wwPDB X-ray Structure Validation Summary Report (i)

Jan 6, 2024 – 08:51 pm GMT

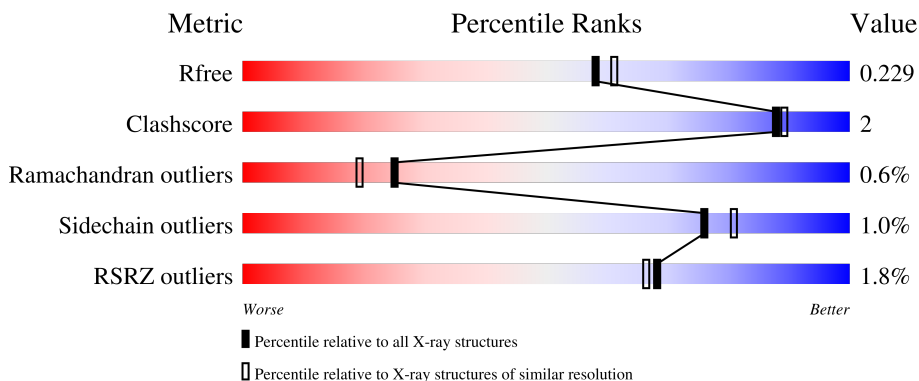|		
PDB ID	:	5MQP
Title	:	Glycoside hydrolase BT_1002
Authors	:	Basle, A.; Ndeh, D.; Rogowski, A.; Cartmell, A.; Luis, A.S.; Venditto, I.; Labourel, A.; Gilbert, H.J.
Deposited on	:	2016-12-20
Resolution	:	2.00 Å(reported)

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 2.00 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.
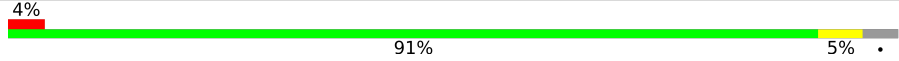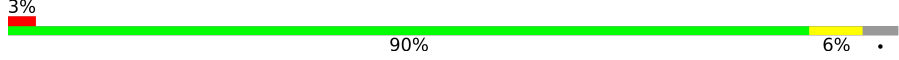
Metric	Percentile Ranks	Value
Rfree		0.229
Clashscore		2
Ramachandran outliers		0.6%
Sidechain outliers		1.0%
RSRZ outliers		1.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	624	% / 90% / 6% ·
1	B	624	2% / 88% / 8% ·
1	C	624	% / 89% / 7% · ·
1	D	624	% / 88% / 7% · ·
1	E	624	% / 89% / 7% ·

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Mol	Chain	Length	Quality of chain
1	F	624	4% 91% 5%
1	G	624	% 87% 8%
1	H	624	3% 90% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41129 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 Glycoside hydrolase BT_1002.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	1	0
			4793	3021	856	894	22			
1	B	599	Total	C	N	O	S	0	1	0
			4784	3015	854	892	23			
1	C	601	Total	C	N	O	S	0	2	0
			4804	3028	857	896	23			
1	D	600	Total	C	N	O	S	0	1	0
			4793	3021	856	894	22			
1	E	602	Total	C	N	O	S	0	1	0
			4807	3030	858	897	22			
1	F	599	Total	C	N	O	S	0	0	0
			4781	3013	854	892	22			
1	G	600	Total	C	N	O	S	0	1	0
			4793	3021	856	894	22			
1	H	600	Total	C	N	O	S	0	1	0
			4793	3021	856	894	22			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
A	-3	GLY	-	expression tag	UNP A0A0P0F5L7
A	-2	SER	-	expression tag	UNP A0A0P0F5L7
A	-1	SER	-	expression tag	UNP A0A0P0F5L7
A	0	HIS	-	expression tag	UNP A0A0P0F5L7
A	1	HIS	-	expression tag	UNP A0A0P0F5L7
A	2	HIS	-	expression tag	UNP A0A0P0F5L7
A	3	HIS	-	expression tag	UNP A0A0P0F5L7
A	4	HIS	-	expression tag	UNP A0A0P0F5L7
A	5	HIS	-	expression tag	UNP A0A0P0F5L7
A	6	SER	-	expression tag	UNP A0A0P0F5L7
A	7	SER	-	expression tag	UNP A0A0P0F5L7
A	8	GLY	-	expression tag	UNP A0A0P0F5L7

