



# wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 05:32 PM JST

PDB ID : 8WDU  
EMDB ID : EMD-37465  
Title : Photosynthetic LH1-RC complex from the purple sulfur bacterium *Allochro-  
matium vinosum* purified by sucrose density  
Authors : Tani, K.; Kanno, R.; Harada, A.; Kobayashi, A.; Minamino, A.; Nakamura,  
N.; Ji, X.-C.; Purba, E.R.; Hall, M.; Yu, L.-J.; Madigan, M.T.; Mizoguchi, A.;  
Iwasaki, K.; Humbel, B.M.; Kimura, Y.; Wang-Otomo, Z.-Y.  
Deposited on : 2023-09-16  
Resolution : 2.24 Å(reported)  
Based on initial model : 7VRJ

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

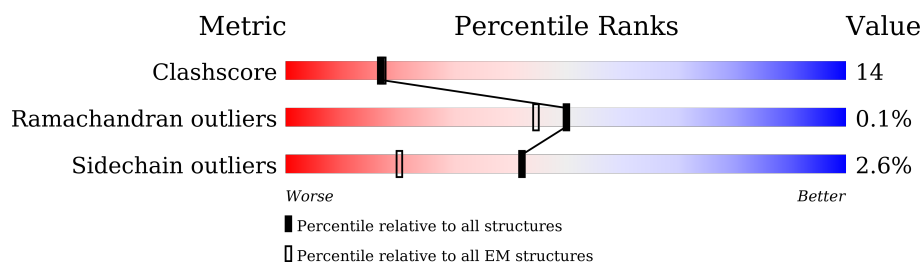
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















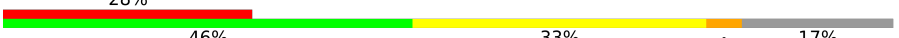











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	C	383	
2	L	278	
3	M	325	
4	H	259	
5	1	44	
5	5	44	
5	7	44	


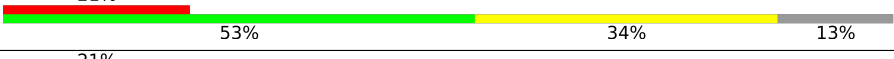

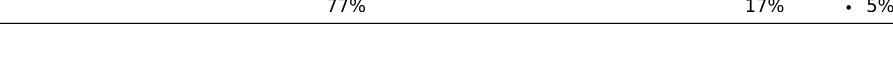
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Mol	Chain	Length	Quality of chain
5	9	44	
5	A	44	
5	I	44	
5	K	44	
5	O	44	
5	Q	44	
6	0	46	
6	2	46	
6	4	46	
6	6	46	
6	8	46	
6	B	46	
6	J	46	
6	N	46	
6	P	46	
6	R	46	
7	D	64	
7	F	64	
7	S	64	
7	U	64	
7	W	64	
7	Y	64	
8	E	47	
8	G	47	
8	T	47	

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Mol	Chain	Length	Quality of chain
8	V	47	
8	X	47	
8	Z	47	
9	3	66	

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 26274 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	311	Total	C	N	O	S	0	0
			2429	1535	418	460	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	277	Total	C	N	O	S	0	0
			2210	1489	354	357	10		

- 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
			2533	1702	405	414	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	259	Total	C	N	O	S	1	0
			1993	1281	339	366	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	I	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	K	44	Total	C	N	O	S	0	0
			366	251	59	55	1		
5	O	44	Total	C	N	O	S	0	0
			366	251	59	55	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	1	43	Total	C	N	O	S	0	0
			359	248	58	52	1		
5	5	43	Total	C	N	O	S	0	0
			355	245	57	52	1		
5	7	42	Total	C	N	O	S	1	0
			359	251	56	51	1		
5	9	43	Total	C	N	O	S	0	0
			359	248	58	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	44	Total	C	N	O	S	0	0
			359	238	58	61	2		
6	J	39	Total	C	N	O	S	0	0
			324	219	52	52	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	40	Total	C	N	O	S	0	0
			331	223	53	54	1		
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	41	Total	C	N	O	S	0	0
			339	228	54	55	2		
6	0	43	Total	C	N	O	S	0	0
			351	234	56	59	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	49	Total	C	N	O	S	0	0
			397	270	62	64	1		
7	F	49	Total	C	N	O	S	0	0
			397	270	62	64	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	50	Total	C	N	O	S	0	0
			402	273	63	65	1		
7	U	50	Total	C	N	O	S	1	0
			407	277	63	65	2		
7	W	50	Total	C	N	O	S	0	0
			402	273	63	65	1		
7	Y	59	Total	C	N	O	S	0	0
			470	317	76	76	1		

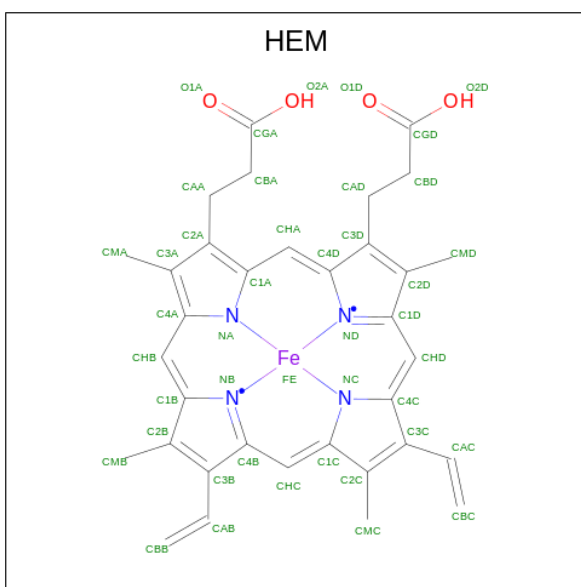
- Molecule 8 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	G	40	Total	C	N	O	S	0	0
			335	226	52	55	2		
8	T	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	V	40	Total	C	N	O	S	0	0
			335	226	52	55	2		
8	X	41	Total	C	N	O	S	0	0
			343	231	53	56	3		
8	Z	41	Total	C	N	O	S	0	0
			343	231	53	56	3		

- Molecule 9 is a protein called Antenna complex alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	63	Total	C	N	O	S	0	0
			498	337	78	80	3		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



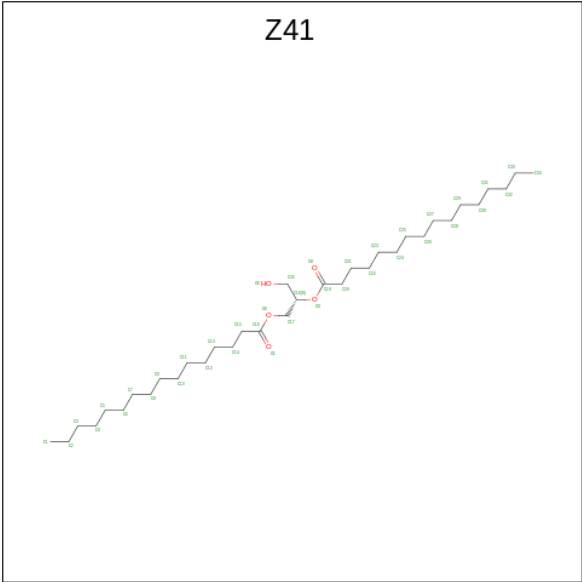
Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0

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

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

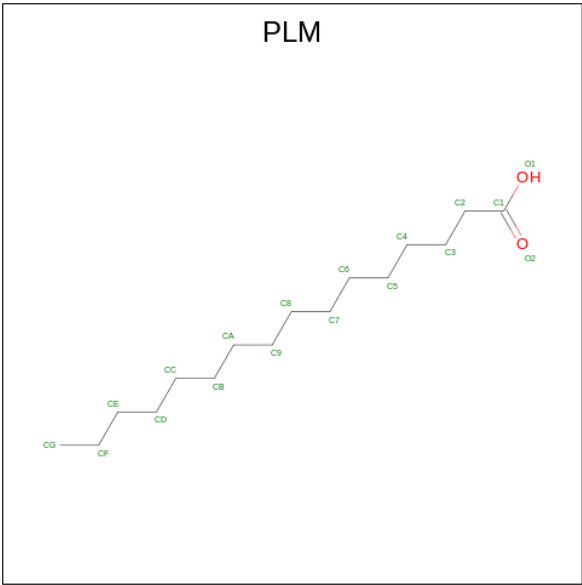
- Molecule 12 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (three-letter code: Z41) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>5</sub>).





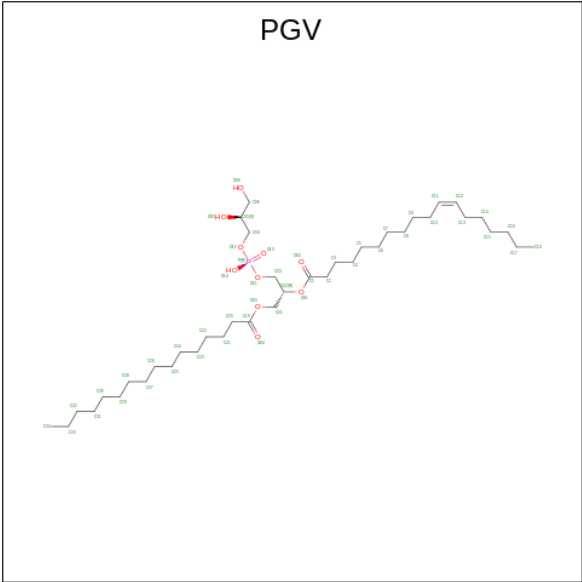
Mol	Chain	Residues	Atoms			AltConf
12	C	1	Total	C	O	0
			35	31	4	

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



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

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



Mol	Chain	Residues	Atoms				AltConf
14	C	1	Total	C	O	P	0
			31	20	10	1	
14	L	1	Total	C	O	P	0
			29	18	10	1	
14	L	1	Total	C	O	P	0
			35	24	10	1	
14	L	1	Total	C	O	P	0
			37	26	10	1	
14	M	1	Total	C	O	P	0
			27	18	8	1	
14	H	1	Total	C	O	P	0
			36	25	10	1	
14	A	1	Total	C	O	P	0
			39	28	10	1	
14	A	1	Total	C	O	P	0
			33	22	10	1	
14	F	1	Total	C	O	P	0
			31	22	8	1	
14	Q	1	Total	C	O	P	0
			24	15	8	1	
14	1	1	Total	C	O	P	0
			27	18	8	1	

- Molecule 15 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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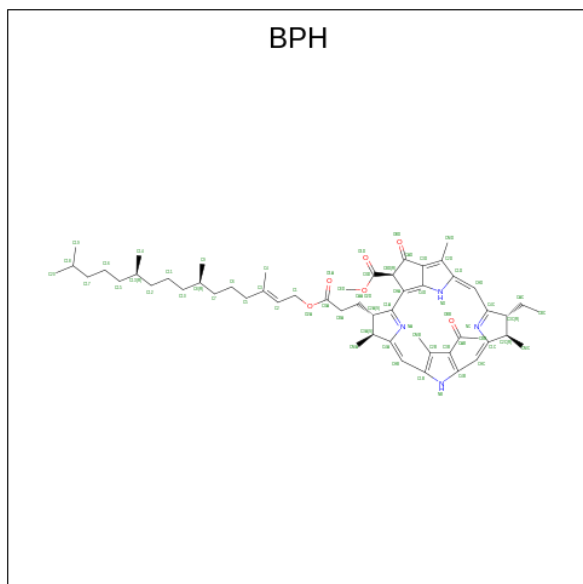
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
15	V	1	Total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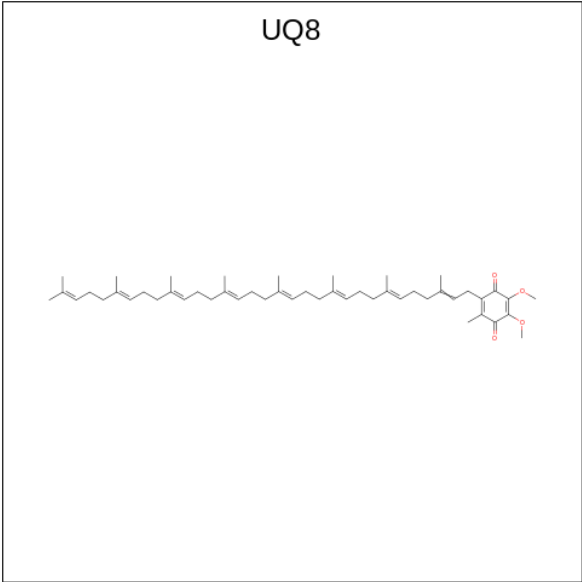
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
15	0	1	66	55	1	4	6	0

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



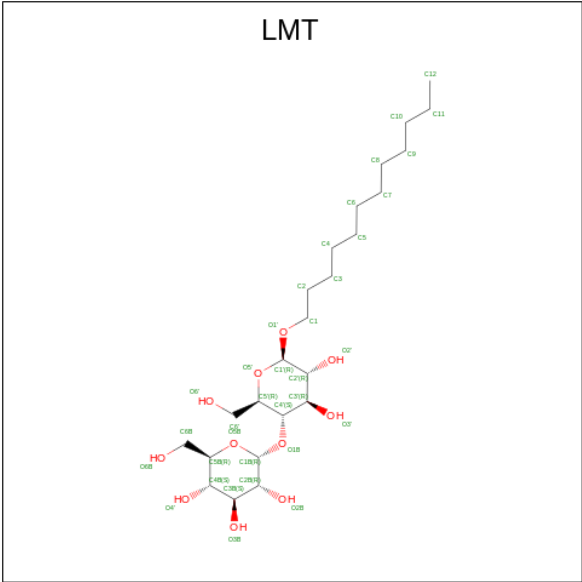
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
16	L	1	65	55	4	6	0
16	M	1	65	55	4	6	0

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



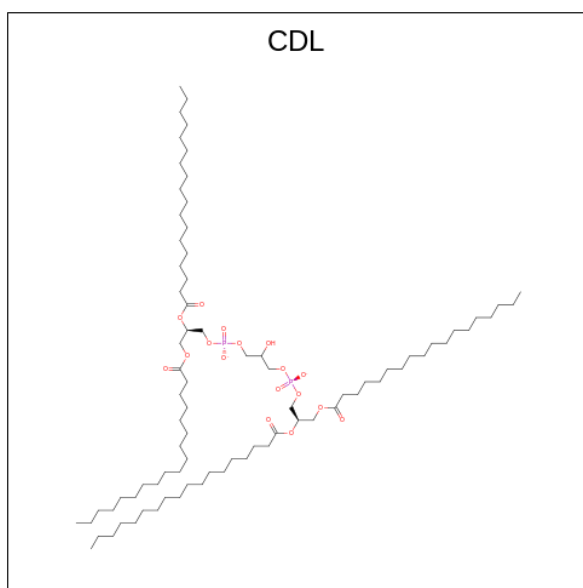
Mol	Chain	Residues	Atoms			AltConf
17	L	1	Total	C	O	0
			33	29	4	
17	L	1	Total	C	O	0
			53	49	4	
17	L	1	Total	C	O	0
			53	49	4	

- Molecule 18 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
18	L	1	Total	C	O	0
			35	24	11	
18	M	1	Total	C	O	0
			35	24	11	
18	M	1	Total	C	O	0
			24	13	11	
18	H	1	Total	C	O	0
			35	24	11	
18	B	1	Total	C	O	0
			35	24	11	
18	E	1	Total	C	O	0
			35	24	11	
18	G	1	Total	C	O	0
			35	24	11	
18	J	1	Total	C	O	0
			35	24	11	
18	J	1	Total	C	O	0
			35	24	11	
18	P	1	Total	C	O	0
			35	24	11	
18	P	1	Total	C	O	0
			35	24	11	
18	R	1	Total	C	O	0
			35	24	11	
18	S	1	Total	C	O	0
			26	15	11	
18	T	1	Total	C	O	0
			35	24	11	
18	X	1	Total	C	O	0
			35	24	11	
18	Z	1	Total	C	O	0
			35	24	11	
18	2	1	Total	C	O	0
			35	24	11	
18	4	1	Total	C	O	0
			35	24	11	
18	4	1	Total	C	O	0
			35	24	11	
18	5	1	Total	C	O	0
			31	20	11	
18	8	1	Total	C	O	0
			35	24	11	
18	8	1	Total	C	O	0
			35	24	11	

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



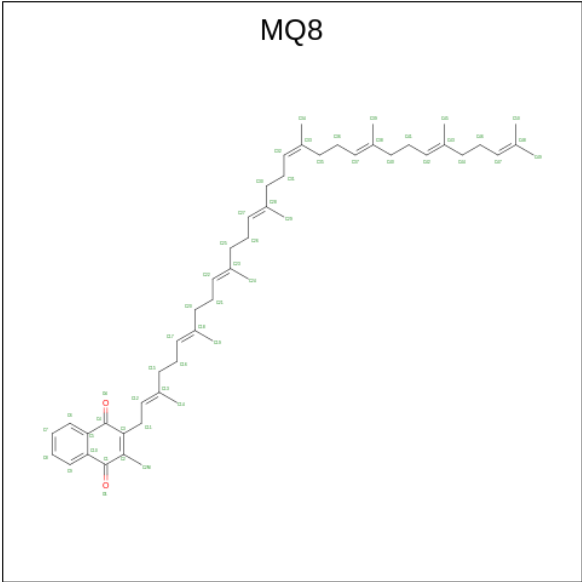
Mol	Chain	Residues	Atoms				AltConf
19	L	1	Total	C	O	P	0
			80	61	17	2	
19	M	1	Total	C	O	P	0
			39	21	16	2	
19	M	1	Total	C	O	P	0
			95	76	17	2	
19	H	1	Total	C	O	P	0
			79	60	17	2	
19	D	1	Total	C	O	P	0
			58	39	17	2	

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

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

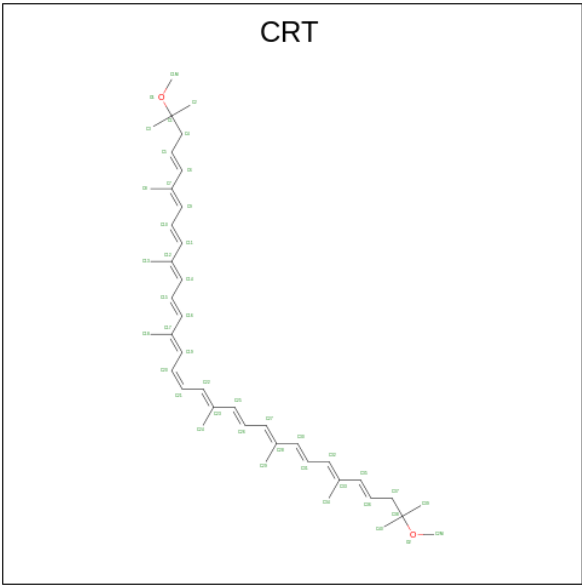
- Molecule 21 is MENAQUINONE 8 (three-letter code: MQ8) (formula:  $C_{51}H_{72}O_2$ ).





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

- Molecule 22 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
22	M	1	Total	C	O	0
			44	42	2	
22	B	1	Total	C	O	0
			44	42	2	
22	E	1	Total	C	O	0
			44	42	2	

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Mol	Chain	Residues	Atoms			AltConf
22	G	1	Total 44	C 42	O 2	0
22	J	1	Total 44	C 42	O 2	0
22	N	1	Total 44	C 42	O 2	0
22	P	1	Total 44	C 42	O 2	0
22	R	1	Total 44	C 42	O 2	0
22	T	1	Total 44	C 42	O 2	0
22	V	1	Total 44	C 42	O 2	0
22	Y	1	Total 44	C 42	O 2	0
22	Z	1	Total 44	C 42	O 2	0
22	2	1	Total 44	C 42	O 2	0
22	4	1	Total 44	C 42	O 2	0
22	6	1	Total 44	C 42	O 2	0
22	9	1	Total 44	C 42	O 2	0
22	0	1	Total 44	C 42	O 2	0

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

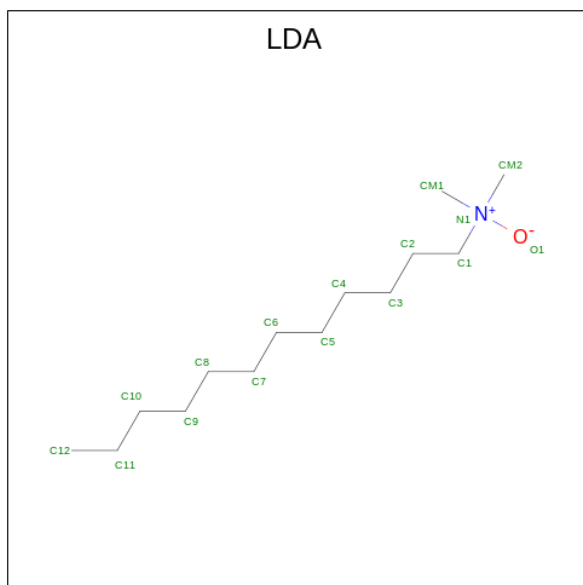
Mol	Chain	Residues	Atoms		AltConf
23	D	1	Total 1	Ca 1	0
23	F	1	Total 1	Ca 1	0
23	S	1	Total 1	Ca 1	0
23	U	1	Total 1	Ca 1	0
23	W	1	Total 1	Ca 1	0

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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	119	Total	O	0
			119	119	
25	L	50	Total	O	0
			50	50	
25	M	77	Total	O	0
			77	77	
25	H	19	Total	O	0
			19	19	
25	A	2	Total	O	0
			2	2	
25	B	1	Total	O	0
			1	1	

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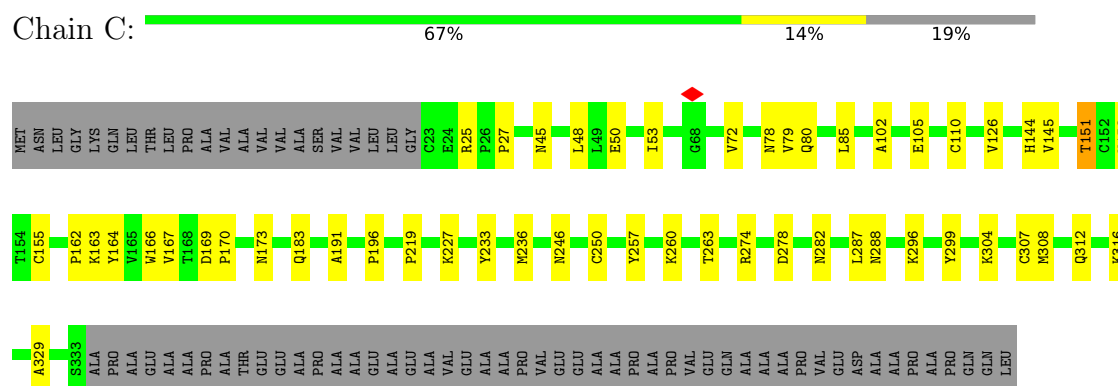
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Mol	Chain	Residues	Atoms		AltConf
25	D	4	Total 4	O 4	0
25	E	2	Total 2	O 2	0
25	F	2	Total 2	O 2	0
25	I	2	Total 2	O 2	0
25	K	1	Total 1	O 1	0
25	O	1	Total 1	O 1	0
25	P	1	Total 1	O 1	0
25	Q	2	Total 2	O 2	0
25	R	1	Total 1	O 1	0
25	S	5	Total 5	O 5	0
25	T	3	Total 3	O 3	0
25	U	10	Total 10	O 10	0
25	V	3	Total 3	O 3	0
25	W	7	Total 7	O 7	0
25	X	1	Total 1	O 1	0
25	Y	5	Total 5	O 5	0
25	1	1	Total 1	O 1	0
25	3	10	Total 10	O 10	0
25	7	1	Total 1	O 1	0
25	9	4	Total 4	O 4	0

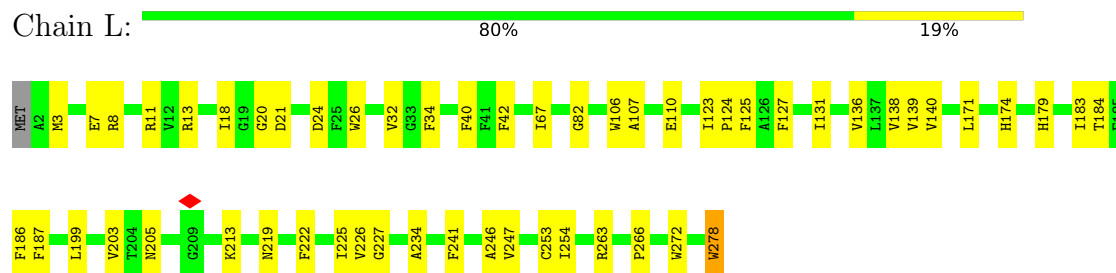
### 3 Residue-property plots

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

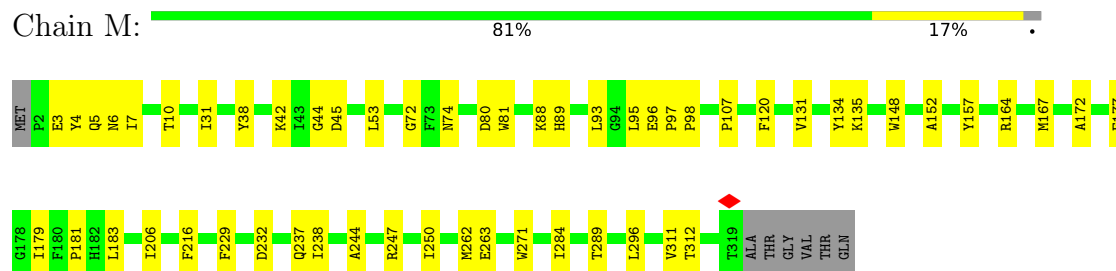
- Molecule 1: Photosynthetic reaction center cytochrome c subunit




- Molecule 2: Reaction center protein L chain

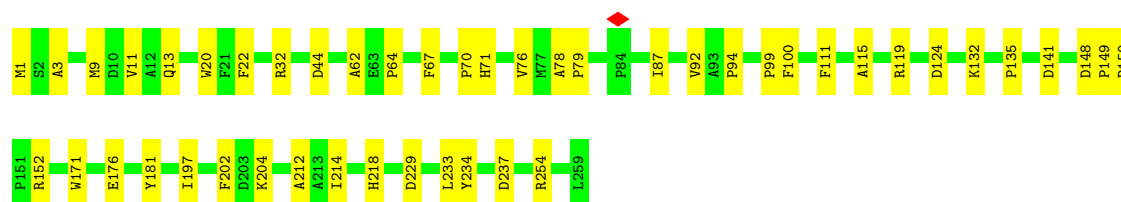


- Molecule 3: Reaction center protein M chain




- Molecule 4: Photosynthetic reaction center H subunit

Chain H:  82% 18%



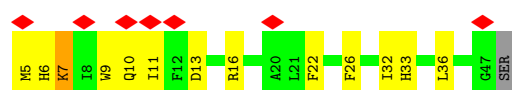
- Molecule 5: Antenna complex alpha/beta subunit

Chain A:  80% 18%




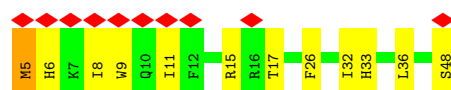
- Molecule 5: Antenna complex alpha/beta subunit

Chain I:  16% 68% 27%



- Molecule 5: Antenna complex alpha/beta subunit

Chain K:  23% 73% 25%



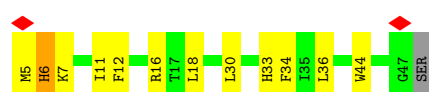
- Molecule 5: Antenna complex alpha/beta subunit

Chain O:  9% 70% 30%



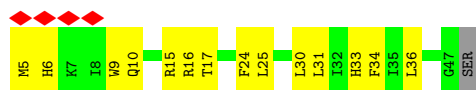
- Molecule 5: Antenna complex alpha/beta subunit

Chain Q:  5% 70% 25%

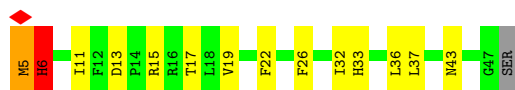


- Molecule 5: Antenna complex alpha/beta subunit

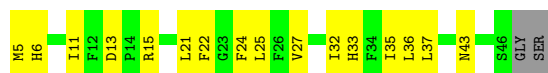
Chain 1:  9% 66% 32%



- Molecule 5: Antenna complex alpha/beta subunit



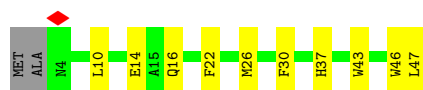
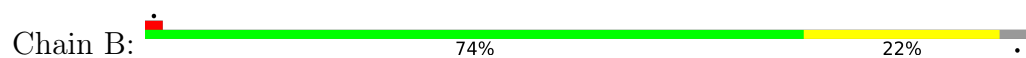
- Molecule 5: Antenna complex alpha/beta subunit



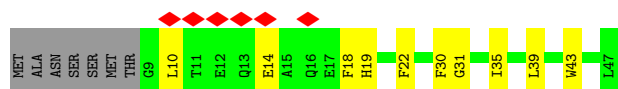
- Molecule 5: Antenna complex alpha/beta subunit



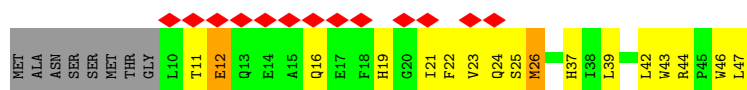
- Molecule 6: Antenna complex alpha/beta subunit



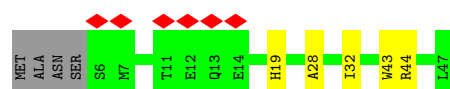
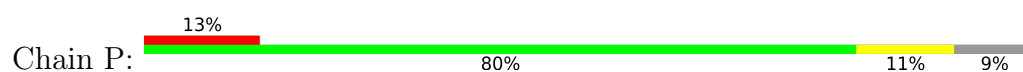
- Molecule 6: Antenna complex alpha/beta subunit



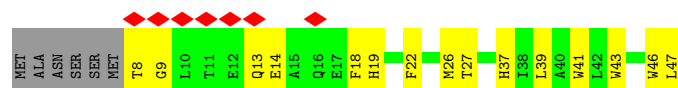
- Molecule 6: Antenna complex alpha/beta subunit



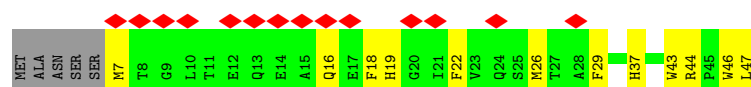
- Molecule 6: Antenna complex alpha/beta subunit



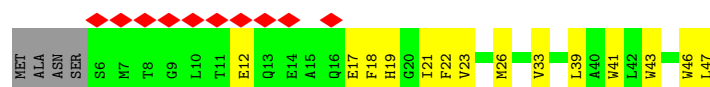
- Molecule 6: Antenna complex alpha/beta subunit



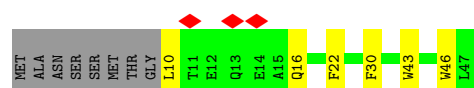
- Molecule 6: Antenna complex alpha/beta subunit



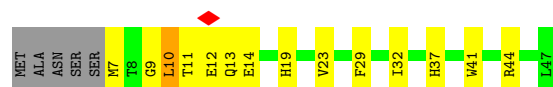
- Molecule 6: Antenna complex alpha/beta subunit



- Molecule 6: Antenna complex alpha/beta subunit



- Molecule 6: Antenna complex alpha/beta subunit

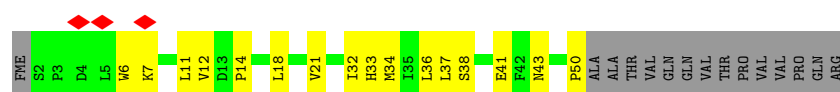


- Molecule 6: Antenna complex alpha/beta subunit

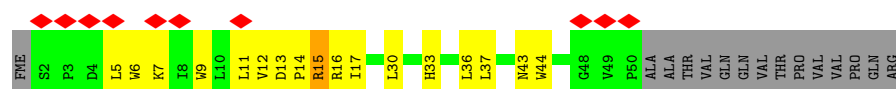




- Molecule 7: Antenna complex alpha/beta subunit



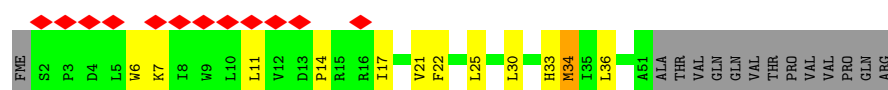
- Molecule 7: Antenna complex alpha/beta subunit



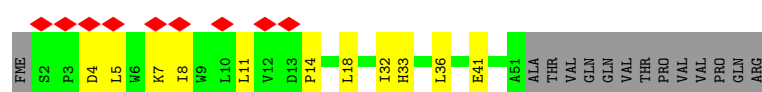
- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit



- Molecule 7: Antenna complex alpha/beta subunit

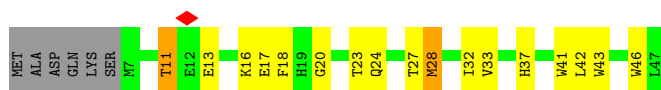


- Molecule 7: Antenna complex alpha/beta subunit

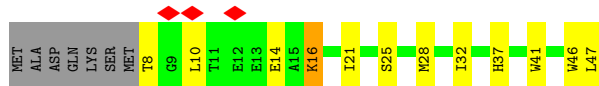


- Molecule 8: Antenna complex alpha/beta subunit

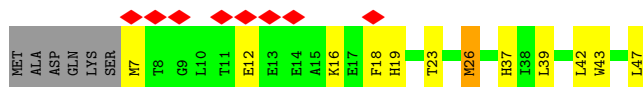




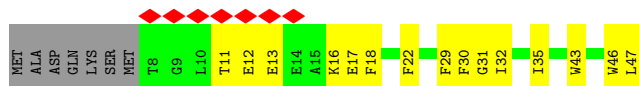
- Molecule 8: Antenna complex alpha/beta subunit



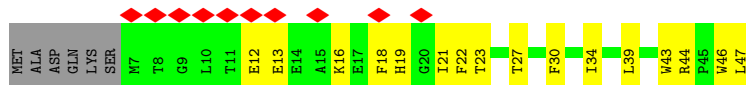
- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit



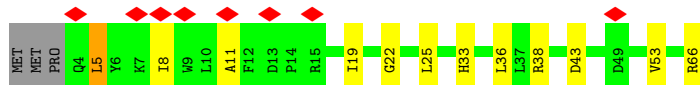
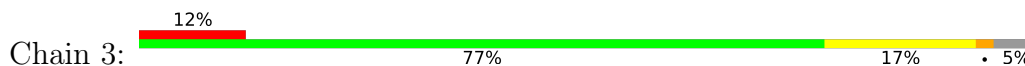
- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 8: Antenna complex alpha/beta subunit



- Molecule 9: Antenna complex alpha/beta subunit



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252230	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size ( $\text{\AA}$ )	290.88, 290.88, 290.88	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.606, 0.606, 0.606	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: FME, CA, BCL, FE, HEM, BPH, PLM, CDL, CRT, LDA, PGV, Z41, MQ8, MG, LMT, 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	0.29	0/2502	0.47	0/3426
2	L	0.29	0/2295	0.45	0/3135
3	M	0.28	0/2632	0.45	0/3601
4	H	0.28	0/2039	0.49	0/2776
5	1	0.25	0/362	0.46	0/492
5	5	0.25	0/358	0.41	0/488
5	7	0.28	0/366	0.45	0/499
5	9	0.27	0/362	0.44	0/492
5	A	0.27	0/362	0.40	0/492
5	I	0.27	0/362	0.44	0/492
5	K	0.25	0/369	0.44	0/500
5	O	0.27	0/369	0.42	0/500
5	Q	0.26	0/362	0.41	0/492
6	0	0.25	0/363	0.39	0/493
6	2	0.24	0/351	0.43	0/477
6	4	0.24	0/357	0.38	0/485
6	6	0.23	0/332	0.35	0/452
6	8	0.25	0/351	0.39	0/477
6	B	0.23	0/371	0.38	0/504
6	J	0.26	0/336	0.39	0/457
6	N	0.24	0/332	0.39	0/452
6	P	0.24	0/357	0.35	0/485
6	R	0.25	0/343	0.41	0/467
7	D	0.25	0/409	0.46	0/561
7	F	0.25	0/409	0.49	0/561
7	S	0.24	0/414	0.46	0/568
7	U	0.24	0/422	0.44	0/578
7	W	0.22	0/414	0.44	0/568
7	Y	0.47	1/483 (0.2%)	0.87	3/663 (0.5%)
8	E	0.26	0/355	0.42	0/480
8	G	0.25	0/347	0.39	0/470
8	T	0.25	0/355	0.41	0/480

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	V	0.24	0/347	0.39	0/470
8	X	0.25	0/355	0.39	0/480
8	Z	0.25	0/355	0.42	0/480
9	3	0.30	0/515	0.55	0/700
All	All	0.27	1/21413 (0.0%)	0.46	3/29193 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	59	PRO	CG-CD	-8.08	1.24	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Y	59	PRO	N-CD-CG	-12.55	84.37	103.20
7	Y	59	PRO	CA-CB-CG	-9.03	86.85	104.00
7	Y	14	PRO	CA-N-CD	-5.20	104.23	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2429	0	2327	55	0
2	L	2210	0	2166	48	0
3	M	2533	0	2490	49	0
4	H	1993	0	1994	35	0
5	1	359	0	371	10	0
5	5	355	0	360	15	0
5	7	359	0	366	19	0
5	9	359	0	371	10	0
5	A	359	0	371	8	0
5	I	359	0	371	14	0
5	K	366	0	376	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	366	0	376	14	0
5	Q	359	0	371	16	0
6	0	351	0	339	10	0
6	2	339	0	329	15	0
6	4	345	0	334	13	0
6	6	320	0	310	5	0
6	8	339	0	329	13	0
6	B	359	0	345	11	0
6	J	324	0	313	10	0
6	N	320	0	310	18	0
6	P	345	0	334	4	0
6	R	331	0	320	16	0
7	D	397	0	413	15	0
7	F	397	0	413	16	0
7	S	402	0	418	12	0
7	U	407	0	427	13	0
7	W	402	0	418	13	0
7	Y	470	0	494	27	0
8	E	343	0	336	16	0
8	G	335	0	327	11	0
8	T	343	0	336	11	0
8	V	335	0	327	13	0
8	X	343	0	336	16	0
8	Z	343	0	336	13	0
9	3	498	0	505	16	0
10	C	172	0	120	21	0
11	C	1	0	0	0	0
12	C	35	0	0	0	0
13	C	12	0	18	2	0
14	1	27	0	25	5	0
14	A	72	0	87	7	0
14	C	31	0	32	2	0
14	F	31	0	35	0	0
14	H	36	0	42	3	0
14	L	101	0	115	13	0
14	M	27	0	27	3	0
14	Q	24	0	21	1	0
15	0	66	0	74	8	0
15	1	66	0	74	11	0
15	2	66	0	74	9	0
15	3	66	0	74	9	0
15	4	66	0	74	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	5	66	0	74	7	0
15	6	66	0	74	7	0
15	7	61	0	61	8	0
15	8	66	0	74	11	0
15	9	66	0	74	5	0
15	A	66	0	74	5	0
15	B	66	0	74	9	0
15	D	66	0	74	4	0
15	E	66	0	74	10	0
15	F	66	0	74	1	0
15	G	66	0	74	9	0
15	I	66	0	74	6	0
15	J	66	0	74	6	0
15	K	66	0	74	8	0
15	L	132	0	148	8	0
15	M	132	0	148	5	0
15	N	66	0	74	10	0
15	O	66	0	74	2	0
15	P	66	0	74	4	0
15	Q	66	0	74	5	0
15	R	66	0	74	6	0
15	S	66	0	74	5	0
15	T	66	0	74	4	0
15	U	66	0	74	6	0
15	V	66	0	74	6	0
15	W	66	0	74	2	0
15	X	66	0	74	5	0
15	Y	66	0	74	4	0
15	Z	66	0	74	6	0
16	L	65	0	76	6	0
16	M	65	0	76	6	0
17	L	139	0	187	24	0
18	2	35	0	46	4	0
18	4	70	0	92	8	0
18	5	31	0	35	1	0
18	8	70	0	92	3	0
18	B	35	0	46	3	0
18	E	35	0	46	2	0
18	G	35	0	46	1	0
18	H	35	0	46	3	0
18	J	70	0	92	4	0
18	L	35	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	M	59	0	67	3	0
18	P	70	0	92	4	0
18	R	35	0	46	4	0
18	S	26	0	25	3	0
18	T	35	0	46	3	0
18	X	35	0	46	3	0
18	Z	35	0	46	2	0
19	D	58	0	60	0	0
19	H	79	0	105	2	0
19	L	80	0	110	7	0
19	M	134	0	168	9	0
20	M	1	0	0	0	0
21	M	53	0	72	8	0
22	0	44	0	60	8	0
22	2	44	0	60	11	0
22	4	44	0	60	10	0
22	6	44	0	60	5	0
22	9	44	0	60	6	0
22	B	44	0	60	6	0
22	E	44	0	60	7	0
22	G	44	0	60	5	0
22	J	44	0	60	9	0
22	M	44	0	60	5	0
22	N	44	0	60	9	0
22	P	44	0	60	3	0
22	R	44	0	60	4	0
22	T	44	0	60	8	0
22	V	44	0	60	9	0
22	Y	44	0	60	6	0
22	Z	44	0	60	7	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	0	0
24	O	16	0	31	1	0
25	1	1	0	0	0	0
25	3	10	0	0	0	0
25	7	1	0	0	0	0
25	9	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	119	0	0	1	0
25	D	4	0	0	0	0
25	E	2	0	0	0	0
25	F	2	0	0	0	0
25	H	19	0	0	0	0
25	I	2	0	0	0	0
25	K	1	0	0	0	0
25	L	50	0	0	0	0
25	M	77	0	0	4	0
25	O	1	0	0	0	0
25	P	1	0	0	0	0
25	Q	2	0	0	0	0
25	R	1	0	0	0	0
25	S	5	0	0	0	0
25	T	3	0	0	0	0
25	U	10	0	0	0	0
25	V	3	0	0	0	0
25	W	7	0	0	0	0
25	X	1	0	0	0	0
25	Y	5	0	0	0	0
All	All	26274	0	26723	718	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 718 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:155:CYS:SG	10:C:402:HEM:HAC	1.60	1.42
1:C:155:CYS:SG	10:C:402:HEM:CAC	2.09	1.41
1:C:250:CYS:SG	10:C:403:HEM:HAC	1.62	1.39
1:C:110:CYS:SG	10:C:401:HEM:HAC	1.71	1.30
1:C:155:CYS:HG	10:C:402:HEM:CAC	1.43	1.29

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	309/383 (81%)	297 (96%)	12 (4%)	0	100	100
2	L	275/278 (99%)	268 (98%)	7 (2%)	0	100	100
3	M	316/325 (97%)	311 (98%)	5 (2%)	0	100	100
4	H	258/259 (100%)	254 (98%)	4 (2%)	0	100	100
5	1	41/44 (93%)	41 (100%)	0	0	100	100
5	5	41/44 (93%)	40 (98%)	0	1 (2%)	5	1
5	7	41/44 (93%)	41 (100%)	0	0	100	100
5	9	41/44 (93%)	40 (98%)	0	1 (2%)	5	1
5	A	41/44 (93%)	41 (100%)	0	0	100	100
5	I	41/44 (93%)	39 (95%)	2 (5%)	0	100	100
5	K	42/44 (96%)	42 (100%)	0	0	100	100
5	O	42/44 (96%)	42 (100%)	0	0	100	100
5	Q	41/44 (93%)	39 (95%)	1 (2%)	1 (2%)	5	1
6	0	41/46 (89%)	41 (100%)	0	0	100	100
6	2	39/46 (85%)	38 (97%)	1 (3%)	0	100	100
6	4	40/46 (87%)	39 (98%)	1 (2%)	0	100	100
6	6	36/46 (78%)	36 (100%)	0	0	100	100
6	8	39/46 (85%)	37 (95%)	2 (5%)	0	100	100
6	B	42/46 (91%)	41 (98%)	1 (2%)	0	100	100
6	J	37/46 (80%)	37 (100%)	0	0	100	100
6	N	36/46 (78%)	36 (100%)	0	0	100	100
6	P	40/46 (87%)	40 (100%)	0	0	100	100
6	R	38/46 (83%)	37 (97%)	1 (3%)	0	100	100
7	D	47/64 (73%)	47 (100%)	0	0	100	100
7	F	47/64 (73%)	47 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S	48/64 (75%)	47 (98%)	1 (2%)	0	100	100
7	U	49/64 (77%)	49 (100%)	0	0	100	100
7	W	48/64 (75%)	48 (100%)	0	0	100	100
7	Y	55/64 (86%)	52 (94%)	3 (6%)	0	100	100
8	E	39/47 (83%)	39 (100%)	0	0	100	100
8	G	38/47 (81%)	37 (97%)	1 (3%)	0	100	100
8	T	39/47 (83%)	39 (100%)	0	0	100	100
8	V	38/47 (81%)	38 (100%)	0	0	100	100
8	X	39/47 (83%)	39 (100%)	0	0	100	100
8	Z	39/47 (83%)	39 (100%)	0	0	100	100
9	3	61/66 (92%)	60 (98%)	1 (2%)	0	100	100
All	All	2504/2833 (88%)	2458 (98%)	43 (2%)	3 (0%)	50	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Q	6	HIS
5	9	6	HIS
5	5	6	HIS

