



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2026 – 05:13 PM UTC

PDB ID : 4U10 / pdb_00004u10
Title : Probing the structure and mechanism of de-N-acetylase from aggregatibacter actinomycetemcomitans
Authors : Varudharasu, D.; Narayanan, R.
Deposited on : 2014-07-14
Resolution : 2.05 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

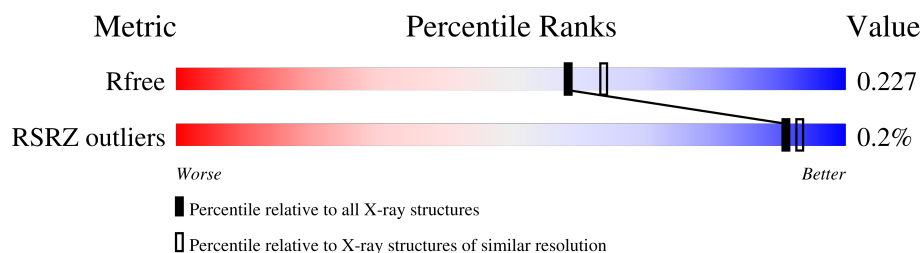
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 4513 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 Poly-beta-1,6-N-acetyl-D-glucosamine N-deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	Se	0	3	0
			2138	1368	368	397	5			
1	B	262	Total	C	N	O	Se	0	0	0
			2106	1348	363	391	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MSE	-	expression tag	UNP A5HJW8
A	152	ASP	GLU	conflict	UNP A5HJW8
A	299	HIS	-	expression tag	UNP A5HJW8
A	300	HIS	-	expression tag	UNP A5HJW8
A	301	HIS	-	expression tag	UNP A5HJW8
A	302	HIS	-	expression tag	UNP A5HJW8
A	303	HIS	-	expression tag	UNP A5HJW8
A	304	HIS	-	expression tag	UNP A5HJW8
B	25	MSE	-	expression tag	UNP A5HJW8
B	152	ASP	GLU	conflict	UNP A5HJW8
B	299	HIS	-	expression tag	UNP A5HJW8
B	300	HIS	-	expression tag	UNP A5HJW8
B	301	HIS	-	expression tag	UNP A5HJW8
B	302	HIS	-	expression tag	UNP A5HJW8
B	303	HIS	-	expression tag	UNP A5HJW8
B	304	HIS	-	expression tag	UNP A5HJW8

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	1
			4	4		
2	B	4	Total	Zn	0	1
			5	5		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total 139	O 139	0	0
4	B	119	Total 119	O 119	0	0

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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	65.24Å 67.10Å 101.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.48 – 2.05 42.48 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.48-2.05) 99.8 (42.48-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.163 , 0.220 0.171 , 0.227	Depositor DCC
R_{free} test set	1542 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4513	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.39 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0887e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

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	259/280 (92%)	-0.23	0	100 100	12, 21, 39, 53	3 (1%)
1	B	258/280 (92%)	-0.22	1 (0%)	88 90	12, 21, 39, 48	0
All	All	517/560 (92%)	-0.22	1 (0%)	91 93	12, 21, 39, 53	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	THR	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	ZN	A	403[A]	1/1	0.99	0.02	14,14,14,14	1
2	ZN	A	403[B]	1/1	0.99	0.02	34,34,34,34	1
2	ZN	B	404	1/1	0.99	0.06	18,18,18,18	1
3	CL	B	405	1/1	0.99	0.02	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	401	1/1	1.00	0.01	14,14,14,14	0
2	ZN	B	402	1/1	1.00	0.01	14,14,14,14	0
2	ZN	B	403[A]	1/1	1.00	0.01	7,7,7,7	1
2	ZN	B	403[B]	1/1	1.00	0.01	19,19,19,19	1
2	ZN	A	401	1/1	1.00	0.01	14,14,14,14	0
3	CL	A	404	1/1	1.00	0.03	16,16,16,16	0
2	ZN	A	402	1/1	1.00	0.01	14,14,14,14	0

5.5 Other polymers [i](#)

There are no such residues in this entry.