wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 12:30 PM EDT

PDB ID	:	4JCQ
Title	:	ClpP1 from Listeria monocytogenes
Authors	:	Zeiler, E.; List, A.; Alte, F.; Gersch, M.; Wachtel, R.; Groll, M.; Sieber, S.
Deposited on	:	2013-02-22
Resolution	:	2.00 Å(reported)

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

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

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

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

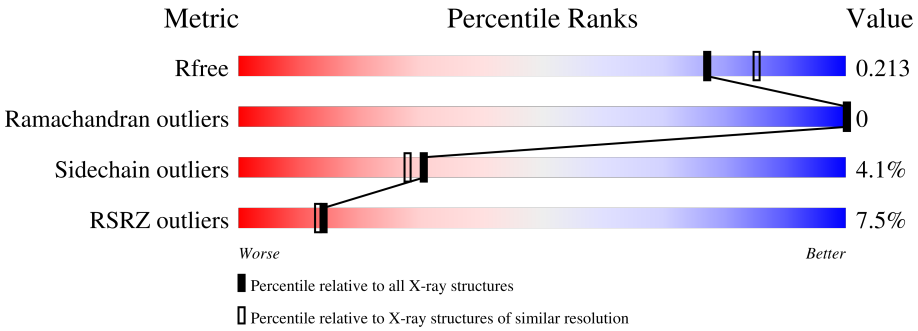
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	201	5% 82% · 15%
1	B	201	5% 82% · 15%
1	C	201	8% 82% · 15%
1	D	201	7% 82% · 15%
1	E	201	7% 81% · 15%
1	F	201	6% 81% · 15%

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Mol	Chain	Length	Quality of chain
1	G	201	7% 81% 15%
1	H	201	5% 81% 15%
1	I	201	7% 82% 15%
1	J	201	7% 82% 15%
1	K	201	6% 81% 15%
1	L	201	6% 82% 15%
1	M	201	6% 80% 15%
1	N	201	5% 81% 15%
1	O	201	8% 82% 15%
1	P	201	5% 82% 15%
1	Q	201	6% 82% 15%
1	R	201	5% 81% 15%
1	S	201	5% 81% 15%
1	T	201	6% 81% 15%
1	U	201	6% 82% 15%
1	V	201	7% 82% 15%
1	W	201	7% 82% 15%
1	X	201	6% 82% 15%
1	Y	201	8% 82% 15%
1	Z	201	6% 82% 15%
1	a	201	6% 81% 15%
1	b	201	6% 81% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 40559 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	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	B	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	C	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	D	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	E	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	F	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	G	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	H	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	I	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	J	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	K	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	L	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	M	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	N	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	O	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	P	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	R	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	S	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	T	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	U	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	V	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	W	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	X	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	Y	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	Z	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	a	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			
