Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 05:38 PM JST

PDB ID	:	4X0V
Title	:	Structure of a GH5 family lichenase from Caldicellulosiruptor sp. F32
Authors	:	Meng, D.; Liu, X.; Wang, X.; Li, F.; Feng, Y.
Deposited on	:	2014-11-24
Resolution	:	2.80 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:

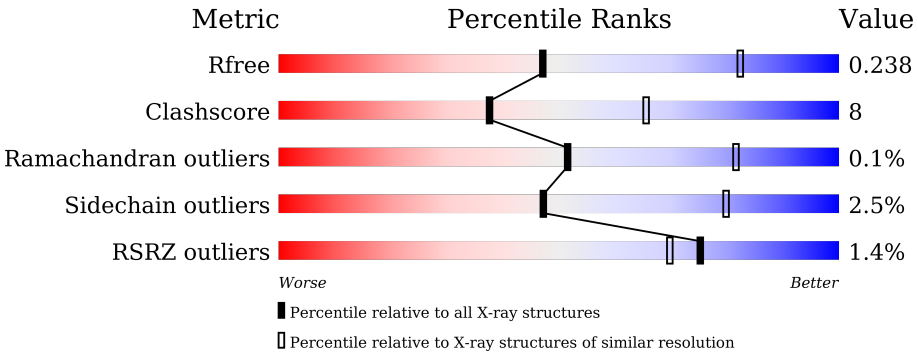
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	396	79% 15% • 5%
1	B	396	78% 16% • 5%
1	C	396	76% 18% • 5%
1	D	396	73% 21% • 5%
1	E	396	3% 74% 19% • 6%
1	F	396	3% 74% 19% • 6%

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Mol	Chain	Length	Quality of chain
1	G	396	2% 76% 17% • 6%
1	H	396	% 76% 18% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24709 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 Beta-1,3-1,4-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			3067	1965	533	555	14			
1	B	375	Total	C	N	O	S	0	0	0
			3067	1965	533	555	14			
1	C	376	Total	C	N	O	S	0	0	0
			3075	1969	535	557	14			
1	D	375	Total	C	N	O	S	0	0	0
			3067	1965	533	555	14			
1	E	373	Total	C	N	O	S	0	0	0
			3044	1953	525	552	14			
1	F	374	Total	C	N	O	S	0	0	0
			3056	1959	529	554	14			
1	G	374	Total	C	N	O	S	0	0	0
			3056	1959	529	554	14			
1	H	373	Total	C	N	O	S	0	0	0
			3044	1953	525	552	14			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP R9RX81
A	2	ARG	-	expression tag	UNP R9RX81
A	3	GLY	-	expression tag	UNP R9RX81
A	4	SER	-	expression tag	UNP R9RX81
A	5	HIS	-	expression tag	UNP R9RX81
A	6	HIS	-	expression tag	UNP R9RX81
A	7	HIS	-	expression tag	UNP R9RX81
A	8	HIS	-	expression tag	UNP R9RX81
A	9	HIS	-	expression tag	UNP R9RX81
A	10	HIS	-	expression tag	UNP R9RX81
A	11	GLY	-	expression tag	UNP R9RX81
A	12	MET	-	expression tag	UNP R9RX81
A	13	ALA	-	expression tag	UNP R9RX81

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SER	-	expression tag	UNP R9RX81
A	15	LEU	-	expression tag	UNP R9RX81
A	16	ASN	-	expression tag	UNP R9RX81
A	17	ARG	-	expression tag	UNP R9RX81
A	18	GLU	-	expression tag	UNP R9RX81
B	1	MET	-	expression tag	UNP R9RX81
B	2	ARG	-	expression tag	UNP R9RX81
B	3	GLY	-	expression tag	UNP R9RX81
B	4	SER	-	expression tag	UNP R9RX81
B	5	HIS	-	expression tag	UNP R9RX81
B	6	HIS	-	expression tag	UNP R9RX81
B	7	HIS	-	expression tag	UNP R9RX81
B	8	HIS	-	expression tag	UNP R9RX81
B	9	HIS	-	expression tag	UNP R9RX81
B	10	HIS	-	expression tag	UNP R9RX81
B	11	GLY	-	expression tag	UNP R9RX81
B	12	MET	-	expression tag	UNP R9RX81
B	13	ALA	-	expression tag	UNP R9RX81
B	14	SER	-	expression tag	UNP R9RX81
B	15	LEU	-	expression tag	UNP R9RX81
B	16	ASN	-	expression tag	UNP R9RX81
B	17	ARG	-	expression tag	UNP R9RX81
B	18	GLU	-	expression tag	UNP R9RX81
C	1	MET	-	expression tag	UNP R9RX81
C	2	ARG	-	expression tag	UNP R9RX81
C	3	GLY	-	expression tag	UNP R9RX81
C	4	SER	-	expression tag	UNP R9RX81
C	5	HIS	-	expression tag	UNP R9RX81
C	6	HIS	-	expression tag	UNP R9RX81
C	7	HIS	-	expression tag	UNP R9RX81
C	8	HIS	-	expression tag	UNP R9RX81
C	9	HIS	-	expression tag	UNP R9RX81
C	10	HIS	-	expression tag	UNP R9RX81
C	11	GLY	-	expression tag	UNP R9RX81
C	12	MET	-	expression tag	UNP R9RX81
C	13	ALA	-	expression tag	UNP R9RX81
C	14	SER	-	expression tag	UNP R9RX81
C	15	LEU	-	expression tag	UNP R9RX81
C	16	ASN	-	expression tag	UNP R9RX81
C	17	ARG	-	expression tag	UNP R9RX81
C	18	GLU	-	expression tag	UNP R9RX81
D	1	MET	-	expression tag	UNP R9RX81

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ARG	-	expression tag	UNP R9RX81
D	3	GLY	-	expression tag	UNP R9RX81
D	4	SER	-	expression tag	UNP R9RX81
D	5	HIS	-	expression tag	UNP R9RX81
D	6	HIS	-	expression tag	UNP R9RX81
D	7	HIS	-	expression tag	UNP R9RX81
D	8	HIS	-	expression tag	UNP R9RX81
D	9	HIS	-	expression tag	UNP R9RX81
D	10	HIS	-	expression tag	UNP R9RX81
D	11	GLY	-	expression tag	UNP R9RX81
D	12	MET	-	expression tag	UNP R9RX81
D	13	ALA	-	expression tag	UNP R9RX81
D	14	SER	-	expression tag	UNP R9RX81
D	15	LEU	-	expression tag	UNP R9RX81
D	16	ASN	-	expression tag	UNP R9RX81
D	17	ARG	-	expression tag	UNP R9RX81
D	18	GLU	-	expression tag	UNP R9RX81
E	1	MET	-	expression tag	UNP R9RX81
E	2	ARG	-	expression tag	UNP R9RX81
E	3	GLY	-	expression tag	UNP R9RX81
E	4	SER	-	expression tag	UNP R9RX81
E	5	HIS	-	expression tag	UNP R9RX81
E	6	HIS	-	expression tag	UNP R9RX81
E	7	HIS	-	expression tag	UNP R9RX81
E	8	HIS	-	expression tag	UNP R9RX81
E	9	HIS	-	expression tag	UNP R9RX81
E	10	HIS	-	expression tag	UNP R9RX81
E	11	GLY	-	expression tag	UNP R9RX81
E	12	MET	-	expression tag	UNP R9RX81
E	13	ALA	-	expression tag	UNP R9RX81
E	14	SER	-	expression tag	UNP R9RX81
E	15	LEU	-	expression tag	UNP R9RX81
E	16	ASN	-	expression tag	UNP R9RX81
E	17	ARG	-	expression tag	UNP R9RX81
E	18	GLU	-	expression tag	UNP R9RX81
F	1	MET	-	expression tag	UNP R9RX81
F	2	ARG	-	expression tag	UNP R9RX81
F	3	GLY	-	expression tag	UNP R9RX81
F	4	SER	-	expression tag	UNP R9RX81
F	5	HIS	-	expression tag	UNP R9RX81
F	6	HIS	-	expression tag	UNP R9RX81
F	7	HIS	-	expression tag	UNP R9RX81

