



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:00 PM BST

PDB ID : 5W18  
Title : Staphylococcus aureus ClpP in complex with (S)-N-((2R,6S,8aS,14aS,20S,23aS)-2,6-dimethyl-5,8,14,19,23-pentaoxooctadecahydro-1H,5H,14H,19H-pyrido[2,1-i]dipyrrolo[2,1-c:2',1'-l][1]oxa[4,7,10,13]tetraazacyclohexadecin-20-yl)-3-phenyl-2-(3-phenylureido)propanamide  
Authors : Lee, R.E.; Griffith, E.C.  
Deposited on : 2017-06-02  
Resolution : 2.44 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

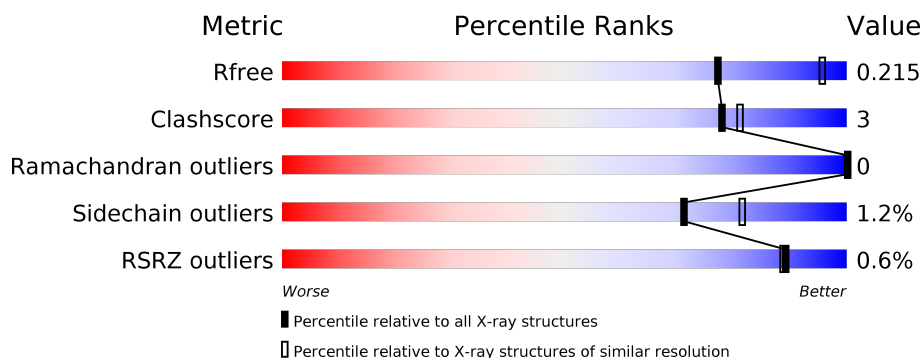
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	203	<div> <div>78%</div> <div>9%</div> <div>12%</div> </div>
1	B	203	<div> <div>80%</div> <div>9%</div> <div>11%</div> </div>
1	C	203	<div> <div>78%</div> <div>10%</div> <div>12%</div> </div>
1	D	203	<div> <div>76%</div> <div>11%</div> <div>11%</div> </div>
1	E	203	<div> <div>76%</div> <div>10%</div> <div>12%</div> </div>
1	F	203	<div> <div>82%</div> <div>6%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	203	
1	I	203	
1	K	203	
1	L	203	
1	M	203	
1	N	203	
1	S	203	
1	T	203	
2	H	7	
2	J	7	
2	O	7	
2	P	7	
2	Q	7	
2	R	7	
2	U	7	
2	V	7	
2	X	7	
2	Y	7	
2	Z	7	
2	a	7	
2	b	7	
2	c	7	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20484 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
			1366	860	233	267	6			
1	B	180	Total	C	N	O	S	0	0	0
			1356	854	229	267	6			
1	C	179	Total	C	N	O	S	0	0	0
			1363	857	232	268	6			
1	D	180	Total	C	N	O	S	0	0	0
			1381	871	234	270	6			
1	E	178	Total	C	N	O	S	0	0	0
			1364	860	232	266	6			
1	F	179	Total	C	N	O	S	0	0	0
			1354	851	231	266	6			
1	G	180	Total	C	N	O	S	0	0	0
			1361	856	230	269	6			
1	I	179	Total	C	N	O	S	0	0	0
			1350	849	229	266	6			
1	K	180	Total	C	N	O	S	0	0	0
			1371	862	234	269	6			
1	L	180	Total	C	N	O	S	0	0	0
			1373	865	232	270	6			
1	M	179	Total	C	N	O	S	0	0	0
			1376	868	233	269	6			
1	N	179	Total	C	N	O	S	0	0	0
			1359	856	229	268	6			
1	S	178	Total	C	N	O	S	0	0	0
			1351	850	228	267	6			
1	T	178	Total	C	N	O	S	0	0	0
			1351	850	231	264	6			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	LEU	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLU	-	expression tag	UNP Q2G036
A	198	HIS	-	expression tag	UNP Q2G036
A	199	HIS	-	expression tag	UNP Q2G036
A	200	HIS	-	expression tag	UNP Q2G036
A	201	HIS	-	expression tag	UNP Q2G036
A	202	HIS	-	expression tag	UNP Q2G036
A	203	HIS	-	expression tag	UNP Q2G036
B	196	LEU	-	expression tag	UNP Q2G036
B	197	GLU	-	expression tag	UNP Q2G036
B	198	HIS	-	expression tag	UNP Q2G036
B	199	HIS	-	expression tag	UNP Q2G036
B	200	HIS	-	expression tag	UNP Q2G036
B	201	HIS	-	expression tag	UNP Q2G036
B	202	HIS	-	expression tag	UNP Q2G036
B	203	HIS	-	expression tag	UNP Q2G036
C	196	LEU	-	expression tag	UNP Q2G036
C	197	GLU	-	expression tag	UNP Q2G036
C	198	HIS	-	expression tag	UNP Q2G036
C	199	HIS	-	expression tag	UNP Q2G036
C	200	HIS	-	expression tag	UNP Q2G036
C	201	HIS	-	expression tag	UNP Q2G036
C	202	HIS	-	expression tag	UNP Q2G036
C	203	HIS	-	expression tag	UNP Q2G036
D	196	LEU	-	expression tag	UNP Q2G036
D	197	GLU	-	expression tag	UNP Q2G036
D	198	HIS	-	expression tag	UNP Q2G036
D	199	HIS	-	expression tag	UNP Q2G036
D	200	HIS	-	expression tag	UNP Q2G036
D	201	HIS	-	expression tag	UNP Q2G036
D	202	HIS	-	expression tag	UNP Q2G036
D	203	HIS	-	expression tag	UNP Q2G036
E	196	LEU	-	expression tag	UNP Q2G036
E	197	GLU	-	expression tag	UNP Q2G036
E	198	HIS	-	expression tag	UNP Q2G036
E	199	HIS	-	expression tag	UNP Q2G036
E	200	HIS	-	expression tag	UNP Q2G036
E	201	HIS	-	expression tag	UNP Q2G036
E	202	HIS	-	expression tag	UNP Q2G036
E	203	HIS	-	expression tag	UNP Q2G036
F	196	LEU	-	expression tag	UNP Q2G036
F	197	GLU	-	expression tag	UNP Q2G036
F	198	HIS	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
F	199	HIS	-	expression tag	UNP Q2G036
F	200	HIS	-	expression tag	UNP Q2G036
F	201	HIS	-	expression tag	UNP Q2G036
F	202	HIS	-	expression tag	UNP Q2G036
F	203	HIS	-	expression tag	UNP Q2G036
G	196	LEU	-	expression tag	UNP Q2G036
G	197	GLU	-	expression tag	UNP Q2G036
G	198	HIS	-	expression tag	UNP Q2G036
G	199	HIS	-	expression tag	UNP Q2G036
G	200	HIS	-	expression tag	UNP Q2G036
G	201	HIS	-	expression tag	UNP Q2G036
G	202	HIS	-	expression tag	UNP Q2G036
G	203	HIS	-	expression tag	UNP Q2G036
I	196	LEU	-	expression tag	UNP Q2G036
I	197	GLU	-	expression tag	UNP Q2G036
I	198	HIS	-	expression tag	UNP Q2G036
I	199	HIS	-	expression tag	UNP Q2G036
I	200	HIS	-	expression tag	UNP Q2G036
I	201	HIS	-	expression tag	UNP Q2G036
I	202	HIS	-	expression tag	UNP Q2G036
I	203	HIS	-	expression tag	UNP Q2G036
K	196	LEU	-	expression tag	UNP Q2G036
K	197	GLU	-	expression tag	UNP Q2G036
K	198	HIS	-	expression tag	UNP Q2G036
K	199	HIS	-	expression tag	UNP Q2G036
K	200	HIS	-	expression tag	UNP Q2G036
K	201	HIS	-	expression tag	UNP Q2G036
K	202	HIS	-	expression tag	UNP Q2G036
K	203	HIS	-	expression tag	UNP Q2G036
L	196	LEU	-	expression tag	UNP Q2G036
L	197	GLU	-	expression tag	UNP Q2G036
L	198	HIS	-	expression tag	UNP Q2G036
L	199	HIS	-	expression tag	UNP Q2G036
L	200	HIS	-	expression tag	UNP Q2G036
L	201	HIS	-	expression tag	UNP Q2G036
L	202	HIS	-	expression tag	UNP Q2G036
L	203	HIS	-	expression tag	UNP Q2G036
M	196	LEU	-	expression tag	UNP Q2G036
M	197	GLU	-	expression tag	UNP Q2G036
M	198	HIS	-	expression tag	UNP Q2G036
M	199	HIS	-	expression tag	UNP Q2G036
M	200	HIS	-	expression tag	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
M	201	HIS	-	expression tag	UNP Q2G036
M	202	HIS	-	expression tag	UNP Q2G036
M	203	HIS	-	expression tag	UNP Q2G036
N	196	LEU	-	expression tag	UNP Q2G036
N	197	GLU	-	expression tag	UNP Q2G036
N	198	HIS	-	expression tag	UNP Q2G036
N	199	HIS	-	expression tag	UNP Q2G036
N	200	HIS	-	expression tag	UNP Q2G036
N	201	HIS	-	expression tag	UNP Q2G036
N	202	HIS	-	expression tag	UNP Q2G036
N	203	HIS	-	expression tag	UNP Q2G036
S	196	LEU	-	expression tag	UNP Q2G036
S	197	GLU	-	expression tag	UNP Q2G036
S	198	HIS	-	expression tag	UNP Q2G036
S	199	HIS	-	expression tag	UNP Q2G036
S	200	HIS	-	expression tag	UNP Q2G036
S	201	HIS	-	expression tag	UNP Q2G036
S	202	HIS	-	expression tag	UNP Q2G036
S	203	HIS	-	expression tag	UNP Q2G036
T	196	LEU	-	expression tag	UNP Q2G036
T	197	GLU	-	expression tag	UNP Q2G036
T	198	HIS	-	expression tag	UNP Q2G036
T	199	HIS	-	expression tag	UNP Q2G036
T	200	HIS	-	expression tag	UNP Q2G036
T	201	HIS	-	expression tag	UNP Q2G036
T	202	HIS	-	expression tag	UNP Q2G036
T	203	HIS	-	expression tag	UNP Q2G036

