



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:56 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (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

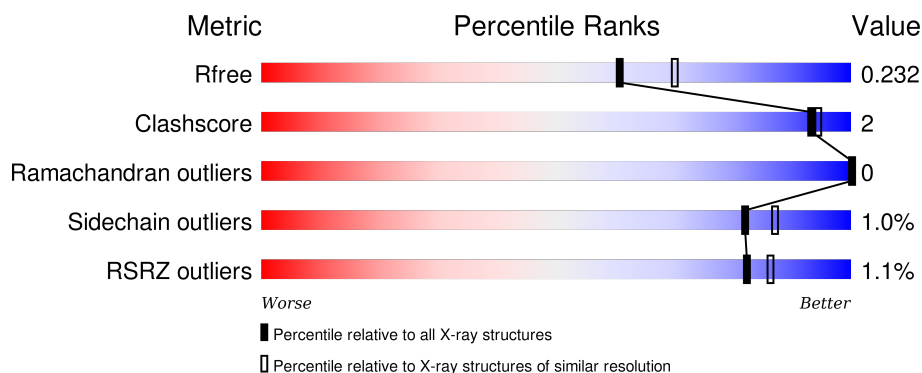
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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>88%</div> <div>8%</div> <div>.</div> </div>
1	B	337	<div> <div>91%</div> <div>.</div> <div>.</div> </div>
1	C	337	<div> <div>87%</div> <div>9%</div> <div>.</div> </div>
1	D	337	<div> <div>88%</div> <div>7%</div> <div>.</div> </div>
1	E	337	<div> <div>89%</div> <div>6%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
1	F	337		•
1	G	337		•
1	H	337		•
1	I	337		•
1	J	337		•
1	K	337		•
1	L	337		•

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
2	GOL	A	326	-	-	-	X

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

Continued on next page...

Continued from previous page...

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
B	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
B	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
G	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
G	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
G	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
G	-2	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
G	-1	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
G	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
G	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
G	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
G	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
G	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
G	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
H	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
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

Continued on next page...

Continued from previous page...

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
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
H	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
H	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
H	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
H	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
H	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
I	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
I	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
I	-9	SER	-	LEADER SEQUENCE	UNP Q9WXT2
I	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXT2
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
I	-3	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
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
I	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
I	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
I	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
I	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
I	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
J	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXT2
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

Continued on next page...

Continued from previous page...

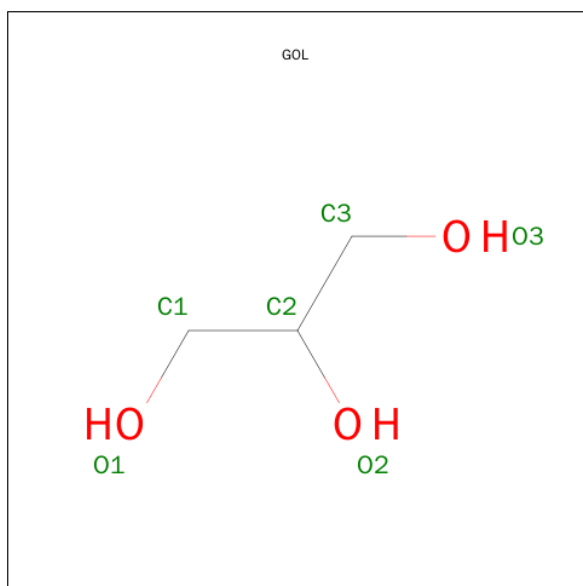
Chain	Residue	Modelled	Actual	Comment	Reference
J	0	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
J	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	47	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	108	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
J	273	MSE	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
K	115	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
K	145	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
K	273	MSE	MET	MODIFIED RESIDUE	UNP Q9WXT2
L	-11	MSE	-	LEADER SEQUENCE	UNP Q9WXT2
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
L	-6	ILE	-	LEADER SEQUENCE	UNP Q9WXT2
L	-5	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
L	-4	HIS	-	LEADER SEQUENCE	UNP Q9WXT2
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

Continued on next page...

