



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 07:47 PM JST

PDB ID : 7WJ9  
Title : Crystal structure of Lactococcus lactis subsp. cremoris GH31 alpha-1,3-glucosidase, P21 space group  
Authors : Ikegaya, M.; Miyazaki, T.  
Deposited on : 2022-01-06  
Resolution : 1.75 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

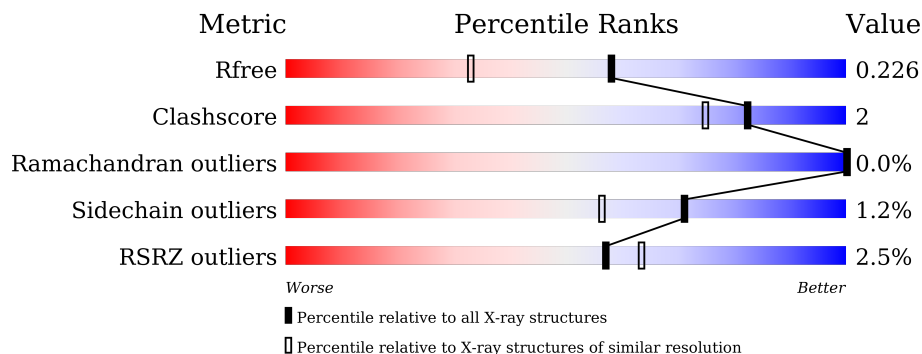
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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  $\leq 5\%$ . 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	759	
1	B	759	
1	C	759	
1	D	759	
1	E	759	
1	F	759	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 39082 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	733	Total 6059	C 3904	N 983	O 1157	S 15	0	6	0
1	B	728	Total 6004	C 3868	N 978	O 1144	S 14	0	3	0
1	C	728	Total 5998	C 3865	N 976	O 1143	S 14	0	2	0
1	D	728	Total 6019	C 3877	N 979	O 1149	S 14	0	6	0
1	F	728	Total 6001	C 3866	N 978	O 1143	S 14	0	2	0
1	E	728	Total 6006	C 3870	N 976	O 1146	S 14	0	4	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A2RM80
A	-18	GLY	-	expression tag	UNP A2RM80
A	-17	SER	-	expression tag	UNP A2RM80
A	-16	SER	-	expression tag	UNP A2RM80
A	-15	HIS	-	expression tag	UNP A2RM80
A	-14	HIS	-	expression tag	UNP A2RM80
A	-13	HIS	-	expression tag	UNP A2RM80
A	-12	HIS	-	expression tag	UNP A2RM80
A	-11	HIS	-	expression tag	UNP A2RM80
A	-10	HIS	-	expression tag	UNP A2RM80
A	-9	SER	-	expression tag	UNP A2RM80
A	-8	SER	-	expression tag	UNP A2RM80
A	-7	GLY	-	expression tag	UNP A2RM80
A	-6	LEU	-	expression tag	UNP A2RM80
A	-5	VAL	-	expression tag	UNP A2RM80
A	-4	PRO	-	expression tag	UNP A2RM80
A	-3	ARG	-	expression tag	UNP A2RM80

