



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:22 pm GMT

PDB ID : 1U0R
Title : Crystal structure of Mycobacterium tuberculosis NAD kinase
Authors : Garavaglia, S.; Raffaelli, N.; Finaurini, L.; Magni, G.; Rizzi, M.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2004-07-14
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

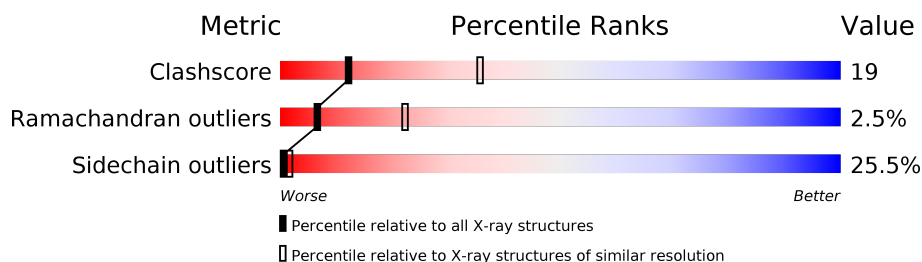
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	
1	B	307	
1	C	307	
1	D	307	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8778 atoms, of which 0 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 Inorganic polyphosphate/ATP-NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2121	1336	384	395	6			
1	B	258	Total	C	N	O	S	0	0	0
			1941	1225	352	358	6			
1	C	285	Total	C	N	O	S	0	0	0
			2156	1353	394	403	6			
1	D	301	Total	C	N	O	S	0	0	0
			2257	1417	412	420	8			

- Molecule 2 is water.

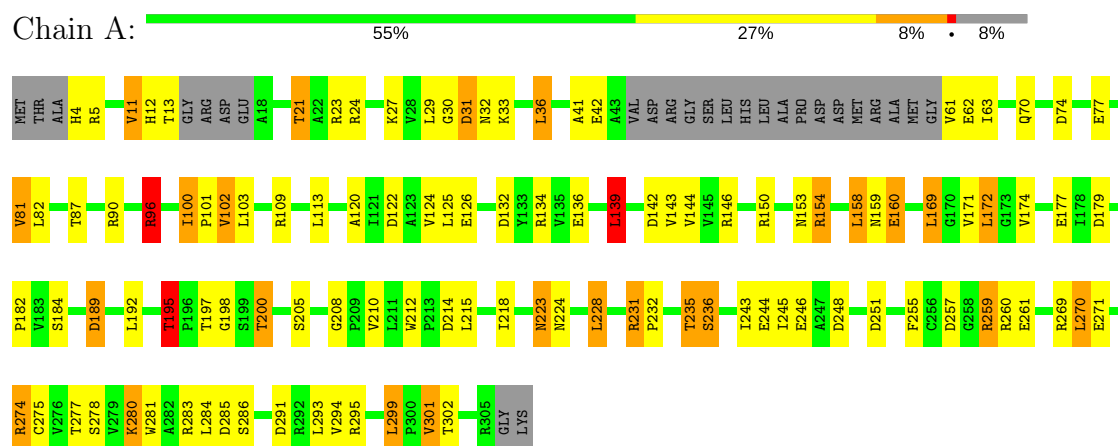
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	81	Total	O	0	0
			81	81		
2	B	56	Total	O	0	0
			56	56		
2	C	90	Total	O	0	0
			90	90		
2	D	76	Total	O	0	0
			76	76		

