



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2017 – 12:43 AM EDT

PDB ID : 3M9B  
Title : Crystal structure of the amino terminal coiled coil domain and the inter domain of the Mycobacterium tuberculosis proteasomal ATPase Mpa  
Authors : Li, H.; Wang, T.  
Deposited on : unknown  
Resolution : 3.94 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

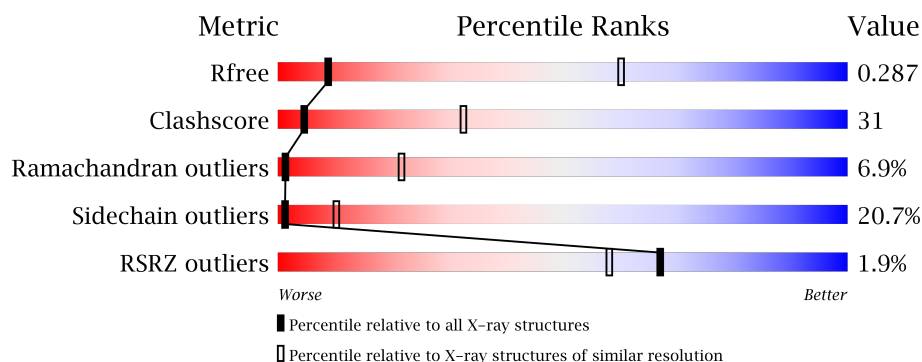
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.94 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))
$R_{free}$	100719	1021 (4.28-3.60)
Clashscore	112137	1117 (4.28-3.60)
Ramachandran outliers	110173	1076 (4.28-3.60)
Sidechain outliers	110143	1067 (4.28-3.60)
RSRZ outliers	101464	1034 (4.28-3.60)

