Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 06:38 PM BST

PDB ID	:	6TTY
Title	:	Structure of ClpP from Staphylococcus aureus (apo, closed state)
Authors	:	Malik, I.T.; Pereira, R.; Vielberg, M.-T.; Mayer, C.; Straetener, J.; Thomy, D.; Famulla, K.; Castro, H.C.; Sass, P.; Groll, M.; Broetz-Oesterheldt, H.
Deposited on	:	2019-12-30
Resolution	:	1.90 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
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:

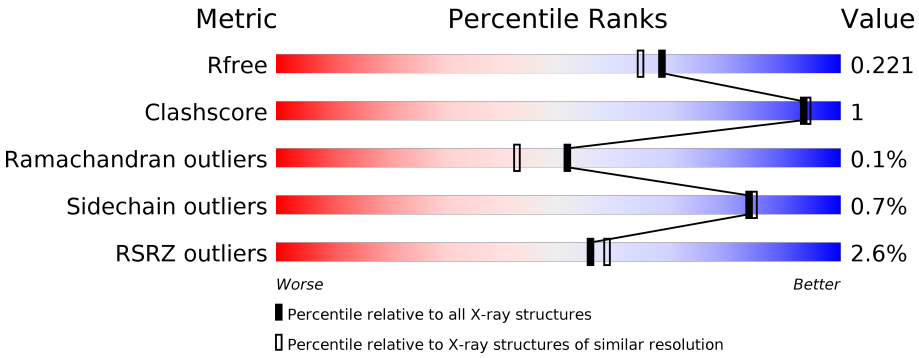
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	92% · 6%
1	B	203	2% 92% · 6%
1	C	203	2% 85% 7% 8%
1	D	203	4% 91% · 6%
1	E	203	90% · 6%
1	F	203	2% 91% · 6%