Continued from previous page...

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 6 3 3	0	0

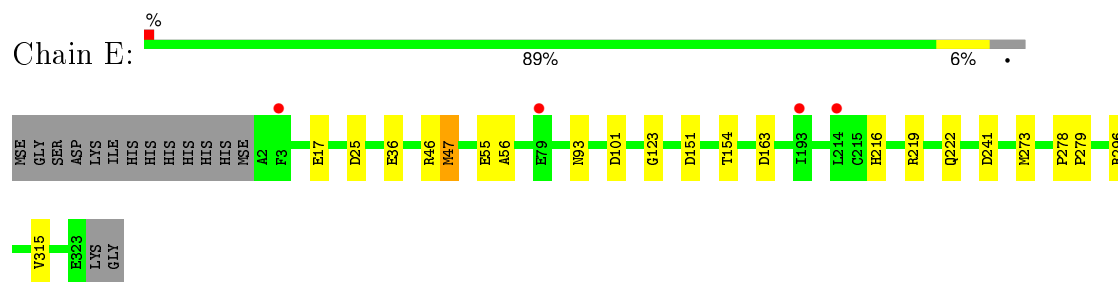
- Molecule 3 is water.

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

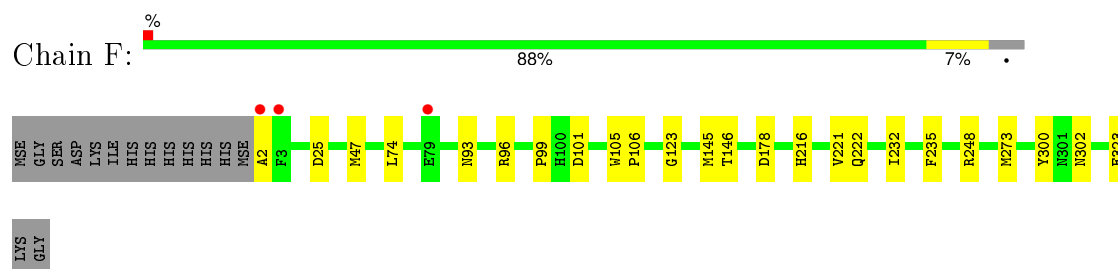
Continued on next page...

Continued from previous page...

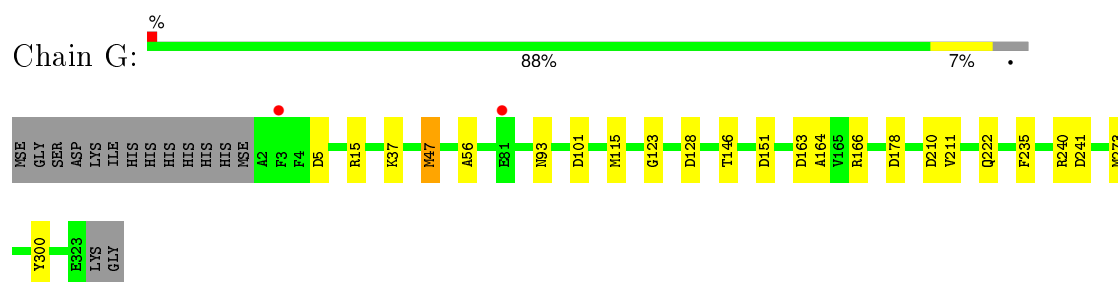
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	173	Total 173	O 173	0	0
3	J	216	Total 216	O 216	0	0
3	K	230	Total 230	O 230	0	0
3	L	245	Total 245	O 245	0	0



