



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:20 AM UTC

PDB ID : 5MQP / pdb_00005mqp
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)

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

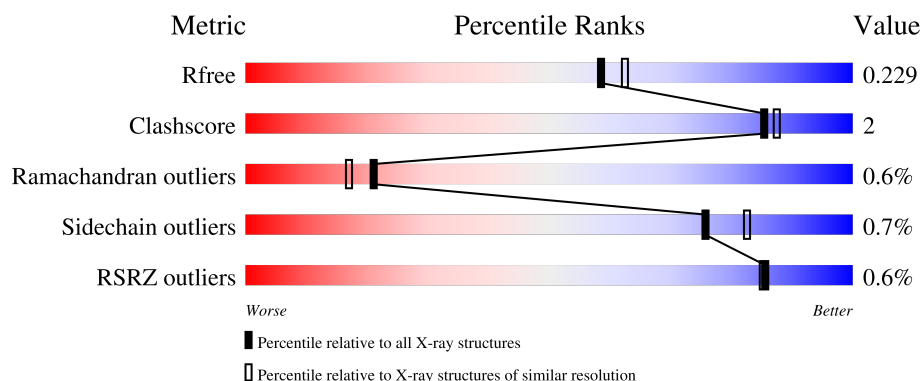
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	624	91% 5% .
1	B	624	% 88% 8% .
1	C	624	% 89% 7% .
1	D	624	89% 7% .
1	E	624	89% 7% .

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Mol	Chain	Length	Quality of chain
1	F	624	% 91% 5% .
1	G	624	% 88% 8% • •
1	H	624	% 90% 6% .

2 Entry composition

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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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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is water.

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

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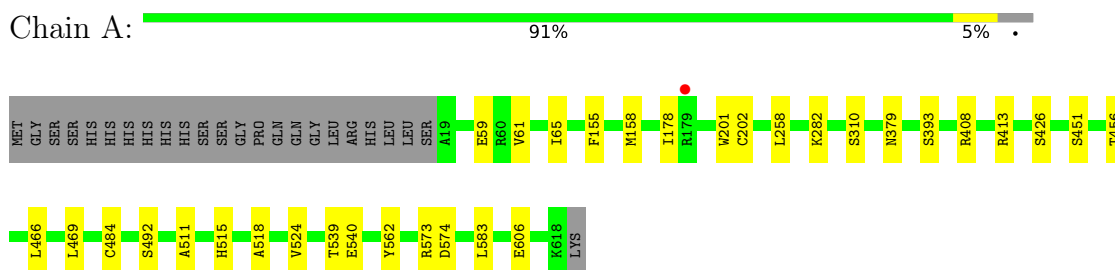
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	383	Total 383	O 383	0	0
3	E	350	Total 350	O 350	0	0
3	F	324	Total 324	O 324	0	0
3	G	289	Total 289	O 289	0	0
3	H	271	Total 271	O 271	0	0

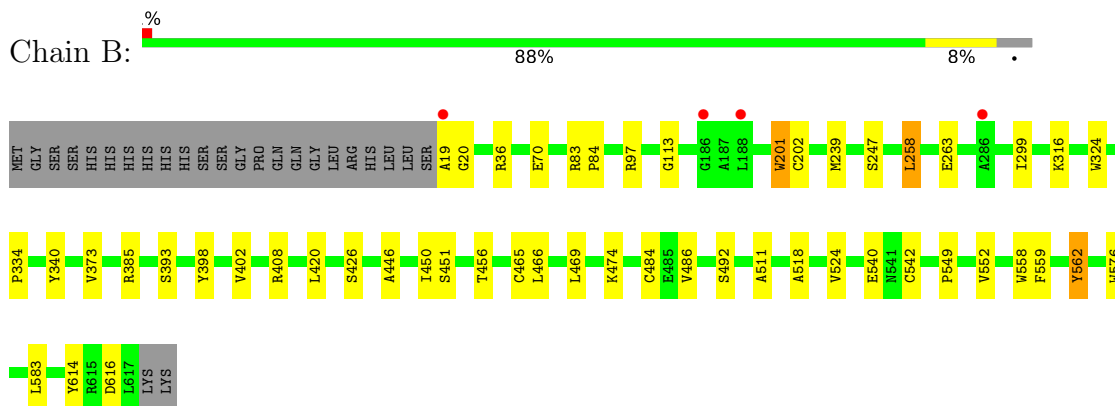
3 Residue-property plots [i](#)

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.

