Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 03:47 AM EDT

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 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

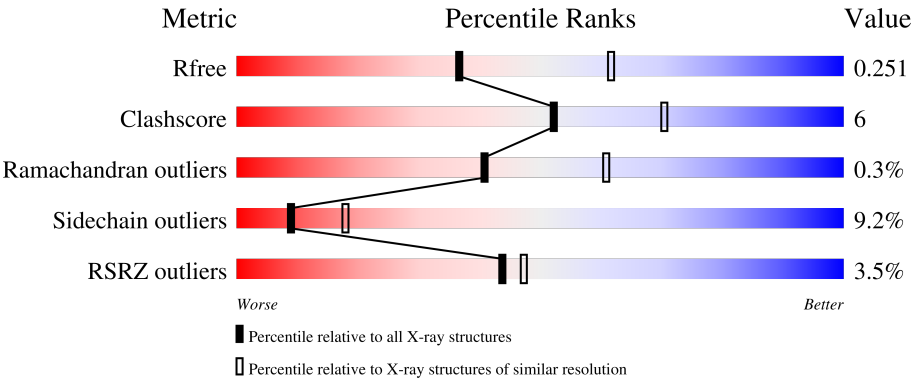
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 of 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	218	2% 64% 12% • 22%
1	B	218	2% 67% 11% • 18%
1	C	218	% 67% 13% • 19%
1	D	218	2% 67% 12% • 18%
1	E	218	3% 62% 15% • 20%

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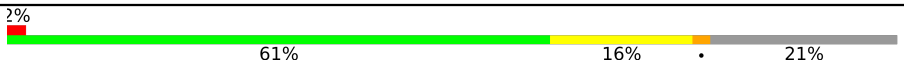
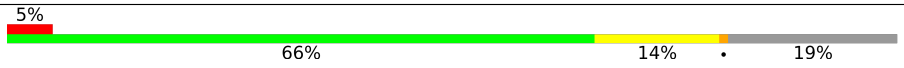
Mol	Chain	Length	Quality of chain
1	F	218	
1	G	218	

2 Entry composition (i)

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
1	A	171	Total	C	N	O	Se		0	0	0
			1315	828	217	258	12				
1	B	178	Total	C	N	O	S	Se	0	0	0
			1373	862	228	270	1	12			
1	C	176	Total	C	N	O	S	Se	0	0	0
			1357	853	226	265	1	12			
1	D	178	Total	C	N	O	S	Se	0	0	0
			1371	859	228	271	1	12			
1	E	174	Total	C	N	O	S	Se	0	0	0
			1340	842	223	262	1	12			
1	F	173	Total	C	N	O	S	Se	0	0	0
			1328	837	219	259	1	12			
1	G	177	Total	C	N	O	Se		0	0	0
			1365	857	227	269	12				

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 mutation	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 mutation	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 mutation	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
D	97	MSE	MET	modified residue	UNP P63788
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 mutation	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
E	124	MSE	MET	modified residue	UNP P63788
E	140	PRO	ALA	engineered mutation	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 mutation	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 mutation	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	A	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	E	1	Total Ca 1 1	0	0
2	F	2	Total Ca 2 2	0	0
2	G	1	Total Ca 1 1	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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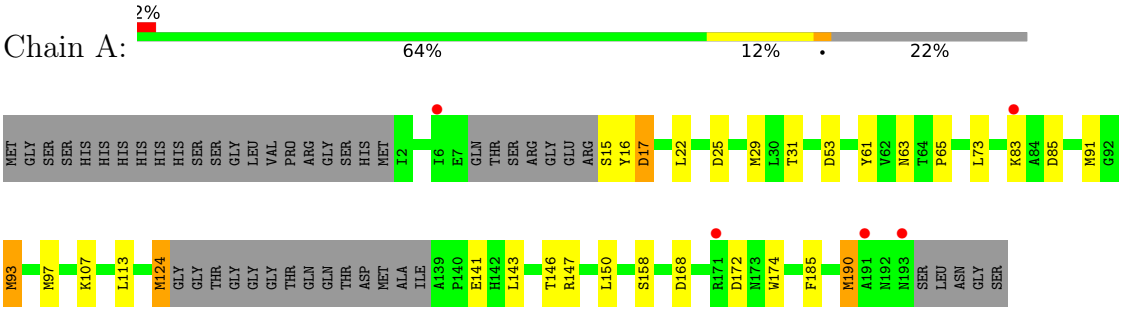
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	30	Total O 30 30	0	0
3	C	28	Total O 28 28	0	0
3	D	17	Total O 17 17	0	0
3	E	13	Total O 13 13	0	0
3	F	11	Total O 11 11	0	0
3	G	17	Total O 17 17	0	0

