



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2023 – 09:18 am GMT

PDB ID : 4BFJ
Title : Superoxide reductase (Neelaredoxin) from *Archaeoglobus fulgidus* E12V mutant
Authors : Bandejas, T.M.; Rodrigues, J.V.; Sousa, C.M.; Barradas, A.R.; Pinho, F.G.; Pinto, A.F.; Teixeira, M.; Matias, P.M.; Romao, C.V.
Deposited on : 2013-03-19
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

<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**
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

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

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.79Å 98.97Å 105.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.54 – 2.80	Depositor
% Data completeness (in resolution range)	96.7 (41.54-2.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.177 , 0.232	Depositor
Wilson B-factor (Å ²)	88.7	Xtrriage
Anisotropy	0.500	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1920	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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.

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](#)

validation-pack failed to run properly - this section is therefore empty.

3.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

3.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

3.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

3.8 Polymer linkage issues

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

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

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

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

4.3 Carbohydrates

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

4.4 Ligands

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

4.5 Other polymers

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