



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:34 PM UTC

PDB ID : 5HXV / pdb_00005hvx
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

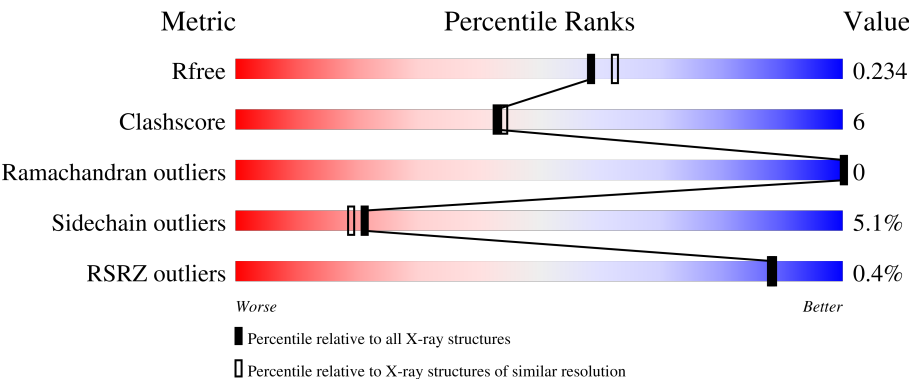
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	86%11%...
1	B	190	88%11%..
1	C	190	% 82%16%..
1	D	190	84%14%..
1	E	190	% 81%16%...

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Mol	Chain	Length	Quality of chain
1	F	190	85%13% %
1	G	190	85%12% %
1	H	190	84%13% %
1	I	190	87%11% 2%
1	J	190	84%12% %
1	K	190	81%17% %
1	L	190	84%13% %

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, 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: 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: 



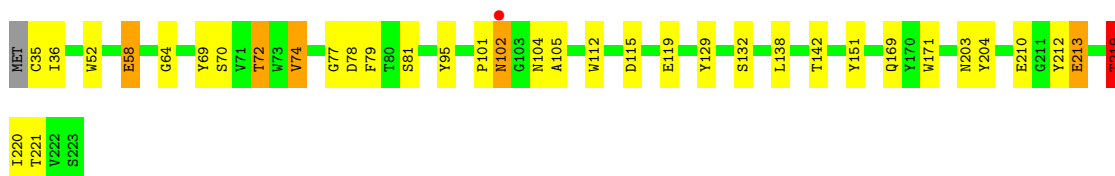
- Molecule 1: Endo-1,4-beta-xylanase

Chain D: 



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

Chain E: 



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

Chain F:  85% 13% ..



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

Chain G:  85% 12% ..



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

Chain H:  84% 13% ...



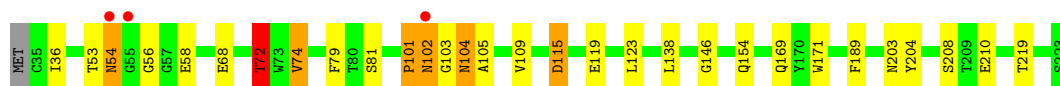
- Molecule 1: Endo-1,4-beta-xylanase

Chain I:  87% 11% ...



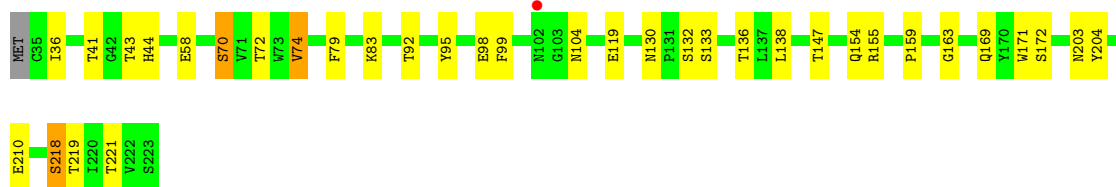
- Molecule 1: Endo-1,4-beta-xylanase

Chain J:  84% 12% ..



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

Chain K:  81% 17% ..



