Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:24 am BST

PDB ID	:	4EMM
Title	:	Crystal structure of Staphylococcus aureus ClpP in compact conformation
Authors	:	Zhang, J.; Liu, H.; Yang, C.-G.
Deposited on	:	2012-04-12
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

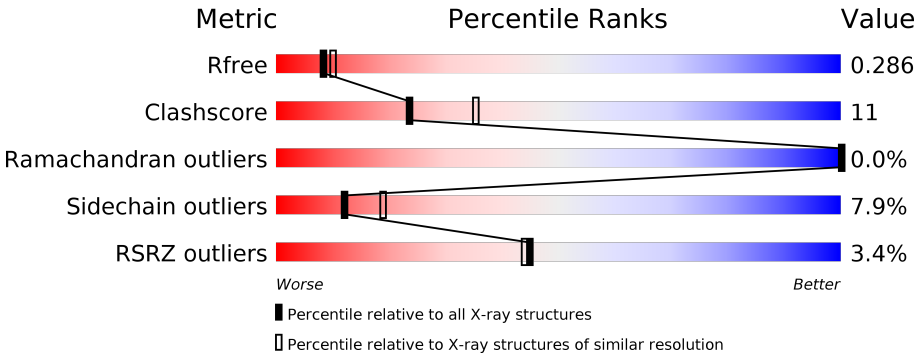
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	203	58% 24% • 15%
1	B	203	3% 59% 22% • 16%
1	C	203	4% 65% 18% • 15%
1	D	203	2% 63% 20% • 16%
1	E	203	2% 60% 22% • 15%
1	F	203	5% 63% 21% • 15%

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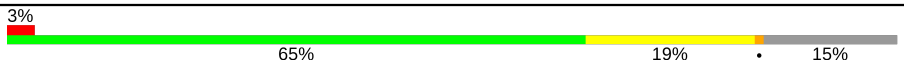
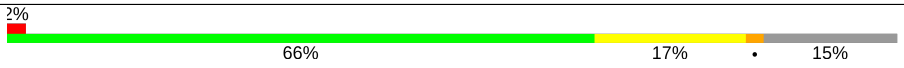
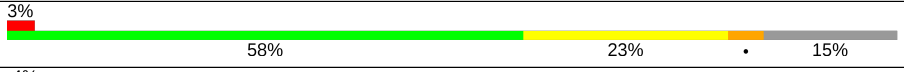
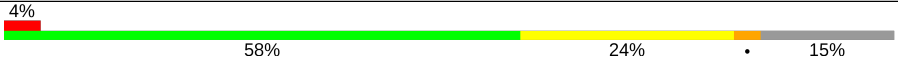
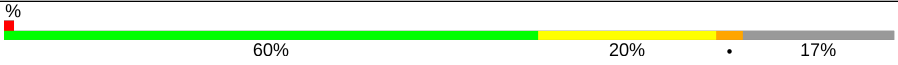
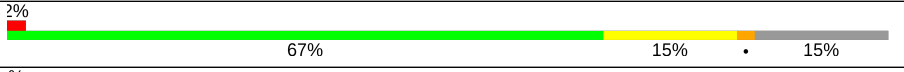
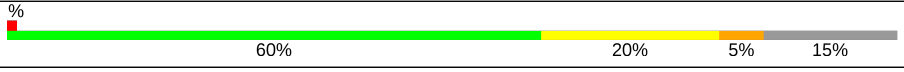
Mol	Chain	Length	Quality of chain
1	G	203	
1	H	203	
1	I	203	
1	J	203	
1	K	203	
1	L	203	
1	M	203	
1	V	203	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18724 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	172	Total	C	N	O	S	0	0	0
			1331	843	225	257	6			
1	A	173	Total	C	N	O	S	0	0	0
			1340	848	226	260	6			
1	B	171	Total	C	N	O	S	0	1	0
			1328	841	224	256	7			
1	C	172	Total	C	N	O	S	0	1	0
			1336	847	225	257	7			
1	D	171	Total	C	N	O	S	0	0	0
			1322	838	224	254	6			
1	E	173	Total	C	N	O	S	0	1	0
			1343	851	226	259	7			
1	F	173	Total	C	N	O	S	0	0	0
			1330	842	226	256	6			
1	G	173	Total	C	N	O	S	0	0	0
			1340	848	226	260	6			
1	H	175	Total	C	N	O	S	0	1	0
			1353	857	228	261	7			
1	I	172	Total	C	N	O	S	0	0	0
			1331	843	225	257	6			
1	J	173	Total	C	N	O	S	0	2	0
			1353	856	228	262	7			
1	K	173	Total	C	N	O	S	0	1	0
			1345	852	226	260	7			
1	L	168	Total	C	N	O	S	0	0	0
			1302	824	221	251	6			
1	M	172	Total	C	N	O	S	0	1	0
			1338	848	225	258	7			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	196	LEU	-	EXPRESSION TAG	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
V	197	GLU	-	EXPRESSION TAG	UNP P63786
V	198	HIS	-	EXPRESSION TAG	UNP P63786
V	199	HIS	-	EXPRESSION TAG	UNP P63786
V	200	HIS	-	EXPRESSION TAG	UNP P63786
V	201	HIS	-	EXPRESSION TAG	UNP P63786
V	202	HIS	-	EXPRESSION TAG	UNP P63786
V	203	HIS	-	EXPRESSION TAG	UNP P63786
A	196	LEU	-	EXPRESSION TAG	UNP P63786
A	197	GLU	-	EXPRESSION TAG	UNP P63786
A	198	HIS	-	EXPRESSION TAG	UNP P63786
A	199	HIS	-	EXPRESSION TAG	UNP P63786
A	200	HIS	-	EXPRESSION TAG	UNP P63786
A	201	HIS	-	EXPRESSION TAG	UNP P63786
A	202	HIS	-	EXPRESSION TAG	UNP P63786
A	203	HIS	-	EXPRESSION TAG	UNP P63786
B	196	LEU	-	EXPRESSION TAG	UNP P63786
B	197	GLU	-	EXPRESSION TAG	UNP P63786
B	198	HIS	-	EXPRESSION TAG	UNP P63786
B	199	HIS	-	EXPRESSION TAG	UNP P63786
B	200	HIS	-	EXPRESSION TAG	UNP P63786
B	201	HIS	-	EXPRESSION TAG	UNP P63786
B	202	HIS	-	EXPRESSION TAG	UNP P63786
B	203	HIS	-	EXPRESSION TAG	UNP P63786
C	196	LEU	-	EXPRESSION TAG	UNP P63786
C	197	GLU	-	EXPRESSION TAG	UNP P63786
C	198	HIS	-	EXPRESSION TAG	UNP P63786
C	199	HIS	-	EXPRESSION TAG	UNP P63786
C	200	HIS	-	EXPRESSION TAG	UNP P63786
C	201	HIS	-	EXPRESSION TAG	UNP P63786
C	202	HIS	-	EXPRESSION TAG	UNP P63786
C	203	HIS	-	EXPRESSION TAG	UNP P63786
D	196	LEU	-	EXPRESSION TAG	UNP P63786
D	197	GLU	-	EXPRESSION TAG	UNP P63786
D	198	HIS	-	EXPRESSION TAG	UNP P63786
D	199	HIS	-	EXPRESSION TAG	UNP P63786
D	200	HIS	-	EXPRESSION TAG	UNP P63786
D	201	HIS	-	EXPRESSION TAG	UNP P63786
D	202	HIS	-	EXPRESSION TAG	UNP P63786
D	203	HIS	-	EXPRESSION TAG	UNP P63786
E	196	LEU	-	EXPRESSION TAG	UNP P63786
E	197	GLU	-	EXPRESSION TAG	UNP P63786
E	198	HIS	-	EXPRESSION TAG	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
E	199	HIS	-	EXPRESSION TAG	UNP P63786
E	200	HIS	-	EXPRESSION TAG	UNP P63786
E	201	HIS	-	EXPRESSION TAG	UNP P63786
E	202	HIS	-	EXPRESSION TAG	UNP P63786
E	203	HIS	-	EXPRESSION TAG	UNP P63786
F	196	LEU	-	EXPRESSION TAG	UNP P63786
F	197	GLU	-	EXPRESSION TAG	UNP P63786
F	198	HIS	-	EXPRESSION TAG	UNP P63786
F	199	HIS	-	EXPRESSION TAG	UNP P63786
F	200	HIS	-	EXPRESSION TAG	UNP P63786
F	201	HIS	-	EXPRESSION TAG	UNP P63786
F	202	HIS	-	EXPRESSION TAG	UNP P63786
F	203	HIS	-	EXPRESSION TAG	UNP P63786
G	196	LEU	-	EXPRESSION TAG	UNP P63786
G	197	GLU	-	EXPRESSION TAG	UNP P63786
G	198	HIS	-	EXPRESSION TAG	UNP P63786
G	199	HIS	-	EXPRESSION TAG	UNP P63786
G	200	HIS	-	EXPRESSION TAG	UNP P63786
G	201	HIS	-	EXPRESSION TAG	UNP P63786
G	202	HIS	-	EXPRESSION TAG	UNP P63786
G	203	HIS	-	EXPRESSION TAG	UNP P63786
H	196	LEU	-	EXPRESSION TAG	UNP P63786
H	197	GLU	-	EXPRESSION TAG	UNP P63786
H	198	HIS	-	EXPRESSION TAG	UNP P63786
H	199	HIS	-	EXPRESSION TAG	UNP P63786
H	200	HIS	-	EXPRESSION TAG	UNP P63786
H	201	HIS	-	EXPRESSION TAG	UNP P63786
H	202	HIS	-	EXPRESSION TAG	UNP P63786
H	203	HIS	-	EXPRESSION TAG	UNP P63786
I	196	LEU	-	EXPRESSION TAG	UNP P63786
I	197	GLU	-	EXPRESSION TAG	UNP P63786
I	198	HIS	-	EXPRESSION TAG	UNP P63786
I	199	HIS	-	EXPRESSION TAG	UNP P63786
I	200	HIS	-	EXPRESSION TAG	UNP P63786
I	201	HIS	-	EXPRESSION TAG	UNP P63786
I	202	HIS	-	EXPRESSION TAG	UNP P63786
I	203	HIS	-	EXPRESSION TAG	UNP P63786
J	196	LEU	-	EXPRESSION TAG	UNP P63786
J	197	GLU	-	EXPRESSION TAG	UNP P63786
J	198	HIS	-	EXPRESSION TAG	UNP P63786
J	199	HIS	-	EXPRESSION TAG	UNP P63786
J	200	HIS	-	EXPRESSION TAG	UNP P63786