### 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	265/311 (85%)	262 (99%)	3 (1%)	70	77
2	L	223/224 (100%)	220 (99%)	3 (1%)	65	73
3	M	252/257 (98%)	249 (99%)	3 (1%)	67	75
4	H	206/206 (100%)	203 (98%)	3 (2%)	60	69
5	1	37/38 (97%)	35 (95%)	2 (5%)	18	17
5	5	36/38 (95%)	35 (97%)	1 (3%)	38	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	7	37/38 (97%)	37 (100%)	0	100	100
5	9	37/38 (97%)	35 (95%)	2 (5%)	18	17
5	A	37/38 (97%)	37 (100%)	0	100	100
5	I	37/38 (97%)	36 (97%)	1 (3%)	40	46
5	K	38/38 (100%)	37 (97%)	1 (3%)	41	47
5	O	38/38 (100%)	37 (97%)	1 (3%)	41	47
5	Q	37/38 (97%)	37 (100%)	0	100	100
6	0	36/38 (95%)	36 (100%)	0	100	100
6	2	34/38 (90%)	31 (91%)	3 (9%)	8	5
6	4	35/38 (92%)	34 (97%)	1 (3%)	37	43
6	6	32/38 (84%)	31 (97%)	1 (3%)	35	41
6	8	34/38 (90%)	32 (94%)	2 (6%)	16	14
6	B	37/38 (97%)	37 (100%)	0	100	100
6	J	32/38 (84%)	32 (100%)	0	100	100
6	N	32/38 (84%)	30 (94%)	2 (6%)	15	12
6	P	35/38 (92%)	35 (100%)	0	100	100
6	R	33/38 (87%)	32 (97%)	1 (3%)	36	42
7	D	43/55 (78%)	42 (98%)	1 (2%)	45	52
7	F	43/55 (78%)	40 (93%)	3 (7%)	12	9
7	S	43/55 (78%)	42 (98%)	1 (2%)	45	52
7	U	44/55 (80%)	42 (96%)	2 (4%)	23	24
7	W	43/55 (78%)	42 (98%)	1 (2%)	45	52
7	Y	51/55 (93%)	47 (92%)	4 (8%)	10	7
8	E	35/40 (88%)	32 (91%)	3 (9%)	8	5
8	G	34/40 (85%)	33 (97%)	1 (3%)	37	43
8	T	35/40 (88%)	33 (94%)	2 (6%)	17	15
8	V	34/40 (85%)	32 (94%)	2 (6%)	16	14
8	X	35/40 (88%)	35 (100%)	0	100	100
8	Z	35/40 (88%)	31 (89%)	4 (11%)	4	2
9	3	49/52 (94%)	47 (96%)	2 (4%)	26	28
All	All	2144/2342 (92%)	2088 (97%)	56 (3%)	42	47

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	T	26	MET
5	9	46	SER
7	Y	16	ARG
5	9	15	ARG
6	4	12	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
5	O	10	GLN
6	R	19	HIS
6	R	13	GLN
5	1	6	HIS
4	H	192	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 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	$\# Z  > 2$
4	FME	H	1	4	8,9,10	0.49	0	7,9,11	1.04	1 (14%)
5	FME	K	5	5	8,9,10	0.50	0	7,9,11	0.92	1 (14%)
5	FME	9	5	5	8,9,10	0.49	0	7,9,11	0.99	1 (14%)
5	FME	A	5	5	8,9,10	0.50	0	7,9,11	1.12	1 (14%)
5	FME	I	5	5	8,9,10	0.50	0	7,9,11	1.10	1 (14%)
5	FME	7	5	5	8,9,10	0.48	0	7,9,11	1.18	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FME	1	5	5	8,9,10	0.52	0	7,9,11	0.83	1 (14%)
5	FME	5	5	5	8,9,10	0.52	0	7,9,11	0.95	1 (14%)
5	FME	Q	5	5	8,9,10	0.53	0	7,9,11	1.00	1 (14%)
5	FME	O	5	5	8,9,10	0.52	0	7,9,11	1.02	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
4	FME	H	1	4	-	0/7/9/11	-
5	FME	K	5	5	-	3/7/9/11	-
5	FME	9	5	5	-	0/7/9/11	-
5	FME	A	5	5	-	0/7/9/11	-
5	FME	I	5	5	-	3/7/9/11	-
5	FME	7	5	5	-	1/7/9/11	-
5	FME	1	5	5	-	2/7/9/11	-
5	FME	5	5	5	-	3/7/9/11	-
5	FME	Q	5	5	-	2/7/9/11	-
5	FME	O	5	5	-	0/7/9/11	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	7	5	FME	O-C-CA	-2.74	117.59	124.78
5	I	5	FME	O-C-CA	-2.68	117.74	124.78
5	A	5	FME	O-C-CA	-2.68	117.76	124.78
5	9	5	FME	O-C-CA	-2.50	118.22	124.78
5	O	5	FME	O-C-CA	-2.48	118.27	124.78

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	K	5	FME	CB-CA-N-CN
5	Q	5	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	5	FME	1	0
5	9	5	FME	1	0
5	5	5	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 8 are monoatomic - leaving 105 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	$\# Z  > 2$
17	UQ8	L	309	-	53,53,53	1.24	2 (3%)	64,67,67	1.55	14 (21%)
19	CDL	M	409	-	94,94,99	0.94	4 (4%)	100,106,111	1.08	7 (7%)
14	PGV	H	301	-	35,35,50	1.09	2 (5%)	38,41,56	1.39	4 (10%)
18	LMT	M	410	-	36,36,36	0.41	0	47,47,47	0.78	1 (2%)
15	BCL	S	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.28	19 (24%)
18	LMT	8	103	-	36,36,36	0.43	0	47,47,47	0.87	1 (2%)
12	Z41	C	406	-	34,34,39	0.28	0	36,36,41	0.30	0
16	BPH	M	404	-	51,70,70	0.50	0	52,101,101	0.69	1 (1%)
22	CRT	R	102	-	41,43,43	0.69	0	50,54,54	1.61	12 (24%)
15	BCL	M	403	-	64,74,74	1.69	14 (21%)	78,115,115	2.36	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CRT	B	103	-	41,43,43	0.71	0	50,54,54	1.69	15 (30%)
15	BCL	R	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.10	21 (26%)
15	BCL	B	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.19	21 (26%)
18	LMT	2	101	-	36,36,36	0.40	0	47,47,47	0.89	2 (4%)
22	CRT	4	103	-	41,43,43	0.70	0	50,54,54	1.89	13 (26%)
15	BCL	I	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.29	19 (24%)
18	LMT	4	101	-	36,36,36	0.40	0	47,47,47	0.75	1 (2%)
14	PGV	Q	101	-	23,23,50	1.40	2 (8%)	27,28,56	1.27	3 (11%)
15	BCL	O	502	-	64,74,74	1.68	12 (18%)	78,115,115	2.31	21 (26%)
22	CRT	M	406	-	41,43,43	0.68	0	50,54,54	2.28	12 (24%)
15	BCL	D	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.25	22 (28%)
18	LMT	B	101	-	36,36,36	0.42	0	47,47,47	0.75	1 (2%)
10	HEM	C	404	1	41,50,50	1.33	3 (7%)	45,82,82	1.77	8 (17%)
14	PGV	M	408	-	26,26,50	1.28	2 (7%)	30,31,56	1.35	5 (16%)
15	BCL	9	102	-	64,74,74	1.68	12 (18%)	78,115,115	2.29	20 (25%)
22	CRT	V	102	-	41,43,43	0.70	0	50,54,54	2.20	19 (38%)
15	BCL	V	101	-	64,74,74	1.67	13 (20%)	78,115,115	2.22	21 (26%)
14	PGV	A	501	-	38,38,50	1.02	2 (5%)	41,44,56	1.19	3 (7%)
10	HEM	C	401	1	41,50,50	1.32	3 (7%)	45,82,82	1.91	10 (22%)
14	PGV	L	305	-	28,28,50	1.23	2 (7%)	31,34,56	1.31	4 (12%)
16	BPH	L	302	-	51,70,70	0.53	0	52,101,101	0.66	1 (1%)
22	CRT	N	102	-	41,43,43	0.73	0	50,54,54	1.82	14 (28%)
15	BCL	N	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.25	20 (25%)
14	PGV	C	408	-	30,30,50	1.17	2 (6%)	33,36,56	1.09	2 (6%)
24	LDA	K	101	-	12,15,15	2.10	1 (8%)	14,17,17	0.53	0
22	CRT	2	103	-	41,43,43	0.74	0	50,54,54	2.07	10 (20%)
18	LMT	4	104	-	36,36,36	0.41	0	47,47,47	0.79	1 (2%)
22	CRT	J	103	-	41,43,43	0.73	0	50,54,54	3.80	14 (28%)
19	CDL	D	101	-	57,57,99	1.11	4 (7%)	63,69,111	1.14	3 (4%)
15	BCL	W	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.27	20 (25%)
15	BCL	J	102	-	64,74,74	1.69	14 (21%)	78,115,115	2.18	20 (25%)
10	HEM	C	402	1	41,50,50	1.31	5 (12%)	45,82,82	1.83	11 (24%)
15	BCL	G	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.21	21 (26%)
18	LMT	P	104	-	36,36,36	0.38	0	47,47,47	0.68	1 (2%)
24	LDA	O	501	-	12,15,15	2.12	1 (8%)	14,17,17	0.50	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	PGV	L	306	-	34,34,50	1.09	2 (5%)	37,40,56	1.05	2 (5%)
15	BCL	Z	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.24	20 (25%)
18	LMT	J	101	-	36,36,36	0.41	0	47,47,47	0.71	0
22	CRT	G	103	-	41,43,43	0.71	0	50,54,54	1.43	8 (16%)
18	LMT	T	103	-	36,36,36	0.42	0	47,47,47	0.83	1 (2%)
15	BCL	O	101	-	64,74,74	1.66	11 (17%)	78,115,115	2.18	20 (25%)
22	CRT	Y	101	-	41,43,43	0.70	0	50,54,54	1.61	9 (18%)
18	LMT	G	101	-	36,36,36	0.44	0	47,47,47	0.82	1 (2%)
18	LMT	E	101	-	36,36,36	0.39	0	47,47,47	0.73	1 (2%)
10	HEM	C	403	1	41,50,50	1.34	5 (12%)	45,82,82	1.81	10 (22%)
14	PGV	L	310	-	36,36,50	1.07	2 (5%)	39,42,56	1.13	3 (7%)
15	BCL	L	301	-	64,74,74	1.65	12 (18%)	78,115,115	2.18	21 (26%)
15	BCL	U	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.33	18 (23%)
15	BCL	F	502	-	64,74,74	1.70	14 (21%)	78,115,115	2.28	19 (24%)
15	BCL	Q	102	-	64,74,74	1.68	12 (18%)	78,115,115	2.33	18 (23%)
15	BCL	5	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.31	20 (25%)
18	LMT	Z	101	-	36,36,36	0.39	0	47,47,47	0.90	2 (4%)
18	LMT	P	101	-	36,36,36	0.38	0	47,47,47	0.73	1 (2%)
13	PLM	C	407	1	11,11,17	0.39	0	10,10,17	0.45	0
15	BCL	1	402	-	64,74,74	1.70	14 (21%)	78,115,115	2.28	19 (24%)
18	LMT	J	104	-	36,36,36	0.38	0	47,47,47	0.69	1 (2%)
15	BCL	M	402	-	64,74,74	1.69	13 (20%)	78,115,115	2.23	21 (26%)
18	LMT	X	101	-	36,36,36	0.45	0	47,47,47	0.85	2 (4%)
17	UQ8	L	303	-	33,33,53	1.46	2 (6%)	40,43,67	1.67	9 (22%)
15	BCL	T	101	-	64,74,74	1.67	11 (17%)	78,115,115	2.16	21 (26%)
15	BCL	8	102	-	64,74,74	1.66	11 (17%)	78,115,115	2.18	21 (26%)
18	LMT	L	307	-	36,36,36	0.39	0	47,47,47	0.79	1 (2%)
15	BCL	2	102	-	64,74,74	1.69	11 (17%)	78,115,115	2.17	22 (28%)
22	CRT	T	102	-	41,43,43	0.70	0	50,54,54	1.79	14 (28%)
21	MQ8	M	405	-	54,54,54	1.34	2 (3%)	66,69,69	1.57	15 (22%)
18	LMT	M	411	-	25,25,36	0.48	0	36,36,47	0.84	1 (2%)
18	LMT	5	101	-	32,32,36	0.41	0	43,43,47	1.30	5 (11%)
22	CRT	9	101	-	41,43,43	0.71	0	50,54,54	1.70	12 (24%)
14	PGV	A	503	-	32,32,50	1.14	2 (6%)	35,38,56	1.17	4 (11%)
15	BCL	X	102	-	64,74,74	1.69	13 (20%)	78,115,115	2.22	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCL	3	101	-	64,74,74	1.68	12 (18%)	78,115,115	2.29	22 (28%)
15	BCL	Y	102	-	64,74,74	1.68	13 (20%)	78,115,115	2.31	21 (26%)
22	CRT	Z	103	-	41,43,43	0.71	0	50,54,54	1.75	9 (18%)
15	BCL	7	101	-	59,69,74	1.74	13 (22%)	72,109,115	2.31	20 (27%)
17	UQ8	L	304	-	53,53,53	1.20	2 (3%)	64,67,67	1.83	19 (29%)
18	LMT	8	101	-	36,36,36	0.39	0	47,47,47	0.76	1 (2%)
15	BCL	A	502	-	64,74,74	1.69	13 (20%)	78,115,115	2.25	19 (24%)
15	BCL	4	102	-	64,74,74	1.68	12 (18%)	78,115,115	2.19	20 (25%)
15	BCL	K	102	-	64,74,74	1.70	13 (20%)	78,115,115	2.34	22 (28%)
15	BCL	6	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.25	19 (24%)
15	BCL	L	308	-	64,74,74	1.70	12 (18%)	78,115,115	2.23	20 (25%)
19	CDL	L	311	-	79,79,99	1.07	4 (5%)	85,91,111	1.11	5 (5%)
14	PGV	1	401	-	26,26,50	1.24	2 (7%)	29,31,56	1.23	4 (13%)
15	BCL	P	102	-	64,74,74	1.66	12 (18%)	78,115,115	2.21	22 (28%)
22	CRT	E	103	-	41,43,43	0.73	0	50,54,54	1.82	14 (28%)
22	CRT	6	102	-	41,43,43	0.67	0	50,54,54	1.70	13 (26%)
15	BCL	E	102	-	64,74,74	1.67	11 (17%)	78,115,115	2.19	20 (25%)
22	CRT	P	103	-	41,43,43	0.71	0	50,54,54	3.62	15 (30%)
19	CDL	M	407	-	38,38,99	1.30	3 (7%)	43,49,111	1.25	5 (11%)
19	CDL	H	302	-	78,78,99	1.02	4 (5%)	84,90,111	1.06	5 (5%)
18	LMT	R	103	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
22	CRT	0	102	-	41,43,43	0.73	0	50,54,54	1.74	16 (32%)
18	LMT	H	303	-	36,36,36	0.43	0	47,47,47	0.78	1 (2%)
18	LMT	S	101	-	27,27,36	0.59	0	37,38,47	1.33	4 (10%)
14	PGV	F	501	-	30,30,50	1.22	2 (6%)	34,35,56	1.34	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	UQ8	L	309	-	-	15/51/75/75	0/1/1/1
19	CDL	M	409	-	-	31/105/105/110	-
14	PGV	H	301	-	-	12/40/40/55	-
18	LMT	M	410	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCL	S	102	-	-	12/37/137/137	-
18	LMT	8	103	-	-	4/21/61/61	0/2/2/2
12	Z41	C	406	-	-	6/35/35/41	-
16	BPH	M	404	-	-	9/37/105/105	0/5/6/6
22	CRT	R	102	-	-	1/51/51/51	-
15	BCL	M	403	-	-	7/37/137/137	-
22	CRT	B	103	-	-	4/51/51/51	-
15	BCL	R	101	-	-	14/37/137/137	-
15	BCL	B	102	-	-	11/37/137/137	-
18	LMT	2	101	-	-	4/21/61/61	0/2/2/2
22	CRT	4	103	-	-	5/51/51/51	-
15	BCL	I	101	-	-	15/37/137/137	-
18	LMT	4	101	-	-	5/21/61/61	0/2/2/2
14	PGV	Q	101	-	-	9/25/25/55	-
15	BCL	O	502	-	-	16/37/137/137	-
22	CRT	M	406	-	-	8/51/51/51	-
15	BCL	D	102	-	-	14/37/137/137	-
18	LMT	B	101	-	-	6/21/61/61	0/2/2/2
10	HEM	C	404	1	-	4/12/54/54	-
14	PGV	M	408	-	-	9/28/28/55	-
15	BCL	9	102	-	-	12/37/137/137	-
22	CRT	V	102	-	-	5/51/51/51	-
15	BCL	V	101	-	-	19/37/137/137	-
14	PGV	A	501	-	-	12/43/43/55	-
10	HEM	C	401	1	-	4/12/54/54	-
14	PGV	L	305	-	-	12/33/33/55	-
16	BPH	L	302	-	-	5/37/105/105	0/5/6/6
22	CRT	N	102	-	-	9/51/51/51	-
15	BCL	N	101	-	-	16/37/137/137	-
14	PGV	C	408	-	-	9/35/35/55	-
24	LDA	K	101	-	-	2/13/13/13	-
22	CRT	2	103	-	-	7/51/51/51	-
18	LMT	4	104	-	-	3/21/61/61	0/2/2/2
22	CRT	J	103	-	-	10/51/51/51	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CDL	D	101	-	-	27/67/67/110	-
15	BCL	W	101	-	-	16/37/137/137	-
15	BCL	J	102	-	-	18/37/137/137	-
10	HEM	C	402	1	-	5/12/54/54	-
15	BCL	G	102	-	-	17/37/137/137	-
18	LMT	P	104	-	-	1/21/61/61	0/2/2/2
24	LDA	O	501	-	-	2/13/13/13	-
14	PGV	L	306	-	-	8/39/39/55	-
15	BCL	Z	102	-	-	15/37/137/137	-
18	LMT	J	101	-	-	2/21/61/61	0/2/2/2
22	CRT	G	103	-	-	9/51/51/51	-
18	LMT	T	103	-	-	10/21/61/61	0/2/2/2
15	BCL	0	101	-	-	17/37/137/137	-
22	CRT	Y	101	-	-	3/51/51/51	-
18	LMT	G	101	-	-	4/21/61/61	0/2/2/2
18	LMT	E	101	-	-	6/21/61/61	0/2/2/2
10	HEM	C	403	1	-	2/12/54/54	-
14	PGV	L	310	-	-	19/41/41/55	-
15	BCL	L	301	-	-	9/37/137/137	-
15	BCL	U	101	-	-	21/37/137/137	-
15	BCL	F	502	-	-	19/37/137/137	-
15	BCL	Q	102	-	-	17/37/137/137	-
15	BCL	5	102	-	-	17/37/137/137	-
18	LMT	Z	101	-	-	4/21/61/61	0/2/2/2
18	LMT	P	101	-	-	5/21/61/61	0/2/2/2
13	PLM	C	407	1	-	1/8/9/15	-
15	BCL	1	402	-	-	11/37/137/137	-
18	LMT	J	104	-	-	4/21/61/61	0/2/2/2
15	BCL	M	402	-	-	6/37/137/137	-
18	LMT	X	101	-	-	5/21/61/61	0/2/2/2
17	UQ8	L	303	-	-	2/27/51/75	0/1/1/1
15	BCL	T	101	-	-	16/37/137/137	-
15	BCL	8	102	-	-	16/37/137/137	-
18	LMT	L	307	-	-	7/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCL	2	102	-	-	15/37/137/137	-
22	CRT	T	102	-	-	9/51/51/51	-
21	MQ8	M	405	-	-	4/47/67/67	0/2/2/2
18	LMT	M	411	-	-	3/10/50/61	0/2/2/2
18	LMT	5	101	-	-	6/17/57/61	0/2/2/2
22	CRT	9	101	-	-	3/51/51/51	-
14	PGV	A	503	-	-	15/37/37/55	-
15	BCL	X	102	-	-	15/37/137/137	-
15	BCL	3	101	-	-	11/37/137/137	-
15	BCL	Y	102	-	-	15/37/137/137	-
22	CRT	Z	103	-	-	13/51/51/51	-
15	BCL	7	101	-	-	13/31/131/137	-
17	UQ8	L	304	-	-	7/51/75/75	0/1/1/1
18	LMT	8	101	-	-	4/21/61/61	0/2/2/2
15	BCL	A	502	-	-	13/37/137/137	-
15	BCL	4	102	-	-	15/37/137/137	-
15	BCL	K	102	-	-	11/37/137/137	-
15	BCL	6	101	-	-	20/37/137/137	-
15	BCL	L	308	-	-	12/37/137/137	-
19	CDL	L	311	-	-	27/89/89/110	-
14	PGV	1	401	-	-	10/30/30/55	-
15	BCL	P	102	-	-	15/37/137/137	-
22	CRT	E	103	-	-	6/51/51/51	-
22	CRT	6	102	-	-	8/51/51/51	-
15	BCL	E	102	-	-	16/37/137/137	-
22	CRT	P	103	-	-	7/51/51/51	-
19	CDL	M	407	-	-	17/48/48/110	-
19	CDL	H	302	-	-	26/89/89/110	-
18	LMT	R	103	-	-	6/21/61/61	0/2/2/2
22	CRT	0	102	-	-	2/51/51/51	-
18	LMT	H	303	-	-	4/21/61/61	0/2/2/2
18	LMT	S	101	-	-	3/12/52/61	0/2/2/2
14	PGV	F	501	-	-	11/32/32/55	-

The worst 5 of 519 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	M	405	MQ8	C3-C2	8.05	1.49	1.35
17	L	309	UQ8	C6-C1	7.69	1.49	1.35
17	L	304	UQ8	C6-C1	7.49	1.48	1.35
17	L	303	UQ8	C6-C1	7.43	1.48	1.35
24	O	501	LDA	O1-N1	-7.31	1.25	1.42

The worst 5 of 1145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	103	CRT	C3-C1-C4	-17.03	84.72	110.86
22	J	103	CRT	C2-C1-C4	-15.82	86.57	110.86
22	P	103	CRT	C3-C1-C4	-15.60	86.91	110.86
22	P	103	CRT	C2-C1-C4	-15.40	87.21	110.86
15	Q	102	BCL	CHD-C1D-ND	-8.78	116.38	124.45

There are no chirality outliers.

5 of 1053 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	401	HEM	C2B-C3B-CAB-CBB
10	C	402	HEM	C2B-C3B-CAB-CBB
10	C	403	HEM	C2B-C3B-CAB-CBB
10	C	403	HEM	C4B-C3B-CAB-CBB
10	C	404	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

100 monomers are involved in 463 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	L	309	UQ8	5	0
19	M	409	CDL	8	0
14	H	301	PGV	3	0
18	M	410	LMT	2	0
15	S	102	BCL	5	0
18	8	103	LMT	3	0
16	M	404	BPH	6	0
22	R	102	CRT	4	0
15	M	403	BCL	2	0
22	B	103	CRT	6	0
15	R	101	BCL	6	0
15	B	102	BCL	9	0
18	2	101	LMT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	4	103	CRT	10	0
15	I	101	BCL	6	0
18	4	101	LMT	6	0
14	Q	101	PGV	1	0
15	O	502	BCL	2	0
22	M	406	CRT	5	0
15	D	102	BCL	4	0
18	B	101	LMT	3	0
10	C	404	HEM	3	0
14	M	408	PGV	3	0
15	9	102	BCL	5	0
22	V	102	CRT	9	0
15	V	101	BCL	6	0
14	A	501	PGV	3	0
10	C	401	HEM	7	0
14	L	305	PGV	5	0
16	L	302	BPH	6	0
22	N	102	CRT	9	0
15	N	101	BCL	10	0
14	C	408	PGV	2	0
22	2	103	CRT	11	0
18	4	104	LMT	2	0
22	J	103	CRT	9	0
15	W	101	BCL	2	0
15	J	102	BCL	6	0
10	C	402	HEM	5	0
15	G	102	BCL	9	0
18	P	104	LMT	3	0
24	O	501	LDA	1	0
14	L	306	PGV	4	0
15	Z	102	BCL	6	0
18	J	101	LMT	3	0
22	G	103	CRT	5	0
18	T	103	LMT	3	0
15	0	101	BCL	8	0
22	Y	101	CRT	6	0
18	G	101	LMT	1	0
18	E	101	LMT	2	0
10	C	403	HEM	6	0
14	L	310	PGV	4	0
15	L	301	BCL	4	0
15	U	101	BCL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	502	BCL	1	0
15	Q	102	BCL	5	0
15	5	102	BCL	7	0
18	Z	101	LMT	2	0
18	P	101	LMT	1	0
13	C	407	PLM	2	0
15	1	402	BCL	11	0
18	J	104	LMT	1	0
15	M	402	BCL	3	0
18	X	101	LMT	3	0
17	L	303	UQ8	4	0
15	T	101	BCL	4	0
15	8	102	BCL	11	0
18	L	307	LMT	3	0
15	2	102	BCL	9	0
22	T	102	CRT	8	0
21	M	405	MQ8	8	0
18	M	411	LMT	1	0
18	5	101	LMT	1	0
22	9	101	CRT	6	0
14	A	503	PGV	4	0
15	X	102	BCL	5	0
15	3	101	BCL	9	0
15	Y	102	BCL	4	0
22	Z	103	CRT	7	0
15	7	101	BCL	8	0
17	L	304	UQ8	15	0
15	A	502	BCL	5	0
15	4	102	BCL	8	0
15	K	102	BCL	8	0
15	6	101	BCL	7	0
15	L	308	BCL	4	0
19	L	311	CDL	7	0
14	1	401	PGV	5	0
15	P	102	BCL	4	0
22	E	103	CRT	7	0
22	6	102	CRT	5	0
15	E	102	BCL	10	0
22	P	103	CRT	3	0
19	M	407	CDL	1	0
19	H	302	CDL	2	0
18	R	103	LMT	4	0

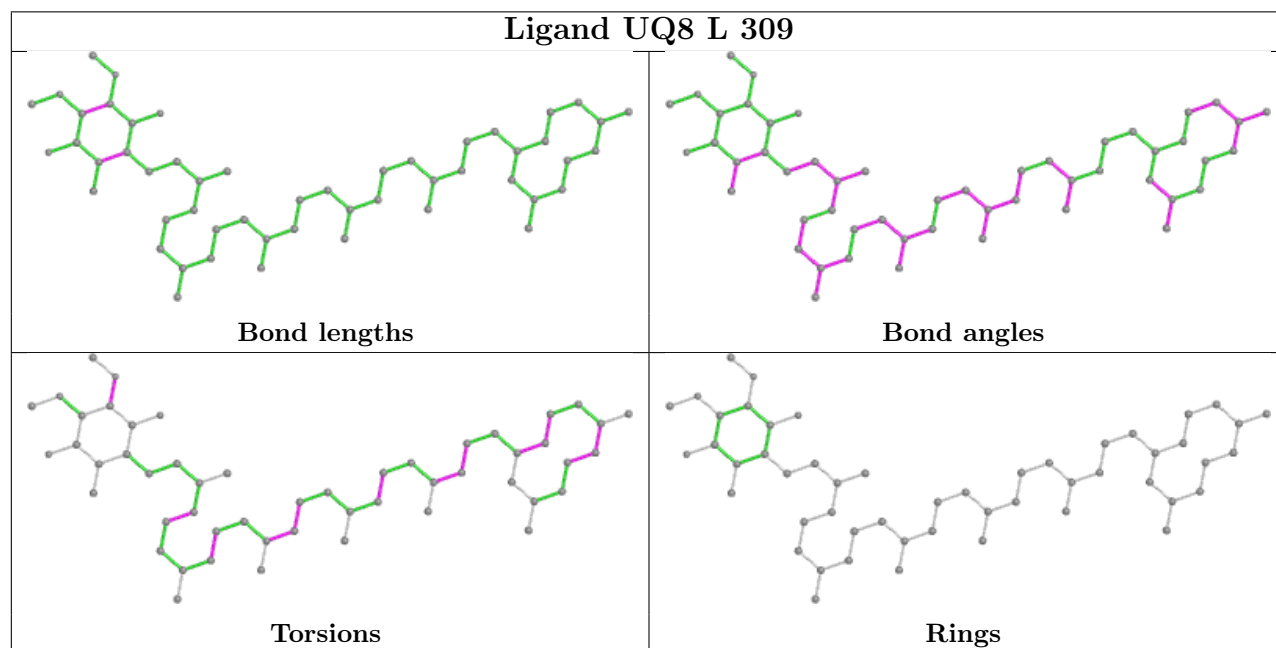
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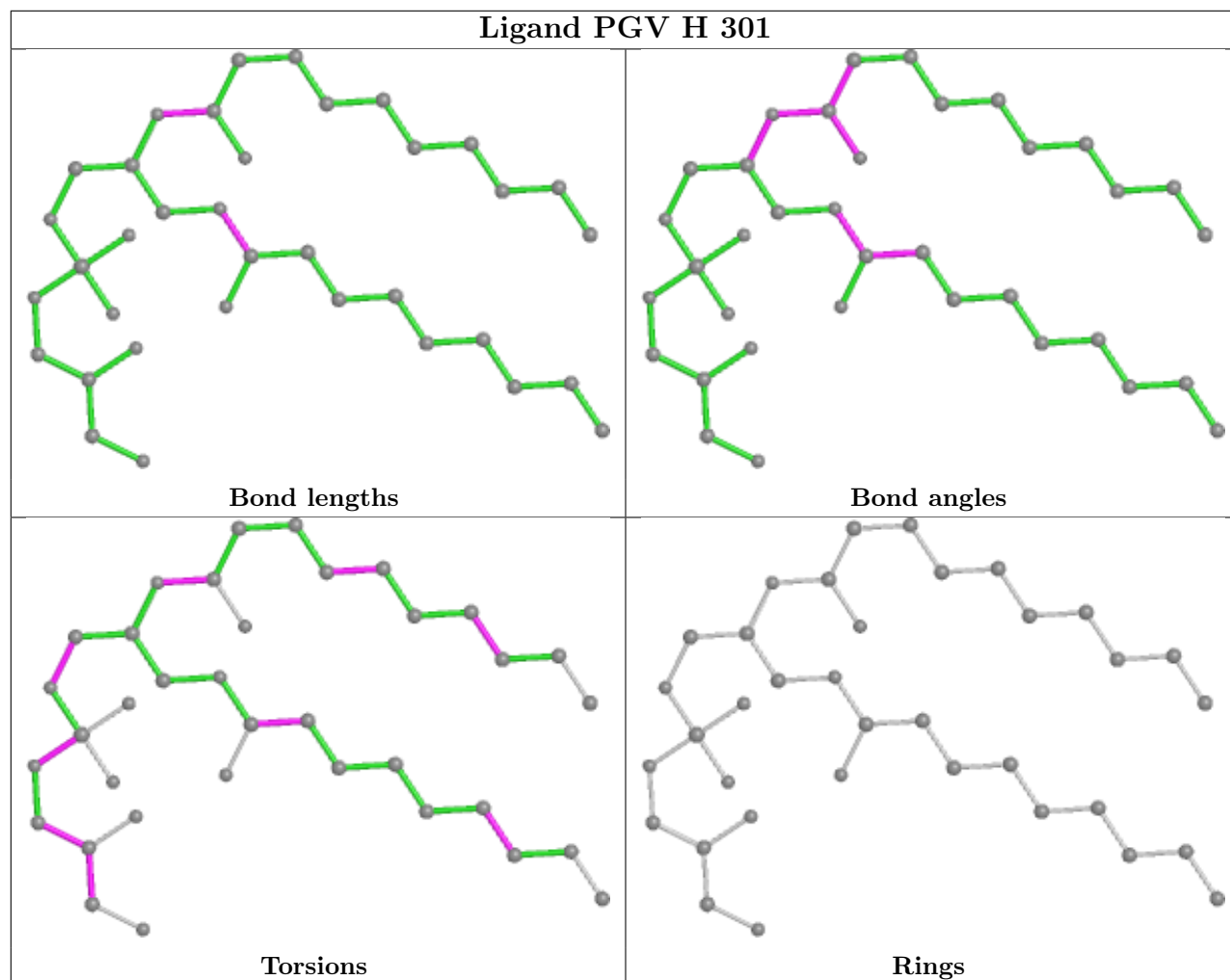
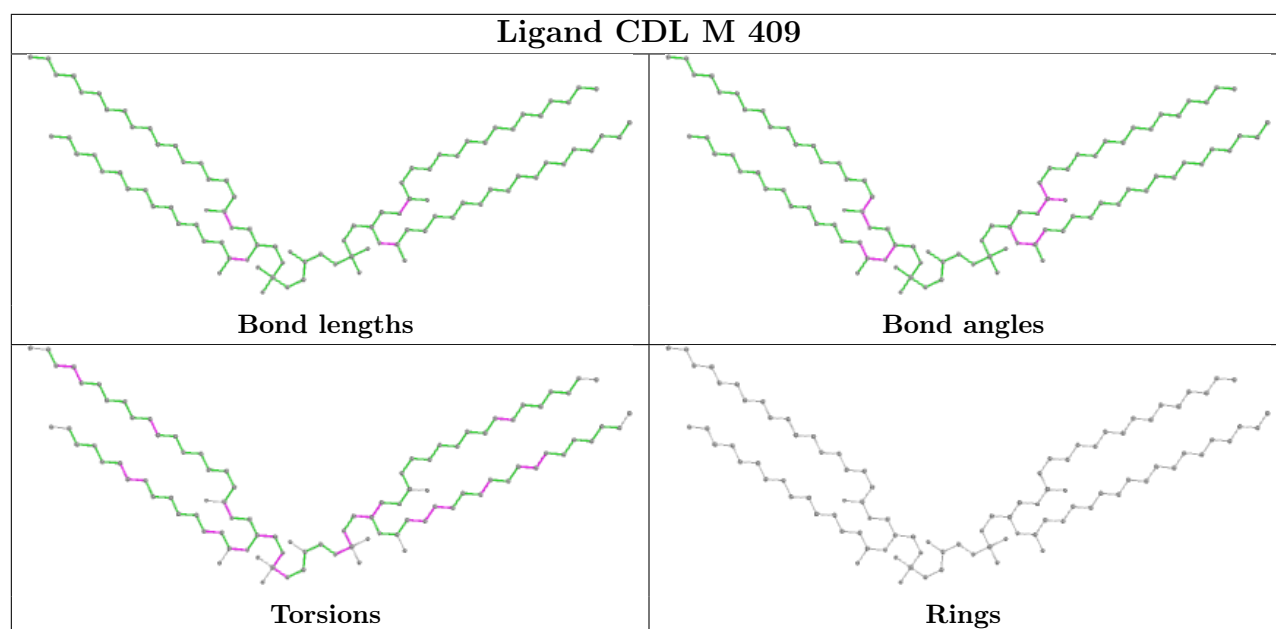


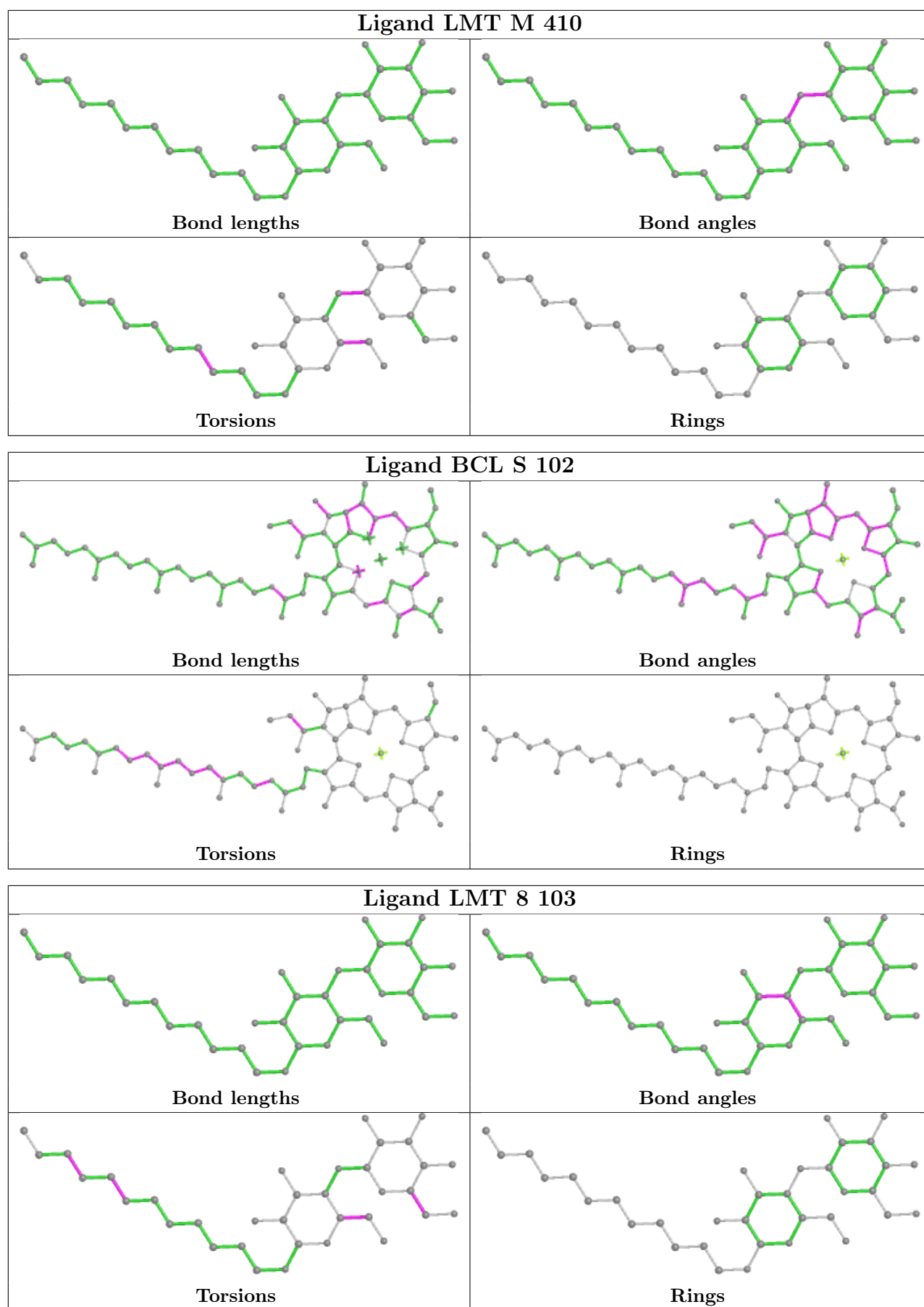
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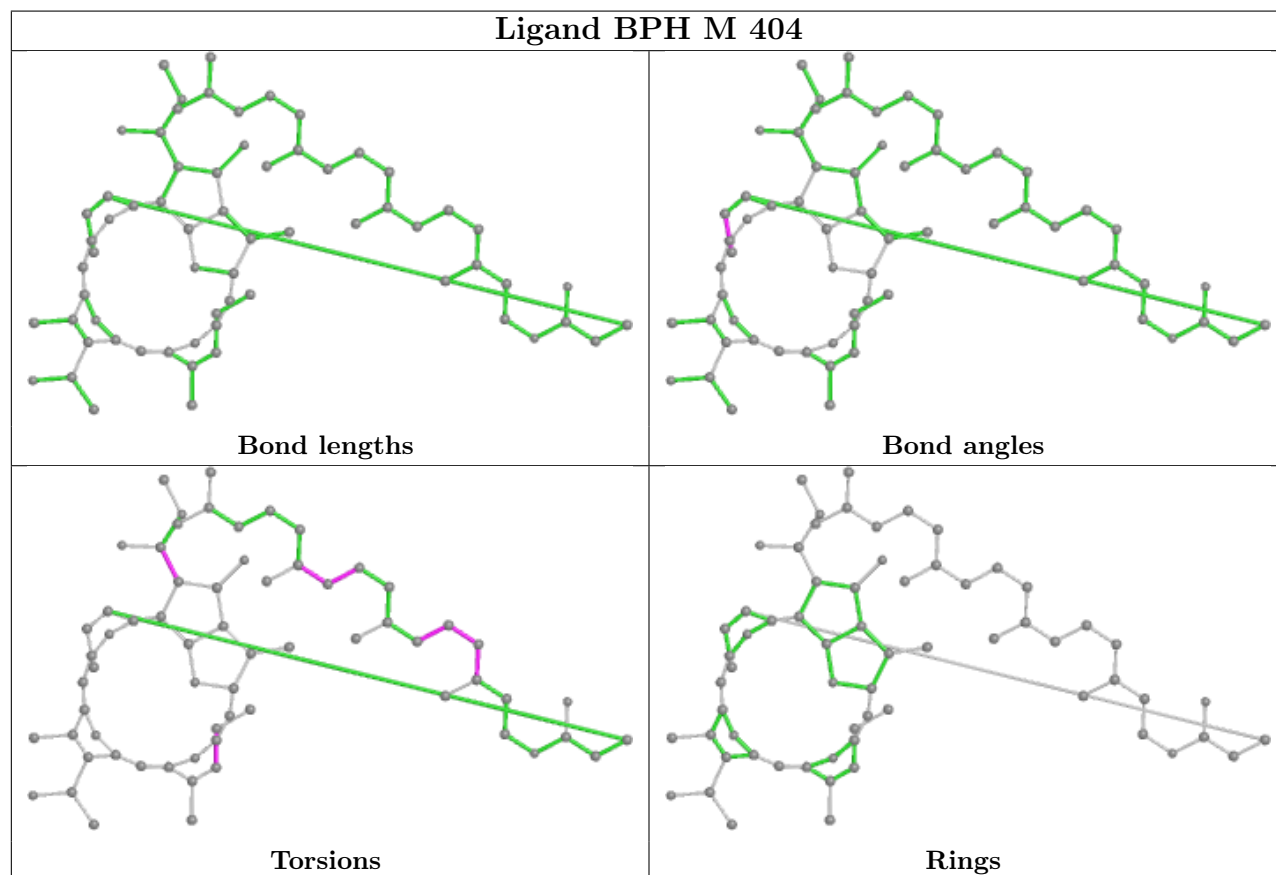
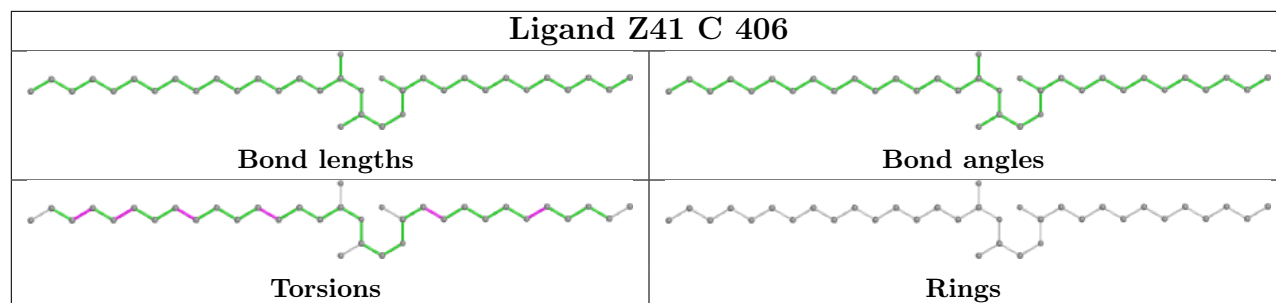
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	0	102	CRT	8	0
18	H	303	LMT	3	0
18	S	101	LMT	3	0

