



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 20, 2025 – 10:57 pm BST

PDB ID : 9G72 / pdb\_00009g72  
Title : Crystal structure of S. epidermidis ClpP in complex with tavaborole - soaking  
Authors : Alves Franca, B.; Rohde, H.; Betzel, C.  
Deposited on : 2024-07-19  
Resolution : 1.91 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

<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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

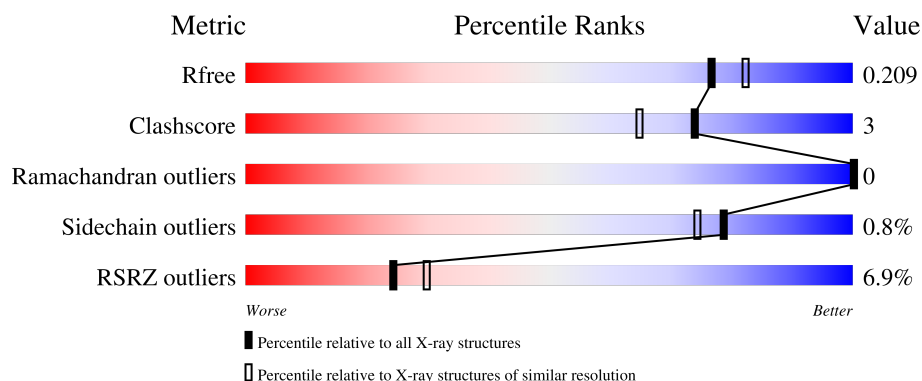
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.91 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.




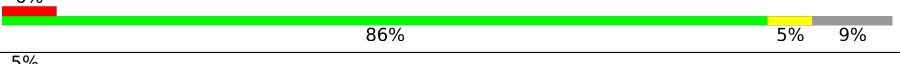
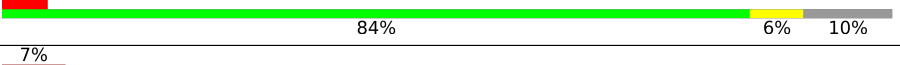

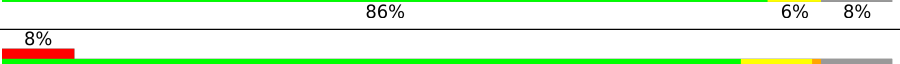
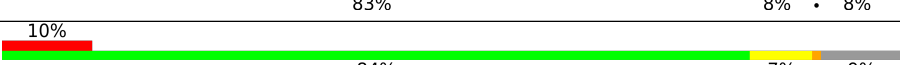
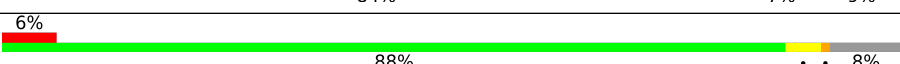
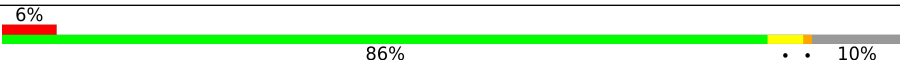

