



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 09:36 PM BST

PDB ID : 3V5I
Title : The crystal structure of the mutant ClpP S98A (Staphylococcus aureus)
Authors : List, A.; Gersch, M.; Groll, M.; Sieber, S.
Deposited on : 2011-12-16
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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
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

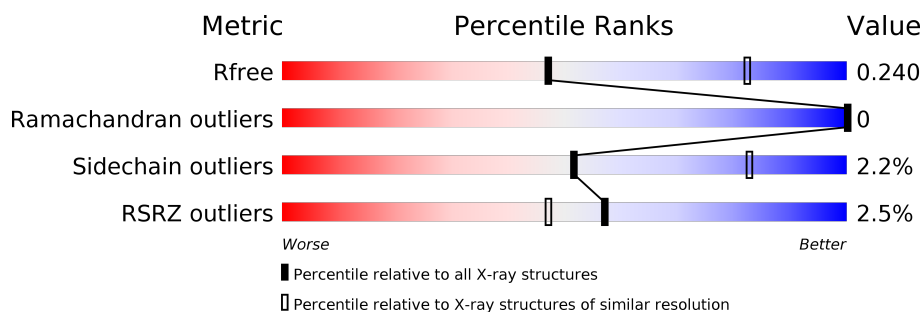
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.













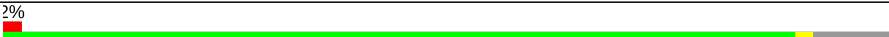

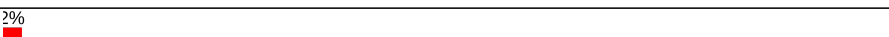
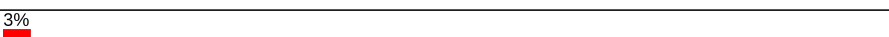
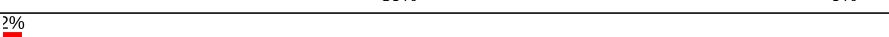
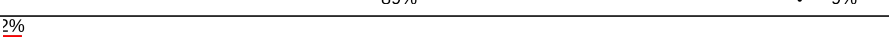

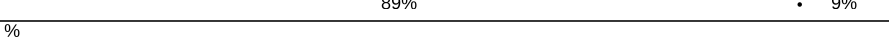


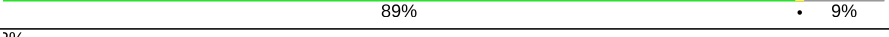
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 ≥ 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></div> <div>89%</div> <div>9%</div> </div>
1	B	203	<div> <div>3%</div> <div>90%</div> <div>9%</div> </div>
1	C	203	<div> <div>2%</div> <div>89%</div> <div>9%</div> </div>
1	D	203	<div> <div>3%</div> <div>89%</div> <div>9%</div> </div>
1	E	203	<div> <div></div> <div>89%</div> <div>9%</div> </div>
1	F	203	<div> <div>6%</div> <div>89%</div> <div>9%</div> </div>
1	G	203	<div> <div></div> <div>89%</div> <div>9%</div> </div>

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40465 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
			1421	896	242	277	6			
1	B	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	C	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	D	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	E	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	F	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	G	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	H	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	I	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	J	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	K	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	L	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	M	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	N	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	O	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	P	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	R	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	S	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	T	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	U	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	V	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	W	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	X	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	Y	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	Z	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	a	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			
1	b	184	Total	C	N	O	S	0	0	0
			1421	896	242	277	6			