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

Chain L:  84% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.00Å 179.88Å 93.34Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.00) 93.9 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.01Å)	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 (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	8.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	1.20	2/1487 (0.1%)	1.12	4/2034 (0.2%)
1	B	1.21	0/1487	1.10	2/2034 (0.1%)
1	C	1.24	4/1487 (0.3%)	1.15	5/2034 (0.2%)
1	D	1.19	4/1487 (0.3%)	1.11	3/2034 (0.1%)
1	E	1.18	2/1487 (0.1%)	1.13	4/2034 (0.2%)
1	F	1.21	3/1487 (0.2%)	1.06	2/2034 (0.1%)
1	G	1.18	2/1487 (0.1%)	1.12	1/2034 (0.0%)
1	H	1.15	1/1487 (0.1%)	1.18	10/2034 (0.5%)
1	I	1.20	2/1487 (0.1%)	1.08	5/2034 (0.2%)
1	J	1.26	7/1487 (0.5%)	1.19	10/2034 (0.5%)
1	K	1.09	1/1487 (0.1%)	1.09	5/2034 (0.2%)
1	L	1.07	2/1487 (0.1%)	1.10	1/2034 (0.0%)
All	All	1.18	30/17844 (0.2%)	1.12	52/24408 (0.2%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	78	ASP	N-CA	-8.11	1.36	1.46
1	I	78	ASP	CB-CG	-7.74	1.32	1.52
1	L	115	ASP	C-O	-7.49	1.20	1.23
1	G	102	ASN	C-O	7.42	1.32	1.24
1	C	102	ASN	C-O	7.38	1.31	1.23
1	F	120	TYR	C-O	6.01	1.31	1.23
1	D	103	GLY	N-CA	5.96	1.54	1.45
1	J	72	THR	CB-CG2	-5.92	1.33	1.52
1	J	154	GLN	CA-C	-5.79	1.45	1.52
1	J	103	GLY	N-CA	5.70	1.53	1.45
1	C	39	SER	C-O	5.52	1.30	1.23
1	D	74	VAL	CA-CB	5.51	1.61	1.54
1	A	72	THR	CB-CG2	-5.50	1.34	1.52
1	C	72	THR	CB-CG2	-5.47	1.34	1.52
1	F	115	ASP	C-O	-5.46	1.21	1.23
1	J	146	GLY	N-CA	5.46	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	58	GLU	CA-C	-5.41	1.46	1.52
1	J	54	ASN	CG-OD1	5.33	1.33	1.23
1	J	54	ASN	N-CA	-5.32	1.40	1.46
1	A	212	TYR	CA-C	5.31	1.58	1.52
1	L	137	LEU	CA-C	5.30	1.59	1.52
1	D	172	SER	C-O	-5.30	1.17	1.24
1	E	115	ASP	CA-C	5.20	1.57	1.53
1	F	140	GLN	CA-C	-5.14	1.46	1.52
1	H	81	SER	C-O	-5.10	1.17	1.24
1	C	209	THR	C-O	5.07	1.30	1.24
1	G	91	GLN	C-O	-5.04	1.17	1.23
1	E	129	TYR	C-O	-5.02	1.18	1.24
1	J	123	LEU	N-CA	-5.02	1.40	1.46
1	K	159	PRO	CA-C	5.01	1.58	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	93	VAL	CB-CA-C	-10.93	94.33	110.62
1	J	53	THR	CA-C-N	-7.15	111.93	122.86
1	J	53	THR	C-N-CA	-7.15	111.93	122.86
1	I	64	GLY	CA-C-N	6.94	126.97	119.89
1	I	64	GLY	C-N-CA	6.94	126.97	119.89
1	A	100	ASN	CA-C-N	6.87	127.42	120.14
1	A	100	ASN	C-N-CA	6.87	127.42	120.14
1	C	74	VAL	CB-CA-C	6.72	120.58	110.63
1	E	64	GLY	CA-C-N	6.55	126.93	119.92
1	E	64	GLY	C-N-CA	6.55	126.93	119.92
1	J	109	VAL	N-CA-C	-6.48	100.33	108.89
1	J	219	THR	OG1-CB-CG2	-6.47	96.35	109.30
1	H	219	THR	CB-CA-C	-6.45	98.37	109.65
1	D	74	VAL	CB-CA-C	6.42	119.09	110.42
1	E	219	THR	CB-CA-C	-6.39	98.47	109.65
1	H	72	THR	CB-CA-C	6.35	121.19	109.70
1	J	102	ASN	CB-CA-C	6.34	120.83	110.24
1	C	122	ILE	N-CA-C	-6.27	96.75	106.72
1	K	163	GLY	N-CA-C	-6.18	103.84	111.45
1	F	203	ASN	N-CA-C	-6.11	103.77	108.78
1	H	101	PRO	CA-C-N	-6.08	111.17	122.60
1	H	101	PRO	C-N-CA	-6.08	111.17	122.60
1	E	77	GLY	N-CA-C	-6.05	104.71	110.21
1	I	219	THR	CB-CA-C	-6.04	97.11	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	133	SER	CB-CA-C	-6.00	101.72	110.06
1	J	74	VAL	CB-CA-C	5.86	118.08	110.12
1	L	203	ASN	N-CA-C	-5.79	104.03	108.78
1	G	219	THR	OG1-CB-CG2	-5.74	97.83	109.30
1	B	129	TYR	N-CA-C	5.68	117.78	108.52
1	K	74	VAL	N-CA-C	5.68	116.06	108.11
1	H	115	ASP	CB-CA-C	-5.60	106.13	111.00
1	B	172	SER	N-CA-C	-5.50	99.44	108.41
1	D	109	VAL	N-CA-C	-5.50	100.40	108.54
1	I	78	ASP	CB-CG-OD1	-5.49	105.77	118.40
1	A	58	GLU	CB-CA-C	5.46	118.77	109.75
1	F	72	THR	CB-CA-C	5.39	119.46	109.70
1	A	203	ASN	N-CA-C	-5.27	104.46	108.78
1	J	101	PRO	CA-C-N	-5.25	112.72	122.60
1	J	101	PRO	C-N-CA	-5.25	112.72	122.60
1	J	189	PHE	N-CA-C	5.23	116.98	111.28
1	I	78	ASP	N-CA-CB	-5.20	101.74	110.32
1	K	41	THR	N-CA-C	-5.17	101.52	109.52
1	J	58	GLU	N-CA-C	5.14	117.28	108.90
1	C	193	LYS	CD-CE-NZ	5.13	128.31	111.90
1	K	92	THR	CB-CA-C	5.12	118.46	110.67
1	H	102	ASN	CB-CA-C	5.11	118.77	110.24
1	C	81	SER	N-CA-C	5.08	116.79	108.76
1	K	155	ARG	N-CA-C	-5.03	101.49	109.59
1	H	141	VAL	CA-C-N	-5.03	115.63	122.93
1	H	141	VAL	C-N-CA	-5.03	115.63	122.93
1	C	93	VAL	N-CA-C	5.02	115.81	108.58
1	D	203	ASN	N-CA-C	-5.01	104.67	108.78

