



wwPDB EM Validation Summary Report ⓘ

Jan 21, 2025 – 12:26 PM JST

PDB ID : 8Z83
EMDB ID : EMD-39837
Title : Photosynthetic LH1-RC 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 : 2.60 Å(reported)
Based on initial model : 5Y5S

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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)

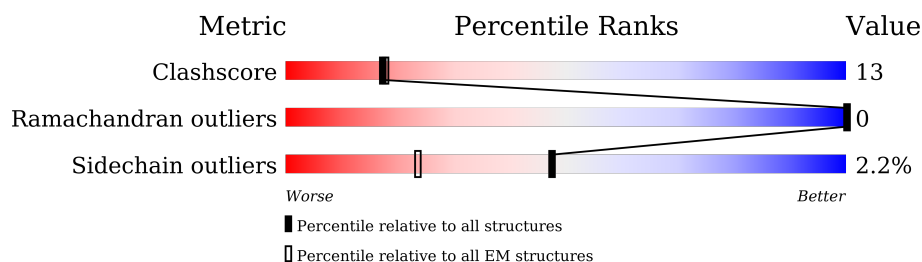
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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 ≥ 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	 71% 20% 8%
2	L	276	 75% 24%
3	M	323	 76% 22%
4	H	278	 76% 22%
5	3	64	 56% 16% 28%
5	7	64	 53% 19% 28%
5	A	64	 55% 17% 28%

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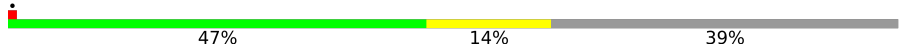
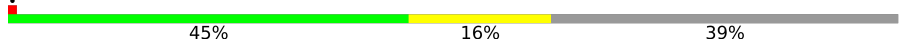
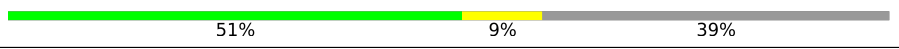

Validation Pipeline (wwPDB-VP) : 2.40

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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	 45% 16% 39%
8	T	74	 51% 9% 39%
8	X	74	 55% 5% 39%

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 27998 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	333	Total	C	N	O	S	0	0
			2618	1603	446	545	24		

- 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

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Chain	Residue	Modelled	Actual	Comment	Reference
M	131	ALA	VAL	conflict	UNP A0A2L1K3T5
M	236	GLU	ASP	conflict	UNP A0A2L1K3T5

- Molecule 4 is a protein called Photosynthetic reaction center H subunit.

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

- 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		
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		

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Mol	Chain	Residues	Atoms					AltConf	Trace
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

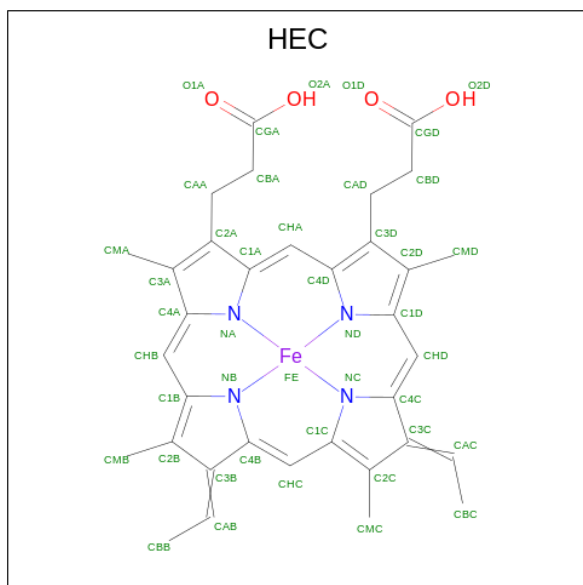
- Molecule 8 is a protein called Antenna complex, alpha/beta subunit.

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

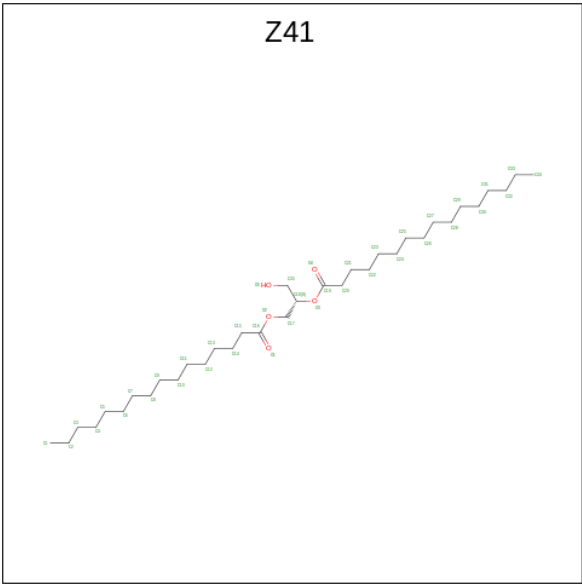


Mol	Chain	Residues	Atoms					AltConf
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

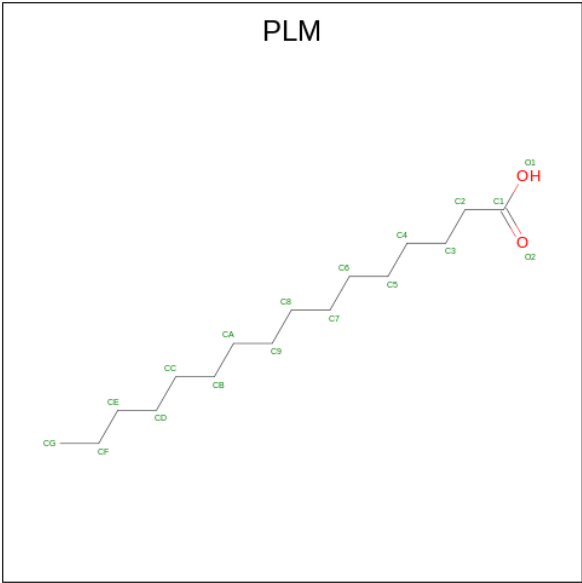
Mol	Chain	Residues	Atoms		AltConf
10	C	1	Total	Mg	0
			1	1	

- Molecule 11 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (three-letter code: Z41) (formula: C₃₅H₆₈O₅).



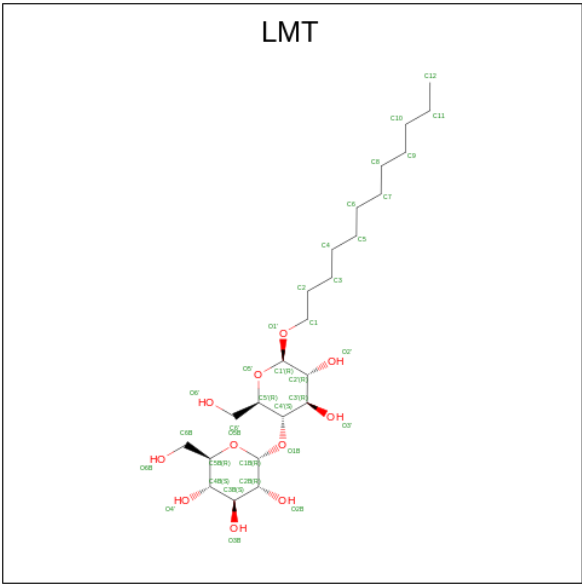
Mol	Chain	Residues	Atoms			AltConf
11	C	1	Total	C	O	0
			31	27	4	

- Molecule 12 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



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

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



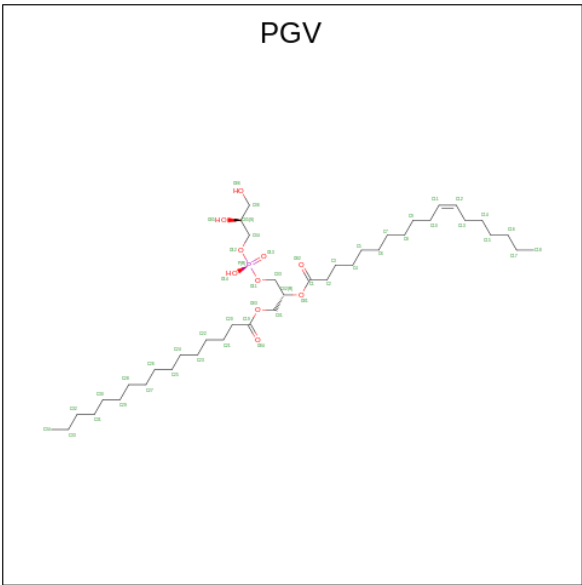
Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			35	24	11	
13	L	1	Total	C	O	0
			25	14	11	
13	H	1	Total	C	O	0
			30	19	11	
13	H	1	Total	C	O	0
			26	15	11	
13	F	1	Total	C	O	0
			33	22	11	
13	K	1	Total	C	O	0
			25	14	11	
13	O	1	Total	C	O	0
			29	18	11	
13	Q	1	Total	C	O	0
			32	21	11	
13	Y	1	Total	C	O	0
			35	24	11	
13	5	1	Total	C	O	0
			24	13	11	
13	7	1	Total	C	O	0
			25	14	11	
13	7	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
13	9	1	Total	C	O	0
			35	24	11	

- 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: C₄₀H₇₇O₁₀P).



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	L	1	Total	C	O	P	0
			36	27	8	1	
14	L	1	Total	C	O	P	0
			41	30	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	H	1	Total	C	O	P	0
			51	40	10	1	
14	B	1	Total	C	O	P	0
			31	20	10	1	
14	B	1	Total	C	O	P	0
			41	32	8	1	

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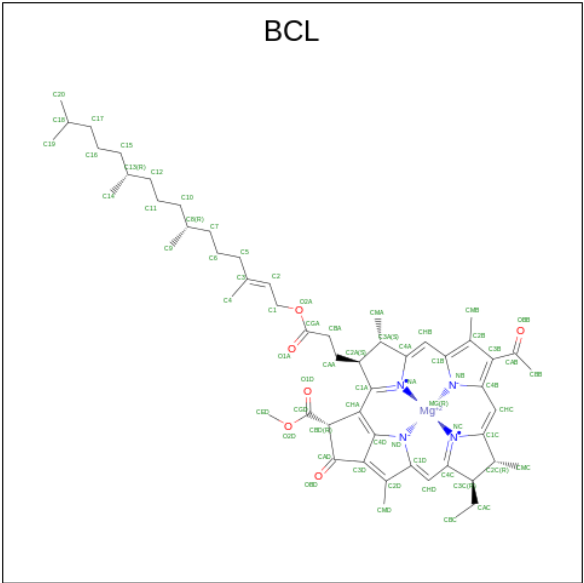
Mol	Chain	Residues	Atoms				AltConf
14	E	1	Total	C	O	P	0
			35	24	10	1	
14	E	1	Total	C	O	P	0
			38	27	10	1	
14	G	1	Total	C	O	P	0
			35	24	10	1	
14	G	1	Total	C	O	P	0
			42	33	8	1	
14	I	1	Total	C	O	P	0
			50	39	10	1	
14	J	1	Total	C	O		0
			29	24	5		
14	N	1	Total	C	O	P	0
			35	24	10	1	
14	N	1	Total	C	O	P	0
			31	20	10	1	
14	N	1	Total	C	O	P	0
			32	23	8	1	
14	P	1	Total	C	O	P	0
			28	19	8	1	
14	P	1	Total	C	O	P	0
			40	31	8	1	
14	R	1	Total	C	O	P	0
			29	18	10	1	
14	R	1	Total	C	O	P	0
			41	32	8	1	
14	T	1	Total	C	O	P	0
			47	36	10	1	
14	V	1	Total	C	O	P	0
			29	18	10	1	
14	V	1	Total	C	O	P	0
			31	20	10	1	
14	V	1	Total	C	O	P	0
			44	33	10	1	
14	X	1	Total	C	O	P	0
			45	34	10	1	
14	Z	1	Total	C	O	P	0
			29	18	10	1	
14	Z	1	Total	C	O	P	0
			32	21	10	1	
14	Z	1	Total	C	O	P	0
			43	34	8	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	1	1	Total 45	34	10	1	0
14	2	1	Total 26	17	8	1	0
14	2	1	Total 34	25	8	1	0
14	3	1	Total 30	21	8	1	0
14	4	1	Total 29	18	10	1	0
14	4	1	Total 41	32	8	1	0
14	6	1	Total 38	29	8	1	0
14	8	1	Total 44	34	9	1	0
14	8	1	Total 43	32	10	1	0
14	0	1	Total 34	23	10	1	0
14	0	1	Total 31	20	10	1	0
14	0	1	Total 32	27	5		0

- Molecule 15 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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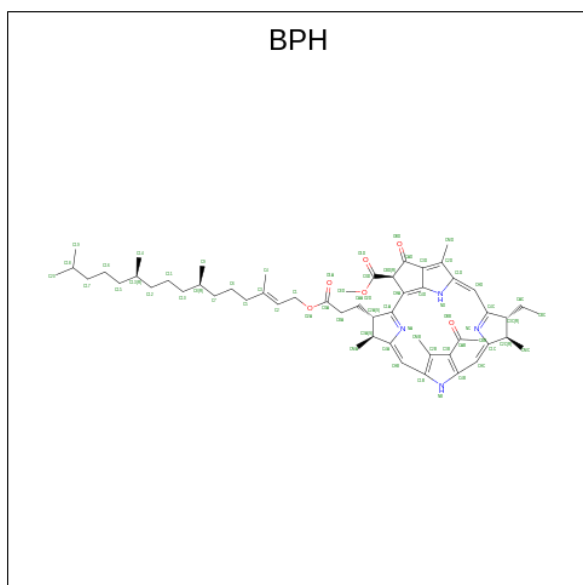
Mol	Chain	Residues	Atoms					AltConf
15	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	9	1	Total 66	C 55	Mg 1	N 4	O 6	0

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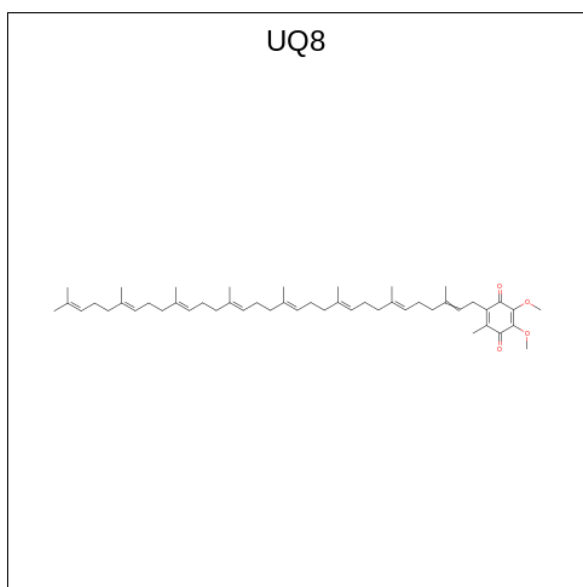
Mol	Chain	Residues	Atoms					AltConf
15	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 16 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



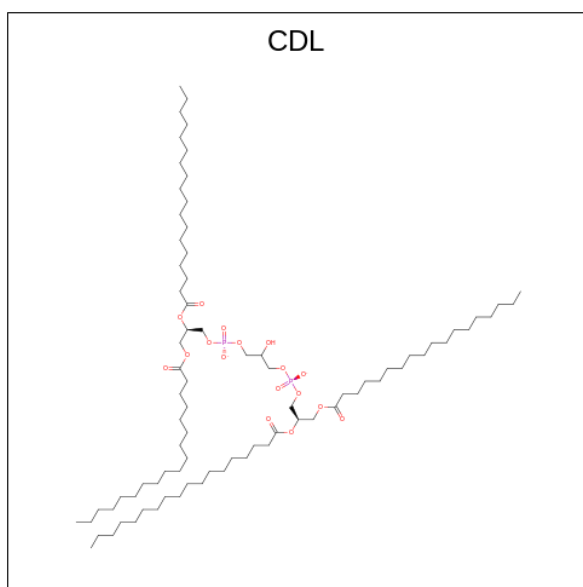
Mol	Chain	Residues	Atoms				AltConf
16	L	1	Total	C	N	O	0
			65	55	4	6	
16	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 17 is Ubiquinone-8 (three-letter code: UQ8) (formula: C₄₉H₇₄O₄).



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

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
18	L	1	Total	C	O	P	0
			73	54	17	2	

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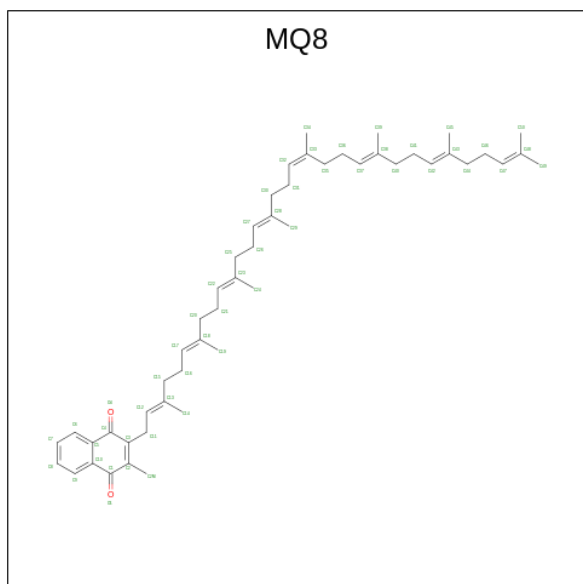
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Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			82	63	17	2	
18	M	1	Total	C	O	P	0
			80	61	17	2	
18	M	1	Total	C	O	P	0
			46	27	17	2	
18	M	1	Total	C	O	P	0
			56	37	17	2	
18	M	1	Total	C	O	P	0
			50	31	17	2	
18	H	1	Total	C	O	P	0
			75	56	17	2	
18	F	1	Total	C	O	P	0
			64	45	17	2	
18	U	1	Total	C	O	P	0
			51	32	17	2	

- Molecule 19 is FE (III) ION (three-letter code: FE) (formula: Fe).

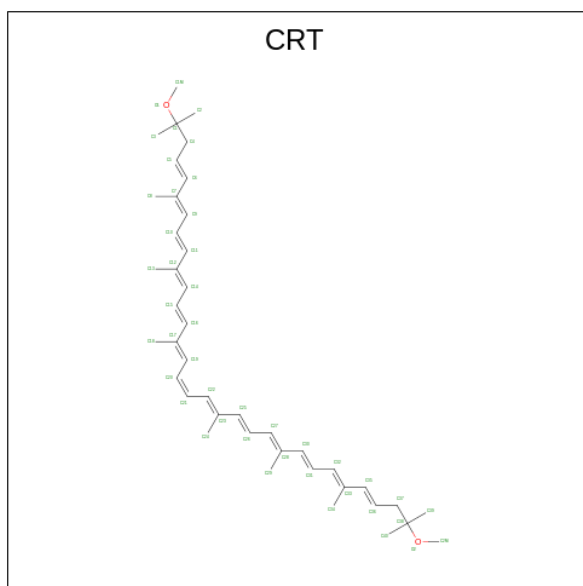
Mol	Chain	Residues	Atoms		AltConf
19	M	1	Total	Fe	0
			1	1	

- Molecule 20 is MENAQUINONE 8 (three-letter code: MQ8) (formula: C₅₁H₇₂O₂).



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

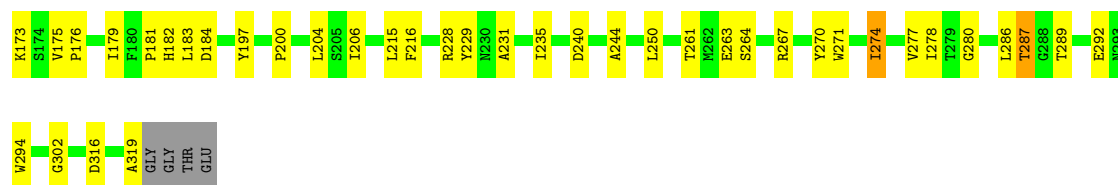
- Molecule 21 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms			AltConf
21	M	1	Total	C	O	0
			44	42	2	
21	B	1	Total	C	O	0
			44	42	2	
21	G	1	Total	C	O	0
			44	42	2	
21	N	1	Total	C	O	0
			44	42	2	
21	R	1	Total	C	O	0
			44	42	2	
21	V	1	Total	C	O	0
			44	42	2	
21	Z	1	Total	C	O	0
			44	42	2	
21	4	1	Total	C	O	0
			44	42	2	
21	8	1	Total	C	O	0
			44	42	2	

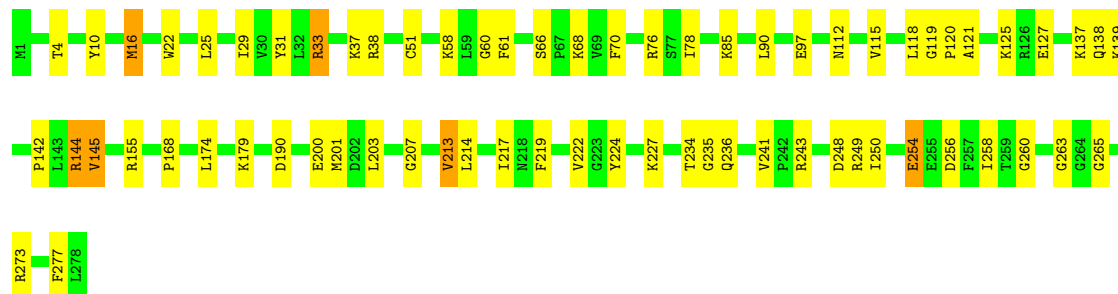
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	C	3	Total 3	O 3	0
22	M	2	Total 2	O 2	0



- Molecule 4: Photosynthetic reaction center H subunit

Chain H: 76% 22%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain A: 55% 17% 28%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain F: 50% 22% 28%



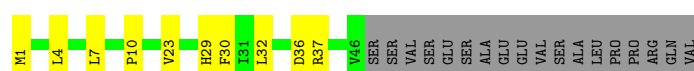
- Molecule 5: Antenna complex, alpha/beta subunit

Chain K: 56% 14% 28%



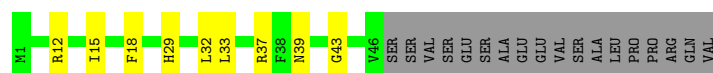
- Molecule 5: Antenna complex, alpha/beta subunit

Chain Q: 56% 16% 28%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain U:  58% 14% 28%



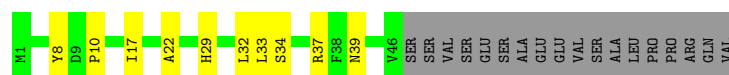
- Molecule 5: Antenna complex, alpha/beta subunit

Chain Y:  53% 19% 28%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain 3:  56% 16% 28%



- Molecule 5: Antenna complex, alpha/beta subunit

Chain 7:  53% 19% 28%



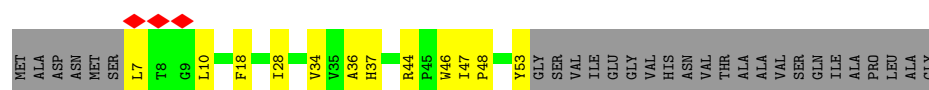
- Molecule 6: Antenna complex, alpha/beta subunit

Chain B:  51% 12% 36%



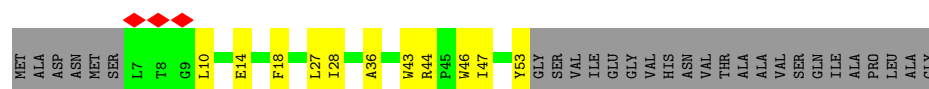
- Molecule 6: Antenna complex, alpha/beta subunit

Chain G:  47% 16% 37%



- Molecule 6: Antenna complex, alpha/beta subunit

Chain N:  48% 15% 37%



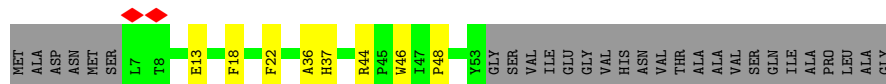
- Molecule 6: Antenna complex, alpha/beta subunit

Chain R:  49% 13% 37%



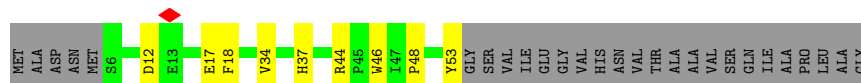
- Molecule 6: Antenna complex, alpha/beta subunit

Chain V:  52% 11% 37%



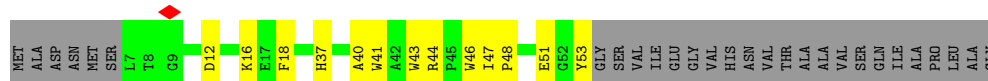
- Molecule 6: Antenna complex, alpha/beta subunit

Chain Z:  52% 12% 36%



- Molecule 6: Antenna complex, alpha/beta subunit

Chain 4:  45% 17% 37%



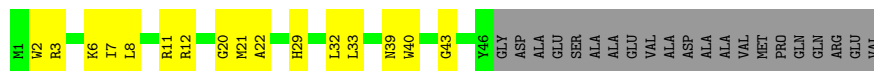
- Molecule 6: Antenna complex, alpha/beta subunit

Chain 8:  52% 11% 37%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain D:  45% 24% 31%



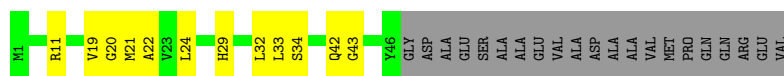
- Molecule 7: Antenna complex, alpha/beta subunit

Chain I:  40% 27% 31%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain O:  51% 18% 31%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain S:  45% 24% 31%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain W:  48% 18% 31%



- Molecule 7: Antenna complex, alpha/beta subunit

Chain 1:  45% 24% 31%



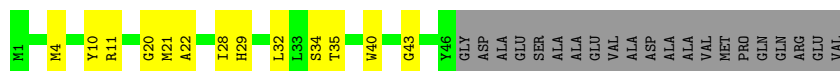
- Molecule 7: Antenna complex, alpha/beta subunit

Chain 5:  48% 21% 31%



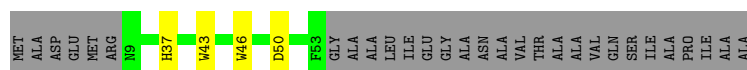
- Molecule 7: Antenna complex, alpha/beta subunit

Chain 9:  49% 19% 31%



- Molecule 8: Antenna complex, alpha/beta subunit

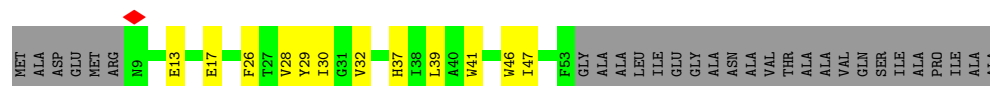
Chain E:  55% 5% 39%



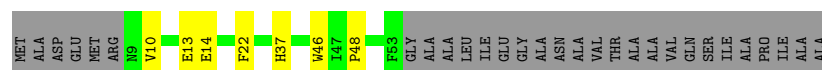
- Molecule 8: Antenna complex, alpha/beta subunit



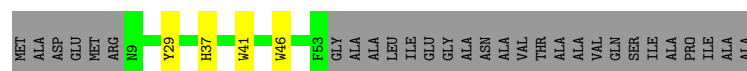
- Molecule 8: Antenna complex, alpha/beta subunit



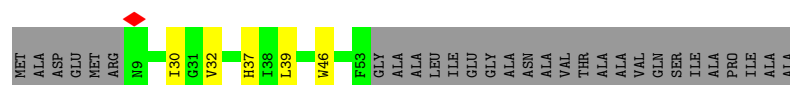
- Molecule 8: Antenna complex, alpha/beta subunit



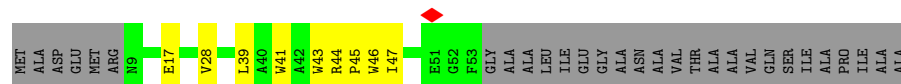
- Molecule 8: Antenna complex, alpha/beta subunit



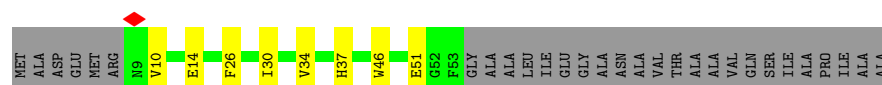
- Molecule 8: Antenna complex, alpha/beta subunit



- Molecule 8: Antenna complex, alpha/beta subunit



- Molecule 8: Antenna complex, alpha/beta subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44938	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	0.223	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (\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 (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/2678	0.49	0/3642
2	L	0.27	0/2252	0.43	0/3082
3	M	0.28	0/2613	0.44	0/3582
4	H	0.27	0/2229	0.49	0/3027
5	3	0.25	0/398	0.44	0/543
5	7	0.25	0/398	0.45	0/543
5	A	0.25	0/398	0.44	0/543
5	F	0.25	0/398	0.46	0/543
5	K	0.25	0/398	0.44	0/543
5	Q	0.25	0/398	0.46	0/543
5	U	0.26	0/398	0.45	0/543
5	Y	0.25	0/398	0.46	0/543
6	4	0.26	0/395	0.36	0/539
6	8	0.25	0/395	0.38	0/539
6	B	0.26	0/401	0.36	0/547
6	G	0.26	0/395	0.36	0/539
6	N	0.26	0/395	0.37	0/539
6	R	0.26	0/395	0.36	0/539
6	V	0.25	0/395	0.36	0/539
6	Z	0.25	0/401	0.37	0/547
7	1	0.25	0/402	0.43	0/547
7	5	0.24	0/402	0.44	0/547
7	9	0.26	0/402	0.44	0/547
7	D	0.27	0/402	0.44	0/547
7	I	0.25	0/402	0.42	0/547
7	O	0.24	0/402	0.44	0/547
7	S	0.26	0/402	0.44	0/547
7	W	0.24	0/402	0.43	0/547
8	0	0.25	0/376	0.34	0/514
8	2	0.25	0/376	0.35	0/514
8	6	0.26	0/376	0.35	0/514
8	E	0.26	0/376	0.35	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	0.26	0/376	0.37	0/514
8	T	0.25	0/376	0.35	0/514
8	X	0.26	0/376	0.36	0/514
All	All	0.26	0/22352	0.43	0/30493

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	2618	0	2377	51	0
2	L	2170	0	2145	60	0
3	M	2518	0	2465	62	0
4	H	2174	0	2131	50	0
5	3	385	0	403	12	0
5	7	385	0	403	15	0
5	A	385	0	403	13	0
5	F	385	0	403	14	0
5	K	385	0	403	9	0
5	Q	385	0	403	14	0
5	U	385	0	403	10	0
5	Y	385	0	403	15	0
6	4	380	0	359	15	0
6	8	380	0	359	8	0
6	B	386	0	364	10	0
6	G	380	0	359	12	0
6	N	380	0	359	11	0
6	R	380	0	359	8	0
6	V	380	0	359	7	0
6	Z	386	0	364	9	0
7	1	390	0	401	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5	390	0	401	15	0
7	9	390	0	401	16	0
7	D	390	0	401	19	0
7	I	390	0	401	21	0
7	O	390	0	401	11	0
7	S	390	0	401	17	0
7	W	390	0	401	15	0
8	0	362	0	333	5	0
8	2	362	0	333	8	0
8	6	362	0	333	10	0
8	E	362	0	333	4	0
8	J	362	0	333	13	0
8	P	362	0	333	12	0
8	T	362	0	333	7	0
8	X	362	0	333	5	0
9	C	172	0	121	8	0
10	C	1	0	0	0	0
11	C	31	0	0	1	0
12	C	12	0	18	5	0
13	5	24	0	21	1	0
13	7	60	0	69	7	0
13	9	35	0	46	2	0
13	C	35	0	46	3	0
13	F	33	0	39	4	0
13	H	56	0	58	3	0
13	K	25	0	23	2	0
13	L	25	0	23	2	0
13	O	29	0	31	2	0
13	Q	32	0	37	3	0
13	Y	35	0	46	1	0
14	0	97	0	113	3	0
14	1	45	0	58	4	0
14	2	60	0	67	3	0
14	3	30	0	31	4	0
14	4	70	0	86	10	0
14	6	38	0	48	3	0
14	8	87	0	109	9	0
14	B	72	0	83	3	0
14	C	32	0	34	5	0
14	E	73	0	84	1	0
14	G	77	0	93	10	0
14	H	129	0	175	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	50	0	71	6	0
14	J	29	0	37	3	0
14	L	120	0	150	11	0
14	N	98	0	107	8	0
14	P	68	0	83	8	0
14	R	70	0	81	2	0
14	T	47	0	65	3	0
14	V	104	0	118	6	0
14	X	45	0	62	2	0
14	Z	104	0	124	6	0
15	0	66	0	74	9	0
15	1	132	0	148	18	0
15	2	66	0	74	9	0
15	3	66	0	74	8	0
15	4	66	0	74	9	0
15	5	132	0	148	13	0
15	6	66	0	74	7	0
15	7	66	0	74	3	0
15	8	66	0	74	8	0
15	9	132	0	148	17	0
15	A	66	0	74	5	0
15	B	66	0	74	3	0
15	D	132	0	148	18	0
15	E	66	0	74	5	0
15	F	66	0	74	3	0
15	G	66	0	74	9	0
15	I	132	0	148	17	0
15	J	66	0	74	9	0
15	K	66	0	74	3	0
15	L	198	0	222	20	0
15	M	66	0	74	5	0
15	N	66	0	74	9	0
15	O	132	0	148	12	0
15	P	66	0	74	10	0
15	Q	66	0	74	5	0
15	R	66	0	74	6	0
15	S	132	0	148	21	0
15	T	66	0	74	9	0
15	U	66	0	74	3	0
15	V	66	0	74	9	0
15	W	132	0	148	14	0
15	X	66	0	74	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Y	132	0	148	12	0
15	Z	66	0	74	9	0
16	L	65	0	76	7	0
16	M	65	0	76	8	0
17	L	88	0	98	13	0
18	F	64	0	72	10	0
18	H	75	0	97	9	0
18	L	73	0	90	3	0
18	M	314	0	354	33	0
18	U	51	0	46	5	0
19	M	1	0	0	0	0
20	M	53	0	72	2	0
21	4	44	0	60	8	0
21	8	44	0	60	7	0
21	B	44	0	60	5	0
21	G	44	0	60	7	0
21	M	44	0	60	7	0
21	N	44	0	60	6	0
21	R	44	0	60	4	0
21	V	44	0	60	9	0
21	Z	44	0	60	8	0
22	C	3	0	0	0	0
22	M	2	0	0	0	0
All	All	27998	0	28404	756	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 13.

The worst 5 of 756 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	9:C:401:HEC:HAB	1.60	1.40
1:C:108:CYS:SG	9:C:401:HEC:CAB	2.14	1.36
21:N:102:CRT:H35	15:O:102:BCL:HMB2	1.57	0.86
3:M:287:THR:HB	3:M:294:TRP:HE1	1.42	0.83
5:7:32:LEU:HD11	15:8:103:BCL:HHD	1.63	0.81

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	331/362 (91%)	317 (96%)	14 (4%)	0	100	100
2	L	272/276 (99%)	261 (96%)	11 (4%)	0	100	100
3	M	316/323 (98%)	306 (97%)	10 (3%)	0	100	100
4	H	276/278 (99%)	274 (99%)	2 (1%)	0	100	100
5	3	44/64 (69%)	44 (100%)	0	0	100	100
5	7	44/64 (69%)	43 (98%)	1 (2%)	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%)	42 (93%)	3 (7%)	0	100	100
6	B	46/75 (61%)	43 (94%)	3 (6%)	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%)	44 (98%)	1 (2%)	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%)	44 (100%)	0	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
All	All	2605/3479 (75%)	2542 (98%)	63 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	285/306 (93%)	277 (97%)	8 (3%)	38	65
2	L	218/219 (100%)	215 (99%)	3 (1%)	62	82
3	M	252/255 (99%)	247 (98%)	5 (2%)	50	74
4	H	228/228 (100%)	217 (95%)	11 (5%)	21	44
5	3	39/55 (71%)	39 (100%)	0	100	100
5	7	39/55 (71%)	39 (100%)	0	100	100
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%)	38 (97%)	1 (3%)	41	67
5	Q	39/55 (71%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	U	39/55 (71%)	39 (100%)	0	100	100
5	Y	39/55 (71%)	39 (100%)	0	100	100
6	4	37/57 (65%)	36 (97%)	1 (3%)	40	66
6	8	37/57 (65%)	37 (100%)	0	100	100
6	B	38/57 (67%)	36 (95%)	2 (5%)	19	40
6	G	37/57 (65%)	37 (100%)	0	100	100
6	N	37/57 (65%)	36 (97%)	1 (3%)	40	66
6	R	37/57 (65%)	36 (97%)	1 (3%)	40	66
6	V	37/57 (65%)	36 (97%)	1 (3%)	40	66
6	Z	38/57 (67%)	37 (97%)	1 (3%)	41	67
7	1	41/55 (74%)	41 (100%)	0	100	100
7	5	41/55 (74%)	40 (98%)	1 (2%)	44	70
7	9	41/55 (74%)	40 (98%)	1 (2%)	44	70
7	D	41/55 (74%)	40 (98%)	1 (2%)	44	70
7	I	41/55 (74%)	40 (98%)	1 (2%)	44	70
7	O	41/55 (74%)	39 (95%)	2 (5%)	21	43
7	S	41/55 (74%)	39 (95%)	2 (5%)	21	43
7	W	41/55 (74%)	39 (95%)	2 (5%)	21	43
8	0	35/52 (67%)	33 (94%)	2 (6%)	17	37
8	2	35/52 (67%)	35 (100%)	0	100	100
8	6	35/52 (67%)	34 (97%)	1 (3%)	37	64
8	E	35/52 (67%)	34 (97%)	1 (3%)	37	64
8	J	35/52 (67%)	35 (100%)	0	100	100
8	P	35/52 (67%)	35 (100%)	0	100	100
8	T	35/52 (67%)	35 (100%)	0	100	100
8	X	35/52 (67%)	35 (100%)	0	100	100
All	All	2201/2760 (80%)	2152 (98%)	49 (2%)	47	72

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	17	GLU
7	O	42	GLN

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Mol	Chain	Res	Type
7	D	3	ARG
5	K	12	ARG
7	S	4	MET

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
7	O	42	GLN
8	6	9	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 132 ligands modelled in this entry, 2 are monoatomic - leaving 130 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	BCL	F	103	-	64,74,74	1.70	13 (20%)	78,115,115	2.25	19 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEC	C	401	1	32,50,50	1.58	4 (12%)	24,82,82	1.57	3 (12%)
14	PGV	L	305	-	42,42,50	0.99	2 (4%)	45,48,56	1.13	3 (6%)
13	LMT	C	408	-	36,36,36	0.38	0	47,47,47	0.88	2 (4%)
15	BCL	3	102	-	64,74,74	1.71	14 (21%)	78,115,115	2.24	19 (24%)
14	PGV	Z	105	-	42,42,50	0.99	2 (4%)	45,47,56	1.15	3 (6%)
15	BCL	I	103	-	64,74,74	1.75	14 (21%)	78,115,115	2.27	20 (25%)
15	BCL	8	103	-	64,74,74	1.69	14 (21%)	78,115,115	2.20	22 (28%)
16	BPH	L	303	-	51,70,70	0.48	0	52,101,101	0.80	2 (3%)
21	CRT	V	102	-	41,43,43	0.77	0	50,54,54	3.68	18 (36%)
15	BCL	J	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.20	20 (25%)
15	BCL	D	102	-	64,74,74	1.74	14 (21%)	78,115,115	2.14	21 (26%)
14	PGV	1	101	-	44,44,50	0.98	2 (4%)	47,50,56	1.05	3 (6%)
14	PGV	3	101	-	29,29,50	1.18	2 (6%)	32,34,56	1.17	2 (6%)
21	CRT	B	101	-	41,43,43	0.75	0	50,54,54	3.46	17 (34%)
14	PGV	R	103	-	28,28,50	1.31	2 (7%)	31,34,56	1.41	4 (12%)
15	BCL	X	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.21	20 (25%)
21	CRT	N	102	-	41,43,43	0.72	0	50,54,54	3.57	13 (26%)
15	BCL	M	403	-	64,74,74	1.71	14 (21%)	78,115,115	2.37	19 (24%)
14	PGV	H	304	-	50,50,50	0.91	2 (4%)	53,56,56	1.04	3 (5%)
15	BCL	O	103	-	64,74,74	1.75	14 (21%)	78,115,115	2.18	19 (24%)
14	PGV	6	102	-	37,37,50	1.10	2 (5%)	41,42,56	1.18	4 (9%)
21	CRT	R	101	-	41,43,43	0.73	0	50,54,54	3.59	18 (36%)
18	CDL	M	408	-	45,45,99	1.41	4 (8%)	51,57,111	1.38	6 (11%)
14	PGV	0	103	-	30,30,50	1.16	2 (6%)	33,36,56	1.11	3 (9%)
14	PGV	J	102	-	28,28,50	1.21	2 (7%)	29,30,56	1.23	2 (6%)
14	PGV	8	101	-	42,43,50	0.99	2 (4%)	45,49,56	1.02	3 (6%)
13	LMT	9	101	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
14	PGV	V	105	-	43,43,50	0.98	2 (4%)	45,49,56	1.00	2 (4%)
15	BCL	1	102	-	64,74,74	1.72	14 (21%)	78,115,115	2.30	23 (29%)
18	CDL	U	101	-	50,50,99	1.29	4 (8%)	56,62,111	1.28	6 (10%)
18	CDL	M	402	-	81,81,99	1.04	4 (4%)	87,93,111	1.01	4 (4%)
15	BCL	V	103	-	64,74,74	1.69	14 (21%)	78,115,115	2.16	19 (24%)
14	PGV	0	101	-	33,33,50	1.10	2 (6%)	36,39,56	1.16	4 (11%)
15	BCL	I	102	-	64,74,74	1.70	14 (21%)	78,115,115	2.30	20 (25%)
9	HEC	C	403	1	32,50,50	1.57	4 (12%)	24,82,82	1.62	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCL	2	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.19	22 (28%)
21	CRT	M	406	-	41,43,43	0.72	0	50,54,54	1.78	12 (24%)
15	BCL	P	101	-	64,74,74	1.68	14 (21%)	78,115,115	2.24	20 (25%)
13	LMT	K	101	-	26,26,36	0.50	0	37,37,47	1.04	1 (2%)
14	PGV	Z	101	-	28,28,50	1.56	3 (10%)	29,33,56	1.23	2 (6%)
15	BCL	Z	103	-	64,74,74	1.69	13 (20%)	78,115,115	2.17	22 (28%)
13	LMT	7	101	-	26,26,36	0.51	0	37,37,47	0.94	1 (2%)
21	CRT	8	102	-	41,43,43	0.75	0	50,54,54	3.53	16 (32%)
13	LMT	H	306	-	27,27,36	0.44	0	37,38,47	0.65	1 (2%)
13	LMT	7	102	-	36,36,36	0.39	0	47,47,47	0.69	0
15	BCL	B	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.20	20 (25%)
14	PGV	P	103	-	39,39,50	1.05	2 (5%)	43,44,56	1.13	4 (9%)
14	PGV	L	309	-	40,40,50	1.02	2 (5%)	42,46,56	1.12	3 (7%)
14	PGV	H	303	-	41,41,50	0.99	2 (4%)	44,47,56	1.04	3 (6%)
15	BCL	5	102	-	64,74,74	1.69	15 (23%)	78,115,115	2.24	25 (32%)
15	BCL	D	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.33	20 (25%)
15	BCL	W	101	-	64,74,74	1.71	14 (21%)	78,115,115	2.26	21 (26%)
17	UQ8	L	306	-	38,38,53	1.38	2 (5%)	46,49,67	1.68	10 (21%)
15	BCL	T	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.21	19 (24%)
15	BCL	5	103	-	64,74,74	1.71	14 (21%)	78,115,115	2.20	23 (29%)
17	UQ8	L	307	-	17,17,53	2.11	2 (11%)	19,23,67	1.01	1 (5%)
14	PGV	V	101	-	28,28,50	1.52	3 (10%)	29,33,56	1.22	2 (6%)
14	PGV	Z	104	-	31,31,50	1.42	3 (9%)	32,36,56	1.19	2 (6%)
18	CDL	F	101	-	63,63,99	1.07	4 (6%)	69,75,111	1.20	4 (5%)
14	PGV	2	102	-	25,25,50	1.64	3 (12%)	27,29,56	1.52	3 (11%)
16	BPH	M	404	-	51,70,70	0.48	0	52,101,101	0.63	0
21	CRT	4	101	-	41,43,43	0.73	0	50,54,54	3.56	15 (30%)
15	BCL	A	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.23	18 (23%)
15	BCL	W	102	-	64,74,74	1.73	14 (21%)	78,115,115	2.24	21 (26%)
15	BCL	6	101	-	64,74,74	1.71	13 (20%)	78,115,115	2.20	21 (26%)
15	BCL	N	103	-	64,74,74	1.71	14 (21%)	78,115,115	2.16	19 (24%)
14	PGV	N	104	-	30,30,50	1.25	2 (6%)	33,36,56	1.30	4 (12%)
15	BCL	R	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.23	19 (24%)
11	Z41	C	406	1	30,30,39	0.29	0	32,32,41	0.35	0
15	BCL	Q	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.28	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PGV	E	102	-	34,34,50	1.08	2 (5%)	37,40,56	1.14	4 (10%)
14	PGV	2	103	-	33,33,50	1.15	2 (6%)	37,38,56	1.27	4 (10%)
15	BCL	S	101	-	64,74,74	1.72	14 (21%)	78,115,115	2.28	24 (30%)
13	LMT	Q	101	-	33,33,36	0.43	0	44,44,47	0.94	1 (2%)
14	PGV	B	104	-	40,40,50	1.02	2 (5%)	42,45,56	1.14	3 (7%)
15	BCL	0	102	-	64,74,74	1.70	14 (21%)	78,115,115	2.23	20 (25%)
15	BCL	U	102	-	64,74,74	1.71	13 (20%)	78,115,115	2.29	21 (26%)
18	CDL	M	407	-	79,79,99	1.01	4 (5%)	85,91,111	1.05	6 (7%)
18	CDL	H	302	-	74,74,99	1.06	4 (5%)	80,86,111	1.10	6 (7%)
14	PGV	4	104	-	40,40,50	1.07	2 (5%)	44,45,56	1.13	3 (6%)
15	BCL	S	102	-	64,74,74	1.73	14 (21%)	78,115,115	2.22	23 (29%)
14	PGV	V	104	-	30,30,50	1.25	2 (6%)	33,36,56	1.33	3 (9%)
15	BCL	9	102	-	64,74,74	1.75	14 (21%)	78,115,115	2.24	20 (25%)
14	PGV	H	301	-	35,35,50	1.09	2 (5%)	38,41,56	1.25	3 (7%)
14	PGV	B	103	-	30,30,50	1.25	2 (6%)	33,36,56	1.39	3 (9%)
14	PGV	N	101	-	34,34,50	1.09	2 (5%)	37,40,56	1.03	2 (5%)
14	PGV	8	104	-	42,42,50	1.01	2 (4%)	45,48,56	1.10	3 (6%)
15	BCL	1	103	-	64,74,74	1.74	14 (21%)	78,115,115	2.22	22 (28%)
14	PGV	G	104	-	41,41,50	1.02	2 (4%)	44,46,56	1.11	4 (9%)
13	LMT	O	101	-	30,30,36	0.44	0	41,41,47	0.90	2 (4%)
14	PGV	G	103	-	34,34,50	1.10	2 (5%)	37,40,56	1.11	3 (8%)
14	PGV	L	308	-	35,35,50	1.08	2 (5%)	38,40,56	1.10	2 (5%)
15	BCL	Y	401	18	64,74,74	1.66	13 (20%)	78,115,115	2.24	21 (26%)
12	PLM	C	407	-	11,11,17	0.40	0	10,10,17	0.45	0
13	LMT	F	102	-	34,34,36	0.49	0	45,45,47	1.14	3 (6%)
15	BCL	L	310	-	64,74,74	1.70	13 (20%)	78,115,115	2.23	21 (26%)
15	BCL	G	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.23	19 (24%)
14	PGV	N	105	-	31,31,50	1.19	2 (6%)	34,36,56	1.26	4 (11%)
15	BCL	O	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.28	19 (24%)
15	BCL	4	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.22	18 (23%)
21	CRT	Z	102	-	41,43,43	0.72	0	50,54,54	3.49	16 (32%)
21	CRT	G	101	-	41,43,43	0.76	0	50,54,54	3.54	16 (32%)
18	CDL	L	312	-	72,72,99	1.08	4 (5%)	78,84,111	1.12	5 (6%)
14	PGV	R	104	-	40,40,50	1.04	2 (5%)	43,45,56	1.16	4 (9%)
20	MQ8	M	405	-	54,54,54	1.31	2 (3%)	66,69,69	1.56	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PGV	T	102	-	46,46,50	0.96	2 (4%)	48,52,56	1.06	3 (6%)
13	LMT	Y	402	-	36,36,36	0.41	0	47,47,47	0.90	1 (2%)
15	BCL	L	311	-	64,74,74	1.71	13 (20%)	78,115,115	2.24	22 (28%)
15	BCL	Y	403	-	64,74,74	1.70	14 (21%)	78,115,115	2.25	18 (23%)
18	CDL	M	410	15	49,49,99	1.30	4 (8%)	55,61,111	1.20	5 (9%)
14	PGV	0	104	-	31,31,50	1.12	2 (6%)	32,33,56	1.17	3 (9%)
14	PGV	4	103	-	28,28,50	1.52	3 (10%)	29,33,56	1.28	2 (6%)
15	BCL	L	302	-	64,74,74	1.69	14 (21%)	78,115,115	2.30	22 (28%)
15	BCL	9	103	-	64,74,74	1.74	14 (21%)	78,115,115	2.19	22 (28%)
13	LMT	5	101	-	25,25,36	0.47	0	36,36,47	0.76	1 (2%)
14	PGV	P	102	-	27,27,50	1.35	2 (7%)	31,32,56	1.51	4 (12%)
17	UQ8	L	304	-	33,33,53	1.50	2 (6%)	40,43,67	1.51	8 (20%)
15	BCL	7	103	-	64,74,74	1.69	12 (18%)	78,115,115	2.30	22 (28%)
9	HEC	C	402	1	32,50,50	1.57	4 (12%)	24,82,82	1.37	1 (4%)
13	LMT	L	301	-	26,26,36	0.45	0	37,37,47	0.80	1 (2%)
18	CDL	M	409	-	55,55,99	1.23	4 (7%)	61,67,111	1.27	6 (9%)
9	HEC	C	404	1	32,50,50	1.54	4 (12%)	24,82,82	1.35	2 (8%)
15	BCL	E	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.19	20 (25%)
14	PGV	I	101	-	49,49,50	0.93	2 (4%)	52,55,56	1.03	4 (7%)
14	PGV	E	103	-	37,37,50	1.05	2 (5%)	39,43,56	1.17	3 (7%)
14	PGV	X	102	-	44,44,50	0.99	2 (4%)	47,50,56	1.09	3 (6%)
15	BCL	K	102	-	64,74,74	1.70	14 (21%)	78,115,115	2.28	19 (24%)
13	LMT	H	305	-	31,31,36	0.44	0	42,42,47	0.97	1 (2%)
14	PGV	C	409	-	31,31,50	1.15	2 (6%)	34,37,56	1.18	3 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCL	F	103	-	-	18/37/137/137	-
9	HEC	C	401	1	-	4/10/54/54	-
14	PGV	L	305	-	-	16/47/47/55	-
13	LMT	C	408	-	-	9/21/61/61	0/2/2/2
15	BCL	3	102	-	-	12/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	PGV	Z	105	-	-	21/46/46/55	-
15	BCL	I	103	-	-	15/37/137/137	-
15	BCL	8	103	-	-	11/37/137/137	-
16	BPH	L	303	-	-	5/37/105/105	0/5/6/6
21	CRT	V	102	-	-	4/51/51/51	-
15	BCL	J	101	-	-	16/37/137/137	-
15	BCL	D	102	-	-	13/37/137/137	-
14	PGV	1	101	-	-	13/49/49/55	-
14	PGV	3	101	-	-	15/33/33/55	-
21	CRT	B	101	-	-	8/51/51/51	-
14	PGV	R	103	-	-	8/32/32/55	-
15	BCL	X	101	-	-	8/37/137/137	-
21	CRT	N	102	-	-	6/51/51/51	-
15	BCL	M	403	-	-	8/37/137/137	-
14	PGV	H	304	-	-	18/55/55/55	-
15	BCL	O	103	-	-	16/37/137/137	-
14	PGV	6	102	-	-	7/39/39/55	-
21	CRT	R	101	-	-	6/51/51/51	-
18	CDL	M	408	-	-	20/55/55/110	-
14	PGV	0	103	-	-	7/35/35/55	-
14	PGV	J	102	-	-	13/30/30/55	-
14	PGV	8	101	-	-	14/47/47/55	-
13	LMT	9	101	-	-	3/21/61/61	0/2/2/2
14	PGV	V	105	-	-	17/48/48/55	-
15	BCL	1	102	-	-	14/37/137/137	-
18	CDL	U	101	-	-	23/61/61/110	-
18	CDL	M	402	-	-	31/92/92/110	-
15	BCL	V	103	-	-	14/37/137/137	-
14	PGV	0	101	-	-	16/38/38/55	-
15	BCL	I	102	-	-	15/37/137/137	-
9	HEC	C	403	1	-	3/10/54/54	-
15	BCL	2	101	-	-	9/37/137/137	-
21	CRT	M	406	-	-	14/51/51/51	-
15	BCL	P	101	-	-	12/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	K	101	-	-	5/11/51/61	0/2/2/2
14	PGV	Z	101	-	-	9/32/32/55	-
15	BCL	Z	103	-	-	18/37/137/137	-
13	LMT	7	101	-	-	5/11/51/61	0/2/2/2
21	CRT	8	102	-	-	5/51/51/51	-
13	LMT	H	306	-	-	3/12/52/61	0/2/2/2
13	LMT	7	102	-	-	2/21/61/61	0/2/2/2
15	BCL	B	102	-	-	8/37/137/137	-
14	PGV	P	103	-	-	15/41/41/55	-
14	PGV	L	309	-	-	17/45/45/55	-
14	PGV	H	303	-	-	13/46/46/55	-
15	BCL	5	102	-	-	16/37/137/137	-
15	BCL	D	101	-	-	20/37/137/137	-
15	BCL	W	101	-	-	15/37/137/137	-
17	UQ8	L	306	-	-	2/33/57/75	0/1/1/1
15	BCL	T	101	-	-	15/37/137/137	-
15	BCL	5	103	-	-	16/37/137/137	-
17	UQ8	L	307	-	-	1/8/32/75	0/1/1/1
14	PGV	V	101	-	-	12/32/32/55	-
14	PGV	Z	104	-	-	13/35/35/55	-
18	CDL	F	101	-	-	23/73/73/110	-
14	PGV	2	102	-	-	9/26/26/55	-
16	BPH	M	404	-	-	6/37/105/105	0/5/6/6
21	CRT	4	101	-	-	5/51/51/51	-
15	BCL	A	101	-	-	21/37/137/137	-
15	BCL	W	102	-	-	14/37/137/137	-
15	BCL	6	101	-	-	5/37/137/137	-
15	BCL	N	103	-	-	14/37/137/137	-
14	PGV	N	104	-	-	18/34/34/55	-
15	BCL	R	102	-	-	15/37/137/137	-
11	Z41	C	406	1	-	12/31/31/41	-
15	BCL	Q	102	-	-	16/37/137/137	-
14	PGV	E	102	-	-	16/39/39/55	-
14	PGV	2	103	-	-	11/35/35/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCL	S	101	-	-	12/37/137/137	-
13	LMT	Q	101	-	-	7/18/58/61	0/2/2/2
14	PGV	B	104	-	-	8/44/44/55	-
15	BCL	O	102	-	-	9/37/137/137	-
15	BCL	U	102	-	-	21/37/137/137	-
18	CDL	M	407	-	-	33/90/90/110	-
18	CDL	H	302	-	-	37/85/85/110	-
14	PGV	4	104	-	-	19/42/42/55	-
15	BCL	S	102	-	-	17/37/137/137	-
14	PGV	V	104	-	-	6/34/34/55	-
15	BCL	9	102	-	-	14/37/137/137	-
14	PGV	H	301	-	-	11/40/40/55	-
14	PGV	B	103	-	-	14/34/34/55	-
14	PGV	N	101	-	-	16/39/39/55	-
14	PGV	8	104	-	-	17/47/47/55	-
15	BCL	1	103	-	-	14/37/137/137	-
14	PGV	G	104	-	-	14/45/45/55	-
13	LMT	O	101	-	-	4/15/55/61	0/2/2/2
14	PGV	G	103	-	-	14/39/39/55	-
14	PGV	L	308	-	-	8/39/39/55	-
15	BCL	Y	401	18	-	12/37/137/137	-
12	PLM	C	407	-	-	0/8/9/15	-
13	LMT	F	102	-	-	8/19/59/61	0/2/2/2
15	BCL	L	310	-	-	16/37/137/137	-
15	BCL	G	102	-	-	16/37/137/137	-
14	PGV	N	105	-	-	9/33/33/55	-
15	BCL	O	102	-	-	9/37/137/137	-
15	BCL	4	102	-	-	13/37/137/137	-
21	CRT	Z	102	-	-	1/51/51/51	-
21	CRT	G	101	-	-	4/51/51/51	-
18	CDL	L	312	-	-	21/83/83/110	-
14	PGV	R	104	-	-	11/42/42/55	-
20	MQ8	M	405	-	-	5/47/67/67	0/2/2/2
14	PGV	T	102	-	-	12/51/51/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	Y	402	-	-	8/21/61/61	0/2/2/2
15	BCL	L	311	-	-	19/37/137/137	-
15	BCL	Y	403	-	-	17/37/137/137	-
18	CDL	M	410	15	-	16/60/60/110	-
14	PGV	0	104	-	-	9/33/33/55	-
14	PGV	4	103	-	-	9/32/32/55	-
15	BCL	L	302	-	-	10/37/137/137	-
15	BCL	9	103	-	-	14/37/137/137	-
13	LMT	5	101	-	-	2/10/50/61	0/2/2/2
14	PGV	P	102	-	-	10/28/28/55	-
17	UQ8	L	304	-	-	6/27/51/75	0/1/1/1
15	BCL	7	103	-	-	14/37/137/137	-
9	HEC	C	402	1	-	2/10/54/54	-
13	LMT	L	301	-	-	5/11/51/61	0/2/2/2
18	CDL	M	409	-	-	21/66/66/110	-
9	HEC	C	404	1	-	2/10/54/54	-
15	BCL	E	101	-	-	13/37/137/137	-
14	PGV	I	101	-	-	11/54/54/55	-
14	PGV	E	103	-	-	8/42/42/55	-
14	PGV	X	102	-	-	15/49/49/55	-
15	BCL	K	102	-	-	18/37/137/137	-
13	LMT	H	305	-	-	4/16/56/61	0/2/2/2
14	PGV	C	409	-	-	11/36/36/55	-

The worst 5 of 762 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	405	MQ8	C3-C2	7.86	1.49	1.35
17	L	307	UQ8	C6-C1	7.78	1.49	1.35
17	L	304	UQ8	C6-C1	7.63	1.49	1.35
17	L	306	UQ8	C6-C1	7.42	1.48	1.35
14	Z	101	PGV	O01-C1	5.80	1.46	1.33

The worst 5 of 1304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	R	101	CRT	C2-C1-C4	-16.40	85.68	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Z	102	CRT	C2-C1-C4	-16.40	85.69	110.86
21	N	102	CRT	C2-C1-C4	-16.23	85.94	110.86
21	4	101	CRT	C2-C1-C4	-16.22	85.95	110.86
21	V	102	CRT	C2-C1-C4	-15.88	86.48	110.86

There are no chirality outliers.

