W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2023 – 03:38 PM JST

PDB ID	:	6JHP
Title	:	Crystal structure of the glycoside hydrolase family 36 alpha-galactosidase from Paecilomyces thermophila
Authors	:	Liu, Y.; Huang, P.; Ma, J.; Jiang, Z.
Deposited on	:	2019-02-18
Resolution	:	2.56 Å(reported)

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

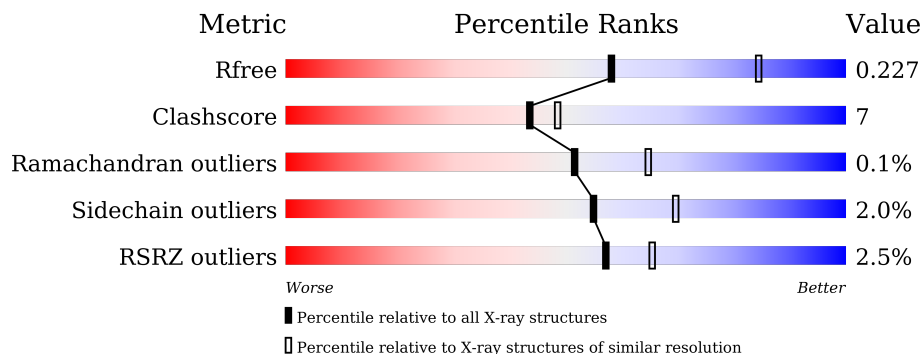|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.56 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		0.227
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		2.0%
RSRZ outliers		2.5%