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.

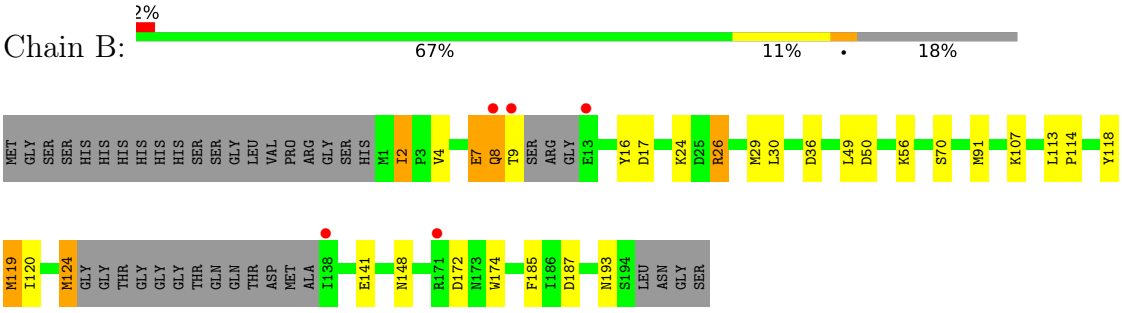
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



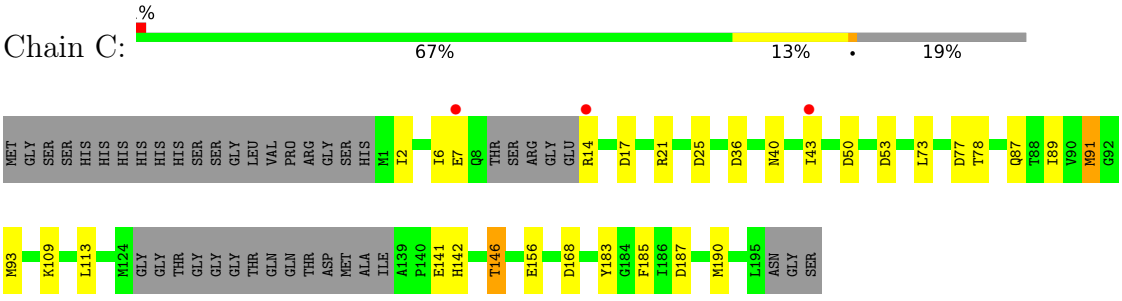
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



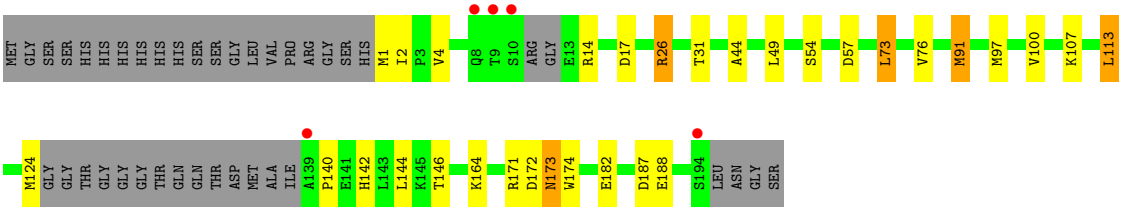
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



