



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:29 PM BST

PDB ID : 6NAQ  
Title : Crystal structure of Neisseria meningitidis ClpP protease in Apo form  
Authors : Houry, W.A.; Mabanglo, M.F.; Pai, E.F.; Eger, B.T.; Bryson, S.  
Deposited on : 2018-12-06  
Resolution : 2.02 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 : 2.13.1  
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) : 2.13.1

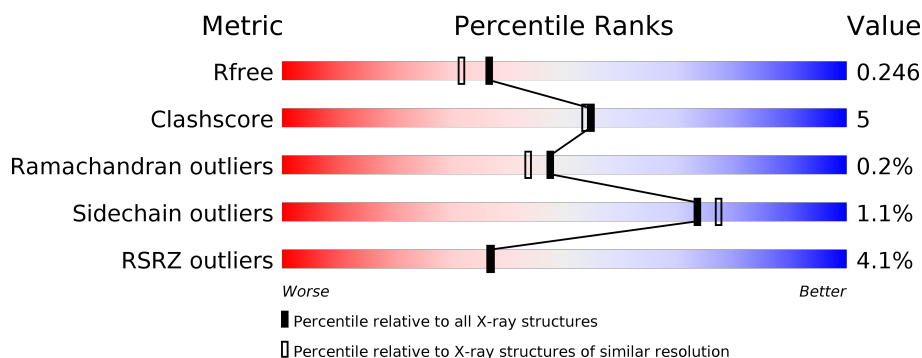
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	218	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>9%</div> <div>16%</div> </div> </div>
1	B	218	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>8%</div> <div>16%</div> </div> </div>
1	C	218	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>17%</div> </div> </div>
1	D	218	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>7%</div> <div>16%</div> </div> </div>
1	E	218	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>10%</div> <div>16%</div> </div> </div>
1	F	218	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>7%</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	218	
1	H	218	
1	I	218	
1	J	218	
1	K	218	
1	L	218	
1	M	218	
1	N	218	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20681 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	184	Total	C	N	O	S	0	0	0
			1428	902	243	275	8			
1	B	183	Total	C	N	O	S	0	0	0
			1422	899	242	273	8			
1	C	182	Total	C	N	O	S	0	0	0
			1415	894	241	272	8			
1	D	183	Total	C	N	O	S	0	0	0
			1422	899	242	273	8			
1	E	184	Total	C	N	O	S	0	0	0
			1430	905	243	274	8			
1	F	183	Total	C	N	O	S	0	0	0
			1422	899	242	273	8			
1	G	187	Total	C	N	O	S	0	0	0
			1456	920	249	279	8			
1	H	187	Total	C	N	O	S	0	0	0
			1455	920	249	278	8			
1	I	185	Total	C	N	O	S	0	0	0
			1436	908	244	276	8			
1	J	186	Total	C	N	O	S	0	0	0
			1448	915	248	277	8			
1	K	184	Total	C	N	O	S	0	0	0
			1428	902	243	275	8			
1	L	183	Total	C	N	O	S	0	0	0
			1423	900	242	273	8			
1	M	183	Total	C	N	O	S	0	0	0
			1421	897	242	274	8			
1	N	184	Total	C	N	O	S	0	0	0
			1428	902	243	275	8			