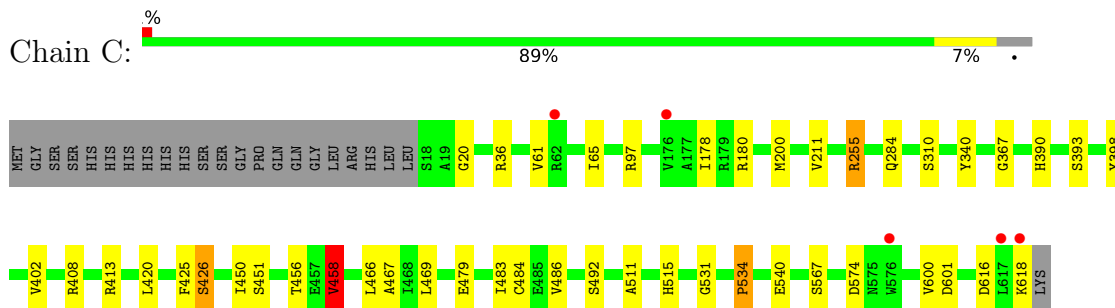
- Molecule 1: Glycoside hydrolase BT_1002



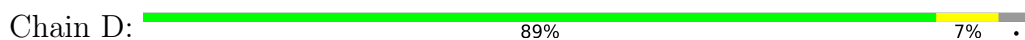
- Molecule 1: Glycoside hydrolase BT_1002

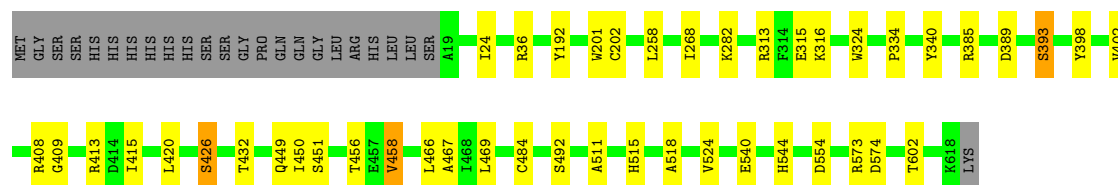


- Molecule 1: Glycoside hydrolase BT_1002



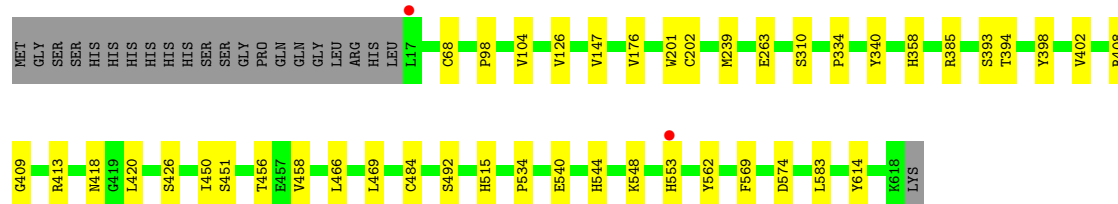
- Molecule 1: Glycoside hydrolase BT_1002





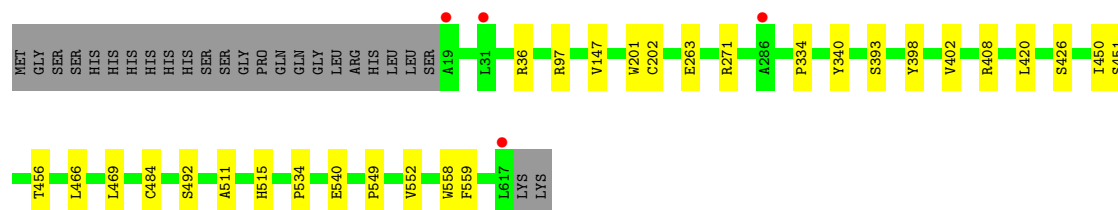
- Molecule 1: Glycoside hydrolase BT_1002

Chain E: 89% 7% .



