



## wwPDB EM Validation Summary Report ⓘ

Mar 24, 2025 – 12:56 PM JST

PDB ID : 8YZ2  
EMDB ID : EMD-39683  
Title : Cryo-EM structure of a tri-heme cytochrome-associated RC-LH1 complex from a marine photoheterotrophic bacterium, purified with magnesium solutions  
Authors : Chen, J.H.; Zheng, Q.; Zhang, X.  
Deposited on : 2024-04-05  
Resolution : 2.68 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>.

---

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

EMDB validation analysis	:	0.0.1.dev117
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)	:	2.41.2

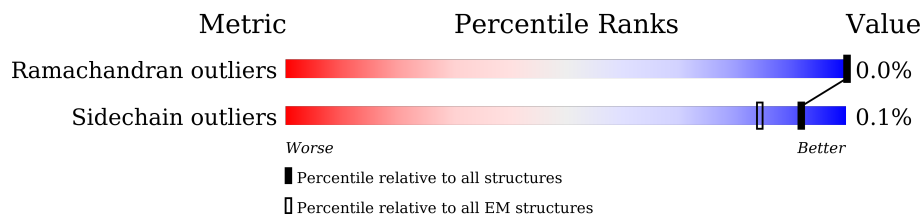
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

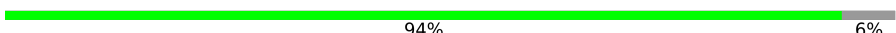
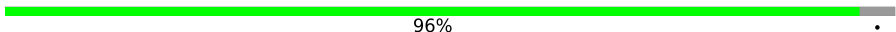
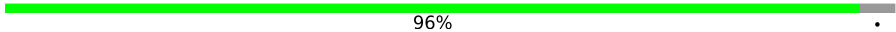
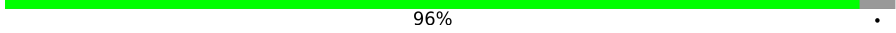
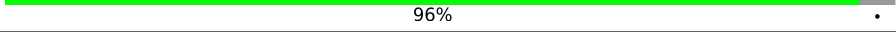
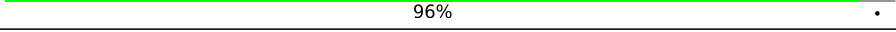
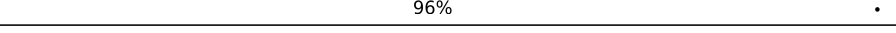
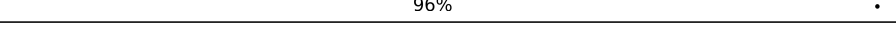
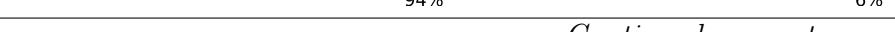
The reported resolution of this entry is 2.68 Å.

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.



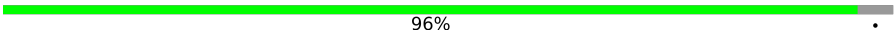
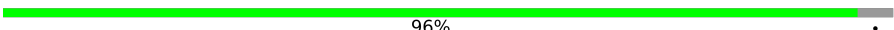
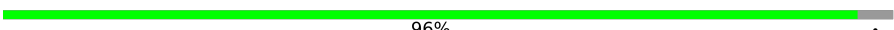
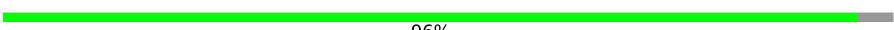
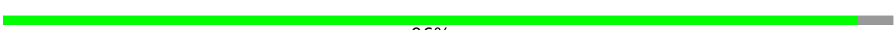





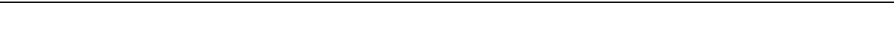

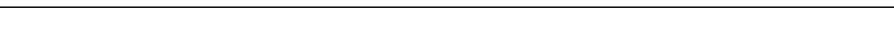
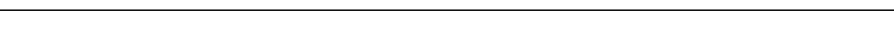











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	53	 94% 6%
1	A	53	 96% .
1	B	53	 96% .
1	D	53	 96% .
1	E	53	 96% .
1	F	53	 96% .
1	G	53	 96% .
1	I	53	 96% .
1	J	53	 94% 6%


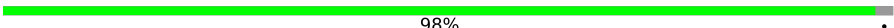
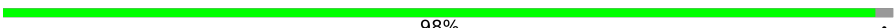
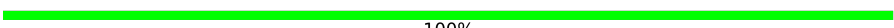
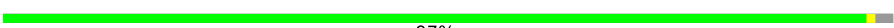
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	K	53	 96% .
1	N	53	 96% .
1	P	53	 96% .
1	Q	53	 96% .
1	R	53	 96% .
1	S	53	 96% .
1	T	53	 96% .
1	V	53	 96% .
2	O	239	 22% 78%
3	2	49	 90% 10%
3	a	49	 90% 10%
3	b	49	 90% 10%
3	d	49	 90% 10%
3	e	49	 90% 10%
3	f	49	 90% 10%
3	g	49	 90% 10%
3	i	49	 88% 12%
3	j	49	 88% 12%
3	k	49	 88% 12%
3	n	49	 90% 10%
3	p	49	 90% 10%
3	q	49	 90% 10%
3	r	49	 88% 12%
3	s	49	 90% 10%
3	t	49	 88% 12%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	v	49	 82%18%
4	M	330	 98%.
5	L	279	 98%.
6	H	256	 100%
7	C	360	 97%..

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28315 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 Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	51	Total	C	N	O	S	0	0
			425	291	68	64	2		
1	V	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	S	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	T	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	Q	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	R	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	1	50	Total	C	N	O	S	0	0
			417	286	67	63	1		
1	N	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	K	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	J	50	Total	C	N	O	S	0	0
			417	286	67	63	1		
1	I	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	G	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	F	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	E	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	D	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	B	51	Total	C	N	O	S	0	0
			422	289	68	64	1		
1	A	51	Total	C	N	O	S	0	0
			422	289	68	64	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	52	Total	C	N	O	S	0	0
			371	249	56	59	7		

- Molecule 3 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	v	40	Total	C	N	O	S	0	0
			325	217	52	55	1		
3	t	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	s	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	r	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	q	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	p	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	2	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	n	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	k	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	j	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	i	43	Total	C	N	O	S	0	0
			350	235	55	59	1		
3	g	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	f	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	e	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	d	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	b	44	Total	C	N	O	S	0	0
			358	239	56	62	1		
3	a	44	Total	C	N	O	S	0	0
			358	239	56	62	1		

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	325	Total	C	N	O	S	0	0
			2633	1752	421	452	8		

- Molecule 5 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	274	Total	C	N	O	S	0	0
			2178	1469	346	354	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	278	ASP	GLY	conflict	UNP A8LQ16
L	279	CYS	LEU	conflict	UNP A8LQ16

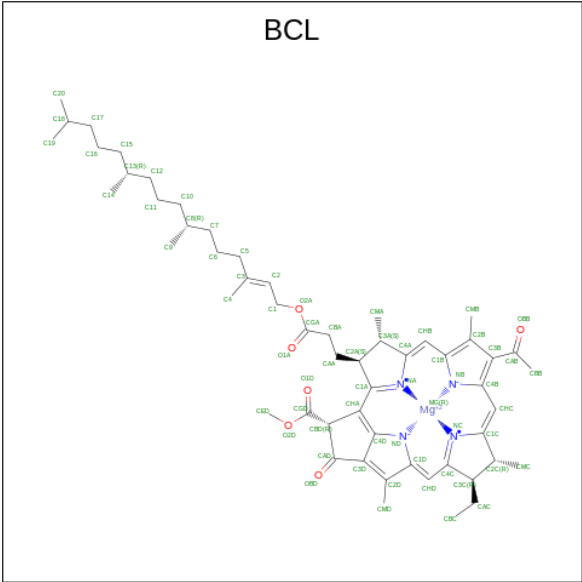
- Molecule 6 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	256	Total	C	N	O	S	0	0
			2022	1283	345	385	9		

- Molecule 7 is a protein called Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	352	Total	C	N	O	S	0	0
			2741	1732	455	540	14		

- 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>).



Mol	Chain	Residues	Atoms					AltConf
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	P	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	v	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	t	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	T	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	s	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	r	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	1	1	Total 66	C 55	Mg 1	N 4	O 6	0

Continued on next page...



*Continued from previous page...*

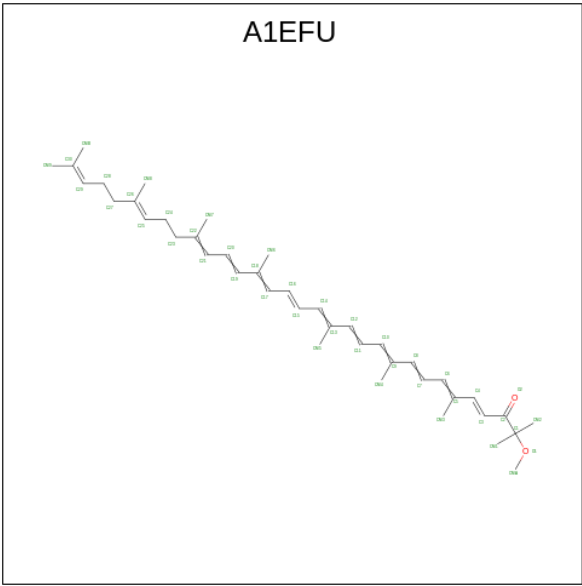
Mol	Chain	Residues	Atoms					AltConf
8	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	e	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	b	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	B	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	a	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0

*Continued on next page...*

Continued from previous page...

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

- Molecule 9 is (4 {E},16 {E},26 {E})-2-methoxy-2,6,10,14,19,23,27,31-octamethyl-dotriaconta-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-3-one (three-letter code: A1EFU) (formula: C<sub>41</sub>H<sub>58</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	v	1	Total	C	O	0
			43	41	2	
9	v	1	Total	C	O	0
			43	41	2	
9	S	1	Total	C	O	0
			43	41	2	
9	t	1	Total	C	O	0
			43	41	2	
9	T	1	Total	C	O	0
			43	41	2	
9	s	1	Total	C	O	0
			43	41	2	
9	Q	1	Total	C	O	0
			43	41	2	

Continued on next page...

*Continued from previous page...*

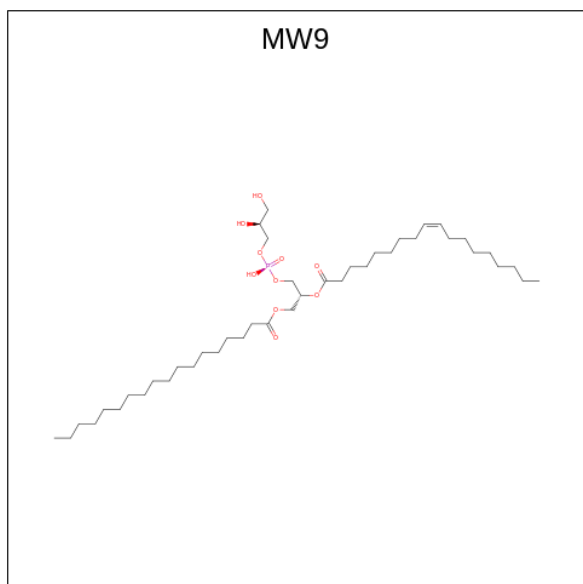
Mol	Chain	Residues	Atoms			AltConf
9	Q	1	Total 43	C 41	O 2	0
9	r	1	Total 43	C 41	O 2	0
9	R	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	1	1	Total 43	C 41	O 2	0
9	1	1	Total 43	C 41	O 2	0
9	N	1	Total 43	C 41	O 2	0
9	N	1	Total 43	C 41	O 2	0
9	k	1	Total 43	C 41	O 2	0
9	K	1	Total 43	C 41	O 2	0
9	J	1	Total 43	C 41	O 2	0
9	J	1	Total 43	C 41	O 2	0
9	I	1	Total 43	C 41	O 2	0
9	I	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	G	1	Total 43	C 41	O 2	0
9	F	1	Total 43	C 41	O 2	0
9	e	1	Total 43	C 41	O 2	0
9	E	1	Total 43	C 41	O 2	0
9	d	1	Total 43	C 41	O 2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
9	D	1	Total	C	O	0
			43	41	2	
9	D	1	Total	C	O	0
			43	41	2	
9	B	1	Total	C	O	0
			43	41	2	
9	a	1	Total	C	O	0
			43	41	2	
9	a	1	Total	C	O	0
			43	41	2	
9	A	1	Total	C	O	0
			43	41	2	
9	M	1	Total	C	O	0
			43	41	2	

- Molecule 10 is (21R,24R,27S)-24,27,28-trihydroxy-18,24-dioxo-19,23,25-trioxa-24lambda a 5 -phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (three-letter code: MW9) (formula: C<sub>42</sub>H<sub>81</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
10	Q	1	Total	C	O	P	0
			45	34	10	1	
10	I	1	Total	C	O	P	0
			40	29	10	1	
10	G	1	Total	C	O	P	0
			49	38	10	1	

*Continued on next page...*

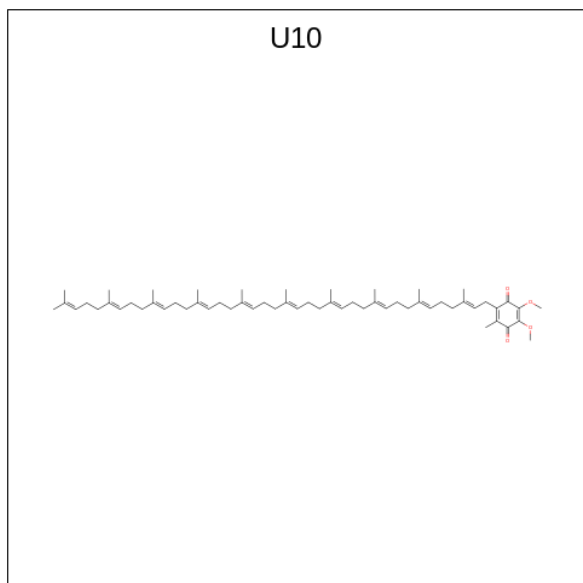
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
10	F	1	Total	C	O	P	0
			43	32	10	1	
10	F	1	Total	C	O	P	0
			48	37	10	1	
10	D	1	Total	C	O		0
			27	22	5		
10	D	1	Total	C	O	P	0
			53	42	10	1	
10	M	1	Total	C	O	P	0
			49	38	10	1	
10	M	1	Total	C	O	P	0
			53	42	10	1	
10	L	1	Total	C	O	P	0
			37	26	10	1	
10	L	1	Total	C	O	P	0
			36	25	10	1	
10	H	1	Total	C	O	P	0
			37	28	8	1	

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

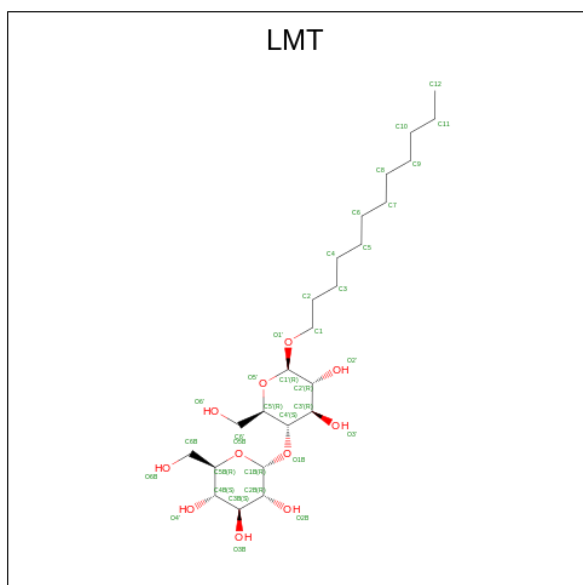
Mol	Chain	Residues	Atoms		AltConf
11	M	1	Total	Fe	0
			1	1	

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



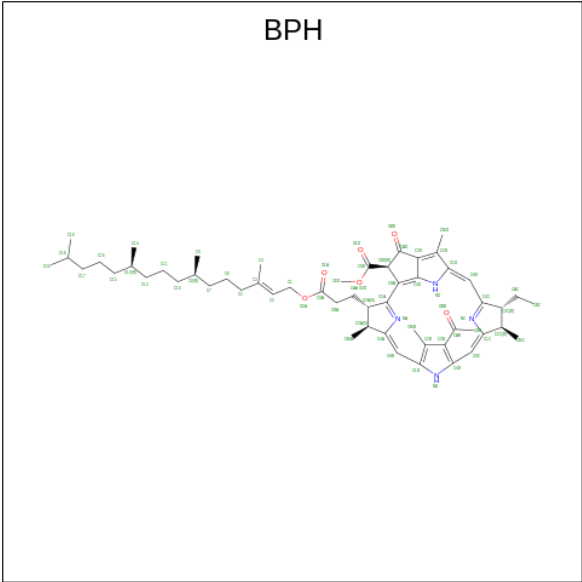
Mol	Chain	Residues	Atoms			AltConf
12	M	1	Total	C	O	0
			63	59	4	
12	L	1	Total	C	O	0
			48	44	4	

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



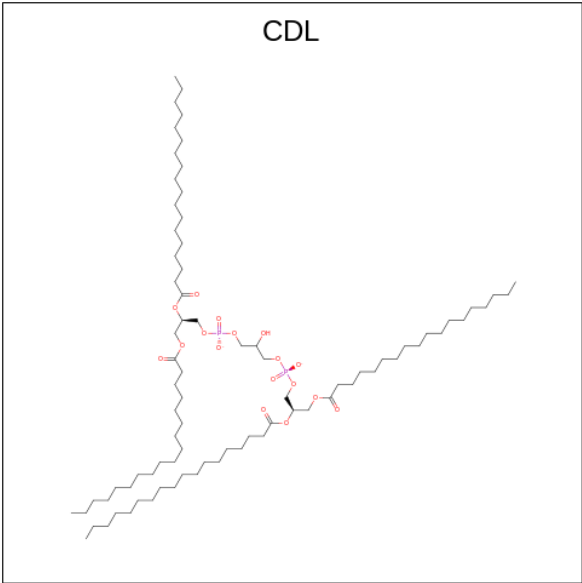
Mol	Chain	Residues	Atoms			AltConf
13	L	1	Total	C	O	0
			35	24	11	
13	L	1	Total	C	O	0
			24	18	6	
13	L	1	Total	C	O	0
			24	19	5	
13	H	1	Total	C	O	0
			24	18	6	
13	C	1	Total	C	O	0
			24	18	6	

- Molecule 14 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



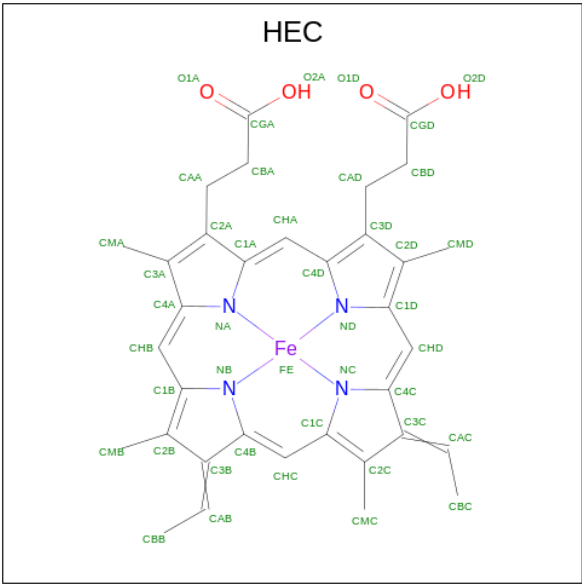
Mol	Chain	Residues	Atoms				AltConf
14	L	1	Total	C	N	O	0
			65	55	4	6	
14	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
15	L	1	Total	C	O	P	0
			67	48	17	2	
15	H	1	Total	C	O	P	0
			91	72	17	2	

- Molecule 16 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



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

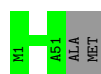


### 3 Residue-property plots [i](#)

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.

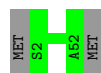
- Molecule 1: Antenna pigment protein alpha chain

Chain P:  96%



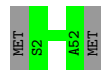
- Molecule 1: Antenna pigment protein alpha chain

Chain V:  96%



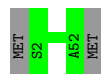
- Molecule 1: Antenna pigment protein alpha chain

Chain S:  96%



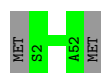
- Molecule 1: Antenna pigment protein alpha chain

Chain T:  96%



- Molecule 1: Antenna pigment protein alpha chain

Chain Q:  96%



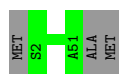
- Molecule 1: Antenna pigment protein alpha chain

Chain R:  96% .



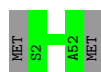
- Molecule 1: Antenna pigment protein alpha chain

Chain 1:  94% 6%



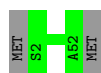
- Molecule 1: Antenna pigment protein alpha chain

Chain N:  96% .



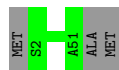
- Molecule 1: Antenna pigment protein alpha chain

Chain K:  96% .



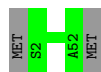
- Molecule 1: Antenna pigment protein alpha chain

Chain J:  94% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain I:  96% .



- Molecule 1: Antenna pigment protein alpha chain

Chain G:  96% .



- Molecule 1: Antenna pigment protein alpha chain

Chain F: 

96%

.



- Molecule 1: Antenna pigment protein alpha chain

Chain E: 

96%

.



- Molecule 1: Antenna pigment protein alpha chain

Chain D: 

96%

.



- Molecule 1: Antenna pigment protein alpha chain

Chain B: 

96%

.



- Molecule 1: Antenna pigment protein alpha chain

Chain A: 

96%

.

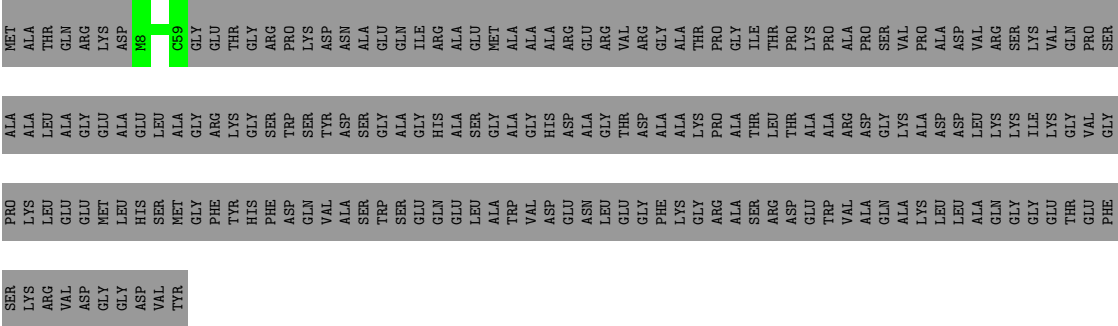


- Molecule 2: Reaction center protein O chain


Chain O: 

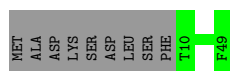
22%

78%




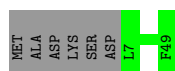
- Molecule 3: Antenna pigment protein beta chain

Chain v:  82% 18%




- Molecule 3: Antenna pigment protein beta chain

Chain t:  88% 12%




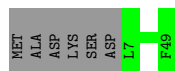
- Molecule 3: Antenna pigment protein beta chain

Chain s:  90% 10%




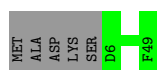
- Molecule 3: Antenna pigment protein beta chain

Chain r:  88% 12%




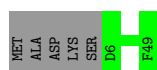
- Molecule 3: Antenna pigment protein beta chain

Chain q:  90% 10%



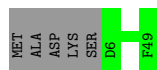
- Molecule 3: Antenna pigment protein beta chain

Chain p:  90% 10%




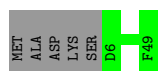
- Molecule 3: Antenna pigment protein beta chain

Chain 2:  90% 10%




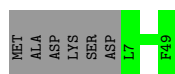
- Molecule 3: Antenna pigment protein beta chain

Chain n:  90% 10%




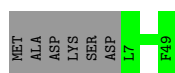
- Molecule 3: Antenna pigment protein beta chain

Chain k:  88% 12%




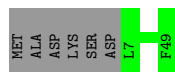
- Molecule 3: Antenna pigment protein beta chain

Chain j:  88% 12%




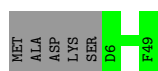
- Molecule 3: Antenna pigment protein beta chain

Chain i:  88% 12%




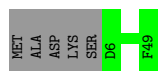
- Molecule 3: Antenna pigment protein beta chain

Chain g:  90% 10%




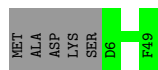
- Molecule 3: Antenna pigment protein beta chain

Chain f:  90% 10%




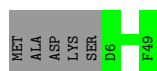
- Molecule 3: Antenna pigment protein beta chain

Chain e:  90% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain d:  90% 10%




- Molecule 3: Antenna pigment protein beta chain

Chain b:  90% 10%



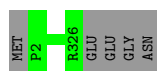
- Molecule 3: Antenna pigment protein beta chain

Chain a:  90% 10%



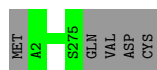
- Molecule 4: Reaction center protein M chain

Chain M:  98% .



- Molecule 5: Reaction center protein L chain

Chain L:  98% .



- Molecule 6: Reaction center protein H chain

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Photosynthetic reaction center cytochrome c subunit

Chain C:  97% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.698	Depositor
Minimum map value	-0.460	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	238.08, 238.08, 238.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, MW9, BCL, U10, HEC, LMT, CDL, A1EFU, FE

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	1	0.26	0/431	0.38	0/585
1	A	0.25	0/436	0.40	0/592
1	B	0.25	0/436	0.40	0/592
1	D	0.25	0/436	0.41	0/592
1	E	0.26	0/436	0.40	0/592
1	F	0.26	0/436	0.40	0/592
1	G	0.26	0/436	0.38	0/592
1	I	0.25	0/436	0.38	0/592
1	J	0.25	0/431	0.38	0/585
1	K	0.25	0/436	0.38	0/592
1	N	0.25	0/436	0.40	0/592
1	P	0.25	0/439	0.41	0/595
1	Q	0.25	0/436	0.38	0/592
1	R	0.25	0/436	0.38	0/592
1	S	0.25	0/436	0.39	0/592
1	T	0.24	0/436	0.38	0/592
1	V	0.24	0/436	0.37	0/592
2	O	0.23	0/378	0.38	0/516
3	2	0.24	0/371	0.40	0/508
3	a	0.24	0/371	0.41	0/508
3	b	0.24	0/371	0.39	0/508
3	d	0.25	0/371	0.39	0/508
3	e	0.24	0/371	0.40	0/508
3	f	0.24	0/371	0.39	0/508
3	g	0.23	0/371	0.37	0/508
3	i	0.24	0/363	0.38	0/497
3	j	0.24	0/363	0.39	0/497
3	k	0.24	0/363	0.44	0/497
3	n	0.23	0/371	0.39	0/508
3	p	0.24	0/371	0.42	0/508
3	q	0.24	0/371	0.44	0/508
3	r	0.23	0/363	0.43	0/497



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	s	0.24	0/371	0.40	0/508
3	t	0.25	0/363	0.39	0/497
3	v	0.23	0/337	0.36	0/462
4	M	0.26	0/2731	0.45	0/3735
5	L	0.27	0/2267	0.44	0/3105
6	H	0.26	0/2072	0.48	0/2804
7	C	0.25	0/2819	0.45	0/3869
All	All	0.25	0/23905	0.42	0/32617

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	1	48/53 (91%)	48 (100%)	0	0	100	100
1	A	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	B	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	D	49/53 (92%)	49 (100%)	0	0	100	100
1	E	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	F	49/53 (92%)	49 (100%)	0	0	100	100
1	G	49/53 (92%)	49 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	49/53 (92%)	49 (100%)	0	0	100	100
1	J	48/53 (91%)	48 (100%)	0	0	100	100
1	K	49/53 (92%)	49 (100%)	0	0	100	100
1	N	49/53 (92%)	49 (100%)	0	0	100	100
1	P	49/53 (92%)	49 (100%)	0	0	100	100
1	Q	49/53 (92%)	49 (100%)	0	0	100	100
1	R	49/53 (92%)	49 (100%)	0	0	100	100
1	S	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	T	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	V	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
2	O	50/239 (21%)	47 (94%)	3 (6%)	0	100	100
3	2	42/49 (86%)	42 (100%)	0	0	100	100
3	a	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	b	42/49 (86%)	42 (100%)	0	0	100	100
3	d	42/49 (86%)	42 (100%)	0	0	100	100
3	e	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	f	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	g	42/49 (86%)	42 (100%)	0	0	100	100
3	i	41/49 (84%)	41 (100%)	0	0	100	100
3	j	41/49 (84%)	41 (100%)	0	0	100	100
3	k	41/49 (84%)	41 (100%)	0	0	100	100
3	n	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	p	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	q	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
3	r	41/49 (84%)	41 (100%)	0	0	100	100
3	s	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	t	41/49 (84%)	41 (100%)	0	0	100	100
3	v	38/49 (78%)	38 (100%)	0	0	100	100
4	M	323/330 (98%)	314 (97%)	9 (3%)	0	100	100
5	L	272/279 (98%)	264 (97%)	8 (3%)	0	100	100
6	H	254/256 (99%)	249 (98%)	5 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	C	350/360 (97%)	334 (95%)	15 (4%)	1 (0%)	37	59
All	All	2785/3198 (87%)	2730 (98%)	54 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	189	VAL