5 of 1553 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	406	Z41	C15-C16-O2-C17
11	C	406	Z41	O1-C16-O2-C17
11	C	406	Z41	O2-C17-C18-O3
13	C	408	LMT	C2-C1-O1'-C1'
13	H	305	LMT	O5B-C1B-O1B-C4'

There are no ring outliers.

123 monomers are involved in 563 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	103	BCL	3	0
9	C	401	HEC	5	0
14	L	305	PGV	4	0
13	C	408	LMT	3	0
15	3	102	BCL	8	0
14	Z	105	PGV	3	0
15	I	103	BCL	10	0
15	8	103	BCL	8	0
16	L	303	BPH	7	0
21	V	102	CRT	9	0
15	J	101	BCL	9	0
15	D	102	BCL	8	0
14	1	101	PGV	4	0
14	3	101	PGV	4	0
21	B	101	CRT	5	0
15	X	101	BCL	4	0
21	N	102	CRT	6	0
15	M	403	BCL	5	0
14	H	304	PGV	9	0
15	O	103	BCL	6	0
14	6	102	PGV	3	0
21	R	101	CRT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	M	408	CDL	3	0
14	J	102	PGV	3	0
14	8	101	PGV	4	0
13	9	101	LMT	2	0
14	V	105	PGV	1	0
15	1	102	BCL	11	0
18	U	101	CDL	5	0
18	M	402	CDL	11	0
15	V	103	BCL	9	0
14	0	101	PGV	1	0
15	I	102	BCL	8	0
9	C	403	HEC	3	0
15	2	101	BCL	9	0
21	M	406	CRT	7	0
15	P	101	BCL	10	0
13	K	101	LMT	2	0
15	Z	103	BCL	9	0
13	7	101	LMT	4	0
21	8	102	CRT	7	0
13	7	102	LMT	3	0
15	B	102	BCL	3	0
14	P	103	PGV	5	0
14	L	309	PGV	5	0
14	H	303	PGV	8	0
15	5	102	BCL	8	0
15	D	101	BCL	10	0
15	W	101	BCL	9	0
17	L	306	UQ8	6	0
15	T	101	BCL	9	0
15	5	103	BCL	6	0
17	L	307	UQ8	1	0
14	V	101	PGV	4	0
14	Z	104	PGV	4	0
18	F	101	CDL	10	0
14	2	102	PGV	2	0
16	M	404	BPH	8	0
21	4	101	CRT	8	0
15	A	101	BCL	5	0
15	W	102	BCL	5	0
15	6	101	BCL	7	0
15	N	103	BCL	9	0
14	N	104	PGV	2	0

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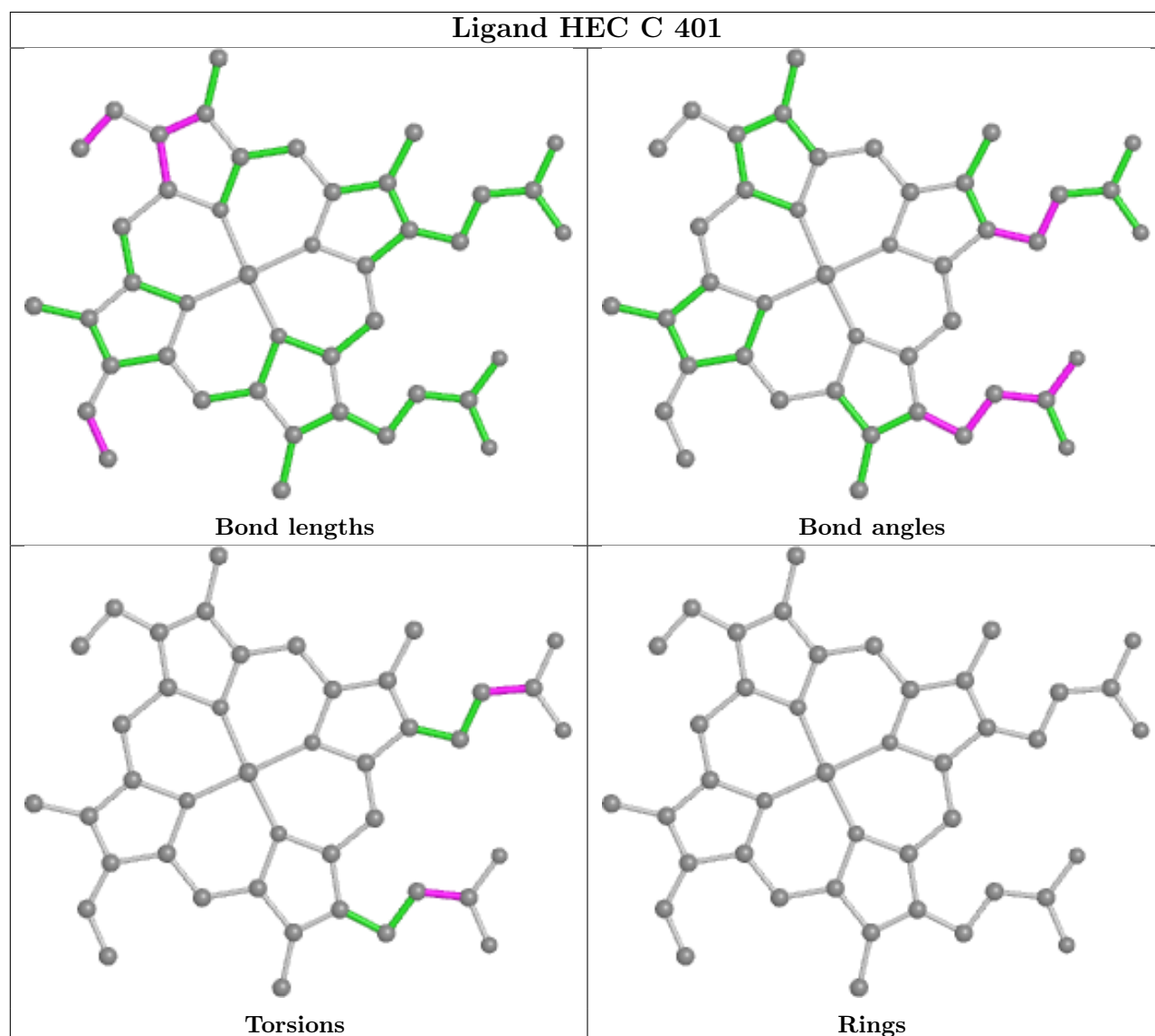
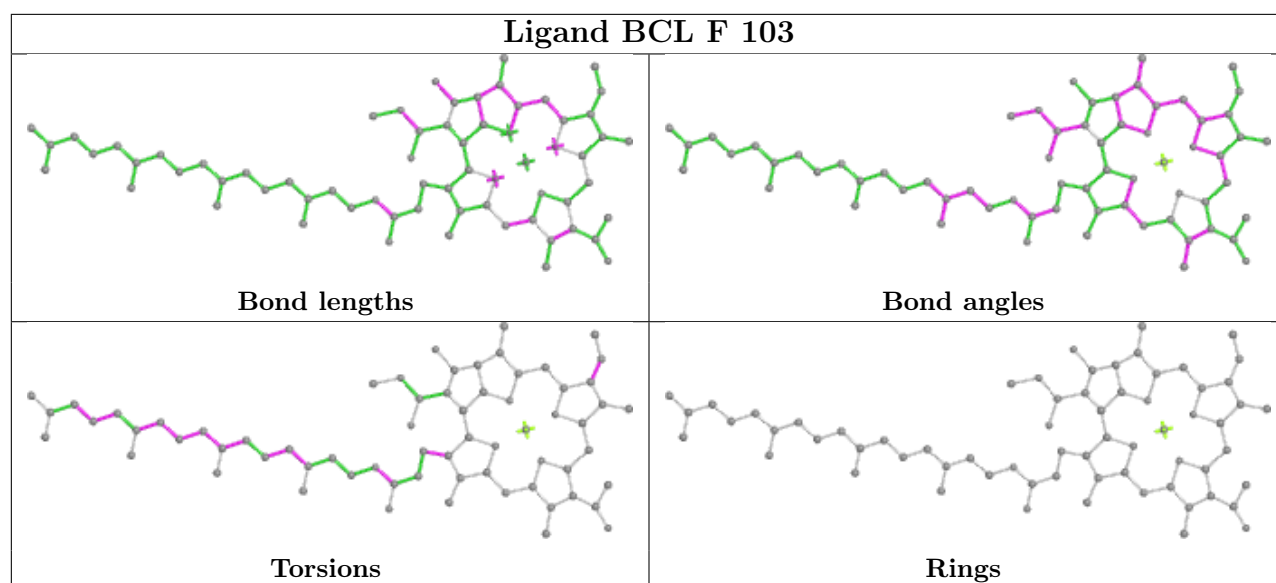
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	R	102	BCL	6	0
11	C	406	Z41	1	0
15	Q	102	BCL	5	0
14	E	102	PGV	1	0
14	2	103	PGV	1	0
15	S	101	BCL	12	0
13	Q	101	LMT	3	0
14	B	104	PGV	2	0
15	0	102	BCL	9	0
15	U	102	BCL	3	0
18	M	407	CDL	10	0
18	H	302	CDL	9	0
14	4	104	PGV	5	0
15	S	102	BCL	10	0
14	V	104	PGV	1	0
15	9	102	BCL	10	0
14	H	301	PGV	3	0
14	B	103	PGV	1	0
14	N	101	PGV	5	0
14	8	104	PGV	5	0
15	1	103	BCL	7	0
14	G	104	PGV	2	0
13	O	101	LMT	2	0
14	G	103	PGV	8	0
14	L	308	PGV	4	0
15	Y	401	BCL	8	0
12	C	407	PLM	5	0
13	F	102	LMT	4	0
15	L	310	BCL	7	0
15	G	102	BCL	9	0
14	N	105	PGV	1	0
15	O	102	BCL	6	0
15	4	102	BCL	9	0
21	Z	102	CRT	8	0
21	G	101	CRT	7	0
18	L	312	CDL	3	0
14	R	104	PGV	2	0
20	M	405	MQ8	2	0
14	T	102	PGV	3	0
13	Y	402	LMT	1	0
15	L	311	BCL	9	0
15	Y	403	BCL	4	0

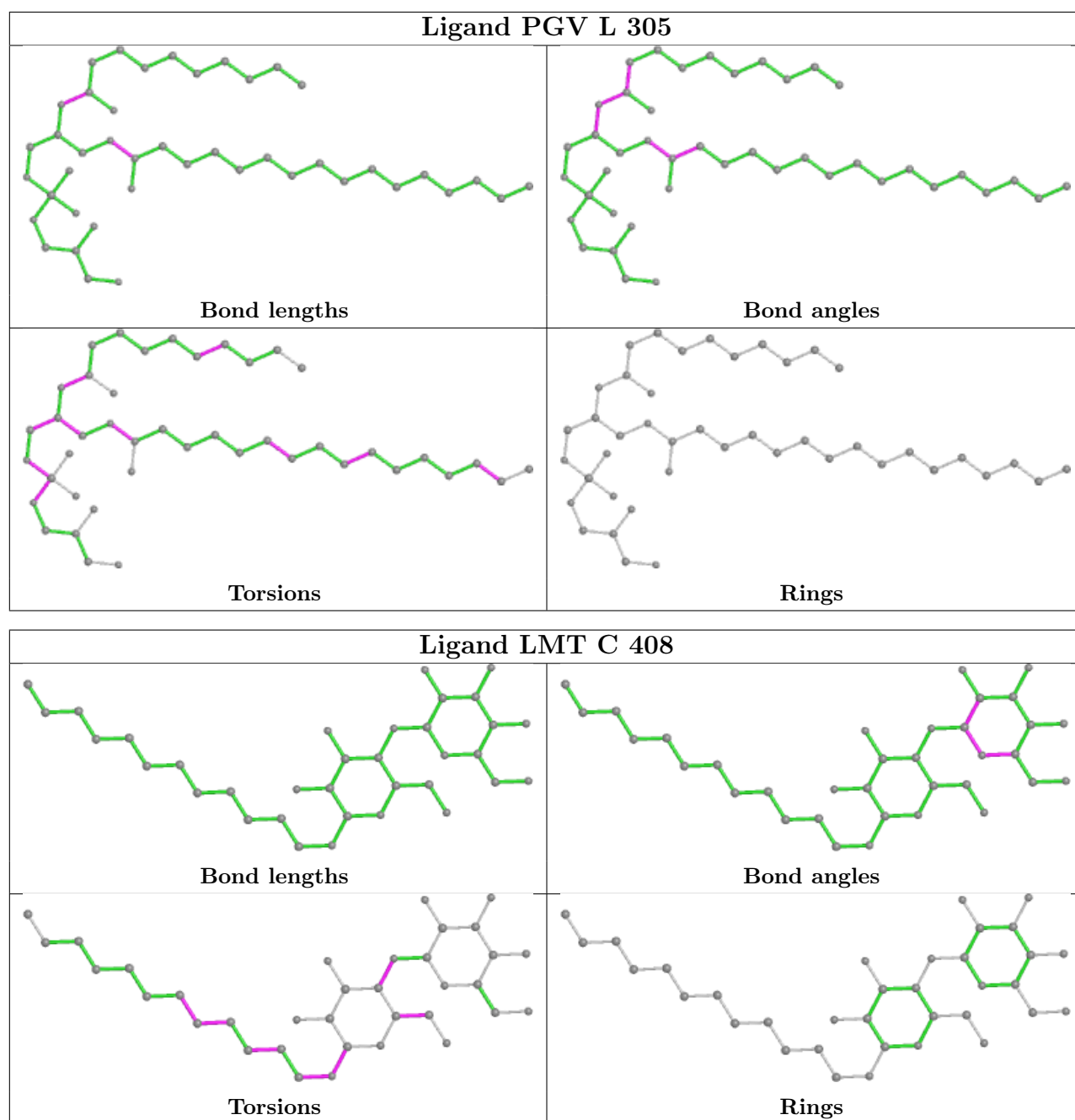
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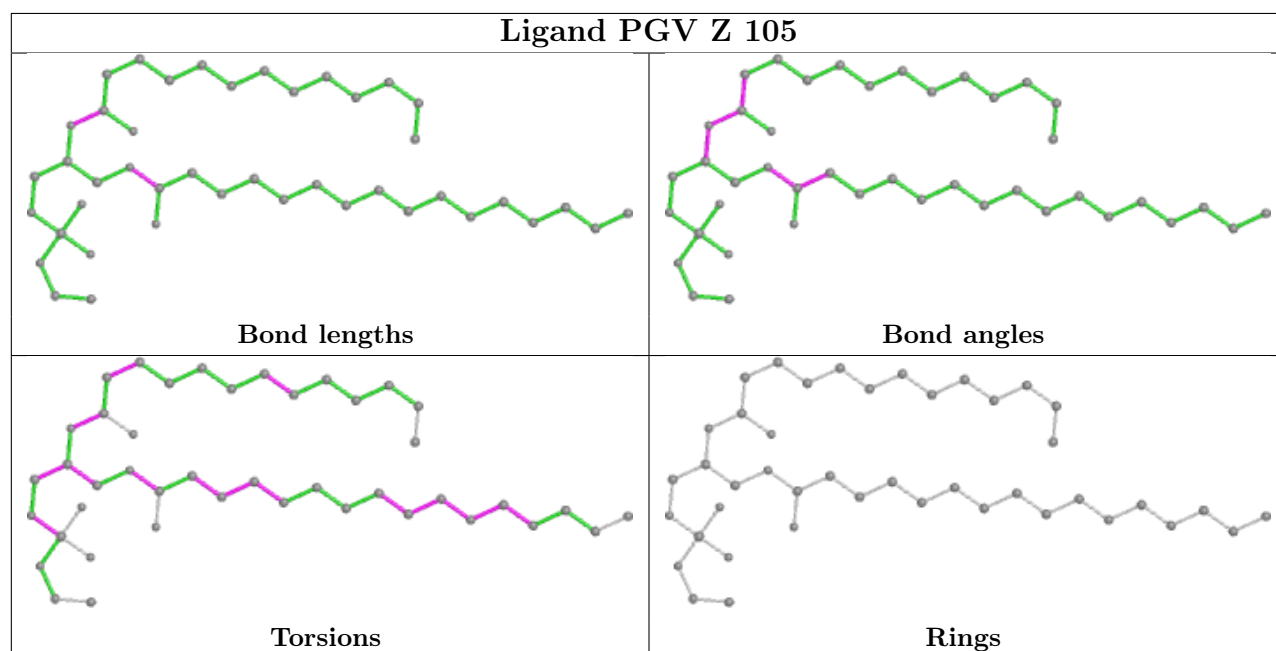
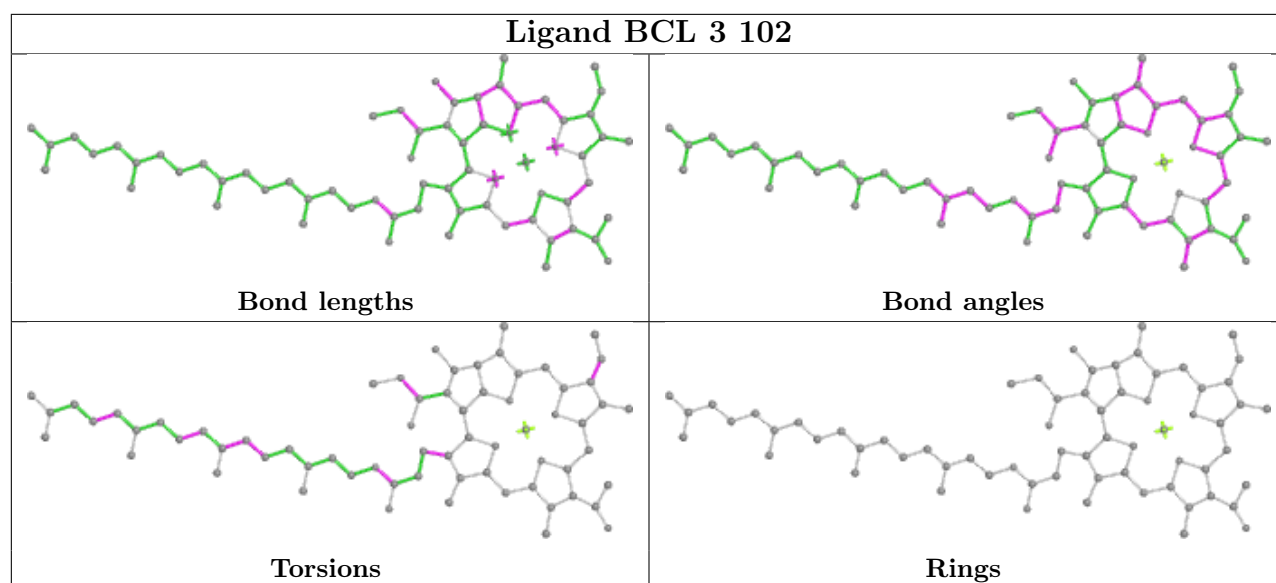
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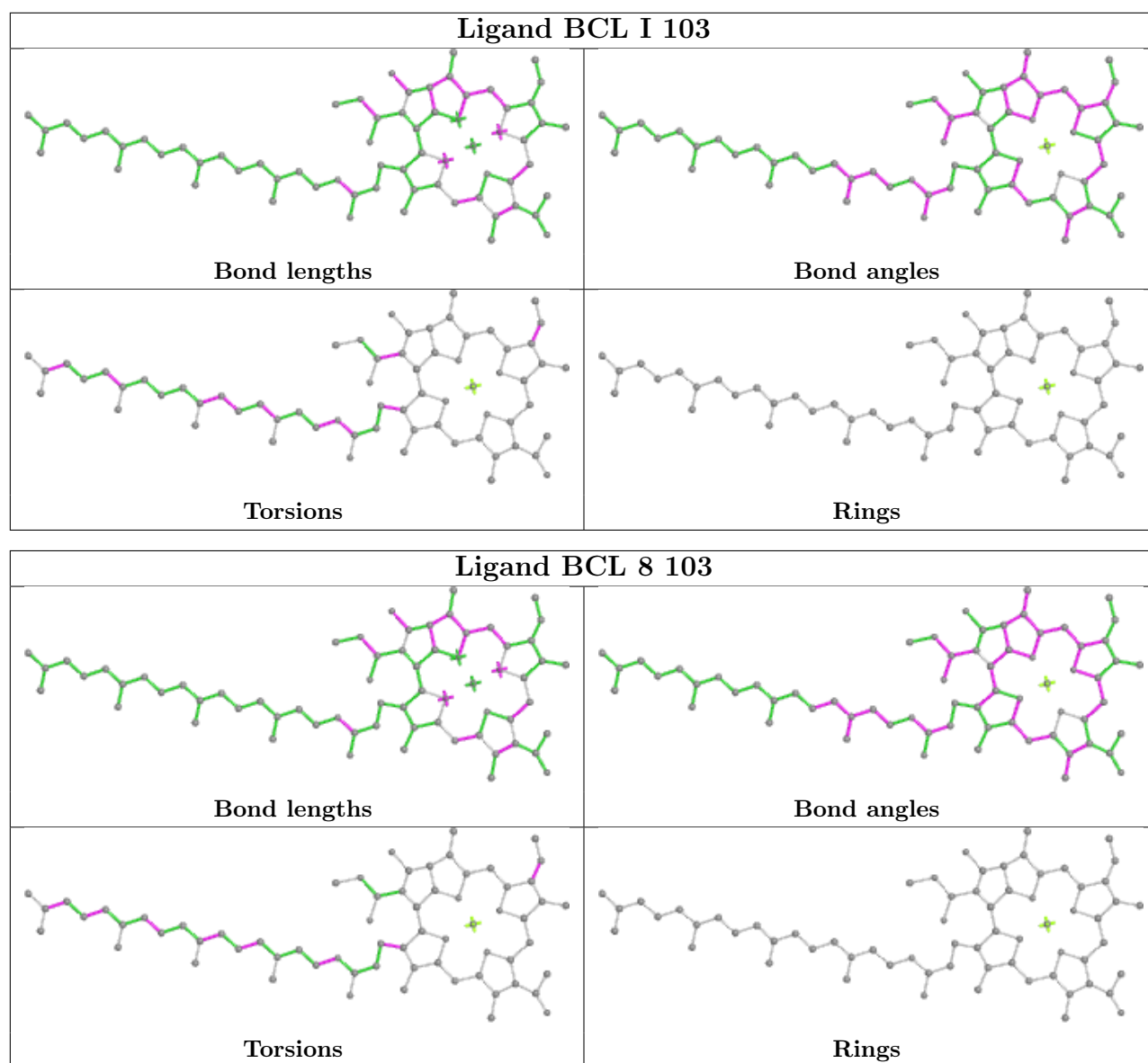
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18	M	410	CDL	5	0
14	0	104	PGV	2	0
14	4	103	PGV	5	0
15	L	302	BCL	4	0
15	9	103	BCL	7	0
13	5	101	LMT	1	0
14	P	102	PGV	4	0
17	L	304	UQ8	6	0
15	7	103	BCL	3	0
13	L	301	LMT	2	0
18	M	409	CDL	5	0
15	E	101	BCL	5	0
14	I	101	PGV	6	0
14	X	102	PGV	2	0
15	K	102	BCL	3	0
13	H	305	LMT	3	0
14	C	409	PGV	5	0

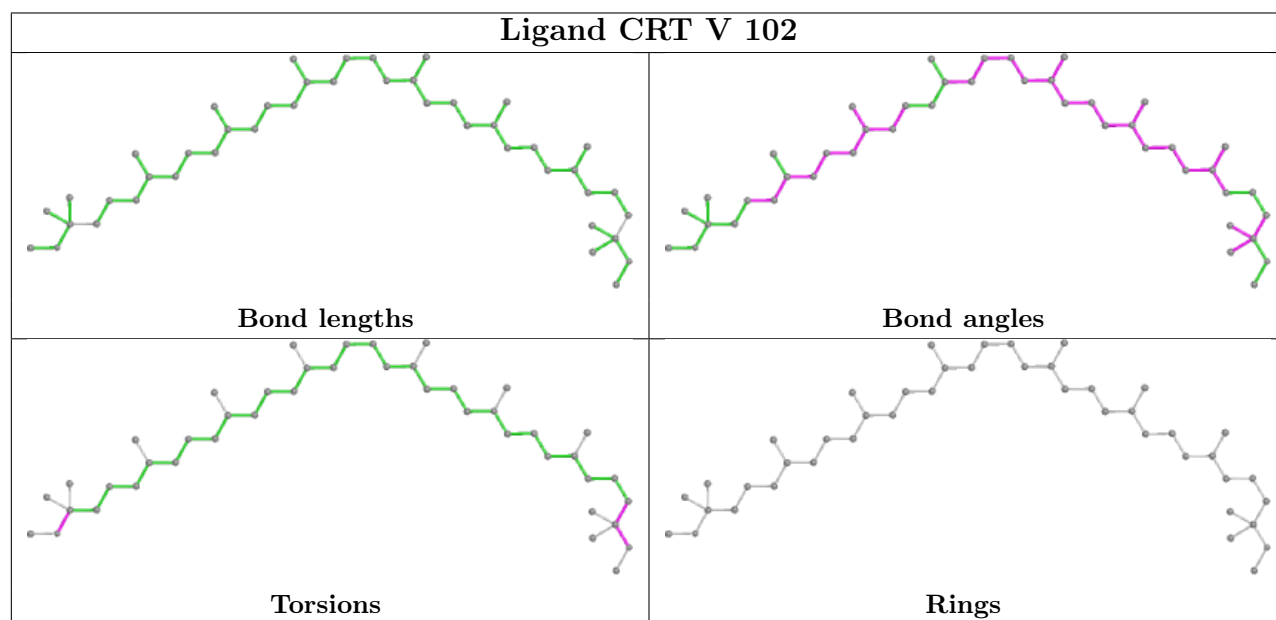
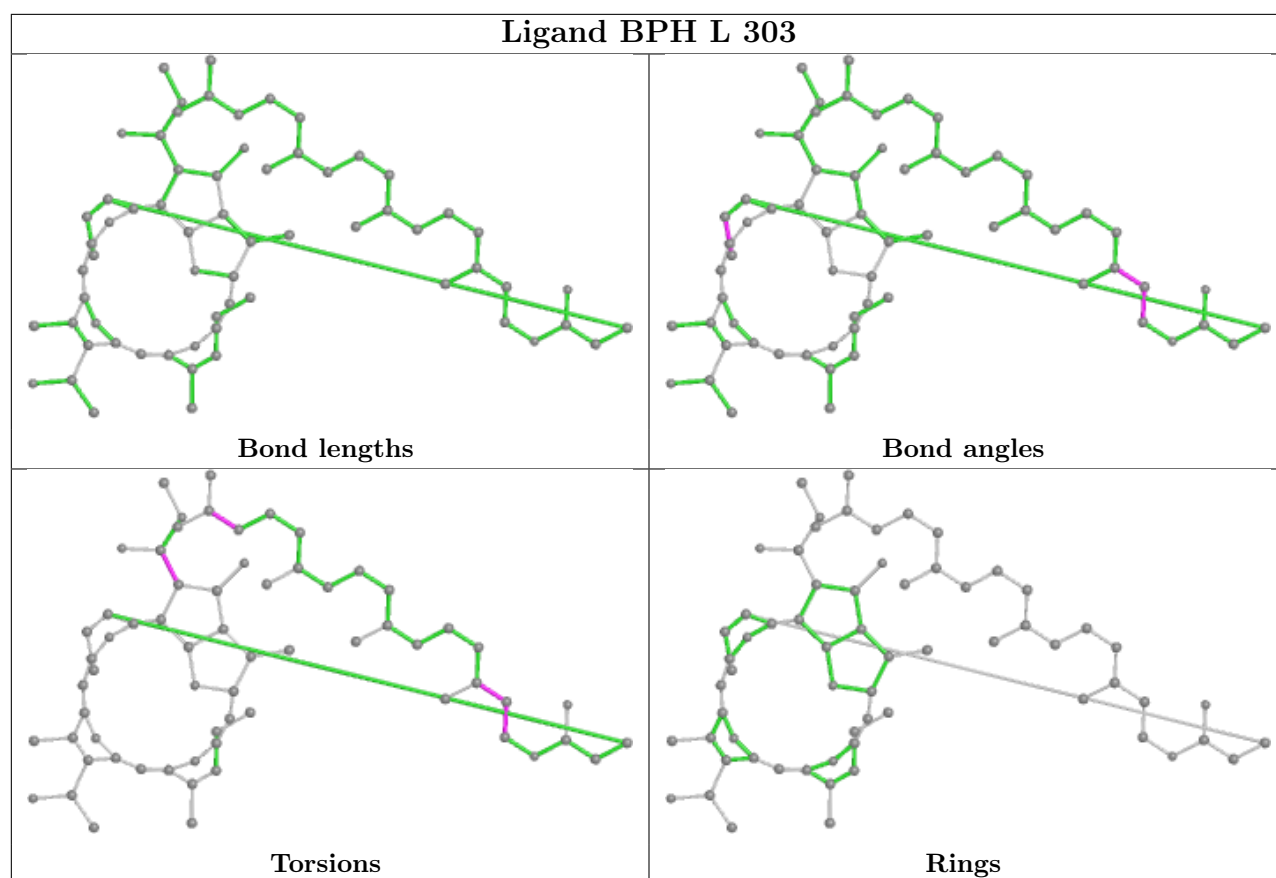
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

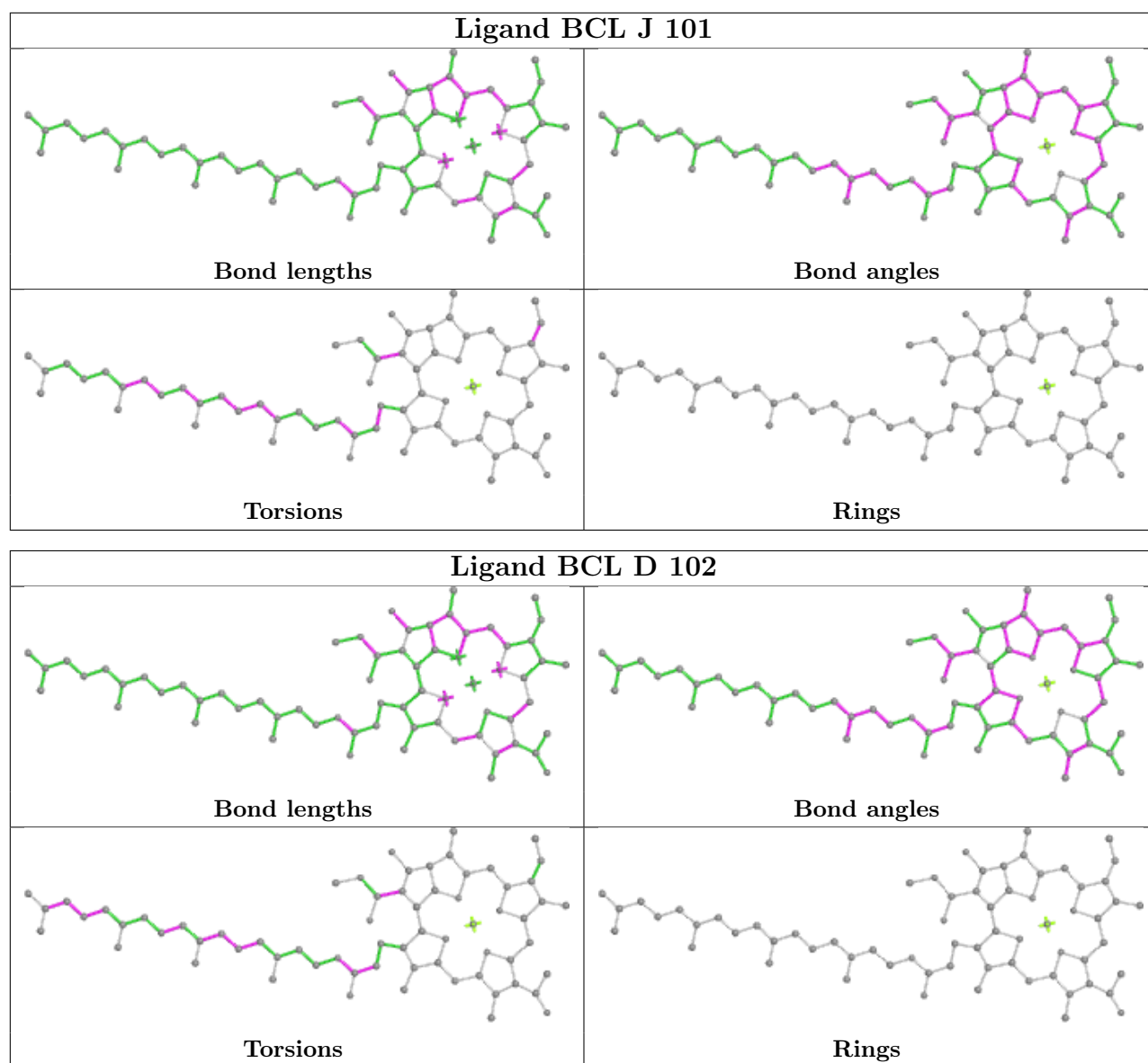


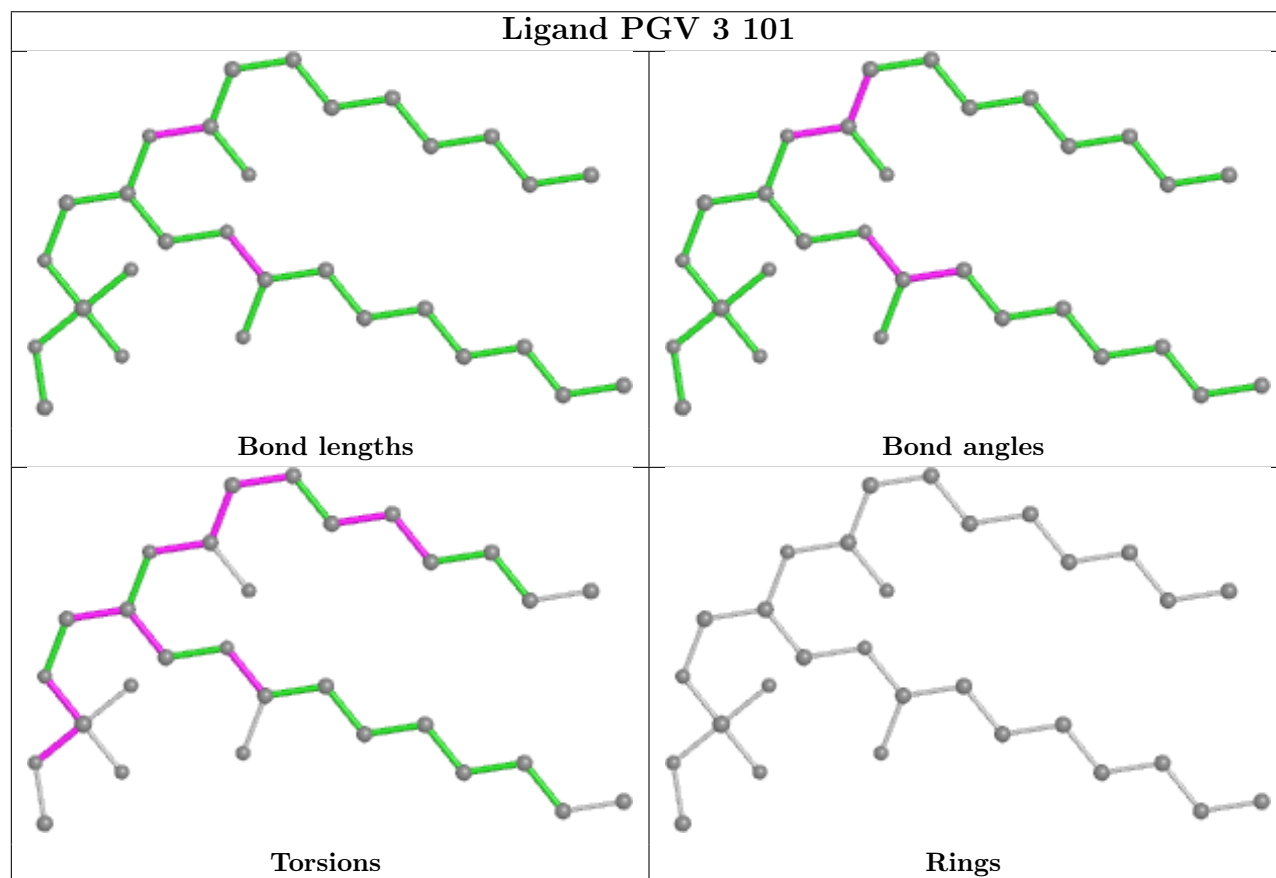
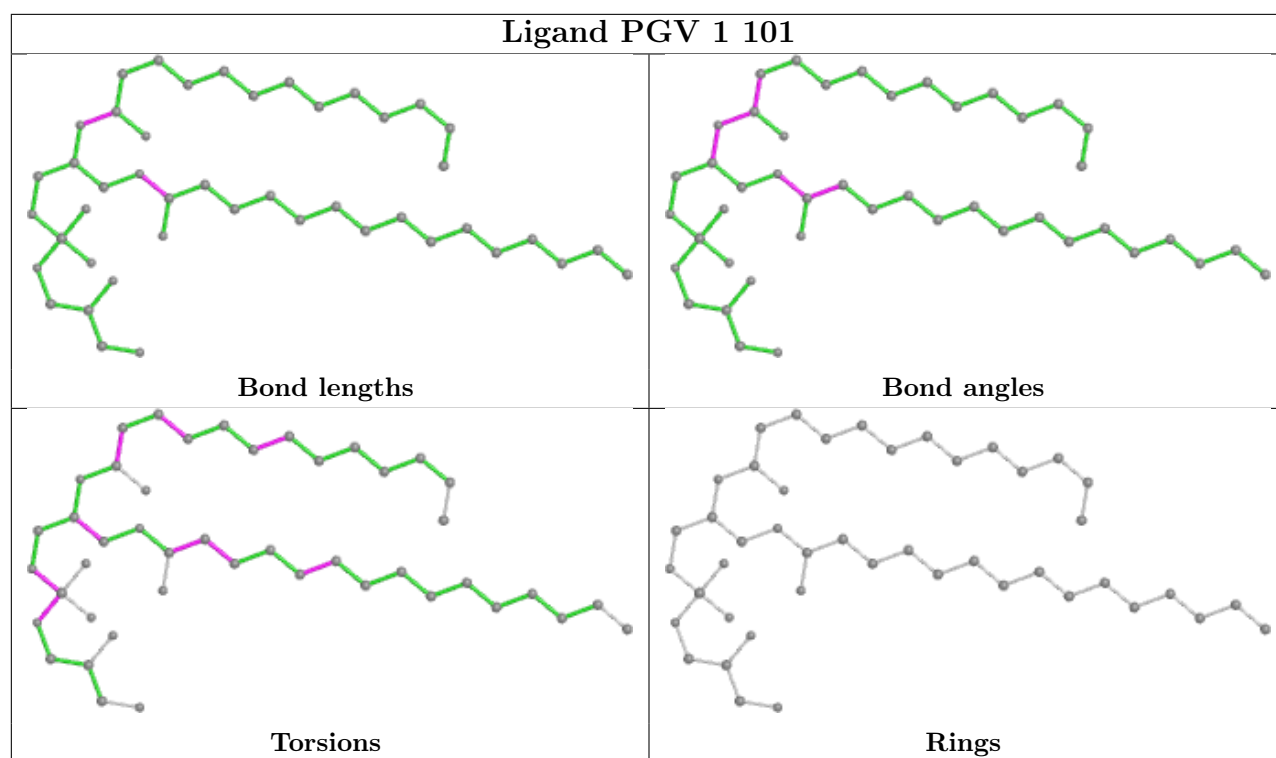


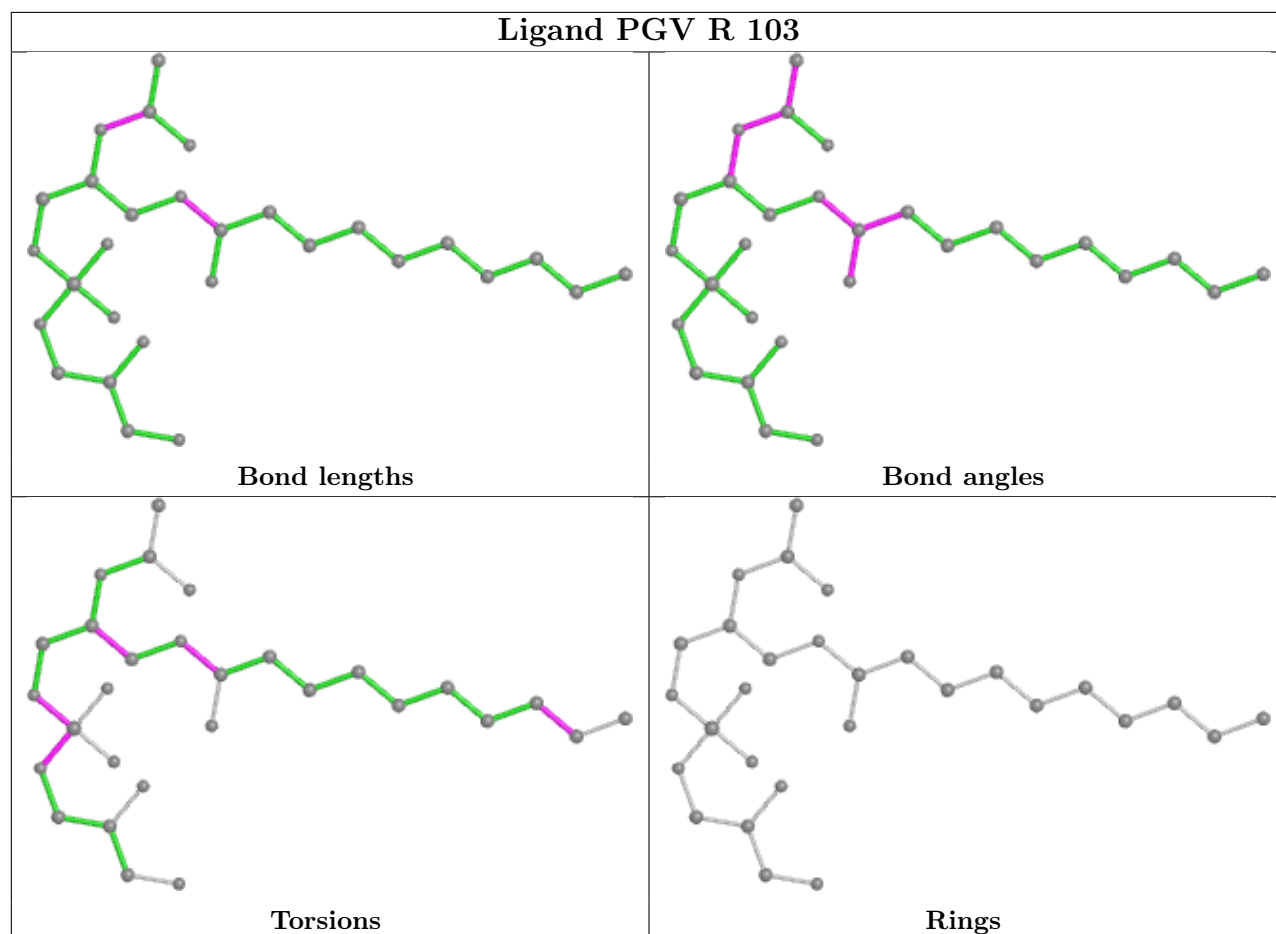
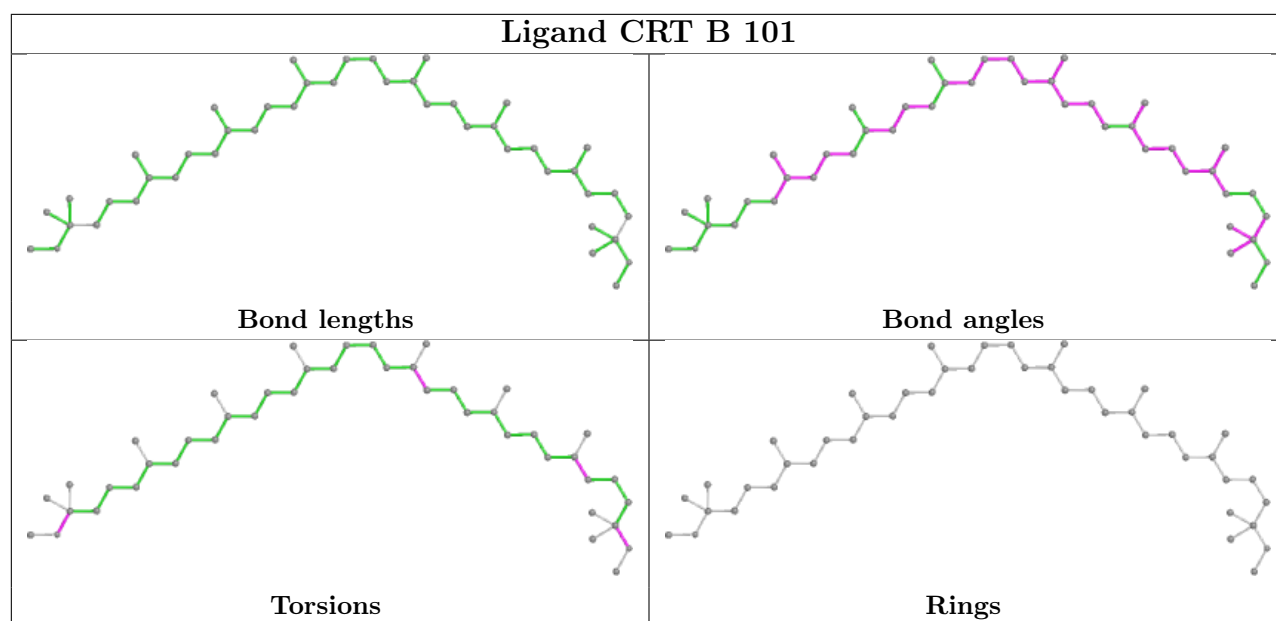


