



# wwPDB X-ray Structure Validation Summary Report

Jan 31, 2016 – 08:37 PM GMT

PDB ID : 1L7J  
Title : X-ray structure of galactose mutarotase from Lactococcus lactis (apo)  
Authors : Holden, H.M.; Thoden, J.B.  
Deposited on : 2002-03-15  
Resolution : 1.90 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

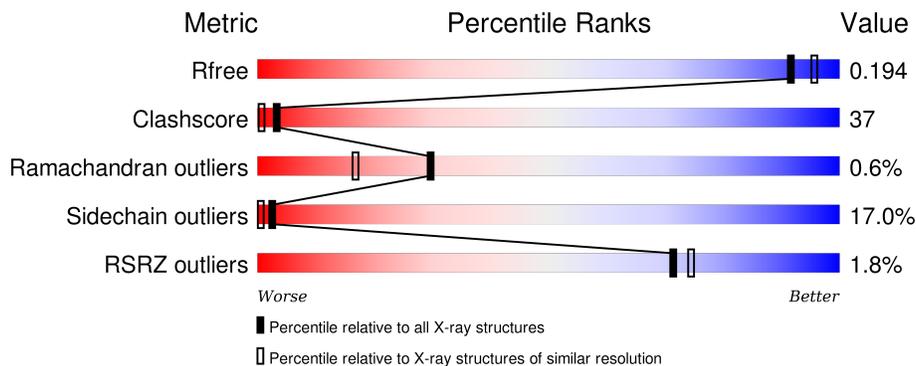
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	347	
1	B	347	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6065 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 galactose mutarotase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2650	1673	447	527	3	0	3	0
1	B	338	2645	1667	446	529	3	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLU	ENGINEERED	UNP Q9ZB17
A	340	LEU	-	EXPRESSION TAG	UNP Q9ZB17
A	341	GLU	-	EXPRESSION TAG	UNP Q9ZB17
A	342	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	343	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	344	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	345	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	346	HIS	-	EXPRESSION TAG	UNP Q9ZB17
A	347	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	2	SER	GLU	ENGINEERED	UNP Q9ZB17
B	340	LEU	-	EXPRESSION TAG	UNP Q9ZB17
B	341	GLU	-	EXPRESSION TAG	UNP Q9ZB17
B	342	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	343	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	344	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	345	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	346	HIS	-	EXPRESSION TAG	UNP Q9ZB17
B	347	HIS	-	EXPRESSION TAG	UNP Q9ZB17

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	376	Total	O	0	0
			376	376		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	B	394	Total 394	O 394	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.50Å 76.10Å 206.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 51.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-1.90) 89.7 (51.70-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 1.79Å)	Xtrriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.189 , 0.267 0.195 , 0.194	Depositor DCC
$R_{free}$ test set	5086 reflections (11.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtrriage
Anisotropy	0.815	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 144.9	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Outliers	0 of 57218 reflections	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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](#)

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	1.00	13/2714 (0.5%)	1.49	53/3672 (1.4%)
1	B	1.02	15/2705 (0.6%)	1.50	56/3661 (1.5%)
All	All	1.01	28/5419 (0.5%)	1.50	109/7333 (1.5%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLU	CD-OE2	7.80	1.34	1.25
1	B	304	GLU	CD-OE2	7.22	1.33	1.25
1	B	138	GLU	CD-OE2	6.38	1.32	1.25
1	A	117	GLU	CD-OE2	6.33	1.32	1.25
1	B	203	GLU	CD-OE2	6.29	1.32	1.25

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	33	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	B	249	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	A	136	LYS	N-CA-CB	-9.18	94.08	110.60
1	B	194	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	B	148	ASP	CB-CG-OD2	-8.56	110.60	118.30

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	2650	0	2592	240	0
1	B	2645	0	2576	155	0
2	A	376	0	0	29	0
2	B	394	0	0	23	0
All	All	6065	0	5168	392	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 37.

The worst 5 of 392 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:B:151:TRP:HH2	1:B:171:VAL:HG21	1.11	1.10
1:A:216:ASP:HB2	1:A:233:MET:HE2	1.26	1.09
1:A:46[A]:LEU:HD13	1:A:172:TYR:HB3	1.32	1.07
1:A:19:ASN:HD21	1:A:21:ALA:HB3	1.21	1.03
1:A:151:TRP:HH2	1:A:171:VAL:HG21	1.28	0.97

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	339/347 (98%)	299 (88%)	36 (11%)	4 (1%)	16	5
1	B	338/347 (97%)	309 (91%)	29 (9%)	0	100	100
All	All	677/694 (98%)	608 (90%)	65 (10%)	4 (1%)	30	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	THR

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Mol	Chain	Res	Type
1	A	311	SER
1	A	40	ASP
1	A	281	ALA

### 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	A	294/300 (98%)	236 (80%)	58 (20%)	<b>1</b> <b>0</b>
1	B	293/300 (98%)	251 (86%)	42 (14%)	<b>4</b> <b>1</b>
All	All	587/600 (98%)	487 (83%)	100 (17%)	<b>2</b> <b>0</b>

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	GLU
1	A	321	SER
1	B	255	LYS
1	A	257	GLN
1	A	288	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	282	ASN
1	B	250	GLN
1	A	237	GLN
1	B	237	GLN

### 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](#)

There are no ligands in this entry.

#### 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	338/347 (97%)	0.35	11 (3%) 50 53	11, 28, 54, 90	0
1	B	338/347 (97%)	0.02	1 (0%) 94 94	9, 22, 45, 68	0
All	All	676/694 (97%)	0.19	12 (1%) 71 74	9, 24, 49, 90	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	THR	5.7
1	A	339	LYS	5.1
1	A	214	ASN	3.8
1	B	214	ASN	3.8
1	A	287	GLY	2.9

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.