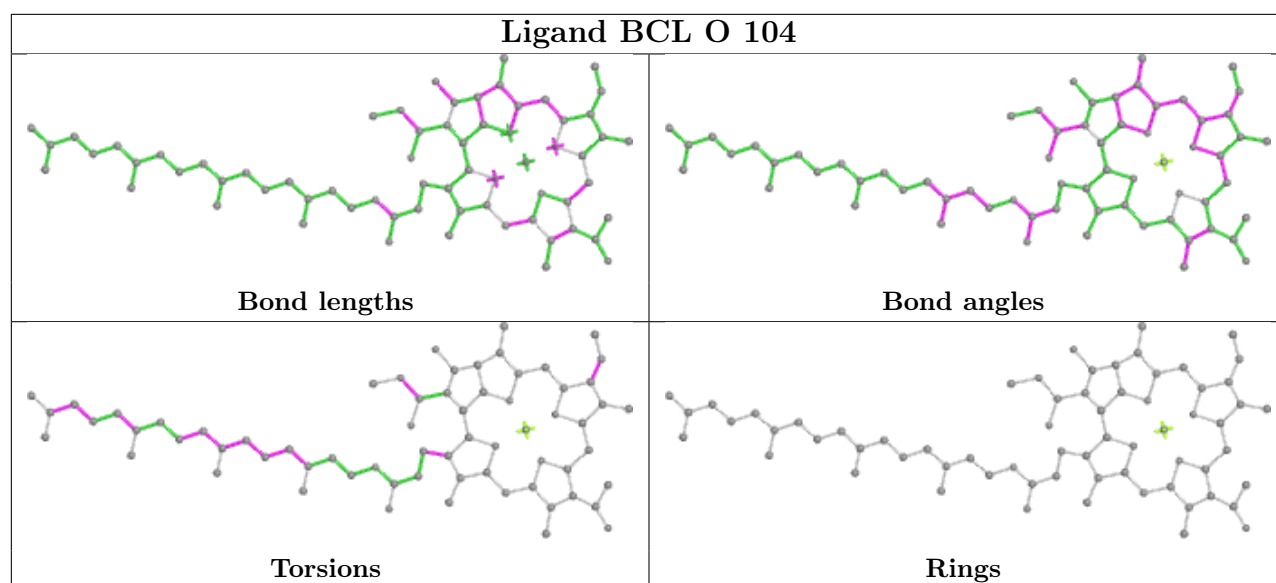


## Ligand PGV 0 104



## Ligand PGV Z 101





## 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.



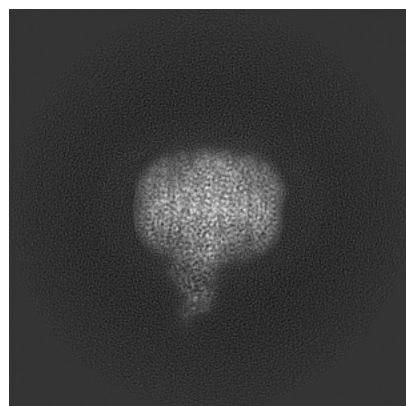
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39836. These allow visual inspection of the internal detail of the map and identification of artifacts.

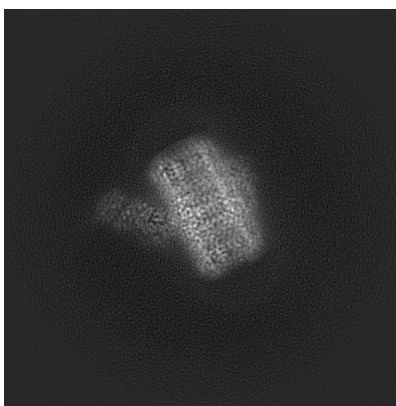
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