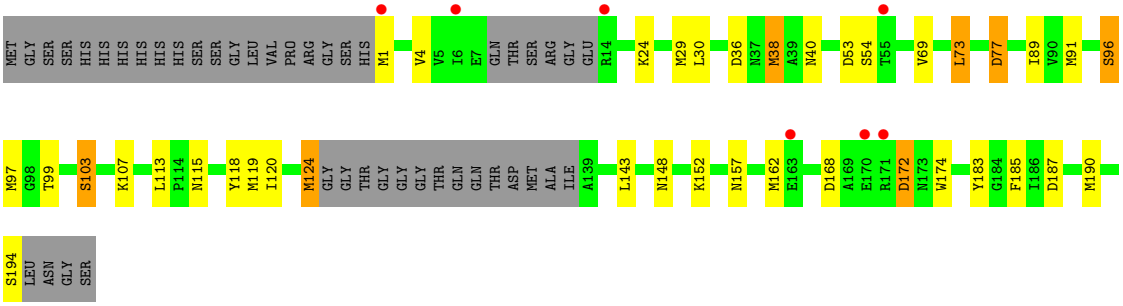
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



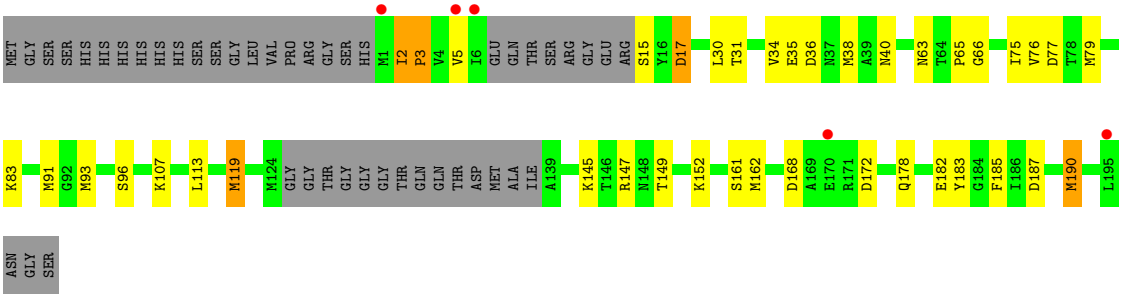
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



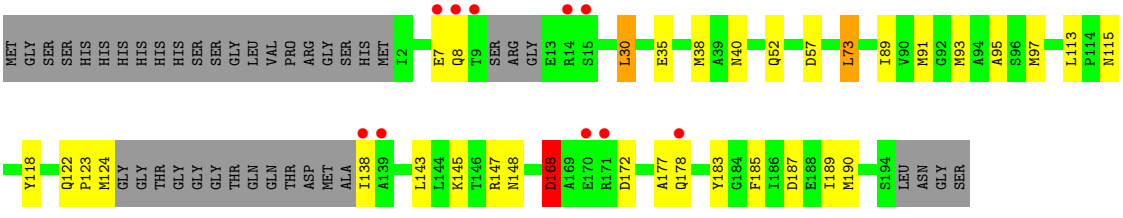
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.49 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.19, CNX 2000.1	Depositor
R, R_{free}	0.186 , 0.248 0.194 , 0.251	Depositor DCC
R_{free} test set	4780 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
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

