



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 10:50 AM EDT

PDB ID : 6N3I
Title : Crystal structure of a double Trp XylE mutants (G58W/L315W)
Authors : Jiang, X.; Wu, J.P.; Yan, N.
Deposited on : 2018-11-15
Resolution : 3.69 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
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)	:	2.35.1

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 3.69 Å.

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

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

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3641 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-xylose transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3641	2411	579	627	24			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP C3SHS4
A	-25	GLY	-	expression tag	UNP C3SHS4
A	-24	SER	-	expression tag	UNP C3SHS4
A	-23	SER	-	expression tag	UNP C3SHS4
A	-22	HIS	-	expression tag	UNP C3SHS4
A	-21	HIS	-	expression tag	UNP C3SHS4
A	-20	HIS	-	expression tag	UNP C3SHS4
A	-19	HIS	-	expression tag	UNP C3SHS4
A	-18	HIS	-	expression tag	UNP C3SHS4
A	-17	HIS	-	expression tag	UNP C3SHS4
A	-16	SER	-	expression tag	UNP C3SHS4
A	-15	SER	-	expression tag	UNP C3SHS4
A	-14	GLY	-	expression tag	UNP C3SHS4
A	-13	LEU	-	expression tag	UNP C3SHS4
A	-12	VAL	-	expression tag	UNP C3SHS4
A	-11	PRO	-	expression tag	UNP C3SHS4
A	-10	ARG	-	expression tag	UNP C3SHS4
A	-9	GLY	-	expression tag	UNP C3SHS4
A	-8	SER	-	expression tag	UNP C3SHS4
A	-7	HIS	-	expression tag	UNP C3SHS4
A	-6	SER	-	expression tag	UNP C3SHS4
A	-5	ASP	-	expression tag	UNP C3SHS4
A	-4	GLU	-	expression tag	UNP C3SHS4
A	-3	VAL	-	expression tag	UNP C3SHS4
A	-2	ASP	-	expression tag	UNP C3SHS4
A	-1	ALA	-	expression tag	UNP C3SHS4
A	0	HIS	-	expression tag	UNP C3SHS4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	58	TRP	GLY	engineered mutation	UNP C3SHS4
A	315	TRP	LEU	engineered mutation	UNP C3SHS4

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.08Å 95.48Å 106.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.60 – 3.69	Depositor
% Data completeness (in resolution range)	98.9 (35.60-3.69)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.291 , 0.330	Depositor
Wilson B-factor (Å ²)	119.5	Xtriage
Anisotropy	0.628	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3641	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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