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WORLDWIDE PDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP A0A0P0F5L7
A	10	GLN	-	expression tag	UNP A0A0P0F5L7
A	11	GLN	-	expression tag	UNP A0A0P0F5L7
A	12	GLY	-	expression tag	UNP A0A0P0F5L7
A	13	LEU	-	expression tag	UNP A0A0P0F5L7
A	14	ARG	-	expression tag	UNP A0A0P0F5L7
B	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
B	-3	GLY	-	expression tag	UNP A0A0P0F5L7
B	-2	SER	-	expression tag	UNP A0A0P0F5L7
B	-1	SER	-	expression tag	UNP A0A0P0F5L7
B	0	HIS	-	expression tag	UNP A0A0P0F5L7
B	1	HIS	-	expression tag	UNP A0A0P0F5L7
B	2	HIS	-	expression tag	UNP A0A0P0F5L7
B	3	HIS	-	expression tag	UNP A0A0P0F5L7
B	4	HIS	-	expression tag	UNP A0A0P0F5L7
B	5	HIS	-	expression tag	UNP A0A0P0F5L7
B	6	SER	-	expression tag	UNP A0A0P0F5L7
B	7	SER	-	expression tag	UNP A0A0P0F5L7
B	8	GLY	-	expression tag	UNP A0A0P0F5L7
B	9	PRO	-	expression tag	UNP A0A0P0F5L7
B	10	GLN	-	expression tag	UNP A0A0P0F5L7
B	11	GLN	-	expression tag	UNP A0A0P0F5L7
B	12	GLY	-	expression tag	UNP A0A0P0F5L7
B	13	LEU	-	expression tag	UNP A0A0P0F5L7
B	14	ARG	-	expression tag	UNP A0A0P0F5L7
C	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
C	-3	GLY	-	expression tag	UNP A0A0P0F5L7
C	-2	SER	-	expression tag	UNP A0A0P0F5L7
C	-1	SER	-	expression tag	UNP A0A0P0F5L7
C	0	HIS	-	expression tag	UNP A0A0P0F5L7
C	1	HIS	-	expression tag	UNP A0A0P0F5L7
C	2	HIS	-	expression tag	UNP A0A0P0F5L7
C	3	HIS	-	expression tag	UNP A0A0P0F5L7
C	4	HIS	-	expression tag	UNP A0A0P0F5L7
C	5	HIS	-	expression tag	UNP A0A0P0F5L7
C	6	SER	-	expression tag	UNP A0A0P0F5L7
C	7	SER	-	expression tag	UNP A0A0P0F5L7
C	8	GLY	-	expression tag	UNP A0A0P0F5L7
C	9	PRO	-	expression tag	UNP A0A0P0F5L7
C	10	GLN	-	expression tag	UNP A0A0P0F5L7
C	11	GLN	-	expression tag	UNP A0A0P0F5L7
C	12	GLY	-	expression tag	UNP A0A0P0F5L7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	13	LEU	-	expression tag	UNP A0A0P0F5L7
C	14	ARG	-	expression tag	UNP A0A0P0F5L7
D	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
D	-3	GLY	-	expression tag	UNP A0A0P0F5L7
D	-2	SER	-	expression tag	UNP A0A0P0F5L7
D	-1	SER	-	expression tag	UNP A0A0P0F5L7
D	0	HIS	-	expression tag	UNP A0A0P0F5L7