Xtriage'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.*

[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

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.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	C	36	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	36	ASP	CB-CG-OD2	6.39	124.06	118.30
1	C	53	ASP	CB-CG-OD2	6.38	124.04	118.30
1	G	187	ASP	CB-CG-OD2	6.29	123.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	187	ASP	CB-CG-OD2	6.26	123.93	118.30
1	F	168	ASP	CB-CG-OD2	6.18	123.87	118.30
1	A	168	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	187	ASP	CB-CG-OD2	6.09	123.78	118.30
1	G	168	ASP	CB-CG-OD2	6.08	123.78	118.30
1	E	53	ASP	CB-CG-OD2	6.01	123.71	118.30
1	F	187	ASP	CB-CG-OD2	5.88	123.59	118.30
1	E	168	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	187	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	17	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	77	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	172	ASP	CB-CG-OD2	5.49	123.25	118.30
1	C	25	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	50	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	25	ASP	CB-CG-OD2	5.33	123.09	118.30
1	E	187	ASP	CB-CG-OD2	5.32	123.08	118.30
1	G	57	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	168	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	172	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	17	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	50	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	26	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	E	172	ASP	CB-CG-OD2	5.00	122.81	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
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
1:A:93:MSE:HE3	1:A:174:TRP:HH2	1.49	0.77
1:E:103:SER:HB3	1:E:157:ASN:HD22	1.48	0.77
1:C:156:GLU:HB3	3:C:1019:HOH:O	1.87	0.74
1:F:75:ILE:HG22	1:F:79:MSE:HE2	1.67	0.74
1:A:31:THR:HG21	1:G:40:ASN:HD21	1.52	0.73
1:A:31:THR:HG21	1:G:40:ASN:ND2	2.06	0.71
1:C:40:ASN:ND2	1:D:31:THR:OG1	2.25	0.70
1:G:113:LEU:HD23	1:G:190:MSE:HE3	1.78	0.65
1:A:113:LEU:HD21	1:A:190:MSE:HE2	1.77	0.65
1:D:44:ALA:HB2	1:E:29:MSE:HE2	1.78	0.65
1:D:91:MSE:HB3	1:D:113:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:GLN:NE2	1:F:182:GLU:OE2	2.30	0.63
1:E:113:LEU:HD23	1:E:190:MSE:HE3	1.81	0.62
1:E:99:THR:O	1:E:103:SER:HB2	1.99	0.61
1:C:113:LEU:HD23	1:C:190:MSE:HE3	1.84	0.59
1:G:30:LEU:HD12	1:G:38:MSE:HE1	1.84	0.59
1:D:91:MSE:HB3	1:D:113:LEU:CD2	2.32	0.59
1:C:142:HIS:O	1:C:146:THR:HG23	2.04	0.58
1:G:138:ILE:HD11	1:G:143:LEU:HD21	1.87	0.57
1:A:93:MSE:HE3	1:A:174:TRP:CH2	2.37	0.57
1:A:65:PRO:HA	1:A:93:MSE:HE2	1.87	0.56
1:F:65:PRO:HA	1:F:93:MSE:HE2	1.88	0.56
1:A:83:LYS:HD2	1:B:193:ASN:HD22	1.73	0.54
1:G:89:ILE:HG23	1:G:190:MSE:HE1	1.88	0.54
1:F:77:ASP:HB2	1:G:113:LEU:HD13	1.90	0.53
1:F:77:ASP:OD2	1:G:115:ASN:HB2	2.09	0.53
1:E:124:MSE:HB3	1:E:143:LEU:HD22	1.92	0.52
1:E:96:SER:OG	1:E:97:MSE:N	2.42	0.51
1:B:16:TYR:CZ	1:B:24:LYS:HE2	2.46	0.51
1:D:26:ARG:NH2	1:D:49:LEU:O	2.44	0.50
1:E:89:ILE:HG23	1:E:190:MSE:HE1	1.93	0.50
1:A:124:MSE:HE1	1:A:147:ARG:HD3	1.94	0.50
1:F:36:ASP:O	1:F:40:ASN:OD1	2.29	0.49
1:B:26:ARG:NH2	1:B:49:LEU:O	2.45	0.49
