



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 02:09 AM EDT

PDB ID : 1R86  
Title : Crystal structure of the extracellular xylanase from *Geobacillus stearothermophilus* T-6 (XT6, monoclinic form): The E159A/E265A mutant at 1.8Å resolution  
Authors : Bar, M.; Golan, G.; Zolotnitsky, G.; Shoham, Y.; Shoham, G.  
Deposited on : 2003-10-23  
Resolution : 1.80 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

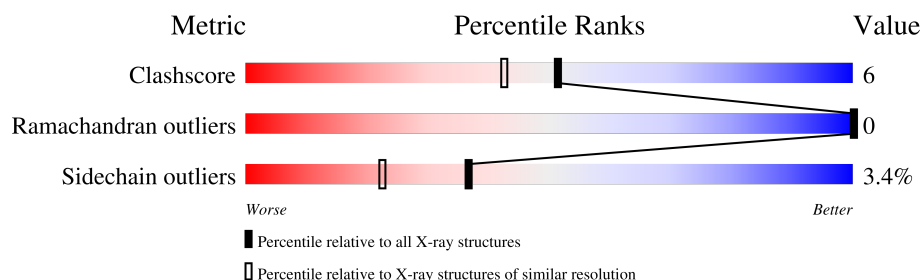
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	379	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3484 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	14	0
			3144	2016	539	582	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ALA	GLU	engineered mutation	UNP P40943
A	265	ALA	GLU	engineered mutation	UNP P40943

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	326	Total	O	0	0
			326	326		



Note EDS was not executed.

- Molecule 1: Endo-1,4-beta-xylanase

## 4 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, $\alpha$ , $\beta$ , $\gamma$	121.24Å 61.25Å 89.46Å 90.00° 119.28° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80	Depositor
% Data completeness (in resolution range)	90.9 (40.00-1.80)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.181 , 0.215	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 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: CL, ZN, SO4

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	0.90	0/3227	0.90	2/4377 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	PRO	N-CA-C	5.53	126.49	112.10
1	A	50	ARG	NE-CZ-NH1	5.34	122.97	120.30

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	3144	0	3068	35	0
2	A	7	0	0	0	0
3	A	2	0	0	0	0
4	A	5	0	0	0	0
5	A	326	0	0	3	0
All	All	3484	0	3068	35	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 6.

All (35) 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:111:LYS:H	1:A:111:LYS:CE	2.01	0.72
1:A:282:ASP:OD1	5:A:1347:HOH:O	2.11	0.69
1:A:111:LYS:H	1:A:111:LYS:CD	2.08	0.66
1:A:76[B]:GLU:CD	1:A:76[B]:GLU:H	2.02	0.62
1:A:218[A]:VAL:HG11	1:A:259:LEU:HD11	1.81	0.61
1:A:110:ASP:HB2	1:A:111:LYS:NZ	2.16	0.60
1:A:64:ILE:HA	1:A:104:PRO:HG3	1.85	0.59
1:A:42[B]:GLU:O	1:A:46[B]:GLN:HG3	2.02	0.59
1:A:111:LYS:H	1:A:111:LYS:HE2	1.68	0.57
1:A:121:ASP:OD2	1:A:123:VAL:HG13	2.04	0.56
1:A:123:VAL:O	1:A:127:GLN:HG3	2.08	0.54
1:A:15[A]:LEU:O	1:A:50:ARG:HD2	2.09	0.53
1:A:111:LYS:H	1:A:111:LYS:HD3	1.73	0.53
1:A:99:TRP:CD2	1:A:101[A]:SER:HB3	2.43	0.53
1:A:111:LYS:CD	1:A:111:LYS:N	2.72	0.52
1:A:111:LYS:HD3	1:A:111:LYS:N	2.25	0.51
1:A:15[A]:LEU:HD21	1:A:43:LYS:HE3	1.93	0.51
1:A:248:GLU:HB2	1:A:302:LEU:HD21	1.93	0.50
1:A:110:ASP:HB2	1:A:111:LYS:HZ3	1.76	0.49
1:A:99:TRP:CE2	1:A:101[A]:SER:HB3	2.47	0.49
1:A:108:PHE:O	1:A:116:MET:HG3	2.12	0.49
1:A:218[A]:VAL:CG1	1:A:259:LEU:HD11	2.43	0.49
1:A:111:LYS:NZ	1:A:128:ASN:OD1	2.47	0.48
1:A:317:GLY:HA3	1:A:360:PHE:CZ	2.49	0.47
1:A:218[A]:VAL:HG21	1:A:231:ILE:HD11	1.99	0.45
1:A:129:LYS:O	1:A:133:LEU:HG	2.18	0.44
1:A:101[B]:SER:O	1:A:102[B]:GLN:O	2.35	0.43
1:A:263:ILE:HB	1:A:313:VAL:HA	2.00	0.43
1:A:119:GLU:OE2	1:A:121:ASP:HB3	2.18	0.42
1:A:134:LYS:HD2	5:A:1256:HOH:O	2.20	0.42
1:A:200:MET:SD	1:A:214:LEU:HD11	2.61	0.41
1:A:9:LYS:HB3	1:A:373:TRP:CD1	2.55	0.41
1:A:101[B]:SER:O	1:A:102[B]:GLN:C	2.58	0.41
1:A:41[B]:ASN:O	1:A:45:VAL:HG23	2.21	0.40
1:A:103[B]:VAL:CG1	5:A:1305:HOH:O	2.70	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	383/379 (101%)	375 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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	334/327 (102%)	322 (96%)	12 (4%)	35	20

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	28	PHE
1	A	103[A]	VAL
1	A	103[B]	VAL
1	A	111	LYS
1	A	123	VAL
1	A	137	GLU
1	A	220	GLN
1	A	301	LYS
1	A	302	LEU
1	A	323	THR
1	A	359	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	118	ASN
1	A	204	ASN
1	A	216	ASN
1	A	338	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	SO4	A	802	-	4,4,4	0.50	0	6,6,6	0.48	0

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.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.