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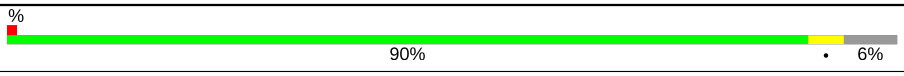
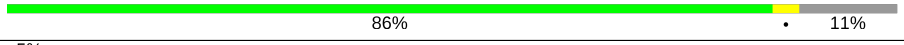
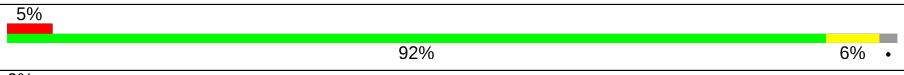
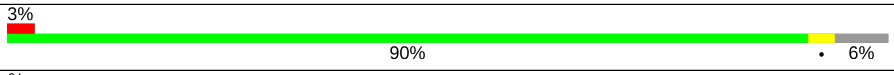
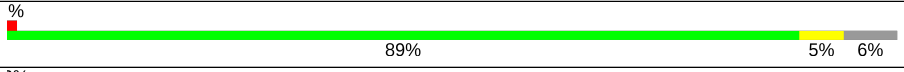
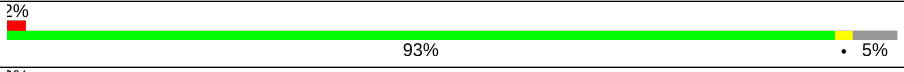
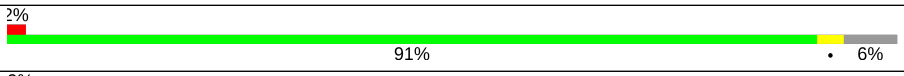
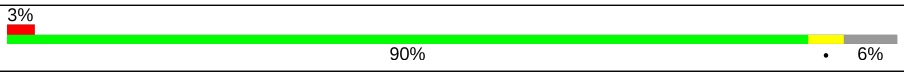
Mol	Chain	Length	Quality of chain
1	G	203	
1	H	203	
1	I	203	
1	J	203	
1	K	203	
1	L	203	
1	M	203	
1	N	203	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22646 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	191	Total	C	N	O	S	0	1	0
			1483	931	255	290	7			
1	B	191	Total	C	N	O	S	0	1	0
			1480	930	254	289	7			
1	C	187	Total	C	N	O	S	0	1	0
			1444	910	246	282	6			
1	D	191	Total	C	N	O	S	0	1	0
			1478	928	254	290	6			
1	E	190	Total	C	N	O	S	0	0	0
			1467	922	252	287	6			
1	F	191	Total	C	N	O	S	0	1	0
			1481	935	249	290	7			
1	G	191	Total	C	N	O	S	0	1	0
			1478	928	254	290	6			
1	H	181	Total	C	N	O	S	0	1	0
			1400	884	236	274	6			
1	I	199	Total	C	N	O	S	0	3	0
			1564	984	267	306	7			
1	J	190	Total	C	N	O	S	0	2	0
			1475	928	252	288	7			
1	K	190	Total	C	N	O	S	0	2	0
			1476	928	252	290	6			
1	L	193	Total	C	N	O	S	0	1	0
			1502	948	256	292	6			
1	M	190	Total	C	N	O	S	0	0	0
			1467	922	252	287	6			
1	N	191	Total	C	N	O	S	0	1	0
			1478	928	254	290	6			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	TRP	-	expression tag	UNP A0A077UUA2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	SER	-	expression tag	UNP A0A077UUA2
A	198	HIS	-	expression tag	UNP A0A077UUA2
A	199	PRO	-	expression tag	UNP A0A077UUA2
A	200	GLN	-	expression tag	UNP A0A077UUA2
A	201	PHE	-	expression tag	UNP A0A077UUA2
A	202	GLU	-	expression tag	UNP A0A077UUA2
A	203	LYS	-	expression tag	UNP A0A077UUA2
B	196	TRP	-	expression tag	UNP A0A077UUA2
B	197	SER	-	expression tag	UNP A0A077UUA2
B	198	HIS	-	expression tag	UNP A0A077UUA2
B	199	PRO	-	expression tag	UNP A0A077UUA2
B	200	GLN	-	expression tag	UNP A0A077UUA2
B	201	PHE	-	expression tag	UNP A0A077UUA2
B	202	GLU	-	expression tag	UNP A0A077UUA2
B	203	LYS	-	expression tag	UNP A0A077UUA2
C	196	TRP	-	expression tag	UNP A0A077UUA2
C	197	SER	-	expression tag	UNP A0A077UUA2
C	198	HIS	-	expression tag	UNP A0A077UUA2
C	199	PRO	-	expression tag	UNP A0A077UUA2
C	200	GLN	-	expression tag	UNP A0A077UUA2
C	201	PHE	-	expression tag	UNP A0A077UUA2
C	202	GLU	-	expression tag	UNP A0A077UUA2
C	203	LYS	-	expression tag	UNP A0A077UUA2
D	196	TRP	-	expression tag	UNP A0A077UUA2
D	197	SER	-	expression tag	UNP A0A077UUA2
D	198	HIS	-	expression tag	UNP A0A077UUA2
D	199	PRO	-	expression tag	UNP A0A077UUA2
D	200	GLN	-	expression tag	UNP A0A077UUA2
D	201	PHE	-	expression tag	UNP A0A077UUA2
D	202	GLU	-	expression tag	UNP A0A077UUA2
D	203	LYS	-	expression tag	UNP A0A077UUA2
E	196	TRP	-	expression tag	UNP A0A077UUA2
E	197	SER	-	expression tag	UNP A0A077UUA2
E	198	HIS	-	expression tag	UNP A0A077UUA2
E	199	PRO	-	expression tag	UNP A0A077UUA2
E	200	GLN	-	expression tag	UNP A0A077UUA2
E	201	PHE	-	expression tag	UNP A0A077UUA2
E	202	GLU	-	expression tag	UNP A0A077UUA2
E	203	LYS	-	expression tag	UNP A0A077UUA2
F	196	TRP	-	expression tag	UNP A0A077UUA2
F	197	SER	-	expression tag	UNP A0A077UUA2
