



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2021 – 04:04 PM GMT

PDB ID : 7NED  
Title : Thiourocyanate hydratase from *Paenibacillus* sp. Soil724D2 in complex with cofactor NAD<sup>+</sup> and urocanate  
Authors : Leisinger, F.; Seebeck, F.P.  
Deposited on : 2021-02-03  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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/XrayValidationReportHelp>

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)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.17

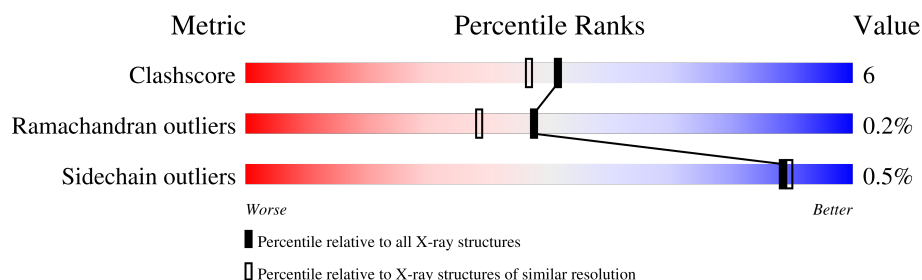
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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	URO	A	701	-	-	X	-
4	EDO	A	703	-	-	X	-

## 2 Entry composition [i](#)

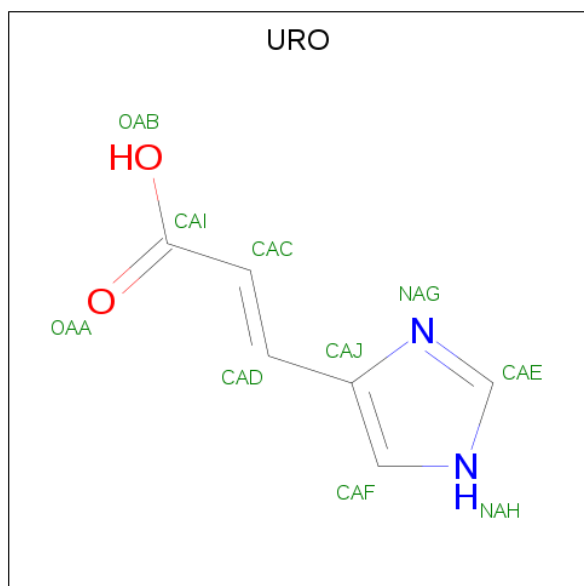
There are 5 unique types of molecules in this entry. The entry contains 4593 atoms, of which 32 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Urocanate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	4232	2664	749	804	15	48	0	0

- Molecule 2 is (2E)-3-(1H-IMIDAZOL-4-YL)ACRYLIC ACID (three-letter code: URO) (formula: C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



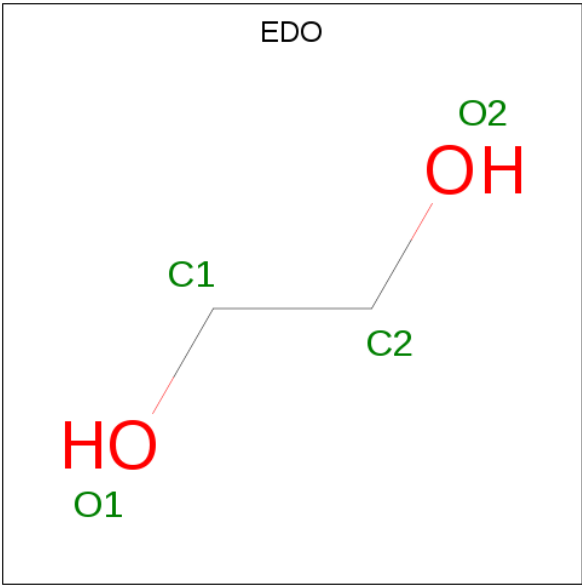
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	6	2	2	0	0

- Molecule 3 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>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	7	0
			70	21	26	7	14	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	271	Total 271	O 271	0	0

SEQUENCE-PLOTS INFOmissingINFO

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.35Å 62.75Å 151.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.32 – 1.90	Depositor
% Data completeness (in resolution range)	99.9 (48.32-1.90)	Depositor
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, $R_{free}$	0.172 , 0.175	Depositor
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtriage
Anisotropy	0.774	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, EDO, URO

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	0.68	3/4311 (0.1%)	0.77	8/5843 (0.1%)

