Full wwPDB X-ray Structure Validation 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)

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:

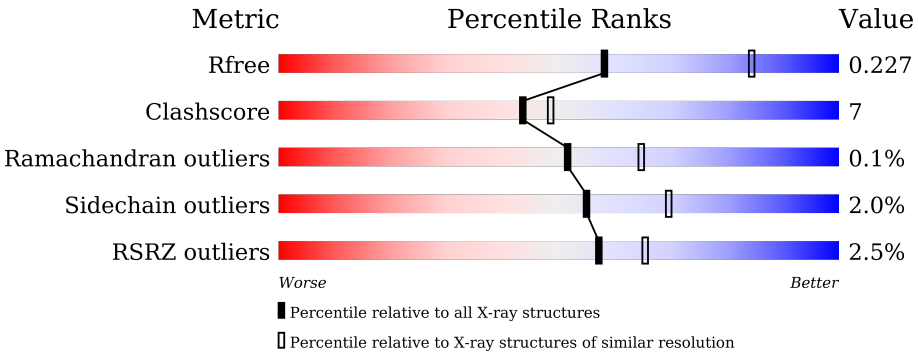
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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	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 (i)

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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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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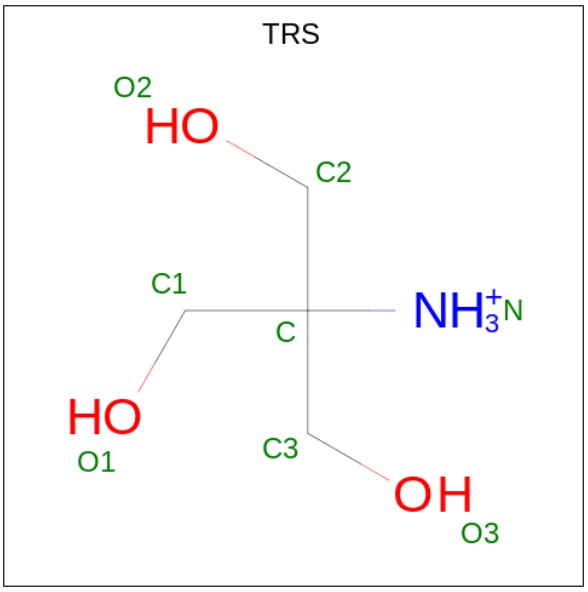
Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP A0A2Z4HIN9
C	25	GLU	-	expression tag	UNP A0A2Z4HIN9
C	26	PHE	-	expression tag	UNP A0A2Z4HIN9
D	-9	MET	-	initiating methionine	UNP A0A2Z4HIN9
D	-8	GLY	-	expression tag	UNP A0A2Z4HIN9
D	-7	SER	-	expression tag	UNP A0A2Z4HIN9
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 C N O 8 4 1 3	0	0
2	A	1	Total C N O 8 4 1 3	0	0
2	B	1	Total C N O 8 4 1 3	0	0
2	C	1	Total C N O 8 4 1 3	0	0

- Molecule 3 is water.

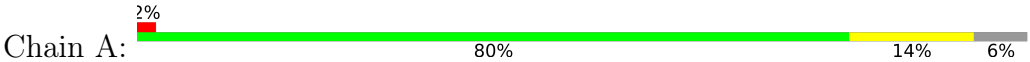
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	87	Total O 87 87	0	0
3	B	88	Total O 88 88	0	0
3	C	77	Total O 77 77	0	0
3	D	73	Total O 73 73	0	0

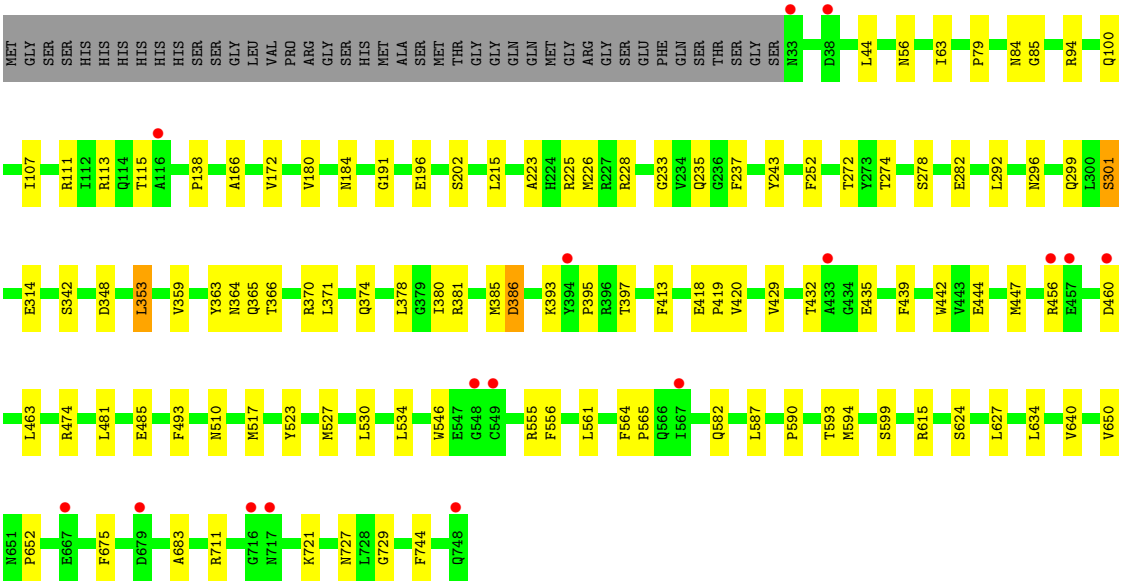
3 Residue-property plots (i)

