



## wwPDB EM Validation Summary Report ⓘ

Jun 16, 2025 – 01:23 PM JST

PDB ID : 9KM0 / pdb\_00009km0  
EMDB ID : EMD-62419  
Title : Cryo-EM structure of a tri-heme cytochrome-associated RC-LH1 complex from a marine photoheterotrophic bacterium, purified with EDTA-2Na-containing solutions  
Authors : Chen, J.H.  
Deposited on : 2024-11-15  
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

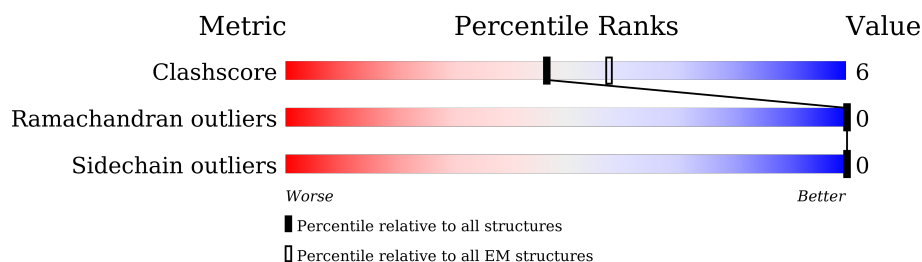
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.78 Å.

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














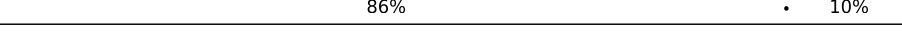







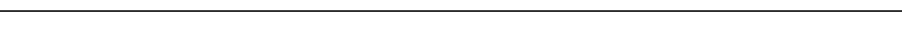

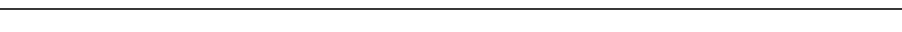
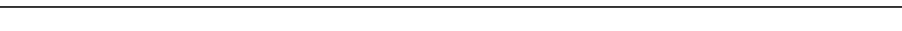


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1	53	83% 11% 6%
1	A	53	83% 13% .
1	B	53	87% 9% .
1	D	53	89% 8% .
1	E	53	77% 19% .
1	F	53	94% . .
1	G	53	89% 8% .
1	I	53	91% 6% .
1	J	53	77% 17% 6%



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Mol	Chain	Length	Quality of chain
1	K	53	 89% 8%
1	N	53	 83% 13%
1	P	53	 91% 6%
1	Q	53	 91% 6%
1	R	53	 81% 15%
1	S	53	 85% 11%
1	T	53	 74% 23%
1	V	53	 77% 19%
2	O	239	 20% 78%
3	2	49	 82% 8% 10%
3	a	49	 86% 10%
3	b	49	 86% 10%
3	d	49	 73% 16% 10%
3	e	49	 82% 8% 10%
3	f	49	 90% 10%
3	g	49	 82% 8% 10%
3	i	49	 82% 6% 12%
3	j	49	 78% 10% 12%
3	k	49	 86% 12%
3	n	49	 86% 10%
3	p	49	 86% 10%
3	q	49	 86% 10%
3	r	49	 73% 14% 12%
3	s	49	 80% 10% 10%
3	t	49	 76% 12% 12%

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Mol	Chain	Length	Quality of chain
3	v	49	 76%6%18%
4	M	330	 82%16%.
5	L	279	 84%14%.
6	H	256	 89%11%
7	C	360	 83%15%.

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	A1EFU	2	102	-	X	-	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28252 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

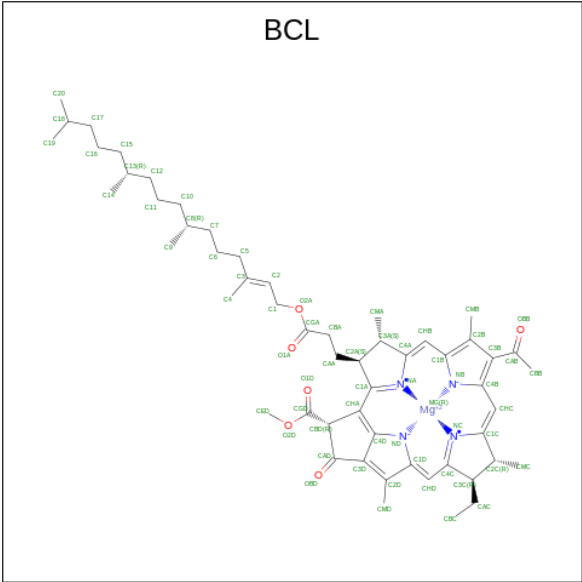
- Molecule 6 is a protein called Reaction center protein H chain.

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 (CCD ID: 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	s	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	2	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

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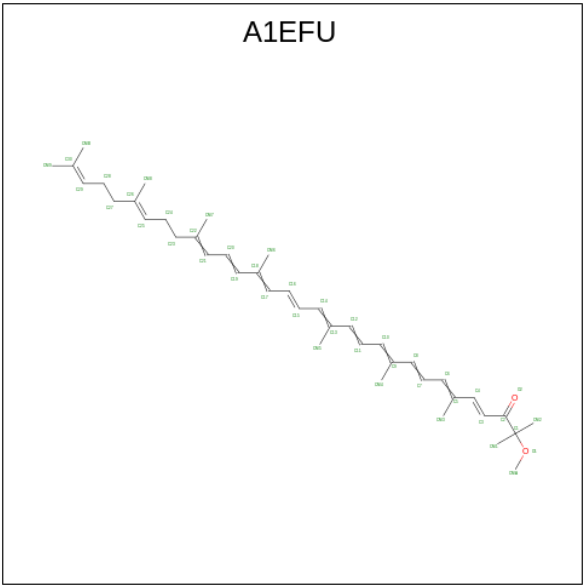
Mol	Chain	Residues	Atoms					AltConf
8	n	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	k	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	j	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	i	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	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

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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-dotriacont a-4,6,8,10,12,14,16,18,20,22,26,30-dodecaen-3-one (CCD ID: 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	P	1	Total	C	O	0
			43	41	2	
9	v	1	Total	C	O	0
			43	41	2	
9	v	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	s	1	Total	C	O	0
			43	41	2	
9	s	1	Total	C	O	0
			43	41	2	

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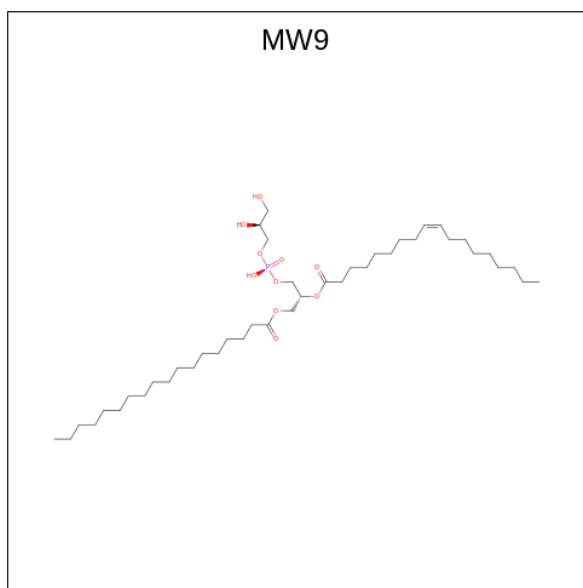
Mol	Chain	Residues	Atoms			AltConf
9	r	1	Total 43	C 41	O 2	0
9	R	1	Total 43	C 41	O 2	0
9	q	1	Total 43	C 41	O 2	0
9	p	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	2	1	Total 43	C 41	O 2	0
9	N	1	Total 43	C 41	O 2	0
9	k	1	Total 43	C 41	O 2	0
9	K	1	Total 43	C 41	O 2	0
9	j	1	Total 43	C 41	O 2	0
9	j	1	Total 43	C 41	O 2	0
9	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	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	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

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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	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	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 5 - phosphaoctacosan-21-yl (9Z)-octadec-9-enoate (CCD ID: MW9) (formula: C<sub>42</sub>H<sub>81</sub>O<sub>10</sub>P).



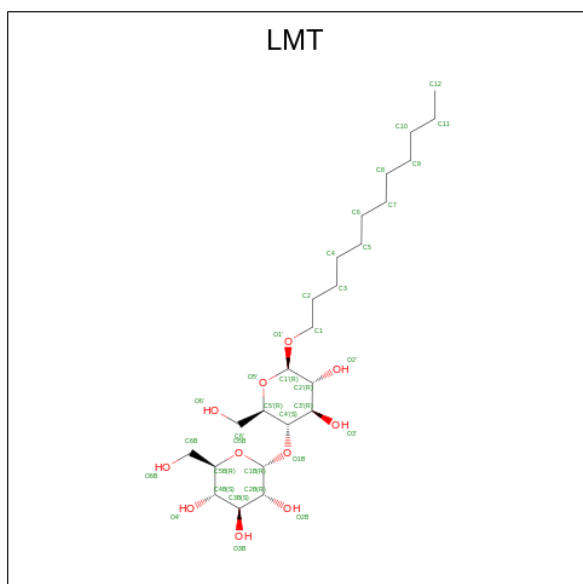
Mol	Chain	Residues	Atoms				AltConf
10	R	1	Total	C	O	P	0
			45	34	10	1	
10	G	1	Total	C	O	P	0
			49	38	10	1	
10	G	1	Total	C	O	P	0
			40	29	10	1	
10	F	1	Total	C	O	P	0
			43	32	10	1	

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Mol	Chain	Residues	Atoms				AltConf
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	H	1	Total	C	O	P	0
			48	37	10	1	
10	H	1	Total	C	O	P	0
			37	28	8	1	

- Molecule 11 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).

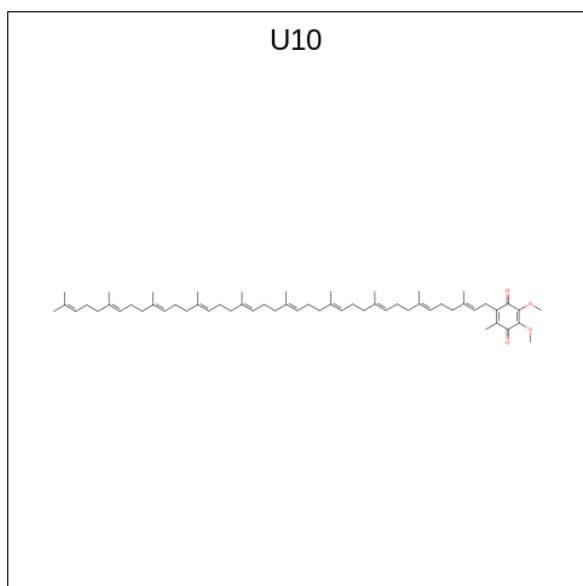


Mol	Chain	Residues	Atoms			AltConf
11	D	1	Total	C	O	0
			35	24	11	
11	L	1	Total	C	O	0
			24	18	6	
11	L	1	Total	C	O	0
			24	19	5	
11	H	1	Total	C	O	0
			24	18	6	
11	C	1	Total	C	O	0
			24	18	6	

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

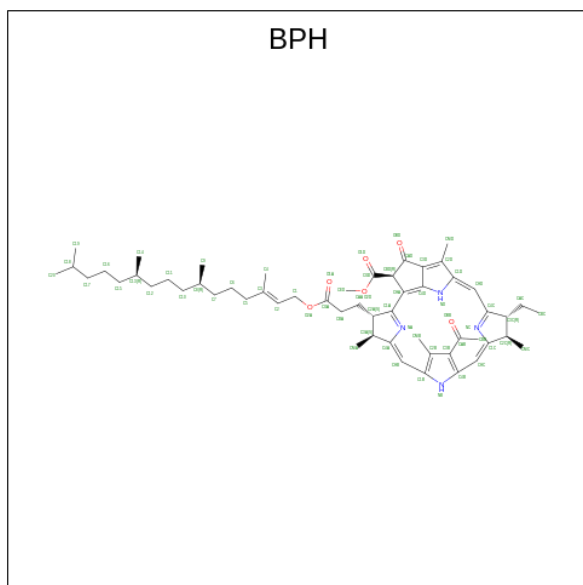
Mol	Chain	Residues	Atoms		AltConf
12	M	1	Total	Fe	0
			1	1	

- Molecule 13 is UBIQUINONE-10 (CCD ID: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



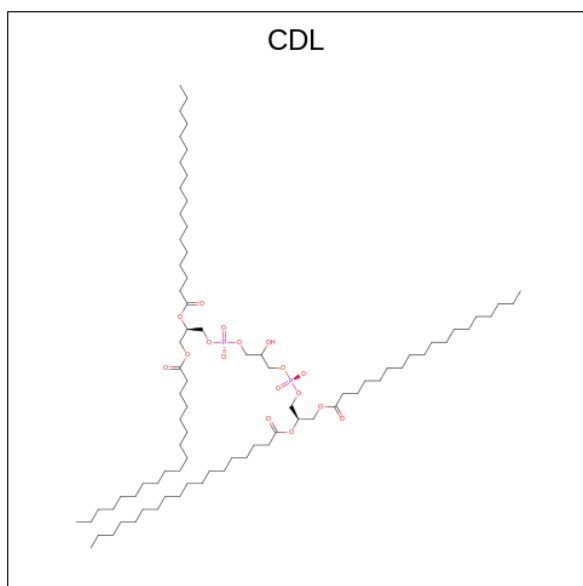
Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			63	59	4	
13	L	1	Total	C	O	0
			48	44	4	

- Molecule 14 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



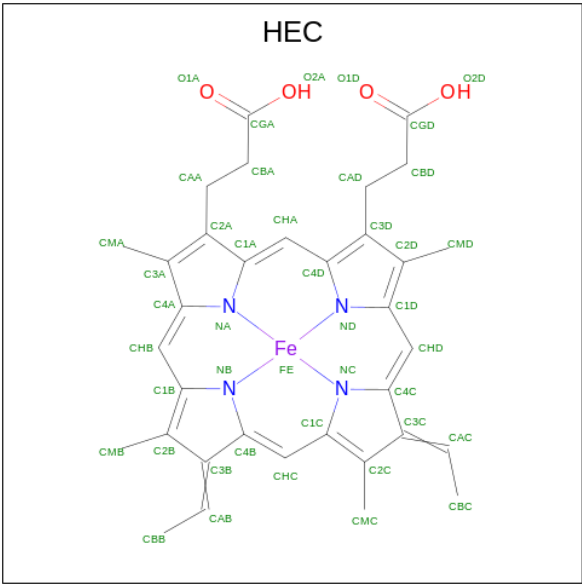
Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	N	O	0
			65	55	4	6	
14	L	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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 (CCD ID: 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	

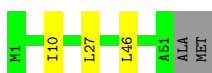


### 3 Residue-property plots


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. 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. 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:  91% 6% .




- Molecule 1: Antenna pigment protein alpha chain

Chain V:  77% 19% .



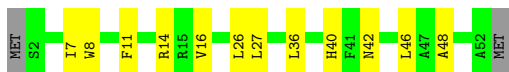
- Molecule 1: Antenna pigment protein alpha chain

Chain S:  85% 11% .



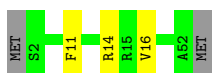
- Molecule 1: Antenna pigment protein alpha chain

Chain T:  74% 23% .




- Molecule 1: Antenna pigment protein alpha chain

Chain Q:  91% 6% .



- Molecule 1: Antenna pigment protein alpha chain

Chain R:  81% 15% .



- Molecule 1: Antenna pigment protein alpha chain

Chain 1: 83% 11% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain N: 83% 13% .



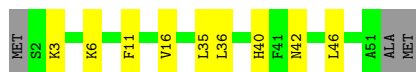
- Molecule 1: Antenna pigment protein alpha chain

Chain K: 89% 8% .



- Molecule 1: Antenna pigment protein alpha chain

Chain J: 77% 17% 6%



- Molecule 1: Antenna pigment protein alpha chain

Chain I: 91% 6% .



- Molecule 1: Antenna pigment protein alpha chain

Chain G: 89% 8% .



- Molecule 1: Antenna pigment protein alpha chain

Chain F: 94% . .



- Molecule 1: Antenna pigment protein alpha chain

Chain E: 77% 19% .



- Molecule 1: Antenna pigment protein alpha chain

Chain D: 89% 8% .



- Molecule 1: Antenna pigment protein alpha chain

Chain B: 87% 9% .



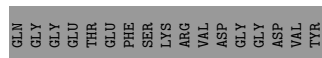
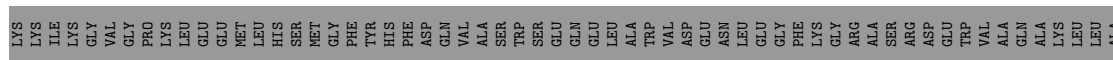
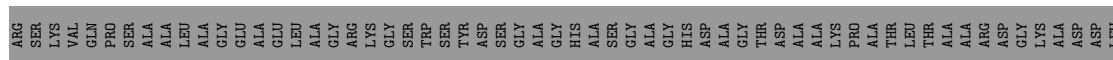
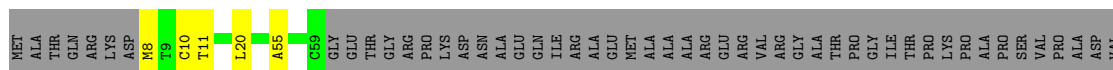
- Molecule 1: Antenna pigment protein alpha chain

Chain A: 83% 13% .



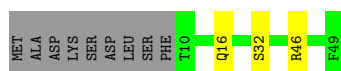
- Molecule 2: Reaction center protein O chain

Chain O: 20% . 78%

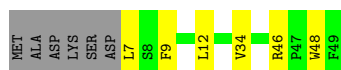
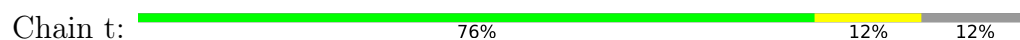


- Molecule 3: Antenna pigment protein beta chain

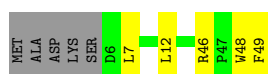
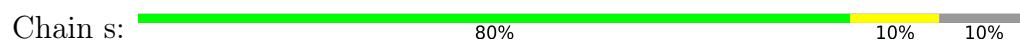
Chain v: 76% 6% 18%



- Molecule 3: Antenna pigment protein beta chain



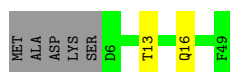
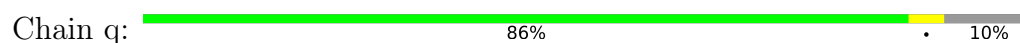
- Molecule 3: Antenna pigment protein beta chain



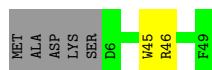
- Molecule 3: Antenna pigment protein beta chain



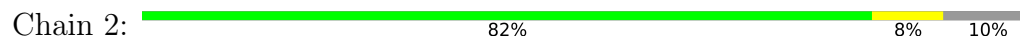
- Molecule 3: Antenna pigment protein beta chain



- Molecule 3: Antenna pigment protein beta chain

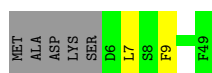


- Molecule 3: Antenna pigment protein beta chain



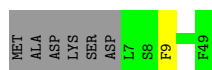
- Molecule 3: Antenna pigment protein beta chain





- Molecule 3: Antenna pigment protein beta chain

Chain k: 86% 12%



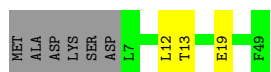
- Molecule 3: Antenna pigment protein beta chain

Chain j: 78% 10% 12%



- Molecule 3: Antenna pigment protein beta chain

Chain i: 82% 6% 12%



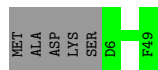
- Molecule 3: Antenna pigment protein beta chain

Chain g: 82% 8% 10%



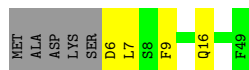
- Molecule 3: Antenna pigment protein beta chain

Chain f: 90% 10%



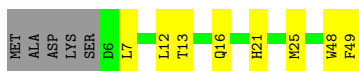
- Molecule 3: Antenna pigment protein beta chain

Chain e: 82% 8% 10%



- Molecule 3: Antenna pigment protein beta chain

Chain d: 73% 16% 10%



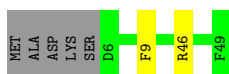
- Molecule 3: Antenna pigment protein beta chain

Chain b: 86% 10%



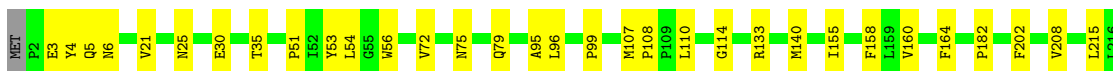
- Molecule 3: Antenna pigment protein beta chain

Chain a: 86% 10%



- Molecule 4: Reaction center protein M chain

Chain M: 82% 16%



- Molecule 5: Reaction center protein L chain

Chain L: 84% 14%



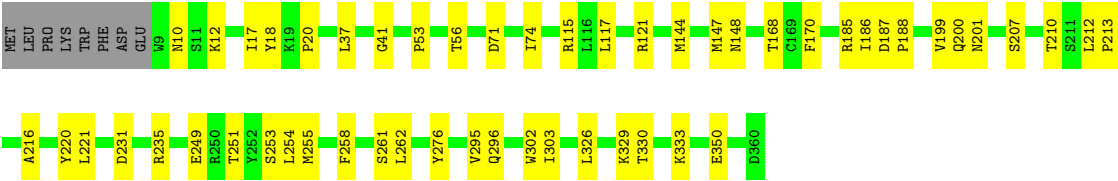
- Molecule 6: Reaction center protein H chain

Chain H: 89% 11%



- Molecule 7: Photosynthetic reaction center cytochrome c subunit

Chain C: 83% 15%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230375	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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



## 5 Model quality

### 5.1 Standard geometry

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

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	0.13	0/431	0.23	0/585
1	A	0.11	0/436	0.22	0/592
1	B	0.13	0/436	0.22	0/592
1	D	0.14	0/436	0.23	0/592
1	E	0.16	0/436	0.24	0/592
1	F	0.14	0/436	0.21	0/592
1	G	0.14	0/436	0.24	0/592
1	I	0.14	0/436	0.26	0/592
1	J	0.13	0/431	0.23	0/585
1	K	0.13	0/436	0.32	0/592
1	N	0.14	0/436	0.28	0/592
1	P	0.12	0/439	0.25	0/595
1	Q	0.11	0/436	0.20	0/592
1	R	0.11	0/436	0.21	0/592
1	S	0.12	0/436	0.24	0/592
1	T	0.12	0/436	0.23	0/592
1	V	0.10	0/436	0.21	0/592
2	O	0.11	0/378	0.24	0/516
3	2	0.12	0/371	0.21	0/508
3	a	0.09	0/371	0.18	0/508
3	b	0.12	0/371	0.19	0/508
3	d	0.14	0/371	0.21	0/508
3	e	0.13	0/371	0.16	0/508
3	f	0.13	0/371	0.20	0/508
3	g	0.12	0/371	0.17	0/508
3	i	0.12	0/363	0.24	0/497
3	j	0.12	0/363	0.24	0/497
3	k	0.11	0/363	0.22	0/497
3	n	0.11	0/371	0.18	0/508
3	p	0.11	0/371	0.28	0/508
3	q	0.11	0/371	0.21	0/508
3	r	0.11	0/363	0.21	0/497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	s	0.12	0/371	0.25	0/508
3	t	0.09	0/363	0.17	0/497
3	v	0.08	0/337	0.15	0/462
4	M	0.16	0/2731	0.27	0/3735
5	L	0.16	0/2267	0.28	0/3105
6	H	0.13	0/2072	0.23	0/2804
7	C	0.15	0/2819	0.31	0/3869
All	All	0.13	0/23905	0.25	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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	417	0	419	5	0
1	A	422	0	426	9	0
1	B	422	0	426	4	0
1	D	422	0	426	4	0
1	E	422	0	426	9	0
1	F	422	0	425	2	0
1	G	422	0	426	3	0
1	I	422	0	426	2	0
1	J	417	0	421	7	0
1	K	422	0	426	3	0
1	N	422	0	426	4	0
1	P	425	0	433	3	0
1	Q	422	0	426	2	0
1	R	422	0	426	6	0
1	S	422	0	426	6	0
1	T	422	0	426	9	0
1	V	422	0	426	8	0
2	O	371	0	395	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	358	0	338	5	0
3	a	358	0	338	2	0
3	b	358	0	338	2	0
3	d	358	0	338	9	0
3	e	358	0	338	5	0
3	f	358	0	338	0	0
3	g	358	0	338	2	0
3	i	350	0	334	2	0
3	j	350	0	334	5	0
3	k	350	0	334	1	0
3	n	358	0	338	5	0
3	p	358	0	338	2	0
3	q	358	0	338	2	0
3	r	350	0	334	6	0
3	s	358	0	338	4	0
3	t	350	0	334	9	0
3	v	325	0	309	4	0
4	M	2633	0	2524	42	0
5	L	2178	0	2118	36	0
6	H	2022	0	1971	23	0
7	C	2741	0	2584	40	0
8	1	66	0	74	0	0
8	2	66	0	74	4	0
8	A	66	0	74	5	0
8	B	66	0	74	4	0
8	D	66	0	74	2	0
8	E	66	0	74	2	0
8	F	132	0	146	4	0
8	G	132	0	146	4	0
8	I	66	0	74	1	0
8	J	66	0	74	3	0
8	K	66	0	74	2	0
8	L	132	0	143	8	0
8	M	132	0	144	5	0
8	N	66	0	74	2	0
8	P	132	0	146	2	0
8	Q	66	0	74	1	0
8	R	66	0	74	6	0
8	S	66	0	74	0	0
8	V	66	0	72	3	0
8	a	66	0	74	2	0
8	b	66	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	d	66	0	74	8	0
8	e	66	0	74	4	0
8	i	66	0	74	2	0
8	j	66	0	74	7	0
8	k	66	0	74	1	0
8	n	66	0	74	3	0
8	q	66	0	74	2	0
8	r	66	0	74	4	0
8	s	132	0	147	8	0
8	t	66	0	73	9	0
8	v	66	0	74	5	0
9	2	129	0	0	0	0
9	A	43	0	0	0	0
9	B	86	0	0	0	0
9	D	86	0	0	0	0
9	E	86	0	0	0	0
9	F	43	0	0	0	0
9	G	86	0	0	0	0
9	I	43	0	0	0	0
9	J	86	0	0	0	0
9	K	43	0	0	0	0
9	M	43	0	0	0	0
9	N	43	0	0	0	0
9	P	43	0	0	0	0
9	R	43	0	0	0	0
9	T	43	0	0	0	0
9	a	43	0	0	0	0
9	f	43	0	0	0	0
9	j	86	0	0	0	0
9	k	43	0	0	0	0
9	p	43	0	0	0	0
9	q	43	0	0	0	0
9	r	43	0	0	0	0
9	s	129	0	0	1	0
9	v	86	0	0	0	0
10	D	53	0	0	0	0
10	F	43	0	0	0	0
10	G	89	0	0	0	0
10	H	85	0	0	0	0
10	L	37	0	0	0	0
10	M	102	0	0	0	0
10	R	45	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	24	0	34	2	0
11	D	35	0	45	1	0
11	H	24	0	34	0	0
11	L	48	0	65	1	0
12	M	1	0	0	0	0
13	L	48	0	63	5	0
13	M	63	0	90	7	0
14	L	65	0	76	0	0
14	M	65	0	73	2	0
15	H	91	0	135	3	0
15	L	67	0	78	1	0
16	C	129	0	88	5	0
All	All	28252	0	26099	322	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 322 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:144:MET:SD	16:C:401:HEC:NC	2.37	0.98
5:L:131:THR:HA	5:L:135:PHE:HB2	1.63	0.81
7:C:144:MET:SD	16:C:401:HEC:FE	1.73	0.80
7:C:144:MET:SD	16:C:401:HEC:NB	2.58	0.77
3:d:48:TRP:CE2	8:d:101:BCL:HHC	2.22	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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%)	48 (98%)	1 (2%)	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%)	49 (100%)	0	0	100	100
1	T	49/53 (92%)	48 (98%)	1 (2%)	0	100	100
1	V	49/53 (92%)	49 (100%)	0	0	100	100
2	O	50/239 (21%)	46 (92%)	4 (8%)	0	100	100
3	2	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	a	42/49 (86%)	42 (100%)	0	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%)	42 (100%)	0	0	100	100
3	g	42/49 (86%)	41 (98%)	1 (2%)	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%)	42 (100%)	0	0	100	100
3	p	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
3	q	42/49 (86%)	42 (100%)	0	0	100	100
3	r	41/49 (84%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	s	42/49 (86%)	40 (95%)	2 (5%)	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%)	312 (97%)	11 (3%)	0	100	100
5	L	272/279 (98%)	266 (98%)	6 (2%)	0	100	100
6	H	254/256 (99%)	250 (98%)	4 (2%)	0	100	100
7	C	350/360 (97%)	330 (94%)	20 (6%)	0	100	100
All	All	2785/3198 (87%)	2729 (98%)	56 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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%)	299 (100%)	0	100	100
All	All	2371/2633 (90%)	2371 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
6	H	34	ASN

