



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:47 am BST

PDB ID : 3FVT
Title : Crystal Structure of Acetyl Xylan Esterase from *Bacillus pumilus*, monoclinic crystal form II
Authors : Krastanova, I.; Cassetta, A.; Lamba, D.
Deposited on : 2009-01-16
Resolution : 1.90 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

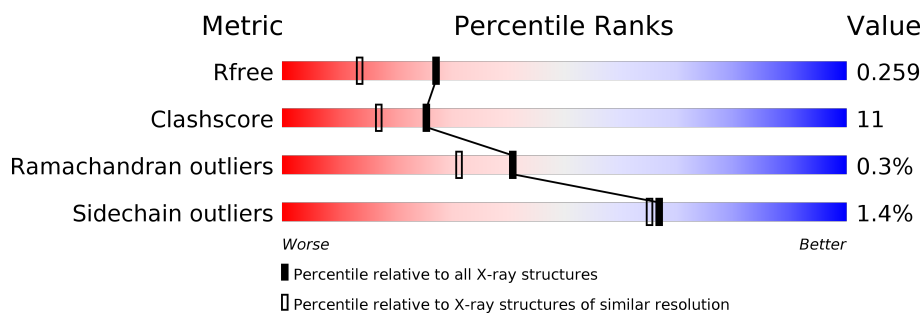
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	320	82% 17% ..
1	B	320	81% 17% ..
1	C	320	80% 18% ..
1	D	320	78% 20% ..
1	E	320	86% 13% ..
1	F	320	78% 20% .
1	G	320	76% 22% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	320	 75%22% ..
1	I	320	 79%19% ..
1	L	320	 76%22% ..
1	M	320	 78%21% ..
1	N	320	 83%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	GOL	G	2274	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33650 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	318	Total	C	N	O	S	0	0	0
			2544	1652	417	471	4			
1	B	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	C	316	Total	C	N	O	S	0	0	0
			2528	1641	415	469	3			
1	D	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	E	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	F	319	Total	C	N	O	S	0	0	0
			2550	1654	418	475	3			
1	G	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	H	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	I	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	L	317	Total	C	N	O	S	0	0	0
			2536	1647	416	470	3			
1	M	318	Total	C	N	O	S	0	0	0
			2544	1652	417	471	4			
1	N	318	Total	C	N	O	S	0	0	0
			2544	1652	417	471	4			

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

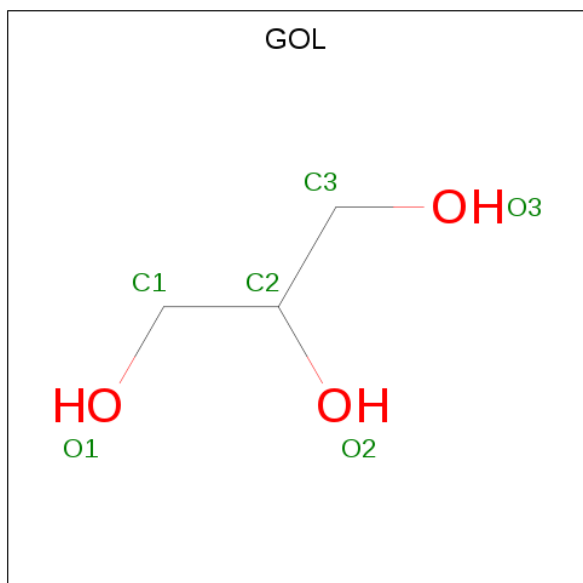
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Cl	0	0
			2	2		
2	D	2	Total	Cl	0	0
			2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

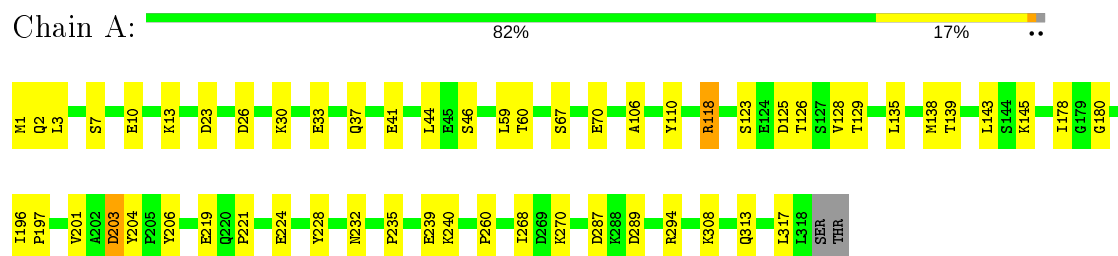
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	332	Total	O	0	0
			332	332		
4	B	303	Total	O	0	0
			303	303		
4	C	296	Total	O	0	0
			296	296		
4	D	266	Total	O	0	0
			266	266		
4	E	295	Total	O	0	0
			295	295		
4	F	267	Total	O	0	0
			267	267		
4	G	196	Total	O	0	0
			196	196		
4	H	206	Total	O	0	0
			206	206		
4	I	270	Total	O	0	0
			270	270		
4	L	265	Total	O	0	0
			265	265		
4	M	213	Total	O	0	0
			213	213		
4	N	243	Total	O	0	0
			243	243		