D	1	HIS	-	expression tag	UNP A0A0P0F5L7
D	2	HIS	-	expression tag	UNP A0A0P0F5L7
D	3	HIS	-	expression tag	UNP A0A0P0F5L7
D	4	HIS	-	expression tag	UNP A0A0P0F5L7
D	5	HIS	-	expression tag	UNP A0A0P0F5L7
D	6	SER	-	expression tag	UNP A0A0P0F5L7
D	7	SER	-	expression tag	UNP A0A0P0F5L7
D	8	GLY	-	expression tag	UNP A0A0P0F5L7
D	9	PRO	-	expression tag	UNP A0A0P0F5L7
D	10	GLN	-	expression tag	UNP A0A0P0F5L7
D	11	GLN	-	expression tag	UNP A0A0P0F5L7
D	12	GLY	-	expression tag	UNP A0A0P0F5L7
D	13	LEU	-	expression tag	UNP A0A0P0F5L7
D	14	ARG	-	expression tag	UNP A0A0P0F5L7
E	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
E	-3	GLY	-	expression tag	UNP A0A0P0F5L7
E	-2	SER	-	expression tag	UNP A0A0P0F5L7
E	-1	SER	-	expression tag	UNP A0A0P0F5L7
E	0	HIS	-	expression tag	UNP A0A0P0F5L7
E	1	HIS	-	expression tag	UNP A0A0P0F5L7
E	2	HIS	-	expression tag	UNP A0A0P0F5L7
E	3	HIS	-	expression tag	UNP A0A0P0F5L7
E	4	HIS	-	expression tag	UNP A0A0P0F5L7
E	5	HIS	-	expression tag	UNP A0A0P0F5L7
E	6	SER	-	expression tag	UNP A0A0P0F5L7
E	7	SER	-	expression tag	UNP A0A0P0F5L7
E	8	GLY	-	expression tag	UNP A0A0P0F5L7
E	9	PRO	-	expression tag	UNP A0A0P0F5L7
E	10	GLN	-	expression tag	UNP A0A0P0F5L7
E	11	GLN	-	expression tag	UNP A0A0P0F5L7
E	12	GLY	-	expression tag	UNP A0A0P0F5L7
E	13	LEU	-	expression tag	UNP A0A0P0F5L7
E	14	ARG	-	expression tag	UNP A0A0P0F5L7
F	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
F	-3	GLY	-	expression tag	UNP A0A0P0F5L7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	SER	-	expression tag	UNP A0A0P0F5L7
F	-1	SER	-	expression tag	UNP A0A0P0F5L7
F	0	HIS	-	expression tag	UNP A0A0P0F5L7
F	1	HIS	-	expression tag	UNP A0A0P0F5L7
F	2	HIS	-	expression tag	UNP A0A0P0F5L7
F	3	HIS	-	expression tag	UNP A0A0P0F5L7
F	4	HIS	-	expression tag	UNP A0A0P0F5L7
F	5	HIS	-	expression tag	UNP A0A0P0F5L7
F	6	SER	-	expression tag	UNP A0A0P0F5L7
F	7	SER	-	expression tag	UNP A0A0P0F5L7
F	8	GLY	-	expression tag	UNP A0A0P0F5L7
F	9	PRO	-	expression tag	UNP A0A0P0F5L7
F	10	GLN	-	expression tag	UNP A0A0P0F5L7
F	11	GLN	-	expression tag	UNP A0A0P0F5L7
F	12	GLY	-	expression tag	UNP A0A0P0F5L7
F	13	LEU	-	expression tag	UNP A0A0P0F5L7