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Chain	Residue	Modelled	Actual	Comment	Reference
J	201	HIS	-	EXPRESSION TAG	UNP P63786
J	202	HIS	-	EXPRESSION TAG	UNP P63786
J	203	HIS	-	EXPRESSION TAG	UNP P63786
K	196	LEU	-	EXPRESSION TAG	UNP P63786
K	197	GLU	-	EXPRESSION TAG	UNP P63786
K	198	HIS	-	EXPRESSION TAG	UNP P63786
K	199	HIS	-	EXPRESSION TAG	UNP P63786
K	200	HIS	-	EXPRESSION TAG	UNP P63786
K	201	HIS	-	EXPRESSION TAG	UNP P63786
K	202	HIS	-	EXPRESSION TAG	UNP P63786
K	203	HIS	-	EXPRESSION TAG	UNP P63786
L	196	LEU	-	EXPRESSION TAG	UNP P63786
L	197	GLU	-	EXPRESSION TAG	UNP P63786
L	198	HIS	-	EXPRESSION TAG	UNP P63786
L	199	HIS	-	EXPRESSION TAG	UNP P63786
L	200	HIS	-	EXPRESSION TAG	UNP P63786
L	201	HIS	-	EXPRESSION TAG	UNP P63786
L	202	HIS	-	EXPRESSION TAG	UNP P63786
L	203	HIS	-	EXPRESSION TAG	UNP P63786
M	196	LEU	-	EXPRESSION TAG	UNP P63786
M	197	GLU	-	EXPRESSION TAG	UNP P63786
M	198	HIS	-	EXPRESSION TAG	UNP P63786
M	199	HIS	-	EXPRESSION TAG	UNP P63786
M	200	HIS	-	EXPRESSION TAG	UNP P63786
M	201	HIS	-	EXPRESSION TAG	UNP P63786
M	202	HIS	-	EXPRESSION TAG	UNP P63786
M	203	HIS	-	EXPRESSION TAG	UNP P63786

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	V	4	Total O 4 4	0	0
2	A	2	Total O 2 2	0	0
2	B	3	Total O 3 3	0	0
2	C	2	Total O 2 2	0	0
2	D	1	Total O 1 1	0	0
2	E	4	Total O 4 4	0	0

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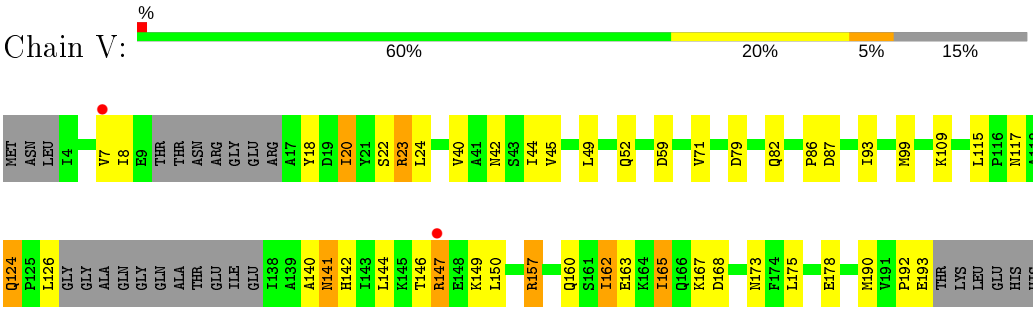
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	2	Total O 2 2	0	0
2	G	4	Total O 4 4	0	0
2	H	1	Total O 1 1	0	0
2	I	3	Total O 3 3	0	0
2	J	1	Total O 1 1	0	0
2	K	1	Total O 1 1	0	0
2	L	3	Total O 3 3	0	0
2	M	1	Total O 1 1	0	0

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 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.

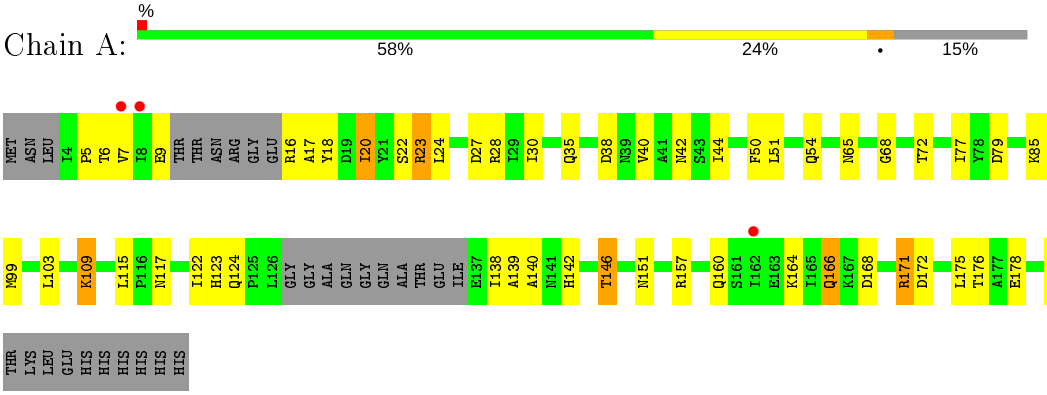
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:



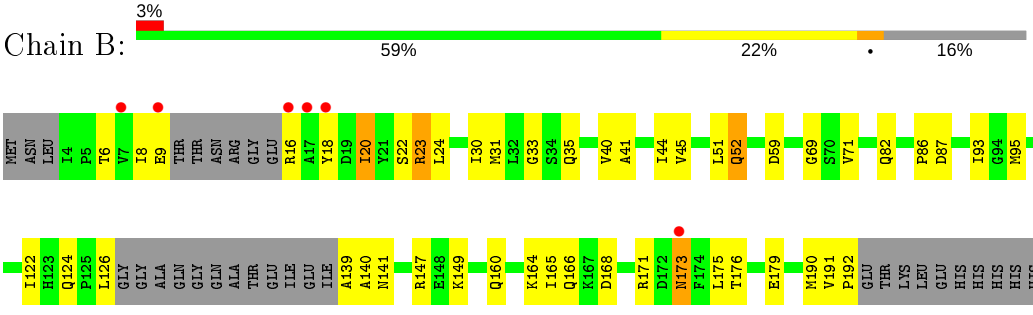
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



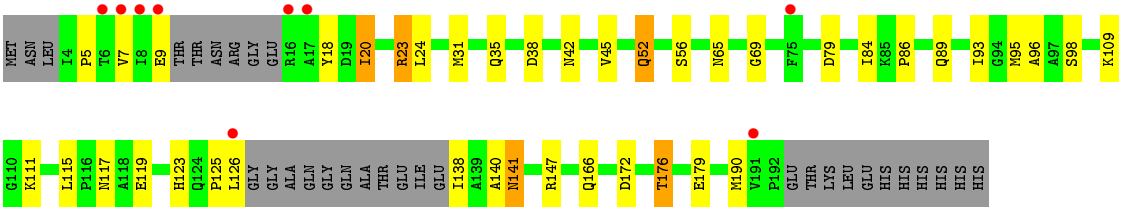
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



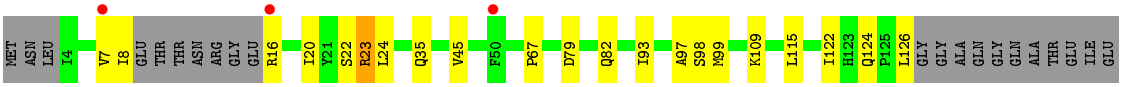
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

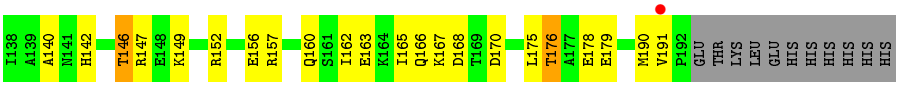
Chain C:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



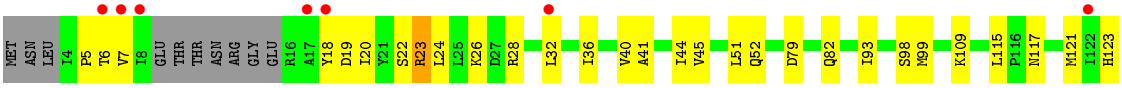


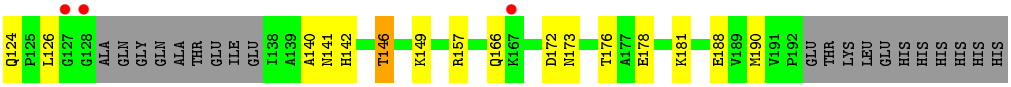
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