F	198	HIS	-	expression tag	UNP A0A077UUA2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	199	PRO	-	expression tag	UNP A0A077UUA2
F	200	GLN	-	expression tag	UNP A0A077UUA2
F	201	PHE	-	expression tag	UNP A0A077UUA2
F	202	GLU	-	expression tag	UNP A0A077UUA2
F	203	LYS	-	expression tag	UNP A0A077UUA2
G	196	TRP	-	expression tag	UNP A0A077UUA2
G	197	SER	-	expression tag	UNP A0A077UUA2
G	198	HIS	-	expression tag	UNP A0A077UUA2
G	199	PRO	-	expression tag	UNP A0A077UUA2
G	200	GLN	-	expression tag	UNP A0A077UUA2
G	201	PHE	-	expression tag	UNP A0A077UUA2
G	202	GLU	-	expression tag	UNP A0A077UUA2
G	203	LYS	-	expression tag	UNP A0A077UUA2
H	196	TRP	-	expression tag	UNP A0A077UUA2
H	197	SER	-	expression tag	UNP A0A077UUA2
H	198	HIS	-	expression tag	UNP A0A077UUA2
H	199	PRO	-	expression tag	UNP A0A077UUA2
H	200	GLN	-	expression tag	UNP A0A077UUA2
H	201	PHE	-	expression tag	UNP A0A077UUA2
H	202	GLU	-	expression tag	UNP A0A077UUA2
H	203	LYS	-	expression tag	UNP A0A077UUA2
I	196	TRP	-	expression tag	UNP A0A077UUA2
I	197	SER	-	expression tag	UNP A0A077UUA2
I	198	HIS	-	expression tag	UNP A0A077UUA2
I	199	PRO	-	expression tag	UNP A0A077UUA2
I	200	GLN	-	expression tag	UNP A0A077UUA2
I	201	PHE	-	expression tag	UNP A0A077UUA2
I	202	GLU	-	expression tag	UNP A0A077UUA2
I	203	LYS	-	expression tag	UNP A0A077UUA2
J	196	TRP	-	expression tag	UNP A0A077UUA2
J	197	SER	-	expression tag	UNP A0A077UUA2
J	198	HIS	-	expression tag	UNP A0A077UUA2
J	199	PRO	-	expression tag	UNP A0A077UUA2
J	200	GLN	-	expression tag	UNP A0A077UUA2
J	201	PHE	-	expression tag	UNP A0A077UUA2
J	202	GLU	-	expression tag	UNP A0A077UUA2
J	203	LYS	-	expression tag	UNP A0A077UUA2
K	196	TRP	-	expression tag	UNP A0A077UUA2
K	197	SER	-	expression tag	UNP A0A077UUA2
K	198	HIS	-	expression tag	UNP A0A077UUA2
K	199	PRO	-	expression tag	UNP A0A077UUA2
K	200	GLN	-	expression tag	UNP A0A077UUA2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	201	PHE	-	expression tag	UNP A0A077UUA2
K	202	GLU	-	expression tag	UNP A0A077UUA2
K	203	LYS	-	expression tag	UNP A0A077UUA2
L	196	TRP	-	expression tag	UNP A0A077UUA2
L	197	SER	-	expression tag	UNP A0A077UUA2
L	198	HIS	-	expression tag	UNP A0A077UUA2
L	199	PRO	-	expression tag	UNP A0A077UUA2
L	200	GLN	-	expression tag	UNP A0A077UUA2
L	201	PHE	-	expression tag	UNP A0A077UUA2
L	202	GLU	-	expression tag	UNP A0A077UUA2
L	203	LYS	-	expression tag	UNP A0A077UUA2
M	196	TRP	-	expression tag	UNP A0A077UUA2
M	197	SER	-	expression tag	UNP A0A077UUA2
M	198	HIS	-	expression tag	UNP A0A077UUA2
M	199	PRO	-	expression tag	UNP A0A077UUA2
M	200	GLN	-	expression tag	UNP A0A077UUA2
M	201	PHE	-	expression tag	UNP A0A077UUA2
M	202	GLU	-	expression tag	UNP A0A077UUA2
M	203	LYS	-	expression tag	UNP A0A077UUA2
N	196	TRP	-	expression tag	UNP A0A077UUA2
N	197	SER	-	expression tag	UNP A0A077UUA2
N	198	HIS	-	expression tag	UNP A0A077UUA2
N	199	PRO	-	expression tag	UNP A0A077UUA2
N	200	GLN	-	expression tag	UNP A0A077UUA2
N	201	PHE	-	expression tag	UNP A0A077UUA2
N	202	GLU	-	expression tag	UNP A0A077UUA2
N	203	LYS	-	expression tag	UNP A0A077UUA2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	145	Total 145	O 145	0	0
2	B	138	Total 138	O 138	0	0
2	C	134	Total 134	O 134	0	0
2	D	140	Total 140	O 140	0	0
2	E	138	Total 138	O 138	0	0
2	F	139	Total 139	O 139	0	0