F	14	ARG	-	expression tag	UNP A0A0P0F5L7
G	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
G	-3	GLY	-	expression tag	UNP A0A0P0F5L7
G	-2	SER	-	expression tag	UNP A0A0P0F5L7
G	-1	SER	-	expression tag	UNP A0A0P0F5L7
G	0	HIS	-	expression tag	UNP A0A0P0F5L7
G	1	HIS	-	expression tag	UNP A0A0P0F5L7
G	2	HIS	-	expression tag	UNP A0A0P0F5L7
G	3	HIS	-	expression tag	UNP A0A0P0F5L7
G	4	HIS	-	expression tag	UNP A0A0P0F5L7
G	5	HIS	-	expression tag	UNP A0A0P0F5L7
G	6	SER	-	expression tag	UNP A0A0P0F5L7
G	7	SER	-	expression tag	UNP A0A0P0F5L7
G	8	GLY	-	expression tag	UNP A0A0P0F5L7
G	9	PRO	-	expression tag	UNP A0A0P0F5L7
G	10	GLN	-	expression tag	UNP A0A0P0F5L7
G	11	GLN	-	expression tag	UNP A0A0P0F5L7
G	12	GLY	-	expression tag	UNP A0A0P0F5L7
G	13	LEU	-	expression tag	UNP A0A0P0F5L7
G	14	ARG	-	expression tag	UNP A0A0P0F5L7
H	-4	MET	-	initiating methionine	UNP A0A0P0F5L7
H	-3	GLY	-	expression tag	UNP A0A0P0F5L7
H	-2	SER	-	expression tag	UNP A0A0P0F5L7
H	-1	SER	-	expression tag	UNP A0A0P0F5L7
H	0	HIS	-	expression tag	UNP A0A0P0F5L7
H	1	HIS	-	expression tag	UNP A0A0P0F5L7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	2	HIS	-	expression tag	UNP A0A0P0F5L7
H	3	HIS	-	expression tag	UNP A0A0P0F5L7
H	4	HIS	-	expression tag	UNP A0A0P0F5L7
H	5	HIS	-	expression tag	UNP A0A0P0F5L7
H	6	SER	-	expression tag	UNP A0A0P0F5L7
H	7	SER	-	expression tag	UNP A0A0P0F5L7
H	8	GLY	-	expression tag	UNP A0A0P0F5L7
H	9	PRO	-	expression tag	UNP A0A0P0F5L7
H	10	GLN	-	expression tag	UNP A0A0P0F5L7
H	11	GLN	-	expression tag	UNP A0A0P0F5L7
H	12	GLY	-	expression tag	UNP A0A0P0F5L7
H	13	LEU	-	expression tag	UNP A0A0P0F5L7
H	14	ARG	-	expression tag	UNP A0A0P0F5L7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	2	Total 2	Ca 2	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0
2	E	2	Total 2	Ca 2	0	0
2	F	1	Total 1	Ca 1	0	0
2	G	1	Total 1	Ca 1	0	0
2	H	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	404	Total 404	O 404	0	0
3	B	399	Total 399	O 399	0	0
3	C	351	Total 351	O 351	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	383	Total 383	O 383	0	0
3	E	350	Total 350	O 350	0	0
3	F	324	Total 324	O 324	0	0
3	G	289	Total 289	O 289	0	0
3	H	271	Total 271	O 271	0	0

