



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:29 am GMT

PDB ID : 1Y7O
Title : The structure of Streptococcus pneumoniae A153P ClpP
Authors : Kimber, M.S.; Gribun, A.; Ching, R.; Sprangers, R.; Fiebig, K.M.; Houry, W.A.
Deposited on : 2004-12-09
Resolution : 2.51 Å(reported)

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

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

A user guide is available at

<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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

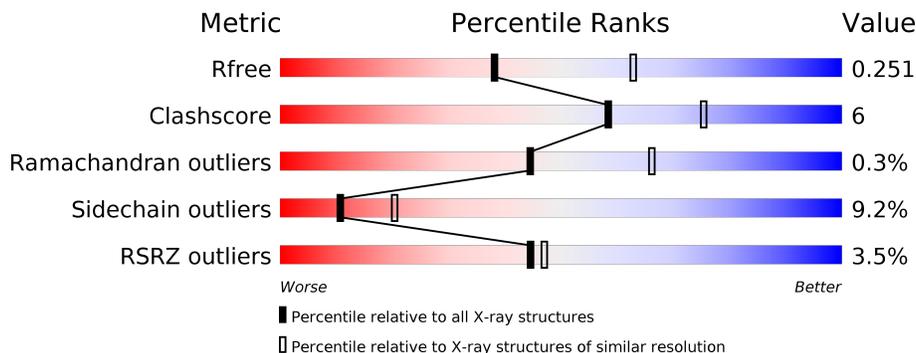
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	218	
1	B	218	
1	C	218	
1	D	218	
1	E	218	
1	F	218	

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Mol	Chain	Length	Quality of chain
1	G	218	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	C	1006	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9601 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
			Total	C	N	O	Se			
1	A	171	1315	828	217	258	12	0	0	0
1	B	178	1373	862	228	270	1	12	0	0
1	C	176	1357	853	226	265	1	12	0	0
1	D	178	1371	859	228	271	1	12	0	0
1	E	174	1340	842	223	262	1	12	0	0
1	F	173	1328	837	219	259	1	12	0	0
1	G	177	1365	857	227	269	12	0	0	0

There are 245 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP P63788
A	-18	GLY	-	CLONING ARTIFACT	UNP P63788
A	-17	SER	-	CLONING ARTIFACT	UNP P63788
A	-16	SER	-	CLONING ARTIFACT	UNP P63788
A	-15	HIS	-	CLONING ARTIFACT	UNP P63788
A	-14	HIS	-	CLONING ARTIFACT	UNP P63788
A	-13	HIS	-	CLONING ARTIFACT	UNP P63788
A	-12	HIS	-	CLONING ARTIFACT	UNP P63788
A	-11	HIS	-	CLONING ARTIFACT	UNP P63788
A	-10	HIS	-	CLONING ARTIFACT	UNP P63788
A	-9	SER	-	CLONING ARTIFACT	UNP P63788
A	-8	SER	-	CLONING ARTIFACT	UNP P63788
A	-7	GLY	-	CLONING ARTIFACT	UNP P63788
A	-6	LEU	-	CLONING ARTIFACT	UNP P63788
A	-5	VAL	-	CLONING ARTIFACT	UNP P63788

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	CLONING ARTIFACT	UNP P63788
A	-3	ARG	-	CLONING ARTIFACT	UNP P63788
A	-2	GLY	-	CLONING ARTIFACT	UNP P63788
A	-1	SER	-	CLONING ARTIFACT	UNP P63788
A	0	HIS	-	CLONING ARTIFACT	UNP P63788
A	29	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	38	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	79	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	91	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	93	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	97	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	112	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	119	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	124	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	140	PRO	ALA	ENGINEERED	UNP P63788
A	162	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	175	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	190	MSE	MET	MODIFIED RESIDUE	UNP P63788
A	197	GLY	-	CLONING ARTIFACT	UNP P63788
A	198	SER	-	CLONING ARTIFACT	UNP P63788
B	-19	MET	-	CLONING ARTIFACT	UNP P63788
B	-18	GLY	-	CLONING ARTIFACT	UNP P63788
B	-17	SER	-	CLONING ARTIFACT	UNP P63788
B	-16	SER	-	CLONING ARTIFACT	UNP P63788
B	-15	HIS	-	CLONING ARTIFACT	UNP P63788
B	-14	HIS	-	CLONING ARTIFACT	UNP P63788
B	-13	HIS	-	CLONING ARTIFACT	UNP P63788
B	-12	HIS	-	CLONING ARTIFACT	UNP P63788
B	-11	HIS	-	CLONING ARTIFACT	UNP P63788
B	-10	HIS	-	CLONING ARTIFACT	UNP P63788
B	-9	SER	-	CLONING ARTIFACT	UNP P63788
B	-8	SER	-	CLONING ARTIFACT	UNP P63788
B	-7	GLY	-	CLONING ARTIFACT	UNP P63788
B	-6	LEU	-	CLONING ARTIFACT	UNP P63788
B	-5	VAL	-	CLONING ARTIFACT	UNP P63788
B	-4	PRO	-	CLONING ARTIFACT	UNP P63788
B	-3	ARG	-	CLONING ARTIFACT	UNP P63788
B	-2	GLY	-	CLONING ARTIFACT	UNP P63788
B	-1	SER	-	CLONING ARTIFACT	UNP P63788
B	0	HIS	-	CLONING ARTIFACT	UNP P63788
B	29	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	38	MSE	MET	MODIFIED RESIDUE	UNP P63788