- Molecule 2 is a protein called 9V7-PHE-SER-PRO-YCP-ALA-MP8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	J	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	O	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	P	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	Q	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	R	7	Total	C	N	O	0	0	0
			54	39	7	8			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	U	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	V	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	X	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	Y	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	Z	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	a	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	b	7	Total	C	N	O	0	0	0
			54	39	7	8			
2	c	7	Total	C	N	O	0	0	0
			54	39	7	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	40	Total	O	0	0
			40	40		
3	C	56	Total	O	0	0
			56	56		
3	D	45	Total	O	0	0
			45	45		
3	E	65	Total	O	0	0
			65	65		
3	F	54	Total	O	0	0
			54	54		
3	G	45	Total	O	0	0
			45	45		
3	I	26	Total	O	0	0
			26	26		
3	K	41	Total	O	0	0
			41	41		
3	L	62	Total	O	0	0
			62	62		
3	M	57	Total	O	0	0
			57	57		

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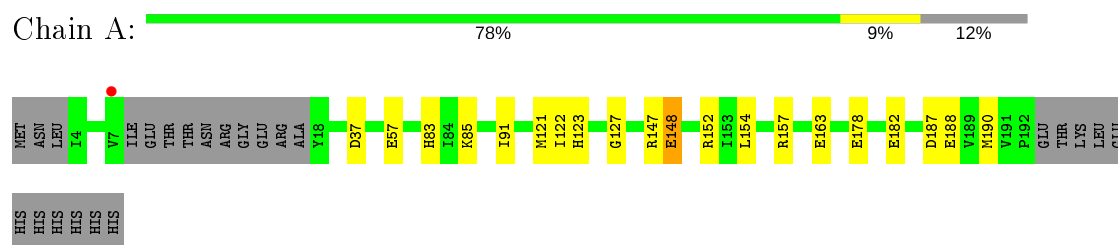
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	62	Total 62	O 62	0	0
3	S	33	Total 33	O 33	0	0
3	T	30	Total 30	O 30	0	0
3	Y	1	Total 1	O 1	0	0
3	Z	1	Total 1	O 1	0	0
3	a	1	Total 1	O 1	0	0

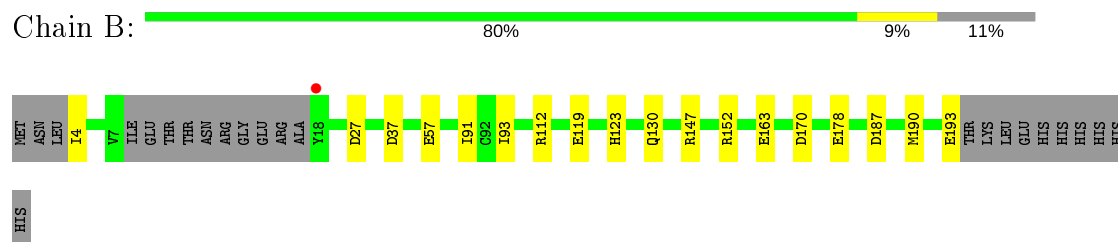
### 3 Residue-property plots [i](#)

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.

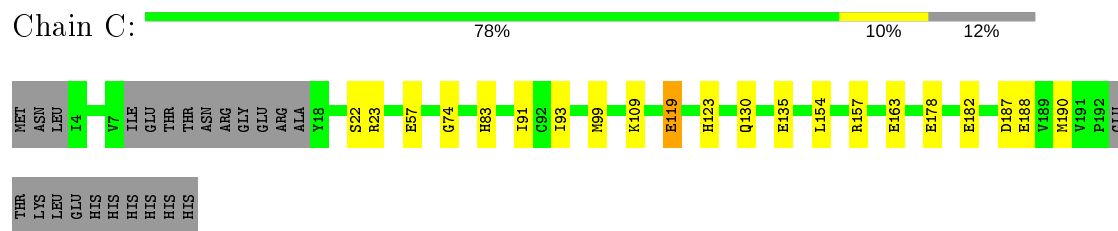
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



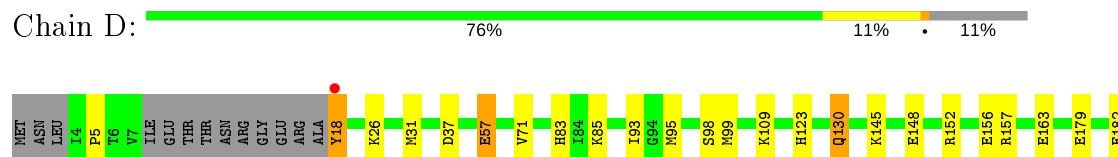
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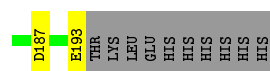


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

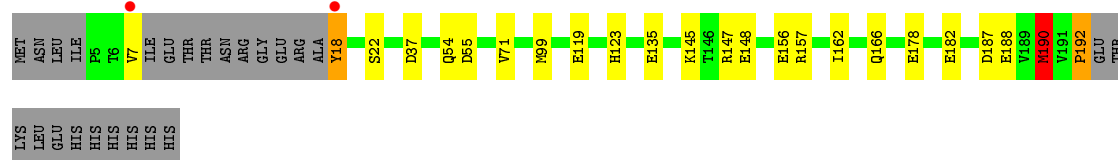
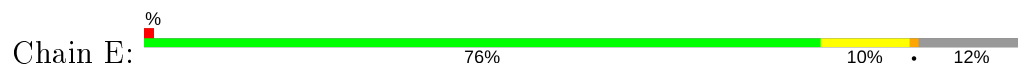


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

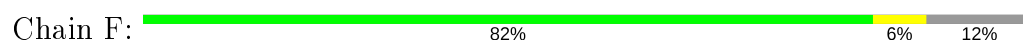




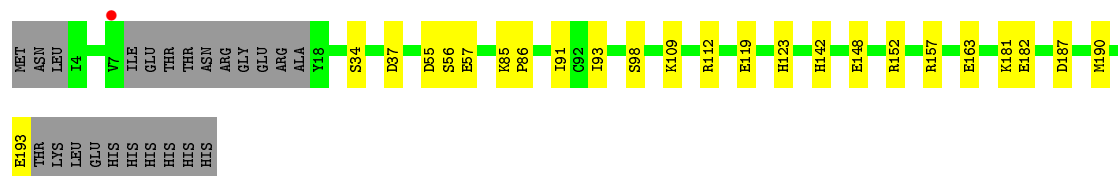
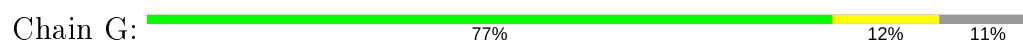
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



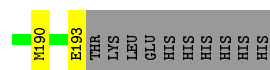
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



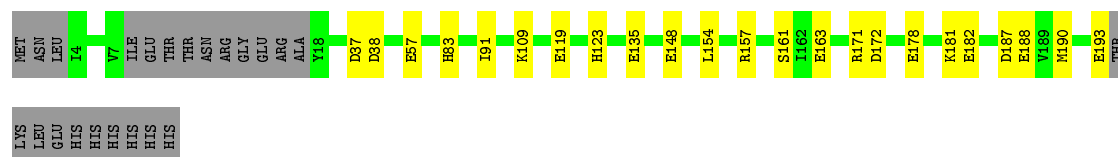
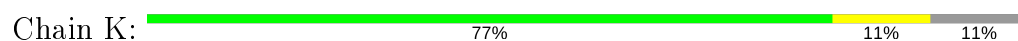
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