1:E:91:MSE:CB	1:E:113:LEU:HD12	2.43	0.48
1:G:168:ASP:N	1:G:168:ASP:OD1	2.46	0.48
1:B:91:MSE:CB	1:B:113:LEU:HD12	2.44	0.48
1:G:123:PRO:O	1:G:124:MSE:HE2	2.12	0.48
1:E:69:VAL:HG12	1:E:73:LEU:HD22	1.95	0.48
1:F:76:VAL:HA	1:F:79:MSE:CE	2.32	0.48
1:F:75:ILE:O	1:F:79:MSE:HG3	2.14	0.48
1:E:183:TYR:CD2	1:E:185:PHE:CE1	3.02	0.47
1:G:113:LEU:CD2	1:G:190:MSE:HE3	2.43	0.47
1:C:87:GLN:NE2	1:C:109:LYS:HD3	2.29	0.47
1:A:29:MSE:HE2	1:A:61:TYR:HB2	1.97	0.47
1:E:40:ASN:ND2	1:F:91:MSE:HE3	2.30	0.47
1:E:152:LYS:HG3	1:E:162:MSE:SE	2.65	0.47
1:E:89:ILE:CG2	1:E:190:MSE:HE1	2.45	0.47
1:A:97:MSE:HE1	1:A:150:LEU:CD1	2.37	0.46
1:B:30:LEU:C	1:B:30:LEU:HD23	2.36	0.46
1:C:89:ILE:HG23	1:C:190:MSE:HE1	1.97	0.46
1:C:91:MSE:HB3	1:C:113:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:LEU:HD13	1:G:97:MSE:HE1	1.97	0.45
1:C:17:ASP:O	1:C:21:ARG:HG3	2.17	0.45
1:B:91:MSE:HB3	1:B:113:LEU:HD12	1.99	0.45
1:F:119:MSE:HE1	1:F:172:ASP:HA	1.98	0.45
1:D:73:LEU:HG	1:E:115:ASN:HB3	1.99	0.45
1:G:30:LEU:HD13	1:G:38:MSE:HE1	1.95	0.45
1:A:97:MSE:CE	1:A:150:LEU:HD13	2.38	0.44
1:G:177:ALA:HB1	1:G:189:ILE:HG12	1.99	0.44
1:A:113:LEU:CD2	1:A:190:MSE:HE2	2.44	0.44
1:B:120:ILE:HG21	1:B:185:PHE:CE1	2.52	0.44
1:F:77:ASP:HB3	1:G:113:LEU:HD22	1.99	0.44
1:A:31:THR:CG2	1:G:40:ASN:HD21	2.25	0.44
1:F:40:ASN:ND2	1:G:91:MSE:HE3	2.32	0.44
1:A:91:MSE:CB	1:A:113:LEU:HD12	2.48	0.43
1:C:43:ILE:HG23	1:C:78:THR:HG21	1.99	0.43
1:D:76:VAL:HG21	1:D:100:VAL:HG12	1.99	0.43
1:A:124:MSE:CG	1:A:143:LEU:HD22	2.47	0.43
1:G:52:GLN:HA	3:G:1014:HOH:O	2.17	0.43
1:G:91:MSE:CB	1:G:113:LEU:HD12	2.49	0.43
1:F:2:ILE:HB	1:F:3:PRO:HD2	2.01	0.43
1:E:120:ILE:HG21	1:E:185:PHE:CE1	2.54	0.43
1:B:7:GLU:HG3	1:B:8:GLN:H	1.84	0.43
1:A:158:SER:HB3	1:A:185:PHE:CE2	2.54	0.42
1:E:30:LEU:CD2	1:E:38:MSE:HE1	2.48	0.42
1:G:138:ILE:HD11	1:G:143:LEU:CD2	2.49	0.42
1:B:7:GLU:HG3	1:B:8:GLN:N	2.34	0.42
1:B:119:MSE:HG3	1:B:174:TRP:CD2	2.55	0.42
1:G:183:TYR:CD2	1:G:185:PHE:CE1	3.08	0.42
1:A:124:MSE:HG2	1:A:143:LEU:HD22	2.02	0.42
1:B:124:MSE:HE2	1:B:124:MSE:HB2	1.87	0.42
1:C:141:GLU:H	1:C:141:GLU:CD	2.23	0.42
1:F:113:LEU:HD23	1:F:190:MSE:HE3	2.02	0.42
1:G:93:MSE:CE	1:G:95:ALA:HB2	2.50	0.42
1:A:31:THR:HA	1:A:63:ASN:O	2.20	0.42
1:E:77:ASP:HB2	1:F:113:LEU:HD13	2.02	0.41
1:F:30:LEU:CD2	1:F:38:MSE:HE1	2.49	0.41
1:C:77:ASP:HB3	1:D:113:LEU:HG	2.03	0.41
1:B:114:PRO:O	3:B:1029:HOH:O	2.22	0.41
1:B:26:ARG:NH1	1:B:56:LYS:O	2.54	0.41
1:C:183:TYR:CD2	1:C:185:PHE:CE1	3.09	0.41
1:E:30:LEU:HD23	1:E:38:MSE:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:GLY:HA3	1:F:96:SER:HB3	2.03	0.41
1:D:142:HIS:ND1	1:E:174:TRP:CD1	2.89	0.40
1:G:122:GLN:HB3	1:G:124:MSE:HE3	2.03	0.40
1:D:173:ASN:ND2	1:D:174:TRP:O	2.54	0.40
1:F:183:TYR:CD2	1:F:185:PHE:CE1	3.09	0.40
1:E:40:ASN:HD21	1:F:63:ASN:HD22	1.69	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	165/218 (76%)	161 (98%)	3 (2%)	1 (1%)	25	43
1	B	172/218 (79%)	164 (95%)	7 (4%)	1 (1%)	25	43
1	C	170/218 (78%)	163 (96%)	7 (4%)	0	100	100
1	D	172/218 (79%)	164 (95%)	7 (4%)	1 (1%)	25	43
1	E	168/218 (77%)	163 (97%)	5 (3%)	0	100	100
1	F	167/218 (77%)	157 (94%)	9 (5%)	1 (1%)	25	43
1	G	171/218 (78%)	165 (96%)	6 (4%)	0	100	100
All	All	1185/1526 (78%)	1137 (96%)	44 (4%)	4 (0%)	41	61