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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  $\geq 3$ , 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	199	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>5% • 10%</div> </div> </div>
1	B	199	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>5% • 10%</div> </div> </div>
1	C	199	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>6% • 9%</div> </div> </div>
1	D	199	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>5% • 9%</div> </div> </div>
1	E	199	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>6% 10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	199	
1	G	199	
1	H	199	
1	I	199	
1	J	199	
1	K	199	
1	L	199	
1	M	199	
1	N	199	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20670 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 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1354	855	231	262	6			
1	B	180	Total	C	N	O	S	0	0	0
			1359	858	232	263	6			
1	C	182	Total	C	N	O	S	0	0	0
			1372	867	234	265	6			
1	D	182	Total	C	N	O	S	0	0	0
			1360	861	234	259	6			
1	E	179	Total	C	N	O	S	0	0	0
			1348	851	231	260	6			
1	F	181	Total	C	N	O	S	0	1	0
			1380	869	235	270	6			
1	G	181	Total	C	N	O	S	0	0	0
			1360	859	233	262	6			
1	H	179	Total	C	N	O	S	0	0	0
			1353	852	232	263	6			
1	I	181	Total	C	N	O	S	0	0	0
			1367	864	233	264	6			
1	J	183	Total	C	N	O	S	0	0	0
			1373	868	235	264	6			
1	K	183	Total	C	N	O	S	0	0	0
			1387	875	238	268	6			
1	L	182	Total	C	N	O	S	0	0	0
			1372	867	234	265	6			
1	M	183	Total	C	N	O	S	0	0	0
			1373	868	235	264	6			
1	N	179	Total	C	N	O	S	0	0	0
			1346	851	231	258	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	HIS	-	expression tag	UNP A0A0N1MQL5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	195	HIS	-	expression tag	UNP A0A0N1MQL5
A	196	HIS	-	expression tag	UNP A0A0N1MQL5
A	197	HIS	-	expression tag	UNP A0A0N1MQL5
A	198	HIS	-	expression tag	UNP A0A0N1MQL5
A	199	HIS	-	expression tag	UNP A0A0N1MQL5
B	194	HIS	-	expression tag	UNP A0A0N1MQL5
B	195	HIS	-	expression tag	UNP A0A0N1MQL5
B	196	HIS	-	expression tag	UNP A0A0N1MQL5
B	197	HIS	-	expression tag	UNP A0A0N1MQL5
B	198	HIS	-	expression tag	UNP A0A0N1MQL5
B	199	HIS	-	expression tag	UNP A0A0N1MQL5
C	194	HIS	-	expression tag	UNP A0A0N1MQL5
C	195	HIS	-	expression tag	UNP A0A0N1MQL5
C	196	HIS	-	expression tag	UNP A0A0N1MQL5
C	197	HIS	-	expression tag	UNP A0A0N1MQL5
C	198	HIS	-	expression tag	UNP A0A0N1MQL5
C	199	HIS	-	expression tag	UNP A0A0N1MQL5
D	194	HIS	-	expression tag	UNP A0A0N1MQL5
D	195	HIS	-	expression tag	UNP A0A0N1MQL5
D	196	HIS	-	expression tag	UNP A0A0N1MQL5
D	197	HIS	-	expression tag	UNP A0A0N1MQL5
D	198	HIS	-	expression tag	UNP A0A0N1MQL5
D	199	HIS	-	expression tag	UNP A0A0N1MQL5
E	194	HIS	-	expression tag	UNP A0A0N1MQL5
E	195	HIS	-	expression tag	UNP A0A0N1MQL5
E	196	HIS	-	expression tag	UNP A0A0N1MQL5
E	197	HIS	-	expression tag	UNP A0A0N1MQL5
E	198	HIS	-	expression tag	UNP A0A0N1MQL5
E	199	HIS	-	expression tag	UNP A0A0N1MQL5
F	194	HIS	-	expression tag	UNP A0A0N1MQL5
F	195	HIS	-	expression tag	UNP A0A0N1MQL5
F	196	HIS	-	expression tag	UNP A0A0N1MQL5
F	197	HIS	-	expression tag	UNP A0A0N1MQL5
F	198	HIS	-	expression tag	UNP A0A0N1MQL5
F	199	HIS	-	expression tag	UNP A0A0N1MQL5
G	194	HIS	-	expression tag	UNP A0A0N1MQL5
G	195	HIS	-	expression tag	UNP A0A0N1MQL5
G	196	HIS	-	expression tag	UNP A0A0N1MQL5
G	197	HIS	-	expression tag	UNP A0A0N1MQL5
G	198	HIS	-	expression tag	UNP A0A0N1MQL5
G	199	HIS	-	expression tag	UNP A0A0N1MQL5
H	194	HIS	-	expression tag	UNP A0A0N1MQL5

