



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 9, 2019 – 02:49 AM EST

PDB ID : 6RD5  
EMDB ID: : EMD-4806  
Title : CryoEM structure of Polytomella F-ATP synthase, focussed refinement of Fo and peripheral stalk, C2 symmetry  
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.  
Deposited on : 2019-04-12  
Resolution : 2.69 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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.

---

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

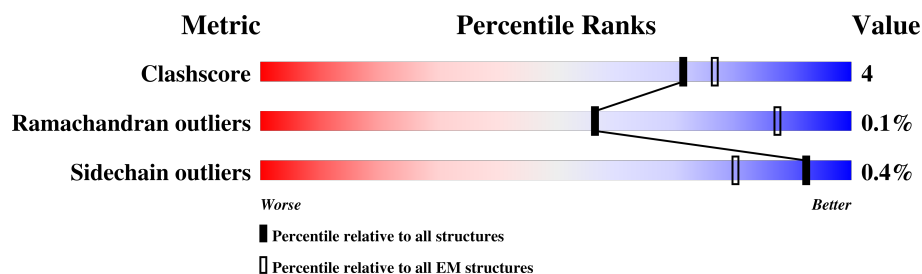
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.69 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	0	82	88% 9% .
2	1	618	89% 8% .
3	3	325	68% 7% 25%
4	5	123	92% 8%
5	6	151	72% 11% 18%
6	8	89	83% 16% .
7	9	97	87% 11% ..
8	M	327	61% 5% 34%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 13000 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	79	Total	C	N	O	S	0	0
			587	376	101	108	2		

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	595	Total	C	N	O	S	0	0
			4661	2958	798	900	5		

- Molecule 3 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	244	Total	C	N	O	S	0	0
			1869	1201	298	369	1		

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	123	Total	C	N	O	S	0	0
			986	640	172	170	4		

- Molecule 5 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 6 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	8	88	Total	C	N	O	0	0
			692	456	115	121		

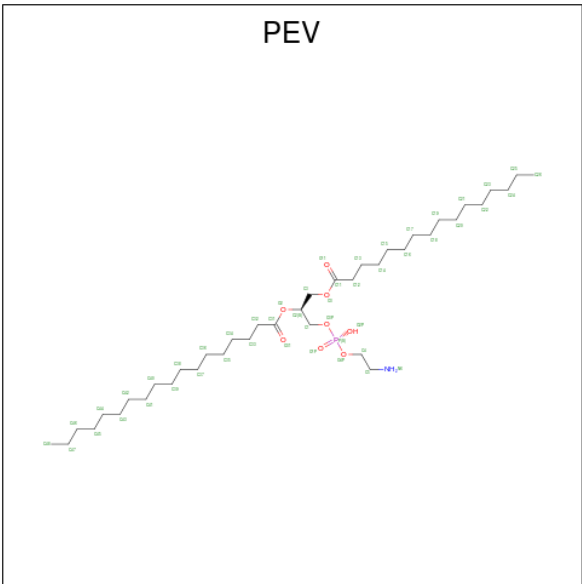
- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	96	Total	C	N	O	S	0	0
			768	509	123	131	5		

- Molecule 8 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

- Molecule 9 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: C<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).



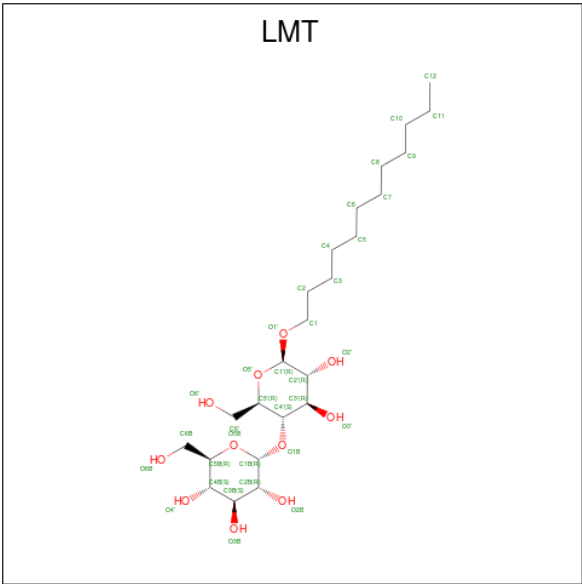
Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total	C	N	O	P	0
			147	117	3	24	3	
9	0	1	Total	C	N	O	P	0
			147	117	3	24	3	
9	0	1	Total	C	N	O	P	0
			147	117	3	24	3	
9	1	1	Total	C	N	O	P	0
			49	39	1	8	1	
9	6	1	Total	C	N	O	P	0
			147	117	3	24	3	
9	6	1	Total	C	N	O	P	0
			147	117	3	24	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	6	1	Total	C	N	O	P	0
			147	117	3	24	3	
9	8	1	Total	C	N	O	P	0
			94	74	2	16	2	
9	8	1	Total	C	N	O	P	0
			94	74	2	16	2	
9	9	1	Total	C	N	O	P	0
			49	39	1	8	1	
9	M	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 10 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
10	6	1	Total	C	O	0
			70	48	22	
10	6	1	Total	C	O	0
			70	48	22	
10	8	1	Total	C	O	0
			70	48	22	
10	8	1	Total	C	O	0
			70	48	22	
10	9	1	Total	C	O	0
			70	48	22	
10	9	1	Total	C	O	0
			70	48	22	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
10	M	1	Total	C	O	0
			70	48	22	
10	M	1	Total	C	O	0
			70	48	22	

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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


- Molecule 12 is water.

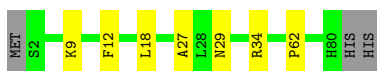
Mol	Chain	Residues	Atoms		AltConf
12	0	1	Total	O	0
			1	1	
12	1	12	Total	O	0
			12	12	
12	3	7	Total	O	0
			7	7	
12	5	2	Total	O	0
			2	2	
12	6	10	Total	O	0
			10	10	
12	8	1	Total	O	0
			1	1	
12	M	22	Total	O	0
			22	22	

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


These plots are drawn for all protein, RNA and DNA 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.