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Mol	Chain	Res	Type
7	C	42	GLN
7	C	321	ASN
7	C	201	ASN
6	H	174	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 98 ligands modelled in this entry, 1 is monoatomic - leaving 97 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	$\# Z  > 2$
9	A1EFU	G	105	-	40,42,42	1.69	8 (20%)	45,52,52	3.57	19 (42%)
9	A1EFU	r	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.78	19 (42%)
8	BCL	R	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.24	27 (34%)
13	U10	L	303	-	48,48,63	0.17	0	58,61,79	0.44	1 (1%)
8	BCL	t	101	-	64,74,74	1.76	13 (20%)	78,115,115	2.09	25 (32%)
10	MW9	F	103	-	42,42,52	1.43	6 (14%)	45,48,58	1.46	3 (6%)
8	BCL	P	102	-	64,74,74	1.73	13 (20%)	78,115,115	2.20	24 (30%)
9	A1EFU	K	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.65	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	K	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.31	27 (34%)
11	LMT	H	302	-	24,24,36	1.04	2 (8%)	29,29,47	1.07	2 (6%)
9	A1EFU	M	407	-	40,42,42	1.68	8 (20%)	45,52,52	3.56	20 (44%)
11	LMT	L	306	-	24,24,36	1.04	2 (8%)	29,29,47	1.18	2 (6%)
9	A1EFU	B	103	-	40,42,42	1.68	8 (20%)	45,52,52	3.68	20 (44%)
8	BCL	s	102	-	64,74,74	1.73	14 (21%)	78,115,115	2.34	28 (35%)
8	BCL	q	102	-	64,74,74	1.72	12 (18%)	78,115,115	2.26	29 (37%)
9	A1EFU	E	103	-	40,42,42	1.68	7 (17%)	45,52,52	3.82	20 (44%)
8	BCL	P	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.24	26 (33%)
9	A1EFU	N	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.69	20 (44%)
8	BCL	2	103	-	64,74,74	1.72	13 (20%)	78,115,115	2.30	28 (35%)
8	BCL	s	103	-	64,74,74	1.72	11 (17%)	78,115,115	2.24	26 (33%)
10	MW9	M	406	-	52,52,52	1.45	6 (11%)	55,58,58	1.47	3 (5%)
9	A1EFU	j	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.99	20 (44%)
8	BCL	e	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.26	27 (34%)
8	BCL	l	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.30	27 (34%)
8	BCL	E	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.30	29 (37%)
10	MW9	H	301	-	47,47,52	1.39	6 (12%)	50,53,58	1.45	4 (8%)
9	A1EFU	q	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.70	21 (46%)
9	A1EFU	P	103	-	40,42,42	1.69	9 (22%)	45,52,52	3.73	20 (44%)
8	BCL	L	301	-	64,74,74	1.71	12 (18%)	78,115,115	2.38	29 (37%)
8	BCL	G	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.27	27 (34%)
9	A1EFU	s	105	-	40,42,42	1.68	9 (22%)	45,52,52	3.80	20 (44%)
14	BPH	M	408	-	51,70,70	0.82	2 (3%)	52,101,101	0.66	1 (1%)
9	A1EFU	2	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.66	20 (44%)
11	LMT	D	102	-	36,36,36	1.17	5 (13%)	47,47,47	0.96	2 (4%)
8	BCL	i	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.32	27 (34%)
8	BCL	G	102	-	64,74,74	1.73	12 (18%)	78,115,115	2.30	27 (34%)
8	BCL	I	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.33	26 (33%)
9	A1EFU	D	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.63	20 (44%)
9	A1EFU	f	101	-	40,42,42	1.68	8 (20%)	45,52,52	3.79	19 (42%)
8	BCL	B	101	-	64,74,74	1.70	11 (17%)	78,115,115	2.29	26 (33%)
9	A1EFU	J	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.56	20 (44%)
8	BCL	L	304	-	64,74,74	1.72	12 (18%)	78,115,115	2.37	29 (37%)
10	MW9	R	103	-	44,44,52	1.47	5 (11%)	47,50,58	1.52	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	HEC	C	402	7	32,50,50	2.04	4 (12%)	24,82,82	2.30	10 (41%)
8	BCL	a	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.29	28 (35%)
9	A1EFU	R	101	-	40,42,42	1.68	8 (20%)	45,52,52	3.67	20 (44%)
9	A1EFU	v	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.73	20 (44%)
9	A1EFU	s	101	-	40,42,42	1.68	7 (17%)	45,52,52	3.88	20 (44%)
8	BCL	F	101	-	64,74,74	1.72	10 (15%)	78,115,115	2.23	29 (37%)
13	U10	M	404	-	63,63,63	0.17	0	76,79,79	0.41	1 (1%)
9	A1EFU	v	103	-	40,42,42	1.67	8 (20%)	45,52,52	3.69	19 (42%)
9	A1EFU	p	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.91	20 (44%)
8	BCL	r	101	-	64,74,74	1.73	12 (18%)	78,115,115	2.25	26 (33%)
9	A1EFU	J	103	-	40,42,42	1.68	9 (22%)	45,52,52	3.93	20 (44%)
8	BCL	D	101	-	64,74,74	1.71	11 (17%)	78,115,115	2.26	27 (34%)
9	A1EFU	j	103	-	40,42,42	1.69	8 (20%)	45,52,52	3.79	20 (44%)
10	MW9	L	307	-	36,36,52	1.47	5 (13%)	39,42,58	1.54	3 (7%)
8	BCL	S	101	-	64,74,74	1.71	12 (18%)	78,115,115	2.25	26 (33%)
10	MW9	G	103	-	48,48,52	1.49	6 (12%)	51,54,58	1.48	4 (7%)
10	MW9	D	103	-	52,52,52	1.45	6 (11%)	55,58,58	1.46	3 (5%)
9	A1EFU	B	102	-	40,42,42	1.69	9 (22%)	45,52,52	3.69	20 (44%)
9	A1EFU	D	105	-	40,42,42	1.68	8 (20%)	45,52,52	3.91	20 (44%)
8	BCL	v	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.25	26 (33%)
8	BCL	Q	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.25	26 (33%)
9	A1EFU	A	102	-	40,42,42	1.70	9 (22%)	45,52,52	3.77	19 (42%)
15	CDL	H	304	-	90,90,99	0.91	8 (8%)	96,102,111	1.14	4 (4%)
8	BCL	M	402	-	64,74,74	1.72	10 (15%)	78,115,115	2.23	24 (30%)
14	BPH	L	302	-	51,70,70	0.52	1 (1%)	52,101,101	0.71	1 (1%)
11	LMT	C	404	-	24,24,36	1.05	2 (8%)	29,29,47	1.06	1 (3%)
16	HEC	C	401	7	32,50,50	2.01	4 (12%)	24,82,82	2.25	11 (45%)
9	A1EFU	2	101	-	40,42,42	1.68	9 (22%)	45,52,52	3.77	20 (44%)
8	BCL	k	102	-	64,74,74	1.73	11 (17%)	78,115,115	2.26	26 (33%)
10	MW9	H	303	-	36,36,52	1.56	7 (19%)	39,41,58	1.88	3 (7%)
8	BCL	N	101	-	64,74,74	1.72	12 (18%)	78,115,115	2.31	26 (33%)
15	CDL	L	308	-	66,66,99	1.05	8 (12%)	72,78,111	1.16	4 (5%)
8	BCL	F	102	-	64,74,74	1.73	12 (18%)	78,115,115	2.30	28 (35%)
9	A1EFU	E	102	-	40,42,42	1.69	7 (17%)	45,52,52	3.67	19 (42%)
8	BCL	V	101	-	64,74,74	1.69	11 (17%)	78,115,115	2.27	29 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BCL	b	101	-	64,74,74	1.72	11 (17%)	78,115,115	2.26	28 (35%)
11	LMT	L	305	-	24,24,36	1.05	2 (8%)	29,29,47	1.10	2 (6%)
8	BCL	M	403	-	64,74,74	1.72	13 (20%)	78,115,115	2.30	28 (35%)
9	A1EFU	T	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.72	20 (44%)
9	A1EFU	F	104	-	40,42,42	1.68	7 (17%)	45,52,52	3.74	19 (42%)
9	A1EFU	I	102	-	40,42,42	1.68	7 (17%)	45,52,52	3.98	20 (44%)
9	A1EFU	G	106	-	40,42,42	1.67	7 (17%)	45,52,52	4.00	19 (42%)
8	BCL	J	101	-	64,74,74	1.73	11 (17%)	78,115,115	2.30	27 (34%)
8	BCL	n	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.25	27 (34%)
10	MW9	M	405	-	48,48,52	1.48	6 (12%)	51,54,58	1.51	3 (5%)
9	A1EFU	s	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.26	20 (44%)
10	MW9	G	104	-	39,39,52	1.42	5 (12%)	42,45,58	1.18	3 (7%)
9	A1EFU	k	101	-	40,42,42	1.69	9 (22%)	45,52,52	3.98	20 (44%)
8	BCL	d	101	-	64,74,74	1.74	11 (17%)	78,115,115	2.26	23 (29%)
9	A1EFU	2	104	-	40,42,42	1.69	9 (22%)	45,52,52	3.48	21 (46%)
8	BCL	j	102	-	64,74,74	1.73	12 (18%)	78,115,115	2.28	27 (34%)
8	BCL	A	101	-	64,74,74	1.73	13 (20%)	78,115,115	2.18	26 (33%)
9	A1EFU	a	102	-	40,42,42	1.70	9 (22%)	45,52,52	4.01	20 (44%)
16	HEC	C	403	7	32,50,50	2.02	4 (12%)	24,82,82	2.32	12 (50%)

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
9	A1EFU	G	105	-	-	25/50/51/51	-
9	A1EFU	r	102	-	-	21/50/51/51	-
8	BCL	R	102	-	-	9/37/137/137	-
13	U10	L	303	-	-	13/45/69/87	0/1/1/1
8	BCL	t	101	-	-	12/37/137/137	-
10	MW9	F	103	-	-	33/47/47/57	-
8	BCL	P	102	-	-	16/37/137/137	-
9	A1EFU	K	102	-	-	21/50/51/51	-
8	BCL	K	101	-	-	10/37/137/137	-
11	LMT	H	302	-	-	6/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1EFU	M	407	-	-	17/50/51/51	-
11	LMT	L	306	-	-	8/15/35/61	0/1/1/2
9	A1EFU	B	103	-	-	19/50/51/51	-
8	BCL	s	102	-	-	10/37/137/137	-
8	BCL	q	102	-	-	14/37/137/137	-
9	A1EFU	E	103	-	-	19/50/51/51	-
8	BCL	P	101	-	-	14/37/137/137	-
9	A1EFU	N	102	-	-	23/50/51/51	-
8	BCL	2	103	-	-	20/37/137/137	-
8	BCL	s	103	-	-	19/37/137/137	-
10	MW9	M	406	-	-	34/57/57/57	-
9	A1EFU	j	101	-	-	25/50/51/51	-
8	BCL	e	101	-	-	11/37/137/137	-
8	BCL	1	101	-	-	13/37/137/137	-
8	BCL	E	101	-	-	10/37/137/137	-
10	MW9	H	301	-	-	27/52/52/57	-
9	A1EFU	q	101	-	-	24/50/51/51	-
9	A1EFU	P	103	-	-	22/50/51/51	-
8	BCL	L	301	-	-	17/37/137/137	-
8	BCL	G	101	-	-	13/37/137/137	-
9	A1EFU	s	105	-	-	24/50/51/51	-
14	BPH	M	408	-	-	10/37/105/105	0/5/6/6
9	A1EFU	2	102	-	-	29/50/51/51	-
11	LMT	D	102	-	-	7/21/61/61	0/2/2/2
8	BCL	i	101	-	-	21/37/137/137	-
8	BCL	G	102	-	-	15/37/137/137	-
8	BCL	I	101	-	-	11/37/137/137	-
9	A1EFU	D	104	-	-	17/50/51/51	-
9	A1EFU	f	101	-	-	18/50/51/51	-
8	BCL	B	101	-	-	15/37/137/137	-
9	A1EFU	J	102	-	-	14/50/51/51	-
8	BCL	L	304	-	-	17/37/137/137	-
10	MW9	R	103	-	-	34/49/49/57	-
16	HEC	C	402	7	-	4/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	a	101	-	-	19/37/137/137	-
9	A1EFU	R	101	-	-	19/50/51/51	-
9	A1EFU	v	102	-	-	23/50/51/51	-
9	A1EFU	s	101	-	-	20/50/51/51	-
8	BCL	F	101	-	-	16/37/137/137	-
13	U10	M	404	-	-	10/63/87/87	0/1/1/1
9	A1EFU	v	103	-	-	24/50/51/51	-
9	A1EFU	p	101	-	-	19/50/51/51	-
8	BCL	r	101	-	-	11/37/137/137	-
9	A1EFU	J	103	-	-	20/50/51/51	-
8	BCL	D	101	-	-	9/37/137/137	-
9	A1EFU	j	103	-	-	19/50/51/51	-
10	MW9	L	307	-	-	15/41/41/57	-
8	BCL	S	101	-	-	13/37/137/137	-
10	MW9	G	103	-	-	27/53/53/57	-
10	MW9	D	103	-	-	29/57/57/57	-
9	A1EFU	B	102	-	-	16/50/51/51	-
9	A1EFU	D	105	-	-	19/50/51/51	-
8	BCL	v	101	-	-	19/37/137/137	-
8	BCL	Q	101	-	-	21/37/137/137	-
9	A1EFU	A	102	-	-	19/50/51/51	-
15	CDL	H	304	-	-	46/101/101/110	-
8	BCL	M	402	-	-	14/37/137/137	-
14	BPH	L	302	-	-	8/37/105/105	0/5/6/6
11	LMT	C	404	-	-	5/15/35/61	0/1/1/2
16	HEC	C	401	7	-	3/10/54/54	-
9	A1EFU	2	101	-	-	20/50/51/51	-
8	BCL	k	102	-	-	10/37/137/137	-
10	MW9	H	303	-	-	22/38/38/57	-
8	BCL	N	101	-	-	10/37/137/137	-
15	CDL	L	308	-	-	41/77/77/110	-
8	BCL	F	102	-	-	10/37/137/137	-
9	A1EFU	E	102	-	-	18/50/51/51	-
8	BCL	V	101	-	-	7/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	b	101	-	-	11/37/137/137	-
11	LMT	L	305	-	-	5/15/35/61	0/1/1/2
8	BCL	M	403	-	-	20/37/137/137	-
9	A1EFU	T	101	-	-	21/50/51/51	-
9	A1EFU	F	104	-	-	21/50/51/51	-
9	A1EFU	I	102	-	-	20/50/51/51	-
9	A1EFU	G	106	-	-	24/50/51/51	-
8	BCL	J	101	-	-	12/37/137/137	-
8	BCL	n	101	-	-	11/37/137/137	-
10	MW9	M	405	-	-	30/53/53/57	-
9	A1EFU	s	104	-	-	22/50/51/51	-
10	MW9	G	104	-	-	27/44/44/57	-
9	A1EFU	k	101	-	-	25/50/51/51	-
8	BCL	d	101	-	-	25/37/137/137	-
9	A1EFU	2	104	-	-	22/50/51/51	-
8	BCL	j	102	-	-	14/37/137/137	-
8	BCL	A	101	-	-	14/37/137/137	-
9	A1EFU	a	102	-	-	18/50/51/51	-
16	HEC	C	403	7	-	2/10/54/54	-

The worst 5 of 843 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	403	HEC	C3C-C2C	-6.44	1.34	1.40
16	C	401	HEC	C2B-C3B	-6.28	1.34	1.40
16	C	402	HEC	C2B-C3B	-6.27	1.34	1.40
16	C	401	HEC	C3C-C2C	-6.20	1.34	1.40

The worst 5 of 1801 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	j	101	A1EFU	C11-C10-C9	-11.21	111.31	127.31
9	k	101	A1EFU	C7-C6-C5	-10.60	112.18	127.31
9	a	102	A1EFU	C7-C6-C5	-10.56	112.24	127.31
9	a	102	A1EFU	C15-C14-C13	-10.54	112.27	127.31
9	I	102	A1EFU	C7-C6-C5	-10.35	112.53	127.31

There are no chirality outliers.

5 of 1706 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	O1A-CGA-O2A-C1
8	P	102	BCL	C1-C2-C3-C4

There are no ring outliers.

46 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	R	102	BCL	6	0
13	L	303	U10	5	0
8	t	101	BCL	9	0
8	P	102	BCL	2	0
8	K	101	BCL	2	0
8	s	102	BCL	7	0
8	q	102	BCL	2	0
8	2	103	BCL	4	0
8	s	103	BCL	2	0
8	e	101	BCL	4	0
8	E	101	BCL	2	0
8	L	301	BCL	3	0
8	G	101	BCL	2	0
14	M	408	BPH	2	0
11	D	102	LMT	1	0
8	i	101	BCL	2	0
8	G	102	BCL	2	0
8	I	101	BCL	1	0
8	B	101	BCL	4	0
8	L	304	BCL	6	0
10	R	103	MW9	1	0
8	a	101	BCL	2	0
8	F	101	BCL	4	0
13	M	404	U10	7	0
8	r	101	BCL	4	0
8	D	101	BCL	2	0
8	v	101	BCL	5	0
8	Q	101	BCL	1	0
15	H	304	CDL	3	0
8	M	402	BCL	3	0

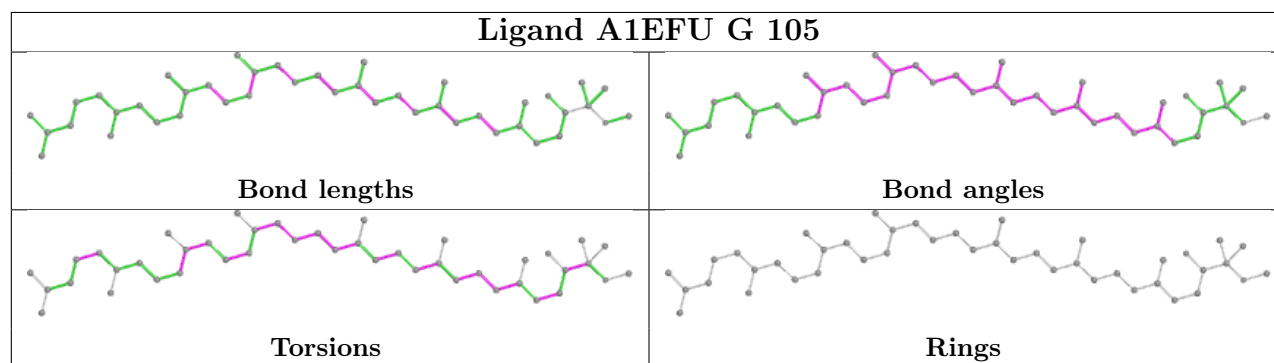
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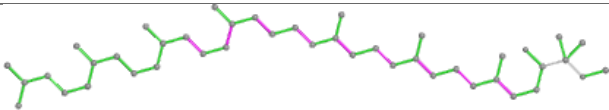
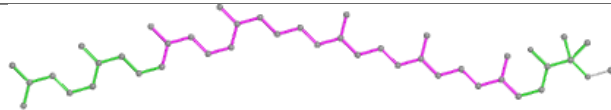
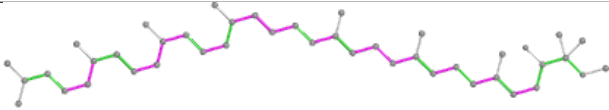
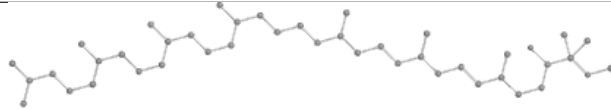


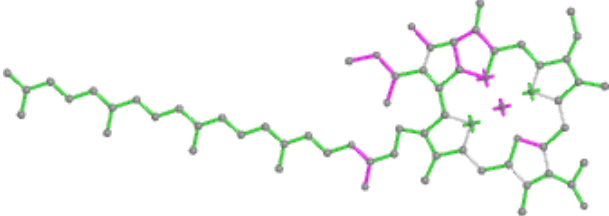
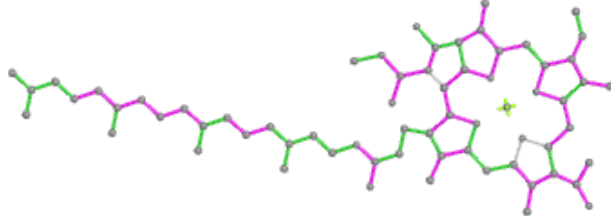
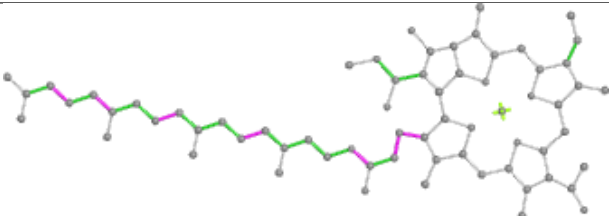
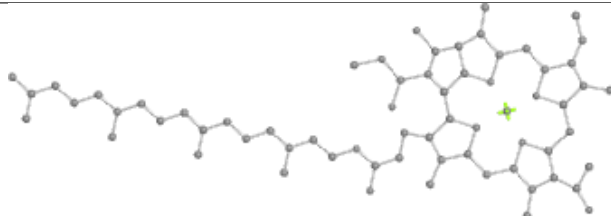
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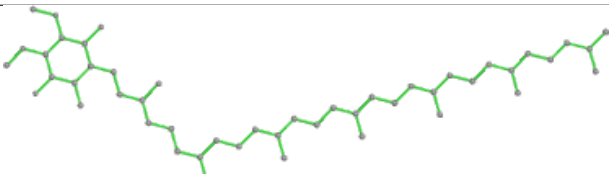
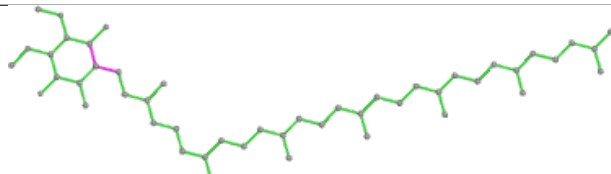
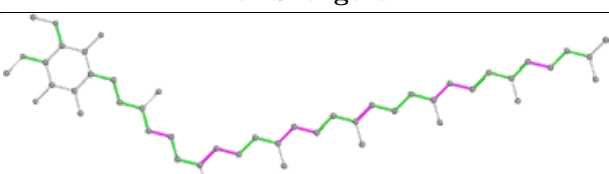
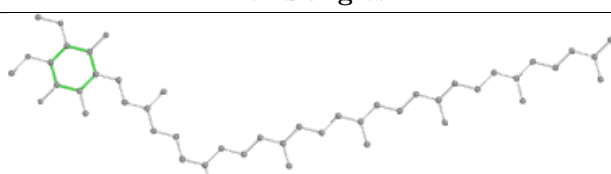
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	404	LMT	2	0
16	C	401	HEC	5	0
8	k	102	BCL	1	0
8	N	101	BCL	2	0
15	L	308	CDL	1	0
8	F	102	BCL	1	0
8	V	101	BCL	3	0
8	b	101	BCL	2	0
11	L	305	LMT	1	0
8	M	403	BCL	3	0
8	J	101	BCL	3	0
8	n	101	BCL	3	0
9	s	104	A1EFU	1	0
8	d	101	BCL	8	0
8	j	102	BCL	7	0
8	A	101	BCL	5	0

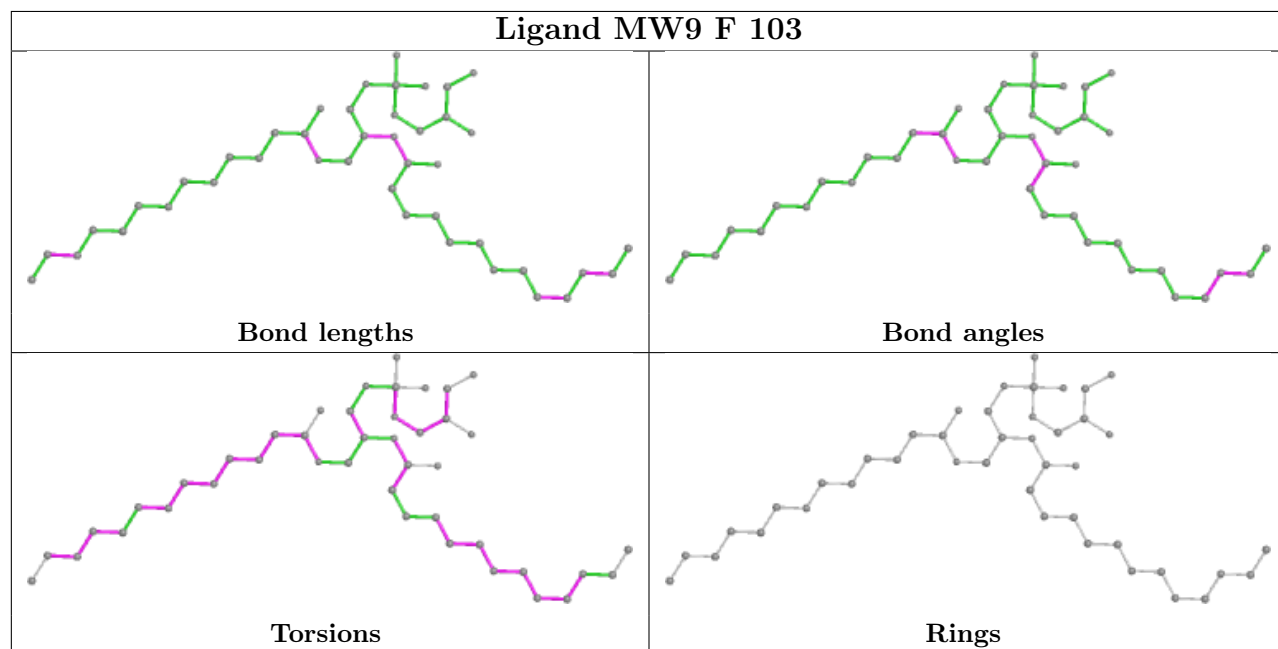
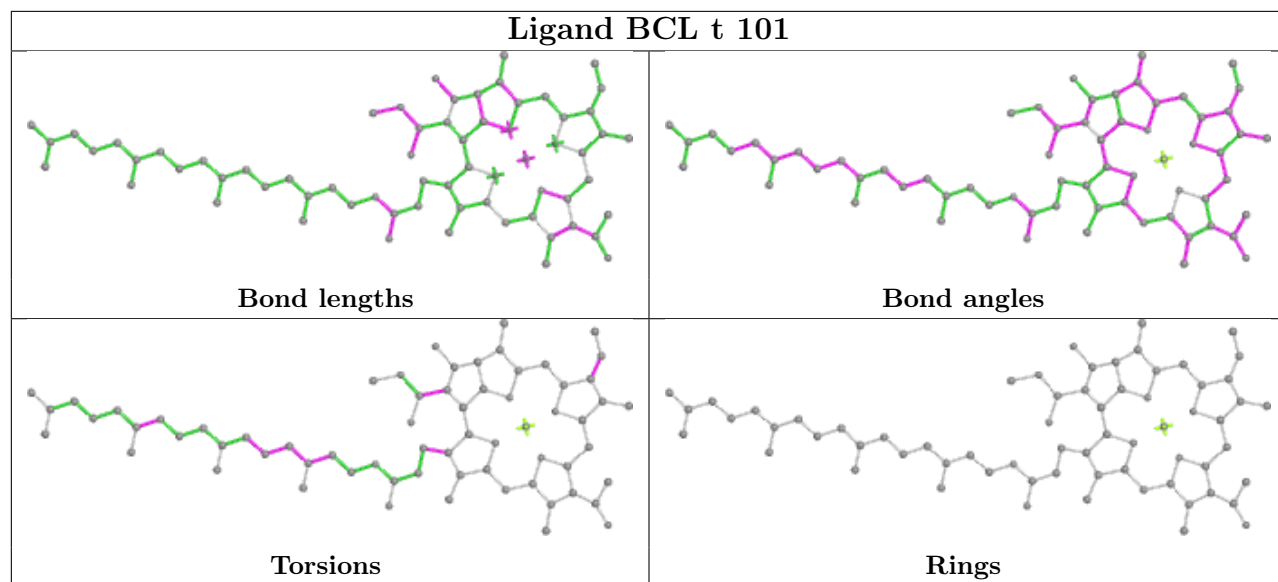
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

