



wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 03:28 AM JST

PDB ID : 7VRJ
EMDB ID : EMD-32100
Title : STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF
Allochrocatium tepidum
Authors : Tani, K.; Kobayashi, K.; Hosogi, N.; Ji, X.-C.; Nagashima, S.; Nagashima,
K.V.P.; Tsukatani, Y.; Kanno, R.; Hall, M.; Yu, L.-J.; Ishikawa, I.; Okura,
Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Kimura, Y.; Wang-Otomo,
Z.-Y.
Deposited on : 2021-10-23
Resolution : 2.81 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:

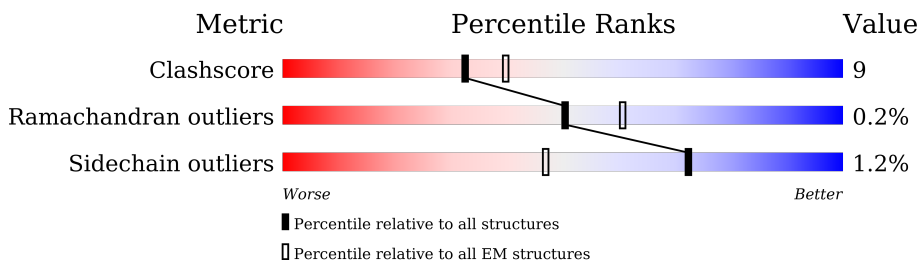
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.81 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.





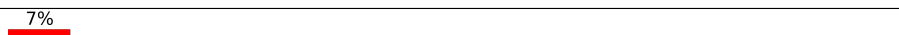
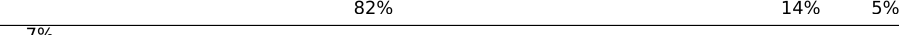


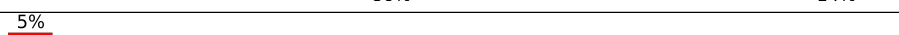



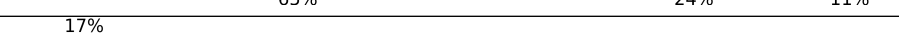


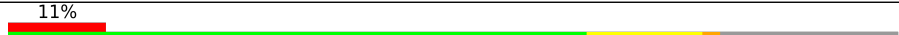
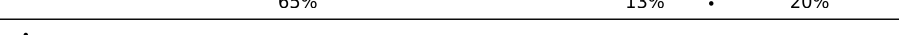



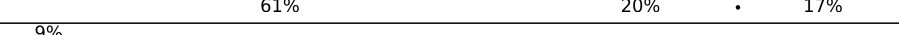


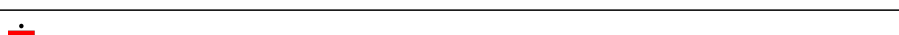



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	405	
2	L	277	
3	M	324	
4	H	259	
5	1	44	
5	5	44	
5	7	44	

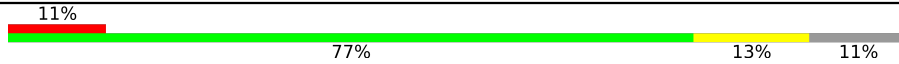

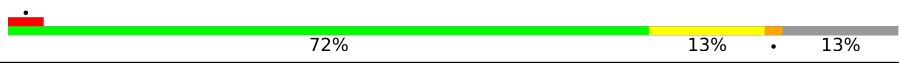
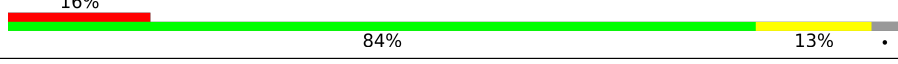
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Mol	Chain	Length	Quality of chain
5	9	44	 80% 18%
5	A	44	 5% 80% 20%
5	I	44	 7% 82% 14% 5%
5	K	44	 7% 82% 16%
5	O	44	 5% 86% 14%
5	Q	44	 5% 77% 20%
6	0	46	 76% 15% 9%
6	2	46	 11% 65% 24% 11%
6	4	46	 17% 83% 9% 9%
6	6	46	 11% 74% 9% 17%
6	8	46	 11% 65% 13% 20%
6	B	46	 83% 13%
6	J	46	 13% 65% 22% 13%
6	N	46	 61% 20% 17%
6	P	46	 9% 76% 15% 9%
6	R	46	 11% 74% 15% 11%
7	D	64	 62% 16% 22%
7	F	64	 62% 14% 23%
7	S	64	 5% 66% 14% 19%
7	U	64	 5% 72% 6% 20%
7	W	64	 14% 69% 17% 12%
7	Y	64	 14% 81% 17%
8	E	47	 81% 11% 9%
8	G	47	 9% 74% 15% 11%
8	T	47	 6% 83% 6% 11%

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Mol	Chain	Length	Quality of chain
8	V	47	
8	X	47	
8	Z	47	
9	3	67	

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 26309 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
			Total	C	N	O	S		
1	C	313	2450	1551	427	455	17	0	0

- Molecule 2 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	277	2212	1491	354	358	9	0	0

- Molecule 3 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	318	2539	1707	409	412	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	259	1989	1280	334	367	8	1	0

- Molecule 5 is a protein called Light-harvesting protein LH1 alpha2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	44	366	251	59	55	1	0	0
5	I	44	366	251	59	55	1	0	0
5	K	44	366	251	59	55	1	0	0
5	O	44	366	251	59	55	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	1	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	5	43	Total	C	N	O	S	0	0
			355	245	57	52	1		
5	7	44	Total	C	N	O	S	0	0
			362	248	58	55	1		
5	9	43	Total	C	N	O	S	0	0
			359	248	58	52	1		

- Molecule 6 is a protein called Light-harvesting protein LH1 beta1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	44	Total	C	N	O	S	0	0
			359	238	58	61	2		
6	J	40	Total	C	N	O	S	0	0
			331	223	53	54	1		
6	N	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	P	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	R	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	2	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	4	42	Total	C	N	O	S	0	0
			345	231	55	57	2		
6	6	38	Total	C	N	O	S	0	0
			320	217	51	51	1		
6	8	37	Total	C	N	O	S	0	0
			312	211	50	50	1		
6	0	42	Total	C	N	O	S	0	0
			345	231	55	57	2		

- Molecule 7 is a protein called Light-harvesting protein LH1 alpha1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	50	Total	C	N	O	S	0	0
			411	279	63	67	2		
7	F	49	Total	C	N	O	S	0	0
			401	273	62	65	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	52	Total	C	N	O	S	0	0
			419	283	65	69	2		
7	U	51	Total	C	N	O	S	0	0
			416	282	64	68	2		
7	W	56	Total	C	N	O	S	0	0
			455	306	72	75	2		
7	Y	63	Total	C	N	O	S	0	0
			510	341	83	84	2		

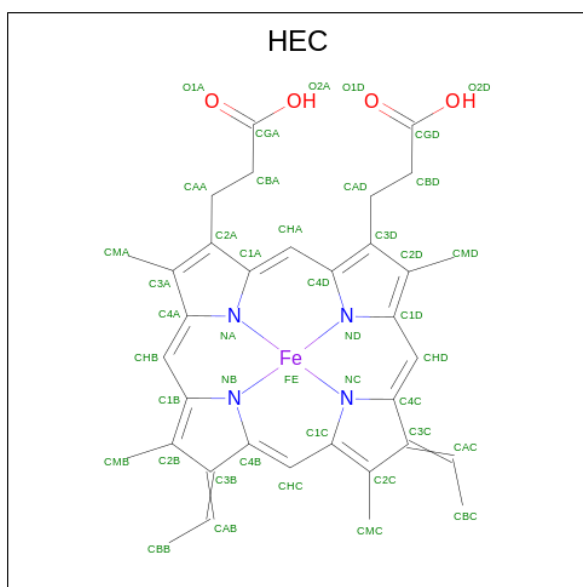
- Molecule 8 is a protein called Light-harvesting protein LH1 beta3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	43	Total	C	N	O	S	0	0
			353	236	55	59	3		
8	G	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	T	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	V	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	X	42	Total	C	N	O	S	0	0
			348	233	54	58	3		
8	Z	41	Total	C	N	O	S	0	0
			342	230	53	56	3		

- Molecule 9 is a protein called Light-harvesting protein LH1 alpha3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	65	Total	C	N	O	S	0	0
			499	337	80	79	3		

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

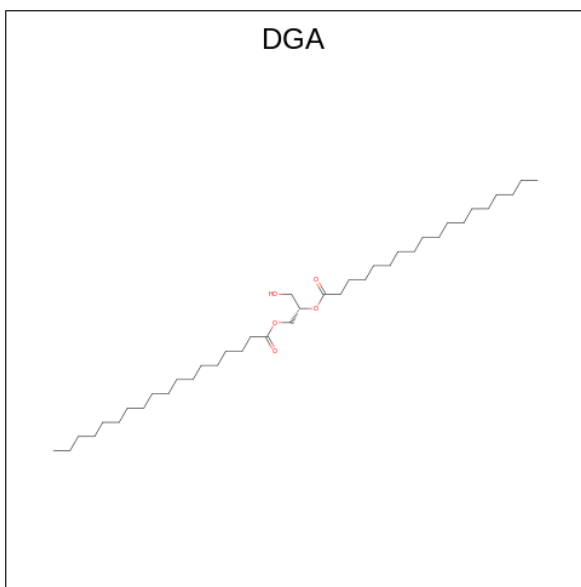


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	
10	C	1	Total	C	Fe	N	O	0
			172	136	4	16	16	

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

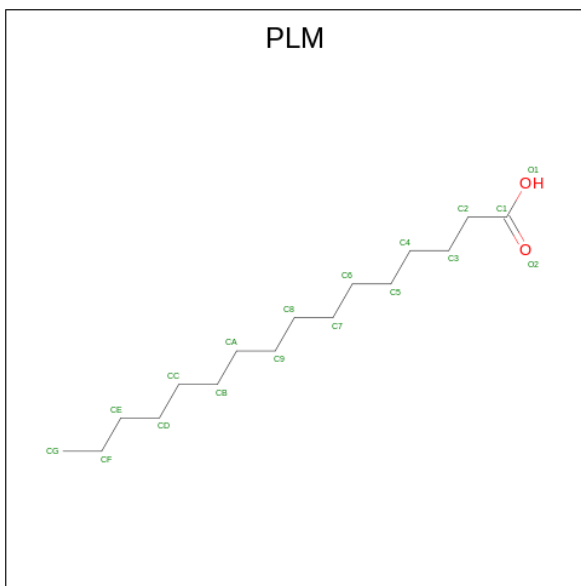
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	C	1	Total	Mg	0
			1	1	

- Molecule 12 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



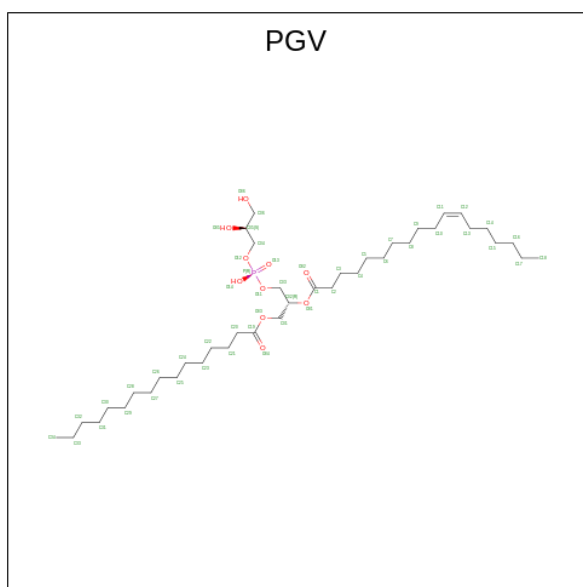
Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			17	13	4	

- Molecule 13 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



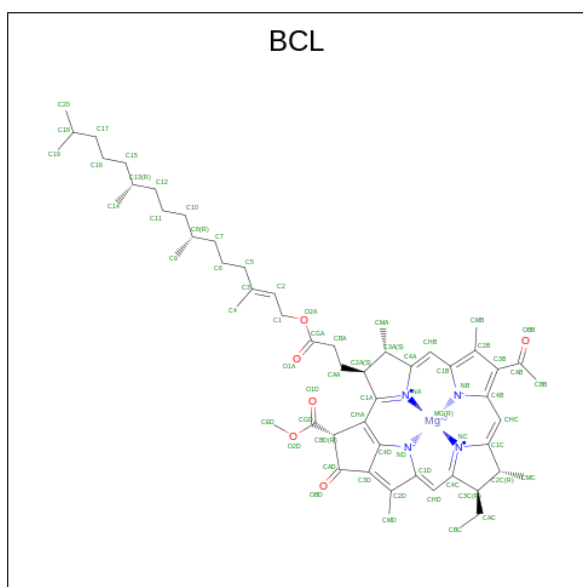
Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	C	O	0
			12	11	1	

- Molecule 14 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
14	C	1	31	20	10	1	0
14	L	1	118	76	38	4	0
14	L	1	118	76	38	4	0
14	L	1	118	76	38	4	0
14	L	1	118	76	38	4	0
14	M	1	104	73	28	3	0
14	M	1	104	73	28	3	0
14	M	1	104	73	28	3	0
14	H	1	36	25	10	1	0
14	D	1	35	24	10	1	0
14	1	1	27	18	8	1	0
14	5	1	44	33	10	1	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
15	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
15	L	1	Total	C	Mg	N	O	0
			198	165	3	12	18	
15	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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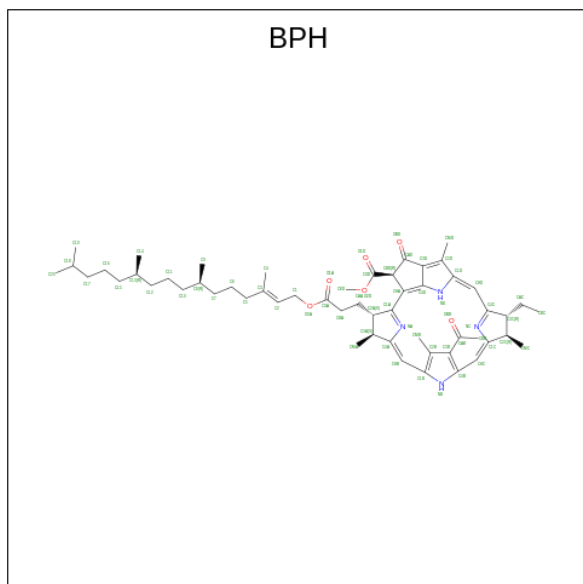
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	V	1	Total 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	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	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	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	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	7	1	Total 61	C 50	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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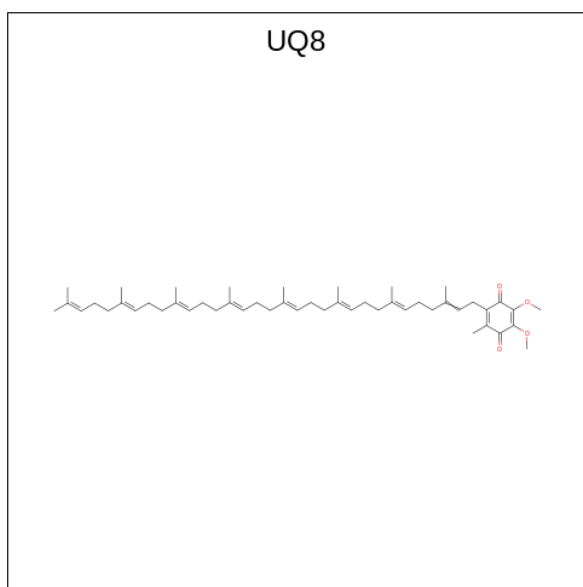
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
15	0	1	66	55	1	4	6	0

- Molecule 16 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



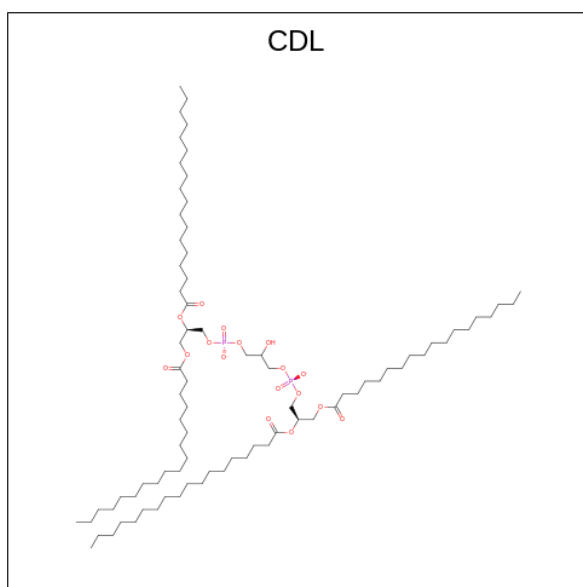
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
16	L	1	65	55	4	6	0
16	M	1	65	55	4	6	0

- Molecule 17 is Ubiquinone-8 (three-letter code: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	L	1	119	107	12	0
17	L	1	119	107	12	0
17	L	1	119	107	12	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	L	1	84	65	17	2	0

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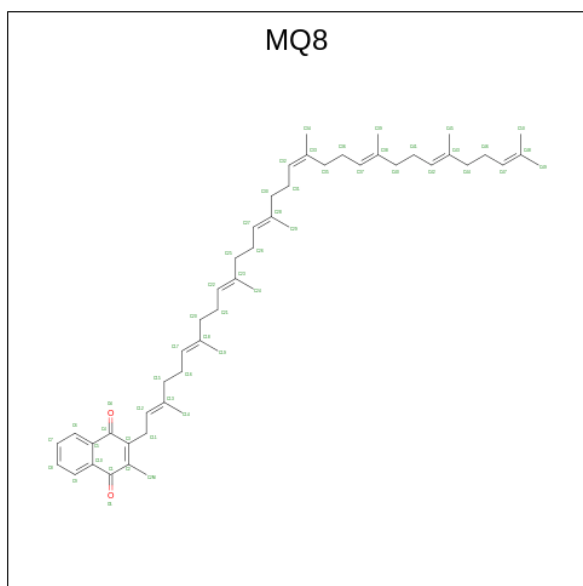
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	M	1	134	97	33	4	0
18	M	1	134	97	33	4	0
18	H	1	114	78	32	4	0
18	H	1	114	78	32	4	0
18	D	1	58	39	17	2	0
18	I	1	51	32	17	2	0
18	S	1	65	46	17	2	0

- 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).



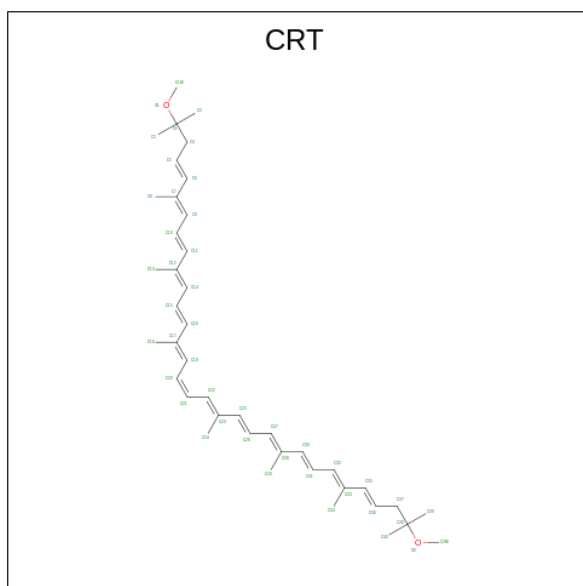
Mol	Chain	Residues	Atoms			AltConf
20	M	1	Total	C	O	0
			106	102	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	M	1	106	102	4	0

- Molecule 21 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C₄₂H₆₀O₂).



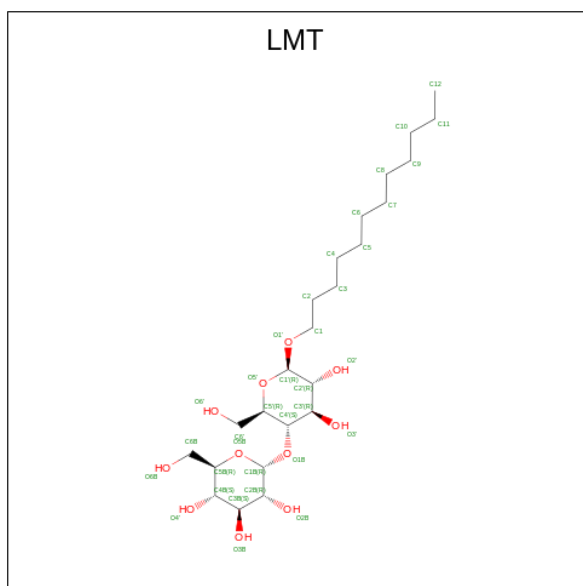
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	M	1	44	42	2	0
21	B	1	44	42	2	0
21	E	1	44	42	2	0
21	G	1	44	42	2	0
21	J	1	44	42	2	0
21	N	1	44	42	2	0
21	P	1	44	42	2	0
21	Q	1	44	42	2	0
21	R	1	44	42	2	0
21	S	1	44	42	2	0

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Mol	Chain	Residues	Atoms			AltConf
21	X	1	Total	C	O	0
			44	42	2	
21	1	1	Total	C	O	0
			44	42	2	
21	2	1	Total	C	O	0
			44	42	2	
21	4	1	Total	C	O	0
			44	42	2	
21	6	1	Total	C	O	0
			44	42	2	
21	7	1	Total	C	O	0
			44	42	2	
21	8	1	Total	C	O	0
			44	42	2	

- Molecule 22 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
22	H	1	Total	C	O	0
			35	24	11	
22	B	1	Total	C	O	0
			35	24	11	
22	E	1	Total	C	O	0
			35	24	11	
22	G	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
22	J	1	Total	C	O	0
			70	48	22	
22	J	1	Total	C	O	0
			70	48	22	
22	K	1	Total	C	O	0
			35	24	11	
22	N	1	Total	C	O	0
			35	24	11	
22	P	1	Total	C	O	0
			35	24	11	
22	T	1	Total	C	O	0
			35	24	11	
22	V	1	Total	C	O	0
			35	24	11	
22	X	1	Total	C	O	0
			35	24	11	
22	Z	1	Total	C	O	0
			35	24	11	
22	2	1	Total	C	O	0
			35	24	11	
22	4	1	Total	C	O	0
			70	48	22	
22	4	1	Total	C	O	0
			70	48	22	
22	8	1	Total	C	O	0
			35	24	11	
22	0	1	Total	C	O	0
			35	24	11	

- Molecule 23 is CALCIUM ION (three-letter code: CA) (formula: Ca).

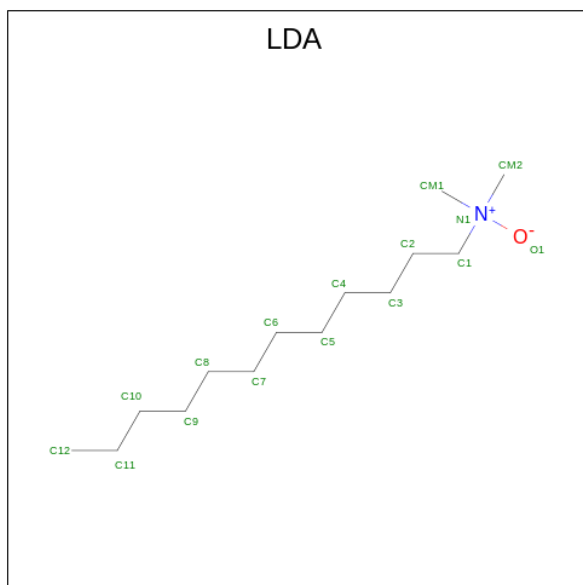
Mol	Chain	Residues	Atoms		AltConf
23	D	1	Total	Ca	0
			1	1	
23	F	1	Total	Ca	0
			1	1	
23	S	1	Total	Ca	0
			1	1	
23	U	1	Total	Ca	0
			1	1	
23	W	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
23	Y	1	Total	Ca	0
			1	1	

- Molecule 24 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				AltConf
24	K	1	Total	C	N	O	0
			16	14	1	1	
24	O	1	Total	C	N	O	0
			16	14	1	1	

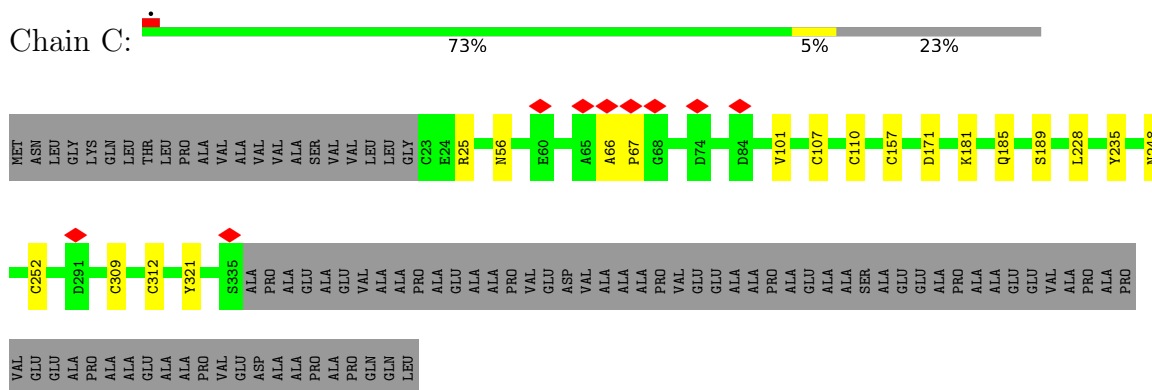
- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	C	18	Total	O	0
			18	18	
25	L	13	Total	O	0
			13	13	
25	M	15	Total	O	0
			15	15	
25	Y	1	Total	O	0
			1	1	
25	3	1	Total	O	0
			1	1	

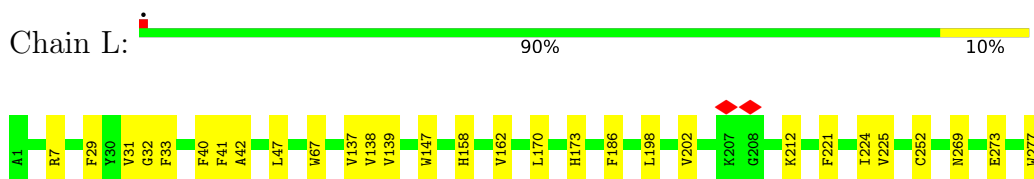
3 Residue-property plots [i](#)

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

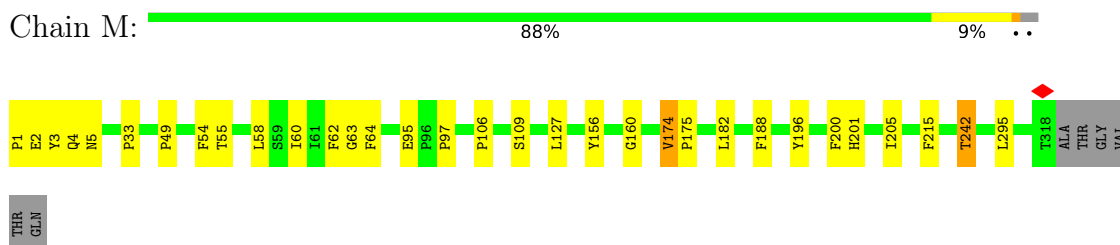
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



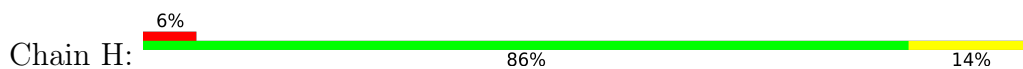
- Molecule 2: Photosynthetic reaction center L subunit

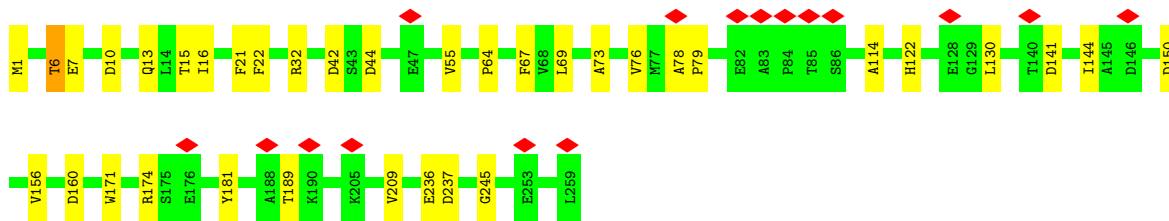


- Molecule 3: Photosynthetic reaction center M subunit

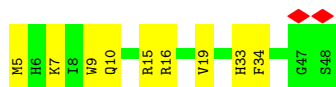
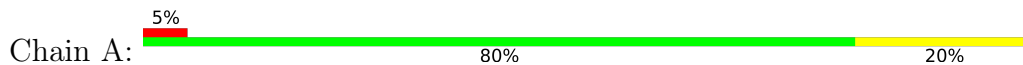


- Molecule 4: Photosynthetic reaction center H subunit

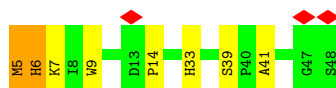
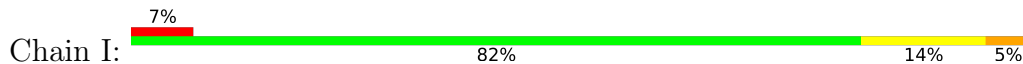




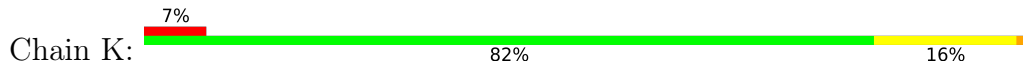
• Molecule 5: Light-harvesting protein LH1 alpha2



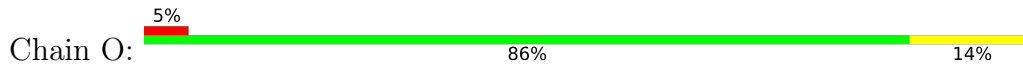
• Molecule 5: Light-harvesting protein LH1 alpha2



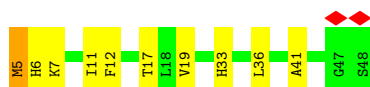
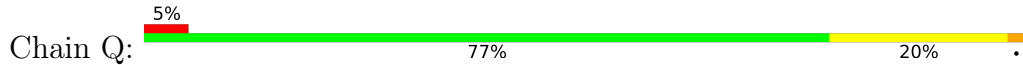
• Molecule 5: Light-harvesting protein LH1 alpha2



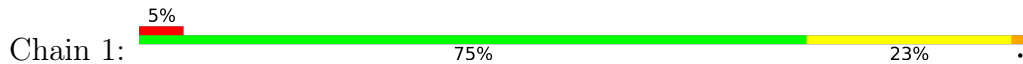
• Molecule 5: Light-harvesting protein LH1 alpha2



• Molecule 5: Light-harvesting protein LH1 alpha2

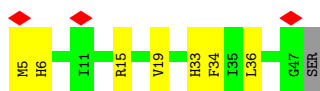
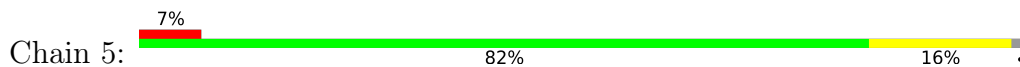


• Molecule 5: Light-harvesting protein LH1 alpha2

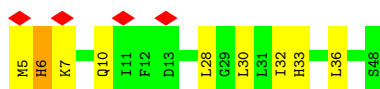
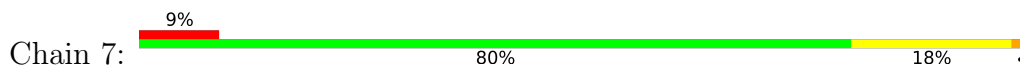




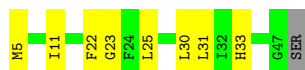
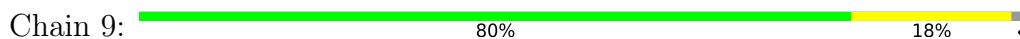
- Molecule 5: Light-harvesting protein LH1 alpha2



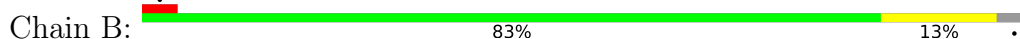
- Molecule 5: Light-harvesting protein LH1 alpha2



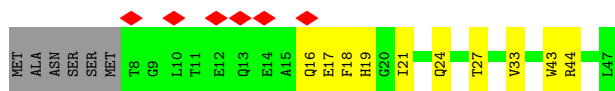
- Molecule 5: Light-harvesting protein LH1 alpha2



- Molecule 6: Light-harvesting protein LH1 beta1



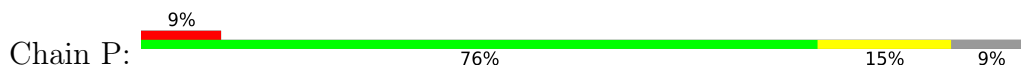
- Molecule 6: Light-harvesting protein LH1 beta1



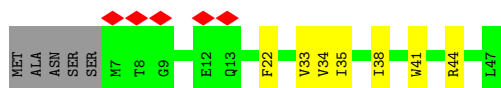
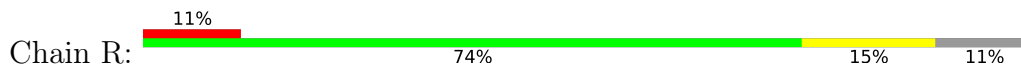
- Molecule 6: Light-harvesting protein LH1 beta1



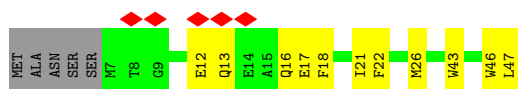
- Molecule 6: Light-harvesting protein LH1 beta1



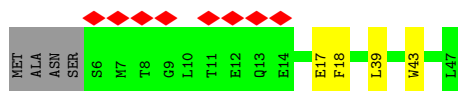
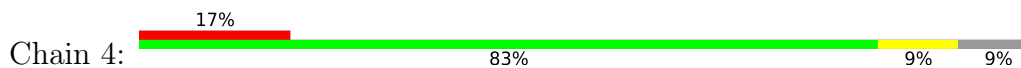
• Molecule 6: Light-harvesting protein LH1 beta1



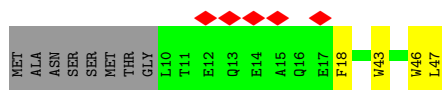
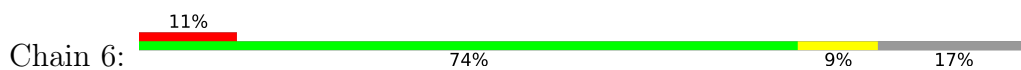
• Molecule 6: Light-harvesting protein LH1 beta1



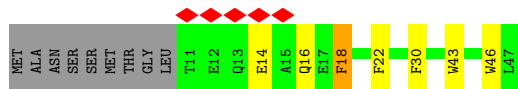
• Molecule 6: Light-harvesting protein LH1 beta1



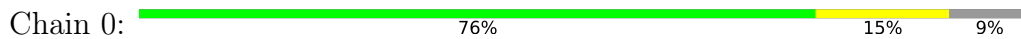
• Molecule 6: Light-harvesting protein LH1 beta1



• Molecule 6: Light-harvesting protein LH1 beta1



• Molecule 6: Light-harvesting protein LH1 beta1



- Molecule 7: Light-harvesting protein LH1 alpha1



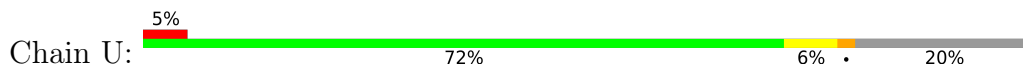
- Molecule 7: Light-harvesting protein LH1 alpha1



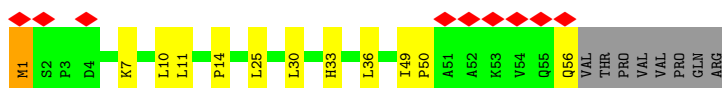
- Molecule 7: Light-harvesting protein LH1 alpha1



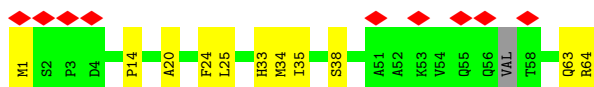
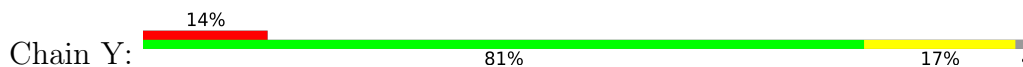
- Molecule 7: Light-harvesting protein LH1 alpha1



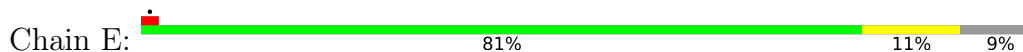
- Molecule 7: Light-harvesting protein LH1 alpha1



- Molecule 7: Light-harvesting protein LH1 alpha1

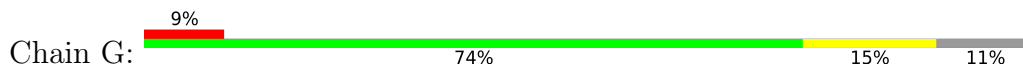


- Molecule 8: Light-harvesting protein LH1 beta3

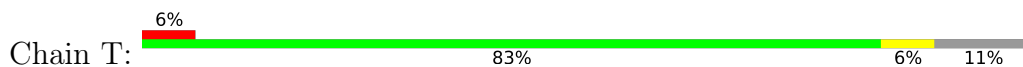




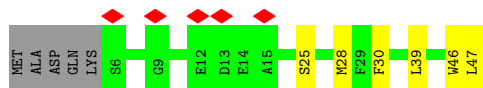
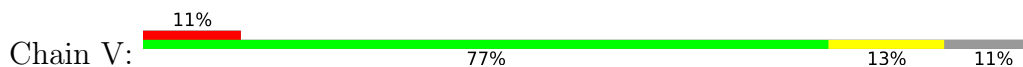
• Molecule 8: Light-harvesting protein LH1 beta3



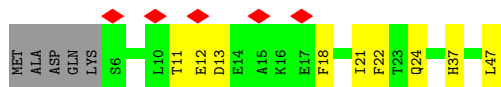
• Molecule 8: Light-harvesting protein LH1 beta3



• Molecule 8: Light-harvesting protein LH1 beta3



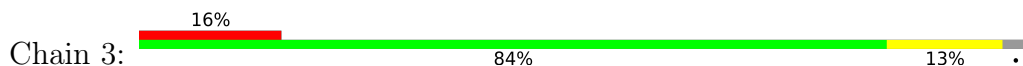
• Molecule 8: Light-harvesting protein LH1 beta3



• Molecule 8: Light-harvesting protein LH1 beta3



• Molecule 9: Light-harvesting protein LH1 alpha3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	156992	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0134	Depositor
Map size (\AA)	325.6, 325.6, 325.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.814, 0.814, 0.814	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.28	0/2524	0.48	0/3453
2	L	0.29	0/2297	0.47	0/3139
3	M	0.29	0/2639	0.46	0/3611
4	H	0.28	0/2045	0.50	0/2782
5	1	0.26	0/369	0.43	0/500
5	5	0.27	0/358	0.43	0/488
5	7	0.27	0/365	0.44	0/496
5	9	0.26	0/362	0.44	0/492
5	A	0.27	0/369	0.43	0/500
5	I	0.27	0/369	0.42	0/500
5	K	0.26	0/369	0.42	0/500
5	O	0.26	0/369	0.43	0/500
5	Q	0.27	0/369	0.43	0/500
6	0	0.26	0/357	0.39	0/485
6	2	0.25	0/351	0.40	0/477
6	4	0.26	0/357	0.39	0/485
6	6	0.25	0/332	0.40	0/452
6	8	0.27	0/324	0.38	0/441
6	B	0.28	0/371	0.45	0/504
6	J	0.26	0/343	0.38	0/467
6	N	0.26	0/332	0.40	0/452
6	P	0.25	0/357	0.40	0/485
6	R	0.26	0/351	0.41	0/477
7	D	0.25	0/413	0.45	0/566
7	F	0.24	0/413	0.47	0/566
7	S	0.25	0/421	0.45	0/577
7	U	0.24	0/418	0.49	0/573
7	W	0.24	0/457	0.46	0/625
7	Y	0.27	0/513	0.47	0/702
8	E	0.25	0/365	0.42	0/494
8	G	0.26	0/360	0.41	0/487
8	T	0.26	0/360	0.41	0/487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	V	0.26	0/360	0.41	0/487
8	X	0.25	0/360	0.41	0/487
8	Z	0.25	0/354	0.40	0/479
9	3	0.26	0/517	0.42	0/704
All	All	0.27	0/21590	0.45	0/29420

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	2450	0	2362	32	0
2	L	2212	0	2173	25	0
3	M	2539	0	2498	23	0
4	H	1989	0	1993	25	0
5	1	366	0	376	13	0
5	5	355	0	360	5	0
5	7	362	0	365	8	0
5	9	359	0	371	7	0
5	A	366	0	376	6	0
5	I	366	0	376	8	0
5	K	366	0	376	6	0
5	O	366	0	376	6	0
5	Q	366	0	376	10	0
6	0	345	0	334	6	0
6	2	339	0	329	11	0
6	4	345	0	334	4	0
6	6	320	0	310	4	0
6	8	312	0	299	9	0
6	B	359	0	345	6	0
6	J	331	0	320	11	0
6	N	320	0	310	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	345	0	334	5	0
6	R	339	0	329	6	0
7	D	411	0	430	8	0
7	F	401	0	419	9	0
7	S	419	0	433	11	0
7	U	416	0	435	6	0
7	W	455	0	478	10	0
7	Y	510	0	537	11	0
8	E	353	0	341	5	0
8	G	348	0	339	7	0
8	T	348	0	339	5	0
8	V	348	0	339	4	0
8	X	348	0	339	6	0
8	Z	342	0	334	7	0
9	3	499	0	506	6	0
10	C	172	0	126	24	0
11	C	1	0	0	0	0
12	C	17	0	15	0	0
13	C	12	0	18	1	0
14	1	27	0	25	2	0
14	5	44	0	56	4	0
14	C	31	0	32	3	0
14	D	35	0	40	0	0
14	H	36	0	42	3	0
14	L	118	0	122	4	0
14	M	104	0	124	3	0
15	0	66	0	74	7	0
15	1	66	0	74	5	0
15	2	66	0	74	6	0
15	3	66	0	74	4	0
15	4	66	0	74	5	0
15	5	66	0	74	4	0
15	6	66	0	74	5	0
15	7	61	0	61	1	0
15	8	66	0	74	9	0
15	9	66	0	74	5	0
15	A	66	0	74	1	0
15	B	66	0	74	7	0
15	D	66	0	74	4	0
15	E	66	0	74	5	0
15	F	66	0	74	6	0
15	G	66	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	I	66	0	74	3	0
15	J	66	0	74	5	0
15	K	66	0	74	8	0
15	L	198	0	222	9	0
15	M	66	0	74	3	0
15	N	66	0	74	7	0
15	O	66	0	74	4	0
15	P	66	0	74	10	0
15	Q	66	0	74	5	0
15	R	66	0	74	10	0
15	S	66	0	74	3	0
15	T	66	0	74	8	0
15	U	66	0	74	3	0
15	V	66	0	74	7	0
15	W	66	0	74	6	0
15	X	66	0	74	4	0
15	Y	66	0	74	7	0
15	Z	66	0	74	5	0
16	L	65	0	76	4	0
16	M	65	0	76	10	0
17	L	119	0	152	20	0
18	D	58	0	60	4	0
18	H	114	0	126	4	0
18	I	51	0	46	1	0
18	L	84	0	121	1	0
18	M	134	0	168	2	0
18	S	65	0	74	5	0
19	M	1	0	0	0	0
20	M	106	0	144	9	0
21	1	44	0	60	8	0
21	2	44	0	60	6	0
21	4	44	0	60	8	0
21	6	44	0	60	5	0
21	7	44	0	60	4	0
21	8	44	0	60	6	0
21	B	44	0	60	8	0
21	E	44	0	60	5	0
21	G	44	0	60	6	0
21	J	44	0	60	5	0
21	M	44	0	60	3	0
21	N	44	0	60	2	0
21	P	44	0	60	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Q	44	0	60	6	0
21	R	44	0	60	5	0
21	S	44	0	60	2	0
21	X	44	0	60	5	0
22	0	35	0	46	2	0
22	2	35	0	46	2	0
22	4	70	0	92	4	0
22	8	35	0	46	1	0
22	B	35	0	46	1	0
22	E	35	0	46	1	0
22	G	35	0	46	3	0
22	H	35	0	46	1	0
22	J	70	0	92	1	0
22	K	35	0	46	1	0
22	N	35	0	46	0	0
22	P	35	0	46	1	0
22	T	35	0	46	0	0
22	V	35	0	46	3	0
22	X	35	0	46	0	0
22	Z	35	0	46	2	0
23	D	1	0	0	0	0
23	F	1	0	0	0	0
23	S	1	0	0	0	0
23	U	1	0	0	0	0
23	W	1	0	0	0	0
23	Y	1	0	0	0	0
24	K	16	0	31	1	0
24	O	16	0	31	2	0
25	3	1	0	0	0	0
25	C	18	0	0	0	0
25	L	13	0	0	0	0
25	M	15	0	0	1	0
25	Y	1	0	0	1	0
All	All	26309	0	27095	498	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 9.

