



# wwPDB EM Model Validation Summary Report ⓘ

May 27, 2020 – 09:52 AM EDT

PDB ID : 6TQH  
EMDB ID : EMD-10551  
Title : Escherichia coli AdhE structure in its extended conformation  
Authors : Fronzes, R.; Pony, P.  
Deposited on : 2019-12-16  
Resolution : 3.40 Å(reported)

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

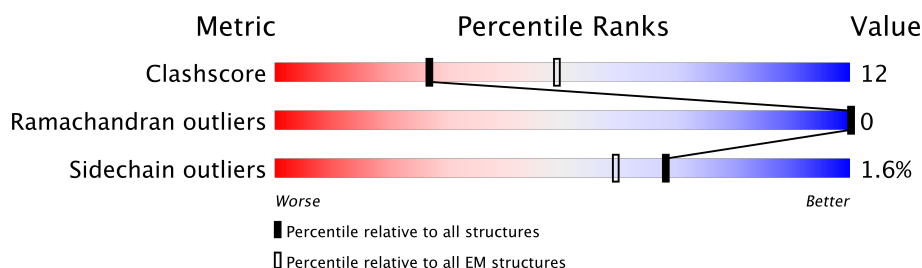
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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	
1	B	891	
1	C	891	
1	F	891	

## 2 Entry composition [i](#)

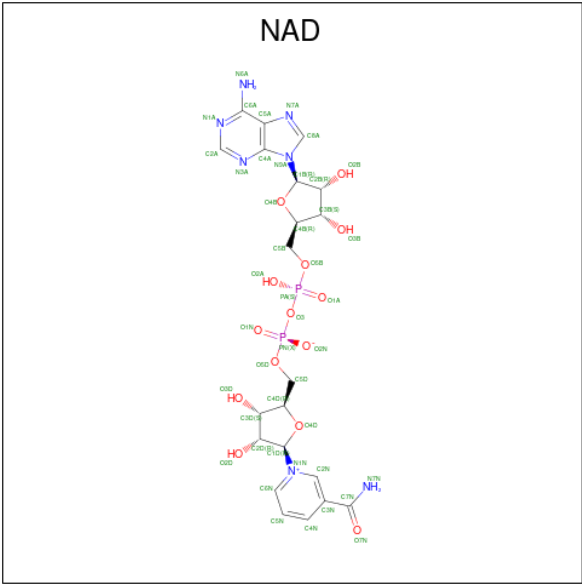
There are 3 unique types of molecules in this entry. The entry contains 39781 atoms, of which 19897 are hydrogens and 0 are deuteriums.

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
			Total	C	H	N	O	S		
1	A	869	Total 13263	4196	6657	1126	1254	30	0	0
1	F	419	Total 6486	2072	3239	552	607	16	0	0
1	C	419	Total 6487	2072	3240	552	607	16	0	0
1	B	869	Total 13263	4196	6657	1126	1254	30	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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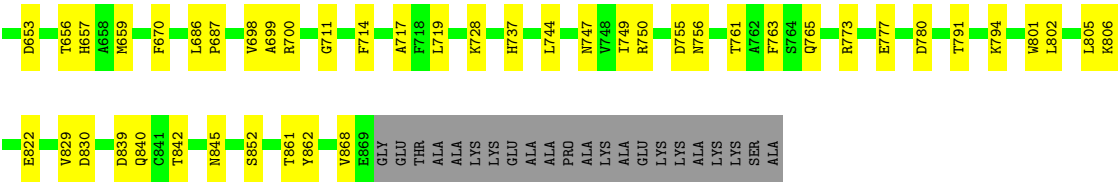
Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H	N	O	P	0
			140	42	52	14	28	4	
2	B	1	Total	C	H	N	O	P	0
			140	42	52	14	28	4	