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
A	196	TRP	-	EXPRESSION TAG	UNP Q2G036
A	197	SER	-	EXPRESSION TAG	UNP Q2G036
A	198	HIS	-	EXPRESSION TAG	UNP Q2G036
A	199	PRO	-	EXPRESSION TAG	UNP Q2G036
A	200	GLN	-	EXPRESSION TAG	UNP Q2G036
A	201	PHE	-	EXPRESSION TAG	UNP Q2G036
A	202	GLU	-	EXPRESSION TAG	UNP Q2G036
A	203	LYS	-	EXPRESSION TAG	UNP Q2G036
B	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
B	196	TRP	-	EXPRESSION TAG	UNP Q2G036
B	197	SER	-	EXPRESSION TAG	UNP Q2G036
B	198	HIS	-	EXPRESSION TAG	UNP Q2G036
B	199	PRO	-	EXPRESSION TAG	UNP Q2G036
B	200	GLN	-	EXPRESSION TAG	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
B	201	PHE	-	EXPRESSION TAG	UNP Q2G036
B	202	GLU	-	EXPRESSION TAG	UNP Q2G036
B	203	LYS	-	EXPRESSION TAG	UNP Q2G036
C	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
C	196	TRP	-	EXPRESSION TAG	UNP Q2G036
C	197	SER	-	EXPRESSION TAG	UNP Q2G036
C	198	HIS	-	EXPRESSION TAG	UNP Q2G036
C	199	PRO	-	EXPRESSION TAG	UNP Q2G036
C	200	GLN	-	EXPRESSION TAG	UNP Q2G036
C	201	PHE	-	EXPRESSION TAG	UNP Q2G036
C	202	GLU	-	EXPRESSION TAG	UNP Q2G036
C	203	LYS	-	EXPRESSION TAG	UNP Q2G036
D	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
D	196	TRP	-	EXPRESSION TAG	UNP Q2G036
D	197	SER	-	EXPRESSION TAG	UNP Q2G036
D	198	HIS	-	EXPRESSION TAG	UNP Q2G036
D	199	PRO	-	EXPRESSION TAG	UNP Q2G036
D	200	GLN	-	EXPRESSION TAG	UNP Q2G036
D	201	PHE	-	EXPRESSION TAG	UNP Q2G036
D	202	GLU	-	EXPRESSION TAG	UNP Q2G036
D	203	LYS	-	EXPRESSION TAG	UNP Q2G036
E	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
E	196	TRP	-	EXPRESSION TAG	UNP Q2G036
E	197	SER	-	EXPRESSION TAG	UNP Q2G036
E	198	HIS	-	EXPRESSION TAG	UNP Q2G036
E	199	PRO	-	EXPRESSION TAG	UNP Q2G036
E	200	GLN	-	EXPRESSION TAG	UNP Q2G036
E	201	PHE	-	EXPRESSION TAG	UNP Q2G036
E	202	GLU	-	EXPRESSION TAG	UNP Q2G036
E	203	LYS	-	EXPRESSION TAG	UNP Q2G036
F	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
F	196	TRP	-	EXPRESSION TAG	UNP Q2G036
F	197	SER	-	EXPRESSION TAG	UNP Q2G036
F	198	HIS	-	EXPRESSION TAG	UNP Q2G036
F	199	PRO	-	EXPRESSION TAG	UNP Q2G036
F	200	GLN	-	EXPRESSION TAG	UNP Q2G036
F	201	PHE	-	EXPRESSION TAG	UNP Q2G036
F	202	GLU	-	EXPRESSION TAG	UNP Q2G036
F	203	LYS	-	EXPRESSION TAG	UNP Q2G036
G	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
G	196	TRP	-	EXPRESSION TAG	UNP Q2G036
G	197	SER	-	EXPRESSION TAG	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
G	198	HIS	-	EXPRESSION TAG	UNP Q2G036
G	199	PRO	-	EXPRESSION TAG	UNP Q2G036
G	200	GLN	-	EXPRESSION TAG	UNP Q2G036
G	201	PHE	-	EXPRESSION TAG	UNP Q2G036
G	202	GLU	-	EXPRESSION TAG	UNP Q2G036
G	203	LYS	-	EXPRESSION TAG	UNP Q2G036
H	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
H	196	TRP	-	EXPRESSION TAG	UNP Q2G036
H	197	SER	-	EXPRESSION TAG	UNP Q2G036
H	198	HIS	-	EXPRESSION TAG	UNP Q2G036
H	199	PRO	-	EXPRESSION TAG	UNP Q2G036
H	200	GLN	-	EXPRESSION TAG	UNP Q2G036
H	201	PHE	-	EXPRESSION TAG	UNP Q2G036
H	202	GLU	-	EXPRESSION TAG	UNP Q2G036
H	203	LYS	-	EXPRESSION TAG	UNP Q2G036
I	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
I	196	TRP	-	EXPRESSION TAG	UNP Q2G036
I	197	SER	-	EXPRESSION TAG	UNP Q2G036
I	198	HIS	-	EXPRESSION TAG	UNP Q2G036
I	199	PRO	-	EXPRESSION TAG	UNP Q2G036
I	200	GLN	-	EXPRESSION TAG	UNP Q2G036
I	201	PHE	-	EXPRESSION TAG	UNP Q2G036
I	202	GLU	-	EXPRESSION TAG	UNP Q2G036
I	203	LYS	-	EXPRESSION TAG	UNP Q2G036
J	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
J	196	TRP	-	EXPRESSION TAG	UNP Q2G036
J	197	SER	-	EXPRESSION TAG	UNP Q2G036
J	198	HIS	-	EXPRESSION TAG	UNP Q2G036
J	199	PRO	-	EXPRESSION TAG	UNP Q2G036
J	200	GLN	-	EXPRESSION TAG	UNP Q2G036
J	201	PHE	-	EXPRESSION TAG	UNP Q2G036
J	202	GLU	-	EXPRESSION TAG	UNP Q2G036
J	203	LYS	-	EXPRESSION TAG	UNP Q2G036
K	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
K	196	TRP	-	EXPRESSION TAG	UNP Q2G036
K	197	SER	-	EXPRESSION TAG	UNP Q2G036
K	198	HIS	-	EXPRESSION TAG	UNP Q2G036
K	199	PRO	-	EXPRESSION TAG	UNP Q2G036
K	200	GLN	-	EXPRESSION TAG	UNP Q2G036
K	201	PHE	-	EXPRESSION TAG	UNP Q2G036
K	202	GLU	-	EXPRESSION TAG	UNP Q2G036
K	203	LYS	-	EXPRESSION TAG	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
L	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
L	196	TRP	-	EXPRESSION TAG	UNP Q2G036
L	197	SER	-	EXPRESSION TAG	UNP Q2G036
L	198	HIS	-	EXPRESSION TAG	UNP Q2G036
L	199	PRO	-	EXPRESSION TAG	UNP Q2G036
L	200	GLN	-	EXPRESSION TAG	UNP Q2G036
L	201	PHE	-	EXPRESSION TAG	UNP Q2G036
L	202	GLU	-	EXPRESSION TAG	UNP Q2G036
L	203	LYS	-	EXPRESSION TAG	UNP Q2G036
M	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
M	196	TRP	-	EXPRESSION TAG	UNP Q2G036
M	197	SER	-	EXPRESSION TAG	UNP Q2G036
M	198	HIS	-	EXPRESSION TAG	UNP Q2G036
