



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:48 AM GMT

PDB ID : 3FYT  
Title : Crystal structure of Bacillus pumilus acetyl xylan esterase S181A mutant in complex with beta-D-xylopyranose  
Authors : Krastanova, I.; Cassetta, A.; Lamba, D.  
Deposited on : 2009-01-23  
Resolution : 2.58 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

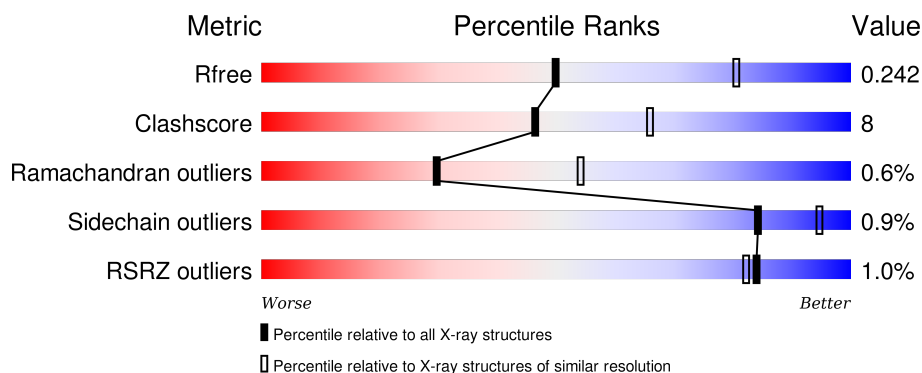
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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))
$R_{free}$	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	320	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 20%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>78%</span> <span>20%</span> </div> </div>
1	B	320	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 20%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>78%</span> <span>20%</span> </div> </div>
1	C	320	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 18%, green 79%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>79%</span> <span>18%</span> </div> </div>
1	D	320	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 21%, green 77%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>77%</span> <span>21%</span> </div> </div>
1	E	320	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 78%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>78%</span> <span>19%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	320	 79% 17% ..
1	G	320	 81% 16% ..
1	H	320	 79% 18% ..
1	I	320	 77% 19% ..
1	L	320	 83% 15% ..
1	M	320	 81% 15% ..
1	N	320	 81% 16% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XYP	C	1002	-	-	-	X
3	XYP	E	1000	-	-	-	X
3	XYP	F	1001	-	-	-	X
3	XYP	H	1005	-	-	-	X
3	XYP	L	1004	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30500 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 Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2518	1636	413	466	3			
1	B	314	Total	C	N	O	S	0	0	0
			2510	1630	412	465	3			
1	C	312	Total	C	N	O	S	0	0	0
			2491	1617	410	461	3			
1	D	315	Total	C	N	O	S	0	0	0
			2518	1636	413	466	3			
1	E	314	Total	C	N	O	S	0	0	0
			2510	1630	412	465	3			
1	F	311	Total	C	N	O	S	0	0	0
			2483	1611	409	460	3			
1	G	312	Total	C	N	O	S	0	0	0
			2491	1617	410	461	3			
1	H	315	Total	C	N	O	S	0	0	0
			2518	1636	413	466	3			
1	I	313	Total	C	N	O	S	0	0	0
			2499	1621	411	464	3			
1	L	316	Total	C	N	O	S	0	0	0
			2524	1639	414	468	3			
1	M	311	Total	C	N	O	S	0	0	0
			2483	1611	409	460	3			
1	N	313	Total	C	N	O	S	0	0	0
			2499	1621	411	464	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	SER	ENGINEERED	UNP Q9K5F2
B	181	ALA	SER	ENGINEERED	UNP Q9K5F2
C	181	ALA	SER	ENGINEERED	UNP Q9K5F2
D	181	ALA	SER	ENGINEERED	UNP Q9K5F2
E	181	ALA	SER	ENGINEERED	UNP Q9K5F2