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Chain	Residue	Modelled	Actual	Comment	Reference
B	79	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	91	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	93	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	97	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	112	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	119	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	124	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	140	PRO	ALA	ENGINEERED	UNP P63788
B	162	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	175	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	190	MSE	MET	MODIFIED RESIDUE	UNP P63788
B	197	GLY	-	CLONING ARTIFACT	UNP P63788
B	198	SER	-	CLONING ARTIFACT	UNP P63788
C	-19	MET	-	CLONING ARTIFACT	UNP P63788
C	-18	GLY	-	CLONING ARTIFACT	UNP P63788
C	-17	SER	-	CLONING ARTIFACT	UNP P63788
C	-16	SER	-	CLONING ARTIFACT	UNP P63788
C	-15	HIS	-	CLONING ARTIFACT	UNP P63788
C	-14	HIS	-	CLONING ARTIFACT	UNP P63788
C	-13	HIS	-	CLONING ARTIFACT	UNP P63788
C	-12	HIS	-	CLONING ARTIFACT	UNP P63788
C	-11	HIS	-	CLONING ARTIFACT	UNP P63788
C	-10	HIS	-	CLONING ARTIFACT	UNP P63788
C	-9	SER	-	CLONING ARTIFACT	UNP P63788
C	-8	SER	-	CLONING ARTIFACT	UNP P63788
C	-7	GLY	-	CLONING ARTIFACT	UNP P63788
C	-6	LEU	-	CLONING ARTIFACT	UNP P63788
C	-5	VAL	-	CLONING ARTIFACT	UNP P63788
C	-4	PRO	-	CLONING ARTIFACT	UNP P63788
C	-3	ARG	-	CLONING ARTIFACT	UNP P63788
C	-2	GLY	-	CLONING ARTIFACT	UNP P63788
C	-1	SER	-	CLONING ARTIFACT	UNP P63788
C	0	HIS	-	CLONING ARTIFACT	UNP P63788
C	29	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	38	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	79	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	91	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	93	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	97	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	112	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	119	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	124	MSE	MET	MODIFIED RESIDUE	UNP P63788