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
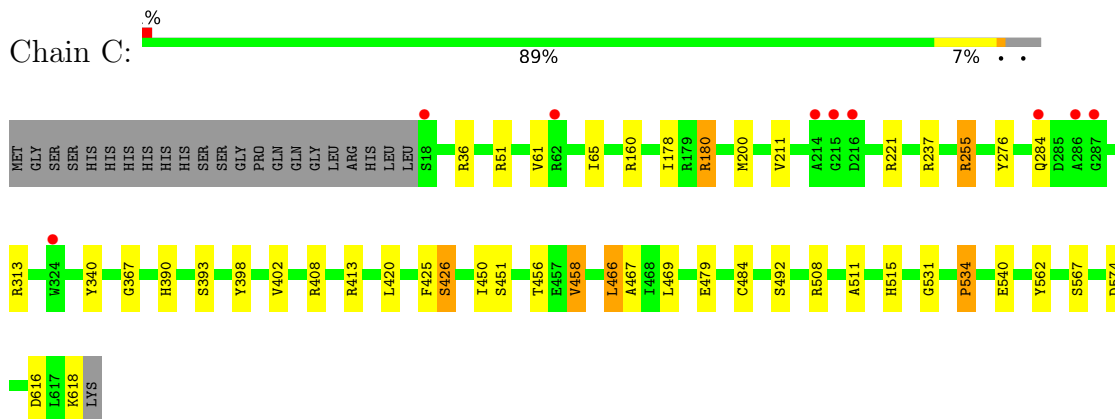
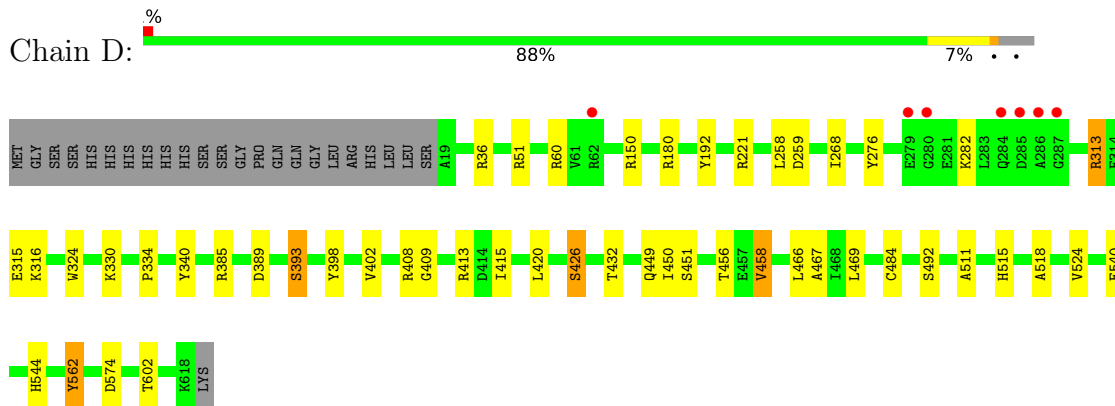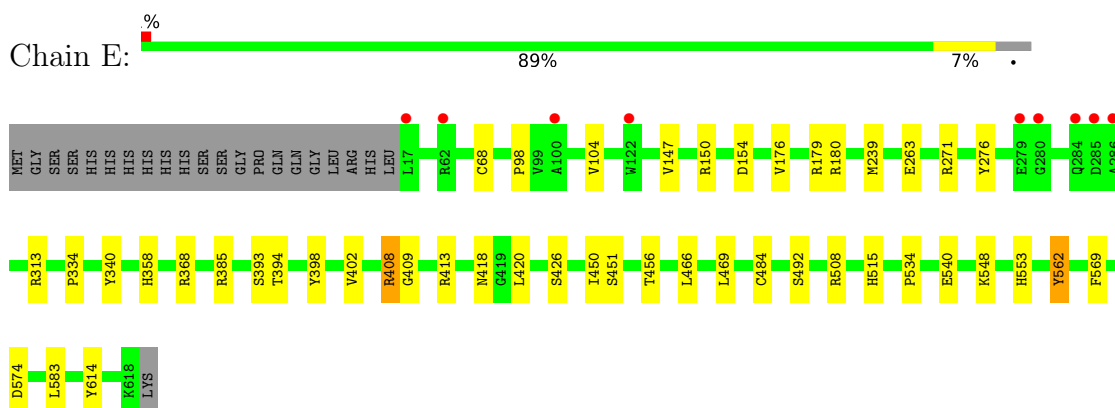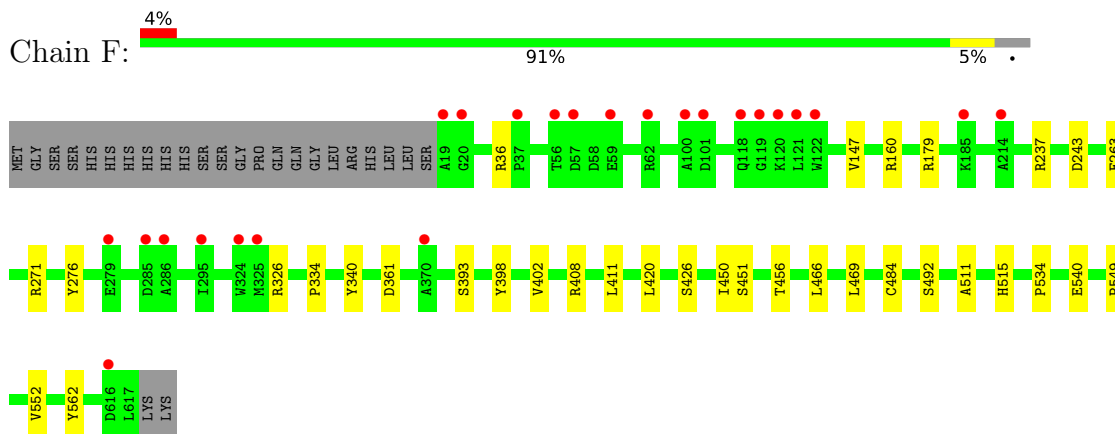