The worst 5 of 498 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:309:CYS:SG	10:C:504:HEC:HAB	1.53	1.48
1:C:252:CYS:SG	10:C:503:HEC:HAC	1.59	1.41
1:C:309:CYS:SG	10:C:504:HEC:CAB	2.07	1.40
1:C:110:CYS:SG	10:C:501:HEC:HAC	1.62	1.40
1:C:157:CYS:SG	10:C:502:HEC:HAC	1.64	1.38

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	311/405 (77%)	297 (96%)	14 (4%)	0	100	100
2	L	275/277 (99%)	268 (98%)	7 (2%)	0	100	100
3	M	316/324 (98%)	309 (98%)	7 (2%)	0	100	100
4	H	258/259 (100%)	245 (95%)	13 (5%)	0	100	100
5	1	42/44 (96%)	40 (95%)	1 (2%)	1 (2%)	6	19
5	5	41/44 (93%)	40 (98%)	0	1 (2%)	6	19
5	7	42/44 (96%)	37 (88%)	4 (10%)	1 (2%)	6	19
5	9	41/44 (93%)	39 (95%)	2 (5%)	0	100	100
5	A	42/44 (96%)	42 (100%)	0	0	100	100
5	I	42/44 (96%)	40 (95%)	1 (2%)	1 (2%)	6	19
5	K	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
5	O	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
5	Q	42/44 (96%)	40 (95%)	1 (2%)	1 (2%)	6	19
6	0	40/46 (87%)	40 (100%)	0	0	100	100
6	2	39/46 (85%)	39 (100%)	0	0	100	100
6	4	40/46 (87%)	38 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	36/46 (78%)	34 (94%)	2 (6%)	0	100	100
6	8	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
6	B	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
6	J	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
6	N	36/46 (78%)	35 (97%)	1 (3%)	0	100	100
6	P	40/46 (87%)	40 (100%)	0	0	100	100
6	R	39/46 (85%)	39 (100%)	0	0	100	100
7	D	48/64 (75%)	46 (96%)	2 (4%)	0	100	100
7	F	47/64 (73%)	47 (100%)	0	0	100	100
7	S	50/64 (78%)	49 (98%)	1 (2%)	0	100	100
7	U	49/64 (77%)	48 (98%)	1 (2%)	0	100	100
7	W	54/64 (84%)	53 (98%)	1 (2%)	0	100	100
7	Y	59/64 (92%)	56 (95%)	3 (5%)	0	100	100
8	E	41/47 (87%)	40 (98%)	1 (2%)	0	100	100
8	G	40/47 (85%)	40 (100%)	0	0	100	100
8	T	40/47 (85%)	40 (100%)	0	0	100	100
8	V	40/47 (85%)	39 (98%)	1 (2%)	0	100	100
8	X	40/47 (85%)	39 (98%)	0	1 (2%)	5	18
8	Z	39/47 (83%)	39 (100%)	0	0	100	100
9	3	63/67 (94%)	59 (94%)	4 (6%)	0	100	100
All	All	2531/2854 (89%)	2451 (97%)	74 (3%)	6 (0%)	50	76

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	X	12	GLU
5	7	6	HIS
5	Q	6	HIS
5	5	6	HIS
5	1	6	HIS

5.3.2 Protein sidechains [i](#)

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	265/322 (82%)	264 (100%)	1 (0%)	91	97
2	L	224/224 (100%)	222 (99%)	2 (1%)	78	93
3	M	252/256 (98%)	248 (98%)	4 (2%)	62	87
4	H	208/208 (100%)	203 (98%)	5 (2%)	49	80
5	1	38/38 (100%)	38 (100%)	0	100	100
5	5	36/38 (95%)	36 (100%)	0	100	100
5	7	37/38 (97%)	37 (100%)	0	100	100
5	9	37/38 (97%)	37 (100%)	0	100	100
5	A	38/38 (100%)	37 (97%)	1 (3%)	46	78
5	I	38/38 (100%)	38 (100%)	0	100	100
5	K	38/38 (100%)	36 (95%)	2 (5%)	22	52
5	O	38/38 (100%)	38 (100%)	0	100	100
5	Q	38/38 (100%)	38 (100%)	0	100	100
6	0	35/38 (92%)	35 (100%)	0	100	100
6	2	34/38 (90%)	34 (100%)	0	100	100
6	4	35/38 (92%)	35 (100%)	0	100	100
6	6	32/38 (84%)	32 (100%)	0	100	100
6	8	31/38 (82%)	30 (97%)	1 (3%)	39	71
6	B	37/38 (97%)	37 (100%)	0	100	100
6	J	33/38 (87%)	33 (100%)	0	100	100
6	N	32/38 (84%)	31 (97%)	1 (3%)	40	72
6	P	35/38 (92%)	32 (91%)	3 (9%)	10	29
6	R	34/38 (90%)	34 (100%)	0	100	100
7	D	44/56 (79%)	44 (100%)	0	100	100
7	F	44/56 (79%)	43 (98%)	1 (2%)	50	80
7	S	43/56 (77%)	42 (98%)	1 (2%)	50	80
7	U	44/56 (79%)	44 (100%)	0	100	100
7	W	48/56 (86%)	47 (98%)	1 (2%)	53	82
7	Y	55/56 (98%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	36/40 (90%)	36 (100%)	0	100	100
8	G	36/40 (90%)	35 (97%)	1 (3%)	43	76
8	T	36/40 (90%)	36 (100%)	0	100	100
8	V	36/40 (90%)	36 (100%)	0	100	100
8	X	36/40 (90%)	35 (97%)	1 (3%)	43	76
8	Z	35/40 (88%)	34 (97%)	1 (3%)	42	74
9	3	49/51 (96%)	48 (98%)	1 (2%)	55	83
All	All	2167/2359 (92%)	2140 (99%)	27 (1%)	72	91

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	G	28	MET
6	N	34	VAL
8	Z	21	ILE
5	K	34	PHE
6	P	11	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
5	7	6	HIS
6	8	16	GLN
6	B	16	GLN
6	J	16	GLN
6	P	13	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FME	D	1	7	8,9,10	0.53	0	7,9,11	1.01	1 (14%)
7	FME	S	1	7	8,9,10	0.51	0	7,9,11	0.97	1 (14%)
5	FME	A	5	5	8,9,10	0.50	0	7,9,11	0.98	1 (14%)
7	FME	Y	1	7	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
5	FME	I	5	5	8,9,10	0.51	0	7,9,11	1.09	1 (14%)
5	FME	K	5	5	8,9,10	0.51	0	7,9,11	1.28	1 (14%)
5	FME	O	5	5	8,9,10	0.53	0	7,9,11	0.98	1 (14%)
5	FME	7	5	5	8,9,10	0.52	0	7,9,11	1.01	1 (14%)
7	FME	U	1	7	8,9,10	0.52	0	7,9,11	1.00	1 (14%)
5	FME	5	5	5	8,9,10	0.54	0	7,9,11	1.03	1 (14%)
5	FME	Q	5	5	8,9,10	0.51	0	7,9,11	0.99	1 (14%)
7	FME	W	1	7	8,9,10	0.52	0	7,9,11	0.97	1 (14%)
5	FME	9	5	5	8,9,10	0.48	0	7,9,11	1.07	1 (14%)
5	FME	1	5	5	8,9,10	0.50	0	7,9,11	1.04	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FME	D	1	7	-	1/7/9/11	-
7	FME	S	1	7	-	2/7/9/11	-
5	FME	A	5	5	-	2/7/9/11	-
7	FME	Y	1	7	-	0/7/9/11	-
5	FME	I	5	5	-	1/7/9/11	-
5	FME	K	5	5	-	1/7/9/11	-
5	FME	O	5	5	-	0/7/9/11	-
5	FME	7	5	5	-	0/7/9/11	-
7	FME	U	1	7	-	0/7/9/11	-
5	FME	5	5	5	-	3/7/9/11	-
5	FME	Q	5	5	-	1/7/9/11	-
7	FME	W	1	7	-	0/7/9/11	-
5	FME	9	5	5	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FME	1	5	5	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	5	FME	O-C-CA	-2.64	117.87	124.78
5	I	5	FME	O-C-CA	-2.62	117.91	124.78
5	Q	5	FME	O-C-CA	-2.54	118.11	124.78
5	7	5	FME	O-C-CA	-2.54	118.11	124.78
5	9	5	FME	O-C-CA	-2.53	118.16	124.78

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5	FME	N-CA-CB-CG
5	K	5	FME	CB-CA-N-CN
5	Q	5	FME	O-C-CA-CB
5	5	5	FME	O1-CN-N-CA
5	5	5	FME	CB-CA-N-CN

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	5	FME	1	0
7	U	1	FME	1	0
5	Q	5	FME	4	0
7	W	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 114 ligands modelled in this entry, 8 are monoatomic - leaving 106 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
22	LMT	J	101	-	36,36,36	0.39	0	47,47,47	0.73	0
15	BCL	6	101	-	58,74,74	1.63	10 (17%)	69,115,115	1.61	14 (20%)
24	LDA	O	501	-	12,15,15	2.08	1 (8%)	14,17,17	0.48	0
22	LMT	N	103	-	36,36,36	0.39	0	47,47,47	0.64	0
22	LMT	P	103	-	36,36,36	0.38	0	47,47,47	0.74	1 (2%)
14	PGV	C	508	-	30,30,50	1.15	2 (6%)	33,36,56	1.28	4 (12%)
21	CRT	1	402	-	41,43,43	0.72	0	50,54,54	1.77	10 (20%)
22	LMT	0	101	-	36,36,36	0.44	0	47,47,47	0.89	1 (2%)
15	BCL	Q	101	-	58,74,74	1.65	10 (17%)	69,115,115	1.64	12 (17%)
14	PGV	M	411	-	35,35,50	1.08	2 (5%)	38,41,56	1.27	4 (10%)
10	HEC	C	503	1	32,50,50	1.56	4 (12%)	24,82,82	1.39	3 (12%)
22	LMT	4	104	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
18	CDL	H	302	-	34,34,99	1.21	3 (8%)	39,44,111	1.12	3 (7%)
21	CRT	6	102	-	41,43,43	0.72	0	50,54,54	1.74	14 (28%)
14	PGV	M	407	-	36,36,50	1.05	2 (5%)	39,42,56	1.14	3 (7%)
15	BCL	N	101	-	58,74,74	1.66	11 (18%)	69,115,115	1.63	15 (21%)
10	HEC	C	502	1	32,50,50	1.57	5 (15%)	24,82,82	1.30	1 (4%)
15	BCL	G	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.64	16 (23%)
17	UQ8	L	505	-	53,53,53	1.21	2 (3%)	64,67,67	1.79	20 (31%)
21	CRT	Q	102	-	41,43,43	0.72	0	50,54,54	1.82	11 (22%)
21	CRT	G	103	-	41,43,43	0.69	0	50,54,54	1.52	11 (22%)
15	BCL	F	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.73	14 (20%)
15	BCL	L	509	-	58,74,74	1.64	11 (18%)	69,115,115	1.67	13 (18%)
22	LMT	2	101	-	36,36,36	0.42	0	47,47,47	0.68	0
16	BPH	L	503	-	51,70,70	0.53	0	52,101,101	0.62	0
14	PGV	L	501	-	16,16,50	1.40	2 (12%)	20,21,56	1.41	3 (15%)
21	CRT	N	102	-	41,43,43	0.71	0	50,54,54	1.71	9 (18%)
22	LMT	Z	101	-	36,36,36	0.39	0	47,47,47	0.79	1 (2%)
15	BCL	I	102	-	58,74,74	1.65	11 (18%)	69,115,115	1.56	13 (18%)
15	BCL	K	103	-	58,74,74	1.68	10 (17%)	69,115,115	1.66	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PLM	C	507	1	11,11,17	0.39	0	10,10,17	0.44	0
22	LMT	H	304	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)
15	BCL	P	101	-	58,74,74	1.65	11 (18%)	69,115,115	1.64	17 (24%)
15	BCL	3	101	-	58,74,74	1.68	11 (18%)	69,115,115	1.58	12 (17%)
14	PGV	1	401	-	26,26,50	1.29	2 (7%)	29,31,56	1.18	2 (6%)
15	BCL	9	101	-	58,74,74	1.63	10 (17%)	69,115,115	1.65	15 (21%)
15	BCL	Z	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.66	15 (21%)
17	UQ8	L	512	-	33,33,53	1.55	2 (6%)	40,43,67	1.51	8 (20%)
14	PGV	D	101	-	34,34,50	1.09	2 (5%)	37,40,56	1.05	2 (5%)
15	BCL	D	103	-	58,74,74	1.63	10 (17%)	69,115,115	1.61	13 (18%)
22	LMT	G	101	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
15	BCL	7	101	-	53,69,74	1.69	8 (15%)	63,109,115	1.77	16 (25%)
20	MQ8	M	404	-	54,54,54	1.29	2 (3%)	66,69,69	1.47	14 (21%)
14	PGV	H	303	-	35,35,50	1.11	2 (5%)	38,41,56	1.09	2 (5%)
21	CRT	E	103	-	41,43,43	0.68	0	50,54,54	1.65	12 (24%)
21	CRT	2	103	-	41,43,43	0.72	0	50,54,54	2.27	15 (30%)
21	CRT	R	102	-	41,43,43	0.70	0	50,54,54	1.59	12 (24%)
21	CRT	X	103	-	41,43,43	0.72	0	50,54,54	1.75	10 (20%)
15	BCL	W	101	-	58,74,74	1.62	8 (13%)	69,115,115	1.76	17 (24%)
21	CRT	J	103	-	41,43,43	0.71	0	50,54,54	3.36	14 (28%)
22	LMT	J	104	-	36,36,36	0.41	0	47,47,47	0.65	0
22	LMT	K	102	-	36,36,36	0.40	0	47,47,47	0.75	0
15	BCL	V	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.64	15 (21%)
21	CRT	M	405	-	41,43,43	0.71	0	50,54,54	1.63	10 (20%)
15	BCL	T	102	-	58,74,74	1.61	9 (15%)	69,115,115	1.61	15 (21%)
10	HEC	C	504	1	32,50,50	1.58	4 (12%)	24,82,82	1.38	3 (12%)
17	UQ8	L	504	-	33,33,53	1.51	2 (6%)	40,43,67	1.51	7 (17%)
15	BCL	0	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.65	14 (20%)
22	LMT	E	101	-	36,36,36	0.42	0	47,47,47	0.92	3 (6%)
16	BPH	M	403	-	51,70,70	0.54	1 (1%)	52,101,101	0.60	0
21	CRT	8	103	-	41,43,43	0.69	0	50,54,54	1.69	10 (20%)
15	BCL	M	402	-	58,74,74	1.65	10 (17%)	69,115,115	1.76	13 (18%)
22	LMT	X	101	-	36,36,36	0.44	0	47,47,47	0.86	3 (6%)
14	PGV	L	511	-	32,32,50	1.12	2 (6%)	35,38,56	1.26	4 (11%)
14	PGV	L	507	-	38,38,50	1.01	2 (5%)	41,44,56	1.14	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCL	U	101	-	58,74,74	1.66	10 (17%)	69,115,115	1.65	13 (18%)
21	CRT	7	102	-	41,43,43	0.70	0	50,54,54	1.59	10 (20%)
12	DGA	C	506	1	16,16,43	1.75	3 (18%)	18,18,45	1.83	4 (22%)
15	BCL	2	102	-	58,74,74	1.65	10 (17%)	69,115,115	1.64	16 (23%)
18	CDL	M	408	-	38,38,99	1.29	3 (7%)	43,49,111	1.24	4 (9%)
15	BCL	B	102	-	58,74,74	1.66	10 (17%)	69,115,115	1.61	18 (26%)
15	BCL	R	101	-	58,74,74	1.62	9 (15%)	69,115,115	1.61	15 (21%)
22	LMT	V	101	-	36,36,36	0.44	0	47,47,47	0.68	0
18	CDL	L	510	-	83,83,99	1.04	4 (4%)	89,95,111	1.21	8 (8%)
15	BCL	1	403	-	58,74,74	1.64	11 (18%)	69,115,115	1.60	13 (18%)
21	CRT	4	103	-	41,43,43	0.67	0	50,54,54	1.60	8 (16%)
18	CDL	H	301	-	78,78,99	1.03	4 (5%)	84,90,111	1.08	5 (5%)
18	CDL	D	102	-	57,57,99	1.11	4 (7%)	63,69,111	1.15	4 (6%)
14	PGV	5	101	-	43,43,50	0.97	2 (4%)	46,49,56	1.03	2 (4%)
20	MQ8	M	406	-	54,54,54	1.33	2 (3%)	66,69,69	1.69	17 (25%)
15	BCL	L	508	-	58,74,74	1.61	9 (15%)	69,115,115	1.75	14 (20%)
10	HEC	C	501	1	32,50,50	1.63	4 (12%)	24,82,82	1.35	1 (4%)
22	LMT	8	101	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
15	BCL	O	502	-	58,74,74	1.65	10 (17%)	69,115,115	1.62	14 (20%)
21	CRT	S	104	-	41,43,43	0.73	0	50,54,54	2.28	16 (32%)
18	CDL	I	101	-	50,50,99	1.28	4 (8%)	56,62,111	1.34	8 (14%)
22	LMT	B	101	-	36,36,36	0.40	0	47,47,47	0.66	0
22	LMT	4	101	-	36,36,36	0.46	0	47,47,47	0.95	1 (2%)
24	LDA	K	101	-	12,15,15	2.08	1 (8%)	14,17,17	0.53	0
15	BCL	5	102	-	58,74,74	1.67	11 (18%)	69,115,115	1.65	16 (23%)
15	BCL	8	102	-	58,74,74	1.64	9 (15%)	69,115,115	1.63	17 (24%)
15	BCL	J	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.65	15 (21%)
14	PGV	L	506	-	28,28,50	1.21	2 (7%)	31,34,56	1.20	4 (12%)
21	CRT	B	103	-	41,43,43	0.72	0	50,54,54	1.71	11 (22%)
15	BCL	A	101	-	58,74,74	1.64	9 (15%)	69,115,115	1.68	15 (21%)
18	CDL	M	410	-	94,94,99	0.95	4 (4%)	100,106,111	1.08	6 (6%)
15	BCL	4	102	-	58,74,74	1.64	10 (17%)	69,115,115	1.69	15 (21%)
15	BCL	E	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.64	16 (23%)
15	BCL	S	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.60	13 (18%)
22	LMT	T	101	-	36,36,36	0.41	0	47,47,47	0.64	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CDL	S	101	-	64,64,99	1.15	4 (6%)	70,76,111	1.15	6 (8%)
15	BCL	X	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.67	16 (23%)
21	CRT	P	102	-	41,43,43	0.71	0	50,54,54	3.54	13 (26%)
15	BCL	Y	101	-	58,74,74	1.66	11 (18%)	69,115,115	1.64	12 (17%)
14	PGV	M	409	-	30,30,50	1.22	2 (6%)	34,35,56	1.28	3 (8%)
15	BCL	L	502	-	58,74,74	1.64	10 (17%)	69,115,115	1.60	14 (20%)

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
22	LMT	J	101	-	-	5/21/61/61	0/2/2/2
15	BCL	6	101	-	-	17/37/137/137	-
24	LDA	O	501	-	-	1/13/13/13	-
22	LMT	N	103	-	-	4/21/61/61	0/2/2/2
22	LMT	P	103	-	-	4/21/61/61	0/2/2/2
14	PGV	C	508	-	-	11/35/35/55	-
21	CRT	1	402	-	-	14/51/51/51	-
22	LMT	0	101	-	-	4/21/61/61	0/2/2/2
15	BCL	Q	101	-	-	16/37/137/137	-
14	PGV	M	411	-	-	12/40/40/55	-
10	HEC	C	503	1	-	0/10/54/54	-
22	LMT	4	104	-	-	1/21/61/61	0/2/2/2
18	CDL	H	302	-	-	14/41/41/110	-
21	CRT	6	102	-	-	7/51/51/51	-
14	PGV	M	407	-	-	5/41/41/55	-
15	BCL	N	101	-	-	13/37/137/137	-
10	HEC	C	502	1	-	5/10/54/54	-
15	BCL	G	102	-	-	14/37/137/137	-
17	UQ8	L	505	-	-	15/51/75/75	0/1/1/1
21	CRT	Q	102	-	-	5/51/51/51	-
21	CRT	G	103	-	-	7/51/51/51	-
15	BCL	F	101	-	-	15/37/137/137	-
15	BCL	L	509	-	-	18/37/137/137	-
22	LMT	2	101	-	-	1/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BPH	L	503	-	-	6/37/105/105	0/5/6/6
14	PGV	L	501	-	-	2/17/17/55	-
21	CRT	N	102	-	-	4/51/51/51	-
22	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
15	BCL	I	102	-	-	16/37/137/137	-
15	BCL	K	103	-	-	16/37/137/137	-
13	PLM	C	507	1	-	0/8/9/15	-
22	LMT	H	304	-	-	1/21/61/61	0/2/2/2
15	BCL	P	101	-	-	25/37/137/137	-
15	BCL	3	101	-	-	12/37/137/137	-
14	PGV	1	401	-	-	12/30/30/55	-
15	BCL	9	101	-	-	13/37/137/137	-
15	BCL	Z	102	-	-	18/37/137/137	-
17	UQ8	L	512	-	-	5/27/51/75	0/1/1/1
14	PGV	D	101	-	-	15/39/39/55	-
15	BCL	D	103	-	-	14/37/137/137	-
22	LMT	G	101	-	-	5/21/61/61	0/2/2/2
15	BCL	7	101	-	-	9/31/131/137	-
20	MQ8	M	404	-	-	6/47/67/67	0/2/2/2
14	PGV	H	303	-	-	10/40/40/55	-
21	CRT	E	103	-	-	4/51/51/51	-
21	CRT	2	103	-	-	5/51/51/51	-
21	CRT	R	102	-	-	2/51/51/51	-
21	CRT	X	103	-	-	6/51/51/51	-
15	BCL	W	101	-	-	17/37/137/137	-
21	CRT	J	103	-	-	3/51/51/51	-
22	LMT	J	104	-	-	1/21/61/61	0/2/2/2
22	LMT	K	102	-	-	4/21/61/61	0/2/2/2
15	BCL	V	102	-	-	19/37/137/137	-
21	CRT	M	405	-	-	8/51/51/51	-
15	BCL	T	102	-	-	12/37/137/137	-
10	HEC	C	504	1	-	2/10/54/54	-
17	UQ8	L	504	-	-	5/27/51/75	0/1/1/1
15	BCL	0	102	-	-	11/37/137/137	-
22	LMT	E	101	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BPH	M	403	-	-	8/37/105/105	0/5/6/6
21	CRT	8	103	-	-	3/51/51/51	-
15	BCL	M	402	-	-	22/37/137/137	-
22	LMT	X	101	-	-	1/21/61/61	0/2/2/2
14	PGV	L	511	-	-	10/37/37/55	-
14	PGV	L	507	-	-	18/43/43/55	-
15	BCL	U	101	-	-	16/37/137/137	-
21	CRT	7	102	-	-	4/51/51/51	-
12	DGA	C	506	1	-	8/16/16/45	-
15	BCL	2	102	-	-	12/37/137/137	-
18	CDL	M	408	-	-	16/48/48/110	-
15	BCL	B	102	-	-	15/37/137/137	-
15	BCL	R	101	-	-	12/37/137/137	-
22	LMT	V	101	-	-	6/21/61/61	0/2/2/2
18	CDL	L	510	-	-	31/93/93/110	-
15	BCL	1	403	-	-	13/37/137/137	-
21	CRT	4	103	-	-	5/51/51/51	-
18	CDL	H	301	-	-	30/89/89/110	-
18	CDL	D	102	-	-	27/67/67/110	-
14	PGV	5	101	-	-	15/48/48/55	-
20	MQ8	M	406	-	-	7/47/67/67	0/2/2/2
15	BCL	L	508	-	-	11/37/137/137	-
10	HEC	C	501	1	-	2/10/54/54	-
22	LMT	8	101	-	-	2/21/61/61	0/2/2/2
15	BCL	O	502	-	-	15/37/137/137	-
21	CRT	S	104	-	-	9/51/51/51	-
18	CDL	I	101	-	-	14/61/61/110	-
22	LMT	B	101	-	-	6/21/61/61	0/2/2/2
22	LMT	4	101	-	-	3/21/61/61	0/2/2/2
24	LDA	K	101	-	-	5/13/13/13	-
15	BCL	5	102	-	-	18/37/137/137	-
15	BCL	8	102	-	-	18/37/137/137	-
15	BCL	J	102	-	-	13/37/137/137	-
14	PGV	L	506	-	-	11/33/33/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CRT	B	103	-	-	9/51/51/51	-
15	BCL	A	101	-	-	16/37/137/137	-
18	CDL	M	410	-	-	35/105/105/110	-
15	BCL	4	102	-	-	20/37/137/137	-
15	BCL	E	102	-	-	16/37/137/137	-
15	BCL	S	102	-	-	14/37/137/137	-
22	LMT	T	101	-	-	5/21/61/61	0/2/2/2
18	CDL	S	101	-	-	20/75/75/110	-
15	BCL	X	102	-	-	18/37/137/137	-
21	CRT	P	102	-	-	8/51/51/51	-
15	BCL	Y	101	-	-	17/37/137/137	-
14	PGV	M	409	-	-	6/32/32/55	-
15	BCL	L	502	-	-	13/37/137/137	-

The worst 5 of 442 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	512	UQ8	C6-C1	7.84	1.49	1.35
20	M	406	MQ8	C3-C2	7.82	1.49	1.35
20	M	404	MQ8	C3-C2	7.78	1.49	1.35
17	L	504	UQ8	C6-C1	7.63	1.49	1.35
17	L	505	UQ8	C6-C1	7.56	1.49	1.35

The worst 5 of 895 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	102	CRT	C3-C1-C4	-16.52	85.50	110.86
21	J	103	CRT	C3-C1-C4	-14.49	88.61	110.86
21	J	103	CRT	C2-C1-C4	-13.85	89.59	110.86
21	P	102	CRT	C2-C1-C4	-13.10	90.74	110.86
21	S	104	CRT	C39-C38-C37	6.04	120.13	110.86

There are no chirality outliers.

5 of 1113 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	506	DGA	OG1-CG1-CG2-OG2
12	C	506	DGA	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
14	C	508	PGV	C03-O11-P-O12
14	C	508	PGV	C04-O12-P-O14
14	L	506	PGV	C03-O11-P-O13

There are no ring outliers.

96 monomers are involved in 386 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	J	101	LMT	1	0
15	6	101	BCL	5	0
24	O	501	LDA	2	0
22	P	103	LMT	1	0
14	C	508	PGV	3	0
21	1	402	CRT	8	0
22	0	101	LMT	2	0
15	Q	101	BCL	5	0
14	M	411	PGV	2	0
10	C	503	HEC	5	0
22	4	104	LMT	1	0
18	H	302	CDL	1	0
21	6	102	CRT	5	0
15	N	101	BCL	7	0
10	C	502	HEC	5	0
15	G	102	BCL	6	0
17	L	505	UQ8	11	0
21	Q	102	CRT	6	0
21	G	103	CRT	6	0
15	F	101	BCL	6	0
15	L	509	BCL	2	0
22	2	101	LMT	2	0
16	L	503	BPH	4	0
21	N	102	CRT	2	0
22	Z	101	LMT	2	0
15	I	102	BCL	3	0
15	K	103	BCL	8	0
13	C	507	PLM	1	0
22	H	304	LMT	1	0
15	P	101	BCL	10	0
15	3	101	BCL	4	0
14	1	401	PGV	2	0
15	9	101	BCL	5	0
15	Z	102	BCL	5	0

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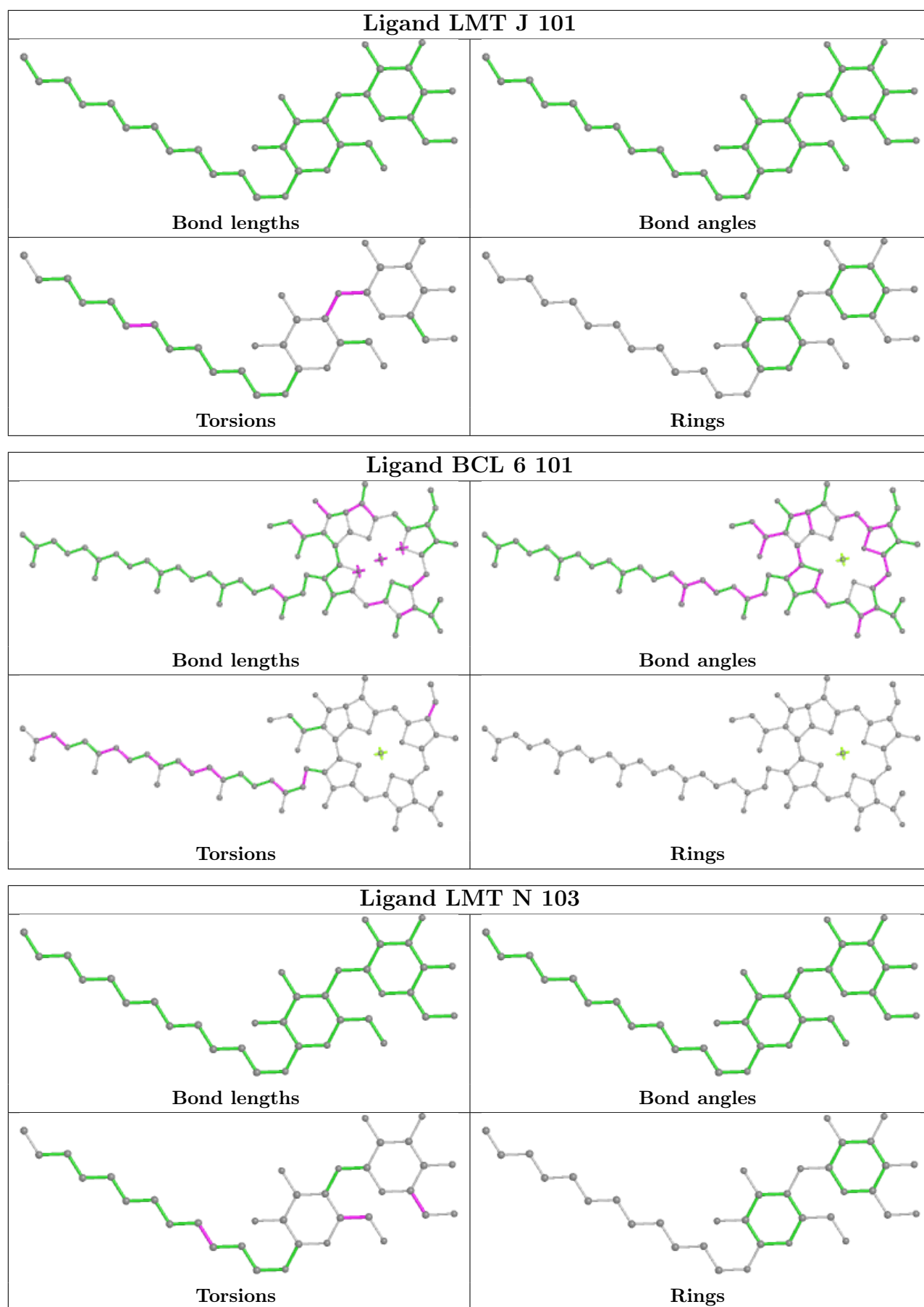
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	512	UQ8	7	0
15	D	103	BCL	4	0
22	G	101	LMT	3	0
15	7	101	BCL	1	0
20	M	404	MQ8	4	0
14	H	303	PGV	3	0
21	E	103	CRT	5	0
21	2	103	CRT	6	0
21	R	102	CRT	5	0
21	X	103	CRT	5	0
15	W	101	BCL	6	0
21	J	103	CRT	5	0
22	K	102	LMT	1	0
15	V	102	BCL	7	0
21	M	405	CRT	3	0
15	T	102	BCL	8	0
10	C	504	HEC	9	0
17	L	504	UQ8	2	0
15	0	102	BCL	7	0
22	E	101	LMT	1	0
16	M	403	BPH	10	0
21	8	103	CRT	6	0
15	M	402	BCL	3	0
15	U	101	BCL	3	0
21	7	102	CRT	4	0
15	2	102	BCL	6	0
18	M	408	CDL	1	0
15	B	102	BCL	7	0
15	R	101	BCL	10	0
22	V	101	LMT	3	0
18	L	510	CDL	1	0
15	1	403	BCL	5	0
21	4	103	CRT	8	0
18	H	301	CDL	3	0
18	D	102	CDL	4	0
14	5	101	PGV	4	0
20	M	406	MQ8	5	0
15	L	508	BCL	5	0
10	C	501	HEC	5	0
22	8	101	LMT	1	0
15	O	502	BCL	4	0
21	S	104	CRT	2	0

