



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 PM UTC

PDB ID : 8T7Z / pdb_00008t7z
Title : Crystal structure of alpha-glucosidase (yicI) from *Klebsiella aerogenes*
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2023-06-21
Resolution : 2.70 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

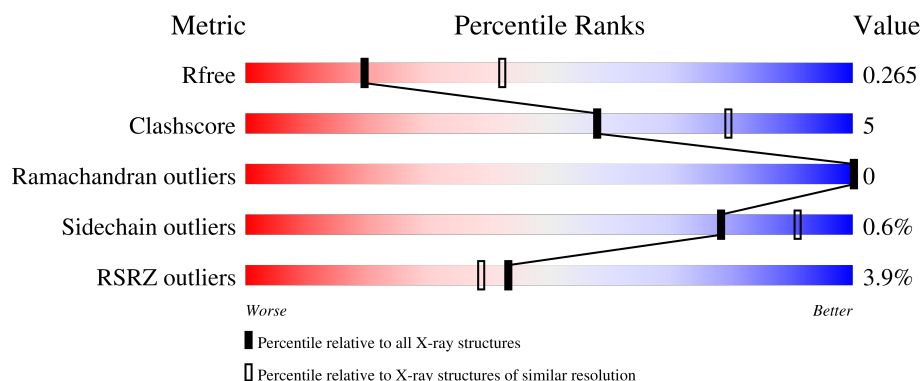
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	780	5% 85% 12% .
1	B	780	3% 85% 12% .
1	C	780	3% 86% 11% .
1	D	780	2% 88% 9% .
1	E	780	5% 86% 10% .

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Mol	Chain	Length	Quality of chain
1	F	780	4% 87% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 36248 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-glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	0	0	0
			6033	3865	1031	1109	28			
1	B	758	Total	C	N	O	S	0	0	0
			6064	3881	1033	1122	28			
1	C	758	Total	C	N	O	S	0	0	0
			6065	3881	1037	1119	28			
1	D	751	Total	C	N	O	S	0	0	0
			6024	3859	1030	1107	28			
1	E	753	Total	C	N	O	S	0	0	0
			6018	3857	1026	1107	28			
1	F	752	Total	C	N	O	S	0	0	0
			6014	3853	1027	1106	28			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0H3FLJ3
A	2	ALA	-	expression tag	UNP A0A0H3FLJ3
A	3	HIS	-	expression tag	UNP A0A0H3FLJ3
A	4	HIS	-	expression tag	UNP A0A0H3FLJ3
A	5	HIS	-	expression tag	UNP A0A0H3FLJ3
A	6	HIS	-	expression tag	UNP A0A0H3FLJ3
A	7	HIS	-	expression tag	UNP A0A0H3FLJ3
A	8	HIS	-	expression tag	UNP A0A0H3FLJ3
A	81	GLN	HIS	engineered mutation	UNP A0A0H3FLJ3
A	87	SER	GLY	engineered mutation	UNP A0A0H3FLJ3
A	702	GLY	ASP	engineered mutation	UNP A0A0H3FLJ3
A	705	ASN	ARG	engineered mutation	UNP A0A0H3FLJ3
A	707	THR	ALA	engineered mutation	UNP A0A0H3FLJ3
A	708	VAL	LEU	engineered mutation	UNP A0A0H3FLJ3
A	718	ALA	VAL	engineered mutation	UNP A0A0H3FLJ3
B	1	MET	-	initiating methionine	UNP A0A0H3FLJ3
B	2	ALA	-	expression tag	UNP A0A0H3FLJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	HIS	-	expression tag	UNP A0A0H3FLJ3
B	4	HIS	-	expression tag	UNP A0A0H3FLJ3
B	5	HIS	-	expression tag	UNP A0A0H3FLJ3
B	6	HIS	-	expression tag	UNP A0A0H3FLJ3
B	7	HIS	-	expression tag	UNP A0A0H3FLJ3
B	8	HIS	-	expression tag	UNP A0A0H3FLJ3
B	81	GLN	HIS	engineered mutation	UNP A0A0H3FLJ3
B	87	SER	GLY	engineered mutation	UNP A0A0H3FLJ3
B	702	GLY	ASP	engineered mutation	UNP A0A0H3FLJ3
B	705	ASN	ARG	engineered mutation	UNP A0A0H3FLJ3
B	707	THR	ALA	engineered mutation	UNP A0A0H3FLJ3
B	708	VAL	LEU	engineered mutation	UNP A0A0H3FLJ3
B	718	ALA	VAL	engineered mutation	UNP A0A0H3FLJ3
C	1	MET	-	initiating methionine	UNP A0A0H3FLJ3
C	2	ALA	-	expression tag	UNP A0A0H3FLJ3
C	3	HIS	-	expression tag	UNP A0A0H3FLJ3
C	4	HIS	-	expression tag	UNP A0A0H3FLJ3
C	5	HIS	-	expression tag	UNP A0A0H3FLJ3
C	6	HIS	-	expression tag	UNP A0A0H3FLJ3
C	7	HIS	-	expression tag	UNP A0A0H3FLJ3
C	8	HIS	-	expression tag	UNP A0A0H3FLJ3
C	81	GLN	HIS	engineered mutation	UNP A0A0H3FLJ3
C	87	SER	GLY	engineered mutation	UNP A0A0H3FLJ3
C	702	GLY	ASP	engineered mutation	UNP A0A0H3FLJ3
C	705	ASN	ARG	engineered mutation	UNP A0A0H3FLJ3
C	707	THR	ALA	engineered mutation	UNP A0A0H3FLJ3
C	708	VAL	LEU	engineered mutation	UNP A0A0H3FLJ3
C	718	ALA	VAL	engineered mutation	UNP A0A0H3FLJ3
D	1	MET	-	initiating methionine	UNP A0A0H3FLJ3
D	2	ALA	-	expression tag	UNP A0A0H3FLJ3
D	3	HIS	-	expression tag	UNP A0A0H3FLJ3
D	4	HIS	-	expression tag	UNP A0A0H3FLJ3
D	5	HIS	-	expression tag	UNP A0A0H3FLJ3
D	6	HIS	-	expression tag	UNP A0A0H3FLJ3
D	7	HIS	-	expression tag	UNP A0A0H3FLJ3
D	8	HIS	-	expression tag	UNP A0A0H3FLJ3
D	81	GLN	HIS	engineered mutation	UNP A0A0H3FLJ3
D	87	SER	GLY	engineered mutation	UNP A0A0H3FLJ3
D	702	GLY	ASP	engineered mutation	UNP A0A0H3FLJ3
D	705	ASN	ARG	engineered mutation	UNP A0A0H3FLJ3
D	707	THR	ALA	engineered mutation	UNP A0A0H3FLJ3
D	708	VAL	LEU	engineered mutation	UNP A0A0H3FLJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	718	ALA	VAL	engineered mutation	UNP A0A0H3FLJ3
E	1	MET	-	initiating methionine	UNP A0A0H3FLJ3
E	2	ALA	-	expression tag	UNP A0A0H3FLJ3
E	3	HIS	-	expression tag	UNP A0A0H3FLJ3
E	4	HIS	-	expression tag	UNP A0A0H3FLJ3
E	5	HIS	-	expression tag	UNP A0A0H3FLJ3
E	6	HIS	-	expression tag	UNP A0A0H3FLJ3
E	7	HIS	-	expression tag	UNP A0A0H3FLJ3
E	8	HIS	-	expression tag	UNP A0A0H3FLJ3
E	81	GLN	HIS	engineered mutation	UNP A0A0H3FLJ3
E	87	SER	GLY	engineered mutation	UNP A0A0H3FLJ3
E	702	GLY	ASP	engineered mutation	UNP A0A0H3FLJ3
E	705	ASN	ARG	engineered mutation	UNP A0A0H3FLJ3
E	707	THR	ALA	engineered mutation	UNP A0A0H3FLJ3
E	708	VAL	LEU	engineered mutation	UNP A0A0H3FLJ3
E	718	ALA	VAL	engineered mutation	UNP A0A0H3FLJ3
F	1	MET	-	initiating methionine	UNP A0A0H3FLJ3
F	2	ALA	-	expression tag	UNP A0A0H3FLJ3
F	3	HIS	-	expression tag	UNP A0A0H3FLJ3
F	4	HIS	-	expression tag	UNP A0A0H3FLJ3
F	5	HIS	-	expression tag	UNP A0A0H3FLJ3
F	6	HIS	-	expression tag	UNP A0A0H3FLJ3
F	7	HIS	-	expression tag	UNP A0A0H3FLJ3
F	8	HIS	-	expression tag	UNP A0A0H3FLJ3
F	81	GLN	HIS	engineered mutation	UNP A0A0H3FLJ3
F	87	SER	GLY	engineered mutation	UNP A0A0H3FLJ3
F	702	GLY	ASP	engineered mutation	UNP A0A0H3FLJ3
F	705	ASN	ARG	engineered mutation	UNP A0A0H3FLJ3
F	707	THR	ALA	engineered mutation	UNP A0A0H3FLJ3
F	708	VAL	LEU	engineered mutation	UNP A0A0H3FLJ3
F	718	ALA	VAL	engineered mutation	UNP A0A0H3FLJ3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	6	Total O 6 6	0	0
2	C	8	Total O 8 8	0	0
2	D	5	Total O 5 5	0	0