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: Alpha-galactosidase

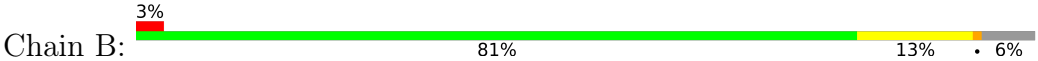
Chain A:

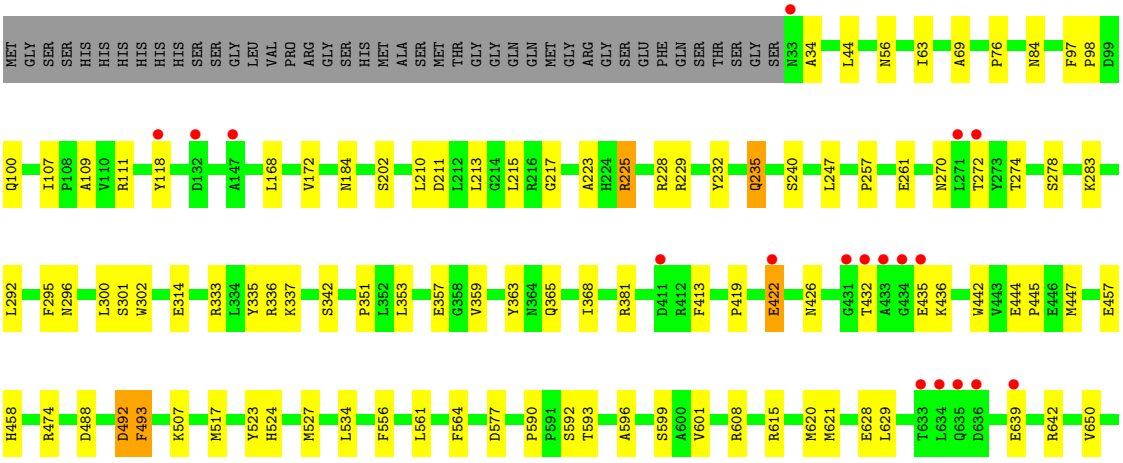


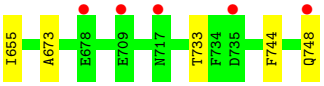


• Molecule 1: Alpha-galactosidase

Chain B:

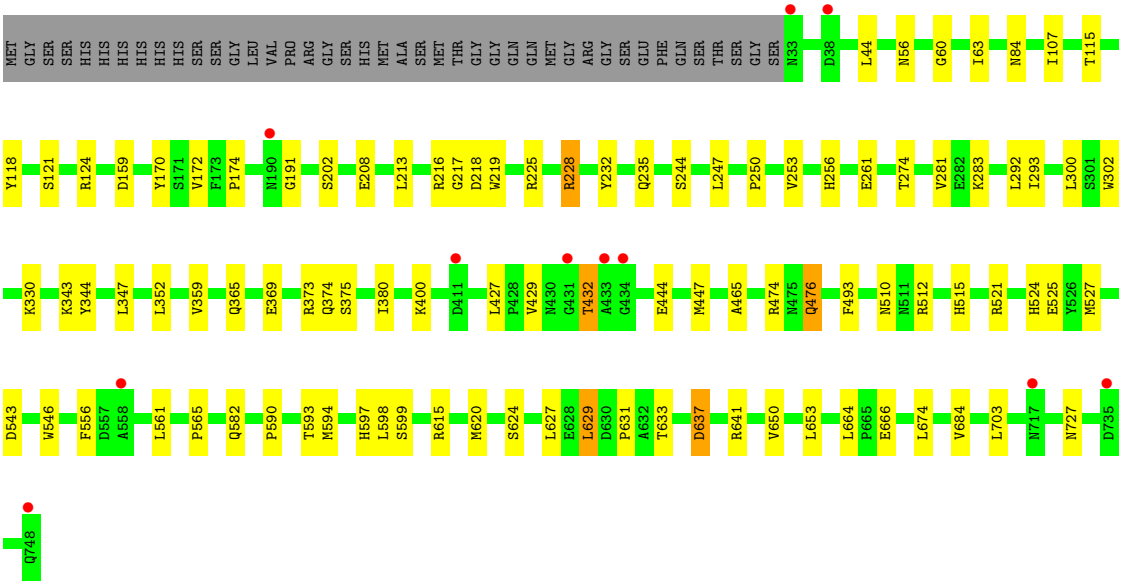






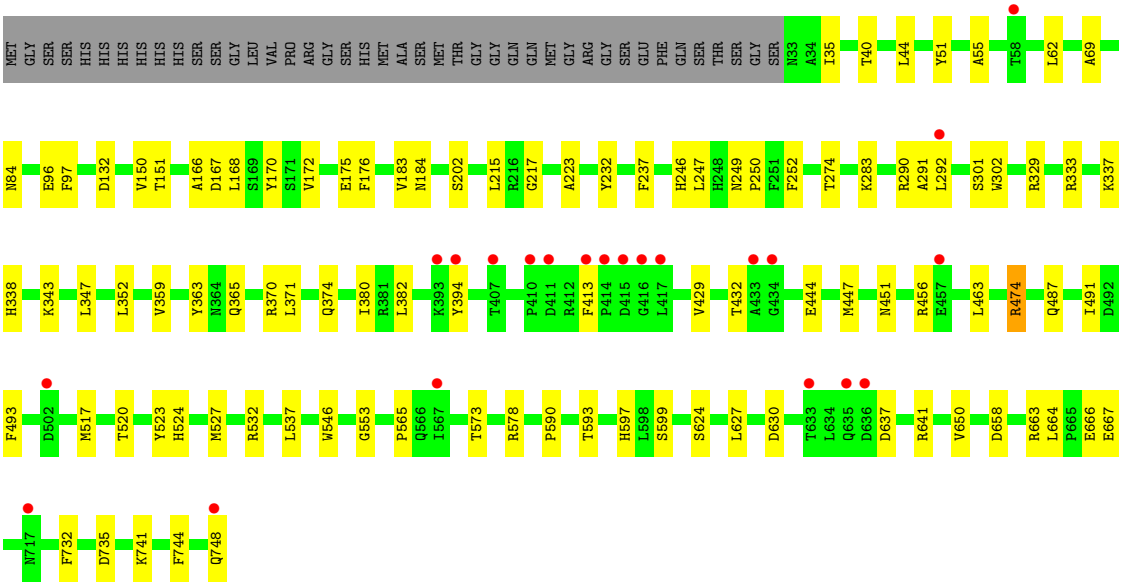
• Molecule 1: Alpha-galactosidase

Chain C:



• Molecule 1: Alpha-galactosidase

Chain D:



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.*

[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.