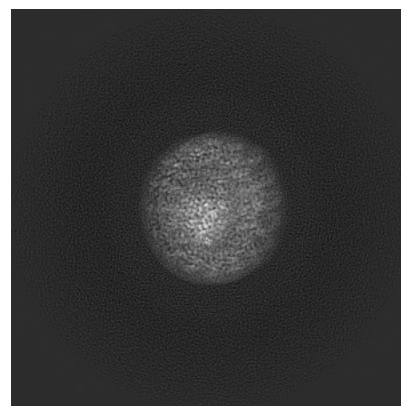
#### 6.1.1 Primary map



X

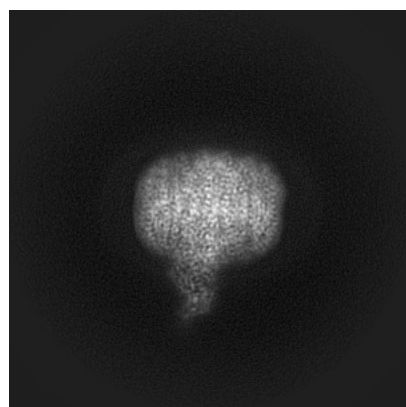


Y

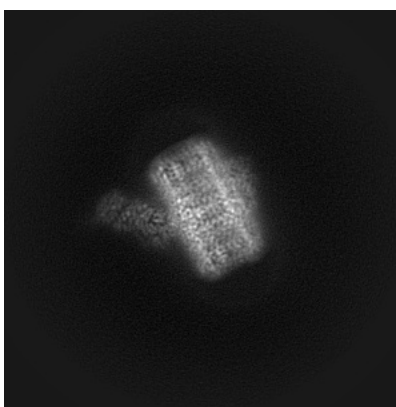


Z

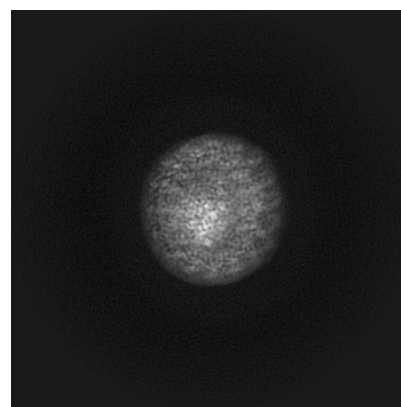
#### 6.1.2 Raw map



X



Y

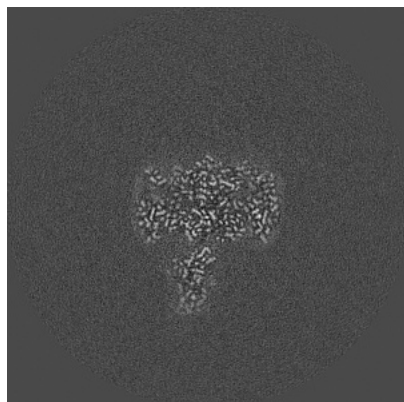


Z

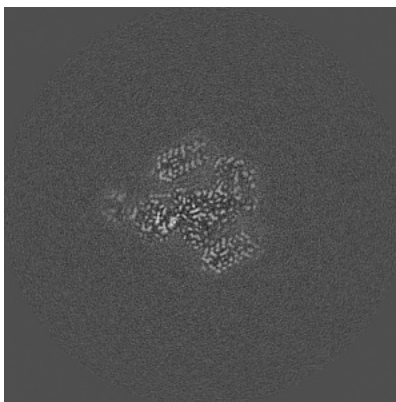
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

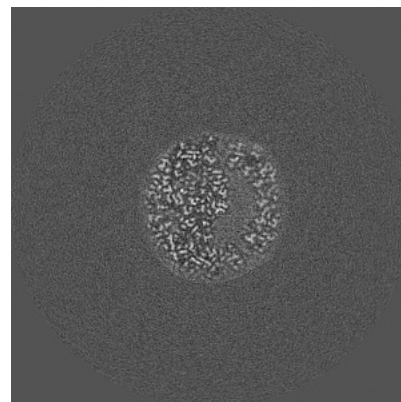
### 6.2.1 Primary map



X Index: 200

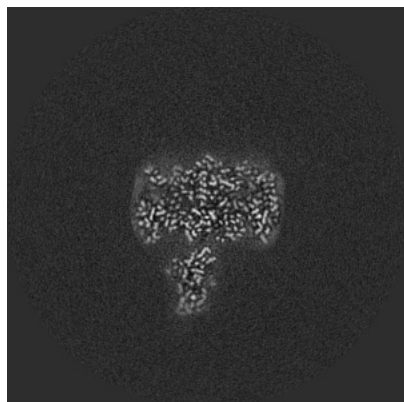


Y Index: 200

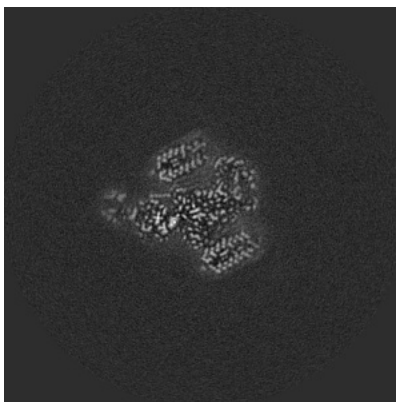


Z Index: 200

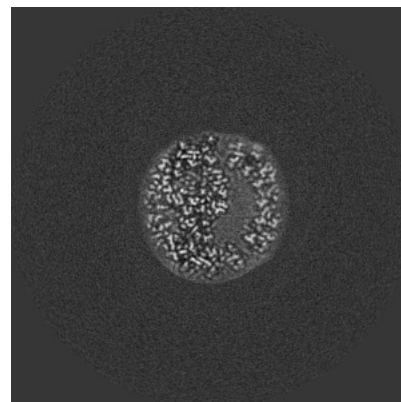
### 6.2.2 Raw map



X Index: 200



Y Index: 200

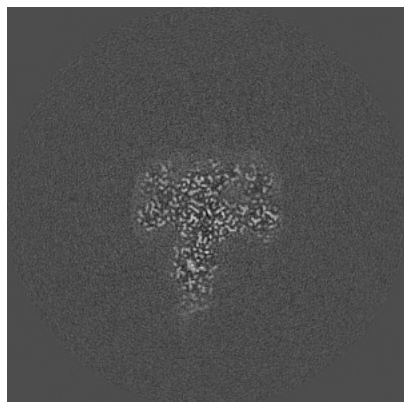


Z Index: 200

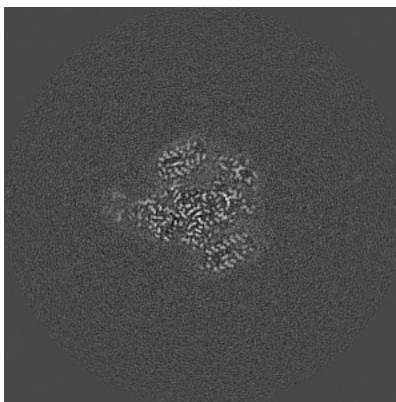
The images above show central slices of the map in three orthogonal directions.