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP I4E574
A	-11	HIS	-	expression tag	UNP I4E574
A	-10	HIS	-	expression tag	UNP I4E574
A	-9	HIS	-	expression tag	UNP I4E574
A	-8	HIS	-	expression tag	UNP I4E574
A	-7	GLU	-	expression tag	UNP I4E574
A	-6	ASN	-	expression tag	UNP I4E574
A	-5	LEU	-	expression tag	UNP I4E574
A	-4	TYR	-	expression tag	UNP I4E574
A	-3	PHE	-	expression tag	UNP I4E574
A	-2	GLN	-	expression tag	UNP I4E574
A	-1	SER	-	expression tag	UNP I4E574
A	0	ASN	-	expression tag	UNP I4E574
B	-13	HIS	-	expression tag	UNP I4E574
B	-12	HIS	-	expression tag	UNP I4E574
B	-11	HIS	-	expression tag	UNP I4E574
B	-10	HIS	-	expression tag	UNP I4E574
B	-9	HIS	-	expression tag	UNP I4E574
B	-8	HIS	-	expression tag	UNP I4E574
B	-7	GLU	-	expression tag	UNP I4E574
B	-6	ASN	-	expression tag	UNP I4E574
B	-5	LEU	-	expression tag	UNP I4E574
B	-4	TYR	-	expression tag	UNP I4E574
B	-3	PHE	-	expression tag	UNP I4E574
B	-2	GLN	-	expression tag	UNP I4E574
B	-1	SER	-	expression tag	UNP I4E574
B	0	ASN	-	expression tag	UNP I4E574
C	-13	HIS	-	expression tag	UNP I4E574
C	-12	HIS	-	expression tag	UNP I4E574
C	-11	HIS	-	expression tag	UNP I4E574
C	-10	HIS	-	expression tag	UNP I4E574
C	-9	HIS	-	expression tag	UNP I4E574
C	-8	HIS	-	expression tag	UNP I4E574
C	-7	GLU	-	expression tag	UNP I4E574
C	-6	ASN	-	expression tag	UNP I4E574
C	-5	LEU	-	expression tag	UNP I4E574
C	-4	TYR	-	expression tag	UNP I4E574
C	-3	PHE	-	expression tag	UNP I4E574
C	-2	GLN	-	expression tag	UNP I4E574
C	-1	SER	-	expression tag	UNP I4E574
C	0	ASN	-	expression tag	UNP I4E574
D	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP I4E574
D	-11	HIS	-	expression tag	UNP I4E574
D	-10	HIS	-	expression tag	UNP I4E574
D	-9	HIS	-	expression tag	UNP I4E574
D	-8	HIS	-	expression tag	UNP I4E574
D	-7	GLU	-	expression tag	UNP I4E574
D	-6	ASN	-	expression tag	UNP I4E574
D	-5	LEU	-	expression tag	UNP I4E574
D	-4	TYR	-	expression tag	UNP I4E574
D	-3	PHE	-	expression tag	UNP I4E574
D	-2	GLN	-	expression tag	UNP I4E574
D	-1	SER	-	expression tag	UNP I4E574
D	0	ASN	-	expression tag	UNP I4E574
E	-13	HIS	-	expression tag	UNP I4E574
E	-12	HIS	-	expression tag	UNP I4E574
E	-11	HIS	-	expression tag	UNP I4E574
E	-10	HIS	-	expression tag	UNP I4E574
E	-9	HIS	-	expression tag	UNP I4E574
E	-8	HIS	-	expression tag	UNP I4E574
E	-7	GLU	-	expression tag	UNP I4E574
E	-6	ASN	-	expression tag	UNP I4E574
E	-5	LEU	-	expression tag	UNP I4E574
E	-4	TYR	-	expression tag	UNP I4E574
E	-3	PHE	-	expression tag	UNP I4E574
E	-2	GLN	-	expression tag	UNP I4E574
E	-1	SER	-	expression tag	UNP I4E574
E	0	ASN	-	expression tag	UNP I4E574
F	-13	HIS	-	expression tag	UNP I4E574
F	-12	HIS	-	expression tag	UNP I4E574
F	-11	HIS	-	expression tag	UNP I4E574
F	-10	HIS	-	expression tag	UNP I4E574
F	-9	HIS	-	expression tag	UNP I4E574
F	-8	HIS	-	expression tag	UNP I4E574
F	-7	GLU	-	expression tag	UNP I4E574
F	-6	ASN	-	expression tag	UNP I4E574
F	-5	LEU	-	expression tag	UNP I4E574
F	-4	TYR	-	expression tag	UNP I4E574
F	-3	PHE	-	expression tag	UNP I4E574
F	-2	GLN	-	expression tag	UNP I4E574
F	-1	SER	-	expression tag	UNP I4E574
F	0	ASN	-	expression tag	UNP I4E574
G	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-12	HIS	-	expression tag	UNP I4E574
G	-11	HIS	-	expression tag	UNP I4E574
G	-10	HIS	-	expression tag	UNP I4E574
G	-9	HIS	-	expression tag	UNP I4E574
G	-8	HIS	-	expression tag	UNP I4E574
G	-7	GLU	-	expression tag	UNP I4E574
G	-6	ASN	-	expression tag	UNP I4E574
G	-5	LEU	-	expression tag	UNP I4E574
G	-4	TYR	-	expression tag	UNP I4E574
G	-3	PHE	-	expression tag	UNP I4E574
G	-2	GLN	-	expression tag	UNP I4E574
G	-1	SER	-	expression tag	UNP I4E574
G	0	ASN	-	expression tag	UNP I4E574
H	-13	HIS	-	expression tag	UNP I4E574
H	-12	HIS	-	expression tag	UNP I4E574
H	-11	HIS	-	expression tag	UNP I4E574
H	-10	HIS	-	expression tag	UNP I4E574
H	-9	HIS	-	expression tag	UNP I4E574
H	-8	HIS	-	expression tag	UNP I4E574
H	-7	GLU	-	expression tag	UNP I4E574
H	-6	ASN	-	expression tag	UNP I4E574
H	-5	LEU	-	expression tag	UNP I4E574
H	-4	TYR	-	expression tag	UNP I4E574
H	-3	PHE	-	expression tag	UNP I4E574
H	-2	GLN	-	expression tag	UNP I4E574
H	-1	SER	-	expression tag	UNP I4E574
H	0	ASN	-	expression tag	UNP I4E574
I	-13	HIS	-	expression tag	UNP I4E574
I	-12	HIS	-	expression tag	UNP I4E574
I	-11	HIS	-	expression tag	UNP I4E574
I	-10	HIS	-	expression tag	UNP I4E574
I	-9	HIS	-	expression tag	UNP I4E574
I	-8	HIS	-	expression tag	UNP I4E574
I	-7	GLU	-	expression tag	UNP I4E574
I	-6	ASN	-	expression tag	UNP I4E574
I	-5	LEU	-	expression tag	UNP I4E574
I	-4	TYR	-	expression tag	UNP I4E574
I	-3	PHE	-	expression tag	UNP I4E574
I	-2	GLN	-	expression tag	UNP I4E574
I	-1	SER	-	expression tag	UNP I4E574
I	0	ASN	-	expression tag	UNP I4E574
J	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-12	HIS	-	expression tag	UNP I4E574
J	-11	HIS	-	expression tag	UNP I4E574
J	-10	HIS	-	expression tag	UNP I4E574
J	-9	HIS	-	expression tag	UNP I4E574
J	-8	HIS	-	expression tag	UNP I4E574
J	-7	GLU	-	expression tag	UNP I4E574
J	-6	ASN	-	expression tag	UNP I4E574
J	-5	LEU	-	expression tag	UNP I4E574
J	-4	TYR	-	expression tag	UNP I4E574
J	-3	PHE	-	expression tag	UNP I4E574
J	-2	GLN	-	expression tag	UNP I4E574
J	-1	SER	-	expression tag	UNP I4E574
J	0	ASN	-	expression tag	UNP I4E574
K	-13	HIS	-	expression tag	UNP I4E574
K	-12	HIS	-	expression tag	UNP I4E574
K	-11	HIS	-	expression tag	UNP I4E574
K	-10	HIS	-	expression tag	UNP I4E574
K	-9	HIS	-	expression tag	UNP I4E574
K	-8	HIS	-	expression tag	UNP I4E574
K	-7	GLU	-	expression tag	UNP I4E574
K	-6	ASN	-	expression tag	UNP I4E574
K	-5	LEU	-	expression tag	UNP I4E574
K	-4	TYR	-	expression tag	UNP I4E574
K	-3	PHE	-	expression tag	UNP I4E574
K	-2	GLN	-	expression tag	UNP I4E574
K	-1	SER	-	expression tag	UNP I4E574
K	0	ASN	-	expression tag	UNP I4E574
L	-13	HIS	-	expression tag	UNP I4E574
L	-12	HIS	-	expression tag	UNP I4E574
L	-11	HIS	-	expression tag	UNP I4E574
L	-10	HIS	-	expression tag	UNP I4E574
L	-9	HIS	-	expression tag	UNP I4E574
L	-8	HIS	-	expression tag	UNP I4E574
L	-7	GLU	-	expression tag	UNP I4E574
L	-6	ASN	-	expression tag	UNP I4E574
L	-5	LEU	-	expression tag	UNP I4E574
L	-4	TYR	-	expression tag	UNP I4E574
L	-3	PHE	-	expression tag	UNP I4E574
L	-2	GLN	-	expression tag	UNP I4E574
L	-1	SER	-	expression tag	UNP I4E574
L	0	ASN	-	expression tag	UNP I4E574
M	-13	HIS	-	expression tag	UNP I4E574

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	HIS	-	expression tag	UNP I4E574
M	-11	HIS	-	expression tag	UNP I4E574
M	-10	HIS	-	expression tag	UNP I4E574
M	-9	HIS	-	expression tag	UNP I4E574
M	-8	HIS	-	expression tag	UNP I4E574
M	-7	GLU	-	expression tag	UNP I4E574
M	-6	ASN	-	expression tag	UNP I4E574
M	-5	LEU	-	expression tag	UNP I4E574
M	-4	TYR	-	expression tag	UNP I4E574
M	-3	PHE	-	expression tag	UNP I4E574
M	-2	GLN	-	expression tag	UNP I4E574
M	-1	SER	-	expression tag	UNP I4E574
M	0	ASN	-	expression tag	UNP I4E574
N	-13	HIS	-	expression tag	UNP I4E574
N	-12	HIS	-	expression tag	UNP I4E574
N	-11	HIS	-	expression tag	UNP I4E574
N	-10	HIS	-	expression tag	UNP I4E574
N	-9	HIS	-	expression tag	UNP I4E574
N	-8	HIS	-	expression tag	UNP I4E574
N	-7	GLU	-	expression tag	UNP I4E574
N	-6	ASN	-	expression tag	UNP I4E574
N	-5	LEU	-	expression tag	UNP I4E574
N	-4	TYR	-	expression tag	UNP I4E574
N	-3	PHE	-	expression tag	UNP I4E574
N	-2	GLN	-	expression tag	UNP I4E574
N	-1	SER	-	expression tag	UNP I4E574
N	0	ASN	-	expression tag	UNP I4E574