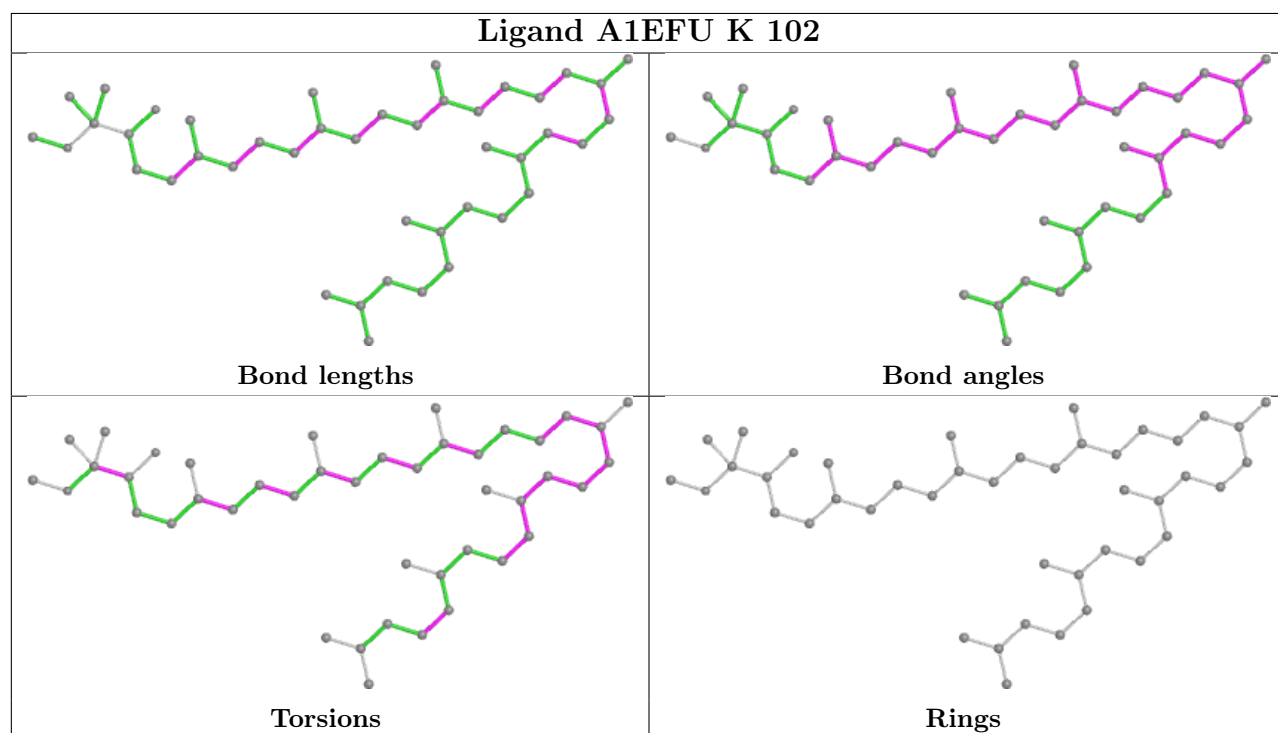
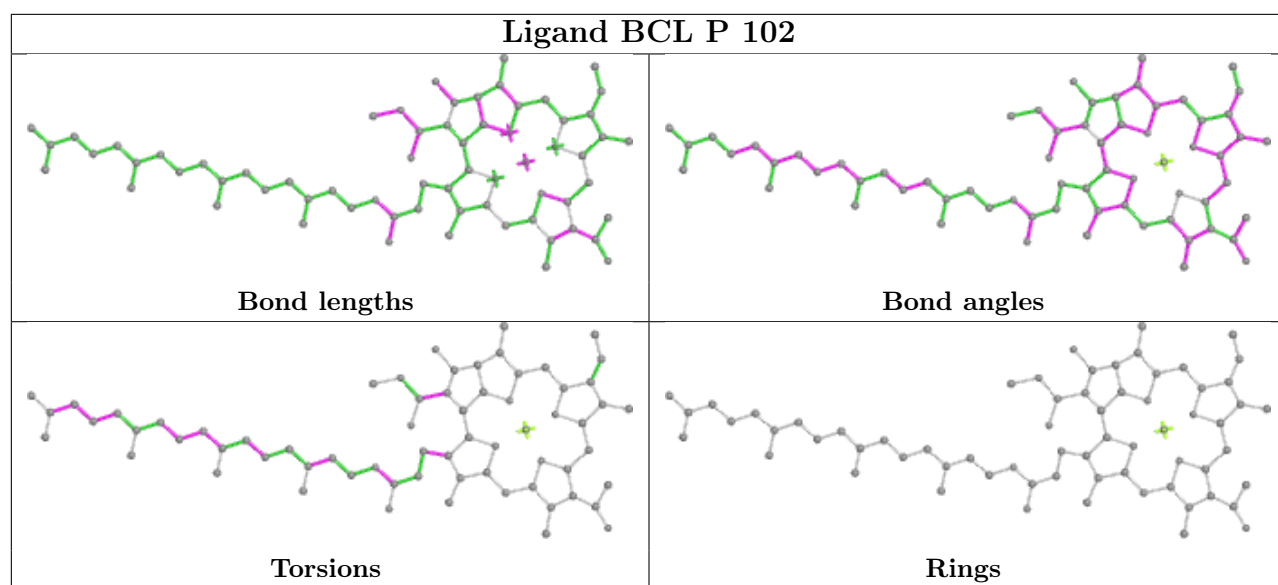


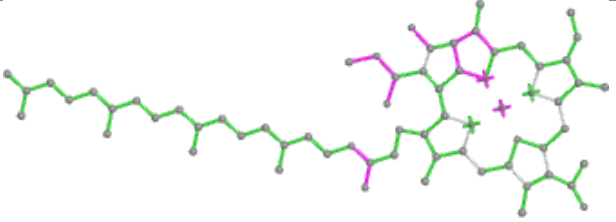
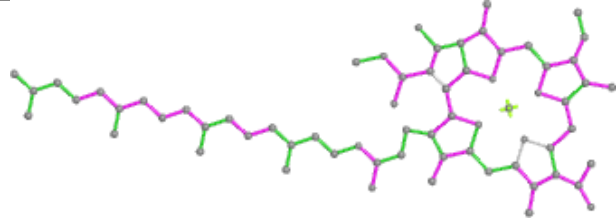
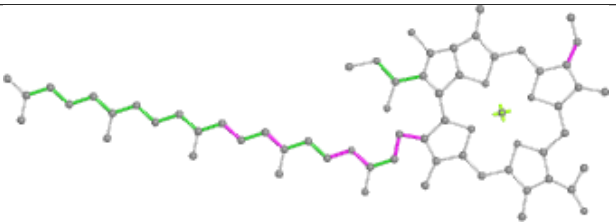
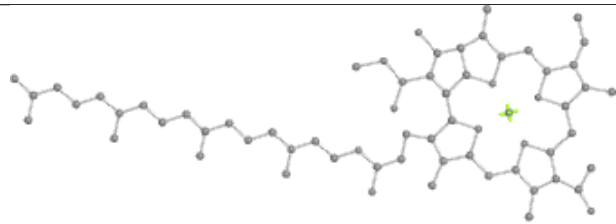
Ligand A1EFU r 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

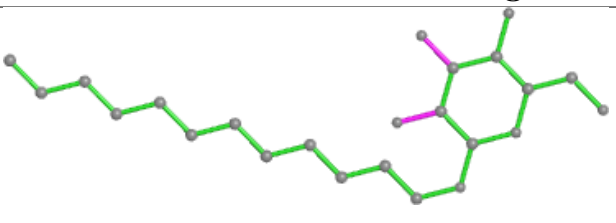
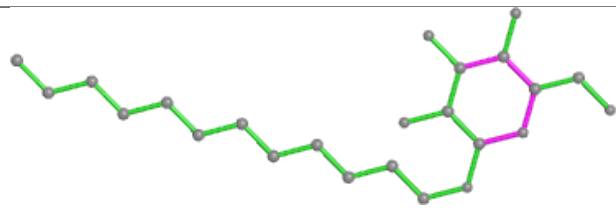
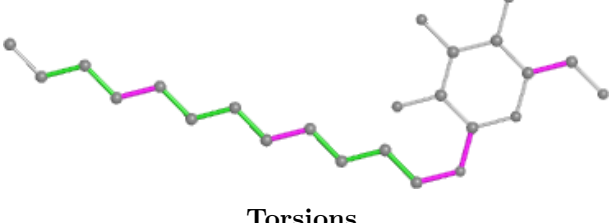
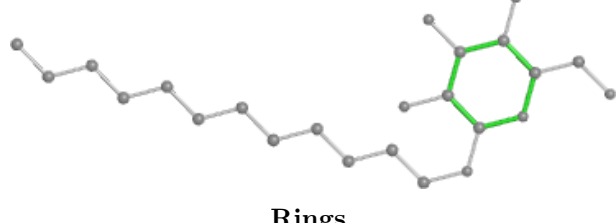
Ligand BCL R 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

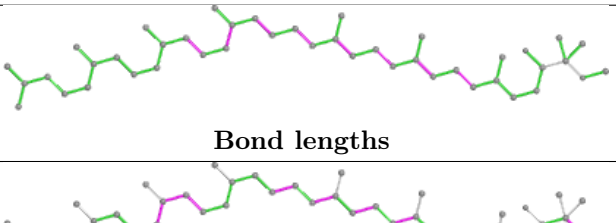
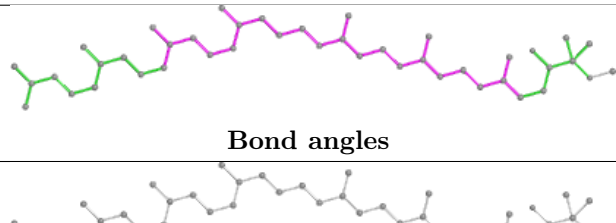


Ligand U10 L 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

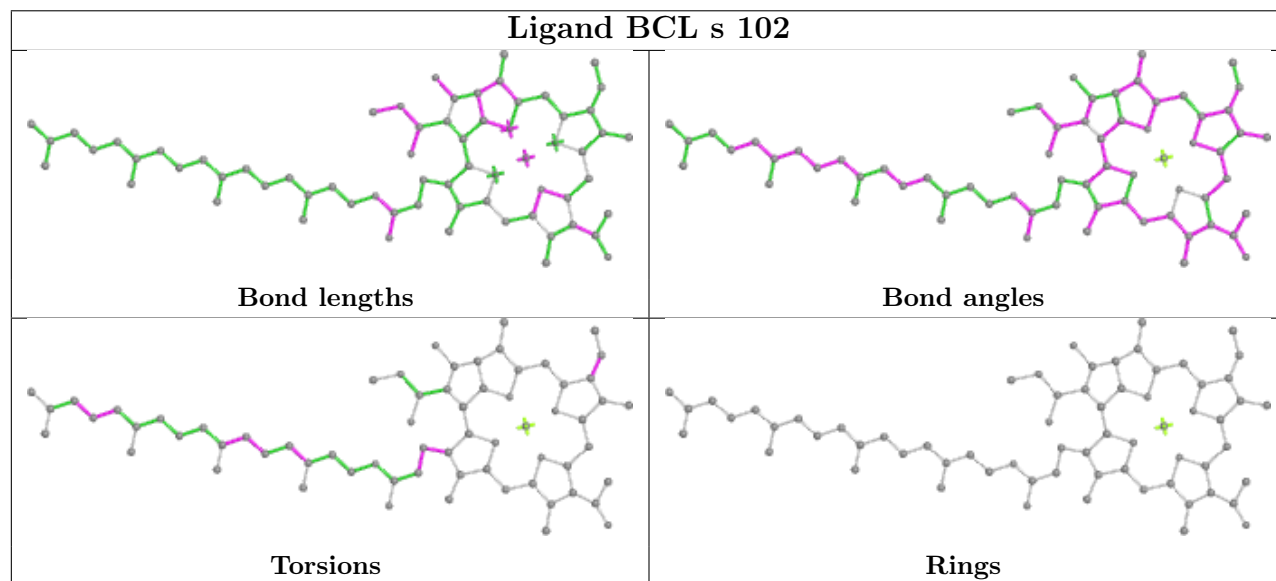
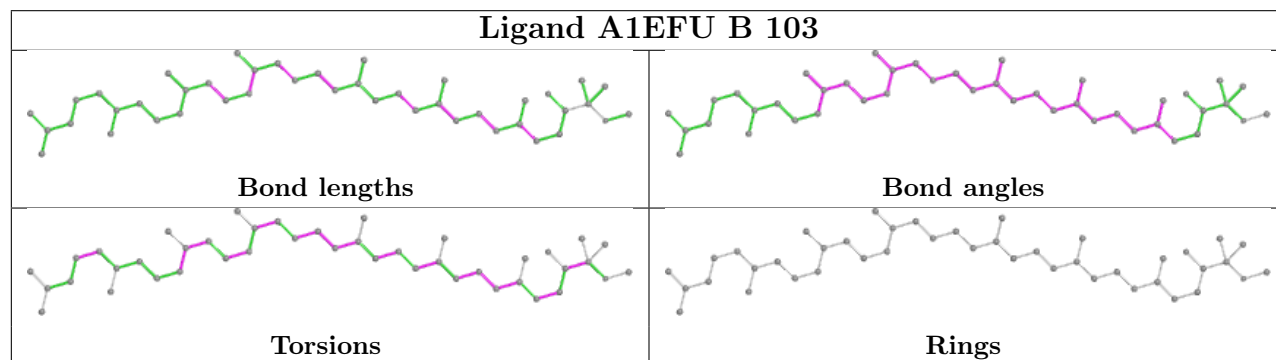
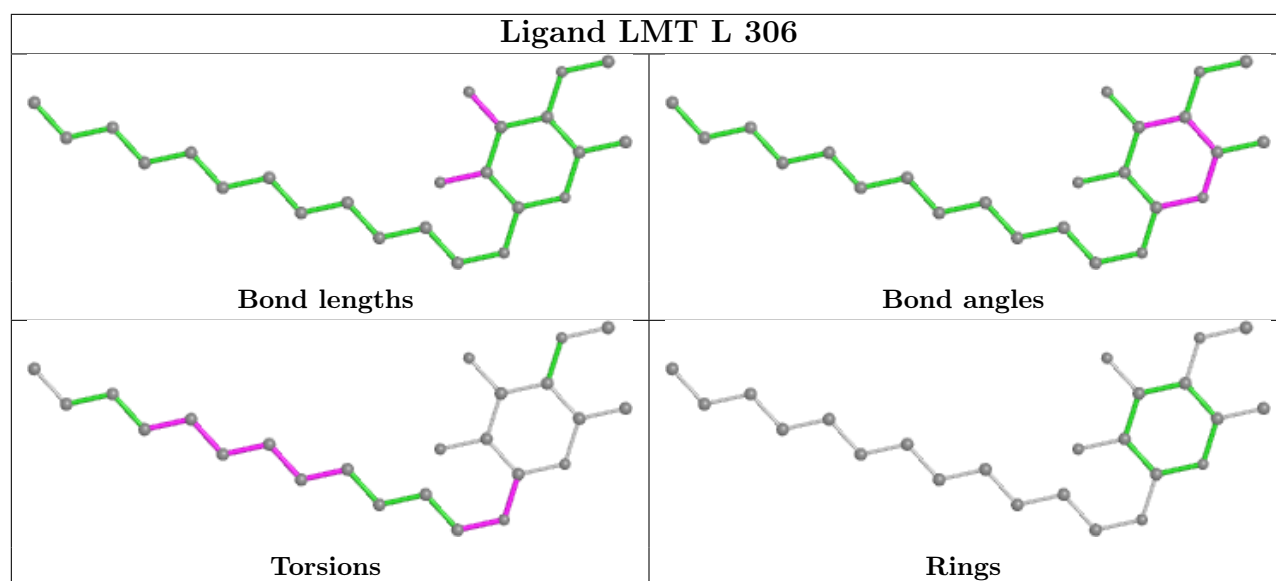


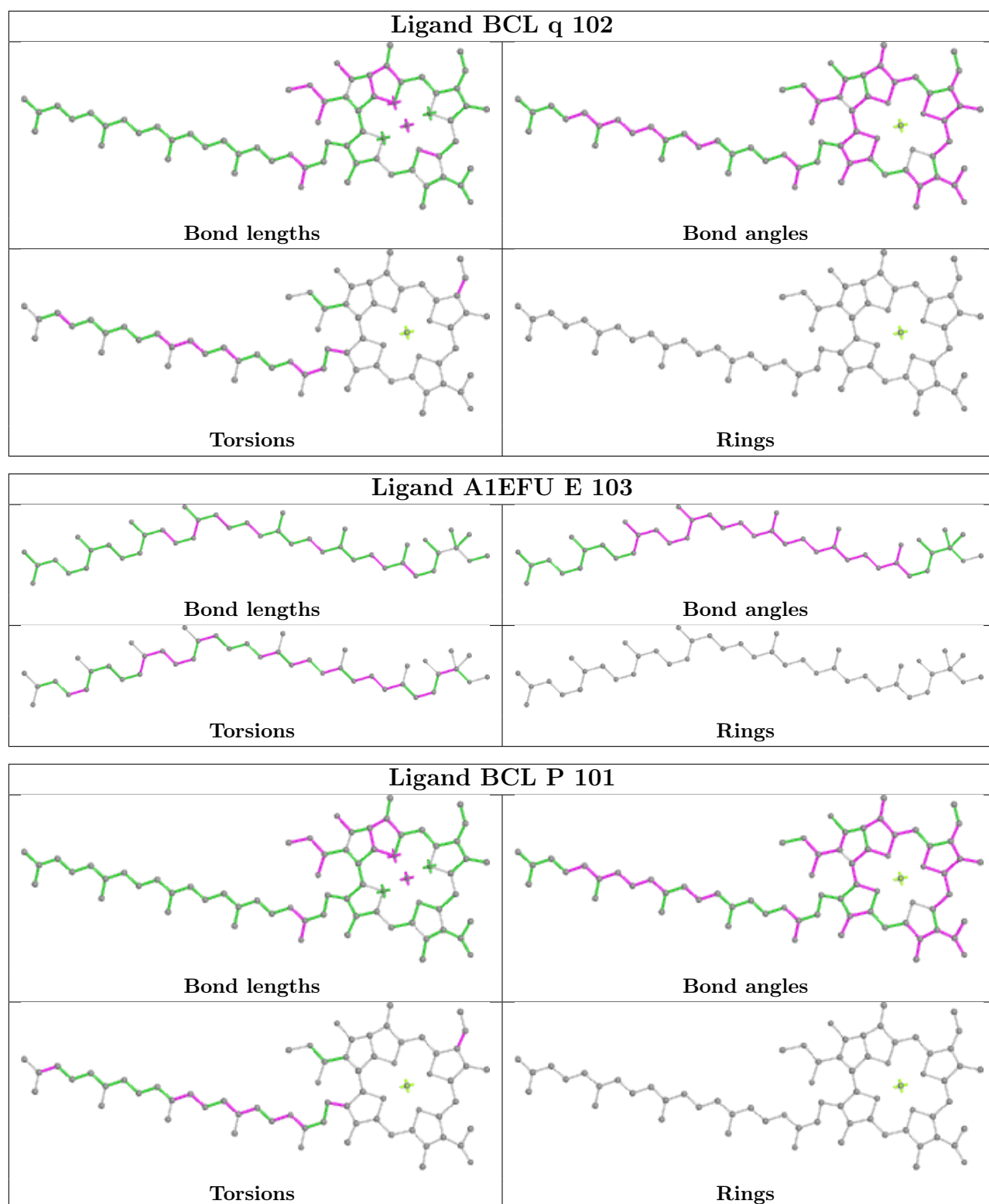


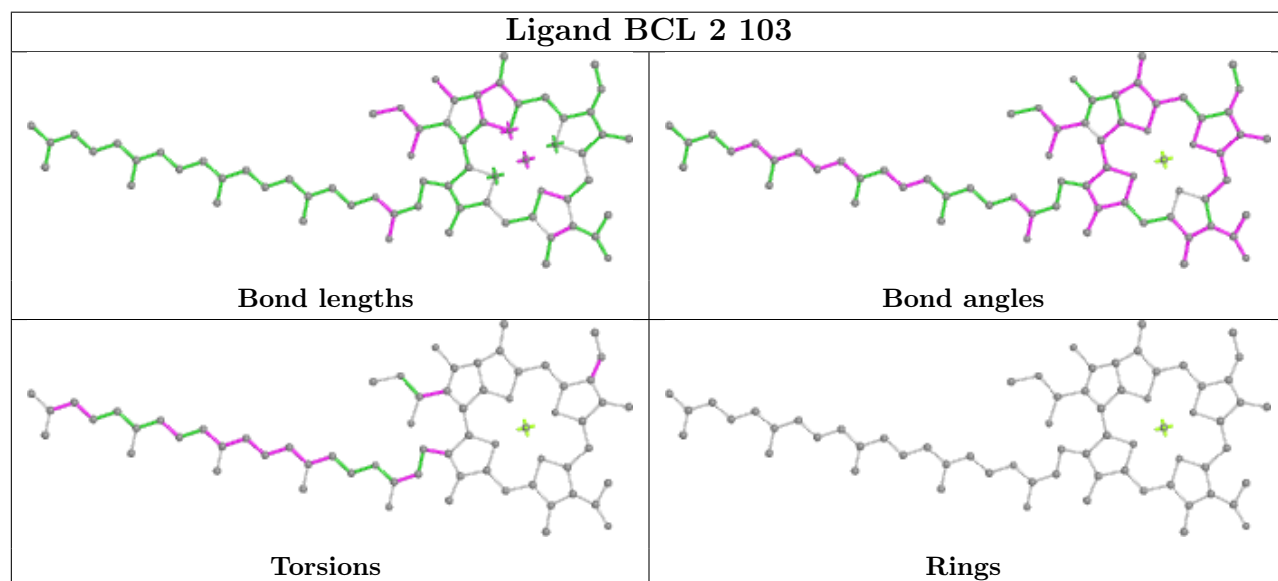
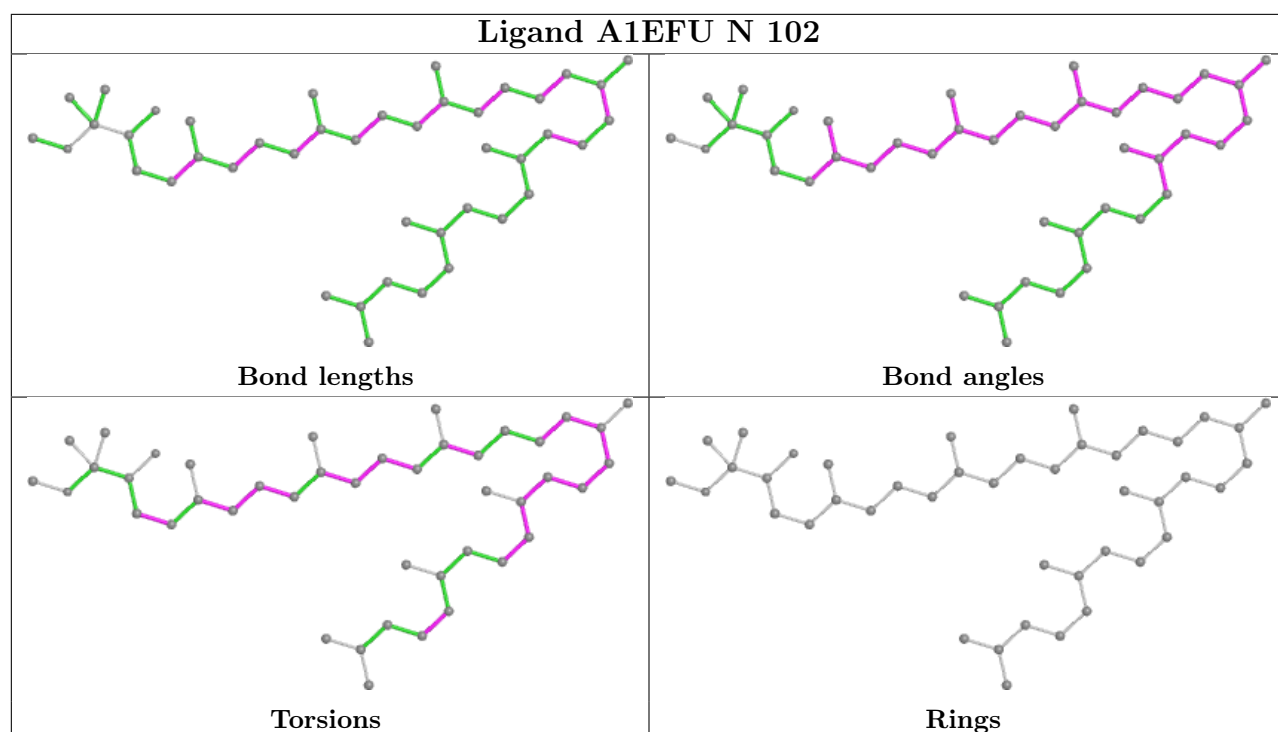
Ligand BCL K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT H 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