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1446	0	1315	13	0
1	C	1446	0	1315	17	0
1	D	1446	0	1315	18	0
1	E	1446	0	1315	24	0
1	F	1446	0	1315	17	0
1	G	1446	0	1315	20	0
1	H	1446	0	1315	26	0
1	I	1446	0	1315	13	0
1	J	1446	0	1315	22	0
1	K	1446	0	1315	15	0
1	L	1446	0	1315	14	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	205	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.

All (205) 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
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
1:B:137:LEU:H	1:E:72:THR:HG21	1.41	0.85
1:K:219:THR:HG22	2:K:354:HOH:O	1.76	0.84
1:C:136:THR:HG22	2:G:382:HOH:O	1.79	0.82
1:C:203:ASN:HD22	1:C:204:TYR:H	1.28	0.80
1:E:70:SER:OG	1:E:219:THR:HG23	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:H	1:G:72:THR:HG21	1.48	0.79
1:J:203:ASN:HD22	1:J:204:TYR:H	1.30	0.78
1:A:70:SER:OG	1:A:219:THR:HG23	1.83	0.78
1:B:169:GLN:HE21	1:B:171:TRP:HE1	1.30	0.78
1:J:36:ILE:HG22	2:J:397:HOH:O	1.84	0.77
1:G:102:ASN:ND2	1:G:215:SER:HB2	2.02	0.74
1:I:70:SER:OG	1:I:219:THR:HG23	1.86	0.74
1:I:137:LEU:H	1:J:72:THR:HG21	1.52	0.74
2:A:369:HOH:O	1:F:43:THR:HB	1.87	0.73
1:C:212:TYR:OH	1:J:54:ASN:ND2	2.21	0.73
1:B:142:THR:HG23	2:B:411:HOH:O	1.88	0.73
1:D:70:SER:OG	1:D:219:THR:HG23	1.91	0.71
1:C:70:SER:OG	1:C:219:THR:HG23	1.91	0.70
1:B:219:THR:HG22	2:B:364:HOH:O	1.91	0.70
1:B:203:ASN:HD22	1:B:204:TYR:H	1.40	0.70
1:F:219:THR:HG22	2:F:385:HOH:O	1.90	0.70
1:H:203:ASN:HD22	1:H:204:TYR:H	1.38	0.69
1:E:212:TYR:CE2	1:E:213:GLU:HG3	2.28	0.69
1:A:72:THR:HG21	1:D:137:LEU:H	1.57	0.68
1:A:72:THR:HG22	2:D:335:HOH:O	1.93	0.68
1:D:158:GLN:OE1	1:I:157:ASP:OD2	2.11	0.67
1:H:115:ASP:HB2	2:H:390:HOH:O	1.94	0.67
1:F:203:ASN:HD22	1:F:204:TYR:H	1.43	0.66
1:H:85:TRP:HH2	1:H:93:VAL:HG13	1.59	0.66
1:F:169:GLN:HE21	1:F:171:TRP:HE1	1.44	0.65
1:K:70:SER:OG	1:K:219:THR:HG23	1.96	0.64
1:E:169:GLN:HE21	1:E:171:TRP:HE1	1.47	0.63
1:K:44:HIS:HD2	1:K:83:LYS:NZ	1.97	0.62
1:A:43:THR:HG23	2:E:315:HOH:O	1.99	0.61
1:D:169:GLN:HE21	1:D:171:TRP:HE1	1.47	0.61
1:C:219:THR:HG22	2:C:368:HOH:O	2.00	0.61
1:L:169:GLN:HE21	1:L:171:TRP:HE1	1.49	0.61
1:E:132:SER:HB2	1:E:151:TYR:CZ	2.37	0.60
1:C:44:HIS:HD2	1:C:83:LYS:NZ	1.99	0.59
1:B:169:GLN:NE2	1:B:171:TRP:HE1	1.99	0.59