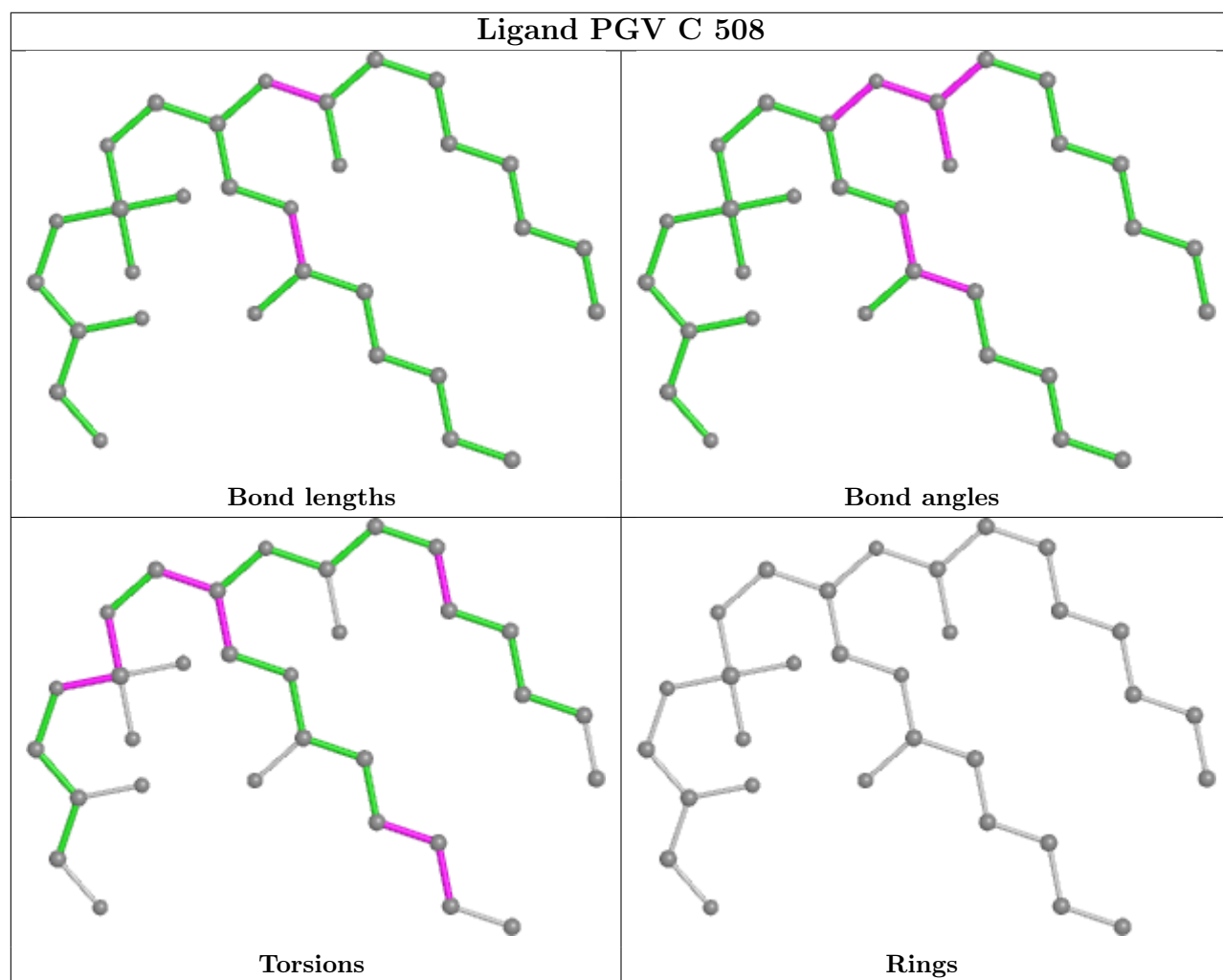
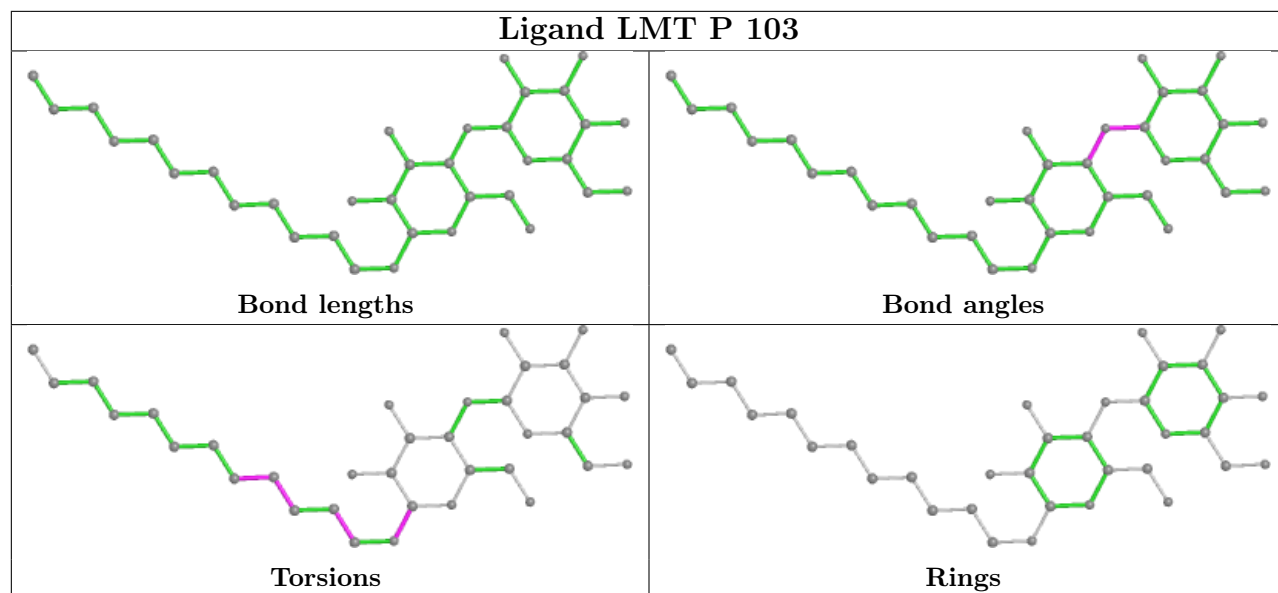
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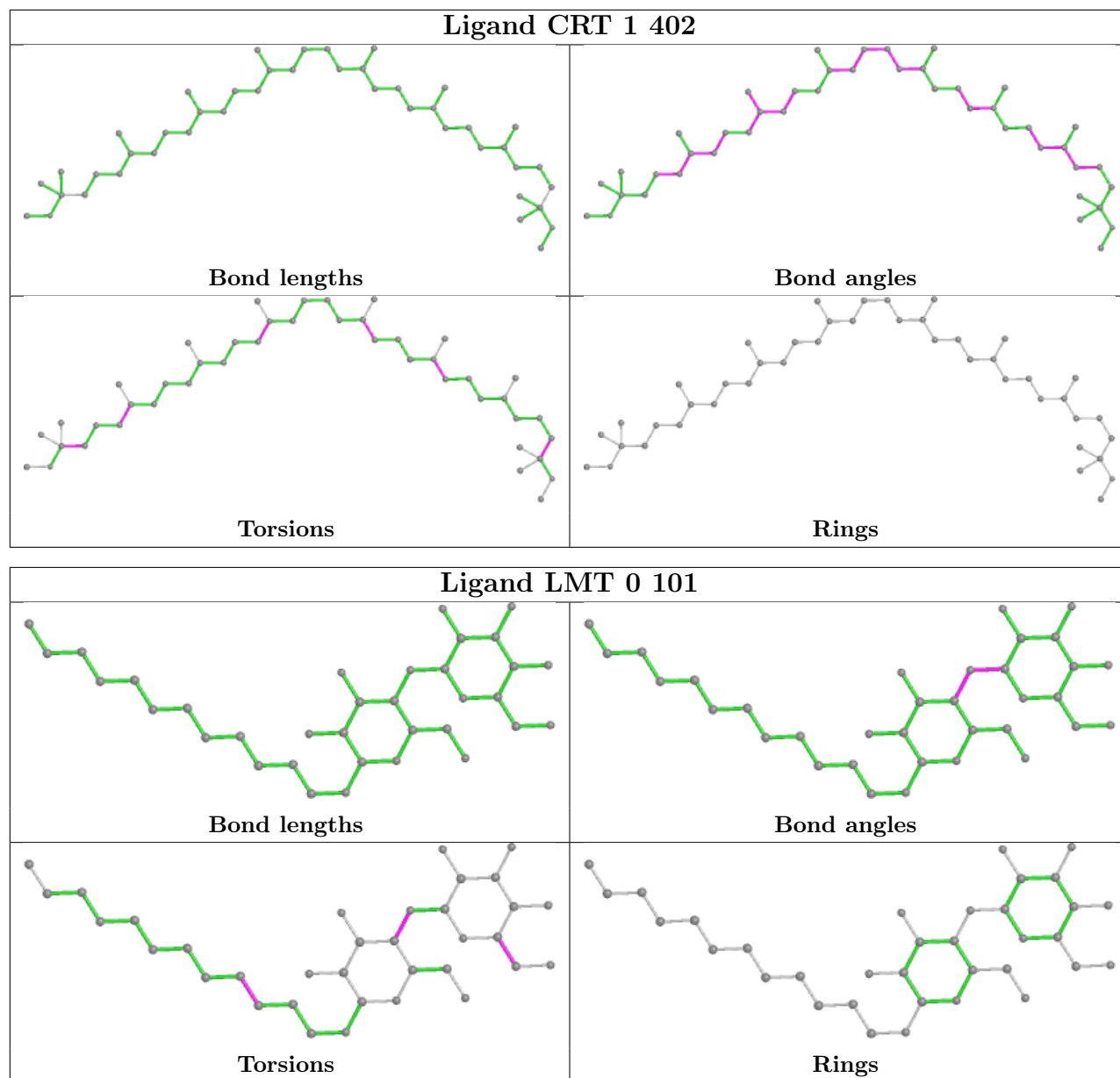
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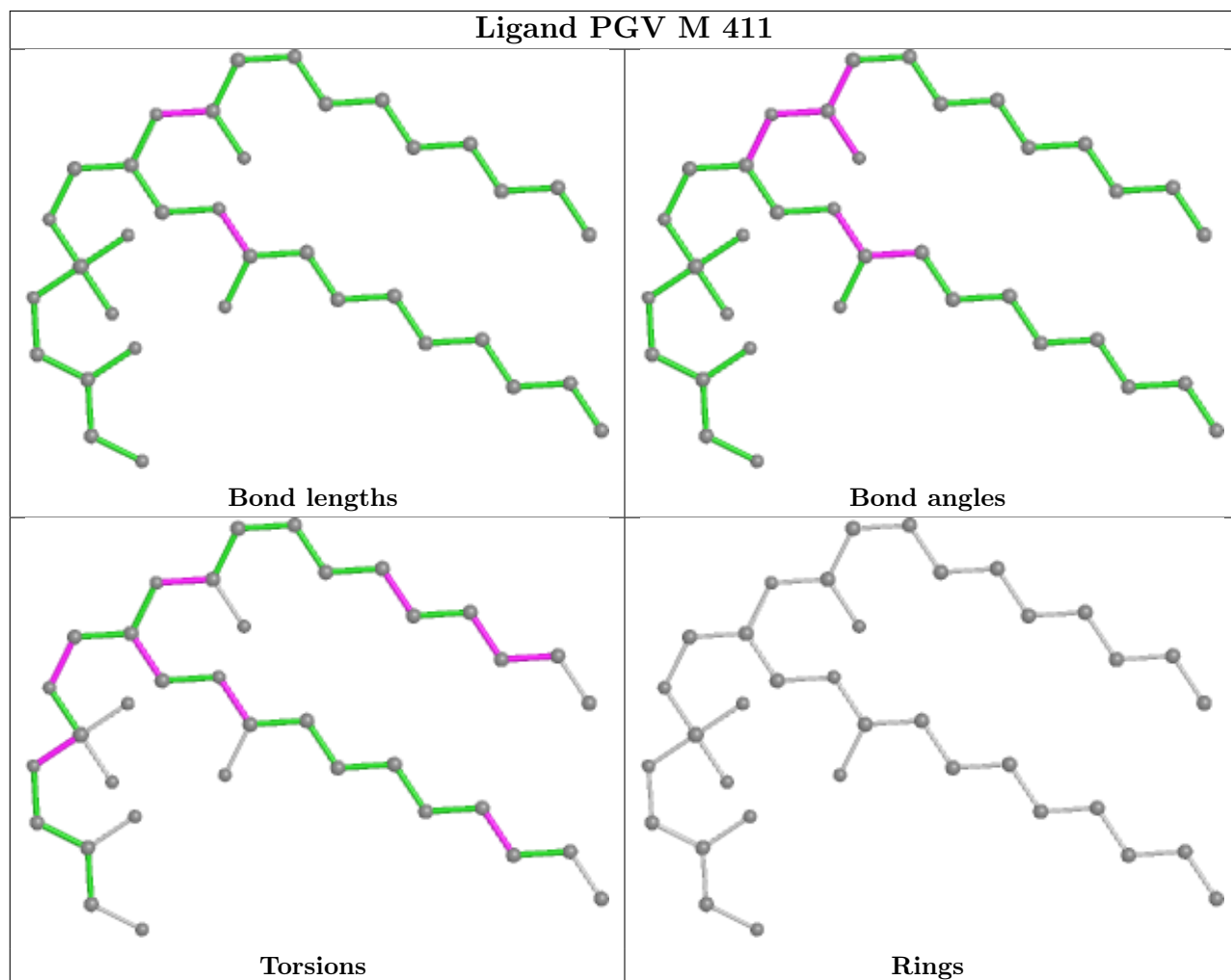
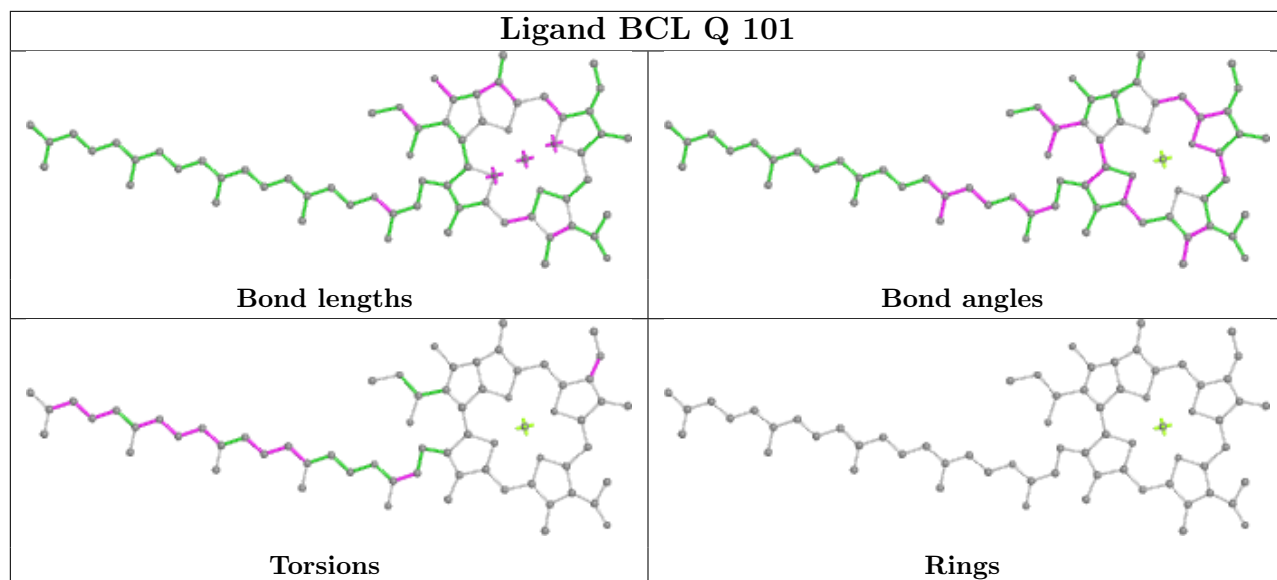
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	I	101	CDL	1	0
22	B	101	LMT	1	0
22	4	101	LMT	3	0
24	K	101	LDA	1	0
15	5	102	BCL	4	0
15	8	102	BCL	9	0
15	J	102	BCL	5	0
14	L	506	PGV	4	0
21	B	103	CRT	8	0
15	A	101	BCL	1	0
18	M	410	CDL	1	0
15	4	102	BCL	5	0
15	E	102	BCL	5	0
15	S	102	BCL	3	0
18	S	101	CDL	5	0
15	X	102	BCL	4	0
21	P	102	CRT	6	0
15	Y	101	BCL	7	0
14	M	409	PGV	1	0
15	L	502	BCL	2	0

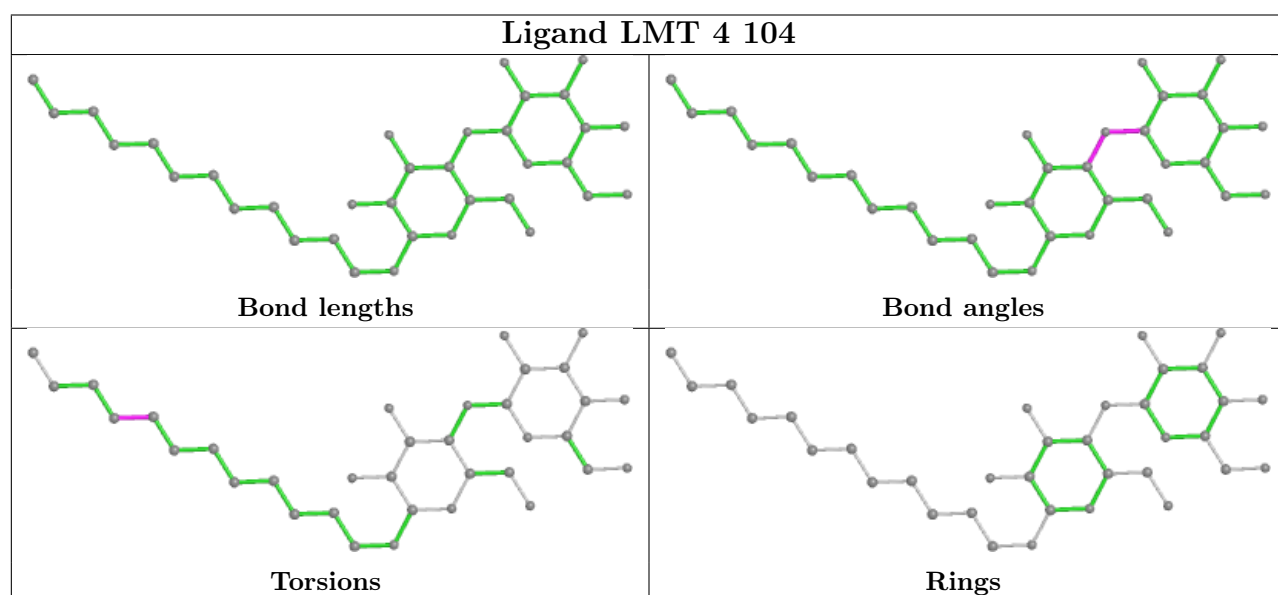
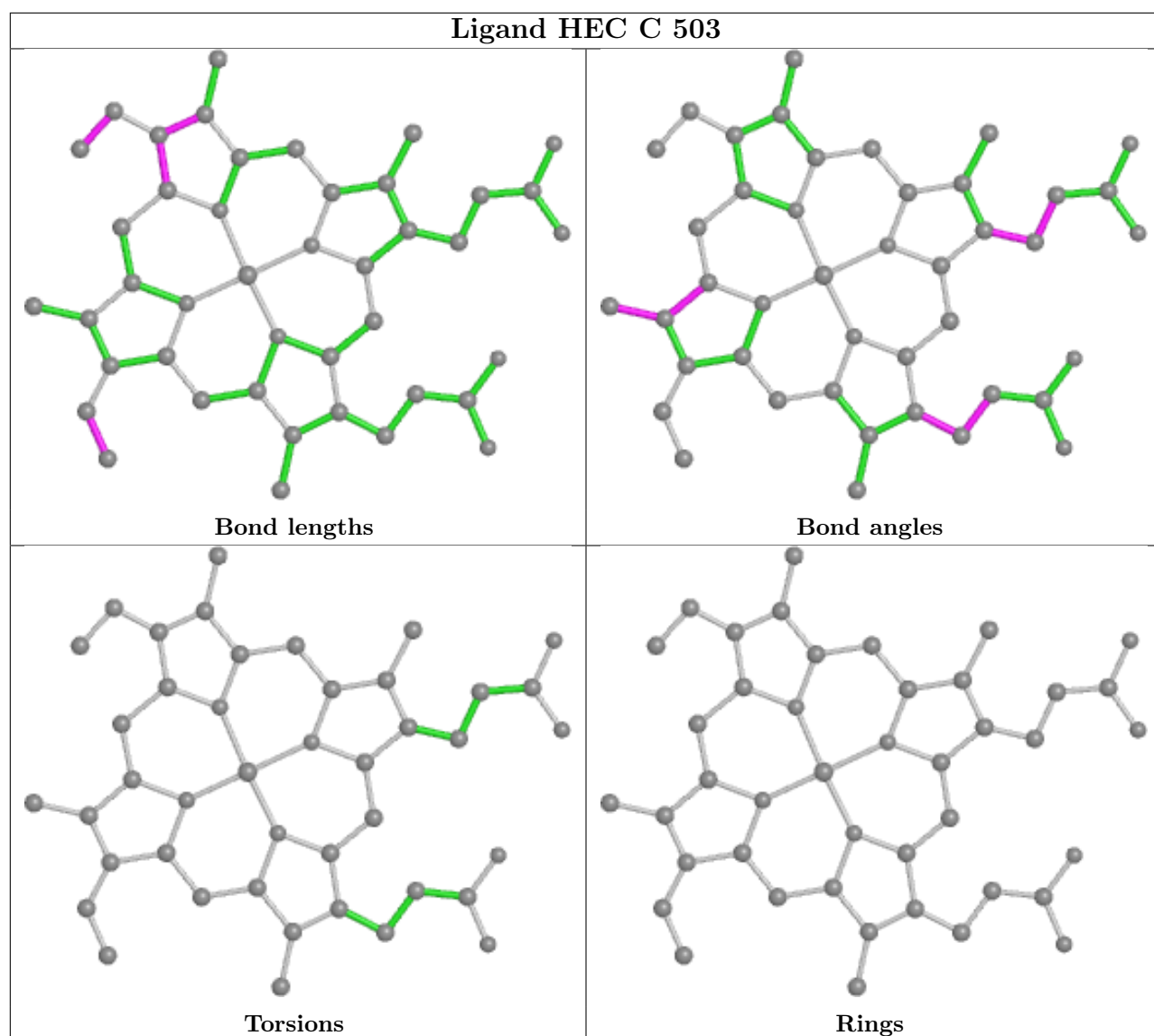
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

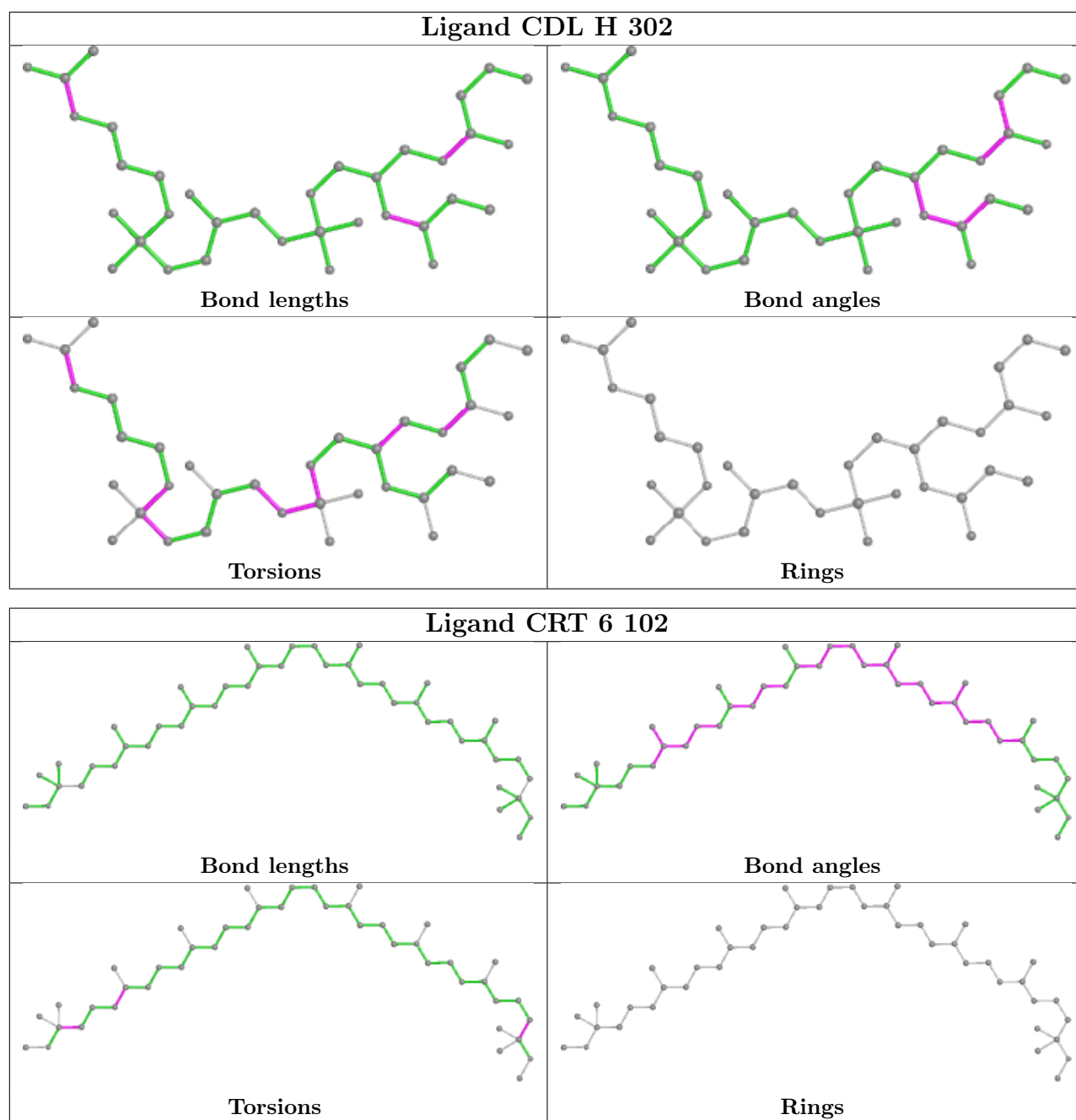


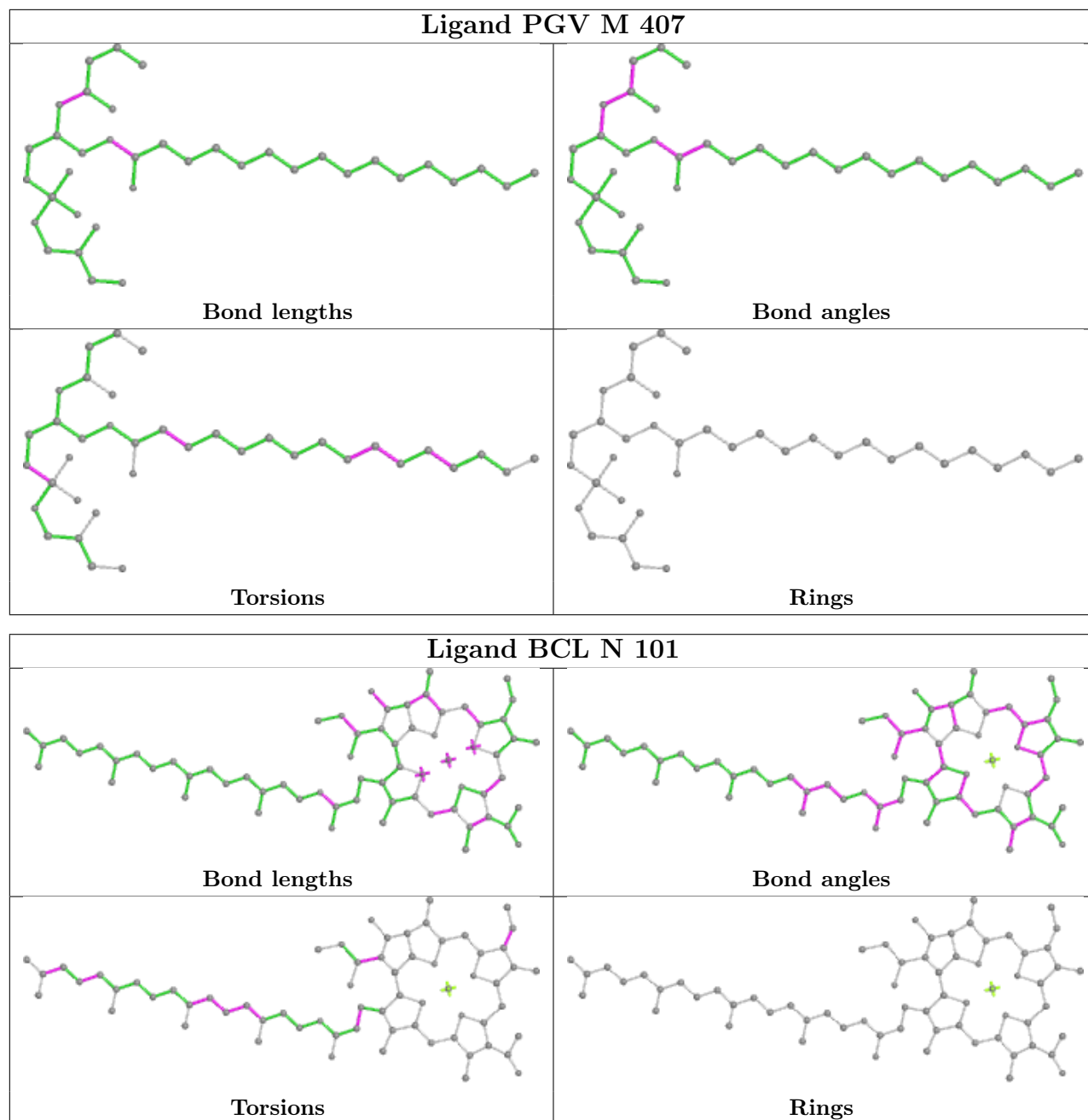


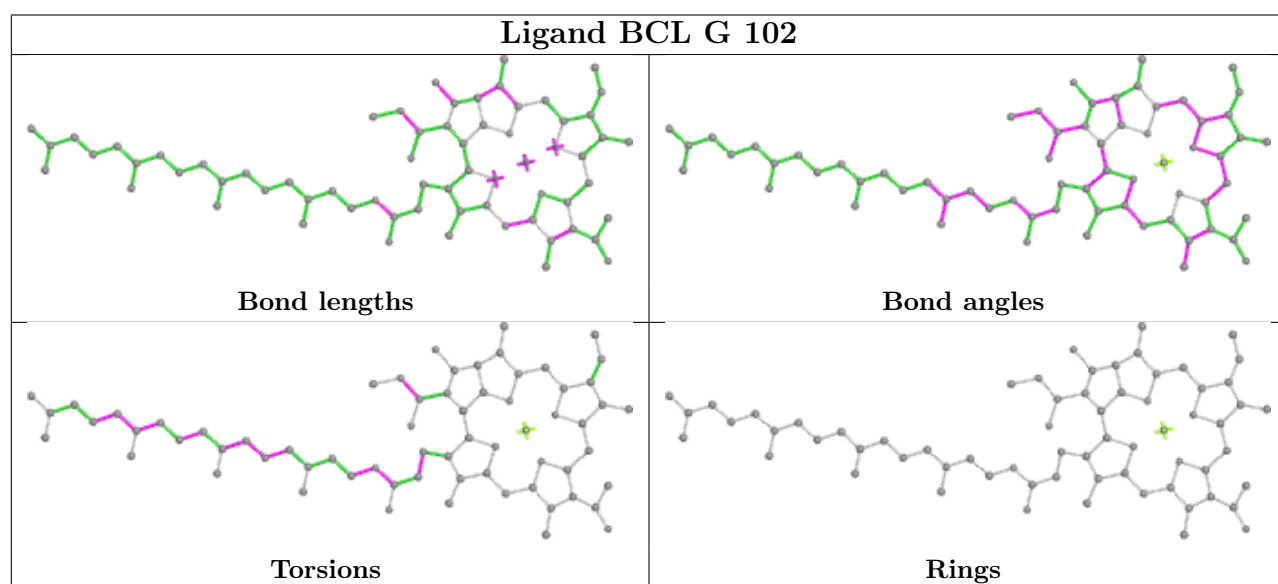
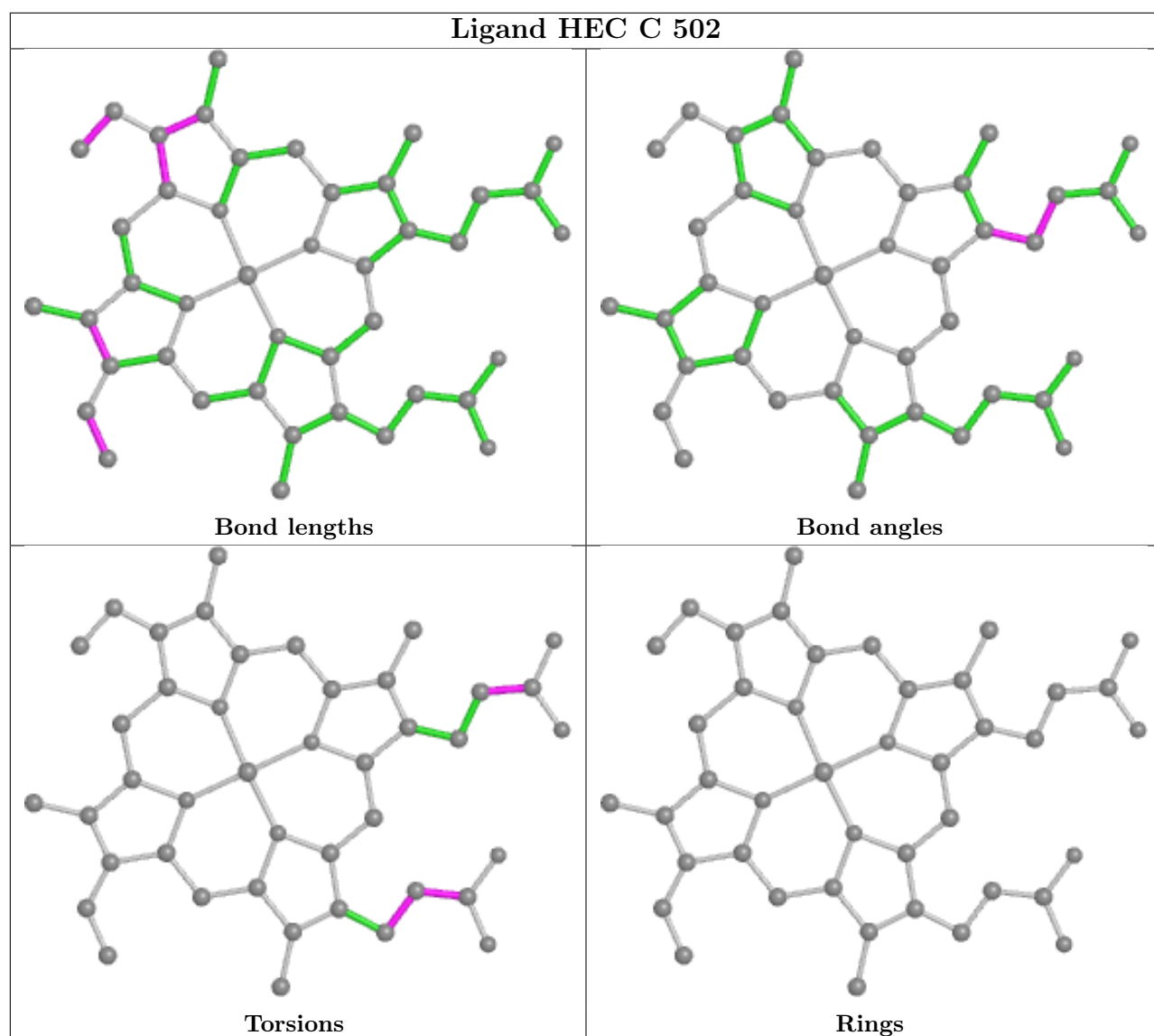


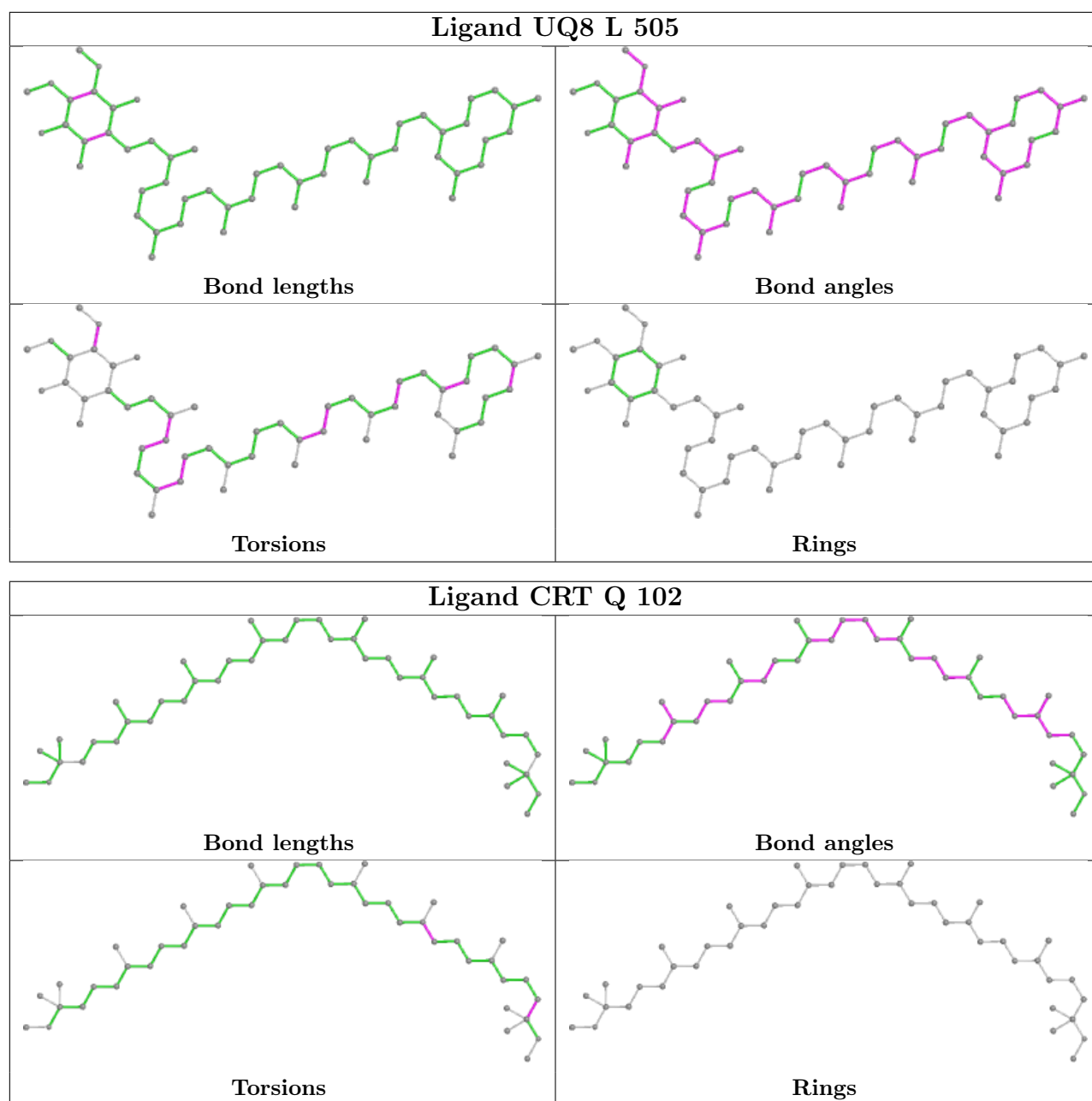


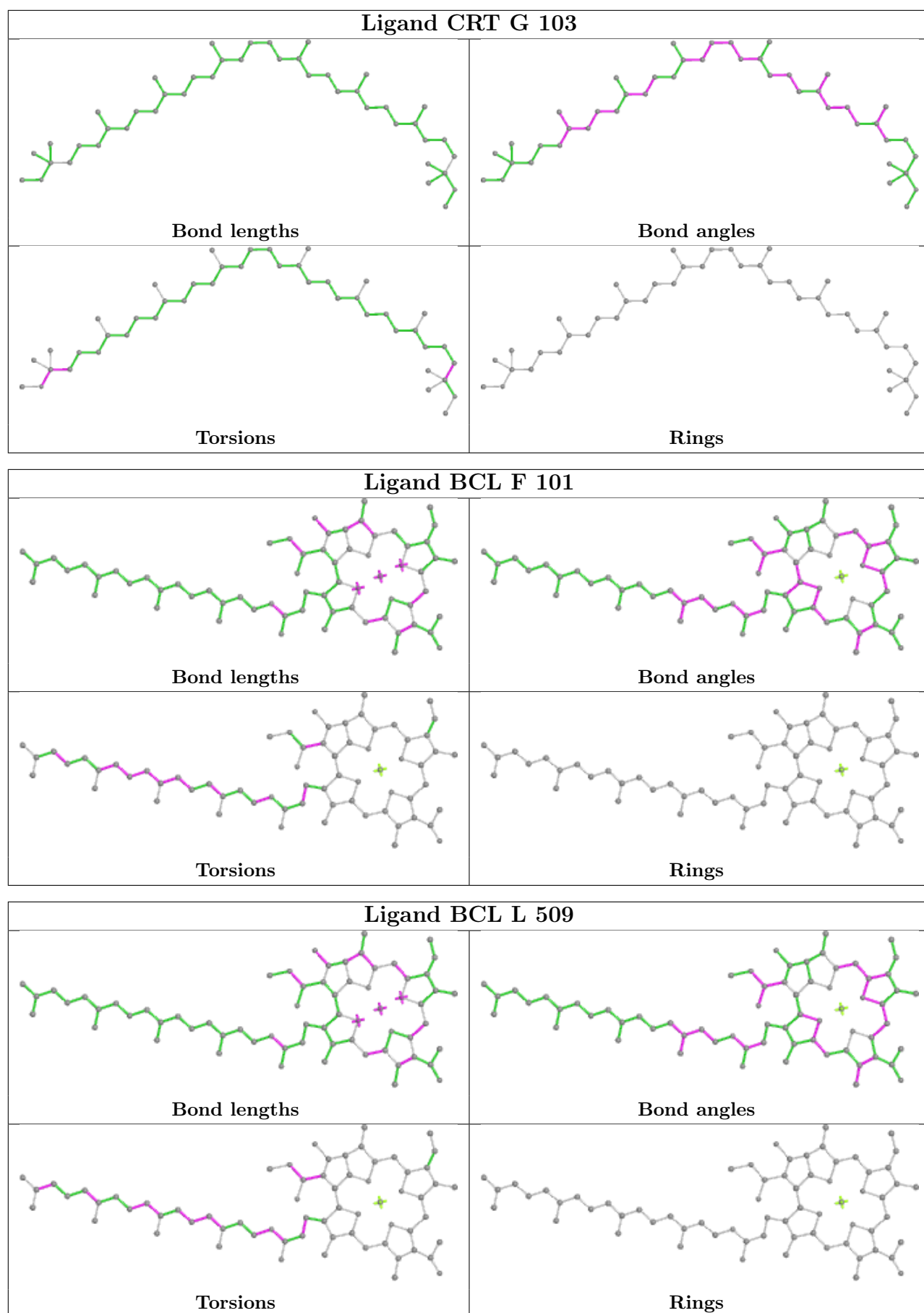


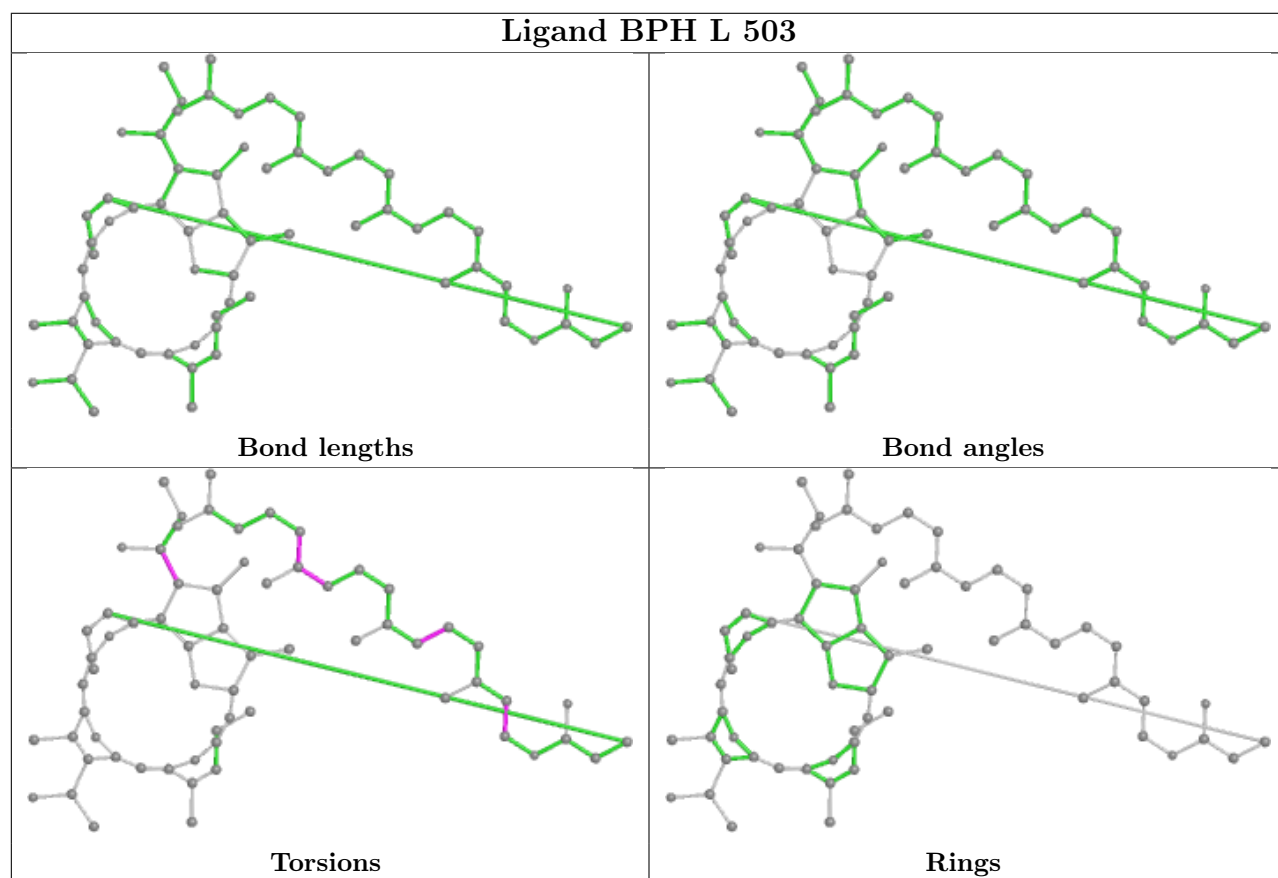
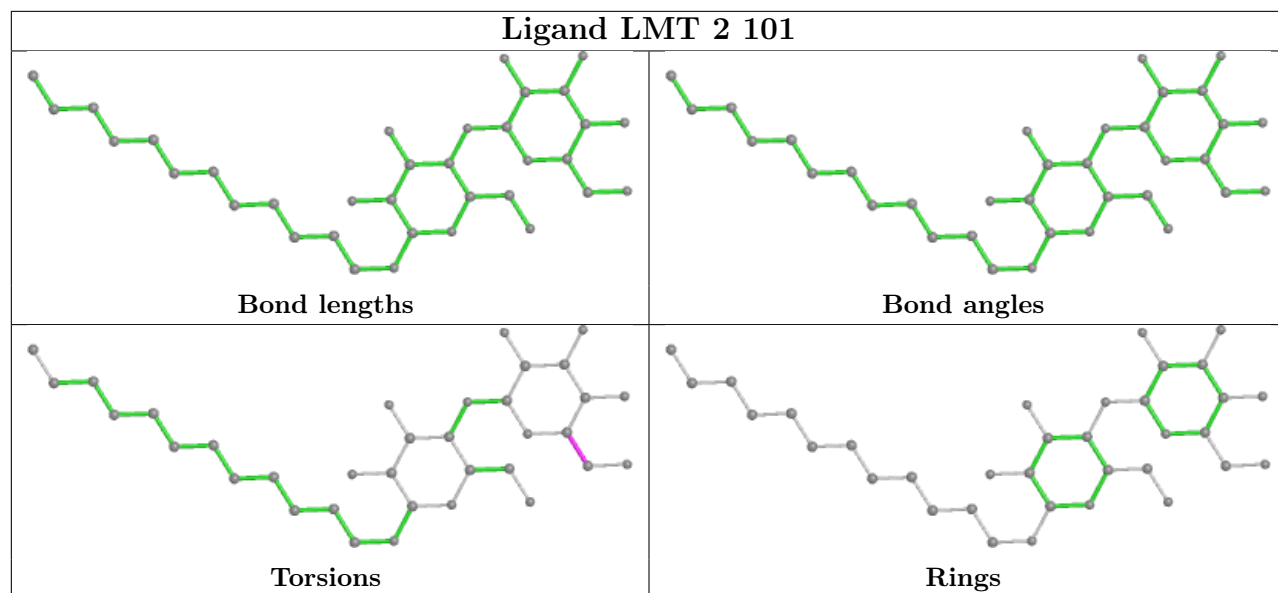