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	251	<div> <div>0.1%</div> <div>28% 34% 12% 26%</div> </div>
1	B	251	<div> <div>3%</div> <div>35% 29% 10% 26%</div> </div>
1	C	251	<div> <div>29% 30% 14% 26%</div> </div>
1	D	251	<div> <div>2%</div> <div>37% 29% 8% 26%</div> </div>
1	E	251	<div> <div>27% 33% 12% 26%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>35%</div><div>30%</div><div>8%</div><div>26%</div></div></div>
1	G	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>25%</div><div>33%</div><div>14%</div><div>26%</div></div></div>
1	H	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>35%</div><div>30%</div><div>9%</div><div>26%</div></div></div>
1	I	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>26%</div><div>36%</div><div>11%</div><div>26%</div></div></div>
1	J	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>35%</div><div>31%</div><div>8%</div><div>26%</div></div></div>
1	K	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>26%</div><div>33%</div><div>14%</div><div>26%</div></div></div>
1	L	251	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>36%</div><div>32%</div><div>6%</div><div>26%</div></div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17172 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 Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	B	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	C	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	D	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	E	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	F	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	G	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	H	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	I	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	J	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	K	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			
1	L	186	Total	C	N	O	S	0	0	0
			1431	888	259	281	3			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	LEU	-	EXPRESSION TAG	UNP P63345
A	236	VAL	-	EXPRESSION TAG	UNP P63345
A	237	PRO	-	EXPRESSION TAG	UNP P63345
A	238	ARG	-	EXPRESSION TAG	UNP P63345
A	239	GLY	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	240	SER	-	EXPRESSION TAG	UNP P63345
A	241	ALA	-	EXPRESSION TAG	UNP P63345
A	242	ALA	-	EXPRESSION TAG	UNP P63345
A	243	ALA	-	EXPRESSION TAG	UNP P63345
A	244	LEU	-	EXPRESSION TAG	UNP P63345
A	245	GLU	-	EXPRESSION TAG	UNP P63345
A	246	HIS	-	EXPRESSION TAG	UNP P63345
A	247	HIS	-	EXPRESSION TAG	UNP P63345
A	248	HIS	-	EXPRESSION TAG	UNP P63345
A	249	HIS	-	EXPRESSION TAG	UNP P63345
A	250	HIS	-	EXPRESSION TAG	UNP P63345
A	251	HIS	-	EXPRESSION TAG	UNP P63345
B	235	LEU	-	EXPRESSION TAG	UNP P63345
B	236	VAL	-	EXPRESSION TAG	UNP P63345
B	237	PRO	-	EXPRESSION TAG	UNP P63345
B	238	ARG	-	EXPRESSION TAG	UNP P63345
B	239	GLY	-	EXPRESSION TAG	UNP P63345
B	240	SER	-	EXPRESSION TAG	UNP P63345
B	241	ALA	-	EXPRESSION TAG	UNP P63345
B	242	ALA	-	EXPRESSION TAG	UNP P63345
B	243	ALA	-	EXPRESSION TAG	UNP P63345
B	244	LEU	-	EXPRESSION TAG	UNP P63345
B	245	GLU	-	EXPRESSION TAG	UNP P63345
B	246	HIS	-	EXPRESSION TAG	UNP P63345
B	247	HIS	-	EXPRESSION TAG	UNP P63345
B	248	HIS	-	EXPRESSION TAG	UNP P63345
B	249	HIS	-	EXPRESSION TAG	UNP P63345
B	250	HIS	-	EXPRESSION TAG	UNP P63345
B	251	HIS	-	EXPRESSION TAG	UNP P63345
C	235	LEU	-	EXPRESSION TAG	UNP P63345
C	236	VAL	-	EXPRESSION TAG	UNP P63345
C	237	PRO	-	EXPRESSION TAG	UNP P63345
C	238	ARG	-	EXPRESSION TAG	UNP P63345
C	239	GLY	-	EXPRESSION TAG	UNP P63345
C	240	SER	-	EXPRESSION TAG	UNP P63345
C	241	ALA	-	EXPRESSION TAG	UNP P63345
C	242	ALA	-	EXPRESSION TAG	UNP P63345
C	243	ALA	-	EXPRESSION TAG	UNP P63345
C	244	LEU	-	EXPRESSION TAG	UNP P63345
C	245	GLU	-	EXPRESSION TAG	UNP P63345
C	246	HIS	-	EXPRESSION TAG	UNP P63345
C	247	HIS	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
C	248	HIS	-	EXPRESSION TAG	UNP P63345
C	249	HIS	-	EXPRESSION TAG	UNP P63345
C	250	HIS	-	EXPRESSION TAG	UNP P63345
C	251	HIS	-	EXPRESSION TAG	UNP P63345
D	235	LEU	-	EXPRESSION TAG	UNP P63345
D	236	VAL	-	EXPRESSION TAG	UNP P63345
D	237	PRO	-	EXPRESSION TAG	UNP P63345
D	238	ARG	-	EXPRESSION TAG	UNP P63345
D	239	GLY	-	EXPRESSION TAG	UNP P63345
D	240	SER	-	EXPRESSION TAG	UNP P63345
D	241	ALA	-	EXPRESSION TAG	UNP P63345
D	242	ALA	-	EXPRESSION TAG	UNP P63345
D	243	ALA	-	EXPRESSION TAG	UNP P63345
D	244	LEU	-	EXPRESSION TAG	UNP P63345
D	245	GLU	-	EXPRESSION TAG	UNP P63345
D	246	HIS	-	EXPRESSION TAG	UNP P63345
D	247	HIS	-	EXPRESSION TAG	UNP P63345
D	248	HIS	-	EXPRESSION TAG	UNP P63345
D	249	HIS	-	EXPRESSION TAG	UNP P63345
D	250	HIS	-	EXPRESSION TAG	UNP P63345
D	251	HIS	-	EXPRESSION TAG	UNP P63345
E	235	LEU	-	EXPRESSION TAG	UNP P63345
E	236	VAL	-	EXPRESSION TAG	UNP P63345
E	237	PRO	-	EXPRESSION TAG	UNP P63345
E	238	ARG	-	EXPRESSION TAG	UNP P63345
E	239	GLY	-	EXPRESSION TAG	UNP P63345
E	240	SER	-	EXPRESSION TAG	UNP P63345
E	241	ALA	-	EXPRESSION TAG	UNP P63345
E	242	ALA	-	EXPRESSION TAG	UNP P63345
E	243	ALA	-	EXPRESSION TAG	UNP P63345
E	244	LEU	-	EXPRESSION TAG	UNP P63345
E	245	GLU	-	EXPRESSION TAG	UNP P63345
E	246	HIS	-	EXPRESSION TAG	UNP P63345
E	247	HIS	-	EXPRESSION TAG	UNP P63345
E	248	HIS	-	EXPRESSION TAG	UNP P63345
E	249	HIS	-	EXPRESSION TAG	UNP P63345
E	250	HIS	-	EXPRESSION TAG	UNP P63345
E	251	HIS	-	EXPRESSION TAG	UNP P63345
F	235	LEU	-	EXPRESSION TAG	UNP P63345
F	236	VAL	-	EXPRESSION TAG	UNP P63345
F	237	PRO	-	EXPRESSION TAG	UNP P63345
F	238	ARG	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
F	239	GLY	-	EXPRESSION TAG	UNP P63345
F	240	SER	-	EXPRESSION TAG	UNP P63345
F	241	ALA	-	EXPRESSION TAG	UNP P63345
F	242	ALA	-	EXPRESSION TAG	UNP P63345
F	243	ALA	-	EXPRESSION TAG	UNP P63345
F	244	LEU	-	EXPRESSION TAG	UNP P63345
F	245	GLU	-	EXPRESSION TAG	UNP P63345
F	246	HIS	-	EXPRESSION TAG	UNP P63345
F	247	HIS	-	EXPRESSION TAG	UNP P63345
F	248	HIS	-	EXPRESSION TAG	UNP P63345
F	249	HIS	-	EXPRESSION TAG	UNP P63345
F	250	HIS	-	EXPRESSION TAG	UNP P63345
F	251	HIS	-	EXPRESSION TAG	UNP P63345
G	235	LEU	-	EXPRESSION TAG	UNP P63345
G	236	VAL	-	EXPRESSION TAG	UNP P63345
G	237	PRO	-	EXPRESSION TAG	UNP P63345
G	238	ARG	-	EXPRESSION TAG	UNP P63345
G	239	GLY	-	EXPRESSION TAG	UNP P63345
G	240	SER	-	EXPRESSION TAG	UNP P63345
G	241	ALA	-	EXPRESSION TAG	UNP P63345
G	242	ALA	-	EXPRESSION TAG	UNP P63345
G	243	ALA	-	EXPRESSION TAG	UNP P63345
G	244	LEU	-	EXPRESSION TAG	UNP P63345
G	245	GLU	-	EXPRESSION TAG	UNP P63345
G	246	HIS	-	EXPRESSION TAG	UNP P63345
G	247	HIS	-	EXPRESSION TAG	UNP P63345
G	248	HIS	-	EXPRESSION TAG	UNP P63345
G	249	HIS	-	EXPRESSION TAG	UNP P63345
G	250	HIS	-	EXPRESSION TAG	UNP P63345
G	251	HIS	-	EXPRESSION TAG	UNP P63345
H	235	LEU	-	EXPRESSION TAG	UNP P63345
H	236	VAL	-	EXPRESSION TAG	UNP P63345
H	237	PRO	-	EXPRESSION TAG	UNP P63345
H	238	ARG	-	EXPRESSION TAG	UNP P63345
H	239	GLY	-	EXPRESSION TAG	UNP P63345
H	240	SER	-	EXPRESSION TAG	UNP P63345
H	241	ALA	-	EXPRESSION TAG	UNP P63345
H	242	ALA	-	EXPRESSION TAG	UNP P63345
H	243	ALA	-	EXPRESSION TAG	UNP P63345
H	244	LEU	-	EXPRESSION TAG	UNP P63345
H	245	GLU	-	EXPRESSION TAG	UNP P63345
H	246	HIS	-	EXPRESSION TAG	UNP P63345