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

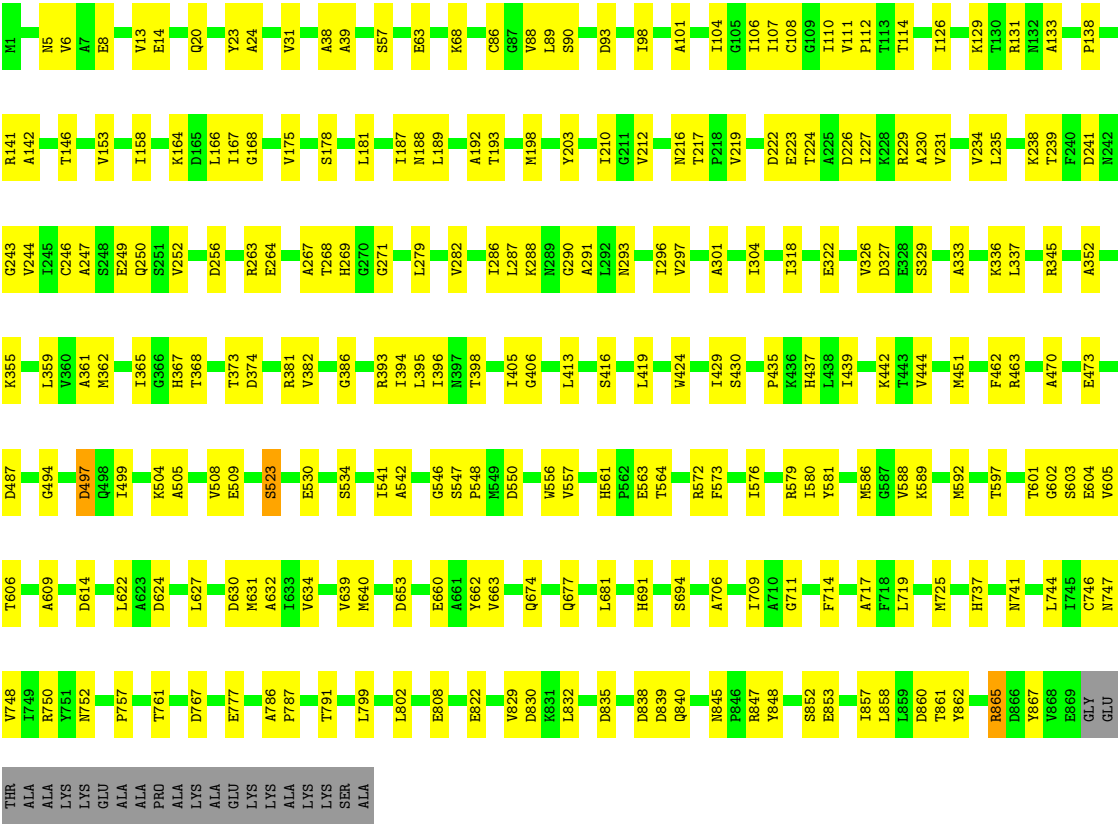
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Fe	0
			1	1	
3	A	1	Total	Fe	0
			1	1	







• Molecule 1: Aldehyde-alcohol dehydrogenase



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	138927	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)	0.5	Depositor
Maximum defocus (nm)	2.5	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: FE, NAD

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	0.56	2/6734 (0.0%)	0.49	0/9134
1	B	0.56	2/6734 (0.0%)	0.49	0/9134
1	C	0.53	1/3318 (0.0%)	0.49	0/4499
1	F	0.53	1/3318 (0.0%)	0.49	0/4499
All	All	0.55	6/20104 (0.0%)	0.49	0/27266

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	865	ARG	C-N	9.47	1.55	1.34
1	A	865	ARG	C-N	9.44	1.55	1.34
1	B	605	VAL	C-N	-5.35	1.21	1.34
1	F	605	VAL	C-N	-5.34	1.21	1.34
1	C	605	VAL	C-N	-5.33	1.21	1.34

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	416	SER	Peptide
1	B	416	SER	Peptide

## 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	6606	6657	6657	179	0
1	B	6606	6657	6657	173	0
1	C	3247	3240	3239	70	0
1	F	3247	3239	3239	76	0
2	A	88	52	52	3	0
2	B	88	52	52	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	19884	19897	19896	473	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 12.

The worst 5 of 473 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:C:579:ARG:NH1	1:C:623:ALA:O	1.95	1.00
1:F:579:ARG:NH1	1:F:623:ALA:O	1.95	0.99
1:A:640:MET:O	1:A:694:SER:OG	1.82	0.96
1:B:640:MET:O	1:B:694:SER:OG	1.81	0.96
1:A:229:ARG:NH2	1:B:767:ASP:OD1	2.00	0.95

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	867/891 (97%)	754 (87%)	113 (13%)	0	100	100
1	B	867/891 (97%)	754 (87%)	113 (13%)	0	100	100
1	C	417/891 (47%)	369 (88%)	48 (12%)	0	100	100
1	F	417/891 (47%)	369 (88%)	48 (12%)	0	100	100
All	All	2568/3564 (72%)	2246 (88%)	322 (12%)	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%)	685 (99%)	10 (1%)	69	87
1	B	695/708 (98%)	685 (99%)	10 (1%)	69	87
1	C	340/708 (48%)	333 (98%)	7 (2%)	56	82
1	F	340/708 (48%)	333 (98%)	7 (2%)	56	82
All	All	2070/2832 (73%)	2036 (98%)	34 (2%)	68	85

