



# wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 10:06 am GMT

PDB ID : 6Z5S  
EMDB ID : EMD-11081  
Title : RC-LH1(14)-W complex from Rhodospseudomonas palustris  
Authors : Swainsbury, D.J.K.; Qian, P.; Hitchcock, A.; Hunter, C.N.  
Deposited on : 2020-05-27  
Resolution : 2.65 Å(reported)

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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

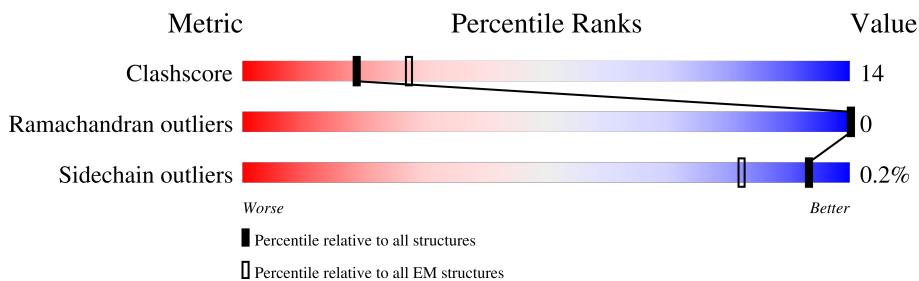
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.65 Å.

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



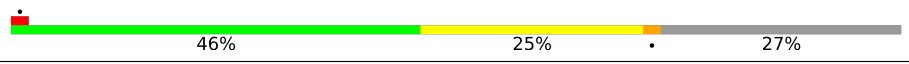
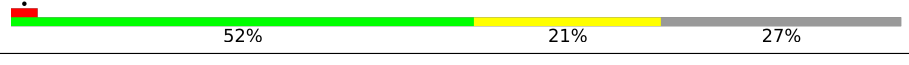


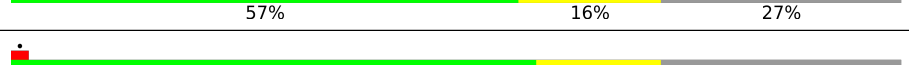

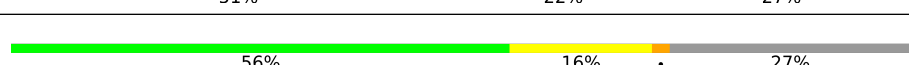
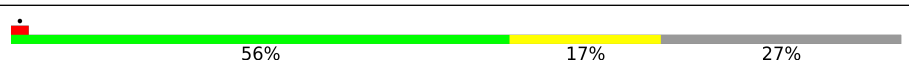

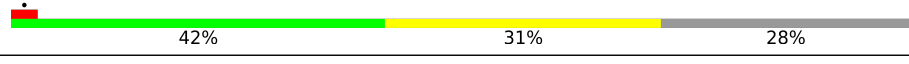
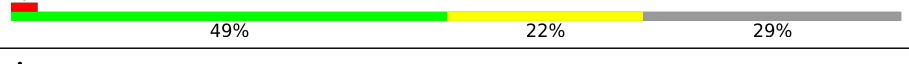
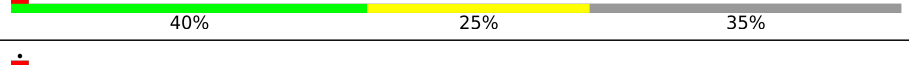

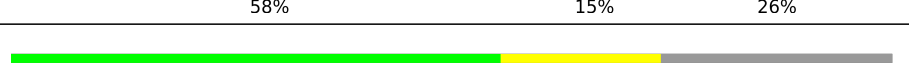


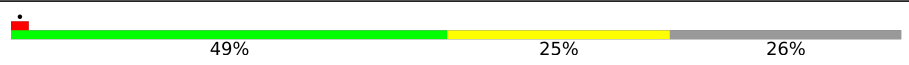

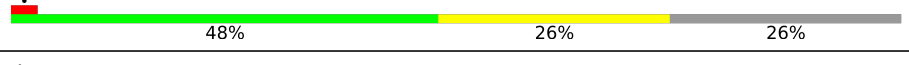


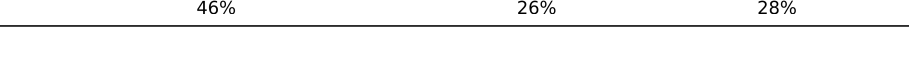
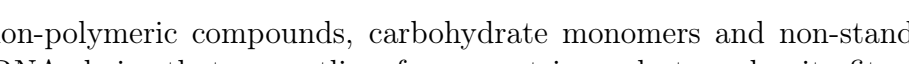
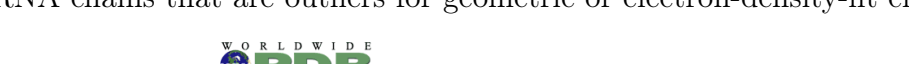
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	W	102	
2	M	307	
3	L	277	
4	H	255	
5	1	63	
5	3	63	
5	5	63	
5	A	63	

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Mol	Chain	Length	Quality of chain
5	C	63	
5	E	63	
5	G	63	
5	J	63	
5	N	63	
5	P	63	
5	R	63	
5	T	63	
5	V	63	
5	Y	63	
6	2	65	
6	4	65	
6	6	65	
6	B	65	
6	D	65	
6	F	65	
6	I	65	
6	K	65	
6	O	65	
6	Q	65	
6	S	65	
6	U	65	
6	X	65	
6	Z	65	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	QAK	M	401	X	-	-	-
9	BPH	L	403	X	-	-	-
9	BPH	M	403	X	-	-	-

## 2 Entry composition i

There are 17 unique types of molecules in this entry. The entry contains 22794 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 Light harvesting complex 1 Protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	W	94	682	455	114	110	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	299	2381	1582	389	398	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	276	2185	1467	350	359	9	0	0

- Molecule 4 is a protein called H subunit of photosynthetic reaction center complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	251	1894	1221	321	347	5	0	0

- Molecule 5 is a protein called Light-harvesting complex 1 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1	46	397	274	67	55	1	0	0
5	5	46	397	274	67	55	1	0	0
5	3	46	397	274	67	55	1	0	0
5	Y	46	397	274	67	55	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	T	46	Total	C	N	O	S	1	0
			408	283	68	56	1		
5	A	40	Total	C	N	O		0	0
			352	248	58	46			
5	C	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	R	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	P	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	N	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	J	45	Total	C	N	O	S	0	0
			392	271	66	54	1		
5	G	46	Total	C	N	O	S	0	0
			397	274	67	55	1		
5	E	46	Total	C	N	O	S	0	0
			397	274	67	55	1		

- Molecule 6 is a protein called Light-harvesting complex 1 beta chain.

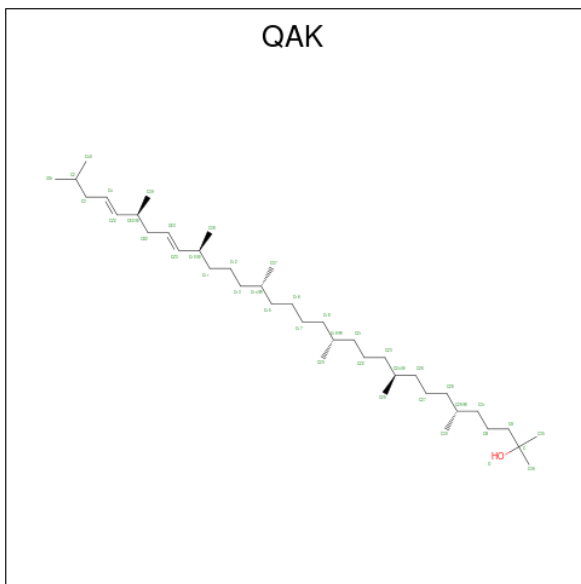
Mol	Chain	Residues	Atoms					AltConf	Trace
6	2	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
6	6	42	Total	C	N	O	S	1	0
			356	247	54	54	1		
6	4	46	Total	C	N	O	S	0	0
			374	256	58	59	1		
6	Z	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
6	X	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
6	U	47	Total	C	N	O	S	1	0
			393	271	60	61	1		
6	B	47	Total	C	N	O	S	0	0
			382	262	59	60	1		
6	D	48	Total	C	N	O	S	1	0
			399	274	61	63	1		
6	S	48	Total	C	N	O	S	1	0
			399	274	61	63	1		

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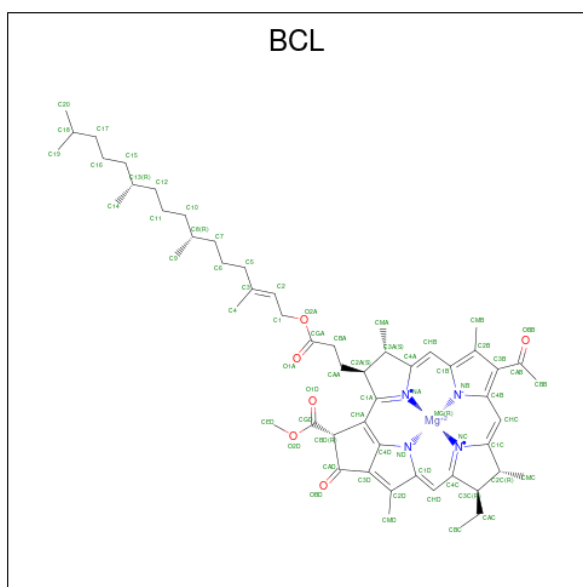
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Q	48	Total 399	C 274	N 61	O 63	S 1	1	0
6	O	48	Total 388	C 265	N 60	O 62	S 1	0	0
6	K	47	Total 382	C 262	N 59	O 60	S 1	0	0
6	I	47	Total 382	C 262	N 59	O 60	S 1	0	0
6	F	48	Total 388	C 265	N 60	O 62	S 1	0	0

- Molecule 7 is (6 {R},10 {S},14 {R},19 {R},23 {S},24 {E},27 {S},28 {E})-2,6,10,14,19,23,27,31-octamethyldotriaconta-24,28-dien-2-ol (three-letter code: QAK) (formula: C<sub>40</sub>H<sub>78</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	M	1	Total 41	C 40	O 1	0

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
8	M	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	M	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	L	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	L	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	5	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	5	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	4	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Y	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	Y	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	V	1	Total 132	C 110	Mg 2	N 8	O 12	0
8	V	1	Total 132	C 110	Mg 2	N 8	O 12	0

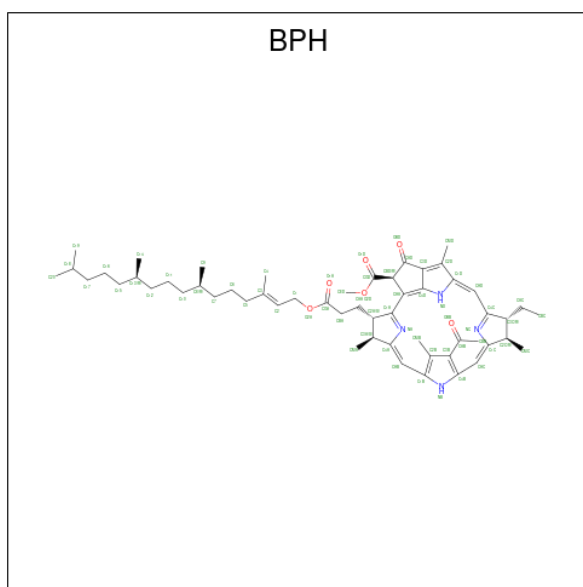
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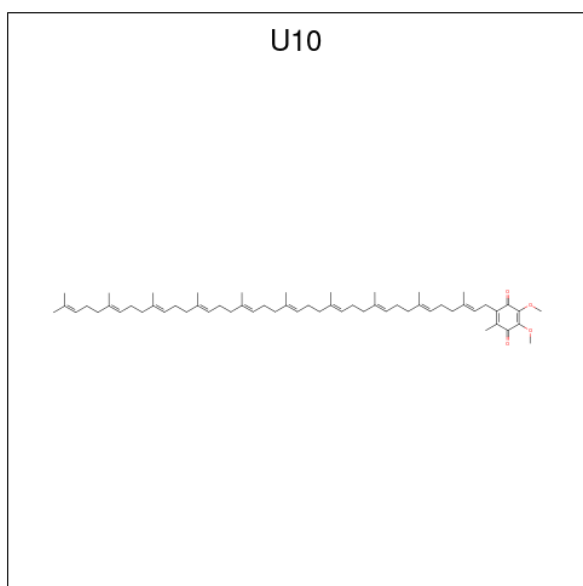
Mol	Chain	Residues	Atoms					AltConf
8	T	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	T	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	A	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	R	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	R	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	P	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	P	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	N	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	N	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	J	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	J	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	G	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	G	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	E	1	Total	C	Mg	N	O	0
			132	110	2	8	12	
8	E	1	Total	C	Mg	N	O	0
			132	110	2	8	12	

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



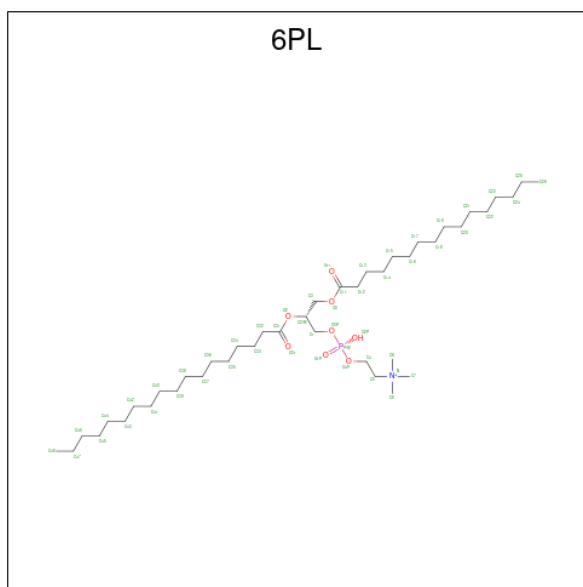
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	M	1	48	44	4	0

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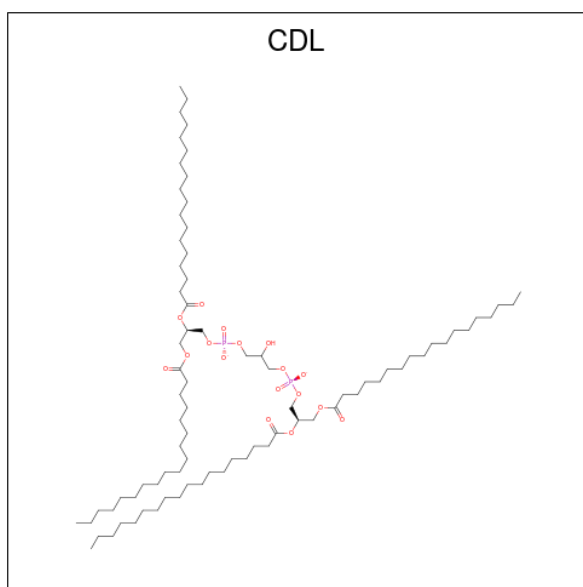
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	L	1	19	15	4	0
10	1	1	40	36	4	0

- Molecule 11 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: 6PL) (formula:  $C_{42}H_{85}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	M	1	52	42	1	8	1	0
11	H	1	52	42	1	8	1	0
11	E	1	40	30	1	8	1	0

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).

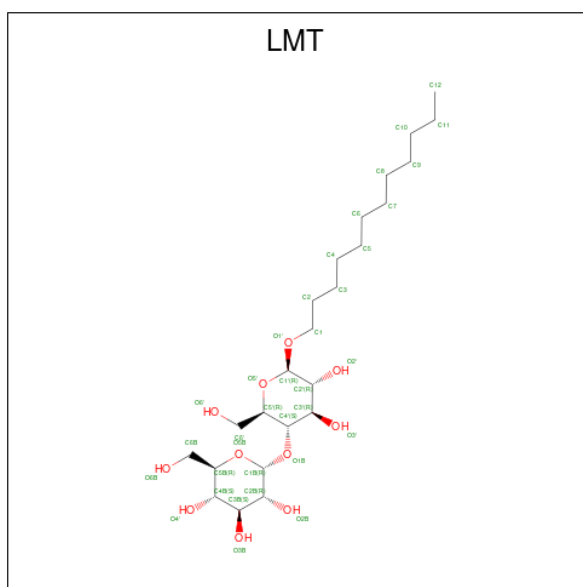


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	M	1	95	76	17	2	0
12	L	1	89	70	17	2	0
12	H	1	87	68	17	2	0
12	3	1	85	66	17	2	0
12	G	1	178	140	34	4	0
12	G	1	178	140	34	4	0

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 14 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



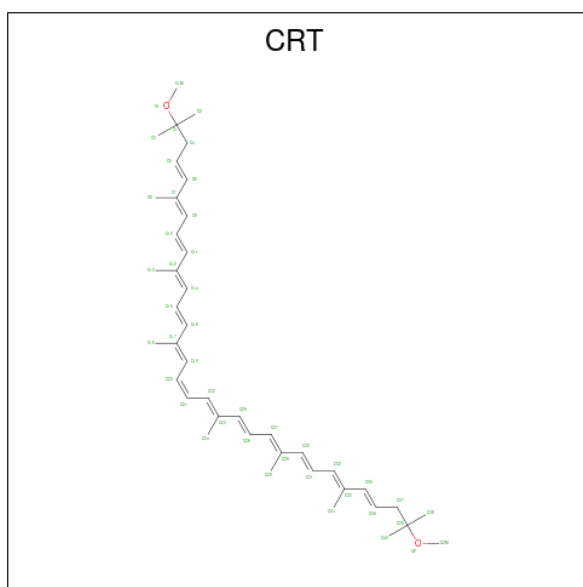
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	M	1	35	24	11	0
14	L	1	35	24	11	0
14	2	1	70	48	22	0
14	2	1	70	48	22	0
14	6	1	35	24	11	0
14	4	1	35	24	11	0
14	Z	1	35	24	11	0
14	X	1	70	48	22	0
14	X	1	70	48	22	0
14	U	1	70	48	22	0
14	U	1	70	48	22	0
14	B	1	70	48	22	0
14	B	1	70	48	22	0
14	D	1	101	68	33	0

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Mol	Chain	Residues	Atoms			AltConf
14	D	1	Total	C	O	0
			101	68	33	
14	D	1	Total	C	O	0
			101	68	33	
14	R	1	Total	C	O	0
			35	24	11	
14	S	1	Total	C	O	0
			70	48	22	
14	S	1	Total	C	O	0
			70	48	22	
14	Q	1	Total	C	O	0
			70	48	22	
14	Q	1	Total	C	O	0
			70	48	22	
14	O	1	Total	C	O	0
			35	24	11	
14	J	1	Total	C	O	0
			35	24	11	
14	K	1	Total	C	O	0
			70	48	22	
14	K	1	Total	C	O	0
			70	48	22	
14	I	1	Total	C	O	0
			70	48	22	
14	I	1	Total	C	O	0
			70	48	22	
14	F	1	Total	C	O	0
			70	48	22	
14	F	1	Total	C	O	0
			70	48	22	

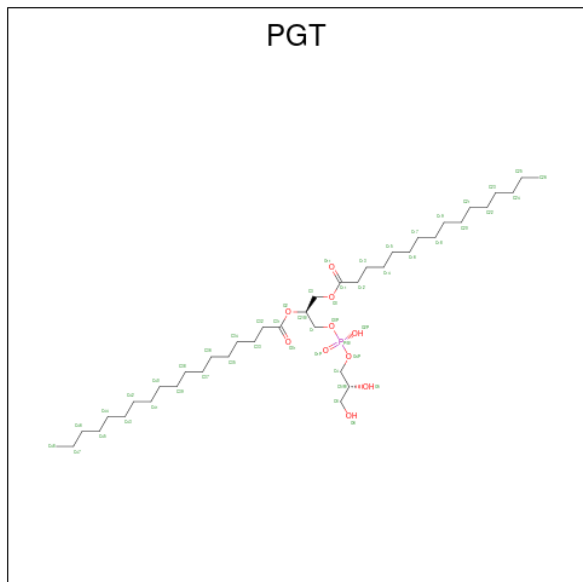
- Molecule 15 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	2	1	44	42	2	0
15	3	1	44	42	2	0
15	Z	1	44	42	2	0
15	X	1	44	42	2	0
15	B	1	44	42	2	0
15	D	1	44	42	2	0
15	R	1	44	42	2	0
15	S	1	44	42	2	0
15	Q	1	44	42	2	0
15	O	1	44	42	2	0
15	K	1	44	42	2	0
15	I	1	44	42	2	0
15	F	1	44	42	2	0

- Molecule 16 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}}(HYDROXY)PHOSPH

ORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	P	1	50	39	10	1	0

- Molecule 17 is water.

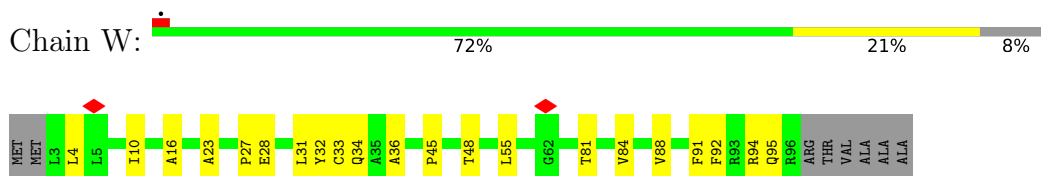
Mol	Chain	Residues	Atoms		AltConf
17	M	3	Total	O	0
			3	3	
17	L	5	Total	O	0
			5	5	
17	H	2	Total	O	0
			2	2	



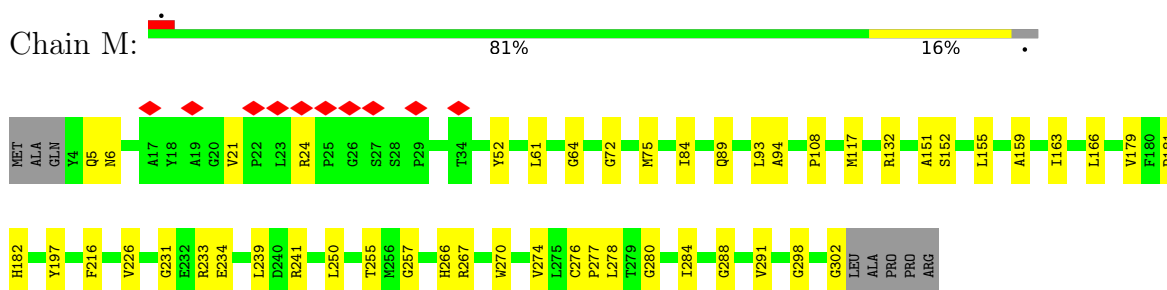
### 3 Residue-property plots [i](#)

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

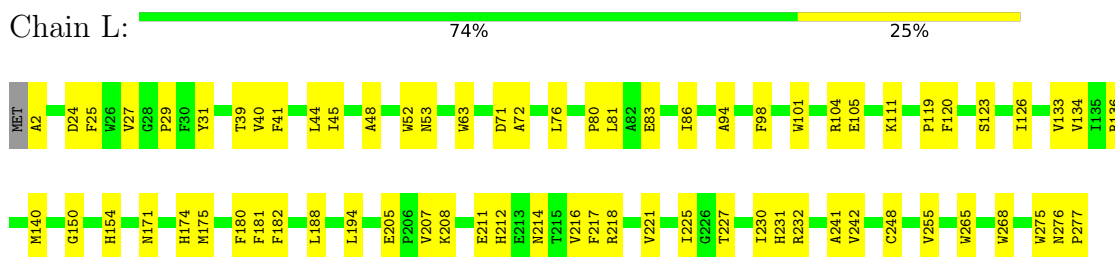
- Molecule 1: Light harvesting complex 1 Protein W



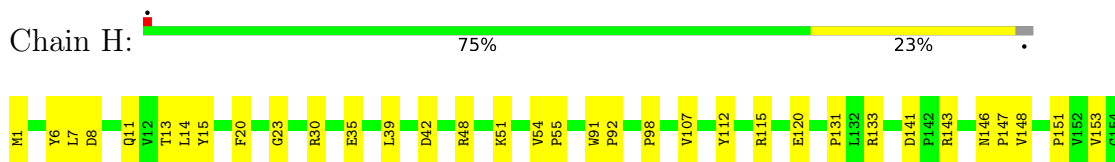
- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein L chain



- Molecule 4: H subunit of photosynthetic reaction center complex

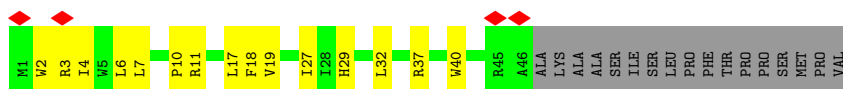




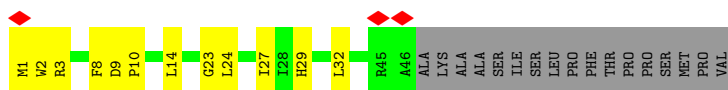
• Molecule 5: Light-harvesting complex 1 alpha chain



• Molecule 5: Light-harvesting complex 1 alpha chain



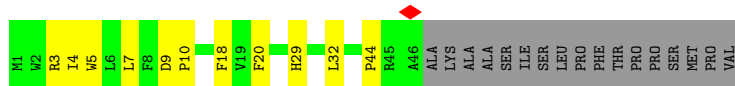
• Molecule 5: Light-harvesting complex 1 alpha chain



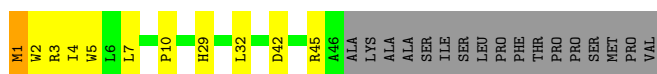
• Molecule 5: Light-harvesting complex 1 alpha chain



• Molecule 5: Light-harvesting complex 1 alpha chain



• Molecule 5: Light-harvesting complex 1 alpha chain



• Molecule 5: Light-harvesting complex 1 alpha chain

Chain A:  43% 21% 37%



• Molecule 5: Light-harvesting complex 1 alpha chain

Chain C:  46% 25% 27%



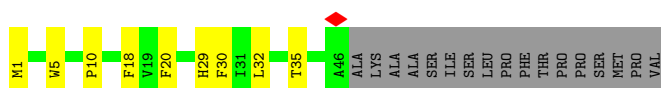
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain R:  51% 22% 27%



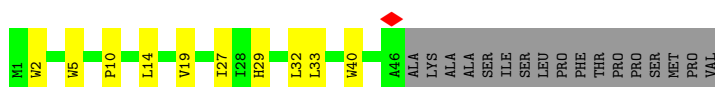
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain P:  59% 14% 27%



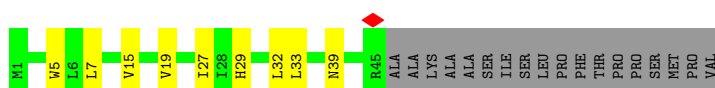
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain N:  57% 16% 27%



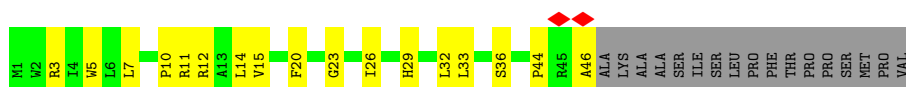
• Molecule 5: Light-harvesting complex 1 alpha chain

Chain J:  57% 14% 29%

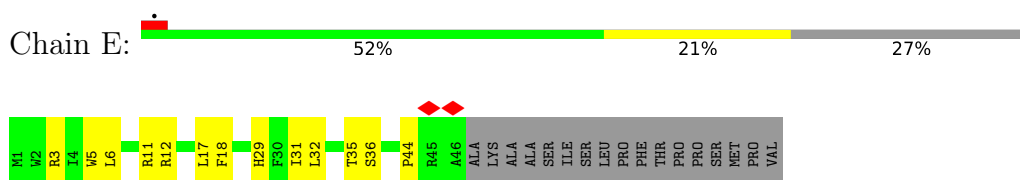


• Molecule 5: Light-harvesting complex 1 alpha chain

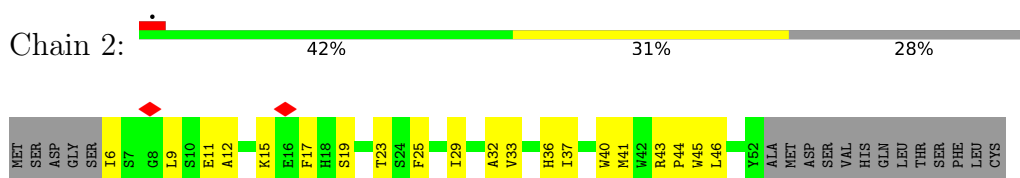
Chain G:  46% 27% 27%



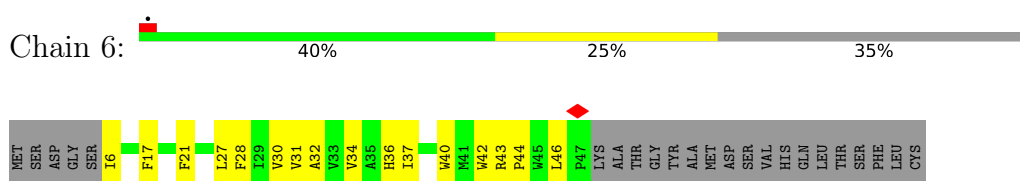
- Molecule 5: Light-harvesting complex 1 alpha chain



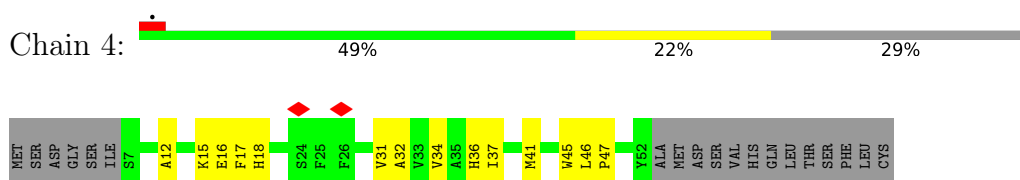
- Molecule 6: Light-harvesting complex 1 beta chain



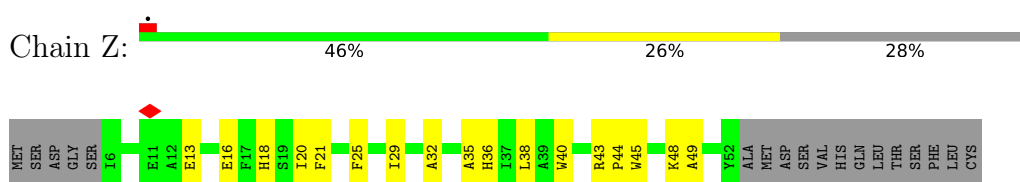
- Molecule 6: Light-harvesting complex 1 beta chain



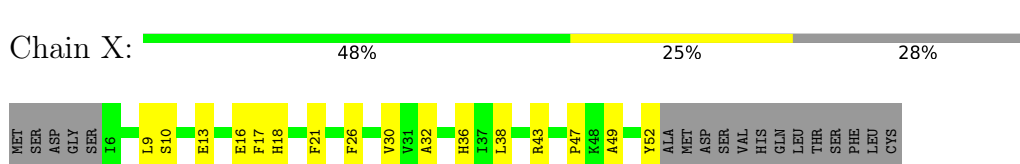
- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain





- Molecule 6: Light-harvesting complex 1 beta chain



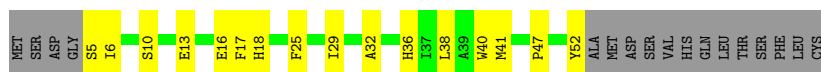
- Molecule 6: Light-harvesting complex 1 beta chain



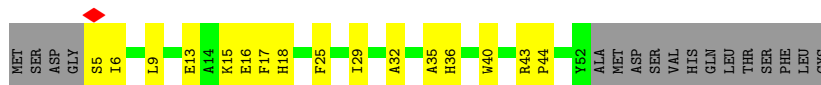
- Molecule 6: Light-harvesting complex 1 beta chain



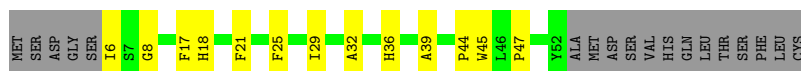
- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain

