



# wwPDB EM Model Validation Summary Report ⓘ

May 27, 2020 – 09:46 AM EDT

PDB ID : 6TQM  
EMDB ID : EMD-10555  
Title : Escherichia coli AdhE structure in its compact conformation  
Authors : Fronzes, R.; Pony, P.  
Deposited on : 2019-12-16  
Resolution : 3.80 Å (reported)  
Based on initial model : 6TQH

This is a wwPDB EM 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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 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) : 2.10.1

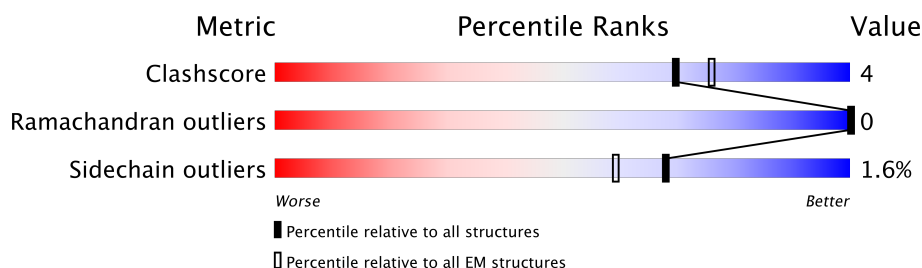
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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 and their fit to the map. 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 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	A	891	86% 11% .
1	B	891	87% 11% .
1	C	891	44% . 53%
1	F	891	43% . 53%

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
3	TXE	A	902	X	-	-	-
3	TXE	B	902	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39670 atoms, of which 19858 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.

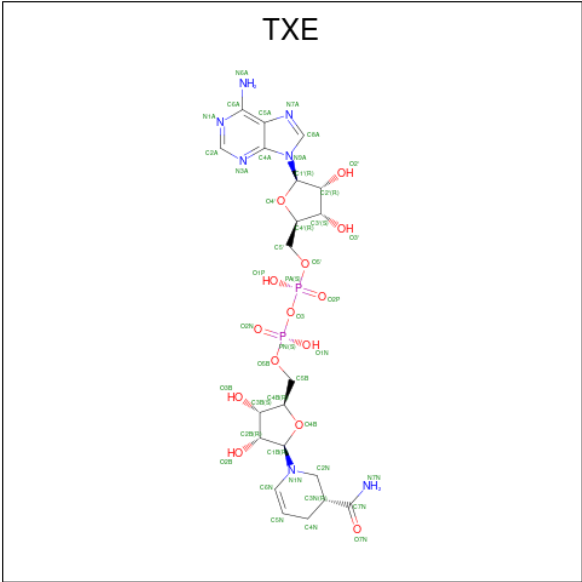
- Molecule 1 is a protein called Aldehyde-alcohol dehydrogenase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F	420	Total	C	H	N	O	S	0	0
			6500	2076	3245	554	609	16		
1	C	420	Total	C	H	N	O	S	0	0
			6500	2076	3245	554	609	16		
1	B	869	Total	C	H	N	O	S	0	0
			13263	4196	6657	1126	1254	30		
1	A	869	Total	C	H	N	O	S	0	0
			13263	4196	6657	1126	1254	30		

