Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:22 PM GMT

PDB ID	:	3QWD
Title	:	Crystal structure of ClpP from Staphylococcus aureus
Authors	:	Geiger, S.R.; Boettcher, T.; Sieber, S.A.; Cramer, P.
Deposited on	:	2011-02-28
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

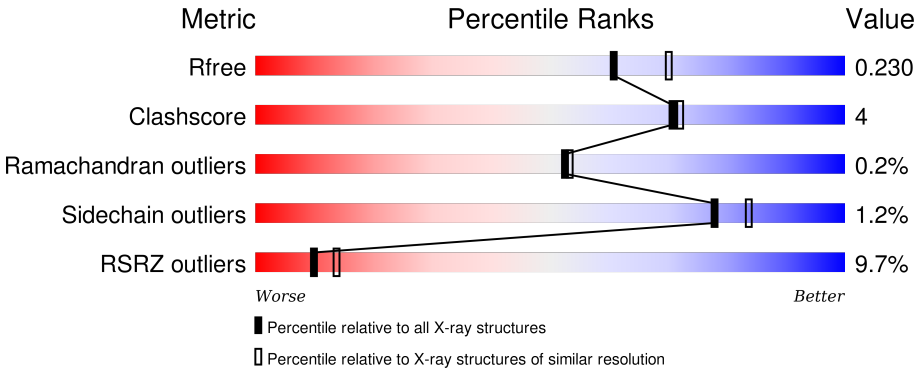
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	8% 80% 12% 8%
1	B	203	12% 81% 11% 8%
1	C	203	10% 80% 10% • 8%
1	D	203	8% 79% 11% 10%
1	E	203	6% 85% 8% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	203	8% 79% 10% 10%
1	G	203	8% 79% 12% 9%
1	H	203	8% 81% 13% 5%
1	I	203	6% 81% 9% 8%
1	J	203	11% 84% 8% 8%
1	K	203	6% 80% 8% 12%
1	L	203	7% 79% 10% 11%
1	M	203	11% 83% 8% 8%
1	N	203	13% 80% 9% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20404 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	187	Total	C	N	O	S	0	3	0
			1455	920	244	283	8			
1	B	187	Total	C	N	O	S	0	3	0
			1454	919	244	284	7			
1	C	186	Total	C	N	O	S	0	2	0
			1444	914	243	280	7			
1	D	182	Total	C	N	O	S	0	2	0
			1413	895	238	273	7			
1	E	188	Total	C	N	O	S	0	3	0
			1459	921	247	284	7			
1	F	182	Total	C	N	O	S	0	2	0
			1418	896	239	276	7			
1	G	185	Total	C	N	O	S	0	1	0
			1424	899	240	278	7			
1	H	192	Total	C	N	O	S	0	2	0
			1489	941	253	288	7			
1	I	186	Total	C	N	O	S	0	2	0
			1442	912	242	281	7			
1	J	186	Total	C	N	O	S	0	2	0
			1437	909	242	279	7			
1	K	179	Total	C	N	O	S	0	4	0
			1411	895	236	273	7			
1	L	180	Total	C	N	O	S	0	3	0
			1413	895	237	274	7			
1	M	186	Total	C	N	O	S	0	1	0
			1436	907	241	281	7			
1	N	183	Total	C	N	O	S	0	1	0
			1409	891	236	275	7			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	196	TRP	-	EXPRESSION TAG	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	SER	-	EXPRESSION TAG	UNP Q2G036
A	198	HIS	-	EXPRESSION TAG	UNP Q2G036
A	199	PRO	-	EXPRESSION TAG	UNP Q2G036
A	200	GLN	-	EXPRESSION TAG	UNP Q2G036
A	201	PHE	-	EXPRESSION TAG	UNP Q2G036
A	202	GLU	-	EXPRESSION TAG	UNP Q2G036
A	203	LYS	-	EXPRESSION TAG	UNP Q2G036
B	196	TRP	-	EXPRESSION TAG	UNP Q2G036
B	197	SER	-	EXPRESSION TAG	UNP Q2G036
B	198	HIS	-	EXPRESSION TAG	UNP Q2G036
B	199	PRO	-	EXPRESSION TAG	UNP Q2G036
B	200	GLN	-	EXPRESSION TAG	UNP Q2G036
B	201	PHE	-	EXPRESSION TAG	UNP Q2G036
B	202	GLU	-	EXPRESSION TAG	UNP Q2G036
B	203	LYS	-	EXPRESSION TAG	UNP Q2G036
C	196	TRP	-	EXPRESSION TAG	UNP Q2G036
C	197	SER	-	EXPRESSION TAG	UNP Q2G036
C	198	HIS	-	EXPRESSION TAG	UNP Q2G036
C	199	PRO	-	EXPRESSION TAG	UNP Q2G036
C	200	GLN	-	EXPRESSION TAG	UNP Q2G036
C	201	PHE	-	EXPRESSION TAG	UNP Q2G036
C	202	GLU	-	EXPRESSION TAG	UNP Q2G036
C	203	LYS	-	EXPRESSION TAG	UNP Q2G036
D	196	TRP	-	EXPRESSION TAG	UNP Q2G036
D	197	SER	-	EXPRESSION TAG	UNP Q2G036
D	198	HIS	-	EXPRESSION TAG	UNP Q2G036
D	199	PRO	-	EXPRESSION TAG	UNP Q2G036
D	200	GLN	-	EXPRESSION TAG	UNP Q2G036
D	201	PHE	-	EXPRESSION TAG	UNP Q2G036
D	202	GLU	-	EXPRESSION TAG	UNP Q2G036
D	203	LYS	-	EXPRESSION TAG	UNP Q2G036
E	196	TRP	-	EXPRESSION TAG	UNP Q2G036
E	197	SER	-	EXPRESSION TAG	UNP Q2G036
E	198	HIS	-	EXPRESSION TAG	UNP Q2G036
E	199	PRO	-	EXPRESSION TAG	UNP Q2G036
E	200	GLN	-	EXPRESSION TAG	UNP Q2G036
E	201	PHE	-	EXPRESSION TAG	UNP Q2G036
E	202	GLU	-	EXPRESSION TAG	UNP Q2G036
E	203	LYS	-	EXPRESSION TAG	UNP Q2G036
F	196	TRP	-	EXPRESSION TAG	UNP Q2G036
F	197	SER	-	EXPRESSION TAG	UNP Q2G036
F	198	HIS	-	EXPRESSION TAG	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	199	PRO	-	EXPRESSION TAG	UNP Q2G036
F	200	GLN	-	EXPRESSION TAG	UNP Q2G036
F	201	PHE	-	EXPRESSION TAG	UNP Q2G036
F	202	GLU	-	EXPRESSION TAG	UNP Q2G036
F	203	LYS	-	EXPRESSION TAG	UNP Q2G036
G	196	TRP	-	EXPRESSION TAG	UNP Q2G036
G	197	SER	-	EXPRESSION TAG	UNP Q2G036
G	198	HIS	-	EXPRESSION TAG	UNP Q2G036
G	199	PRO	-	EXPRESSION TAG	UNP Q2G036
G	200	GLN	-	EXPRESSION TAG	UNP Q2G036
G	201	PHE	-	EXPRESSION TAG	UNP Q2G036
G	202	GLU	-	EXPRESSION TAG	UNP Q2G036
G	203	LYS	-	EXPRESSION TAG	UNP Q2G036
H	196	TRP	-	EXPRESSION TAG	UNP Q2G036
H	197	SER	-	EXPRESSION TAG	UNP Q2G036
H	198	HIS	-	EXPRESSION TAG	UNP Q2G036
H	199	PRO	-	EXPRESSION TAG	UNP Q2G036
H	200	GLN	-	EXPRESSION TAG	UNP Q2G036
H	201	PHE	-	EXPRESSION TAG	UNP Q2G036
H	202	GLU	-	EXPRESSION TAG	UNP Q2G036
H	203	LYS	-	EXPRESSION TAG	UNP Q2G036
I	196	TRP	-	EXPRESSION TAG	UNP Q2G036
I	197	SER	-	EXPRESSION TAG	UNP Q2G036
I	198	HIS	-	EXPRESSION TAG	UNP Q2G036
I	199	PRO	-	EXPRESSION TAG	UNP Q2G036
I	200	GLN	-	EXPRESSION TAG	UNP Q2G036
I	201	PHE	-	EXPRESSION TAG	UNP Q2G036
I	202	GLU	-	EXPRESSION TAG	UNP Q2G036
I	203	LYS	-	EXPRESSION TAG	UNP Q2G036
J	196	TRP	-	EXPRESSION TAG	UNP Q2G036
J	197	SER	-	EXPRESSION TAG	UNP Q2G036
J	198	HIS	-	EXPRESSION TAG	UNP Q2G036
J	199	PRO	-	EXPRESSION TAG	UNP Q2G036
J	200	GLN	-	EXPRESSION TAG	UNP Q2G036
J	201	PHE	-	EXPRESSION TAG	UNP Q2G036
J	202	GLU	-	EXPRESSION TAG	UNP Q2G036
J	203	LYS	-	EXPRESSION TAG	UNP Q2G036
K	196	TRP	-	EXPRESSION TAG	UNP Q2G036
K	197	SER	-	EXPRESSION TAG	UNP Q2G036
K	198	HIS	-	EXPRESSION TAG	UNP Q2G036
K	199	PRO	-	EXPRESSION TAG	UNP Q2G036
K	200	GLN	-	EXPRESSION TAG	UNP Q2G036

