



# wwPDB X-ray Structure Validation Summary Report

Aug 11, 2014 – 11:28 PM EDT

PDB ID : 3P14  
Title : Crystal structure of L-rhamnose isomerase with a novel high thermo-stability from *Bacillus halodurans*  
Authors : Doan, T.T.N.; Prabhu, P.; Kang, L.W.; Lee, J.K.  
Deposited on : 2010-09-30  
Resolution : 2.51 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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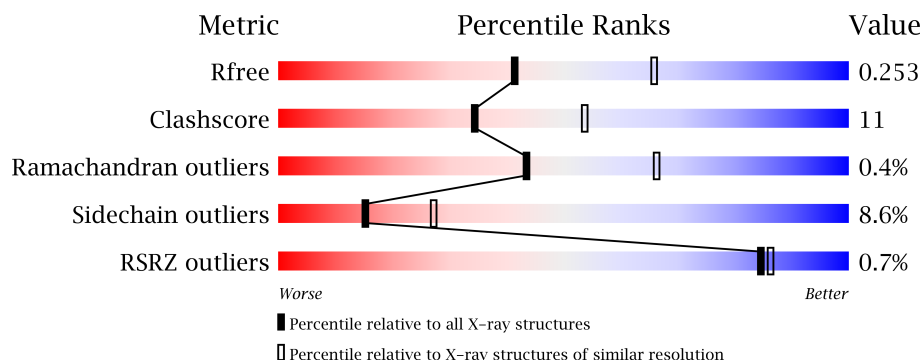
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.51 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	424	
1	B	424	
1	C	424	
1	D	424	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13611 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-rhamnose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3290	2109	566	606	9			
1	B	403	Total	C	N	O	S	0	0	0
			3298	2114	567	607	10			
1	C	402	Total	C	N	O	S	0	0	0
			3294	2112	566	606	10			
1	D	401	Total	C	N	O	S	0	0	0
			3278	2103	561	604	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
A	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
B	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
C	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-5	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-4	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-3	HIS	-	EXPRESSION TAG	UNP Q9KCL9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	-1	HIS	-	EXPRESSION TAG	UNP Q9KCL9
D	0	HIS	-	EXPRESSION TAG	UNP Q9KCL9

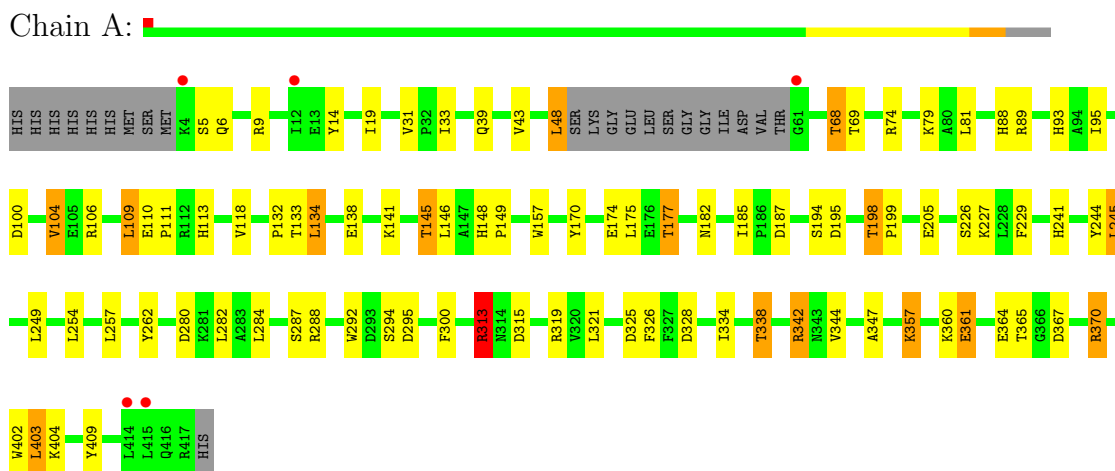
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total 114	O 114	0	0
2	B	114	Total 114	O 114	0	0
2	C	119	Total 119	O 119	0	0
2	D	104	Total 104	O 104	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

