



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:48 PM GMT

PDB ID : 4JCQ
Title : ClpP1 from *Listeria monocytogenes*
Authors : Zeiler, E.; List, A.; Alte, F.; Gersch, M.; Wachtel, R.; Groll, M.; Sieber, S.
Deposited on : 2013-02-22
Resolution : 2.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

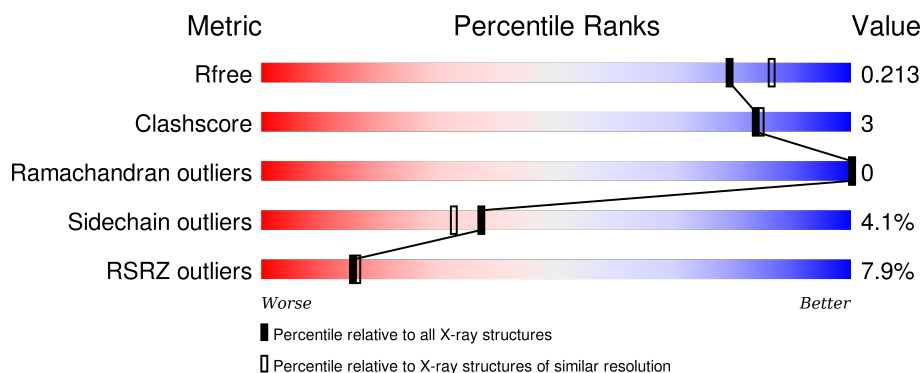
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	201	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
1	B	201	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>15%</div> </div> </div>
1	C	201	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div>15%</div> </div> </div>
1	D	201	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>
1	E	201	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>8%</div> <div>15%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	201	
1	G	201	
1	H	201	
1	I	201	
1	J	201	
1	K	201	
1	L	201	
1	M	201	
1	N	201	
1	O	201	
1	P	201	
1	Q	201	
1	R	201	
1	S	201	
1	T	201	
1	U	201	
1	V	201	
1	W	201	
1	X	201	
1	Y	201	
1	Z	201	
1	a	201	
1	b	201	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40559 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	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	B	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	C	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	D	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	E	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	F	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	G	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	H	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	I	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	J	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	K	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	L	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	M	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	N	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	O	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	P	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	R	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	S	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	T	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	U	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	V	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	W	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	X	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	Y	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	Z	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	a	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	b	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			

There are 308 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
A	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
A	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
A	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
A	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
A	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
A	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
A	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
A	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
A	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
A	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
B	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
B	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
B	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
B	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
B	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
B	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
B	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
B	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
B	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
B	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
C	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
C	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
C	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
C	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
C	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
C	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
C	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
C	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
C	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
C	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
C	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
D	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
D	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
D	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
D	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
D	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
D	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
D	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
D	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
D	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
D	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
D	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
E	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
E	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
E	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
E	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
E	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
E	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
E	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
E	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
E	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
E	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
E	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
F	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
F	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
F	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
F	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
F	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
F	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
F	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
F	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
F	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
F	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
G	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
G	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
G	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
G	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
G	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
G	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
G	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
G	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
G	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
G	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
G	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
H	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
H	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
H	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
H	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
H	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
H	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
H	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
H	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
H	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
H	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
H	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
I	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
I	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
I	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
I	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
I	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
I	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
I	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
I	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
I	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
I	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
I	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
J	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
J	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
J	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
J	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
J	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
J	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
J	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
J	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
J	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
J	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
K	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
K	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
K	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
K	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
K	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
K	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
K	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
K	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
K	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
K	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
K	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
L	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
L	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
L	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
L	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
L	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
L	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
L	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
L	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
L	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
L	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
L	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
M	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
M	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
M	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
M	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
M	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
M	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
M	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
M	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
M	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
M	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
N	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
N	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
N	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
N	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
N	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
N	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
N	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
N	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
N	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
N	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
N	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
O	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
O	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
O	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
O	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
O	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
O	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
O	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
O	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
O	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
O	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
O	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
P	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
P	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
P	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
P	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
P	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
P	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
P	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
P	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
P	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
P	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
P	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
Q	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
R	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
R	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
R	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
R	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
R	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
R	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
R	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
R	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
R	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
R	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
R	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
S	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
S	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
S	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
S	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
S	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
S	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
S	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
S	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
S	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
S	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
S	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
T	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
T	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
T	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
T	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
T	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
T	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
T	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
T	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
T	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
T	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
T	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
U	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
U	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
U	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
U	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
U	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
U	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
U	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
U	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
U	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
U	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
V	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
V	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
V	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
V	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
V	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
V	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
V	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
V	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
V	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
V	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
V	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
W	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
W	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
W	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
W	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
W	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
W	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
W	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
W	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
W	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
W	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
W	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
X	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
X	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
X	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
X	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
X	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
X	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
X	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
X	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
X	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
X	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
X	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
Y	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
Z	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
a	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
a	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
a	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
a	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
a	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
a	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
a	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
a	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
a	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
a	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
a	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1
b	191	MET	-	EXPRESSION TAG	UNP Q8Y7Y1
b	192	ALA	-	EXPRESSION TAG	UNP Q8Y7Y1
b	193	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
b	194	TRP	-	EXPRESSION TAG	UNP Q8Y7Y1
b	195	SER	-	EXPRESSION TAG	UNP Q8Y7Y1
b	196	HIS	-	EXPRESSION TAG	UNP Q8Y7Y1
b	197	PRO	-	EXPRESSION TAG	UNP Q8Y7Y1
b	198	GLN	-	EXPRESSION TAG	UNP Q8Y7Y1
b	199	PHE	-	EXPRESSION TAG	UNP Q8Y7Y1
b	200	GLU	-	EXPRESSION TAG	UNP Q8Y7Y1
b	201	LYS	-	EXPRESSION TAG	UNP Q8Y7Y1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	88	Total O 88 88	0	0
2	B	93	Total O 93 93	0	0
2	C	80	Total O 80 80	0	0
2	D	72	Total O 72 72	0	0
2	E	102	Total O 102 102	0	0
2	F	135	Total O 135 135	0	0
2	G	107	Total O 107 107	0	0
2	H	89	Total O 89 89	0	0
2	I	81	Total O 81 81	0	0
2	J	87	Total O 87 87	0	0
2	K	111	Total O 111 111	0	0
2	L	108	Total O 108 108	0	0
2	M	134	Total O 134 134	0	0
2	N	147	Total O 147 147	0	0
2	O	83	Total O 83 83	0	0
2	P	76	Total O 76 76	0	0
2	Q	100	Total O 100 100	0	0
2	R	99	Total O 99 99	0	0
2	S	124	Total O 124 124	0	0
2	T	157	Total O 157 157	0	0
2	U	93	Total O 93 93	0	0
2	V	106	Total O 106 106	0	0

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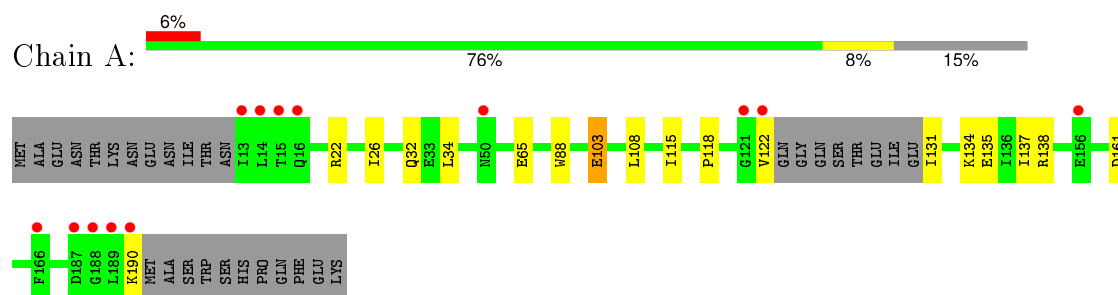
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	W	93	Total 93	O 93	0	0
2	X	84	Total 84	O 84	0	0
2	Y	90	Total 90	O 90	0	0
2	Z	93	Total 93	O 93	0	0
2	a	124	Total 124	O 124	0	0
2	b	143	Total 143	O 143	0	0

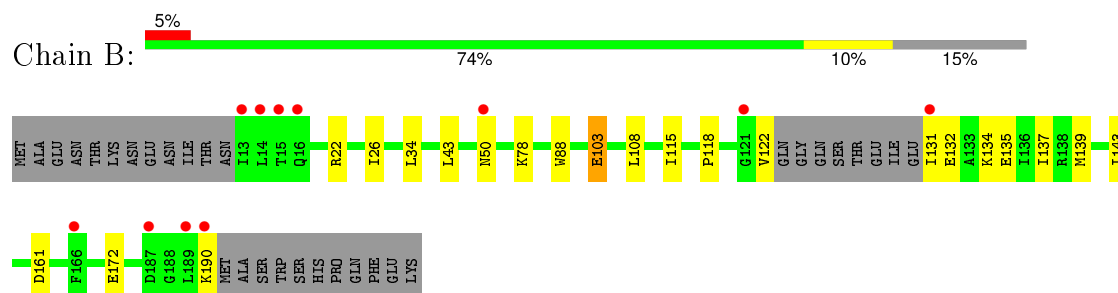
3 Residue-property plots [i](#)