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	201	PHE	-	EXPRESSION TAG	UNP Q2G036
K	202	GLU	-	EXPRESSION TAG	UNP Q2G036
K	203	LYS	-	EXPRESSION TAG	UNP Q2G036
L	196	TRP	-	EXPRESSION TAG	UNP Q2G036
L	197	SER	-	EXPRESSION TAG	UNP Q2G036
L	198	HIS	-	EXPRESSION TAG	UNP Q2G036
L	199	PRO	-	EXPRESSION TAG	UNP Q2G036
L	200	GLN	-	EXPRESSION TAG	UNP Q2G036
L	201	PHE	-	EXPRESSION TAG	UNP Q2G036
L	202	GLU	-	EXPRESSION TAG	UNP Q2G036
L	203	LYS	-	EXPRESSION TAG	UNP Q2G036
M	196	TRP	-	EXPRESSION TAG	UNP Q2G036
M	197	SER	-	EXPRESSION TAG	UNP Q2G036
M	198	HIS	-	EXPRESSION TAG	UNP Q2G036
M	199	PRO	-	EXPRESSION TAG	UNP Q2G036
M	200	GLN	-	EXPRESSION TAG	UNP Q2G036
M	201	PHE	-	EXPRESSION TAG	UNP Q2G036
M	202	GLU	-	EXPRESSION TAG	UNP Q2G036
M	203	LYS	-	EXPRESSION TAG	UNP Q2G036
N	196	TRP	-	EXPRESSION TAG	UNP Q2G036
N	197	SER	-	EXPRESSION TAG	UNP Q2G036
N	198	HIS	-	EXPRESSION TAG	UNP Q2G036
N	199	PRO	-	EXPRESSION TAG	UNP Q2G036
N	200	GLN	-	EXPRESSION TAG	UNP Q2G036
N	201	PHE	-	EXPRESSION TAG	UNP Q2G036
N	202	GLU	-	EXPRESSION TAG	UNP Q2G036
N	203	LYS	-	EXPRESSION TAG	UNP Q2G036

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	L	2	Total Cl 2 2	0	0
2	M	1	Total Cl 1 1	0	0

- Molecule 3 is water.

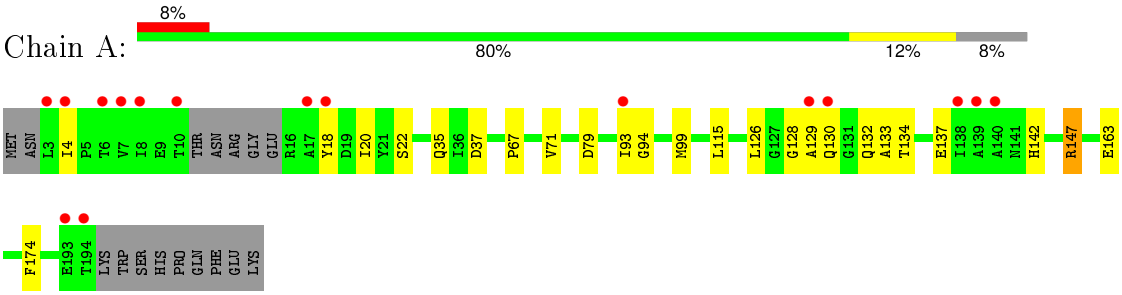
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	28	Total O 28 28	0	0
3	C	19	Total O 19 19	0	0
3	D	16	Total O 16 16	0	0
3	E	25	Total O 25 25	0	0
3	F	10	Total O 10 10	0	0
3	G	27	Total O 27 27	0	0
3	H	22	Total O 22 22	0	0
3	I	23	Total O 23 23	0	0
3	J	16	Total O 16 16	0	0
3	K	17	Total O 17 17	0	0
3	L	22	Total O 22 22	0	0
3	M	9	Total O 9 9	0	0
3	N	20	Total O 20 20	0	0

