



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:38 AM UTC

PDB ID : 3AUS / pdb\_00003aus  
Title : Crystal structure of Bacillus megaterium glucose dehydrogenase 4 in ligand-free form  
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Deposited on : 2011-02-16  
Resolution : 2.00 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](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                     | : | <b>FAILED</b>                                                    |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

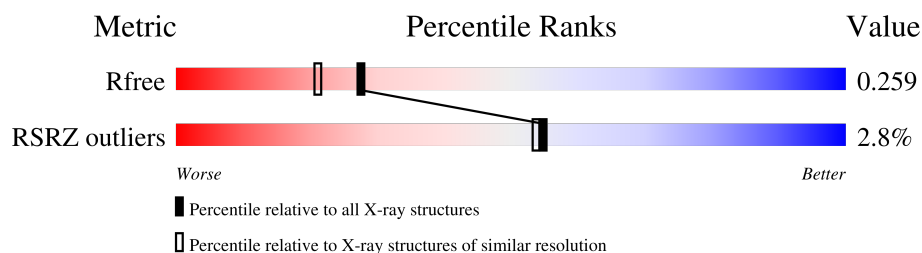
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric        | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|---------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$    | 180053                      | 10052 (2.00-2.00)                                     |
| RSRZ outliers | 180081                      | 10067 (2.00-2.00)                                     |

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

GLOBAL-STATISTICS INFOmissingINFO

## 2 Model quality [i](#)

### 2.1 Standard geometry [i](#)

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

### 2.2 Too-close contacts [i](#)

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

### 2.3 Torsion angles [i](#)

#### 2.3.1 Protein backbone [i](#)

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

#### 2.3.2 Protein sidechains [i](#)

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

#### 2.3.3 RNA [i](#)

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

### 2.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 2.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 2.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 2.7 Other polymers [i](#)

There are no such residues in this entry.

## 2.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

### 3 Fit of model and data ⓘ

#### 3.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | 1-A   | 109/269 (40%) | 0.63   | 3 (2%) 55 54 | 30, 42, 56, 59        | 0     |

All (3) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | 1-A   | 20  | GLY  | 2.8  |
| 1   | 1-A   | 80  | ILE  | 2.7  |
| 1   | 1-A   | 41  | ASN  | 2.0  |

#### 3.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

#### 3.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

#### 3.4 Ligands ⓘ

There are no ligands in this entry.

#### 3.5 Other polymers ⓘ

There are no such residues in this entry.