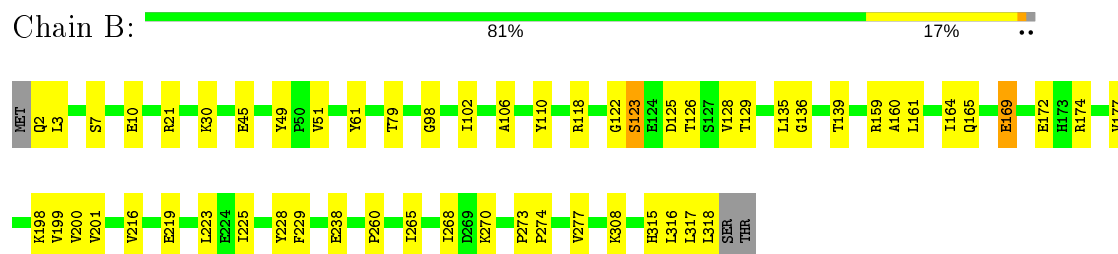
3 Residue-property plots [i](#)

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. 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. 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.

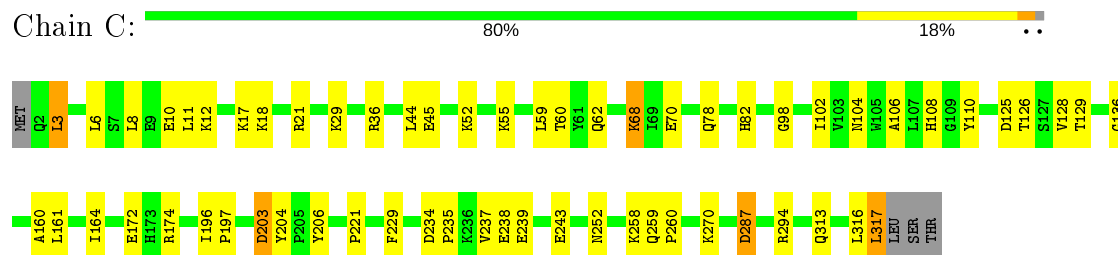
- Molecule 1: Acetyl xylan esterase



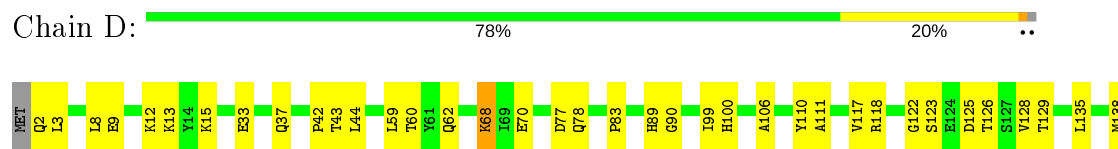
- Molecule 1: Acetyl xylan esterase



- Molecule 1: Acetyl xylan esterase

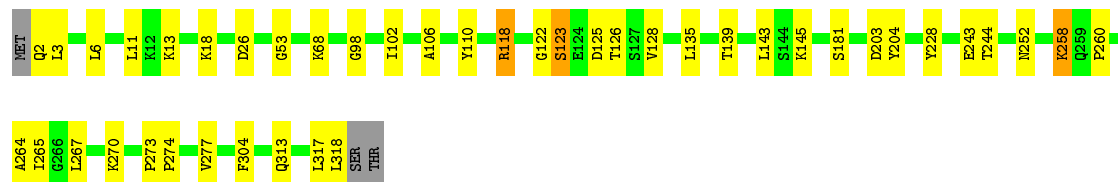
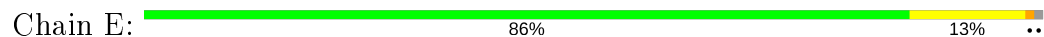