3 Residue-property plots (i)

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

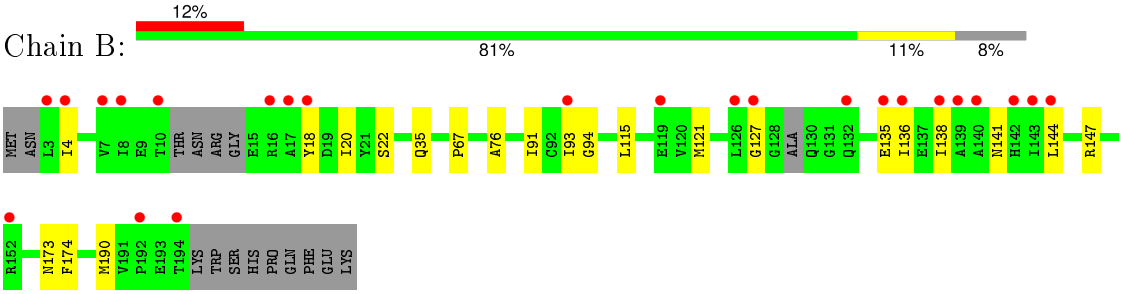
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



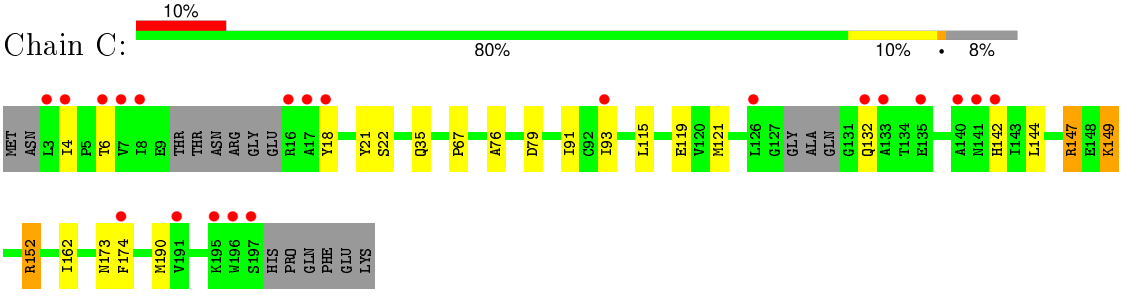
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



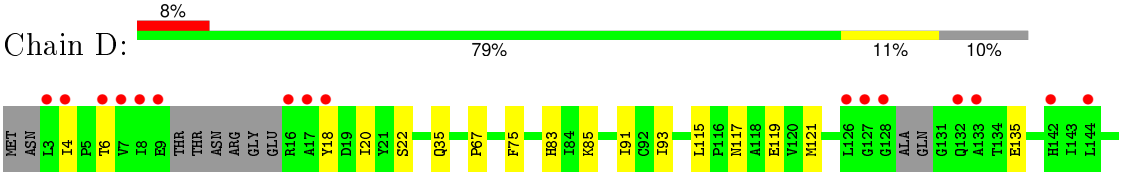
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:

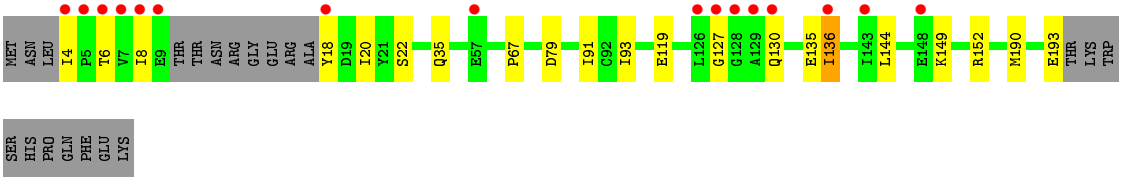


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:

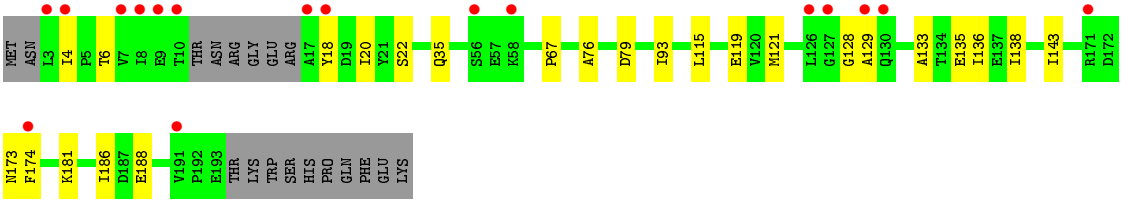
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



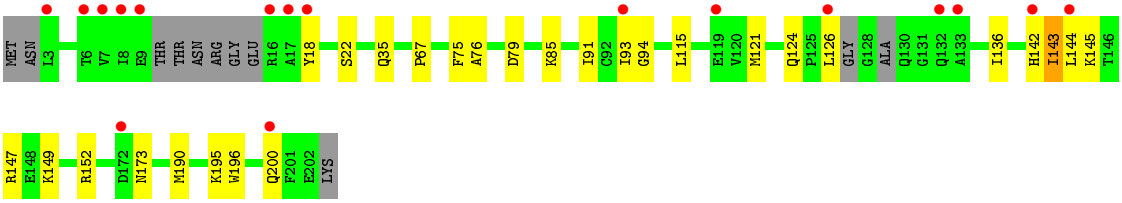
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



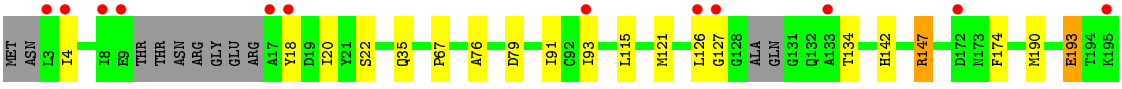
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

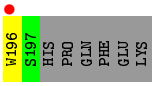
Chain H:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

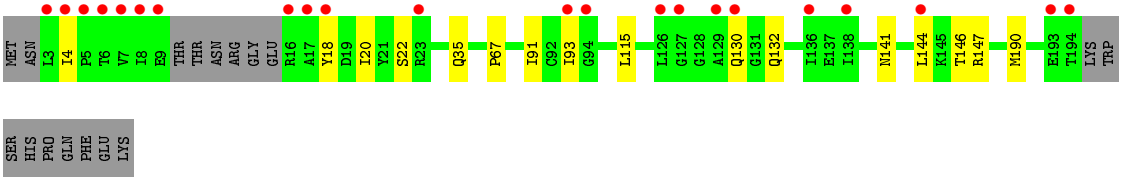
Chain I:





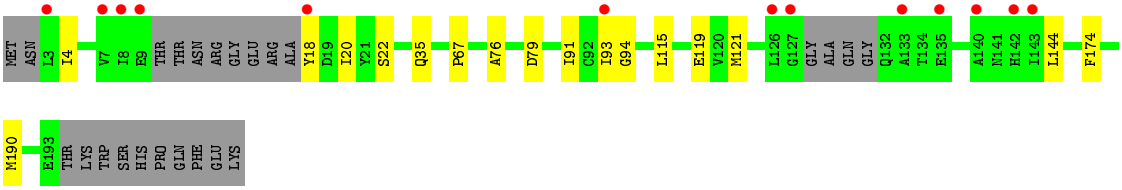
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



