



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:53 pm BST

PDB ID : 2C8T  
Title : The 3.0 Å Resolution Structure of Caseinolytic Clp Protease 1 from Mycobacterium tuberculosis  
Authors : Ingvarsson, H.; Hogbom, M.; Jones, T.A.; Unge, T.  
Deposited on : 2005-12-07  
Resolution : 3.00 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

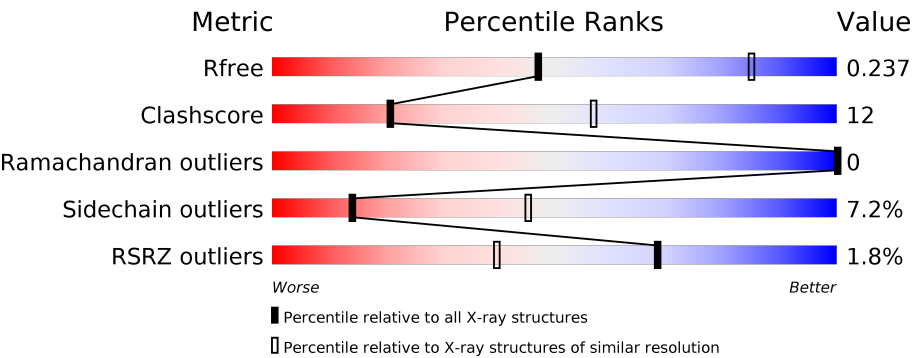
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	206	<div><div>%</div><div><div></div><div>63%</div><div>17%</div><div>•</div><div>17%</div></div></div>
1	B	206	<div><div>%</div><div><div></div><div>65%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	C	206	<div><div>2%</div><div><div></div><div>65%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	D	206	<div><div>2%</div><div><div></div><div>64%</div><div>15%</div><div>•</div><div>17%</div></div></div>
1	E	206	<div><div>%</div><div><div></div><div>62%</div><div>17%</div><div>•</div><div>17%</div></div></div>
1	F	206	<div><div>2%</div><div><div></div><div>62%</div><div>18%</div><div>•</div><div>17%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	206	
1	H	206	
1	I	206	
1	J	206	
1	K	206	
1	L	206	
1	M	206	
1	N	206	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18482 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 ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUB-UNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1322	839	224	250	9			
1	B	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	C	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	D	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	E	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	F	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	G	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	H	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	I	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	J	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	K	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	L	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	M	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			
1	N	171	Total	C	N	O	S	0	0	0
			1320	839	223	249	9			

There are 98 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP P0A526
A	1	ALA	-	expression tag	UNP P0A526
A	201	GLY	-	expression tag	UNP P0A526
A	202	HIS	-	expression tag	UNP P0A526
A	203	HIS	-	expression tag	UNP P0A526
A	204	HIS	-	expression tag	UNP P0A526
A	205	HIS	-	expression tag	UNP P0A526
B	0	MET	-	expression tag	UNP P0A526
B	1	ALA	-	expression tag	UNP P0A526
B	201	GLY	-	expression tag	UNP P0A526
B	202	HIS	-	expression tag	UNP P0A526
B	203	HIS	-	expression tag	UNP P0A526
B	204	HIS	-	expression tag	UNP P0A526
B	205	HIS	-	expression tag	UNP P0A526
C	0	MET	-	expression tag	UNP P0A526
C	1	ALA	-	expression tag	UNP P0A526
C	201	GLY	-	expression tag	UNP P0A526
C	202	HIS	-	expression tag	UNP P0A526
C	203	HIS	-	expression tag	UNP P0A526
C	204	HIS	-	expression tag	UNP P0A526
C	205	HIS	-	expression tag	UNP P0A526
D	0	MET	-	expression tag	UNP P0A526
D	1	ALA	-	expression tag	UNP P0A526
D	201	GLY	-	expression tag	UNP P0A526
D	202	HIS	-	expression tag	UNP P0A526
D	203	HIS	-	expression tag	UNP P0A526
D	204	HIS	-	expression tag	UNP P0A526
D	205	HIS	-	expression tag	UNP P0A526
E	0	MET	-	expression tag	UNP P0A526
E	1	ALA	-	expression tag	UNP P0A526
E	201	GLY	-	expression tag	UNP P0A526
E	202	HIS	-	expression tag	UNP P0A526
E	203	HIS	-	expression tag	UNP P0A526
E	204	HIS	-	expression tag	UNP P0A526
E	205	HIS	-	expression tag	UNP P0A526
F	0	MET	-	expression tag	UNP P0A526
F	1	ALA	-	expression tag	UNP P0A526
F	201	GLY	-	expression tag	UNP P0A526
F	202	HIS	-	expression tag	UNP P0A526
F	203	HIS	-	expression tag	UNP P0A526
F	204	HIS	-	expression tag	UNP P0A526
F	205	HIS	-	expression tag	UNP P0A526
G	0	MET	-	expression tag	UNP P0A526

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	expression tag	UNP P0A526
G	201	GLY	-	expression tag	UNP P0A526
G	202	HIS	-	expression tag	UNP P0A526
G	203	HIS	-	expression tag	UNP P0A526
G	204	HIS	-	expression tag	UNP P0A526
G	205	HIS	-	expression tag	UNP P0A526
H	0	MET	-	expression tag	UNP P0A526
H	1	ALA	-	expression tag	UNP P0A526
H	201	GLY	-	expression tag	UNP P0A526
H	202	HIS	-	expression tag	UNP P0A526
H	203	HIS	-	expression tag	UNP P0A526
H	204	HIS	-	expression tag	UNP P0A526
H	205	HIS	-	expression tag	UNP P0A526
I	0	MET	-	expression tag	UNP P0A526
I	1	ALA	-	expression tag	UNP P0A526
I	201	GLY	-	expression tag	UNP P0A526
I	202	HIS	-	expression tag	UNP P0A526
I	203	HIS	-	expression tag	UNP P0A526
I	204	HIS	-	expression tag	UNP P0A526
I	205	HIS	-	expression tag	UNP P0A526
J	0	MET	-	expression tag	UNP P0A526
J	1	ALA	-	expression tag	UNP P0A526
J	201	GLY	-	expression tag	UNP P0A526
J	202	HIS	-	expression tag	UNP P0A526
J	203	HIS	-	expression tag	UNP P0A526
J	204	HIS	-	expression tag	UNP P0A526
J	205	HIS	-	expression tag	UNP P0A526
K	0	MET	-	expression tag	UNP P0A526
K	1	ALA	-	expression tag	UNP P0A526
K	201	GLY	-	expression tag	UNP P0A526
K	202	HIS	-	expression tag	UNP P0A526
K	203	HIS	-	expression tag	UNP P0A526
K	204	HIS	-	expression tag	UNP P0A526
K	205	HIS	-	expression tag	UNP P0A526
L	0	MET	-	expression tag	UNP P0A526
L	1	ALA	-	expression tag	UNP P0A526
L	201	GLY	-	expression tag	UNP P0A526
L	202	HIS	-	expression tag	UNP P0A526
L	203	HIS	-	expression tag	UNP P0A526
L	204	HIS	-	expression tag	UNP P0A526
L	205	HIS	-	expression tag	UNP P0A526
M	0	MET	-	expression tag	UNP P0A526

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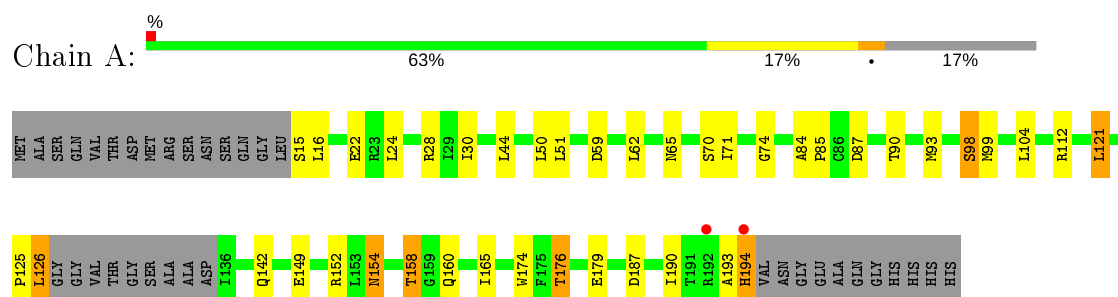
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Chain	Residue	Modelled	Actual	Comment	Reference
M	1	ALA	-	expression tag	UNP P0A526
M	201	GLY	-	expression tag	UNP P0A526
M	202	HIS	-	expression tag	UNP P0A526
M	203	HIS	-	expression tag	UNP P0A526
M	204	HIS	-	expression tag	UNP P0A526
M	205	HIS	-	expression tag	UNP P0A526
N	0	MET	-	expression tag	UNP P0A526
N	1	ALA	-	expression tag	UNP P0A526
N	201	GLY	-	expression tag	UNP P0A526
N	202	HIS	-	expression tag	UNP P0A526
N	203	HIS	-	expression tag	UNP P0A526
N	204	HIS	-	expression tag	UNP P0A526
N	205	HIS	-	expression tag	UNP P0A526

