



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 12:59 AM JST

PDB ID : 4YDR  
Title : Crystal structure of oxidized homoserine dehydrogenase of *Sulfolobus tokodaii*  
Authors : Goto, M.; Yoshimune, K.; Kaneko, R.  
Deposited on : 2015-02-23  
Resolution : 1.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

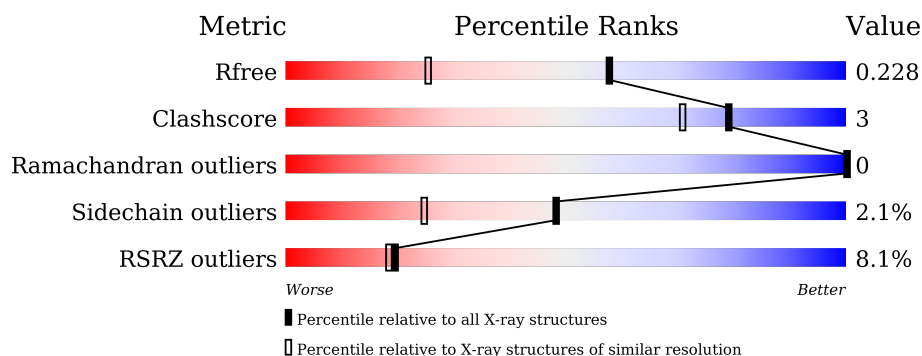
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	304	
1	B	304	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4979 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 Homoserine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2301	1473	387	435	6			
1	B	300	Total	C	N	O	S	0	0	0
			2275	1459	380	430	6			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

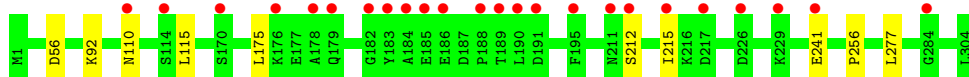
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	205	Total	O	0	0
			205	205		
3	B	197	Total	O	0	0
			197	197		

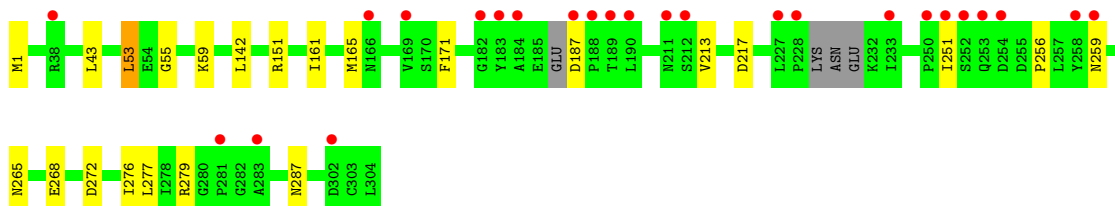
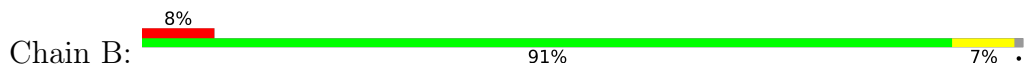
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Homoserine dehydrogenase



- Molecule 1: Homoserine dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.82Å 78.91Å 65.81Å 90.00° 105.79° 90.00°	Depositor
Resolution (Å)	28.50 – 1.60 28.50 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.50-1.60) 99.2 (28.50-1.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.01 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.197 , 0.228 0.197 , 0.228	Depositor DCC
$R_{free}$ test set	3747 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
NA

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	0.42	0/2338	0.64	1/3169 (0.0%)
1	B	0.41	0/2310	0.64	0/3127
All	All	0.41	0/4648	0.64	1/6296 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ASP	CB-CG-OD1	6.12	123.81	118.30

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	A	2301	0	2331	5	0
1	B	2275	0	2311	22	0
2	A	1	0	0	0	0
3	A	205	0	0	0	0
3	B	197	0	0	0	0
All	All	4979	0	4642	24	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.