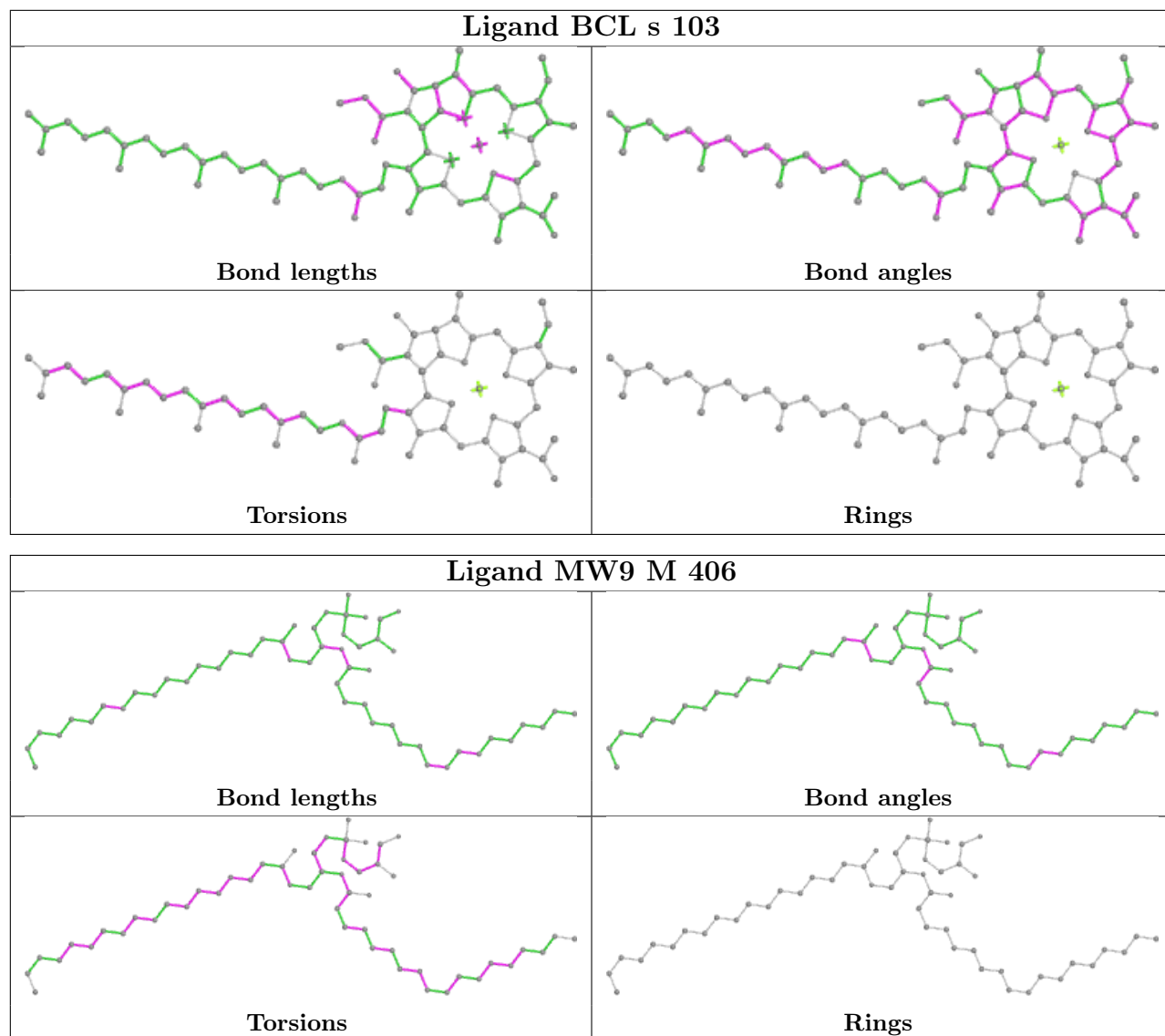
Ligand A1EFU M 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

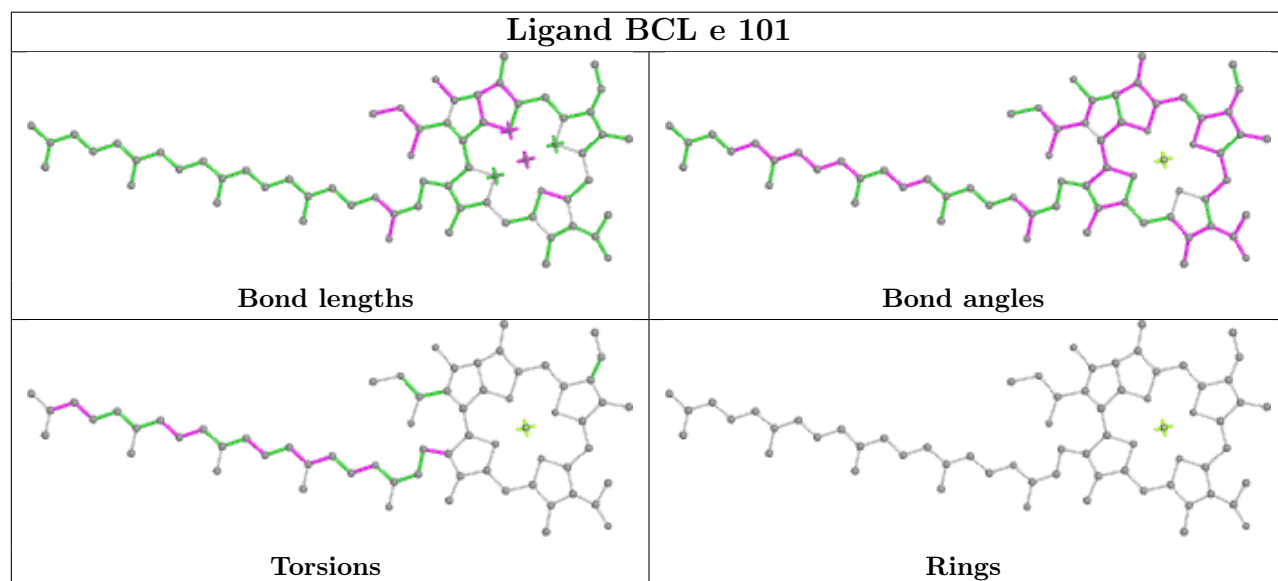
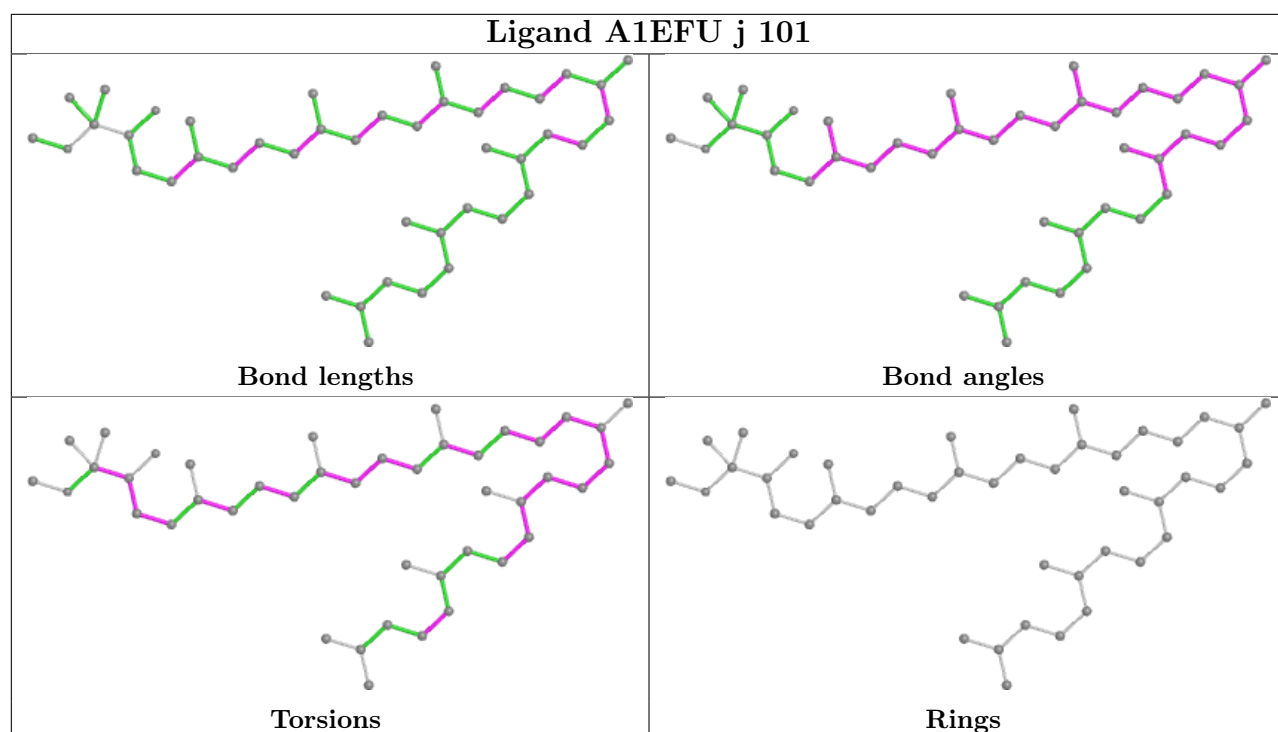


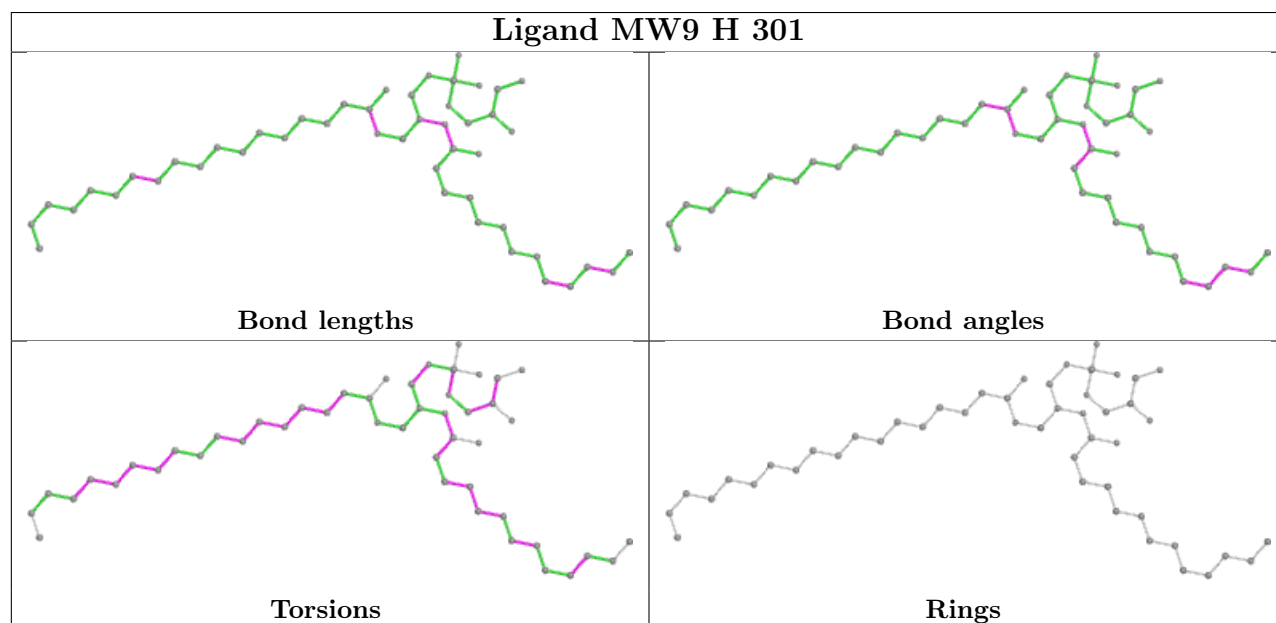
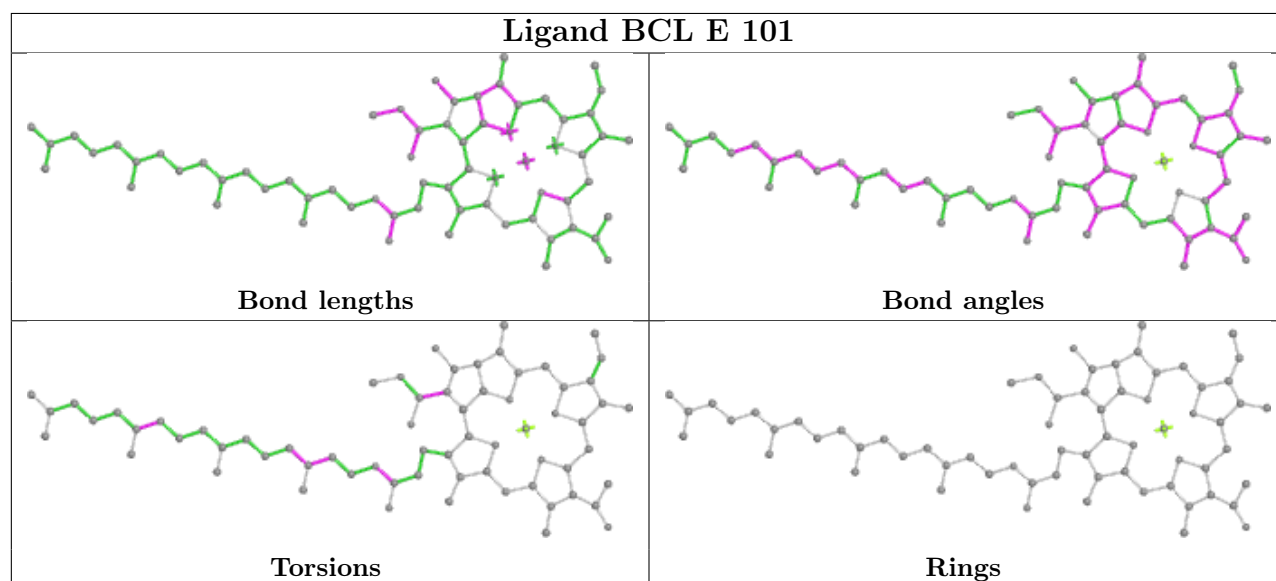
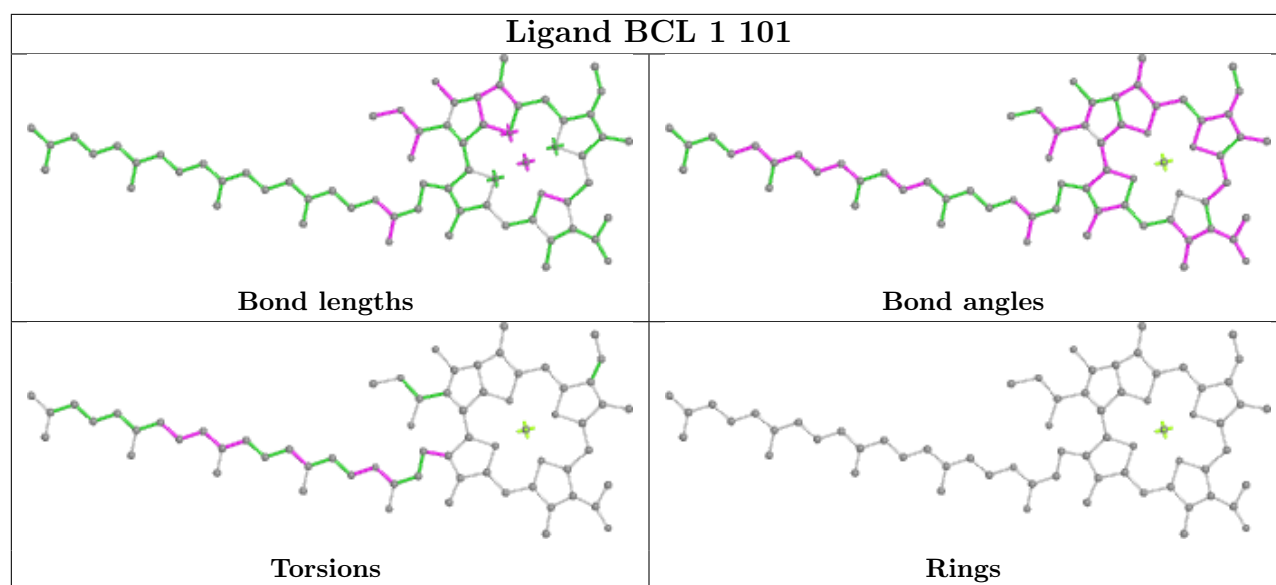


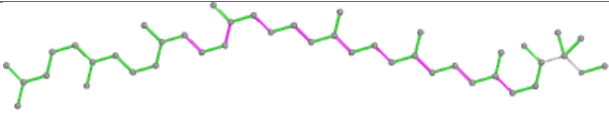
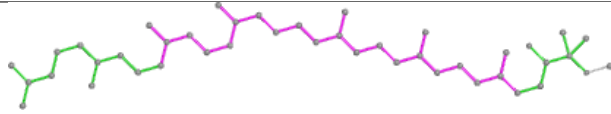
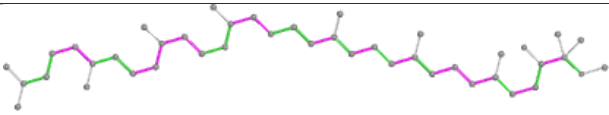
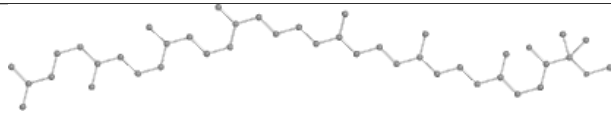


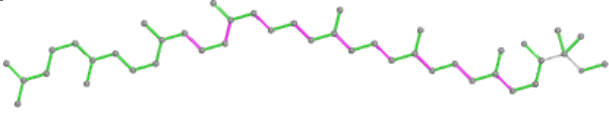
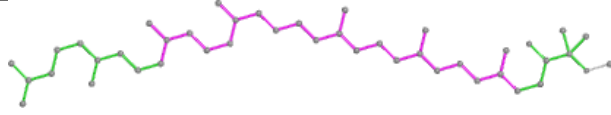
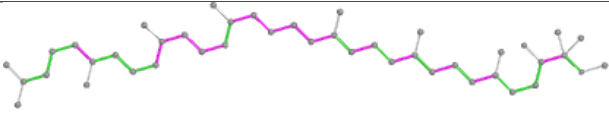
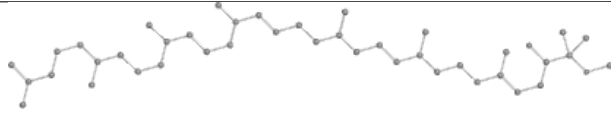


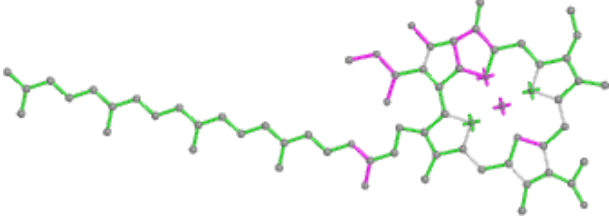
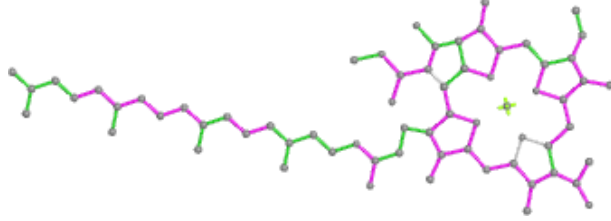
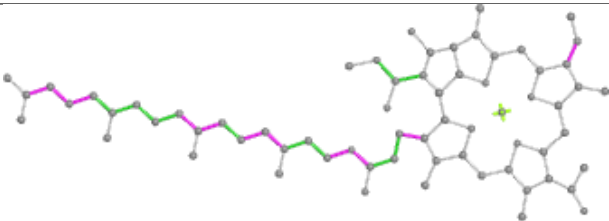
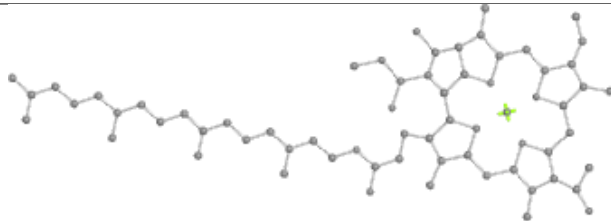


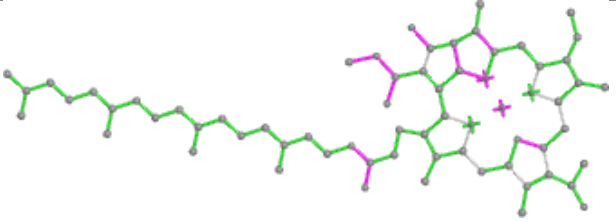
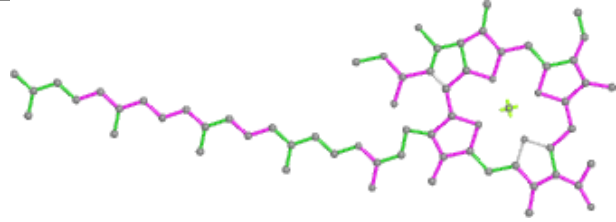
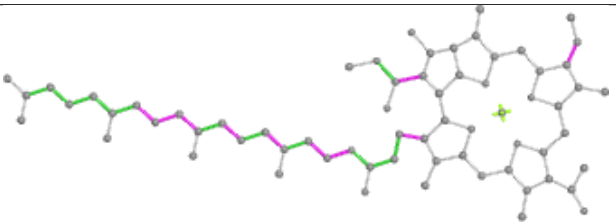
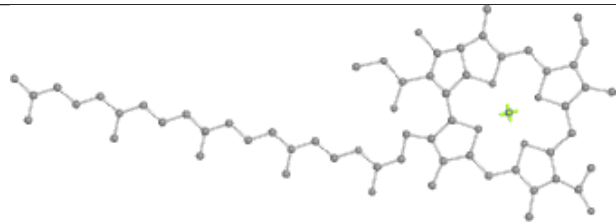


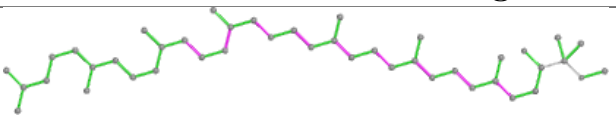
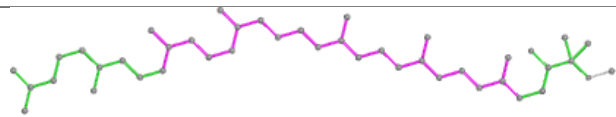
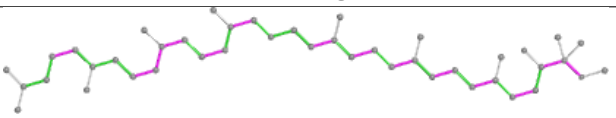
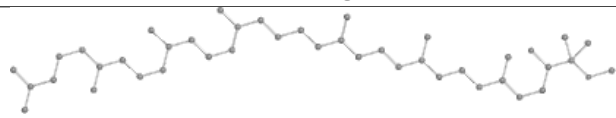


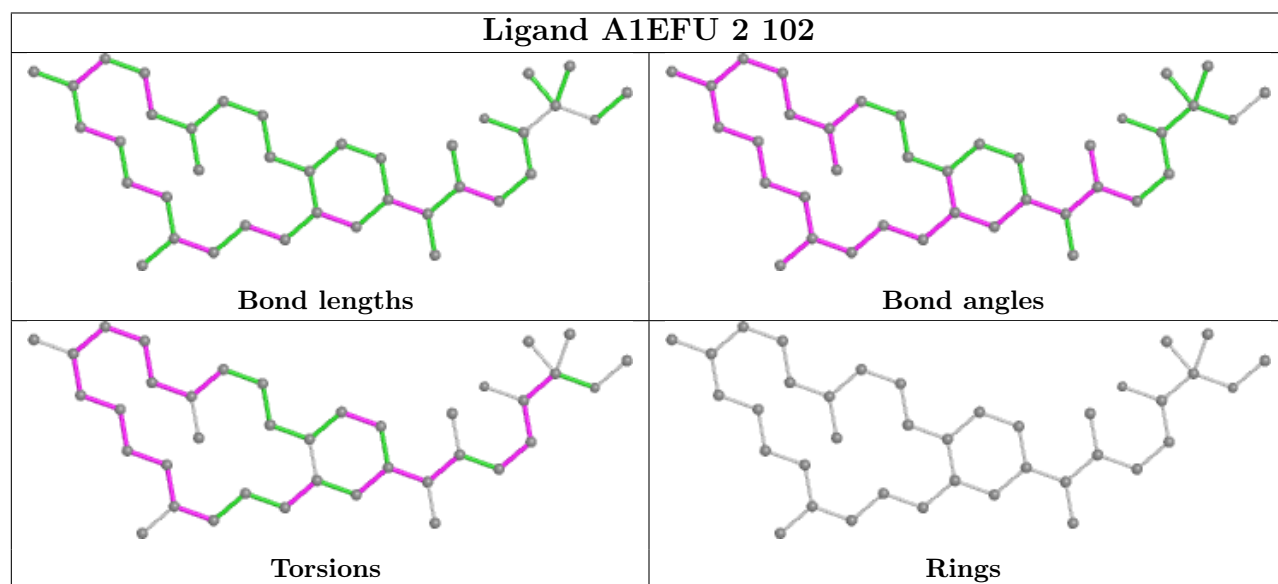
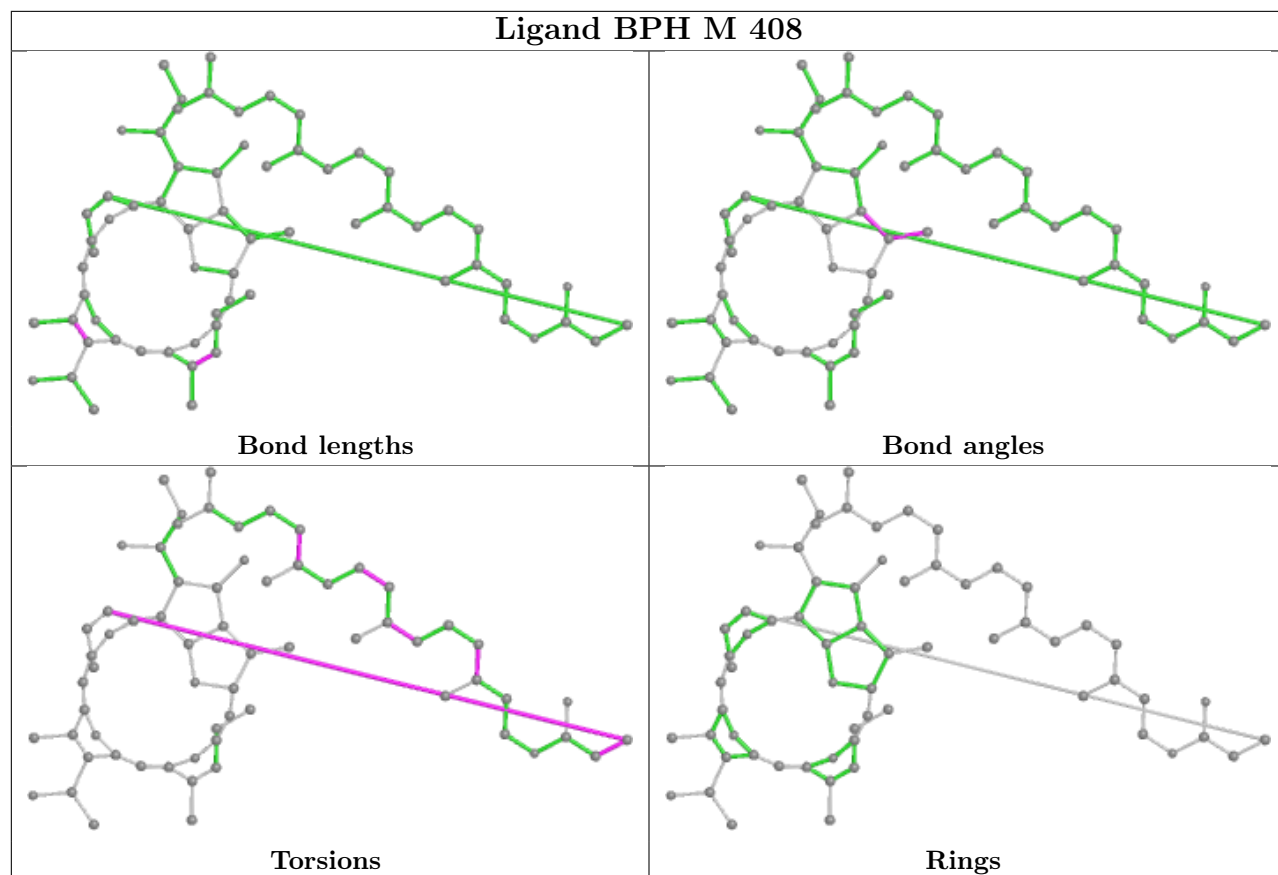
Ligand A1EFU q 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

