



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2025 – 01:49 pm BST

PDB ID : 9GPC / pdb_00009gpc
Title : The crystal structure of ManDH5 E303Q mutant at 1.4 Angstroms Resolution
- a beta-D-Mannanase of GH5 family from Dictyoglomus thermophilum
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Deposited on : 2024-09-07
Resolution : 1.40 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 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	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

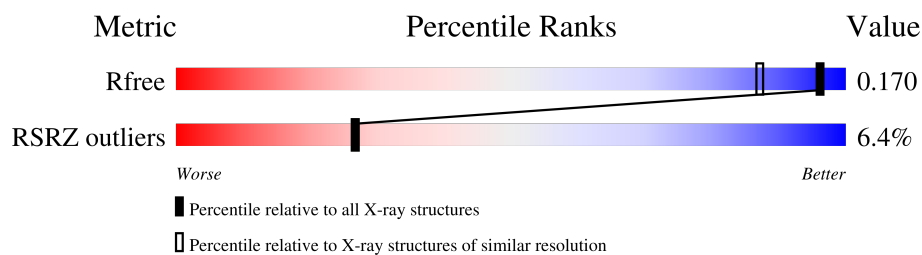
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2247 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9809 atoms, of which 4568 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.

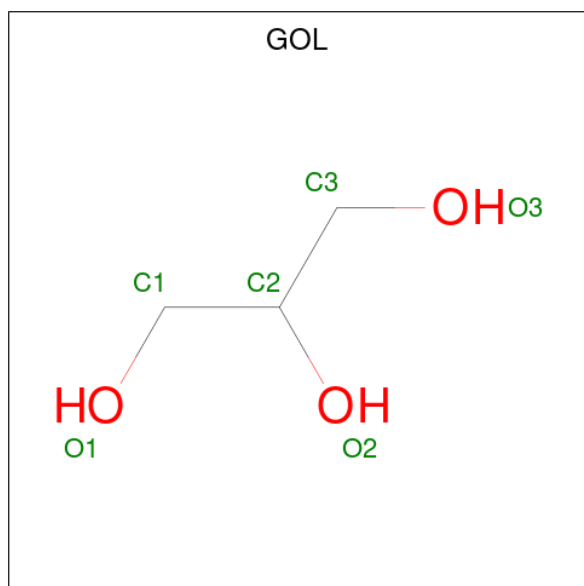
- Molecule 1 is a protein called DUF5060 domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	563	9299	3113	4560	763	854	9	0	3	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	GLN	GLU	engineered mutation	UNP A0A7C3MIF0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	14	3	8	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	496	Total 496	O 496	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.50Å 99.13Å 154.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.44 – 1.40 83.44 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.44-1.40) 99.9 (83.44-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.147 , 0.169 0.149 , 0.170	Depositor DCC
R_{free} test set	7410 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9809	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	601	-	5,5,5	0.88	0	5,5,5	0.95	0

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	GOL	A	601	-	-	0/4/4/4	-

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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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	563/568 (99%)	-0.24	36 (6%)	27 27	9, 18, 39, 50	3 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	TRP	5.4
1	A	506	PRO	5.1
1	A	474	ASN	5.0
1	A	475	ARG	3.9
1	A	520	LEU	3.8
1	A	124	TYR	3.4
1	A	521	ILE	3.4
1	A	466	THR	3.4
1	A	507	ASN	3.3
1	A	508	MET	3.3
1	A	522	LYS	3.1
1	A	467	ASN	3.1
1	A	519	LEU	3.1
1	A	354	ILE	3.0
1	A	20	MET	2.9
1	A	544	ASP	2.9
1	A	465	LEU	2.9
1	A	19	LYS	2.9
1	A	472	VAL	2.8
1	A	496	LYS	2.8
1	A	400	ASN	2.7
1	A	505	ILE	2.7
1	A	538	ILE	2.7
1	A	398	GLY	2.7
1	A	399	GLY	2.7
1	A	397	ALA	2.6
1	A	119	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	454	ASP	2.4
1	A	523	PRO	2.4
1	A	564	LEU	2.3
1	A	502	LYS	2.3
1	A	396	ASP	2.3
1	A	563	LEU	2.3
1	A	512	LYS	2.3
1	A	547	VAL	2.2
1	A	511	SER	2.1

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 oligosaccharides 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
2	GOL	A	601	6/6	0.93	0.09	30,36,39,39	0

5.5 Other polymers [i](#)

There are no such residues in this entry.