- Molecule 1: Acetyl xylan esterase

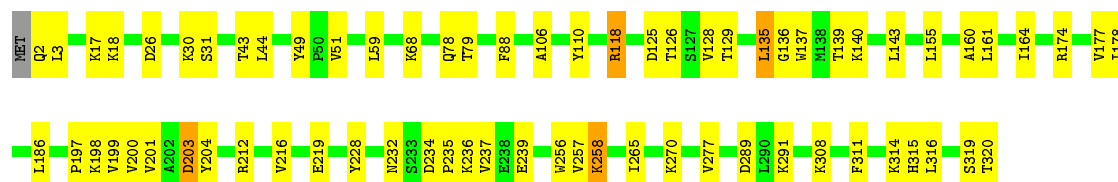




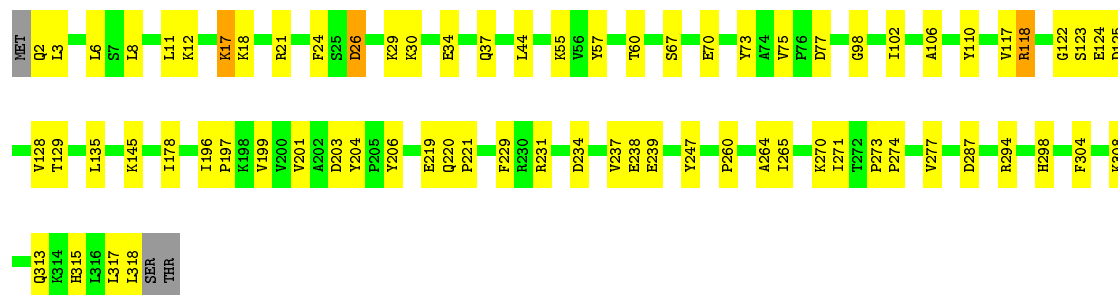
- Molecule 1: Acetyl xylan esterase



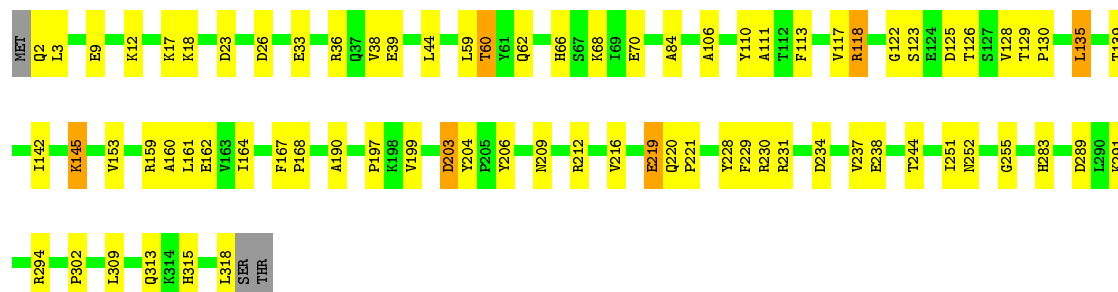
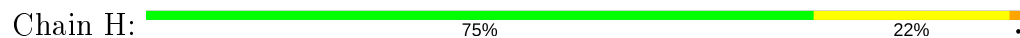
- Molecule 1: Acetyl xylan esterase



