

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 03:53 PM EDT

PDB ID : 6NZA

Title : Crystal structure of E. coli fumarase C K324A variant with closed SS Loop at

1.41 angstrom resolution

Authors: Weaver, T.M.; May, J.F.; Bhattacharyya, B.

Deposited on : 2019-02-13

Resolution : 1.41 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 1.41 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 8043 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 Fumarate hydratase class II.

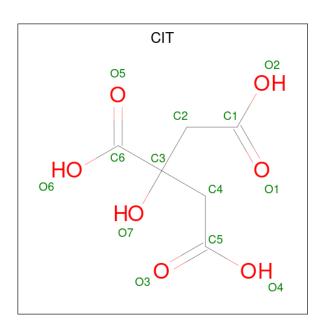
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	461	Total 3546	C 2214	N 630	O 677	S 25	0	10	0
1	В	459	Total 3547	C 2217	N 629	O 677	S 24	0	12	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	ALA	LYS	engineered mutation	UNP P05042
A	468	HIS	-	expression tag	UNP P05042
A	469	HIS	-	expression tag	UNP P05042
A	470	HIS	-	expression tag	UNP P05042
A	471	HIS	-	expression tag	UNP P05042
A	472	HIS	-	expression tag	UNP P05042
В	324	ALA	LYS	engineered mutation	UNP P05042
В	468	HIS	-	expression tag	UNP P05042
В	469	HIS	_	expression tag	UNP P05042
В	470	HIS	-	expression tag	UNP P05042
В	471	HIS	-	expression tag	UNP P05042
В	472	HIS	-	expression tag	UNP P05042

• Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	В	1	Total C O 13 6 7	0	0

• Molecule 3 is water.

Mol	Chain	Residues Atoms		ZeroOcc	AltConf
3	A	500	Total O 500 500	0	0
3	В	424	Total O 424 424	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	C 2 2 21	Depositor
Cell constants	103.23Å 217.56Å 86.38Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.34 - 1.41	Depositor
% Data completeness	100.0 (59.34-1.41)	Depositor
(in resolution range)	` ´	
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.22 (at 1.41Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.145 , 0.170	Depositor
Wilson B-factor (\mathring{A}^2)	14.0	Xtriage
Anisotropy	0.487	Xtriage
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8043	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.86% 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)

2 ligands are modelled in this entry.

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).

Mol	Mal True Chain Das		Res Link		Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	501	-	12,12,12	1.09	0	17,17,17	1.37	1 (5%)
2	CIT	В	601	-	12,12,12	1.05	0	17,17,17	1.58	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	501	-	-	3/16/16/16	-
2	CIT	В	601	-	-	0/16/16/16	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	В	601	CIT	O6-C6-C3	4.02	120.04	113.05
2	A	501	CIT	O6-C6-C3	3.18	118.58	113.05
2	В	601	CIT	O2-C1-C2	2.01	120.80	114.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C2-C3-C4-C5
2	A	501	CIT	O7-C3-C4-C5
2	A	501	CIT	C6-C3-C4-C5

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.