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

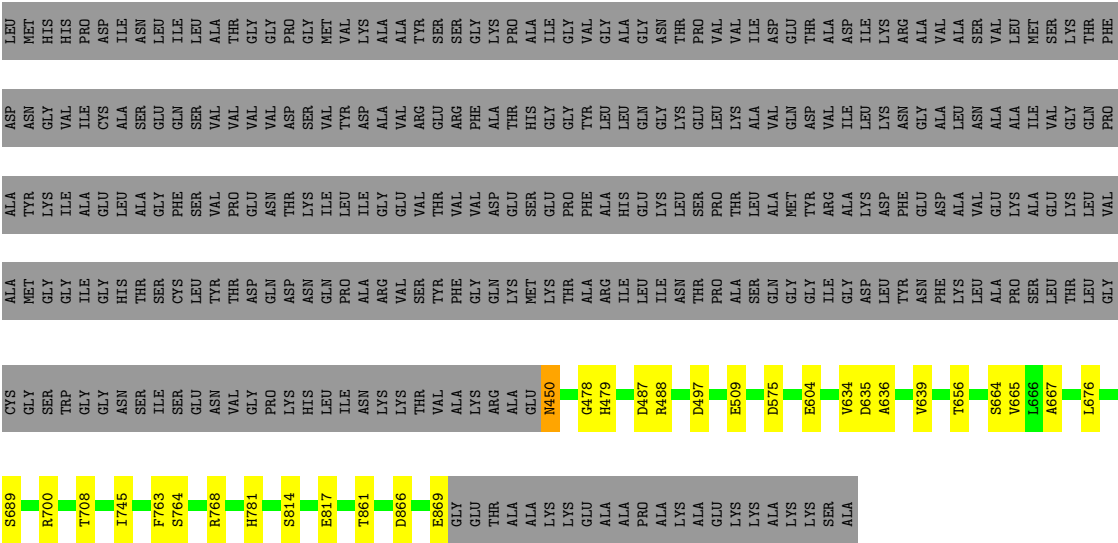
Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Fe	0
			1	1	
2	A	1	Total	Fe	0
			1	1	

- Molecule 3 is [[(2R,3S,4R,5R)-5-[(3R)-3-aminocarbonyl-3,4-dihydro-2H-pyridin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanidyl-phosphoryl] [(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl phosphate (three-letter code: TXE) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



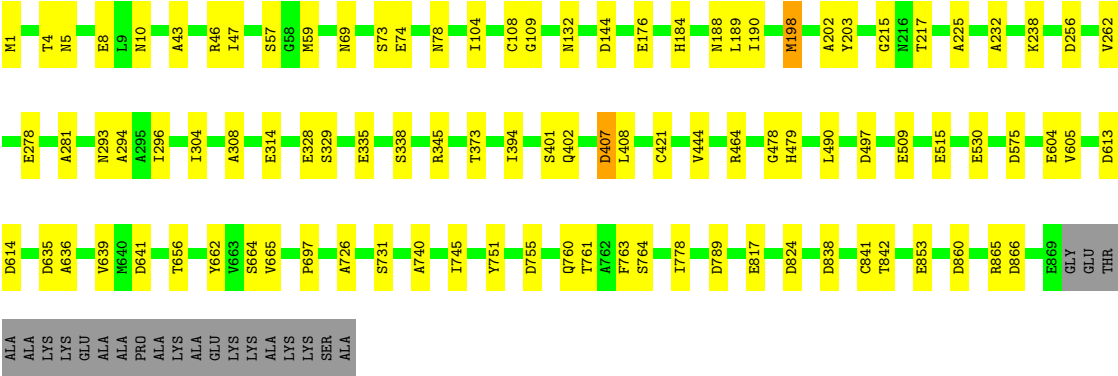
Mol	Chain	Residues	Atoms						AltConf
3	B	1	Total	C	H	N	O	P	0
			71	21	27	7	14	2	
3	A	1	Total	C	H	N	O	P	0
			71	21	27	7	14	2	





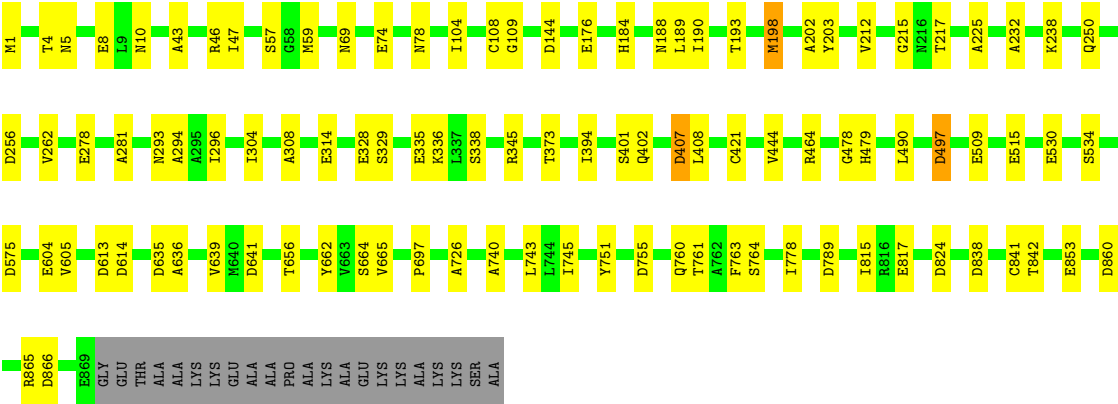
• Molecule 1: Aldehyde-alcohol dehydrogenase

