

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

#### May 14, 2020 – 10:18 pm BST

PDB ID : 4DVJ

Title : Crystal structure of a putative zinc-dependent alcohol dehydrogenase protein

from Rhizobium etli CFN 42

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Deposited on : 2012-02-23

Resolution : 1.99 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

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

Xtriage (Phenix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

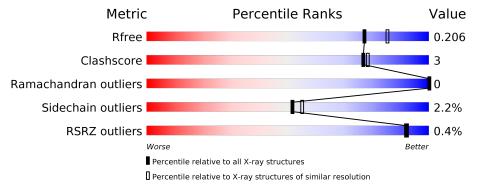
Validation Pipeline (wwPDB-VP) : 2.11

# 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 1.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	A	363	85%	8%	• 6%
1	В	363	85%	8%	• 6%



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5582 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 Putative zinc-dependent alcohol dehydrogenase protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	341	Total 2569	C 1637		O 474		0	0	0
1	В	342	Total 2573	C 1638		O 477		0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q2JZD9
A	2	HIS	-	EXPRESSION TAG	UNP Q2JZD9
A	3	HIS	-	EXPRESSION TAG	UNP Q2JZD9
A	4	HIS	-	EXPRESSION TAG	UNP Q2JZD9
A	5	HIS	=	EXPRESSION TAG	UNP Q2JZD9
A	6	HIS	-	EXPRESSION TAG	UNP Q2JZD9
A	7	HIS	-	EXPRESSION TAG	UNP Q2JZD9
A	8	SER	-	EXPRESSION TAG	UNP Q2JZD9
A	9	SER	-	EXPRESSION TAG	UNP Q2JZD9
A	10	GLY	=	EXPRESSION TAG	UNP Q2JZD9
A	11	VAL	-	EXPRESSION TAG	UNP Q2JZD9
A	12	ASP	-	EXPRESSION TAG	UNP Q2JZD9
A	13	LEU	=	EXPRESSION TAG	UNP Q2JZD9
A	14	GLY	=	EXPRESSION TAG	UNP Q2JZD9
A	15	THR	=	EXPRESSION TAG	UNP Q2JZD9
A	16	GLU	=	EXPRESSION TAG	UNP Q2JZD9
A	17	ASN	=	EXPRESSION TAG	UNP Q2JZD9
A	18	LEU	=	EXPRESSION TAG	UNP Q2JZD9
A	19	TYR	=	EXPRESSION TAG	UNP Q2JZD9
A	20	PHE	=	EXPRESSION TAG	UNP Q2JZD9
A	21	GLN	-	EXPRESSION TAG	UNP Q2JZD9
A	22	SER	=	EXPRESSION TAG	UNP Q2JZD9
В	1	MSE	-	EXPRESSION TAG	UNP Q2JZD9
В	2	HIS	ı	EXPRESSION TAG	UNP Q2JZD9
В	3	HIS	-	EXPRESSION TAG	UNP Q2JZD9

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Chain	Residue	Modelled	Actual	Comment	Reference
В	4	HIS	-	EXPRESSION TAG	UNP Q2JZD9
В	5	HIS	-	EXPRESSION TAG	UNP Q2JZD9
В	6	HIS	-	EXPRESSION TAG	UNP Q2JZD9
В	7	HIS	-	EXPRESSION TAG	UNP Q2JZD9
В	8	SER	_	EXPRESSION TAG	UNP Q2JZD9
В	9	SER	_	EXPRESSION TAG	UNP Q2JZD9
В	10	GLY	-	EXPRESSION TAG	UNP Q2JZD9
В	11	VAL	_	EXPRESSION TAG	UNP Q2JZD9
В	12	ASP	-	EXPRESSION TAG	UNP Q2JZD9
В	13	LEU	-	EXPRESSION TAG	UNP Q2JZD9
В	14	GLY	_	EXPRESSION TAG	UNP Q2JZD9
В	15	THR	-	EXPRESSION TAG	UNP Q2JZD9
В	16	GLU	_	EXPRESSION TAG	UNP Q2JZD9
В	17	ASN	-	EXPRESSION TAG	UNP Q2JZD9
В	18	LEU	_	EXPRESSION TAG	UNP Q2JZD9
В	19	TYR	=	EXPRESSION TAG	UNP Q2JZD9
В	20	PHE	-	EXPRESSION TAG	UNP Q2JZD9
В	21	GLN	=	EXPRESSION TAG	UNP Q2JZD9
В	22	SER	-	EXPRESSION TAG	UNP Q2JZD9