### 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	1	42/44 (96%)	42 (100%)	0	100	100
1	A	42/44 (96%)	42 (100%)	0	100	100
1	B	42/44 (96%)	42 (100%)	0	100	100
1	D	42/44 (96%)	42 (100%)	0	100	100
1	E	42/44 (96%)	42 (100%)	0	100	100
1	F	42/44 (96%)	42 (100%)	0	100	100
1	G	42/44 (96%)	42 (100%)	0	100	100
1	I	42/44 (96%)	42 (100%)	0	100	100
1	J	42/44 (96%)	42 (100%)	0	100	100
1	K	42/44 (96%)	42 (100%)	0	100	100
1	N	42/44 (96%)	42 (100%)	0	100	100
1	P	43/44 (98%)	43 (100%)	0	100	100
1	Q	42/44 (96%)	42 (100%)	0	100	100
1	R	42/44 (96%)	42 (100%)	0	100	100
1	S	42/44 (96%)	42 (100%)	0	100	100
1	T	42/44 (96%)	42 (100%)	0	100	100
1	V	42/44 (96%)	42 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	39/174 (22%)	39 (100%)	0	100	100
3	2	37/41 (90%)	37 (100%)	0	100	100
3	a	37/41 (90%)	37 (100%)	0	100	100
3	b	37/41 (90%)	37 (100%)	0	100	100
3	d	37/41 (90%)	37 (100%)	0	100	100
3	e	37/41 (90%)	37 (100%)	0	100	100
3	f	37/41 (90%)	37 (100%)	0	100	100
3	g	37/41 (90%)	37 (100%)	0	100	100
3	i	36/41 (88%)	36 (100%)	0	100	100
3	j	36/41 (88%)	36 (100%)	0	100	100
3	k	36/41 (88%)	36 (100%)	0	100	100
3	n	37/41 (90%)	37 (100%)	0	100	100
3	p	37/41 (90%)	37 (100%)	0	100	100
3	q	37/41 (90%)	37 (100%)	0	100	100
3	r	36/41 (88%)	36 (100%)	0	100	100
3	s	37/41 (90%)	37 (100%)	0	100	100
3	t	36/41 (88%)	36 (100%)	0	100	100
3	v	33/41 (80%)	33 (100%)	0	100	100
4	M	266/270 (98%)	266 (100%)	0	100	100
5	L	218/223 (98%)	218 (100%)	0	100	100
6	H	214/214 (100%)	214 (100%)	0	100	100
7	C	299/307 (97%)	297 (99%)	2 (1%)	81	92
All	All	2371/2633 (90%)	2369 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	143	ASN
7	C	148	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	40	HIS
3	q	16	GLN
3	e	16	GLN
5	L	167	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 1 is monoatomic - leaving 99 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	$\# Z  > 2$
8	BCL	t	101	-	64,74,74	1.76	12 (18%)	78,115,115	2.07	24 (30%)
9	A1EFU	N	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.70	20 (44%)
9	A1EFU	2	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.68	21 (46%)
13	LMT	C	404	-	24,24,36	1.02	2 (8%)	29,29,47	1.07	1 (3%)
8	BCL	v	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.30	28 (35%)
8	BCL	L	303	-	64,74,74	1.70	12 (18%)	78,115,115	2.36	29 (37%)
8	BCL	T	102	-	64,74,74	1.73	13 (20%)	78,115,115	2.27	29 (37%)
8	BCL	G	102	-	64,74,74	1.73	11 (17%)	78,115,115	2.29	27 (34%)
8	BCL	k	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.27	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	E	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.31	27 (34%)
14	BPH	L	302	-	51,70,70	0.81	2 (3%)	52,101,101	0.66	1 (1%)
16	HEC	C	401	7	32,50,50	2.00	4 (12%)	24,82,82	2.26	12 (50%)
12	U10	L	305	-	48,48,63	0.17	0	58,61,79	0.46	1 (1%)
8	BCL	V	101	-	64,74,74	1.69	10 (15%)	78,115,115	2.25	29 (37%)
9	A1EFU	I	101	-	40,42,42	1.69	8 (20%)	45,52,52	3.79	19 (42%)
9	A1EFU	a	103	-	40,42,42	1.70	9 (22%)	45,52,52	4.01	20 (44%)
9	A1EFU	t	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.80	19 (42%)
8	BCL	a	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.26	28 (35%)
13	LMT	L	308	-	24,24,36	1.05	2 (8%)	29,29,47	1.17	2 (6%)
8	BCL	L	306	-	64,74,74	1.70	12 (18%)	78,115,115	2.36	29 (37%)
8	BCL	K	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.26	27 (34%)
9	A1EFU	A	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.72	20 (44%)
10	MW9	F	104	-	47,47,52	1.39	6 (12%)	50,53,58	1.44	3 (6%)
9	A1EFU	N	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.81	20 (44%)
8	BCL	i	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.28	26 (33%)
9	A1EFU	l	101	-	40,42,42	1.70	9 (22%)	45,52,52	3.83	20 (44%)
10	MW9	F	103	-	42,42,52	1.43	6 (14%)	45,48,58	1.46	3 (6%)
9	A1EFU	J	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.91	20 (44%)
8	BCL	S	101	-	64,74,74	1.71	10 (15%)	78,115,115	2.24	27 (34%)
8	BCL	Q	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.24	26 (33%)
8	BCL	l	103	-	64,74,74	1.72	11 (17%)	78,115,115	2.28	27 (34%)
10	MW9	D	103	-	52,52,52	1.45	6 (11%)	55,58,58	1.46	4 (7%)
10	MW9	M	406	-	52,52,52	1.45	6 (11%)	55,58,58	1.47	4 (7%)
8	BCL	B	101	-	64,74,74	1.72	13 (20%)	78,115,115	2.25	27 (34%)
8	BCL	d	101	-	64,74,74	1.74	11 (17%)	78,115,115	2.23	22 (28%)
8	BCL	l	102	-	64,74,74	1.70	11 (17%)	78,115,115	2.25	25 (32%)
10	MW9	M	405	-	48,48,52	1.49	6 (12%)	51,54,58	1.50	3 (5%)
8	BCL	q	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.26	26 (33%)
9	A1EFU	T	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.71	20 (44%)
9	A1EFU	Q	103	-	40,42,42	1.70	9 (22%)	45,52,52	3.88	20 (44%)
8	BCL	M	402	-	64,74,74	1.71	11 (17%)	78,115,115	2.22	24 (30%)
9	A1EFU	Q	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.73	21 (46%)
13	LMT	H	301	-	24,24,36	1.04	2 (8%)	29,29,47	1.06	1 (3%)
8	BCL	N	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.28	27 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	M	403	-	64,74,74	1.71	13 (20%)	78,115,115	2.31	27 (34%)
9	A1EFU	E	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.73	19 (42%)
8	BCL	R	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.27	27 (34%)
9	A1EFU	F	105	-	40,42,42	1.69	7 (17%)	45,52,52	3.80	19 (42%)
8	BCL	j	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.29	29 (37%)
9	A1EFU	e	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.80	19 (42%)
10	MW9	D	102	-	26,26,52	1.42	4 (15%)	28,28,58	1.29	2 (7%)
9	A1EFU	G	104	-	40,42,42	1.69	8 (20%)	45,52,52	3.68	19 (42%)
9	A1EFU	s	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.40	20 (44%)
9	A1EFU	D	105	-	40,42,42	1.68	9 (22%)	45,52,52	3.92	20 (44%)
9	A1EFU	r	102	-	40,42,42	1.68	8 (20%)	45,52,52	3.72	19 (42%)
8	BCL	G	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.25	27 (34%)
10	MW9	L	309	-	36,36,52	1.47	5 (13%)	39,42,58	1.53	3 (7%)
14	BPH	L	304	-	51,70,70	0.62	2 (3%)	52,101,101	0.73	1 (1%)
16	HEC	C	402	7	32,50,50	2.05	4 (12%)	24,82,82	2.23	11 (45%)
8	BCL	F	101	-	64,74,74	1.73	10 (15%)	78,115,115	2.14	23 (29%)
9	A1EFU	M	407	-	40,42,42	1.68	9 (22%)	45,52,52	3.67	19 (42%)
12	U10	M	404	-	63,63,63	0.15	0	76,79,79	0.42	1 (1%)
9	A1EFU	I	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.90	20 (44%)
8	BCL	P	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.19	25 (32%)
9	A1EFU	D	104	-	40,42,42	1.70	9 (22%)	45,52,52	3.72	19 (42%)
9	A1EFU	v	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.87	20 (44%)
9	A1EFU	K	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.66	20 (44%)
10	MW9	Q	104	-	44,44,52	1.48	5 (11%)	47,50,58	1.52	3 (6%)
8	BCL	r	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.22	26 (33%)
8	BCL	P	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.27	26 (33%)
8	BCL	e	102	-	64,74,74	1.72	11 (17%)	78,115,115	2.25	26 (33%)
8	BCL	I	102	-	64,74,74	1.72	11 (17%)	78,115,115	2.31	27 (34%)
8	BCL	s	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.24	27 (34%)
10	MW9	G	103	-	48,48,52	1.49	6 (12%)	51,54,58	1.48	4 (7%)
8	BCL	F	102	-	64,74,74	1.74	10 (15%)	78,115,115	2.27	28 (35%)
9	A1EFU	S	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.84	20 (44%)
8	BCL	D	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.24	28 (35%)
13	LMT	L	301	-	36,36,36	1.16	5 (13%)	47,47,47	0.96	1 (2%)
13	LMT	L	307	-	24,24,36	1.03	2 (8%)	29,29,47	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MW9	I	104	-	39,39,52	1.43	5 (12%)	42,45,58	1.17	3 (7%)
8	BCL	n	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.21	27 (34%)
8	BCL	J	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.28	27 (34%)
8	BCL	A	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.19	26 (33%)
9	A1EFU	1	104	-	40,42,42	1.71	9 (22%)	45,52,52	3.61	21 (46%)
10	MW9	H	302	-	36,36,52	1.57	8 (22%)	39,41,58	1.87	3 (7%)
9	A1EFU	d	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.75	20 (44%)
9	A1EFU	R	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.73	20 (44%)
9	A1EFU	2	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.76	20 (44%)
9	A1EFU	J	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.64	20 (44%)
9	A1EFU	v	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.72	20 (44%)
8	BCL	b	101	-	64,74,74	1.72	10 (15%)	78,115,115	2.24	25 (32%)
16	HEC	C	403	7	32,50,50	1.99	4 (12%)	24,82,82	2.32	14 (58%)
9	A1EFU	B	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.75	20 (44%)
9	A1EFU	G	105	-	40,42,42	1.68	9 (22%)	45,52,52	3.96	20 (44%)
15	CDL	H	303	-	90,90,99	0.91	8 (8%)	96,102,111	1.12	4 (4%)
9	A1EFU	k	102	-	40,42,42	1.68	9 (22%)	45,52,52	3.88	19 (42%)
10	MW9	L	310	-	35,35,52	1.25	3 (8%)	38,41,58	1.14	2 (5%)
15	CDL	L	311	-	66,66,99	1.05	8 (12%)	72,78,111	1.16	4 (5%)
9	A1EFU	a	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.76	20 (44%)

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
8	BCL	t	101	-	-	13/37/137/137	-
9	A1EFU	N	102	-	-	23/50/51/51	-
9	A1EFU	2	102	-	-	25/50/51/51	-
13	LMT	C	404	-	-	5/15/35/61	0/1/1/2
8	BCL	v	101	-	-	20/37/137/137	-
8	BCL	L	303	-	-	16/37/137/137	-
8	BCL	T	102	-	-	10/37/137/137	-
8	BCL	G	102	-	-	15/37/137/137	-
8	BCL	k	101	-	-	9/37/137/137	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	E	101	-	-	12/37/137/137	-
14	BPH	L	302	-	-	10/37/105/105	0/5/6/6
16	HEC	C	401	7	-	4/10/54/54	-
12	U10	L	305	-	-	13/45/69/87	0/1/1/1
8	BCL	V	101	-	-	11/37/137/137	-
9	A1EFU	I	101	-	-	18/50/51/51	-
9	A1EFU	a	103	-	-	19/50/51/51	-
9	A1EFU	t	102	-	-	25/50/51/51	-
8	BCL	a	102	-	-	21/37/137/137	-
13	LMT	L	308	-	-	6/15/35/61	0/1/1/2
8	BCL	L	306	-	-	17/37/137/137	-
8	BCL	K	101	-	-	11/37/137/137	-
9	A1EFU	A	102	-	-	17/50/51/51	-
10	MW9	F	104	-	-	29/52/52/57	-
9	A1EFU	N	103	-	-	25/50/51/51	-
8	BCL	i	101	-	-	19/37/137/137	-
9	A1EFU	1	101	-	-	20/50/51/51	-
10	MW9	F	103	-	-	34/47/47/57	-
9	A1EFU	J	103	-	-	22/50/51/51	-
8	BCL	S	101	-	-	13/37/137/137	-
8	BCL	Q	101	-	-	18/37/137/137	-
8	BCL	1	103	-	-	9/37/137/137	-
10	MW9	D	103	-	-	28/57/57/57	-
10	MW9	M	406	-	-	33/57/57/57	-
8	BCL	B	101	-	-	16/37/137/137	-
8	BCL	d	101	-	-	25/37/137/137	-
8	BCL	1	102	-	-	19/37/137/137	-
10	MW9	M	405	-	-	33/53/53/57	-
8	BCL	q	101	-	-	16/37/137/137	-
9	A1EFU	T	101	-	-	25/50/51/51	-
9	A1EFU	Q	103	-	-	19/50/51/51	-
8	BCL	M	402	-	-	11/37/137/137	-
9	A1EFU	Q	102	-	-	18/50/51/51	-
13	LMT	H	301	-	-	6/15/35/61	0/1/1/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	N	101	-	-	11/37/137/137	-
8	BCL	M	403	-	-	17/37/137/137	-
9	A1EFU	E	102	-	-	19/50/51/51	-
8	BCL	R	102	-	-	14/37/137/137	-
9	A1EFU	F	105	-	-	20/50/51/51	-
8	BCL	j	101	-	-	15/37/137/137	-
9	A1EFU	e	101	-	-	15/50/51/51	-
10	MW9	D	102	-	-	19/28/28/57	-
9	A1EFU	G	104	-	-	24/50/51/51	-
9	A1EFU	s	102	-	-	25/50/51/51	-
9	A1EFU	D	105	-	-	19/50/51/51	-
9	A1EFU	r	102	-	-	22/50/51/51	-
8	BCL	G	101	-	-	14/37/137/137	-
10	MW9	L	309	-	-	19/41/41/57	-
14	BPH	L	304	-	-	8/37/105/105	0/5/6/6
16	HEC	C	402	7	-	3/10/54/54	-
8	BCL	F	101	-	-	10/37/137/137	-
9	A1EFU	M	407	-	-	21/50/51/51	-
12	U10	M	404	-	-	10/63/87/87	0/1/1/1
9	A1EFU	I	103	-	-	20/50/51/51	-
8	BCL	P	102	-	-	13/37/137/137	-
9	A1EFU	D	104	-	-	19/50/51/51	-
9	A1EFU	v	103	-	-	25/50/51/51	-
9	A1EFU	K	102	-	-	25/50/51/51	-
10	MW9	Q	104	-	-	25/49/49/57	-
8	BCL	r	101	-	-	12/37/137/137	-
8	BCL	P	101	-	-	10/37/137/137	-
8	BCL	e	102	-	-	11/37/137/137	-
8	BCL	I	102	-	-	10/37/137/137	-
8	BCL	s	101	-	-	21/37/137/137	-
10	MW9	G	103	-	-	24/53/53/57	-
8	BCL	F	102	-	-	9/37/137/137	-
9	A1EFU	S	102	-	-	18/50/51/51	-
8	BCL	D	101	-	-	15/37/137/137	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	LMT	L	301	-	-	9/21/61/61	0/2/2/2
13	LMT	L	307	-	-	5/15/35/61	0/1/1/2
10	MW9	I	104	-	-	29/44/44/57	-
8	BCL	n	101	-	-	12/37/137/137	-
8	BCL	J	101	-	-	14/37/137/137	-
8	BCL	A	101	-	-	16/37/137/137	-
9	A1EFU	1	104	-	-	21/50/51/51	-
10	MW9	H	302	-	-	22/38/38/57	-
9	A1EFU	d	102	-	-	17/50/51/51	-
9	A1EFU	R	101	-	-	19/50/51/51	-
9	A1EFU	2	101	-	-	18/50/51/51	-
9	A1EFU	J	102	-	-	19/50/51/51	-
9	A1EFU	v	102	-	-	19/50/51/51	-
8	BCL	b	101	-	-	13/37/137/137	-
16	HEC	C	403	7	-	2/10/54/54	-
9	A1EFU	B	102	-	-	15/50/51/51	-
9	A1EFU	G	105	-	-	21/50/51/51	-
15	CDL	H	303	-	-	40/101/101/110	-
9	A1EFU	k	102	-	-	24/50/51/51	-
10	MW9	L	310	-	-	28/40/40/57	-
15	CDL	L	311	-	-	36/77/77/110	-
9	A1EFU	a	101	-	-	15/50/51/51	-

The worst 5 of 853 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	402	HEC	C3C-C2C	-6.54	1.33	1.40
16	C	402	HEC	C2B-C3B	-6.36	1.34	1.40
8	t	101	BCL	MG-ND	-6.28	1.93	2.05
16	C	401	HEC	C2B-C3B	-6.27	1.34	1.40
16	C	403	HEC	C3C-C2C	-6.24	1.34	1.40

The worst 5 of 1799 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	k	102	A1EFU	C11-C10-C9	-10.75	111.97	127.31
9	Q	103	A1EFU	C16-C17-C18	-10.61	112.17	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	103	A1EFU	C15-C14-C13	-10.53	112.29	127.31
9	a	103	A1EFU	C7-C6-C5	-10.43	112.42	127.31
9	Q	102	A1EFU	C16-C17-C18	-10.32	112.58	127.31

There are no chirality outliers.

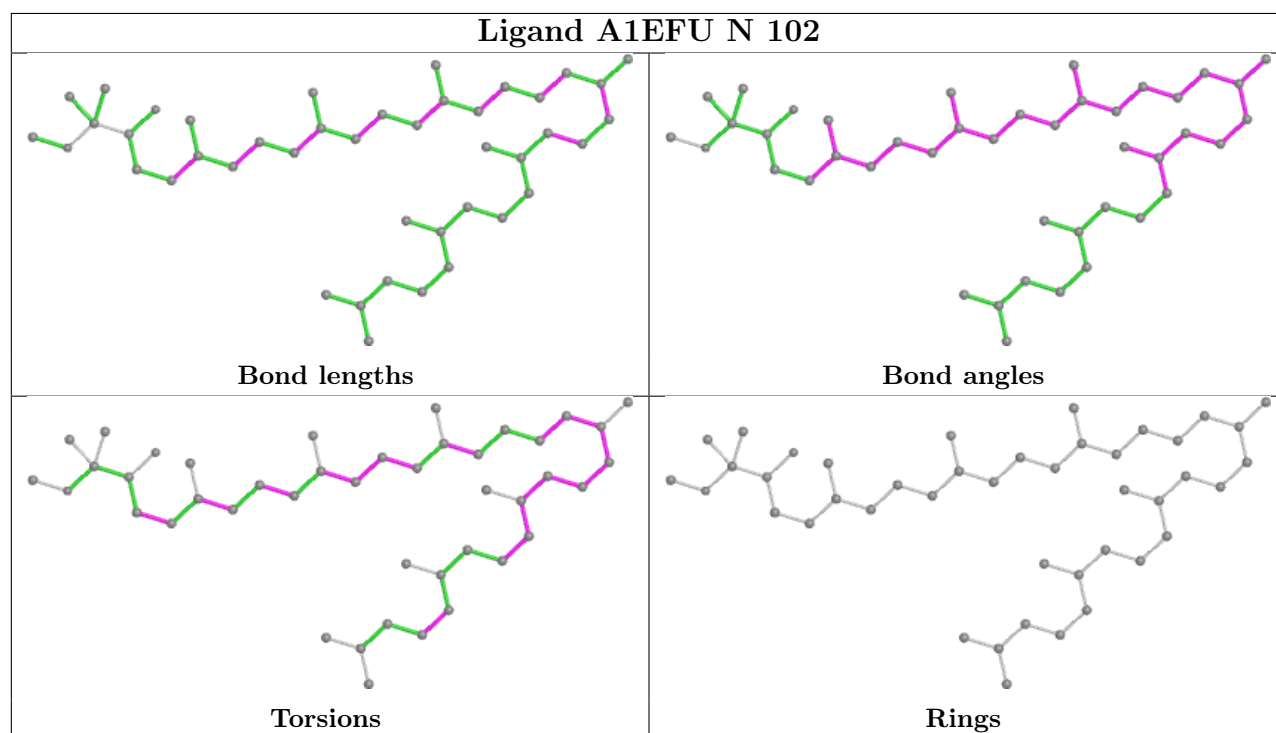
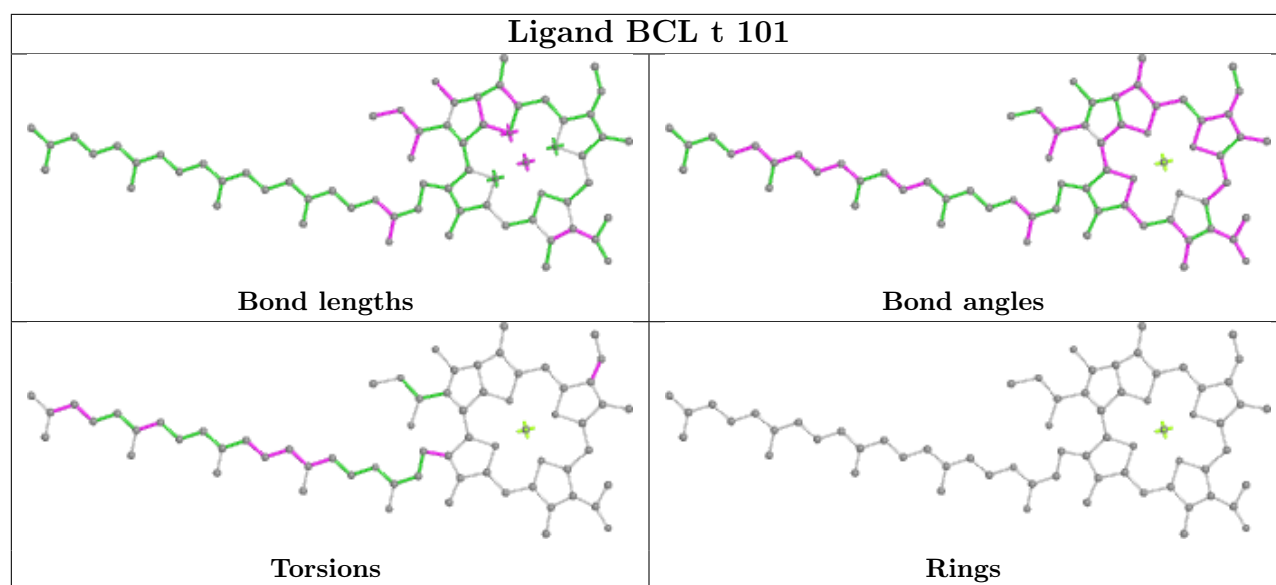
5 of 1734 torsion outliers are listed below:

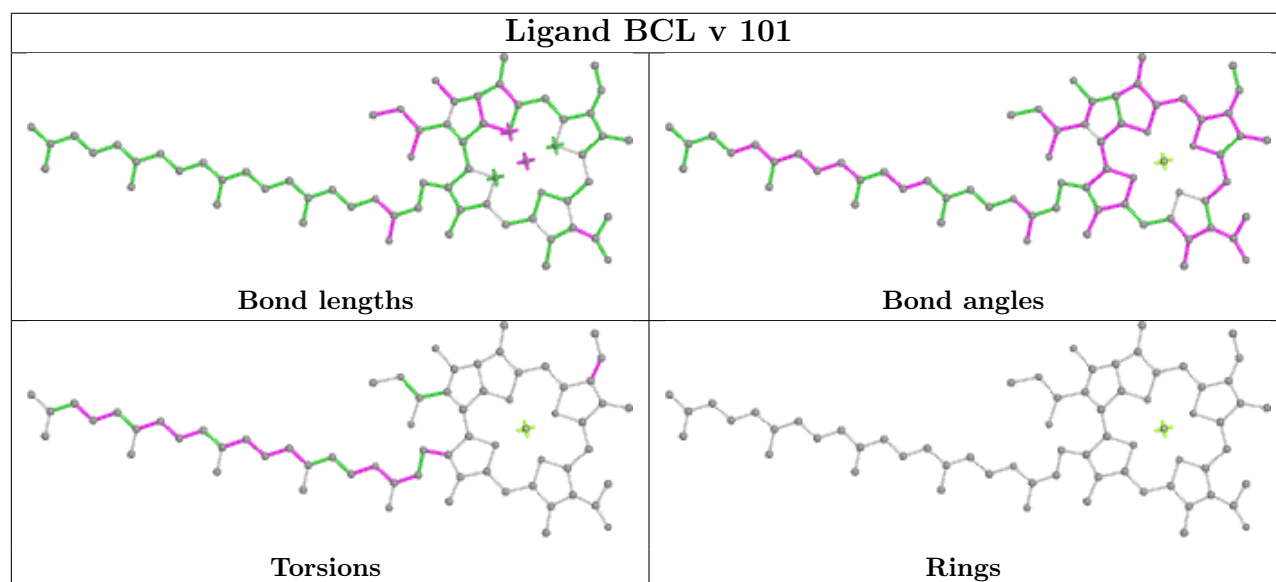
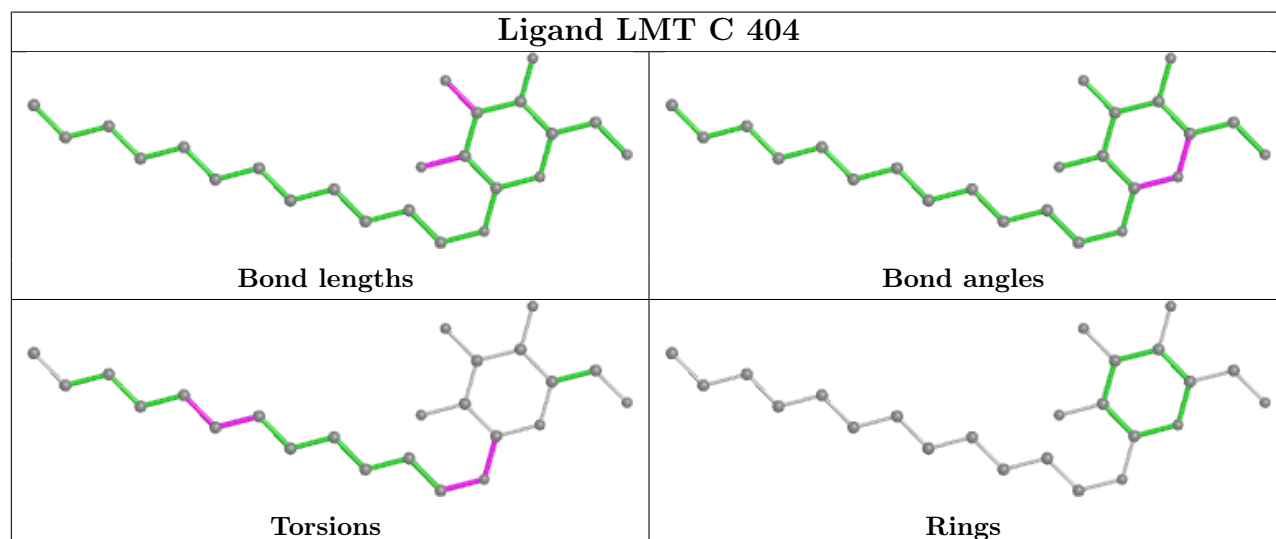
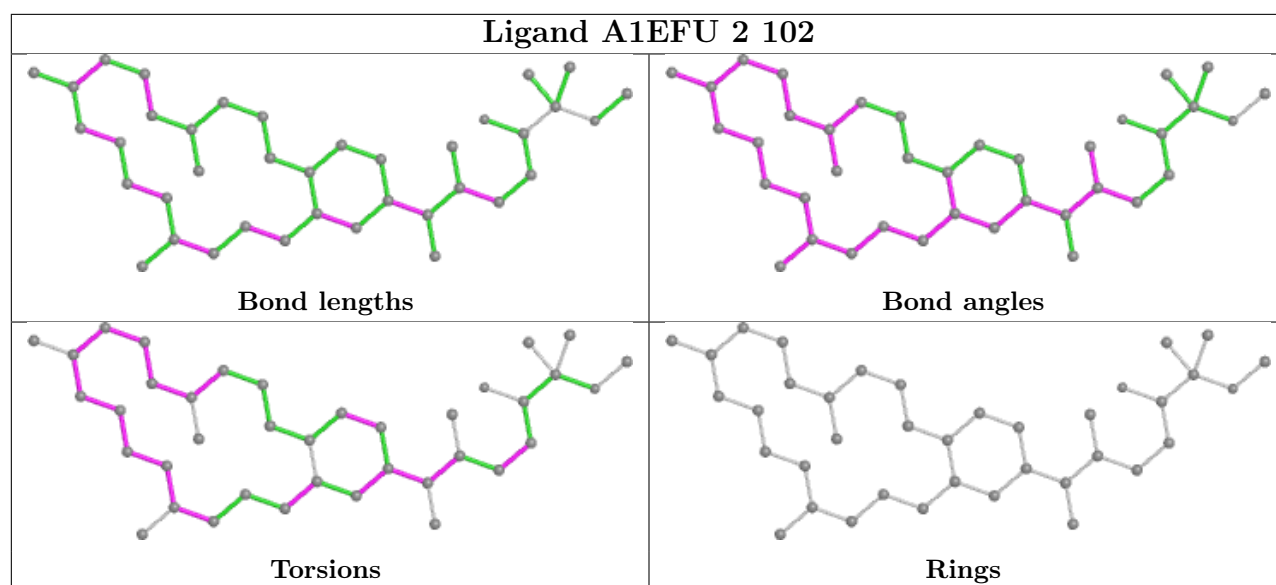
Mol	Chain	Res	Type	Atoms
8	P	101	BCL	C1A-C2A-CAA-CBA
8	P	101	BCL	C3A-C2A-CAA-CBA
8	P	101	BCL	C4C-C3C-CAC-CBC
8	P	102	BCL	C1-C2-C3-C4
8	V	101	BCL	C1A-C2A-CAA-CBA

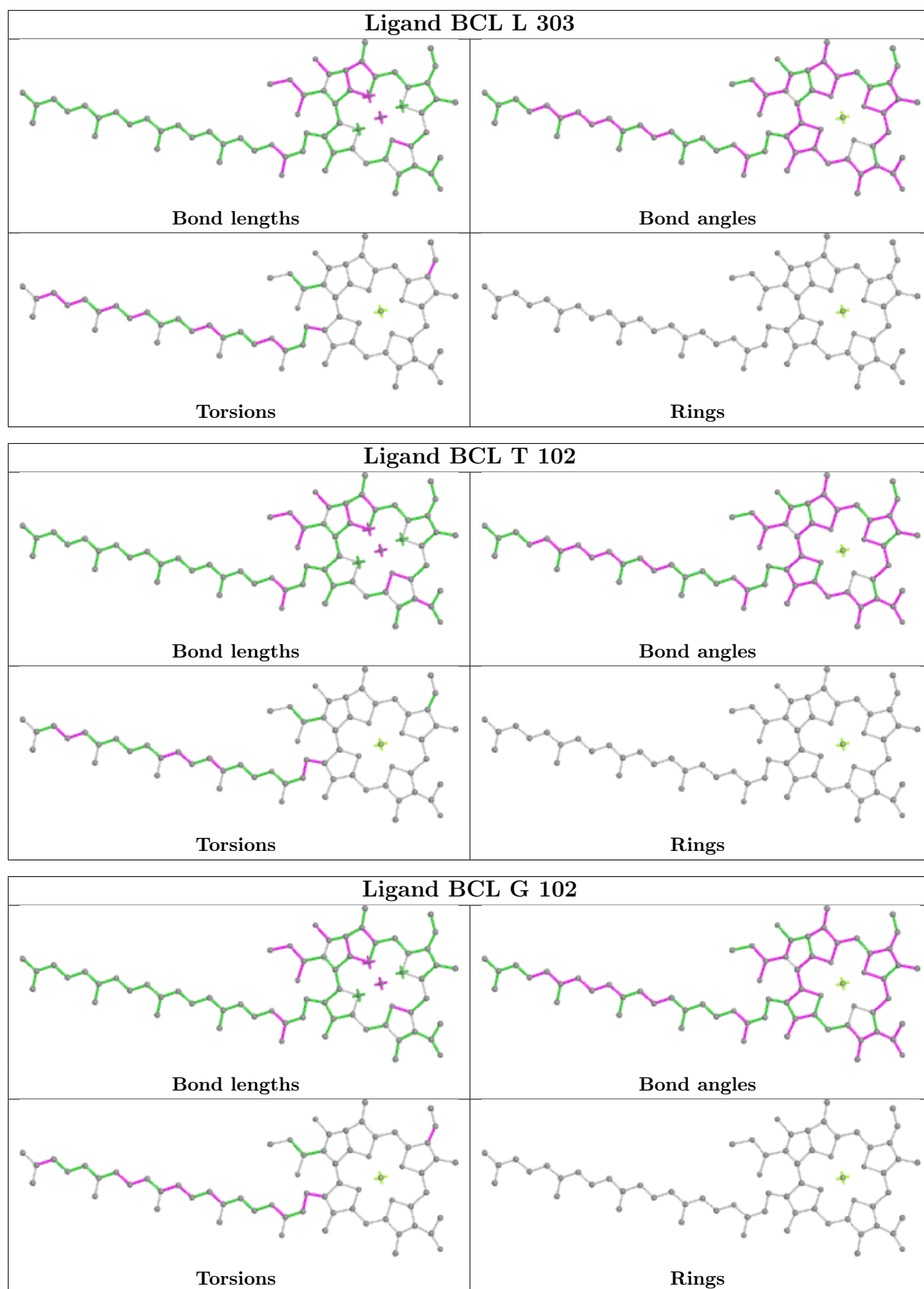
There are no ring outliers.

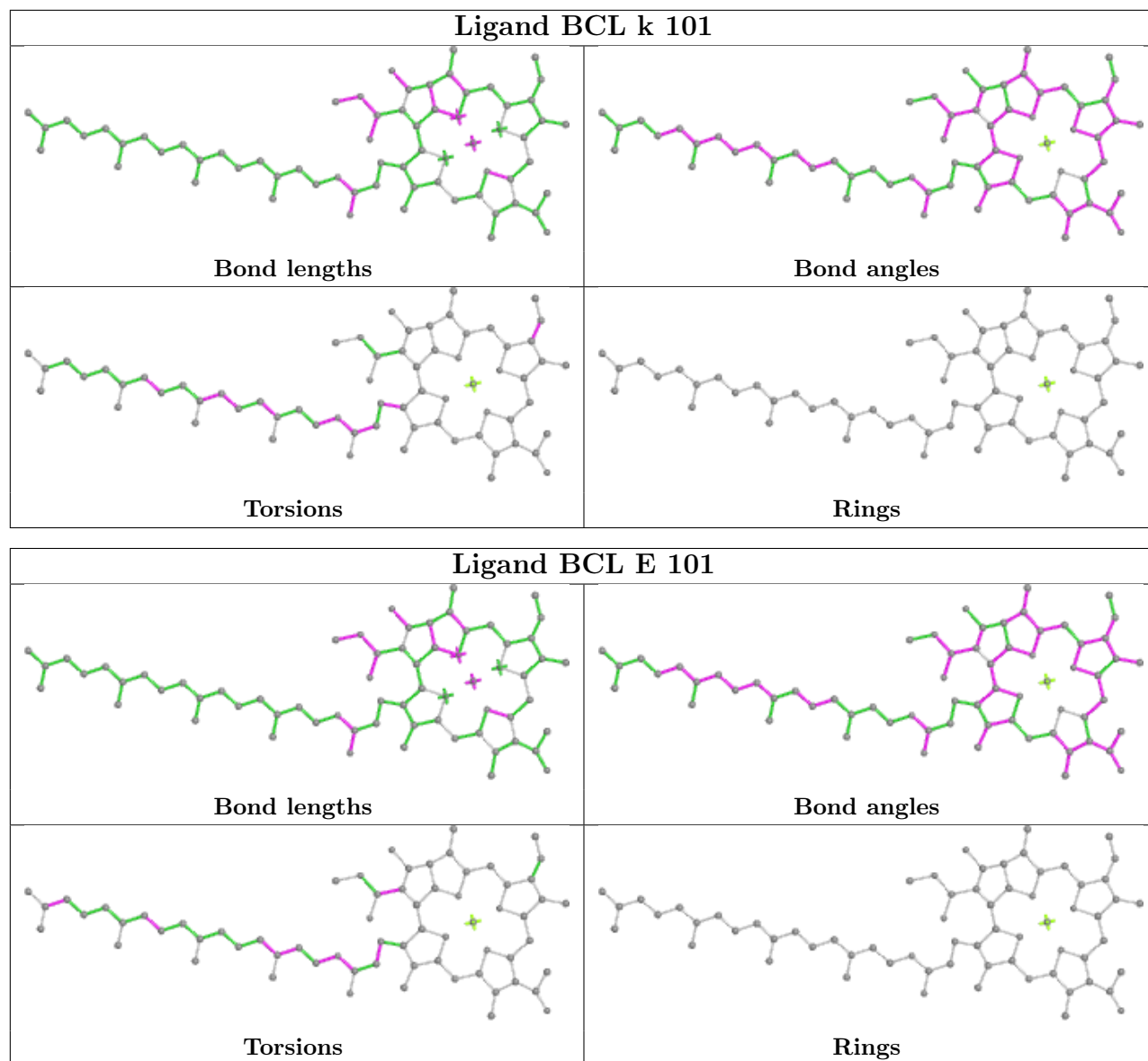
No monomer is involved in short contacts.