3 Residue-property plots

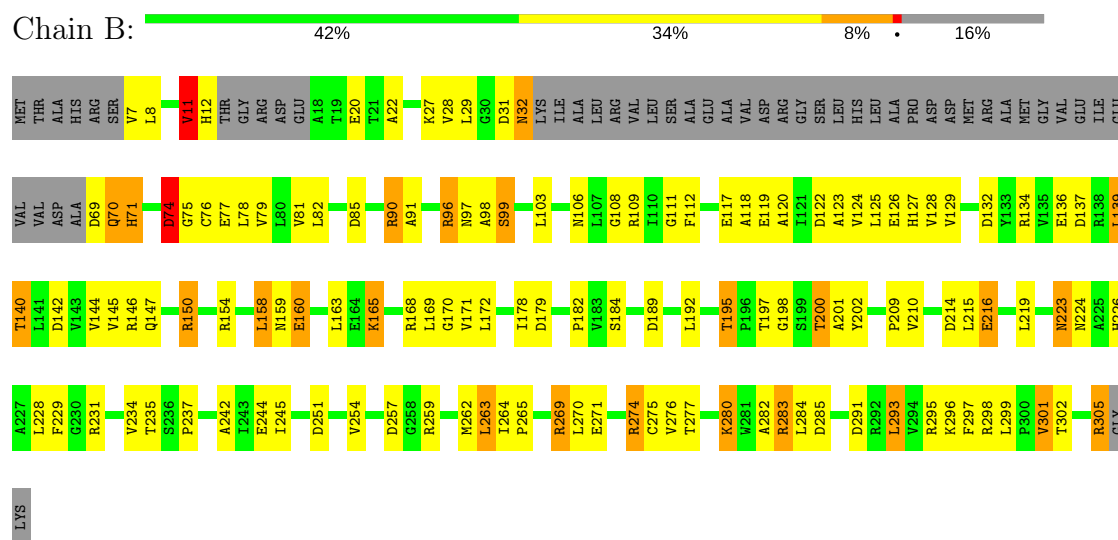
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: Inorganic polyphosphate/ATP-NAD kinase

