

wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 04:45 AM EDT

PDB ID : 1MMZ

Title: Crystal structure of galactose mutarotase from Lactococcus lactis complexed

with L-arabinose

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Deposited on : 2002-09-04

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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.23.2

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

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

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

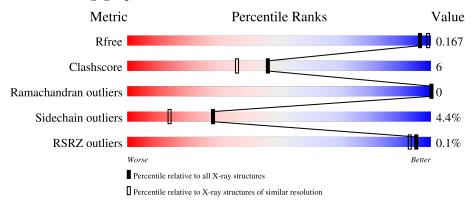
Validation Pipeline (wwPDB-VP) : 2.23.2

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 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 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	347	69%	24%	• • • • • • • • • • • • • • • • • • • •			
1	В	347	78%	18%	•			

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:



N	Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
	2	ARB	A	348[A]	X	-	-	-
	2	ARB	A	348[B]	X	-	-	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5846 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 Aldose 1-epimerase.

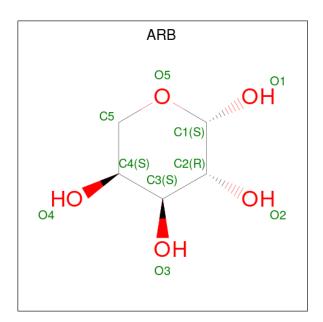
\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	339	Total	С	N	О	S	0	3	0
		330	2658	1677	448	530	3	Ů	9	
1	B	346	Total	С	N	O	S	0	2	0
1	Ъ	940	2732	1721	467	541	3		3	U

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLU	engineered mutation	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
В	2	SER	GLU	engineered mutation	UNP Q9ZB17
В	340	LEU	-	expression tag	UNP Q9ZB17
В	341	GLU	-	expression tag	UNP Q9ZB17
В	342	HIS	-	expression tag	UNP Q9ZB17
В	343	HIS	-	expression tag	UNP Q9ZB17
В	344	HIS	-	expression tag	UNP Q9ZB17
В	345	HIS	-	expression tag	UNP Q9ZB17
В	346	HIS	-	expression tag	UNP Q9ZB17
В	347	HIS	_	expression tag	UNP Q9ZB17

• Molecule 2 is beta-L-arabinopyranose (three-letter code: ARB) (formula: C₅H₁₀O₅).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 11 5 6	0	1
2	В	1	Total C O 10 5 5	0	0

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

• Molecule 4 is water.

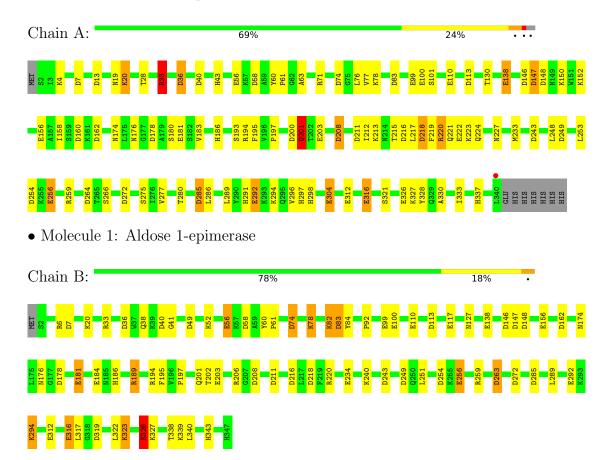
\mathbf{N}	Iol	Chain	Residues	Atoms	ZeroOcc	AltConf
	4	A	195	Total O 195 195	0	0
	4	В	239	Total O 239 239	0	0



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: Aldose 1-epimerase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	44.90Å 76.30Å 210.90Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 1.80	Depositor
Resolution (A)	71.75 - 1.74	EDS
% Data completeness	95.3 (30.00-1.80)	Depositor
(in resolution range)	93.0 (71.75-1.74)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) > 1$	1.89 (at 1.74Å)	Xtriage
Refinement program	TNT	Depositor
D D.	0.169 , 0.230	Depositor
R, R_{free}	0.165 , 0.167	DCC
R_{free} test set	7131 reflections (10.20%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 96.0	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5846	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.79% 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: NA, ARB