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

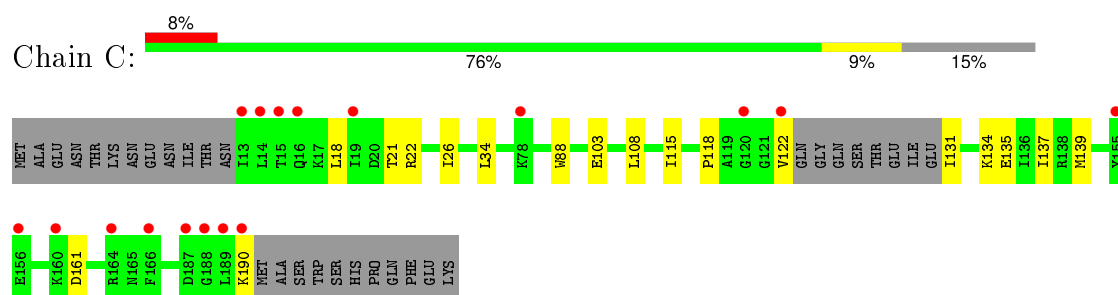
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



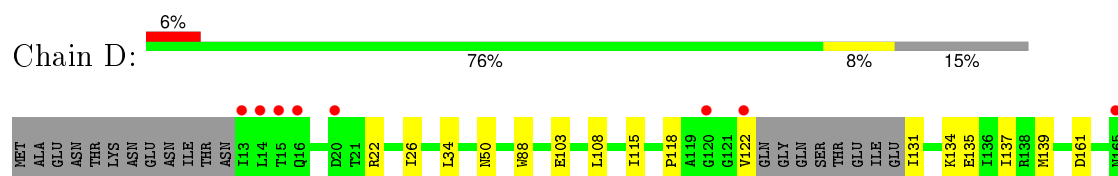
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

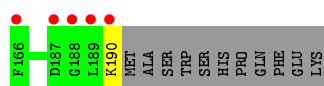


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

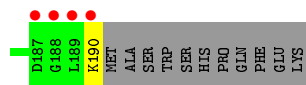
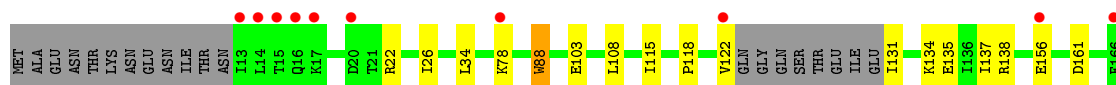
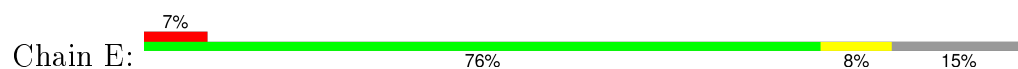


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

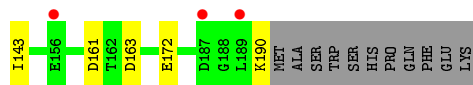
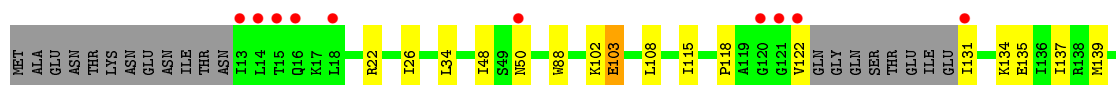
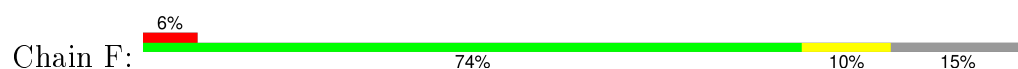




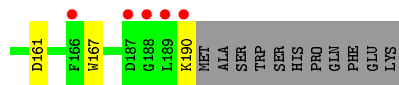
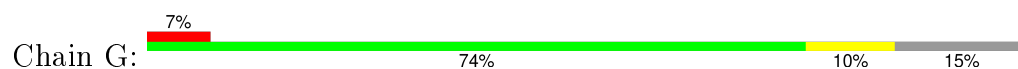
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



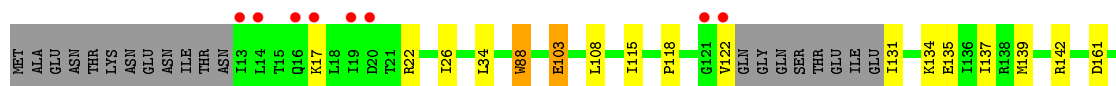
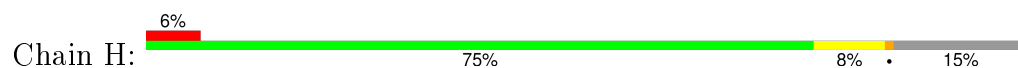
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



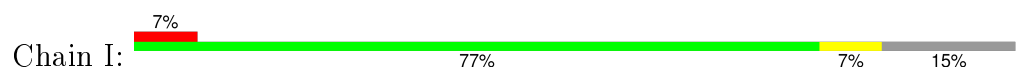
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

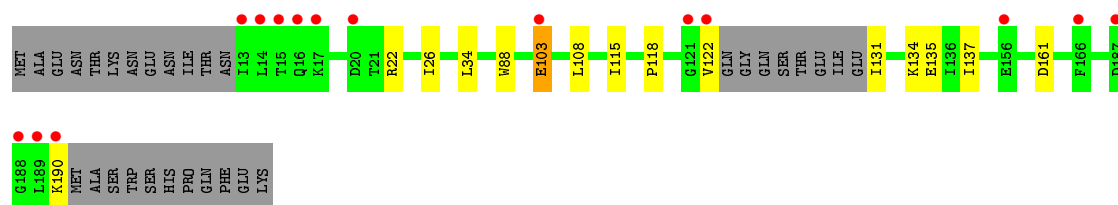


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

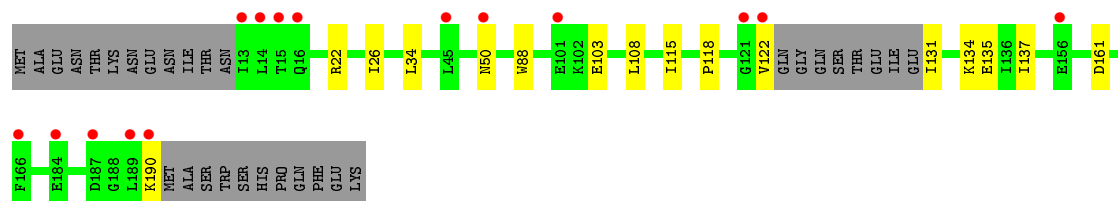
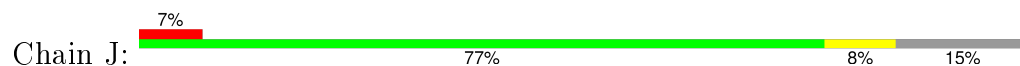


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

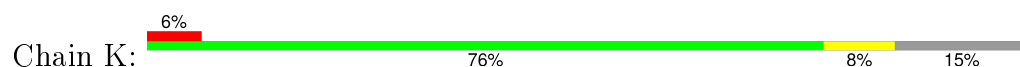




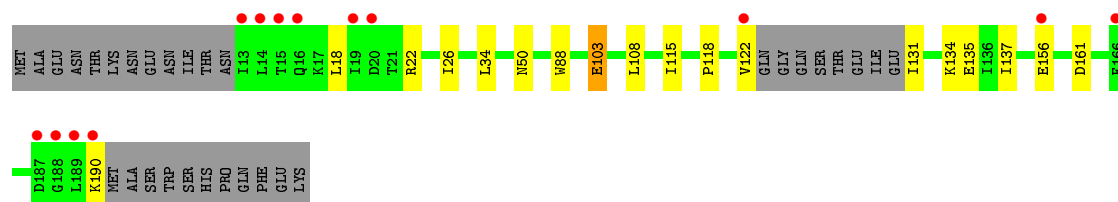
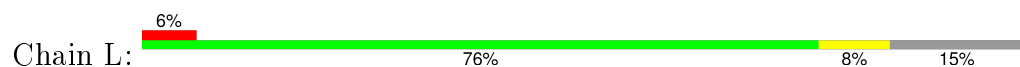
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



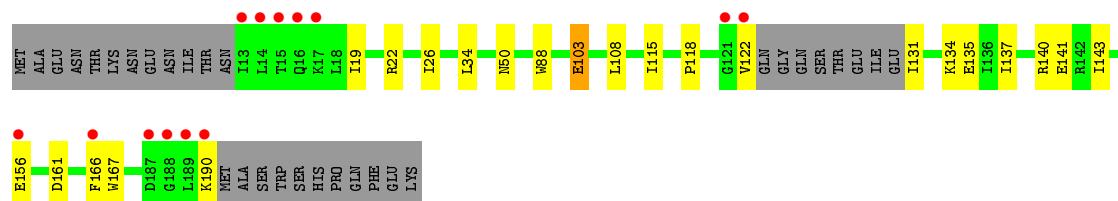
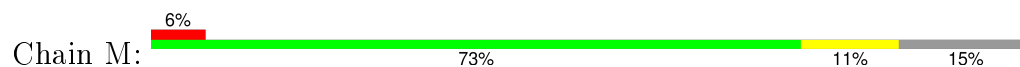
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



