



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:26 PM UTC

PDB ID : 3MUF / pdb_00003muf
Title : Shikimate kinase from Helicobacter pylori in complex with shikimate-3-phosphate and ADP
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Deposited on : 2010-05-03
Resolution : 2.30 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

<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	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

PERCENTILES INFOmissingINFO

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

1 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	98.82Å 98.82Å 42.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.30) 99.5 (30.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.231 , 0.277 (Not available) , 0.233	Depositor DCC
R_{free} test set	502 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	1.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1201	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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.

2 Model quality [i](#)

2.1 Standard geometry [i](#)

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

2.2 Too-close contacts [i](#)

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

2.3 Torsion angles [i](#)

2.3.1 Protein backbone [i](#)

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

2.3.2 Protein sidechains [i](#)

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

2.3.3 RNA [i](#)

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

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

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

2.5 Carbohydrates [i](#)

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

2.6 Ligand geometry [i](#)

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

2.7 Other polymers [i](#)

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

2.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	32/168 (19%)	0.26	0 100 100	38, 50, 60, 69	0

There are no RSRZ outliers to report.

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

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

3.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

3.4 Other polymers [i](#)

There are no such residues in this entry.