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	K	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	I	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	N	1	Total K 1 1	0	0
2	L	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0
2	M	1	Total K 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	54	Total O 54 54	0	0
3	C	45	Total O 45 45	0	0
3	D	43	Total O 43 43	0	0
3	E	31	Total O 31 31	0	0
3	F	37	Total O 37 37	0	0
3	G	51	Total O 51 51	0	0
3	H	32	Total O 32 32	0	0
3	I	29	Total O 29 29	0	0
3	J	44	Total O 44 44	0	0
3	K	48	Total O 48 48	0	0

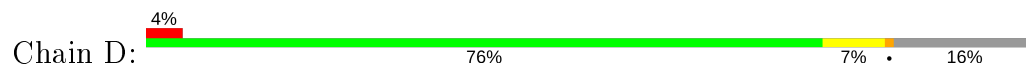
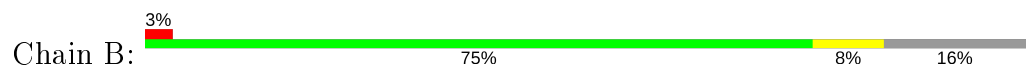
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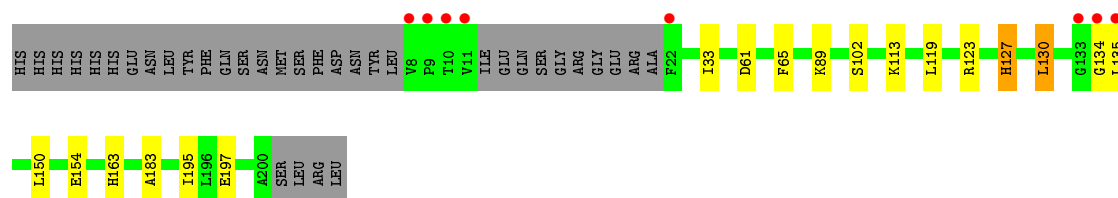
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	54	Total 54	O 54	0	0
3	M	58	Total 58	O 58	0	0
3	N	52	Total 52	O 52	0	0

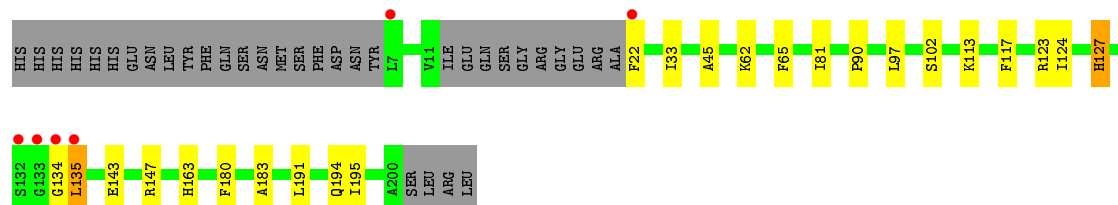
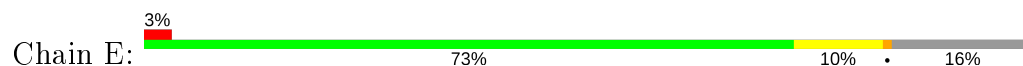
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Chain A: 

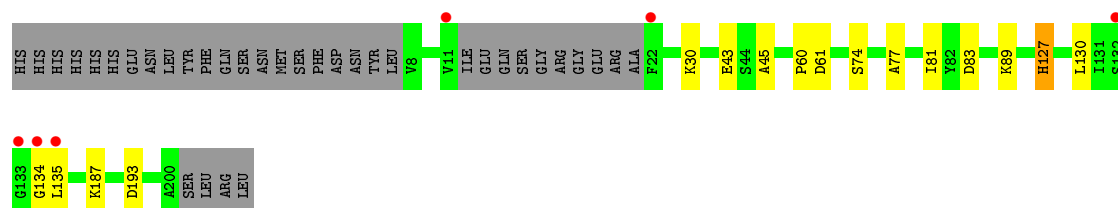
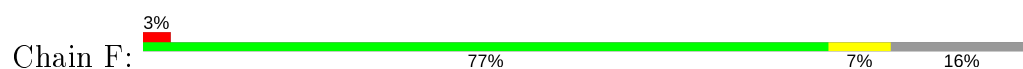




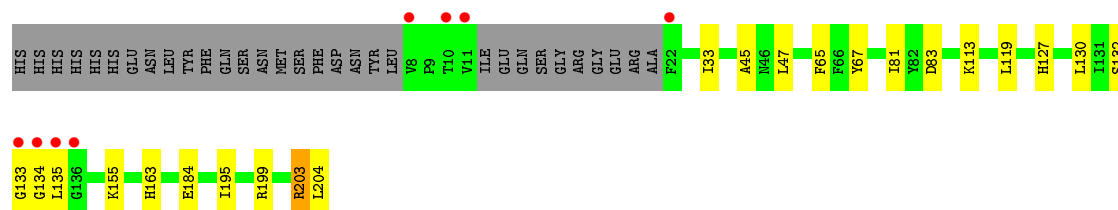
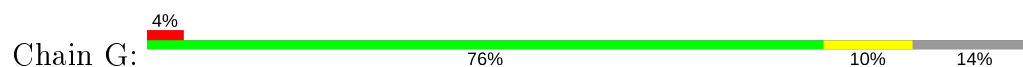
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



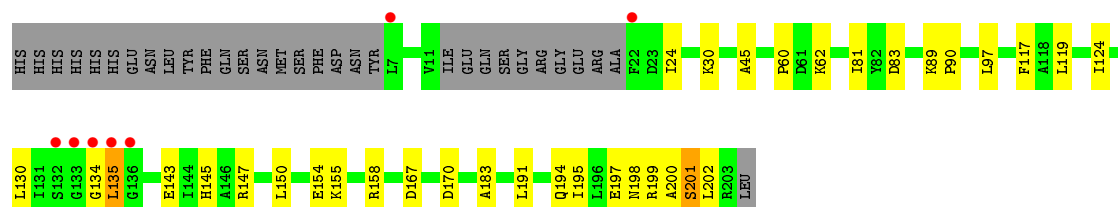
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



