



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 04:59 AM EDT

PDB ID : 1TYY / pdb_00001tyy
Title : Crystal structure of aminoimidazole riboside kinase from Salmonella enterica
Authors : Zhang, Y.; Dougherty, M.; Downs, D.M.; Ealick, S.E.
Deposited on : 2004-07-08
Resolution : 2.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4429 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 putative sugar kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	Se	0	0	0
			2195	1392	371	418	10	4			
1	B	296	Total	C	N	O	S	Se	0	0	0
			2176	1373	370	420	10	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP Q8ZKR2
A	-18	GLY	-	cloning artifact	UNP Q8ZKR2
A	-17	SER	-	cloning artifact	UNP Q8ZKR2
A	-16	SER	-	cloning artifact	UNP Q8ZKR2
A	-15	HIS	-	expression tag	UNP Q8ZKR2
A	-14	HIS	-	expression tag	UNP Q8ZKR2
A	-13	HIS	-	expression tag	UNP Q8ZKR2
A	-12	HIS	-	expression tag	UNP Q8ZKR2
A	-11	HIS	-	expression tag	UNP Q8ZKR2
A	-10	HIS	-	expression tag	UNP Q8ZKR2
A	-9	SER	-	expression tag	UNP Q8ZKR2
A	-8	SER	-	cloning artifact	UNP Q8ZKR2
A	-7	GLY	-	cloning artifact	UNP Q8ZKR2
A	-6	LEU	-	cloning artifact	UNP Q8ZKR2
A	-5	VAL	-	cloning artifact	UNP Q8ZKR2
A	-4	PRO	-	cloning artifact	UNP Q8ZKR2
A	-3	ARG	-	cloning artifact	UNP Q8ZKR2
A	-2	GLY	-	cloning artifact	UNP Q8ZKR2
A	-1	SER	-	cloning artifact	UNP Q8ZKR2
A	0	HIS	-	cloning artifact	UNP Q8ZKR2
A	148	MSE	MET	modified residue	UNP Q8ZKR2
A	165	MSE	MET	modified residue	UNP Q8ZKR2
A	286	MSE	MET	modified residue	UNP Q8ZKR2
A	294	MSE	MET	modified residue	UNP Q8ZKR2
B	-19	MET	-	cloning artifact	UNP Q8ZKR2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	cloning artifact	UNP Q8ZKR2
B	-17	SER	-	cloning artifact	UNP Q8ZKR2
B	-16	SER	-	cloning artifact	UNP Q8ZKR2
B	-15	HIS	-	expression tag	UNP Q8ZKR2
B	-14	HIS	-	expression tag	UNP Q8ZKR2
B	-13	HIS	-	expression tag	UNP Q8ZKR2
B	-12	HIS	-	expression tag	UNP Q8ZKR2
B	-11	HIS	-	expression tag	UNP Q8ZKR2
B	-10	HIS	-	expression tag	UNP Q8ZKR2
B	-9	SER	-	expression tag	UNP Q8ZKR2
B	-8	SER	-	cloning artifact	UNP Q8ZKR2
B	-7	GLY	-	cloning artifact	UNP Q8ZKR2
B	-6	LEU	-	cloning artifact	UNP Q8ZKR2
B	-5	VAL	-	cloning artifact	UNP Q8ZKR2
B	-4	PRO	-	cloning artifact	UNP Q8ZKR2
B	-3	ARG	-	cloning artifact	UNP Q8ZKR2
B	-2	GLY	-	cloning artifact	UNP Q8ZKR2
B	-1	SER	-	cloning artifact	UNP Q8ZKR2
B	0	HIS	-	cloning artifact	UNP Q8ZKR2
B	148	MSE	MET	modified residue	UNP Q8ZKR2
B	165	MSE	MET	modified residue	UNP Q8ZKR2
B	286	MSE	MET	modified residue	UNP Q8ZKR2
B	294	MSE	MET	modified residue	UNP Q8ZKR2

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	B	2	Total K 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	26	Total O 26 26	0	0
3	B	28	Total O 28 28	0	0

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.43Å 53.99Å 89.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.01 – 2.60	Depositor
% Data completeness (in resolution range)	82.8 (32.01-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.293	Depositor
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.687	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4429	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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