



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:09 AM UTC

PDB ID : 3AUB / pdb_00003aub
Title : A simplified BPTI variant stabilized by the A14G and A38V substitutions
Authors : Islam, M.M.; Kato, A.; Khan, M.M.A.; Noguchi, K.; Yohda, M.; Kidokoro, S.I.; Kuroda, Y.
Deposited on : 2011-02-03
Resolution : 1.00 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

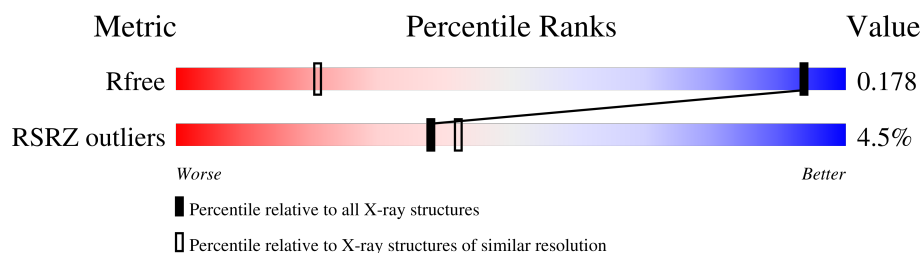
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.00 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))
R_{free}	180053	1358 (1.04-0.96)
RSRZ outliers	180081	1355 (1.04-0.96)

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

GLOBAL-STATISTICS INFOmissingINFO

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](#)

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

2.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

2.6 Ligand geometry [i](#)

There are no ligands in this entry.

2.7 Other polymers [i](#)

There are no such residues in this entry.

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	22/58 (37%)	0.52	1 (4%) 38 42	4, 9, 12, 12	4 (18%)
1	-15.990-A	0/58	-	-	-	-
All	All	22/116 (18%)	0.52	1 (4%) 38 42	4, 9, 12, 12	4 (18%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	6	LEU	3.1

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.

3.4 Ligands [i](#)

There are no ligands in this entry.

3.5 Other polymers [i](#)

There are no such residues in this entry.