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Chain	Residue	Modelled	Actual	Comment	Reference
F	8	HIS	-	expression tag	UNP R9RX81
F	9	HIS	-	expression tag	UNP R9RX81
F	10	HIS	-	expression tag	UNP R9RX81
F	11	GLY	-	expression tag	UNP R9RX81
F	12	MET	-	expression tag	UNP R9RX81
F	13	ALA	-	expression tag	UNP R9RX81
F	14	SER	-	expression tag	UNP R9RX81
F	15	LEU	-	expression tag	UNP R9RX81
F	16	ASN	-	expression tag	UNP R9RX81
F	17	ARG	-	expression tag	UNP R9RX81
F	18	GLU	-	expression tag	UNP R9RX81
G	1	MET	-	expression tag	UNP R9RX81
G	2	ARG	-	expression tag	UNP R9RX81
G	3	GLY	-	expression tag	UNP R9RX81
G	4	SER	-	expression tag	UNP R9RX81
G	5	HIS	-	expression tag	UNP R9RX81
G	6	HIS	-	expression tag	UNP R9RX81
G	7	HIS	-	expression tag	UNP R9RX81
G	8	HIS	-	expression tag	UNP R9RX81
G	9	HIS	-	expression tag	UNP R9RX81
G	10	HIS	-	expression tag	UNP R9RX81
G	11	GLY	-	expression tag	UNP R9RX81
G	12	MET	-	expression tag	UNP R9RX81
G	13	ALA	-	expression tag	UNP R9RX81
G	14	SER	-	expression tag	UNP R9RX81
G	15	LEU	-	expression tag	UNP R9RX81
G	16	ASN	-	expression tag	UNP R9RX81
G	17	ARG	-	expression tag	UNP R9RX81
G	18	GLU	-	expression tag	UNP R9RX81
H	1	MET	-	expression tag	UNP R9RX81
H	2	ARG	-	expression tag	UNP R9RX81
H	3	GLY	-	expression tag	UNP R9RX81
H	4	SER	-	expression tag	UNP R9RX81
H	5	HIS	-	expression tag	UNP R9RX81
H	6	HIS	-	expression tag	UNP R9RX81
H	7	HIS	-	expression tag	UNP R9RX81
H	8	HIS	-	expression tag	UNP R9RX81
H	9	HIS	-	expression tag	UNP R9RX81
H	10	HIS	-	expression tag	UNP R9RX81
H	11	GLY	-	expression tag	UNP R9RX81
H	12	MET	-	expression tag	UNP R9RX81
H	13	ALA	-	expression tag	UNP R9RX81

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Chain	Residue	Modelled	Actual	Comment	Reference
H	14	SER	-	expression tag	UNP R9RX81
H	15	LEU	-	expression tag	UNP R9RX81
H	16	ASN	-	expression tag	UNP R9RX81
H	17	ARG	-	expression tag	UNP R9RX81
H	18	GLU	-	expression tag	UNP R9RX81

- Molecule 2 is water.

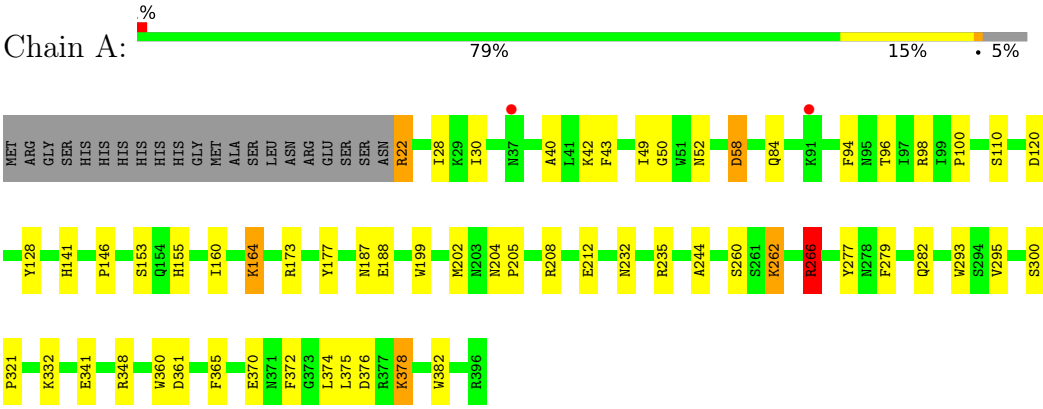
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	36	Total O 36 36	0	0
2	C	37	Total O 37 37	0	0
2	D	45	Total O 45 45	0	0
2	E	17	Total O 17 17	0	0
2	F	30	Total O 30 30	0	0
2	G	14	Total O 14 14	0	0
2	H	25	Total O 25 25	0	0

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.

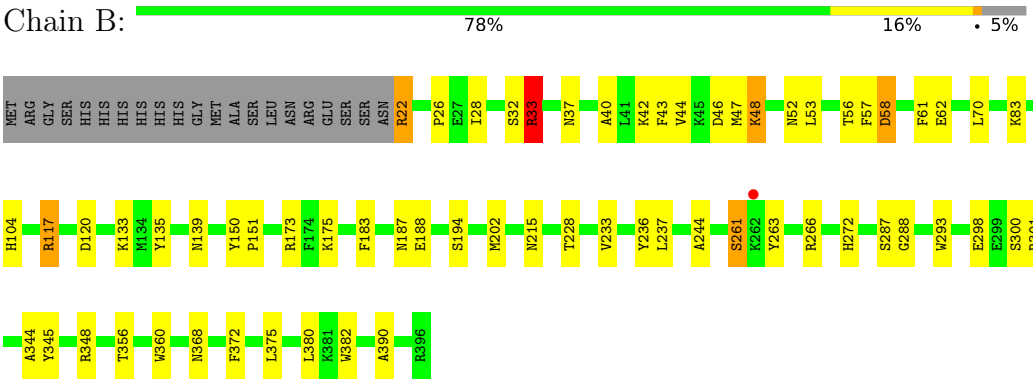
• Molecule 1: Beta-1,3-1,4-glucanase

Chain A:



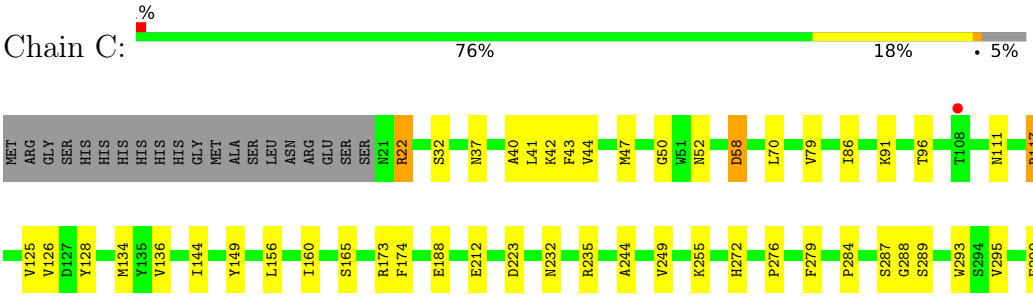
• Molecule 1: Beta-1,3-1,4-glucanase

Chain B:



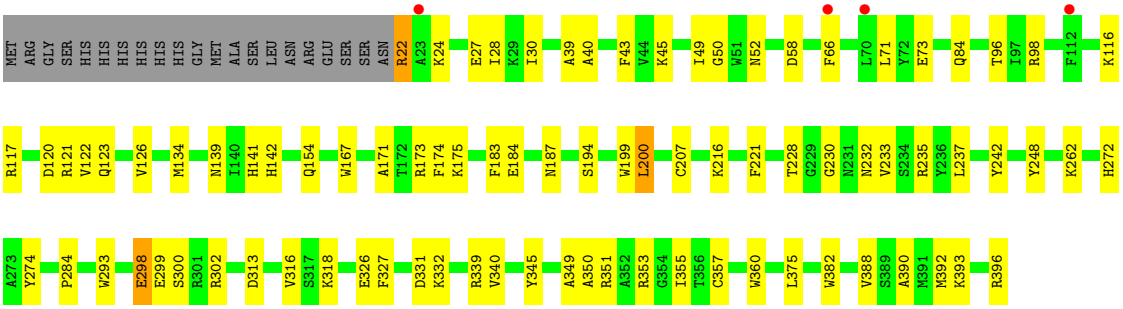
• Molecule 1: Beta-1,3-1,4-glucanase

Chain C:



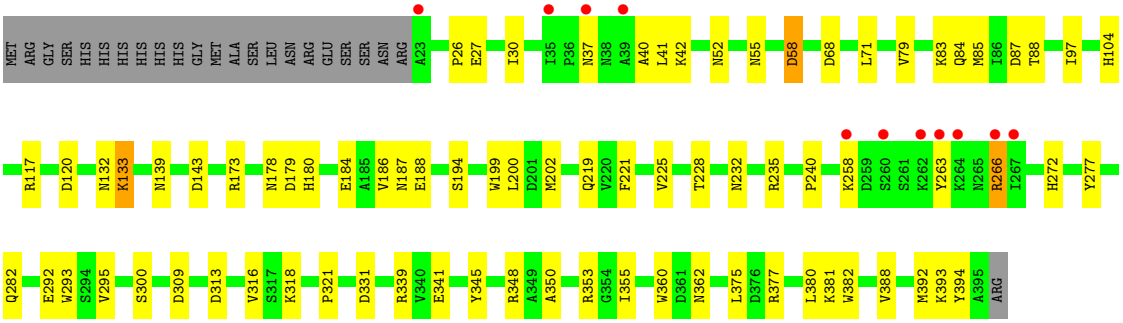
• Molecule 1: Beta-1,3-1,4-glucanase

Chain D:



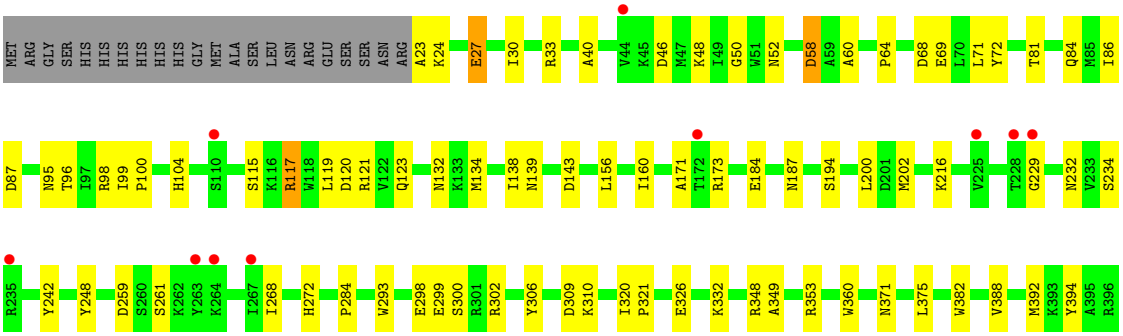
• Molecule 1: Beta-1,3-1,4-glucanase

Chain E:



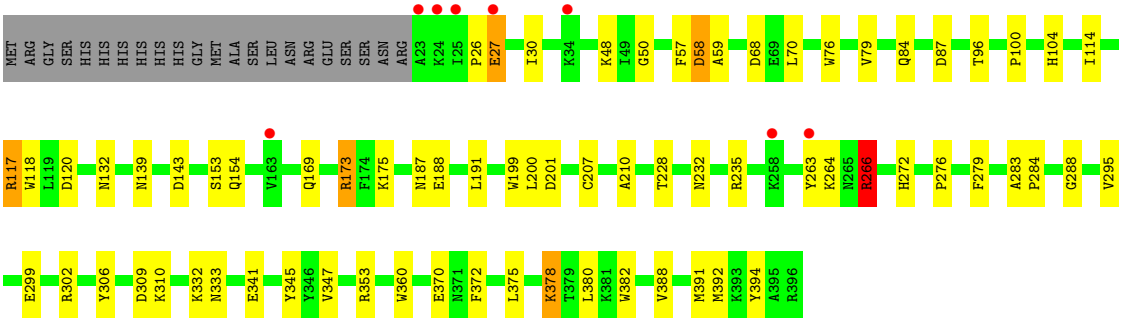
• Molecule 1: Beta-1,3-1,4-glucanase

Chain F:



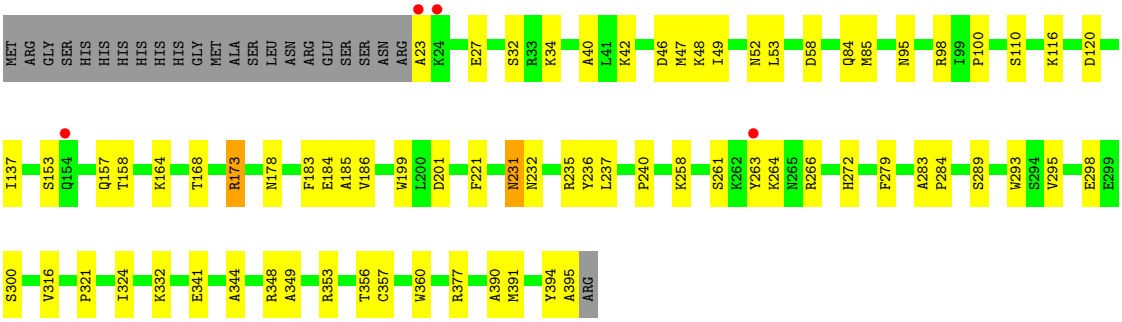
• Molecule 1: Beta-1,3-1,4-glucanase

Chain G:



• Molecule 1: Beta-1,3-1,4-glucanase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.66Å 157.78Å 120.80Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	46.65 – 2.80 46.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.3 (46.65-2.80) 92.0 (46.65-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.183 , 0.238 0.185 , 0.238	Depositor DCC
R_{free} test set	1994 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24709	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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	0.48	0/3149	0.63	1/4266 (0.0%)
1	B	0.48	0/3149	0.63	1/4266 (0.0%)
1	C	0.53	0/3157	0.66	0/4277
1	D	0.50	0/3149	0.63	0/4266
1	E	0.47	0/3126	0.62	0/4238
1	F	0.44	0/3138	0.60	0/4252
1	G	0.46	0/3138	0.61	1/4252 (0.0%)
1	H	0.46	0/3126	0.62	0/4238
All	All	0.48	0/25132	0.63	3/34055 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	G	266	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	266	ARG	NE-CZ-NH1	5.16	122.88	120.30

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	3067	0	3004	44	0
1	B	3067	0	3004	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3075	0	3010	49	0
1	D	3067	0	3004	54	0
1	E	3044	0	2978	46	0
1	F	3056	0	2991	56	0
1	G	3056	0	2991	49	0
1	H	3044	0	2978	46	0
2	A	29	0	0	1	0
2	B	36	0	0	1	0
2	C	37	0	0	4	0
2	D	45	0	0	2	0
2	E	17	0	0	2	0
2	F	30	0	0	10	0
2	G	14	0	0	0	0
2	H	25	0	0	8	0
All	All	24709	0	23960	373	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 8.