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Chain	Residue	Modelled	Actual	Comment	Reference
H	247	HIS	-	EXPRESSION TAG	UNP P63345
H	248	HIS	-	EXPRESSION TAG	UNP P63345
H	249	HIS	-	EXPRESSION TAG	UNP P63345
H	250	HIS	-	EXPRESSION TAG	UNP P63345
H	251	HIS	-	EXPRESSION TAG	UNP P63345
I	235	LEU	-	EXPRESSION TAG	UNP P63345
I	236	VAL	-	EXPRESSION TAG	UNP P63345
I	237	PRO	-	EXPRESSION TAG	UNP P63345
I	238	ARG	-	EXPRESSION TAG	UNP P63345
I	239	GLY	-	EXPRESSION TAG	UNP P63345
I	240	SER	-	EXPRESSION TAG	UNP P63345
I	241	ALA	-	EXPRESSION TAG	UNP P63345
I	242	ALA	-	EXPRESSION TAG	UNP P63345
I	243	ALA	-	EXPRESSION TAG	UNP P63345
I	244	LEU	-	EXPRESSION TAG	UNP P63345
I	245	GLU	-	EXPRESSION TAG	UNP P63345
I	246	HIS	-	EXPRESSION TAG	UNP P63345
I	247	HIS	-	EXPRESSION TAG	UNP P63345
I	248	HIS	-	EXPRESSION TAG	UNP P63345
I	249	HIS	-	EXPRESSION TAG	UNP P63345
I	250	HIS	-	EXPRESSION TAG	UNP P63345
I	251	HIS	-	EXPRESSION TAG	UNP P63345
J	235	LEU	-	EXPRESSION TAG	UNP P63345
J	236	VAL	-	EXPRESSION TAG	UNP P63345
J	237	PRO	-	EXPRESSION TAG	UNP P63345
J	238	ARG	-	EXPRESSION TAG	UNP P63345
J	239	GLY	-	EXPRESSION TAG	UNP P63345
J	240	SER	-	EXPRESSION TAG	UNP P63345
J	241	ALA	-	EXPRESSION TAG	UNP P63345
J	242	ALA	-	EXPRESSION TAG	UNP P63345
J	243	ALA	-	EXPRESSION TAG	UNP P63345
J	244	LEU	-	EXPRESSION TAG	UNP P63345
J	245	GLU	-	EXPRESSION TAG	UNP P63345
J	246	HIS	-	EXPRESSION TAG	UNP P63345
J	247	HIS	-	EXPRESSION TAG	UNP P63345
J	248	HIS	-	EXPRESSION TAG	UNP P63345
J	249	HIS	-	EXPRESSION TAG	UNP P63345
J	250	HIS	-	EXPRESSION TAG	UNP P63345
J	251	HIS	-	EXPRESSION TAG	UNP P63345
K	235	LEU	-	EXPRESSION TAG	UNP P63345
K	236	VAL	-	EXPRESSION TAG	UNP P63345
K	237	PRO	-	EXPRESSION TAG	UNP P63345