M	199	PRO	-	EXPRESSION TAG	UNP Q2G036
M	200	GLN	-	EXPRESSION TAG	UNP Q2G036
M	201	PHE	-	EXPRESSION TAG	UNP Q2G036
M	202	GLU	-	EXPRESSION TAG	UNP Q2G036
M	203	LYS	-	EXPRESSION TAG	UNP Q2G036
N	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
N	196	TRP	-	EXPRESSION TAG	UNP Q2G036
N	197	SER	-	EXPRESSION TAG	UNP Q2G036
N	198	HIS	-	EXPRESSION TAG	UNP Q2G036
N	199	PRO	-	EXPRESSION TAG	UNP Q2G036
N	200	GLN	-	EXPRESSION TAG	UNP Q2G036
N	201	PHE	-	EXPRESSION TAG	UNP Q2G036
N	202	GLU	-	EXPRESSION TAG	UNP Q2G036
N	203	LYS	-	EXPRESSION TAG	UNP Q2G036
O	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
O	196	TRP	-	EXPRESSION TAG	UNP Q2G036
O	197	SER	-	EXPRESSION TAG	UNP Q2G036
O	198	HIS	-	EXPRESSION TAG	UNP Q2G036
O	199	PRO	-	EXPRESSION TAG	UNP Q2G036
O	200	GLN	-	EXPRESSION TAG	UNP Q2G036
O	201	PHE	-	EXPRESSION TAG	UNP Q2G036
O	202	GLU	-	EXPRESSION TAG	UNP Q2G036
O	203	LYS	-	EXPRESSION TAG	UNP Q2G036
P	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
P	196	TRP	-	EXPRESSION TAG	UNP Q2G036
P	197	SER	-	EXPRESSION TAG	UNP Q2G036
P	198	HIS	-	EXPRESSION TAG	UNP Q2G036
P	199	PRO	-	EXPRESSION TAG	UNP Q2G036
P	200	GLN	-	EXPRESSION TAG	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
P	201	PHE	-	EXPRESSION TAG	UNP Q2G036
P	202	GLU	-	EXPRESSION TAG	UNP Q2G036
P	203	LYS	-	EXPRESSION TAG	UNP Q2G036
Q	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
Q	196	TRP	-	EXPRESSION TAG	UNP Q2G036
Q	197	SER	-	EXPRESSION TAG	UNP Q2G036
Q	198	HIS	-	EXPRESSION TAG	UNP Q2G036
Q	199	PRO	-	EXPRESSION TAG	UNP Q2G036
Q	200	GLN	-	EXPRESSION TAG	UNP Q2G036
Q	201	PHE	-	EXPRESSION TAG	UNP Q2G036
Q	202	GLU	-	EXPRESSION TAG	UNP Q2G036
Q	203	LYS	-	EXPRESSION TAG	UNP Q2G036
R	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
R	196	TRP	-	EXPRESSION TAG	UNP Q2G036
R	197	SER	-	EXPRESSION TAG	UNP Q2G036
R	198	HIS	-	EXPRESSION TAG	UNP Q2G036
R	199	PRO	-	EXPRESSION TAG	UNP Q2G036
R	200	GLN	-	EXPRESSION TAG	UNP Q2G036
R	201	PHE	-	EXPRESSION TAG	UNP Q2G036
R	202	GLU	-	EXPRESSION TAG	UNP Q2G036
R	203	LYS	-	EXPRESSION TAG	UNP Q2G036
S	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
S	196	TRP	-	EXPRESSION TAG	UNP Q2G036
S	197	SER	-	EXPRESSION TAG	UNP Q2G036
S	198	HIS	-	EXPRESSION TAG	UNP Q2G036
S	199	PRO	-	EXPRESSION TAG	UNP Q2G036
S	200	GLN	-	EXPRESSION TAG	UNP Q2G036
S	201	PHE	-	EXPRESSION TAG	UNP Q2G036
S	202	GLU	-	EXPRESSION TAG	UNP Q2G036
S	203	LYS	-	EXPRESSION TAG	UNP Q2G036
T	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
T	196	TRP	-	EXPRESSION TAG	UNP Q2G036
T	197	SER	-	EXPRESSION TAG	UNP Q2G036
T	198	HIS	-	EXPRESSION TAG	UNP Q2G036
T	199	PRO	-	EXPRESSION TAG	UNP Q2G036
T	200	GLN	-	EXPRESSION TAG	UNP Q2G036
T	201	PHE	-	EXPRESSION TAG	UNP Q2G036
T	202	GLU	-	EXPRESSION TAG	UNP Q2G036
T	203	LYS	-	EXPRESSION TAG	UNP Q2G036
U	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
U	196	TRP	-	EXPRESSION TAG	UNP Q2G036
U	197	SER	-	EXPRESSION TAG	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
U	198	HIS	-	EXPRESSION TAG	UNP Q2G036
U	199	PRO	-	EXPRESSION TAG	UNP Q2G036
U	200	GLN	-	EXPRESSION TAG	UNP Q2G036
U	201	PHE	-	EXPRESSION TAG	UNP Q2G036
U	202	GLU	-	EXPRESSION TAG	UNP Q2G036
U	203	LYS	-	EXPRESSION TAG	UNP Q2G036
V	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
V	196	TRP	-	EXPRESSION TAG	UNP Q2G036
V	197	SER	-	EXPRESSION TAG	UNP Q2G036
V	198	HIS	-	EXPRESSION TAG	UNP Q2G036
V	199	PRO	-	EXPRESSION TAG	UNP Q2G036
V	200	GLN	-	EXPRESSION TAG	UNP Q2G036
V	201	PHE	-	EXPRESSION TAG	UNP Q2G036
V	202	GLU	-	EXPRESSION TAG	UNP Q2G036
V	203	LYS	-	EXPRESSION TAG	UNP Q2G036
W	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
W	196	TRP	-	EXPRESSION TAG	UNP Q2G036
W	197	SER	-	EXPRESSION TAG	UNP Q2G036
W	198	HIS	-	EXPRESSION TAG	UNP Q2G036
W	199	PRO	-	EXPRESSION TAG	UNP Q2G036
W	200	GLN	-	EXPRESSION TAG	UNP Q2G036
W	201	PHE	-	EXPRESSION TAG	UNP Q2G036
W	202	GLU	-	EXPRESSION TAG	UNP Q2G036
W	203	LYS	-	EXPRESSION TAG	UNP Q2G036
X	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
X	196	TRP	-	EXPRESSION TAG	UNP Q2G036
X	197	SER	-	EXPRESSION TAG	UNP Q2G036
X	198	HIS	-	EXPRESSION TAG	UNP Q2G036
X	199	PRO	-	EXPRESSION TAG	UNP Q2G036
X	200	GLN	-	EXPRESSION TAG	UNP Q2G036
X	201	PHE	-	EXPRESSION TAG	UNP Q2G036
X	202	GLU	-	EXPRESSION TAG	UNP Q2G036
X	203	LYS	-	EXPRESSION TAG	UNP Q2G036
Y	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
Y	196	TRP	-	EXPRESSION TAG	UNP Q2G036
Y	197	SER	-	EXPRESSION TAG	UNP Q2G036
Y	198	HIS	-	EXPRESSION TAG	UNP Q2G036
Y	199	PRO	-	EXPRESSION TAG	UNP Q2G036
Y	200	GLN	-	EXPRESSION TAG	UNP Q2G036
Y	201	PHE	-	EXPRESSION TAG	UNP Q2G036
Y	202	GLU	-	EXPRESSION TAG	UNP Q2G036
Y	203	LYS	-	EXPRESSION TAG	UNP Q2G036