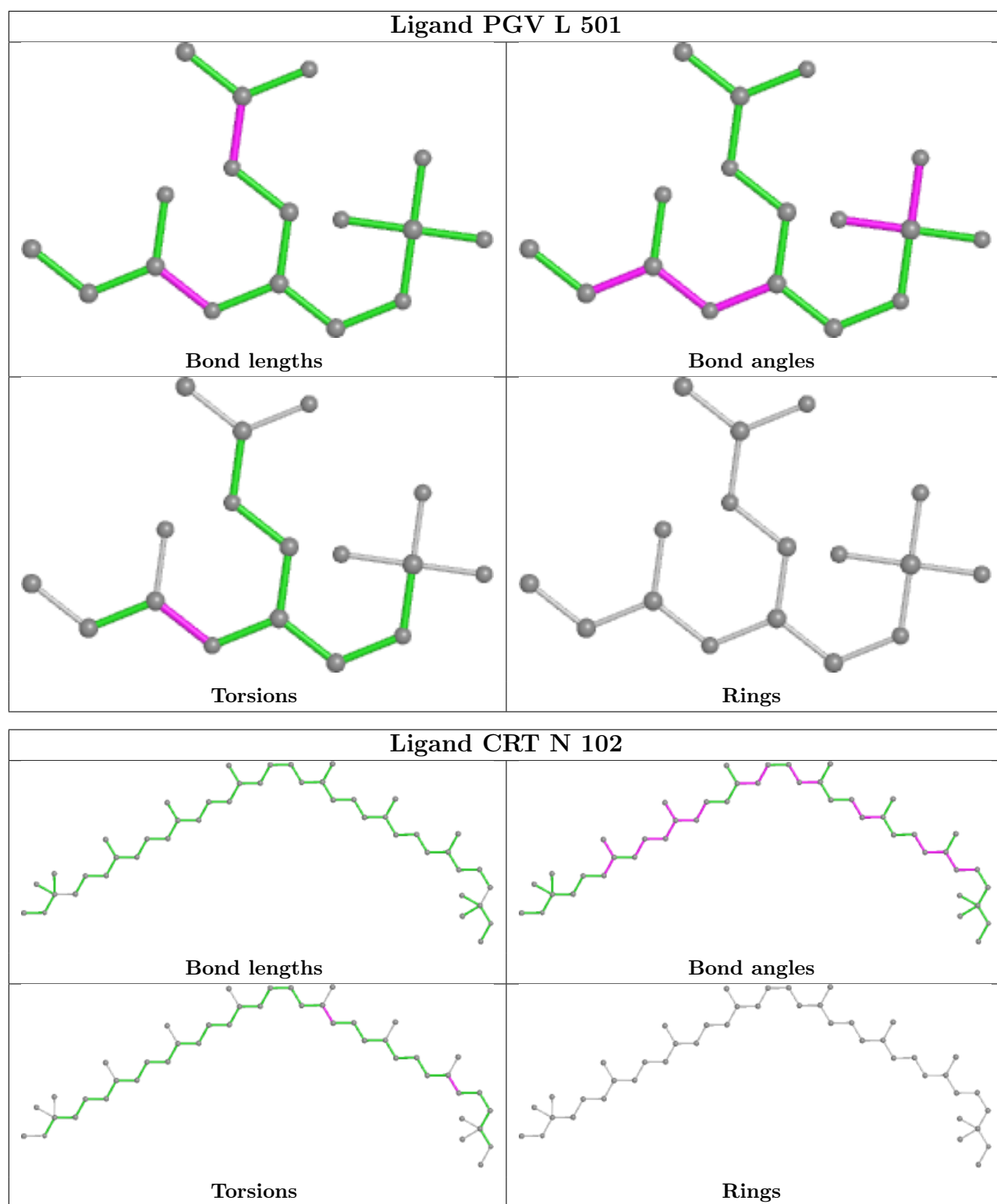


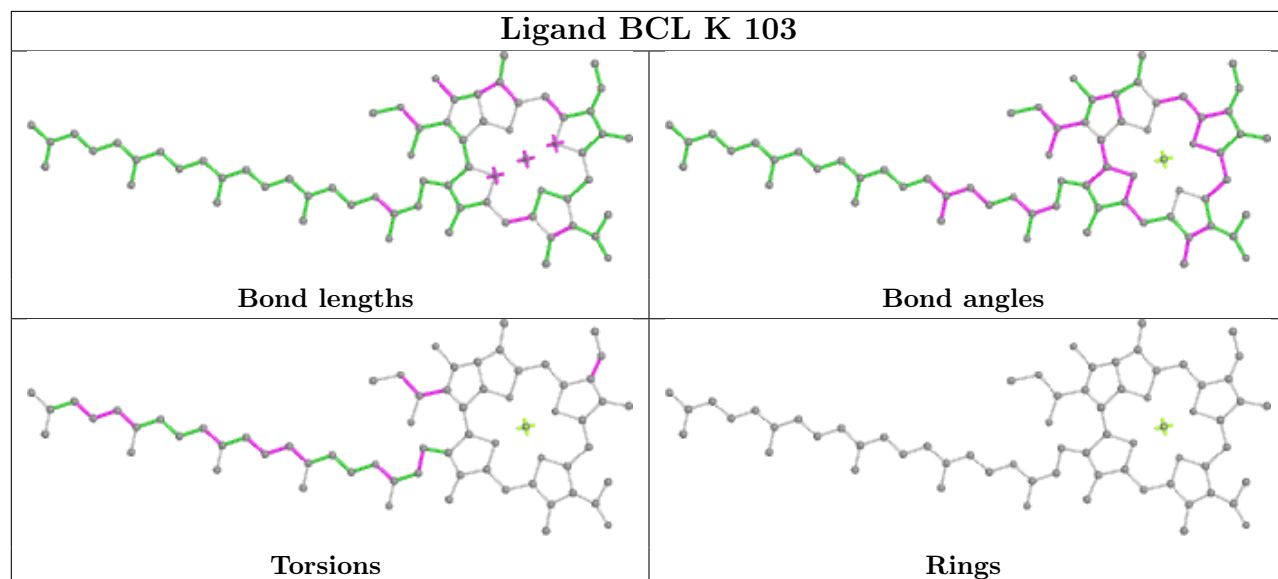
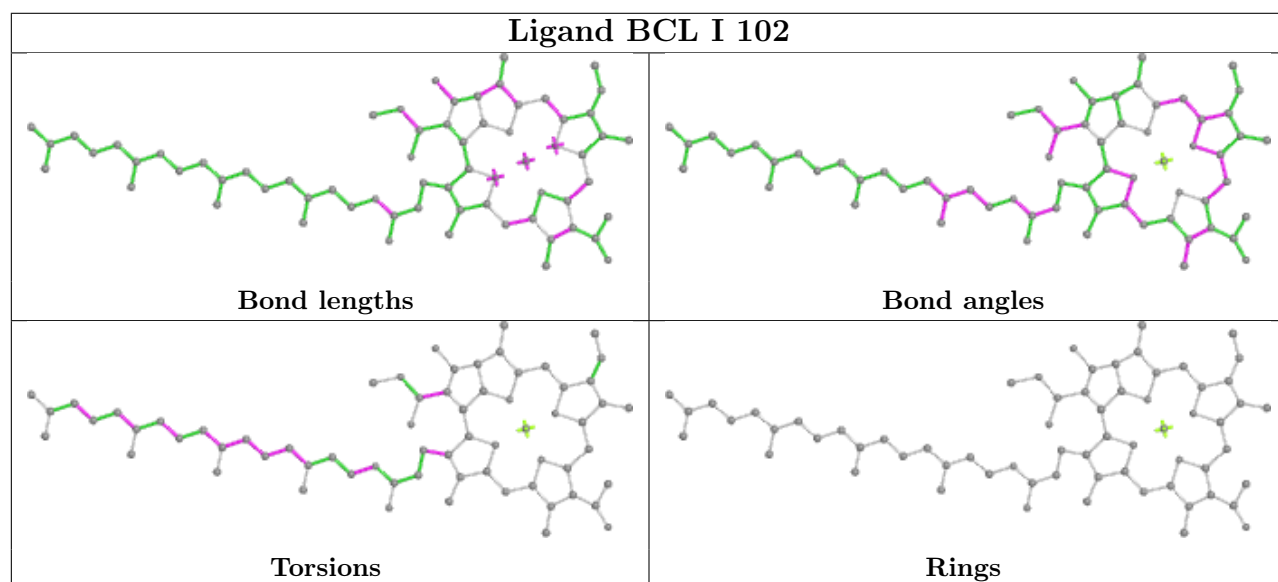
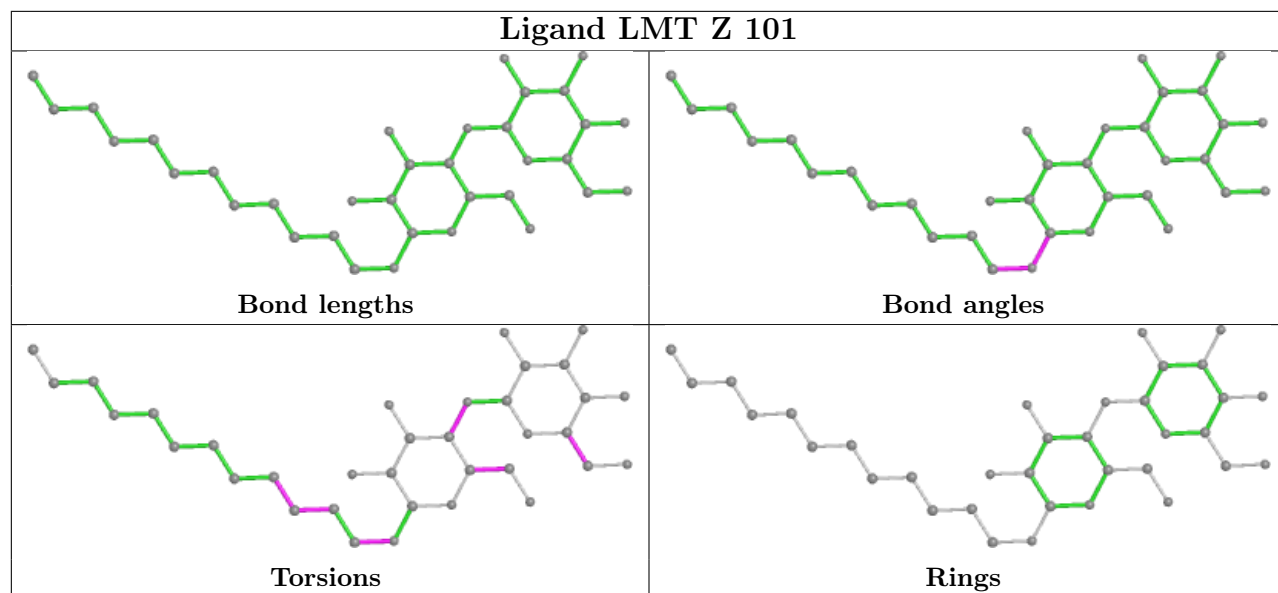


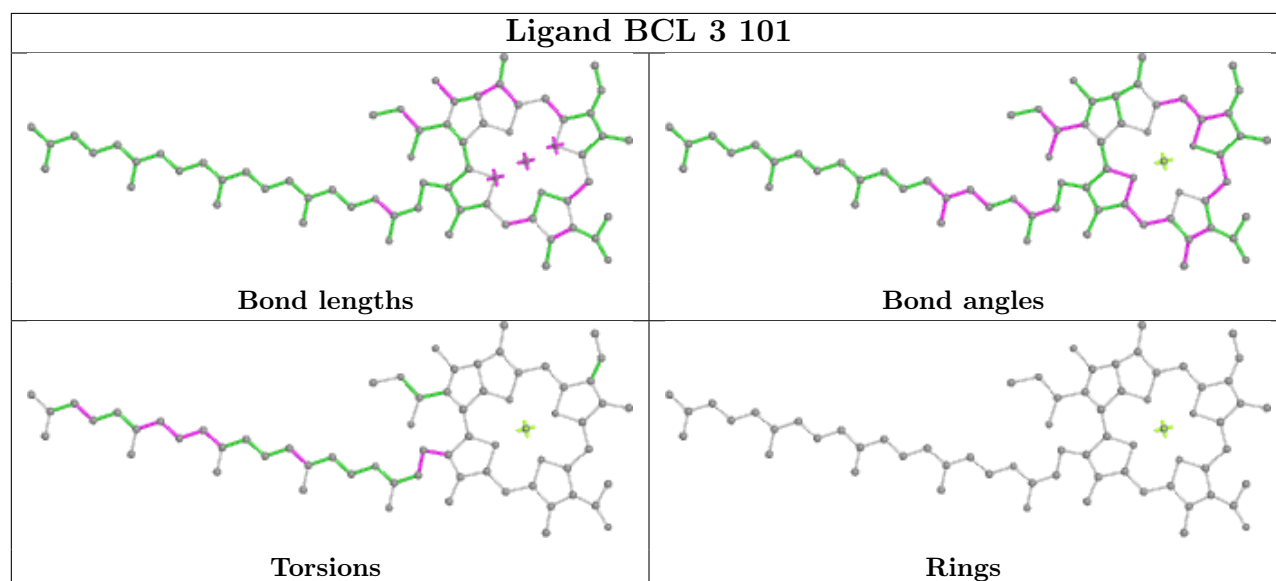
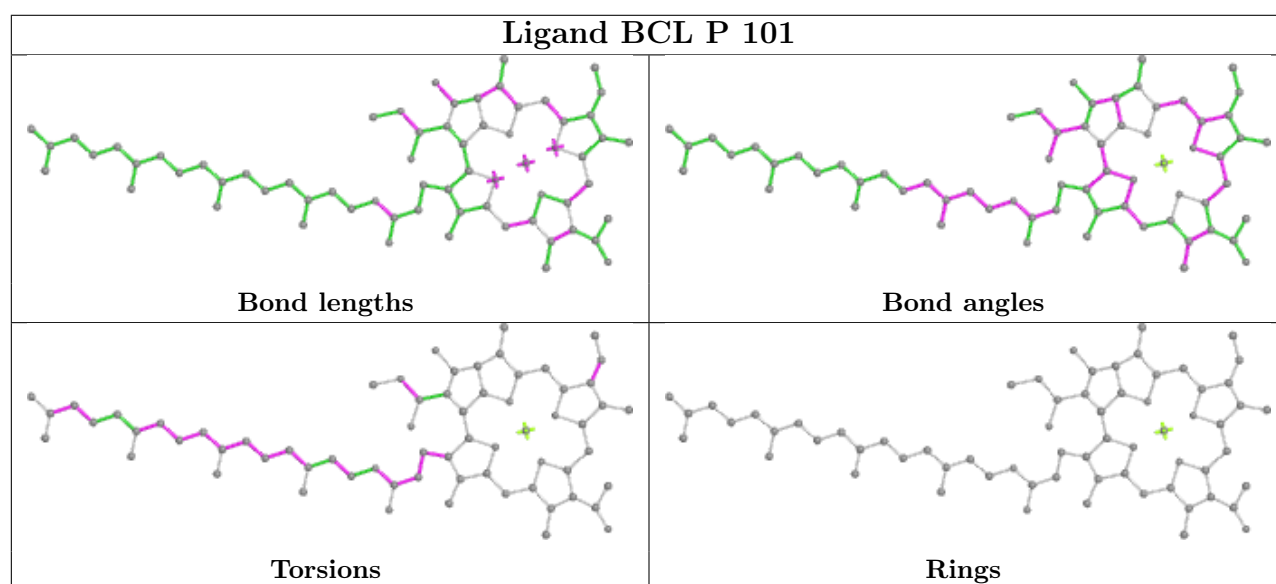
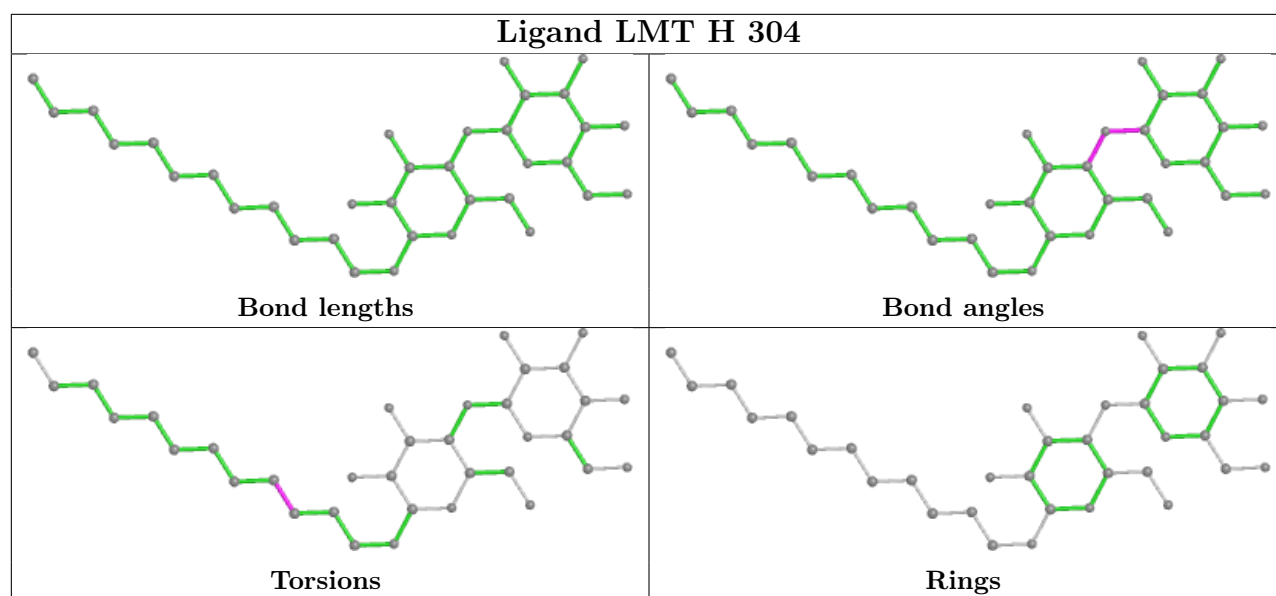


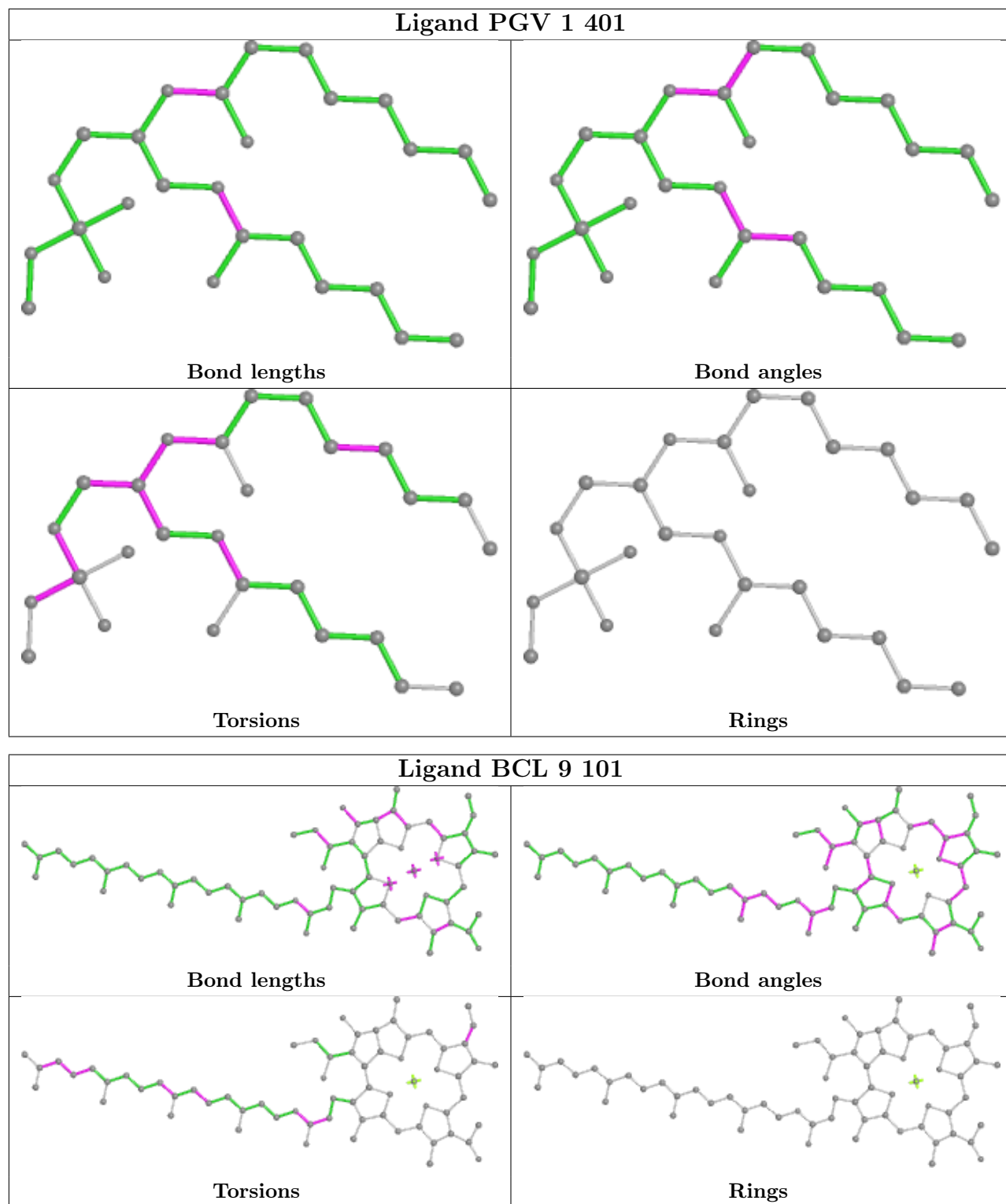


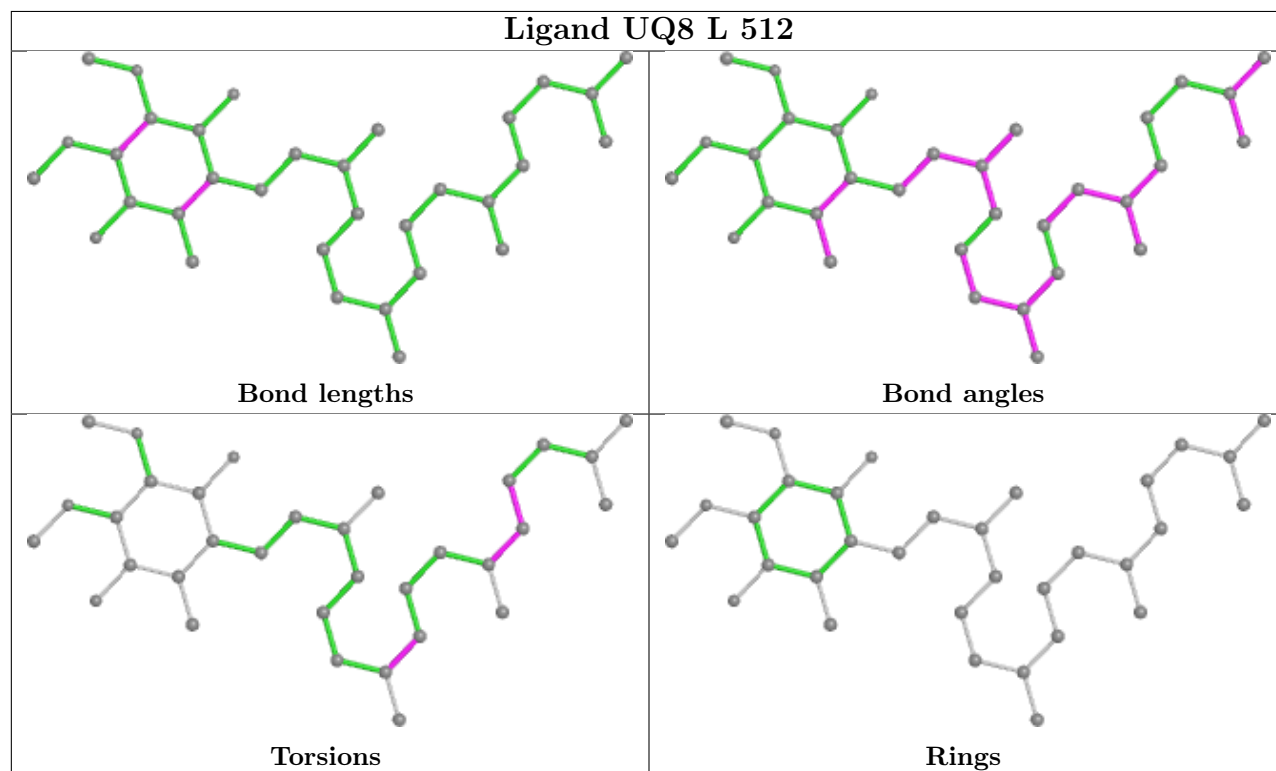
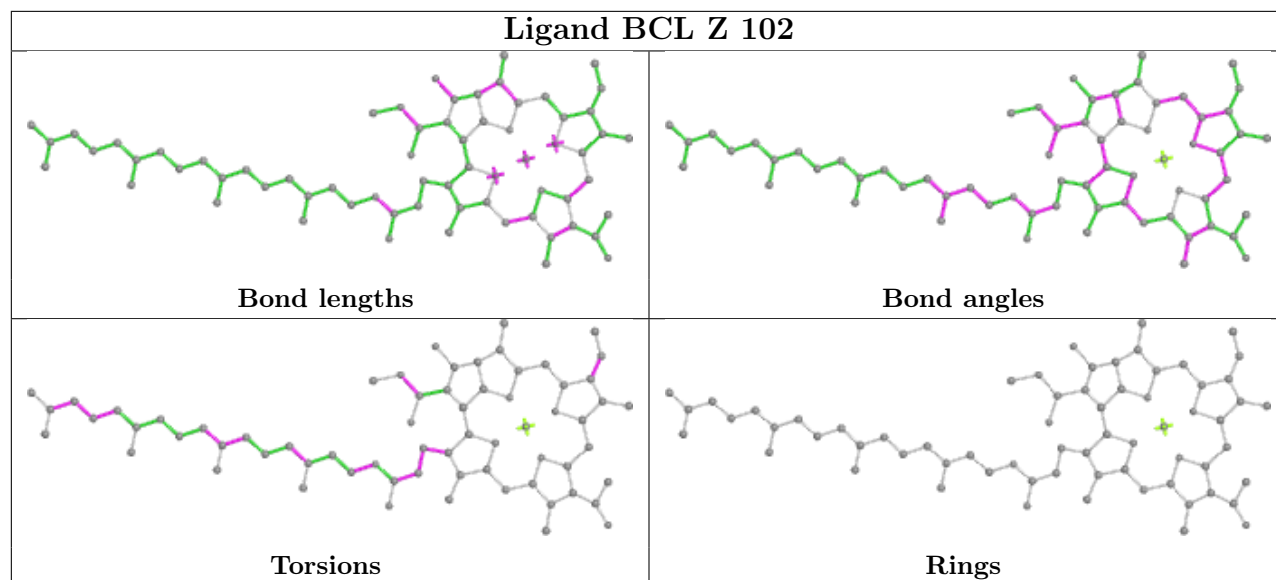


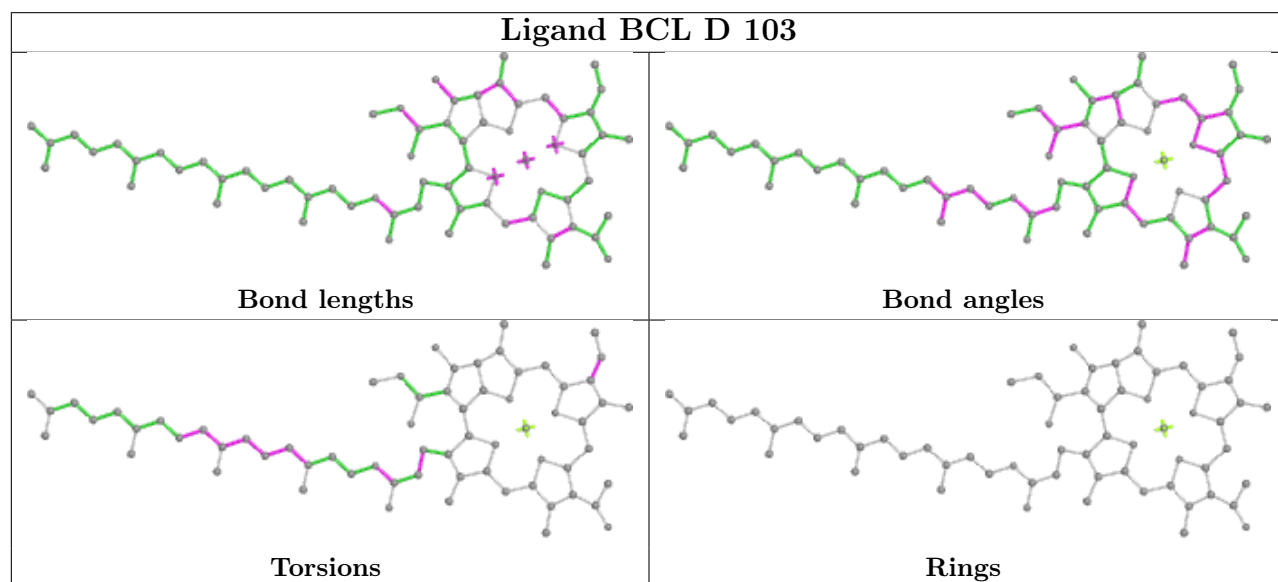
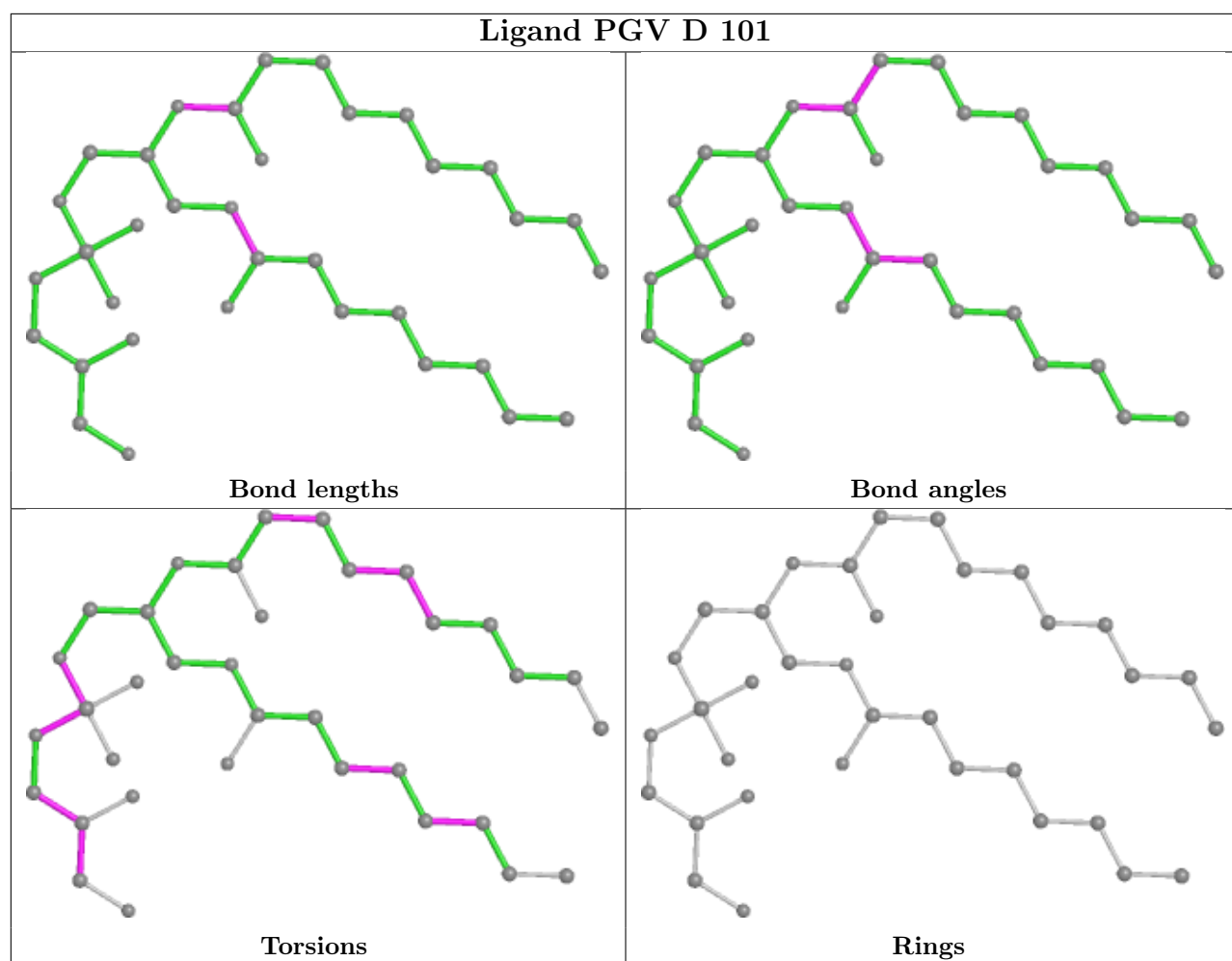