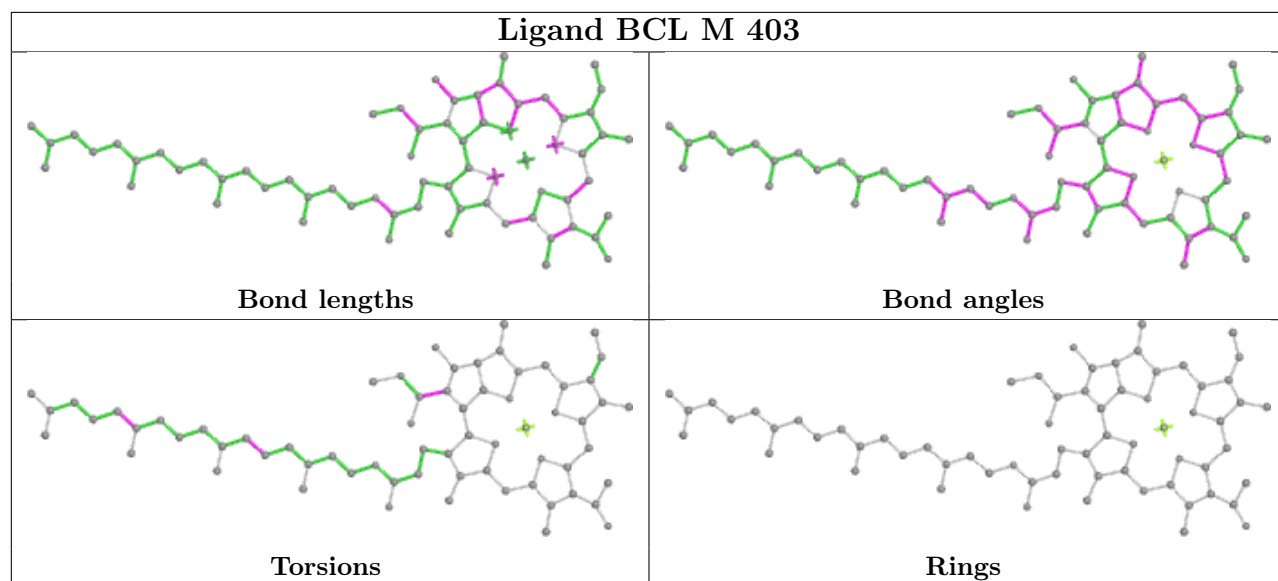
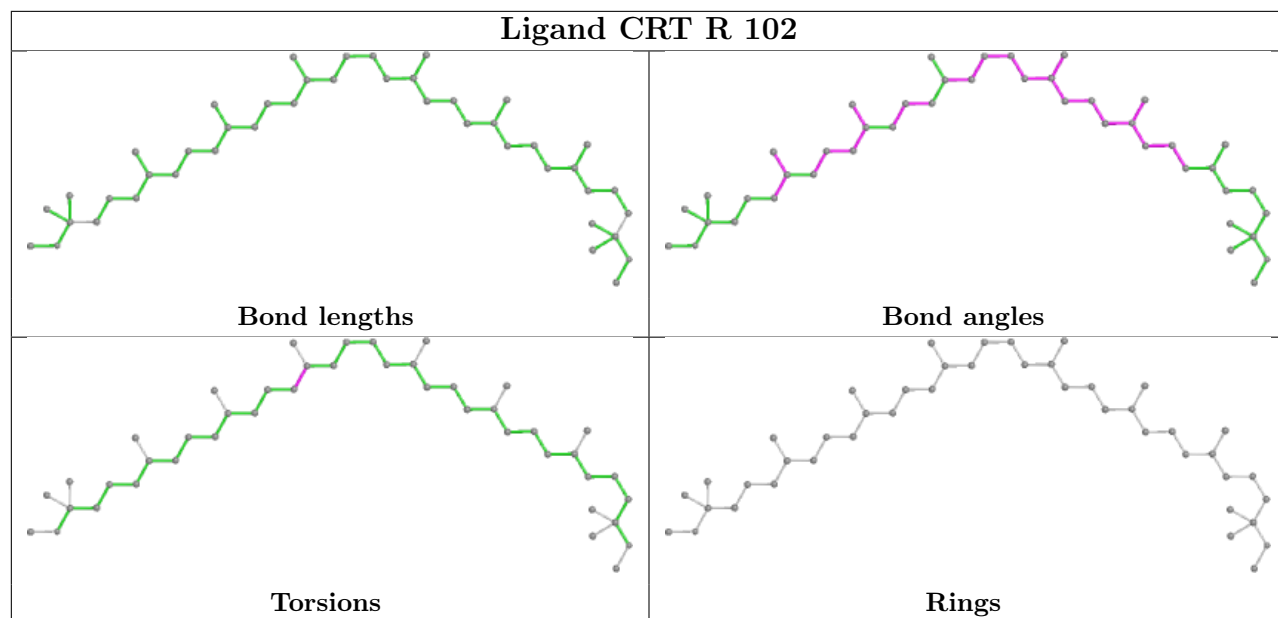
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

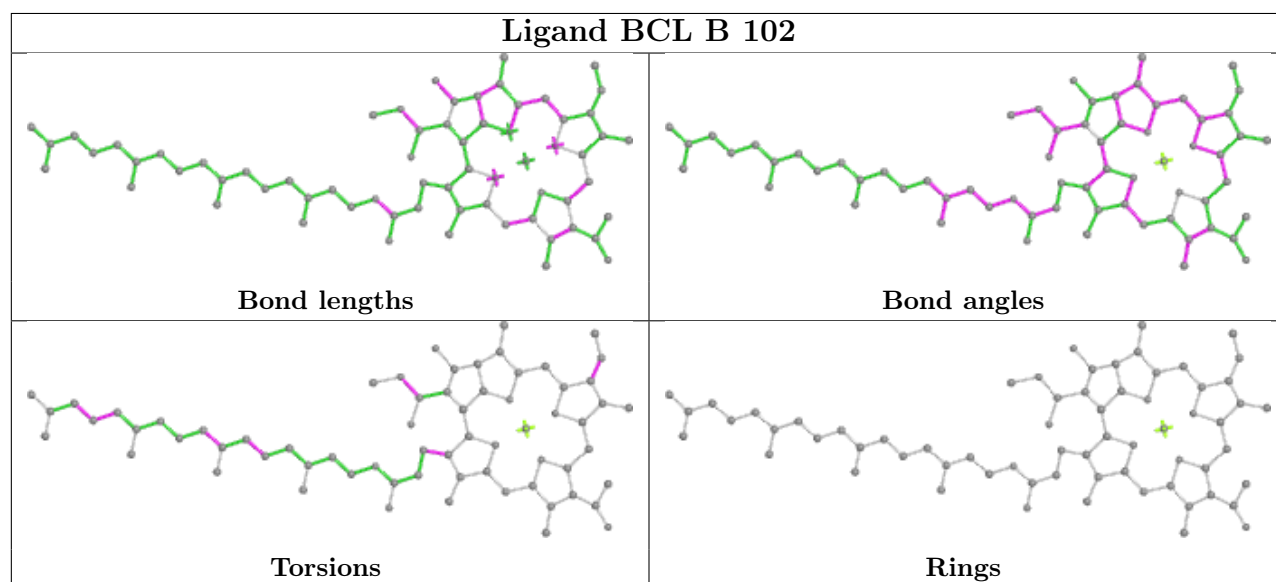
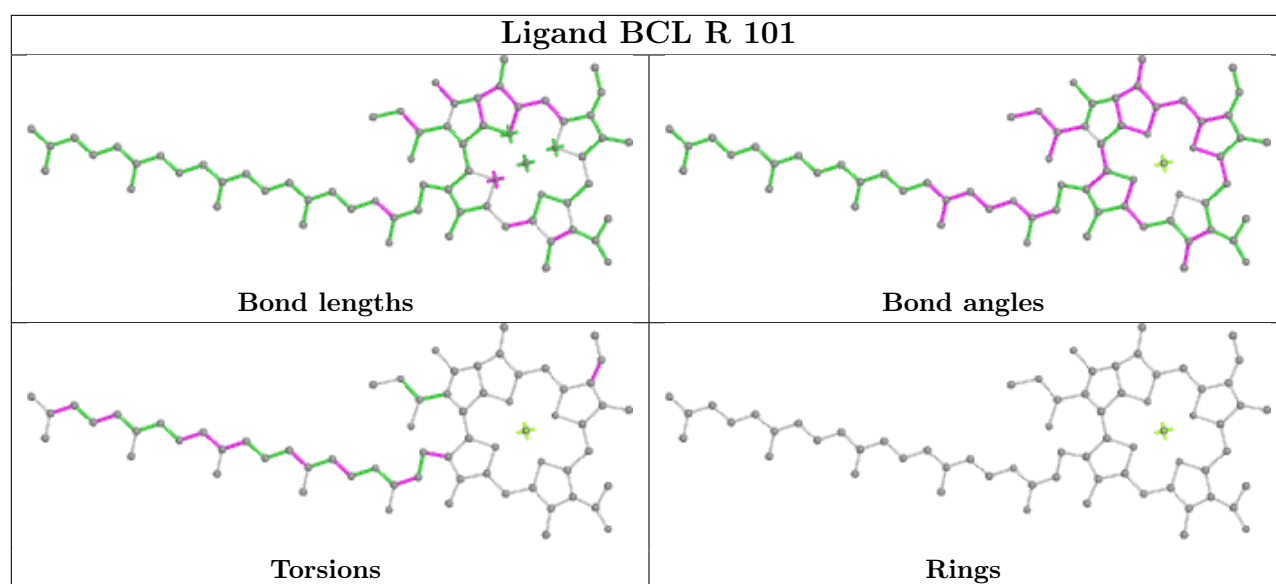
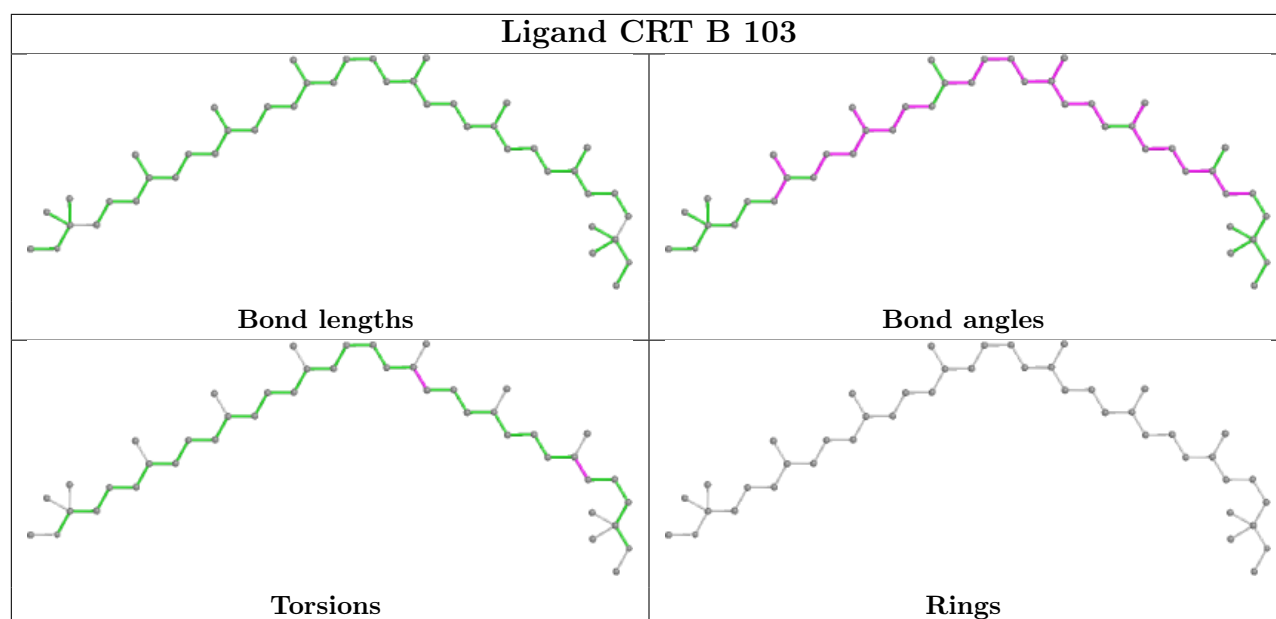


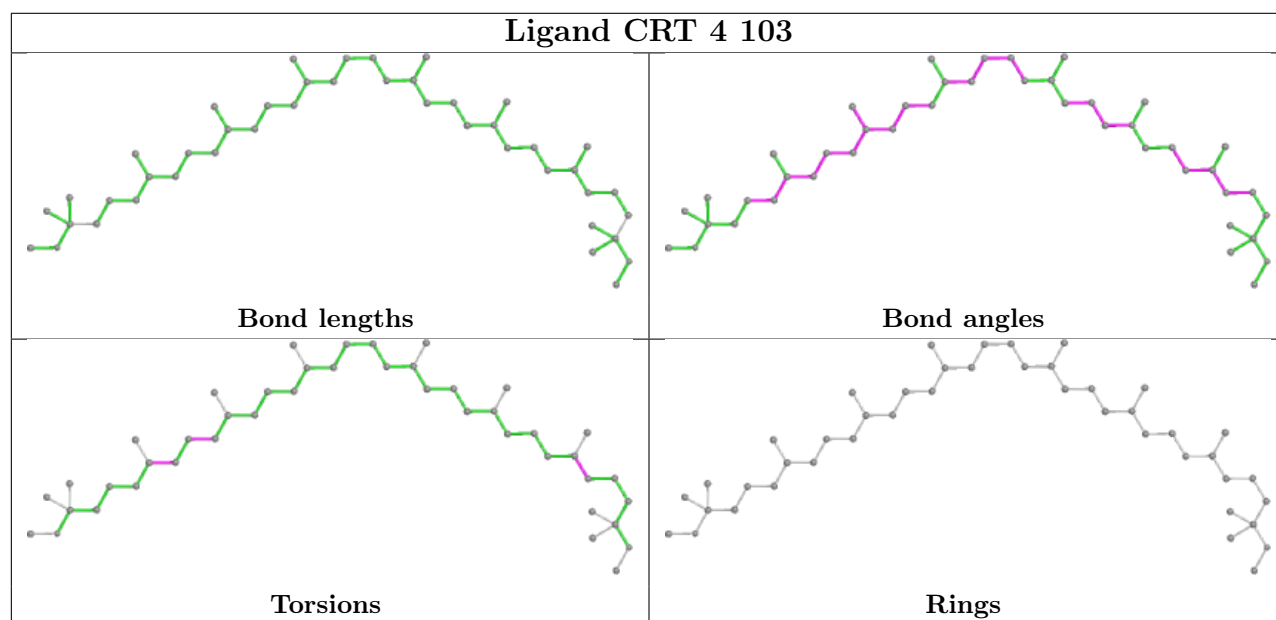
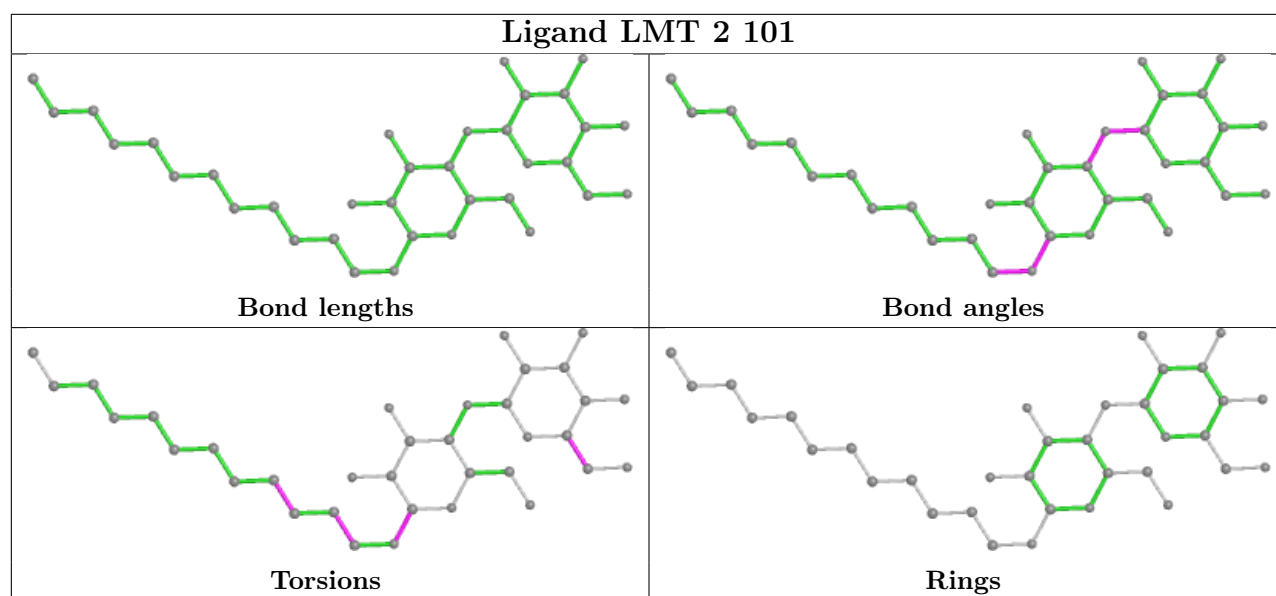


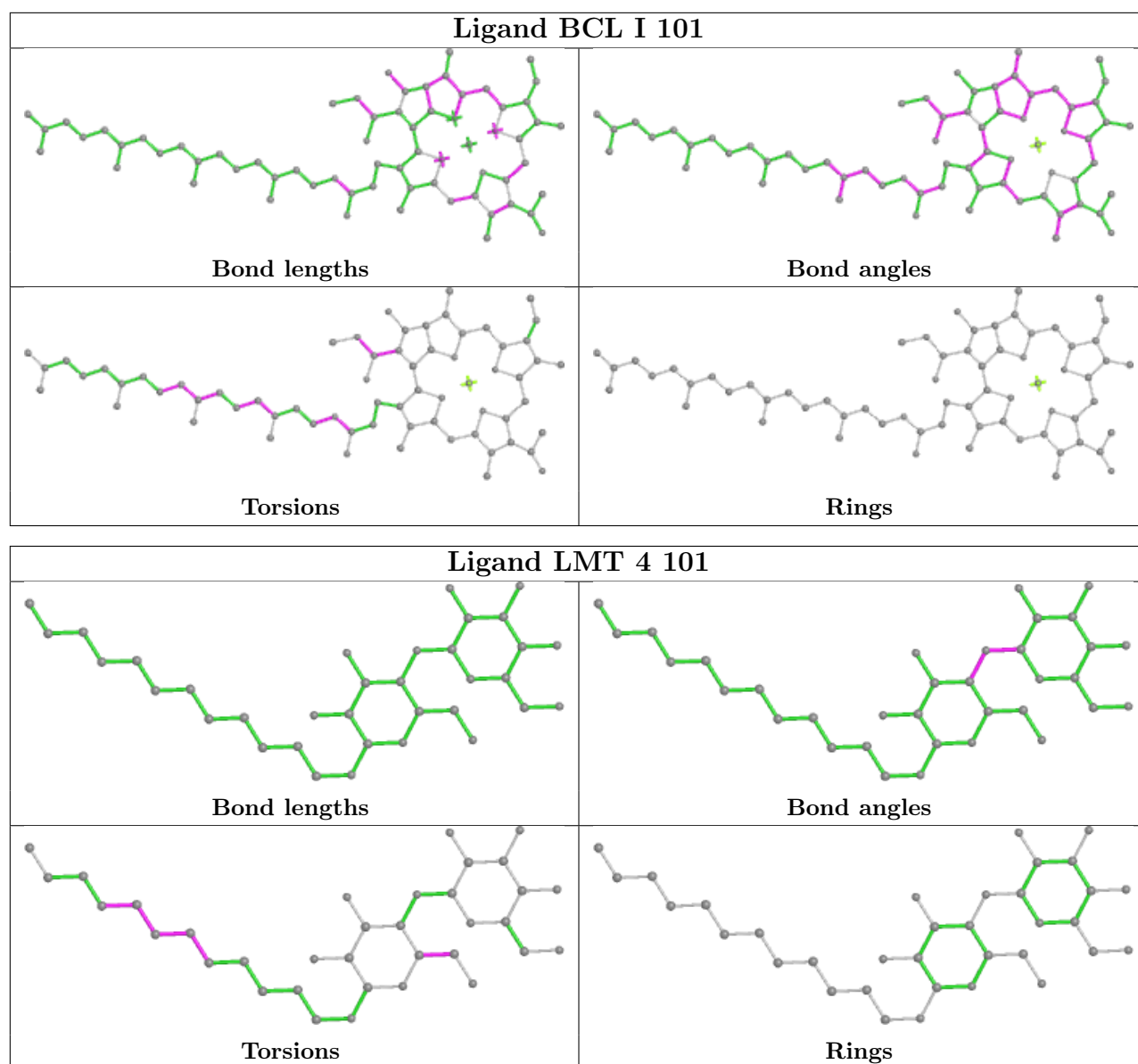




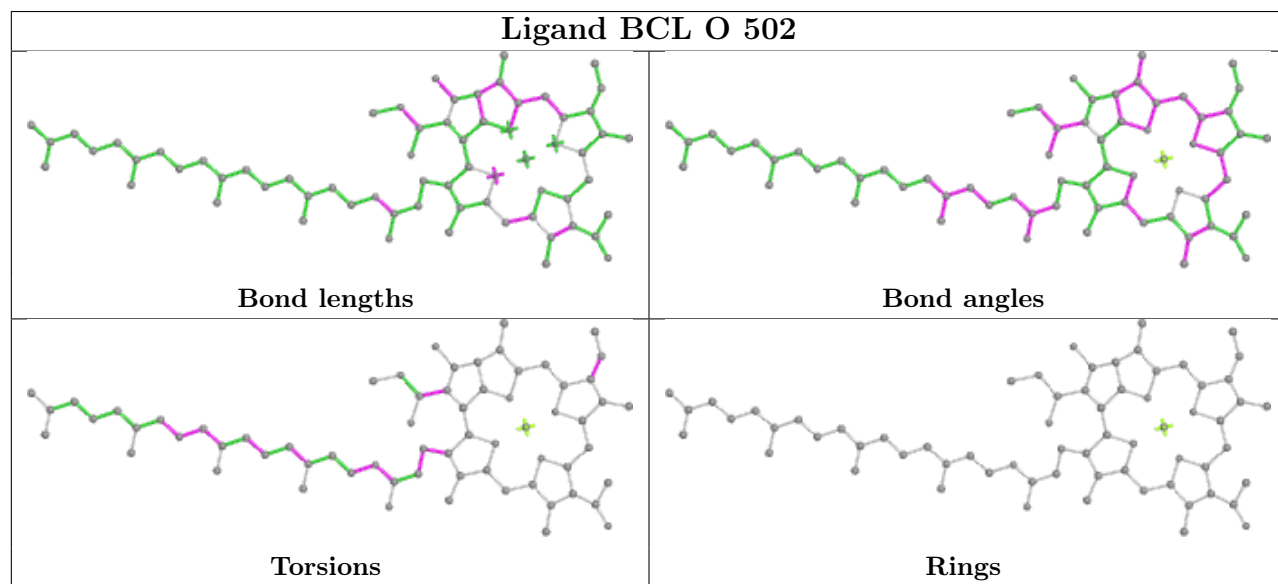
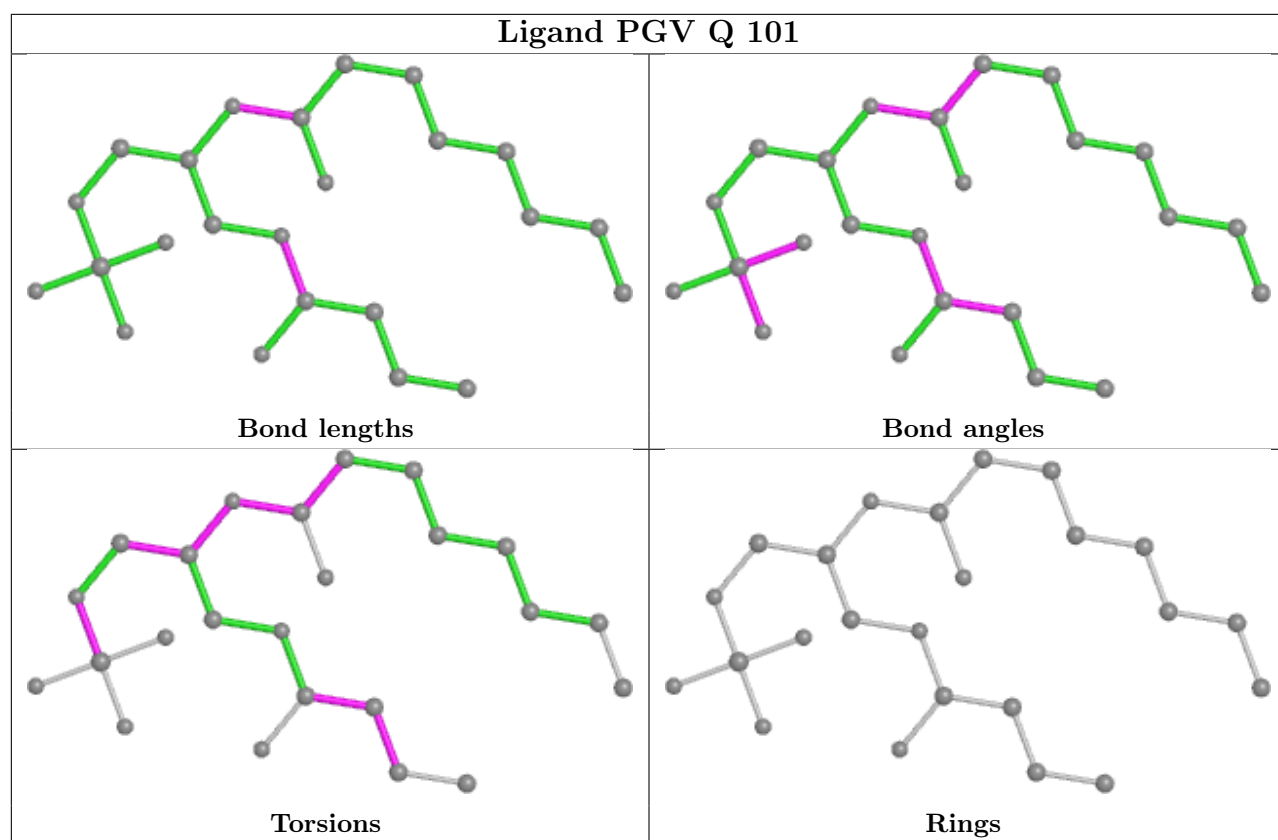


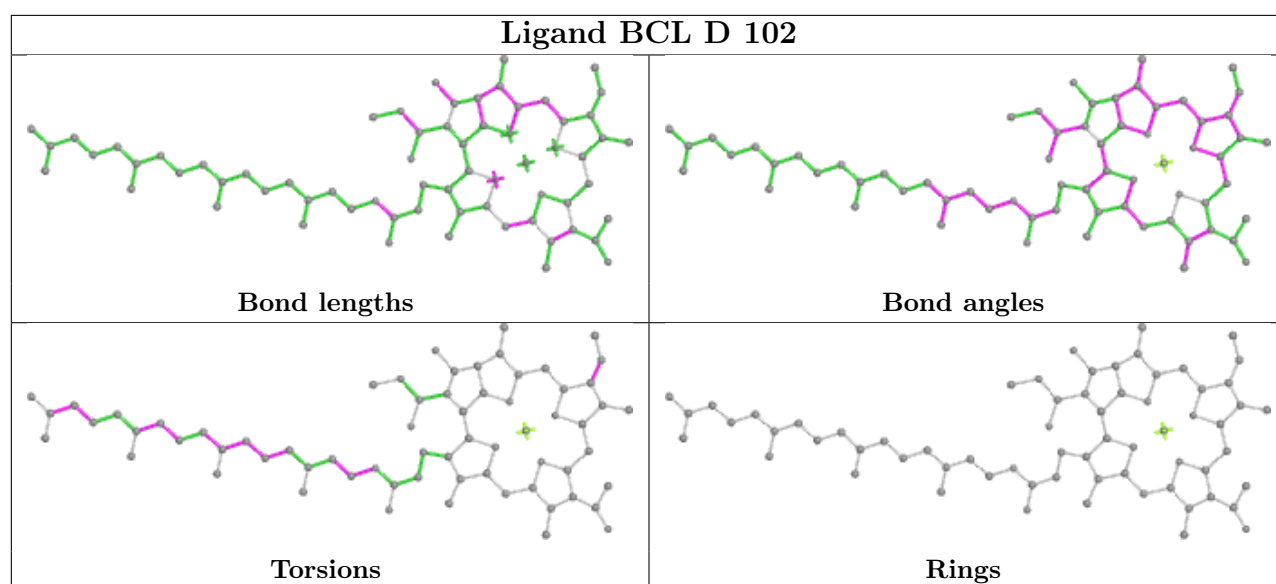
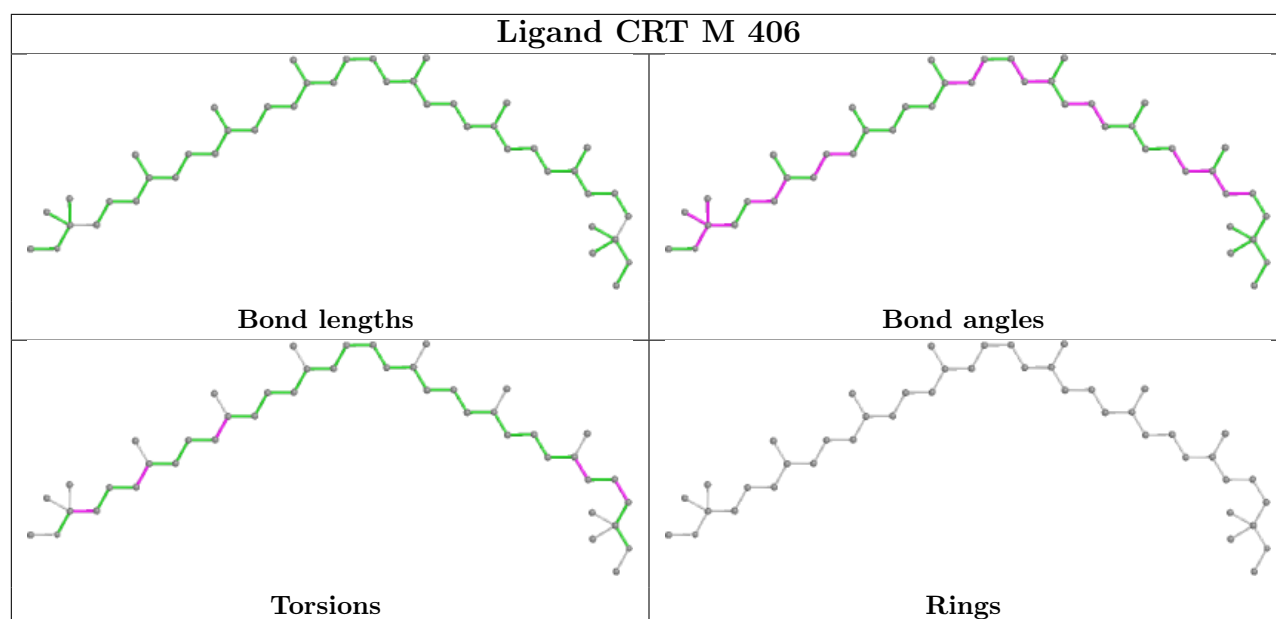


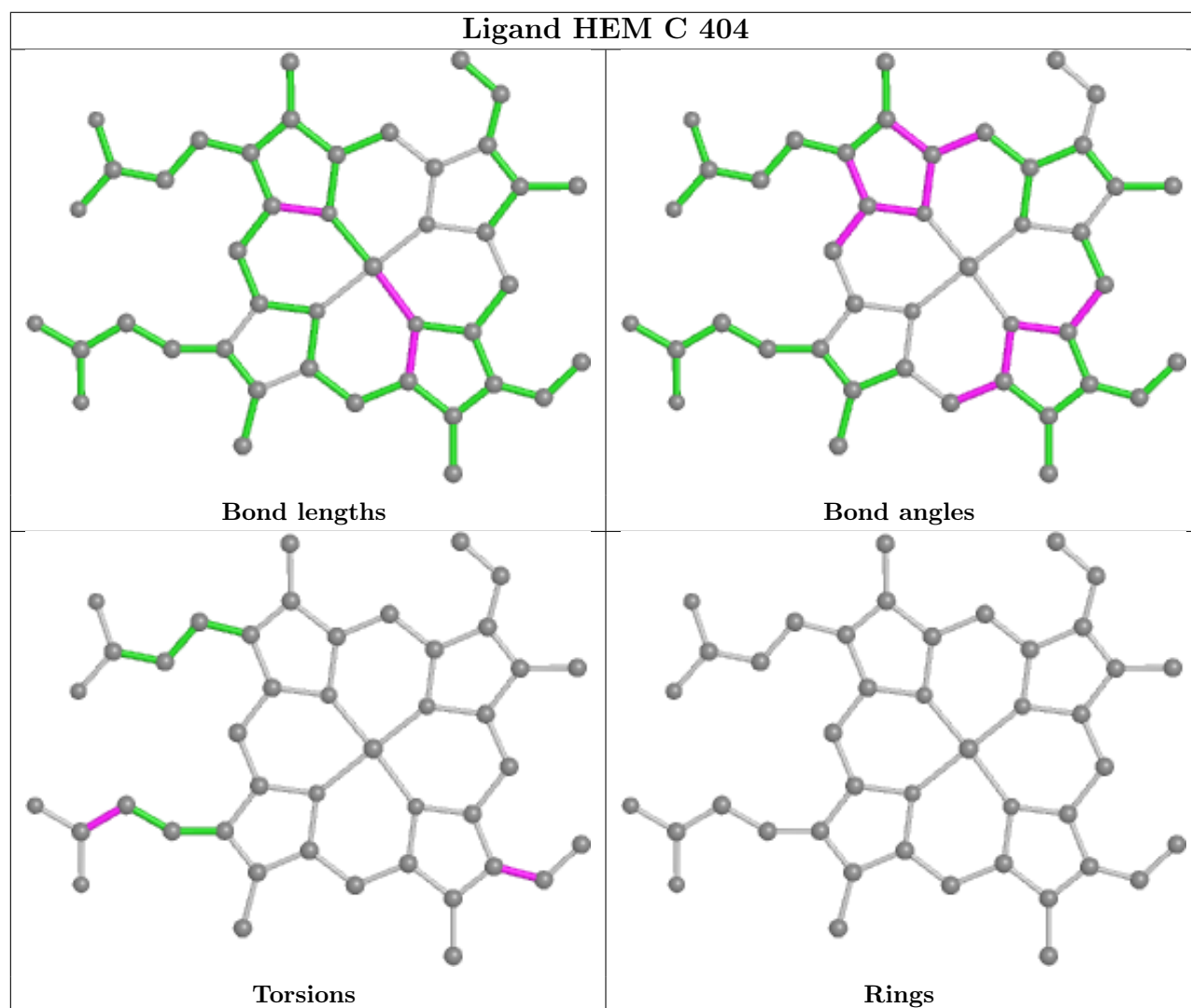
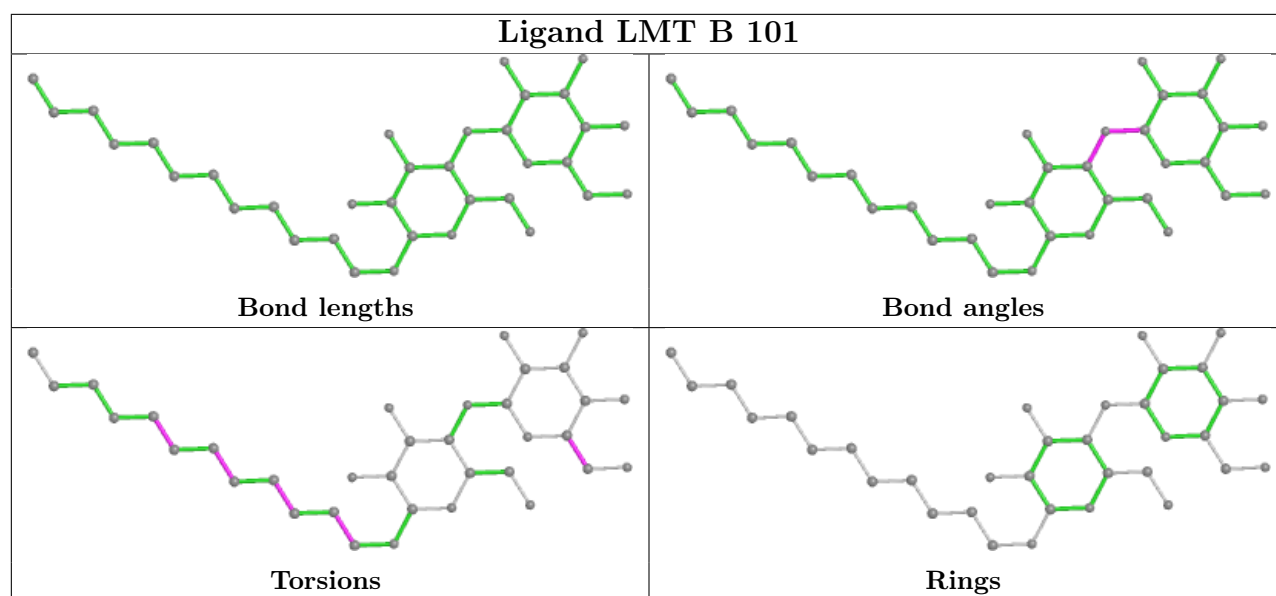


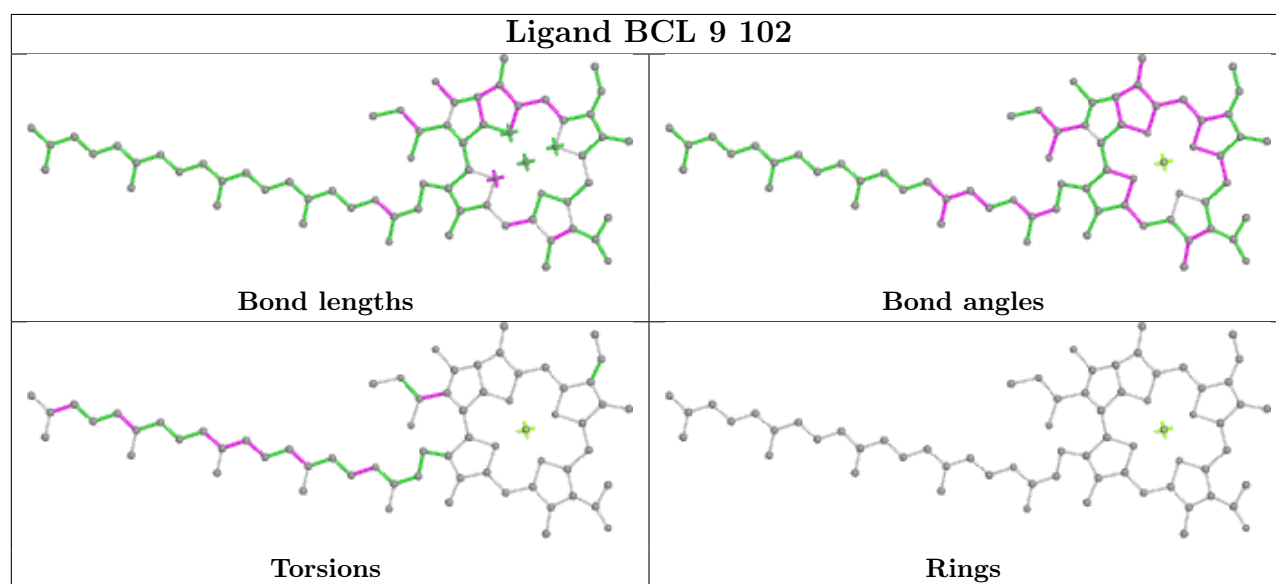
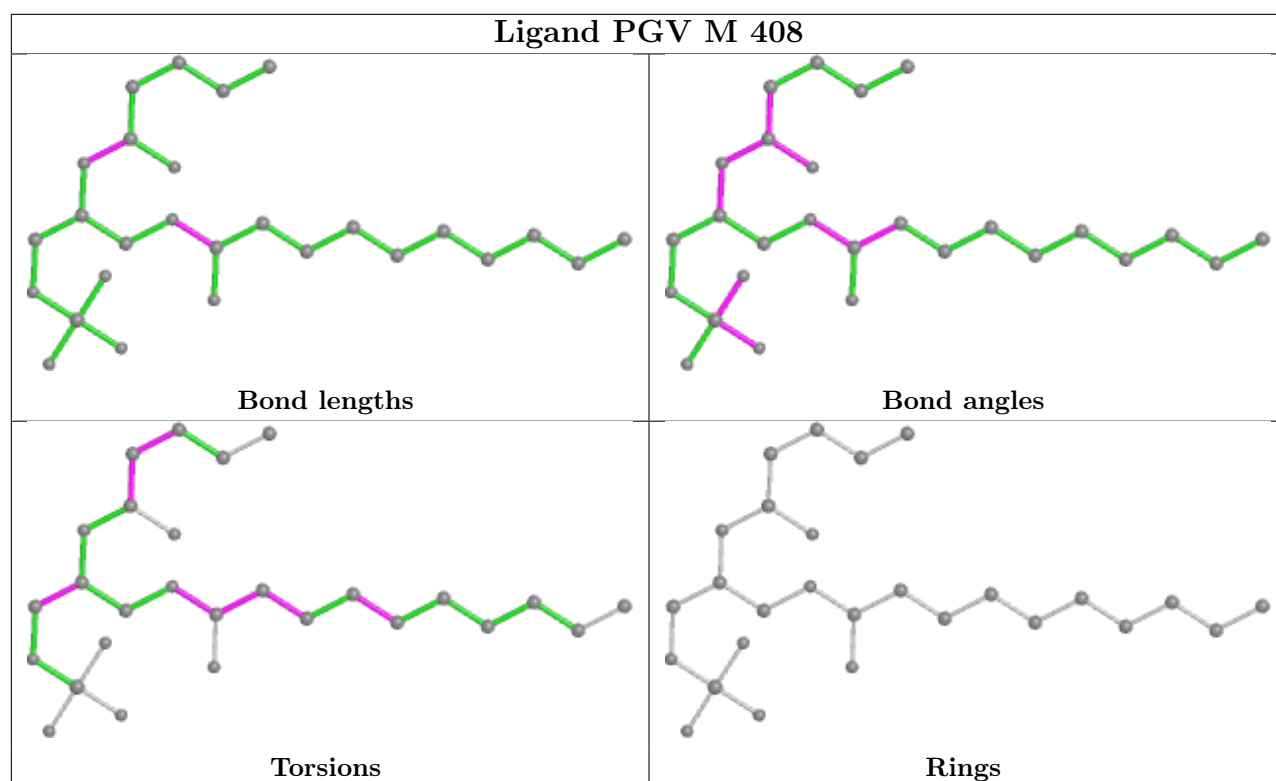