All (373) 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:E:309:ASP:OD1	1:E:353:ARG:NH1	2.01	0.92
1:D:39:ALA:O	2:D:439:HOH:O	1.89	0.90
1:E:202:MET:SD	2:E:405:HOH:O	2.29	0.89
1:H:120:ASP:OD1	1:H:173:ARG:NH2	2.07	0.88
1:C:223:ASP:OD2	2:C:414:HOH:O	1.92	0.87
1:H:232:ASN:OD1	1:H:235:ARG:NH1	2.08	0.87
1:H:391:MET:O	2:H:404:HOH:O	1.95	0.85
1:E:120:ASP:OD1	1:E:173:ARG:NH1	2.14	0.80
1:E:179:ASP:OD2	2:E:410:HOH:O	1.99	0.80
1:D:120:ASP:OD1	1:D:173:ARG:NH1	2.14	0.79
1:D:45:LYS:HZ1	1:D:396:ARG:HH11	1.29	0.78
1:G:120:ASP:OD1	1:G:173:ARG:NH2	2.17	0.78
1:F:23:ALA:N	2:F:403:HOH:O	2.17	0.77
1:H:279:PHE:O	1:H:332:LYS:NZ	2.18	0.77
1:H:266:ARG:NH1	2:H:410:HOH:O	2.16	0.77
1:A:232:ASN:OD1	1:A:235:ARG:NH1	2.19	0.75
1:H:298:GLU:OE1	2:H:409:HOH:O	2.05	0.74
1:H:395:ALA:N	2:H:404:HOH:O	2.20	0.74
1:C:120:ASP:OD1	1:C:173:ARG:NH2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:ARG:NH2	1:H:184:GLU:OE2	2.20	0.72
1:F:298:GLU:OE1	2:F:414:HOH:O	2.06	0.72
1:G:263:TYR:HB3	1:G:266:ARG:NH1	2.04	0.72
1:F:248:TYR:O	2:F:418:HOH:O	2.07	0.72
1:G:68:ASP:OD1	1:G:117:ARG:NH1	2.22	0.71
1:C:279:PHE:O	1:C:332:LYS:NZ	2.24	0.71
1:F:40:ALA:HB1	1:F:321:PRO:HG3	1.70	0.71
1:H:344:ALA:HB2	1:H:390:ALA:HB1	1.72	0.71
1:F:187:ASN:O	2:F:424:HOH:O	2.09	0.70
1:B:215:ASN:O	2:B:420:HOH:O	2.10	0.69
1:D:200:LEU:HG	1:D:207:CYS:HB3	1.73	0.69
1:C:212:GLU:OE2	1:C:255:LYS:NZ	2.26	0.68
1:C:47:MET:O	1:C:96:THR:OG1	2.12	0.68
1:B:62:GLU:OE2	1:B:104:HIS:NE2	2.27	0.68
1:D:98:ARG:NH1	1:D:184:GLU:OE1	2.28	0.67
1:E:232:ASN:OD1	1:E:235:ARG:NH1	2.24	0.67
1:E:27:GLU:OE1	1:E:393:LYS:NZ	2.26	0.67
1:D:187:ASN:OD1	1:D:272:HIS:HE1	1.76	0.67
1:A:266:ARG:HG3	1:A:266:ARG:HH11	1.60	0.66
1:F:299:GLU:HG2	1:F:302:ARG:HH22	1.61	0.66
1:E:200:LEU:HD13	1:E:202:MET:HE3	1.78	0.65
1:F:123:GLN:OE1	1:F:173:ARG:NH1	2.28	0.65
1:F:119:LEU:HD21	1:F:173:ARG:HG3	1.78	0.65
1:G:266:ARG:HG3	1:G:266:ARG:HH11	1.60	0.65
1:G:309:ASP:OD1	1:G:353:ARG:NH1	2.30	0.65
1:C:79:VAL:O	2:C:404:HOH:O	2.14	0.64
1:E:375:LEU:HB2	1:E:382:TRP:CZ3	2.33	0.64
1:D:375:LEU:HB2	1:D:382:TRP:CZ3	2.33	0.64
1:F:375:LEU:HB2	1:F:382:TRP:CZ3	2.33	0.64
1:E:40:ALA:HB1	1:E:321:PRO:HG3	1.81	0.63
1:D:139:ASN:ND2	1:D:184:GLU:OE2	2.19	0.63
1:C:348:ARG:HH12	1:C:396:ARG:HH21	1.46	0.62
1:H:52:ASN:HB2	1:H:360:TRP:HA	1.80	0.62
1:A:120:ASP:OD1	1:A:173:ARG:NH1	2.29	0.61
1:G:375:LEU:HB2	1:G:382:TRP:CZ3	2.36	0.61
1:F:120:ASP:OD1	1:F:173:ARG:NH2	2.28	0.61
1:A:40:ALA:HB1	1:A:321:PRO:HG3	1.82	0.60
1:D:199:TRP:N	2:D:433:HOH:O	2.11	0.60
1:B:293:TRP:CE2	1:B:300:SER:HB3	2.36	0.60
1:F:268:ILE:HG23	1:F:321:PRO:HB2	1.81	0.60
1:F:299:GLU:HG2	1:F:302:ARG:NH2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:HIS:O	2:F:422:HOH:O	2.17	0.60
1:F:298:GLU:HG2	1:G:154:GLN:O	2.01	0.60
1:G:232:ASN:OD1	1:G:235:ARG:NH1	2.35	0.60
1:A:302:ARG:HD2	1:F:216:LYS:NZ	2.16	0.60
1:F:171:ALA:O	1:F:232:ASN:ND2	2.28	0.60
1:F:52:ASN:HB2	1:F:360:TRP:HA	1.84	0.59
1:E:68:ASP:HB3	1:E:71:LEU:HD13	1.85	0.59
1:A:293:TRP:CE2	1:A:300:SER:HB3	2.38	0.59
1:D:45:LYS:HZ1	1:D:396:ARG:HD3	1.68	0.58
1:E:221:PHE:O	1:E:225:VAL:HG23	2.03	0.58
1:G:199:TRP:CH2	1:G:201:ASP:HB2	2.38	0.58
1:A:365:PHE:O	2:A:405:HOH:O	2.16	0.58
1:E:186:VAL:O	1:E:240:PRO:HG3	2.02	0.58
1:F:58:ASP:HB3	1:F:100:PRO:HB2	1.85	0.58
1:E:85:MET:HG3	1:E:380:LEU:HD21	1.84	0.58
1:B:233:VAL:O	1:B:261:SER:HB2	2.03	0.58
1:D:116:LYS:NZ	1:D:173:ARG:HH21	2.02	0.57
1:H:183:PHE:HB2	1:H:237:LEU:HD22	1.85	0.57
1:A:30:ILE:HD12	1:A:348:ARG:HG3	1.85	0.57
1:B:139:ASN:ND2	1:B:187:ASN:HB2	2.20	0.57
1:F:87:ASP:OD1	1:F:132:ASN:ND2	2.37	0.57
1:C:293:TRP:HB3	1:C:338:SER:HB3	1.87	0.57
1:D:183:PHE:HB2	1:D:237:LEU:HD22	1.87	0.56
1:E:295:VAL:HG13	1:E:341:GLU:HB3	1.87	0.56
1:E:348:ARG:HD3	1:E:394:TYR:CD1	2.40	0.56
1:G:191:LEU:HD11	1:G:210:ALA:HB2	1.87	0.56
1:C:122:VAL:O	1:C:126:VAL:HG23	2.06	0.56
1:G:284:PRO:HG3	1:G:332:LYS:HG2	1.86	0.56
1:E:313:ASP:O	1:E:318:LYS:NZ	2.39	0.56
1:A:141:HIS:HA	1:A:187:ASN:HB3	1.88	0.55
1:A:84:GLN:OE1	1:A:84:GLN:N	2.37	0.55
1:B:183:PHE:HB2	1:B:237:LEU:HD22	1.88	0.55
1:F:68:ASP:OD1	1:F:117:ARG:NH1	2.27	0.55
1:C:174:PHE:O	1:C:235:ARG:NH2	2.39	0.55
1:G:87:ASP:HA	1:G:132:ASN:HD21	1.71	0.55
1:B:33:ARG:HH11	1:B:33:ARG:CG	2.19	0.55
1:A:28:ILE:HG22	1:A:30:ILE:HG13	1.89	0.55
1:A:370:GLU:HG3	1:C:368:ASN:HD21	1.72	0.55
1:E:26:PRO:HG3	1:E:341:GLU:HG2	1.88	0.55
1:F:156:LEU:O	1:F:160:ILE:HG13	2.07	0.55
1:H:40:ALA:HB1	1:H:321:PRO:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ASN:HA	2:F:423:HOH:O	2.06	0.54
1:B:53:LEU:HG	1:B:56:THR:OG1	2.08	0.54
1:A:279:PHE:O	1:A:332:LYS:NZ	2.33	0.54
1:H:263:TYR:HB3	1:H:266:ARG:HE	1.71	0.54
1:D:175:LYS:HE3	1:D:228:THR:O	2.07	0.54
1:C:188:GLU:HG2	1:C:244:ALA:HB3	1.90	0.54
1:C:348:ARG:NH1	1:C:396:ARG:HH21	2.06	0.54
1:F:132:ASN:HB3	1:F:134:MET:HE2	1.90	0.54
1:D:293:TRP:CE2	1:D:300:SER:HB3	2.42	0.53
1:A:125:VAL:HA	1:A:128:TYR:CD2	2.44	0.53
1:F:293:TRP:CE2	1:F:300:SER:HB3	2.42	0.53
1:G:295:VAL:HG23	1:G:341:GLU:OE1	2.08	0.53
1:G:266:ARG:HH11	1:G:266:ARG:CG	2.20	0.53
1:F:69:GLU:OE2	1:F:115:SER:OG	2.24	0.53
1:G:188:GLU:OE2	1:G:272:HIS:HD2	1.92	0.53
1:G:306:TYR:CZ	1:G:310:LYS:HE2	2.43	0.53
1:F:27:GLU:N	2:F:406:HOH:O	2.35	0.52
1:G:84:GLN:OE1	1:G:84:GLN:N	2.39	0.52
1:H:157:GLN:CD	1:H:157:GLN:H	2.13	0.52
1:B:187:ASN:OD1	1:B:272:HIS:HE1	1.93	0.52
1:D:45:LYS:NZ	1:D:396:ARG:HH11	2.05	0.52
1:G:232:ASN:HA	1:G:235:ARG:HH11	1.75	0.52
1:C:188:GLU:OE2	1:C:272:HIS:HD2	1.92	0.52
1:H:295:VAL:HG23	1:H:341:GLU:OE1	2.09	0.52
1:E:139:ASN:HB3	1:E:184:GLU:HB3	1.91	0.52
1:B:120:ASP:OD1	1:B:173:ARG:NH2	2.43	0.52
