



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:21 PM GMT

PDB ID : 1D8W  
Title : L-RHAMNOSE ISOMERASE  
Authors : Korndorfer, I.P.; Matthews, B.W.  
Deposited on : 1999-10-26  
Resolution : 1.60 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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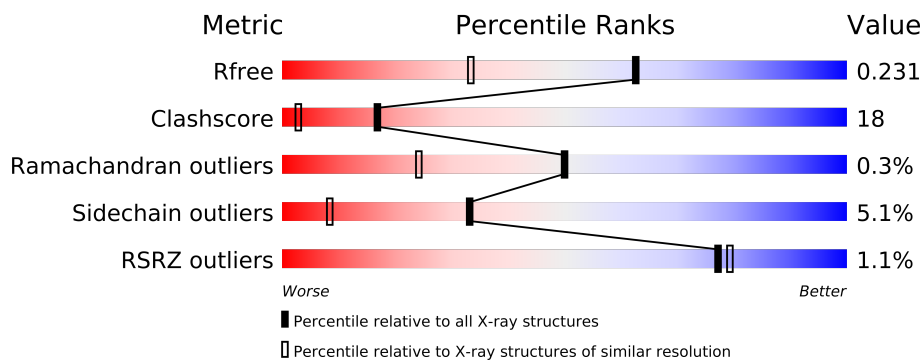
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (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 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	426	
1	B	426	
1	C	426	
1	D	426	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14687 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	Se	0	0	0
			3219	2037	571	598	5	8			
1	B	402	Total	C	N	O	S	Se	0	0	0
			3218	2037	570	598	5	8			
1	C	401	Total	C	N	O	S	Se	0	0	0
			3211	2033	569	596	5	8			
1	D	403	Total	C	N	O	S	Se	0	0	0
			3226	2042	571	599	5	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	45	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	91	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	190	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	198	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	254	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	285	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	353	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	398	MSE	MET	MODIFIED RESIDUE	UNP P32170
A	2	GLY	-	RECOMBINANT HIS TAG	UNP P32170
A	3	HIS	-	RECOMBINANT HIS TAG	UNP P32170
A	4	HIS	-	RECOMBINANT HIS TAG	UNP P32170
A	5	HIS	-	RECOMBINANT HIS TAG	UNP P32170
A	6	HIS	-	RECOMBINANT HIS TAG	UNP P32170
A	7	HIS	-	RECOMBINANT HIS TAG	UNP P32170
A	8	HIS	-	RECOMBINANT HIS TAG	UNP P32170
B	9	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	45	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	91	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	190	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	198	MSE	MET	MODIFIED RESIDUE	UNP P32170

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Chain	Residue	Modelled	Actual	Comment	Reference
B	254	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	285	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	353	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	398	MSE	MET	MODIFIED RESIDUE	UNP P32170
B	2	GLY	-	RECOMBINANT HIS TAG	UNP P32170
B	3	HIS	-	RECOMBINANT HIS TAG	UNP P32170
B	4	HIS	-	RECOMBINANT HIS TAG	UNP P32170
B	5	HIS	-	RECOMBINANT HIS TAG	UNP P32170
B	6	HIS	-	RECOMBINANT HIS TAG	UNP P32170
B	7	HIS	-	RECOMBINANT HIS TAG	UNP P32170
B	8	HIS	-	RECOMBINANT HIS TAG	UNP P32170
C	9	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	45	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	91	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	190	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	198	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	254	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	285	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	353	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	398	MSE	MET	MODIFIED RESIDUE	UNP P32170
C	2	GLY	-	RECOMBINANT HIS TAG	UNP P32170
C	3	HIS	-	RECOMBINANT HIS TAG	UNP P32170
C	4	HIS	-	RECOMBINANT HIS TAG	UNP P32170
C	5	HIS	-	RECOMBINANT HIS TAG	UNP P32170
C	6	HIS	-	RECOMBINANT HIS TAG	UNP P32170
C	7	HIS	-	RECOMBINANT HIS TAG	UNP P32170
C	8	HIS	-	RECOMBINANT HIS TAG	UNP P32170
D	9	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	45	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	91	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	190	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	198	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	254	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	285	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	353	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	398	MSE	MET	MODIFIED RESIDUE	UNP P32170
D	2	GLY	-	RECOMBINANT HIS TAG	UNP P32170
D	3	HIS	-	RECOMBINANT HIS TAG	UNP P32170
D	4	HIS	-	RECOMBINANT HIS TAG	UNP P32170
D	5	HIS	-	RECOMBINANT HIS TAG	UNP P32170
D	6	HIS	-	RECOMBINANT HIS TAG	UNP P32170
D	7	HIS	-	RECOMBINANT HIS TAG	UNP P32170