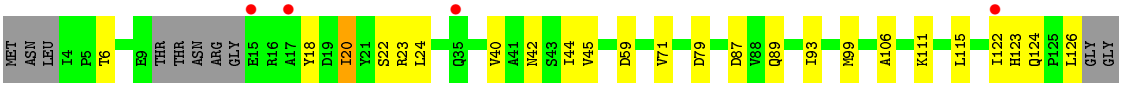
Chain F:

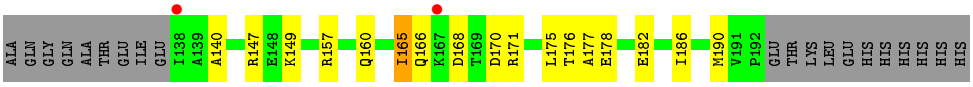




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

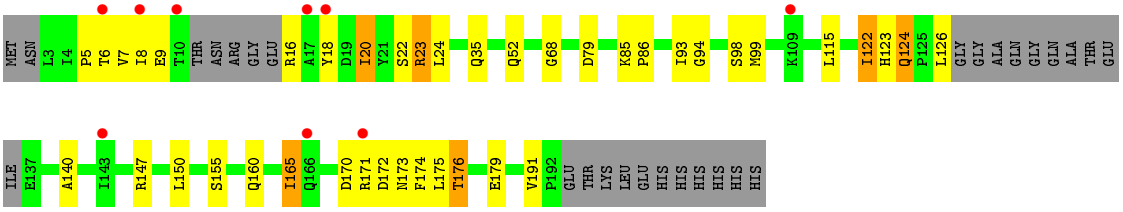
Chain G:





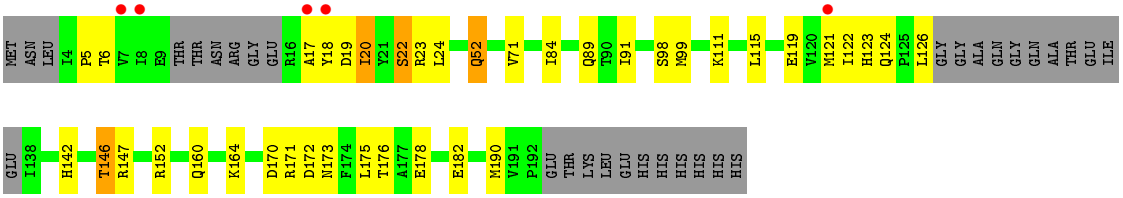
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H:



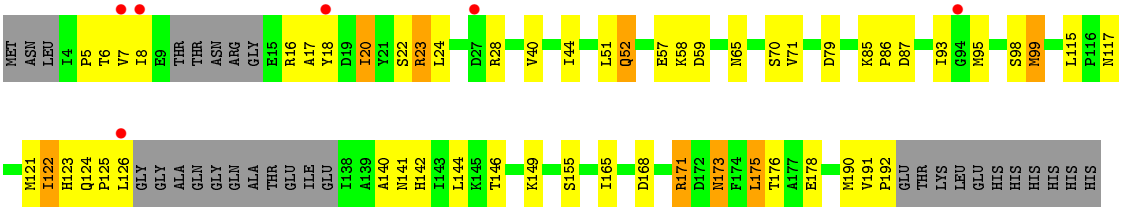
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:



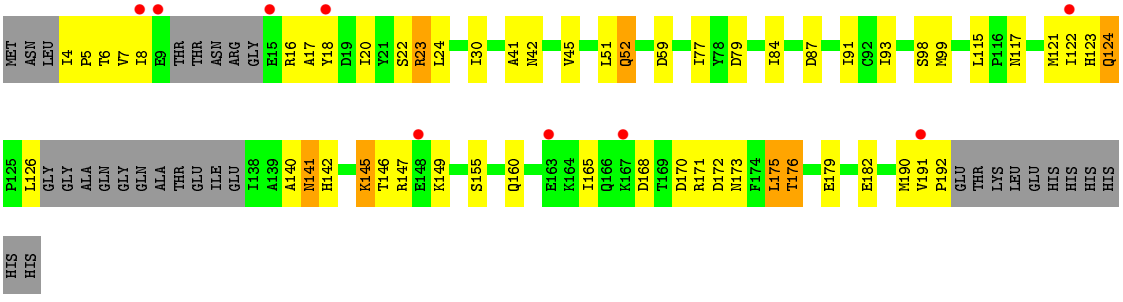
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:



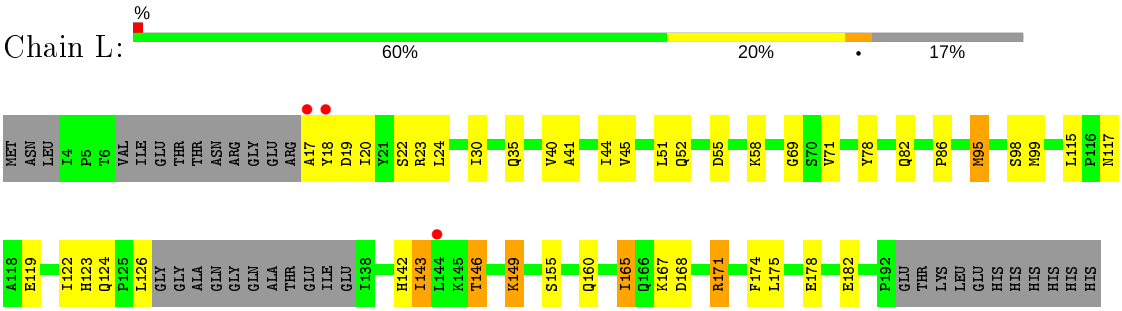
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:



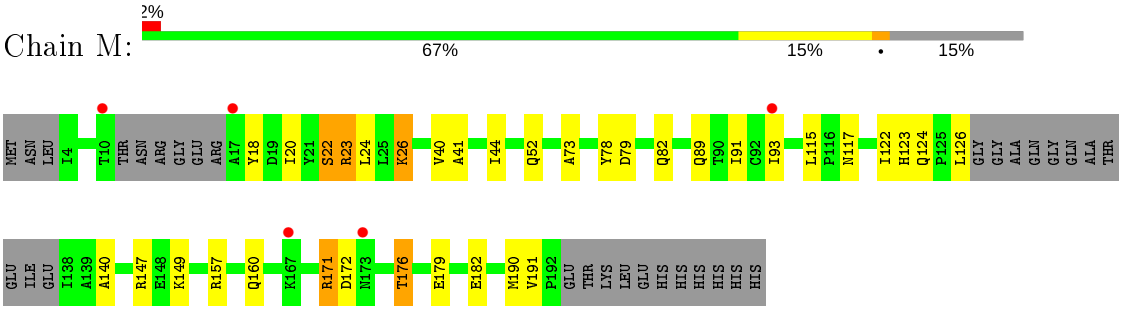
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.38Å 170.05Å 96.33Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 49.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-2.40) 95.6 (49.06-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.286 0.239 , 0.286	Depositor DCC
R_{free} test set	5666 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.286 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18724	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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	0.53	0/1357	0.67	0/1831
1	B	0.59	0/1348	0.68	0/1818
1	C	0.50	0/1356	0.63	0/1829
1	D	0.55	0/1339	0.68	0/1807
1	E	0.52	0/1363	0.65	0/1839
1	F	0.52	0/1347	0.63	0/1817
1	G	0.50	0/1357	0.64	0/1831
1	H	0.49	0/1373	0.61	0/1853
1	I	0.52	0/1348	0.65	0/1819
1	J	0.57	0/1373	0.68	1/1852 (0.1%)
1	K	0.48	0/1365	0.63	0/1841
1	L	0.51	0/1319	0.65	0/1779
1	M	0.50	0/1358	0.61	0/1832
1	V	0.60	0/1348	0.71	0/1819
All	All	0.53	0/18951	0.65	1/25567 (0.0%)

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	E	0	1

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	J	175	LEU	CA-CB-CG	5.74	128.49	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	172	ASP	Peptide

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	1340	0	1351	57	0
1	B	1328	0	1343	53	0
1	C	1336	0	1354	32	0
1	D	1322	0	1339	30	0
1	E	1343	0	1361	44	0
1	F	1330	0	1345	34	0
1	G	1340	0	1351	31	0
1	H	1353	0	1365	28	0
1	I	1331	0	1345	28	0
1	J	1353	0	1365	45	0
1	K	1345	0	1360	42	0
1	L	1302	0	1317	35	0
1	M	1338	0	1359	22	0
1	V	1331	0	1345	49	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	4	0	0	1	0
2	F	2	0	0	0	0
2	G	4	0	0	1	0
2	H	1	0	0	0	0
2	I	3	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	3	0	0	0	0
2	M	1	0	0	0	0
2	V	4	0	0	0	0
All	All	18724	0	18900	422	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 11.