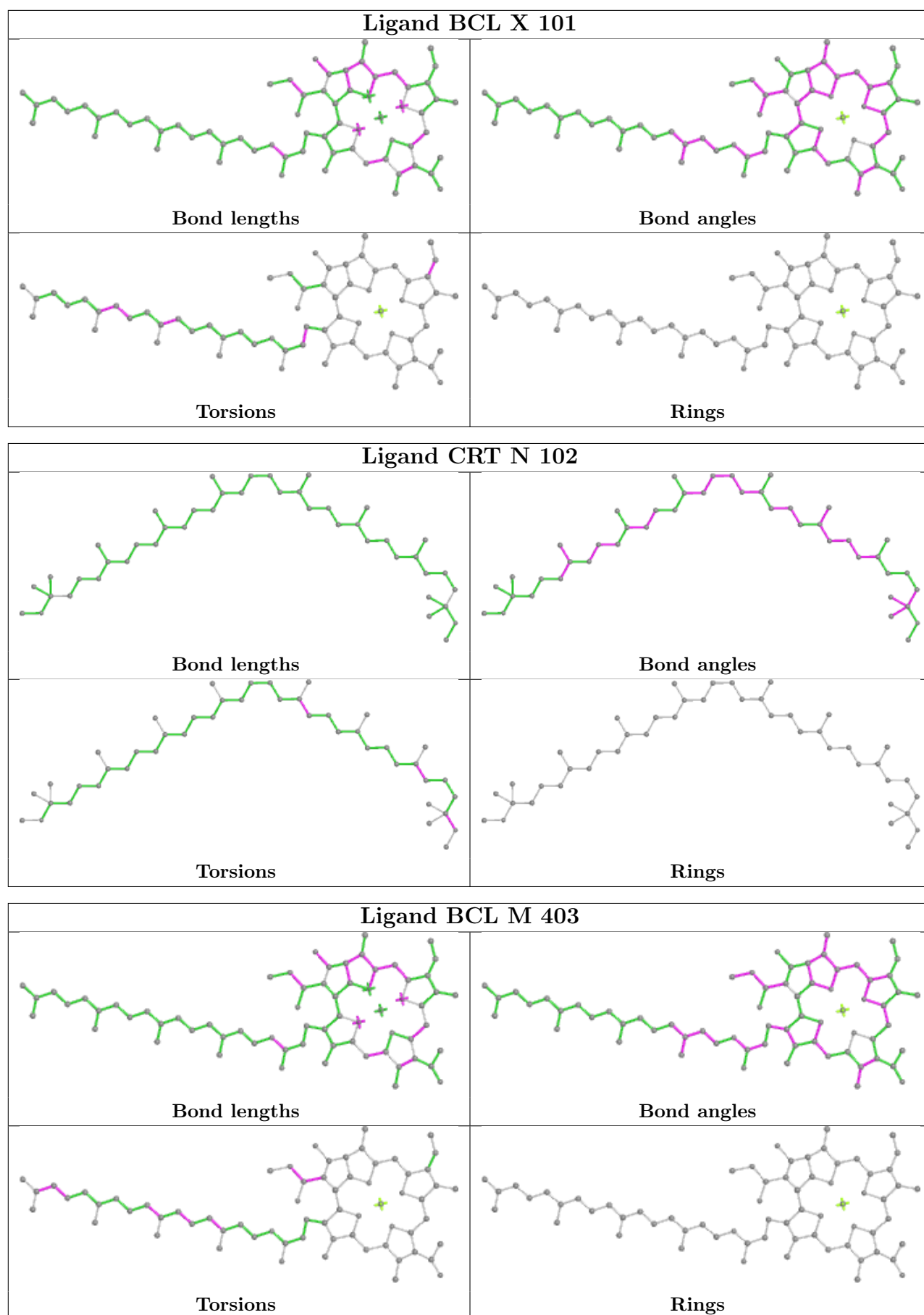


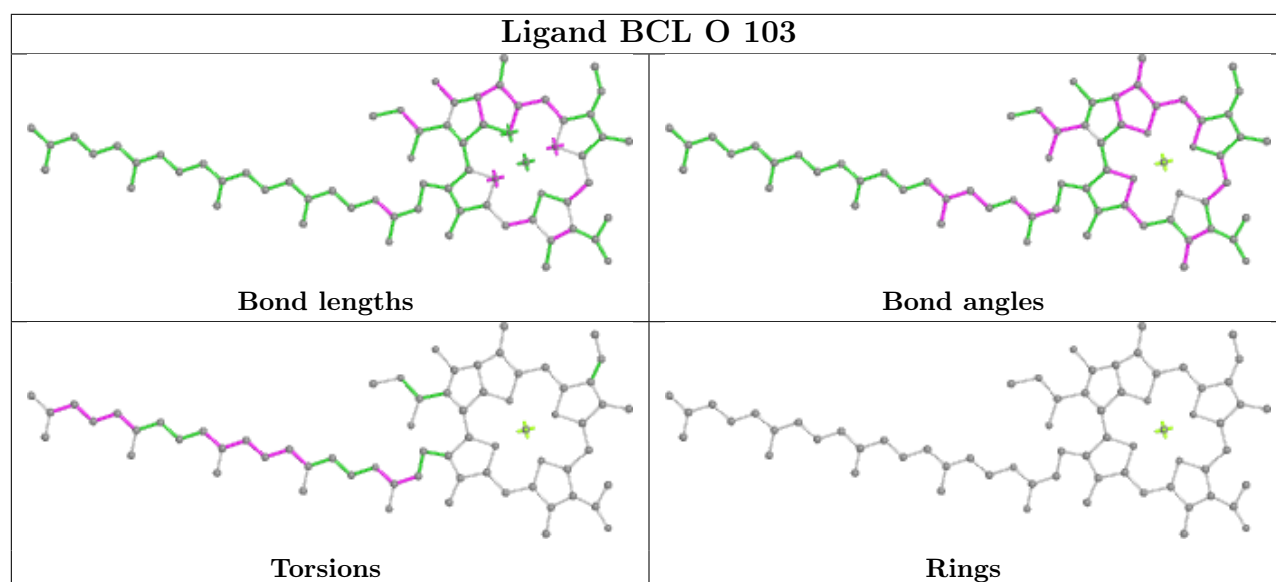
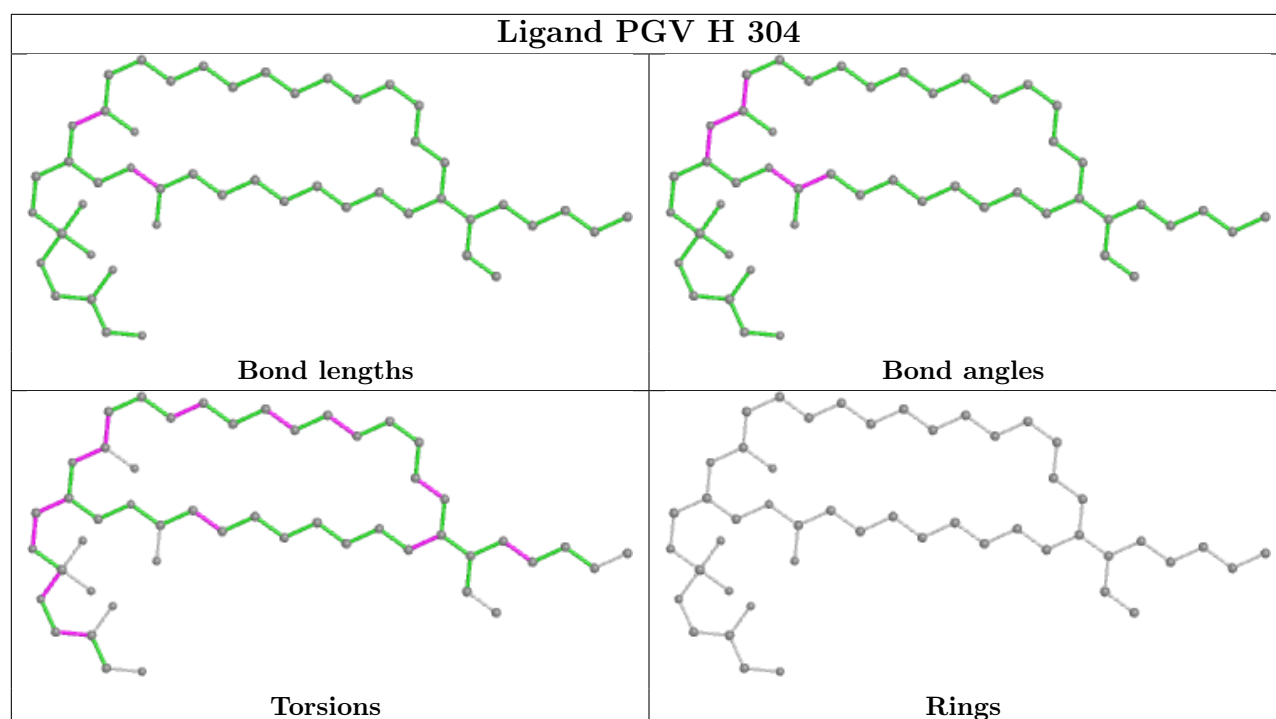


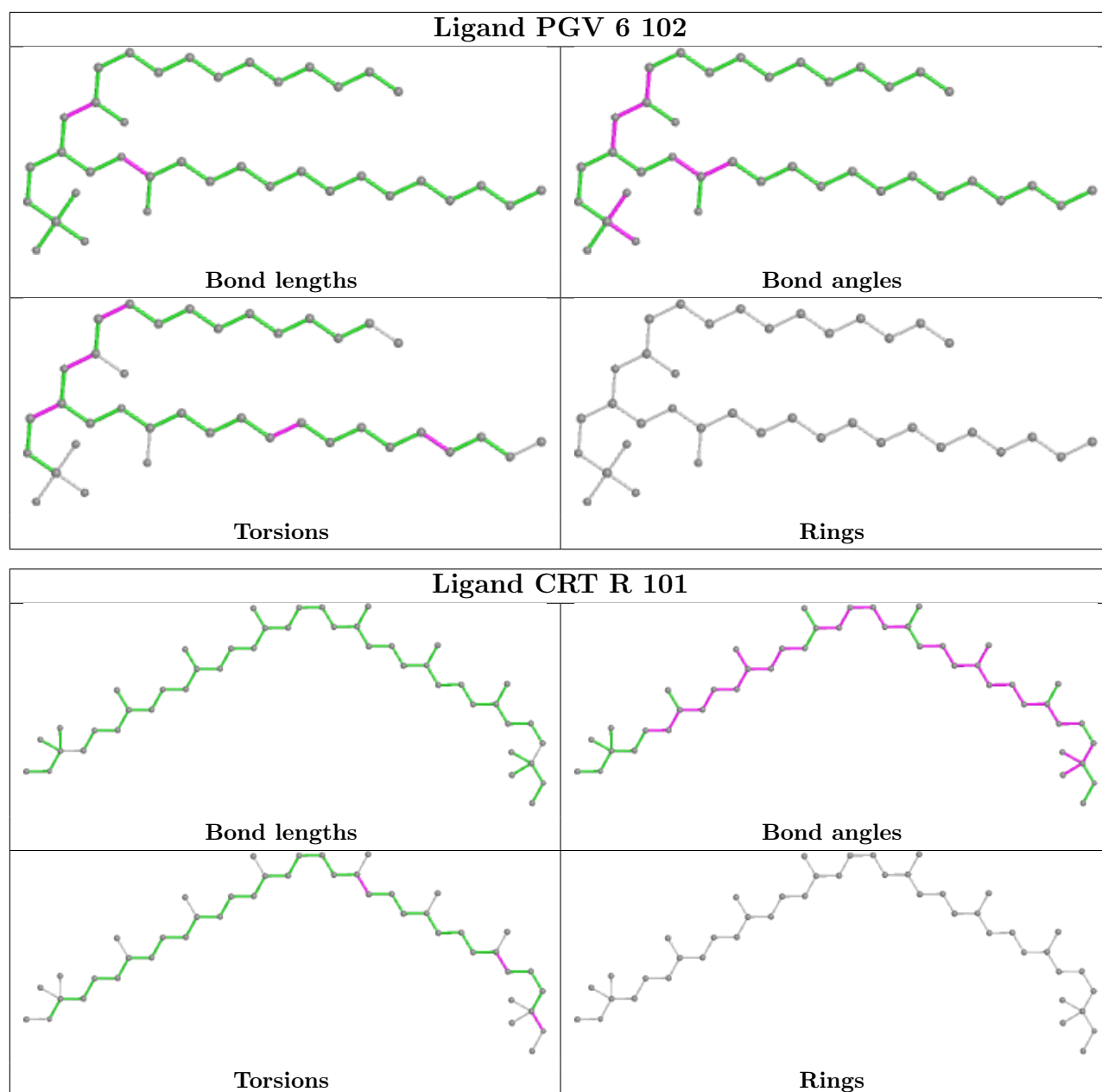


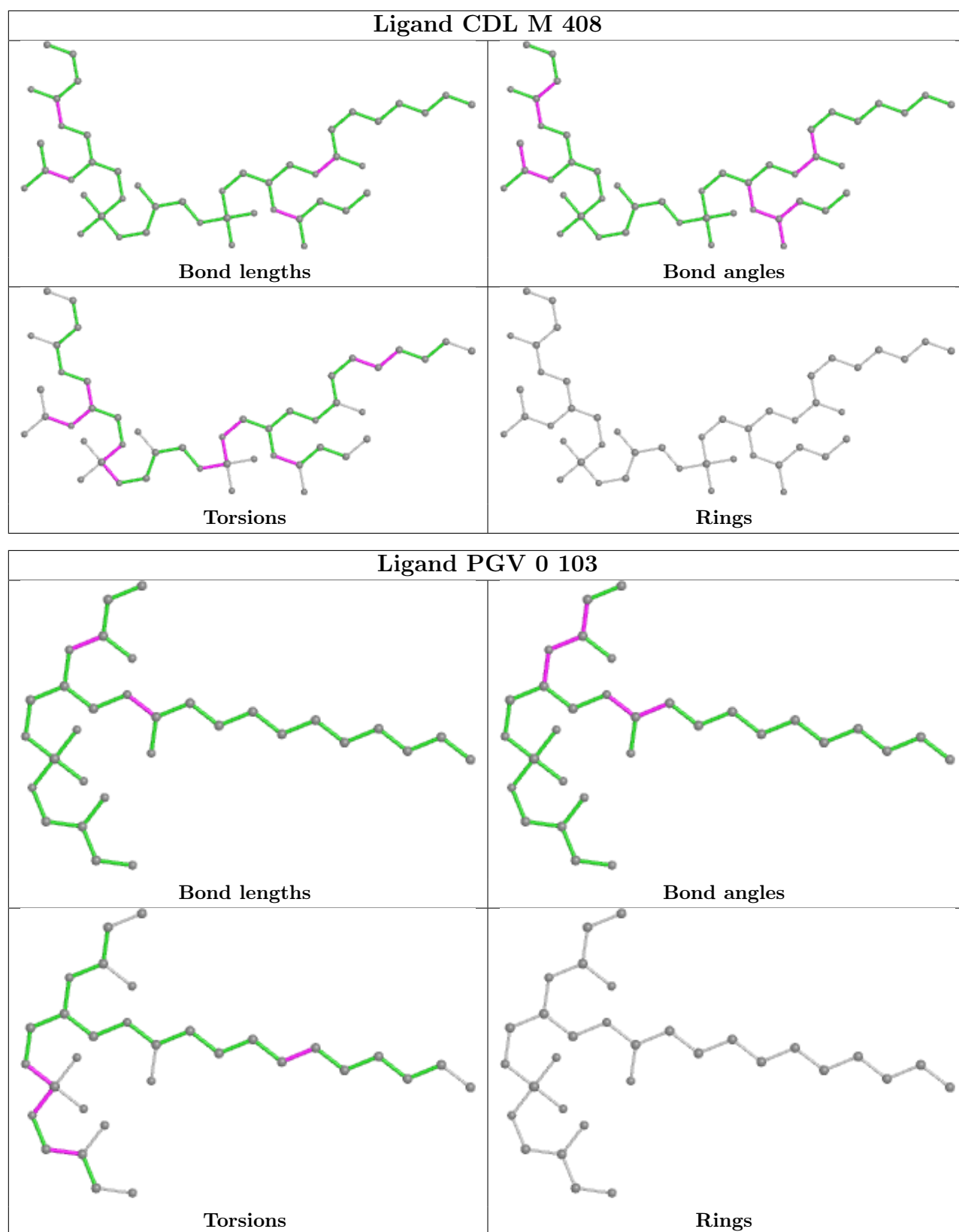


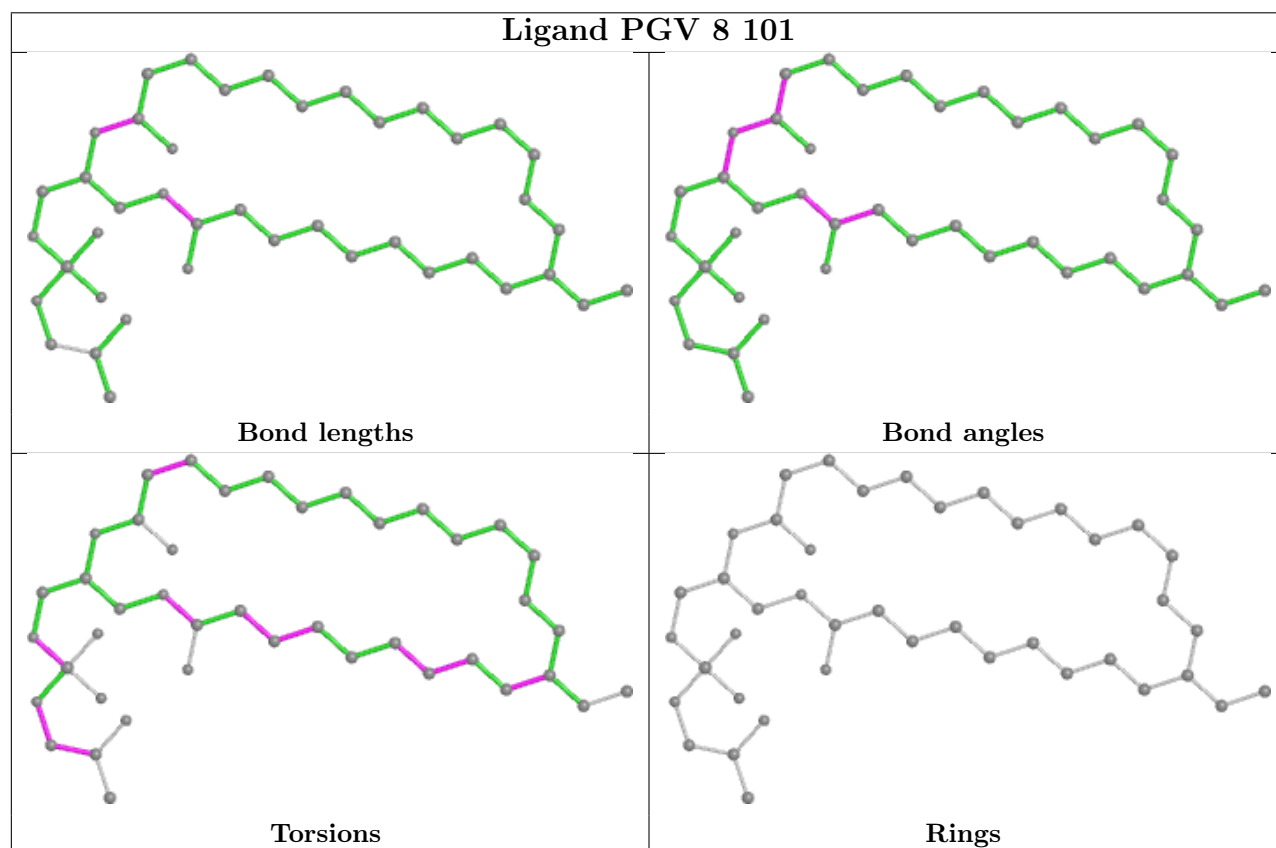
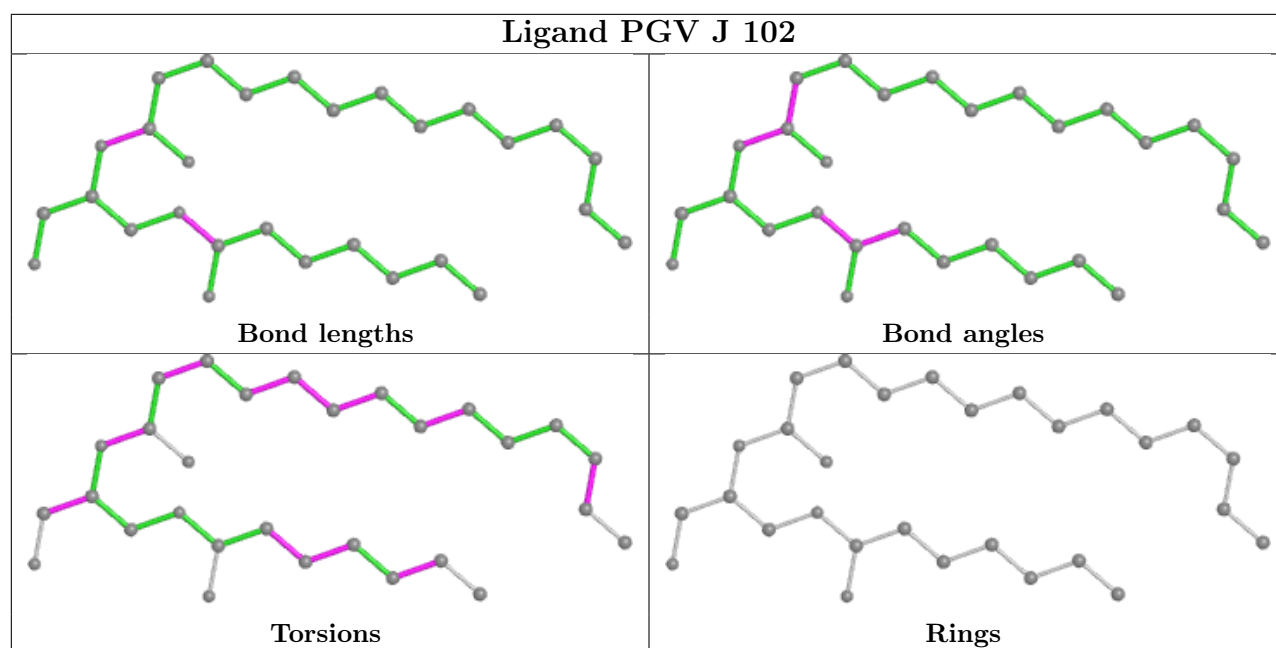


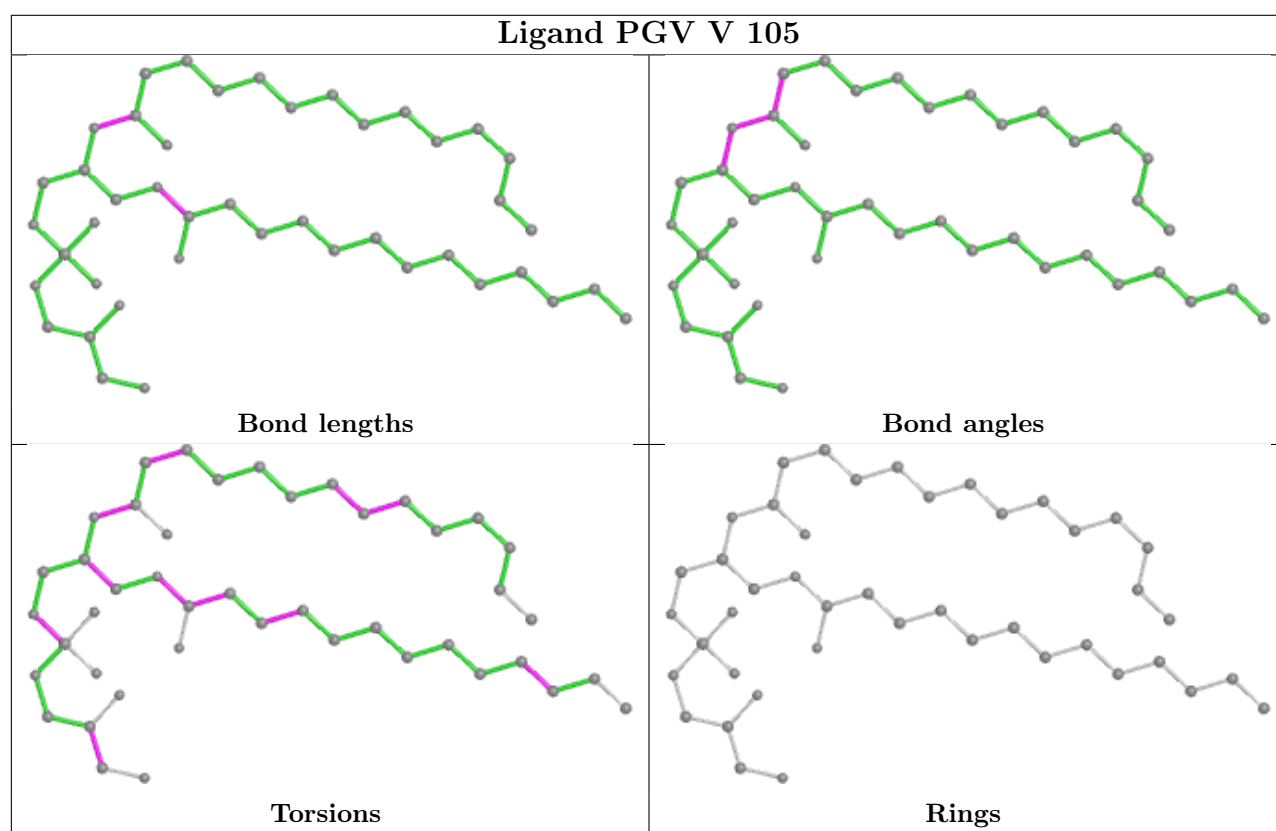
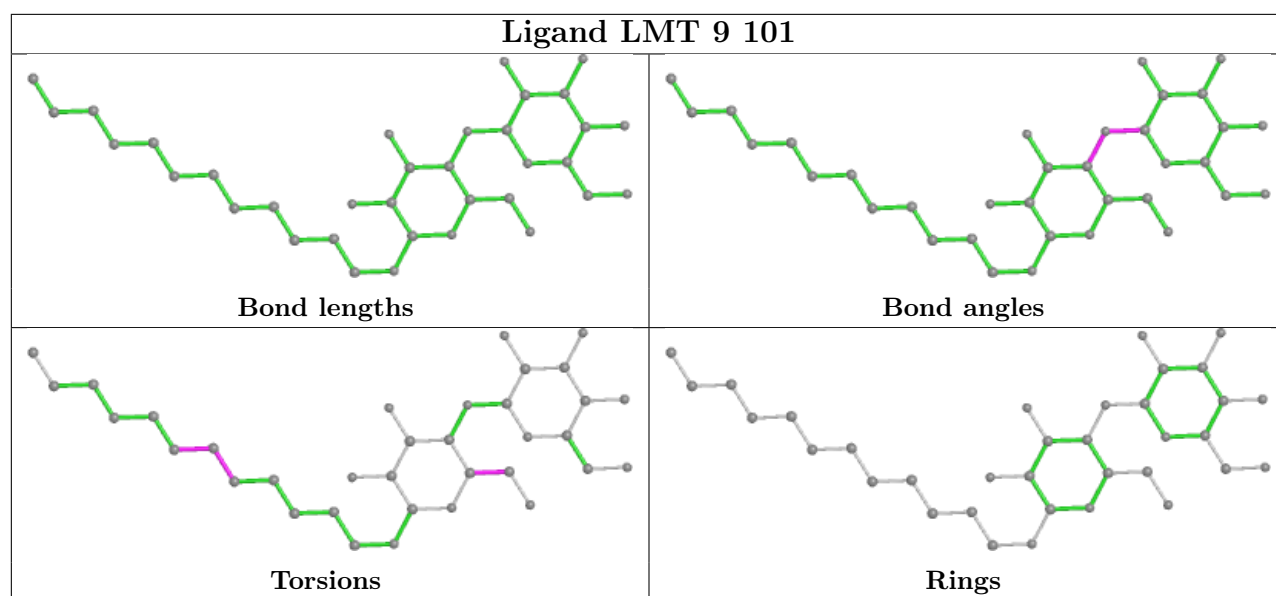


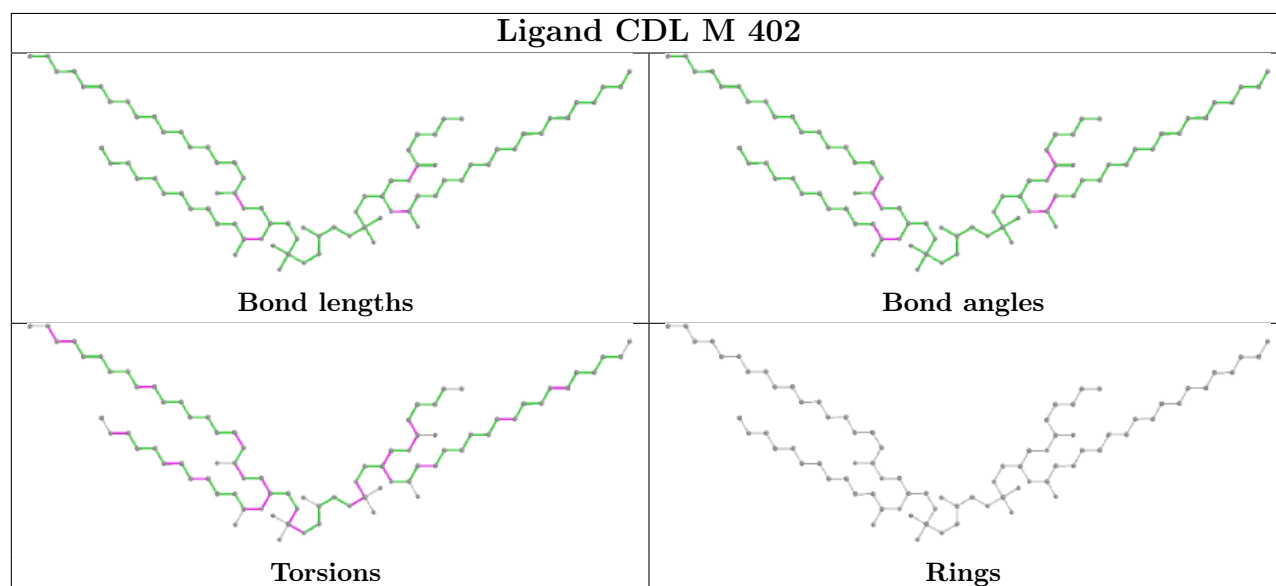
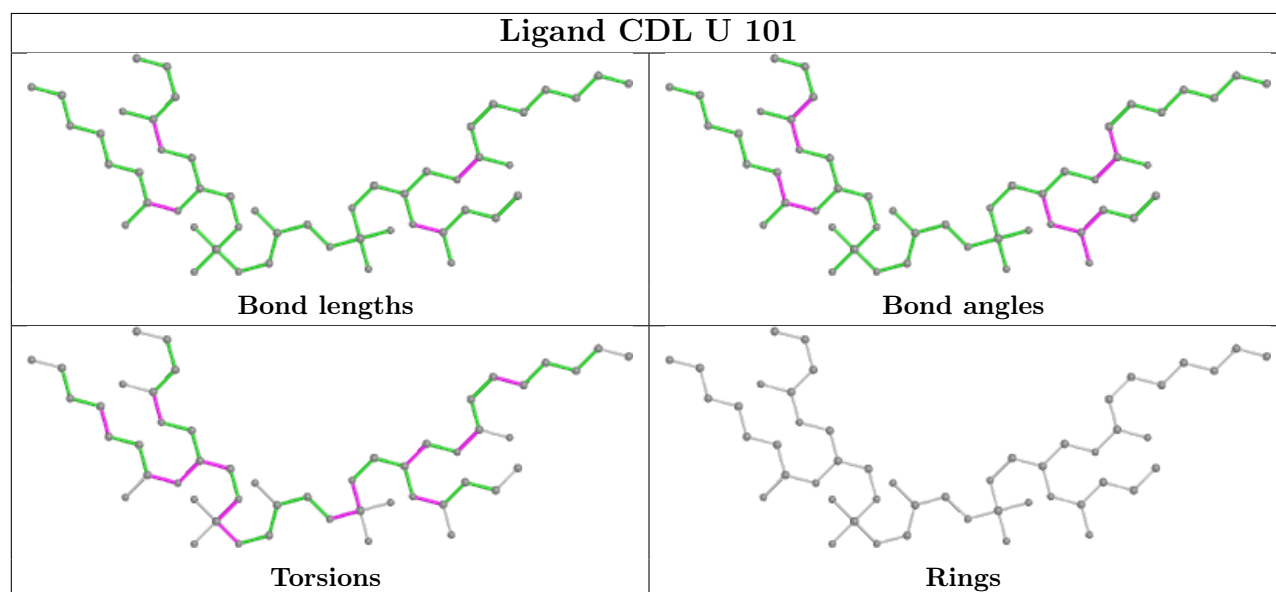
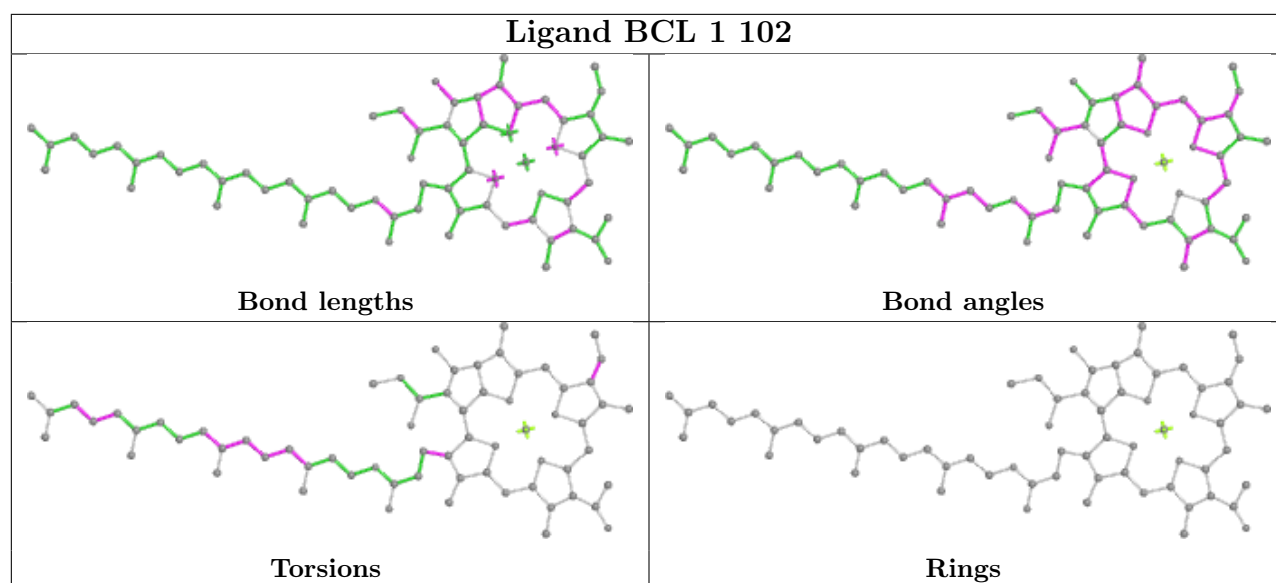


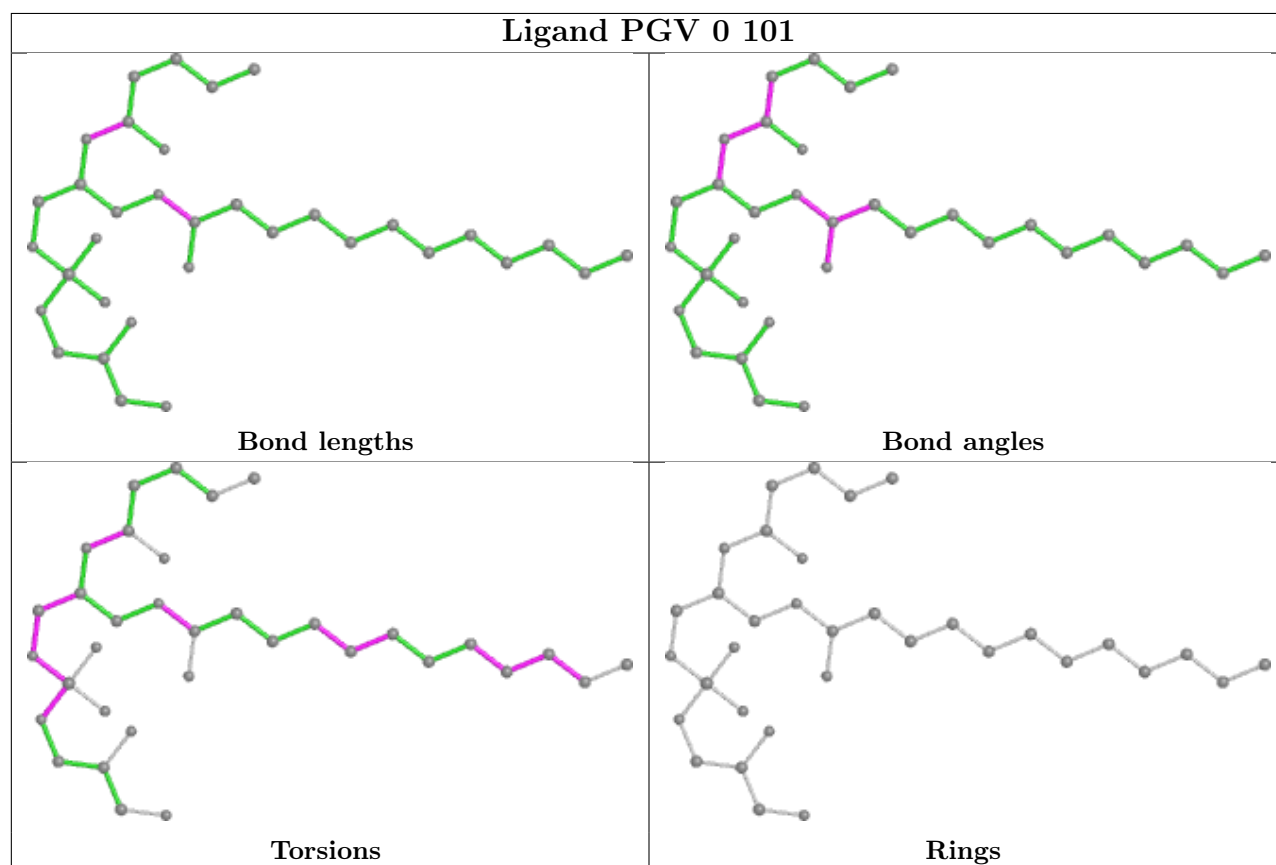
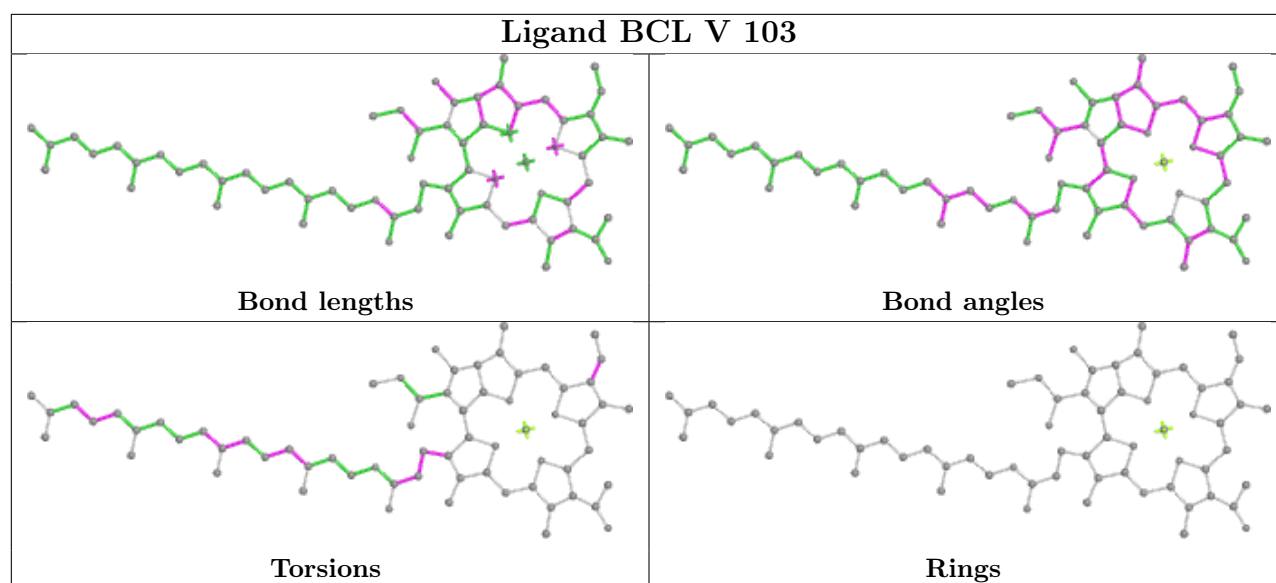


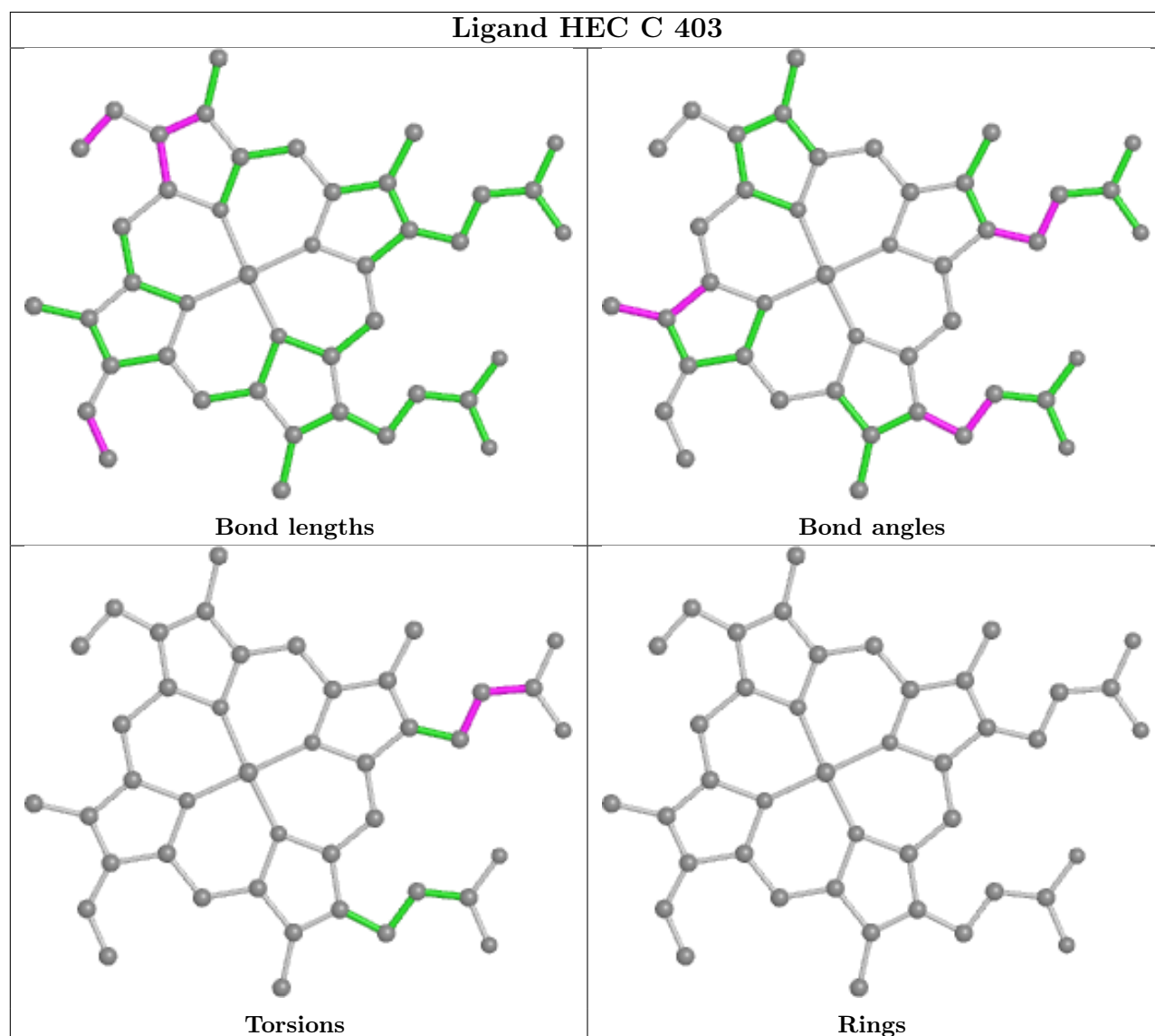
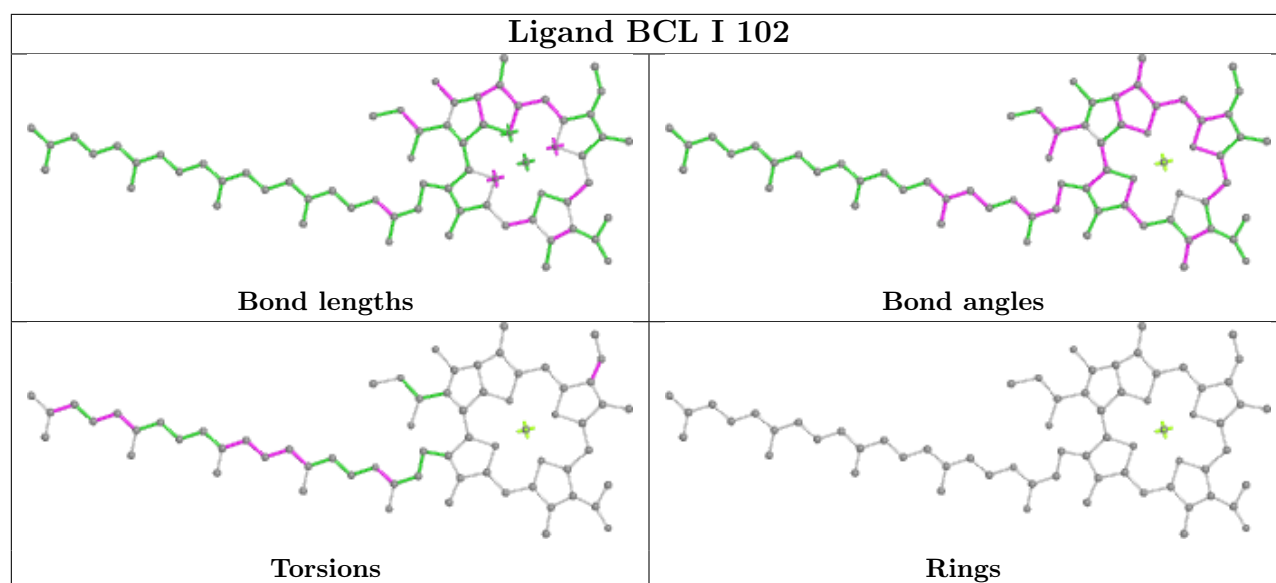


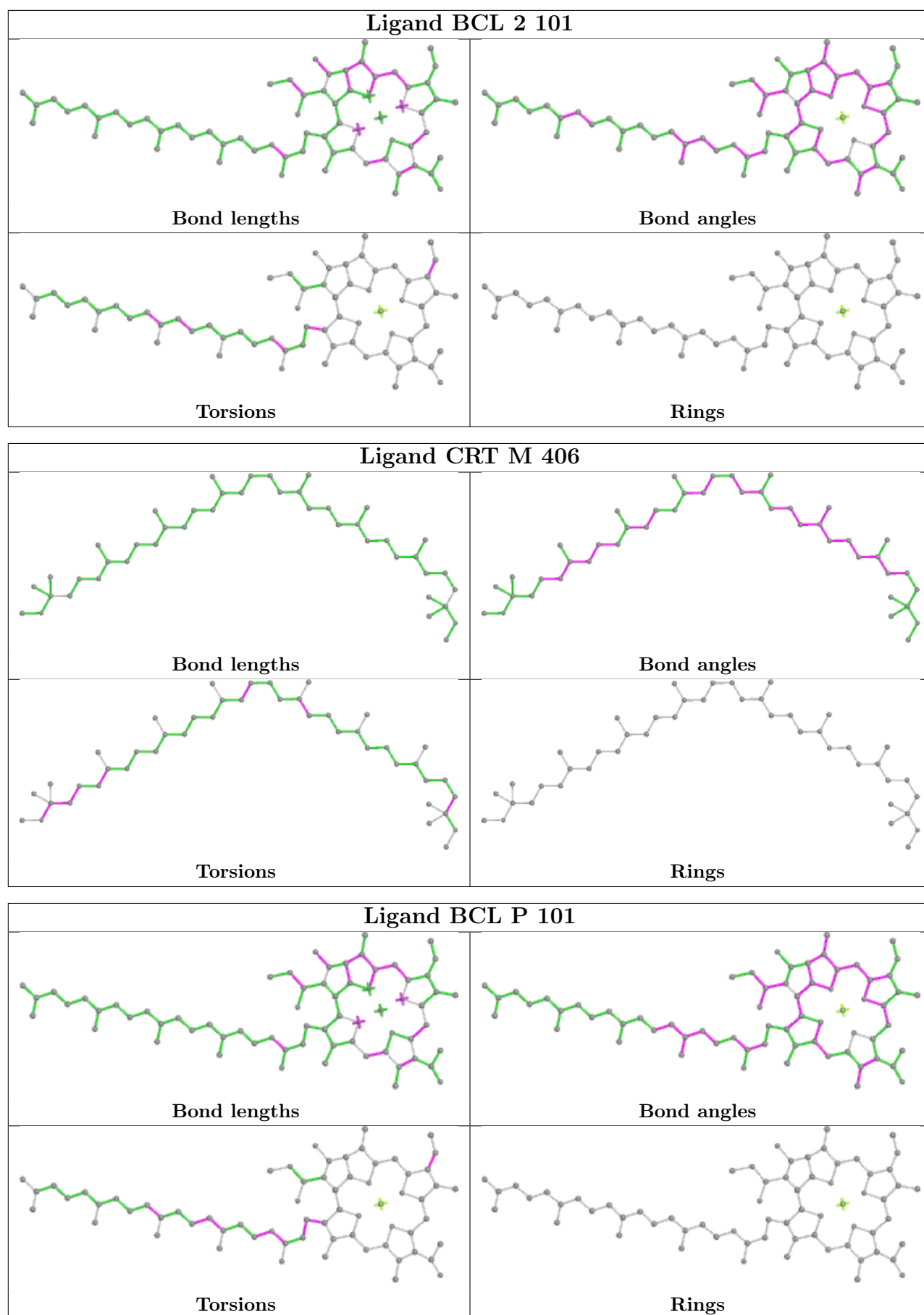


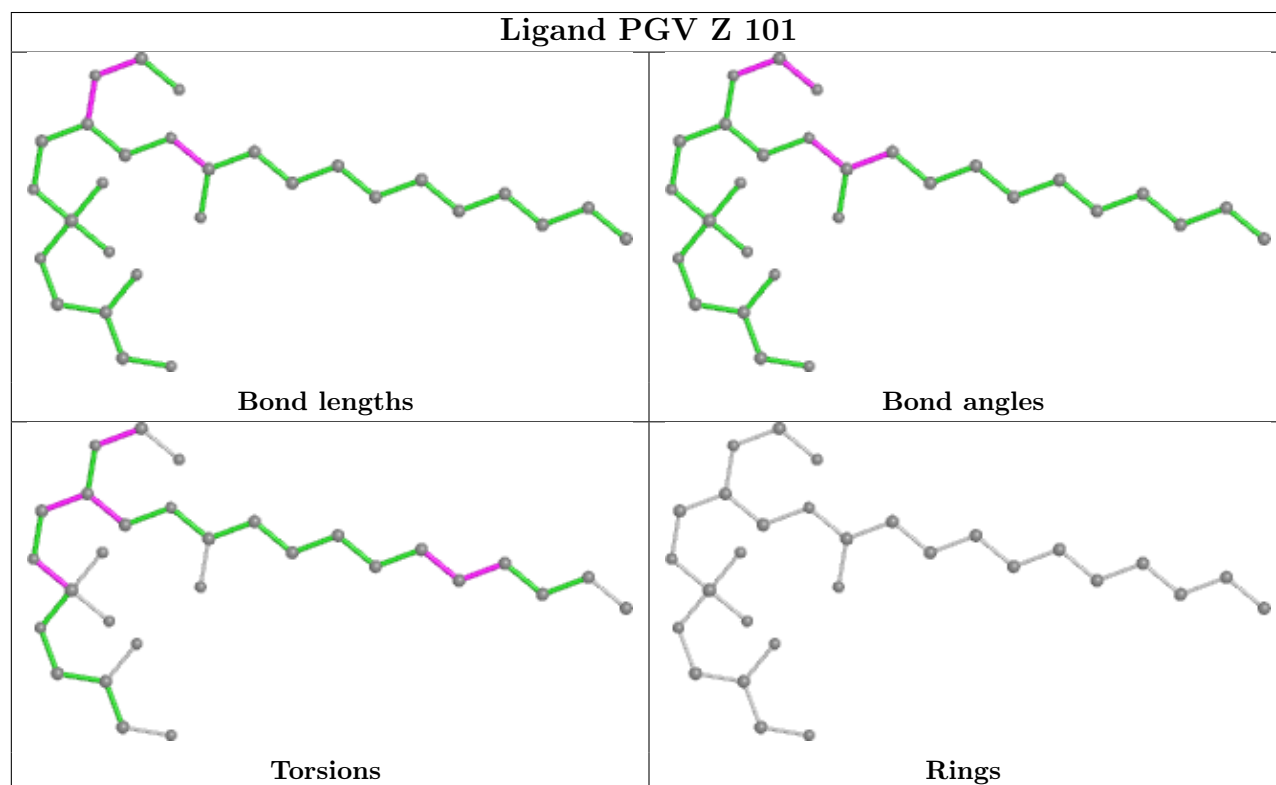
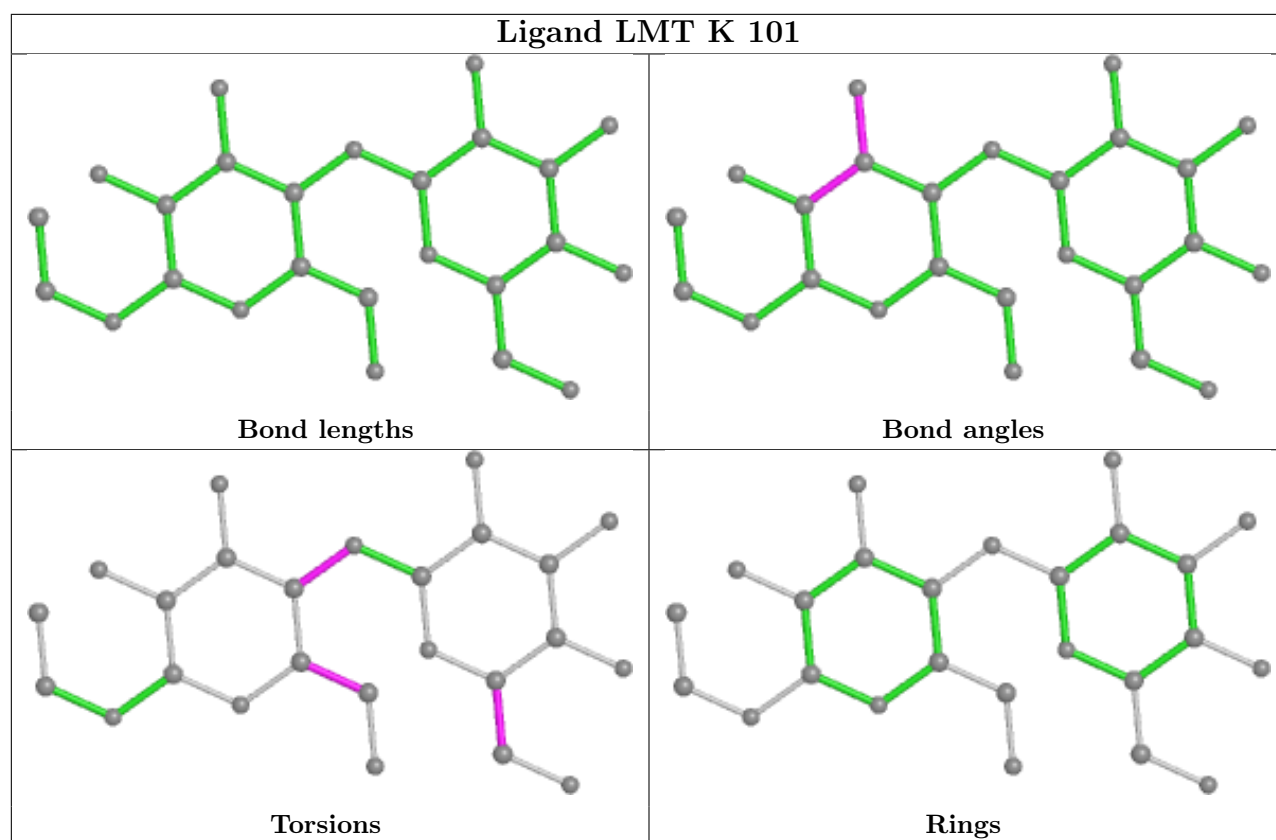