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Chain	Residue	Modelled	Actual	Comment	Reference
C	140	PRO	ALA	ENGINEERED	UNP P63788
C	162	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	175	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	190	MSE	MET	MODIFIED RESIDUE	UNP P63788
C	197	GLY	-	CLONING ARTIFACT	UNP P63788
C	198	SER	-	CLONING ARTIFACT	UNP P63788
D	-19	MET	-	CLONING ARTIFACT	UNP P63788
D	-18	GLY	-	CLONING ARTIFACT	UNP P63788
D	-17	SER	-	CLONING ARTIFACT	UNP P63788
D	-16	SER	-	CLONING ARTIFACT	UNP P63788
D	-15	HIS	-	CLONING ARTIFACT	UNP P63788
D	-14	HIS	-	CLONING ARTIFACT	UNP P63788
D	-13	HIS	-	CLONING ARTIFACT	UNP P63788
D	-12	HIS	-	CLONING ARTIFACT	UNP P63788
D	-11	HIS	-	CLONING ARTIFACT	UNP P63788
D	-10	HIS	-	CLONING ARTIFACT	UNP P63788
D	-9	SER	-	CLONING ARTIFACT	UNP P63788
D	-8	SER	-	CLONING ARTIFACT	UNP P63788
D	-7	GLY	-	CLONING ARTIFACT	UNP P63788
D	-6	LEU	-	CLONING ARTIFACT	UNP P63788
D	-5	VAL	-	CLONING ARTIFACT	UNP P63788
D	-4	PRO	-	CLONING ARTIFACT	UNP P63788
D	-3	ARG	-	CLONING ARTIFACT	UNP P63788
D	-2	GLY	-	CLONING ARTIFACT	UNP P63788
D	-1	SER	-	CLONING ARTIFACT	UNP P63788
D	0	HIS	-	CLONING ARTIFACT	UNP P63788
D	29	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	38	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	79	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	91	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	93	MSE	MET	MODIFIED RESIDUE	UNP P63788
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D	112	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	119	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	124	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	140	PRO	ALA	ENGINEERED	UNP P63788
D	162	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	175	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	190	MSE	MET	MODIFIED RESIDUE	UNP P63788
D	197	GLY	-	CLONING ARTIFACT	UNP P63788
D	198	SER	-	CLONING ARTIFACT	UNP P63788
E	-19	MET	-	CLONING ARTIFACT	UNP P63788

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	GLY	-	CLONING ARTIFACT	UNP P63788
E	-17	SER	-	CLONING ARTIFACT	UNP P63788
E	-16	SER	-	CLONING ARTIFACT	UNP P63788
E	-15	HIS	-	CLONING ARTIFACT	UNP P63788
E	-14	HIS	-	CLONING ARTIFACT	UNP P63788
E	-13	HIS	-	CLONING ARTIFACT	UNP P63788
E	-12	HIS	-	CLONING ARTIFACT	UNP P63788
E	-11	HIS	-	CLONING ARTIFACT	UNP P63788
E	-10	HIS	-	CLONING ARTIFACT	UNP P63788
E	-9	SER	-	CLONING ARTIFACT	UNP P63788
E	-8	SER	-	CLONING ARTIFACT	UNP P63788
E	-7	GLY	-	CLONING ARTIFACT	UNP P63788
E	-6	LEU	-	CLONING ARTIFACT	UNP P63788
E	-5	VAL	-	CLONING ARTIFACT	UNP P63788
E	-4	PRO	-	CLONING ARTIFACT	UNP P63788
E	-3	ARG	-	CLONING ARTIFACT	UNP P63788
E	-2	GLY	-	CLONING ARTIFACT	UNP P63788
E	-1	SER	-	CLONING ARTIFACT	UNP P63788
E	0	HIS	-	CLONING ARTIFACT	UNP P63788
E	29	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	38	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	79	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	91	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	93	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	97	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	112	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	119	MSE	MET	MODIFIED RESIDUE	UNP P63788
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E	140	PRO	ALA	ENGINEERED	UNP P63788
E	162	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	175	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	190	MSE	MET	MODIFIED RESIDUE	UNP P63788
E	197	GLY	-	CLONING ARTIFACT	UNP P63788
E	198	SER	-	CLONING ARTIFACT	UNP P63788
F	-19	MET	-	CLONING ARTIFACT	UNP P63788
F	-18	GLY	-	CLONING ARTIFACT	UNP P63788
F	-17	SER	-	CLONING ARTIFACT	UNP P63788
F	-16	SER	-	CLONING ARTIFACT	UNP P63788
F	-15	HIS	-	CLONING ARTIFACT	UNP P63788
F	-14	HIS	-	CLONING ARTIFACT	UNP P63788
F	-13	HIS	-	CLONING ARTIFACT	UNP P63788
F	-12	HIS	-	CLONING ARTIFACT	UNP P63788