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.

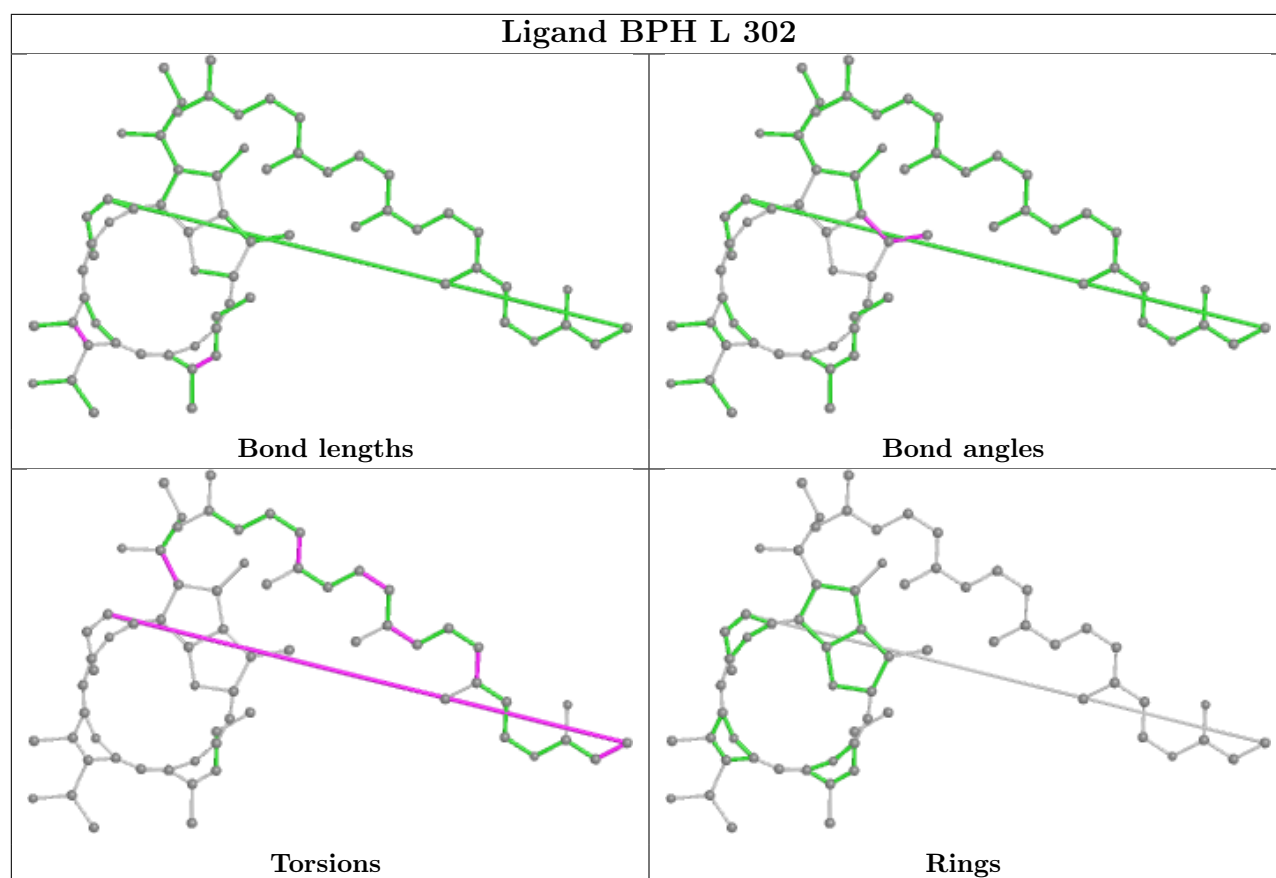




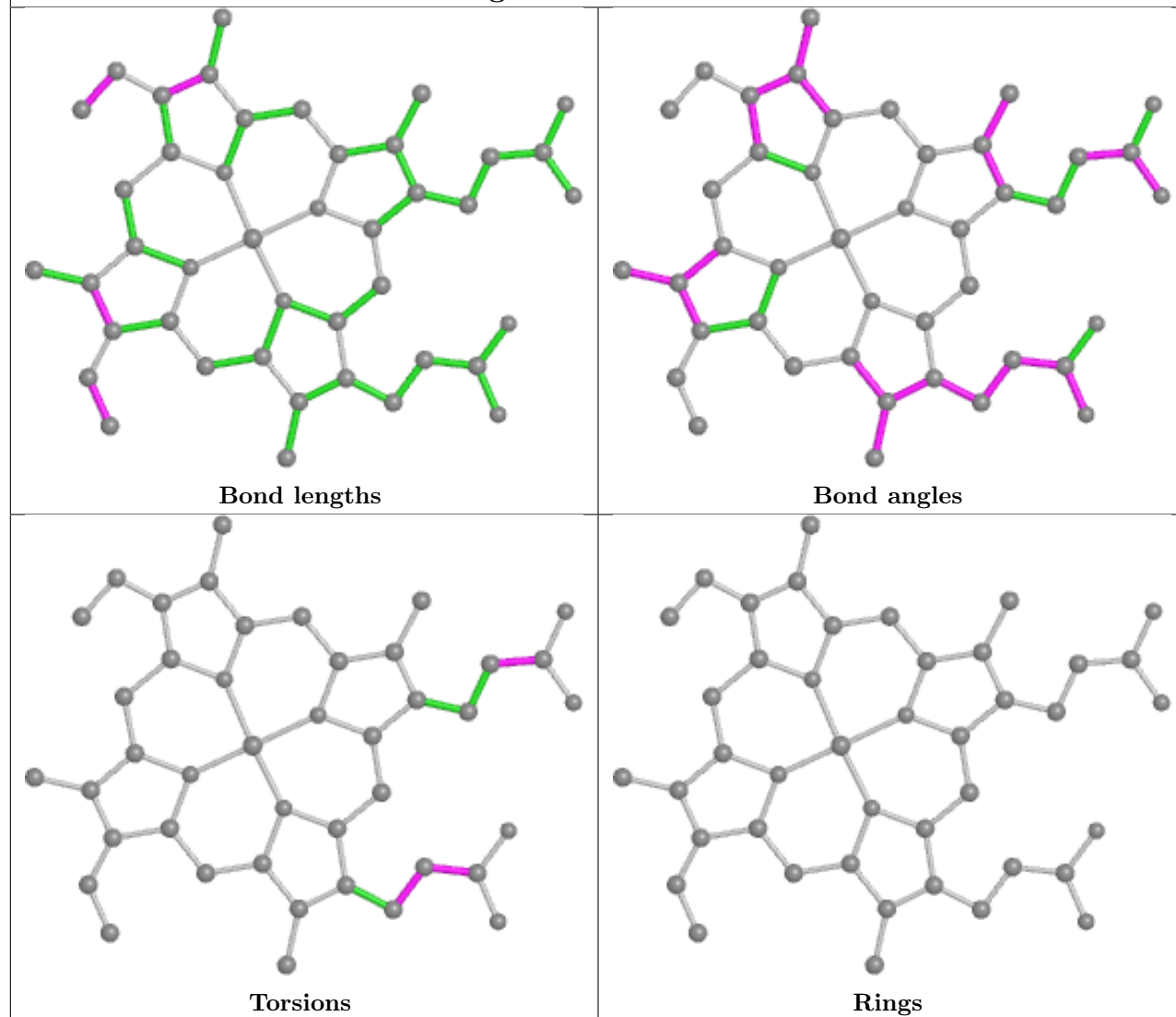




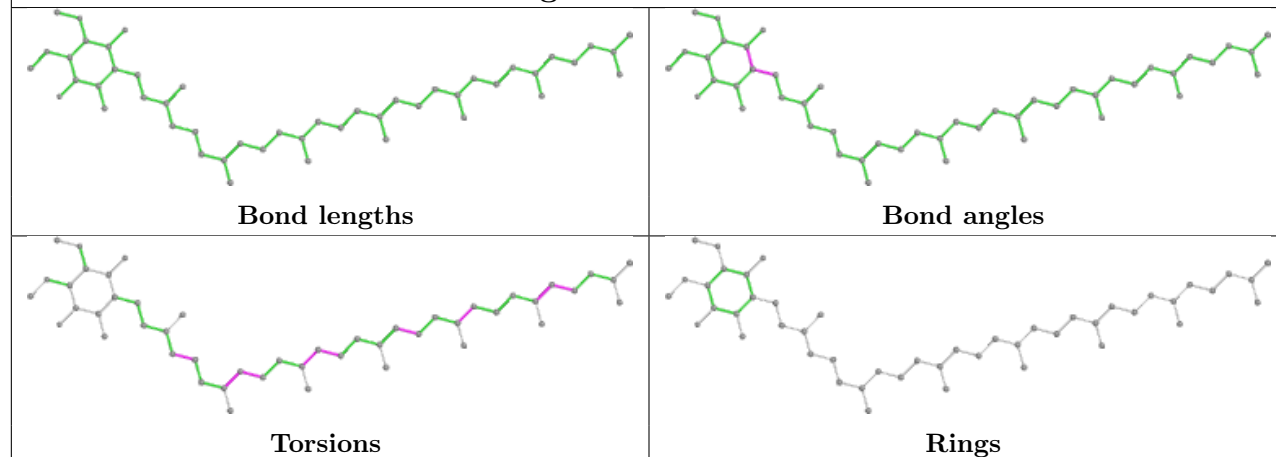


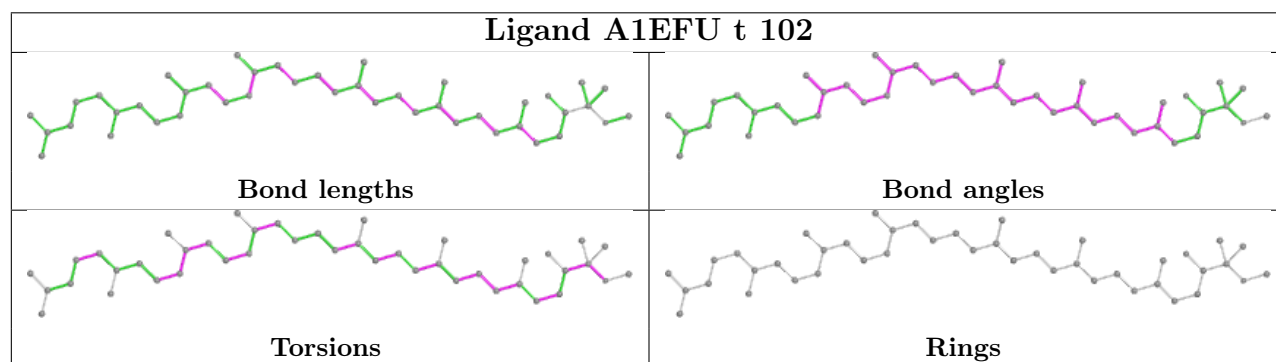
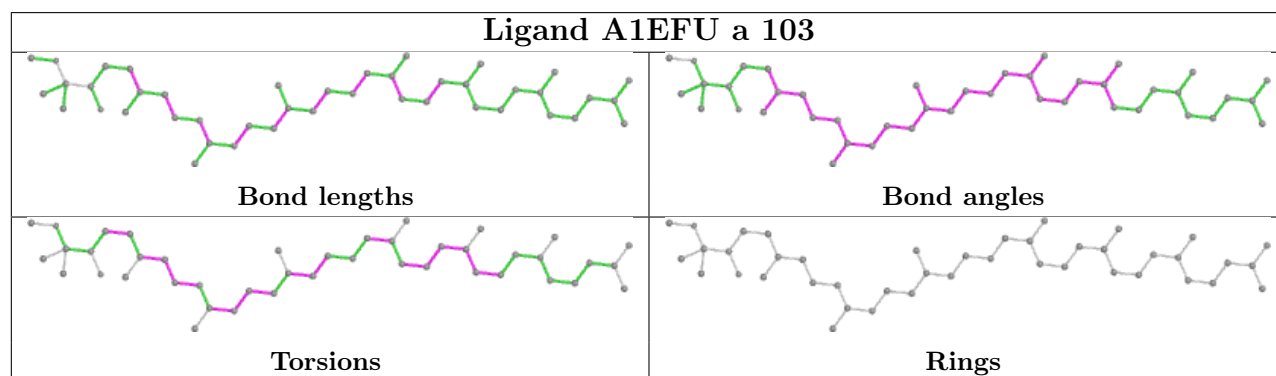
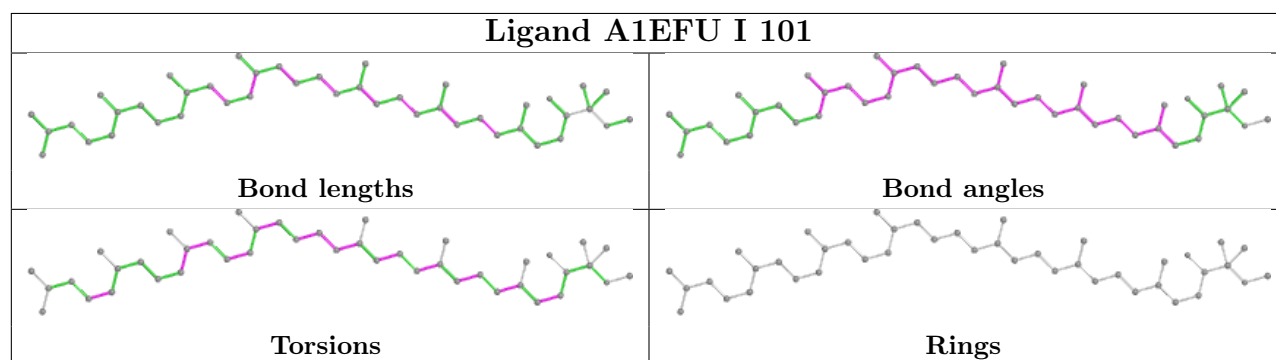
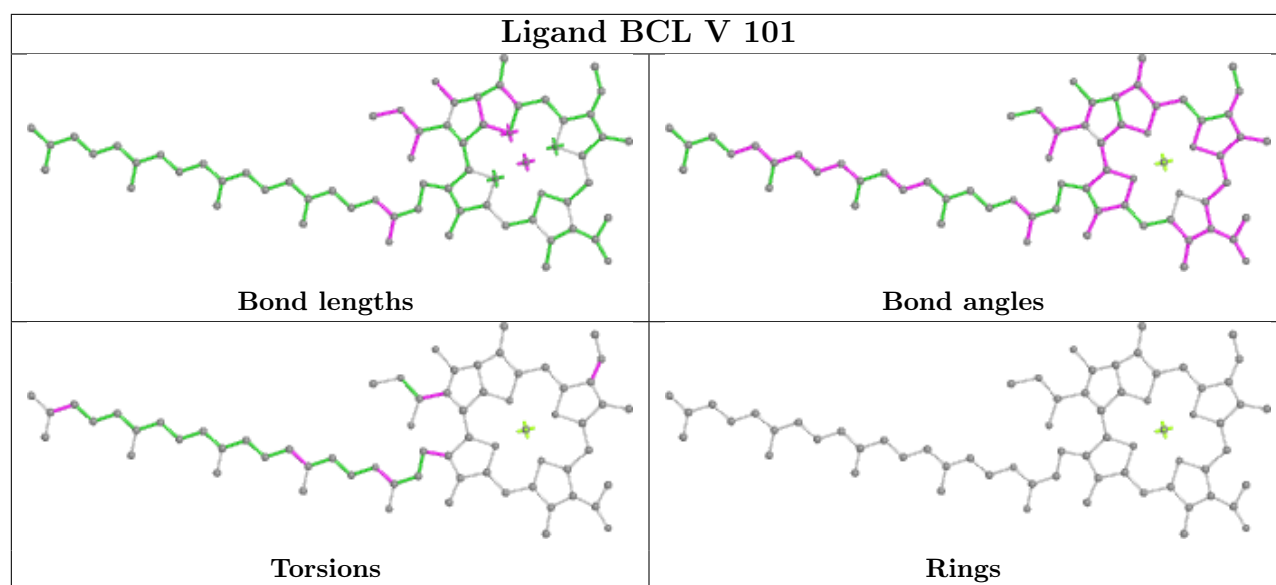


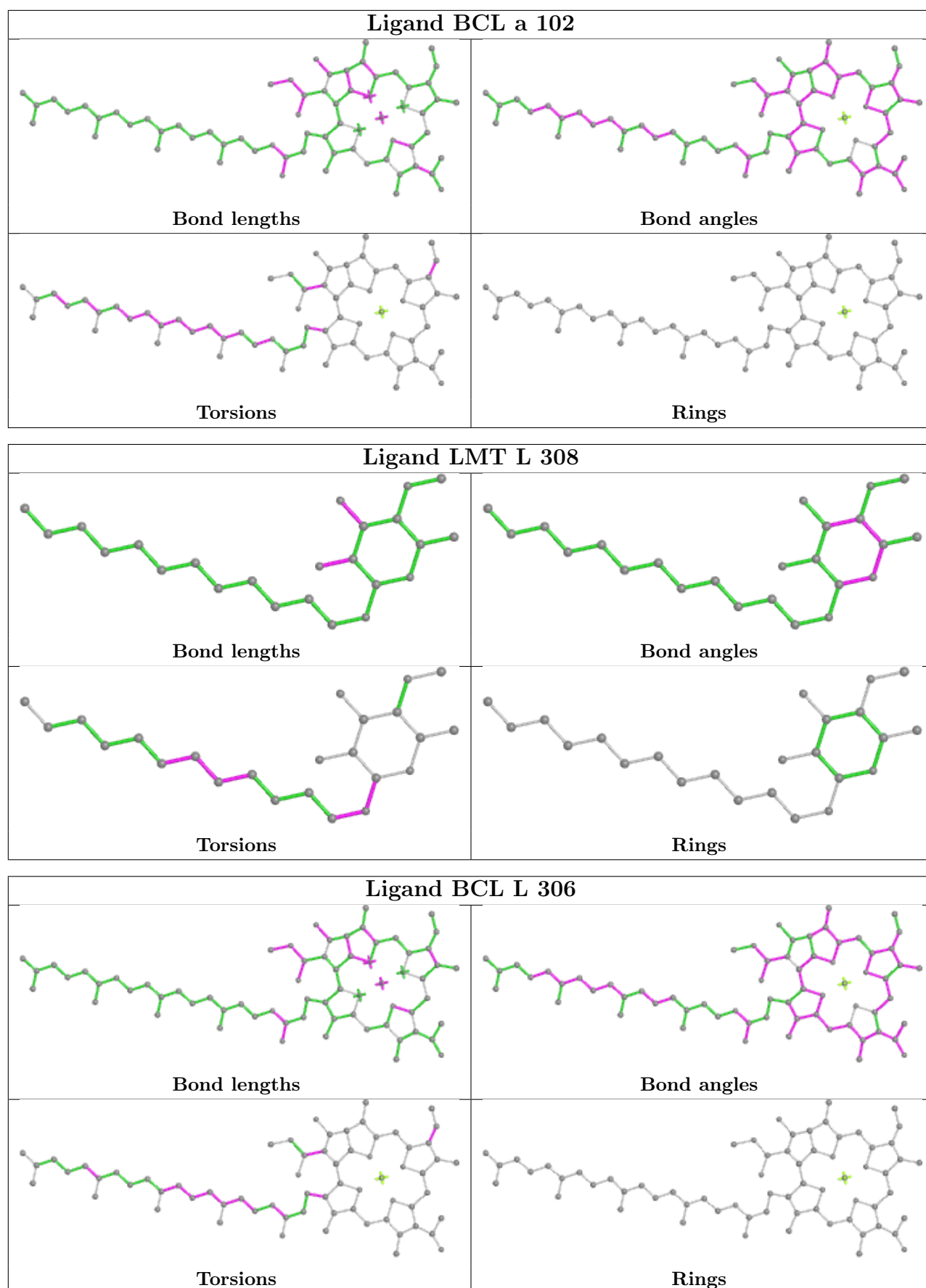
## Ligand HEC C 401

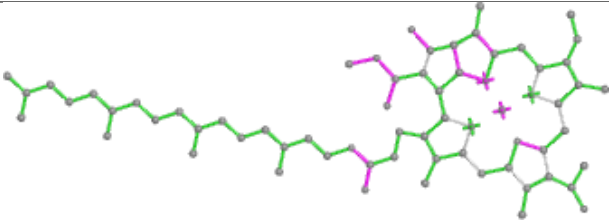
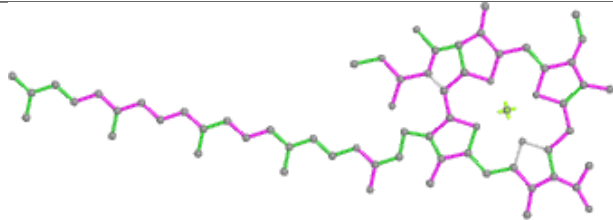
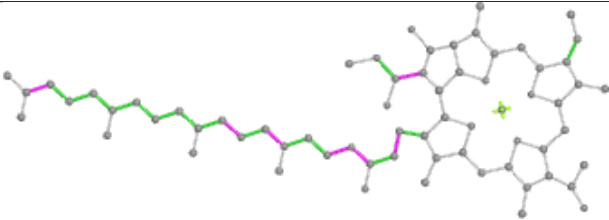
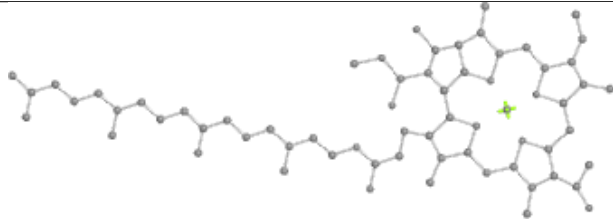


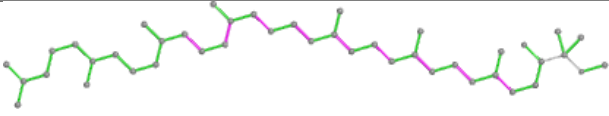
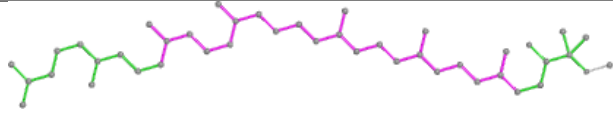
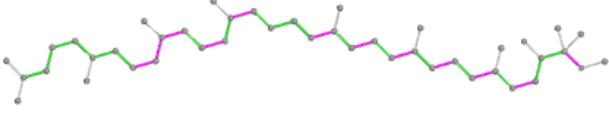
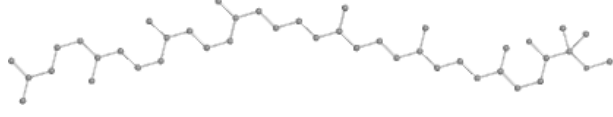
## Ligand U10 L 305

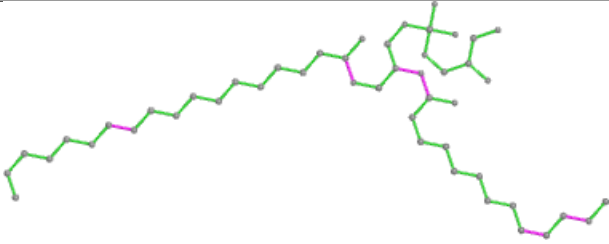
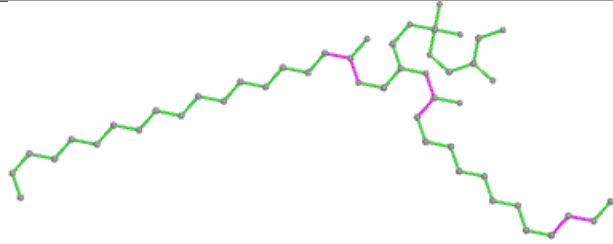
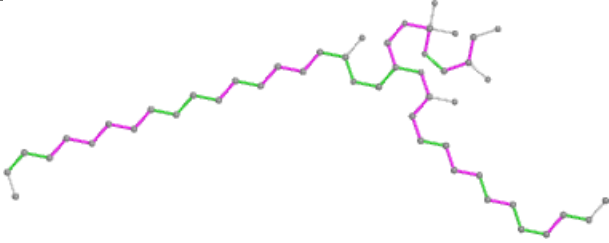
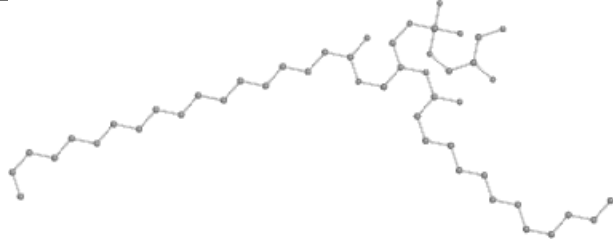


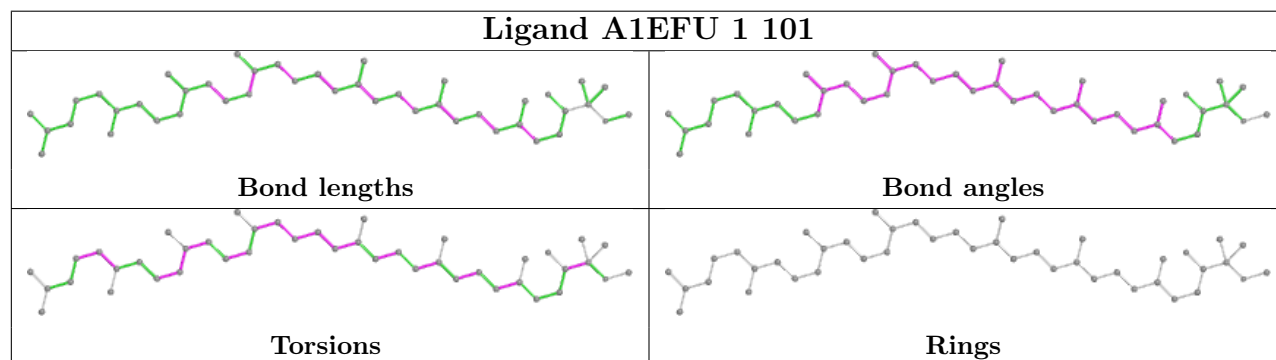
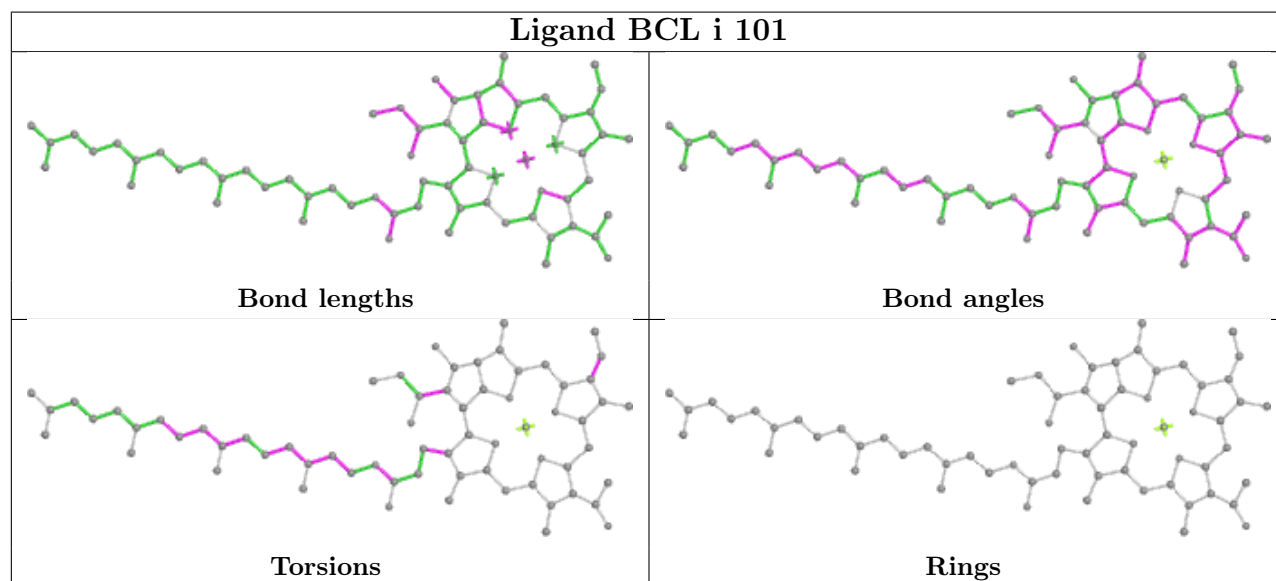
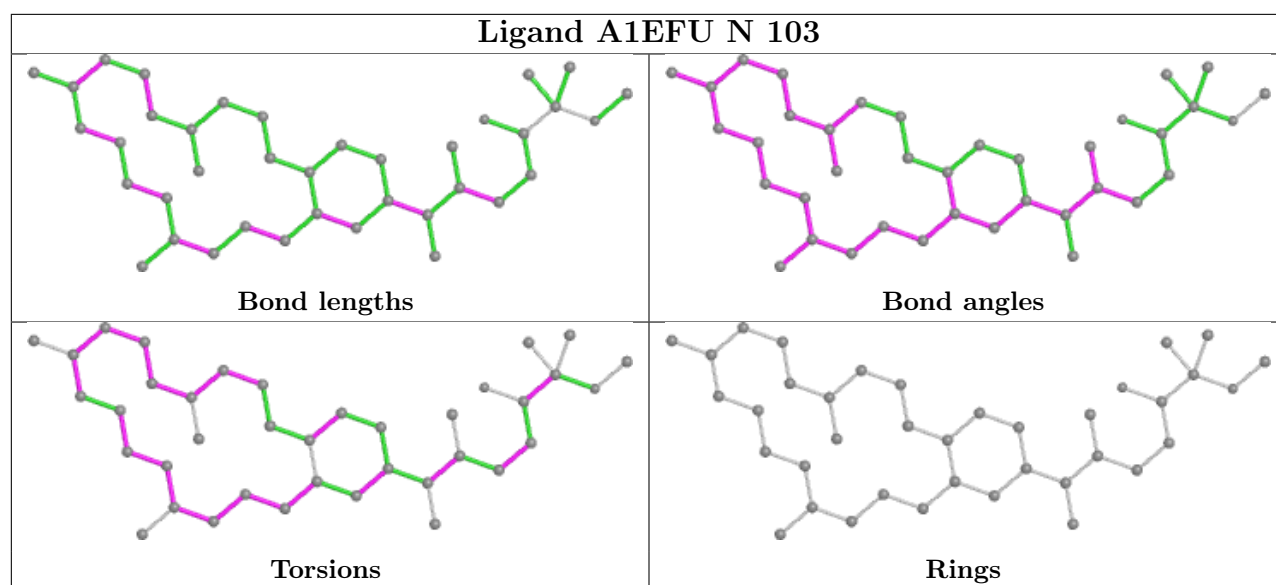