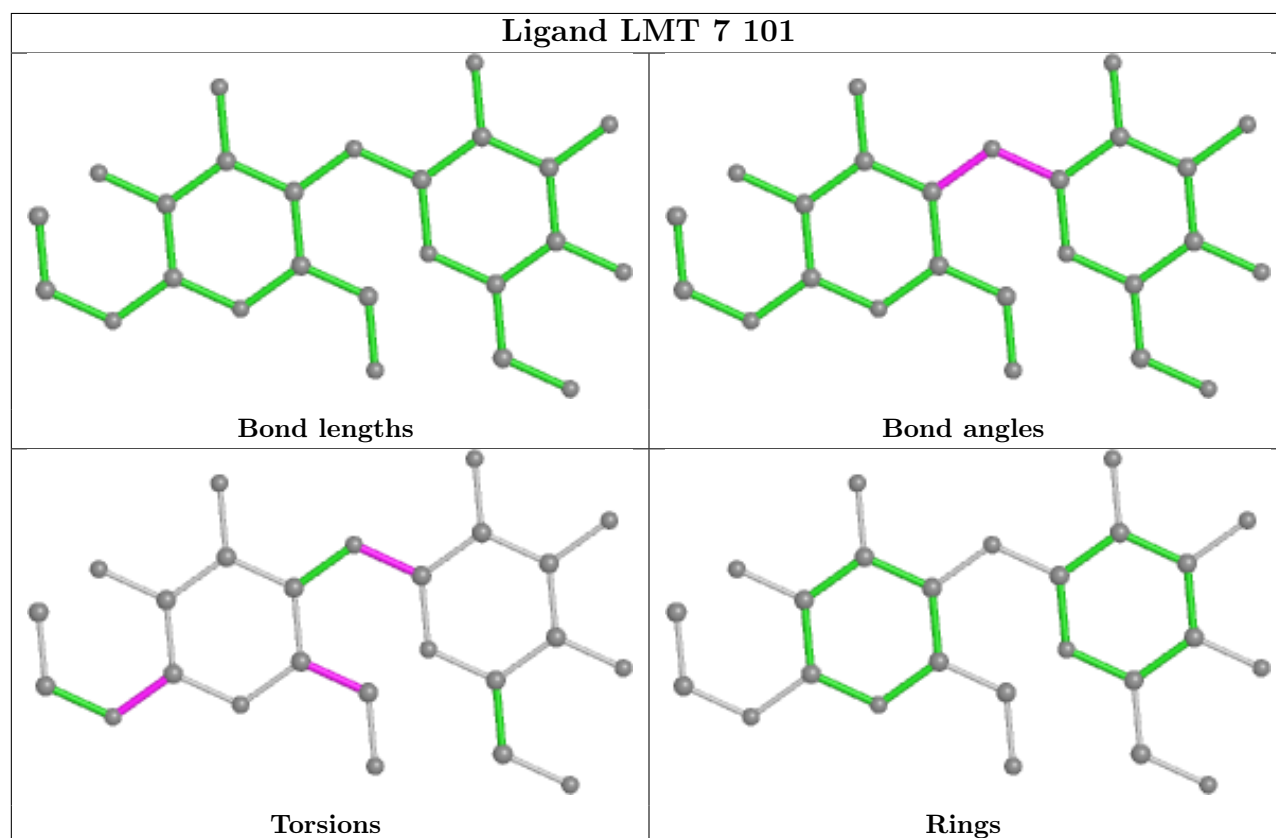
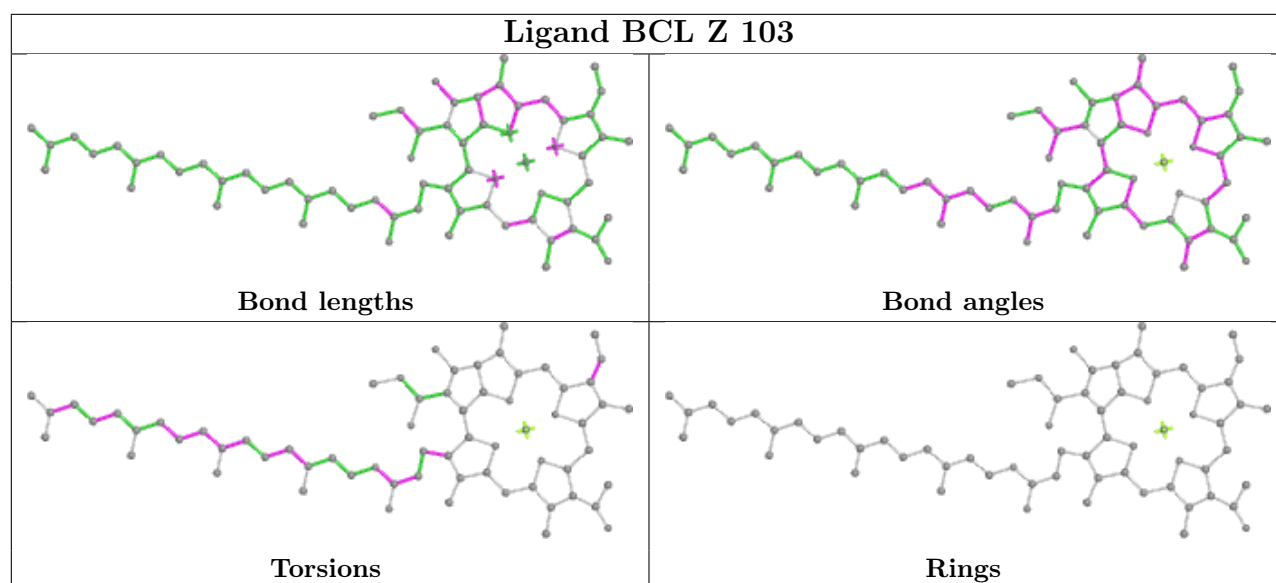


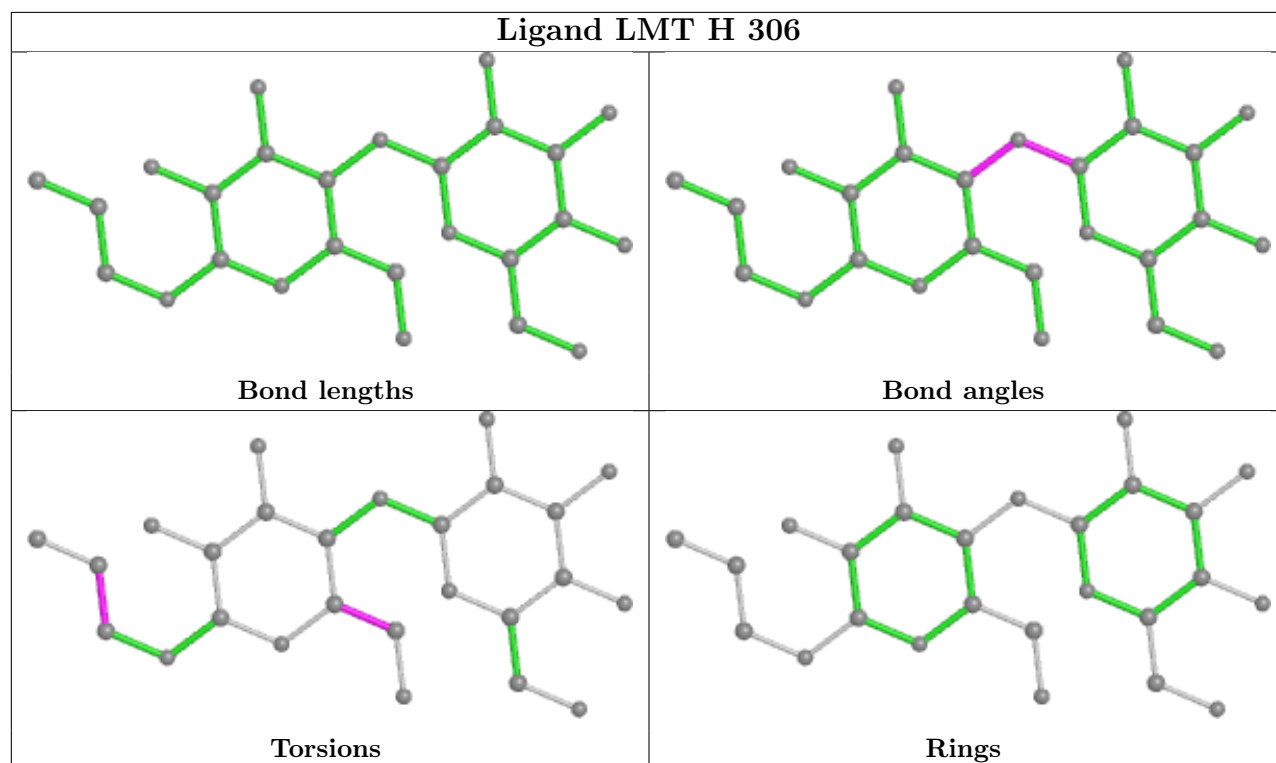
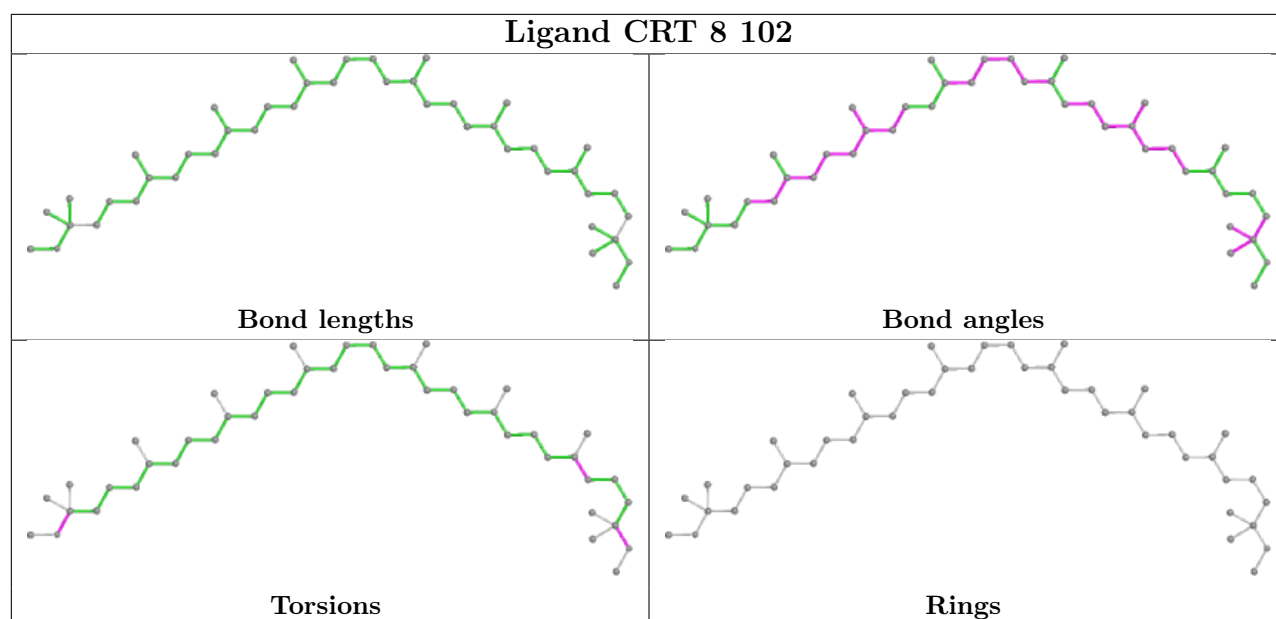


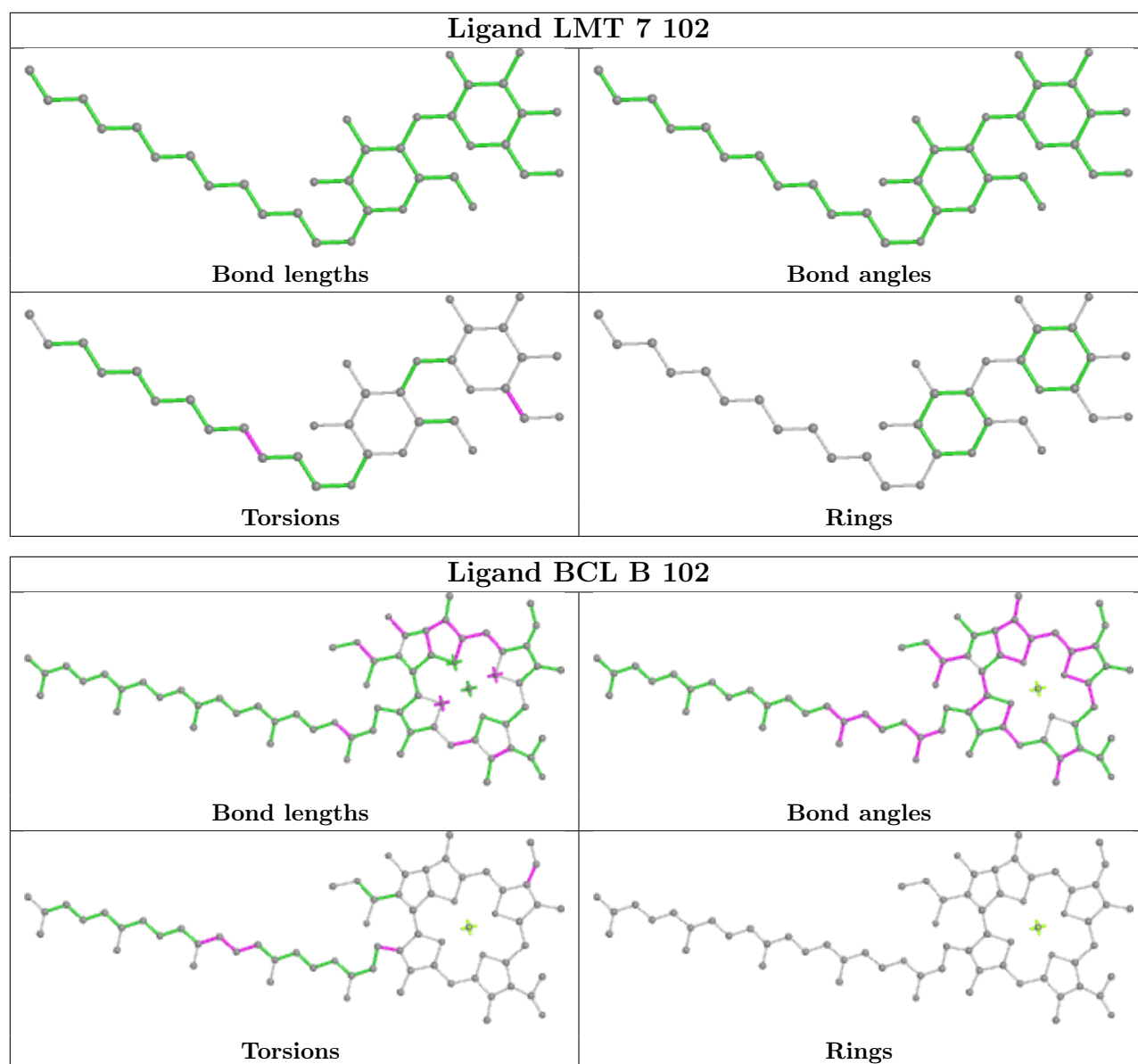


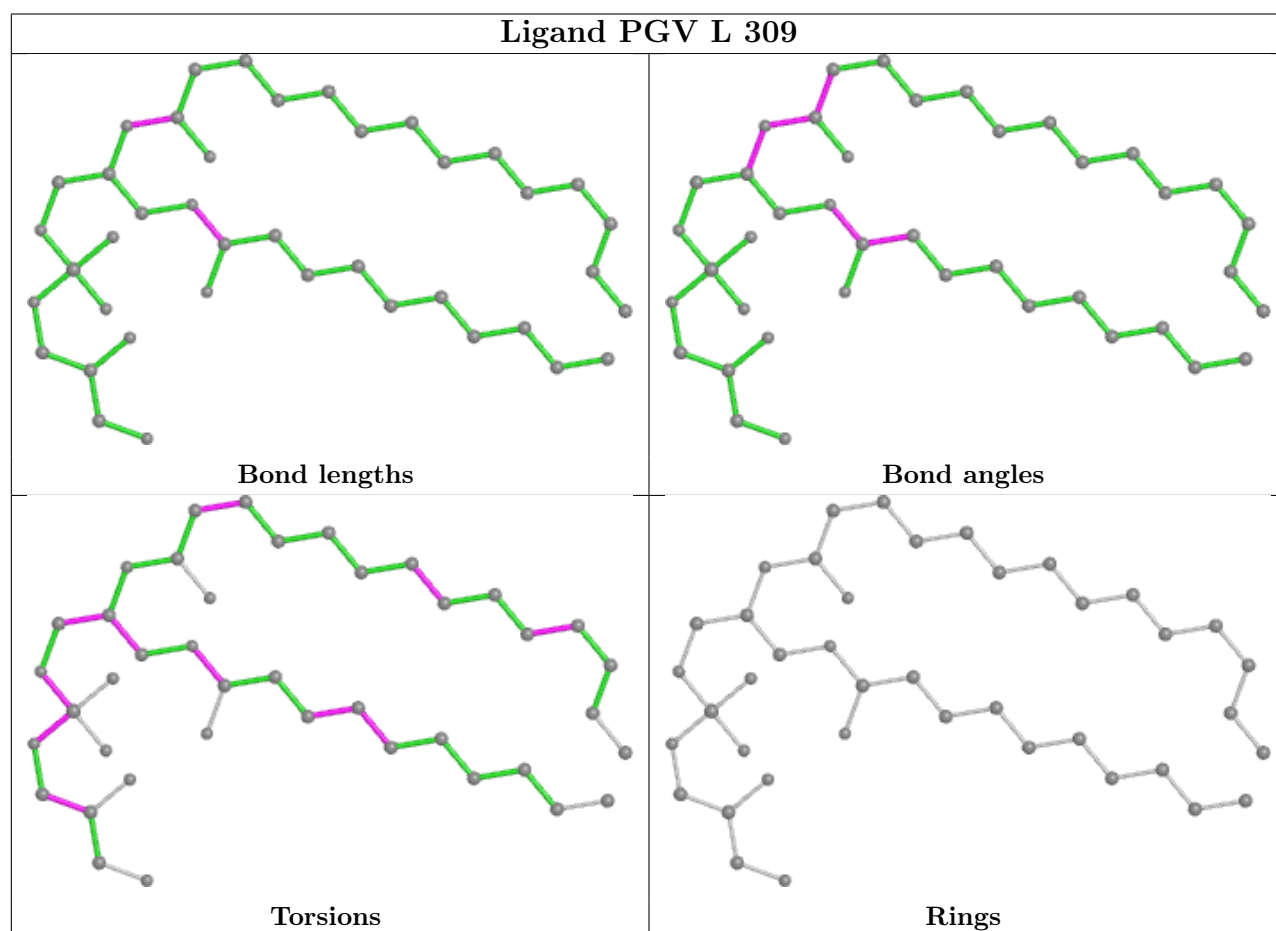
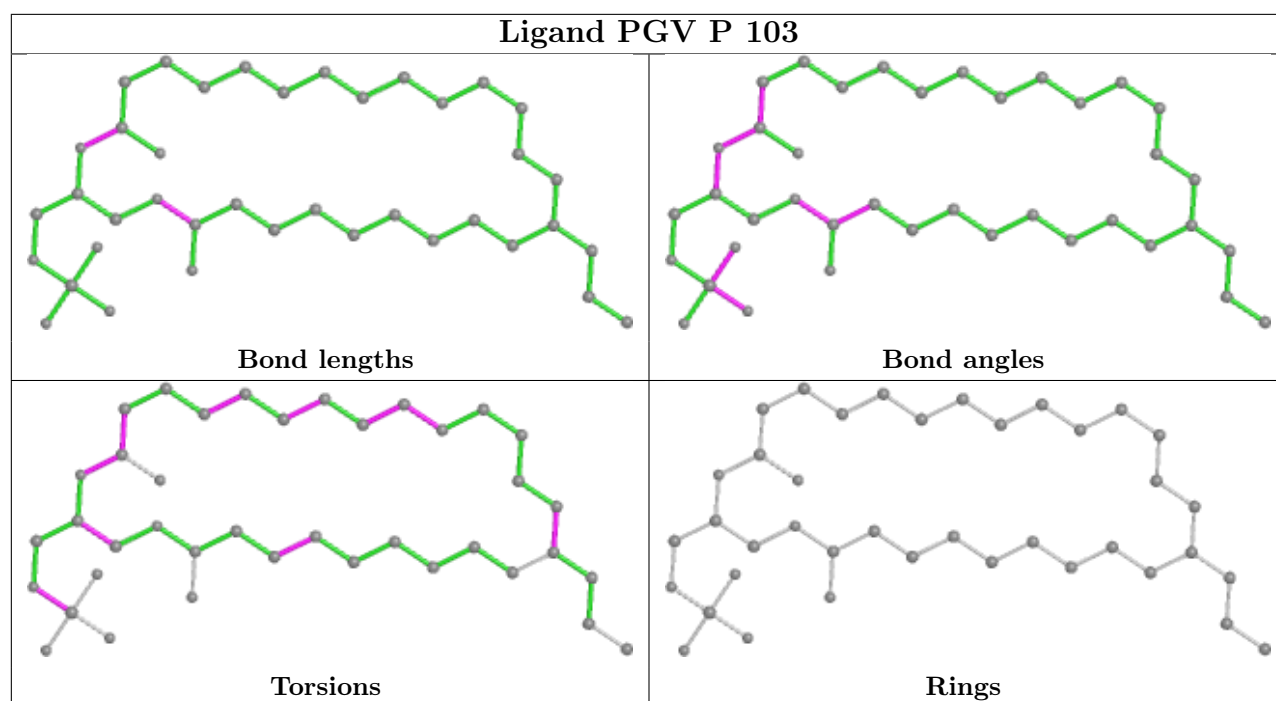


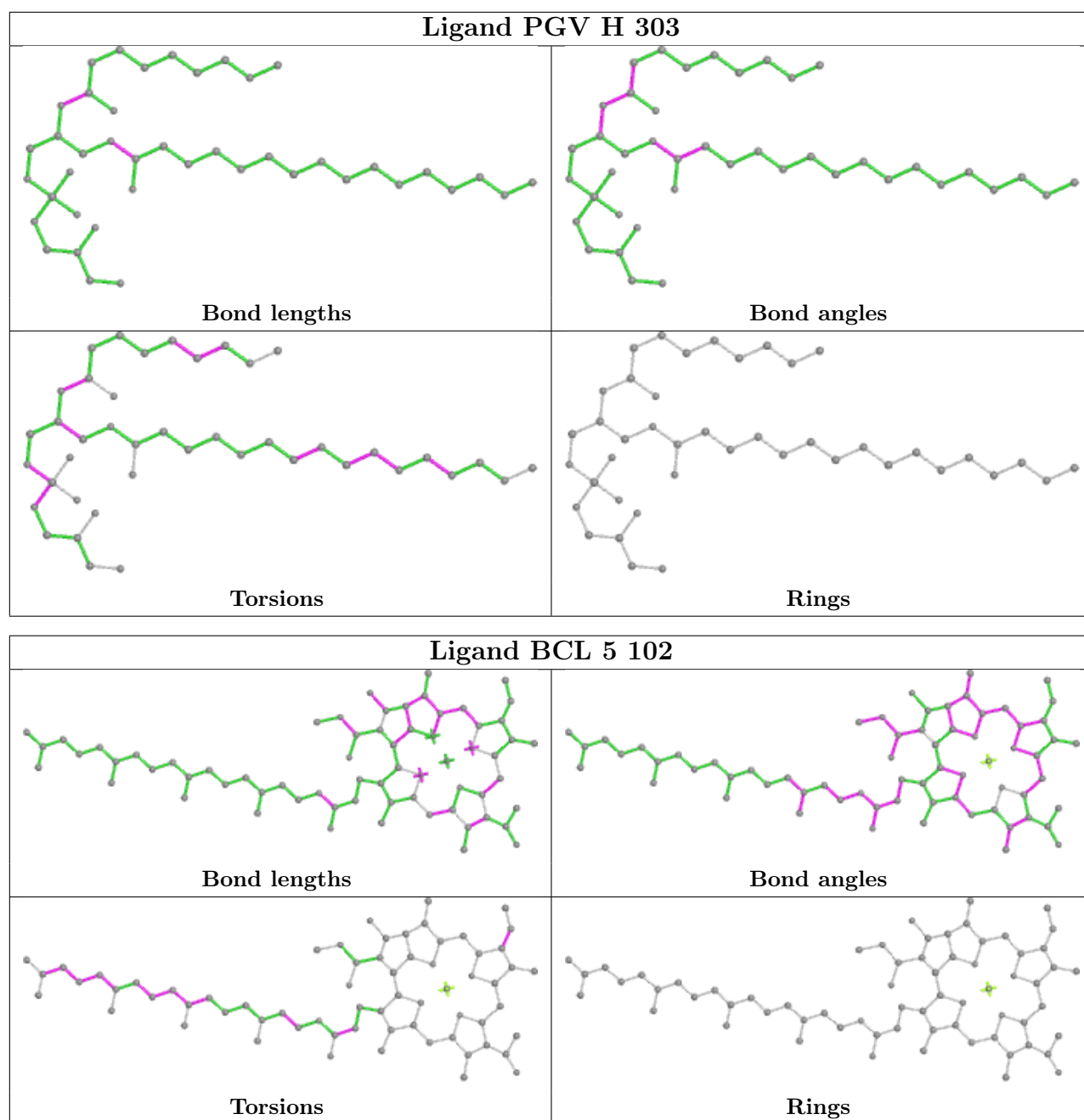


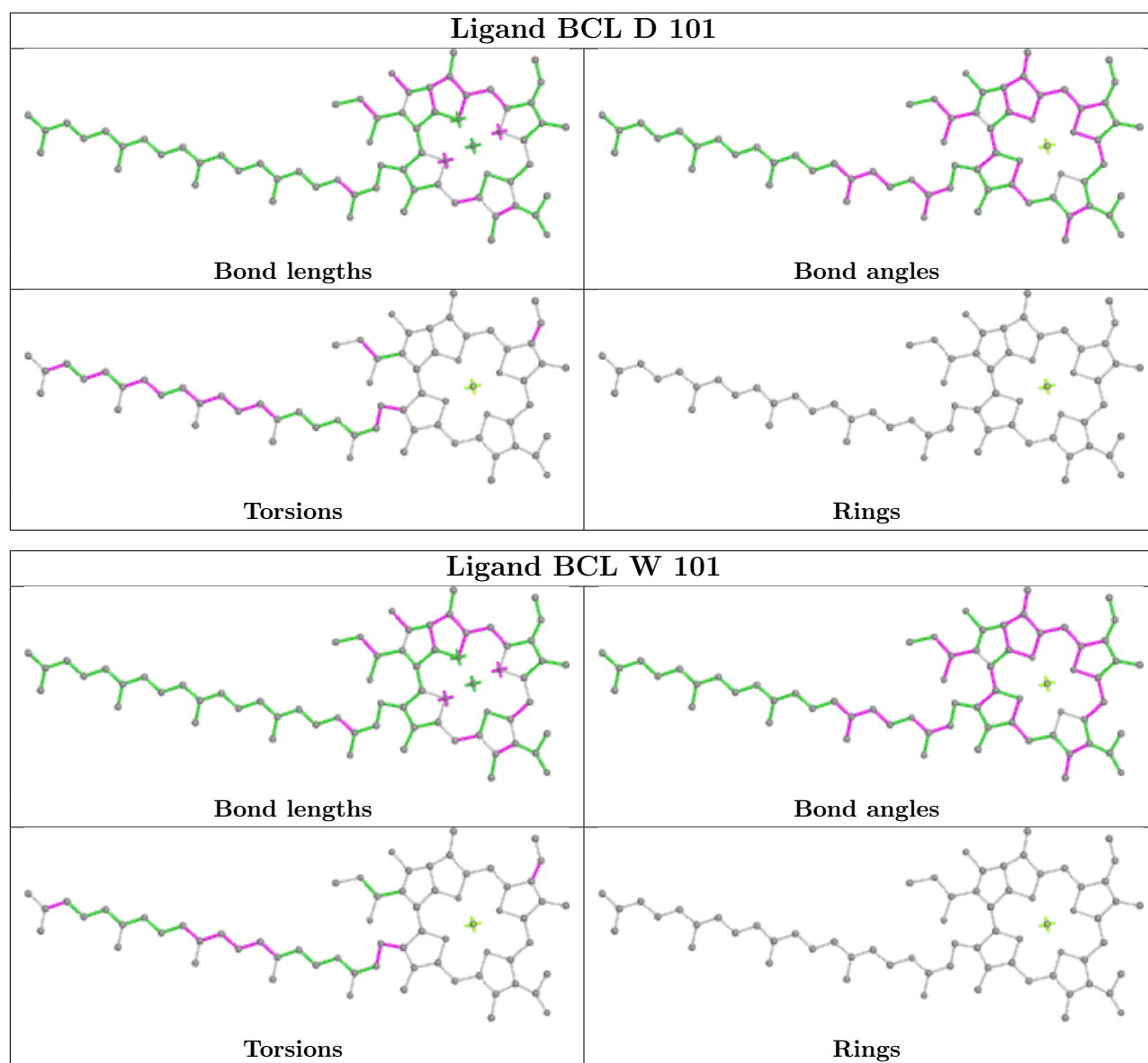


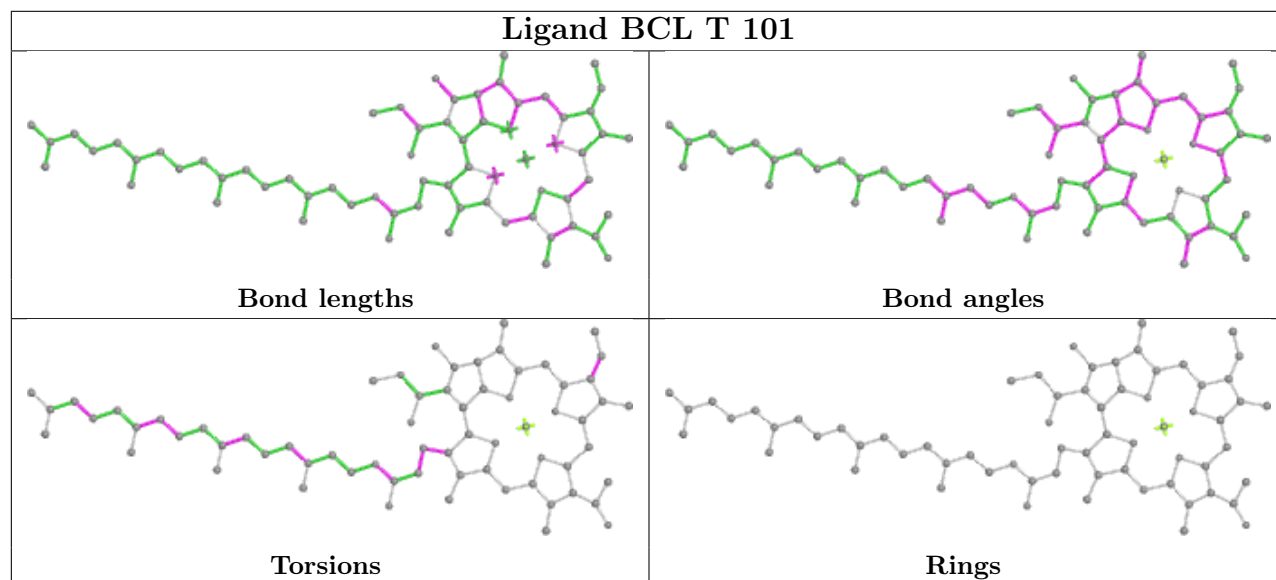
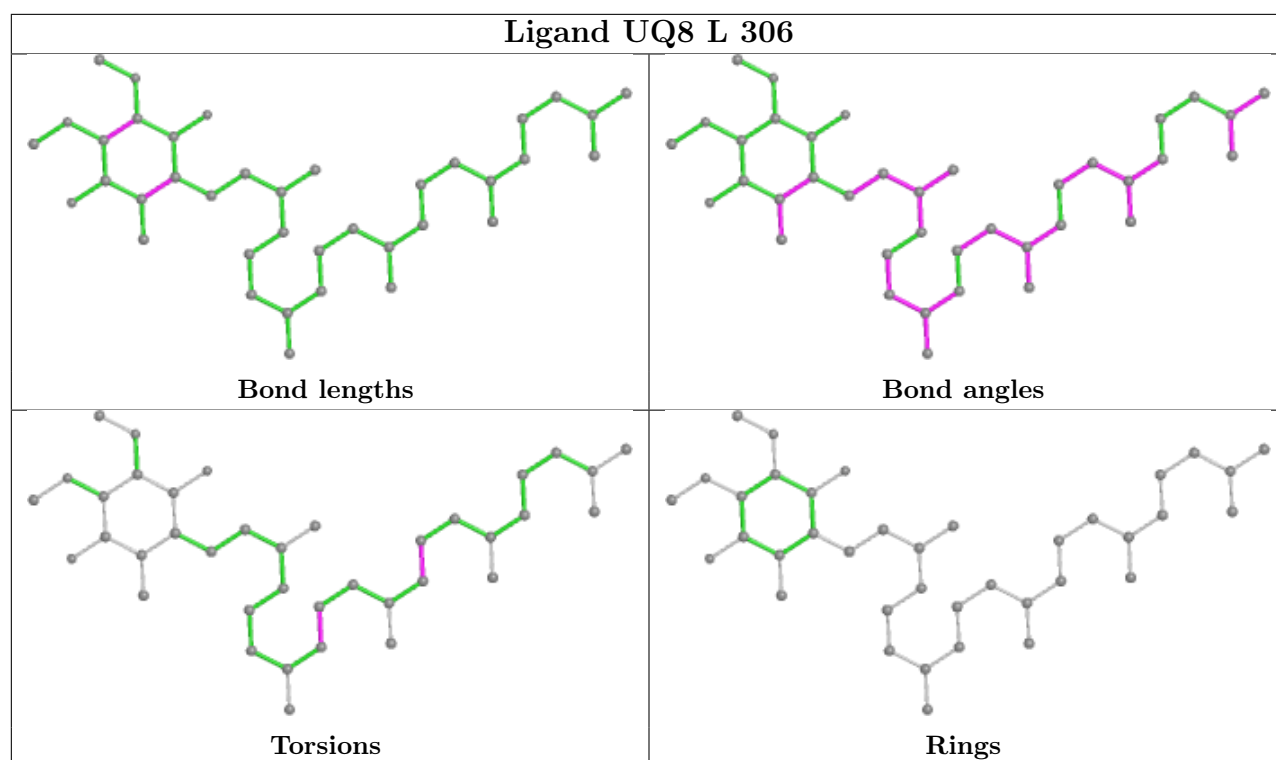


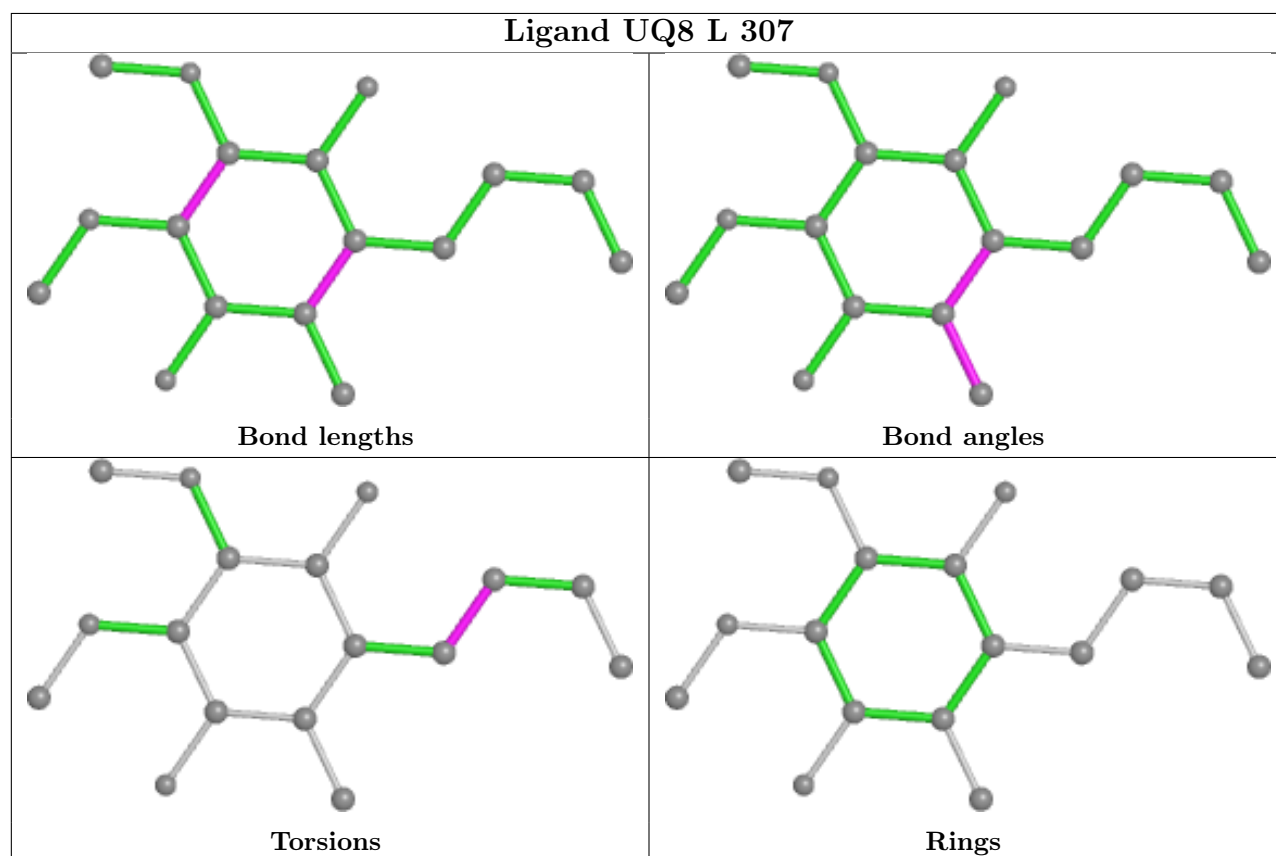
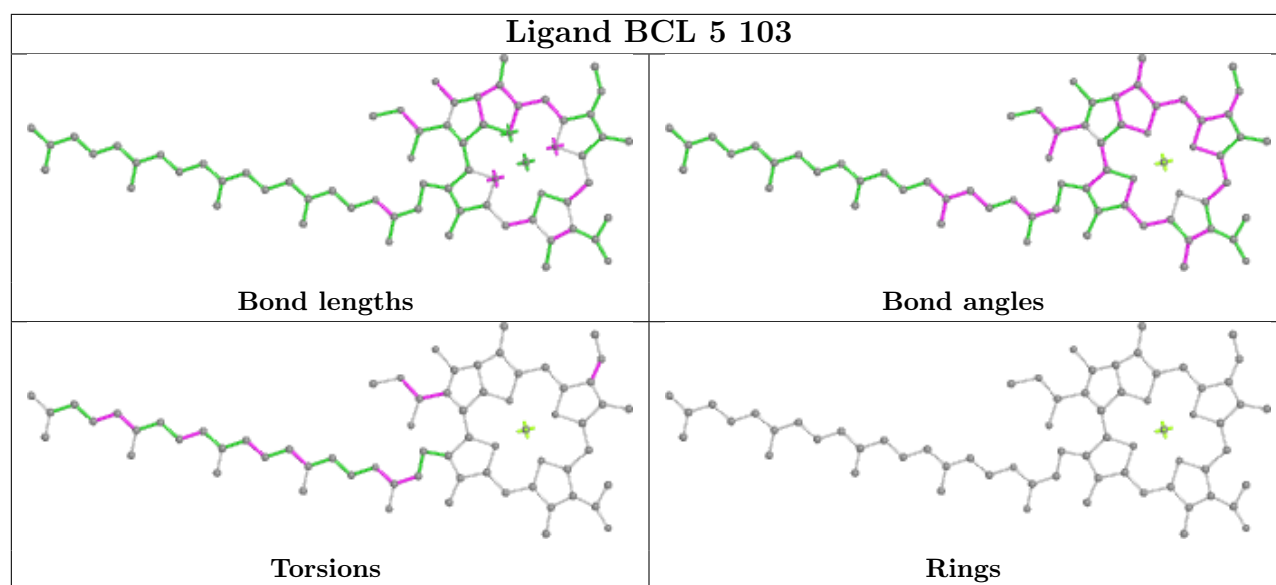


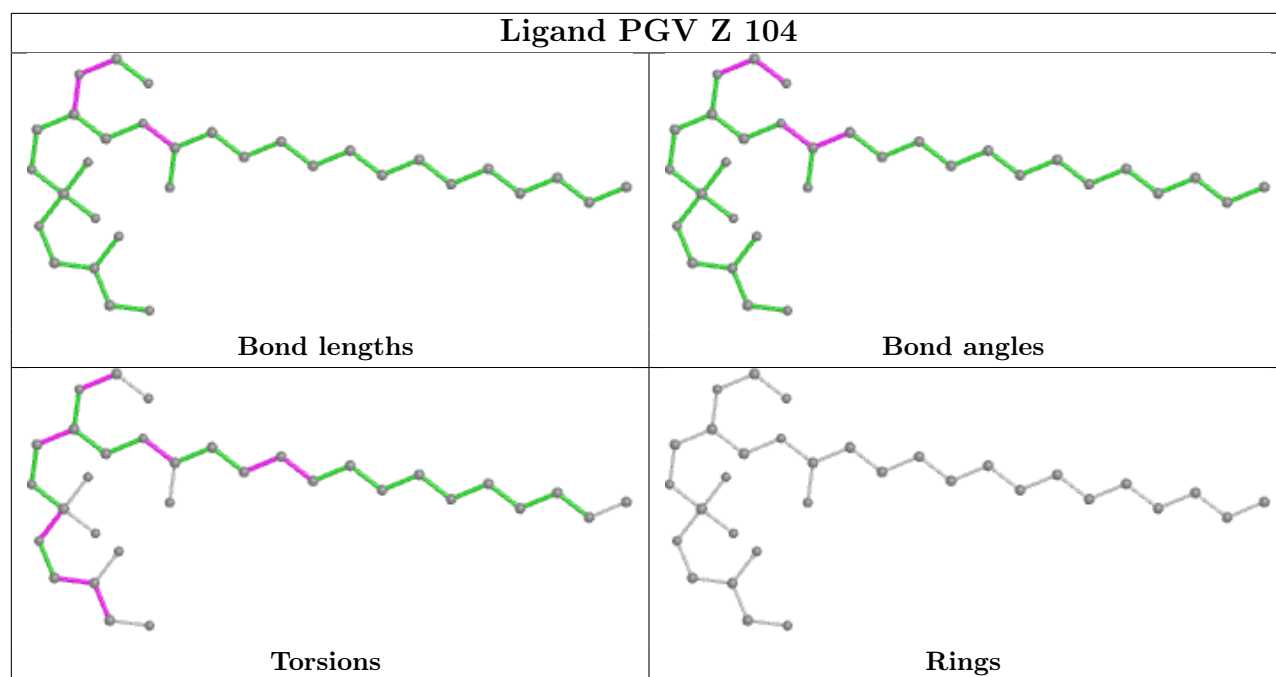
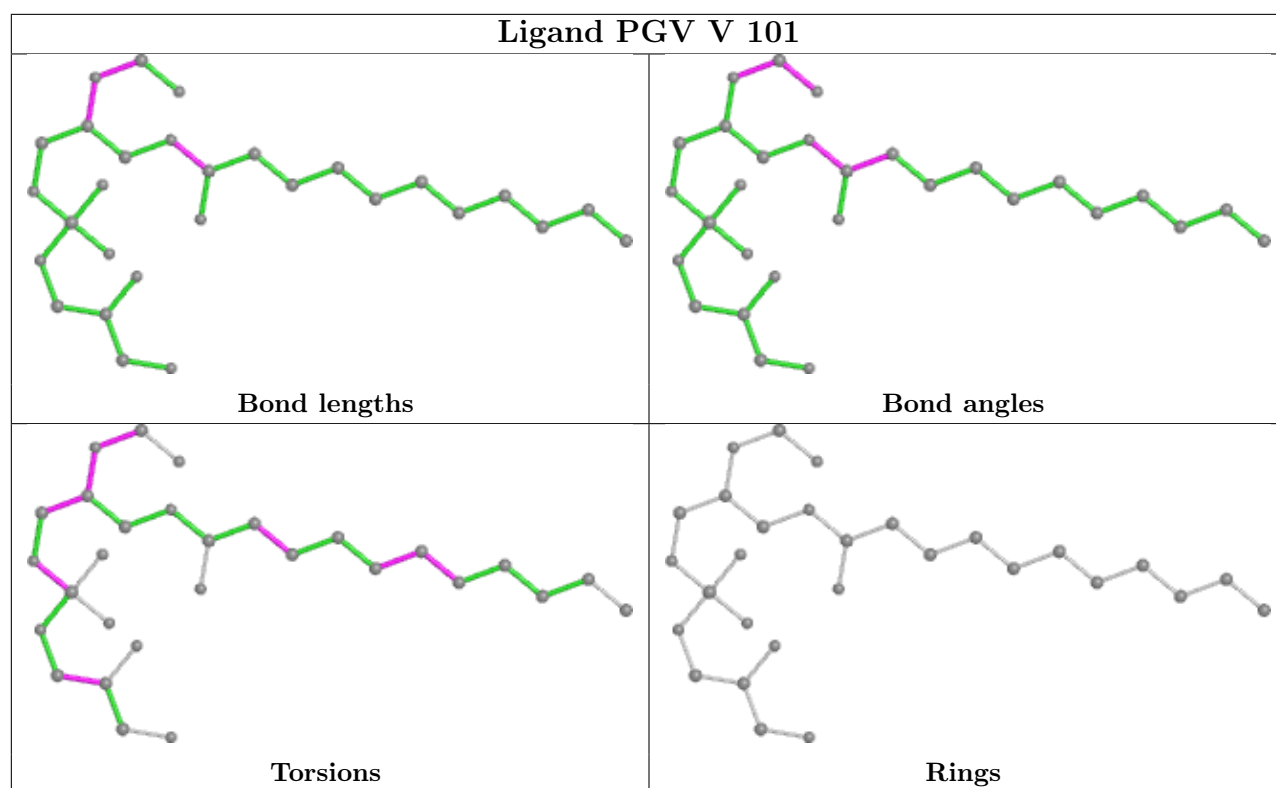


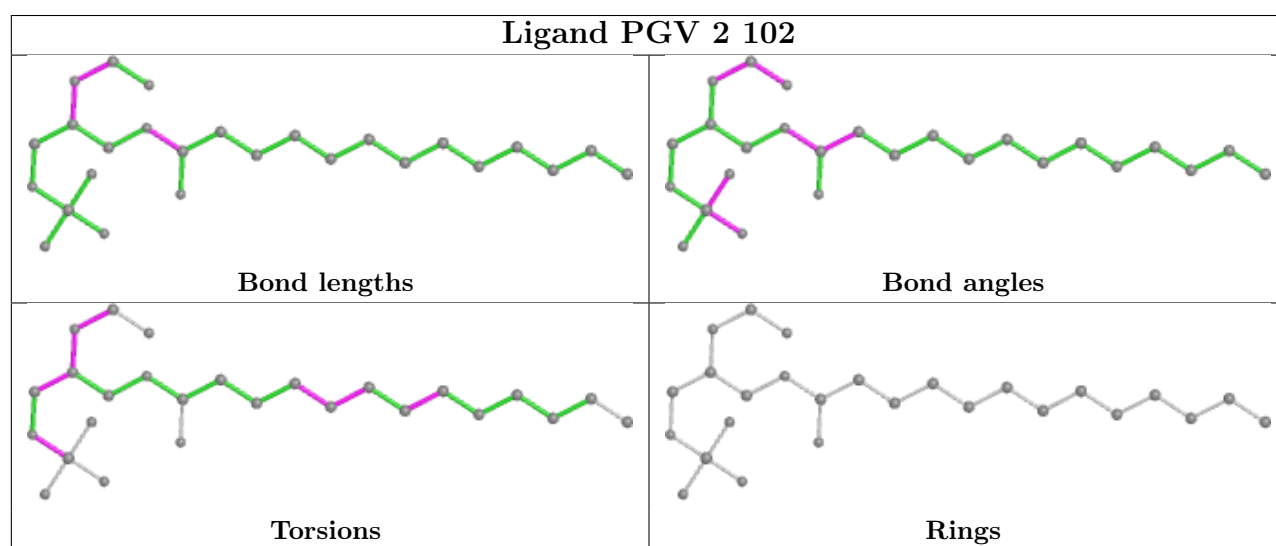
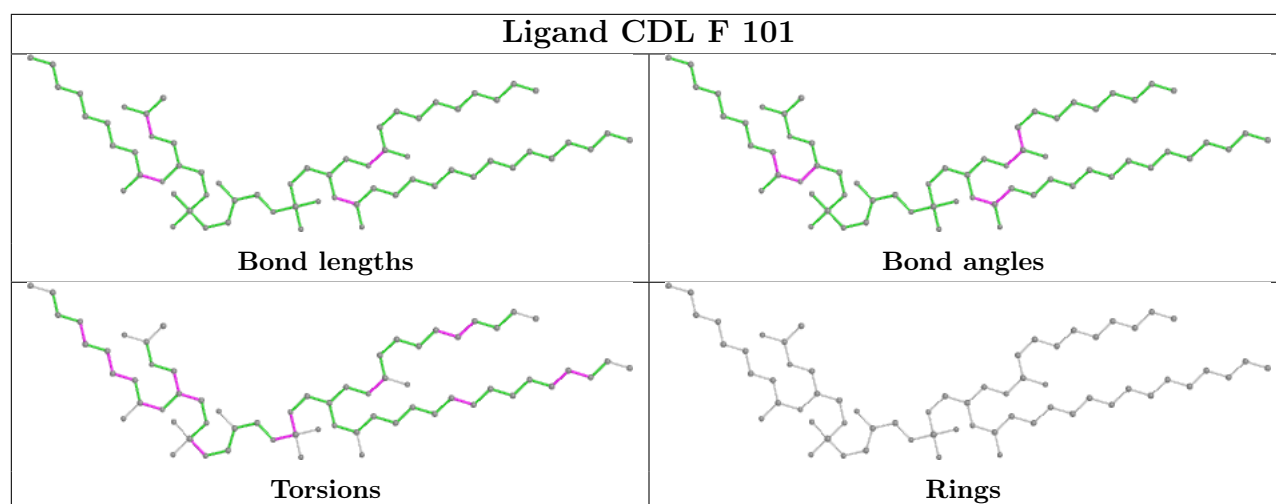