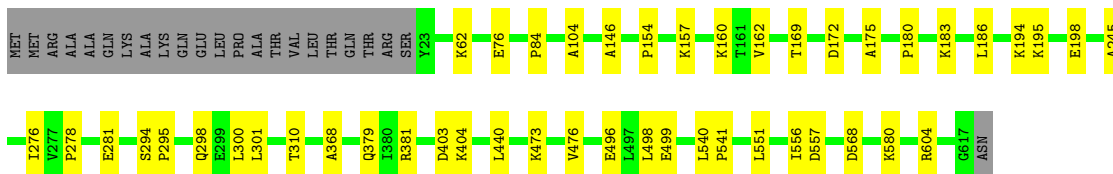
- Molecule 1: ASA-10: *Polytomella* F-ATP synthase associated subunit 10

Chain 0: 



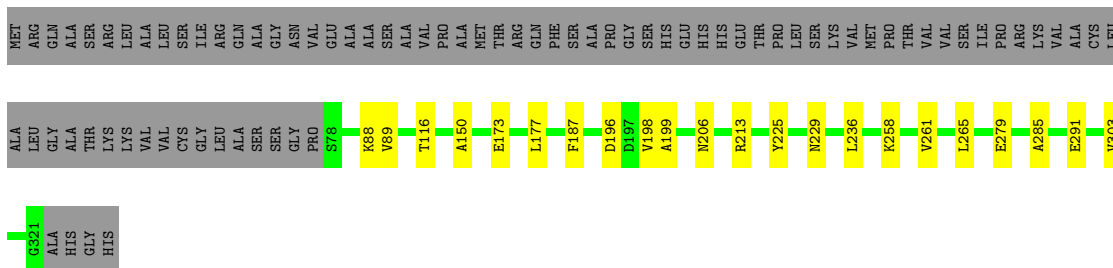
- Molecule 2: ATP synthase associated protein ASA1

Chain 1: 



- Molecule 3: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3: 



- Molecule 4: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5: 

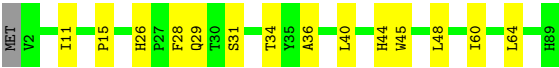
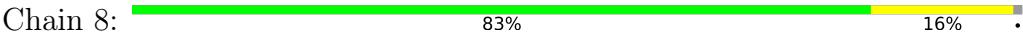


- Molecule 5: Mitochondrial ATP synthase subunit ASA6

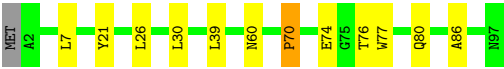
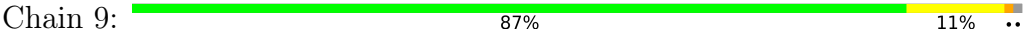
Chain 6: 



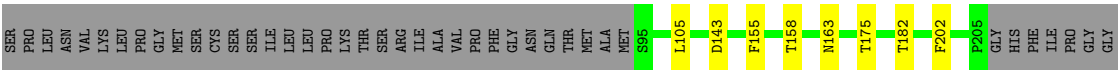
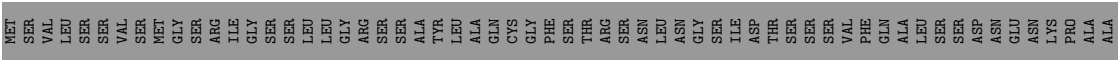
● Molecule 6: Mitochondrial ATP synthase subunit ASA8



● Molecule 7: Mitochondrial ATP synthase subunit ASA9



● Molecule 8: Mitochondrial ATP synthase subunit 6





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	388670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, LMT, PEV

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  >2	RMSZ	# Z  >2
1	0	0.33	0/606	0.49	0/826
2	1	0.30	0/4750	0.44	0/6434
3	3	0.32	0/1906	0.46	0/2594
4	5	0.33	0/1011	0.48	0/1376
5	6	0.30	0/946	0.43	0/1287
6	8	0.35	0/715	0.52	0/974
7	9	0.29	0/794	0.45	0/1074
8	M	0.32	0/1683	0.49	0/2295
All	All	0.31	0/12411	0.46	0/16860

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	0	587	0	570	7	0
2	1	4661	0	4695	28	0
3	3	1869	0	1824	12	0
4	5	986	0	1021	10	0
5	6	926	0	941	13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	8	692	0	694	12	0
7	9	768	0	745	6	0
8	M	1640	0	1665	12	0
9	0	147	0	231	9	0
9	1	49	0	77	3	0
9	6	147	0	231	7	0
9	8	94	0	143	5	0
9	9	49	0	77	3	0
9	M	49	0	77	2	0
10	6	70	0	88	4	0
10	8	70	0	90	1	0
10	9	70	0	90	0	0
10	M	70	0	91	3	0
11	M	1	0	0	0	0
12	0	1	0	0	0	0
12	1	12	0	0	0	0
12	3	7	0	0	0	0
12	5	2	0	0	0	0
12	6	10	0	0	0	0
12	8	1	0	0	0	0
12	M	22	0	0	0	0
All	All	13000	0	13350	99	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 4.

The worst 5 of 99 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)
6:8:26:HIS:H	6:8:29:GLN:HE21	1.45	0.64
2:1:62:LYS:HD3	2:1:146:ALA:HB2	1.79	0.63
6:8:26:HIS:HD2	6:8:28:PHE:H	1.46	0.63
2:1:278:PRO:HG2	2:1:281:GLU:HB2	1.82	0.61
2:1:368:ALA:O	2:1:379:GLN:NE2	2.33	0.59

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
2	1	593/618 (96%)	584 (98%)	9 (2%)	0	100	100
3	3	242/325 (74%)	241 (100%)	1 (0%)	0	100	100
4	5	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
5	6	122/151 (81%)	120 (98%)	2 (2%)	0	100	100
6	8	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
7	9	94/97 (97%)	83 (88%)	9 (10%)	2 (2%)	8	20
8	M	213/327 (65%)	205 (96%)	8 (4%)	0	100	100
All	All	1548/1812 (85%)	1504 (97%)	42 (3%)	2 (0%)	56	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	9	74	GLU
7	9	70	PRO

### 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	0	61/64 (95%)	61 (100%)	0	100	100
2	1	493/512 (96%)	491 (100%)	2 (0%)	92	97
3	3	195/258 (76%)	194 (100%)	1 (0%)	90	97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	5	107/107 (100%)	107 (100%)	0	100	100
5	6	96/115 (84%)	96 (100%)	0	100	100
6	8	71/72 (99%)	71 (100%)	0	100	100
7	9	78/79 (99%)	77 (99%)	1 (1%)	71	89
8	M	178/272 (65%)	177 (99%)	1 (1%)	87	96
All	All	1279/1479 (86%)	1274 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	195	LYS
2	1	310	THR
3	3	187	PHE
7	9	76	THR
8	M	314	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	206	ASN
4	5	29	GLN
6	8	29	GLN
2	1	562	ASN
6	8	26	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	PEV	0	101	-	48,48,48	0.84	2 (4%)	51,53,53	0.91	3 (5%)
9	PEV	0	102	-	48,48,48	0.88	3 (6%)	51,53,53	0.87	2 (3%)
9	PEV	0	103	-	48,48,48	0.88	4 (8%)	51,53,53	0.87	2 (3%)
9	PEV	1	701	-	48,48,48	0.88	4 (8%)	51,53,53	0.90	2 (3%)
10	LMT	6	201	-	36,36,36	1.26	5 (13%)	47,47,47	1.28	4 (8%)
10	LMT	6	202	-	36,36,36	1.22	5 (13%)	47,47,47	1.05	5 (10%)
9	PEV	6	203	-	48,48,48	0.87	3 (6%)	51,53,53	0.97	2 (3%)
9	PEV	6	204	-	48,48,48	0.87	4 (8%)	51,53,53	0.80	2 (3%)
9	PEV	6	205	-	48,48,48	0.87	3 (6%)	51,53,53	0.84	3 (5%)
10	LMT	8	101	-	36,36,36	1.23	6 (16%)	47,47,47	1.13	3 (6%)
9	PEV	8	102	-	44,44,48	0.92	4 (9%)	47,49,53	0.91	2 (4%)
10	LMT	8	103	-	36,36,36	1.22	5 (13%)	47,47,47	1.16	3 (6%)
9	PEV	8	104	-	48,48,48	0.88	4 (8%)	51,53,53	0.87	2 (3%)
10	LMT	9	101	-	36,36,36	1.20	5 (13%)	47,47,47	0.98	3 (6%)
9	PEV	9	102	-	48,48,48	0.88	3 (6%)	51,53,53	0.92	2 (3%)
10	LMT	9	103	-	36,36,36	1.21	6 (16%)	47,47,47	1.24	5 (10%)
9	PEV	M	402	-	48,48,48	0.88	4 (8%)	51,53,53	0.86	2 (3%)
10	LMT	M	403	-	36,36,36	1.18	5 (13%)	47,47,47	0.96	3 (6%)
10	LMT	M	404	-	36,36,36	1.22	4 (11%)	47,47,47	1.02	2 (4%)