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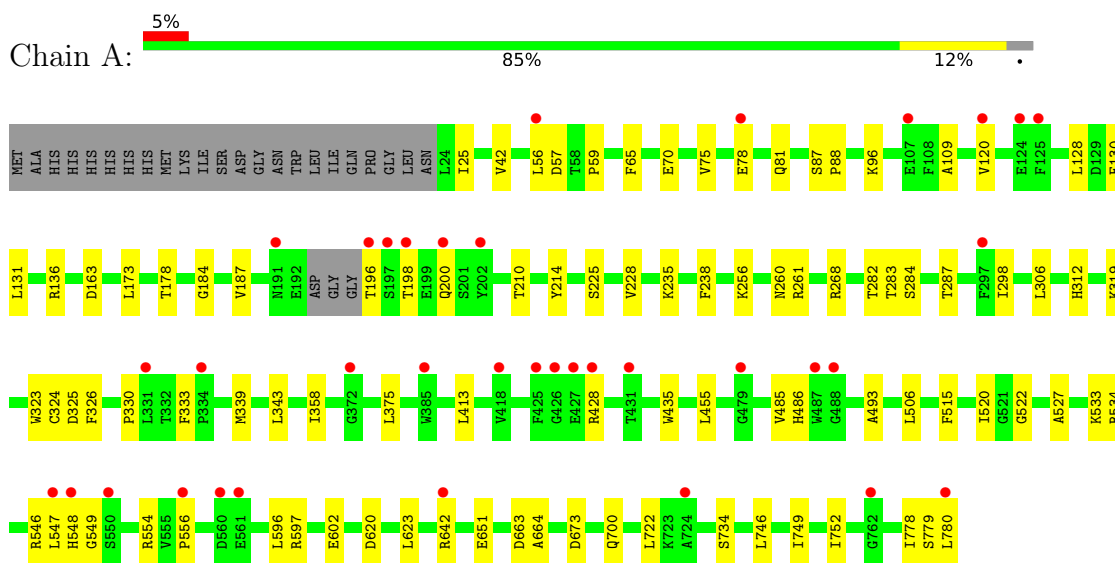
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	4	Total	O	0	0
			4	4		
2	F	4	Total	O	0	0
			4	4		

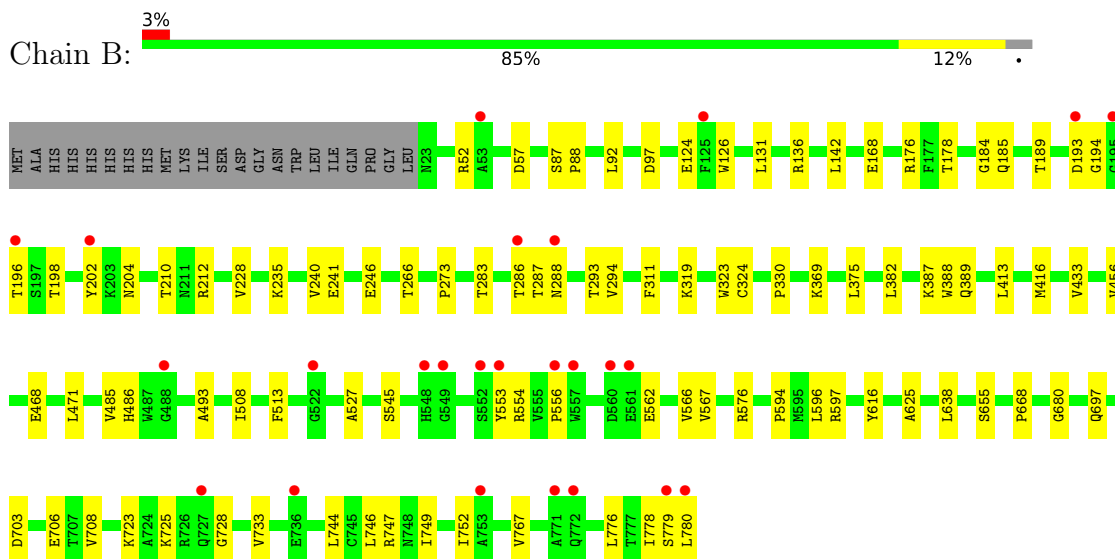
3 Residue-property plots [i](#)

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.