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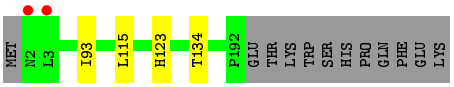
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	145	Total O 145 145	0	0
2	H	145	Total O 145 145	0	0
2	I	138	Total O 138 138	0	0
2	J	123	Total O 123 123	0	0
2	K	142	Total O 142 142	0	0
2	L	164	Total O 164 164	0	0
2	M	131	Total O 131 131	0	0
2	N	151	Total O 151 151	0	0

3 Residue-property plots (i)

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

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:

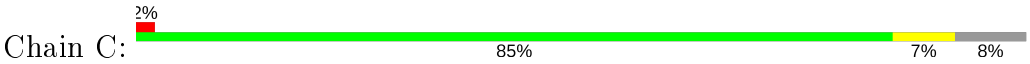


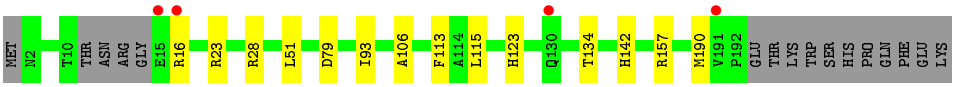
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:

- Molecule 1: ATP-dependent Clp protease proteolytic subunit

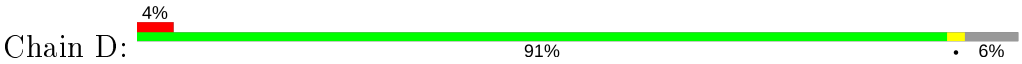
Chain C:

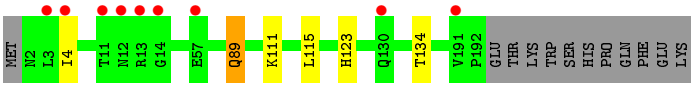




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

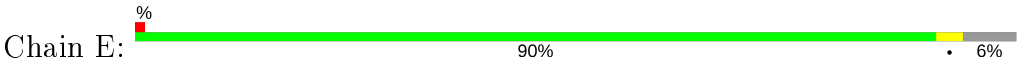
Chain D:





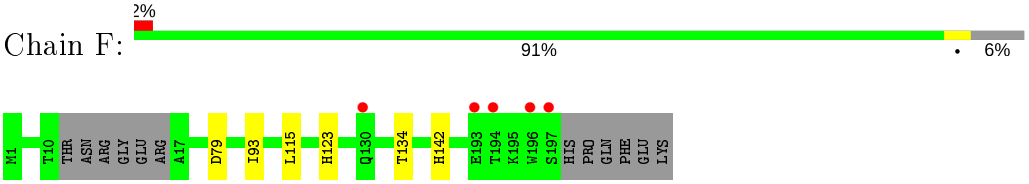
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



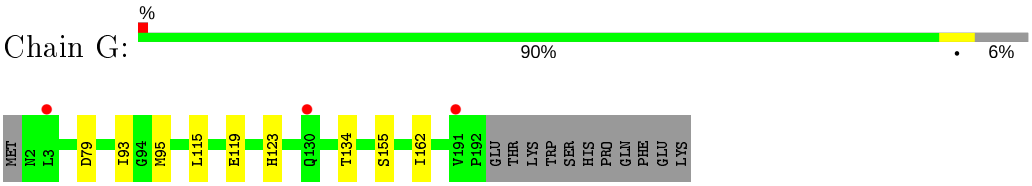
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



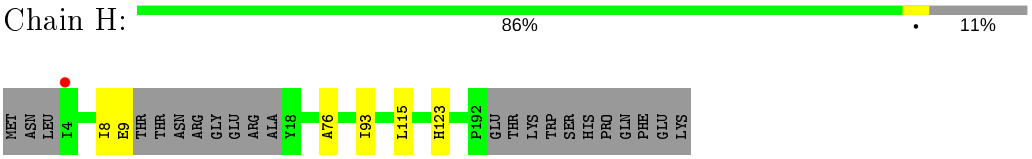
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



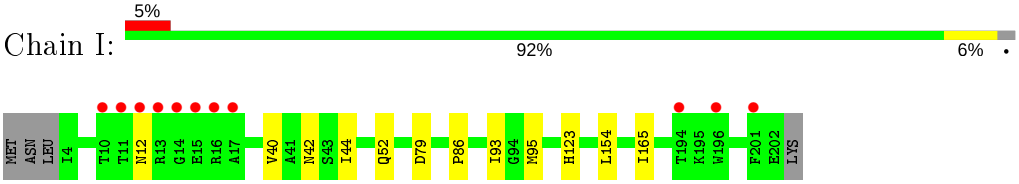
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



