



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 11:36 AM UTC

PDB ID : 1R85 / pdb_00001r85
Title : Crystal structure of the extracellular xylanase from *Geobacillus stearothermophilus* T-6 (XT6): The WT enzyme (monoclinic form) at 1.45Å resolution
Authors : Bar, M.; Golan, G.; Nechama, M.; Zolotnitsky, G.; Shoham, Y.; Shoham, G.
Deposited on : 2003-10-23
Resolution : 1.45 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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 1.45 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3816 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	32	0
			3172	2038	543	584	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Zn	0	0
			7	7		

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

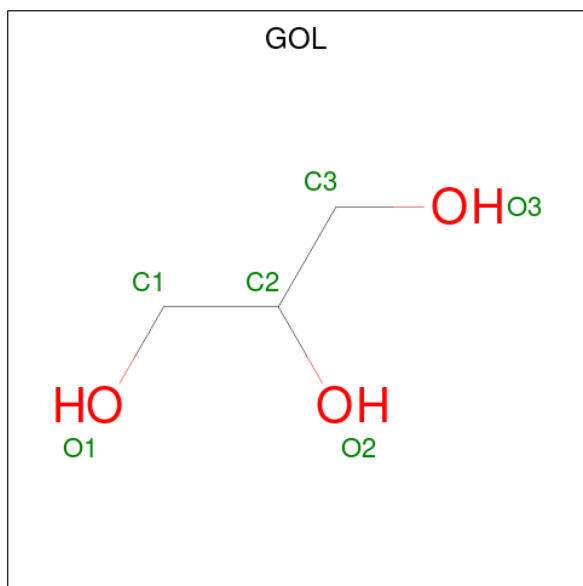
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 12 6 6	0	1
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	1
			12	6	6		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	494	Total	O	0	0
			494	494		

MolProbity failed to run properly; EDS was not executed - this section is therefore empty.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.51Å 61.71Å 89.09Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	40.00 – 1.45	Depositor
% Data completeness (in resolution range)	94.1 (40.00-1.45)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.126 , 0.181	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3816	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

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 33 ligands modelled in this entry, 9 are monoatomic - leaving 24 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	SO4	A	802	-	4,4,4	0.26	0	6,6,6	0.42	0
5	GOL	A	519	-	5,5,5	0.49	0	5,5,5	0.91	0
5	GOL	A	517	-	5,5,5	0.66	0	5,5,5	0.41	0
5	GOL	A	501	-	5,5,5	0.58	0	5,5,5	0.60	0
5	GOL	A	505	-	5,5,5	0.68	0	5,5,5	0.28	0
5	GOL	A	506[A]	-	5,5,5	0.58	0	5,5,5	0.87	0
5	GOL	A	504	-	5,5,5	0.71	0	5,5,5	0.36	0
5	GOL	A	509	-	5,5,5	0.56	0	5,5,5	0.55	0
4	SO4	A	803	-	4,4,4	0.34	0	6,6,6	0.14	0
5	GOL	A	510	2	5,5,5	0.91	0	5,5,5	0.85	0
5	GOL	A	502	-	5,5,5	0.52	0	5,5,5	1.77	2 (40%)
5	GOL	A	516[B]	-	5,5,5	0.56	0	5,5,5	1.26	0
5	GOL	A	515	-	5,5,5	0.61	0	5,5,5	0.61	0
5	GOL	A	512	-	5,5,5	0.59	0	5,5,5	0.59	0
5	GOL	A	506[B]	-	5,5,5	0.76	0	5,5,5	0.77	0
5	GOL	A	507	-	5,5,5	0.65	0	5,5,5	0.83	0
5	GOL	A	513	-	5,5,5	0.68	0	5,5,5	0.69	0
4	SO4	A	801	-	4,4,4	0.34	0	6,6,6	0.27	0
5	GOL	A	508	-	5,5,5	0.78	0	5,5,5	0.36	0
5	GOL	A	518	2	5,5,5	0.54	0	5,5,5	1.35	0
5	GOL	A	514	-	5,5,5	0.68	0	5,5,5	0.38	0
5	GOL	A	503	-	5,5,5	0.79	0	5,5,5	0.56	0
5	GOL	A	516[A]	-	5,5,5	0.67	0	5,5,5	0.31	0
5	GOL	A	511	-	5,5,5	0.55	0	5,5,5	0.52	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
5	GOL	A	519	-	-	4/4/4/4	-
5	GOL	A	517	-	-	3/4/4/4	-
5	GOL	A	501	-	-	4/4/4/4	-
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	A	506[A]	-	-	4/4/4/4	-
5	GOL	A	504	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	509	-	-	4/4/4/4	-
5	GOL	A	510	2	-	3/4/4/4	-
5	GOL	A	502	-	-	2/4/4/4	-
5	GOL	A	516[B]	-	-	2/4/4/4	-
5	GOL	A	515	-	-	2/4/4/4	-
5	GOL	A	512	-	-	2/4/4/4	-
5	GOL	A	506[B]	-	-	4/4/4/4	-
5	GOL	A	507	-	-	1/4/4/4	-
5	GOL	A	513	-	-	4/4/4/4	-
5	GOL	A	508	-	-	0/4/4/4	-
5	GOL	A	518	2	-	1/4/4/4	-
5	GOL	A	514	-	-	4/4/4/4	-
5	GOL	A	503	-	-	2/4/4/4	-
5	GOL	A	516[A]	-	-	4/4/4/4	-
5	GOL	A	511	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	GOL	O2-C2-C1	2.36	118.95	109.18
5	A	502	GOL	C3-C2-C1	2.36	120.45	111.80