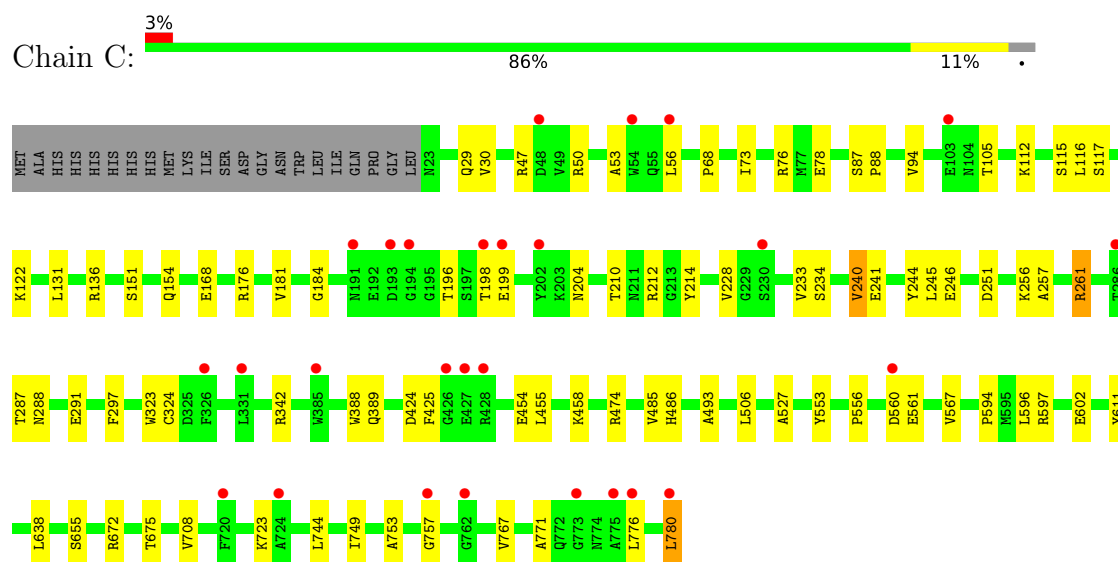
• Molecule 1: Alpha-glucosidase yicI



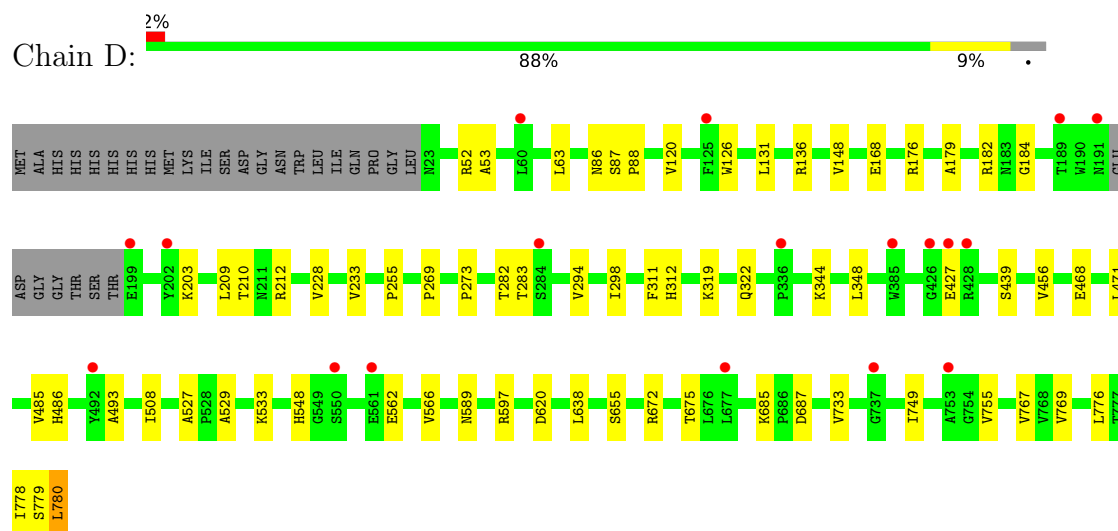
• Molecule 1: Alpha-glucosidase yicI



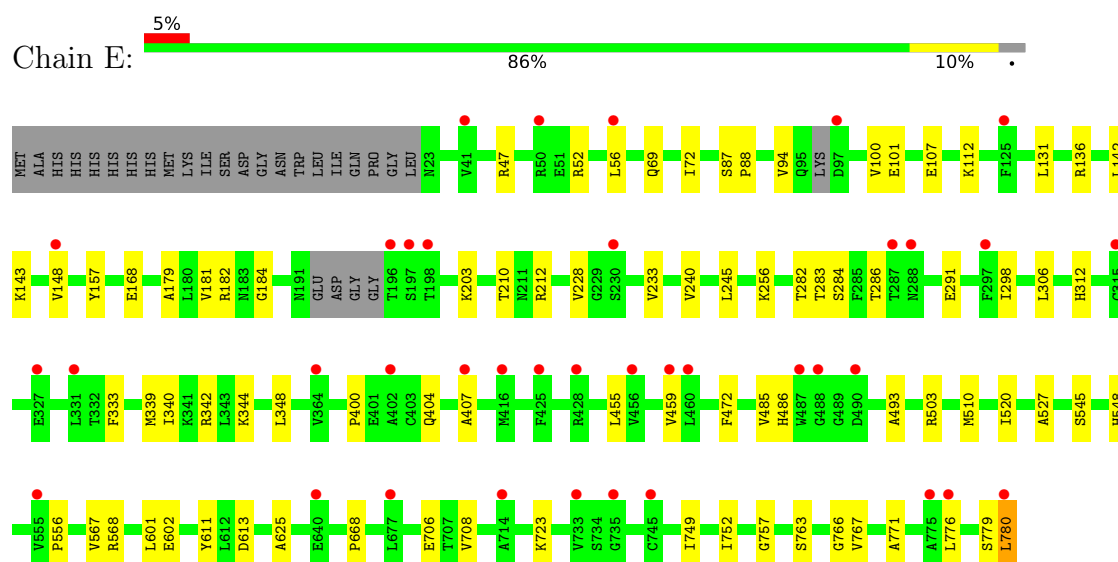
• Molecule 1: Alpha-glucosidase yicI



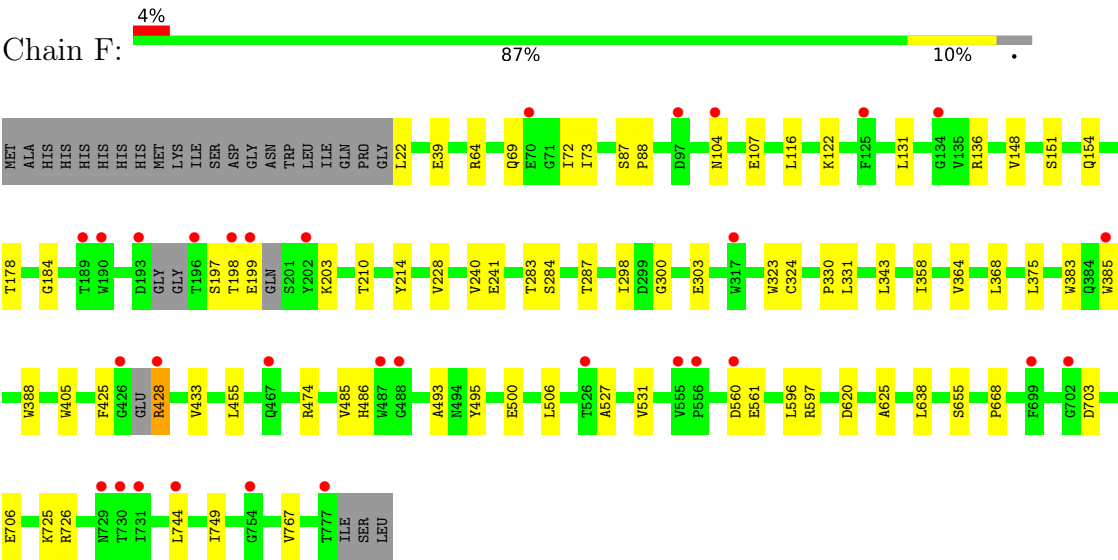
• Molecule 1: Alpha-glucosidase yicI



• Molecule 1: Alpha-glucosidase yicI



● Molecule 1: Alpha-glucosidase yicI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.79Å 208.51Å 280.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.25 – 2.70 29.25 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.25-2.70) 99.9 (29.25-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.21rc1_4933: ???)	Depositor
R, R_{free}	0.229 , 0.263 0.233 , 0.265	Depositor DCC
R_{free} test set	6573 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	36248	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.16	0/6211	0.36	0/8441
1	B	0.16	0/6243	0.36	0/8485
1	C	0.16	0/6244	0.36	0/8486
1	D	0.15	0/6202	0.35	0/8427
1	E	0.17	0/6195	0.36	0/8419
1	F	0.15	0/6190	0.35	0/8412
All	All	0.16	0/37285	0.36	0/50670

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 [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	6033	0	5756	74	0
1	B	6064	0	5776	56	0
1	C	6065	0	5783	64	0
1	D	6024	0	5751	39	0
1	E	6018	0	5730	53	0
1	F	6014	0	5729	47	0
2	A	3	0	0	0	0
2	B	6	0	0	1	0
2	C	8	0	0	0	0
2	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	4	0	0	0	0
2	F	4	0	0	0	0
All	All	36248	0	34525	320	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 5.

