

Full wwPDB X-ray Structure Validation Report (i)

May 4, 2024 – 06:08 pm BST

PDB ID : 6RCZ

Title : The structure of Burkholderia pseudomallei trehalose-6-phosphatase

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Resolution : 1.74 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) : NOT EXECUTED EDS : NOT EXECUTED

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) : 2.36.2

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 1.74 Å.

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

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4072 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 Trehalose 6-phosphate phosphatase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	265	Total 1997	C 1263	N 365	O 365	S 4	0	3	0
1	Е	254	Total 1899		N 342	O 352	S 4	2	1	0

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	Е	1	Total Mg 1 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total O 100 100	0	0
4	Е	73	Total O 73 73	0	0

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.



3 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	75.93Å 83.84Å 84.98Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	59.68 - 1.74	Depositor	
% Data completeness	62.4 (59.68-1.74)	Depositor	
(in resolution range)	02.4 (03.00 1.14)	Depositor	
R_{merge}	0.16	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	PHENIX (1.13_2998: ???)	Depositor	
R, R_{free}	0.191 , 0.229	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4072	wwPDB-VP	
Average B, all atoms (Å ²)	32.0	wwPDB-VP	



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)

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

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)

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

4.5 Carbohydrates (i)

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

4.6 Ligand geometry (i)

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

4.7 Other polymers (i)

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



4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

5.4 Ligands (i)

EDS was not executed - this section is therefore empty.

5.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