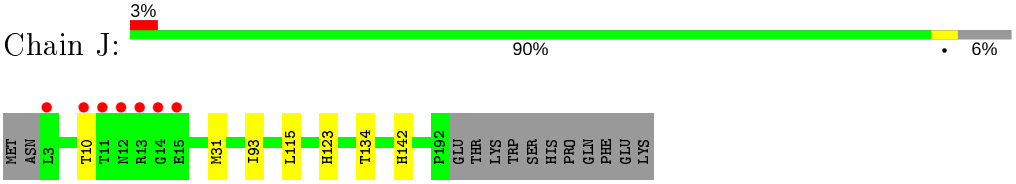
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



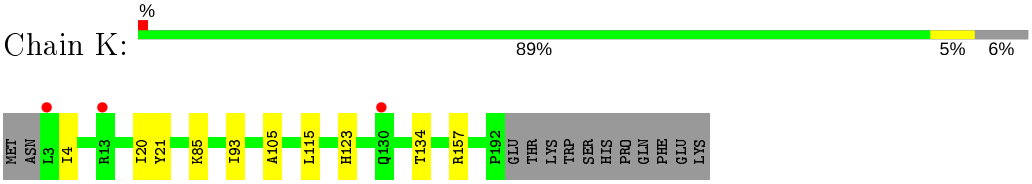
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



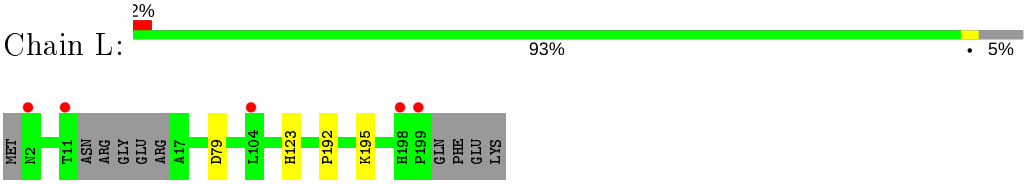
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



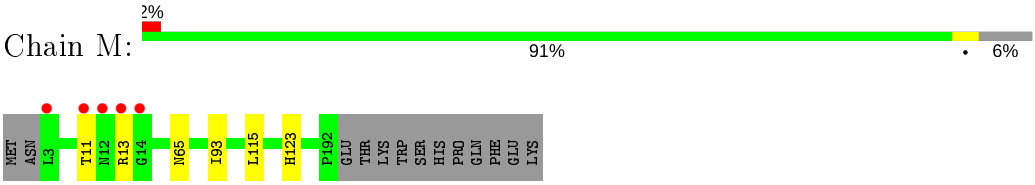
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



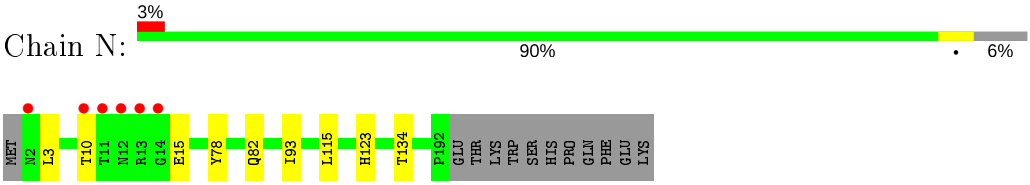
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	95.19Å 99.25Å 107.47Å 105.22° 101.27° 117.70°	Depositor
Resolution (Å)	30.00 – 1.90 29.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.4 (30.00-1.90) 87.5 (29.73-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.173 , 0.217 0.174 , 0.221	Depositor DCC
R_{free} test set	10750 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22646	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.51	0/1502	0.62	0/2028
1	B	0.53	0/1502	0.64	0/2028
1	C	0.47	0/1465	0.60	0/1978
1	D	0.51	0/1500	0.62	0/2026
1	E	0.51	0/1486	0.63	0/2007
1	F	0.51	0/1504	0.61	0/2031
1	G	0.54	0/1500	0.63	0/2026
1	H	0.49	0/1421	0.60	0/1918
1	I	0.49	0/1594	0.61	0/2153
1	J	0.50	0/1500	0.61	0/2025
1	K	0.50	0/1501	0.64	0/2027
1	L	0.48	0/1527	0.62	0/2064
1	M	0.48	0/1486	0.63	0/2007
1	N	0.50	0/1500	0.62	0/2026
All	All	0.50	0/20988	0.62	0/28344