1:A:72:THR:CG2	2:D:335:HOH:O	2.50	0.59
1:E:35:CYS:N	2:E:301:HOH:O	2.36	0.58
1:J:104:ASN:HD22	1:J:104:ASN:C	2.12	0.58
2:B:354:HOH:O	1:C:43:THR:HG23	2.03	0.57
1:L:58:GLU:HG2	1:L:74:VAL:CG1	2.34	0.57
1:C:203:ASN:ND2	1:C:204:TYR:H	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:GLU:O	1:D:169:GLN:HA	2.05	0.57
2:I:325:HOH:O	1:J:72:THR:CG2	2.53	0.57
1:K:99:PHE:HA	1:K:218:SER:HB2	1.86	0.57
1:K:119:GLU:O	1:K:169:GLN:HA	2.05	0.57
1:G:203:ASN:HD22	1:G:204:TYR:H	1.53	0.57
1:H:70:SER:HG	1:H:219:THR:HG23	1.68	0.57
1:L:119:GLU:O	1:L:169:GLN:HA	2.04	0.57
1:I:44:HIS:HD2	1:I:83:LYS:NZ	2.03	0.56
1:J:54:ASN:ND2	2:J:302:HOH:O	2.38	0.56
1:G:99:PHE:HA	1:G:218:SER:HB2	1.88	0.55
2:C:325:HOH:O	1:G:72:THR:CG2	2.53	0.55
1:L:58:GLU:HG2	1:L:74:VAL:HG13	1.87	0.55
1:F:70:SER:OG	1:F:219:THR:HG23	2.05	0.55
1:J:79:PHE:O	1:J:210:GLU:HG3	2.06	0.55
1:B:119:GLU:O	1:B:169:GLN:HA	2.07	0.55
1:H:70:SER:OG	1:H:219:THR:CG2	2.50	0.54
1:C:169:GLN:HE21	1:C:171:TRP:HE1	1.56	0.54
1:K:203:ASN:HD22	1:K:204:TYR:H	1.56	0.54
1:J:203:ASN:ND2	1:J:204:TYR:H	2.03	0.53
1:I:157:ASP:HB3	2:I:372:HOH:O	2.06	0.53
1:H:163:GLY:C	2:H:355:HOH:O	2.52	0.53
2:I:325:HOH:O	1:J:72:THR:HG22	2.09	0.53
1:C:169:GLN:NE2	1:C:171:TRP:HE1	2.07	0.53
1:H:104:ASN:C	1:H:104:ASN:HD22	2.17	0.53
1:D:104:ASN:HD22	1:D:105:ALA:N	2.07	0.52
1:D:169:GLN:NE2	1:D:171:TRP:HE1	2.06	0.52
1:H:85:TRP:CH2	1:H:93:VAL:HG13	2.43	0.52
1:F:135:LEU:HD22	1:F:153:THR:HB	1.92	0.52
1:I:157:ASP:CB	2:I:372:HOH:O	2.56	0.52
2:C:325:HOH:O	1:G:72:THR:HG22	2.09	0.52
1:I:155:ARG:NH2	2:I:301:HOH:O	2.30	0.52
1:G:158:GLN:HB3	1:G:159:PRO:HD2	1.92	0.51
1:E:169:GLN:NE2	1:E:171:TRP:HE1	2.08	0.51
1:E:104:ASN:HD22	1:E:105:ALA:N	2.08	0.51
1:H:163:GLY:HA2	2:H:355:HOH:O	2.10	0.51
1:D:219:THR:HG22	2:D:338:HOH:O	2.10	0.51
1:A:219:THR:HG22	2:A:409:HOH:O	2.11	0.50
1:D:44:HIS:HD2	1:D:83:LYS:NZ	2.09	0.50
1:H:169:GLN:NE2	1:H:171:TRP:HE1	2.10	0.50
1:K:203:ASN:ND2	1:K:204:TYR:H	2.09	0.50
1:F:203:ASN:ND2	1:F:204:TYR:H	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:GLU:HG2	1:E:74:VAL:HG13	1.92	0.50
1:H:36:ILE:O	1:H:36:ILE:HG13	2.11	0.50
1:J:54:ASN:OD1	1:J:54:ASN:C	2.55	0.50
1:C:119:GLU:O	1:C:169:GLN:HA	2.11	0.49
1:K:104:ASN:ND2	2:K:302:HOH:O	2.40	0.49
1:B:203:ASN:ND2	1:B:204:TYR:H	2.10	0.49