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%)	11 22
1	B	151/168 (90%)	138 (91%)	13 (9%)	10 20
1	C	149/168 (89%)	142 (95%)	7 (5%)	26 49
1	D	151/168 (90%)	132 (87%)	19 (13%)	4 8
1	E	147/168 (88%)	131 (89%)	16 (11%)	6 12
1	F	146/168 (87%)	129 (88%)	17 (12%)	5 10
1	G	150/168 (89%)	139 (93%)	11 (7%)	14 27
All	All	1038/1176 (88%)	943 (91%)	95 (9%)	9 18

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	16	TYR
1	A	17	ASP
1	A	22	LEU
1	A	73	LEU
1	A	93	MSE
1	A	107	LYS
1	A	124	MSE
1	A	141	GLU
1	A	146	THR
1	A	172	ASP
1	A	190	MSE
1	B	2	ILE
1	B	4	VAL
1	B	7	GLU
1	B	8	GLN
1	B	9	THR
1	B	29	MSE
1	B	70	SER
1	B	107	LYS

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Mol	Chain	Res	Type
1	B	118	TYR
1	B	119	MSE
1	B	124	MSE
1	B	141	GLU
1	B	148	ASN
1	C	6	ILE
1	C	7	GLU
1	C	14	ARG
1	C	73	LEU
1	C	91	MSE
1	C	93	MSE
1	C	146	THR
1	D	1	MET
1	D	2	ILE
1	D	4	VAL
1	D	14	ARG
1	D	26	ARG
1	D	54	SER
1	D	73	LEU
1	D	91	MSE
1	D	97	MSE
1	D	107	LYS
1	D	113	LEU
1	D	124	MSE
1	D	144	LEU
1	D	146	THR
1	D	164	LYS
1	D	171	ARG
1	D	173	ASN
1	D	182	GLU
1	D	188	GLU
1	E	1	MET
1	E	4	VAL
1	E	24	LYS
1	E	36	ASP
1	E	38	MSE
1	E	54	SER
1	E	73	LEU
1	E	96	SER
1	E	103	SER
1	E	107	LYS
1	E	118	TYR