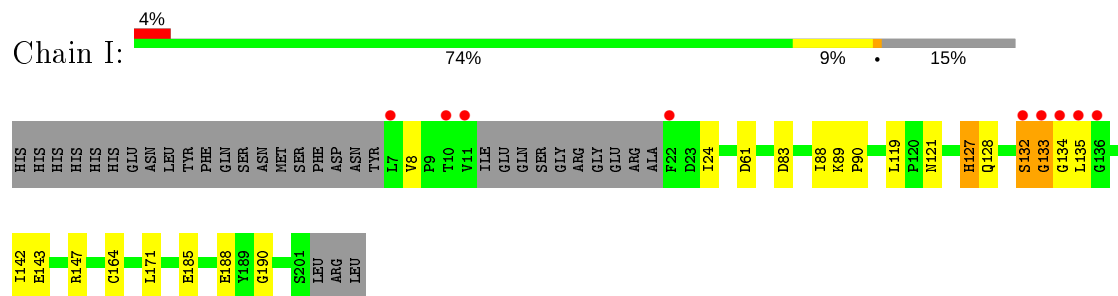
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



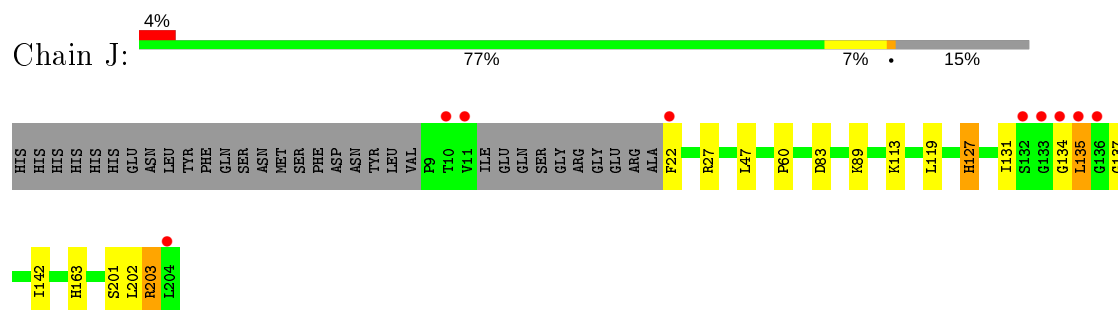
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



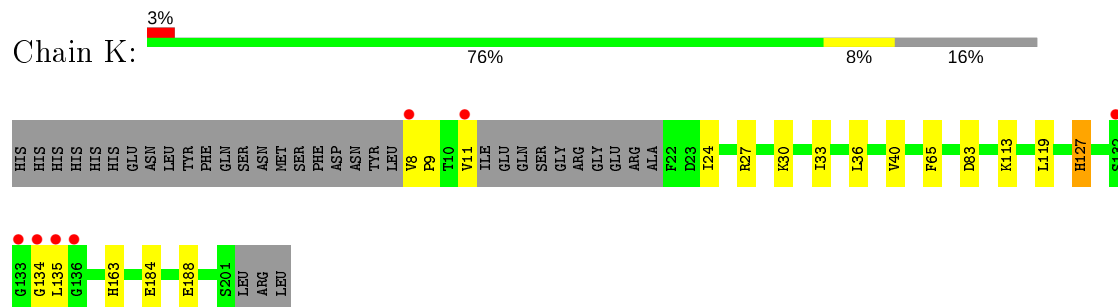
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



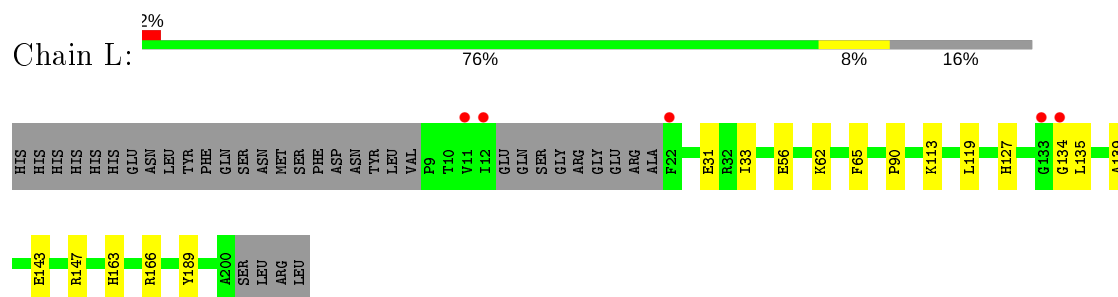
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



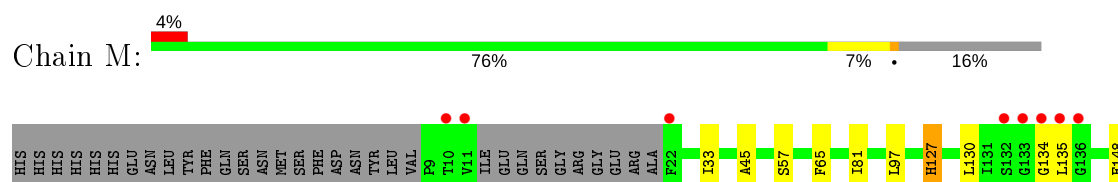
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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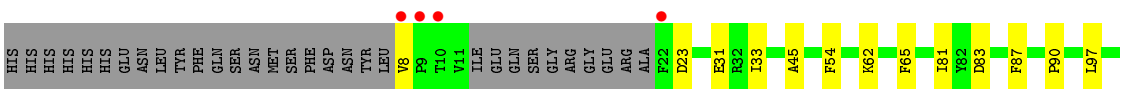


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





- 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, $\alpha$ , $\beta$ , $\gamma$	98.58Å 127.94Å 120.19Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	51.39 – 2.02 51.39 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.7 (51.39-2.02) 97.3 (51.39-2.02)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.8.4 _1496	Depositor
R, $R_{free}$	0.207 , 0.246 0.209 , 0.246	Depositor DCC
$R_{free}$ test set	9516 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.936	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 23.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.370 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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

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

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	0.45	0/1449	0.58	0/1951
1	B	0.41	0/1443	0.56	0/1943
1	C	0.42	0/1436	0.60	1/1932 (0.1%)
1	D	0.39	0/1443	0.57	1/1943 (0.1%)
1	E	0.38	0/1451	0.64	1/1954 (0.1%)
1	F	0.38	0/1443	0.57	0/1943
1	G	0.44	0/1477	0.60	1/1987 (0.1%)
1	H	0.42	0/1476	0.64	1/1987 (0.1%)
1	I	0.41	0/1457	0.57	0/1962
1	J	0.41	0/1469	0.59	1/1976 (0.1%)
1	K	0.41	0/1449	0.56	0/1951
1	L	0.41	0/1444	0.54	0/1943
1	M	0.42	0/1442	0.57	0/1940
1	N	0.41	0/1449	0.57	0/1951
All	All	0.41	0/20328	0.59	6/27363 (0.0%)

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	C	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	135	LEU	CA-CB-CG	11.74	142.29	115.30
1	G	133	GLY	N-CA-C	-6.56	96.69	113.10
1	H	135	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	J	135	LEU	CA-CB-CG	5.82	128.69	115.30
1	D	130	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	133	GLY	N-CA-C	-5.37	99.68	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	132	SER	Peptide
1	G	132	SER	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	1428	0	1434	16	0
1	B	1422	0	1429	18	0
1	C	1415	0	1421	27	0
1	D	1422	0	1429	15	0
1	E	1430	0	1440	22	0
1	F	1422	0	1429	14	0
1	G	1456	0	1469	16	0
1	H	1455	0	1469	30	0
1	I	1436	0	1445	20	0
1	J	1448	0	1461	31	0
1	K	1428	0	1434	18	0
1	L	1423	0	1432	11	0
1	M	1421	0	1426	12	0
1	N	1428	0	1434	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	55	0	0	1	0
3	B	54	0	0	0	0
3	C	45	0	0	0	0
3	D	43	0	0	0	0
3	E	31	0	0	0	0
3	F	37	0	0	2	0
3	G	51	0	0	0	0
3	H	32	0	0	0	0
3	I	29	0	0	0	0
3	J	44	0	0	0	0
3	K	48	0	0	1	0
3	L	54	0	0	1	0
3	M	58	0	0	0	0
3	N	52	0	0	0	0
All	All	20681	0	20152	209	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 5.