All (320) 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:F:210:THR:HG22	1:F:214:TYR:O	1.86	0.76
1:D:168:GLU:OE2	1:D:210:THR:HG21	1.87	0.74
1:B:168:GLU:OE2	1:B:210:THR:HG21	1.88	0.73
1:A:210:THR:HG22	1:A:214:TYR:O	1.89	0.73
1:A:324:CYS:C	1:A:358:ILE:HD13	2.15	0.72
1:A:642:ARG:CZ	1:A:651:GLU:HB3	2.19	0.72
1:B:746:LEU:HD11	1:B:778:ILE:HD13	1.73	0.71
1:C:287:THR:HG21	1:C:553:TYR:CE1	2.26	0.71
1:B:287:THR:HG21	1:B:553:TYR:CE1	2.27	0.69
1:A:109:ALA:HB3	1:A:120:VAL:CG2	2.23	0.69
1:C:168:GLU:OE2	1:C:210:THR:HG21	1.94	0.68
1:B:131:LEU:HD23	1:B:136:ARG:HA	1.74	0.68
1:F:131:LEU:HD23	1:F:136:ARG:HA	1.75	0.67
1:D:298:ILE:HD12	1:D:348:LEU:HD11	1.78	0.66
1:E:556:PRO:HG3	1:E:567:VAL:HG21	1.77	0.66
1:F:506:LEU:HD23	1:F:596:LEU:HD23	1.79	0.65
1:A:324:CYS:N	1:A:358:ILE:HD12	2.10	0.65
1:E:148:VAL:CG1	1:E:157:TYR:HB2	2.27	0.65
1:A:642:ARG:NH2	1:A:651:GLU:OE1	2.29	0.64
1:A:325:ASP:HB3	1:A:358:ILE:HD11	1.79	0.64
1:C:131:LEU:HD23	1:C:136:ARG:HA	1.78	0.64
1:B:703:ASP:OD1	1:B:728:GLY:N	2.30	0.64
1:F:493:ALA:HB1	1:F:527:ALA:HB2	1.81	0.63
1:C:506:LEU:HD23	1:C:596:LEU:HD23	1.80	0.63
1:E:168:GLU:OE2	1:E:210:THR:HG21	1.99	0.62
1:A:324:CYS:O	1:A:358:ILE:HD13	2.00	0.62
1:A:642:ARG:CG	1:A:700:GLN:HG3	2.27	0.62
1:C:556:PRO:HG3	1:C:567:VAL:HG21	1.82	0.62
1:C:757:GLY:HA3	1:C:776:LEU:HD23	1.81	0.61
1:A:642:ARG:NH2	1:A:651:GLU:CB	2.64	0.60
1:C:291:GLU:OE2	1:C:342:ARG:NH2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ILE:HB	1:A:547:LEU:HD23	1.83	0.60
1:F:210:THR:HG21	1:F:214:TYR:CE2	2.37	0.60
1:C:757:GLY:C	1:C:776:LEU:CD2	2.74	0.59
1:E:757:GLY:C	1:E:776:LEU:CD2	2.75	0.59
1:C:757:GLY:HA3	1:C:776:LEU:CD2	2.31	0.59
1:A:752:ILE:HA	1:A:780:LEU:HD22	1.85	0.59
1:A:493:ALA:HB1	1:A:527:ALA:HB2	1.83	0.59
1:D:269:PRO:O	1:D:589:ASN:ND2	2.33	0.59
1:A:131:LEU:HD23	1:A:136:ARG:HA	1.85	0.59
1:A:326:PHE:HD1	1:A:413:LEU:HD11	1.67	0.59
1:E:757:GLY:HA3	1:E:776:LEU:HD23	1.84	0.59
1:A:642:ARG:HG2	1:A:700:GLN:CD	2.28	0.59
1:E:131:LEU:HD23	1:E:136:ARG:HA	1.84	0.59
1:C:757:GLY:C	1:C:776:LEU:HD21	2.29	0.58
1:A:485:VAL:HG12	1:A:486:HIS:H	1.69	0.58
1:A:324:CYS:C	1:A:358:ILE:CD1	2.76	0.58
1:A:65:PHE:CD1	1:A:75:VAL:HG22	2.39	0.57
1:D:282:THR:HG23	1:D:312:HIS:HD2	1.69	0.57
1:A:642:ARG:NH2	1:A:651:GLU:HB3	2.20	0.57
1:B:210:THR:HG22	1:B:212:ARG:H	1.68	0.57
1:C:210:THR:HG22	1:C:212:ARG:H	1.69	0.57
1:C:757:GLY:O	1:C:776:LEU:HD21	2.05	0.57
1:C:73:ILE:HD12	1:C:116:LEU:HG	1.87	0.56
1:A:319:LYS:HE3	1:A:330:PRO:HD2	1.86	0.56
1:C:493:ALA:HB1	1:C:527:ALA:HB2	1.87	0.56
1:A:57:ASP:OD1	1:C:388:TRP:N	2.37	0.56
1:E:298:ILE:HD12	1:E:348:LEU:HD11	1.87	0.56
1:B:194:GLY:HA3	1:B:198:THR:HG21	1.88	0.56
1:C:560:ASP:OD1	1:C:561:GLU:N	2.37	0.56
1:D:597:ARG:NH1	1:D:620:ASP:OD1	2.37	0.55
1:D:282:THR:HG21	1:D:548:HIS:ND1	2.21	0.55
1:E:256:LYS:NZ	1:E:602:GLU:OE1	2.31	0.55
1:B:556:PRO:HG3	1:B:567:VAL:HG21	1.90	0.54
1:C:233:VAL:HG12	1:F:178:THR:HG22	1.88	0.54
1:C:196:THR:HG22	1:C:196:THR:O	2.05	0.54
1:E:240:VAL:HG12	1:E:245:LEU:HD13	1.90	0.54
1:F:298:ILE:CD1	1:F:343:LEU:HD22	2.38	0.54
1:D:485:VAL:HG12	1:D:486:HIS:H	1.73	0.53
1:C:240:VAL:HG12	1:C:245:LEU:HD13	1.91	0.53
1:E:210:THR:HG22	1:E:212:ARG:H	1.74	0.53
1:A:210:THR:HG21	1:A:214:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ASP:OD1	1:B:202:TYR:OH	2.26	0.53
1:B:52:ARG:NH1	1:F:287:THR:O	2.40	0.53
1:D:210:THR:HG22	1:D:212:ARG:H	1.73	0.53
1:B:184:GLY:N	1:B:228:VAL:O	2.37	0.52
1:A:642:ARG:NH2	1:A:651:GLU:HB2	2.24	0.52
1:F:69:GLN:HB3	1:F:72:ILE:HD12	1.92	0.52
1:B:485:VAL:HG12	1:B:486:HIS:H	1.73	0.52
1:D:282:THR:HG22	1:D:283:THR:N	2.24	0.52
1:A:534:ARG:NH1	1:A:663:ASP:O	2.43	0.52
1:B:196:THR:HG22	1:B:196:THR:O	2.09	0.52