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	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	GLU	CD-OE1	-6.29	1.18	1.25
1	A	190	GLU	CD-OE2	-5.96	1.19	1.25
1	A	439	SER	CB-OG	-5.33	1.35	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	PHE	CB-CG-CD2	-8.29	115.00	120.80
1	A	455	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	37	LYS	CB-CG-CD	-6.46	94.80	111.60
1	A	192	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	A	118	ILE	CB-CG1-CD1	-5.81	97.64	113.90
1	A	37	LYS	CA-CB-CG	5.53	125.57	113.40
1	A	351	PHE	CB-CG-CD1	-5.39	117.03	120.80
1	A	192	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	PHE	Sidechain
1	A	351	PHE	Sidechain
1	A	455	ASP	Sidechain

## 4.2 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	4232	0	4183	39	0
2	A	10	0	5	9	0
3	A	44	26	26	6	0
4	A	4	6	6	7	0
5	A	271	0	0	2	0
All	All	4561	32	4220	47	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.

All (47) 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:A:3:ARG:HE	4:A:703:EDO:H22	1.07	1.11
1:A:47:LYS:HD2	1:A:118:ILE:HD11	1.43	0.99
1:A:3:ARG:HE	4:A:703:EDO:C2	1.82	0.93
2:A:701:URO:HAF	3:A:702:NAD:C4N	2.00	0.91
1:A:3:ARG:NE	4:A:703:EDO:H22	1.84	0.91
2:A:701:URO:HAF	3:A:702:NAD:C5N	2.09	0.83
2:A:701:URO:HAE	5:A:822:HOH:O	1.78	0.82
2:A:701:URO:CAF	3:A:702:NAD:C4N	2.67	0.72
2:A:701:URO:HAH	3:A:702:NAD:C3N	2.02	0.72
1:A:47:LYS:HD2	1:A:118:ILE:CD1	2.21	0.69
1:A:269:TYR:OH	1:A:288:ASP:OD2	2.08	0.69
2:A:701:URO:CAE	5:A:822:HOH:O	2.38	0.68
1:A:36:GLN:HB3	4:A:703:EDO:H21	1.76	0.66
1:A:368:GLU:OE2	1:A:388:ARG:NH1	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:701:URO:NAH	3:A:702:NAD:C3N	2.65	0.59
1:A:3:ARG:HH11	4:A:703:EDO:C2	2.17	0.57
1:A:42:TYR:OH	2:A:701:URO:NAG	2.29	0.57
1:A:270:ARG:HB2	1:A:273:GLU:OE1	2.07	0.55
1:A:471:SER:O	1:A:472:MET:HB2	2.07	0.53
2:A:701:URO:CAF	3:A:702:NAD:C5N	2.85	0.52
1:A:29:VAL:HG11	1:A:127:TRP:HA	1.90	0.52
1:A:159:PHE:CD1	1:A:216:ILE:HG21	2.44	0.52
1:A:117:LEU:C	1:A:117:LEU:HD12	2.31	0.50
1:A:420:ARG:HB2	1:A:500:GLY:O	2.12	0.49
1:A:472:MET:HB3	1:A:507:ARG:HG2	1.94	0.49
1:A:8:ARG:HG3	1:A:358:GLY:HA3	1.95	0.48
1:A:414:ALA:O	1:A:418:MET:HG3	2.14	0.48
1:A:380:ILE:HG12	1:A:403:PHE:CZ	2.50	0.47
1:A:266:PRO:HB2	1:A:269:TYR:CD2	2.50	0.47
1:A:440:MET:HG2	1:A:446:MET:HB2	1.97	0.46
1:A:3:ARG:NE	4:A:703:EDO:C2	2.61	0.46
1:A:96:CYS:HB2	1:A:118:ILE:O	2.16	0.45
1:A:47:LYS:CD	1:A:118:ILE:HD11	2.30	0.45
1:A:118:ILE:HA	1:A:118:ILE:HD12	1.59	0.45
1:A:119:TRP:CZ2	1:A:121:GLY:HA2	2.52	0.45
1:A:265:VAL:HG22	1:A:274:LEU:HD11	1.99	0.44
1:A:172:GLN:N	1:A:173:PRO:HD2	2.32	0.44
1:A:472:MET:CE	1:A:506:ILE:HG22	2.48	0.44
1:A:3:ARG:CZ	4:A:703:EDO:H22	2.47	0.43
1:A:258:HIS:O	1:A:484:GLY:HA3	2.19	0.42
1:A:353:TRP:HA	1:A:429:ALA:O	2.20	0.42
1:A:336:THR:HG21	1:A:446:MET:HA	2.01	0.41
1:A:52:TRP:N	1:A:53:PRO:CD	2.83	0.41
1:A:427:PRO:HB3	1:A:499:ASP:HA	2.01	0.41
1:A:73:ILE:HB	1:A:93:MET:HB3	2.01	0.41
1:A:434:HIS:HB3	1:A:491:SER:HB2	2.02	0.41
1:A:349:GLY:O	1:A:402:TRP:HA	2.21	0.40