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
Z	196	TRP	-	EXPRESSION TAG	UNP Q2G036
Z	197	SER	-	EXPRESSION TAG	UNP Q2G036
Z	198	HIS	-	EXPRESSION TAG	UNP Q2G036
Z	199	PRO	-	EXPRESSION TAG	UNP Q2G036
Z	200	GLN	-	EXPRESSION TAG	UNP Q2G036
Z	201	PHE	-	EXPRESSION TAG	UNP Q2G036
Z	202	GLU	-	EXPRESSION TAG	UNP Q2G036
Z	203	LYS	-	EXPRESSION TAG	UNP Q2G036
a	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
a	196	TRP	-	EXPRESSION TAG	UNP Q2G036
a	197	SER	-	EXPRESSION TAG	UNP Q2G036
a	198	HIS	-	EXPRESSION TAG	UNP Q2G036
a	199	PRO	-	EXPRESSION TAG	UNP Q2G036
a	200	GLN	-	EXPRESSION TAG	UNP Q2G036
a	201	PHE	-	EXPRESSION TAG	UNP Q2G036
a	202	GLU	-	EXPRESSION TAG	UNP Q2G036
a	203	LYS	-	EXPRESSION TAG	UNP Q2G036
b	98	ALA	SER	ENGINEERED MUTATION	UNP Q2G036
b	196	TRP	-	EXPRESSION TAG	UNP Q2G036
b	197	SER	-	EXPRESSION TAG	UNP Q2G036
b	198	HIS	-	EXPRESSION TAG	UNP Q2G036
b	199	PRO	-	EXPRESSION TAG	UNP Q2G036
b	200	GLN	-	EXPRESSION TAG	UNP Q2G036
b	201	PHE	-	EXPRESSION TAG	UNP Q2G036
b	202	GLU	-	EXPRESSION TAG	UNP Q2G036
b	203	LYS	-	EXPRESSION TAG	UNP Q2G036

