



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2016 – 12:26 AM EDT

PDB ID : 5HXV  
Title : The crystal structure of thermostable xylanase mutant  
Authors : Watanabe, M.; Ishikawa, K.  
Deposited on : 2016-01-31  
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

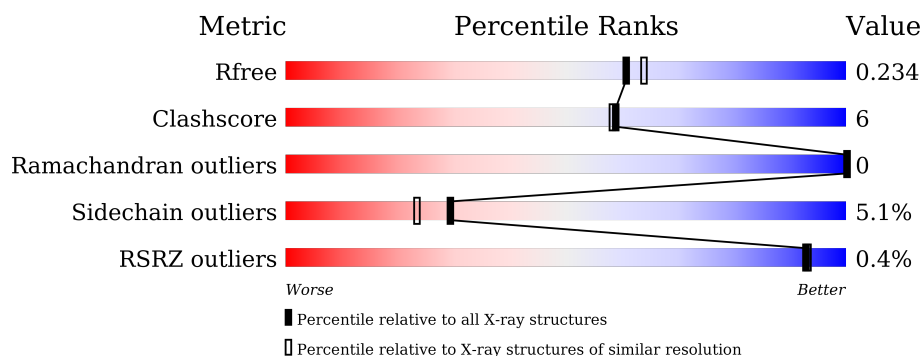
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	190	<div> <div>88%</div> <div>11% ...</div> </div>
1	B	190	<div> <div>88%</div> <div>10% ..</div> </div>
1	C	190	<div> <div>82%</div> <div>16% ..</div> </div>
1	D	190	<div> <div>85%</div> <div>13% ..</div> </div>
1	E	190	<div> <div>%</div> <div>83%</div> <div>14% ..</div> </div>
1	F	190	<div> <div>87%</div> <div>12% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	190	<div><div>%</div><div><div></div><div>84%</div><div>13%</div><div>...</div></div></div>
1	H	190	<div><div>%</div><div><div></div><div>86%</div><div>12%</div><div>...</div></div></div>
1	I	190	<div><div></div><div><div></div><div>89%</div><div>9%</div><div>...</div></div></div>
1	J	190	<div><div>2%</div><div><div></div><div>87%</div><div>11%</div><div>...</div></div></div>
1	K	190	<div><div>%</div><div><div></div><div>84%</div><div>14%</div><div>..</div></div></div>
1	L	190	<div><div>%</div><div><div></div><div>84%</div><div>14%</div><div>..</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18554 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	B	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	C	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	D	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	E	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	F	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	G	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	H	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	I	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	J	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	K	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			
1	L	189	Total	C	N	O	S	0	0	0
			1446	910	229	301	6			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	expression tag	UNP W8VR85
A	35	CYS	SER	engineered mutation	UNP W8VR85
A	44	HIS	ASN	engineered mutation	UNP W8VR85
A	61	MET	TYR	engineered mutation	UNP W8VR85
A	62	CYS	THR	engineered mutation	UNP W8VR85