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

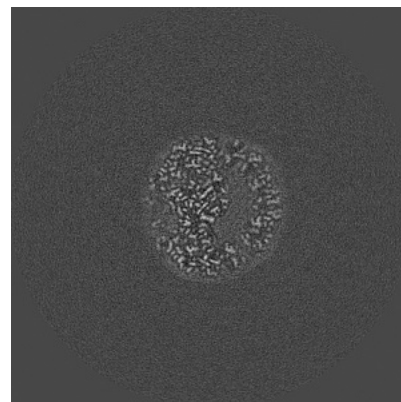
### 6.3.1 Primary map



X Index: 193

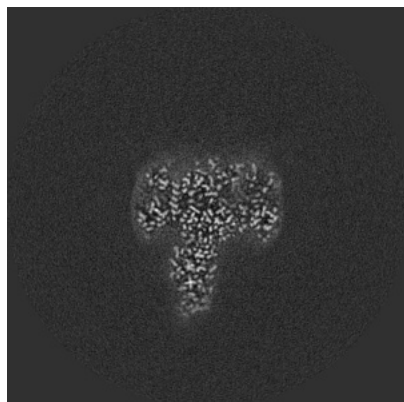


Y Index: 202

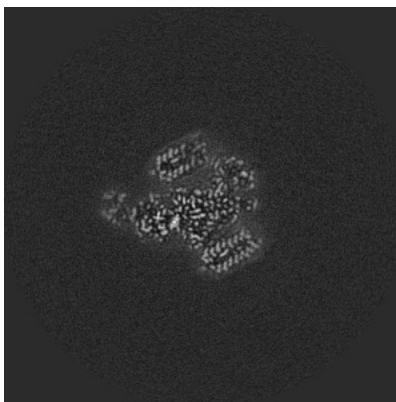


Z Index: 196

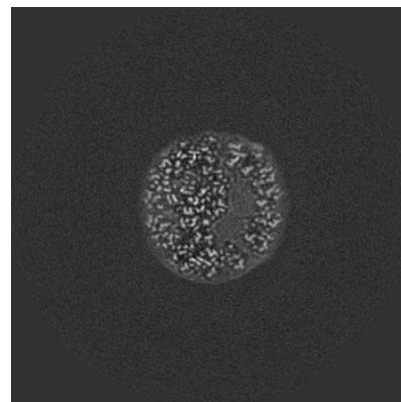
### 6.3.2 Raw map



X Index: 194



Y Index: 199

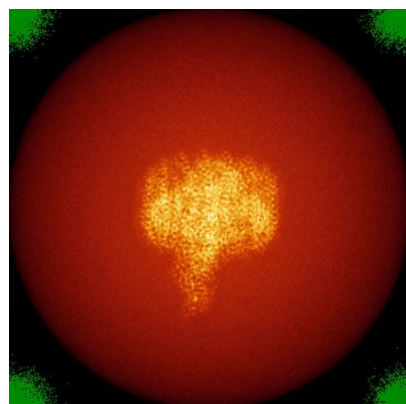


Z Index: 199

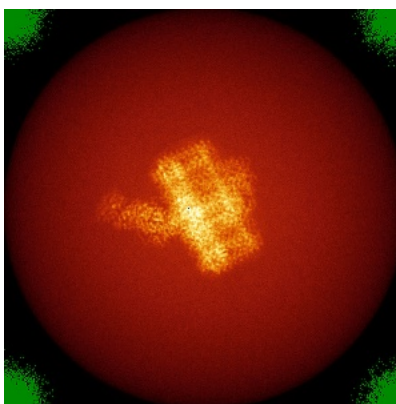
The images above show the largest variance slices of the map in three orthogonal directions.