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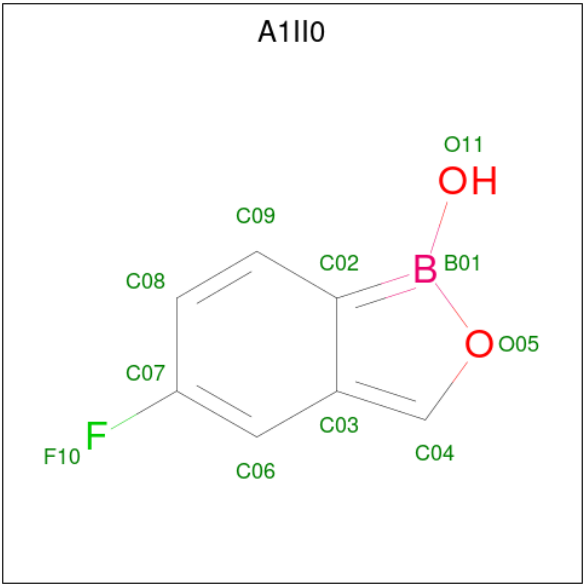
Chain	Residue	Modelled	Actual	Comment	Reference
H	195	HIS	-	expression tag	UNP A0A0N1MQL5
H	196	HIS	-	expression tag	UNP A0A0N1MQL5
H	197	HIS	-	expression tag	UNP A0A0N1MQL5
H	198	HIS	-	expression tag	UNP A0A0N1MQL5
H	199	HIS	-	expression tag	UNP A0A0N1MQL5
I	194	HIS	-	expression tag	UNP A0A0N1MQL5
I	195	HIS	-	expression tag	UNP A0A0N1MQL5
I	196	HIS	-	expression tag	UNP A0A0N1MQL5
I	197	HIS	-	expression tag	UNP A0A0N1MQL5
I	198	HIS	-	expression tag	UNP A0A0N1MQL5
I	199	HIS	-	expression tag	UNP A0A0N1MQL5
J	194	HIS	-	expression tag	UNP A0A0N1MQL5
J	195	HIS	-	expression tag	UNP A0A0N1MQL5
J	196	HIS	-	expression tag	UNP A0A0N1MQL5
J	197	HIS	-	expression tag	UNP A0A0N1MQL5
J	198	HIS	-	expression tag	UNP A0A0N1MQL5
J	199	HIS	-	expression tag	UNP A0A0N1MQL5
K	194	HIS	-	expression tag	UNP A0A0N1MQL5
K	195	HIS	-	expression tag	UNP A0A0N1MQL5
K	196	HIS	-	expression tag	UNP A0A0N1MQL5
K	197	HIS	-	expression tag	UNP A0A0N1MQL5
K	198	HIS	-	expression tag	UNP A0A0N1MQL5
K	199	HIS	-	expression tag	UNP A0A0N1MQL5
L	194	HIS	-	expression tag	UNP A0A0N1MQL5
L	195	HIS	-	expression tag	UNP A0A0N1MQL5
L	196	HIS	-	expression tag	UNP A0A0N1MQL5
L	197	HIS	-	expression tag	UNP A0A0N1MQL5
L	198	HIS	-	expression tag	UNP A0A0N1MQL5
L	199	HIS	-	expression tag	UNP A0A0N1MQL5
M	194	HIS	-	expression tag	UNP A0A0N1MQL5
M	195	HIS	-	expression tag	UNP A0A0N1MQL5
M	196	HIS	-	expression tag	UNP A0A0N1MQL5
M	197	HIS	-	expression tag	UNP A0A0N1MQL5
M	198	HIS	-	expression tag	UNP A0A0N1MQL5
M	199	HIS	-	expression tag	UNP A0A0N1MQL5
N	194	HIS	-	expression tag	UNP A0A0N1MQL5
N	195	HIS	-	expression tag	UNP A0A0N1MQL5
N	196	HIS	-	expression tag	UNP A0A0N1MQL5
N	197	HIS	-	expression tag	UNP A0A0N1MQL5
N	198	HIS	-	expression tag	UNP A0A0N1MQL5
N	199	HIS	-	expression tag	UNP A0A0N1MQL5

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	M	1	Total	C	O	0	0
			4	2	2		
2	N	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 3-fluoranyl-7-oxidanyl-8-oxa-7 $\lambda$ <sup>4</sup>-borabicyclo[4.3.0]nona-1(9),2,4,6-tetraene (CCD ID: A1II0) (formula: C<sub>7</sub>H<sub>5</sub>BF<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	B	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	C	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	D	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	E	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	F	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	G	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	H	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	I	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	J	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	K	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	L	1	Total	B	C	F	O	0	0
			11	1	7	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	M	1	Total	B	C	F	O	0	0
			11	1	7	1	2		
3	N	1	Total	B	C	F	O	0	0
			11	1	7	1	2		

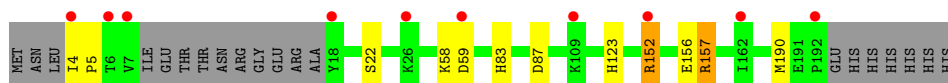
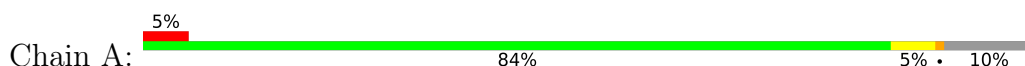
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	B	106	Total	O	0	0
			106	106		
4	C	102	Total	O	0	0
			102	102		
4	D	105	Total	O	0	0
			105	105		
4	E	106	Total	O	0	0
			106	106		
4	F	106	Total	O	0	0
			106	106		
4	G	94	Total	O	0	0
			94	94		
4	H	105	Total	O	0	0
			105	105		
4	I	90	Total	O	0	0
			90	90		
4	J	99	Total	O	0	0
			99	99		
4	K	97	Total	O	0	0
			97	97		
4	L	93	Total	O	0	0
			93	93		
4	M	74	Total	O	0	0
			74	74		
4	N	79	Total	O	0	0
			79	79		