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	PEV	0	101	-	-	30/52/52/52	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PEV	0	102	-	-	23/52/52/52	-
9	PEV	0	103	-	-	26/52/52/52	-
9	PEV	1	701	-	-	28/52/52/52	-
10	LMT	6	201	-	-	14/21/61/61	0/2/2/2
10	LMT	6	202	-	-	9/21/61/61	0/2/2/2
9	PEV	6	203	-	-	31/52/52/52	-
9	PEV	6	204	-	-	29/52/52/52	-
9	PEV	6	205	-	-	33/52/52/52	-
10	LMT	8	101	-	-	11/21/61/61	0/2/2/2
9	PEV	8	102	-	-	22/48/48/52	-
10	LMT	8	103	-	-	14/21/61/61	0/2/2/2
9	PEV	8	104	-	-	32/52/52/52	-
10	LMT	9	101	-	-	7/21/61/61	0/2/2/2
9	PEV	9	102	-	-	26/52/52/52	-
10	LMT	9	103	-	-	7/21/61/61	0/2/2/2
9	PEV	M	402	-	-	25/52/52/52	-
10	LMT	M	403	-	-	10/21/61/61	0/2/2/2
10	LMT	M	404	-	-	8/21/61/61	0/2/2/2

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	6	201	LMT	O2'-C2'	-3.02	1.35	1.43
10	6	202	LMT	O3'-C3'	-2.90	1.36	1.43
10	9	101	LMT	O3'-C3'	-2.90	1.36	1.43
10	9	103	LMT	O3'-C3'	-2.82	1.36	1.43
10	6	202	LMT	O2'-C2'	-2.71	1.36	1.43

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	6	203	PEV	O2-C31-C32	4.65	121.67	111.51
9	8	102	PEV	O2-C31-C32	4.32	120.94	111.51
9	9	102	PEV	O2-C31-C32	4.12	120.51	111.51
9	1	701	PEV	O2-C31-C32	4.09	120.44	111.51
9	0	103	PEV	O2-C31-C32	4.08	120.42	111.51

There are no chirality outliers.

5 of 385 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	1	701	PEV	C32-C31-O2-C2
9	1	701	PEV	O31-C31-O2-C2
9	1	701	PEV	C4-O4P-P-O3P
9	1	701	PEV	C4-O4P-P-O1P
9	1	701	PEV	C4-O4P-P-O2P

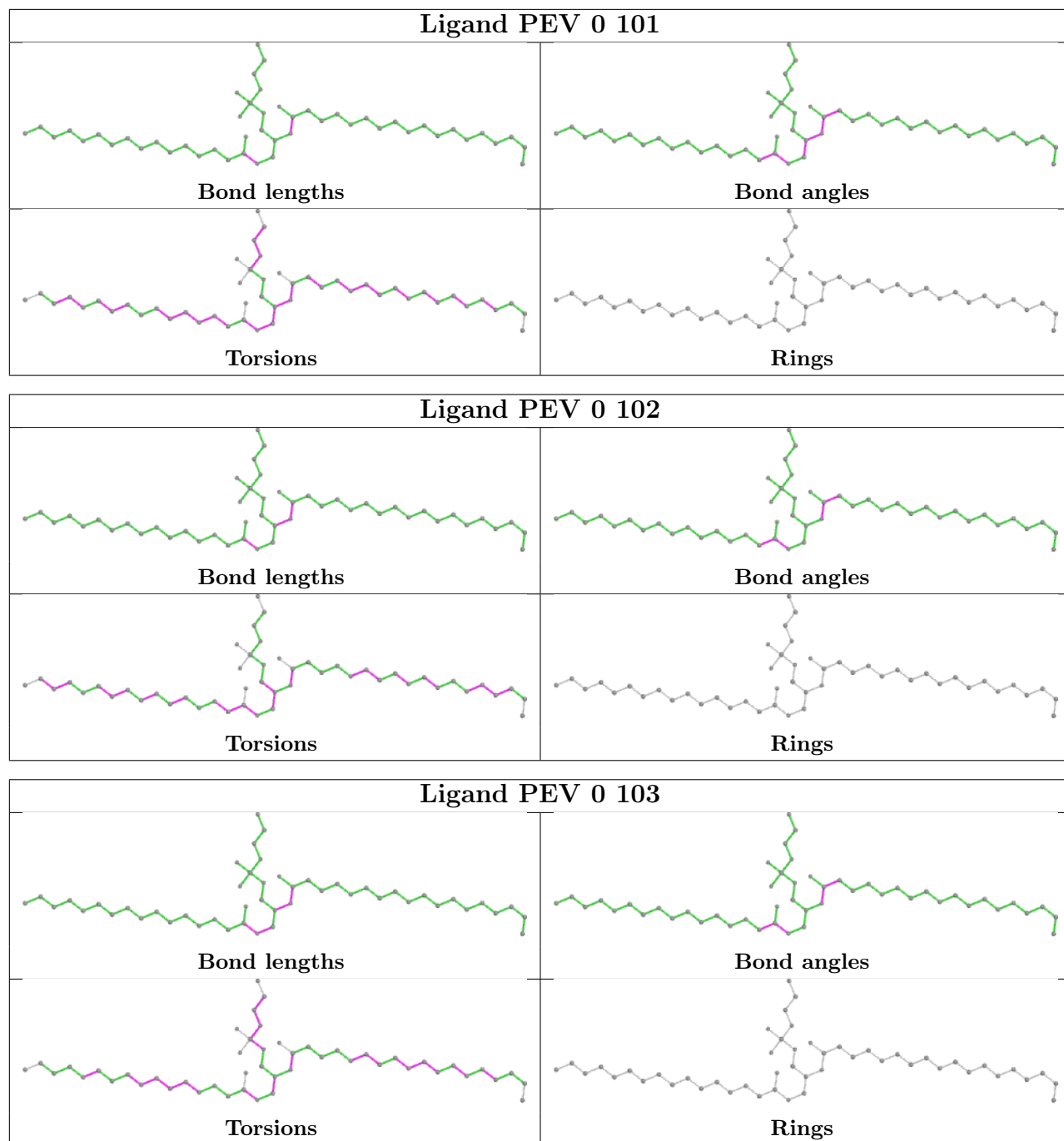
There are no ring outliers.