All (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
1:B:228:ARG:HH22	1:C:228:ARG:CD	1.73	1.02
1:B:228:ARG:NH2	1:C:228:ARG:HD3	1.81	0.95
1:B:213:LEU:HD21	1:B:225:ARG:HH21	1.32	0.94
1:D:291:ALA:O	1:D:292:LEU:HD12	1.73	0.87
1:B:357:GLU:HB2	1:B:628:GLU:HG2	1.57	0.85
2:B:801:TRS:H11	1:C:474:ARG:HD2	1.59	0.84
1:C:107:ILE:HD12	1:C:292:LEU:HD21	1.68	0.75
1:C:107:ILE:HD12	1:C:292:LEU:CD2	2.17	0.74
1:B:84:ASN:HA	2:B:801:TRS:N	2.03	0.73
1:C:674:LEU:HD22	1:C:703:LEU:HD12	1.71	0.73
1:B:629:LEU:HD12	1:B:629:LEU:O	1.89	0.73
1:C:598:LEU:HB3	1:C:627:LEU:HD23	1.70	0.73
1:B:228:ARG:NH2	1:C:228:ARG:CD	2.48	0.71
1:C:429:VAL:O	1:C:432:THR:HG22	1.91	0.71
1:D:380:ILE:HD11	1:D:627:LEU:HD22	1.70	0.71
1:B:642:ARG:NH2	3:B:902:HOH:O	2.23	0.71
1:B:639:GLU:OE2	1:B:642:ARG:NH1	2.24	0.70
1:C:666:GLU:OE2	1:C:666:GLU:N	2.21	0.70
2:A:802:TRS:H22	1:D:474:ARG:HD2	1.74	0.69
1:B:84:ASN:HA	2:B:801:TRS:HN3	1.57	0.69
1:B:213:LEU:HD21	1:B:225:ARG:NH2	2.06	0.68
1:B:107:ILE:HG13	1:B:292:LEU:HD21	1.74	0.67
1:C:84:ASN:HA	2:C:801:TRS:HN1	1.59	0.67
1:D:290:ARG:HG3	1:D:292:LEU:HD11	1.75	0.67
1:A:418:GLU:HG2	1:A:419:PRO:HD3	1.78	0.65
1:B:56:ASN:HB2	1:B:63:ILE:CD1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:LEU:HB3	1:C:666:GLU:OE2	1.97	0.64
1:D:292:LEU:HD12	1:D:292:LEU:N	2.08	0.64
1:B:432:THR:HG21	1:B:435:GLU:HB2	1.79	0.64
1:A:432:THR:HG21	1:A:435:GLU:HB2	1.80	0.63
1:B:107:ILE:CD1	1:B:292:LEU:HD21	2.28	0.63
1:D:202:SER:OG	1:D:292:LEU:HG	1.98	0.63
1:B:44:LEU:HD23	1:B:172:VAL:HG13	1.81	0.62
1:B:444:GLU:OE2	1:B:447:MET:HG3	2.00	0.62
1:B:228:ARG:NH2	1:C:228:ARG:HH11	1.98	0.62
1:D:637:ASP:HB3	1:D:641:ARG:HH21	1.63	0.62
1:A:561:LEU:HD21	1:A:593:THR:HG23	1.81	0.62
1:D:291:ALA:C	1:D:292:LEU:CD1	2.51	0.61
1:C:627:LEU:HB3	1:C:629:LEU:CD1	2.30	0.61
1:B:272:THR:HB	1:B:314:GLU:HG3	1.81	0.61
1:B:44:LEU:HB3	1:B:172:VAL:HG11	1.83	0.61
1:C:561:LEU:HD21	1:C:593:THR:HG23	1.82	0.61
1:B:44:LEU:HB3	1:B:172:VAL:CG1	2.31	0.60
1:C:629:LEU:C	1:C:629:LEU:HD22	2.22	0.60
1:A:84:ASN:HA	2:A:802:TRS:N	2.16	0.60
2:A:801:TRS:HN2	1:D:84:ASN:HA	1.66	0.60
1:D:274:THR:HB	1:D:527:MET:HE1	1.83	0.60
1:A:292:LEU:HD12	1:A:292:LEU:C	2.21	0.60
1:C:633:THR:HG22	1:C:633:THR:O	2.01	0.60
1:C:60:GLY:HA3	1:C:124:ARG:HG2	1.84	0.60
1:C:44:LEU:HD21	1:C:170:TYR:HB3	1.84	0.59
1:C:429:VAL:HB	1:C:432:THR:HG21	1.85	0.59
1:B:274:THR:HB	1:B:527:MET:HE1	1.84	0.58
1:C:84:ASN:HA	2:C:801:TRS:N	2.17	0.58
1:A:711:ARG:HG3	1:A:711:ARG:HH11	1.66	0.58
1:A:56:ASN:HB2	1:A:63:ILE:CD1	2.34	0.58
1:D:590:PRO:O	1:D:593:THR:HB	2.04	0.58
1:B:228:ARG:HH22	1:C:228:ARG:HH11	1.52	0.58
1:C:235:GLN:NE2	1:C:281:VAL:O	2.34	0.58
1:D:429:VAL:O	1:D:432:THR:OG1	2.20	0.57
1:C:474:ARG:O	1:C:474:ARG:HG2	2.03	0.57
1:B:359:VAL:HG11	1:B:363:TYR:HB3	1.85	0.57
2:A:801:TRS:N	1:D:84:ASN:HA	2.20	0.57
1:C:653:LEU:HD13	1:C:684:VAL:HG23	1.86	0.57
1:A:274:THR:HB	1:A:527:MET:HE1	1.85	0.57
1:D:650:VAL:HG12	1:D:744:PHE:CZ	2.40	0.57
1:C:274:THR:HB	1:C:527:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:GLY:O	1:D:247:LEU:HA	2.05	0.56
1:A:84:ASN:HA	2:A:802:TRS:HN2	1.70	0.56
1:A:721:LYS:HD2	1:A:721:LYS:N	2.20	0.56