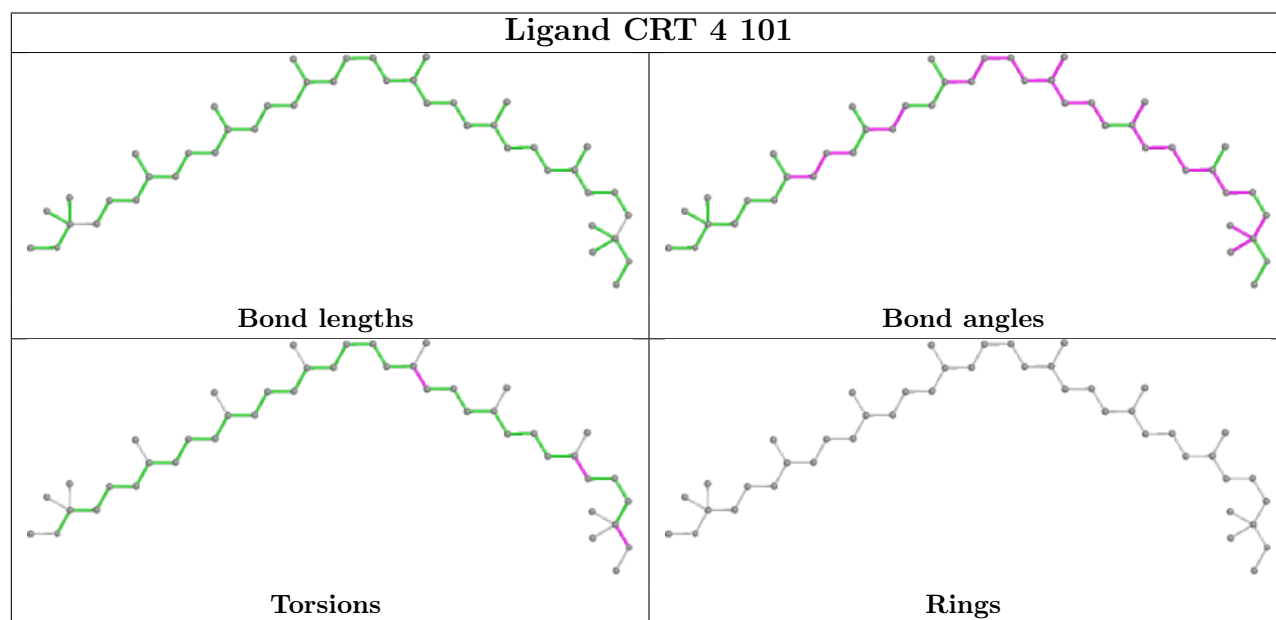
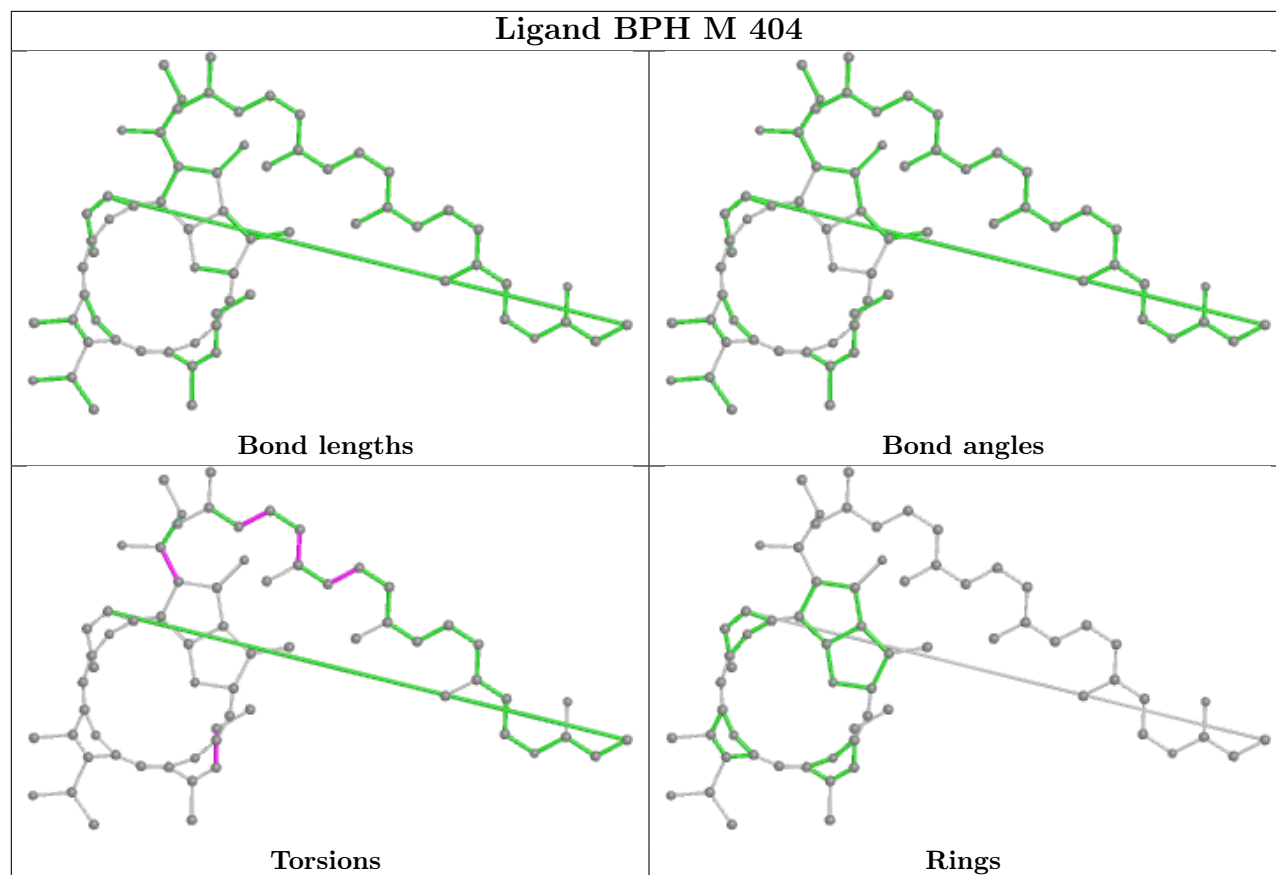


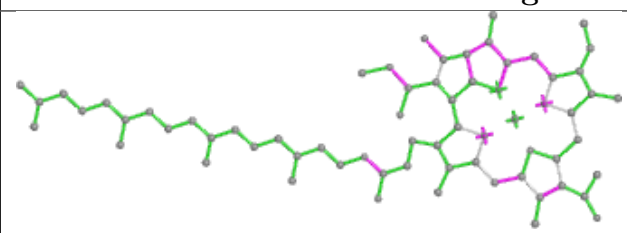
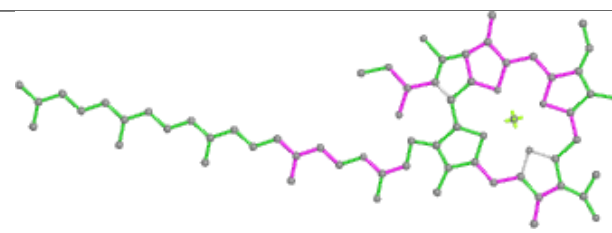
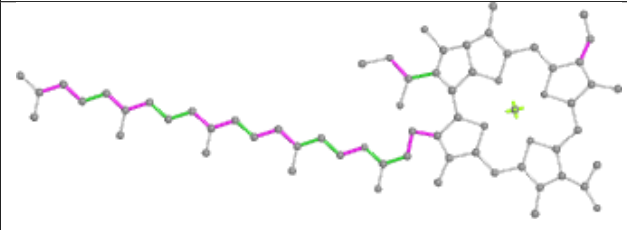
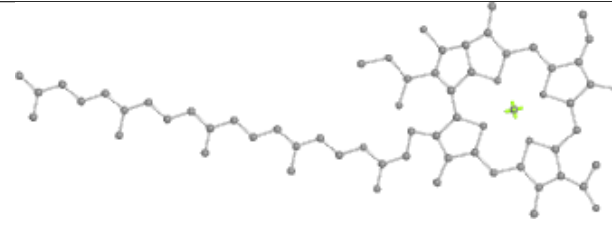
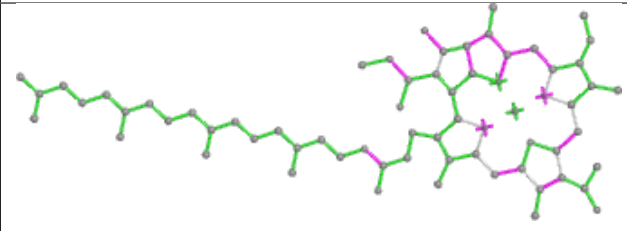
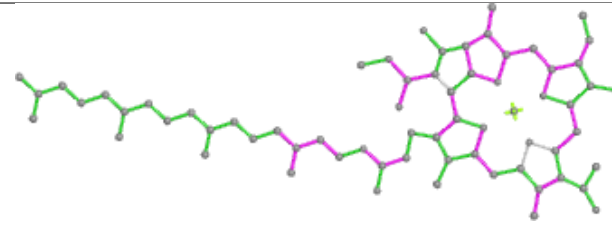
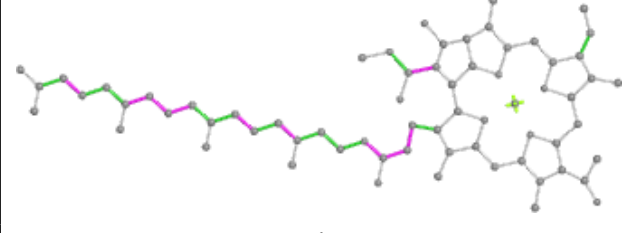
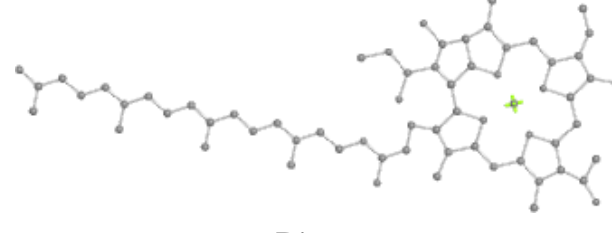
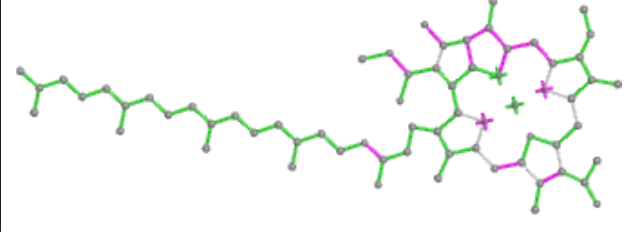
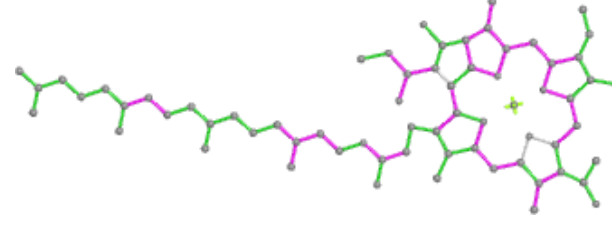
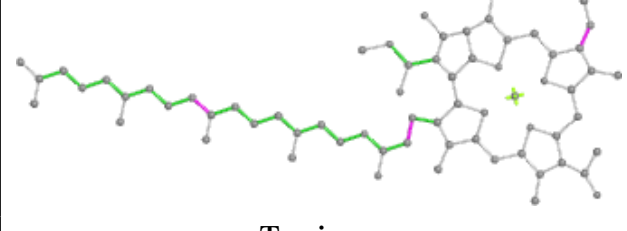
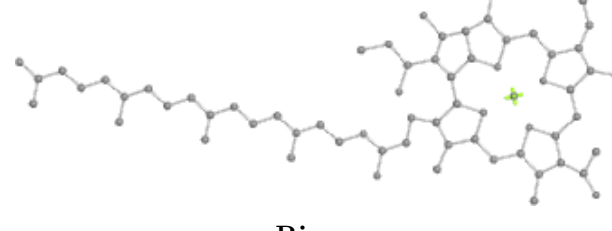


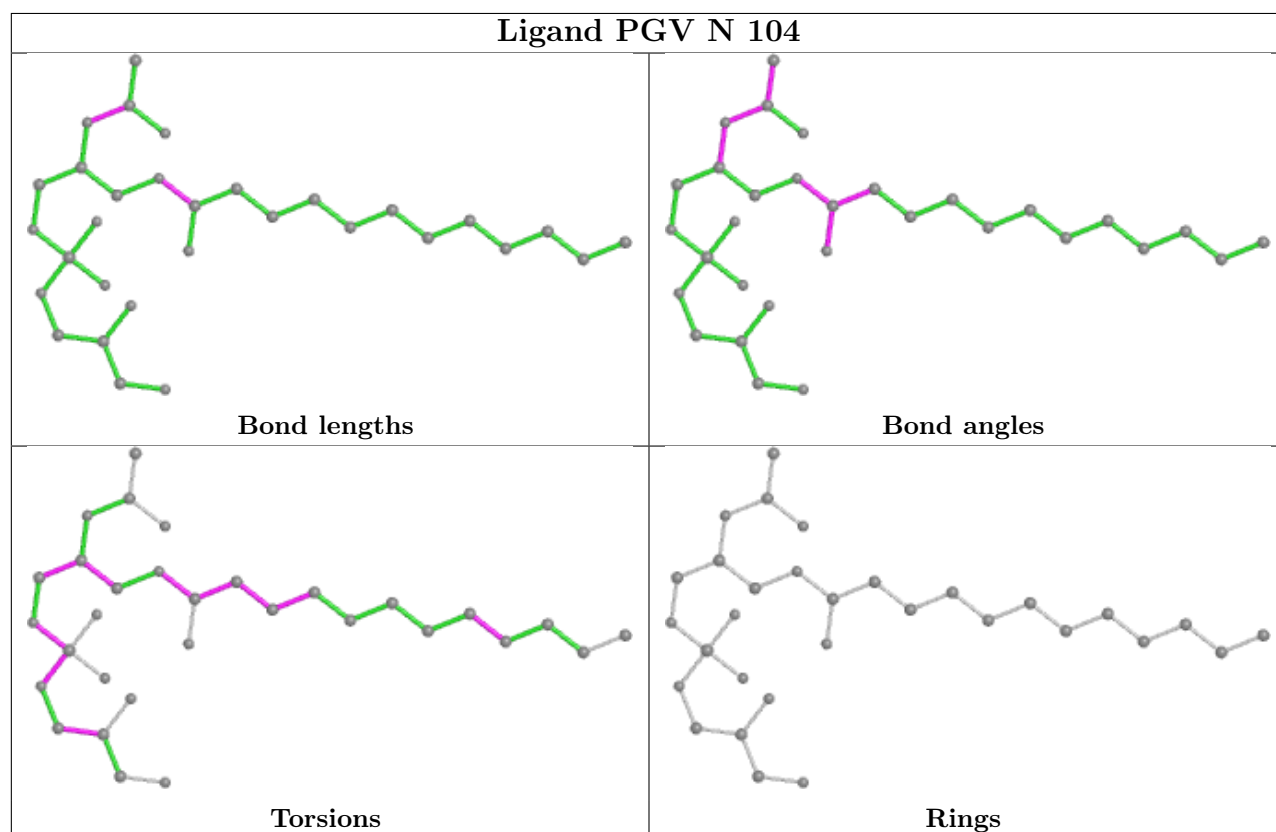
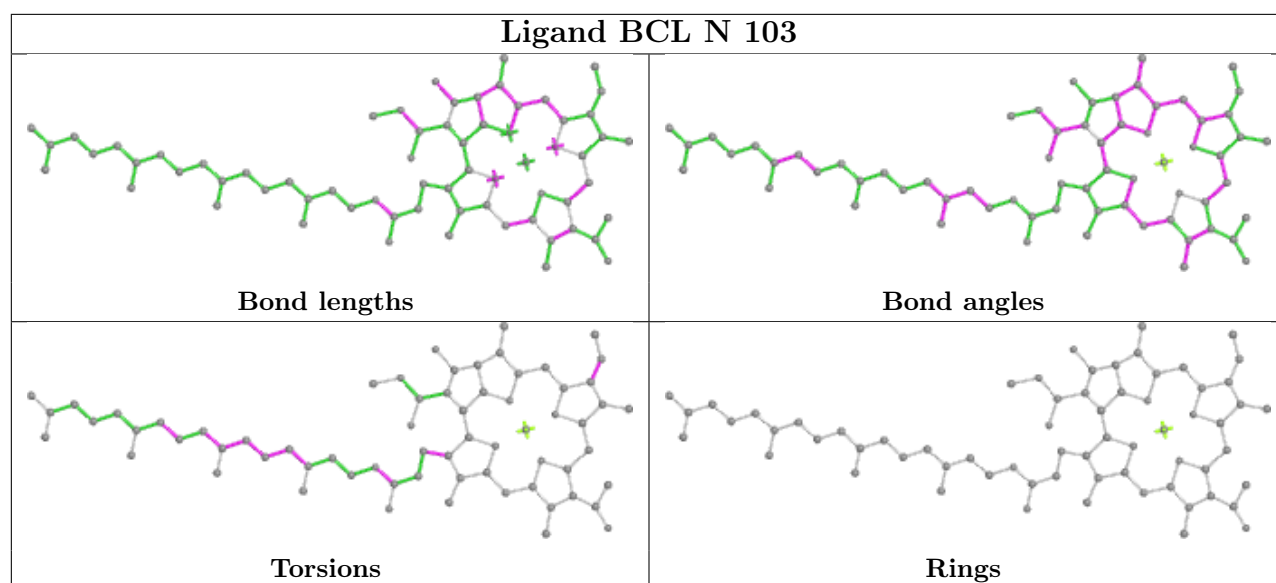


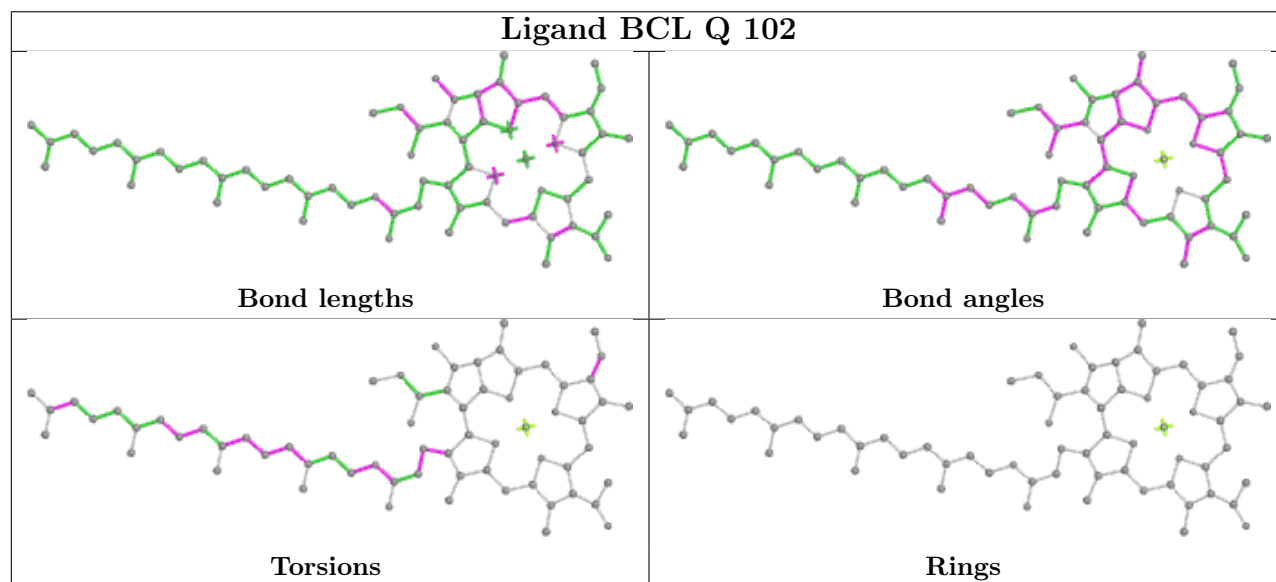
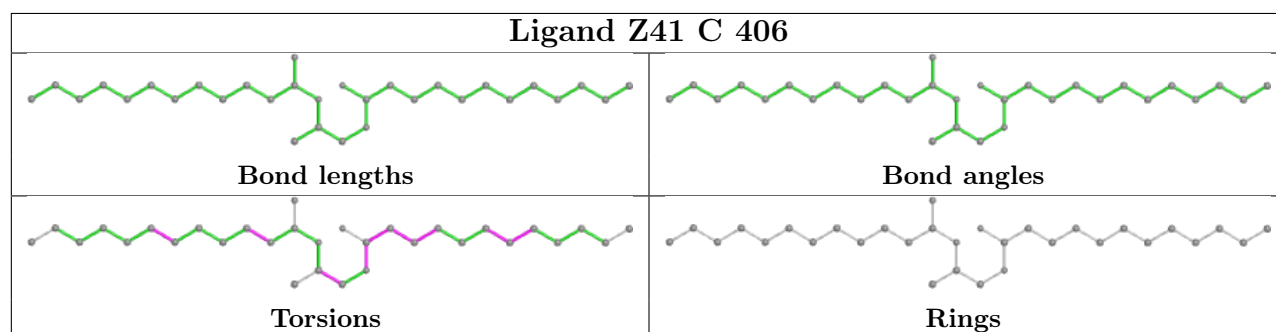
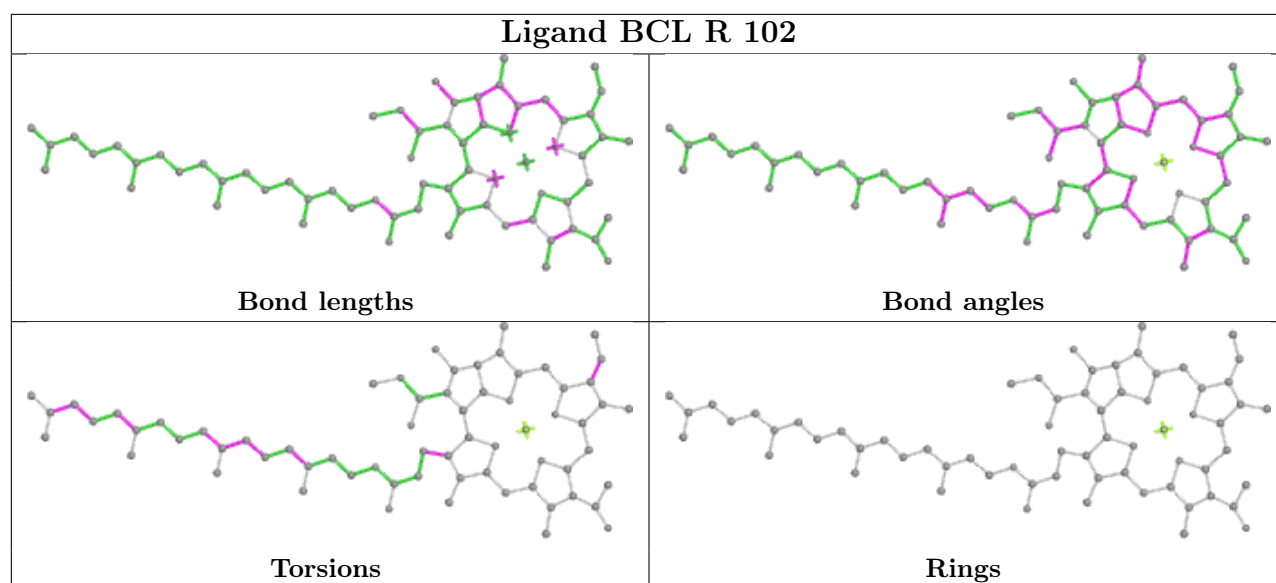


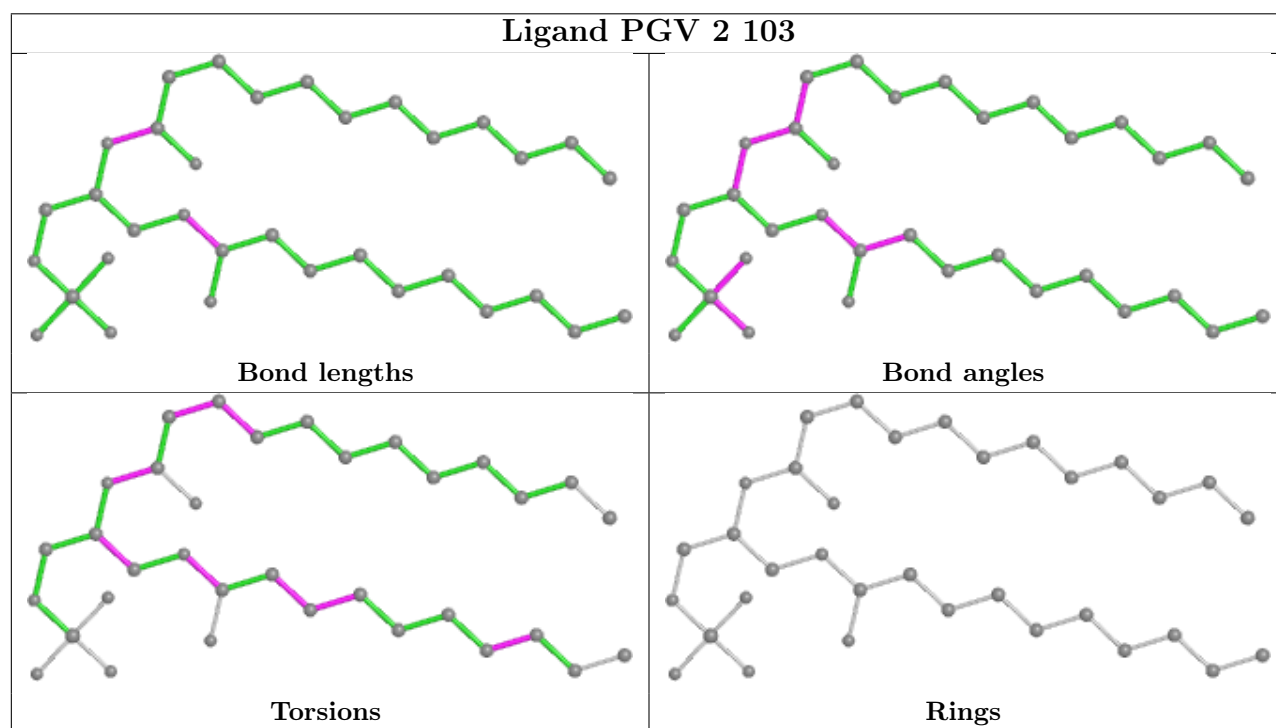
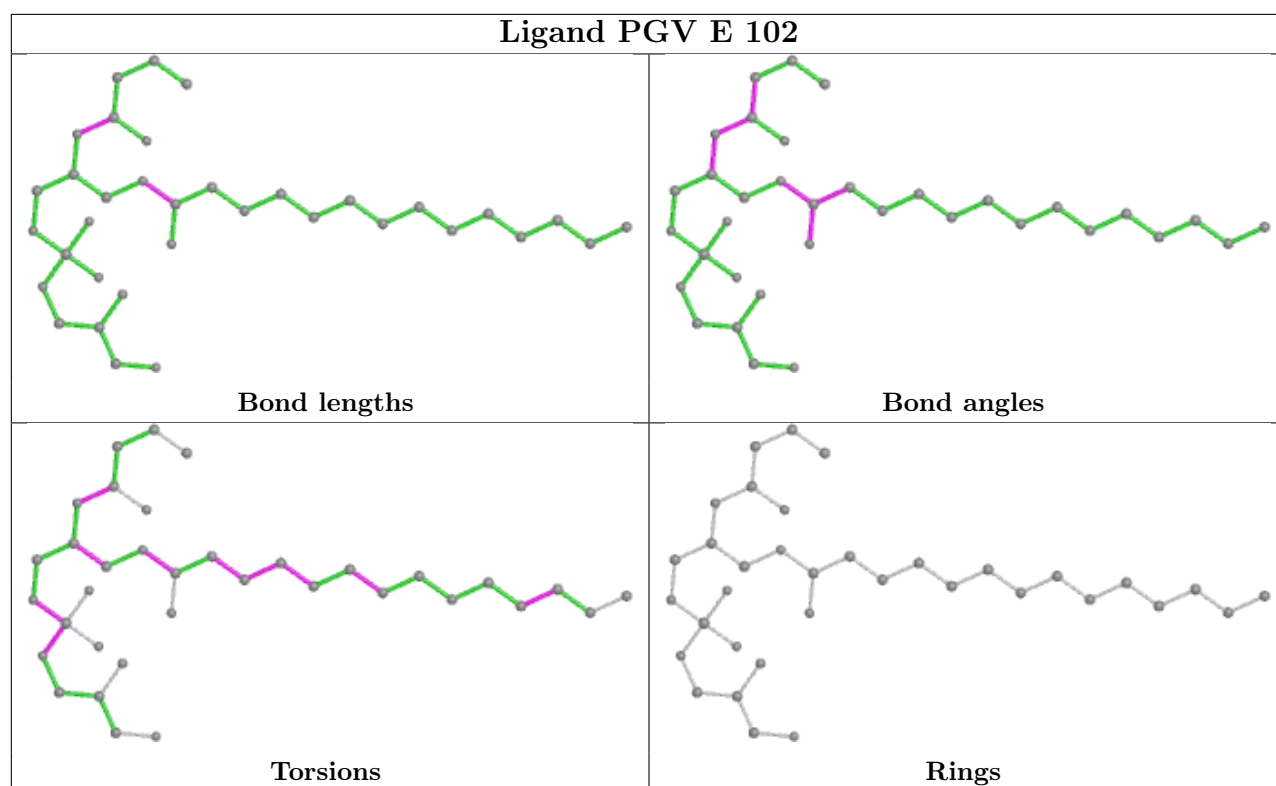


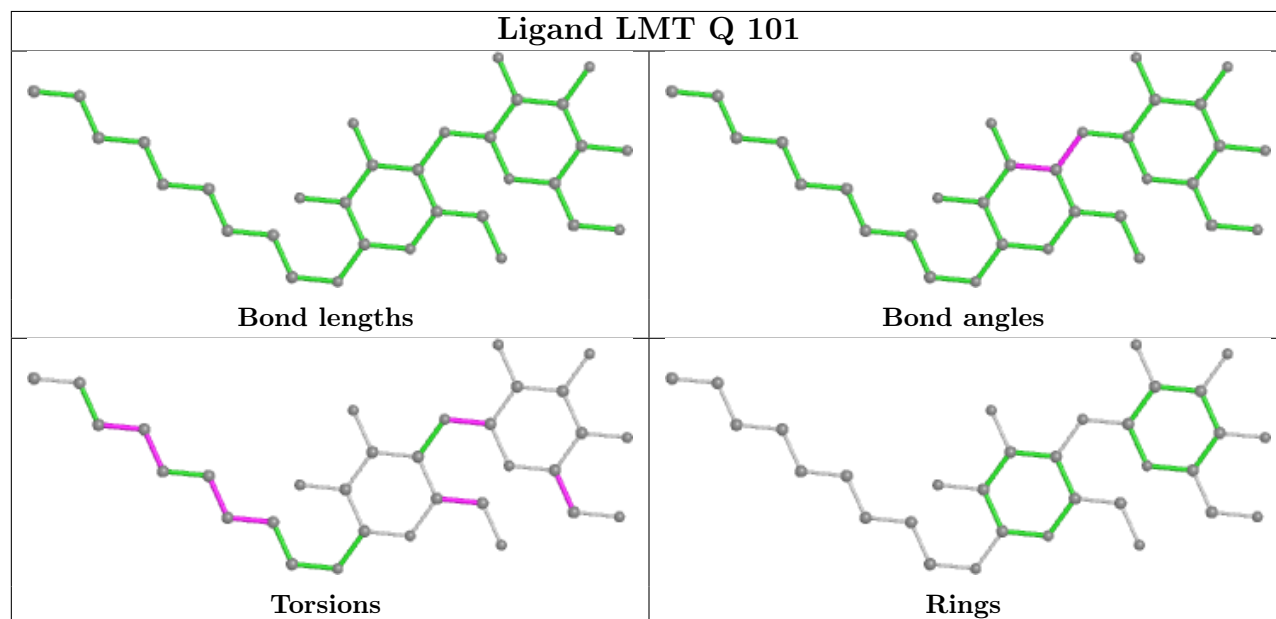
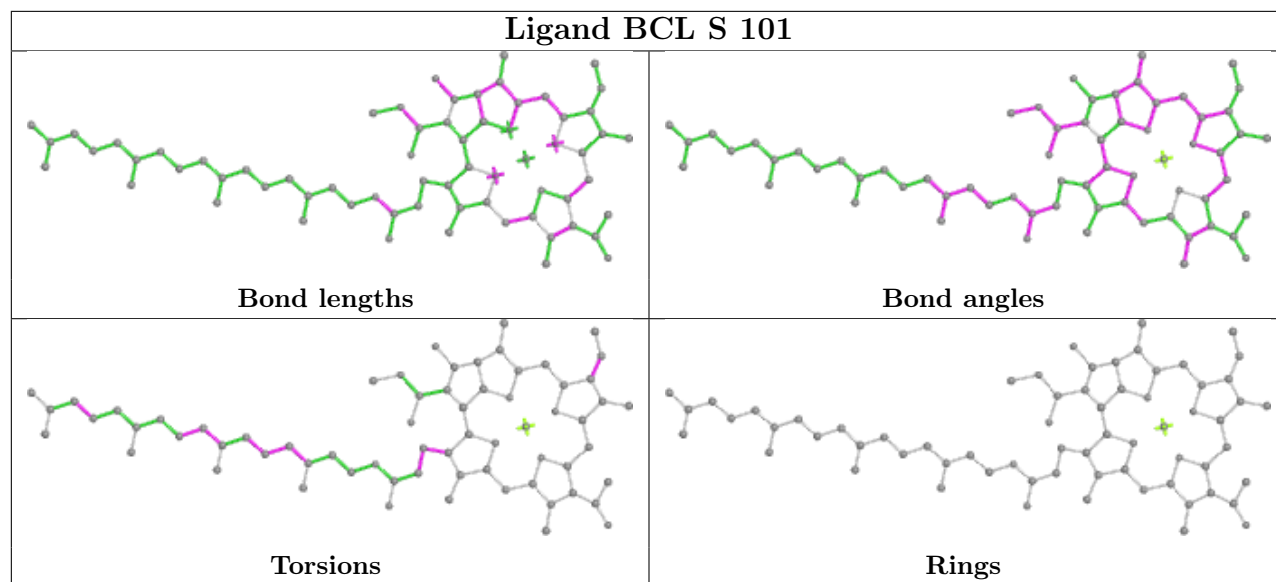


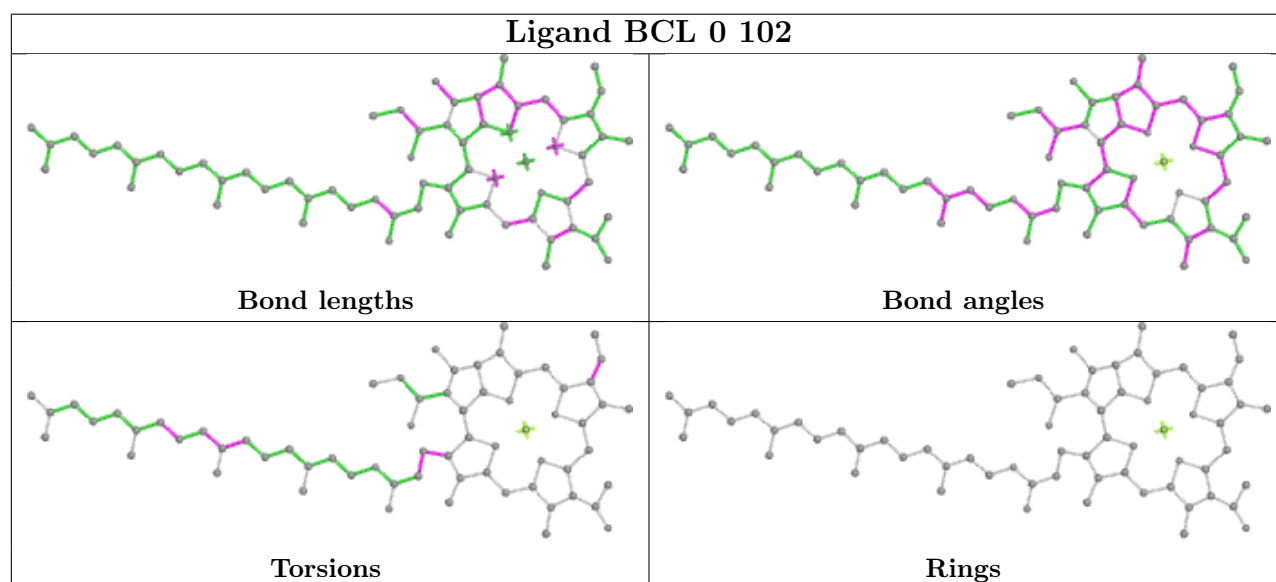
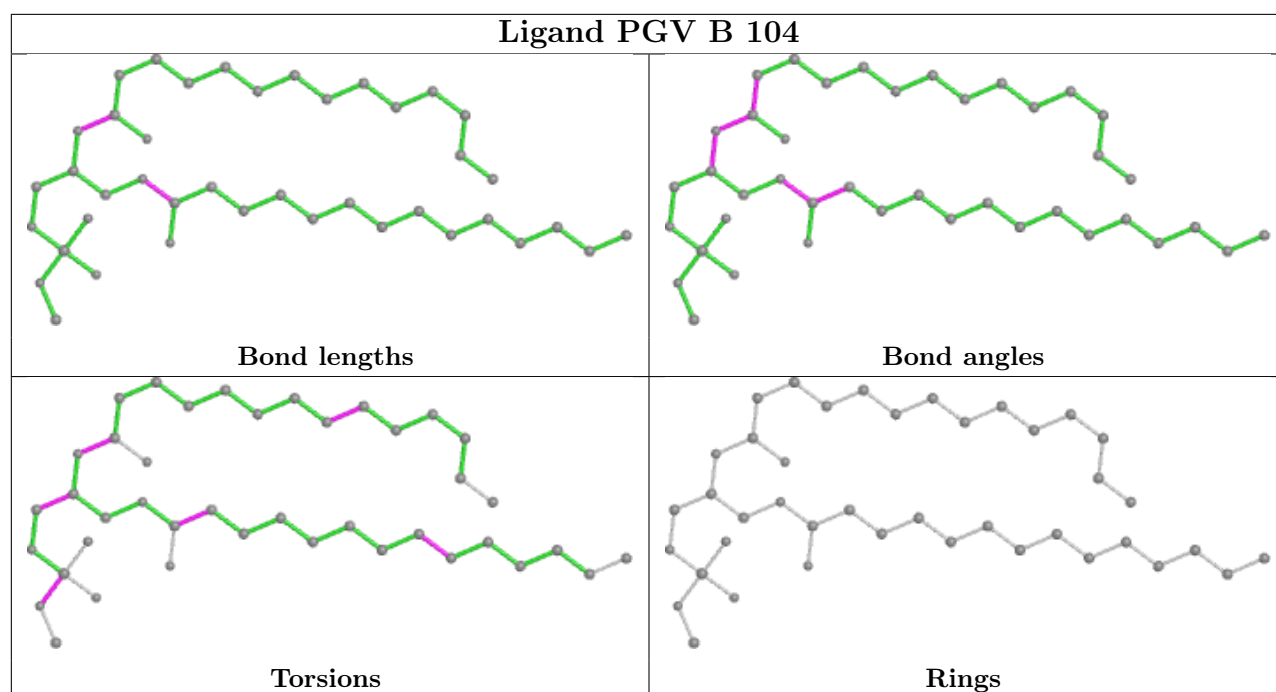
Ligand BCL A 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL W 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCL 6 101	
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 <p>Torsions</p>	 <p>Rings</p>

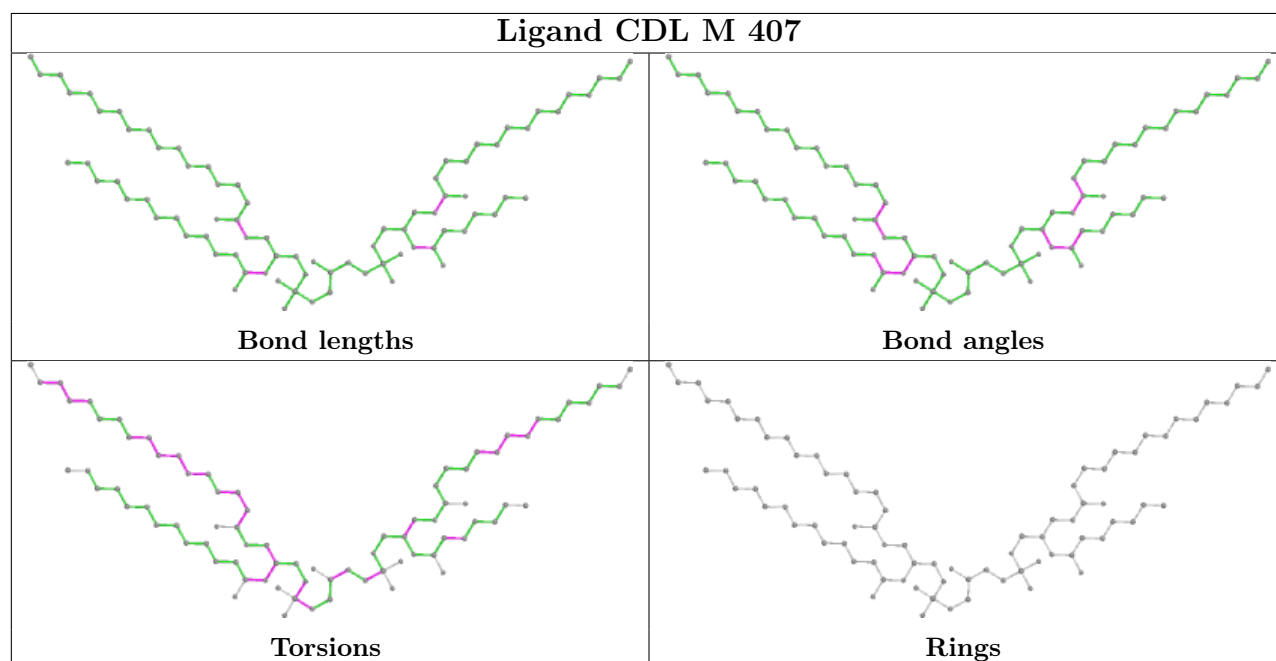
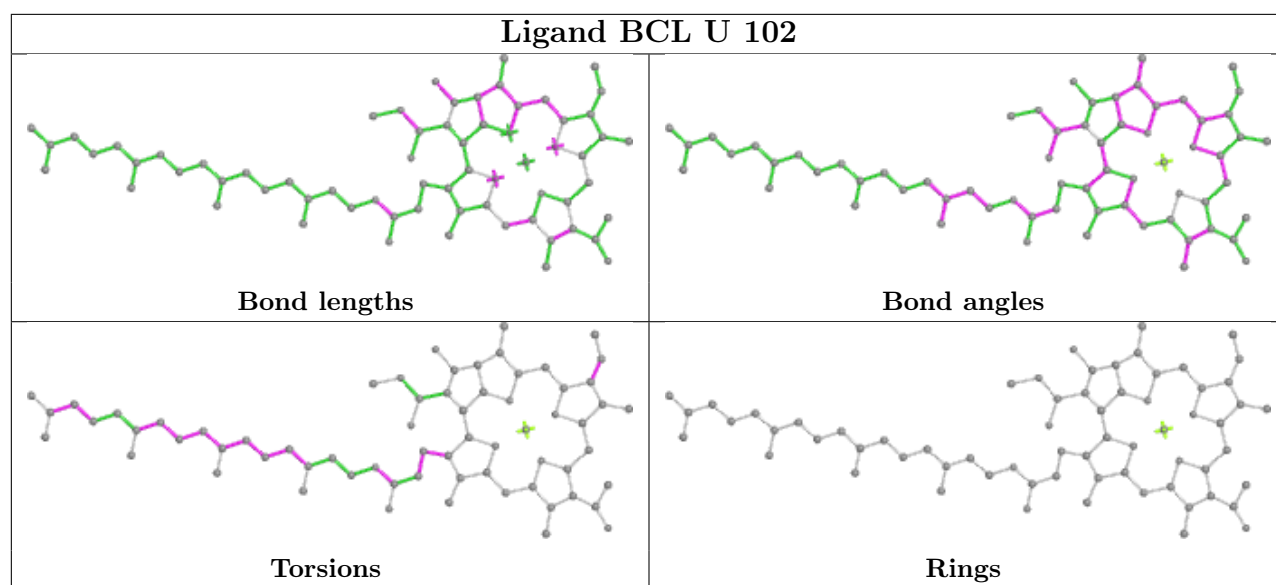


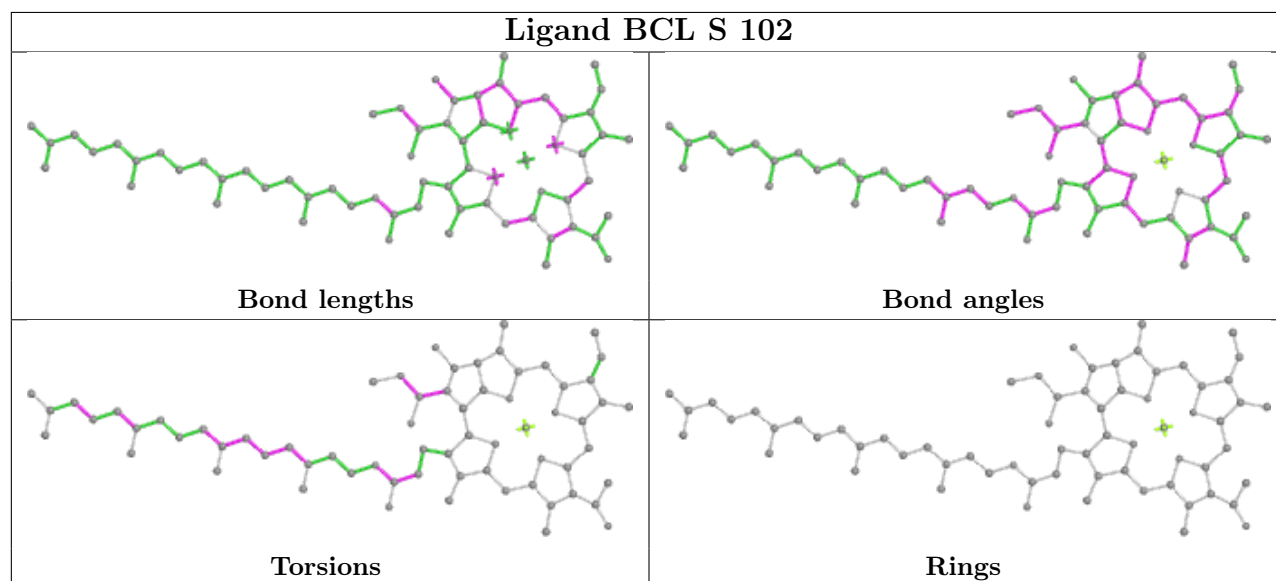
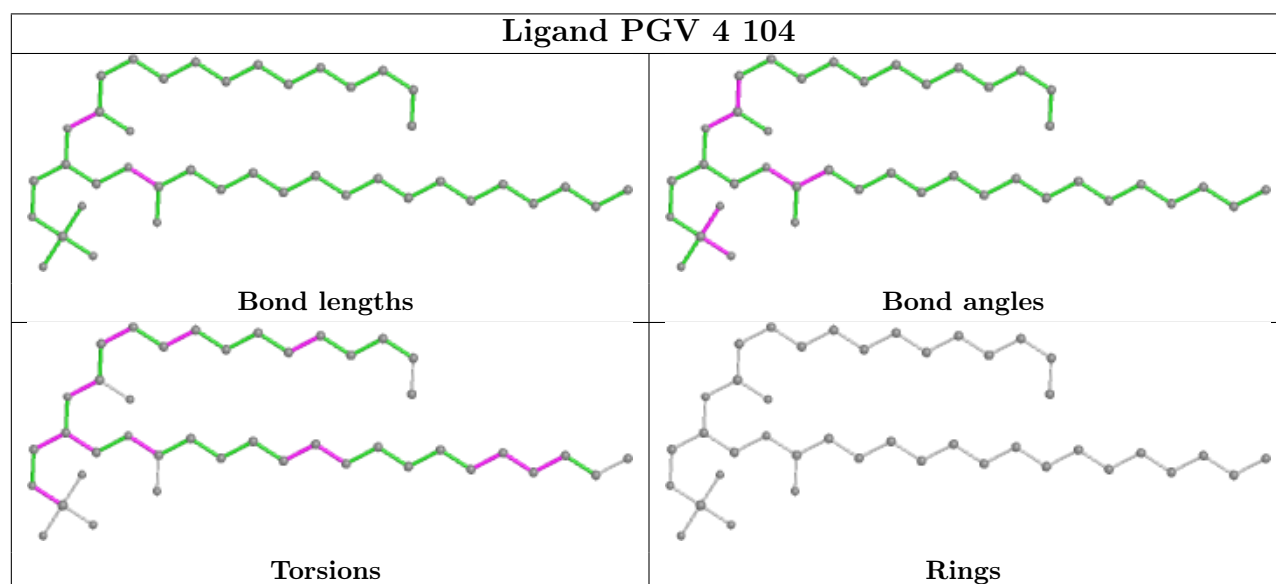
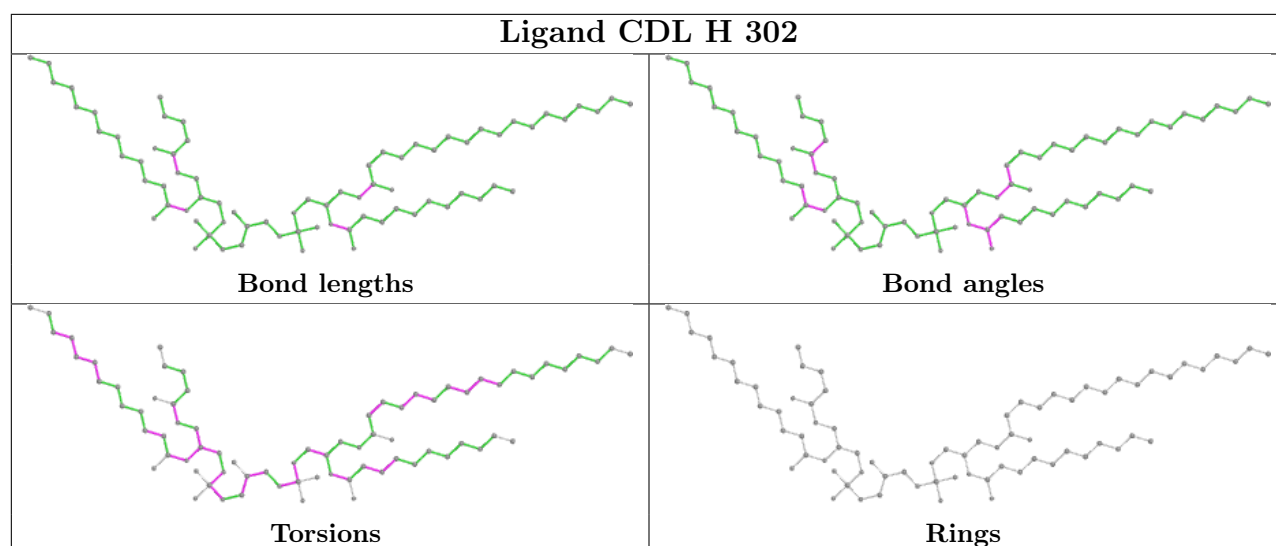