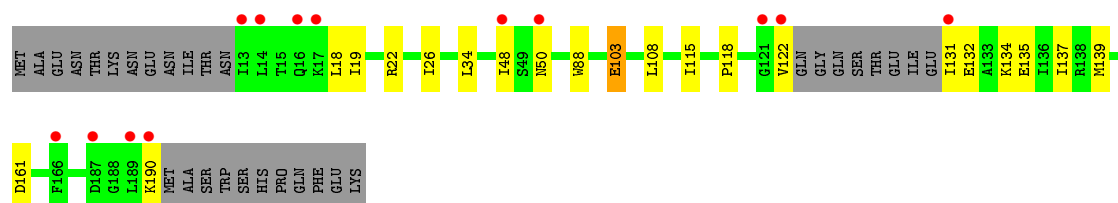
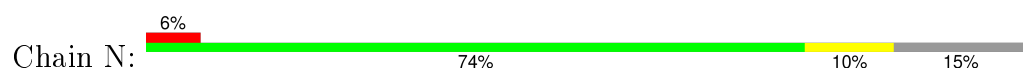
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



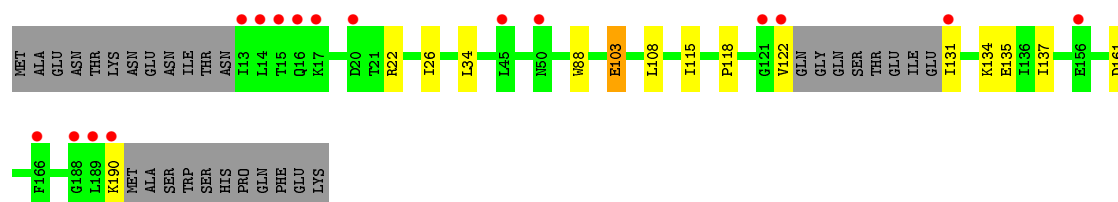
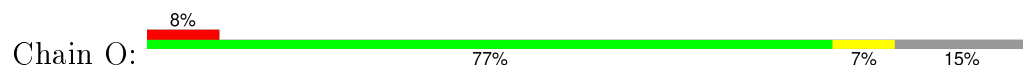
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



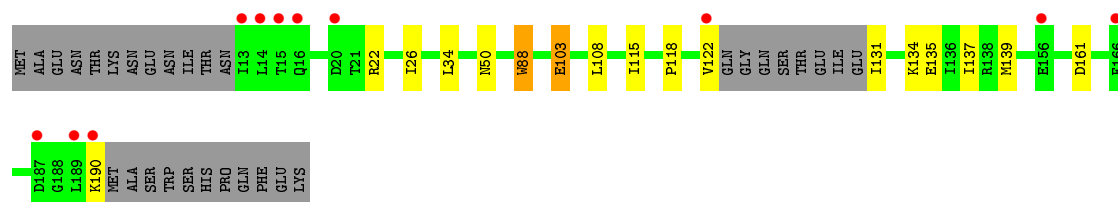
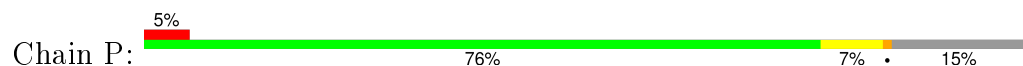
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



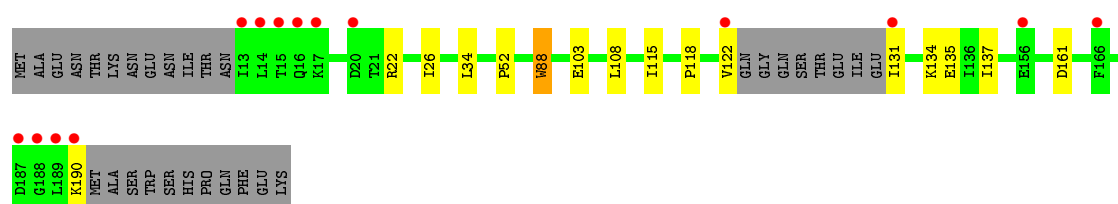
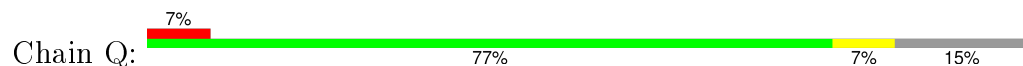
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



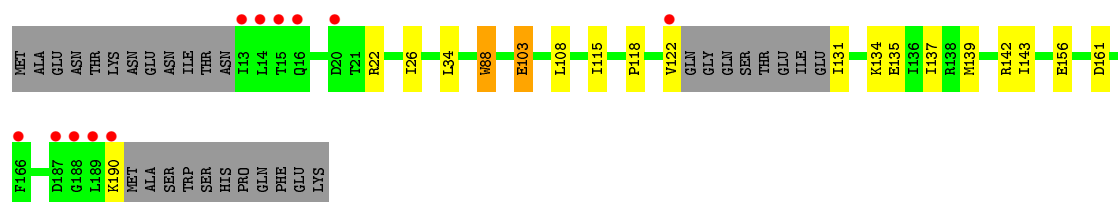
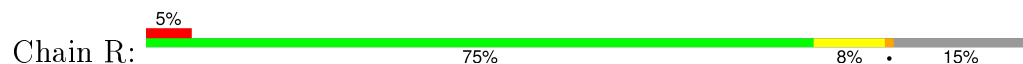
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



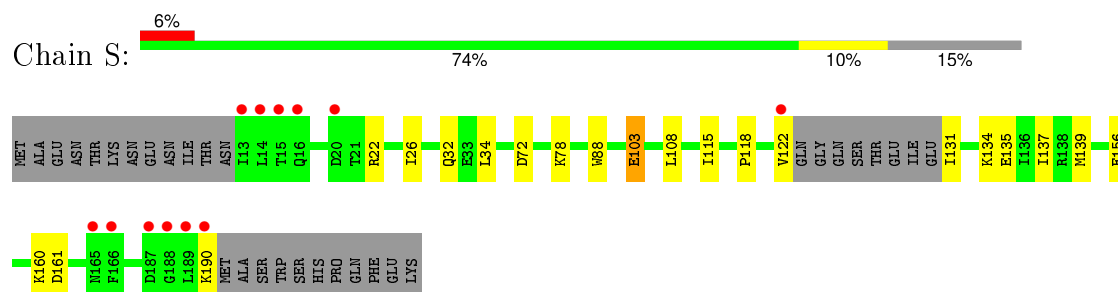
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



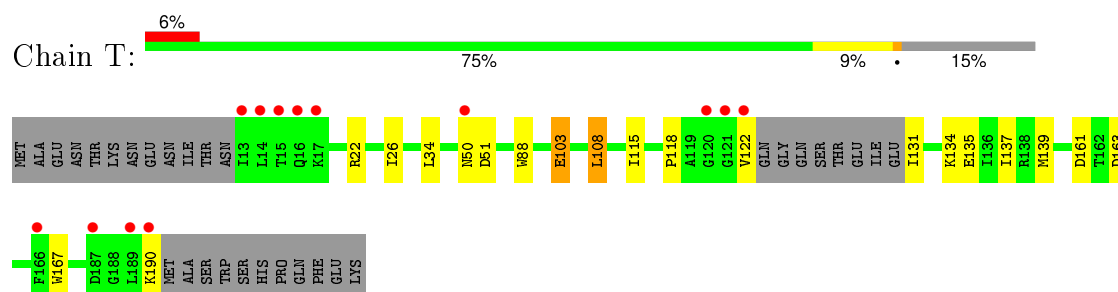
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



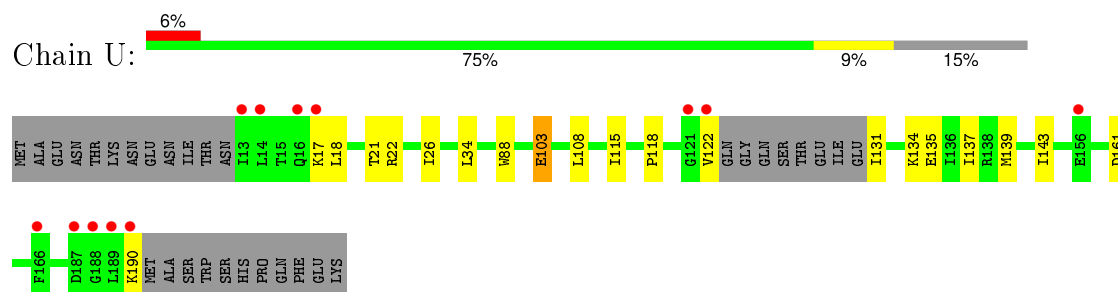
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



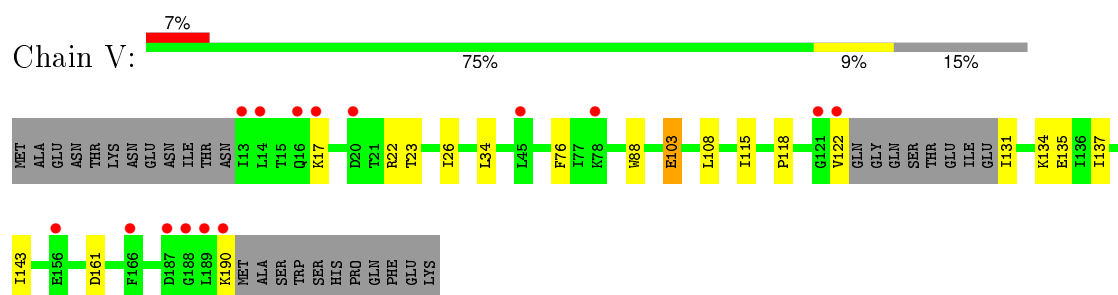
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



