



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:33 AM GMT

PDB ID : 3ITX  
Title : Mn<sup>2+</sup> bound form of Pseudomonas stutzeri L-rhamnose isomerase  
Authors : Yoshida, H.; Yamaji, M.; Ishii, T.; Izumori, K.; Kamitori, S.  
Deposited on : 2009-08-28  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

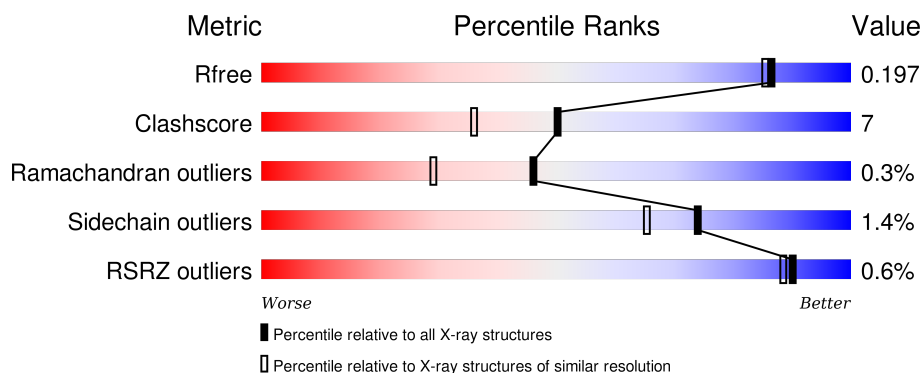
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	438	<div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	B	438	<div> <div>%</div> <div>81%</div> <div>13%</div> <div>5%</div> </div>
1	C	438	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>5%</div> </div>
1	D	438	<div> <div>%</div> <div>80%</div> <div>15%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	D	508	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14758 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	A	420	Total	C	N	O	S	0	0	0
			3255	2045	583	618	9			
1	B	418	Total	C	N	O	S	0	0	0
			3242	2037	581	615	9			
1	C	418	Total	C	N	O	S	0	0	0
			3242	2037	581	615	9			
1	D	418	Total	C	N	O	S	0	0	0
			3242	2037	581	615	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	ASN	ASP	ENGINEERED	UNP Q75WH8
A	431	GLY	-	EXPRESSION TAG	UNP Q75WH8
A	432	SER	-	EXPRESSION TAG	UNP Q75WH8
A	433	HIS	-	EXPRESSION TAG	UNP Q75WH8
A	434	HIS	-	EXPRESSION TAG	UNP Q75WH8
A	435	HIS	-	EXPRESSION TAG	UNP Q75WH8
A	436	HIS	-	EXPRESSION TAG	UNP Q75WH8
A	437	HIS	-	EXPRESSION TAG	UNP Q75WH8
A	438	HIS	-	EXPRESSION TAG	UNP Q75WH8
B	150	ASN	ASP	ENGINEERED	UNP Q75WH8
B	431	GLY	-	EXPRESSION TAG	UNP Q75WH8
B	432	SER	-	EXPRESSION TAG	UNP Q75WH8
B	433	HIS	-	EXPRESSION TAG	UNP Q75WH8
B	434	HIS	-	EXPRESSION TAG	UNP Q75WH8
B	435	HIS	-	EXPRESSION TAG	UNP Q75WH8
B	436	HIS	-	EXPRESSION TAG	UNP Q75WH8
B	437	HIS	-	EXPRESSION TAG	UNP Q75WH8
B	438	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	150	ASN	ASP	ENGINEERED	UNP Q75WH8
C	431	GLY	-	EXPRESSION TAG	UNP Q75WH8
C	432	SER	-	EXPRESSION TAG	UNP Q75WH8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	433	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	434	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	435	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	436	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	437	HIS	-	EXPRESSION TAG	UNP Q75WH8
C	438	HIS	-	EXPRESSION TAG	UNP Q75WH8
D	150	ASN	ASP	ENGINEERED	UNP Q75WH8
D	431	GLY	-	EXPRESSION TAG	UNP Q75WH8
D	432	SER	-	EXPRESSION TAG	UNP Q75WH8
D	433	HIS	-	EXPRESSION TAG	UNP Q75WH8
D	434	HIS	-	EXPRESSION TAG	UNP Q75WH8
D	435	HIS	-	EXPRESSION TAG	UNP Q75WH8
D	436	HIS	-	EXPRESSION TAG	UNP Q75WH8
D	437	HIS	-	EXPRESSION TAG	UNP Q75WH8
D	438	HIS	-	EXPRESSION TAG	UNP Q75WH8

