Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 07:22 PM EST

PDB ID	:	3STA
Title	:	Crystal structure of ClpP in tetradecameric form from Staphylococcus aureus
Authors	:	Zhang, J.; Ye, F.; Lan, L.; Jiang, H.; Luo, C.; Yang, C.-G.
Deposited on	:	2011-07-09
Resolution	:	2.28 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

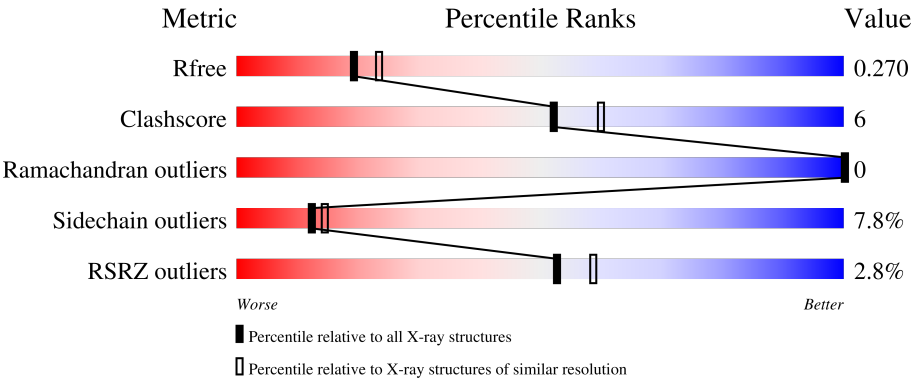
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	197	2% 80% 13% • •
1	B	197	% 80% 11% • 8%
1	C	197	2% 79% 13% • 6%
1	E	197	2% 82% 11% • 6%
1	F	197	4% 81% 11% • 6%

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Mol	Chain	Length	Quality of chain
1	G	197	2% 78% 12% 9%
1	I	197	4% 80% 13%
1	K	197	4% 75% 16% 6%
1	L	197	4% 75% 16% 7%
1	M	197	2% 79% 14% 6%
1	N	197	4% 79% 12% 6%
1	S	197	4% 77% 13% 7%
1	T	197	3% 81% 11% 6%
1	V	197	% 80% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20755 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	V	189	Total	C	N	O	S	0	2	0
			1469	922	252	287	8			
1	A	189	Total	C	N	O	S	0	2	0
			1466	921	251	286	8			
1	B	182	Total	C	N	O	S	0	1	0
			1404	886	237	274	7			
1	C	185	Total	C	N	O	S	0	2	0
			1434	904	243	279	8			
1	E	185	Total	C	N	O	S	0	2	0
			1436	905	243	280	8			
1	F	185	Total	C	N	O	S	0	1	0
			1431	901	243	280	7			
1	G	180	Total	C	N	O	S	0	1	0
			1390	878	235	270	7			
1	I	189	Total	C	N	O	S	0	0	0
			1456	913	251	286	6			
1	K	186	Total	C	N	O	S	0	1	0
			1435	903	244	281	7			
1	L	184	Total	C	N	O	S	0	1	0
			1422	896	242	277	7			
1	M	185	Total	C	N	O	S	0	1	0
			1431	901	243	280	7			
1	N	185	Total	C	N	O	S	0	1	0
			1431	901	243	280	7			
1	S	184	Total	C	N	O	S	0	2	0
			1429	901	242	278	8			
1	T	186	Total	C	N	O	S	0	1	0
			1435	903	244	281	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-1	GLY	-	expression tag	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
V	0	SER	-	expression tag	UNP P63786
A	-1	GLY	-	expression tag	UNP P63786
A	0	SER	-	expression tag	UNP P63786
B	-1	GLY	-	expression tag	UNP P63786
B	0	SER	-	expression tag	UNP P63786
C	-1	GLY	-	expression tag	UNP P63786
C	0	SER	-	expression tag	UNP P63786
E	-1	GLY	-	expression tag	UNP P63786
E	0	SER	-	expression tag	UNP P63786
F	-1	GLY	-	expression tag	UNP P63786
F	0	SER	-	expression tag	UNP P63786
G	-1	GLY	-	expression tag	UNP P63786
G	0	SER	-	expression tag	UNP P63786
I	-1	GLY	-	expression tag	UNP P63786
I	0	SER	-	expression tag	UNP P63786
K	-1	GLY	-	expression tag	UNP P63786
K	0	SER	-	expression tag	UNP P63786
L	-1	GLY	-	expression tag	UNP P63786
L	0	SER	-	expression tag	UNP P63786
M	-1	GLY	-	expression tag	UNP P63786
M	0	SER	-	expression tag	UNP P63786
N	-1	GLY	-	expression tag	UNP P63786
N	0	SER	-	expression tag	UNP P63786
S	-1	GLY	-	expression tag	UNP P63786
S	0	SER	-	expression tag	UNP P63786
T	-1	GLY	-	expression tag	UNP P63786
T	0	SER	-	expression tag	UNP P63786

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	V	58	Total O 58 58	0	0
2	A	53	Total O 53 53	0	0
2	B	59	Total O 59 59	0	0
2	C	57	Total O 57 57	0	0
2	E	42	Total O 42 42	0	0
2	F	48	Total O 48 48	0	0

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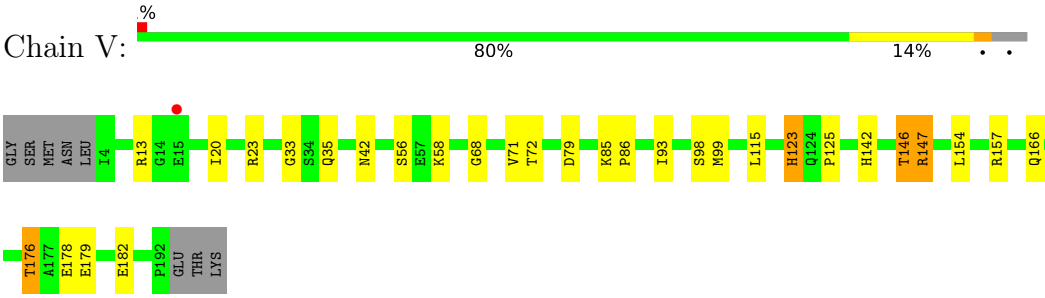
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	52	Total O 52 52	0	0
2	I	53	Total O 53 53	0	0
2	K	43	Total O 43 43	0	0
2	L	27	Total O 27 27	0	0
2	M	28	Total O 28 28	0	0
2	N	46	Total O 46 46	0	0
2	S	64	Total O 64 64	0	0
2	T	56	Total O 56 56	0	0

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.

