wwPDB EM Validation Summary Report (i)

Aug 29, 2023 – 12:23 PM EDT

PDB ID	:	3M9I
Title	:	Electron crystallographic structure of lens Aquaporin-0 (AQP0) (lens MIP) in E. coli polar lipids
Authors	:	Hite, R.K.; Li, Z.; Walz, T.
Deposited on	:	2010-03-22
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

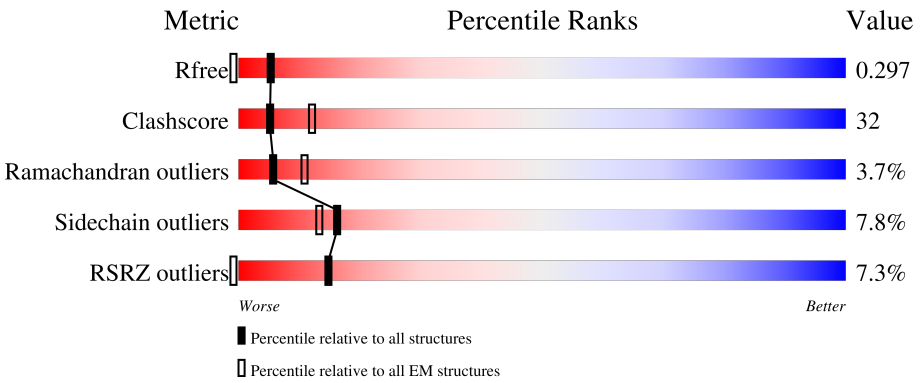
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.50 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)
R_{free}	130704	0
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RSRZ outliers	127900	0

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	220	7% 51% 41% 7%

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
2	3PE	A	307	-	-	-	X

2 Entry composition (i)

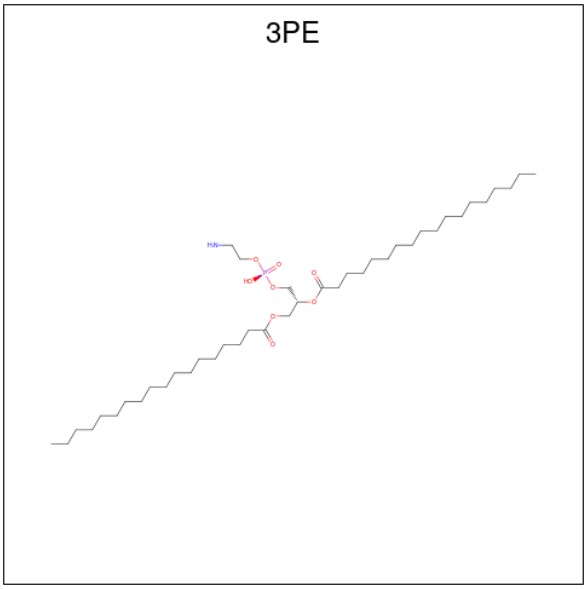
There are 3 unique types of molecules in this entry. The entry contains 1949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lens fiber major intrinsic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	220	1668	1110	279	274	5	0	0

- Molecule 2 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	28	18	1	8	1	0
2	A	1	37	27	1	8	1	0
2	A	1	42	32	1	8	1	0
2	A	1	40	30	1	8	1	0
2	A	1	38	28	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	48	38	1	8	1	0
			Total	C	N	O	P	
2	A	1	40	30	1	8	1	0

- Molecule 3 is water.

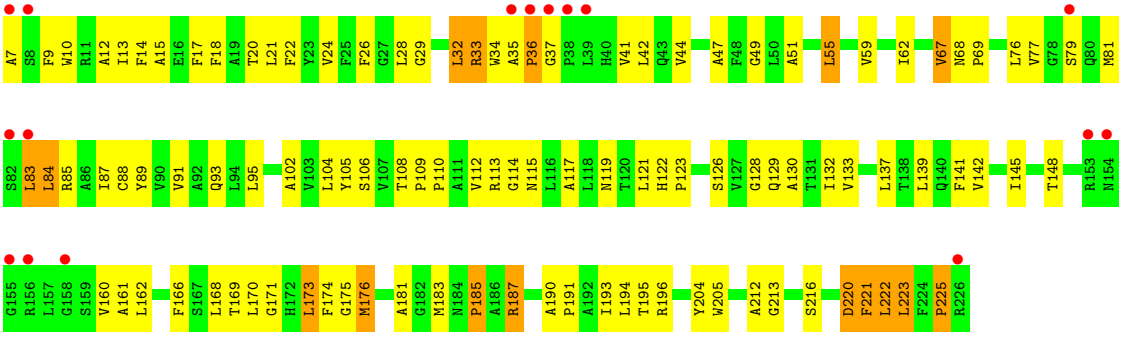
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
3	A	8	8	8	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: Lens fiber major intrinsic protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	65.50Å 65.50Å 200.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.89 – 2.50 15.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (15.89-2.50) 89.9 (15.89-2.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	3.12 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.250 , 0.284 0.266 , 0.297	Depositor DCC
R_{free} test set	1453 reflections (10.19%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	1949	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 3PE

