

wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2024 – 01:55 PM EST

PDB ID : 3UU0

Title : Crystal structure of L-rhamnose isomerase from Bacillus halodurans in com-

plex with Mn

Authors: Doan, T.T.N.; Prabhu, P.; Kim, J.K.; Jeya, M.; Kang, L.W.; Lee, J.K.

Deposited on : 2011-11-27

Resolution : 2.70 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

Phenix) : 1.13 EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

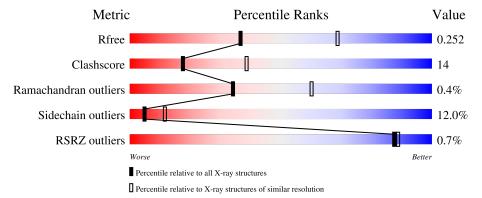
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.70 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\mathring{A}))$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 >=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	424	67%	22%	5% 5%			
1	В	424	70%	20%	• 5%			
1	С	424	69%	21%	5% 5%			
1	D	424	62%	28%	• 5%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13491 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 L-rhamnose isomerase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	401	Total	С	N	О	S	0	0	0
1	A	401	3286	2107	565	605	9	0	U	0
1	В	402	Total	С	N	О	S	0	0	0
1	Ъ	402	3290	2109	566	606	9	0	0	0
1	С	403	Total	С	N	О	S	0	0	0
1		405	3296	2112	567	608	9	0	0	0
1	D	404	Total	С	N	О	S	0	0	0
1	D	404	3304	2117	568	609	10	U	U	U

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
В	-5	HIS	-	expression tag	UNP Q9KCL9
В	-4	HIS	-	expression tag	UNP Q9KCL9
В	-3	HIS	-	expression tag	UNP Q9KCL9
В	-2	HIS	-	expression tag	UNP Q9KCL9
В	-1	HIS	-	expression tag	UNP Q9KCL9
В	0	HIS	-	expression tag	UNP Q9KCL9
С	-5	HIS	-	expression tag	UNP Q9KCL9
С	-4	HIS	-	expression tag	UNP Q9KCL9
С	-3	HIS	-	expression tag	UNP Q9KCL9
С	-2	HIS	-	expression tag	UNP Q9KCL9
С	-1	HIS	-	expression tag	UNP Q9KCL9
С	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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	В	2	Total Mn 2 2	0	0
2	С	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

• Molecule 3 is water.

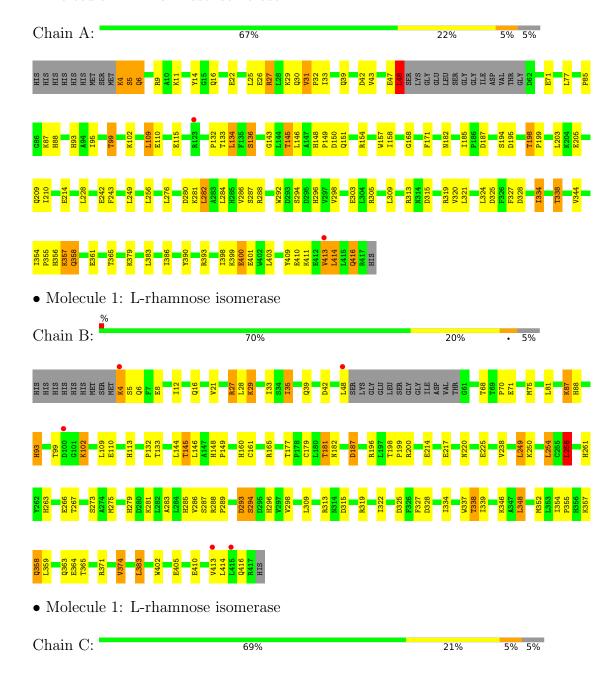
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	78	Total O 78 78	0	0
3	В	83	Total O 83 83	0	0
3	С	73	Total O 73 73	0	0
3	D	73	Total O 73 73	0	0



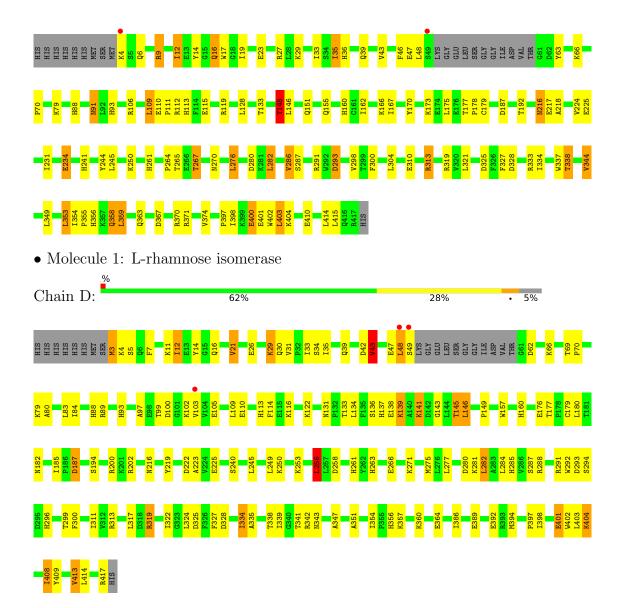
3 Residue-property plots (i)