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1483	0	1499	3	0
1	B	1480	0	1500	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1444	0	1462	10	0
1	D	1478	0	1496	5	0
1	E	1467	0	1485	3	0
1	F	1481	0	1500	4	0
1	G	1478	0	1496	8	0
1	H	1400	0	1418	3	0
1	I	1564	0	1570	7	0
1	J	1475	0	1499	7	0
1	K	1476	0	1496	6	0
1	L	1502	0	1517	3	0
1	M	1467	0	1485	4	0
1	N	1478	0	1496	4	0
2	A	145	0	0	1	0
2	B	138	0	0	1	0
2	C	134	0	0	1	0
2	D	140	0	0	1	0
2	E	138	0	0	1	0
2	F	139	0	0	0	0
2	G	145	0	0	1	0
2	H	145	0	0	1	0
2	I	138	0	0	4	0
2	J	123	0	0	1	0
2	K	142	0	0	1	0
2	L	164	0	0	1	0
2	M	131	0	0	1	0
2	N	151	0	0	1	0
All	All	22646	0	20919	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:GLN:HG3	1:D:111:LYS:HB3	1.53	0.91
1:H:93:ILE:HG22	1:H:115:LEU:HD12	1.64	0.79
1:M:93:ILE:HG22	1:M:115:LEU:HD12	1.68	0.74
1:G:134:THR:HG21	2:L:302:HOH:O	1.88	0.72
1:J:10:THR:HG23	1:J:10:THR:O	1.89	0.71
1:G:95:MET:HG3	2:G:385:HOH:O	1.96	0.66
1:C:79:ASP:HB3	1:D:115:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:ILE:HG22	1:G:115:LEU:HD12	1.78	0.65
1:I:95[A]:MET:SD	2:I:302:HOH:O	2.56	0.63
1:F:93:ILE:HG22	1:F:115:LEU:HD12	1.80	0.62
1:G:155:SER:CB	1:G:162:ILE:HD12	2.30	0.62
1:F:134:THR:HG21	2:M:301:HOH:O	2.00	0.61
1:A:134:THR:HG21	2:K:302:HOH:O	2.00	0.60
1:E:93:ILE:HG22	1:E:115:LEU:HD12	1.84	0.59
1:I:79:ASP:HB3	1:J:115:LEU:HD13	1.89	0.55
2:B:302:HOH:O	1:J:134:THR:HG21	2.06	0.54
1:J:10:THR:CG2	1:J:10:THR:O	2.53	0.54
2:A:305:HOH:O	1:K:134:THR:HG21	2.08	0.54
1:B:93:ILE:HG22	1:B:115:LEU:HD12	1.89	0.54
1:C:134:THR:HG21	2:I:306:HOH:O	2.08	0.53
2:I:403:HOH:O	1:J:31:MET:HB3	2.07	0.53
1:K:93:ILE:HG22	1:K:115:LEU:HD12	1.91	0.52
1:E:134:THR:HG21	2:N:315:HOH:O	2.10	0.52
1:J:93:ILE:HG22	1:J:115:LEU:HD12	1.92	0.51
1:L:192:PRO:O	1:L:195:LYS:HB2	2.10	0.51
1:A:93:ILE:HG22	1:A:115:LEU:HD12	1.93	0.51
1:D:134:THR:HG23	2:D:301:HOH:O	2.10	0.50
2:E:303:HOH:O	1:N:134:THR:HG21	2.14	0.48
1:H:8:ILE:HG22	1:H:9:GLU:HG3	1.95	0.48
1:I:42:ASN:HB3	2:I:403:HOH:O	2.12	0.48
1:N:93:ILE:HG22	1:N:115:LEU:HD12	1.96	0.48
1:C:93:ILE:HG22	1:C:115:LEU:HD12	1.96	0.47
1:L:79:ASP:HB3	1:M:115:LEU:HD13	1.96	0.47
1:G:155:SER:HB2	1:G:162:ILE:HD12	1.97	0.47
1:F:79:ASP:HB3	1:G:115:LEU:HD13	1.96	0.47
1:I:52:GLN:HG3	1:I:86:PRO:HD3	1.97	0.46
1:H:76:ALA:HB1	1:I:93:ILE:HD12	1.96	0.46
1:N:10:THR:HG22	1:N:15:GLU:HB3	1.97	0.46
1:N:78:TYR:O	1:N:82:GLN:HG2	2.16	0.45
1:B:50:PHE:CE1	1:C:23:ARG:HG2	2.52	0.45
1:D:134:THR:HG21	2:H:302:HOH:O	2.16	0.45
1:C:142:HIS:HD2	2:C:414:HOH:O	2.00	0.44
1:I:154:LEU:HD23	1:I:165:ILE:HD12	2.00	0.44
1:K:105:ALA:O	1:K:157:ARG:HD2	2.17	0.43
1:F:142:HIS:HE1	1:G:119:GLU:OE1	2.01	0.43
1:J:142:HIS:HD2	2:J:415:HOH:O	2.00	0.43
1:B:79:ASP:HB3	1:C:115:LEU:HD13	2.01	0.42
1:I:40:VAL:O	1:I:44:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:ASN:HB2	1:M:93:ILE:HG13	2.01	0.41
1:E:56:SER:HB2	1:E:85:LYS:HD2	2.01	0.41
1:C:16:ARG:NH2	1:D:4:ILE:O	2.44	0.41
1:K:4:ILE:HD12	1:K:21:TYR:HE2	1.85	0.41
1:C:28:ARG:HG2	1:C:51:LEU:HD22	2.02	0.41
1:C:106:ALA:HA	1:C:157:ARG:HD2	2.03	0.41
1:K:85:LYS:HA	1:L:195:LYS:HD3	2.03	0.41
1:A:115:LEU:HD13	1:G:79:ASP:HB3	2.03	0.41
1:C:113:PHE:HB3	1:C:190:MET:HG3	2.03	0.40
1:K:4:ILE:CG2	1:K:20:ILE:HG22	2.52	0.40
1:M:11:THR:HG23	1:M:13:ARG:H	1.87	0.40