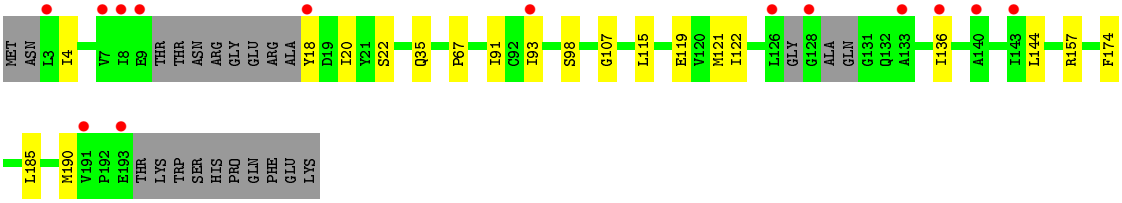
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



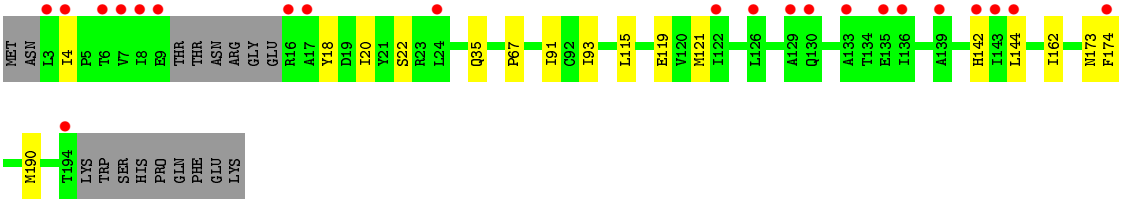
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



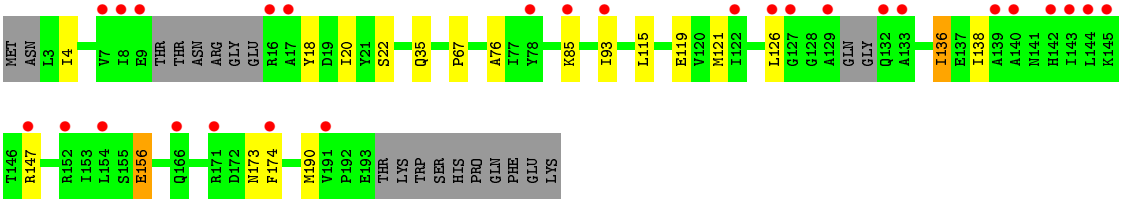
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:


MET
ASN
L3
I4
V7
I8
E9
THR
THR
ASN
ARG
GLY
GLU
R16
A17
Y18
D19
I20
Y21
S22
Q35
P67
A76
I77
Y78
K85
I93
L115
E119
V120
M121
I122
L126
G127
G128
A129
GLN
GLY
Q132
A133
I136
E137
I138
A139
A140
N141
H142
I143
L144
K145
T146
R147
R152
I153
L154
S155
E156
Q166
R171
D172
N173
F174
M190
V191
P192
E193
THR
LYS
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	172.05Å 177.97Å 100.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.99 – 2.10 88.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (88.99-2.10) 99.5 (88.99-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.208 , 0.226 0.226 , 0.230	Depositor DCC
R_{free} test set	8961 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.3	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 179406 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20404	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	0/1483	0.67	0/2002
1	B	0.48	0/1481	0.65	0/1998
1	C	0.53	0/1468	0.67	0/1980
1	D	0.52	0/1437	0.69	0/1938
1	E	0.56	0/1487	0.70	0/2007
1	F	0.49	0/1443	0.66	0/1947
1	G	0.50	0/1445	0.67	0/1951
1	H	0.48	0/1516	0.67	0/2046
1	I	0.51	0/1467	0.65	0/1980
1	J	0.47	0/1462	0.68	0/1974
1	K	0.45	0/1441	0.64	0/1944
1	L	0.48	0/1439	0.66	0/1939
1	M	0.45	0/1457	0.65	0/1967
1	N	0.47	0/1429	0.69	1/1928 (0.1%)
All	All	0.49	0/20455	0.67	1/27601 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	156	GLU	CB-CG-CD	5.21	128.28	114.20

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	1455	0	1476	17	0
1	B	1454	0	1464	16	0
1	C	1444	0	1460	23	0
1	D	1413	0	1433	16	0
1	E	1459	0	1472	13	0
1	F	1418	0	1435	16	0
1	G	1424	0	1438	19	0
1	H	1489	0	1480	17	0
1	I	1442	0	1446	17	0
1	J	1437	0	1449	11	0
1	K	1411	0	1434	14	0
1	L	1413	0	1434	15	0
1	M	1436	0	1453	11	0
1	N	1409	0	1419	14	0
2	A	1	0	0	1	0
2	B	1	0	0	0	0
2	C	1	0	0	1	0
2	D	1	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
3	A	39	0	0	0	0
3	B	28	0	0	1	0
3	C	19	0	0	1	0
3	D	16	0	0	0	0
3	E	25	0	0	0	0
3	F	10	0	0	0	0
3	G	27	0	0	1	0
3	H	22	0	0	0	0
3	I	23	0	0	0	0
3	J	16	0	0	0	0
3	K	17	0	0	1	0
3	L	22	0	0	0	0
3	M	9	0	0	0	0
3	N	20	0	0	1	0
All	All	20404	0	20293	178	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 4.