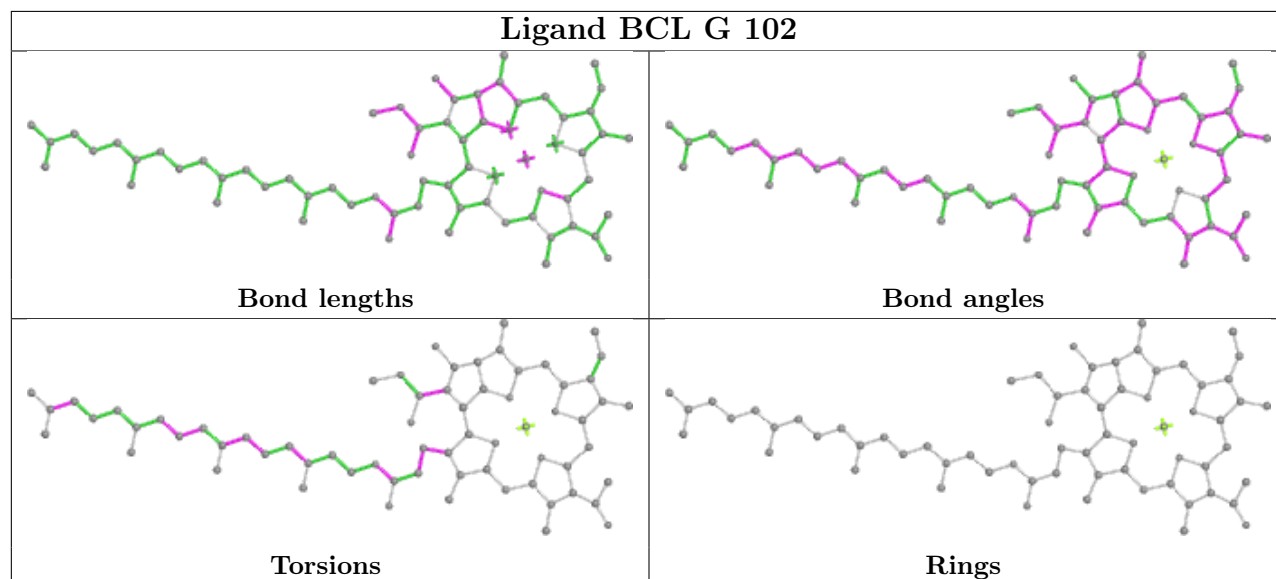
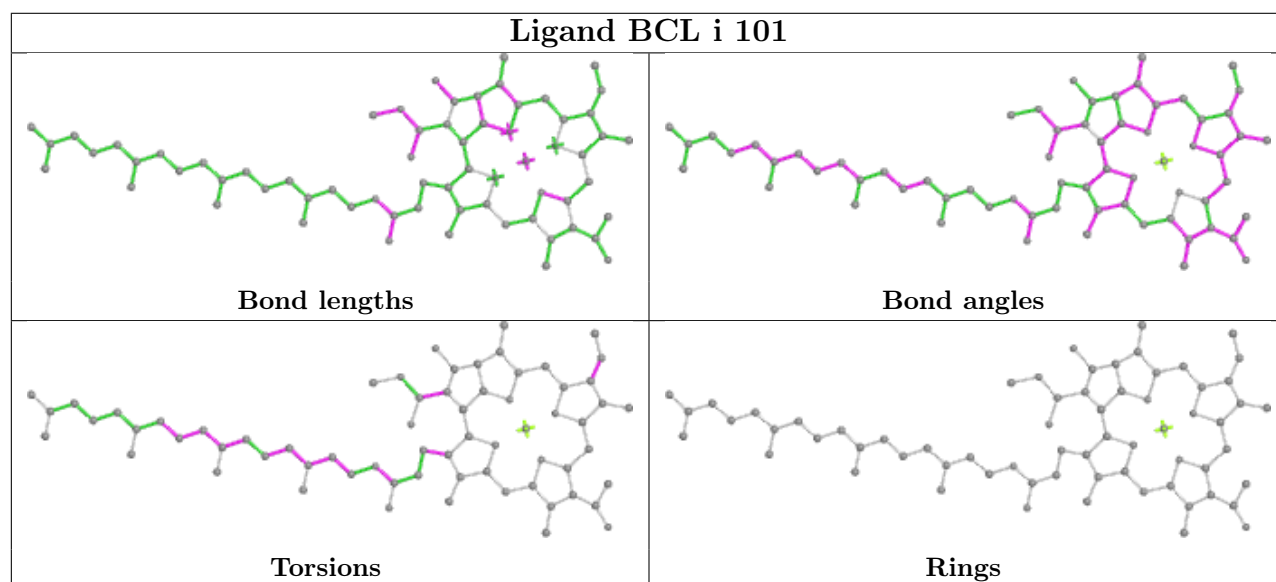
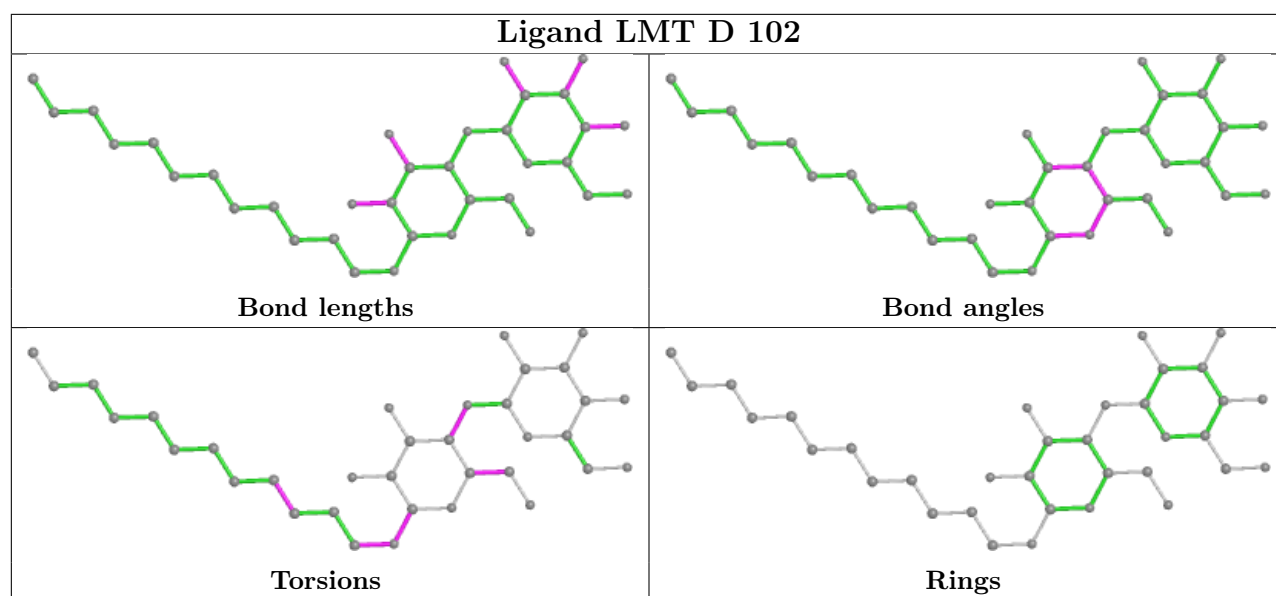
Ligand A1EFU P 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

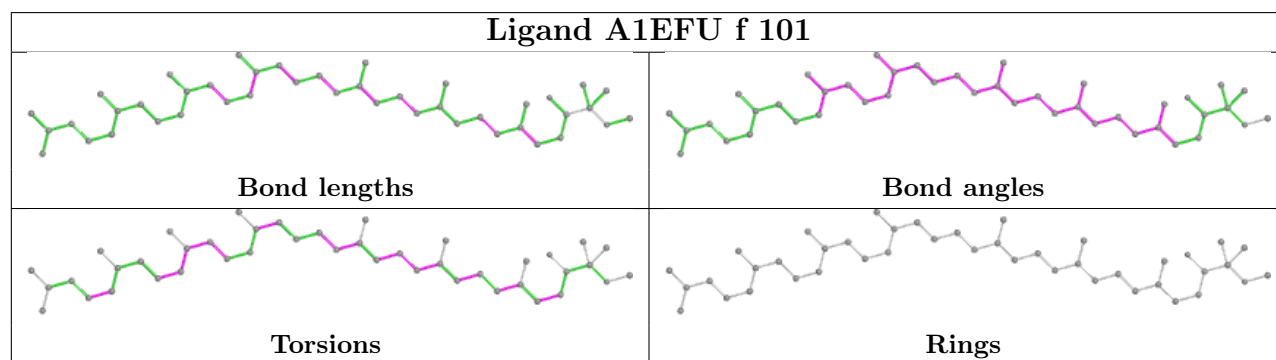
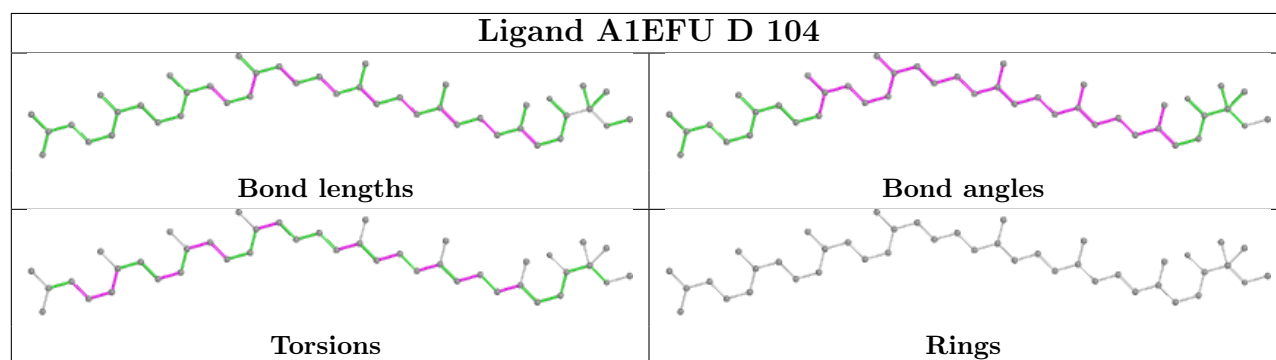
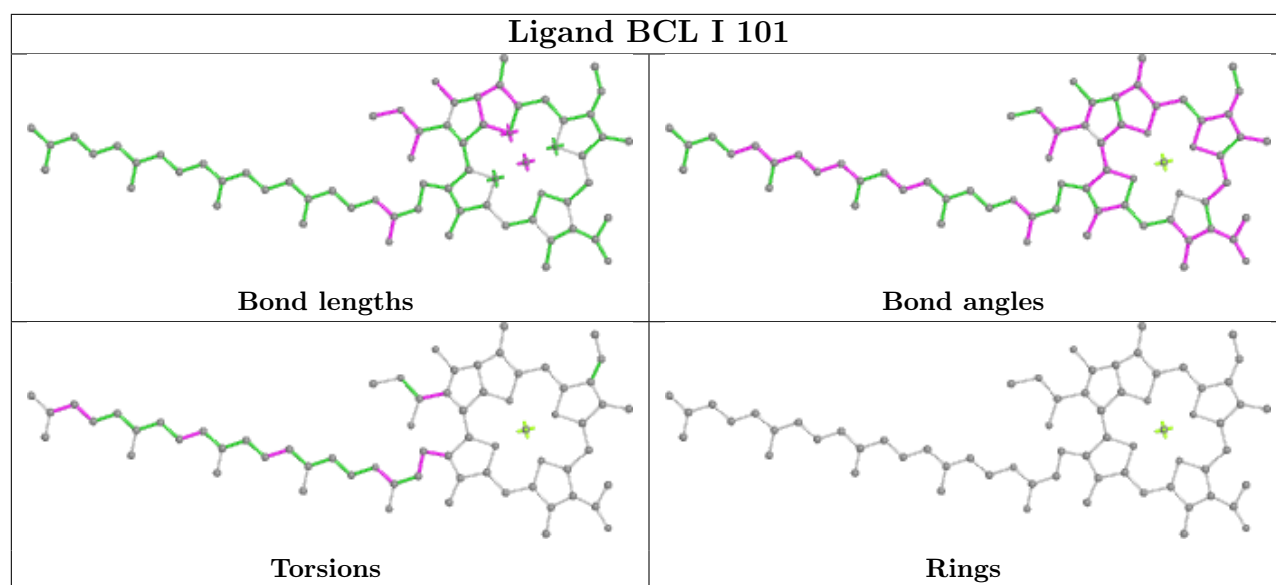
Ligand BCL L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCL G 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

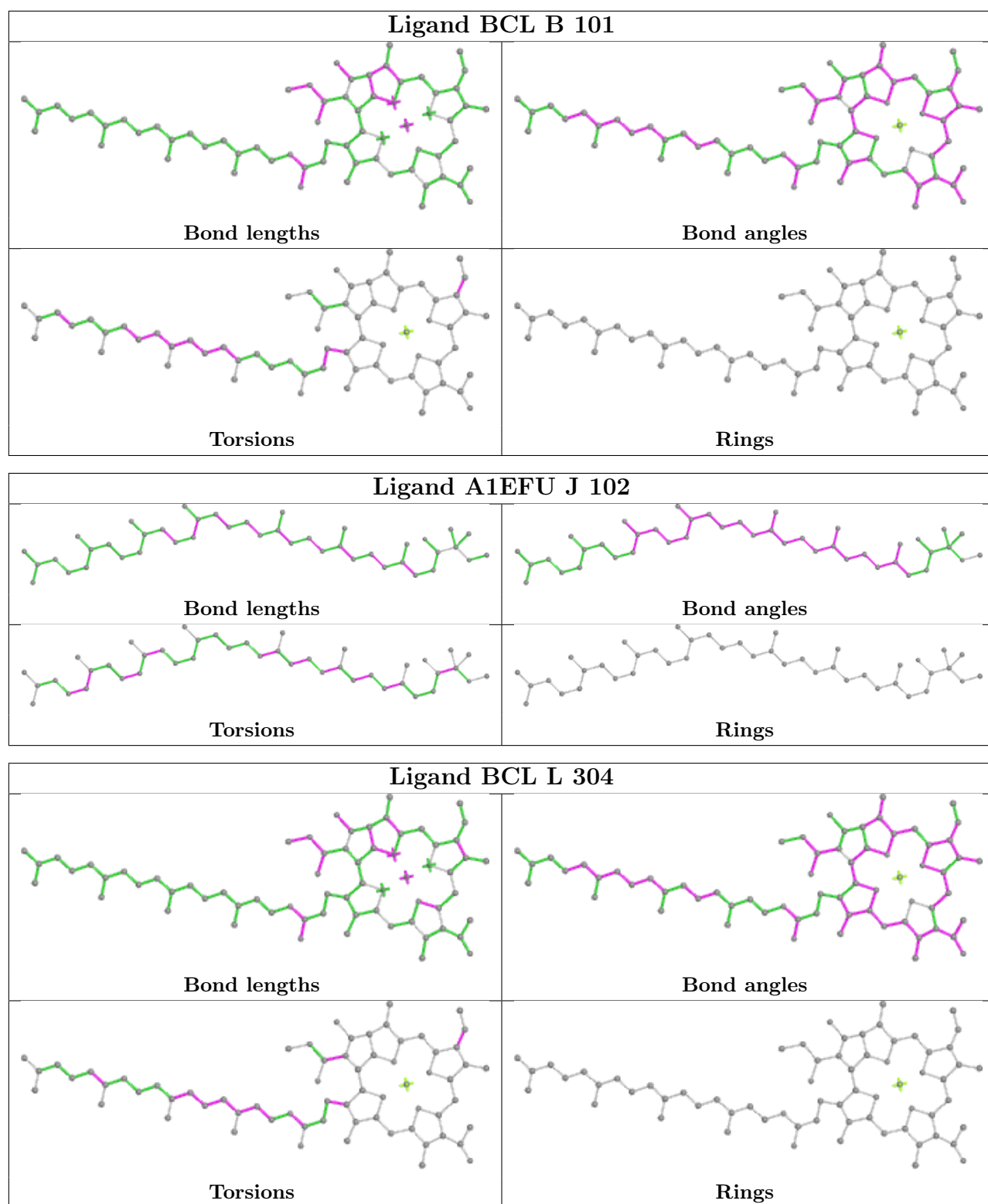
Ligand A1EFU s 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

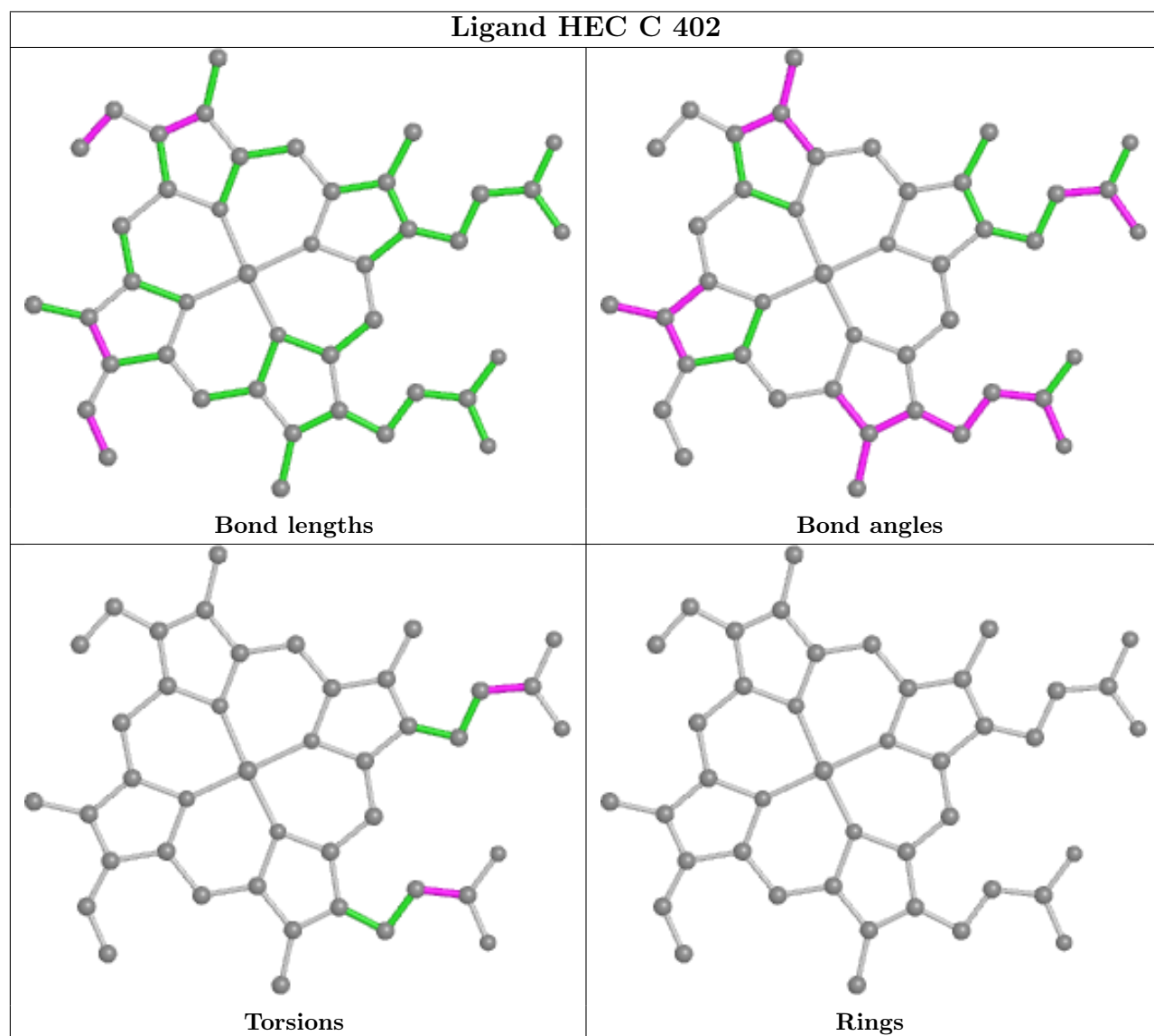
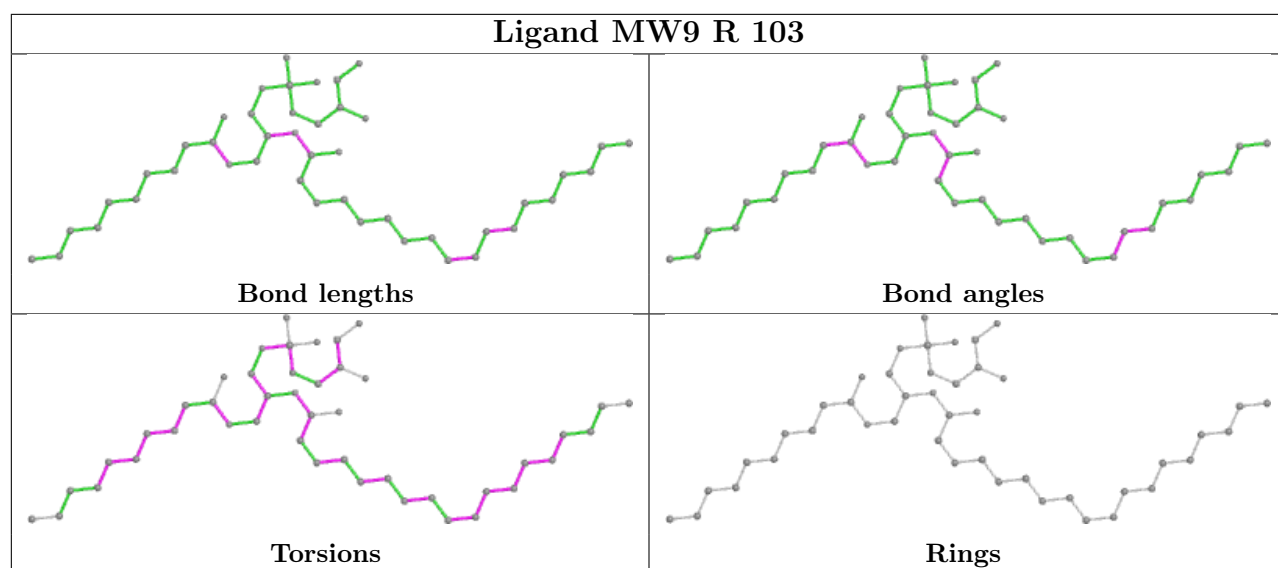










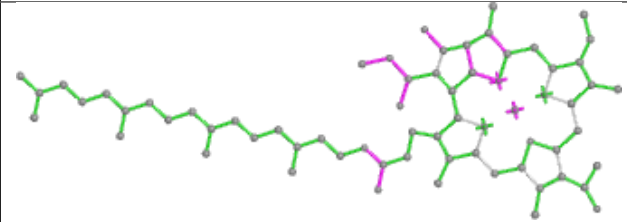
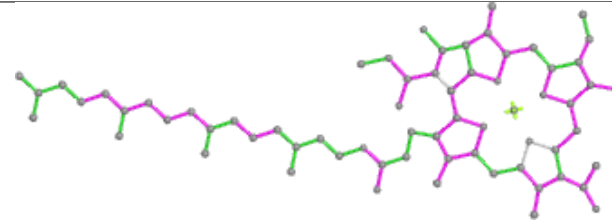
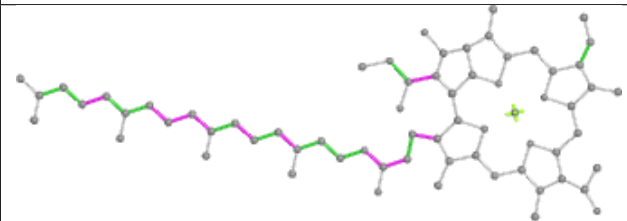
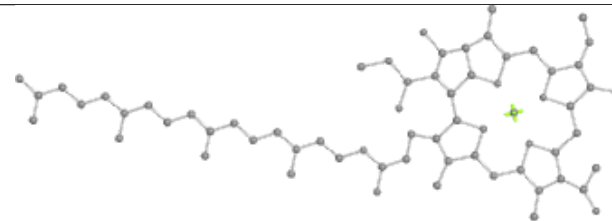


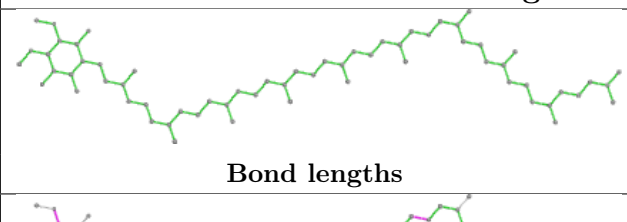
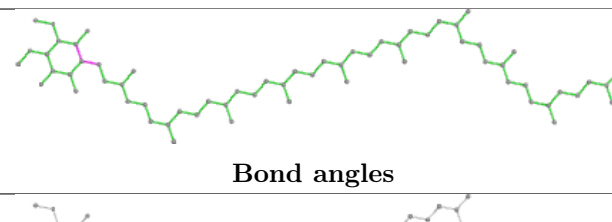
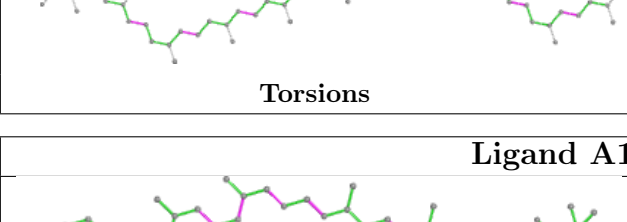