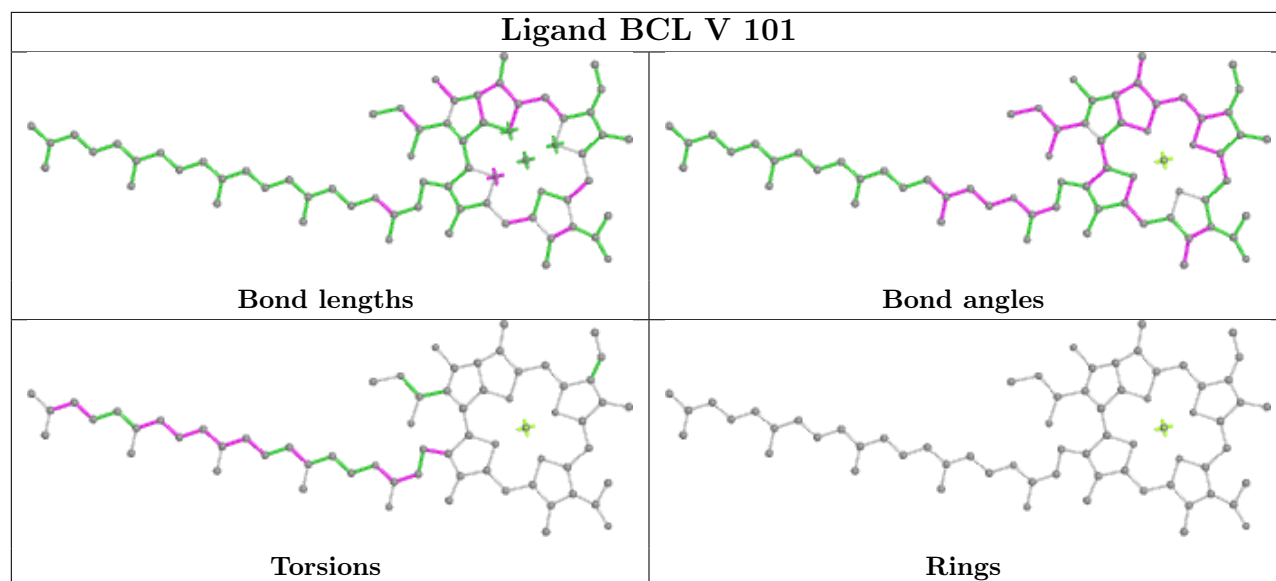
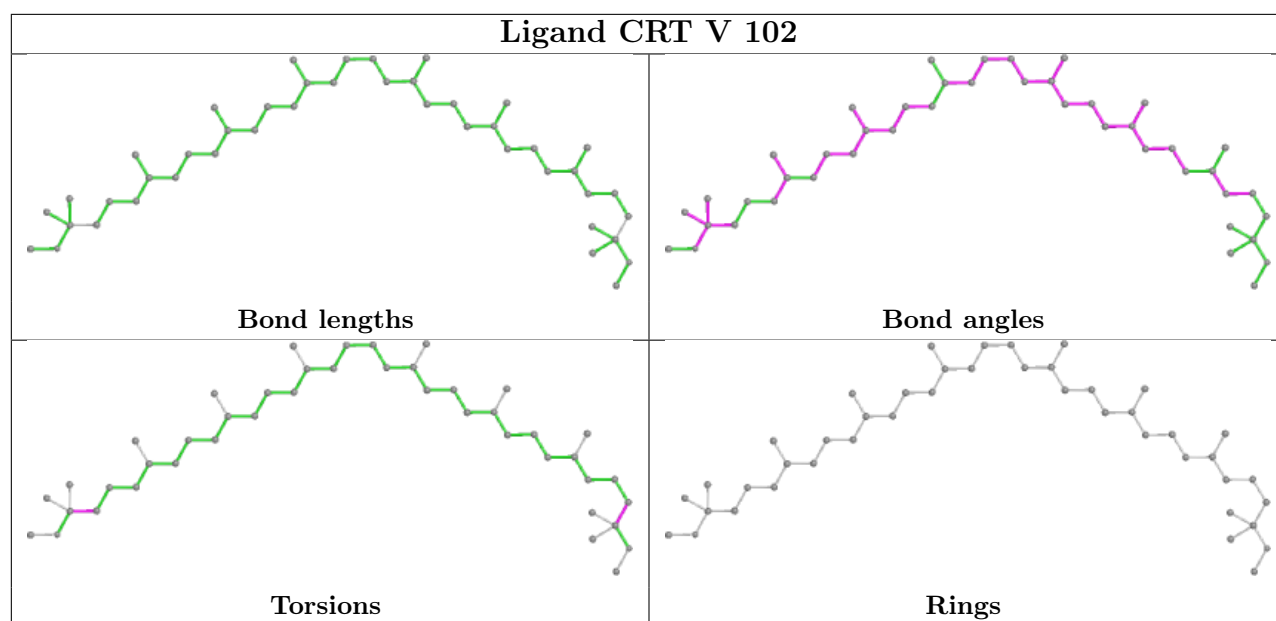


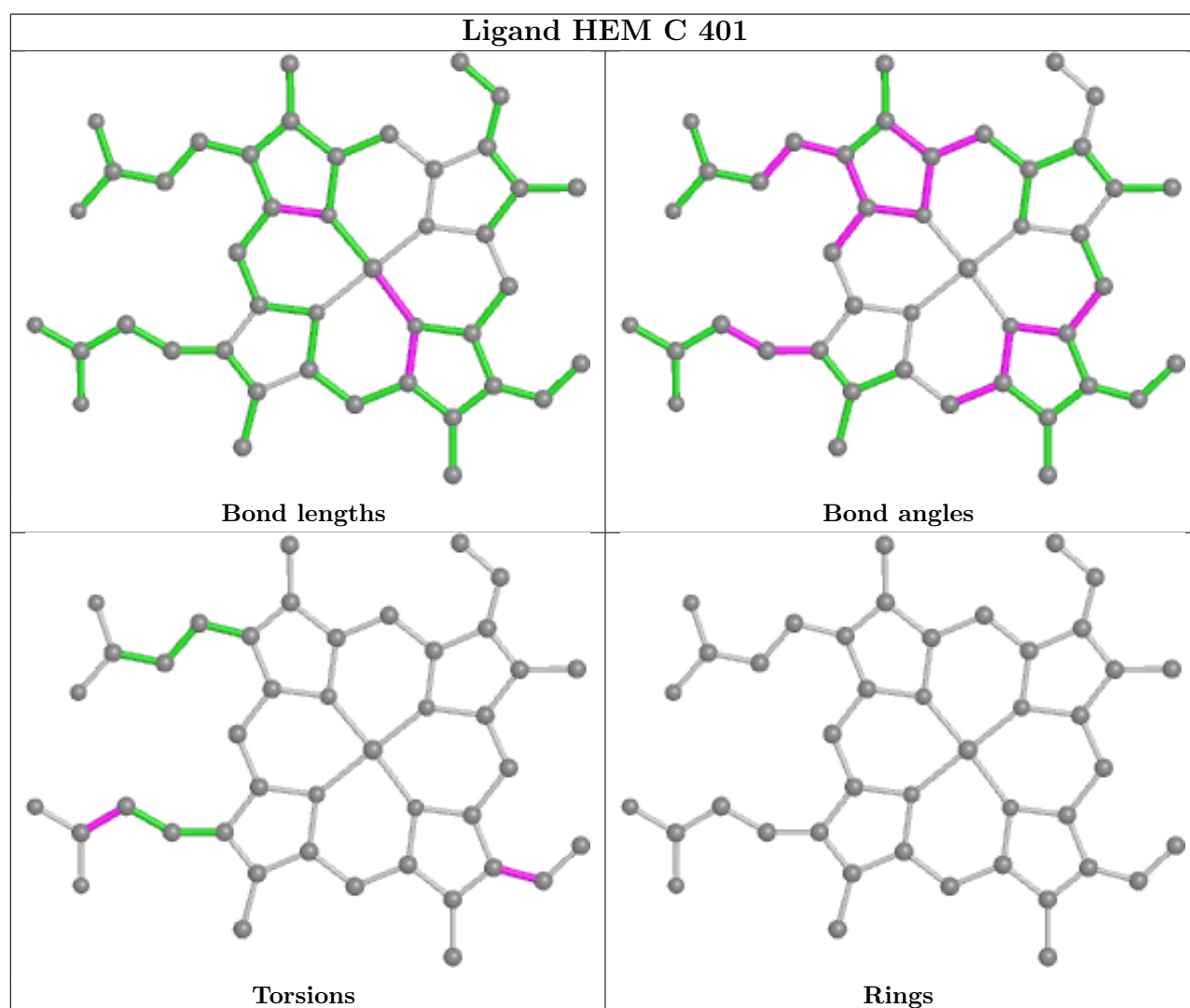
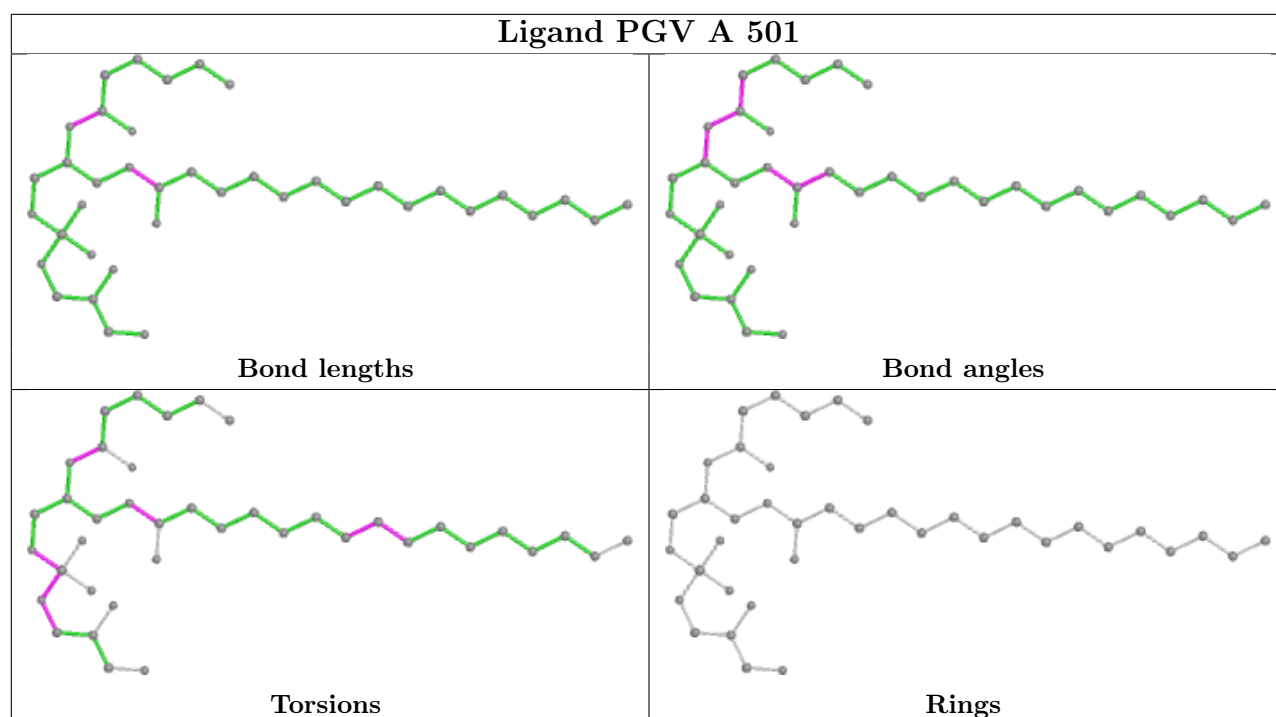


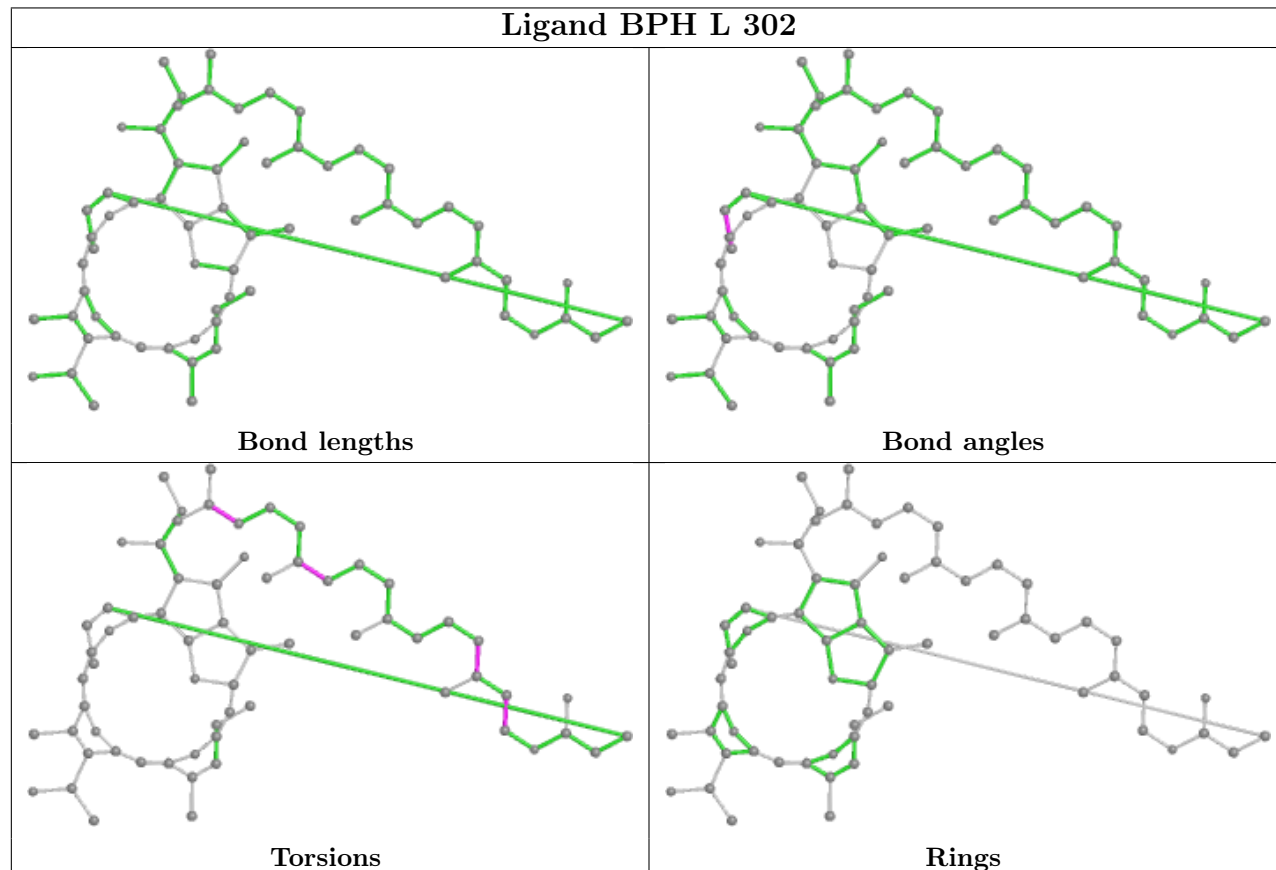
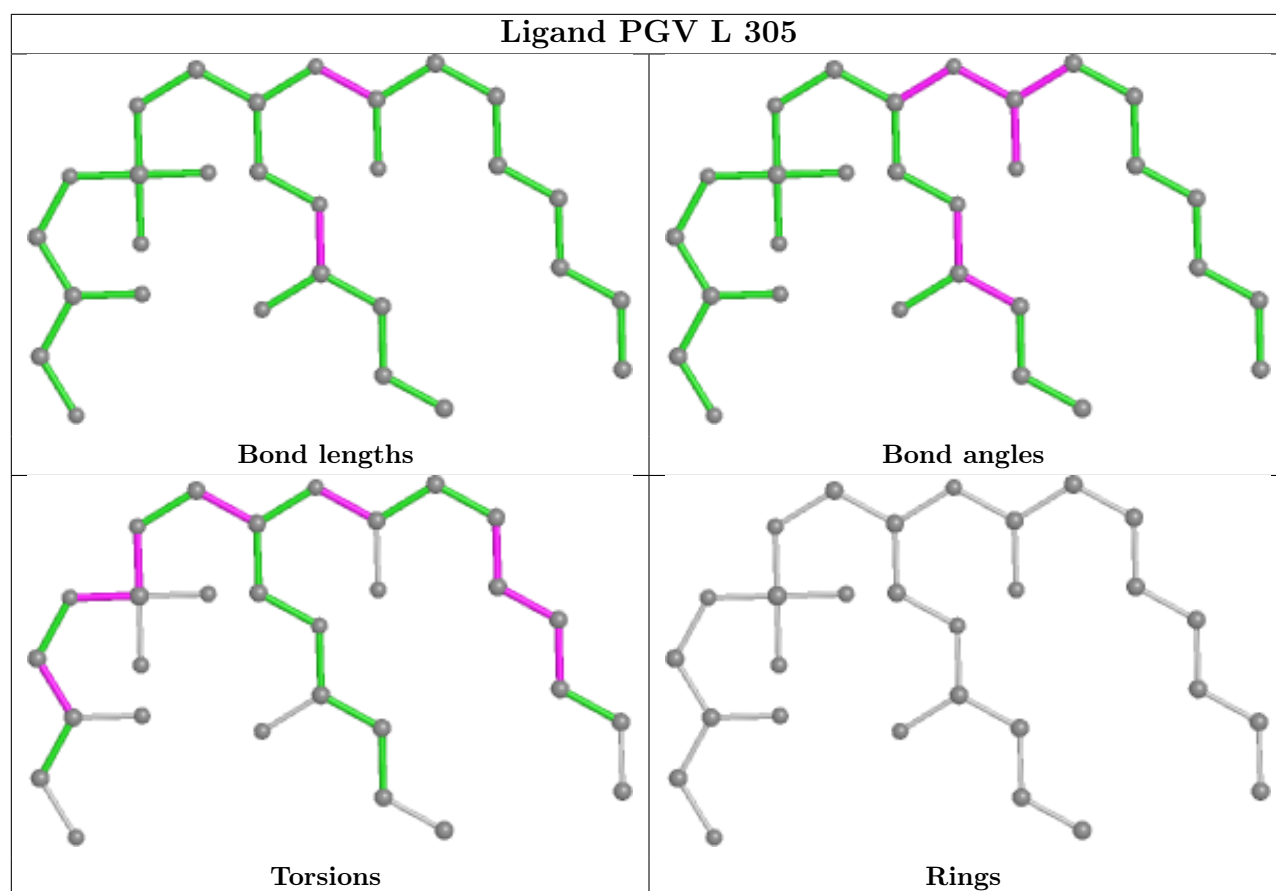


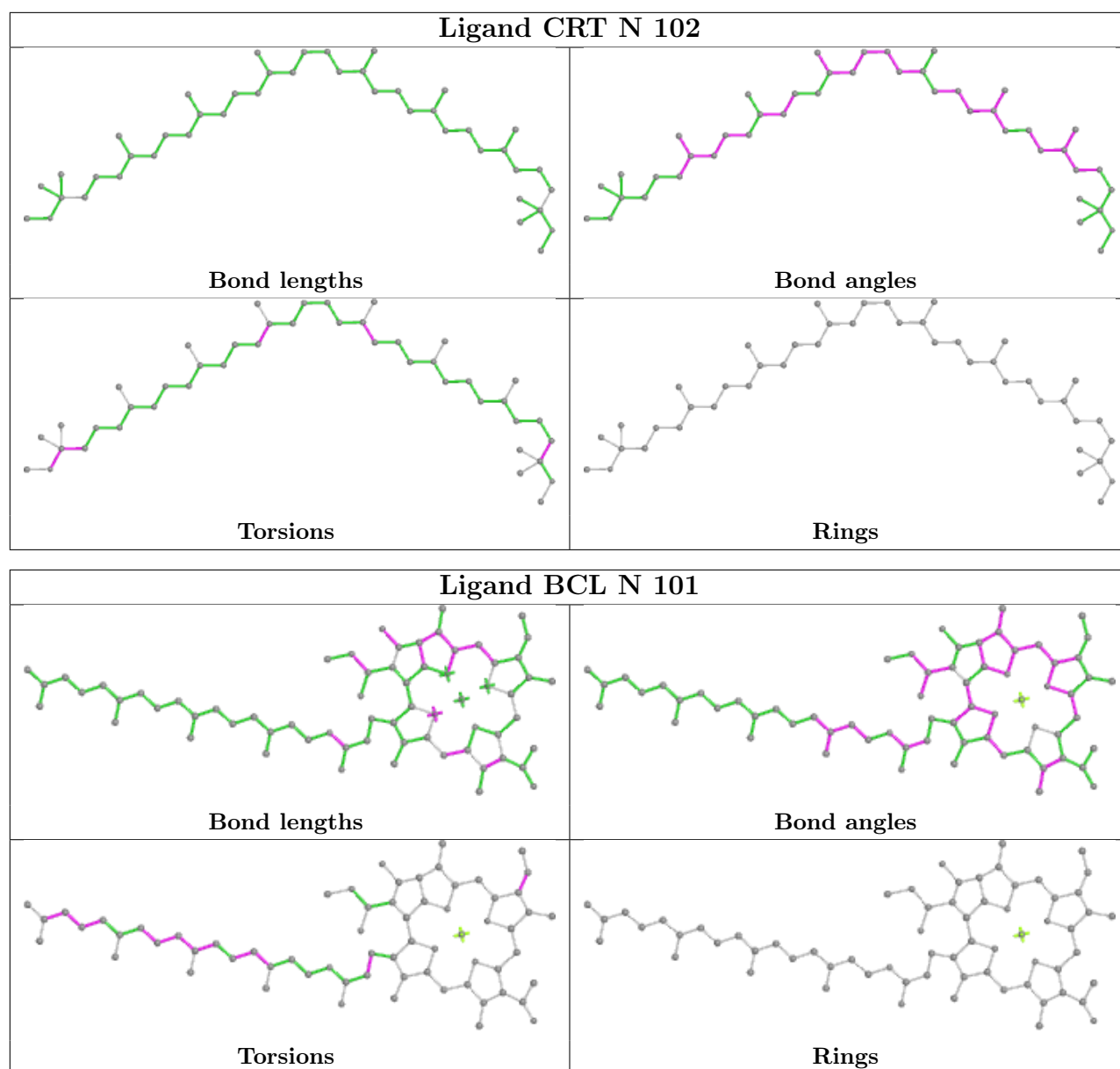




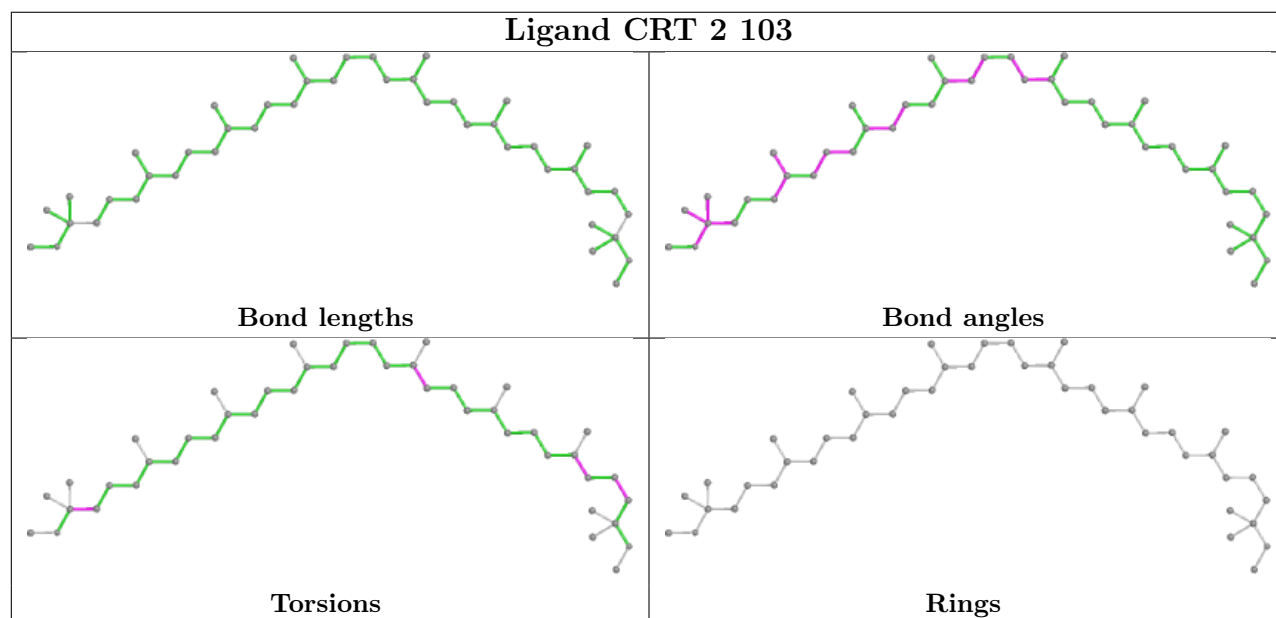
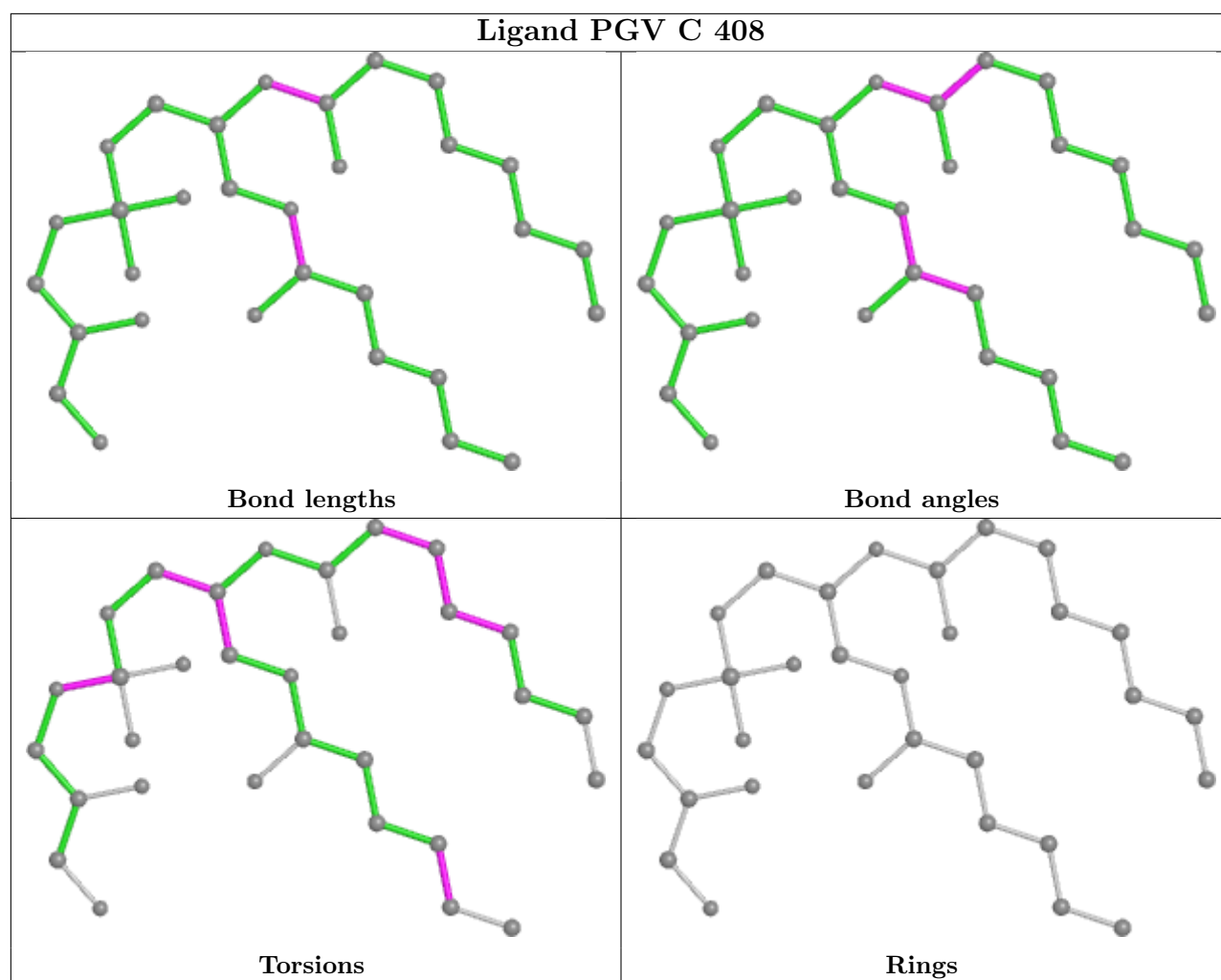


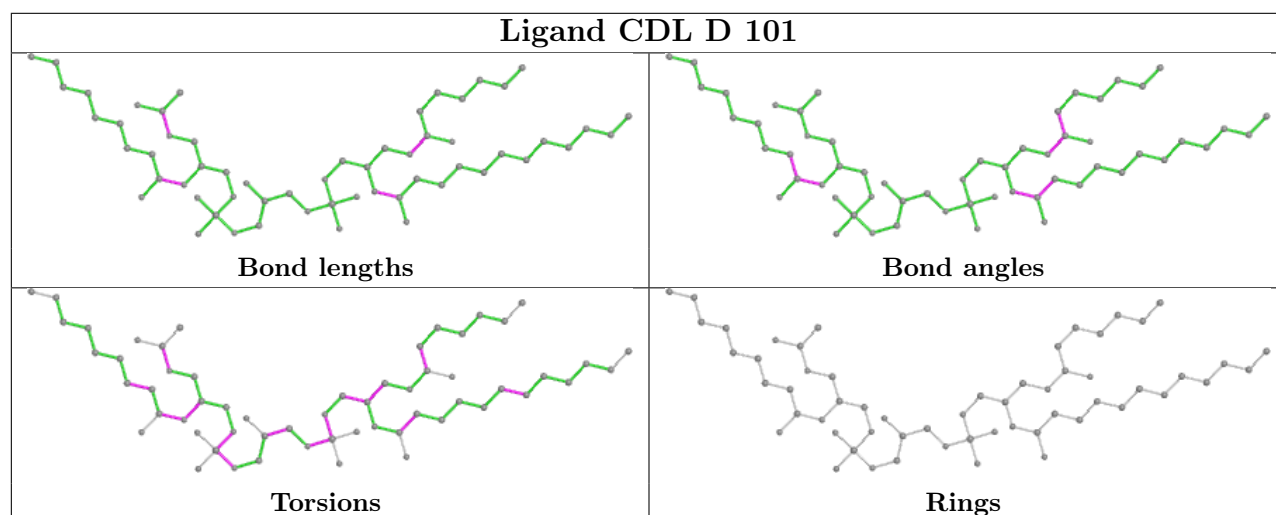
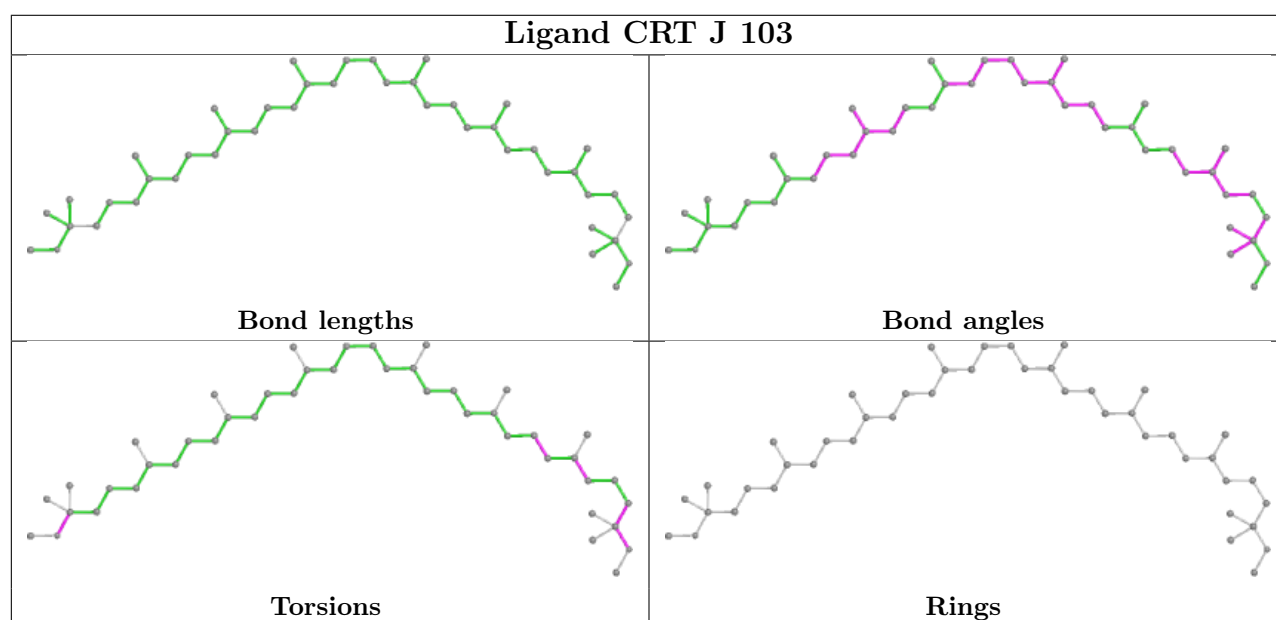
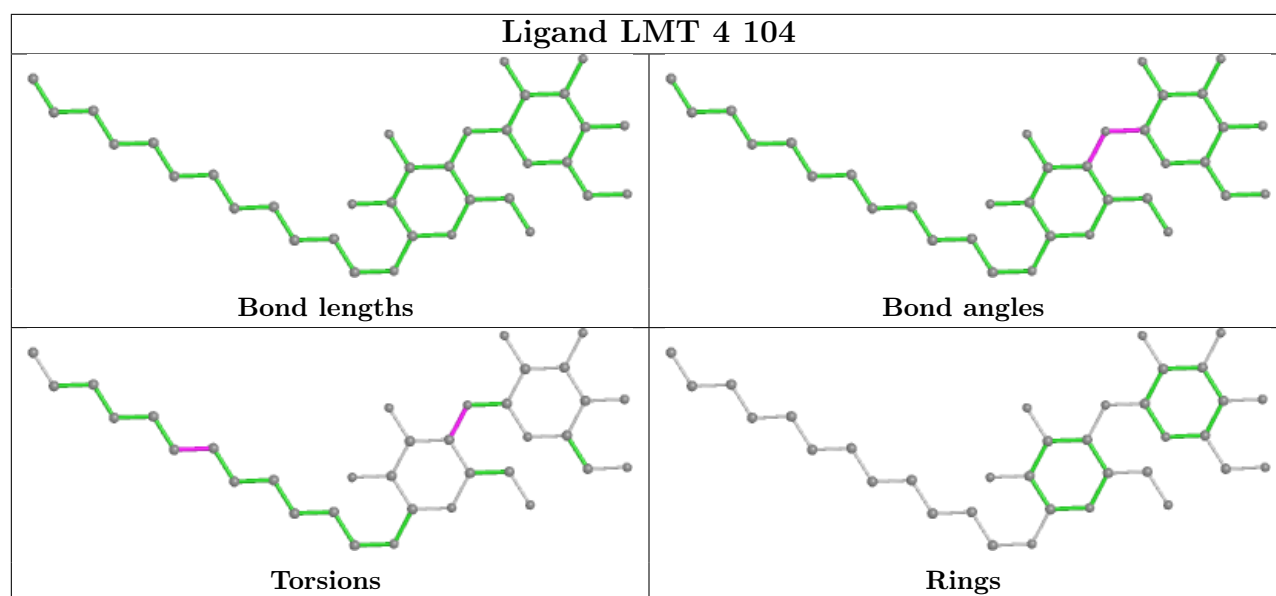


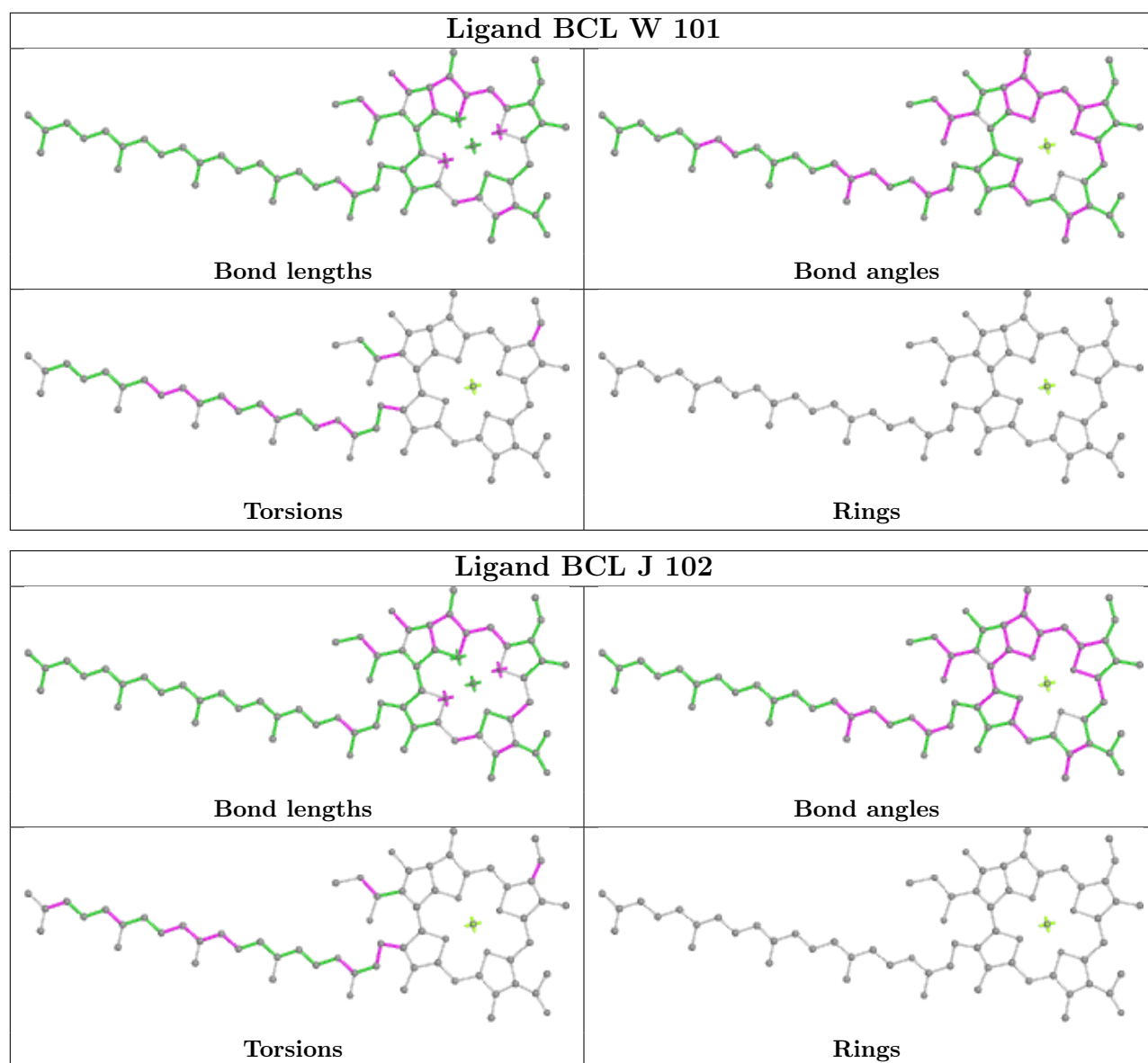


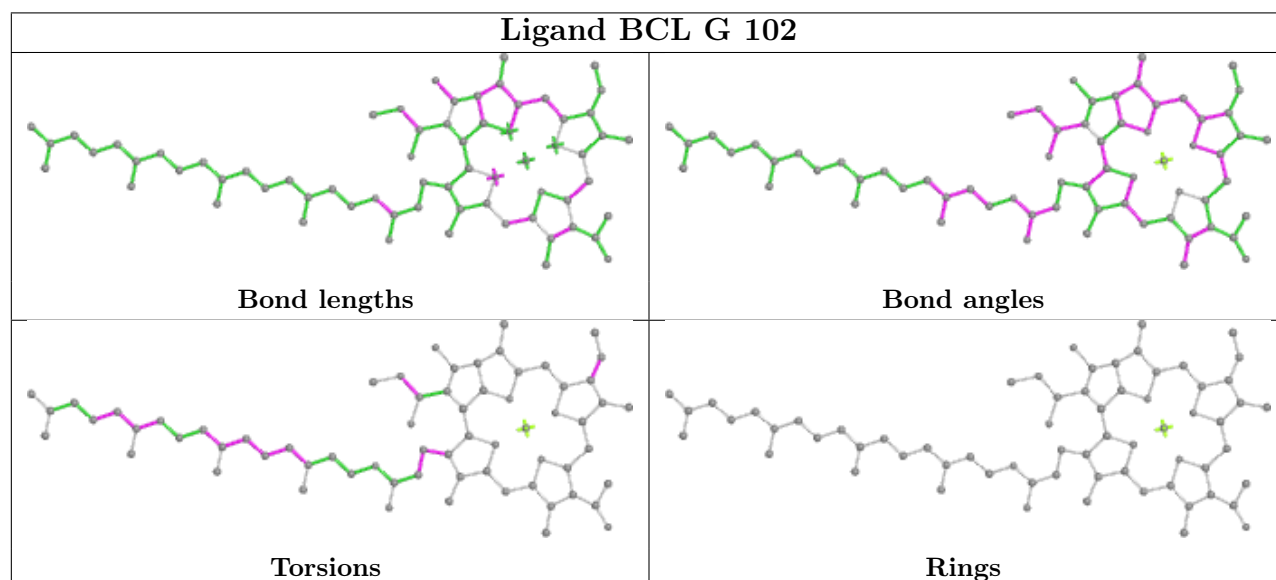
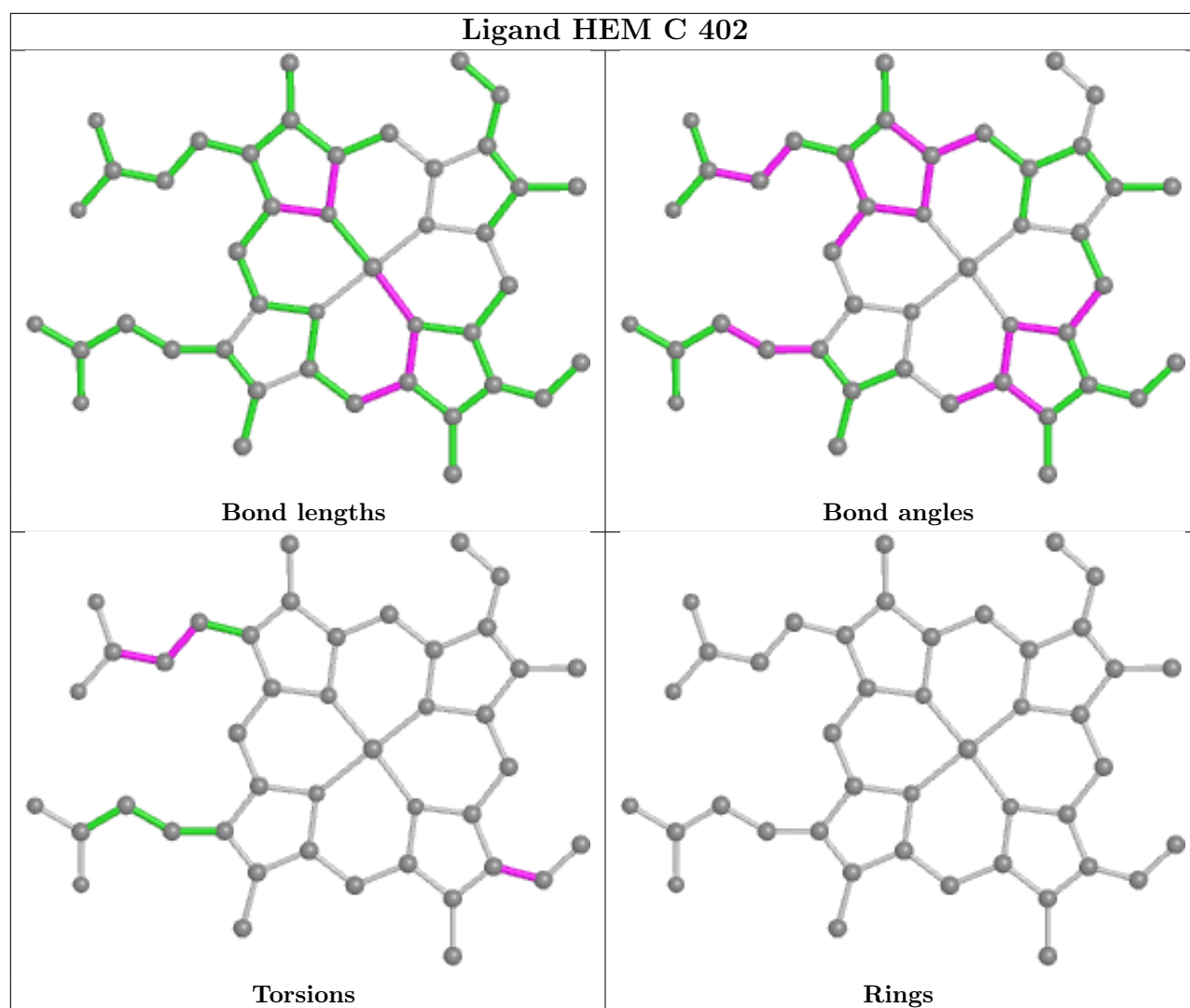