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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	758	2% 80% 14% 6%
1	B	758	3% 81% 13% · 6%
1	C	758	% 82% 12% · 6%
1	D	758	3% 81% 13% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TRS	A	802	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 22793 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 Alpha-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	716	Total	C	N	O	S	0	0	0
			5609	3557	984	1051	17			
1	B	716	Total	C	N	O	S	0	0	0
			5609	3557	984	1051	17			
1	C	716	Total	C	N	O	S	0	0	0
			5609	3557	984	1051	17			
1	D	716	Total	C	N	O	S	0	0	0
			5609	3557	984	1051	17			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A2Z4HIN9
A	-8	GLY	-	expression tag	UNP A0A2Z4HIN9
A	-7	SER	-	expression tag	UNP A0A2Z4HIN9
A	-6	SER	-	expression tag	UNP A0A2Z4HIN9
A	-5	HIS	-	expression tag	UNP A0A2Z4HIN9
A	-4	HIS	-	expression tag	UNP A0A2Z4HIN9
A	-3	HIS	-	expression tag	UNP A0A2Z4HIN9
A	-2	HIS	-	expression tag	UNP A0A2Z4HIN9
A	-1	HIS	-	expression tag	UNP A0A2Z4HIN9
A	0	HIS	-	expression tag	UNP A0A2Z4HIN9
A	1	SER	-	expression tag	UNP A0A2Z4HIN9
A	2	SER	-	expression tag	UNP A0A2Z4HIN9
A	3	GLY	-	expression tag	UNP A0A2Z4HIN9
A	4	LEU	-	expression tag	UNP A0A2Z4HIN9
A	5	VAL	-	expression tag	UNP A0A2Z4HIN9
A	6	PRO	-	expression tag	UNP A0A2Z4HIN9
A	7	ARG	-	expression tag	UNP A0A2Z4HIN9
A	8	GLY	-	expression tag	UNP A0A2Z4HIN9
A	9	SER	-	expression tag	UNP A0A2Z4HIN9
A	10	HIS	-	expression tag	UNP A0A2Z4HIN9
A	11	MET	-	expression tag	UNP A0A2Z4HIN9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	-	expression tag	UNP A0A2Z4HIN9
A	13	SER	-	expression tag	UNP A0A2Z4HIN9
A	14	MET	-	expression tag	UNP A0A2Z4HIN9
A	15	THR	-	expression tag	UNP A0A2Z4HIN9
A	16	GLY	-	expression tag	UNP A0A2Z4HIN9
A	17	GLY	-	expression tag	UNP A0A2Z4HIN9
A	18	GLN	-	expression tag	UNP A0A2Z4HIN9
A	19	GLN	-	expression tag	UNP A0A2Z4HIN9
A	20	MET	-	expression tag	UNP A0A2Z4HIN9
A	21	GLY	-	expression tag	UNP A0A2Z4HIN9
A	22	ARG	-	expression tag	UNP A0A2Z4HIN9
A	23	GLY	-	expression tag	UNP A0A2Z4HIN9
A	24	SER	-	expression tag	UNP A0A2Z4HIN9
A	25	GLU	-	expression tag	UNP A0A2Z4HIN9
A	26	PHE	-	expression tag	UNP A0A2Z4HIN9
B	-9	MET	-	initiating methionine	UNP A0A2Z4HIN9
B	-8	GLY	-	expression tag	UNP A0A2Z4HIN9
B	-7	SER	-	expression tag	UNP A0A2Z4HIN9
B	-6	SER	-	expression tag	UNP A0A2Z4HIN9
B	-5	HIS	-	expression tag	UNP A0A2Z4HIN9
B	-4	HIS	-	expression tag	UNP A0A2Z4HIN9
B	-3	HIS	-	expression tag	UNP A0A2Z4HIN9
B	-2	HIS	-	expression tag	UNP A0A2Z4HIN9
B	-1	HIS	-	expression tag	UNP A0A2Z4HIN9
B	0	HIS	-	expression tag	UNP A0A2Z4HIN9
B	1	SER	-	expression tag	UNP A0A2Z4HIN9
B	2	SER	-	expression tag	UNP A0A2Z4HIN9
B	3	GLY	-	expression tag	UNP A0A2Z4HIN9
B	4	LEU	-	expression tag	UNP A0A2Z4HIN9
B	5	VAL	-	expression tag	UNP A0A2Z4HIN9
B	6	PRO	-	expression tag	UNP A0A2Z4HIN9
B	7	ARG	-	expression tag	UNP A0A2Z4HIN9
B	8	GLY	-	expression tag	UNP A0A2Z4HIN9
B	9	SER	-	expression tag	UNP A0A2Z4HIN9
B	10	HIS	-	expression tag	UNP A0A2Z4HIN9
B	11	MET	-	expression tag	UNP A0A2Z4HIN9
B	12	ALA	-	expression tag	UNP A0A2Z4HIN9
B	13	SER	-	expression tag	UNP A0A2Z4HIN9
B	14	MET	-	expression tag	UNP A0A2Z4HIN9
B	15	THR	-	expression tag	UNP A0A2Z4HIN9
B	16	GLY	-	expression tag	UNP A0A2Z4HIN9
B	17	GLY	-	expression tag	UNP A0A2Z4HIN9