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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	HIS	-	RECOMBINANT HIS TAG	UNP P32170

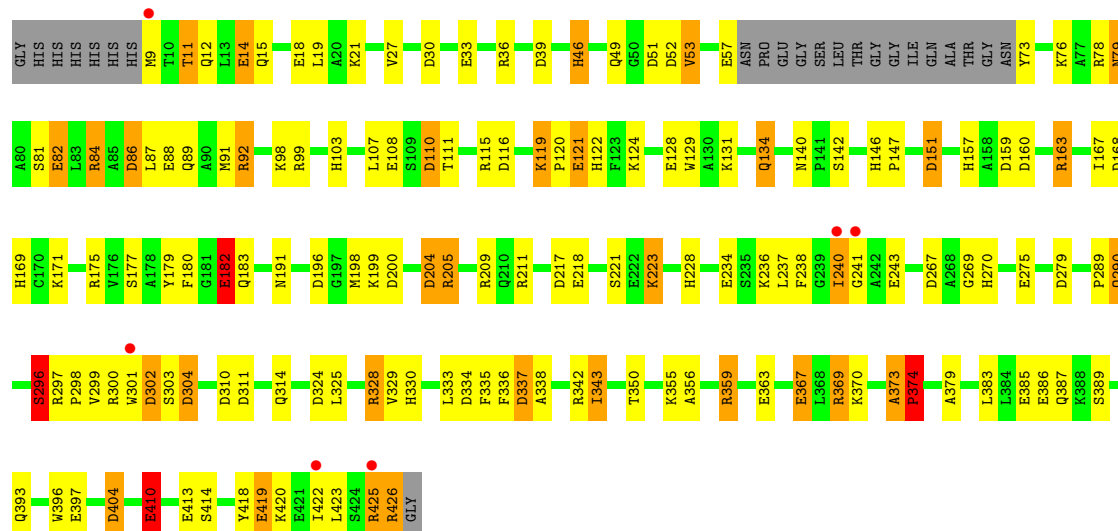
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	424	Total O 424 424	0	0
3	B	518	Total O 518 518	0	0
3	C	475	Total O 475 475	0	0
3	D	392	Total O 392 392	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.85Å 163.10Å 78.15Å 90.00° 110.32° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 28.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-1.60) 96.5 (28.81-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.174 , 0.241 0.173 , 0.231	Depositor DCC
$R_{free}$ test set	12796 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 87.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 252170 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14687	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 4.19% 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

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

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	1.12	22/3289 (0.7%)	1.65	67/4451 (1.5%)
1	B	1.16	24/3288 (0.7%)	1.71	62/4450 (1.4%)
1	C	1.15	22/3281 (0.7%)	1.78	64/4440 (1.4%)
1	D	1.09	19/3296 (0.6%)	1.67	72/4460 (1.6%)
All	All	1.13	87/13154 (0.7%)	1.70	265/17801 (1.5%)

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	GLU	CD-OE2	9.35	1.35	1.25
1	C	359	ARG	CZ-NH1	8.74	1.44	1.33
1	B	218	GLU	CD-OE2	7.99	1.34	1.25
1	B	385	GLU	CD-OE2	7.88	1.34	1.25
1	B	413	GLU	CD-OE2	7.84	1.34	1.25