1	b	170	Total	C	N	O	S	0	0	0
			1345	850	232	260	3			

There are 308 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	MET	-	expression tag	UNP Q8Y7Y1
A	192	ALA	-	expression tag	UNP Q8Y7Y1
A	193	SER	-	expression tag	UNP Q8Y7Y1
A	194	TRP	-	expression tag	UNP Q8Y7Y1
A	195	SER	-	expression tag	UNP Q8Y7Y1
A	196	HIS	-	expression tag	UNP Q8Y7Y1
A	197	PRO	-	expression tag	UNP Q8Y7Y1
A	198	GLN	-	expression tag	UNP Q8Y7Y1
A	199	PHE	-	expression tag	UNP Q8Y7Y1
A	200	GLU	-	expression tag	UNP Q8Y7Y1
A	201	LYS	-	expression tag	UNP Q8Y7Y1
B	191	MET	-	expression tag	UNP Q8Y7Y1
B	192	ALA	-	expression tag	UNP Q8Y7Y1
B	193	SER	-	expression tag	UNP Q8Y7Y1
B	194	TRP	-	expression tag	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	SER	-	expression tag	UNP Q8Y7Y1
B	196	HIS	-	expression tag	UNP Q8Y7Y1
B	197	PRO	-	expression tag	UNP Q8Y7Y1
B	198	GLN	-	expression tag	UNP Q8Y7Y1
B	199	PHE	-	expression tag	UNP Q8Y7Y1
B	200	GLU	-	expression tag	UNP Q8Y7Y1
B	201	LYS	-	expression tag	UNP Q8Y7Y1
C	191	MET	-	expression tag	UNP Q8Y7Y1
C	192	ALA	-	expression tag	UNP Q8Y7Y1
C	193	SER	-	expression tag	UNP Q8Y7Y1
C	194	TRP	-	expression tag	UNP Q8Y7Y1
C	195	SER	-	expression tag	UNP Q8Y7Y1
C	196	HIS	-	expression tag	UNP Q8Y7Y1
C	197	PRO	-	expression tag	UNP Q8Y7Y1
C	198	GLN	-	expression tag	UNP Q8Y7Y1
C	199	PHE	-	expression tag	UNP Q8Y7Y1
C	200	GLU	-	expression tag	UNP Q8Y7Y1
C	201	LYS	-	expression tag	UNP Q8Y7Y1
D	191	MET	-	expression tag	UNP Q8Y7Y1
D	192	ALA	-	expression tag	UNP Q8Y7Y1
D	193	SER	-	expression tag	UNP Q8Y7Y1
D	194	TRP	-	expression tag	UNP Q8Y7Y1
D	195	SER	-	expression tag	UNP Q8Y7Y1
D	196	HIS	-	expression tag	UNP Q8Y7Y1
D	197	PRO	-	expression tag	UNP Q8Y7Y1
D	198	GLN	-	expression tag	UNP Q8Y7Y1
D	199	PHE	-	expression tag	UNP Q8Y7Y1
D	200	GLU	-	expression tag	UNP Q8Y7Y1
D	201	LYS	-	expression tag	UNP Q8Y7Y1
E	191	MET	-	expression tag	UNP Q8Y7Y1
E	192	ALA	-	expression tag	UNP Q8Y7Y1
E	193	SER	-	expression tag	UNP Q8Y7Y1
E	194	TRP	-	expression tag	UNP Q8Y7Y1
E	195	SER	-	expression tag	UNP Q8Y7Y1
E	196	HIS	-	expression tag	UNP Q8Y7Y1
E	197	PRO	-	expression tag	UNP Q8Y7Y1
E	198	GLN	-	expression tag	UNP Q8Y7Y1
E	199	PHE	-	expression tag	UNP Q8Y7Y1
E	200	GLU	-	expression tag	UNP Q8Y7Y1
E	201	LYS	-	expression tag	UNP Q8Y7Y1
F	191	MET	-	expression tag	UNP Q8Y7Y1
F	192	ALA	-	expression tag	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	193	SER	-	expression tag	UNP Q8Y7Y1
F	194	TRP	-	expression tag	UNP Q8Y7Y1
F	195	SER	-	expression tag	UNP Q8Y7Y1
F	196	HIS	-	expression tag	UNP Q8Y7Y1