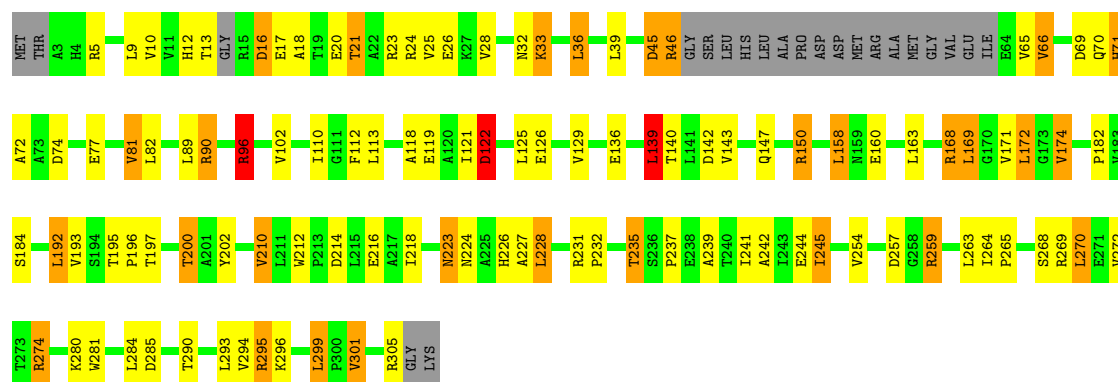


• Molecule 1: Inorganic polyphosphate/ATP-NAD kinase



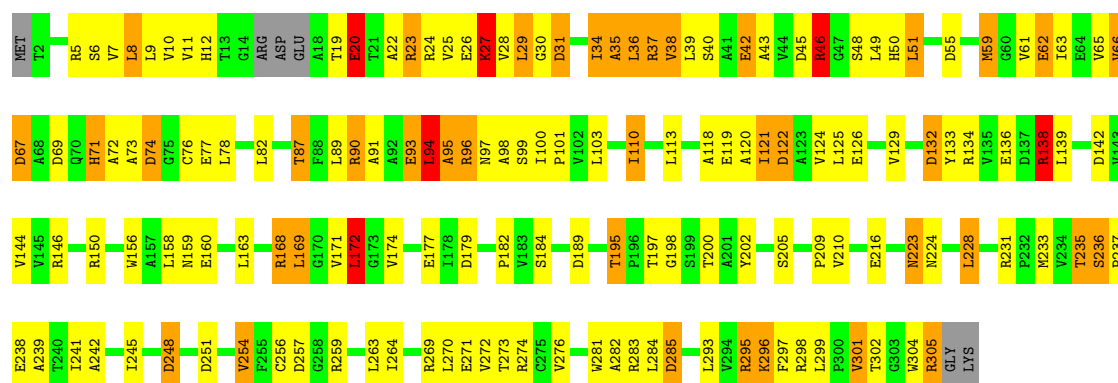
• Molecule 1: Inorganic polyphosphate/ATP-NAD kinase





- Molecule 1: Inorganic polyphosphate/ATP-NAD kinase

Chain D: 48% 35% 13% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.51Å 118.51Å 222.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.2 (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8778	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.89	1/2154 (0.0%)	1.08	19/2931 (0.6%)
1	B	0.77	0/1973	1.04	14/2685 (0.5%)
1	C	0.88	1/2189 (0.0%)	1.06	10/2977 (0.3%)
1	D	0.84	0/2293	1.07	14/3119 (0.4%)
All	All	0.85	2/8609 (0.0%)	1.06	57/11712 (0.5%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	THR	CB-OG1	5.13	1.53	1.43
1	C	74	ASP	CB-CG	5.08	1.62	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	257	ASP	CB-CG-OD2	8.10	125.59	118.30
1	B	214	ASP	CB-CG-OD2	7.88	125.39	118.30
1	B	257	ASP	CB-CG-OD2	7.40	124.96	118.30
1	A	142	ASP	CB-CG-OD2	7.21	124.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	VAL	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	2121	0	2150	65	0
1	B	1941	0	1958	83	0
1	C	2156	0	2178	73	0
1	D	2257	0	2277	126	0
2	A	81	0	0	7	1
2	B	56	0	0	4	0
2	C	90	0	0	8	0
2	D	76	0	0	10	1
All	All	8778	0	8563	324	1

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 19.

The worst 5 of 324 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:D:12:HIS:CE1	2:D:379:HOH:O	1.80	1.28
1:C:72:ALA:HB3	2:C:321:HOH:O	1.49	1.12
1:A:158:LEU:O	1:A:195:THR:HG21	1.57	1.04
1:D:30:GLY:HA3	1:D:61:VAL:HG12	1.42	1.00
1:D:6:SER:HA	1:D:35:ALA:HB2	1.45	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:316:HOH:O	2:D:320:HOH:O[4_555]	2.14	0.06

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 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	275/307 (90%)	261 (95%)	12 (4%)	2 (1%)	25	59
1	B	252/307 (82%)	225 (89%)	19 (8%)	8 (3%)	5	16
1	C	279/307 (91%)	253 (91%)	24 (9%)	2 (1%)	25	59
1	D	297/307 (97%)	256 (86%)	25 (8%)	16 (5%)	2	6
All	All	1103/1228 (90%)	995 (90%)	80 (7%)	28 (2%)	6	22

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	GLY
1	B	119	GLU
1	D	20	GLU
1	D	62	GLU
1	D	72	ALA

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 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	223/242 (92%)	169 (76%)	54 (24%)	1	2
1	B	202/242 (84%)	148 (73%)	54 (27%)	0	1
1	C	226/242 (93%)	175 (77%)	51 (23%)	1	3
1	D	235/242 (97%)	168 (72%)	67 (28%)	0	1
All	All	886/968 (92%)	660 (74%)	226 (26%)	0	2

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	ARG
1	C	122	ASP
1	D	248	ASP
1	B	301	VAL
1	C	33	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	127	HIS
1	B	223	ASN
1	D	106	ASN
1	B	106	ASN
1	C	223	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.