The worst 5 of 265 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	ARG	NE-CZ-NH2	-33.88	103.36	120.30
1	B	328	ARG	NE-CZ-NH1	27.62	134.11	120.30
1	C	359	ARG	NE-CZ-NH1	26.19	133.40	120.30
1	D	205	ARG	NE-CZ-NH1	26.08	133.34	120.30
1	C	328	ARG	NE-CZ-NH1	24.38	132.49	120.30

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	3219	0	3145	135	0
1	B	3218	0	3146	102	0
1	C	3211	0	3139	129	0
1	D	3226	0	3155	120	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	424	0	0	16	0
3	B	518	0	0	24	0
3	C	475	0	0	26	2
3	D	392	0	0	20	0
All	All	14687	0	12585	452	2

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 18.

The worst 5 of 452 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:10:THR:HG22	1:B:15:GLN:HG3	1.23	1.19
1:B:10:THR:HG23	1:B:14:GLU:HB3	1.35	1.08
1:A:22:GLN:NE2	1:D:12:GLN:HE22	1.50	1.08
1:C:11:THR:HG23	1:C:15:GLN:HE21	1.21	1.04
1:A:142:SER:H	1:A:169:HIS:HE1	1.02	1.00

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	Distance(Å)	Clash(Å)
3:C:660:HOH:O	3:C:660:HOH:O[2_556]	0.96	1.24
3:C:934:HOH:O	3:C:934:HOH:O[2_556]	2.06	0.14

## 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	398/426 (93%)	379 (95%)	17 (4%)	2 (0%)	38	13
1	B	398/426 (93%)	385 (97%)	13 (3%)	0	100	100
1	C	397/426 (93%)	382 (96%)	14 (4%)	1 (0%)	50	24
1	D	399/426 (94%)	388 (97%)	10 (2%)	1 (0%)	50	24
All	All	1592/1704 (93%)	1534 (96%)	54 (3%)	4 (0%)	50	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	LEU
1	A	73	TYR
1	C	53	VAL
1	D	53	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	342/350 (98%)	327 (96%)	15 (4%)	39	12
1	B	342/350 (98%)	326 (95%)	16 (5%)	36	10
1	C	341/350 (97%)	326 (96%)	15 (4%)	39	12
1	D	343/350 (98%)	319 (93%)	24 (7%)	21	4
All	All	1368/1400 (98%)	1298 (95%)	70 (5%)	33	8

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	11	THR
1	C	128	GLU
1	D	369	ARG
1	C	27	VAL
1	C	81	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	ASN
1	C	15	GLN
1	D	140	ASN
1	B	169	HIS
1	B	314	GLN

### 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 ⓘ

Of 4 ligands modelled in this entry, 4 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.

## 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	402/426 (94%)	-0.39	5 (1%) 75 76	12, 21, 47, 96	0
1	B	402/426 (94%)	-0.50	3 (0%) 84 87	12, 19, 42, 62	0
1	C	401/426 (94%)	-0.48	3 (0%) 84 87	11, 20, 45, 69	0
1	D	403/426 (94%)	-0.35	6 (1%) 70 71	14, 22, 49, 87	0
All	All	1608/1704 (94%)	-0.43	17 (1%) 77 79	11, 21, 47, 96	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	ARG	3.3
1	D	301	TRP	2.9
1	A	422	ILE	2.8
1	D	425	ARG	2.7
1	A	72	ASN	2.7

### 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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	450	1/1	0.06	-0.91	40,40,40,40	1
2	ZN	B	450	1/1	0.04	-1.33	26,26,26,26	1
2	ZN	D	450	1/1	0.05	-1.46	39,39,39,39	1
2	ZN	A	450	1/1	0.05	-1.49	31,31,31,31	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.