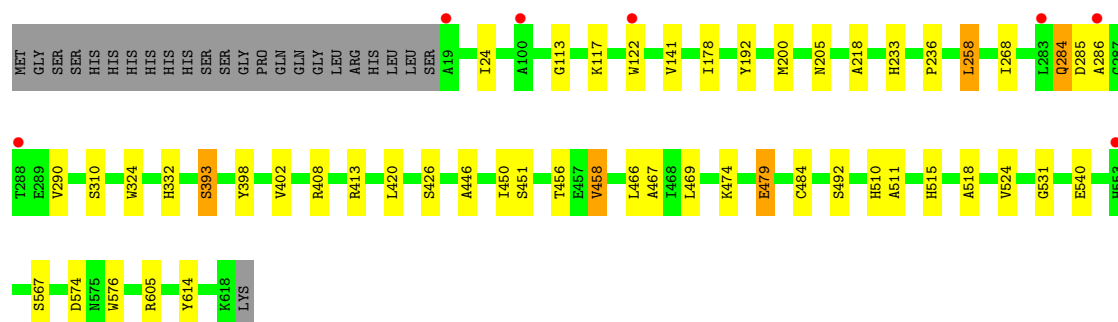
- Molecule 1: Glycoside hydrolase BT_1002

Chain F: 91% 5% .



- Molecule 1: Glycoside hydrolase BT_1002

Chain G: 88% 8% . .



- Molecule 1: Glycoside hydrolase BT_1002

Chain H: 90% 6% .





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 49.16 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.16-2.00) 99.8 (49.16-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	20383 reflections (5.00%)	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)	0.33 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: 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	0.96	0/4923	0.96	0/6693
1	B	1.00	2/4914 (0.0%)	1.01	5/6681 (0.1%)
1	C	0.93	1/4937 (0.0%)	0.96	6/6711 (0.1%)
1	D	0.90	0/4923	0.96	0/6693
1	E	0.85	0/4937	0.92	4/6712 (0.1%)
1	F	0.89	0/4908	0.93	1/6673 (0.0%)
1	G	0.89	1/4923 (0.0%)	0.95	2/6693 (0.0%)
1	H	0.87	0/4923	0.92	2/6693 (0.0%)
All	All	0.91	4/39388 (0.0%)	0.95	20/53549 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	GLY	N-CA	8.78	1.51	1.44
1	G	113	GLY	N-CA	8.10	1.50	1.44
1	C	483	ILE	N-CA	-5.52	1.39	1.46
1	B	201	TRP	CA-C	5.04	1.59	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	GLY	N-CA-C	7.22	122.23	110.97
1	F	97	ARG	N-CA-C	7.04	114.56	108.22
1	B	616	ASP	N-CA-C	6.62	120.81	112.87
1	C	97	ARG	N-CA-C	6.30	113.89	108.22
1	B	486	VAL	N-CA-C	-6.17	104.13	109.19
1	C	458	VAL	N-CA-C	-5.62	100.50	109.20
1	C	458	VAL	CB-CA-C	5.38	118.88	111.19
1	C	486	VAL	N-CA-C	-5.34	102.97	109.01
1	G	310	SER	N-CA-C	5.34	117.30	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	126	VAL	CA-C-N	-5.31	115.11	120.21
1	E	126	VAL	C-N-CA	-5.31	115.11	120.21
1	H	531	GLY	N-CA-C	5.26	119.48	112.65
1	E	544	HIS	N-CA-C	5.24	116.26	108.60
1	B	562	TYR	CA-CB-CG	5.23	123.31	113.90
1	C	310	SER	N-CA-C	5.14	117.00	109.24
1	H	479	GLU	N-CA-C	5.11	117.15	109.23
1	C	20	GLY	N-CA-C	-5.11	106.71	112.33
1	E	310	SER	N-CA-C	5.07	116.90	109.24
1	G	479	GLU	N-CA-C	5.04	117.47	109.50
1	B	465	CYS	N-CA-C	5.00	116.99	110.53

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	16	0
1	B	4784	0	4596	27	0
1	C	4804	0	4623	21	0
1	D	4793	0	4609	26	0
1	E	4807	0	4625	21	0
1	F	4781	0	4591	15	0
1	G	4793	0	4609	26	0
1	H	4793	0	4609	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	168	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.