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	22	Total O 22 22	0	0
2	C	16	Total O 16 16	0	0
2	D	22	Total O 22 22	0	0
2	E	31	Total O 31 31	0	0
2	F	44	Total O 44 44	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	33	Total O 33 33	0	0
2	H	38	Total O 38 38	0	0
2	I	31	Total O 31 31	0	0
2	J	20	Total O 20 20	0	0
2	K	41	Total O 41 41	0	0
2	L	31	Total O 31 31	0	0
2	M	31	Total O 31 31	0	0
2	N	28	Total O 28 28	0	0
2	O	19	Total O 19 19	0	0
2	P	18	Total O 18 18	0	0
2	Q	18	Total O 18 18	0	0
2	R	21	Total O 21 21	0	0
2	S	14	Total O 14 14	0	0
2	T	19	Total O 19 19	0	0
2	U	14	Total O 14 14	0	0
2	V	20	Total O 20 20	0	0
2	W	16	Total O 16 16	0	0
2	X	20	Total O 20 20	0	0
2	Y	20	Total O 20 20	0	0
2	Z	16	Total O 16 16	0	0
2	a	20	Total O 20 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	b	25	Total	O	0	0
			25	25		

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.

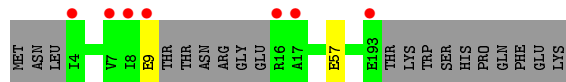
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B: 




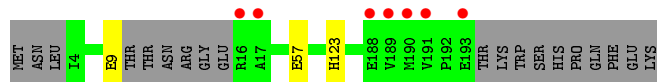
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D: 

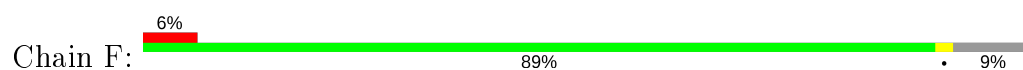


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

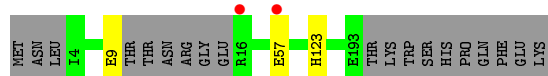
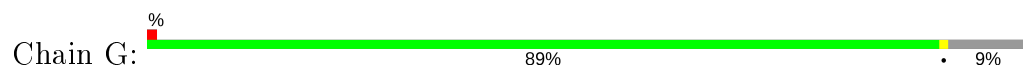
Chain E: 



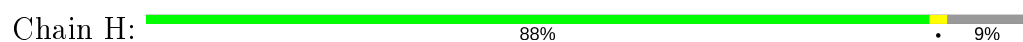
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



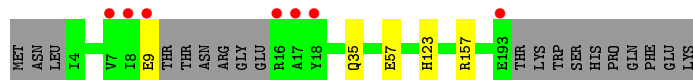
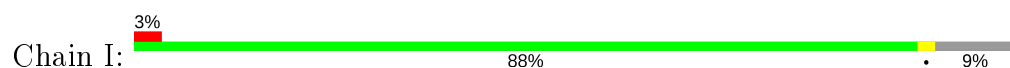
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



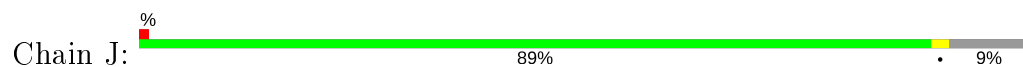
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



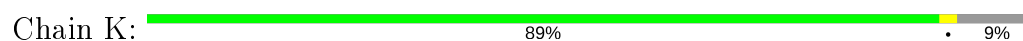
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