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	CLONING ARTIFACT	UNP P63788
F	-10	HIS	-	CLONING ARTIFACT	UNP P63788
F	-9	SER	-	CLONING ARTIFACT	UNP P63788
F	-8	SER	-	CLONING ARTIFACT	UNP P63788
F	-7	GLY	-	CLONING ARTIFACT	UNP P63788
F	-6	LEU	-	CLONING ARTIFACT	UNP P63788
F	-5	VAL	-	CLONING ARTIFACT	UNP P63788
F	-4	PRO	-	CLONING ARTIFACT	UNP P63788
F	-3	ARG	-	CLONING ARTIFACT	UNP P63788
F	-2	GLY	-	CLONING ARTIFACT	UNP P63788
F	-1	SER	-	CLONING ARTIFACT	UNP P63788
F	0	HIS	-	CLONING ARTIFACT	UNP P63788
F	29	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	38	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	79	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	91	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	93	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	97	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	112	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	119	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	124	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	140	PRO	ALA	ENGINEERED	UNP P63788
F	162	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	175	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	190	MSE	MET	MODIFIED RESIDUE	UNP P63788
F	197	GLY	-	CLONING ARTIFACT	UNP P63788
F	198	SER	-	CLONING ARTIFACT	UNP P63788
G	-19	MET	-	CLONING ARTIFACT	UNP P63788
G	-18	GLY	-	CLONING ARTIFACT	UNP P63788
G	-17	SER	-	CLONING ARTIFACT	UNP P63788
G	-16	SER	-	CLONING ARTIFACT	UNP P63788
G	-15	HIS	-	CLONING ARTIFACT	UNP P63788
G	-14	HIS	-	CLONING ARTIFACT	UNP P63788
G	-13	HIS	-	CLONING ARTIFACT	UNP P63788
G	-12	HIS	-	CLONING ARTIFACT	UNP P63788
G	-11	HIS	-	CLONING ARTIFACT	UNP P63788
G	-10	HIS	-	CLONING ARTIFACT	UNP P63788
G	-9	SER	-	CLONING ARTIFACT	UNP P63788
G	-8	SER	-	CLONING ARTIFACT	UNP P63788
G	-7	GLY	-	CLONING ARTIFACT	UNP P63788
G	-6	LEU	-	CLONING ARTIFACT	UNP P63788
G	-5	VAL	-	CLONING ARTIFACT	UNP P63788

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	PRO	-	CLONING ARTIFACT	UNP P63788
G	-3	ARG	-	CLONING ARTIFACT	UNP P63788
G	-2	GLY	-	CLONING ARTIFACT	UNP P63788
G	-1	SER	-	CLONING ARTIFACT	UNP P63788
G	0	HIS	-	CLONING ARTIFACT	UNP P63788
G	29	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	38	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	79	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	91	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	93	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	97	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	112	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	119	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	124	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	140	PRO	ALA	ENGINEERED	UNP P63788
G	162	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	175	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	190	MSE	MET	MODIFIED RESIDUE	UNP P63788
G	197	GLY	-	CLONING ARTIFACT	UNP P63788
G	198	SER	-	CLONING ARTIFACT	UNP P63788

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	2	Total Ca 2 2	0	0
2	A	1	Total Ca 1 1	0	0
2	F	2	Total Ca 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	28	Total O 28 28	0	0

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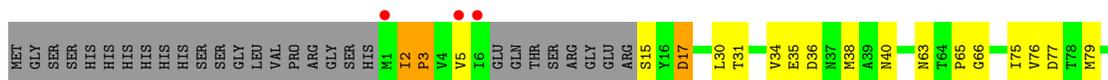
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	30	Total O 30 30	0	0
3	C	28	Total O 28 28	0	0
3	D	17	Total O 17 17	0	0
3	E	13	Total O 13 13	0	0
3	F	11	Total O 11 11	0	0
3	G	17	Total O 17 17	0	0



• Molecule 1: ATP-dependent Clp protease proteolytic subunit



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.65Å 105.65Å 236.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.50 – 2.51 29.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.50-2.51) 90.6 (29.84-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.186 , 0.248 0.194 , 0.251	Depositor DCC
R_{free} test set	4760 reflections (10.97%)	DCC
Wilson B-factor (Å ²)	34.5	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9601	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.58	0/1321	0.80	4/1764 (0.2%)
1	B	0.59	0/1379	0.82	6/1841 (0.3%)
1	C	0.61	0/1363	0.82	6/1819 (0.3%)
1	D	0.55	0/1377	0.79	4/1838 (0.2%)
1	E	0.53	0/1346	0.77	5/1796 (0.3%)
1	F	0.60	0/1334	0.80	3/1781 (0.2%)
1	G	0.52	0/1371	0.78	4/1831 (0.2%)
All	All	0.57	0/9491	0.80	32/12670 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	17	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	85	ASP	CB-CG-OD2	7.54	125.08	118.30
1	B	17	ASP	CB-CG-OD2	6.95	124.55	118.30
1	G	172	ASP	CB-CG-OD2	6.64	124.28	118.30
1	D	57	ASP	CB-CG-OD2	6.53	124.18	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2	ILE	Peptide

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	1315	0	1311	19	0
1	B	1373	0	1373	15	0
1	C	1357	0	1360	12	0
1	D	1371	0	1367	10	0
1	E	1340	0	1341	20	0
1	F	1328	0	1333	20	0
1	G	1365	0	1361	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
3	A	28	0	0	0	0
3	B	30	0	0	3	0
3	C	28	0	0	1	0
3	D	17	0	0	0	0
3	E	13	0	0	0	0
3	F	11	0	0	0	0
3	G	17	0	0	1	0
All	All	9601	0	9446	104	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 6.