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A2RM80
A	-1	SER	-	expression tag	UNP A2RM80
A	0	HIS	-	expression tag	UNP A2RM80
B	-19	MET	-	initiating methionine	UNP A2RM80
B	-18	GLY	-	expression tag	UNP A2RM80
B	-17	SER	-	expression tag	UNP A2RM80
B	-16	SER	-	expression tag	UNP A2RM80
B	-15	HIS	-	expression tag	UNP A2RM80
B	-14	HIS	-	expression tag	UNP A2RM80
B	-13	HIS	-	expression tag	UNP A2RM80
B	-12	HIS	-	expression tag	UNP A2RM80
B	-11	HIS	-	expression tag	UNP A2RM80
B	-10	HIS	-	expression tag	UNP A2RM80
B	-9	SER	-	expression tag	UNP A2RM80
B	-8	SER	-	expression tag	UNP A2RM80
B	-7	GLY	-	expression tag	UNP A2RM80
B	-6	LEU	-	expression tag	UNP A2RM80
B	-5	VAL	-	expression tag	UNP A2RM80
B	-4	PRO	-	expression tag	UNP A2RM80
B	-3	ARG	-	expression tag	UNP A2RM80
B	-2	GLY	-	expression tag	UNP A2RM80
B	-1	SER	-	expression tag	UNP A2RM80
B	0	HIS	-	expression tag	UNP A2RM80
C	-19	MET	-	initiating methionine	UNP A2RM80
C	-18	GLY	-	expression tag	UNP A2RM80
C	-17	SER	-	expression tag	UNP A2RM80
C	-16	SER	-	expression tag	UNP A2RM80
C	-15	HIS	-	expression tag	UNP A2RM80
C	-14	HIS	-	expression tag	UNP A2RM80
C	-13	HIS	-	expression tag	UNP A2RM80
C	-12	HIS	-	expression tag	UNP A2RM80
C	-11	HIS	-	expression tag	UNP A2RM80
C	-10	HIS	-	expression tag	UNP A2RM80
C	-9	SER	-	expression tag	UNP A2RM80
C	-8	SER	-	expression tag	UNP A2RM80
C	-7	GLY	-	expression tag	UNP A2RM80
C	-6	LEU	-	expression tag	UNP A2RM80
C	-5	VAL	-	expression tag	UNP A2RM80
C	-4	PRO	-	expression tag	UNP A2RM80
C	-3	ARG	-	expression tag	UNP A2RM80
C	-2	GLY	-	expression tag	UNP A2RM80
C	-1	SER	-	expression tag	UNP A2RM80

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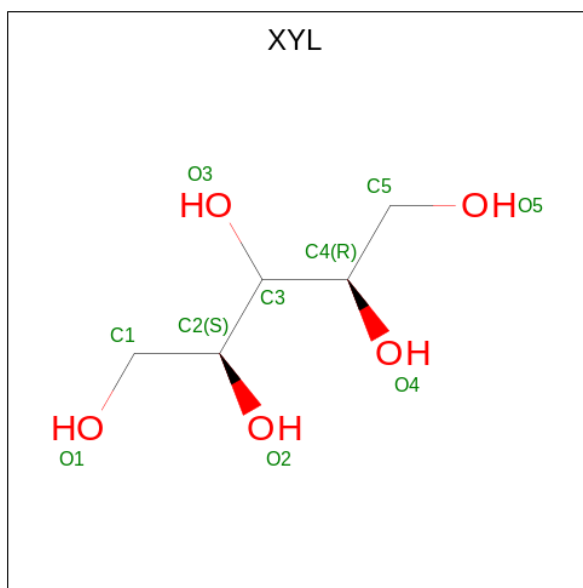
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP A2RM80
D	-19	MET	-	initiating methionine	UNP A2RM80
D	-18	GLY	-	expression tag	UNP A2RM80
D	-17	SER	-	expression tag	UNP A2RM80
D	-16	SER	-	expression tag	UNP A2RM80
D	-15	HIS	-	expression tag	UNP A2RM80
D	-14	HIS	-	expression tag	UNP A2RM80
D	-13	HIS	-	expression tag	UNP A2RM80
D	-12	HIS	-	expression tag	UNP A2RM80
D	-11	HIS	-	expression tag	UNP A2RM80
D	-10	HIS	-	expression tag	UNP A2RM80
D	-9	SER	-	expression tag	UNP A2RM80
D	-8	SER	-	expression tag	UNP A2RM80
D	-7	GLY	-	expression tag	UNP A2RM80
D	-6	LEU	-	expression tag	UNP A2RM80
D	-5	VAL	-	expression tag	UNP A2RM80
D	-4	PRO	-	expression tag	UNP A2RM80
D	-3	ARG	-	expression tag	UNP A2RM80
D	-2	GLY	-	expression tag	UNP A2RM80
D	-1	SER	-	expression tag	UNP A2RM80
D	0	HIS	-	expression tag	UNP A2RM80
F	-19	MET	-	initiating methionine	UNP A2RM80
F	-18	GLY	-	expression tag	UNP A2RM80
F	-17	SER	-	expression tag	UNP A2RM80
F	-16	SER	-	expression tag	UNP A2RM80
F	-15	HIS	-	expression tag	UNP A2RM80
F	-14	HIS	-	expression tag	UNP A2RM80
F	-13	HIS	-	expression tag	UNP A2RM80
F	-12	HIS	-	expression tag	UNP A2RM80
F	-11	HIS	-	expression tag	UNP A2RM80
F	-10	HIS	-	expression tag	UNP A2RM80
F	-9	SER	-	expression tag	UNP A2RM80
F	-8	SER	-	expression tag	UNP A2RM80
F	-7	GLY	-	expression tag	UNP A2RM80
F	-6	LEU	-	expression tag	UNP A2RM80
F	-5	VAL	-	expression tag	UNP A2RM80
F	-4	PRO	-	expression tag	UNP A2RM80
F	-3	ARG	-	expression tag	UNP A2RM80
F	-2	GLY	-	expression tag	UNP A2RM80
F	-1	SER	-	expression tag	UNP A2RM80
F	0	HIS	-	expression tag	UNP A2RM80
E	-19	MET	-	initiating methionine	UNP A2RM80