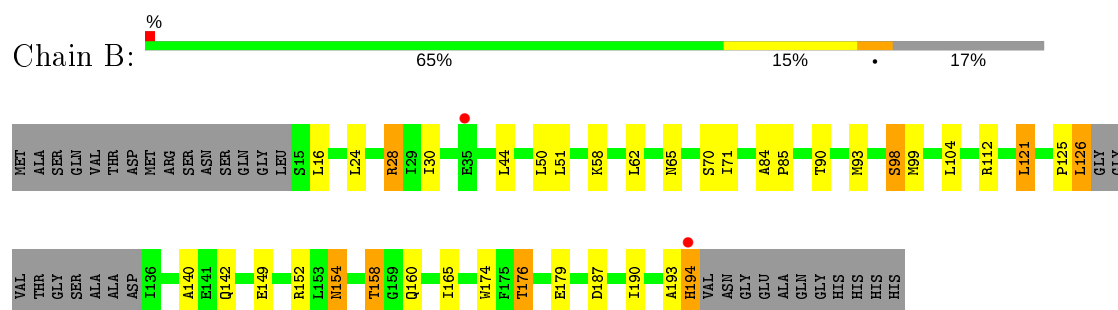
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

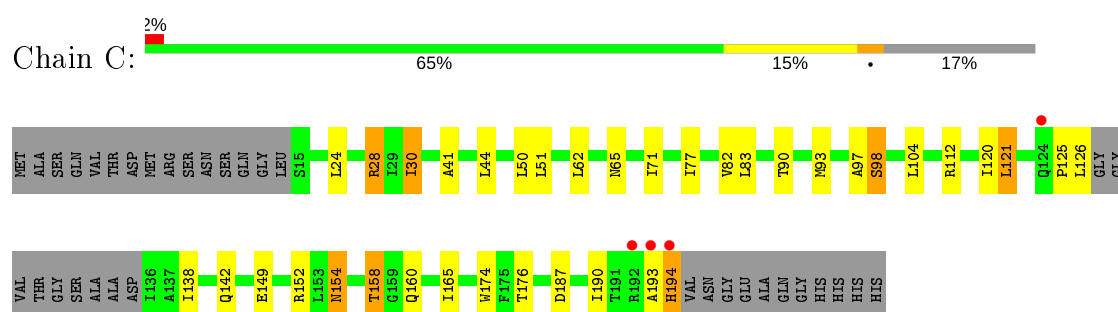
#### • Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



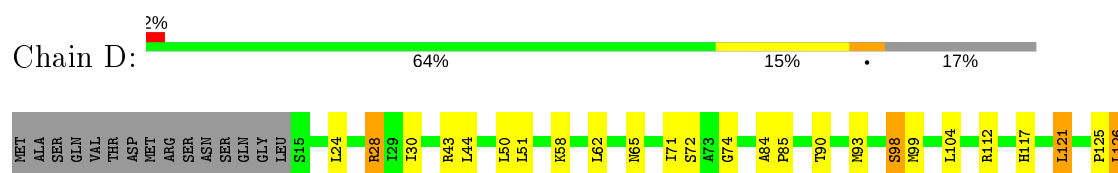
#### • Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



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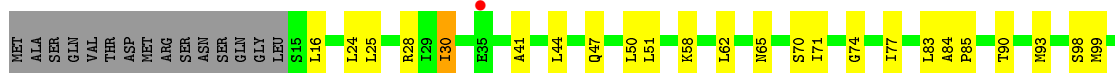




- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



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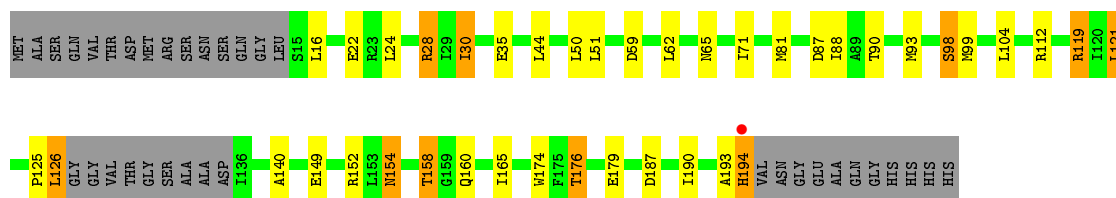


- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1

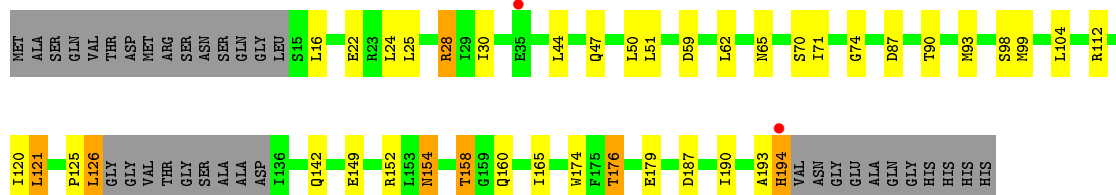


- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1

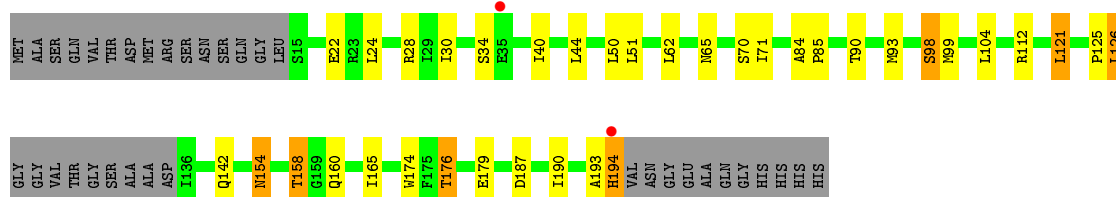




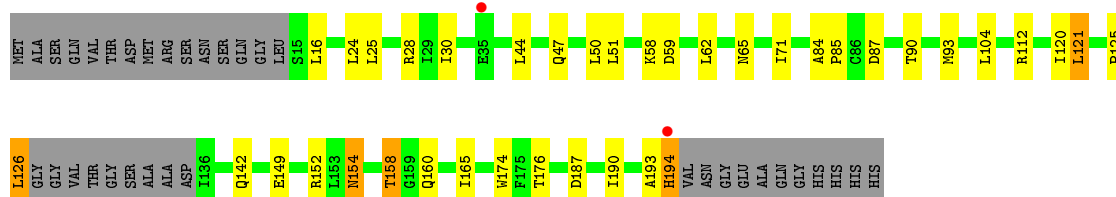
- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



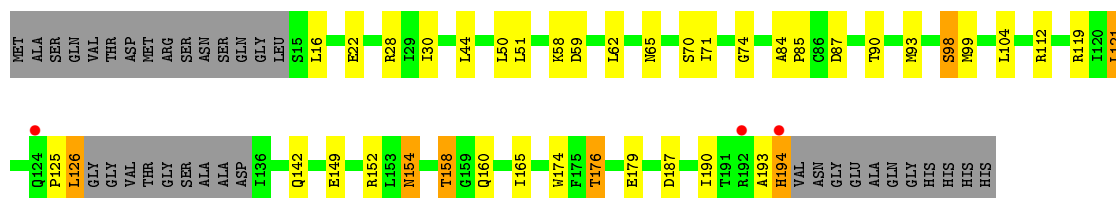
- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