All (209) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:202:LEU:O	1:J:203:ARG:HD2	1.51	1.09
1:J:203:ARG:HH11	1:J:203:ARG:HG2	1.28	0.99
1:F:135:LEU:H	1:N:135:LEU:H	1.24	0.86
1:F:134:GLY:HA3	1:N:134:GLY:HA3	1.61	0.82
1:C:134:GLY:HA3	1:J:134:GLY:HA3	1.62	0.81
1:F:135:LEU:HB2	1:N:135:LEU:HB2	1.61	0.81
1:D:135:LEU:HB2	1:I:135:LEU:HG	1.63	0.79
1:A:148:GLU:OE1	3:A:401:HOH:O	2.03	0.76
1:A:166:ARG:NH1	1:A:170:ASP:OD2	2.20	0.74
1:G:135:LEU:HB2	1:M:135:LEU:HB2	1.67	0.73
1:H:60:PRO:HB2	1:H:89:LYS:HD3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:HB2	1:K:135:LEU:HB2	1.69	0.73
1:E:135:LEU:HD12	1:H:135:LEU:HD22	1.71	0.73
1:D:134:GLY:HA3	1:I:134:GLY:HA3	1.72	0.71
1:N:8:VAL:HG12	1:N:23:ASP:HB2	1.73	0.70
1:J:202:LEU:C	1:J:203:ARG:HD2	2.12	0.70
1:K:184:GLU:OE2	3:K:401:HOH:O	2.10	0.69
1:B:135:LEU:H	1:K:135:LEU:H	1.40	0.69
1:L:33:ILE:HD13	1:L:65:PHE:HB2	1.74	0.68
1:J:135:LEU:HD21	1:J:142:ILE:HG12	1.76	0.67
1:C:11:VAL:HG21	1:C:27:ARG:HB2	1.74	0.67
1:K:33:ILE:HD13	1:K:65:PHE:HB2	1.78	0.66
1:C:33:ILE:HD13	1:C:65:PHE:HB2	1.76	0.66
1:H:154:GLU:OE2	1:H:158:ARG:NH2	2.28	0.66
1:J:203:ARG:NH1	1:J:203:ARG:HG2	2.03	0.65
1:D:33:ILE:HD13	1:D:65:PHE:HB2	1.79	0.63
1:E:135:LEU:H	1:H:135:LEU:H	1.45	0.63
1:B:33:ILE:HD13	1:B:65:PHE:HB2	1.81	0.63
1:L:143:GLU:OE2	1:L:147:ARG:NH1	2.32	0.63
1:F:135:LEU:N	1:N:135:LEU:H	1.96	0.62
1:C:135:LEU:HD12	1:J:135:LEU:HD22	1.81	0.62
1:C:135:LEU:H	1:J:135:LEU:H	1.48	0.61
1:B:135:LEU:H	1:K:135:LEU:N	1.98	0.61
1:B:134:GLY:HA3	1:K:134:GLY:HA3	1.83	0.61
1:C:135:LEU:HB2	1:J:135:LEU:HB3	1.81	0.60
1:H:199:ARG:O	1:H:201:SER:N	2.34	0.60
1:J:135:LEU:HD21	1:J:142:ILE:HG23	1.84	0.60
1:E:134:GLY:HA3	1:H:134:GLY:HA3	1.83	0.60
1:J:113:LYS:HE2	1:J:163:HIS:O	2.02	0.60
1:N:33:ILE:HD13	1:N:65:PHE:HB2	1.82	0.60
1:F:135:LEU:H	1:N:135:LEU:N	1.96	0.59
1:C:10:THR:OG1	1:C:22:PHE:O	2.17	0.59
1:J:202:LEU:C	1:J:203:ARG:CD	2.71	0.59
1:B:135:LEU:N	1:K:135:LEU:H	2.01	0.58
1:E:135:LEU:H	1:H:135:LEU:N	2.02	0.58
1:J:202:LEU:O	1:J:203:ARG:CD	2.40	0.58
1:G:134:GLY:HA3	1:M:134:GLY:HA3	1.86	0.58
1:D:135:LEU:H	1:I:135:LEU:H	1.52	0.58
1:J:47:LEU:HD11	1:K:9:PRO:HD2	1.85	0.58
1:A:33:ILE:HD13	1:A:65:PHE:HB2	1.85	0.57
1:D:150:LEU:O	1:D:154:GLU:HG3	2.03	0.57
1:E:135:LEU:CD1	1:H:135:LEU:HD22	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:HIS:CD2	1:I:128:GLN:O	2.59	0.56
1:G:135:LEU:H	1:M:135:LEU:H	1.50	0.56
1:H:117:PHE:CD1	1:H:194:GLN:HB2	2.41	0.56
1:G:113:LYS:HE2	1:G:163:HIS:O	2.06	0.56
1:J:135:LEU:CD2	1:J:142:ILE:HG12	2.36	0.55
1:F:60:PRO:HB2	1:F:89:LYS:HD3	1.88	0.55
1:N:45:ALA:HA	1:N:81:ILE:HD11	1.89	0.55
1:C:113:LYS:HE2	1:C:163:HIS:O	2.06	0.55
1:H:155:LYS:HE2	1:I:121:ASN:OD1	2.07	0.54
1:M:200:ALA:O	1:M:201:SER:HB3	2.08	0.54
1:B:143:GLU:O	1:B:147:ARG:HG3	2.08	0.53
1:A:121:ASN:OD1	1:G:155:LYS:HE2	2.09	0.53
1:M:97:LEU:HD23	1:M:97:LEU:H	1.74	0.53
1:L:56:GLU:OE1	1:M:199:ARG:NH2	2.42	0.53
1:M:148:GLU:HA	1:M:151:LYS:HE3	1.92	0.52
1:E:183:ALA:HB1	1:E:195:ILE:HG12	1.91	0.52
1:E:33:ILE:HD13	1:E:65:PHE:HB2	1.92	0.52
1:K:27:ARG:O	1:K:30:LYS:HB2	2.09	0.52
1:E:117:PHE:CE1	1:E:194:GLN:HB2	2.45	0.52
1:J:22:PHE:HE1	1:J:27:ARG:HD3	1.76	0.51
1:I:83:ASP:HB3	1:J:119:LEU:HB3	1.92	0.51
1:C:135:LEU:N	1:J:135:LEU:H	2.08	0.51
1:J:203:ARG:CG	1:J:203:ARG:NH1	2.71	0.51
1:E:62:LYS:O	1:E:90:PRO:HB3	2.10	0.51
1:H:167:ASP:HB2	1:H:170:ASP:OD2	2.10	0.51
1:H:135:LEU:HD21	1:H:145:HIS:HB2	1.92	0.51
1:N:97:LEU:HD23	1:N:97:LEU:H	1.76	0.51
1:A:113:LYS:HE2	1:A:163:HIS:O	2.10	0.51
1:C:10:THR:HA	1:C:23:ASP:HA	1.93	0.50
1:H:117:PHE:HD1	1:H:194:GLN:HB2	1.74	0.50
1:L:113:LYS:HE2	1:L:163:HIS:O	2.11	0.50
1:J:60:PRO:HB2	1:J:89:LYS:HD3	1.93	0.50
1:A:135:LEU:H	1:L:135:LEU:N	2.09	0.50
1:A:45:ALA:HA	1:A:81:ILE:HD11	1.93	0.50
1:K:8:VAL:HG23	1:K:24:ILE:HG22	1.93	0.50
1:J:203:ARG:HH11	1:J:203:ARG:CG	2.09	0.50
1:I:143:GLU:O	1:I:147:ARG:HG3	2.11	0.49
1:L:62:LYS:O	1:L:90:PRO:HB3	2.12	0.49
1:M:57:SER:OG	1:N:31:GLU:OE2	2.29	0.49
1:A:83:ASP:HB3	1:B:119:LEU:HB3	1.94	0.49
1:I:88:ILE:HD12	1:I:90:PRO:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:31:GLU:HB2	1:L:33:ILE:HG12	1.94	0.49
1:N:113:LYS:HE2	1:N:163:HIS:O	2.12	0.49
1:A:9:PRO:HD2	1:G:47:LEU:HD11	1.94	0.49
1:B:26:SER:HG	1:C:10:THR:N	2.10	0.49
1:I:135:LEU:HD12	1:I:135:LEU:O	2.12	0.49
1:B:166:ARG:HD2	1:B:189:TYR:O	2.13	0.49
1:N:127:HIS:CD2	1:N:128:GLN:O	2.66	0.49
1:D:183:ALA:HB1	1:D:195:ILE:HG12	1.95	0.48
1:C:97:LEU:HD23	1:C:97:LEU:H	1.78	0.48
1:J:22:PHE:HE1	1:J:27:ARG:HB2	1.77	0.48
1:B:127:HIS:CD2	1:B:127:HIS:C	2.86	0.48
1:A:119:LEU:HB3	1:G:83:ASP:HB3	1.96	0.48
1:B:113:LYS:HE2	1:B:163:HIS:O	2.13	0.48
1:I:135:LEU:HD13	1:I:142:ILE:HG12	1.95	0.48
1:J:127:HIS:C	1:J:127:HIS:CD2	2.85	0.47
1:H:202:LEU:HA	1:H:202:LEU:HD23	1.62	0.47
1:J:22:PHE:CE1	1:J:27:ARG:HB2	2.50	0.47
1:I:8:VAL:HG13	1:I:24:ILE:HG22	1.96	0.47
1:I:185:GLU:O	1:I:188:GLU:HG2	2.14	0.47
1:I:127:HIS:CD2	1:I:127:HIS:C	2.88	0.47
1:B:26:SER:HG	1:C:10:THR:H	1.63	0.46
1:B:83:ASP:HB3	1:C:119:LEU:HB3	1.96	0.46
1:H:198:ASN:HA	1:N:87:PHE:HA	1.96	0.46
1:F:187:LYS:HE3	1:F:193:ASP:O	2.15	0.46
1:N:155:LYS:HG3	1:N:158:ARG:HH21	1.81	0.46
1:B:8:VAL:HG13	1:B:24:ILE:HG22	1.98	0.46
1:I:61:ASP:OD1	1:I:89:LYS:HE3	2.15	0.46
1:F:61:ASP:OD1	1:F:89:LYS:HE3	2.16	0.46
1:H:97:LEU:HD23	1:H:97:LEU:H	1.81	0.45
1:D:113:LYS:HE2	1:D:163:HIS:O	2.17	0.45
1:G:45:ALA:HA	1:G:81:ILE:HD11	1.97	0.45
1:H:62:LYS:O	1:H:90:PRO:HB3	2.16	0.45
1:K:127:HIS:C	1:K:127:HIS:CD2	2.90	0.45
1:K:83:ASP:HB3	1:L:119:LEU:HB3	1.98	0.45
1:N:62:LYS:O	1:N:90:PRO:HB3	2.16	0.45
1:C:135:LEU:H	1:J:135:LEU:N	2.11	0.45
1:H:183:ALA:HB1	1:H:195:ILE:HG12	1.98	0.45
1:J:201:SER:O	1:J:203:ARG:HD3	2.17	0.45
1:J:22:PHE:CE1	1:J:27:ARG:HD3	2.51	0.45
1:F:43:GLU:HG2	3:F:428:HOH:O	2.16	0.45
1:L:166:ARG:HD2	1:L:189:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:O	1:L:134:GLY:HA2	2.17	0.45
1:G:184:GLU:HA	1:G:195:ILE:HD11	1.99	0.44
1:J:127:HIS:HD2	1:J:127:HIS:O	2.00	0.44
1:E:22:PHE:N	1:E:22:PHE:CD1	2.84	0.44
1:F:83:ASP:HB3	1:G:119:LEU:HB3	1.98	0.44
1:A:87:PHE:CZ	1:B:199:ARG:HG2	2.53	0.44
1:C:27:ARG:O	1:C:30:LYS:HB2	2.17	0.44
1:G:33:ILE:HD13	1:G:65:PHE:HB2	1.99	0.44
1:H:83:ASP:HB3	1:I:119:LEU:HB3	1.99	0.44
1:M:127:HIS:C	1:M:127:HIS:CD2	2.90	0.44
1:A:127:HIS:C	1:A:127:HIS:CD2	2.91	0.44
1:E:143:GLU:OE2	1:E:147:ARG:NE	2.51	0.44
1:C:83:ASP:HB3	1:D:119:LEU:HB3	2.00	0.44
1:N:127:HIS:C	1:N:127:HIS:CD2	2.91	0.44
1:H:124:ILE:HG21	1:H:191:LEU:HD13	1.99	0.44
1:E:124:ILE:HG21	1:E:191:LEU:HD13	2.00	0.44
1:I:132:SER:O	1:I:133:GLY:C	2.56	0.44
3:F:406:HOH:O	1:G:199:ARG:HG3	2.18	0.43
1:I:164:CYS:HA	1:I:190:GLY:O	2.19	0.43
1:D:135:LEU:N	1:I:135:LEU:H	2.15	0.43
1:A:10:THR:HA	1:A:23:ASP:HA	2.01	0.43
1:E:113:LYS:HZ1	1:E:163:HIS:HA	1.84	0.43
1:C:127:HIS:CD2	1:C:127:HIS:C	2.92	0.43
1:C:152:ILE:HD11	1:D:123:ARG:NH2	2.34	0.43
1:H:143:GLU:HG2	1:H:147:ARG:NH1	2.34	0.43
1:E:135:LEU:HB2	1:H:135:LEU:H	1.83	0.43
1:M:45:ALA:HA	1:M:81:ILE:HD11	2.00	0.43
1:H:24:ILE:HD11	1:N:54:PHE:CB	2.49	0.43
1:H:119:LEU:HB3	1:N:83:ASP:HB3	2.00	0.43
1:E:117:PHE:CD1	1:E:194:GLN:HB2	2.53	0.43
1:D:127:HIS:C	1:D:127:HIS:CD2	2.92	0.42
1:D:61:ASP:OD1	1:D:89:LYS:NZ	2.43	0.42
1:C:131:ILE:O	1:J:137:GLY:N	2.52	0.42
1:H:135:LEU:HD21	1:H:145:HIS:CB	2.49	0.42
1:K:113:LYS:HE2	1:K:163:HIS:O	2.19	0.42
1:N:97:LEU:N	1:N:97:LEU:HD23	2.34	0.42
1:J:83:ASP:HB3	1:K:119:LEU:HB3	2.02	0.42
1:C:152:ILE:HD11	1:D:123:ARG:HH21	1.84	0.42
1:E:123:ARG:HD3	1:E:180:PHE:CE1	2.54	0.42
1:F:30:LYS:HD3	1:F:30:LYS:HA	1.88	0.42
1:G:33:ILE:HD12	1:G:67:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLY:HA2	1:I:135:LEU:O	2.20	0.42
1:F:45:ALA:HA	1:F:81:ILE:HD11	2.01	0.42
1:H:197:GLU:HG3	1:H:198:ASN:N	2.35	0.42
1:H:45:ALA:HA	1:H:81:ILE:HD11	2.02	0.42
1:M:33:ILE:HD13	1:M:65:PHE:HB2	2.02	0.42
1:C:120:PRO:HD3	1:C:196:LEU:O	2.20	0.41
1:C:71:PRO:HA	1:C:101:ALA:HB3	2.02	0.41
1:E:143:GLU:O	1:E:147:ARG:HG3	2.20	0.41
1:E:97:LEU:H	1:E:97:LEU:HD23	1.85	0.41
1:M:170:ASP:OD1	1:M:173:ARG:NH1	2.46	0.41
1:C:61:ASP:OD1	1:C:89:LYS:NZ	2.50	0.41
1:I:171:LEU:HA	1:I:171:LEU:HD13	1.97	0.41
1:B:135:LEU:N	1:K:135:LEU:N	2.66	0.41
1:K:11:VAL:HG21	1:K:27:ARG:HG2	2.02	0.41
1:G:203:ARG:O	1:G:204:LEU:OXT	2.38	0.41
1:H:30:LYS:HE3	1:H:30:LYS:HB3	1.91	0.41
1:C:102:SER:HG	1:C:127:HIS:CE1	2.38	0.41
1:E:45:ALA:HA	1:E:81:ILE:HD11	2.03	0.41
1:E:143:GLU:OE1	1:H:150:LEU:HD11	2.21	0.41
1:F:127:HIS:CD2	1:F:127:HIS:C	2.94	0.41
1:K:184:GLU:O	1:K:188:GLU:HG3	2.21	0.41
1:L:139:ALA:HB1	3:L:408:HOH:O	2.21	0.41
1:C:148:GLU:HA	1:C:151:LYS:HE3	2.03	0.41
1:E:102:SER:HG	1:E:127:HIS:CE1	2.38	0.41
1:F:74:SER:HB3	1:F:77:ALA:HB3	2.03	0.41
1:G:135:LEU:HA	1:G:135:LEU:HD23	1.91	0.41
1:C:60:PRO:HB2	1:C:89:LYS:HD3	2.02	0.40
1:G:203:ARG:HA	1:G:203:ARG:HD3	1.71	0.40
1:D:102:SER:OG	1:D:127:HIS:CE1	2.74	0.40
1:K:36:LEU:HD21	1:K:40:VAL:HG22	2.03	0.40
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.89	0.40
1:E:143:GLU:HB2	1:H:150:LEU:HD21	2.04	0.40
1:A:155:LYS:HE2	1:B:121:ASN:OD1	2.22	0.40
1:J:131:ILE:HA	1:J:131:ILE:HD13	1.94	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	180/218 (83%)	176 (98%)	3 (2%)	1 (1%)	25	18
1	B	179/218 (82%)	176 (98%)	3 (2%)	0	100	100
1	C	178/218 (82%)	176 (99%)	2 (1%)	0	100	100
1	D	179/218 (82%)	176 (98%)	3 (2%)	0	100	100
1	E	180/218 (83%)	178 (99%)	2 (1%)	0	100	100
1	F	179/218 (82%)	176 (98%)	3 (2%)	0	100	100
1	G	183/218 (84%)	180 (98%)	3 (2%)	0	100	100
1	H	183/218 (84%)	177 (97%)	5 (3%)	1 (0%)	29	22
1	I	181/218 (83%)	175 (97%)	4 (2%)	2 (1%)	14	7
1	J	182/218 (84%)	180 (99%)	2 (1%)	0	100	100
1	K	180/218 (83%)	178 (99%)	2 (1%)	0	100	100
1	L	179/218 (82%)	175 (98%)	4 (2%)	0	100	100
1	M	179/218 (82%)	177 (99%)	2 (1%)	0	100	100
1	N	180/218 (83%)	177 (98%)	2 (1%)	1 (1%)	25	18
All	All	2522/3052 (83%)	2477 (98%)	40 (2%)	5 (0%)	47	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	200	ALA
1	I	133	GLY
1	A	200	ALA
1	I	132	SER
1	N	200	ALA