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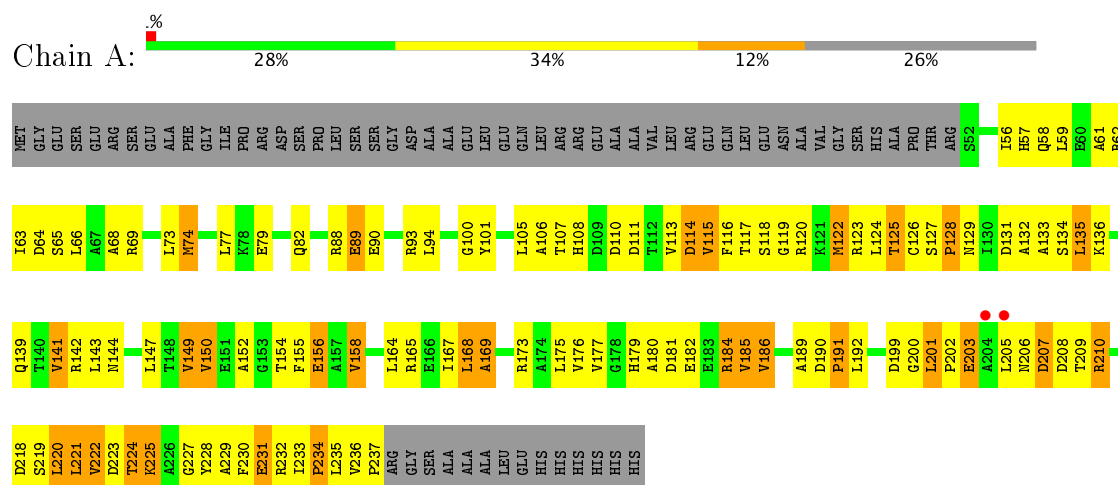
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Chain	Residue	Modelled	Actual	Comment	Reference
K	238	ARG	-	EXPRESSION TAG	UNP P63345
K	239	GLY	-	EXPRESSION TAG	UNP P63345
K	240	SER	-	EXPRESSION TAG	UNP P63345
K	241	ALA	-	EXPRESSION TAG	UNP P63345
K	242	ALA	-	EXPRESSION TAG	UNP P63345
K	243	ALA	-	EXPRESSION TAG	UNP P63345
K	244	LEU	-	EXPRESSION TAG	UNP P63345
K	245	GLU	-	EXPRESSION TAG	UNP P63345
K	246	HIS	-	EXPRESSION TAG	UNP P63345
K	247	HIS	-	EXPRESSION TAG	UNP P63345
K	248	HIS	-	EXPRESSION TAG	UNP P63345
K	249	HIS	-	EXPRESSION TAG	UNP P63345
K	250	HIS	-	EXPRESSION TAG	UNP P63345
K	251	HIS	-	EXPRESSION TAG	UNP P63345
L	235	LEU	-	EXPRESSION TAG	UNP P63345
L	236	VAL	-	EXPRESSION TAG	UNP P63345
L	237	PRO	-	EXPRESSION TAG	UNP P63345
L	238	ARG	-	EXPRESSION TAG	UNP P63345
L	239	GLY	-	EXPRESSION TAG	UNP P63345
L	240	SER	-	EXPRESSION TAG	UNP P63345
L	241	ALA	-	EXPRESSION TAG	UNP P63345
L	242	ALA	-	EXPRESSION TAG	UNP P63345
L	243	ALA	-	EXPRESSION TAG	UNP P63345
L	244	LEU	-	EXPRESSION TAG	UNP P63345
L	245	GLU	-	EXPRESSION TAG	UNP P63345
L	246	HIS	-	EXPRESSION TAG	UNP P63345
L	247	HIS	-	EXPRESSION TAG	UNP P63345
L	248	HIS	-	EXPRESSION TAG	UNP P63345
L	249	HIS	-	EXPRESSION TAG	UNP P63345
L	250	HIS	-	EXPRESSION TAG	UNP P63345
L	251	HIS	-	EXPRESSION TAG	UNP P63345

