



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6Y0S  
Title : X-ray structure of Lactobacillus brevis alcohol dehydrogenase mutant T102E  
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Deposited on : 2020-02-10  
Resolution : 1.44 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.

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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 : 2.13  
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) : 2.13

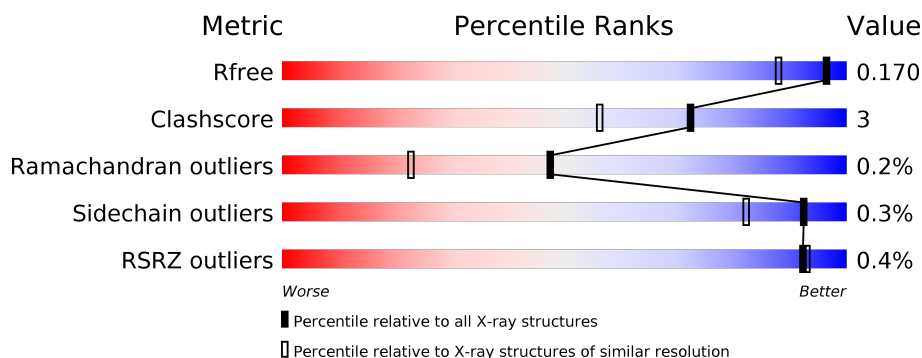
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.44 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))
$R_{free}$	130704	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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 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	AAA	262	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>87%</span> <span>8%</span> <span>• •</span> </div> </div>
1	BBB	262	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>89%</span> <span>6%</span> <span>•</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8656 atoms, of which 3918 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 R-specific alcohol dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	251	Total	C	H	N	O	S	92	17	0
			3994	1255	1989	337	402	11			
1	BBB	251	Total	C	H	N	O	S	86	10	0
			3881	1221	1929	328	392	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-10	MET	-	initiating methionine	UNP Q84EX5
AAA	-9	GLY	-	expression tag	UNP Q84EX5
AAA	-8	HIS	-	expression tag	UNP Q84EX5
AAA	-7	HIS	-	expression tag	UNP Q84EX5
AAA	-6	HIS	-	expression tag	UNP Q84EX5
AAA	-5	HIS	-	expression tag	UNP Q84EX5
AAA	-4	HIS	-	expression tag	UNP Q84EX5
AAA	-3	HIS	-	expression tag	UNP Q84EX5
AAA	-2	GLY	-	expression tag	UNP Q84EX5
AAA	-1	SER	-	expression tag	UNP Q84EX5
AAA	0	GLY	-	expression tag	UNP Q84EX5
AAA	102	GLU	THR	engineered mutation	UNP Q84EX5
BBB	-10	MET	-	initiating methionine	UNP Q84EX5
BBB	-9	GLY	-	expression tag	UNP Q84EX5
BBB	-8	HIS	-	expression tag	UNP Q84EX5
BBB	-7	HIS	-	expression tag	UNP Q84EX5
BBB	-6	HIS	-	expression tag	UNP Q84EX5
BBB	-5	HIS	-	expression tag	UNP Q84EX5
BBB	-4	HIS	-	expression tag	UNP Q84EX5
BBB	-3	HIS	-	expression tag	UNP Q84EX5
BBB	-2	GLY	-	expression tag	UNP Q84EX5
BBB	-1	SER	-	expression tag	UNP Q84EX5
BBB	0	GLY	-	expression tag	UNP Q84EX5
BBB	102	GLU	THR	engineered mutation	UNP Q84EX5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BBB	6	Total 6	Mg 6	0	0
2	AAA	3	Total 3	Mg 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	382	Total 382	O 382	0	0
3	BBB	390	Total 390	O 390	0	0

### 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: R-specific alcohol dehydrogenase



- Molecule 1: R-specific alcohol dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.62Å 81.15Å 115.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.07 – 1.44 47.07 – 1.44	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.07-1.44) 99.6 (47.07-1.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 1.44Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.130 , 0.168 0.131 , 0.170	Depositor DCC
$R_{free}$ test set	4748 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8656	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	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 64.63 % 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 8.0441e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

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

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	AAA	0.64	0/2046	0.68	0/2759
1	BBB	0.62	0/1986	0.69	0/2682
All	All	0.63	0/4032	0.69	0/5441

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	AAA	2005	1989	1978	16	0
1	BBB	1952	1929	1921	13	0
2	AAA	3	0	0	0	0
2	BBB	6	0	0	0	0
3	AAA	382	0	0	4	2
3	BBB	390	0	0	2	0
All	All	4738	3918	3899	27	2