### 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	156/187 (83%)	154 (99%)	2 (1%)	69	72
1	B	155/187 (83%)	153 (99%)	2 (1%)	69	72
1	C	154/187 (82%)	153 (99%)	1 (1%)	86	89
1	D	155/187 (83%)	152 (98%)	3 (2%)	57	59
1	E	156/187 (83%)	155 (99%)	1 (1%)	86	89
1	F	155/187 (83%)	153 (99%)	2 (1%)	69	72
1	G	159/187 (85%)	156 (98%)	3 (2%)	57	59
1	H	159/187 (85%)	157 (99%)	2 (1%)	69	72
1	I	157/187 (84%)	156 (99%)	1 (1%)	86	89
1	J	158/187 (84%)	156 (99%)	2 (1%)	69	72
1	K	156/187 (83%)	155 (99%)	1 (1%)	86	89
1	L	155/187 (83%)	154 (99%)	1 (1%)	86	89
1	M	155/187 (83%)	152 (98%)	3 (2%)	57	59
1	N	156/187 (83%)	155 (99%)	1 (1%)	86	89
All	All	2186/2618 (84%)	2161 (99%)	25 (1%)	73	77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	127	HIS
1	B	127	HIS
1	B	130	LEU
1	C	127	HIS
1	D	127	HIS
1	D	130	LEU
1	D	197	GLU
1	E	127	HIS
1	F	127	HIS
1	F	130	LEU

