



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 05:05 am BST

PDB ID : 1VLQ
Title : Crystal structure of Acetyl xylan esterase (TM0077) from *Thermotoga maritima* at 2.10 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2004-08-09
Resolution : 2.10 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 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	:	2.11
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)	:	2.11

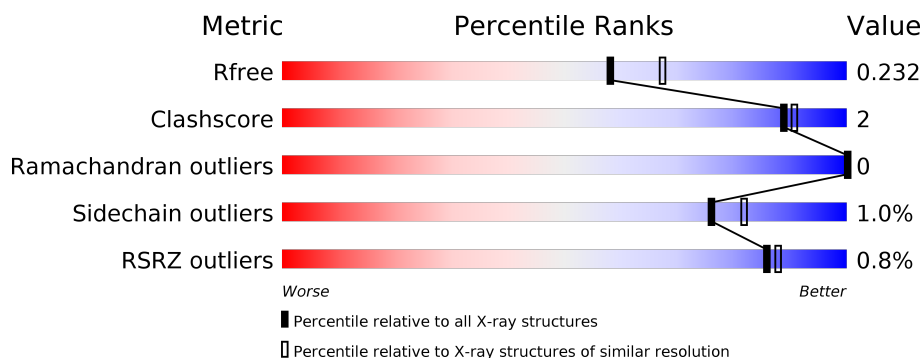
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	337	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>.</div> </div> </div>
1	B	337	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>.</div> <div>.</div> </div> </div>
1	C	337	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	337	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>.</div> </div> </div>
1	E	337	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>.</div> </div> </div>
1	F	337	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	337	<div><div></div><div>88%</div><div>7%</div><div></div></div>
1	H	337	<div>%<div><div></div><div>88%</div><div>7%</div><div></div></div></div>
1	I	337	<div>%<div><div></div><div>90%</div><div>6%</div><div></div></div></div>
1	J	337	<div>%<div><div></div><div>87%</div><div>8%</div><div></div></div></div>
1	K	337	<div>%<div><div></div><div>89%</div><div>6%</div><div></div></div></div>
1	L	337	<div>%<div><div></div><div>91%</div><div>5%</div><div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33653 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	322	Total	C	N	O	S	Se	0	1	0
			2604	1694	432	468	5	5			
1	B	322	Total	C	N	O	S	Se	0	0	0
			2588	1685	430	463	5	5			
1	C	322	Total	C	N	O	S	Se	0	0	0
			2599	1690	427	472	5	5			
1	D	322	Total	C	N	O	S	Se	0	0	0
			2591	1686	427	468	5	5			
1	E	322	Total	C	N	O	S	Se	0	0	0
			2602	1691	431	470	5	5			
1	F	322	Total	C	N	O	S	Se	0	0	0
			2595	1687	430	468	5	5			
1	G	322	Total	C	N	O	S	Se	0	0	0
			2600	1690	430	470	5	5			
1	H	322	Total	C	N	O	S	Se	0	0	0
			2602	1691	431	470	5	5			
1	I	322	Total	C	N	O	S	Se	0	0	0
			2599	1691	432	466	5	5			
1	J	322	Total	C	N	O	S	Se	0	1	0
			2596	1689	429	468	5	5			
1	K	322	Total	C	N	O	S	Se	0	0	0
			2598	1690	430	468	5	5			
1	L	322	Total	C	N	O	S	Se	0	1	0
			2609	1694	432	473	5	5			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
A	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
A	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
A	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
A	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
A	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
B	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
B	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
B	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
B	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
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C	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
C	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
C	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
C	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
C	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
C	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
D	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
D	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
D	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
D	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
D	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
D	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
E	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
E	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
E	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
E	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
E	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
E	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
E	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
E	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
E	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
E	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
E	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
E	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
E	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
E	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
E	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
E	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
F	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
F	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
F	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
F	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
F	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
F	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
F	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
F	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
F	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
F	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
F	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
F	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
F	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
F	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
F	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
F	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
F	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
G	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
G	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
G	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
G	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
G	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
G	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
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H	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
H	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
H	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
H	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
H	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
H	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
H	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
H	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
H	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
H	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
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I	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
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I	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
I	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
I	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
I	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
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I	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
I	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
I	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
I	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
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I	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
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J	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
J	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
J	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
J	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
J	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
J	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
J	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
J	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
J	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2