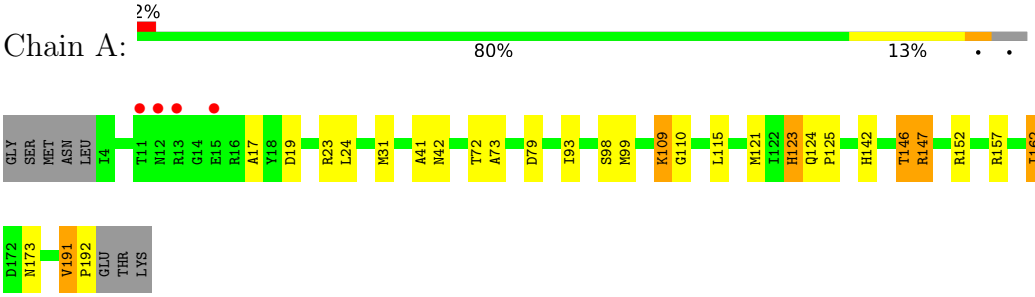
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:



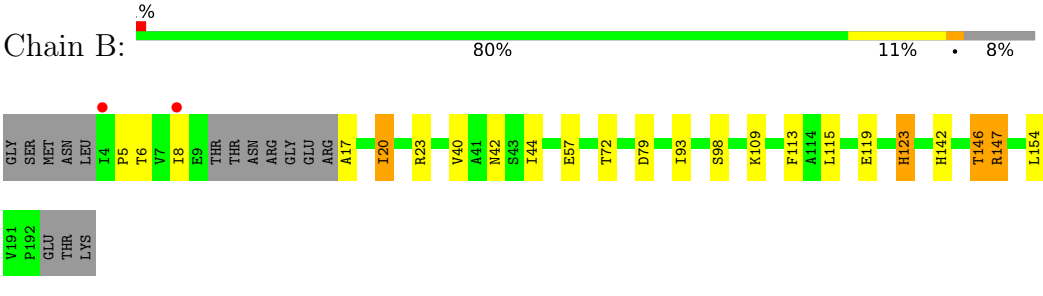
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



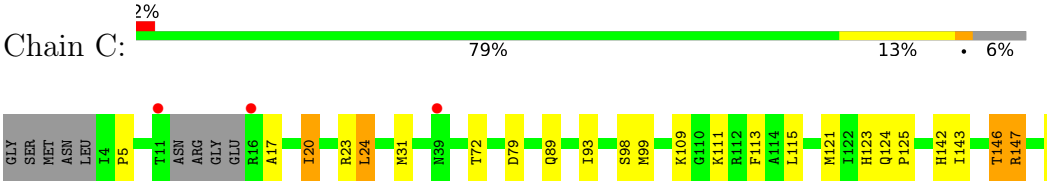
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



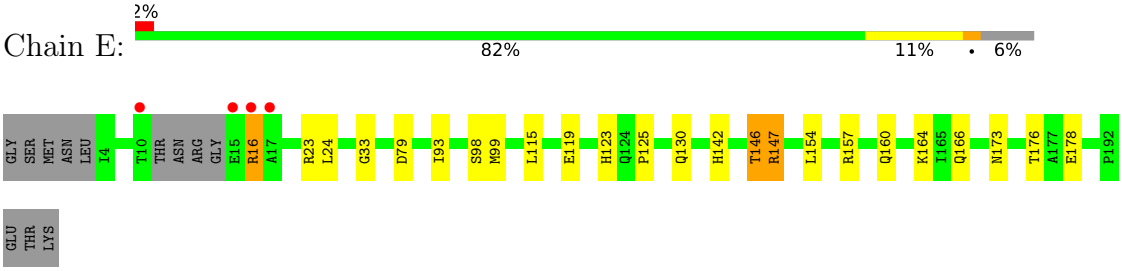
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



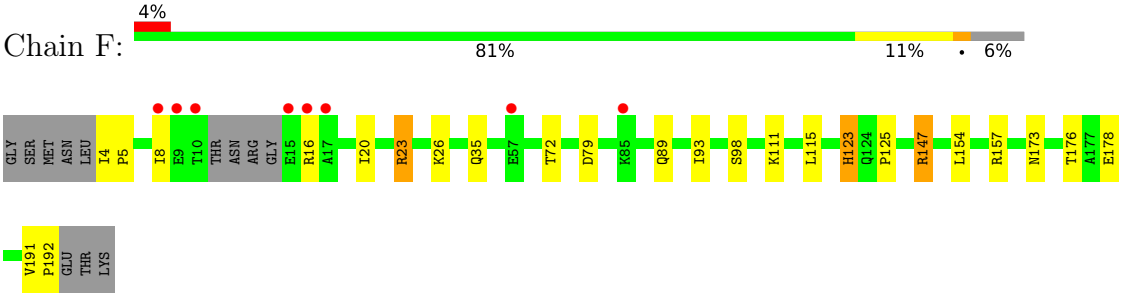
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



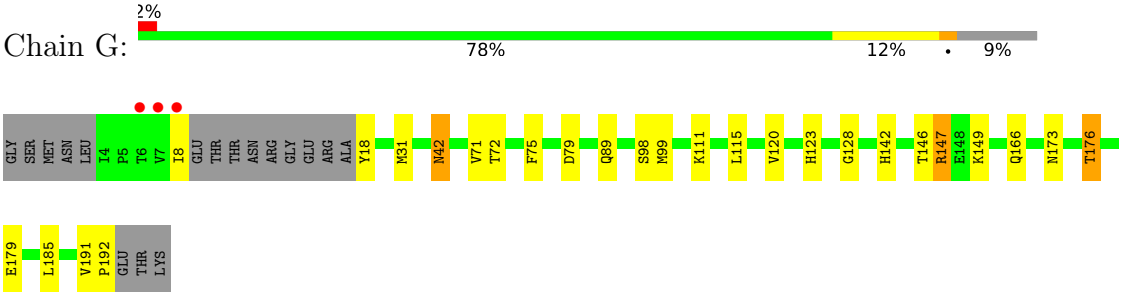
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



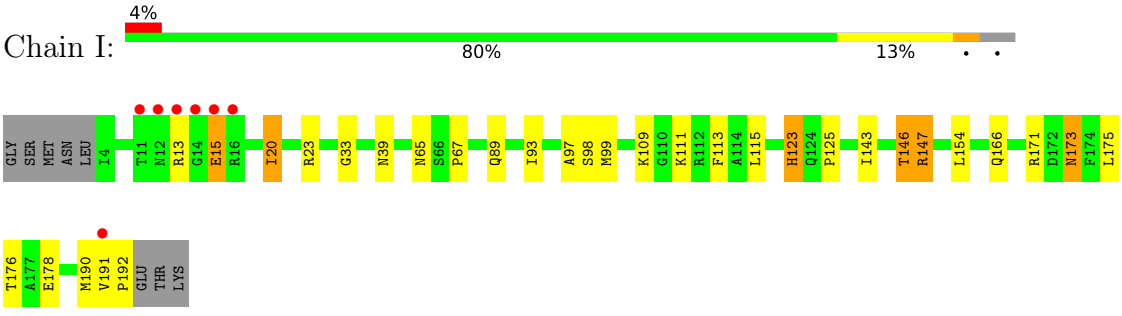
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