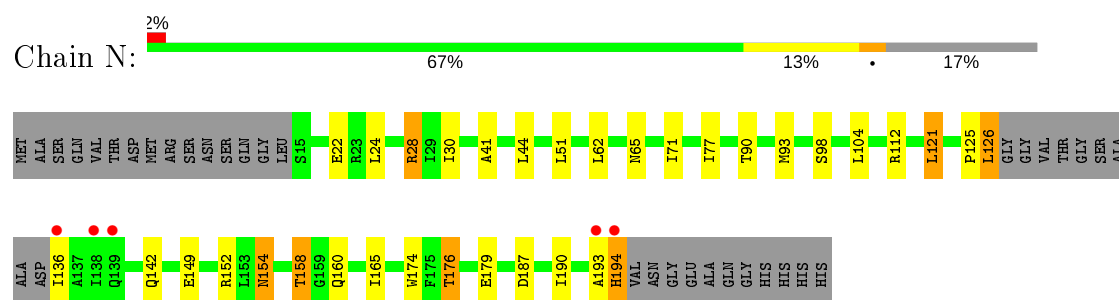
- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



- Molecule 1: ATP-DEPENDENT CLP PROTEASE PROTEOLYTIC SUBUNIT 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.72Å 168.22Å 103.76Å 90.00° 114.60° 90.00°	Depositor
Resolution (Å)	19.87 – 3.00 19.87 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.87-3.00) 100.0 (19.87-3.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.213 , 0.238 0.215 , 0.237	Depositor DCC
$R_{free}$ test set	3036 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18482	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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	0.55	0/1344	0.66	1/1815 (0.1%)
1	B	0.60	0/1342	0.70	1/1812 (0.1%)
1	C	0.68	0/1342	0.75	1/1812 (0.1%)
1	D	0.72	0/1342	0.74	1/1812 (0.1%)
1	E	0.66	0/1342	0.73	1/1812 (0.1%)
1	F	0.76	0/1342	0.79	2/1812 (0.1%)
1	G	0.68	0/1342	0.70	1/1812 (0.1%)
1	H	0.70	0/1342	0.74	1/1812 (0.1%)
1	I	0.76	0/1342	0.81	2/1812 (0.1%)
1	J	0.62	0/1342	0.71	2/1812 (0.1%)
1	K	0.60	0/1342	0.72	1/1812 (0.1%)
1	L	0.72	0/1342	0.77	1/1812 (0.1%)
1	M	0.59	0/1342	0.68	1/1812 (0.1%)
1	N	0.58	0/1342	0.70	1/1812 (0.1%)
All	All	0.66	0/18790	0.73	17/25371 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	121	LEU	CA-CB-CG	7.06	131.55	115.30
1	K	121	LEU	CA-CB-CG	6.73	130.78	115.30
1	N	121	LEU	CA-CB-CG	6.71	130.74	115.30
1	A	121	LEU	CA-CB-CG	6.57	130.41	115.30
1	B	121	LEU	CA-CB-CG	6.46	130.17	115.30
1	I	121	LEU	CA-CB-CG	6.46	130.15	115.30
1	F	121	LEU	CA-CB-CG	6.16	129.48	115.30
1	M	121	LEU	CA-CB-CG	6.05	129.21	115.30
1	C	121	LEU	CA-CB-CG	6.05	129.21	115.30
1	D	121	LEU	CA-CB-CG	5.96	129.01	115.30
1	J	121	LEU	CA-CB-CG	5.93	128.93	115.30
1	E	121	LEU	CA-CB-CG	5.89	128.84	115.30
1	L	121	LEU	CA-CB-CG	5.81	128.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	121	LEU	CA-CB-CG	5.72	128.47	115.30
1	F	173	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	I	119	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	J	28	ARG	NE-CZ-NH2	5.03	122.82	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	1322	0	1316	41	0
1	B	1320	0	1315	37	0
1	C	1320	0	1315	33	0
1	D	1320	0	1315	37	0
1	E	1320	0	1315	39	0
1	F	1320	0	1315	40	0
1	G	1320	0	1315	44	0
1	H	1320	0	1315	31	0
1	I	1320	0	1315	34	0
1	J	1320	0	1315	41	0
1	K	1320	0	1315	34	0
1	L	1320	0	1315	36	0
1	M	1320	0	1315	37	0
1	N	1320	0	1315	34	0
All	All	18482	0	18411	450	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 12.