All (178) 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:C:162:ILE:CG1	1:C:162:ILE:CD1	1.75	1.57
1:N:93:ILE:HG23	1:N:115:LEU:HD12	1.73	0.69
1:F:144:LEU:HD12	1:G:119:GLU:HG2	1.77	0.67
1:A:142[A]:HIS:CE1	2:A:204:CL:CL	2.88	0.64
1:F:35:GLN:HG3	1:F:67:PRO:HG2	1.82	0.62
1:G:35:GLN:HG3	1:G:67:PRO:HG2	1.82	0.61
1:E:144:LEU:HD12	1:F:119:GLU:HG2	1.81	0.61
1:E:35:GLN:HG3	1:E:67:PRO:HG2	1.82	0.61
1:H:124:GLN:O	1:H:147:ARG:NH2	2.34	0.61
1:C:152:ARG:NH1	1:C:162:ILE:HD11	2.15	0.61
1:A:35:GLN:HG3	1:A:67:PRO:HG2	1.83	0.60
1:J:35:GLN:HG3	1:J:67:PRO:HG2	1.83	0.60
1:D:35:GLN:HG3	1:D:67:PRO:HG2	1.83	0.60
1:C:4:ILE:HD12	1:C:21:TYR:HE1	1.64	0.60
1:C:35:GLN:HG3	1:C:67:PRO:HG2	1.83	0.60
1:B:35:GLN:HG3	1:B:67:PRO:HG2	1.83	0.60
1:H:35:GLN:HG3	1:H:67:PRO:HG2	1.85	0.59
1:M:35:GLN:HG3	1:M:67:PRO:HG2	1.82	0.59
1:L:35:GLN:HG3	1:L:67:PRO:HG2	1.85	0.59
1:A:128:GLY:HA3	1:A:133:ALA:HB3	1.83	0.59
1:K:35[A]:GLN:HG2	1:K:67:PRO:HG2	1.85	0.58
1:B:91:ILE:HG23	1:B:190:MET:HE2	1.86	0.58
1:N:35:GLN:HG3	1:N:67:PRO:HG2	1.85	0.58
1:A:93:ILE:HG23	1:A:115:LEU:HD12	1.86	0.57
1:F:136:ILE:HG22	1:G:174:PHE:HZ	1.69	0.57
1:I:35:GLN:HG3	1:I:67:PRO:HG2	1.87	0.56
1:G:128:GLY:HA3	1:G:133:ALA:HB3	1.86	0.56
1:C:93:ILE:HG23	1:C:115:LEU:HD12	1.88	0.56
1:F:4:ILE:HG23	1:F:20:ILE:HG22	1.88	0.56
1:M:4:ILE:HG23	1:M:20:ILE:HG22	1.87	0.55
1:N:4:ILE:HG23	1:N:20:ILE:HG22	1.87	0.55
1:B:4:ILE:HG23	1:B:20:ILE:HG22	1.87	0.55
1:L:4:ILE:HG23	1:L:20:ILE:HG22	1.89	0.55
1:J:4:ILE:HG23	1:J:20:ILE:HG22	1.89	0.55
1:C:142[B]:HIS:CE1	2:C:204:CL:CL	2.96	0.55
1:K:4:ILE:HG23	1:K:20:ILE:HG22	1.90	0.54
1:B:93:ILE:HG23	1:B:115:LEU:HD12	1.89	0.54
1:A:4:ILE:HG23	1:A:20:ILE:HG22	1.89	0.54
1:H:143:ILE:HG12	1:H:145:LYS:HD3	1.91	0.53
1:H:195:LYS:HA	1:N:85:LYS:HE2	1.90	0.53
1:I:4:ILE:HG23	1:I:20:ILE:HG22	1.90	0.53
1:H:76:ALA:HB1	1:I:93:ILE:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:79:ASP:HB3	1:J:115:LEU:HD13	1.91	0.52
1:N:115:LEU:HD23	1:N:190:MET:HB2	1.91	0.52
1:G:135:GLU:HA	1:G:138:ILE:HD12	1.92	0.52
1:A:79:ASP:HB3	1:B:115:LEU:HD13	1.91	0.52
1:H:136:ILE:HG23	1:I:174:PHE:HZ	1.74	0.52
1:C:144:LEU:HD12	1:D:119:GLU:HG2	1.91	0.52
1:G:93:ILE:HG23	1:G:115:LEU:HD12	1.93	0.51
1:D:4:ILE:HG23	1:D:20:ILE:HG22	1.91	0.51
1:F:93:ILE:O	1:F:93:ILE:HG13	2.10	0.51
1:H:93:ILE:HG22	1:N:76:ALA:HB1	1.92	0.51
1:H:79:ASP:HB3	1:I:115:LEU:HD13	1.93	0.50
1:E:4:ILE:HG23	1:E:20:ILE:HG22	1.93	0.50
1:A:126:LEU:HD23	1:A:147:ARG:HH21	1.77	0.50
1:M:121:MET:HG3	1:M:173:ASN:O	2.12	0.50
1:K:91:ILE:HG23	1:K:190:MET:HE2	1.93	0.50
1:J:144:LEU:HD12	1:K:119:GLU:HG2	1.94	0.50
1:H:85:LYS:HG2	1:I:193:GLU:HG2	1.94	0.50
1:B:18:TYR:HB3	1:B:22:SER:HB2	1.94	0.50
1:I:126:LEU:O	1:I:142:HIS:CE1	2.64	0.50
1:G:4:ILE:HG23	1:G:20:ILE:HG22	1.94	0.49
1:C:147:ARG:NH1	3:C:217:HOH:O	2.45	0.49
1:M:144:LEU:HD12	1:N:119:GLU:HG2	1.95	0.49
1:B:76:ALA:HB1	1:C:93:ILE:HG22	1.95	0.49
1:A:174:PHE:CE2	1:G:143:ILE:HD13	2.48	0.49
1:M:93:ILE:HG23	1:M:115:LEU:HD12	1.95	0.49
1:M:18:TYR:HB3	1:M:22:SER:HB2	1.95	0.49
1:M:121:MET:HB2	1:M:174:PHE:CE1	2.48	0.48
1:N:18:TYR:HB3	1:N:22:SER:HB2	1.95	0.48
1:B:91:ILE:HG23	1:B:190:MET:CE	2.43	0.48
1:N:136:ILE:H	1:N:136:ILE:HD12	1.78	0.48
1:E:18:TYR:HB3	1:E:22:SER:HB2	1.95	0.48
1:J:141:ASN:HA	1:J:146:THR:HG23	1.95	0.48
1:J:93:ILE:HG23	1:J:115:LEU:HD12	1.95	0.48
1:K:18:TYR:HB3	1:K:22:SER:HB2	1.95	0.48
1:A:37:ASP:HB3	1:A:132:GLN:HG3	1.95	0.48
1:K:93:ILE:HG23	1:K:115:LEU:HD12	1.96	0.48
1:H:93:ILE:HG23	1:H:115:LEU:HD12	1.95	0.48
1:I:18:TYR:HB3	1:I:22:SER:HB2	1.96	0.48
1:C:91:ILE:HG23	1:C:190:MET:CE	2.43	0.48
1:K:190:MET:HE3	1:K:190:MET:HB2	1.67	0.47
1:L:18:TYR:HB3	1:L:22:SER:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:HG22	1:A:99:MET:HE3	1.96	0.47
1:C:18:TYR:HB3	1:C:22:SER:HB2	1.96	0.47
1:E:134:THR:HG22	1:E:137:GLU:OE1	2.14	0.47
1:D:83:HIS:O	1:E:193:GLU:HG2	2.15	0.47
1:L:93:ILE:HG23	1:L:115:LEU:HD12	1.97	0.47
1:L:107:GLY:O	1:L:157:ARG:NH2	2.48	0.47
1:I:193:GLU:HA	1:I:196:TRP:CD1	2.50	0.47
1:D:93:ILE:HG23	1:D:115:LEU:HD12	1.97	0.47
1:B:22:SER:HB3	1:C:6:THR:O	2.15	0.47
1:F:18:TYR:HB3	1:F:22:SER:HB2	1.97	0.46
1:K:144:LEU:HD12	1:L:119:GLU:HG2	1.96	0.46
1:B:94:GLY:HA2	3:B:215:HOH:O	2.15	0.46
1:J:18:TYR:HB3	1:J:22:SER:HB2	1.97	0.46
1:K:91:ILE:HG23	1:K:190:MET:CE	2.45	0.46
1:I:193:GLU:HA	1:I:196:TRP:HD1	1.80	0.46
1:A:93:ILE:HG22	1:G:76:ALA:HB1	1.98	0.46
1:I:190:MET:HE3	1:I:190:MET:HB2	1.70	0.46
1:H:18:TYR:HB3	1:H:22:SER:HB2	1.97	0.45
1:D:18:TYR:HB3	1:D:22:SER:HB2	1.97	0.45
1:E:17:ALA:O	1:F:8:ILE:HD11	2.17	0.45
1:N:126:LEU:HA	1:N:147:ARG:NH2	2.31	0.45
1:A:94:GLY:HA2	3:G:211:HOH:O	2.16	0.45
1:G:18:TYR:HB3	1:G:22:SER:HB2	1.97	0.45