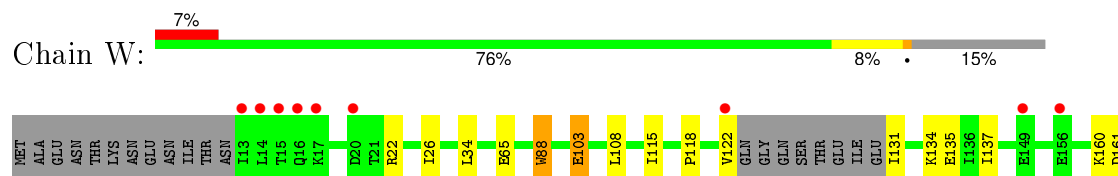
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

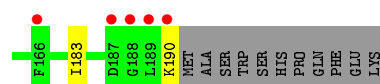


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

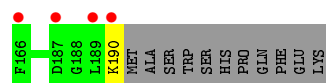
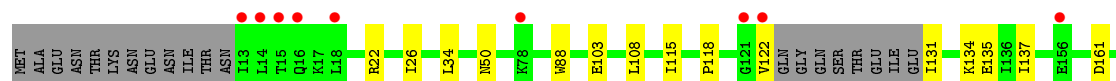


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

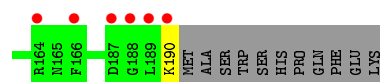




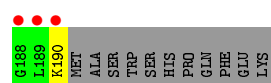
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



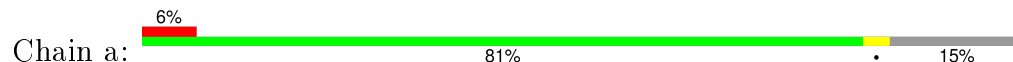
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



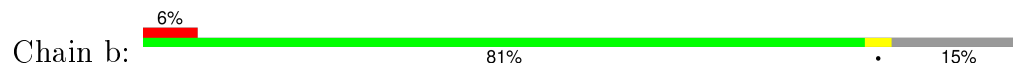
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



GLU
RTD
SMT

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	140.95Å 109.06Å 196.26Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 15.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.00) 99.7 (15.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.192 , 0.213 0.192 , 0.213	Depositor DCC
R_{free} test set	19880 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 397588 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40559	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.0334e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/1363	0.49	0/1841
1	B	0.40	0/1363	0.49	0/1841
1	C	0.40	0/1363	0.49	0/1841
1	D	0.40	0/1363	0.48	0/1841
1	E	0.41	1/1363 (0.1%)	0.49	0/1841
1	F	0.41	0/1363	0.49	0/1841
1	G	0.40	1/1363 (0.1%)	0.49	0/1841
1	H	0.41	2/1363 (0.1%)	0.49	0/1841
1	I	0.40	0/1363	0.48	0/1841
1	J	0.40	0/1363	0.49	0/1841
1	K	0.40	0/1363	0.49	0/1841
1	L	0.40	0/1363	0.49	0/1841
1	M	0.41	1/1363 (0.1%)	0.49	0/1841
1	N	0.41	0/1363	0.49	0/1841
1	O	0.40	0/1363	0.49	0/1841
1	P	0.40	1/1363 (0.1%)	0.49	0/1841
1	Q	0.41	1/1363 (0.1%)	0.49	0/1841
1	R	0.40	1/1363 (0.1%)	0.49	0/1841
1	S	0.41	0/1363	0.49	0/1841
1	T	0.41	1/1363 (0.1%)	0.49	0/1841
1	U	0.40	0/1363	0.49	0/1841
1	V	0.41	0/1363	0.49	0/1841
1	W	0.41	1/1363 (0.1%)	0.49	0/1841
1	X	0.40	0/1363	0.48	0/1841
1	Y	0.41	0/1363	0.48	0/1841
1	Z	0.40	0/1363	0.48	0/1841
1	a	0.41	0/1363	0.49	0/1841
1	b	0.41	0/1363	0.49	0/1841
All	All	0.40	10/38164 (0.0%)	0.49	0/51548

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	88	TRP	CD2-CE2	5.07	1.47	1.41
1	Q	88	TRP	CD2-CE2	5.05	1.47	1.41
1	M	167	TRP	CD2-CE2	5.04	1.47	1.41
1	H	167	TRP	CD2-CE2	5.03	1.47	1.41
1	P	88	TRP	CD2-CE2	5.03	1.47	1.41
1	H	88	TRP	CD2-CE2	5.02	1.47	1.41
1	W	88	TRP	CD2-CE2	5.01	1.47	1.41
1	G	167	TRP	CD2-CE2	5.00	1.47	1.41
1	T	167	TRP	CD2-CE2	5.00	1.47	1.41
1	E	88	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1345	0	1363	10	0
1	B	1345	0	1363	16	0
1	C	1345	0	1363	8	0
1	D	1345	0	1363	7	0
1	E	1345	0	1363	8	1
1	F	1345	0	1363	13	1
1	G	1345	0	1363	14	1
1	H	1345	0	1363	10	1
1	I	1345	0	1363	6	0
1	J	1345	0	1363	6	0
1	K	1345	0	1363	6	1
1	L	1345	0	1363	12	0
1	M	1345	0	1363	12	1
1	N	1345	0	1363	12	1
1	O	1345	0	1363	6	0
1	P	1345	0	1363	8	0
1	Q	1345	0	1363	8	0
1	R	1345	0	1363	11	1
1	S	1345	0	1363	11	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1345	0	1363	12	1
1	U	1345	0	1363	13	0
1	V	1345	0	1363	10	0
1	W	1345	0	1363	9	0
1	X	1345	0	1363	6	0
1	Y	1345	0	1363	6	0
1	Z	1345	0	1363	6	0
1	a	1345	0	1363	0	2
1	b	1345	0	1363	0	1
2	A	88	0	0	2	0
2	B	93	0	0	10	0
2	C	80	0	0	1	0
2	D	72	0	0	2	0
2	E	102	0	0	2	1
2	F	135	0	0	5	0
2	G	107	0	0	6	0
2	H	89	0	0	3	0
2	I	81	0	0	0	0
2	J	87	0	0	1	0
2	K	111	0	0	1	0
2	L	108	0	0	3	0
2	M	134	0	0	7	1
2	N	147	0	0	6	0
2	O	83	0	0	0	0
2	P	76	0	0	2	0
2	Q	100	0	0	0	0
2	R	99	0	0	6	0
2	S	124	0	0	3	0
2	T	157	0	0	8	0
2	U	93	0	0	4	0
2	V	106	0	0	1	0
2	W	93	0	0	1	0
2	X	84	0	0	2	0
2	Y	90	0	0	1	0
2	Z	93	0	0	1	0
2	a	124	0	0	0	0
2	b	143	0	0	0	1
All	All	40559	0	38164	220	8