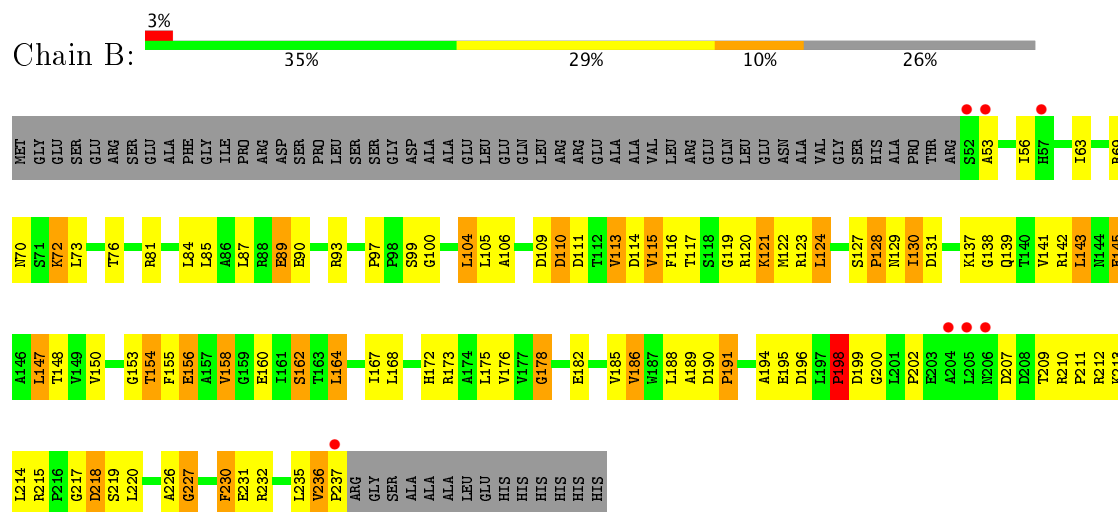
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

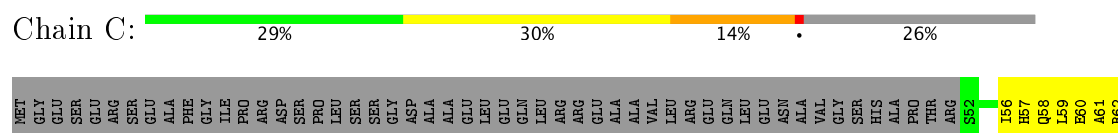
#### • Molecule 1: Proteasome-associated ATPase



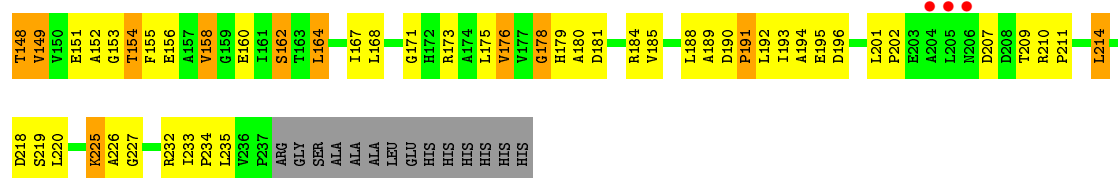
#### • Molecule 1: Proteasome-associated ATPase



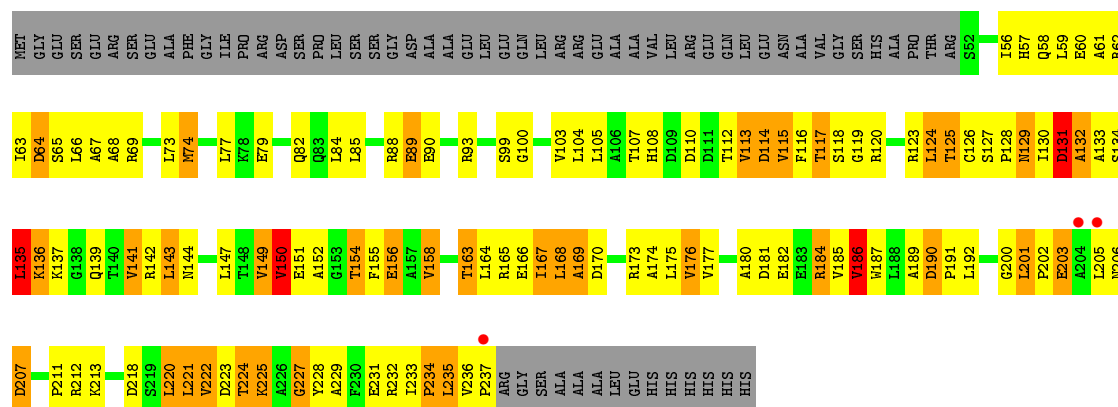
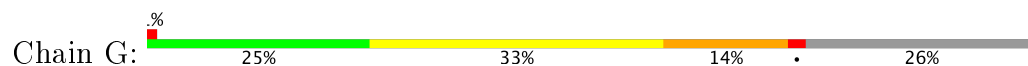
#### • Molecule 1: Proteasome-associated ATPase