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	852	SER
1	C	501	SER
1	B	534	SER
1	C	475	ILE
1	A	530	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	723	HIS
1	F	781	HIS
1	B	677	GLN
1	A	845	ASN
1	B	752	ASN

### 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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	NAD	B	902	-	42,48,48	1.51	7 (16%)	50,73,73	1.86	13 (26%)
2	NAD	A	901	-	42,48,48	1.40	6 (14%)	50,73,73	1.78	12 (24%)
2	NAD	A	902	-	42,48,48	1.47	4 (9%)	50,73,73	1.72	10 (20%)
2	NAD	B	901	-	42,48,48	1.40	3 (7%)	50,73,73	1.68	12 (24%)

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	NAD	B	902	-	-	11/26/62/62	0/5/5/5
2	NAD	A	901	-	-	18/26/62/62	0/5/5/5
2	NAD	A	902	-	-	11/26/62/62	0/5/5/5
2	NAD	B	901	-	-	7/26/62/62	0/5/5/5

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	NAD	PN-O5D	4.67	1.78	1.59
2	A	902	NAD	PN-O5D	4.62	1.78	1.59
2	A	901	NAD	PN-O5D	4.53	1.77	1.59
2	B	902	NAD	PN-O5D	4.15	1.76	1.59
2	A	902	NAD	PA-O5B	3.89	1.75	1.59

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	NAD	PN-O3-PA	-5.64	113.48	132.83
2	A	901	NAD	PN-O3-PA	-5.61	113.56	132.83
2	A	902	NAD	PN-O3-PA	-5.53	113.86	132.83
2	B	901	NAD	PN-O3-PA	-5.04	115.52	132.83
2	A	901	NAD	O2A-PA-O1A	3.89	131.46	112.24

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

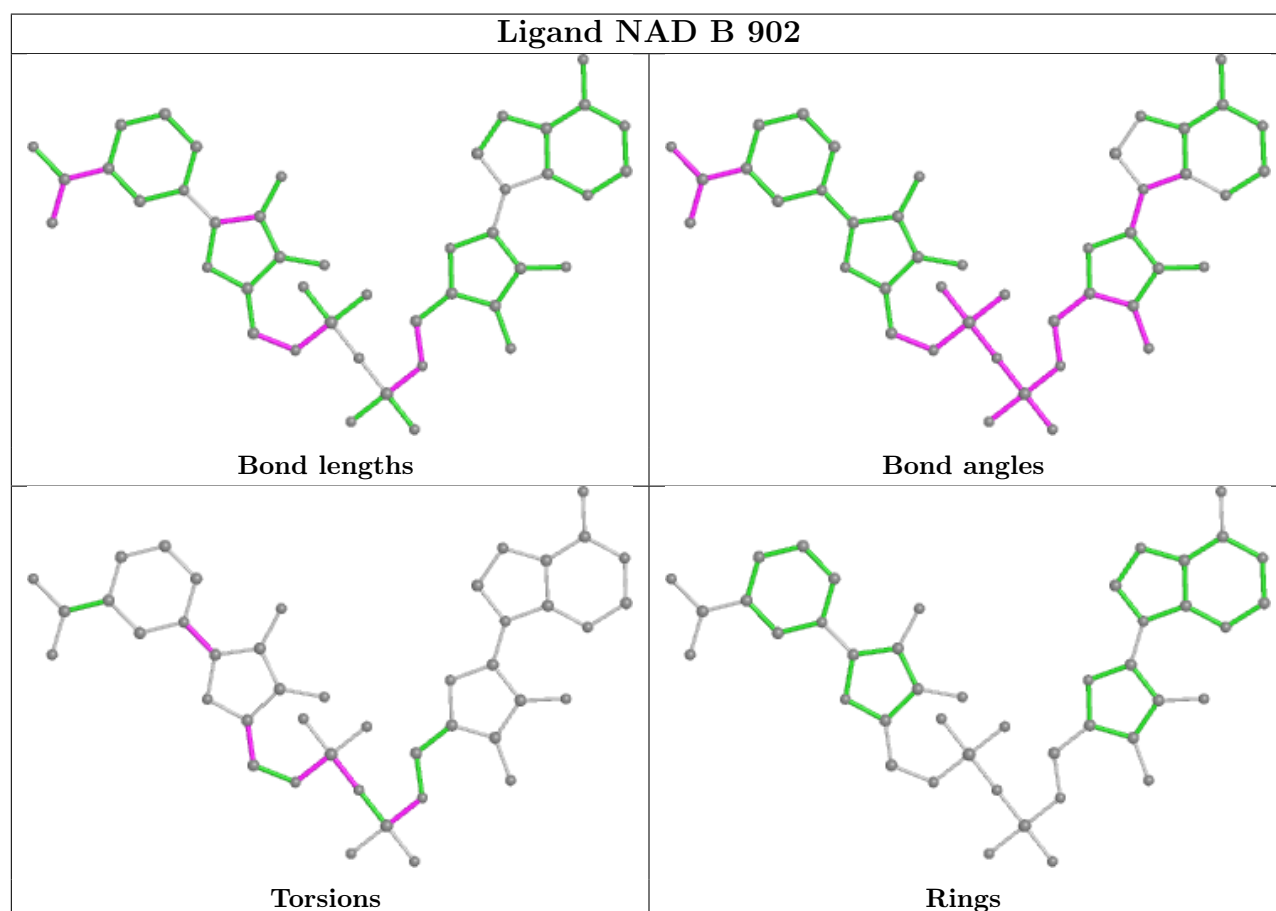
Mol	Chain	Res	Type	Atoms
2	B	902	NAD	C5B-O5B-PA-O2A
2	B	902	NAD	O4D-C4D-C5D-O5D
2	B	902	NAD	C3D-C4D-C5D-O5D
2	B	902	NAD	O4D-C1D-N1N-C2N
2	B	902	NAD	O4D-C1D-N1N-C6N