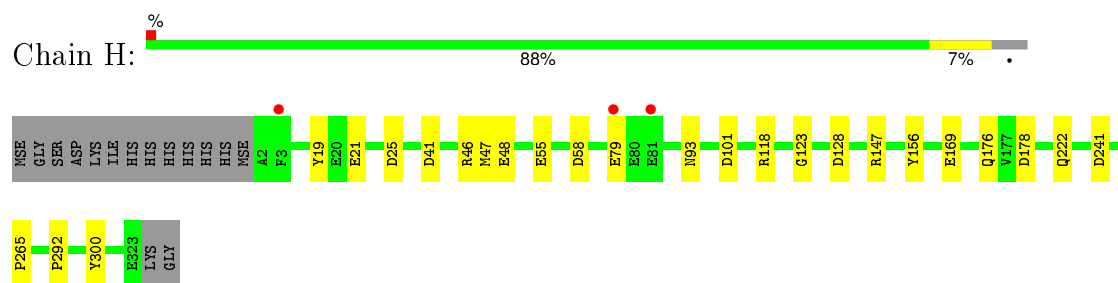
- Molecule 1: acetyl xylan esterase



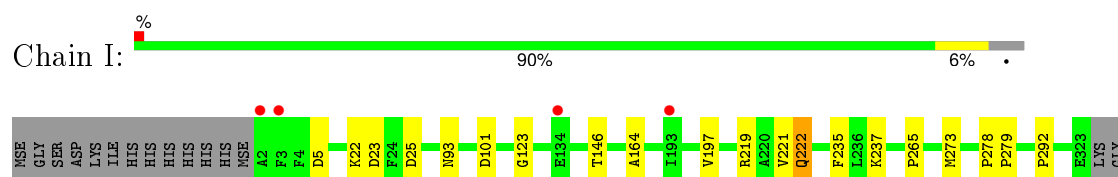
- Molecule 1: acetyl xylan esterase



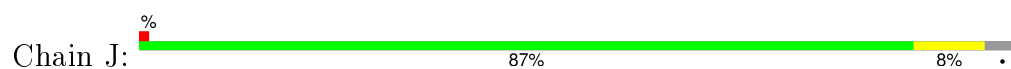
- Molecule 1: acetyl xylan esterase

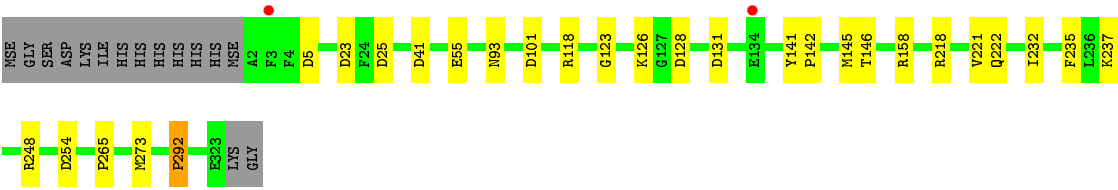


- Molecule 1: acetyl xylan esterase

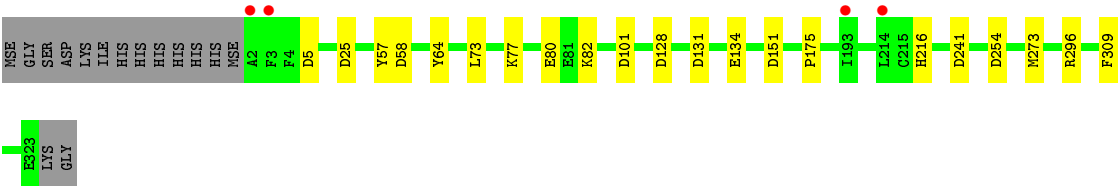
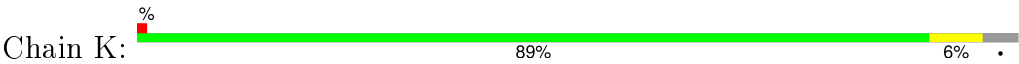