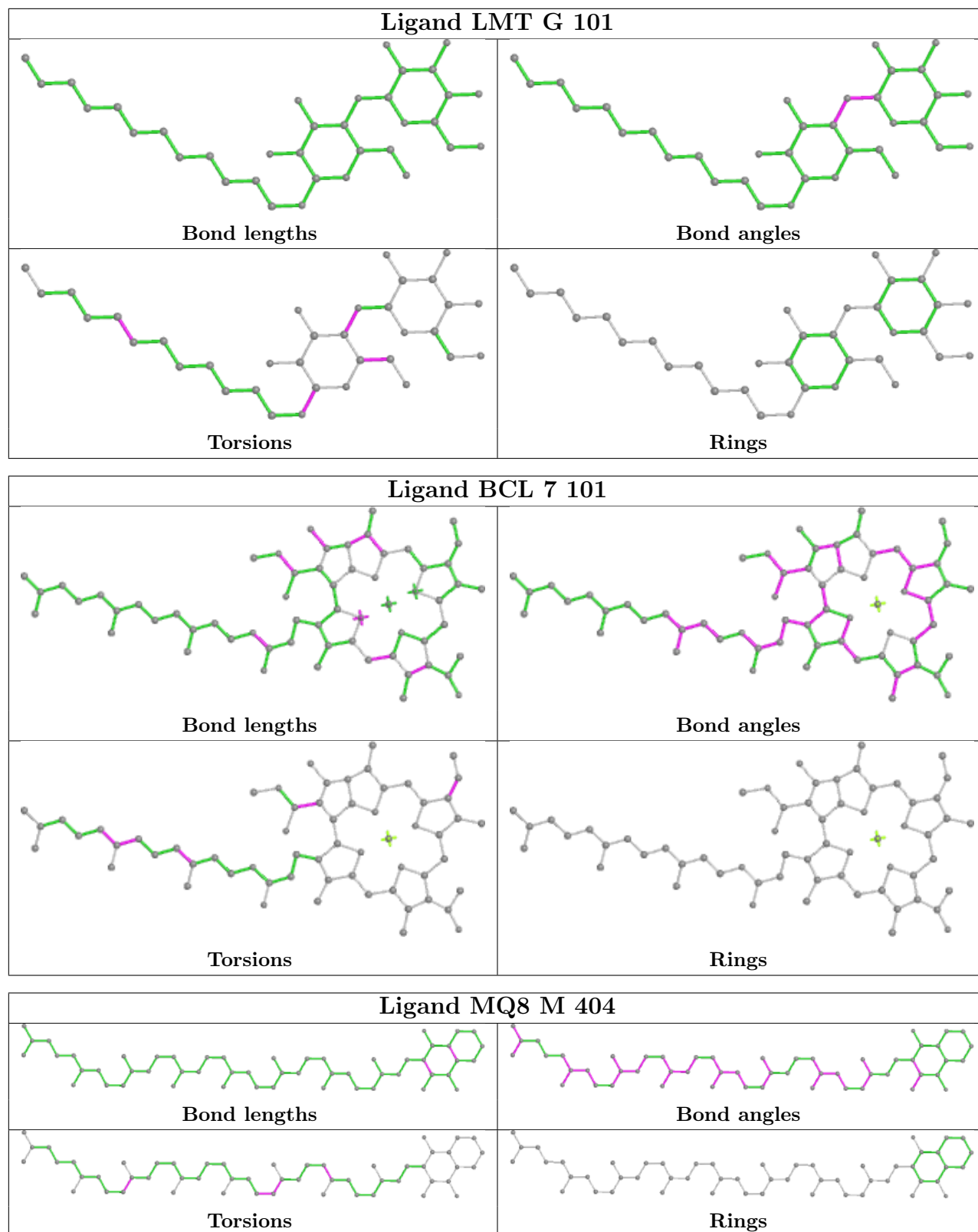


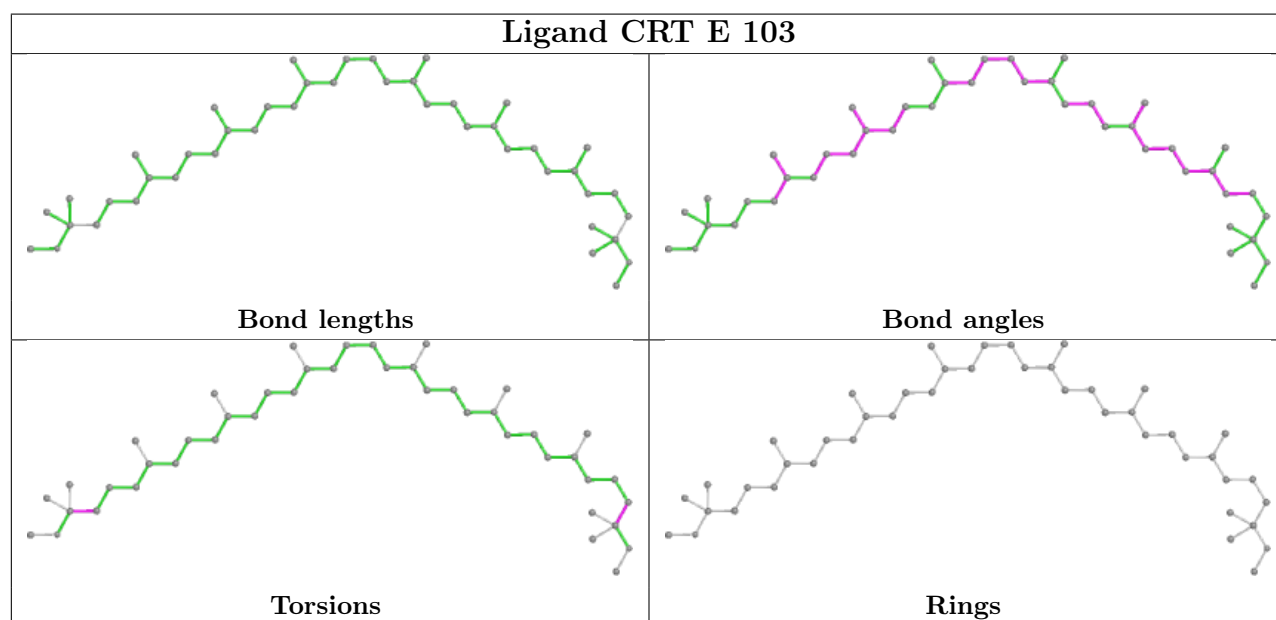
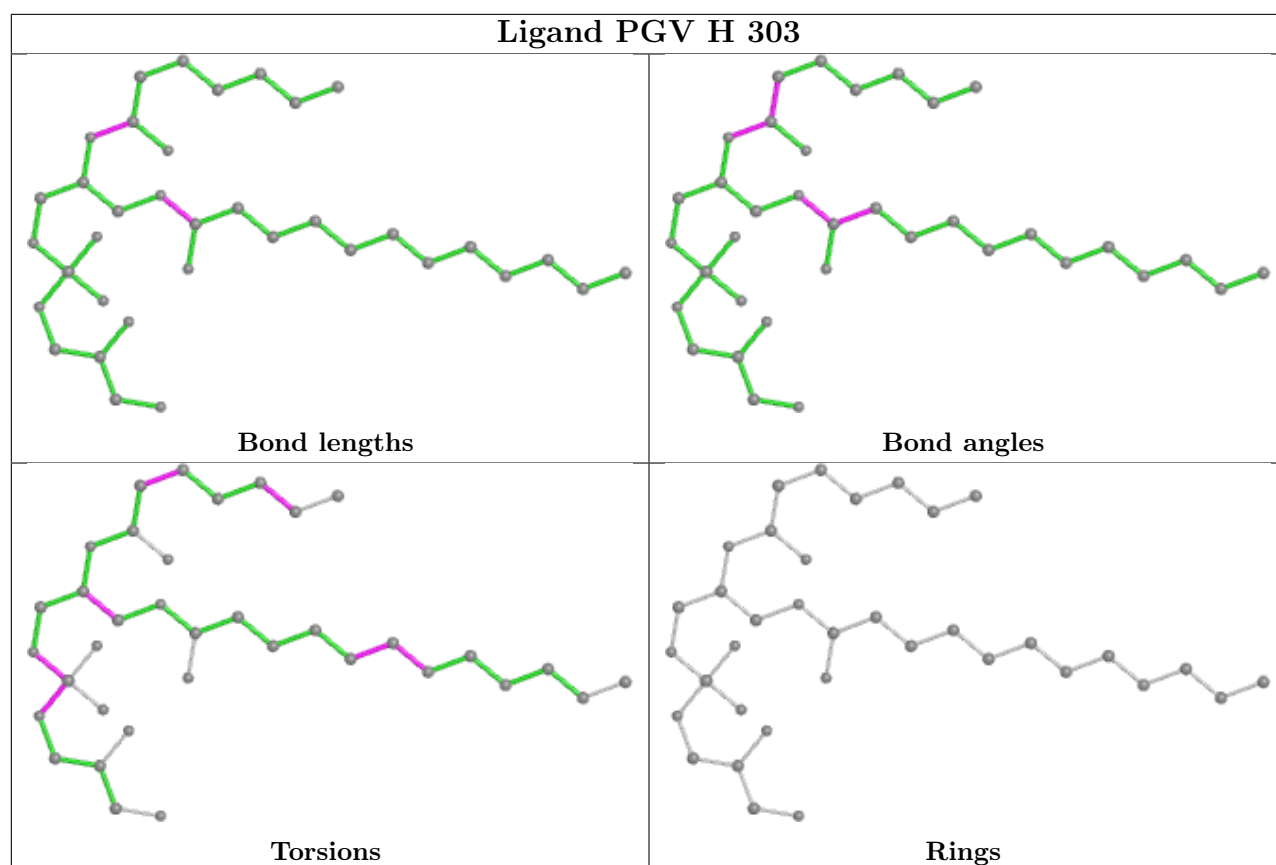


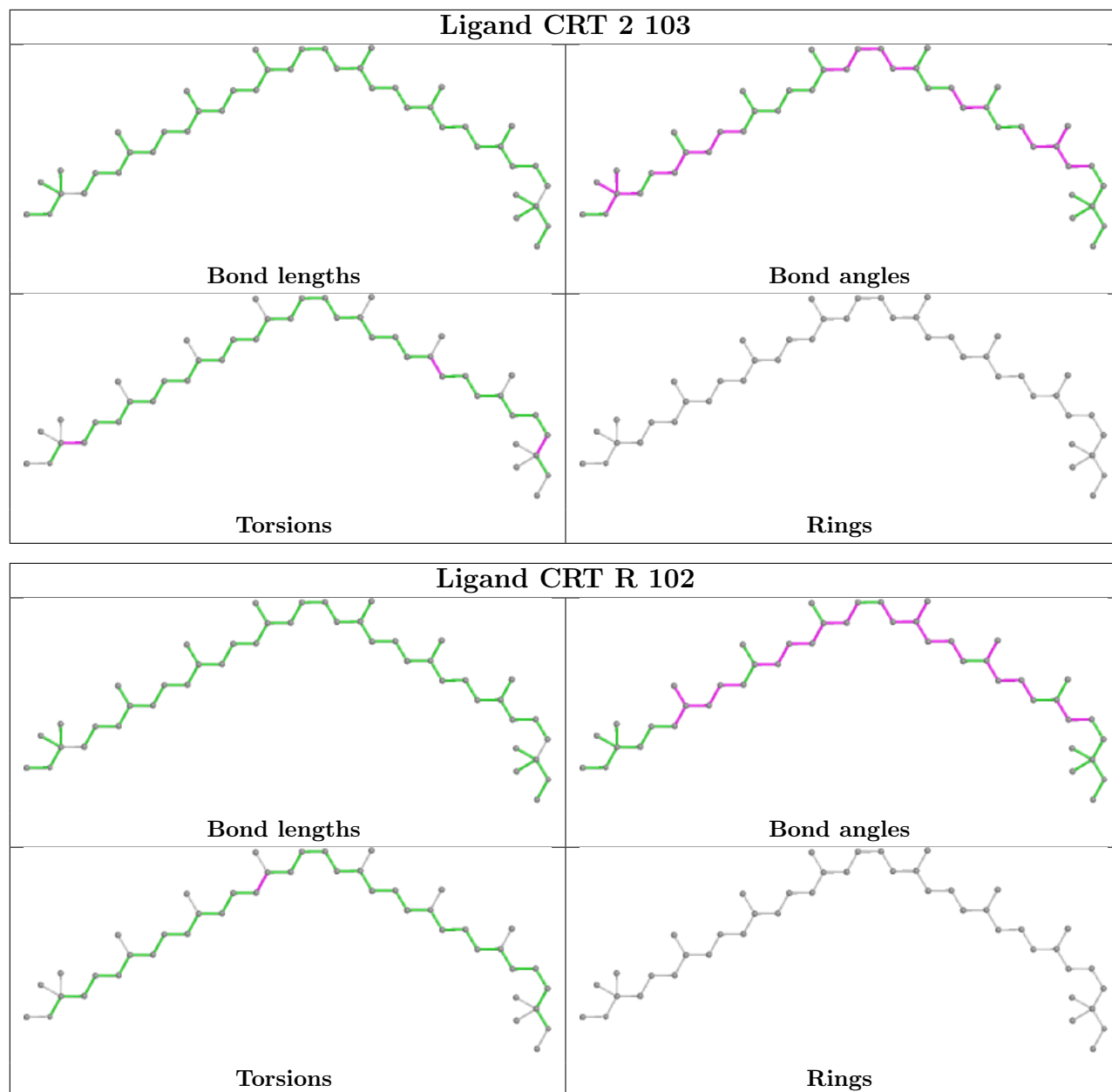


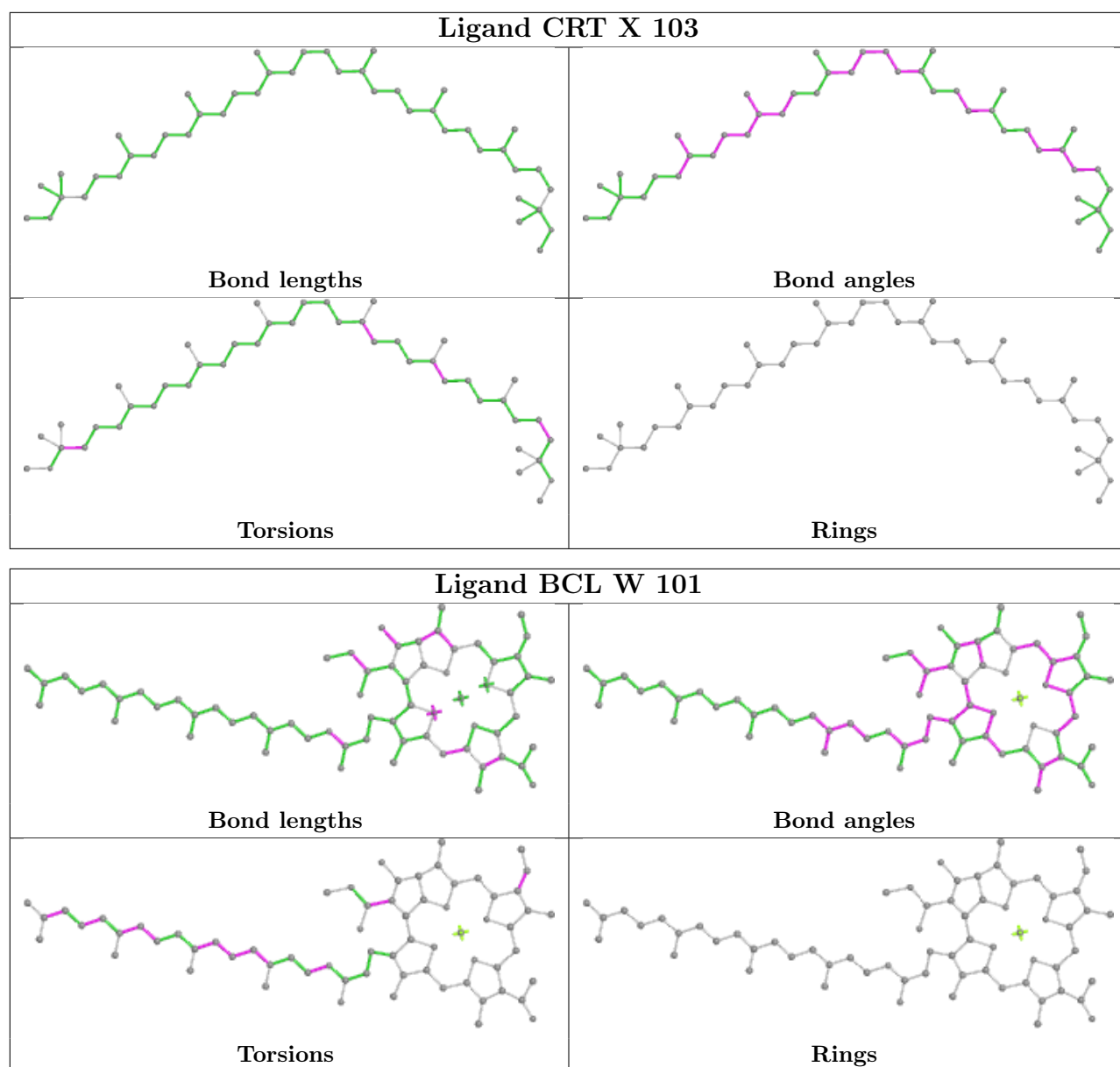


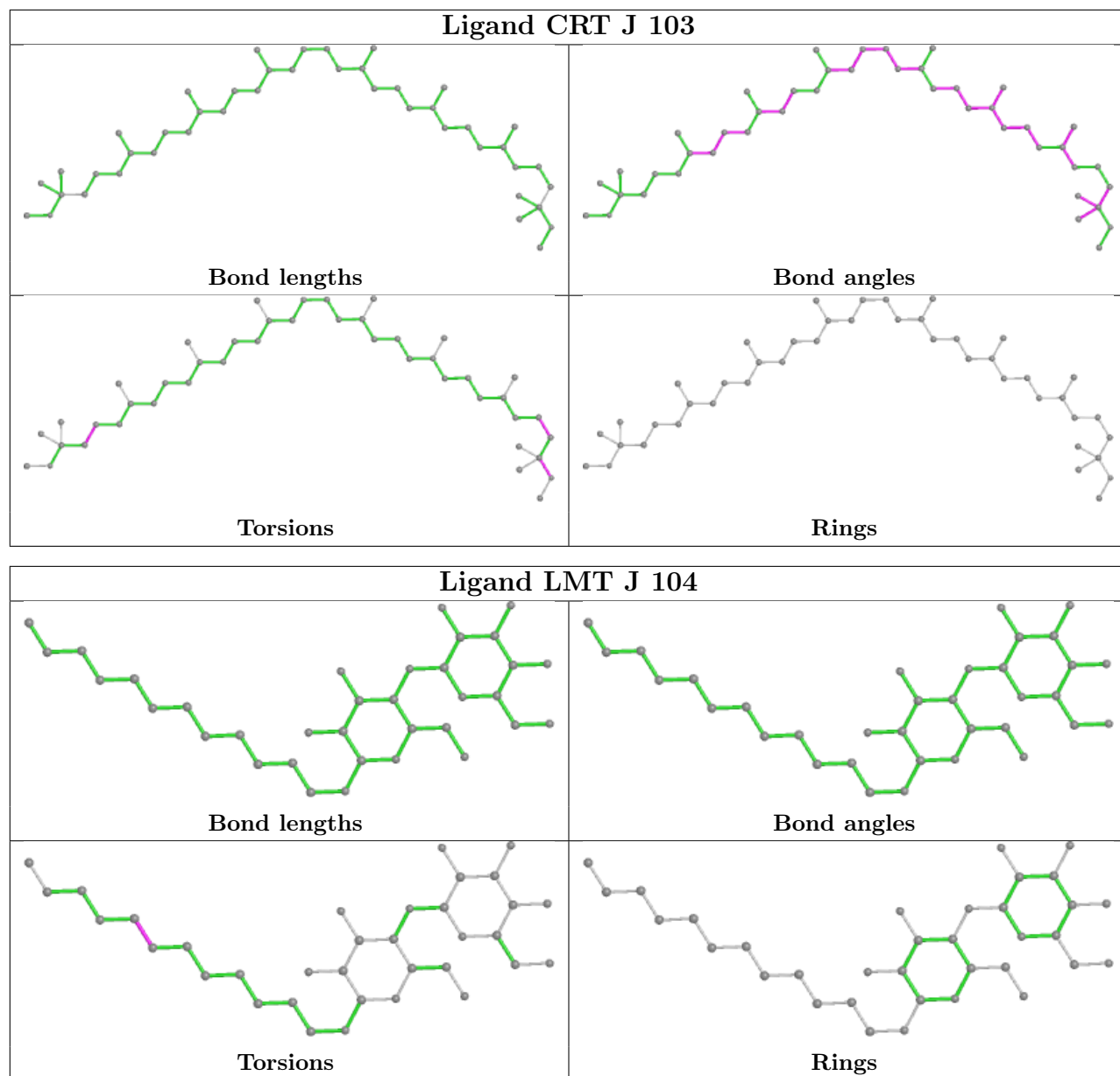


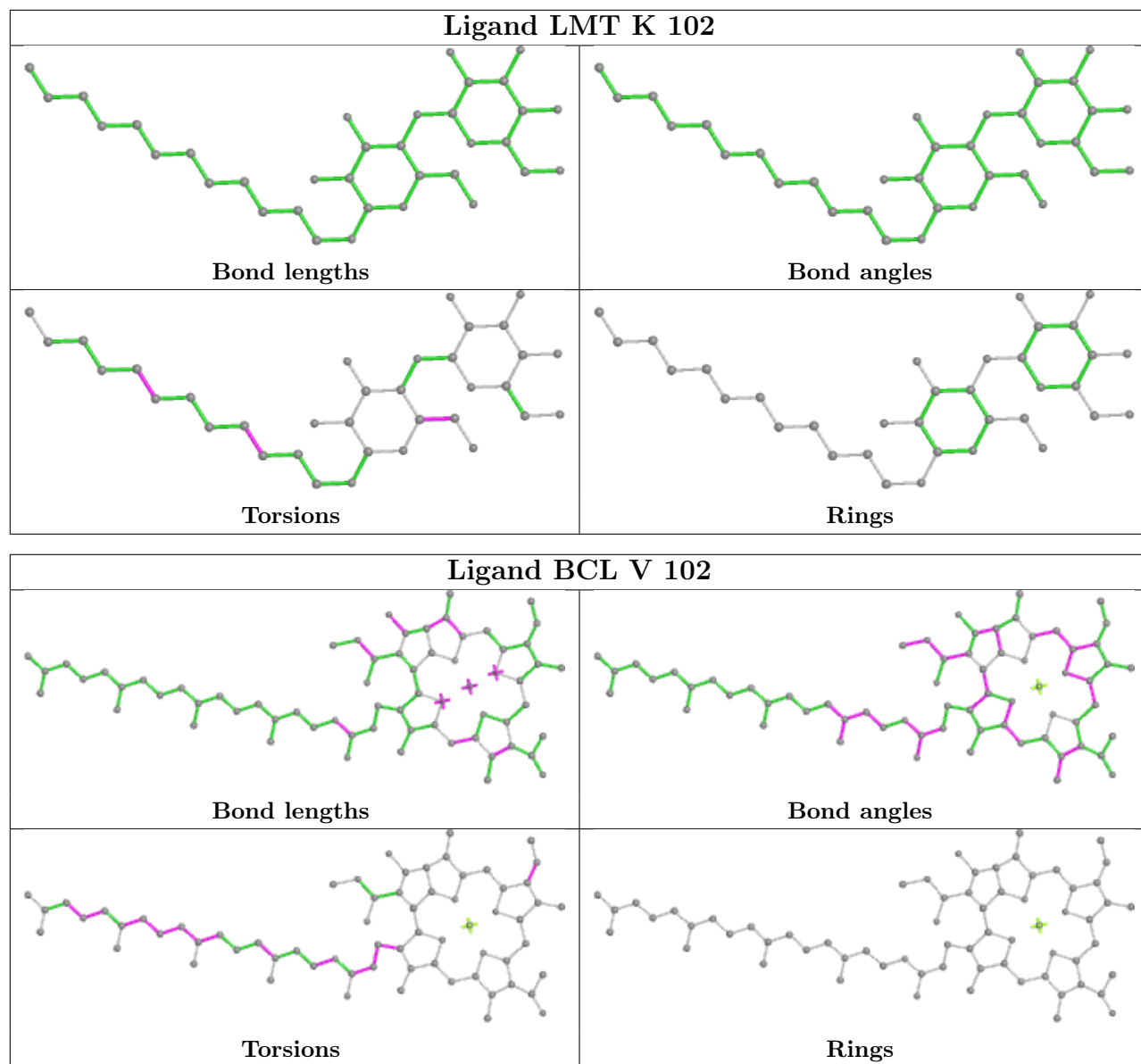


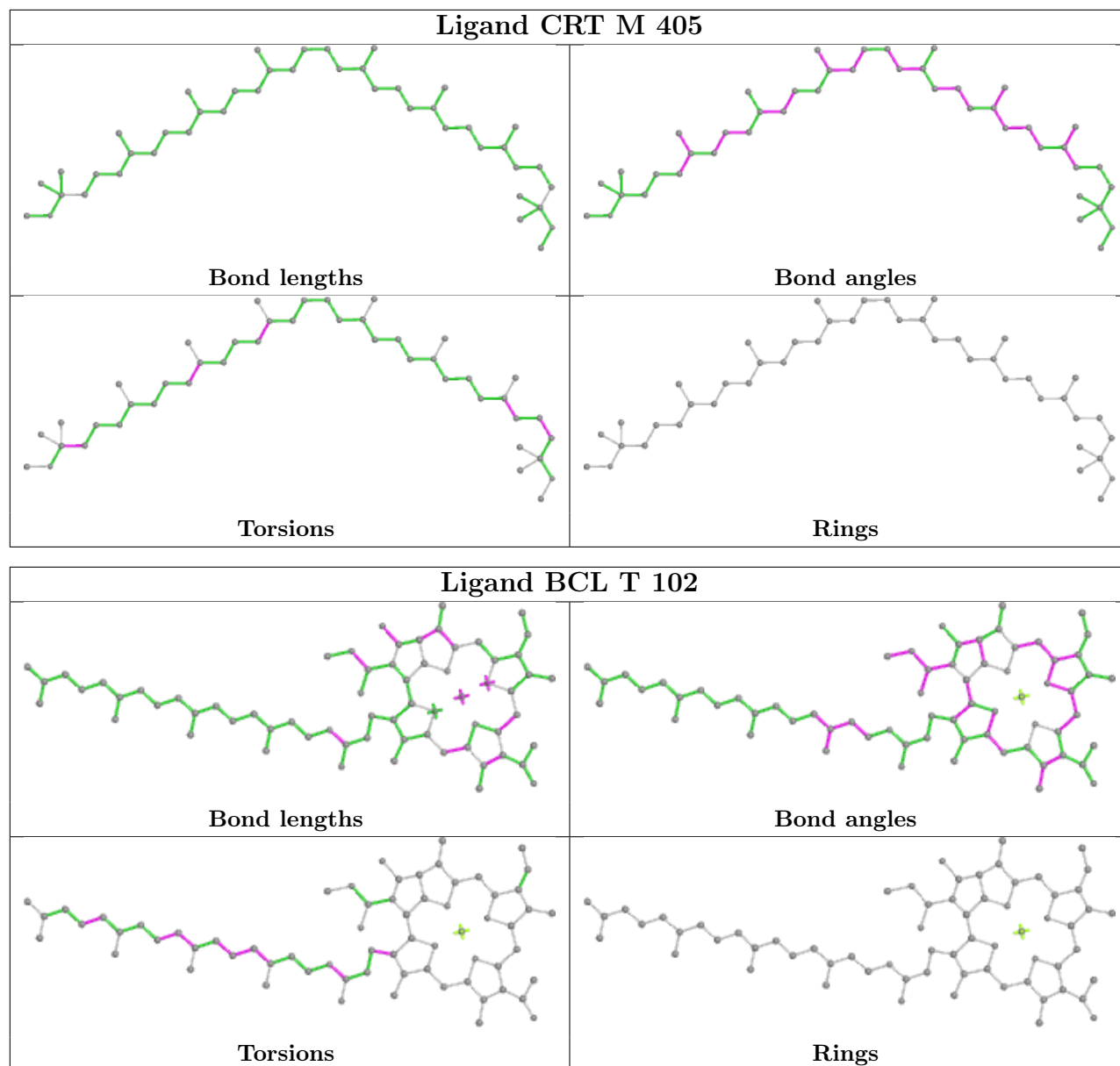


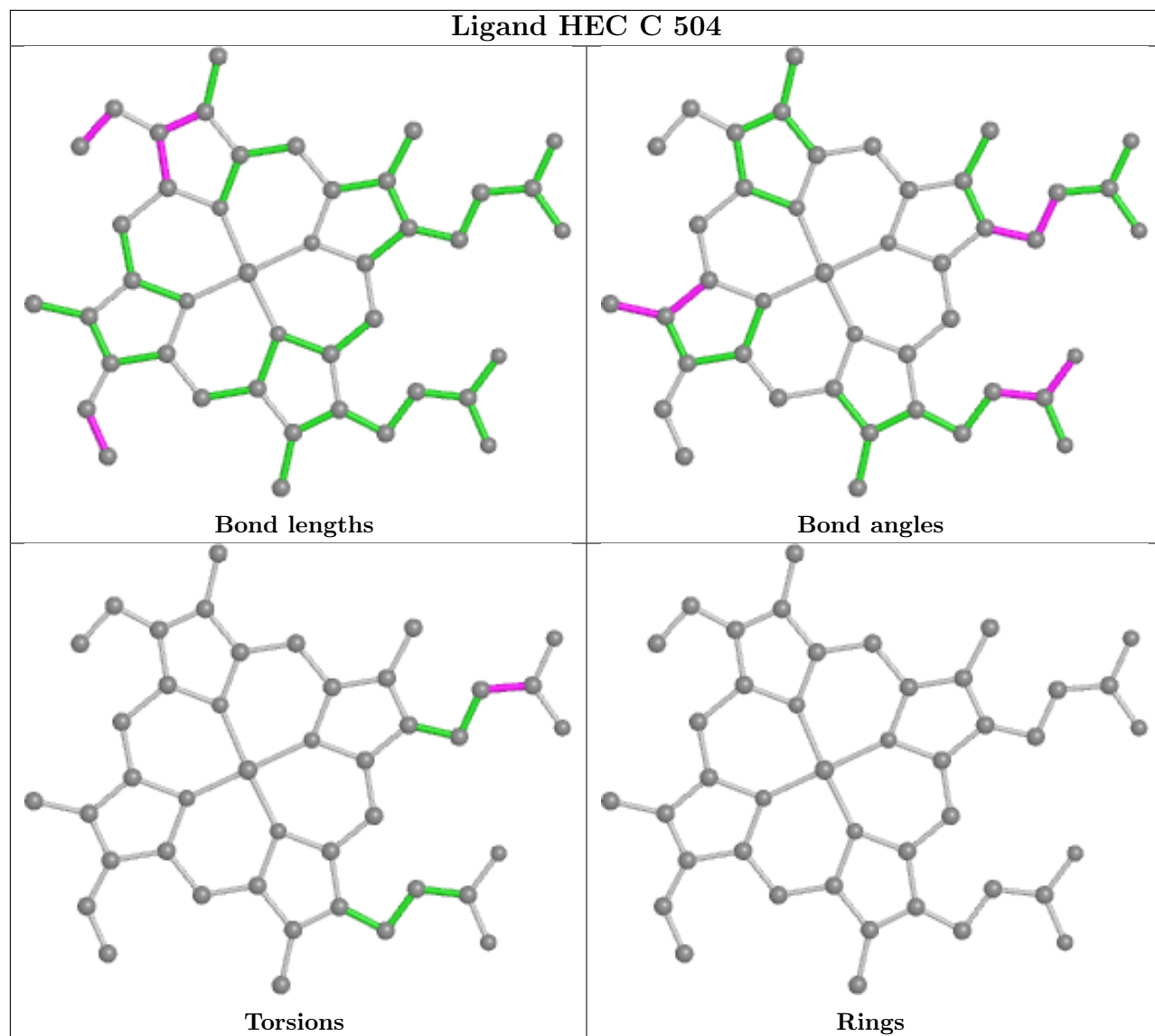


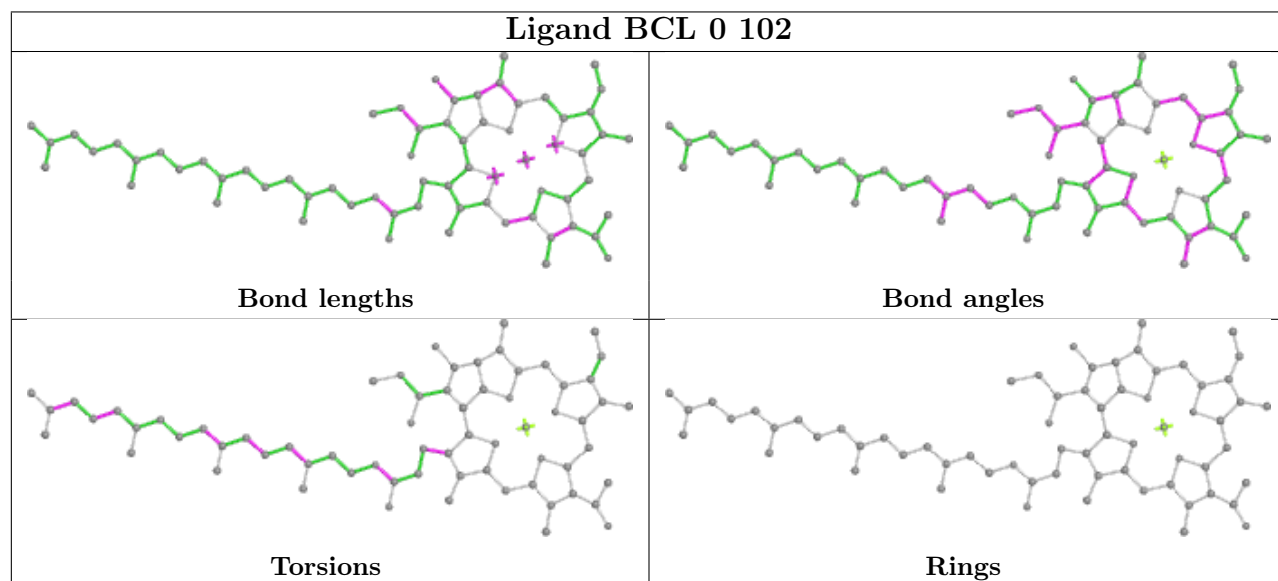
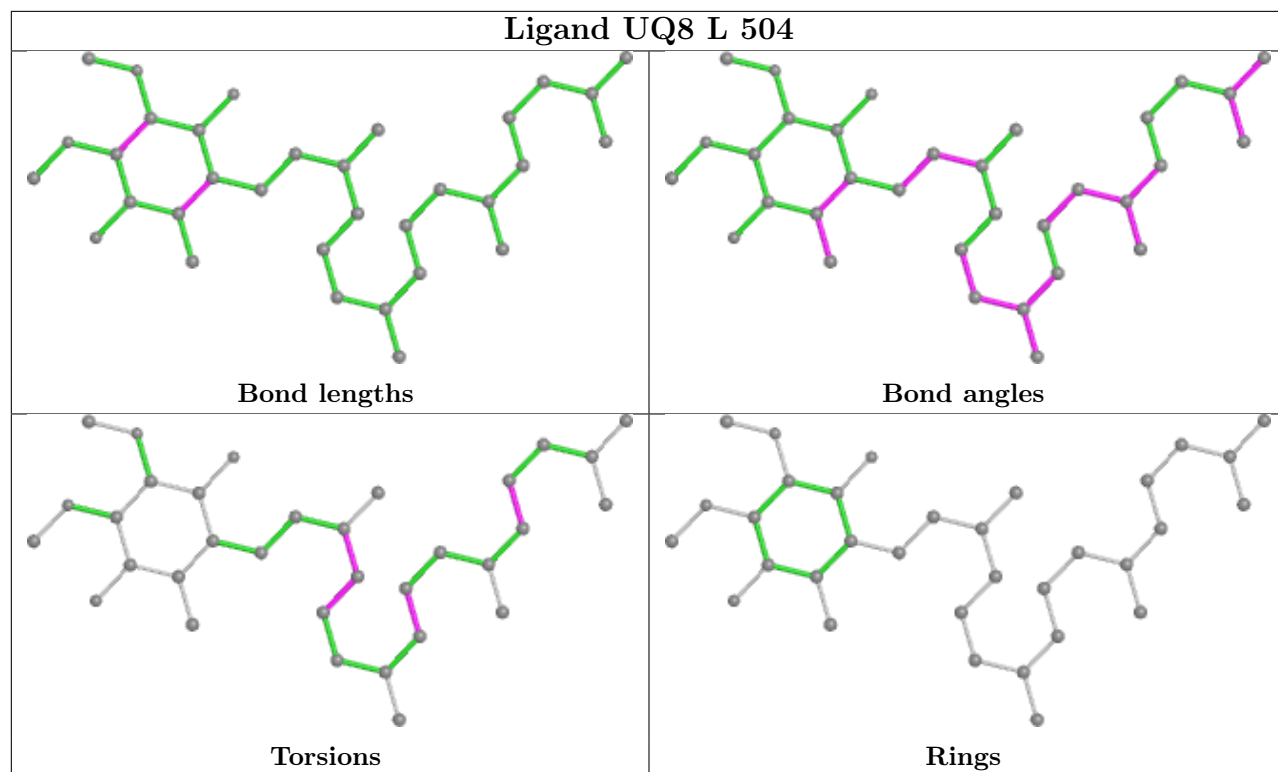


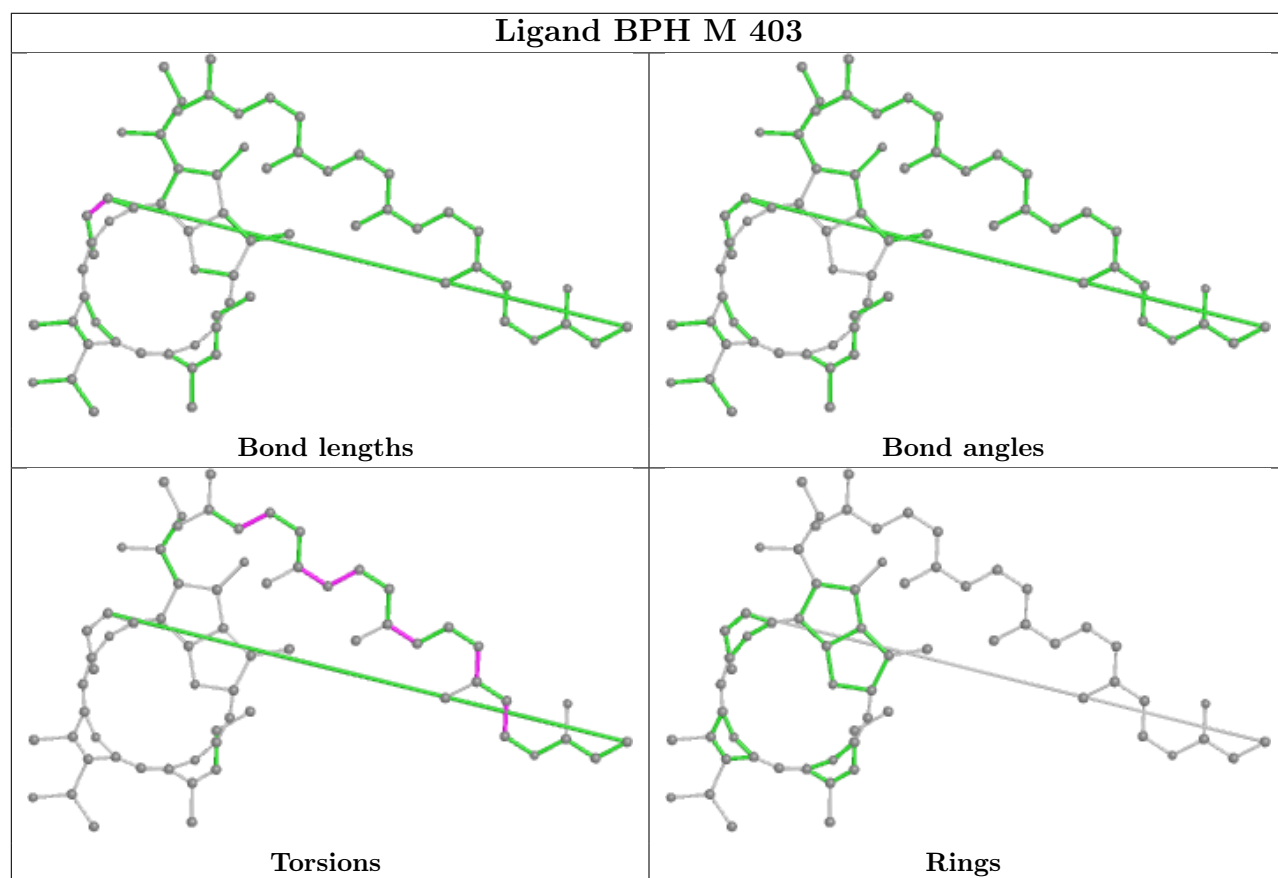
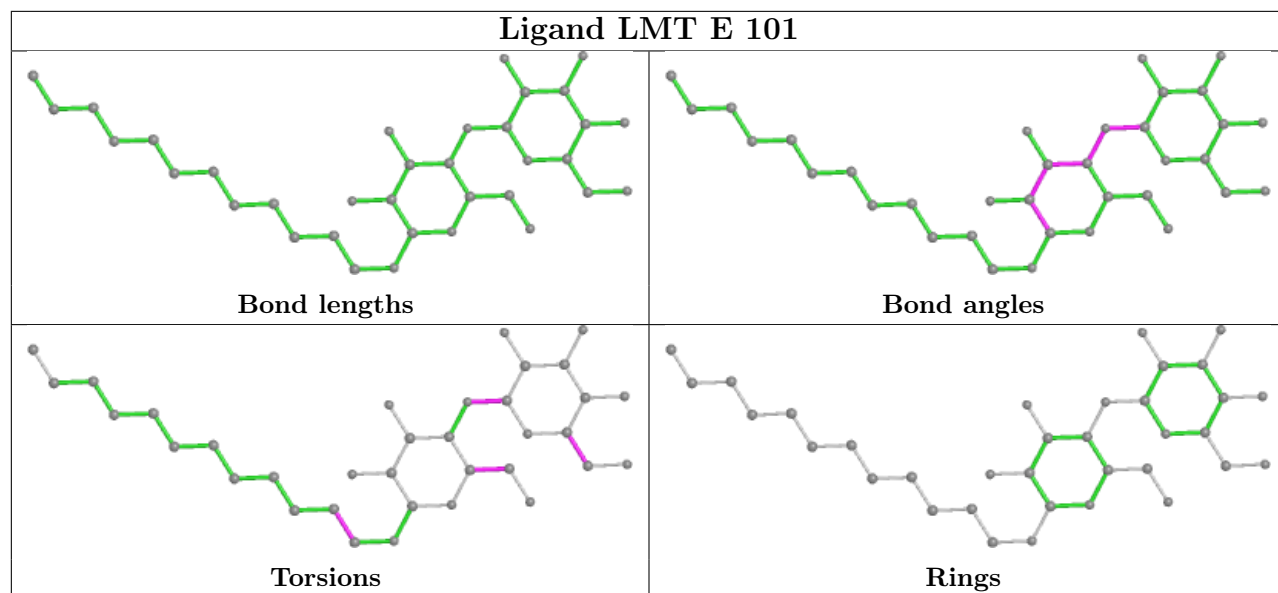