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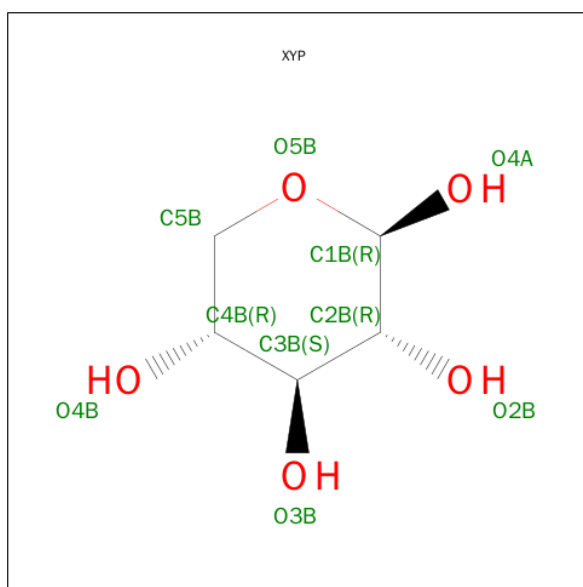
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Chain	Residue	Modelled	Actual	Comment	Reference
F	181	ALA	SER	ENGINEERED	UNP Q9K5F2
G	181	ALA	SER	ENGINEERED	UNP Q9K5F2
H	181	ALA	SER	ENGINEERED	UNP Q9K5F2
I	181	ALA	SER	ENGINEERED	UNP Q9K5F2
L	181	ALA	SER	ENGINEERED	UNP Q9K5F2
M	181	ALA	SER	ENGINEERED	UNP Q9K5F2
N	181	ALA	SER	ENGINEERED	UNP Q9K5F2

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Cl 2 2	0	0
2	D	3	Total Cl 3 3	0	0
2	E	2	Total Cl 2 2	0	0
2	H	3	Total Cl 3 3	0	0
2	B	3	Total Cl 3 3	0	0
2	I	3	Total Cl 3 3	0	0
2	C	3	Total Cl 3 3	0	0
2	A	3	Total Cl 3 3	0	0
2	N	3	Total Cl 3 3	0	0
2	L	3	Total Cl 3 3	0	0
2	F	3	Total Cl 3 3	0	0
2	M	3	Total Cl 3 3	0	0

- Molecule 3 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	F	1	Total	C	O	0	0
			10	5	5		
3	H	1	Total	C	O	0	0
			10	5	5		
3	L	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	19	Total	O	0	0
			19	19		
4	C	25	Total	O	0	0
			25	25		
4	D	15	Total	O	0	0
			15	15		
4	E	26	Total	O	0	0
			26	26		
4	F	30	Total	O	0	0
			30	30		

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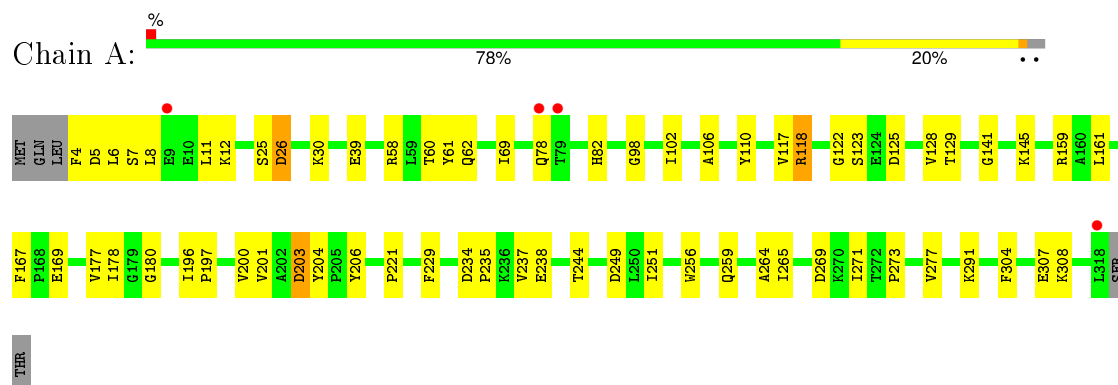
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	39	Total 39	O 39	0	0
4	H	39	Total 39	O 39	0	0
4	I	39	Total 39	O 39	0	0
4	L	26	Total 26	O 26	0	0
4	M	36	Total 36	O 36	0	0
4	N	37	Total 37	O 37	0	0