All (450) 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:M:121:LEU:HD11	1:N:142:GLN:HE22	1.18	1.09
1:D:142:GLN:HE22	1:E:121:LEU:HD11	1.13	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:THR:HG22	1:L:104:LEU:HD12	1.34	1.06
1:E:90:THR:HG22	1:E:104:LEU:HD12	1.36	1.06
1:M:90:THR:HG22	1:M:104:LEU:HD12	1.37	1.04
1:J:90:THR:HG22	1:J:104:LEU:HD12	1.40	1.04
1:A:90:THR:HG22	1:A:104:LEU:HD12	1.37	1.04
1:N:90:THR:HG22	1:N:104:LEU:HD12	1.40	1.03
1:H:90:THR:HG22	1:H:104:LEU:HD12	1.38	1.03
1:B:90:THR:HG22	1:B:104:LEU:HD12	1.37	1.02
1:C:90:THR:HG22	1:C:104:LEU:HD12	1.39	1.02
1:G:90:THR:HG22	1:G:104:LEU:HD12	1.40	1.02
1:F:90:THR:HG22	1:F:104:LEU:HD12	1.37	1.01
1:D:90:THR:HG22	1:D:104:LEU:HD12	1.42	1.00
1:K:90:THR:HG22	1:K:104:LEU:HD12	1.40	1.00
1:I:90:THR:HG22	1:I:104:LEU:HD12	1.43	0.98
1:D:142:GLN:NE2	1:E:121:LEU:HD11	1.78	0.97
1:M:121:LEU:HD11	1:N:142:GLN:NE2	1.84	0.92
1:A:90:THR:HG21	1:A:104:LEU:HA	1.54	0.89
1:C:90:THR:HG21	1:C:104:LEU:HA	1.53	0.89
1:E:90:THR:CG2	1:E:104:LEU:HD12	2.02	0.89
1:M:90:THR:HG21	1:M:104:LEU:HA	1.54	0.87
1:A:90:THR:CG2	1:A:104:LEU:HD12	2.05	0.86
1:B:90:THR:CG2	1:B:104:LEU:HD12	2.04	0.86
1:G:90:THR:HG21	1:G:104:LEU:HA	1.58	0.86
1:F:50:LEU:HB2	1:G:24:LEU:HD13	1.58	0.86
1:L:90:THR:CG2	1:L:104:LEU:HD12	2.06	0.86
1:D:90:THR:CG2	1:D:104:LEU:HD12	2.07	0.85
1:N:90:THR:CG2	1:N:104:LEU:HD12	2.07	0.85
1:F:90:THR:CG2	1:F:104:LEU:HD12	2.05	0.85
1:J:90:THR:CG2	1:J:104:LEU:HD12	2.05	0.85
1:C:90:THR:CG2	1:C:104:LEU:HD12	2.07	0.84
1:G:126:LEU:O	1:N:136:ILE:CD1	2.25	0.84
1:H:90:THR:CG2	1:H:104:LEU:HD12	2.07	0.84
1:A:121:LEU:HD11	1:G:142:GLN:HE22	1.43	0.83
1:N:90:THR:HG21	1:N:104:LEU:HA	1.58	0.83
1:G:90:THR:CG2	1:G:104:LEU:HD12	2.08	0.83
1:L:90:THR:HG21	1:L:104:LEU:HA	1.61	0.83
1:H:90:THR:HG21	1:H:104:LEU:HA	1.60	0.82
1:K:90:THR:HG21	1:K:104:LEU:HA	1.60	0.82
1:M:90:THR:CG2	1:M:104:LEU:HD12	2.09	0.82
1:H:50:LEU:HB2	1:N:24:LEU:HD13	1.59	0.81
1:K:90:THR:CG2	1:K:104:LEU:HD12	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:90:THR:CG2	1:I:104:LEU:HD12	2.10	0.81
1:B:90:THR:HG21	1:B:104:LEU:HA	1.62	0.80
1:D:90:THR:HG21	1:D:104:LEU:HA	1.63	0.80
1:E:90:THR:HG21	1:E:104:LEU:HA	1.63	0.80
1:G:126:LEU:O	1:N:136:ILE:HD12	1.82	0.79
1:I:28:ARG:NH1	1:I:51:LEU:HB3	1.98	0.79
1:N:158:THR:HG21	1:N:165:ILE:HD11	1.65	0.78
1:J:90:THR:HG21	1:J:104:LEU:HA	1.64	0.78
1:A:126:LEU:O	1:H:136:ILE:HD12	1.83	0.78
1:G:158:THR:HG21	1:G:165:ILE:HD11	1.65	0.77
1:K:24:LEU:HD13	1:L:50:LEU:HB2	1.66	0.77
1:A:158:THR:HG21	1:A:165:ILE:HD11	1.65	0.77
1:M:158:THR:HG21	1:M:165:ILE:HD11	1.66	0.77
1:F:158:THR:HG21	1:F:165:ILE:HD11	1.68	0.76
1:N:28:ARG:NH1	1:N:51:LEU:HB3	1.99	0.76
1:E:158:THR:HG21	1:E:165:ILE:HD11	1.68	0.76
1:K:193:ALA:O	1:K:194:HIS:HB2	1.85	0.76
1:H:28:ARG:NH1	1:H:51:LEU:HB3	2.01	0.76
1:J:30:ILE:HG22	1:J:62:LEU:HD13	1.68	0.76
1:L:158:THR:HG21	1:L:165:ILE:HD11	1.67	0.76
1:K:158:THR:HG21	1:K:165:ILE:HD11	1.68	0.75
1:C:158:THR:HG21	1:C:165:ILE:HD11	1.67	0.75
1:H:158:THR:HG21	1:H:165:ILE:HD11	1.67	0.75
1:B:158:THR:HG21	1:B:165:ILE:HD11	1.68	0.75
1:C:50:LEU:HB2	1:D:24:LEU:HD13	1.68	0.75
1:D:193:ALA:O	1:D:194:HIS:HB2	1.86	0.75
1:H:193:ALA:O	1:H:194:HIS:HB2	1.87	0.75
1:J:121:LEU:HD11	1:K:142:GLN:HE22	1.51	0.75
1:I:90:THR:HG21	1:I:104:LEU:HA	1.69	0.75
1:J:28:ARG:NH1	1:J:51:LEU:HB3	2.02	0.75
1:F:90:THR:HG21	1:F:104:LEU:HA	1.67	0.74
1:N:193:ALA:O	1:N:194:HIS:HB2	1.88	0.74
1:E:193:ALA:O	1:E:194:HIS:HB2	1.88	0.73
1:I:193:ALA:O	1:I:194:HIS:HB2	1.88	0.73
1:K:28:ARG:NH1	1:K:51:LEU:HB3	2.04	0.73
1:B:193:ALA:O	1:B:194:HIS:HB2	1.88	0.72
1:M:28:ARG:NH1	1:M:51:LEU:HB3	2.04	0.71
1:B:28:ARG:NH1	1:B:51:LEU:HB3	2.05	0.71
1:C:28:ARG:NH1	1:C:51:LEU:HB3	2.05	0.71
1:G:193:ALA:O	1:G:194:HIS:HB2	1.89	0.71
1:M:193:ALA:O	1:M:194:HIS:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:193:ALA:O	1:J:194:HIS:HB2	1.90	0.71
1:J:158:THR:HG21	1:J:165:ILE:HD11	1.71	0.71
1:F:193:ALA:O	1:F:194:HIS:HB2	1.89	0.70
1:E:71:ILE:HD11	1:E:125:PRO:HG2	1.74	0.70
1:H:65:ASN:HB2	1:H:93:MET:O	1.91	0.69
1:D:71:ILE:HD11	1:D:125:PRO:HG2	1.75	0.69
1:I:158:THR:HG21	1:I:165:ILE:HD11	1.74	0.69
1:M:90:THR:CG2	1:M:104:LEU:HA	2.22	0.69
1:K:90:THR:CG2	1:K:104:LEU:HA	2.23	0.68
1:G:90:THR:CG2	1:G:104:LEU:HA	2.23	0.68
1:C:193:ALA:O	1:C:194:HIS:HB2	1.93	0.68
1:L:28:ARG:NH1	1:L:51:LEU:HB3	2.08	0.68
1:N:90:THR:CG2	1:N:104:LEU:HA	2.23	0.68
1:C:90:THR:CG2	1:C:104:LEU:HA	2.21	0.68
1:F:28:ARG:NH1	1:F:51:LEU:HB3	2.09	0.68
1:D:158:THR:HG21	1:D:165:ILE:HD11	1.74	0.67
1:E:28:ARG:NH1	1:E:51:LEU:HB3	2.10	0.67
1:A:193:ALA:O	1:A:194:HIS:HB2	1.93	0.67
1:B:90:THR:CG2	1:B:104:LEU:HA	2.25	0.67
1:L:193:ALA:O	1:L:194:HIS:HB2	1.93	0.67
1:D:50:LEU:HB2	1:E:24:LEU:HD13	1.76	0.67
1:A:28:ARG:NH1	1:A:51:LEU:HB3	2.09	0.67
1:A:90:THR:CG2	1:A:104:LEU:HA	2.23	0.66
1:A:174:TRP:CE2	1:G:142:GLN:HG2	2.30	0.66
1:A:71:ILE:HD11	1:A:125:PRO:HG2	1.78	0.66
1:G:28:ARG:NH1	1:G:51:LEU:HB3	2.11	0.66
1:D:28:ARG:NH1	1:D:51:LEU:HB3	2.11	0.65
1:E:90:THR:CG2	1:E:104:LEU:HA	2.26	0.65
1:H:90:THR:CG2	1:H:104:LEU:HA	2.26	0.65
1:B:50:LEU:HB2	1:C:24:LEU:HD13	1.78	0.65
1:I:121:LEU:HD11	1:J:142:GLN:HE22	1.61	0.65
1:D:30:ILE:HG22	1:D:62:LEU:HD13	1.79	0.65
1:H:71:ILE:HD11	1:H:125:PRO:HG2	1.78	0.65
1:F:30:ILE:HG22	1:F:62:LEU:HD13	1.79	0.64
1:L:90:THR:CG2	1:L:104:LEU:HA	2.26	0.64
1:B:30:ILE:HG22	1:B:62:LEU:HD13	1.80	0.64
1:L:71:ILE:HD11	1:L:125:PRO:HG2	1.79	0.64
1:J:24:LEU:HD13	1:K:50:LEU:HB2	1.79	0.63
1:B:142:GLN:HE22	1:C:121:LEU:HD11	1.62	0.63
1:C:71:ILE:HD11	1:C:125:PRO:HG2	1.80	0.63
1:N:30:ILE:HG22	1:N:62:LEU:HD13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:HG21	1:B:104:LEU:O	1.99	0.63
1:I:71:ILE:HD11	1:I:125:PRO:HG2	1.80	0.63
1:L:30:ILE:HG22	1:L:62:LEU:HD13	1.80	0.62
1:N:71:ILE:HD11	1:N:125:PRO:HG2	1.80	0.62
1:D:90:THR:CG2	1:D:104:LEU:HA	2.29	0.62
1:G:71:ILE:HD11	1:G:125:PRO:HG2	1.81	0.62
1:J:158:THR:HG23	1:J:160:GLN:HG2	1.80	0.62
1:N:121:LEU:HD13	1:N:174:TRP:HB3	1.82	0.62
1:F:71:ILE:HD11	1:F:125:PRO:HG2	1.81	0.61
1:B:71:ILE:HD11	1:B:125:PRO:HG2	1.81	0.61
1:K:30:ILE:HG22	1:K:62:LEU:HD13	1.82	0.61
1:B:65:ASN:HB2	1:B:93:MET:O	2.01	0.61
1:L:65:ASN:HB2	1:L:93:MET:O	1.99	0.61
1:F:90:THR:CG2	1:F:104:LEU:HA	2.31	0.61
1:A:90:THR:HG21	1:A:104:LEU:CA	2.30	0.60
1:I:90:THR:CG2	1:I:104:LEU:HA	2.31	0.60
1:M:71:ILE:HD11	1:M:125:PRO:HG2	1.83	0.60
1:E:142:GLN:HG2	1:F:174:TRP:CE2	2.37	0.60
1:A:121:LEU:HD11	1:G:142:GLN:NE2	2.15	0.60
1:I:90:THR:HG21	1:I:104:LEU:O	2.02	0.60
1:G:90:THR:HG21	1:G:104:LEU:CA	2.31	0.60
1:C:154:ASN:O	1:C:158:THR:HB	2.02	0.59
1:E:112:ARG:HD3	1:E:187:ASP:OD2	2.02	0.59
1:E:50:LEU:HB2	1:F:24:LEU:HD13	1.83	0.59
1:H:24:LEU:HD13	1:I:50:LEU:HB2	1.83	0.59
1:J:121:LEU:HD11	1:K:142:GLN:NE2	2.16	0.59
1:C:30:ILE:HG22	1:C:62:LEU:HD13	1.84	0.59
1:L:174:TRP:CE2	1:M:142:GLN:HG2	2.36	0.59
1:M:90:THR:HG21	1:M:104:LEU:CA	2.29	0.59
1:J:71:ILE:HD11	1:J:125:PRO:HG2	1.83	0.59
1:K:90:THR:HG21	1:K:104:LEU:CA	2.31	0.59
1:E:90:THR:HG21	1:E:104:LEU:O	2.03	0.59
1:F:158:THR:HG23	1:F:160:GLN:HG2	1.85	0.59
1:C:121:LEU:HD13	1:C:174:TRP:HB3	1.85	0.59