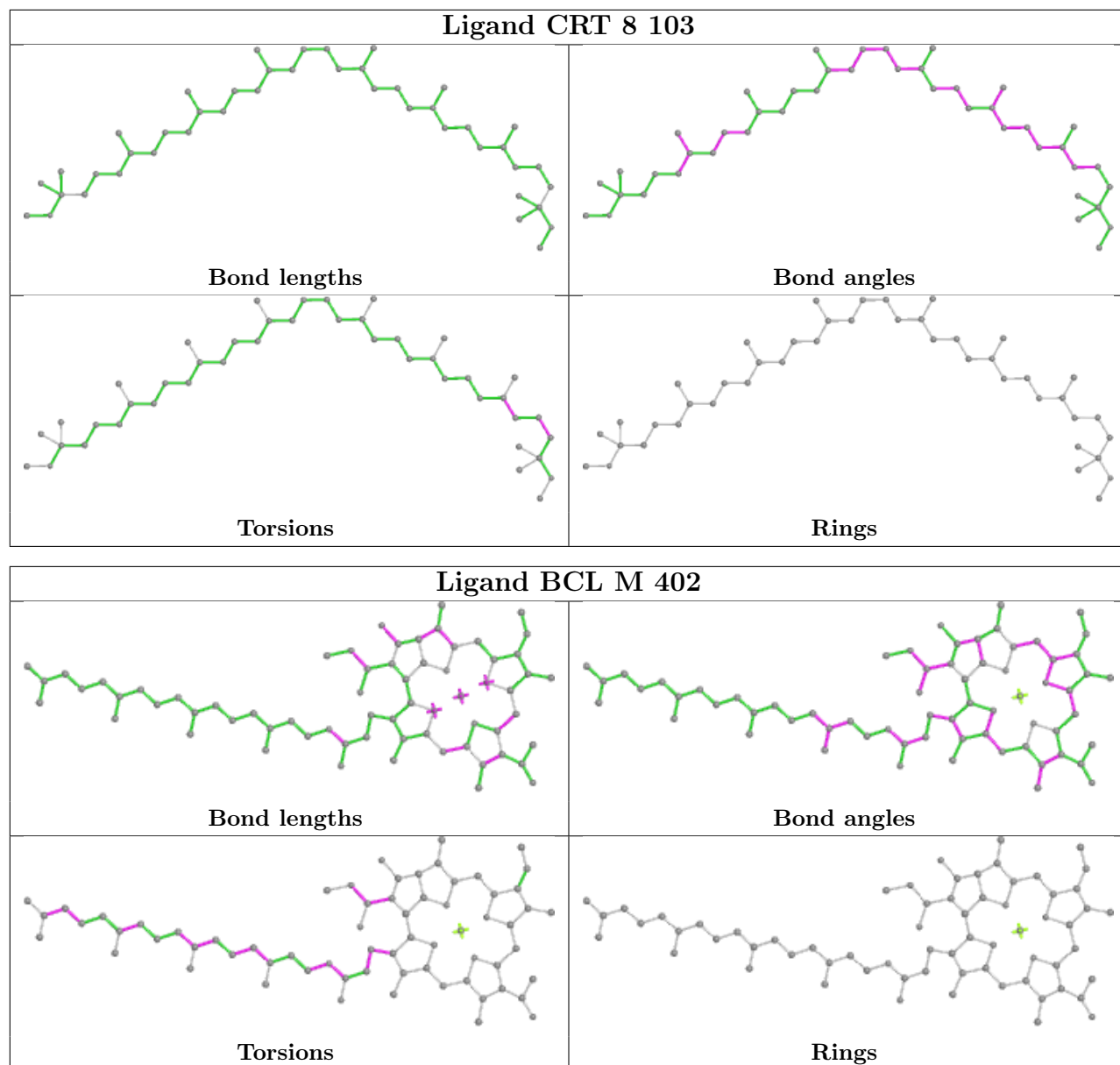


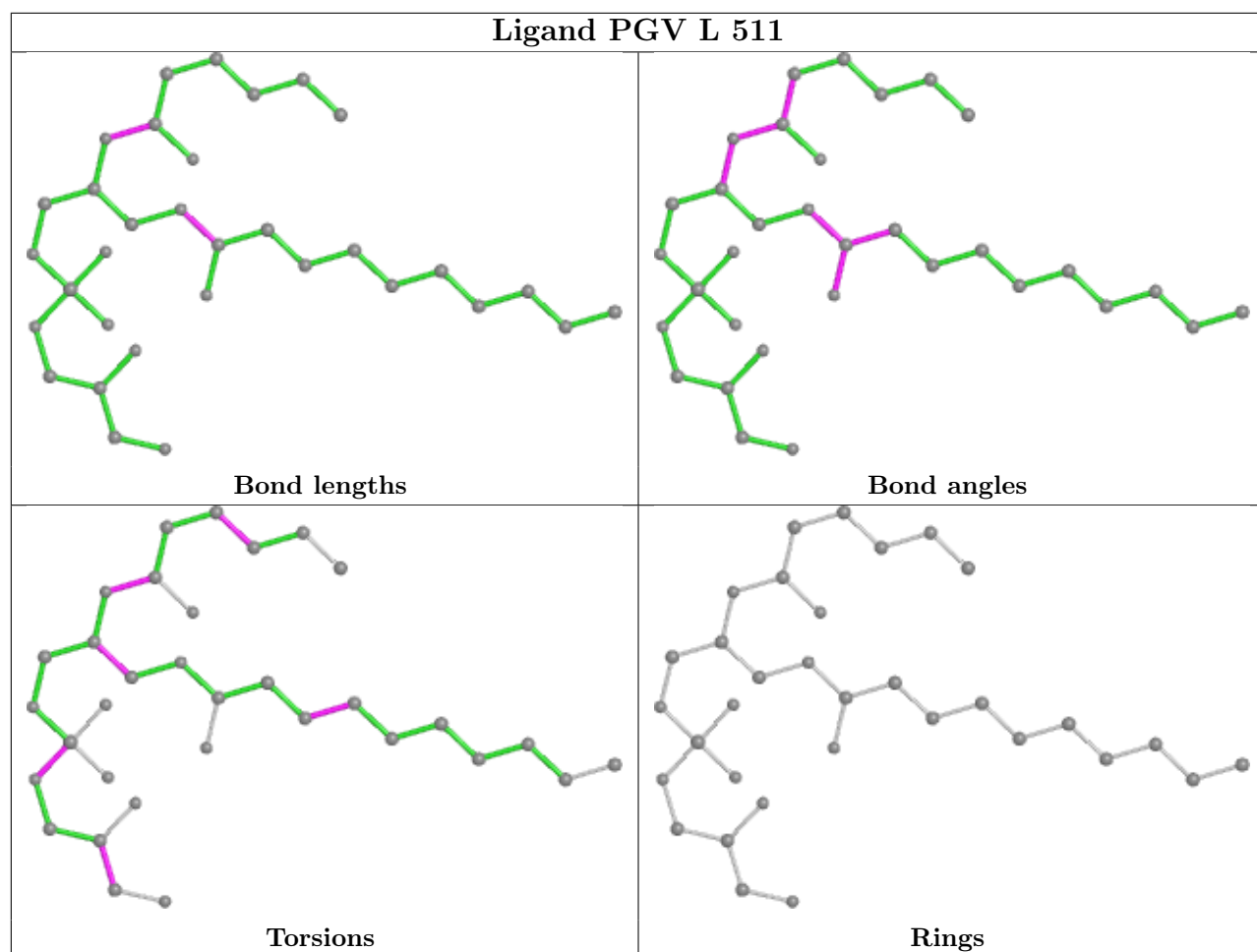
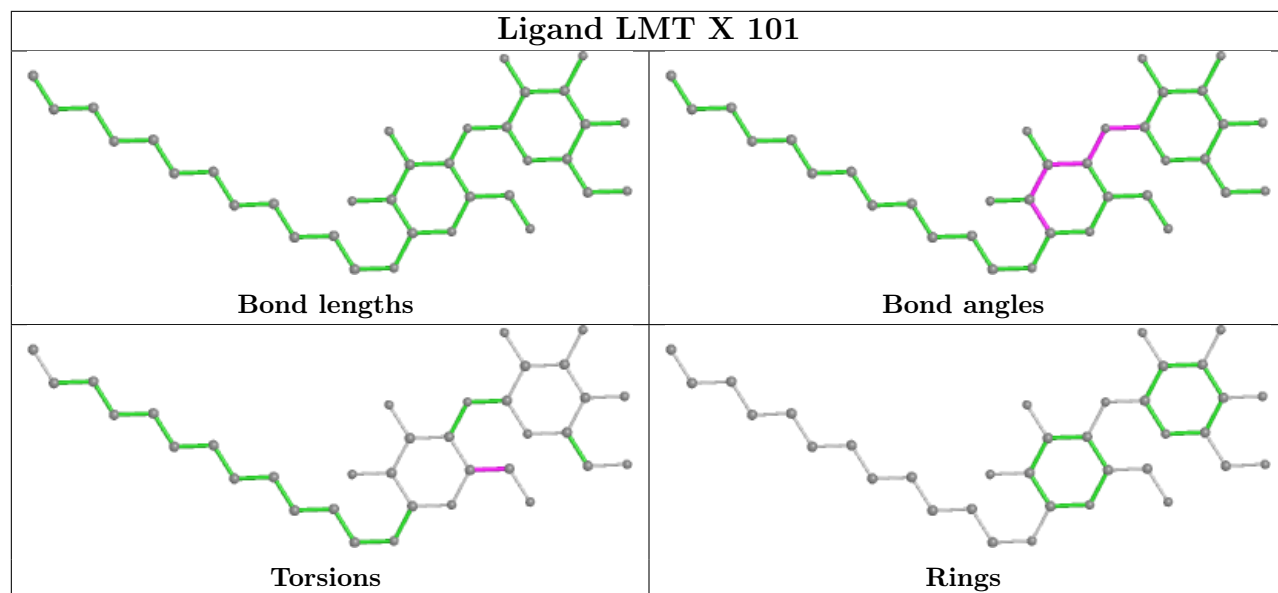


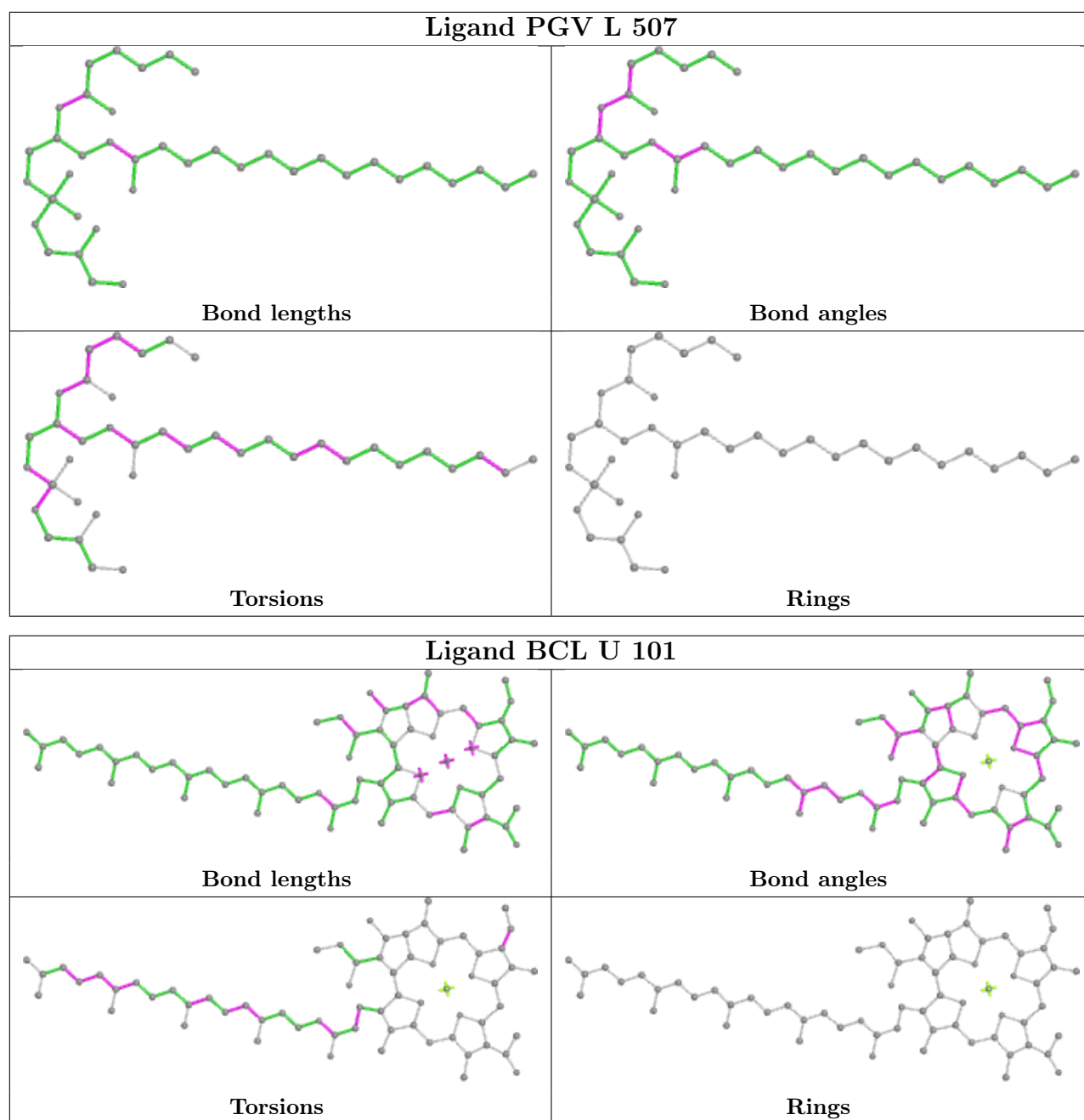


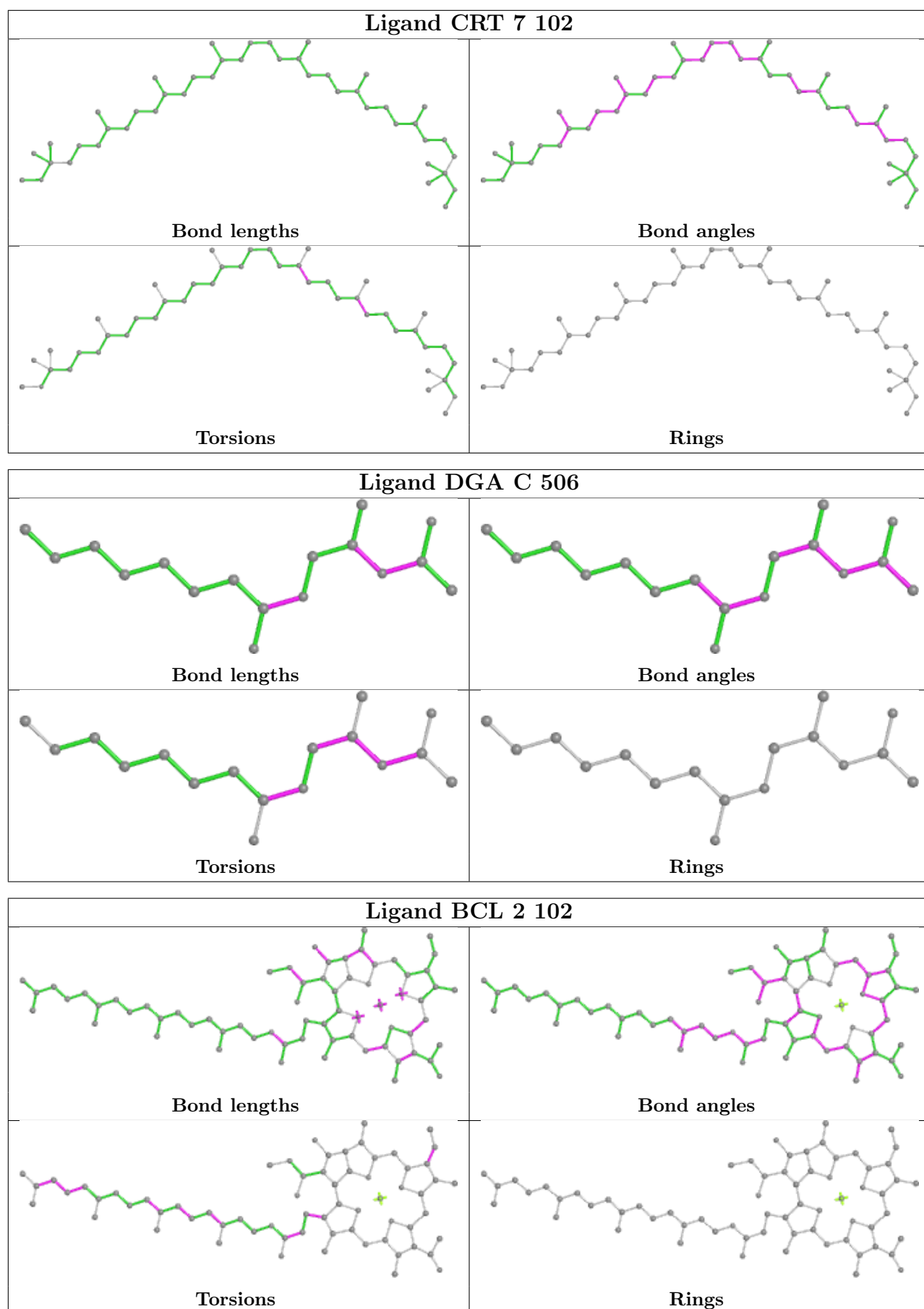


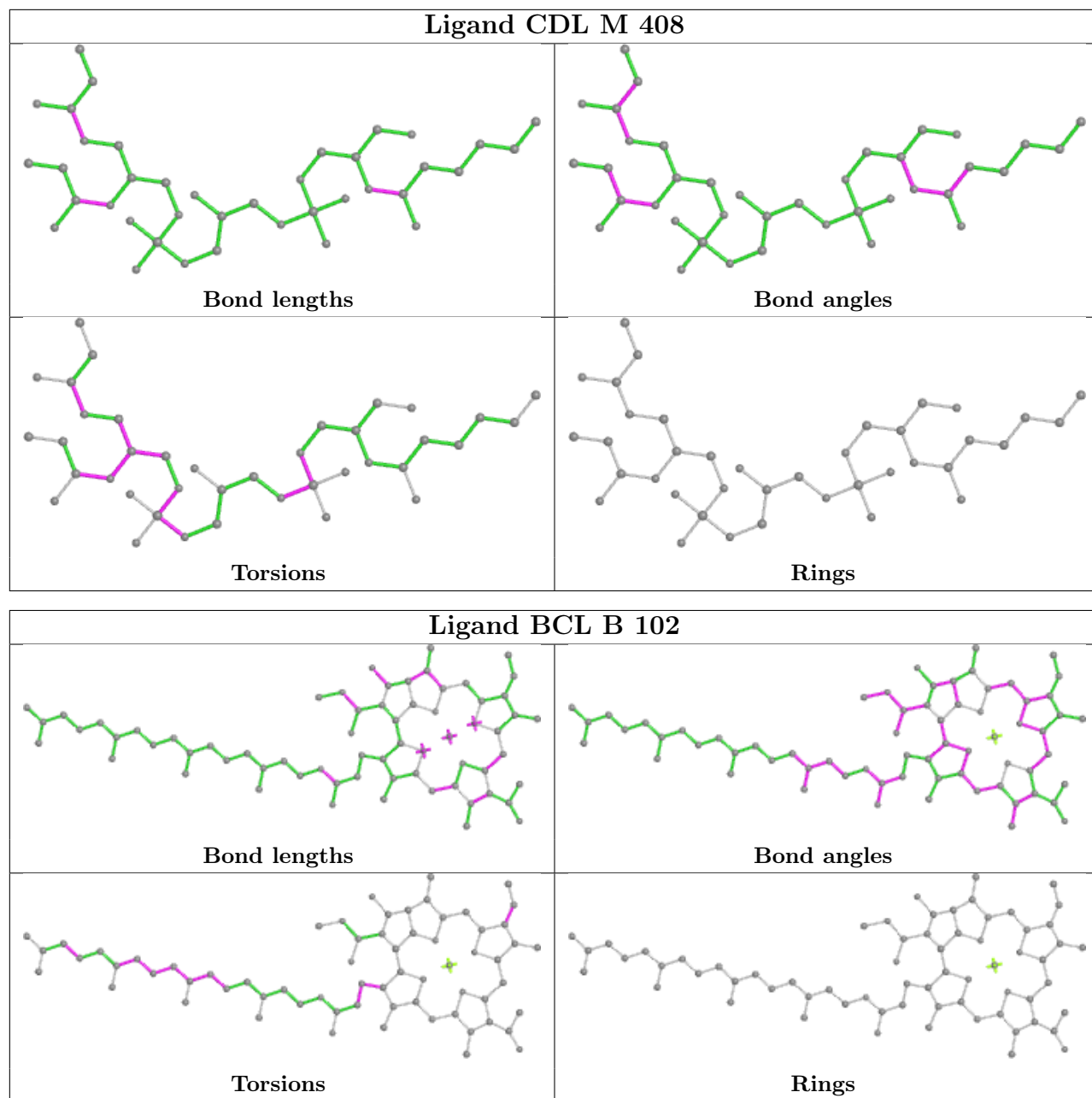


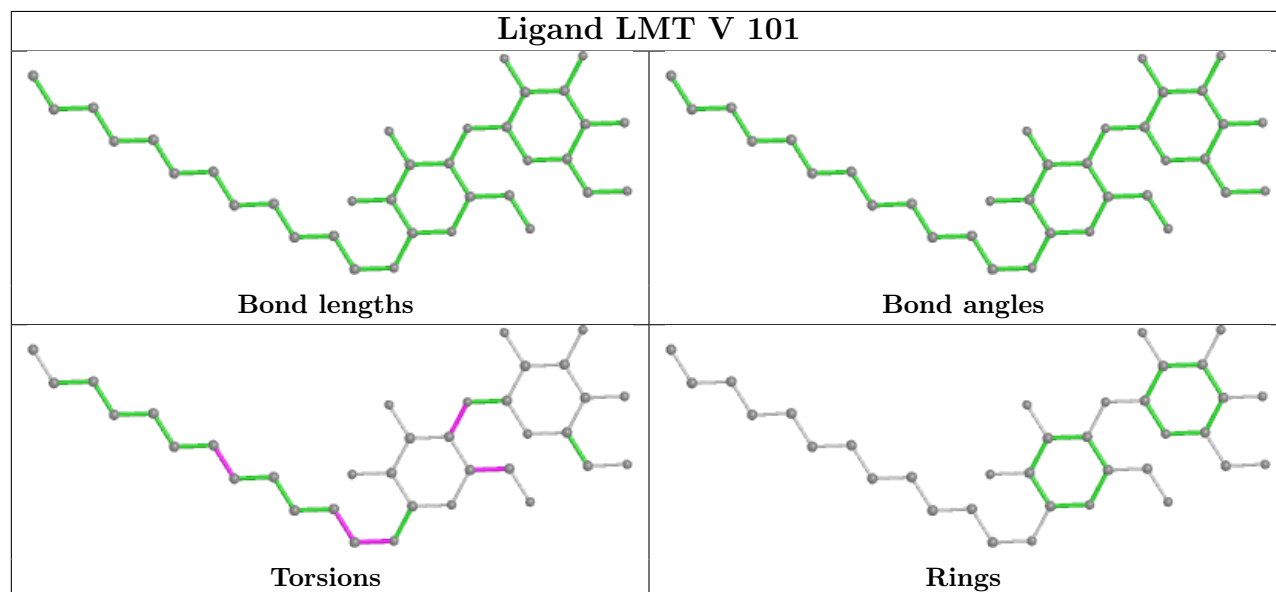
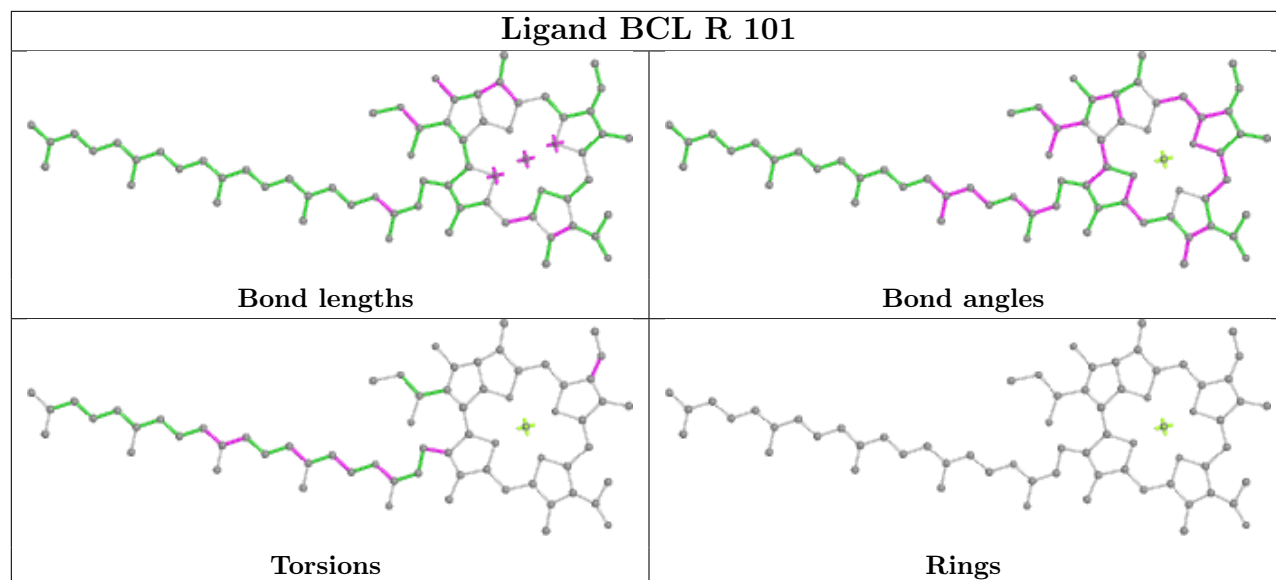


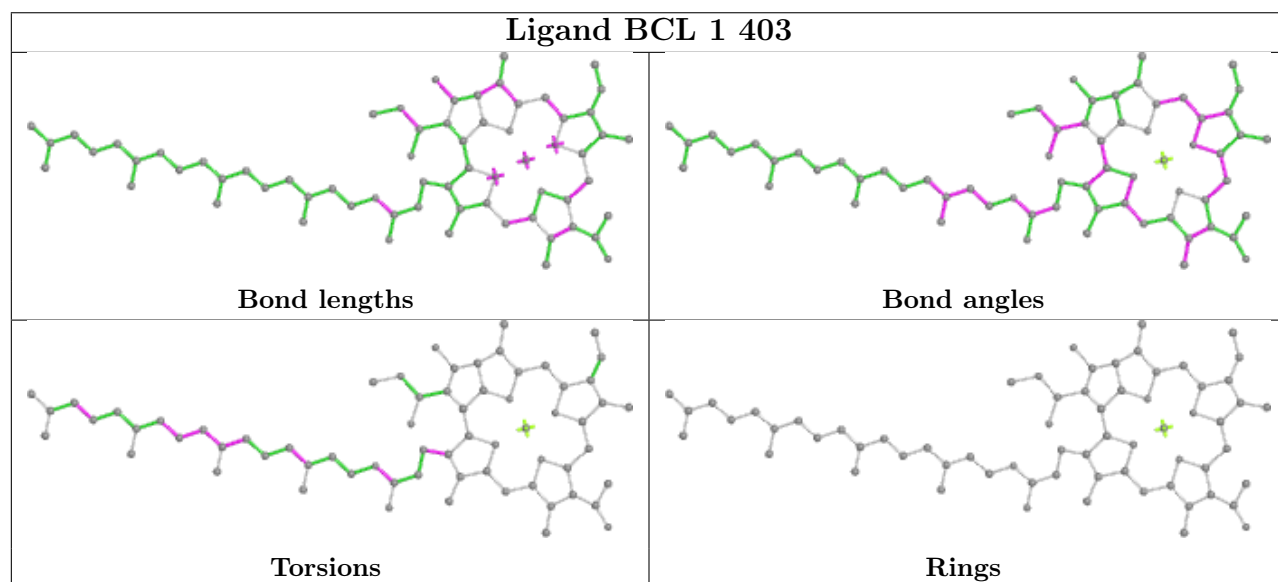
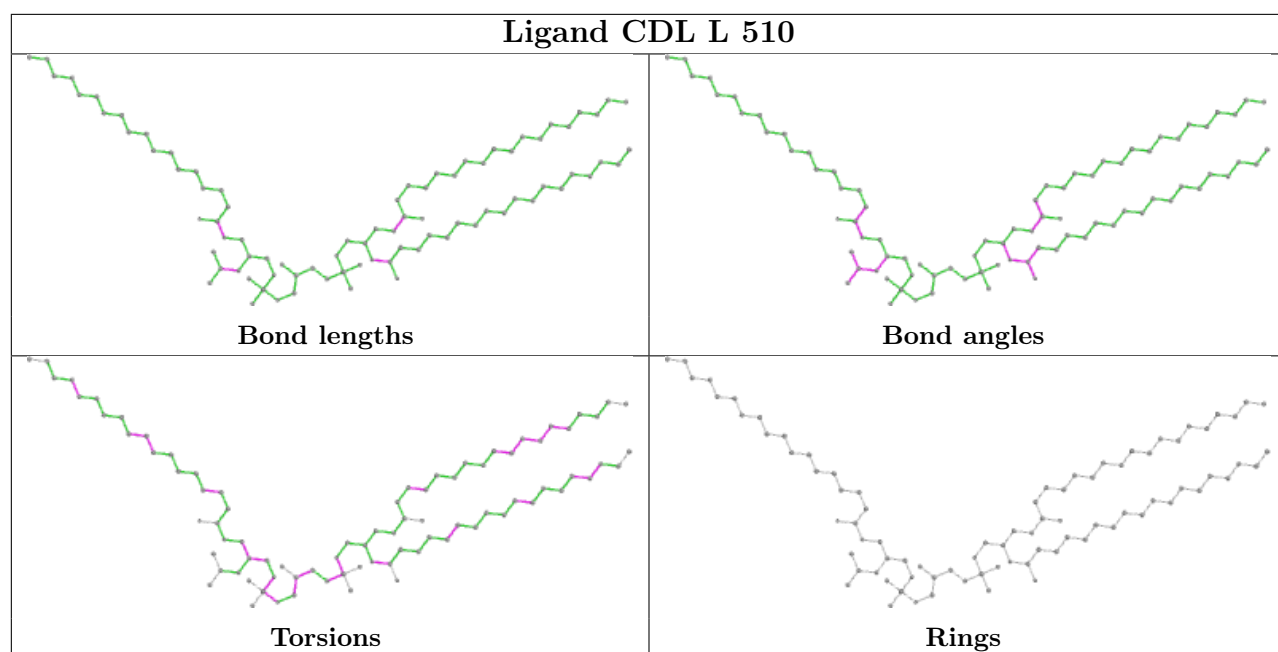


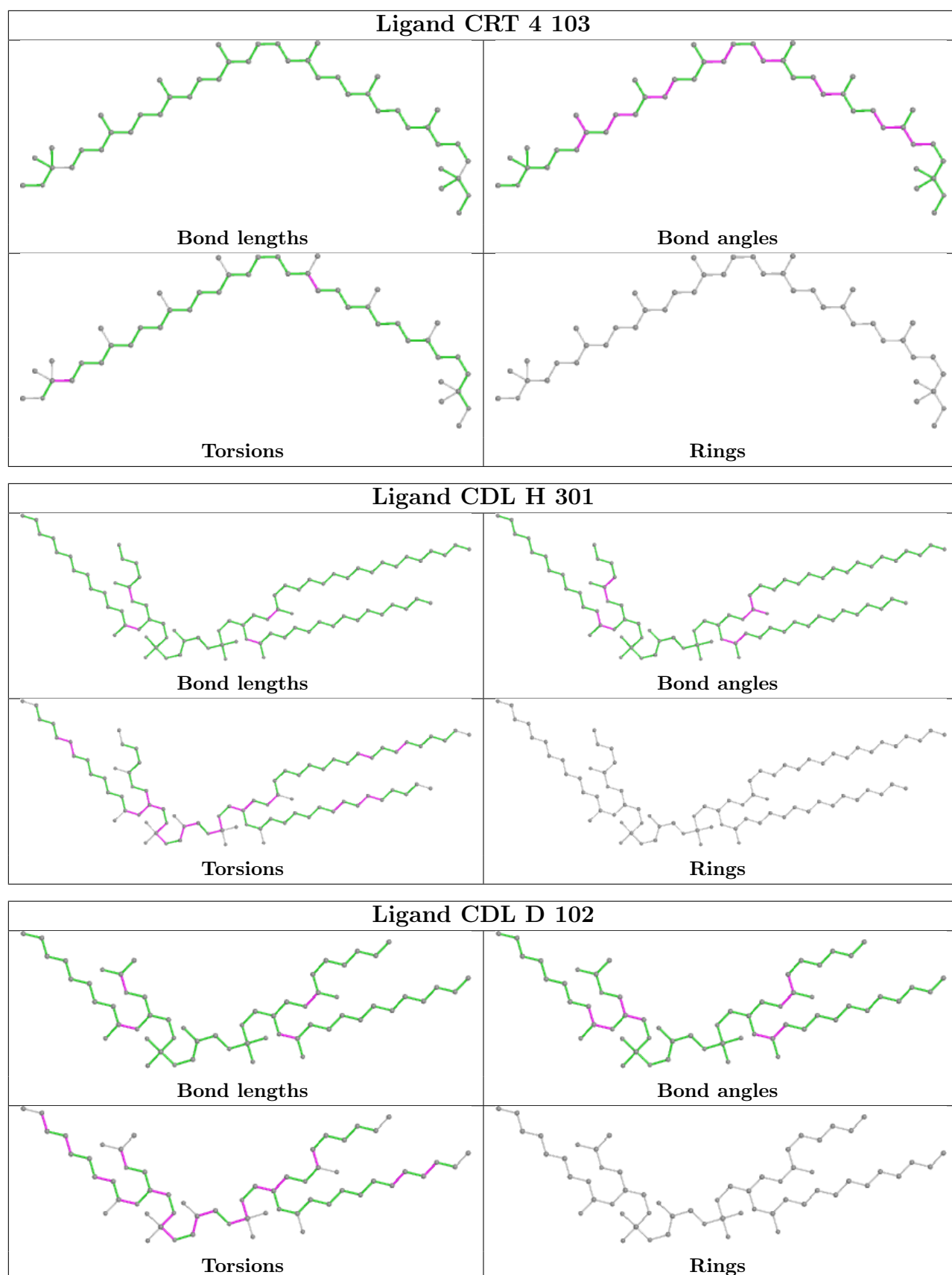


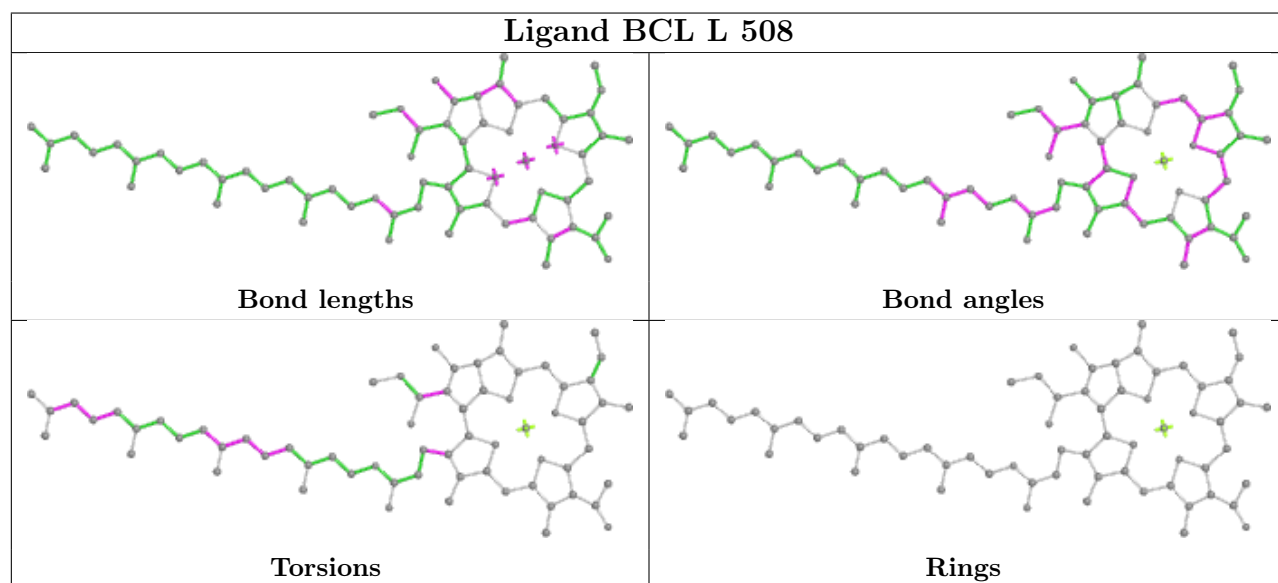
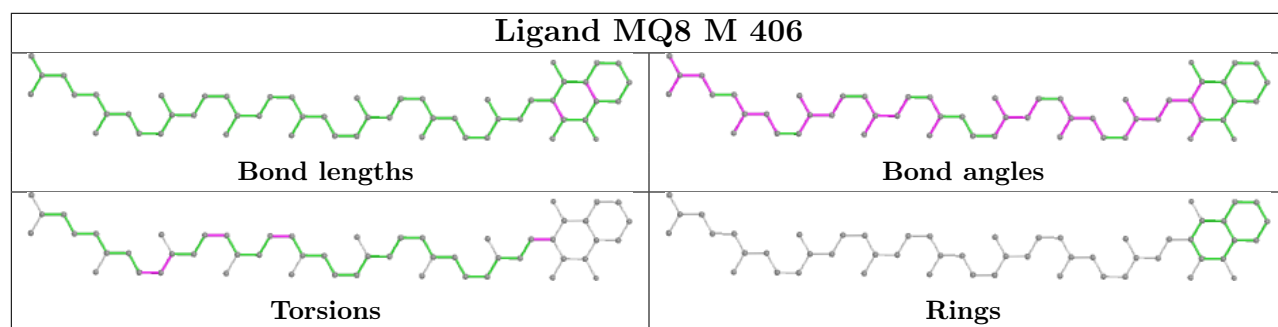
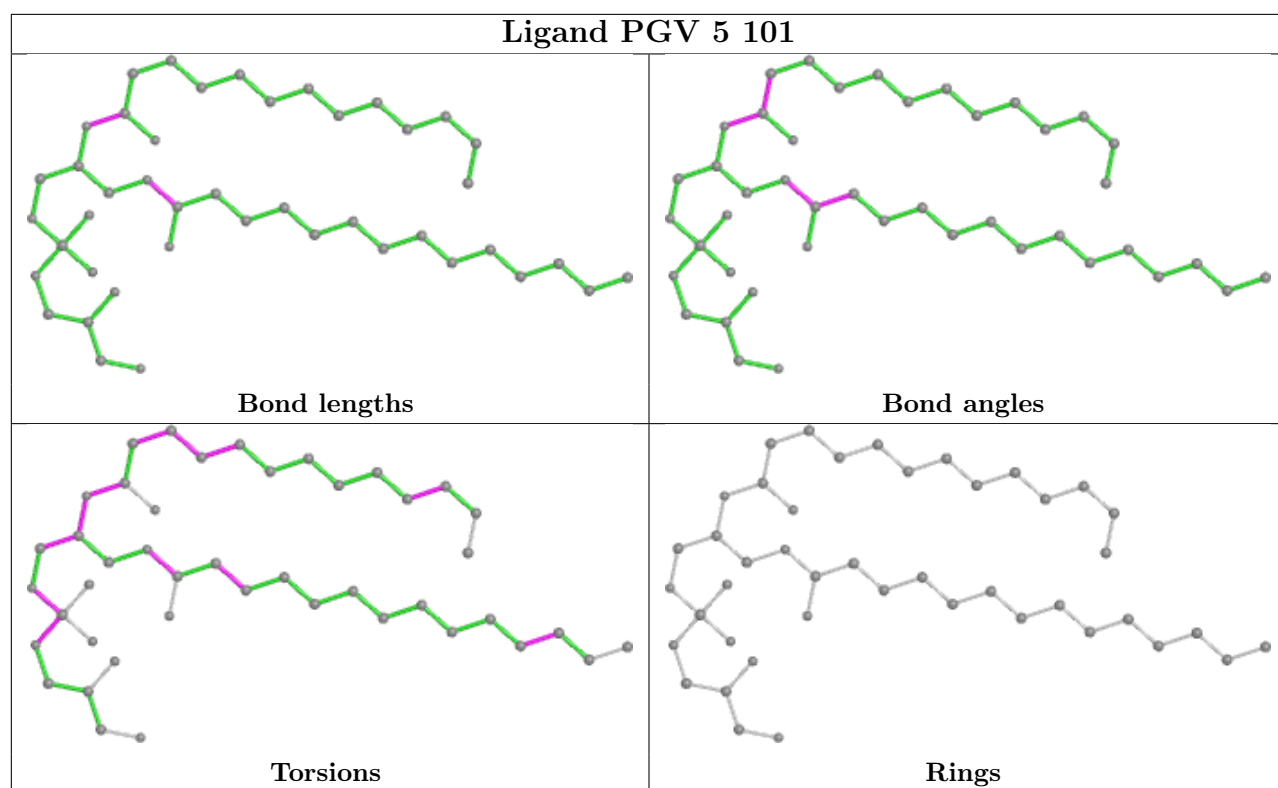


