

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

#### Oct 1, 2023 – 10:20 PM EDT

PDB ID	:	6MZZ
Title	:	Fluoroacetate dehalogenase, room temperature structure, using first 1 degree
		of total 3 degree oscillation
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Deposited on	:	2018-11-06
Resolution	:	1.80  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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	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:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 1.80 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.



#### 6MZZ

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4972 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 Fluoroacetate dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	297	Total	С	Ν	0	S	0	4	0
			2386	1536	418	423	9			
1	В	B 298 Total C 2368 1524	Ν	0	S	0	1	0		
1	I D		2368	1524	413	422	9	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6NAM1
А	0	HIS	-	expression tag	UNP Q6NAM1
A	303	GLY	-	expression tag	UNP Q6NAM1
А	304	SER	-	expression tag	UNP Q6NAM1
В	-1	GLY	-	expression tag	UNP Q6NAM1
В	0	HIS	-	expression tag	UNP Q6NAM1
В	303	GLY	-	expression tag	UNP Q6NAM1
В	304	SER	-	expression tag	UNP Q6NAM1

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

Mol	Chain	Residues	Ator	ns	ZeroOcc	AltConf
2	В	1	Total 1	Ca 1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	115	Total O 115 115	0	0
3	В	102	Total O 102 102	0	0

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



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	41.60Å 79.10Å 83.80Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $103.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	39.55 - 1.80	Depositor
% Data completeness	99.0 (39.55-1.80)	Depositor
(in resolution range)		-
$R_{merge}$	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.04 (at 1.79 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
$R, R_{free}$	0.175 , $0.209$	Depositor
Wilson B-factor $(Å^2)$	34.4	Xtriage
Anisotropy	0.340	Xtriage
L-test for twinning <sup>2</sup>	$<  L  > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
Total number of atoms	4972	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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 1 ligands modelled in this entry, 1 is 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)

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