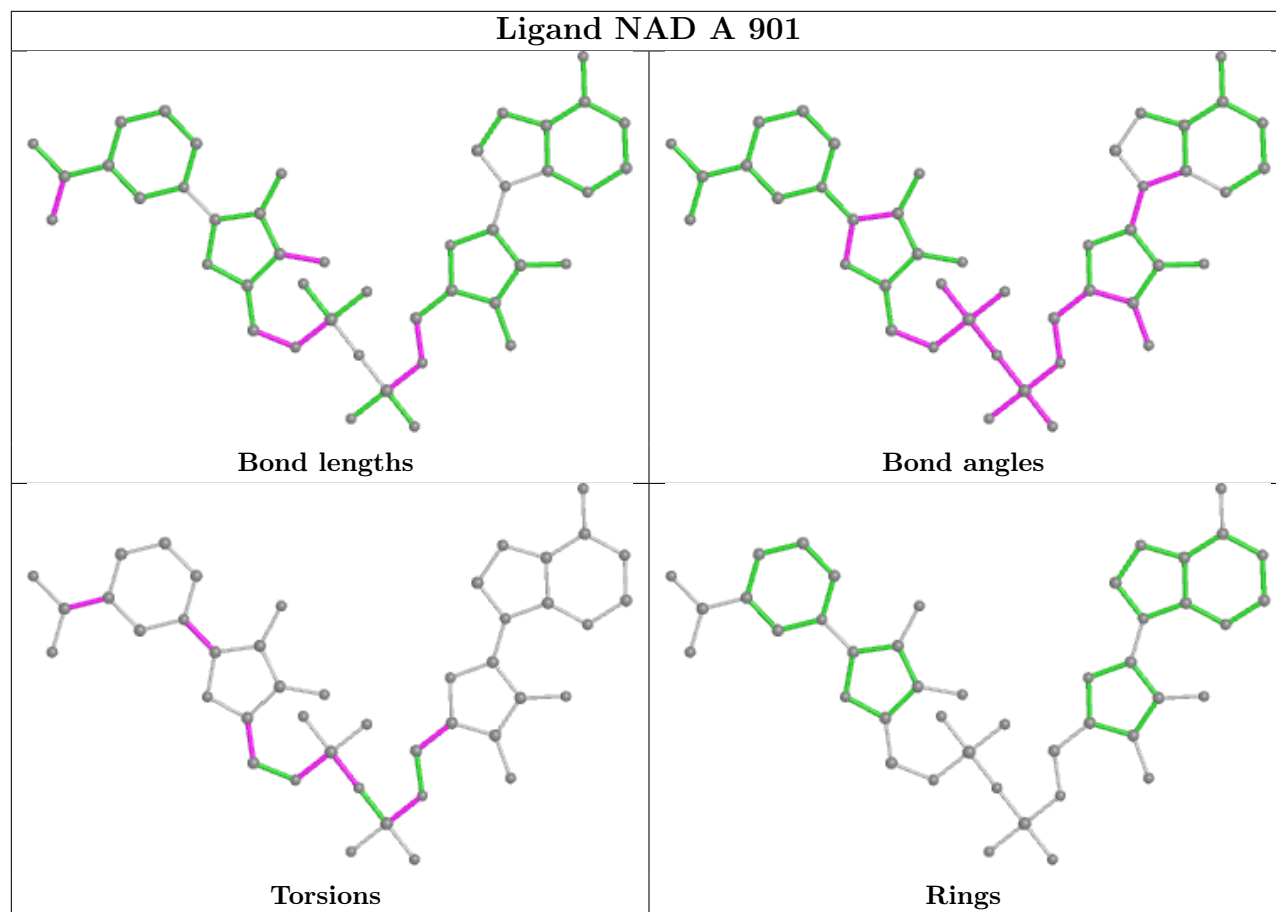
There are no ring outliers.