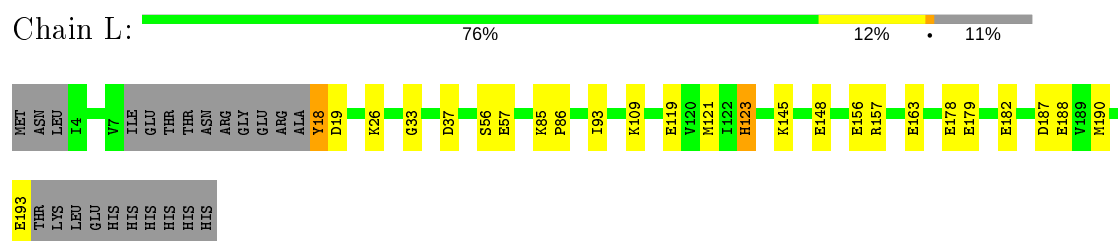
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



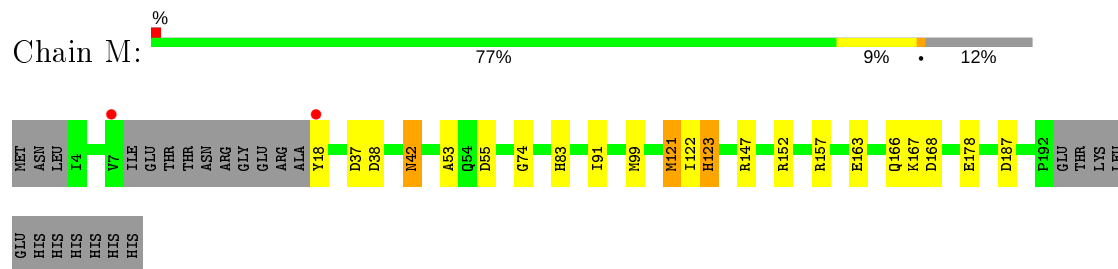
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



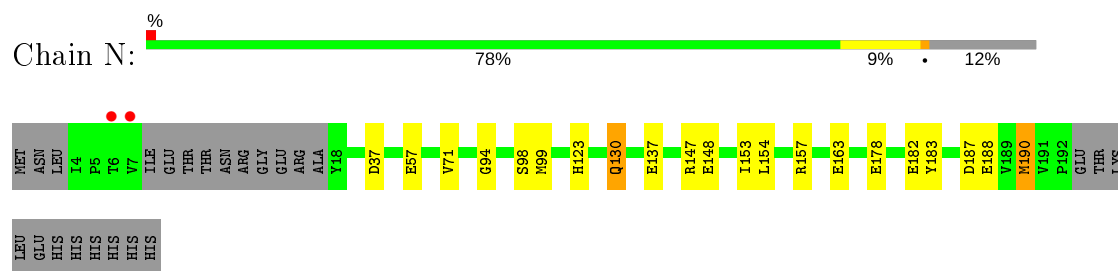
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



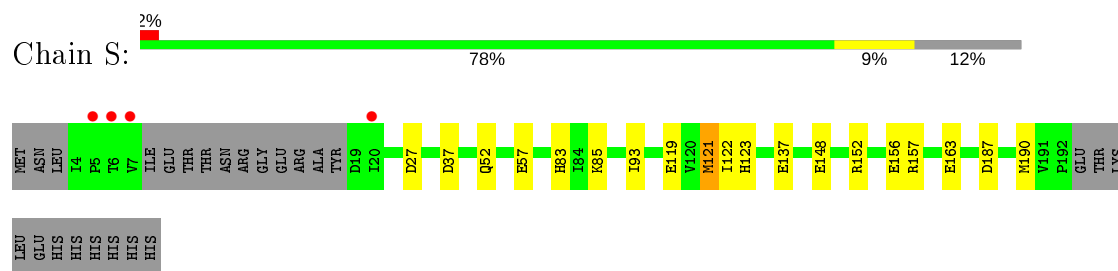
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



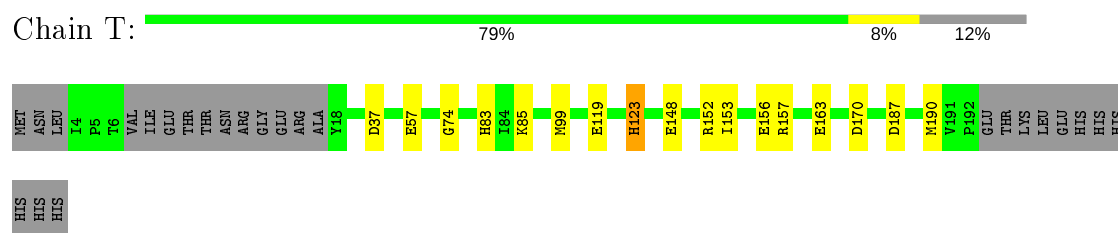
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



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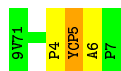
- Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain H:  43% 43% 14%



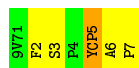
• Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain J:  57% 29% 14%



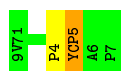
• Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain O:  29% 57% 14%



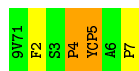
• Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain P:  71% 14% 14%



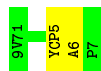
• Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain Q:  43% 29% 29%



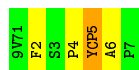
• Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain R:  71% 29%



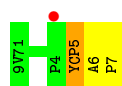
• Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain U:  43% 43% 14%



• Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain V:  14% 57% 29% 14%



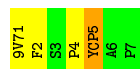
- Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain X: 43% 43% 14%



- Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain Y: 43% 43% 14%



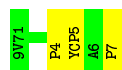
- Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain Z: 43% 57%



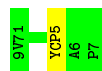
- Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain a: 57% 43%



- Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain b: 86% 14%



- Molecule 2: 9V7-PHE-SER-PRO-YCP-ALA-MP8

Chain c: 57% 43%



## 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 126.38Å 146.06Å 90.00° 93.42° 90.00°	Depositor
Resolution (Å)	50.00 – 2.44 48.94 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.44) 99.6 (48.94-2.44)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.26 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.189 , 0.210 0.193 , 0.215	Depositor DCC
$R_{free}$ test set	6556 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: 9V7, MP8, YCP

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	1.22	7/1383 (0.5%)	1.04	7/1867 (0.4%)
1	B	1.19	9/1373 (0.7%)	1.00	9/1859 (0.5%)
1	C	1.31	13/1380 (0.9%)	1.02	5/1865 (0.3%)
1	D	1.38	15/1399 (1.1%)	1.03	6/1890 (0.3%)
1	E	1.33	11/1382 (0.8%)	1.08	9/1866 (0.5%)
1	F	1.26	7/1371 (0.5%)	1.00	5/1855 (0.3%)
1	G	1.29	13/1378 (0.9%)	0.99	7/1864 (0.4%)
1	I	1.22	13/1367 (1.0%)	1.01	9/1849 (0.5%)
1	K	1.34	14/1388 (1.0%)	1.06	10/1875 (0.5%)
1	L	1.43	21/1391 (1.5%)	1.01	4/1882 (0.2%)
1	M	1.25	7/1394 (0.5%)	1.05	7/1883 (0.4%)
1	N	1.29	13/1376 (0.9%)	1.01	6/1861 (0.3%)
1	S	1.22	9/1368 (0.7%)	1.00	5/1850 (0.3%)
1	T	1.21	8/1368 (0.6%)	1.01	5/1848 (0.3%)
2	H	1.35	1/29 (3.4%)	0.77	0/37
2	J	1.27	0/29	0.90	0/37
2	O	1.29	1/29 (3.4%)	0.97	0/37
2	P	1.28	0/29	1.12	0/37
2	Q	1.72	1/29 (3.4%)	1.15	0/37
2	R	1.47	0/29	0.82	0/37
2	U	0.96	0/29	0.87	0/37
2	V	1.27	0/29	0.84	0/37
2	X	1.40	0/29	0.87	0/37
2	Y	1.22	0/29	0.94	0/37
2	Z	1.43	1/29 (3.4%)	1.08	0/37
2	a	1.60	1/29 (3.4%)	0.69	0/37
2	b	1.16	0/29	0.70	0/37
2	c	1.56	1/29 (3.4%)	0.83	0/37
All	All	1.29	166/19724 (0.8%)	1.02	94/26632 (0.4%)