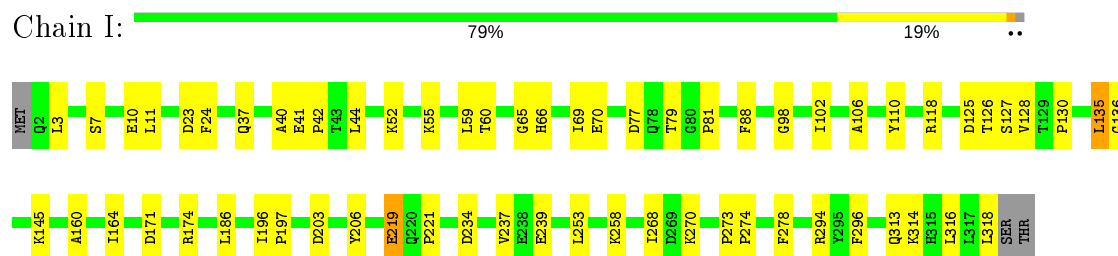
- Molecule 1: Acetyl xylan esterase



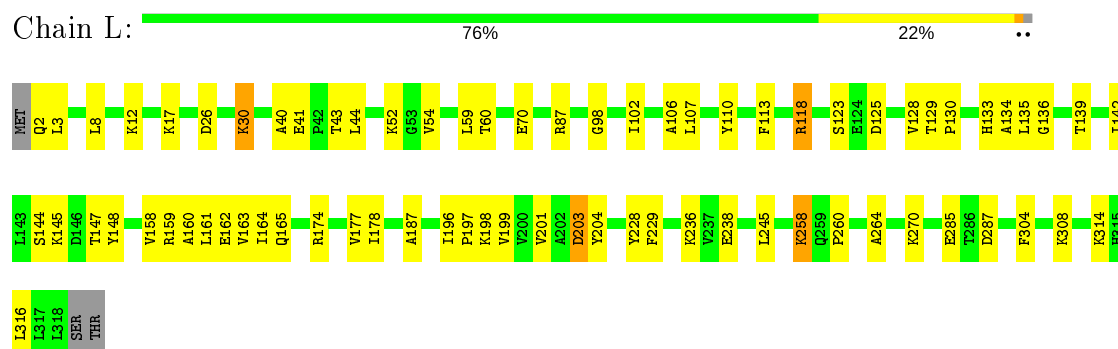
- Molecule 1: Acetyl xylan esterase



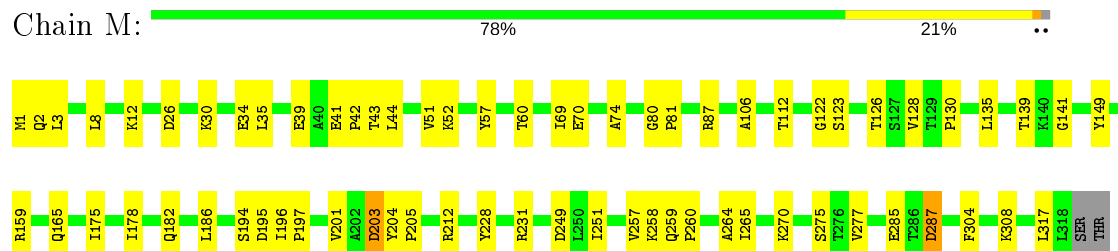
- Molecule 1: Acetyl xylan esterase



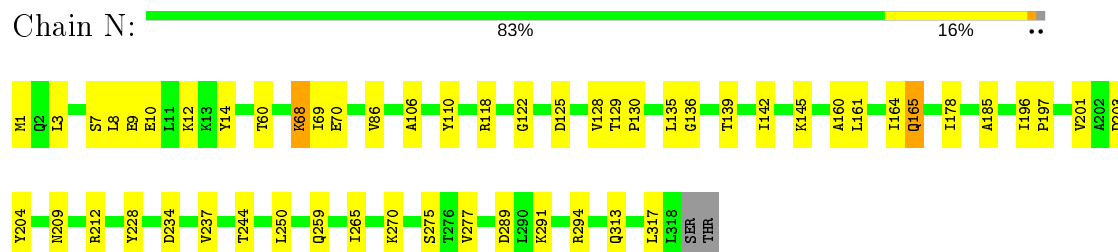
- Molecule 1: Acetyl xylan esterase



- 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	144.04 Å 87.20 Å 184.82 Å 90.00° 112.87° 90.00°	Depositor
Resolution (Å)	29.74 – 1.90 29.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.9 (29.74-1.90) 89.7 (29.74-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.89 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.211 , 0.264 0.207 , 0.259	Depositor DCC
R_{free} test set	29799 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.296 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	33650	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.52	0/2616	0.70	0/3551
1	B	0.53	0/2608	0.69	0/3541
1	C	0.50	0/2600	0.70	0/3530
1	D	0.51	0/2608	0.68	1/3541 (0.0%)
1	E	0.51	0/2608	0.68	0/3541
1	F	0.49	0/2622	0.70	0/3559
1	G	0.44	0/2608	0.65	0/3541
1	H	0.44	0/2608	0.65	0/3541
1	I	0.50	0/2608	0.69	0/3541
1	L	0.50	0/2608	0.67	0/3541
1	M	0.44	0/2616	0.65	0/3551
1	N	0.49	0/2616	0.67	0/3551
All	All	0.49	0/31326	0.68	1/42529 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	111	ALA	N-CA-C	-5.11	97.21	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2544	0	2494	56	0
1	B	2536	0	2482	48	0
1	C	2528	0	2471	46	0
1	D	2536	0	2482	55	0
1	E	2536	0	2482	39	0
1	F	2550	0	2494	75	0
1	G	2536	0	2482	68	0
1	H	2536	0	2482	68	0
1	I	2536	0	2482	54	0
1	L	2536	0	2482	65	0
1	M	2544	0	2494	60	0
1	N	2544	0	2494	41	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	1	0
2	N	2	0	0	0	0
3	E	6	0	8	1	0
3	G	6	0	8	8	0
4	A	332	0	0	6	0
4	B	303	0	0	13	0
4	C	296	0	0	11	0
4	D	266	0	0	11	0
4	E	295	0	0	9	0
4	F	267	0	0	6	0
4	G	196	0	0	3	0
4	H	206	0	0	6	0
4	I	270	0	0	5	0
4	L	265	0	0	8	0
4	M	213	0	0	12	0
4	N	243	0	0	1	0
All	All	33650	0	29837	639	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 11.

