Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 06:56 AM EDT

PDB ID	:	6MS2
Title	:	Crystal structure of the GH43 BlXynB protein from Bacillus licheniformis
Authors	:	Zanphorlin, L.M.; Morais, M.A.B.; Diogo, J.A.; Murakami, M.T.
Deposited on	:	2018-10-16
Resolution	:	2.49 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 (i)) 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 (i)

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

The reported resolution of this entry is 2.49 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 (i)

There are 3 unique types of molecules in this entry. The entry contains 4132 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 Glycoside Hydrolase Family 43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	511	4073	2590	706	765	12	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP Q65MB6
A	-21	GLY	-	expression tag	UNP Q65MB6
A	-20	SER	-	expression tag	UNP Q65MB6
A	-19	SER	-	expression tag	UNP Q65MB6
A	-18	HIS	-	expression tag	UNP Q65MB6
A	-17	HIS	-	expression tag	UNP Q65MB6
A	-16	HIS	-	expression tag	UNP Q65MB6
A	-15	HIS	-	expression tag	UNP Q65MB6
A	-14	HIS	-	expression tag	UNP Q65MB6
A	-13	HIS	-	expression tag	UNP Q65MB6
A	-12	SER	-	expression tag	UNP Q65MB6
A	-11	SER	-	expression tag	UNP Q65MB6
A	-10	GLY	-	expression tag	UNP Q65MB6
A	-9	LEU	-	expression tag	UNP Q65MB6
A	-8	VAL	-	expression tag	UNP Q65MB6
A	-7	PRO	-	expression tag	UNP Q65MB6
A	-6	ARG	-	expression tag	UNP Q65MB6
A	-5	GLY	-	expression tag	UNP Q65MB6
A	-4	SER	-	expression tag	UNP Q65MB6
A	-3	HIS	-	expression tag	UNP Q65MB6
A	-2	MET	-	expression tag	UNP Q65MB6
A	-1	ALA	-	expression tag	UNP Q65MB6
A	0	SER	-	expression tag	UNP Q65MB6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	58	58	58	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.86Å 41.90Å 71.81Å 90.00° 91.70° 90.00°	Depositor
Resolution (Å)	33.31 – 2.49	Depositor
% Data completeness (in resolution range)	87.8 (33.31-2.49)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.10_2148	Depositor
R, R_{free}	0.197 , 0.242	Depositor
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.544	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
Total number of atoms	4132	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

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)

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - 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.

4.7 Other polymers (i)

There are no such residues in this entry.

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 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)

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