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: L-rhamnose isomerase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	83.58Å 165.55Å 92.47Å	Denogitor
a, b, c, α , β , γ	90.00° 115.82° 90.00°	Depositor
Resolution (Å)	46.62 - 2.70	Depositor
rtesolution (A)	46.62 - 2.70	EDS
% Data completeness	96.0 (46.62-2.70)	Depositor
(in resolution range)	96.0 (46.62-2.70)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.29 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
Ρ. Р.	0.180 , 0.255	Depositor
R, R_{free}	0.183 , 0.252	DCC
R_{free} test set	3022 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 40.1	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13491	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MN

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).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.88	1/3367~(0.0%)	0.87	4/4559 (0.1%)	
1	В	0.91	$1/3371 \ (0.0\%)$	0.89	4/4564 (0.1%)	
1	С	0.88	$2/3377 \ (0.1\%)$	0.88	$2/4572 \ (0.0\%)$	
1	D	0.87	1/3385~(0.0%)	0.88	$4/4582 \ (0.1\%)$	
All	All	0.89	5/13500~(0.0%)	0.88	14/18277 (0.1%)	

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	225	GLU	CD-OE1	-5.71	1.19	1.25
1	С	63	TYR	CE2-CZ	-5.52	1.31	1.38
1	С	63	TYR	CD2-CE2	-5.44	1.31	1.39
1	D	225	GLU	CD-OE1	-5.41	1.19	1.25
1	A	214	GLU	CG-CD	5.33	1.59	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	293	ASP	CB-CG-OD2	7.62	125.16	118.30
1	В	293	ASP	CB-CG-OD1	7.29	124.86	118.30
1	D	256	LEU	CA-CB-CG	6.39	130.01	115.30
1	В	254	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	48	LEU	CA-CB-CG	5.92	128.92	115.30

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	3286	0	3241	90	0
1	В	3290	0	3244	84	0
1	С	3296	0	3249	83	0
1	D	3304	0	3258	112	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
3	A	78	0	0	1	0
3	В	83	0	0	2	0
3	С	73	0	0	0	0
3	D	73	0	0	5	0
All	All	13491	0	12992	359	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 14.

The worst 5 of 359 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:D:48:LEU:HD22	1:D:49:SER:N	1.53	1.19	
1:D:145:THR:CG2	1:D:146:LEU:H	1.60	1.13	
1:D:48:LEU:HG	1:D:103:VAL:HG12	1.24	1.12	
1:B:145:THR:HG22	1:B:146:LEU:H	1.00	1.11	
1:C:286:VAL:HG23	1:C:298:VAL:HG21	1.33	1.09	

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	ntiles
1	A	397/424 (94%)	377 (95%)	19 (5%)	1 (0%)	41	66
1	В	398/424 (94%)	368 (92%)	30 (8%)	0	100	100
1	C	399/424 (94%)	379 (95%)	18 (4%)	2 (0%)	29	54
1	D	400/424 (94%)	373 (93%)	24 (6%)	3 (1%)	19	43
All	All	1594/1696 (94%)	1497 (94%)	91 (6%)	6 (0%)	34	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	300	PHE
1	С	145	THR
1	A	136	SER
1	D	136	SER
1	D	291	ARG

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	P	erc	entiles
1	A	351/370 (95%)	308 (88%)	43 (12%)		4	11
1	В	351/370~(95%)	309 (88%)	42 (12%)		5	11
1	\mathbf{C}	352/370~(95%)	313 (89%)	39 (11%)		6	14
1	D	353/370 (95%)	308 (87%)	45 (13%)		4	10
All	All	1407/1480 (95%)	1238 (88%)	169 (12%)		5	11

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	321	LEU
1	D	139	LYS
1	С	358	GLN

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Mol	Chain	Res	Type
1	D	31	VAL
1	D	187	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	160	HIS
1	D	30	GLN
1	С	216	ASN
1	С	358	GLN
1	D	113	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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^{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></rsrz>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	401/424 (94%)	-0.36	2 (0%) 91 92	16, 30, 45, 80	0
1	В	402/424 (94%)	-0.27	5 (1%) 79 80	16, 30, 50, 78	0
1	С	403/424 (95%)	-0.32	2 (0%) 91 92	19, 31, 45, 66	0
1	D	404/424 (95%)	-0.28	3 (0%) 87 89	19, 32, 54, 83	0
All	All	1610/1696 (94%)	-0.31	12 (0%) 87 89	16, 31, 50, 83	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	SER	5.7
1	В	4	LYS	3.6
1	С	4	LYS	3.3
1	С	49	SER	3.1
1	D	103	VAL	3.0

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 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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MN	С	419	1/1	0.75	0.15	44,44,44,44	0
2	MN	С	420	1/1	0.82	0.12	53,53,53,53	0
2	MN	A	420	1/1	0.83	0.16	51,51,51,51	0
2	MN	В	419	1/1	0.84	0.15	37,37,37,37	0
2	MN	D	420	1/1	0.91	0.16	55,55,55,55	0
2	MN	В	420	1/1	0.93	0.25	63,63,63,63	0
2	MN	A	419	1/1	0.96	0.12	45,45,45,45	0
2	MN	D	419	1/1	0.97	0.11	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.

