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

Oct 5, 2023 – 04:19 AM EDT

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|---|---|---|
| PDB ID | : | 6V9K |
| Title | : | CRYSTAL STRUCTURE OF THE HYBRID C-TERMINAL DOMAIN OF ENZYME I OF THE BACTERIAL PHOSPHOTRANSFERASE SYSTEM FORMED BY HYBRIDIZING THE SCAFFOLD OF THE ESCHERICHIA COLI ENZYME WITH THE ACTIVE SITE LOOPS FROM THE THERMOANAEROBACTER TENGCONGENSIS ENZYME |
| Authors | : | Stewart Jr., C.E. |
| Deposited on | : | 2019-12-13 |
| Resolution | : | 1.90 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 (i) 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 (i)) were used in the production of this report:

| | | |
|---|---|---|
| MolProbity | : | FAILED |
| Xtriage (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 (i)

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

The reported resolution of this entry is 1.90 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 (i)

There are 3 unique types of molecules in this entry. The entry contains 10416 atoms, of which 4929 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 Phosphoenolpyruvate-protein phosphotransferase.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 310 | Total | C | H | N | O | S | 0 | 4 | 0 |
| | | | 4956 | 1563 | 2483 | 422 | 472 | 16 | | | |
| 1 | B | 310 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 4880 | 1538 | 2446 | 415 | 466 | 15 | | | |

There are 44 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 260 | MET | - | initiating methionine | UNP A0A4S4CN20 |
| A | 278 | PRO | VAL | engineered mutation | UNP A0A4S4CN20 |
| A | 279 | LYS | ARG | engineered mutation | UNP A0A4S4CN20 |
| A | 301 | TYR | PHE | engineered mutation | UNP A0A4S4CN20 |
| A | 305 | ASN | ASP | engineered mutation | UNP A0A4S4CN20 |
| A | 306 | SER | ALA | engineered mutation | UNP A0A4S4CN20 |
| A | 309 | SER | THR | engineered mutation | UNP A0A4S4CN20 |
| A | 334 | LEU | MET | engineered mutation | UNP A0A4S4CN20 |
| A | 345 | LEU | MET | engineered mutation | UNP A0A4S4CN20 |
| A | 346 | ASP | ASN | engineered mutation | UNP A0A4S4CN20 |
| A | 347 | MET | PHE | engineered mutation | UNP A0A4S4CN20 |
| A | 351 | MET | GLU | engineered mutation | UNP A0A4S4CN20 |
| A | 357 | TYR | TRP | engineered mutation | UNP A0A4S4CN20 |
| A | 466 | MET | GLY | engineered mutation | UNP A0A4S4CN20 |
| A | 468 | GLU | ASP | engineered mutation | UNP A0A4S4CN20 |
| A | 469 | HIS | MET | engineered mutation | UNP A0A4S4CN20 |
| A | 470 | VAL | ILE | engineered mutation | UNP A0A4S4CN20 |
| A | 471 | LYS | SER | engineered mutation | UNP A0A4S4CN20 |
| A | 472 | GLU | HIS | engineered mutation | UNP A0A4S4CN20 |
| A | 473 | TYR | LEU | engineered mutation | UNP A0A4S4CN20 |
| A | 477 | PHE | MET | engineered mutation | UNP A0A4S4CN20 |
| A | 478 | HIS | SER | engineered mutation | UNP A0A4S4CN20 |
| B | 260 | MET | - | initiating methionine | UNP A0A4S4CN20 |
| B | 278 | PRO | VAL | engineered mutation | UNP A0A4S4CN20 |
| B | 279 | LYS | ARG | engineered mutation | UNP A0A4S4CN20 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 301 | TYR | PHE | engineered mutation | UNP A0A4S4CN20 |
| B | 305 | ASN | ASP | engineered mutation | UNP A0A4S4CN20 |
| B | 306 | SER | ALA | engineered mutation | UNP A0A4S4CN20 |
| B | 309 | SER | THR | engineered mutation | UNP A0A4S4CN20 |
| B | 334 | LEU | MET | engineered mutation | UNP A0A4S4CN20 |
| B | 345 | LEU | MET | engineered mutation | UNP A0A4S4CN20 |
| B | 346 | ASP | ASN | engineered mutation | UNP A0A4S4CN20 |
| B | 347 | MET | PHE | engineered mutation | UNP A0A4S4CN20 |
| B | 351 | MET | GLU | engineered mutation | UNP A0A4S4CN20 |
| B | 357 | TYR | TRP | engineered mutation | UNP A0A4S4CN20 |
| B | 466 | MET | GLY | engineered mutation | UNP A0A4S4CN20 |
| B | 468 | GLU | ASP | engineered mutation | UNP A0A4S4CN20 |
| B | 469 | HIS | MET | engineered mutation | UNP A0A4S4CN20 |
| B | 470 | VAL | ILE | engineered mutation | UNP A0A4S4CN20 |
| B | 471 | LYS | SER | engineered mutation | UNP A0A4S4CN20 |
| B | 472 | GLU | HIS | engineered mutation | UNP A0A4S4CN20 |
| B | 473 | TYR | LEU | engineered mutation | UNP A0A4S4CN20 |
| B | 477 | PHE | MET | engineered mutation | UNP A0A4S4CN20 |
| B | 478 | HIS | SER | engineered mutation | UNP A0A4S4CN20 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 1 | Total Mg<br>1 1 | 0 | 0 |
| 2 | B | 1 | Total Mg<br>1 1 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 279 | Total O<br>279 279 | 0 | 0 |
| 3 | B | 299 | Total O<br>299 299 | 0 | 0 |

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

# 3 Data and refinement statistics (i)

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

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 57.38Å 69.53Å 84.66Å<br>90.00° 108.73° 90.00° | Depositor |
| Resolution (Å) | 42.81 – 1.90 | Depositor |
| % Data completeness<br>(in resolution range) | 98.8 (42.81-1.90) | Depositor |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.28 (at 1.89Å) | Xtriage |
| Refinement program | PHENIX 1.14.3260 | Depositor |
| R, $R_{free}$ | 0.161 , 0.204 | Depositor |
| Wilson B-factor (Å$^2$) | 19.0 | Xtriage |
| Anisotropy | 0.225 | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.51$, $< L^2 > = 0.34$ | Xtriage |
| Estimated twinning fraction | 0.027 for h,-k,-h-l | Xtriage |
| Total number of atoms | 10416 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 28.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 4 Model quality

## 4.1 Standard geometry

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

## 4.2 Too-close contacts

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

## 4.3 Torsion angles

### 4.3.1 Protein backbone

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

### 4.3.2 Protein sidechains

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

### 4.3.3 RNA

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

## 4.4 Non-standard residues in protein, DNA, RNA chains

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

## 4.5 Carbohydrates

There are no monosaccharides in this entry.

## 4.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - 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.

## 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

## 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

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