F	197	PRO	-	expression tag	UNP Q8Y7Y1
F	198	GLN	-	expression tag	UNP Q8Y7Y1
F	199	PHE	-	expression tag	UNP Q8Y7Y1
F	200	GLU	-	expression tag	UNP Q8Y7Y1
F	201	LYS	-	expression tag	UNP Q8Y7Y1
G	191	MET	-	expression tag	UNP Q8Y7Y1
G	192	ALA	-	expression tag	UNP Q8Y7Y1
G	193	SER	-	expression tag	UNP Q8Y7Y1
G	194	TRP	-	expression tag	UNP Q8Y7Y1
G	195	SER	-	expression tag	UNP Q8Y7Y1
G	196	HIS	-	expression tag	UNP Q8Y7Y1
G	197	PRO	-	expression tag	UNP Q8Y7Y1
G	198	GLN	-	expression tag	UNP Q8Y7Y1
G	199	PHE	-	expression tag	UNP Q8Y7Y1
G	200	GLU	-	expression tag	UNP Q8Y7Y1
G	201	LYS	-	expression tag	UNP Q8Y7Y1
H	191	MET	-	expression tag	UNP Q8Y7Y1
H	192	ALA	-	expression tag	UNP Q8Y7Y1
H	193	SER	-	expression tag	UNP Q8Y7Y1
H	194	TRP	-	expression tag	UNP Q8Y7Y1
H	195	SER	-	expression tag	UNP Q8Y7Y1
H	196	HIS	-	expression tag	UNP Q8Y7Y1
H	197	PRO	-	expression tag	UNP Q8Y7Y1
H	198	GLN	-	expression tag	UNP Q8Y7Y1
H	199	PHE	-	expression tag	UNP Q8Y7Y1
H	200	GLU	-	expression tag	UNP Q8Y7Y1
H	201	LYS	-	expression tag	UNP Q8Y7Y1
I	191	MET	-	expression tag	UNP Q8Y7Y1
I	192	ALA	-	expression tag	UNP Q8Y7Y1
I	193	SER	-	expression tag	UNP Q8Y7Y1
I	194	TRP	-	expression tag	UNP Q8Y7Y1
I	195	SER	-	expression tag	UNP Q8Y7Y1
I	196	HIS	-	expression tag	UNP Q8Y7Y1
I	197	PRO	-	expression tag	UNP Q8Y7Y1
I	198	GLN	-	expression tag	UNP Q8Y7Y1
I	199	PHE	-	expression tag	UNP Q8Y7Y1
I	200	GLU	-	expression tag	UNP Q8Y7Y1
I	201	LYS	-	expression tag	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	191	MET	-	expression tag	UNP Q8Y7Y1
J	192	ALA	-	expression tag	UNP Q8Y7Y1
J	193	SER	-	expression tag	UNP Q8Y7Y1
J	194	TRP	-	expression tag	UNP Q8Y7Y1
J	195	SER	-	expression tag	UNP Q8Y7Y1
J	196	HIS	-	expression tag	UNP Q8Y7Y1
J	197	PRO	-	expression tag	UNP Q8Y7Y1
J	198	GLN	-	expression tag	UNP Q8Y7Y1
J	199	PHE	-	expression tag	UNP Q8Y7Y1
J	200	GLU	-	expression tag	UNP Q8Y7Y1
J	201	LYS	-	expression tag	UNP Q8Y7Y1
K	191	MET	-	expression tag	UNP Q8Y7Y1
K	192	ALA	-	expression tag	UNP Q8Y7Y1
K	193	SER	-	expression tag	UNP Q8Y7Y1
K	194	TRP	-	expression tag	UNP Q8Y7Y1
K	195	SER	-	expression tag	UNP Q8Y7Y1
K	196	HIS	-	expression tag	UNP Q8Y7Y1
K	197	PRO	-	expression tag	UNP Q8Y7Y1
K	198	GLN	-	expression tag	UNP Q8Y7Y1
K	199	PHE	-	expression tag	UNP Q8Y7Y1
K	200	GLU	-	expression tag	UNP Q8Y7Y1
K	201	LYS	-	expression tag	UNP Q8Y7Y1
L	191	MET	-	expression tag	UNP Q8Y7Y1
L	192	ALA	-	expression tag	UNP Q8Y7Y1
L	193	SER	-	expression tag	UNP Q8Y7Y1
L	194	TRP	-	expression tag	UNP Q8Y7Y1
L	195	SER	-	expression tag	UNP Q8Y7Y1
L	196	HIS	-	expression tag	UNP Q8Y7Y1
L	197	PRO	-	expression tag	UNP Q8Y7Y1
L	198	GLN	-	expression tag	UNP Q8Y7Y1