All (168) 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
1:B:201:TRP:CD1	1:B:202:CYS:HG	2.17	0.63
1:E:420:LEU:HD21	1:E:450:ILE:HD12	1.82	0.62
1:F:201:TRP:CD1	1:F:202:CYS:HG	2.21	0.58
1:C:420:LEU:HD21	1:C:450:ILE:HD12	1.86	0.58
1:E:176:VAL:HG23	3:E:2022:HOH:O	2.05	0.57
1:D:316:LYS:HA	1:D:385:ARG:O	2.06	0.56
1:H:239:MET:HE2	1:H:553:HIS:HB2	1.88	0.56
1:A:408:ARG:HA	1:A:451:SER:O	2.07	0.55
1:A:61:VAL:HG22	1:A:65:ILE:HD11	1.88	0.55
1:F:466:LEU:HD22	1:F:492:SER:HB2	1.88	0.55
1:H:420:LEU:HD21	1:H:450:ILE:HD12	1.88	0.55
1:F:511:ALA:HA	1:F:540:GLU:O	2.06	0.55
1:F:408:ARG:HA	1:F:451:SER:O	2.08	0.54
1:C:408:ARG:HA	1:C:451:SER:O	2.08	0.54
1:E:408:ARG:HA	1:E:451:SER:O	2.07	0.54
1:D:415:ILE:HB	1:D:458:VAL:HG22	1.90	0.54
1:D:420:LEU:HD21	1:D:450:ILE:HD12	1.89	0.54
1:H:398:TYR:CD2	1:H:402:VAL:HG11	2.43	0.54
1:G:420:LEU:HD21	1:G:450:ILE:HD12	1.89	0.54
1:F:420:LEU:HD21	1:F:450:ILE:HD12	1.91	0.53
1:A:466:LEU:HD13	1:A:469:LEU:HD13	1.91	0.53
1:B:316:LYS:HA	1:B:385:ARG:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:LEU:HD13	1:F:469:LEU:HD13	1.92	0.52
1:D:408:ARG:HA	1:D:451:SER:O	2.09	0.52
1:H:562:TYR:CE1	1:H:583:LEU:HD23	2.43	0.52
1:C:61:VAL:HG22	1:C:65:ILE:HD11	1.90	0.52
1:E:398:TYR:HD2	1:E:402:VAL:HG11	1.75	0.52
1:B:258:LEU:HD13	1:B:263:GLU:HB2	1.92	0.51
1:B:408:ARG:HD3	1:B:614:TYR:CZ	2.46	0.51
1:E:466:LEU:HD13	1:E:469:LEU:HD13	1.94	0.50
1:D:201:TRP:CD1	1:D:202:CYS:HG	2.29	0.50
1:A:201:TRP:CD1	1:A:202:CYS:HG	2.29	0.50
1:E:466:LEU:HD22	1:E:492:SER:HB2	1.92	0.50
1:C:180:ARG:NH2	3:C:804:HOH:O	2.32	0.50
1:B:511:ALA:HA	1:B:540:GLU:O	2.12	0.50
1:D:398:TYR:CD2	1:D:402:VAL:HG11	2.46	0.50
1:E:201:TRP:CD1	1:E:202:CYS:HG	2.29	0.50
1:C:425:PHE:O	1:C:426[B]:SER:CB	2.59	0.49
1:G:466:LEU:HD13	1:G:469:LEU:HD13	1.93	0.49
1:E:398:TYR:CD2	1:E:402:VAL:HG11	2.47	0.49
1:A:606:GLU:O	1:B:36:ARG:NH2	2.46	0.49
1:D:192:TYR:CZ	1:D:268:ILE:HD11	2.48	0.49
1:F:484:CYS:HA	1:F:515:HIS:O	2.12	0.49
1:A:511:ALA:HA	1:A:540:GLU:O	2.13	0.49
1:C:466:LEU:HD13	1:C:469:LEU:HD13	1.95	0.49
1:C:458:VAL:HG11	1:C:467:ALA:HA	1.95	0.49
1:B:518:ALA:HB2	1:B:524:VAL:HG21	1.95	0.48
1:B:562:TYR:CE1	1:B:583:LEU:HD23	2.48	0.48
1:C:466:LEU:HD22	1:C:492:SER:HB2	1.95	0.48
1:H:201:TRP:CD1	1:H:202:CYS:HG	2.31	0.48
1:C:398:TYR:CD2	1:C:402:VAL:HG11	2.48	0.48
1:E:239:MET:HG3	1:E:553:HIS:HB3	1.95	0.48
1:D:398:TYR:HD2	1:D:402:VAL:HG11	1.77	0.48