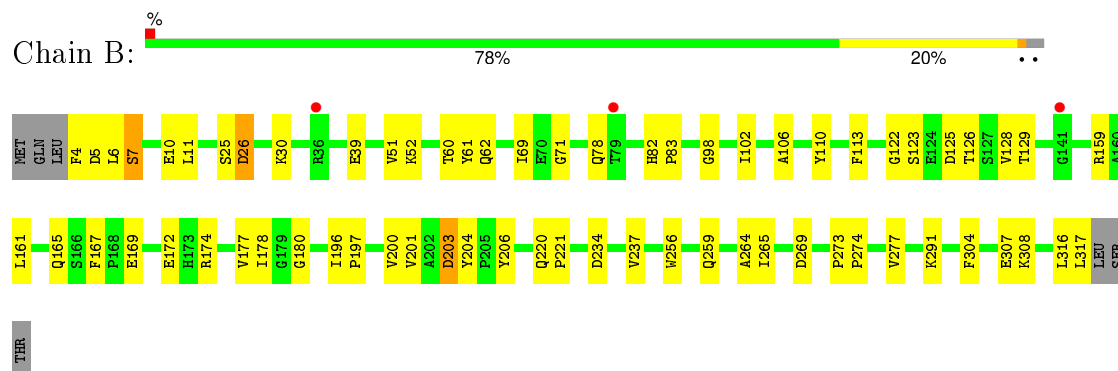
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

