



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:17 AM UTC

PDB ID : 2XVK / pdb_00002xvk
Title : crystal structure of alpha-xylosidase (GH31) from Cellvibrio japonicus in complex with 5-fluoro-alpha-D-xylopyranosyl fluoride
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Deposited on : 2010-10-26
Resolution : 2.50 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	:	4-5-2 with Phenix2.0
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

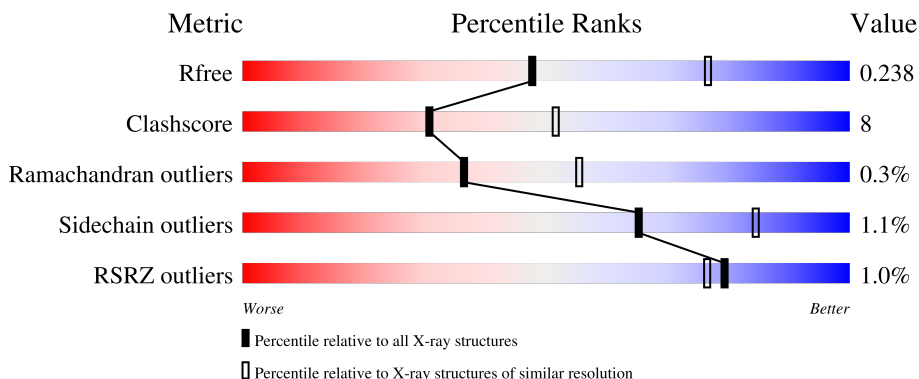
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1020	73% 19% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7673 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 ALPHA-XYLOSIDASE, PUTATIVE, XYL31A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	944	Total	C	N	O	S	44	1	0
			7575	4841	1293	1426	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	989	LYS	-	expression tag	UNP B3PBD9
A	990	VAL	-	expression tag	UNP B3PBD9
A	991	VAL	-	expression tag	UNP B3PBD9
A	992	ILE	-	expression tag	UNP B3PBD9
A	993	ASN	-	expression tag	UNP B3PBD9
A	994	SER	-	expression tag	UNP B3PBD9
A	995	LYS	-	expression tag	UNP B3PBD9
A	996	LEU	-	expression tag	UNP B3PBD9
A	997	GLU	-	expression tag	UNP B3PBD9
A	998	GLY	-	expression tag	UNP B3PBD9
A	999	LYS	-	expression tag	UNP B3PBD9
A	1000	PRO	-	expression tag	UNP B3PBD9
A	1001	ILE	-	expression tag	UNP B3PBD9
A	1002	PRO	-	expression tag	UNP B3PBD9
A	1003	ASN	-	expression tag	UNP B3PBD9
A	1004	PRO	-	expression tag	UNP B3PBD9
A	1005	LEU	-	expression tag	UNP B3PBD9
A	1006	LEU	-	expression tag	UNP B3PBD9
A	1007	GLY	-	expression tag	UNP B3PBD9
A	1008	LEU	-	expression tag	UNP B3PBD9
A	1009	ASP	-	expression tag	UNP B3PBD9
A	1010	SER	-	expression tag	UNP B3PBD9
A	1011	THR	-	expression tag	UNP B3PBD9
A	1012	ARG	-	expression tag	UNP B3PBD9
A	1013	THR	-	expression tag	UNP B3PBD9
A	1014	GLY	-	expression tag	UNP B3PBD9
A	1015	HIS	-	expression tag	UNP B3PBD9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1016	HIS	-	expression tag	UNP B3PBD9
A	1017	HIS	-	expression tag	UNP B3PBD9
A	1018	HIS	-	expression tag	UNP B3PBD9
A	1019	HIS	-	expression tag	UNP B3PBD9
A	1020	HIS	-	expression tag	UNP B3PBD9

