Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 06:55 AM EDT

PDB ID	:	6VBL
Title	:	Crystal structure of the transpeptidase domain of PBP2 from the Neisseria gonorrhoeae cephalosporin decreased susceptibility strain 35/02
Authors	:	Singh, A.; Davies, C.
Deposited on	:	2019-12-19
Resolution	:	1.93 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 ⓘ 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 (i)

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

The reported resolution of this entry is 1.93 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 2 unique types of molecules in this entry. The entry contains 2560 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 Probable peptidoglycan D,D-transpeptidase PenA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	2	0
			2460	1564	426	461	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q8RR30
A	233	SER	-	expression tag	UNP Q8RR30
A	234	GLY	-	expression tag	UNP Q8RR30
A	235	GLY	-	expression tag	UNP Q8RR30
A	236	ALA	-	expression tag	UNP Q8RR30
A	297	GLY	ALA	conflict	UNP Q8RR30
A	?	-	TYR	deletion	UNP Q8RR30
A	?	-	GLU	deletion	UNP Q8RR30
A	?	-	PRO	deletion	UNP Q8RR30
A	?	-	ASN	deletion	UNP Q8RR30
A	?	-	LYS	deletion	UNP Q8RR30
A	?	-	PRO	deletion	UNP Q8RR30
A	?	-	GLY	deletion	UNP Q8RR30
A	?	-	GLN	deletion	UNP Q8RR30
A	?	-	ALA	deletion	UNP Q8RR30
A	?	-	ASP	deletion	UNP Q8RR30
A	?	-	SER	deletion	UNP Q8RR30
A	?	-	GLU	deletion	UNP Q8RR30
A	?	-	GLN	deletion	UNP Q8RR30
A	?	-	ARG	deletion	UNP Q8RR30

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	100	Total	O	0	0
			100	100		

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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.62Å 61.09Å 109.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.72 – 1.93	Depositor
% Data completeness (in resolution range)	99.5 (31.72-1.93)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.96 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.183 , 0.205	Depositor
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.101	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2560	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

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

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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