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Mol	Chain	Res	Type
1	G	127	HIS
1	G	130	LEU
1	G	203	ARG
1	H	130	LEU
1	H	201	SER
1	I	127	HIS
1	J	127	HIS
1	J	203	ARG
1	K	127	HIS
1	L	127	HIS
1	M	127	HIS
1	M	130	LEU
1	M	201	SER
1	N	127	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	D	127	HIS
1	F	127	HIS
1	K	127	HIS
1	L	127	HIS
1	N	127	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	184/218 (84%)	-0.11	7 (3%) 40 40	13, 20, 50, 95	0
1	B	183/218 (83%)	-0.20	7 (3%) 40 40	15, 21, 50, 94	0
1	C	182/218 (83%)	-0.18	9 (4%) 29 29	14, 20, 46, 96	0
1	D	183/218 (83%)	-0.22	8 (4%) 34 33	15, 21, 53, 96	0
1	E	184/218 (84%)	-0.07	6 (3%) 46 46	17, 24, 45, 97	0
1	F	183/218 (83%)	-0.17	6 (3%) 46 46	17, 23, 45, 95	0
1	G	187/218 (85%)	-0.10	8 (4%) 35 34	14, 21, 50, 95	0
1	H	187/218 (85%)	-0.09	7 (3%) 41 41	17, 24, 44, 96	0
1	I	185/218 (84%)	0.00	9 (4%) 29 29	17, 24, 51, 96	0
1	J	186/218 (85%)	-0.07	9 (4%) 30 30	16, 21, 44, 97	0
1	K	184/218 (84%)	-0.11	7 (3%) 40 40	14, 20, 43, 96	0
1	L	183/218 (83%)	-0.22	5 (2%) 54 54	11, 20, 48, 91	0
1	M	183/218 (83%)	-0.21	8 (4%) 34 33	14, 20, 46, 96	0
1	N	184/218 (84%)	-0.18	9 (4%) 29 29	15, 21, 54, 96	0
All	All	2578/3052 (84%)	-0.14	105 (4%) 37 37	11, 22, 50, 97	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	134	GLY	14.3
1	M	134	GLY	12.3
1	E	134	GLY	10.1
1	H	134	GLY	10.0
1	D	134	GLY	9.4
1	C	134	GLY	9.3
1	L	133	GLY	9.3
1	K	133	GLY	9.2