All (166) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	182	GLU	CD-OE1	13.86	1.41	1.25
1	C	119	GLU	CD-OE1	12.62	1.39	1.25
1	D	57	GLU	CD-OE2	12.53	1.39	1.25
1	G	57	GLU	CD-OE2	12.35	1.39	1.25
1	T	163	GLU	CD-OE1	11.61	1.38	1.25
1	I	148	GLU	CD-OE1	10.10	1.36	1.25
1	L	156	GLU	CD-OE1	9.46	1.36	1.25
1	A	148	GLU	CD-OE2	9.23	1.35	1.25
1	S	148	GLU	CD-OE2	9.22	1.35	1.25
1	D	156	GLU	CD-OE2	9.12	1.35	1.25
1	C	188	GLU	CD-OE1	9.09	1.35	1.25
1	G	193	GLU	N-CA	8.96	1.64	1.46
1	F	163	GLU	CD-OE1	8.87	1.35	1.25
1	F	119	GLU	CD-OE2	8.84	1.35	1.25
1	C	57	GLU	CD-OE2	8.75	1.35	1.25
1	I	119	GLU	CD-OE2	8.72	1.35	1.25
1	S	163	GLU	CD-OE1	8.61	1.35	1.25
1	L	148	GLU	CD-OE2	8.57	1.35	1.25
1	N	137	GLU	CD-OE1	8.56	1.35	1.25
1	T	119	GLU	CD-OE2	8.51	1.35	1.25
1	D	148	GLU	CD-OE1	8.50	1.35	1.25
1	D	57	GLU	CD-OE1	8.26	1.34	1.25
1	F	163	GLU	CD-OE2	8.24	1.34	1.25
1	G	57	GLU	CD-OE1	8.20	1.34	1.25
1	G	148	GLU	CD-OE2	8.19	1.34	1.25
1	L	163	GLU	CG-CD	8.17	1.64	1.51
1	C	178	GLU	CD-OE1	8.16	1.34	1.25
1	N	178	GLU	CD-OE1	8.16	1.34	1.25
1	E	156	GLU	CD-OE2	7.98	1.34	1.25
1	N	163	GLU	CD-OE1	7.93	1.34	1.25
1	S	57	GLU	CD-OE2	7.89	1.34	1.25
1	E	182	GLU	CD-OE1	7.85	1.34	1.25
1	L	182	GLU	CD-OE1	7.84	1.34	1.25
1	A	178	GLU	CD-OE1	7.80	1.34	1.25
1	L	57	GLU	CD-OE1	7.76	1.34	1.25
1	G	163	GLU	CG-CD	7.71	1.63	1.51
1	G	182	GLU	CD-OE1	7.70	1.34	1.25
1	S	163	GLU	CD-OE2	7.67	1.34	1.25
1	A	182	GLU	CD-OE2	7.66	1.34	1.25
1	G	119	GLU	CD-OE1	7.65	1.34	1.25
1	K	182	GLU	CD-OE2	7.64	1.34	1.25
1	B	57	GLU	CD-OE2	7.58	1.33	1.25
1	I	193	GLU	N-CA	7.57	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	163	GLU	CG-CD	7.51	1.63	1.51
1	L	148	GLU	CD-OE1	7.43	1.33	1.25
1	K	178	GLU	CD-OE1	7.28	1.33	1.25
1	D	163	GLU	CD-OE1	7.21	1.33	1.25
1	B	193	GLU	C-O	7.20	1.37	1.23
1	K	148	GLU	CD-OE1	7.14	1.33	1.25
1	E	188	GLU	CD-OE1	7.12	1.33	1.25
1	L	188	GLU	CD-OE1	7.10	1.33	1.25
1	I	163	GLU	CD-OE1	7.08	1.33	1.25
1	L	182	GLU	CD-OE2	7.02	1.33	1.25
1	B	119	GLU	CD-OE2	7.01	1.33	1.25
1	F	182	GLU	CD-OE1	7.00	1.33	1.25
1	I	148	GLU	CD-OE2	6.98	1.33	1.25
1	I	5	PRO	C-O	6.97	1.37	1.23
1	M	163	GLU	CD-OE2	6.96	1.33	1.25
1	G	152	ARG	CZ-NH2	6.95	1.42	1.33
1	K	188	GLU	CD-OE1	6.95	1.33	1.25
1	D	193	GLU	N-CA	6.90	1.60	1.46
1	B	163	GLU	CD-OE2	6.90	1.33	1.25
2	Q	4	PRO	N-CD	6.90	1.57	1.47
1	T	156	GLU	CD-OE1	6.89	1.33	1.25
1	B	57	GLU	CD-OE1	6.86	1.33	1.25
1	K	57	GLU	CD-OE2	6.79	1.33	1.25
1	C	163	GLU	CG-CD	6.77	1.62	1.51
1	B	178	GLU	CD-OE1	6.74	1.33	1.25
1	S	152	ARG	CZ-NH2	6.70	1.41	1.33
1	T	148	GLU	CD-OE1	6.69	1.33	1.25
1	L	119	GLU	CD-OE2	6.68	1.32	1.25
1	B	193	GLU	N-CA	6.66	1.59	1.46
2	c	3	SER	CB-OG	6.63	1.50	1.42
1	T	57	GLU	CD-OE2	6.61	1.32	1.25
1	K	57	GLU	CD-OE1	6.58	1.32	1.25
1	D	163	GLU	CG-CD	6.57	1.61	1.51
1	N	188	GLU	CD-OE2	6.53	1.32	1.25
1	I	163	GLU	CG-CD	6.47	1.61	1.51
1	L	163	GLU	CD-OE2	-6.47	1.18	1.25
1	K	193	GLU	C-O	6.39	1.35	1.23
1	I	182	GLU	CD-OE1	6.36	1.32	1.25
1	D	163	GLU	CD-OE2	6.35	1.32	1.25
1	L	156	GLU	CD-OE2	6.35	1.32	1.25
1	N	188	GLU	CD-OE1	6.29	1.32	1.25
1	A	163	GLU	CG-CD	6.19	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	156	GLU	CD-OE1	6.15	1.32	1.25
1	E	178	GLU	CD-OE1	6.13	1.32	1.25
1	N	178	GLU	CD-OE2	6.13	1.32	1.25
1	G	56	SER	CB-OG	-6.12	1.34	1.42
1	F	156	GLU	CD-OE1	6.12	1.32	1.25
1	I	182	GLU	CD-OE2	6.11	1.32	1.25
1	K	119	GLU	CD-OE2	6.10	1.32	1.25
1	N	148	GLU	CD-OE1	6.08	1.32	1.25
1	K	135	GLU	CD-OE1	6.05	1.32	1.25
1	E	148	GLU	CD-OE2	6.05	1.32	1.25
1	D	145	LYS	CE-NZ	6.04	1.64	1.49
1	K	193	GLU	N-CA	6.01	1.58	1.46
1	D	179	GLU	CD-OE2	-5.98	1.19	1.25
1	F	178	GLU	CD-OE2	5.96	1.32	1.25
1	L	163	GLU	CD-OE1	5.95	1.32	1.25
1	E	22	SER	CB-OG	5.94	1.50	1.42
1	I	152	ARG	CZ-NH2	5.91	1.40	1.33
1	T	119	GLU	CG-CD	5.91	1.60	1.51
1	I	193	GLU	C-O	5.89	1.34	1.23
1	G	163	GLU	CD-OE2	5.89	1.32	1.25
1	L	179	GLU	CD-OE2	-5.88	1.19	1.25
1	G	193	GLU	C-O	5.84	1.34	1.23
1	G	148	GLU	CD-OE1	5.84	1.32	1.25
1	K	182	GLU	CG-CD	5.82	1.60	1.51
1	F	178	GLU	CD-OE1	5.77	1.31	1.25
1	E	18	TYR	CE1-CZ	5.74	1.46	1.38
1	S	57	GLU	CG-CD	-5.72	1.43	1.51
1	A	188	GLU	CD-OE1	5.71	1.31	1.25
2	a	4	PRO	N-CD	5.70	1.55	1.47
1	L	56	SER	CB-OG	5.67	1.49	1.42
1	C	57	GLU	CD-OE1	5.66	1.31	1.25
1	L	182	GLU	CG-CD	5.66	1.60	1.51
1	I	178	GLU	CD-OE2	5.65	1.31	1.25
1	N	182	GLU	CD-OE1	5.62	1.31	1.25
1	L	193	GLU	C-O	5.60	1.33	1.23
1	L	193	GLU	N-CA	5.59	1.57	1.46
1	C	109	LYS	C-O	-5.58	1.12	1.23
1	D	109	LYS	C-O	-5.57	1.12	1.23
1	M	18	TYR	CZ-OH	5.54	1.47	1.37
1	N	57	GLU	CD-OE1	5.49	1.31	1.25
1	D	130	GLN	CD-NE2	5.49	1.46	1.32
1	L	19	ASP	CG-OD2	5.44	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	54	GLN	CD-OE1	5.43	1.35	1.24
1	G	109	LYS	C-O	-5.42	1.13	1.23
1	B	130	GLN	CD-OE1	5.40	1.35	1.24
1	M	157	ARG	CG-CD	-5.40	1.38	1.51
1	S	57	GLU	CD-OE1	5.40	1.31	1.25
1	C	119	GLU	CG-CD	5.39	1.60	1.51
1	N	130	GLN	CD-OE1	5.38	1.35	1.24
1	E	119	GLU	CD-OE2	5.37	1.31	1.25
1	N	182	GLU	CD-OE2	5.36	1.31	1.25
1	K	161	SER	CB-OG	-5.35	1.35	1.42
1	D	5	PRO	C-O	5.35	1.33	1.23
1	M	178	GLU	CD-OE1	5.34	1.31	1.25
1	T	57	GLU	CD-OE1	5.33	1.31	1.25
1	E	145	LYS	CE-NZ	5.33	1.62	1.49
1	E	188	GLU	CD-OE2	5.32	1.31	1.25
1	L	178	GLU	CD-OE2	5.31	1.31	1.25
1	M	163	GLU	CD-OE1	5.30	1.31	1.25
1	M	42	ASN	CG-OD1	5.29	1.35	1.24
1	N	94	GLY	N-CA	5.29	1.53	1.46
1	D	152	ARG	CD-NE	5.27	1.55	1.46
1	L	145	LYS	CE-NZ	5.27	1.62	1.49
1	C	182	GLU	CG-CD	5.22	1.59	1.51
2	O	3	SER	CB-OG	5.22	1.49	1.42
1	I	148	GLU	CG-CD	5.19	1.59	1.51
1	B	147	ARG	CZ-NH1	5.18	1.39	1.33
1	A	127	GLY	C-O	-5.17	1.15	1.23
1	A	178	GLU	CD-OE2	5.14	1.31	1.25
1	S	119	GLU	CD-OE2	5.13	1.31	1.25
1	C	130	GLN	CD-NE2	5.13	1.45	1.32
1	C	22	SER	CB-OG	5.09	1.48	1.42
2	Z	4	PRO	N-CD	5.09	1.54	1.47
1	C	163	GLU	CD-OE1	5.09	1.31	1.25
1	M	123	HIS	C-O	-5.07	1.13	1.23
1	C	182	GLU	CD-OE2	5.06	1.31	1.25
1	K	109	LYS	C-O	-5.06	1.13	1.23
1	L	109	LYS	C-O	-5.05	1.13	1.23
1	D	152	ARG	CZ-NH2	5.04	1.39	1.33
1	T	123	HIS	C-O	-5.02	1.13	1.23
2	H	3	SER	CB-OG	5.00	1.48	1.42