1:D:466:LEU:HD13	1:D:469:LEU:HD13	1.96	0.48
1:E:562:TYR:CE1	1:E:583:LEU:HD23	2.49	0.48
1:H:466:LEU:HD13	1:H:469:LEU:HD13	1.95	0.48
1:G:398:TYR:HD2	1:G:402:VAL:HG11	1.79	0.48
1:B:466:LEU:HD22	1:B:492:SER:HB2	1.96	0.47
1:G:141:VAL:HG22	1:G:290:VAL:HG22	1.95	0.47
1:D:515:HIS:HA	1:D:544:HIS:O	2.14	0.47
1:G:122:TRP:CH2	1:G:284:GLN:HG3	2.50	0.47
1:B:398:TYR:CD2	1:B:402:VAL:HG11	2.50	0.47
1:G:518:ALA:HB2	1:G:524:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:540:GLU:HA	1:H:574:ASP:O	2.15	0.47
1:B:420:LEU:HD21	1:B:450:ILE:HD12	1.96	0.47
1:G:408:ARG:HA	1:G:451:SER:O	2.15	0.47
1:E:147:VAL:O	1:E:263:GLU:HA	2.15	0.46
1:G:576:TRP:CG	1:G:605:ARG:HG3	2.50	0.46
1:H:511:ALA:HA	1:H:540:GLU:O	2.16	0.46
1:D:313:ARG:NH1	1:D:315:GLU:OE2	2.48	0.46
1:C:511:ALA:HA	1:C:540:GLU:O	2.16	0.46
1:A:155:PHE:HB3	1:A:158:MET:HE2	1.98	0.46
1:G:413:ARG:HA	1:G:456:THR:O	2.16	0.46
1:D:466:LEU:HD22	1:D:492:SER:HB2	1.98	0.46
1:A:413:ARG:HA	1:A:456:THR:O	2.15	0.46
1:H:398:TYR:HD2	1:H:402:VAL:HG11	1.79	0.45
1:C:540:GLU:HA	1:C:574:ASP:O	2.16	0.45
1:B:299:ILE:HB	1:B:373:VAL:HG13	1.98	0.45
1:G:511:ALA:HA	1:G:540:GLU:O	2.17	0.45
1:E:413:ARG:HA	1:E:456:THR:O	2.16	0.45
1:C:36:ARG:NH1	3:C:801:HOH:O	2.26	0.45
1:D:385:ARG:HA	1:D:409:GLY:O	2.17	0.45
1:A:562:TYR:CE1	1:A:583:LEU:HD23	2.51	0.45
1:E:385:ARG:HA	1:E:409:GLY:O	2.17	0.45
1:E:394:THR:HA	1:E:418:ASN:O	2.17	0.45
1:E:408:ARG:HD3	1:E:614:TYR:OH	2.17	0.45
1:A:518:ALA:HB2	1:A:524:VAL:HG21	1.99	0.45
1:B:408:ARG:HA	1:B:451:SER:O	2.16	0.45
1:E:540:GLU:HA	1:E:574:ASP:O	2.17	0.45
1:G:192:TYR:CZ	1:G:268:ILE:HD11	2.52	0.44
1:A:540:GLU:HA	1:A:574:ASP:O	2.17	0.44
1:G:540:GLU:HA	1:G:574:ASP:O	2.17	0.44
1:A:466:LEU:HD22	1:A:492:SER:HB2	2.00	0.44
1:D:334:PRO:HA	1:D:340:TYR:HA	2.00	0.44
1:D:511:ALA:HA	1:D:540:GLU:O	2.18	0.43
1:F:334:PRO:HA	1:F:340:TYR:HA	2.00	0.43
1:H:451:SER:HA	1:H:479:GLU:O	2.18	0.43
1:F:398:TYR:CD2	1:F:402:VAL:HG11	2.54	0.43
1:A:178:ILE:C	1:A:178:ILE:HD12	2.43	0.43
1:B:324:TRP:HB2	1:B:393:SER:HB2	2.00	0.43
1:C:600:VAL:O	1:C:601:ASP:C	2.62	0.43
1:C:178:ILE:HD13	1:C:211:VAL:HG11	2.01	0.43
1:D:458:VAL:HG11	1:D:467:ALA:HA	2.00	0.43
1:G:458:VAL:HG11	1:G:467:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:GLY:O	1:C:567:SER:HA	2.18	0.43
1:E:569:PHE:CE1	1:H:569:PHE:HB3	2.54	0.43
1:F:456:THR:HA	1:F:484:CYS:O	2.18	0.43