All (422) 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:A:42:ASN:HD22	1:B:31[A]:MET:CE	1.60	1.13
1:B:149:LYS:HE3	1:K:117:ASN:HD22	1.23	1.02
1:D:149:LYS:HE3	1:F:117:ASN:HD22	1.21	1.00
1:J:117:ASN:HD22	1:L:149:LYS:HE2	1.21	0.98
1:M:176:THR:HG22	1:M:179:GLU:H	1.26	0.98
1:J:117:ASN:ND2	1:L:149:LYS:HE2	1.78	0.98
1:G:122:ILE:HD11	1:G:168:ASP:HB3	1.46	0.97
1:H:124:GLN:O	1:H:147:ARG:NH2	1.99	0.94
1:B:122:ILE:HD11	1:B:168:ASP:HB3	1.50	0.93
1:D:160:GLN:HB2	1:D:165:ILE:CD1	2.01	0.91
1:M:124:GLN:O	1:M:147:ARG:NH2	2.06	0.88
1:C:9:GLU:HG3	1:C:23:ARG:HD3	1.55	0.87
1:D:160:GLN:HB2	1:D:165:ILE:HD11	1.53	0.87
1:H:176:THR:HG22	1:H:179:GLU:H	1.39	0.87
1:A:17:ALA:O	1:B:8:ILE:HD11	1.76	0.86
1:I:18:TYR:HB3	1:I:22:SER:HB2	1.59	0.85
1:A:140:ALA:H	1:J:123:HIS:HE1	1.24	0.84
1:C:140:ALA:H	1:H:123:HIS:HE1	1.25	0.84
1:V:109:LYS:HZ3	1:V:157:ARG:NH1	1.75	0.83
1:A:42:ASN:HD22	1:B:31[A]:MET:HE3	1.45	0.82
1:J:117:ASN:HD22	1:L:149:LYS:CE	1.92	0.82
1:C:123:HIS:HE1	1:H:140:ALA:H	1.26	0.82
1:B:140:ALA:H	1:L:123:HIS:HE1	1.27	0.82
1:C:176:THR:HG22	1:C:179:GLU:H	1.42	0.81
1:D:122:ILE:HD11	1:D:168:ASP:HB3	1.63	0.81
1:K:140:ALA:H	1:M:123:HIS:HE1	1.29	0.81
1:B:124:GLN:O	1:B:147:ARG:NH2	2.15	0.80
1:A:115:LEU:HD23	1:A:190:MET:HE3	1.64	0.80
1:A:79:ASP:HB3	1:B:115:LEU:HD13	1.64	0.80
1:E:117:ASN:HD22	1:K:149:LYS:HE3	1.47	0.79
1:L:122:ILE:HD11	1:L:168:ASP:HB3	1.64	0.79
1:A:123:HIS:HE1	1:J:140:ALA:H	1.28	0.79
1:L:115:LEU:HD13	1:M:79:ASP:HB3	1.64	0.79
1:A:42:ASN:HB3	1:B:31[A]:MET:HE1	1.65	0.79
1:C:52:GLN:HG3	1:C:84:ILE:HB	1.65	0.78
1:A:42:ASN:ND2	1:B:31[A]:MET:CE	2.44	0.78
1:K:122:ILE:HD11	1:K:168:ASP:HB3	1.64	0.78
1:V:119:GLU:OE1	1:J:142:HIS:HE1	1.68	0.77
1:V:42:ASN:OD1	1:C:31[A]:MET:SD	2.43	0.77
1:B:115:LEU:HD23	1:B:190:MET:HE3	1.66	0.76
1:V:7:VAL:HB	1:V:23:ARG:HG3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:ALA:H	1:F:123:HIS:HE1	1.31	0.76
1:B:149:LYS:HE3	1:K:117:ASN:ND2	2.01	0.76
1:A:22:SER:HB3	1:B:6:THR:O	1.86	0.76
1:V:140:ALA:H	1:G:123:HIS:HE1	1.34	0.75
1:V:109:LYS:NZ	1:V:157:ARG:NH1	2.33	0.75
1:J:71:VAL:HG22	1:J:99:MET:HE3	1.66	0.74
1:E:22:SER:HB3	1:I:6:THR:O	1.88	0.74
1:A:176:THR:HG22	1:A:178:GLU:H	1.52	0.73
1:B:22:SER:HB3	1:K:6:THR:O	1.87	0.73
1:E:52:GLN:HG3	1:E:84:ILE:HB	1.71	0.73
1:L:55:ASP:OD2	1:L:58:LYS:HG3	1.88	0.72
1:E:176:THR:HG22	1:E:179:GLU:H	1.57	0.70
1:A:42:ASN:HD22	1:B:31[A]:MET:HE1	1.57	0.70
1:F:7:VAL:HB	1:F:23:ARG:HG3	1.73	0.70
1:H:23:ARG:O	1:H:23:ARG:HD3	1.91	0.70
1:A:23:ARG:NH2	1:A:27:ASP:OD1	2.24	0.70
1:L:18:TYR:HB3	1:L:22:SER:HB2	1.74	0.69
1:D:140:ALA:H	1:I:123:HIS:HE1	1.38	0.69
1:D:176:THR:HG22	1:D:179:GLU:H	1.58	0.69
1:C:140:ALA:H	1:H:123:HIS:CE1	2.09	0.68
1:G:124:GLN:O	1:G:147:ARG:NH2	2.26	0.68
1:G:147:ARG:NH1	1:G:170:ASP:OD2	2.27	0.68
1:F:23:ARG:HH21	1:F:26:LYS:HB3	1.58	0.68
1:A:42:ASN:ND2	1:B:33:GLY:HA3	2.09	0.67
1:H:5:PRO:HD2	1:H:20:ILE:HG12	1.77	0.67
1:E:122:ILE:HD11	1:E:168:ASP:HB3	1.78	0.66
1:E:19:ASP:OD2	1:E:22:SER:OG	2.07	0.66
1:A:123:HIS:CE1	1:J:140:ALA:H	2.11	0.66
1:V:123:HIS:HE1	1:G:140:ALA:H	1.44	0.66
1:V:119:GLU:OE1	1:J:142:HIS:CE1	2.49	0.66
1:A:171:ARG:HE	1:J:141[A]:ASN:HD22	1.42	0.66
1:D:149:LYS:HE3	1:F:117:ASN:ND2	2.04	0.66
1:K:176:THR:HG22	1:K:179:GLU:H	1.61	0.66
1:E:160:GLN:HB2	1:E:165:ILE:CD1	2.26	0.65
1:H:8:ILE:HA	1:H:16:ARG:O	1.96	0.65
1:C:126:LEU:HD21	1:C:147:ARG:HD2	1.77	0.65
1:A:140:ALA:H	1:J:123:HIS:CE1	2.11	0.64
1:C:89:GLN:HG2	1:C:111:LYS:HB3	1.79	0.64
1:V:141:ASN:HB3	1:G:170:ASP:HB3	1.79	0.64
1:D:22:SER:HB3	1:F:6:THR:O	1.98	0.64
1:D:163:GLU:O	1:D:167:LYS:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:TYR:HB3	1:F:22:SER:HB2	1.81	0.63
1:H:176:THR:CG2	1:H:179:GLU:H	2.12	0.63
1:B:126:LEU:HD12	1:L:143:ILE:HG12	1.80	0.62
1:K:124:GLN:O	1:K:147:ARG:NH2	2.32	0.62
1:D:79:ASP:HB3	1:F:115:LEU:HD13	1.81	0.62
1:A:50:PHE:CD1	1:B:23:ARG:HD2	2.36	0.61
1:B:18:TYR:HB3	1:B:22:SER:HB2	1.81	0.61
1:A:50:PHE:CE1	1:B:23:ARG:HD2	2.35	0.61
1:A:79:ASP:CB	1:B:115:LEU:HD13	2.31	0.61
1:A:7:VAL:HG11	1:A:23:ARG:HG3	1.81	0.61
1:I:121:MET:HG3	1:I:173:ASN:O	2.01	0.60
1:H:8:ILE:HD11	1:I:17:ALA:O	2.02	0.60
1:A:6:THR:HA	1:A:18:TYR:O	2.01	0.60
1:E:18:TYR:HB3	1:E:22:SER:HB2	1.83	0.60
1:V:82:GLN:HA	1:V:82:GLN:NE2	2.17	0.60
1:E:79:ASP:HB3	1:I:115:LEU:HD13	1.83	0.59
1:B:35:GLN:HE21	1:B:69:GLY:HA2	1.67	0.59
1:K:93:ILE:HG22	1:K:115:LEU:HD12	1.84	0.59
1:J:176:THR:HG22	1:J:178:GLU:H	1.68	0.59
1:E:123:HIS:HE1	1:F:140:ALA:H	1.49	0.59
1:I:176:THR:HG22	1:I:178:GLU:H	1.68	0.59
1:K:140:ALA:H	1:M:123:HIS:CE1	2.16	0.58
1:E:160:GLN:NE2	1:E:164:LYS:HD3	2.18	0.58
1:L:142:HIS:O	1:L:146:THR:HG22	2.03	0.58
1:V:79:ASP:HB3	1:C:115:LEU:HD13	1.84	0.58
1:V:142:HIS:CE1	1:C:119:GLU:OE1	2.57	0.58
1:E:35:GLN:HE21	1:E:69:GLY:HA2	1.68	0.58
1:A:176:THR:HG22	1:A:178:GLU:N	2.18	0.58
1:K:41:ALA:O	1:K:45:VAL:HG23	2.03	0.58
1:A:42:ASN:CB	1:B:31[A]:MET:HE1	2.33	0.58
1:E:82:GLN:HA	1:E:82:GLN:NE2	2.18	0.58
1:E:99:MET:HE2	1:E:124:GLN:HE22	1.69	0.58
1:I:142:HIS:O	1:I:146:THR:HG22	2.03	0.58
1:G:115:LEU:HD23	1:G:190:MET:HE3	1.86	0.57
1:C:45:VAL:HG11	1:D:93:ILE:HD13	1.85	0.57
1:D:124:GLN:O	1:D:147:ARG:NH2	2.30	0.57
1:K:18:TYR:HB3	1:K:22:SER:HB2	1.86	0.57
1:M:18:TYR:HB3	1:M:22:SER:HB2	1.85	0.57
1:B:115:LEU:HD23	1:B:190:MET:CE	2.34	0.57
1:C:123:HIS:CE1	1:H:140:ALA:H	2.15	0.57
1:V:59:ASP:OD1	1:V:87:ASP:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:PRO:O	1:D:97:ALA:HB3	2.05	0.57
1:I:122:ILE:O	1:I:124:GLN:NE2	2.38	0.56
1:C:35:GLN:HE21	1:C:69:GLY:HA2	1.69	0.56
1:L:167:LYS:O	1:L:171:ARG:HD2	2.06	0.56
1:I:89:GLN:HG2	1:I:111:LYS:HB3	1.87	0.56
1:F:176:THR:HG22	1:F:178:GLU:H	1.71	0.56
1:J:123:HIS:HB2	1:J:171:ARG:O	2.06	0.56
1:K:123:HIS:HE1	1:M:140:ALA:H	1.53	0.56
1:F:141:ASN:OD1	1:F:142:HIS:N	2.39	0.55
1:G:176:THR:HG22	1:G:178:GLU:H	1.70	0.55
1:E:115:LEU:HD13	1:K:79:ASP:HB3	1.88	0.55
1:F:149:LYS:NZ	1:M:117:ASN:HD22	2.04	0.55
1:G:93:ILE:HG13	1:G:93:ILE:O	2.07	0.55
1:J:7:VAL:HB	1:J:23:ARG:HG3	1.87	0.55
1:V:124:GLN:HG2	1:V:150:LEU:HD13	1.87	0.55
1:A:42:ASN:ND2	1:B:31[A]:MET:HE3	2.12	0.55
1:V:163:GLU:O	1:V:167:LYS:HG3	2.07	0.55
1:V:42:ASN:OD1	1:C:31[A]:MET:CG	2.55	0.54
1:G:18:TYR:HB3	1:G:22:SER:HB2	1.90	0.54
1:G:42:ASN:ND2	2:G:302:HOH:O	2.41	0.54
1:H:124:GLN:HG2	1:H:150:LEU:HD13	1.90	0.54
1:J:52:GLN:HG3	1:J:86:PRO:HD3	1.89	0.54
1:E:126:LEU:HD13	1:F:126:LEU:HD22	1.90	0.54
