



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3KSU  
Title : Crystal structure of short-chain dehydrogenase from oenococcus oeni psu-1  
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Deposited on : 2009-11-23  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

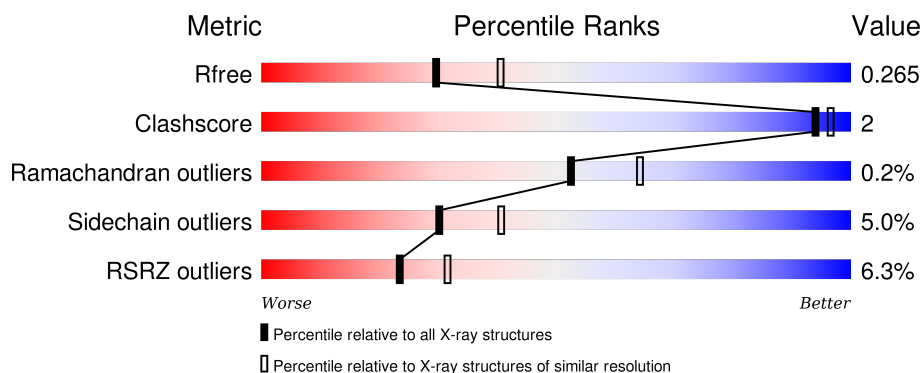
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	262	<div> <div>5%</div> <div>81% 8% 11%</div> </div>
1	B	262	<div> <div>6%</div> <div>77% 8% 15%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3651 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 3-oxoacyl-acyl carrier protein reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	1	0
			1830	1173	300	352	5			
1	B	223	Total	C	N	O	S	0	0	0
			1735	1114	284	333	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q04HJ2
A	1	LEU	-	expression tag	UNP Q04HJ2
A	253	GLU	-	expression tag	UNP Q04HJ2
A	254	GLY	-	expression tag	UNP Q04HJ2
A	255	HIS	-	expression tag	UNP Q04HJ2
A	256	HIS	-	expression tag	UNP Q04HJ2
A	257	HIS	-	expression tag	UNP Q04HJ2
A	258	HIS	-	expression tag	UNP Q04HJ2
A	259	HIS	-	expression tag	UNP Q04HJ2
A	260	HIS	-	expression tag	UNP Q04HJ2
B	0	SER	-	expression tag	UNP Q04HJ2
B	1	LEU	-	expression tag	UNP Q04HJ2
B	253	GLU	-	expression tag	UNP Q04HJ2
B	254	GLY	-	expression tag	UNP Q04HJ2
B	255	HIS	-	expression tag	UNP Q04HJ2
B	256	HIS	-	expression tag	UNP Q04HJ2
B	257	HIS	-	expression tag	UNP Q04HJ2
B	258	HIS	-	expression tag	UNP Q04HJ2
B	259	HIS	-	expression tag	UNP Q04HJ2
B	260	HIS	-	expression tag	UNP Q04HJ2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total 42	O 42	0	0
2	B	44	Total 44	O 44	0	0



- Molecule 1: 3-oxoacyl-acyl carrier protein reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.59Å 84.21Å 87.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 38.95 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.1 (40.00-2.30) 94.1 (38.95-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.230 , 0.286 0.221 , 0.265	Depositor DCC
$R_{free}$ test set	727 reflections (3.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.2	EDS
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22490 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.40	0/1867	0.52	0/2523
1	B	0.37	0/1767	0.52	0/2389
All	All	0.39	0/3634	0.52	0/4912

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	96	THR	Peptide

### 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	A	1830	0	1824	6	0
1	B	1735	0	1735	7	0
2	A	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	0	0	0
All	All	3651	0	3559	13	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 2.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:VAL:HG13	1:B:98:GLY:H	1.58	0.69
1:A:35:ASN:HD22	1:A:62:LYS:HB2	1.74	0.52
1:B:15:ALA:HA	1:B:39:HIS:HB3	1.93	0.50
1:B:18:ILE:HG12	1:B:40:TYR:HB3	1.96	0.47
1:A:15:ALA:HA	1:A:39:HIS:HB3	1.96	0.47
1:B:18:ILE:HA	1:B:52:LEU:HD22	1.99	0.44
1:B:12:ILE:HG12	1:B:92:ILE:HB	2.00	0.42
1:A:41:HIS:HA	1:A:68:SER:O	2.20	0.41
1:A:164:ALA:HA	1:A:165:PRO:HD3	1.81	0.41
1:B:46:SER:O	1:B:50:ASN:ND2	2.54	0.41
1:A:12:ILE:HG12	1:A:92:ILE:HB	2.02	0.41
1:B:225:ALA:N	1:B:226:PRO:HD2	2.36	0.41
1:A:67:GLN:HE21	1:A:67:GLN:HB2	1.72	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	Percentiles	
1	A	229/262 (87%)	225 (98%)	4 (2%)	0	100	100
1	B	217/262 (83%)	211 (97%)	5 (2%)	1 (0%)	34	41
All	All	446/524 (85%)	436 (98%)	9 (2%)	1 (0%)	52	64



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	VAL

### 5.3.2 Protein sidechains ⓘ

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	194/216 (90%)	182 (94%)	12 (6%)	23	30
1	B	184/216 (85%)	177 (96%)	7 (4%)	40	54
All	All	378/432 (88%)	359 (95%)	19 (5%)	30	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	37	VAL
1	A	44	LYS
1	A	59	GLN
1	A	67	GLN
1	A	106	VAL
1	A	112	GLU
1	A	155	PHE
1	A	171	ARG
1	A	201	GLU
1	A	229	LYS
1	A	250	THR
1	B	59	GLN
1	B	67	GLN
1	B	84	GLU
1	B	86	GLU
1	B	178	MET
1	B	179	LYS
1	B	191	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	59	GLN
1	A	67	GLN
1	A	200	GLN
1	B	67	GLN
1	B	121	ASN
1	B	241	GLN

### 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	234/262 (89%)	0.39	14 (5%) 25 33	31, 51, 86, 109	0
1	B	223/262 (85%)	0.41	15 (6%) 21 29	32, 50, 93, 113	0
All	All	457/524 (87%)	0.40	29 (6%) 23 31	31, 50, 92, 113	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	PHE	7.2
1	B	155	PHE	6.6
1	B	156	TYR	6.4
1	B	157	SER	5.4
1	B	195	SER	4.7
1	B	216	ASN	4.5
1	B	99	LYS	4.5
1	B	158	THR	4.5
1	B	98	GLY	4.0
1	B	196	PHE	4.0
1	B	101	LEU	3.8
1	A	215	GLY	3.8
1	A	157	SER	3.6
1	A	158	THR	3.4
1	A	214	MET	3.3
1	A	6	ASP	3.2
1	B	3	LYS	2.8
1	B	100	VAL	2.8
1	B	249	TYR	2.7
1	B	152	TYR	2.7
1	A	98	GLY	2.6
1	B	5	HIS	2.4
1	A	153	THR	2.4
1	A	251	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	142	ILE	2.1
1	A	232	THR	2.1
1	A	154	GLY	2.1
1	A	220	LYS	2.1
1	A	195	SER	2.0

## 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.