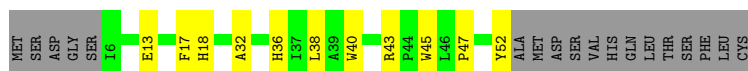


- Molecule 6: Light-harvesting complex 1 beta chain



- Molecule 6: Light-harvesting complex 1 beta chain

Chain I:  55% 17% 28%



- Molecule 6: Light-harvesting complex 1 beta chain

Chain F:  55% 18% 26%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	377703	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.804	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: QAK, PGT, FE, LMT, FME, U10, CRT, BCL, CDL, BPH, 6PL

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	W	0.31	0/696	0.47	0/949
2	M	0.41	0/2470	0.44	0/3379
3	L	0.45	0/2271	0.44	0/3109
4	H	0.39	0/1946	0.48	0/2663
5	1	0.37	0/401	0.44	0/546
5	3	0.33	0/401	0.46	0/546
5	5	0.29	0/401	0.46	0/546
5	A	0.38	0/365	0.42	0/497
5	C	0.42	0/401	0.43	0/546
5	E	0.42	0/401	0.42	0/546
5	G	0.41	0/401	0.42	0/546
5	J	0.39	0/396	0.39	0/539
5	N	0.39	0/401	0.41	0/546
5	P	0.39	0/401	0.42	0/546
5	R	0.40	0/401	0.46	0/546
5	T	0.40	0/413	0.47	0/562
5	V	0.38	0/401	0.47	0/546
5	Y	0.36	0/401	0.43	0/546
6	2	0.37	0/409	0.42	0/558
6	4	0.32	0/389	0.45	0/531
6	6	0.36	0/371	0.41	0/507
6	B	0.41	0/397	0.43	0/542
6	D	0.41	0/415	0.41	0/566
6	F	0.41	0/403	0.47	0/550
6	I	0.41	0/397	0.42	0/542
6	K	0.41	0/397	0.39	0/542
6	O	0.38	0/403	0.46	0/550
6	Q	0.39	0/415	0.46	0/566
6	S	0.40	0/415	0.42	0/566
6	U	0.39	0/409	0.41	0/558
6	X	0.39	0/409	0.48	0/558
6	Z	0.41	0/409	0.46	0/558



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.40	0/18606	0.44	0/25398

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	682	0	727	15	0
2	M	2381	0	2323	41	0
3	L	2185	0	2130	54	0
4	H	1894	0	1909	45	0
5	1	397	0	415	23	0
5	3	397	0	415	19	0
5	5	397	0	415	17	0
5	A	352	0	372	15	0
5	C	397	0	415	17	0
5	E	397	0	415	16	0
5	G	397	0	415	17	0
5	J	392	0	410	11	0
5	N	397	0	415	11	0
5	P	397	0	415	10	0
5	R	397	0	415	14	0
5	T	408	0	423	14	0
5	V	397	0	415	14	0
5	Y	397	0	415	16	0
6	2	393	0	388	21	0
6	4	374	0	369	17	0
6	6	356	0	351	15	0
6	B	382	0	380	10	0
6	D	399	0	393	11	0
6	F	388	0	385	14	0
6	I	382	0	380	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	382	0	380	14	0
6	O	388	0	385	15	0
6	Q	399	0	393	18	0
6	S	399	0	393	15	0
6	U	393	0	388	13	0
6	X	393	0	388	17	0
6	Z	393	0	388	20	0
7	M	41	0	0	0	0
8	1	66	0	74	11	0
8	2	66	0	74	5	0
8	3	66	0	74	6	0
8	4	66	0	74	5	0
8	5	132	0	148	15	0
8	A	132	0	148	19	0
8	C	66	0	74	5	0
8	D	66	0	74	6	0
8	E	132	0	148	13	0
8	G	132	0	148	11	0
8	J	132	0	148	16	0
8	L	132	0	148	7	0
8	M	132	0	148	9	0
8	N	132	0	148	17	0
8	P	132	0	148	6	0
8	R	132	0	148	10	0
8	T	132	0	148	10	0
8	V	132	0	148	9	0
8	Y	132	0	148	17	0
9	L	65	0	76	6	0
9	M	65	0	76	6	0
10	1	40	0	51	2	0
10	L	19	0	17	1	0
10	M	48	0	63	6	0
11	E	40	0	54	9	0
11	H	52	0	84	9	0
11	M	52	0	84	5	0
12	3	85	0	117	10	0
12	G	178	0	259	20	0
12	H	87	0	121	12	0
12	L	89	0	124	9	0
12	M	95	0	143	12	0
13	M	1	0	0	0	0
14	2	70	0	89	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	4	35	0	45	1	0
14	6	35	0	44	3	0
14	B	70	0	88	6	0
14	D	101	0	124	9	0
14	F	70	0	90	5	0
14	I	70	0	91	4	0
14	J	35	0	45	2	0
14	K	70	0	90	4	0
14	L	35	0	44	3	0
14	M	35	0	45	2	0
14	O	35	0	45	3	0
14	Q	70	0	90	2	0
14	R	35	0	44	4	0
14	S	70	0	90	3	0
14	U	70	0	90	2	0
14	X	70	0	91	5	0
14	Z	35	0	45	3	0
15	2	44	0	60	7	0
15	3	44	0	60	5	0
15	B	44	0	60	3	0
15	D	44	0	60	1	0
15	F	44	0	60	6	0
15	I	44	0	60	5	0
15	K	44	0	60	6	0
15	O	44	0	60	3	0
15	Q	44	0	60	2	0
15	R	44	0	60	2	0
15	S	44	0	60	1	0
15	X	44	0	60	8	0
15	Z	44	0	60	13	0
16	P	50	0	73	3	0
17	H	2	0	0	0	0
17	L	5	0	0	0	0
17	M	3	0	0	1	0
All	All	22794	0	24000	674	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 674 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)
12:H:302:CDL:H581	11:E:101:6PL:H381	1.52	0.90
3:L:63:TRP:HE1	11:H:301:6PL:H61	1.39	0.87
3:L:221:VAL:HG23	8:L:401:BCL:H112	1.57	0.84
5:C:32:LEU:HD11	8:D:104:BCL:HHD	1.64	0.80
8:5:101:BCL:HMB2	15:3:103:CRT:H35	1.64	0.79

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	92/102 (90%)	83 (90%)	9 (10%)	0	100	100
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
3	L	274/277 (99%)	266 (97%)	8 (3%)	0	100	100
4	H	249/255 (98%)	226 (91%)	23 (9%)	0	100	100
5	1	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	3	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
5	5	44/63 (70%)	38 (86%)	6 (14%)	0	100	100
5	A	38/63 (60%)	35 (92%)	3 (8%)	0	100	100
5	C	44/63 (70%)	44 (100%)	0	0	100	100
5	E	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	G	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
5	J	43/63 (68%)	42 (98%)	1 (2%)	0	100	100
5	N	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
5	P	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
5	R	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
5	T	45/63 (71%)	41 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	V	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
5	Y	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
6	2	46/65 (71%)	42 (91%)	4 (9%)	0	100	100
6	4	44/65 (68%)	41 (93%)	3 (7%)	0	100	100
6	6	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
6	B	45/65 (69%)	41 (91%)	4 (9%)	0	100	100
6	D	47/65 (72%)	45 (96%)	2 (4%)	0	100	100
6	F	46/65 (71%)	41 (89%)	5 (11%)	0	100	100
6	I	45/65 (69%)	42 (93%)	3 (7%)	0	100	100
6	K	45/65 (69%)	43 (96%)	2 (4%)	0	100	100
6	O	46/65 (71%)	42 (91%)	4 (9%)	0	100	100
6	Q	47/65 (72%)	45 (96%)	2 (4%)	0	100	100
6	S	47/65 (72%)	43 (92%)	4 (8%)	0	100	100
6	U	46/65 (71%)	42 (91%)	4 (9%)	0	100	100
6	X	46/65 (71%)	44 (96%)	2 (4%)	0	100	100
6	Z	46/65 (71%)	44 (96%)	2 (4%)	0	100	100
All	All	2159/2733 (79%)	2037 (94%)	122 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	65/70 (93%)	65 (100%)	0	100	100
2	M	241/247 (98%)	241 (100%)	0	100	100
3	L	222/223 (100%)	220 (99%)	2 (1%)	78	87
4	H	199/203 (98%)	199 (100%)	0	100	100
5	1	40/54 (74%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	3	40/54 (74%)	40 (100%)	0	100	100
5	5	40/54 (74%)	39 (98%)	1 (2%)	47	66
5	A	37/54 (68%)	37 (100%)	0	100	100
5	C	40/54 (74%)	40 (100%)	0	100	100
5	E	40/54 (74%)	40 (100%)	0	100	100
5	G	40/54 (74%)	40 (100%)	0	100	100
5	J	40/54 (74%)	40 (100%)	0	100	100
5	N	40/54 (74%)	40 (100%)	0	100	100
5	P	40/54 (74%)	40 (100%)	0	100	100
5	R	40/54 (74%)	40 (100%)	0	100	100
5	T	41/54 (76%)	41 (100%)	0	100	100
5	V	40/54 (74%)	40 (100%)	0	100	100
5	Y	40/54 (74%)	39 (98%)	1 (2%)	47	66
6	2	40/55 (73%)	40 (100%)	0	100	100
6	4	38/55 (69%)	38 (100%)	0	100	100
6	6	37/55 (67%)	37 (100%)	0	100	100
6	B	39/55 (71%)	39 (100%)	0	100	100
6	D	41/55 (74%)	41 (100%)	0	100	100
6	F	40/55 (73%)	40 (100%)	0	100	100
6	I	39/55 (71%)	39 (100%)	0	100	100
6	K	39/55 (71%)	39 (100%)	0	100	100
6	O	40/55 (73%)	40 (100%)	0	100	100
6	Q	41/55 (74%)	41 (100%)	0	100	100
6	S	41/55 (74%)	41 (100%)	0	100	100
6	U	40/55 (73%)	40 (100%)	0	100	100
6	X	40/55 (73%)	40 (100%)	0	100	100
6	Z	40/55 (73%)	40 (100%)	0	100	100
All	All	1840/2269 (81%)	1836 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	248	CYS

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Mol	Chain	Res	Type
3	L	275	TRP
5	5	3	ARG
5	Y	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
6	O	18	HIS
6	F	18	HIS
6	I	18	HIS
6	X	18	HIS
6	Q	18	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FME	R	1	5	8,9,10	0.94	0	7,9,11	0.92	0
5	FME	V	1	5	8,9,10	0.96	0	7,9,11	0.99	0
5	FME	C	1	5	8,9,10	0.98	1 (12%)	7,9,11	1.11	1 (14%)
5	FME	N	1	5	8,9,10	0.94	0	7,9,11	0.75	0
5	FME	E	1	5	8,9,10	0.93	0	7,9,11	0.76	0
5	FME	Y	1	5	8,9,10	0.93	0	7,9,11	1.14	0
5	FME	G	1	5	8,9,10	0.96	0	7,9,11	0.82	0
5	FME	5	1	5	8,9,10	0.95	0	7,9,11	0.89	0
5	FME	T	1	5	8,9,10	0.89	0	7,9,11	1.79	2 (28%)
5	FME	1	1	5	8,9,10	0.96	0	7,9,11	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	FME	J	1	5	8,9,10	0.96	0	7,9,11	1.06	0
5	FME	P	1	5	8,9,10	0.94	0	7,9,11	1.25	1 (14%)
5	FME	3	1	5	8,9,10	0.98	0	7,9,11	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FME	R	1	5	-	1/7/9/11	-
5	FME	V	1	5	-	2/7/9/11	-
5	FME	C	1	5	-	3/7/9/11	-
5	FME	N	1	5	-	2/7/9/11	-
5	FME	E	1	5	-	3/7/9/11	-
5	FME	Y	1	5	-	3/7/9/11	-
5	FME	G	1	5	-	2/7/9/11	-
5	FME	5	1	5	-	5/7/9/11	-
5	FME	T	1	5	-	3/7/9/11	-
5	FME	1	1	5	-	0/7/9/11	-
5	FME	J	1	5	-	3/7/9/11	-
5	FME	P	1	5	-	5/7/9/11	-
5	FME	3	1	5	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	FME	CA-N	-2.03	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	1	FME	CA-N-CN	3.39	128.03	122.82
5	T	1	FME	C-CA-N	3.03	115.19	109.73
5	P	1	FME	C-CA-N	2.62	114.45	109.73
5	C	1	FME	C-CA-N	2.06	113.44	109.73

There are no chirality outliers.

5 of 34 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
5	5	1	FME	N-CA-CB-CG
5	5	1	FME	O-C-CA-CB
5	5	1	FME	CA-CB-CG-SD
5	Y	1	FME	N-CA-CB-CG
5	Y	1	FME	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	FME	1	0
5	Y	1	FME	2	0
5	T	1	FME	2	0
5	1	1	FME	1	0
5	3	1	FME	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 1 is monoatomic - leaving 90 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CRT	O	102	-	41,43,43	1.89	12 (29%)	50,54,54	1.71	12 (24%)
8	BCL	E	103	-	58,74,74	1.63	8 (13%)	69,115,115	1.62	12 (17%)
15	CRT	K	103	-	41,43,43	1.90	12 (29%)	50,54,54	1.70	14 (28%)
15	CRT	B	103	-	41,43,43	1.88	12 (29%)	50,54,54	1.62	14 (28%)
14	LMT	U	101	-	36,36,36	1.21	6 (16%)	47,47,47	1.02	2 (4%)
15	CRT	3	103	-	41,43,43	1.94	12 (29%)	50,54,54	1.71	13 (26%)
8	BCL	L	402	-	58,74,74	1.63	9 (15%)	69,115,115	1.71	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	CDL	G	101	-	87,87,99	0.30	0	93,99,111	0.41	0
8	BCL	P	103	-	58,74,74	1.64	9 (15%)	69,115,115	1.71	14 (20%)
15	CRT	2	102	-	41,43,43	1.96	12 (29%)	50,54,54	1.76	15 (30%)
8	BCL	J	103	-	58,74,74	1.65	9 (15%)	69,115,115	1.72	13 (18%)
8	BCL	V	102	-	58,74,74	1.65	9 (15%)	69,115,115	1.65	12 (17%)
11	6PL	H	301	-	51,51,51	0.30	0	57,59,59	0.40	0
14	LMT	F	101	-	36,36,36	1.20	6 (16%)	47,47,47	1.01	1 (2%)
8	BCL	M	407	-	58,74,74	1.63	9 (15%)	69,115,115	1.83	14 (20%)
14	LMT	D	102	-	36,36,36	1.16	4 (11%)	47,47,47	0.95	2 (4%)
14	LMT	S	101	-	36,36,36	1.19	5 (13%)	47,47,47	1.03	2 (4%)
9	BPH	L	403	-	51,70,70	0.60	2 (3%)	52,101,101	0.75	2 (3%)
8	BCL	Y	102	-	58,74,74	1.64	8 (13%)	69,115,115	1.64	13 (18%)
12	CDL	G	104	-	89,89,99	0.29	0	95,101,111	0.41	0
14	LMT	F	102	-	36,36,36	1.12	5 (13%)	47,47,47	0.97	2 (4%)
14	LMT	I	101	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	3 (6%)
8	BCL	A	101	-	58,74,74	1.62	9 (15%)	69,115,115	1.68	16 (23%)
12	CDL	M	406	-	94,94,99	0.28	0	100,106,111	0.35	0
14	LMT	Q	102	-	36,36,36	1.25	6 (16%)	47,47,47	1.11	3 (6%)
8	BCL	Y	101	-	58,74,74	1.62	8 (13%)	69,115,115	1.74	13 (18%)
8	BCL	V	101	-	58,74,74	1.61	9 (15%)	69,115,115	1.72	13 (18%)
14	LMT	I	102	-	36,36,36	1.22	6 (16%)	47,47,47	1.02	1 (2%)
14	LMT	O	101	-	36,36,36	1.13	5 (13%)	47,47,47	1.07	2 (4%)
12	CDL	H	302	-	86,86,99	0.30	0	92,98,111	0.39	0
7	QAK	M	401	-	40,40,40	1.28	3 (7%)	45,49,49	0.81	2 (4%)
8	BCL	J	102	-	58,74,74	1.61	9 (15%)	69,115,115	1.75	13 (18%)
8	BCL	3	101	-	58,74,74	1.65	11 (18%)	69,115,115	1.69	13 (18%)
14	LMT	M	409	-	36,36,36	1.25	6 (16%)	47,47,47	1.03	3 (6%)
8	BCL	G	102	-	58,74,74	1.61	8 (13%)	69,115,115	1.70	14 (20%)
8	BCL	D	104	-	58,74,74	1.64	10 (17%)	69,115,115	1.69	13 (18%)
14	LMT	K	102	-	36,36,36	1.18	6 (16%)	47,47,47	1.05	3 (6%)
15	CRT	X	102	-	41,43,43	1.94	12 (29%)	50,54,54	1.71	14 (28%)
8	BCL	G	103	-	58,74,74	1.64	8 (13%)	69,115,115	1.68	12 (17%)
14	LMT	2	104	-	36,36,36	1.19	5 (13%)	47,47,47	0.97	2 (4%)
14	LMT	X	101	-	36,36,36	1.28	8 (22%)	47,47,47	1.13	4 (8%)
14	LMT	K	101	-	36,36,36	1.18	5 (13%)	47,47,47	0.96	1 (2%)
14	LMT	4	102	-	36,36,36	1.21	5 (13%)	47,47,47	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	LMT	U	102	-	36,36,36	1.17	5 (13%)	47,47,47	1.04	3 (6%)
15	CRT	R	101	-	41,43,43	1.86	12 (29%)	50,54,54	1.58	12 (24%)
12	CDL	3	102	-	84,84,99	0.30	0	90,96,111	0.42	0
14	LMT	Q	101	-	36,36,36	1.22	5 (13%)	47,47,47	1.06	3 (6%)
11	6PL	M	405	-	51,51,51	0.29	0	57,59,59	0.35	0
8	BCL	1	101	-	58,74,74	1.62	10 (17%)	69,115,115	1.72	14 (20%)
16	PGT	P	102	-	49,49,50	0.28	0	52,55,56	0.41	0
8	BCL	R	103	-	58,74,74	1.64	8 (13%)	69,115,115	1.69	12 (17%)
8	BCL	N	102	-	58,74,74	1.63	8 (13%)	69,115,115	1.71	14 (20%)
14	LMT	X	103	-	36,36,36	1.21	6 (16%)	47,47,47	1.03	2 (4%)
12	CDL	L	404	-	87,87,99	0.29	0	91,98,111	0.38	0
8	BCL	E	102	-	58,74,74	1.63	10 (17%)	69,115,115	1.78	15 (21%)
10	U10	L	406	-	19,19,63	2.78	8 (42%)	23,26,79	1.37	3 (13%)
8	BCL	5	102	-	58,74,74	1.70	11 (18%)	69,115,115	1.59	11 (15%)
9	BPH	M	403	-	51,70,70	0.64	2 (3%)	52,101,101	0.72	1 (1%)
14	LMT	Z	102	-	36,36,36	1.17	6 (16%)	47,47,47	1.02	3 (6%)
14	LMT	R	102	-	36,36,36	1.24	6 (16%)	47,47,47	0.97	1 (2%)
14	LMT	D	101	-	36,36,36	1.24	6 (16%)	47,47,47	1.06	3 (6%)
8	BCL	P	101	-	58,74,74	1.59	9 (15%)	69,115,115	1.72	13 (18%)
15	CRT	Z	101	-	41,43,43	1.93	12 (29%)	50,54,54	1.88	13 (26%)
8	BCL	M	402	-	58,74,74	1.65	10 (17%)	69,115,115	1.87	18 (26%)
14	LMT	6	101	-	36,36,36	1.15	5 (13%)	47,47,47	0.94	1 (2%)
10	U10	M	404	-	48,48,63	2.65	14 (29%)	58,61,79	1.71	13 (22%)
8	BCL	5	101	-	58,74,74	1.64	10 (17%)	69,115,115	1.65	16 (23%)
14	LMT	S	102	-	36,36,36	1.18	5 (13%)	47,47,47	1.18	3 (6%)
8	BCL	T	102	-	58,74,74	1.63	9 (15%)	69,115,115	1.64	13 (18%)
14	LMT	B	101	-	36,36,36	1.21	6 (16%)	47,47,47	0.97	1 (2%)
8	BCL	R	104	-	58,74,74	1.65	10 (17%)	69,115,115	1.72	12 (17%)
14	LMT	2	103	-	36,36,36	1.22	6 (16%)	47,47,47	1.03	2 (4%)
15	CRT	I	103	-	41,43,43	1.86	13 (31%)	50,54,54	1.57	12 (24%)
14	LMT	J	101	-	36,36,36	1.20	4 (11%)	47,47,47	1.16	2 (4%)
14	LMT	D	103	-	32,32,36	1.33	7 (21%)	43,43,47	1.16	3 (6%)
15	CRT	F	103	-	41,43,43	1.90	12 (29%)	50,54,54	1.64	13 (26%)
8	BCL	N	101	-	58,74,74	1.61	8 (13%)	69,115,115	1.69	13 (18%)
8	BCL	L	401	-	58,74,74	1.63	9 (15%)	69,115,115	1.77	16 (23%)
11	6PL	E	101	-	39,39,51	0.33	0	45,47,59	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CRT	D	105	-	41,43,43	1.90	12 (29%)	50,54,54	1.64	14 (28%)
15	CRT	S	103	-	41,43,43	1.86	12 (29%)	50,54,54	1.65	13 (26%)
8	BCL	C	100	-	58,74,74	1.61	8 (13%)	69,115,115	1.74	15 (21%)
10	U10	1	102	-	40,40,63	2.69	11 (27%)	48,51,79	1.75	13 (27%)
15	CRT	Q	103	-	41,43,43	1.87	12 (29%)	50,54,54	1.59	13 (26%)
8	BCL	4	101	-	58,74,74	1.71	12 (20%)	69,115,115	1.60	12 (17%)
8	BCL	T	101	-	58,74,74	1.62	8 (13%)	69,115,115	1.73	14 (20%)
14	LMT	B	102	-	36,36,36	1.17	5 (13%)	47,47,47	1.10	3 (6%)
8	BCL	A	102	-	58,74,74	1.64	8 (13%)	69,115,115	1.64	12 (17%)
14	LMT	L	405	-	36,36,36	1.19	5 (13%)	47,47,47	1.12	3 (6%)
8	BCL	2	101	-	58,74,74	1.67	10 (17%)	69,115,115	1.63	12 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CRT	O	102	-	-	1/51/51/51	-
8	BCL	E	103	-	-	13/37/137/137	-
15	CRT	K	103	-	-	0/51/51/51	-
15	CRT	B	103	-	-	0/51/51/51	-
14	LMT	U	101	-	-	8/21/61/61	0/2/2/2
15	CRT	3	103	-	-	1/51/51/51	-
8	BCL	L	402	-	-	10/37/137/137	-
12	CDL	G	101	-	-	24/98/98/110	-
8	BCL	P	103	-	-	15/37/137/137	-
15	CRT	2	102	-	-	3/51/51/51	-
8	BCL	J	103	-	-	20/37/137/137	-
8	BCL	V	102	-	-	14/37/137/137	-
11	6PL	H	301	-	-	16/55/55/55	-
14	LMT	F	101	-	-	8/21/61/61	0/2/2/2
8	BCL	M	407	-	-	4/37/137/137	-
14	LMT	D	102	-	-	8/21/61/61	0/2/2/2
14	LMT	S	101	-	-	13/21/61/61	0/2/2/2
9	BPH	L	403	-	2/2/18/22	7/37/105/105	0/5/6/6
8	BCL	Y	102	-	-	19/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	G	104	-	-	22/100/100/110	-
14	LMT	F	102	-	-	14/21/61/61	0/2/2/2
14	LMT	I	101	-	-	9/21/61/61	0/2/2/2
8	BCL	A	101	-	-	15/37/137/137	-
12	CDL	M	406	-	-	25/105/105/110	-
14	LMT	Q	102	-	-	8/21/61/61	0/2/2/2
8	BCL	Y	101	-	-	16/37/137/137	-
8	BCL	V	101	-	-	16/37/137/137	-
14	LMT	I	102	-	-	8/21/61/61	0/2/2/2
14	LMT	O	101	-	-	6/21/61/61	0/2/2/2
12	CDL	H	302	-	-	19/97/97/110	-
7	QAK	M	401	-	1/1/8/12	25/44/44/44	-
8	BCL	J	102	-	-	16/37/137/137	-
8	BCL	3	101	-	-	15/37/137/137	-
14	LMT	M	409	-	-	9/21/61/61	0/2/2/2
8	BCL	G	102	-	-	14/37/137/137	-
8	BCL	D	104	-	-	12/37/137/137	-
14	LMT	K	102	-	-	10/21/61/61	0/2/2/2
15	CRT	X	102	-	-	2/51/51/51	-
8	BCL	G	103	-	-	20/37/137/137	-
14	LMT	2	104	-	-	9/21/61/61	0/2/2/2
14	LMT	X	101	-	-	13/21/61/61	0/2/2/2
14	LMT	K	101	-	-	11/21/61/61	0/2/2/2
14	LMT	4	102	-	-	6/21/61/61	0/2/2/2
14	LMT	U	102	-	-	13/21/61/61	0/2/2/2
15	CRT	R	101	-	-	0/51/51/51	-
12	CDL	3	102	-	-	14/95/95/110	-
14	LMT	Q	101	-	-	13/21/61/61	0/2/2/2
11	6PL	M	405	-	-	6/55/55/55	-
8	BCL	1	101	-	-	17/37/137/137	-
16	PGT	P	102	-	-	15/54/54/55	-
8	BCL	R	103	-	-	15/37/137/137	-
8	BCL	N	102	-	-	16/37/137/137	-
14	LMT	X	103	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CDL	L	404	-	-	12/96/96/110	-
8	BCL	E	102	-	-	14/37/137/137	-
10	U10	L	406	-	-	1/11/35/87	0/1/1/1
8	BCL	5	102	-	-	15/37/137/137	-
9	BPH	M	403	-	2/2/18/22	2/37/105/105	0/5/6/6
14	LMT	Z	102	-	-	11/21/61/61	0/2/2/2
14	LMT	R	102	-	-	8/21/61/61	0/2/2/2
14	LMT	D	101	-	-	9/21/61/61	0/2/2/2
8	BCL	P	101	-	-	15/37/137/137	-
15	CRT	Z	101	-	-	0/51/51/51	-
8	BCL	M	402	-	-	13/37/137/137	-
14	LMT	6	101	-	-	10/21/61/61	0/2/2/2
10	U10	M	404	-	-	10/45/69/87	0/1/1/1
8	BCL	5	101	-	-	16/37/137/137	-
14	LMT	S	102	-	-	12/21/61/61	0/2/2/2
8	BCL	T	102	-	-	17/37/137/137	-
14	LMT	B	101	-	-	12/21/61/61	0/2/2/2
8	BCL	R	104	-	-	14/37/137/137	-
14	LMT	2	103	-	-	12/21/61/61	0/2/2/2
15	CRT	I	103	-	-	0/51/51/51	-
14	LMT	J	101	-	-	7/21/61/61	0/2/2/2
14	LMT	D	103	-	-	9/17/57/61	0/2/2/2
15	CRT	F	103	-	-	3/51/51/51	-
8	BCL	N	101	-	-	13/37/137/137	-
8	BCL	L	401	-	-	23/37/137/137	-
11	6PL	E	101	-	-	9/43/43/55	-
15	CRT	D	105	-	-	2/51/51/51	-
15	CRT	S	103	-	-	0/51/51/51	-
8	BCL	C	100	-	-	20/37/137/137	-
10	U10	1	102	-	-	16/36/60/87	0/1/1/1
15	CRT	Q	103	-	-	1/51/51/51	-
8	BCL	4	101	-	-	16/37/137/137	-
8	BCL	T	101	-	-	20/37/137/137	-
14	LMT	B	102	-	-	7/21/61/61	0/2/2/2
8	BCL	A	102	-	-	15/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LMT	L	405	-	-	12/21/61/61	0/2/2/2
8	BCL	2	101	-	-	14/37/137/137	-

The worst 5 of 648 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1	102	U10	C18-C19	6.20	1.47	1.33
10	L	406	U10	C8-C9	6.08	1.47	1.33
10	1	102	U10	C23-C24	6.01	1.47	1.33
10	1	102	U10	C28-C29	6.00	1.47	1.33
10	1	102	U10	C13-C14	5.96	1.47	1.33

The worst 5 of 704 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	401	BCL	O2D-CGD-CBD	6.01	121.96	111.27
8	M	407	BCL	O2D-CGD-CBD	5.83	121.62	111.27
8	M	402	BCL	CHD-C4C-NC	5.25	130.91	125.08
8	5	102	BCL	C4B-CHC-C1C	-5.19	119.84	130.12
8	T	101	BCL	CMB-C2B-C3B	5.08	134.18	124.68

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	401	QAK	CE2
9	M	403	BPH	C8
9	M	403	BPH	C13
9	L	403	BPH	C8
9	L	403	BPH	C13

5 of 1012 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	401	QAK	CE3-CD2-CE2-CZ2
7	M	401	QAK	CE3-CD2-CE2-C39
7	M	401	QAK	C37-C14-C15-C16
7	M	401	QAK	C22-C23-C24-C25
8	M	407	BCL	C4C-C3C-CAC-CBC

There are no ring outliers.