2:A:802:TRS:O3	2:A:802:TRS:O1	2.10	0.56
2:B:801:TRS:H11	1:C:474:ARG:CD	2.33	0.56
1:D:44:LEU:HD11	1:D:170:TYR:HB3	1.86	0.56
1:D:215:LEU:HB3	1:D:223:ALA:HA	1.88	0.56
1:B:274:THR:HB	1:B:527:MET:CE	2.36	0.56
1:A:113:ARG:NH2	1:D:520:THR:OG1	2.39	0.56
1:B:599:SER:O	1:B:615:ARG:NH1	2.38	0.55
1:D:97:PHE:HB2	1:D:168:LEU:HD21	1.87	0.55
1:B:107:ILE:CG1	1:B:292:LEU:HD21	2.36	0.55
1:A:107:ILE:HD12	1:A:292:LEU:HD23	1.87	0.55
1:A:721:LYS:HD2	1:A:721:LYS:H	1.72	0.55
1:B:426:ASN:HA	1:B:436:LYS:HD2	1.87	0.55
1:C:582:GLN:HB3	1:C:594:MET:HE1	1.89	0.55
1:D:290:ARG:HG2	1:D:292:LEU:HD13	1.79	0.55
1:B:590:PRO:O	1:B:593:THR:HB	2.06	0.55
1:D:35:ILE:HD12	1:D:151:THR:HG22	1.89	0.55
1:A:474:ARG:HD2	2:A:801:TRS:H22	1.89	0.55
1:A:278:SER:HB2	1:A:296:ASN:HA	1.88	0.55
1:C:637:ASP:HB3	1:C:641:ARG:NH2	2.22	0.55
1:D:663:ARG:HB3	3:D:821:HOH:O	2.06	0.55
1:C:653:LEU:CD1	1:C:684:VAL:HG23	2.38	0.54
1:B:56:ASN:HB2	1:B:63:ILE:HD11	1.88	0.54
1:B:365:GLN:HG3	1:B:413:PHE:HA	1.90	0.54
1:B:474:ARG:HG3	2:C:801:TRS:H21	1.90	0.54
1:D:246:HIS:ND1	3:D:803:HOH:O	2.32	0.54
2:B:801:TRS:H12	1:C:474:ARG:HB2	1.89	0.54
1:D:44:LEU:HD13	1:D:172:VAL:HG22	1.90	0.54
1:C:629:LEU:HD13	1:C:629:LEU:N	2.22	0.54
1:D:444:GLU:OE2	1:D:447:MET:HG3	2.08	0.54
1:D:517:MET:HG3	1:D:523:TYR:CZ	2.42	0.54
1:A:444:GLU:OE2	1:A:447:MET:HG3	2.07	0.54
1:B:213:LEU:CD2	1:B:225:ARG:HH21	2.15	0.54
1:C:637:ASP:HB3	1:C:641:ARG:HH21	1.72	0.54
1:D:370:ARG:HE	1:D:374:GLN:HE22	1.56	0.54
1:A:292:LEU:HD12	1:A:292:LEU:O	2.08	0.54
1:D:291:ALA:O	1:D:292:LEU:CD1	2.53	0.54
1:D:370:ARG:HG2	1:D:374:GLN:NE2	2.22	0.54
1:A:381:ARG:HH22	1:A:435:GLU:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLN:HB3	1:A:523:TYR:CD2	2.43	0.53
2:A:801:TRS:O3	2:A:801:TRS:O1	2.23	0.53
1:B:620:MET:HB3	1:B:650:VAL:HG21	1.91	0.53
1:A:378:LEU:HB2	1:A:380:ILE:HD12	1.90	0.53
1:A:364:ASN:OD1	1:A:366:THR:HB	2.08	0.53
1:D:291:ALA:CA	1:D:292:LEU:HD12	2.35	0.53
1:B:98:PRO:HD2	1:B:109:ALA:HB2	1.91	0.53
1:A:226:MET:HG3	1:A:228:ARG:HH12	1.74	0.52
1:A:485:GLU:OE1	1:A:485:GLU:N	2.23	0.52
1:B:336:ARG:NH2	3:B:907:HOH:O	2.42	0.52
1:A:100:GLN:OE1	1:A:111:ARG:NH2	2.42	0.52
1:C:629:LEU:CD1	1:C:629:LEU:N	2.73	0.52
1:A:365:GLN:HG3	1:A:413:PHE:HA	1.91	0.52
2:A:802:TRS:H22	1:D:474:ARG:CD	2.39	0.52
1:A:727:ASN:HB3	1:B:69:ALA:HB3	1.92	0.51
1:B:592:SER:HB3	1:B:655:ILE:HA	1.92	0.51
1:B:359:VAL:CG1	1:B:363:TYR:HB3	2.40	0.51
1:D:292:LEU:CD1	1:D:292:LEU:N	2.74	0.51
1:B:56:ASN:HB2	1:B:63:ILE:HD13	1.92	0.51
1:C:218:ASP:OD1	1:C:219:TRP:N	2.38	0.50
1:C:561:LEU:HD11	1:C:593:THR:HG21	1.93	0.50
1:A:180:VAL:HG11	1:A:314:GLU:OE1	2.11	0.50
1:A:274:THR:HB	1:A:527:MET:CE	2.42	0.50
1:A:395:PRO:HB2	1:A:397:THR:HG23	1.94	0.50
1:B:184:ASN:ND2	3:B:909:HOH:O	2.44	0.50
1:A:590:PRO:O	1:A:593:THR:HB	2.13	0.49
1:C:582:GLN:CB	1:C:594:MET:HE1	2.43	0.49
1:A:166:ALA:HA	1:A:184:ASN:O	2.13	0.49
1:A:418:GLU:H	1:A:418:GLU:CD	2.15	0.49
1:B:118:TYR:CG	1:C:465:ALA:HB1	2.47	0.49
1:B:232:TYR:HA	1:B:283:LYS:HB3	1.94	0.49
1:C:44:LEU:HD23	1:C:172:VAL:HG22	1.94	0.49
1:A:107:ILE:HD12	1:A:292:LEU:CD2	2.43	0.49
1:B:278:SER:HB2	1:B:296:ASN:HA	1.94	0.49
1:D:274:THR:HB	1:D:527:MET:CE	2.43	0.49