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	A	0.42	0/1718	0.66	2/2350 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	PHE	CB-CA-C	9.15	128.70	110.40
1	A	223	LEU	N-CA-CB	-7.25	95.90	110.40

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	A	1668	0	1687	108	0
2	A	273	0	364	32	0
3	A	8	0	0	0	0
All	All	1949	0	2051	128	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 32.

The worst 5 of 128 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)
2:A:303:3PE:C2E	2:A:306:3PE:C39	2.36	1.03
1:A:222:LEU:O	1:A:225:PRO:HD3	1.63	0.98
2:A:303:3PE:C2E	2:A:306:3PE:H391	1.94	0.97
2:A:303:3PE:C2E	2:A:306:3PE:C3A	2.44	0.94
2:A:304:3PE:C3E	2:A:307:3PE:H3A1	1.97	0.94

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	A	218/220 (99%)	181 (83%)	29 (13%)	8 (4%)	3 4

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	36	PRO
1	A	181	ALA
1	A	114	GLY
1	A	220	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	166/166 (100%)	153 (92%)	13 (8%)	12 24

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LEU
1	A	173	LEU
1	A	222	LEU
1	A	185	PRO
1	A	187	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	122	HIS
1	A	200	ASN
1	A	66	HIS
1	A	57	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	3PE	A	306	-	47,47,50	0.48	0	50,52,55	1.08	3 (6%)
2	3PE	A	305	-	37,37,50	0.52	0	40,42,55	1.16	3 (7%)
2	3PE	A	301	-	27,27,50	0.59	0	30,32,55	1.28	3 (10%)
2	3PE	A	304	-	39,39,50	0.51	0	42,44,55	1.14	3 (7%)
2	3PE	A	302	-	36,36,50	0.53	0	39,41,55	1.17	3 (7%)
2	3PE	A	307	-	39,39,50	0.51	0	42,44,55	1.14	3 (7%)
2	3PE	A	303	-	41,41,50	0.50	0	44,46,55	1.12	3 (6%)

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
2	3PE	A	306	-	-	40/51/51/54	-
2	3PE	A	305	-	-	21/41/41/54	-
2	3PE	A	301	-	-	18/31/31/54	-
2	3PE	A	304	-	-	23/43/43/54	-
2	3PE	A	302	-	-	31/40/40/54	-
2	3PE	A	307	-	-	24/43/43/54	-
2	3PE	A	303	-	-	25/45/45/54	-

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	305	3PE	O31-C31-O32	-4.46	112.33	123.59
2	A	306	3PE	O31-C31-O32	-4.46	112.34	123.59
2	A	301	3PE	O31-C31-O32	-4.45	112.36	123.59
2	A	307	3PE	O31-C31-O32	-4.45	112.36	123.59
2	A	303	3PE	O31-C31-O32	-4.45	112.37	123.59

There are no chirality outliers.

5 of 182 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	3PE	C1-O11-P-O14
2	A	301	3PE	O21-C2-C3-O31
2	A	301	3PE	O22-C21-O21-C2
2	A	302	3PE	C1-O11-P-O14
2	A	302	3PE	C11-O13-P-O11