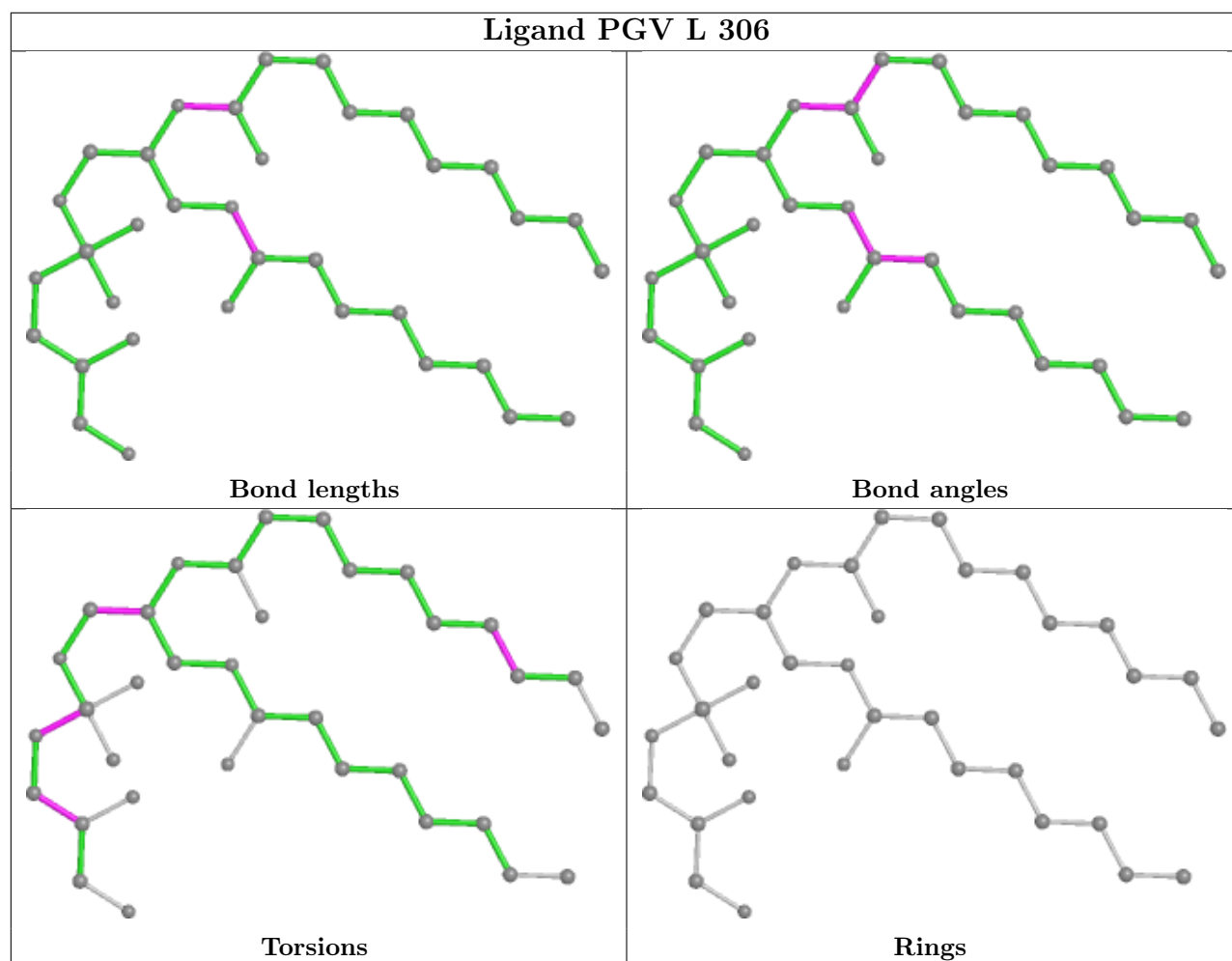
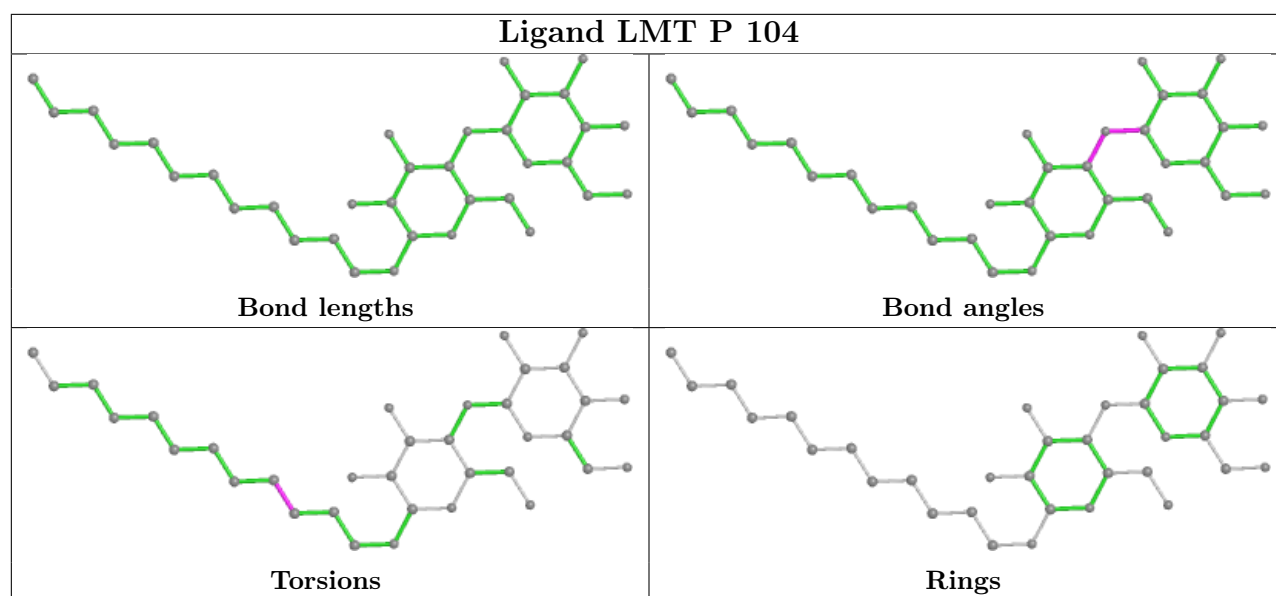


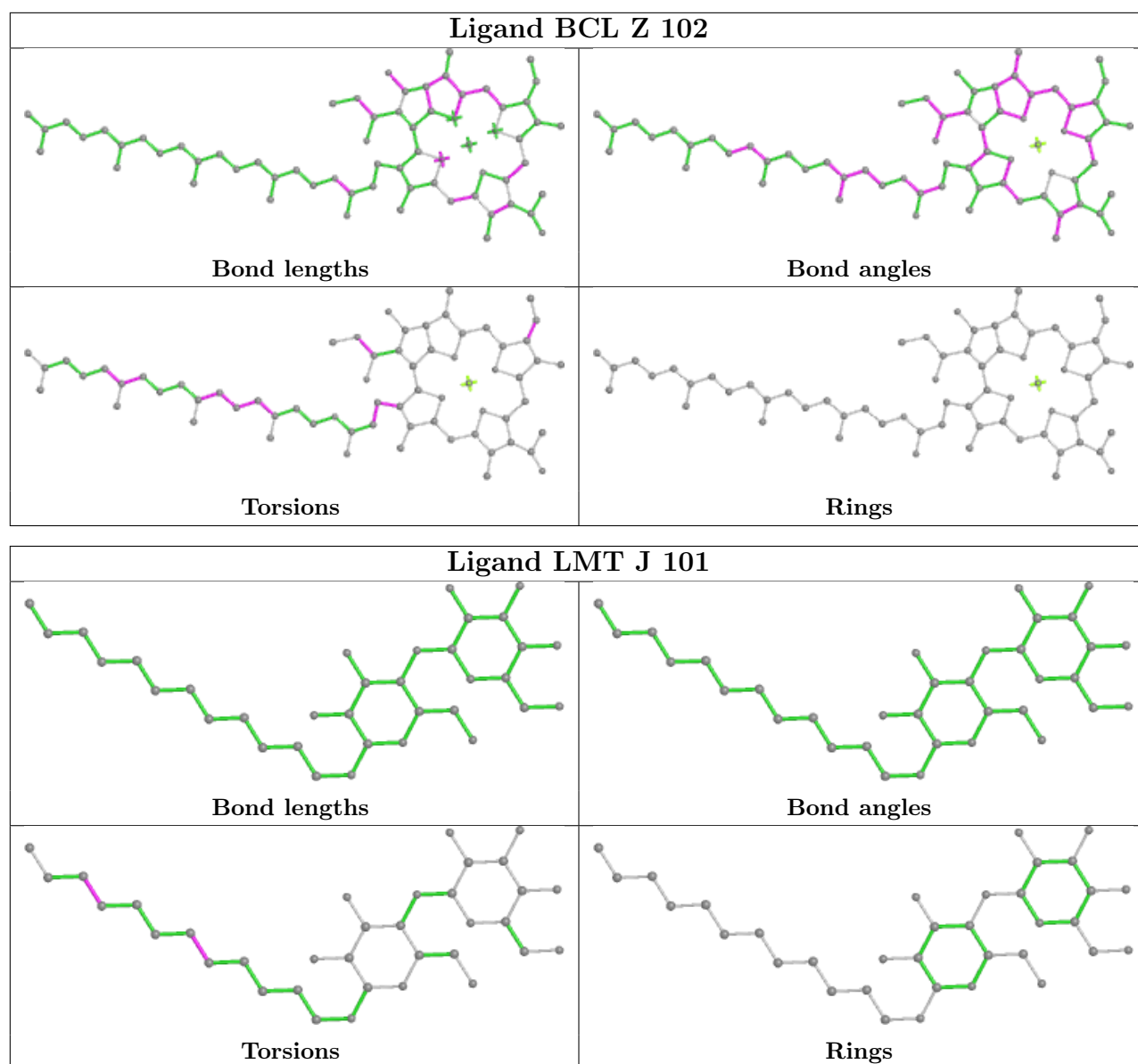


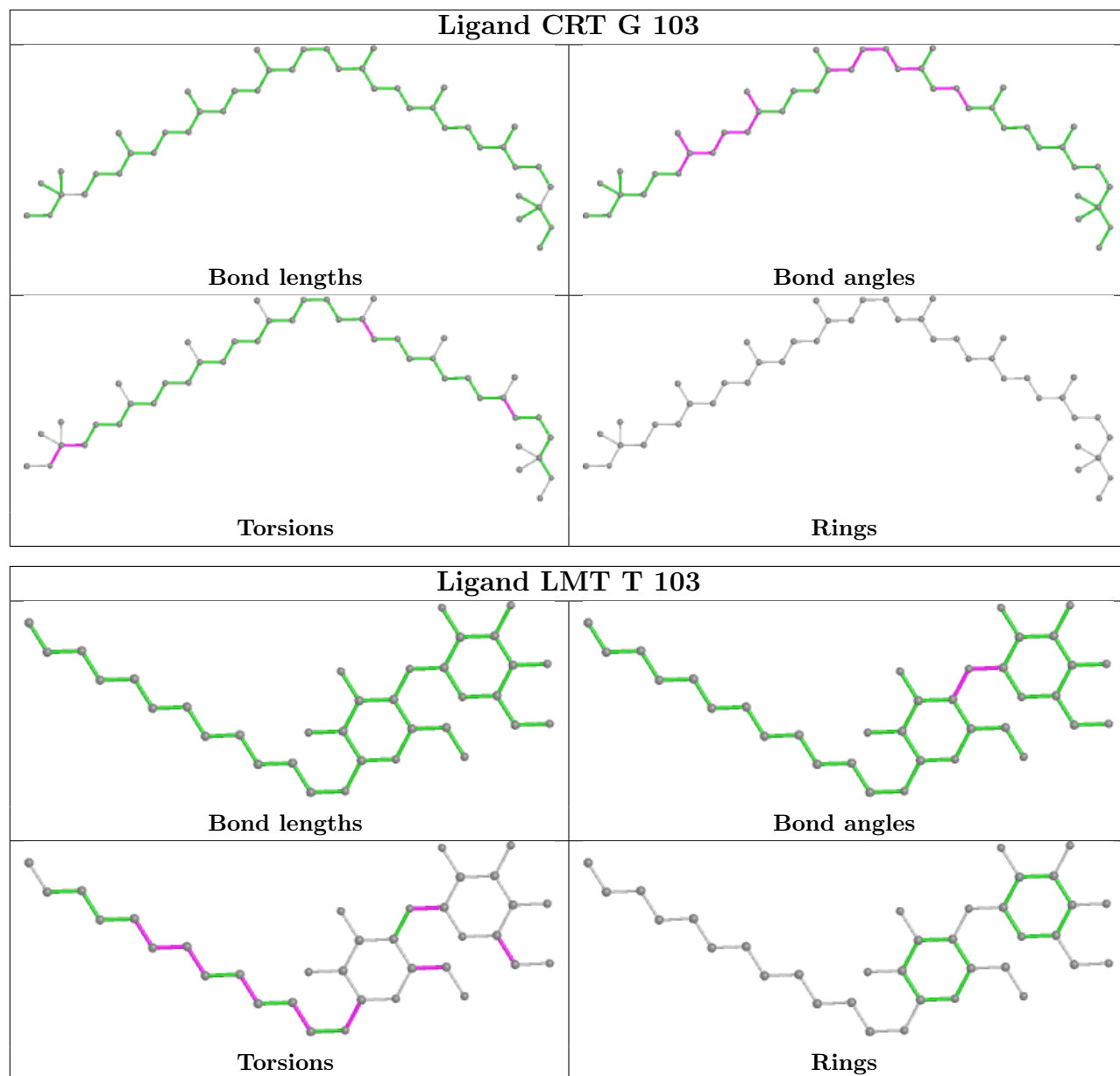


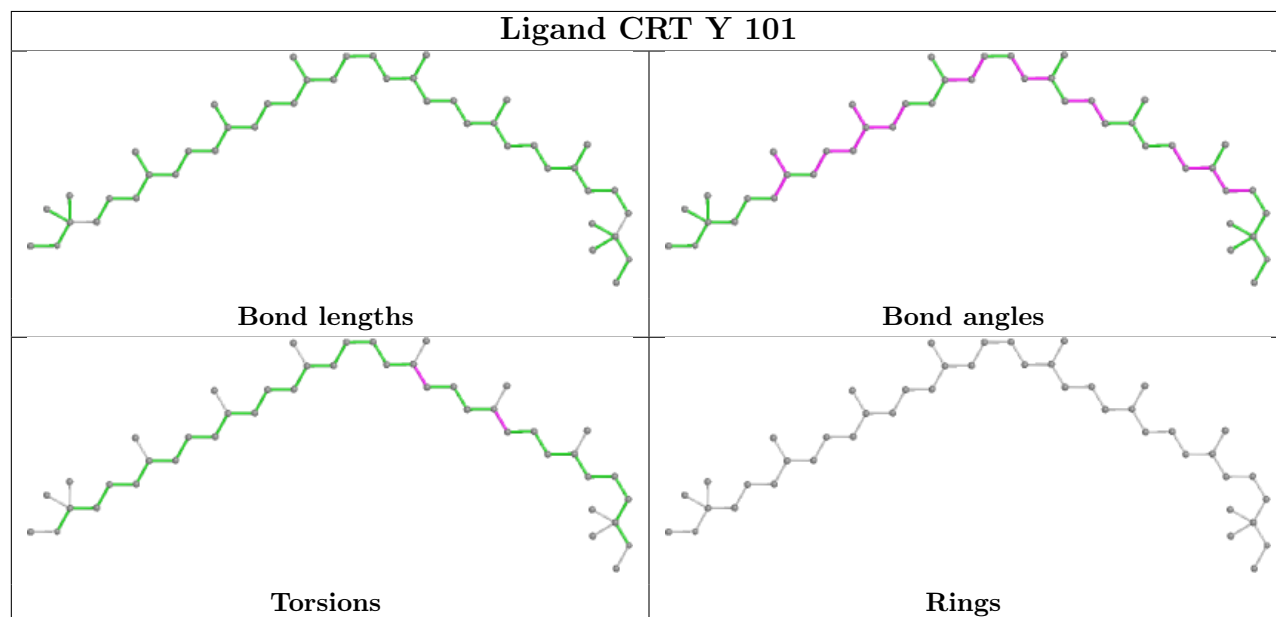
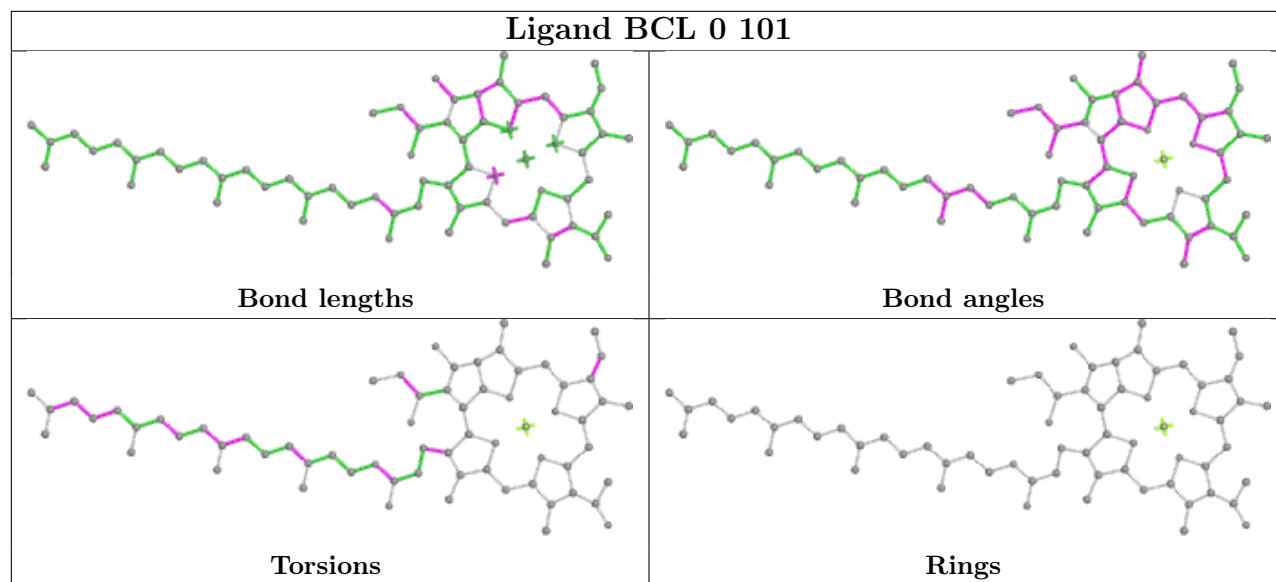




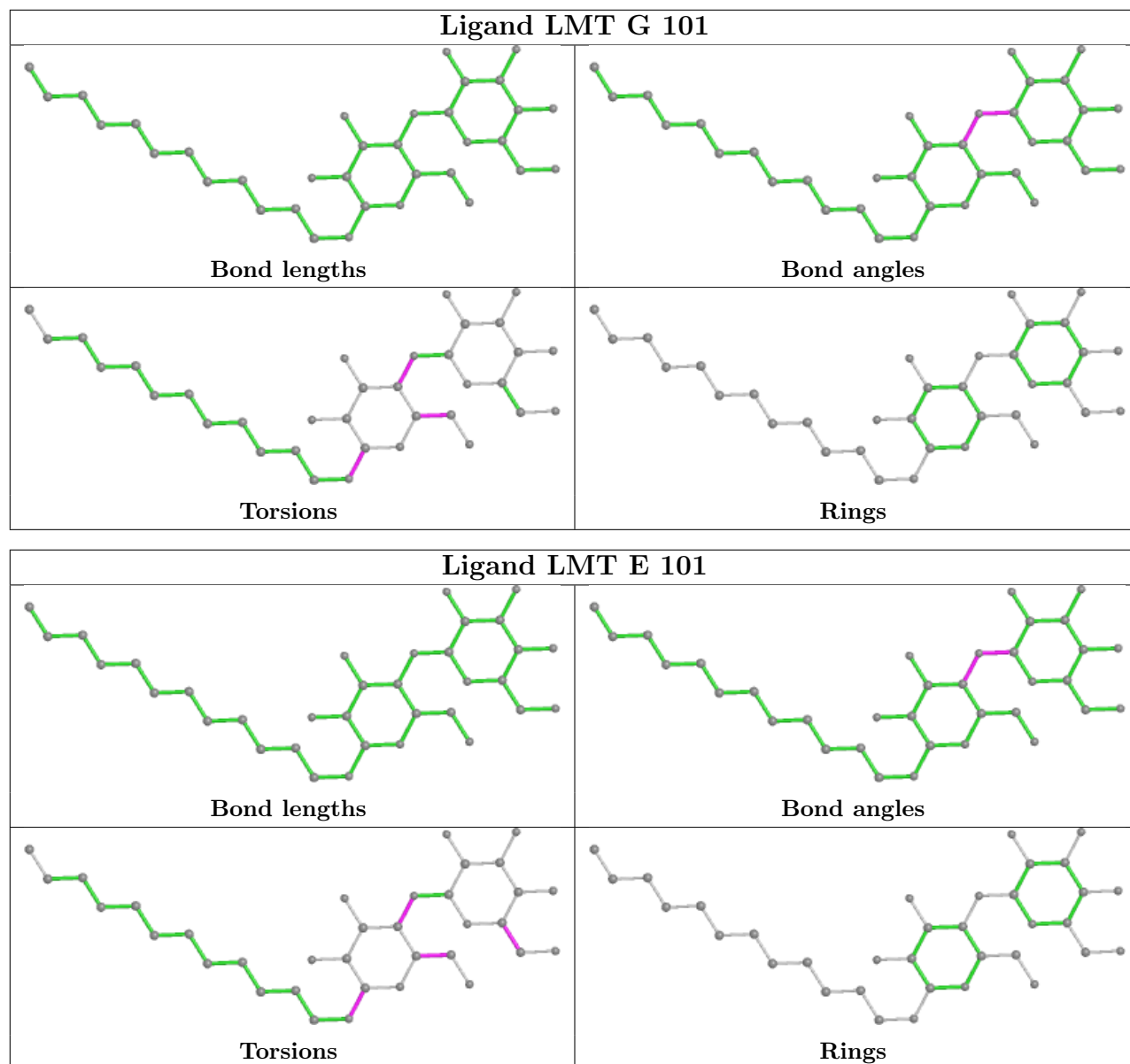


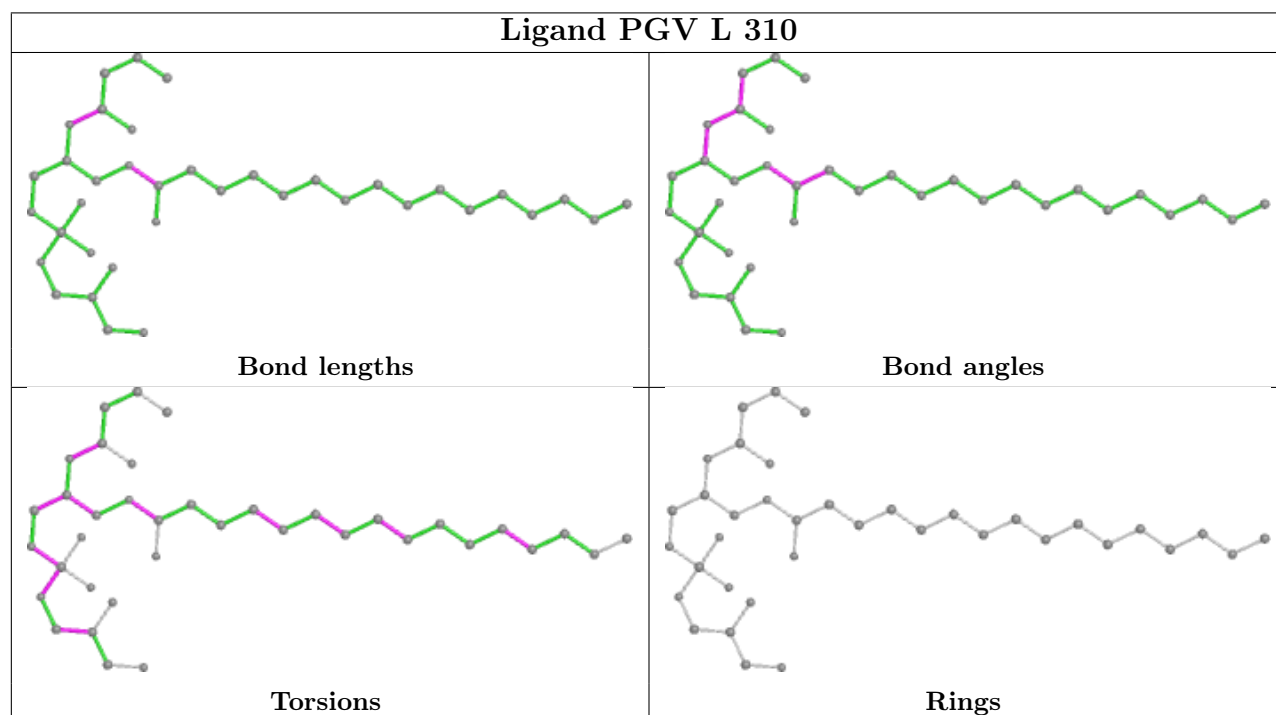
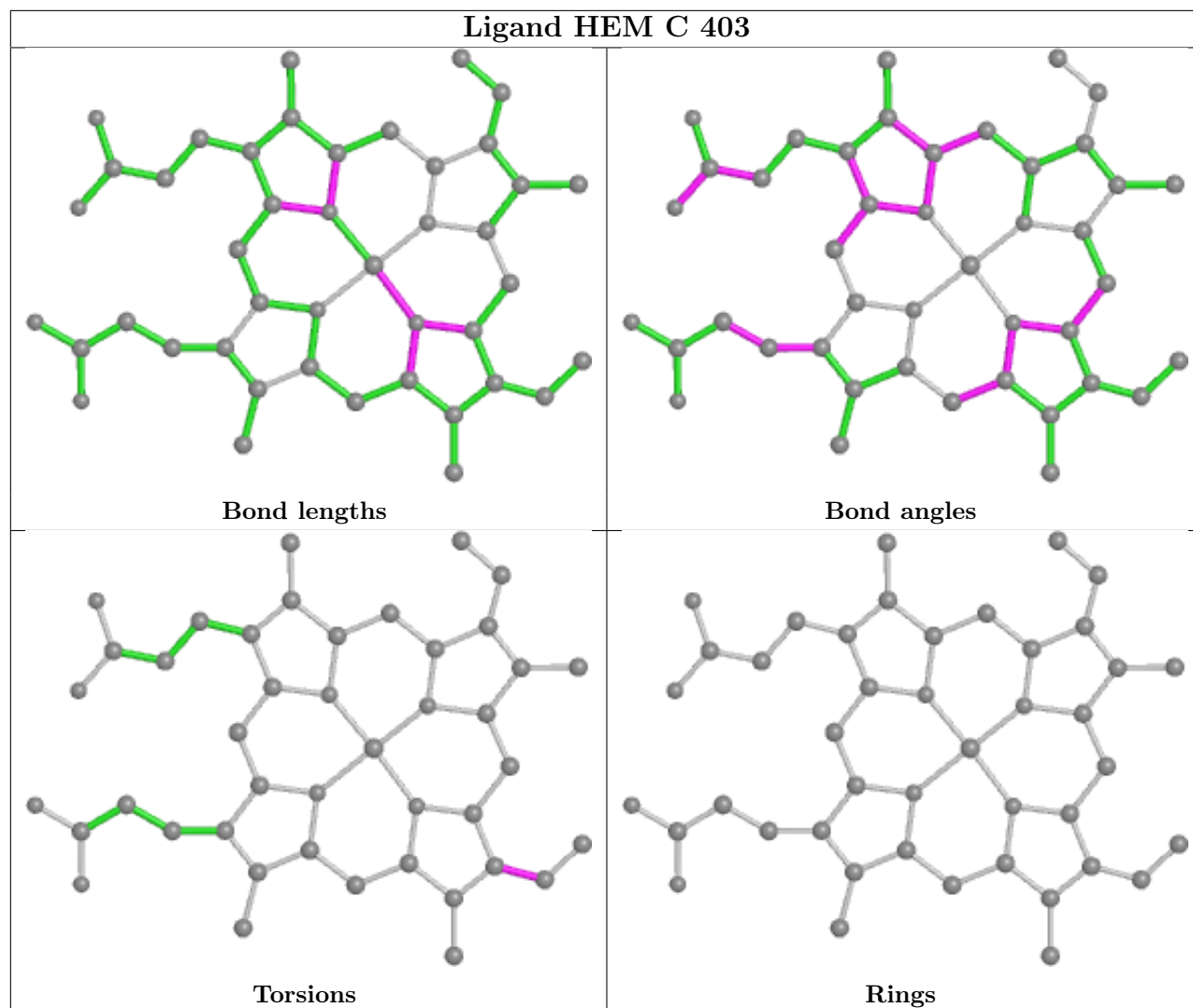


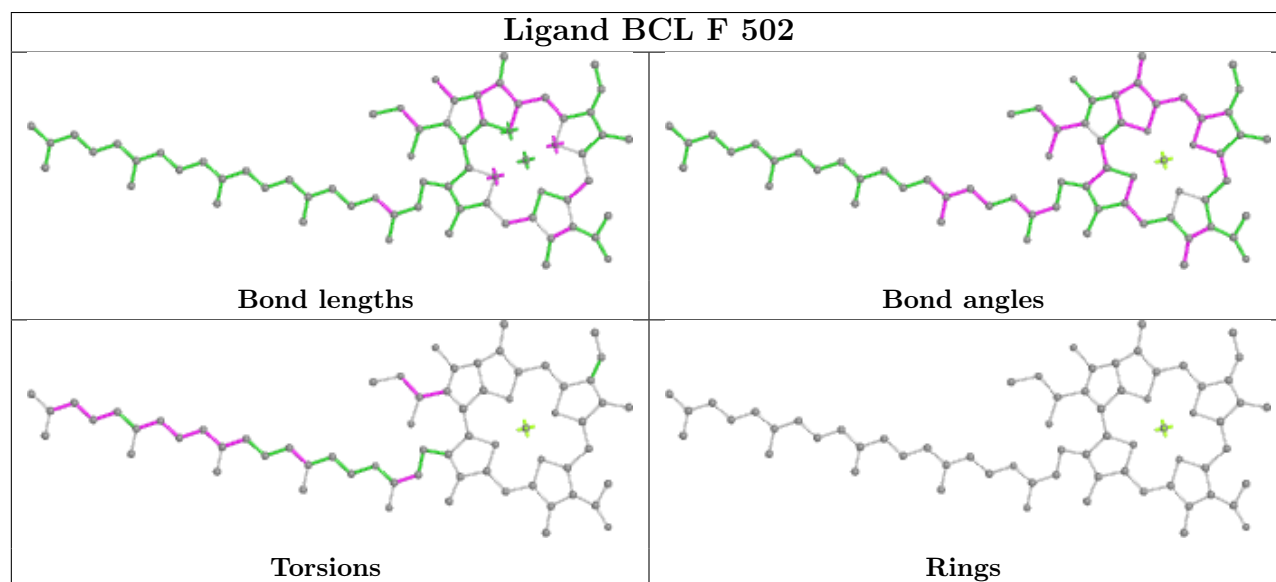
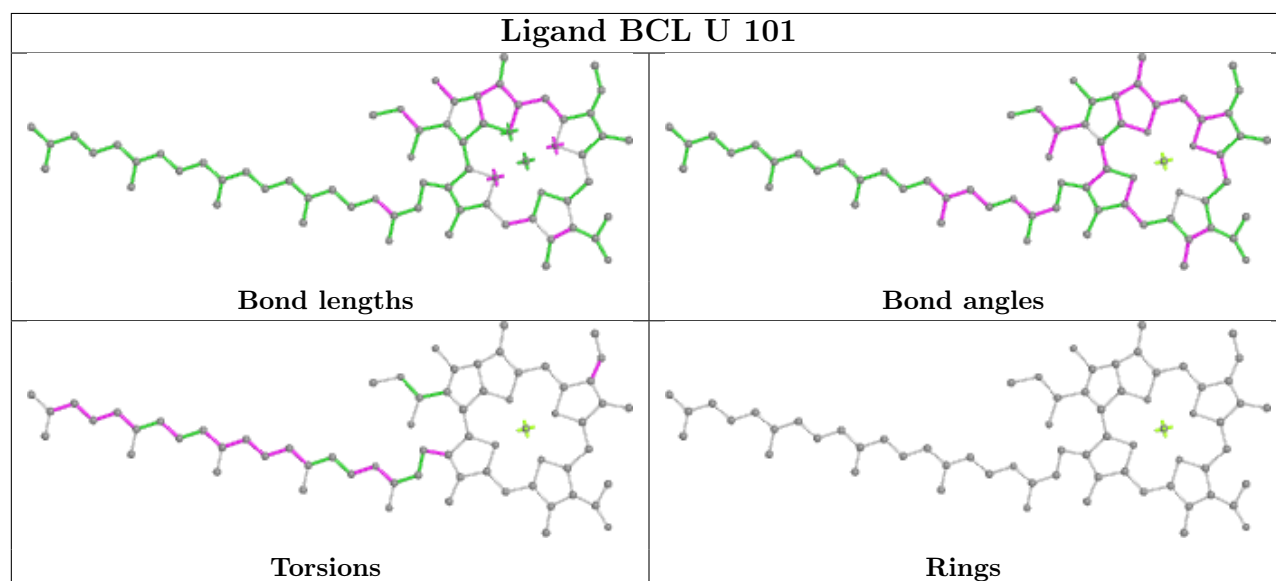
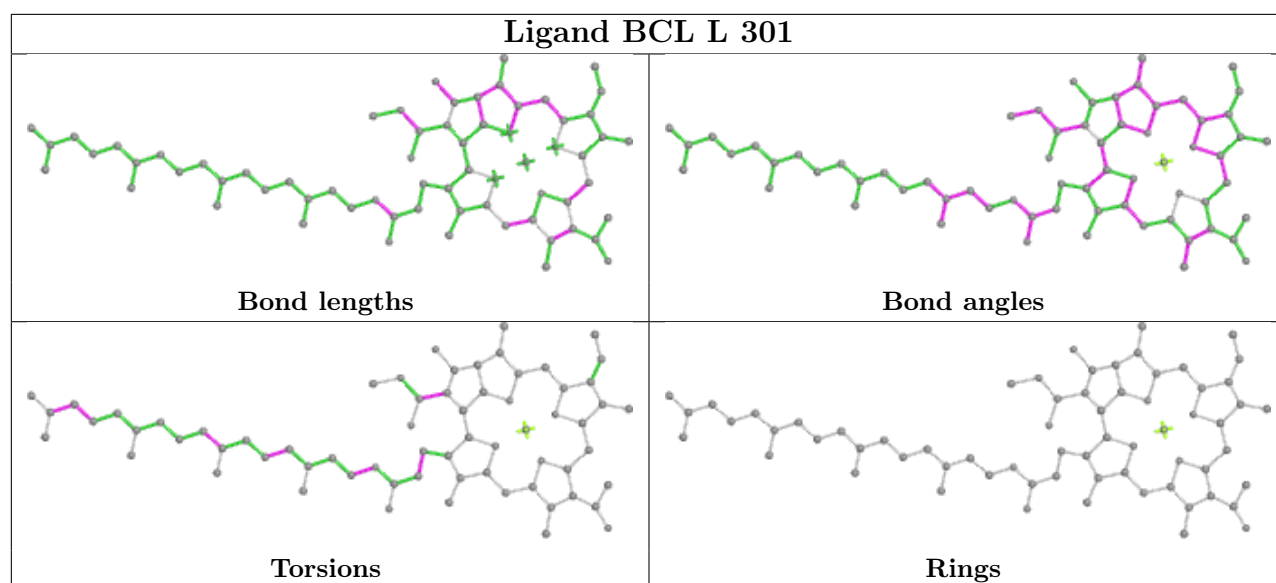


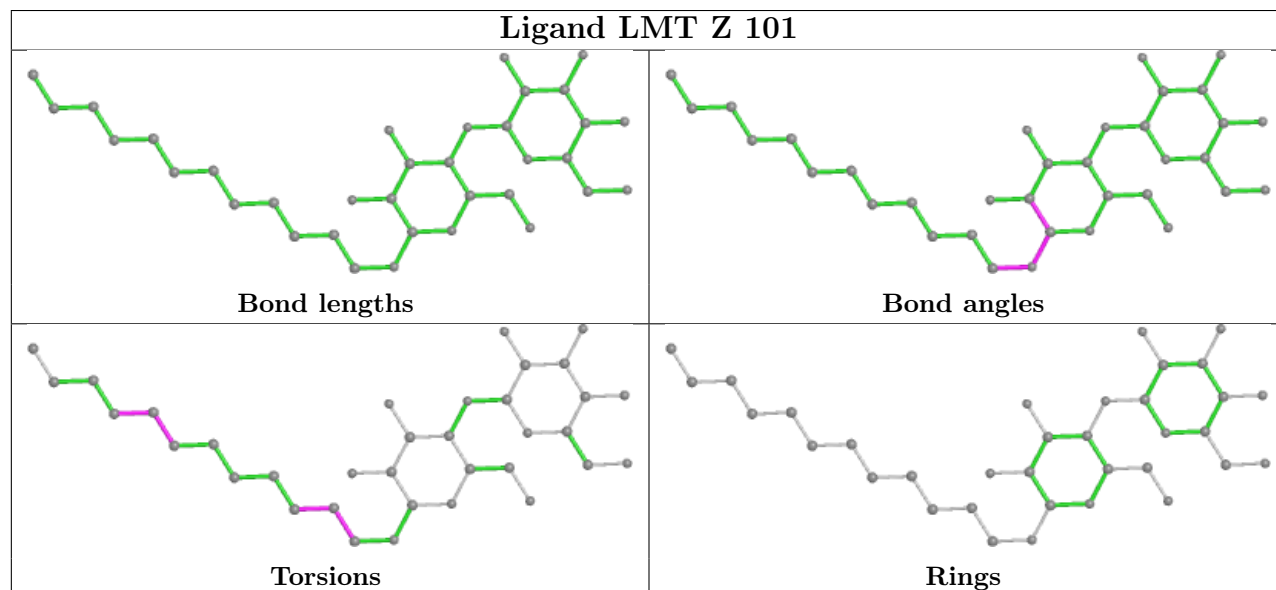
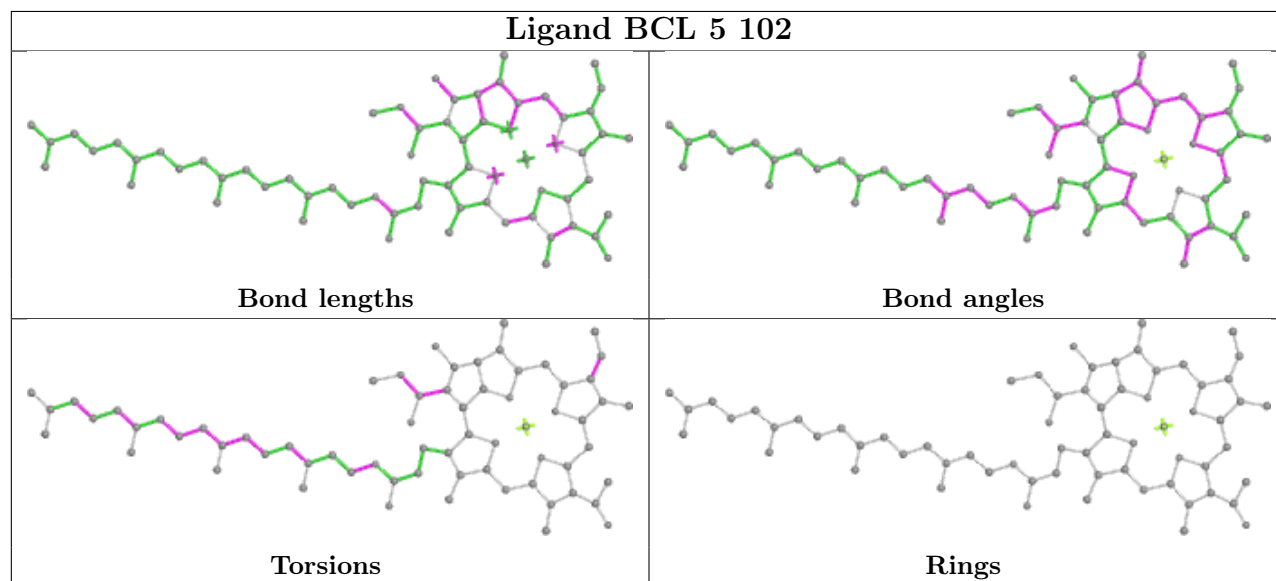
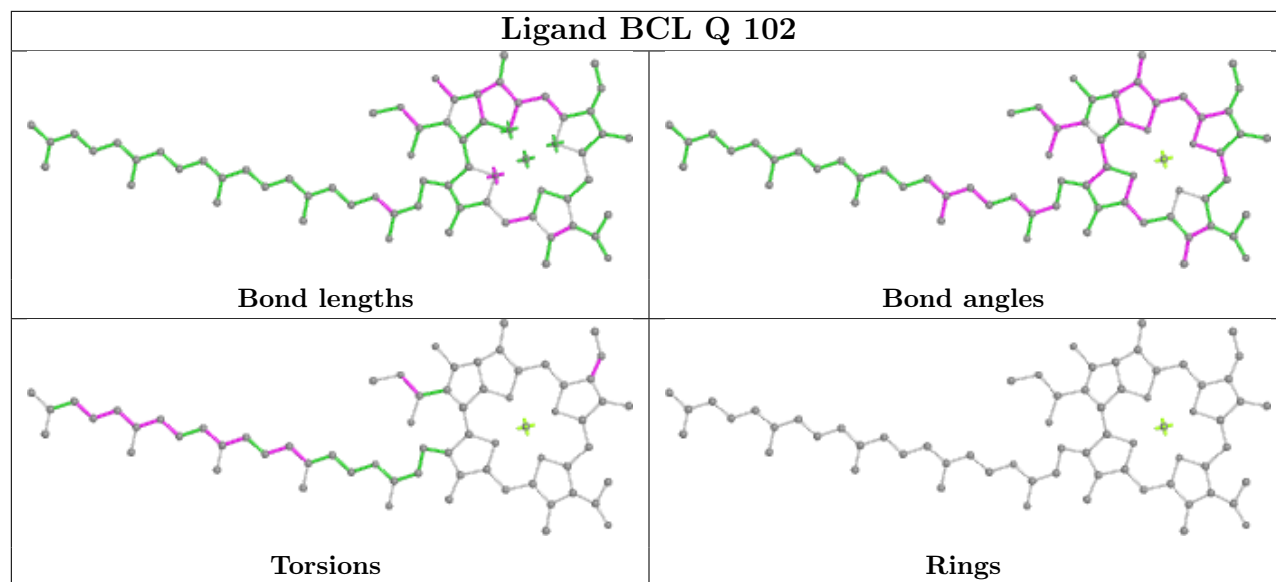