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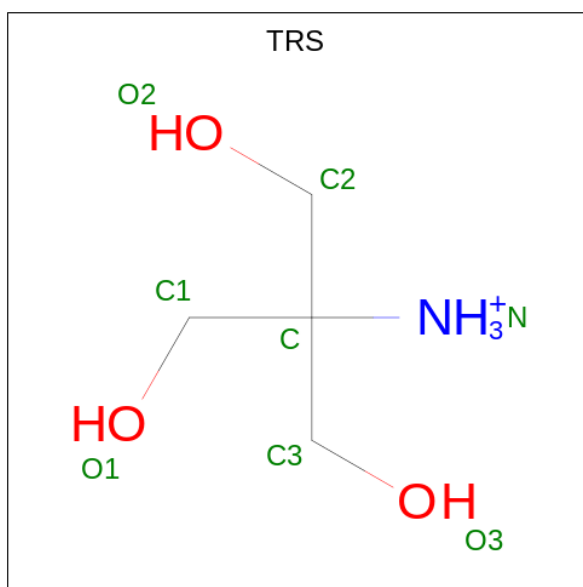
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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	GLN	-	expression tag	UNP A0A2Z4HIN9
B	19	GLN	-	expression tag	UNP A0A2Z4HIN9
B	20	MET	-	expression tag	UNP A0A2Z4HIN9
B	21	GLY	-	expression tag	UNP A0A2Z4HIN9
B	22	ARG	-	expression tag	UNP A0A2Z4HIN9
B	23	GLY	-	expression tag	UNP A0A2Z4HIN9
B	24	SER	-	expression tag	UNP A0A2Z4HIN9
B	25	GLU	-	expression tag	UNP A0A2Z4HIN9
B	26	PHE	-	expression tag	UNP A0A2Z4HIN9
C	-9	MET	-	initiating methionine	UNP A0A2Z4HIN9
C	-8	GLY	-	expression tag	UNP A0A2Z4HIN9
C	-7	SER	-	expression tag	UNP A0A2Z4HIN9
C	-6	SER	-	expression tag	UNP A0A2Z4HIN9
C	-5	HIS	-	expression tag	UNP A0A2Z4HIN9
C	-4	HIS	-	expression tag	UNP A0A2Z4HIN9
C	-3	HIS	-	expression tag	UNP A0A2Z4HIN9
C	-2	HIS	-	expression tag	UNP A0A2Z4HIN9
C	-1	HIS	-	expression tag	UNP A0A2Z4HIN9
C	0	HIS	-	expression tag	UNP A0A2Z4HIN9
C	1	SER	-	expression tag	UNP A0A2Z4HIN9
C	2	SER	-	expression tag	UNP A0A2Z4HIN9
C	3	GLY	-	expression tag	UNP A0A2Z4HIN9
C	4	LEU	-	expression tag	UNP A0A2Z4HIN9
C	5	VAL	-	expression tag	UNP A0A2Z4HIN9
C	6	PRO	-	expression tag	UNP A0A2Z4HIN9
C	7	ARG	-	expression tag	UNP A0A2Z4HIN9
C	8	GLY	-	expression tag	UNP A0A2Z4HIN9
C	9	SER	-	expression tag	UNP A0A2Z4HIN9
C	10	HIS	-	expression tag	UNP A0A2Z4HIN9
C	11	MET	-	expression tag	UNP A0A2Z4HIN9
C	12	ALA	-	expression tag	UNP A0A2Z4HIN9
C	13	SER	-	expression tag	UNP A0A2Z4HIN9
C	14	MET	-	expression tag	UNP A0A2Z4HIN9
C	15	THR	-	expression tag	UNP A0A2Z4HIN9
C	16	GLY	-	expression tag	UNP A0A2Z4HIN9
C	17	GLY	-	expression tag	UNP A0A2Z4HIN9
C	18	GLN	-	expression tag	UNP A0A2Z4HIN9
C	19	GLN	-	expression tag	UNP A0A2Z4HIN9
C	20	MET	-	expression tag	UNP A0A2Z4HIN9
C	21	GLY	-	expression tag	UNP A0A2Z4HIN9
C	22	ARG	-	expression tag	UNP A0A2Z4HIN9
C	23	GLY	-	expression tag	UNP A0A2Z4HIN9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP A0A2Z4HIN9
C	25	GLU	-	expression tag	UNP A0A2Z4HIN9
C	26	PHE	-	expression tag	UNP A0A2Z4HIN9
D	-9	MET	-	initiating methionine	UNP A0A2Z4HIN9
D	-8	GLY	-	expression tag	UNP A0A2Z4HIN9
D	-7	SER	-	expression tag	UNP A0A2Z4HIN9
D	-6	SER	-	expression tag	UNP A0A2Z4HIN9
D	-5	HIS	-	expression tag	UNP A0A2Z4HIN9
D	-4	HIS	-	expression tag	UNP A0A2Z4HIN9
D	-3	HIS	-	expression tag	UNP A0A2Z4HIN9
D	-2	HIS	-	expression tag	UNP A0A2Z4HIN9
D	-1	HIS	-	expression tag	UNP A0A2Z4HIN9
D	0	HIS	-	expression tag	UNP A0A2Z4HIN9
D	1	SER	-	expression tag	UNP A0A2Z4HIN9
D	2	SER	-	expression tag	UNP A0A2Z4HIN9
D	3	GLY	-	expression tag	UNP A0A2Z4HIN9
D	4	LEU	-	expression tag	UNP A0A2Z4HIN9
D	5	VAL	-	expression tag	UNP A0A2Z4HIN9
D	6	PRO	-	expression tag	UNP A0A2Z4HIN9
D	7	ARG	-	expression tag	UNP A0A2Z4HIN9
D	8	GLY	-	expression tag	UNP A0A2Z4HIN9
D	9	SER	-	expression tag	UNP A0A2Z4HIN9
D	10	HIS	-	expression tag	UNP A0A2Z4HIN9
D	11	MET	-	expression tag	UNP A0A2Z4HIN9
D	12	ALA	-	expression tag	UNP A0A2Z4HIN9
D	13	SER	-	expression tag	UNP A0A2Z4HIN9
D	14	MET	-	expression tag	UNP A0A2Z4HIN9
D	15	THR	-	expression tag	UNP A0A2Z4HIN9
D	16	GLY	-	expression tag	UNP A0A2Z4HIN9
D	17	GLY	-	expression tag	UNP A0A2Z4HIN9
D	18	GLN	-	expression tag	UNP A0A2Z4HIN9
D	19	GLN	-	expression tag	UNP A0A2Z4HIN9
D	20	MET	-	expression tag	UNP A0A2Z4HIN9
D	21	GLY	-	expression tag	UNP A0A2Z4HIN9
D	22	ARG	-	expression tag	UNP A0A2Z4HIN9
D	23	GLY	-	expression tag	UNP A0A2Z4HIN9
D	24	SER	-	expression tag	UNP A0A2Z4HIN9
D	25	GLU	-	expression tag	UNP A0A2Z4HIN9
D	26	PHE	-	expression tag	UNP A0A2Z4HIN9