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	543/546 (100%)	522 (96%)	20 (4%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	ILE

### 4.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	436/437 (100%)	434 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	ARG
1	A	546	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 4.6 Ligand geometry ⓘ

3 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	URO	A	701	-	5,10,10	1.01	1 (20%)	4,12,12	2.00	1 (25%)
4	EDO	A	703	-	3,3,3	0.25	0	2,2,2	0.25	0
3	NAD	A	702	-	42,48,48	1.68	11 (26%)	50,73,73	1.95	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	URO	A	701	-	-	0/1/5/5	0/1/1/1
4	EDO	A	703	-	-	0/1/1/1	-
3	NAD	A	702	-	-	1/26/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAD	C3D-C4D	3.57	1.62	1.53
3	A	702	NAD	PN-O5D	3.33	1.72	1.59
3	A	702	NAD	C7N-N7N	3.13	1.38	1.33
3	A	702	NAD	C2N-N1N	2.98	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAD	C5B-C4B	2.78	1.60	1.51
3	A	702	NAD	PA-O5B	2.63	1.69	1.59
3	A	702	NAD	O4B-C1B	2.50	1.44	1.41
3	A	702	NAD	O3B-C3B	-2.47	1.37	1.43
3	A	702	NAD	O2D-C2D	-2.39	1.37	1.43
3	A	702	NAD	C3N-C7N	2.25	1.54	1.50
2	A	701	URO	CAJ-CAD	-2.07	1.42	1.47
3	A	702	NAD	O4B-C4B	-2.03	1.40	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAD	C3D-C2D-C1D	-6.74	90.83	100.98
3	A	702	NAD	PN-O3-PA	-3.74	119.98	132.83
3	A	702	NAD	O7N-C7N-C3N	3.70	124.06	119.63
3	A	702	NAD	C2N-N1N-C1D	-3.68	110.93	119.14
2	A	701	URO	CAJ-CAD-CAC	-3.29	112.07	125.32
3	A	702	NAD	C5D-C4D-C3D	-3.26	102.98	115.18
3	A	702	NAD	C5B-C4B-C3B	-3.17	103.30	115.18
3	A	702	NAD	O2A-PA-O1A	2.77	125.94	112.24
3	A	702	NAD	O7N-C7N-N7N	-2.70	118.74	122.58
3	A	702	NAD	C5N-C6N-N1N	-2.54	116.75	120.40
3	A	702	NAD	O5D-PN-O1N	-2.39	99.73	109.07
3	A	702	NAD	C4N-C3N-C7N	2.08	126.61	121.04
3	A	702	NAD	C6N-N1N-C2N	2.01	123.80	121.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NAD	O4B-C4B-C5B-O5B

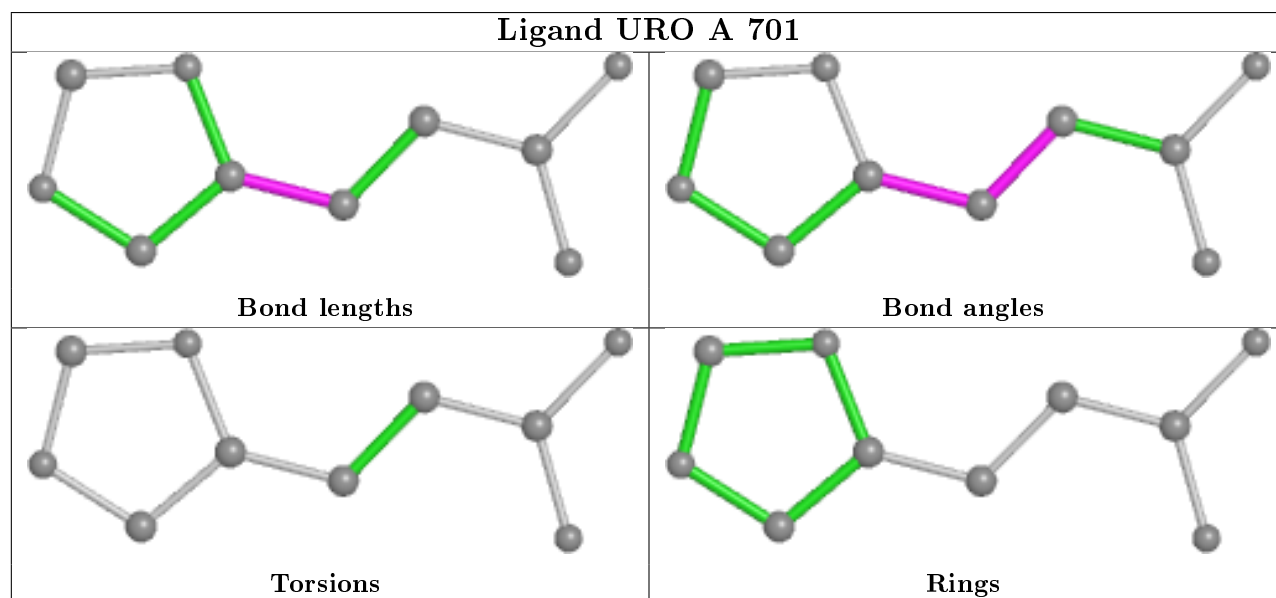
There are no ring outliers.

