



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 21, 2024 – 12:43 PM EDT

PDB ID : 1TZ9
Title : Crystal Structure of the Putative Mannonate Dehydratase from *Enterococcus faecalis*, Northeast Structural Genomics Target EfR41
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Deposited on : 2004-07-09
Resolution : 2.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

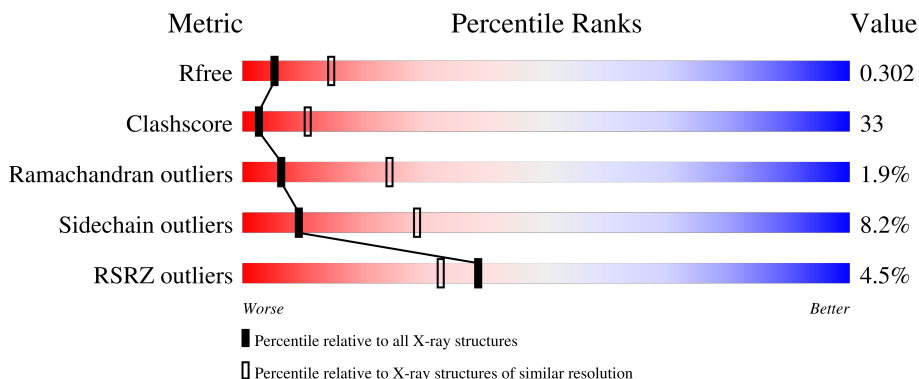
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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 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 $\leq 5\%$. 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	367	
1	B	367	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5495 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 Mannonate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	Se	0	0	0
			2731	1742	464	511	4	10			
1	B	344	Total	C	N	O	S	Se	0	0	0
			2731	1742	464	511	4	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	cloning artifact	UNP Q82ZC9
A	-8	GLY	-	cloning artifact	UNP Q82ZC9
A	-7	HIS	-	cloning artifact	UNP Q82ZC9
A	-6	HIS	-	cloning artifact	UNP Q82ZC9
A	-5	HIS	-	cloning artifact	UNP Q82ZC9
A	-4	HIS	-	cloning artifact	UNP Q82ZC9
A	-3	HIS	-	cloning artifact	UNP Q82ZC9
A	-2	HIS	-	cloning artifact	UNP Q82ZC9
A	-1	SER	-	cloning artifact	UNP Q82ZC9
A	0	HIS	-	cloning artifact	UNP Q82ZC9
A	1	MSE	MET	modified residue	UNP Q82ZC9
A	138	MSE	MET	modified residue	UNP Q82ZC9
A	143	MSE	MET	modified residue	UNP Q82ZC9
A	173	MSE	MET	modified residue	UNP Q82ZC9
A	204	MSE	MET	modified residue	UNP Q82ZC9
A	260	MSE	MET	modified residue	UNP Q82ZC9
A	298	MSE	MET	modified residue	UNP Q82ZC9
A	302	MSE	MET	modified residue	UNP Q82ZC9
A	328	MSE	MET	modified residue	UNP Q82ZC9
A	338	MSE	MET	modified residue	UNP Q82ZC9
B	-9	MET	-	cloning artifact	UNP Q82ZC9
B	-8	GLY	-	cloning artifact	UNP Q82ZC9
B	-7	HIS	-	cloning artifact	UNP Q82ZC9
B	-6	HIS	-	cloning artifact	UNP Q82ZC9
B	-5	HIS	-	cloning artifact	UNP Q82ZC9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	cloning artifact	UNP Q82ZC9
B	-3	HIS	-	cloning artifact	UNP Q82ZC9
B	-2	HIS	-	cloning artifact	UNP Q82ZC9
B	-1	SER	-	cloning artifact	UNP Q82ZC9
B	0	HIS	-	cloning artifact	UNP Q82ZC9
B	1	MSE	MET	modified residue	UNP Q82ZC9
B	138	MSE	MET	modified residue	UNP Q82ZC9
B	143	MSE	MET	modified residue	UNP Q82ZC9
B	173	MSE	MET	modified residue	UNP Q82ZC9
B	204	MSE	MET	modified residue	UNP Q82ZC9
B	260	MSE	MET	modified residue	UNP Q82ZC9
B	298	MSE	MET	modified residue	UNP Q82ZC9
B	302	MSE	MET	modified residue	UNP Q82ZC9
B	328	MSE	MET	modified residue	UNP Q82ZC9
B	338	MSE	MET	modified residue	UNP Q82ZC9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	16	Total O 16 16	0	0

V308	V313	I314	R315	P316	D317	H318	A321	I322	E325	K326	L333	Y334	M338	G339	L340	T341	Y342	I343	Q344	G345	L346	A349	T350	K351	A352	K353	GLN	ASN	ARG	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.34Å 89.94Å 156.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.90 29.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (29.61-2.90) 96.6 (29.61-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.292 0.226 , 0.302	Depositor DCC
R_{free} test set	1539 reflections (9.62%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5495	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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.

5 Model quality

5.1 Standard geometry

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	0.45	0/2785	0.62	0/3760
1	B	0.42	0/2785	0.60	0/3760
All	All	0.44	0/5570	0.61	0/7520

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

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	2731	0	2682	190	0
1	B	2731	0	2682	177	0
2	A	17	0	0	3	0
2	B	16	0	0	5	0
All	All	5495	0	5364	354	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 33.

The worst 5 of 354 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:A:39:GLY:H	1:A:68:ALA:HB1	1.13	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLY:H	1:B:68:ALA:HB1	1.13	1.08
1:B:326:LYS:NZ	1:B:326:LYS:H	1.73	0.86
1:B:296:LEU:HB3	1:B:298:MSE:HE3	1.56	0.85
1:A:206:ILE:HG12	1:A:222:THR:HG21	1.60	0.84

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	340/367 (93%)	294 (86%)	40 (12%)	6 (2%)	7	25
1	B	340/367 (93%)	290 (85%)	43 (13%)	7 (2%)	5	22
All	All	680/734 (93%)	584 (86%)	83 (12%)	13 (2%)	6	24

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	108	PRO
1	A	222	THR
1	B	77	THR
1	B	108	PRO

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	288/298 (97%)	264 (92%)	24 (8%)	9	28
1	B	288/298 (97%)	265 (92%)	23 (8%)	10	30
All	All	576/596 (97%)	529 (92%)	47 (8%)	9	29

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	LEU
1	B	203	LYS
1	B	78	ASP
1	B	143	MSE
1	B	222	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	HIS
1	B	289	HIS
1	B	303	GLN
1	B	272	HIS
1	A	266	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 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	334/367 (91%)	0.26	15 (4%) 39 32	6, 26, 52, 64	0
1	B	334/367 (91%)	0.31	15 (4%) 39 32	6, 28, 58, 91	0
All	All	668/734 (91%)	0.29	30 (4%) 39 32	6, 27, 55, 91	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	ALA	5.1
1	B	13	ASP	4.6
1	A	9	GLY	3.8
1	B	159	TRP	3.8
1	A	68	ALA	3.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.