



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 05:03 AM EDT

PDB ID : 6VFM  
Title : Crystal structure of SpeG allosteric polyamine acetyltransferase from *Bacillus thuringiensis*  
Authors : Tsimbalyuk, S.; Shornikov, A.; Le, V.T.B.; Kuhn, M.L.; Forwood, J.K.  
Deposited on : 2020-01-05  
Resolution : 2.67 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
Xtrriage (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

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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

There is only 1 type of molecule in this entry. The entry contains 2842 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 Spermidine N1-acetyltransferase.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 1   | A     | 167      | 1421  | 915 | 234 | 264 | 8 | 0       | 0       | 0     |
| 1   | B     | 167      | 1421  | 915 | 234 | 264 | 8 | 0       | 0       | 0     |

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

### 3 Data and refinement statistics

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

| Property                                                 | Value                                                       | Source    |
|----------------------------------------------------------|-------------------------------------------------------------|-----------|
| Space group                                              | P 63 2 2                                                    | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 159.37Å 159.37Å 106.20Å<br>90.00° 90.00° 120.00°            | Depositor |
| Resolution (Å)                                           | 63.74 – 2.67                                                | Depositor |
| % Data completeness<br>(in resolution range)             | 99.7 (63.74-2.67)                                           | Depositor |
| $R_{merge}$                                              | 0.32                                                        | Depositor |
| $R_{sym}$                                                | (Not available)                                             | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 2.37 (at 2.65Å)                                             | Xtrriage  |
| Refinement program                                       | PHENIX 1.12_2829                                            | Depositor |
| R, $R_{free}$                                            | 0.274 , 0.293                                               | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 42.1                                                        | Xtrriage  |
| Anisotropy                                               | 0.328                                                       | Xtrriage  |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$ | Xtrriage  |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtrriage  |
| Total number of atoms                                    | 2842                                                        | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 45.0                                                        | wwPDB-VP  |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9683e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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](#)

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### 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

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

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