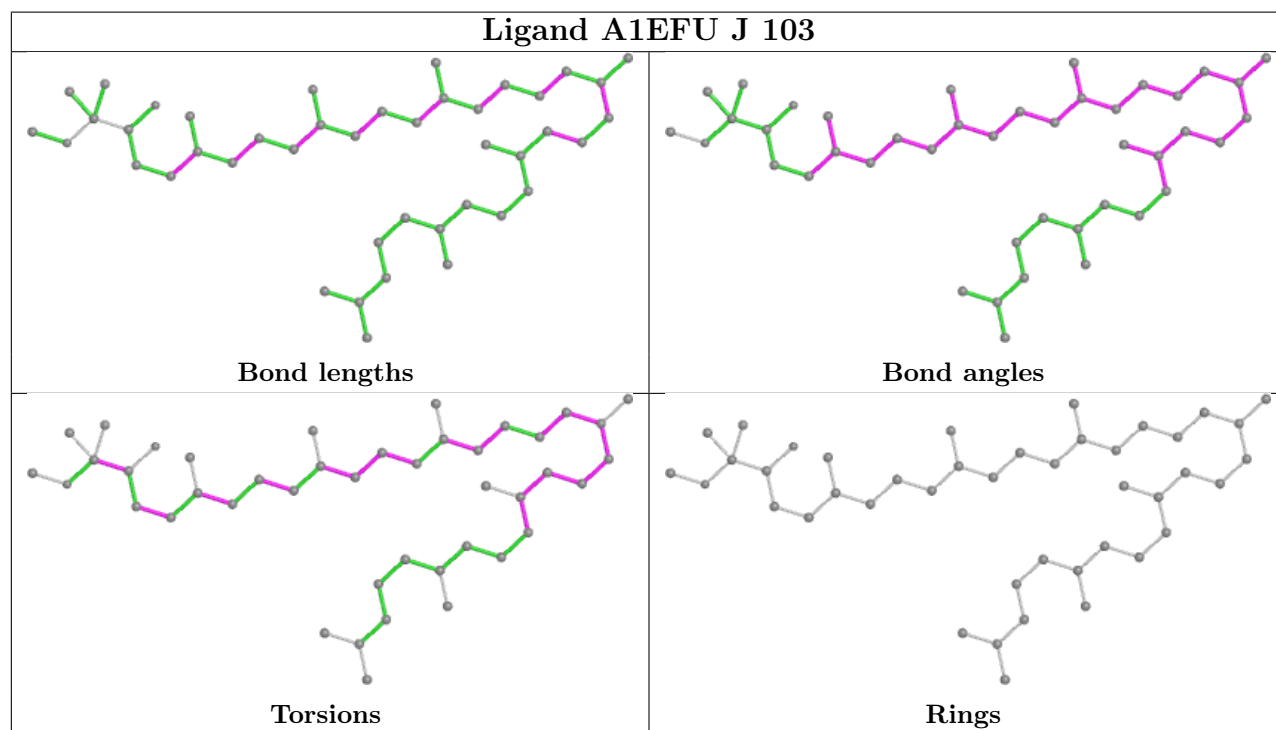
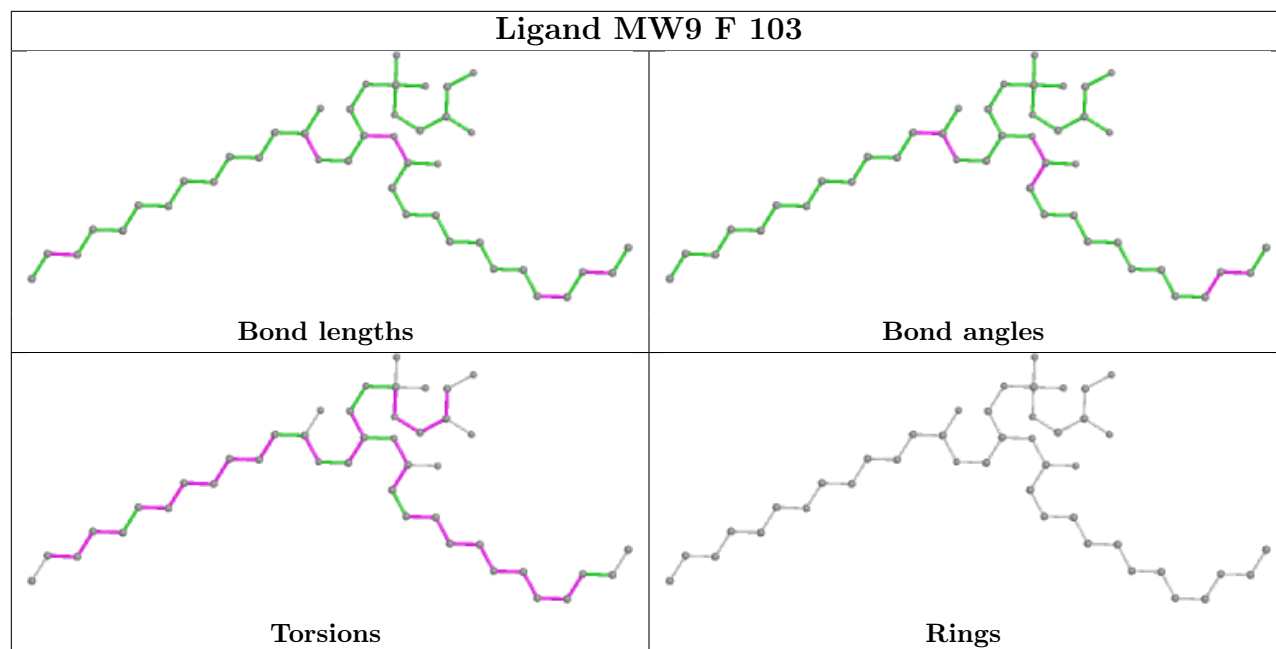


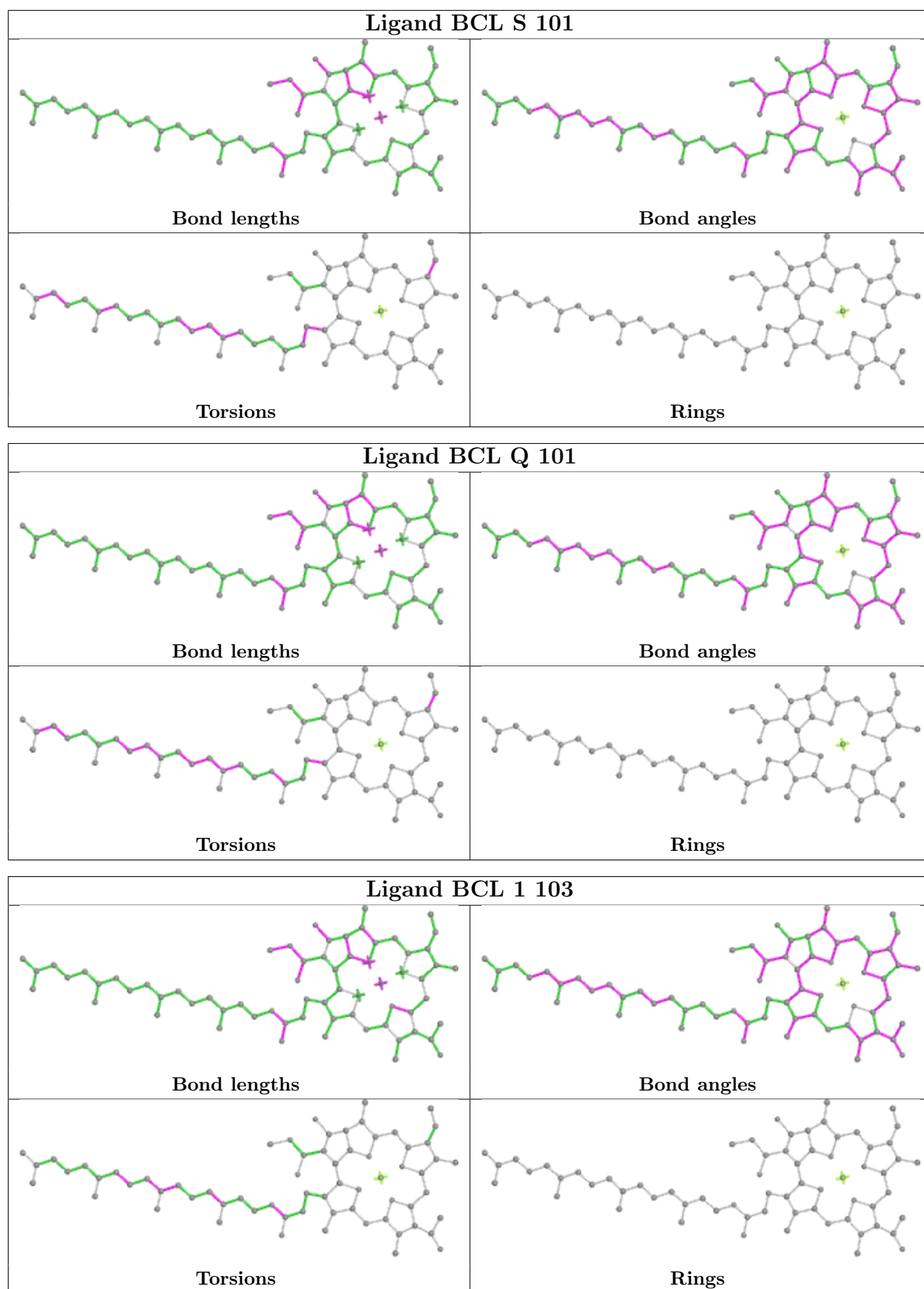
Ligand BCL K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EFU A 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

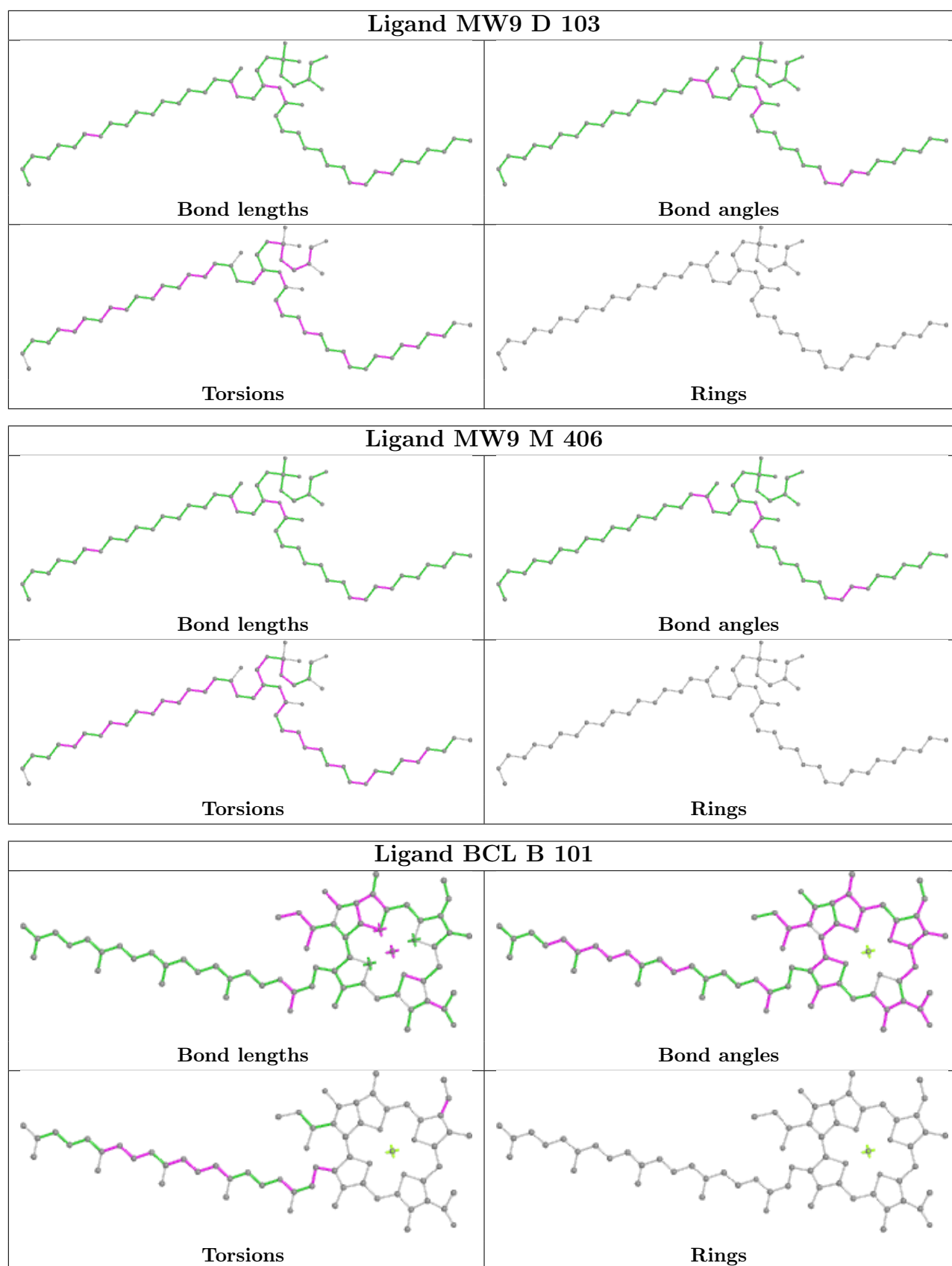
Ligand MW9 F 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

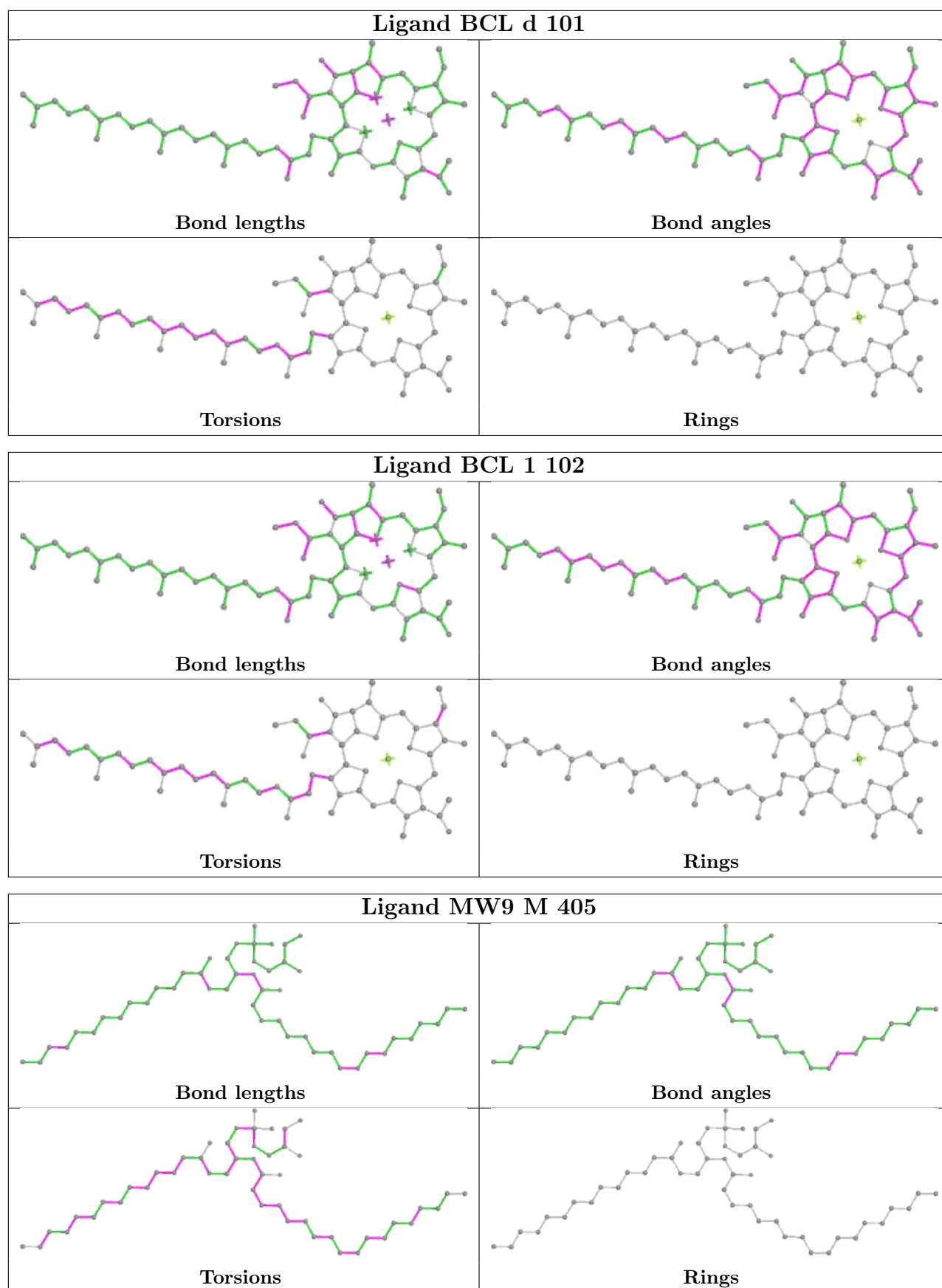


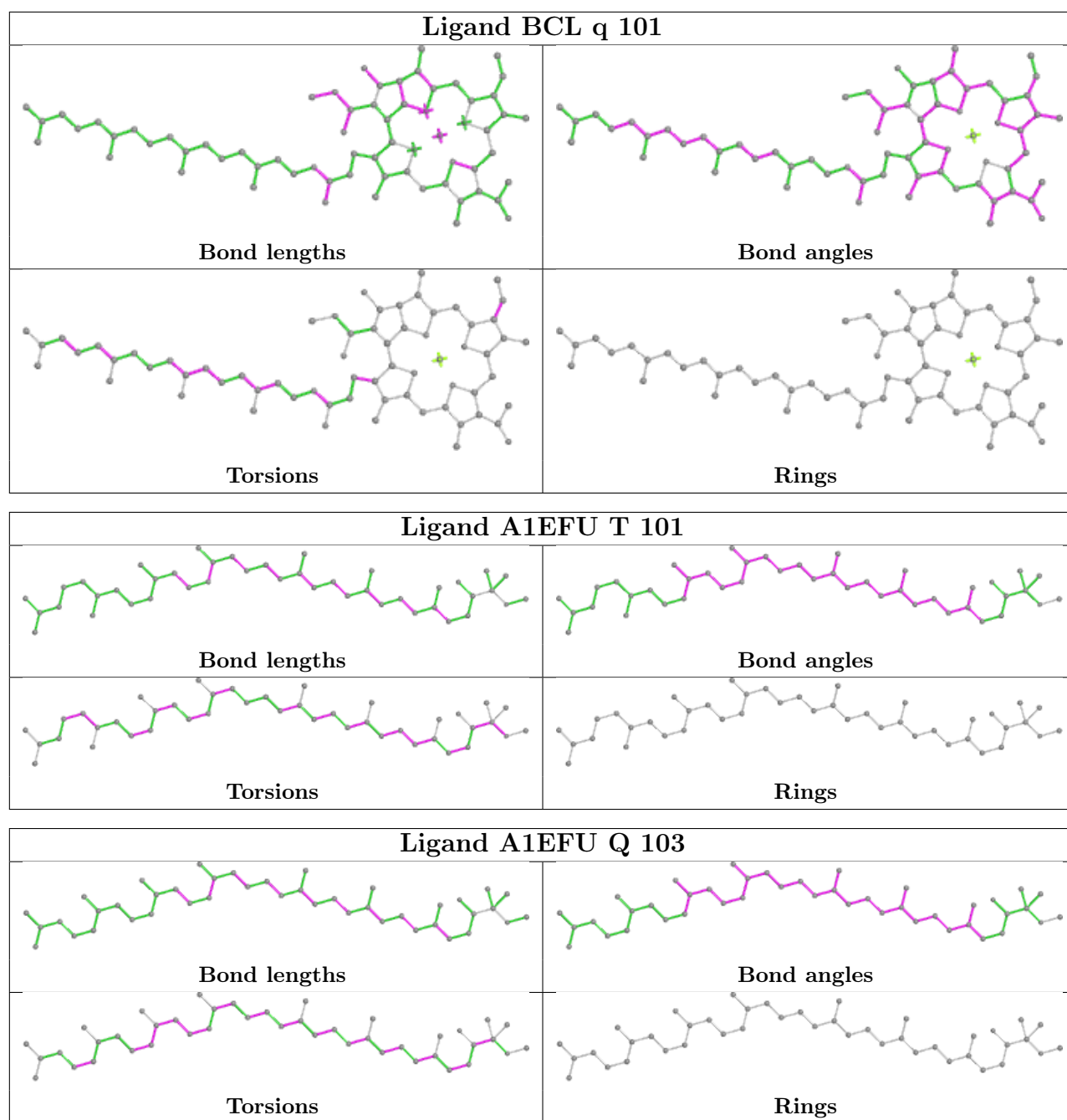


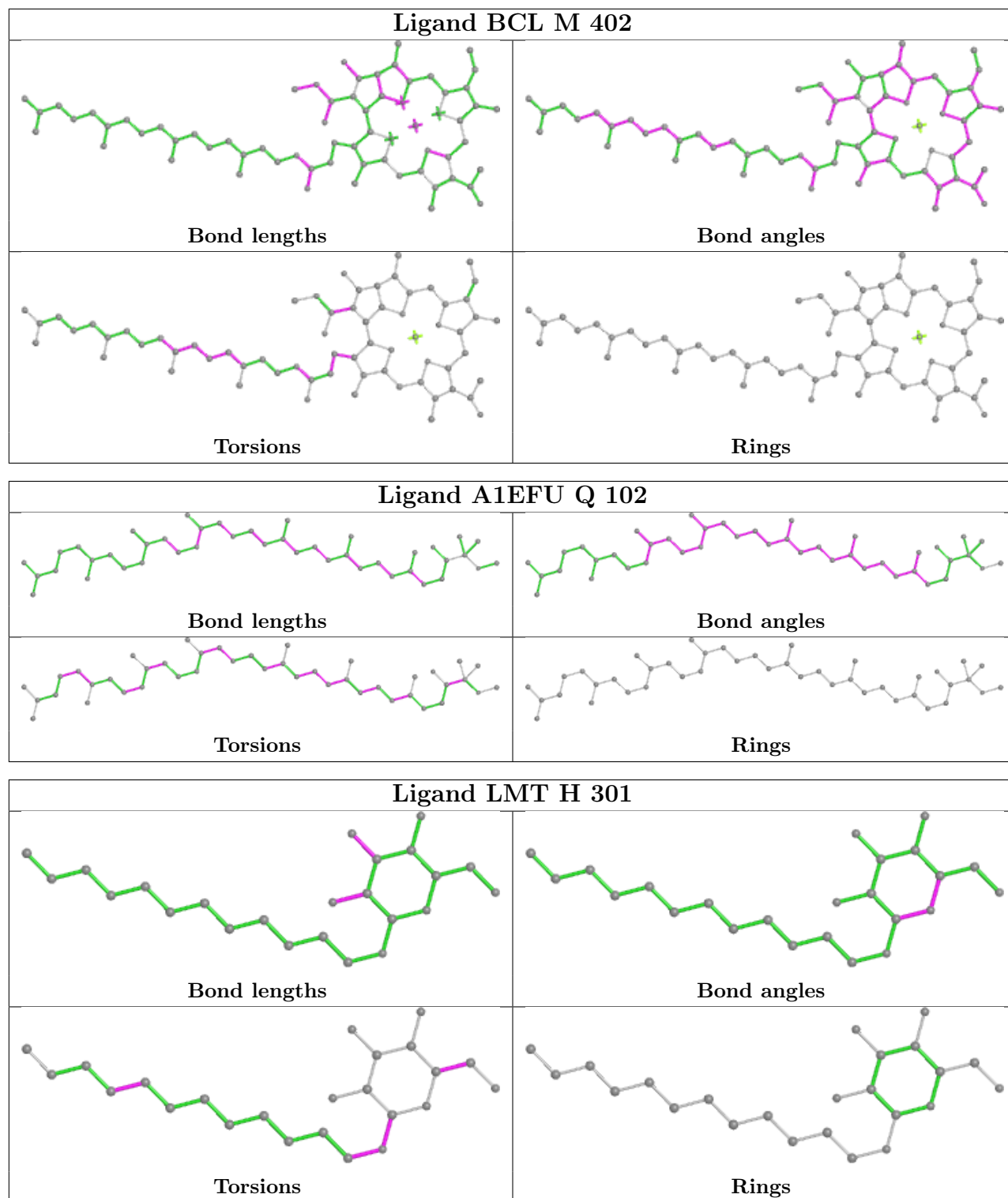


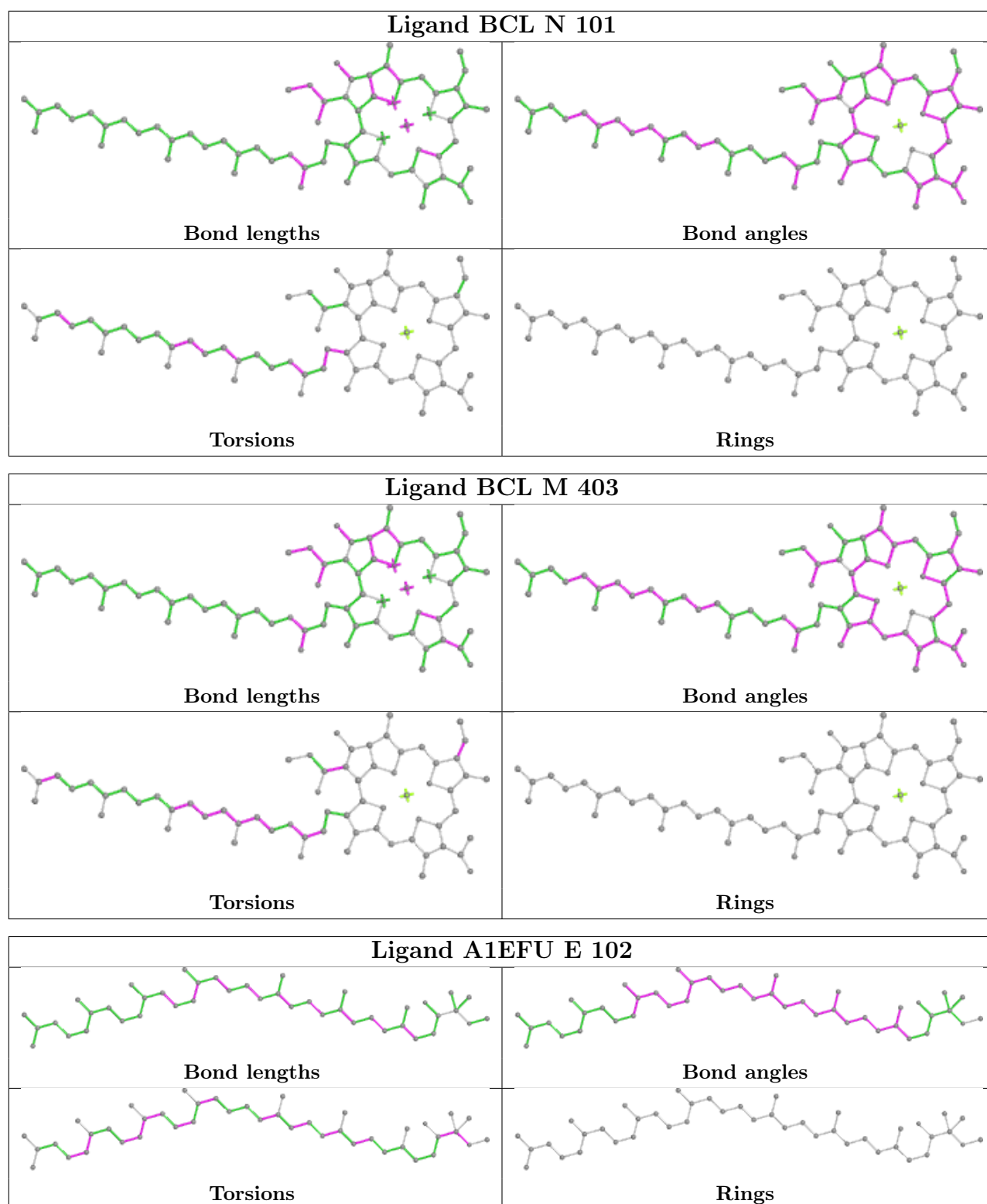


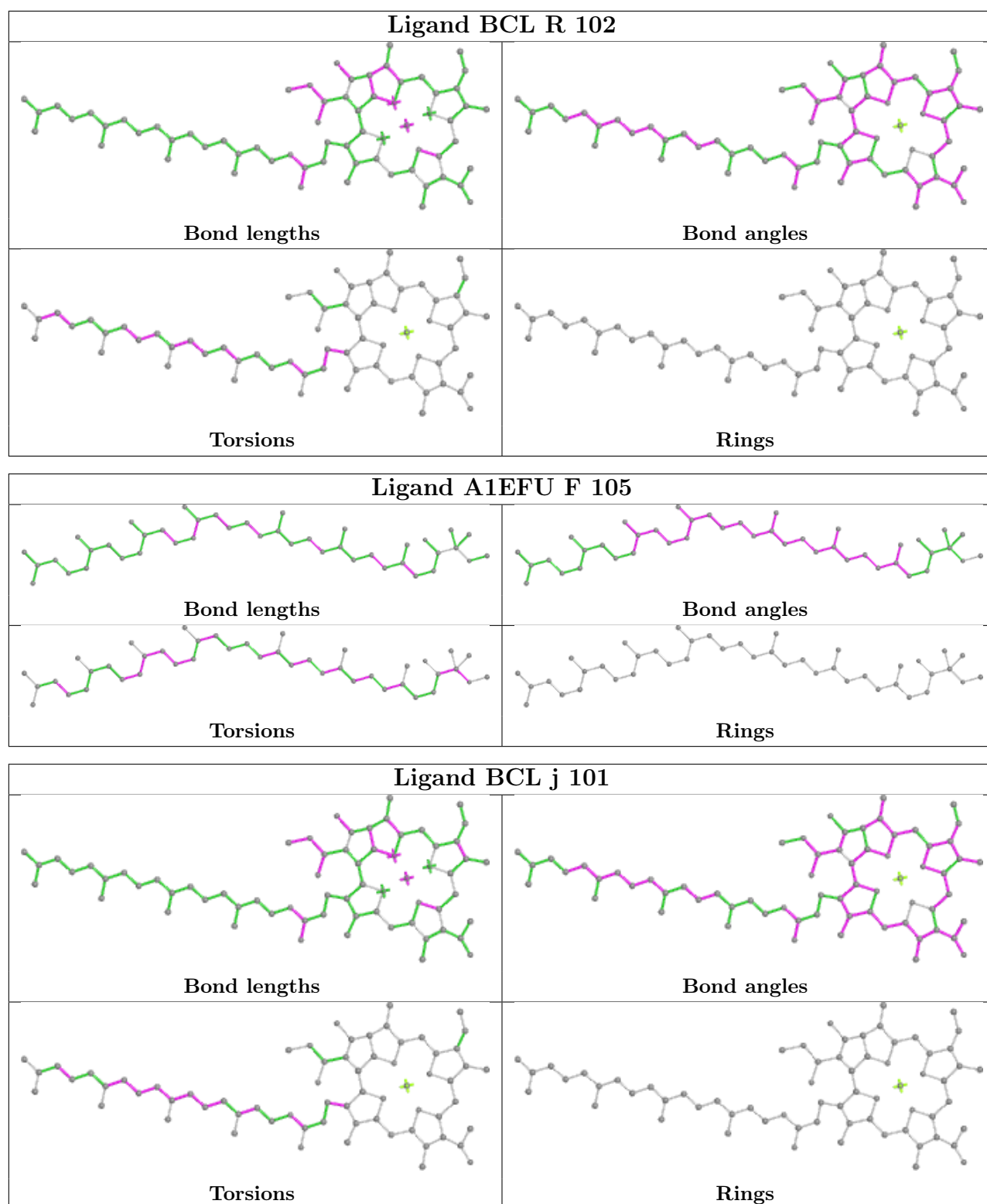


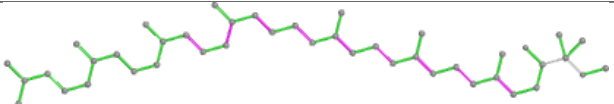
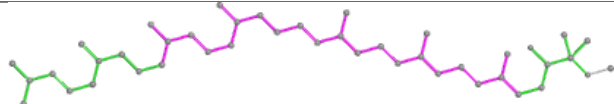
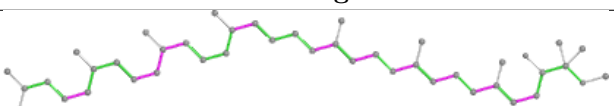




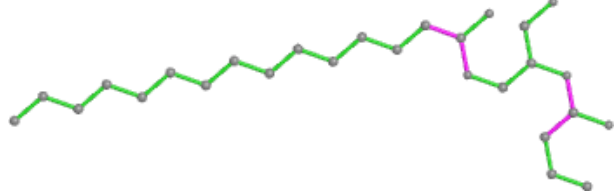
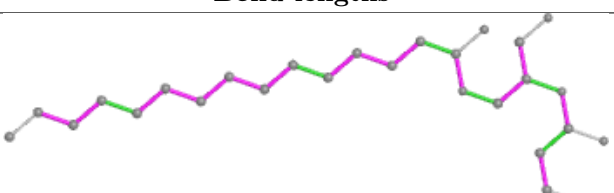



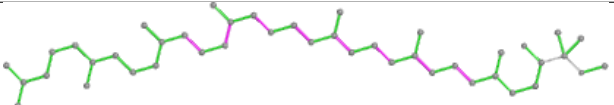
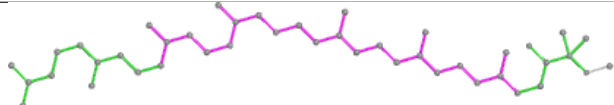
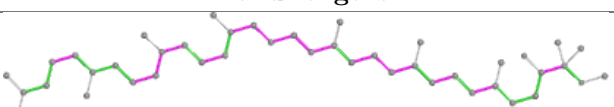
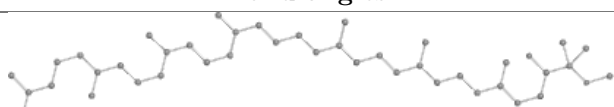


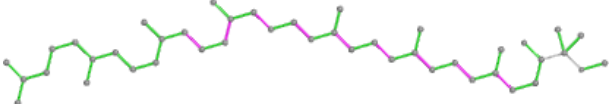
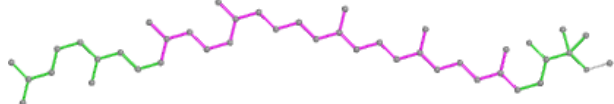
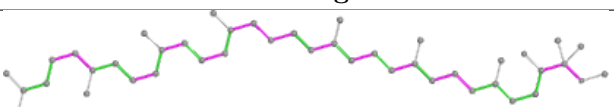
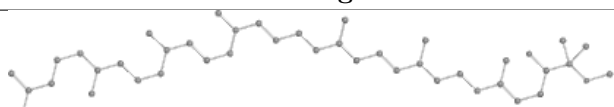