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	GLY	-	expression tag	UNP A2RM80
E	-17	SER	-	expression tag	UNP A2RM80
E	-16	SER	-	expression tag	UNP A2RM80
E	-15	HIS	-	expression tag	UNP A2RM80
E	-14	HIS	-	expression tag	UNP A2RM80
E	-13	HIS	-	expression tag	UNP A2RM80
E	-12	HIS	-	expression tag	UNP A2RM80
E	-11	HIS	-	expression tag	UNP A2RM80
E	-10	HIS	-	expression tag	UNP A2RM80
E	-9	SER	-	expression tag	UNP A2RM80
E	-8	SER	-	expression tag	UNP A2RM80
E	-7	GLY	-	expression tag	UNP A2RM80
E	-6	LEU	-	expression tag	UNP A2RM80
E	-5	VAL	-	expression tag	UNP A2RM80
E	-4	PRO	-	expression tag	UNP A2RM80
E	-3	ARG	-	expression tag	UNP A2RM80
E	-2	GLY	-	expression tag	UNP A2RM80
E	-1	SER	-	expression tag	UNP A2RM80
E	0	HIS	-	expression tag	UNP A2RM80

- Molecule 2 is Xylitol (three-letter code: XYL) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>5</sub>).



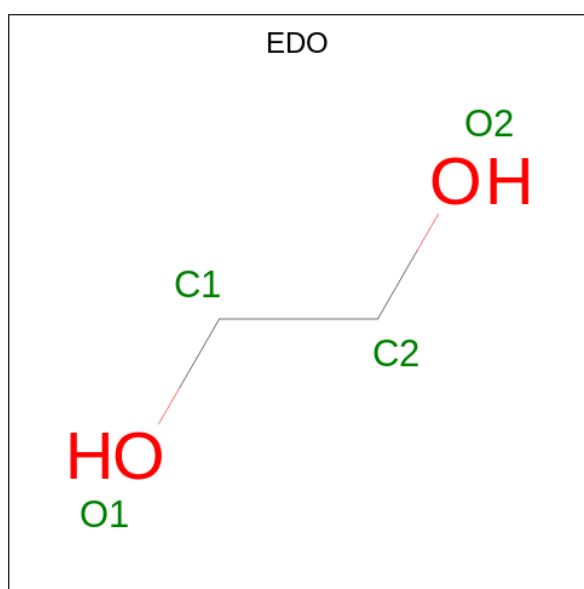
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		
2	E	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