1:F:68:ASP:HB3	1:F:71:LEU:HD13	1.90	0.52
1:A:155:HIS:ND1	1:D:298:GLU:HG2	2.25	0.52
1:C:40:ALA:HB1	1:C:321:PRO:HG3	1.93	0.51
1:E:350:ALA:HB1	1:E:355:ILE:HB	1.91	0.51
1:H:23:ALA:N	2:H:407:HOH:O	2.43	0.51
1:H:199:TRP:CH2	1:H:201:ASP:HB2	2.45	0.51
1:A:123:GLN:OE1	1:A:173:ARG:HD3	2.09	0.51
1:B:37:ASN:OD1	1:B:42:LYS:NZ	2.35	0.51
1:D:27:GLU:OE1	1:D:393:LYS:NZ	2.40	0.51
1:C:86:ILE:HG23	1:C:134:MET:HE1	1.92	0.51
1:H:263:TYR:HB3	1:H:266:ARG:NE	2.26	0.51
1:D:123:GLN:OE1	1:D:173:ARG:HD3	2.11	0.51
1:D:299:GLU:HG2	1:D:302:ARG:HH22	1.75	0.51
1:F:27:GLU:HA	1:F:394:TYR:OH	2.11	0.51
1:E:84:GLN:OE1	1:E:84:GLN:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:ASN:HA	1:G:235:ARG:NH1	2.26	0.51
1:C:375:LEU:HB2	1:C:382:TRP:CZ3	2.46	0.50
1:E:83:LYS:NZ	1:E:87:ASP:OD1	2.44	0.50
1:D:45:LYS:NZ	1:D:396:ARG:HD3	2.26	0.50
1:D:299:GLU:HG2	1:D:302:ARG:NH2	2.25	0.50
1:E:228:THR:OG1	1:E:232:ASN:ND2	2.40	0.50
1:H:316:VAL:HG11	1:H:353:ARG:O	2.12	0.50
1:F:259:ASP:C	1:F:261:SER:H	2.15	0.50
1:D:66:PHE:CD2	1:D:71:LEU:HB2	2.47	0.50
1:F:24:LYS:NZ	2:F:428:HOH:O	2.44	0.50
1:A:52:ASN:OD1	1:A:98:ARG:HD3	2.11	0.50
1:B:175:LYS:HE3	1:B:228:THR:O	2.12	0.50
1:D:154:GLN:NE2	1:G:288:GLY:HA2	2.26	0.50
1:H:232:ASN:HA	1:H:235:ARG:NH1	2.27	0.50
1:B:188:GLU:HG2	1:B:244:ALA:HB3	1.94	0.50
1:F:104:HIS:ND1	1:F:143:ASP:OD1	2.35	0.50
1:B:236:TYR:CE1	1:B:266:ARG:HD3	2.47	0.50
1:C:312:TYR:O	1:C:317:SER:HB3	2.12	0.50
1:F:248:TYR:HB3	2:F:418:HOH:O	2.10	0.50
1:B:46:ASP:O	1:B:95:ASN:ND2	2.39	0.49
1:D:313:ASP:O	1:D:318:LYS:NZ	2.45	0.49
1:E:263:TYR:HB3	1:E:266:ARG:NH1	2.27	0.49
1:C:289:SER:OG	1:C:332:LYS:HE2	2.11	0.49
1:F:371:ASN:ND2	2:F:427:HOH:O	2.38	0.49
1:B:83:LYS:NZ	1:B:87:ASP:OD1	2.45	0.49
1:B:368:ASN:HD21	1:G:370:GLU:HG3	1.76	0.49
1:C:223:ASP:OD1	2:C:401:HOH:O	2.19	0.49
1:H:356:THR:HA	2:H:403:HOH:O	2.11	0.49
1:D:388:VAL:O	1:D:392:MET:HG2	2.11	0.49
1:F:139:ASN:ND2	1:F:187:ASN:HB2	2.28	0.49
1:B:298:GLU:HA	1:B:301:ARG:HH21	1.76	0.49
1:D:28:ILE:HG22	1:D:30:ILE:HG13	1.94	0.49
1:B:301:ARG:NH2	1:H:157:GLN:HE21	2.11	0.49
1:B:40:ALA:HB1	1:B:321:PRO:HG3	1.94	0.48
1:B:52:ASN:HB2	1:B:360:TRP:HA	1.95	0.48
1:D:171:ALA:O	1:D:232:ASN:ND2	2.37	0.48
1:B:301:ARG:HG2	1:B:345:TYR:CZ	2.48	0.48
1:D:351:ARG:HG2	1:D:396:ARG:HB3	1.95	0.48
1:F:284:PRO:HG3	1:F:332:LYS:HG2	1.94	0.48
1:G:79:VAL:HG21	1:G:378:LYS:HG2	1.94	0.48
1:C:156:LEU:O	1:C:160:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:ILE:HD11	1:G:345:TYR:CE2	2.48	0.48
1:D:73:GLU:OE2	1:D:121:ARG:NH2	2.41	0.48
1:H:293:TRP:CE2	1:H:300:SER:HB3	2.48	0.48
1:C:91:LYS:HB2	1:C:91:LYS:HE3	1.61	0.48
1:E:232:ASN:HA	1:E:235:ARG:NH1	2.28	0.48
1:B:70:LEU:HD22	1:B:117:ARG:NH2	2.28	0.47
1:D:122:VAL:O	1:D:126:VAL:HG23	2.14	0.47
1:G:87:ASP:HA	1:G:132:ASN:ND2	2.29	0.47
1:H:58:ASP:HB3	1:H:100:PRO:HB2	1.94	0.47
1:C:344:ALA:HB2	1:C:390:ALA:HB1	1.97	0.47
1:G:235:ARG:HH11	1:G:235:ARG:HB2	1.80	0.47
1:D:284:PRO:HG3	1:D:332:LYS:HG2	1.96	0.47
1:H:46:ASP:O	1:H:95:ASN:ND2	2.41	0.47
1:B:360:TRP:O	1:B:372:PHE:HB3	2.15	0.47
1:E:293:TRP:CE2	1:E:300:SER:HB3	2.50	0.47
1:E:316:VAL:HG11	1:E:353:ARG:O	2.14	0.47
1:H:348:ARG:HD3	1:H:394:TYR:HD2	1.79	0.47
1:A:262:LYS:O	1:A:262:LYS:HG2	2.14	0.47
1:B:32:SER:HB2	1:B:348:ARG:HH22	1.79	0.47
1:E:381:LYS:HD3	1:E:381:LYS:HA	1.64	0.47
1:D:174:PHE:O	1:D:235:ARG:NH2	2.48	0.47
1:D:316:VAL:HG11	1:D:353:ARG:O	2.15	0.47
1:B:22:ARG:HA	1:B:22:ARG:HD3	1.54	0.47
1:E:84:GLN:O	1:E:88:THR:OG1	2.22	0.47
1:B:26:PRO:HG2	1:B:28:ILE:HD11	1.96	0.46
1:E:178:ASN:OD1	1:E:180:HIS:HB2	2.15	0.46
1:F:46:ASP:O	1:F:95:ASN:ND2	2.48	0.46
1:G:59:ALA:HA	1:G:76:TRP:CZ3	2.50	0.46
1:G:299:GLU:HA	1:G:299:GLU:OE1	2.15	0.46
1:F:242:TYR:HB3	1:F:248:TYR:CD2	2.51	0.46
1:A:52:ASN:HB2	1:A:360:TRP:HA	1.96	0.46
1:B:344:ALA:HB2	1:B:390:ALA:HB1	1.97	0.46
1:B:287:SER:HA	1:B:288:GLY:HA2	1.54	0.46
1:C:144:ILE:HA	1:C:149:TYR:O	2.16	0.46
1:B:202:MET:HB2	1:E:199:TRP:CE3	2.51	0.46
1:G:276:PRO:HG2	1:G:279:PHE:HB3	1.97	0.46
1:H:236:TYR:OH	2:H:410:HOH:O	2.20	0.46
1:B:43:PHE:CE1	1:B:135:TYR:HE1	2.33	0.46
1:G:347:VAL:HG21	1:G:391:MET:HG2	1.98	0.46
1:A:50:GLY:HA2	1:A:96:THR:HB	1.98	0.46
1:D:242:TYR:HB3	1:D:248:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:TRP:O	1:G:372:PHE:HB3	2.16	0.46
1:H:289:SER:OG	1:H:332:LYS:HE2	2.16	0.46
1:F:60:ALA:HB1	1:F:104:HIS:CE1	2.51	0.45
1:H:84:GLN:N	1:H:84:GLN:OE1	2.48	0.45
1:A:302:ARG:HD2	1:F:216:LYS:HZ3	1.82	0.45
1:F:30:ILE:HD12	1:F:348:ARG:HG3	1.98	0.45
1:F:306:TYR:OH	1:F:310:LYS:HE2	2.17	0.45
1:C:388:VAL:O	1:C:392:MET:HG2	2.15	0.45
1:A:361:ASP:OD2	1:A:374:LEU:HB2	2.17	0.45
1:C:272:HIS:CG	1:C:326:GLU:HB2	2.52	0.45
1:A:360:TRP:O	1:A:372:PHE:HB3	2.17	0.45
1:B:33:ARG:HH11	1:B:33:ARG:HG2	1.82	0.45
1:B:58:ASP:OD1	1:B:58:ASP:N	2.45	0.45
1:C:331:ASP:HB2	1:C:339:ARG:NH1	2.32	0.45
1:D:30:ILE:HD11	1:D:345:TYR:CE1	2.51	0.45
1:F:64:PRO:HG3	1:F:72:TYR:OH	2.17	0.45
1:H:349:ALA:O	1:H:353:ARG:NH1	2.50	0.45
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.27	0.45
1:C:22:ARG:HA	1:C:22:ARG:HD3	1.49	0.45
1:C:360:TRP:O	1:C:372:PHE:HB3	2.17	0.45
1:D:40:ALA:O	1:D:43:PHE:HB3	2.16	0.45
1:C:287:SER:HA	1:C:288:GLY:HA2	1.66	0.45
1:C:44:VAL:O	1:C:47:MET:HB2	2.17	0.44
1:G:27:GLU:HA	1:G:394:TYR:OH	2.17	0.44
1:D:22:ARG:HA	1:D:22:ARG:HD3	1.54	0.44
1:A:177:TYR:O	1:A:235:ARG:NH2	2.51	0.44
1:A:302:ARG:HD2	1:F:216:LYS:HZ1	1.82	0.44
1:F:81:THR:O	1:F:121:ARG:NH2	2.48	0.44
1:C:58:ASP:OD1	1:C:58:ASP:N	2.41	0.44
1:G:235:ARG:NH1	1:G:235:ARG:HB2	2.31	0.44
1:C:382:TRP:O	1:C:385:PRO:HD3	2.17	0.44
1:H:32:SER:HG	1:H:348:ARG:HH22	1.62	0.44
1:D:50:GLY:HA2	1:D:96:THR:HB	2.00	0.44