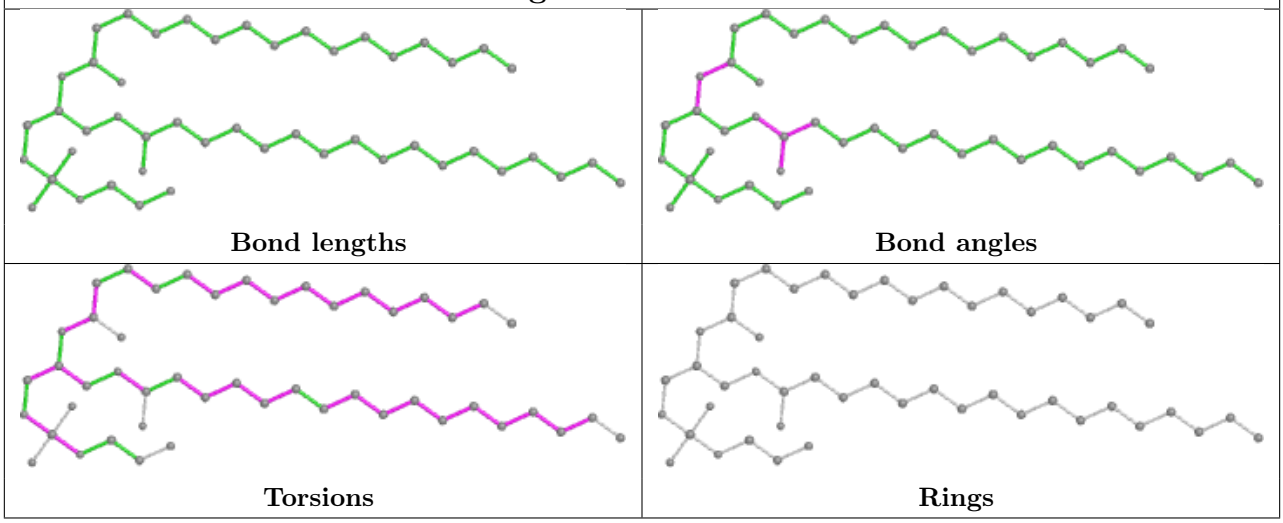
There are no ring outliers.

5 monomers are involved in 32 short contacts:

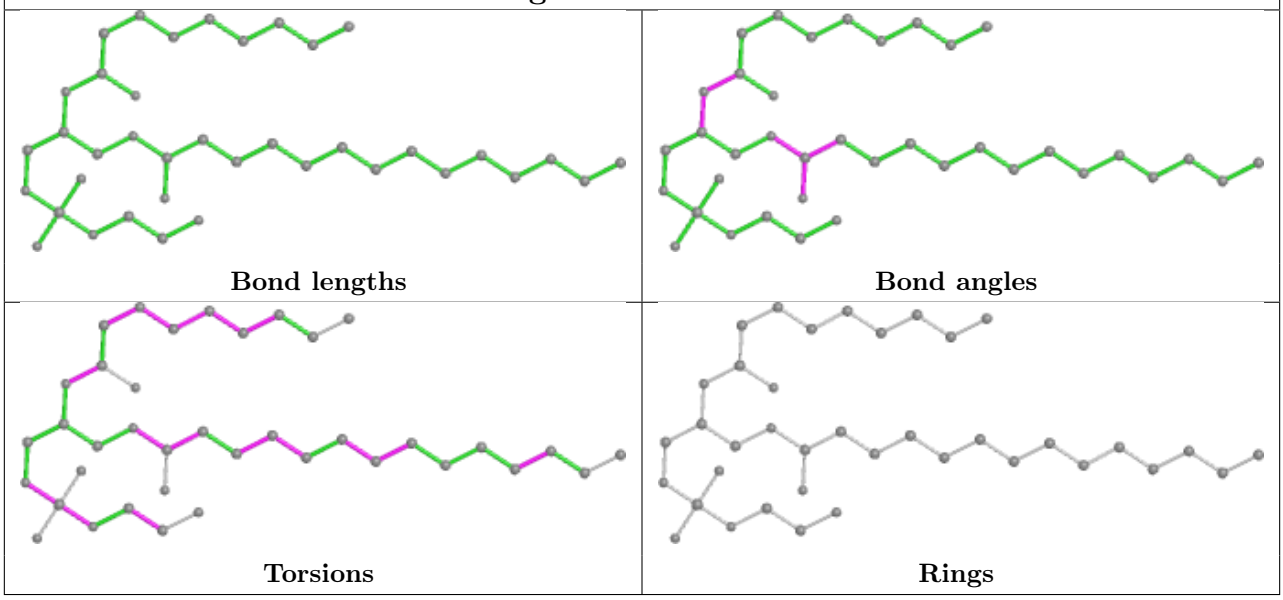
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	306	3PE	12	0
2	A	304	3PE	9	0
2	A	302	3PE	1	0
2	A	307	3PE	10	0
2	A	303	3PE	15	0

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 then 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.