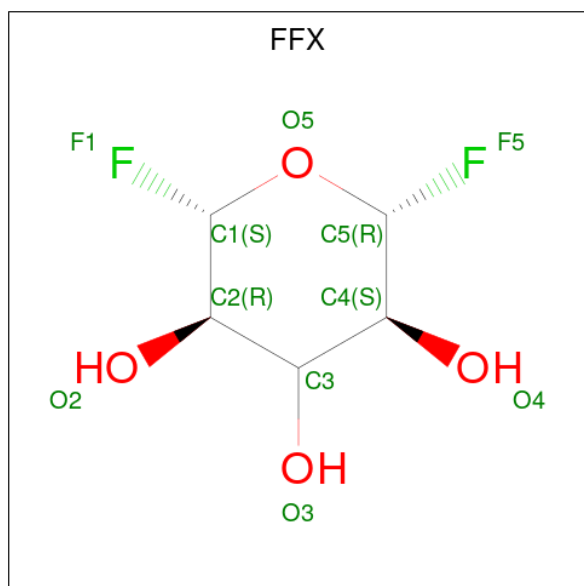
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cl 4 4	0	0

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 4 is (2R,3S,5R,6S)-2,6-DIFLUOROOXANE-3,4,5-TRIOL (CCD ID: FFX) (formula: C₅H₈F₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F O 10 5 1 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total 83	O 83	0	0

- Molecule 1: ALPHA-XYLOSIDASE, PUTATIVE, XYL31A



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.52Å 156.52Å 227.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.98 – 2.50 49.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-2.50) 99.8 (49.98-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.195 , 0.240 0.194 , 0.238	Depositor DCC
R_{free} test set	2905 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7673	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FFX, CL, NI

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	0.49	0/7787	0.84	15/10579 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ASN	N-CA-C	7.03	119.54	108.79
1	A	489	PHE	CA-C-N	6.02	125.57	119.19
1	A	489	PHE	C-N-CA	6.02	125.57	119.19
1	A	798	PHE	CA-C-N	5.95	125.63	119.56
1	A	798	PHE	C-N-CA	5.95	125.63	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7575	0	7271	122	0
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	10	0	7	0	0
5	A	83	0	0	2	0
All	All	7673	0	7278	122	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 8.

The worst 5 of 122 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:697:ARG:HB2	1:A:716:GLN:NE2	2.05	0.71
1:A:320:HIS:ND1	1:A:381:HIS:HE1	1.92	0.68
1:A:454:LEU:HD23	1:A:502:MET:HE3	1.75	0.66
1:A:586:PRO:HG3	1:A:616:TYR:CD2	2.32	0.64
1:A:279:GLN:HB2	1:A:378:HIS:HB2	1.80	0.64

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	943/1020 (92%)	899 (95%)	41 (4%)	3 (0%)	36 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	GLU
1	A	269	LEU
1	A	284	GLY

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	792/856 (92%)	783 (99%)	9 (1%)	65 84

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	758	VAL
1	A	838	SER
1	A	543	ILE
1	A	660	ILE
1	A	661	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	HIS
1	A	466	ASN
1	A	574	HIS
1	A	227	ASN
1	A	190	ASN

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 ⓘ

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	FFX	A	1994	1	10,10,11	1.51	2 (20%)	14,14,16	0.88	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
4	FFX	A	1994	1	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1994	FFX	O5-C5	3.49	1.44	1.39
4	A	1994	FFX	C4-C5	2.96	1.54	1.52

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.

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	944/1020 (92%)	-0.16	9 (0%) 79 76	31, 68, 121, 176	13 (1%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	3.6
1	A	347	TRP	3.1
1	A	293	GLU	3.0
1	A	390	GLN	3.0
1	A	988	ARG	2.8

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 oligosaccharides in this entry.

6.4 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
4	FFX	A	1994	10/11	0.94	0.08	59,68,77,81	0
2	CL	A	1991	1/1	0.96	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	1989	1/1	0.96	0.06	60,60,60,60	0
2	CL	A	1990	1/1	0.97	0.06	67,67,67,67	0
2	CL	A	1992	1/1	0.98	0.05	58,58,58,58	0
3	NI	A	1993	1/1	1.00	0.02	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.