88 monomers are involved in 368 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	102	CRT	3	0
8	E	103	BCL	5	0
15	K	103	CRT	6	0
15	B	103	CRT	3	0
14	U	101	LMT	2	0
15	3	103	CRT	5	0
8	L	402	BCL	1	0
12	G	101	CDL	13	0
8	P	103	BCL	4	0
15	2	102	CRT	7	0
8	J	103	BCL	9	0
8	V	102	BCL	7	0
11	H	301	6PL	9	0
14	F	101	LMT	5	0
8	M	407	BCL	3	0
14	D	102	LMT	3	0
14	S	101	LMT	3	0
9	L	403	BPH	6	0
8	Y	102	BCL	9	0
12	G	104	CDL	8	0
14	F	102	LMT	1	0
14	I	101	LMT	2	0
8	A	101	BCL	8	0
12	M	406	CDL	12	0
8	Y	101	BCL	8	0
8	V	101	BCL	2	0
14	I	102	LMT	2	0
14	O	101	LMT	3	0
12	H	302	CDL	12	0
8	J	102	BCL	7	0
8	3	101	BCL	6	0
14	M	409	LMT	2	0
8	G	102	BCL	3	0
8	D	104	BCL	6	0
14	K	102	LMT	1	0
15	X	102	CRT	8	0
8	G	103	BCL	8	0
14	2	104	LMT	2	0
14	X	101	LMT	3	0
14	K	101	LMT	3	0
14	4	102	LMT	1	0
14	U	102	LMT	1	0
15	R	101	CRT	2	0

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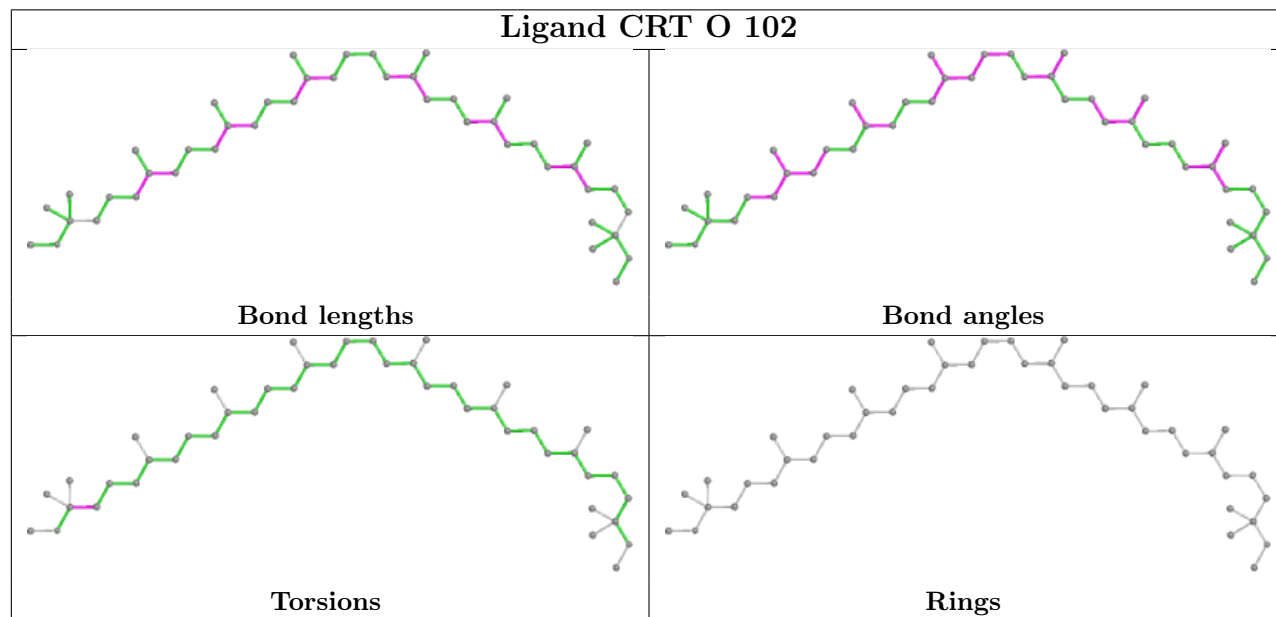
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	3	102	CDL	10	0
14	Q	101	LMT	2	0
11	M	405	6PL	5	0
8	1	101	BCL	11	0
16	P	102	PGT	3	0
8	R	103	BCL	6	0
8	N	102	BCL	7	0
14	X	103	LMT	2	0
12	L	404	CDL	9	0
8	E	102	BCL	8	0
10	L	406	U10	1	0
8	5	102	BCL	6	0
9	M	403	BPH	6	0
14	Z	102	LMT	3	0
14	R	102	LMT	4	0
14	D	101	LMT	6	0
8	P	101	BCL	2	0
15	Z	101	CRT	13	0
8	M	402	BCL	6	0
14	6	101	LMT	3	0
10	M	404	U10	6	0
8	5	101	BCL	9	0
14	S	102	LMT	1	0
8	T	102	BCL	8	0
14	B	101	LMT	3	0
8	R	104	BCL	4	0
14	2	103	LMT	3	0
15	I	103	CRT	5	0
14	J	101	LMT	2	0
14	D	103	LMT	2	0
15	F	103	CRT	6	0
8	N	101	BCL	10	0
8	L	401	BCL	6	0
11	E	101	6PL	9	0
15	D	105	CRT	1	0
15	S	103	CRT	1	0
8	C	100	BCL	5	0
10	1	102	U10	2	0
15	Q	103	CRT	2	0
8	4	101	BCL	5	0
8	T	101	BCL	2	0
14	B	102	LMT	3	0

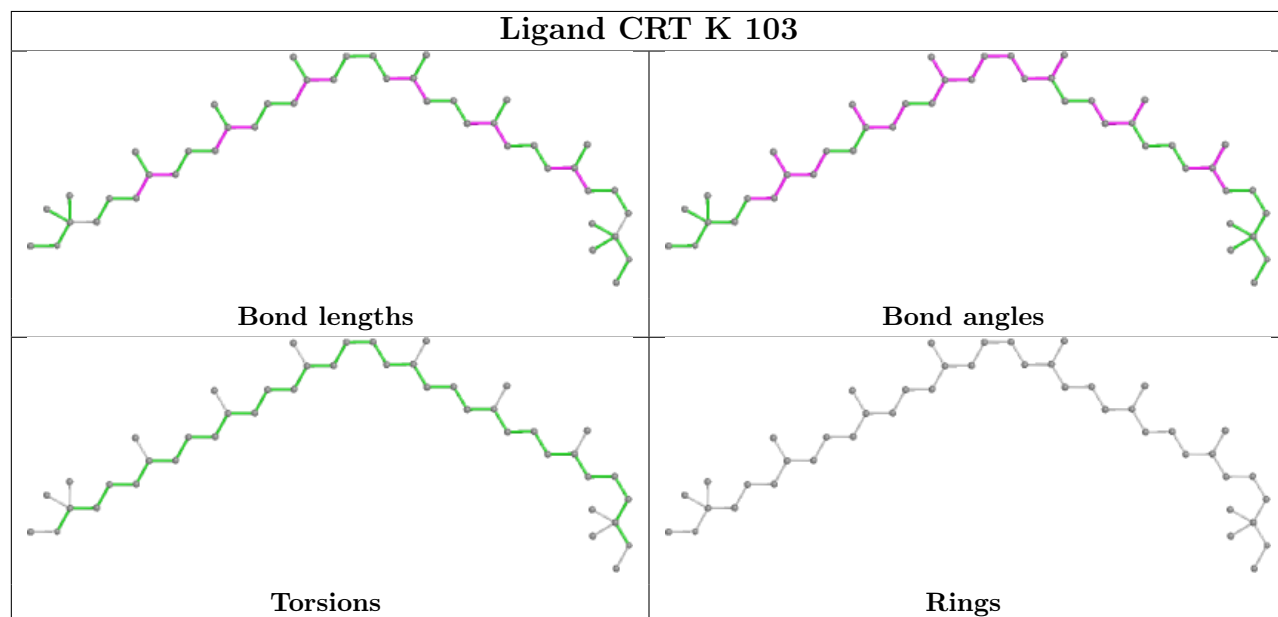
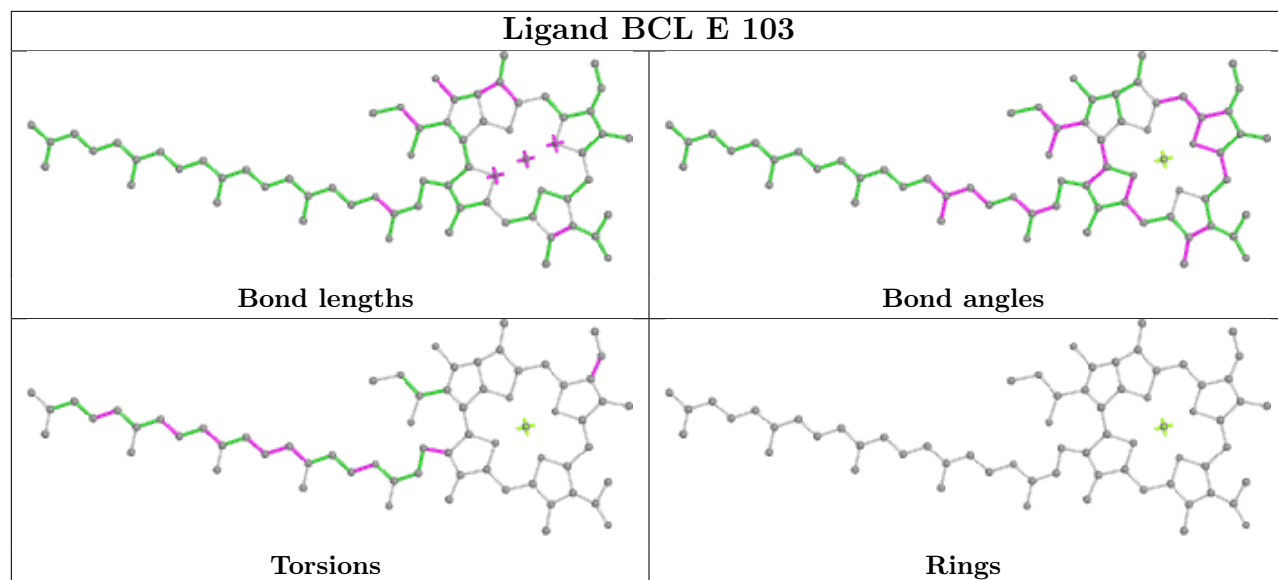
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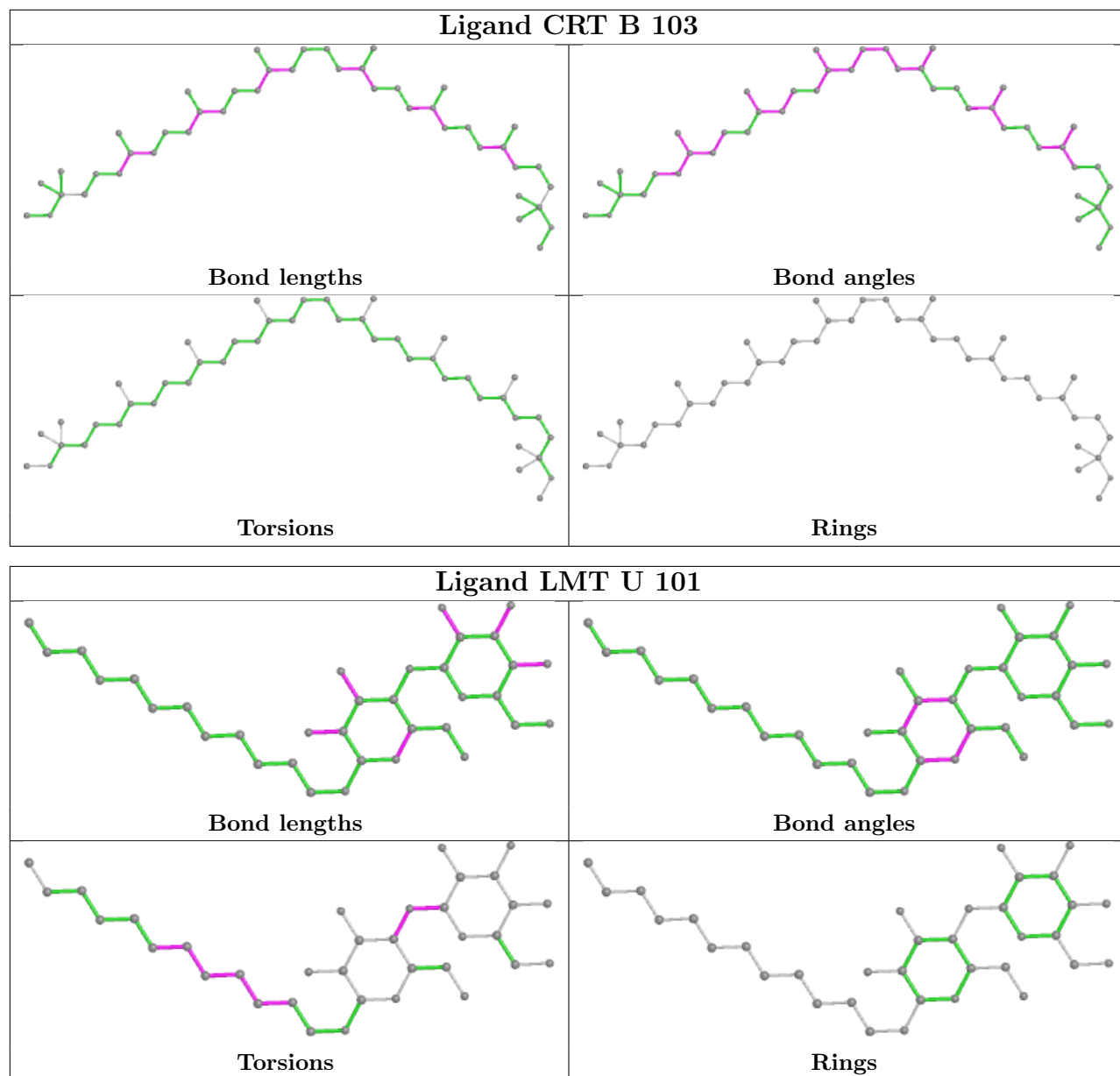
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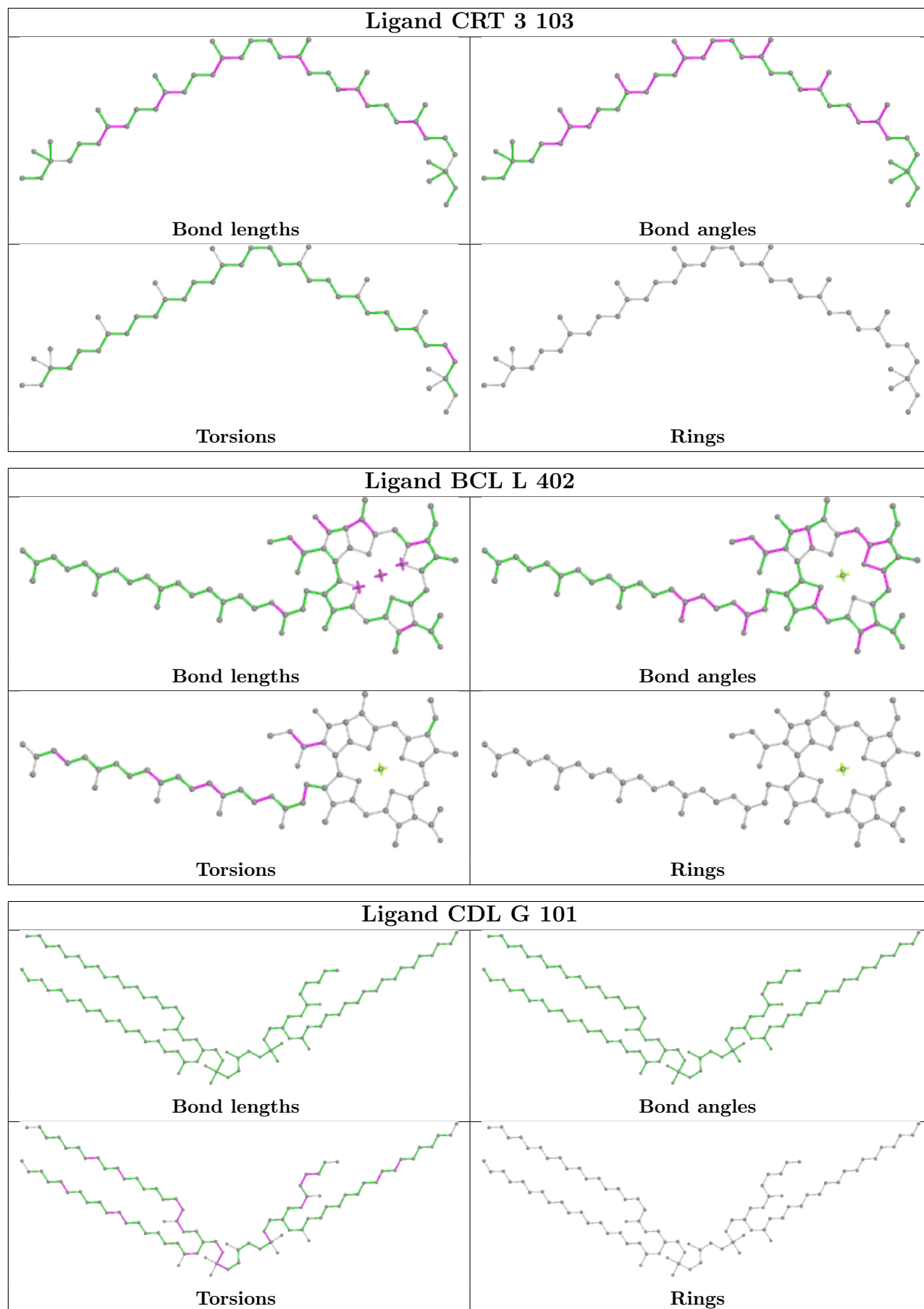
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	102	BCL	11	0
14	L	405	LMT	3	0
8	2	101	BCL	5	0

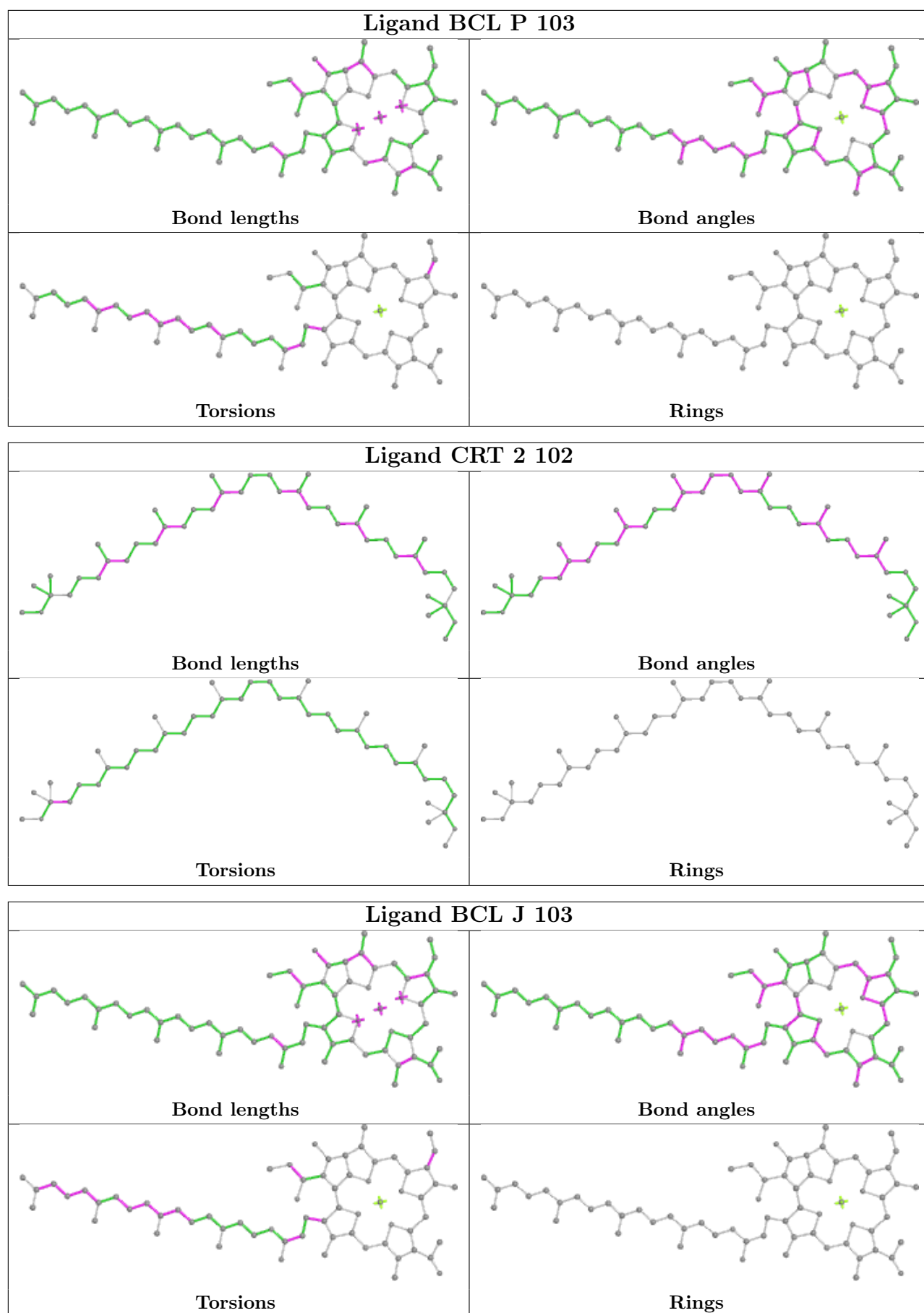
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

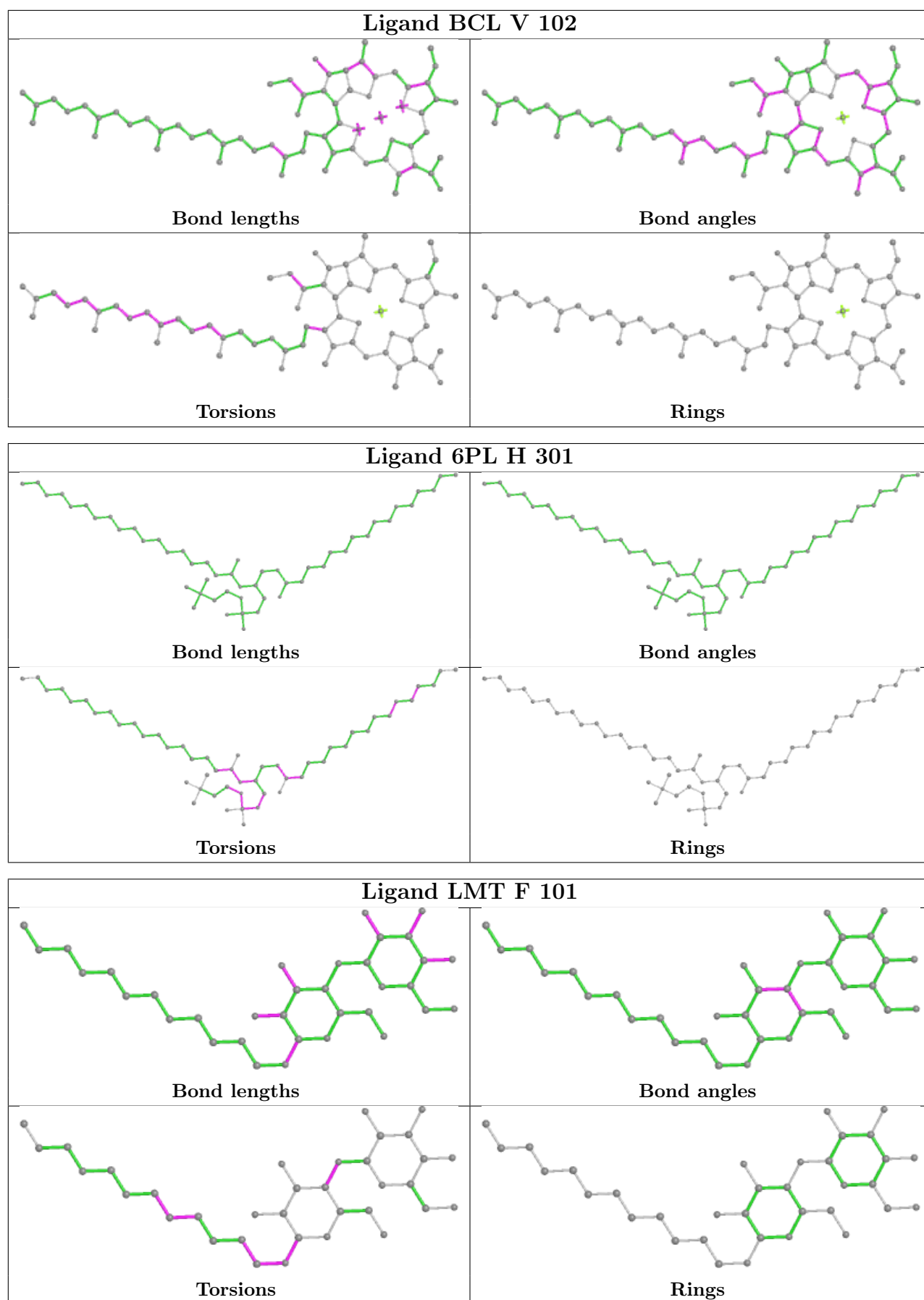


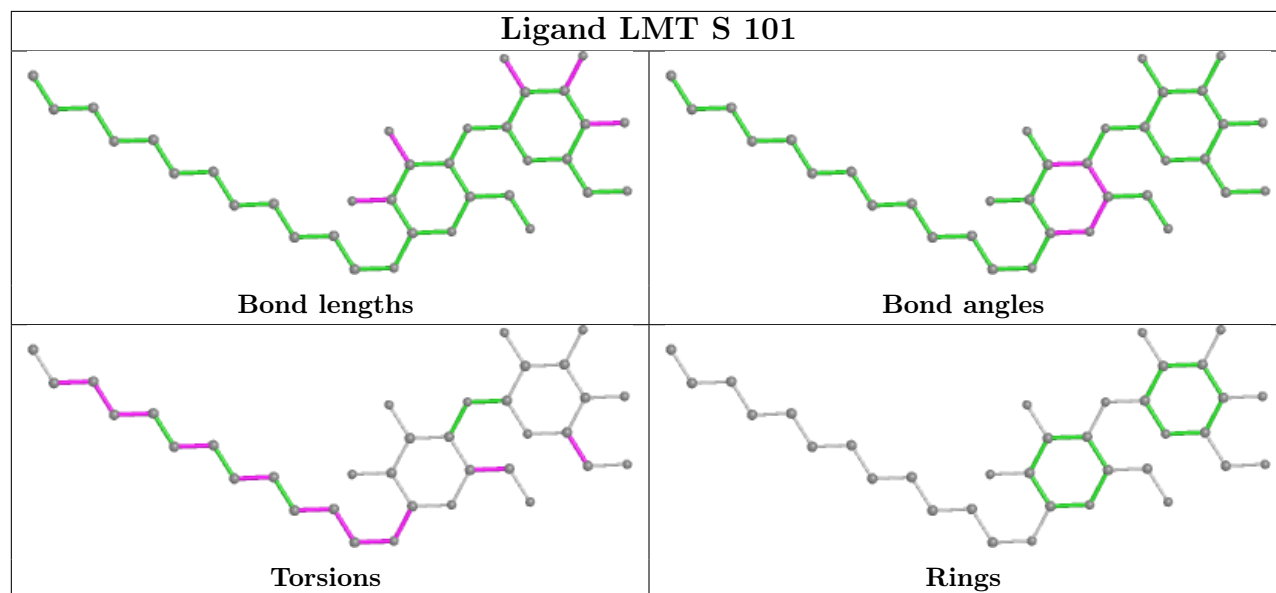
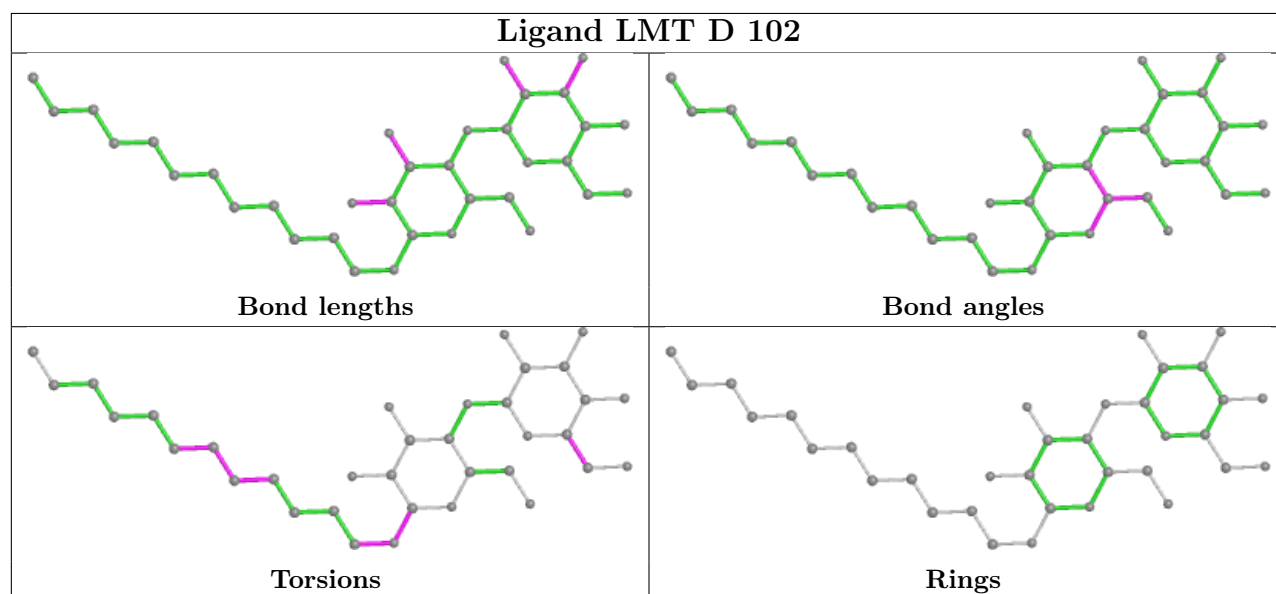
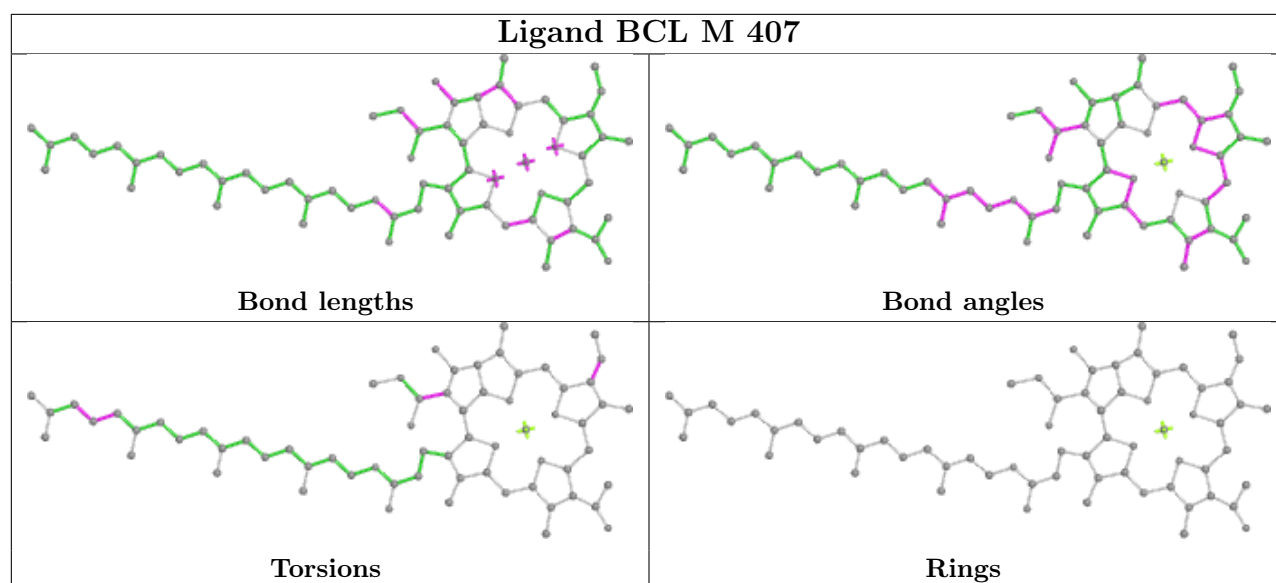