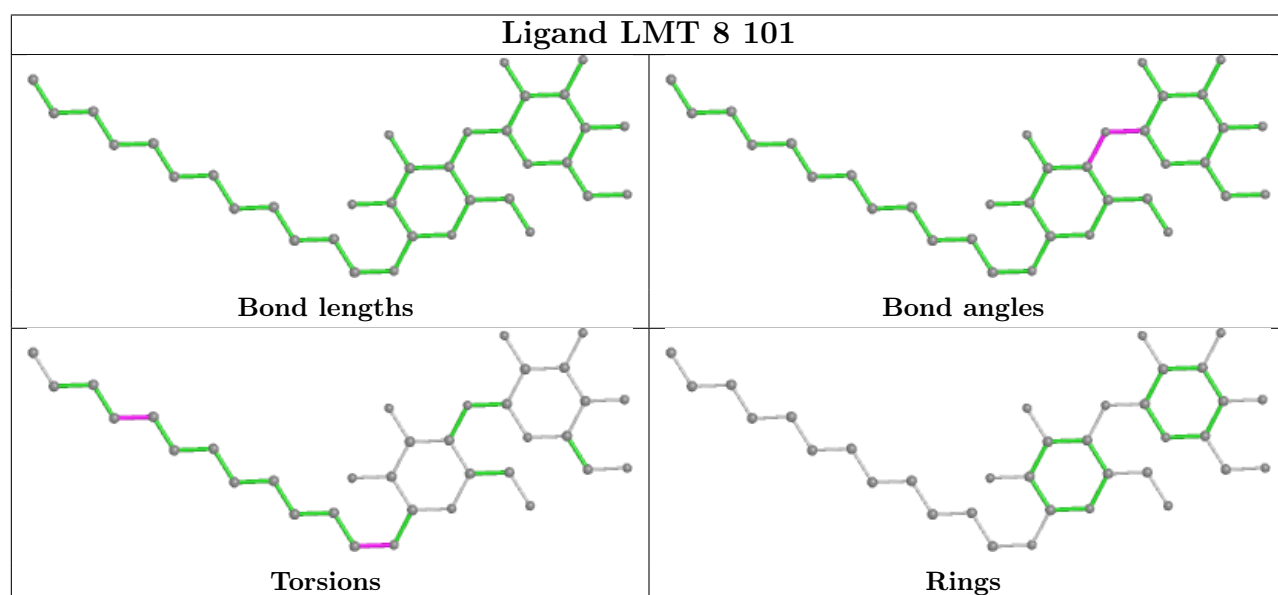
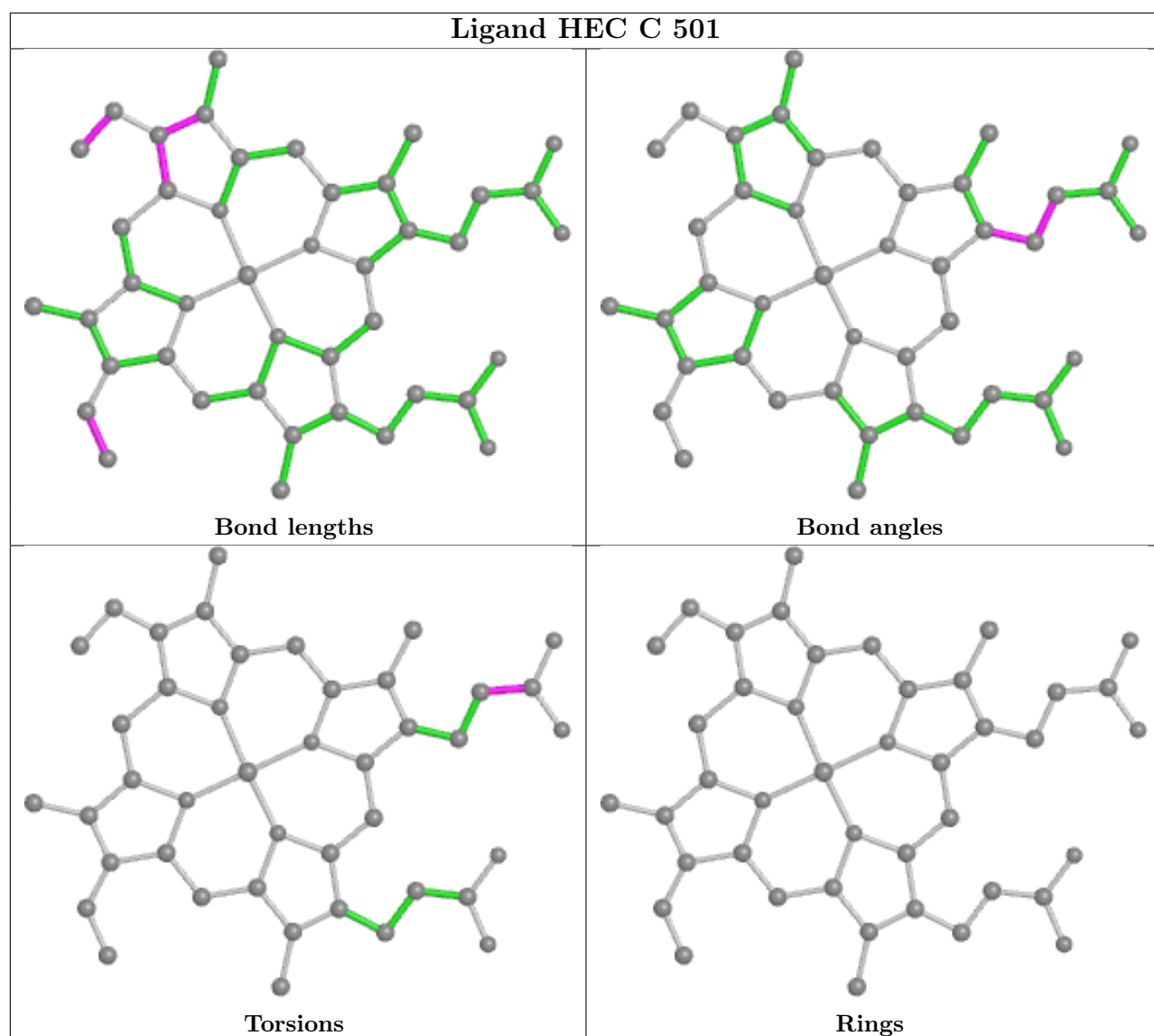


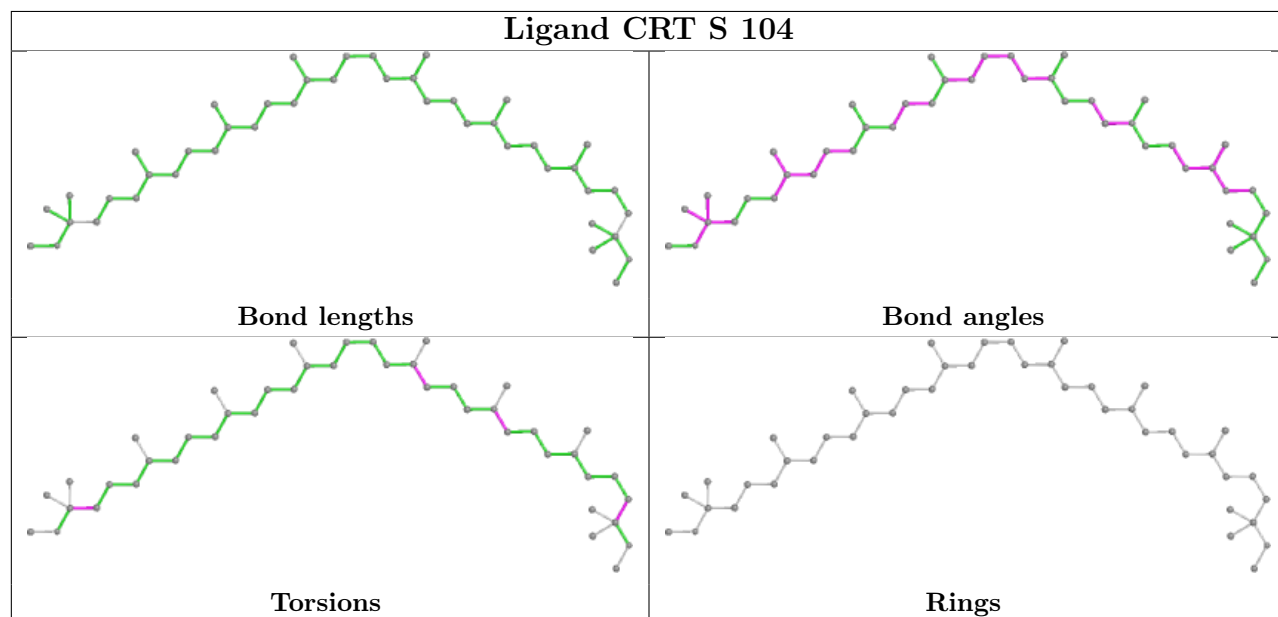
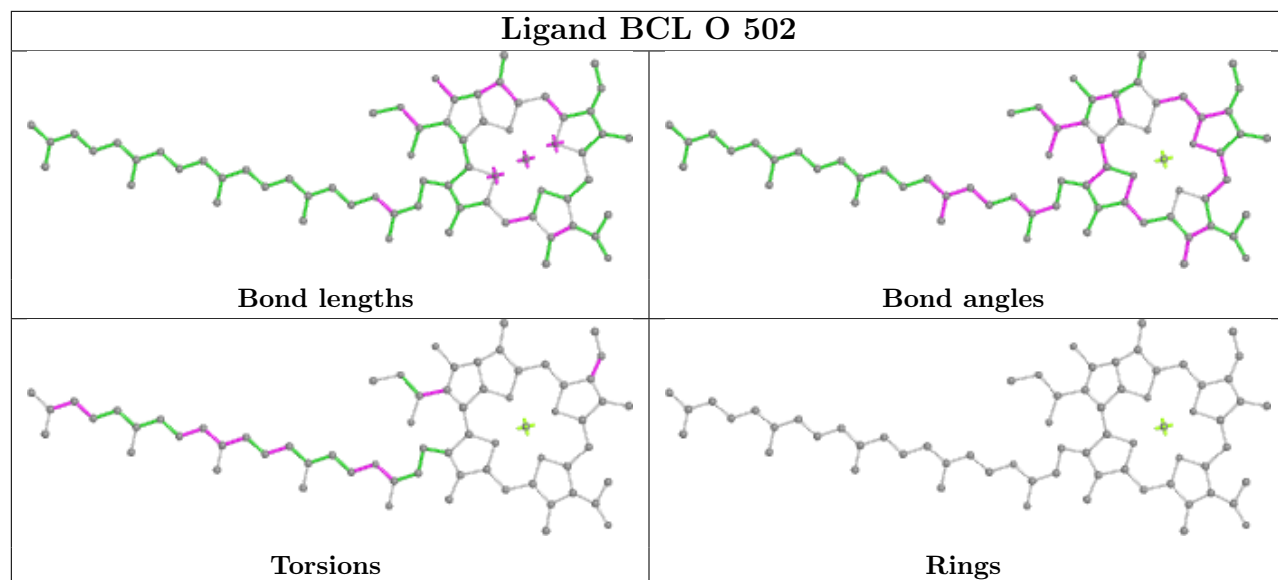


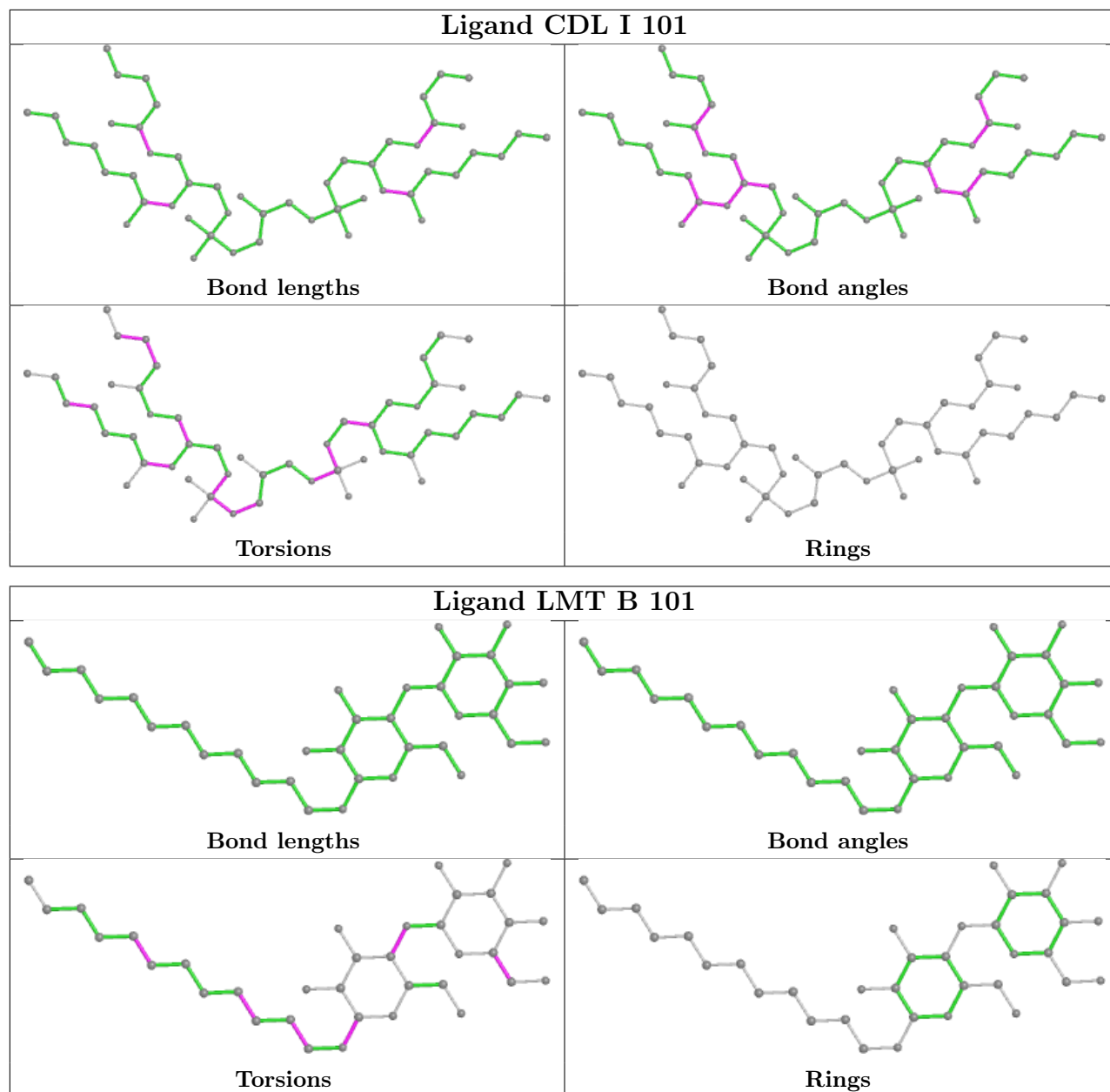


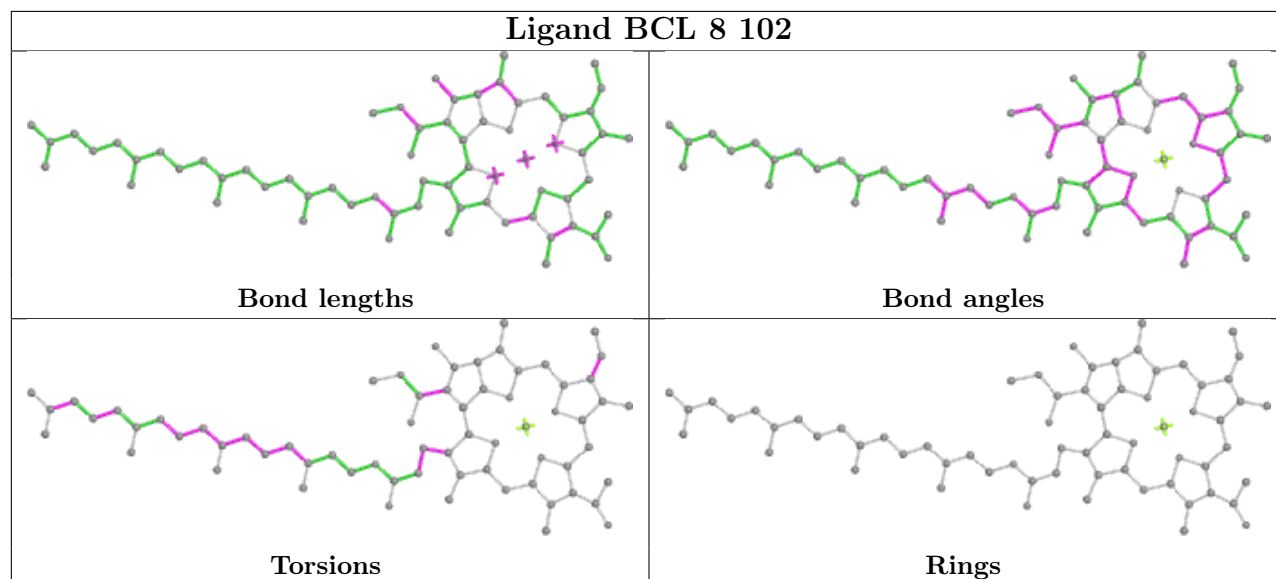
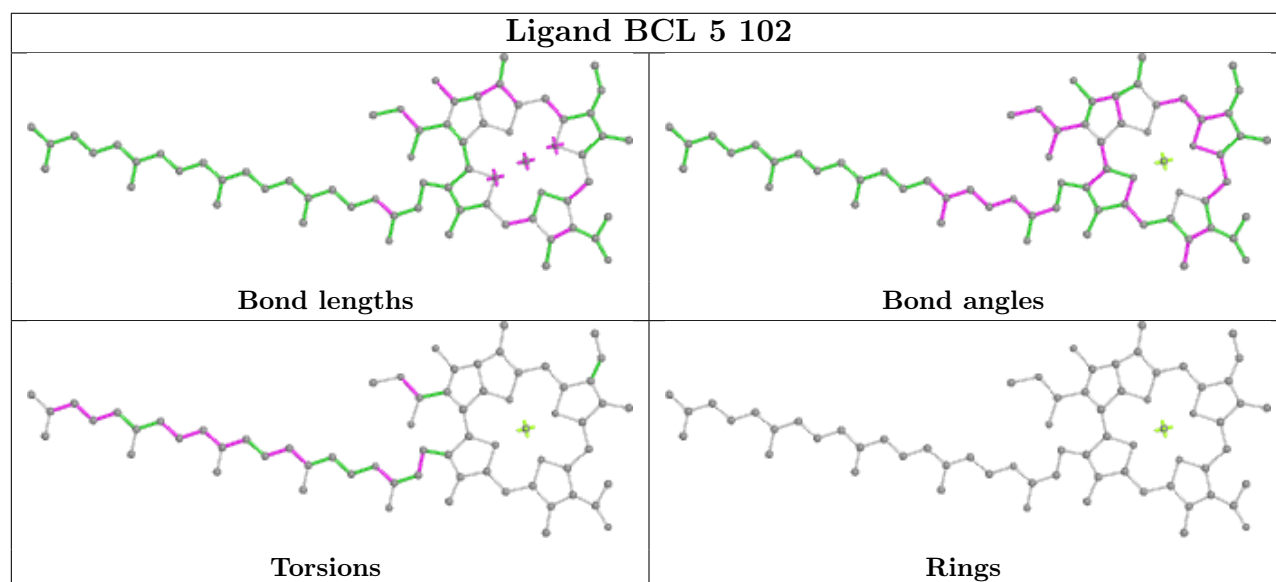
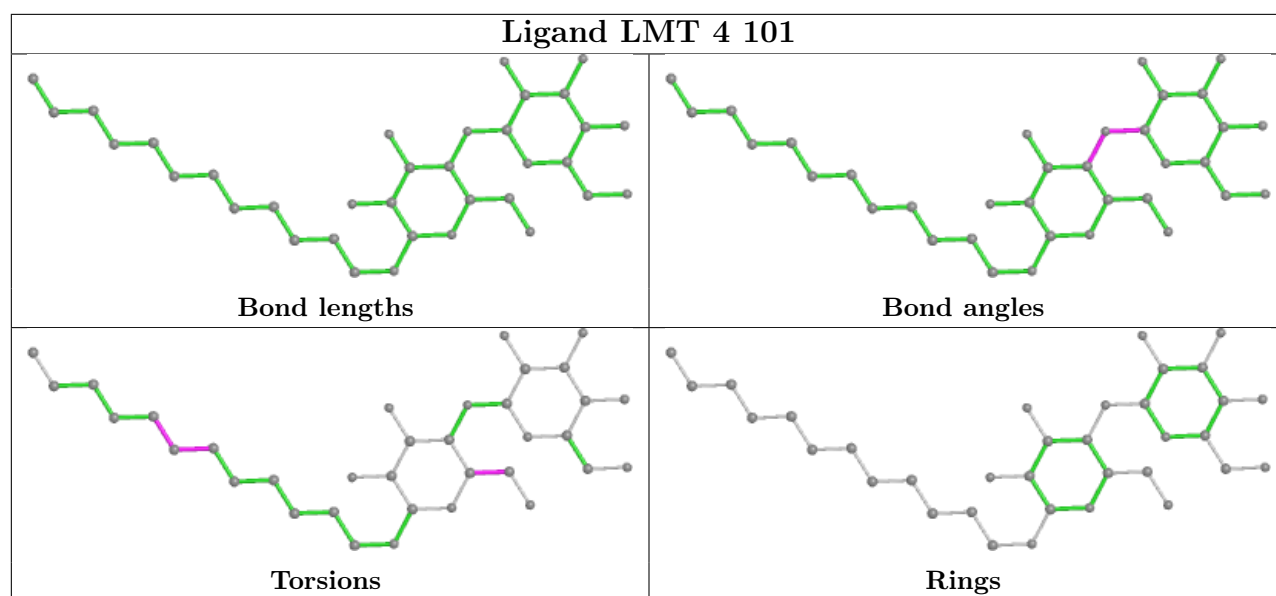


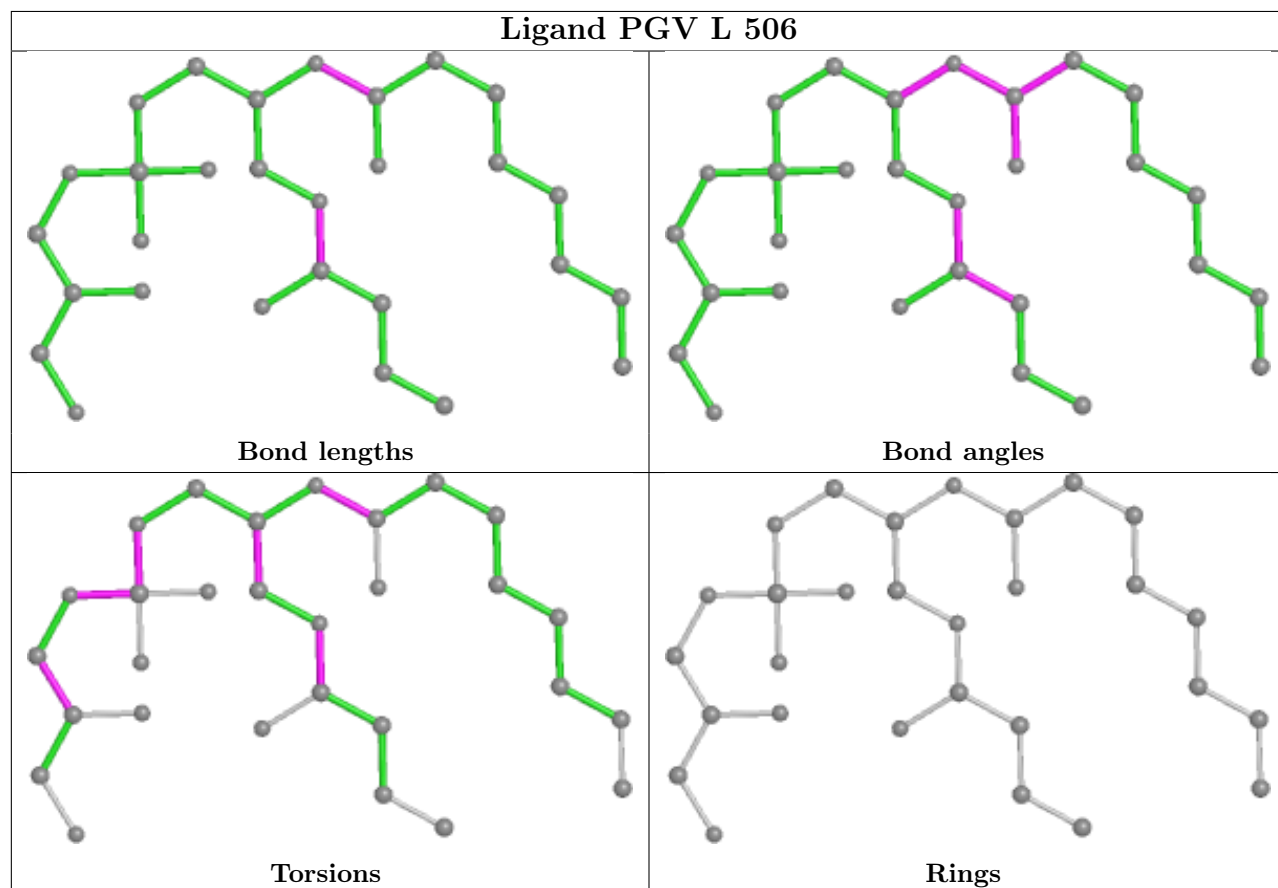
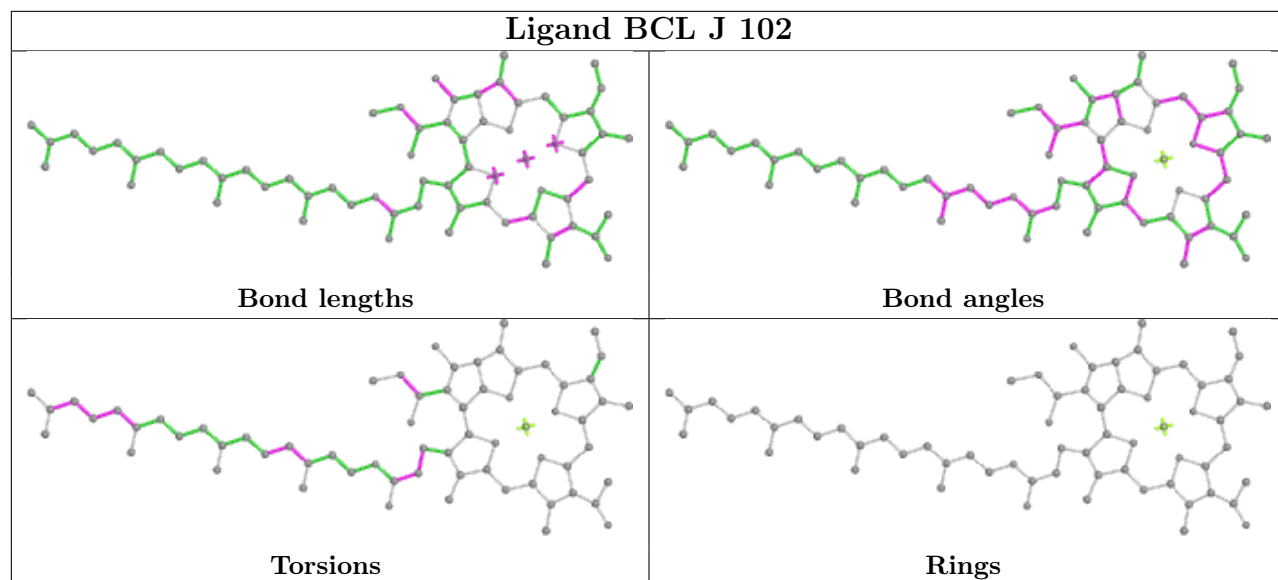


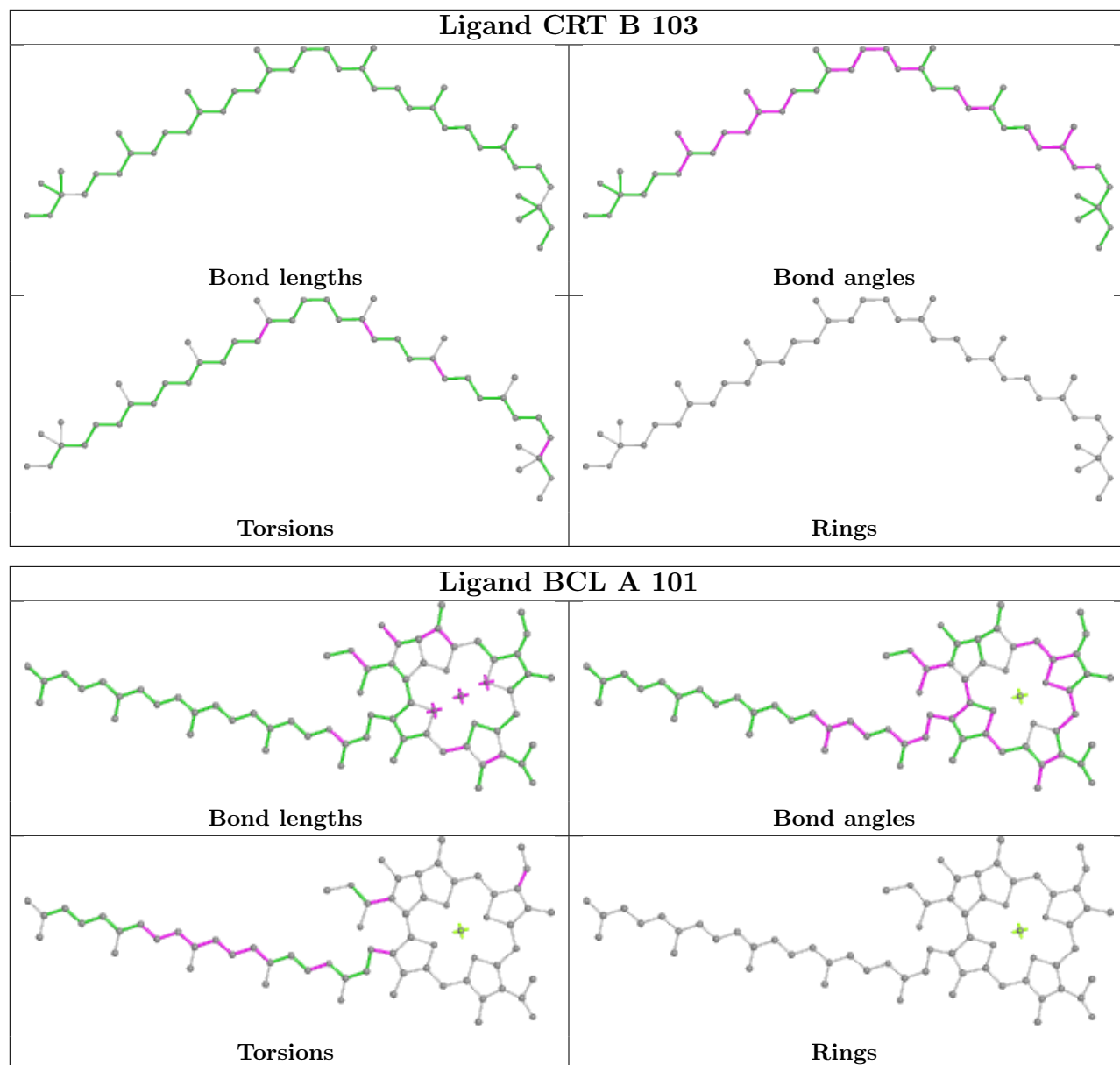


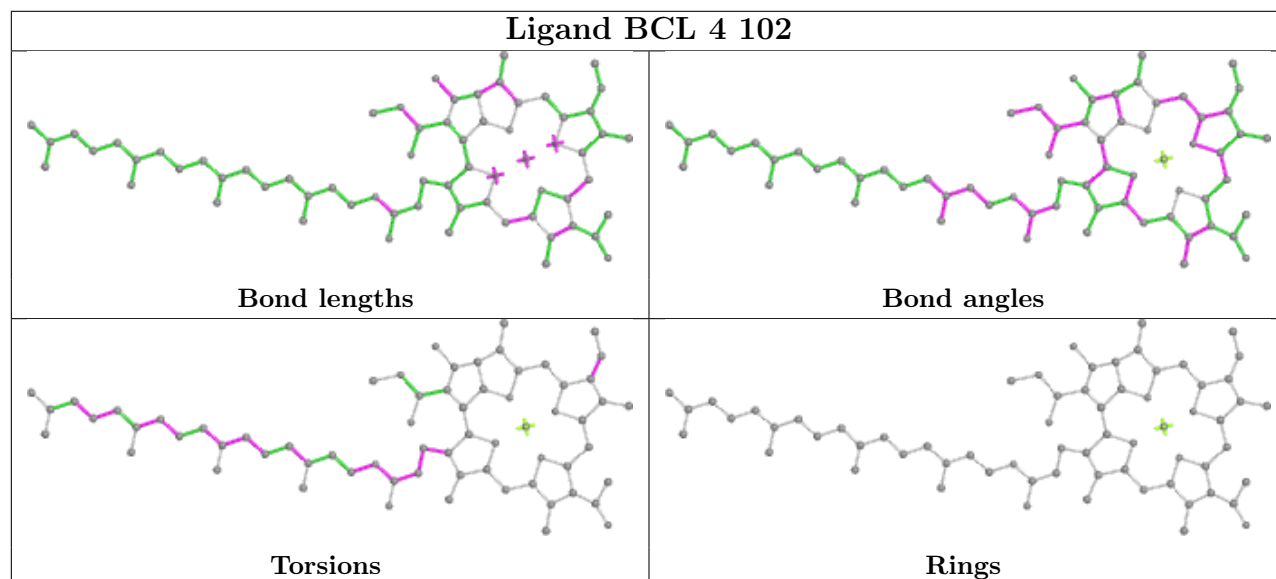
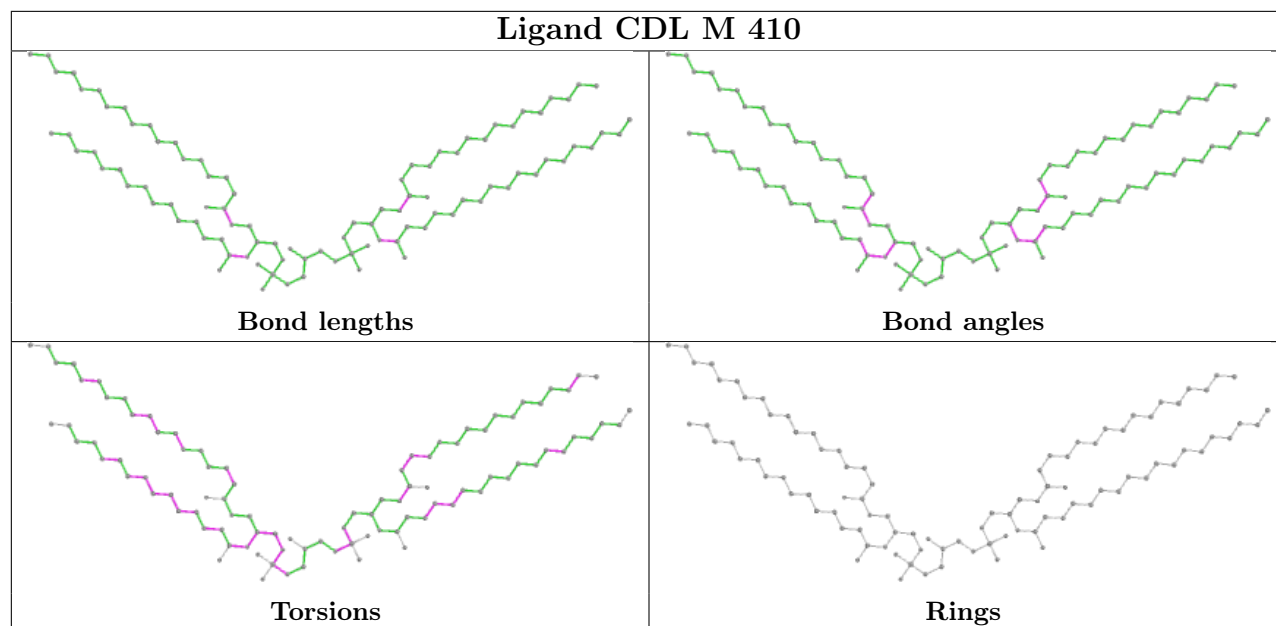


