wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 01:54 AM EDT

PDB ID	:	6VBJ
Title	:	CRYSTAL STRUCTURE OF THE HYBRID C-TERMINAL DOMAIN OF ENZYME I OF THE BACTERIAL PHOSPHOTRANSFERASE SYSTEM FORMED BY HYBRIDIZING THE SCAFFOLD OF THE THERMOANAEROBACTER TENGCONGENSIS ENZYME WITH THE ACTIVE SITE LOOPS FROM THE ESCHERICHIA COLI ENZYME
Authors	:	Stewart Jr., C.E.
Deposited on	:	2019-12-19
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*
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 2.00 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 2 unique types of molecules in this entry. The entry contains 10266 atoms, of which 4962 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	313	Total	C	H	N	O	S	0	0	0
			4909	1540	2478	405	466	20			
1	B	313	Total	C	H	N	O	S	0	1	0
			4924	1545	2484	406	469	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	MET	-	initiating methionine	UNP Q8R7R4
A	278	VAL	PRO	engineered mutation	UNP Q8R7R4
A	279	ARG	LYS	engineered mutation	UNP Q8R7R4
A	301	PHE	TYR	engineered mutation	UNP Q8R7R4
A	305	ASP	ASN	engineered mutation	UNP Q8R7R4
A	306	ALA	SER	engineered mutation	UNP Q8R7R4
A	309	THR	SER	engineered mutation	UNP Q8R7R4
A	334	MET	LEU	engineered mutation	UNP Q8R7R4
A	345	MET	LEU	engineered mutation	UNP Q8R7R4
A	346	ASN	ASP	engineered mutation	UNP Q8R7R4
A	347	PHE	MET	engineered mutation	UNP Q8R7R4
A	351	GLU	MET	engineered mutation	UNP Q8R7R4
A	357	TRP	TYR	engineered mutation	UNP Q8R7R4
A	466	GLY	MET	engineered mutation	UNP Q8R7R4
A	468	ASP	GLU	engineered mutation	UNP Q8R7R4
A	469	MET	HIS	engineered mutation	UNP Q8R7R4
A	470	ILE	VAL	engineered mutation	UNP Q8R7R4
A	471	SER	LYS	engineered mutation	UNP Q8R7R4
A	472	HIS	GLU	engineered mutation	UNP Q8R7R4
A	473	LEU	TYR	engineered mutation	UNP Q8R7R4
A	477	MET	PHE	engineered mutation	UNP Q8R7R4
A	478	SER	HIS	engineered mutation	UNP Q8R7R4
B	260	MET	-	initiating methionine	UNP Q8R7R4
B	278	VAL	PRO	engineered mutation	UNP Q8R7R4
B	279	ARG	LYS	engineered mutation	UNP Q8R7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	PHE	TYR	engineered mutation	UNP Q8R7R4
B	305	ASP	ASN	engineered mutation	UNP Q8R7R4
B	306	ALA	SER	engineered mutation	UNP Q8R7R4
B	309	THR	SER	engineered mutation	UNP Q8R7R4
B	334	MET	LEU	engineered mutation	UNP Q8R7R4
B	345	MET	LEU	engineered mutation	UNP Q8R7R4
B	346	ASN	ASP	engineered mutation	UNP Q8R7R4
B	347	PHE	MET	engineered mutation	UNP Q8R7R4
B	351	GLU	MET	engineered mutation	UNP Q8R7R4
B	357	TRP	TYR	engineered mutation	UNP Q8R7R4
B	466	GLY	MET	engineered mutation	UNP Q8R7R4
B	468	ASP	GLU	engineered mutation	UNP Q8R7R4
B	469	MET	HIS	engineered mutation	UNP Q8R7R4
B	470	ILE	VAL	engineered mutation	UNP Q8R7R4
B	471	SER	LYS	engineered mutation	UNP Q8R7R4
B	472	HIS	GLU	engineered mutation	UNP Q8R7R4
B	473	LEU	TYR	engineered mutation	UNP Q8R7R4
B	477	MET	PHE	engineered mutation	UNP Q8R7R4
B	478	SER	HIS	engineered mutation	UNP Q8R7R4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	232	Total O 232 232	0	0
2	B	201	Total O 201 201	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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.43Å 85.42Å 95.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.71 – 2.00	Depositor
% Data completeness (in resolution range)	97.9 (42.71-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.191 , 0.230	Depositor
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.724	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10266	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4096e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

There are no ligands in this entry.

4.7 Other polymers

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

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