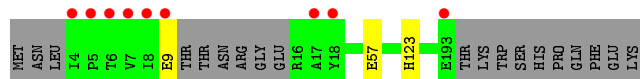
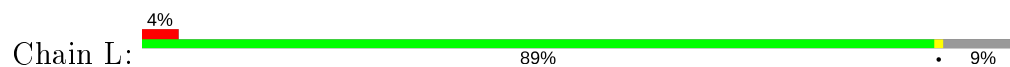
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



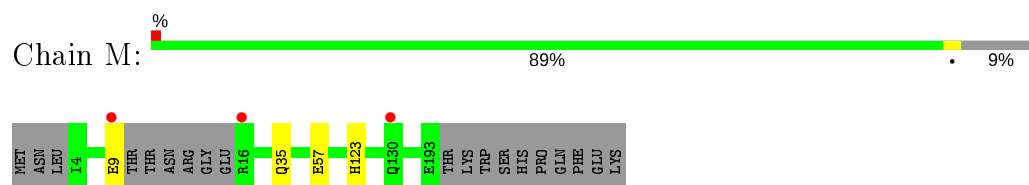
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



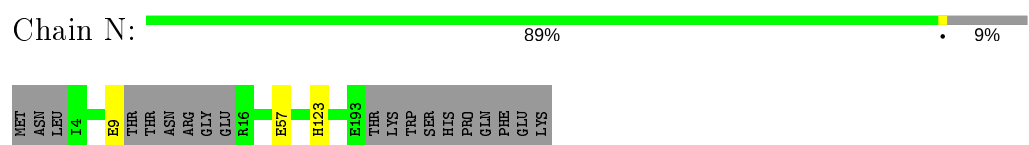
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



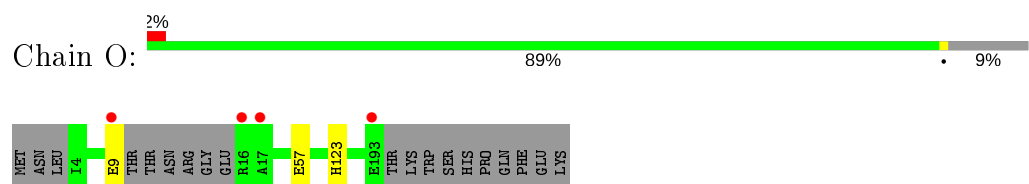
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



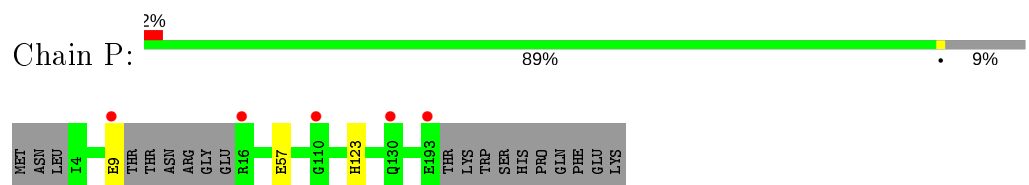
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



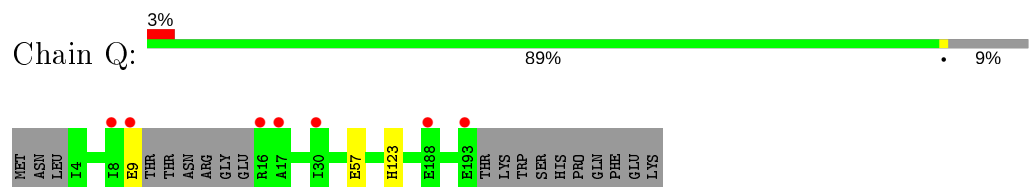
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



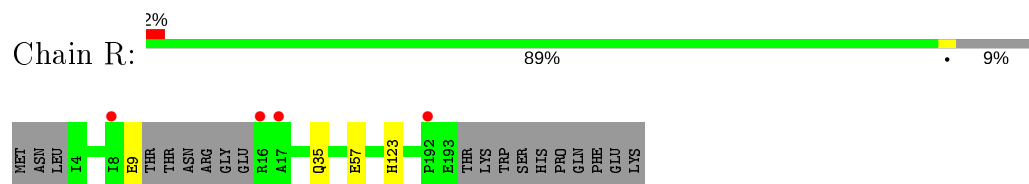
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



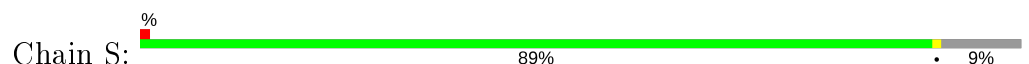
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

