

Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 11:32 am GMT

PDB ID	:	2X3B
Title	:	AsaP1 inactive mutant E294A, an extracellular toxic zinc metalloendopepti-
		dase
Authors	:	Bogdanovic, X.; Palm, G.J.; Singh, R.K.; Hinrichs, W.
Deposited on	:	2010-01-22
Resolution	:	2.28 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO



2 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	57.85Å 60.20 Å 183.61 Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	91.81 - 2.28	Depositor	
% Data completeness	99.7 (91.81-2.28)	Depositor	
(in resolution range)			
R_{merge}	0.13	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$3.08 (at 2.28 \text{\AA})$	Xtriage	
Refinement program	REFMAC 5.5.0072	Depositor	
R, R_{free}	0.244 , 0.293	Depositor	
Wilson B-factor $(Å^2)$	34.5	Xtriage	
Anisotropy	0.107	Xtriage	
L-test for twinning ²	$< L >=0.48, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	0.060 for k,h,-l	Xtriage	
Total number of atoms	4805	wwPDB-VP	
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP	

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.32% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

3 Model quality (i)

3.1 Standard geometry (i)

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

3.2 Too-close contacts (i)

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

3.3 Torsion angles (i)

3.3.1 Protein backbone (i)

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

3.3.2 Protein sidechains (i)

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

3.3.3 RNA (i)

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

3.4 Non-standard residues in protein, DNA, RNA chains (i)

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



4 Fit of model and data (i)

4.1 Protein, DNA and RNA chains (i)

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

4.2 Non-standard residues in protein, DNA, RNA chains (i)

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

4.3 Carbohydrates (i)

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

4.4 Ligands (i)

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

4.5 Other polymers (i)

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