1:J:90:THR:CG2	1:J:104:LEU:HA	2.30	0.59
1:F:154:ASN:O	1:F:158:THR:HB	2.02	0.58
1:G:126:LEU:O	1:N:136:ILE:HD11	2.03	0.58
1:A:16:LEU:HD12	1:G:22:GLU:HG3	1.84	0.58
1:G:121:LEU:HD13	1:G:174:TRP:HB3	1.84	0.58
1:H:90:THR:HG21	1:H:104:LEU:CA	2.32	0.58
1:N:90:THR:HG21	1:N:104:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:ASN:HB2	1:I:93:MET:O	2.03	0.58
1:M:121:LEU:HD13	1:M:174:TRP:HB3	1.85	0.58
1:G:90:THR:HG21	1:G:104:LEU:O	2.03	0.58
1:K:90:THR:HG21	1:K:104:LEU:O	2.04	0.58
1:J:121:LEU:HD13	1:J:174:TRP:HB3	1.86	0.57
1:K:71:ILE:HD11	1:K:125:PRO:HG2	1.85	0.57
1:L:158:THR:HG23	1:L:160:GLN:HG2	1.86	0.57
1:E:65:ASN:HB2	1:E:93:MET:O	2.04	0.57
1:A:121:LEU:HD13	1:A:174:TRP:HB3	1.86	0.57
1:B:90:THR:HG21	1:B:104:LEU:CA	2.32	0.57
1:A:126:LEU:O	1:H:136:ILE:CD1	2.52	0.57
1:F:90:THR:HG21	1:F:104:LEU:O	2.04	0.57
1:A:22:GLU:HG3	1:B:16:LEU:HD12	1.87	0.57
1:E:22:GLU:HG3	1:F:16:LEU:HD12	1.85	0.57
1:A:24:LEU:HD13	1:G:50:LEU:HB2	1.85	0.57
1:F:65:ASN:HB2	1:F:93:MET:O	2.05	0.57
1:G:154:ASN:O	1:G:158:THR:HB	2.05	0.57
1:J:154:ASN:O	1:J:158:THR:HB	2.04	0.57
1:E:90:THR:HG21	1:E:104:LEU:CA	2.34	0.57
1:B:142:GLN:NE2	1:C:121:LEU:HD11	2.21	0.56
1:L:16:LEU:HD12	1:M:22:GLU:HG3	1.87	0.56
1:C:90:THR:HG21	1:C:104:LEU:CA	2.29	0.56
1:K:121:LEU:HD13	1:K:174:TRP:HB3	1.87	0.56
1:N:28:ARG:HH11	1:N:51:LEU:HB3	1.68	0.56
1:N:90:THR:HG21	1:N:104:LEU:CA	2.31	0.56
1:G:136:ILE:HD11	1:N:126:LEU:O	2.06	0.56
1:I:30:ILE:HG22	1:I:62:LEU:HD13	1.86	0.56
1:E:158:THR:HG23	1:E:160:GLN:HG2	1.88	0.56
1:D:112:ARG:HD3	1:D:187:ASP:OD2	2.06	0.56
1:C:65:ASN:HB2	1:C:93:MET:O	2.06	0.56
1:B:158:THR:HG23	1:B:160:GLN:HG2	1.88	0.56
1:D:154:ASN:O	1:D:158:THR:HB	2.06	0.56
1:G:158:THR:HG23	1:G:160:GLN:HG2	1.88	0.56
1:L:154:ASN:O	1:L:158:THR:HB	2.06	0.56
1:N:158:THR:HG23	1:N:160:GLN:HG2	1.87	0.56
1:D:158:THR:HG23	1:D:160:GLN:HG2	1.88	0.55
1:I:24:LEU:HD13	1:J:50:LEU:HB2	1.88	0.55
1:H:154:ASN:O	1:H:158:THR:HB	2.07	0.55
1:I:149:GLU:OE2	1:I:152:ARG:NH1	2.40	0.55
1:D:90:THR:HG21	1:D:104:LEU:CA	2.36	0.55
1:L:158:THR:HG23	1:L:160:GLN:CG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:ARG:HD3	1:L:187:ASP:OD2	2.07	0.55
1:L:90:THR:HG21	1:L:104:LEU:CA	2.33	0.55
1:H:30:ILE:HG22	1:H:62:LEU:HD13	1.88	0.54
1:F:158:THR:HG23	1:F:160:GLN:CG	2.37	0.54
1:H:90:THR:HG21	1:H:104:LEU:O	2.07	0.54
1:J:28:ARG:HH11	1:J:51:LEU:HB3	1.73	0.54
1:M:28:ARG:HH11	1:M:51:LEU:HB3	1.71	0.54
1:A:30:ILE:HG22	1:A:62:LEU:HD13	1.90	0.54
1:I:28:ARG:HH11	1:I:51:LEU:HB3	1.70	0.54
1:D:74:GLY:HA3	1:D:99:MET:HE2	1.89	0.54
1:L:90:THR:HG21	1:L:104:LEU:O	2.06	0.54
1:A:154:ASN:O	1:A:158:THR:HB	2.07	0.54
1:C:120:ILE:HD12	1:C:120:ILE:N	2.23	0.54
1:C:28:ARG:HH11	1:C:51:LEU:HB3	1.72	0.53
1:I:71:ILE:H	1:I:126:LEU:HD11	1.71	0.53
1:K:158:THR:HG23	1:K:160:GLN:HG2	1.91	0.53
1:G:158:THR:HG23	1:G:160:GLN:CG	2.38	0.53
1:I:121:LEU:HD11	1:J:142:GLN:NE2	2.23	0.53
1:N:154:ASN:O	1:N:158:THR:HB	2.09	0.53
1:N:65:ASN:HB2	1:N:93:MET:O	2.09	0.53
1:C:149:GLU:OE2	1:C:152:ARG:NH1	2.42	0.53
1:D:121:LEU:HD13	1:D:174:TRP:HB3	1.90	0.53
1:G:176:THR:HG22	1:G:179:GLU:H	1.73	0.53
1:F:121:LEU:HD13	1:F:174:TRP:HB3	1.91	0.53
1:J:90:THR:HG21	1:J:104:LEU:O	2.09	0.53
1:L:24:LEU:HD13	1:M:50:LEU:HB2	1.90	0.53
1:D:71:ILE:H	1:D:126:LEU:HD11	1.74	0.53
1:G:74:GLY:HA3	1:G:99:MET:HE2	1.91	0.53
1:I:16:LEU:HD12	1:J:22:GLU:HG3	1.91	0.53
1:E:154:ASN:O	1:E:158:THR:HB	2.09	0.52
1:K:121:LEU:HD11	1:L:142:GLN:HE22	1.75	0.52
1:J:158:THR:HG23	1:J:160:GLN:CG	2.38	0.52
1:B:28:ARG:HH11	1:B:51:LEU:HB3	1.74	0.52
1:C:158:THR:HG23	1:C:160:GLN:HG2	1.90	0.52
1:H:121:LEU:HD13	1:H:174:TRP:HB3	1.91	0.52
1:I:154:ASN:O	1:I:158:THR:HB	2.09	0.52
1:B:154:ASN:O	1:B:158:THR:HB	2.10	0.51
1:M:30:ILE:HG22	1:M:62:LEU:HD13	1.92	0.51
1:A:50:LEU:HB2	1:B:24:LEU:HD13	1.92	0.51
1:K:121:LEU:HD11	1:L:142:GLN:NE2	2.26	0.51
1:D:90:THR:HG21	1:D:104:LEU:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:ASN:HB2	1:G:93:MET:O	2.10	0.51
1:J:71:ILE:H	1:J:126:LEU:HD11	1.74	0.51
1:G:30:ILE:HG22	1:G:62:LEU:HD13	1.93	0.51
1:H:158:THR:HG23	1:H:160:GLN:HG2	1.93	0.51
1:I:28:ARG:HH12	1:I:51:LEU:HB3	1.74	0.51
1:E:176:THR:HG22	1:E:179:GLU:H	1.74	0.51
1:H:65:ASN:CB	1:H:93:MET:O	2.59	0.51
1:D:30:ILE:HG22	1:D:62:LEU:CD1	2.40	0.50
1:F:83:LEU:HA	1:G:191:THR:O	2.11	0.50
1:M:65:ASN:HB2	1:M:93:MET:O	2.11	0.50
1:J:149:GLU:OE2	1:J:152:ARG:NH1	2.44	0.50
1:K:154:ASN:O	1:K:158:THR:HB	2.11	0.50
1:K:28:ARG:HH11	1:K:51:LEU:HB3	1.73	0.50
1:A:112:ARG:HD3	1:A:187:ASP:OD2	2.11	0.50
1:D:158:THR:HG23	1:D:160:GLN:CG	2.41	0.50
1:I:176:THR:HG22	1:I:179:GLU:H	1.76	0.50
1:G:136:ILE:CD1	1:N:126:LEU:O	2.58	0.50
1:I:158:THR:HG23	1:I:160:GLN:CG	2.41	0.50
1:N:158:THR:HG23	1:N:160:GLN:CG	2.42	0.50
1:B:121:LEU:HD13	1:B:174:TRP:HB3	1.94	0.50
1:M:90:THR:HG21	1:M:104:LEU:O	2.12	0.50
1:M:74:GLY:HA3	1:M:99:MET:HE2	1.94	0.50
1:F:83:LEU:CD1	1:G:190:ILE:HD12	2.41	0.50
1:M:112:ARG:HD3	1:M:187:ASP:OD2	2.12	0.50
1:F:90:THR:HG21	1:F:104:LEU:CA	2.39	0.49
1:C:90:THR:HG21	1:C:104:LEU:O	2.12	0.49
1:J:90:THR:HG21	1:J:104:LEU:CA	2.38	0.49
1:C:149:GLU:HG2	1:D:117:HIS:CD2	2.47	0.49
1:I:90:THR:HG21	1:I:104:LEU:CA	2.40	0.49
1:C:158:THR:HG23	1:C:160:GLN:CG	2.43	0.49
1:E:158:THR:HG23	1:E:160:GLN:CG	2.43	0.49
1:H:16:LEU:HD12	1:I:22:GLU:HG3	1.94	0.49
1:L:28:ARG:NH2	1:L:58:LYS:O	2.45	0.49
1:L:30:ILE:HG22	1:L:62:LEU:CD1	2.41	0.49
1:A:90:THR:HG21	1:A:104:LEU:O	2.12	0.49
1:N:28:ARG:HH12	1:N:51:LEU:HB3	1.78	0.49
1:K:71:ILE:H	1:K:126:LEU:HD11	1.78	0.48
1:A:174:TRP:CD2	1:G:142:GLN:HG2	2.49	0.48
1:A:158:THR:HG23	1:A:160:GLN:HG2	1.94	0.48
1:G:112:ARG:HD3	1:G:187:ASP:OD2	2.13	0.48
1:J:30:ILE:HG22	1:J:62:LEU:CD1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:HB2	1:A:93:MET:O	2.14	0.48
1:B:149:GLU:OE2	1:B:152:ARG:NH1	2.47	0.48
1:L:16:LEU:CD1	1:M:22:GLU:HG3	2.44	0.48
1:H:28:ARG:HH11	1:H:51:LEU:HB3	1.73	0.48
1:K:65:ASN:HB2	1:K:93:MET:O	2.14	0.48
1:A:74:GLY:HA3	1:A:99:MET:HE2	1.95	0.47
1:L:121:LEU:HD13	1:L:174:TRP:HB3	1.96	0.47
1:D:65:ASN:HB2	1:D:93:MET:O	2.14	0.47
1:E:98:SER:HB3	1:E:99:MET:H	1.46	0.47
1:L:149:GLU:OE2	1:L:152:ARG:NH1	2.48	0.47
1:E:30:ILE:HG22	1:E:62:LEU:HD13	1.97	0.47
1:G:149:GLU:OE2	1:G:152:ARG:NH1	2.48	0.47
1:J:74:GLY:HA3	1:J:99:MET:HE2	1.97	0.47
1:B:112:ARG:HD3	1:B:187:ASP:OD2	2.15	0.47
1:M:158:THR:HG23	1:M:160:GLN:HG2	1.96	0.47
1:C:30:ILE:HG22	1:C:62:LEU:CD1	2.45	0.47
1:J:176:THR:HG22	1:J:179:GLU:H	1.79	0.47
1:C:82:VAL:HG12	1:D:191:THR:O	2.15	0.47
1:K:176:THR:HG22	1:K:179:GLU:H	1.80	0.47
1:B:28:ARG:NH2	1:B:58:LYS:O	2.48	0.47
1:M:71:ILE:H	1:M:126:LEU:HD11	1.79	0.46
1:E:121:LEU:HD13	1:E:174:TRP:HB3	1.97	0.46
1:F:83:LEU:O	1:G:193:ALA:N	2.47	0.46
1:A:158:THR:HG23	1:A:160:GLN:CG	2.45	0.46
1:B:71:ILE:H	1:B:126:LEU:HD11	1.81	0.46
1:E:59:ASP:OD1	1:E:87:ASP:HB2	2.15	0.46
1:J:112:ARG:HD3	1:J:187:ASP:OD2	2.14	0.46
1:A:22:GLU:HG3	1:B:16:LEU:CD1	2.45	0.46
1:E:22:GLU:HG3	1:F:16:LEU:CD1	2.45	0.46
1:A:98:SER:HB3	1:A:99:MET:H	1.47	0.46
1:B:84:ALA:HA	1:B:85:PRO:HD3	1.84	0.46
1:M:154:ASN:O	1:M:158:THR:HB	2.16	0.46
1:I:121:LEU:HD13	1:I:174:TRP:HB3	1.97	0.46