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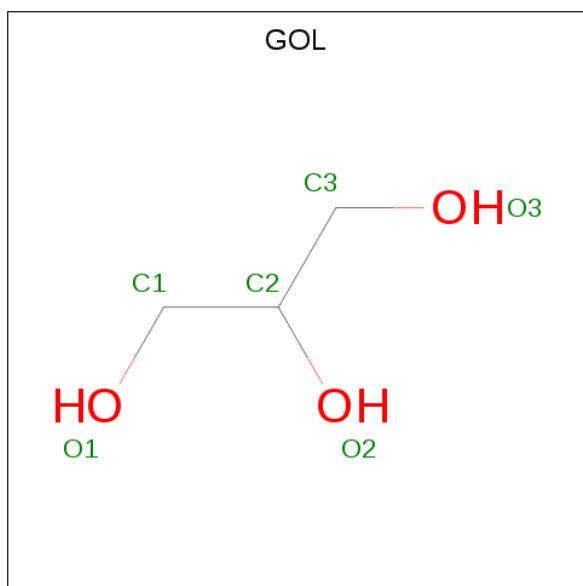
Chain	Residue	Modelled	Actual	Comment	Reference
J	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
J	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
K	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
K	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
K	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
K	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
K	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
K	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
K	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
K	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
K	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
K	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
K	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
K	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
K	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
K	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
K	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
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K	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
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L	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
L	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
L	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
L	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXT2
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L	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
L	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
L	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
L	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
L	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
L	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
L	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
L	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
L	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	213	Total	O	0	0
			213	213		
3	B	186	Total	O	0	0
			186	186		
3	C	176	Total	O	0	0
			176	176		
3	D	194	Total	O	0	0
			194	194		
3	E	206	Total	O	0	0
			206	206		
3	F	218	Total	O	0	0
			218	218		
3	G	228	Total	O	0	0
			228	228		
3	H	179	Total	O	0	0
			179	179		

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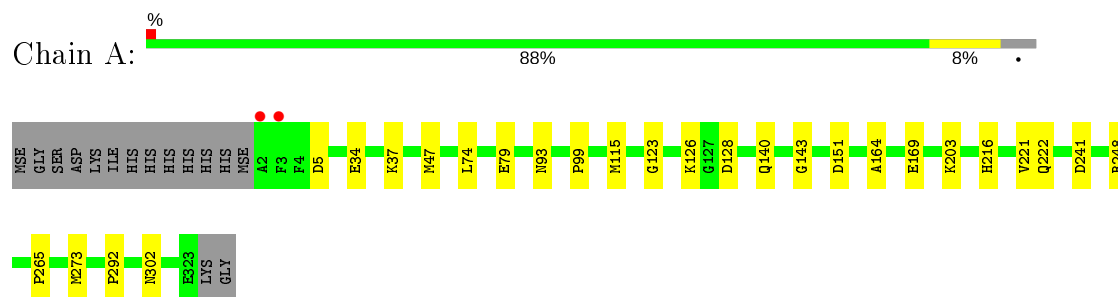
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	173	Total 173	O 173	0	0
3	J	216	Total 216	O 216	0	0
3	K	230	Total 230	O 230	0	0
3	L	245	Total 245	O 245	0	0

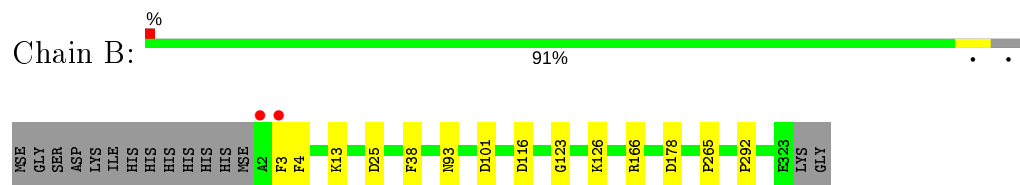
3 Residue-property plots [i](#)