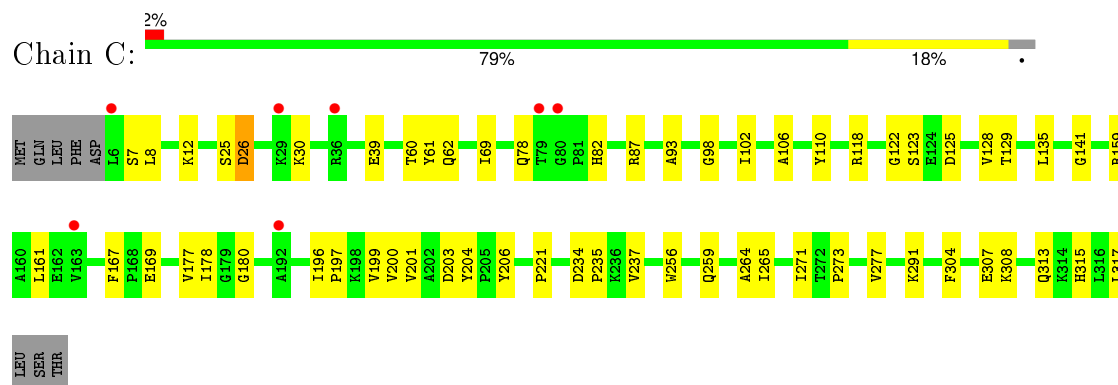
- Molecule 1: Acetyl xylan esterase



- Molecule 1: Acetyl xylan esterase

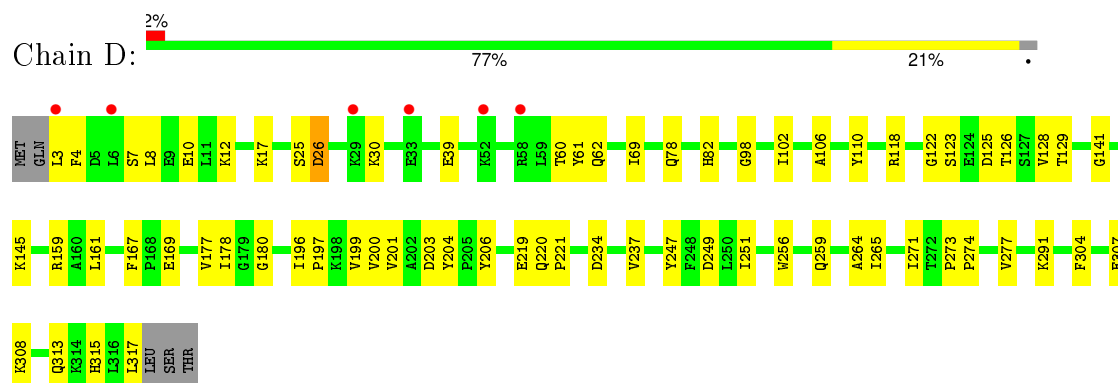


- Molecule 1: Acetyl xylan esterase

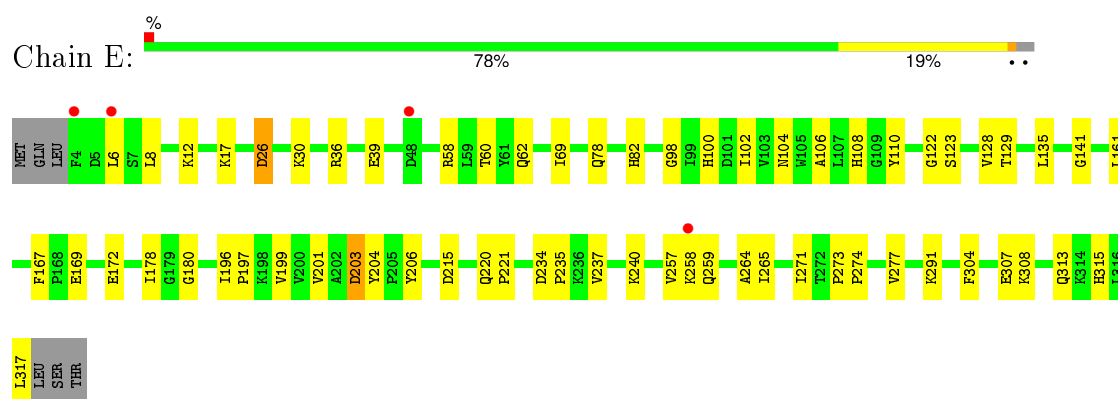




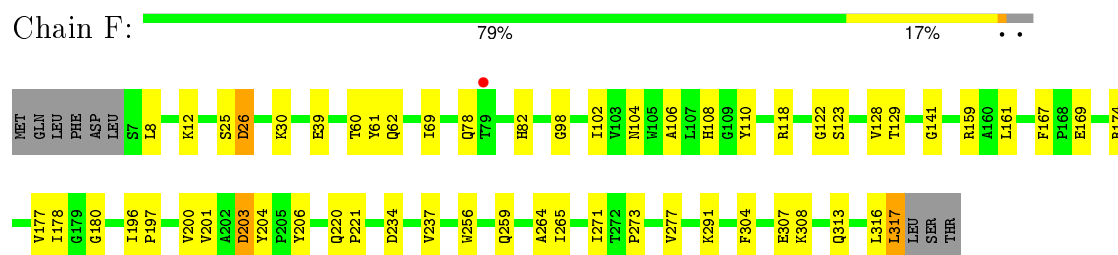
- Molecule 1: Acetyl xylan esterase



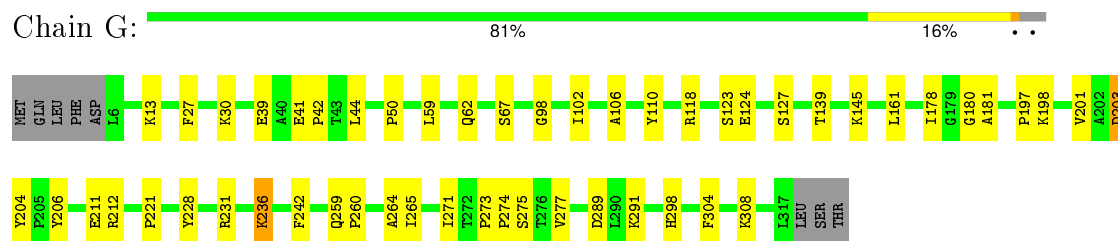
- Molecule 1: Acetyl xylan esterase



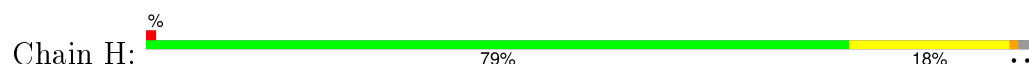
- Molecule 1: Acetyl xylan esterase