1:I:98:SER:HB3	1:I:99:MET:H	1.46	0.46
1:J:16:LEU:HD12	1:K:22:GLU:HG3	1.98	0.46
1:L:28:ARG:HH11	1:L:51:LEU:HB3	1.78	0.46
1:B:158:THR:HG23	1:B:160:GLN:CG	2.46	0.46
1:F:176:THR:HG22	1:F:179:GLU:H	1.81	0.46
1:K:158:THR:HG23	1:K:160:GLN:CG	2.45	0.45
1:M:16:LEU:HD12	1:N:22:GLU:HG3	1.97	0.45
1:D:43:ARG:HG3	1:E:17:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:149:GLU:OE2	1:E:152:ARG:NH1	2.50	0.45
1:G:98:SER:HB3	1:G:99:MET:H	1.49	0.45
1:I:112:ARG:HD3	1:I:187:ASP:OD2	2.17	0.45
1:J:65:ASN:HB2	1:J:93:MET:O	2.16	0.45
1:M:154:ASN:HA	1:M:154:ASN:HD22	1.52	0.45
1:H:149:GLU:OE2	1:H:152:ARG:NH1	2.50	0.45
1:M:149:GLU:OE2	1:M:152:ARG:NH1	2.49	0.45
1:I:158:THR:HG23	1:I:160:GLN:HG2	1.98	0.45
1:E:71:ILE:H	1:E:126:LEU:HD11	1.82	0.45
1:F:28:ARG:HD2	1:F:51:LEU:HD22	1.99	0.45
1:J:30:ILE:HD13	1:J:30:ILE:HG21	1.71	0.45
1:K:28:ARG:HD2	1:K:51:LEU:HD22	1.99	0.45
1:M:59:ASP:OD1	1:M:87:ASP:HB2	2.17	0.45
1:B:140:ALA:HB2	1:I:140:ALA:HB2	1.98	0.45
1:A:176:THR:HG22	1:A:179:GLU:H	1.82	0.45
1:B:98:SER:HB3	1:B:99:MET:H	1.48	0.45
1:A:28:ARG:HH11	1:A:51:LEU:HB3	1.82	0.45
1:E:138:ILE:O	1:E:142:GLN:HG3	2.17	0.45
1:M:98:SER:HB3	1:M:99:MET:H	1.50	0.45
1:N:112:ARG:HD3	1:N:187:ASP:OD2	2.17	0.44
1:A:59:ASP:OD1	1:A:87:ASP:HB2	2.17	0.44
1:E:25:LEU:HD13	1:E:47:GLN:HE21	1.83	0.44
1:A:142:GLN:HE22	1:B:121:LEU:HD11	1.83	0.44
1:G:154:ASN:HD22	1:G:154:ASN:HA	1.57	0.44
1:A:84:ALA:HA	1:A:85:PRO:HD3	1.83	0.44
1:B:176:THR:HG22	1:B:179:GLU:H	1.82	0.44
1:B:154:ASN:HA	1:B:154:ASN:HD22	1.53	0.44
1:A:142:GLN:HG2	1:B:174:TRP:CE2	2.53	0.44
1:H:71:ILE:H	1:H:126:LEU:HD11	1.83	0.44
1:J:25:LEU:HD13	1:J:47:GLN:HE21	1.83	0.44
1:E:154:ASN:HA	1:E:154:ASN:HD22	1.61	0.44
1:N:28:ARG:HD2	1:N:51:LEU:HD22	1.99	0.44
1:F:74:GLY:HA3	1:F:99:MET:HE2	2.00	0.44
1:E:28:ARG:HH11	1:E:51:LEU:HB3	1.80	0.44
1:F:149:GLU:OE2	1:F:152:ARG:NH1	2.51	0.44
1:I:59:ASP:OD1	1:I:87:ASP:HB2	2.18	0.44
1:D:176:THR:HG22	1:D:179:GLU:H	1.83	0.43
1:E:30:ILE:HG21	1:E:30:ILE:HD13	1.73	0.43
1:A:71:ILE:H	1:A:126:LEU:HD11	1.83	0.43
1:E:74:GLY:HA3	1:E:99:MET:HE2	2.01	0.43
1:C:83:LEU:HD13	1:D:190:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:LEU:HD13	1:F:47:GLN:HE21	1.82	0.43
1:J:98:SER:HB3	1:J:99:MET:H	1.50	0.43
1:M:84:ALA:HA	1:M:85:PRO:HD3	1.83	0.43
1:C:41:ALA:HA	1:C:77:ILE:HD11	2.00	0.43
1:I:81:MET:HG2	1:I:88:ILE:HD13	2.00	0.43
1:K:30:ILE:HG22	1:K:62:LEU:CD1	2.48	0.43
1:L:71:ILE:H	1:L:126:LEU:HD11	1.84	0.43
1:N:176:THR:HG22	1:N:179:GLU:H	1.83	0.43
1:C:83:LEU:CD1	1:D:190:ILE:HD12	2.48	0.43
1:D:98:SER:HB3	1:D:99:MET:H	1.53	0.43
1:M:158:THR:HG23	1:M:160:GLN:CG	2.49	0.43
1:N:149:GLU:OE2	1:N:152:ARG:NH1	2.51	0.43
1:A:149:GLU:OE2	1:A:152:ARG:NH1	2.51	0.43
1:F:28:ARG:HH12	1:F:51:LEU:HB3	1.82	0.43
1:L:84:ALA:HA	1:L:85:PRO:HD3	1.84	0.43
1:F:84:ALA:HA	1:F:85:PRO:HD3	1.81	0.42
1:G:30:ILE:HG12	1:G:47:GLN:NE2	2.34	0.42
1:H:112:ARG:HD3	1:H:187:ASP:OD2	2.19	0.42
1:A:28:ARG:HH12	1:A:51:LEU:HB3	1.82	0.42
1:B:28:ARG:HH12	1:B:51:LEU:HB3	1.83	0.42
1:J:59:ASP:OD1	1:J:87:ASP:HB2	2.19	0.42
1:K:28:ARG:HH12	1:K:51:LEU:HB3	1.82	0.42
1:N:30:ILE:HG22	1:N:62:LEU:CD1	2.46	0.42
1:D:28:ARG:NH2	1:D:58:LYS:O	2.52	0.42
1:M:176:THR:HG22	1:M:179:GLU:H	1.84	0.42
1:D:72:SER:HB3	1:E:119:ARG:HH22	1.84	0.42
1:G:30:ILE:HG12	1:G:47:GLN:HE21	1.85	0.42
1:G:28:ARG:HH12	1:G:51:LEU:HB3	1.85	0.42
1:L:28:ARG:HD2	1:L:51:LEU:HD22	2.01	0.42
1:M:28:ARG:NH2	1:M:58:LYS:O	2.53	0.42
1:E:84:ALA:HA	1:E:85:PRO:HD3	1.84	0.42
1:J:24:LEU:HA	1:J:24:LEU:HD12	1.82	0.42
1:M:28:ARG:HD2	1:M:51:LEU:HD22	2.02	0.42
1:N:41:ALA:HA	1:N:77:ILE:HD11	2.02	0.42
1:J:28:ARG:HH12	1:J:51:LEU:HB3	1.79	0.42
1:H:81:MET:HG2	1:H:88:ILE:HD13	2.01	0.42
1:H:84:ALA:HA	1:H:85:PRO:HD3	1.86	0.42
1:L:120:ILE:HD12	1:L:120:ILE:N	2.35	0.42
1:L:154:ASN:HA	1:L:154:ASN:HD22	1.66	0.42
1:F:83:LEU:HD13	1:G:190:ILE:HD12	2.01	0.41
1:H:74:GLY:HA3	1:H:99:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:TRP:CE2	1:K:142:GLN:HG2	2.55	0.41
1:C:138:ILE:O	1:C:142:GLN:HG3	2.20	0.41
1:F:30:ILE:HG21	1:F:30:ILE:HD13	1.77	0.41
1:K:112:ARG:HD3	1:K:187:ASP:OD2	2.20	0.41
1:C:30:ILE:HG21	1:C:30:ILE:HD13	1.67	0.41
1:I:16:LEU:CD1	1:J:22:GLU:HG3	2.51	0.41
1:N:71:ILE:H	1:N:126:LEU:HD11	1.86	0.41
1:D:84:ALA:HA	1:D:85:PRO:HD3	1.86	0.41
1:F:50:LEU:HB2	1:G:24:LEU:CD1	2.40	0.41
1:D:30:ILE:CG2	1:D:62:LEU:HD13	2.46	0.41
1:F:120:ILE:N	1:F:120:ILE:HD12	2.36	0.41
1:F:28:ARG:HH11	1:F:51:LEU:HB3	1.83	0.41
1:H:28:ARG:HH12	1:H:51:LEU:HB3	1.77	0.41
1:K:84:ALA:HA	1:K:85:PRO:HD3	1.80	0.41
1:L:59:ASP:OD1	1:L:87:ASP:HB2	2.20	0.41
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.91	0.41
1:K:34:SER:OG	1:K:40:ILE:HD13	2.21	0.41
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.85	0.41
1:D:193:ALA:O	1:D:194:HIS:CB	2.65	0.41
1:D:28:ARG:HH11	1:D:51:LEU:HB3	1.83	0.41
1:B:28:ARG:HD2	1:B:51:LEU:HD22	2.03	0.41
1:J:30:ILE:CG2	1:J:62:LEU:HD13	2.44	0.41
1:A:154:ASN:HA	1:A:154:ASN:HD22	1.57	0.40
1:C:112:ARG:HD3	1:C:187:ASP:OD2	2.21	0.40
1:F:83:LEU:HD11	1:G:190:ILE:HD12	2.03	0.40
1:I:30:ILE:HG22	1:I:62:LEU:CD1	2.51	0.40
1:F:41:ALA:HA	1:F:77:ILE:HD11	2.03	0.40
1:G:84:ALA:HA	1:G:85:PRO:HD3	1.82	0.40
1:L:174:TRP:CZ2	1:M:142:GLN:HG2	2.56	0.40
1:H:30:ILE:HD13	1:H:30:ILE:HG21	1.73	0.40
1:J:120:ILE:N	1:J:120:ILE:HD12	2.37	0.40
1:C:97:ALA:O	1:C:98:SER:C	2.57	0.40
1:L:25:LEU:HD13	1:L:47:GLN:HE21	1.85	0.40
1:E:149:GLU:HG2	1:F:117:HIS:CD2	2.57	0.40
1:F:28:ARG:NH2	1:F:58:LYS:O	2.55	0.40
1:H:59:ASP:OD1	1:H:87:ASP:HB2	2.21	0.40
1:K:98:SER:HB3	1:K:99:MET:H	1.49	0.40
1:M:30:ILE:HG21	1:M:30:ILE:HD13	1.79	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	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	B	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	C	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	D	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	E	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	F	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	G	167/206 (81%)	160 (96%)	7 (4%)	0	100	100
1	H	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	I	167/206 (81%)	162 (97%)	5 (3%)	0	100	100
1	J	167/206 (81%)	160 (96%)	7 (4%)	0	100	100
1	K	167/206 (81%)	161 (96%)	6 (4%)	0	100	100
1	L	167/206 (81%)	160 (96%)	7 (4%)	0	100	100
1	M	167/206 (81%)	159 (95%)	8 (5%)	0	100	100
1	N	167/206 (81%)	160 (96%)	7 (4%)	0	100	100
All	All	2338/2884 (81%)	2249 (96%)	89 (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	136/161 (84%)	126 (93%)	10 (7%)	13	44
1	B	135/161 (84%)	125 (93%)	10 (7%)	13	44
1	C	135/161 (84%)	125 (93%)	10 (7%)	13	44
1	D	135/161 (84%)	125 (93%)	10 (7%)	13	44
1	E	135/161 (84%)	127 (94%)	8 (6%)	19	54
1	F	135/161 (84%)	125 (93%)	10 (7%)	13	44
1	G	135/161 (84%)	125 (93%)	10 (7%)	13	44
1	H	135/161 (84%)	122 (90%)	13 (10%)	8	32
1	I	135/161 (84%)	123 (91%)	12 (9%)	9	35
1	J	135/161 (84%)	127 (94%)	8 (6%)	19	54
1	K	135/161 (84%)	126 (93%)	9 (7%)	16	49
1	L	135/161 (84%)	128 (95%)	7 (5%)	23	59
1	M	135/161 (84%)	125 (93%)	10 (7%)	13	44
1	N	135/161 (84%)	126 (93%)	9 (7%)	16	49
All	All	1891/2254 (84%)	1755 (93%)	136 (7%)	14	45