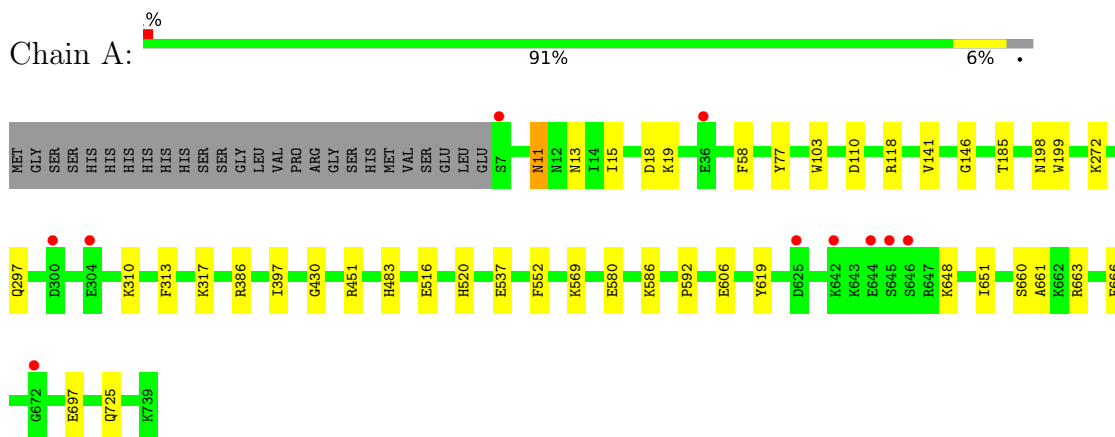
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	576	Total O 576 576	0	0
4	B	459	Total O 459 459	0	0
4	C	407	Total O 407 407	0	0
4	D	504	Total O 504 504	0	0
4	F	401	Total O 401 401	0	0
4	E	532	Total O 532 532	0	0



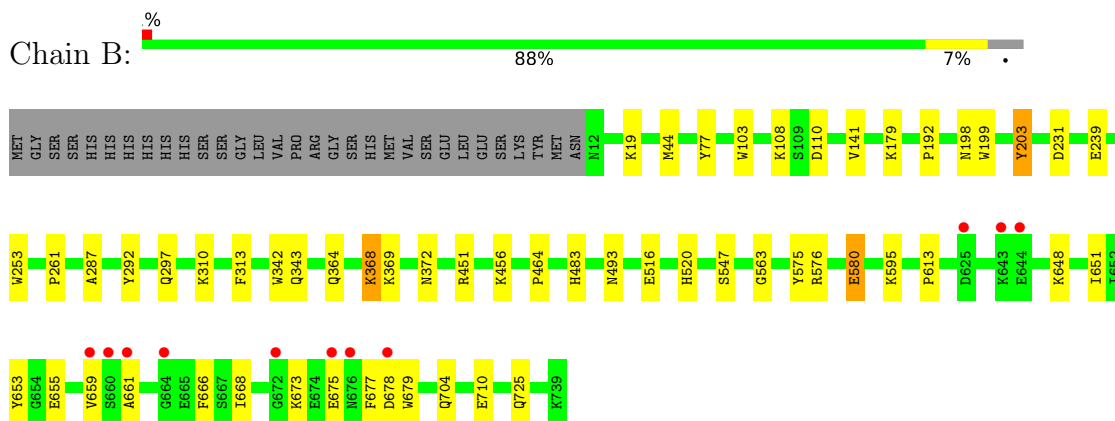
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