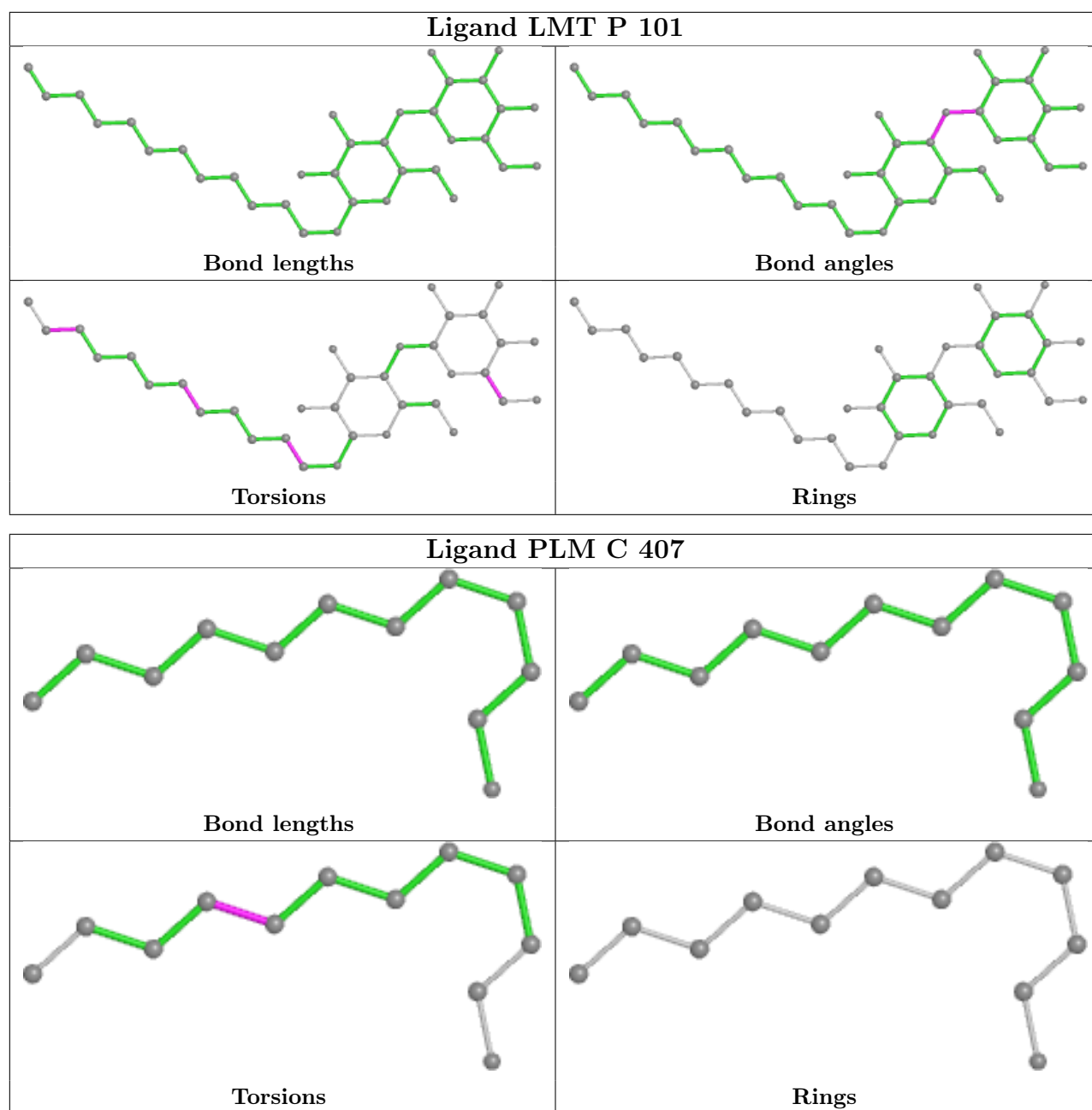


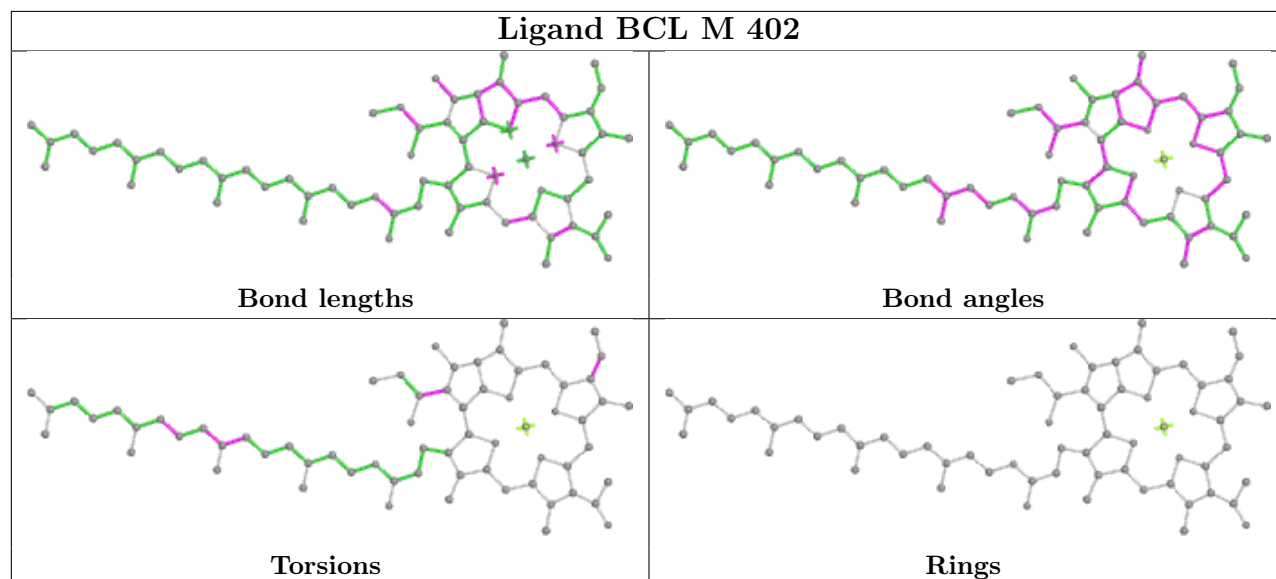
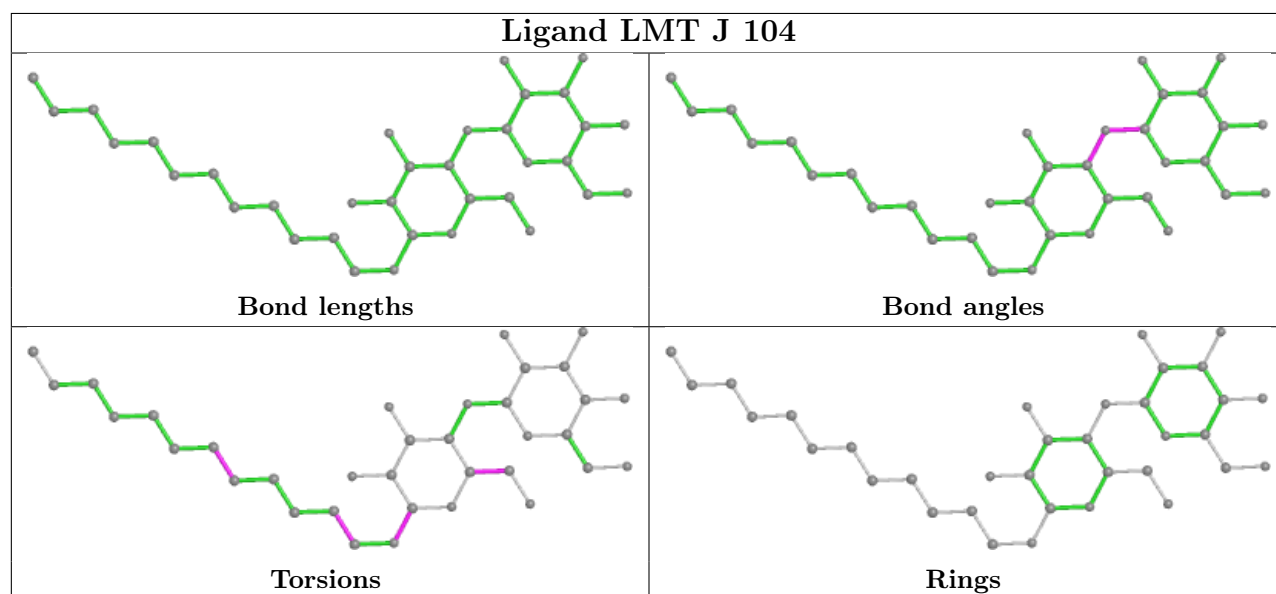
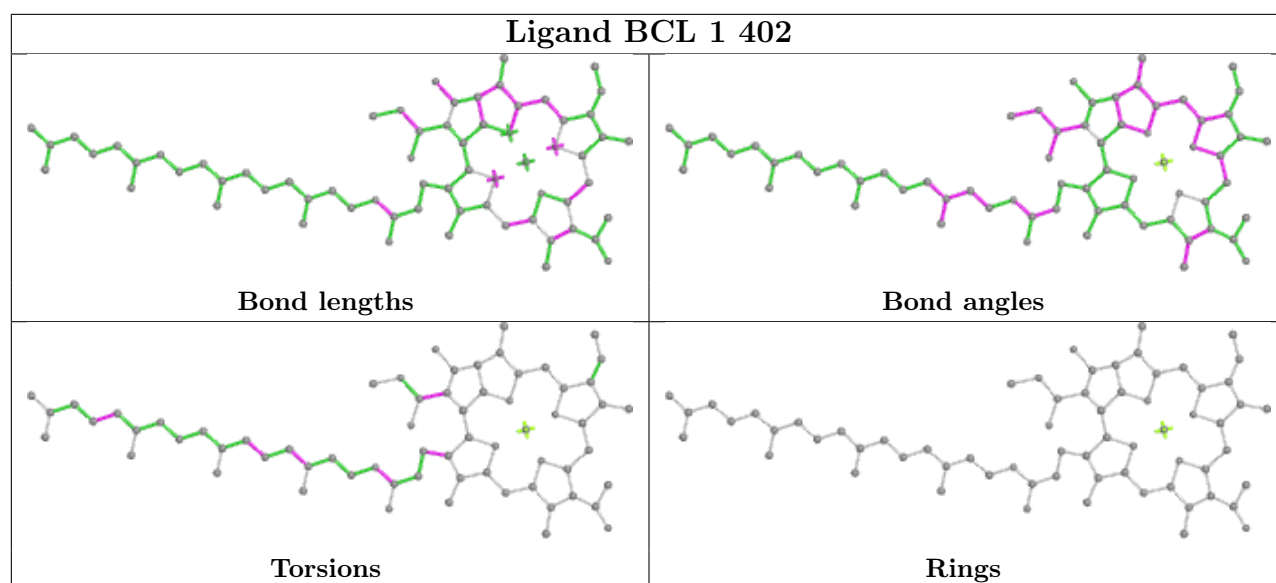


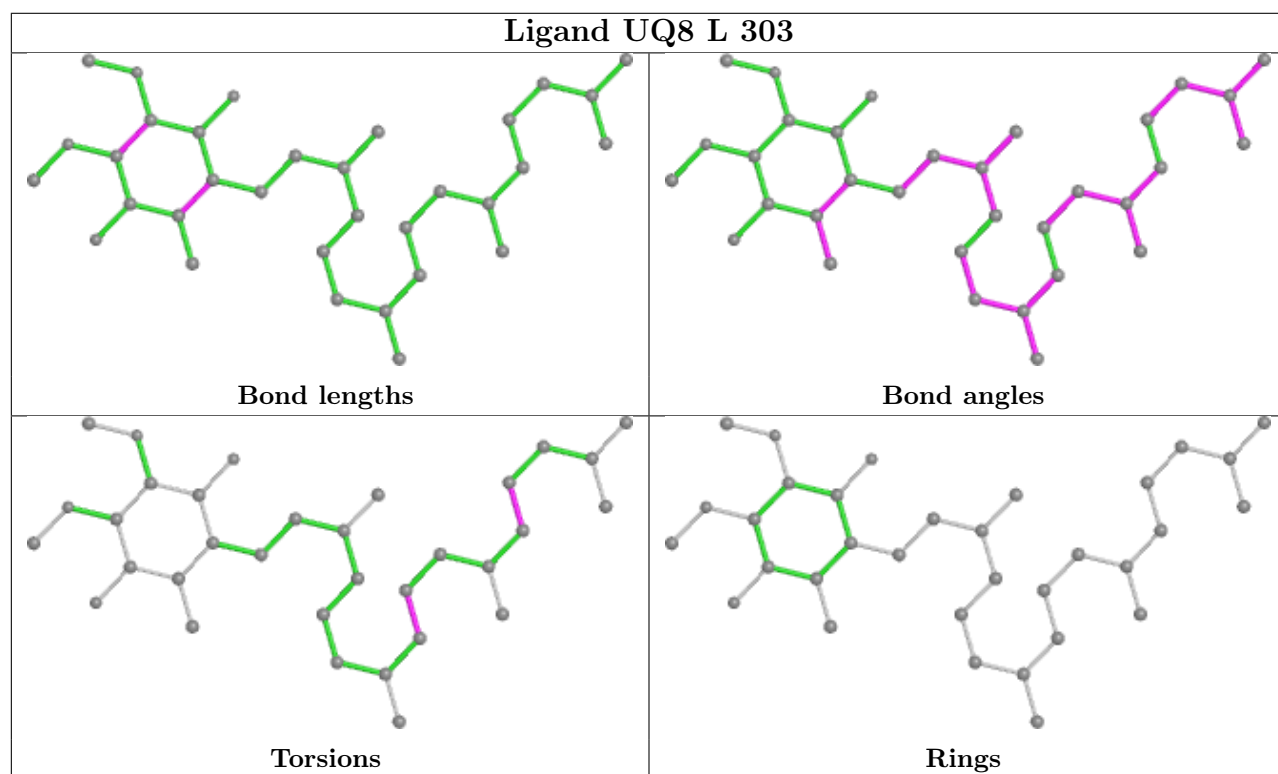
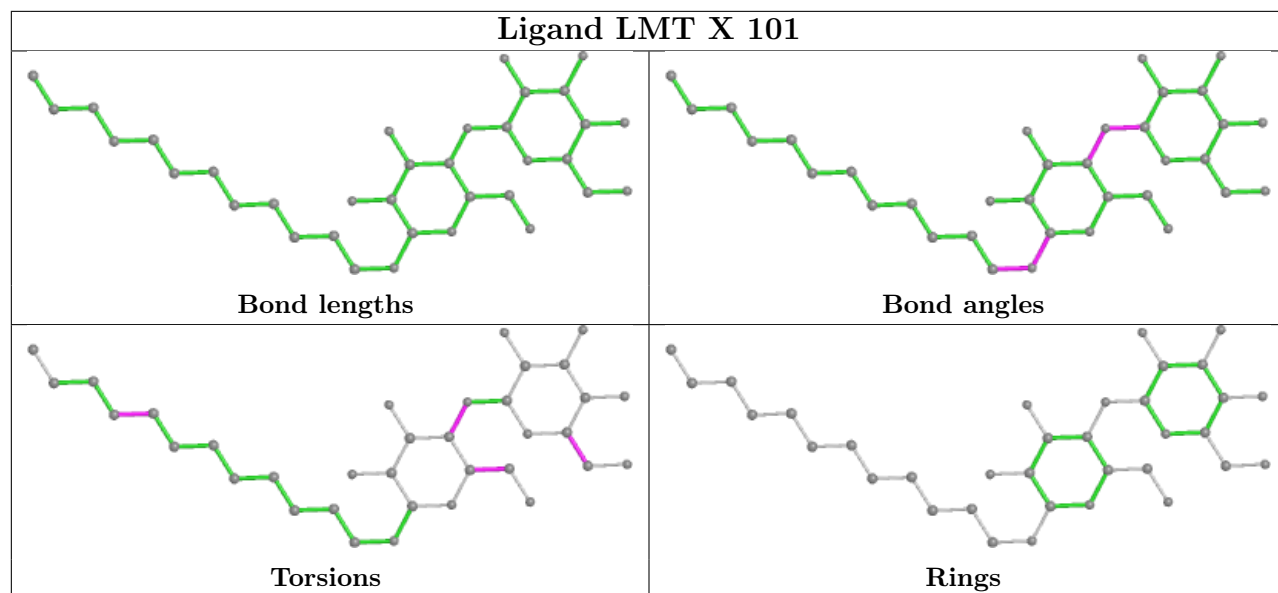


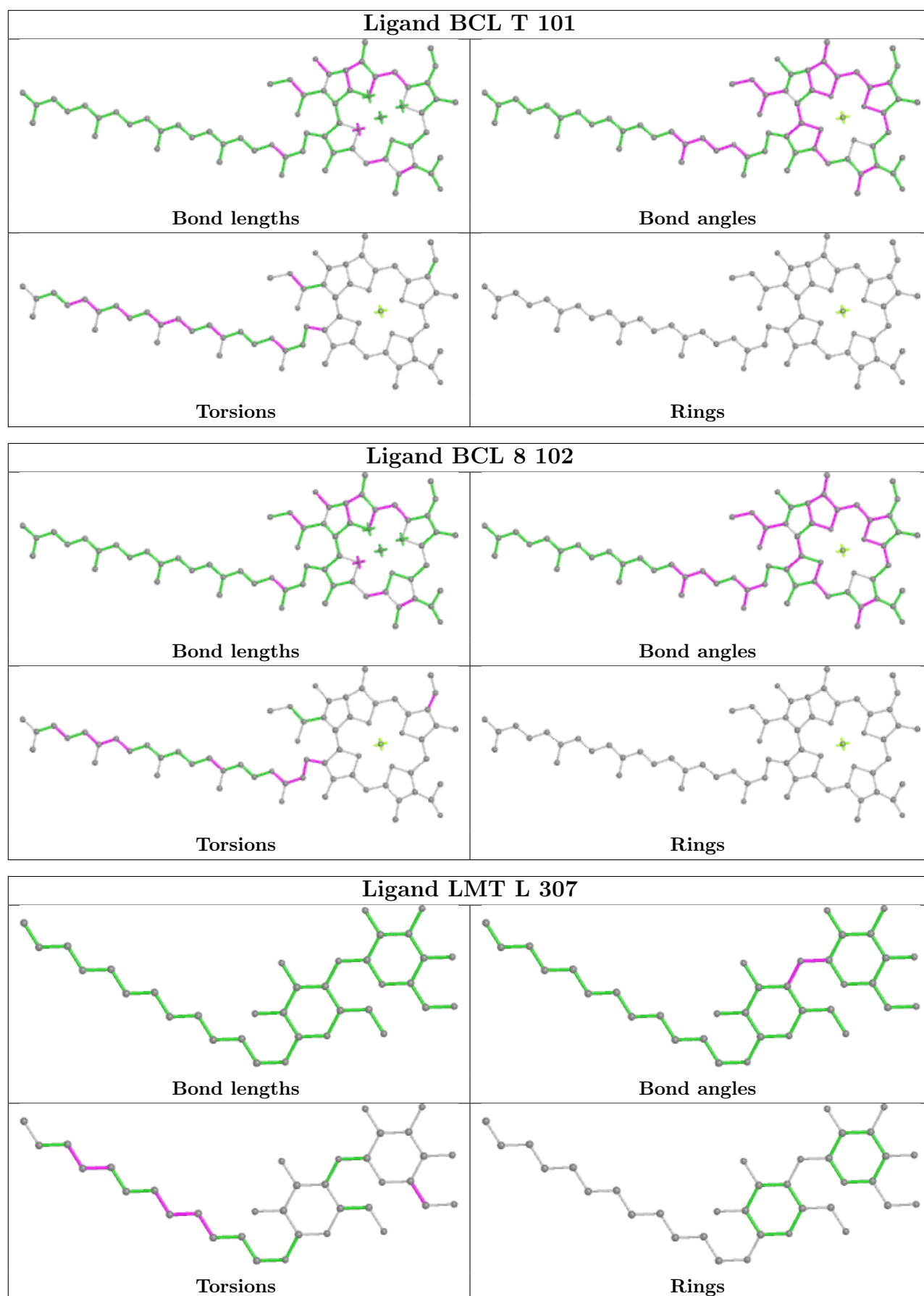




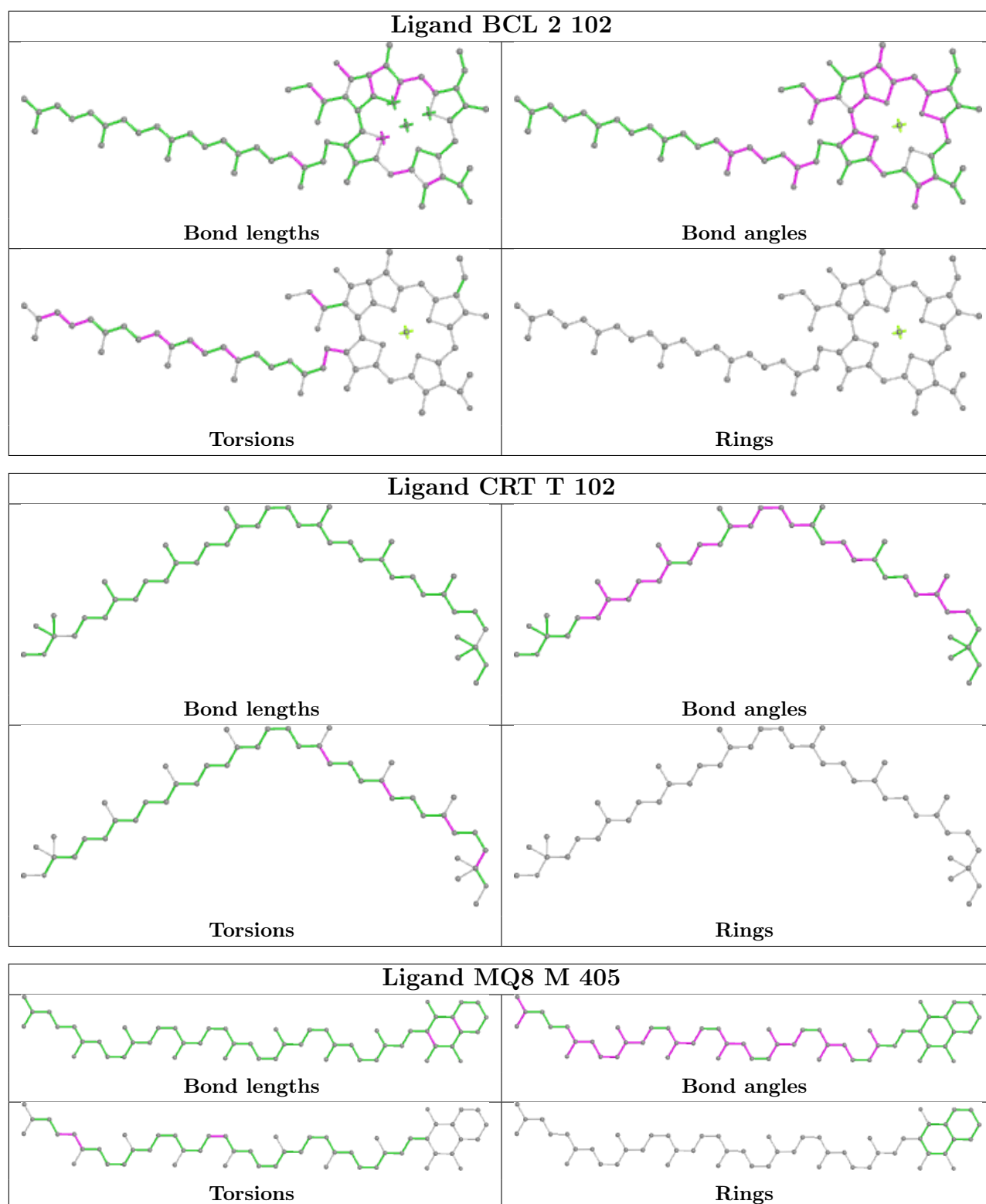


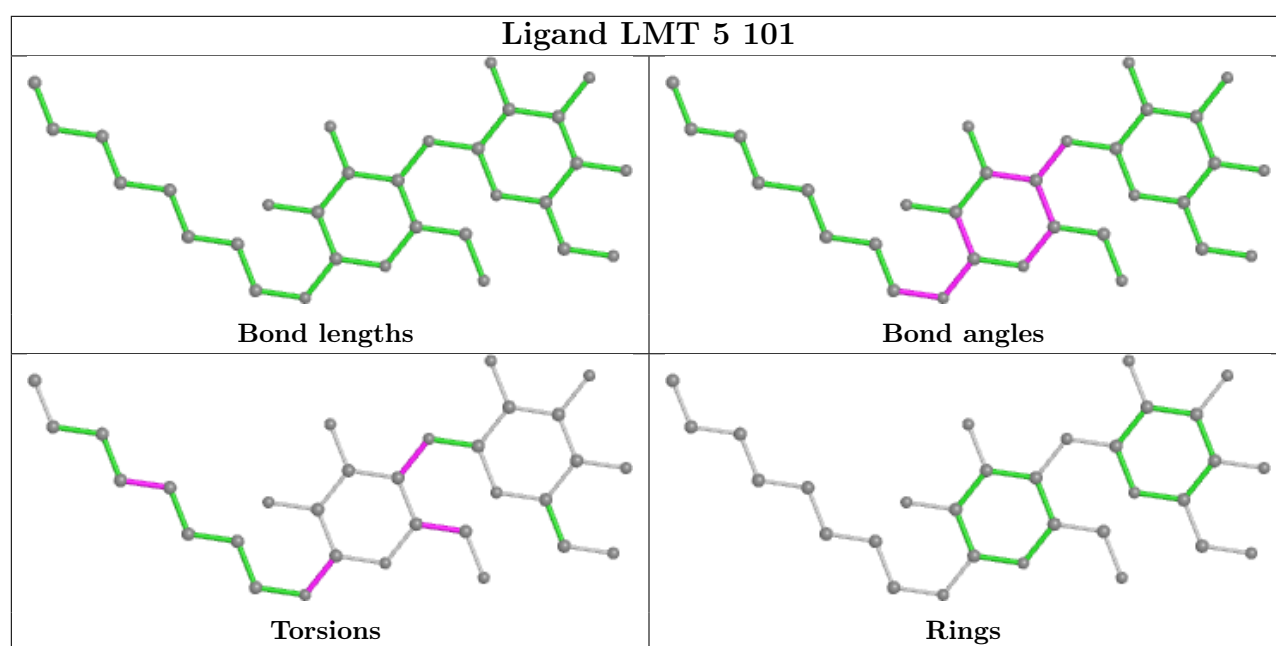
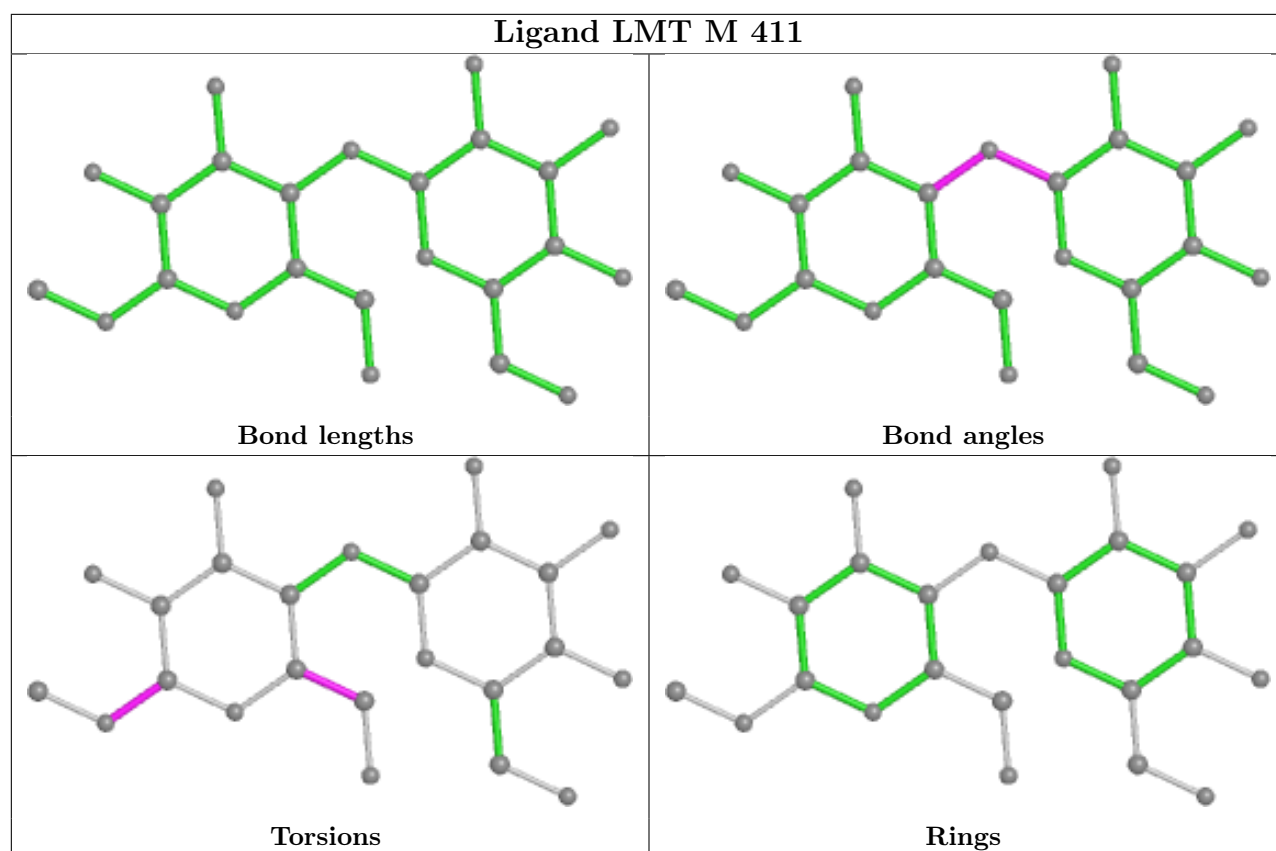


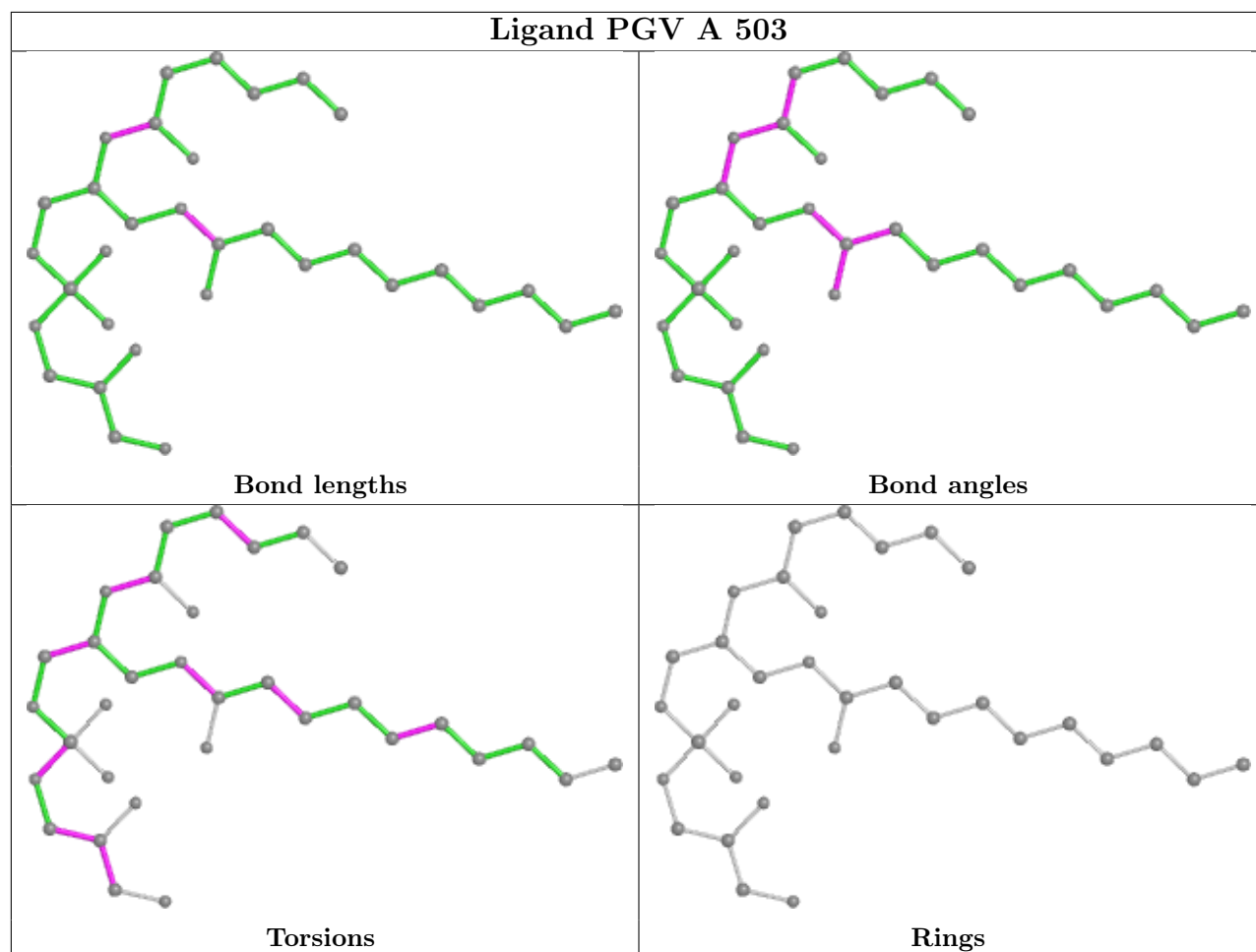
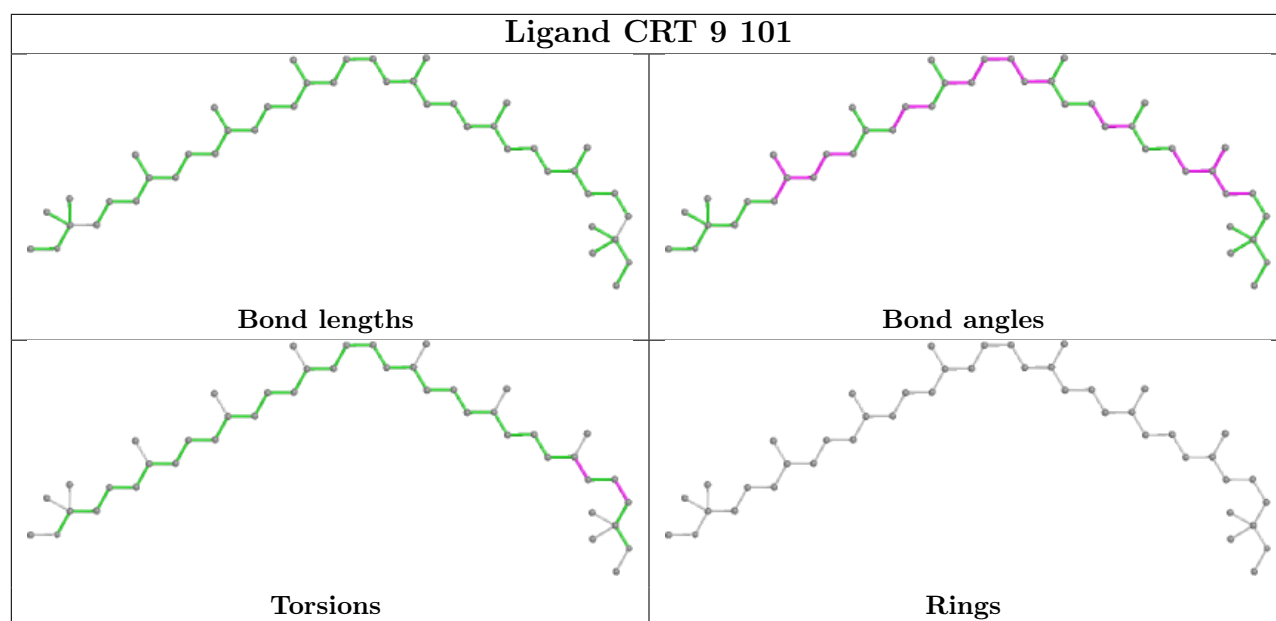


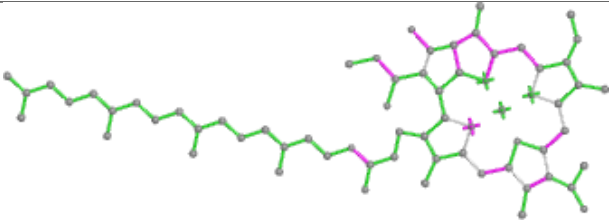
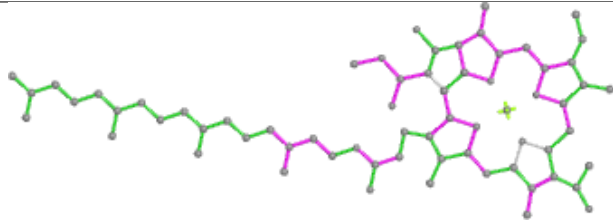
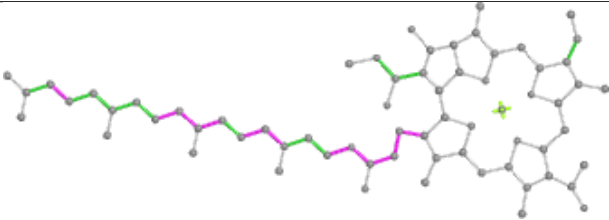
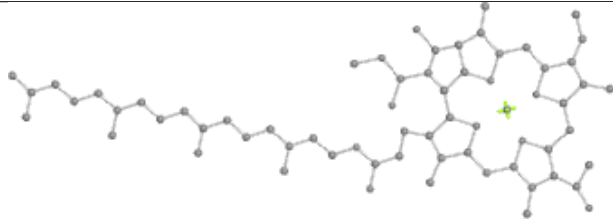


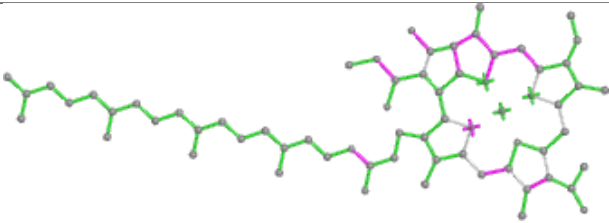
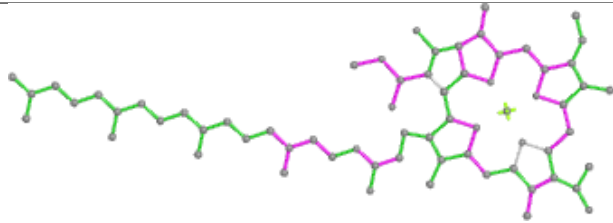
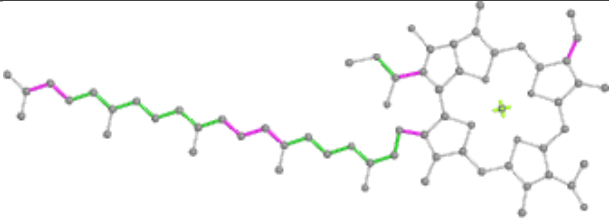
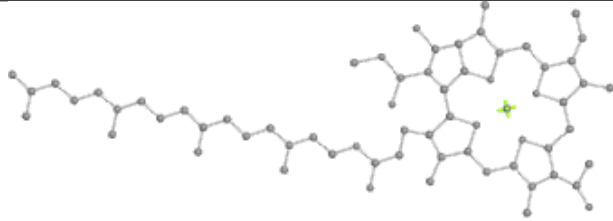


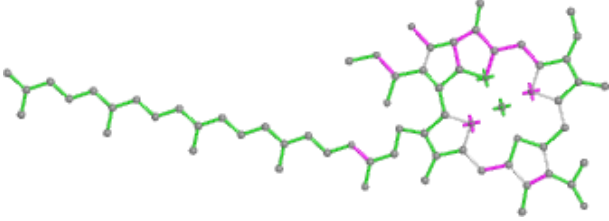
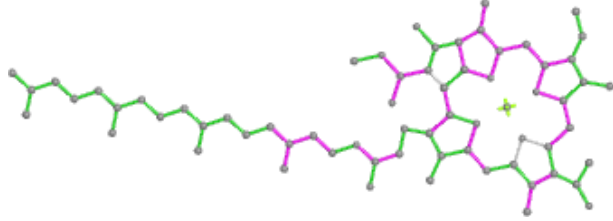
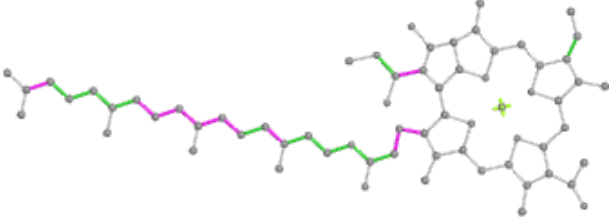
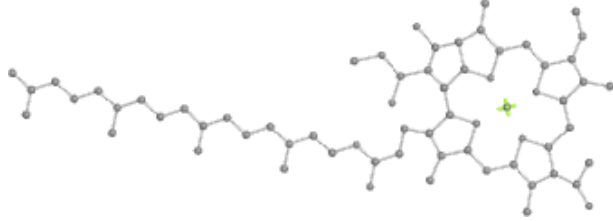


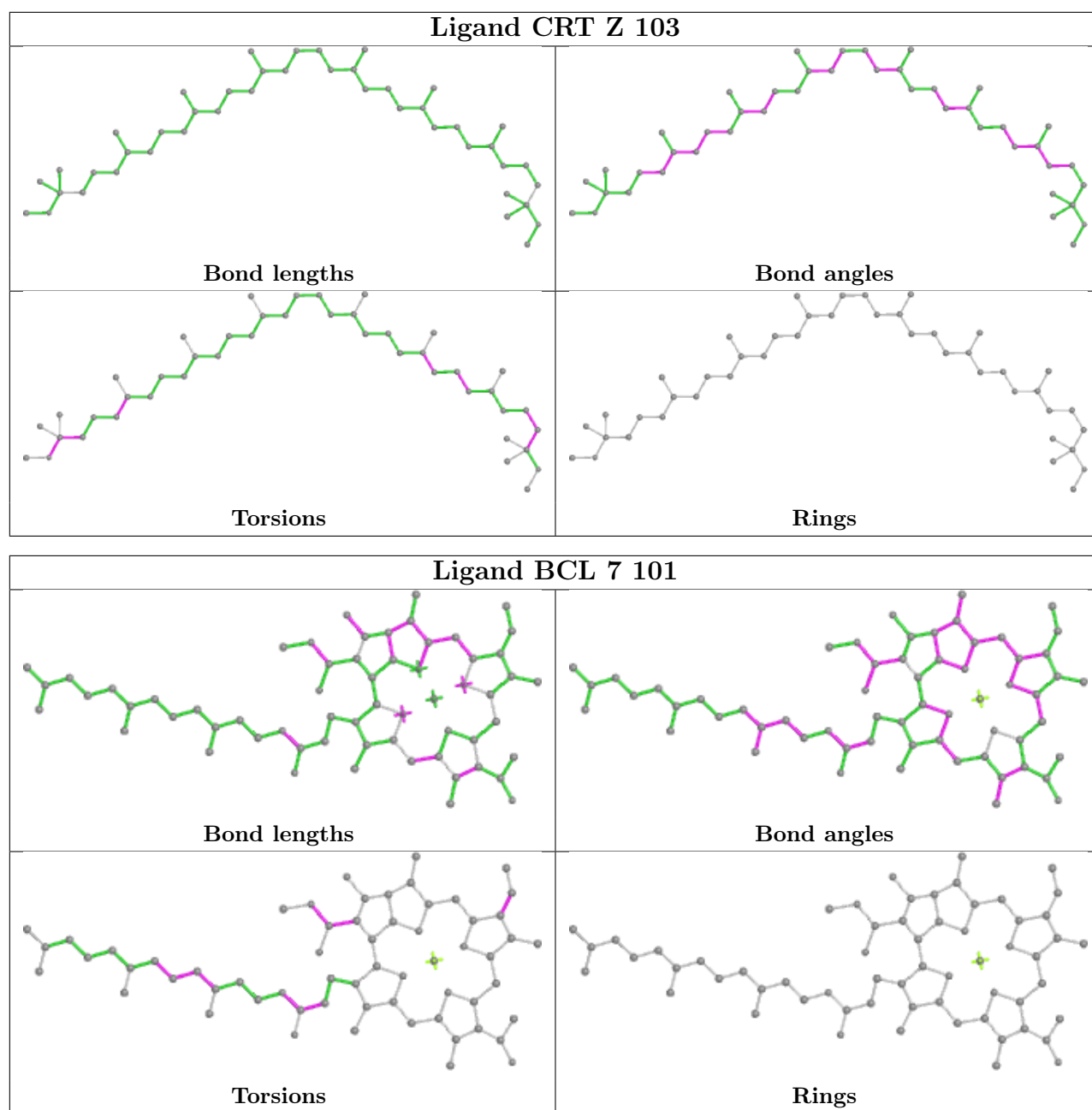


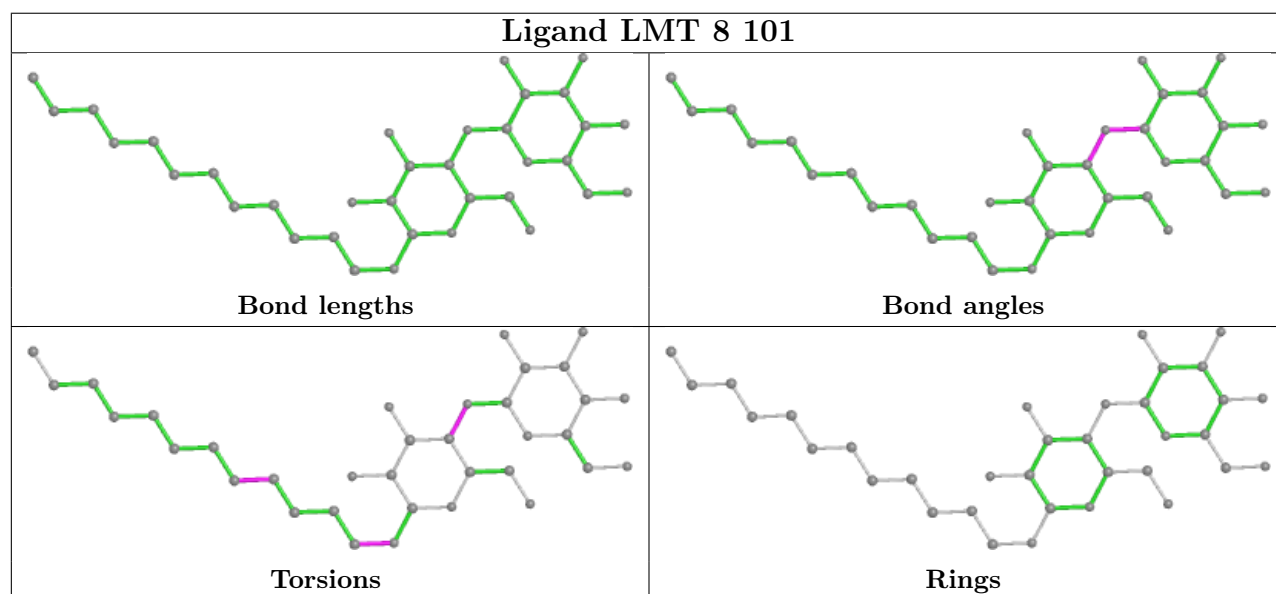
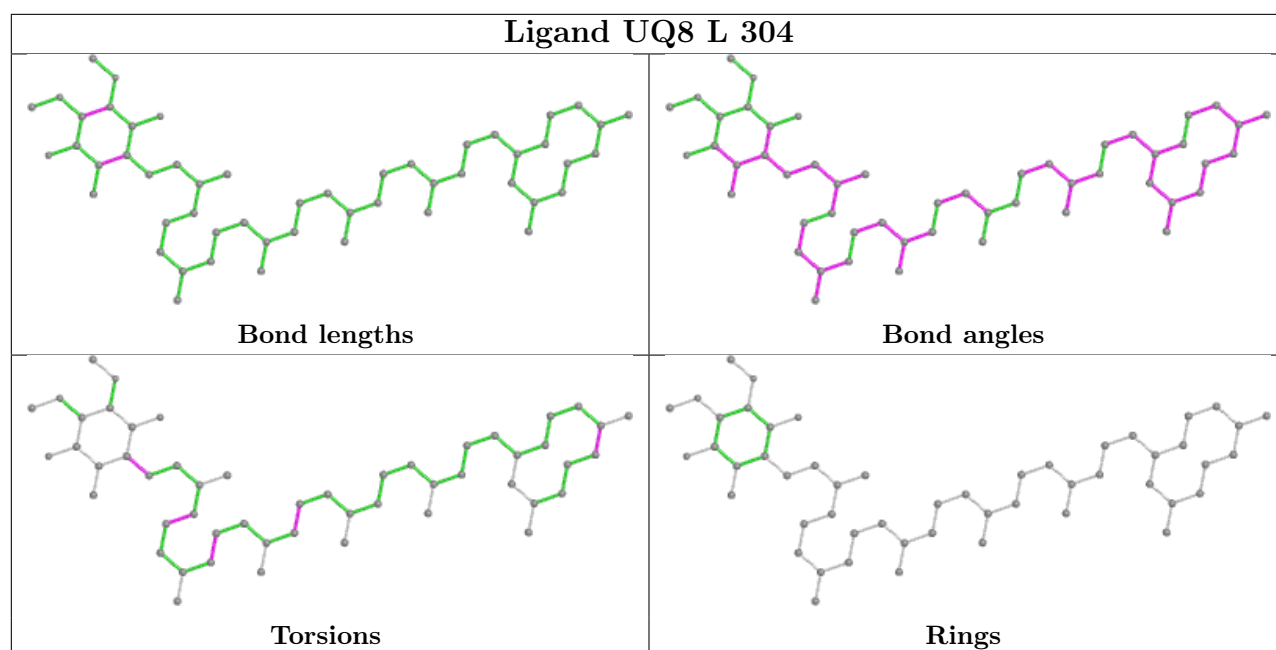