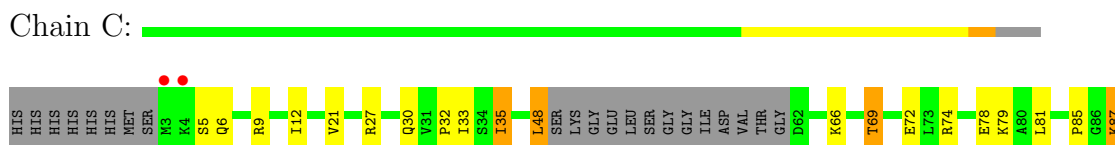
#### • Molecule 1: L-rhamnose isomerase



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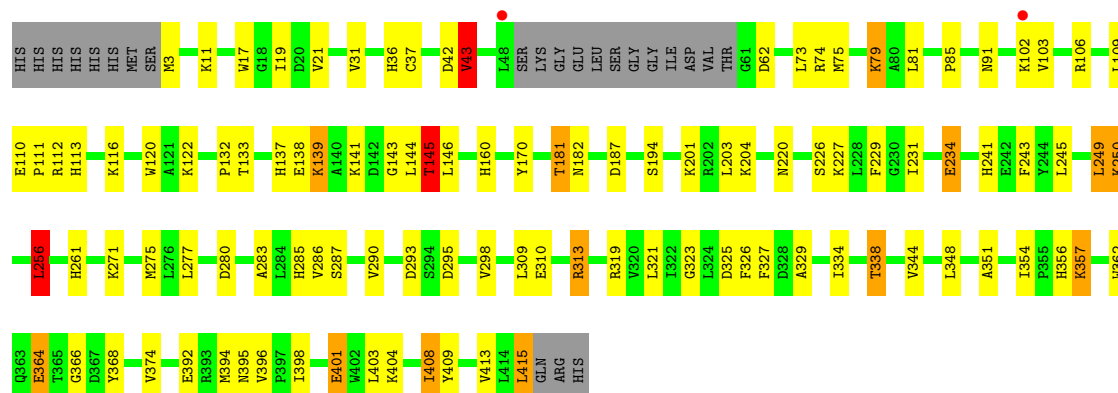
#### • Molecule 1: L-rhamnose isomerase





• Molecule 1: L-rhamnose isomerase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.24Å 164.88Å 92.01Å 90.00° 115.97° 90.00°	Depositor
Resolution (Å)	45.78 – 2.51 45.78 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.78-2.51) 97.7 (45.78-2.51)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.185 , 0.256 0.186 , 0.253	Depositor DCC
$R_{free}$ test set	3751 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.4	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 18.3	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 74739 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13611	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.91	1/3371 (0.0%)	0.90	5/4564 (0.1%)
1	B	0.90	1/3379 (0.0%)	0.91	13/4574 (0.3%)
1	C	0.93	3/3375 (0.1%)	0.89	1/4569 (0.0%)
1	D	0.90	0/3359	0.90	7/4548 (0.2%)
All	All	0.91	5/13484 (0.0%)	0.90	26/18255 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	392	GLU	CG-CD	9.23	1.65	1.51
1	C	255	CYS	CB-SG	-5.53	1.72	1.81
1	C	392	GLU	CB-CG	5.37	1.62	1.52
1	B	71	GLU	CG-CD	5.24	1.59	1.51
1	A	205	GLU	CG-CD	5.07	1.59	1.51

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	256	LEU	CA-CB-CG	7.60	132.79	115.30
1	B	202	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	C	282	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	B	415	LEU	CA-CB-CG	6.71	130.72	115.30
1	B	403	LEU	CA-CB-CG	6.59	130.47	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,



and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3290	0	3244	66	0
1	B	3298	0	3253	71	0
1	C	3294	0	3250	80	0
1	D	3278	0	3232	72	0
2	A	114	0	0	2	0
2	B	114	0	0	1	0
2	C	119	0	0	2	0
2	D	104	0	0	2	0
All	All	13611	0	12979	281	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 281 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:TYR:HB3	1:A:19:ILE:CD1	1.62	1.27
1:A:14:TYR:CB	1:A:19:ILE:HD11	1.64	1.26
1:B:145:THR:HG22	1:B:146:LEU:H	1.11	1.14
1:A:145:THR:HG22	1:A:146:LEU:H	1.13	1.08
1:C:99:THR:HG21	1:C:102:LYS:O	1.51	1.08

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	398/424 (94%)	382 (96%)	15 (4%)	1 (0%)	50 73
1	B	399/424 (94%)	379 (95%)	19 (5%)	1 (0%)	50 73
1	C	398/424 (94%)	380 (96%)	17 (4%)	1 (0%)	50 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	397/424 (94%)	373 (94%)	20 (5%)	4 (1%)	22	38
All	All	1592/1696 (94%)	1514 (95%)	71 (4%)	7 (0%)	43	66

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	293	ASP
1	D	112	ARG
1	D	43	VAL
1	D	145	THR
1	C	138	GLU

### 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	351/370 (95%)	324 (92%)	27 (8%)	18	33
1	B	352/370 (95%)	325 (92%)	27 (8%)	18	33
1	C	352/370 (95%)	319 (91%)	33 (9%)	13	23
1	D	350/370 (95%)	316 (90%)	34 (10%)	12	21
All	All	1405/1480 (95%)	1284 (91%)	121 (9%)	15	27

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	5	SER
1	C	103	VAL
1	D	338	THR
1	C	21	VAL
1	C	69	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	388	ASN
1	C	131	ASN
1	D	241	HIS
1	C	39	GLN
1	C	160	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

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	402/424 (94%)	-0.28	5 (1%) 75 77	17, 30, 45, 66	0
1	B	403/424 (95%)	-0.36	3 (0%) 84 86	17, 30, 50, 85	0
1	C	402/424 (94%)	-0.33	2 (0%) 88 90	19, 30, 45, 81	0
1	D	401/424 (94%)	-0.29	2 (0%) 88 90	18, 31, 50, 71	0
All	All	1608/1696 (94%)	-0.31	12 (0%) 84 86	17, 30, 48, 85	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	LYS	4.3
1	B	3	MET	4.2
1	A	4	LYS	3.6
1	B	415	LEU	3.3
1	A	61	GLY	3.3

### 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 carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.