1:D:115:LEU:HD21	1:D:190:MET:CE	2.38	0.53
1:E:142:HIS:O	1:E:146:THR:HG23	2.07	0.53
1:V:18:TYR:HB3	1:V:22:SER:HB2	1.89	0.53
1:L:178:GLU:O	1:L:182:GLU:HG3	2.09	0.53
1:A:117:ASN:ND2	1:G:149:LYS:HD3	2.24	0.53
1:I:19:ASP:OD2	1:I:22:SER:OG	2.25	0.53
1:C:79:ASP:HB3	1:D:115:LEU:HD13	1.91	0.53
1:E:122:ILE:HD11	1:E:168:ASP:CB	2.39	0.53
1:L:98:SER:OG	1:L:99:MET:N	2.42	0.53
1:D:142:HIS:O	1:D:146:THR:HG23	2.09	0.52
1:I:160:GLN:NE2	1:I:164:LYS:HD2	2.24	0.52
1:J:18:TYR:HB3	1:J:22:SER:HB2	1.91	0.52
1:F:121:MET:HG3	1:F:173:ASN:O	2.08	0.52
1:L:35:GLN:HE21	1:L:69:GLY:HA2	1.74	0.52
1:V:109:LYS:HZ3	1:V:157:ARG:HH12	1.53	0.52
1:A:42:ASN:HD21	1:B:33:GLY:HA3	1.75	0.52
1:J:93:ILE:HG22	1:J:115:LEU:CD1	2.39	0.52
1:F:5:PRO:O	1:F:19:ASP:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:GLN:HB2	1:G:165:ILE:HD12	1.92	0.52
1:G:115:LEU:HD13	1:H:79:ASP:HB3	1.92	0.52
1:G:40:VAL:O	1:G:44:ILE:HG12	2.09	0.52
1:A:109:LYS:NZ	1:A:157:ARG:HA	2.25	0.52
1:B:52:GLN:HG3	1:B:86:PRO:HD3	1.92	0.52
1:A:115:LEU:HD13	1:G:79:ASP:CB	2.40	0.52
1:H:160:GLN:HB2	1:H:165:ILE:HD12	1.92	0.52
1:J:57:GLU:OE2	1:J:85:LYS:HE2	2.10	0.52
1:E:140:ALA:H	1:F:123:HIS:CE1	2.20	0.51
1:I:52:GLN:HG3	1:I:84:ILE:HB	1.91	0.51
1:V:109:LYS:NZ	1:V:157:ARG:HH11	2.04	0.51
1:E:35:GLN:NE2	1:E:69:GLY:HA2	2.26	0.51
1:A:115:LEU:HD13	1:G:79:ASP:HB3	1.93	0.51
1:E:142:HIS:ND1	2:E:304:HOH:O	2.34	0.51
1:E:82:GLN:HA	1:E:82:GLN:HE21	1.76	0.51
1:C:93:ILE:HG22	1:C:115:LEU:HD12	1.92	0.51
1:F:32:LEU:HD21	1:F:36:ILE:HD11	1.92	0.51
1:A:171:ARG:HE	1:J:141[A]:ASN:ND2	2.08	0.51
1:K:52:GLN:HG3	1:K:84:ILE:HB	1.92	0.51
1:J:99:MET:CE	1:J:124:GLN:OE1	2.58	0.51
1:A:28:ARG:HG2	1:A:51:LEU:HD22	1.93	0.51
1:G:115:LEU:CD2	1:G:190:MET:HE3	2.41	0.51
1:V:149:LYS:HE3	1:C:117:ASN:HD22	1.75	0.51
1:E:124:GLN:O	1:E:147:ARG:NH2	2.41	0.51
1:I:5:PRO:HD2	1:I:20:ILE:CG1	2.41	0.51
1:I:71:VAL:HG22	1:I:99:MET:HE3	1.94	0.50
1:V:115:LEU:HD13	1:J:79:ASP:HB3	1.93	0.50
1:G:89:GLN:HG2	1:G:111:LYS:HB3	1.94	0.50
1:M:41:ALA:HB2	1:M:73:ALA:HB1	1.94	0.50
1:C:138:ILE:O	1:C:138:ILE:HG22	2.10	0.50
1:I:124:GLN:O	1:I:147:ARG:NH2	2.33	0.50
1:V:160:GLN:HB2	1:V:165:ILE:CD1	2.41	0.50
1:F:142:HIS:O	1:F:146:THR:HG23	2.12	0.50
1:H:35:GLN:HG3	1:H:68:GLY:O	2.12	0.50
1:L:40:VAL:O	1:L:44:ILE:HG12	2.11	0.50
1:F:40:VAL:O	1:F:44:ILE:HG12	2.12	0.50
1:V:122:ILE:CD1	1:V:168:ASP:HB3	2.42	0.50
1:B:141:ASN:ND2	1:L:171:ARG:NH2	2.60	0.50
1:D:147:ARG:NH1	1:D:170:ASP:OD1	2.41	0.50
1:K:7:VAL:HB	1:K:23:ARG:HG3	1.92	0.50
1:L:160:GLN:HB2	1:L:165:ILE:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:HIS:HB2	1:G:171:ARG:O	2.12	0.49
1:H:7:VAL:N	1:H:18:TYR:O	2.42	0.49
1:C:5:PRO:HD2	1:C:20:ILE:HG12	1.94	0.49
1:D:98:SER:OG	1:D:99:MET:N	2.44	0.49
1:C:141:ASN:HB3	1:H:170:ASP:HB3	1.94	0.49
1:E:41:ALA:HB2	1:E:73:ALA:HB1	1.94	0.49
1:E:35:GLN:HE21	1:E:69:GLY:CA	2.25	0.49
1:B:52:GLN:HG3	1:B:86:PRO:CD	2.43	0.49
1:B:71:VAL:HG22	1:B:99:MET:HE3	1.95	0.49
1:D:99:MET:HE2	1:D:124:GLN:HE22	1.78	0.49
1:A:16:ARG:CB	1:B:8:ILE:HG21	2.41	0.49
1:A:142:HIS:O	1:A:146:THR:HG23	2.12	0.49
1:J:121:MET:HG3	1:J:173:ASN:O	2.12	0.49
1:K:126:LEU:HD13	1:M:126:LEU:HD22	1.95	0.49
1:A:85:LYS:N	1:A:86:PRO:HD2	2.27	0.49
1:B:160:GLN:HB2	1:B:165:ILE:CD1	2.43	0.49
1:M:93:ILE:HG22	1:M:115:LEU:HD12	1.94	0.49
1:D:7:VAL:HB	1:D:23:ARG:HG3	1.95	0.48
1:B:140:ALA:H	1:L:123:HIS:CE1	2.18	0.48
1:V:142:HIS:O	1:V:146:THR:HG23	2.13	0.48
1:F:93:ILE:HG22	1:F:115:LEU:CD1	2.43	0.48
1:H:122:ILE:H	1:H:122:ILE:HD13	1.78	0.48
1:B:40:VAL:O	1:B:44:ILE:HG12	2.13	0.48
1:D:152:ARG:O	1:D:156:GLU:HG3	2.13	0.48
1:K:142:HIS:O	1:K:146:THR:HG23	2.13	0.48
1:V:144:LEU:O	1:V:147:ARG:HG3	2.13	0.48
1:D:45:VAL:HG11	1:F:93:ILE:HD12	1.95	0.48
1:B:41:ALA:O	1:B:45:VAL:HG23	2.14	0.48
1:L:160:GLN:HB2	1:L:165:ILE:HD12	1.95	0.48
1:L:155:SER:HA	1:L:165:ILE:HD13	1.96	0.48
1:K:8:ILE:HA	1:K:16:ARG:O	2.14	0.48
1:B:59:ASP:OD1	1:B:87:ASP:HB2	2.14	0.47
1:L:41:ALA:O	1:L:45:VAL:HG23	2.14	0.47
1:E:52:GLN:HB3	1:E:52:GLN:HE21	1.56	0.47
1:V:52:GLN:HG3	1:V:86:PRO:HD3	1.94	0.47
1:A:9:GLU:HG3	1:A:23:ARG:HD3	1.95	0.47
1:D:93:ILE:HG13	1:D:93:ILE:O	2.14	0.47
1:V:42:ASN:OD1	1:C:31[A]:MET:HG2	2.13	0.47
1:G:122:ILE:HD11	1:G:168:ASP:CB	2.32	0.47
1:A:164:LYS:NZ	1:A:168:ASP:OD2	2.47	0.47
1:C:95:MET:HG3	1:C:96:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:SER:OG	1:H:99:MET:N	2.44	0.47
1:K:91:ILE:HG23	1:K:190:MET:CE	2.44	0.47
1:L:95:MET:HE2	1:L:95:MET:HB2	1.78	0.47
1:V:109:LYS:HE3	1:V:157:ARG:O	2.15	0.47
1:B:176:THR:HG22	1:B:179:GLU:H	1.78	0.47
1:D:140:ALA:H	1:I:123:HIS:CE1	2.26	0.47
1:J:142:HIS:O	1:J:146:THR:HG23	2.14	0.47
1:A:40:VAL:O	1:A:44:ILE:HG12	2.15	0.47
1:L:123:HIS:HB2	1:L:171:ARG:O	2.15	0.47
1:V:115:LEU:HD23	1:V:190:MET:HE3	1.97	0.47
1:C:7:VAL:N	1:C:18:TYR:O	2.45	0.47
1:G:177:ALA:O	1:G:186:ILE:HD11	2.15	0.47
1:J:98:SER:OG	1:J:99:MET:N	2.47	0.47
1:V:140:ALA:H	1:G:123:HIS:CE1	2.23	0.47
1:V:109:LYS:HZ1	1:V:157:ARG:HH11	1.61	0.47
1:D:115:LEU:CD2	1:D:190:MET:HE2	2.44	0.47
1:E:120:VAL:HG11	1:E:185:LEU:HD13	1.97	0.47
1:I:152:ARG:HD2	1:I:152:ARG:C	2.35	0.47
1:K:41:ALA:HA	1:K:77:ILE:HD11	1.97	0.47
1:A:123:HIS:HB2	1:A:172:ASP:HA	1.96	0.46
1:J:99:MET:HE1	1:J:124:GLN:OE1	2.15	0.46
1:K:121:MET:HG3	1:K:173:ASN:O	2.15	0.46
1:L:78:TYR:O	1:L:82:GLN:HG2	2.14	0.46
1:V:117:ASN:HD22	1:J:149:LYS:HE3	1.80	0.46
1:V:190:MET:HE3	1:V:190:MET:HB2	1.74	0.46
1:A:42:ASN:ND2	1:B:31[A]:MET:SD	2.85	0.46
1:F:99:MET:HE2	1:F:124:GLN:HE22	1.81	0.46
1:K:191:VAL:HA	1:K:192:PRO:HD3	1.83	0.46
1:V:122:ILE:H	1:V:122:ILE:HG13	1.54	0.46
1:E:123:HIS:CE1	1:F:140:ALA:H	2.32	0.46
1:E:8:ILE:HD11	1:K:17:ALA:O	2.15	0.46
1:F:98:SER:OG	1:F:99:MET:N	2.48	0.46
1:J:59:ASP:OD1	1:J:87:ASP:HB2	2.15	0.46
1:K:6:THR:HG23	1:K:18:TYR:O	2.16	0.46
1:B:122:ILE:CD1	1:B:168:ASP:HB3	2.34	0.46
1:G:115:LEU:HD13	1:H:79:ASP:CB	2.46	0.46
1:M:171:ARG:HB2	1:M:171:ARG:NH1	2.31	0.46
1:M:40:VAL:O	1:M:44:ILE:HG12	2.16	0.45
1:E:160:GLN:HB2	1:E:165:ILE:HD13	1.96	0.45
1:F:6:THR:HA	1:F:18:TYR:O	2.16	0.45
1:J:122:ILE:HD12	1:J:168:ASP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:O	1:C:93:ILE:HG13	2.15	0.45
1:V:7:VAL:CB	1:V:23:ARG:HG3	2.42	0.45
1:G:106:ALA:HA	1:G:157:ARG:HD3	1.98	0.45
1:K:141:ASN:O	1:K:145:LYS:HE3	2.17	0.45
1:E:93:ILE:HD12	1:K:45:VAL:HG11	1.97	0.45
1:D:82:GLN:HA	1:D:82:GLN:NE2	2.31	0.45
1:K:175:LEU:HG	1:K:179:GLU:HB3	1.99	0.45