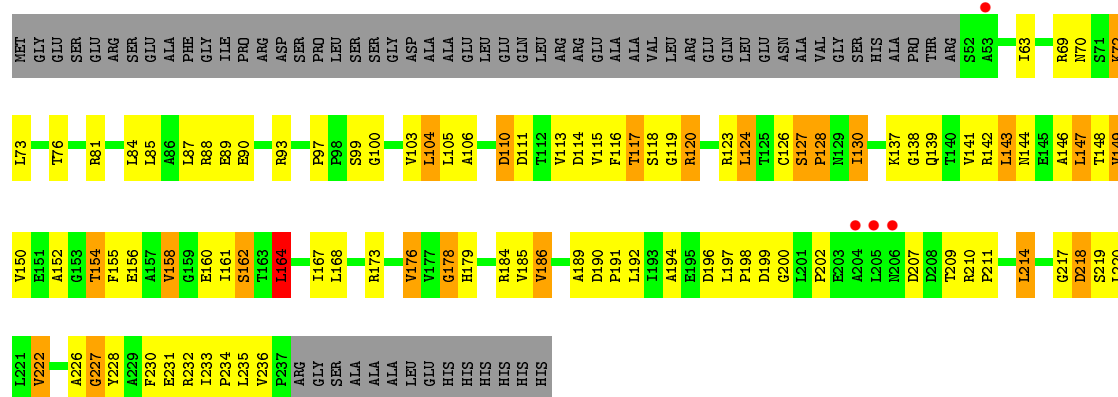




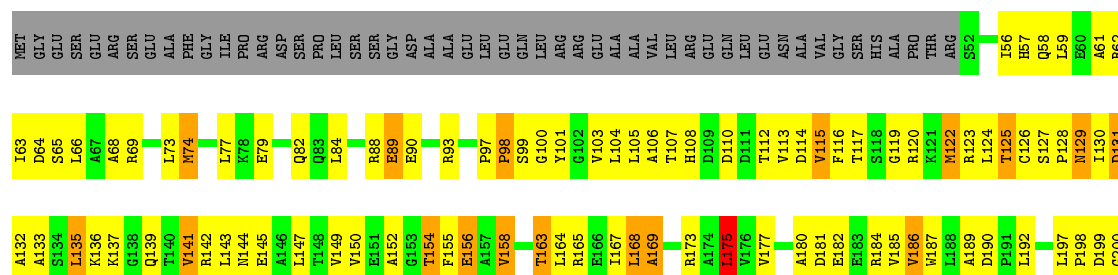
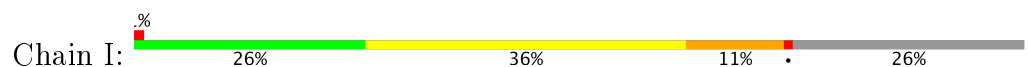
• Molecule 1: Proteasome-associated ATPase



• Molecule 1: Proteasome-associated ATPase

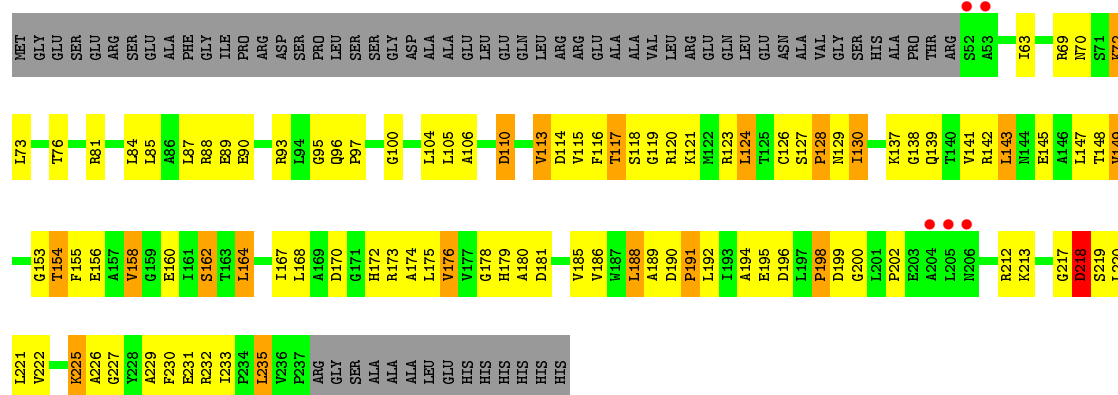


• Molecule 1: Proteasome-associated ATPase

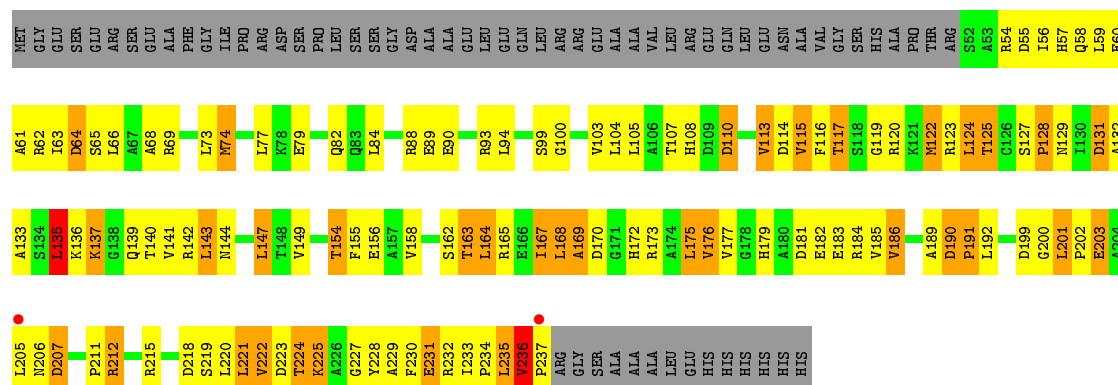
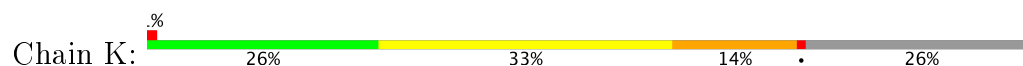