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 (220) 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:L:156:GLU:OE1	1:Q:52:PRO:HD2	1.40	1.17
1:T:50:ASN:HB2	2:T:441:HOH:O	1.62	0.98
1:W:65:GLU:HG2	2:X:383:HOH:O	1.62	0.97
1:F:137:ILE:HD11	1:N:137:ILE:HD11	1.47	0.94
1:R:139:MET:HG3	2:R:397:HOH:O	1.69	0.91
1:B:137:ILE:HD11	1:T:137:ILE:HD11	88.79	0.90
1:R:142:ARG:NH1	2:R:397:HOH:O	2.09	0.85
1:N:103:GLU:HG3	2:N:355:HOH:O	1.87	0.75
1:F:50:ASN:ND2	2:F:320:HOH:O	2.22	0.72
1:M:140:ARG:HG2	2:M:426:HOH:O	1.88	0.72
1:S:78:LYS:HE3	2:S:358:HOH:O	1.90	0.71
1:B:137:ILE:HD11	1:K:137:ILE:HD11	1.73	0.71
1:T:139:MET:HB2	2:T:397:HOH:O	1.91	0.71
1:G:137:ILE:HD11	1:M:137:ILE:HD11	1.71	0.71
1:G:50:ASN:ND2	2:G:399:HOH:O	2.25	0.69
1:A:137:ILE:HD11	1:L:137:ILE:HD11	1.75	0.69
1:T:50:ASN:ND2	2:T:318:HOH:O	2.25	0.68
1:B:103:GLU:HG3	2:B:368:HOH:O	30.46	0.68
1:F:103:GLU:HG3	2:F:386:HOH:O	1.94	0.68
1:E:137:ILE:HD11	1:H:137:ILE:HD11	1.77	0.67
1:N:50:ASN:ND2	2:N:344:HOH:O	2.28	0.67
1:D:139:MET:HB2	2:D:372:HOH:O	1.94	0.66
1:S:137:ILE:HD11	1:V:137:ILE:HD11	1.76	0.66
1:G:122:VAL:CG2	2:G:400:HOH:O	2.43	0.66
1:S:139:MET:HB2	2:S:416:HOH:O	1.95	0.66
1:D:50:ASN:ND2	2:D:335:HOH:O	2.28	0.65
1:T:103:GLU:HG3	2:T:451:HOH:O	1.97	0.65
1:P:137:ILE:HD11	1:Y:137:ILE:HD11	1.79	0.65
1:Q:137:ILE:HD11	1:X:137:ILE:HD11	1.79	0.65
1:L:50:ASN:ND2	2:L:378:HOH:O	2.29	0.64
1:P:139:MET:HB2	2:P:346:HOH:O	1.98	0.64
1:M:143:ILE:HG12	2:M:427:HOH:O	1.97	0.64
1:B:50:ASN:ND2	2:B:323:HOH:O	18.85	0.63
1:U:139:MET:HB2	2:U:389:HOH:O	1.98	0.63
1:O:137:ILE:HD11	1:Z:137:ILE:HD11	1.80	0.63
1:F:143:ILE:HG12	2:F:426:HOH:O	1.97	0.62
1:R:139:MET:HB2	2:R:398:HOH:O	2.02	0.60
1:A:137:ILE:HD11	1:U:137:ILE:HD11	91.87	0.60
1:P:50:ASN:ND2	2:P:336:HOH:O	2.35	0.60
1:M:50:ASN:ND2	2:M:410:HOH:O	2.33	0.59
1:Z:50:ASN:ND2	2:Z:331:HOH:O	2.34	0.59
1:D:26:ILE:HG23	1:D:34:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:457:HOH:O	1:U:18:LEU:HD12	2.03	0.59
1:U:26:ILE:HG23	1:U:34:LEU:HD11	1.85	0.59
1:B:143:ILE:HG12	2:B:324:HOH:O	2.03	0.59
1:A:26:ILE:HG23	1:A:34:LEU:HD11	1.85	0.58
1:A:65:GLU:HG2	2:B:388:HOH:O	2.04	0.58
1:Q:26:ILE:HG23	1:Q:34:LEU:HD11	1.86	0.58
2:A:385:HOH:O	1:G:65:GLU:HG2	2.02	0.58
1:O:26:ILE:HG23	1:O:34:LEU:HD11	1.86	0.57
1:C:26:ILE:HG23	1:C:34:LEU:HD11	1.85	0.57
1:G:26:ILE:HG23	1:G:34:LEU:HD11	1.86	0.57
1:R:26:ILE:HG23	1:R:34:LEU:HD11	1.85	0.57
2:T:359:HOH:O	1:U:17:LYS:HE2	2.05	0.57
1:X:50:ASN:ND2	2:X:368:HOH:O	2.37	0.57
1:T:26:ILE:HG23	1:T:34:LEU:HD11	1.86	0.57
1:S:26:ILE:HG23	1:S:34:LEU:HD11	1.85	0.57
1:L:156:GLU:OE1	1:Q:52:PRO:CD	2.34	0.57
1:F:139:MET:HB2	2:F:367:HOH:O	2.05	0.56
1:K:26:ILE:HG23	1:K:34:LEU:HD11	1.87	0.56
1:P:26:ILE:HG23	1:P:34:LEU:HD11	1.86	0.56
1:L:26:ILE:HG23	1:L:34:LEU:HD11	1.87	0.56
1:R:137:ILE:HD11	1:W:137:ILE:HD11	1.87	0.56
1:G:122:VAL:HG23	2:G:400:HOH:O	2.05	0.56
1:N:26:ILE:HG23	1:N:34:LEU:HD11	1.87	0.56
1:B:26:ILE:HG23	1:B:34:LEU:HD11	1.87	0.56
1:K:76:PHE:HD1	2:L:408:HOH:O	1.87	0.56
1:H:26:ILE:HG23	1:H:34:LEU:HD11	1.88	0.56
1:H:17:LYS:HE2	2:N:431:HOH:O	2.05	0.55
1:E:26:ILE:HG23	1:E:34:LEU:HD11	1.88	0.55
1:I:26:ILE:HG23	1:I:34:LEU:HD11	1.88	0.55
1:M:26:ILE:HG23	1:M:34:LEU:HD11	1.87	0.55
1:J:50:ASN:ND2	2:J:328:HOH:O	2.39	0.55
1:G:103:GLU:HG3	2:G:342:HOH:O	2.05	0.55
1:J:26:ILE:HG23	1:J:34:LEU:HD11	1.88	0.55
1:V:26:ILE:HG23	1:V:34:LEU:HD11	1.89	0.55
1:V:143:ILE:HG12	2:V:361:HOH:O	2.07	0.55
1:F:26:ILE:HG23	1:F:34:LEU:HD11	1.87	0.55
1:X:26:ILE:HG23	1:X:34:LEU:HD11	1.89	0.54
2:K:406:HOH:O	1:L:18:LEU:HD12	2.08	0.54
1:Y:26:ILE:HG23	1:Y:34:LEU:HD11	1.90	0.54
2:B:337:HOH:O	1:V:17:LYS:HE2	115.71	0.53
1:D:137:ILE:HD11	1:I:137:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:26:ILE:HG23	1:W:34:LEU:HD11	1.90	0.53
1:S:32:GLN:HB3	2:T:452:HOH:O	2.08	0.53
1:R:139:MET:CG	2:R:397:HOH:O	2.39	0.52
1:G:122:VAL:HG21	2:G:400:HOH:O	2.08	0.52
1:Z:26:ILE:HG23	1:Z:34:LEU:HD11	1.89	0.52
1:M:103:GLU:HG3	2:M:400:HOH:O	2.08	0.52
1:H:139:MET:HB2	2:H:388:HOH:O	2.10	0.51
1:M:156:GLU:HB2	2:M:310:HOH:O	2.09	0.51
1:Y:118:PRO:HG3	1:Y:122:VAL:HG22	1.93	0.51
2:B:390:HOH:O	1:C:21:THR:HG21	2.12	0.50
1:C:137:ILE:HD11	1:J:137:ILE:HD11	1.92	0.50
1:N:139:MET:HB2	2:N:435:HOH:O	2.11	0.50
1:E:156:GLU:HB2	2:E:311:HOH:O	2.12	0.50
1:A:118:PRO:HG3	1:A:122:VAL:HG22	1.96	0.50
1:C:118:PRO:HG3	1:C:122:VAL:HG22	1.95	0.49
1:B:139:MET:HB2	2:B:352:HOH:O	31.28	0.49
1:V:118:PRO:HG3	1:V:122:VAL:HG22	1.93	0.49
1:B:118:PRO:HG3	1:B:122:VAL:HG22	1.96	0.49
1:W:118:PRO:HG3	1:W:122:VAL:HG22	1.94	0.48
1:E:78:LYS:HE3	2:E:387:HOH:O	2.11	0.48
1:R:103:GLU:HG3	2:R:364:HOH:O	2.13	0.48
1:Q:118:PRO:HG3	1:Q:122:VAL:HG22	1.96	0.48
1:G:118:PRO:HG3	1:G:122:VAL:HG22	1.95	0.48
1:Z:118:PRO:HG3	1:Z:122:VAL:HG22	1.94	0.48
1:R:118:PRO:HG3	1:R:122:VAL:HG22	1.95	0.48
1:A:138:ARG:HH22	1:B:172:GLU:CD	2.41	0.48
1:L:156:GLU:CD	1:Q:52:PRO:HD2	2.25	0.47
2:B:390:HOH:O	1:C:18:LEU:HD12	2.13	0.47
1:F:118:PRO:HG3	1:F:122:VAL:HG22	1.95	0.47
1:R:143:ILE:HD11	2:R:397:HOH:O	2.13	0.47
1:N:18:LEU:HD23	2:N:436:HOH:O	2.14	0.47
1:X:118:PRO:HG3	1:X:122:VAL:HG22	1.94	0.47
1:E:118:PRO:HG3	1:E:122:VAL:HG22	1.95	0.47
1:O:118:PRO:HG3	1:O:122:VAL:HG22	1.96	0.47
1:S:118:PRO:HG3	1:S:122:VAL:HG22	1.95	0.47
1:T:115:ILE:HD11	1:T:161:ASP:HB2	1.96	0.47
1:D:118:PRO:HG3	1:D:122:VAL:HG22	1.96	0.47
1:E:138:ARG:HH22	1:F:172:GLU:CD	2.18	0.47
1:S:156:GLU:HB2	2:S:306:HOH:O	2.14	0.47
1:U:118:PRO:HG3	1:U:122:VAL:HG22	1.96	0.46
1:H:142:ARG:NH2	2:H:385:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:GLU:HG3	2:H:335:HOH:O	2.15	0.46
1:N:131:ILE:HA	2:N:437:HOH:O	2.16	0.46
1:P:118:PRO:HG3	1:P:122:VAL:HG22	1.96	0.46
2:A:385:HOH:O	1:G:32:GLN:HG2	2.15	0.46
1:T:118:PRO:HG3	1:T:122:VAL:HG22	1.96	0.46
1:U:131:ILE:HG23	1:U:135:GLU:HB3	1.98	0.46
1:B:78:LYS:HE3	2:B:347:HOH:O	2.16	0.46
1:R:115:ILE:HD11	1:R:161:ASP:HB2	1.98	0.46
1:R:131:ILE:HG23	1:R:135:GLU:HB3	1.98	0.46
1:A:115:ILE:HD11	1:A:161:ASP:HB2	1.98	0.46
1:G:78:LYS:HE3	2:G:407:HOH:O	2.16	0.46
1:K:118:PRO:HG3	1:K:122:VAL:HG22	1.98	0.46
1:O:131:ILE:HG23	1:O:135:GLU:HB3	1.98	0.46
1:U:122:VAL:CG2	2:U:386:HOH:O	2.65	0.45
1:M:141:GLU:HG3	2:M:380:HOH:O	2.15	0.45
1:P:131:ILE:HG23	1:P:135:GLU:HB3	1.98	0.45
1:Z:131:ILE:HG23	1:Z:135:GLU:HB3	1.99	0.45
1:S:131:ILE:HG23	1:S:135:GLU:HB3	1.99	0.45
1:W:131:ILE:HG23	1:W:135:GLU:HB3	1.99	0.45
1:B:131:ILE:HG23	1:B:135:GLU:HB3	1.99	0.45
1:D:131:ILE:HG23	1:D:135:GLU:HB3	1.99	0.45
1:U:115:ILE:HD11	1:U:161:ASP:HB2	1.98	0.45
1:L:131:ILE:HG23	1:L:135:GLU:HB3	1.99	0.45
1:O:115:ILE:HD11	1:O:161:ASP:HB2	1.98	0.45
1:B:132:GLU:HB3	1:T:163:ASP:OD2	92.88	0.45
1:Q:131:ILE:HG23	1:Q:135:GLU:HB3	1.98	0.45
1:G:131:ILE:HG23	1:G:135:GLU:HB3	1.99	0.45
1:N:118:PRO:HG3	1:N:122:VAL:HG22	1.98	0.45
1:M:118:PRO:HG3	1:M:122:VAL:HG22	1.98	0.45
1:C:115:ILE:HD11	1:C:161:ASP:HB2	1.99	0.45
1:P:115:ILE:HD11	1:P:161:ASP:HB2	1.99	0.45
1:E:131:ILE:HG23	1:E:135:GLU:HB3	1.99	0.44
1:S:115:ILE:HD11	1:S:161:ASP:HB2	1.99	0.44
1:W:103:GLU:HG3	1:W:103:GLU:H	1.63	0.44
1:T:131:ILE:HG23	1:T:135:GLU:HB3	1.98	0.44
1:Q:115:ILE:HD11	1:Q:161:ASP:HB2	1.99	0.44
1:H:118:PRO:HG3	1:H:122:VAL:HG22	1.99	0.44
1:A:131:ILE:HG23	1:A:135:GLU:HB3	1.99	0.44
1:H:131:ILE:HG23	1:H:135:GLU:HB3	2.00	0.44
1:X:131:ILE:HG23	1:X:135:GLU:HB3	1.99	0.44
1:F:115:ILE:HD11	1:F:161:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:HG23	1:C:135:GLU:HB3	1.99	0.44
1:C:139:MET:HB2	2:C:336:HOH:O	2.18	0.44
1:Y:131:ILE:HG23	1:Y:135:GLU:HB3	1.99	0.44
1:S:72:ASP:HB3	1:T:108:LEU:HG	2.00	0.44
1:F:131:ILE:HG23	1:F:135:GLU:HB3	1.99	0.44
1:V:131:ILE:HG23	1:V:135:GLU:HB3	2.00	0.44
1:E:115:ILE:HD11	1:E:161:ASP:HB2	2.00	0.44
1:D:115:ILE:HD11	1:D:161:ASP:HB2	1.99	0.44
1:J:118:PRO:HG3	1:J:122:VAL:HG22	1.99	0.44
1:J:131:ILE:HG23	1:J:135:GLU:HB3	2.00	0.43
1:I:131:ILE:HG23	1:I:135:GLU:HB3	2.00	0.43
1:W:115:ILE:HD11	1:W:161:ASP:HB2	2.00	0.43
1:U:122:VAL:HG21	2:U:386:HOH:O	2.18	0.43
1:M:115:ILE:HD11	1:M:161:ASP:HB2	2.00	0.43
1:I:115:ILE:HD11	1:I:161:ASP:HB2	2.00	0.43
1:U:143:ILE:HG12	2:U:379:HOH:O	2.18	0.43
1:G:115:ILE:HD11	1:G:161:ASP:HB2	2.00	0.43
1:V:115:ILE:HD11	1:V:161:ASP:HB2	2.00	0.43
1:Y:115:ILE:HD11	1:Y:161:ASP:HB2	2.01	0.43
1:N:131:ILE:HG23	1:N:135:GLU:HB3	2.00	0.43
1:K:115:ILE:HD11	1:K:161:ASP:HB2	2.01	0.43
1:K:131:ILE:HG23	1:K:135:GLU:HB3	2.00	0.43
1:M:131:ILE:HG23	1:M:135:GLU:HB3	2.00	0.43
1:I:118:PRO:HG3	1:I:122:VAL:HG22	1.99	0.43
1:F:102:LYS:HE3	2:F:376:HOH:O	2.19	0.43
1:L:118:PRO:HG3	1:L:122:VAL:HG22	1.99	0.43
1:B:43:LEU:HD13	1:V:23:THR:HG21	123.52	0.43
1:X:115:ILE:HD11	1:X:161:ASP:HB2	2.00	0.43
1:B:115:ILE:HD11	1:B:161:ASP:HB2	2.00	0.42
1:L:103:GLU:HG3	2:L:364:HOH:O	2.19	0.42
1:M:166:PHE:HZ	2:M:355:HOH:O	1.99	0.42
1:B:103:GLU:H	1:B:103:GLU:HG3	1.64	0.42
1:A:32:GLN:HG2	2:B:388:HOH:O	2.20	0.42
1:H:103:GLU:H	1:H:103:GLU:HG3	1.63	0.42
1:O:103:GLU:HG3	1:O:103:GLU:H	1.63	0.42
1:A:103:GLU:H	1:A:103:GLU:HG3	1.64	0.42
1:L:115:ILE:HD11	1:L:161:ASP:HB2	2.00	0.42
1:N:115:ILE:HD11	1:N:161:ASP:HB2	2.00	0.42
1:Z:115:ILE:HD11	1:Z:161:ASP:HB2	2.00	0.42
2:T:457:HOH:O	1:U:21:THR:HG21	2.19	0.42
1:J:115:ILE:HD11	1:J:161:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:103:GLU:H	1:P:103:GLU:HG3	1.64	0.41
1:I:103:GLU:H	1:I:103:GLU:HG3	1.61	0.41
1:W:160:LYS:NZ	2:W:389:HOH:O	2.52	0.41
1:V:76:PHE:HE1	1:W:183:ILE:HD12	1.86	0.41
1:S:103:GLU:H	1:S:103:GLU:HG3	1.63	0.41
1:H:115:ILE:HD11	1:H:161:ASP:HB2	2.01	0.41
1:F:137:ILE:CD1	1:N:137:ILE:HD11	2.34	0.41
1:L:103:GLU:HG3	1:L:103:GLU:H	1.63	0.41
1:G:103:GLU:H	1:G:103:GLU:HG3	1.65	0.41
1:Y:139:MET:HB2	2:Y:384:HOH:O	2.21	0.41
1:U:103:GLU:H	1:U:103:GLU:HG3	1.64	0.41
1:F:163:ASP:OD2	1:N:132:GLU:HB3	2.21	0.41
1:B:132:GLU:HB3	1:T:163:ASP:CG	93.64	0.40
1:V:103:GLU:HG3	1:V:103:GLU:H	1.65	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:156:GLU:OE2	1:b:48:ILE:CG2[2_354]	1.60	0.60
1:K:52:PRO:CG	1:R:156:GLU:OE1[1_565]	1.72	0.48
1:E:156:GLU:OE2	1:F:48:ILE:CG2[2_555]	1.92	0.28
1:H:17:LYS:NZ	2:M:310:HOH:O[2_455]	2.03	0.17
1:S:160:LYS:NZ	1:T:51:ASP:OD2[2_444]	2.04	0.16
1:M:156:GLU:OE2	1:N:48:ILE:CG2[2_445]	2.09	0.11
1:a:156:GLU:OE1	2:b:365:HOH:O[2_354]	2.13	0.07
1:G:17:LYS:NZ	2:E:311:HOH:O[2_545]	2.15	0.05