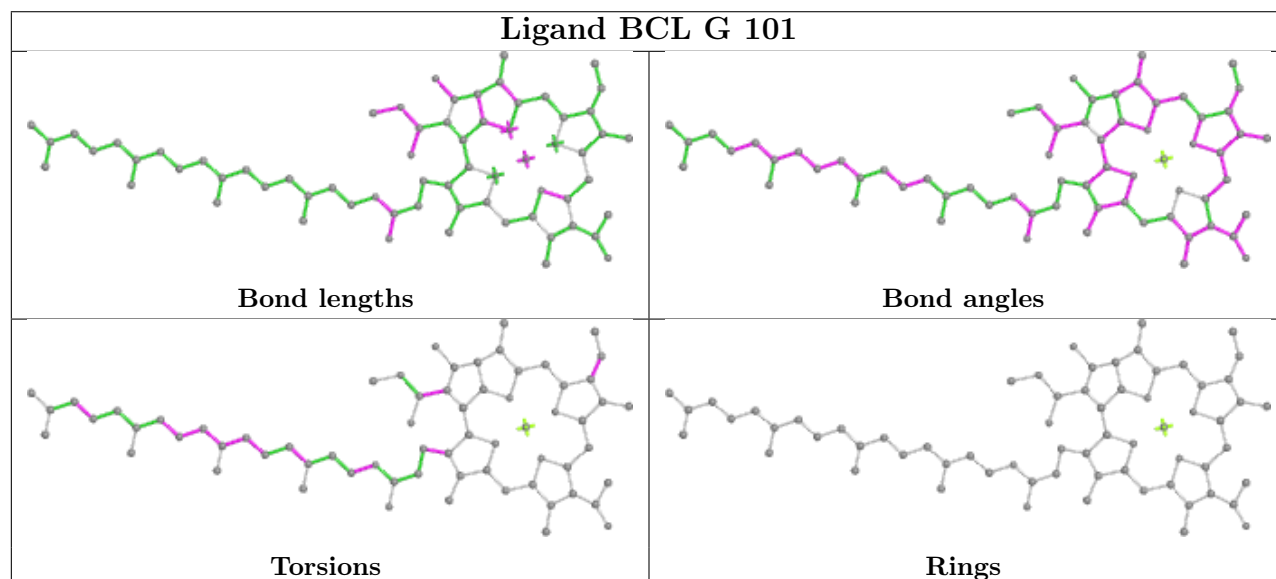
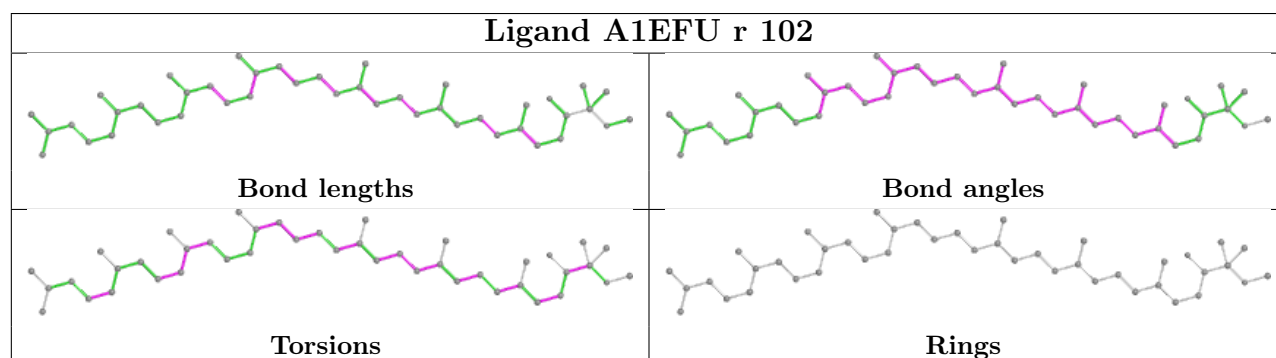
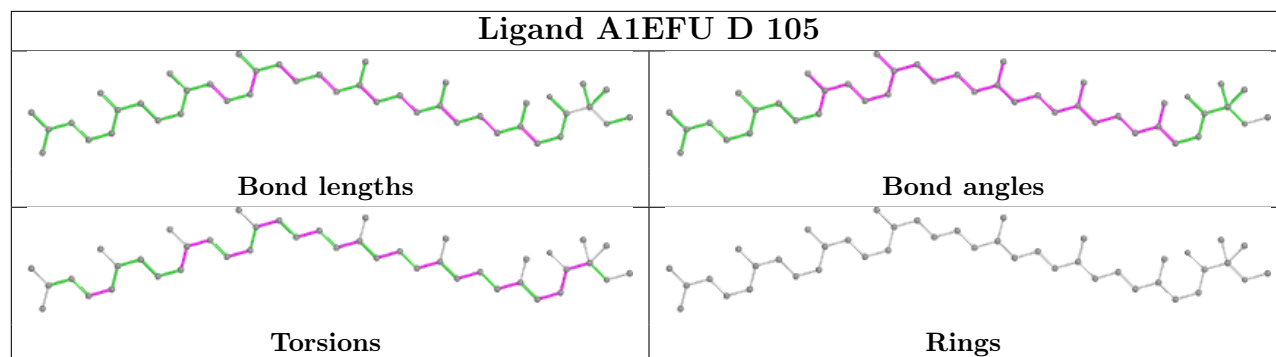


Ligand A1EFU e 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

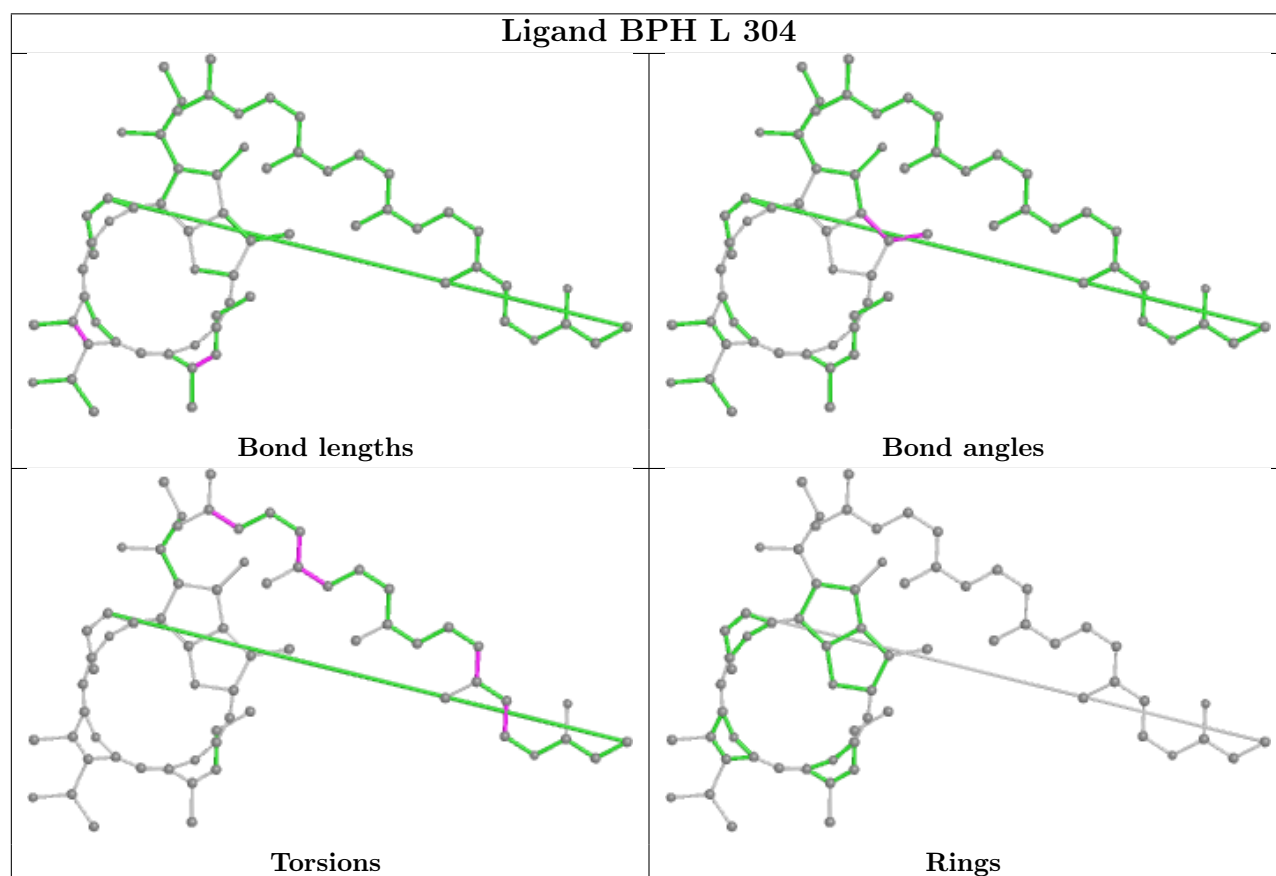
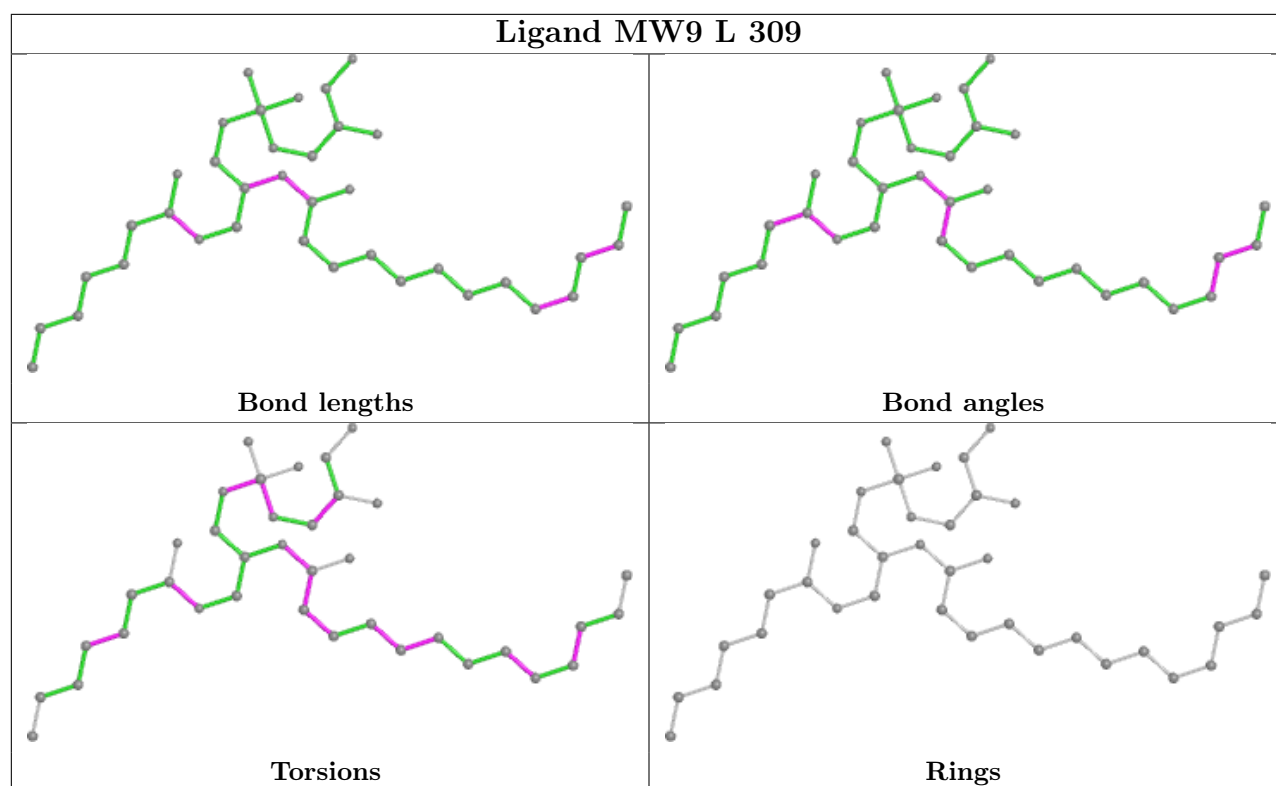
Ligand MW9 D 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

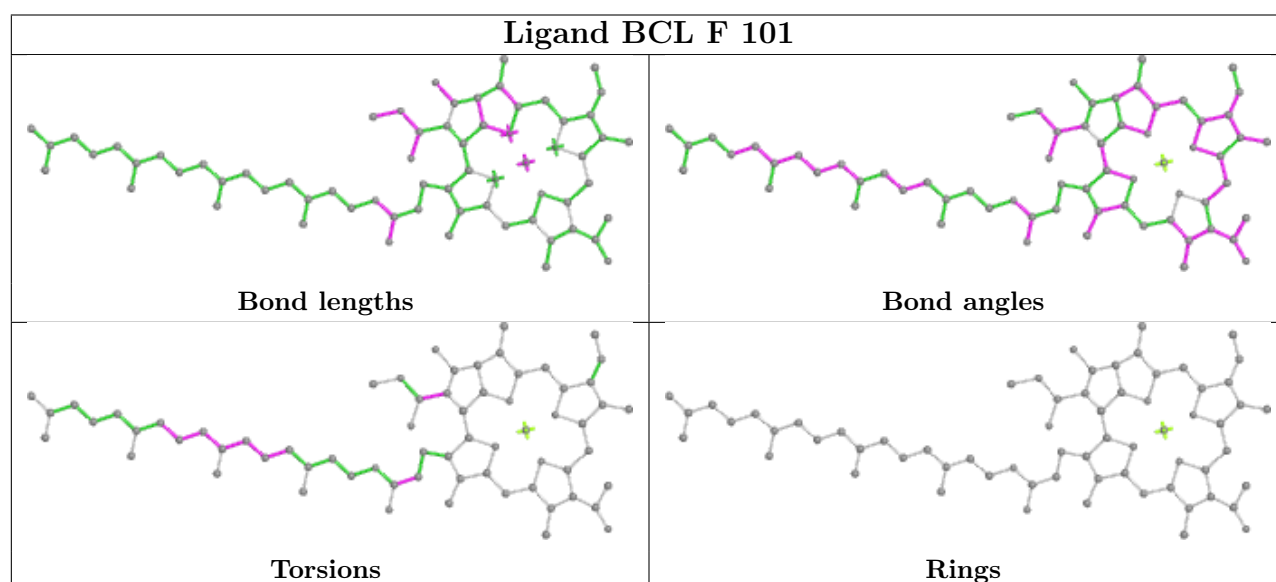
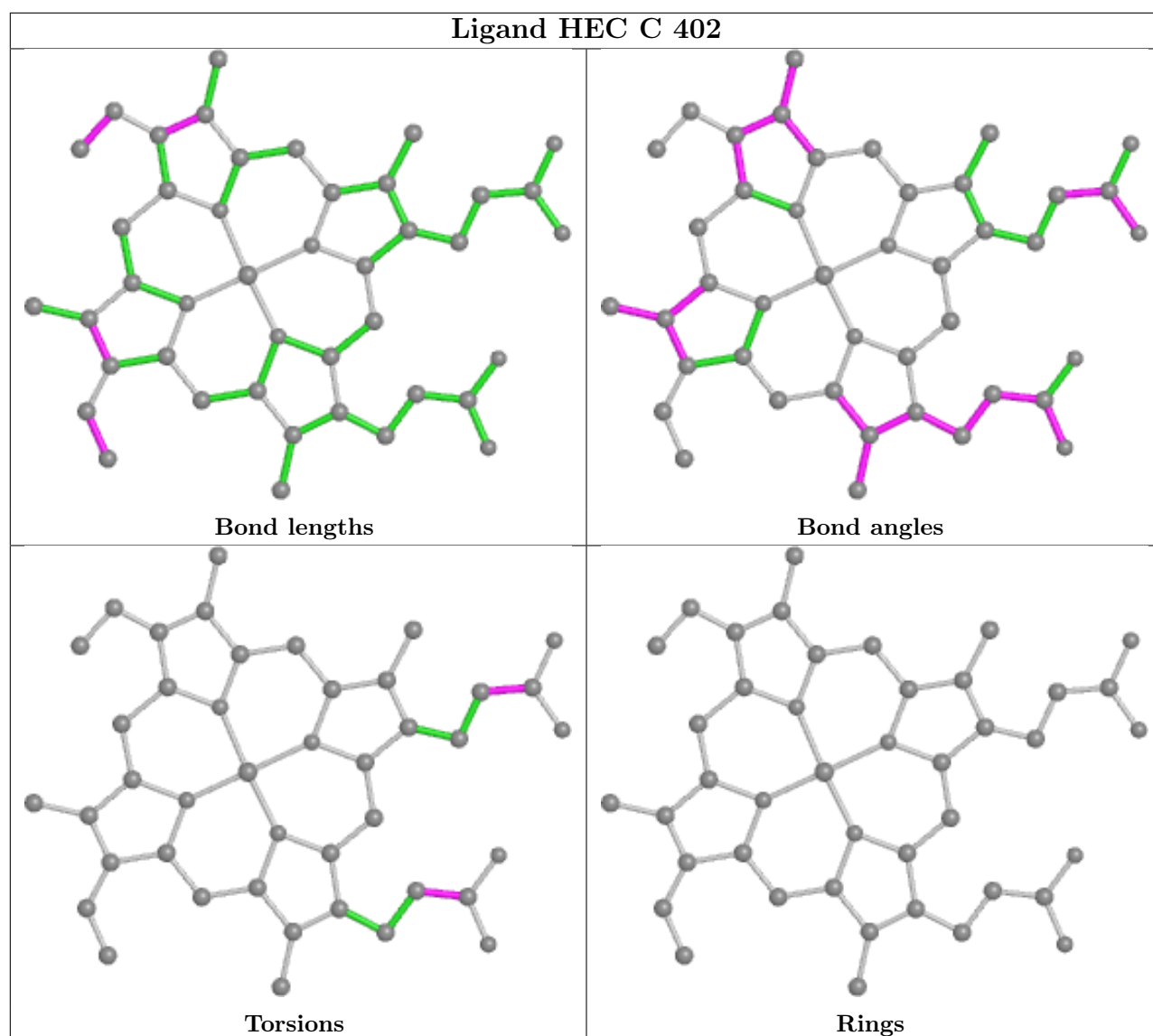
Ligand A1EFU G 104	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

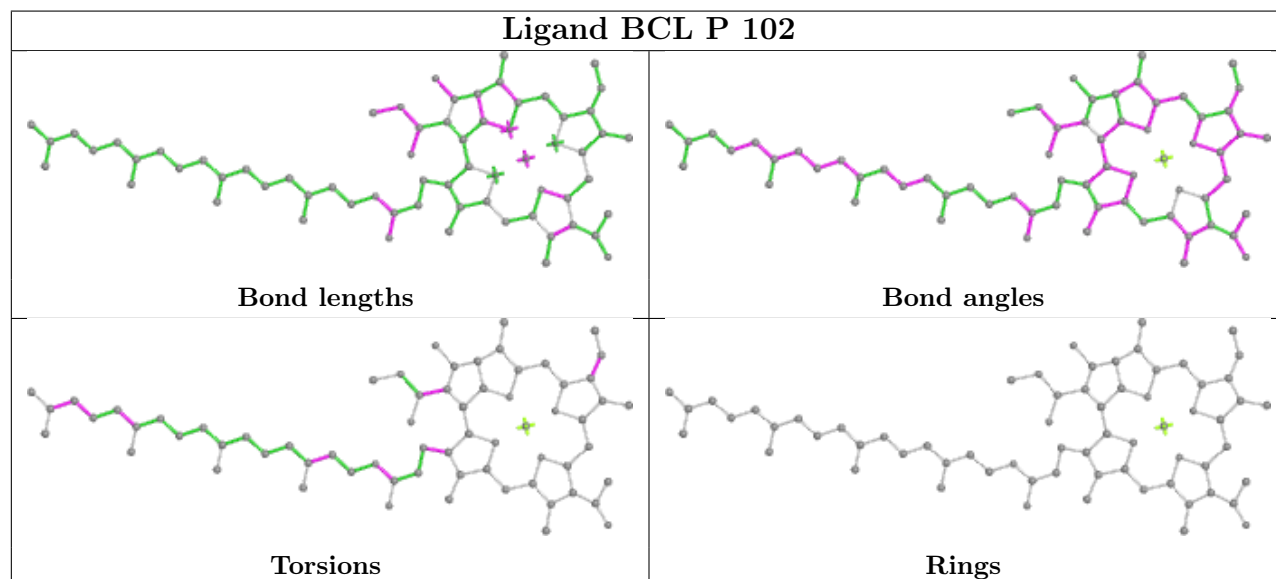
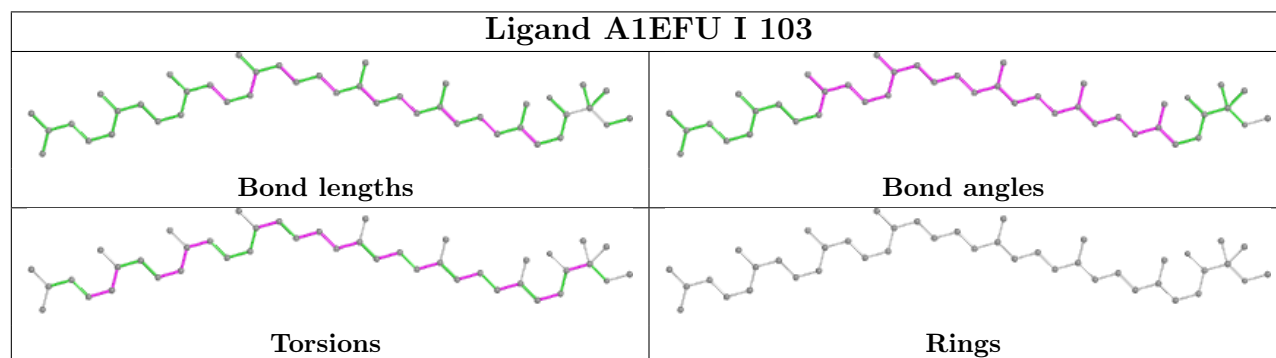
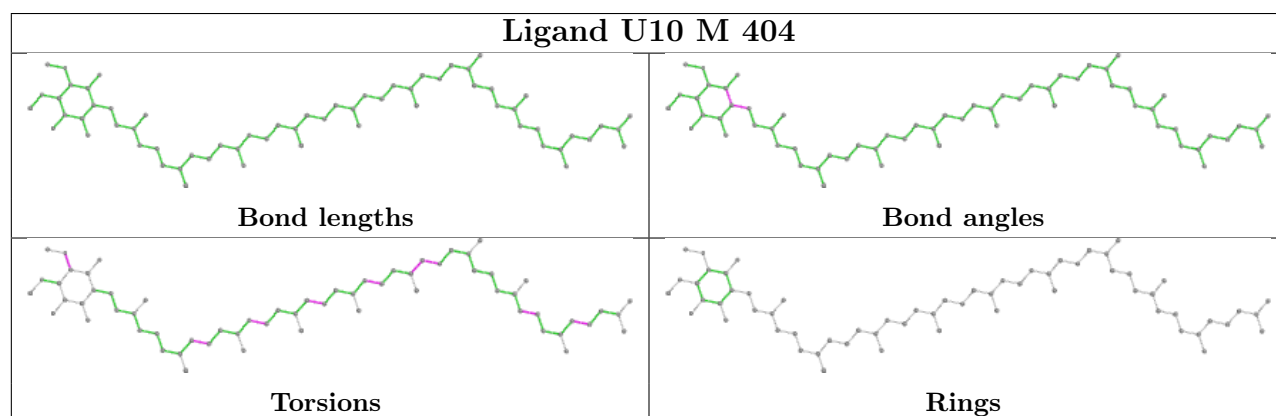
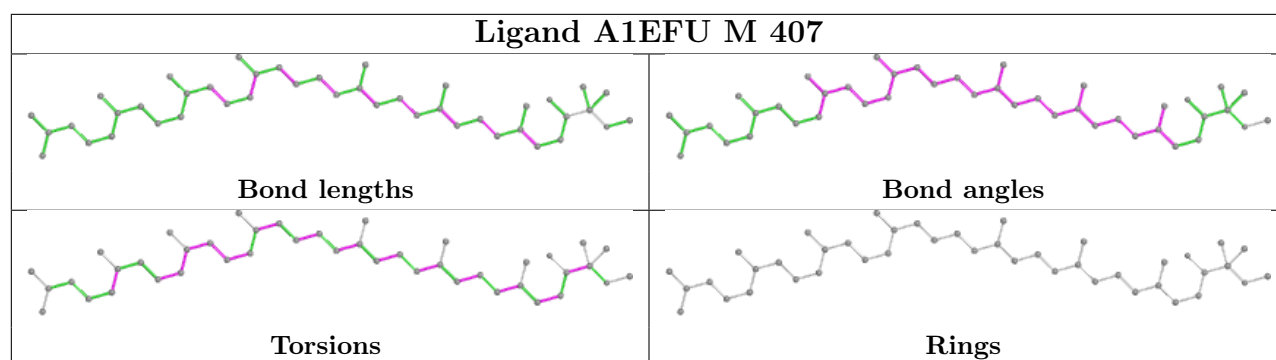
Ligand A1EFU s 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

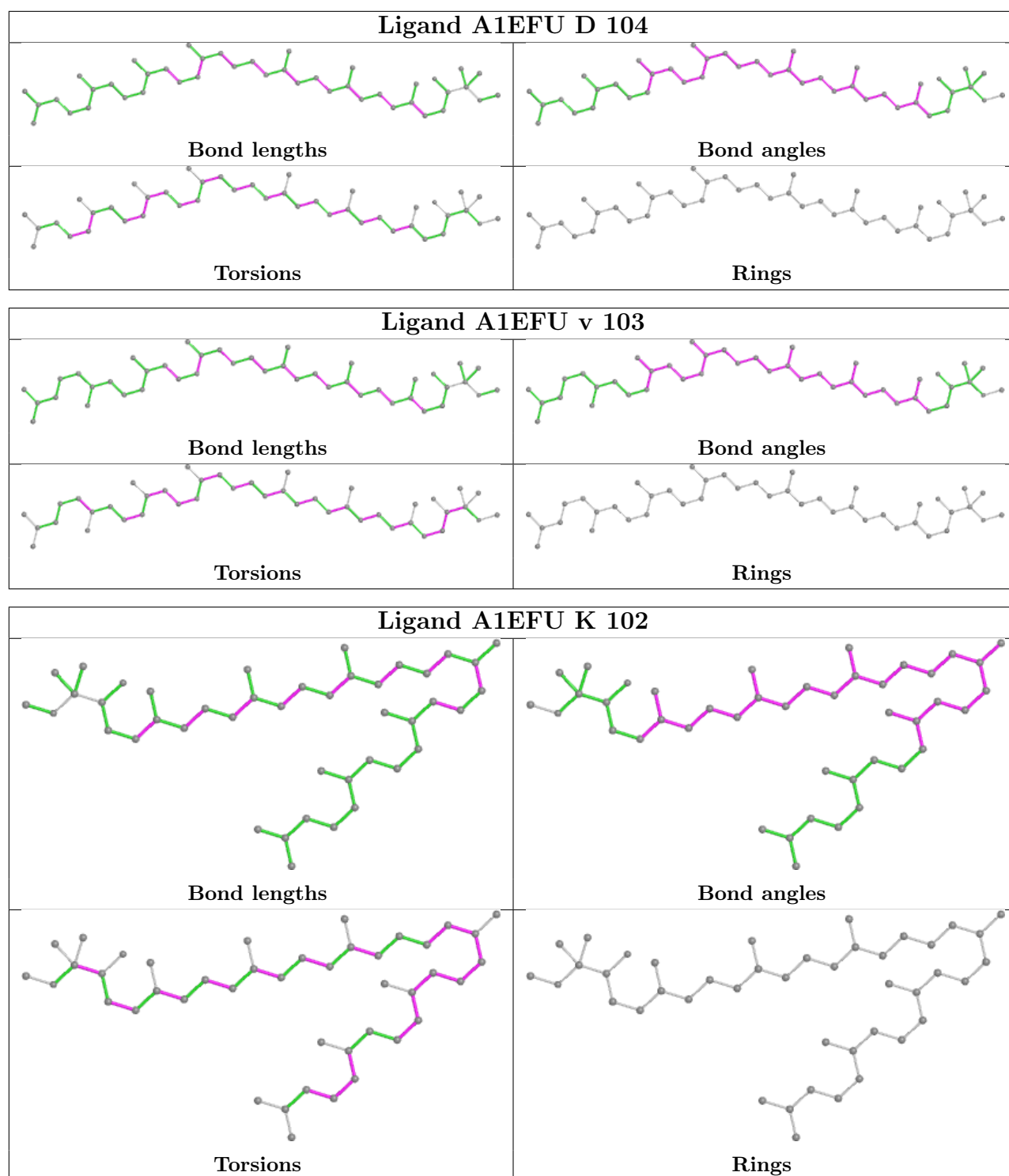


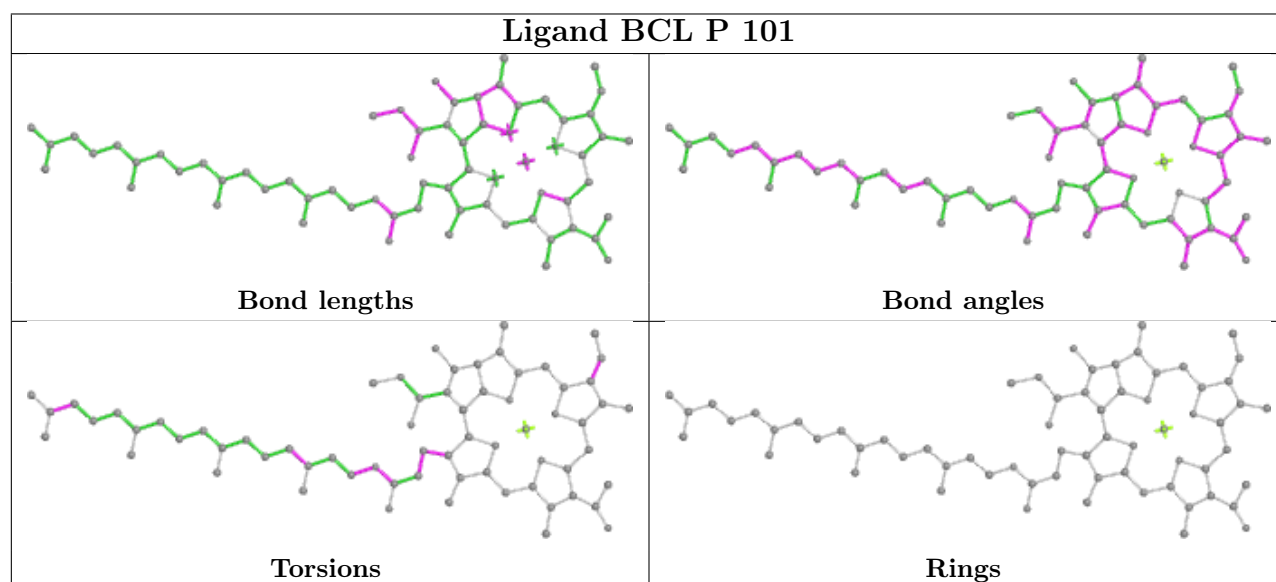
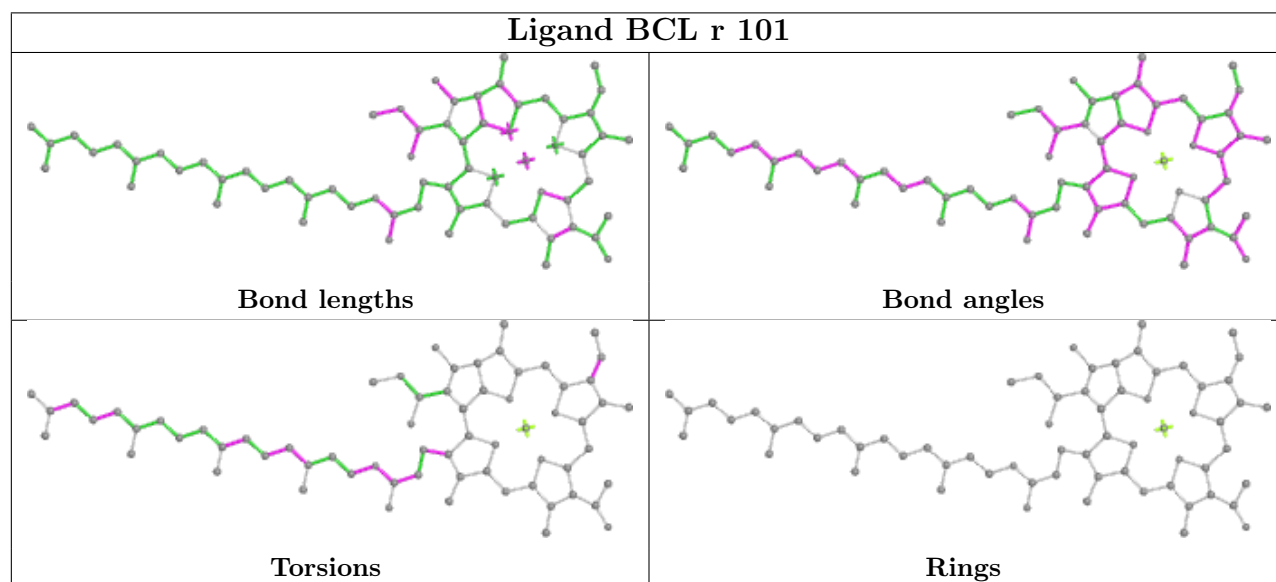
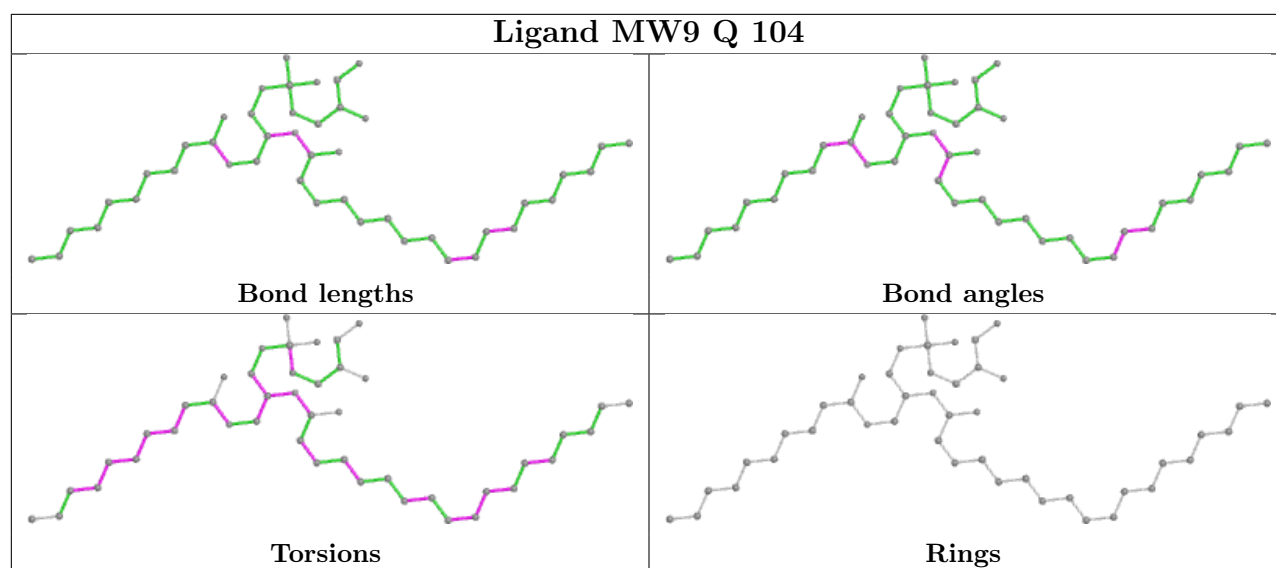