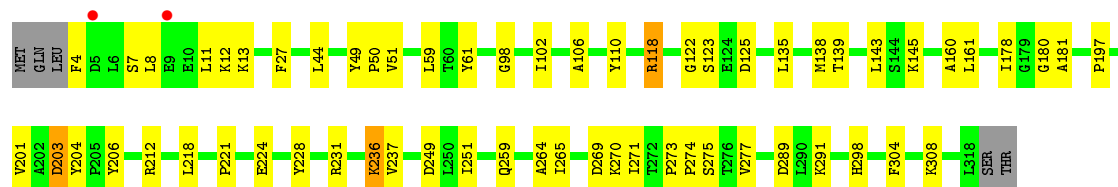


- Molecule 1: Acetyl xylan esterase



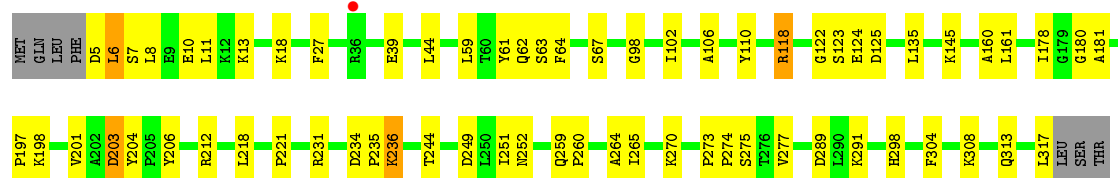
- Molecule 1: Acetyl xylan esterase





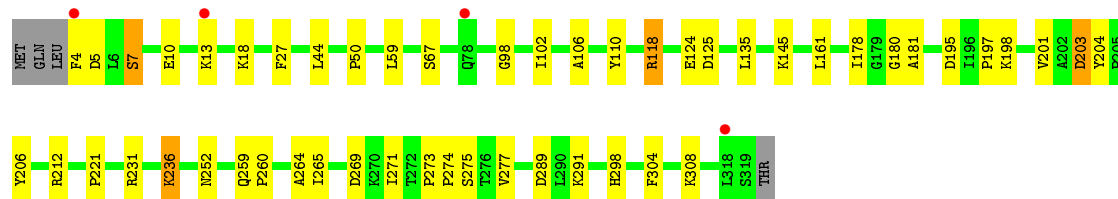
- Molecule 1: Acetyl xylan esterase

Chain I: 77% 19% ..



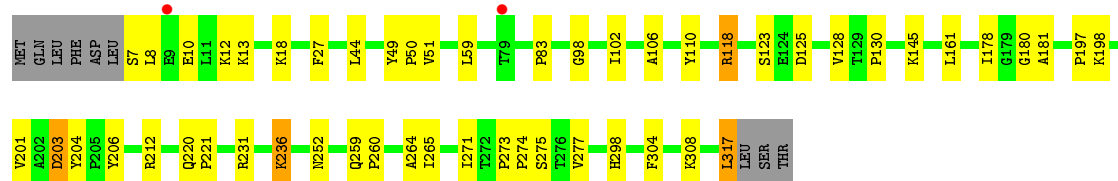
- Molecule 1: Acetyl xylan esterase

Chain L: 83% 15% ..



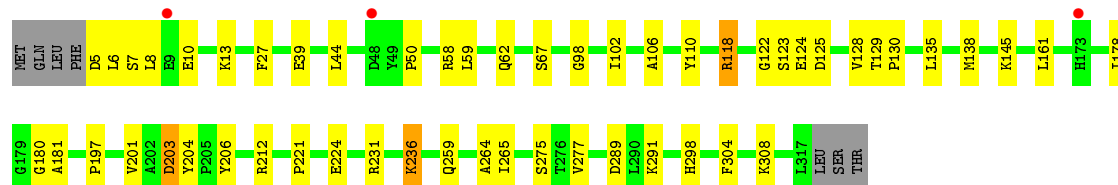
- Molecule 1: Acetyl xylan esterase

Chain M: 81% 15% ..



