

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

#### Oct 2, 2023 – 05:41 AM EDT

PDB ID	:	6NQ9
Title	:	Crystal structure of YetJ mutant from Bacillus Subtilis - D195E
Authors	:	Guo, G.; Chang, Y.; Liu, Q.
Deposited on		
Resolution	:	3.10  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:

:	FAILED
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber $(2001)$
:	Parkinson et al. (1996)
:	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 3.10 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.



#### 6NQ9

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6416 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	1 A	208	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
			1620	1102	245	265	8			0
1	1 B	207	Total	С	Ν	0	S	0	0	0
			1612	1096	245	263	8			
1	1 C	203	Total	С	Ν	0	S	0	0	0
			1583	1081	238	256	8			
1 D	Л	207	Total	С	Ν	0	S	0	0	0
	207	1601	1089	242	262	8	0	0	U	

• Molecule 1 is a protein called Uncharacterized protein YetJ.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	195	GLU	ASP	engineered mutation	UNP O31539
В	195	GLU	ASP	engineered mutation	UNP O31539
С	195	GLU	ASP	engineered mutation	UNP O31539
D	195	GLU	ASP	engineered mutation	UNP O31539

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



# 3 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 1 2 1	Depositor	
Cell constants	217.33Å 118.20Å 51.89Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $93.23^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	39.96 - 3.10	Depositor	
% Data completeness	99.4 (39.96-3.10)	Depositor	
(in resolution range)	· · · · · · · · · · · · · · · · · · ·	-	
R <sub>merge</sub>	(Not available)	Depositor	
R <sub>sym</sub>	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.43 (at 3.12 \text{\AA})$	Xtriage	
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor	
$R, R_{free}$	0.247 , $0.276$	Depositor	
Wilson B-factor $(Å^2)$	67.2	Xtriage	
Anisotropy	0.347	Xtriage	
L-test for twinning <sup>2</sup>	$ < L >=0.47, < L^2>=0.30$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	6416	wwPDB-VP	
Average B, all atoms $(Å^2)$	68.0	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 4.65% 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)

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 (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.