1:V:142:HIS:HE1	1:C:119:GLU:OE1	2.00	0.45
1:D:115:LEU:CD2	1:D:190:MET:CE	2.94	0.45
1:J:155:SER:HA	1:J:165:ILE:HD12	1.99	0.45
1:K:172:ASP:N	1:K:172:ASP:OD2	2.44	0.45
1:V:126:LEU:HD13	1:G:126:LEU:HD22	1.98	0.45
1:H:18:TYR:HB3	1:H:22:SER:HB2	1.98	0.45
1:V:8:ILE:HD11	1:J:17:ALA:O	2.17	0.45
1:J:40:VAL:O	1:J:44:ILE:HG12	2.17	0.45
1:L:71:VAL:HG22	1:L:99:MET:HE3	1.98	0.45
1:I:91:ILE:HG23	1:I:190:MET:HE2	1.98	0.45
1:J:5:PRO:HD2	1:J:20:ILE:HG12	1.99	0.45
1:K:155:SER:HA	1:K:165:ILE:HD13	1.99	0.45
1:M:91:ILE:HD12	1:M:91:ILE:N	2.32	0.45
1:G:20:ILE:H	1:G:20:ILE:HG13	1.63	0.45
1:A:93:ILE:HD13	1:G:45:VAL:HG11	2.00	0.44
1:J:93:ILE:HG22	1:J:115:LEU:HD11	1.98	0.44
1:D:8:ILE:HA	1:D:16:ARG:O	2.17	0.44
1:M:123:HIS:HB2	1:M:172:ASP:HA	1.99	0.44
1:B:30:ILE:HD11	1:B:51:LEU:HD12	1.99	0.44
1:F:190:MET:HE3	1:F:190:MET:HB2	1.57	0.44
1:V:20:ILE:HG13	1:V:20:ILE:H	1.66	0.44
1:A:72:THR:HG21	1:B:95:MET:HB2	2.00	0.44
1:V:8:ILE:HD12	1:J:18:TYR:CZ	2.53	0.44
1:A:99:MET:HE2	1:A:124:GLN:HE22	1.83	0.44
1:C:38:ASP:O	1:C:42:ASN:ND2	2.50	0.44
1:F:109:LYS:NZ	1:F:157:ARG:O	2.51	0.44
1:E:160:GLN:HB2	1:E:165:ILE:HD12	2.00	0.44
1:F:79:ASP:HB3	1:M:115:LEU:HD13	1.99	0.44
1:F:82:GLN:HA	1:F:82:GLN:NE2	2.32	0.44
1:H:155:SER:HA	1:H:165:ILE:HD13	2.00	0.44
1:J:191:VAL:HA	1:J:192:PRO:HD3	1.89	0.44
1:V:40:VAL:O	1:V:44:ILE:HG12	2.18	0.44
1:A:65:ASN:HB2	1:A:93:ILE:HG13	1.99	0.43
1:C:98:SER:HB3	1:C:125:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:SER:HA	1:K:124:GLN:HE21	1.83	0.43
1:E:162:ILE:O	1:E:166:GLN:HB2	2.18	0.43
1:I:20:ILE:HG13	1:I:20:ILE:H	1.67	0.43
1:J:28:ARG:HG2	1:J:51:LEU:HD22	2.00	0.43
1:K:98:SER:OG	1:K:99:MET:N	2.52	0.43
1:L:115:LEU:HD13	1:M:79:ASP:CB	2.40	0.43
1:V:119:GLU:CD	1:J:142:HIS:CE1	2.91	0.43
1:H:93:ILE:HG22	1:H:115:LEU:HD12	2.01	0.43
1:V:162:ILE:H	1:V:162:ILE:HG12	1.52	0.43
1:A:42:ASN:HD21	1:B:33:GLY:CA	2.31	0.43
1:C:56:SER:HA	1:C:86:PRO:HG3	1.99	0.43
1:K:59:ASP:OD1	1:K:87:ASP:HB2	2.17	0.43
1:I:5:PRO:HD2	1:I:20:ILE:HG12	1.99	0.43
1:J:28:ARG:NH2	1:J:58:LYS:O	2.48	0.43
1:L:117:ASN:HD22	1:M:149:LYS:HE3	1.84	0.43
1:B:191:VAL:HA	1:B:192:PRO:HD3	1.86	0.43
1:C:190:MET:HB2	1:C:190:MET:HE3	1.84	0.43
1:K:93:ILE:O	1:K:93:ILE:HG13	2.19	0.43
1:M:190:MET:HB2	1:M:190:MET:HE3	1.82	0.43
1:E:142:HIS:HE1	1:I:119:GLU:OE1	2.01	0.43
1:J:155:SER:HA	1:J:165:ILE:CD1	2.49	0.43
1:K:147:ARG:NH1	1:K:170:ASP:OD1	2.52	0.43
1:A:151:ASN:OD1	1:A:166:GLN:NE2	2.52	0.42
1:B:20:ILE:HG13	1:B:20:ILE:H	1.60	0.42
1:M:23:ARG:HH21	1:M:26:LYS:HD3	1.84	0.42
1:B:173:ASN:HD22	1:B:173:ASN:HA	1.69	0.42
1:E:5:PRO:HD2	1:E:20:ILE:HG12	2.01	0.42
1:I:147:ARG:NH1	1:I:170:ASP:OD1	2.42	0.42
1:L:52:GLN:HG3	1:L:86:PRO:HD3	2.02	0.42
1:G:71:VAL:HG13	1:G:99:MET:HE3	2.02	0.42
1:B:82:GLN:HA	1:B:82:GLN:NE2	2.35	0.42
1:E:85:LYS:N	1:E:86:PRO:CD	2.82	0.42
1:B:98:SER:HB2	1:B:99:MET:H	1.52	0.42
1:D:126:LEU:HD22	1:I:126:LEU:HD13	2.01	0.42
1:H:85:LYS:N	1:H:86:PRO:CD	2.83	0.42
1:B:9:GLU:HG2	1:B:18:TYR:HE1	1.84	0.42
1:G:59:ASP:OD1	1:G:87:ASP:HB2	2.20	0.42
1:K:4:ILE:HA	1:K:5:PRO:HD3	1.93	0.42
1:A:38:ASP:O	1:A:42:ASN:OD1	2.38	0.42
1:A:77:ILE:HG21	1:A:103:LEU:HD13	2.02	0.42
1:A:138:ILE:HG22	1:A:139:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ILE:HD11	1:K:51:LEU:HD12	2.02	0.42
1:A:30:ILE:HD11	1:A:51:LEU:HD12	2.01	0.42
1:B:93:ILE:HG13	1:B:93:ILE:O	2.19	0.42
1:I:190:MET:HE3	1:I:190:MET:HB2	1.55	0.42
1:H:6:THR:O	1:I:22:SER:HB3	2.20	0.42
1:D:176:THR:HG22	1:D:178:GLU:N	2.35	0.41
1:E:99:MET:HE1	1:E:150:LEU:HD11	2.02	0.41
1:I:91:ILE:HG23	1:I:190:MET:CE	2.50	0.41
1:J:8:ILE:HD11	1:L:17:ALA:O	2.19	0.41
1:L:126:LEU:CD2	1:L:143:ILE:HD11	2.51	0.41
1:A:160:GLN:HE21	1:A:160:GLN:HA	1.86	0.41
1:F:18:TYR:CD1	1:F:23:ARG:HG2	2.54	0.41
1:A:171:ARG:NE	1:J:141[A]:ASN:HD22	2.14	0.41
1:E:171:ARG:HB3	1:F:141:ASN:ND2	2.35	0.41
1:G:6:THR:O	1:H:22:SER:HB3	2.21	0.41
1:H:123:HIS:HB2	1:H:172:ASP:HA	2.01	0.41
1:H:176:THR:HG22	1:H:179:GLU:N	2.21	0.41
1:K:123:HIS:HB2	1:K:171:ARG:O	2.21	0.41
1:A:35:GLN:HG3	1:A:68:GLY:O	2.21	0.41
1:J:65:ASN:HB2	1:J:93:ILE:HG13	2.03	0.41
1:J:8:ILE:HA	1:J:16:ARG:O	2.20	0.41
1:A:160:GLN:NE2	1:A:160:GLN:HA	2.36	0.41
1:A:5:PRO:HD2	1:A:20:ILE:HG12	2.01	0.41
1:F:28:ARG:HG2	1:F:51:LEU:HD22	2.02	0.41
1:V:71:VAL:HG22	1:V:99:MET:CE	2.51	0.41
1:C:5:PRO:HD2	1:C:20:ILE:CG1	2.50	0.41
1:K:155:SER:CA	1:K:165:ILE:HD13	2.51	0.41
1:F:181:LYS:HD2	1:F:188:GLU:HA	2.03	0.41
1:B:164:LYS:NZ	1:B:168:ASP:OD2	2.54	0.41
1:E:33:GLY:O	1:K:42:ASN:ND2	2.51	0.41
1:L:167:LYS:O	1:L:171:ARG:CD	2.69	0.41
1:M:115:LEU:HD23	1:M:190:MET:HE3	2.03	0.41
1:M:78:TYR:O	1:M:82:GLN:HG2	2.21	0.41
1:A:17:ALA:O	1:B:8:ILE:CD1	2.57	0.40
1:V:144:LEU:HA	1:V:147:ARG:HG3	2.03	0.40
1:V:45:VAL:O	1:V:49:LEU:HG	2.21	0.40
1:E:123:HIS:HB2	1:E:172:ASP:HA	2.04	0.40
1:E:142:HIS:CE1	1:I:119:GLU:OE1	2.74	0.40
1:B:139:ALA:HA	1:L:123:HIS:CE1	2.56	0.40
1:J:6:THR:O	1:L:22:SER:HB3	2.20	0.40
1:V:192:PRO:HA	1:V:193:GLU:HA	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:93:ILE:HG22	1:V:115:LEU:CD1	2.52	0.40
1:E:119:GLU:OE1	1:K:142:HIS:NE2	2.55	0.40
1:K:160:GLN:HB2	1:K:165:ILE:CD1	2.51	0.40
1:A:123:HIS:HB2	1:A:171:ARG:O	2.22	0.40
1:B:8:ILE:HA	1:B:16:ARG:O	2.21	0.40
1:J:124:GLN:HA	1:J:125:PRO:HD2	1.92	0.40
1:V:82:GLN:HA	1:V:82:GLN:HE21	1.84	0.40
1:C:65:ASN:HB2	1:C:93:ILE:O	2.22	0.40
1:E:37:ASP:OD2	1:E:37:ASP:C	2.60	0.40
1:F:41:ALA:O	1:F:45:VAL:HG23	2.22	0.40
1:L:119:GLU:HG2	1:L:174:PHE:HD1	1.86	0.40
1:L:30:ILE:HD11	1:L:51:LEU:HD12	2.02	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	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
1	B	166/203 (82%)	162 (98%)	4 (2%)	0	100	100
1	C	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
1	D	165/203 (81%)	159 (96%)	6 (4%)	0	100	100
1	E	168/203 (83%)	165 (98%)	3 (2%)	0	100	100
1	F	167/203 (82%)	163 (98%)	4 (2%)	0	100	100
1	G	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
1	H	170/203 (84%)	166 (98%)	3 (2%)	1 (1%)	25	36
1	I	166/203 (82%)	162 (98%)	4 (2%)	0	100	100
1	J	169/203 (83%)	166 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	168/203 (83%)	164 (98%)	4 (2%)	0	100	100
1	L	162/203 (80%)	159 (98%)	3 (2%)	0	100	100
1	M	167/203 (82%)	161 (96%)	6 (4%)	0	100	100
1	V	166/203 (82%)	162 (98%)	4 (2%)	0	100	100
All	All	2335/2842 (82%)	2281 (98%)	53 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	94	GLY