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

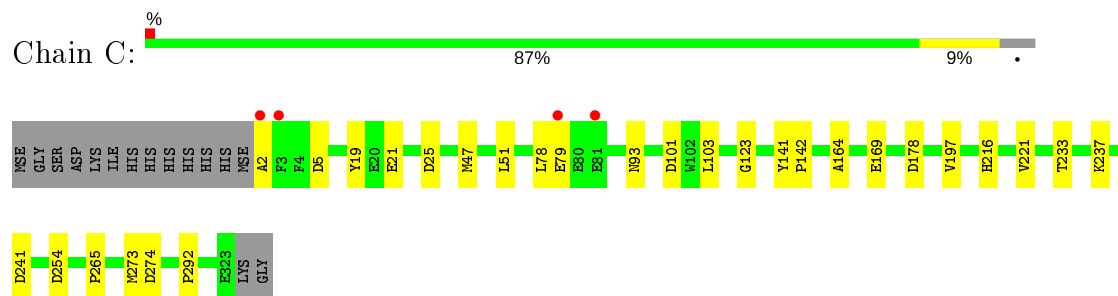
- Molecule 1: acetyl xylan esterase



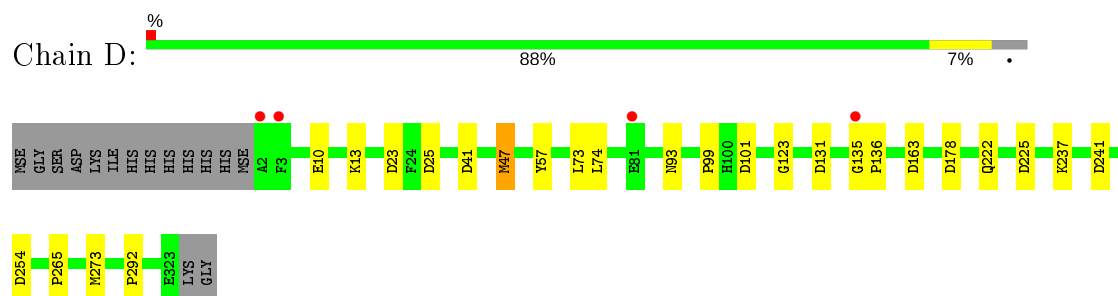
- Molecule 1: acetyl xylan esterase



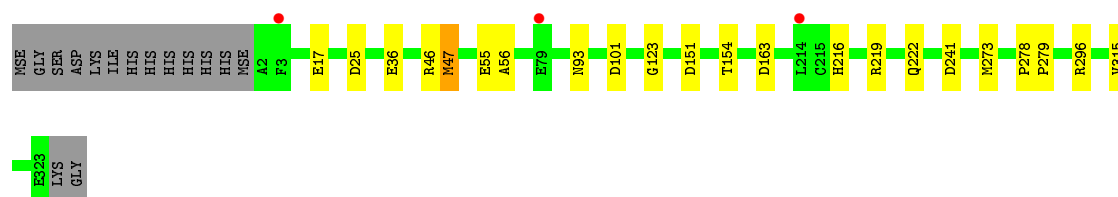
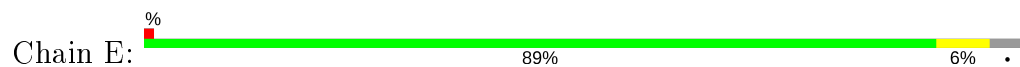
- Molecule 1: acetyl xylan esterase



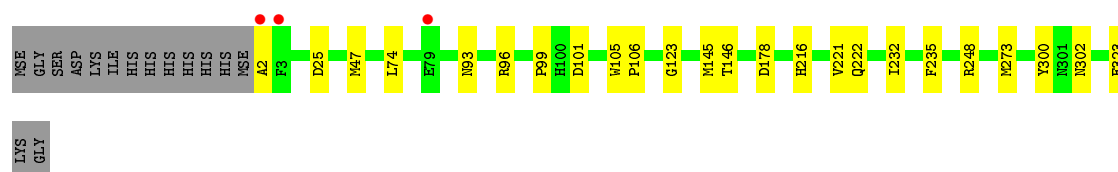
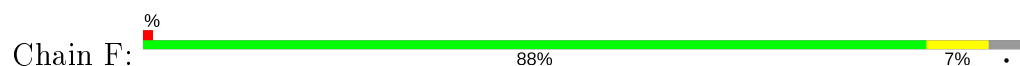
- Molecule 1: acetyl xylan esterase