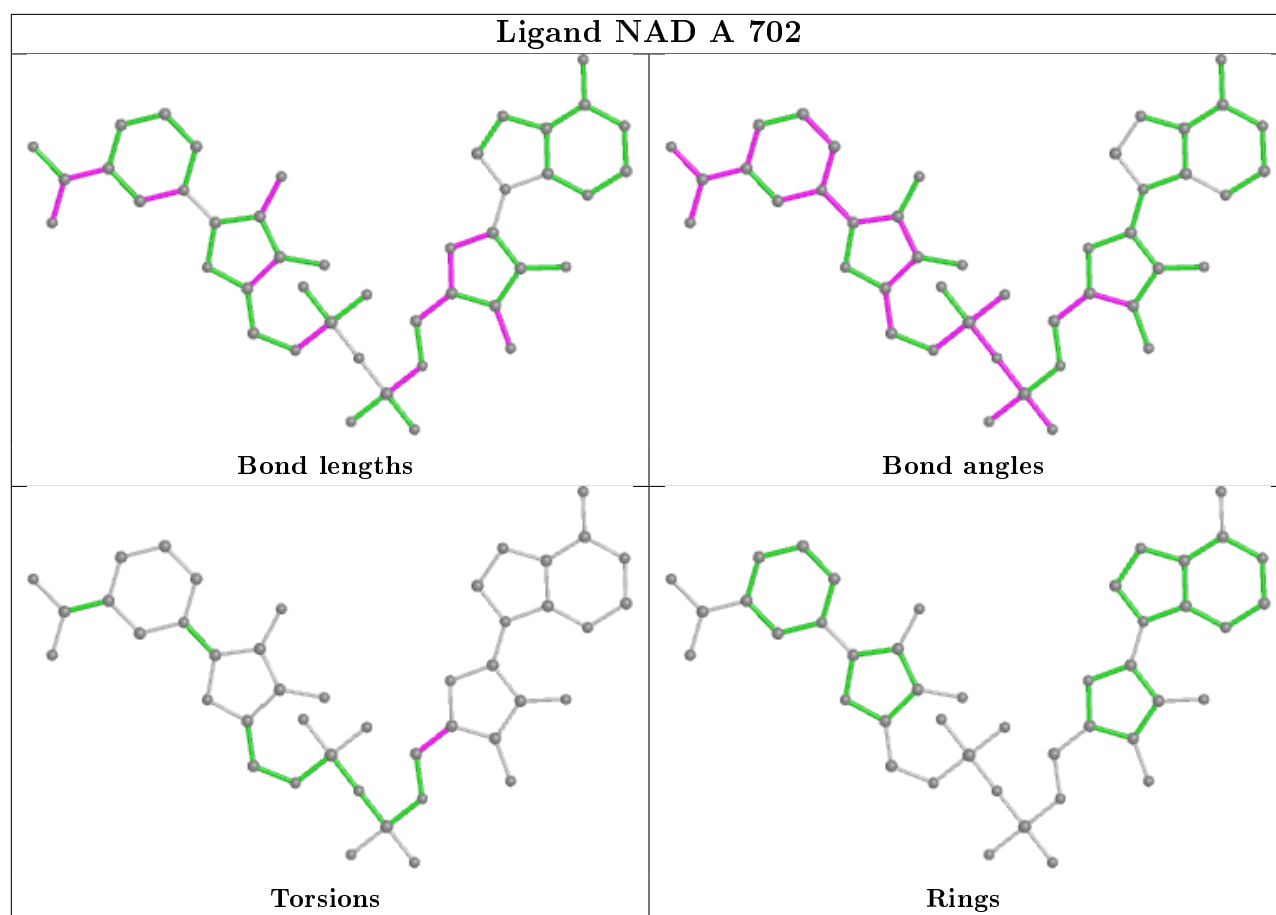
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	URO	9	0
4	A	703	EDO	7	0
3	A	702	NAD	6	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.





#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.