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	55	ASP	CB-CG-OD2	-13.87	105.82	118.30
1	L	157	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	D	157	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	K	157	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	S	157	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	I	175	LEU	CB-CG-CD1	8.48	125.42	111.00
1	A	190	MET	CG-SD-CE	-8.41	86.75	100.20
1	A	157	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	L	163	GLU	OE1-CD-OE2	-7.73	114.03	123.30
1	C	135	GLU	OE1-CD-OE2	-7.53	114.26	123.30
1	C	23	ARG	NE-CZ-NH1	-7.50	116.55	120.30
1	K	38	ASP	CB-CG-OD1	7.45	125.01	118.30
1	K	163	GLU	OE1-CD-OE2	-7.39	114.43	123.30
1	C	163	GLU	OE1-CD-OE2	-7.37	114.46	123.30
1	M	157	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	187	ASP	CB-CG-OD2	7.16	124.75	118.30
1	A	163	GLU	OE1-CD-OE2	-7.14	114.73	123.30
1	G	55	ASP	CB-CG-OD2	7.03	124.63	118.30
1	I	157	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	D	57	GLU	OE1-CD-OE2	6.61	131.23	123.30
1	E	147	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	E	187	ASP	CB-CG-OD2	6.43	124.09	118.30
1	N	190	MET	CG-SD-CE	-6.42	89.92	100.20
1	B	152	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	M	152	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	I	135	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	D	182	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	F	23	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	B	187	ASP	CB-CG-OD2	6.27	123.94	118.30
1	M	187	ASP	CB-CG-OD2	6.26	123.93	118.30
1	M	55	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	C	157	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	K	187	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	147	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	E	190	MET	CG-SD-CE	-6.01	90.58	100.20
1	L	187	ASP	CB-CG-OD2	5.99	123.69	118.30
1	T	37	ASP	CB-CG-OD1	5.90	123.61	118.30
1	I	187	ASP	CB-CG-OD2	5.89	123.60	118.30
1	I	119	GLU	OE1-CD-OE2	5.86	130.33	123.30
1	E	157	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	I	58	LYS	CD-CE-NZ	5.79	125.03	111.70
1	S	187	ASP	CB-CG-OD2	5.75	123.47	118.30
1	K	181	LYS	CD-CE-NZ	-5.74	98.50	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	183	TYR	CB-CG-CD1	-5.72	117.56	121.00
1	F	187	ASP	CB-CG-OD2	5.72	123.44	118.30
1	S	137	GLU	OE1-CD-OE2	-5.72	116.44	123.30
1	N	154	LEU	CB-CG-CD1	5.69	120.67	111.00
1	B	27	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	152	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	N	183	TYR	CB-CG-CD2	5.63	124.38	121.00
1	T	187	ASP	CB-CG-OD2	5.62	123.36	118.30
1	G	187	ASP	CB-CG-OD2	5.61	123.35	118.30
1	G	112	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	T	152	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	M	38	ASP	CB-CG-OD1	5.58	123.33	118.30
1	C	187	ASP	CB-CG-OD2	5.57	123.31	118.30
1	M	37	ASP	CB-CG-OD1	5.52	123.27	118.30
1	E	7	VAL	CA-CB-CG2	5.48	119.12	110.90
1	G	152	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	E	135	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	I	112	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	T	85	LYS	CD-CE-NZ	-5.44	99.18	111.70
1	G	181	LYS	CD-CE-NZ	-5.44	99.19	111.70
1	I	37	ASP	CB-CG-OD1	5.43	123.19	118.30
1	N	187	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	37	ASP	CB-CG-OD1	5.41	123.17	118.30
1	D	187	ASP	CB-CG-OD2	5.40	123.16	118.30
1	K	154	LEU	CB-CG-CD1	5.39	120.17	111.00
1	K	37	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	37	ASP	CB-CG-OD1	5.38	123.14	118.30
1	E	37	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	170	ASP	CB-CG-OD2	5.35	123.11	118.30
1	K	171	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	F	23	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	G	37	ASP	CB-CG-OD1	5.24	123.01	118.30
1	L	37	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	154	LEU	CB-CG-CD1	5.19	119.82	111.00
1	G	157	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	K	172	ASP	CB-CG-OD1	5.16	122.94	118.30
1	M	37	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	37	ASP	CB-CG-OD1	5.12	122.91	118.30
1	T	170	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	K	157	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	N	37	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	112	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	37	ASP	CB-CG-OD1	5.07	122.87	118.30
1	F	37	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	31	MET	CG-SD-CE	-5.05	92.11	100.20
1	I	28	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	37	ASP	OD1-CG-OD2	-5.03	113.75	123.30
1	F	171	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	B	37	ASP	CB-CG-OD2	5.02	122.81	118.30
1	S	27	ASP	CB-CG-OD2	5.01	122.81	118.30
1	E	192	PRO	CA-C-O	-5.01	108.18	120.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1366	0	1374	9	0
1	B	1356	0	1343	5	0
1	C	1363	0	1360	10	0
1	D	1381	0	1387	12	0
1	E	1364	0	1371	6	0
1	F	1354	0	1343	2	0
1	G	1361	0	1349	11	0
1	I	1350	0	1336	11	0
1	K	1371	0	1371	6	0
1	L	1373	0	1365	10	0
1	M	1376	0	1385	10	0
1	N	1359	0	1356	7	0
1	S	1351	0	1345	10	0
1	T	1351	0	1350	7	0
2	H	54	0	43	2	0
2	J	54	0	43	2	0
2	O	54	0	43	3	0
2	P	54	0	43	1	0
2	Q	54	0	43	3	0
2	R	54	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	U	54	0	43	3	0
2	V	54	0	43	2	0
2	X	54	0	43	3	0
2	Y	54	0	43	4	0
2	Z	54	0	43	1	0
2	a	54	0	43	0	0
2	b	54	0	43	0	0
2	c	54	0	43	0	0
3	A	33	0	0	1	0
3	B	40	0	0	0	0
3	C	56	0	0	1	0
3	D	45	0	0	2	0
3	E	65	0	0	2	0
3	F	54	0	0	0	0
3	G	45	0	0	2	0
3	I	26	0	0	1	0
3	K	41	0	0	0	0
3	L	62	0	0	0	0
3	M	57	0	0	0	0
3	N	62	0	0	3	0
3	S	33	0	0	0	0
3	T	30	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
3	a	1	0	0	0	0
All	All	20484	0	19637	105	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 3.