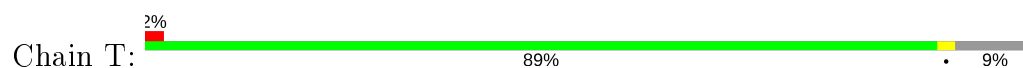


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

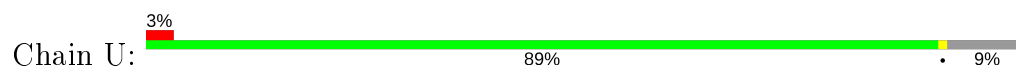




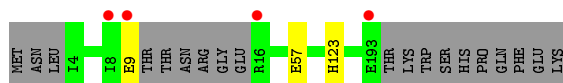
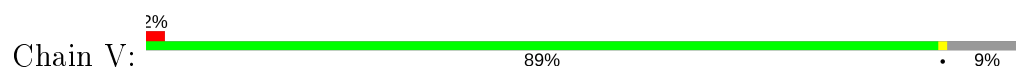
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



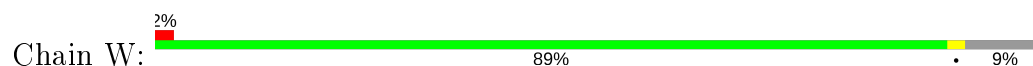
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



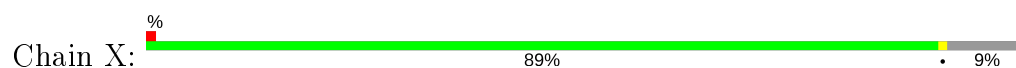
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



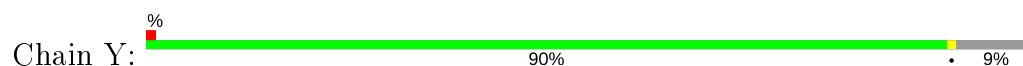
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



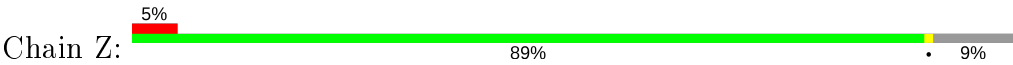
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



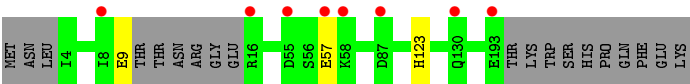
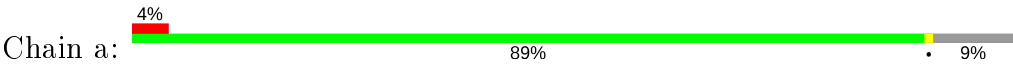
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



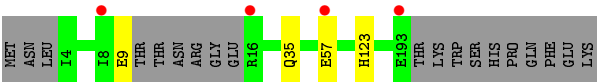
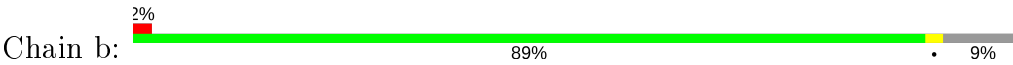
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.55Å 109.73Å 171.41Å 73.10° 78.68° 71.46°	Depositor
Resolution (Å)	24.80 – 2.80 24.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.80-2.80) 95.7 (24.81-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.216 , 0.242 0.216 , 0.240	Depositor DCC
R_{free} test set	7542 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	40465	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/1439	0.67	0/1942
1	B	0.52	0/1439	0.65	0/1942
1	C	0.57	0/1439	0.62	0/1942
1	D	0.63	0/1439	0.66	0/1942
1	E	0.76	0/1439	0.77	1/1942 (0.1%)
1	F	0.76	0/1439	0.72	0/1942
1	G	0.68	0/1439	0.70	0/1942
1	H	0.74	0/1439	0.73	1/1942 (0.1%)
1	I	0.67	0/1439	0.70	1/1942 (0.1%)
1	J	0.60	0/1439	0.65	0/1942
1	K	0.69	0/1439	0.70	0/1942
1	L	0.69	0/1439	0.69	0/1942
1	M	0.72	0/1439	0.71	0/1942
1	N	0.75	0/1439	0.73	0/1942
1	O	0.61	0/1439	0.65	0/1942
1	P	0.63	0/1439	0.66	0/1942
1	Q	0.64	0/1439	0.65	0/1942
1	R	0.59	0/1439	0.64	0/1942
1	S	0.65	0/1439	0.66	0/1942
1	T	0.62	0/1439	0.63	0/1942
1	U	0.56	0/1439	0.62	0/1942
1	V	0.61	0/1439	0.66	0/1942
1	W	0.61	0/1439	0.66	0/1942
1	X	0.62	0/1439	0.63	0/1942
1	Y	0.60	0/1439	0.65	0/1942
1	Z	0.53	0/1439	0.63	0/1942
1	a	0.55	0/1439	0.64	0/1942
1	b	0.63	0/1439	0.67	0/1942
All	All	0.64	0/40292	0.67	3/54376 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	157	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	147	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	H	157	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	B	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	C	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	D	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	E	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	F	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	G	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	H	180/203 (89%)	174 (97%)	6 (3%)	0	100	100
1	I	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	J	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	K	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	L	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	M	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	N	180/203 (89%)	177 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	P	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	Q	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	R	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	S	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	T	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	U	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	V	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	W	180/203 (89%)	176 (98%)	4 (2%)	0	100	100
1	X	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	Y	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	Z	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	a	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
1	b	180/203 (89%)	177 (98%)	3 (2%)	0	100	100
All	All	5040/5684 (89%)	4942 (98%)	98 (2%)	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	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	B	152/170 (89%)	150 (99%)	2 (1%)	69	91
1	C	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	D	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	E	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	F	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	G	152/170 (89%)	149 (98%)	3 (2%)	55	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	I	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	J	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	K	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	L	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	M	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	N	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	O	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	P	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	Q	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	R	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	S	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	T	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	U	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	V	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	W	152/170 (89%)	148 (97%)	4 (3%)	46	79
1	X	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	Y	152/170 (89%)	150 (99%)	2 (1%)	69	91
1	Z	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	a	152/170 (89%)	149 (98%)	3 (2%)	55	84
1	b	152/170 (89%)	148 (97%)	4 (3%)	46	79
All	All	4256/4760 (89%)	4163 (98%)	93 (2%)	52	83