1:C:22:SER:HB3	1:D:6:THR:O	2.17	0.45
1:J:91:ILE:HG23	1:J:190:MET:CE	2.47	0.45
1:A:18:TYR:HB3	1:A:22:SER:HB2	1.99	0.45
1:E:22:SER:HB3	1:F:6:THR:O	2.16	0.45
1:H:91:ILE:HG23	1:H:190:MET:CE	2.47	0.45
1:F:135:GLU:H	1:F:135:GLU:CD	2.20	0.45
1:E:93:ILE:O	1:E:93:ILE:HG13	2.16	0.44
1:N:121:MET:HG3	1:N:173:ASN:O	2.16	0.44
1:L:144:LEU:HD12	1:M:119:GLU:HG2	2.00	0.44
1:M:91:ILE:HG23	1:M:190:MET:CE	2.47	0.44
1:B:190:MET:HB2	1:B:190:MET:HE3	1.66	0.44
1:M:190:MET:HE3	1:M:190:MET:HB2	1.73	0.44
1:H:121:MET:HG3	1:H:173:ASN:O	2.17	0.44
1:G:136:ILE:H	1:G:136:ILE:HD12	1.83	0.43
1:B:121:MET:HB2	1:B:174:PHE:CE1	2.52	0.43
1:C:35:GLN:HB3	1:C:132:GLN:NE2	2.33	0.43
1:H:94:GLY:HA2	3:N:206:HOH:O	2.18	0.43
1:A:128:GLY:CA	1:A:133:ALA:HB3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:121:MET:HB2	1:K:174:PHE:CE1	2.52	0.43
1:G:121:MET:HG3	1:G:173:ASN:O	2.19	0.43
1:H:195:LYS:HG2	1:N:85:LYS:HG2	2.00	0.43
1:F:22:SER:HB3	1:G:6:THR:O	2.19	0.43
1:D:190:MET:HB2	1:D:190:MET:HE3	1.72	0.43
1:C:162:ILE:CB	1:C:162:ILE:CD1	2.84	0.43
1:B:138:ILE:O	1:B:141:ASN:HB2	2.18	0.43
1:I:76:ALA:HB1	1:J:93:ILE:HG22	2.01	0.43
1:D:135:GLU:HB2	1:E:130:GLN:NE2	2.34	0.43
1:C:76:ALA:HB1	1:D:93:ILE:HG22	2.00	0.42
1:B:121:MET:HG3	1:B:173:ASN:O	2.19	0.42
1:I:126:LEU:HG	1:I:147:ARG:HH21	1.84	0.42
1:C:79:ASP:HB3	1:D:115:LEU:HD13	2.02	0.42
1:F:67:PRO:HB2	1:F:130:GLN:HE22	1.84	0.42
1:K:76:ALA:HB1	1:L:93:ILE:HG22	2.00	0.42
1:D:121:MET:HG3	1:D:173:ASN:O	2.19	0.42
1:I:93:ILE:HG23	1:I:115:LEU:HD12	2.01	0.42
1:D:91:ILE:HG23	1:D:190:MET:CE	2.50	0.42
1:C:121:MET:HG3	1:C:173:ASN:O	2.19	0.42
1:C:149:LYS:HE3	1:D:117:ASN:OD1	2.19	0.42
1:A:134:THR:HG22	1:A:137:GLU:HG3	2.02	0.42
1:B:144:LEU:HD12	1:C:119:GLU:HG2	2.00	0.42
1:N:126:LEU:HA	1:N:147:ARG:HH22	1.84	0.42
1:H:149:LYS:HD2	1:H:152:ARG:HH22	1.85	0.42
1:A:115:LEU:HD13	1:G:79:ASP:HB3	2.01	0.42
1:F:79:ASP:HB3	1:G:115:LEU:HD13	2.02	0.41
1:G:121:MET:HB2	1:G:174:PHE:CE1	2.55	0.41
1:L:122:ILE:HG21	1:L:185:LEU:HD11	2.01	0.41
1:C:121:MET:HB2	1:C:174:PHE:CE1	2.55	0.41
1:K:79:ASP:HB3	1:L:115:LEU:HD13	2.03	0.41
1:L:91:ILE:HG23	1:L:190:MET:HE2	2.02	0.41
1:C:91:ILE:HG23	1:C:190:MET:HE1	2.03	0.41
1:A:130:GLN:HE21	1:G:136:ILE:HD13	1.84	0.41
1:D:121:MET:HB2	1:D:174:PHE:CE1	2.55	0.41
1:D:85:LYS:HE3	1:E:194:THR:O	2.21	0.41
1:J:190:MET:HB2	1:J:190:MET:HE3	1.71	0.41
1:F:149:LYS:HE2	1:F:152:ARG:HH12	1.86	0.41
1:G:181:LYS:HA	1:G:186:ILE:HG13	2.02	0.41
1:E:83:HIS:O	1:F:193:GLU:HG2	2.20	0.41
1:L:121:MET:HB2	1:L:174:PHE:CE1	2.56	0.41
1:N:121:MET:HB2	1:N:174:PHE:CE1	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ILE:HG22	1:C:174:PHE:HZ	1.86	0.40
1:F:91:ILE:HG23	1:F:190:MET:CE	2.51	0.40
1:J:35:GLN:HB3	1:J:132:GLN:NE2	2.36	0.40
1:L:190:MET:HE3	1:L:190:MET:HB2	1.68	0.40
1:K:94:GLY:HA2	3:K:208:HOH:O	2.21	0.40
1:L:136:ILE:HG22	1:M:174:PHE:HZ	1.86	0.40
1:H:126:LEU:HD22	1:H:142[A]:HIS:HE1	1.86	0.40
1:I:91:ILE:HG23	1:I:190:MET:CE	2.51	0.40
1:G:181:LYS:HD3	1:G:188:GLU:HA	2.03	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	186/203 (92%)	182 (98%)	3 (2%)	1 (0%)	34	30
1	B	184/203 (91%)	180 (98%)	3 (2%)	1 (0%)	34	30
1	C	182/203 (90%)	178 (98%)	4 (2%)	0	100	100
1	D	178/203 (88%)	173 (97%)	5 (3%)	0	100	100
1	E	187/203 (92%)	180 (96%)	7 (4%)	0	100	100
1	F	180/203 (89%)	174 (97%)	5 (3%)	1 (1%)	30	24
1	G	182/203 (90%)	177 (97%)	4 (2%)	1 (0%)	34	30
1	H	187/203 (92%)	181 (97%)	6 (3%)	0	100	100
1	I	182/203 (90%)	179 (98%)	2 (1%)	1 (0%)	34	30
1	J	184/203 (91%)	178 (97%)	5 (3%)	1 (0%)	34	30
1	K	177/203 (87%)	173 (98%)	4 (2%)	0	100	100
1	L	176/203 (87%)	174 (99%)	2 (1%)	0	100	100
1	M	183/203 (90%)	180 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	178/203 (88%)	173 (97%)	5 (3%)	0	100 100
All	All	2546/2842 (90%)	2482 (98%)	58 (2%)	6 (0%)	52 53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ALA
1	G	129	ALA
1	J	130	GLN
1	B	127	GLY
1	F	127	GLY
1	I	127	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	158/171 (92%)	156 (99%)	2 (1%)	76 82
1	B	157/171 (92%)	155 (99%)	2 (1%)	76 82
1	C	156/171 (91%)	153 (98%)	3 (2%)	65 70
1	D	153/171 (90%)	150 (98%)	3 (2%)	63 68
1	E	157/171 (92%)	157 (100%)	0	100 100
1	F	154/171 (90%)	153 (99%)	1 (1%)	90 94
1	G	153/171 (90%)	153 (100%)	0	100 100
1	H	159/171 (93%)	154 (97%)	5 (3%)	47 50
1	I	155/171 (91%)	152 (98%)	3 (2%)	65 70
1	J	154/171 (90%)	153 (99%)	1 (1%)	90 94
1	K	155/171 (91%)	155 (100%)	0	100 100
1	L	155/171 (91%)	154 (99%)	1 (1%)	90 94
1	M	155/171 (91%)	153 (99%)	2 (1%)	76 82
1	N	151/171 (88%)	148 (98%)	3 (2%)	63 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2172/2394 (91%)	2146 (99%)	26 (1%)	78 84