Ligand BCL a 101	
Bond lengths	Bond angles
Torsions	Rings

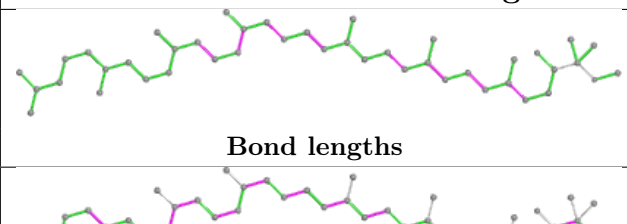
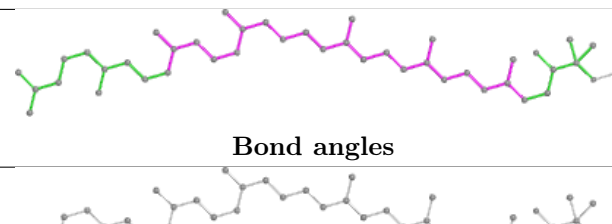
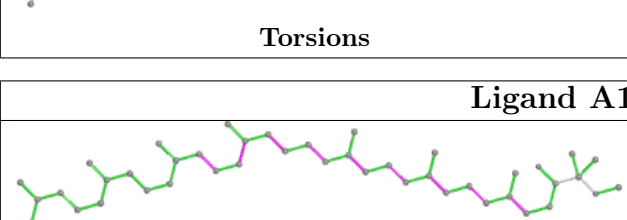
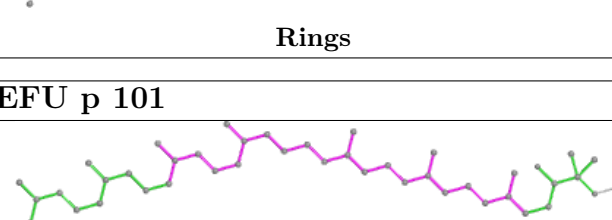
Ligand A1EFU R 101	
Bond lengths	Bond angles
Torsions	Rings

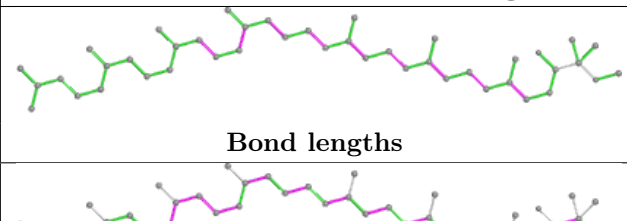
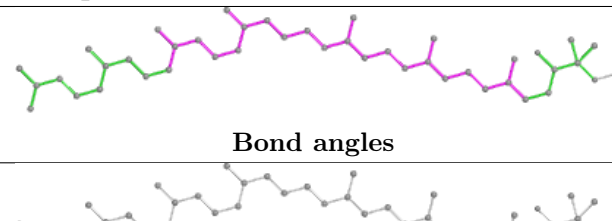


Ligand A1EFU v 102	
Bond lengths	Bond angles
Torsions	Rings

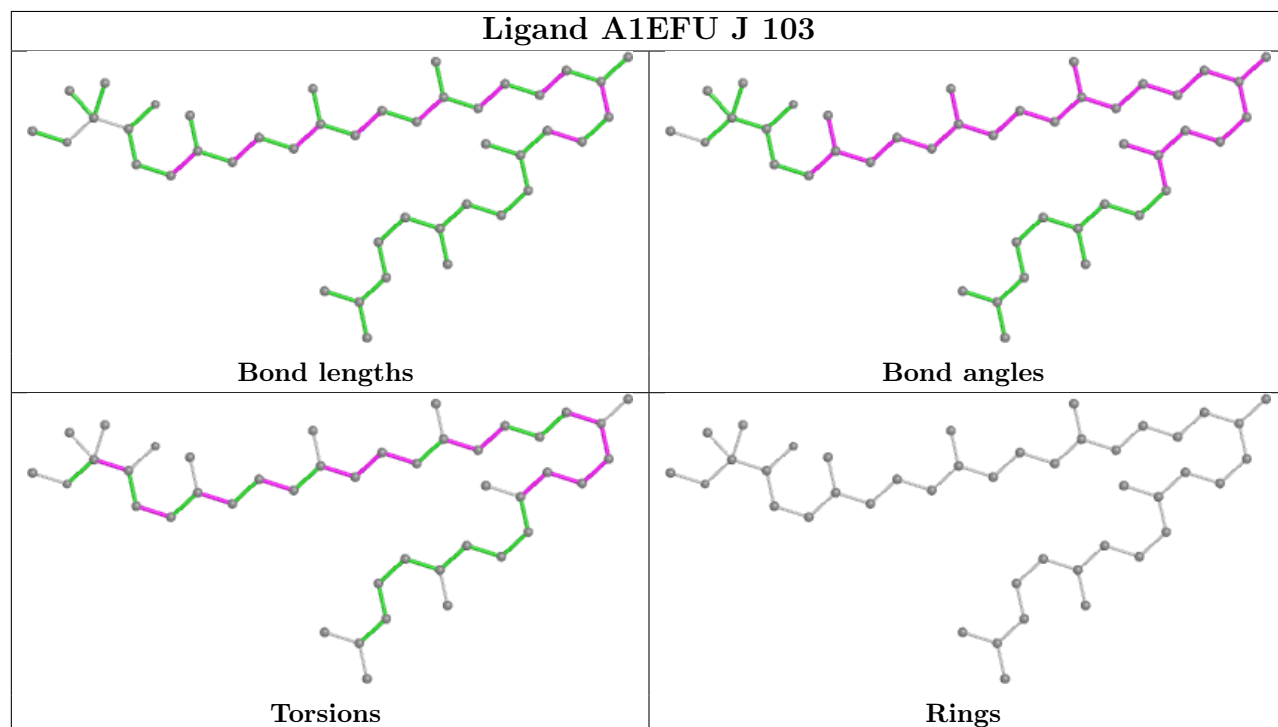
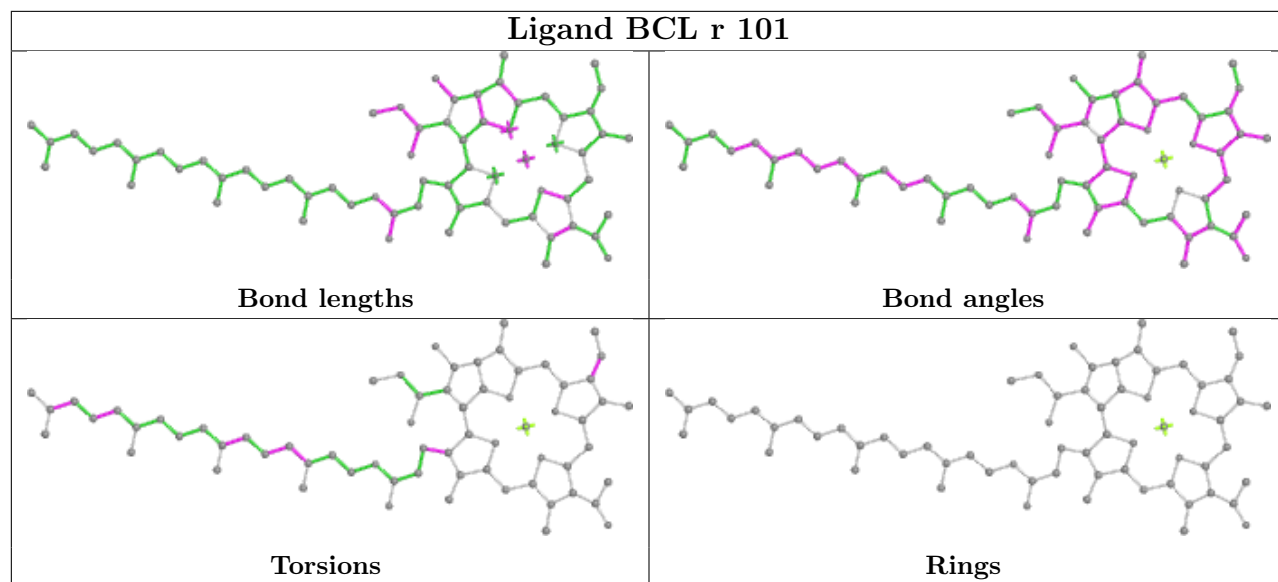
Ligand A1EFU s 101	
Bond lengths	Bond angles
Torsions	Rings

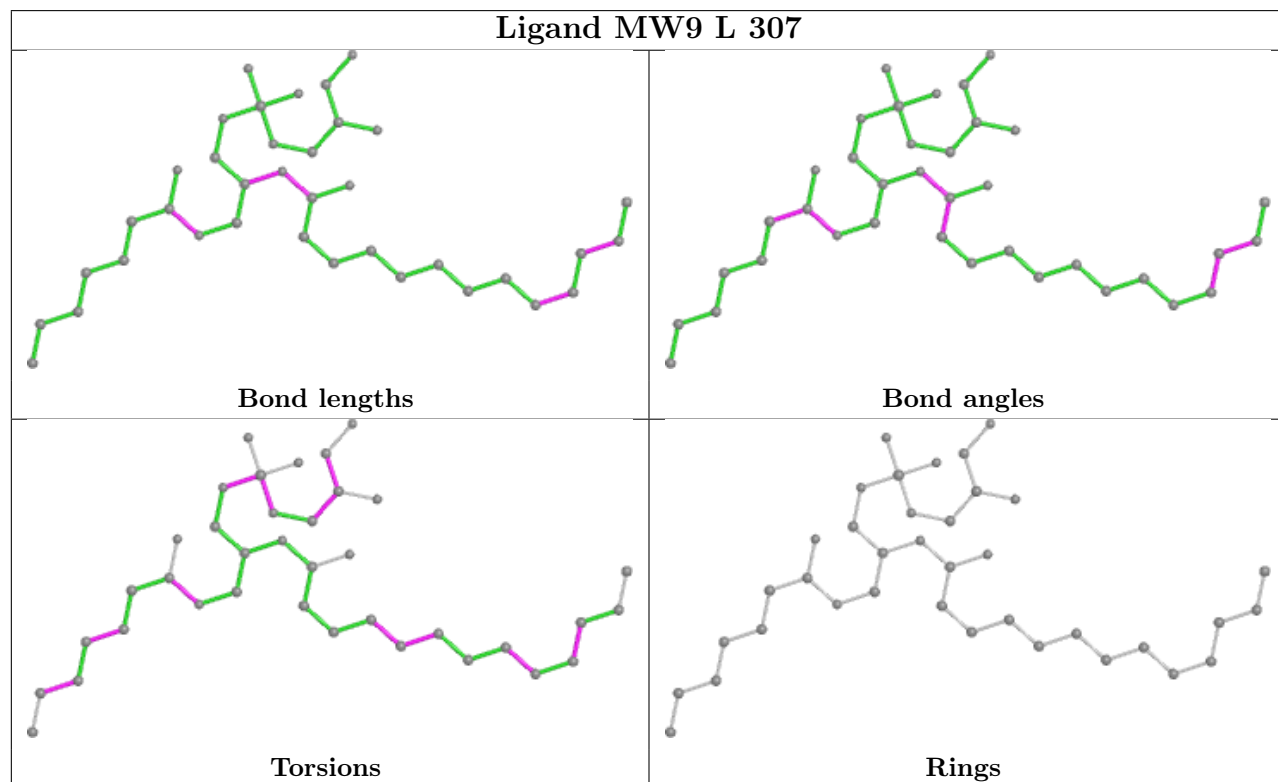
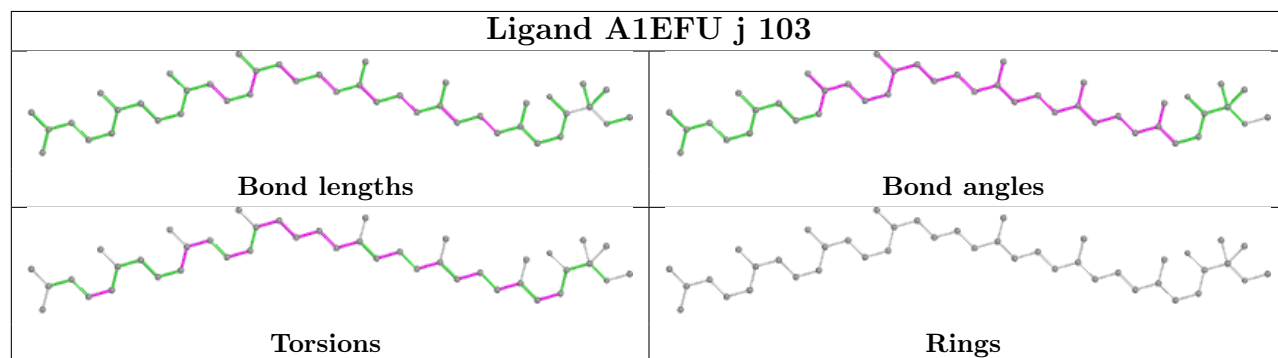
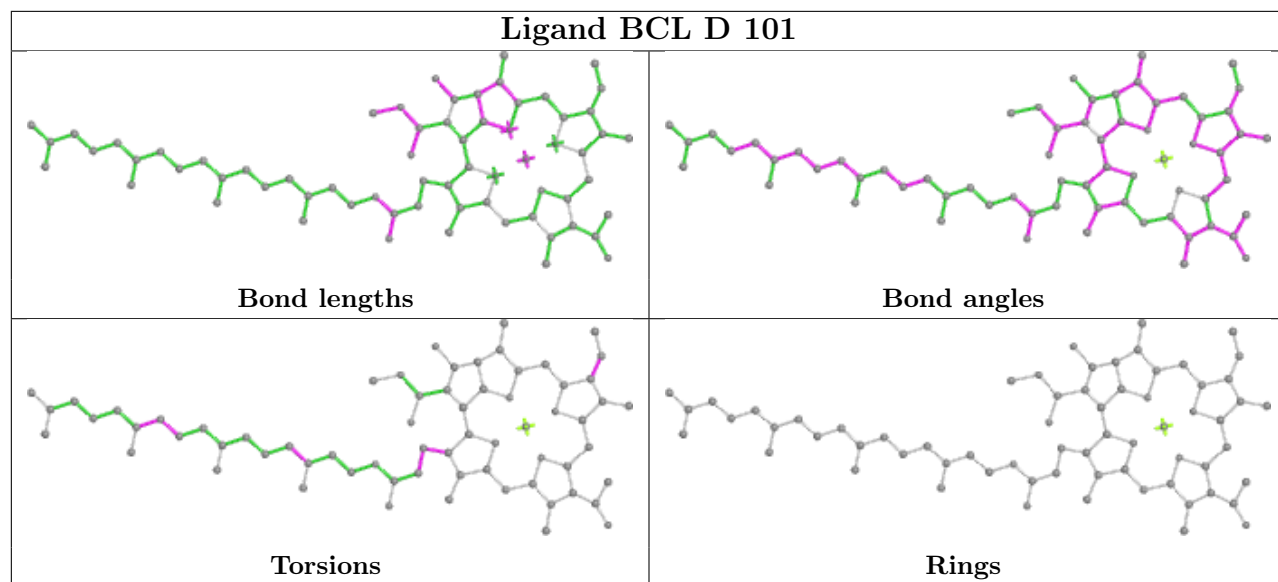
Ligand BCL F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

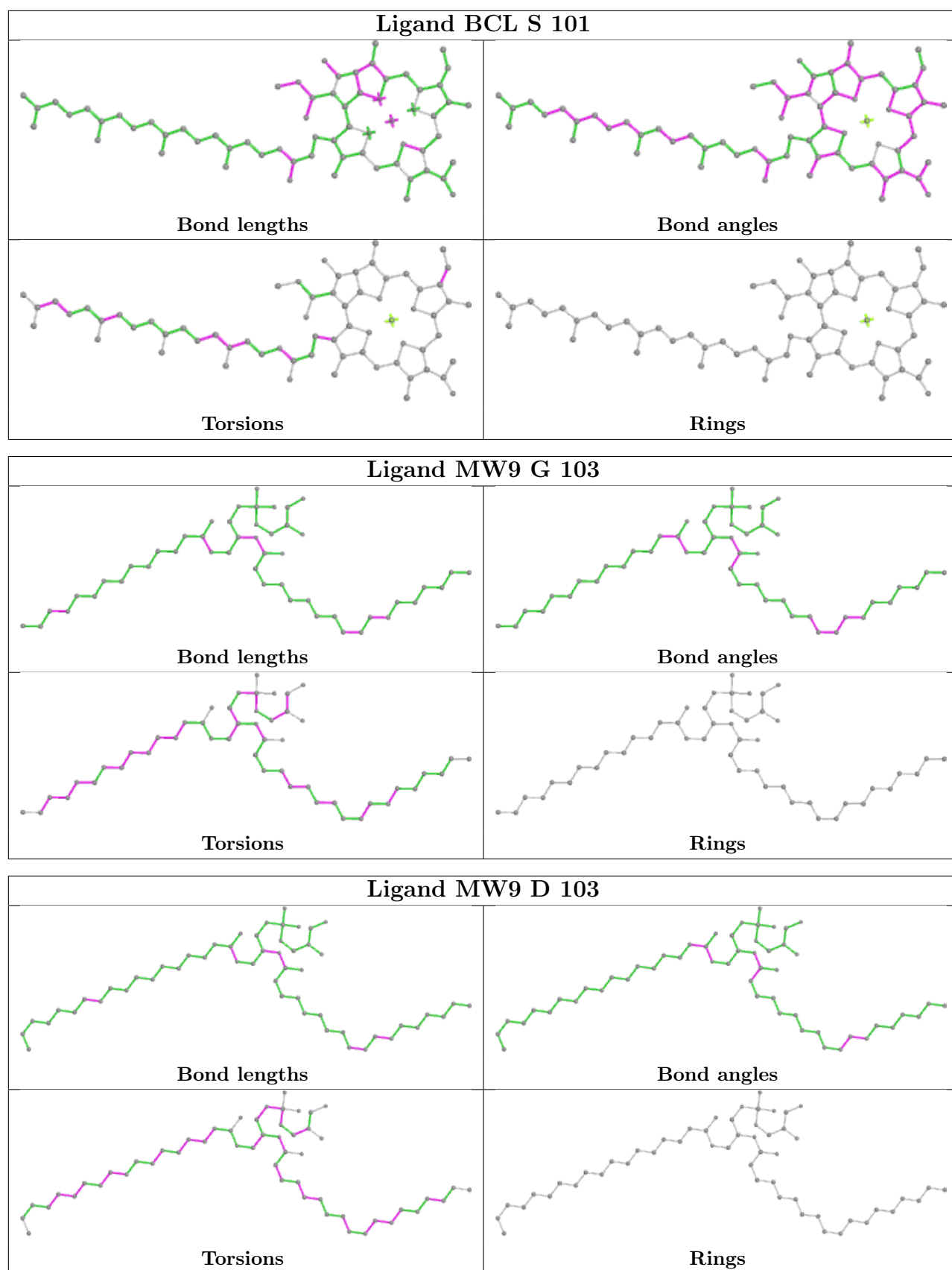
Ligand U10 M 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

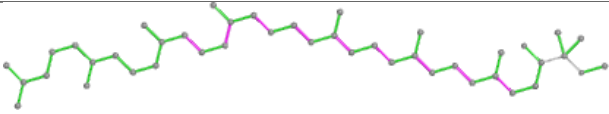
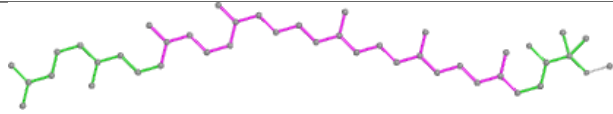
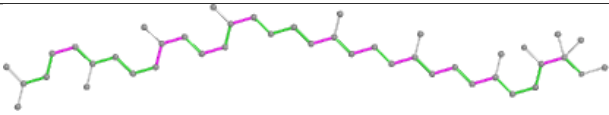
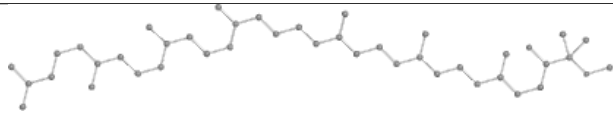
Ligand A1EFU v 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

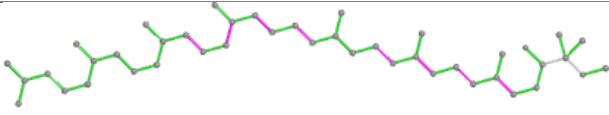
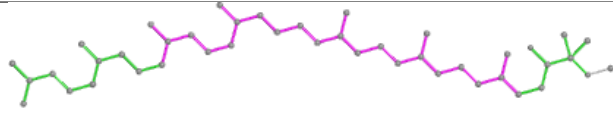
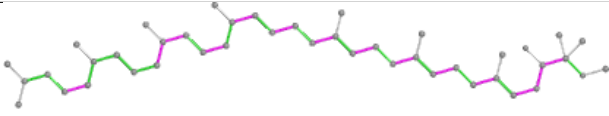
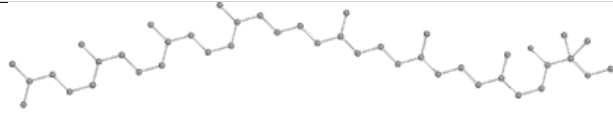
Ligand A1EFU p 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

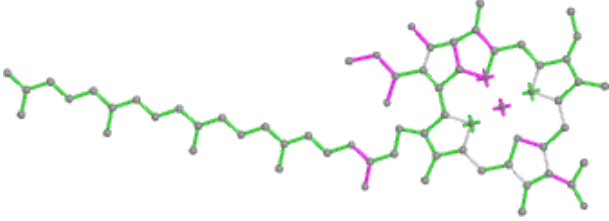
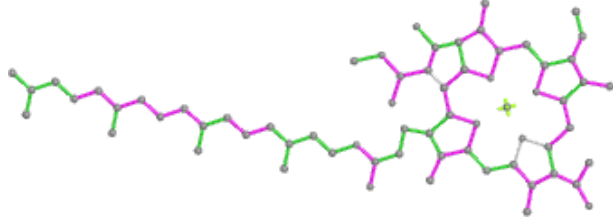
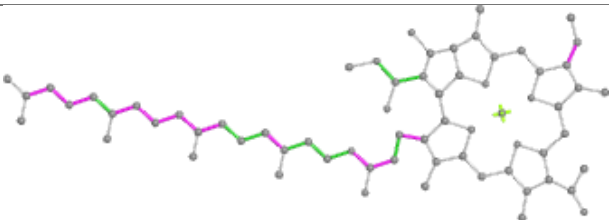
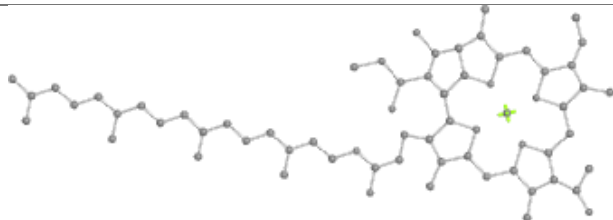




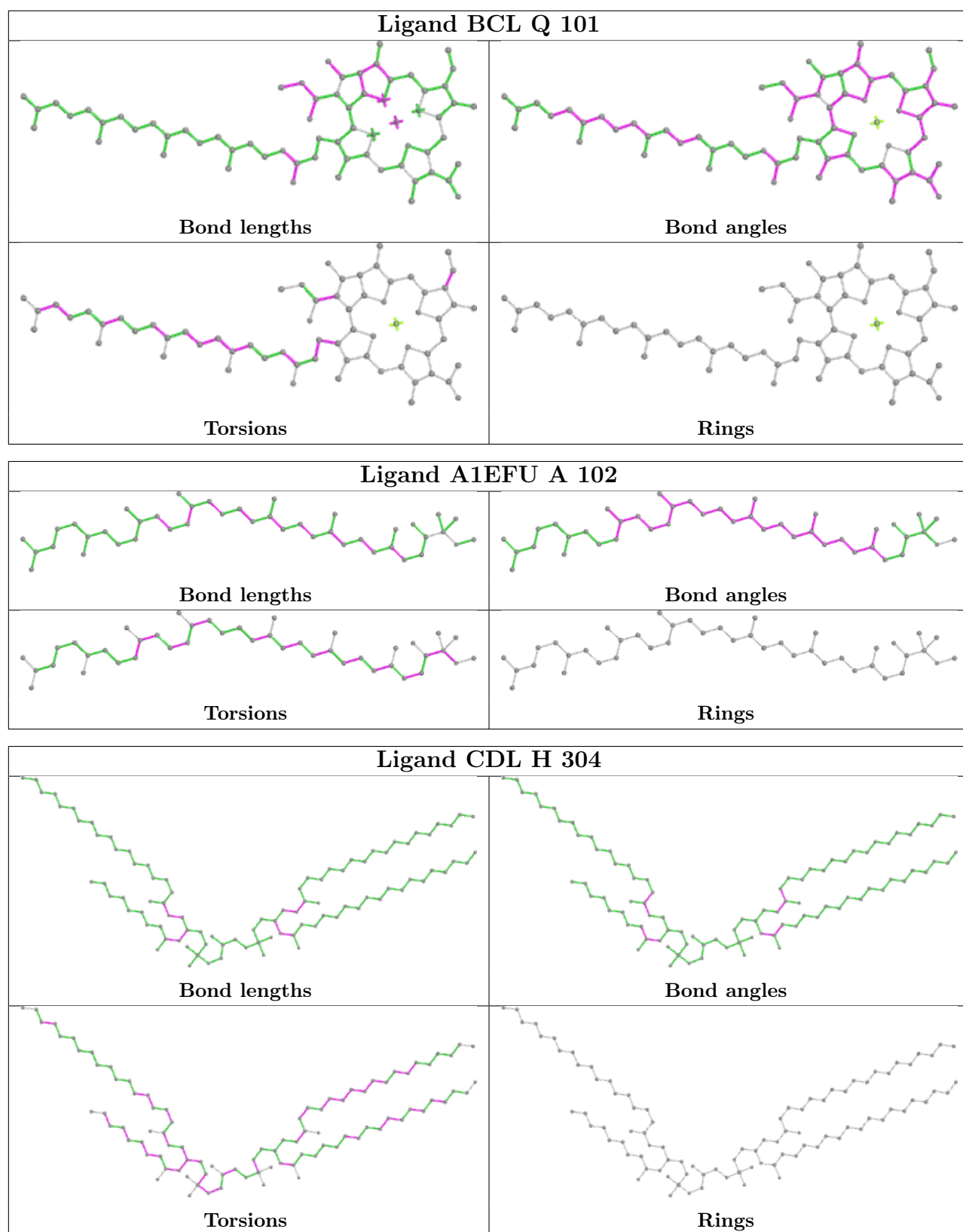


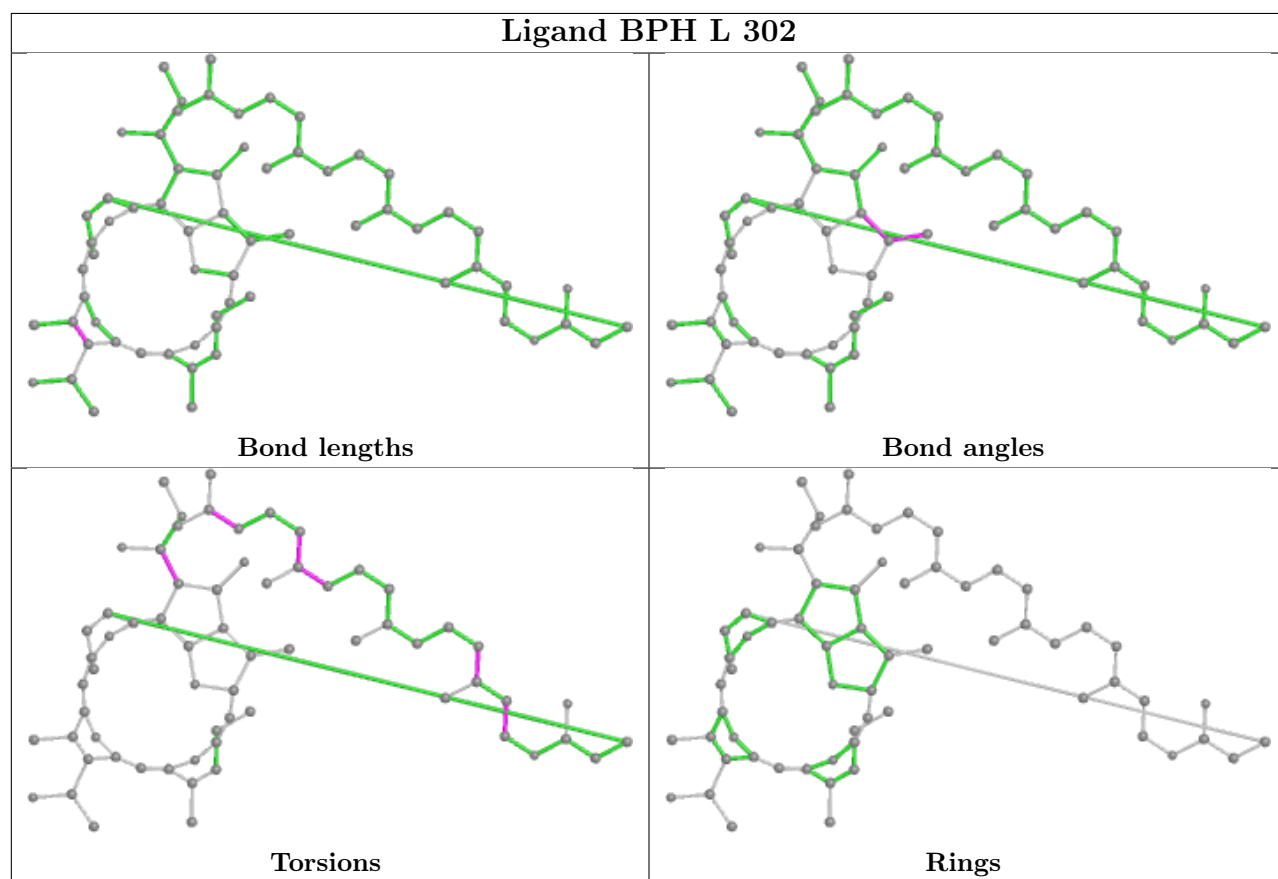
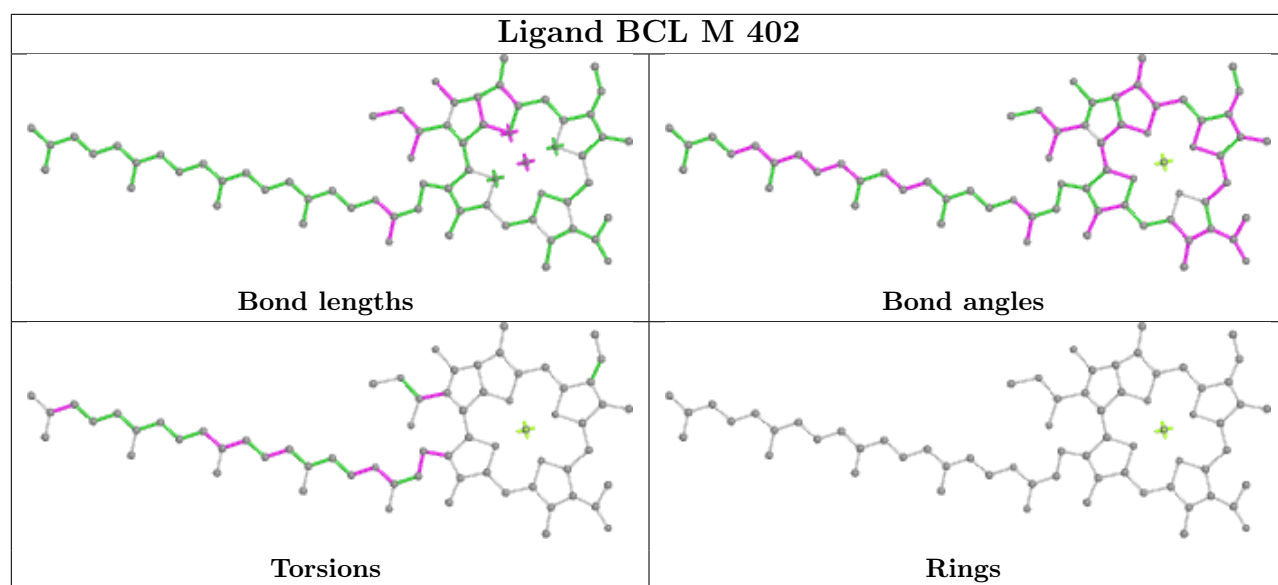
Ligand A1EFU B 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

