Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2023 – 06:08 PM EDT

PDB ID	:	8T7Z
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:

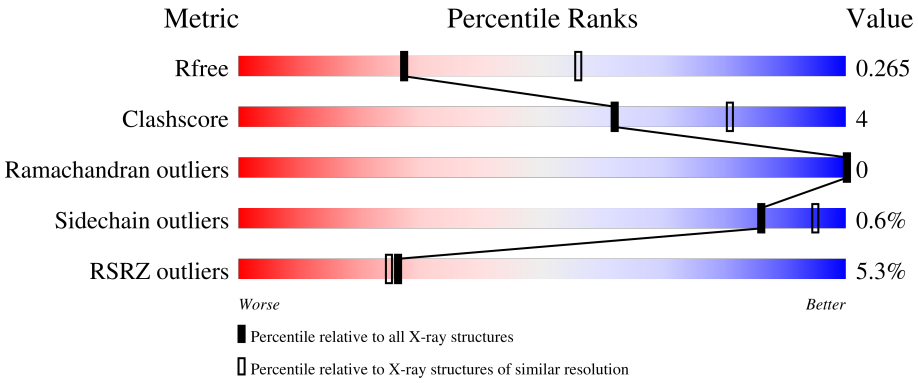
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	7% 86% 11% ·
1	D	780	3% 88% 8% ·
1	E	780	8% 86% 10% ·

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Mol	Chain	Length	Quality of chain
1	F	780	

2 Entry composition (i)

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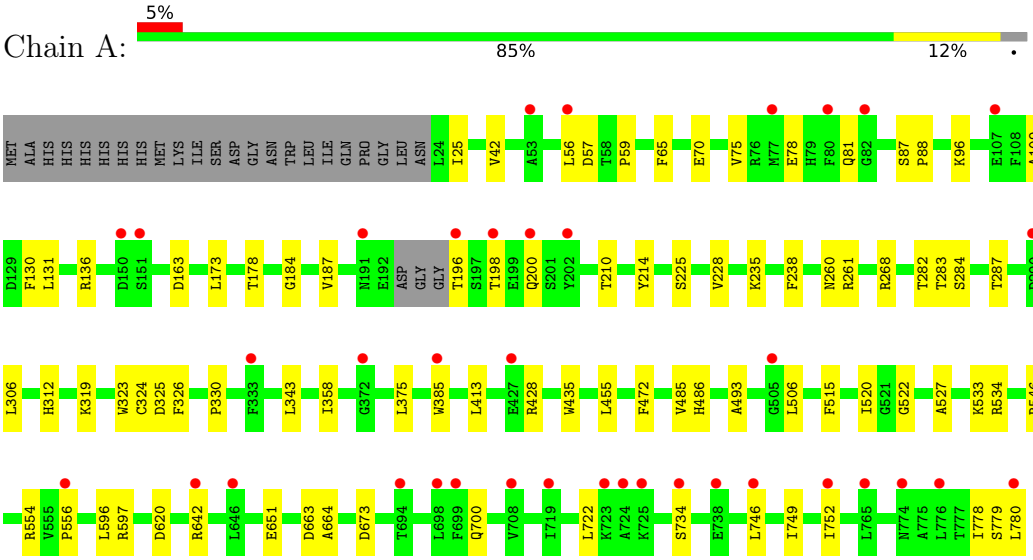
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	4	Total O 4 4	0	0
2	F	4	Total O 4 4	0	0

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.