L	199	PHE	-	expression tag	UNP Q8Y7Y1
L	200	GLU	-	expression tag	UNP Q8Y7Y1
L	201	LYS	-	expression tag	UNP Q8Y7Y1
M	191	MET	-	expression tag	UNP Q8Y7Y1
M	192	ALA	-	expression tag	UNP Q8Y7Y1
M	193	SER	-	expression tag	UNP Q8Y7Y1
M	194	TRP	-	expression tag	UNP Q8Y7Y1
M	195	SER	-	expression tag	UNP Q8Y7Y1
M	196	HIS	-	expression tag	UNP Q8Y7Y1
M	197	PRO	-	expression tag	UNP Q8Y7Y1
M	198	GLN	-	expression tag	UNP Q8Y7Y1
M	199	PHE	-	expression tag	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	200	GLU	-	expression tag	UNP Q8Y7Y1
M	201	LYS	-	expression tag	UNP Q8Y7Y1
N	191	MET	-	expression tag	UNP Q8Y7Y1
N	192	ALA	-	expression tag	UNP Q8Y7Y1
N	193	SER	-	expression tag	UNP Q8Y7Y1
N	194	TRP	-	expression tag	UNP Q8Y7Y1
N	195	SER	-	expression tag	UNP Q8Y7Y1
N	196	HIS	-	expression tag	UNP Q8Y7Y1
N	197	PRO	-	expression tag	UNP Q8Y7Y1
N	198	GLN	-	expression tag	UNP Q8Y7Y1
N	199	PHE	-	expression tag	UNP Q8Y7Y1
N	200	GLU	-	expression tag	UNP Q8Y7Y1
N	201	LYS	-	expression tag	UNP Q8Y7Y1
O	191	MET	-	expression tag	UNP Q8Y7Y1
O	192	ALA	-	expression tag	UNP Q8Y7Y1
O	193	SER	-	expression tag	UNP Q8Y7Y1
O	194	TRP	-	expression tag	UNP Q8Y7Y1
O	195	SER	-	expression tag	UNP Q8Y7Y1
O	196	HIS	-	expression tag	UNP Q8Y7Y1
O	197	PRO	-	expression tag	UNP Q8Y7Y1
O	198	GLN	-	expression tag	UNP Q8Y7Y1
O	199	PHE	-	expression tag	UNP Q8Y7Y1
O	200	GLU	-	expression tag	UNP Q8Y7Y1
O	201	LYS	-	expression tag	UNP Q8Y7Y1
P	191	MET	-	expression tag	UNP Q8Y7Y1
P	192	ALA	-	expression tag	UNP Q8Y7Y1
P	193	SER	-	expression tag	UNP Q8Y7Y1
P	194	TRP	-	expression tag	UNP Q8Y7Y1
P	195	SER	-	expression tag	UNP Q8Y7Y1
P	196	HIS	-	expression tag	UNP Q8Y7Y1
P	197	PRO	-	expression tag	UNP Q8Y7Y1
P	198	GLN	-	expression tag	UNP Q8Y7Y1
P	199	PHE	-	expression tag	UNP Q8Y7Y1
P	200	GLU	-	expression tag	UNP Q8Y7Y1
P	201	LYS	-	expression tag	UNP Q8Y7Y1
Q	191	MET	-	expression tag	UNP Q8Y7Y1
Q	192	ALA	-	expression tag	UNP Q8Y7Y1
Q	193	SER	-	expression tag	UNP Q8Y7Y1
Q	194	TRP	-	expression tag	UNP Q8Y7Y1
Q	195	SER	-	expression tag	UNP Q8Y7Y1
Q	196	HIS	-	expression tag	UNP Q8Y7Y1
Q	197	PRO	-	expression tag	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	198	GLN	-	expression tag	UNP Q8Y7Y1
Q	199	PHE	-	expression tag	UNP Q8Y7Y1
Q	200	GLU	-	expression tag	UNP Q8Y7Y1
Q	201	LYS	-	expression tag	UNP Q8Y7Y1
R	191	MET	-	expression tag	UNP Q8Y7Y1
R	192	ALA	-	expression tag	UNP Q8Y7Y1
R	193	SER	-	expression tag	UNP Q8Y7Y1
R	194	TRP	-	expression tag	UNP Q8Y7Y1
R	195	SER	-	expression tag	UNP Q8Y7Y1
R	196	HIS	-	expression tag	UNP Q8Y7Y1
R	197	PRO	-	expression tag	UNP Q8Y7Y1
R	198	GLN	-	expression tag	UNP Q8Y7Y1
R	199	PHE	-	expression tag	UNP Q8Y7Y1