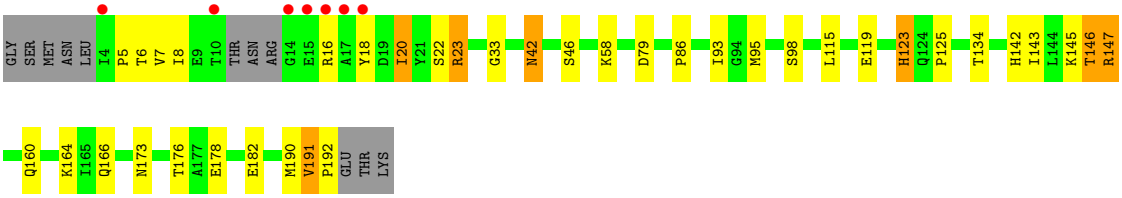
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:

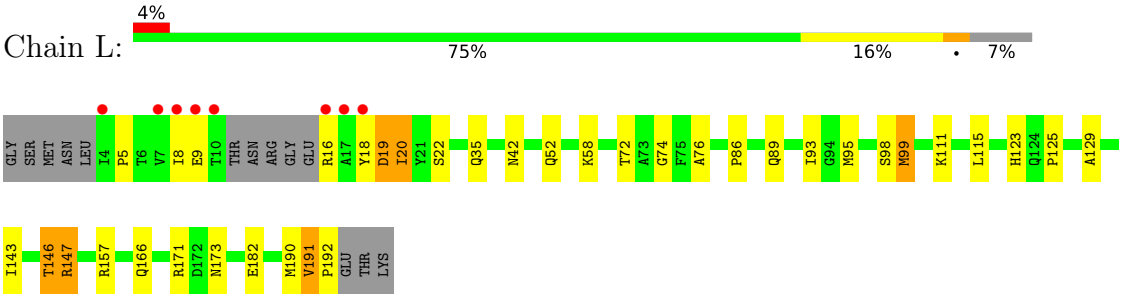


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

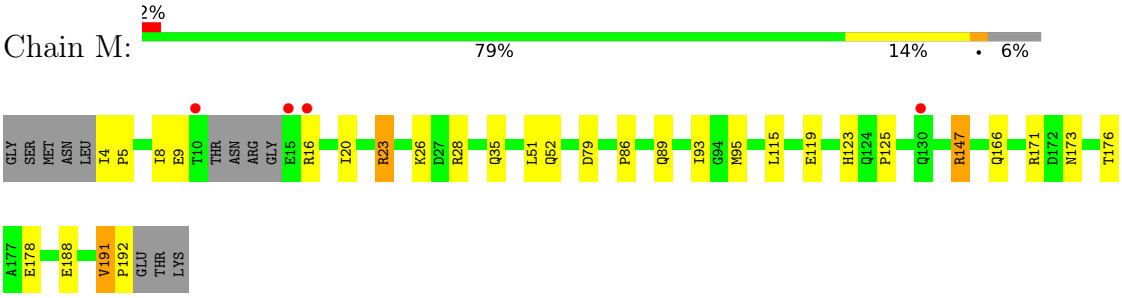
Chain K:



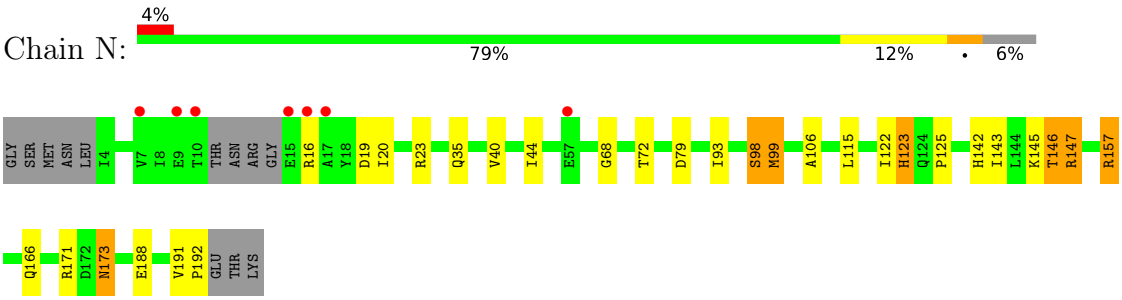
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



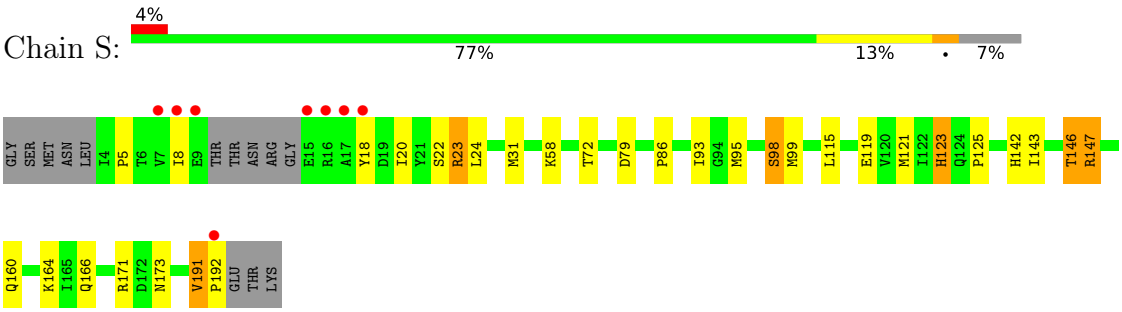
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

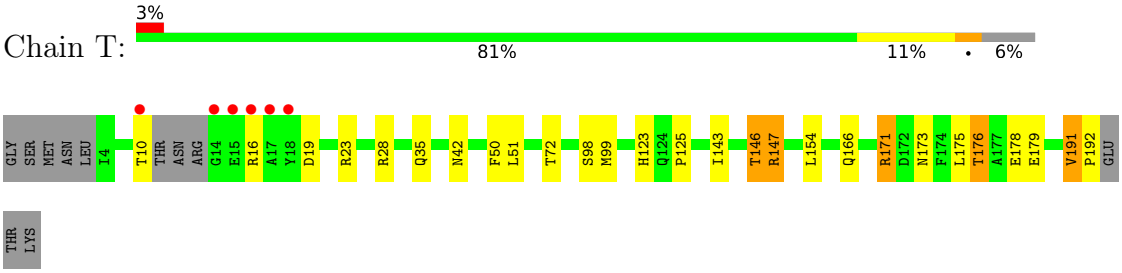


• Molecule 1: ATP-dependent Clp protease proteolytic subunit



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T:


3%
81%
11%
6%
GLY
SER
MET
ASN
LEU
I4
T10
THR
ASN
ARG
G14
E15
R16
A17
Y18
D19
R23
R28
Q35
N42
F50
L51
T72
S98
M99
H123
Q124
P125
I143
T146
R147
L154
Q166
R171
D172
N173
F174
L175
T176
A177
E178
E179
V191
P192
GLU
THR
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.57Å 96.29Å 192.61Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.28 41.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.28) 95.1 (41.94-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.269 0.224 , 0.270	Depositor DCC
R_{free} test set	7425 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.013 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.018 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.020 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20755	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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	0.35	0/1491	0.53	0/2012
1	B	0.36	0/1425	0.54	0/1923
1	C	0.35	0/1458	0.52	0/1967
1	E	0.34	0/1460	0.50	0/1969
1	F	0.34	0/1452	0.50	0/1959
1	G	0.35	0/1411	0.50	0/1904
1	I	0.35	0/1475	0.51	0/1992
1	K	0.35	0/1456	0.50	0/1964
1	L	0.34	0/1443	0.51	0/1947
1	M	0.33	0/1452	0.50	0/1959
1	N	0.34	0/1452	0.50	0/1959
1	S	0.36	0/1453	0.53	0/1959
1	T	0.34	0/1456	0.51	0/1964
1	V	0.35	0/1491	0.53	0/2012
All	All	0.35	0/20375	0.51	0/27490