- Molecule 1: acetyl xylan esterase

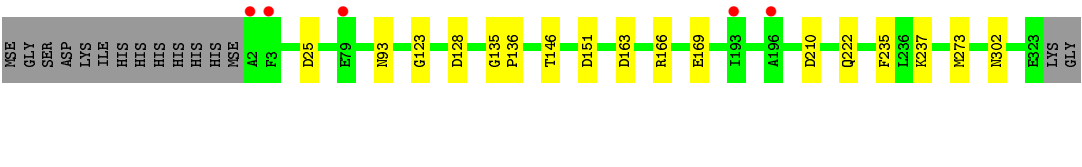
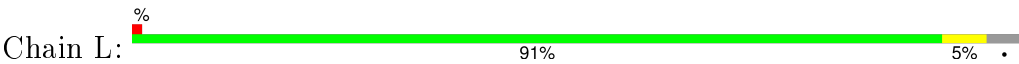




• Molecule 1: acetyl xylan esterase



• 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 (5.29%)	DCC
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 , 56.9	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	2 of 293097 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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

All (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
1	J	55	GLU	CD-OE1	5.03	1.31	1.25

All (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
1	D	41	ASP	CB-CG-OD1	7.06	124.65	118.30
1	D	131	ASP	CB-CG-OD2	6.85	124.46	118.30
1	K	58	ASP	CB-CG-OD2	6.79	124.41	118.30
1	J	41	ASP	CB-CG-OD1	6.74	124.37	118.30
1	H	101	ASP	CB-CG-OD2	6.72	124.35	118.30
1	H	241	ASP	CB-CG-OD1	6.68	124.32	118.30
1	C	274	ASP	CB-CG-OD2	6.47	124.13	118.30
1	C	178	ASP	CB-CG-OD2	6.47	124.12	118.30
1	I	5	ASP	CB-CG-OD2	6.47	124.12	118.30
1	E	25	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	5	ASP	CB-CG-OD2	6.41	124.07	118.30
1	H	128	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	101	ASP	CB-CG-OD2	6.26	123.94	118.30
1	K	5	ASP	CB-CG-OD2	6.25	123.93	118.30
1	F	101	ASP	CB-CG-OD2	6.23	123.90	118.30
1	D	241	ASP	CB-CG-OD1	6.17	123.85	118.30
1	I	25	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	25	ASP	CB-CG-OD2	6.01	123.71	118.30
1	H	58	ASP	CB-CG-OD2	5.97	123.67	118.30
1	J	248	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	128	ASP	CB-CG-OD2	5.90	123.61	118.30
1	J	25	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	101	ASP	CB-CG-OD2	5.86	123.57	118.30
1	I	23	ASP	CB-CG-OD2	5.82	123.54	118.30
1	G	101	ASP	CB-CG-OD2	5.79	123.52	118.30
1	K	131	ASP	CB-CG-OD1	5.79	123.51	118.30
1	G	178	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	241	ASP	CB-CG-OD1	5.77	123.50	118.30
1	F	25	ASP	CB-CG-OD2	5.77	123.50	118.30
1	K	101	ASP	CB-CG-OD2	5.77	123.50	118.30
1	E	101	ASP	CB-CG-OD2	5.74	123.47	118.30
1	K	241	ASP	CB-CG-OD1	5.72	123.45	118.30
1	J	5	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	25	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	178	ASP	CB-CG-OD2	5.70	123.43	118.30
1	E	296	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	J	131	ASP	CB-CG-OD2	5.67	123.40	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	248	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	L	163	ASP	CB-CG-OD1	5.60	123.34	118.30
1	G	241	ASP	CB-CG-OD1	5.58	123.33	118.30
1	I	101	ASP	CB-CG-OD2	5.57	123.31	118.30
1	G	128	ASP	CB-CG-OD2	5.56	123.31	118.30
1	H	41	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	5	ASP	CB-CG-OD2	5.54	123.28	118.30
1	F	178	ASP	CB-CG-OD2	5.51	123.26	118.30
1	L	25	ASP	CB-CG-OD2	5.51	123.26	118.30
1	K	296	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	J	158	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	L	128	ASP	CB-CG-OD2	5.40	123.16	118.30
1	H	178	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	296	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	25	ASP	CB-CG-OD2	5.37	123.14	118.30
1	D	163	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	241	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	116	ASP	CB-CG-OD2	5.33	123.10	118.30
1	J	254	ASP	CB-CG-OD2	5.32	123.09	118.30
1	J	118	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	F	96	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	248	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	25	ASP	CB-CG-OD2	5.18	122.97	118.30
1	G	163	ASP	CB-CG-OD1	5.18	122.96	118.30
1	H	118	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	K	254	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	163	ASP	CB-CG-OD1	5.13	122.92	118.30
1	K	25	ASP	CB-CG-OD2	5.11	122.90	118.30
1	K	151	ASP	CB-CG-OD1	5.11	122.90	118.30
1	L	210	ASP	CB-CG-OD2	5.09	122.88	118.30
1	L	151	ASP	CB-CG-OD1	5.08	122.87	118.30
1	J	23	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	225	ASP	CB-CG-OD2	5.07	122.86	118.30
1	G	5	ASP	CB-CG-OD2	5.07	122.86	118.30
1	G	210	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	254	ASP	CB-CG-OD2	5.04	122.83	118.30
1	K	128	ASP	CB-CG-OD2	5.02	122.82	118.30
1	D	178	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	254	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	23	ASP	CB-CG-OD2	5.01	122.81	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