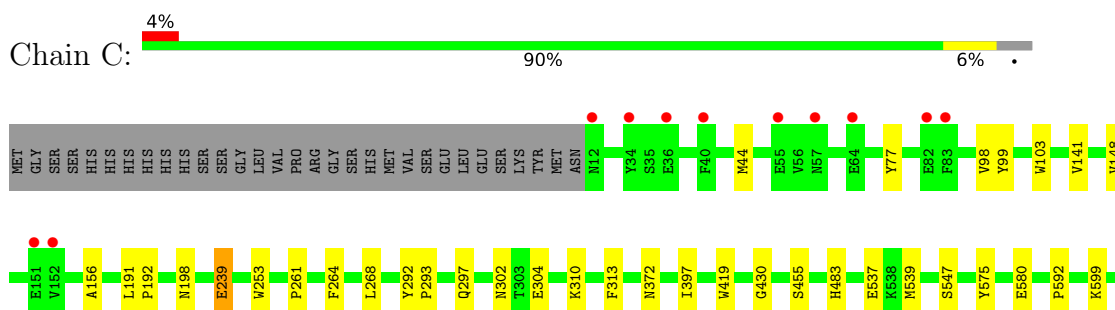
- Molecule 1: Alpha-xylosidase

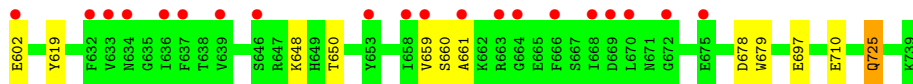


- Molecule 1: Alpha-xylosidase

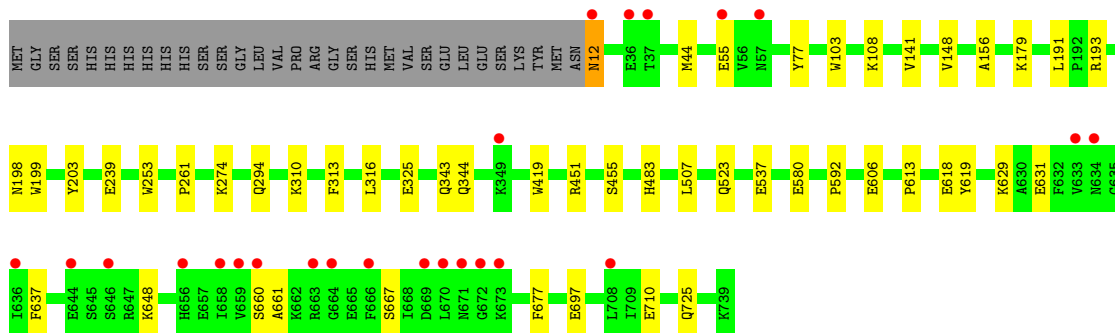
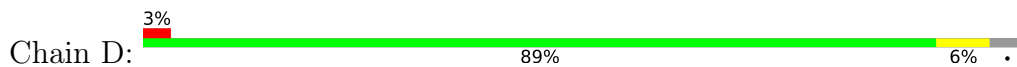


- Molecule 1: Alpha-xylosidase

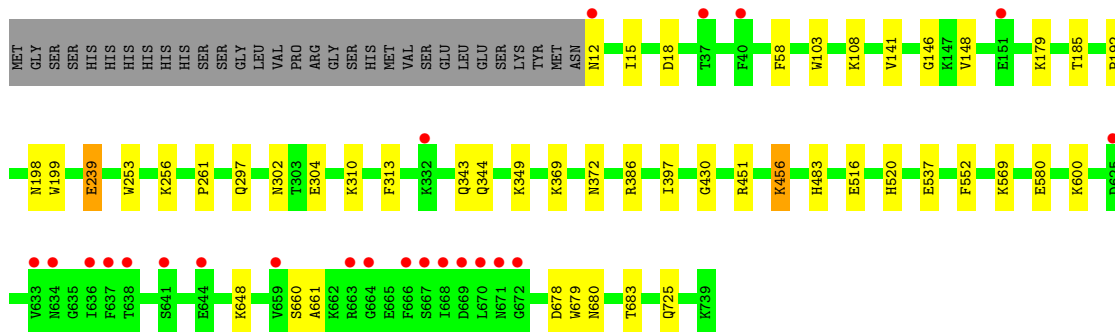
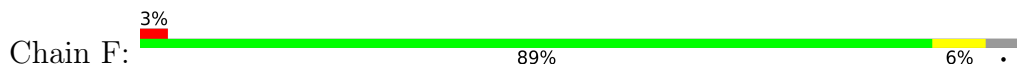