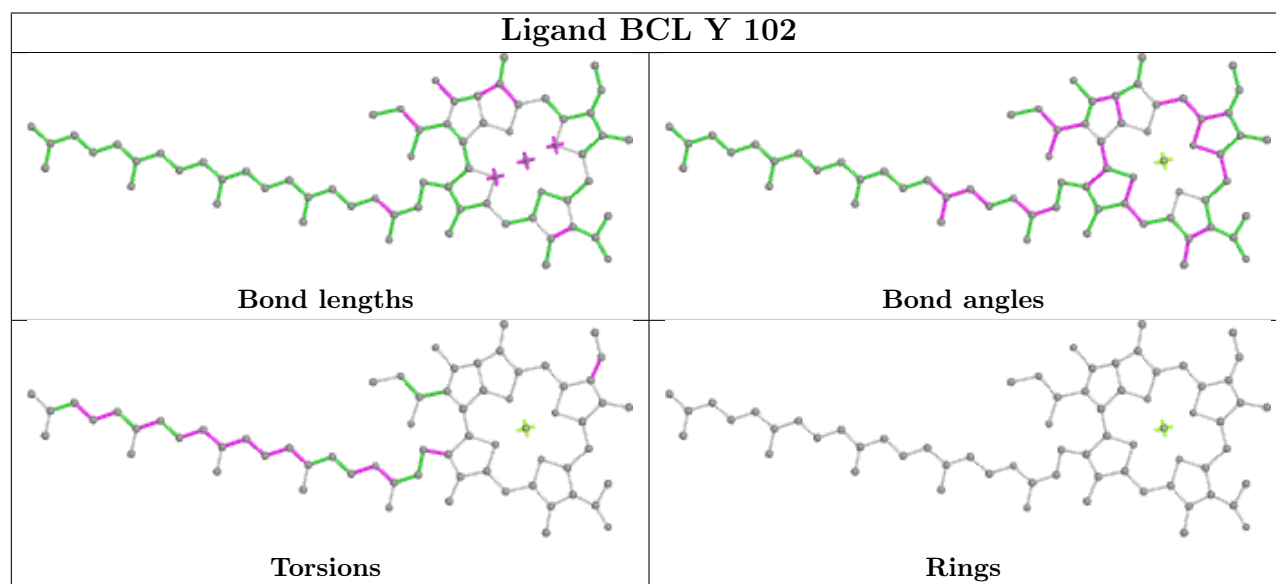
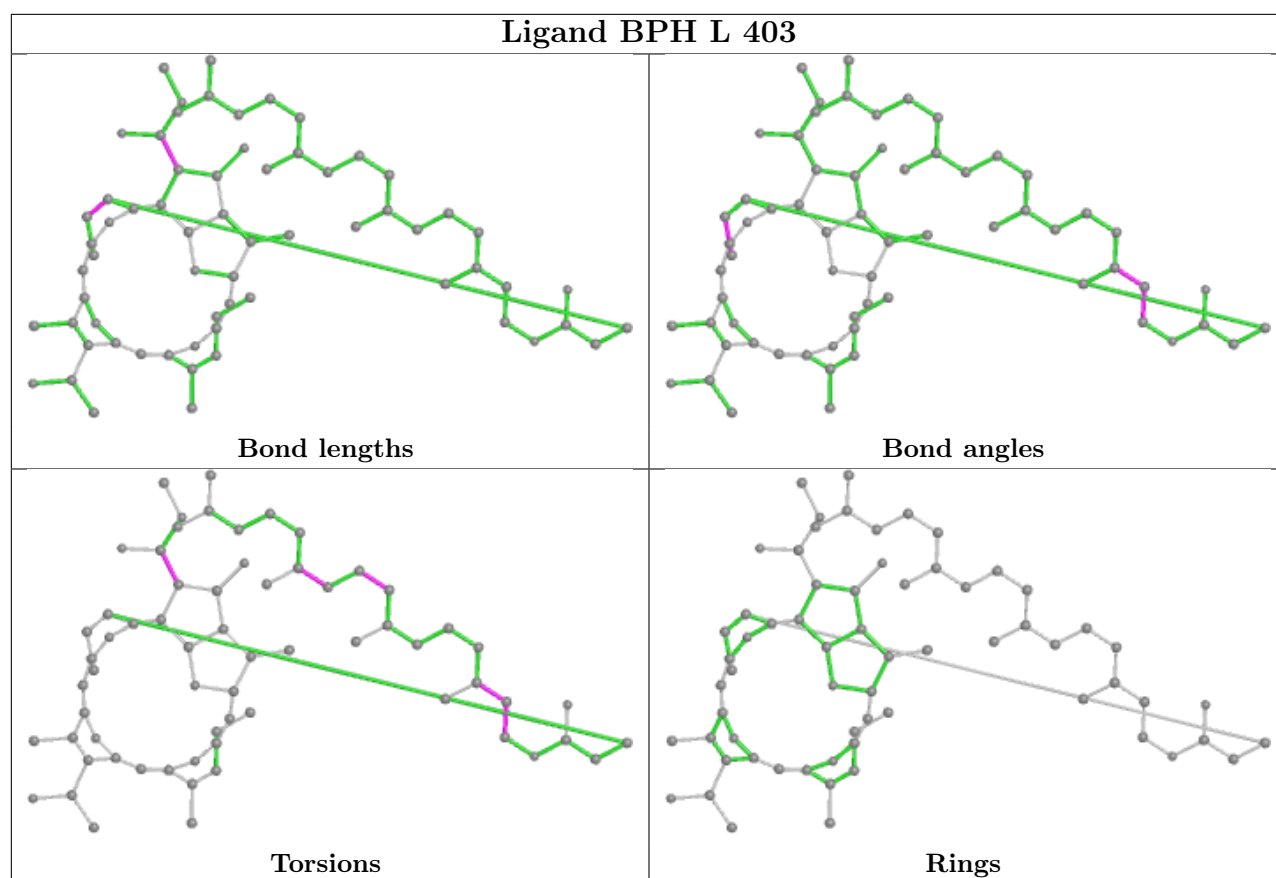


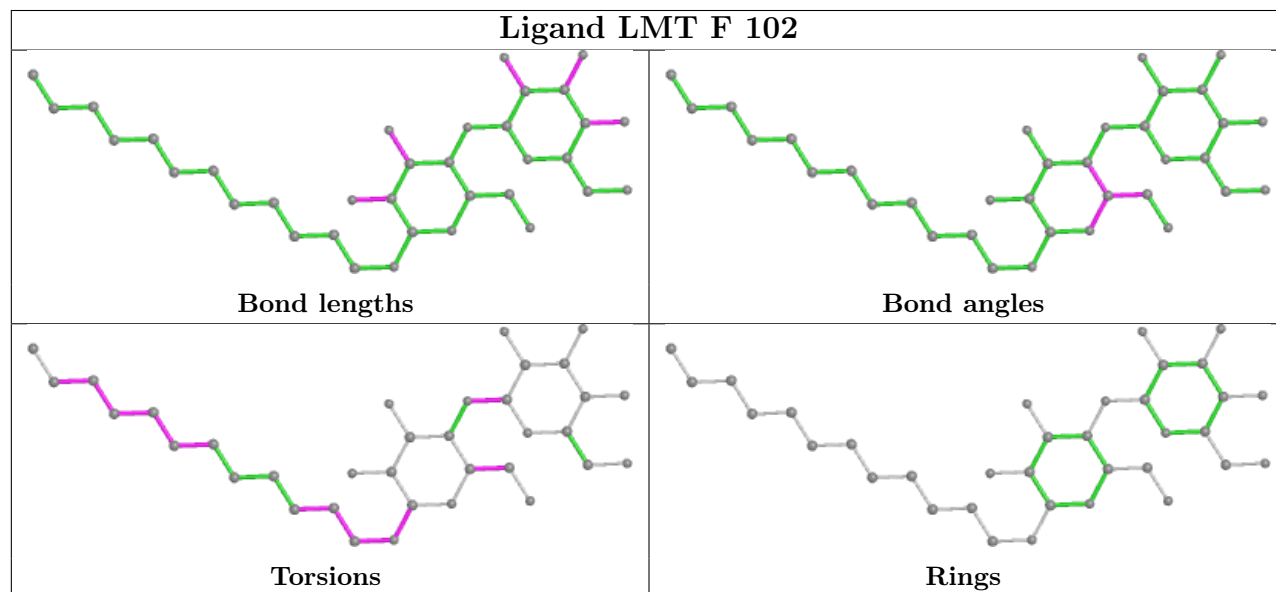
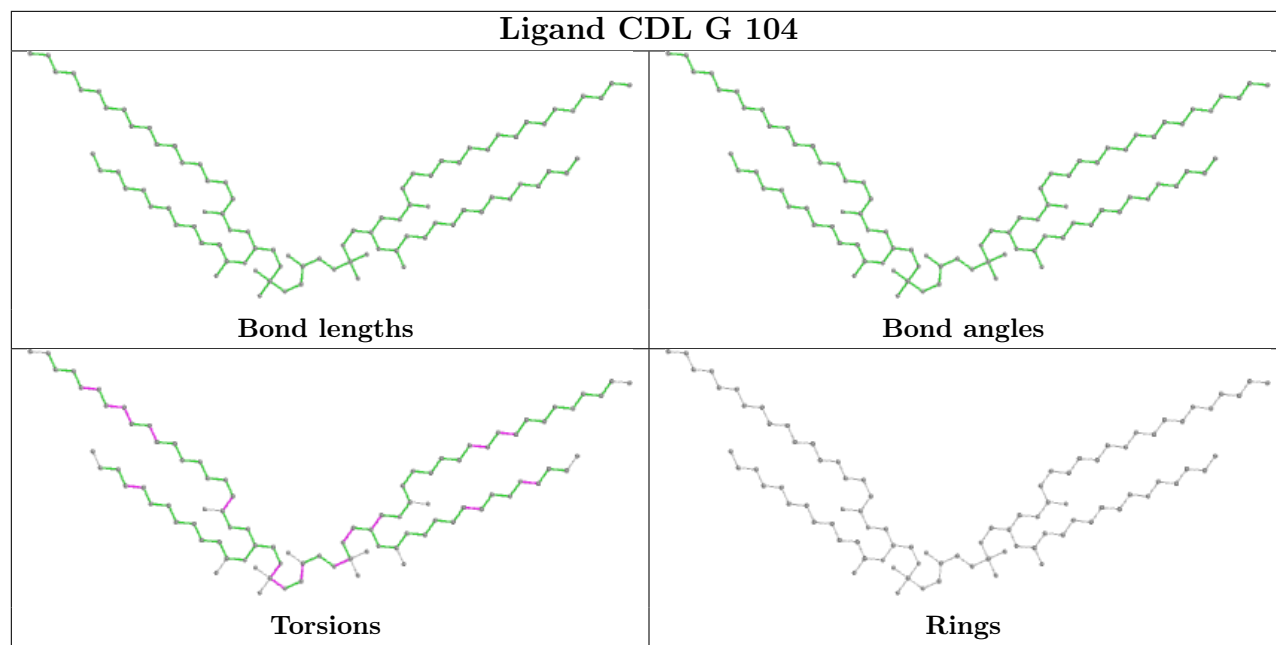


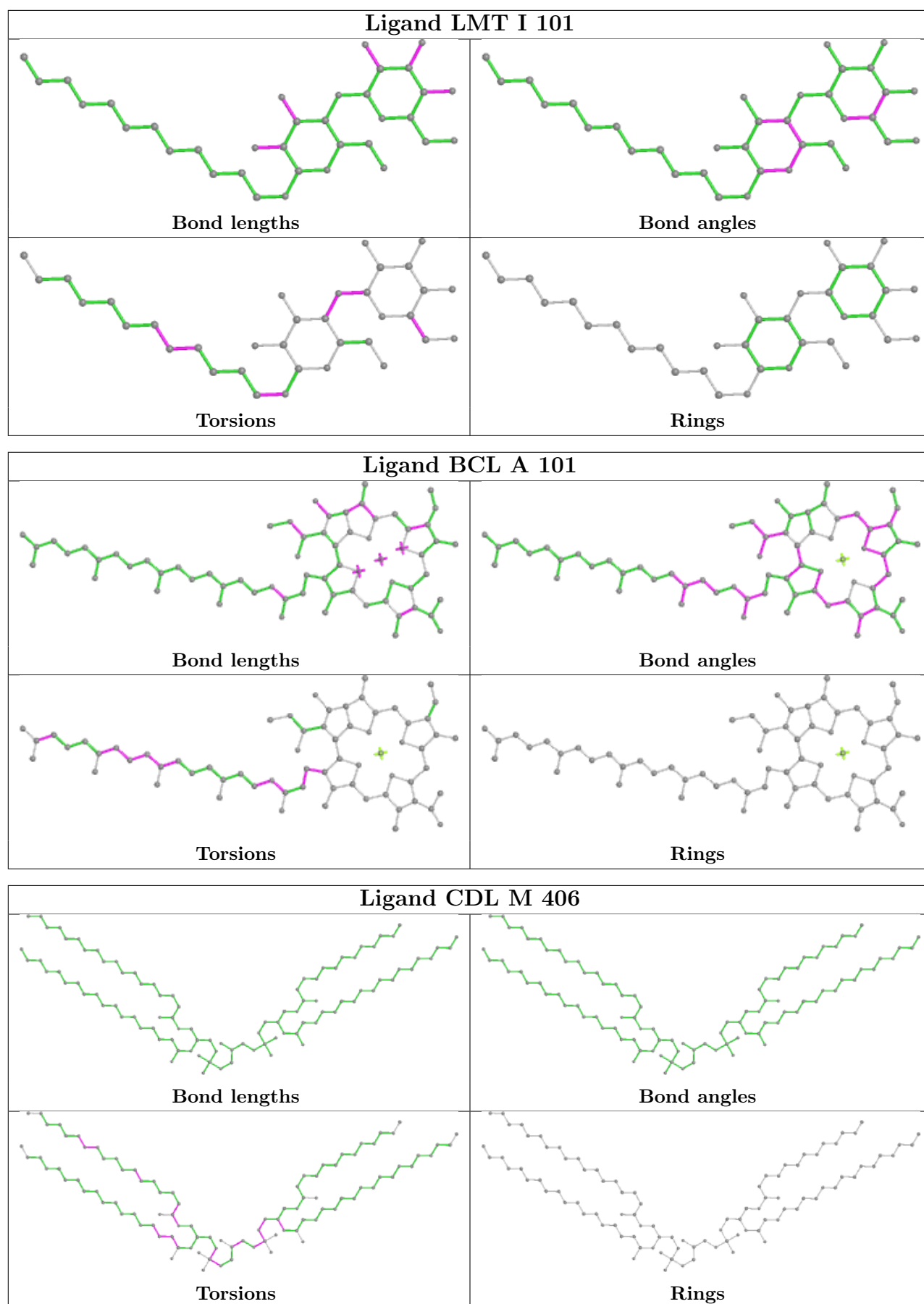


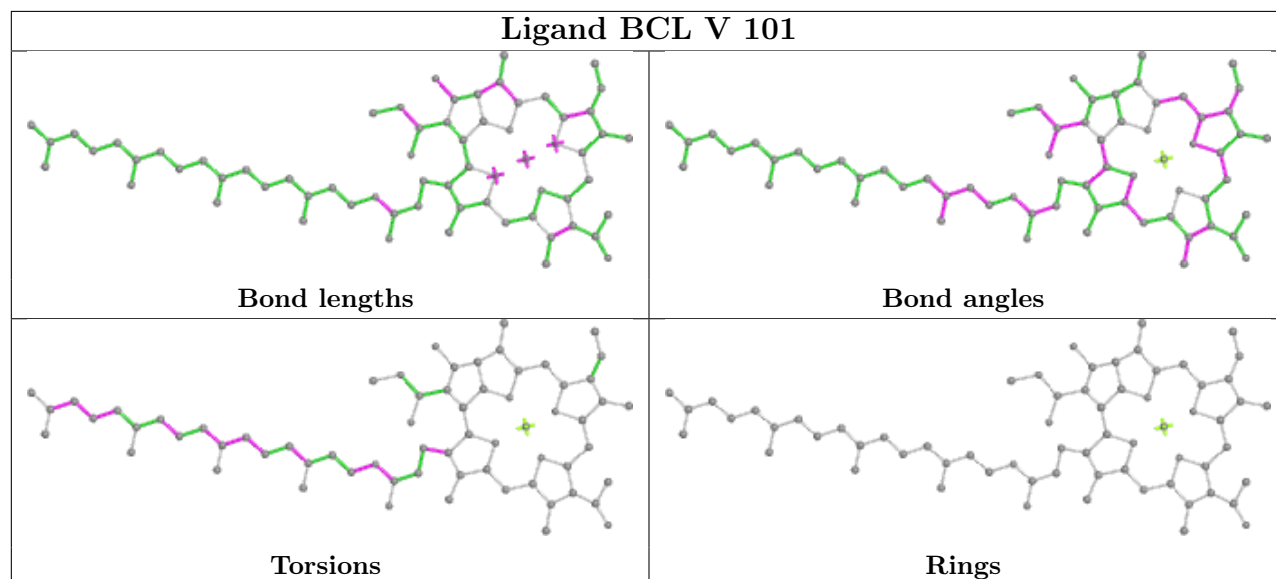
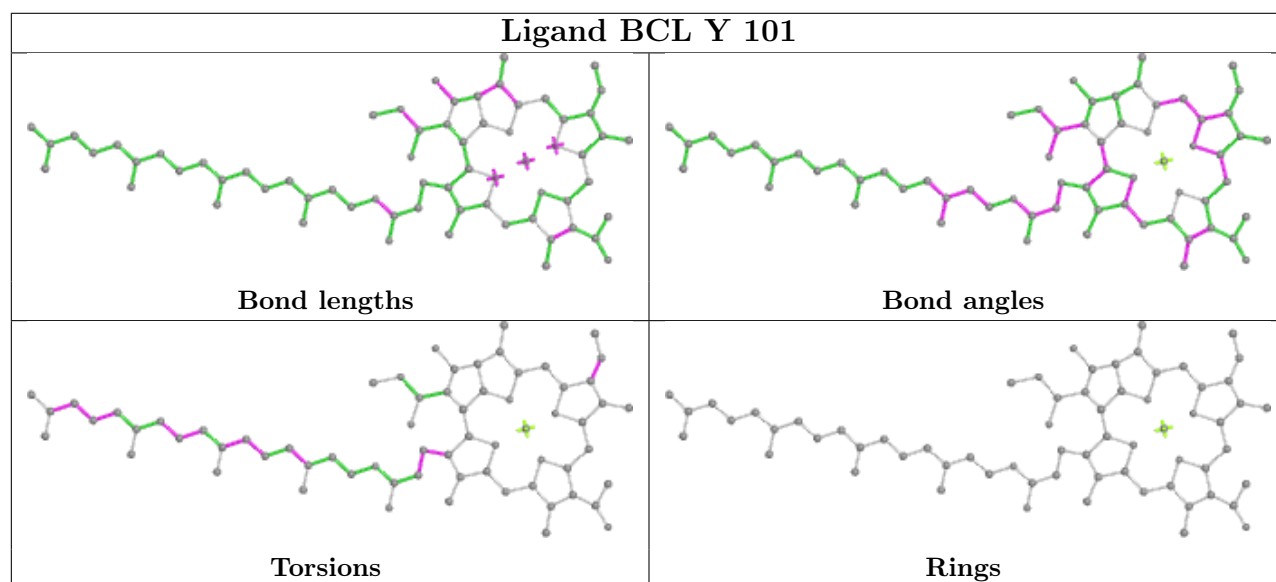
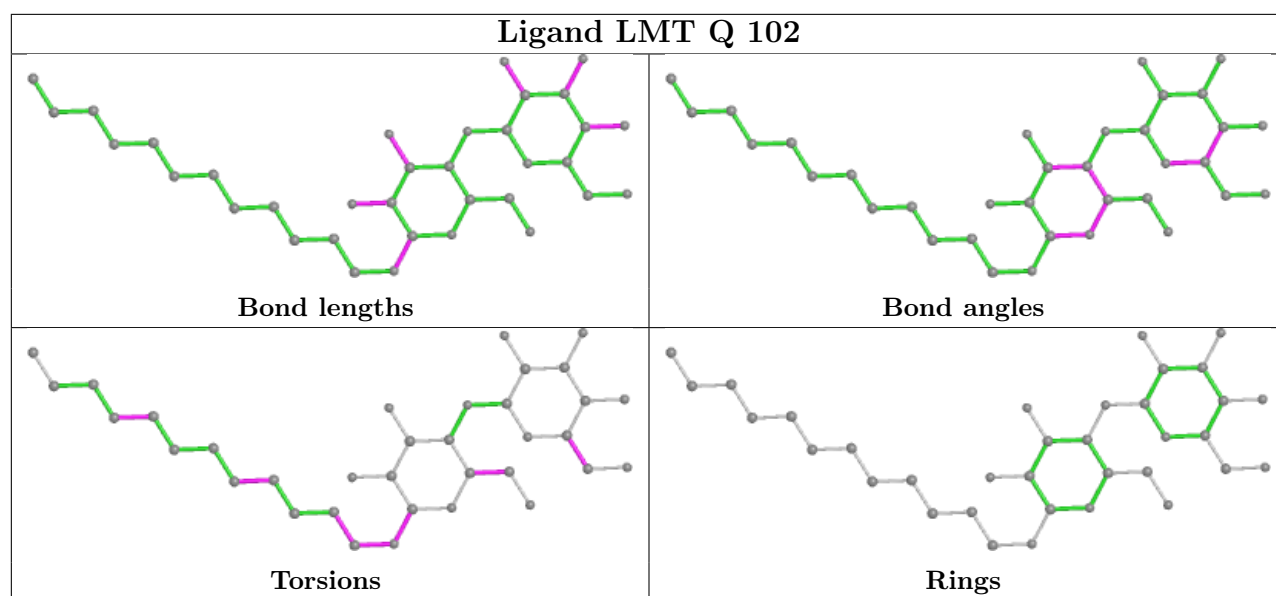


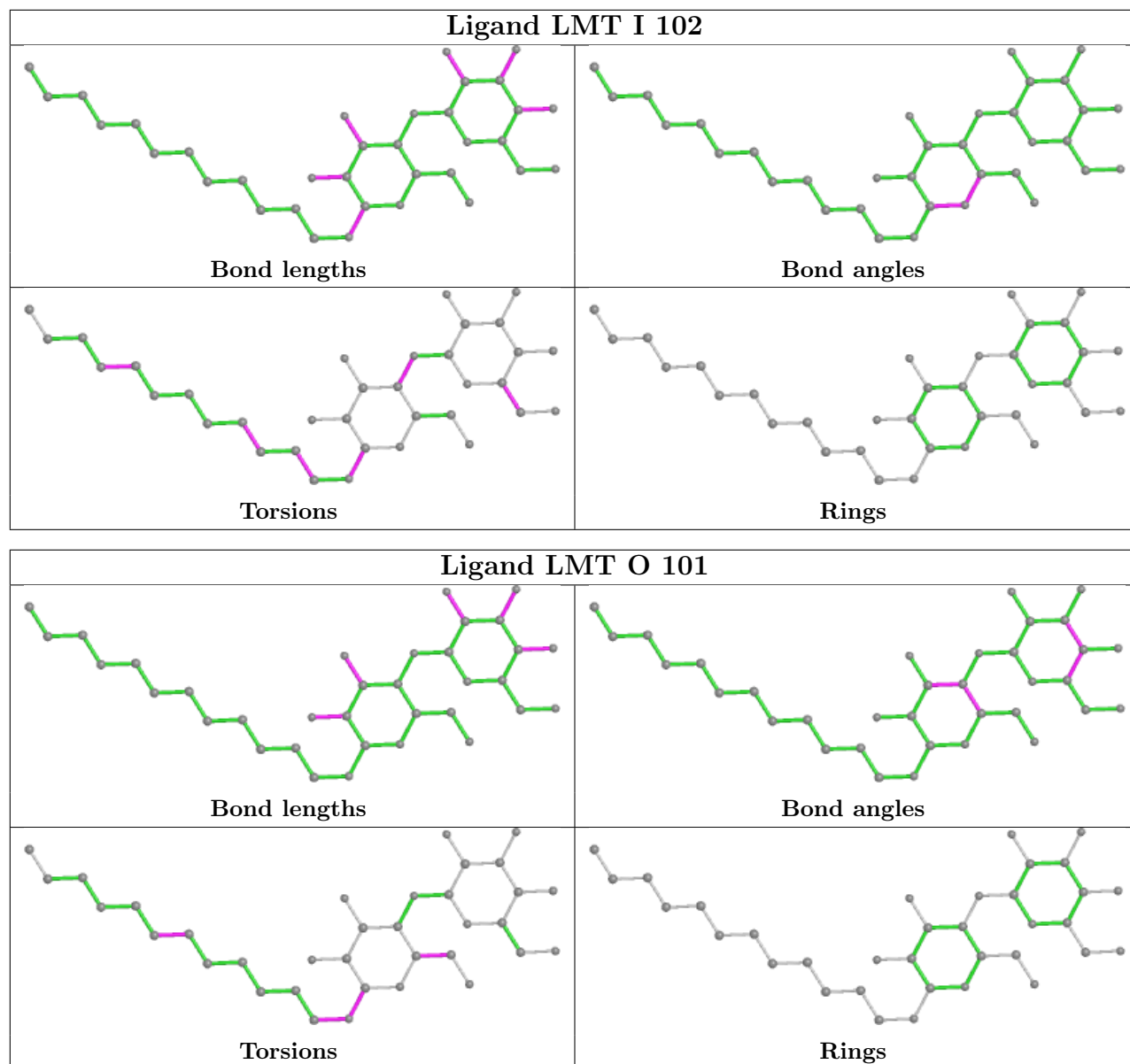


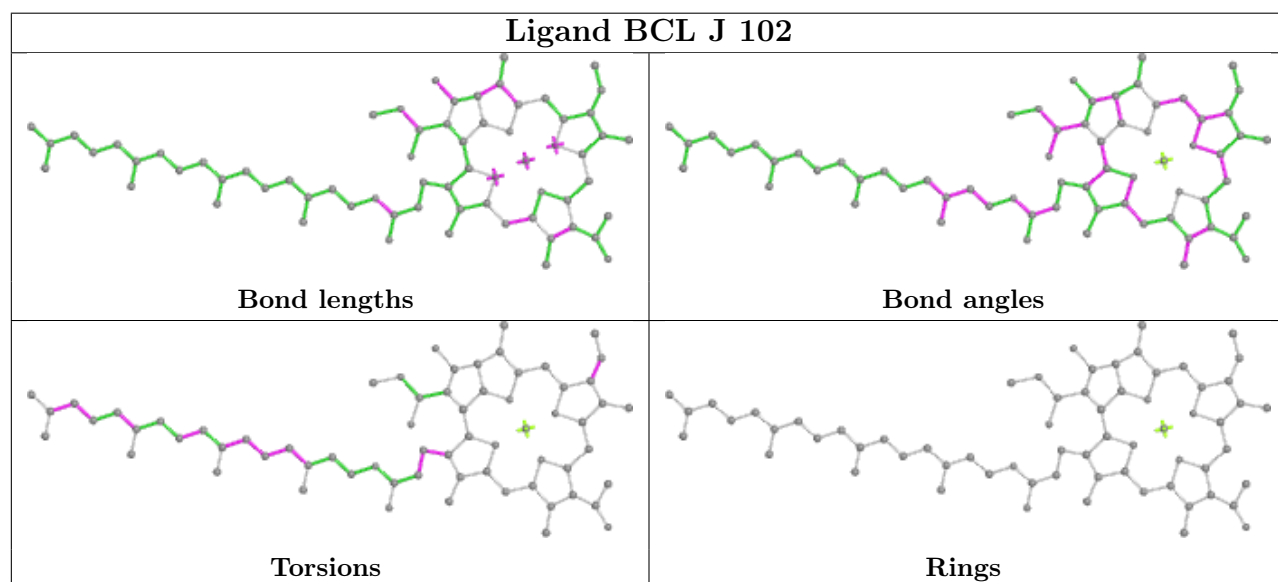
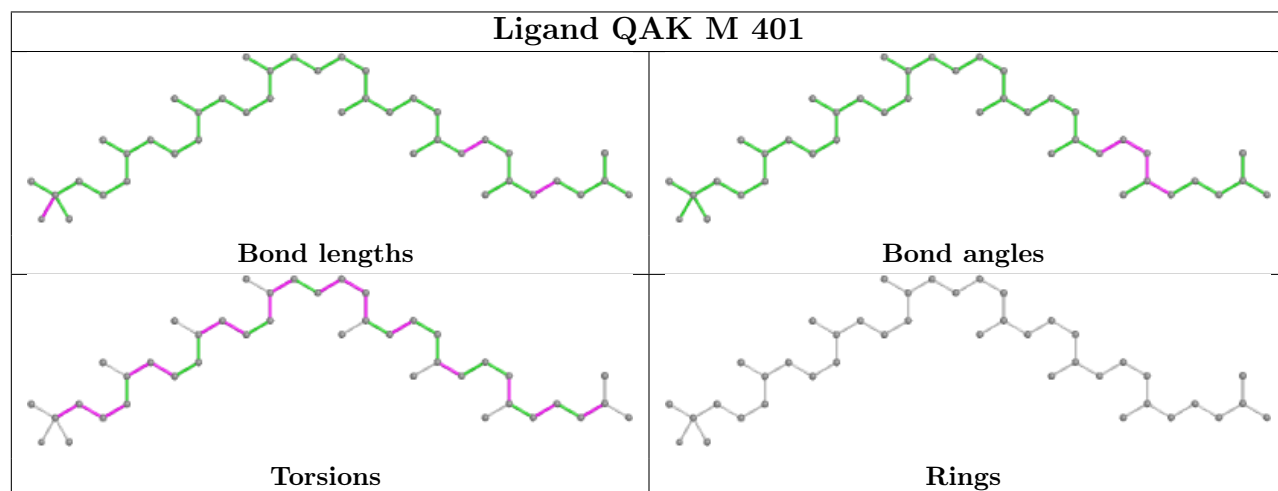
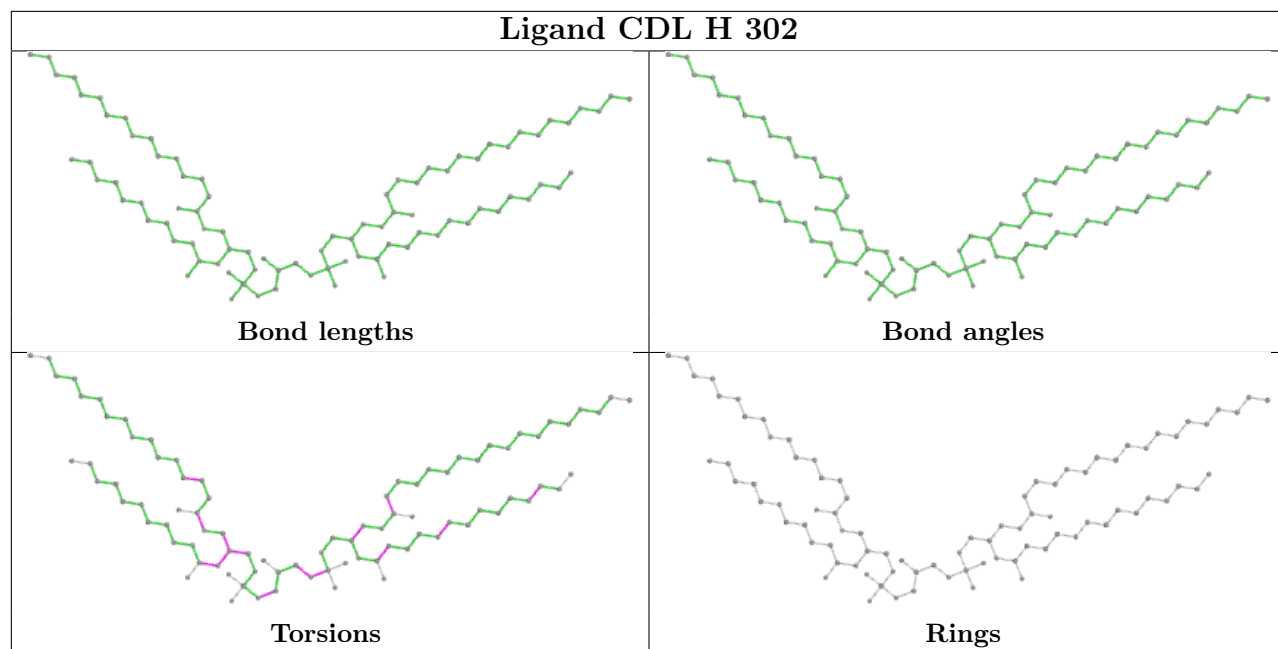