- Molecule 1: Acetyl xylan esterase

Chain N: 81% 16% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.19Å 167.99Å 144.47Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	24.83 – 2.58 24.83 – 2.58	Depositor EDS
% Data completeness (in resolution range)	77.4 (24.83-2.58) 73.5 (24.83-2.58)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.66 (at 2.57Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.188 , 0.241 0.189 , 0.242	Depositor DCC
$R_{free}$ test set	10126 reflections (10.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.0	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.115 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 100895 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	30500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: XYP, CL

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	0.39	0/2590	0.58	0/3517
1	B	0.38	0/2582	0.57	0/3506
1	C	0.37	0/2562	0.57	0/3479
1	D	0.37	0/2590	0.57	0/3517
1	E	0.38	0/2582	0.57	0/3506
1	F	0.39	0/2554	0.58	0/3468
1	G	0.38	0/2562	0.59	0/3479
1	H	0.39	0/2590	0.59	0/3517
1	I	0.39	0/2570	0.60	0/3490
1	L	0.39	0/2596	0.59	0/3525
1	M	0.39	0/2554	0.59	0/3468
1	N	0.40	0/2570	0.60	0/3490
All	All	0.39	0/30902	0.58	0/41962

There are no bond length outliers.

There are no bond angle outliers.

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	2518	0	2463	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2510	0	2452	44	0
1	C	2491	0	2439	41	0
1	D	2518	0	2463	45	0
1	E	2510	0	2452	41	0
1	F	2483	0	2428	35	0
1	G	2491	0	2439	32	0
1	H	2518	0	2463	37	0
1	I	2499	0	2443	44	0
1	L	2524	0	2468	33	0
1	M	2483	0	2428	35	0
1	N	2499	0	2443	35	0
2	A	3	0	0	1	0
2	B	3	0	0	0	0
2	C	3	0	0	1	0
2	D	3	0	0	1	0
2	E	2	0	0	0	0
2	F	3	0	0	1	0
2	G	2	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	1	0
2	L	3	0	0	0	0
2	M	3	0	0	0	0
2	N	3	0	0	0	0
3	C	20	0	20	3	0
3	E	10	0	10	0	0
3	F	10	0	10	0	0
3	H	10	0	10	0	0
3	L	10	0	10	0	0
4	A	31	0	0	2	0
4	B	19	0	0	0	0
4	C	25	0	0	0	0
4	D	15	0	0	1	0
4	E	26	0	0	5	0
4	F	30	0	0	0	0
4	G	39	0	0	2	0
4	H	39	0	0	1	0
4	I	39	0	0	1	0
4	L	26	0	0	0	0
4	M	36	0	0	0	0
4	N	37	0	0	1	0
All	All	30500	0	29441	455	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 455 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:M:201:VAL:HG11	1:M:308:LYS:HG3	1.55	0.88
1:I:201:VAL:HG11	1:I:308:LYS:HG3	1.55	0.88
1:H:201:VAL:HG11	1:H:308:LYS:HG3	1.58	0.85
1:G:201:VAL:HG11	1:G:308:LYS:HG3	1.59	0.84
1:E:206:TYR:OH	1:E:221:PRO:HG2	1.81	0.81

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	313/320 (98%)	293 (94%)	19 (6%)	1 (0%)	46	70
1	B	312/320 (98%)	294 (94%)	17 (5%)	1 (0%)	46	70
1	C	310/320 (97%)	293 (94%)	17 (6%)	0	100	100
1	D	313/320 (98%)	295 (94%)	16 (5%)	2 (1%)	30	54
1	E	312/320 (98%)	293 (94%)	19 (6%)	0	100	100
1	F	309/320 (97%)	293 (95%)	15 (5%)	1 (0%)	46	70
1	G	310/320 (97%)	295 (95%)	12 (4%)	3 (1%)	19	38
1	H	313/320 (98%)	297 (95%)	14 (4%)	2 (1%)	30	54
1	I	311/320 (97%)	297 (96%)	12 (4%)	2 (1%)	30	54
1	L	314/320 (98%)	298 (95%)	13 (4%)	3 (1%)	19	38
1	M	309/320 (97%)	295 (96%)	11 (4%)	3 (1%)	19	38
1	N	311/320 (97%)	294 (94%)	14 (4%)	3 (1%)	19	38
All	All	3737/3840 (97%)	3537 (95%)	179 (5%)	21 (1%)	30	54