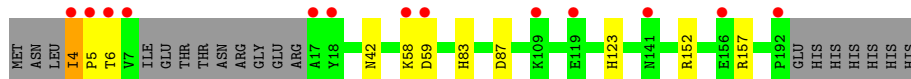
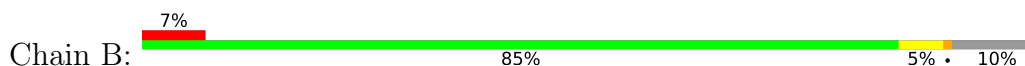
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

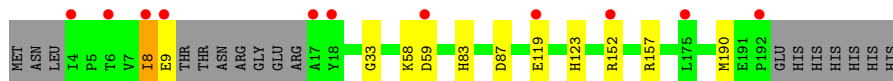
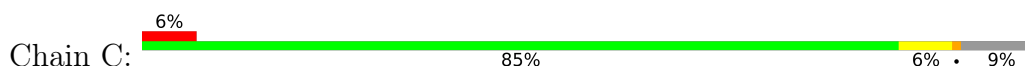
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



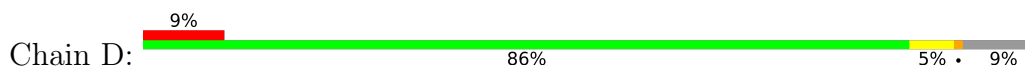
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



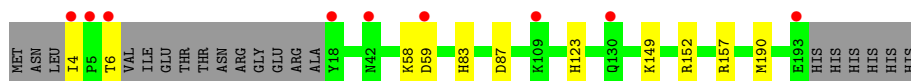
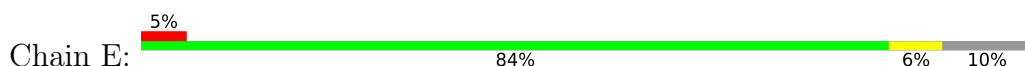
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



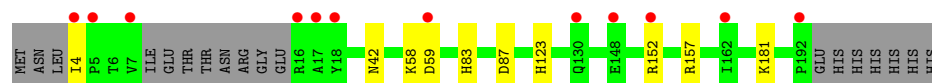
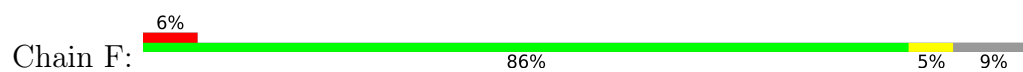
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



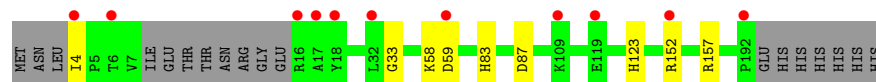
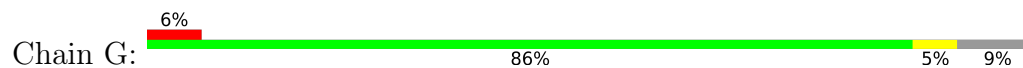
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



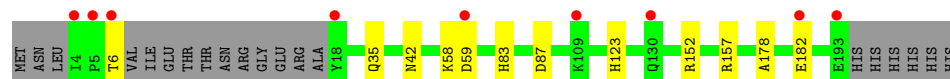
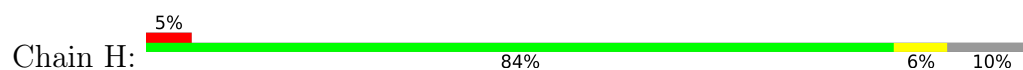
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



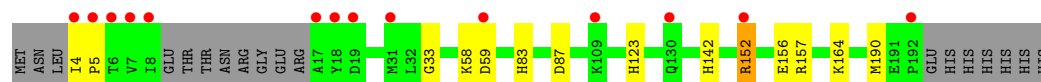
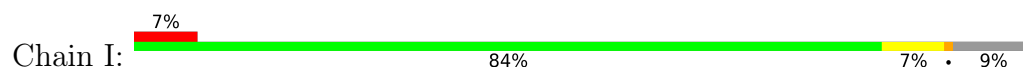
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



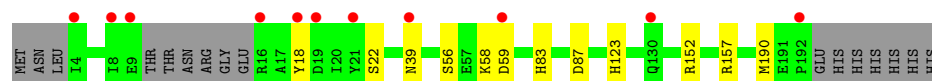
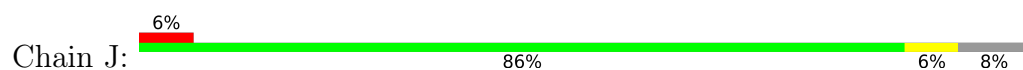
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