### • Molecule 2 is water.

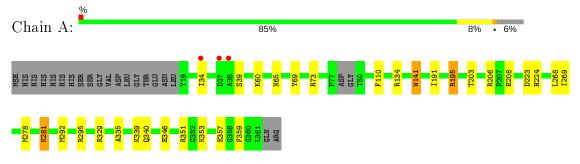
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
2	A	203	Total O 203 203	0	0
2	В	237	Total O 237 237	0	0



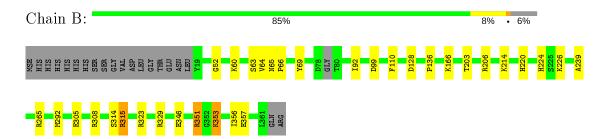
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Putative zinc-dependent alcohol dehydrogenase protein



• Molecule 1: Putative zinc-dependent alcohol dehydrogenase protein





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	185.31Å 42.24Å 111.27Å	Danagitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $122.39^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	48.66 - 1.99	Depositor
Resolution (A)	48.66 - 1.99	EDS
% Data completeness	99.5 (48.66-1.99)	Depositor
(in resolution range)	99.5 (48.66-1.99)	EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	5.01 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
P. P.	0.162 , 0.206	Depositor
$R, R_{free}$	0.164 , $0.206$	DCC
$R_{free}$ test set	2559 reflections $(5.08\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 40.6	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5582	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.38% of the height of the origin peak. No significant pseudotranslation is detected.

<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.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bo	nd lengths	Bond angles		
WIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	1.21	$1/2622 \ (0.0\%)$	0.96	$2/3565 \ (0.1\%)$	
1	В	1.27	$3/2626 \ (0.1\%)$	0.98	7/3572 (0.2%)	
All	All	1.24	4/5248 (0.1%)	0.97	9/7137 (0.1%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	В	64	VAL	CB-CG1	5.84	1.65	1.52
1	В	239	ALA	CA-CB	5.74	1.64	1.52
1	В	351	ARG	CB-CG	-5.29	1.38	1.52
1	A	141	TRP	CE3-CZ3	5.20	1.47	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	В	128	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	В	206	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	В	353	LYS	CD-CE-NZ	5.47	124.28	111.70
1	A	223	ASP	CB-CG-OD1	5.32	123.09	118.30
1	В	265	ARG	NE-CZ-NH2	-5.30	117.65	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Α	2569	0	2585	16	0
1	В	2573	0	2578	15	0
2	A	203	0	0	3	0
2	В	237	0	0	6	0
All	All	5582	0	5163	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 31 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:203:THR:OG1	1:A:224:HIS:HD2	1.70	0.75
1:A:278:MSE:HE1	1:A:281:LYS:HE2	1.74	0.69
1:B:214:LYS:HE3	2:B:579:HOH:O	1.94	0.67
1:B:220:HIS:HE1	2:B:634:HOH:O	1.78	0.66
1:A:65:ASN:OD1	1:A:353:LYS:NZ	2.30	0.63

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	$\mathbf{ntiles}$
1	A	337/363 (93%)	329 (98%)	8 (2%)	0	100	100
1	В	338/363 (93%)	329 (97%)	9 (3%)	0	100	100
All	All	675/726 (93%)	658 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.



#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/285 (94%)	261 (97%)	7 (3%)	46 48	
1	В	$268/285 \; (94\%)$	263 (98%)	5 (2%)	57 61	
All	All	536/570 (94%)	524 (98%)	12 (2%)	52 55	

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	351	ARG
1	В	110	PHE
1	A	281	LYS
1	В	66	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	HIS
1	В	220	HIS
1	В	224	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

# 5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.



# 5.6 Ligand geometry (i)

There are no ligands in this entry.

# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB( m \AA^2)$	Q < 0.9
1	A	$336/363 \ (92\%)$	-0.45	3 (0%) 84 83	12, 21, 38, 58	0
1	В	337/363 (92%)	-0.44	0 100 100	10, 19, 33, 44	0
All	All	673/726 (92%)	-0.45	3 (0%) 92 92	10, 20, 35, 58	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	4.9
1	A	38	ALA	3.2
1	A	34	ILE	2.6

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

### 6.4 Ligands (i)

There are no ligands in this entry.

### 6.5 Other polymers (i)

There are no such residues in this entry.