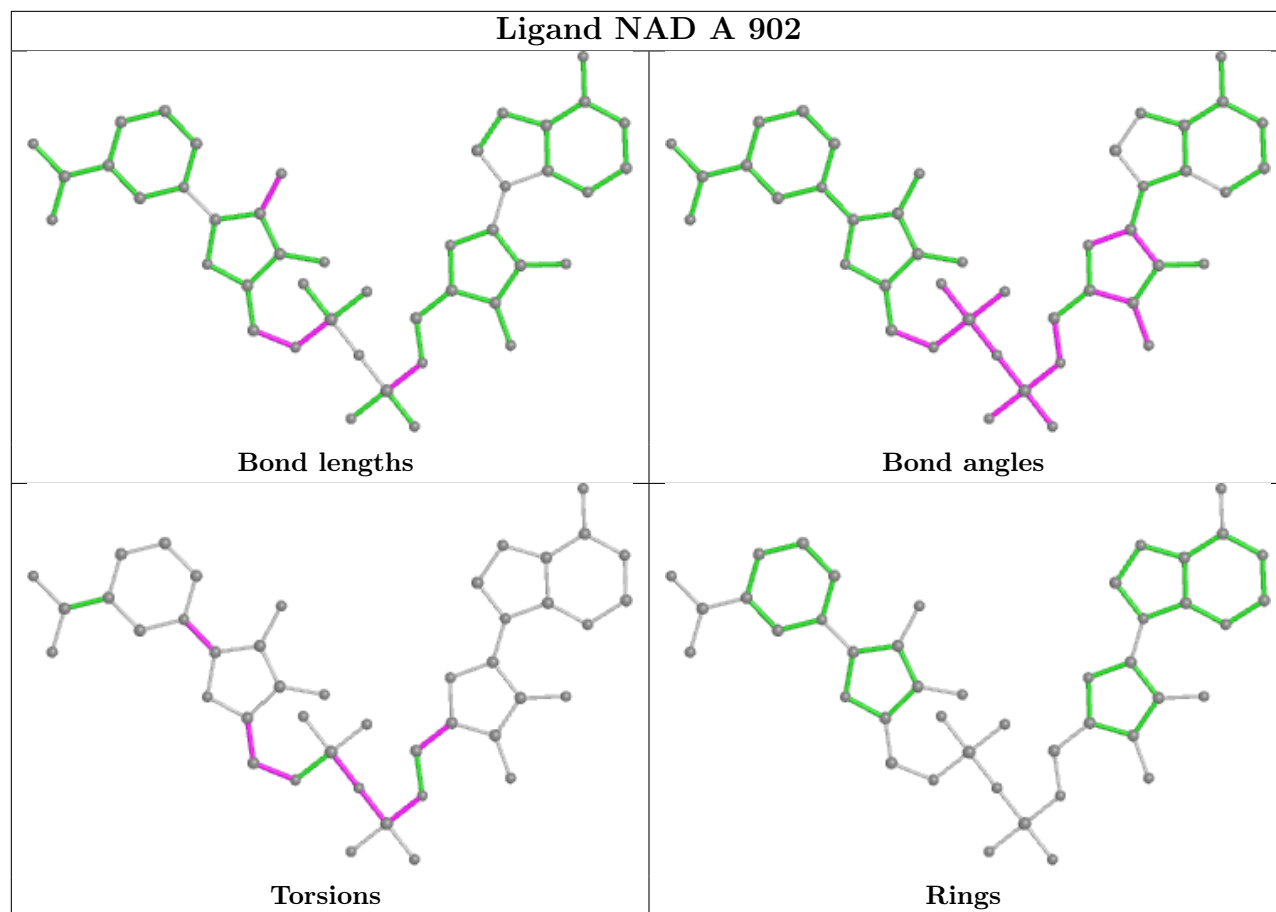
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	NAD	4	0
2	A	901	NAD	2	0
2	A	902	NAD	1	0
2	B	901	NAD	2	0