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

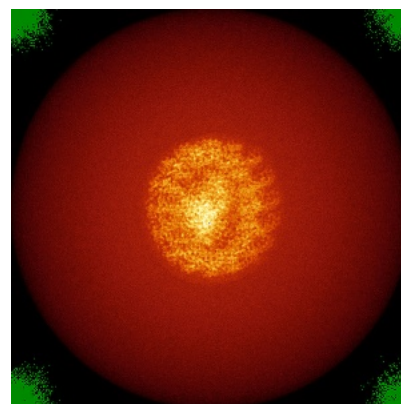
### 6.4.1 Primary map



X

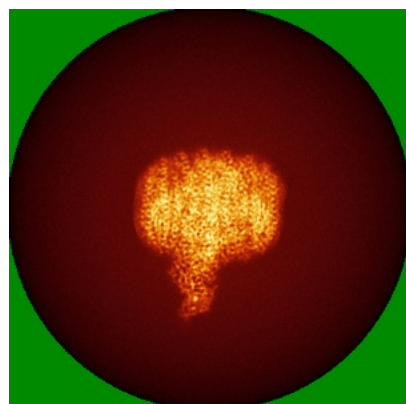


Y

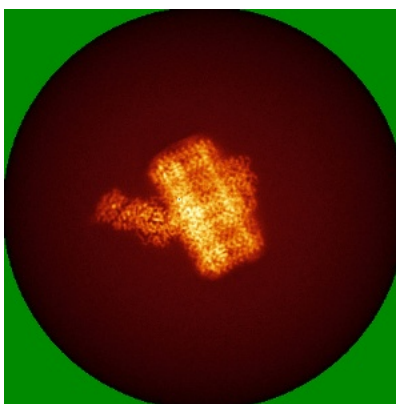


Z

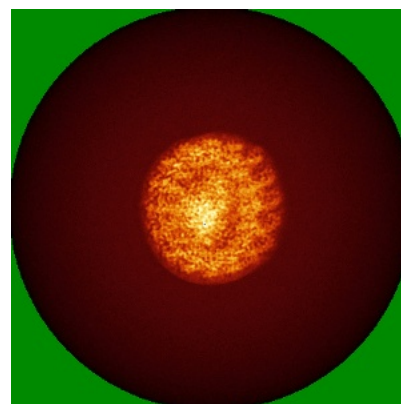
### 6.4.2 Raw map



X



Y



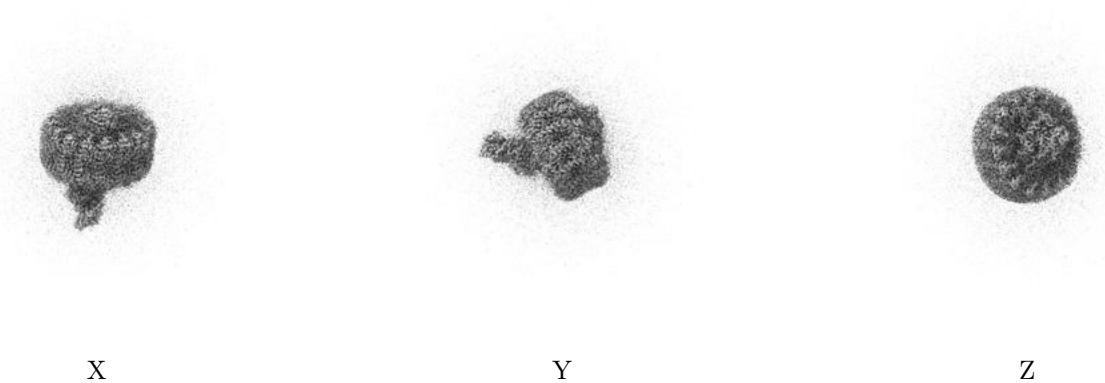
Z

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.



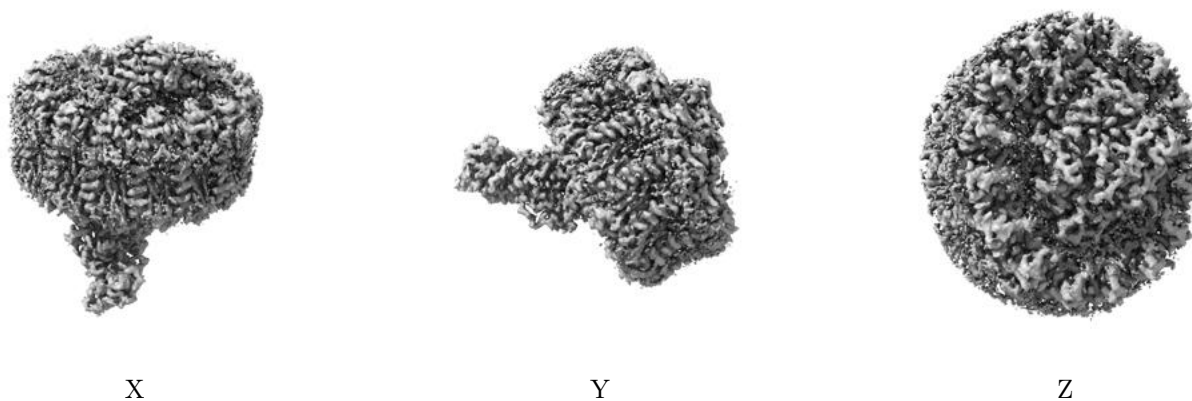
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

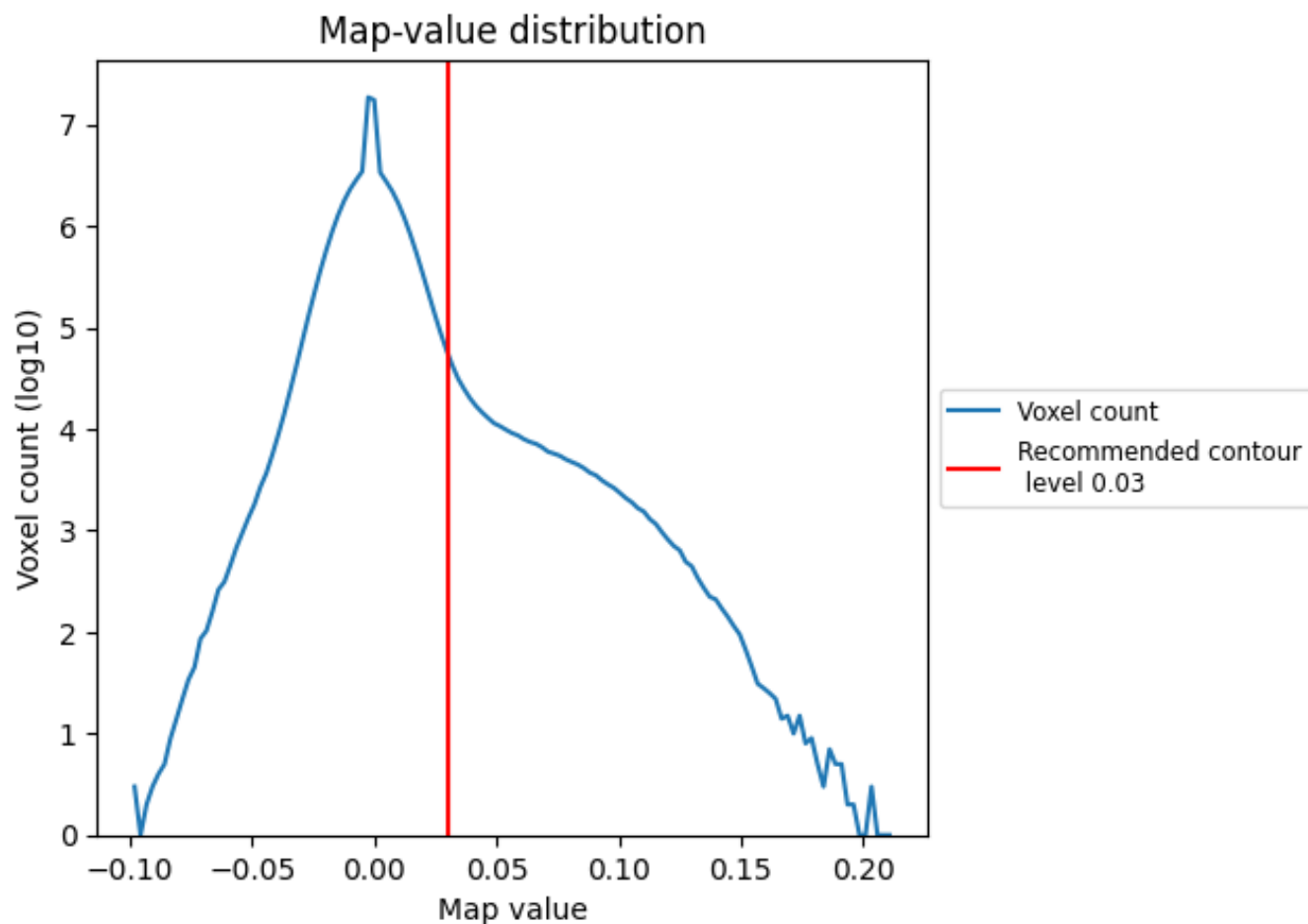
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