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	35	GLN
1	P	57	GLU
1	Z	123	HIS
1	M	57	GLU
1	N	123	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	52	GLN
1	Q	42	ASN
1	Z	124	GLN
1	N	82	GLN
1	O	123	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no 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, 95th 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 ²)	Q<0.9
1	A	184/203 (90%)	-0.40	0 100 100	73, 82, 110, 172	0
1	B	184/203 (90%)	-0.16	7 (3%) 40 30	80, 89, 155, 224	0
1	C	184/203 (90%)	-0.23	4 (2%) 62 52	78, 91, 111, 150	0
1	D	184/203 (90%)	-0.23	7 (3%) 40 30	65, 82, 112, 392	0
1	E	184/203 (90%)	-0.39	1 (0%) 91 88	59, 69, 94, 122	0
1	F	184/203 (90%)	-0.03	12 (6%) 18 11	60, 68, 108, 206	0
1	G	184/203 (90%)	-0.33	2 (1%) 80 75	65, 74, 94, 137	0
1	H	184/203 (90%)	-0.41	1 (0%) 91 88	58, 69, 97, 127	0
1	I	184/203 (90%)	-0.29	7 (3%) 40 30	64, 77, 101, 197	0
1	J	184/203 (90%)	-0.29	3 (1%) 72 66	71, 85, 105, 146	0
1	K	184/203 (90%)	-0.40	1 (0%) 91 88	67, 80, 96, 126	0
1	L	184/203 (90%)	-0.10	9 (4%) 29 20	64, 76, 118, 281	0
1	M	184/203 (90%)	-0.32	3 (1%) 72 66	64, 73, 91, 124	0
1	N	184/203 (90%)	-0.41	0 100 100	60, 70, 98, 244	0
1	O	184/203 (90%)	-0.18	4 (2%) 62 52	71, 86, 111, 190	0
1	P	184/203 (90%)	-0.33	5 (2%) 54 44	67, 80, 115, 175	0
1	Q	184/203 (90%)	-0.27	7 (3%) 40 30	67, 79, 120, 161	0
1	R	184/203 (90%)	-0.30	4 (2%) 62 52	74, 87, 134, 227	0
1	S	184/203 (90%)	-0.40	3 (1%) 72 66	70, 81, 102, 128	0
1	T	184/203 (90%)	-0.23	5 (2%) 54 44	70, 83, 105, 149	0
1	U	184/203 (90%)	-0.28	6 (3%) 46 36	74, 91, 111, 149	0
1	V	184/203 (90%)	-0.27	4 (2%) 62 52	72, 84, 102, 172	0
1	W	184/203 (90%)	-0.24	5 (2%) 54 44	73, 85, 122, 240	0
1	X	184/203 (90%)	-0.30	3 (1%) 72 66	69, 81, 115, 167	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	184/203 (90%)	-0.29	3 (1%) 72 66	74, 88, 132, 161	0
1	Z	184/203 (90%)	0.17	10 (5%) 25 17	89, 100, 168, 303	0
1	a	184/203 (90%)	-0.11	8 (4%) 35 25	79, 99, 124, 154	0
1	b	184/203 (90%)	-0.40	4 (2%) 62 52	69, 80, 122, 159	0
All	All	5152/5684 (90%)	-0.26	128 (2%) 57 47	58, 82, 116, 392	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	17	ALA	13.7
1	F	9	GLU	13.5
1	F	8	ILE	10.7
1	L	9	GLU	9.6
1	Z	8	ILE	8.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.