1:F:549:PRO:HG2	1:F:552:VAL:HG13	2.01	0.43
1:H:316:LYS:HA	1:H:385:ARG:O	2.19	0.43
1:B:558:TRP:C	1:B:559:PHE:CG	2.96	0.43
1:F:558:TRP:C	1:F:559:PHE:CG	2.97	0.43
1:G:446:ALA:HA	1:G:474:LYS:O	2.18	0.43
1:B:542:CYS:HA	1:B:576:TRP:O	2.19	0.43
1:G:178:ILE:HD11	1:G:218:ALA:HB2	2.01	0.43
1:H:409:GLY:O	1:H:617:LEU:HD21	2.19	0.43
1:F:271:ARG:HG2	3:F:950:HOH:O	2.19	0.42
1:G:408:ARG:HD3	1:G:614:TYR:CZ	2.54	0.42
1:C:425:PHE:O	1:C:426[B]:SER:HB2	2.18	0.42
1:C:484:CYS:HA	1:C:515:HIS:O	2.19	0.42
1:D:602:THR:HG23	3:D:1109:HOH:O	2.19	0.42
1:E:484:CYS:HA	1:E:515:HIS:O	2.20	0.42
1:D:518:ALA:HB2	1:D:524:VAL:HG21	2.01	0.42
1:A:539:THR:HA	1:A:573:ARG:O	2.19	0.42
1:D:426[A]:SER:OG	1:D:432:THR:HA	2.19	0.42
1:G:576:TRP:CD2	1:G:605:ARG:HG3	2.54	0.42
1:B:549:PRO:HG2	1:B:552:VAL:CG1	2.50	0.42
1:G:324:TRP:HB2	1:G:393:SER:HB2	2.01	0.42
1:H:558:TRP:CE2	1:H:581:LYS:HE3	2.55	0.42
1:D:456:THR:HA	1:D:484:CYS:O	2.20	0.42
1:E:358:HIS:HE1	3:E:2038:HOH:O	2.02	0.41
1:B:83:ARG:HB2	1:B:84:PRO:HD2	2.01	0.41
1:B:258:LEU:C	1:B:258:LEU:HD12	2.45	0.41
1:D:554:ASP:OD1	1:D:554:ASP:C	2.63	0.41
1:G:233:HIS:NE2	1:G:236:PRO:O	2.53	0.41
1:F:147:VAL:O	1:F:263:GLU:HA	2.20	0.41
1:F:466:LEU:HD22	1:F:492:SER:CB	2.51	0.41
1:G:398:TYR:CD2	1:G:402:VAL:HG11	2.55	0.41
1:H:170:ILE:HD11	1:H:221:ARG:NH2	2.35	0.41
1:B:446:ALA:HA	1:B:474:LYS:O	2.20	0.41
1:D:389:ASP:HA	1:D:413:ARG:O	2.21	0.41
1:G:258:LEU:HD12	1:G:258:LEU:C	2.46	0.41
1:C:413:ARG:HA	1:C:456:THR:O	2.20	0.41
1:E:98:PRO:HB3	1:E:104:VAL:HG23	2.02	0.41
1:H:385:ARG:HA	1:H:409:GLY:O	2.20	0.41
1:D:540:GLU:HA	1:D:574:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:ARG:HG2	1:D:574:ASP:CG	2.46	0.41
1:C:340:TYR:CZ	1:C:367:GLY:HA3	2.56	0.41
1:D:466:LEU:HD22	1:D:492:SER:CB	2.51	0.41
1:C:451:SER:HA	1:C:479:GLU:O	2.20	0.41
1:E:334:PRO:HA	1:E:340:TYR:HA	2.02	0.41
1:G:484:CYS:HA	1:G:515:HIS:O	2.21	0.40
1:B:334:PRO:HA	1:B:340:TYR:HA	2.03	0.40
1:D:324:TRP:HB2	1:D:393:SER:HB2	2.03	0.40
1:G:531:GLY:O	1:G:567:SER:HA	2.21	0.40
1:H:394:THR:HA	1:H:418:ASN:O	2.22	0.40
1:B:456:THR:HA	1:B:484:CYS:O	2.21	0.40
1:G:205:ASN:HB2	1:G:332:HIS:HB3	2.02	0.40
1:G:466:LEU:HD22	1:G:492:SER:CB	2.52	0.40
1:A:310:SER:HA	1:A:379:ASN:O	2.21	0.40
1:A:484:CYS:HA	1:A:515:HIS:O	2.21	0.40
1:B:239:MET:N	1:B:247:SER:OG	2.47	0.40
1:G:479:GLU:HA	1:G:510:HIS:O	2.22	0.40
1:H:334:PRO:HA	1:H:340:TYR:HA	2.02	0.40