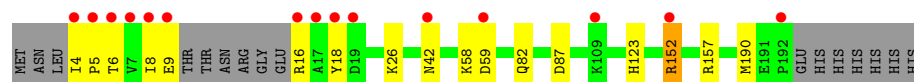
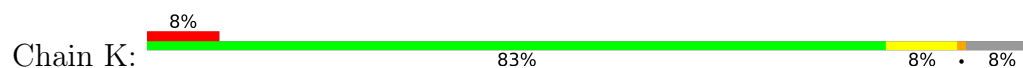
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



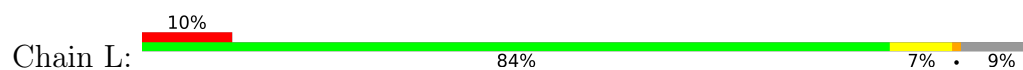
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

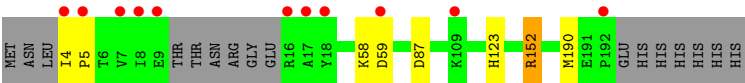
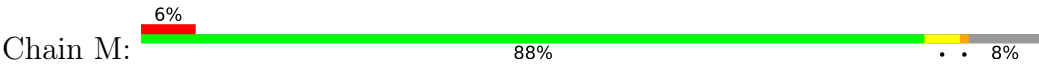


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

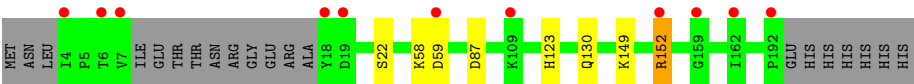
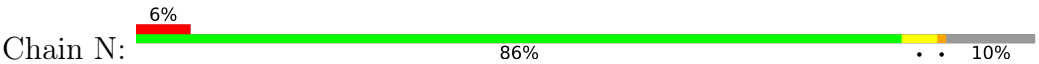


HIS

● Molecule 1: ATP-dependent Clp protease proteolytic subunit



● Molecule 1: ATP-dependent Clp protease proteolytic subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.92Å 123.52Å 127.03Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	75.25 – 1.91 75.25 – 1.91	Depositor EDS
% Data completeness (in resolution range)	98.7 (75.25-1.91) 98.6 (75.25-1.91)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.91Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, $R_{free}$	0.200 , 0.210 0.200 , 0.209	Depositor DCC
$R_{free}$ test set	1989 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.003 for -h,-l,-k 0.014 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1II0, ACT

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	0.56	0/1372	0.67	2/1856 (0.1%)
1	B	0.56	0/1377	0.69	3/1863 (0.2%)
1	C	0.56	0/1390	0.68	2/1881 (0.1%)
1	D	0.58	0/1378	0.68	3/1866 (0.2%)
1	E	0.56	0/1366	0.67	2/1848 (0.1%)
1	F	0.55	0/1398	0.66	2/1891 (0.1%)
1	G	0.56	0/1378	0.66	2/1865 (0.1%)
1	H	0.56	0/1371	0.67	2/1854 (0.1%)
1	I	0.56	0/1385	0.69	2/1874 (0.1%)
1	J	0.56	0/1391	0.68	2/1883 (0.1%)
1	K	0.56	0/1405	0.67	2/1900 (0.1%)
1	L	0.58	0/1390	0.70	2/1881 (0.1%)
1	M	0.55	0/1391	0.66	2/1883 (0.1%)
1	N	0.55	0/1364	0.66	2/1846 (0.1%)
All	All	0.56	0/19356	0.68	30/26191 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ILE	CA-CB-CG1	7.14	122.54	110.40
1	D	58	LYS	CA-C-N	-6.06	108.49	121.45
1	D	58	LYS	C-N-CA	-6.06	108.49	121.45
1	F	58	LYS	CA-C-N	-6.05	108.49	121.45
1	F	58	LYS	C-N-CA	-6.05	108.49	121.45

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Sidechain
1	B	152	ARG	Sidechain
1	C	152	ARG	Sidechain
1	D	152	ARG	Sidechain
1	E	152	ARG	Sidechain