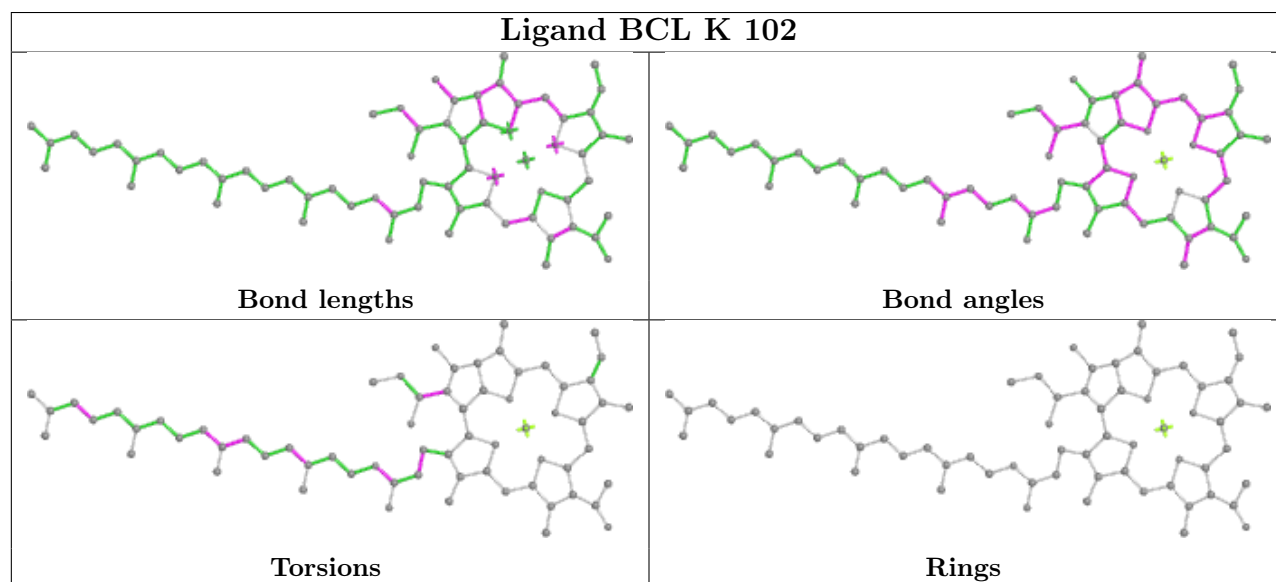
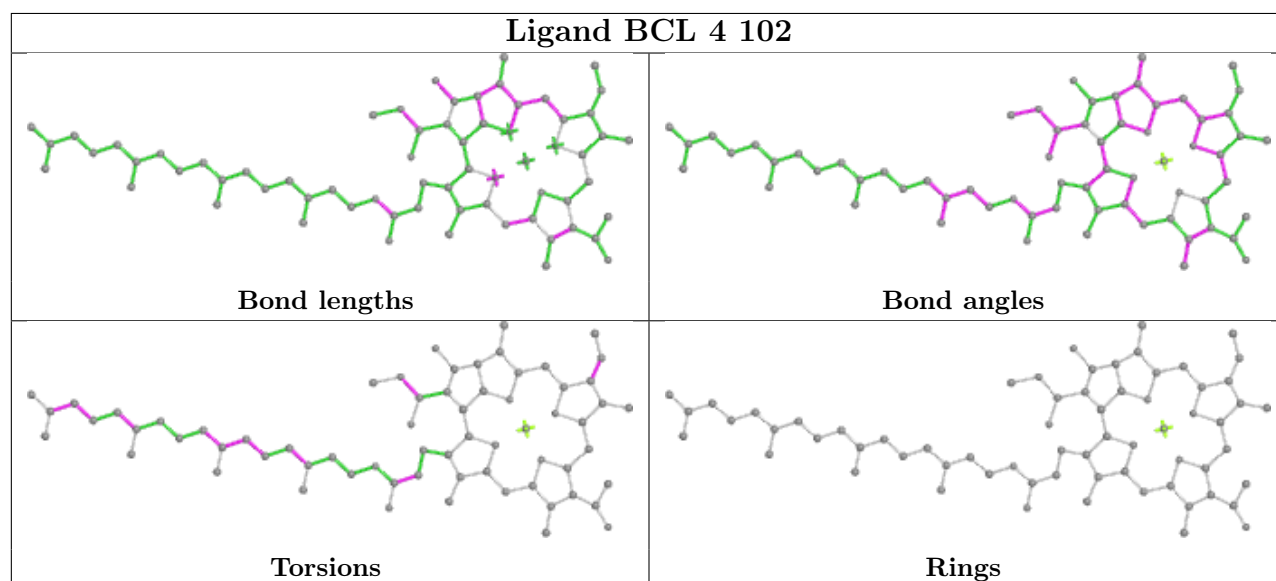
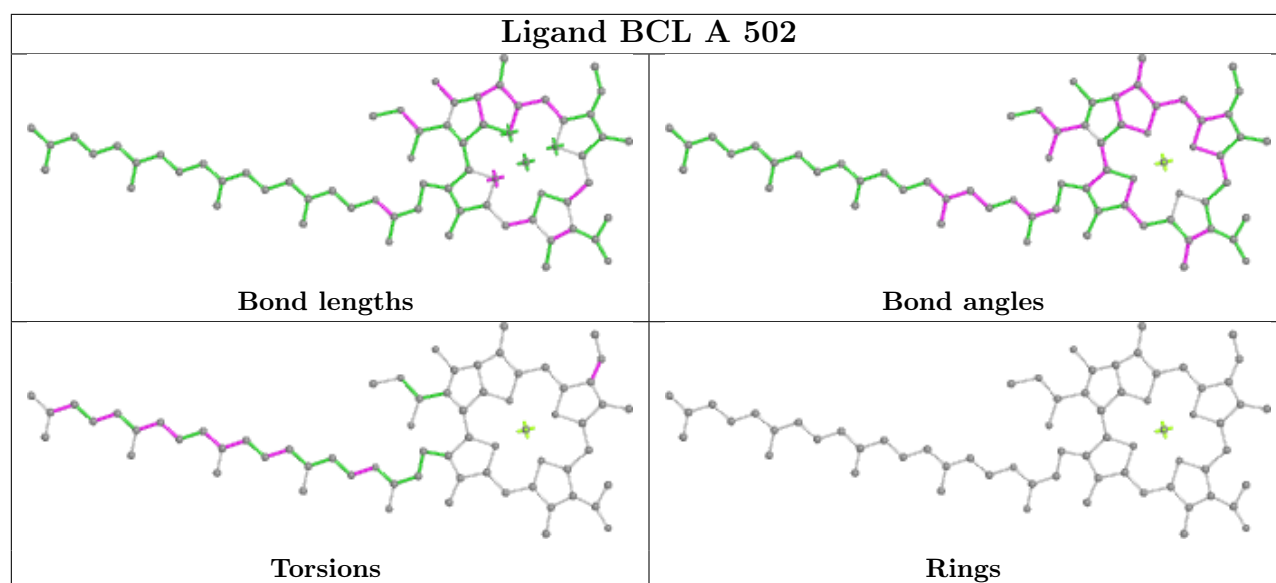
Ligand BCL X 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

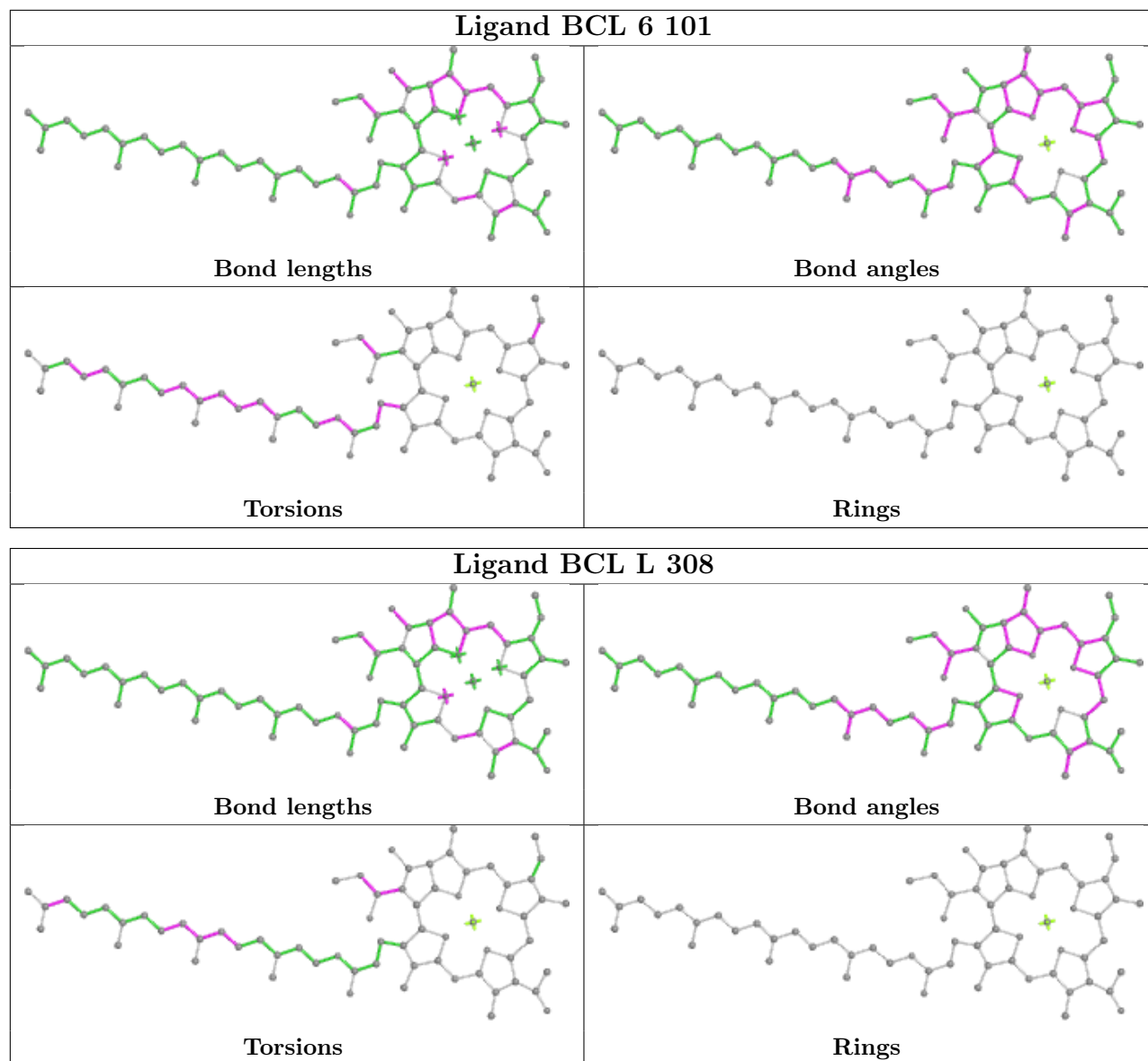
Ligand BCL 3 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL Y 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

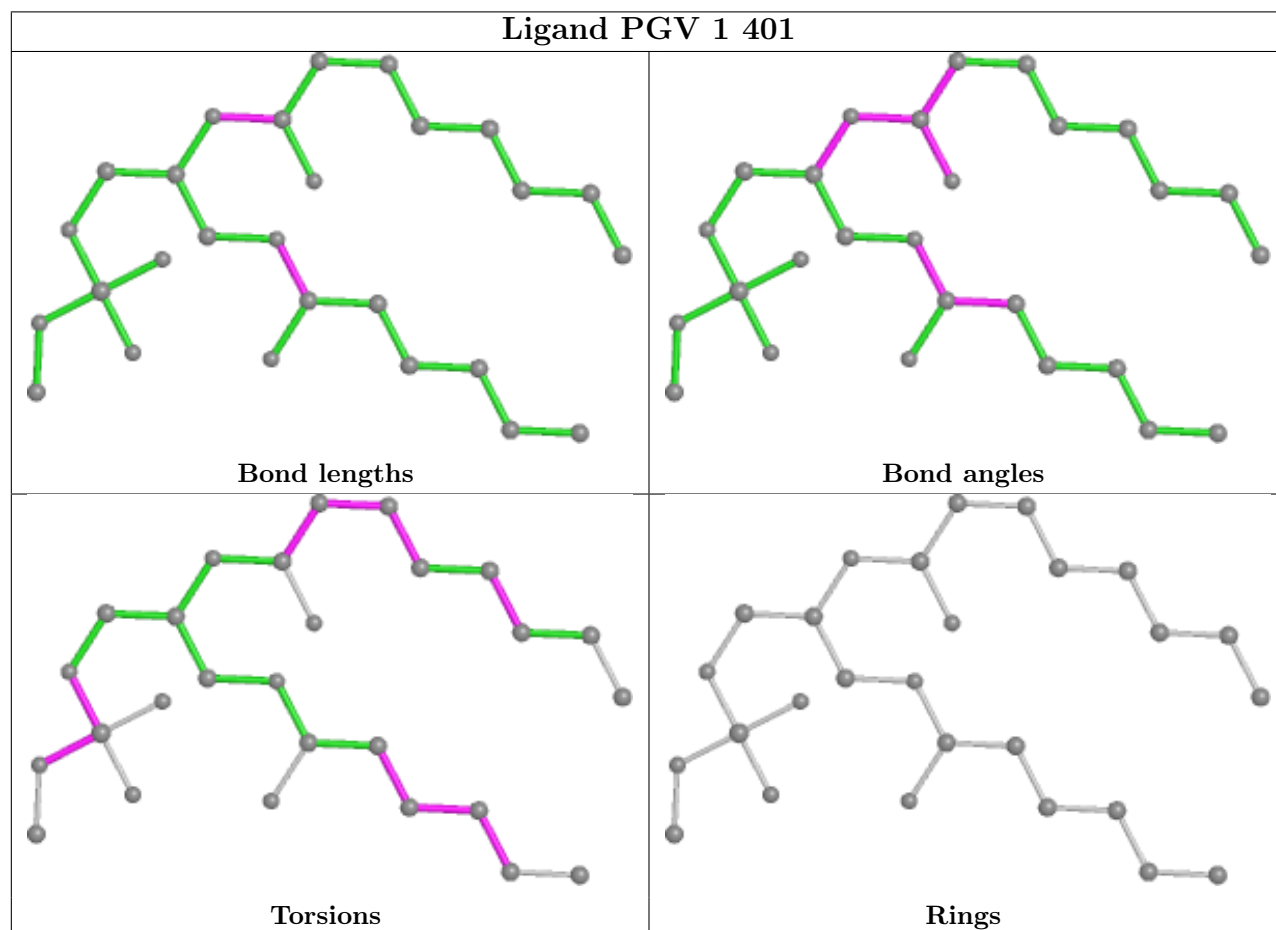
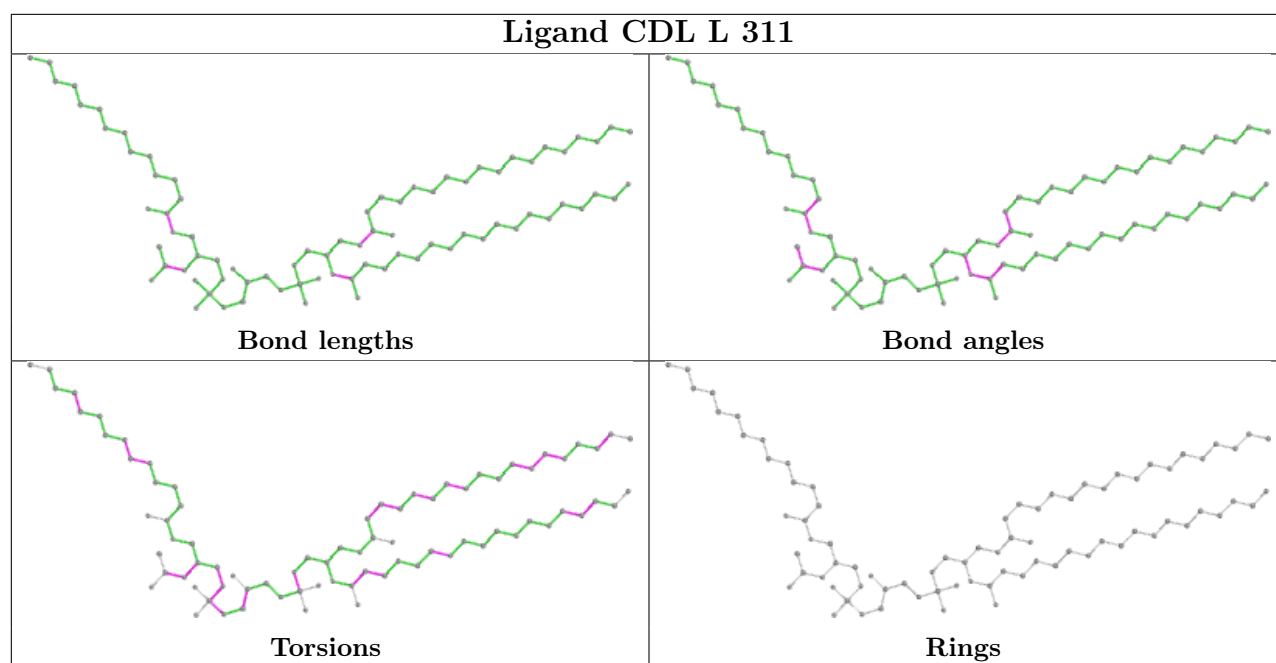


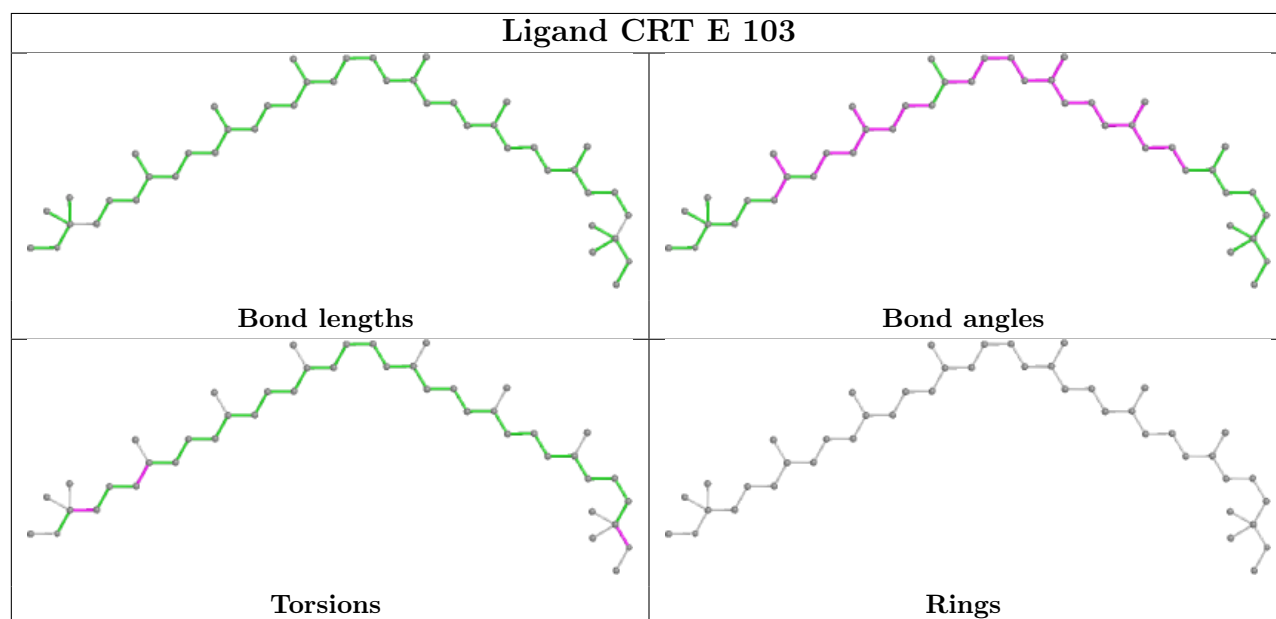
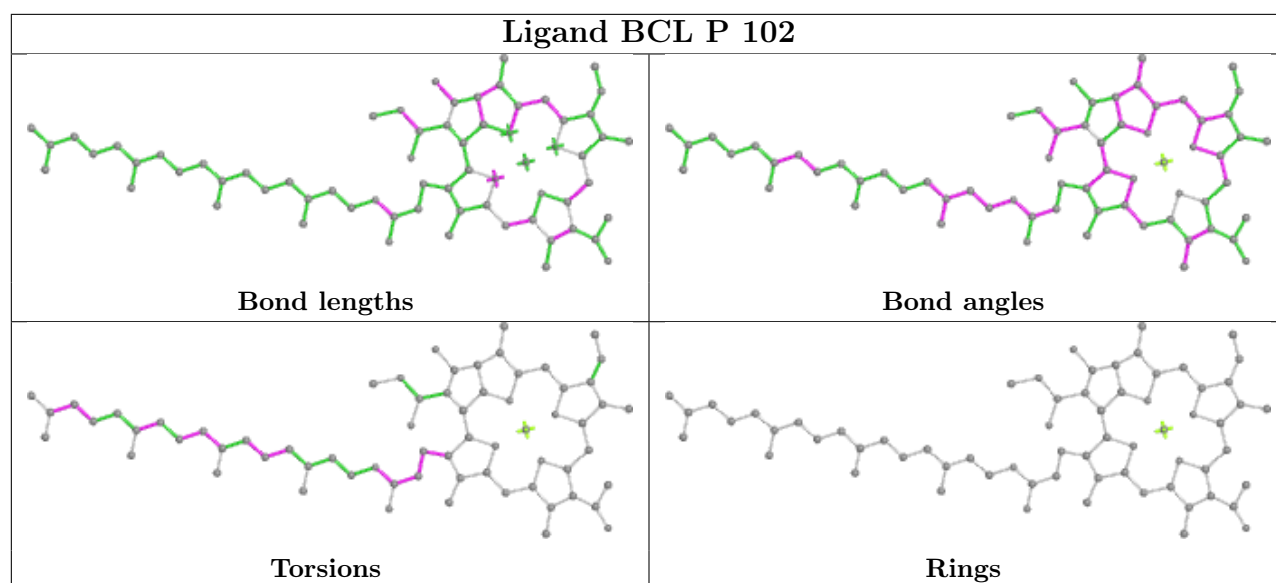


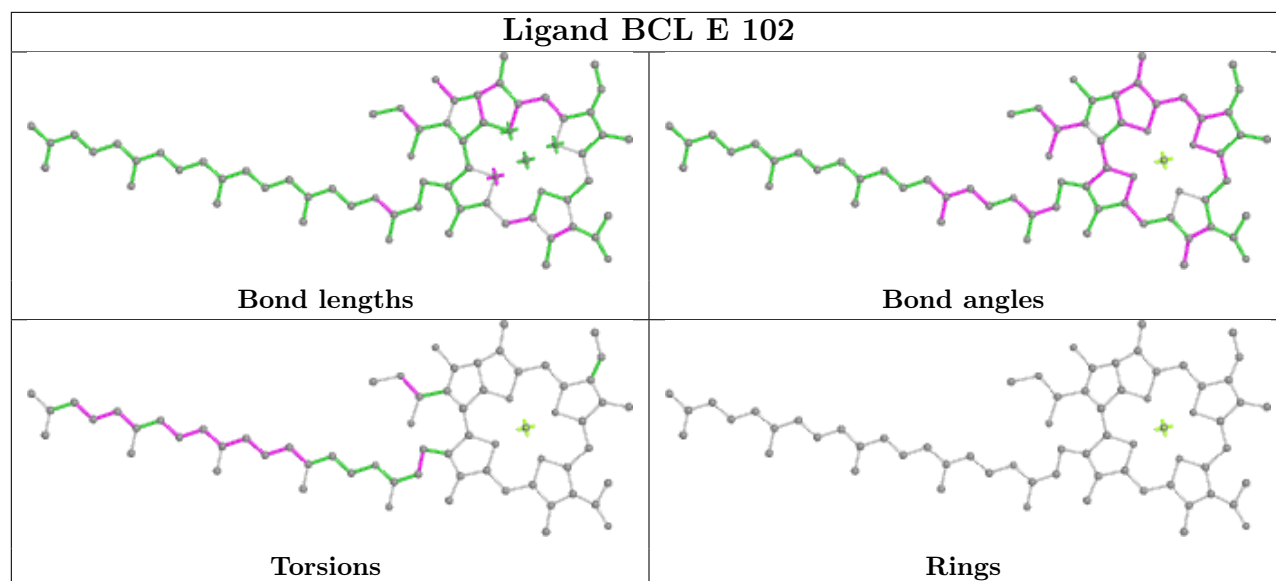
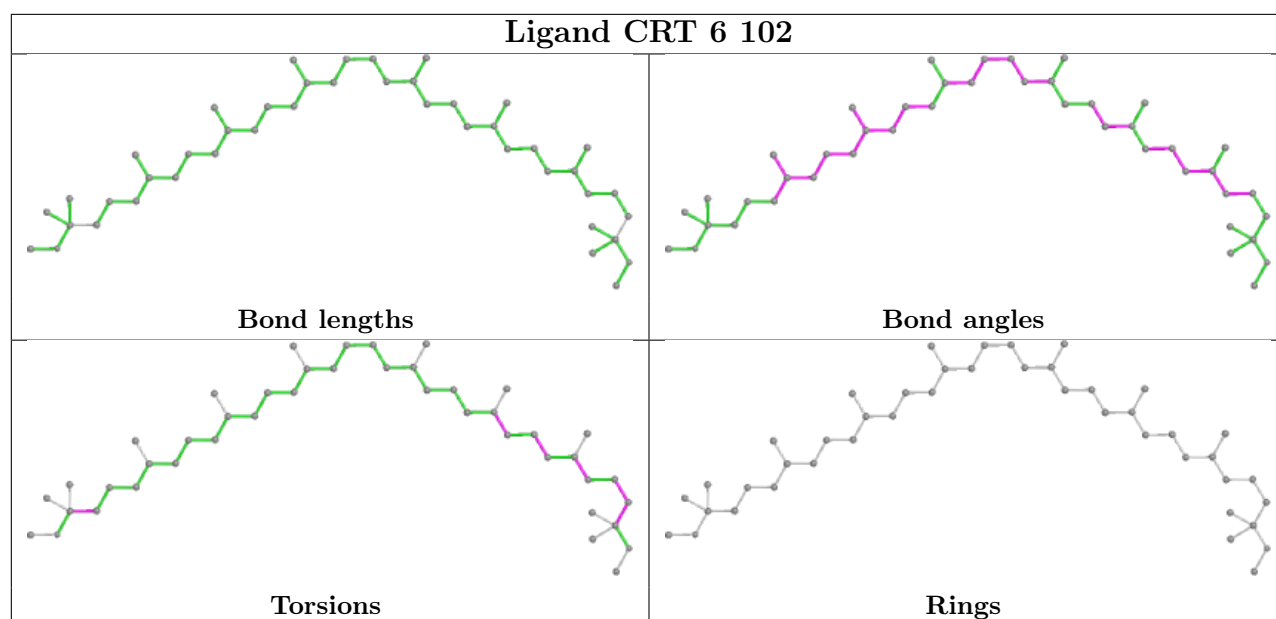


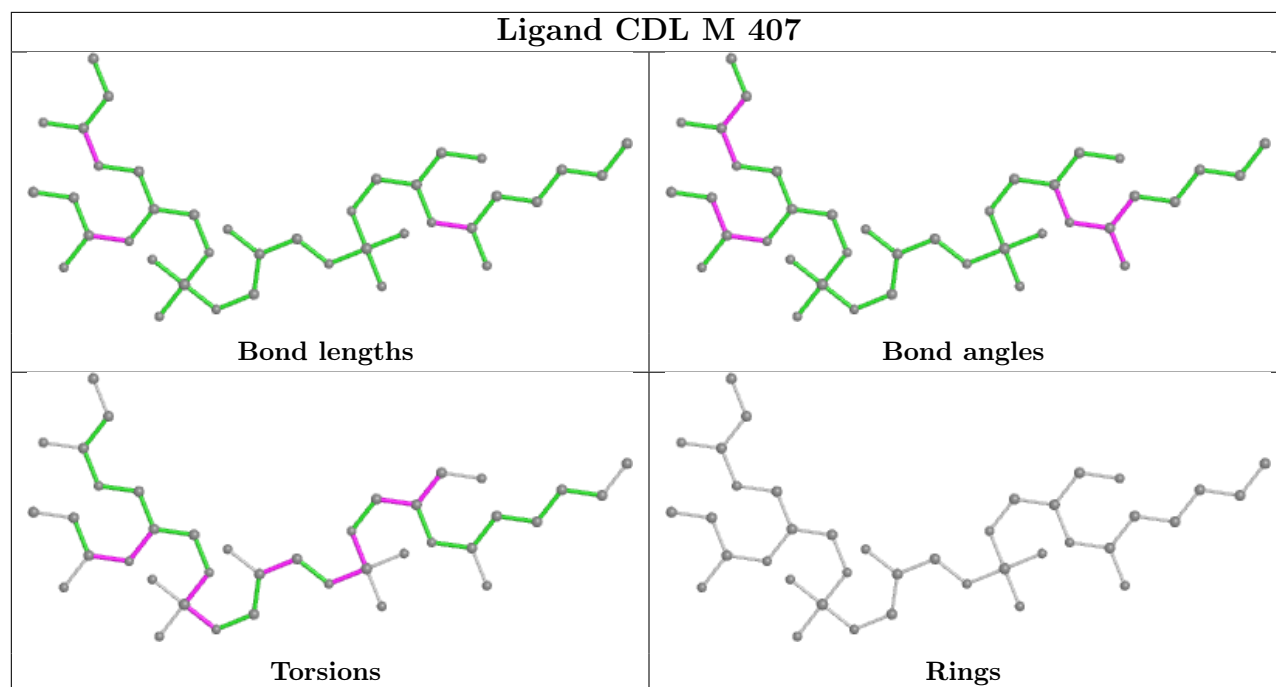
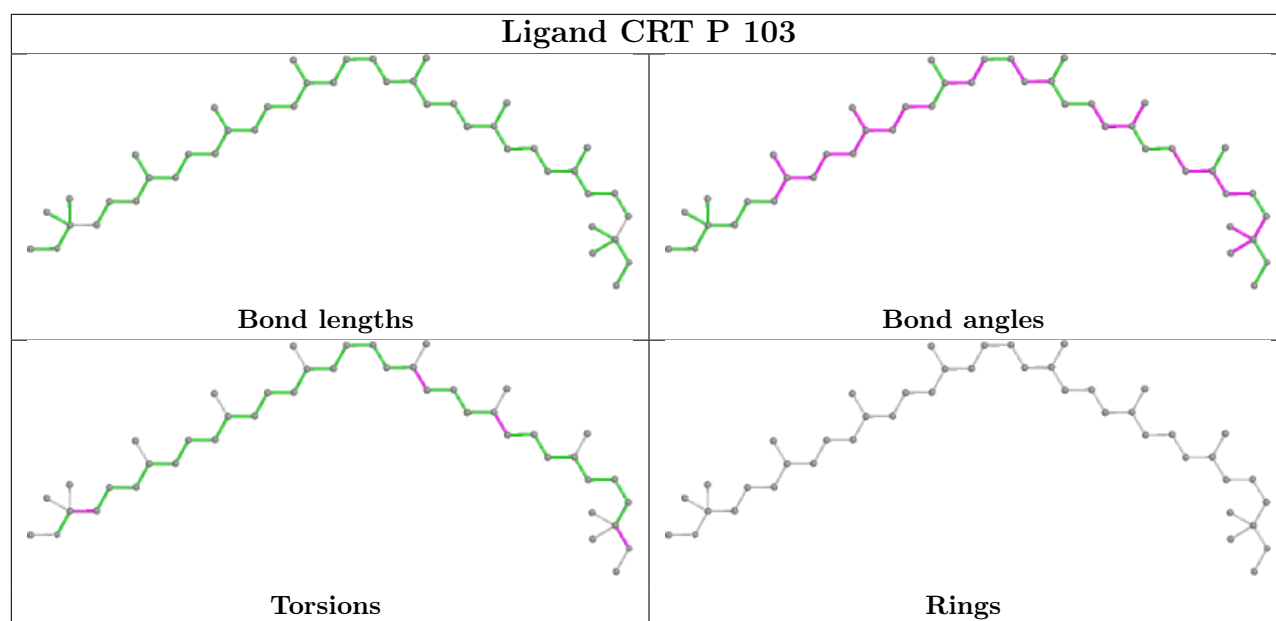


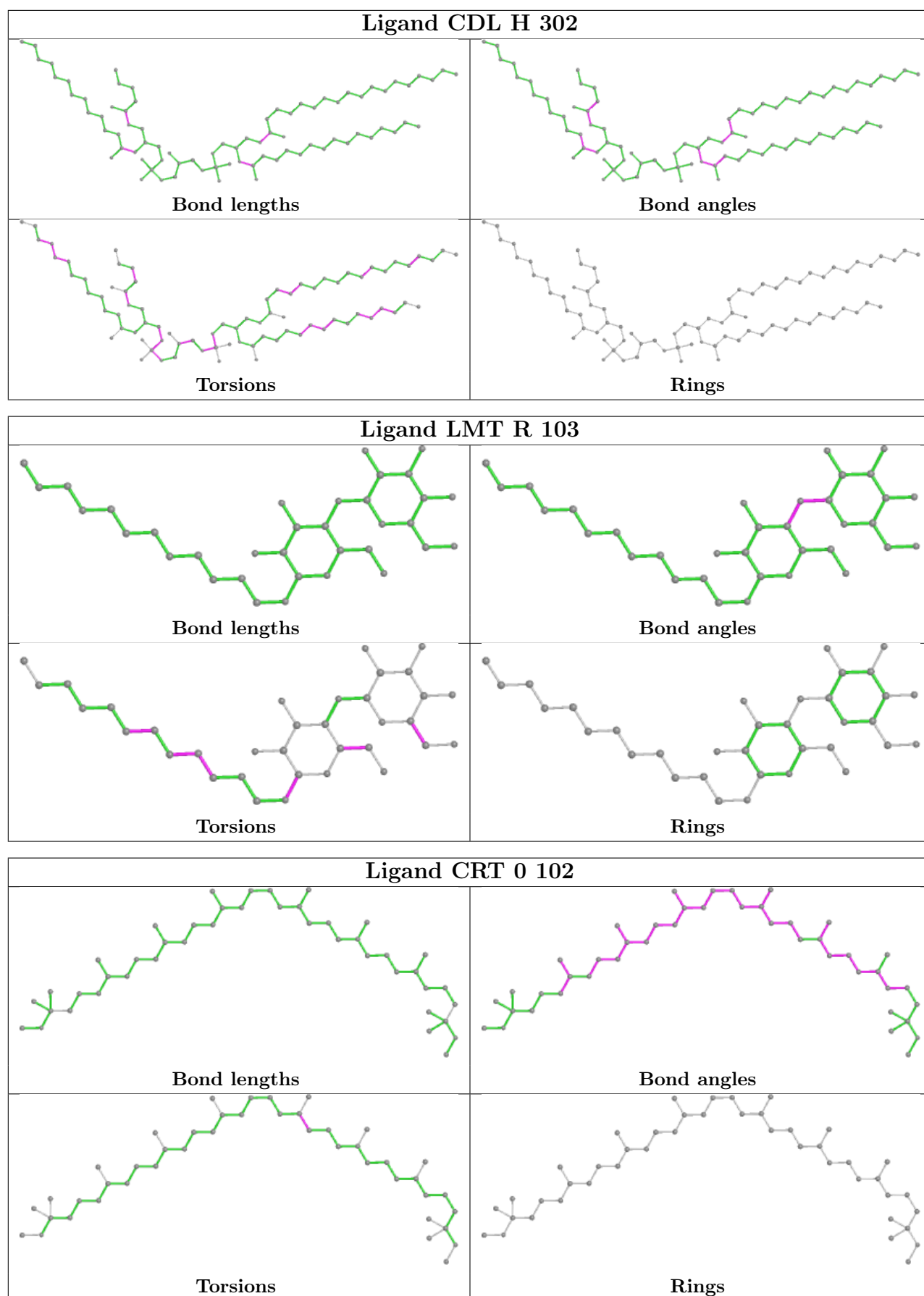


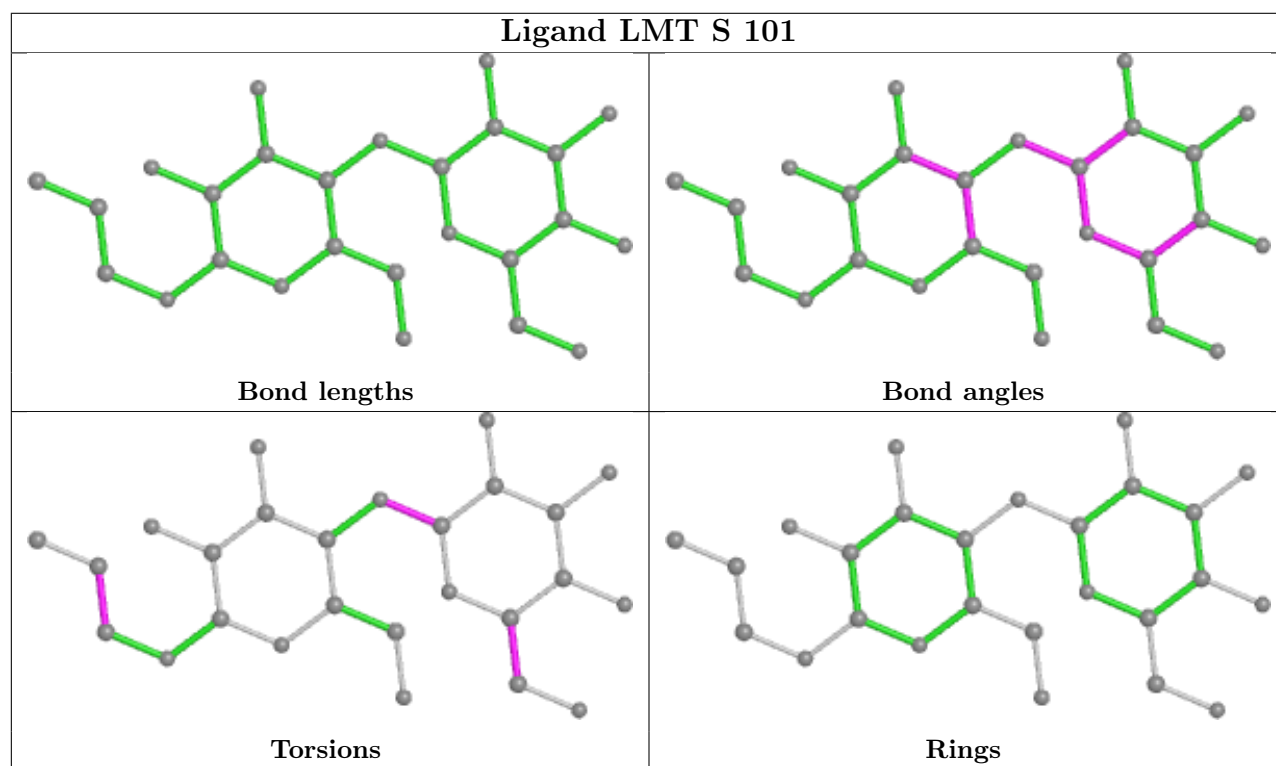
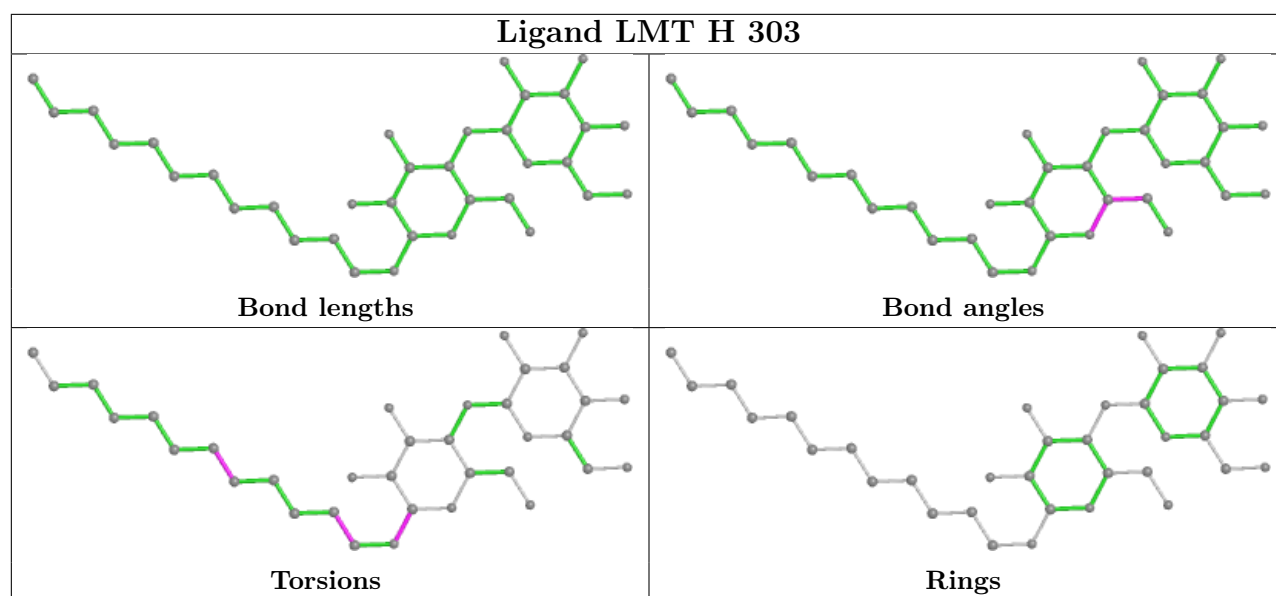


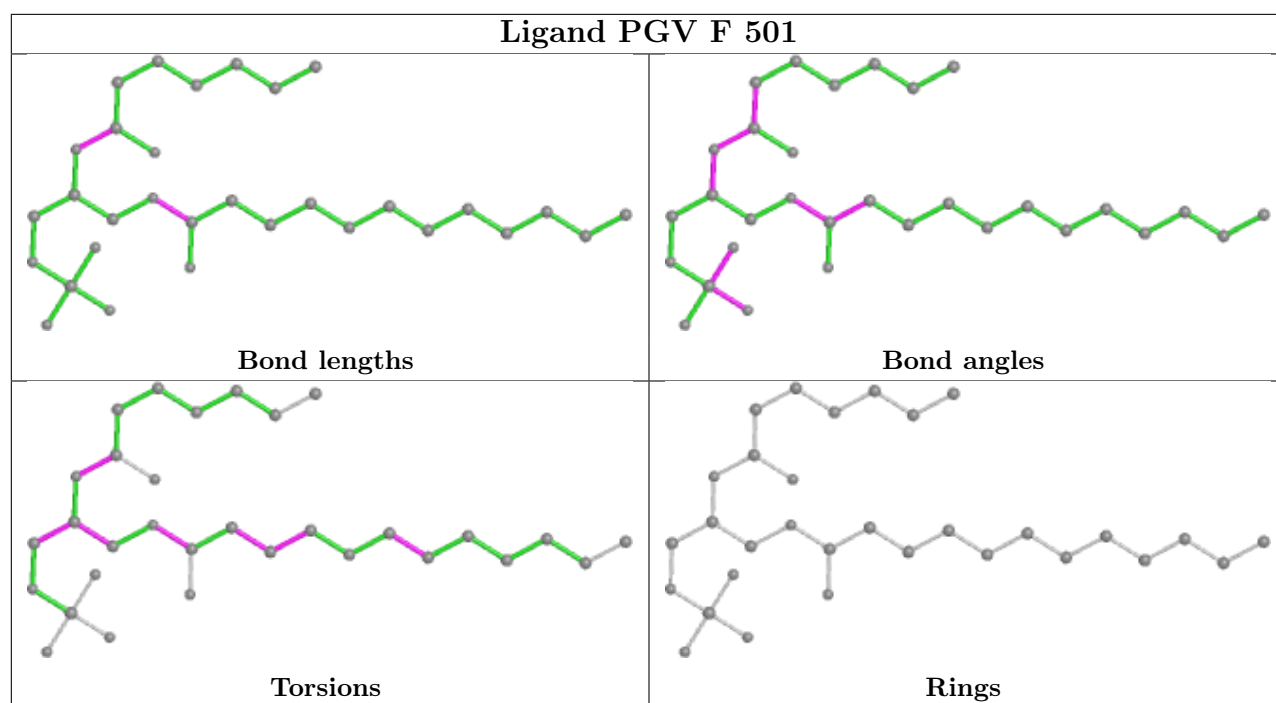












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

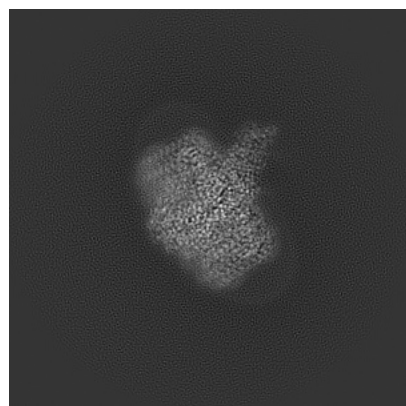
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37465. These allow visual inspection of the internal detail of the map and identification of artifacts.

