



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:42 pm GMT

PDB ID : 1MMX
Title : Crystal structure of galactose mutarotase from *Lactococcus lactis* complexed with D-fucose
Authors : Thoden, J.B.; Kim, J.; Raushel, F.M.; Holden, H.M.
Deposited on : 2002-09-04
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

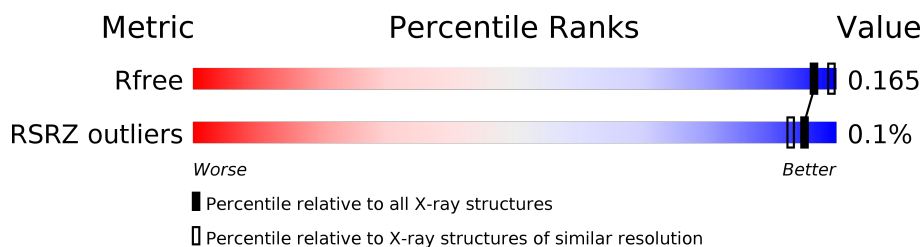
1 Overall quality at a glance

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}	111664	5253 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5937 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	5	0
			2666	1683	449	531	3			
1	B	346	Total	C	N	O	S	0	5	0
			2740	1726	467	543	4			

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 ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			12	6	6		
2	B	1	Total	C	O	0	1
			12	6	6		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	234	Total	O	0	0
			234	234		
4	B	272	Total	O	0	0
			272	272		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.90Å 76.30Å 210.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 76.30 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-1.80) 93.3 (76.30-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 1.71Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.168 , 0.229 0.165 , 0.165	Depositor DCC
R_{free} test set	7403 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5937	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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4.5 Carbohydrates [i](#)

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4.6 Ligand geometry [i](#)

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4.7 Other polymers [i](#)

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4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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, 95th 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 ²)	Q<0.9
1	A	339/347 (97%)	-0.87	1 (0%) 93 92	12, 23, 54, 92	0
1	B	346/347 (99%)	-0.94	0 100 100	12, 20, 44, 60	0
All	All	685/694 (98%)	-0.91	1 (0%) 95 93	12, 21, 52, 92	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	2.9

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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, 95th 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	B-factors(Å ²)	Q<0.9
3	NA	A	349	1/1	0.97	0.23	28,28,28,28	0
2	FUC	B	348[A]	11/11	0.97	0.06	7,18,22,26	1
2	FUC	B	348[B]	11/11	0.97	0.06	15,19,24,26	1
2	FUC	A	348[B]	11/11	0.98	0.05	11,17,22,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FUC	A	348[A]	11/11	0.98	0.05	11,18,22,26	1

5.5 Other polymers [i](#)

There are no such residues in this entry.