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Mol	Chain	Res	Type	RSRZ
1	C	22	PHE	8.7
1	I	134	GLY	8.1
1	A	133	GLY	7.5
1	C	133	GLY	7.4
1	N	22	PHE	7.3
1	N	10	THR	7.1
1	J	133	GLY	6.9
1	N	134	GLY	6.8
1	J	22	PHE	6.6
1	G	134	GLY	6.5
1	G	135	LEU	6.4
1	M	22	PHE	6.4
1	G	133	GLY	6.4
1	H	135	LEU	6.4
1	K	134	GLY	6.0
1	B	22	PHE	5.9
1	A	134	GLY	5.8
1	I	135	LEU	5.8
1	E	132	SER	5.4
1	D	133	GLY	5.3
1	N	133	GLY	5.3
1	M	132	SER	5.2
1	I	22	PHE	5.1
1	J	135	LEU	5.1
1	E	22	PHE	5.0
1	F	134	GLY	4.9
1	I	133	GLY	4.9
1	E	135	LEU	4.8
1	D	22	PHE	4.7
1	I	11	VAL	4.7
1	F	22	PHE	4.7
1	D	10	THR	4.6
1	L	134	GLY	4.6
1	A	22	PHE	4.6
1	C	10	THR	4.5
1	M	133	GLY	4.4
1	H	132	SER	4.3
1	K	135	LEU	4.3
1	M	10	THR	4.2
1	F	11	VAL	4.2
1	F	132	SER	4.2
1	I	136	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	9	PRO	4.1
1	G	136	GLY	4.1
1	B	134	GLY	4.0
1	J	204	LEU	4.0
1	G	22	PHE	3.8
1	H	7	LEU	3.8
1	K	136	GLY	3.8
1	A	10	THR	3.7
1	D	11	VAL	3.7
1	G	8	VAL	3.6
1	L	11	VAL	3.5
1	C	135	LEU	3.5
1	B	133	GLY	3.5
1	L	12	ILE	3.4
1	A	132	SER	3.4
1	G	11	VAL	3.4
1	K	11	VAL	3.4
1	D	8	VAL	3.4
1	M	135	LEU	3.3
1	K	132	SER	3.3
1	E	133	GLY	3.2
1	K	8	VAL	3.2
1	C	136	GLY	3.2
1	N	132	SER	3.1
1	D	135	LEU	3.1
1	E	7	LEU	3.1
1	J	132	SER	3.1
1	L	22	PHE	3.0
1	M	136	GLY	3.0
1	I	10	THR	2.9
1	H	22	PHE	2.8
1	A	135	LEU	2.7
1	N	201	SER	2.7
1	I	7	LEU	2.7
1	B	8	VAL	2.6
1	H	133	GLY	2.5
1	B	135	LEU	2.4
1	M	11	VAL	2.4
1	F	133	GLY	2.4
1	N	8	VAL	2.4
1	N	135	LEU	2.3
1	B	9	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	132	SER	2.3
1	I	132	SER	2.3
1	B	10	THR	2.3
1	H	136	GLY	2.3
1	N	9	PRO	2.2
1	G	10	THR	2.2
1	A	11	VAL	2.2
1	C	11	VAL	2.2
1	J	11	VAL	2.1
1	J	10	THR	2.1
1	C	130	LEU	2.1
1	J	136	GLY	2.1
1	F	135	LEU	2.0

## 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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
2	K	F	301	1/1	0.97	0.12	29,29,29,29	0
2	K	E	301	1/1	0.97	0.11	33,33,33,33	0
2	K	G	301	1/1	0.97	0.08	18,18,18,18	0
2	K	I	301	1/1	0.97	0.08	33,33,33,33	0
2	K	K	301	1/1	0.97	0.07	16,16,16,16	0
2	K	D	301	1/1	0.98	0.06	22,22,22,22	0
2	K	A	301	1/1	0.98	0.07	15,15,15,15	0
2	K	L	301	1/1	0.99	0.07	21,21,21,21	0
2	K	J	301	1/1	0.99	0.06	17,17,17,17	0
2	K	N	301	1/1	0.99	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	H	301	1/1	0.99	0.08	28,28,28,28	0
2	K	B	301	1/1	0.99	0.07	20,20,20,20	0
2	K	C	301	1/1	0.99	0.06	18,18,18,18	0
2	K	M	301	1/1	1.00	0.05	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.