1:F:485:VAL:HG12	1:F:486:HIS:H	1.74	0.52
1:D:131:LEU:HD23	1:D:136:ARG:HA	1.92	0.51
1:F:560:ASP:OD1	1:F:561:GLU:N	2.43	0.51
1:A:173:LEU:HD13	1:A:187:VAL:HG21	1.92	0.51
1:A:109:ALA:O	1:A:120:VAL:HG22	2.10	0.51
1:B:294:VAL:HG13	1:B:311:PHE:CZ	2.45	0.51
1:A:522:GLY:O	1:A:554:ARG:NH2	2.43	0.51
1:B:126:TRP:HB3	1:B:142:LEU:HD13	1.92	0.51
1:C:105:THR:O	1:C:122:LYS:NZ	2.39	0.51
1:E:749:ILE:O	1:E:767:VAL:HG23	2.10	0.51
1:A:546:ARG:CD	1:A:548:HIS:HB2	2.41	0.51
1:B:189:THR:HG23	1:B:204:ASN:HB3	1.93	0.51
1:B:178:THR:HG22	1:E:233:VAL:HG12	1.91	0.51
1:B:697:GLN:OE1	1:B:747:ARG:NH1	2.42	0.51
1:F:330:PRO:HG2	1:F:331:LEU:HD12	1.92	0.50
1:A:485:VAL:HG12	1:A:486:HIS:N	2.26	0.50
1:B:369:LYS:HG3	1:B:382:LEU:HD11	1.94	0.50
1:E:107:GLU:OE1	1:E:107:GLU:N	2.45	0.50
1:D:755:VAL:HG23	1:D:778:ILE:HD13	1.93	0.50
1:E:493:ALA:HB1	1:E:527:ALA:HB2	1.94	0.50
1:F:485:VAL:HG12	1:F:486:HIS:N	2.26	0.50
1:D:749:ILE:O	1:D:767:VAL:HG23	2.12	0.50
1:E:757:GLY:C	1:E:776:LEU:HD21	2.37	0.50
1:F:184:GLY:N	1:F:228:VAL:O	2.41	0.49
1:D:493:ALA:HB1	1:D:527:ALA:HB2	1.93	0.49
1:F:22:LEU:HD11	1:F:148:VAL:CG1	2.42	0.49
1:B:749:ILE:O	1:B:767:VAL:HG23	2.12	0.49
1:D:203:LYS:HD2	1:D:508:ILE:HD12	1.94	0.49
1:B:286:THR:HG21	1:D:53:ALA:HA	1.94	0.49
1:D:485:VAL:HG12	1:D:486:HIS:N	2.27	0.49
1:B:273:PRO:HG3	1:B:468:GLU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:ILE:HA	1:B:780:LEU:HD22	1.94	0.49
1:E:100:VAL:HG13	1:E:112:LYS:O	2.12	0.49
1:B:485:VAL:HG12	1:B:486:HIS:N	2.28	0.49
1:C:749:ILE:O	1:C:767:VAL:HG23	2.13	0.49
1:E:485:VAL:HG12	1:E:486:HIS:N	2.28	0.49
1:C:638:LEU:O	1:C:655:SER:N	2.46	0.49
1:A:196:THR:O	1:A:196:THR:HG22	2.12	0.49
1:A:722:LEU:HD12	1:A:734:SER:O	2.13	0.49
1:B:375:LEU:HD21	1:B:433:VAL:HG21	1.94	0.49
1:B:638:LEU:O	1:B:655:SER:N	2.47	0.48
1:A:184:GLY:N	1:A:228:VAL:O	2.43	0.48
1:C:184:GLY:N	1:C:228:VAL:O	2.38	0.48
1:F:107:GLU:N	1:F:107:GLU:OE1	2.46	0.48
1:F:358:ILE:HD13	1:F:368:LEU:HD12	1.95	0.48
1:A:56:LEU:N	1:A:56:LEU:HD23	2.28	0.48
1:B:493:ALA:HB1	1:B:527:ALA:HB2	1.95	0.48
1:C:454:GLU:HG2	1:C:458:LYS:HE3	1.95	0.48
1:C:757:GLY:CA	1:C:776:LEU:CD2	2.92	0.48
1:E:485:VAL:HG12	1:E:486:HIS:H	1.77	0.48
1:C:485:VAL:HG12	1:C:486:HIS:H	1.79	0.48
1:A:333:PHE:CD1	1:A:339:MET:HE1	2.49	0.48
1:E:47:ARG:NH2	1:E:56:LEU:O	2.46	0.47
1:B:697:GLN:HB3	1:B:747:ARG:HD2	1.96	0.47
1:A:642:ARG:NE	1:A:651:GLU:HB3	2.28	0.47
1:A:642:ARG:HG3	1:A:700:GLN:HG3	1.95	0.47
1:C:78:GLU:HG2	1:C:244:TYR:HB3	1.95	0.47
1:E:184:GLY:N	1:E:228:VAL:O	2.40	0.47
1:C:78:GLU:HG2	1:C:244:TYR:CB	2.45	0.47
1:B:594:PRO:O	1:B:597:ARG:NE	2.48	0.47
1:D:779:SER:O	1:D:780:LEU:CB	2.62	0.47
1:E:752:ILE:HA	1:E:780:LEU:HD22	1.96	0.47
1:C:256:LYS:NZ	1:C:602:GLU:OE1	2.34	0.47
1:E:282:THR:HG22	1:E:283:THR:N	2.30	0.47
1:E:708:VAL:HG22	1:E:723:LYS:HG2	1.97	0.47
1:B:57:ASP:OD1	1:F:388:TRP:N	2.45	0.47
1:B:287:THR:HG21	1:B:553:TYR:CZ	2.50	0.47
1:F:364:VAL:HG11	1:F:405:TRP:CZ2	2.49	0.47
1:C:198:THR:HG22	1:C:199:GLU:N	2.30	0.46
1:F:151:SER:O	1:F:154:GLN:NE2	2.44	0.46
1:A:298:ILE:CD1	1:A:343:LEU:HD22	2.45	0.46
1:A:282:THR:HG23	1:A:546:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ALA:O	1:C:261:ARG:HG2	2.15	0.46
1:C:708:VAL:HG22	1:C:723:LYS:HG2	1.96	0.46
1:C:672:ARG:O	1:C:675:THR:OG1	2.29	0.46
1:C:753:ALA:HB2	1:C:780:LEU:HD22	1.97	0.46
1:D:184:GLY:N	1:D:228:VAL:O	2.43	0.46
1:E:779:SER:O	1:E:780:LEU:CB	2.64	0.46
1:A:282:THR:HG22	1:A:312:HIS:HB3	1.97	0.46
1:B:596:LEU:HD12	1:B:616:TYR:CD2	2.50	0.46
1:F:203:LYS:HE2	1:F:486:HIS:HB3	1.98	0.46
1:E:69:GLN:HB3	1:E:72:ILE:HD12	1.98	0.46
1:A:178:THR:HG22	1:D:233:VAL:HG12	1.98	0.46
1:A:506:LEU:HD23	1:A:596:LEU:HD23	1.98	0.45
1:C:594:PRO:O	1:C:597:ARG:NE	2.49	0.45
1:A:163:ASP:OD1	1:A:235:LYS:HE3	2.16	0.45