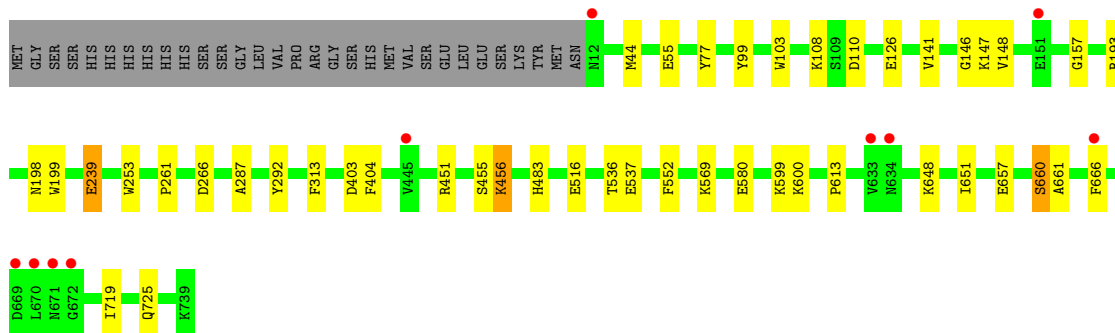
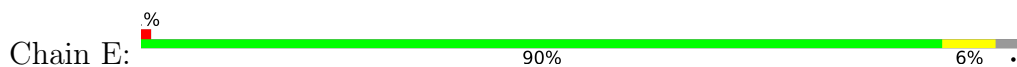
• Molecule 1: Alpha-xylosidase



• Molecule 1: Alpha-xylosidase



• Molecule 1: Alpha-xylosidase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.40Å 207.85Å 117.90Å 90.00° 103.63° 90.00°	Depositor
Resolution (Å)	47.19 – 1.75 47.15 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.19-1.75) 97.9 (47.15-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.186 , 0.217 0.197 , 0.226	Depositor DCC
$R_{free}$ test set	26657 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.016 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	39082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: XYL, EDO

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	0.78	1/6245 (0.0%)	0.85	1/8454 (0.0%)
1	B	0.72	1/6177 (0.0%)	0.84	1/8364 (0.0%)
1	C	0.73	1/6171 (0.0%)	0.84	2/8356 (0.0%)
1	D	0.75	1/6198 (0.0%)	0.85	2/8392 (0.0%)
1	E	0.75	2/6185 (0.0%)	0.85	3/8375 (0.0%)
1	F	0.73	1/6171 (0.0%)	0.82	3/8356 (0.0%)
All	All	0.74	7/37147 (0.0%)	0.84	12/50297 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	580	GLU	CD-OE1	9.97	1.36	1.25
1	A	580	GLU	CD-OE1	9.96	1.36	1.25
1	C	580	GLU	CD-OE1	8.64	1.35	1.25
1	E	580	GLU	CD-OE1	8.54	1.35	1.25
1	F	580	GLU	CD-OE1	6.64	1.32	1.25

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	E	193	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	E	239	GLU	CB-CA-C	-6.07	98.25	110.40
1	A	118	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	239	GLU	CB-CA-C	-5.67	99.07	110.40

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	6059	0	5809	29	1
1	B	6004	0	5751	37	0
1	C	5998	0	5745	28	0
1	D	6019	0	5766	37	0
1	E	6006	0	5754	27	1
1	F	6001	0	5746	26	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
2	C	10	0	12	0	0
2	D	10	0	12	0	0
2	E	10	0	12	0	0
2	F	10	0	12	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
3	D	12	0	18	1	0
3	E	12	0	18	0	0
3	F	8	0	12	0	0
4	A	576	0	0	9	0
4	B	459	0	0	9	0
4	C	407	0	0	9	0
4	D	504	0	0	11	0
4	E	532	0	0	8	0
4	F	401	0	0	5	0
All	All	39082	0	34727	174	1

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 2.