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	1466	0	1483	21	0
1	B	1404	0	1418	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1434	0	1454	15	0
1	E	1436	0	1453	12	0
1	F	1431	0	1444	16	0
1	G	1390	0	1407	20	0
1	I	1456	0	1465	20	0
1	K	1435	0	1447	27	0
1	L	1422	0	1438	27	0
1	M	1431	0	1444	16	0
1	N	1431	0	1444	16	0
1	S	1429	0	1446	22	0
1	T	1435	0	1447	15	0
1	V	1469	0	1482	20	0
2	A	53	0	0	3	0
2	B	59	0	0	1	0
2	C	57	0	0	0	0
2	E	42	0	0	1	0
2	F	48	0	0	1	0
2	G	52	0	0	3	0
2	I	53	0	0	0	0
2	K	43	0	0	0	0
2	L	27	0	0	0	0
2	M	28	0	0	0	0
2	N	46	0	0	0	0
2	S	64	0	0	1	0
2	T	56	0	0	0	0
2	V	58	0	0	1	0
All	All	20755	0	20272	223	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 (223) 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:S:23:ARG:HG2	1:S:23:ARG:HH11	1.22	1.00
1:A:152:ARG:HA	1:A:162:ILE:HD11	1.46	0.97
1:N:98:SER:HB3	1:N:123:HIS:CE1	2.02	0.95
1:S:191:VAL:HG22	1:S:192:PRO:HA	1.53	0.91
1:T:191:VAL:HG22	1:T:192:PRO:HA	1.57	0.85
1:S:8:ILE:HG21	1:T:16:ARG:HG2	1.59	0.83
1:I:33:GLY:HA3	1:K:42:ASN:OD1	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:VAL:HG22	1:K:192:PRO:HA	1.62	0.81
1:F:98:SER:HB3	1:F:123:HIS:CE1	2.17	0.80
1:K:33:GLY:HA3	1:L:42:ASN:HD21	1.46	0.79
1:L:191:VAL:HG22	1:L:192:PRO:HA	1.64	0.78
1:B:93:ILE:HG22	1:B:115:LEU:HD12	1.67	0.76
1:K:8:ILE:HG21	1:L:16:ARG:HG3	1.68	0.74
1:F:191:VAL:HG22	1:F:192:PRO:HA	1.70	0.73
1:C:191:VAL:HG22	1:C:192:PRO:HA	1.69	0.73
1:L:9:GLU:HB2	1:L:16:ARG:HD3	1.72	0.72
1:M:191:VAL:HG22	1:M:192:PRO:HA	1.72	0.71
1:N:93:ILE:HG22	1:N:115:LEU:HD12	1.71	0.71
1:E:93:ILE:HG22	1:E:115:LEU:HD12	1.71	0.71
1:S:23:ARG:HG2	1:S:23:ARG:NH1	1.98	0.70
1:V:93:ILE:HG22	1:V:115:LEU:HD12	1.74	0.69
1:L:125:PRO:HD2	1:L:147:ARG:HG2	1.74	0.69
1:I:93:ILE:HG22	1:I:115:LEU:HD12	1.76	0.67
1:K:33:GLY:HA3	1:L:42:ASN:ND2	2.10	0.67
1:K:6:THR:O	1:L:22:SER:HB3	1.95	0.66
1:F:93:ILE:HG22	1:F:115:LEU:HD12	1.79	0.65
1:G:98:SER:OG	2:G:528:HOH:O	2.14	0.64
1:M:93:ILE:HG22	1:M:115:LEU:HD12	1.79	0.63
1:E:79:ASP:HB3	1:F:115:LEU:HD13	1.81	0.62
1:S:98:SER:OG	1:S:99:MET:N	2.31	0.62
1:E:125:PRO:HD2	1:E:147:ARG:HG2	1.81	0.62
1:N:99:MET:HA	1:N:99:MET:CE	2.30	0.62
1:C:24:LEU:HD23	1:C:31[A]:MET:HE1	1.82	0.61
1:V:125:PRO:HD2	1:V:147:ARG:HG2	1.81	0.61
1:F:98:SER:CB	1:F:123:HIS:CE1	2.84	0.61
1:T:176:THR:HG22	1:T:179:GLU:H	1.66	0.61
1:A:93:ILE:HG22	1:A:115:LEU:HD12	1.83	0.60
1:L:5:PRO:HD2	1:L:20:ILE:HD11	1.84	0.60
1:M:8:ILE:HG21	1:N:16:ARG:HG2	1.83	0.60
1:L:89:GLN:HG2	1:L:111:LYS:HB3	1.85	0.58
1:E:33:GLY:HA3	1:G:42:ASN:OD1	2.03	0.57
1:E:119:GLU:OE2	1:G:142:HIS:HE1	1.87	0.57
1:M:176:THR:HG22	1:M:178:GLU:H	1.69	0.57
1:A:142:HIS:O	1:A:146:THR:HG23	2.06	0.56
1:V:33:GLY:HA3	1:B:42:ASN:OD1	2.05	0.56
1:A:125:PRO:HD2	1:A:147:ARG:HG2	1.88	0.55
1:S:143:ILE:HA	1:S:146:THR:HG23	1.87	0.55
1:E:142:HIS:O	1:E:146:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:GLN:HG2	1:G:111:LYS:HB3	1.87	0.55
1:L:8:ILE:HD13	1:M:16:ARG:HB2	1.88	0.55
1:L:143:ILE:HA	1:L:146:THR:HG23	1.88	0.55
1:A:121:MET:HE3	1:A:123:HIS:HB3	1.88	0.55
1:N:125:PRO:HD2	1:N:147:ARG:HG2	1.89	0.55
1:S:23:ARG:HD3	1:S:23:ARG:C	2.27	0.55
1:G:142:HIS:O	1:G:146:THR:HG23	2.08	0.54
1:S:142:HIS:O	1:S:146:THR:HG22	2.08	0.54
1:C:93:ILE:HG22	1:C:115:LEU:HD12	1.89	0.53
1:I:20:ILE:HD12	1:K:46:SER:HB3	1.89	0.53
1:V:79:ASP:HB3	1:A:115:LEU:HD13	1.91	0.53
1:A:98:SER:OG	1:A:99:MET:N	2.40	0.53
1:A:109:LYS:HD2	1:A:110:GLY:N	2.24	0.53
1:F:176:THR:HG22	1:F:178:GLU:H	1.74	0.52
1:L:115:LEU:HD23	1:L:190:MET:HB2	1.89	0.52
1:M:125:PRO:HD2	1:M:147:ARG:HG2	1.91	0.52
1:K:8:ILE:HA	1:K:16:ARG:O	2.09	0.52
1:S:5:PRO:HD2	1:S:20:ILE:HG12	1.91	0.52
1:K:5:PRO:HD2	1:K:20:ILE:HD11	1.91	0.52
1:L:74:GLY:HA3	1:L:99:MET:HG2	1.92	0.52
1:C:89:GLN:HG2	1:C:111:LYS:HB3	1.91	0.52
1:K:115:LEU:HD23	1:K:190:MET:HB2	1.91	0.52
1:L:191:VAL:CG2	1:L:192:PRO:HA	2.37	0.52
1:G:176:THR:HG22	1:G:179:GLU:H	1.74	0.52
1:F:191:VAL:CG2	1:F:192:PRO:HA	2.38	0.51
1:B:40:VAL:O	1:B:44:ILE:HG12	2.11	0.51
1:L:125:PRO:CD	1:L:147:ARG:HG2	2.37	0.51
1:A:79:ASP:HB3	1:G:115:LEU:HD13	1.92	0.51
1:I:13:ARG:HD2	1:T:10:THR:HG21	1.91	0.51
1:S:98:SER:HB2	1:S:123:HIS:CE1	2.46	0.51
1:B:98:SER:CB	1:B:123:HIS:CE1	2.94	0.51
1:V:42:ASN:OD1	1:A:31[A]:MET:HG3	2.12	0.50
1:V:125:PRO:CD	1:V:147:ARG:HG2	2.41	0.50
1:S:8:ILE:CG2	1:T:16:ARG:HG2	2.36	0.50
1:S:23:ARG:HD2	1:T:50:PHE:HD1	1.76	0.50
1:T:28:ARG:HG2	1:T:51:LEU:HD22	1.93	0.50
1:I:125:PRO:HD2	1:I:147:ARG:HG2	1.93	0.50
1:S:31[A]:MET:HG2	1:T:42:ASN:HD21	1.77	0.50
1:L:93:ILE:HG22	1:L:115:LEU:HD12	1.93	0.50
1:S:147:ARG:HD3	2:S:203:HOH:O	2.12	0.50
1:A:41:ALA:HB2	1:A:73:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ILE:HG22	1:B:115:LEU:CD1	2.39	0.50
1:K:143:ILE:HA	1:K:146:THR:HG23	1.92	0.50
1:K:176:THR:HG22	1:K:178:GLU:H	1.77	0.50
1:S:93:ILE:HG22	1:S:115:LEU:HD12	1.94	0.50
1:B:142:HIS:O	1:B:146:THR:HG23	2.12	0.49
1:N:142:HIS:O	1:N:146:THR:HG22	2.12	0.49
1:B:98:SER:HB2	1:B:123:HIS:CE1	2.48	0.49
1:B:115:LEU:HD13	1:C:79:ASP:HB3	1.94	0.49
1:I:115:LEU:HD13	1:K:79:ASP:HB3	1.94	0.49
1:V:98:SER:HB2	1:V:123:HIS:CE1	2.48	0.49
1:L:19:ASP:OD2	1:L:22:SER:OG	2.26	0.49
1:C:115:LEU:HD13	1:F:79:ASP:HB3	1.95	0.48
1:F:147:ARG:HD3	2:F:571:HOH:O	2.13	0.48
1:F:191:VAL:HG22	1:F:192:PRO:CA	2.42	0.48
1:K:33:GLY:CA	1:L:42:ASN:HD21	2.23	0.48
1:K:7:VAL:HB	1:K:23:ARG:HG3	1.94	0.48
1:B:6:THR:HG23	1:B:17:ALA:HB1	1.95	0.48
1:F:89:GLN:HG2	1:F:111:LYS:HB3	1.95	0.48
1:A:98:SER:OG	2:A:447:HOH:O	2.20	0.48
1:B:113:PHE:HB3	1:B:190:MET:HG3	1.95	0.47
1:I:13:ARG:HD2	1:T:10:THR:CG2	2.44	0.47
1:N:99:MET:HA	1:N:99:MET:HE2	1.96	0.47
1:N:125:PRO:CD	1:N:147:ARG:HG2	2.42	0.47
1:B:98:SER:HB3	1:B:123:HIS:CE1	2.50	0.47
1:C:125:PRO:HD2	1:C:147:ARG:HG2	1.97	0.47
1:A:121:MET:CE	1:A:123:HIS:HB3	2.45	0.47
1:C:5:PRO:HG2	1:C:20:ILE:HG12	1.97	0.47
1:E:115:LEU:HD13	1:G:79:ASP:HB3	1.96	0.47
1:L:125:PRO:HD2	1:L:147:ARG:CG	2.42	0.47
1:K:98:SER:HB3	1:K:123:HIS:CE1	2.50	0.47