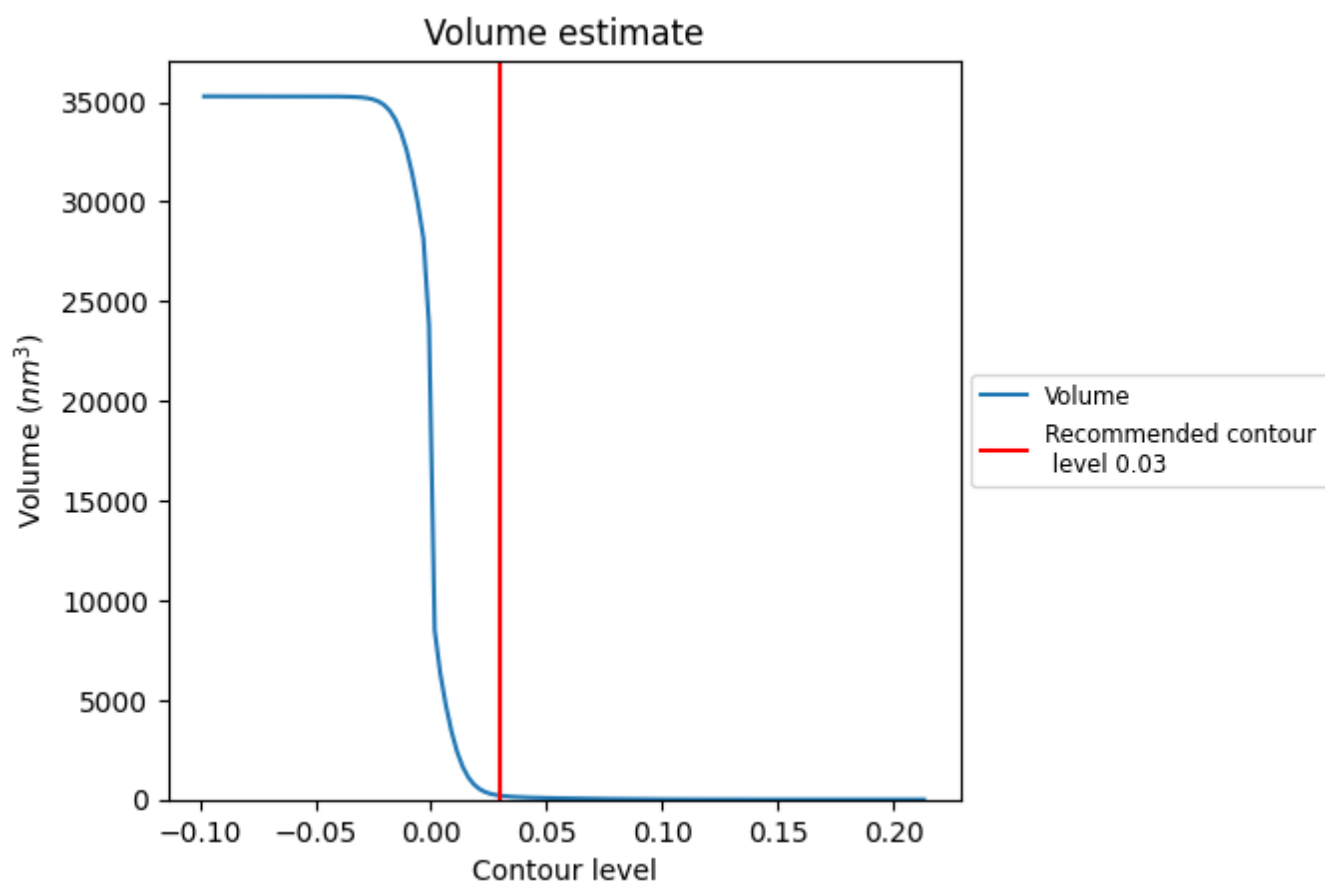
This section contains the results of statistical analysis of the map.