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.99	$15/2722 \ (0.6\%)$	1.40	52/3683 (1.4%)	
1	В	0.99	$17/2802 \ (0.6\%)$	1.35	46/3790 (1.2%)	
All	All	0.99	32/5524~(0.6%)	1.37	98/7473 (1.3%)	

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
1	A	100	GLU	CD-OE2	7.90	1.34	1.25
1	A	326	GLU	CD-OE2	7.84	1.34	1.25
1	A	99	GLU	CD-OE2	6.55	1.32	1.25
1	A	110	GLU	CD-OE2	6.46	1.32	1.25
1	A	292	GLU	CD-OE2	6.26	1.32	1.25

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}(^{o})$
1	A	71	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	146	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	В	249	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	A	249	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	A	218	ASP	CB-CG-OD2	-8.65	110.52	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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	A	2658	0	2596	48	0
1	В	2732	0	2647	20	0
2	A	11	0	4	0	0
2	В	10	0	10	0	0
3	A	1	0	0	0	0
4	A	195	0	0	5	0
4	В	239	0	0	0	0
All	All	5846	0	5257	67	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 6.

The worst 5 of 67 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:215:THR:HB	1:A:233:MET:HE3	1.55	0.86
1:B:338:THR:HG22	1:B:339:LYS:HG3	1.57	0.85
1:A:180:SER:HA	1:A:296:VAL:HG13	1.64	0.77
1:A:294:LYS:HB3	1:A:294:LYS:NZ	2.03	0.74
1:B:338:THR:CG2	1:B:339:LYS:HG3	2.21	0.70

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	entiles
1	A	340/347 (98%)	320 (94%)	20 (6%)	0	100	100
1	В	347/347 (100%)	331 (95%)	16 (5%)	0	100	100
All	All	687/694 (99%)	651 (95%)	36 (5%)	0	100	100



There are no Ramachandran outliers to report.

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	Percen	tiles
1	A	295/300 (98%)	283 (96%)	12 (4%)	30	16
1	В	302/300 (101%)	287 (95%)	15 (5%)	24	10
All	All	597/600 (100%)	570 (96%)	27 (4%)	28	13

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	82	LYS
1	В	195	PHE
1	В	326[A]	GLU
1	В	189	ARG
1	В	201	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	227	ASN
1	В	38	GLN
1	В	88	GLN
1	В	224	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Tuno	Chain	Res	Link	Во	ond leng	gths	В	ond ang	cles
IVIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ARB	A	348[B]	-	10,10,10	0.88	0	14,14,14	1.20	1 (7%)
2	ARB	A	348[A]	-	10,10,10	0.86	0	14,14,14	1.22	1 (7%)
2	ARB	В	348	-	10,10,10	0.89	0	14,14,14	1.69	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARB	A	348[B]	-	1/1/4/4	-	0/1/1/1
2	ARB	A	348[A]	-	1/1/4/4	-	0/1/1/1
2	ARB	В	348	-	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	В	348	ARB	C5-O5-C1	4.66	120.56	112.71
2	В	348	ARB	C5-C4-C3	-2.65	106.41	109.67
2	В	348	ARB	O4-C4-C3	2.27	114.68	110.14
2	A	348[A]	ARB	O2-C2-C1	2.06	113.94	109.16
2	A	348[B]	ARB	O2-C2-C1	2.06	113.94	109.16

All (2) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
2	A	348[A]	ARB	C1
2	A	348[B]	ARB	C1

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 > 2	$OWAB(A^2)$	Q < 0.9
1	A	339/347 (97%)	-0.89	1 (0%) 94 92	15, 26, 58, 89	0
1	В	346/347 (99%)	-0.98	0 100 100	13, 23, 51, 62	0
All	All	685/694 (98%)	-0.93	1 (0%) 95 93	13, 24, 55, 89	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	2.6

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
3	NA	A	349	1/1	0.85	0.12	40,40,40,40	0
2	ARB	A	348[B]	10/10	0.96	0.07	18,29,31,50	1
2	ARB	В	348	10/10	0.96	0.09	19,28,38,39	0
2	ARB	A	348[A]	10/10	0.96	0.07	18,25,31,50	1



6.5 Other polymers (i)

There are no such residues in this entry.