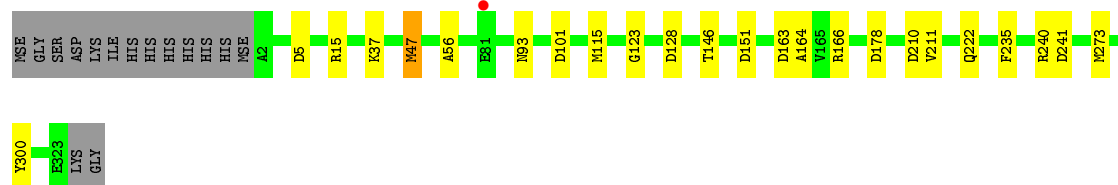
- Molecule 1: acetyl xylan esterase



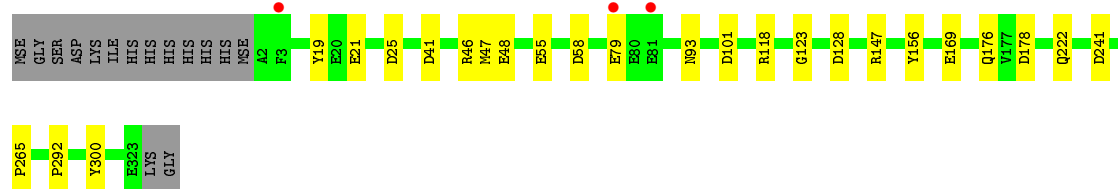
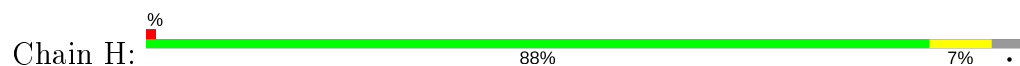
- Molecule 1: acetyl xylan esterase



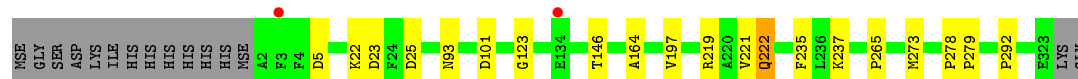
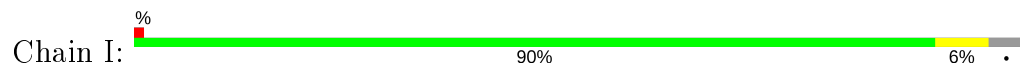
- Molecule 1: acetyl xylan esterase