1:E:94:VAL:HG23	1:E:94:VAL:O	2.16	0.45
1:E:520:ILE:HD11	1:E:545:SER:HB3	1.97	0.45
1:B:779:SER:O	1:B:780:LEU:CB	2.63	0.45
1:D:63:LEU:HD22	1:D:126:TRP:HH2	1.82	0.45
1:C:485:VAL:HG12	1:C:486:HIS:N	2.31	0.45
1:A:651:GLU:OE2	1:A:700:GLN:NE2	2.50	0.45
1:C:115:SER:OG	1:C:251:ASP:OD2	2.31	0.45
1:C:323:TRP:HA	1:C:324:CYS:HA	1.81	0.45
1:F:73:ILE:HD12	1:F:116:LEU:HG	1.99	0.45
1:F:364:VAL:HG11	1:F:405:TRP:HZ2	1.81	0.45
1:A:455:LEU:C	1:A:455:LEU:HD23	2.42	0.45
1:E:282:THR:HG23	1:E:312:HIS:ND1	2.32	0.45
1:C:455:LEU:C	1:C:455:LEU:HD13	2.42	0.45
1:D:209:LEU:HD21	1:D:255:PRO:HB3	1.98	0.45
1:A:746:LEU:HD11	1:A:778:ILE:HG21	1.98	0.45
1:B:625:ALA:HB3	1:B:668:PRO:HB2	1.99	0.45
1:A:323:TRP:C	1:A:358:ILE:HD12	2.41	0.45
1:D:456:VAL:HG12	1:D:471:LEU:HD21	1.99	0.45
1:D:685:LYS:HG2	1:D:687:ASP:OD1	2.17	0.45
1:A:779:SER:O	1:A:780:LEU:CB	2.65	0.45
1:A:306:LEU:HD13	1:A:556:PRO:HG2	1.99	0.44
1:B:576:ARG:O	1:B:680:GLY:N	2.47	0.44
1:E:625:ALA:HB3	1:E:668:PRO:HB2	1.99	0.44
1:C:176:ARG:NH1	1:C:204:ASN:OD1	2.50	0.44
1:C:233:VAL:HG22	1:F:197:SER:HA	1.99	0.44
1:C:744:LEU:C	1:C:744:LEU:HD23	2.41	0.44
1:A:323:TRP:O	1:A:358:ILE:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLN:HG2	1:E:184:GLY:O	2.18	0.44
1:D:87:SER:HB3	1:D:88:PRO:HA	2.00	0.44
1:E:407:ALA:HB1	1:E:459:VAL:HG22	2.00	0.44
1:F:104:ASN:OD1	1:F:122:LYS:NZ	2.51	0.44
1:B:733:VAL:HB	1:B:776:LEU:HG	2.00	0.44
1:C:76:ARG:NE	1:C:78:GLU:OE2	2.50	0.44
1:C:388:TRP:CD1	1:C:389:GLN:HG2	2.53	0.44
1:D:638:LEU:O	1:D:655:SER:N	2.51	0.44
1:B:287:THR:O	1:D:52:ARG:NH1	2.50	0.44
1:C:287:THR:HG22	1:C:288:ASN:N	2.32	0.44
1:E:771:ALA:CB	1:E:776:LEU:HD11	2.48	0.44
1:C:454:GLU:O	1:C:458:LYS:HG3	2.18	0.43
1:E:340:ILE:O	1:E:344:LYS:HG2	2.18	0.43
1:E:771:ALA:HB2	1:E:776:LEU:HD11	2.00	0.43
1:F:87:SER:HB3	1:F:88:PRO:HA	1.99	0.43
1:F:638:LEU:O	1:F:655:SER:N	2.51	0.43
1:A:260:ASN:OD1	1:A:268:ARG:NH1	2.45	0.43
1:D:344:LYS:HD2	1:D:348:LEU:O	2.18	0.43
1:F:744:LEU:C	1:F:744:LEU:HD23	2.43	0.43
1:A:642:ARG:HB3	1:A:673:ASP:HB3	2.00	0.43
1:E:291:GLU:OE2	1:E:342:ARG:NH2	2.52	0.43
1:A:287:THR:O	1:E:52:ARG:NH1	2.49	0.43
1:D:319:LYS:HE3	1:D:322:GLN:OE1	2.18	0.43
1:F:198:THR:HG22	1:F:199:GLU:N	2.33	0.43
1:C:68:PRO:HB3	1:C:94:VAL:HG13	2.00	0.43
1:D:179:ALA:O	1:D:182:ARG:NH1	2.52	0.43
1:E:510:MET:HG2	1:E:601:LEU:HD11	2.01	0.43
1:F:455:LEU:C	1:F:455:LEU:HD23	2.42	0.43
1:C:29:GLN:HE22	1:C:50:ARG:HG3	1.83	0.43
1:D:769:VAL:HG21	1:D:778:ILE:HD11	1.99	0.43
1:F:625:ALA:HB3	1:F:668:PRO:HB2	1.99	0.43
1:A:78:GLU:OE2	1:A:81:GLN:HG2	2.19	0.43
1:E:503:ARG:HG2	1:E:613:ASP:HB2	2.00	0.43
1:F:383:TRP:HH2	1:F:385:TRP:CE2	2.37	0.43
1:A:87:SER:HB3	1:A:88:PRO:HA	2.00	0.43
1:A:128:LEU:HD21	1:A:130:PHE:CE2	2.54	0.43
1:A:256:LYS:NZ	1:A:602:GLU:OE1	2.50	0.43
1:F:495:TYR:CZ	1:F:531:VAL:HG22	2.54	0.43
1:A:25:ILE:HD13	1:A:59:PRO:HG2	2.00	0.43
1:C:424:ASP:OD1	1:C:474:ARG:HD3	2.19	0.43
1:E:87:SER:HB3	1:E:88:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:455:LEU:HD23	1:E:455:LEU:C	2.44	0.43
1:F:706:GLU:HB3	1:F:725:LYS:HD3	2.01	0.43
1:D:562:GLU:O	1:D:566:VAL:HG23	2.19	0.42
1:B:92:LEU:CD2	1:B:266:THR:HG22	2.49	0.42
1:C:297:PHE:HZ	1:C:553:TYR:CE1	2.36	0.42
1:B:87:SER:HB3	1:B:88:PRO:HA	2.02	0.42
1:C:87:SER:HB3	1:C:88:PRO:HA	2.01	0.42
1:D:273:PRO:HG3	1:D:468:GLU:HA	2.00	0.42
1:C:181:VAL:HG21	1:C:611:TYR:CD1	2.54	0.42
1:C:425:PHE:HA	1:C:474:ARG:NH2	2.34	0.42
1:C:771:ALA:HA	1:C:776:LEU:HD11	2.00	0.42
1:E:179:ALA:O	1:E:182:ARG:NH1	2.53	0.42
1:E:306:LEU:HD23	1:E:568:ARG:HB2	2.02	0.42
1:E:282:THR:HG21	1:E:548:HIS:ND1	2.34	0.42
1:D:63:LEU:HD22	1:D:126:TRP:CH2	2.53	0.42
1:A:549:GLY:HA3	1:A:554:ARG:HE	1.85	0.42
1:B:744:LEU:C	1:B:744:LEU:HD23	2.45	0.42