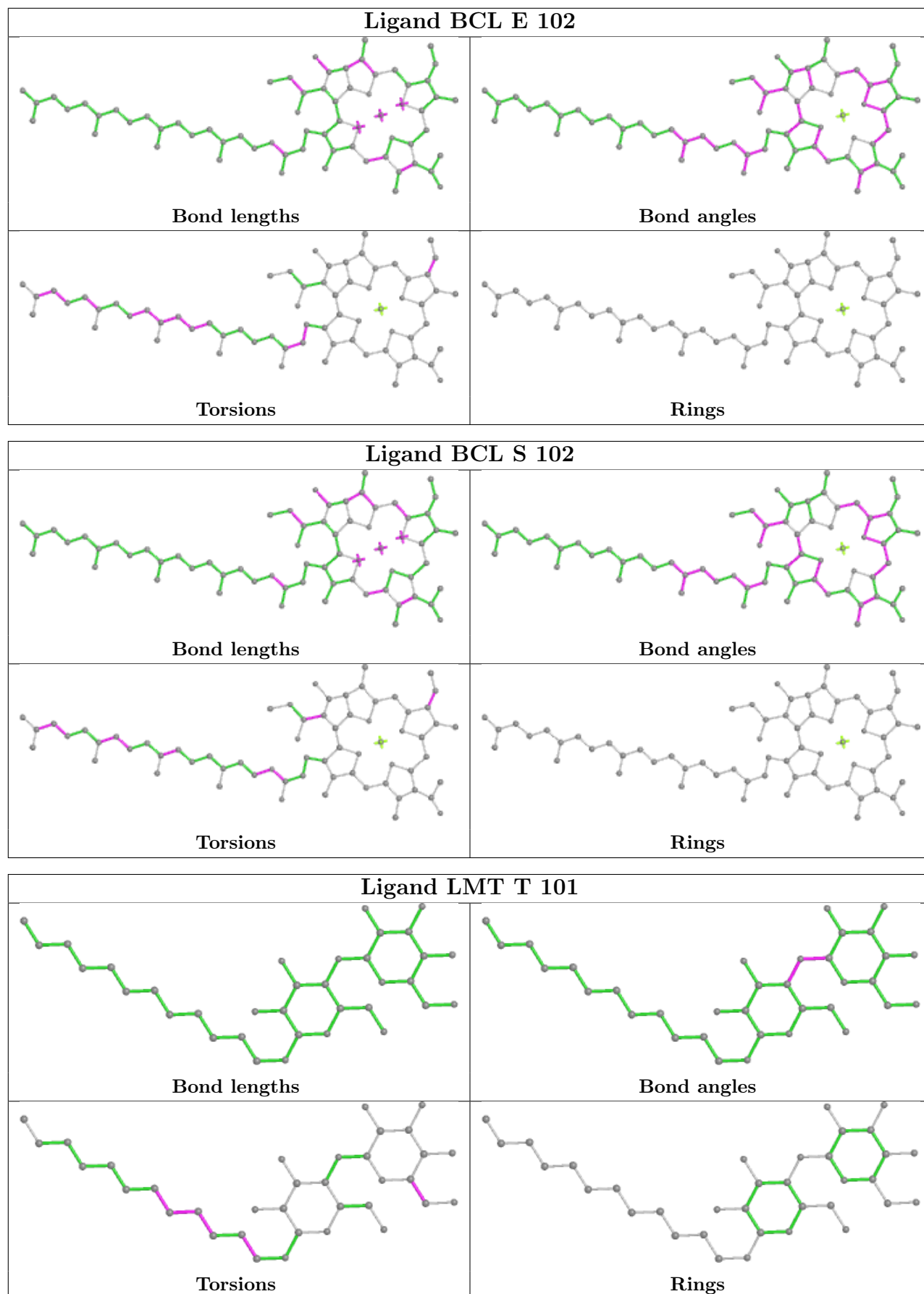


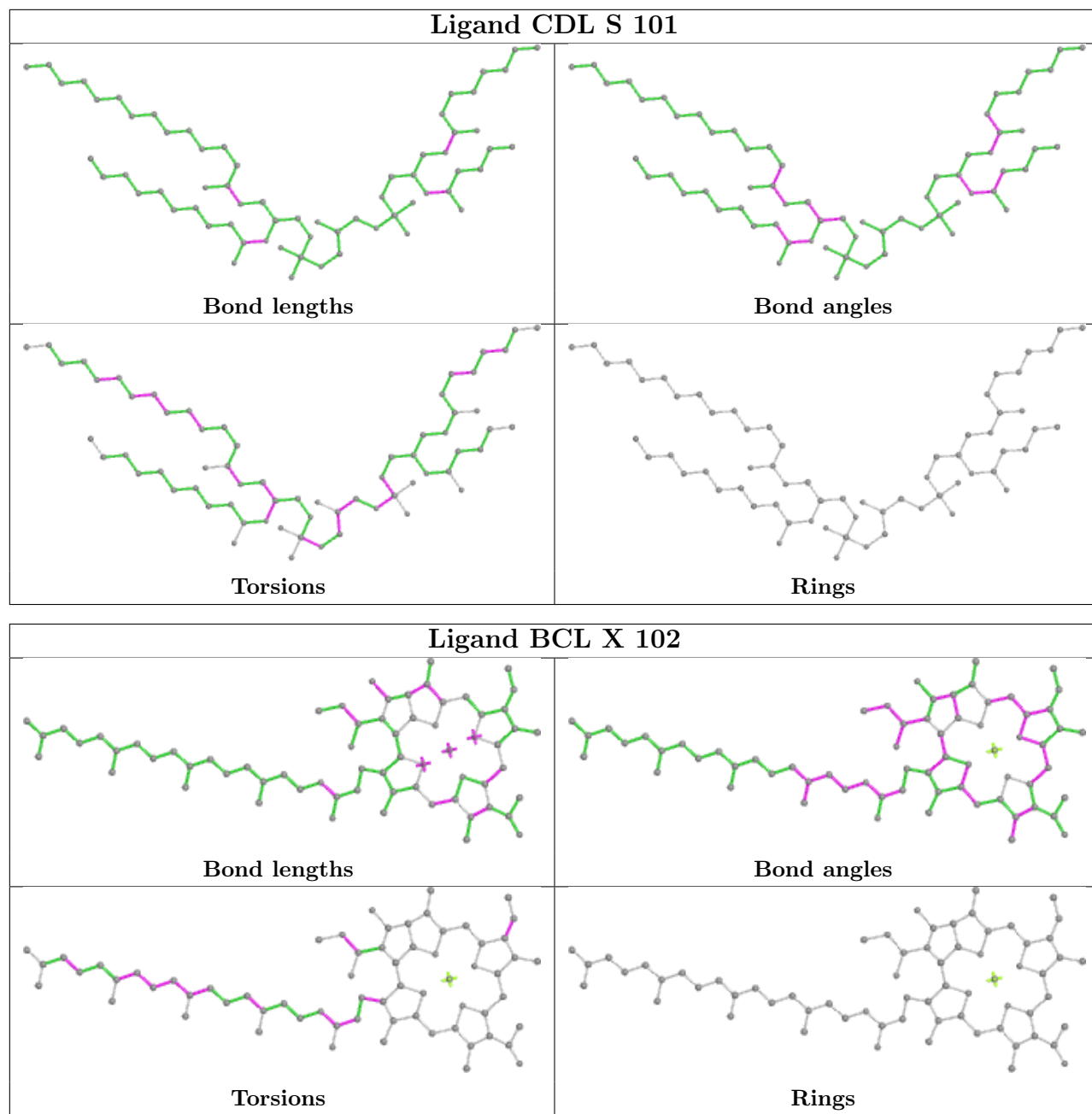


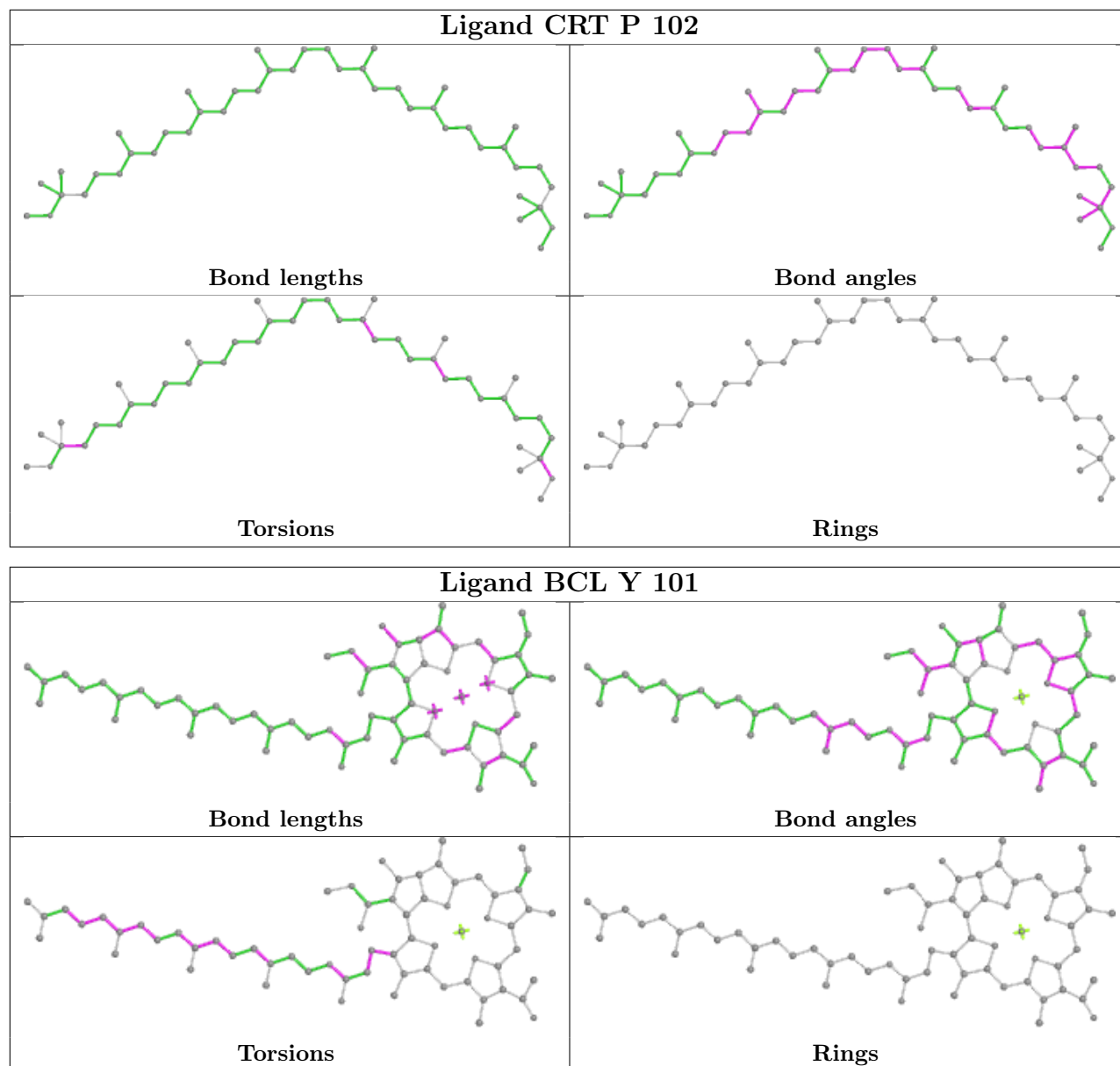


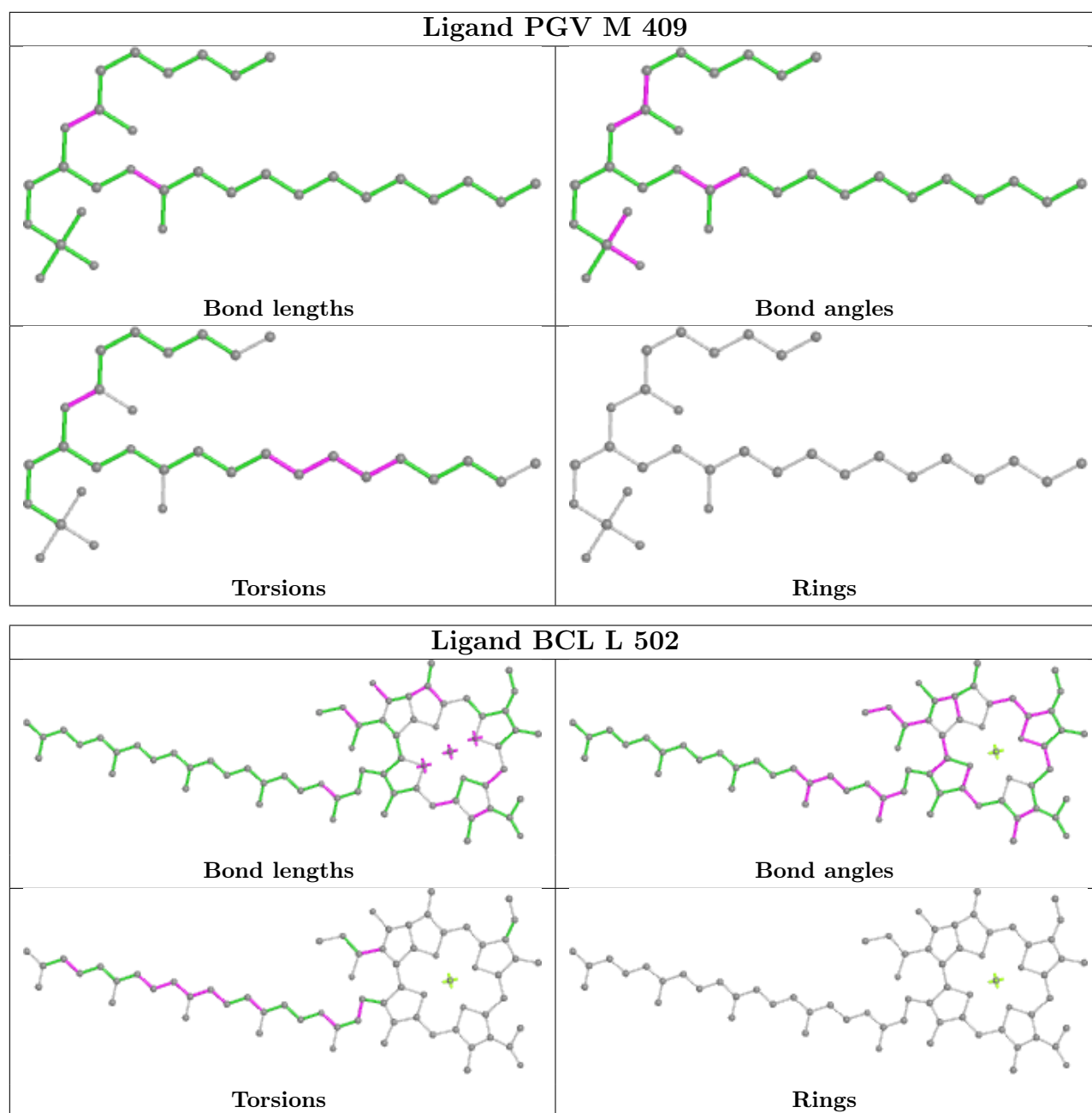












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

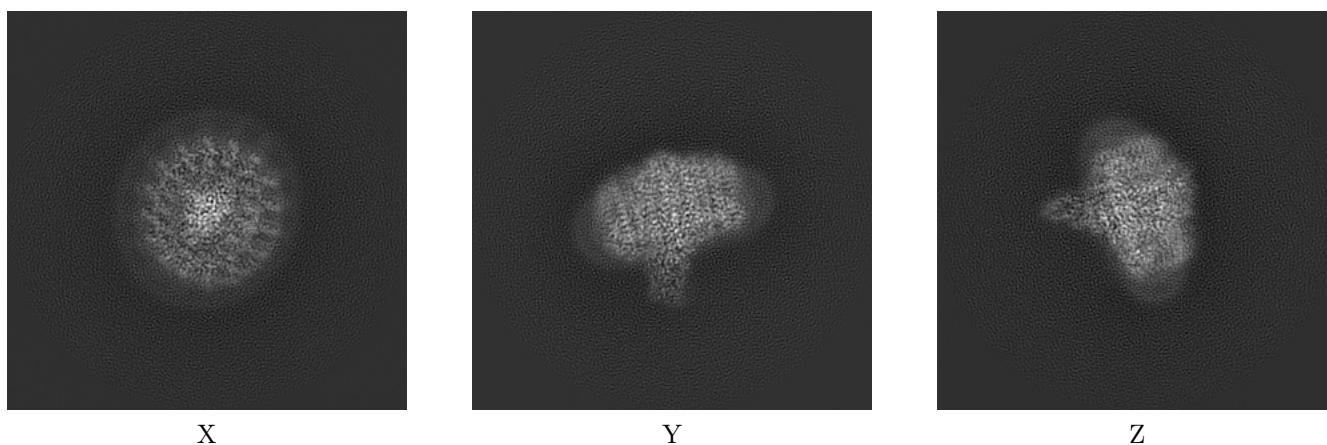
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32100. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

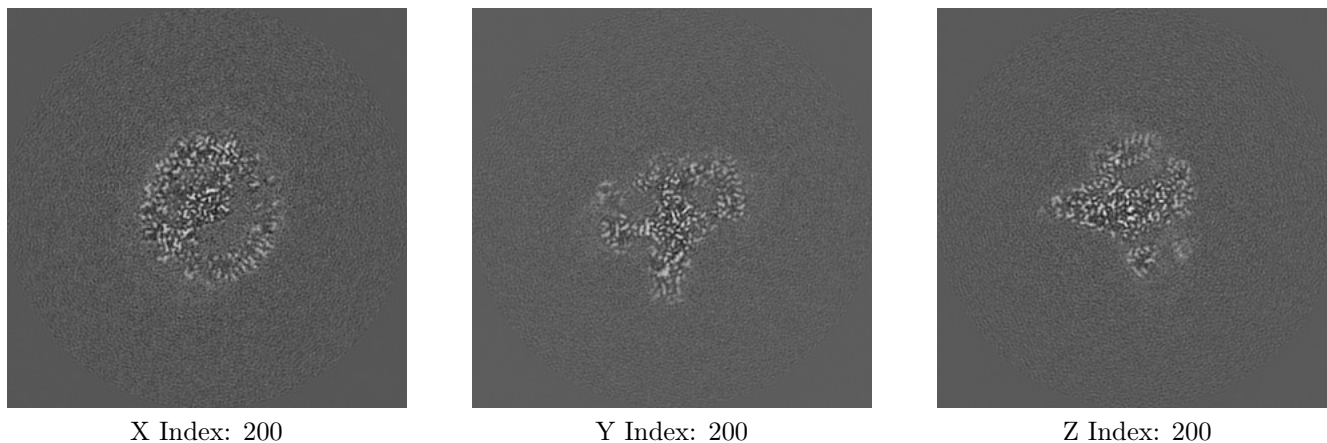
6.1.1 Primary map



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

6.2 Central slices [i](#)

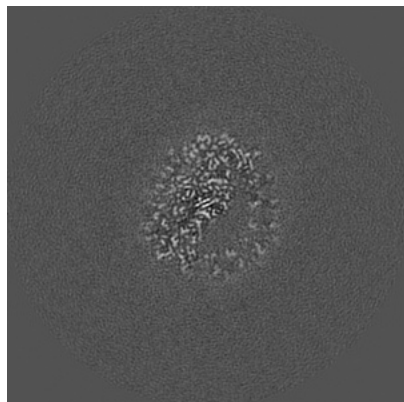
6.2.1 Primary map



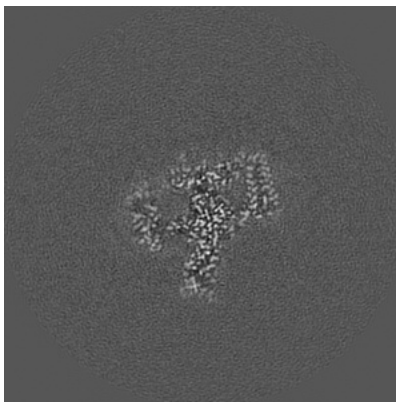
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

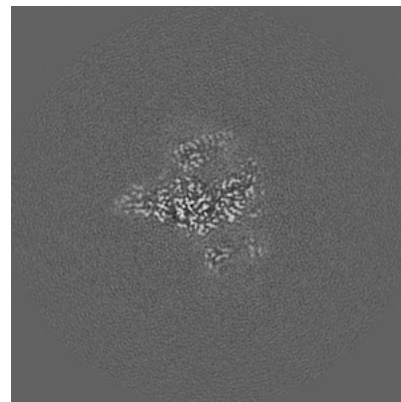
6.3.1 Primary map



X Index: 193



Y Index: 203

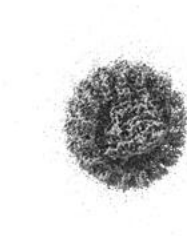


Z Index: 205

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0134. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

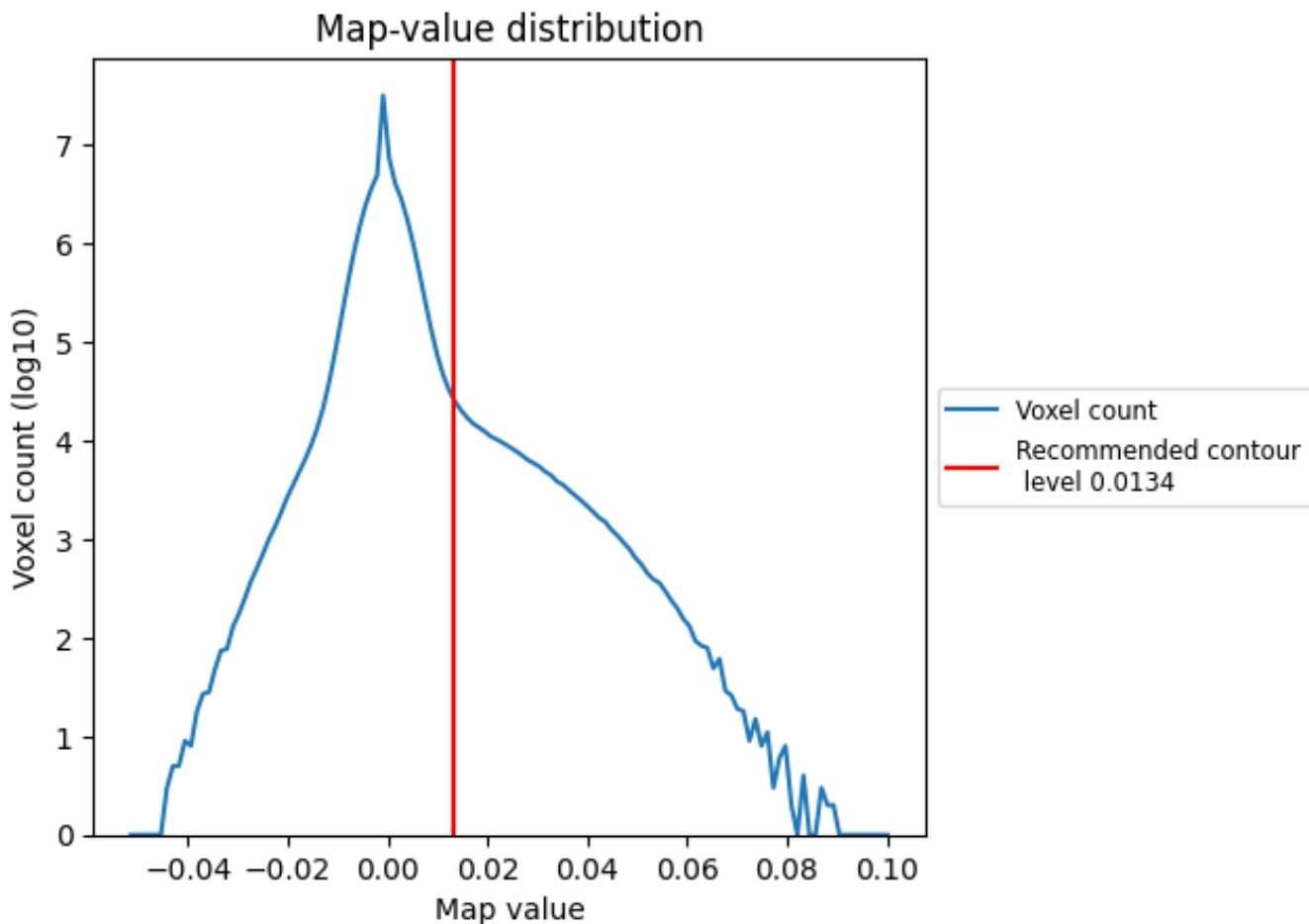
6.5 Mask visualisation

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

7 Map analysis [i](#)

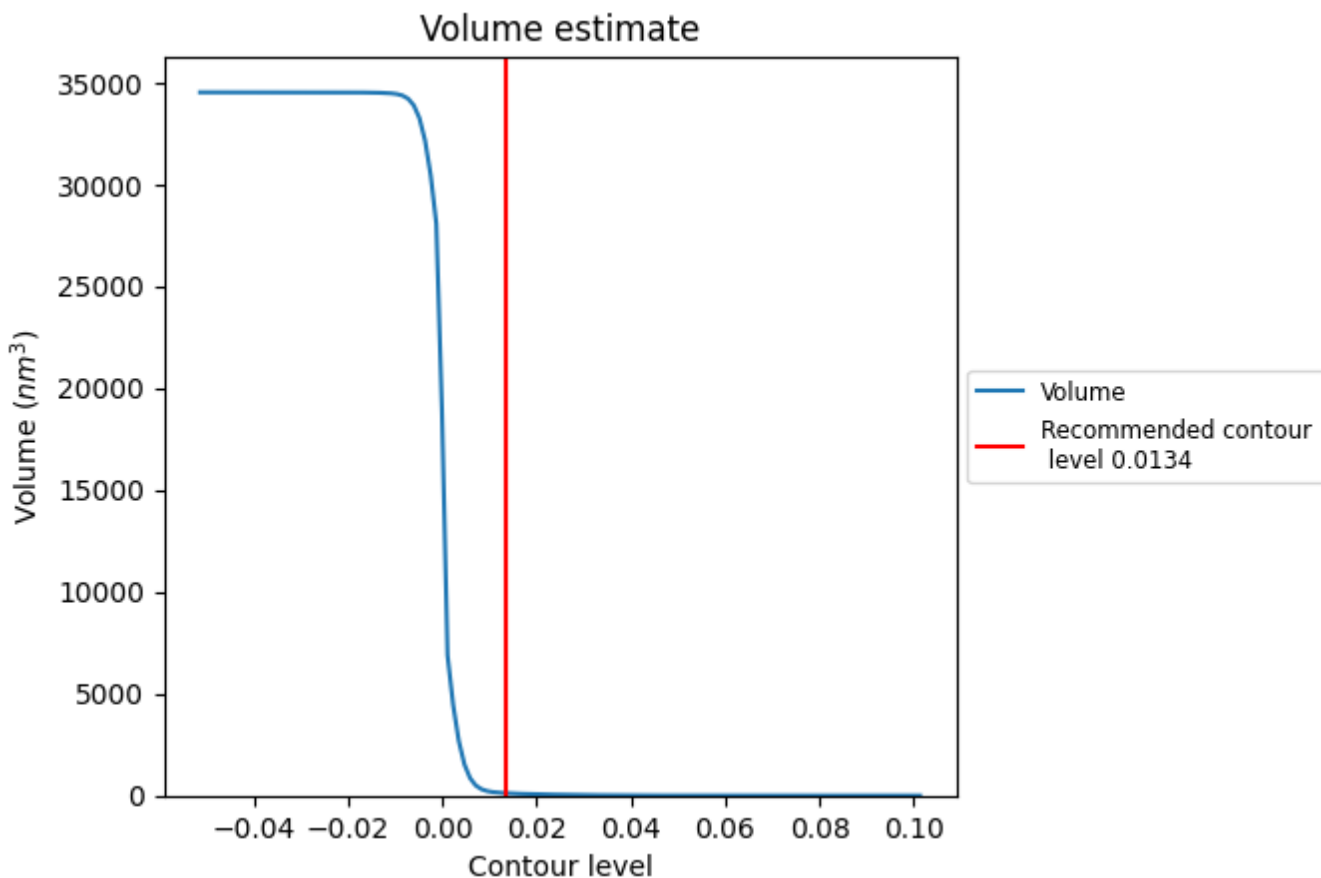
This section contains the results of statistical analysis of the map.

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.

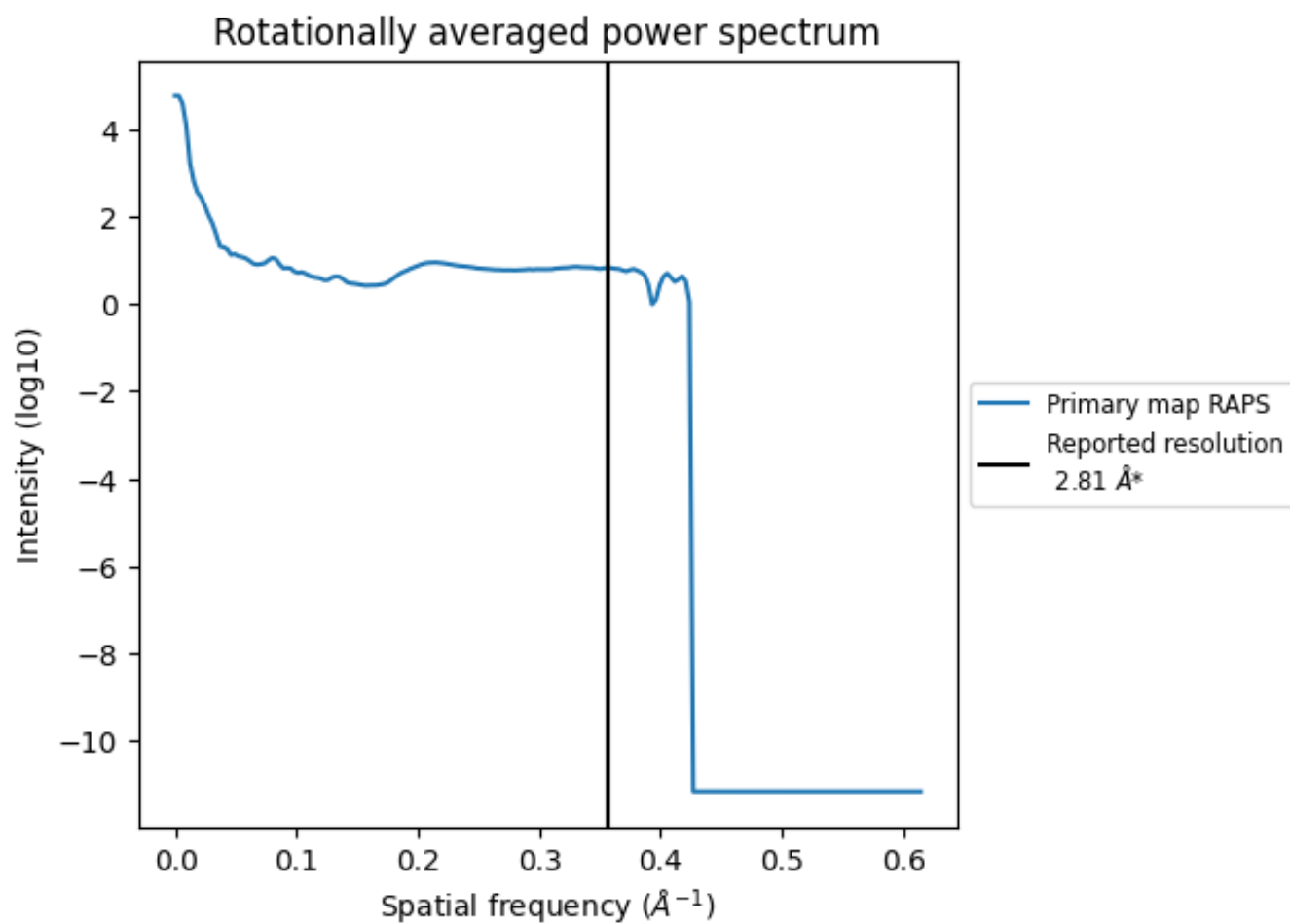
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 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 [\(i\)](#)

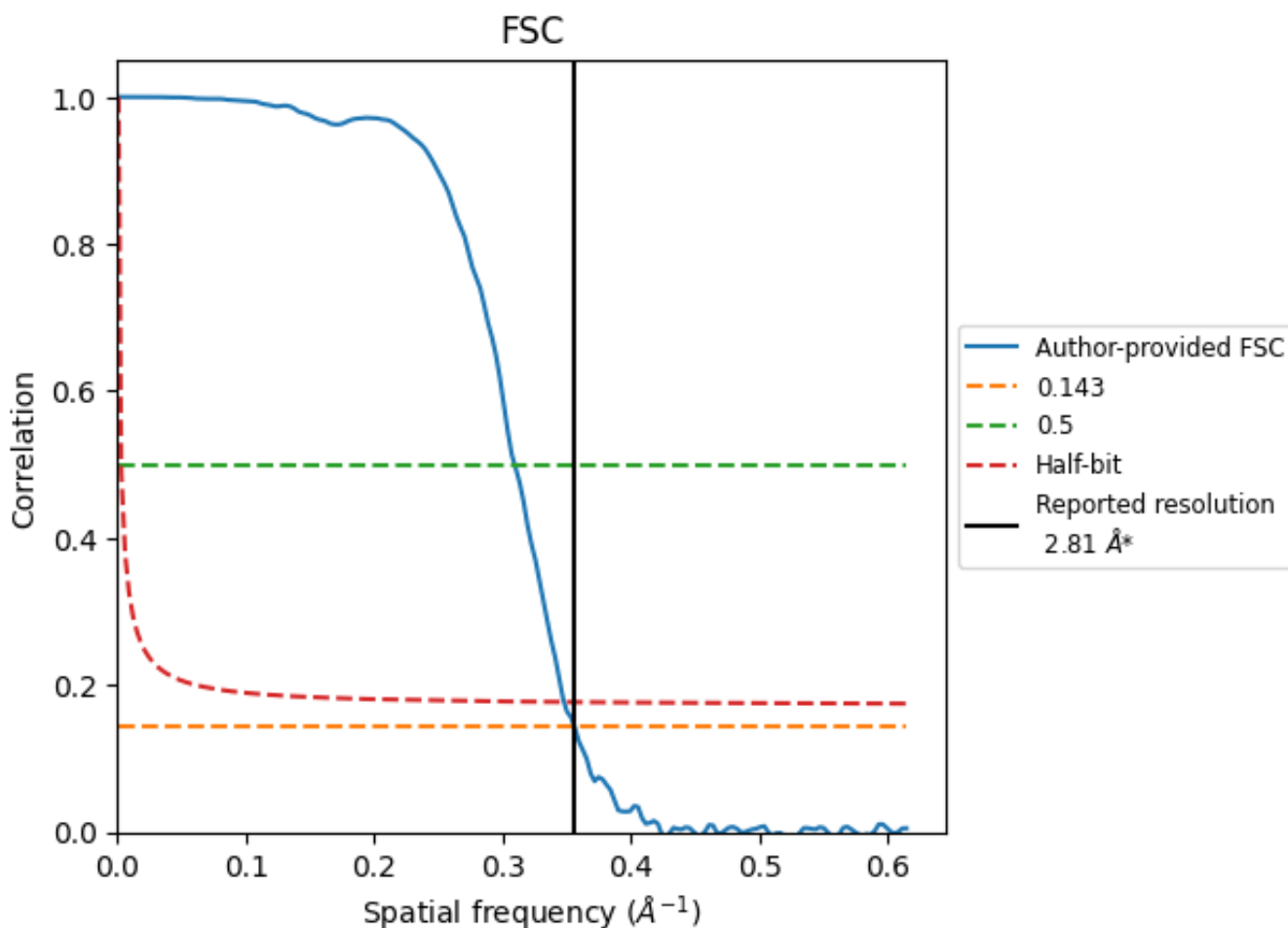


*Reported resolution corresponds to spatial frequency of 0.356\AA^{-1}

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 0.356 Å⁻¹

8.2 Resolution estimates [i](#)

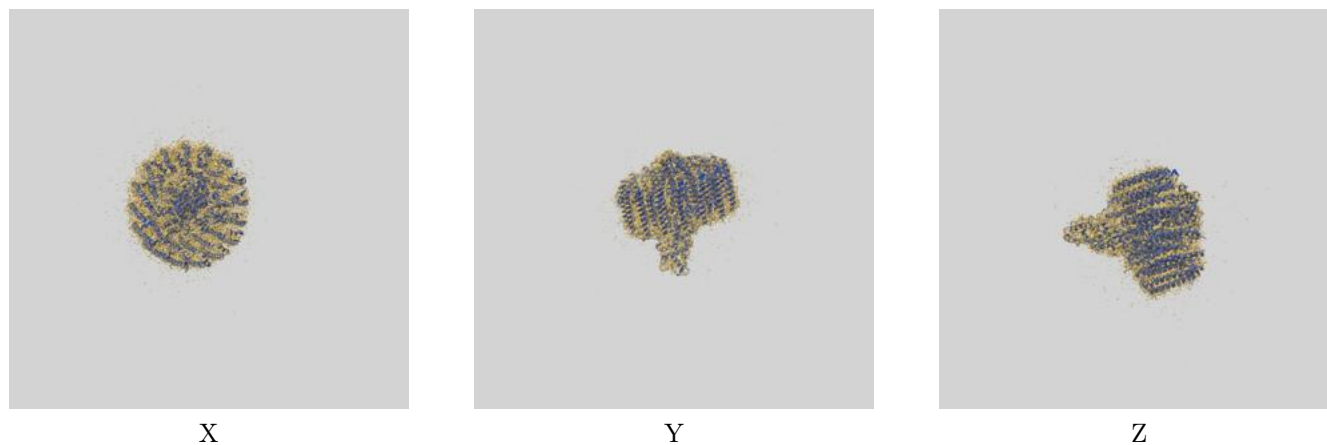
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.23	2.88
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

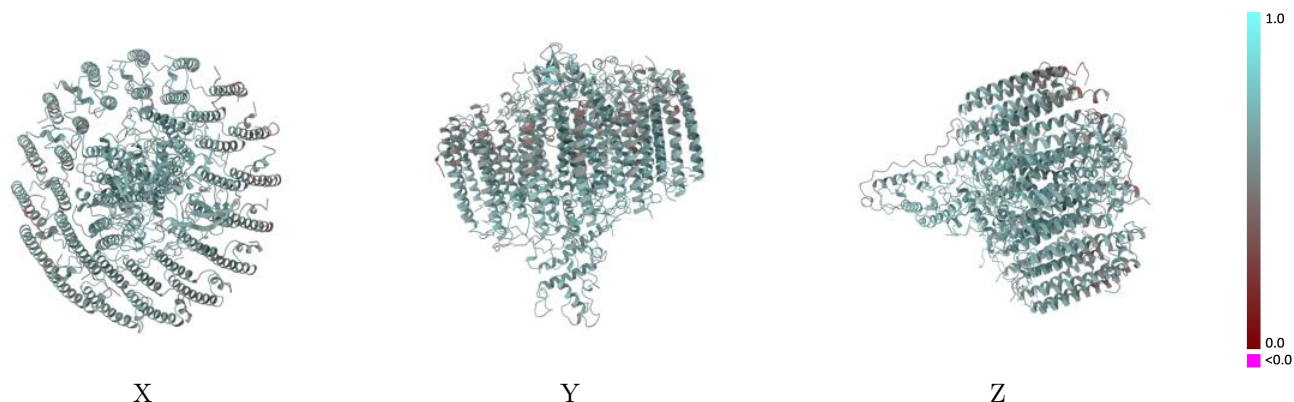
This section contains information regarding the fit between EMDB map EMD-32100 and PDB model 7VRJ. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



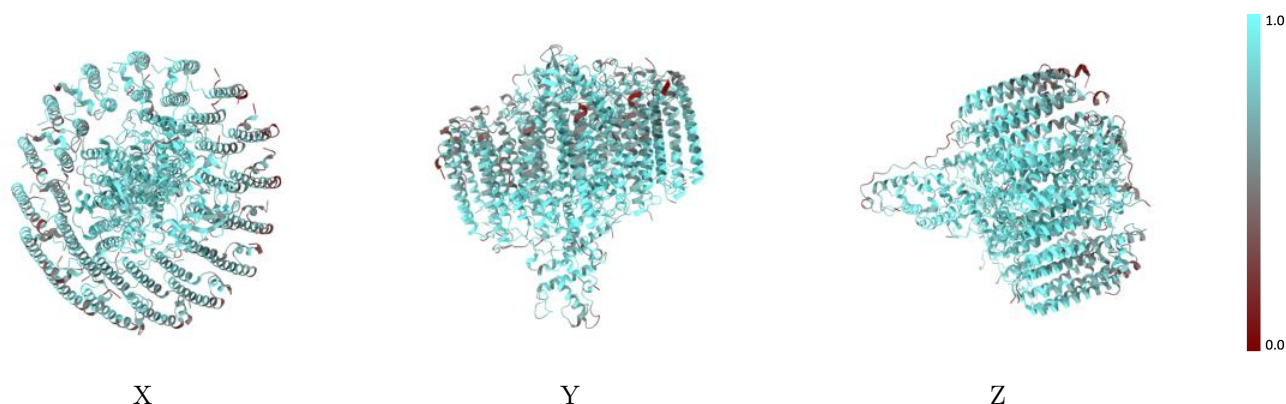
The images above show the 3D surface view of the map at the recommended contour level 0.0134 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



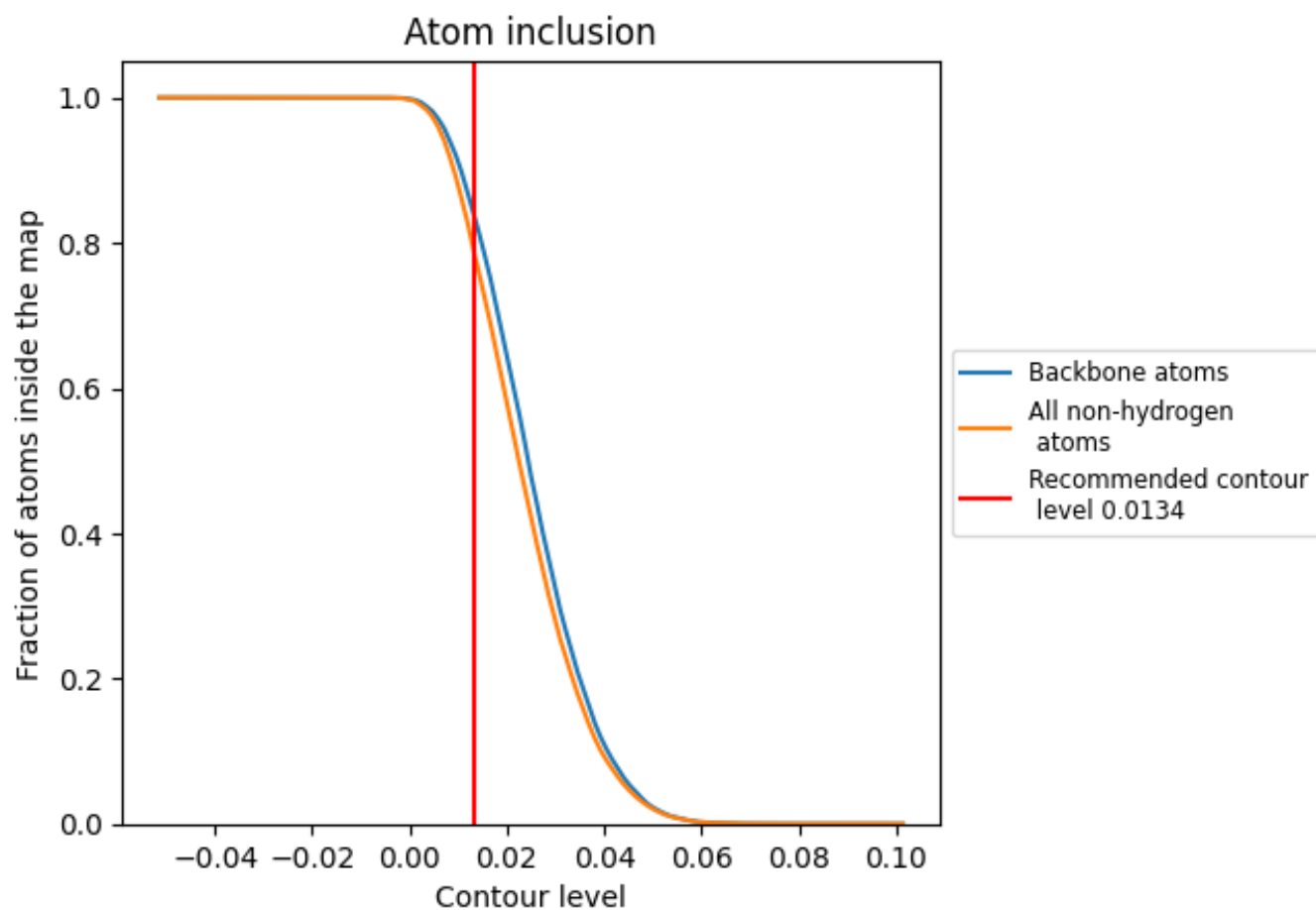
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0134).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.0134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7827	 0.6010
0	 0.7689	 0.5950
1	 0.6795	 0.5680
2	 0.6653	 0.5520
3	 0.6908	 0.5680
4	 0.5988	 0.5280
5	 0.6989	 0.5870
6	 0.6580	 0.5420
7	 0.7352	 0.5770
8	 0.6942	 0.5620
9	 0.8361	 0.6280
A	 0.8483	 0.6200
B	 0.7556	 0.5840
C	 0.8854	 0.6370
D	 0.7804	 0.6070
E	 0.7607	 0.5900
F	 0.7746	 0.5920
G	 0.7149	 0.5660
H	 0.7567	 0.5950
I	 0.6829	 0.5630
J	 0.6534	 0.5400
K	 0.6723	 0.5660
L	 0.8893	 0.6500
M	 0.8854	 0.6510
N	 0.6689	 0.5590
O	 0.7648	 0.5980
P	 0.6965	 0.5620
Q	 0.8026	 0.6110
R	 0.7523	 0.5790
S	 0.7192	 0.5810
T	 0.7341	 0.5790
U	 0.7754	 0.5870
V	 0.7045	 0.5640
W	 0.7397	 0.5890
X	 0.6983	 0.5650



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.6968	 0.5770
Z	 0.7028	 0.5600