### 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.

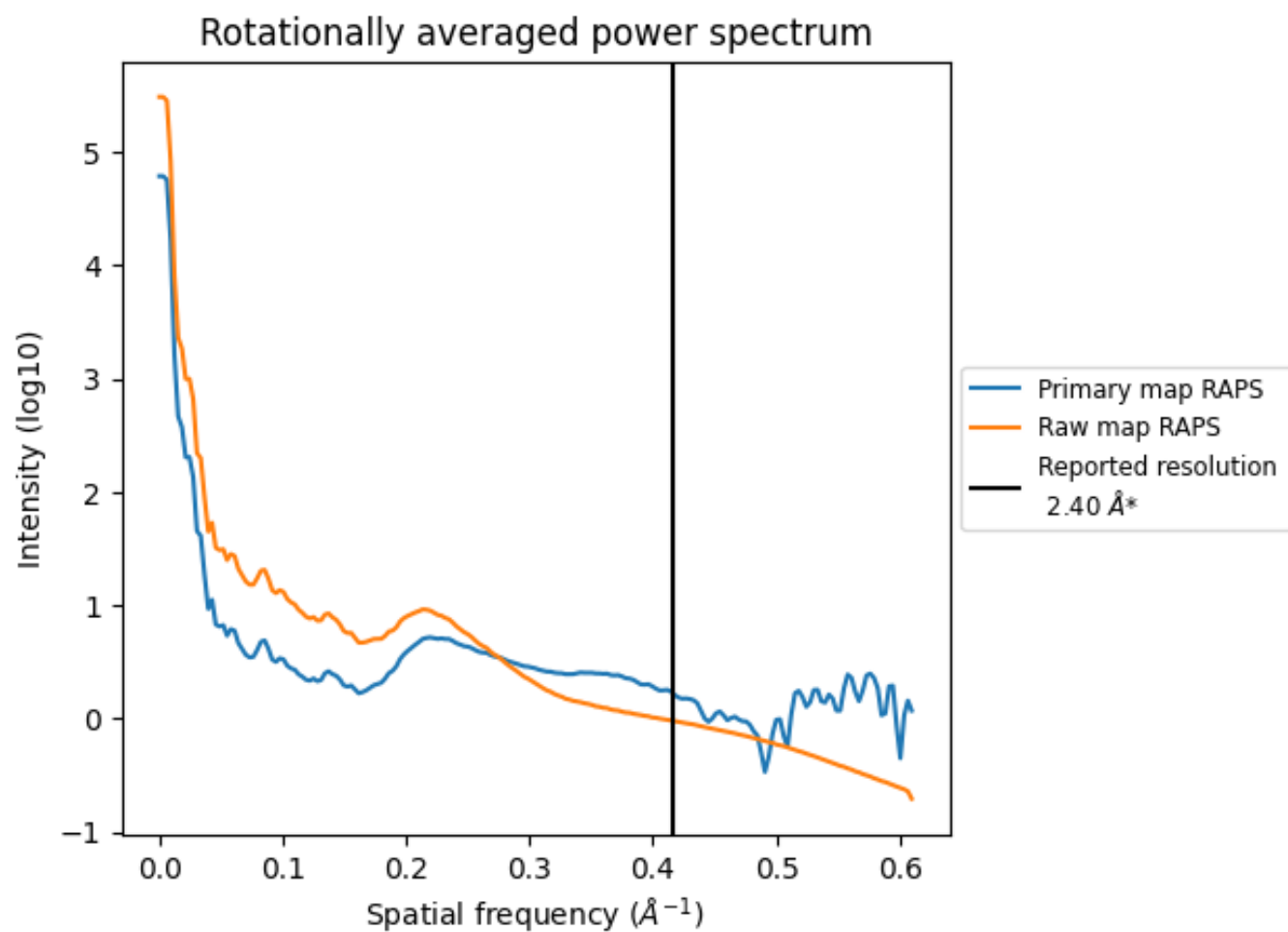
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm<sup>3</sup>; this corresponds to an approximate mass of 178 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 ⓘ



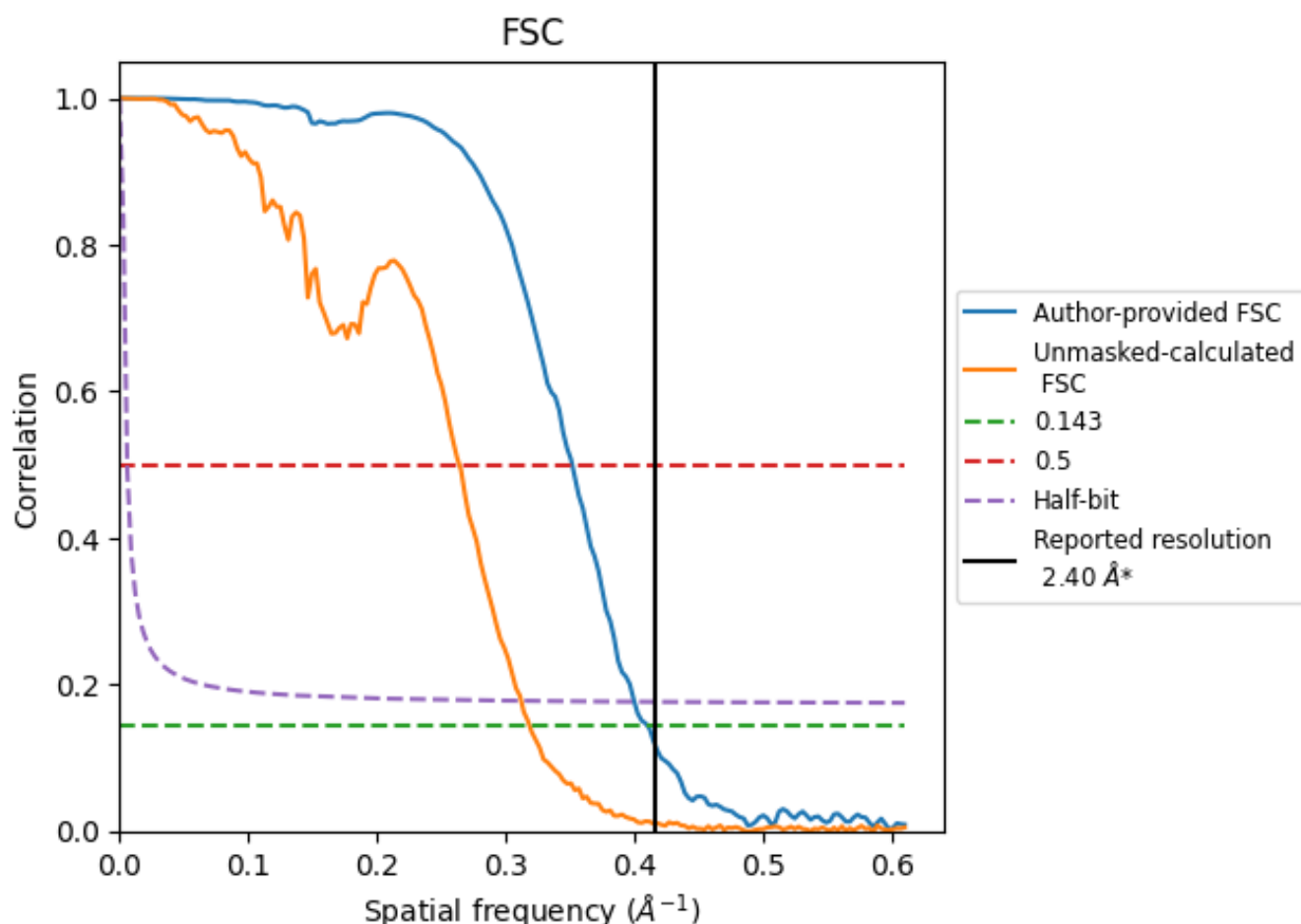
\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