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Mol	Chain	Res	Type
1	E	119	MSE
1	E	124	MSE
1	E	148	ASN
1	E	172	ASP
1	E	194	SER
1	F	2	ILE
1	F	5	VAL
1	F	15	SER
1	F	17	ASP
1	F	31	THR
1	F	34	VAL
1	F	35	GLU
1	F	83	LYS
1	F	107	LYS
1	F	119	MSE
1	F	145	LYS
1	F	147	ARG
1	F	149	THR
1	F	152	LYS
1	F	161	SER
1	F	162	MSE
1	F	190	MSE
1	G	7	GLU
1	G	8	GLN
1	G	30	LEU
1	G	35	GLU
1	G	73	LEU
1	G	118	TYR
1	G	145	LYS
1	G	147	ARG
1	G	148	ASN
1	G	168	ASP
1	G	178	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	B	80	ASN
1	C	40	ASN
1	C	148	ASN
1	D	87	GLN

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Mol	Chain	Res	Type
1	D	148	ASN
1	D	173	ASN
1	E	40	ASN
1	E	87	GLN
1	E	157	ASN
1	F	40	ASN
1	F	87	GLN
1	F	121	HIS
1	F	148	ASN
1	F	173	ASN
1	F	178	GLN
1	G	40	ASN
1	G	173	ASN

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

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

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	159/218 (72%)	-0.03	5 (3%)	49	52	15, 27, 51, 60	0
1	B	166/218 (76%)	-0.11	5 (3%)	50	53	15, 25, 50, 59	0
1	C	164/218 (75%)	-0.08	3 (1%)	68	71	13, 22, 41, 53	0
1	D	166/218 (76%)	0.07	5 (3%)	50	53	21, 30, 52, 59	0
1	E	162/218 (74%)	0.16	7 (4%)	35	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%)	21	22	19, 32, 58, 72	0
All	All	1143/1526 (74%)	0.01	40 (3%)	44	47	13, 29, 54, 72	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	THR	5.9
1	D	8	GLN	4.6
1	D	10	SER	4.5
1	D	9	THR	4.0
1	F	1	MET	3.7
1	B	138	ILE	3.6
1	E	6	ILE	3.6
1	E	171	ARG	3.6
1	E	170	GLU	3.4
1	G	14	ARG	3.4
1	G	170	GLU	3.2
1	A	193	ASN	3.2
1	F	195	LEU	3.2
1	B	171	ARG	3.1
1	F	6	ILE	3.0
1	G	15	SER	2.8
1	B	8	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	8	GLN	2.6
1	A	191	ALA	2.6
1	D	194	SER	2.6
1	B	9	THR	2.5
1	G	139	ALA	2.5
1	B	13	GLU	2.5
1	C	14	ARG	2.5
1	D	139	ALA	2.5
1	G	138	ILE	2.4
1	A	6	ILE	2.4
1	F	5	VAL	2.3
1	E	55	THR	2.3
1	E	1	MET	2.2
1	E	163	GLU	2.2
1	E	14	ARG	2.1
1	G	7	GLU	2.1
1	F	170	GLU	2.1
1	A	171	ARG	2.1
1	C	43	ILE	2.1
1	G	178	GLN	2.1
1	A	83	LYS	2.1
1	C	7	GLU	2.0
1	G	171	ARG	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	F	1003	1/1	0.71	0.09	61,61,61,61	0
2	CA	A	1001	1/1	0.86	0.10	60,60,60,60	0
2	CA	E	1007	1/1	0.88	0.13	60,60,60,60	0
2	CA	F	1008	1/1	0.89	0.18	59,59,59,59	0
2	CA	B	1004	1/1	0.96	0.06	52,52,52,52	0
2	CA	G	1005	1/1	0.97	0.04	53,53,53,53	0
2	CA	C	1002	1/1	0.98	0.18	56,56,56,56	0
2	CA	C	1006	1/1	0.98	0.20	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.