

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 11:35 PM EDT

PDB ID : 6V2N

Title : Crystal structure of E. coli phosphoenolpyruvate carboxykinase mutant

Lys254Ser

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Deposited on : 2019-11-25

Resolution : 1.65 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

Mogul : 1.8.5 (274361), CSD as541be (2020)

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 1.65 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.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	602	-	X	-	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4553 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 Phosphoenolpyruvate carboxykinase (ATP).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	518	Total 4025	C 2563	N 677	O 771	S 14	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	CYS	conflict	UNP A0A400L9R1
A	240	ALA	LYS	conflict	UNP A0A400L9R1
A	262	ALA	LYS	conflict	UNP A0A400L9R1
A	285	SER	CYS	conflict	UNP A0A400L9R1
A	302	ALA	ASN	conflict	UNP A0A400L9R1
A	315	LYS	VAL	$\operatorname{conflict}$	UNP A0A400L9R1
A	318	ASN	ASP	conflict	UNP A0A400L9R1
A	492	GLY	LYS	conflict	UNP A0A400L9R1
A	539	ALA	LYS	conflict	UNP A0A400L9R1

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	523	Total O 523 523	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	54.91Å 76.65Å 65.42Å	Depositor	
a, b, c, α , β , γ	90.00° 96.38° 90.00°	Depositor	
Resolution (Å)	44.29 - 1.65	Depositor	
% Data completeness	99.8 (44.29-1.65)	Depositor	
(in resolution range)	33.0 (44.23-1.00)	Depositor	
R_{merge}	0.08	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	0.07 (at 1.31Å)	Xtriage	
Refinement program	PHENIX 1.17.1_3660	Depositor	
R, R_{free}	0.146 , 0.174	Depositor	
Wilson B-factor (Å ²)	11.6	Xtriage	
Anisotropy	0.417	Xtriage	
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	4553	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	19.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

ſ	Mol	Type	Chain	Pog	Link	В	ond len	gths	Bond angles		
	MIOI	туре		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	3	ACT	A	602	-	3,3,3	2.79	3 (100%)	3,3,3	1.70	1 (33%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
3	A	602	ACT	O-C	3.49	1.38	1.22
3	A	602	ACT	OXT-C	-2.53	1.18	1.30
3	A	602	ACT	СН3-С	-2.20	1.39	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	602	ACT	OXT-C-O	2.48	131.19	122.05

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)

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

