WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2023 – 03:32 am GMT

PDB ID	:	4D74
Title	:	1.57 Å crystal structure of erwinia amylovora tyrosine phosphatase amsI
Authors	:	Benini, S.; Salomone-Stagni, M.; Caputi, L.; Cianci, M.
Deposited on	:	2014-11-19
Resolution	:	1.57 Å(reported)

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 1.57 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	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	66.03Å 66.03Å 72.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.18 – 1.57	Depositor
% Data completeness (in resolution range)	99.9 (57.18-1.57)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.17 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.169 , 0.179	Depositor
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.673	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
Total number of atoms	1284	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality ⓘ

3.1 Standard geometry ⓘ

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

3.2 Too-close contacts ⓘ

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

3.3 Torsion angles ⓘ

3.3.1 Protein backbone ⓘ

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

3.3.2 Protein sidechains ⓘ

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

3.3.3 RNA ⓘ

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

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

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

3.5 Carbohydrates ⓘ

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

3.6 Ligand geometry ⓘ

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

3.7 Other polymers ⓘ

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

3.8 Polymer linkage issues (i)

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.