

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

#### Oct 2, 2023 – 05:24 AM EDT

PDB ID : 6MVU

Title: Structure of a bacterial ALDH16 active site mutant C295A complexed with

p-nitrophenylacetate

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Deposited on : 2018-10-28

Resolution : 1.49 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

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:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.49 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 5 unique types of molecules in this entry. The entry contains 12481 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.

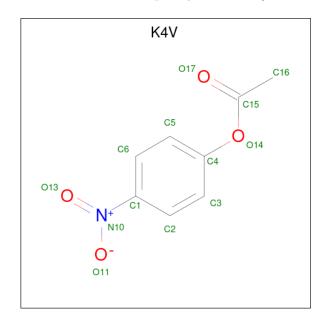
• Molecule 1 is a protein called Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	752	Total 5588	C 3541	N 982	O 1040	S 25	0	8	0
1	В	752	Total 5577	C 3533	N 976	O 1043	S 25	0	8	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A0Q3EUQ3
A	295	ALA	CYS	engineered mutation	UNP A0A0Q3EUQ3
В	0	SER	-	expression tag	UNP A0A0Q3EUQ3
В	295	ALA	CYS	engineered mutation	UNP A0A0Q3EUQ3

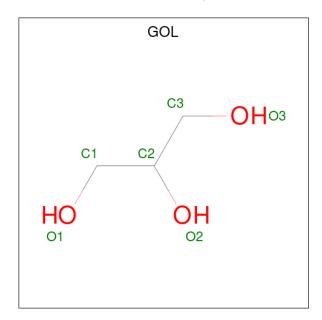
• Molecule 2 is 4-nitrophenyl acetate (three-letter code: K4V) (formula: C<sub>8</sub>H<sub>7</sub>NO<sub>4</sub>).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
2	A	1	Total 13	C 8		O 4	0	0
2	В	1	Total 13	C 8	N 1	O 4	0	0

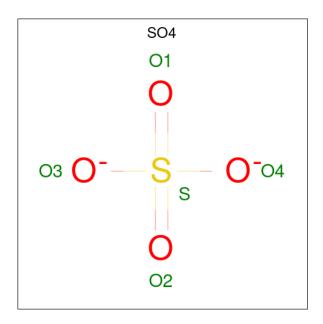
 $\bullet$  Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 



$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	1
3	В	1	Total C O 12 6 6	0	1

 $\bullet$  Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 





Mol	Chain	Residues	Ato	${f Atoms}$			AltConf	
4	A	1	Total	О	S	0	0	
4	A	1	5	4	1	0	U	
4	A	1	Total	О	S	0	0	
4	A	1	5	4	1	0	U	
4	A	1	Total	О	S	0	0	
4	Λ	1	5	4	1	0	U	
4	A	1	Total	Ο	$\mathbf{S}$	0	0	
4	Λ	1	5	4	1			
4	В	1	Total	О	S	0	0	
4	Ъ	1	5	4	1	U	U	
4	В	1	Total	Ο	S	0	0	
4	ט	1	5	4	1		U	
4	В	1	Total	О	S	0	0	
4	В	1	5	4	1	U	U	

### $\bullet$ Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	597	Total O 602 602	0	5
5	В	627	Total O 629 629	0	4

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	79.38Å 119.62Å 158.67Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.52 - 1.49	Depositor
% Data completeness	98.2 (95.52-1.49)	Depositor
(in resolution range)	30.2 (30.02-1.43)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.50  (at  1.49Å)	Xtriage
Refinement program	PHENIX	Depositor
$R, R_{free}$	0.192 , 0.216	Depositor
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.110	Xtriage
L-test for twinning <sup>2</sup>	$ < L >=0.52, < L^2>=0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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 47.39 % 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 9.9910e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>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.



<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)

13 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	Tuno	Chain	Res	Link	Во	ond leng	ths	В	ond ang	cles
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	В	803	-	4,4,4	0.15	0	6,6,6	0.15	0
4	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.18	0
2	K4V	A	801	-	12,13,13	3.17	2 (16%)	15,17,17	2.23	4 (26%)
4	SO4	A	806	-	4,4,4	0.13	0	6,6,6	0.22	0
3	GOL	A	802[A]	-	5,5,5	0.95	0	5,5,5	0.91	0
3	GOL	A	802[B]	-	5,5,5	0.96	0	5,5,5	0.77	0
2	K4V	В	801	-	12,13,13	3.20	3 (25%)	15,17,17	2.19	4 (26%)
3	GOL	В	802[A]	-	5,5,5	0.97	0	5,5,5	0.86	0
3	GOL	В	802[B]	-	5,5,5	0.94	0	5,5,5	0.78	0
4	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	В	805	-	4,4,4	0.12	0	6,6,6	0.21	0
4	SO4	В	804	-	4,4,4	0.15	0	6,6,6	0.19	0
4	SO4	A	805	-	4,4,4	0.12	0	6,6,6	0.19	0

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	K4V	A	801	-	-	6/6/8/8	0/1/1/1
3	GOL	A	802[A]	-	ı	1/4/4/4	-
3	GOL	A	802[B]	-	-	2/4/4/4	-
2	K4V	В	801	-	-	6/6/8/8	0/1/1/1
3	GOL	В	802[A]	-	-	1/4/4/4	-
3	GOL	В	802[B]	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
2	В	801	K4V	O13-N10	10.37	1.40	1.22
2	A	801	K4V	O13-N10	10.31	1.40	1.22
2	В	801	K4V	O14-C15	2.99	1.46	1.35
2	A	801	K4V	O14-C15	2.97	1.46	1.35
2	В	801	K4V	C1-N10	-2.02	1.40	1.45

The worst 5 of 8 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	801	K4V	O14-C15-C16	6.36	125.08	110.98
2	A	801	K4V	O14-C15-C16	6.31	124.98	110.98
2	A	801	K4V	C4-O14-C15	3.81	133.43	118.27
2	В	801	K4V	C4-O14-C15	3.64	132.76	118.27
2	A	801	K4V	O14-C15-O17	-3.13	115.35	122.41

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	K4V	C2-C1-N10-O13
2	A	801	K4V	C6-C1-N10-O13
2	В	801	K4V	C2-C1-N10-O13
2	В	801	K4V	C6-C1-N10-O13
2	В	801	K4V	C16-C15-O14-C4

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.