1:L:115:LEU:HD13	1:M:79:ASP:HB3	1.97	0.47
1:M:9:GLU:HB2	1:M:16:ARG:HG3	1.97	0.46
1:S:125:PRO:HD2	1:S:147:ARG:HG2	1.97	0.46
1:C:113:PHE:HB3	1:C:190:MET:HG3	1.98	0.46
1:I:191:VAL:HB	1:I:192:PRO:HA	1.98	0.46
1:B:5:PRO:HD2	1:B:20:ILE:HB	1.96	0.46
1:S:23:ARG:NH1	1:S:23:ARG:CG	2.72	0.46
1:V:93:ILE:HG22	1:V:115:LEU:CD1	2.45	0.46
1:C:143:ILE:HA	1:C:146:THR:HG23	1.97	0.46
1:G:71:VAL:HG22	1:G:99:MET:CE	2.45	0.46
1:V:123:HIS:ND1	1:V:123:HIS:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:ARG:HD3	2:G:266:HOH:O	2.16	0.46
1:V:35:GLN:HG3	1:V:68:GLY:O	2.15	0.45
1:L:18:TYR:HB3	1:L:22:SER:HB2	1.98	0.45
1:I:176:THR:HG22	1:I:178:GLU:H	1.81	0.45
1:L:52:GLN:HG3	1:L:86:PRO:HD3	1.97	0.45
1:A:109:LYS:HD2	1:A:110:GLY:H	1.82	0.45
1:I:15:GLU:HG2	1:K:16:ARG:HG2	1.98	0.45
1:M:176:THR:HG22	1:M:178:GLU:N	2.32	0.45
1:C:93:ILE:HG22	1:C:115:LEU:CD1	2.47	0.45
1:I:98:SER:OG	1:I:99:MET:N	2.50	0.45
1:A:162:ILE:HG12	2:A:282:HOH:O	2.16	0.45
1:N:115:LEU:HD13	1:S:79:ASP:HB3	1.97	0.45
1:V:115:LEU:HD13	1:B:79:ASP:HB3	1.99	0.44
1:A:79:ASP:HB3	1:G:115:LEU:CD1	2.47	0.44
1:M:28:ARG:HG2	1:M:51:LEU:HD22	2.00	0.44
1:S:58:LYS:O	1:S:86:PRO:HB3	2.18	0.44
1:G:75:PHE:CZ	1:G:149:LYS:HD2	2.52	0.44
1:I:89:GLN:HG2	1:I:111:LYS:HB3	2.00	0.44
1:M:52:GLN:HG3	1:M:86:PRO:HD3	2.00	0.44
1:V:176:THR:HG22	1:V:179:GLU:H	1.83	0.44
1:A:42:ASN:HD21	1:G:31:MET:HB3	1.83	0.44
1:G:120:VAL:HG11	1:G:185:LEU:HD13	1.99	0.44
1:K:93:ILE:HG22	1:K:115:LEU:HD12	1.99	0.44
1:E:176:THR:HG22	1:E:178:GLU:H	1.82	0.44
1:G:191:VAL:CG2	1:G:192:PRO:HA	2.48	0.44
1:I:173:ASN:C	1:I:173:ASN:HD22	2.21	0.43
1:K:95[B]:MET:HG2	1:K:119:GLU:HB2	2.00	0.43
1:L:98:SER:OG	1:L:99:MET:N	2.51	0.43
1:N:143:ILE:HA	1:N:146:THR:HG23	2.00	0.43
1:T:171:ARG:HE	1:T:171:ARG:HB3	1.62	0.43
1:K:160:GLN:NE2	1:K:164:LYS:HD3	2.33	0.43
1:E:147:ARG:HD3	2:E:531:HOH:O	2.17	0.43
1:T:176:THR:CG2	1:T:179:GLU:H	2.31	0.43
1:E:98:SER:OG	1:E:99:MET:N	2.51	0.43
1:I:113:PHE:HB3	1:I:190:MET:HG3	2.01	0.43
1:N:106:ALA:HA	1:N:157:ARG:HD2	2.00	0.43
1:S:18:TYR:HB3	1:S:22:SER:HB2	2.01	0.43
1:T:98:SER:OG	1:T:99:MET:N	2.50	0.43
1:C:98:SER:OG	1:C:99:MET:N	2.52	0.43
1:I:67:PRO:HA	1:I:97:ALA:HB3	2.00	0.43
1:S:160:GLN:HE21	1:S:164:LYS:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:LYS:O	1:L:86:PRO:HB3	2.19	0.43
1:I:33:GLY:HA2	1:I:65:ASN:O	2.18	0.43
1:S:95[B]:MET:HG2	1:S:119:GLU:HB2	1.99	0.43
1:A:17:ALA:HB3	1:G:8:ILE:HG13	2.00	0.43
1:I:123:HIS:C	1:I:123:HIS:ND1	2.71	0.43
1:B:119:GLU:OE2	1:C:142:HIS:HE1	2.01	0.43
1:F:4:ILE:HA	1:F:5:PRO:HD3	1.87	0.43
1:F:125:PRO:HD2	1:F:147:ARG:HG2	2.01	0.42
1:I:125:PRO:CD	1:I:147:ARG:HG2	2.48	0.42
1:M:23:ARG:HH21	1:M:26:LYS:HD3	1.82	0.42
1:T:143:ILE:HA	1:T:146:THR:HG23	2.01	0.42
1:V:56:SER:HB2	1:V:85:LYS:HD3	2.01	0.42
1:V:176:THR:HG23	2:V:247:HOH:O	2.18	0.42
1:E:160:GLN:HG3	1:E:164:LYS:HD3	2.01	0.42
1:I:93:ILE:HG22	1:I:115:LEU:CD1	2.47	0.42
1:F:16:ARG:NH1	1:F:26:LYS:HE2	2.34	0.42
1:M:95[B]:MET:HG2	1:M:119:GLU:HB2	2.01	0.42
1:M:115:LEU:HD13	1:N:79:ASP:HB3	2.01	0.42
1:V:123:HIS:C	1:V:123:HIS:HD1	2.22	0.42
1:I:143:ILE:HA	1:I:146:THR:HG23	2.01	0.42
1:V:58:LYS:O	1:V:86:PRO:HB3	2.19	0.42
1:V:71:VAL:HG22	1:V:99:MET:HE3	2.01	0.42
1:N:40:VAL:O	1:N:44:ILE:HG12	2.19	0.42
1:G:191:VAL:HG22	1:G:192:PRO:HA	2.02	0.42
1:T:125:PRO:HD2	1:T:147:ARG:HG2	2.01	0.42
1:A:124:GLN:HE22	1:K:134:THR:HG23	1.85	0.42
1:V:176:THR:HG22	1:V:178:GLU:H	1.85	0.42
1:N:35:GLN:HG3	1:N:68:GLY:O	2.19	0.42
1:G:98:SER:OG	1:G:99:MET:N	2.53	0.41
1:K:125:PRO:HD2	1:K:147:ARG:HG2	2.02	0.41
1:G:176:THR:HG23	2:G:468:HOH:O	2.19	0.41
1:K:93:ILE:HD12	1:L:76:ALA:HB1	2.02	0.41
1:G:128:GLY:HA2	1:L:129:ALA:O	2.21	0.41
1:M:89:GLN:HE21	1:M:89:GLN:HB3	1.70	0.41
1:N:122:ILE:HG13	1:N:173:ASN:HB3	2.03	0.41
1:V:20:ILE:H	1:V:20:ILE:HG13	1.65	0.41
1:A:147:ARG:HD3	2:A:361:HOH:O	2.21	0.41
1:K:142:HIS:O	1:K:146:THR:HG22	2.21	0.41
1:B:147:ARG:HD3	2:B:207:HOH:O	2.21	0.41
1:K:98:SER:CB	1:K:123:HIS:CE1	3.04	0.41
1:N:191:VAL:CG2	1:N:192:PRO:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:HG22	1:A:192:PRO:HD2	2.02	0.40
1:F:23:ARG:HH21	1:F:26:LYS:HB3	1.86	0.40
1:B:8:ILE:HB	1:C:17:ALA:HB3	2.03	0.40
1:M:4:ILE:HA	1:M:5:PRO:HD3	1.91	0.40
1:K:58:LYS:O	1:K:86:PRO:HB3	2.22	0.40
1:T:176:THR:HG23	1:T:178:GLU:H	1.85	0.40
1:V:142:HIS:O	1:V:146:THR:HG22	2.22	0.40
1:C:142:HIS:O	1:C:146:THR:CG2	2.69	0.40
1:E:16:ARG:HB2	1:F:8:ILE:HD13	2.04	0.40
1:K:18:TYR:HD2	1:K:22:SER:HB3	1.85	0.40
1:L:191:VAL:HG22	1:L:192:PRO:CA	2.43	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	189/197 (96%)	184 (97%)	5 (3%)	0	100	100
1	B	179/197 (91%)	175 (98%)	4 (2%)	0	100	100
1	C	183/197 (93%)	180 (98%)	3 (2%)	0	100	100
1	E	183/197 (93%)	180 (98%)	3 (2%)	0	100	100
1	F	182/197 (92%)	179 (98%)	3 (2%)	0	100	100
1	G	177/197 (90%)	174 (98%)	3 (2%)	0	100	100
1	I	187/197 (95%)	184 (98%)	3 (2%)	0	100	100
1	K	183/197 (93%)	180 (98%)	3 (2%)	0	100	100
1	L	181/197 (92%)	179 (99%)	2 (1%)	0	100	100
1	M	182/197 (92%)	176 (97%)	6 (3%)	0	100	100
1	N	182/197 (92%)	179 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	182/197 (92%)	179 (98%)	3 (2%)	0	100	100
1	T	183/197 (93%)	181 (99%)	2 (1%)	0	100	100
1	V	189/197 (96%)	187 (99%)	2 (1%)	0	100	100
All	All	2562/2758 (93%)	2517 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	158/164 (96%)	144 (91%)	14 (9%)	9	10
1	B	151/164 (92%)	141 (93%)	10 (7%)	16	20
1	C	155/164 (94%)	142 (92%)	13 (8%)	11	12
1	E	155/164 (94%)	144 (93%)	11 (7%)	14	17
1	F	154/164 (94%)	145 (94%)	9 (6%)	20	25
1	G	150/164 (92%)	142 (95%)	8 (5%)	22	29
1	I	156/164 (95%)	143 (92%)	13 (8%)	11	12
1	K	154/164 (94%)	143 (93%)	11 (7%)	14	17
1	L	153/164 (93%)	137 (90%)	16 (10%)	7	7
1	M	154/164 (94%)	144 (94%)	10 (6%)	17	21
1	N	154/164 (94%)	139 (90%)	15 (10%)	8	8
1	S	154/164 (94%)	142 (92%)	12 (8%)	12	14
1	T	154/164 (94%)	140 (91%)	14 (9%)	9	10
1	V	158/164 (96%)	145 (92%)	13 (8%)	11	13
All	All	2160/2296 (94%)	1991 (92%)	169 (8%)	12	14