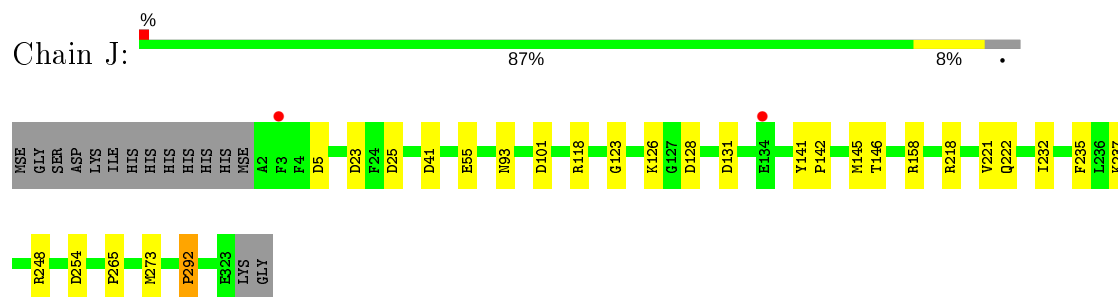
- Molecule 1: acetyl xylan esterase



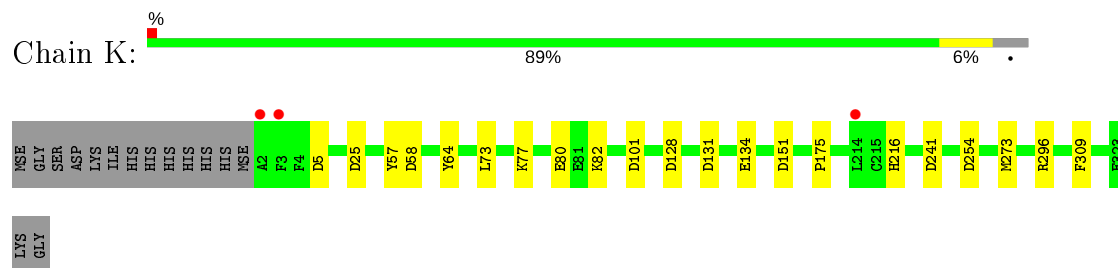
- Molecule 1: acetyl xylan esterase



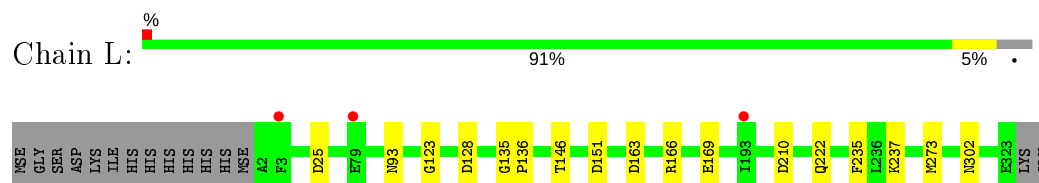
- Molecule 1: acetyl xylan esterase



- Molecule 1: acetyl xylan esterase



- Molecule 1: acetyl xylan esterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.64Å 130.95Å 157.81Å 90.00° 118.93° 90.00°	Depositor
Resolution (Å)	29.56 – 2.10 29.56 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.8 (29.56-2.10) 92.8 (29.56-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.223 0.195 , 0.232	Depositor DCC
R_{free} test set	14726 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.050 for h,-k,-h-l 0.000 for l,-k,h 0.000 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33653	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0664e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.81	1/2684 (0.0%)	0.84	5/3630 (0.1%)
1	B	0.81	0/2663	0.84	4/3604 (0.1%)
1	C	0.83	0/2674	0.86	7/3619 (0.2%)
1	D	0.86	1/2666 (0.0%)	0.88	10/3608 (0.3%)
1	E	0.81	1/2677 (0.0%)	0.87	6/3622 (0.2%)
1	F	0.80	0/2670	0.85	5/3614 (0.1%)
1	G	0.82	2/2675 (0.1%)	0.86	8/3620 (0.2%)
1	H	0.82	0/2677	0.86	8/3622 (0.2%)
1	I	0.82	0/2674	0.83	4/3617 (0.1%)
1	J	0.85	1/2677 (0.0%)	0.88	10/3622 (0.3%)
1	K	0.81	0/2673	0.86	10/3617 (0.3%)
1	L	0.82	0/2689	0.83	5/3638 (0.1%)
All	All	0.82	6/32099 (0.0%)	0.85	82/43433 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	315	VAL	CB-CG1	6.29	1.66	1.52
1	D	47	MSE	SE-CE	5.84	2.29	1.95
1	G	47	MSE	SE-CE	5.58	2.28	1.95
1	G	164	ALA	CA-CB	-5.21	1.41	1.52
1	A	164	ALA	CA-CB	-5.13	1.41	1.52

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	241	ASP	CB-CG-OD1	8.21	125.69	118.30
1	G	151	ASP	CB-CG-OD1	8.04	125.54	118.30
1	D	101	ASP	CB-CG-OD2	8.00	125.50	118.30
1	J	101	ASP	CB-CG-OD2	7.85	125.36	118.30
1	A	151	ASP	CB-CG-OD1	7.52	125.07	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2	ALA	Peptide

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	2604	0	2523	11	0
1	B	2588	0	2500	4	0
1	C	2599	0	2502	12	0
1	D	2591	0	2495	10	0
1	E	2602	0	2514	12	0
1	F	2595	0	2501	11	0
1	G	2600	0	2507	10	0
1	H	2602	0	2514	10	0
1	I	2599	0	2519	10	0
1	J	2596	0	2505	12	0
1	K	2598	0	2507	8	0
1	L	2609	0	2520	13	0
2	A	6	0	8	0	0
3	A	213	0	0	2	0
3	B	186	0	0	0	0
3	C	176	0	0	5	0
3	D	194	0	0	3	0
3	E	206	0	0	1	0
3	F	218	0	0	0	0
3	G	228	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	179	0	0	2	0
3	I	173	0	0	0	0
3	J	216	0	0	1	0
3	K	230	0	0	2	0
3	L	245	0	0	3	0
All	All	33653	0	30115	115	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 2.