1:A:79:PRO:HG2	1:B:733:THR:HG23	1.95	0.49
1:A:463:LEU:HD13	1:A:517:MET:SD	2.53	0.48
1:B:100:GLN:OE1	1:B:111:ARG:NH2	2.45	0.48
1:B:215:LEU:HB3	1:B:223:ALA:HA	1.94	0.48
1:B:517:MET:HG3	1:B:523:TYR:CZ	2.48	0.48
1:B:621:MET:HE1	1:B:673:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LYS:HG2	1:D:338:HIS:CD2	2.48	0.48
1:C:590:PRO:O	1:C:593:THR:HB	2.13	0.48
1:A:365:GLN:HG2	1:A:420:VAL:HG21	1.95	0.48
1:D:487:GLN:O	1:D:491:ILE:HG13	2.13	0.48
1:C:274:THR:HB	1:C:527:MET:CE	2.43	0.48
1:D:232:TYR:HA	1:D:283:LYS:HB3	1.94	0.48
1:D:237:PHE:HZ	1:D:252:PHE:HB3	1.77	0.48
1:D:463:LEU:HD13	1:D:517:MET:SD	2.54	0.48
1:C:343:LYS:HE2	1:C:543:ASP:OD1	2.14	0.48
1:C:107:ILE:HD12	1:C:292:LEU:HD23	1.93	0.47
1:B:295:PHE:CB	1:B:300:LEU:HD22	2.45	0.47
1:A:386:ASP:HA	1:A:442:TRP:HB2	1.96	0.47
1:A:115:THR:HG21	1:A:191:GLY:HA3	1.97	0.47
1:A:370:ARG:O	1:A:374:GLN:HG3	2.15	0.47
1:B:445:PRO:HB3	1:B:493:PHE:CZ	2.50	0.47
1:A:44:LEU:HB3	1:A:172:VAL:CG2	2.45	0.47
1:A:44:LEU:HB3	1:A:172:VAL:HG21	1.97	0.47
1:A:215:LEU:HB3	1:A:223:ALA:HA	1.97	0.46
1:D:732:PHE:CD1	1:D:741:LYS:HD3	2.50	0.46
1:A:385:MET:HE1	1:A:439:PHE:HZ	1.80	0.46
1:B:302:TRP:CZ3	1:B:524:HIS:HB3	2.51	0.46
1:D:359:VAL:HG11	1:D:363:TYR:HB3	1.98	0.46
1:A:359:VAL:HG11	1:A:363:TYR:HB3	1.96	0.46
1:A:359:VAL:HG21	1:A:371:LEU:HD11	1.97	0.46
1:A:359:VAL:CG1	1:A:363:TYR:HB3	2.44	0.46
1:B:97:PHE:HB2	1:B:168:LEU:HD21	1.97	0.46
1:B:488:ASP:O	1:B:492:ASP:HB2	2.16	0.46
1:C:330:LYS:NZ	3:C:909:HOH:O	2.44	0.46
1:B:442:TRP:HD1	1:B:507:LYS:HE3	1.81	0.46
1:B:270:ASN:ND2	1:B:335:TYR:OH	2.36	0.45
1:C:512:ARG:HH21	1:C:515:HIS:CD2	2.34	0.45
1:A:711:ARG:HG3	1:A:711:ARG:NH1	2.30	0.45
1:B:419:PRO:O	1:B:422:GLU:HG3	2.16	0.45
1:C:599:SER:O	1:C:615:ARG:NH1	2.45	0.45
1:D:44:LEU:HB2	1:D:51:TYR:HB3	1.98	0.45
1:C:302:TRP:CZ3	1:C:524:HIS:HB3	2.52	0.45
1:C:627:LEU:HB3	1:C:629:LEU:HD11	1.99	0.45
1:B:474:ARG:HG3	2:C:801:TRS:C2	2.46	0.45
1:C:232:TYR:HA	1:C:283:LYS:HB3	1.99	0.45
1:D:352:LEU:HA	1:D:382:LEU:O	2.16	0.45
1:A:63:ILE:HG23	1:A:94:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLY:O	1:B:247:LEU:HA	2.17	0.45
1:B:596:ALA:HB1	3:B:964:HOH:O	2.17	0.45
1:C:727:ASN:HB3	1:D:69:ALA:HB3	1.98	0.45
1:D:44:LEU:HB3	1:D:172:VAL:CG2	2.47	0.45
1:B:457:GLU:OE2	1:B:458:HIS:NE2	2.50	0.45
1:D:370:ARG:NH2	1:D:630:ASP:OD1	2.50	0.45
1:D:546:TRP:O	1:D:565:PRO:HD2	2.16	0.44
1:A:378:LEU:HB2	1:A:380:ILE:CD1	2.47	0.44
1:C:344:TYR:HA	1:C:347:LEU:HB2	1.99	0.44
1:A:237:PHE:HZ	1:A:252:PHE:HB3	1.82	0.44
1:B:577:ASP:OD1	1:B:608:ARG:NH2	2.50	0.44
1:A:429:VAL:O	1:A:432:THR:HB	2.16	0.44
1:A:582:GLN:HB3	1:A:594:MET:HE1	1.99	0.44
1:A:56:ASN:HB2	1:A:63:ILE:HD11	1.99	0.44
1:A:393:LYS:HB2	1:A:393:LYS:HE2	1.70	0.44
1:B:534:LEU:HD22	1:B:564:PHE:CZ	2.52	0.44
1:C:107:ILE:CD1	1:C:292:LEU:HD23	2.48	0.44
1:C:629:LEU:HD13	1:C:629:LEU:H	1.83	0.44
1:D:553:GLY:O	3:D:801:HOH:O	2.21	0.44
1:A:534:LEU:HD22	1:A:564:PHE:CZ	2.53	0.44
1:C:444:GLU:OE2	1:C:447:MET:HG3	2.18	0.43
1:D:175:GLU:HG3	1:D:176:PHE:CZ	2.53	0.43
1:D:365:GLN:HG3	1:D:413:PHE:HA	2.00	0.43
1:B:210:LEU:O	1:B:229:ARG:HD3	2.18	0.43
1:B:228:ARG:NH1	1:B:235:GLN:OE1	2.51	0.43
1:B:445:PRO:HB3	1:B:493:PHE:HZ	1.83	0.43