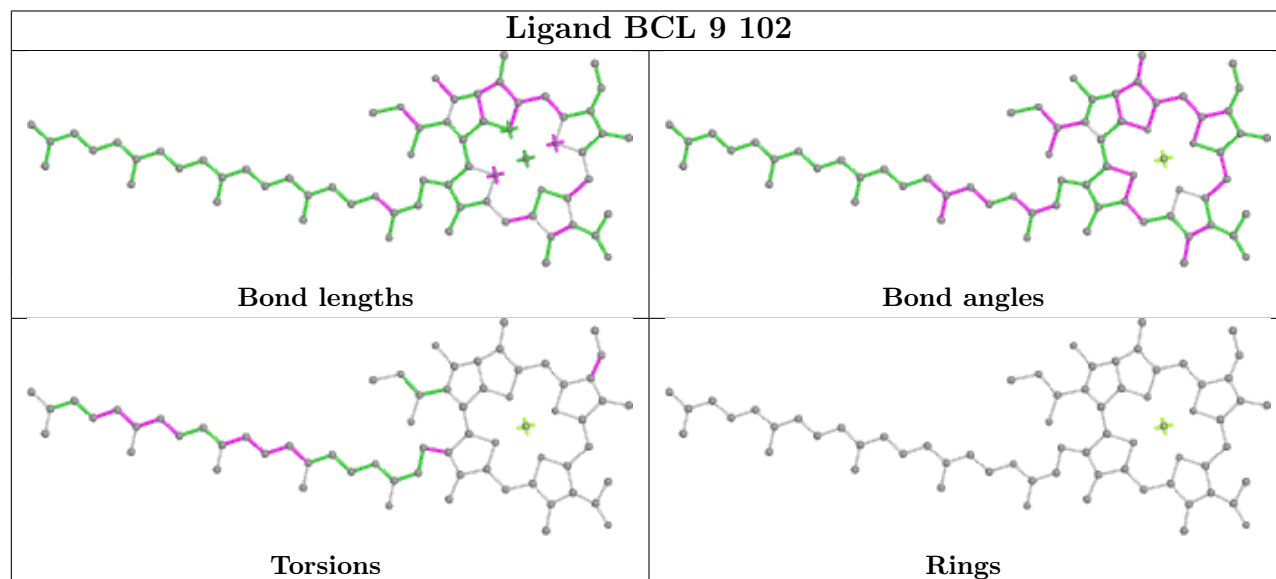
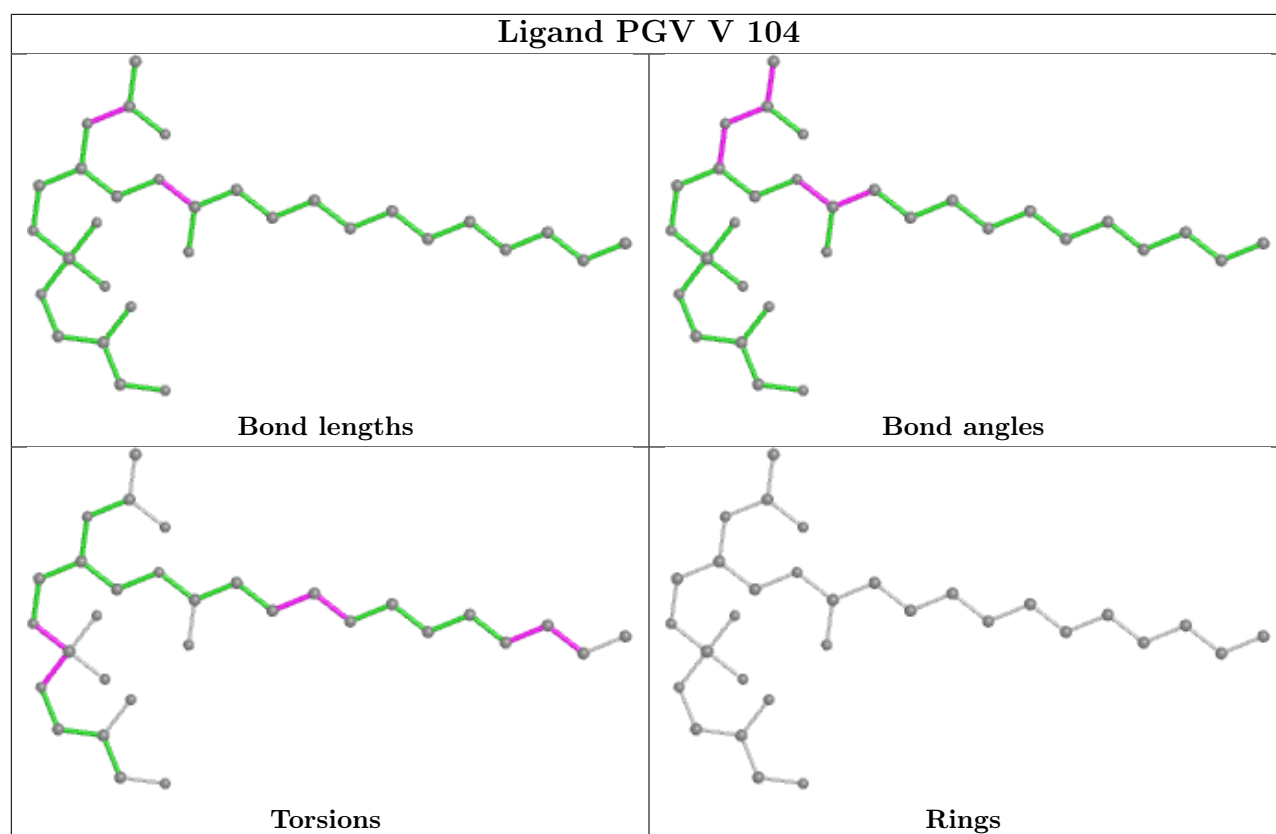


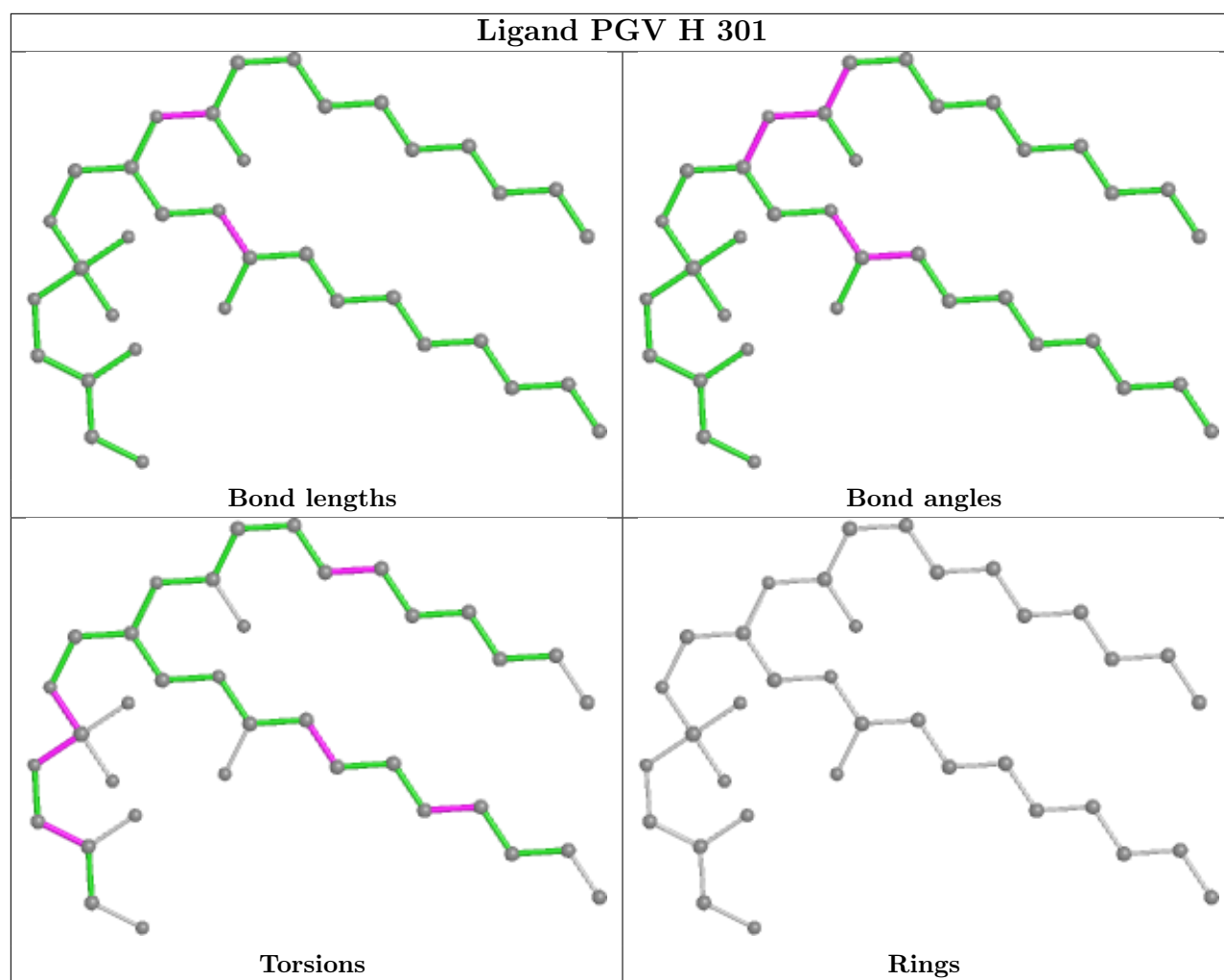


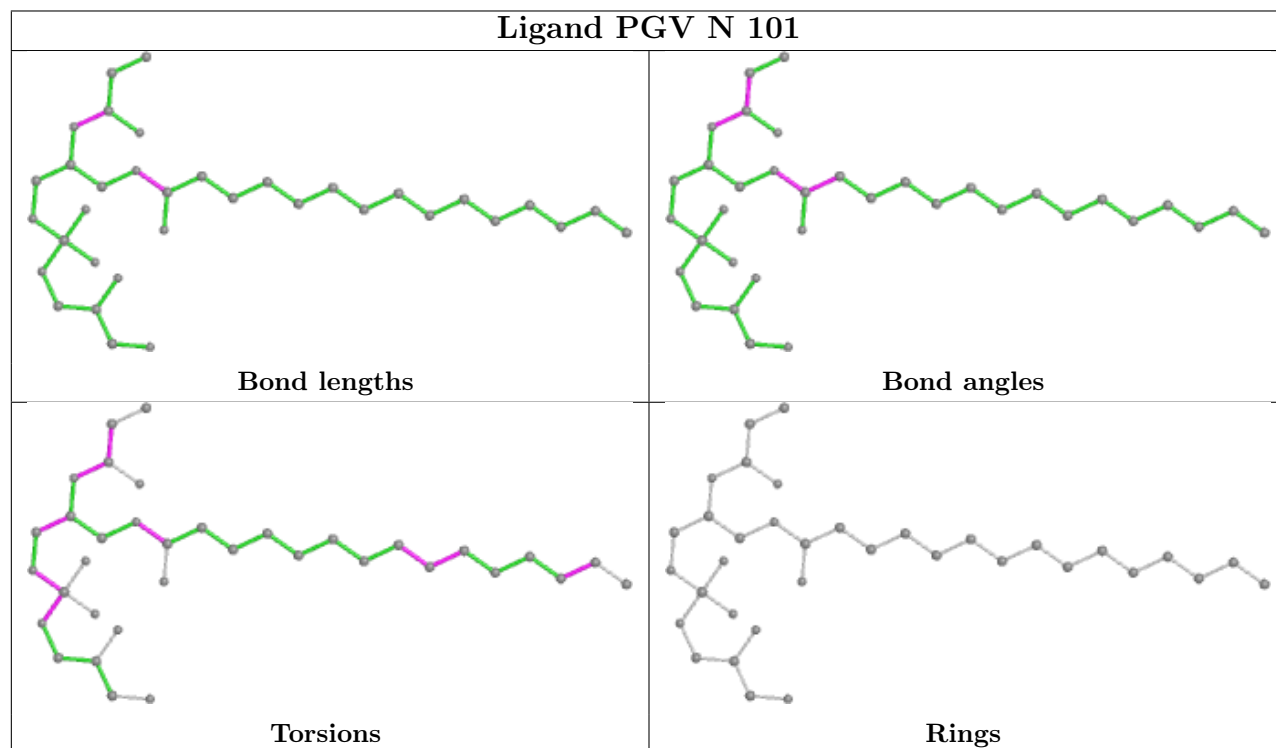
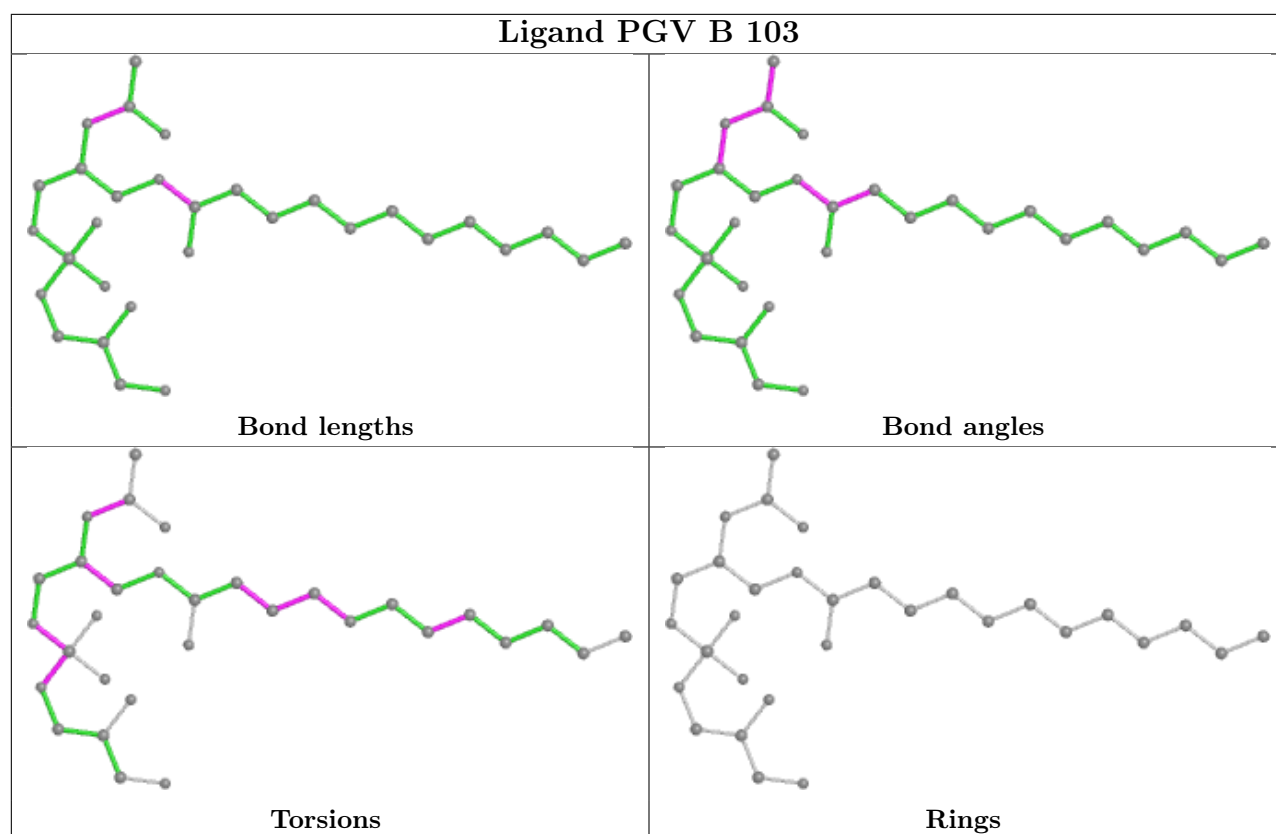


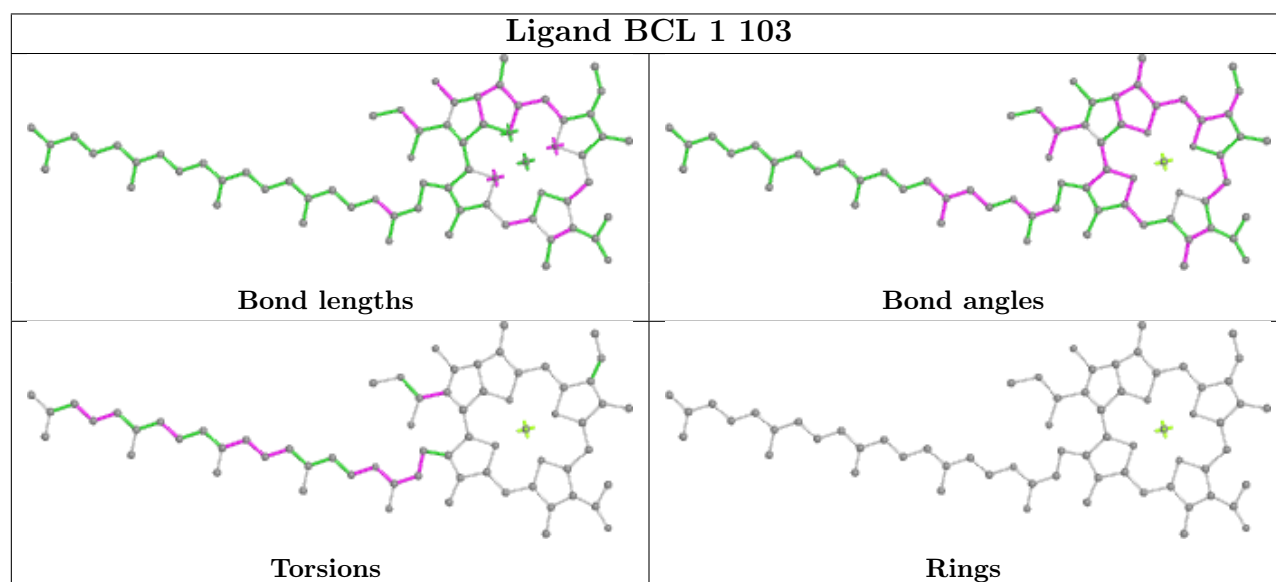
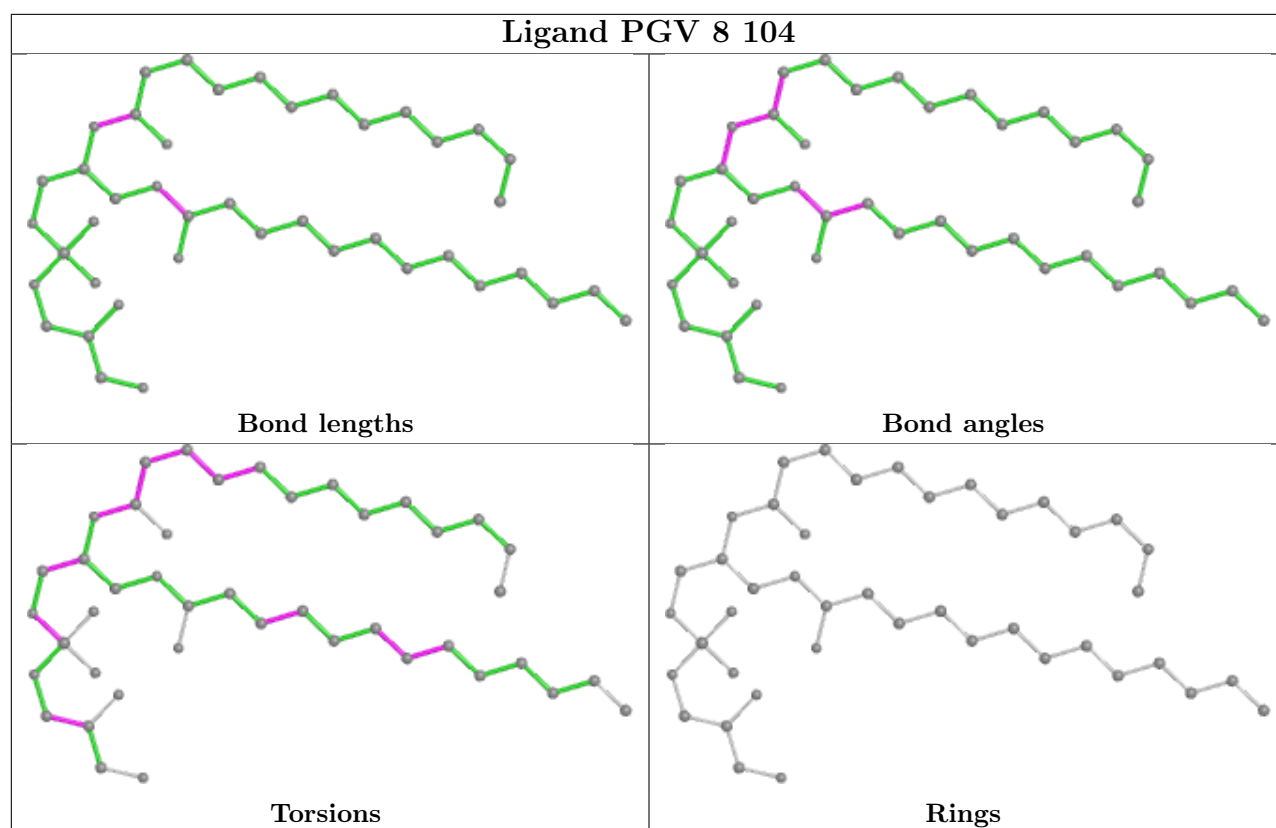


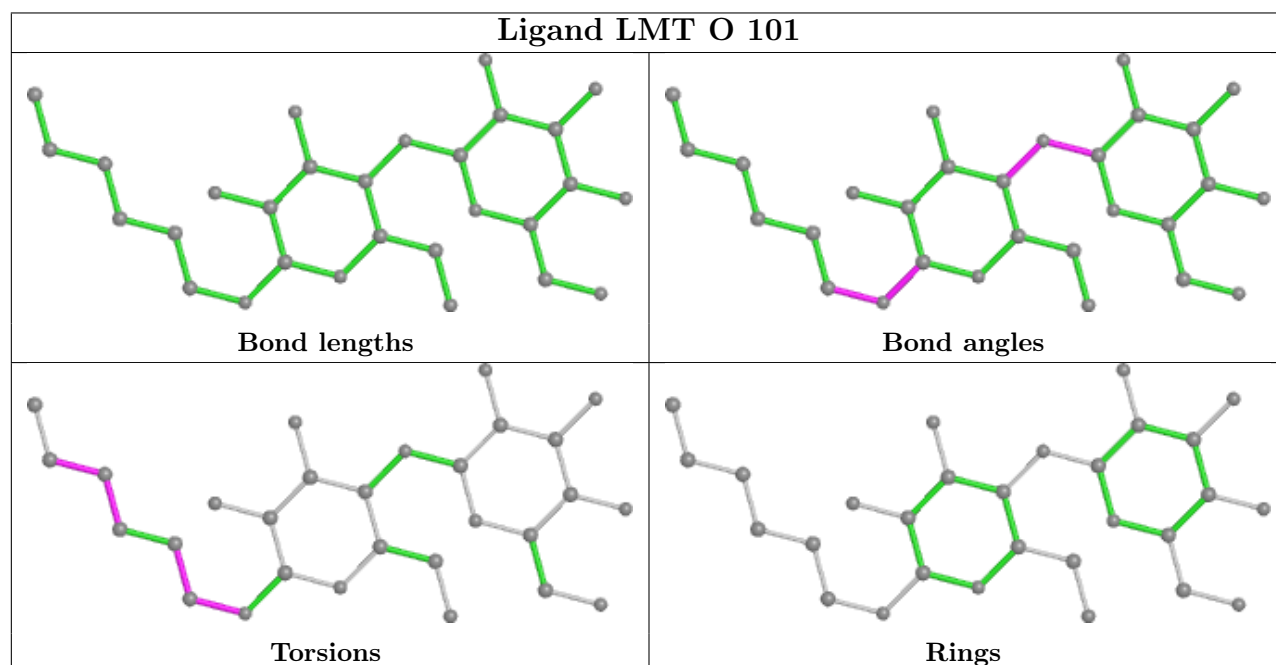
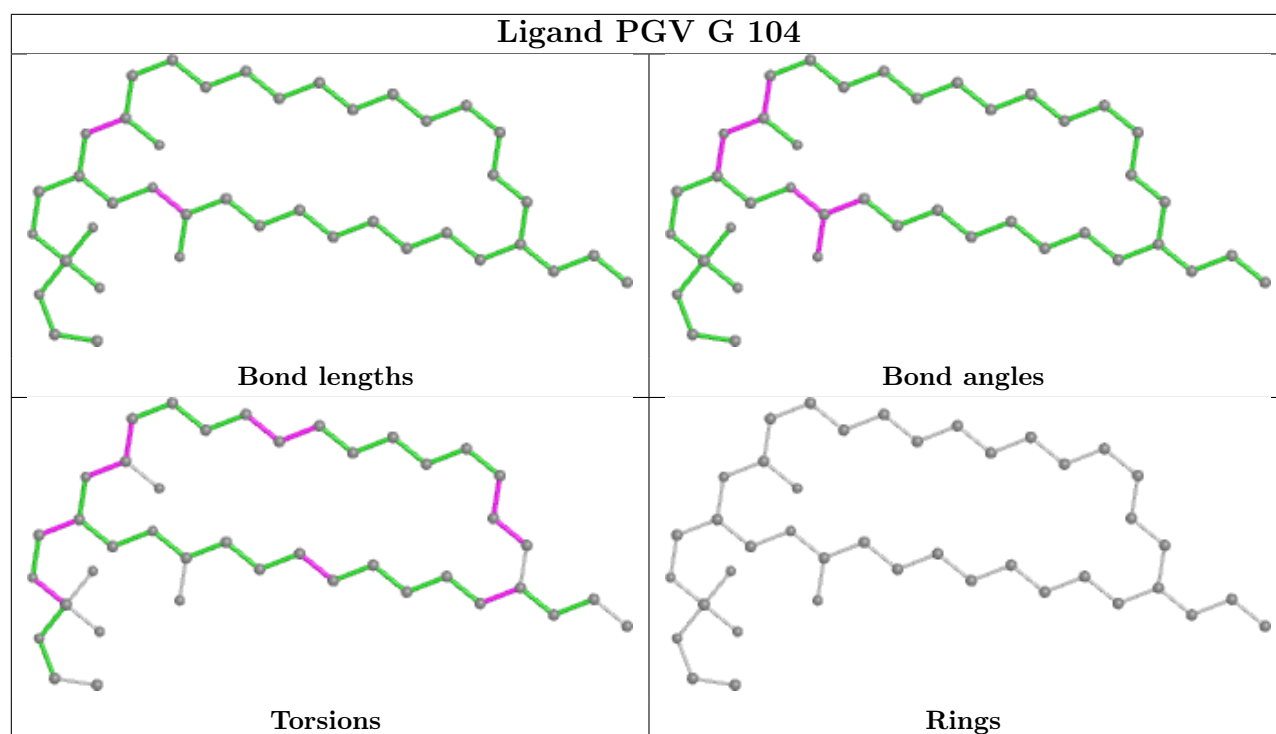


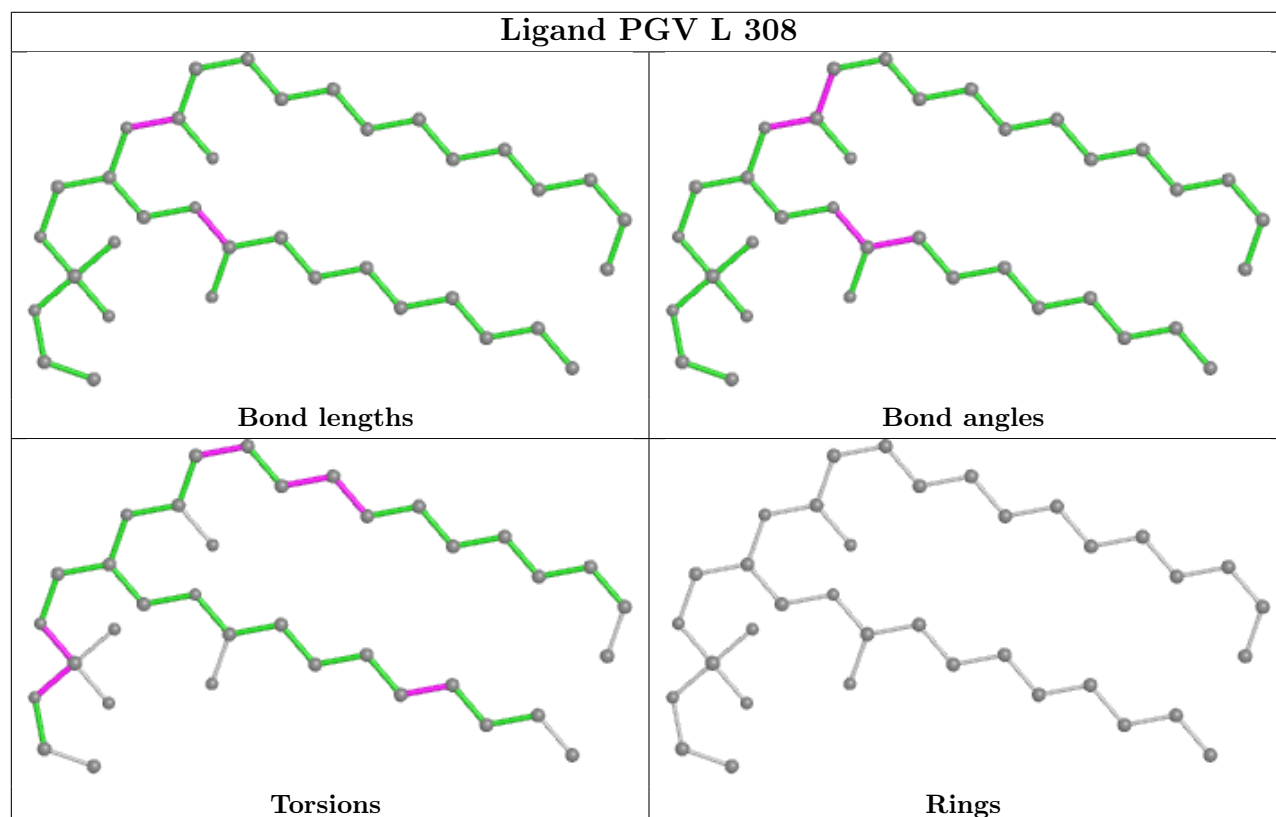
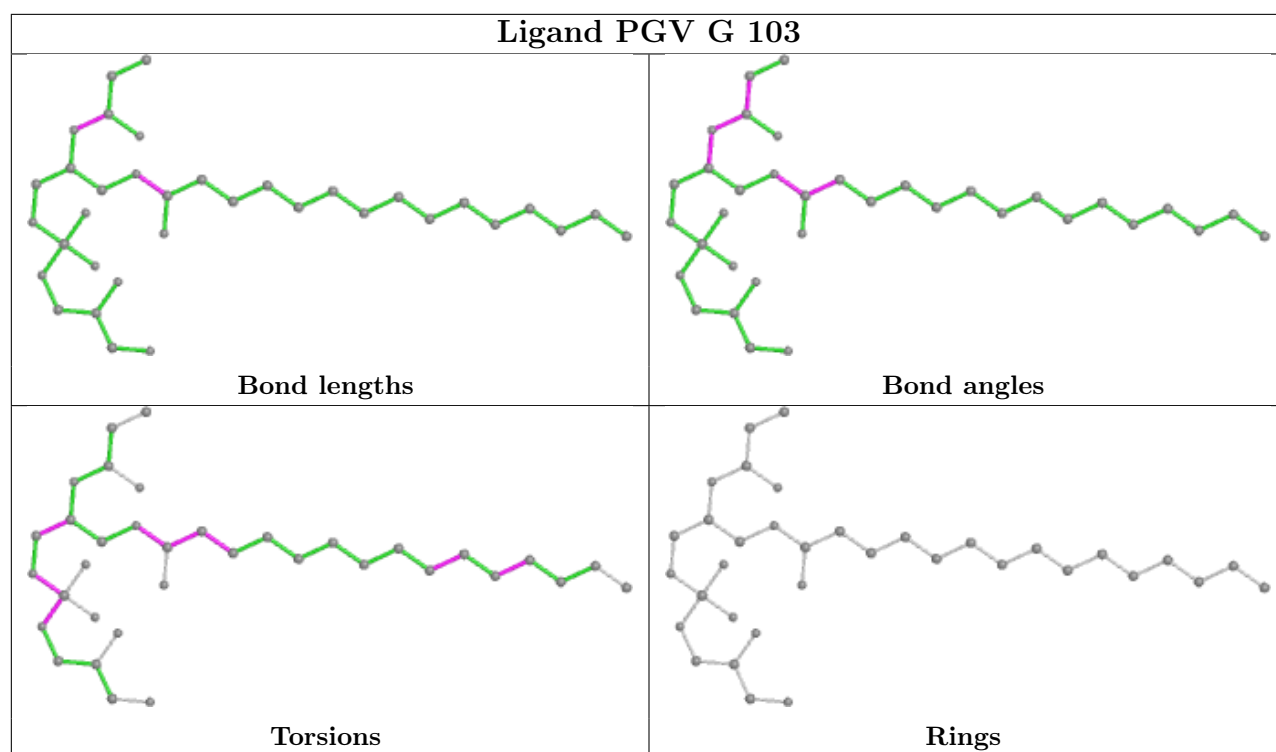


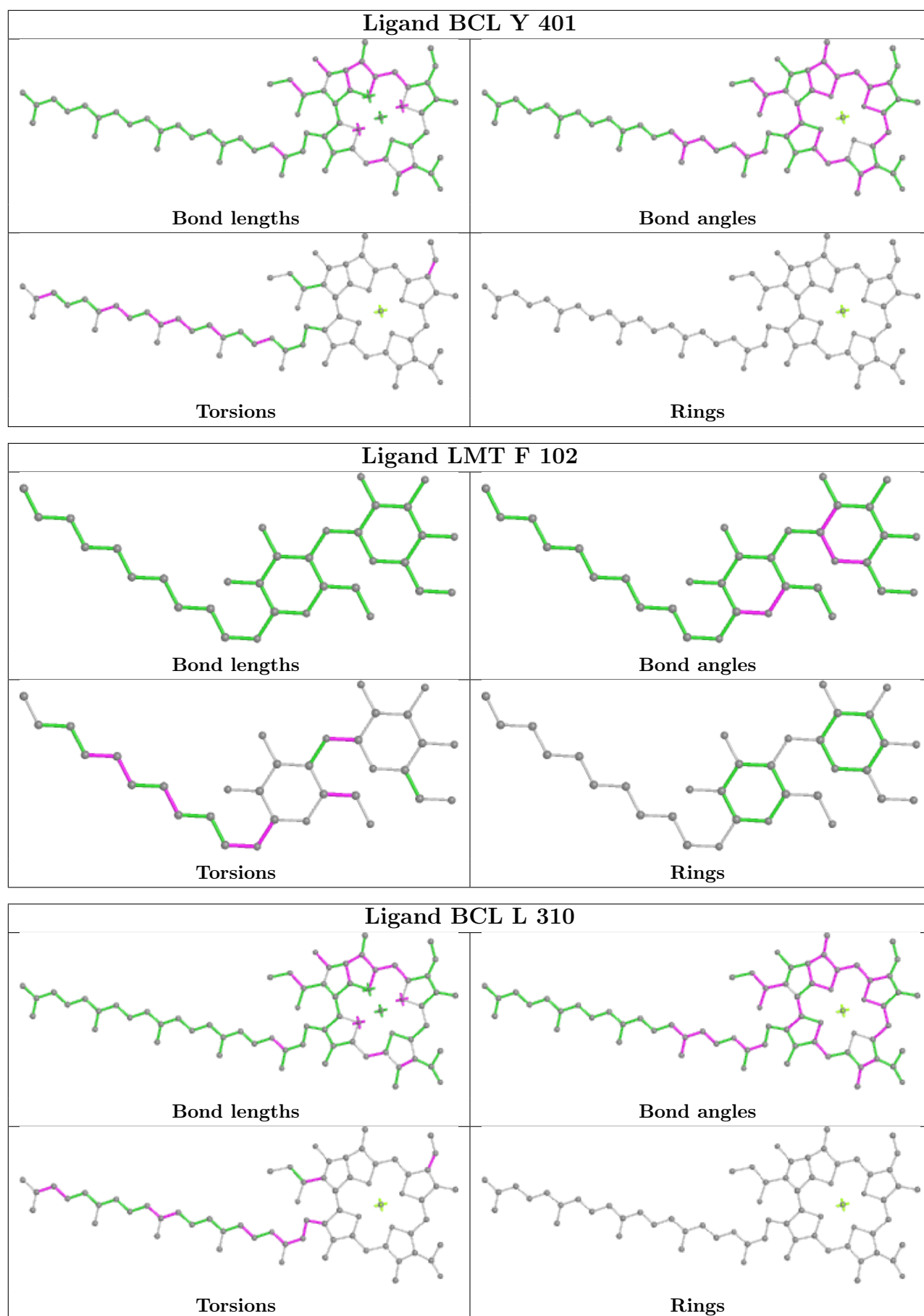


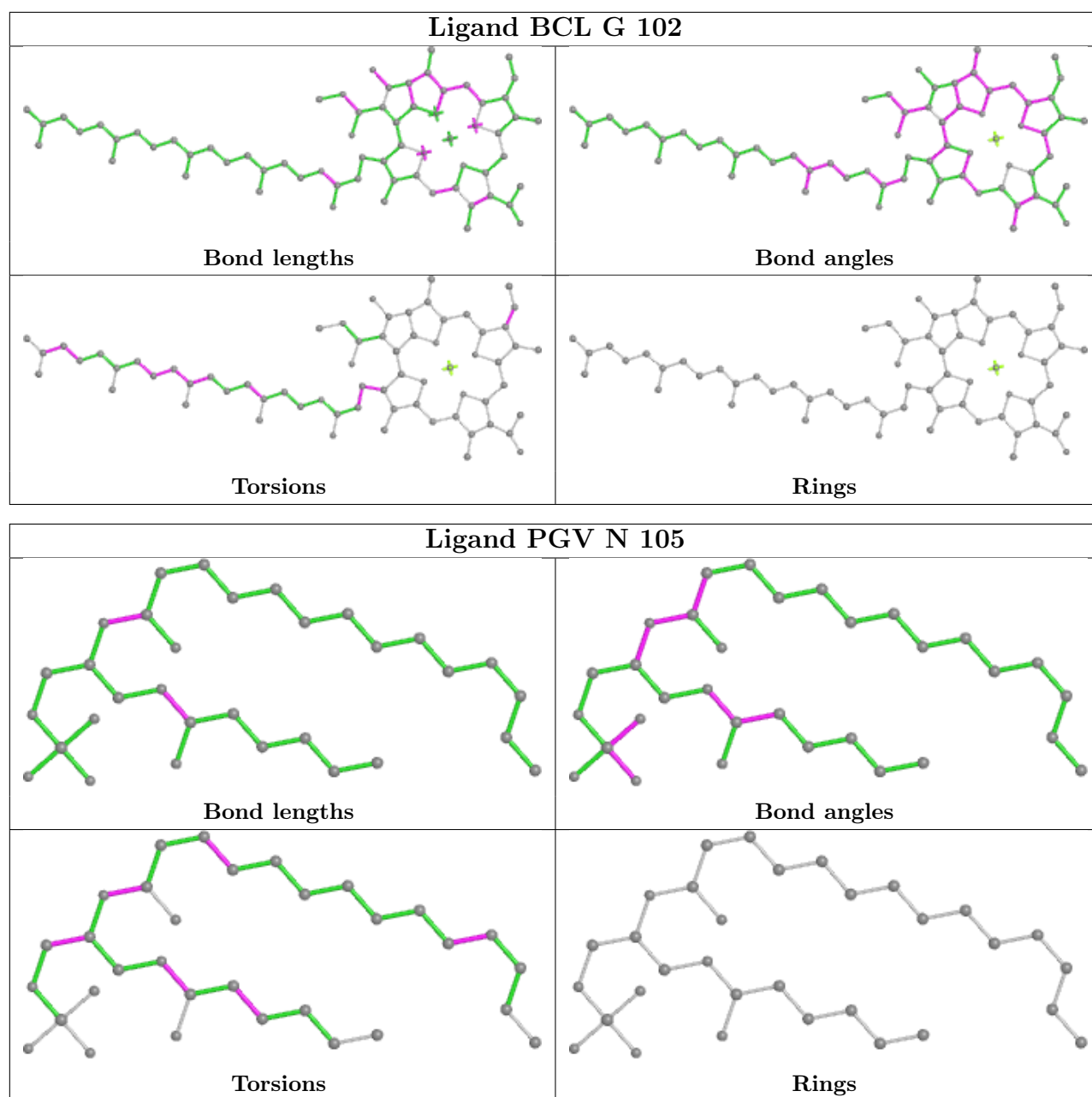


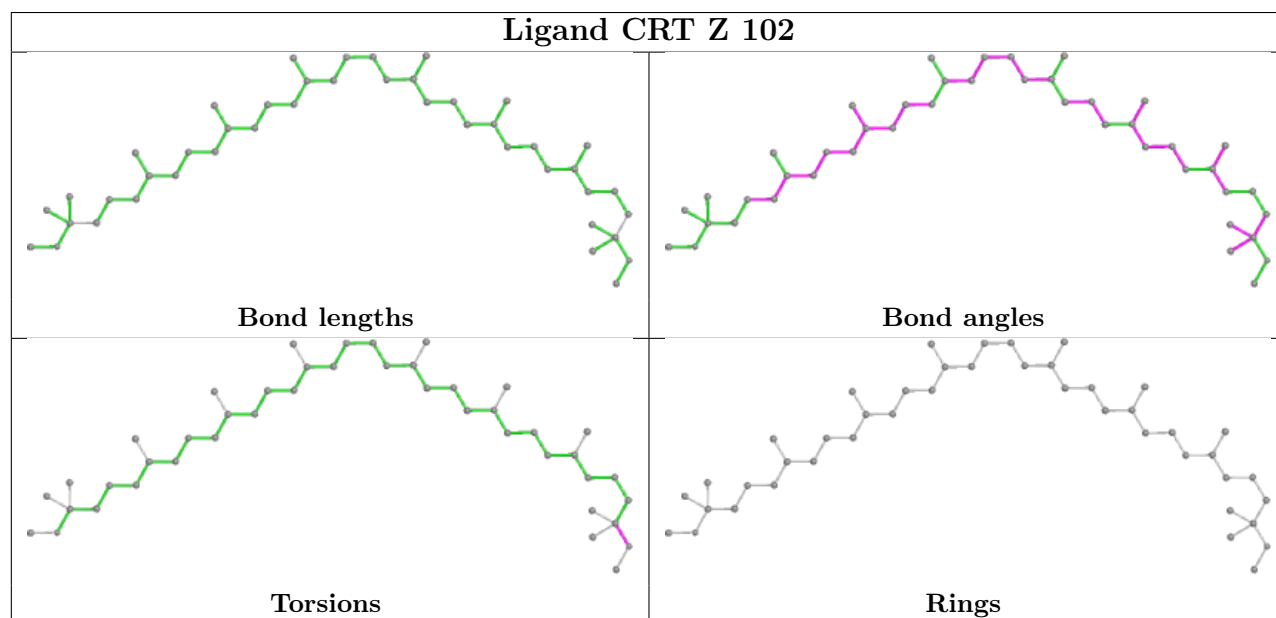
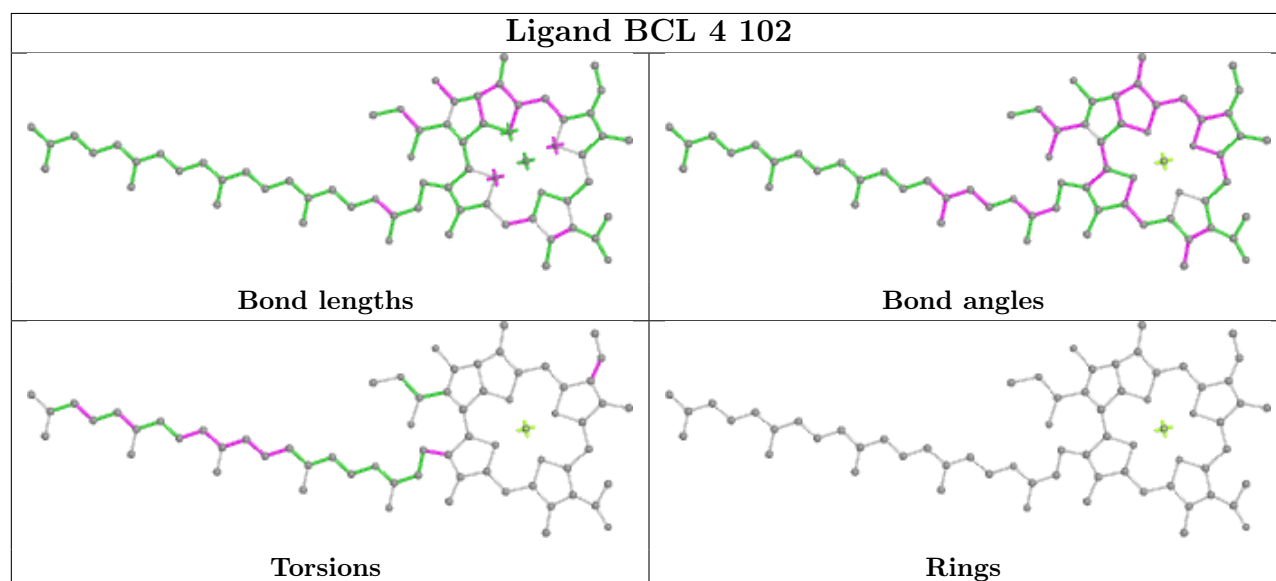
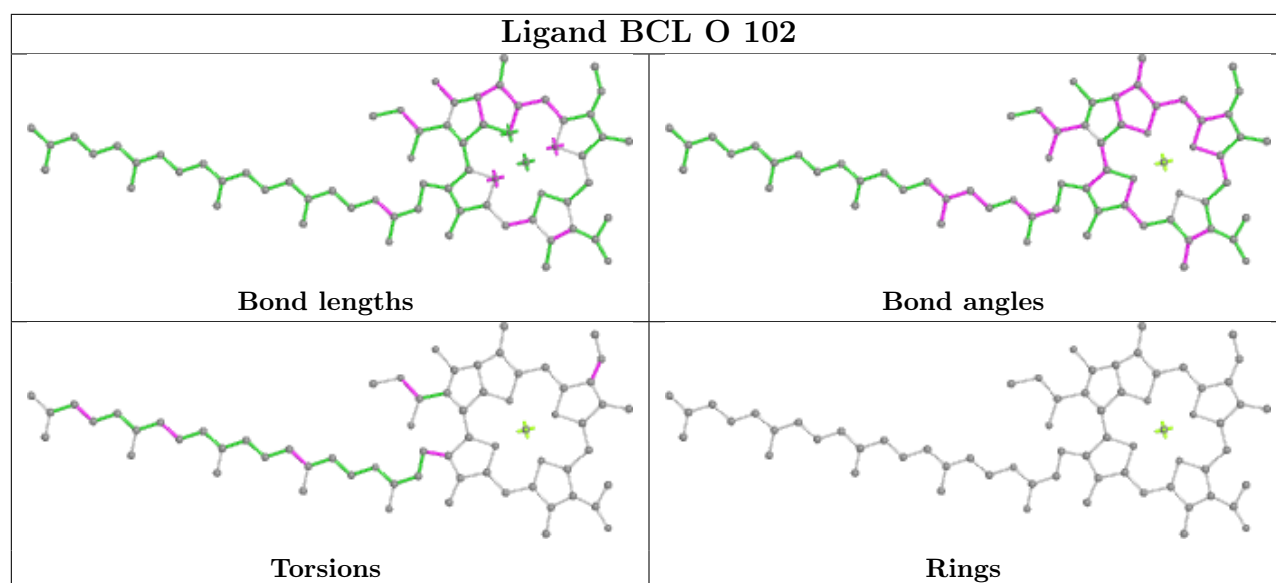


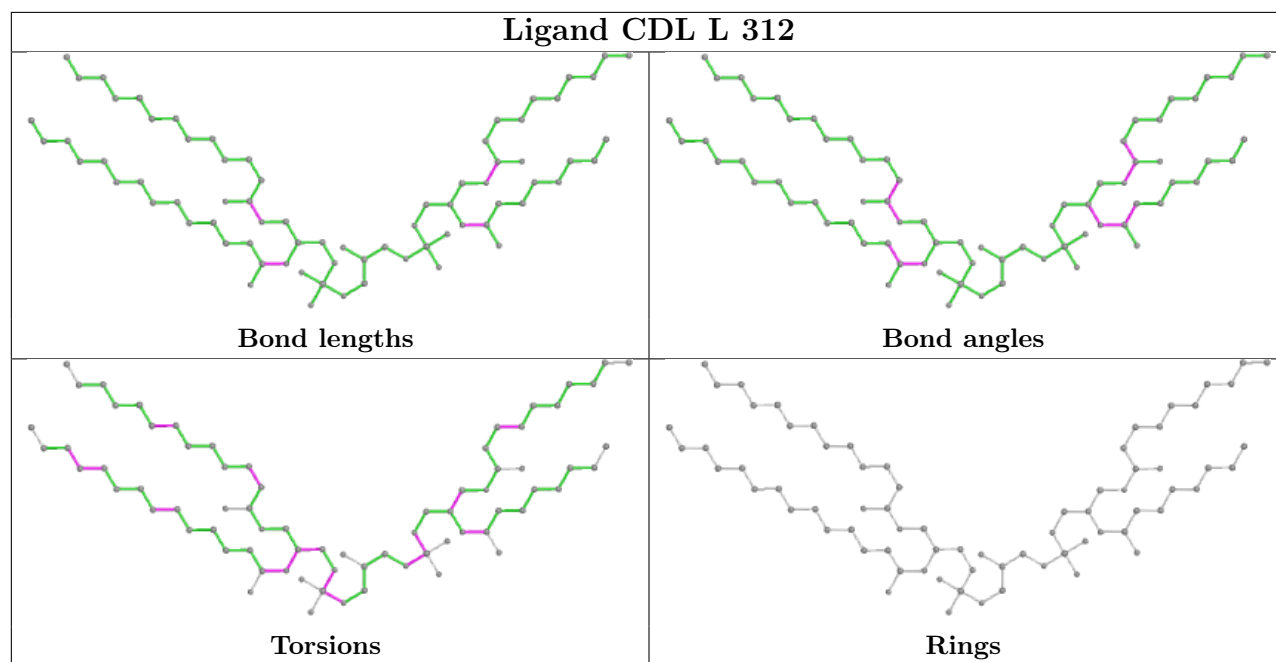
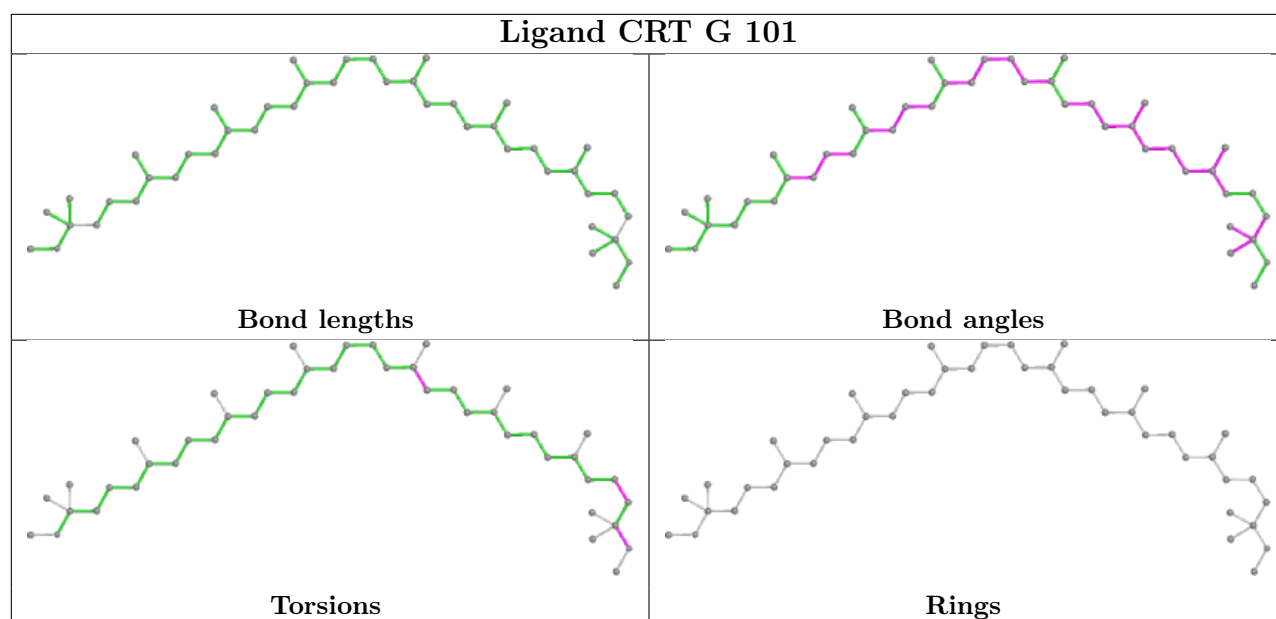