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	13	ARG
1	V	23	ARG
1	V	72	THR
1	V	123	HIS
1	V	146	THR
1	V	147	ARG
1	V	154	LEU
1	V	157	ARG
1	V	166	GLN
1	V	171	ARG
1	V	173	ASN
1	V	176	THR
1	V	182	GLU
1	A	19	ASP
1	A	23	ARG
1	A	24	LEU
1	A	72	THR
1	A	109	LYS
1	A	123	HIS
1	A	146	THR
1	A	147	ARG
1	A	157	ARG
1	A	162	ILE
1	A	166	GLN
1	A	171	ARG
1	A	173	ASN
1	A	191	VAL
1	B	20	ILE
1	B	23	ARG
1	B	57	GLU
1	B	72	THR
1	B	109	LYS
1	B	123	HIS
1	B	146	THR
1	B	147	ARG
1	B	154	LEU
1	B	166	GLN
1	C	20	ILE
1	C	23	ARG
1	C	24	LEU
1	C	72	THR
1	C	109	LYS
1	C	121	MET

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Mol	Chain	Res	Type
1	C	123	HIS
1	C	124	GLN
1	C	146	THR
1	C	147	ARG
1	C	166	GLN
1	C	171	ARG
1	C	173	ASN
1	E	16	ARG
1	E	23	ARG
1	E	24	LEU
1	E	123	HIS
1	E	130	GLN
1	E	146	THR
1	E	147	ARG
1	E	154	LEU
1	E	157	ARG
1	E	166	GLN
1	E	173	ASN
1	F	20	ILE
1	F	23	ARG
1	F	35	GLN
1	F	72	THR
1	F	123	HIS
1	F	147	ARG
1	F	154	LEU
1	F	157	ARG
1	F	173	ASN
1	G	18	TYR
1	G	42	ASN
1	G	72	THR
1	G	123	HIS
1	G	147	ARG
1	G	166	GLN
1	G	173	ASN
1	G	176	THR
1	I	15	GLU
1	I	20	ILE
1	I	23	ARG
1	I	39	ASN
1	I	109	LYS
1	I	123	HIS
1	I	146	THR

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Mol	Chain	Res	Type
1	I	147	ARG
1	I	154	LEU
1	I	166	GLN
1	I	171	ARG
1	I	173	ASN
1	I	175	LEU
1	K	20	ILE
1	K	23	ARG
1	K	42	ASN
1	K	123	HIS
1	K	145	LYS
1	K	146	THR
1	K	147	ARG
1	K	166	GLN
1	K	173	ASN
1	K	182	GLU
1	K	191	VAL
1	L	19	ASP
1	L	20	ILE
1	L	35	GLN
1	L	72	THR
1	L	95[A]	MET
1	L	95[B]	MET
1	L	99	MET
1	L	123	HIS
1	L	146	THR
1	L	147	ARG
1	L	157	ARG
1	L	166	GLN
1	L	171	ARG
1	L	173	ASN
1	L	182	GLU
1	L	191	VAL
1	M	20	ILE
1	M	23	ARG
1	M	35	GLN
1	M	123	HIS
1	M	147	ARG
1	M	166	GLN
1	M	171	ARG
1	M	173	ASN
1	M	188	GLU