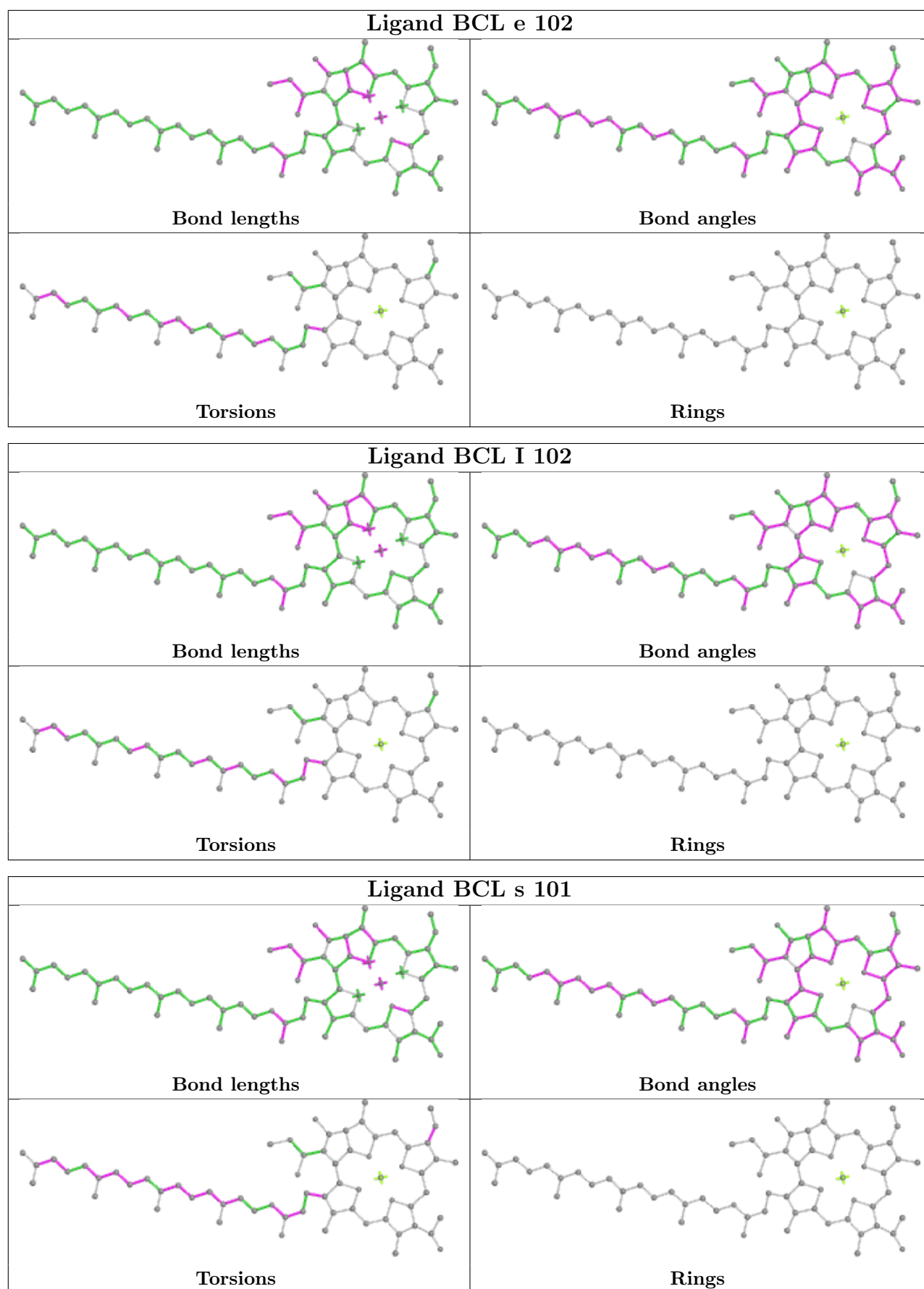


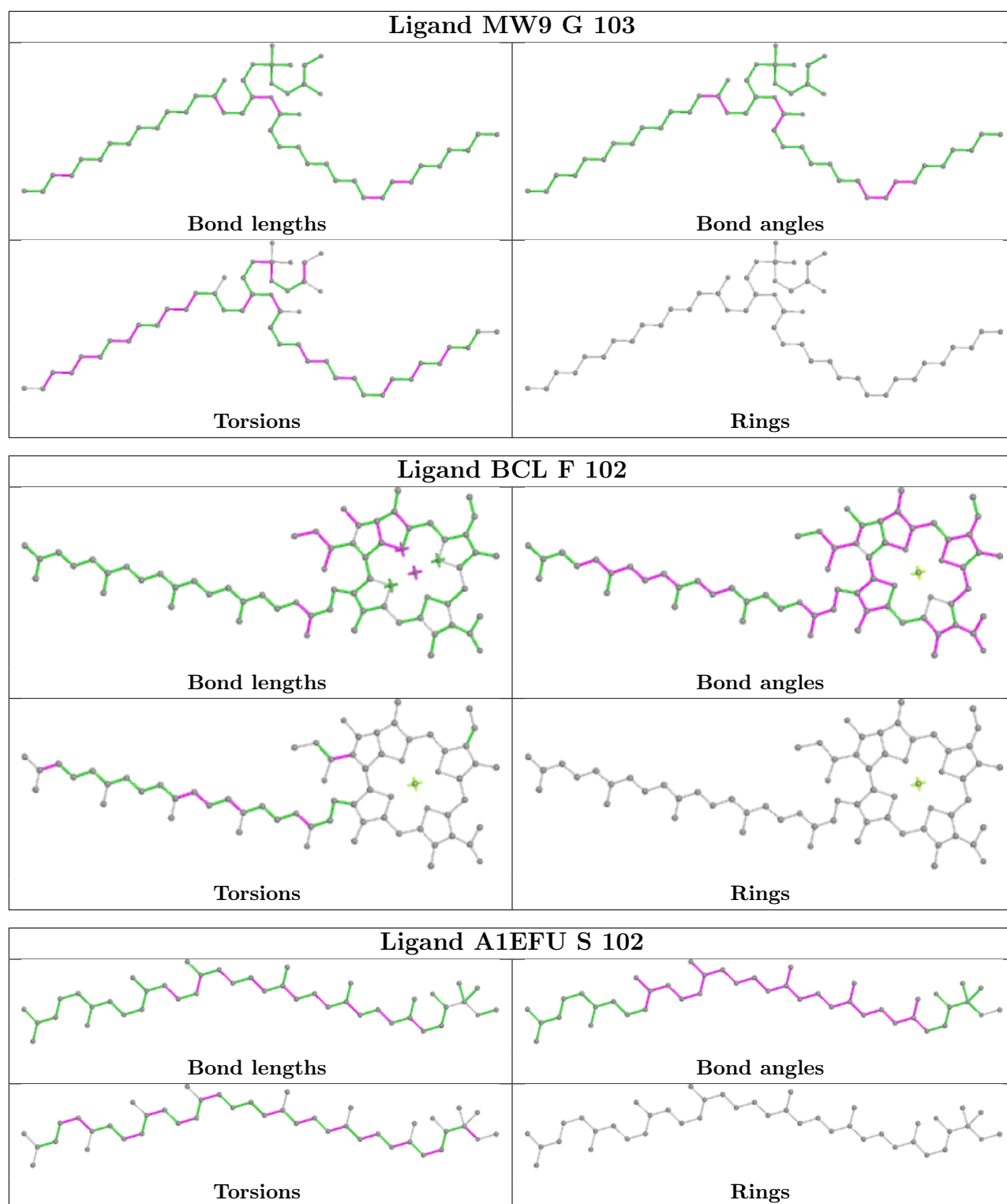


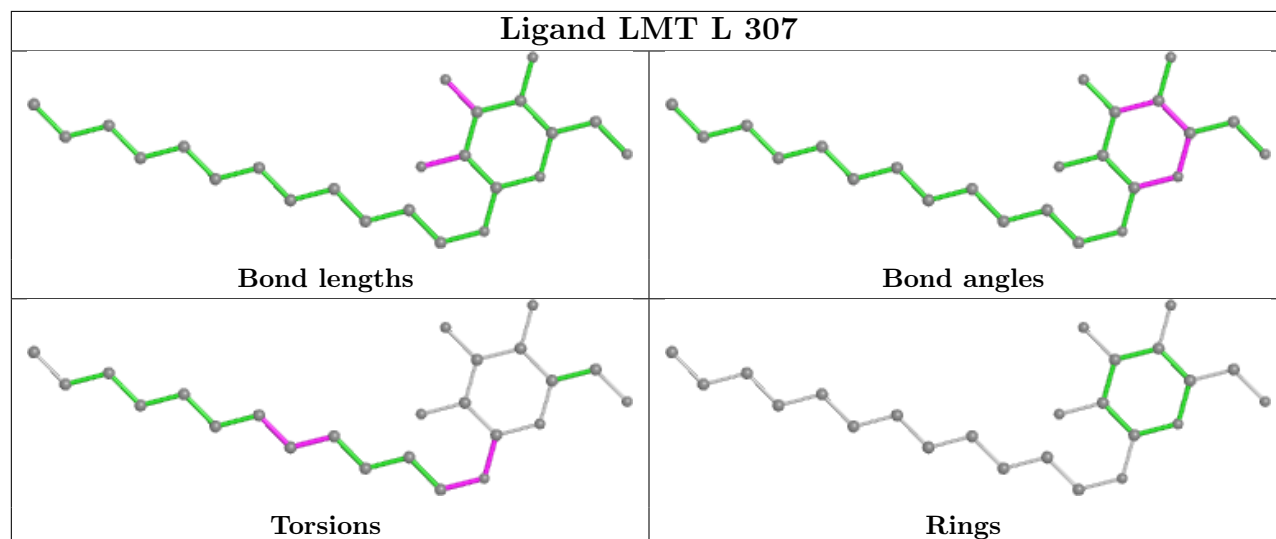
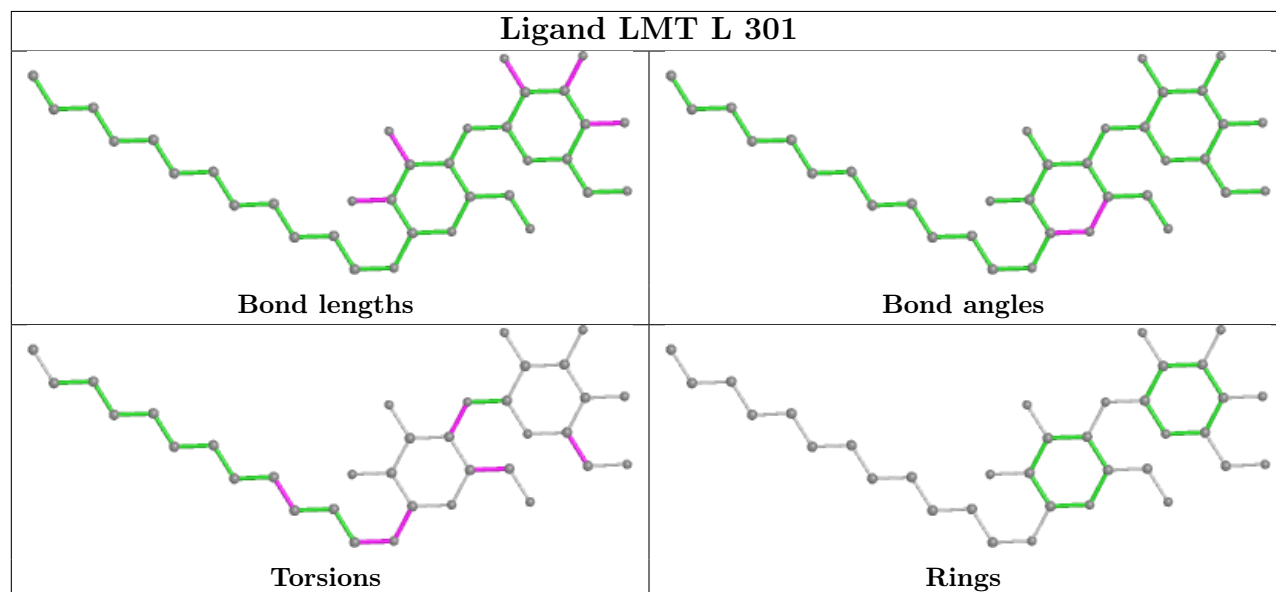
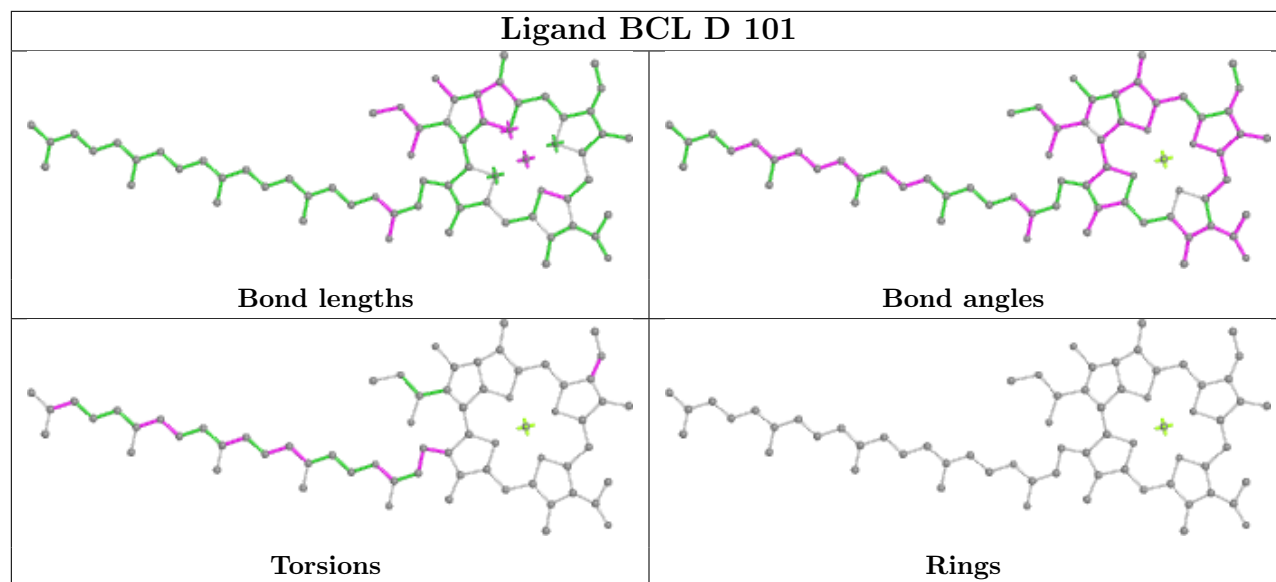




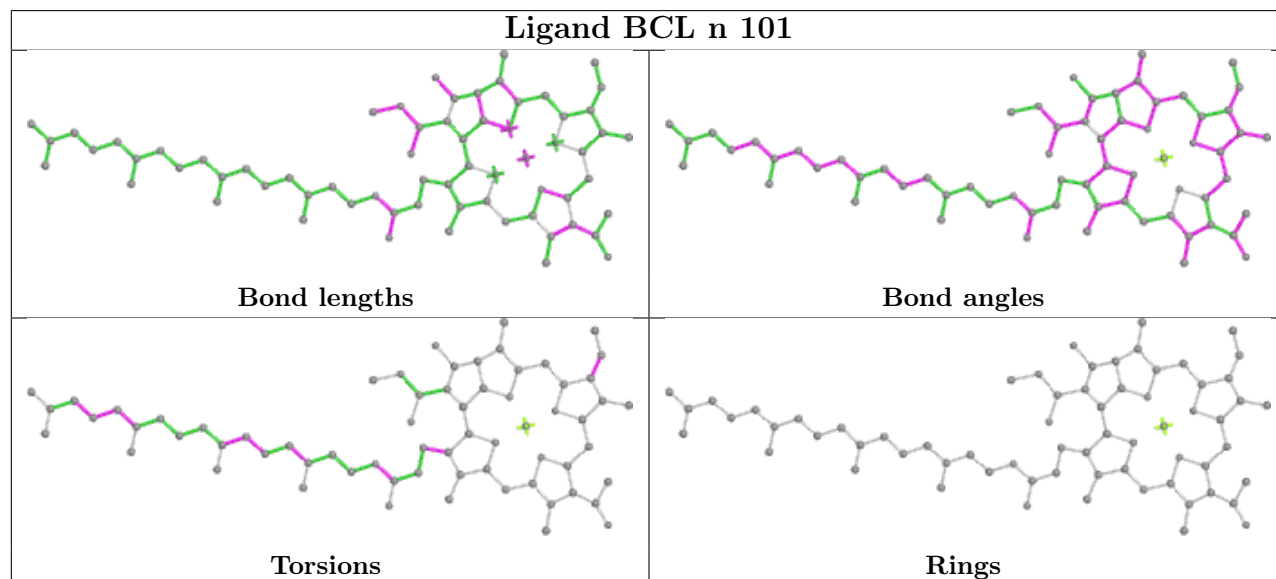
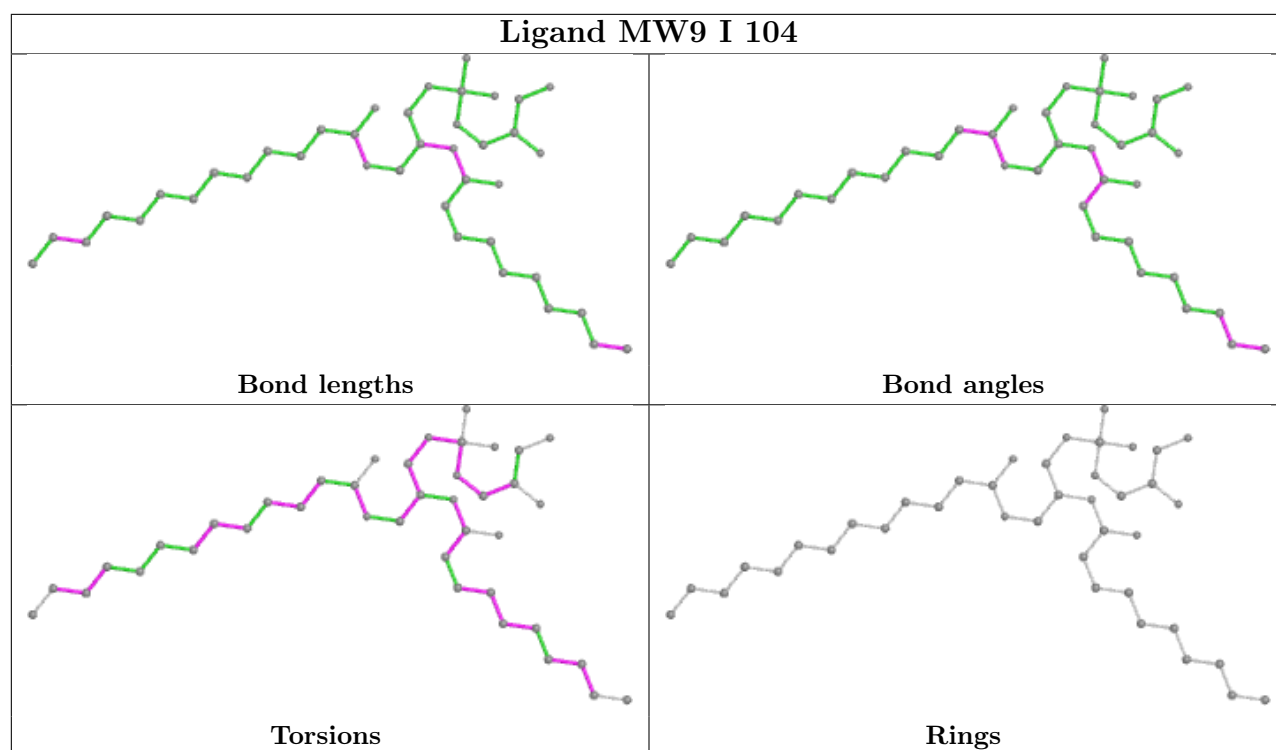


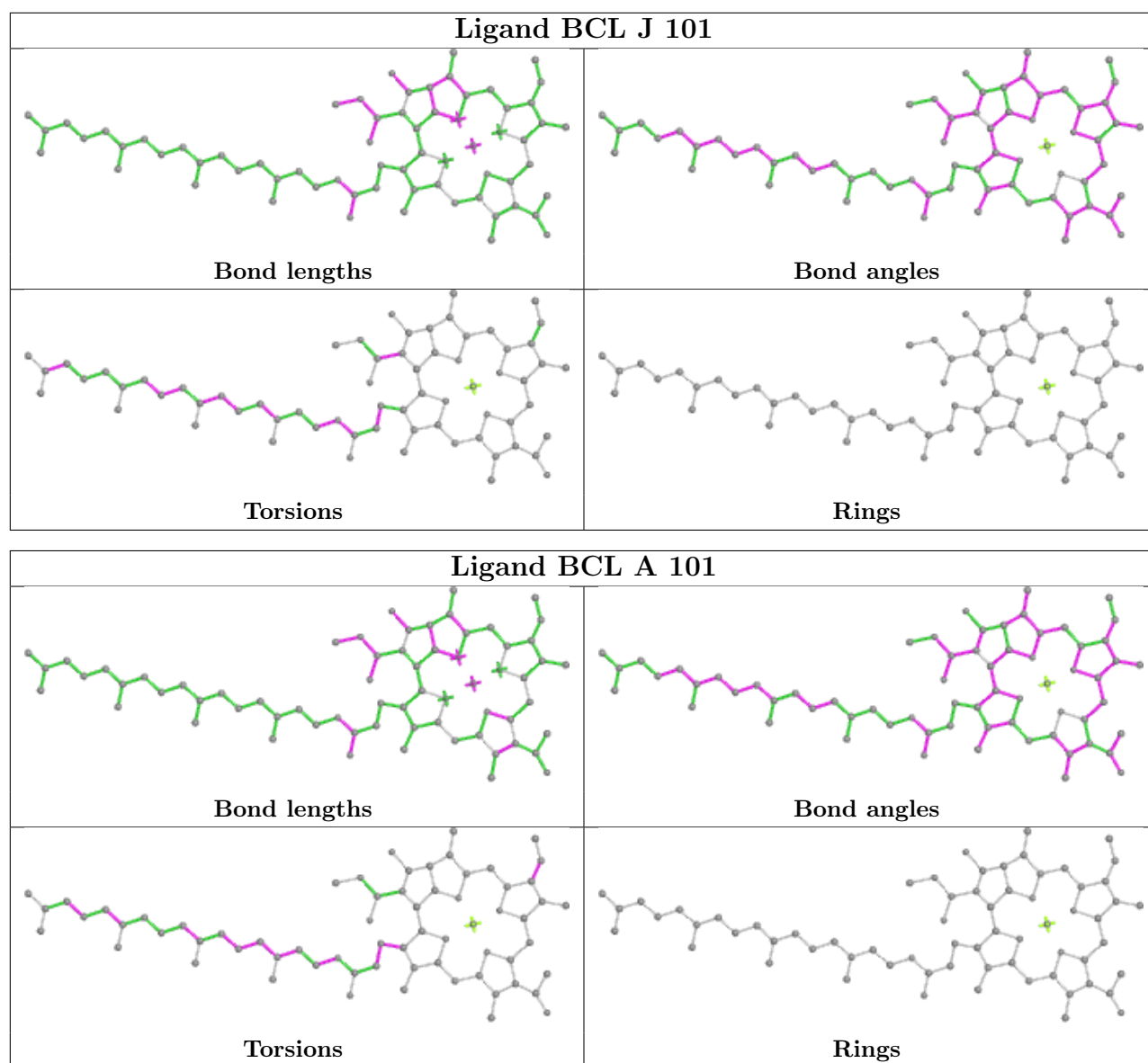


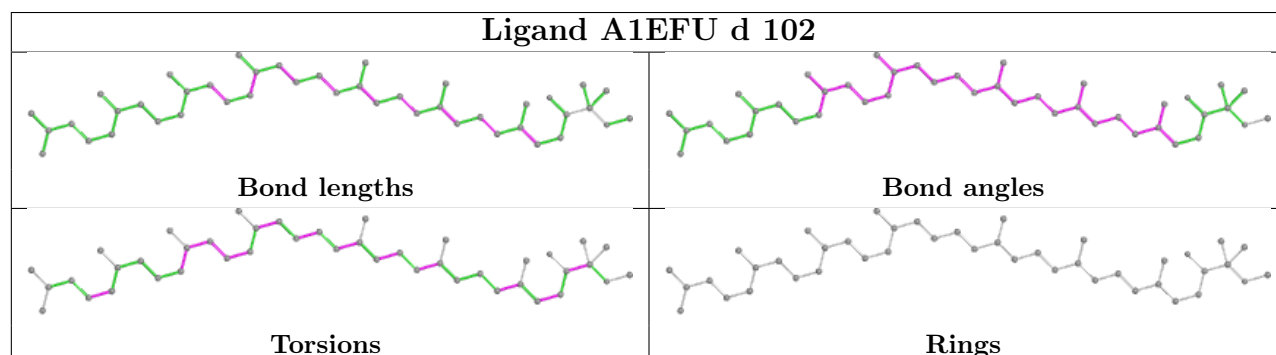
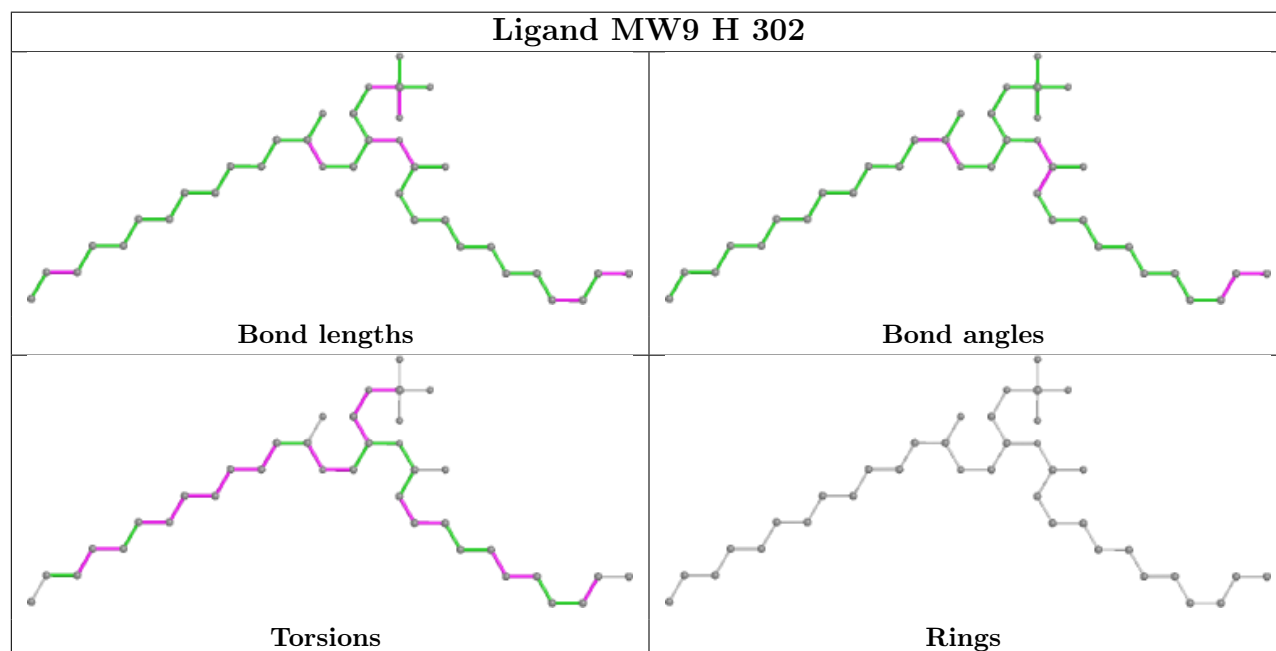
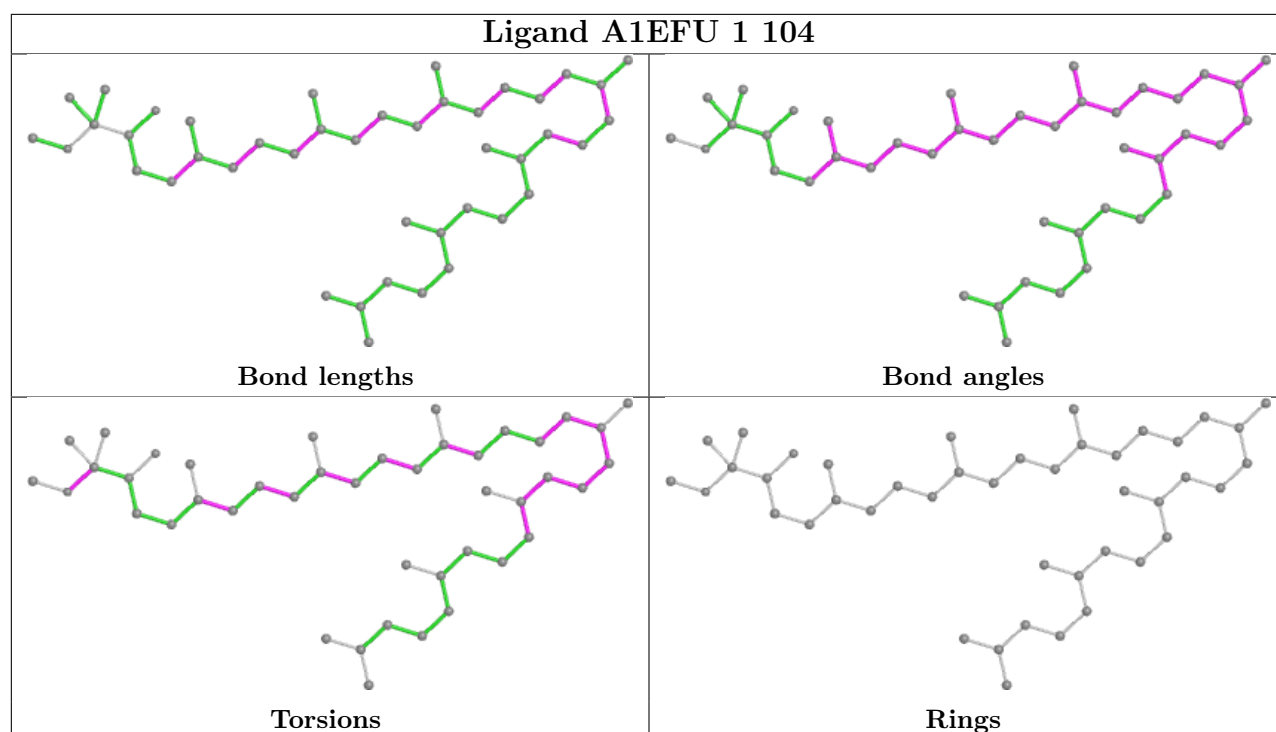