## 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	1354	0	1351	9	1
1	B	1359	0	1356	10	0
1	C	1372	0	1369	7	0
1	D	1360	0	1357	8	0
1	E	1348	0	1340	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1380	0	1371	6	0
1	G	1360	0	1354	5	0
1	H	1353	0	1341	11	0
1	I	1367	0	1367	11	0
1	J	1373	0	1367	7	1
1	K	1387	0	1386	19	1
1	L	1372	0	1369	12	2
1	M	1373	0	1367	6	0
1	N	1346	0	1343	9	0
2	A	4	0	3	1	0
2	B	4	0	3	1	0
2	C	4	0	3	1	0
2	D	4	0	3	1	0
2	E	4	0	3	1	0
2	F	4	0	3	1	0
2	G	4	0	3	1	0
2	H	4	0	3	1	0
2	I	4	0	3	1	0
2	J	4	0	3	1	0
2	K	4	0	3	1	0
2	L	4	0	3	1	0
2	M	4	0	3	1	0
2	N	4	0	3	1	0
3	A	11	0	0	1	0
3	B	11	0	0	1	0
3	C	11	0	0	1	0
3	D	11	0	0	1	0
3	E	11	0	0	1	0
3	F	11	0	0	1	0
3	G	11	0	0	1	0
3	H	11	0	0	1	0
3	I	11	0	0	1	0
3	J	11	0	0	1	0
3	K	11	0	0	1	0
3	L	11	0	0	1	0
3	M	11	0	0	1	0
3	N	11	0	0	1	0
4	A	100	0	0	2	0
4	B	106	0	0	1	0
4	C	102	0	0	2	0
4	D	105	0	0	1	1
4	E	106	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	106	0	0	2	0
4	G	94	0	0	2	0
4	H	105	0	0	2	0
4	I	90	0	0	3	0
4	J	99	0	0	1	0
4	K	97	0	0	5	0
4	L	93	0	0	2	0
4	M	74	0	0	1	0
4	N	79	0	0	5	0
All	All	20670	0	19080	116	3

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 3.

The worst 5 of 116 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:N:152:ARG:NE	4:N:301:HOH:O	2.05	0.86
1:N:152:ARG:NH2	4:N:301:HOH:O	2.01	0.83
1:D:152:ARG:NH2	4:D:301:HOH:O	2.08	0.83
1:J:18:TYR:OH	1:K:8:ILE:HB	1.83	0.79
1:M:4:ILE:HG13	1:M:5:PRO:HD3	1.66	0.76

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:SER:OG	1:L:152:ARG:NH2[2_545]	1.97	0.23
1:K:26:LYS:NZ	1:L:163:GLU:OE2[2_545]	2.05	0.15
1:A:156:GLU:O	4:D:301:HOH:O[1_655]	2.13	0.07

## 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	175/199 (88%)	173 (99%)	2 (1%)	0	100	100
1	B	176/199 (88%)	174 (99%)	2 (1%)	0	100	100
1	C	178/199 (89%)	176 (99%)	2 (1%)	0	100	100
1	D	178/199 (89%)	176 (99%)	2 (1%)	0	100	100
1	E	175/199 (88%)	173 (99%)	2 (1%)	0	100	100
1	F	178/199 (89%)	176 (99%)	2 (1%)	0	100	100
1	G	177/199 (89%)	175 (99%)	2 (1%)	0	100	100
1	H	175/199 (88%)	173 (99%)	2 (1%)	0	100	100
1	I	177/199 (89%)	175 (99%)	2 (1%)	0	100	100
1	J	179/199 (90%)	177 (99%)	2 (1%)	0	100	100
1	K	179/199 (90%)	177 (99%)	2 (1%)	0	100	100
1	L	178/199 (89%)	176 (99%)	2 (1%)	0	100	100
1	M	179/199 (90%)	177 (99%)	2 (1%)	0	100	100
1	N	175/199 (88%)	173 (99%)	2 (1%)	0	100	100
All	All	2479/2786 (89%)	2451 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/166 (86%)	141 (99%)	1 (1%)	81	77
1	B	142/166 (86%)	141 (99%)	1 (1%)	81	77
1	C	143/166 (86%)	141 (99%)	2 (1%)	62	51
1	D	140/166 (84%)	139 (99%)	1 (1%)	81	77
1	E	140/166 (84%)	139 (99%)	1 (1%)	81	77
1	F	145/166 (87%)	143 (99%)	2 (1%)	62	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	141/166 (85%)	140 (99%)	1 (1%)	81	77
1	H	141/166 (85%)	140 (99%)	1 (1%)	81	77
1	I	143/166 (86%)	142 (99%)	1 (1%)	81	77
1	J	142/166 (86%)	141 (99%)	1 (1%)	81	77
1	K	145/166 (87%)	144 (99%)	1 (1%)	81	77
1	L	143/166 (86%)	141 (99%)	2 (1%)	62	51
1	M	142/166 (86%)	142 (100%)	0	100	100
1	N	140/166 (84%)	140 (100%)	0	100	100
All	All	1989/2324 (86%)	1974 (99%)	15 (1%)	79	74

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	157	ARG
1	L	4	ILE
1	G	157	ARG
1	L	157	ARG
1	J	157	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	39	ASN
1	M	39	ASN
1	N	39	ASN
1	L	39	ASN
1	E	83	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