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	44	LEU
1	A	70	SER
1	A	98	SER
1	A	126	LEU
1	A	154	ASN
1	A	158	THR
1	A	176	THR
1	A	190	ILE
1	A	194	HIS
1	B	28	ARG
1	B	44	LEU
1	B	70	SER
1	B	98	SER
1	B	126	LEU
1	B	154	ASN
1	B	158	THR
1	B	176	THR
1	B	190	ILE

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Mol	Chain	Res	Type
1	B	194	HIS
1	C	28	ARG
1	C	30	ILE
1	C	44	LEU
1	C	98	SER
1	C	126	LEU
1	C	154	ASN
1	C	158	THR
1	C	176	THR
1	C	190	ILE
1	C	194	HIS
1	D	28	ARG
1	D	44	LEU
1	D	98	SER
1	D	126	LEU
1	D	154	ASN
1	D	158	THR
1	D	176	THR
1	D	186	VAL
1	D	190	ILE
1	D	194	HIS
1	E	44	LEU
1	E	98	SER
1	E	126	LEU
1	E	154	ASN
1	E	158	THR
1	E	176	THR
1	E	190	ILE
1	E	194	HIS
1	F	30	ILE
1	F	44	LEU
1	F	70	SER
1	F	98	SER
1	F	126	LEU
1	F	154	ASN
1	F	158	THR
1	F	176	THR
1	F	190	ILE
1	F	194	HIS
1	G	44	LEU
1	G	70	SER
1	G	98	SER