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	GOL	C1-C2-C3-O3
5	A	503	GOL	O1-C1-C2-C3
5	A	504	GOL	O1-C1-C2-C3
5	A	504	GOL	C1-C2-C3-O3
5	A	506[A]	GOL	O1-C1-C2-C3
5	A	506[A]	GOL	C1-C2-C3-O3
5	A	506[B]	GOL	C1-C2-C3-O3
5	A	509	GOL	C1-C2-C3-O3
5	A	510	GOL	O1-C1-C2-O2
5	A	510	GOL	O1-C1-C2-C3
5	A	511	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	512	GOL	O1-C1-C2-O2
5	A	512	GOL	O1-C1-C2-C3
5	A	513	GOL	O1-C1-C2-C3
5	A	513	GOL	C1-C2-C3-O3
5	A	514	GOL	O1-C1-C2-C3
5	A	516[A]	GOL	C1-C2-C3-O3
5	A	516[A]	GOL	O2-C2-C3-O3
5	A	516[B]	GOL	O1-C1-C2-C3
5	A	517	GOL	C1-C2-C3-O3
5	A	519	GOL	C1-C2-C3-O3
5	A	519	GOL	O2-C2-C3-O3
5	A	502	GOL	O1-C1-C2-O2
5	A	511	GOL	O2-C2-C3-O3
5	A	501	GOL	O1-C1-C2-C3
5	A	501	GOL	C1-C2-C3-O3
5	A	505	GOL	O1-C1-C2-C3
5	A	506[B]	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	A	509	GOL	O1-C1-C2-C3
5	A	511	GOL	O1-C1-C2-C3
5	A	514	GOL	C1-C2-C3-O3
5	A	515	GOL	C1-C2-C3-O3
5	A	516[A]	GOL	O1-C1-C2-C3
5	A	518	GOL	O1-C1-C2-C3
5	A	519	GOL	O1-C1-C2-C3
5	A	501	GOL	O2-C2-C3-O3
5	A	503	GOL	O1-C1-C2-O2
5	A	504	GOL	O1-C1-C2-O2
5	A	504	GOL	O2-C2-C3-O3
5	A	505	GOL	O1-C1-C2-O2
5	A	506[A]	GOL	O1-C1-C2-O2
5	A	513	GOL	O1-C1-C2-O2
5	A	514	GOL	O1-C1-C2-O2
5	A	514	GOL	O2-C2-C3-O3
5	A	516[B]	GOL	O1-C1-C2-O2
5	A	519	GOL	O1-C1-C2-O2
5	A	506[A]	GOL	O2-C2-C3-O3
5	A	506[B]	GOL	O2-C2-C3-O3
5	A	509	GOL	O2-C2-C3-O3
5	A	517	GOL	O2-C2-C3-O3
5	A	511	GOL	O1-C1-C2-O2
5	A	506[B]	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	509	GOL	O1-C1-C2-O2
5	A	516[A]	GOL	O1-C1-C2-O2
5	A	517	GOL	O1-C1-C2-O2
5	A	510	GOL	C1-C2-C3-O3
5	A	501	GOL	O1-C1-C2-O2
5	A	515	GOL	O2-C2-C3-O3
5	A	513	GOL	O2-C2-C3-O3

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 ⓘ

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

5.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

5.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.