

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 5, 2023 – 12:32 AM EDT

PDB ID	:	6USS
Title	:	Catalytic S88C mutant of gut microbial sulfatase from Bacteroides fragilis
		CAG:558
Authors	:	Ervin, S.M.; Redinbo, M.R.
Deposited on	:	2019-10-28
Resolution	:	2.50 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 (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)	:	1.13
$\mathrm{EDS}$	:	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:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 2.50 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 8068 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 Sulfatase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A	485	Total	С	Ν	0	$\mathbf{S}$	0	0	0
			3840	2448	658	716	18			
1	р	485	Total	С	Ν	0	S	0	0	0
	I D		3840	2448	658	716	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	88	CYS	SER	engineered mutation	UNP A0A081TVR9
В	88	CYS	SER	engineered mutation	UNP A0A081TVR9

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ca 1 1	0	0
2	В	1	Total Ca 1 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	208	Total O   208 208	0	0
3	В	178	Total O 178 178	0	0

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



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	122.63Å 180.38Å 123.69Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 - 2.50	Depositor
% Data completeness	99.1 (49.48-2.50)	Depositor
(in resolution range)		-
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.96 (at 2.51 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
$R, R_{free}$	0.186 , $0.240$	Depositor
Wilson B-factor $(Å^2)$	21.2	Xtriage
Anisotropy	0.359	Xtriage
L-test for twinning <sup>2</sup>	$ < L >=0.52, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8068	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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 2 ligands modelled in this entry, 2 are 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.