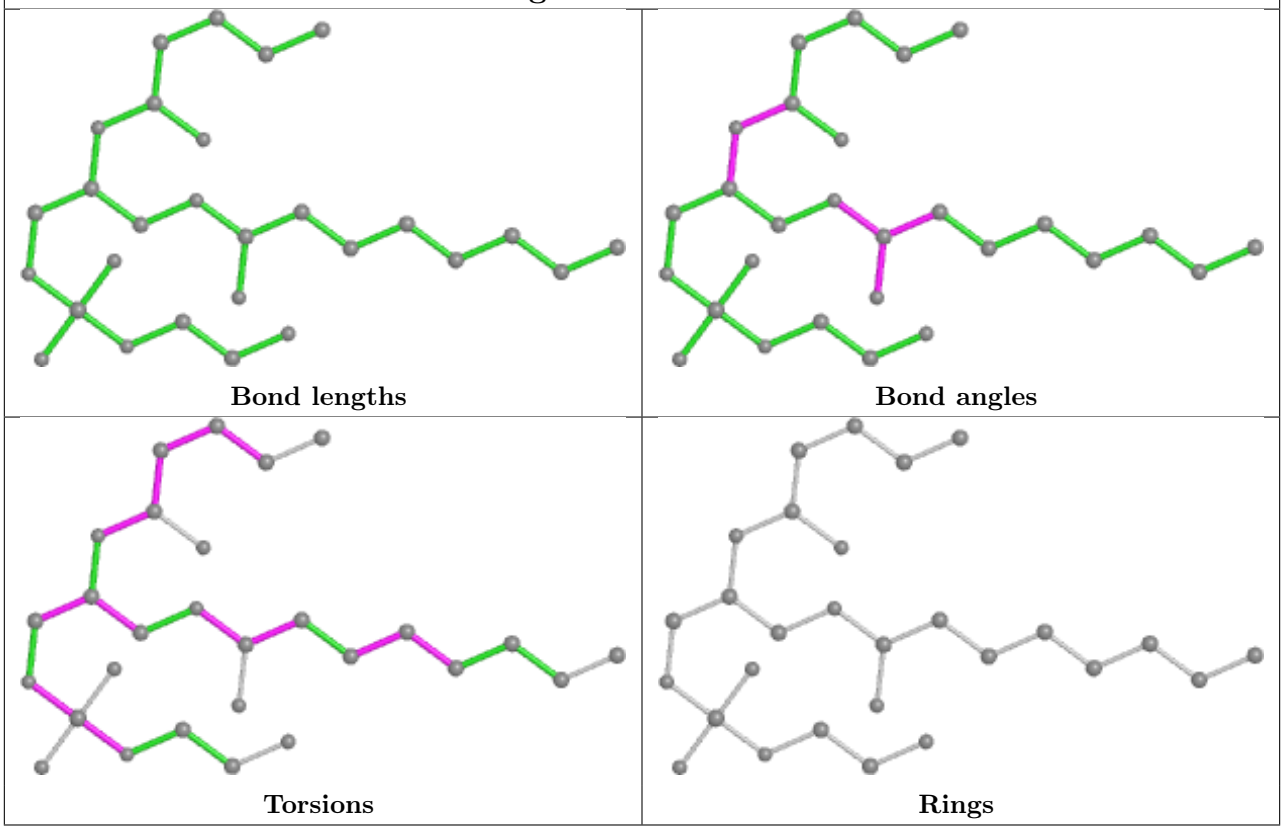
Ligand 3PE A 306

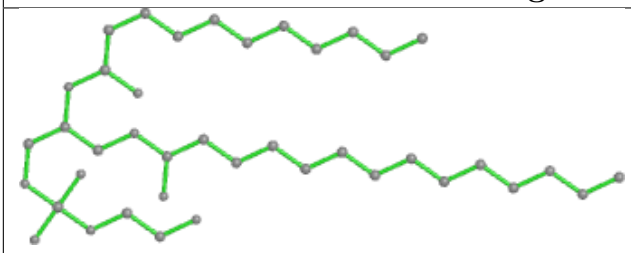
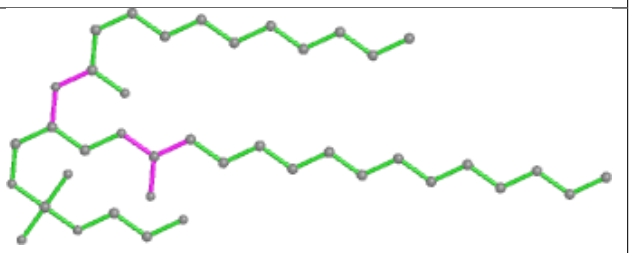
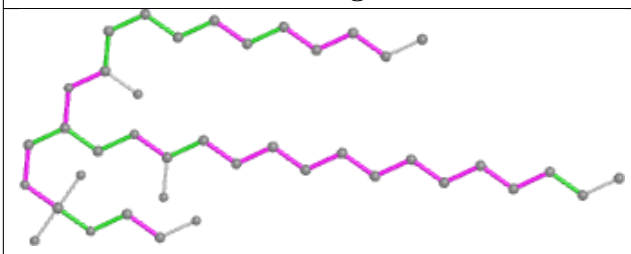
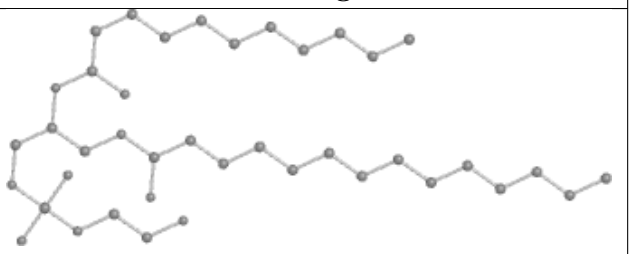