1:D:79:PHE:O	1:D:210:GLU:HG3	2.12	0.49
1:H:169:GLN:HE21	1:H:171:TRP:HE1	1.59	0.49
1:G:104:ASN:HD22	1:G:104:ASN:C	2.21	0.49
1:L:103:GLY:HA3	2:L:325:HOH:O	2.12	0.49
1:D:138:LEU:HB2	1:D:150:ILE:O	2.13	0.49
1:E:104:ASN:HD22	1:E:104:ASN:C	2.20	0.48
1:D:198:GLU:HG2	2:D:366:HOH:O	2.12	0.48
1:K:169:GLN:HE21	1:K:171:TRP:HE1	1.60	0.48
1:D:104:ASN:HD22	1:D:104:ASN:C	2.21	0.48
1:B:137:LEU:H	1:E:72:THR:CG2	2.19	0.48
1:F:137:LEU:H	1:H:72:THR:CG2	2.15	0.48
2:B:328:HOH:O	1:E:72:THR:HG22	2.14	0.48
1:A:51:PHE:HD1	1:A:81:SER:HB2	1.79	0.48
1:H:115:ASP:CB	2:H:390:HOH:O	2.59	0.47
1:A:119:GLU:O	1:A:169:GLN:HA	2.14	0.47
1:H:203:ASN:ND2	1:H:204:TYR:H	2.08	0.47
1:J:119:GLU:O	1:J:169:GLN:HA	2.14	0.47
1:E:79:PHE:O	1:E:210:GLU:HG3	2.15	0.47
1:K:44:HIS:HD2	1:K:83:LYS:HZ3	1.60	0.47
1:D:203:ASN:HD22	1:D:204:TYR:H	1.63	0.46
1:K:79:PHE:O	1:K:210:GLU:HG3	2.14	0.46
1:J:54:ASN:O	1:J:54:ASN:CG	2.58	0.46
1:C:44:HIS:HD2	1:C:83:LYS:HZ3	1.61	0.46
1:F:132:SER:HA	1:F:135:LEU:HD12	1.98	0.46
1:H:79:PHE:CD1	1:H:79:PHE:C	2.94	0.46
1:K:169:GLN:NE2	1:K:171:TRP:HE1	2.13	0.46
1:H:163:GLY:CA	2:H:355:HOH:O	2.63	0.46
1:E:203:ASN:HD22	1:E:204:TYR:H	1.64	0.46
1:I:154:GLN:HG3	2:I:339:HOH:O	2.15	0.45
1:J:101:PRO:HB3	1:J:105:ALA:HB3	1.99	0.45
1:H:112:TRP:CZ3	1:H:119:GLU:HB2	2.52	0.45
1:L:203:ASN:HD22	1:L:204:TYR:H	1.65	0.45
1:A:150:ILE:HA	1:A:171:TRP:O	2.17	0.45
1:G:169:GLN:NE2	1:G:171:TRP:HE1	2.13	0.45
1:E:70:SER:HG	1:E:219:THR:HG23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLN:HE21	1:A:171:TRP:HE1	1.64	0.45
1:A:203:ASN:HD22	1:A:204:TYR:H	1.65	0.45
1:E:102:ASN:HD22	1:E:102:ASN:HA	1.67	0.45
1:B:44:HIS:HD2	1:B:83:LYS:NZ	2.15	0.44
1:I:102:ASN:OD1	1:I:102:ASN:C	2.60	0.44
1:H:70:SER:HG	1:H:219:THR:CG2	2.29	0.44
1:J:104:ASN:HD22	1:J:105:ALA:N	2.16	0.44
1:A:219:THR:OG1	1:D:137:LEU:HD21	2.17	0.44
1:D:112:TRP:CZ3	1:D:119:GLU:HB2	2.53	0.44
1:D:198:GLU:CG	2:D:366:HOH:O	2.66	0.44
2:I:325:HOH:O	1:J:72:THR:HG23	2.18	0.43
1:C:112:TRP:HA	1:C:118:VAL:O	2.18	0.43
1:F:169:GLN:NE2	1:F:171:TRP:HE1	2.11	0.43
1:I:115:ASP:HB3	2:I:387:HOH:O	2.18	0.43
1:J:115:ASP:O	1:J:115:ASP:CG	2.61	0.43
1:L:77:GLY:O	1:L:212:TYR:HA	2.18	0.43
1:K:95:TYR:HA	1:K:221:THR:O	2.18	0.43
1:F:101:PRO:HB3	1:F:105:ALA:HB3	2.01	0.43
