Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 04:19 AM EDT

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 Full wwPDB X-ray Structure Validation 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.

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
			Total	C	H	N	O	S			
1	A	310	4956	1563	2483	422	472	16	0	4	0
1	B	310	4880	1538	2446	415	466	15	0	0	0

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
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B	301	TYR	PHE	engineered mutation	UNP A0A4S4CN20
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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
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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 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	279	Total O 279 279	0	0
3	B	299	Total O 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 a, b, c, α, β, γ	57.38Å 69.53Å 84.66Å 90.00° 108.73° 90.00°	Depositor
Resolution (Å)	42.81 – 1.90	Depositor
% Data completeness (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 (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 monosaccharides in this entry.

4.6 Ligand geometry (i)

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 (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)

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