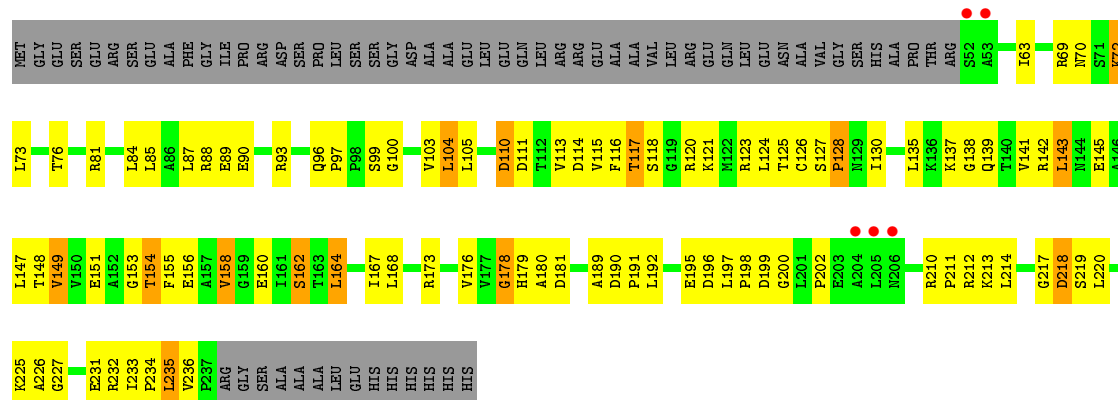
● Molecule 1: Proteasome-associated ATPase



● Molecule 1: Proteasome-associated ATPase



● Molecule 1: Proteasome-associated ATPase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.79Å 176.65Å 176.63Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	25.00 – 3.94 25.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-3.94) 99.4 (25.00-3.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 3.85Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.275 , 0.304 0.262 , 0.287	Depositor DCC
$R_{free}$ test set	4860 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	152.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l 0.007 for -k,-h,-l 0.002 for l,k,-h 0.006 for -h,-l,-k 0.003 for -h,l,k 0.449 for l,h,k 0.449 for k,l,h 0.448 for -k,-l,h 0.448 for l,-h,-k 0.450 for -h,-k,l 0.005 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	239.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	1.24	8/1451 (0.6%)	1.15	4/1969 (0.2%)
1	B	1.08	3/1451 (0.2%)	1.09	4/1969 (0.2%)
1	C	1.24	8/1451 (0.6%)	1.13	5/1969 (0.3%)
1	D	1.09	3/1451 (0.2%)	1.11	8/1969 (0.4%)
1	E	1.27	9/1451 (0.6%)	1.16	6/1969 (0.3%)
1	F	1.08	4/1451 (0.3%)	1.09	6/1969 (0.3%)
1	G	1.22	6/1451 (0.4%)	1.14	8/1969 (0.4%)
1	H	1.10	3/1451 (0.2%)	1.10	8/1969 (0.4%)
1	I	1.20	5/1451 (0.3%)	1.13	4/1969 (0.2%)
1	J	1.10	3/1451 (0.2%)	1.12	6/1969 (0.3%)
1	K	1.22	5/1451 (0.3%)	1.12	6/1969 (0.3%)
1	L	1.07	3/1451 (0.2%)	1.10	5/1969 (0.3%)
All	All	1.16	60/17412 (0.3%)	1.12	70/23628 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	1
1	I	0	1
1	K	0	1
All	All	0	5

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	160	GLU	CG-CD	9.62	1.66	1.51
1	A	93	ARG	CZ-NH1	9.08	1.44	1.33
1	E	93	ARG	CZ-NH1	8.66	1.44	1.33
1	F	160	GLU	CG-CD	8.66	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	ARG	CZ-NH1	8.65	1.44	1.33

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	NE-CZ-NH2	-12.81	113.90	120.30
1	E	93	ARG	NE-CZ-NH1	12.61	126.60	120.30
1	E	93	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	A	93	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	C	93	ARG	NE-CZ-NH1	12.16	126.38	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	PRO	Peptide
1	B	236	VAL	Peptide
1	D	198	PRO	Peptide
1	I	236	VAL	Peptide
1	K	236	VAL	Peptide

## 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	1431	0	1443	117	0
1	B	1431	0	1443	82	0
1	C	1431	0	1443	113	0
1	D	1431	0	1443	74	0
1	E	1431	0	1443	112	0
1	F	1431	0	1443	81	0
1	G	1431	0	1443	106	0
1	H	1431	0	1443	78	0
1	I	1431	0	1443	124	0
1	J	1431	0	1443	74	0
1	K	1431	0	1443	113	0
1	L	1431	0	1443	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17172	0	17316	1071	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 31.