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 [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	599/624 (96%)	570 (95%)	26 (4%)	3 (0%)	24 21
1	B	598/624 (96%)	572 (96%)	25 (4%)	1 (0%)	43 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	601/624 (96%)	571 (95%)	23 (4%)	7 (1%)	10	6
1	D	599/624 (96%)	568 (95%)	28 (5%)	3 (0%)	24	21
1	E	601/624 (96%)	570 (95%)	27 (4%)	4 (1%)	18	14
1	F	597/624 (96%)	571 (96%)	23 (4%)	3 (0%)	24	21
1	G	599/624 (96%)	568 (95%)	25 (4%)	6 (1%)	12	8
1	H	599/624 (96%)	564 (94%)	29 (5%)	6 (1%)	12	8
All	All	4793/4992 (96%)	4554 (95%)	206 (4%)	33 (1%)	21	14

All (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
1	B	426	SER
1	C	426[A]	SER
1	C	426[B]	SER
1	D	426[A]	SER
1	D	426[B]	SER
1	E	426[A]	SER
1	E	426[B]	SER
1	G	200	MET
1	G	286	ALA
1	H	390	HIS
1	H	393	SER
1	H	426[A]	SER
1	H	426[B]	SER
1	H	616	ASP
1	A	393	SER
1	A	426[A]	SER
1	A	426[B]	SER
1	C	393	SER
1	D	393	SER
1	E	393	SER
1	F	426	SER
1	G	426[A]	SER
1	G	426[B]	SER
1	C	390	HIS