1:B:779:SER:O	1:B:780:LEU:HB3	2.19	0.42
1:E:333:PHE:CD1	1:E:339:MET:HE1	2.55	0.42
1:F:385:TRP:HZ2	1:F:428:ARG:HG3	1.85	0.42
1:B:387:LYS:O	1:B:388:TRP:HB3	2.20	0.42
1:C:251:ASP:O	1:C:261:ARG:HD2	2.19	0.42
1:D:672:ARG:O	1:D:675:THR:OG1	2.34	0.42
1:F:597:ARG:NH1	1:F:620:ASP:OD1	2.45	0.42
1:B:545:SER:HA	2:B:801:HOH:O	2.20	0.42
1:D:294:VAL:HG22	1:D:311:PHE:CZ	2.54	0.42
1:E:181:VAL:HG21	1:E:611:TYR:CD1	2.55	0.42
1:E:706:GLU:OE2	1:E:723:LYS:HD3	2.20	0.42
1:B:319:LYS:HE3	1:B:330:PRO:HD2	2.00	0.41
1:F:39:GLU:OE1	1:F:64:ARG:NH1	2.51	0.41
1:F:375:LEU:HD21	1:F:433:VAL:HG21	2.02	0.41
1:A:65:PHE:HD1	1:A:75:VAL:HG22	1.81	0.41
1:E:763:SER:OG	1:E:766:GLY:O	2.30	0.41
1:F:240:VAL:HG22	1:F:241:GLU:N	2.35	0.41
1:B:562:GLU:O	1:B:566:VAL:HG23	2.20	0.41
1:C:151:SER:O	1:C:154:GLN:NE2	2.50	0.41
1:D:88:PRO:HD3	1:D:439:SER:HB3	2.03	0.41
1:D:529:ALA:HB1	1:D:533:LYS:NZ	2.34	0.41
1:F:300:GLY:HA2	1:F:303:GLU:HG2	2.01	0.41
1:A:198:THR:HG22	1:A:200:GLN:H	1.85	0.41
1:B:323:TRP:HA	1:B:324:CYS:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:TRP:CD1	1:B:389:GLN:HG2	2.56	0.41
1:C:214:TYR:CD1	1:C:214:TYR:C	2.98	0.41
1:C:287:THR:HG21	1:C:553:TYR:CZ	2.54	0.41
1:A:597:ARG:NH1	1:A:620:ASP:OD1	2.38	0.41
1:C:30:VAL:HG11	1:C:122:LYS:HG2	2.02	0.41
1:C:112:LYS:HG2	1:C:117:SER:CB	2.50	0.41
1:A:282:THR:OG1	1:A:548:HIS:HA	2.19	0.41
1:B:240:VAL:HG22	1:B:241:GLU:N	2.36	0.41
1:B:508:ILE:HG12	1:B:513:PHE:HB2	2.03	0.41
1:C:240:VAL:HG22	1:C:241:GLU:N	2.35	0.41
1:D:529:ALA:HB1	1:D:533:LYS:HZ2	1.85	0.41
1:F:703:ASP:HA	1:F:726:ARG:HD3	2.02	0.41
1:A:42:VAL:HG21	1:A:120:VAL:HG11	2.02	0.41
1:A:283:THR:O	1:A:284:SER:HB2	2.21	0.41
1:A:623:LEU:HD23	1:A:623:LEU:C	2.46	0.41
1:B:413:LEU:O	1:B:416:MET:HG2	2.20	0.41
1:B:706:GLU:HB3	1:B:725:LYS:HD3	2.03	0.41
1:E:100:VAL:HG12	1:E:101:GLU:N	2.35	0.41
1:E:142:LEU:HG	1:E:143:LYS:HG3	2.02	0.41
1:E:400:PRO:O	1:E:404:GLN:HG3	2.21	0.41
1:A:282:THR:CG2	1:A:546:ARG:HD3	2.51	0.41
1:C:47:ARG:NH2	1:C:56:LEU:O	2.54	0.41
1:C:234:SER:HB3	1:F:500:GLU:OE2	2.21	0.41
1:E:148:VAL:HG12	1:E:157:TYR:HB2	2.01	0.41
1:E:283:THR:O	1:E:284:SER:HB2	2.19	0.41
1:B:283:THR:HG22	1:B:311:PHE:HZ	1.86	0.41
1:B:287:THR:HG22	1:B:288:ASN:N	2.35	0.41
1:A:375:LEU:HD13	1:A:435:TRP:CE3	2.56	0.40
1:F:323:TRP:HA	1:F:324:CYS:HA	1.78	0.40
1:F:425:PHE:HA	1:F:474:ARG:NH2	2.36	0.40
1:A:70:GLU:OE1	1:A:261:ARG:NH1	2.39	0.40
1:A:549:GLY:CA	1:A:554:ARG:HE	2.34	0.40
1:A:746:LEU:HB3	1:A:749:ILE:HD12	2.02	0.40
1:C:53:ALA:HA	1:E:286:THR:HG21	2.02	0.40
1:F:749:ILE:O	1:F:767:VAL:HG23	2.21	0.40
1:A:225:SER:O	1:A:238:PHE:HA	2.21	0.40
1:A:485:VAL:HG13	1:A:515:PHE:CB	2.51	0.40
1:A:533:LYS:HD3	1:A:664:ALA:HB1	2.02	0.40
1:B:456:VAL:HG12	1:B:471:LEU:HD21	2.04	0.40
1:D:733:VAL:HB	1:D:776:LEU:HG	2.03	0.40
1:B:708:VAL:HG22	1:B:723:LYS:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:THR:O	1:F:284:SER:HB2	2.21	0.40
1:F:131:LEU:HD23	1:F:136:ARG:CA	2.48	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	750/780 (96%)	727 (97%)	23 (3%)	0	100	100
1	B	756/780 (97%)	728 (96%)	28 (4%)	0	100	100
1	C	756/780 (97%)	731 (97%)	25 (3%)	0	100	100
1	D	747/780 (96%)	718 (96%)	29 (4%)	0	100	100
1	E	747/780 (96%)	722 (97%)	25 (3%)	0	100	100
1	F	744/780 (95%)	718 (96%)	26 (4%)	0	100	100
All	All	4500/4680 (96%)	4344 (96%)	156 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	634/660 (96%)	632 (100%)	2 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	638/660 (97%)	631 (99%)	7 (1%)	65	85
1	C	638/660 (97%)	634 (99%)	4 (1%)	78	91
1	D	634/660 (96%)	628 (99%)	6 (1%)	70	87
1	E	631/660 (96%)	628 (100%)	3 (0%)	81	92
1	F	632/660 (96%)	631 (100%)	1 (0%)	87	95
All	All	3807/3960 (96%)	3784 (99%)	23 (1%)	78	91