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	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	B	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	C	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	D	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	E	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	F	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	G	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	H	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	I	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	J	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	K	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	L	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	M	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	N	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	O	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	P	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	Q	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	R	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	S	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	T	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	U	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	V	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	W	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	X	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	Y	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	Z	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	a	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	b	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
All	All	4648/5628 (83%)	4536 (98%)	112 (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	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	B	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	C	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	D	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	E	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	F	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	G	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	H	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	I	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	J	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	K	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	L	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	M	147/175 (84%)	140 (95%)	7 (5%)	31	26
1	N	147/175 (84%)	140 (95%)	7 (5%)	31	26
1	O	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	P	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	Q	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	R	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	S	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	T	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	U	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	V	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	W	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	X	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	Y	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	Z	147/175 (84%)	141 (96%)	6 (4%)	37	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	147/175 (84%)	141 (96%)	6 (4%)	37	32
1	b	147/175 (84%)	141 (96%)	6 (4%)	37	32
All	All	4116/4900 (84%)	3946 (96%)	170 (4%)	37	32

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	88	TRP
1	A	103	GLU
1	A	108	LEU
1	A	134	LYS
1	A	190	LYS
1	B	22	ARG
1	B	88	TRP
1	B	103	GLU
1	B	108	LEU
1	B	134	LYS
1	B	190	LYS
1	C	22	ARG
1	C	88	TRP
1	C	103	GLU
1	C	108	LEU
1	C	134	LYS
1	C	190	LYS
1	D	22	ARG
1	D	88	TRP
1	D	103	GLU
1	D	108	LEU
1	D	134	LYS
1	D	190	LYS
1	E	22	ARG
1	E	88	TRP
1	E	103	GLU
1	E	108	LEU
1	E	134	LYS
1	E	190	LYS
1	F	22	ARG
1	F	88	TRP
1	F	103	GLU
1	F	108	LEU

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Mol	Chain	Res	Type
1	F	134	LYS
1	F	190	LYS
1	G	22	ARG
1	G	88	TRP
1	G	103	GLU
1	G	108	LEU
1	G	134	LYS
1	G	190	LYS
1	H	22	ARG
1	H	88	TRP
1	H	103	GLU
1	H	108	LEU
1	H	134	LYS
1	H	190	LYS
1	I	22	ARG
1	I	88	TRP
1	I	103	GLU
1	I	108	LEU
1	I	134	LYS
1	I	190	LYS
1	J	22	ARG
1	J	88	TRP
1	J	103	GLU
1	J	108	LEU
1	J	134	LYS
1	J	190	LYS
1	K	22	ARG
1	K	88	TRP
1	K	103	GLU
1	K	108	LEU
1	K	134	LYS
1	K	190	LYS
1	L	22	ARG
1	L	88	TRP
1	L	103	GLU
1	L	108	LEU
1	L	134	LYS
1	L	190	LYS
1	M	19	ILE
1	M	22	ARG
1	M	88	TRP
1	M	103	GLU