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Chain	Residue	Modelled	Actual	Comment	Reference
A	63	LEU	ASN	engineered mutation	UNP W8VR85
A	65	PRO	ASP	engineered mutation	UNP W8VR85
A	66	GLY	ASN	engineered mutation	UNP W8VR85
A	101	PRO	THR	engineered mutation	UNP W8VR85
A	102	ASN	SER	engineered mutation	UNP W8VR85
B	34	MET	-	expression tag	UNP W8VR85
B	35	CYS	SER	engineered mutation	UNP W8VR85
B	44	HIS	ASN	engineered mutation	UNP W8VR85
B	61	MET	TYR	engineered mutation	UNP W8VR85
B	62	CYS	THR	engineered mutation	UNP W8VR85
B	63	LEU	ASN	engineered mutation	UNP W8VR85
B	65	PRO	ASP	engineered mutation	UNP W8VR85
B	66	GLY	ASN	engineered mutation	UNP W8VR85
B	101	PRO	THR	engineered mutation	UNP W8VR85
B	102	ASN	SER	engineered mutation	UNP W8VR85
C	34	MET	-	expression tag	UNP W8VR85
C	35	CYS	SER	engineered mutation	UNP W8VR85
C	44	HIS	ASN	engineered mutation	UNP W8VR85
C	61	MET	TYR	engineered mutation	UNP W8VR85
C	62	CYS	THR	engineered mutation	UNP W8VR85
C	63	LEU	ASN	engineered mutation	UNP W8VR85
C	65	PRO	ASP	engineered mutation	UNP W8VR85
C	66	GLY	ASN	engineered mutation	UNP W8VR85
C	101	PRO	THR	engineered mutation	UNP W8VR85
C	102	ASN	SER	engineered mutation	UNP W8VR85
D	34	MET	-	expression tag	UNP W8VR85
D	35	CYS	SER	engineered mutation	UNP W8VR85
D	44	HIS	ASN	engineered mutation	UNP W8VR85
D	61	MET	TYR	engineered mutation	UNP W8VR85
D	62	CYS	THR	engineered mutation	UNP W8VR85
D	63	LEU	ASN	engineered mutation	UNP W8VR85
D	65	PRO	ASP	engineered mutation	UNP W8VR85
D	66	GLY	ASN	engineered mutation	UNP W8VR85
D	101	PRO	THR	engineered mutation	UNP W8VR85
D	102	ASN	SER	engineered mutation	UNP W8VR85
E	34	MET	-	expression tag	UNP W8VR85
E	35	CYS	SER	engineered mutation	UNP W8VR85
E	44	HIS	ASN	engineered mutation	UNP W8VR85
E	61	MET	TYR	engineered mutation	UNP W8VR85
E	62	CYS	THR	engineered mutation	UNP W8VR85
E	63	LEU	ASN	engineered mutation	UNP W8VR85
E	65	PRO	ASP	engineered mutation	UNP W8VR85

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Chain	Residue	Modelled	Actual	Comment	Reference
E	66	GLY	ASN	engineered mutation	UNP W8VR85
E	101	PRO	THR	engineered mutation	UNP W8VR85
E	102	ASN	SER	engineered mutation	UNP W8VR85
F	34	MET	-	expression tag	UNP W8VR85
F	35	CYS	SER	engineered mutation	UNP W8VR85
F	44	HIS	ASN	engineered mutation	UNP W8VR85
F	61	MET	TYR	engineered mutation	UNP W8VR85
F	62	CYS	THR	engineered mutation	UNP W8VR85
F	63	LEU	ASN	engineered mutation	UNP W8VR85
F	65	PRO	ASP	engineered mutation	UNP W8VR85
F	66	GLY	ASN	engineered mutation	UNP W8VR85
F	101	PRO	THR	engineered mutation	UNP W8VR85
F	102	ASN	SER	engineered mutation	UNP W8VR85
G	34	MET	-	expression tag	UNP W8VR85
G	35	CYS	SER	engineered mutation	UNP W8VR85
G	44	HIS	ASN	engineered mutation	UNP W8VR85
G	61	MET	TYR	engineered mutation	UNP W8VR85
G	62	CYS	THR	engineered mutation	UNP W8VR85
G	63	LEU	ASN	engineered mutation	UNP W8VR85
G	65	PRO	ASP	engineered mutation	UNP W8VR85
G	66	GLY	ASN	engineered mutation	UNP W8VR85
G	101	PRO	THR	engineered mutation	UNP W8VR85
G	102	ASN	SER	engineered mutation	UNP W8VR85
H	34	MET	-	expression tag	UNP W8VR85
H	35	CYS	SER	engineered mutation	UNP W8VR85
H	44	HIS	ASN	engineered mutation	UNP W8VR85
H	61	MET	TYR	engineered mutation	UNP W8VR85
H	62	CYS	THR	engineered mutation	UNP W8VR85
H	63	LEU	ASN	engineered mutation	UNP W8VR85
H	65	PRO	ASP	engineered mutation	UNP W8VR85
H	66	GLY	ASN	engineered mutation	UNP W8VR85
H	101	PRO	THR	engineered mutation	UNP W8VR85
H	102	ASN	SER	engineered mutation	UNP W8VR85
I	34	MET	-	expression tag	UNP W8VR85
I	35	CYS	SER	engineered mutation	UNP W8VR85
I	44	HIS	ASN	engineered mutation	UNP W8VR85
I	61	MET	TYR	engineered mutation	UNP W8VR85
I	62	CYS	THR	engineered mutation	UNP W8VR85
I	63	LEU	ASN	engineered mutation	UNP W8VR85
I	65	PRO	ASP	engineered mutation	UNP W8VR85
I	66	GLY	ASN	engineered mutation	UNP W8VR85
I	101	PRO	THR	engineered mutation	UNP W8VR85