1:A:650:VAL:HG12	1:A:744:PHE:CZ	2.54	0.43
1:C:674:LEU:HD12	1:C:684:VAL:O	2.18	0.43
1:D:337:LYS:HE2	1:D:338:HIS:NE2	2.34	0.43
1:B:629:LEU:HD12	1:B:629:LEU:C	2.37	0.43
1:B:561:LEU:HD21	1:B:593:THR:HG23	2.00	0.43
1:C:244:SER:HB2	1:C:250:PRO:HD3	2.01	0.43
1:D:537:LEU:HD23	1:D:537:LEU:HA	1.87	0.43
1:A:599:SER:O	1:A:615:ARG:NH1	2.50	0.43
1:C:172:VAL:O	1:C:174:PRO:HD3	2.19	0.43
1:D:40:THR:HB	1:D:55:ALA:HB3	2.00	0.43
1:D:337:LYS:HE2	1:D:338:HIS:CE1	2.54	0.43
1:D:352:LEU:HD11	1:D:597:HIS:NE2	2.34	0.43
1:C:620:MET:HB3	1:C:650:VAL:HG21	2.01	0.43
1:A:85:GLY:H	2:A:802:TRS:H12	1.83	0.42
1:B:34:ALA:HB1	1:B:172:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ARG:HA	1:C:427:LEU:HD13	2.01	0.42
1:C:374:GLN:HB3	1:C:631:PRO:HB2	2.01	0.42
1:A:481:LEU:HD23	1:A:530:LEU:HA	2.01	0.42
1:C:561:LEU:HD23	1:C:561:LEU:HA	1.91	0.42
1:C:546:TRP:O	1:C:565:PRO:HD2	2.20	0.42
1:C:217:GLY:O	1:C:247:LEU:HA	2.20	0.42
1:C:352:LEU:HD11	1:C:597:HIS:CE1	2.55	0.42
1:D:359:VAL:HG21	1:D:371:LEU:HD11	2.02	0.42
1:A:353:LEU:HD12	1:A:627:LEU:CB	2.49	0.42
1:B:351:PRO:HD2	1:B:381:ARG:HG3	2.02	0.42
1:B:601:VAL:HG22	3:B:987:HOH:O	2.19	0.42
1:C:115:THR:HG21	1:C:191:GLY:HA3	2.02	0.42
1:C:347:LEU:HD23	1:C:347:LEU:HA	1.84	0.42
1:A:196:GLU:OE2	1:A:301:SER:OG	2.33	0.41
1:A:233:GLY:O	1:A:282:GLU:HA	2.20	0.41
1:A:272:THR:HB	1:A:314:GLU:HG2	2.02	0.41
1:A:546:TRP:O	1:A:565:PRO:HD2	2.20	0.41
1:C:208:GLU:OE1	1:C:256:HIS:NE2	2.51	0.41
1:D:664:LEU:HB2	1:D:667:GLU:HG2	2.02	0.41
1:D:302:TRP:CZ3	1:D:524:HIS:HB3	2.55	0.41
1:D:370:ARG:NE	1:D:374:GLN:HE22	2.17	0.41
1:A:348:ASP:OD2	1:A:652:PRO:HG3	2.20	0.41
1:B:225:ARG:NH1	1:B:261:GLU:OE2	2.49	0.41
1:C:213:LEU:HB2	1:C:253:VAL:HB	2.01	0.41
1:C:365:GLN:O	1:C:369:GLU:HG3	2.20	0.41
1:C:474:ARG:O	1:C:476:GLN:HG2	2.21	0.41
1:D:573:THR:HB	1:D:599:SER:HB2	2.02	0.41
1:A:243:TYR:CD1	1:A:555:ARG:HD3	2.56	0.41
1:C:375:SER:O	1:C:380:ILE:HB	2.21	0.41
1:C:225:ARG:NH1	1:C:261:GLU:OE2	2.48	0.41
1:C:521:ARG:HG2	1:C:525:GLU:HG3	2.03	0.41
1:D:343:LYS:O	1:D:347:LEU:HG	2.21	0.41
1:B:333:ARG:HD3	1:B:333:ARG:HA	1.75	0.41
1:B:368:ILE:HD13	1:B:368:ILE:HA	1.90	0.41
1:D:150:VAL:HA	1:D:172:VAL:O	2.20	0.41
1:D:333:ARG:HA	1:D:333:ARG:HD3	1.71	0.41
1:A:675:PHE:O	1:A:683:ALA:HA	2.21	0.41
1:A:729:GLY:O	1:B:76:PRO:HG2	2.21	0.41
1:C:293:ILE:HD13	1:C:293:ILE:HG21	1.79	0.41
1:D:664:LEU:HB3	1:D:666:GLU:OE1	2.22	0.41
1:A:353:LEU:HD12	1:A:627:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:VAL:HB	1:C:432:THR:CG2	2.50	0.40
1:D:167:ASP:O	1:D:183:VAL:HA	2.21	0.40
1:D:394:TYR:CE2	1:D:456:ARG:NH2	2.89	0.40
1:A:138:PRO:O	3:A:901:HOH:O	2.22	0.40
1:B:302:TRP:HZ3	1:B:524:HIS:HB3	1.85	0.40
1:D:62:LEU:HB2	1:D:96:GLU:HB2	2.02	0.40
1:D:166:ALA:HA	1:D:184:ASN:O	2.21	0.40
1:D:329:ARG:HD2	1:D:658:ASP:HB3	2.02	0.40
1:B:211:ASP:OD2	1:B:257:PRO:HA	2.21	0.40
1:C:56:ASN:HB2	1:C:63:ILE:CD1	2.51	0.40
1:D:578:ARG:HD3	1:D:578:ARG:HA	1.89	0.40
1:B:650:VAL:HG12	1:B:744:PHE:CZ	2.57	0.40
1:C:159:ASP:C	1:C:159:ASP:OD1	2.60	0.40
1:D:249:ASN:CG	1:D:250:PRO:HD2	2.42	0.40
1:A:587:LEU:HD12	1:A:587:LEU:HA	1.84	0.40
1:A:634:LEU:HD13	1:A:640:VAL:HG21	2.03	0.40