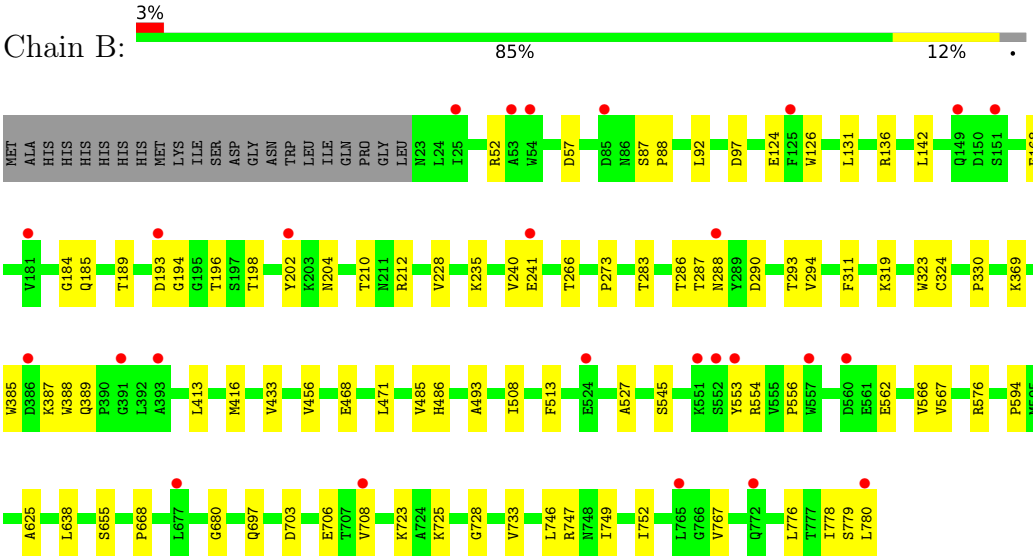
• Molecule 1: Alpha-glucosidase yicI

Chain A:



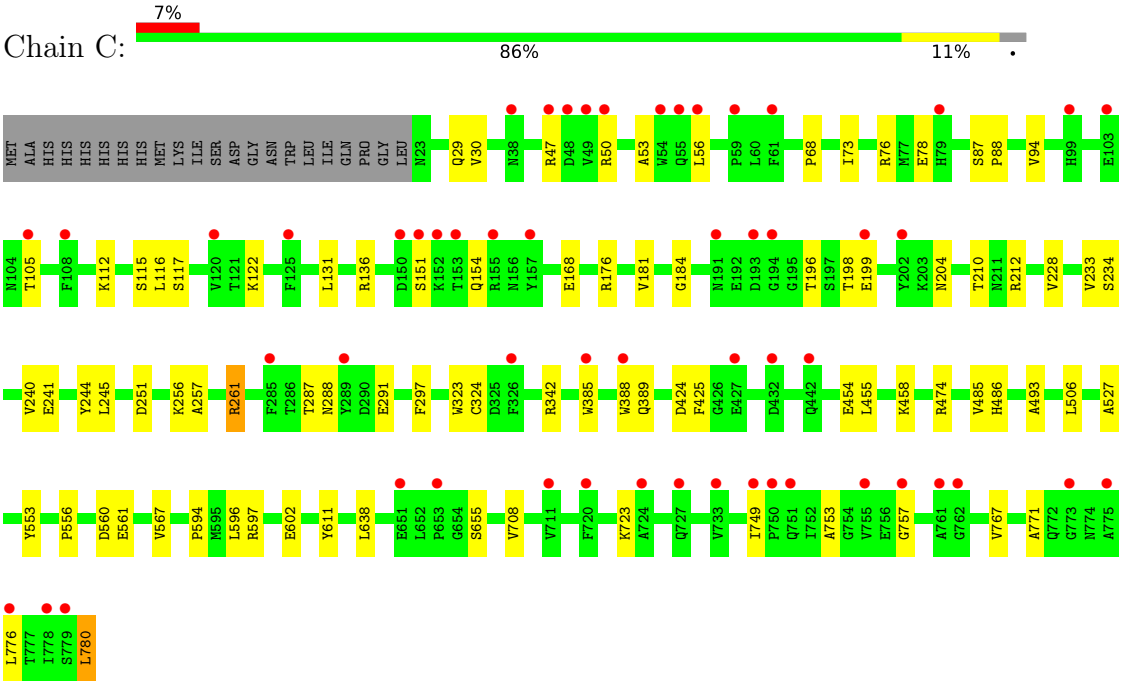
• Molecule 1: Alpha-glucosidase yicI

Chain B:



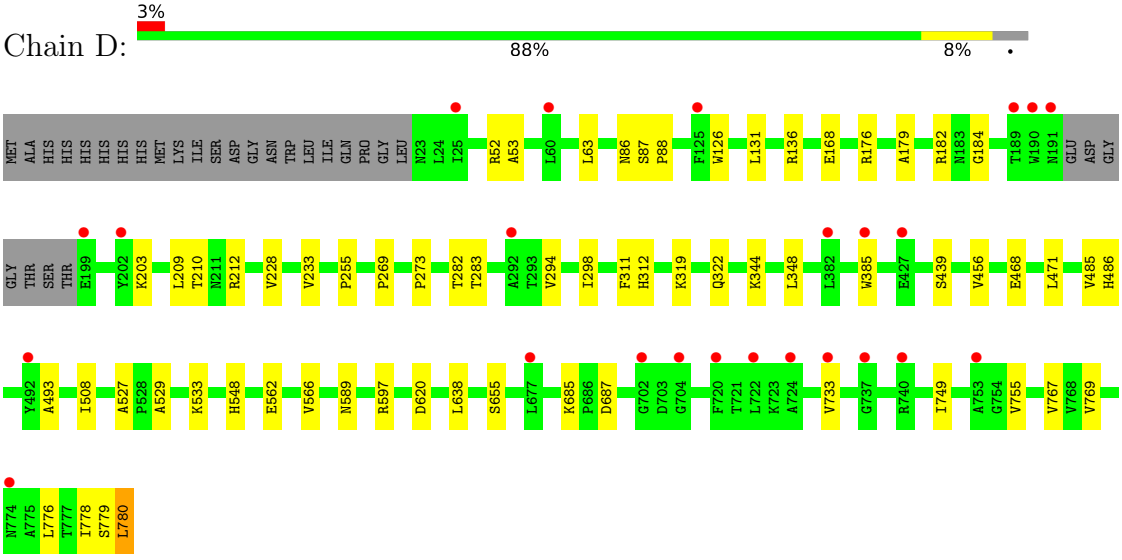
• Molecule 1: Alpha-glucosidase yicI

Chain C:



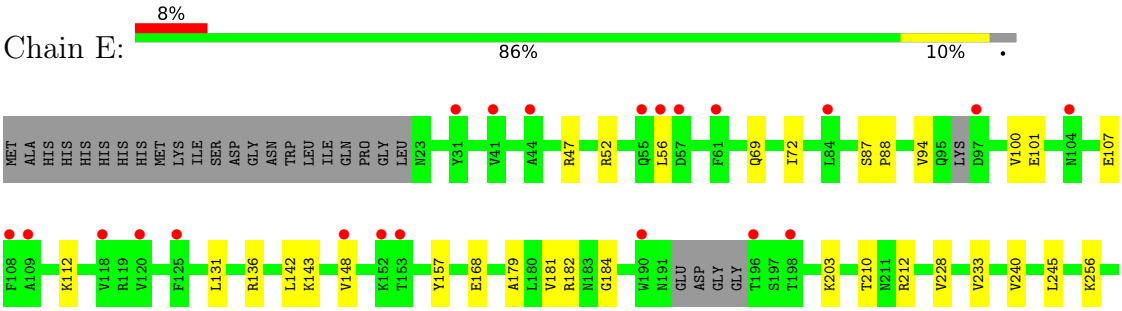
• Molecule 1: Alpha-glucosidase yicI

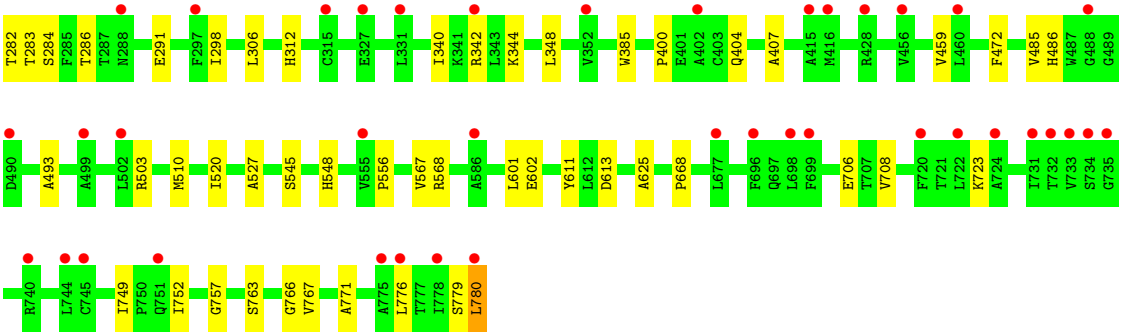
Chain D:



• Molecule 1: Alpha-glucosidase yicI

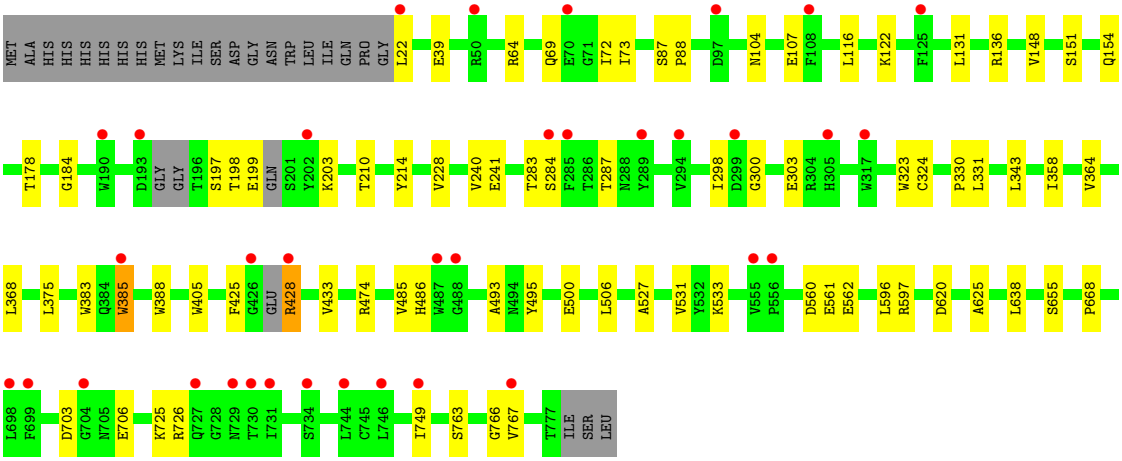
Chain E:





• Molecule 1: Alpha-glucosidase yicI

Chain F:



4 Data and refinement statistics (i)

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 49.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.25-2.70) 100.0 (49.55-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	6572 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)	0.34 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	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.*

[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

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	0.28	0/6211	0.52	0/8441
1	B	0.28	0/6243	0.52	0/8485
1	C	0.28	0/6244	0.53	0/8486
1	D	0.27	0/6202	0.52	0/8427
1	E	0.29	0/6195	0.52	0/8419
1	F	0.27	0/6190	0.51	0/8412
All	All	0.28	0/37285	0.52	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

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	70	0
1	B	6064	0	5776	56	0
1	C	6065	0	5783	61	0
1	D	6024	0	5751	37	0
1	E	6018	0	5730	51	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	309	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 4.