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 8	C 4	N 1	O 3	0	0
2	A	1	Total 8	C 4	N 1	O 3	0	0
2	B	1	Total 8	C 4	N 1	O 3	0	0
2	C	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 3 is water.

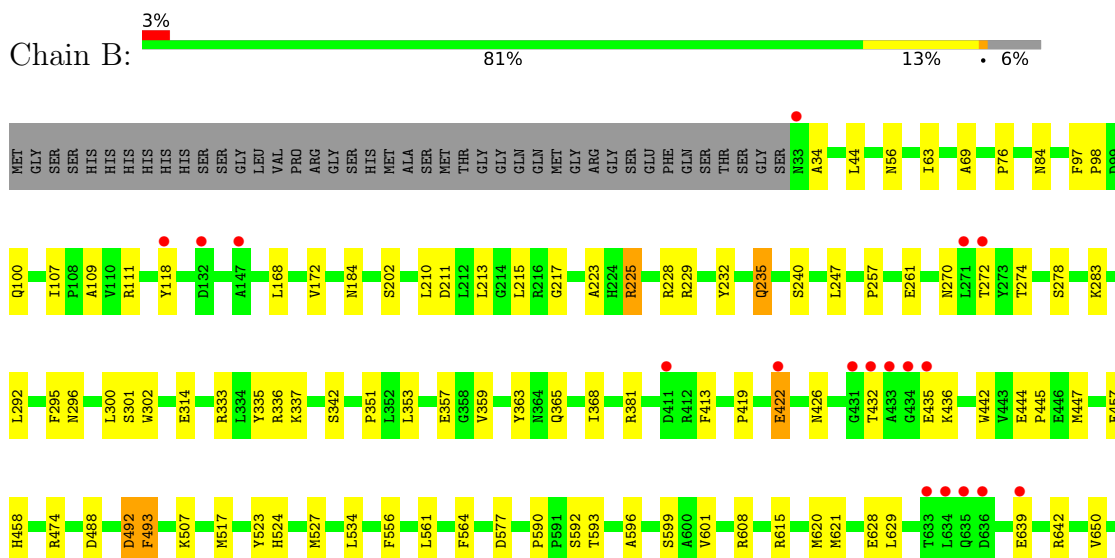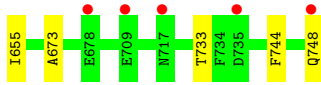| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total 87	O 87	0	0
3	B	88	Total 88	O 88	0	0
3	C	77	Total 77	O 77	0	0
3	D	73	Total 73	O 73	0	0