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Chain	Residue	Modelled	Actual	Comment	Reference
I	102	ASN	SER	engineered mutation	UNP W8VR85
J	34	MET	-	expression tag	UNP W8VR85
J	35	CYS	SER	engineered mutation	UNP W8VR85
J	44	HIS	ASN	engineered mutation	UNP W8VR85
J	61	MET	TYR	engineered mutation	UNP W8VR85
J	62	CYS	THR	engineered mutation	UNP W8VR85
J	63	LEU	ASN	engineered mutation	UNP W8VR85
J	65	PRO	ASP	engineered mutation	UNP W8VR85
J	66	GLY	ASN	engineered mutation	UNP W8VR85
J	101	PRO	THR	engineered mutation	UNP W8VR85
J	102	ASN	SER	engineered mutation	UNP W8VR85
K	34	MET	-	expression tag	UNP W8VR85
K	35	CYS	SER	engineered mutation	UNP W8VR85
K	44	HIS	ASN	engineered mutation	UNP W8VR85
K	61	MET	TYR	engineered mutation	UNP W8VR85
K	62	CYS	THR	engineered mutation	UNP W8VR85
K	63	LEU	ASN	engineered mutation	UNP W8VR85
K	65	PRO	ASP	engineered mutation	UNP W8VR85
K	66	GLY	ASN	engineered mutation	UNP W8VR85
K	101	PRO	THR	engineered mutation	UNP W8VR85
K	102	ASN	SER	engineered mutation	UNP W8VR85
L	34	MET	-	expression tag	UNP W8VR85
L	35	CYS	SER	engineered mutation	UNP W8VR85
L	44	HIS	ASN	engineered mutation	UNP W8VR85
L	61	MET	TYR	engineered mutation	UNP W8VR85
L	62	CYS	THR	engineered mutation	UNP W8VR85
L	63	LEU	ASN	engineered mutation	UNP W8VR85
L	65	PRO	ASP	engineered mutation	UNP W8VR85
L	66	GLY	ASN	engineered mutation	UNP W8VR85
L	101	PRO	THR	engineered mutation	UNP W8VR85
L	102	ASN	SER	engineered mutation	UNP W8VR85

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	114	Total O 114 114	0	0
2	B	114	Total O 114 114	0	0
2	C	121	Total O 121 121	0	0
2	D	107	Total O 107 107	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	103	Total 103	O 103	0	0
2	F	119	Total 119	O 119	0	0
2	G	86	Total 86	O 86	0	0
2	H	107	Total 107	O 107	0	0
2	I	95	Total 95	O 95	0	0
2	J	105	Total 105	O 105	0	0
2	K	74	Total 74	O 74	0	0
2	L	57	Total 57	O 57	0	0



### 3 Residue-property plots


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Endo-1,4-beta-xylanase

Chain A: 




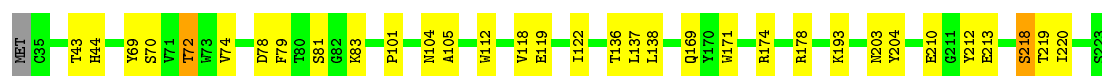
- Molecule 1: Endo-1,4-beta-xylanase

Chain B: 




- Molecule 1: Endo-1,4-beta-xylanase

Chain C: 




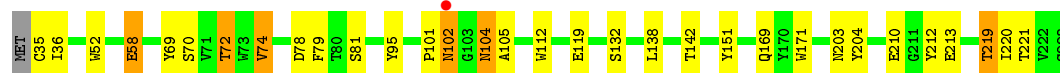
- Molecule 1: Endo-1,4-beta-xylanase

Chain D: 




- Molecule 1: Endo-1,4-beta-xylanase

Chain E: 

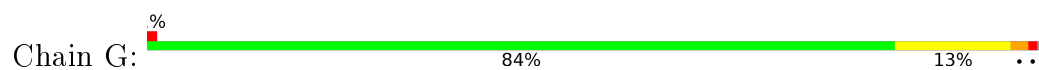


- Molecule 1: Endo-1,4-beta-xylanase

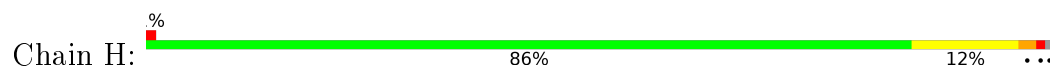
Chain F: 