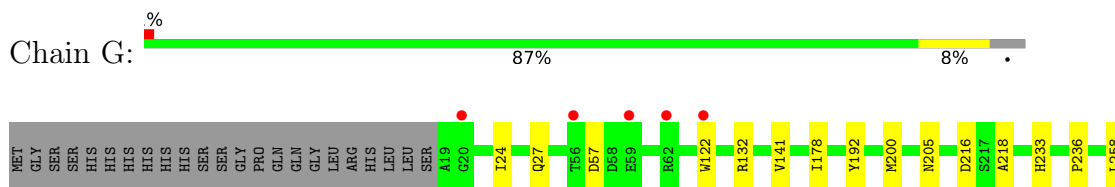• Molecule 1: Glycoside hydrolase BT_1002
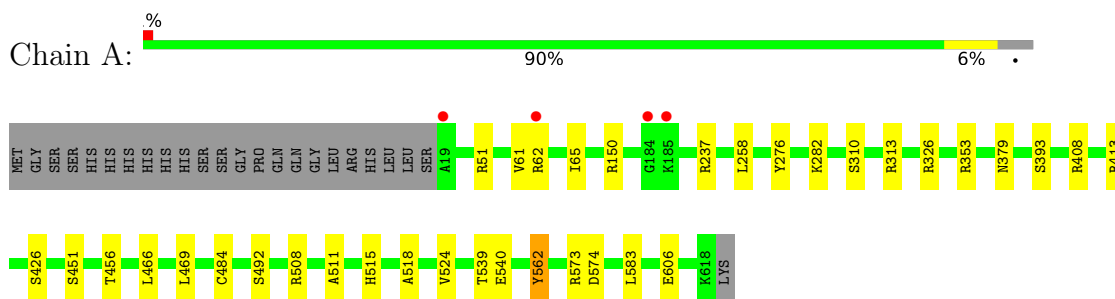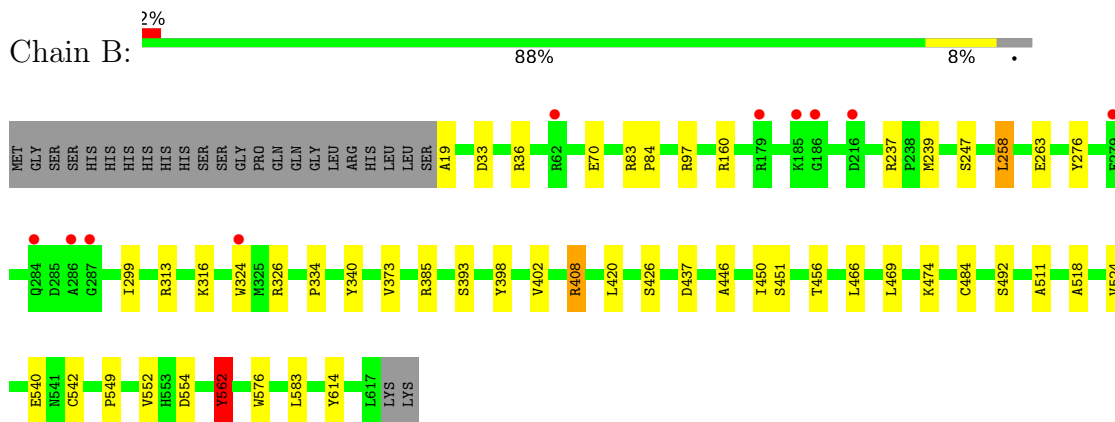
• Molecule 1: Glycoside hydrolase BT_1002