The worst 5 of 174 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:D:618:GLU:OE2	1:D:629:LYS:HE2	1.65	0.97
1:A:697:GLU:HG2	4:A:908:HOH:O	1.69	0.92
1:B:44:MET:HG2	4:B:1262:HOH:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ASN:H	1:E:483:HIS:HE1	1.26	0.83
1:A:272:LYS:HE3	4:A:1175:HOH:O	1.81	0.79

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ARG:NH2	1:E:266[B]:ASP:OD2[1_554]	1.81	0.39

## 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	737/759 (97%)	715 (97%)	22 (3%)	0	100	100
1	B	729/759 (96%)	704 (97%)	25 (3%)	0	100	100
1	C	728/759 (96%)	700 (96%)	28 (4%)	0	100	100
1	D	732/759 (96%)	713 (97%)	17 (2%)	2 (0%)	41	22
1	E	730/759 (96%)	709 (97%)	19 (3%)	2 (0%)	41	22
1	F	728/759 (96%)	701 (96%)	27 (4%)	0	100	100
All	All	4384/4554 (96%)	4242 (97%)	138 (3%)	4 (0%)	100	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	455[A]	SER
1	E	455[B]	SER
1	D	455[A]	SER
1	D	455[B]	SER

### 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	656/673 (98%)	651 (99%)	5 (1%)	81	72
1	B	648/673 (96%)	638 (98%)	10 (2%)	65	49
1	C	647/673 (96%)	640 (99%)	7 (1%)	73	60
1	D	651/673 (97%)	643 (99%)	8 (1%)	71	56
1	E	649/673 (96%)	642 (99%)	7 (1%)	73	60
1	F	647/673 (96%)	637 (98%)	10 (2%)	65	49
All	All	3898/4038 (96%)	3851 (99%)	47 (1%)	71	56

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	667	SER
1	F	297	GLN
1	D	710	GLU
1	F	148	VAL
1	F	369	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	362	GLN
1	D	483	HIS
1	E	365	ASN
1	D	372	ASN
1	D	680	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](#)

20 ligands are modelled in this entry.