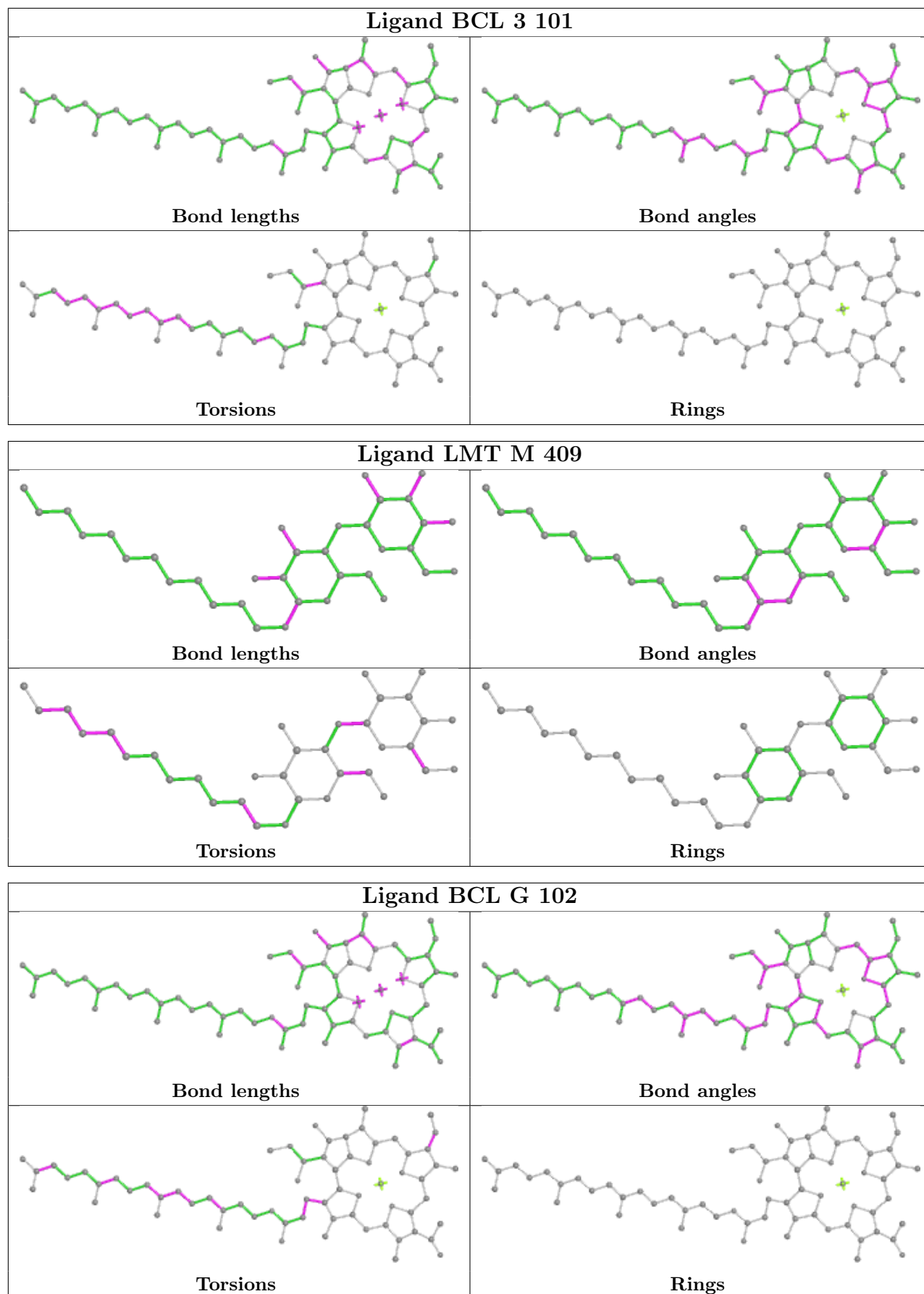


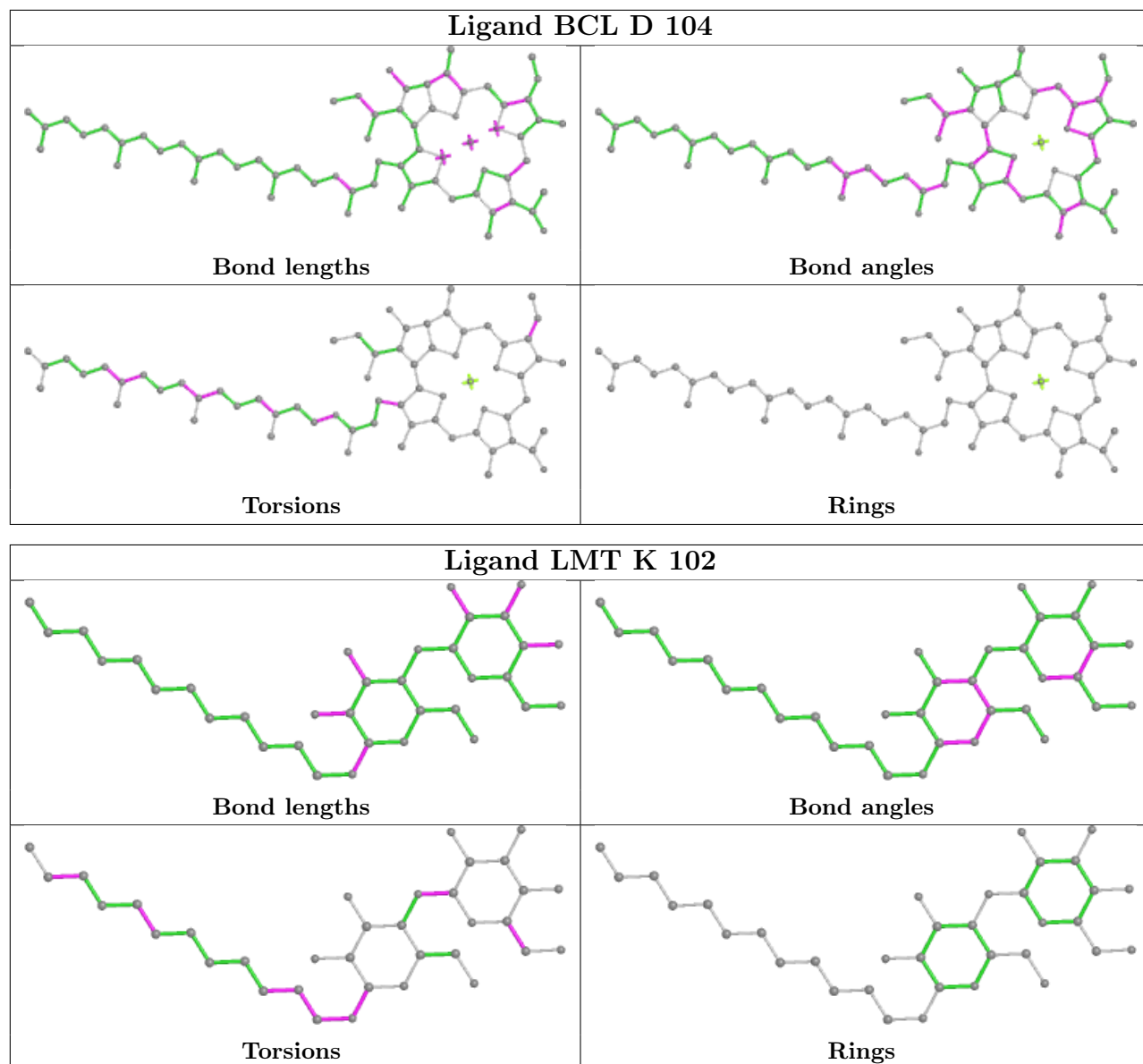




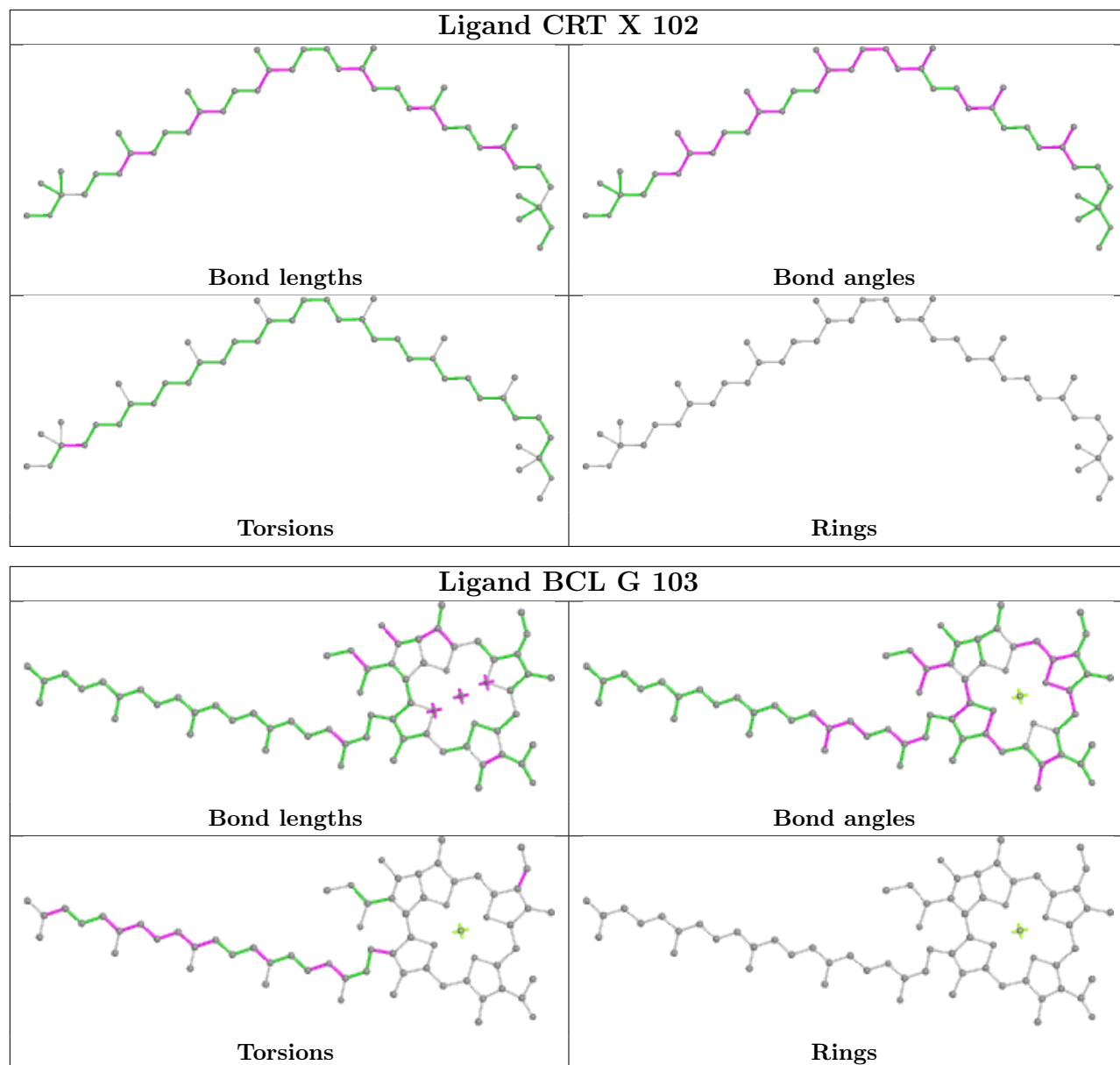


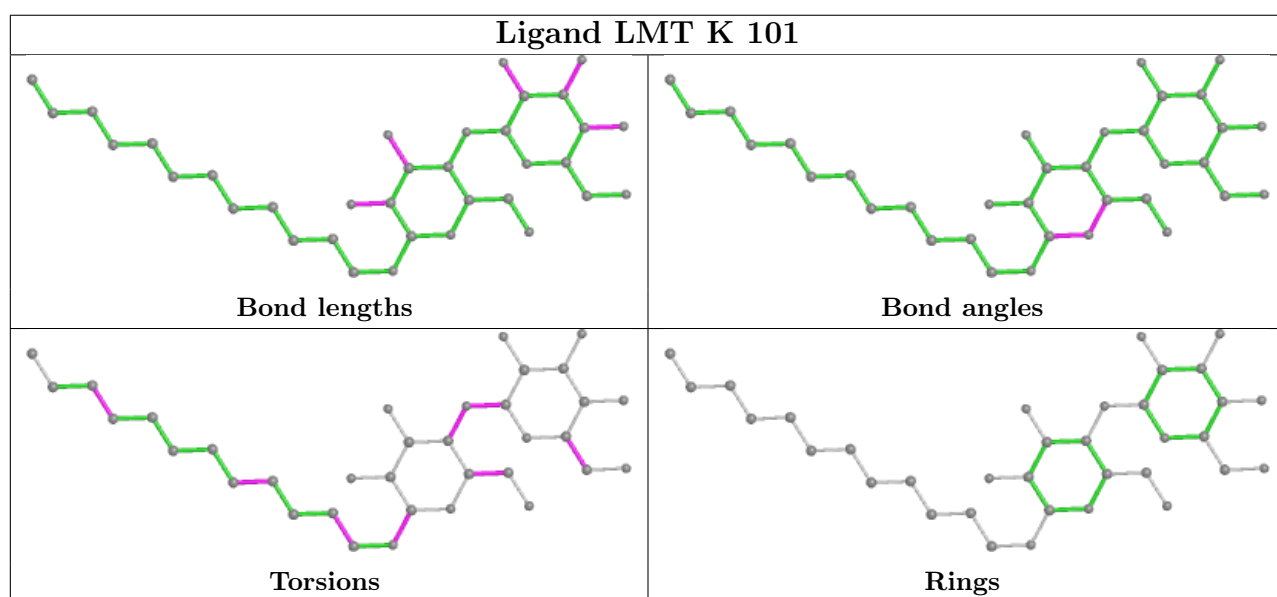
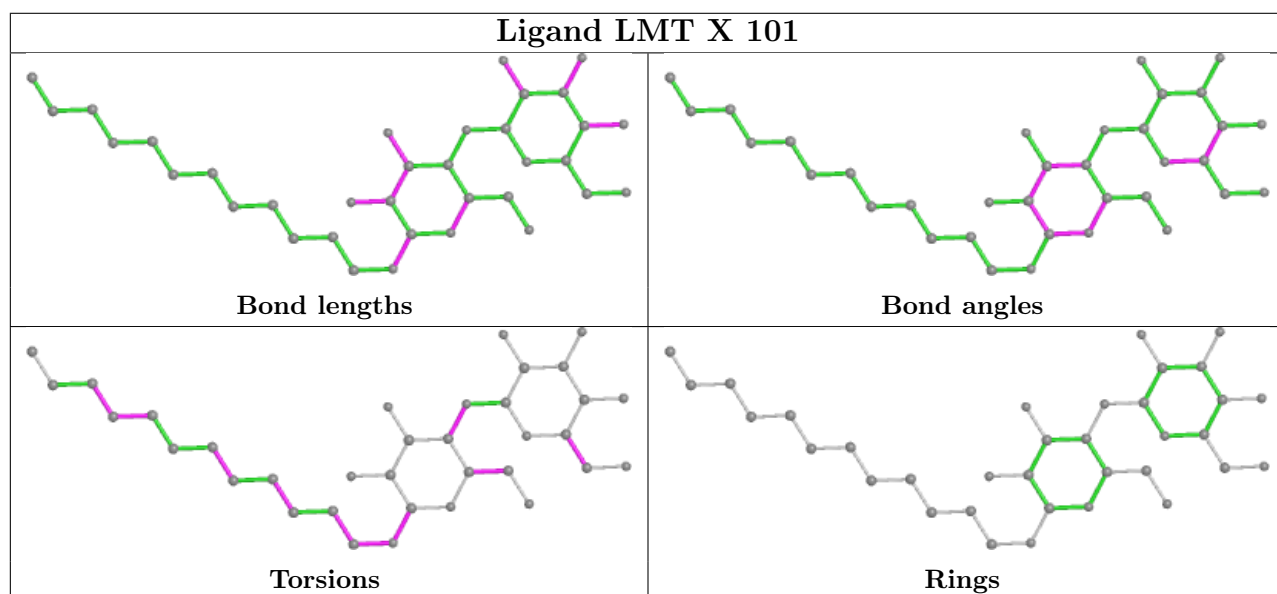
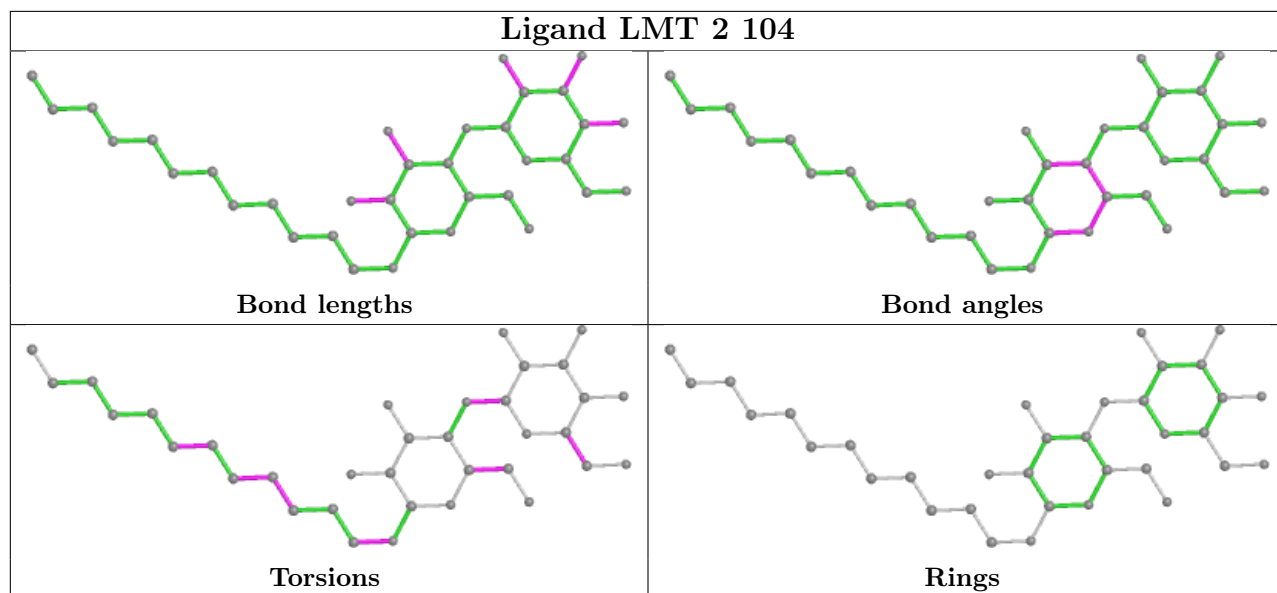


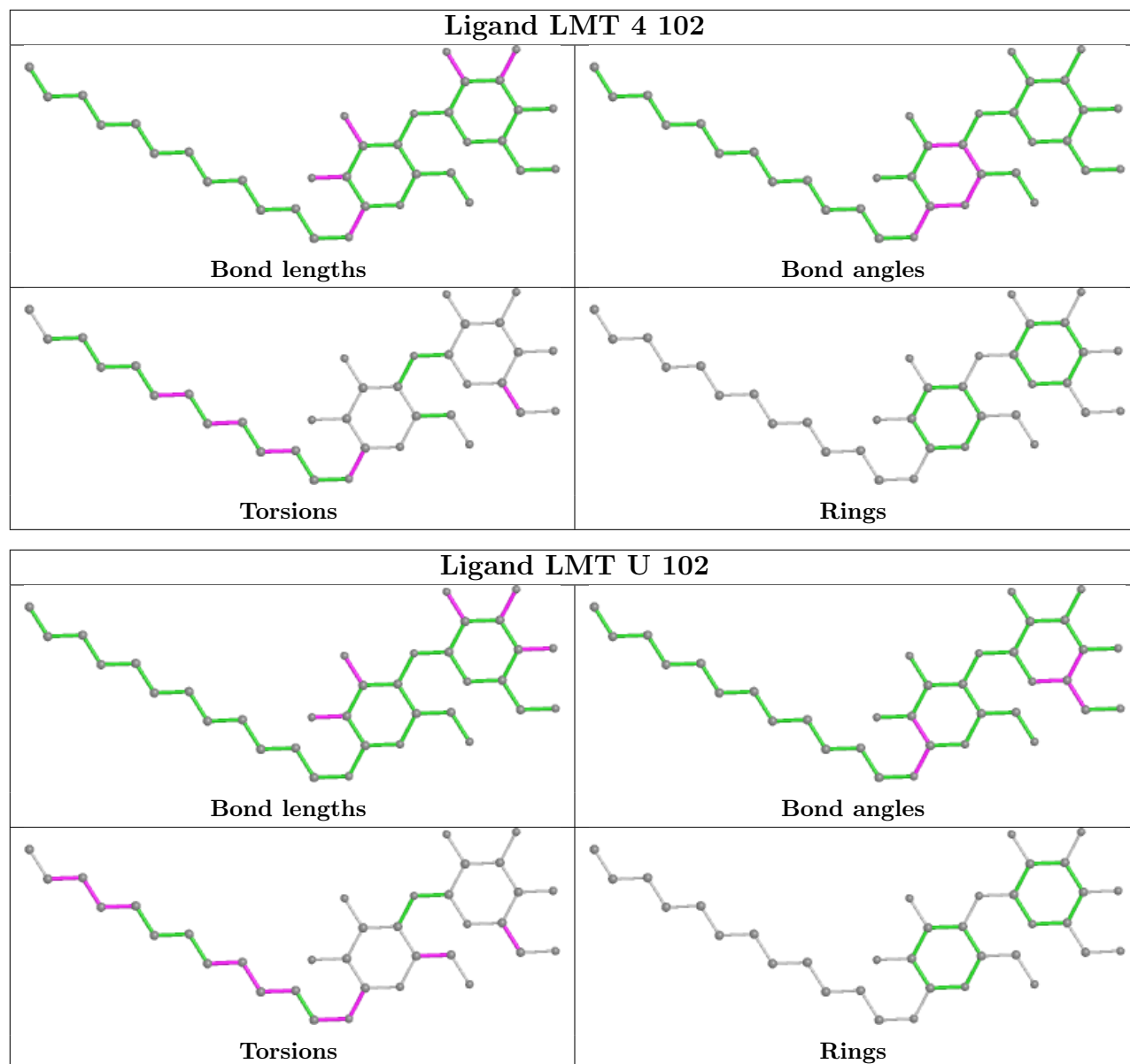


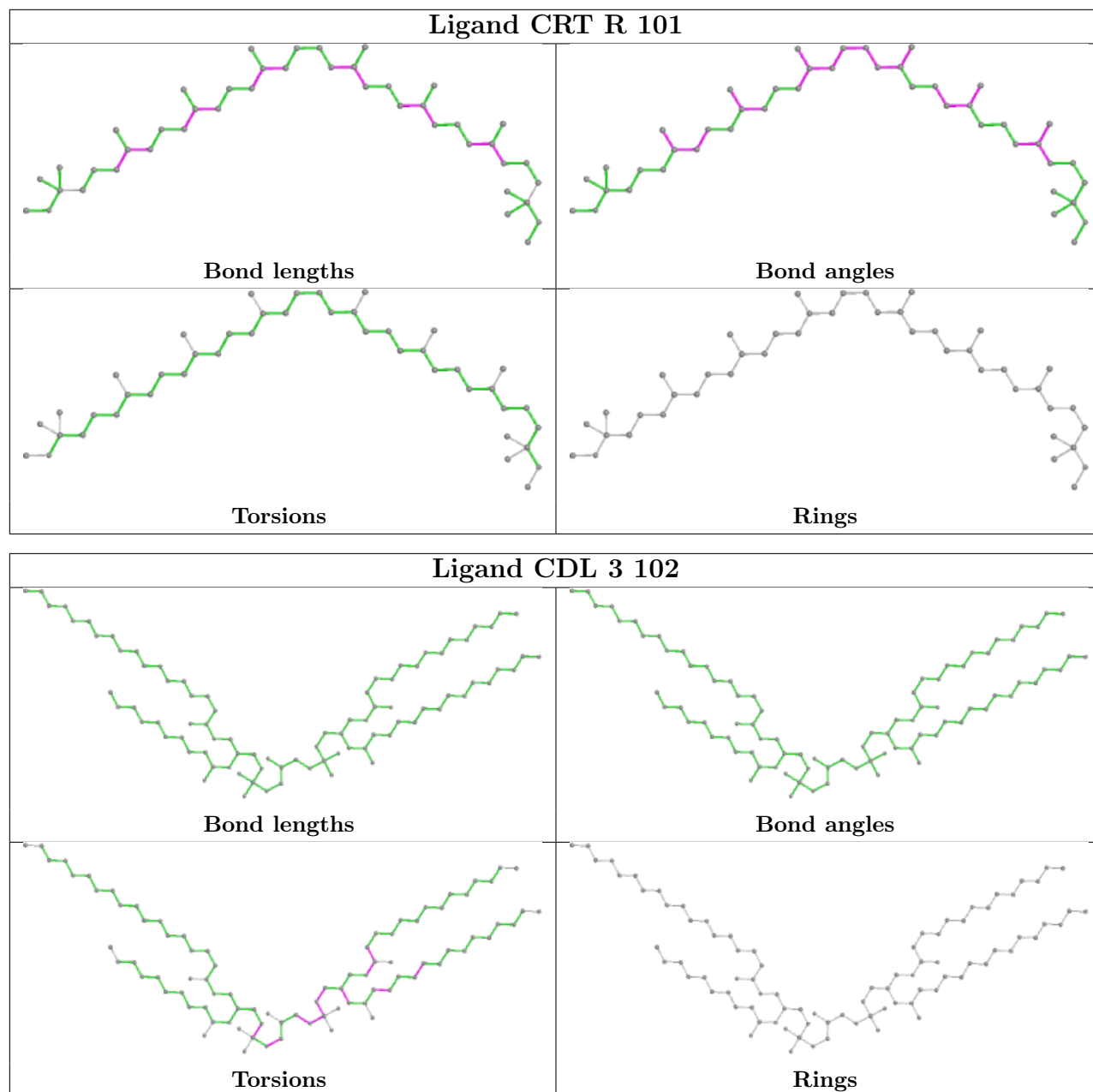


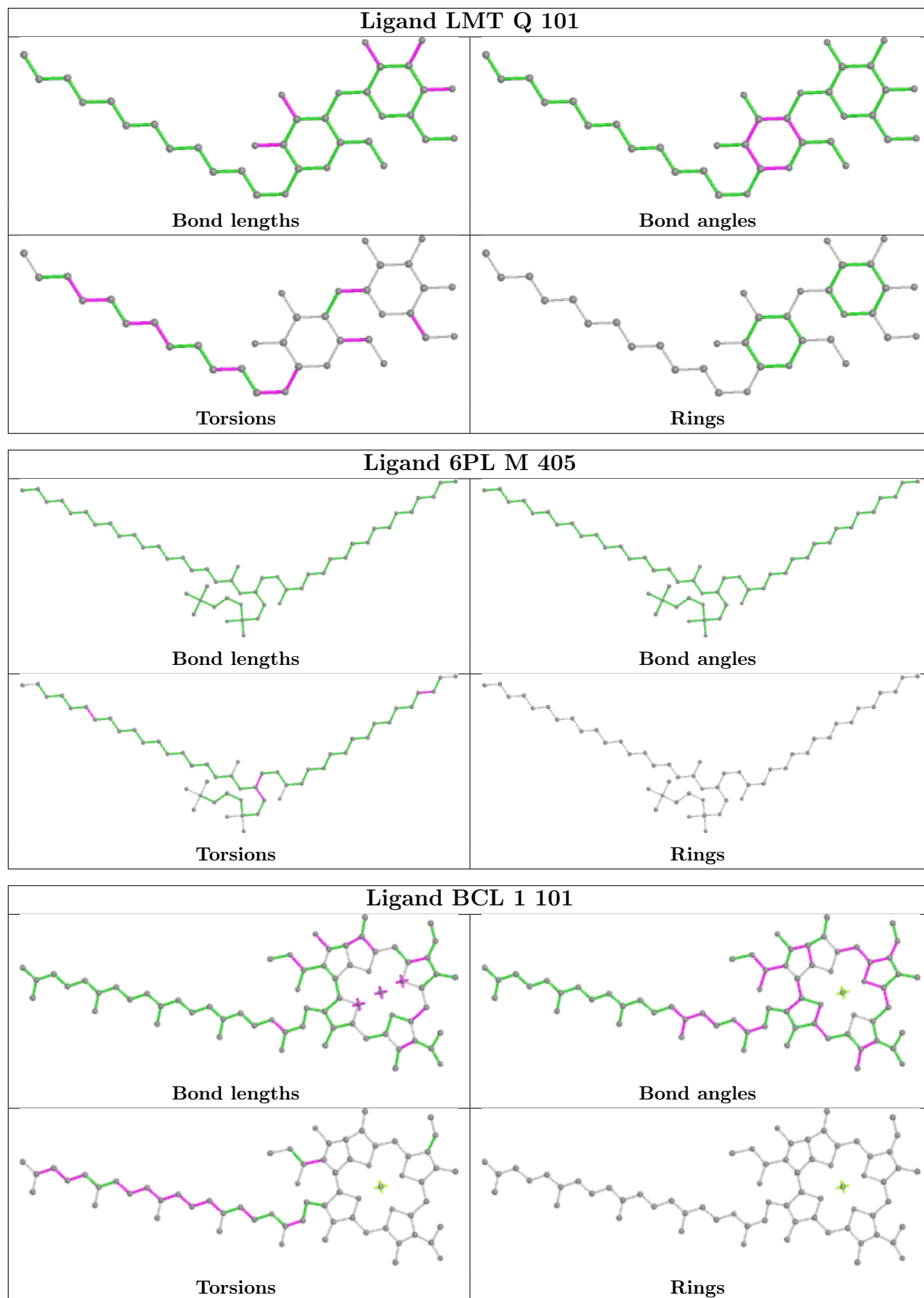


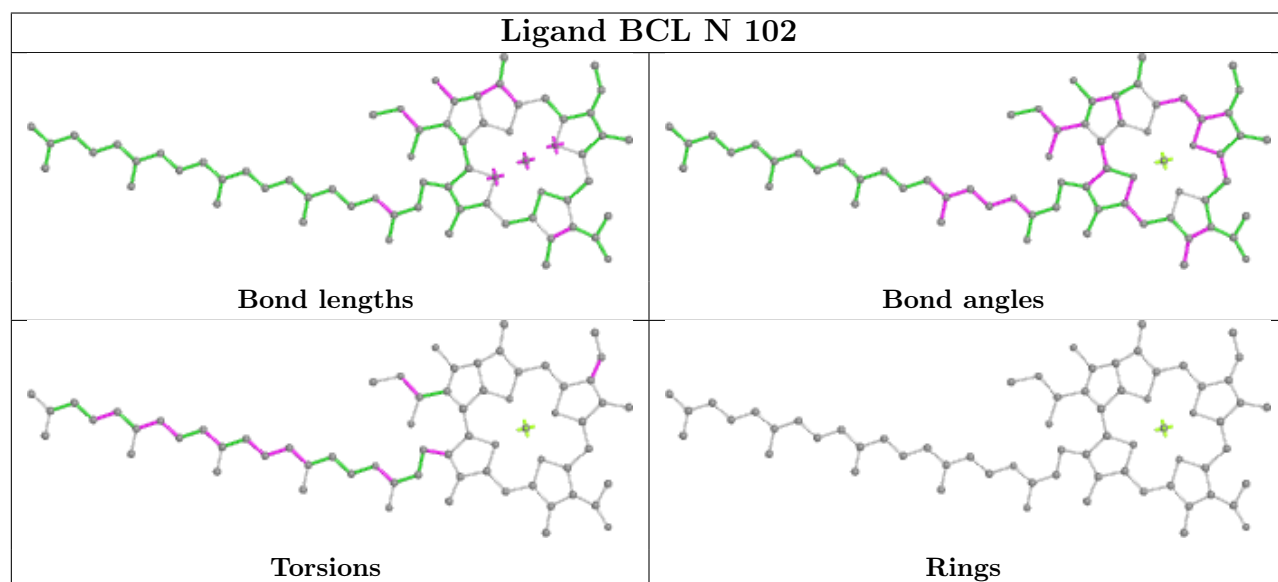
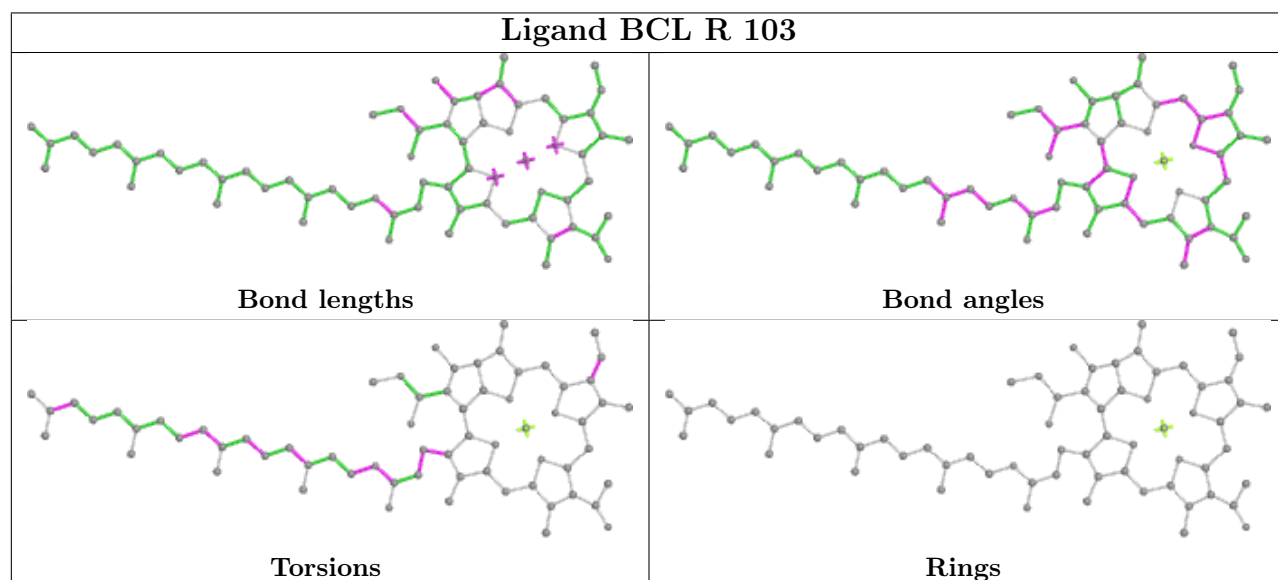
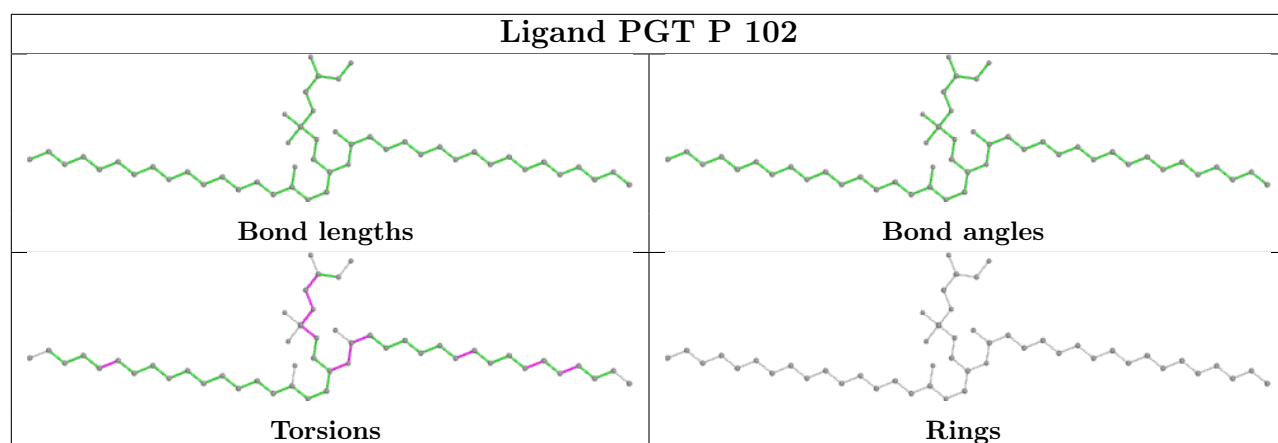