All (309) 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: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:A:324:CYS:C	1:A:358:ILE:HD13	2.15	0.67
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: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:E:131:LEU:HD23	1:E:136:ARG:HA	1.84	0.59
1:A:485:VAL:HG12	1:A:486:HIS:H	1.69	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:C:757:GLY:C	1:C:776:LEU:CD2	2.74	0.55
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:E:757:GLY:C	1:E:776:LEU:CD2	2.75	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:A:642:ARG:HG2	1:A:700:GLN:CD	2.28	0.54
1:F:298:ILE:CD1	1:F:343:LEU:HD22	2.38	0.54
1:C:757:GLY:C	1:C:776:LEU:HD21	2.29	0.53
1:D:485:VAL:HG12	1:D:486:HIS:H	1.73	0.53
1:A:324:CYS:C	1:A:358:ILE:CD1	2.76	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:C:256:LYS:NZ	1:C:602:GLU:OE1	2.34	0.50
1:D:749:ILE:O	1:D:767:VAL:HG23	2.12	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:A:196:THR:O	1:A:196:THR:HG22	2.12	0.49
1:C:638:LEU:O	1:C:655:SER:N	2.46	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: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: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
1:C:115:SER:OG	1:C:251:ASP:OD2	2.31	0.46
1:C:257:ALA:O	1:C:261:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:VAL:HG22	1:C:723:LYS:HG2	1.96	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: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:E:282:THR:HG23	1:E:312:HIS:ND1	2.32	0.45
1:E:757:GLY:C	1:E:776:LEU:HD21	2.37	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: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:B:290:ASP:H	1:B:293:THR:HG1	1.65	0.44
1:A:323:TRP:O	1:A:358:ILE:HA	2.18	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:F:706:GLU:HB3	1:F:725:LYS:HD3	2.01	0.43
1:F:763:SER:OG	1:F:766:GLY:O	2.28	0.43
1:D:562:GLU:O	1:D:566:VAL:HG23	2.19	0.42
1:E:283:THR:O	1:E:284:SER:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:779:SER:O	1:B:780:LEU:HB3	2.19	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: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
1:B:388:TRP:CD1	1:B:389:GLN:HG2	2.56	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:F:533:LYS:NZ	1:F:562:GLU:OE1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:455:LEU:HD23	1:A:455:LEU:C	2.42	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
1:C:455:LEU:C	1:C:455:LEU:HD13	2.42	0.40
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%)	630 (99%)	4 (1%)	86	95
1	B	638/660 (97%)	632 (99%)	6 (1%)	78	92
1	C	638/660 (97%)	635 (100%)	3 (0%)	88	96
1	D	634/660 (96%)	630 (99%)	4 (1%)	86	95
1	E	631/660 (96%)	627 (99%)	4 (1%)	86	95
1	F	632/660 (96%)	630 (100%)	2 (0%)	92	98
All	All	3807/3960 (96%)	3784 (99%)	23 (1%)	86	95