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Mol	Chain	Res	Type
1	C	534	PRO
1	H	534	PRO
1	F	534	PRO
1	E	534	PRO

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%)	503 (99%)	3 (1%)	78	85
1	B	505/526 (96%)	504 (100%)	1 (0%)	87	92
1	C	508/526 (97%)	503 (99%)	5 (1%)	68	75
1	D	506/526 (96%)	500 (99%)	6 (1%)	63	70
1	E	508/526 (97%)	505 (99%)	3 (1%)	78	85
1	F	504/526 (96%)	503 (100%)	1 (0%)	87	92
1	G	506/526 (96%)	501 (99%)	5 (1%)	68	75
1	H	506/526 (96%)	502 (99%)	4 (1%)	73	80
All	All	4049/4208 (96%)	4021 (99%)	28 (1%)	76	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	258	LEU
1	A	282	LYS
1	B	258	LEU
1	C	255	ARG
1	C	284	GLN
1	C	458	VAL
1	C	534	PRO
1	C	618	LYS
1	D	24	ILE
1	D	36	ARG

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Mol	Chain	Res	Type
1	D	258	LEU
1	D	282	LYS
1	D	449	GLN
1	D	458	VAL
1	E	68	CYS
1	E	458	VAL
1	E	548	LYS
1	F	36	ARG
1	G	24	ILE
1	G	117	LYS
1	G	258	LEU
1	G	284	GLN
1	G	458	VAL
1	H	27	GLN
1	H	176	VAL
1	H	282	LYS
1	H	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	GLN
1	A	379	ASN
1	A	403	GLN
1	A	506	ASN
1	B	223	HIS
1	B	403	GLN
1	C	199	GLN
1	C	230	GLN
1	C	379	ASN
1	C	449	GLN
1	D	363	GLN
1	E	27	GLN
1	E	358	HIS
1	E	379	ASN
1	E	380	GLN
1	E	587	ASN
1	F	168	ASN
1	F	449	GLN
1	G	363	GLN
1	G	449	GLN
1	H	27	GLN

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Mol	Chain	Res	Type
1	H	223	HIS
1	H	379	ASN
1	H	380	GLN
1	H	449	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	600/624 (96%)	-0.39	1 (0%) 91 90	19, 31, 51, 79	1 (0%)
1	B	599/624 (95%)	-0.12	4 (0%) 84 84	21, 33, 56, 85	1 (0%)
1	C	601/624 (96%)	-0.17	5 (0%) 82 82	18, 34, 55, 78	2 (0%)
1	D	600/624 (96%)	-0.26	0 100 100	18, 33, 56, 74	1 (0%)
1	E	602/624 (96%)	-0.19	2 (0%) 90 89	18, 37, 58, 74	1 (0%)
1	F	599/624 (95%)	-0.04	4 (0%) 84 84	23, 37, 63, 81	0
1	G	600/624 (96%)	0.09	7 (1%) 76 76	23, 40, 65, 84	1 (0%)
1	H	600/624 (96%)	0.15	5 (0%) 82 82	23, 42, 63, 89	1 (0%)
All	All	4801/4992 (96%)	-0.11	28 (0%) 85 85	18, 36, 59, 89	8 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	ALA	4.0
1	H	19	ALA	4.0
1	E	17	LEU	3.7
1	G	19	ALA	3.3
1	G	283	LEU	3.0
1	C	618	LYS	3.0
1	A	179	ARG	2.8
1	G	286	ALA	2.8
1	G	553	HIS	2.7
1	H	286	ALA	2.6
1	C	62	ARG	2.6
1	F	19	ALA	2.5
1	F	286	ALA	2.5
1	H	548	LYS	2.5
1	C	576	TRP	2.4
1	C	617	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	100	ALA	2.3
1	F	617	LEU	2.3
1	G	122	TRP	2.2
1	C	176	VAL	2.2
1	G	288	THR	2.2
1	B	186	GLY	2.2
1	B	286	ALA	2.1
1	F	31	LEU	2.1
1	H	602	THR	2.1
1	E	553	HIS	2.1
1	H	101	ASP	2.0
1	B	188	LEU	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CA	E	702	1/1	0.98	0.04	54,54,54,54	0
2	CA	B	701	1/1	0.99	0.02	40,40,40,40	0
2	CA	B	702	1/1	0.99	0.10	51,51,51,51	0
2	CA	D	701	1/1	0.99	0.03	36,36,36,36	0
2	CA	E	701	1/1	0.99	0.03	39,39,39,39	0
2	CA	A	701	1/1	0.99	0.02	34,34,34,34	0
2	CA	F	701	1/1	0.99	0.03	41,41,41,41	0
2	CA	G	701	1/1	0.99	0.03	43,43,43,43	0
2	CA	H	701	1/1	0.99	0.03	42,42,42,42	0
2	CA	C	701	1/1	1.00	0.02	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.