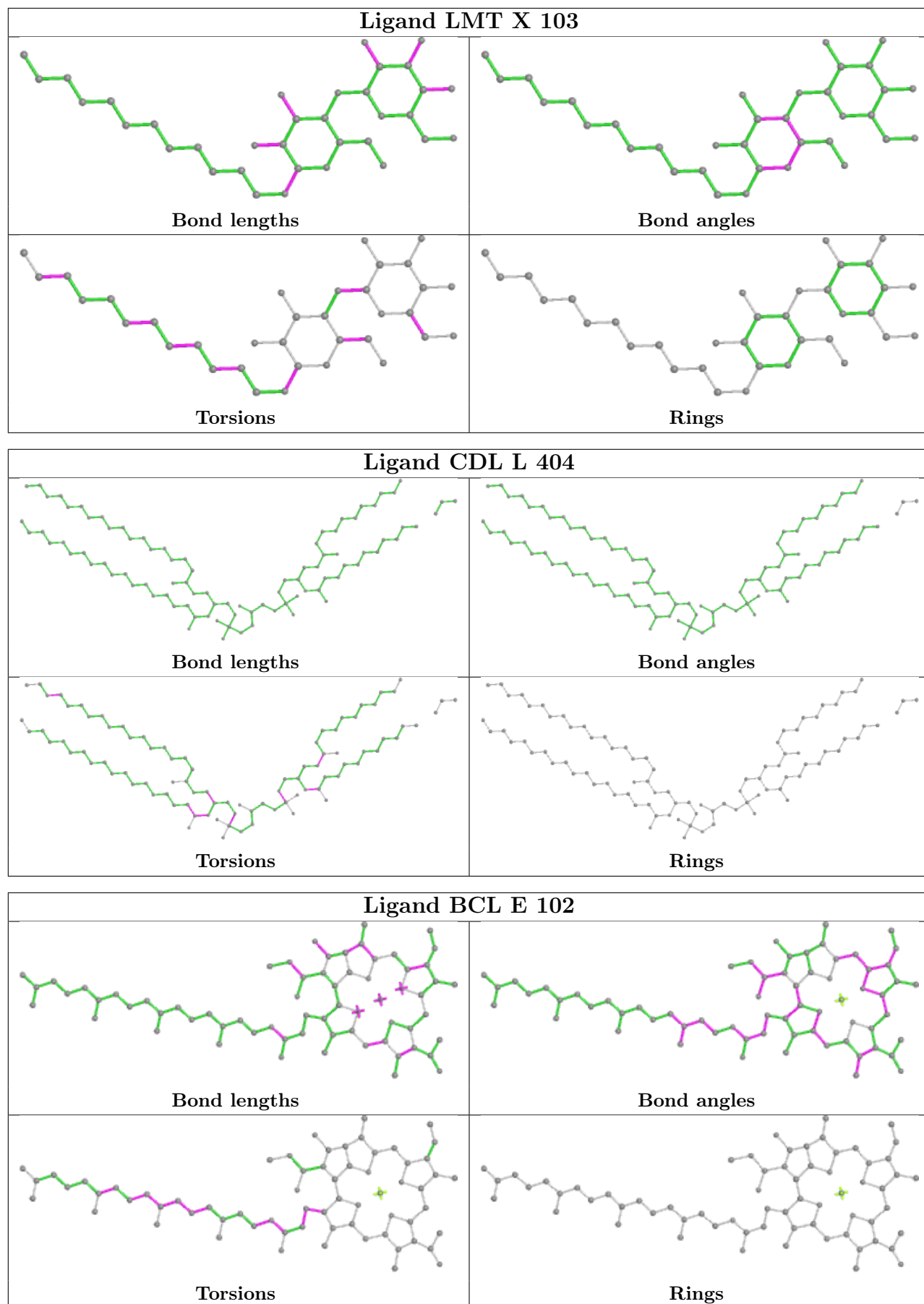


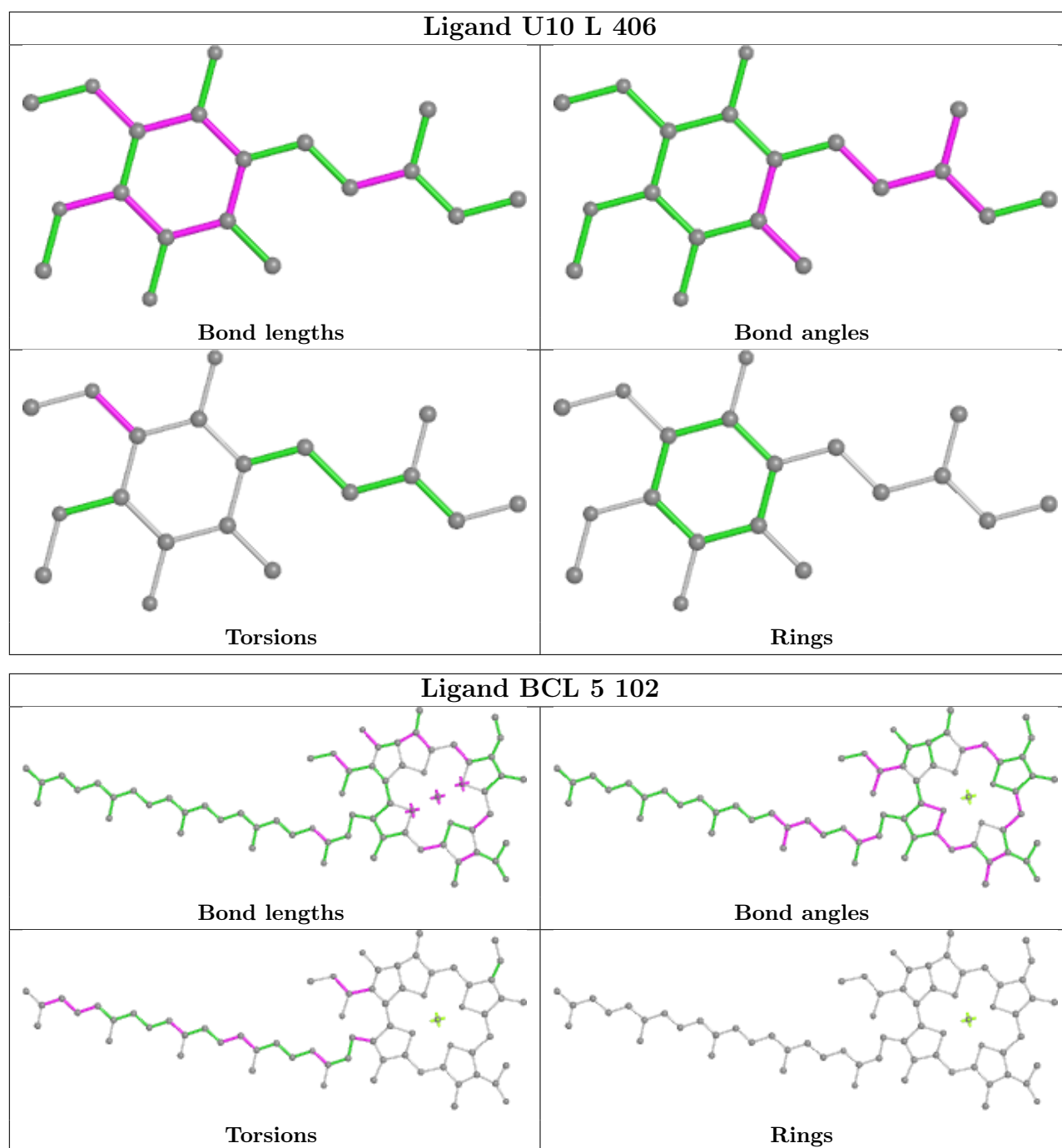




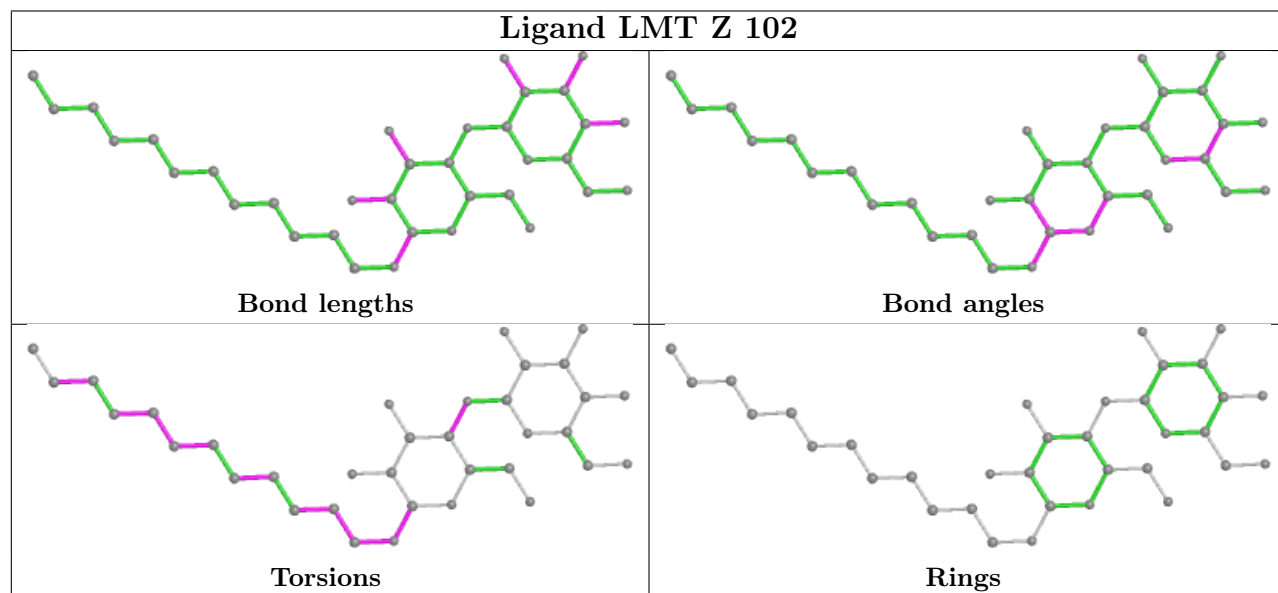
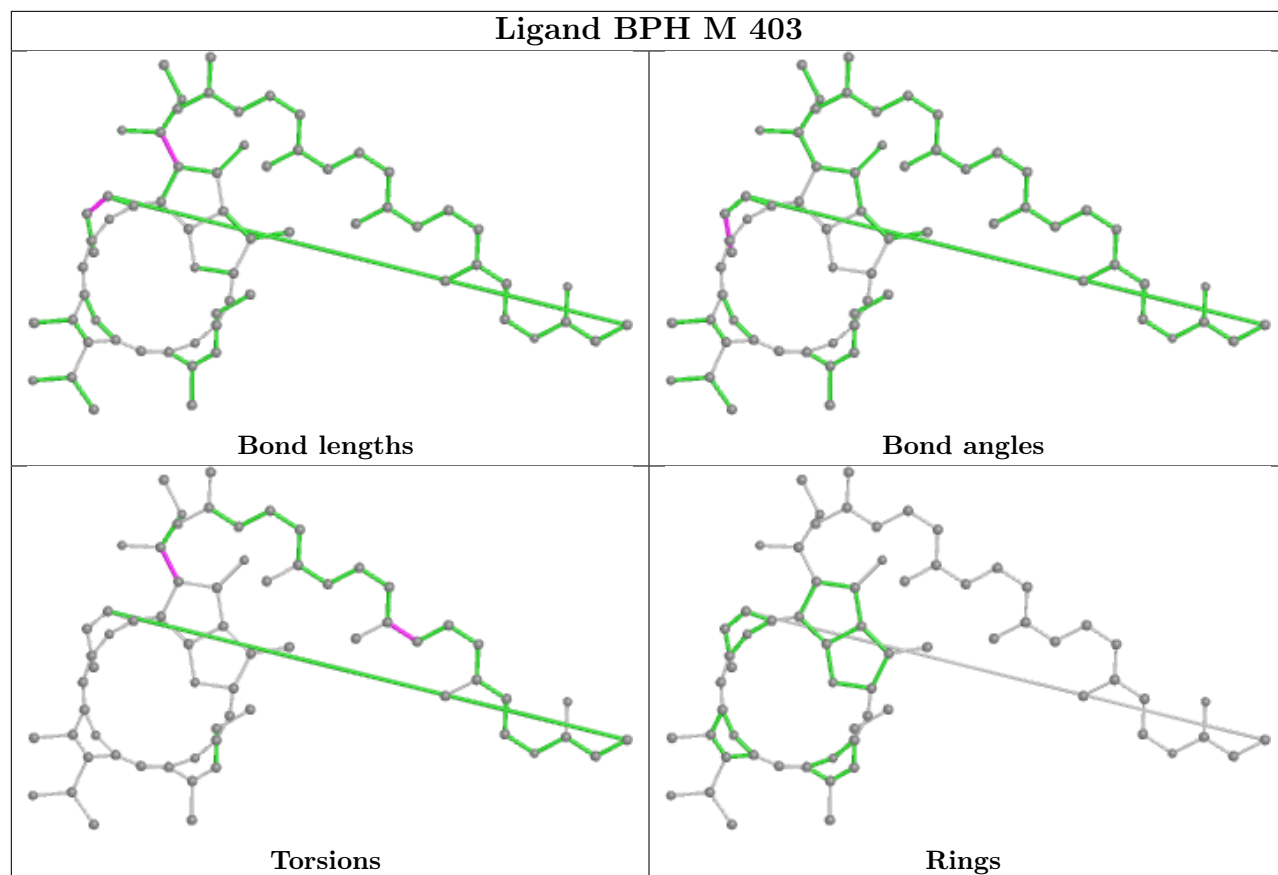