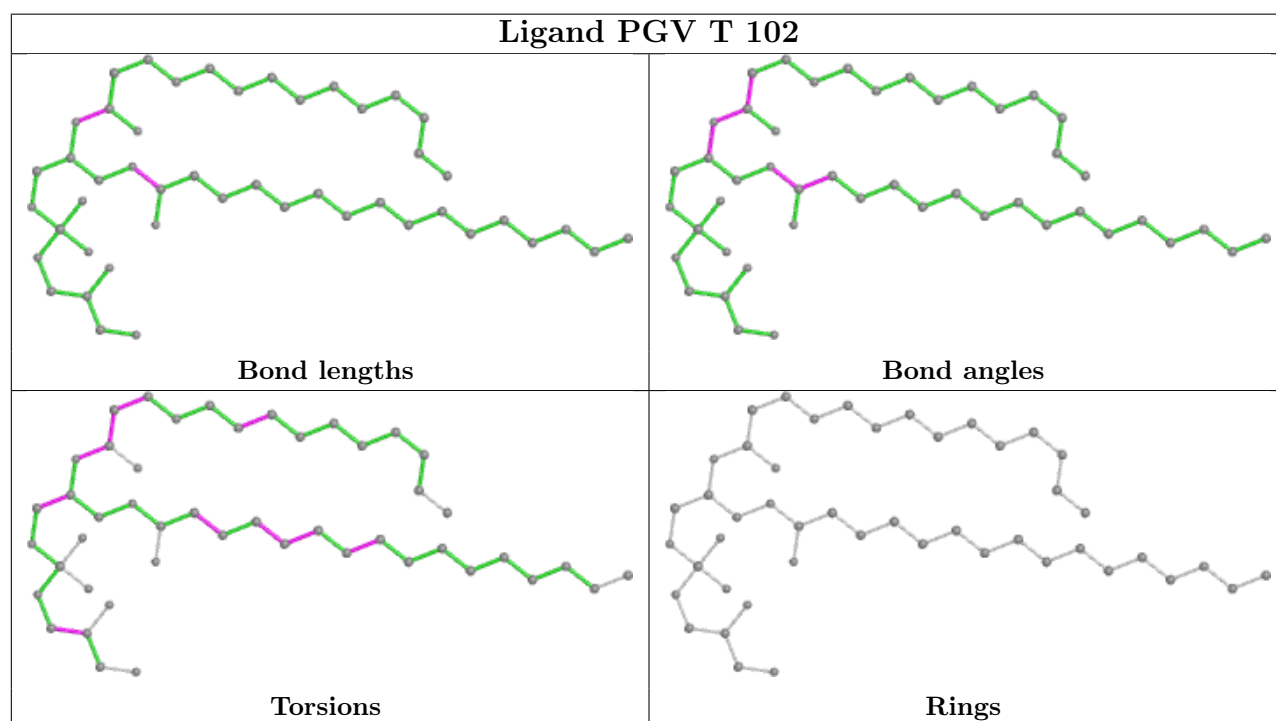
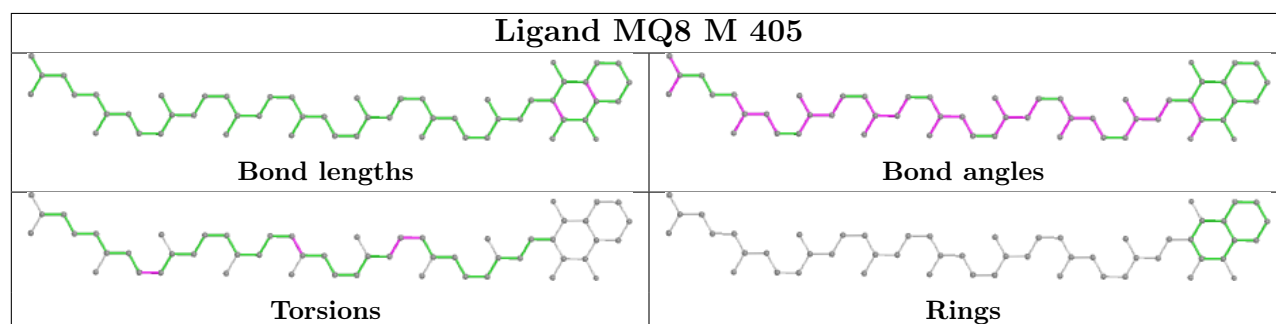
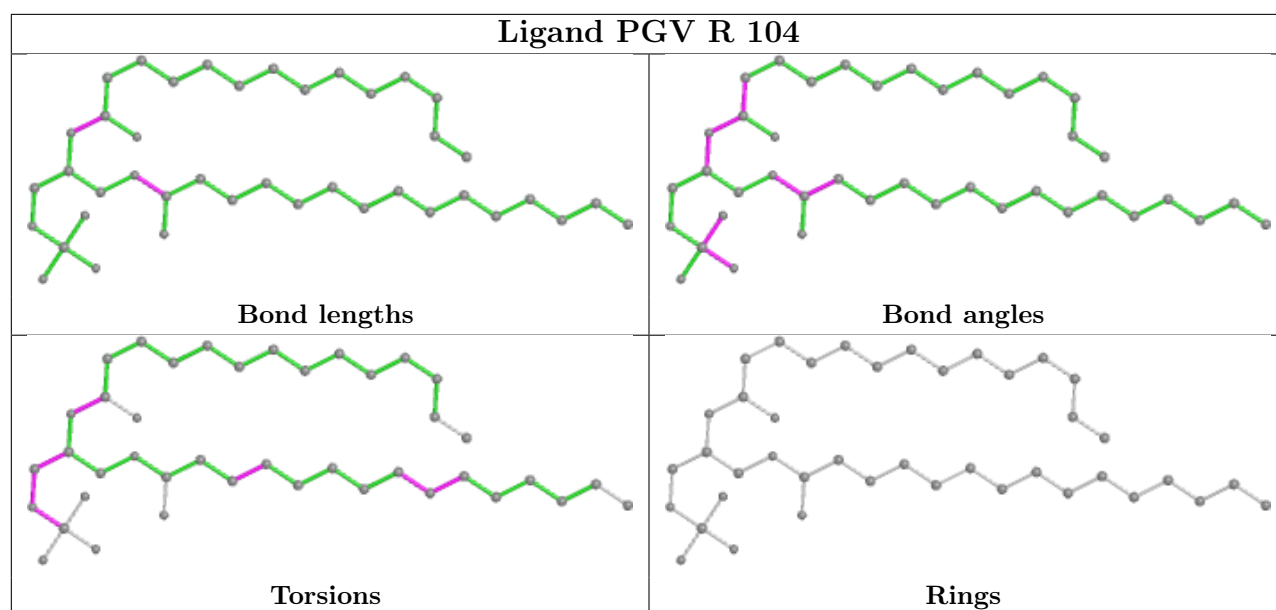


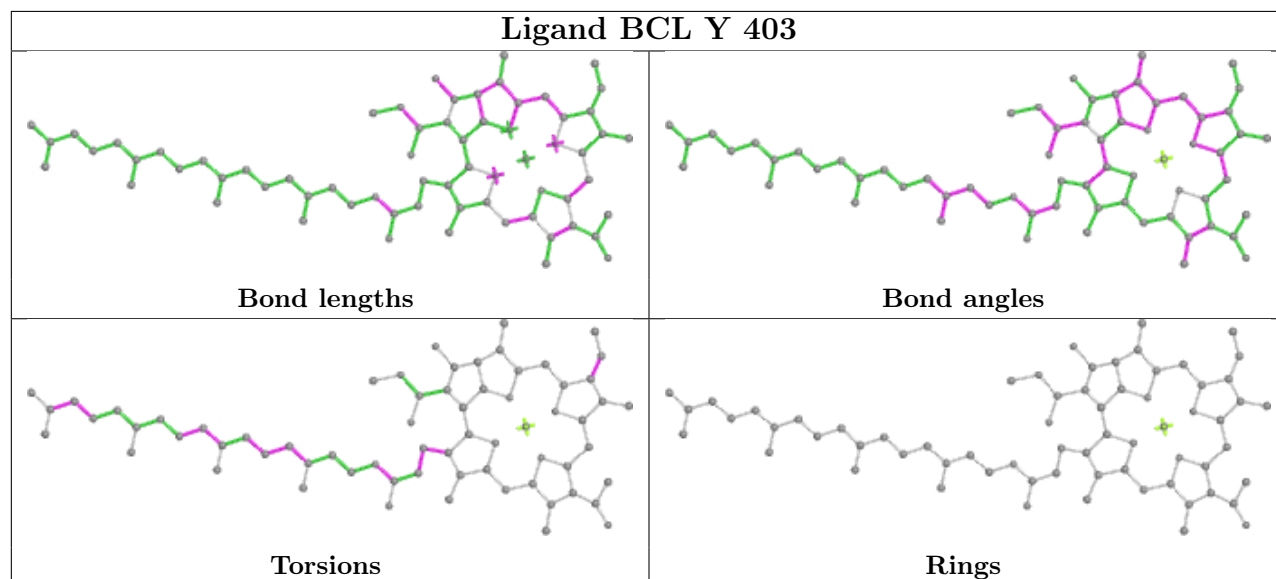
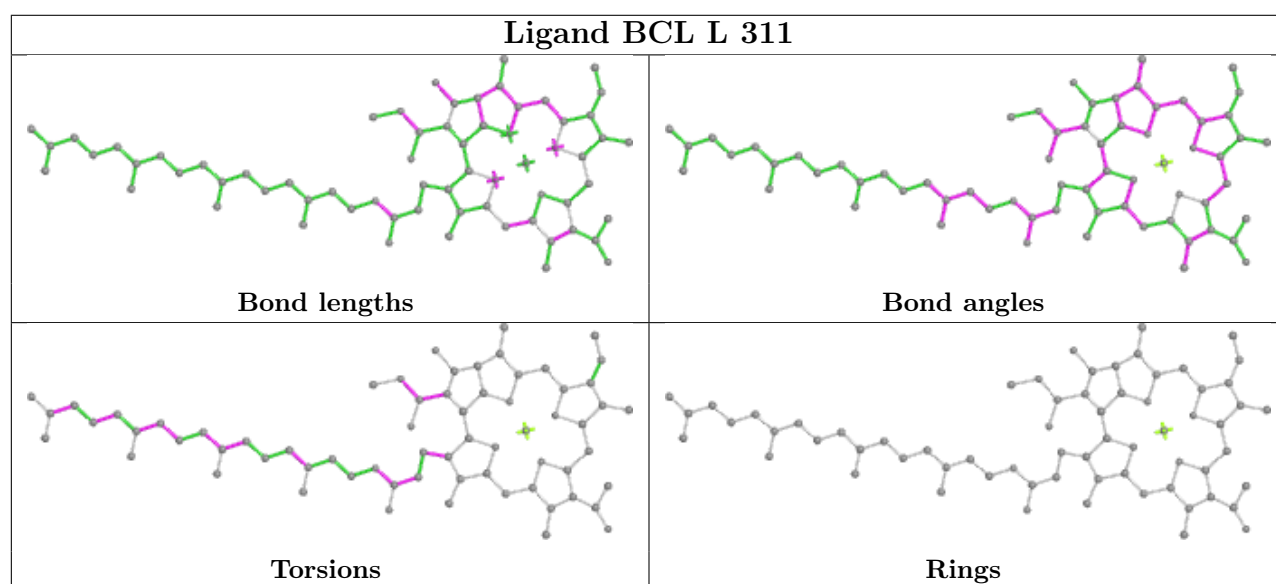
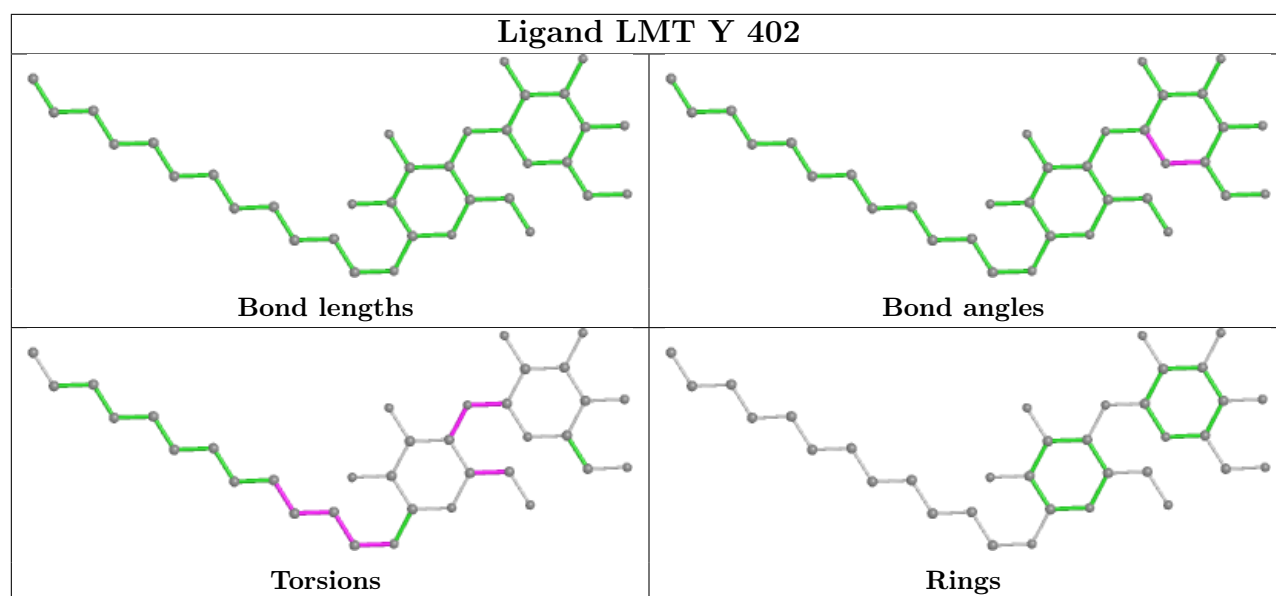


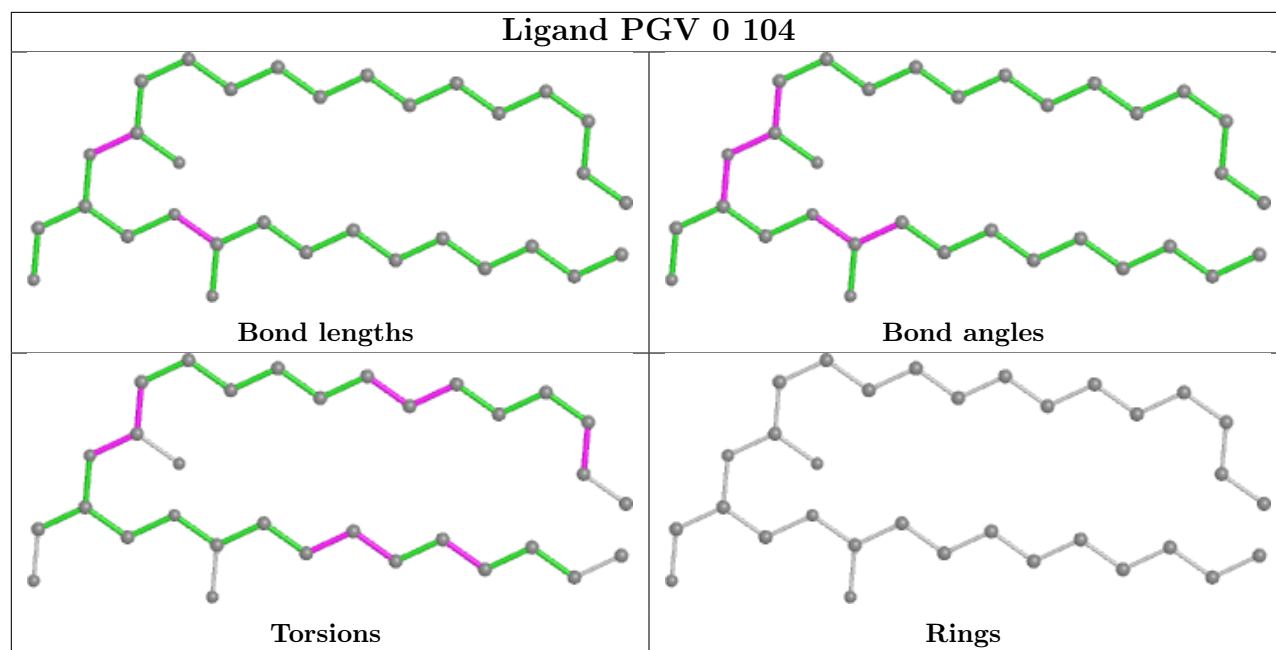
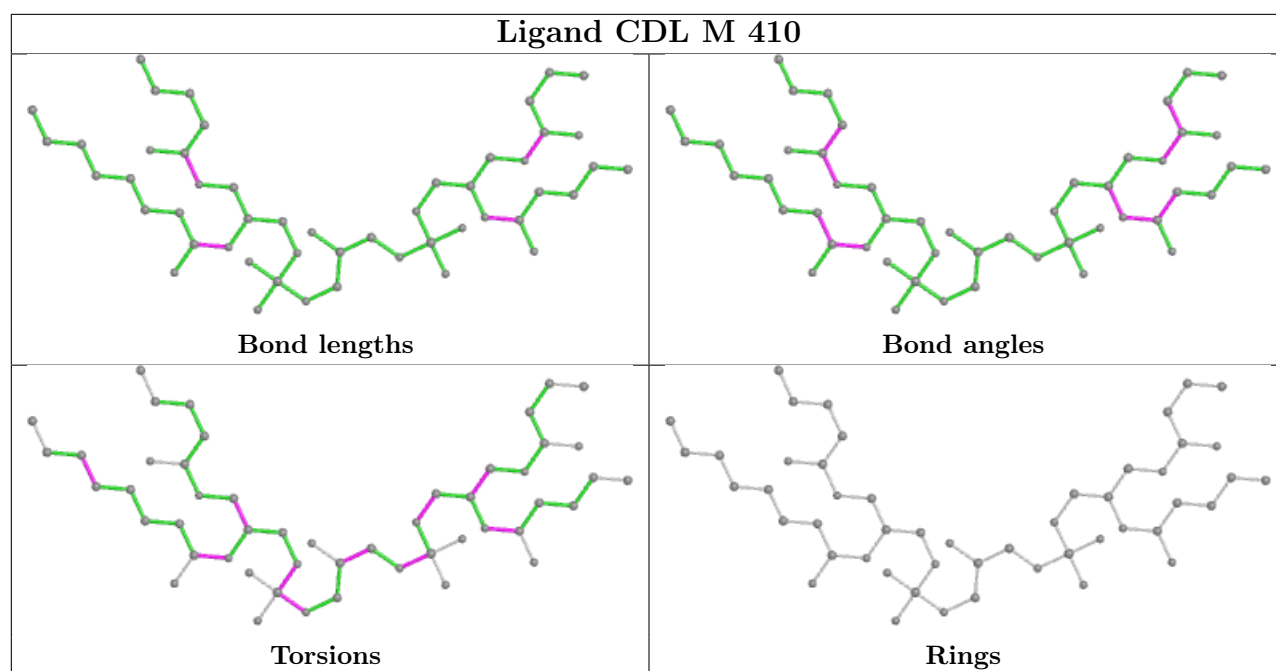


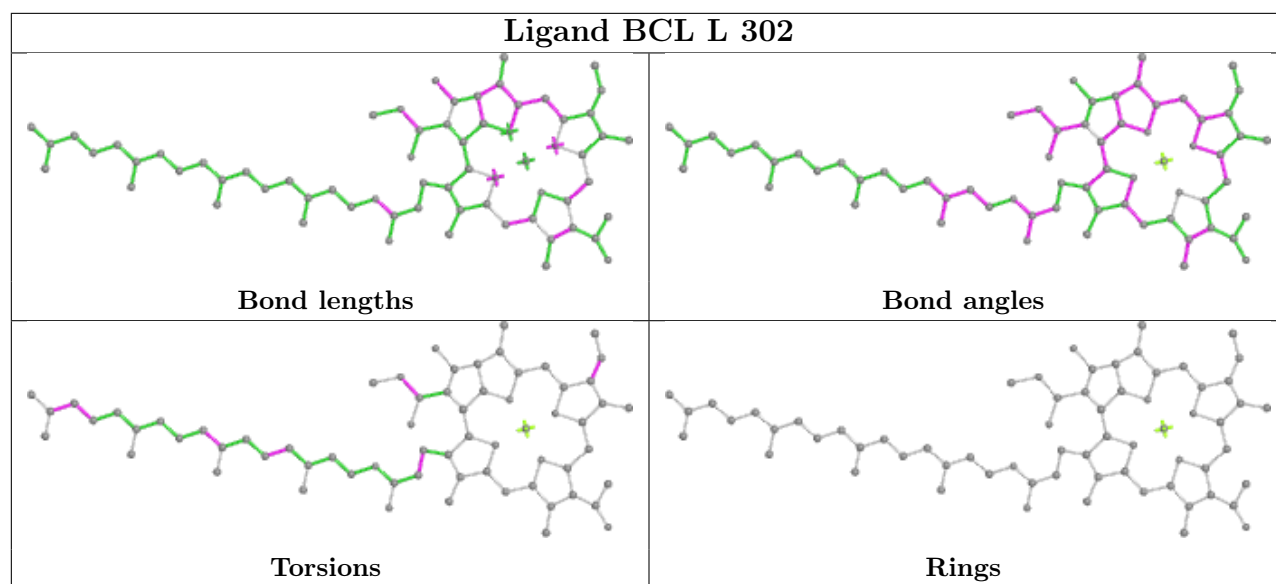
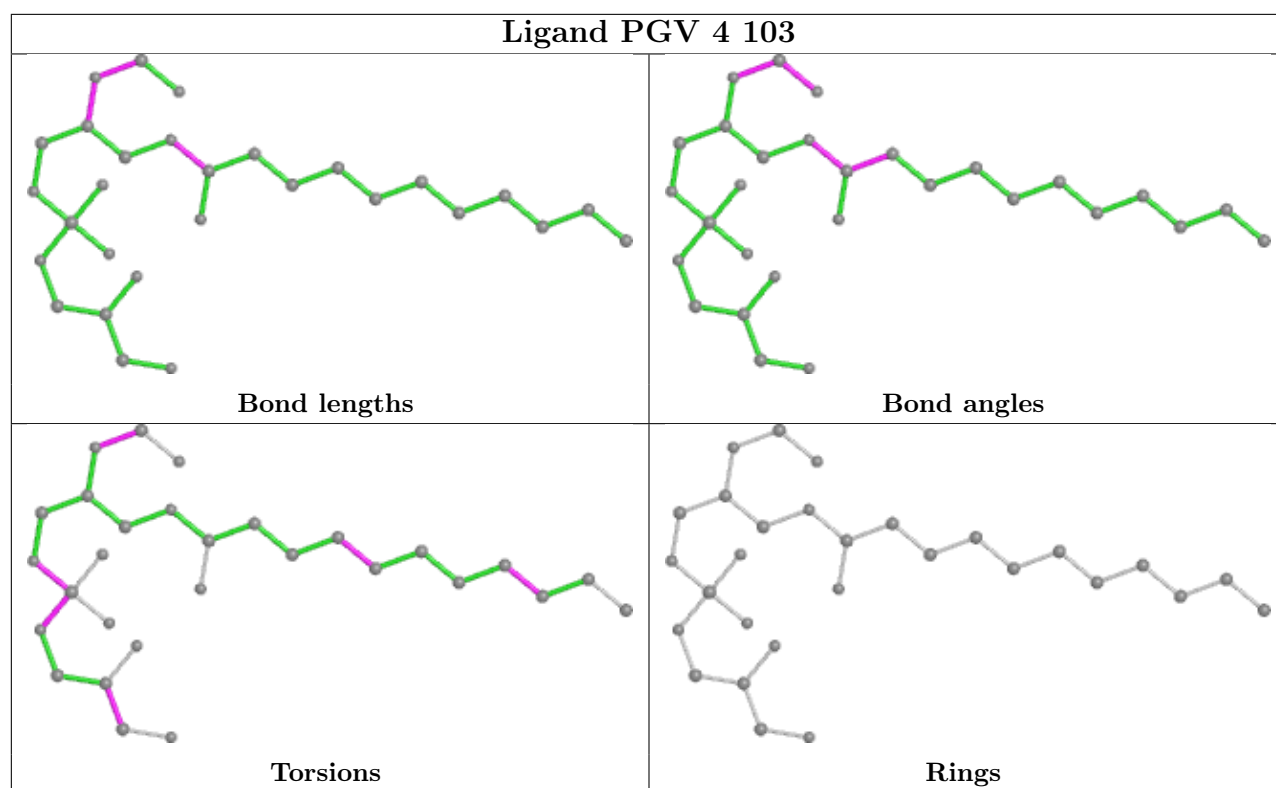


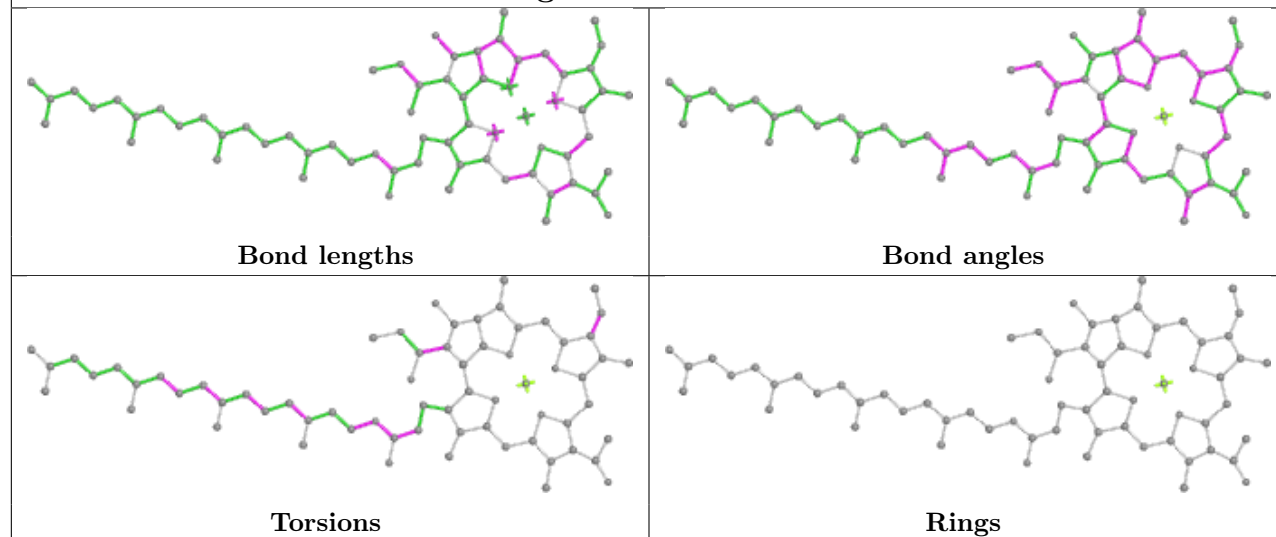
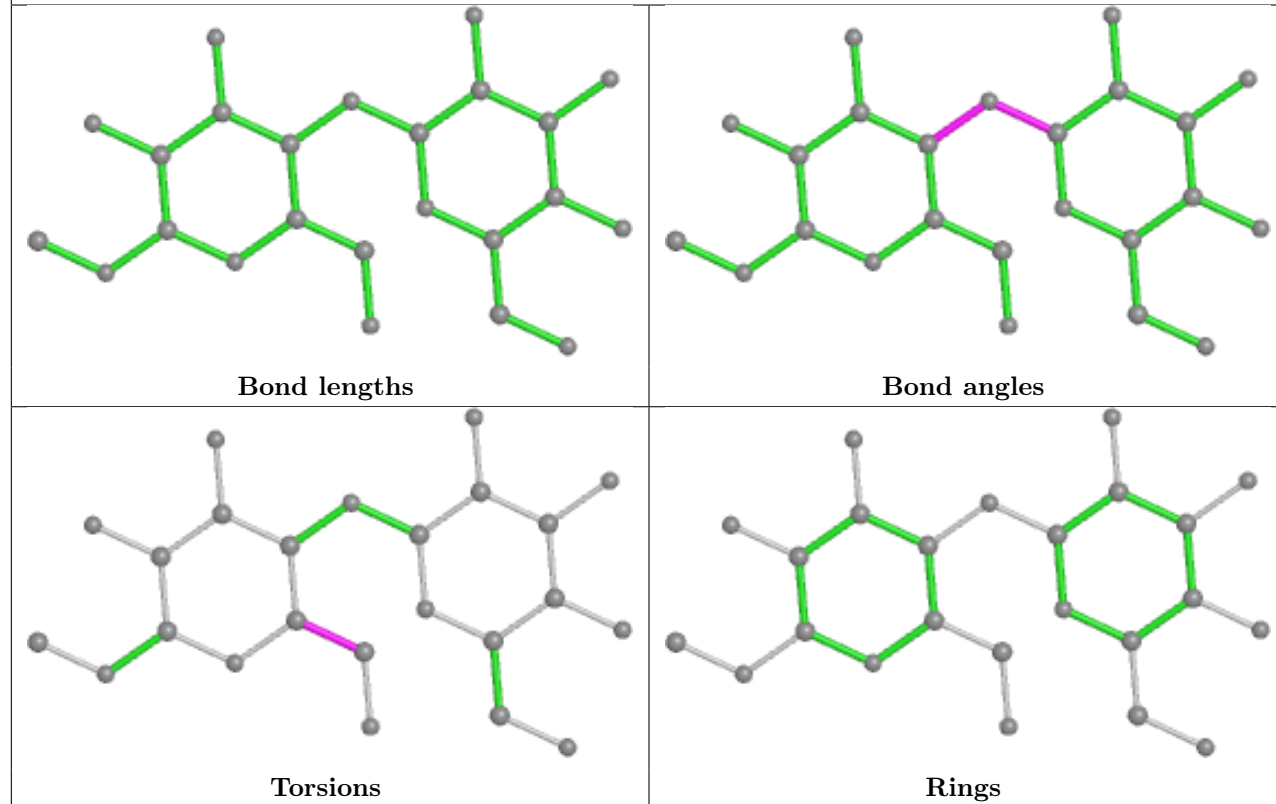


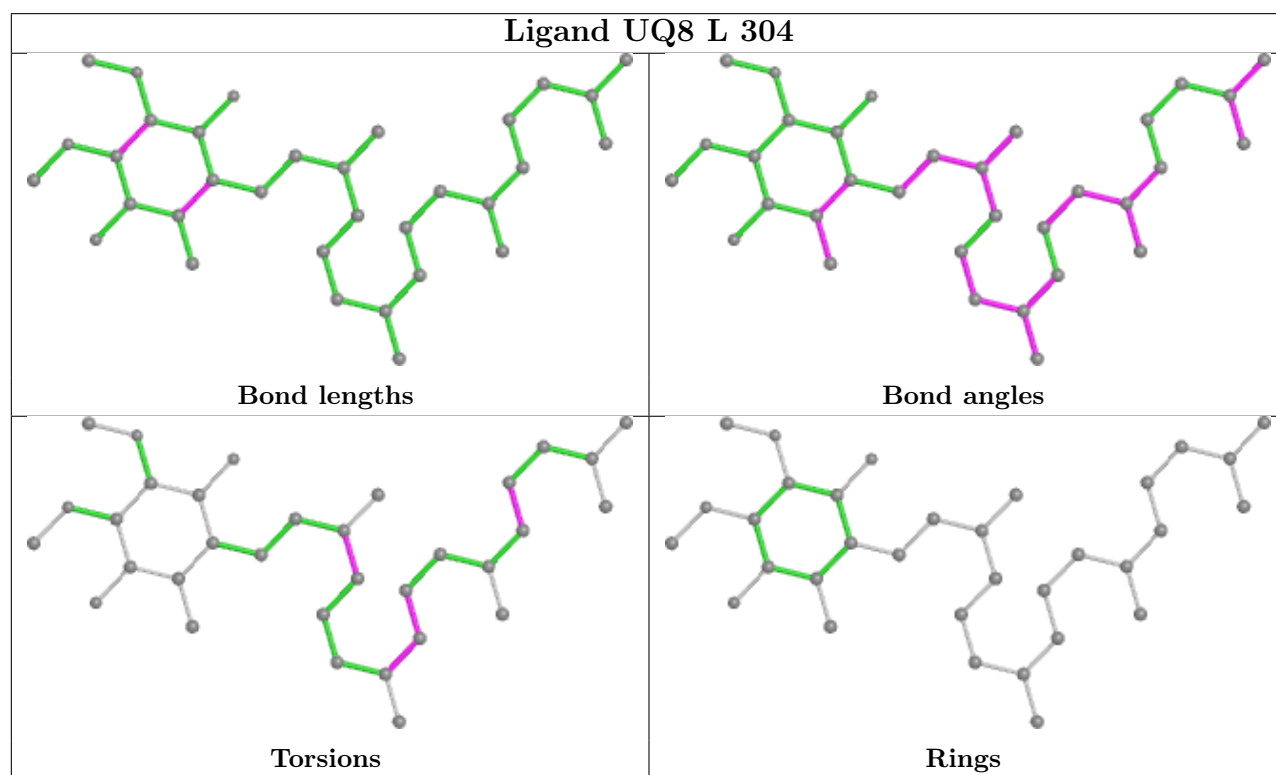
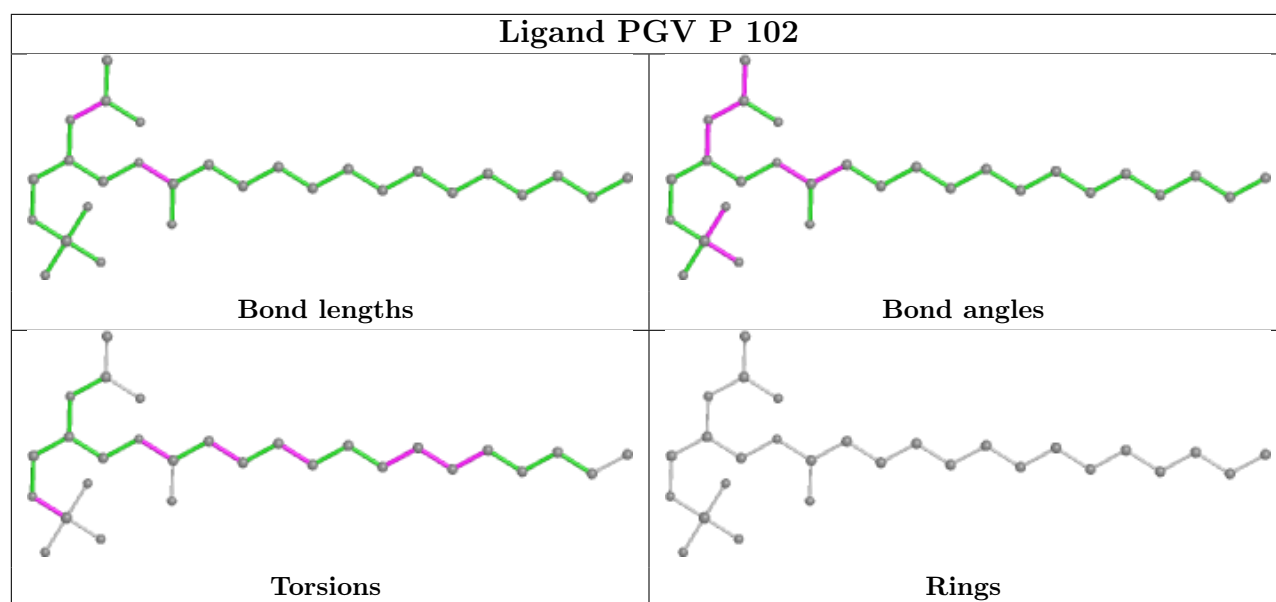




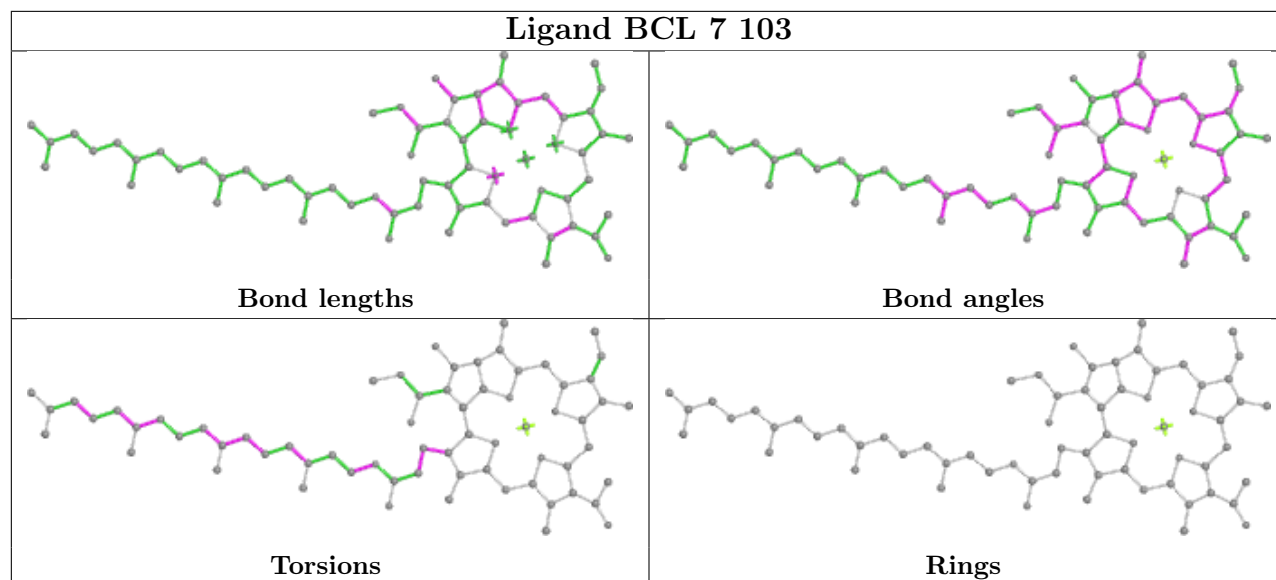




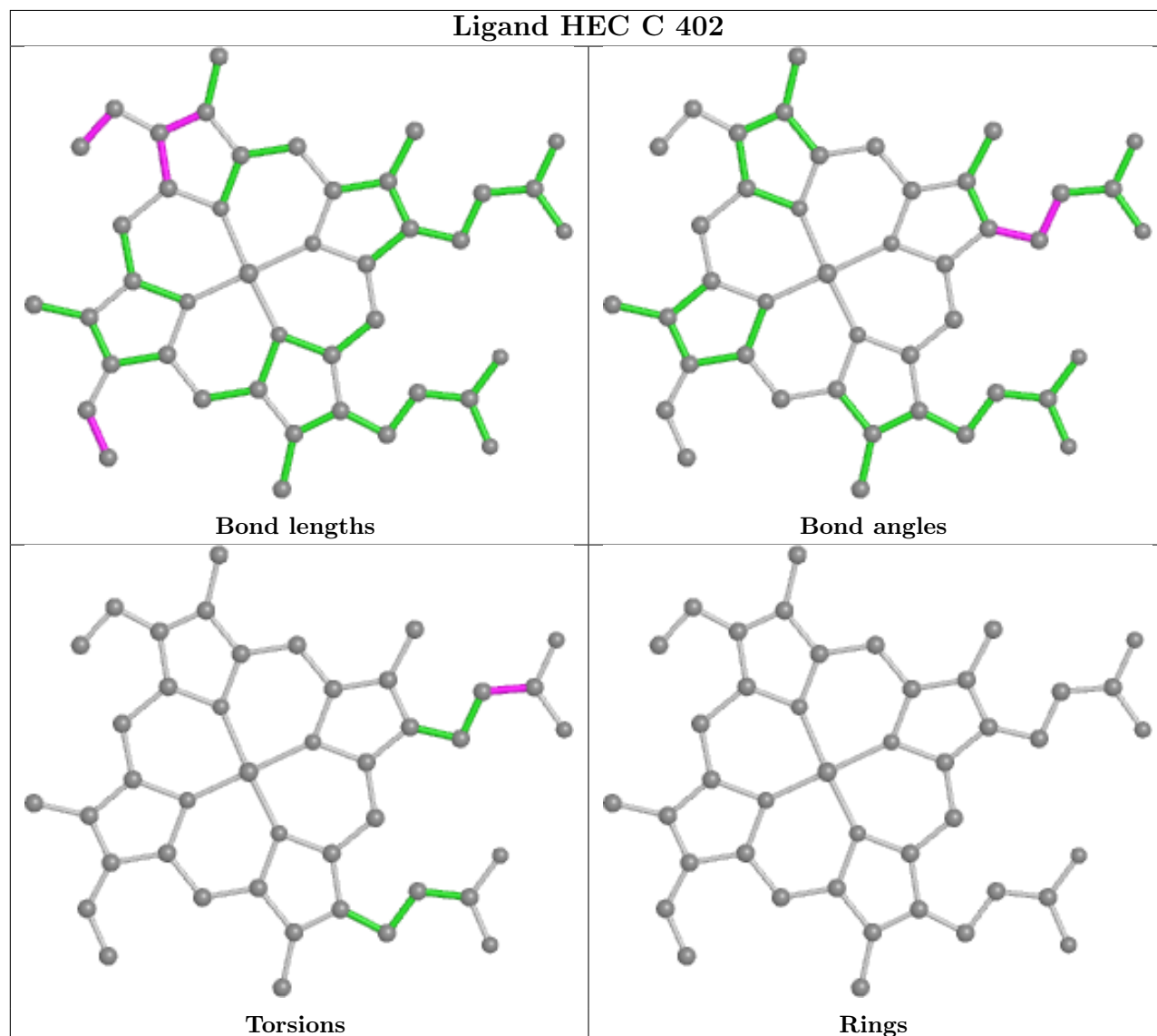
Ligand BCL 9 103**Ligand LMT 5 101**

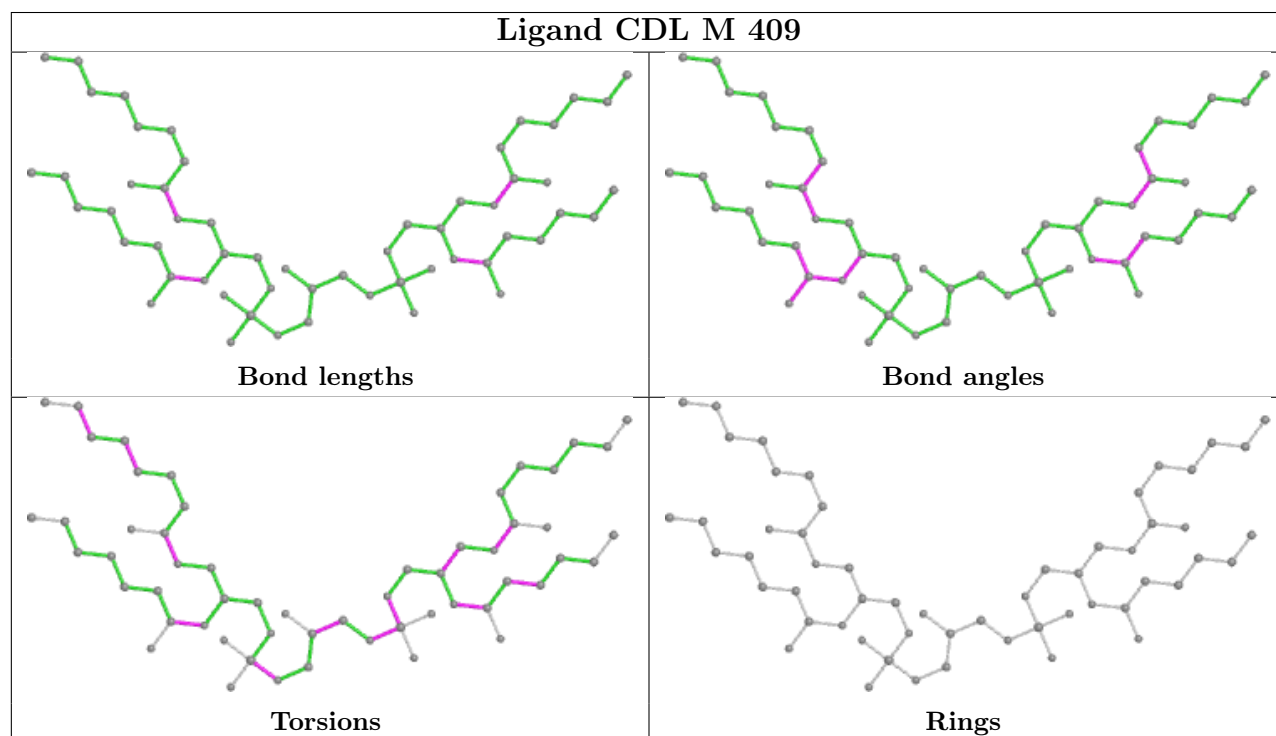
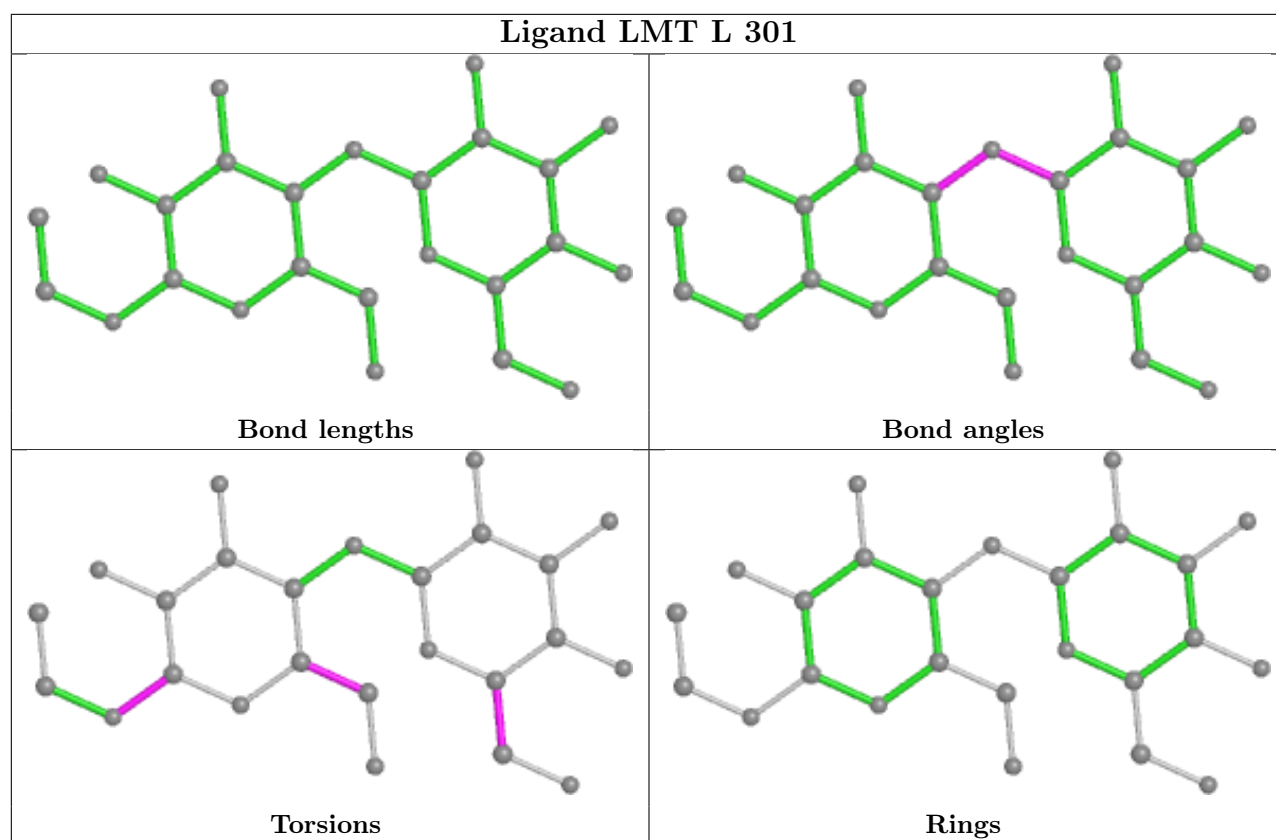


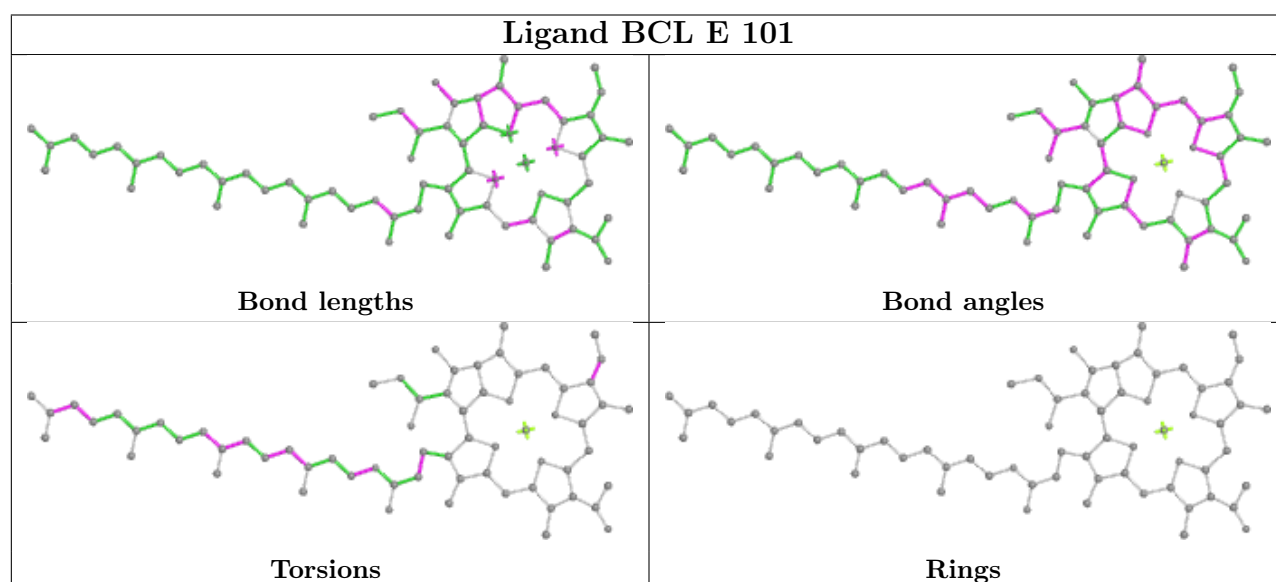
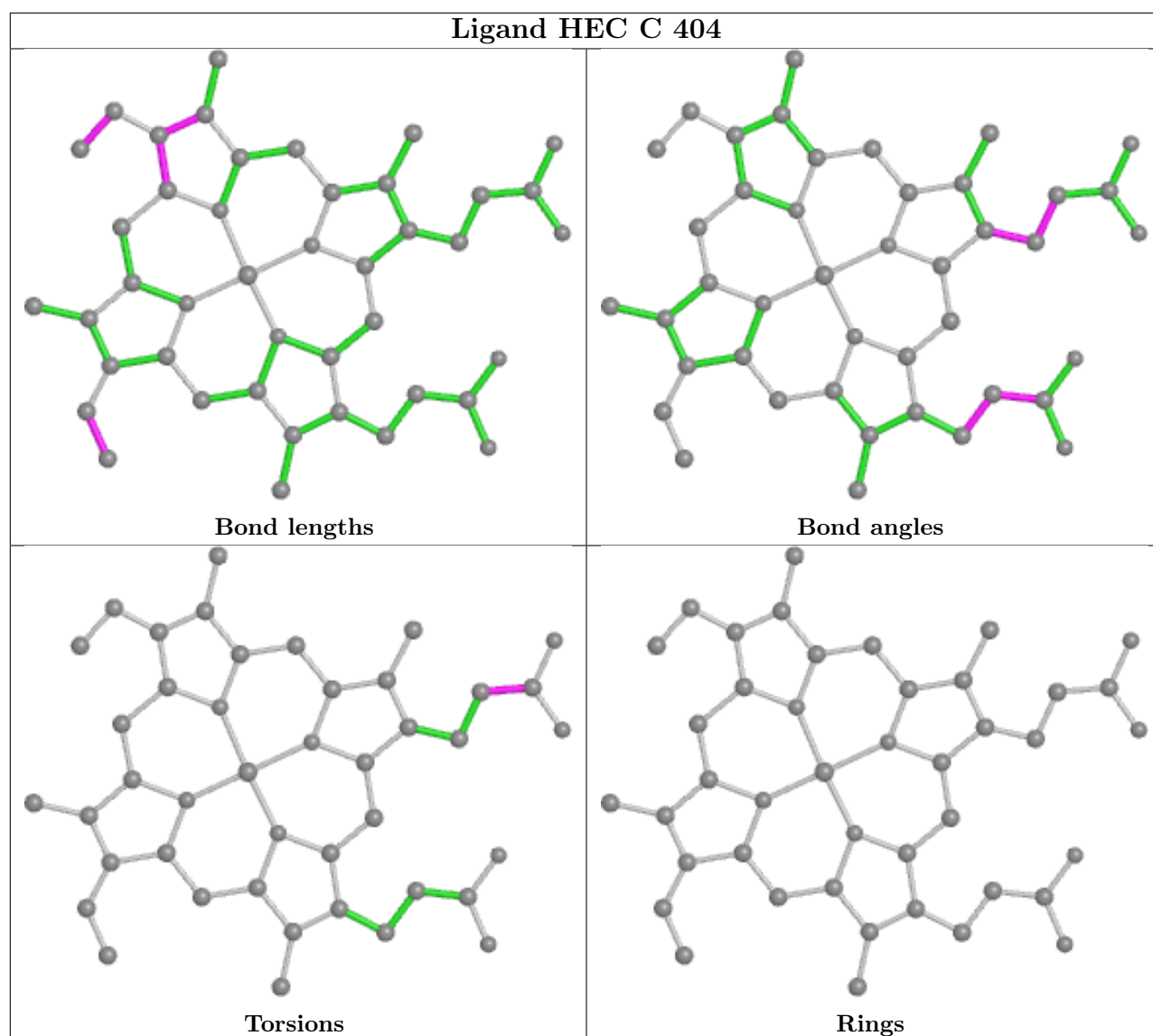
Ligand BCL 7 103