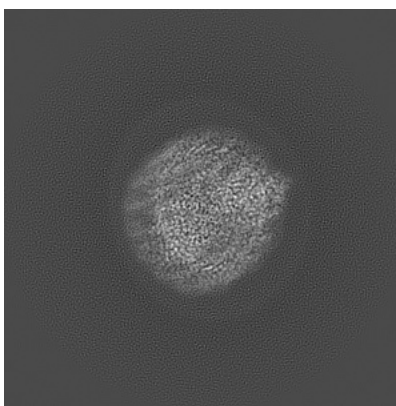
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

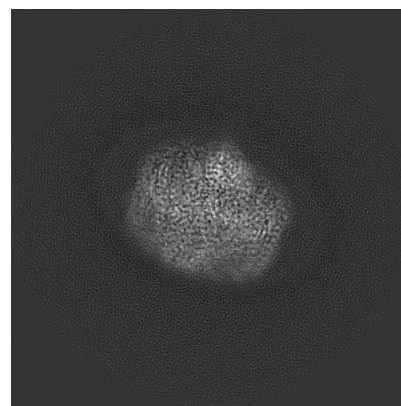
#### 6.1.1 Primary map



X

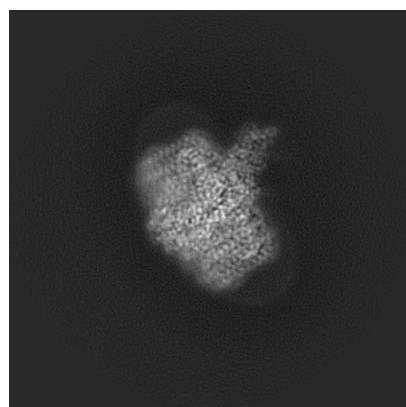


Y

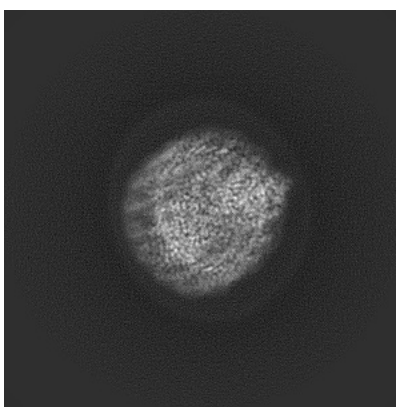


Z

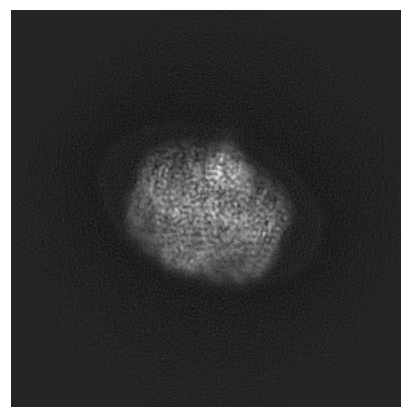
#### 6.1.2 Raw map



X



Y



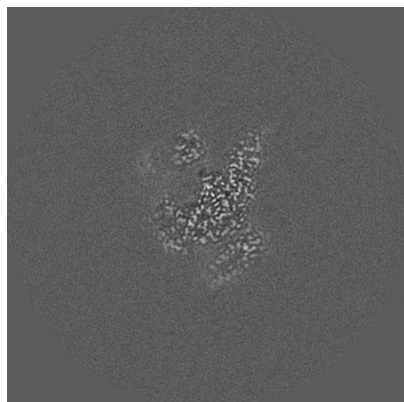
Z

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

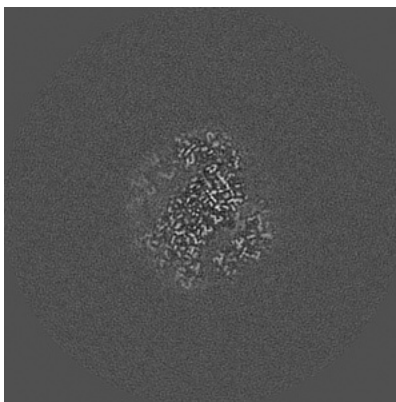


## 6.2 Central slices [i](#)

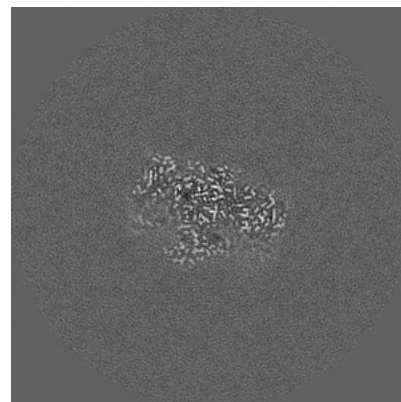
### 6.2.1 Primary map



X Index: 240

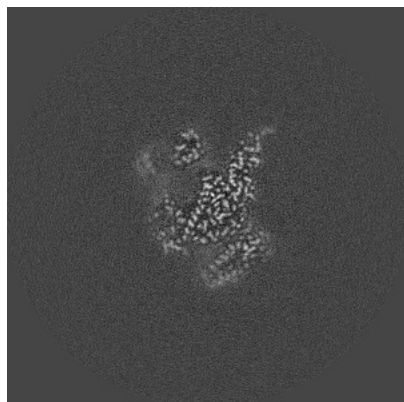


Y Index: 240

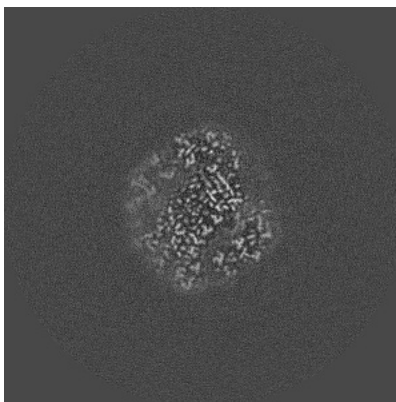


Z Index: 240

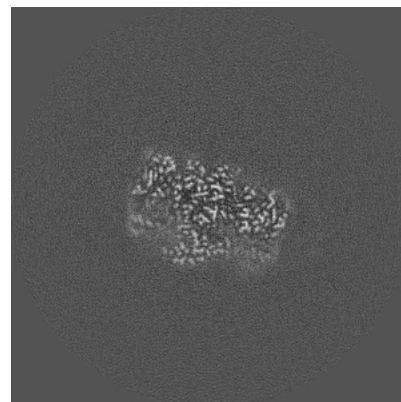
### 6.2.2 Raw map



X Index: 240



Y Index: 240

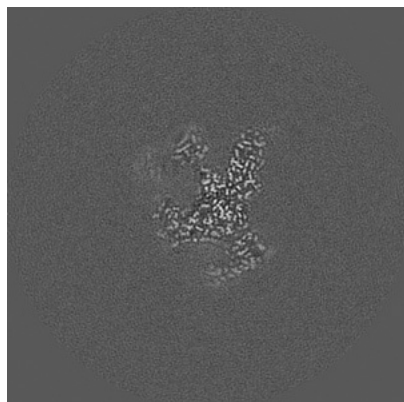


Z Index: 240

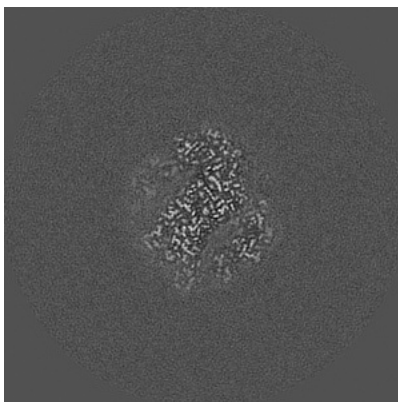
The images above show central slices of the map in three orthogonal directions.

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

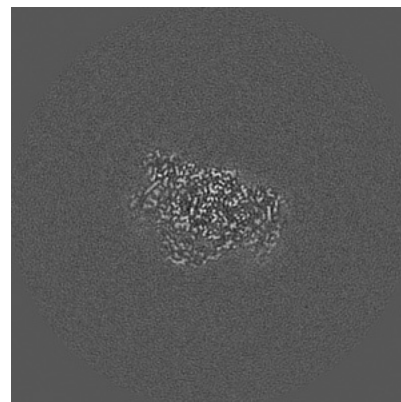
### 6.3.1 Primary map



X Index: 246

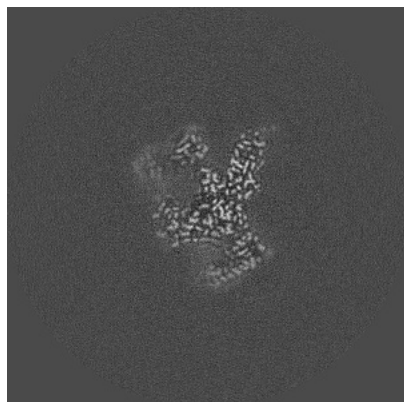


Y Index: 238

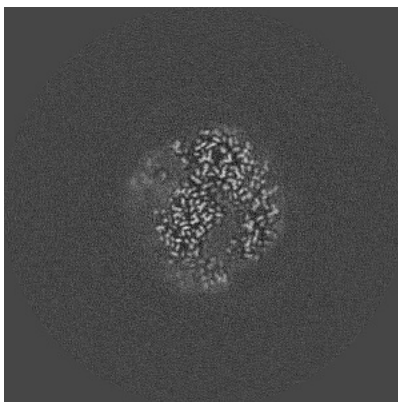


Z Index: 231

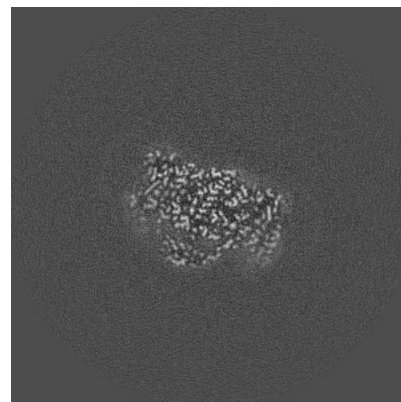
### 6.3.2 Raw map



X Index: 246



Y Index: 228

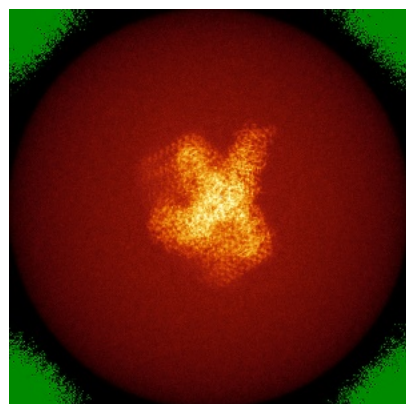


Z Index: 231

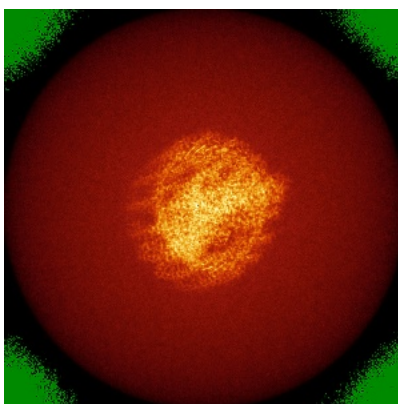
The images above show the largest variance slices of the map in three orthogonal directions.

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

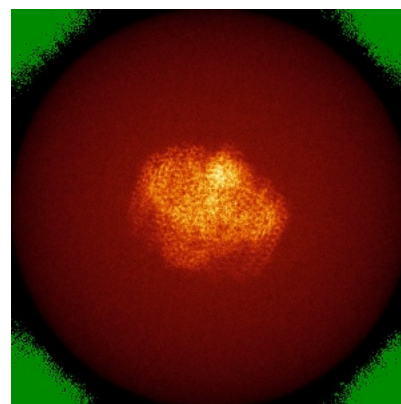
### 6.4.1 Primary map



X

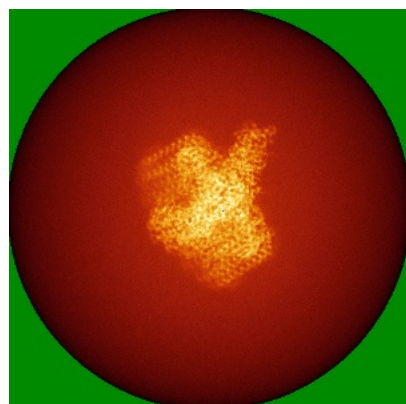


Y

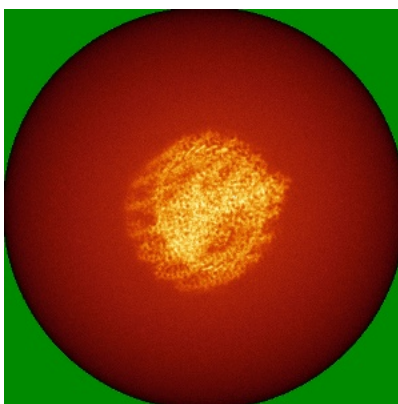


Z

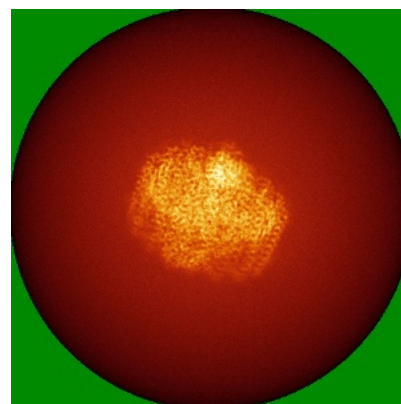
### 6.4.2 Raw map



X



Y

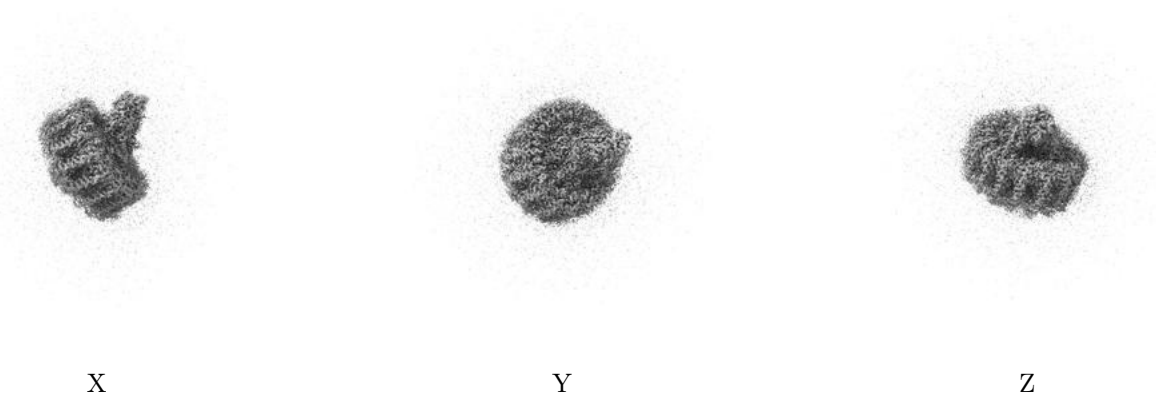


Z

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.

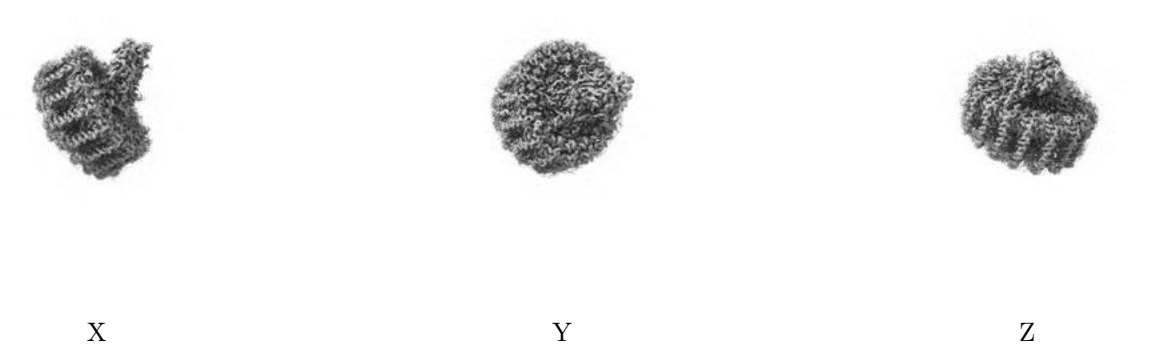
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

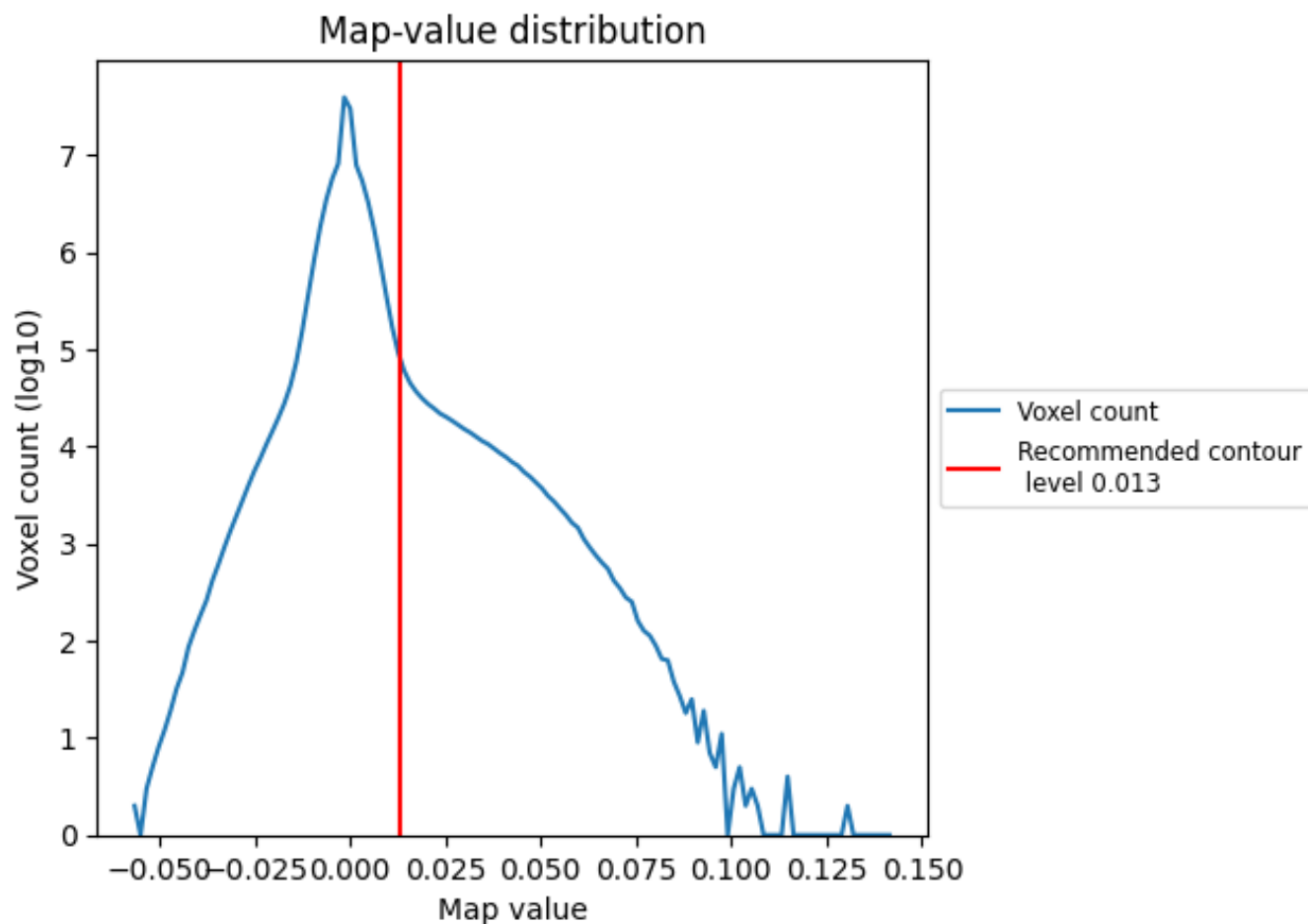
## 6.6 Mask visualisation [i](#)

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.

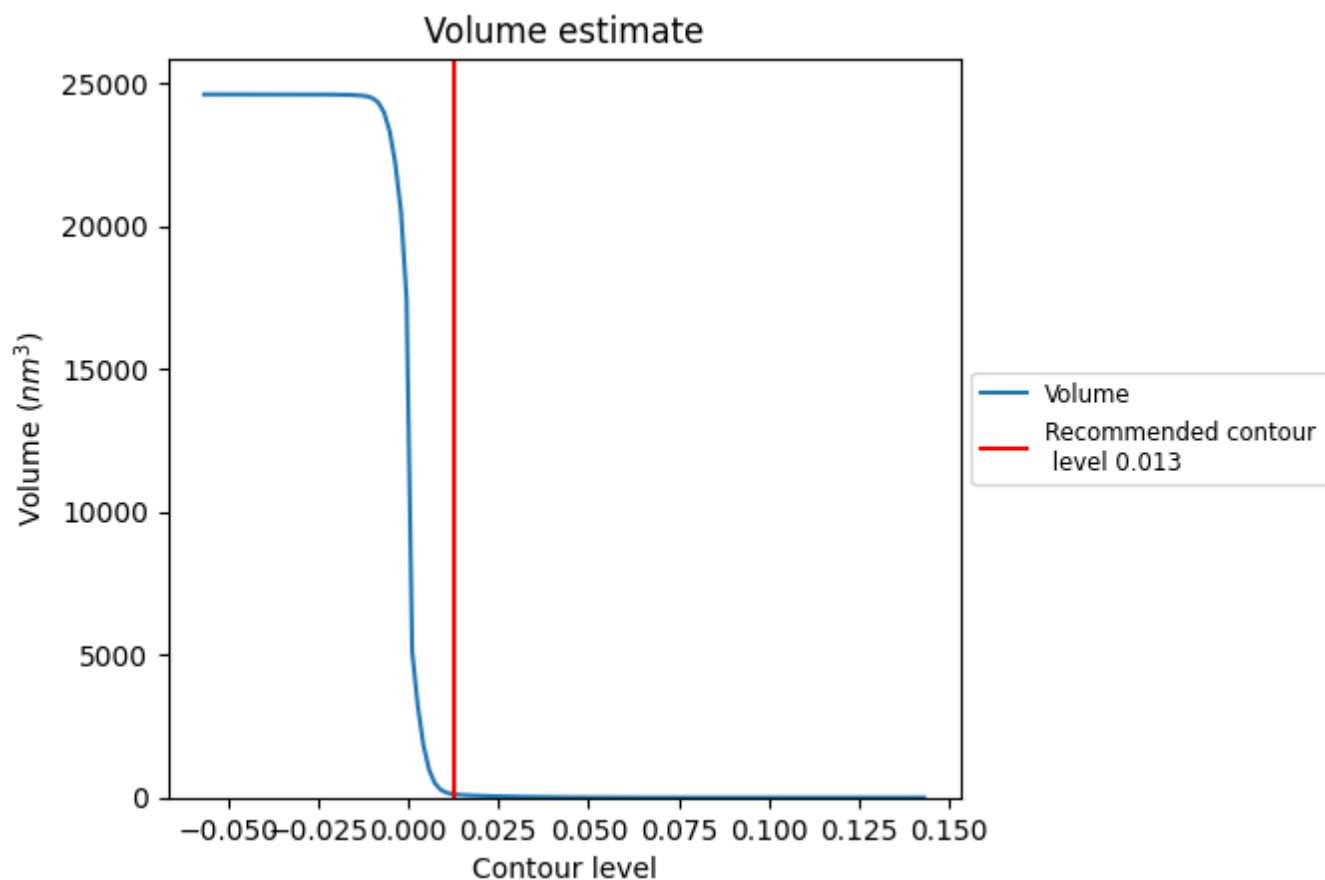
### 7.1 Map-value distribution [i](#)



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.



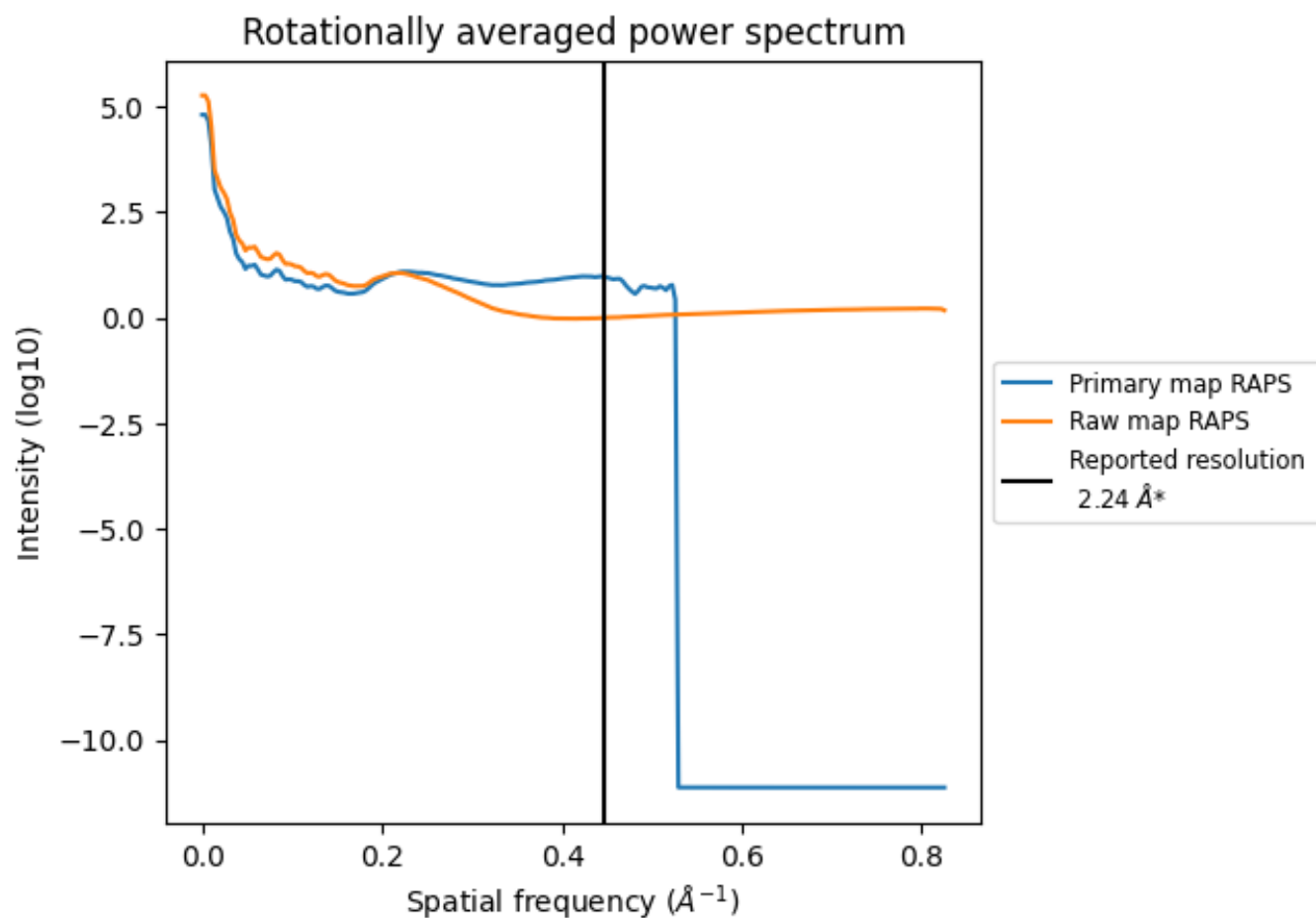
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115  $\text{nm}^3$ ; this corresponds to an approximate mass of 103 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 ⓘ

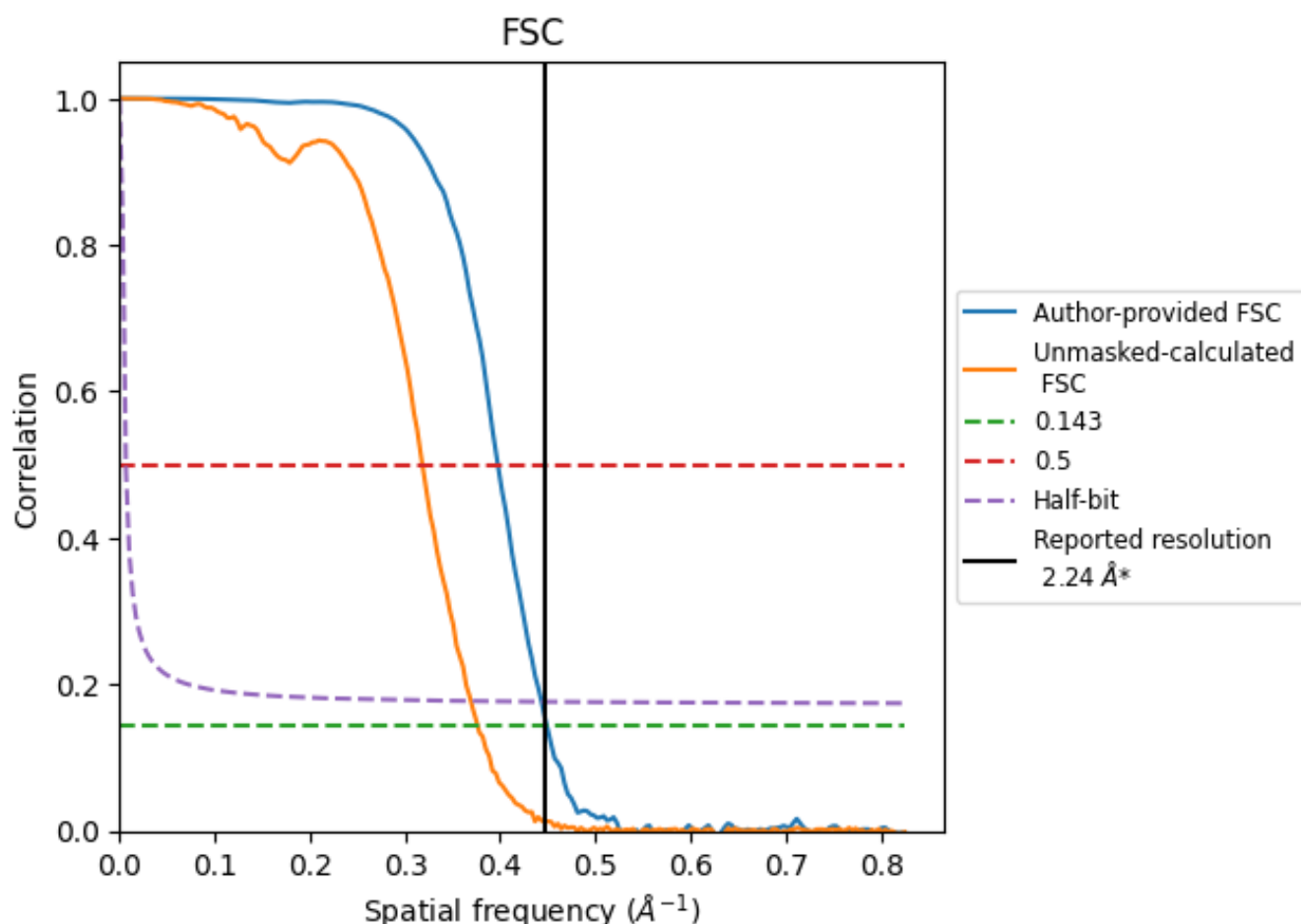


\*Reported resolution corresponds to spatial frequency of 0.446 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.446 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

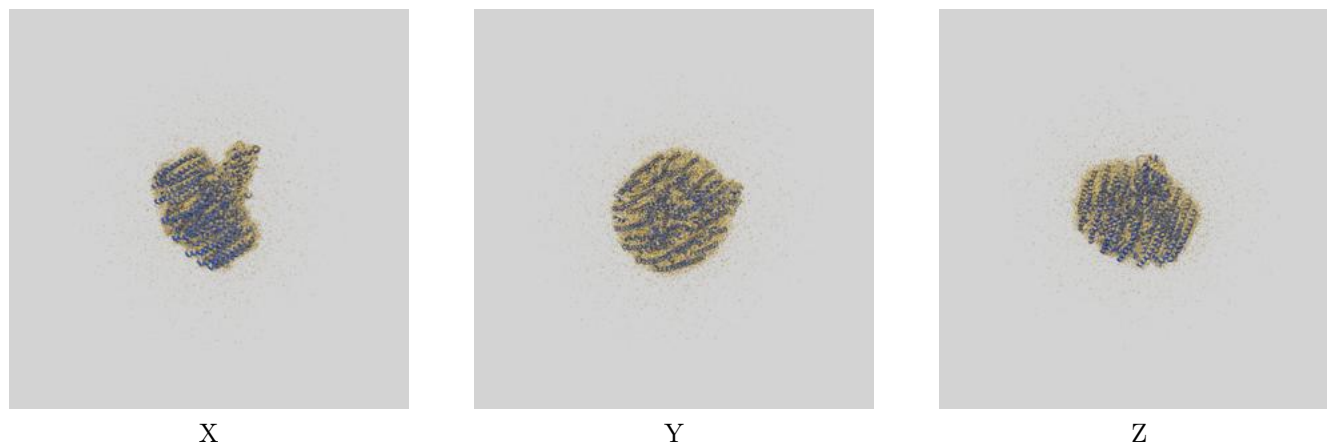
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.23	2.52	2.25
Unmasked-calculated*	2.66	3.14	2.71

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.66 differs from the reported value 2.24 by more than 10 %

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

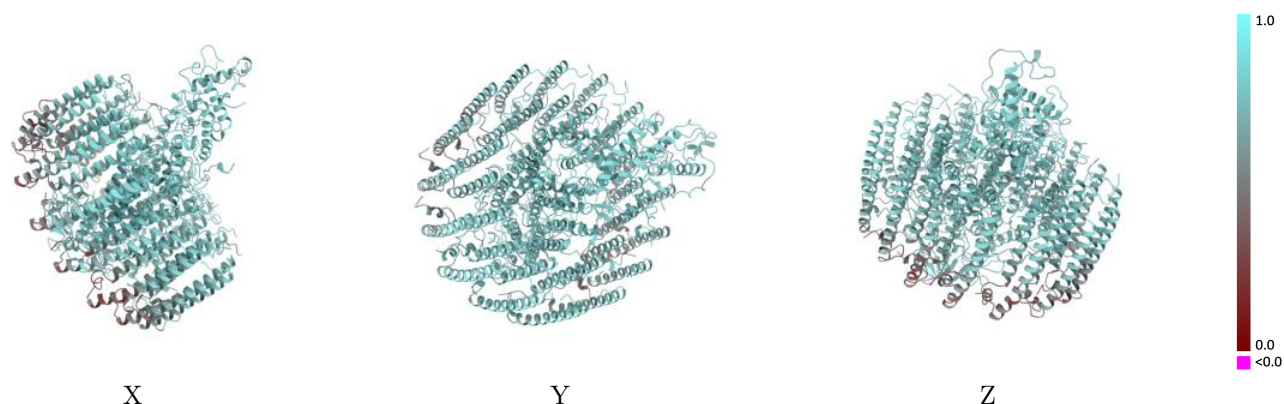
This section contains information regarding the fit between EMDB map EMD-37465 and PDB model 8WDU. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

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



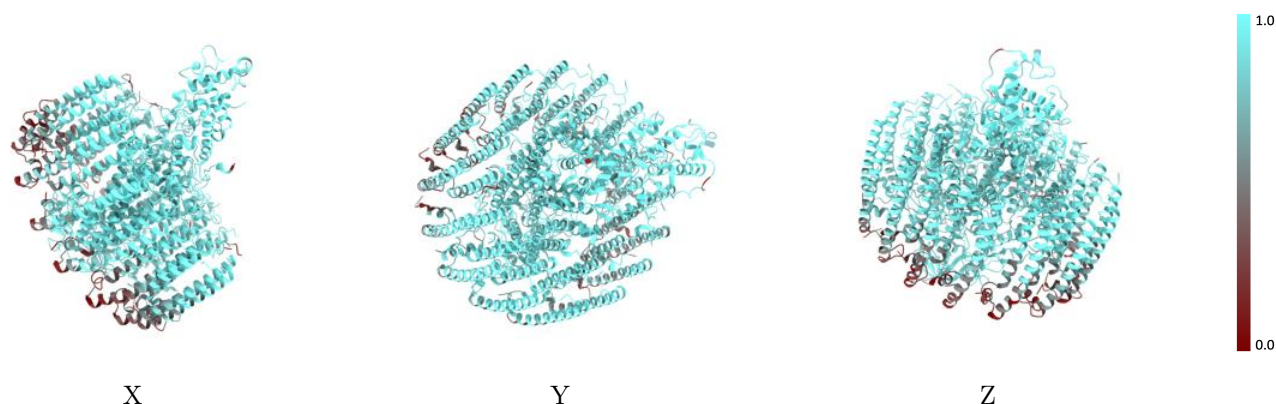
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



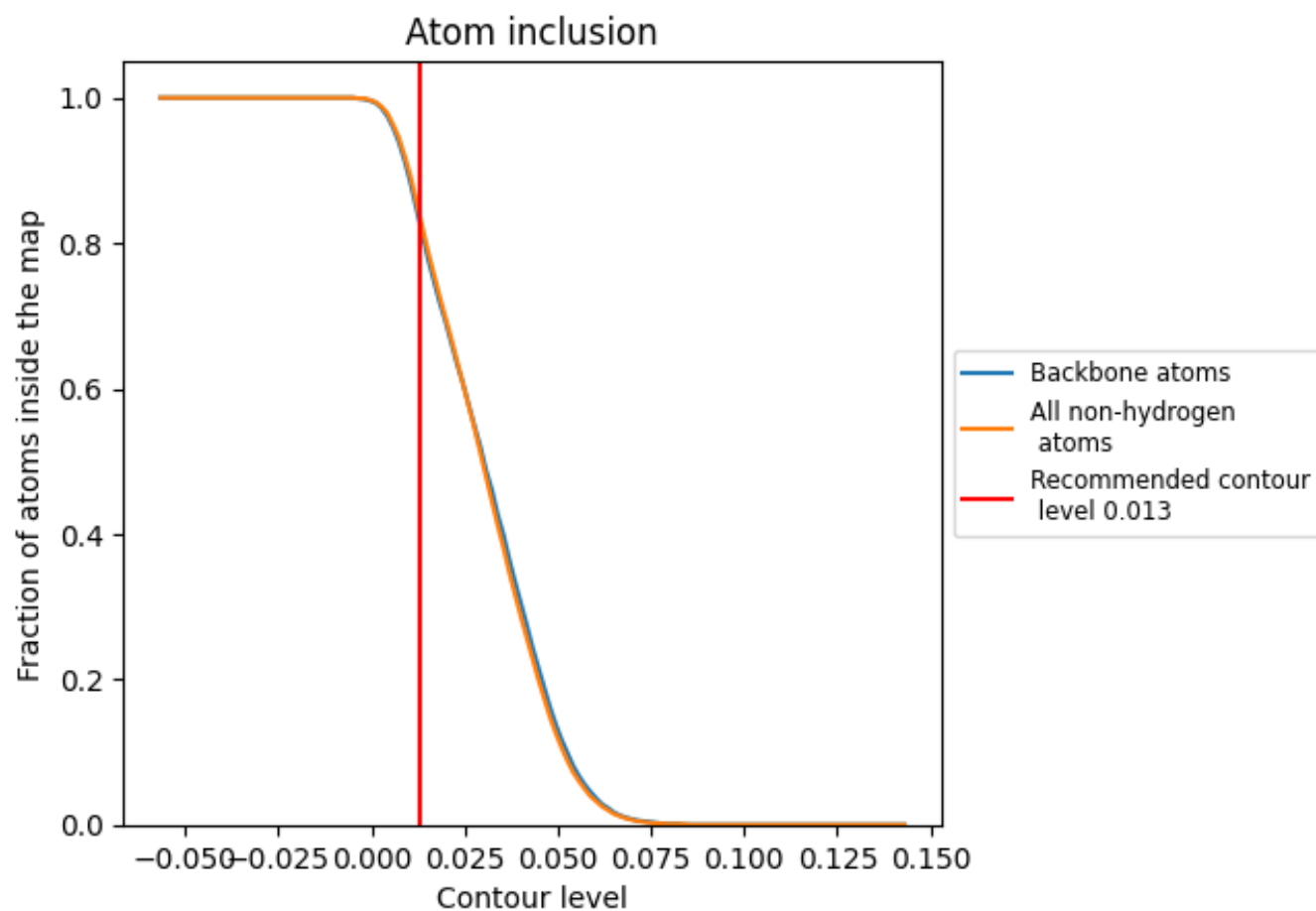
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.6760
0	 0.9090	 0.7090
1	 0.7440	 0.6370
2	 0.5920	 0.5390
3	 0.7870	 0.6490
4	 0.6360	 0.5700
5	 0.8460	 0.6710
6	 0.8050	 0.6540
7	 0.9350	 0.7170
8	 0.8050	 0.6450
9	 0.9480	 0.7270
A	 0.9240	 0.7070
B	 0.8770	 0.6870
C	 0.9620	 0.7430
D	 0.8530	 0.6830
E	 0.7970	 0.6520
F	 0.7340	 0.6280
G	 0.7390	 0.6240
H	 0.9220	 0.7140
I	 0.7470	 0.6370
J	 0.6730	 0.5870
K	 0.6900	 0.5930
L	 0.9300	 0.7400
M	 0.9460	 0.7430
N	 0.6370	 0.5700
O	 0.8080	 0.6510
P	 0.7110	 0.5980
Q	 0.8220	 0.6620
R	 0.7710	 0.6370
S	 0.7500	 0.6510
T	 0.7120	 0.6050
U	 0.7360	 0.6320
V	 0.7320	 0.6130
W	 0.7180	 0.6230
X	 0.6760	 0.5960



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Chain	Atom inclusion	Q-score
Y	 0.6850	 0.5950
Z	 0.6680	 0.5650