All (105) 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:D:95:MET:HG3	3:D:301:HOH:O	1.59	1.00
1:S:190:MET:CE	1:T:83:HIS:CE1	2.55	0.89
1:B:190:MET:HE2	1:C:83:HIS:CE1	2.11	0.84
1:A:148:GLU:OE1	1:A:152:ARG:NH2	2.09	0.84
1:A:83:HIS:CE1	1:G:190:MET:CE	2.62	0.82
1:E:190:MET:HE3	2:Q:2:PHE:HB3	1.60	0.81
1:C:190:MET:CE	1:D:83:HIS:CE1	2.69	0.76
1:I:190:MET:HE2	1:K:83:HIS:NE2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:190:MET:CE	1:M:83:HIS:CE1	2.72	0.72
1:M:147:ARG:NH1	1:M:166:GLN:OE1	2.22	0.72
1:S:190:MET:HE2	1:T:83:HIS:CE1	2.26	0.70
1:B:190:MET:CE	1:C:83:HIS:CE1	2.76	0.68
1:D:95:MET:CE	3:E:301:HOH:O	2.42	0.68
1:A:83:HIS:CE1	1:G:190:MET:HE2	2.30	0.67
1:A:83:HIS:CE1	1:G:190:MET:HE3	2.30	0.66
1:D:95:MET:HE3	3:E:301:HOH:O	1.96	0.66
1:I:190:MET:CE	1:K:83:HIS:NE2	2.58	0.66
1:S:52:GLN:HE21	1:S:85:LYS:H	1.42	0.65
1:K:190:MET:HE3	2:X:2:PHE:HB3	1.78	0.64
1:T:153:ILE:O	1:T:157:ARG:HG2	1.99	0.63
1:D:57:GLU:OE2	1:D:85:LYS:NZ	2.32	0.62
1:D:71:VAL:HG22	1:D:99:MET:HE3	1.82	0.61
1:D:71:VAL:HG22	1:D:99:MET:CE	2.32	0.60
1:I:190:MET:HE2	1:K:83:HIS:CD2	2.37	0.60
1:S:190:MET:HE3	1:T:83:HIS:CE1	2.35	0.59
1:L:190:MET:HE2	1:M:83:HIS:CE1	2.36	0.59
1:N:71:VAL:HG22	1:N:99:MET:CE	2.34	0.58
1:I:83:HIS:NE2	1:T:190:MET:HE2	2.18	0.58
1:M:167:LYS:NZ	1:M:168:ASP:OD1	2.37	0.57
1:I:71:VAL:HG22	1:I:99:MET:CE	2.36	0.56
1:E:190:MET:CE	2:Q:2:PHE:HB3	2.34	0.55
1:A:57:GLU:OE2	1:A:85:LYS:NZ	2.40	0.54
1:E:162:ILE:O	1:E:166:GLN:HG3	2.07	0.54
1:E:71:VAL:HG22	1:E:99:MET:CE	2.37	0.54
1:C:190:MET:HE2	1:D:83:HIS:CE1	2.42	0.53
3:I:321:HOH:O	1:K:83:HIS:HD2	1.92	0.52
1:L:121:MET:HE2	1:L:121:MET:C	2.30	0.51
1:L:190:MET:CE	2:Y:2:PHE:HB3	2.41	0.51
1:G:142:HIS:HD2	3:G:345:HOH:O	1.93	0.51
1:C:119:GLU:OE2	3:C:301:HOH:O	2.19	0.51
1:S:52:GLN:NE2	1:S:85:LYS:H	2.09	0.51
1:M:53:ALA:HB2	2:Y:1:9V7:C4	2.41	0.50
1:N:153:ILE:O	1:N:157:ARG:HG2	2.11	0.50
1:D:98:SER:HB3	3:D:342:HOH:O	2.11	0.49
1:T:74:GLY:HA3	1:T:99:MET:HE2	1.95	0.48
1:L:121:MET:HE3	1:L:123:HIS:HB3	1.95	0.47
1:N:71:VAL:HG22	1:N:99:MET:HE3	1.96	0.47
1:S:121:MET:HE2	1:S:121:MET:C	2.35	0.47
1:A:121:MET:C	1:A:121:MET:HE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:MET:HE1	2:O:2:PHE:HB3	1.97	0.47
1:L:190:MET:HE3	2:Y:2:PHE:HB3	1.96	0.46
1:N:71:VAL:HG22	1:N:99:MET:HE1	1.98	0.46
1:I:83:HIS:NE2	1:T:190:MET:CE	2.79	0.46
1:S:121:MET:HE3	1:S:122:ILE:C	2.37	0.46
1:S:190:MET:HE2	1:S:190:MET:HB3	1.83	0.45
1:B:4:ILE:O	1:B:4:ILE:HG13	2.16	0.45
1:G:98:SER:HB3	3:G:332:HOH:O	2.16	0.45
1:G:190:MET:HE3	2:U:2:PHE:HB3	1.99	0.45
1:G:93:ILE:HG13	1:G:93:ILE:O	2.16	0.45
3:N:348:HOH:O	1:S:83:HIS:HD2	2.00	0.44
1:D:18:TYR:OH	1:D:26:LYS:HD3	2.17	0.44
1:A:148:GLU:CD	1:A:152:ARG:NH2	2.70	0.44
1:I:71:VAL:HG22	1:I:99:MET:HE3	1.98	0.44
1:E:71:VAL:HG22	1:E:99:MET:HE3	1.98	0.44
1:M:74:GLY:HA3	1:M:99:MET:HE2	2.00	0.44
2:U:4:PRO:HA	2:U:5:YCP:HA	1.77	0.44
1:C:91:ILE:HD11	2:O:6:ALA:HB1	2.00	0.44
1:I:91:ILE:HD11	2:V:6:ALA:HB1	1.99	0.44
2:J:4:PRO:HA	2:J:5:YCP:HA	1.78	0.44
1:K:91:ILE:HD11	2:X:6:ALA:HB1	1.99	0.44
1:C:93:ILE:HG13	1:C:93:ILE:O	2.16	0.44
1:D:93:ILE:HG13	1:D:93:ILE:O	2.18	0.44
1:A:91:ILE:HD11	2:H:6:ALA:HB1	1.98	0.44
1:M:121:MET:C	1:M:121:MET:HE2	2.38	0.44
1:F:91:ILE:HD11	2:R:6:ALA:HB1	1.99	0.44
2:O:5:YCP:HA	2:O:7:MP8:O	2.18	0.43
1:G:91:ILE:HD11	2:U:6:ALA:HB1	2.00	0.43
1:I:113:PHE:CZ	2:V:5:YCP:HD	2.52	0.43
1:B:93:ILE:O	1:B:93:ILE:HG13	2.18	0.43
1:L:93:ILE:O	1:L:93:ILE:HG13	2.19	0.43
1:I:71:VAL:HG22	1:I:99:MET:HE1	1.99	0.42
2:P:4:PRO:HA	2:P:5:YCP:HA	1.78	0.42
1:E:71:VAL:HG22	1:E:99:MET:HE1	1.99	0.42
1:L:33:GLY:HA3	1:M:42:ASN:ND2	2.35	0.42
1:M:91:ILE:HD11	2:Z:6:ALA:HB1	2.02	0.42
1:B:91:ILE:HD11	2:J:6:ALA:HB1	2.01	0.42
1:S:93:ILE:HG13	1:S:93:ILE:O	2.19	0.42
1:I:93:ILE:O	1:I:93:ILE:HG13	2.19	0.42
1:A:121:MET:HE3	1:A:122:ILE:C	2.40	0.42
1:G:190:MET:HE2	1:G:190:MET:HB3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:MET:HE3	1:D:83:HIS:CE1	2.53	0.41
1:N:98:SER:HB3	3:N:342:HOH:O	2.20	0.41
1:N:147:ARG:HD3	3:N:332:HOH:O	2.19	0.41
2:Q:4:PRO:HA	2:Q:5:YCP:HA	1.74	0.41
2:H:4:PRO:HA	2:H:5:YCP:HA	1.85	0.41
1:M:121:MET:HE3	1:M:122:ILE:C	2.41	0.41
1:G:85:LYS:N	1:G:86:PRO:CD	2.84	0.41
1:N:190:MET:HE2	1:N:190:MET:HB3	1.87	0.41
1:C:74:GLY:HA3	1:C:99:MET:HE2	2.03	0.40
3:A:318:HOH:O	1:G:34:SER:HA	2.20	0.40
1:L:85:LYS:N	1:L:86:PRO:CD	2.84	0.40
2:X:4:PRO:HA	2:X:5:YCP:HA	1.67	0.40
2:Y:4:PRO:HA	2:Y:5:YCP:HA	1.81	0.40
1:F:93:ILE:O	1:F:93:ILE:HG13	2.20	0.40
1:L:18:TYR:OH	1:L:26:LYS:HD2	2.21	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	175/203 (86%)	172 (98%)	3 (2%)	0	100	100
1	B	176/203 (87%)	172 (98%)	4 (2%)	0	100	100
1	C	175/203 (86%)	172 (98%)	3 (2%)	0	100	100
1	D	176/203 (87%)	171 (97%)	5 (3%)	0	100	100
1	E	174/203 (86%)	170 (98%)	4 (2%)	0	100	100
1	F	175/203 (86%)	171 (98%)	4 (2%)	0	100	100
1	G	176/203 (87%)	172 (98%)	4 (2%)	0	100	100
1	I	175/203 (86%)	171 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	176/203 (87%)	171 (97%)	5 (3%)	0	100	100
1	L	176/203 (87%)	171 (97%)	5 (3%)	0	100	100
1	M	175/203 (86%)	170 (97%)	5 (3%)	0	100	100
1	N	175/203 (86%)	172 (98%)	3 (2%)	0	100	100
1	S	174/203 (86%)	170 (98%)	4 (2%)	0	100	100
1	T	174/203 (86%)	170 (98%)	4 (2%)	0	100	100
2	H	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	J	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	O	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	P	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	Q	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	R	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	U	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	V	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	X	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	Y	4/7 (57%)	2 (50%)	2 (50%)	0	100	100
2	Z	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	a	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	b	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	c	4/7 (57%)	2 (50%)	2 (50%)	0	100	100
All	All	2508/2940 (85%)	2435 (97%)	73 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	146/171 (85%)	145 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	143/171 (84%)	142 (99%)	1 (1%)	84	90
1	C	145/171 (85%)	143 (99%)	2 (1%)	67	78
1	D	148/171 (86%)	145 (98%)	3 (2%)	55	67
1	E	146/171 (85%)	142 (97%)	4 (3%)	44	57
1	F	143/171 (84%)	142 (99%)	1 (1%)	84	90
1	G	144/171 (84%)	143 (99%)	1 (1%)	84	90
1	I	142/171 (83%)	141 (99%)	1 (1%)	84	90
1	K	146/171 (85%)	145 (99%)	1 (1%)	84	90
1	L	146/171 (85%)	144 (99%)	2 (1%)	67	78
1	M	148/171 (86%)	146 (99%)	2 (1%)	67	78
1	N	145/171 (85%)	143 (99%)	2 (1%)	67	78
1	S	144/171 (84%)	142 (99%)	2 (1%)	67	78
1	T	143/171 (84%)	142 (99%)	1 (1%)	84	90
2	H	3/3 (100%)	3 (100%)	0	100	100
2	J	3/3 (100%)	3 (100%)	0	100	100
2	O	3/3 (100%)	3 (100%)	0	100	100
2	P	3/3 (100%)	3 (100%)	0	100	100
2	Q	3/3 (100%)	3 (100%)	0	100	100
2	R	3/3 (100%)	3 (100%)	0	100	100
2	U	3/3 (100%)	3 (100%)	0	100	100
2	V	3/3 (100%)	3 (100%)	0	100	100
2	X	3/3 (100%)	3 (100%)	0	100	100
2	Y	3/3 (100%)	3 (100%)	0	100	100
2	Z	3/3 (100%)	3 (100%)	0	100	100
2	a	3/3 (100%)	3 (100%)	0	100	100
2	b	3/3 (100%)	3 (100%)	0	100	100
2	c	3/3 (100%)	3 (100%)	0	100	100
All	All	2071/2436 (85%)	2047 (99%)	24 (1%)	71	81