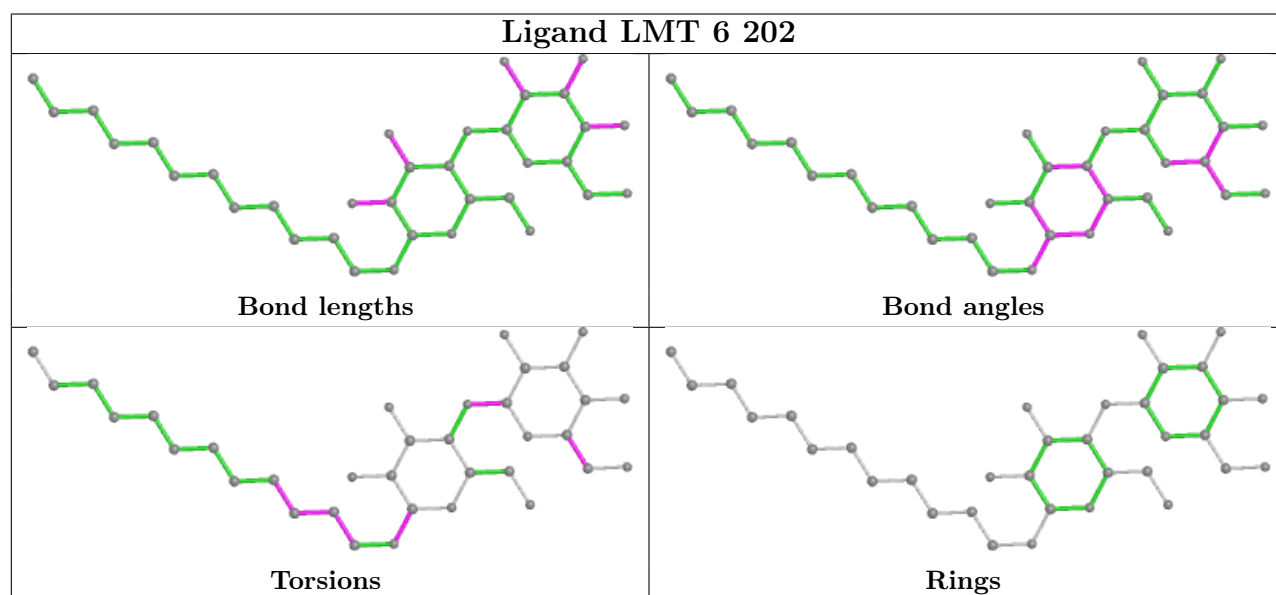
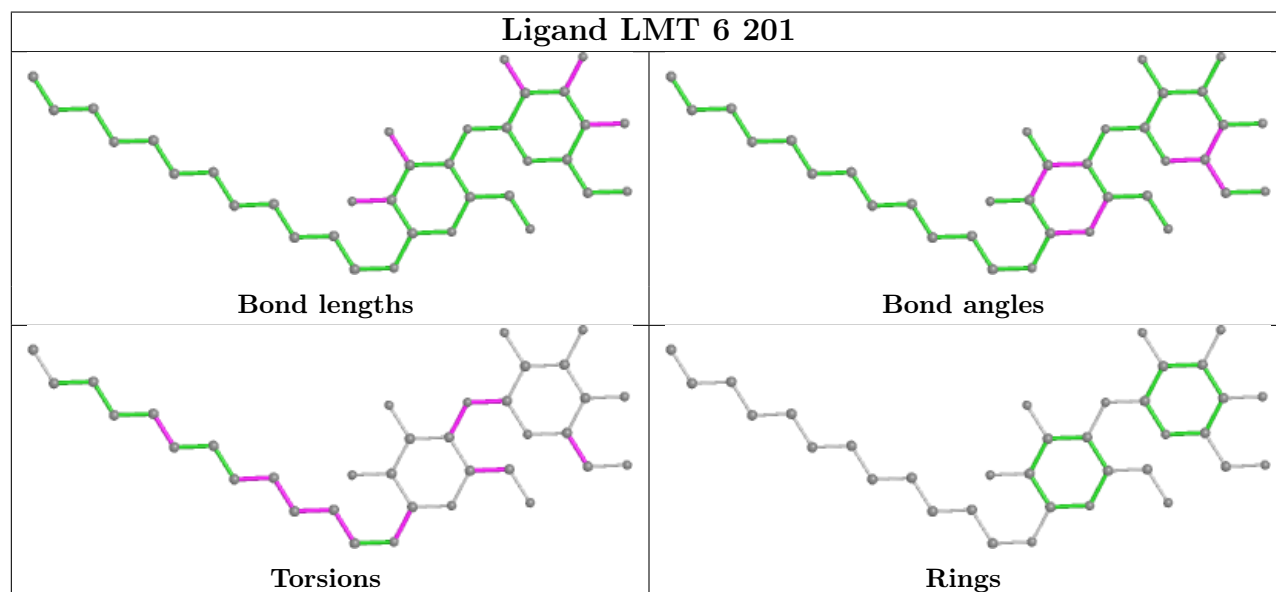
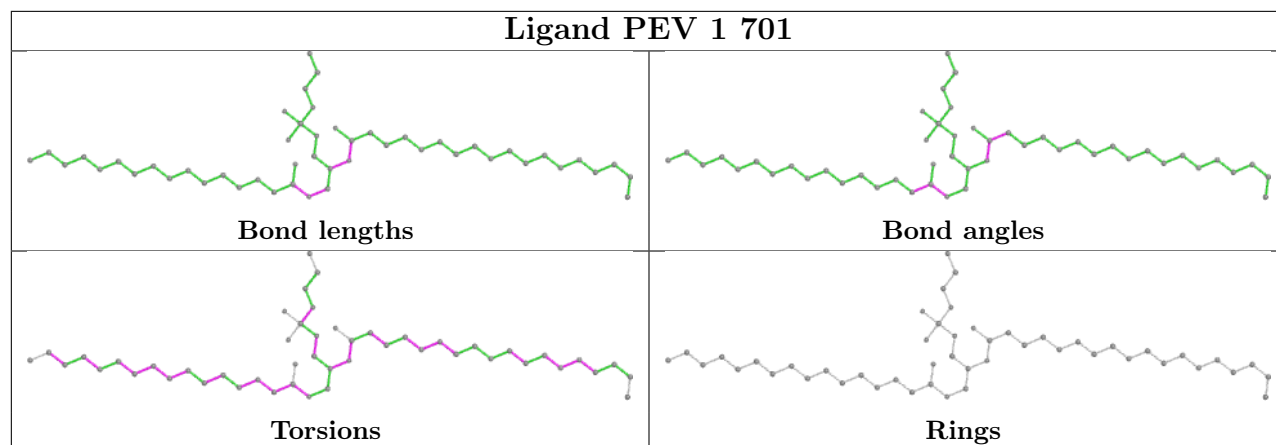
15 monomers are involved in 30 short contacts:

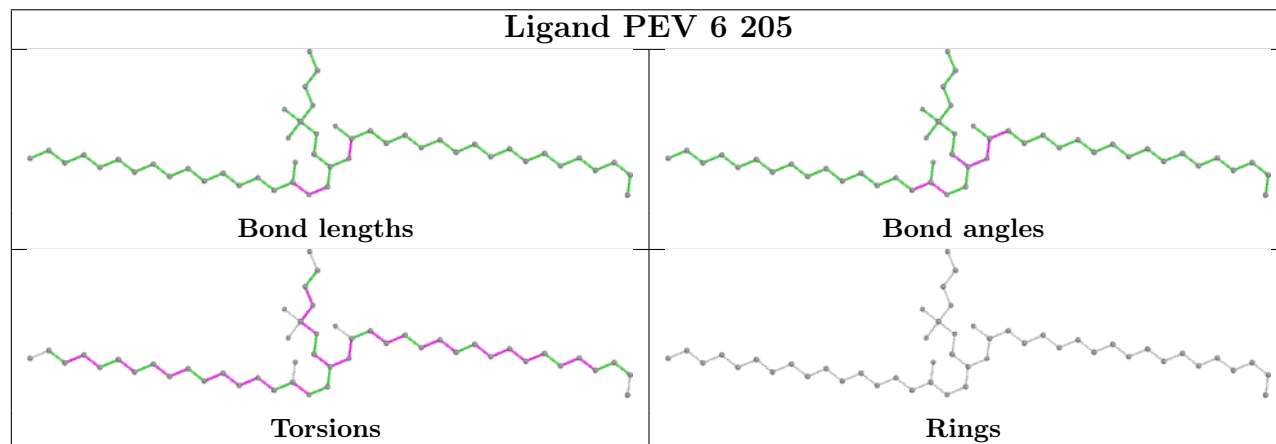
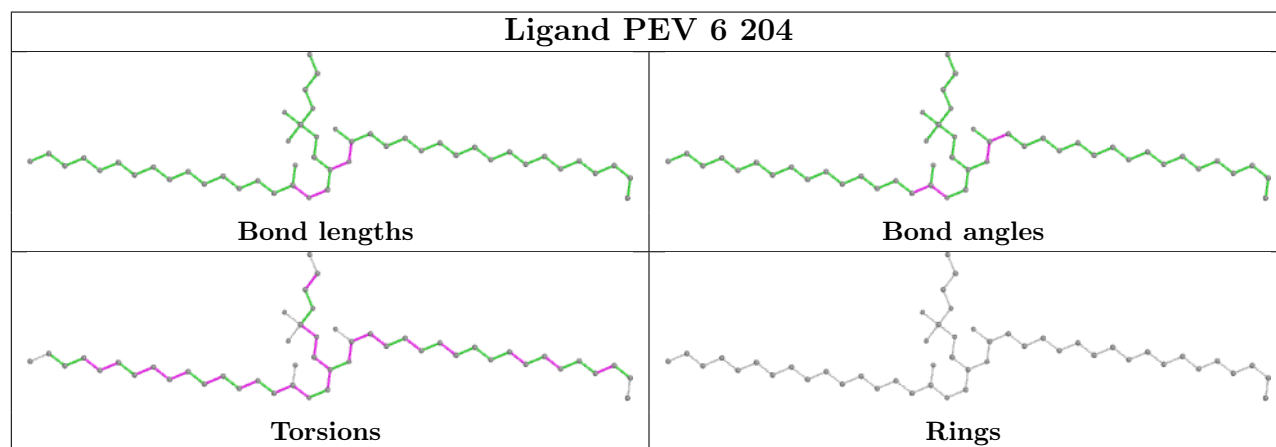
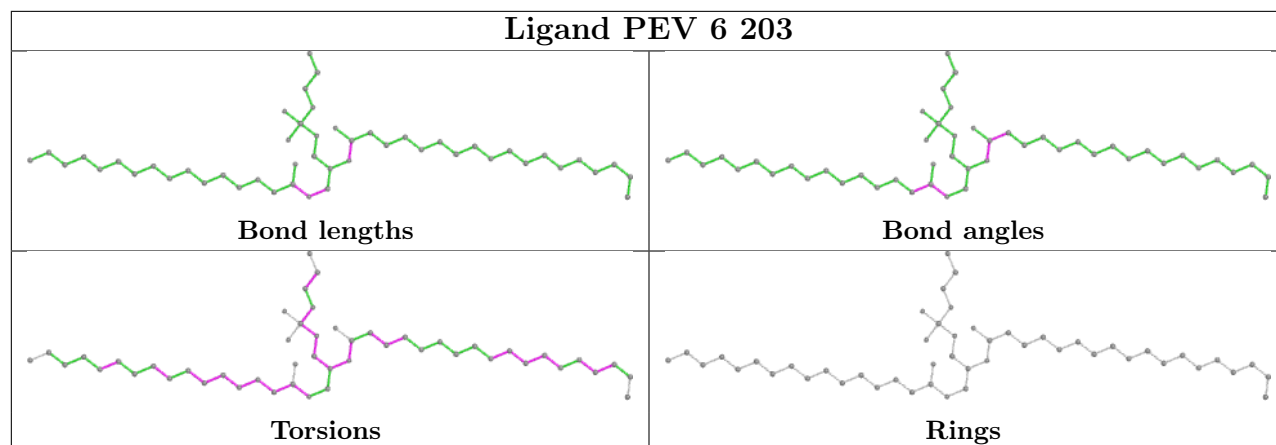
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	0	101	PEV	3	0
9	0	102	PEV	3	0
9	0	103	PEV	3	0
9	1	701	PEV	3	0
10	6	201	LMT	3	0
10	6	202	LMT	2	0
9	6	203	PEV	2	0
9	6	204	PEV	2	0
9	6	205	PEV	3	0
9	8	102	PEV	3	0
10	8	103	LMT	1	0
9	8	104	PEV	2	0
9	9	102	PEV	3	0
9	M	402	PEV	2	0
10	M	404	LMT	3	0