Chain B: 87% 11%



• Molecule 1: Aldehyde-alcohol dehydrogenase

Chain A: 86% 11%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	226646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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: TXE, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.58	0/6734	0.60	0/9134
1	B	0.58	0/6734	0.60	0/9134
1	C	0.46	0/3326	0.57	0/4510
1	F	0.50	0/3326	0.60	0/4510
All	All	0.55	0/20120	0.60	0/27288

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	47	ILE	Peptide
1	B	47	ILE	Peptide



## 5.2 Too-close contacts

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	6606	6657	6657	59	0
1	B	6606	6657	6657	57	0
1	C	3255	3245	3245	21	0
1	F	3255	3245	3245	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	27	27	2	0
3	B	44	27	27	2	0
All	All	19812	19858	19858	158	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 158 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)
1:F:450:ASN:HD22	1:F:450:ASN:N	1.73	0.86
1:B:256:ASP:OD1	1:B:345:ARG:NH1	2.16	0.79
1:A:256:ASP:OD1	1:A:345:ARG:NH1	2.16	0.78
1:A:238:LYS:NZ	1:A:338:SER:O	2.23	0.72
1:A:108:CYS:SG	1:A:109:GLY:N	2.63	0.72

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	A	867/891 (97%)	730 (84%)	137 (16%)	0	100	100
1	B	867/891 (97%)	729 (84%)	138 (16%)	0	100	100
1	C	418/891 (47%)	369 (88%)	49 (12%)	0	100	100
1	F	418/891 (47%)	369 (88%)	49 (12%)	0	100	100
All	All	2570/3564 (72%)	2197 (86%)	373 (14%)	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	A	695/708 (98%)	680 (98%)	15 (2%)	55	79
1	B	695/708 (98%)	680 (98%)	15 (2%)	55	79
1	C	341/708 (48%)	340 (100%)	1 (0%)	93	97
1	F	341/708 (48%)	339 (99%)	2 (1%)	87	94
All	All	2072/2832 (73%)	2039 (98%)	33 (2%)	68	85

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	641	ASP
1	A	4	THR
1	A	755	ASP
1	B	755	ASP
1	B	760	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
3	TXE	A	902	-	41,48,48	4.80	15 (36%)	44,73,73	2.26	8 (18%)
3	TXE	B	902	-	41,48,48	4.80	14 (34%)	44,73,73	2.26	8 (18%)

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
3	TXE	A	902	-	1/1/15/15	12/26/72/72	0/5/5/5
3	TXE	B	902	-	1/1/15/15	12/26/72/72	0/5/5/5

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	TXE	O4'-C1'	15.86	1.63	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	TXE	O4'-C1'	15.86	1.63	1.41
3	A	902	TXE	C2'-C1'	-15.61	1.30	1.53
3	B	902	TXE	C2'-C1'	-15.59	1.30	1.53
3	A	902	TXE	C6N-C5N	11.61	1.54	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	TXE	C5A-C6A-N6A	8.45	133.19	120.35
3	A	902	TXE	C5A-C6A-N6A	8.42	133.14	120.35
3	B	902	TXE	N6A-C6A-N1A	-6.05	106.01	118.57
3	A	902	TXE	N6A-C6A-N1A	-6.04	106.03	118.57
3	A	902	TXE	C1'-N9A-C4A	5.21	135.79	126.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	TXE	C3N
3	B	902	TXE	C3N