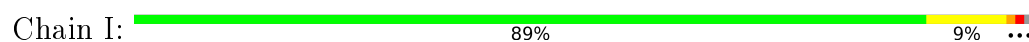
- Molecule 1: Endo-1,4-beta-xylanase



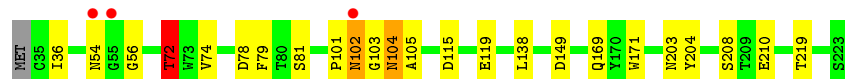
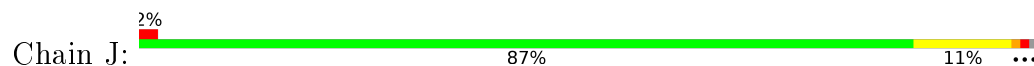
- Molecule 1: Endo-1,4-beta-xylanase



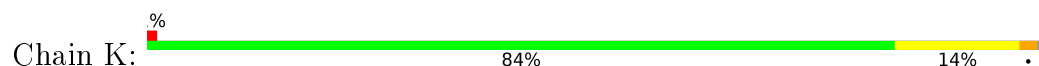
- Molecule 1: Endo-1,4-beta-xylanase



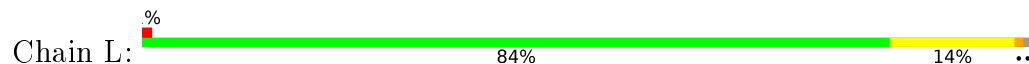
- Molecule 1: Endo-1,4-beta-xylanase



- Molecule 1: Endo-1,4-beta-xylanase



- Molecule 1: Endo-1,4-beta-xylanase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.00 Å 179.88 Å 93.34 Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.00) 94.0 (19.98-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.01 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.176 , 0.229 0.184 , 0.234	Depositor DCC
$R_{free}$ test set	7690 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	8.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 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	0.98	1/1487 (0.1%)	0.93	0/2034
1	B	0.99	0/1487	0.95	3/2034 (0.1%)
1	C	0.99	3/1487 (0.2%)	1.02	7/2034 (0.3%)
1	D	0.95	1/1487 (0.1%)	0.94	2/2034 (0.1%)
1	E	0.96	0/1487	0.92	0/2034
1	F	0.97	0/1487	0.89	0/2034
1	G	0.92	1/1487 (0.1%)	0.96	3/2034 (0.1%)
1	H	0.94	0/1487	0.98	4/2034 (0.2%)
1	I	0.98	2/1487 (0.1%)	0.97	4/2034 (0.2%)
1	J	1.00	2/1487 (0.1%)	0.98	5/2034 (0.2%)
1	K	0.88	0/1487	0.94	3/2034 (0.1%)
1	L	0.83	0/1487	0.87	0/2034
All	All	0.95	10/17844 (0.1%)	0.95	31/24408 (0.1%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	78	ASP	CB-CG	-9.07	1.32	1.51
1	J	72	THR	CB-CG2	-5.86	1.33	1.52
1	C	81	SER	CB-OG	-5.64	1.34	1.42
1	I	70	SER	CB-OG	-5.62	1.34	1.42
1	A	72	THR	CB-CG2	-5.44	1.34	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	78	ASP	CB-CG-OD1	-13.93	105.77	118.30
1	H	93	VAL	CB-CA-C	-8.98	94.33	111.40
1	B	78	ASP	CB-CG-OD1	8.89	126.30	118.30
1	K	78	ASP	CB-CG-OD1	8.84	126.26	118.30
1	C	78	ASP	CB-CG-OD1	8.01	125.51	118.30

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	1446	0	1315	16	0
1	B	1446	0	1315	13	0
1	C	1446	0	1315	16	0
1	D	1446	0	1315	18	0
1	E	1446	0	1315	23	0
1	F	1446	0	1315	16	0
1	G	1446	0	1315	20	0
1	H	1446	0	1315	22	0
1	I	1446	0	1315	11	0
1	J	1446	0	1315	21	0
1	K	1446	0	1315	14	0
1	L	1446	0	1315	13	0
2	A	114	0	0	2	0
2	B	114	0	0	6	0
2	C	121	0	0	4	0
2	D	107	0	0	5	0
2	E	103	0	0	2	0
2	F	119	0	0	1	0
2	G	86	0	0	4	0
2	H	107	0	0	5	0
2	I	95	0	0	9	0
2	J	105	0	0	4	0
2	K	74	0	0	2	0
2	L	57	0	0	1	0
All	All	18554	0	15780	193	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 6.