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
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.

All (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
1:K:273:MSE:SE	1:K:273:MSE:CE	2.16	1.42
1:A:115:MSE:SE	1:A:115:MSE:CE	2.17	1.41
1:J:273:MSE:SE	1:J:273:MSE:CE	2.17	1.41
1:A:273:MSE:SE	1:A:273:MSE:CE	2.20	1.40
1:G:273:MSE:CE	1:G:273:MSE:SE	2.19	1.40
1:A:47:MSE:CE	1:A:47:MSE:SE	2.20	1.40
1:D:273:MSE:CE	1:D:273:MSE:SE	2.19	1.40
1:C:47:MSE:SE	1:C:47:MSE:CE	2.20	1.39
1:E:47:MSE:SE	1:E:47:MSE:CE	2.21	1.38
1:L:273:MSE:SE	1:L:273:MSE:CE	2.22	1.37
1:I:273:MSE:CE	1:I:273:MSE:SE	2.24	1.35
1:G:47:MSE:CE	1:G:47:MSE:SE	2.28	1.32
1:D:47:MSE:CE	1:D:47:MSE:SE	2.29	1.29
1:A:302:ASN:HB2	3:C:488:HOH:O	1.75	0.83
3:D:486:HOH:O	1:F:302:ASN:HB2	1.84	0.77
1:C:169:GLU:HG3	3:C:421:HOH:O	1.87	0.74
1:E:47:MSE:HB3	1:E:47:MSE:CE	2.24	0.68
1:H:93:ASN:HB3	1:H:123:GLY:HA3	1.79	0.63
1:L:93:ASN:HB3	1:L:123:GLY:HA3	1.79	0.63
1:E:47:MSE:HB3	1:E:47:MSE:HE2	1.81	0.62
1:J:237:LYS:NZ	1:L:302[B]:ASN:ND2	2.48	0.62
1:C:273:MSE:HE3	3:C:477:HOH:O	1.99	0.62
1:H:176:GLN:OE1	3:H:473:HOH:O	2.16	0.61
1:C:93:ASN:HB3	1:C:123:GLY:HA3	1.83	0.60
1:C:237:LYS:NZ	3:C:488:HOH:O	2.36	0.59
1:A:169:GLU:OE1	1:A:203:LYS:NZ	2.36	0.58
1:J:126[B]:LYS:NZ	1:J:128:ASP:OD1	2.36	0.56
1:E:93:ASN:HB3	1:E:123:GLY:HA3	1.87	0.56
1:G:93:ASN:HB3	1:G:123:GLY:HA3	1.88	0.55
1:I:219:ARG:HH11	1:I:222:GLN:HE21	1.54	0.55
1:F:47:MSE:CG	1:F:47:MSE:CE	2.84	0.55
1:A:93:ASN:HB3	1:A:123:GLY:HA3	1.89	0.54
1:B:93:ASN:HB3	1:B:123:GLY:HA3	1.90	0.54
1:J:93:ASN:HB3	1:J:123:GLY:HA3	1.90	0.54
1:D:237:LYS:NZ	3:D:486:HOH:O	2.42	0.53
1:L:237:LYS:HE3	3:L:563:HOH:O	2.08	0.53
1:E:46:ARG:NH2	1:E:55:GLU:HG2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:OE1	3:A:537:HOH:O	2.19	0.52
1:I:146:THR:HG21	1:I:235:PHE:HB2	1.92	0.52
1:D:93:ASN:HB3	1:D:123:GLY:HA3	1.92	0.51