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	TXE	C5'-O5'-PA-O2P
3	A	902	TXE	O4B-C1B-N1N-C2N
3	B	902	TXE	C5'-O5'-PA-O2P
3	B	902	TXE	O4B-C1B-N1N-C2N
3	A	902	TXE	O4'-C4'-C5'-O5'

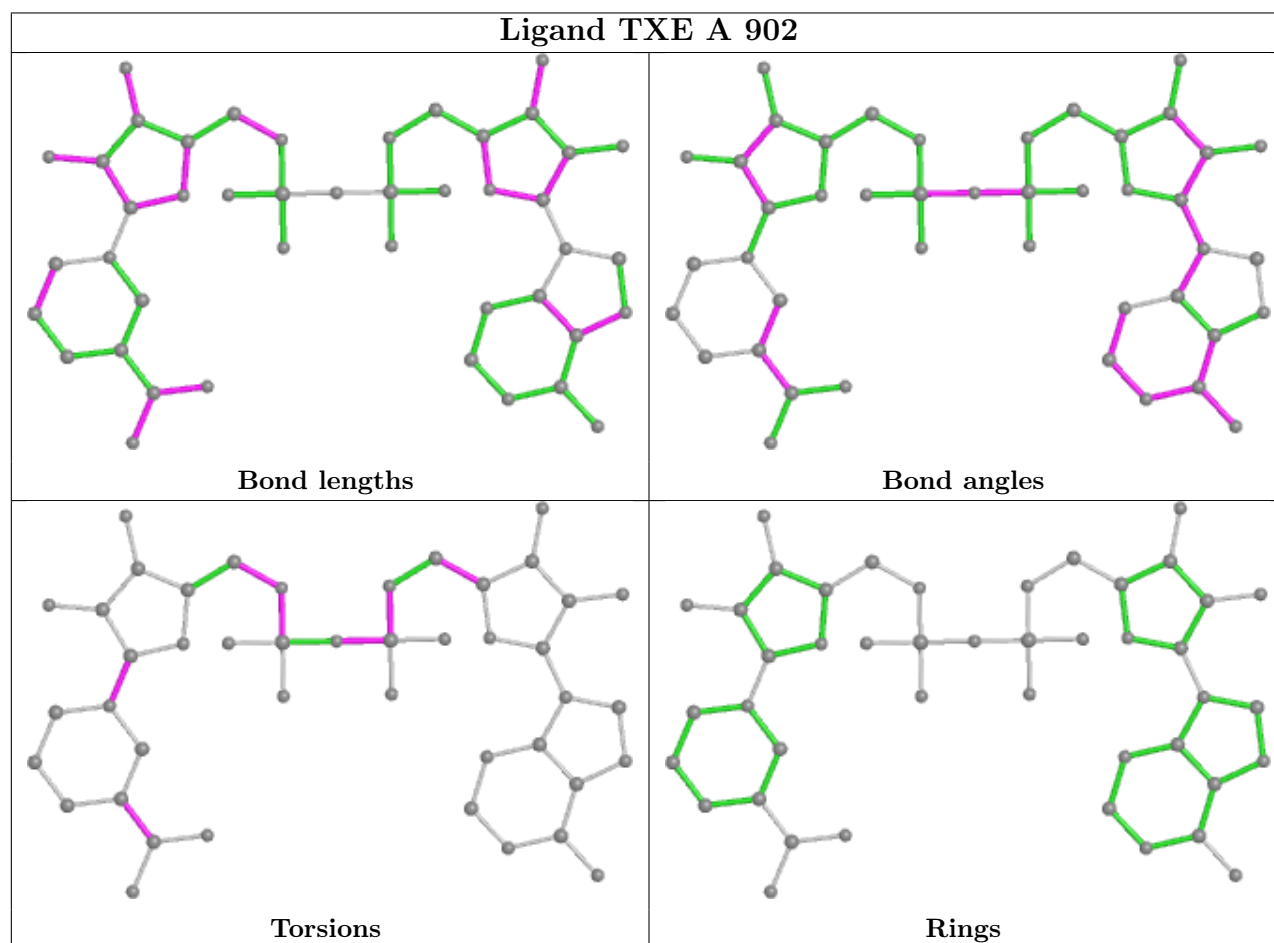
There are no ring outliers.