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	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 (i)

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

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	SER
1	A	225	ARG
1	A	235	GLN
1	A	301	SER
1	A	342	SER
1	A	353	LEU
1	A	456	ARG
1	A	460	ASP
1	A	493	PHE
1	A	556	PHE
1	A	624	SER
1	B	202	SER
1	B	225	ARG
1	B	235	GLN
1	B	240	SER
1	B	301	SER
1	B	337	LYS
1	B	342	SER

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Mol	Chain	Res	Type
1	B	353	LEU
1	B	422	GLU
1	B	492	ASP
1	B	493	PHE
1	B	556	PHE
1	B	748	GLN
1	C	118	TYR
1	C	121	SER
1	C	202	SER
1	C	216	ARG
1	C	228	ARG
1	C	300	LEU
1	C	400	LYS
1	C	432	THR
1	C	476	GLN
1	C	493	PHE
1	C	556	PHE
1	C	624	SER
1	C	629	LEU
1	C	637	ASP
1	D	132	ASP
1	D	301	SER
1	D	451	ASN
1	D	474	ARG
1	D	493	PHE
1	D	532	ARG
1	D	624	SER
1	D	735	ASP
1	D	748	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	GLN
1	B	270	ASN
1	C	280	GLN
1	C	689	GLN
1	D	190	ASN
1	D	374	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.

All (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
2	C	801	TRS	C3-C-C1-O1
2	C	801	TRS	N-C-C1-O1
2	C	801	TRS	N-C-C3-O3
2	A	801	TRS	C1-C-C2-O2
2	A	801	TRS	N-C-C3-O3
2	A	802	TRS	C3-C-C1-O1
2	A	802	TRS	N-C-C1-O1
2	A	802	TRS	C1-C-C3-O3
2	A	802	TRS	N-C-C3-O3
2	B	801	TRS	C3-C-C1-O1
2	B	801	TRS	C1-C-C3-O3
2	B	801	TRS	N-C-C3-O3
2	C	801	TRS	C1-C-C2-O2
2	C	801	TRS	N-C-C2-O2
2	A	801	TRS	C1-C-C3-O3
2	A	801	TRS	C2-C-C3-O3
2	A	802	TRS	C2-C-C1-O1
2	A	802	TRS	C2-C-C3-O3
2	B	801	TRS	C2-C-C3-O3
2	A	801	TRS	C3-C-C2-O2
2	A	801	TRS	N-C-C2-O2
2	B	801	TRS	C3-C-C2-O2
2	C	801	TRS	C3-C-C2-O2

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 (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, 95^{th} 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

All (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
1	D	633	THR	4.2
1	C	748	GLN	3.9
1	C	434	GLY	3.9
1	B	748	GLN	3.8
1	B	432	THR	3.7
1	B	635	GLN	3.6
1	D	433	ALA	3.6
1	B	634	LEU	3.6
1	D	394	TYR	3.5
1	C	433	ALA	3.5
1	D	411	ASP	3.5
1	B	33	ASN	3.4
1	C	431	GLY	3.3
1	D	434	GLY	3.3
1	D	393	LYS	3.2
1	D	414	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	717	ASN	3.1
1	B	431	GLY	3.1
1	B	118	TYR	3.1
1	A	394	TYR	3.0
1	A	456	ARG	3.0
1	B	272	THR	3.0
1	B	735	ASP	2.9
1	A	717	ASN	2.9
1	A	33	ASN	2.9
1	D	407	THR	2.9
1	B	132	ASP	2.8
1	D	748	GLN	2.7
1	A	716	GLY	2.6
1	D	410	PRO	2.6
1	D	417	LEU	2.6
1	A	433	ALA	2.6
1	D	58	THR	2.6
1	C	735	ASP	2.5
1	C	558	ALA	2.5
1	B	709	GLU	2.5
1	B	271	LEU	2.4
1	B	411	ASP	2.4
1	B	717	ASN	2.4
1	C	190	ASN	2.4
1	D	717	ASN	2.4
1	A	38	ASP	2.4
1	D	636	ASP	2.4
1	D	292	LEU	2.4
1	C	33	ASN	2.4
1	D	567	ILE	2.4
1	B	147	ALA	2.3
1	A	548	GLY	2.3
1	A	457	GLU	2.3
1	B	678	GLU	2.2
1	A	116	ALA	2.2
1	D	502	ASP	2.2
1	A	549	CYS	2.2
1	A	748	GLN	2.2
1	D	413	PHE	2.2
1	C	38	ASP	2.1
1	C	411	ASP	2.1
1	A	567	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	422	GLU	2.1
1	D	457	GLU	2.1
1	D	416	GLY	2.1
1	A	460	ASP	2.1
1	A	679	ASP	2.1
1	D	415	ASP	2.1
1	A	667	GLU	2.1
1	B	639	GLU	2.0
1	B	435	GLU	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 monosaccharides 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, 95^{th} 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	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 (i)

There are no such residues in this entry.