1:F:145:MSE:HE3	1:F:232:ILE:HD11	1.94	0.50
1:C:19:TYR:OH	1:C:21:GLU:OE2	2.21	0.49
1:J:237:LYS:NZ	1:L:302[B]:ASN:HD22	2.09	0.49
1:J:145:MSE:HE3	1:J:232:ILE:HD11	1.95	0.48
1:G:166:ARG:NH2	3:G:428:HOH:O	2.44	0.48
1:E:219:ARG:HA	1:E:222:GLN:HG2	1.95	0.48
1:H:19:TYR:OH	1:H:21:GLU:OE2	2.13	0.48
1:J:237:LYS:HZ3	1:L:302[B]:ASN:ND2	2.11	0.48
1:C:51:LEU:HD21	1:C:103:LEU:HD21	1.96	0.47
1:I:219:ARG:HH11	1:I:222:GLN:NE2	2.12	0.47
1:F:93:ASN:HB3	1:F:123:GLY:HA3	1.98	0.46
3:D:343:HOH:O	1:F:2:ALA:HB2	2.15	0.46
1:G:146:THR:HG21	1:G:235:PHE:HB2	1.96	0.46
1:D:10:GLU:HA	1:D:13:LYS:HE2	1.97	0.46
1:G:240:ARG:HD2	1:K:309:PHE:CD1	2.51	0.46
1:I:164:ALA:HB1	1:I:197:VAL:HG21	1.98	0.46
1:L:146:THR:HG21	1:L:235:PHE:HB2	1.98	0.46
1:K:64:TYR:HE2	1:K:134:GLU:OE2	1.99	0.45
1:H:300:TYR:O	1:L:237:LYS:HG2	2.16	0.45
1:H:169:GLU:HG3	3:H:435:HOH:O	2.17	0.45
1:B:265:PRO:HA	1:B:292:PRO:O	2.16	0.45
1:E:222:GLN:NE2	3:E:477:HOH:O	2.49	0.45
1:A:37:LYS:HE2	3:A:459:HOH:O	2.17	0.45
1:H:265:PRO:HA	1:H:292:PRO:O	2.17	0.45
1:L:169:GLU:HG3	3:L:508:HOH:O	2.16	0.44
1:H:46:ARG:NH2	1:H:55:GLU:HG2	2.31	0.44
1:D:57:TYR:HB2	1:D:73:LEU:HB3	1.99	0.44
1:C:141:TYR:CG	1:C:142:PRO:HD2	2.53	0.44
1:H:47:MSE:CE	1:H:47:MSE:CG	2.94	0.44
1:H:147:ARG:HB3	1:H:156:TYR:HB2	2.00	0.44
1:I:93:ASN:HB3	1:I:123:GLY:HA3	1.99	0.43
1:K:77:LYS:NZ	3:K:530:HOH:O	2.51	0.43
1:C:78:LEU:O	3:C:431:HOH:O	2.21	0.43
1:G:300:TYR:O	1:I:237:LYS:HG2	2.19	0.43
1:L:273:MSE:O	1:L:302[B]:ASN:OD1	2.37	0.43
1:J:146:THR:HG21	1:J:235:PHE:HB2	2.00	0.43
1:J:237:LYS:HZ3	1:L:302[B]:ASN:HD22	1.64	0.43
1:F:74:LEU:HD21	1:F:99:PRO:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:GLU:N	3:K:528:HOH:O	2.52	0.43
1:L:166:ARG:NH2	3:L:475:HOH:O	2.50	0.43
1:J:265:PRO:HA	1:J:292:PRO:O	2.20	0.42
1:J:218:ARG:HB3	3:J:405:HOH:O	2.19	0.42
1:I:219:ARG:NH1	1:I:222:GLN:HE21	2.17	0.42