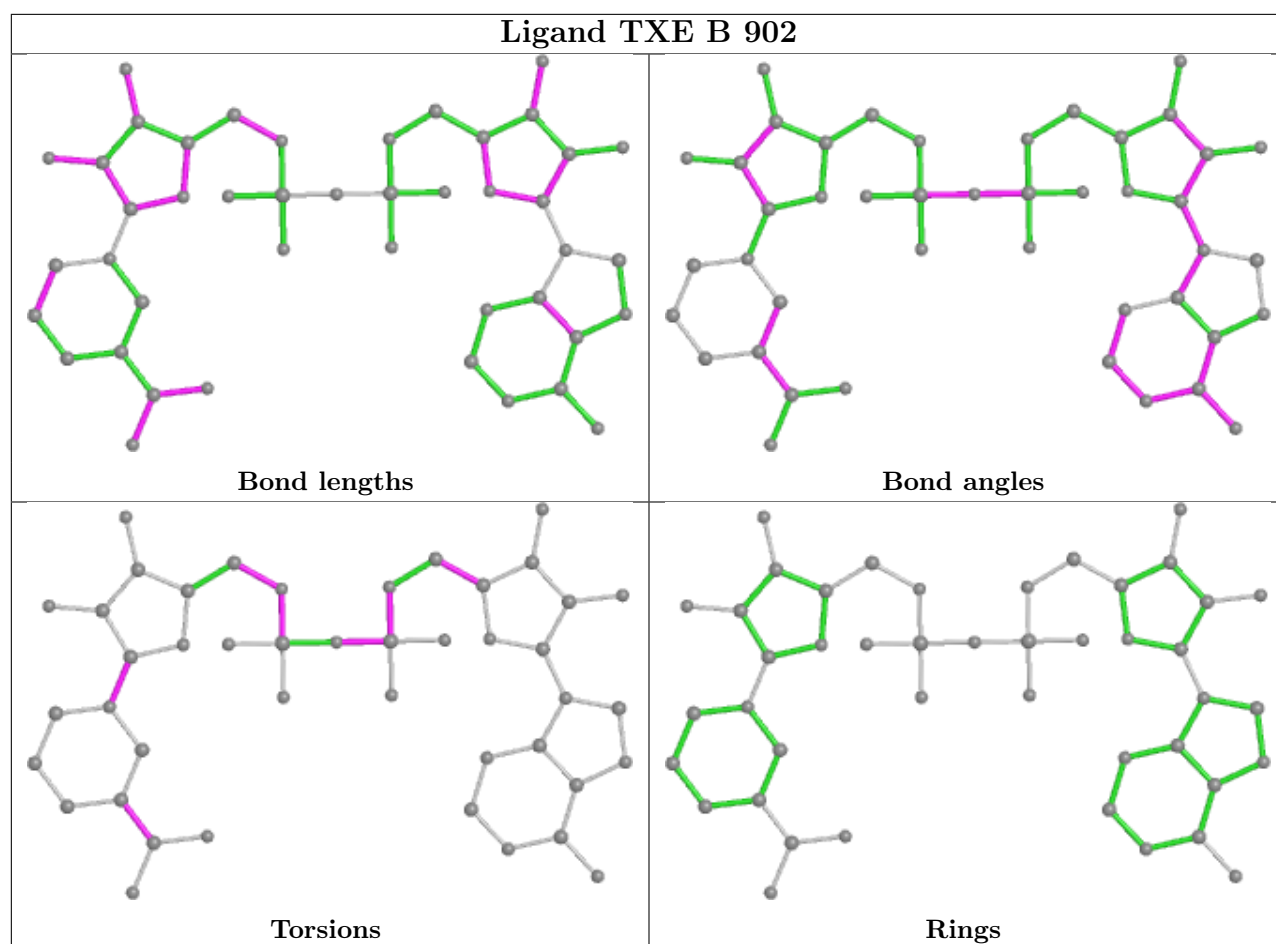
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	TXE	2	0
3	B	902	TXE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.