There are no symmetry-related clashes.

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	190/203 (94%)	188 (99%)	2 (1%)	0	100	100
1	B	190/203 (94%)	187 (98%)	3 (2%)	0	100	100
1	C	184/203 (91%)	180 (98%)	4 (2%)	0	100	100
1	D	190/203 (94%)	186 (98%)	4 (2%)	0	100	100
1	E	188/203 (93%)	186 (99%)	2 (1%)	0	100	100
1	F	188/203 (93%)	184 (98%)	4 (2%)	0	100	100
1	G	190/203 (94%)	186 (98%)	4 (2%)	0	100	100
1	H	178/203 (88%)	173 (97%)	5 (3%)	0	100	100
1	I	200/203 (98%)	196 (98%)	3 (2%)	1 (0%)	29	18
1	J	190/203 (94%)	185 (97%)	5 (3%)	0	100	100
1	K	190/203 (94%)	185 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	190/203 (94%)	186 (98%)	4 (2%)	0	100 100
1	M	188/203 (93%)	186 (99%)	2 (1%)	0	100 100
1	N	190/203 (94%)	183 (96%)	6 (3%)	1 (0%)	29 18
All	All	2646/2842 (93%)	2591 (98%)	53 (2%)	2 (0%)	51 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	12	ASN
1	N	3	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	160/171 (94%)	159 (99%)	1 (1%)	86 87
1	B	160/171 (94%)	159 (99%)	1 (1%)	86 87
1	C	156/171 (91%)	155 (99%)	1 (1%)	86 87
1	D	160/171 (94%)	158 (99%)	2 (1%)	69 68
1	E	158/171 (92%)	156 (99%)	2 (1%)	69 68
1	F	161/171 (94%)	160 (99%)	1 (1%)	86 87
1	G	160/171 (94%)	159 (99%)	1 (1%)	86 87
1	H	152/171 (89%)	151 (99%)	1 (1%)	84 84
1	I	170/171 (99%)	169 (99%)	1 (1%)	86 87
1	J	160/171 (94%)	159 (99%)	1 (1%)	86 87
1	K	160/171 (94%)	159 (99%)	1 (1%)	86 87
1	L	163/171 (95%)	162 (99%)	1 (1%)	86 87
1	M	158/171 (92%)	157 (99%)	1 (1%)	86 87
1	N	160/171 (94%)	159 (99%)	1 (1%)	86 87
All	All	2238/2394 (94%)	2222 (99%)	16 (1%)	84 84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	B	123	HIS
1	C	123	HIS
1	D	89	GLN
1	D	123	HIS
1	E	39	ASN
1	E	123	HIS
1	F	123	HIS
1	G	123	HIS
1	H	123	HIS
1	I	123	HIS
1	J	123	HIS
1	K	123	HIS
1	L	123	HIS
1	M	123	HIS
1	N	123	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	191/203 (94%)	-0.23	2 (1%)	82	84	17, 24, 37, 44	0
1	B	191/203 (94%)	-0.23	5 (2%)	56	58	17, 24, 36, 45	0
1	C	187/203 (92%)	-0.19	4 (2%)	63	66	19, 25, 38, 48	0
1	D	191/203 (94%)	-0.21	9 (4%)	31	34	19, 24, 44, 68	0
1	E	190/203 (93%)	-0.33	2 (1%)	80	82	17, 24, 34, 45	0
1	F	191/203 (94%)	-0.27	5 (2%)	56	58	18, 24, 37, 64	0
1	G	191/203 (94%)	-0.31	3 (1%)	72	74	19, 24, 35, 47	0
1	H	181/203 (89%)	-0.41	1 (0%)	89	90	16, 22, 33, 44	0
1	I	199/203 (98%)	-0.06	11 (5%)	25	28	17, 24, 52, 97	0
1	J	190/203 (93%)	-0.04	7 (3%)	41	44	18, 25, 44, 91	0
1	K	190/203 (93%)	-0.38	3 (1%)	72	74	18, 24, 37, 59	0
1	L	193/203 (95%)	-0.15	5 (2%)	56	58	19, 24, 37, 56	0
1	M	190/203 (93%)	-0.11	5 (2%)	56	58	19, 25, 43, 83	0
1	N	191/203 (94%)	-0.03	6 (3%)	49	51	18, 25, 49, 95	0
All	All	2666/2842 (93%)	-0.21	68 (2%)	56	58	16, 24, 40, 97	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	11	THR	10.0
1	N	2	ASN	8.4
1	J	13	ARG	8.3
1	I	13	ARG	8.0
1	N	11	THR	7.7
1	J	10	THR	7.6
1	J	12	ASN	7.3
1	I	11	THR	7.0