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	6	LEU
1	B	7	SER
1	D	4	PHE
1	N	6	LEU
1	A	118	ARG

### 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	264/269 (98%)	262 (99%)	2 (1%)	86	95
1	B	263/269 (98%)	260 (99%)	3 (1%)	80	93
1	C	261/269 (97%)	259 (99%)	2 (1%)	86	95
1	D	264/269 (98%)	263 (100%)	1 (0%)	93	98
1	E	263/269 (98%)	260 (99%)	3 (1%)	80	93
1	F	260/269 (97%)	257 (99%)	3 (1%)	78	92
1	G	261/269 (97%)	259 (99%)	2 (1%)	86	95
1	H	264/269 (98%)	262 (99%)	2 (1%)	86	95
1	I	262/269 (97%)	260 (99%)	2 (1%)	86	95
1	L	265/269 (98%)	262 (99%)	3 (1%)	80	93
1	M	260/269 (97%)	257 (99%)	3 (1%)	78	92
1	N	262/269 (97%)	259 (99%)	3 (1%)	80	93
All	All	3149/3228 (98%)	3120 (99%)	29 (1%)	84	94

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	317	LEU
1	H	203	ASP
1	N	5	ASP
1	G	203	ASP

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Mol	Chain	Res	Type
1	H	236	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	313	GLN
1	E	82	HIS
1	L	108	HIS
1	D	82	HIS
1	G	108	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 34 are monoatomic - leaving 6 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	$\# Z  > 2$
3	XYP	C	1002	-	10,10,10	0.95	0	12,14,14	0.91	0
3	XYP	C	1003	-	10,10,10	1.15	1 (10%)	12,14,14	0.89	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	XYP	E	1000	-	10,10,10	1.02	0	12,14,14	0.95	0
3	XYP	F	1001	-	10,10,10	1.08	1 (10%)	12,14,14	0.97	0
3	XYP	H	1005	-	10,10,10	1.03	1 (10%)	12,14,14	0.95	0
3	XYP	L	1004	-	10,10,10	0.98	0	12,14,14	0.96	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
3	XYP	C	1002	-	-	0/0/17/17	0/1/1/1
3	XYP	C	1003	-	-	0/0/17/17	0/1/1/1
3	XYP	E	1000	-	-	0/0/17/17	0/1/1/1
3	XYP	F	1001	-	-	0/0/17/17	0/1/1/1
3	XYP	H	1005	-	-	0/0/17/17	0/1/1/1
3	XYP	L	1004	-	-	0/0/17/17	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1005	XYP	O5B-C1B	-2.27	1.39	1.43
3	F	1001	XYP	O5B-C1B	-2.03	1.40	1.43
3	C	1003	XYP	O5B-C5B	2.01	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1003	XYP	3	0

## 5.7 Other polymers [i](#)

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 [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	315/320 (98%)	-0.13	4 (1%) 79 77	10, 25, 48, 63	0
1	B	314/320 (98%)	-0.01	3 (0%) 84 82	11, 30, 49, 60	0
1	C	312/320 (97%)	0.07	7 (2%) 65 61	14, 32, 54, 72	0
1	D	315/320 (98%)	0.09	6 (1%) 70 66	15, 32, 54, 64	0
1	E	314/320 (98%)	0.05	4 (1%) 79 77	15, 32, 51, 65	0
1	F	311/320 (97%)	-0.13	1 (0%) 94 94	12, 25, 47, 62	0
1	G	312/320 (97%)	-0.23	0 100 100	10, 24, 43, 59	0
1	H	315/320 (98%)	-0.16	2 (0%) 90 89	8, 23, 45, 60	0
1	I	313/320 (97%)	-0.18	1 (0%) 94 94	9, 24, 45, 61	0
1	L	316/320 (98%)	-0.08	4 (1%) 79 77	10, 26, 48, 60	0
1	M	311/320 (97%)	-0.16	2 (0%) 90 89	10, 25, 45, 64	0
1	N	313/320 (97%)	-0.21	3 (0%) 84 82	6, 22, 43, 65	0
All	All	3761/3840 (97%)	-0.09	37 (0%) 84 82	6, 27, 48, 72	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36	ARG	3.8
1	E	6	LEU	3.7
1	D	6	LEU	3.4
1	L	78	GLN	3.2
1	D	52	LYS	3.0