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

Mol	Chain	Res	Type
1	A	96	LYS
1	A	385	TRP
1	A	428	ARG

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Mol	Chain	Res	Type
1	A	472	PHE
1	B	97	ASP
1	B	124	GLU
1	B	176	ARG
1	B	235	LYS
1	B	385	TRP
1	B	554	ARG
1	C	261	ARG
1	C	385	TRP
1	C	780	LEU
1	D	86	ASN
1	D	176	ARG
1	D	385	TRP
1	D	780	LEU
1	E	203	LYS
1	E	385	TRP
1	E	472	PHE
1	E	780	LEU
1	F	385	TRP
1	F	428	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	29	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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, 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	754/780 (96%)	0.47	42 (5%)	24	23	35, 51, 76, 107	0
1	B	758/780 (97%)	0.33	26 (3%)	45	45	35, 49, 82, 126	0
1	C	758/780 (97%)	0.47	55 (7%)	15	13	38, 51, 78, 129	0
1	D	751/780 (96%)	0.30	24 (3%)	47	48	35, 48, 68, 102	0
1	E	753/780 (96%)	0.64	60 (7%)	12	10	38, 56, 80, 123	0
1	F	752/780 (96%)	0.37	35 (4%)	31	30	36, 50, 76, 106	0
All	All	4526/4680 (96%)	0.43	242 (5%)	26	25	35, 51, 77, 129	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	753	ALA	6.5
1	C	776	LEU	6.5
1	E	731	ILE	6.4
1	E	733	VAL	5.9
1	E	402	ALA	5.5
1	A	724	ALA	5.3
1	F	426	GLY	5.1
1	C	103	GLU	4.9
1	F	730	THR	4.8
1	E	776	LEU	4.7
1	E	56	LEU	4.6
1	F	202	TYR	4.6
1	F	729	ASN	4.4
1	E	778	ILE	4.4
1	A	550	SER	4.2
1	E	677	LEU	4.2
1	C	724	ALA	4.2
1	B	553	TYR	4.1
1	B	151	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	107	GLU	3.9
1	F	698	LEU	3.8
1	F	385	TRP	3.7
1	C	720	PHE	3.7
1	D	722	LEU	3.6
1	E	125	PHE	3.6
1	E	775	ALA	3.6
1	A	56	LEU	3.6
1	E	153	THR	3.5
1	E	720	PHE	3.5
1	C	48	ASP	3.5
1	F	744	LEU	3.5
1	B	393	ALA	3.5
1	E	331	LEU	3.4
1	B	780	LEU	3.4
1	F	727	GLN	3.4
1	E	722	LEU	3.4
1	E	315	CYS	3.4
1	E	297	PHE	3.4
1	A	120	VAL	3.4
1	A	198	THR	3.4
1	A	752	ILE	3.4
1	A	725	LYS	3.3
1	C	157	TYR	3.3
1	C	653	PRO	3.3
1	C	199	GLU	3.3
1	A	698	LEU	3.3
1	D	733	VAL	3.2
1	A	719	ILE	3.2
1	C	155	ARG	3.2
1	E	109	ALA	3.2
1	B	202	TYR	3.1
1	C	105	THR	3.1
1	D	737	GLY	3.1
1	C	757	GLY	3.0
1	F	294	VAL	3.0
1	E	152	LYS	3.0
1	C	385	TRP	3.0
1	E	724	ALA	3.0
1	F	305	HIS	3.0
1	F	699	PHE	3.0
1	E	327	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	193	ASP	2.9
1	C	762	GLY	2.9
1	E	342	ARG	2.9
1	C	54	TRP	2.9
1	D	191	ASN	2.9
1	A	372	GLY	2.9
1	C	202	TYR	2.9
1	F	285	PHE	2.9
1	A	765	LEU	2.9
1	B	551	LYS	2.8
1	E	456	VAL	2.8
1	E	428	ARG	2.8
1	E	416	MET	2.8
1	B	552	SER	2.8
1	E	488	GLY	2.8
1	C	727	GLN	2.8
1	E	698	LEU	2.8
1	E	735	GLY	2.8
1	F	317	TRP	2.8
1	E	31	TYR	2.8
1	B	557	TRP	2.7
1	B	765	LEU	2.7
1	F	731	ILE	2.7
1	C	153	THR	2.7
1	E	148	VAL	2.7
1	B	560	ASP	2.7
1	E	740	ARG	2.7
1	A	196	THR	2.7
1	E	745	CYS	2.7
1	B	386	ASP	2.7