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Mol	Chain	Res	Type
1	M	108	LEU
1	M	134	LYS
1	M	190	LYS
1	N	19	ILE
1	N	22	ARG
1	N	88	TRP
1	N	103	GLU
1	N	108	LEU
1	N	134	LYS
1	N	190	LYS
1	O	22	ARG
1	O	88	TRP
1	O	103	GLU
1	O	108	LEU
1	O	134	LYS
1	O	190	LYS
1	P	22	ARG
1	P	88	TRP
1	P	103	GLU
1	P	108	LEU
1	P	134	LYS
1	P	190	LYS
1	Q	22	ARG
1	Q	88	TRP
1	Q	103	GLU
1	Q	108	LEU
1	Q	134	LYS
1	Q	190	LYS
1	R	22	ARG
1	R	88	TRP
1	R	103	GLU
1	R	108	LEU
1	R	134	LYS
1	R	190	LYS
1	S	22	ARG
1	S	88	TRP
1	S	103	GLU
1	S	108	LEU
1	S	134	LYS
1	S	190	LYS
1	T	22	ARG
1	T	88	TRP

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Mol	Chain	Res	Type
1	T	103	GLU
1	T	108	LEU
1	T	134	LYS
1	T	190	LYS
1	U	22	ARG
1	U	88	TRP
1	U	103	GLU
1	U	108	LEU
1	U	134	LYS
1	U	190	LYS
1	V	22	ARG
1	V	88	TRP
1	V	103	GLU
1	V	108	LEU
1	V	134	LYS
1	V	190	LYS
1	W	22	ARG
1	W	88	TRP
1	W	103	GLU
1	W	108	LEU
1	W	134	LYS
1	W	190	LYS
1	X	22	ARG
1	X	88	TRP
1	X	103	GLU
1	X	108	LEU
1	X	134	LYS
1	X	190	LYS
1	Y	22	ARG
1	Y	88	TRP
1	Y	103	GLU
1	Y	108	LEU
1	Y	134	LYS
1	Y	190	LYS
1	Z	22	ARG
1	Z	88	TRP
1	Z	103	GLU
1	Z	108	LEU
1	Z	134	LYS
1	Z	190	LYS
1	a	22	ARG
1	a	88	TRP

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Mol	Chain	Res	Type
1	a	103	GLU
1	a	108	LEU
1	a	134	LYS
1	a	190	LYS
1	b	22	ARG
1	b	88	TRP
1	b	103	GLU
1	b	108	LEU
1	b	134	LYS
1	b	190	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	B	180	ASN
1	E	180	ASN
1	F	50	ASN
1	F	185	ASN
1	G	180	ASN
1	L	63	HIS
1	M	50	ASN
1	N	50	ASN
1	O	180	ASN
1	P	16	GLN
1	R	180	ASN
1	S	180	ASN
1	T	50	ASN
1	T	180	ASN
1	U	63	HIS
1	U	180	ASN
1	V	16	GLN
1	W	16	GLN
1	Z	63	HIS
1	b	16	GLN
1	b	50	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	170/201 (84%)	0.20	13 (7%) 17 18	19, 30, 67, 111	0
1	B	170/201 (84%)	0.25	11 (6%) 22 23	23, 35, 71, 116	0
1	C	170/201 (84%)	0.39	17 (10%) 9 10	24, 36, 74, 121	0
1	D	170/201 (84%)	0.49	13 (7%) 17 18	23, 36, 74, 118	0
1	E	170/201 (84%)	0.26	14 (8%) 14 15	16, 27, 66, 111	0
1	F	170/201 (84%)	0.17	13 (7%) 17 18	15, 25, 60, 102	0
1	G	170/201 (84%)	0.18	14 (8%) 14 15	16, 27, 65, 107	0
1	H	170/201 (84%)	0.23	13 (7%) 17 18	17, 29, 63, 106	0
1	I	170/201 (84%)	0.43	15 (8%) 12 13	22, 34, 69, 112	0
1	J	170/201 (84%)	0.32	15 (8%) 12 13	25, 36, 67, 114	0
1	K	170/201 (84%)	0.34	13 (7%) 17 18	22, 32, 72, 114	0
1	L	170/201 (84%)	0.23	13 (7%) 17 18	18, 30, 66, 112	0
1	M	170/201 (84%)	0.19	13 (7%) 17 18	13, 23, 62, 108	0
1	N	170/201 (84%)	0.14	13 (7%) 17 18	13, 23, 55, 101	0
1	O	170/201 (84%)	0.32	16 (9%) 11 11	21, 33, 67, 114	0
1	P	170/201 (84%)	0.29	11 (6%) 22 23	23, 35, 70, 114	0
1	Q	170/201 (84%)	0.26	14 (8%) 14 15	20, 31, 69, 112	0
1	R	170/201 (84%)	0.15	11 (6%) 22 23	18, 28, 66, 110	0
1	S	170/201 (84%)	0.18	12 (7%) 19 20	13, 23, 65, 109	0
1	T	170/201 (84%)	0.09	13 (7%) 17 18	13, 23, 50, 100	0
1	U	170/201 (84%)	0.23	12 (7%) 19 20	17, 28, 63, 108	0
1	V	170/201 (84%)	0.19	15 (8%) 12 13	16, 27, 65, 109	0
1	W	170/201 (84%)	0.26	14 (8%) 14 15	17, 28, 65, 110	0
1	X	170/201 (84%)	0.23	13 (7%) 17 18	21, 33, 68, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	Y	170/201 (84%)	0.40	16 (9%)	11 11	21, 32, 69, 116	0
1	Z	170/201 (84%)	0.27	13 (7%)	17 18	21, 32, 70, 114	0
1	a	170/201 (84%)	0.18	13 (7%)	17 18	15, 25, 65, 107	0
1	b	170/201 (84%)	0.16	12 (7%)	19 20	14, 23, 59, 102	0
All	All	4760/5628 (84%)	0.25	375 (7%)	15 16	13, 30, 73, 121	0

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	14	LEU	15.7
1	K	13	ILE	14.8
1	I	14	LEU	14.4
1	D	188	GLY	12.4
1	W	14	LEU	12.3
1	C	14	LEU	12.3
1	E	14	LEU	12.1
1	J	14	LEU	12.1
1	Q	188	GLY	11.7
1	R	190	LYS	11.6
1	X	14	LEU	11.4
1	P	14	LEU	11.4
1	W	13	ILE	11.3
1	Z	14	LEU	11.3
1	Y	13	ILE	11.0
1	I	13	ILE	10.5
1	Y	14	LEU	10.5
1	O	13	ILE	10.2
1	O	14	LEU	10.1
1	U	14	LEU	9.9
1	P	190	LYS	9.7
1	R	14	LEU	9.6
1	Q	13	ILE	9.5
1	M	14	LEU	9.4
1	U	13	ILE	9.2
1	P	15	THR	9.0
1	X	13	ILE	8.8
1	V	13	ILE	8.8
1	L	14	LEU	8.8
1	C	188	GLY	8.8
1	H	13	ILE	8.5
1	S	188	GLY	8.5