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	HIS

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Mol	Chain	Res	Type
1	B	123	HIS
1	C	123	HIS
1	C	154	LEU
1	D	18	TYR
1	D	123	HIS
1	D	130	GLN
1	E	18	TYR
1	E	123	HIS
1	E	190	MET
1	E	192	PRO
1	F	123	HIS
1	G	123	HIS
1	I	123	HIS
1	K	123	HIS
1	L	18	TYR
1	L	123	HIS
1	M	121	MET
1	M	123	HIS
1	N	123	HIS
1	N	130	GLN
1	S	121	MET
1	S	123	HIS
1	T	123	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	151	ASN
1	E	166	GLN
1	G	151	ASN
1	K	47	GLN
1	L	151	ASN
1	S	52	GLN
1	T	39	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 non-standard protein/DNA/RNA residues 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
2	YCP	O	5	2	6,8,9	1.47	1 (16%)	5,9,11	1.63	1 (20%)
2	MP8	a	7	2	5,8,9	1.30	1 (20%)	3,10,12	0.87	0
2	YCP	b	5	2	6,8,9	1.60	1 (16%)	5,9,11	1.47	1 (20%)
2	MP8	V	7	2	5,8,9	1.24	1 (20%)	3,10,12	0.64	0
2	MP8	Q	7	2	5,8,9	1.61	1 (20%)	3,10,12	0.67	0
2	YCP	Y	5	2	6,8,9	1.16	1 (16%)	5,9,11	1.78	1 (20%)
2	MP8	U	7	2	5,8,9	0.75	0	3,10,12	0.43	0
2	YCP	a	5	2	6,8,9	1.41	1 (16%)	5,9,11	1.32	1 (20%)
2	YCP	R	5	2	6,8,9	1.25	1 (16%)	5,9,11	1.34	1 (20%)
2	MP8	b	7	2	5,8,9	0.92	0	3,10,12	0.97	0
2	YCP	Z	5	2	6,8,9	1.16	1 (16%)	5,9,11	1.51	1 (20%)
2	YCP	H	5	2	6,8,9	1.34	1 (16%)	5,9,11	1.20	1 (20%)
2	YCP	Q	5	2	6,8,9	1.19	1 (16%)	5,9,11	1.67	1 (20%)
2	MP8	P	7	2	5,8,9	0.91	0	3,10,12	1.16	0
2	YCP	J	5	2	6,8,9	1.56	1 (16%)	5,9,11	1.82	1 (20%)
2	YCP	X	5	2	6,8,9	1.27	1 (16%)	5,9,11	1.76	1 (20%)
2	MP8	c	7	2	5,8,9	1.03	1 (20%)	3,10,12	0.70	0
2	MP8	J	7	2	5,8,9	0.76	0	3,10,12	0.88	0
2	YCP	U	5	2	6,8,9	1.61	2 (33%)	5,9,11	1.37	1 (20%)
2	MP8	H	7	2	5,8,9	0.61	0	3,10,12	0.83	0
2	MP8	O	7	2	5,8,9	0.45	0	3,10,12	0.81	0
2	MP8	R	7	2	5,8,9	0.82	0	3,10,12	0.80	0
2	YCP	P	5	2	6,8,9	1.42	1 (16%)	5,9,11	1.37	1 (20%)
2	MP8	Z	7	2	5,8,9	1.30	1 (20%)	3,10,12	0.73	0
2	MP8	X	7	2	5,8,9	0.79	0	3,10,12	1.00	0
2	YCP	V	5	2	6,8,9	0.73	0	5,9,11	1.61	1 (20%)
2	MP8	Y	7	2	5,8,9	0.69	0	3,10,12	0.99	0
2	YCP	c	5	2	6,8,9	1.37	1 (16%)	5,9,11	1.51	1 (20%)