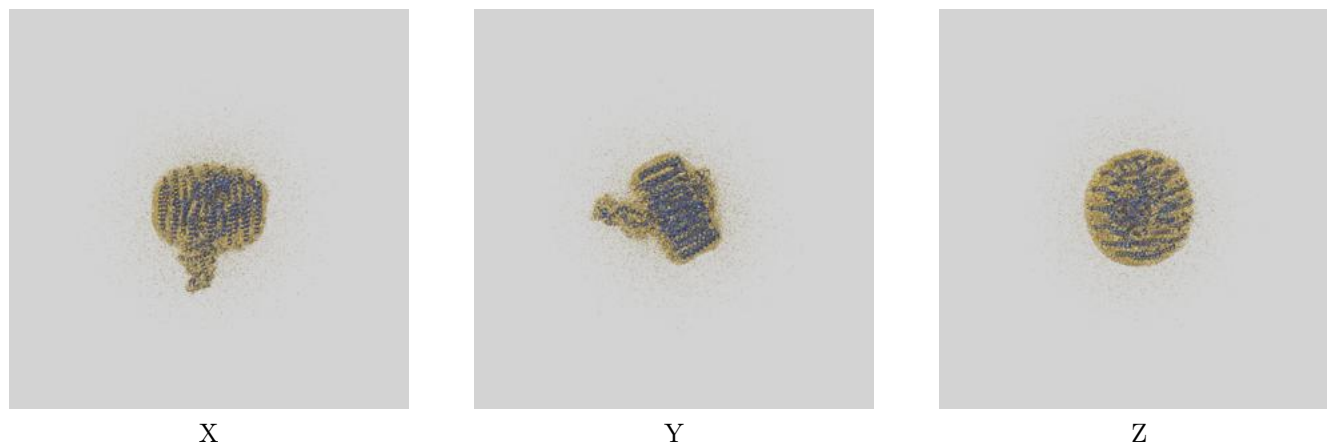
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.84	2.50
Unmasked-calculated*	3.14	3.79	3.21

\*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 3.14 differs from the reported value 2.4 by more than 10 %

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

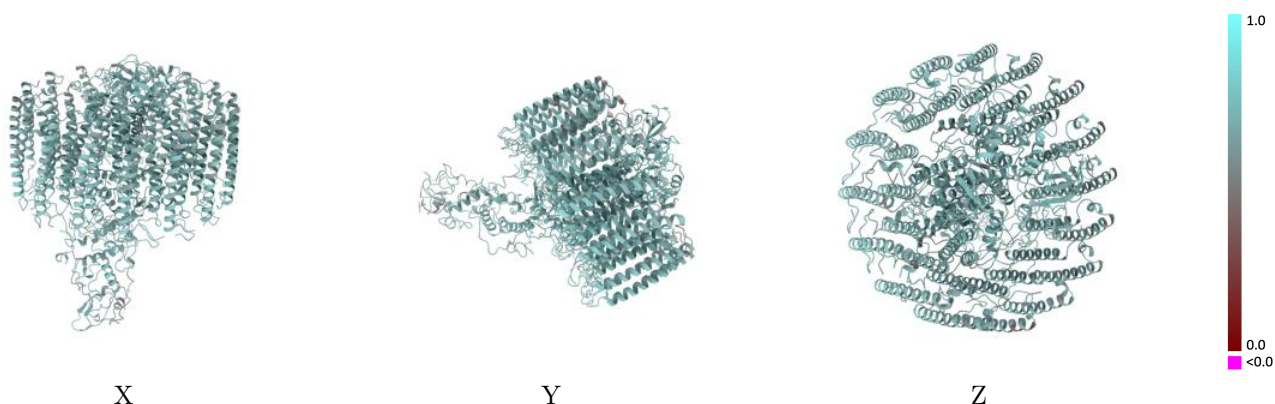
This section contains information regarding the fit between EMDB map EMD-39836 and PDB model 8Z82. Per-residue inclusion information can be found in section 3 on page 24.

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



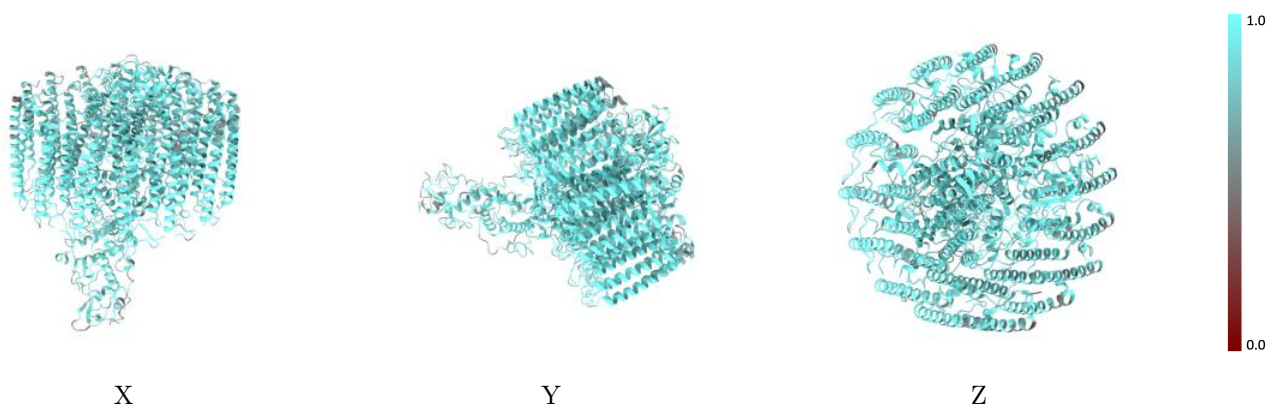
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