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Mol	Chain	Res	Type	RSRZ
1	R	13	ILE	8.4
1	J	15	THR	8.3
1	I	15	THR	8.3
1	Z	188	GLY	8.1
1	a	14	LEU	8.1
1	D	13	ILE	8.1
1	A	14	LEU	8.1
1	Y	188	GLY	8.1
1	E	13	ILE	8.0
1	M	122	VAL	8.0
1	M	188	GLY	7.9
1	a	13	ILE	7.9
1	G	13	ILE	7.9
1	Q	190	LYS	7.8
1	S	14	LEU	7.8
1	L	190	LYS	7.8
1	D	15	THR	7.7
1	H	14	LEU	7.7
1	D	189	LEU	7.6
1	N	14	LEU	7.6
1	I	190	LYS	7.5
1	A	13	ILE	7.3
1	L	189	LEU	7.3
1	C	190	LYS	7.3
1	O	16	GLN	7.2
1	T	14	LEU	7.2
1	H	122	VAL	7.1
1	Z	122	VAL	7.1
1	Y	190	LYS	7.0
1	P	13	ILE	7.0
1	Z	189	LEU	6.9
1	C	13	ILE	6.9
1	K	187	ASP	6.8
1	S	15	THR	6.8
1	W	15	THR	6.8
1	J	190	LYS	6.8
1	V	122	VAL	6.7
1	G	14	LEU	6.6
1	B	14	LEU	6.5
1	B	190	LYS	6.5
1	Y	187	ASP	6.4
1	Q	14	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	U	122	VAL	6.4
1	B	16	GLN	6.4
1	V	189	LEU	6.4
1	N	13	ILE	6.3
1	E	188	GLY	6.3
1	V	14	LEU	6.2
1	V	190	LYS	6.1
1	D	122	VAL	6.1
1	S	16	GLN	6.0
1	b	15	THR	5.9
1	I	122	VAL	5.9
1	G	122	VAL	5.8
1	a	188	GLY	5.7
1	A	189	LEU	5.6
1	I	16	GLN	5.5
1	D	190	LYS	5.5
1	Q	16	GLN	5.4
1	T	187	ASP	5.4
1	Z	190	LYS	5.4
1	b	13	ILE	5.4
1	E	15	THR	5.4
1	A	190	LYS	5.4
1	S	190	LYS	5.4
1	F	13	ILE	5.3
1	K	190	LYS	5.3
1	Z	15	THR	5.3
1	P	16	GLN	5.3
1	O	15	THR	5.3
1	K	15	THR	5.3
1	K	122	VAL	5.2
1	T	13	ILE	5.2
1	M	189	LEU	5.2
1	M	190	LYS	5.2
1	L	13	ILE	5.1
1	K	14	LEU	5.1
1	V	188	GLY	5.1
1	C	189	LEU	5.1
1	E	189	LEU	5.1
1	Y	15	THR	5.0
1	Z	13	ILE	5.0
1	D	187	ASP	5.0
1	J	13	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	R	188	GLY	5.0
1	L	16	GLN	5.0
1	S	122	VAL	5.0
1	W	190	LYS	4.9
1	C	15	THR	4.9
1	a	15	THR	4.9
1	A	15	THR	4.9
1	D	16	GLN	4.9
1	C	166	PHE	4.8
1	Y	16	GLN	4.8
1	L	188	GLY	4.8
1	S	189	LEU	4.8
1	Z	16	GLN	4.8
1	I	188	GLY	4.8
1	O	17	LYS	4.8
1	B	13	ILE	4.7
1	R	122	VAL	4.7
1	H	190	LYS	4.7
1	W	188	GLY	4.7
1	B	15	THR	4.7
1	Q	122	VAL	4.7
1	Q	189	LEU	4.7
1	a	189	LEU	4.6
1	K	166	PHE	4.6
1	F	187	ASP	4.6
1	L	15	THR	4.6
1	b	14	LEU	4.6
1	C	187	ASP	4.5
1	J	16	GLN	4.5
1	K	16	GLN	4.5
1	Q	187	ASP	4.5
1	G	190	LYS	4.5
1	W	122	VAL	4.5
1	Y	189	LEU	4.4
1	a	187	ASP	4.4
1	W	16	GLN	4.4
1	M	16	GLN	4.3
1	Y	166	PHE	4.3
1	G	189	LEU	4.3
1	O	188	GLY	4.3
1	P	187	ASP	4.2
1	S	166	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	Q	15	THR	4.2
1	W	166	PHE	4.2
1	E	166	PHE	4.1
1	X	16	GLN	4.1
1	E	187	ASP	4.1
1	M	15	THR	4.1
1	K	188	GLY	4.1
1	L	122	VAL	4.1
1	V	16	GLN	4.1
1	F	122	VAL	4.1
1	U	187	ASP	4.0
1	E	190	LYS	4.0
1	R	189	LEU	4.0
1	C	122	VAL	4.0
1	R	16	GLN	4.0
1	G	188	GLY	4.0
1	O	190	LYS	4.0
1	U	189	LEU	4.0
1	T	122	VAL	4.0
1	M	166	PHE	4.0
1	a	156	GLU	4.0
1	b	122	VAL	4.0
1	F	14	LEU	3.9
1	U	190	LYS	3.9
1	A	122	VAL	3.9
1	X	122	VAL	3.9
1	K	131	ILE	3.9
1	D	166	PHE	3.9
1	N	122	VAL	3.8
1	I	187	ASP	3.8
1	H	189	LEU	3.7
1	a	16	GLN	3.7
1	G	17	LYS	3.7
1	W	189	LEU	3.7
1	X	15	THR	3.6
1	C	16	GLN	3.6
1	V	166	PHE	3.6
1	A	121	GLY	3.6
1	T	15	THR	3.6
1	H	187	ASP	3.6
1	I	121	GLY	3.5
1	A	16	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	U	16	GLN	3.5
1	K	189	LEU	3.5
1	E	122	VAL	3.5
1	O	189	LEU	3.5
1	J	187	ASP	3.5
1	M	187	ASP	3.5
1	a	166	PHE	3.5
1	G	15	THR	3.4
1	P	189	LEU	3.4
1	N	187	ASP	3.4
1	X	190	LYS	3.4
1	Q	166	PHE	3.4
1	G	166	PHE	3.4
1	J	189	LEU	3.4
1	F	50	ASN	3.3
1	b	187	ASP	3.3
1	I	166	PHE	3.3
1	Y	122	VAL	3.3
1	P	166	PHE	3.3
1	L	20	ASP	3.2
1	X	189	LEU	3.2
1	C	120	GLY	3.2
1	C	19	ILE	3.2
1	E	16	GLN	3.2
1	J	166	PHE	3.2
1	E	156	GLU	3.2
1	R	187	ASP	3.2
1	F	16	GLN	3.2
1	O	20	ASP	3.1
1	Z	187	ASP	3.1
1	a	190	LYS	3.1
1	X	78	LYS	3.1
1	B	131	ILE	3.1
1	B	187	ASP	3.1
1	H	17	LYS	3.1
1	T	16	GLN	3.1
1	N	166	PHE	3.1
1	b	50	ASN	3.1
1	V	20	ASP	3.1
1	T	189	LEU	3.0
1	Z	166	PHE	3.0
1	R	15	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	121	GLY	3.0
1	G	187	ASP	3.0
1	V	187	ASP	3.0
1	N	17	LYS	3.0
1	a	122	VAL	3.0
1	X	121	GLY	2.9
1	A	166	PHE	2.9
1	O	166	PHE	2.9
1	G	16	GLN	2.9
1	O	121	GLY	2.9
1	W	17	LYS	2.9
1	E	78	LYS	2.8
1	V	17	LYS	2.8
1	L	187	ASP	2.8
1	B	166	PHE	2.8
1	M	17	LYS	2.8
1	A	188	GLY	2.8
1	N	50	ASN	2.8
1	T	166	PHE	2.8
1	T	190	LYS	2.8
1	H	188	GLY	2.8
1	F	189	LEU	2.7
1	F	156	GLU	2.7
1	S	187	ASP	2.7
1	B	121	GLY	2.7
1	D	120	GLY	2.7
1	L	166	PHE	2.7
1	F	15	THR	2.7
1	D	20	ASP	2.7
1	U	121	GLY	2.7
1	U	156	GLU	2.7
1	G	156	GLU	2.7
1	G	18	LEU	2.7
1	Y	131	ILE	2.7
1	P	20	ASP	2.7
1	Y	120	GLY	2.7
1	E	17	LYS	2.6
1	S	13	ILE	2.6
1	U	17	LYS	2.6
1	U	166	PHE	2.6
1	I	20	ASP	2.6
1	C	78	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	Y	164	ARG	2.6
1	R	166	PHE	2.6
1	N	189	LEU	2.6
1	P	122	VAL	2.6
1	W	187	ASP	2.6
1	M	13	ILE	2.6
1	b	131	ILE	2.6
1	b	190	LYS	2.5
1	O	156	GLU	2.5
1	W	156	GLU	2.5
1	C	164	ARG	2.5
1	C	155	TYR	2.5
1	X	187	ASP	2.5
1	D	165	ASN	2.5
1	b	16	GLN	2.5
1	X	166	PHE	2.5
1	V	121	GLY	2.5
1	Y	78	LYS	2.5
1	O	122	VAL	2.5
1	O	131	ILE	2.5
1	X	156	GLU	2.5
1	Q	17	LYS	2.5
1	b	166	PHE	2.4
1	P	156	GLU	2.4
1	F	131	ILE	2.4
1	M	156	GLU	2.4
1	E	20	ASP	2.4
1	V	156	GLU	2.4
1	Z	165	ASN	2.4
1	H	166	PHE	2.4
1	U	188	GLY	2.4
1	I	17	LYS	2.4
1	J	156	GLU	2.4
1	Q	156	GLU	2.4
1	Z	17	LYS	2.4
1	I	156	GLU	2.4
1	V	78	LYS	2.4
1	J	101	GLU	2.3
1	V	45	LEU	2.3
1	J	122	VAL	2.3
1	A	50	ASN	2.3
1	H	20	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	b	18	LEU	2.3
1	N	48	ILE	2.3
1	K	20	ASP	2.3
1	I	189	LEU	2.3
1	Q	20	ASP	2.3
1	S	20	ASP	2.3
1	b	20	ASP	2.3
1	Q	131	ILE	2.3
1	T	17	LYS	2.3
1	a	17	LYS	2.3
1	C	156	GLU	2.2
1	G	78	LYS	2.2
1	N	131	ILE	2.2
1	F	121	GLY	2.2
1	K	17	LYS	2.2
1	H	16	GLN	2.2
1	O	45	LEU	2.2
1	L	156	GLU	2.2
1	N	190	LYS	2.2
1	N	16	GLN	2.2
1	W	20	ASP	2.2
1	B	50	ASN	2.2
1	Y	155	TYR	2.2
1	F	120	GLY	2.2
1	T	121	GLY	2.2
1	O	50	ASN	2.2
1	T	50	ASN	2.2
1	F	18	LEU	2.2
1	R	20	ASP	2.1
1	Y	20	ASP	2.1
1	A	187	ASP	2.1
1	Z	20	ASP	2.1
1	N	121	GLY	2.1
1	T	120	GLY	2.1
1	H	121	GLY	2.1
1	J	184	GLU	2.1
1	W	149	GLU	2.1
1	J	45	LEU	2.1
1	S	165	ASN	2.1
1	X	18	LEU	2.1
1	B	189	LEU	2.0
1	M	121	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLU	2.0
1	C	160	LYS	2.0
1	J	50	ASN	2.0
1	a	165	ASN	2.0
1	H	19	ILE	2.0
1	L	19	ILE	2.0
1	I	103	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.