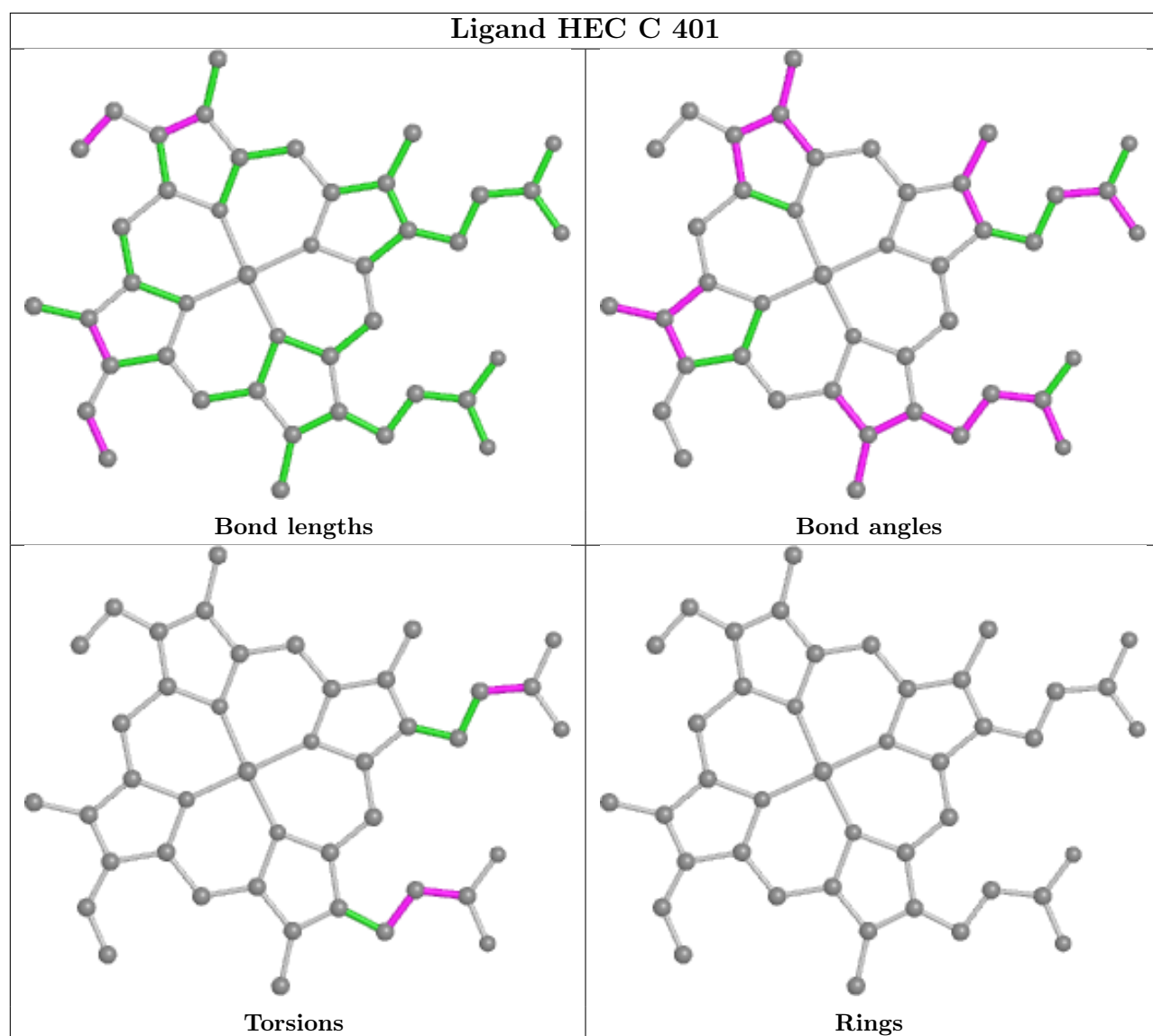
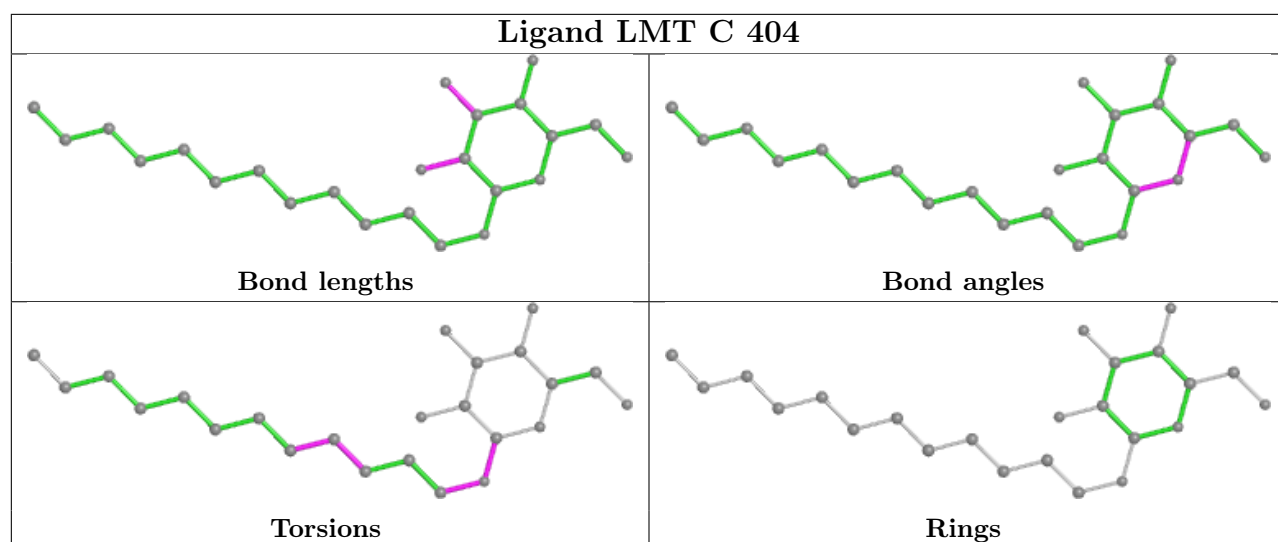
Ligand A1EFU D 105	
	
Bond lengths	Bond angles
	
Torsions	Rings

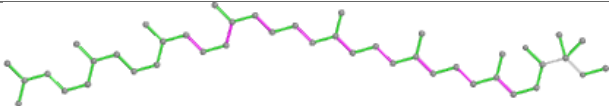
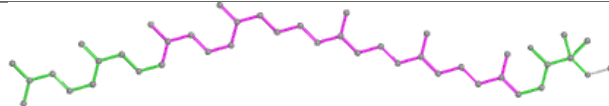
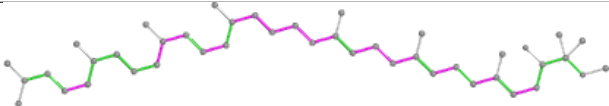
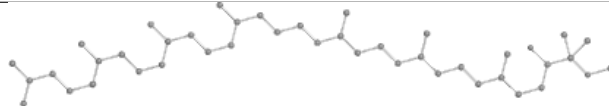
Ligand BCL v 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

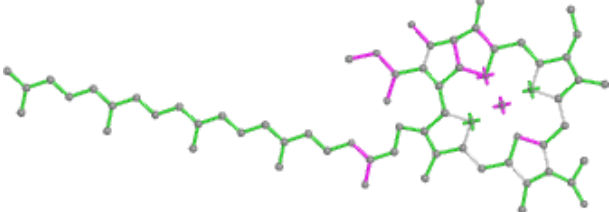
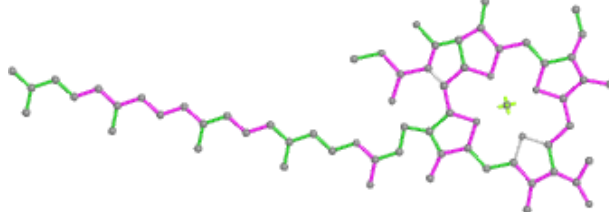
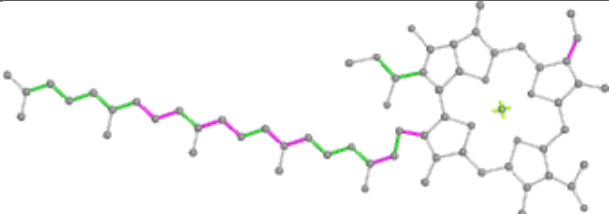
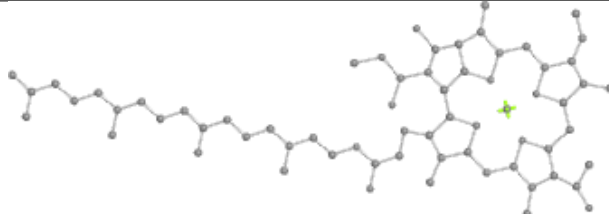


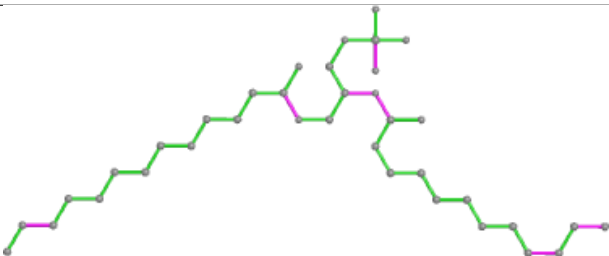
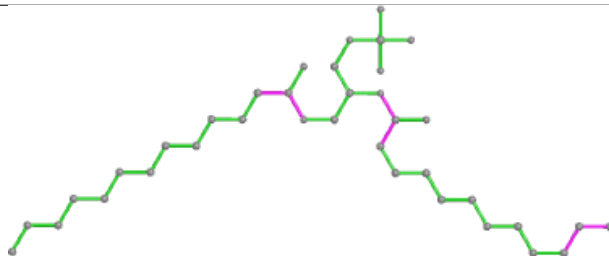
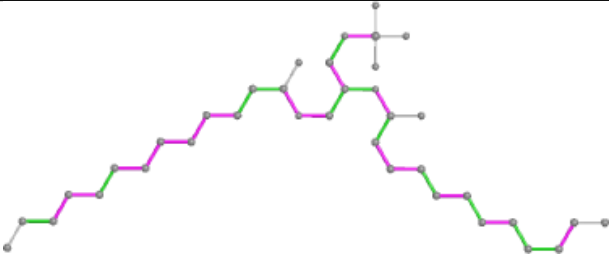
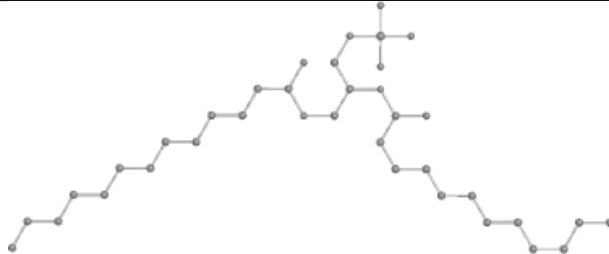


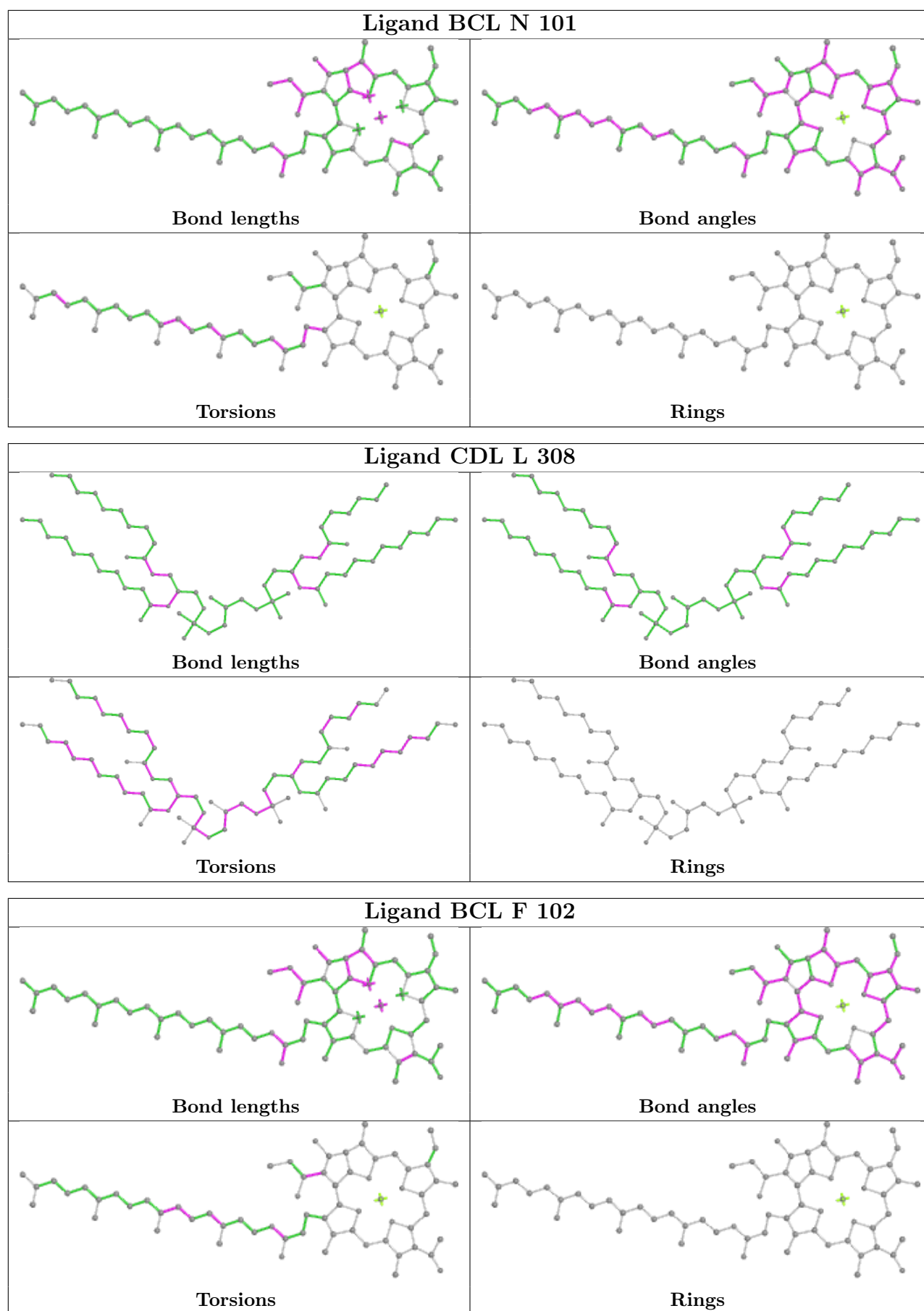


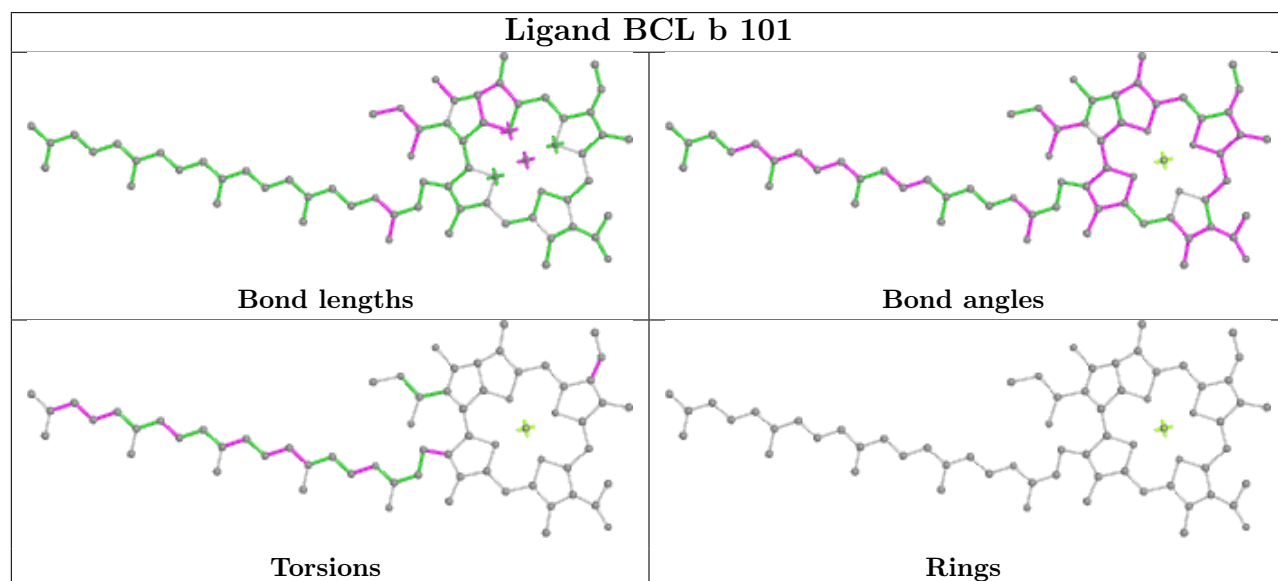
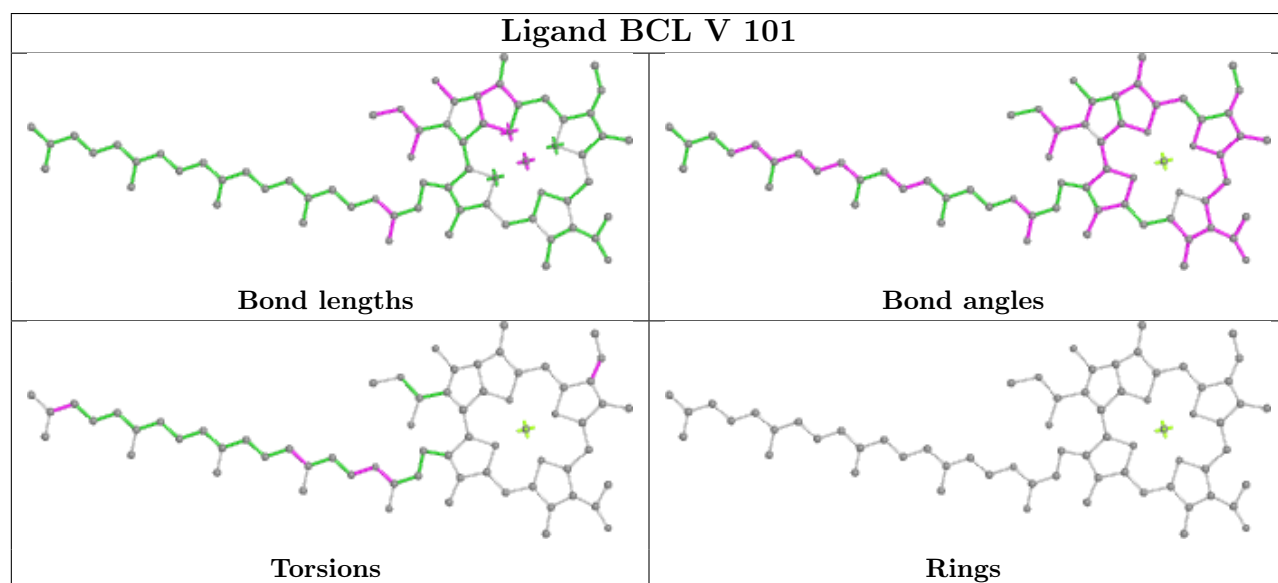
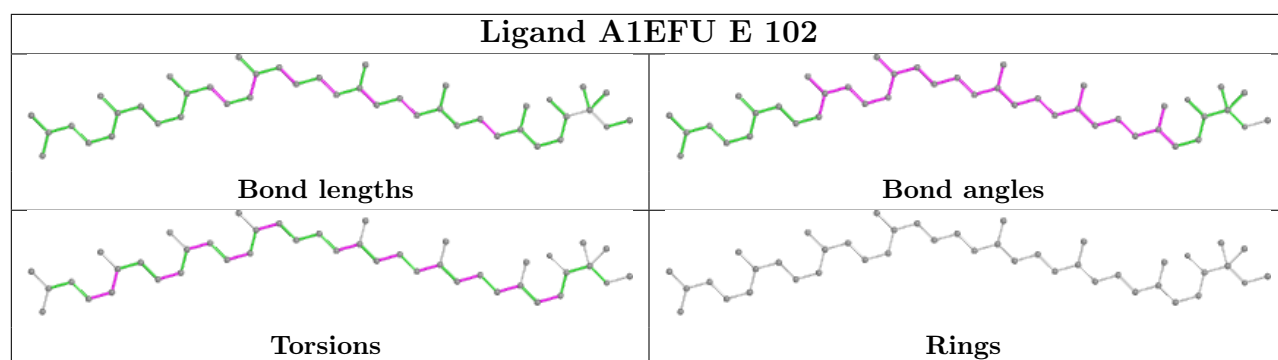


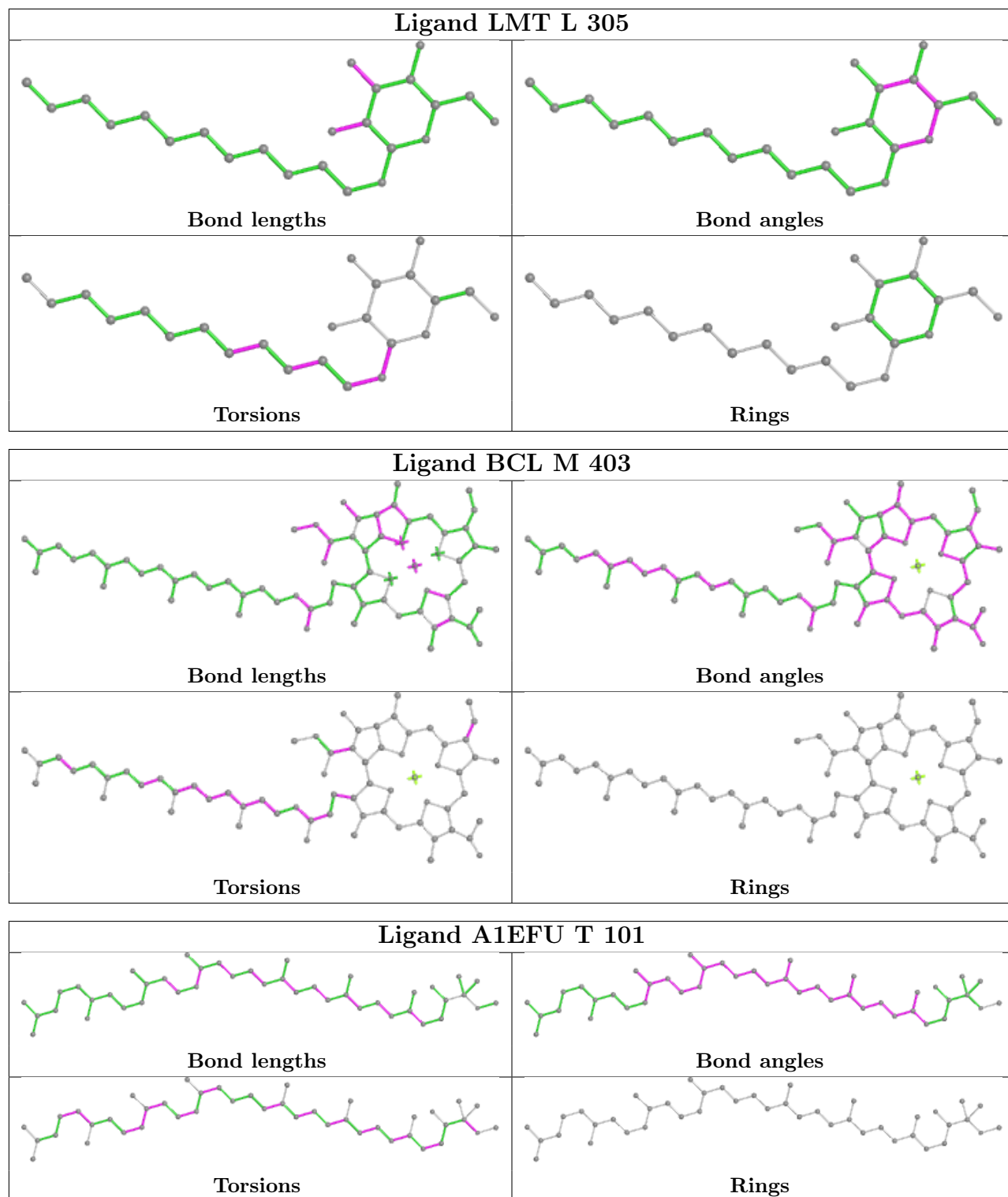
Ligand A1EFU 2 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