The worst 5 of 1071 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:ASP:OD1	1:E:123:ARG:HG3	1.44	1.16
1:K:186:VAL:HG12	1:K:227:GLY:O	1.48	1.13
1:C:120:ARG:HE	1:C:122:MET:CE	1.59	1.12
1:K:235:LEU:HD11	1:K:237:PRO:HD3	1.37	1.05
1:D:154:THR:HG22	1:D:155:PHE:H	1.15	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/251 (73%)	137 (74%)	33 (18%)	14 (8%)	1	19
1	B	184/251 (73%)	148 (80%)	21 (11%)	15 (8%)	1	16
1	C	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	19
1	D	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	2	28
1	E	184/251 (73%)	139 (76%)	31 (17%)	14 (8%)	1	19
1	F	184/251 (73%)	152 (83%)	23 (12%)	9 (5%)	2	29
1	G	184/251 (73%)	138 (75%)	28 (15%)	18 (10%)	1	13
1	H	184/251 (73%)	148 (80%)	27 (15%)	9 (5%)	2	29
1	I	184/251 (73%)	136 (74%)	34 (18%)	14 (8%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	184/251 (73%)	147 (80%)	24 (13%)	13 (7%)	1	21
1	K	184/251 (73%)	135 (73%)	36 (20%)	13 (7%)	1	21
1	L	184/251 (73%)	147 (80%)	27 (15%)	10 (5%)	2	28
All	All	2208/3012 (73%)	1713 (78%)	342 (16%)	153 (7%)	1	22

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ALA
1	A	169	ALA
1	A	203	GLU
1	A	207	ASP
1	B	128	PRO

### 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	154/204 (76%)	121 (79%)	33 (21%)	1	9
1	B	154/204 (76%)	126 (82%)	28 (18%)	2	15
1	C	154/204 (76%)	118 (77%)	36 (23%)	1	7
1	D	154/204 (76%)	126 (82%)	28 (18%)	2	15
1	E	154/204 (76%)	114 (74%)	40 (26%)	0	5
1	F	154/204 (76%)	127 (82%)	27 (18%)	2	17
1	G	154/204 (76%)	115 (75%)	39 (25%)	0	6
1	H	154/204 (76%)	126 (82%)	28 (18%)	2	15
1	I	154/204 (76%)	123 (80%)	31 (20%)	1	12
1	J	154/204 (76%)	125 (81%)	29 (19%)	2	14
1	K	154/204 (76%)	115 (75%)	39 (25%)	0	6
1	L	154/204 (76%)	129 (84%)	25 (16%)	3	20
All	All	1848/2448 (76%)	1465 (79%)	383 (21%)	1	10

5 of 383 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	115	VAL
1	G	163	THR
1	K	224	THR
1	F	143	LEU
1	G	82	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	70	ASN
1	E	96	GLN
1	I	70	ASN
1	D	70	ASN
1	J	70	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 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 ⓘ

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	186/251 (74%)	0.00	2 (1%) 80 72	166, 225, 345, 406	0
1	B	186/251 (74%)	0.03	7 (3%) 41 32	158, 212, 412, 527	0
1	C	186/251 (74%)	-0.03	0 100 100	168, 226, 338, 403	0
1	D	186/251 (74%)	0.00	5 (2%) 55 45	155, 210, 417, 544	0
1	E	186/251 (74%)	-0.04	1 (0%) 90 86	164, 220, 340, 398	0
1	F	186/251 (74%)	0.02	5 (2%) 55 45	156, 212, 419, 539	0
1	G	186/251 (74%)	0.00	3 (1%) 72 62	167, 224, 343, 406	0
1	H	186/251 (74%)	-0.02	4 (2%) 62 53	157, 210, 406, 520	0
1	I	186/251 (74%)	-0.01	3 (1%) 72 62	166, 222, 339, 402	0
1	J	186/251 (74%)	-0.03	5 (2%) 55 45	156, 210, 417, 538	0
1	K	186/251 (74%)	-0.04	2 (1%) 80 72	165, 223, 335, 409	0
1	L	186/251 (74%)	0.02	5 (2%) 55 45	157, 213, 423, 548	0
All	All	2232/3012 (74%)	-0.01	42 (1%) 67 58	155, 218, 384, 548	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	204	ALA	7.8
1	J	204	ALA	7.2
1	L	53	ALA	6.3
1	L	204	ALA	6.3
1	B	204	ALA	6.1

### 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.