1:D:216:LYS:HE3	1:G:302:ARG:HD2	1.99	0.44
1:D:84:GLN:OE1	1:D:84:GLN:N	2.45	0.44
1:D:331:ASP:HB2	1:D:339:ARG:NH1	2.33	0.44
1:E:52:ASN:HB2	1:E:360:TRP:HA	2.00	0.44
1:E:55:ASN:ND2	1:E:362:ASN:HB2	2.33	0.44
1:C:52:ASN:HB2	1:C:360:TRP:HA	1.99	0.44
1:C:295:VAL:HG12	1:C:341:GLU:OE1	2.18	0.44
1:A:58:ASP:OD1	1:A:58:ASP:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:TYR:OH	1:D:326:GLU:OE1	2.27	0.43
1:H:186:VAL:O	1:H:240:PRO:HG3	2.18	0.43
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.76	0.43
1:D:167:TRP:CD1	1:D:221:PHE:HD1	2.36	0.43
1:E:133:LYS:HB3	1:E:133:LYS:HE3	1.47	0.43
1:H:53:LEU:HD12	1:H:377:ARG:NH2	2.33	0.43
1:C:70:LEU:HD11	1:C:117:ARG:HD2	2.01	0.43
1:D:52:ASN:HB2	1:D:360:TRP:HA	2.00	0.43
1:E:331:ASP:HB2	1:E:339:ARG:NH1	2.33	0.43
1:F:349:ALA:O	1:F:353:ARG:NH1	2.50	0.43
1:E:188:GLU:OE2	1:E:272:HIS:HD2	2.01	0.43
1:G:388:VAL:O	1:G:392:MET:HG2	2.18	0.43
1:H:157:GLN:HG2	1:H:158:THR:N	2.33	0.43
1:F:139:ASN:HB3	1:F:184:GLU:HB3	2.01	0.43
1:H:85:MET:HE1	1:H:377:ARG:HB3	2.01	0.43
1:H:185:ALA:HB2	1:H:221:PHE:CD2	2.53	0.43
1:C:126:VAL:HG13	1:C:136:VAL:HG11	1.99	0.43
1:C:40:ALA:O	1:C:43:PHE:HB3	2.19	0.43
1:G:26:PRO:HG3	1:G:341:GLU:HG2	2.00	0.43
1:G:114:ILE:HG13	1:G:169:GLN:OE1	2.17	0.43
1:G:139:ASN:ND2	1:G:187:ASN:HB2	2.34	0.43
1:G:175:LYS:HE3	1:G:228:THR:O	2.19	0.43
1:H:178:ASN:ND2	2:H:421:HOH:O	2.47	0.43
1:A:58:ASP:HB3	1:A:100:PRO:HB2	2.01	0.43
1:A:49:ILE:HG23	1:A:94:PHE:HA	2.01	0.43
1:F:50:GLY:HA2	1:F:96:THR:O	2.19	0.43
1:G:58:ASP:HB3	1:G:100:PRO:HB2	2.01	0.43
1:H:231:ASN:OD1	1:H:231:ASN:N	2.52	0.43
1:A:40:ALA:O	1:A:43:PHE:HB3	2.19	0.42
1:C:293:TRP:CH2	1:C:304:ILE:HD12	2.54	0.42
1:E:139:ASN:ND2	1:E:187:ASN:HB2	2.34	0.42
1:A:199:TRP:CE3	1:F:202:MET:HB2	2.53	0.42
1:B:375:LEU:HB2	1:B:382:TRP:CZ3	2.55	0.42
1:C:125:VAL:HA	1:C:128:TYR:CD2	2.54	0.42
1:F:320:ILE:HA	1:F:321:PRO:HD3	1.83	0.42
1:A:375:LEU:HB2	1:A:382:TRP:CZ3	2.54	0.42
1:E:30:ILE:HD11	1:E:345:TYR:CE1	2.54	0.42
1:C:293:TRP:CD1	1:C:293:TRP:C	2.93	0.42
1:E:87:ASP:OD1	1:E:132:ASN:ND2	2.45	0.42
1:A:376:ASP:OD1	1:A:378:LYS:HG3	2.19	0.42
1:B:48:LYS:O	1:B:356:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:HIS:CG	1:B:326:GLU:HB2	2.55	0.42
1:F:99:ILE:HB	1:F:138:ILE:HG22	2.02	0.42
1:G:50:GLY:HA2	1:G:96:THR:O	2.19	0.42
1:G:283:ALA:HA	1:G:284:PRO:HD3	1.92	0.42
1:F:98:ARG:NH1	1:F:184:GLU:OE1	2.52	0.42
1:B:261:SER:OG	1:B:263:TYR:O	2.37	0.42
1:C:50:GLY:HA2	1:C:96:THR:O	2.19	0.42
1:C:348:ARG:HH12	1:C:396:ARG:NH2	2.14	0.42
1:D:24:LYS:HD3	1:D:24:LYS:HA	1.83	0.42
1:D:134:MET:HB2	1:D:134:MET:HE3	1.83	0.42
1:E:104:HIS:ND1	1:E:143:ASP:OD1	2.42	0.42
1:A:22:ARG:HA	1:A:22:ARG:HD3	1.53	0.42
1:A:146:PRO:HB3	1:A:155:HIS:CE1	2.55	0.42
1:B:56:THR:HB	1:B:57:PHE:H	1.68	0.42
1:D:139:ASN:HB3	1:D:184:GLU:HB3	2.01	0.42
1:F:200:LEU:HB2	1:F:248:TYR:CZ	2.54	0.42
1:C:111:ASN:O	1:C:165:SER:OG	2.18	0.41
1:E:58:ASP:OD1	1:E:58:ASP:N	2.49	0.41
1:E:388:VAL:O	1:E:392:MET:HG2	2.20	0.41
1:G:70:LEU:HG	1:G:117:ARG:NH1	2.34	0.41
1:D:349:ALA:O	1:D:353:ARG:NH1	2.52	0.41
1:A:160:ILE:O	1:A:164:LYS:HB2	2.21	0.41
1:E:37:ASN:OD1	1:E:42:LYS:HD2	2.21	0.41
1:A:202:MET:HE3	1:A:208:ARG:HG2	2.02	0.41
1:E:79:VAL:HG11	1:E:377:ARG:HB2	2.02	0.41
1:H:98:ARG:HG3	1:H:137:ILE:HB	2.02	0.41
1:D:141:HIS:HB3	1:D:142:HIS:H	1.69	0.41
1:D:340:VAL:HG13	1:D:390:ALA:HB2	2.02	0.41
1:A:188:GLU:HG2	1:A:244:ALA:HB3	2.02	0.41
1:B:61:PHE:CZ	1:G:333:ASN:HB3	2.56	0.41
1:F:272:HIS:CG	1:F:326:GLU:HB2	2.55	0.41
1:H:258:LYS:HD2	1:H:258:LYS:HA	1.59	0.41
1:F:388:VAL:O	1:F:392:MET:HG2	2.21	0.41
1:A:277:TYR:CE2	1:A:282:GLN:HB2	2.56	0.41
1:F:33:ARG:NH2	1:F:309:ASP:OD1	2.53	0.41
1:G:57:PHE:HD1	1:G:118:TRP:CH2	2.39	0.41
1:G:200:LEU:HD22	1:G:207:CYS:HB3	2.03	0.41
1:H:47:MET:O	1:H:49:ILE:N	2.54	0.41
1:A:204:ASN:HA	1:A:205:PRO:HD3	1.92	0.41
1:A:295:VAL:HG13	1:A:341:GLU:HB3	2.03	0.41
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:PRO:HB3	2:C:403:HOH:O	2.21	0.41
1:C:284:PRO:HG3	1:C:332:LYS:HG2	2.02	0.41
1:C:293:TRP:CZ3	1:C:300:SER:O	2.74	0.41
1:D:116:LYS:HG3	1:D:173:ARG:NH2	2.36	0.41
1:E:277:TYR:CE2	1:E:282:GLN:HB2	2.56	0.41
1:F:229:GLY:O	1:F:232:ASN:HB2	2.21	0.41
1:H:42:LYS:HA	1:H:42:LYS:HD2	1.79	0.41
1:C:232:ASN:OD1	1:C:235:ARG:NE	2.47	0.41
1:E:219:GLN:OE1	1:E:258:LYS:HG3	2.21	0.41
1:G:264:LYS:HE2	1:G:264:LYS:HB3	1.90	0.41
1:H:283:ALA:HA	1:H:284:PRO:HD3	1.95	0.41
1:H:293:TRP:NE1	1:H:300:SER:HB3	2.35	0.41
1:H:324:ILE:HD12	1:H:357:CYS:SG	2.61	0.41
1:B:44:VAL:O	1:B:47:MET:HB2	2.21	0.40
1:B:150:TYR:HA	1:B:151:PRO:HD3	1.86	0.40
1:D:230:GLY:O	1:D:233:VAL:HG22	2.21	0.40
1:A:293:TRP:HZ3	1:A:295:VAL:HG12	1.86	0.40
1:A:320:ILE:HA	1:A:321:PRO:HD3	1.95	0.40
1:E:41:LEU:HA	1:E:41:LEU:HD23	1.87	0.40
1:G:104:HIS:ND1	1:G:143:ASP:OD1	2.39	0.40
1:G:378:LYS:HB3	1:G:378:LYS:HE2	1.82	0.40
1:A:125:VAL:O	1:A:128:TYR:HB2	2.21	0.40
1:D:350:ALA:HB1	1:D:355:ILE:HB	2.04	0.40
1:D:49:ILE:HD12	1:D:357:CYS:O	2.22	0.40
1:G:380:LEU:HD23	1:G:380:LEU:HA	1.89	0.40
1:H:164:LYS:O	1:H:168:THR:OG1	2.32	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	373/396 (94%)	362 (97%)	11 (3%)	0	100	100
1	B	373/396 (94%)	359 (96%)	13 (4%)	1 (0%)	41	72
1	C	374/396 (94%)	358 (96%)	16 (4%)	0	100	100
1	D	373/396 (94%)	359 (96%)	14 (4%)	0	100	100
1	E	371/396 (94%)	361 (97%)	10 (3%)	0	100	100
1	F	372/396 (94%)	356 (96%)	15 (4%)	1 (0%)	41	72
1	G	372/396 (94%)	359 (96%)	12 (3%)	1 (0%)	41	72
1	H	371/396 (94%)	355 (96%)	15 (4%)	1 (0%)	41	72
All	All	2979/3168 (94%)	2869 (96%)	106 (4%)	4 (0%)	51	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	48	LYS
1	B	48	LYS
1	F	48	LYS
1	G	48	LYS