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	145/171 (85%)	135 (93%)	10 (7%)	15	25
1	B	144/171 (84%)	134 (93%)	10 (7%)	15	25
1	C	145/171 (85%)	136 (94%)	9 (6%)	18	29
1	D	143/171 (84%)	131 (92%)	12 (8%)	11	16
1	E	146/171 (85%)	131 (90%)	15 (10%)	7	10
1	F	143/171 (84%)	136 (95%)	7 (5%)	25	40
1	G	145/171 (85%)	138 (95%)	7 (5%)	25	41
1	H	146/171 (85%)	131 (90%)	15 (10%)	7	10
1	I	144/171 (84%)	133 (92%)	11 (8%)	13	20
1	J	147/171 (86%)	133 (90%)	14 (10%)	8	12
1	K	146/171 (85%)	136 (93%)	10 (7%)	16	25
1	L	141/171 (82%)	129 (92%)	12 (8%)	10	16
1	M	146/171 (85%)	132 (90%)	14 (10%)	8	12
1	V	144/171 (84%)	130 (90%)	14 (10%)	8	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2025/2394 (85%)	1865 (92%)	160 (8%)	12 19

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	20	ILE
1	V	23	ARG
1	V	24	LEU
1	V	119	GLU
1	V	122	ILE
1	V	124	GLN
1	V	141	ASN
1	V	147	ARG
1	V	157	ARG
1	V	162	ILE
1	V	165	ILE
1	V	173	ASN
1	V	175	LEU
1	V	178	GLU
1	A	20	ILE
1	A	23	ARG
1	A	24	LEU
1	A	54	GLN
1	A	109	LYS
1	A	122	ILE
1	A	146	THR
1	A	166	GLN
1	A	171	ARG
1	A	175	LEU
1	B	20	ILE
1	B	23	ARG
1	B	24	LEU
1	B	52	GLN
1	B	98	SER
1	B	99	MET
1	B	166	GLN
1	B	171	ARG
1	B	173	ASN
1	B	175	LEU
1	C	20	ILE
1	C	23	ARG
1	C	24	LEU