The worst 5 of 193 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:J:54:ASN:HB2	2:J:302:HOH:O	1.45	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:ASN:OD1	1:G:103:GLY:N	1.96	0.98
1:H:70:SER:OG	1:H:219:THR:HG23	1.65	0.94
1:G:219:THR:HG22	2:G:328:HOH:O	1.69	0.92
1:F:137:LEU:H	1:H:72:THR:HG21	1.35	0.89

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/190 (98%)	181 (97%)	6 (3%)	0	100	100
1	B	187/190 (98%)	182 (97%)	5 (3%)	0	100	100
1	C	187/190 (98%)	181 (97%)	6 (3%)	0	100	100
1	D	187/190 (98%)	180 (96%)	7 (4%)	0	100	100
1	E	187/190 (98%)	178 (95%)	9 (5%)	0	100	100
1	F	187/190 (98%)	181 (97%)	6 (3%)	0	100	100
1	G	187/190 (98%)	181 (97%)	6 (3%)	0	100	100
1	H	187/190 (98%)	179 (96%)	8 (4%)	0	100	100
1	I	187/190 (98%)	180 (96%)	7 (4%)	0	100	100
1	J	187/190 (98%)	181 (97%)	6 (3%)	0	100	100
1	K	187/190 (98%)	181 (97%)	6 (3%)	0	100	100
1	L	187/190 (98%)	175 (94%)	12 (6%)	0	100	100
All	All	2244/2280 (98%)	2160 (96%)	84 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/156 (99%)	150 (97%)	5 (3%)	46	44
1	B	155/156 (99%)	148 (96%)	7 (4%)	34	29
1	C	155/156 (99%)	149 (96%)	6 (4%)	39	35
1	D	155/156 (99%)	148 (96%)	7 (4%)	34	29
1	E	155/156 (99%)	145 (94%)	10 (6%)	21	15
1	F	155/156 (99%)	149 (96%)	6 (4%)	39	35
1	G	155/156 (99%)	146 (94%)	9 (6%)	25	19
1	H	155/156 (99%)	147 (95%)	8 (5%)	29	23
1	I	155/156 (99%)	145 (94%)	10 (6%)	21	15
1	J	155/156 (99%)	149 (96%)	6 (4%)	39	35
1	K	155/156 (99%)	143 (92%)	12 (8%)	16	10
1	L	155/156 (99%)	146 (94%)	9 (6%)	25	19
All	All	1860/1872 (99%)	1765 (95%)	95 (5%)	29	23

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	74	VAL
1	H	104	ASN
1	L	68	GLU
1	G	136	THR
1	G	198	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	203	ASN
1	G	45	ASN
1	L	40	GLN
1	F	44	HIS

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Mol	Chain	Res	Type
1	F	169	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 carbohydrates 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	189/190 (99%)	-0.54	0 100 100	4, 8, 17, 26	0
1	B	189/190 (99%)	-0.58	0 100 100	4, 7, 16, 25	0
1	C	189/190 (99%)	-0.60	0 100 100	4, 7, 13, 23	0
1	D	189/190 (99%)	-0.45	0 100 100	5, 10, 20, 29	0
1	E	189/190 (99%)	-0.45	1 (0%) 91 92	5, 10, 20, 33	0
1	F	189/190 (99%)	-0.57	0 100 100	4, 9, 15, 27	0
1	G	189/190 (99%)	-0.32	1 (0%) 91 92	5, 11, 26, 37	0
1	H	189/190 (99%)	-0.45	2 (1%) 82 83	4, 9, 22, 36	0
1	I	189/190 (99%)	-0.41	0 100 100	6, 11, 20, 29	0
1	J	189/190 (99%)	-0.47	3 (1%) 74 75	5, 9, 18, 36	0
1	K	189/190 (99%)	-0.22	1 (0%) 91 92	8, 15, 24, 33	0
1	L	189/190 (99%)	-0.11	2 (1%) 82 83	9, 17, 27, 36	0
All	All	2268/2280 (99%)	-0.43	10 (0%) 93 93	4, 10, 21, 37	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	55	GLY	7.0
1	E	102	ASN	2.9
1	J	54	ASN	2.9
1	G	102	ASN	2.8
1	K	102	ASN	2.7

### 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 carbohydrates 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.