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	328/346 (95%)	317 (97%)	11 (3%)	37	71
1	B	328/346 (95%)	321 (98%)	7 (2%)	53	84
1	C	329/346 (95%)	320 (97%)	9 (3%)	44	78
1	D	328/346 (95%)	320 (98%)	8 (2%)	49	81
1	E	326/346 (94%)	319 (98%)	7 (2%)	53	84
1	F	327/346 (94%)	320 (98%)	7 (2%)	53	84
1	G	327/346 (94%)	320 (98%)	7 (2%)	53	84
1	H	326/346 (94%)	316 (97%)	10 (3%)	40	74
All	All	2619/2768 (95%)	2553 (98%)	66 (2%)	47	80

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	42	LYS
1	A	58	ASP
1	A	110	SER
1	A	153	SER
1	A	164	LYS
1	A	212	GLU
1	A	260	SER
1	A	262	LYS
1	A	266	ARG
1	A	378	LYS
1	B	22	ARG
1	B	33	ARG
1	B	58	ASP
1	B	117	ARG
1	B	133	LYS
1	B	194	SER
1	B	261	SER
1	C	22	ARG
1	C	32	SER
1	C	37	ASN
1	C	42	LYS
1	C	58	ASP
1	C	117	ARG
1	C	249	VAL
1	C	299	GLU
1	C	317	SER
1	D	22	ARG
1	D	58	ASP
1	D	117	ARG
1	D	194	SER
1	D	200	LEU
1	D	262	LYS
1	D	298	GLU
1	D	327	PHE
1	E	58	ASP
1	E	97	ILE
1	E	117	ARG
1	E	133	LYS
1	E	194	SER
1	E	266	ARG
1	E	292	GLU