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
2	YCP	O	5	2	-	0/1/10/12	0/1/1/1
2	MP8	a	7	2	-	0/0/11/13	0/1/1/1
2	YCP	b	5	2	-	0/1/10/12	0/1/1/1
2	MP8	V	7	2	-	0/0/11/13	0/1/1/1
2	MP8	Q	7	2	-	0/0/11/13	0/1/1/1
2	YCP	Y	5	2	-	0/1/10/12	0/1/1/1
2	MP8	U	7	2	-	0/0/11/13	0/1/1/1
2	YCP	a	5	2	-	0/1/10/12	0/1/1/1
2	YCP	R	5	2	-	0/1/10/12	0/1/1/1
2	MP8	b	7	2	-	0/0/11/13	0/1/1/1
2	YCP	Z	5	2	-	0/1/10/12	0/1/1/1
2	YCP	H	5	2	-	0/1/10/12	0/1/1/1
2	YCP	Q	5	2	-	0/1/10/12	0/1/1/1
2	MP8	P	7	2	-	0/0/11/13	0/1/1/1
2	YCP	J	5	2	-	0/1/10/12	0/1/1/1
2	YCP	X	5	2	-	0/1/10/12	0/1/1/1
2	MP8	c	7	2	-	0/0/11/13	0/1/1/1
2	MP8	J	7	2	-	0/0/11/13	0/1/1/1
2	YCP	U	5	2	-	0/1/10/12	0/1/1/1
2	MP8	H	7	2	-	0/0/11/13	0/1/1/1
2	MP8	O	7	2	-	0/0/11/13	0/1/1/1
2	MP8	R	7	2	-	0/0/11/13	0/1/1/1
2	YCP	P	5	2	-	0/1/10/12	0/1/1/1
2	MP8	Z	7	2	-	0/0/11/13	0/1/1/1
2	MP8	X	7	2	-	0/0/11/13	0/1/1/1
2	YCP	V	5	2	-	0/1/10/12	0/1/1/1
2	MP8	Y	7	2	-	0/0/11/13	0/1/1/1
2	YCP	c	5	2	-	0/1/10/12	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	5	YCP	CG-CD	3.33	1.64	1.51
2	Q	7	MP8	CB-CA	-3.24	1.47	1.54
2	H	5	YCP	CD-CE	3.00	1.63	1.49
2	b	5	YCP	CG-CD	2.92	1.63	1.51
2	O	5	YCP	CG-CD	2.78	1.62	1.51
2	U	5	YCP	CG-CD	2.77	1.62	1.51
2	a	5	YCP	CG-CD	2.74	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	7	MP8	CB-CA	-2.69	1.48	1.54
2	a	7	MP8	CB-CA	-2.64	1.48	1.54
2	V	7	MP8	CB-CA	-2.56	1.48	1.54
2	U	5	YCP	CD-CE	2.44	1.61	1.49
2	P	5	YCP	CD-CE	2.32	1.60	1.49
2	R	5	YCP	CG-CD	2.25	1.60	1.51
2	c	5	YCP	CG-CD	2.24	1.60	1.51
2	Q	5	YCP	CG-CD	2.22	1.60	1.51
2	Y	5	YCP	CD-CE	2.20	1.60	1.49
2	X	5	YCP	CD-CE	2.15	1.59	1.49
2	c	7	MP8	CB-CA	-2.08	1.49	1.54
2	Z	5	YCP	CG-CD	2.04	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	5	YCP	O-C-CA	-3.99	114.33	124.78
2	X	5	YCP	O-C-CA	-3.90	114.56	124.78
2	Q	5	YCP	O-C-CA	-3.69	115.11	124.78
2	Y	5	YCP	O-C-CA	-3.60	115.34	124.78
2	V	5	YCP	O-C-CA	-3.55	115.48	124.78
2	O	5	YCP	O-C-CA	-3.44	115.77	124.78
2	Z	5	YCP	O-C-CA	-3.23	116.32	124.78
2	b	5	YCP	O-C-CA	-3.17	116.47	124.78
2	P	5	YCP	O-C-CA	-2.98	116.98	124.78
2	U	5	YCP	O-C-CA	-2.95	117.04	124.78
2	R	5	YCP	O-C-CA	-2.95	117.06	124.78
2	a	5	YCP	O-C-CA	-2.91	117.16	124.78
2	c	5	YCP	O-C-CA	-2.89	117.22	124.78
2	H	5	YCP	O-C-CA	-2.51	118.21	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	5	YCP	1	0
2	Y	5	YCP	1	0
2	H	5	YCP	1	0
2	Q	5	YCP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	5	YCP	1	0
2	X	5	YCP	1	0
2	U	5	YCP	1	0
2	O	7	MP8	1	0
2	P	5	YCP	1	0
2	V	5	YCP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	179/203 (88%)	-0.36	1 (0%) 89 89	30, 35, 44, 53	0
1	B	180/203 (88%)	-0.30	1 (0%) 89 89	30, 35, 43, 52	0
1	C	179/203 (88%)	-0.32	0 100 100	26, 32, 41, 48	0
1	D	180/203 (88%)	-0.37	1 (0%) 89 89	24, 30, 39, 46	0
1	E	178/203 (87%)	-0.33	2 (1%) 80 79	24, 30, 38, 49	0
1	F	179/203 (88%)	-0.33	1 (0%) 89 89	24, 31, 42, 50	0
1	G	180/203 (88%)	-0.42	1 (0%) 89 89	30, 35, 43, 51	0
1	I	179/203 (88%)	-0.32	0 100 100	32, 37, 44, 52	0
1	K	180/203 (88%)	-0.36	0 100 100	28, 33, 42, 50	0
1	L	180/203 (88%)	-0.36	0 100 100	25, 31, 38, 47	0
1	M	179/203 (88%)	-0.25	2 (1%) 80 79	26, 31, 41, 48	0
1	N	179/203 (88%)	-0.46	2 (1%) 80 79	26, 32, 41, 51	0
1	S	178/203 (87%)	-0.20	4 (2%) 62 58	30, 37, 45, 51	0
1	T	178/203 (87%)	-0.17	0 100 100	33, 38, 46, 50	0
2	H	4/7 (57%)	-0.69	0 100 100	37, 38, 41, 44	0
2	J	4/7 (57%)	-0.31	0 100 100	36, 39, 40, 43	0
2	O	4/7 (57%)	-0.50	0 100 100	33, 36, 38, 41	0
2	P	4/7 (57%)	-0.71	0 100 100	30, 32, 34, 37	0
2	Q	4/7 (57%)	-0.27	0 100 100	32, 33, 35, 39	0
2	R	4/7 (57%)	-0.75	0 100 100	35, 37, 38, 40	0
2	U	4/7 (57%)	0.10	0 100 100	38, 40, 41, 44	0
2	V	4/7 (57%)	0.54	1 (25%) 0 0	40, 42, 44, 48	0
2	X	4/7 (57%)	-0.38	0 100 100	35, 35, 38, 41	0
2	Y	4/7 (57%)	-0.86	0 100 100	34, 36, 36, 41	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	Z	4/7 (57%)	-0.05	0 100 100	32, 35, 38, 41	0
2	a	4/7 (57%)	-0.44	0 100 100	36, 37, 40, 41	0
2	b	4/7 (57%)	0.12	0 100 100	40, 43, 43, 44	0
2	c	4/7 (57%)	-0.01	0 100 100	41, 43, 44, 46	0
All	All	2564/2940 (87%)	-0.33	16 (0%) 89 89	24, 34, 43, 53	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	7	VAL	6.5
1	S	6	THR	4.9
1	N	7	VAL	4.7
1	D	18	TYR	4.1
1	G	7	VAL	3.5
1	A	7	VAL	3.3
1	N	6	THR	3.3
1	E	18	TYR	3.1
1	F	7	VAL	2.8
1	M	7	VAL	2.7
2	V	4	PRO	2.5
1	S	5	PRO	2.5
1	E	7	VAL	2.3
1	B	18	TYR	2.2
1	M	18	TYR	2.2
1	S	20	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	MP8	b	7	8/9	0.94	0.14	40,42,44,45	0
2	MP8	O	7	8/9	0.94	0.14	35,36,37,39	0
2	MP8	Z	7	8/9	0.94	0.10	34,35,37,38	0
2	MP8	Y	7	8/9	0.94	0.12	35,36,36,38	0
2	YCP	R	5	8/9	0.95	0.13	37,39,40,40	0
2	YCP	O	5	8/9	0.95	0.15	38,38,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MP8	c	7	8/9	0.95	0.15	42,43,43,44	0
2	YCP	b	5	8/9	0.95	0.20	43,43,44,44	0
2	MP8	R	7	8/9	0.95	0.12	37,38,39,41	0
2	MP8	V	7	8/9	0.95	0.09	39,40,42,46	0
2	MP8	U	7	8/9	0.95	0.15	39,40,41,42	0
2	YCP	a	5	8/9	0.96	0.12	37,37,38,38	0
2	MP8	J	7	8/9	0.96	0.12	38,39,40,40	0
2	MP8	Q	7	8/9	0.96	0.13	33,34,34,37	0
2	MP8	a	7	8/9	0.96	0.11	36,37,38,40	0
2	YCP	P	5	8/9	0.96	0.13	34,35,36,36	0
2	YCP	Z	5	8/9	0.96	0.18	37,38,38,38	0
2	YCP	V	5	8/9	0.96	0.14	43,44,45,45	0
2	YCP	X	5	8/9	0.96	0.09	37,38,39,40	0
2	YCP	Q	5	8/9	0.97	0.12	33,35,36,36	0
2	YCP	J	5	8/9	0.97	0.19	40,41,41,42	0
2	YCP	U	5	8/9	0.97	0.20	41,42,43,44	0
2	MP8	X	7	8/9	0.97	0.14	35,36,37,39	0
2	MP8	H	7	8/9	0.97	0.11	37,38,39,41	0
2	YCP	H	5	8/9	0.97	0.10	39,40,41,41	0
2	YCP	c	5	8/9	0.97	0.15	43,44,44,44	0
2	YCP	Y	5	8/9	0.98	0.10	37,38,39,40	0
2	MP8	P	7	8/9	0.98	0.13	31,32,34,34	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.