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.
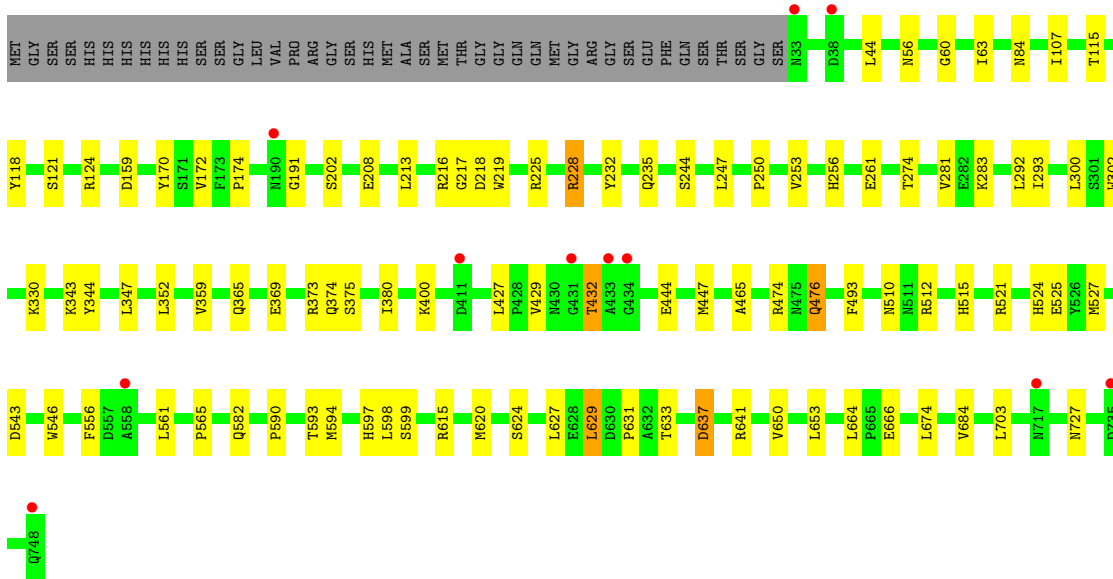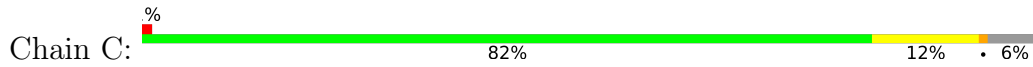
- Molecule 1: Alpha-galactosidase
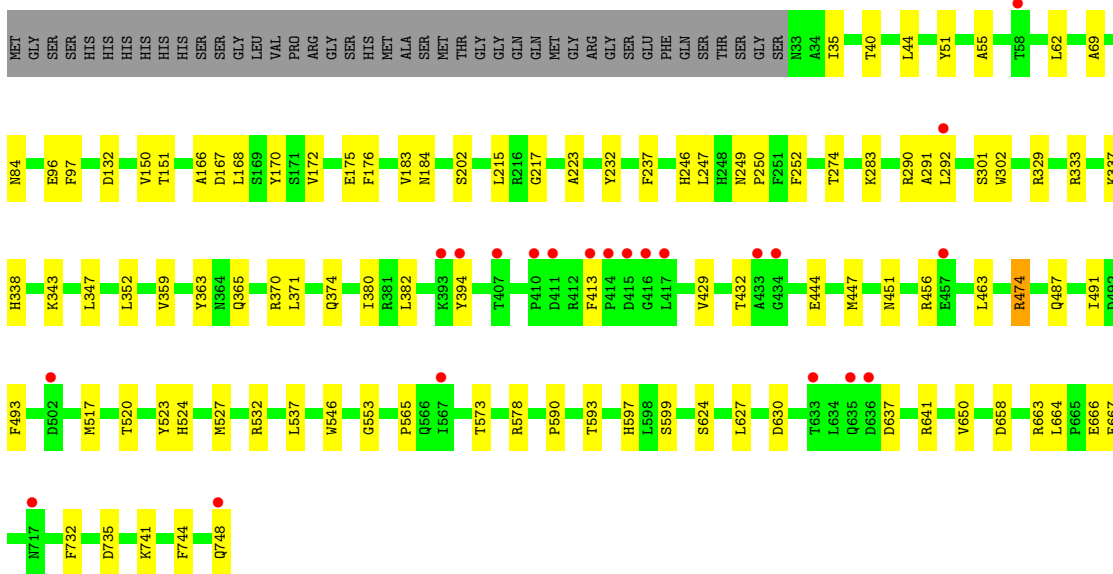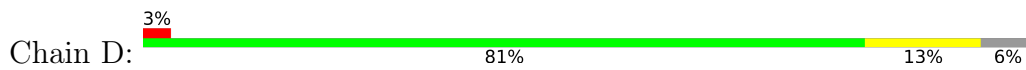