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Mol	Chain	Res	Type
1	F	27	GLU
1	F	58	ASP
1	F	84	GLN
1	F	86	ILE
1	F	117	ARG
1	F	194	SER
1	F	234	SER
1	G	27	GLU
1	G	58	ASP
1	G	117	ARG
1	G	153	SER
1	G	173	ARG
1	G	266	ARG
1	G	378	LYS
1	H	27	GLU
1	H	34	LYS
1	H	110	SER
1	H	116	LYS
1	H	153	SER
1	H	173	ARG
1	H	231	ASN
1	H	261	SER
1	H	264	LYS
1	H	272	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	272	HIS
1	B	142	HIS
1	B	272	HIS
1	D	142	HIS
1	D	272	HIS
1	F	141	HIS
1	F	142	HIS
1	G	154	GLN
1	G	363	ASN
1	H	155	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	375/396 (94%)	-0.14	2 (0%)	91	88	18, 32, 50, 67	0
1	B	375/396 (94%)	-0.09	1 (0%)	94	93	23, 34, 48, 74	0
1	C	376/396 (94%)	-0.12	2 (0%)	91	88	18, 32, 50, 78	0
1	D	375/396 (94%)	-0.04	4 (1%)	80	75	21, 34, 52, 72	0
1	E	373/396 (94%)	0.09	11 (2%)	51	41	23, 41, 61, 85	0
1	F	374/396 (94%)	0.29	10 (2%)	54	44	24, 45, 69, 92	0
1	G	374/396 (94%)	0.02	8 (2%)	63	54	26, 39, 57, 81	0
1	H	373/396 (94%)	0.03	4 (1%)	80	75	18, 40, 58, 92	0
All	All	2995/3168 (94%)	0.01	42 (1%)	75	70	18, 37, 58, 92	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	263	TYR	4.4
1	E	263	TYR	4.2
1	F	264	LYS	4.2
1	E	262	LYS	3.5
1	E	37	ASN	3.2
1	E	264	LYS	3.2
1	G	263	TYR	2.9
1	F	228	THR	2.9
1	D	66	PHE	2.9
1	E	266	ARG	2.8
1	E	260	SER	2.7
1	F	267	ILE	2.7
1	G	258	LYS	2.6
1	F	229	GLY	2.6
1	G	25	ILE	2.6
1	B	262	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	267	ILE	2.6
1	D	70	LEU	2.5
1	H	23	ALA	2.5
1	F	172	THR	2.5
1	G	163	VAL	2.4
1	G	23	ALA	2.4
1	F	44	VAL	2.4
1	C	108	THR	2.4
1	F	225	VAL	2.3
1	E	35	ILE	2.3
1	G	24	LYS	2.3
1	E	258	LYS	2.3
1	G	27	GLU	2.2
1	C	396	ARG	2.2
1	H	154	GLN	2.2
1	F	110	SER	2.1
1	E	39	ALA	2.1
1	E	23	ALA	2.1
1	A	37	ASN	2.1
1	H	24	LYS	2.1
1	A	91	LYS	2.0
1	H	263	TYR	2.0
1	D	112	PHE	2.0
1	D	23	ALA	2.0
1	F	235	ARG	2.0
1	G	34	LYS	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.