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	428	ARG
1	B	97	ASP
1	B	124	GLU
1	B	176	ARG
1	B	235	LYS
1	B	246	GLU
1	B	293	THR
1	B	554	ARG
1	C	240	VAL
1	C	246	GLU
1	C	261	ARG
1	C	780	LEU
1	D	86	ASN
1	D	120	VAL
1	D	148	VAL
1	D	176	ARG
1	D	427	GLU
1	D	780	LEU
1	E	203	LYS
1	E	472	PHE
1	E	780	LEU
1	F	428	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	295	ASN

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Mol	Chain	Res	Type
1	A	384	GLN
1	A	442	GLN
1	A	486	HIS
1	A	584	GLN
1	A	684	GLN
1	B	95	GLN
1	B	404	GLN
1	B	442	GLN
1	B	584	GLN
1	C	29	GLN
1	C	295	ASN
1	C	447	HIS
1	C	569	HIS
1	C	584	GLN
1	D	23	ASN
1	D	93	ASN
1	D	156	ASN
1	D	453	ASN
1	D	584	GLN
1	E	26	GLN
1	E	447	HIS
1	E	584	GLN
1	E	684	GLN
1	E	748	ASN
1	F	23	ASN
1	F	26	GLN
1	F	93	ASN
1	F	149	GLN
1	F	447	HIS
1	F	482	GLN
1	F	525	ASN
1	F	748	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	754/780 (96%)	0.49	36 (4%) 35 32	35, 51, 76, 107	0
1	B	758/780 (97%)	0.41	25 (3%) 49 45	35, 49, 82, 126	0
1	C	758/780 (97%)	0.54	27 (3%) 46 42	38, 51, 78, 129	0
1	D	751/780 (96%)	0.33	18 (2%) 59 56	35, 48, 68, 102	0
1	E	753/780 (96%)	0.64	38 (5%) 34 30	38, 56, 80, 123	0
1	F	752/780 (96%)	0.45	31 (4%) 41 37	36, 50, 76, 106	0
All	All	4526/4680 (96%)	0.48	175 (3%) 43 39	35, 51, 77, 129	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	426	GLY	6.9
1	E	402	ALA	5.8
1	B	288	ASN	5.3
1	D	753	ALA	5.3
1	E	428	ARG	4.7
1	B	553	TYR	4.5
1	C	427	GLU	4.4
1	C	776	LEU	4.3
1	F	777	THR	4.2
1	C	199	GLU	4.2
1	A	550	SER	4.2
1	E	776	LEU	4.1
1	B	125	PHE	4.0
1	F	199	GLU	3.8
1	B	560	ASP	3.7
1	C	103	GLU	3.7
1	A	427	GLU	3.7
1	E	125	PHE	3.6
1	A	125	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	720	PHE	3.6
1	B	193	ASP	3.5
1	F	754	GLY	3.5
1	E	780	LEU	3.5
1	D	189	THR	3.5
1	A	556	PRO	3.4
1	C	202	TYR	3.4
1	F	202	TYR	3.4
1	C	780	LEU	3.4
1	D	385	TRP	3.3
1	D	191	ASN	3.3
1	B	202	TYR	3.3
1	A	196	THR	3.2
1	E	456	VAL	3.1
1	E	56	LEU	3.1
1	D	199	GLU	3.1
1	E	315	CYS	3.1
1	F	428	ARG	3.1
1	A	120	VAL	3.1
1	E	230	SER	3.1
1	F	744	LEU	3.0
1	C	426	GLY	3.0
1	A	372	GLY	3.0
1	B	552	SER	3.0
1	A	762	GLY	2.9
1	B	196	THR	2.9
1	C	385	TRP	2.9
1	E	198	THR	2.9
1	E	733	VAL	2.9
1	C	194	GLY	2.9
1	A	198	THR	2.9
1	C	724	ALA	2.9
1	B	488	GLY	2.9
1	A	642	ARG	2.8
1	A	560	ASP	2.8
1	B	195	GLY	2.8
1	A	56	LEU	2.8
1	A	425	PHE	2.8
1	F	125	PHE	2.8
1	A	385	TRP	2.8
1	E	288	ASN	2.8
1	B	736	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	125	PHE	2.8
1	E	677	LEU	2.7
1	B	557	TRP	2.7
1	C	48	ASP	2.7
1	F	555	VAL	2.7
1	A	107	GLU	2.7
1	A	124	GLU	2.7
1	A	200	GLN	2.7
1	F	729	ASN	2.7
1	B	522	GLY	2.6
1	E	327	GLU	2.6
1	F	488	GLY	2.6
1	D	550	SER	2.6
1	E	196	THR	2.6
1	E	490	ASP	2.6
1	E	460	LEU	2.6
1	F	487	TRP	2.6
1	E	297	PHE	2.6
1	A	487	TRP	2.5
1	F	699	PHE	2.5
1	F	385	TRP	2.5
1	B	780	LEU	2.5
1	F	198	THR	2.5
1	D	737	GLY	2.5
1	B	772	GLN	2.5
1	F	730	THR	2.4
1	F	731	ILE	2.4
1	E	459	VAL	2.4
1	F	526	THR	2.4
1	A	547	LEU	2.4
1	A	426	GLY	2.4
1	C	757	GLY	2.4
1	E	745	CYS	2.4
1	E	555	VAL	2.4
1	A	780	LEU	2.4
1	A	191	ASN	2.4
1	A	561	GLU	2.4
1	C	193	ASP	2.4
1	F	193	ASP	2.4
1	E	775	ALA	2.4
1	D	427	GLU	2.3
1	C	560	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	97	ASP	2.3
1	A	334	PRO	2.3
1	A	479	GLY	2.3
1	F	702	GLY	2.3
1	C	428	ARG	2.3
1	C	286	THR	2.3
1	F	190	TRP	2.3
1	B	549	GLY	2.3
1	E	197	SER	2.3
1	A	488	GLY	2.3
1	E	148	VAL	2.3
1	D	677	LEU	2.3
1	B	556	PRO	2.3
1	D	336	PRO	2.3
1	E	640	GLU	2.2
1	E	364	VAL	2.2
1	A	428	ARG	2.2
1	C	191	ASN	2.2
1	E	735	GLY	2.2
1	A	331	LEU	2.2
1	B	548	HIS	2.2
1	A	724	ALA	2.2
1	D	561	GLU	2.2
1	F	189	THR	2.2
1	D	492	TYR	2.2
1	F	467	GLN	2.2
1	E	97	ASP	2.2
1	A	418	VAL	2.2
1	C	54	TRP	2.2
1	F	104	ASN	2.2
1	C	331	LEU	2.2
1	C	773	GLY	2.2
1	D	426	GLY	2.2
1	A	197	SER	2.2
1	E	41	VAL	2.2
1	A	297	PHE	2.2
1	E	287	THR	2.1
1	C	56	LEU	2.1
1	D	60	LEU	2.1
1	A	548	HIS	2.1
1	C	230	SER	2.1
1	B	753	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	714	ALA	2.1
1	E	488	GLY	2.1
1	F	134	GLY	2.1
1	E	425	PHE	2.1
1	C	775	ALA	2.1
1	F	70	GLU	2.1
1	D	428	ARG	2.1
1	E	487	TRP	2.1
1	B	286	THR	2.1
1	B	727	GLN	2.1
1	A	202	TYR	2.1
1	C	326	PHE	2.1
1	F	560	ASP	2.1
1	A	78	GLU	2.1
1	B	53	ALA	2.1
1	B	771	ALA	2.1
1	F	556	PRO	2.1
1	E	50	ARG	2.0
1	D	284	SER	2.0
1	F	317	TRP	2.0
1	A	431	THR	2.0
1	C	198	THR	2.0
1	F	196	THR	2.0
1	E	331	LEU	2.0
1	C	762	GLY	2.0
1	B	561	GLU	2.0
1	E	407	ALA	2.0
1	B	779	SER	2.0
1	E	416	MET	2.0
1	D	202	TYR	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.