The worst 5 of 104 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:F:76:VAL:HA	1:F:79:MSE:HE3	1.47	0.94
1:B:26:ARG:HG2	3:B:1011:HOH:O	1.72	0.88
1:B:26:ARG:NE	3:B:1011:HOH:O	2.02	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MSE:HE1	1:A:150:LEU:HD13	1.58	0.83
1:G:30:LEU:CD1	1:G:38:MSE:HE1	2.14	0.77

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	165/218 (76%)	161 (98%)	3 (2%)	1 (1%)	28	48
1	B	172/218 (79%)	164 (95%)	7 (4%)	1 (1%)	28	48
1	C	170/218 (78%)	163 (96%)	7 (4%)	0	100	100
1	D	172/218 (79%)	164 (95%)	7 (4%)	1 (1%)	28	48
1	E	168/218 (77%)	163 (97%)	5 (3%)	0	100	100
1	F	167/218 (77%)	157 (94%)	9 (5%)	1 (1%)	28	48
1	G	171/218 (78%)	165 (96%)	6 (4%)	0	100	100
All	All	1185/1526 (78%)	1137 (96%)	44 (4%)	4 (0%)	44	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	3	PRO
1	B	2	ILE
1	A	53	ASP
1	D	140	PRO

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	144/168 (86%)	132 (92%)	12 (8%)	13	25
1	B	151/168 (90%)	138 (91%)	13 (9%)	12	23
1	C	149/168 (89%)	142 (95%)	7 (5%)	30	54
1	D	151/168 (90%)	132 (87%)	19 (13%)	5	10
1	E	147/168 (88%)	131 (89%)	16 (11%)	7	14
1	F	146/168 (87%)	129 (88%)	17 (12%)	6	12
1	G	150/168 (89%)	139 (93%)	11 (7%)	16	31
All	All	1038/1176 (88%)	943 (91%)	95 (9%)	11	20

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	113	LEU
1	E	24	LYS
1	G	35	GLU
1	D	144	LEU
1	D	173	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	87	GLN
1	E	157	ASN
1	F	173	ASN
1	D	173	ASN
1	E	40	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	159/218 (72%)	-0.03	5 (3%) 49 52	15, 27, 51, 60	0
1	B	166/218 (76%)	-0.11	5 (3%) 51 53	15, 25, 50, 59	0
1	C	164/218 (75%)	-0.08	3 (1%) 69 70	13, 22, 41, 53	0
1	D	166/218 (76%)	0.07	5 (3%) 51 53	21, 30, 52, 59	0
1	E	162/218 (74%)	0.16	7 (4%) 36 38	27, 36, 56, 66	0
1	F	161/218 (73%)	-0.06	5 (3%) 49 52	20, 31, 56, 69	0
1	G	165/218 (75%)	0.15	10 (6%) 22 22	19, 32, 58, 72	0
All	All	1143/1526 (74%)	0.01	40 (3%) 44 47	13, 29, 54, 72	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	THR	5.9
1	D	8	GLN	4.7
1	D	10	SER	4.5
1	D	9	THR	3.9
1	F	1	MET	3.7

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	C	1006	1/1	0.98	0.20	3.40	35,35,35,35	0
2	CA	F	1008	1/1	0.89	0.18	0.87	59,59,59,59	0
2	CA	C	1002	1/1	0.98	0.18	0.10	56,56,56,56	0
2	CA	E	1007	1/1	0.88	0.13	-0.47	60,60,60,60	0
2	CA	A	1001	1/1	0.86	0.10	-0.72	60,60,60,60	0
2	CA	B	1004	1/1	0.97	0.06	-2.32	52,52,52,52	0
2	CA	G	1005	1/1	0.97	0.04	-2.51	53,53,53,53	0
2	CA	F	1003	1/1	0.72	0.09	-	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.