1:C:221:VAL:HG13	1:C:233:THR:OG1	2.19	0.42
1:E:47:MSE:CE	1:E:47:MSE:CB	2.97	0.42
1:E:278:PRO:HA	1:E:279:PRO:HD3	1.92	0.42
1:C:164:ALA:HB1	1:C:197:VAL:HG21	2.01	0.42
1:E:47:MSE:HG3	1:E:56:ALA:O	2.20	0.41
1:L:135:GLY:HA3	1:L:136:PRO:HD3	1.95	0.41
1:G:47:MSE:HG3	1:G:56:ALA:O	2.21	0.41
1:I:265:PRO:HA	1:I:292:PRO:O	2.21	0.41
1:D:237:LYS:HG2	1:F:300:TYR:O	2.21	0.41
1:A:140:GLN:NE2	1:A:143:GLY:O	2.52	0.41
1:D:265:PRO:HA	1:D:292:PRO:O	2.20	0.41
1:E:151:ASP:HB3	1:E:154:THR:OG1	2.21	0.41
1:F:146:THR:HG21	1:F:235:PHE:HB2	2.02	0.41
1:K:57:TYR:HB2	1:K:73:LEU:HB3	2.03	0.41
1:B:3:PHE:CG	1:B:4:PHE:N	2.89	0.40
1:K:64:TYR:CE2	1:K:134:GLU:OE2	2.74	0.40
1:K:82:LYS:NZ	1:K:175:PRO:O	2.26	0.40
1:A:265:PRO:HA	1:A:292:PRO:O	2.21	0.40
1:D:74:LEU:HD21	1:D:99:PRO:HB3	2.04	0.40
1:J:141:TYR:CG	1:J:142:PRO:HD2	2.57	0.40
1:I:278:PRO:HA	1:I:279:PRO:HD3	1.94	0.40
1:A:74:LEU:HD21	1:A:99:PRO:HB3	2.03	0.40
1:F:105:TRP:N	1:F:106:PRO:CD	2.84	0.40
1:D:135:GLY:HA3	1:D:136:PRO:HD3	1.97	0.40
1:B:38:PHE:O	1:B:166:ARG:NH2	2.54	0.40
1:C:265:PRO:HA	1:C:292:PRO:O	2.22	0.40
1:G:211:VAL:O	1:G:211:VAL:HG23	2.21	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	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
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%)	60	64
1	B	266/278 (96%)	264 (99%)	2 (1%)	86	91
1	C	269/278 (97%)	267 (99%)	2 (1%)	88	92
1	D	267/278 (96%)	266 (100%)	1 (0%)	93	96
1	E	270/278 (97%)	266 (98%)	4 (2%)	72	78
1	F	268/278 (96%)	264 (98%)	4 (2%)	72	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	269/278 (97%)	266 (99%)	3 (1%)	80	85
1	H	270/278 (97%)	267 (99%)	3 (1%)	80	85
1	I	269/278 (97%)	266 (99%)	3 (1%)	80	85
1	J	269/278 (97%)	266 (99%)	3 (1%)	80	85
1	K	268/278 (96%)	266 (99%)	2 (1%)	88	92
1	L	272/278 (98%)	271 (100%)	1 (0%)	93	96
All	All	3227/3336 (97%)	3193 (99%)	34 (1%)	82	85