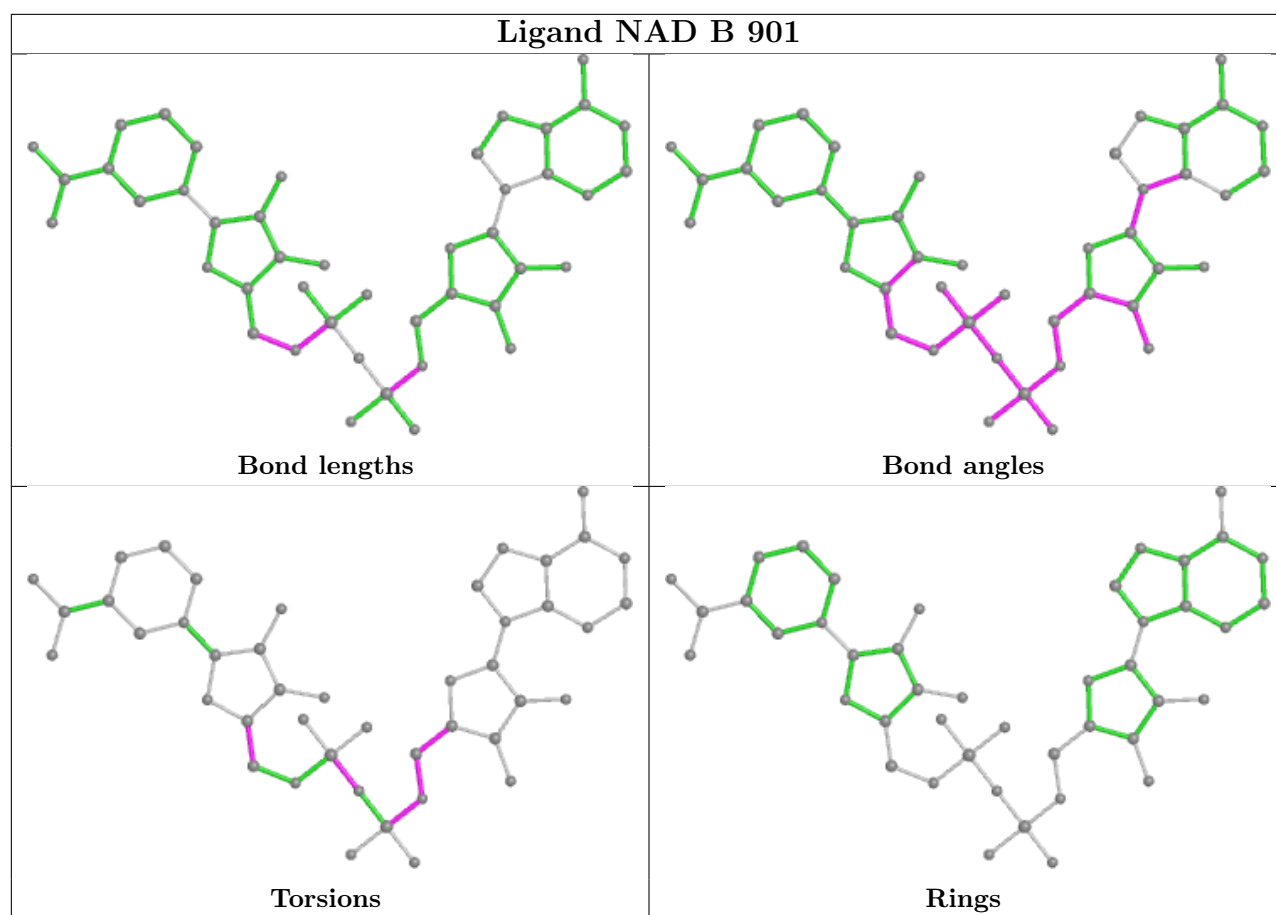
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.