• Molecule 1: Glycoside hydrolase BT_1002

• Molecule 1: Glycoside hydrolase BT_1002

Chain D:

• Molecule 1: Glycoside hydrolase BT_1002

Chain E:

• Molecule 1: Glycoside hydrolase BT_1002

Chain F:

• Molecule 1: Glycoside hydrolase BT_1002

Chain G:

I268 Y276 E279 Q284 D285 A286 V290 W324 H332 S393 Y398 V402 R408 R413 L420 S426 A446 I450 S451 T456 E457 V458 L466 A467 I468 L469 K474 E479 C484 S492 H510 A511 H515 A518

V524 G531 E540 Y562 S567 D574 N575 W576 R605 Y614 K618 LYS

• Molecule 1: Glycoside hydrolase BT_1002

Chain H:

3%

90%   6%   •

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY PRO GLN GLN GLY LEU ARG HIS LEU LEU SER A19 G20 Q27 E59 R62 D101 R137 I170 V176 R179 A214 G215 D216 S217 R221 R271 Y276 E279 Q284 D285 A286 G287

R313 K316 P334 Y340 R385 H390 S393 T394 Y398 V402 G409 N418 G419 L420 S426 D437 I450 S451 L466 L469 E479 A511 P534 E540 W558 Y562 F569 D574 K581 Y582 L583 D616 L617 K618 LYS
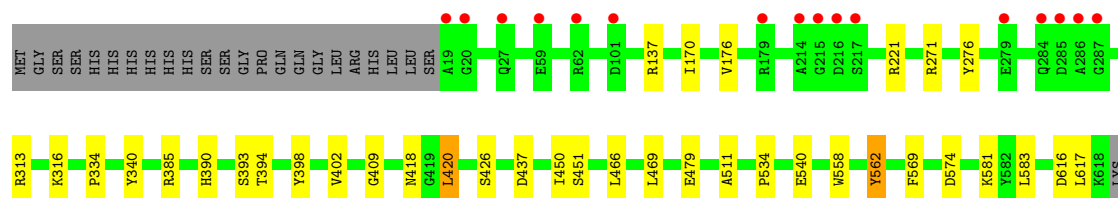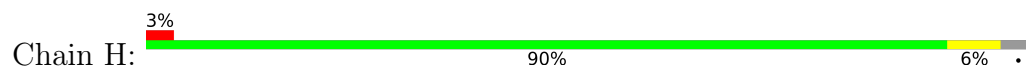
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.23Å 133.24Å 224.08Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	49.16 – 2.00 48.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.16-2.00) 99.8 (48.58-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.183 , 0.224 0.190 , 0.229	Depositor DCC
R_{free} test set	20382 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	41129	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.74	0/4923	0.87	9/6693 (0.1%)
1	B	0.75	0/4914	0.90	14/6681 (0.2%)
1	C	0.70	0/4937	0.89	11/6711 (0.2%)
1	D	0.68	0/4923	0.89	12/6693 (0.2%)
1	E	0.65	0/4937	0.85	11/6712 (0.2%)
1	F	0.68	0/4908	0.84	6/6673 (0.1%)
1	G	0.66	0/4923	0.84	2/6693 (0.0%)
1	H	0.63	0/4923	0.82	5/6693 (0.1%)
All	All	0.69	0/39388	0.86	70/53549 (0.1%)

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	313	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	B	408	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	D	313	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	C	313	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	313	ARG	NE-CZ-NH1	6.97	123.78	120.30

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	4793	0	4609	13	0
1	B	4784	0	4596	24	0
1	C	4804	0	4623	20	0
1	D	4793	0	4609	23	0
1	E	4807	0	4625	20	0
1	F	4781	0	4591	13	0
1	G	4793	0	4609	25	0
1	H	4793	0	4609	16	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	404	0	0	0	0
3	B	399	0	0	0	0
3	C	351	0	0	3	1
3	D	383	0	0	1	0
3	E	350	0	0	2	1
3	F	324	0	0	1	0
3	G	289	0	0	0	0
3	H	271	0	0	0	0
All	All	41129	0	36871	152	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 152 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:B:36:ARG:NH1	1:B:70:GLU:OE1	2.25	0.69
1:B:466:LEU:HD13	1:B:469:LEU:HD13	1.77	0.66
1:B:19:ALA:HB3	1:B:97:ARG:HH21	1.61	0.66
1:B:408:ARG:HD3	1:B:614:TYR:OH	1.96	0.65
1:C:255:ARG:NH1	3:C:802:HOH:O	2.31	0.63