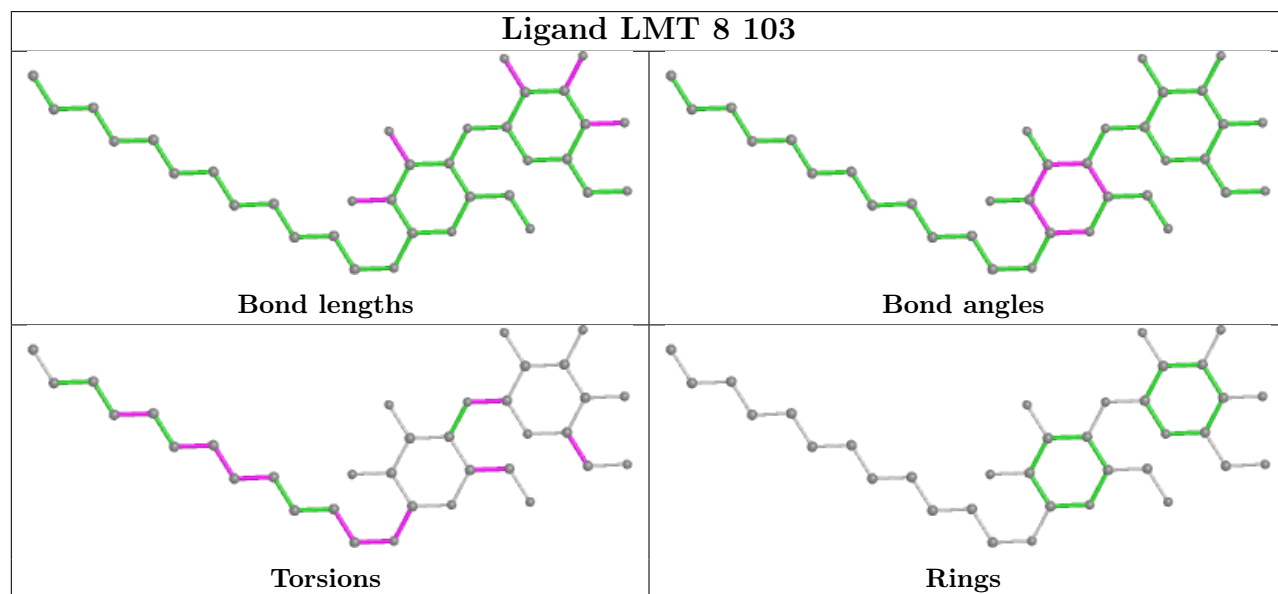
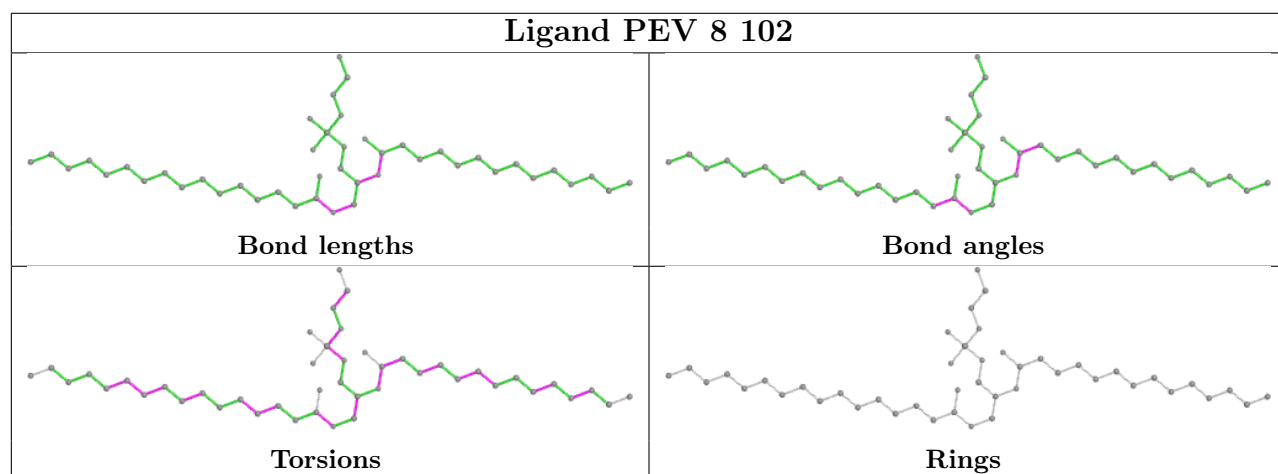
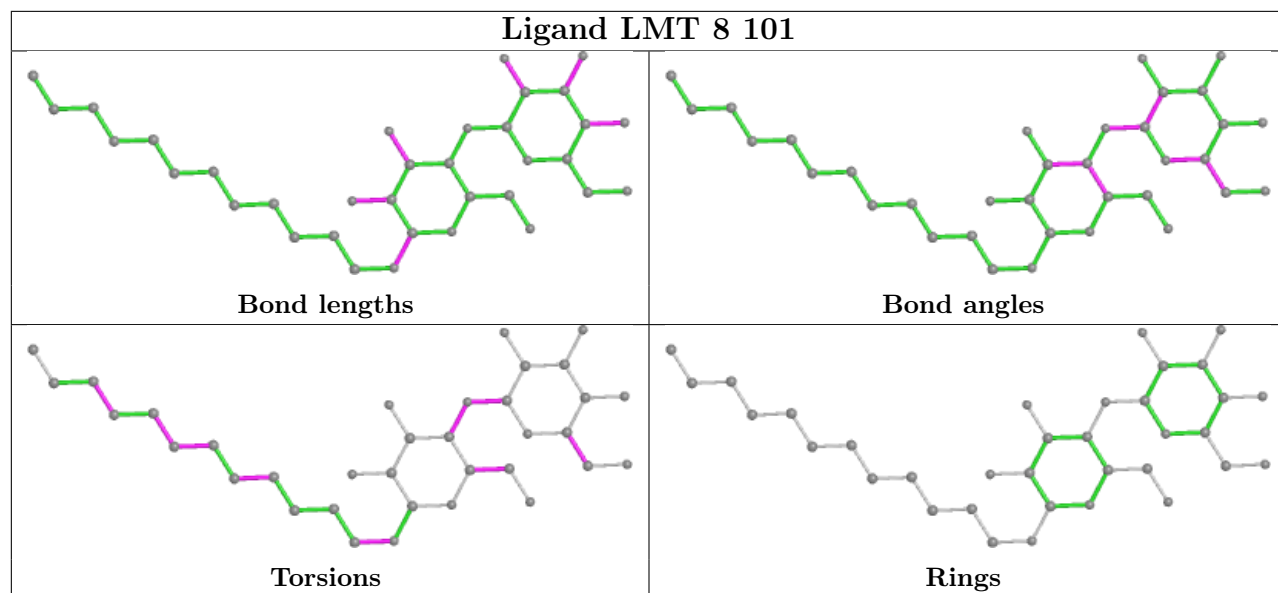
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