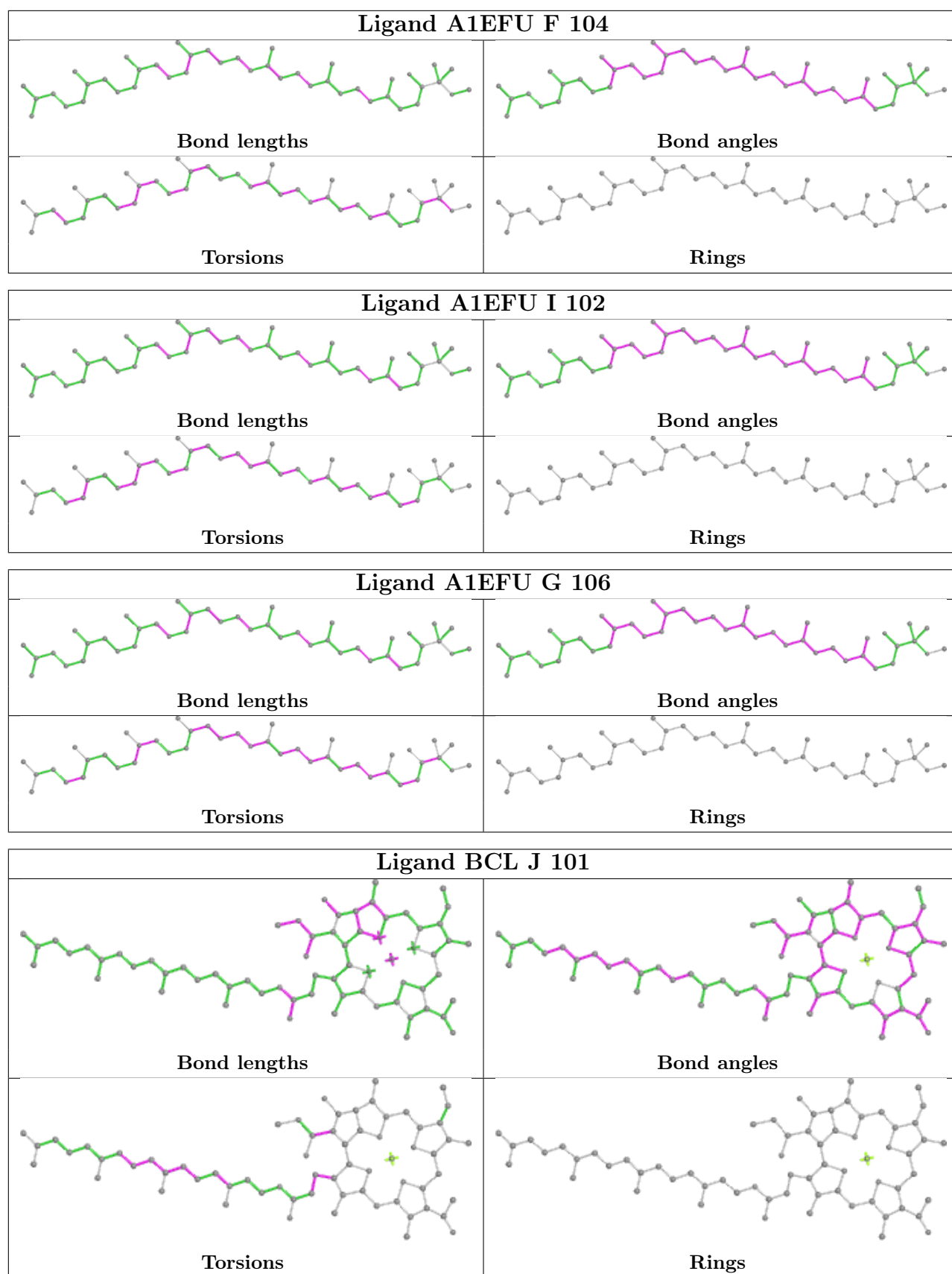
Ligand BCL k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand MW9 H 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

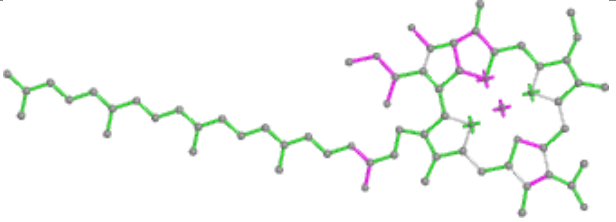
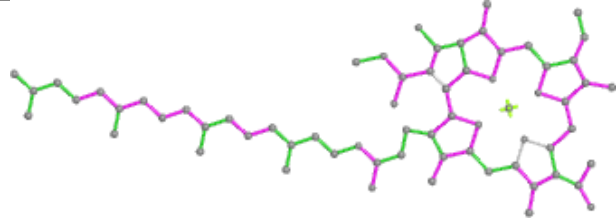
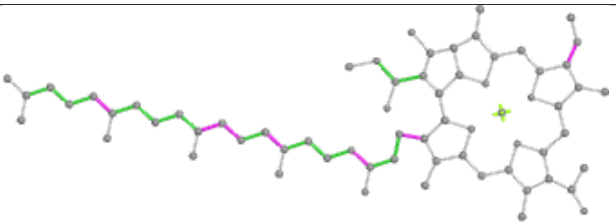
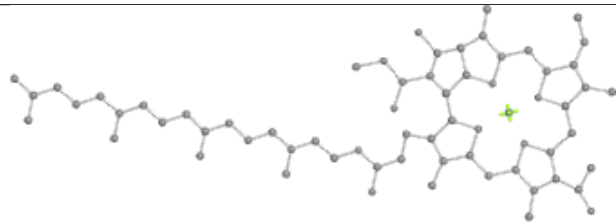


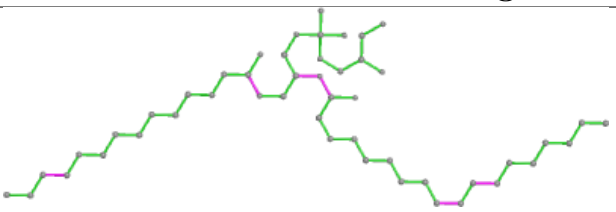
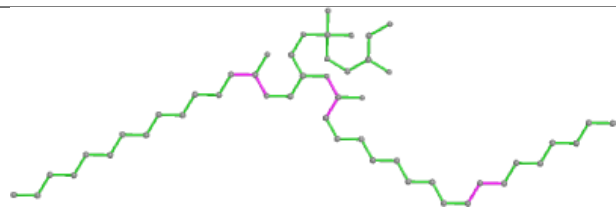
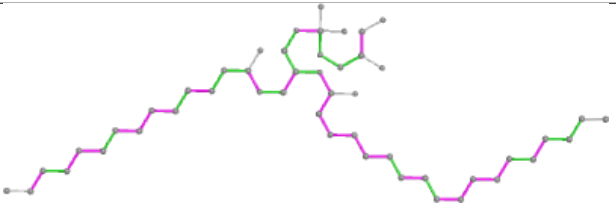
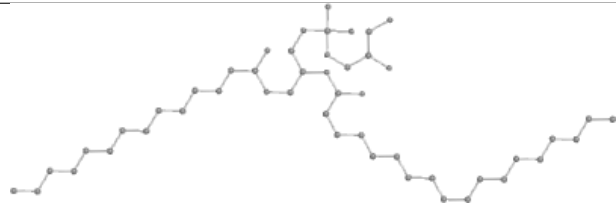


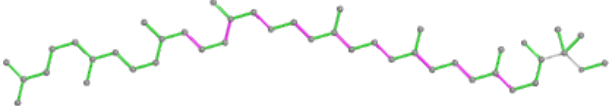
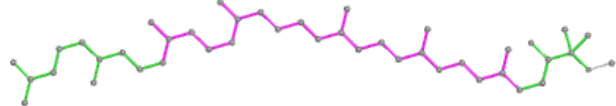
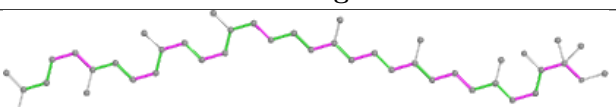
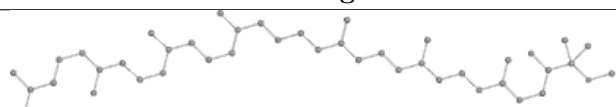


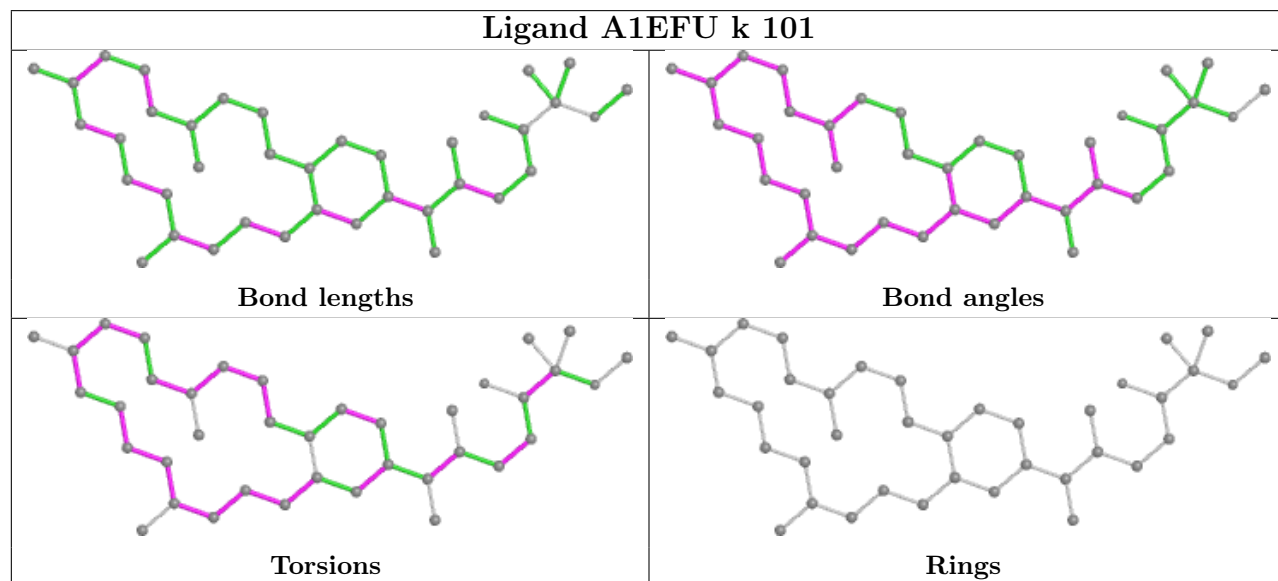
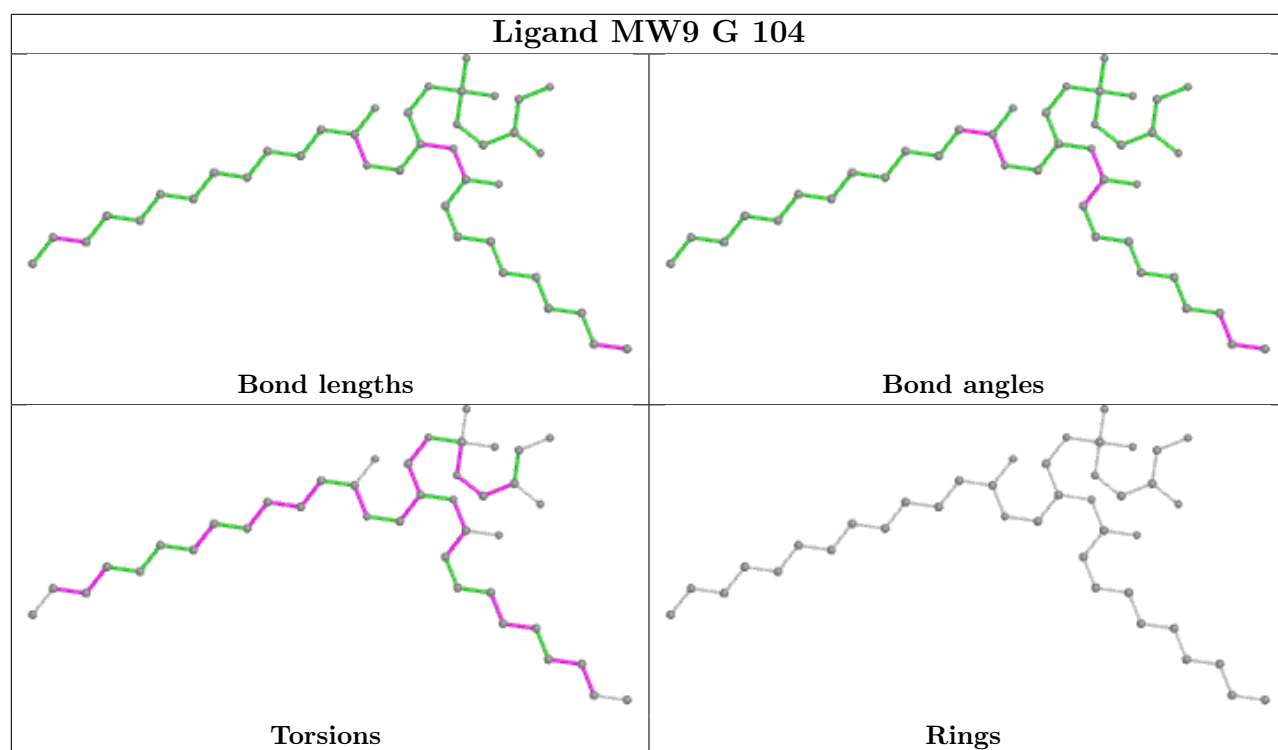


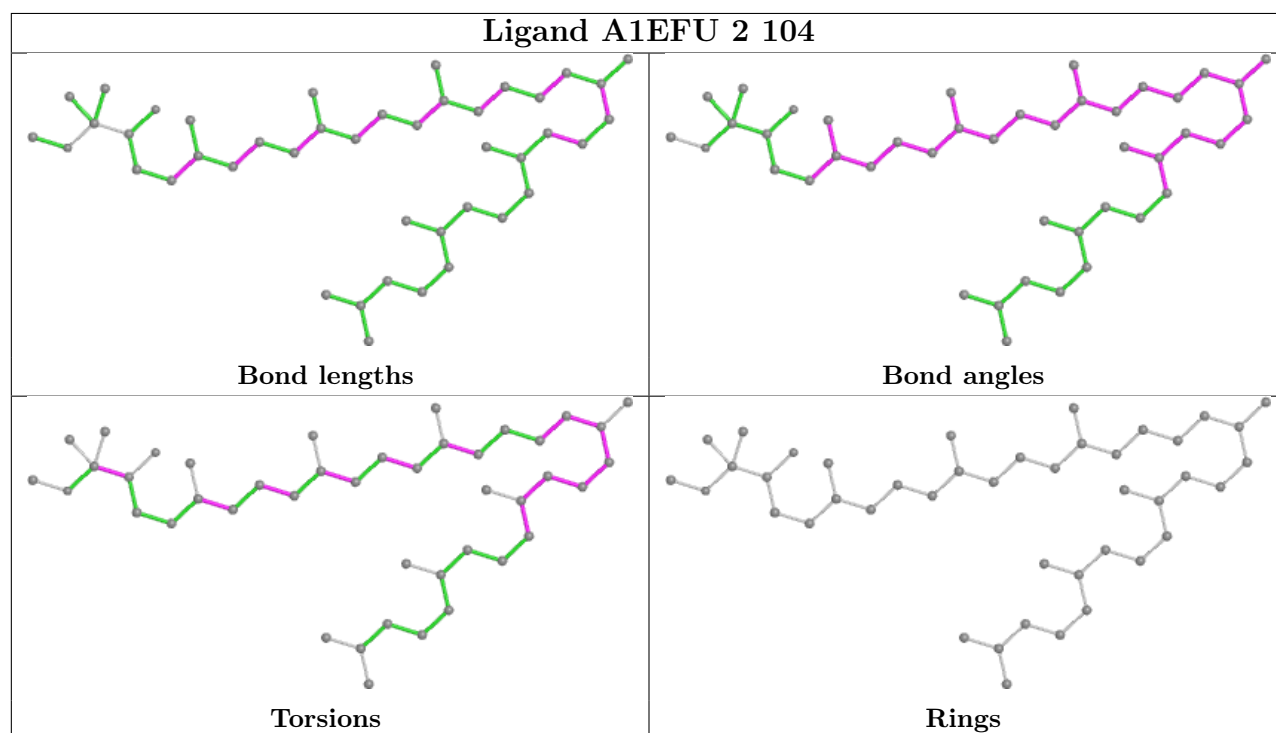
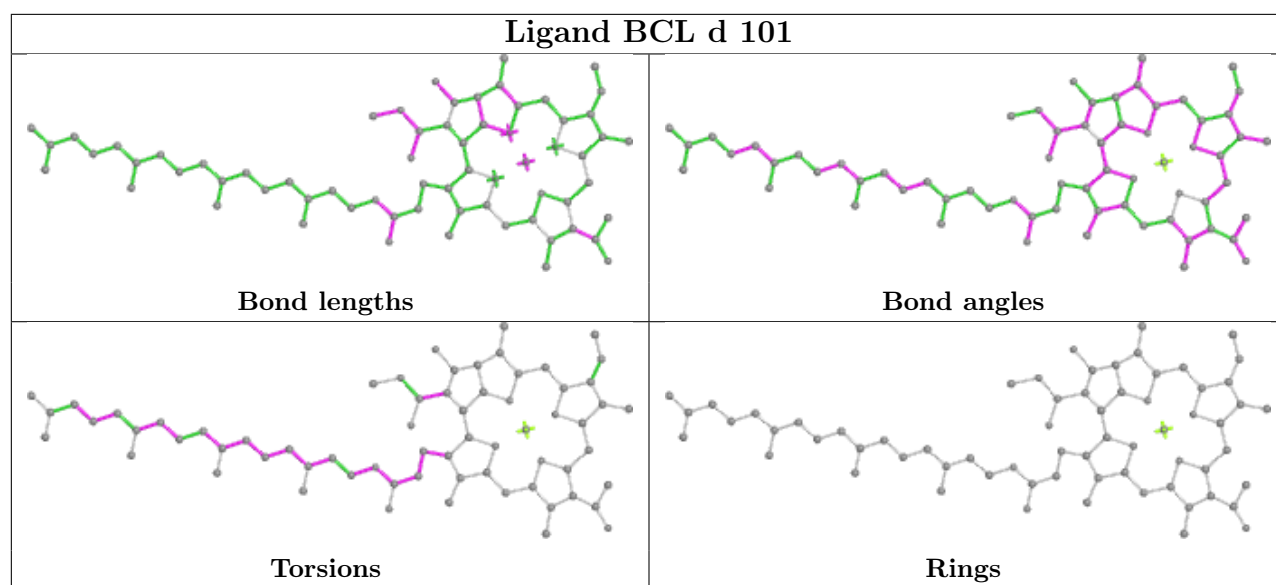


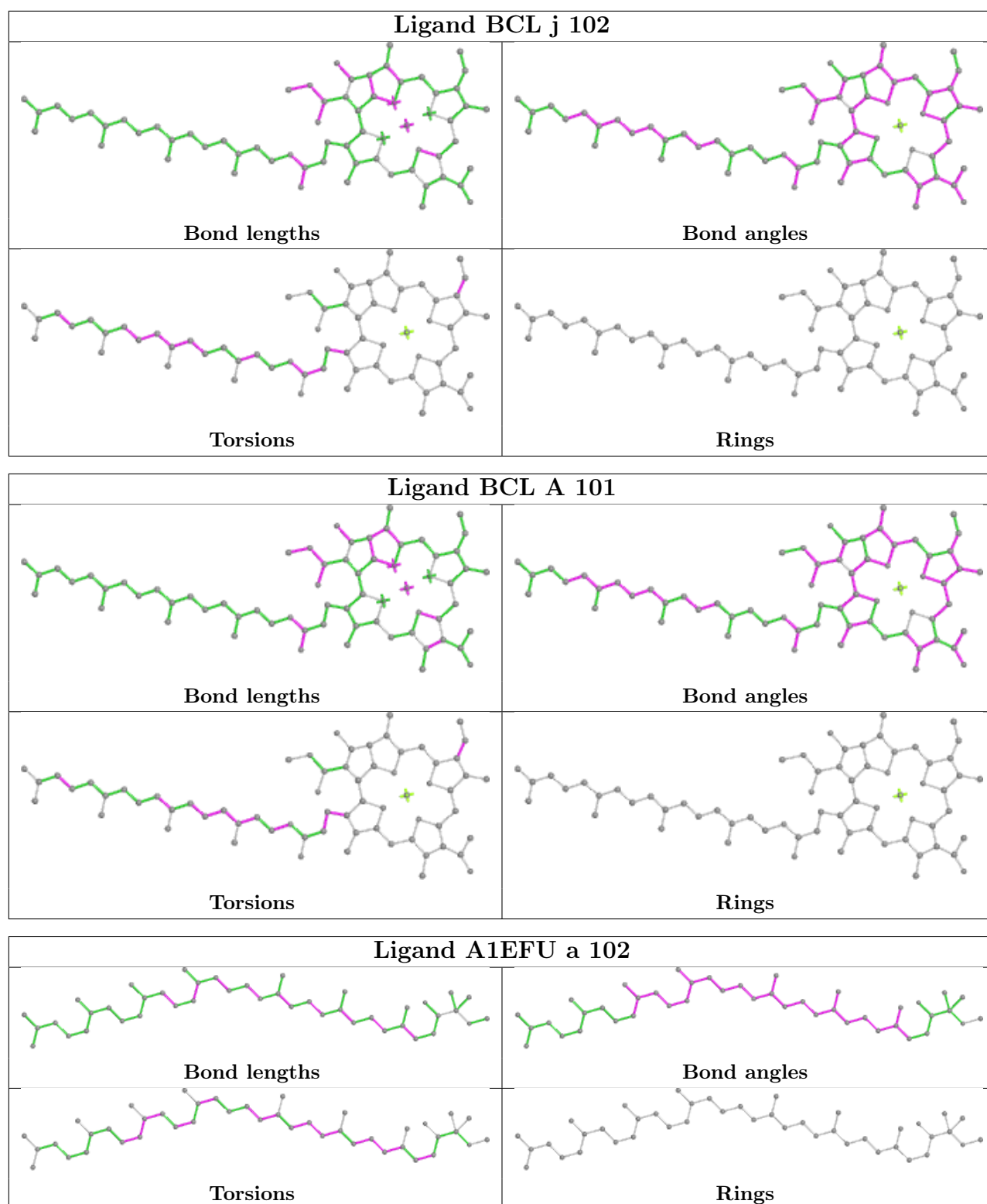
Ligand BCL n 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

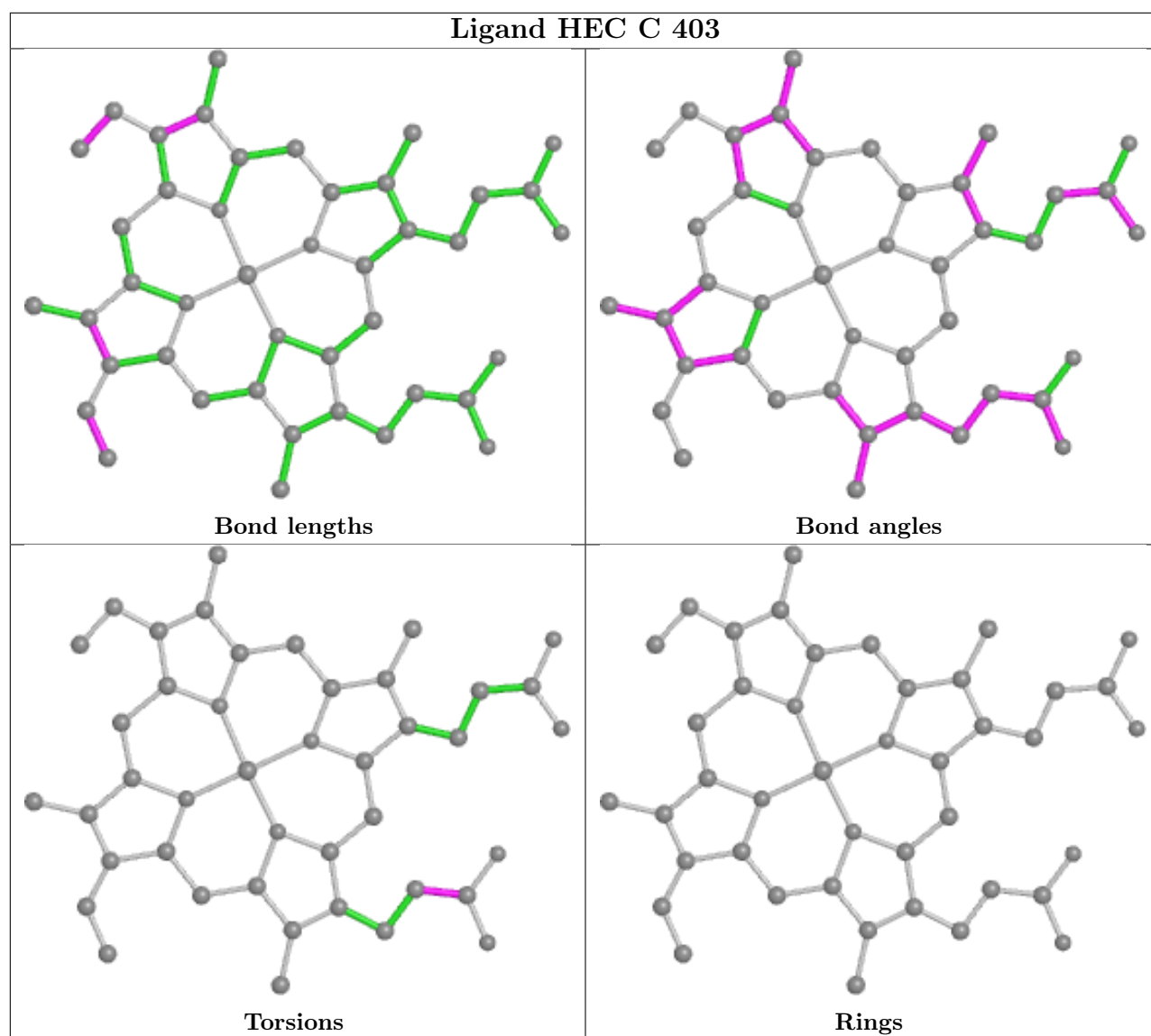
Ligand MW9 M 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A1EFU s 104	
	
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.