Chain A:

- Molecule 1: Alpha-galactosidase

Chain B:

I655 A673 E678 E709 N717 T733 F734 D735 F744 Q748

• Molecule 1: Alpha-galactosidase

Chain C:

%

82%   12%   •   6%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER GLU PHE GLN SER THR SER GLY SER N33 D38 L44 N56 G60 I63 N84 I107 T115

Y118 S121 R124 D159 Y170 S171 V172 F173 P174 N190 G191 S202 E208 L213 R216 G217 D218 W219 R225 R228 Y232 Q235 S244 L247 P250 V253 H256 E261 T274 V281 E282 K283 L292 I293 L300 S301 W302

K330 K343 Y344 L347 L352 V359 Q365 E369 R373 Q374 S375 I380 K400 D411 L427 F428 V429 N430 G431 T432 A433 G434 E444 M447 A465 R474 N475 Q476 F493 N510 N511 R512 H515 R521 H524 E525 Y526 M527

D543 W546 F556 D557 A558 L561 P565 Q582 P590 T593 M594 H597 L598 S599 R615 M620 S624 L627 E628 L629 D630 P631 A632 T633 D637 R641 V650 L653 L664 P665 E666 L674 V684 L703 N717 N727 D735

Q748

• Molecule 1: Alpha-galactosidase

Chain D:

3%

81%   13%   6%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER SER HIS MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER GLU PHE GLN SER THR SER GLY SER N33 A34 I35 T40 L44 Y51 A55 T58 L62 A69

N84 E96 F97 D132 V150 T151 A166 D167 L168 S169 Y170 S171 V172 E175 F176 V183 N184 S202 L215 R216 G217 A223 Y232 F237 H246 L247 H248 N249 P250 F251 F252 T274 K283 R290 A291 L292 S301 W302 R329 R333 K337

H338 K343 L347 L352 V359 Y363 N364 Q365 R370 L371 Q374 I380 R381 L382 K393 Y394 T407 P410 D411 R412 F413 P414 D415 G416 L417 V429 T432 A433 G434 E444 M447 N451 R456 E457 L463 R474 Q487 I491 D492

F493 D502 M517 T520 Y523 H524 M527 R532 L537 W546 G553 P565 Q566 I567 T573 R578 P590 T593 H597 L598 S599 S624 L627 D630 T633 L634 Q635 D636 D637 R641 V650 D658 R663 L664 P665 E666 E667

N717 F732 D735 K741 F744 Q748

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.25Å 173.04Å 177.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.78 – 2.56 43.78 – 2.56	Depositor EDS
% Data completeness (in resolution range)	92.2 (43.78-2.56) 92.2 (43.78-2.56)	Depositor EDS
R_{merge}	0.89	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.51 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.167 , 0.226 0.167 , 0.227	Depositor DCC
R_{free} test set	4746 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 29.4	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22793	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.50	0/5765	0.62	0/7852
1	B	0.51	0/5765	0.63	0/7852
1	C	0.51	0/5765	0.62	0/7852
1	D	0.47	0/5765	0.62	0/7852
All	All	0.50	0/23060	0.62	0/31408

There are no bond length outliers.

There are no bond angle outliers.