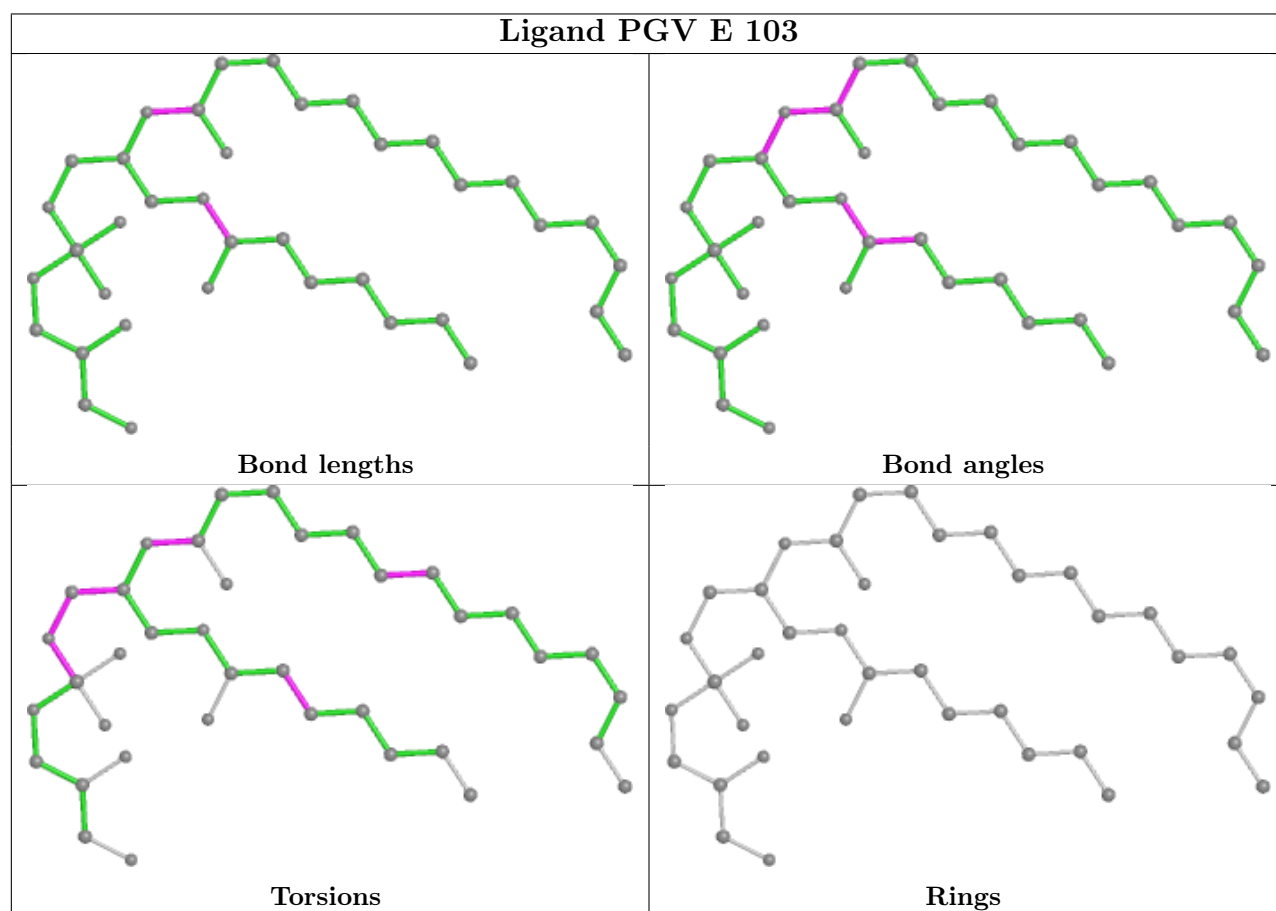
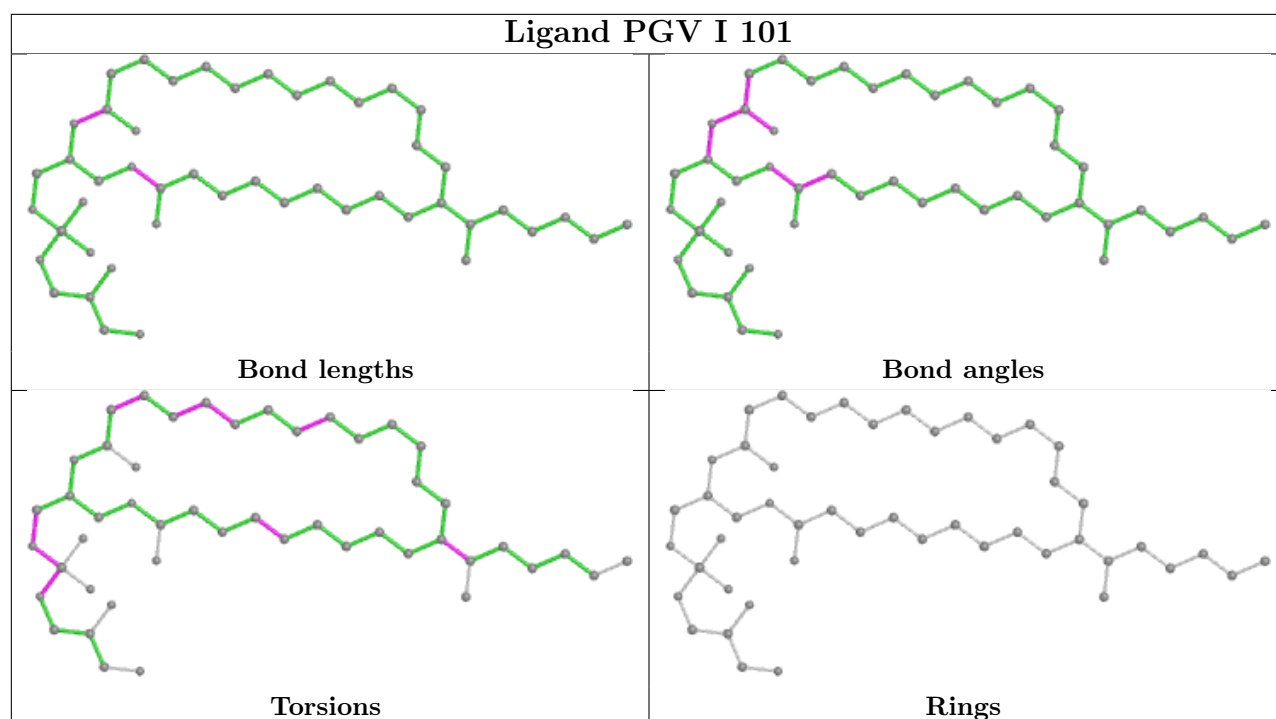


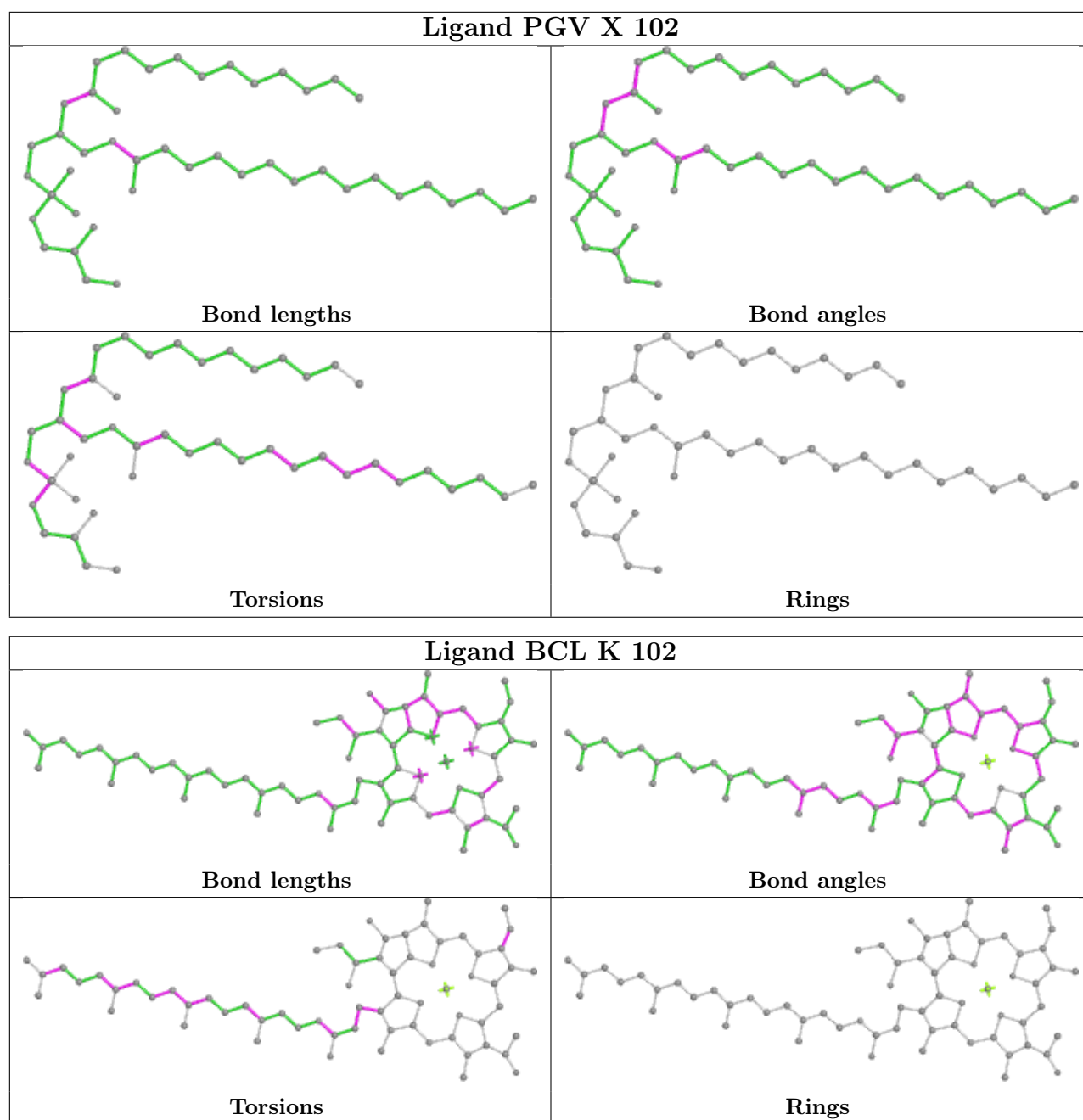
Ligand HEC C 402

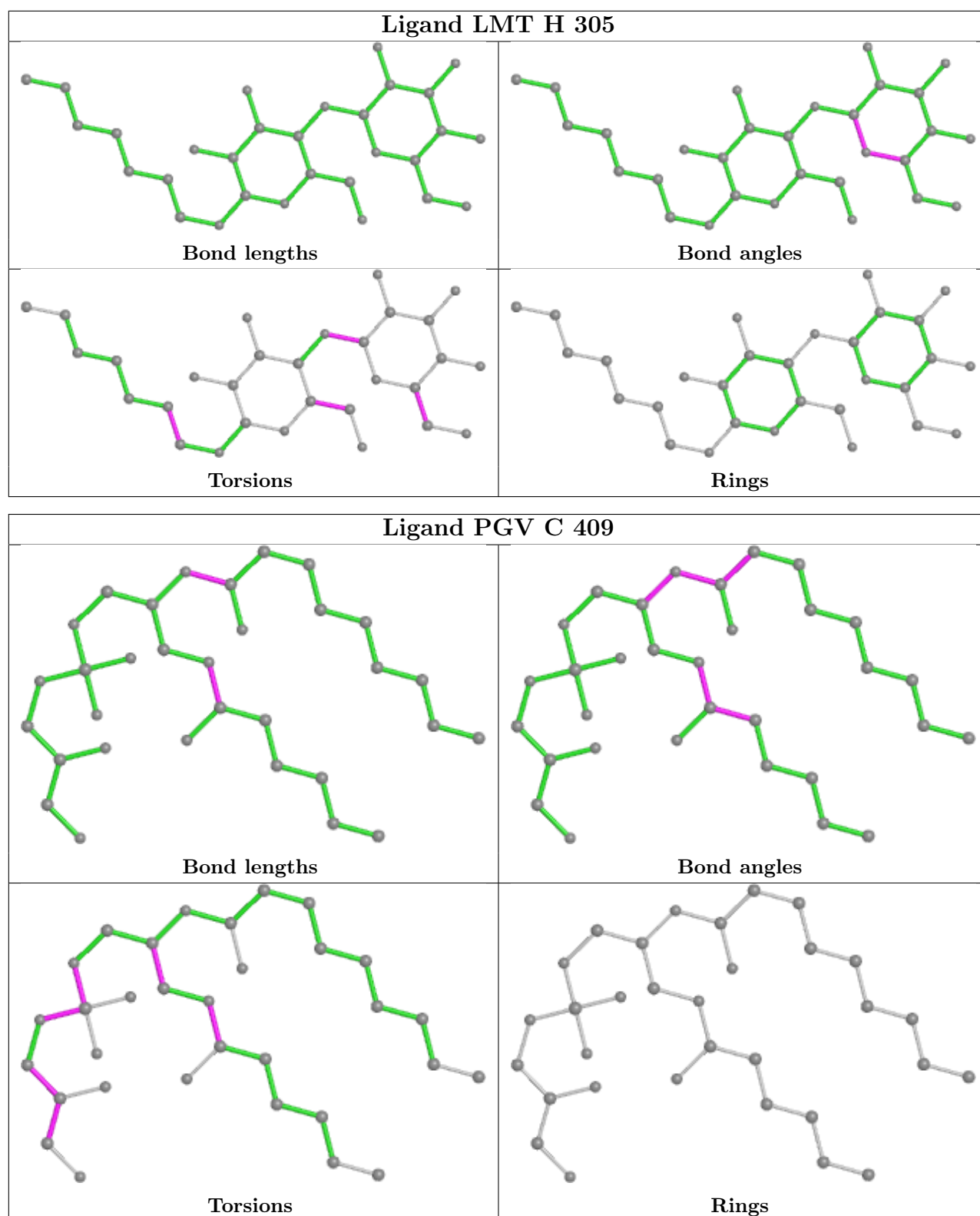












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

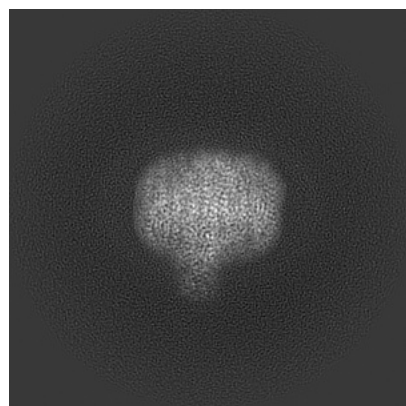
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39837. These allow visual inspection of the internal detail of the map and identification of artifacts.

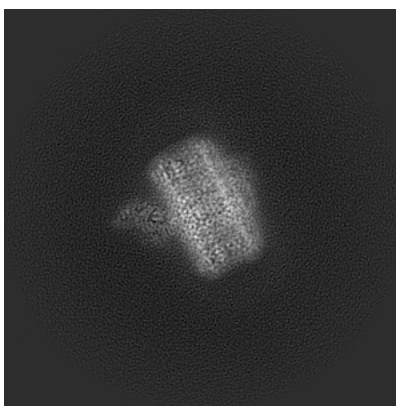
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

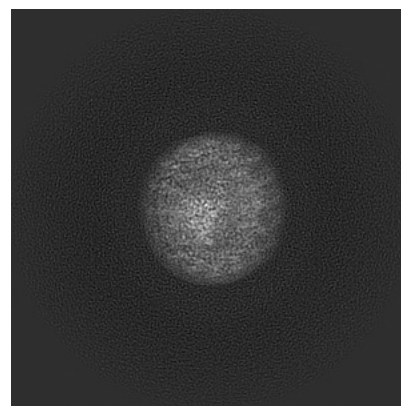
6.1.1 Primary map



X

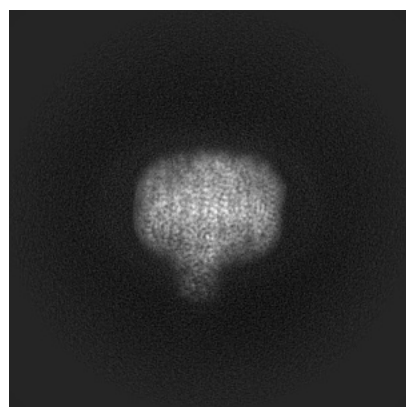


Y

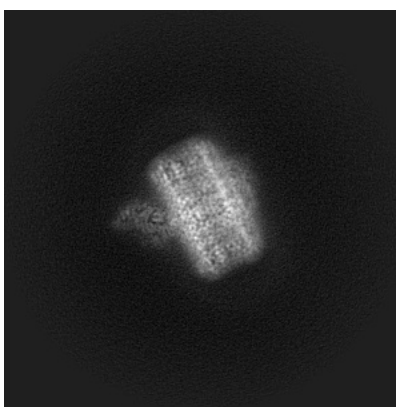


Z

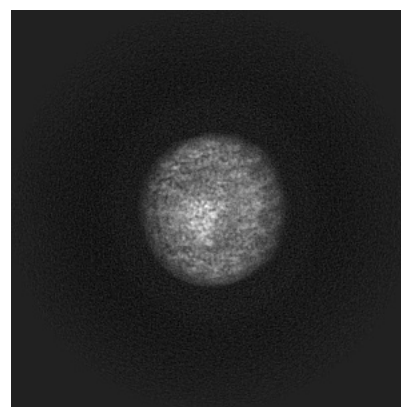
6.1.2 Raw map



X



Y

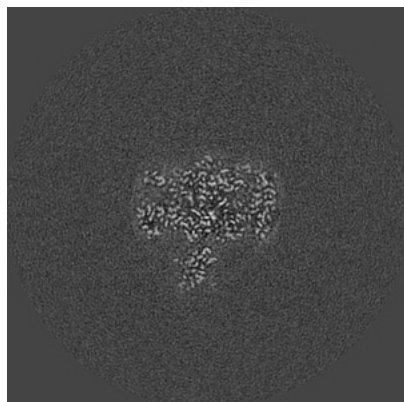


Z

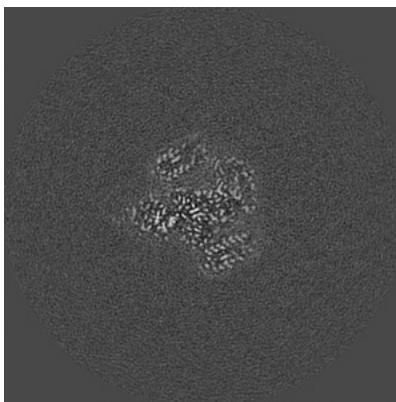
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

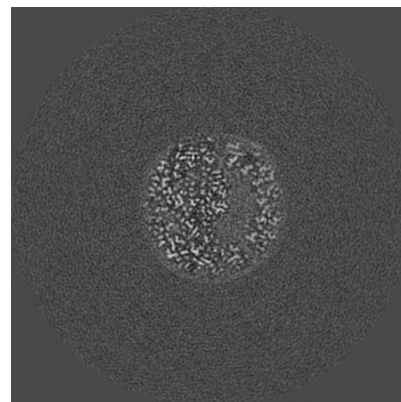
6.2.1 Primary map



X Index: 200

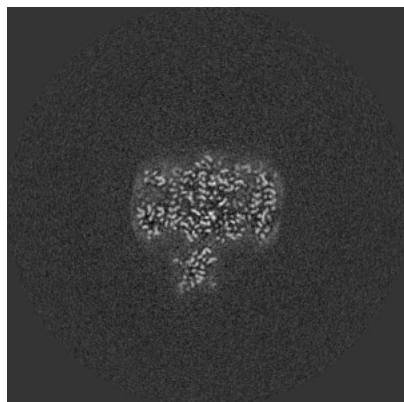


Y Index: 200

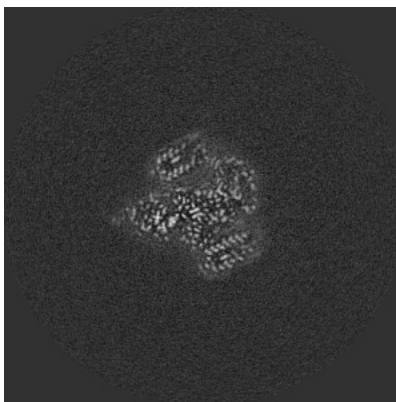


Z Index: 200

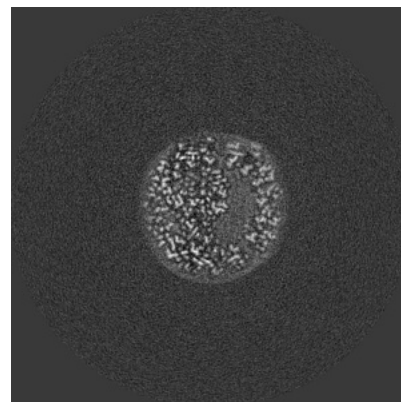
6.2.2 Raw map



X Index: 200



Y Index: 200

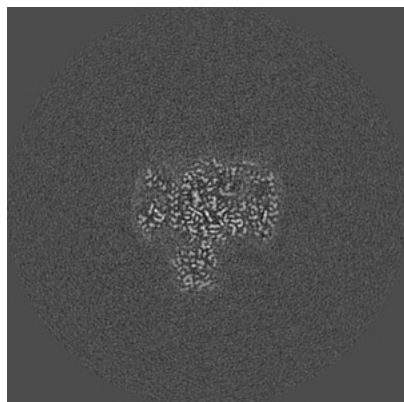


Z Index: 200

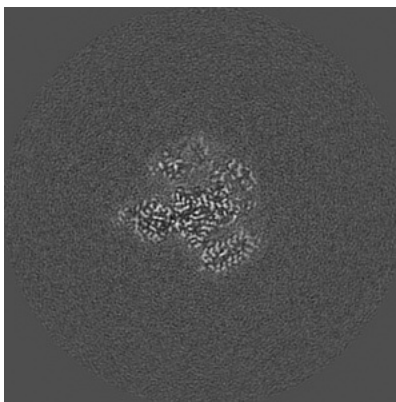
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

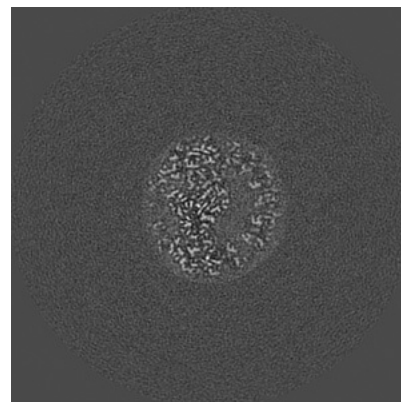
6.3.1 Primary map



X Index: 197

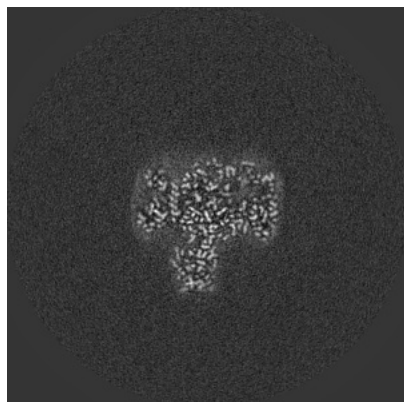


Y Index: 197

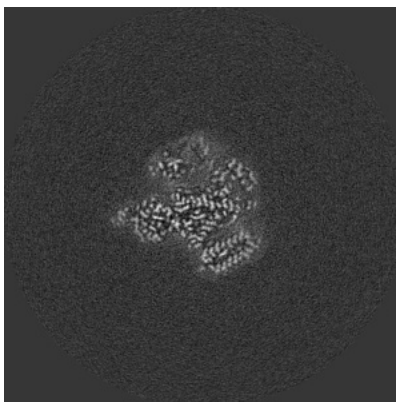


Z Index: 195

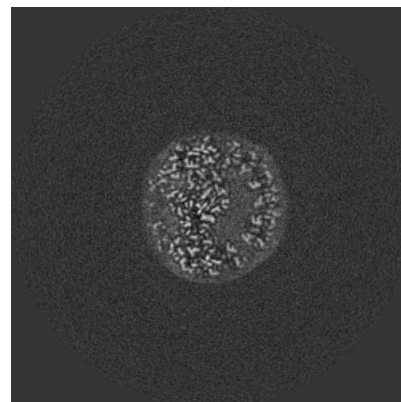
6.3.2 Raw map



X Index: 196



Y Index: 197

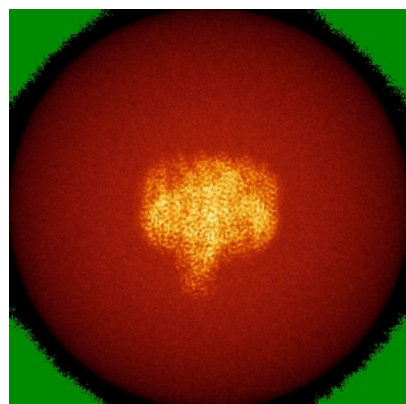


Z Index: 195

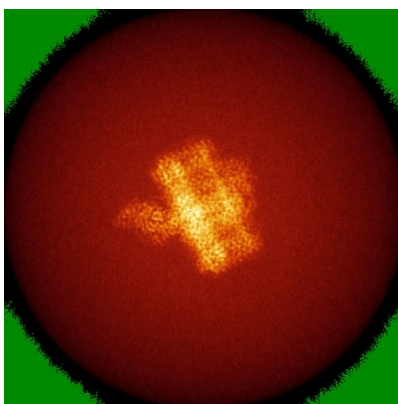
The images above show the largest variance slices of the map in three orthogonal directions.

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

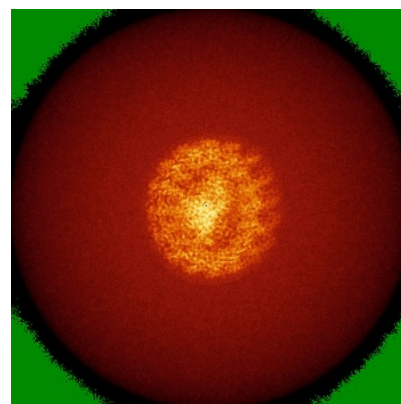
6.4.1 Primary map



X

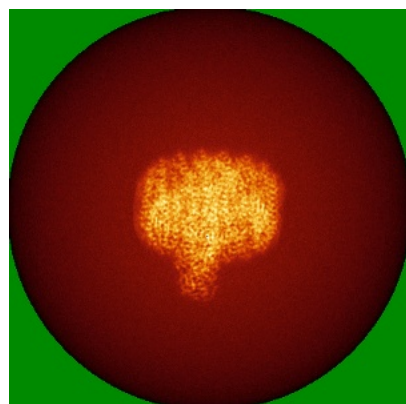


Y

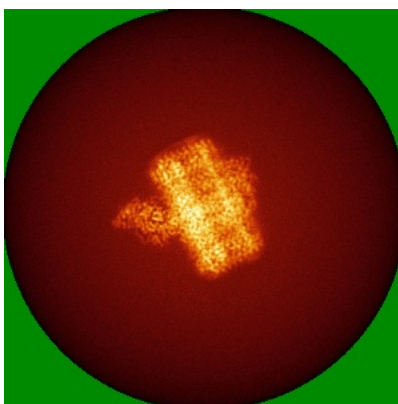


Z

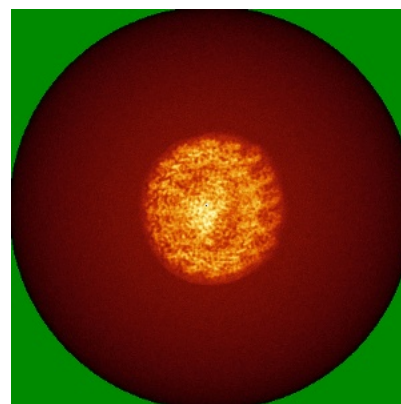
6.4.2 Raw map



X



Y

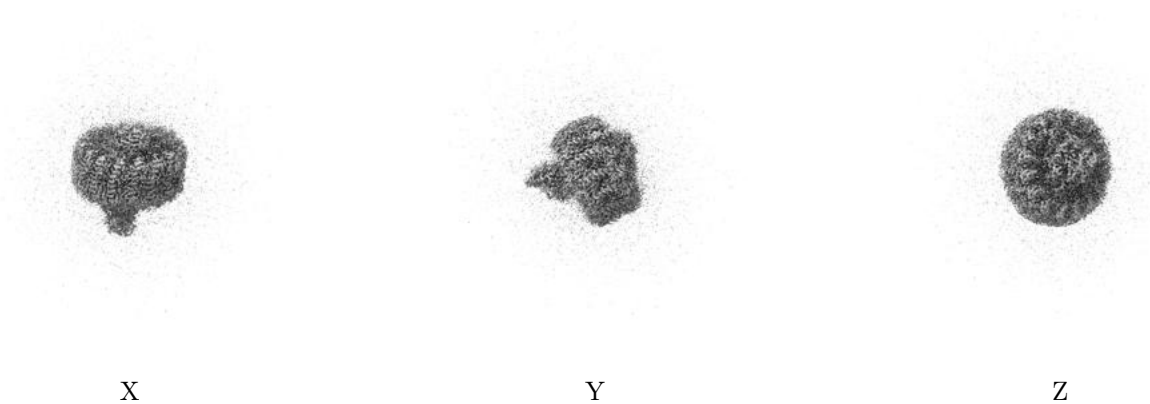


Z

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.

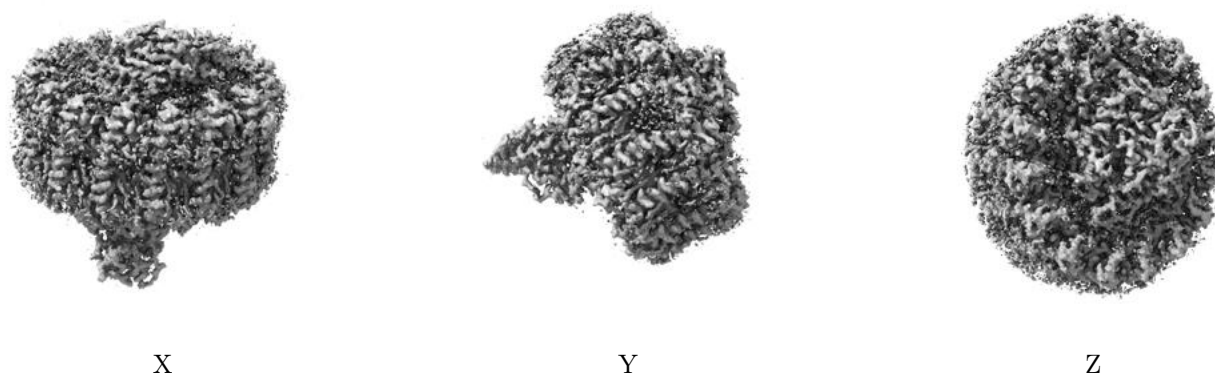
6.5 Orthogonal surface views [i](#)

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.

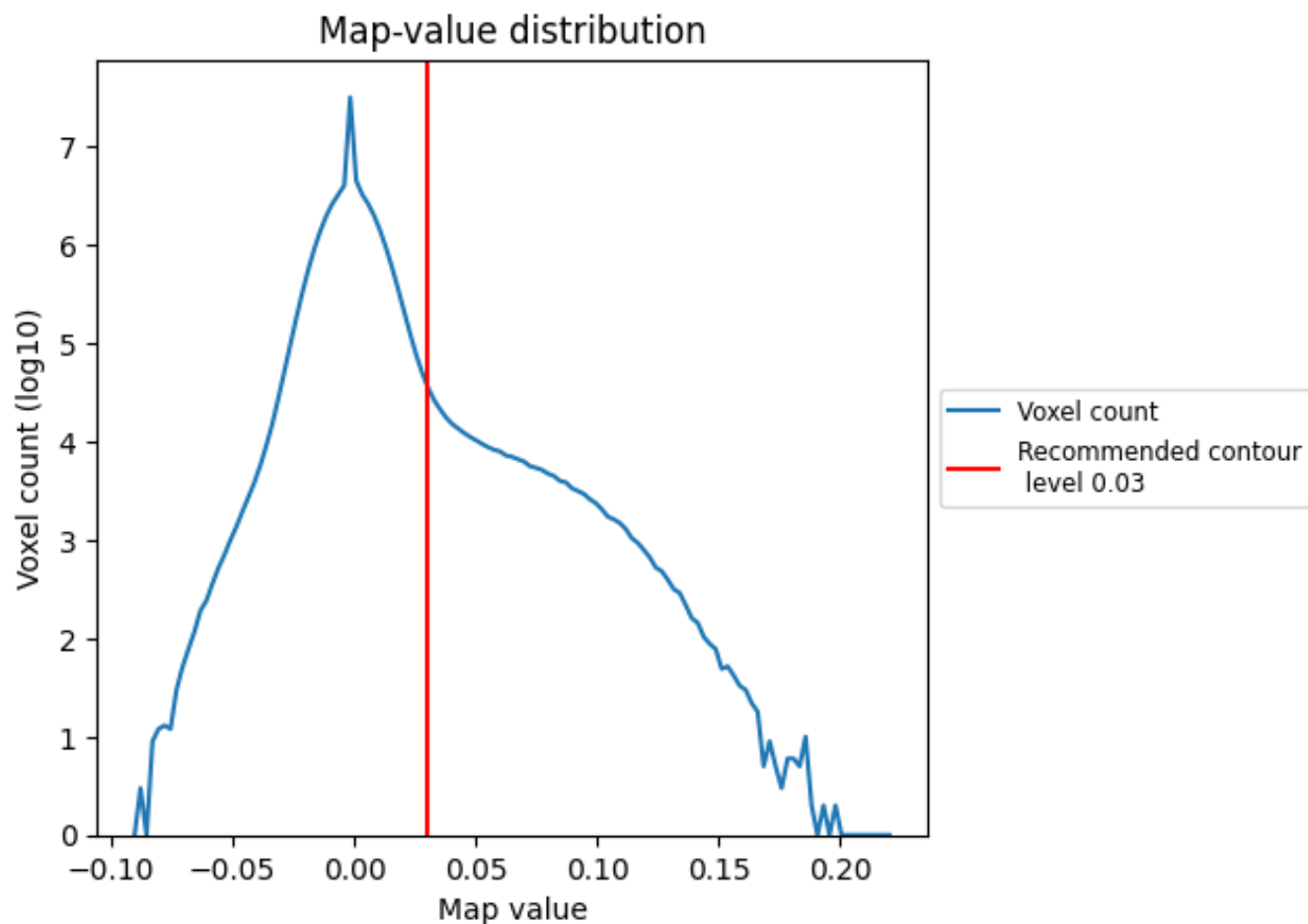
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

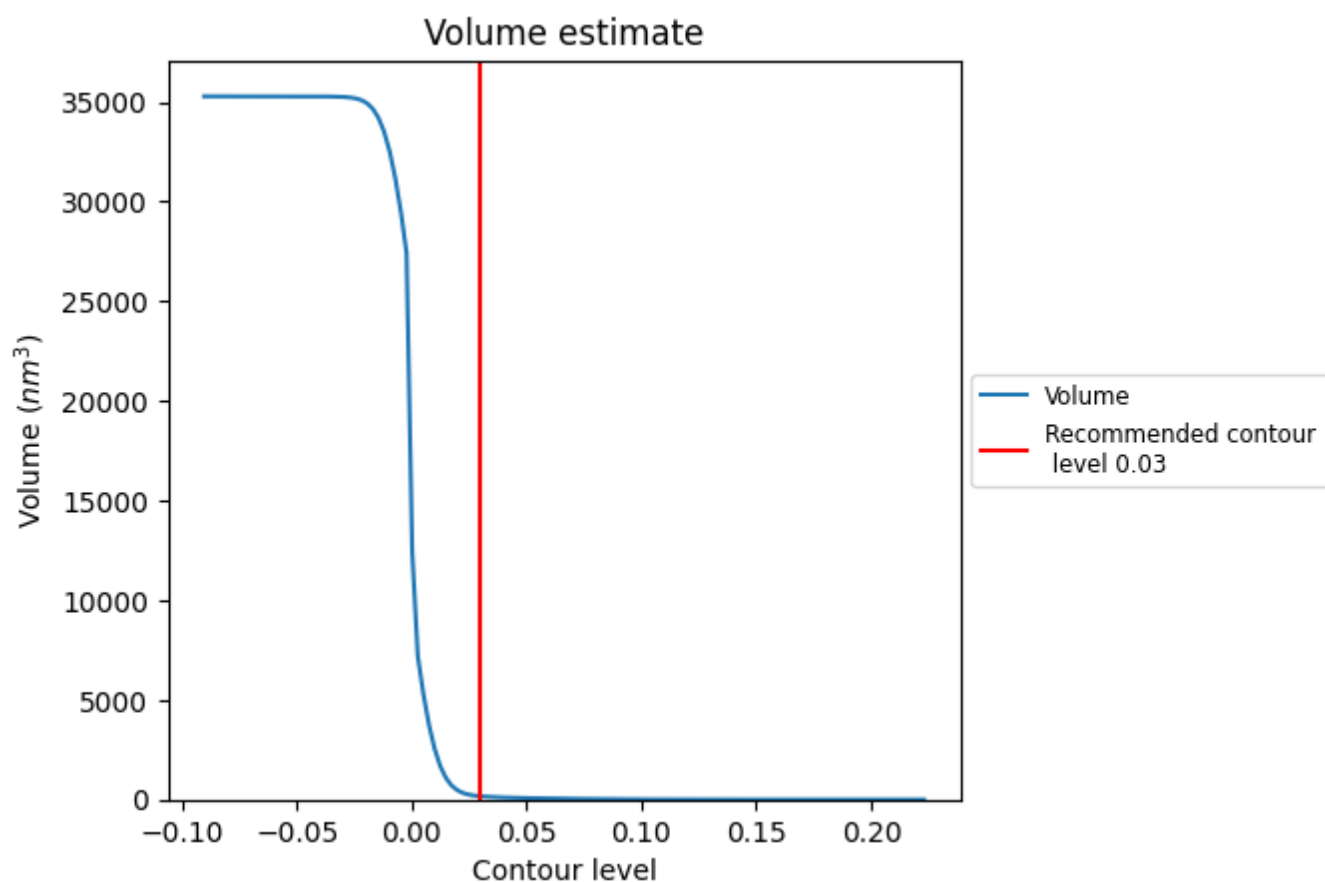
This section contains the results of statistical analysis of the map.

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.

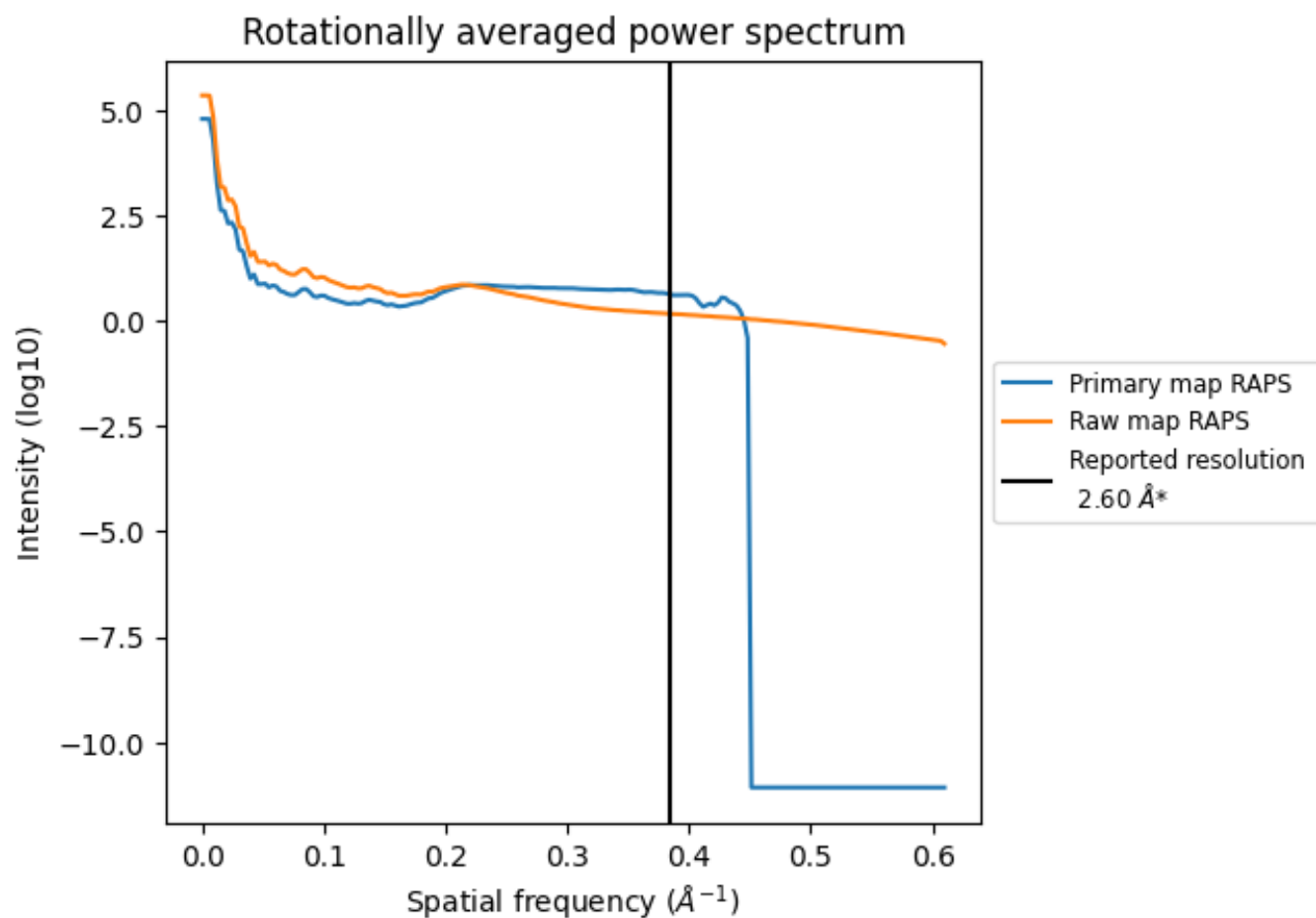
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm³; this corresponds to an approximate mass of 149 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 ⓘ

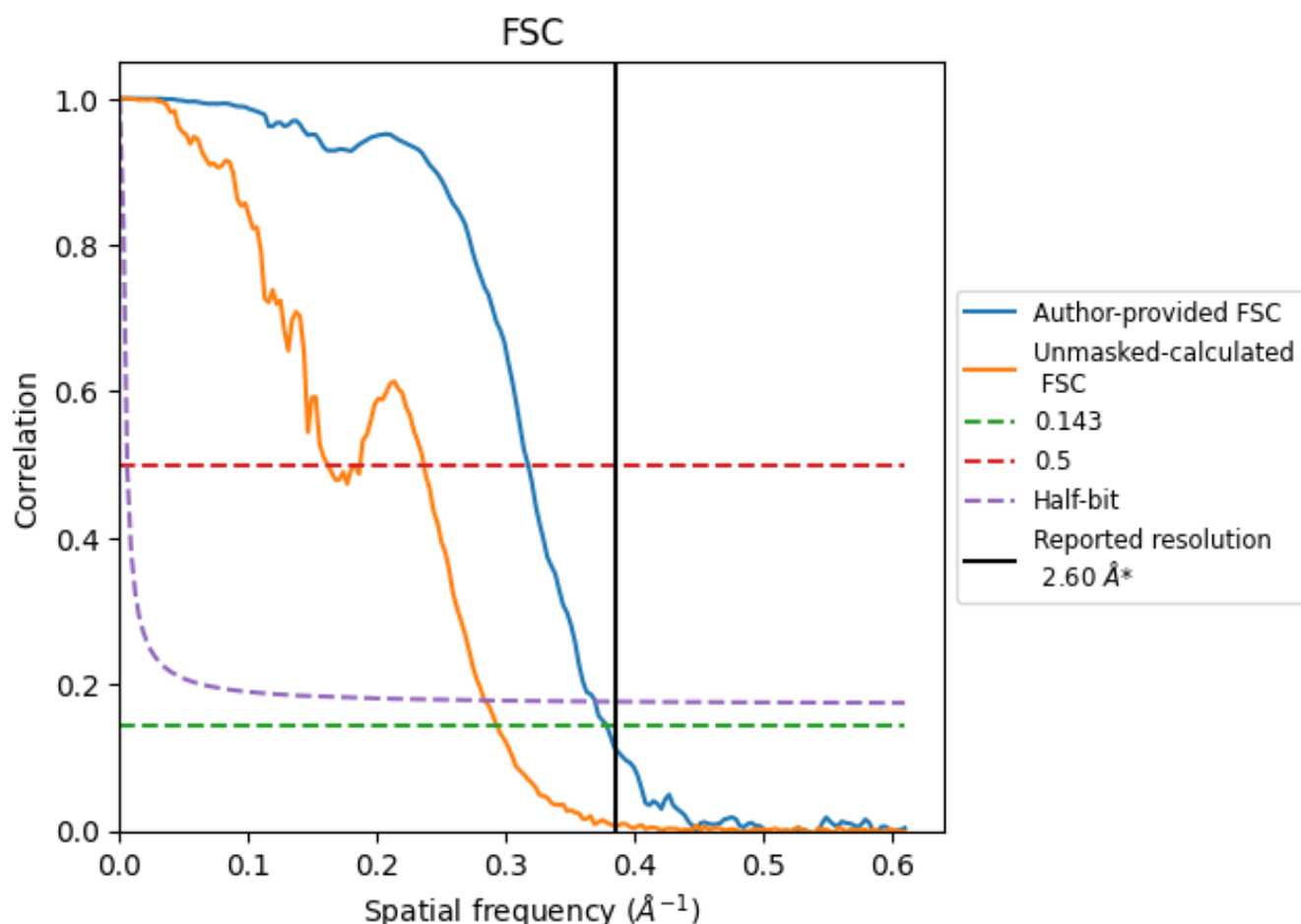


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

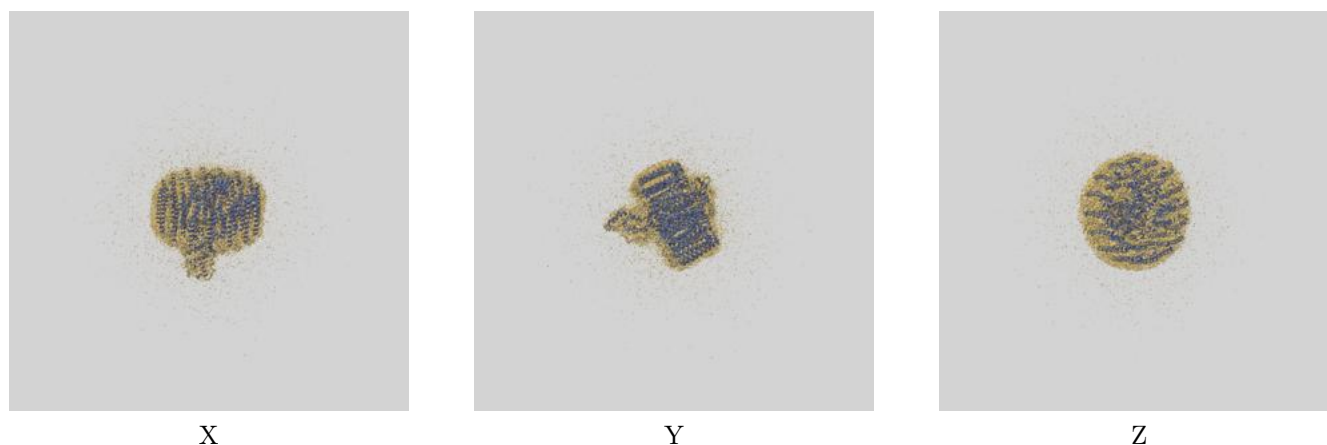
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.64	3.15	2.71
Unmasked-calculated*	3.41	6.19	3.53

*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 3.41 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

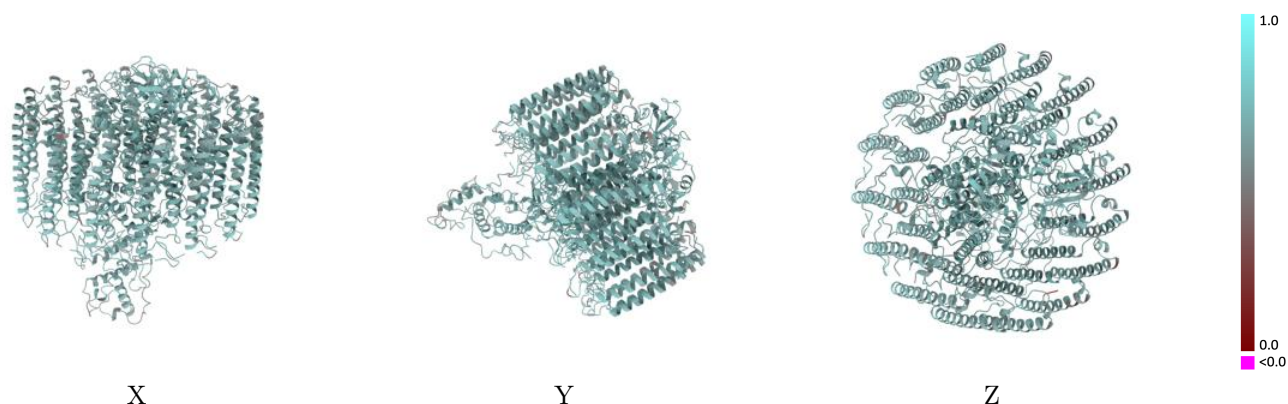
This section contains information regarding the fit between EMDB map EMD-39837 and PDB model 8Z83. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



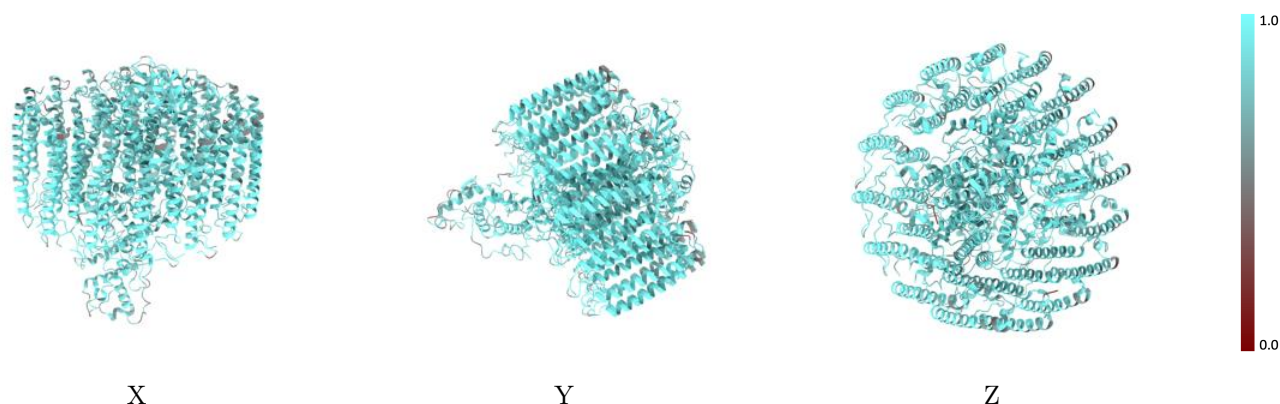
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



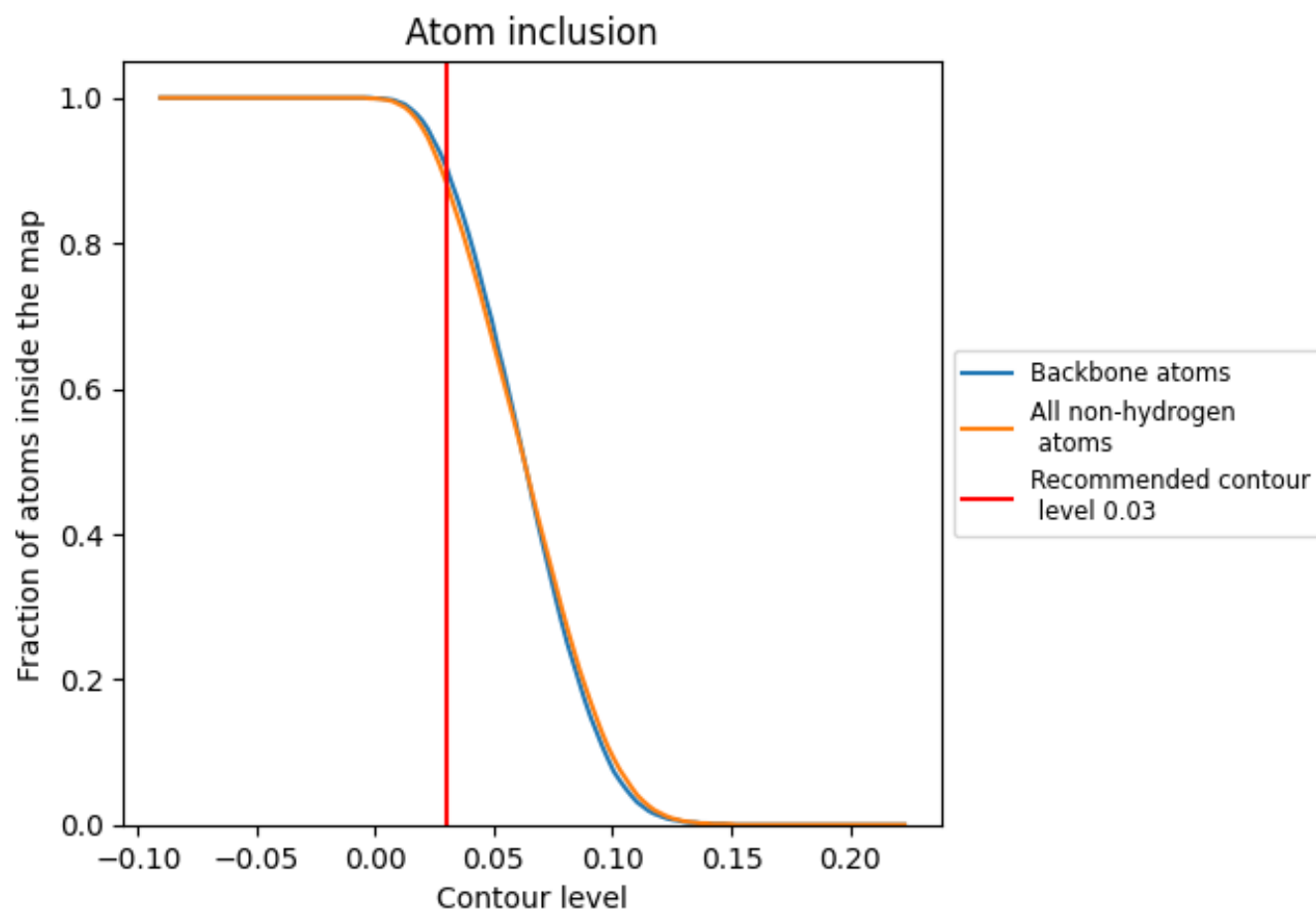
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ




The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.6320
0	 0.8430	 0.6070
1	 0.8650	 0.6210
2	 0.8450	 0.6130
3	 0.8730	 0.6200
4	 0.8270	 0.6090
5	 0.8800	 0.6210
6	 0.8440	 0.6070
7	 0.8580	 0.6040
8	 0.8130	 0.6010
9	 0.9070	 0.6220
A	 0.9290	 0.6480
B	 0.8820	 0.6300
C	 0.8910	 0.6450
D	 0.9420	 0.6470
E	 0.8600	 0.6110
F	 0.8830	 0.6220
G	 0.8460	 0.6200
H	 0.8800	 0.6360
I	 0.8970	 0.6330
J	 0.8790	 0.6300
K	 0.8720	 0.6110
L	 0.9290	 0.6610
M	 0.9320	 0.6610
N	 0.8300	 0.6050
O	 0.8780	 0.6240
P	 0.8560	 0.6070
Q	 0.8910	 0.6120
R	 0.8470	 0.6190
S	 0.9030	 0.6410
T	 0.8580	 0.6230
U	 0.8840	 0.6200
V	 0.8100	 0.6110
W	 0.9140	 0.6400
X	 0.8550	 0.6200



Continued on next page...

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Chain	Atom inclusion	Q-score
Y	 0.8720	 0.6320
Z	 0.8370	 0.6090