



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 11:08 PM UTC

PDB ID : 5F7C / pdb_00005f7c
Title : Crystal structure of Family 31 alpha-glucosidase (BT_0339) from Bacteroides
thetaiotaomicron
Authors : Chaudet, M.M.; Rose, D.R.
Deposited on : 2015-12-07
Resolution : 2.60 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	:	FAILED
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

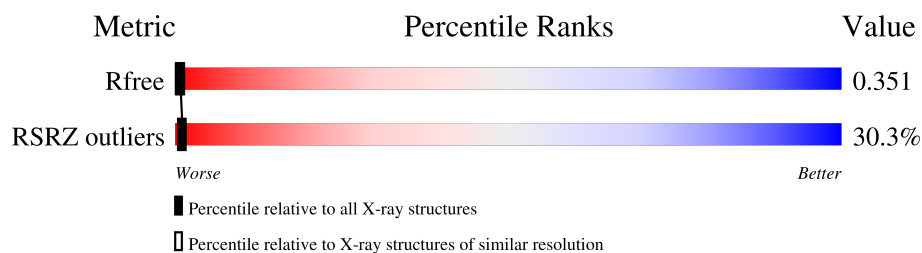
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34019 atoms, of which 14026 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 Alpha-glucosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	625	Total	C	H	N	O	S	0	0	0
			8422	3229	3426	837	901	29			
1	B	611	Total	C	H	N	O	S	0	0	0
			8403	3150	3512	832	881	28			
1	C	632	Total	C	H	N	O	S	0	0	0
			8637	3278	3548	865	917	29			
1	D	623	Total	C	H	N	O	S	0	0	0
			8490	3185	3540	840	895	30			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	LEU	PHE	conflict	UNP Q8AAX3
A	13	PHE	LEU	conflict	UNP Q8AAX3
A	750	HIS	-	expression tag	UNP Q8AAX3
A	751	HIS	-	expression tag	UNP Q8AAX3
A	752	HIS	-	expression tag	UNP Q8AAX3
A	753	HIS	-	expression tag	UNP Q8AAX3
A	754	HIS	-	expression tag	UNP Q8AAX3
A	755	HIS	-	expression tag	UNP Q8AAX3
A	756	LEU	-	expression tag	UNP Q8AAX3
A	757	ARG	-	expression tag	UNP Q8AAX3
A	758	VAL	-	expression tag	UNP Q8AAX3
A	759	PRO	-	expression tag	UNP Q8AAX3
A	760	ARG	-	expression tag	UNP Q8AAX3
A	761	GLY	-	expression tag	UNP Q8AAX3
A	762	SER	-	expression tag	UNP Q8AAX3
B	12	LEU	PHE	conflict	UNP Q8AAX3
B	13	PHE	LEU	conflict	UNP Q8AAX3
B	750	HIS	-	expression tag	UNP Q8AAX3
B	751	HIS	-	expression tag	UNP Q8AAX3
B	752	HIS	-	expression tag	UNP Q8AAX3
B	753	HIS	-	expression tag	UNP Q8AAX3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	754	HIS	-	expression tag	UNP Q8AAX3
B	755	HIS	-	expression tag	UNP Q8AAX3
B	756	LEU	-	expression tag	UNP Q8AAX3
B	757	ARG	-	expression tag	UNP Q8AAX3
B	758	VAL	-	expression tag	UNP Q8AAX3
B	759	PRO	-	expression tag	UNP Q8AAX3
B	760	ARG	-	expression tag	UNP Q8AAX3
B	761	GLY	-	expression tag	UNP Q8AAX3
B	762	SER	-	expression tag	UNP Q8AAX3
C	12	LEU	PHE	conflict	UNP Q8AAX3
C	13	PHE	LEU	conflict	UNP Q8AAX3
C	750	HIS	-	expression tag	UNP Q8AAX3
C	751	HIS	-	expression tag	UNP Q8AAX3
C	752	HIS	-	expression tag	UNP Q8AAX3
C	753	HIS	-	expression tag	UNP Q8AAX3
C	754	HIS	-	expression tag	UNP Q8AAX3
C	755	HIS	-	expression tag	UNP Q8AAX3
C	756	LEU	-	expression tag	UNP Q8AAX3
C	757	ARG	-	expression tag	UNP Q8AAX3
C	758	VAL	-	expression tag	UNP Q8AAX3
C	759	PRO	-	expression tag	UNP Q8AAX3
C	760	ARG	-	expression tag	UNP Q8AAX3
C	761	GLY	-	expression tag	UNP Q8AAX3
C	762	SER	-	expression tag	UNP Q8AAX3
D	12	LEU	PHE	conflict	UNP Q8AAX3
D	13	PHE	LEU	conflict	UNP Q8AAX3
D	750	HIS	-	expression tag	UNP Q8AAX3
D	751	HIS	-	expression tag	UNP Q8AAX3
D	752	HIS	-	expression tag	UNP Q8AAX3
D	753	HIS	-	expression tag	UNP Q8AAX3
D	754	HIS	-	expression tag	UNP Q8AAX3
D	755	HIS	-	expression tag	UNP Q8AAX3
D	756	LEU	-	expression tag	UNP Q8AAX3
D	757	ARG	-	expression tag	UNP Q8AAX3
D	758	VAL	-	expression tag	UNP Q8AAX3
D	759	PRO	-	expression tag	UNP Q8AAX3
D	760	ARG	-	expression tag	UNP Q8AAX3
D	761	GLY	-	expression tag	UNP Q8AAX3
D	762	SER	-	expression tag	UNP Q8AAX3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total 23	O 23	0	0
2	B	9	Total 9	O 9	0	0
2	C	18	Total 18	O 18	0	0
2	D	17	Total 17	O 17	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.34Å 75.00Å 232.86Å 90.00° 95.14° 90.00°	Depositor
Resolution (Å)	48.81 – 2.60 48.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.81-2.60) 100.0 (48.81-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.302 , 0.349 0.307 , 0.351	Depositor DCC
R_{free} test set	2000 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	34019	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

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	625/761 (82%)	1.30	159 (25%) 1 1	24, 48, 82, 101	0
1	B	611/761 (80%)	1.82	220 (36%) 1 1	51, 69, 92, 104	0
1	C	632/761 (83%)	1.48	193 (30%) 1 1	28, 53, 86, 102	0
1	D	623/761 (81%)	1.55	184 (29%) 1 1	34, 58, 91, 106	0
All	All	2491/3044 (81%)	1.54	756 (30%) 1 1	24, 61, 90, 106	0

The worst 5 of 756 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ILE	6.7
1	A	470	VAL	6.4
1	D	323	PHE	6.2
1	C	35	TYR	6.2
1	C	54	ASN	5.9

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 oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.