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Mol	Chain	Res	Type
1	G	119	ARG
1	G	126	LEU
1	G	154	ASN
1	G	158	THR
1	G	176	THR
1	G	190	ILE
1	G	194	HIS
1	H	28	ARG
1	H	30	ILE
1	H	35	GLU
1	H	44	LEU
1	H	98	SER
1	H	121	LEU
1	H	126	LEU
1	H	154	ASN
1	H	158	THR
1	H	176	THR
1	H	186	VAL
1	H	190	ILE
1	H	194	HIS
1	I	28	ARG
1	I	30	ILE
1	I	35	GLU
1	I	44	LEU
1	I	98	SER
1	I	119	ARG
1	I	126	LEU
1	I	154	ASN
1	I	158	THR
1	I	176	THR
1	I	190	ILE
1	I	194	HIS
1	J	44	LEU
1	J	70	SER
1	J	126	LEU
1	J	154	ASN
1	J	158	THR
1	J	176	THR
1	J	190	ILE
1	J	194	HIS
1	K	44	LEU
1	K	70	SER

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Mol	Chain	Res	Type
1	K	98	SER
1	K	126	LEU
1	K	154	ASN
1	K	158	THR
1	K	176	THR
1	K	190	ILE
1	K	194	HIS
1	L	44	LEU
1	L	126	LEU
1	L	154	ASN
1	L	158	THR
1	L	176	THR
1	L	190	ILE
1	L	194	HIS
1	M	44	LEU
1	M	70	SER
1	M	98	SER
1	M	119	ARG
1	M	126	LEU
1	M	154	ASN
1	M	158	THR
1	M	176	THR
1	M	190	ILE
1	M	194	HIS
1	N	28	ARG
1	N	44	LEU
1	N	98	SER
1	N	126	LEU
1	N	154	ASN
1	N	158	THR
1	N	176	THR
1	N	190	ILE
1	N	194	HIS

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

Mol	Chain	Res	Type
1	A	47	GLN
1	A	154	ASN
1	B	47	GLN
1	B	142	GLN
1	B	154	ASN

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Mol	Chain	Res	Type
1	C	47	GLN
1	C	154	ASN
1	D	47	GLN
1	D	154	ASN
1	E	47	GLN
1	E	154	ASN
1	F	47	GLN
1	F	154	ASN
1	G	47	GLN
1	G	142	GLN
1	G	154	ASN
1	H	47	GLN
1	H	154	ASN
1	I	47	GLN
1	I	154	ASN
1	J	47	GLN
1	J	142	GLN
1	J	154	ASN
1	K	47	GLN
1	K	142	GLN
1	K	154	ASN
1	L	47	GLN
1	L	142	GLN
1	L	154	ASN
1	M	47	GLN
1	M	154	ASN
1	N	47	GLN
1	N	142	GLN
1	N	154	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates 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<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	171/206 (83%)	-0.24	2 (1%) 79 54	12, 14, 20, 23	0
1	B	171/206 (83%)	-0.29	2 (1%) 79 54	12, 14, 20, 23	0
1	C	171/206 (83%)	-0.39	4 (2%) 60 31	12, 14, 20, 23	0
1	D	171/206 (83%)	-0.42	4 (2%) 60 31	12, 14, 20, 23	0
1	E	171/206 (83%)	-0.37	2 (1%) 79 54	12, 14, 20, 23	0
1	F	171/206 (83%)	-0.42	4 (2%) 60 31	12, 14, 20, 23	0
1	G	171/206 (83%)	-0.30	5 (2%) 51 23	12, 14, 20, 23	0
1	H	171/206 (83%)	-0.42	4 (2%) 60 31	12, 14, 20, 23	0
1	I	171/206 (83%)	-0.52	1 (0%) 89 72	12, 14, 20, 23	0
1	J	171/206 (83%)	-0.39	2 (1%) 79 54	12, 14, 20, 23	0
1	K	171/206 (83%)	-0.36	2 (1%) 79 54	12, 14, 20, 23	0
1	L	171/206 (83%)	-0.42	2 (1%) 79 54	12, 14, 20, 23	0
1	M	171/206 (83%)	-0.34	3 (1%) 68 40	12, 14, 20, 23	0
1	N	171/206 (83%)	-0.24	5 (2%) 51 23	12, 14, 20, 23	0
All	All	2394/2884 (83%)	-0.37	42 (1%) 68 40	12, 14, 20, 23	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	194	HIS	6.1
1	G	138	ILE	5.4
1	D	194	HIS	5.3
1	N	138	ILE	4.5
1	H	194	HIS	4.5
1	N	194	HIS	4.4
1	B	194	HIS	4.3
1	C	194	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	M	194	HIS	4.1
1	N	139	GLN	3.7
1	F	194	HIS	3.7
1	G	193	ALA	3.6
1	L	194	HIS	3.5
1	D	193	ALA	3.5
1	M	192	ARG	3.4
1	G	192	ARG	3.4
1	K	194	HIS	3.3
1	J	194	HIS	3.2
1	E	194	HIS	3.1
1	D	192	ARG	3.1
1	G	139	GLN	3.0
1	A	194	HIS	3.0
1	E	192	ARG	3.0
1	N	193	ALA	2.7
1	C	124	GLN	2.6
1	C	192	ARG	2.6
1	A	192	ARG	2.6
1	N	136	ILE	2.6
1	I	194	HIS	2.5
1	D	191	THR	2.5
1	H	192	ARG	2.5
1	L	35	GLU	2.4
1	F	35	GLU	2.3
1	K	35	GLU	2.3
1	J	35	GLU	2.3
1	H	139	GLN	2.3
1	C	193	ALA	2.3
1	H	35	GLU	2.2
1	B	35	GLU	2.1
1	F	136	ILE	2.1
1	M	124	GLN	2.1
1	F	192	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [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.