1:G:169:GLN:HE21	1:G:171:TRP:HE1	1.66	0.43
1:L:104:ASN:C	1:L:104:ASN:HD22	2.26	0.43
1:F:104:ASN:C	1:F:104:ASN:HD22	2.27	0.43
1:D:51:PHE:HD1	1:D:81:SER:HB2	1.84	0.43
1:G:198:GLU:HG2	2:G:372:HOH:O	2.19	0.43
1:G:219:THR:CG2	2:G:328:HOH:O	2.44	0.43
1:E:52:TRP:HZ3	1:E:78:ASP:OD2	2.01	0.43
1:F:104:ASN:HD22	1:F:105:ALA:N	2.17	0.42
1:E:58:GLU:CG	1:E:74:VAL:HG13	2.49	0.42
1:L:132:SER:HB2	1:L:151:TYR:CZ	2.53	0.42
1:B:142:THR:CG2	2:B:411:HOH:O	2.59	0.42
1:H:95:TYR:HA	1:H:221:THR:O	2.19	0.42
1:H:104:ASN:C	1:H:104:ASN:ND2	2.77	0.42
2:B:328:HOH:O	1:E:72:THR:CG2	2.67	0.42
1:G:161:ILE:HG13	1:G:162:GLU:HG3	2.02	0.42
1:A:81:SER:O	1:A:208:SER:HA	2.19	0.42
1:E:101:PRO:HB3	1:E:105:ALA:HB3	2.02	0.42
1:A:155:ARG:O	1:A:166:THR:HA	2.20	0.42
1:J:56:GLY:N	2:J:303:HOH:O	2.39	0.42
1:C:69:TYR:CE1	1:C:220:ILE:HB	2.55	0.42
1:I:219:THR:C	1:I:220:ILE:HG12	2.45	0.42
1:K:132:SER:O	1:K:133:SER:C	2.63	0.42
1:L:68:GLU:HG3	1:L:221:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:SER:O	1:L:208:SER:HA	2.19	0.41
1:C:101:PRO:HB3	1:C:105:ALA:HB3	2.03	0.41
1:G:73:TRP:CD1	1:G:215:SER:HA	2.55	0.41
1:H:104:ASN:HD22	1:H:105:ALA:N	2.18	0.41
1:A:93:VAL:O	1:A:182:THR:HA	2.20	0.41
1:F:79:PHE:O	1:F:210:GLU:HG3	2.20	0.41
1:L:97:GLY:HA3	1:L:219:THR:O	2.21	0.41
1:E:95:TYR:HA	1:E:221:THR:O	2.19	0.41
1:K:130:ASN:O	1:K:133:SER:OG	2.29	0.41
1:C:79:PHE:O	1:C:210:GLU:HG3	2.21	0.41
1:J:81:SER:O	1:J:208:SER:HA	2.21	0.41
1:E:119:GLU:O	1:E:169:GLN:HA	2.21	0.41
1:F:44:HIS:HD2	1:F:83:LYS:NZ	2.19	0.41
1:G:112:TRP:CH2	1:G:160:SER:HA	2.56	0.41
1:G:119:GLU:O	1:G:169:GLN:HA	2.20	0.41
1:I:169:GLN:NE2	1:I:171:TRP:HE1	2.19	0.41
1:B:104:ASN:HD22	1:B:105:ALA:N	2.18	0.41
1:J:203:ASN:HD22	1:J:204:TYR:N	2.08	0.41
1:E:112:TRP:CZ3	1:E:119:GLU:HB2	2.56	0.41
1:H:101:PRO:HB3	1:H:105:ALA:HB3	2.02	0.41
1:I:157:ASP:HB2	2:I:372:HOH:O	2.21	0.41
1:A:76:CYS:O	1:A:213:GLU:HA	2.21	0.40
1:G:44:HIS:HD2	1:G:83:LYS:NZ	2.19	0.40
1:H:130:ASN:OD1	1:H:130:ASN:C	2.63	0.40
1:J:169:GLN:HE21	1:J:171:TRP:HE1	1.69	0.40
1:E:69:TYR:CE1	1:E:220:ILE:HB	2.56	0.40
1:B:95:TYR:HA	1:B:221:THR:O	2.22	0.40
2:C:325:HOH:O	1:G:72:THR:HG23	2.19	0.40
1:F:79:PHE:O	1:F:210:GLU:HA	2.20	0.40
1:L:99:PHE:HA	1:L:218:SER:HB2	2.04	0.40
1:L:101:PRO:HB3	1:L:105:ALA:HB3	2.03	0.40