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	$\# Z  > 2$
2	XYL	B	801	-	9,9,9	0.42	0	11,11,11	0.97	0
3	EDO	E	802	-	3,3,3	0.07	0	2,2,2	0.23	0
2	XYL	A	801	-	9,9,9	0.22	0	11,11,11	0.78	0
3	EDO	A	802	-	3,3,3	0.32	0	2,2,2	0.24	0
2	XYL	E	801	-	9,9,9	0.23	0	11,11,11	0.94	0
3	EDO	F	802	-	3,3,3	0.31	0	2,2,2	0.41	0
3	EDO	D	802	-	3,3,3	0.14	0	2,2,2	0.35	0
3	EDO	F	803	-	3,3,3	0.05	0	2,2,2	0.24	0
3	EDO	D	804	-	3,3,3	0.15	0	2,2,2	0.13	0
3	EDO	C	803	-	3,3,3	0.21	0	2,2,2	0.58	0
2	XYL	D	801	-	9,9,9	0.42	0	11,11,11	1.02	0
3	EDO	E	804	-	3,3,3	0.10	0	2,2,2	0.08	0
3	EDO	E	803	-	3,3,3	0.19	0	2,2,2	0.21	0
2	XYL	F	801	-	9,9,9	0.20	0	11,11,11	0.85	0
3	EDO	A	803	-	3,3,3	0.33	0	2,2,2	0.27	0
3	EDO	B	802	-	3,3,3	0.24	0	2,2,2	0.28	0
2	XYL	C	801	-	9,9,9	0.48	0	11,11,11	0.77	0
3	EDO	C	802	-	3,3,3	0.08	0	2,2,2	0.12	0
3	EDO	D	803	-	3,3,3	0.40	0	2,2,2	0.52	0
3	EDO	B	803	-	3,3,3	0.21	0	2,2,2	0.25	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYL	B	801	-	-	1/12/12/12	-
3	EDO	E	802	-	-	0/1/1/1	-
2	XYL	A	801	-	-	0/12/12/12	-
3	EDO	A	802	-	-	0/1/1/1	-
2	XYL	E	801	-	-	1/12/12/12	-
3	EDO	F	802	-	-	0/1/1/1	-
3	EDO	D	802	-	-	0/1/1/1	-
3	EDO	F	803	-	-	0/1/1/1	-
3	EDO	D	804	-	-	0/1/1/1	-
3	EDO	C	803	-	-	1/1/1/1	-
2	XYL	D	801	-	-	0/12/12/12	-
3	EDO	E	804	-	-	1/1/1/1	-
3	EDO	E	803	-	-	0/1/1/1	-
2	XYL	F	801	-	-	1/12/12/12	-
3	EDO	A	803	-	-	1/1/1/1	-
3	EDO	B	802	-	-	0/1/1/1	-
2	XYL	C	801	-	-	0/12/12/12	-
3	EDO	C	802	-	-	0/1/1/1	-
3	EDO	D	803	-	-	0/1/1/1	-
3	EDO	B	803	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	EDO	O1-C1-C2-O2
3	C	803	EDO	O1-C1-C2-O2
2	E	801	XYL	O1-C1-C2-O2
2	F	801	XYL	O1-C1-C2-O2
2	B	801	XYL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	804	EDO	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	733/759 (96%)	-0.24	10 (1%) 75 82	17, 25, 45, 64	0
1	B	728/759 (95%)	-0.17	11 (1%) 73 80	21, 30, 52, 93	0
1	C	728/759 (95%)	0.06	31 (4%) 35 41	20, 32, 58, 82	0
1	D	728/759 (95%)	-0.16	24 (3%) 46 53	18, 26, 52, 72	0
1	E	728/759 (95%)	-0.18	10 (1%) 75 82	17, 26, 49, 73	0
1	F	728/759 (95%)	-0.07	23 (3%) 47 54	22, 31, 58, 80	0
All	All	4373/4554 (96%)	-0.13	109 (2%) 57 63	17, 28, 53, 93	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	672	GLY	5.5
1	B	676	ASN	4.5
1	E	672	GLY	4.5
1	B	661	ALA	4.4
1	D	666	PHE	4.2

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	B	802	4/4	0.91	0.10	42,45,46,51	0
3	EDO	E	802	4/4	0.91	0.10	43,43,44,45	0
3	EDO	D	804	4/4	0.94	0.09	33,39,40,41	0
3	EDO	F	802	4/4	0.94	0.07	43,43,45,47	0
3	EDO	A	802	4/4	0.94	0.07	37,37,37,38	0
3	EDO	E	804	4/4	0.94	0.09	42,45,46,48	0
3	EDO	B	803	4/4	0.95	0.10	28,32,39,41	0
3	EDO	F	803	4/4	0.95	0.08	26,30,33,40	0
3	EDO	D	802	4/4	0.95	0.09	36,43,43,44	0
3	EDO	E	803	4/4	0.95	0.10	27,31,36,38	0
2	XYL	B	801	10/10	0.95	0.11	23,26,29,30	0
3	EDO	C	802	4/4	0.96	0.08	25,33,38,40	0
2	XYL	C	801	10/10	0.96	0.10	21,24,25,28	0
3	EDO	D	803	4/4	0.96	0.08	22,27,33,35	0
2	XYL	D	801	10/10	0.97	0.06	19,20,22,24	0
2	XYL	F	801	10/10	0.97	0.08	22,25,28,30	0
2	XYL	E	801	10/10	0.97	0.09	18,20,21,26	0
3	EDO	C	803	4/4	0.97	0.09	42,44,45,45	0
2	XYL	A	801	10/10	0.97	0.08	20,22,24,25	0
3	EDO	A	803	4/4	0.97	0.06	28,34,39,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.