The worst 5 of 115 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:F:273:MSE:SE	1:F:273:MSE:CE	2.15	1.45
1:E:273:MSE:SE	1:E:273:MSE:CE	2.15	1.44
1:G:115:MSE:SE	1:G:115:MSE:CE	2.15	1.43
1:H:47:MSE:SE	1:H:47:MSE:CE	2.17	1.42
1:F:47:MSE:SE	1:F:47:MSE:CE	2.16	1.42

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	321/337 (95%)	314 (98%)	7 (2%)	0	100	100
1	B	320/337 (95%)	310 (97%)	10 (3%)	0	100	100
1	C	320/337 (95%)	314 (98%)	6 (2%)	0	100	100
1	D	320/337 (95%)	312 (98%)	8 (2%)	0	100	100
1	E	320/337 (95%)	311 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	320/337 (95%)	311 (97%)	9 (3%)	0	100	100
1	G	320/337 (95%)	311 (97%)	9 (3%)	0	100	100
1	H	320/337 (95%)	313 (98%)	7 (2%)	0	100	100
1	I	320/337 (95%)	309 (97%)	11 (3%)	0	100	100
1	J	321/337 (95%)	313 (98%)	8 (2%)	0	100	100
1	K	320/337 (95%)	312 (98%)	8 (2%)	0	100	100
1	L	321/337 (95%)	312 (97%)	9 (3%)	0	100	100
All	All	3843/4044 (95%)	3742 (97%)	101 (3%)	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	270/278 (97%)	264 (98%)	6 (2%)	52	57
1	B	266/278 (96%)	264 (99%)	2 (1%)	81	86
1	C	269/278 (97%)	267 (99%)	2 (1%)	84	88
1	D	267/278 (96%)	266 (100%)	1 (0%)	91	94
1	E	270/278 (97%)	266 (98%)	4 (2%)	65	71
1	F	268/278 (96%)	264 (98%)	4 (2%)	65	71
1	G	269/278 (97%)	266 (99%)	3 (1%)	73	79
1	H	270/278 (97%)	267 (99%)	3 (1%)	73	79
1	I	269/278 (97%)	266 (99%)	3 (1%)	73	79
1	J	269/278 (97%)	266 (99%)	3 (1%)	73	79
1	K	268/278 (96%)	266 (99%)	2 (1%)	84	88
1	L	272/278 (98%)	271 (100%)	1 (0%)	91	94
All	All	3227/3336 (97%)	3193 (99%)	34 (1%)	76	79

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	216	HIS
1	G	15	ARG
1	K	80	GLU
1	F	222	GLN
1	B	13	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	222	GLN
1	L	50	HIS
1	I	222	GLN
1	E	222	GLN
1	H	222	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	GOL	A	326	-	5,5,5	0.42	0	5,5,5	0.57	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
2	GOL	A	326	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	326	GOL	O1-C1-C2-C3
2	A	326	GOL	C1-C2-C3-O3
2	A	326	GOL	O1-C1-C2-O2
2	A	326	GOL	O2-C2-C3-O3

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	317/337 (94%)	-0.52	2 (0%) 89 91	18, 24, 40, 64	0
1	B	317/337 (94%)	-0.58	2 (0%) 89 91	19, 25, 40, 68	0
1	C	317/337 (94%)	-0.53	4 (1%) 77 80	19, 25, 43, 67	0
1	D	317/337 (94%)	-0.51	4 (1%) 77 80	19, 25, 41, 66	0
1	E	317/337 (94%)	-0.46	3 (0%) 84 86	19, 24, 40, 63	0
1	F	317/337 (94%)	-0.48	3 (0%) 84 86	18, 24, 41, 65	0
1	G	317/337 (94%)	-0.50	1 (0%) 94 94	18, 24, 41, 64	0
1	H	317/337 (94%)	-0.49	3 (0%) 84 86	19, 25, 42, 64	0
1	I	317/337 (94%)	-0.51	2 (0%) 89 91	19, 25, 43, 68	0
1	J	317/337 (94%)	-0.46	2 (0%) 89 91	17, 24, 40, 64	1 (0%)
1	K	317/337 (94%)	-0.44	3 (0%) 84 86	18, 24, 41, 64	0
1	L	317/337 (94%)	-0.43	3 (0%) 84 86	17, 24, 40, 63	0
All	All	3804/4044 (94%)	-0.49	32 (0%) 86 88	17, 24, 41, 68	1 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PHE	3.8
1	D	2	ALA	3.6
1	L	3	PHE	3.3
1	K	3	PHE	3.0
1	F	79	GLU	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 [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
2	GOL	A	326	6/6	0.86	0.22	40,50,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.