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%)	149 (96%)	6 (4%)	28	28
1	B	155/156 (99%)	148 (96%)	7 (4%)	24	23
1	C	155/156 (99%)	149 (96%)	6 (4%)	28	28
1	D	155/156 (99%)	148 (96%)	7 (4%)	24	23
1	E	155/156 (99%)	145 (94%)	10 (6%)	15	12
1	F	155/156 (99%)	149 (96%)	6 (4%)	28	28
1	G	155/156 (99%)	148 (96%)	7 (4%)	24	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	155/156 (99%)	147 (95%)	8 (5%)	21	18
1	I	155/156 (99%)	145 (94%)	10 (6%)	15	12
1	J	155/156 (99%)	148 (96%)	7 (4%)	24	23
1	K	155/156 (99%)	142 (92%)	13 (8%)	10	7
1	L	155/156 (99%)	147 (95%)	8 (5%)	21	18
All	All	1860/1872 (99%)	1765 (95%)	95 (5%)	21	19

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	72	THR
1	A	74	VAL
1	A	81	SER
1	A	138	LEU
1	A	165	SER
1	B	58	GLU
1	B	72	THR
1	B	74	VAL
1	B	81	SER
1	B	138	LEU
1	B	142	THR
1	B	165	SER
1	C	72	THR
1	C	74	VAL
1	C	138	LEU
1	C	193	LYS
1	C	213	GLU
1	C	218	SER
1	D	72	THR
1	D	74	VAL
1	D	115	ASP
1	D	138	LEU
1	D	162	GLU
1	D	165	SER
1	D	198	GLU
1	E	36	ILE
1	E	58	GLU
1	E	72	THR
1	E	74	VAL