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Mol	Chain	Res	Type	RSRZ
1	M	13	ARG	6.5
1	M	12	ASN	6.5
1	N	12	ASN	5.7
1	N	13	ARG	5.6
1	L	2	ASN	5.3
1	J	3	LEU	5.0
1	J	14	GLY	5.0
1	B	2	ASN	4.8
1	I	12	ASN	4.8
1	L	11	THR	4.5
1	N	14	GLY	4.4
1	D	12	ASN	4.3
1	M	11	THR	4.2
1	H	4	ILE	4.2
1	M	14	GLY	4.2
1	E	3	LEU	4.1
1	K	3	LEU	4.1
1	I	14	GLY	3.9
1	K	13	ARG	3.9
1	D	14	GLY	3.9
1	D	3	LEU	3.8
1	J	15	GLU	3.7
1	I	201	PHE	3.6
1	L	199	PRO	3.5
1	E	191	VAL	3.3
1	C	15	GLU	3.0
1	F	193	GLU	3.0
1	I	10	THR	3.0
1	N	10	THR	2.9
1	F	196	TRP	2.8
1	A	2	ASN	2.8
1	I	16	ARG	2.8
1	I	15	GLU	2.8
1	D	11	THR	2.7
1	C	16	ARG	2.7
1	B	3	LEU	2.7
1	D	13	ARG	2.6
1	G	3	LEU	2.6
1	F	194	THR	2.6
1	C	130	GLN	2.5
1	D	130	GLN	2.4
1	D	191	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	197	SER	2.3
1	B	102	PHE	2.3
1	A	3	LEU	2.3
1	I	194	THR	2.3
1	I	17	ALA	2.2
1	C	191	VAL	2.2
1	L	104	LEU	2.1
1	B	105	ALA	2.1
1	D	4	ILE	2.1
1	F	130	GLN	2.1
1	K	130	GLN	2.1
1	M	3	LEU	2.1
1	G	130	GLN	2.0
1	I	196	TRP	2.0
1	L	198	HIS	2.0
1	G	191	VAL	2.0
1	D	57	GLU	2.0
1	B	104	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.