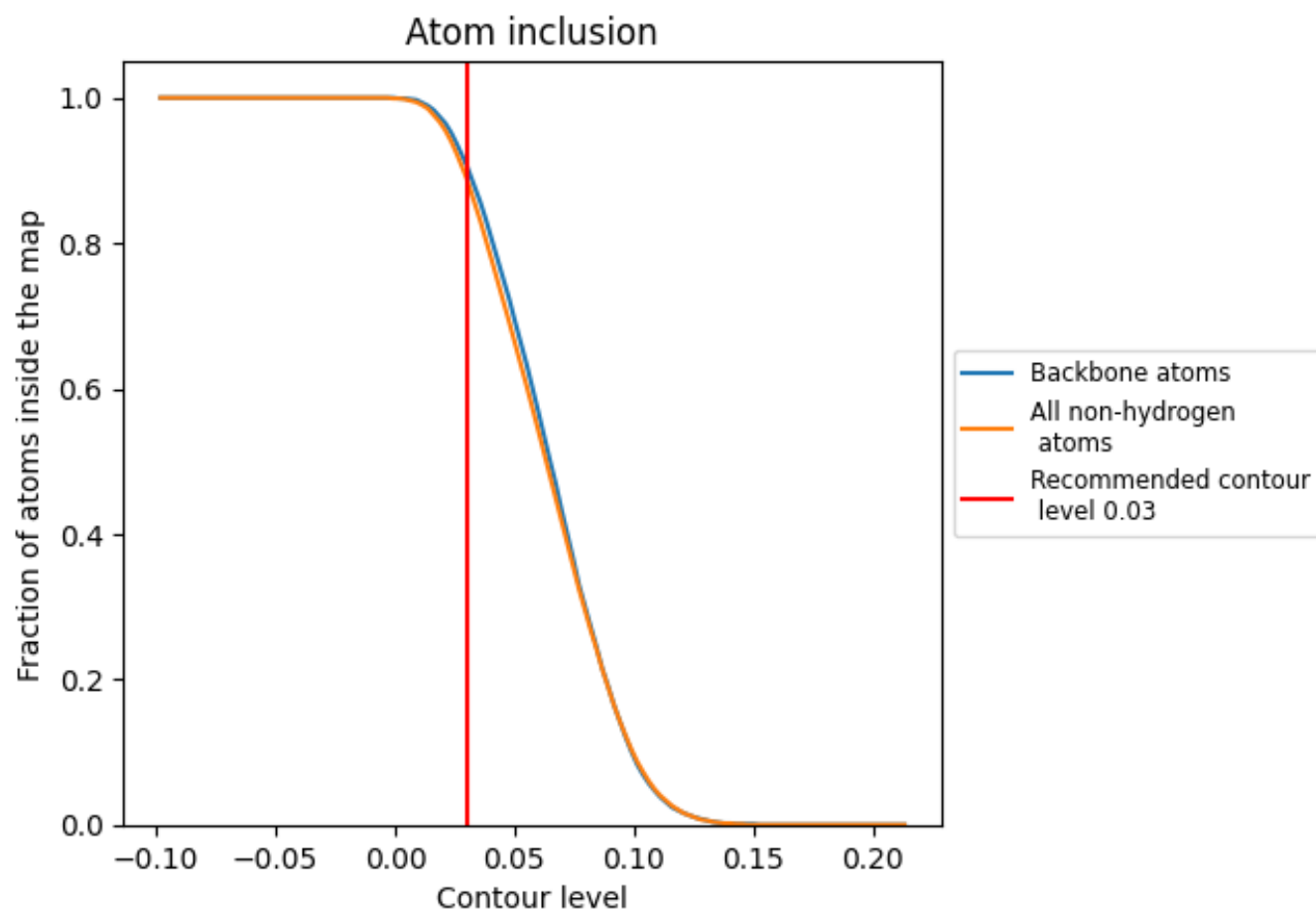
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8890	 0.6390
0	 0.8240	 0.6130
1	 0.9000	 0.6370
2	 0.8600	 0.6160
3	 0.8840	 0.6280
4	 0.8570	 0.6190
5	 0.8590	 0.6130
6	 0.7950	 0.5990
7	 0.8560	 0.6050
8	 0.8430	 0.6190
9	 0.9300	 0.6440
A	 0.9540	 0.6570
B	 0.8740	 0.6360
C	 0.9140	 0.6570
D	 0.9560	 0.6700
E	 0.9060	 0.6440
F	 0.9050	 0.6410
G	 0.8420	 0.6230
H	 0.9030	 0.6450
I	 0.8860	 0.6280
J	 0.8540	 0.6270
K	 0.9310	 0.6460
L	 0.9500	 0.6730
M	 0.9380	 0.6680
N	 0.8160	 0.6140
O	 0.8430	 0.6130
P	 0.8500	 0.6190
Q	 0.9160	 0.6350
R	 0.8810	 0.6330
S	 0.9020	 0.6410
T	 0.8290	 0.6060
U	 0.9310	 0.6540
V	 0.8240	 0.6040
W	 0.9200	 0.6430
X	 0.8530	 0.6350



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Chain	Atom inclusion	Q-score
Y	 0.9200	 0.6470
Z	 0.8120	 0.6000
a	 0.7460	 0.5640