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	5609	0	5387	72	0
1	B	5609	0	5387	79	0
1	C	5609	0	5387	78	0
1	D	5609	0	5387	74	0
2	A	16	0	24	10	0
2	B	8	0	12	5	0
2	C	8	0	12	4	0
3	A	87	0	0	1	0
3	B	88	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	77	0	0	1	0
3	D	73	0	0	3	0
All	All	22793	0	21596	293	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 7.

The worst 5 of 293 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:D:291:ALA:C	1:D:292:LEU:HD12	1.57	1.24
1:D:290:ARG:CG	1:D:292:LEU:HD11	1.76	1.14
1:D:290:ARG:HG2	1:D:292:LEU:CD1	1.77	1.14
1:B:228:ARG:HH22	1:C:228:ARG:HD3	1.07	1.13
1:D:290:ARG:HG2	1:D:292:LEU:HD11	1.13	1.08

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	714/758 (94%)	686 (96%)	26 (4%)	2 (0%)	41	50
1	B	714/758 (94%)	677 (95%)	37 (5%)	0	100	100
1	C	714/758 (94%)	685 (96%)	27 (4%)	2 (0%)	41	50
1	D	714/758 (94%)	680 (95%)	34 (5%)	0	100	100
All	All	2856/3032 (94%)	2728 (96%)	124 (4%)	4 (0%)	51	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	ASN
1	C	510	ASN
1	A	386	ASP
1	C	359	VAL

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	594/629 (94%)	583 (98%)	11 (2%)	57	71
1	B	594/629 (94%)	581 (98%)	13 (2%)	52	66
1	C	594/629 (94%)	580 (98%)	14 (2%)	49	63
1	D	594/629 (94%)	585 (98%)	9 (2%)	65	77
All	All	2376/2516 (94%)	2329 (98%)	47 (2%)	55	69

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	228	ARG
1	C	624	SER
1	C	300	LEU
1	C	476	GLN
1	C	637	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	689	GLN
1	D	190	ASN
1	D	374	GLN
1	B	270	ASN
1	A	365	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 ⓘ

4 ligands are 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	TRS	A	801	-	7,7,7	0.42	0	9,9,9	0.68	0
2	TRS	A	802	-	7,7,7	0.29	0	9,9,9	0.32	0
2	TRS	B	801	-	7,7,7	0.30	0	9,9,9	0.32	0
2	TRS	C	801	-	7,7,7	0.42	0	9,9,9	0.73	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	TRS	A	801	-	-	9/9/9/9	-
2	TRS	A	802	-	-	6/9/9/9	-
2	TRS	B	801	-	-	6/9/9/9	-
2	TRS	C	801	-	-	7/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	TRS	C2-C-C1-O1
2	A	801	TRS	C3-C-C1-O1
2	A	801	TRS	N-C-C1-O1
2	B	801	TRS	N-C-C1-O1
2	C	801	TRS	C2-C-C1-O1

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	TRS	4	0
2	A	802	TRS	6	0
2	B	801	TRS	5	0
2	C	801	TRS	4	0

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(Å^2)	Q<0.9
1	A	716/758 (94%)	-0.14	16 (2%)	62	70	24, 35, 50, 63	0
1	B	716/758 (94%)	-0.08	23 (3%)	47	57	24, 35, 55, 80	0
1	C	716/758 (94%)	-0.19	11 (1%)	73	80	23, 34, 52, 80	0
1	D	716/758 (94%)	-0.07	22 (3%)	49	58	24, 35, 55, 92	0
All	All	2864/3032 (94%)	-0.12	72 (2%)	57	65	23, 35, 53, 92	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	635	GLN	7.3
1	B	434	GLY	6.4
1	B	433	ALA	4.9
1	B	633	THR	4.4
1	B	636	ASP	4.3

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(Å²)	Q<0.9
2	TRS	A	802	8/8	0.81	0.32	49,53,56,67	0
2	TRS	C	801	8/8	0.88	0.32	47,52,53,59	0
2	TRS	B	801	8/8	0.90	0.18	43,48,51,57	0
2	TRS	A	801	8/8	0.93	0.31	48,48,54,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.