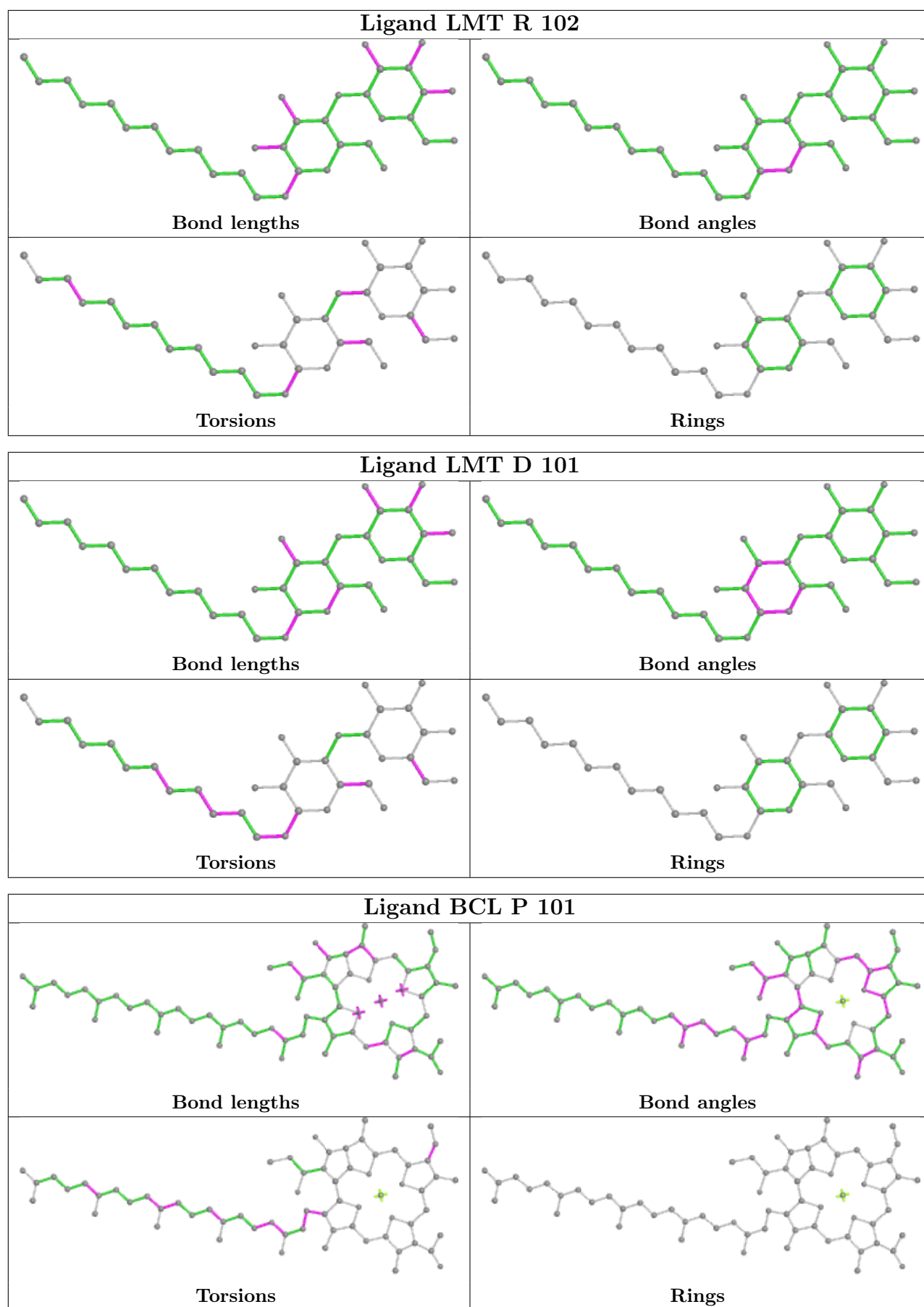


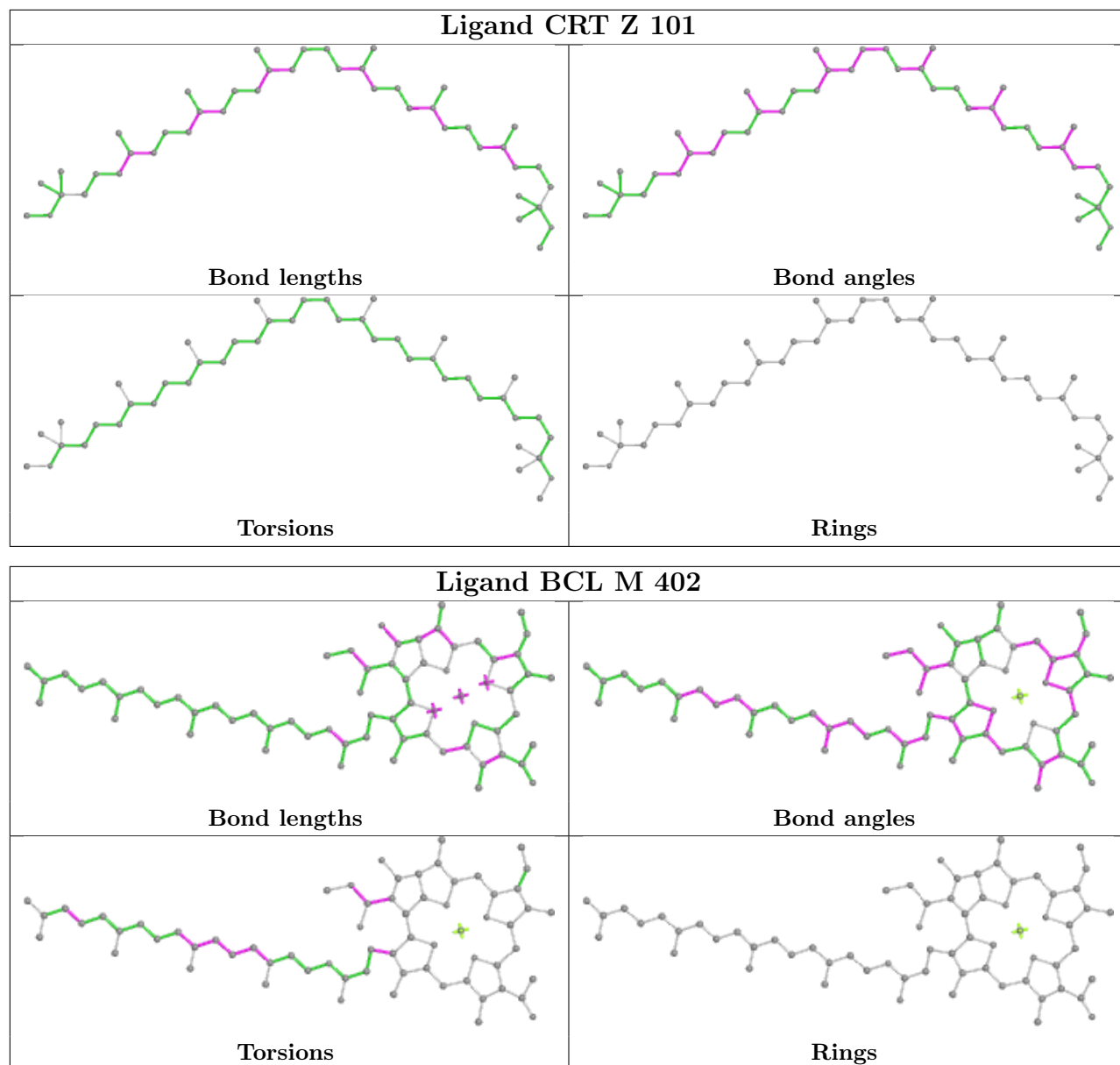


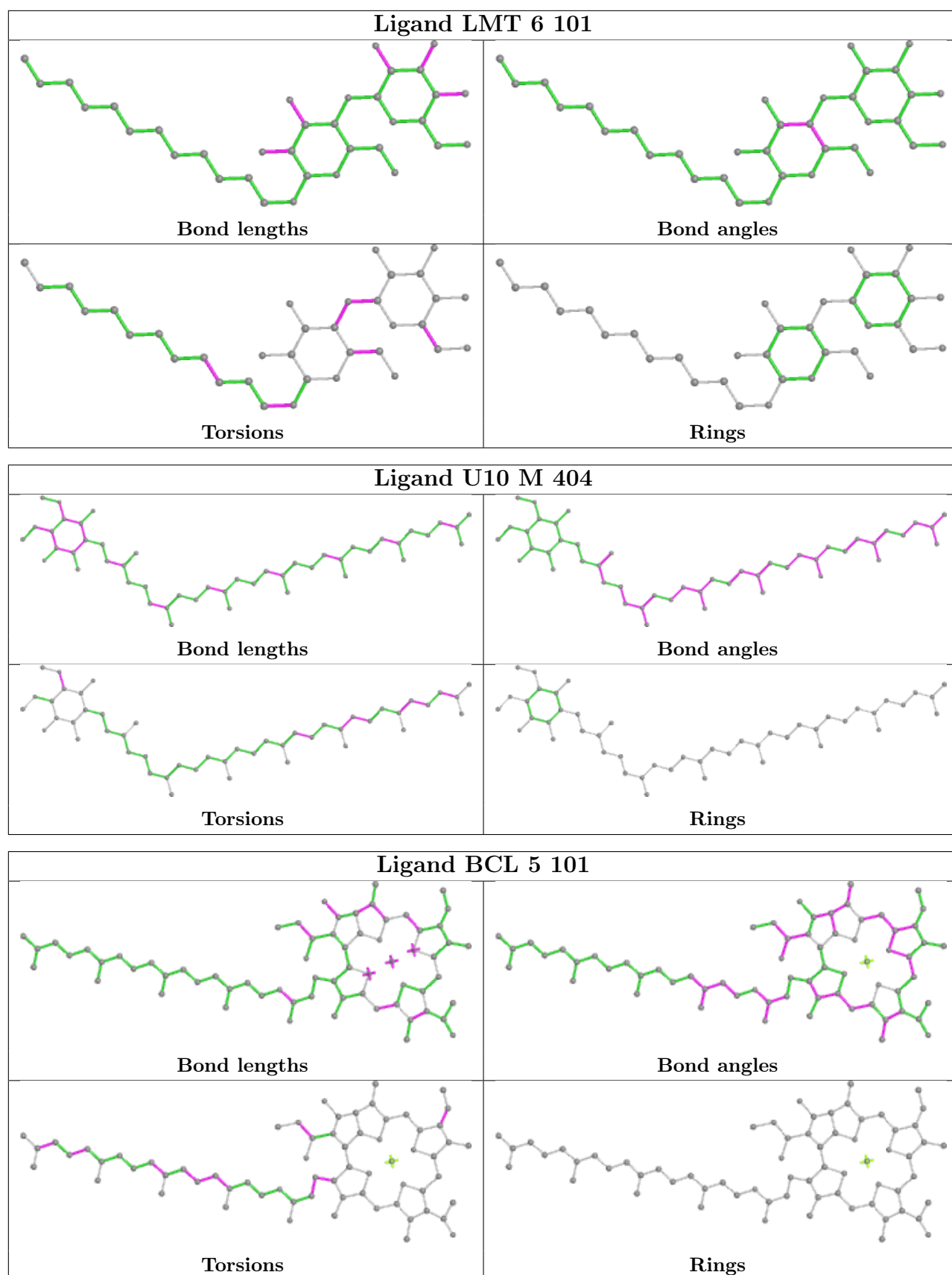


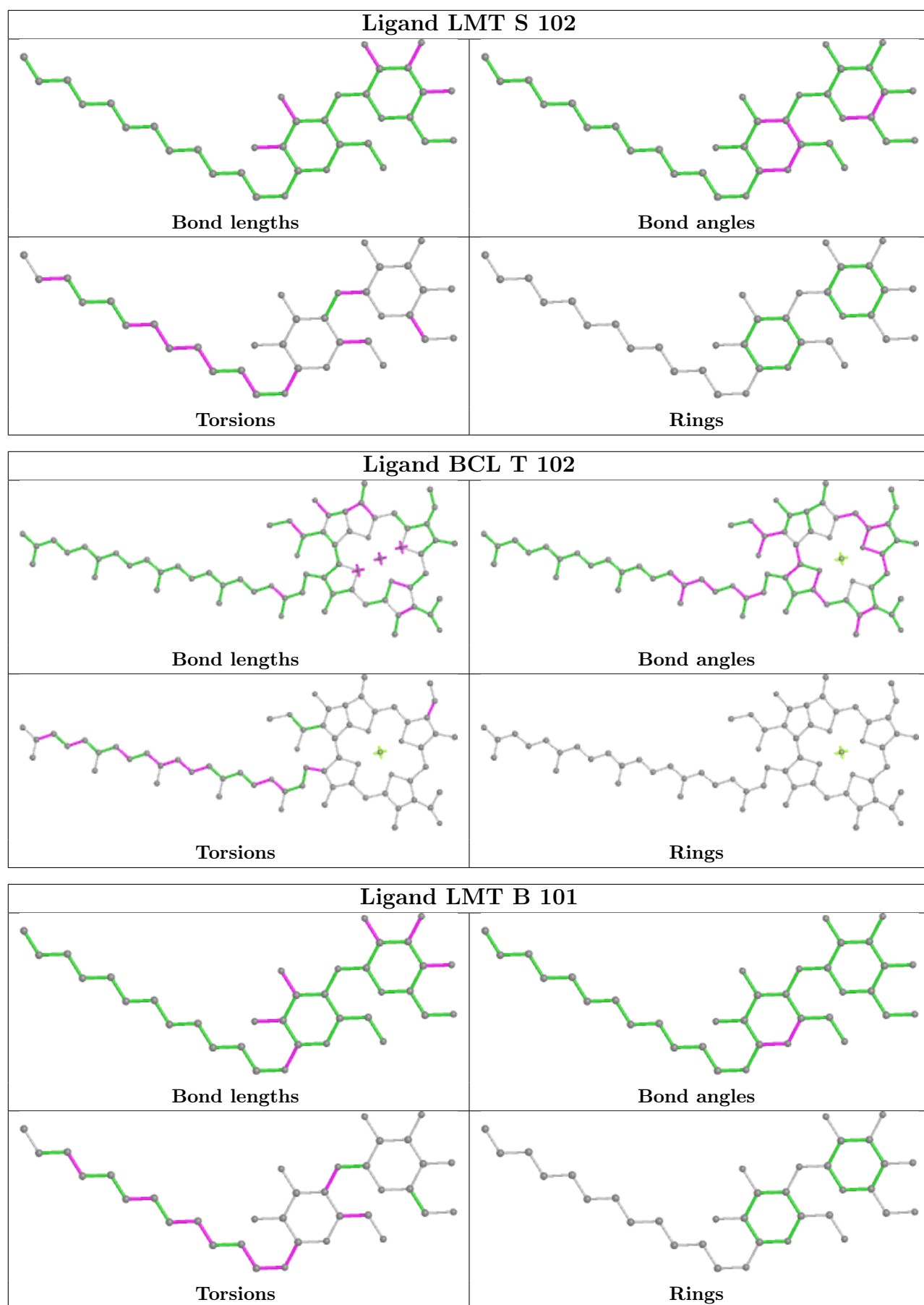


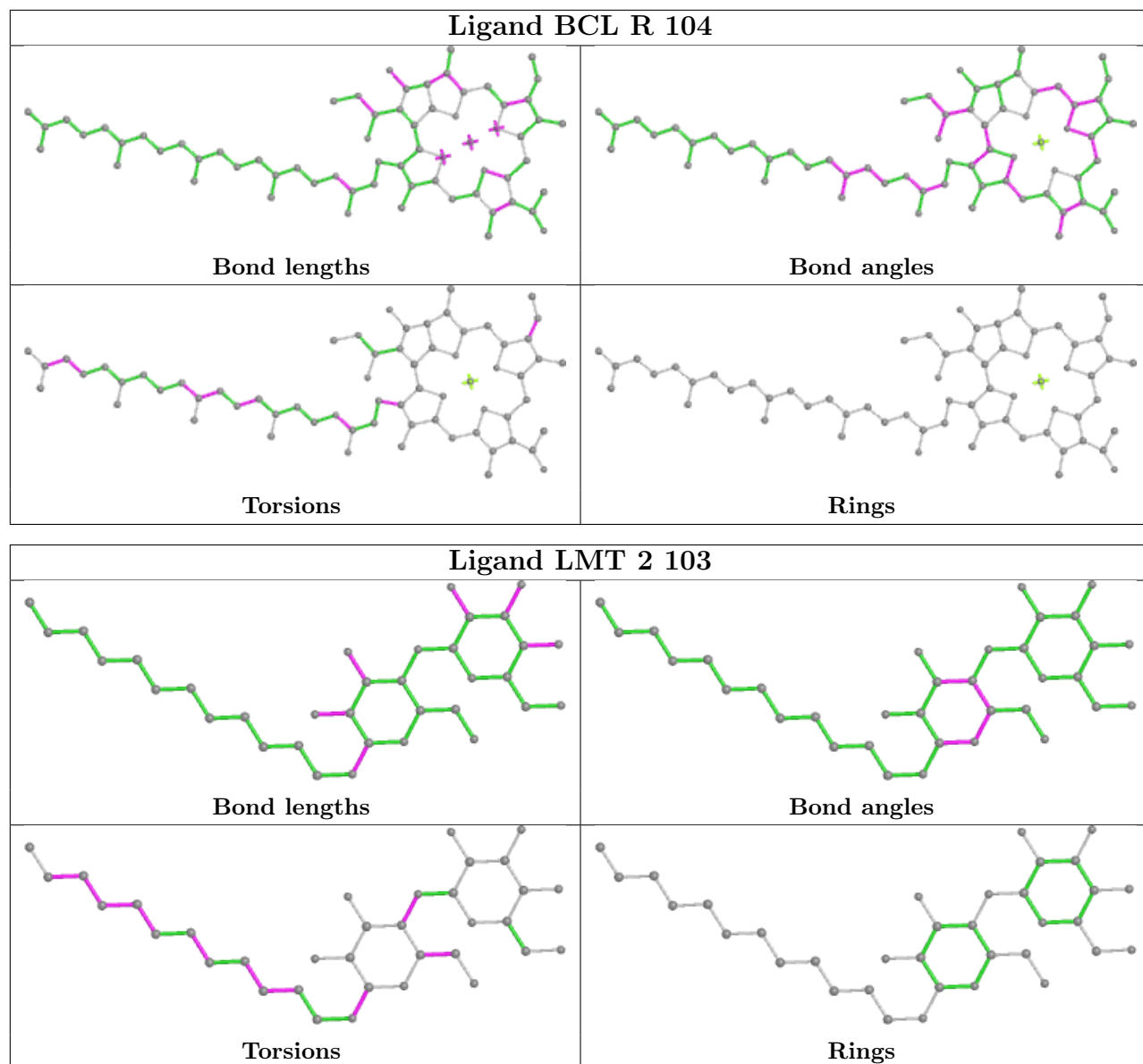


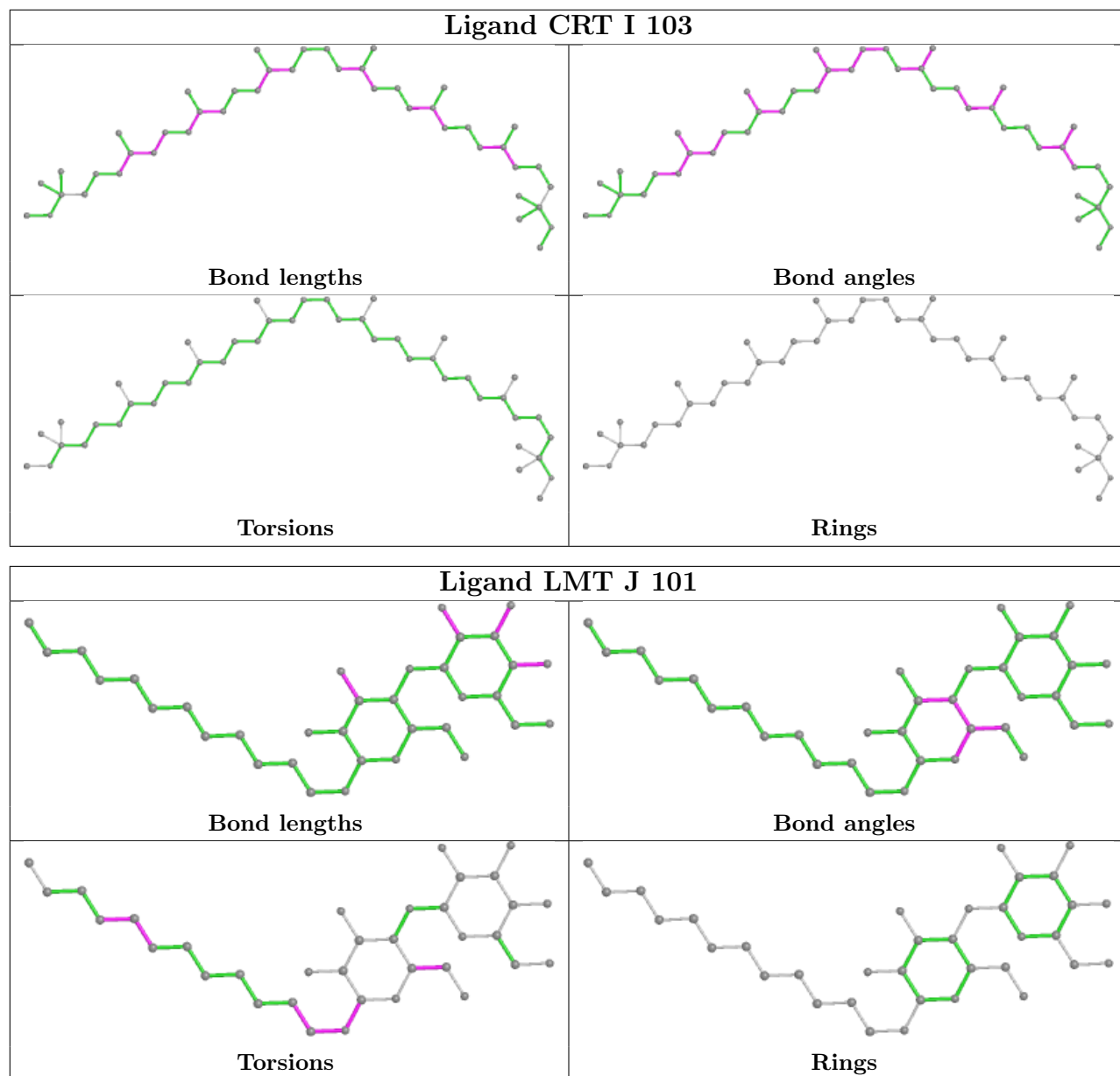


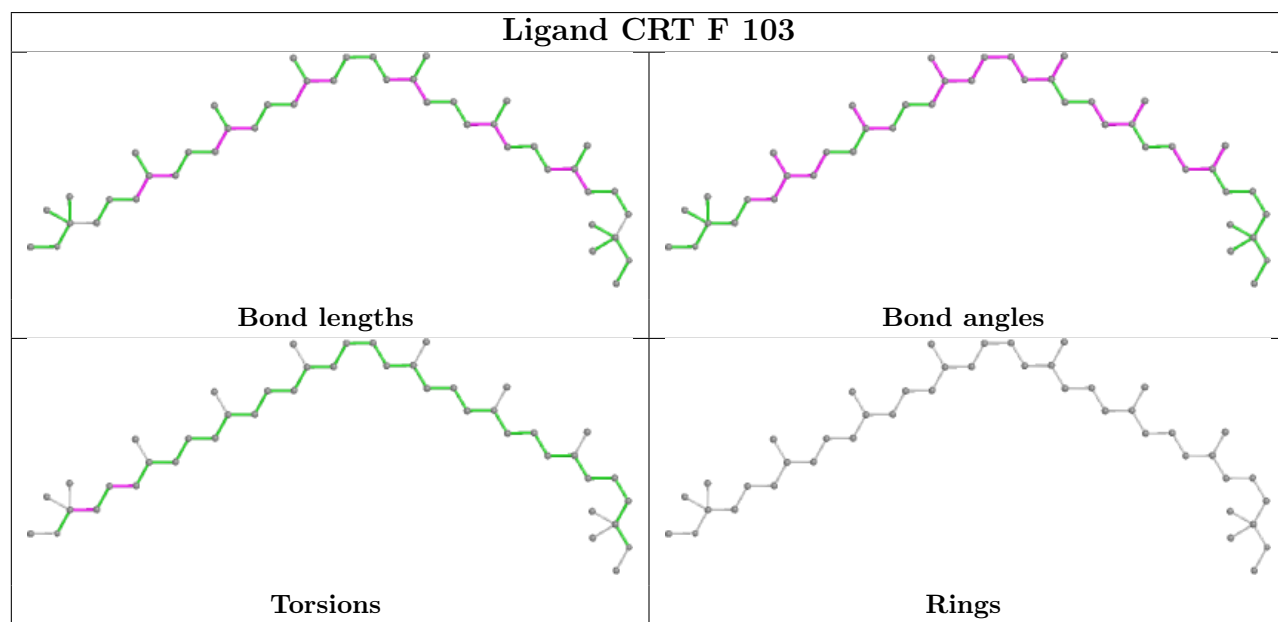
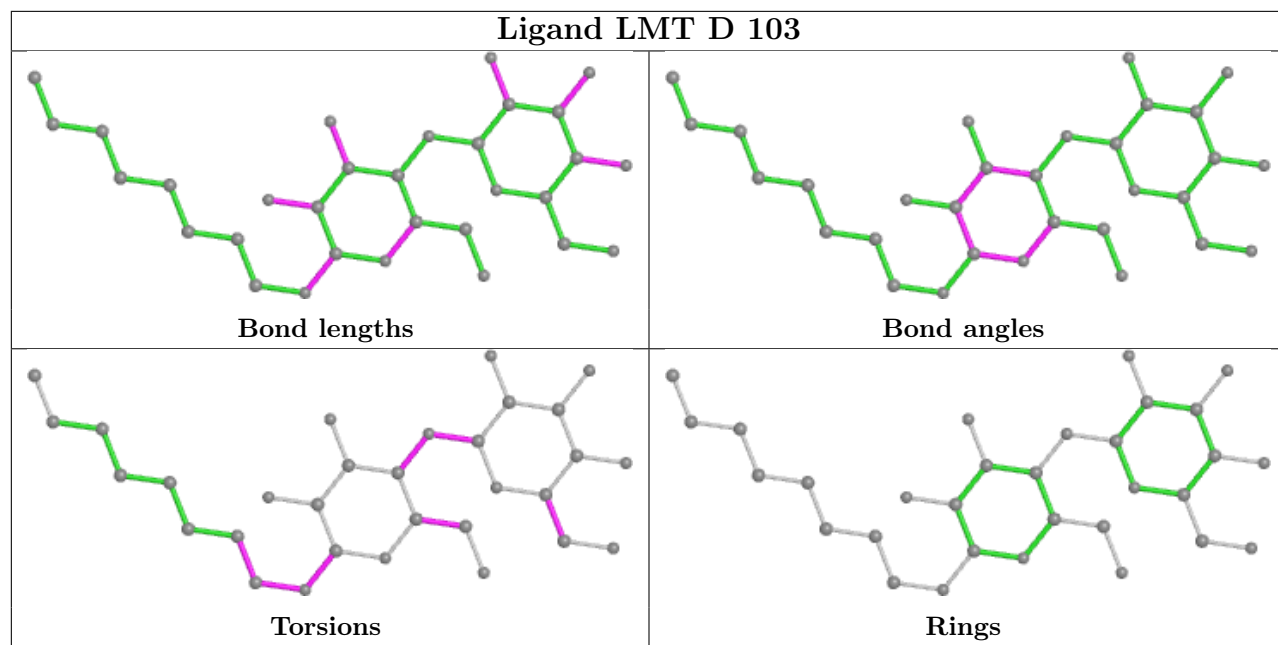




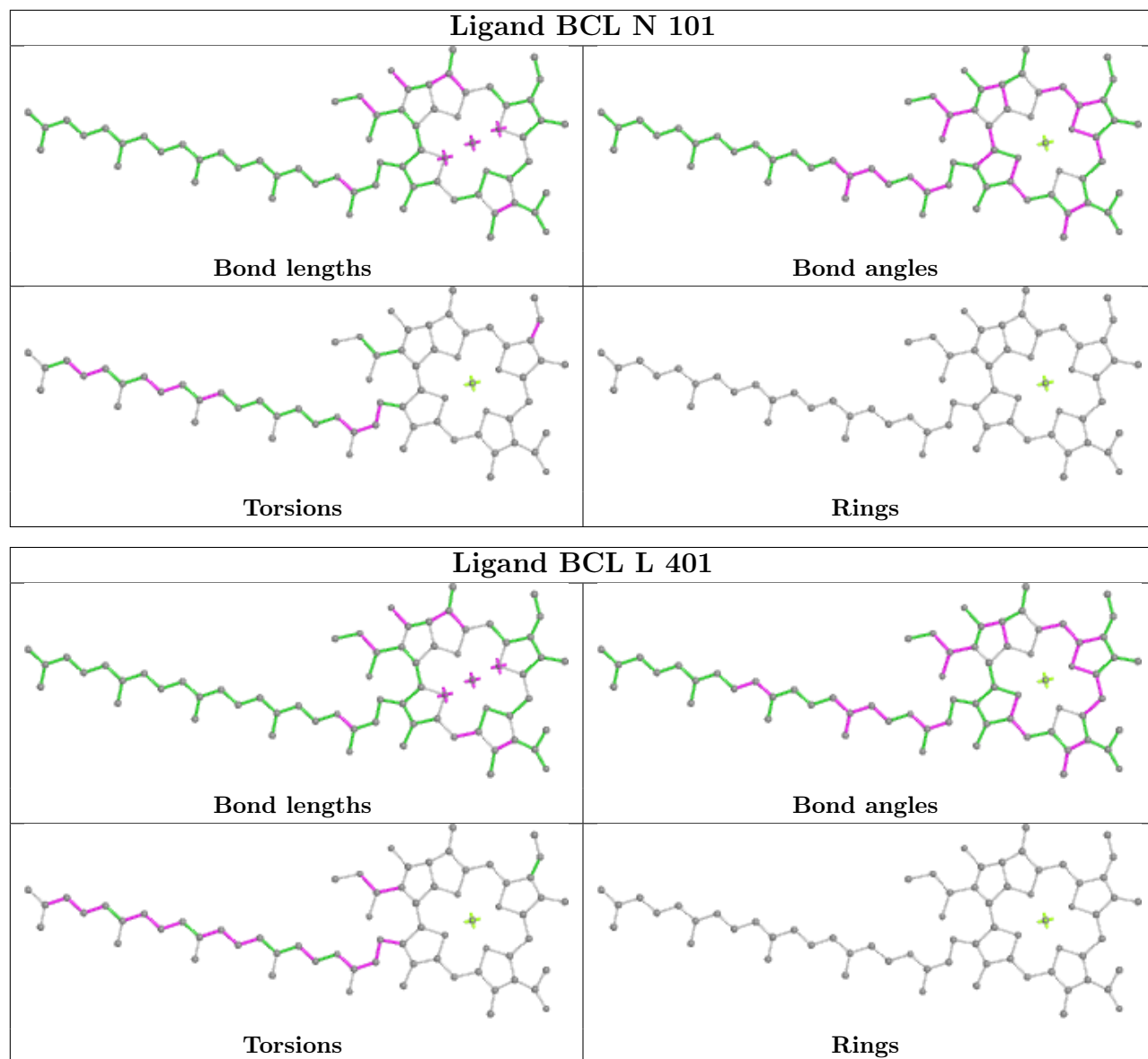


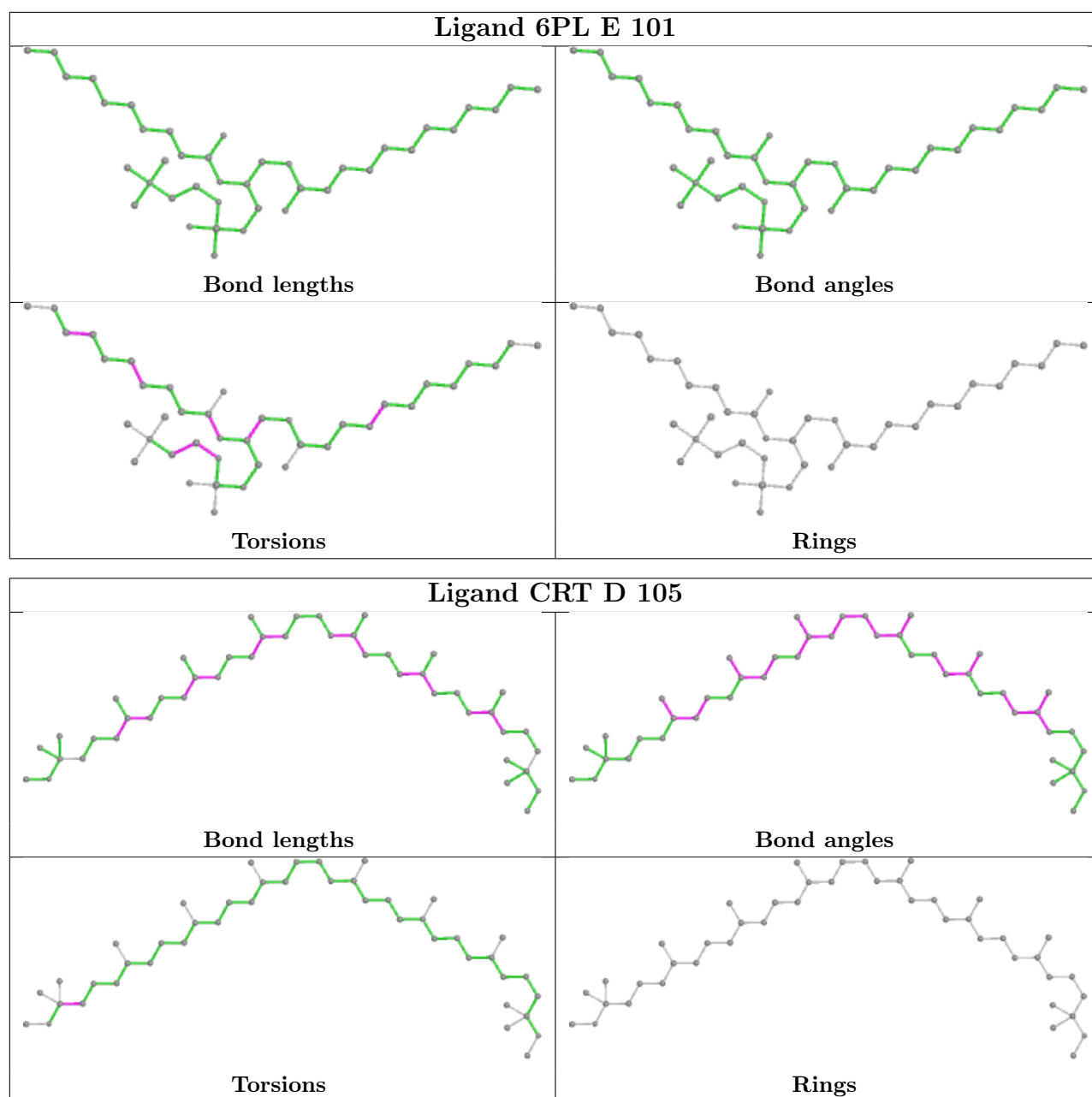


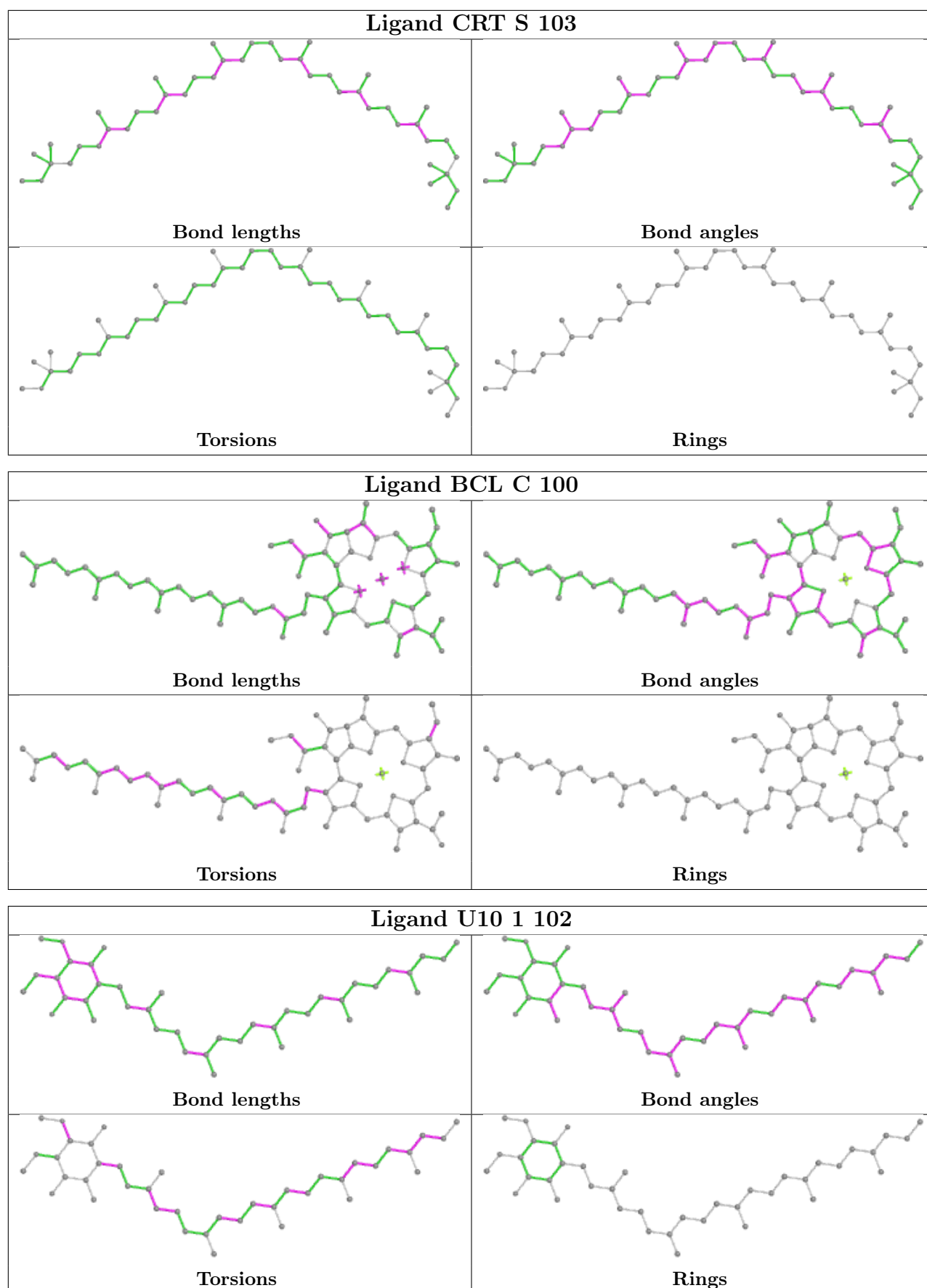


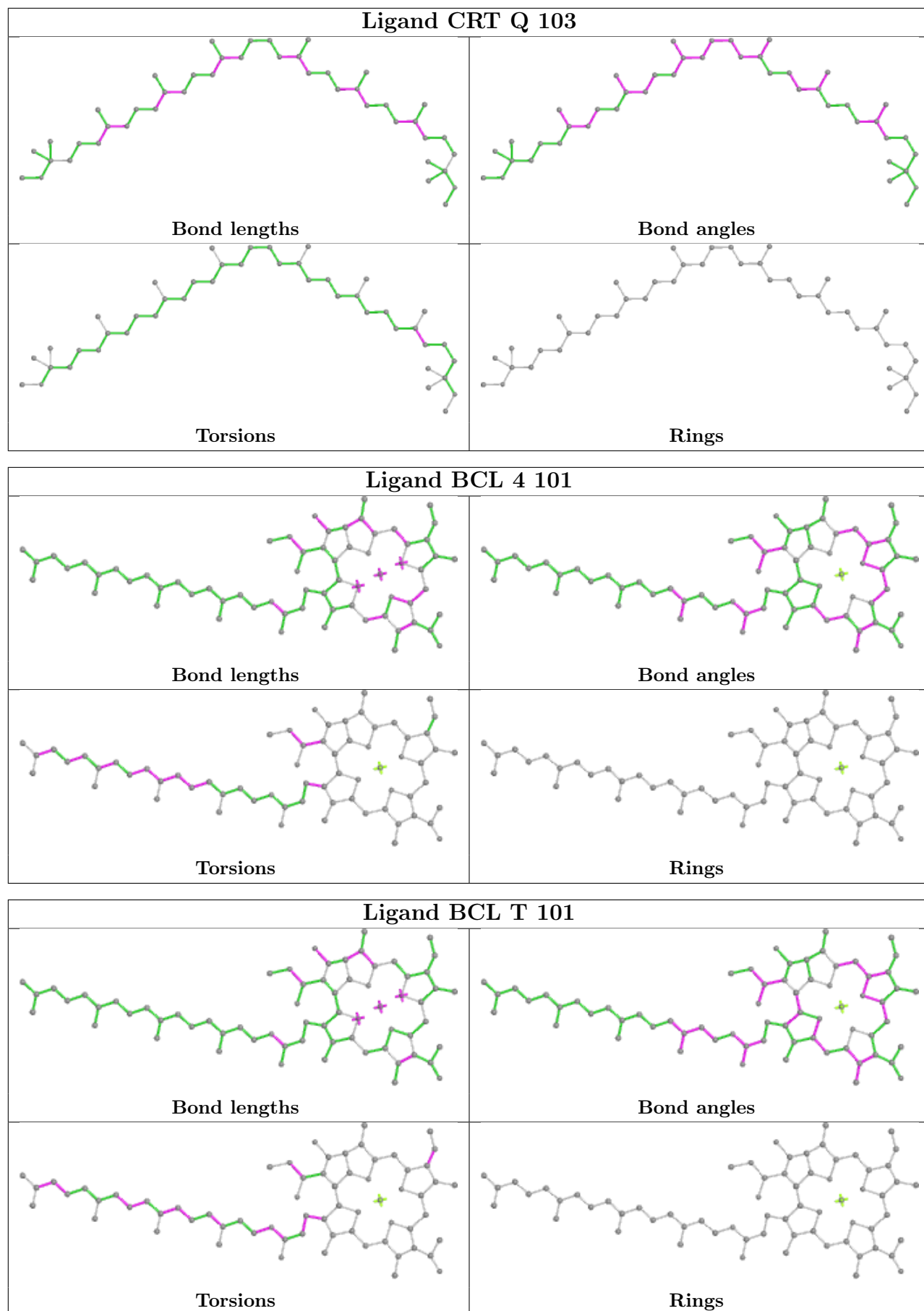


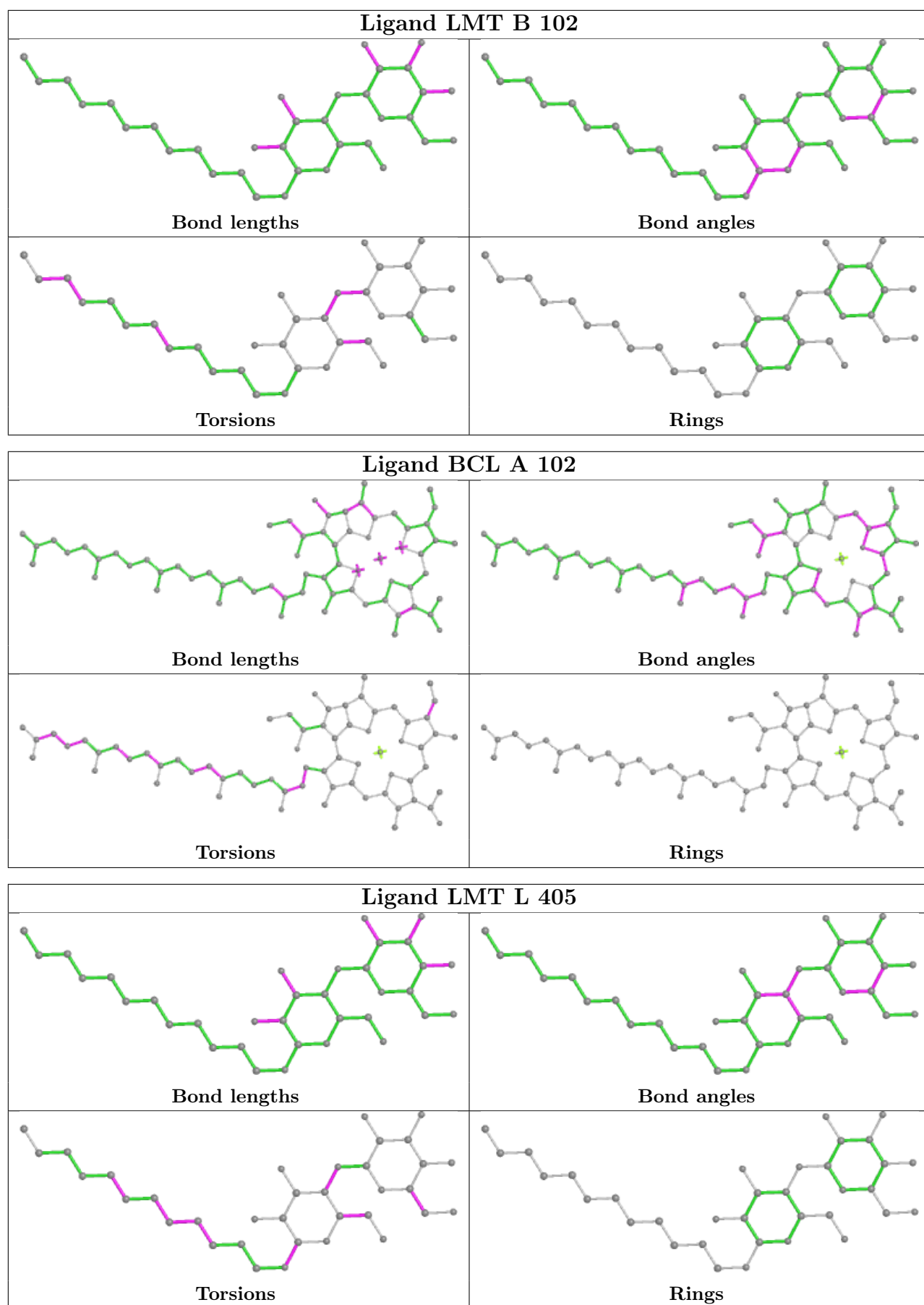


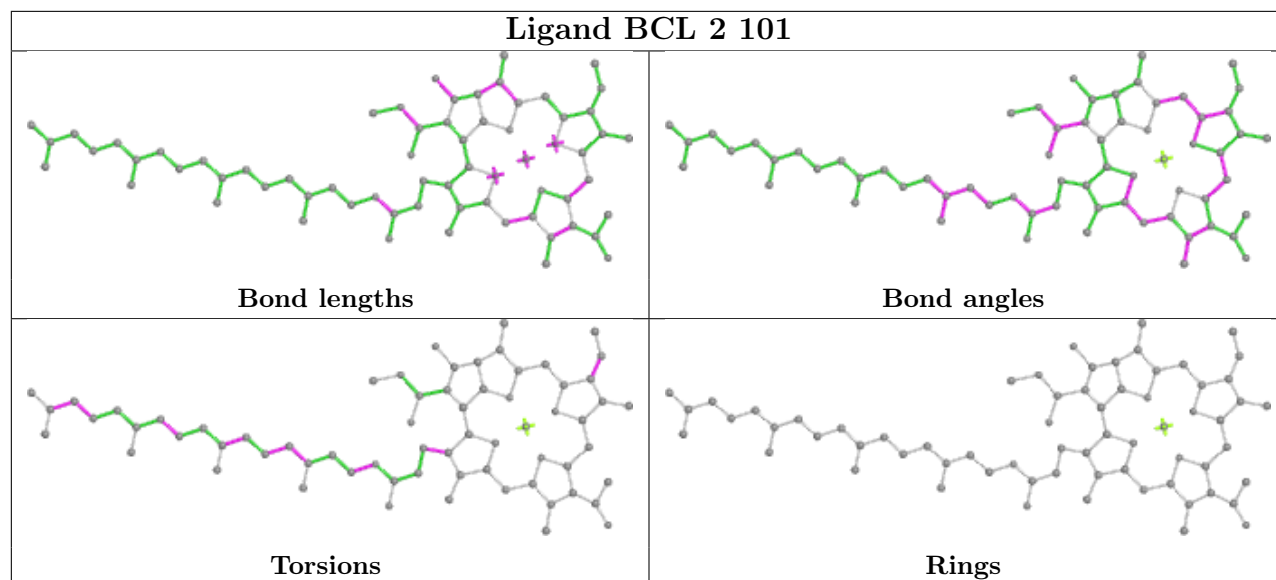












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

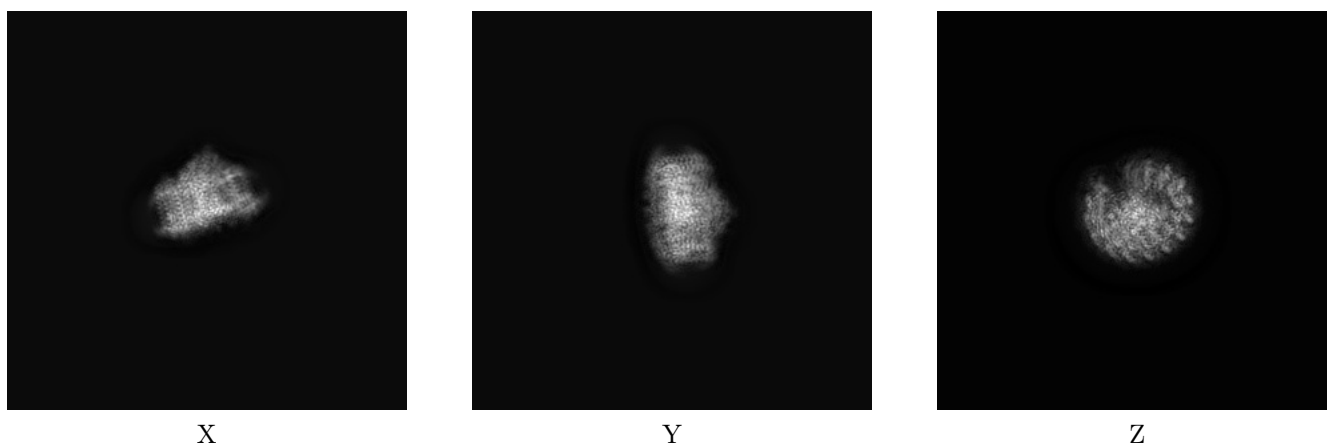
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11081. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