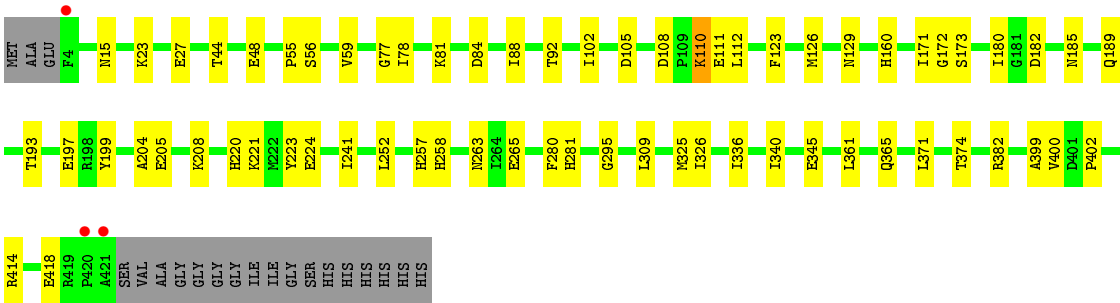
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	499	Total O 499 499	0	0
3	B	420	Total O 420 420	0	0
3	C	403	Total O 403 403	0	0
3	D	447	Total O 447 447	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.65Å 105.11Å 102.53Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	43.36 – 1.80 43.35 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (43.36-1.80) 96.6 (43.35-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.91 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.165 , 0.197 0.165 , 0.197	Depositor DCC
$R_{free}$ test set	14487 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 145217 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/3327	0.55	0/4511
1	B	0.29	0/3314	0.54	0/4493
1	C	0.29	0/3314	0.52	0/4493
1	D	0.30	0/3314	0.53	0/4493
All	All	0.29	0/13269	0.54	0/17990

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 [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	3255	0	3160	35	0
1	B	3242	0	3146	45	0
1	C	3242	0	3146	37	0
1	D	3242	0	3146	62	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	499	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	420	0	0	3	0
3	C	403	0	0	2	0
3	D	447	0	0	1	0
All	All	14758	0	12598	179	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 7.

The worst 5 of 179 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:D:78:ILE:HD12	1:D:105:ASP:HB3	1.45	0.95
1:A:129:ASN:H	1:A:160:HIS:HE1	1.13	0.90
1:C:129:ASN:H	1:C:160:HIS:HE1	1.20	0.89
1:B:40:ILE:HD11	1:B:388:ILE:HG12	1.56	0.88
1:B:129:ASN:H	1:B:160:HIS:HE1	1.16	0.87

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	418/438 (95%)	407 (97%)	10 (2%)	1 (0%)	52	35
1	B	416/438 (95%)	402 (97%)	12 (3%)	2 (0%)	34	17
1	C	416/438 (95%)	406 (98%)	9 (2%)	1 (0%)	52	35
1	D	416/438 (95%)	406 (98%)	9 (2%)	1 (0%)	52	35
All	All	1666/1752 (95%)	1621 (97%)	40 (2%)	5 (0%)	46	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	317	VAL
1	A	224	GLU
1	B	224	GLU
1	C	224	GLU
1	D	224	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	330/341 (97%)	327 (99%)	3 (1%)	84	80
1	B	328/341 (96%)	320 (98%)	8 (2%)	57	41
1	C	328/341 (96%)	324 (99%)	4 (1%)	78	71
1	D	328/341 (96%)	324 (99%)	4 (1%)	78	71
All	All	1314/1364 (96%)	1295 (99%)	19 (1%)	74	65

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	318	LYS
1	B	374	THR
1	D	110	LYS
1	B	283	ASN
1	D	325	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	352	GLN
1	C	139	HIS
1	D	189	GLN
1	C	8	GLN
1	C	97	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 carbohydrates 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<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	420/438 (95%)	-0.53	1 (0%) 95 93	4, 10, 21, 34	0
1	B	418/438 (95%)	-0.42	3 (0%) 89 87	5, 12, 24, 44	0
1	C	418/438 (95%)	-0.31	3 (0%) 89 87	5, 14, 28, 42	0
1	D	418/438 (95%)	-0.38	3 (0%) 89 87	5, 11, 25, 40	0
All	All	1674/1752 (95%)	-0.41	10 (0%) 90 88	4, 11, 25, 44	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	GLY	3.8
1	D	4	PHE	3.8
1	C	4	PHE	3.2
1	D	420	PRO	3.0
1	B	317	VAL	2.4

### 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	D	508	1/1	1.00	0.12	2.52	30,30,30,30	0
2	MN	A	502	1/1	0.98	0.09	1.35	30,30,30,30	0
2	MN	C	506	1/1	0.98	0.10	1.02	30,30,30,30	0
2	MN	B	504	1/1	0.99	0.08	-0.98	26,26,26,26	0
2	MN	A	501	1/1	0.98	0.06	-1.82	14,14,14,14	0
2	MN	C	505	1/1	0.93	0.07	-	22,22,22,22	0
2	MN	B	503	1/1	0.98	0.06	-	17,17,17,17	0
2	MN	D	507	1/1	0.98	0.04	-	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.