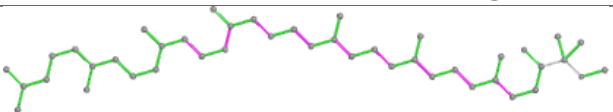
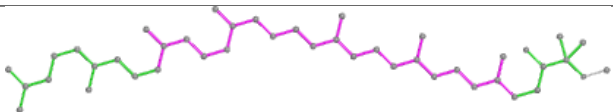
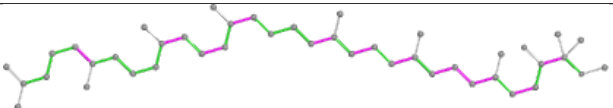
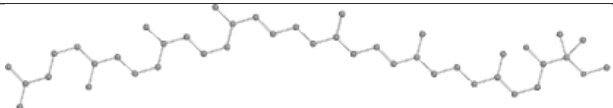
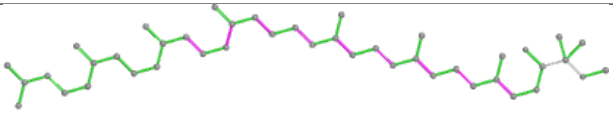
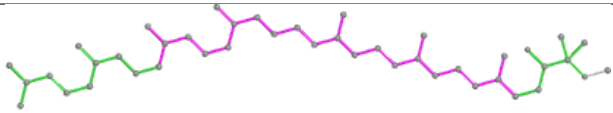
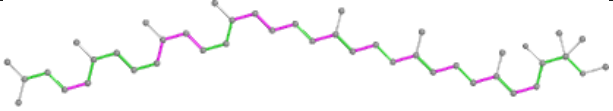
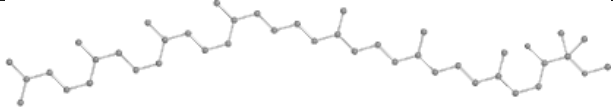
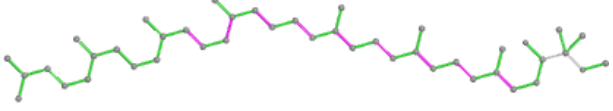
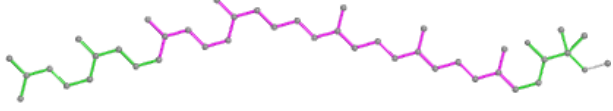
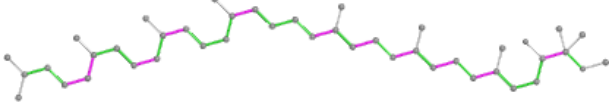
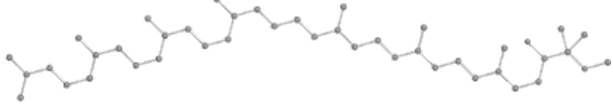
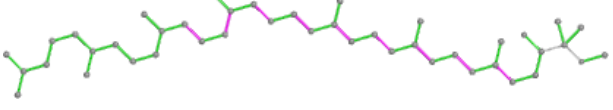
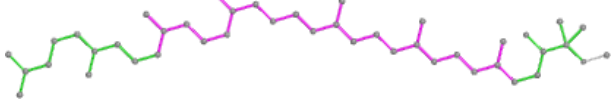
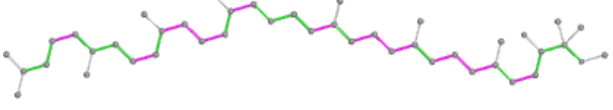
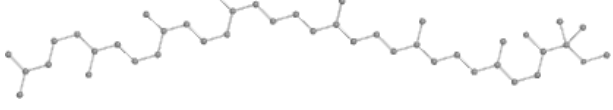


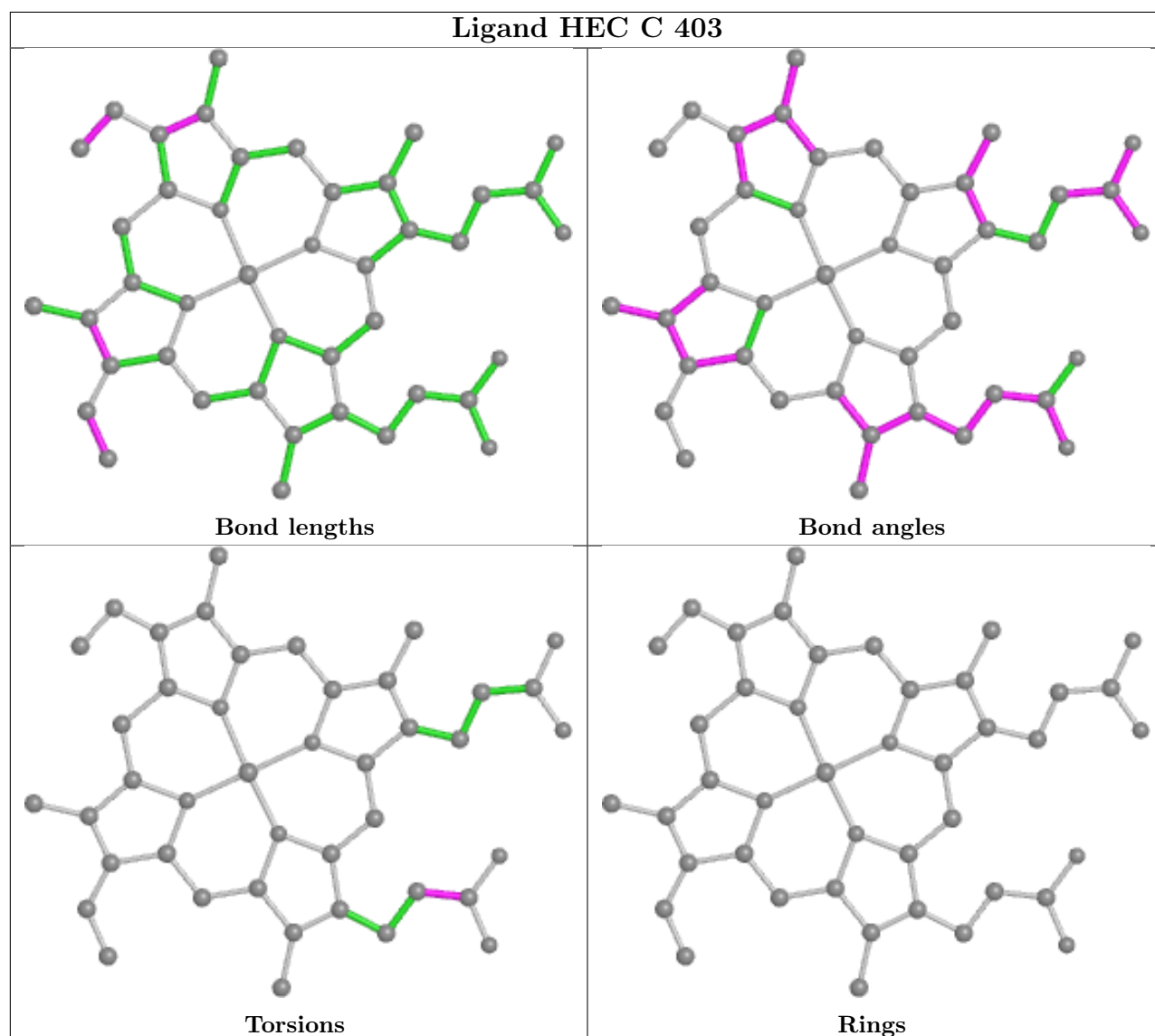
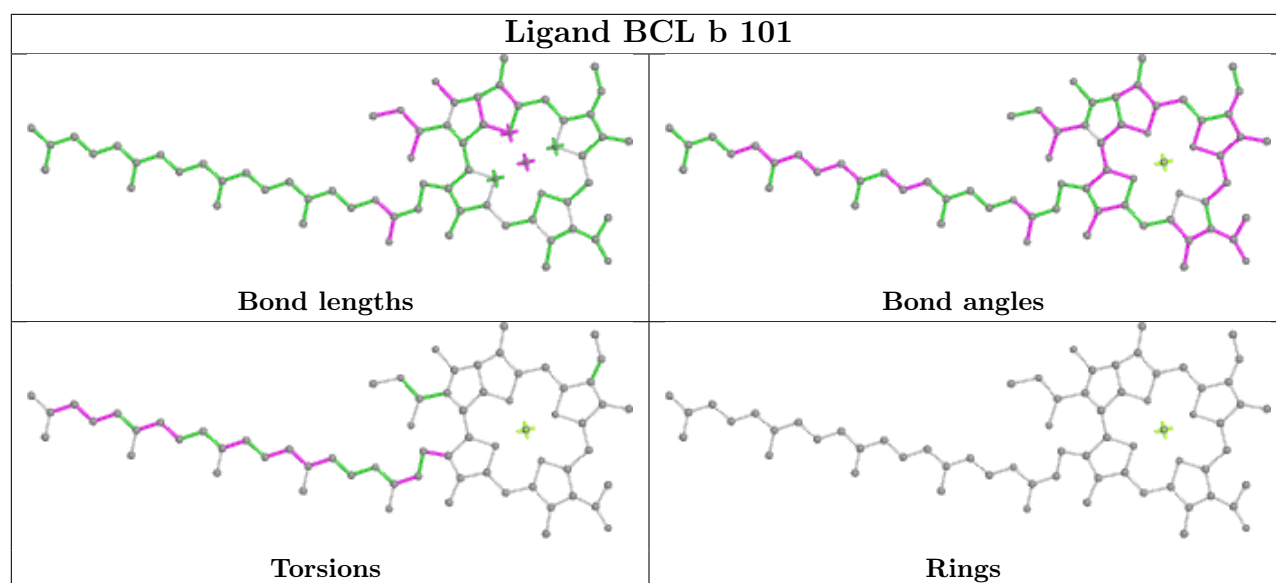


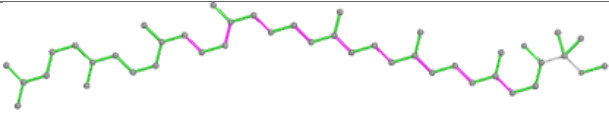
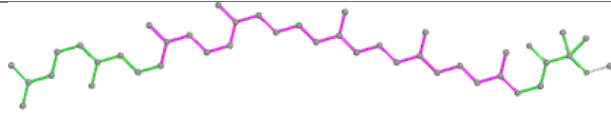
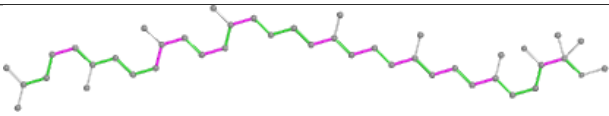
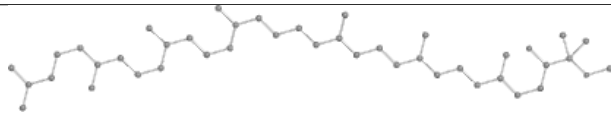


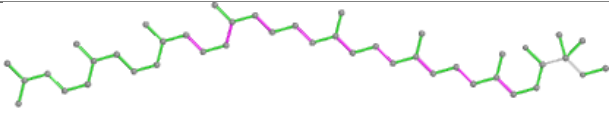
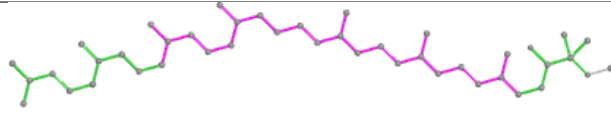
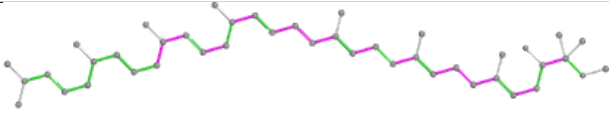
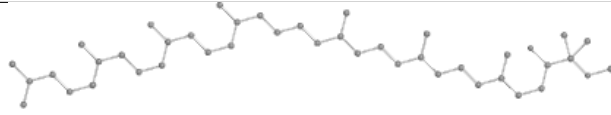


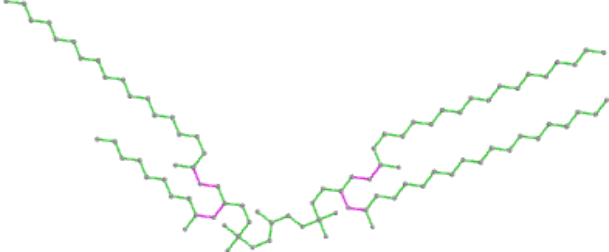
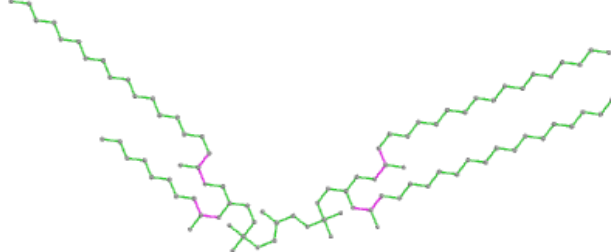
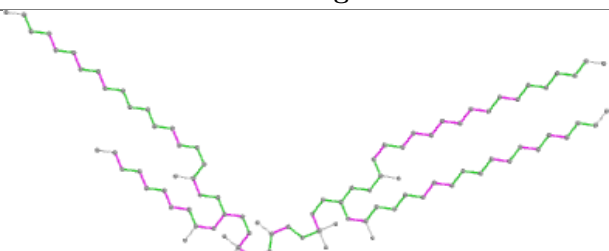
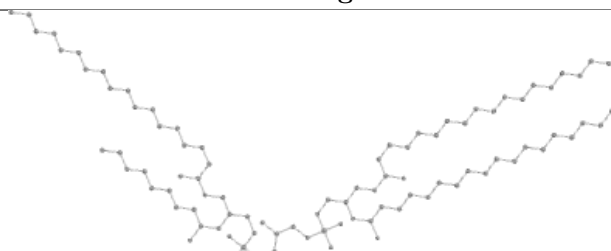


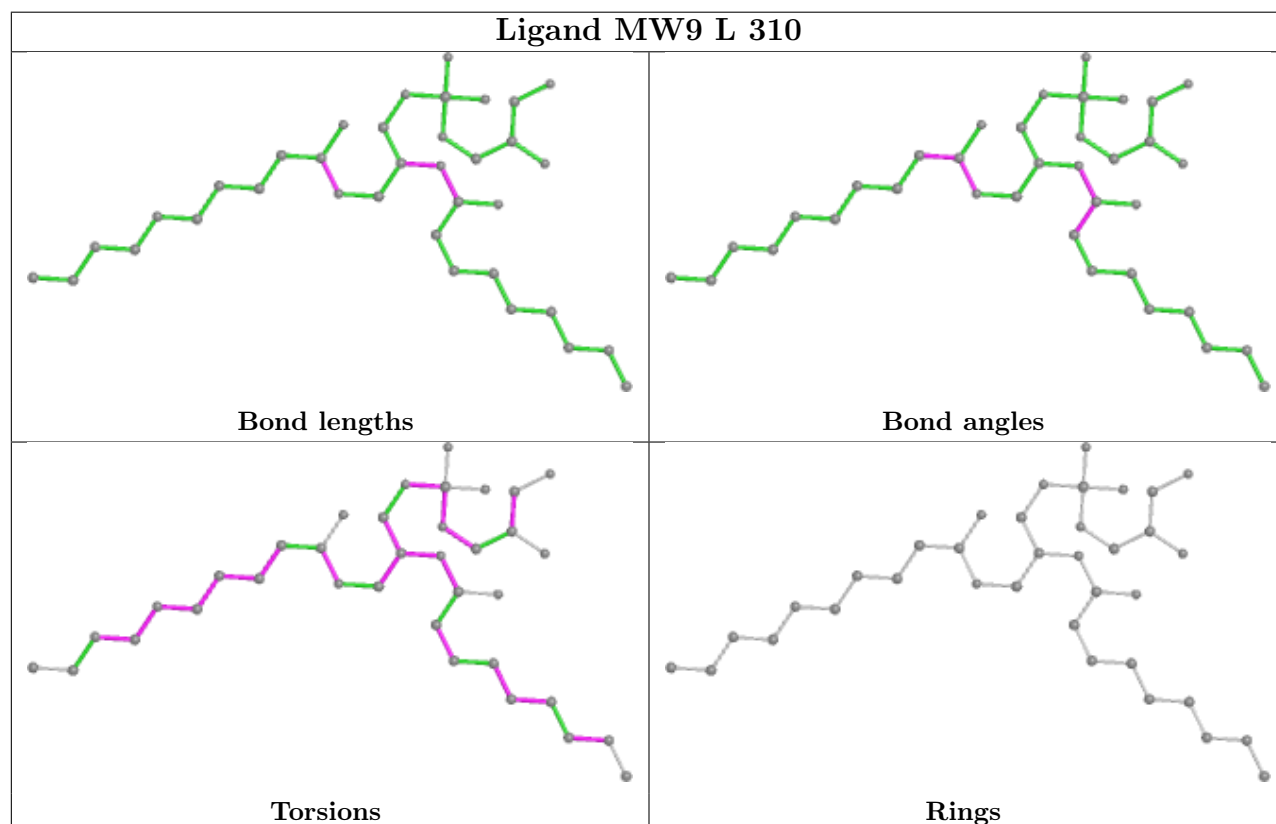
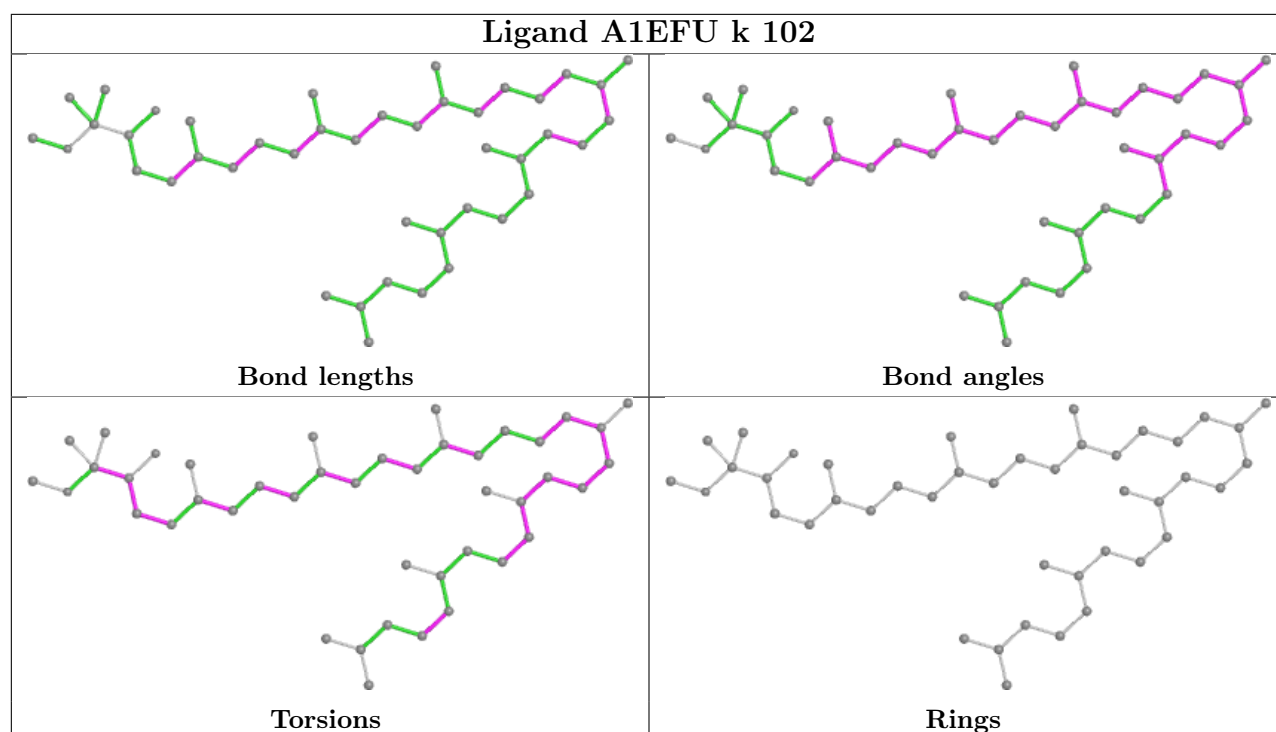
Ligand A1EFU R 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU 2 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A1EFU v 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

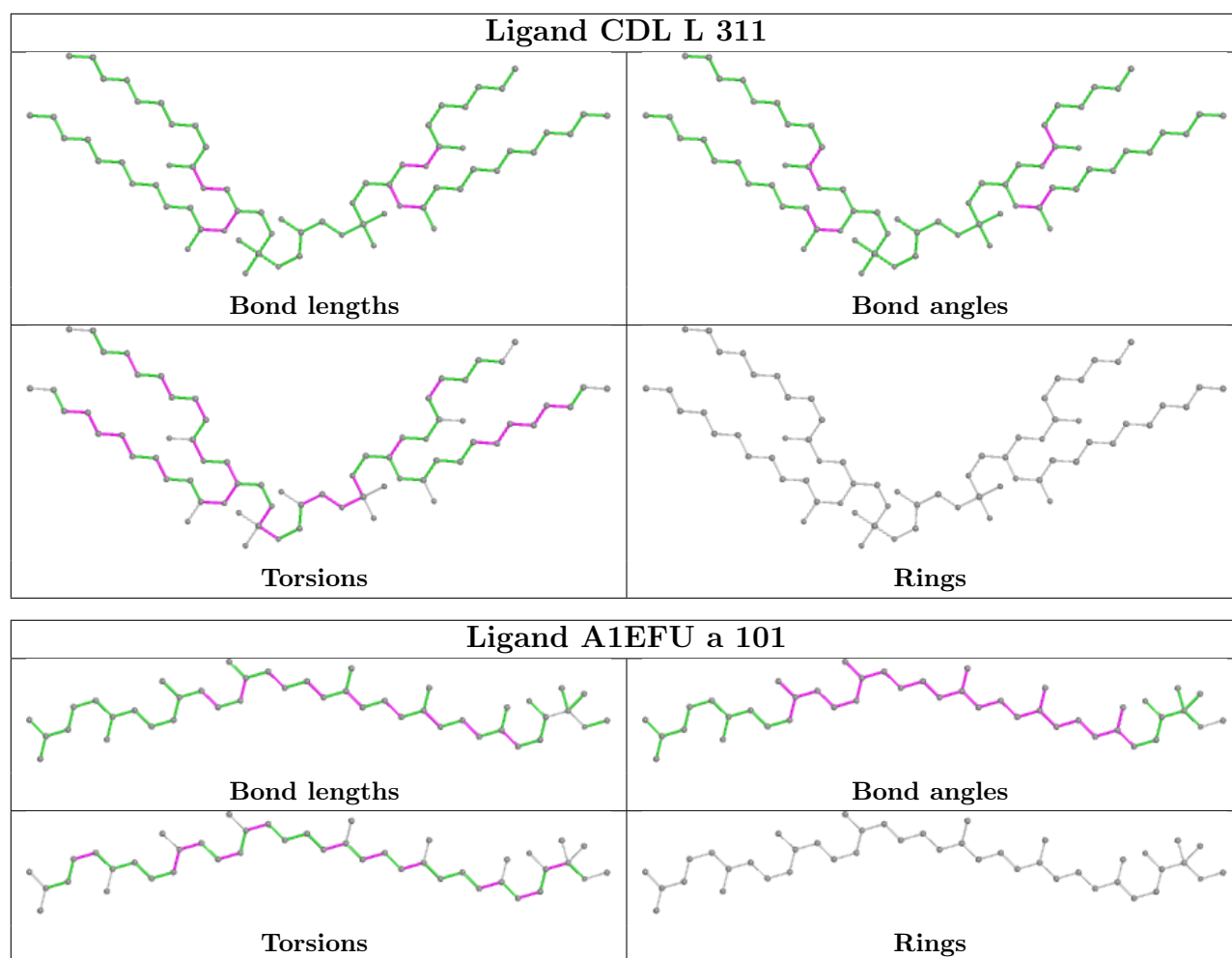


Ligand A1EFU B 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EFU G 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CDL H 303	
	
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.



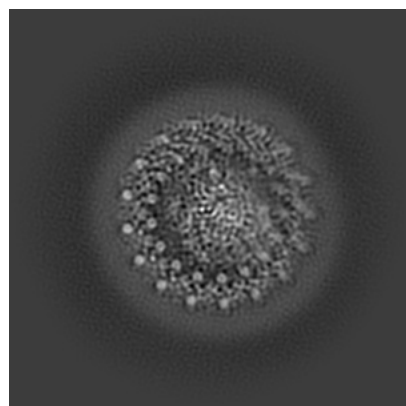
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39683. These allow visual inspection of the internal detail of the map and identification of artifacts.

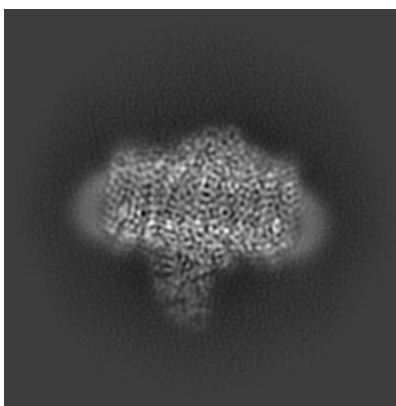
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

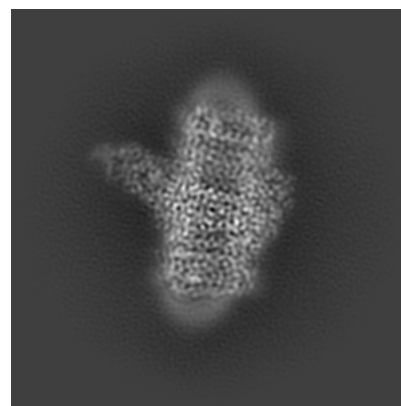
#### 6.1.1 Primary map



X

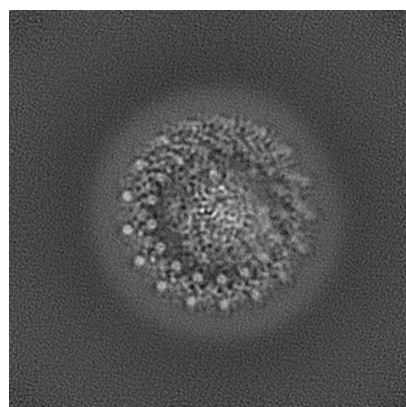


Y

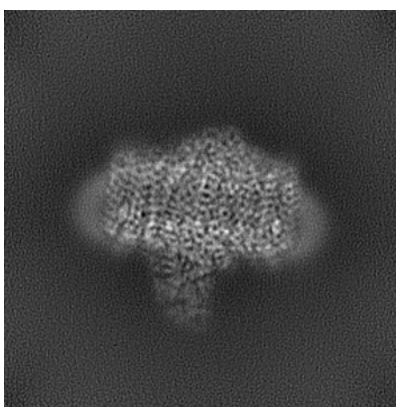


Z

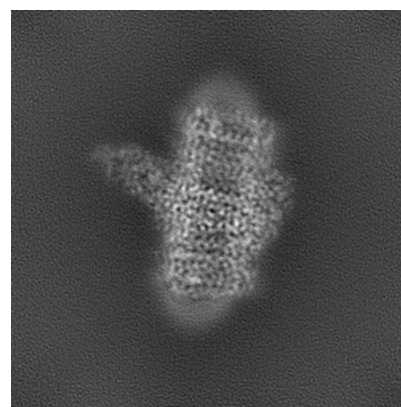
#### 6.1.2 Raw map



X



Y

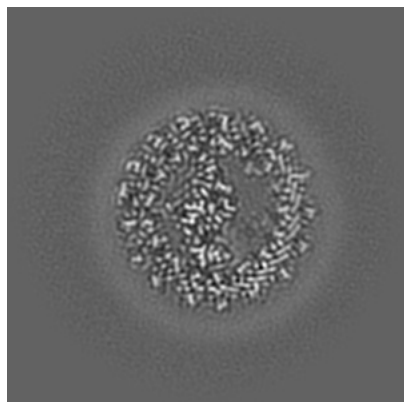


Z

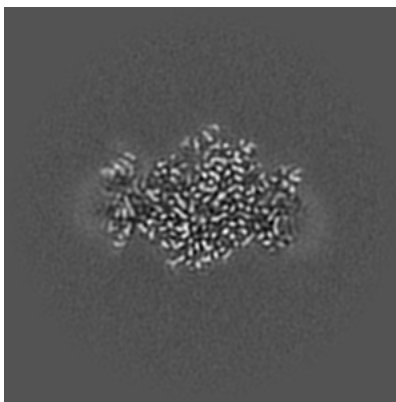
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

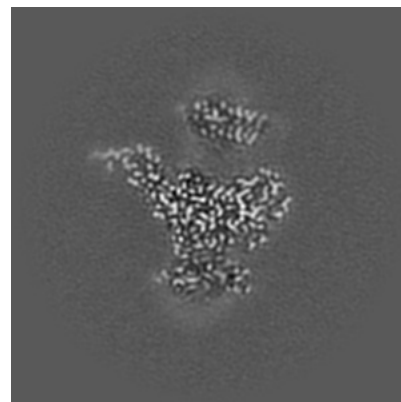
### 6.2.1 Primary map



X Index: 128

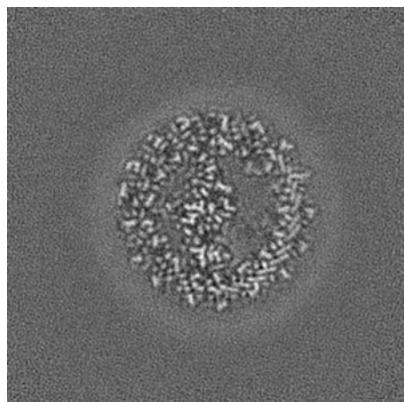


Y Index: 128

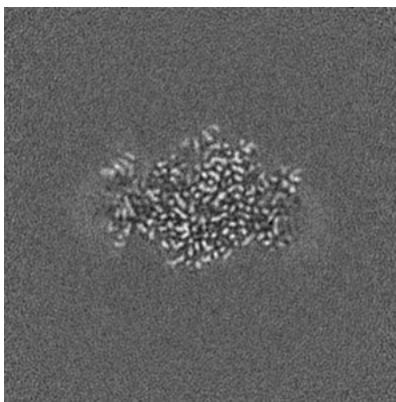


Z Index: 128

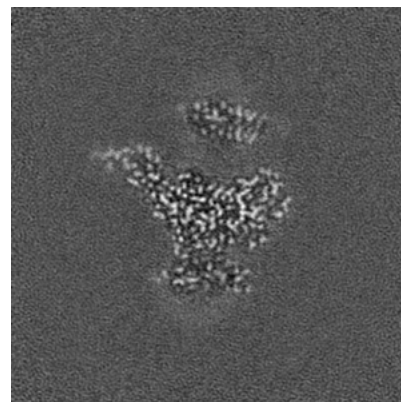
### 6.2.2 Raw map



X Index: 128



Y Index: 128

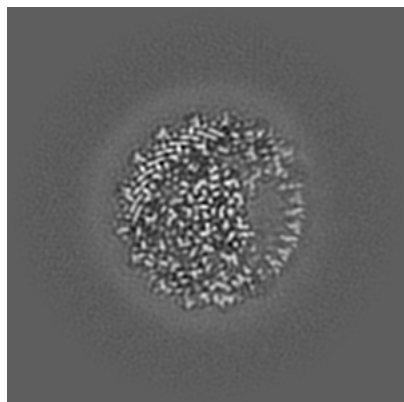


Z Index: 128

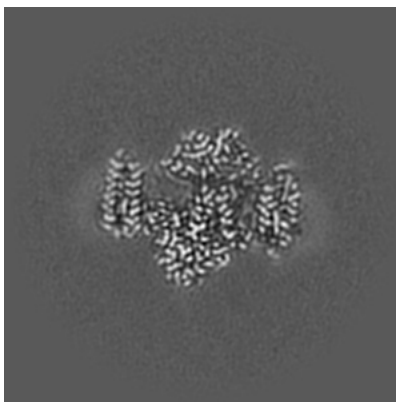
The images above show central slices of the map in three orthogonal directions.

