# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2024 – 09:47 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 1ZGH |
| Title | : | Methionyl-tRNA formyltransferase from Clostridium thermocellum |
| Authors | : | Yang, H.; Kataeva, I.; Xu, H.; Zhao, M.; Chang, J.; Liu, Z.; Chen, L.; Tempel, W.; Habel, J.; Zhou, W.; Lee, D.; Lin, D.; Chang, S.; Arendall III, W.B.; Richardson, J.S.; Richardson, D.C.; Rose, J.P.; Wang, B.; Southeast Collaboratory for Structural Genomics (SECSG) |
| Deposited on | : | 2005-04-21 |
| Resolution | : | 2.05 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 ⓘ 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:

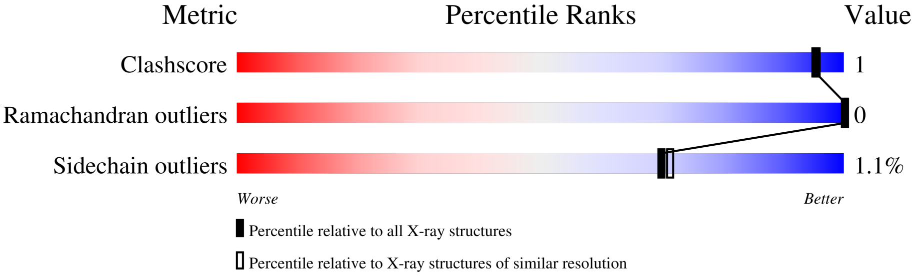
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| Xtriage (Phenix) | : | 1.20.1 |
| EDS | : | FAILED |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.39 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 180529 | 2229 (2.04-2.04) |
| Ramachandran outliers | 177936 | 2217 (2.04-2.04) |
| Sidechain outliers | 177891 | 2217 (2.04-2.04) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 260 |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1873 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 Methionyl-tRNA formyltransferase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | Se | | | |
| 1 | A | 227 | 1809 | 1176 | 293 | 333 | 1 | 6 | 0 | 0 | 0 |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -29 | MSE | - | cloning artifact | GB 48859327 |
| A | -28 | GLY | - | cloning artifact | GB 48859327 |
| A | -27 | SER | - | cloning artifact | GB 48859327 |
| A | -26 | SER | - | cloning artifact | GB 48859327 |
| A | -25 | HIS | - | expression tag | GB 48859327 |
| A | -24 | HIS | - | expression tag | GB 48859327 |
| A | -23 | HIS | - | expression tag | GB 48859327 |
| A | -22 | HIS | - | expression tag | GB 48859327 |
| A | -21 | HIS | - | expression tag | GB 48859327 |
| A | -20 | HIS | - | expression tag | GB 48859327 |
| A | -19 | SER | - | cloning artifact | GB 48859327 |
| A | -18 | SER | - | cloning artifact | GB 48859327 |
| A | -17 | GLY | - | cloning artifact | GB 48859327 |
| A | -16 | LEU | - | cloning artifact | GB 48859327 |
| A | -15 | VAL | - | cloning artifact | GB 48859327 |
| A | -14 | PRO | - | cloning artifact | GB 48859327 |
| A | -13 | ARG | - | cloning artifact | GB 48859327 |
| A | -12 | GLY | - | cloning artifact | GB 48859327 |
| A | -11 | SER | - | cloning artifact | GB 48859327 |
| A | -10 | GLN | - | cloning artifact | GB 48859327 |
| A | -9 | SER | - | cloning artifact | GB 48859327 |
| A | -8 | THR | - | cloning artifact | GB 48859327 |
| A | -7 | SER | - | cloning artifact | GB 48859327 |
| A | -6 | LEU | - | cloning artifact | GB 48859327 |
| A | -5 | TYR | - | cloning artifact | GB 48859327 |
| A | -4 | LYS | - | cloning artifact | GB 48859327 |
| A | -3 | LYS | - | cloning artifact | GB 48859327 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -2 | ALA | - | cloning artifact | GB 48859327 |
| A | -1 | GLY | - | cloning artifact | GB 48859327 |
| A | 0 | LEU | - | cloning artifact | GB 48859327 |
| A | 1 | MSE | MET | modified residue | GB 48859327 |
| A | 75 | MSE | MET | modified residue | GB 48859327 |
| A | 131 | MSE | MET | modified residue | GB 48859327 |
| A | 141 | MSE | MET | modified residue | GB 48859327 |
| A | 187 | MSE | MET | modified residue | GB 48859327 |
| A | 212 | MSE | MET | modified residue | GB 48859327 |

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | A | 17 | Total<br>17 | X<br>17 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | A | 47 | Total<br>47 | O<br>47 | 0 | 0 |

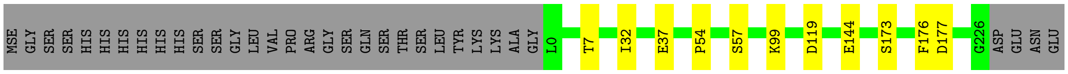
# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

- Molecule 1: Methionyl-tRNA formyltransferase

Chain A:



# 4 Data and refinement statistics ⓘ

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

| **Property** | **Value** | **Source** |
|---|---|---|
| Space group | P 42 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 85.40Å 85.40Å 104.27Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.19 – 2.05 | Depositor |
| % Data completeness<br>(in resolution range) | 99.9 (30.19-2.05) | Depositor |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 4.34 (at 2.05Å) | Xtriage |
| Refinement program | REFMAC refmac_5.2.0005 | Depositor |
| R, $R_{free}$ | 0.209 , 0.237 | Depositor |
| Wilson B-factor (Å$^2$) | 28.7 | Xtriage |
| Anisotropy | 0.202 | Xtriage |
| L-test for twinning[2] | $< \lvert L \rvert > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 1873 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 30.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UNX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.71 | 0/1844 | 0.71 | 1/2483 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 1 | A | 177 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1809 | 0 | 1779 | 4 | 0 |
| 2 | A | 17 | 0 | 0 | 0 | 0 |
| 3 | A | 47 | 0 | 0 | 0 | 0 |
| All | All | 1873 | 0 | 1779 | 4 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (4) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:32:ILE:HG23 | 1:A:37:GLU:HB2 | 1.93 | 0.51 |
| 1:A:99:LYS:NZ | 1:A:119:ASP:OD1 | 2.44 | 0.50 |
| 1:A:173:SER:HB3 | 1:A:176:PHE:CE1 | 2.50 | 0.46 |
| 1:A:7:THR:HB | 1:A:54:PRO:HD2 | 2.00 | 0.43 |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 225/260 (86%) | 219 (97%) | 6 (3%) | 0 | 100 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 189/225 (84%) | 187 (99%) | 2 (1%) | 70 71 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 57 | SER |
| 1 | A | 144 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 17 are unknown - 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data ⓘ

## 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

## 6.3 Carbohydrates ⓘ

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

## 6.4 Ligands ⓘ

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

## 6.5 Other polymers ⓘ

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