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:978:HOH:O	3:E:2128:HOH:O[3_544]	2.16	0.04

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	599/624 (96%)	570 (95%)	26 (4%)	3 (0%)	29	23
1	B	598/624 (96%)	572 (96%)	25 (4%)	1 (0%)	47	44
1	C	601/624 (96%)	571 (95%)	23 (4%)	7 (1%)	13	7
1	D	599/624 (96%)	568 (95%)	28 (5%)	3 (0%)	29	23
1	E	601/624 (96%)	570 (95%)	27 (4%)	4 (1%)	22	16
1	F	597/624 (96%)	571 (96%)	23 (4%)	3 (0%)	29	23
1	G	599/624 (96%)	568 (95%)	25 (4%)	6 (1%)	15	9
1	H	599/624 (96%)	564 (94%)	29 (5%)	6 (1%)	15	9
All	All	4793/4992 (96%)	4554 (95%)	206 (4%)	33 (1%)	25	16

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	285	ASP
1	C	200	MET
1	C	616	ASP
1	F	393	SER
1	G	393	SER

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	506/526 (96%)	501 (99%)	5 (1%)	76	81
1	B	505/526 (96%)	502 (99%)	3 (1%)	86	90
1	C	508/526 (97%)	501 (99%)	7 (1%)	67	72
1	D	506/526 (96%)	499 (99%)	7 (1%)	67	72
1	E	508/526 (97%)	504 (99%)	4 (1%)	81	86
1	F	504/526 (96%)	500 (99%)	4 (1%)	81	86
1	G	506/526 (96%)	498 (98%)	8 (2%)	62	67
1	H	506/526 (96%)	502 (99%)	4 (1%)	81	86
All	All	4049/4208 (96%)	4007 (99%)	42 (1%)	76	81

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	411	LEU
1	G	276	TYR
1	F	562	TYR
1	G	57	ASP
1	G	562	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	449	GLN
1	E	358	HIS
1	F	449	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 monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	600/624 (96%)	-0.28	4 (0%)	87	87	22, 31, 51, 79	0
1	B	599/624 (95%)	-0.11	10 (1%)	70	68	21, 33, 56, 85	0
1	C	601/624 (96%)	-0.20	9 (1%)	73	72	22, 34, 55, 78	0
1	D	600/624 (96%)	-0.23	7 (1%)	79	78	23, 33, 56, 74	0
1	E	602/624 (96%)	-0.29	9 (1%)	73	72	24, 37, 58, 74	0
1	F	599/624 (95%)	-0.04	24 (4%)	38	37	23, 37, 63, 81	0
1	G	600/624 (96%)	-0.07	7 (1%)	79	78	28, 40, 65, 84	0
1	H	600/624 (96%)	-0.04	16 (2%)	54	53	28, 42, 63, 89	0
All	All	4801/4992 (96%)	-0.16	86 (1%)	68	66	21, 36, 59, 89	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	19	ALA	6.4
1	H	286	ALA	4.8
1	E	100	ALA	4.3
1	F	19	ALA	4.2
1	F	59	GLU	4.1

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 monosaccharides 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. 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(Å^2)	Q<0.9
2	CA	B	702	1/1	0.97	0.10	51,51,51,51	0
2	CA	E	702	1/1	0.97	0.05	54,54,54,54	0
2	CA	H	701	1/1	0.97	0.05	42,42,42,42	0
2	CA	F	701	1/1	0.98	0.04	41,41,41,41	0
2	CA	G	701	1/1	0.98	0.06	43,43,43,43	0
2	CA	E	701	1/1	0.98	0.06	39,39,39,39	0
2	CA	D	701	1/1	0.99	0.03	36,36,36,36	0
2	CA	B	701	1/1	0.99	0.05	40,40,40,40	0
2	CA	A	701	1/1	0.99	0.06	34,34,34,34	0
2	CA	C	701	1/1	1.00	0.07	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.