28 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	A1II0	K	202	1	7,12,12	2.75	3 (42%)	6,17,17	1.38	1 (16%)
3	A1II0	D	202	1	7,12,12	2.77	3 (42%)	6,17,17	1.35	1 (16%)
2	ACT	J	201	-	3,3,3	0.68	0	3,3,3	1.09	0
3	A1II0	A	202	1	7,12,12	2.78	3 (42%)	6,17,17	1.37	1 (16%)
3	A1II0	L	202	1	7,12,12	2.75	3 (42%)	6,17,17	1.37	1 (16%)
3	A1II0	H	202	1	7,12,12	2.80	3 (42%)	6,17,17	1.35	1 (16%)
3	A1II0	F	202	1	7,12,12	2.79	3 (42%)	6,17,17	1.37	1 (16%)
3	A1II0	I	202	1	7,12,12	2.75	3 (42%)	6,17,17	1.36	1 (16%)
2	ACT	K	201	-	3,3,3	0.68	0	3,3,3	1.09	0
2	ACT	M	201	-	3,3,3	0.68	0	3,3,3	1.09	0
3	A1II0	M	202	1	7,12,12	2.74	3 (42%)	6,17,17	1.37	1 (16%)
2	ACT	N	201	-	3,3,3	0.68	0	3,3,3	1.09	0
3	A1II0	N	202	1	7,12,12	2.77	3 (42%)	6,17,17	1.39	1 (16%)
2	ACT	E	201	-	3,3,3	0.67	0	3,3,3	1.09	0
2	ACT	G	201	-	3,3,3	0.68	0	3,3,3	1.09	0
2	ACT	L	201	-	3,3,3	0.67	0	3,3,3	1.09	0
2	ACT	D	201	-	3,3,3	0.68	0	3,3,3	1.09	0
2	ACT	H	201	-	3,3,3	0.68	0	3,3,3	1.09	0
2	ACT	B	201	-	3,3,3	0.68	0	3,3,3	1.09	0
2	ACT	F	201	-	3,3,3	0.67	0	3,3,3	1.08	0
3	A1II0	E	202	1	7,12,12	2.78	3 (42%)	6,17,17	1.37	1 (16%)
2	ACT	I	201	-	3,3,3	0.68	0	3,3,3	1.09	0
3	A1II0	G	202	1	7,12,12	2.78	3 (42%)	6,17,17	1.39	1 (16%)
2	ACT	C	201	-	3,3,3	0.69	0	3,3,3	1.10	0
2	ACT	A	201	-	3,3,3	0.67	0	3,3,3	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	A1II0	B	202	1	7,12,12	2.79	3 (42%)	6,17,17	1.34	1 (16%)
3	A1II0	C	202	1	7,12,12	2.76	3 (42%)	6,17,17	1.39	1 (16%)
3	A1II0	J	202	1	7,12,12	2.79	3 (42%)	6,17,17	1.37	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1II0	E	202	1	-	-	0/2/2/2
3	A1II0	K	202	1	-	-	0/2/2/2
3	A1II0	D	202	1	-	-	0/2/2/2
3	A1II0	M	202	1	-	-	0/2/2/2
3	A1II0	G	202	1	-	-	0/2/2/2
3	A1II0	A	202	1	-	-	0/2/2/2
3	A1II0	L	202	1	-	-	0/2/2/2
3	A1II0	N	202	1	-	-	0/2/2/2
3	A1II0	H	202	1	-	-	0/2/2/2
3	A1II0	F	202	1	-	-	0/2/2/2
3	A1II0	I	202	1	-	-	0/2/2/2
3	A1II0	B	202	1	-	-	0/2/2/2
3	A1II0	C	202	1	-	-	0/2/2/2
3	A1II0	J	202	1	-	-	0/2/2/2

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	202	A1II0	C06-C07	4.83	1.44	1.36
3	J	202	A1II0	C06-C07	4.82	1.44	1.36
3	H	202	A1II0	C06-C07	4.81	1.44	1.36
3	N	202	A1II0	C06-C07	4.81	1.44	1.36
3	A	202	A1II0	C06-C07	4.80	1.44	1.36

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	202	A1II0	C08-C07-C06	-2.54	120.42	123.23
3	C	202	A1II0	C08-C07-C06	-2.53	120.43	123.23
3	N	202	A1II0	C08-C07-C06	-2.53	120.44	123.23
3	K	202	A1II0	C08-C07-C06	-2.52	120.45	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	202	A1II0	C08-C07-C06	-2.52	120.45	123.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	202	A1II0	1	0
3	D	202	A1II0	1	0
2	J	201	ACT	1	0
3	A	202	A1II0	1	0
3	L	202	A1II0	1	0
3	H	202	A1II0	1	0
3	F	202	A1II0	1	0
3	I	202	A1II0	1	0
2	K	201	ACT	1	0
2	M	201	ACT	1	0
3	M	202	A1II0	1	0
2	N	201	ACT	1	0
3	N	202	A1II0	1	0
2	E	201	ACT	1	0
2	G	201	ACT	1	0
2	L	201	ACT	1	0
2	D	201	ACT	1	0
2	H	201	ACT	1	0
2	B	201	ACT	1	0
2	F	201	ACT	1	0
3	E	202	A1II0	1	0
2	I	201	ACT	1	0
3	G	202	A1II0	1	0
2	C	201	ACT	1	0
2	A	201	ACT	1	0
3	B	202	A1II0	1	0
3	C	202	A1II0	1	0
3	J	202	A1II0	1	0