The worst 5 of 639 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:H:62:GLN:NE2	1:H:68:LYS:HD3	1.73	1.04
1:A:1:MET:HG2	1:A:2:GLN:H	1.23	1.04
3:G:2274:GOL:H11	1:M:135:LEU:HD11	1.38	1.03
1:C:8:LEU:HG	1:C:12:LYS:HE2	1.44	0.98
1:C:68:LYS:HZ2	1:C:68:LYS:HB2	1.26	0.98

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	316/320 (99%)	303 (96%)	11 (4%)	2 (1%)	25	15
1	B	315/320 (98%)	302 (96%)	11 (4%)	2 (1%)	25	15
1	C	314/320 (98%)	298 (95%)	16 (5%)	0	100	100
1	D	315/320 (98%)	296 (94%)	19 (6%)	0	100	100
1	E	315/320 (98%)	303 (96%)	10 (3%)	2 (1%)	25	15
1	F	317/320 (99%)	303 (96%)	13 (4%)	1 (0%)	41	31
1	G	315/320 (98%)	298 (95%)	16 (5%)	1 (0%)	41	31
1	H	315/320 (98%)	298 (95%)	15 (5%)	2 (1%)	25	15
1	I	315/320 (98%)	303 (96%)	12 (4%)	0	100	100
1	L	315/320 (98%)	299 (95%)	14 (4%)	2 (1%)	25	15
1	M	316/320 (99%)	296 (94%)	19 (6%)	1 (0%)	41	31
1	N	316/320 (99%)	297 (94%)	19 (6%)	0	100	100
All	All	3784/3840 (98%)	3596 (95%)	175 (5%)	13 (0%)	41	31

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	317	LEU
1	B	118	ARG
1	E	118	ARG
1	F	118	ARG
1	G	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	268/270 (99%)	266 (99%)	2 (1%)	84	84
1	B	267/270 (99%)	266 (100%)	1 (0%)	91	91
1	C	266/270 (98%)	261 (98%)	5 (2%)	57	53
1	D	267/270 (99%)	264 (99%)	3 (1%)	73	73
1	E	267/270 (99%)	262 (98%)	5 (2%)	57	53
1	F	269/270 (100%)	264 (98%)	5 (2%)	57	53
1	G	267/270 (99%)	263 (98%)	4 (2%)	65	62
1	H	267/270 (99%)	262 (98%)	5 (2%)	57	53
1	I	267/270 (99%)	263 (98%)	4 (2%)	65	62
1	L	267/270 (99%)	261 (98%)	6 (2%)	52	47
1	M	268/270 (99%)	265 (99%)	3 (1%)	73	73
1	N	268/270 (99%)	265 (99%)	3 (1%)	73	73
All	All	3208/3240 (99%)	3162 (99%)	46 (1%)	67	65

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	258	LYS
1	H	60	THR
1	M	287	ASP
1	G	17	LYS
1	G	57	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	37	GLN
1	G	220	GLN
1	N	37	GLN
1	F	62	GLN
1	G	37	GLN

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 26 ligands modelled in this entry, 24 are monoatomic - leaving 2 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	GOL	G	2274	-	5,5,5	0.31	0	5,5,5	0.13	0
3	GOL	E	2273	-	5,5,5	0.33	0	5,5,5	0.18	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	GOL	G	2274	-	-	0/4/4/4	-
3	GOL	E	2273	-	-	0/4/4/4	-

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.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2274	GOL	8	0
3	E	2273	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.