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	A	163	GLU
1	B	135	GLU
1	B	147	ARG
1	C	147	ARG
1	C	149	LYS
1	C	152	ARG
1	D	75	PHE
1	D	147	ARG
1	D	157	ARG
1	F	136	ILE
1	H	75	PHE
1	H	143	ILE
1	H	144	LEU
1	H	196	TRP
1	H	200	GLN
1	I	134	THR
1	I	147	ARG
1	I	193	GLU
1	J	147	ARG
1	L	98	SER
1	M	142	HIS
1	M	162	ILE
1	N	136	ILE
1	N	138	ILE
1	N	156	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	GLN
1	H	200	GLN
1	I	142	HIS
1	J	132	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	187/203 (92%)	0.58	16 (8%)	13	18	35, 57, 108, 157	0
1	B	187/203 (92%)	0.78	24 (12%)	5	6	51, 69, 118, 151	0
1	C	186/203 (91%)	0.66	21 (11%)	7	9	43, 61, 114, 142	0
1	D	182/203 (89%)	0.66	16 (8%)	12	17	42, 56, 101, 145	0
1	E	188/203 (92%)	0.48	13 (6%)	20	27	32, 50, 100, 132	0
1	F	182/203 (89%)	0.47	16 (8%)	12	17	40, 62, 99, 163	0
1	G	185/203 (91%)	0.68	17 (9%)	11	15	40, 61, 106, 175	0
1	H	192/203 (94%)	0.57	17 (8%)	12	16	45, 66, 114, 146	0
1	I	186/203 (91%)	0.55	13 (6%)	19	26	41, 56, 104, 157	0
1	J	186/203 (91%)	0.75	22 (11%)	6	8	50, 70, 114, 149	0
1	K	179/203 (88%)	0.53	13 (7%)	18	24	49, 69, 110, 158	0
1	L	180/203 (88%)	0.50	14 (7%)	16	22	44, 63, 109, 166	0
1	M	186/203 (91%)	0.80	22 (11%)	6	8	50, 75, 114, 148	0
1	N	183/203 (90%)	1.04	27 (14%)	3	5	55, 79, 117, 175	0
All	All	2589/2842 (91%)	0.65	251 (9%)	10	14	32, 65, 113, 175	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	17	ALA	13.4
1	K	8	ILE	9.9
1	C	3	LEU	8.7
1	G	126	LEU	8.2
1	B	3	LEU	8.0
1	N	143	ILE	8.0
1	J	17	ALA	7.8
1	N	126	LEU	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	17	ALA	7.8
1	M	17	ALA	7.8
1	N	133	ALA	7.4
1	J	129	ALA	7.4
1	H	8	ILE	7.3
1	G	8	ILE	7.2
1	A	3	LEU	7.2
1	L	8	ILE	7.0
1	A	17	ALA	7.0
1	G	130	GLN	6.8
1	I	3	LEU	6.8
1	I	8	ILE	6.8
1	B	8	ILE	6.6
1	H	17	ALA	6.6
1	J	3	LEU	6.5
1	B	7	VAL	6.3
1	H	7	VAL	6.3
1	B	139	ALA	6.3
1	A	8	ILE	6.1
1	F	8	ILE	6.0
1	N	127	GLY	6.0
1	B	140	ALA	5.8
1	J	7	VAL	5.7
1	M	8	ILE	5.7
1	J	8	ILE	5.6
1	K	18	TYR	5.6
1	F	129	ALA	5.6
1	G	7	VAL	5.5
1	C	142[A]	HIS	5.3
1	B	142[A]	HIS	5.3
1	G	129	ALA	5.3
1	K	3	LEU	5.3
1	M	133	ALA	5.2
1	N	8	ILE	5.2
1	C	133	ALA	5.2
1	N	132	GLN	5.2
1	E	126	LEU	5.1
1	D	3	LEU	5.1
1	A	7	VAL	4.9
1	N	7	VAL	4.9
1	J	16	ARG	4.9
1	E	18	TYR	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	126	LEU	4.8
1	G	191	VAL	4.8
1	B	17	ALA	4.8
1	E	133	ALA	4.8
1	C	8	ILE	4.7
1	M	139	ALA	4.6
1	C	132	GLN	4.6
1	D	144	LEU	4.5
1	M	144	LEU	4.5
1	H	16	ARG	4.5
1	M	16	ARG	4.5
1	B	126	LEU	4.5
1	M	3	LEU	4.5
1	K	135	GLU	4.5
1	J	130	GLN	4.5
1	E	130	GLN	4.5
1	F	7	VAL	4.5
1	D	126	LEU	4.4
1	M	7	VAL	4.4
1	A	194	THR	4.4
1	D	17	ALA	4.4
1	B	143	ILE	4.4
1	M	4	ILE	4.3
1	K	133	ALA	4.3
1	E	142[A]	HIS	4.3
1	N	142	HIS	4.3
1	L	143	ILE	4.3
1	A	193	GLU	4.3
1	B	16	ARG	4.3
1	N	174	PHE	4.2
1	H	142[A]	HIS	4.2
1	H	126	LEU	4.2
1	D	7	VAL	4.2
1	G	127	GLY	4.2
1	D	132	GLN	4.1
1	B	18	TYR	4.1
1	F	18	TYR	4.1
1	L	3	LEU	4.0
1	N	147	ARG	4.0
1	N	17	ALA	4.0
1	D	16	ARG	4.0
1	C	17	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	17	ALA	3.9
1	E	129	ALA	3.9
