



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:37 PM EDT

PDB ID : 1SQ1 / pdb\_00001sq1  
Title : Crystal Structure of the Chorismate Synthase from *Campylobacter jejuni*,  
Northeast Structural Genomics Target BR19  
Authors : Forouhar, F.; Lee, I.; Vorobiev, S.M.; Xiao, R.; Acton, T.B.; Montelione, G.T.;  
Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2004-03-17  
Resolution : 2.80 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                     | : | <b>FAILED</b>                                                    |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | <b>FAILED</b>                                                    |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| 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 2.80 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 are 3 unique types of molecules in this entry. The entry contains 2168 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 Chorismate synthase.

| Mol | Chain | Residues | Atoms |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S | Se |         |         |       |
| 1   | A     | 288      | 2151  | 1359 | 370 | 409 | 6 | 7  | 0       | 0       | 0     |

There are 15 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | MSE      | MET    | modified residue | UNP Q9PM41 |
| A     | 28      | MSE      | MET    | modified residue | UNP Q9PM41 |
| A     | 140     | MSE      | MET    | modified residue | UNP Q9PM41 |
| A     | 214     | MSE      | MET    | modified residue | UNP Q9PM41 |
| A     | 235     | MSE      | MET    | modified residue | UNP Q9PM41 |
| A     | 254     | MSE      | MET    | modified residue | UNP Q9PM41 |
| A     | 335     | MSE      | MET    | modified residue | UNP Q9PM41 |
| A     | 363     | LEU      | -      | cloning artifact | UNP Q9PM41 |
| A     | 364     | GLU      | -      | cloning artifact | UNP Q9PM41 |
| A     | 365     | HIS      | -      | cloning artifact | UNP Q9PM41 |
| A     | 366     | HIS      | -      | cloning artifact | UNP Q9PM41 |
| A     | 367     | HIS      | -      | cloning artifact | UNP Q9PM41 |
| A     | 368     | HIS      | -      | cloning artifact | UNP Q9PM41 |
| A     | 369     | HIS      | -      | cloning artifact | UNP Q9PM41 |
| A     | 370     | HIS      | -      | cloning artifact | UNP Q9PM41 |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | A     | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |

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                                              | I 41 2 2                                                    | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 73.60Å 73.60Å 338.56Å<br>90.00° 90.00° 90.00°               | Depositor |
| Resolution (Å)                                           | 29.60 – 2.80                                                | Depositor |
| % Data completeness<br>(in resolution range)             | 9.5 (29.60-2.80)                                            | Depositor |
| $R_{merge}$                                              | 0.06                                                        | Depositor |
| $R_{sym}$                                                | 0.06                                                        | Depositor |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>               | 4.43 (at 2.80Å)                                             | Xtriage   |
| Refinement program                                       | CNS                                                         | Depositor |
| R, $R_{free}$                                            | 0.224 , 0.279                                               | Depositor |
| Wilson B-factor (Å <sup>2</sup> )                        | 59.0                                                        | Xtriage   |
| Anisotropy                                               | 0.897                                                       | Xtriage   |
| L-test for twinning <sup>2</sup>                         | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$ | Xtriage   |
| Estimated twinning fraction                              | No twinning to report.                                      | Xtriage   |
| Total number of atoms                                    | 2168                                                        | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 70.0                                                        | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<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](#)

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 oligosaccharides in this entry.

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

2 ligands are modelled in this entry.

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

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 [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.