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	XYP	H	1005	10/10	0.87	0.28	15.13	49,55,61,68	0
3	XYP	L	1004	10/10	0.90	0.31	9.54	32,44,52,61	0
3	XYP	E	1000	10/10	0.92	0.26	7.09	40,48,60,65	0
3	XYP	F	1001	10/10	0.85	0.23	4.40	34,44,57,70	0
3	XYP	C	1002	10/10	0.86	0.22	3.86	27,38,55,55	0
3	XYP	C	1003	10/10	0.85	0.17	0.15	29,39,48,49	0
2	CL	N	322	1/1	0.97	0.14	-0.07	43,43,43,43	0
2	CL	D	322	1/1	0.99	0.13	-0.56	39,39,39,39	0
2	CL	B	322	1/1	0.98	0.12	-0.67	44,44,44,44	0
2	CL	A	321	1/1	0.98	0.11	-0.87	40,40,40,40	0
2	CL	L	322	1/1	0.97	0.11	-0.92	44,44,44,44	0
2	CL	I	321	1/1	0.96	0.12	-0.96	36,36,36,36	0
2	CL	H	321	1/1	0.96	0.10	-1.24	30,30,30,30	0
2	CL	C	321	1/1	0.99	0.09	-1.39	29,29,29,29	0
2	CL	B	321	1/1	0.97	0.08	-1.52	30,30,30,30	0
2	CL	H	322	1/1	0.98	0.08	-1.84	29,29,29,29	0
2	CL	G	321	1/1	0.99	0.08	-1.85	28,28,28,28	0
2	CL	N	321	1/1	0.95	0.10	-1.92	31,31,31,31	0
2	CL	I	322	1/1	0.98	0.08	-2.24	27,27,27,27	0
2	CL	L	321	1/1	0.98	0.07	-2.25	35,35,35,35	0
2	CL	F	321	1/1	0.98	0.05	-2.89	30,30,30,30	0
2	CL	E	321	1/1	0.98	0.05	-2.94	28,28,28,28	0
2	CL	D	321	1/1	0.99	0.04	-3.17	35,35,35,35	0
2	CL	F	322	1/1	0.98	0.07	-3.30	30,30,30,30	0
2	CL	M	321	1/1	0.99	0.05	-3.32	26,26,26,26	0
2	CL	A	322	1/1	0.99	0.04	-3.55	29,29,29,29	0
2	CL	M	322	1/1	0.99	0.06	-5.21	24,24,24,24	0
2	CL	C	322	1/1	0.98	0.06	-5.92	27,27,27,27	0
2	CL	I	323	1/1	0.98	0.05	-	31,31,31,31	0
2	CL	E	322	1/1	0.96	0.08	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	M	323	1/1	0.97	0.07	-	32,32,32,32	0
2	CL	G	322	1/1	0.97	0.07	-	30,30,30,30	0
2	CL	F	323	1/1	0.99	0.07	-	30,30,30,30	0
2	CL	D	323	1/1	0.98	0.07	-	47,47,47,47	0
2	CL	H	323	1/1	0.98	0.06	-	36,36,36,36	0
2	CL	A	323	1/1	0.97	0.08	-	45,45,45,45	0
2	CL	L	323	1/1	0.99	0.12	-	33,33,33,33	0
2	CL	N	323	1/1	0.97	0.12	-	31,31,31,31	0
2	CL	B	323	1/1	0.98	0.08	-	26,26,26,26	0
2	CL	C	323	1/1	0.99	0.04	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.