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	GLU
1	A	126[A]	LYS
1	A	126[B]	LYS
1	A	216	HIS
1	A	221	VAL
1	A	222	GLN
1	B	13	LYS
1	B	126	LYS
1	C	79	GLU
1	C	216	HIS
1	D	222	GLN
1	E	17	GLU
1	E	36	GLU
1	E	47	MSE
1	E	216	HIS
1	F	216	HIS
1	F	221	VAL
1	F	222	GLN
1	F	323	GLU
1	G	15	ARG
1	G	37	LYS
1	G	222	GLN
1	H	48	GLU
1	H	79	GLU
1	H	222	GLN
1	I	22	LYS
1	I	221	VAL
1	I	222	GLN
1	J	221	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	222	GLN
1	J	292	PRO
1	K	80	GLU
1	K	216	HIS
1	L	222	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	100	HIS
1	E	50	HIS
1	E	222	GLN
1	G	50	HIS
1	G	222	GLN
1	H	222	GLN
1	I	222	GLN
1	K	50	HIS
1	L	50	HIS

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	0.39	0	5,5,5	0.61	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	-	-	0/4/4/4	0/0/0/0

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 [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.48	4 (1%)	79 84	18, 24, 40, 64	0
1	B	317/337 (94%)	-0.54	2 (0%)	90 92	19, 25, 40, 68	0
1	C	317/337 (94%)	-0.50	4 (1%)	79 84	19, 25, 43, 67	0
1	D	317/337 (94%)	-0.48	4 (1%)	79 84	19, 25, 41, 66	0
1	E	317/337 (94%)	-0.42	4 (1%)	79 84	19, 24, 40, 63	0
1	F	317/337 (94%)	-0.44	3 (0%)	85 88	18, 24, 41, 65	0
1	G	317/337 (94%)	-0.46	2 (0%)	90 92	18, 24, 41, 64	0
1	H	317/337 (94%)	-0.45	3 (0%)	85 88	19, 25, 42, 64	0
1	I	317/337 (94%)	-0.47	4 (1%)	79 84	19, 25, 43, 68	0
1	J	317/337 (94%)	-0.42	2 (0%)	90 92	17, 24, 40, 64	1 (0%)
1	K	317/337 (94%)	-0.40	4 (1%)	79 84	18, 24, 41, 64	0
1	L	317/337 (94%)	-0.38	5 (1%)	74 79	17, 24, 40, 63	0
All	All	3804/4044 (94%)	-0.45	41 (1%)	82 86	17, 24, 41, 68	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	PHE	4.0
1	D	2	ALA	3.9
1	L	3	PHE	3.5
1	K	3	PHE	3.2
1	F	3	PHE	3.2
1	A	2	ALA	3.1
1	E	3	PHE	3.1
1	F	79	GLU	3.1
1	B	2	ALA	3.1
1	C	2	ALA	3.0
1	A	3	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	2	ALA	2.9
1	C	79	GLU	2.8
1	G	81	GLU	2.8
1	E	79	GLU	2.8
1	H	3	PHE	2.8
1	D	135	GLY	2.7
1	C	3	PHE	2.7
1	I	3	PHE	2.7
1	I	134	GLU	2.5
1	L	193	ILE	2.5
1	D	81	GLU	2.4
1	H	79	GLU	2.4
1	F	2	ALA	2.4
1	J	3	PHE	2.4
1	H	81	GLU	2.4
1	L	79	GLU	2.4
1	C	81	GLU	2.3
1	D	3	PHE	2.2
1	K	214	LEU	2.2
1	E	214	LEU	2.2
1	I	2	ALA	2.1
1	A	79	GLU	2.1
1	J	134	GLU	2.1
1	E	193	ILE	2.1
1	I	193	ILE	2.1
1	K	193	ILE	2.1
1	A	323	GLU	2.1
1	L	196	ALA	2.1
1	G	3	PHE	2.1
1	L	2	ALA	2.0

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

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 [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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	A	326	6/6	0.86	0.22	5.04	40,50,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.