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Mol	Chain	Res	Type
1	M	191	VAL
1	N	19	ASP
1	N	20	ILE
1	N	23	ARG
1	N	72	THR
1	N	98	SER
1	N	99	MET
1	N	123	HIS
1	N	145	LYS
1	N	146	THR
1	N	147	ARG
1	N	157	ARG
1	N	166	GLN
1	N	171	ARG
1	N	173	ASN
1	N	188	GLU
1	S	23	ARG
1	S	24	LEU
1	S	72	THR
1	S	98	SER
1	S	121	MET
1	S	123	HIS
1	S	146	THR
1	S	147	ARG
1	S	166	GLN
1	S	171	ARG
1	S	173	ASN
1	S	191	VAL
1	T	19	ASP
1	T	23	ARG
1	T	35	GLN
1	T	72	THR
1	T	123	HIS
1	T	146	THR
1	T	147	ARG
1	T	154	LEU
1	T	166	GLN
1	T	171	ARG
1	T	173	ASN
1	T	175	LEU
1	T	176	THR
1	T	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	83	HIS
1	V	89	GLN
1	V	117	ASN
1	V	160	GLN
1	V	166	GLN
1	V	173	ASN
1	A	39	ASN
1	A	42	ASN
1	A	82	GLN
1	A	89	GLN
1	A	117	ASN
1	A	123	HIS
1	A	124	GLN
1	A	151	ASN
1	A	160	GLN
1	A	166	GLN
1	A	173	ASN
1	B	39	ASN
1	B	82	GLN
1	B	89	GLN
1	B	117	ASN
1	B	123	HIS
1	B	151	ASN
1	B	160	GLN
1	B	166	GLN
1	B	173	ASN
1	C	83	HIS
1	C	89	GLN
1	C	142	HIS
1	C	151	ASN
1	C	160	GLN
1	C	166	GLN
1	C	173	ASN
1	E	39	ASN
1	E	82	GLN
1	E	89	GLN
1	E	117	ASN
1	E	130	GLN
1	E	151	ASN
1	E	160	GLN
1	E	166	GLN

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Mol	Chain	Res	Type
1	E	173	ASN
1	F	39	ASN
1	F	82	GLN
1	F	83	HIS
1	F	89	GLN
1	F	117	ASN
1	F	123	HIS
1	F	151	ASN
1	F	160	GLN
1	F	166	GLN
1	F	173	ASN
1	G	39	ASN
1	G	82	GLN
1	G	89	GLN
1	G	142	HIS
1	G	151	ASN
1	G	160	GLN
1	G	166	GLN
1	G	173	ASN
1	I	39	ASN
1	I	82	GLN
1	I	89	GLN
1	I	117	ASN
1	I	151	ASN
1	I	160	GLN
1	I	166	GLN
1	I	173	ASN
1	K	82	GLN
1	K	89	GLN
1	K	123	HIS
1	K	151	ASN
1	K	160	GLN
1	K	166	GLN
1	K	173	ASN
1	L	39	ASN
1	L	42	ASN
1	L	89	GLN
1	L	117	ASN
1	L	142	HIS
1	L	151	ASN
1	L	160	GLN
1	L	166	GLN

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Mol	Chain	Res	Type
1	L	173	ASN
1	M	39	ASN
1	M	42	ASN
1	M	82	GLN
1	M	89	GLN
1	M	117	ASN
1	M	160	GLN
1	M	166	GLN
1	M	173	ASN
1	N	39	ASN
1	N	89	GLN
1	N	142	HIS
1	N	151	ASN
1	N	166	GLN
1	N	173	ASN
1	S	39	ASN
1	S	89	GLN
1	S	117	ASN
1	S	142	HIS
1	S	151	ASN
1	S	160	GLN
1	S	166	GLN
1	S	173	ASN
1	T	35	GLN
1	T	42	ASN
1	T	82	GLN
1	T	89	GLN
1	T	117	ASN
1	T	151	ASN
1	T	160	GLN
1	T	166	GLN
1	T	173	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	189/197 (95%)	-0.04	4 (2%)	63	69	20, 25, 46, 55	0
1	B	182/197 (92%)	-0.17	2 (1%)	80	84	19, 24, 36, 60	0
1	C	185/197 (93%)	0.02	3 (1%)	72	77	18, 26, 43, 56	0
1	E	185/197 (93%)	-0.03	4 (2%)	62	68	23, 30, 44, 57	0
1	F	185/197 (93%)	0.08	8 (4%)	35	40	24, 31, 45, 64	0
1	G	180/197 (91%)	-0.09	3 (1%)	70	75	22, 29, 37, 61	0
1	I	189/197 (95%)	0.08	7 (3%)	41	47	20, 27, 51, 59	0
1	K	186/197 (94%)	0.02	7 (3%)	40	45	23, 30, 52, 62	0
1	L	184/197 (93%)	0.27	8 (4%)	35	40	28, 34, 51, 75	0
1	M	185/197 (93%)	0.10	4 (2%)	62	68	27, 33, 47, 56	0
1	N	185/197 (93%)	-0.00	7 (3%)	40	45	24, 29, 44, 59	0
1	S	184/197 (93%)	-0.04	8 (4%)	35	40	20, 25, 42, 63	0
1	T	186/197 (94%)	-0.07	6 (3%)	47	53	20, 25, 48, 62	0
1	V	189/197 (95%)	-0.14	1 (0%)	91	93	19, 25, 43, 52	0
All	All	2594/2758 (94%)	-0.00	72 (2%)	53	59	18, 28, 48, 75	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	17	ALA	7.5
1	L	10	THR	6.8
1	L	9	GLU	6.6
1	L	8	ILE	6.6
1	L	16	ARG	6.2
1	K	15	GLU	5.8
1	S	17	ALA	5.6
1	N	16	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
1	K	17	ALA	5.3
1	I	14	GLY	5.2
1	T	14	GLY	5.0
1	N	15	GLU	5.0
1	S	15	GLU	4.9
1	K	14	GLY	4.6
1	S	8	ILE	4.6
1	A	13	ARG	4.5
1	K	10	THR	4.4
1	F	15	GLU	4.4
1	S	16	ARG	4.3
1	F	10	THR	4.3
1	G	8	ILE	4.2
1	I	16	ARG	4.1
1	T	17	ALA	4.1
1	I	12	ASN	4.1
1	I	11	THR	4.1
1	E	16	ARG	4.0
1	I	13	ARG	4.0
1	A	11	THR	3.9
1	A	12	ASN	3.9
1	I	15	GLU	3.9
1	T	16	ARG	3.8
1	M	16	ARG	3.7
1	V	15	GLU	3.5
1	E	15	GLU	3.5
1	T	15	GLU	3.4
1	E	10	THR	3.4
1	M	10	THR	3.4
1	N	10	THR	3.3
1	F	16	ARG	3.3
1	B	4	ILE	3.3
1	C	16	ARG	3.2
1	S	9	GLU	3.1
1	E	17	ALA	3.1
1	A	15	GLU	3.0
1	K	4	ILE	3.0
1	G	7	VAL	2.9
1	T	10	THR	2.9
1	N	17	ALA	2.9
1	S	7	VAL	2.8
1	F	9	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	191	VAL	2.8
1	N	9	GLU	2.8
1	L	7	VAL	2.7
1	M	15	GLU	2.7
1	K	16	ARG	2.7
1	T	18	TYR	2.6
1	L	4	ILE	2.6
1	C	11	THR	2.5
1	K	18	TYR	2.3
1	F	8	ILE	2.3
1	F	85	LYS	2.3
1	S	18	TYR	2.2
1	S	192	PRO	2.2
1	M	130	GLN	2.2
1	N	7	VAL	2.2
1	G	6	THR	2.2
1	F	57	GLU	2.2
1	F	17	ALA	2.1
1	B	8	ILE	2.1
1	N	57	GLU	2.1
1	C	39	ASN	2.0
1	L	18	TYR	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.