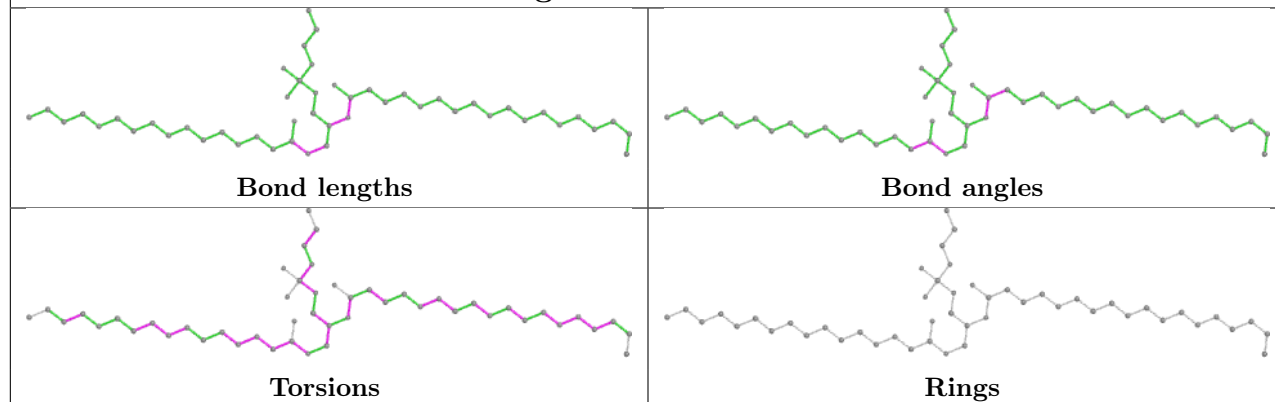
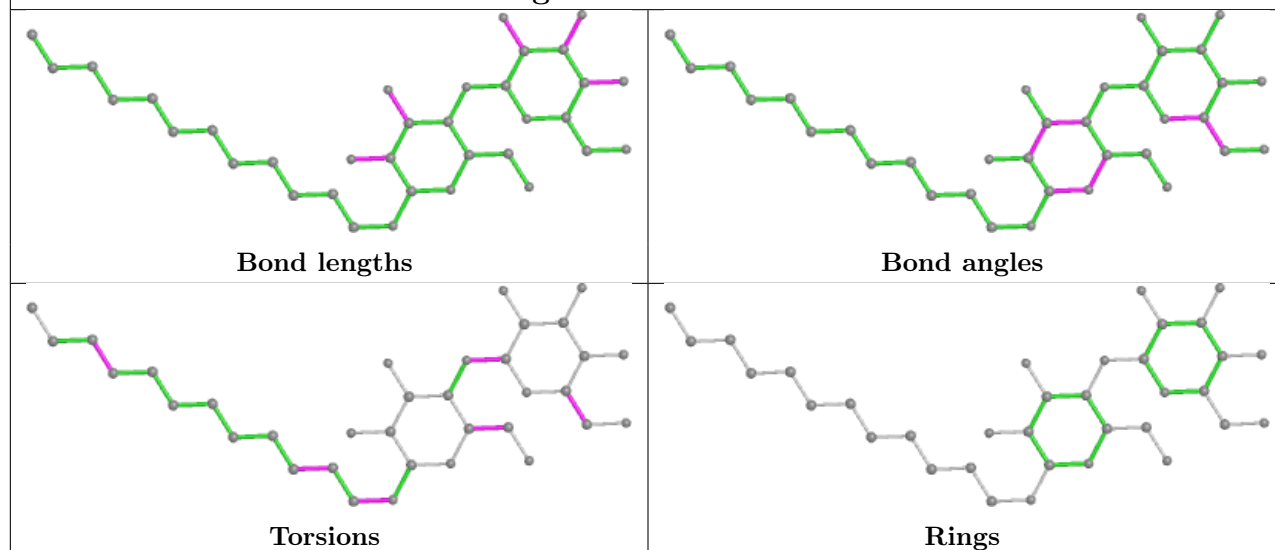
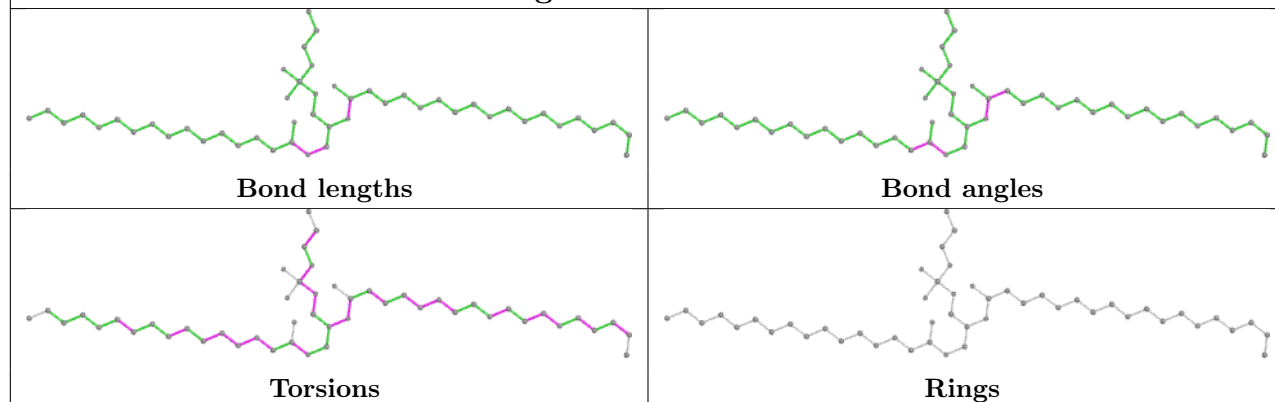