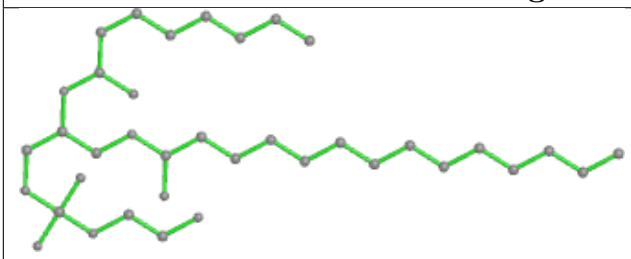
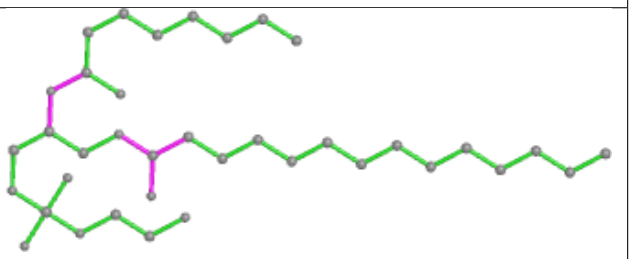
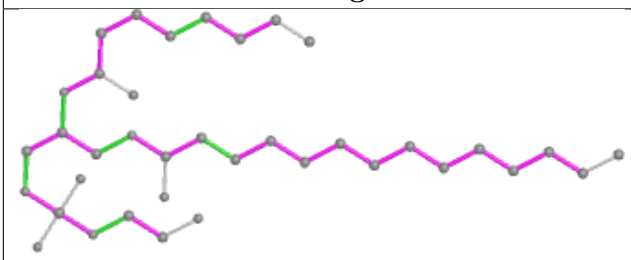
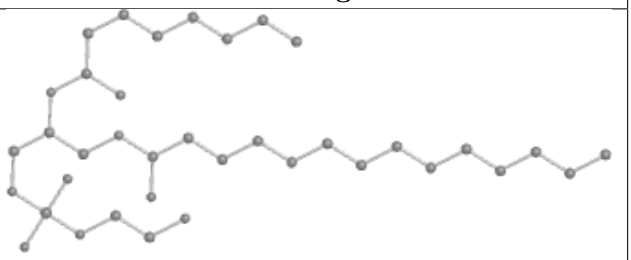
Ligand 3PE A 305