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

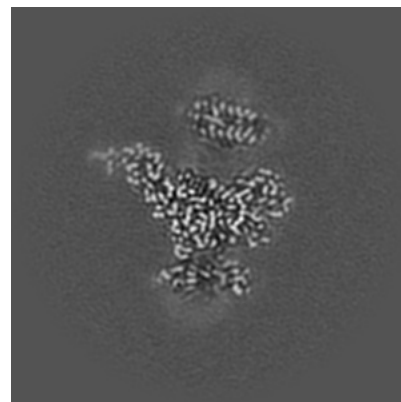
### 6.3.1 Primary map



X Index: 114

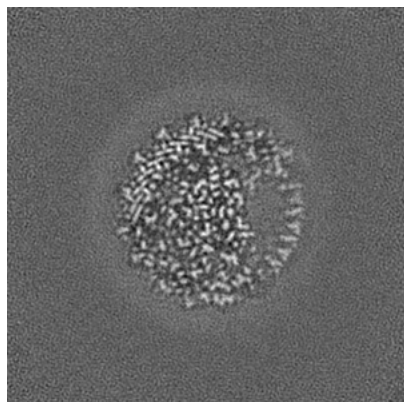


Y Index: 137

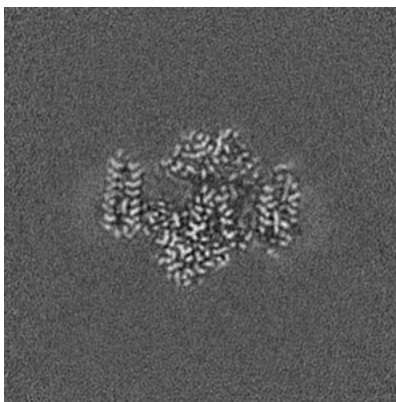


Z Index: 127

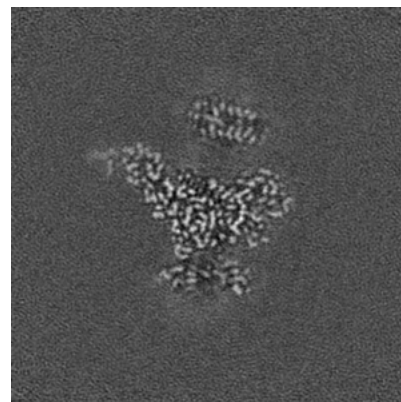
### 6.3.2 Raw map



X Index: 114



Y Index: 137

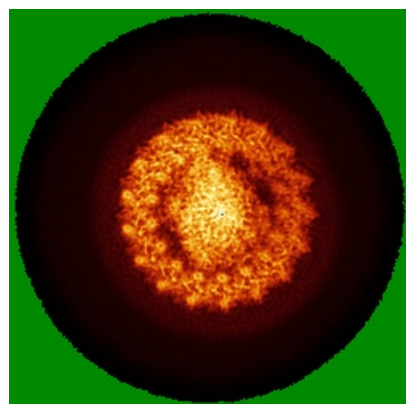


Z Index: 127

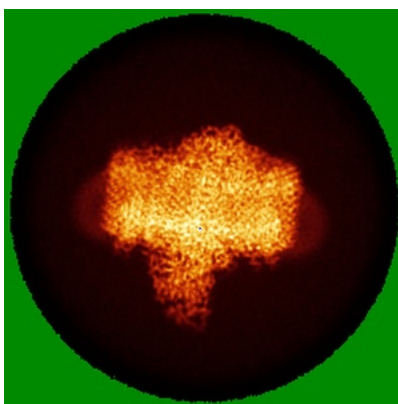
The images above show the largest variance slices of the map in three orthogonal directions.

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

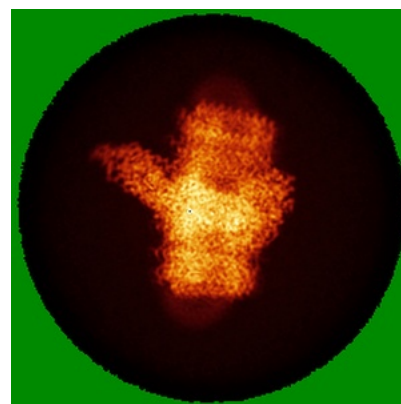
### 6.4.1 Primary map



X

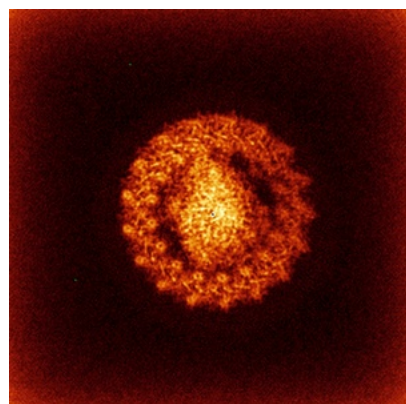


Y

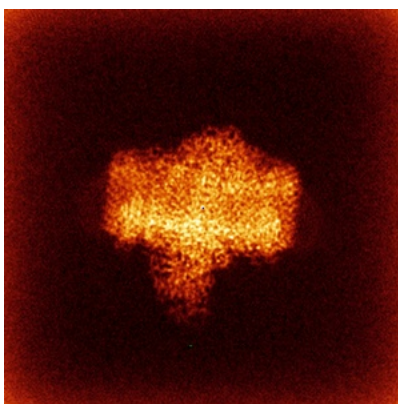


Z

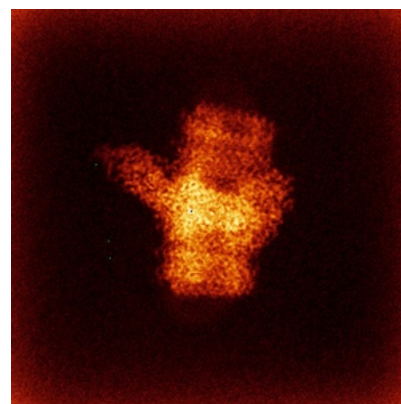
### 6.4.2 Raw map



X



Y



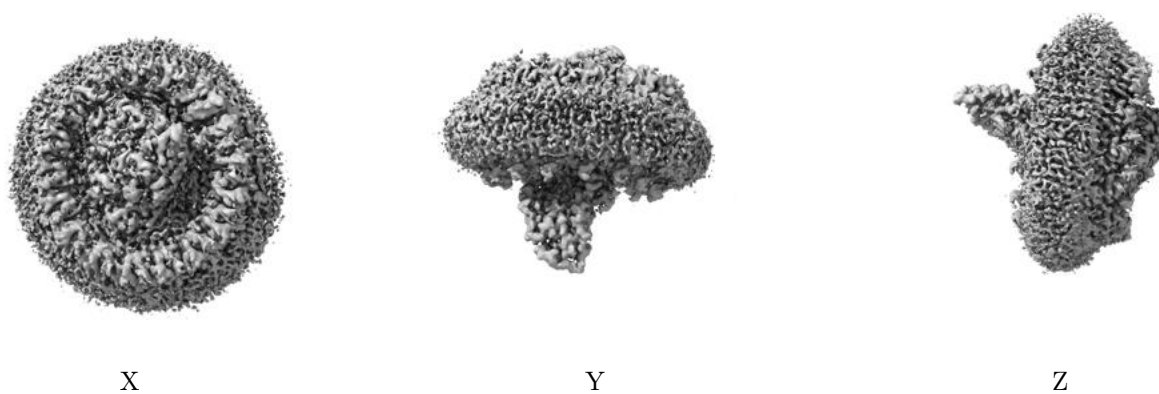
Z

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.



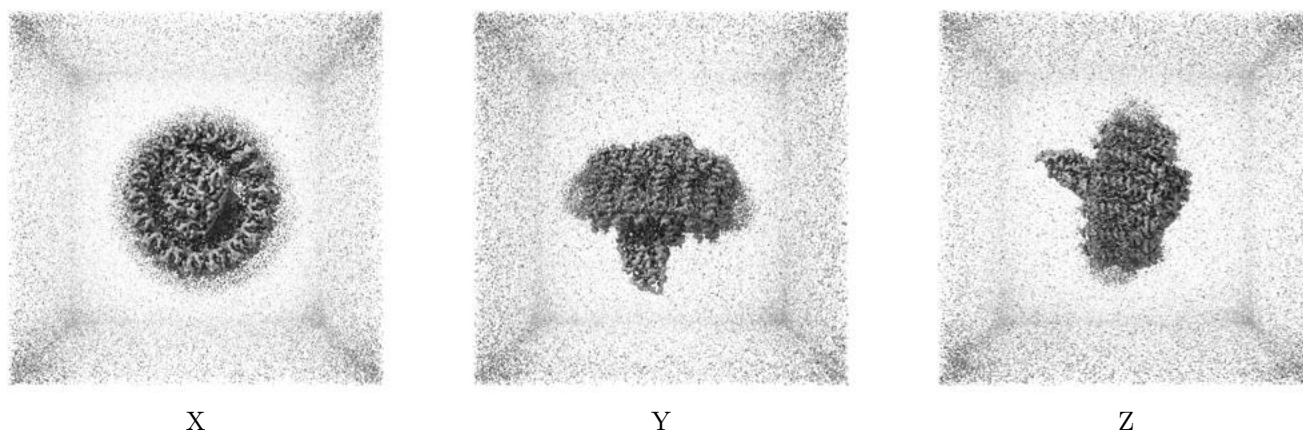
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

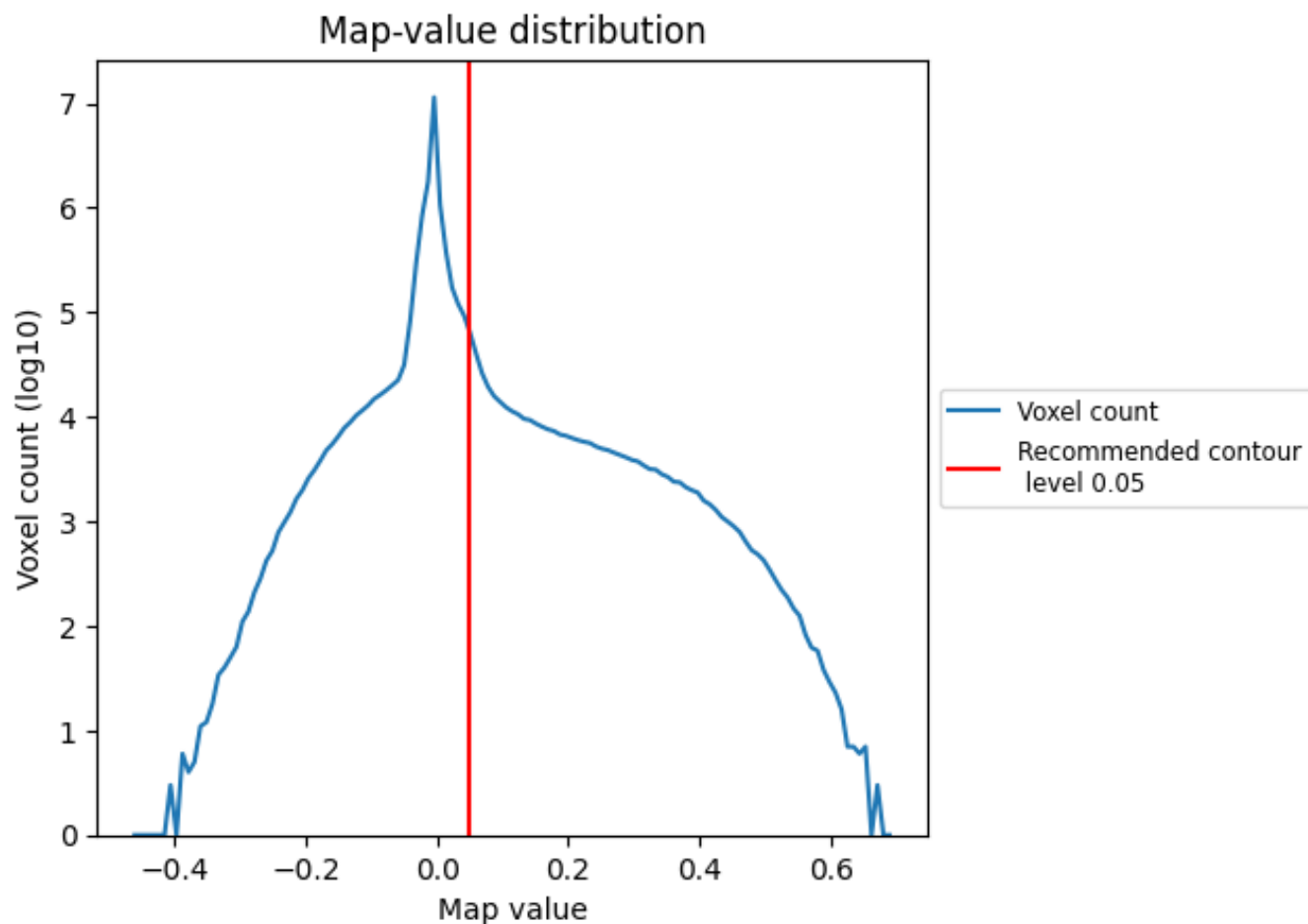
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

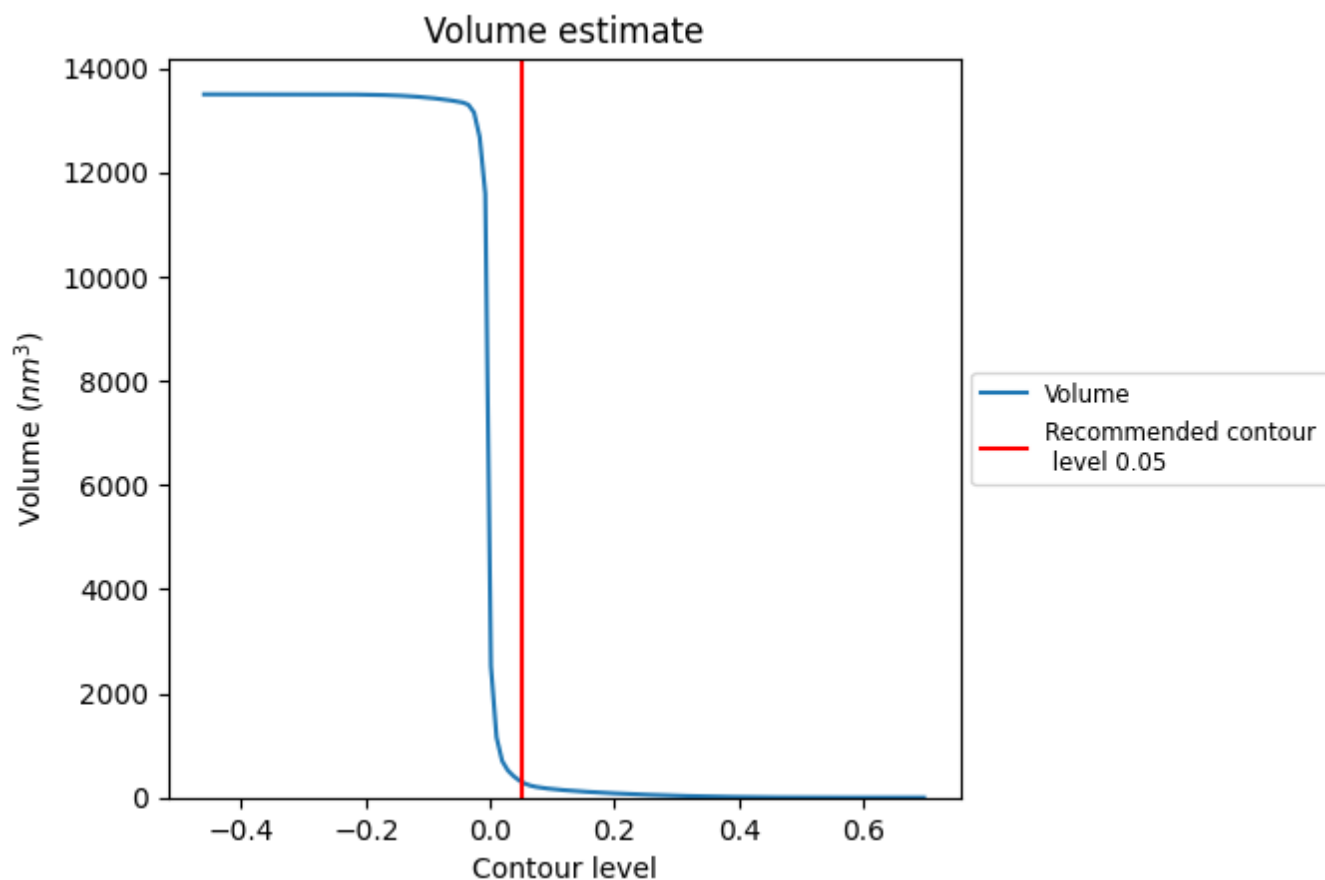
This section contains the results of statistical analysis of the map.

### 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.

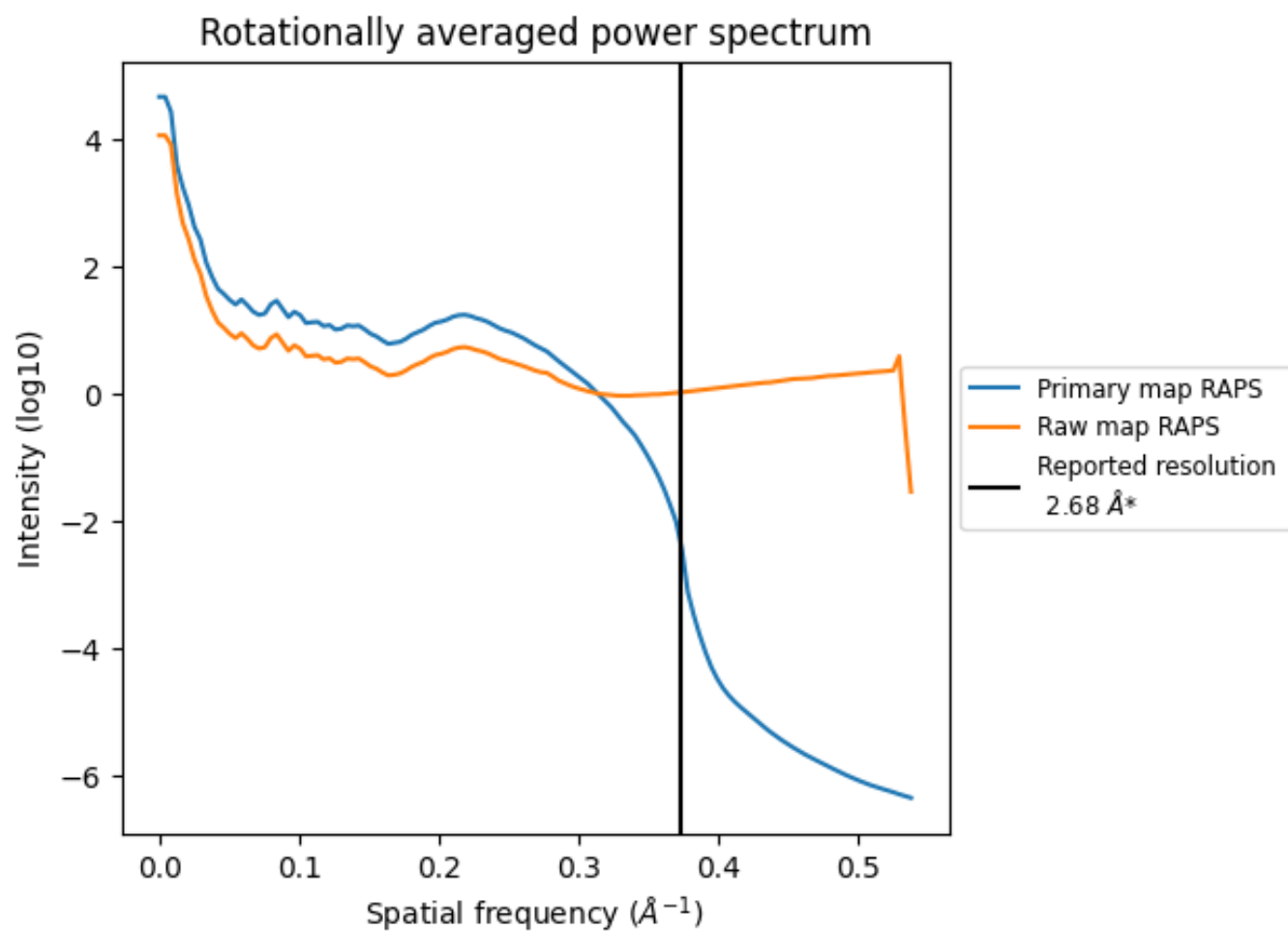
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 307 nm<sup>3</sup>; this corresponds to an approximate mass of 277 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 ⓘ



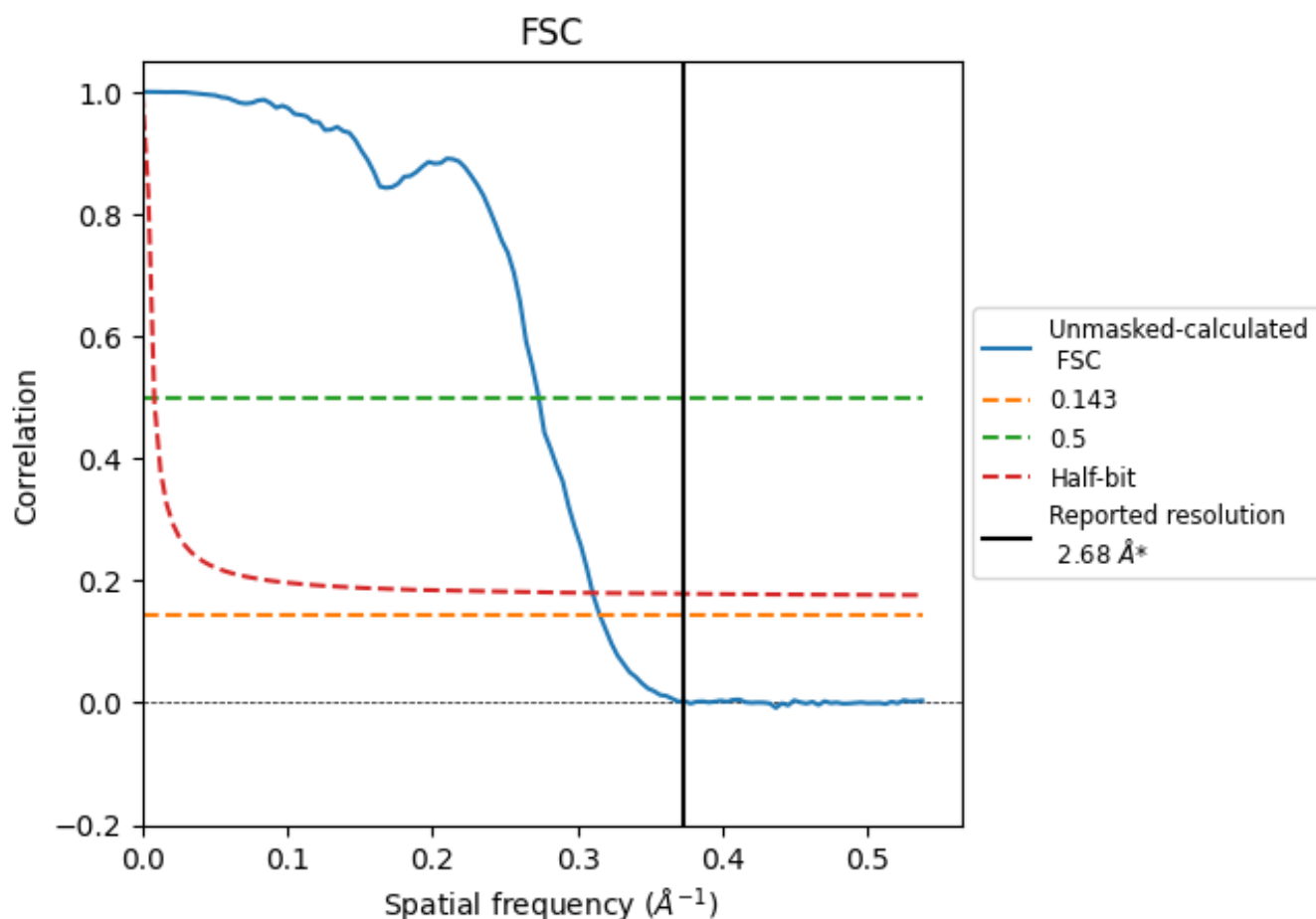
\*Reported resolution corresponds to spatial frequency of 0.373 Å<sup>-1</sup>



## 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 0.373 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

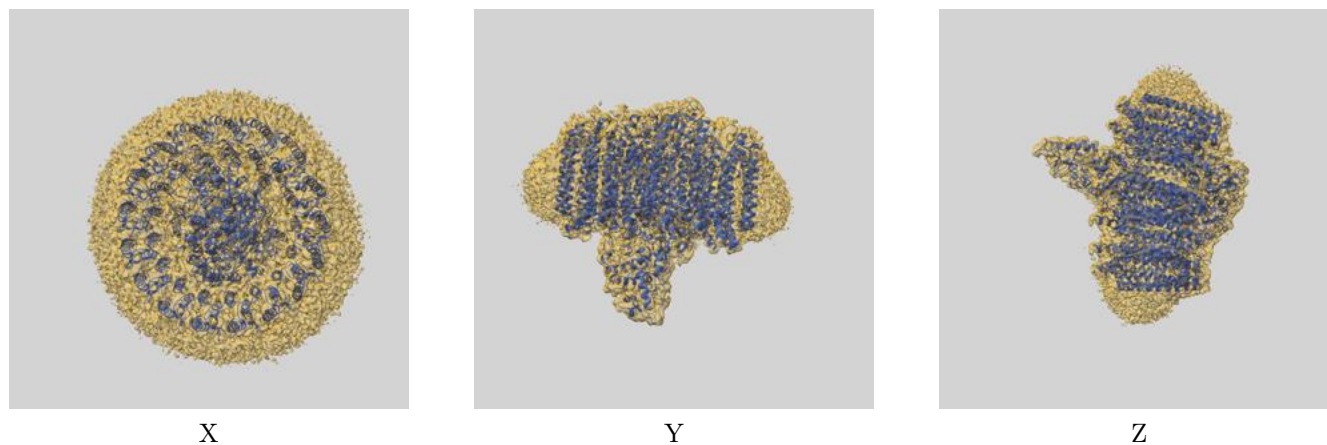
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.66	3.22

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.17 differs from the reported value 2.68 by more than 10 %

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

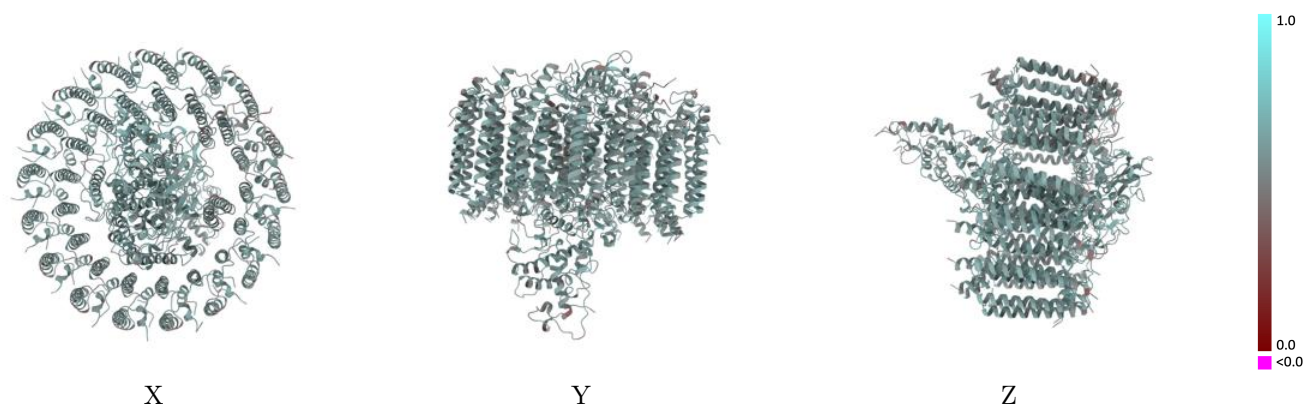
This section contains information regarding the fit between EMDB map EMD-39683 and PDB model 8YZ2. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



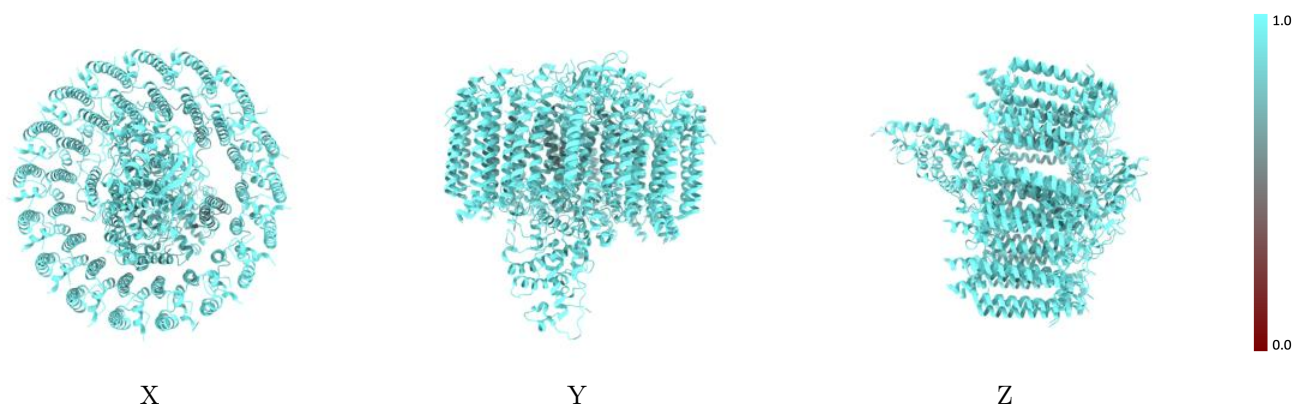
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



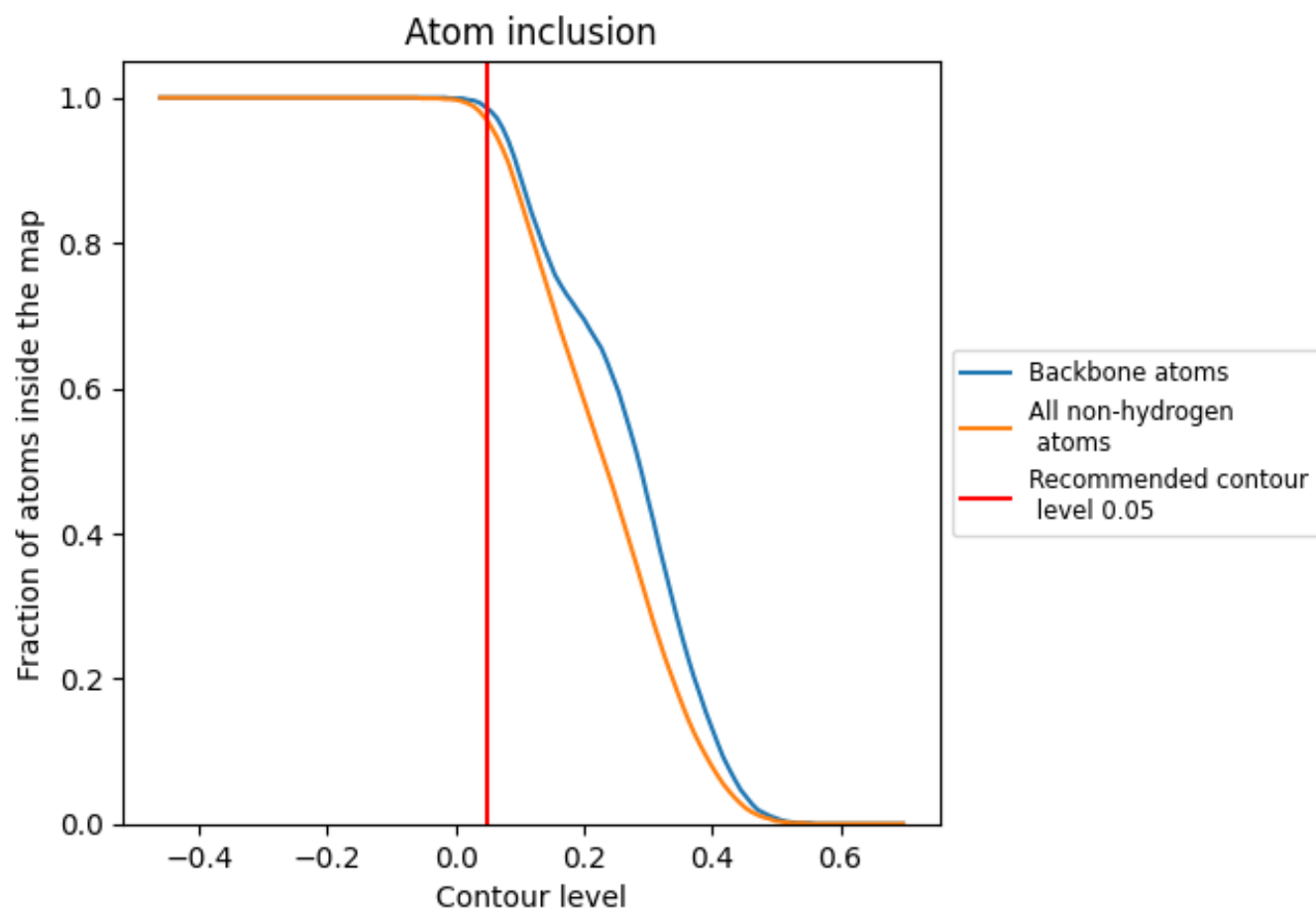
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.5800
1	 0.9600	 0.5810
2	 0.9520	 0.5530
A	 0.9520	 0.5690
B	 0.9770	 0.5810
C	 0.9760	 0.5720
D	 0.9670	 0.5890
E	 0.9750	 0.5900
F	 0.9750	 0.5920
G	 0.9610	 0.5930
H	 0.9780	 0.5910
I	 0.9770	 0.5850
J	 0.9770	 0.5900
K	 0.9770	 0.5830
L	 0.9730	 0.6040
M	 0.9790	 0.6030
N	 0.9500	 0.5600
O	 0.8260	 0.5340
P	 0.9630	 0.5820
Q	 0.9570	 0.5780
R	 0.9790	 0.5810
S	 0.9650	 0.5760
T	 0.9580	 0.5730
V	 0.9500	 0.5440
a	 0.9520	 0.5520
b	 0.9760	 0.5760
d	 0.9650	 0.5670
e	 0.9800	 0.5820
f	 0.9860	 0.5840
g	 0.9860	 0.5820
i	 0.9750	 0.5830
j	 0.9830	 0.5750
k	 0.9620	 0.5540
n	 0.9610	 0.5570
p	 0.9830	 0.5600



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
q	 0.9690	 0.5700
r	 0.9690	 0.5700
s	 0.9610	 0.5680
t	 0.9560	 0.5480
v	 0.9290	 0.5390