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Mol	Chain	Res	Type
1	E	81	SER
1	E	102	ASN
1	E	138	LEU
1	E	142	THR
1	E	213	GLU
1	E	219	THR
1	F	36	ILE
1	F	72	THR
1	F	74	VAL
1	F	138	LEU
1	F	178	ARG
1	F	198	GLU
1	G	72	THR
1	G	74	VAL
1	G	136	THR
1	G	138	LEU
1	G	154	GLN
1	G	198	GLU
1	G	218	SER
1	H	72	THR
1	H	74	VAL
1	H	93	VAL
1	H	138	LEU
1	H	142	THR
1	H	178	ARG
1	H	219	THR
1	H	222	VAL
1	I	43	THR
1	I	58	GLU
1	I	63	LEU
1	I	70	SER
1	I	72	THR
1	I	74	VAL
1	I	138	LEU
1	I	162	GLU
1	I	218	SER
1	I	219	THR
1	J	68	GLU
1	J	72	THR
1	J	74	VAL
1	J	102	ASN
1	J	104	ASN

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Mol	Chain	Res	Type
1	J	115	ASP
1	J	138	LEU
1	K	36	ILE
1	K	43	THR
1	K	58	GLU
1	K	70	SER
1	K	72	THR
1	K	74	VAL
1	K	98	GLU
1	K	136	THR
1	K	138	LEU
1	K	147	THR
1	K	154	GLN
1	K	172	SER
1	K	218	SER
1	L	58	GLU
1	L	68	GLU
1	L	72	THR
1	L	104	ASN
1	L	138	LEU
1	L	142	THR
1	L	176	GLU
1	L	218	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	154	GLN
1	A	203	ASN
1	B	44	HIS
1	B	45	ASN
1	B	100	ASN
1	B	104	ASN
1	B	169	GLN
1	B	203	ASN
1	C	44	HIS
1	C	75	ASN
1	C	100	ASN
1	C	104	ASN
1	C	140	GLN
1	C	169	GLN

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Mol	Chain	Res	Type
1	C	203	ASN
1	D	44	HIS
1	D	104	ASN
1	D	169	GLN
1	D	203	ASN
1	E	100	ASN
1	E	102	ASN
1	E	104	ASN
1	E	169	GLN
1	F	40	GLN
1	F	44	HIS
1	F	104	ASN
1	F	169	GLN
1	F	203	ASN
1	G	44	HIS
1	G	100	ASN
1	G	104	ASN
1	G	140	GLN
1	G	169	GLN
1	G	203	ASN
1	H	104	ASN
1	H	168	ASN
1	H	169	GLN
1	H	203	ASN
1	I	44	HIS
1	I	100	ASN
1	I	104	ASN
1	I	203	ASN
1	J	104	ASN
1	J	158	GLN
1	J	168	ASN
1	J	203	ASN
1	K	44	HIS
1	K	45	ASN
1	K	100	ASN
1	K	104	ASN
1	K	169	GLN
1	K	203	ASN
1	L	40	GLN
1	L	45	ASN
1	L	104	ASN
1	L	169	GLN

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Mol	Chain	Res	Type
1	L	203	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	189/190 (99%)	-0.62	0 100 100	4, 8, 17, 26	0
1	B	189/190 (99%)	-0.68	0 100 100	4, 7, 16, 25	0
1	C	189/190 (99%)	-0.66	1 (0%) 87 87	4, 7, 13, 23	0
1	D	189/190 (99%)	-0.52	0 100 100	5, 10, 20, 29	0
1	E	189/190 (99%)	-0.51	1 (0%) 87 87	4, 10, 20, 33	0
1	F	189/190 (99%)	-0.64	0 100 100	4, 9, 15, 27	0
1	G	189/190 (99%)	-0.42	2 (1%) 78 77	5, 11, 26, 37	0
1	H	189/190 (99%)	-0.49	1 (0%) 87 87	4, 9, 22, 36	0
1	I	189/190 (99%)	-0.48	0 100 100	6, 11, 20, 29	0
1	J	189/190 (99%)	-0.45	3 (1%) 70 70	5, 9, 18, 36	0
1	K	189/190 (99%)	-0.29	1 (0%) 87 87	8, 15, 24, 33	0
1	L	189/190 (99%)	-0.19	1 (0%) 87 87	9, 17, 27, 36	0
All	All	2268/2280 (99%)	-0.50	10 (0%) 88 88	4, 10, 21, 37	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	55	GLY	8.4
1	G	102	ASN	4.2
1	J	54	ASN	4.2
1	E	102	ASN	3.9
1	H	102	ASN	3.7
1	J	102	ASN	3.6
1	K	102	ASN	2.9
1	G	163	GLY	2.4
1	C	102	ASN	2.2
1	L	163	GLY	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.