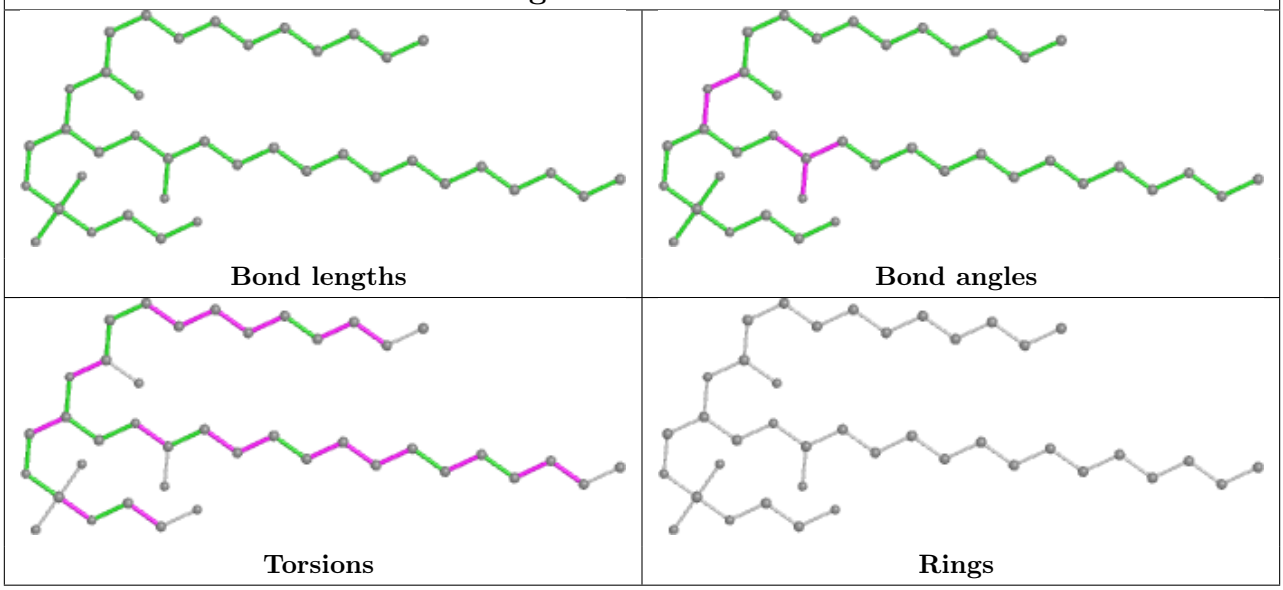
Ligand 3PE A 301



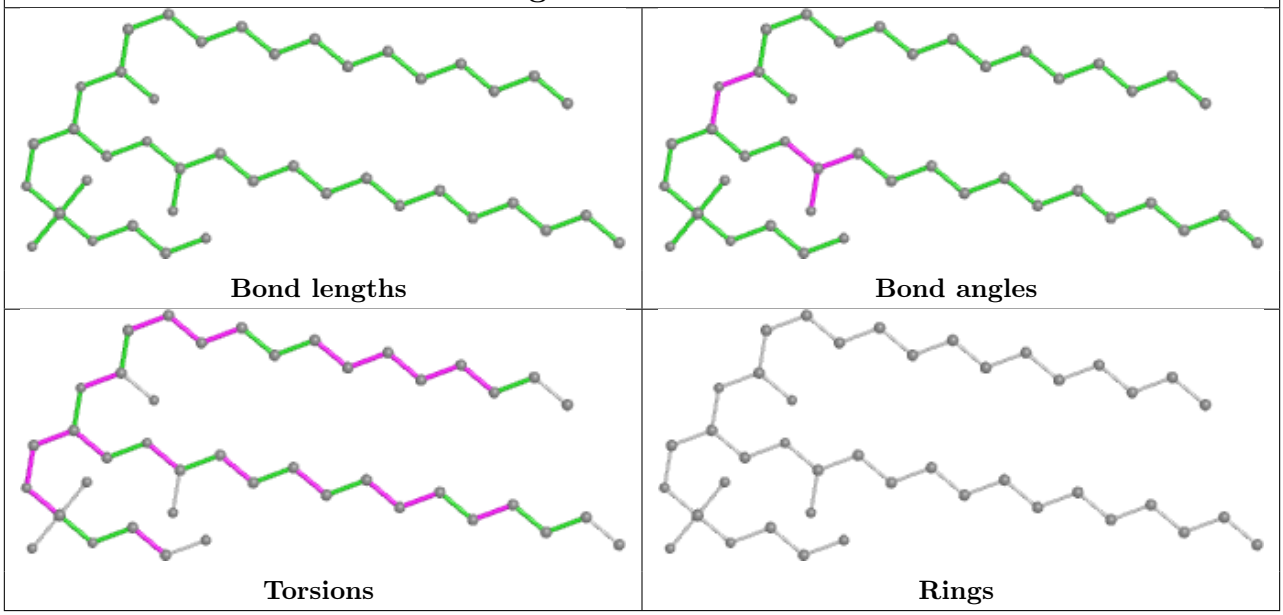
Ligand 3PE A 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE A 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE A 307



Ligand 3PE A 303



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.