## 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	179/199 (89%)	0.38	10 (5%) 31 36	27, 34, 60, 81	0
1	B	180/199 (90%)	0.45	13 (7%) 23 29	27, 34, 63, 105	0
1	C	182/199 (91%)	0.39	11 (6%) 29 33	27, 34, 63, 131	0
1	D	182/199 (91%)	0.62	17 (9%) 16 20	27, 34, 60, 128	0
1	E	179/199 (89%)	0.33	9 (5%) 35 40	27, 34, 60, 112	0
1	F	181/199 (90%)	0.37	12 (6%) 26 31	20, 34, 63, 81	1 (0%)
1	G	181/199 (90%)	0.46	11 (6%) 28 33	27, 34, 60, 96	0
1	H	179/199 (89%)	0.42	9 (5%) 35 40	27, 34, 61, 81	0
1	I	181/199 (90%)	0.54	14 (7%) 21 26	27, 34, 60, 106	0
1	J	183/199 (91%)	0.40	11 (6%) 29 33	27, 34, 61, 145	0
1	K	183/199 (91%)	0.56	15 (8%) 19 24	27, 34, 63, 176	0
1	L	182/199 (91%)	0.58	20 (10%) 12 15	27, 34, 63, 118	0
1	M	183/199 (91%)	0.43	11 (6%) 29 33	27, 34, 63, 135	0
1	N	179/199 (89%)	0.52	11 (6%) 28 33	27, 34, 60, 81	0
All	All	2534/2786 (90%)	0.46	174 (6%) 24 30	20, 34, 63, 176	1 (0%)

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	17	ALA	9.5
1	B	4	ILE	9.3
1	K	4	ILE	8.7
1	I	8	ILE	8.6
1	J	8	ILE	8.5



## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	C	201	4/4	0.84	0.17	32,38,42,49	0
2	ACT	L	201	4/4	0.85	0.16	32,38,42,49	0
2	ACT	B	201	4/4	0.86	0.16	32,38,42,49	0
2	ACT	K	201	4/4	0.88	0.16	32,38,42,49	0
2	ACT	G	201	4/4	0.89	0.14	32,38,42,49	0
3	A1II0	D	202	11/11	0.89	0.13	31,35,115,131	0
2	ACT	I	201	4/4	0.90	0.15	32,38,42,49	0
2	ACT	F	201	4/4	0.90	0.13	32,38,42,49	0
2	ACT	M	201	4/4	0.91	0.13	32,38,42,49	0
2	ACT	D	201	4/4	0.91	0.12	32,38,42,49	0
3	A1II0	J	202	11/11	0.91	0.13	31,35,115,131	0
3	A1II0	N	202	11/11	0.91	0.11	31,35,115,131	0
2	ACT	A	201	4/4	0.92	0.12	32,38,42,49	0
2	ACT	N	201	4/4	0.92	0.11	32,38,42,49	0
2	ACT	J	201	4/4	0.92	0.13	32,38,42,49	0
3	A1II0	G	202	11/11	0.92	0.12	31,35,115,131	0
3	A1II0	H	202	11/11	0.92	0.11	31,35,115,131	0
2	ACT	E	201	4/4	0.92	0.11	32,38,42,49	0
2	ACT	H	201	4/4	0.92	0.12	32,38,42,49	0
3	A1II0	F	202	11/11	0.93	0.11	31,35,115,131	0
3	A1II0	B	202	11/11	0.93	0.12	31,35,115,131	0
3	A1II0	C	202	11/11	0.93	0.11	31,35,115,131	0
3	A1II0	A	202	11/11	0.93	0.10	31,35,115,131	0
3	A1II0	M	202	11/11	0.93	0.11	31,35,115,131	0
3	A1II0	E	202	11/11	0.93	0.11	31,35,115,131	0
3	A1II0	L	202	11/11	0.94	0.10	31,35,115,131	0
3	A1II0	K	202	11/11	0.95	0.10	31,35,115,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1II0	I	202	11/11	0.96	0.09	31,35,115,131	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.