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Mol	Chain	Res	Type
1	C	52	GLN
1	C	109	LYS
1	C	141	ASN
1	C	166	GLN
1	C	172	ASP
1	C	176	THR
1	D	20	ILE
1	D	23	ARG
1	D	24	LEU
1	D	35	GLN
1	D	109	LYS
1	D	146	THR
1	D	157	ARG
1	D	162	ILE
1	D	166	GLN
1	D	175	LEU
1	D	176	THR
1	D	191	VAL
1	E	10	THR
1	E	20	ILE
1	E	23	ARG
1	E	24	LEU
1	E	52	GLN
1	E	70	SER
1	E	150	LEU
1	E	157	ARG
1	E	164	LYS
1	E	165	ILE
1	E	171	ARG
1	E	173	ASN
1	E	175	LEU
1	E	176	THR
1	E	190	MET
1	F	20	ILE
1	F	23	ARG
1	F	24	LEU
1	F	52	GLN
1	F	146	THR
1	F	166	GLN
1	F	172	ASP
1	G	20	ILE
1	G	23	ARG

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Mol	Chain	Res	Type
1	G	24	LEU
1	G	165	ILE
1	G	166	GLN
1	G	175	LEU
1	G	182	GLU
1	H	9	GLU
1	H	20	ILE
1	H	23	ARG
1	H	24	LEU
1	H	52	GLN
1	H	122	ILE
1	H	124	GLN
1	H	126	LEU
1	H	165	ILE
1	H	171	ARG
1	H	173	ASN
1	H	174	PHE
1	H	175	LEU
1	H	176	THR
1	H	191	VAL
1	I	20	ILE
1	I	22	SER
1	I	23	ARG
1	I	24	LEU
1	I	52	GLN
1	I	98	SER
1	I	146	THR
1	I	171	ARG
1	I	172	ASP
1	I	175	LEU
1	I	182	GLU
1	J	20	ILE
1	J	23	ARG
1	J	24	LEU
1	J	52	GLN
1	J	70	SER
1	J	95	MET
1	J	99	MET
1	J	122	ILE
1	J	126	LEU
1	J	144	LEU
1	J	171	ARG

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Mol	Chain	Res	Type
1	J	173	ASN
1	J	175	LEU
1	J	190	MET
1	K	20	ILE
1	K	23	ARG
1	K	24	LEU
1	K	52	GLN
1	K	124	GLN
1	K	141	ASN
1	K	145	LYS
1	K	175	LEU
1	K	176	THR
1	K	182	GLU
1	L	19	ASP
1	L	20	ILE
1	L	23	ARG
1	L	24	LEU
1	L	95	MET
1	L	124	GLN
1	L	143	ILE
1	L	146	THR
1	L	149	LYS
1	L	165	ILE
1	L	171	ARG
1	L	175	LEU
1	M	20	ILE
1	M	22	SER
1	M	23	ARG
1	M	24	LEU
1	M	26	LYS
1	M	52	GLN
1	M	89	GLN
1	M	122	ILE
1	M	157	ARG
1	M	160	GLN
1	M	171	ARG
1	M	176	THR
1	M	182	GLU
1	M	191	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	39	ASN
1	V	82	GLN
1	V	89	GLN
1	V	117	ASN
1	V	123	HIS
1	V	142	HIS
1	V	151	ASN
1	V	160	GLN
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	160	GLN
1	A	166	GLN
1	B	35	GLN
1	B	39	ASN
1	B	82	GLN
1	B	89	GLN
1	B	117	ASN
1	B	124	GLN
1	B	141	ASN
1	B	151	ASN
1	B	160	GLN
1	B	173	ASN
1	C	35	GLN
1	C	52	GLN
1	C	82	GLN
1	C	89	GLN
1	C	117	ASN
1	C	123	HIS
1	C	142	HIS
1	C	151	ASN
1	C	160	GLN
1	C	166	GLN
1	D	42	ASN
1	D	82	GLN
1	D	89	GLN
1	D	117	ASN
1	D	124	GLN
1	D	151	ASN

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Mol	Chain	Res	Type
1	D	160	GLN
1	E	35	GLN
1	E	52	GLN
1	E	82	GLN
1	E	89	GLN
1	E	117	ASN
1	E	123	HIS
1	E	124	GLN
1	E	142	HIS
1	E	151	ASN
1	E	160	GLN
1	E	173	ASN
1	F	82	GLN
1	F	89	GLN
1	F	117	ASN
1	F	123	HIS
1	F	124	GLN
1	F	151	ASN
1	F	160	GLN
1	F	166	GLN
1	G	39	ASN
1	G	82	GLN
1	G	117	ASN
1	G	123	HIS
1	G	124	GLN
1	G	151	ASN
1	G	160	GLN
1	H	89	GLN
1	H	117	ASN
1	H	123	HIS
1	H	142	HIS
1	H	160	GLN
1	I	39	ASN
1	I	42	ASN
1	I	82	GLN
1	I	89	GLN
1	I	117	ASN
1	I	123	HIS
1	I	151	ASN
1	I	160	GLN
1	J	39	ASN
1	J	82	GLN

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Mol	Chain	Res	Type
1	J	89	GLN
1	J	117	ASN
1	J	123	HIS
1	J	142	HIS
1	J	151	ASN
1	J	160	GLN
1	K	52	GLN
1	K	82	GLN
1	K	89	GLN
1	K	117	ASN
1	K	123	HIS
1	K	151	ASN
1	K	160	GLN
1	K	166	GLN
1	K	173	ASN
1	L	35	GLN
1	L	39	ASN
1	L	82	GLN
1	L	89	GLN
1	L	117	ASN
1	L	123	HIS
1	L	151	ASN
1	L	160	GLN
1	M	39	ASN
1	M	82	GLN
1	M	89	GLN
1	M	117	ASN
1	M	123	HIS
1	M	124	GLN
1	M	151	ASN
1	M	160	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	173/203 (85%)	0.45	3 (1%)	70	68	36, 49, 66, 85	0
1	B	171/203 (84%)	0.51	6 (3%)	44	43	35, 46, 61, 79	0
1	C	172/203 (84%)	0.64	9 (5%)	27	26	40, 53, 69, 90	0
1	D	171/203 (84%)	0.47	4 (2%)	60	58	37, 49, 63, 71	0
1	E	173/203 (85%)	0.61	4 (2%)	60	58	37, 49, 68, 92	0
1	F	173/203 (85%)	0.60	10 (5%)	23	22	37, 51, 70, 79	0
1	G	173/203 (85%)	0.51	6 (3%)	44	43	39, 51, 68, 80	0
1	H	175/203 (86%)	0.53	9 (5%)	28	26	40, 52, 69, 87	0
1	I	172/203 (84%)	0.45	5 (2%)	51	50	37, 49, 67, 92	0
1	J	173/203 (85%)	0.42	6 (3%)	44	43	35, 48, 72, 83	0
1	K	173/203 (85%)	0.53	9 (5%)	27	26	39, 53, 72, 88	0
1	L	168/203 (82%)	0.43	3 (1%)	68	66	38, 50, 62, 73	0
1	M	172/203 (84%)	0.51	5 (2%)	51	50	38, 53, 66, 82	0
1	V	172/203 (84%)	0.41	2 (1%)	79	77	30, 46, 59, 76	0
All	All	2411/2842 (84%)	0.51	81 (3%)	45	44	30, 50, 68, 92	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	17	ALA	7.1
1	L	17	ALA	6.5
1	K	122	ILE	5.7
1	B	17	ALA	5.3
1	I	17	ALA	4.9
1	J	8	ILE	4.3
1	C	7	VAL	4.2
1	J	7	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	10	THR	3.9
1	F	7	VAL	3.9
1	J	18	TYR	3.7
1	F	128	GLY	3.7
1	F	6	THR	3.5
1	E	10	THR	3.5
1	H	10	THR	3.3
1	C	6	THR	3.3
1	F	17	ALA	3.3
1	A	8	ILE	3.3
1	E	126	LEU	3.2
1	I	7	VAL	3.2
1	K	15	GLU	3.2
1	M	93	ILE	3.2
1	B	16	ARG	3.1
1	A	7	VAL	3.1
1	D	16	ARG	3.1
1	L	144	LEU	3.1
1	F	122	ILE	3.1
1	C	75	PHE	3.0
1	E	17	ALA	3.0
1	G	15	GLU	2.8
1	H	171	ARG	2.8
1	L	18	TYR	2.8
1	B	9	GLU	2.8
1	G	122	ILE	2.7
1	K	8	ILE	2.7
1	C	8	ILE	2.6
1	F	18	TYR	2.6
1	F	127	GLY	2.6
1	H	166	GLN	2.6
1	B	18	TYR	2.6
1	D	50	PHE	2.6
1	K	9	GLU	2.6
1	E	8	ILE	2.5
1	G	167	LYS	2.5
1	I	18	TYR	2.5
1	J	27	ASP	2.5
1	D	7	VAL	2.4
1	K	148	GLU	2.4
1	G	138	ILE	2.4
1	H	18	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	V	7	VAL	2.4
1	H	17	ALA	2.4
1	C	16	ARG	2.4
1	A	162	ILE	2.3
1	K	163	GLU	2.3
1	J	126	LEU	2.3
1	F	32	LEU	2.3
1	H	143	ILE	2.3
1	B	7	VAL	2.2
1	I	8	ILE	2.2
1	M	173	ASN	2.2
1	F	8	ILE	2.2
1	M	167	LYS	2.2
1	V	147	ARG	2.2
1	K	167	LYS	2.2
1	G	17	ALA	2.2
1	H	8	ILE	2.1
1	M	17	ALA	2.1
1	J	94	GLY	2.1
1	K	18	TYR	2.1
1	C	126	LEU	2.1
1	D	191	VAL	2.1
1	G	35	GLN	2.1
1	C	191	VAL	2.1
1	B	173	ASN	2.1
1	C	9	GLU	2.1
1	F	167	LYS	2.1
1	I	121	MET	2.0
1	H	109	LYS	2.0
1	H	6	THR	2.0
1	K	191	VAL	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.