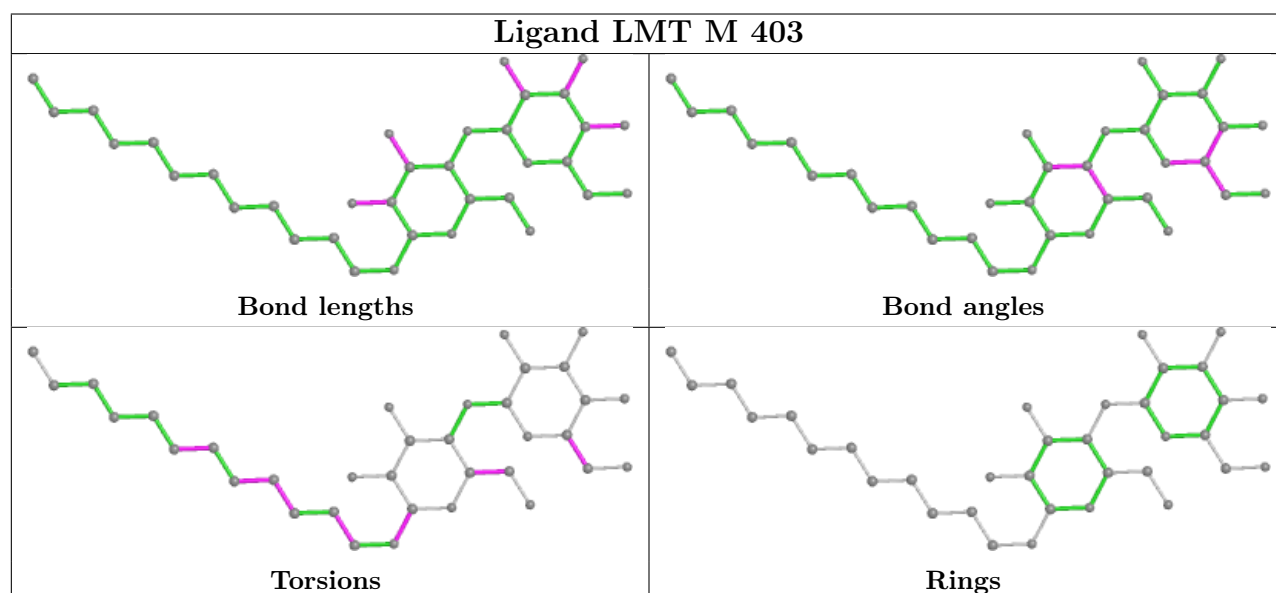
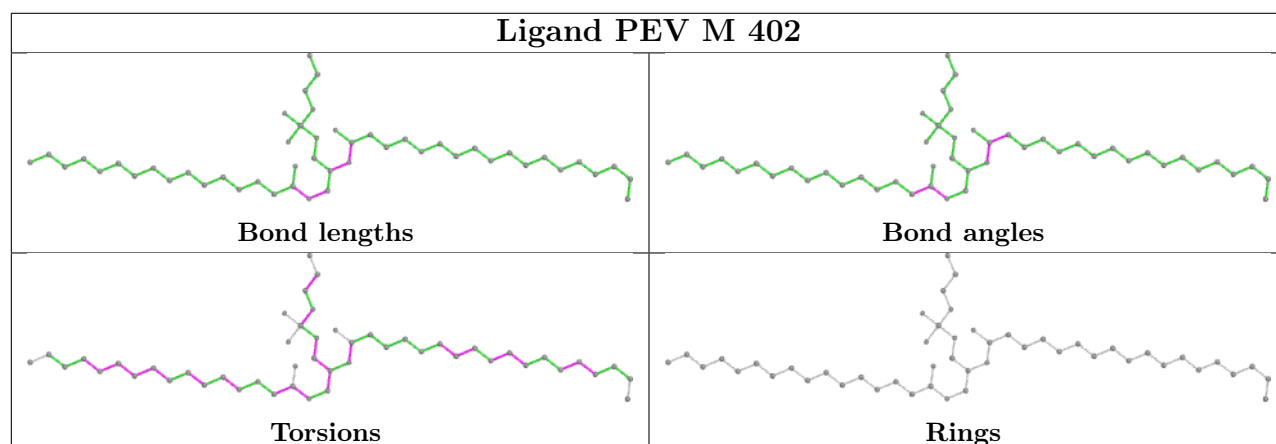
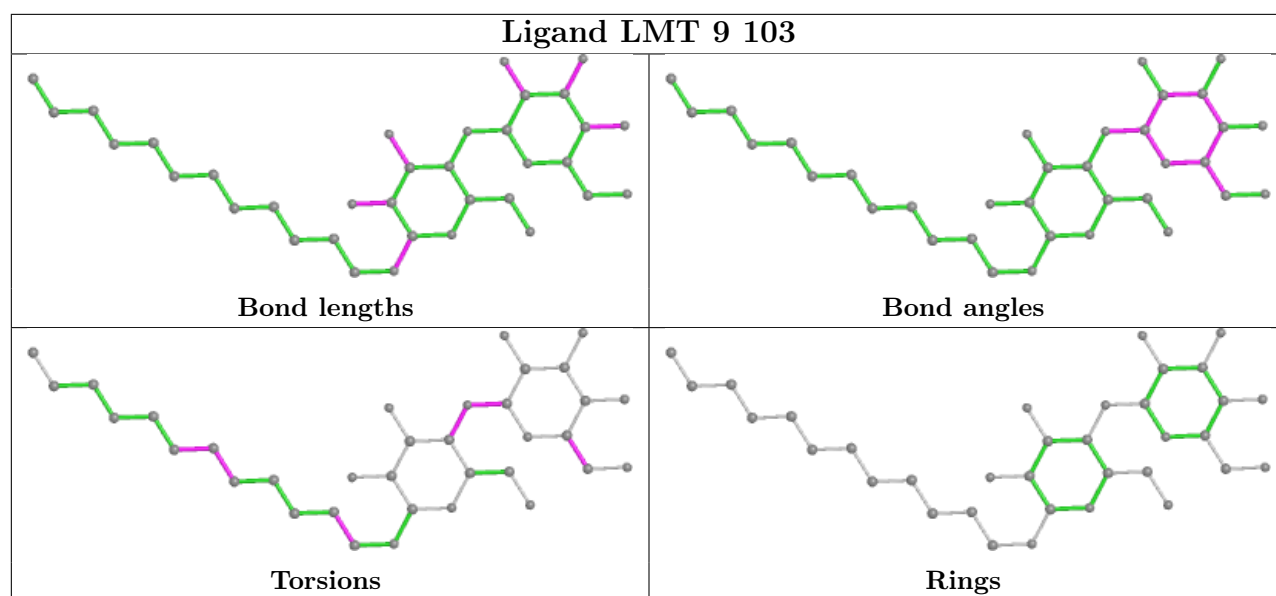


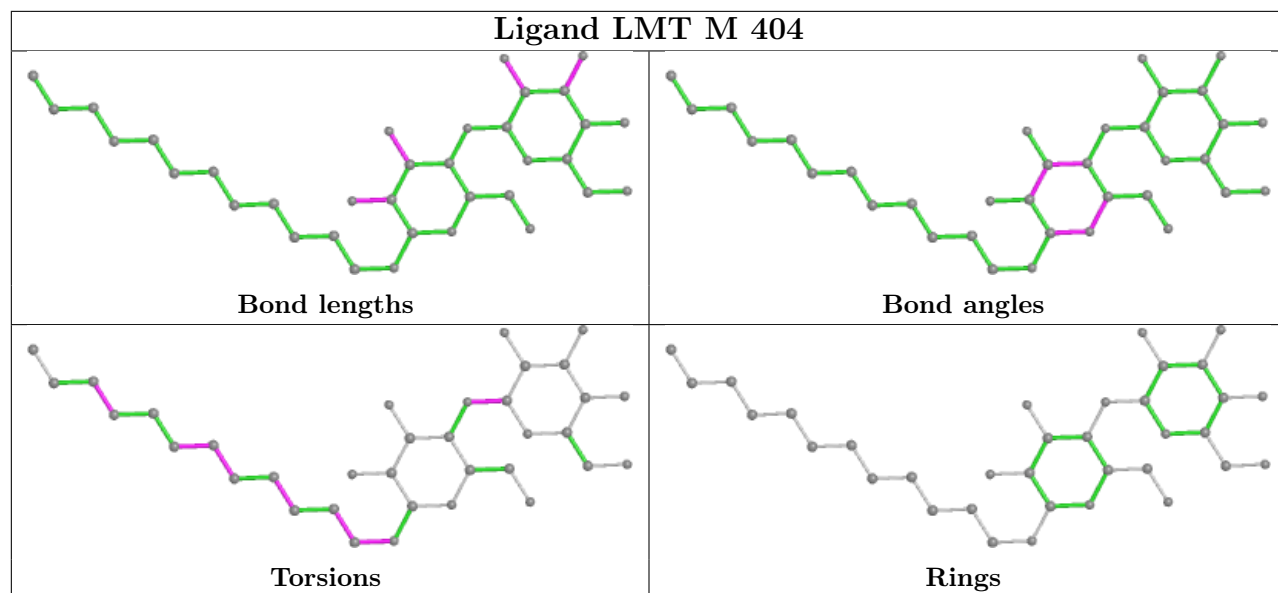






**Ligand PEV 8 104****Ligand LMT 9 101****Ligand PEV 9 102**





## 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.