All (24) 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:161:ILE:HG22	1:B:165:MET:HE3	1.54	0.87
1:B:161:ILE:HG22	1:B:165:MET:CE	2.10	0.80
1:B:165:MET:HE2	1:B:171:PHE:CD1	2.20	0.77
1:B:161:ILE:CG2	1:B:165:MET:HE3	2.17	0.73
1:B:165:MET:CE	1:B:171:PHE:HD1	2.11	0.64
1:B:161:ILE:CG2	1:B:165:MET:CE	2.77	0.60
1:B:213:VAL:HG23	1:B:217:ASP:HB2	1.83	0.59
1:B:165:MET:CE	1:B:171:PHE:CD1	2.85	0.58
1:B:151:ARG:HD3	1:B:268:GLU:OE1	2.03	0.57
1:A:277:LEU:HB3	1:B:279:ARG:CG	2.38	0.54
1:B:165:MET:HE2	1:B:171:PHE:HA	1.90	0.54
1:B:165:MET:HE2	1:B:171:PHE:HD1	1.65	0.53
1:A:277:LEU:HB3	1:B:279:ARG:HG3	1.92	0.52
1:B:43:LEU:CD1	1:B:53:LEU:HD11	2.41	0.50
1:B:142:LEU:HD11	1:B:276:ILE:HD11	1.93	0.50
1:A:256:PRO:HA	1:B:259:ASN:HD22	1.79	0.48
1:B:161:ILE:HG22	1:B:165:MET:HE1	1.93	0.46
1:B:55:GLY:HA3	1:B:59:LYS:HD3	1.96	0.46
1:A:92:LYS:HB3	1:A:92:LYS:HE2	1.73	0.44
1:B:256:PRO:HB2	1:B:277:LEU:HD13	2.00	0.43
1:B:213:VAL:CG2	1:B:217:ASP:HB2	2.47	0.43
1:A:110:ASN:HD21	1:A:212:SER:HB2	1.83	0.43
1:B:43:LEU:HD11	1:B:53:LEU:HD11	2.02	0.42
1:B:287:ASN:HD22	1:B:287:ASN:H	1.68	0.41

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	Percentiles	
1	A	302/304 (99%)	290 (96%)	12 (4%)	0	100	100
1	B	294/304 (97%)	286 (97%)	8 (3%)	0	100	100
All	All	596/608 (98%)	576 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	244/256 (95%)	240 (98%)	4 (2%)	58	37
1	B	242/256 (94%)	236 (98%)	6 (2%)	42	19
All	All	486/512 (95%)	476 (98%)	10 (2%)	48	25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	175	LEU
1	A	215	ILE
1	A	241	GLU
1	B	1	MET
1	B	53	LEU
1	B	187	ASP
1	B	251	ILE
1	B	265	ASN
1	B	272	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	110	ASN
1	A	265	ASN

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Mol	Chain	Res	Type
1	B	287	ASN

### 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 oligosaccharides in this entry.

### 5.6 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.

### 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	304/304 (100%)	0.36	24 (7%)	20 19	13, 21, 40, 49	0
1	B	300/304 (98%)	0.43	25 (8%)	19 18	14, 22, 39, 53	0
All	All	604/608 (99%)	0.40	49 (8%)	19 18	13, 22, 39, 53	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	GLY	6.5
1	A	188	PRO	5.7
1	B	251	ILE	5.0
1	A	184	ALA	4.6
1	B	252	SER	4.3
1	A	185	GLU	4.2
1	B	258	TYR	3.9
1	A	189	THR	3.7
1	B	187	ASP	3.7
1	A	178	ALA	3.7
1	B	228	PRO	3.6
1	B	253	GLN	3.4
1	B	259	ASN	3.4
1	A	170	SER	3.2
1	A	191	ASP	3.1
1	A	183	TYR	3.0
1	B	212	SER	2.8
1	A	179	GLN	2.8
1	B	190	LEU	2.8
1	A	186	GLU	2.7
1	A	226	ASP	2.7
1	B	283	ALA	2.7
1	A	110	ASN	2.6
1	B	227	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	184	ALA	2.6
1	A	190	LEU	2.5
1	B	281	PRO	2.5
1	B	302	ASP	2.5
1	B	250	PRO	2.5
1	A	212	SER	2.4
1	B	189	THR	2.4
1	B	211	ASN	2.4
1	B	182	GLY	2.3
1	A	114	SER	2.3
1	A	176	LYS	2.3
1	B	254	ASP	2.2
1	A	211	ASN	2.2
1	A	217	ASP	2.2
1	B	188	PRO	2.2
1	A	284	GLY	2.2
1	B	166	ASN	2.2
1	B	38	ARG	2.2
1	B	183	TYR	2.2
1	A	195	PHE	2.1
1	B	233	ILE	2.1
1	A	229	LYS	2.1
1	A	241	GLU	2.1
1	B	169	VAL	2.1
1	A	215	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NA	A	401	1/1	0.94	0.08	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.