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 (27) 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:BBB:124:GLY:O	1:BBB:128[B]:MET:HG2	1.51	1.08
1:AAA:141[A]:SER:O	3:AAA:401:HOH:O	1.87	0.92
1:AAA:218[A]:GLU:OE1	3:AAA:402:HOH:O	1.91	0.86
1:AAA:141[B]:SER:O	3:AAA:401:HOH:O	1.97	0.81
1:AAA:142:SER:OG	1:AAA:144[B]:GLU:OE2	2.02	0.77
1:AAA:124:GLY:O	1:AAA:128[B]:MET:HG2	1.97	0.64
1:AAA:28[A]:GLU:HG3	3:AAA:588:HOH:O	1.98	0.63
1:BBB:141[A]:SER:HB2	3:BBB:404:HOH:O	2.03	0.58
1:AAA:189[B]:TYR:CD2	1:AAA:205:MET:HB3	2.42	0.54
1:BBB:84:SER:O	1:BBB:135:ALA:HA	2.09	0.52
1:BBB:52:THR:OG1	1:BBB:54[A]:ASP:OD1	2.15	0.52
1:AAA:161:ALA:HB2	1:BBB:161:ALA:HB2	1.93	0.50
1:AAA:67:ASP:O	1:AAA:70[B]:THR:HG22	2.12	0.49
1:AAA:84:SER:O	1:AAA:135:ALA:HA	2.15	0.47
1:AAA:141[B]:SER:O	1:AAA:142:SER:CB	2.62	0.47
1:AAA:33:VAL:O	1:AAA:56:ILE:HA	2.15	0.46
1:AAA:52:THR:OG1	1:AAA:54[A]:ASP:OD1	2.16	0.46
1:BBB:33:VAL:O	1:BBB:56:ILE:HA	2.16	0.45
1:BBB:43:GLY:HA3	1:BBB:58:PHE:CE1	2.51	0.45
1:AAA:141[A]:SER:HB3	1:AAA:186:HIS:CE1	2.52	0.44
1:AAA:156:ASN:OD1	1:BBB:168:SER:HB2	2.17	0.44
1:AAA:12:THR:HA	1:AAA:36:THR:OG1	2.18	0.43
1:BBB:124:GLY:O	1:BBB:128[B]:MET:CG	2.42	0.43
1:BBB:218[B]:GLU:OE2	3:BBB:401:HOH:O	2.15	0.43
1:BBB:12:THR:HA	1:BBB:36:THR:OG1	2.18	0.42
1:BBB:43:GLY:HA3	1:BBB:58:PHE:CD1	2.55	0.41
1:BBB:141[A]:SER:HB3	1:BBB:186:HIS:CE1	2.56	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AAA:438:HOH:O	3:AAA:438:HOH:O[2_555]	1.69	0.51
3:AAA:497:HOH:O	3:AAA:497:HOH:O[2_555]	1.74	0.46



## 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	AAA	266/262 (102%)	259 (97%)	6 (2%)	1 (0%)	34	13
1	BBB	259/262 (99%)	253 (98%)	6 (2%)	0	100	100
All	All	525/524 (100%)	512 (98%)	12 (2%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	142	SER

### 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	AAA	215/206 (104%)	213 (99%)	2 (1%)	78	54
1	BBB	208/206 (101%)	208 (100%)	0	100	100
All	All	423/412 (103%)	421 (100%)	2 (0%)	92	74

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	218[A]	GLU
1	AAA	218[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are 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 [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<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	AAA	251/262 (95%)	-0.71	2 (0%) 86 86	10, 14, 23, 42	2 (0%)
1	BBB	251/262 (95%)	-0.71	0 100 100	10, 15, 24, 39	3 (1%)
All	All	502/524 (95%)	-0.71	2 (0%) 92 93	10, 14, 24, 42	5 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	199	PRO	2.3
1	AAA	198	LEU	2.1

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

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(Å <sup>2</sup> )	Q<0.9
2	MG	BBB	301	1/1	0.81	0.13	66,66,66,66	0
2	MG	BBB	303	1/1	0.89	0.11	49,49,49,49	0
2	MG	AAA	301	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	BBB	304	1/1	0.95	0.09	57,57,57,57	0
2	MG	AAA	302	1/1	0.97	0.13	43,43,43,43	0
2	MG	AAA	303	1/1	0.99	0.04	27,27,27,27	0
2	MG	BBB	302	1/1	0.99	0.09	36,36,36,36	0
2	MG	BBB	306	1/1	1.00	0.07	12,12,12,12	0
2	MG	BBB	305	1/1	1.00	0.03	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.