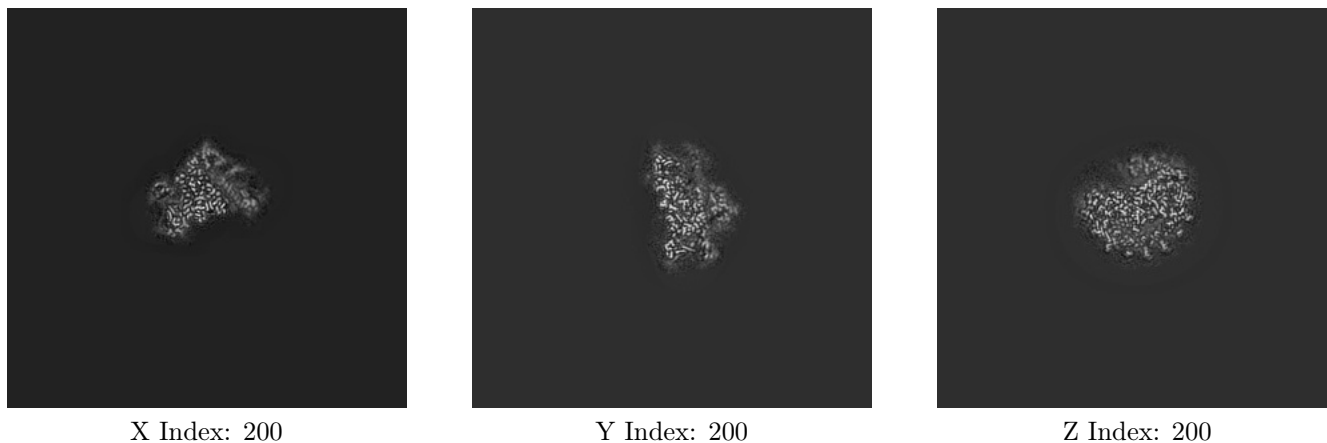
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



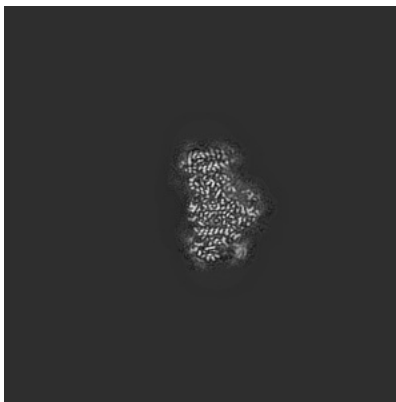
The images above show central slices of the map in three orthogonal directions.

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

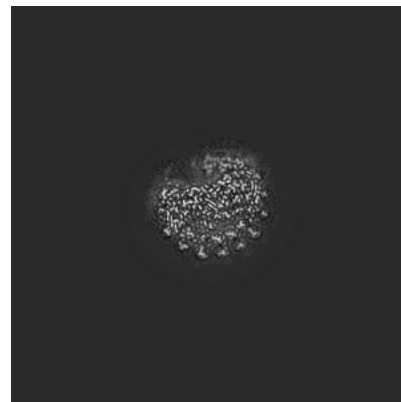
### 6.3.1 Primary map



X Index: 199



Y Index: 193

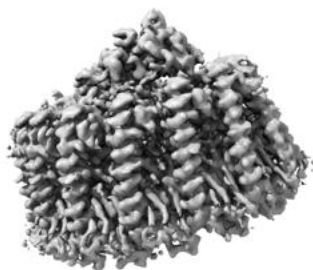


Z Index: 202

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

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

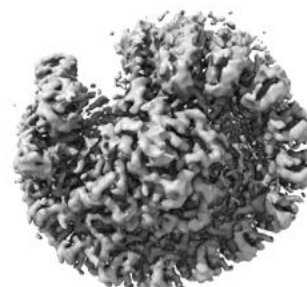
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



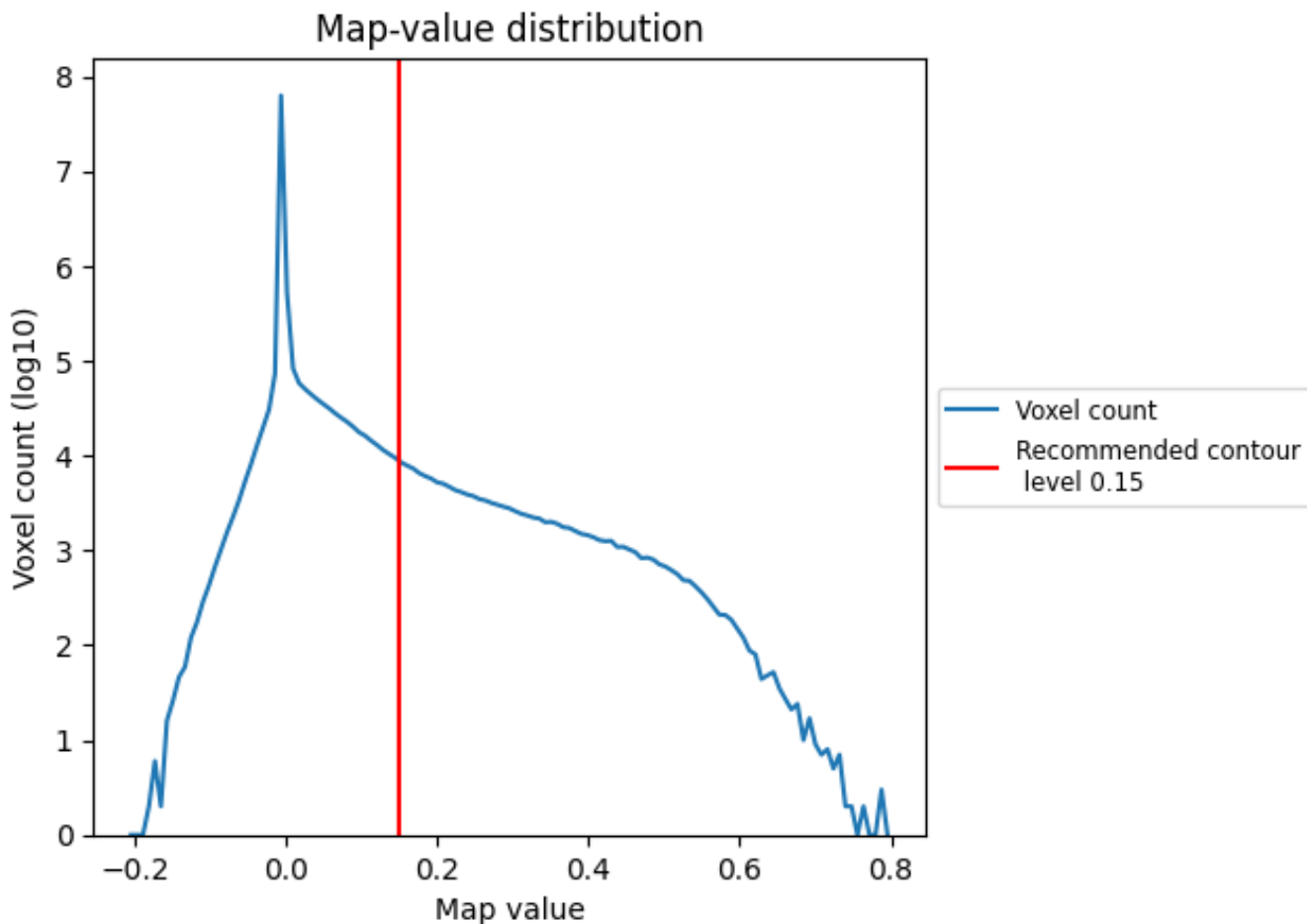
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

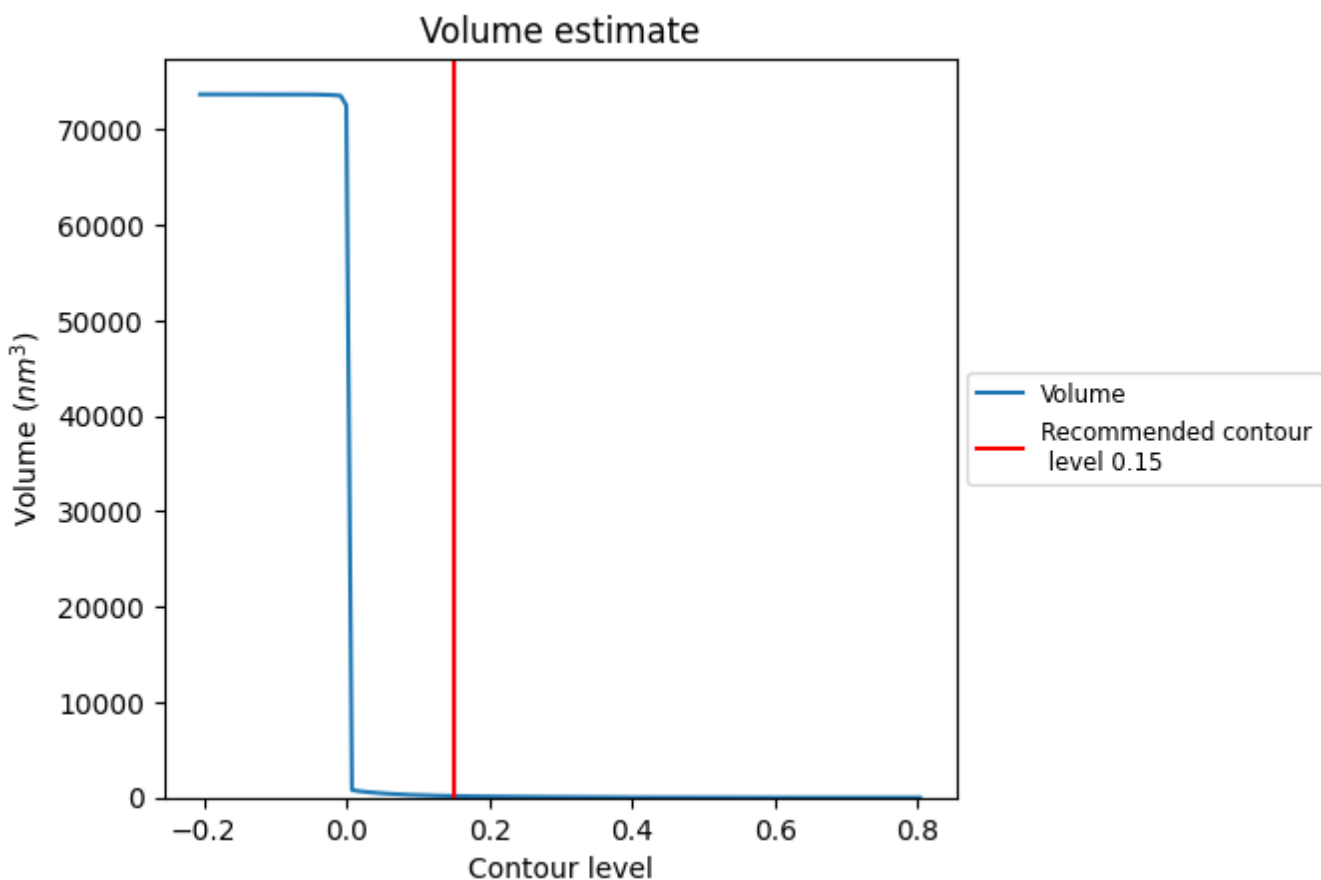
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

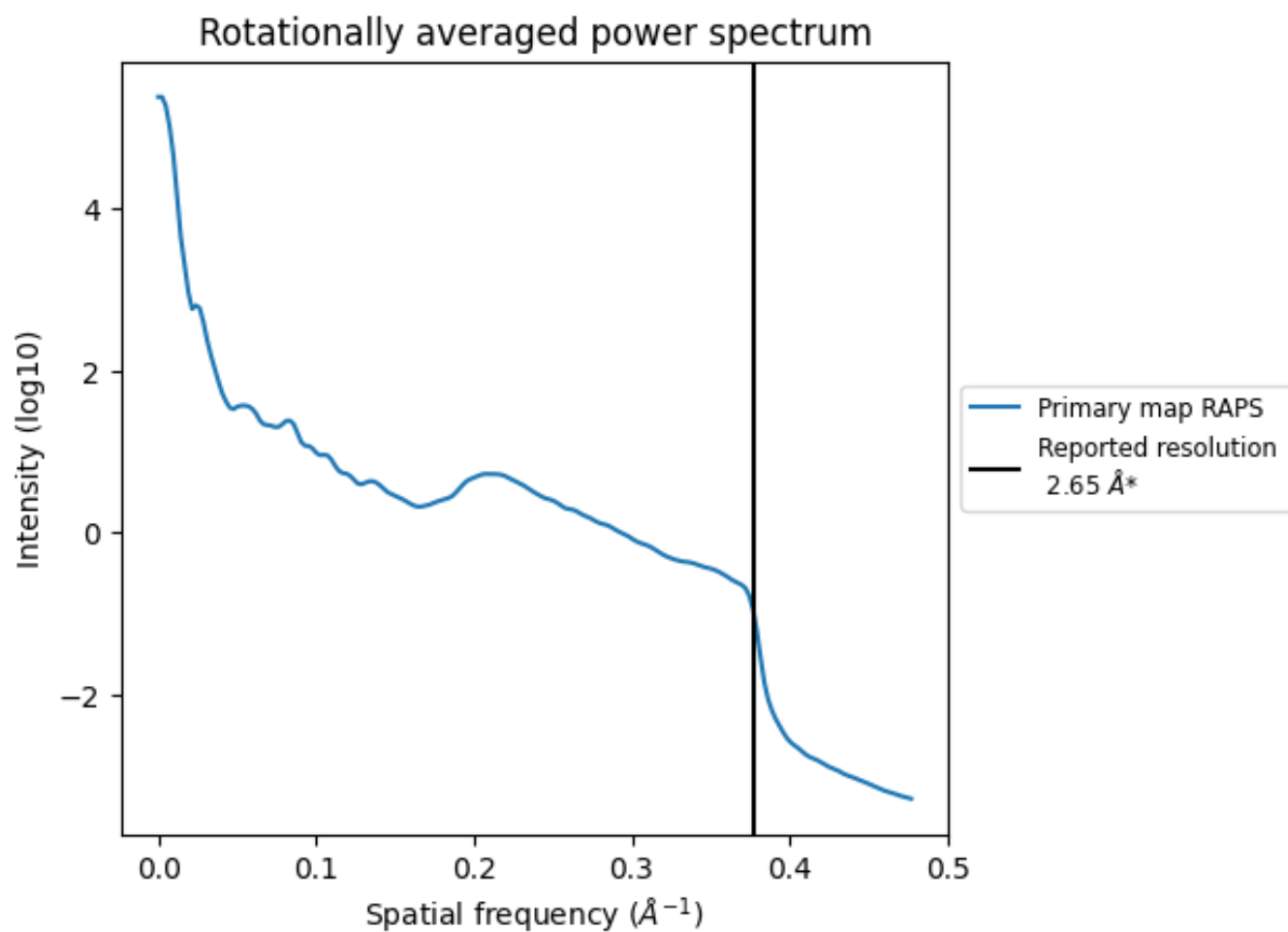
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 159 nm<sup>3</sup>; this corresponds to an approximate mass of 143 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

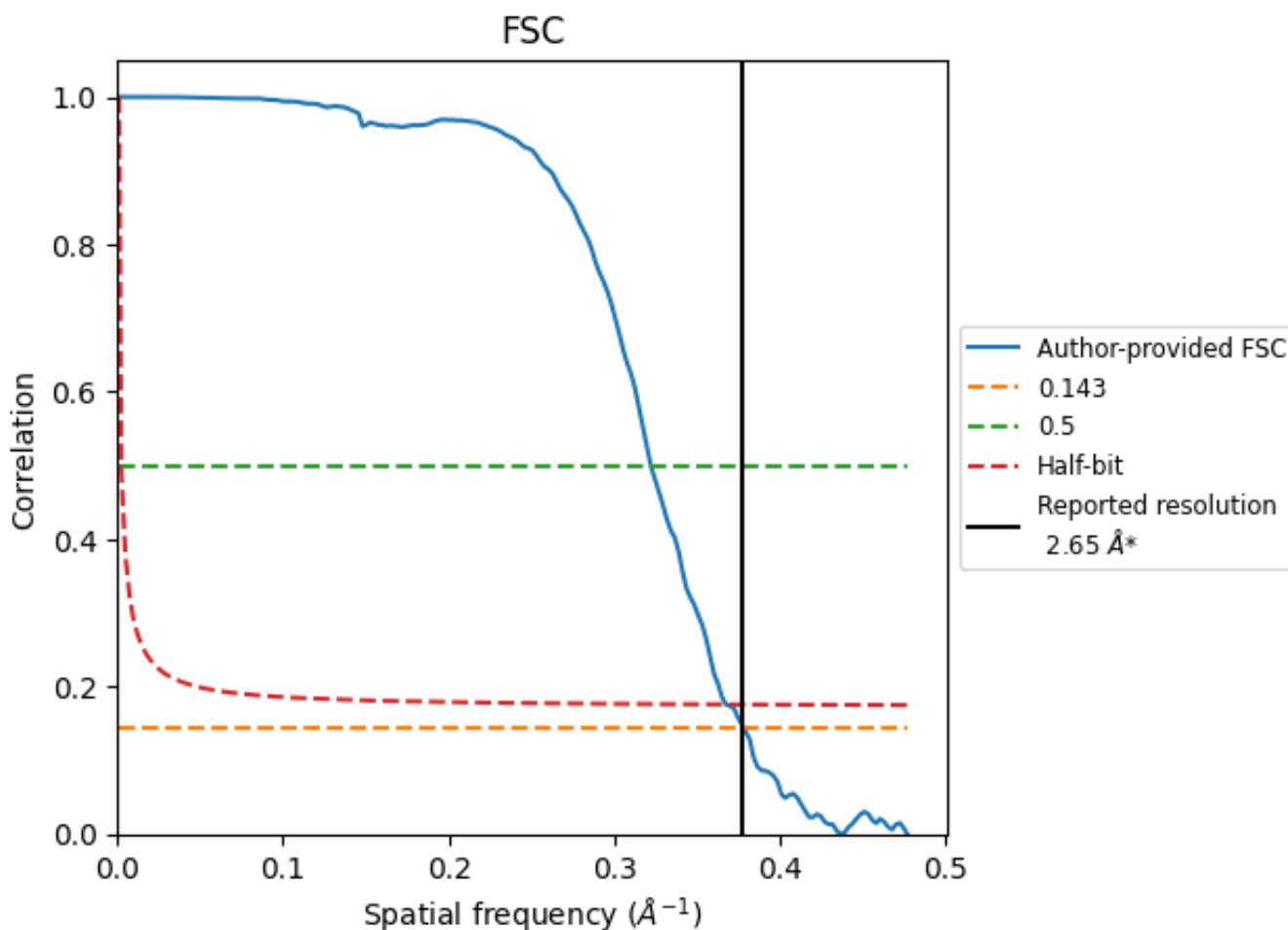


\*Reported resolution corresponds to spatial frequency of  $0.377 \text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.377 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

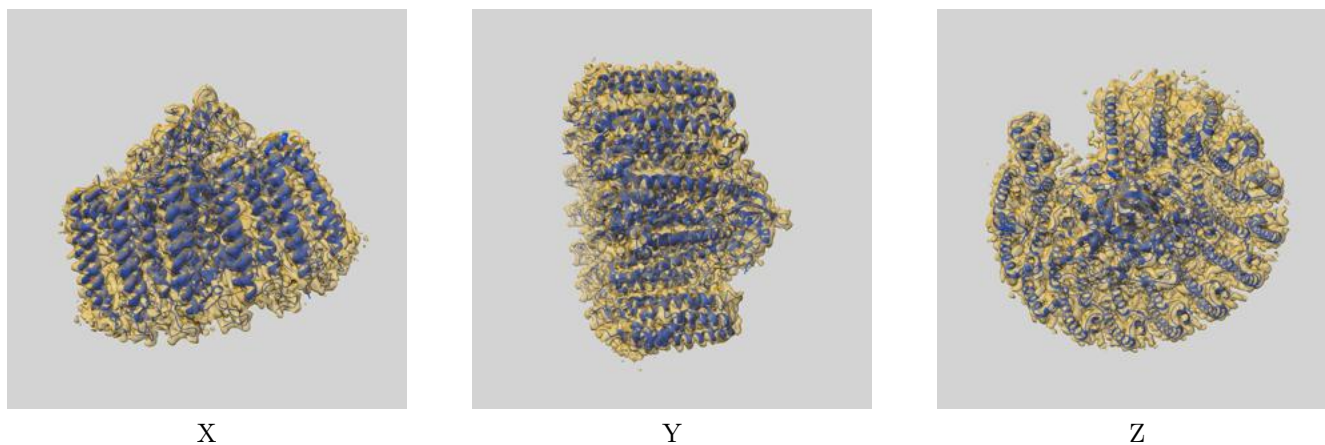
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.64	3.11	2.72
Unmasked-calculated*	-	-	-

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

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

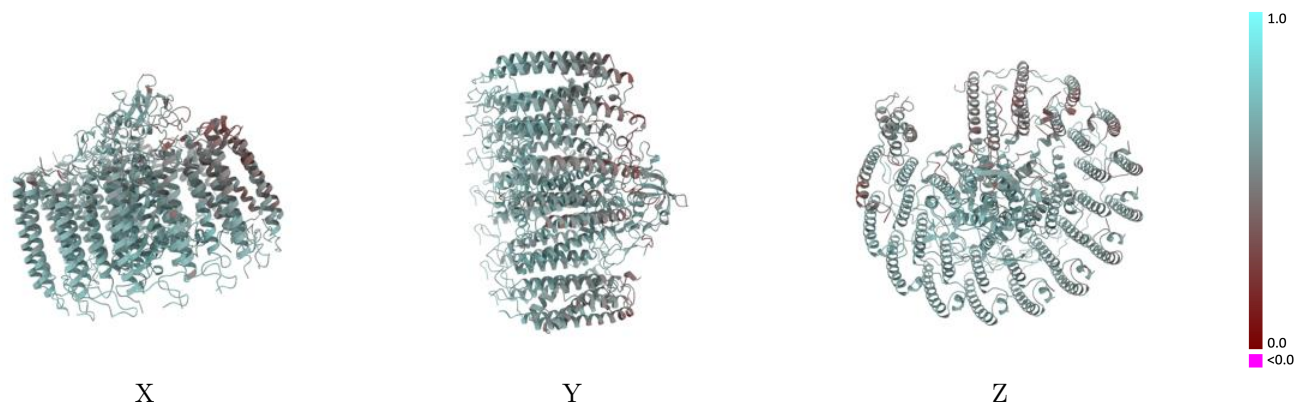
This section contains information regarding the fit between EMDB map EMD-11081 and PDB model 6Z5S. Per-residue inclusion information can be found in section 3 on page 17.

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



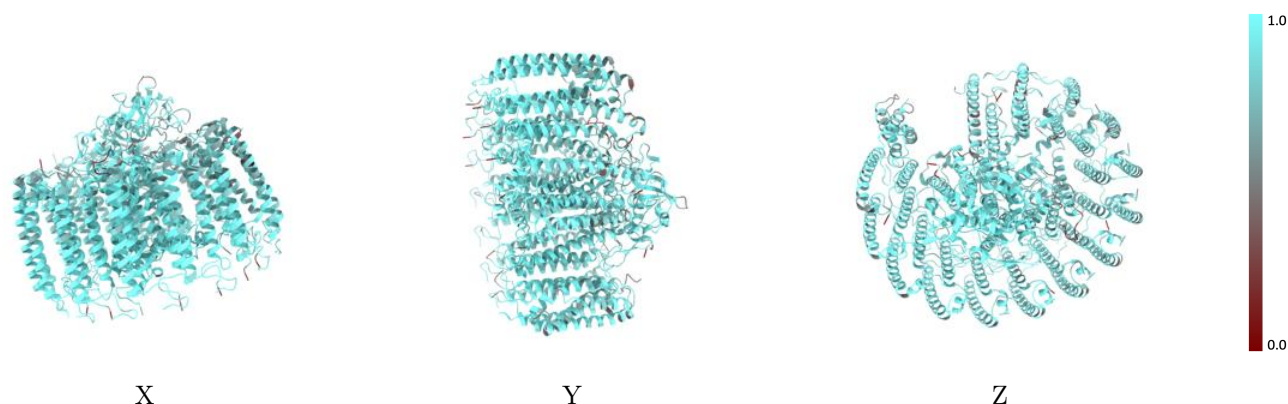
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

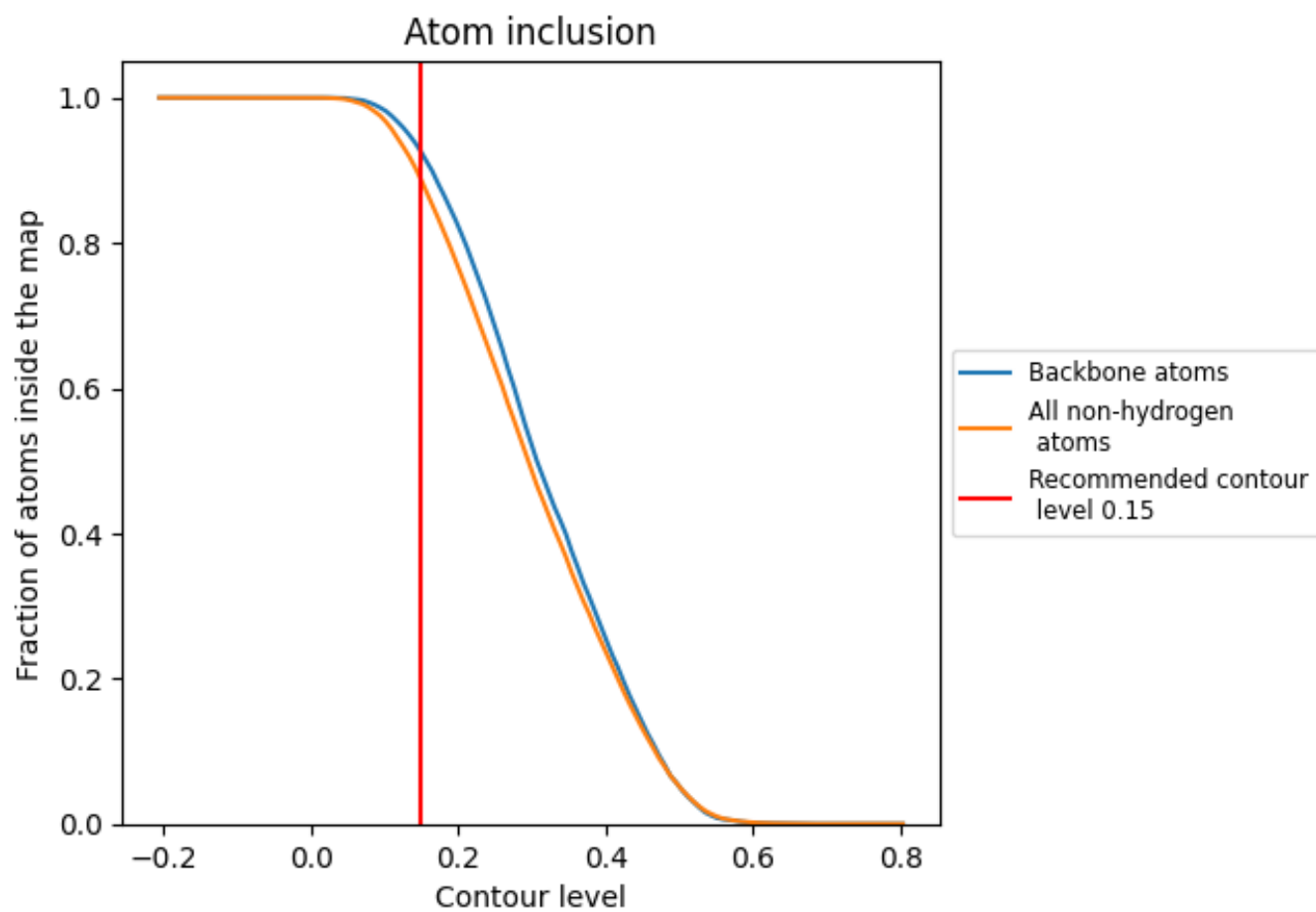
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.15).





































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8863	 0.5930
1	 0.8580	 0.5470
2	 0.7337	 0.4980
3	 0.7617	 0.5030
4	 0.7699	 0.4670
5	 0.7598	 0.5030
6	 0.7467	 0.4680
A	 0.9118	 0.5960
B	 0.8204	 0.5510
C	 0.9776	 0.6390
D	 0.8625	 0.6160
E	 0.9434	 0.6270
F	 0.8649	 0.6060
G	 0.9446	 0.6200
H	 0.9116	 0.5870
I	 0.8816	 0.6100
J	 0.9405	 0.6220
K	 0.8735	 0.6110
L	 0.9733	 0.6500
M	 0.9303	 0.6330
N	 0.9409	 0.6280
O	 0.9024	 0.6050
P	 0.9391	 0.6170
Q	 0.8548	 0.5960
R	 0.9302	 0.6160
S	 0.8327	 0.5840
T	 0.9173	 0.6080
U	 0.8386	 0.5890
V	 0.8917	 0.5980
W	 0.7746	 0.5000
X	 0.8184	 0.5560
Y	 0.8740	 0.5790
Z	 0.8176	 0.5360