1	E	132	GLN	3.9
1	J	18	TYR	3.9
1	D	4	ILE	3.9
1	E	8	ILE	3.8
1	B	127	GLY	3.8
1	L	7	VAL	3.7
1	B	10	THR	3.7
1	C	16	ARG	3.7
1	N	152	ARG	3.7
1	C	196	TRP	3.7
1	H	18	TYR	3.7
1	G	4	ILE	3.7
1	H	133	ALA	3.7
1	M	130	GLN	3.6
1	N	144	LEU	3.6
1	M	6	THR	3.6
1	M	142	HIS	3.6
1	D	142[A]	HIS	3.6
1	H	3	LEU	3.6
1	I	195	LYS	3.6
1	B	93	ILE	3.5
1	J	127	GLY	3.5
1	B	4	ILE	3.5
1	F	126	LEU	3.4
1	H	144	LEU	3.4
1	I	18	TYR	3.4
1	J	194	THR	3.4
1	L	18	TYR	3.4
1	L	128	GLY	3.4
1	N	191	VAL	3.4
1	N	140	ALA	3.4
1	N	122	ILE	3.4
1	B	138	ILE	3.3
1	B	194	THR	3.3
1	E	7	VAL	3.3
1	N	9	GLU	3.3
1	G	18	TYR	3.2
1	L	126	LEU	3.2
1	A	140	ALA	3.2
1	H	9	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	128	GLY	3.2
1	M	129	ALA	3.1
1	D	18	TYR	3.0
1	N	16	ARG	3.0
1	D	127	GLY	3.0
1	E	4	ILE	3.0
1	C	191	VAL	3.0
1	I	133	ALA	3.0
1	F	4	ILE	2.9
1	H	93	ILE	2.9
1	I	172	ASP	2.9
1	D	8	ILE	2.9
1	I	196	TRP	2.9
1	C	197	SER	2.9
1	M	9	GLU	2.9
1	B	136	ILE	2.9
1	A	129	ALA	2.8
1	I	4	ILE	2.8
1	C	7	VAL	2.8
1	N	154	LEU	2.8
1	N	145	LYS	2.8
1	H	6	THR	2.8
1	A	139	ALA	2.7
1	A	138	ILE	2.7
1	F	9	GLU	2.7
1	G	56	SER	2.7
1	G	171	ARG	2.7
1	D	6	THR	2.7
1	G	10	THR	2.7
1	K	7	VAL	2.7
1	C	18	TYR	2.7
1	J	126	LEU	2.7
1	C	4	ILE	2.7
1	A	4	ILE	2.6
1	M	136	ILE	2.6
1	L	136	ILE	2.6
1	N	171	ARG	2.6
1	N	85	LYS	2.6
1	M	143	ILE	2.6
1	E	3	LEU	2.6
1	N	139	ALA	2.6
1	G	174	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	3	LEU	2.5
1	K	142[A]	HIS	2.5
1	J	6	THR	2.5
1	M	174	PHE	2.5
1	C	6	THR	2.5
1	F	130	GLN	2.5
1	K	140	ALA	2.5
1	B	144	LEU	2.5
1	H	132	GLN	2.5
1	F	148	GLU	2.4
1	N	78	TYR	2.4
1	K	127	GLY	2.4
1	C	93	ILE	2.4
1	F	136	ILE	2.4
1	G	9	GLU	2.4
1	B	152	ARG	2.4
1	C	174	PHE	2.4
1	I	127	GLY	2.4
1	K	126	LEU	2.4
1	L	193	GLU	2.4
1	N	93	ILE	2.3
1	M	194	THR	2.3
1	F	5	PRO	2.3
1	J	5	PRO	2.3
1	L	140	ALA	2.3
1	L	191	VAL	2.3
1	K	93	ILE	2.3
1	A	18	TYR	2.3
1	J	193	GLU	2.3
1	I	93	ILE	2.3
1	D	133	ALA	2.3
1	A	10	THR	2.2
1	E	136	ILE	2.2
1	C	135	GLU	2.2
1	F	57	GLU	2.2
1	F	143	ILE	2.2
1	M	126	LEU	2.2
1	J	94	GLY	2.2
1	N	166	GLN	2.2
1	C	141	ASN	2.2
1	A	6	THR	2.2
1	B	192	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	126	LEU	2.2
1	J	144	LEU	2.2
1	J	23	ARG	2.2
1	A	93	ILE	2.2
1	C	140	ALA	2.1
1	N	129	ALA	2.1
1	J	138	ILE	2.1
1	C	195	LYS	2.1
1	G	58	LYS	2.1
1	H	200	GLN	2.1
1	L	133	ALA	2.1
1	H	172	ASP	2.1
1	J	4	ILE	2.1
1	F	6	THR	2.1
1	M	135	GLU	2.1
1	D	128	GLY	2.1
1	J	136	ILE	2.1
1	B	119[A]	GLU	2.1
1	K	9	GLU	2.1
1	L	93	ILE	2.1
1	M	122	ILE	2.1
1	M	24	LEU	2.1
1	H	119	GLU	2.0
1	I	9	GLU	2.0
1	J	93	ILE	2.0
1	K	143	ILE	2.0
1	F	127	GLY	2.0
1	B	135	GLU	2.0
1	D	9	GLU	2.0
1	L	9	GLU	2.0
1	A	130	GLN	2.0
1	B	132	GLN	2.0
1	J	9	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	L	204	1/1	0.87	0.12	-	98,98,98,98	0
2	CL	C	204	1/1	0.88	0.19	-	82,82,82,82	0
2	CL	B	204	1/1	0.75	0.17	-	99,99,99,99	0
2	CL	L	205	1/1	0.92	0.15	-	81,81,81,81	0
2	CL	D	204	1/1	0.94	0.25	-	78,78,78,78	0
2	CL	M	204	1/1	0.78	0.11	-	93,93,93,93	0
2	CL	A	204	1/1	0.97	0.21	-	81,81,81,81	0

6.5 Other polymers

There are no such residues in this entry.