1	A	708	VAL	2.7
1	D	702	GLY	2.7
1	C	285	PHE	2.7
1	D	202	TYR	2.7
1	B	125	PHE	2.7
1	D	427	GLU	2.6
1	A	723	LYS	2.6
1	A	290	ASP	2.6
1	A	53	ALA	2.6
1	D	720	PHE	2.6
1	A	385	TRP	2.6
1	E	196	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	388	TRP	2.6
1	D	774	ASN	2.6
1	A	150	ASP	2.6
1	C	125	PHE	2.6
1	C	651	GLU	2.6
1	B	54	TRP	2.6
1	F	289	TYR	2.6
1	F	704	GLY	2.6
1	C	711	VAL	2.6
1	C	755	VAL	2.6
1	A	427	GLU	2.6
1	C	773	GLY	2.6
1	F	749	ILE	2.5
1	C	751	GLN	2.5
1	B	149	GLN	2.5
1	C	427	GLU	2.5
1	E	104	ASN	2.5
1	E	460	LEU	2.5
1	F	746	LEU	2.5
1	A	77	MET	2.5
1	A	151	SER	2.5
1	B	193	ASP	2.5
1	F	193	ASP	2.5
1	D	704	GLY	2.5
1	E	41	VAL	2.5
1	A	556	PRO	2.5
1	A	642	ARG	2.5
1	B	85	ASP	2.5
1	F	50	ARG	2.5
1	C	61	PHE	2.5
1	C	47	ARG	2.5
1	C	56	LEU	2.4
1	A	776	LEU	2.4
1	F	22	LEU	2.4
1	A	780	LEU	2.4
1	D	677	LEU	2.4
1	B	25	ILE	2.4
1	C	55	GLN	2.4
1	E	61	PHE	2.4
1	E	586	ALA	2.4
1	E	555	VAL	2.4
1	F	428	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	547	LEU	2.4
1	C	194	GLY	2.4
1	E	732	THR	2.4
1	F	284	SER	2.4
1	F	125	PHE	2.4
1	C	79	HIS	2.3
1	C	733	VAL	2.3
1	E	699	PHE	2.3
1	A	202	TYR	2.3
1	C	750	PRO	2.3
1	A	734	SER	2.3
1	D	60	LEU	2.3
1	D	189	THR	2.3
1	E	415	ALA	2.3
1	C	50	ARG	2.3
1	F	556	PRO	2.3
1	A	646	LEU	2.3
1	D	292	ALA	2.3
1	A	200	GLN	2.3
1	E	120	VAL	2.3
1	E	696	PHE	2.3
1	D	492	TYR	2.3
1	E	751	GLN	2.3
1	E	190	TRP	2.3
1	E	744	LEU	2.3
1	B	772	GLN	2.3
1	C	108	PHE	2.3
1	B	677	LEU	2.3
1	E	44	ALA	2.3
1	D	199	GLU	2.3
1	F	555	VAL	2.3
1	A	774	ASN	2.3
1	C	191	ASN	2.3
1	C	779	SER	2.3
1	E	502	LEU	2.2
1	D	25	ILE	2.2
1	A	699	PHE	2.2
1	C	326	PHE	2.2
1	C	432	ASP	2.2
1	B	181	VAL	2.2
1	C	778	ILE	2.2
1	E	352	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	746	LEU	2.2
1	F	190	TRP	2.2
1	D	724	ALA	2.2
1	E	108	PHE	2.2
1	A	191	ASN	2.2
1	E	288	ASN	2.2
1	E	57	ASP	2.2
1	E	499	ALA	2.2
1	A	694	THR	2.2
1	C	99	HIS	2.2
1	E	84	LEU	2.2
1	C	749	ILE	2.1
1	F	70	GLU	2.1
1	E	198	THR	2.1
1	F	767	VAL	2.1
1	E	490	ASP	2.1
1	C	761	ALA	2.1
1	F	487	TRP	2.1
1	A	297	PHE	2.1
1	E	55	GLN	2.1
1	C	289	TYR	2.1
1	D	382	LEU	2.1
1	C	59	PRO	2.1
1	F	97	ASP	2.1
1	C	152	LYS	2.1
1	C	775	ALA	2.1
1	C	151	SER	2.1
1	D	125	PHE	2.1
1	B	391	GLY	2.1
1	D	740	ARG	2.1
1	A	80	PHE	2.1
1	B	241	GLU	2.1
1	A	333	PHE	2.1
1	F	108	PHE	2.1
1	F	488	GLY	2.1
1	C	49	VAL	2.1
1	E	734	SER	2.1
1	E	97	ASP	2.1
1	C	38	ASN	2.1
1	A	82	GLY	2.1
1	A	505	GLY	2.1
1	D	385	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	299	ASP	2.1
1	C	120	VAL	2.0
1	E	118	VAL	2.0
1	C	150	ASP	2.0
1	B	708	VAL	2.0
1	B	524	GLU	2.0
1	B	288	ASN	2.0
1	C	442	GLN	2.0
1	D	190	TRP	2.0
1	E	780	LEU	2.0
1	A	738	GLU	2.0
1	B	53	ALA	2.0
1	F	734	SER	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.