R	200	GLU	-	expression tag	UNP Q8Y7Y1
R	201	LYS	-	expression tag	UNP Q8Y7Y1
S	191	MET	-	expression tag	UNP Q8Y7Y1
S	192	ALA	-	expression tag	UNP Q8Y7Y1
S	193	SER	-	expression tag	UNP Q8Y7Y1
S	194	TRP	-	expression tag	UNP Q8Y7Y1
S	195	SER	-	expression tag	UNP Q8Y7Y1
S	196	HIS	-	expression tag	UNP Q8Y7Y1
S	197	PRO	-	expression tag	UNP Q8Y7Y1
S	198	GLN	-	expression tag	UNP Q8Y7Y1
S	199	PHE	-	expression tag	UNP Q8Y7Y1
S	200	GLU	-	expression tag	UNP Q8Y7Y1
S	201	LYS	-	expression tag	UNP Q8Y7Y1
T	191	MET	-	expression tag	UNP Q8Y7Y1
T	192	ALA	-	expression tag	UNP Q8Y7Y1
T	193	SER	-	expression tag	UNP Q8Y7Y1
T	194	TRP	-	expression tag	UNP Q8Y7Y1
T	195	SER	-	expression tag	UNP Q8Y7Y1
T	196	HIS	-	expression tag	UNP Q8Y7Y1
T	197	PRO	-	expression tag	UNP Q8Y7Y1
T	198	GLN	-	expression tag	UNP Q8Y7Y1
T	199	PHE	-	expression tag	UNP Q8Y7Y1
T	200	GLU	-	expression tag	UNP Q8Y7Y1
T	201	LYS	-	expression tag	UNP Q8Y7Y1
U	191	MET	-	expression tag	UNP Q8Y7Y1
U	192	ALA	-	expression tag	UNP Q8Y7Y1
U	193	SER	-	expression tag	UNP Q8Y7Y1
U	194	TRP	-	expression tag	UNP Q8Y7Y1
U	195	SER	-	expression tag	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	196	HIS	-	expression tag	UNP Q8Y7Y1
U	197	PRO	-	expression tag	UNP Q8Y7Y1
U	198	GLN	-	expression tag	UNP Q8Y7Y1
U	199	PHE	-	expression tag	UNP Q8Y7Y1
U	200	GLU	-	expression tag	UNP Q8Y7Y1
U	201	LYS	-	expression tag	UNP Q8Y7Y1
V	191	MET	-	expression tag	UNP Q8Y7Y1
V	192	ALA	-	expression tag	UNP Q8Y7Y1
V	193	SER	-	expression tag	UNP Q8Y7Y1
V	194	TRP	-	expression tag	UNP Q8Y7Y1
V	195	SER	-	expression tag	UNP Q8Y7Y1
V	196	HIS	-	expression tag	UNP Q8Y7Y1
V	197	PRO	-	expression tag	UNP Q8Y7Y1
V	198	GLN	-	expression tag	UNP Q8Y7Y1
V	199	PHE	-	expression tag	UNP Q8Y7Y1
V	200	GLU	-	expression tag	UNP Q8Y7Y1
V	201	LYS	-	expression tag	UNP Q8Y7Y1
W	191	MET	-	expression tag	UNP Q8Y7Y1
W	192	ALA	-	expression tag	UNP Q8Y7Y1
W	193	SER	-	expression tag	UNP Q8Y7Y1
W	194	TRP	-	expression tag	UNP Q8Y7Y1
W	195	SER	-	expression tag	UNP Q8Y7Y1
W	196	HIS	-	expression tag	UNP Q8Y7Y1
W	197	PRO	-	expression tag	UNP Q8Y7Y1
W	198	GLN	-	expression tag	UNP Q8Y7Y1
W	199	PHE	-	expression tag	UNP Q8Y7Y1
W	200	GLU	-	expression tag	UNP Q8Y7Y1
W	201	LYS	-	expression tag	UNP Q8Y7Y1
X	191	MET	-	expression tag	UNP Q8Y7Y1
X	192	ALA	-	expression tag	UNP Q8Y7Y1
X	193	SER	-	expression tag	UNP Q8Y7Y1
X	194	TRP	-	expression tag	UNP Q8Y7Y1
X	195	SER	-	expression tag	UNP Q8Y7Y1
X	196	HIS	-	expression tag	UNP Q8Y7Y1
X	197	PRO	-	expression tag	UNP Q8Y7Y1
X	198	GLN	-	expression tag	UNP Q8Y7Y1
X	199	PHE	-	expression tag	UNP Q8Y7Y1
X	200	GLU	-	expression tag	UNP Q8Y7Y1
X	201	LYS	-	expression tag	UNP Q8Y7Y1
Y	191	MET	-	expression tag	UNP Q8Y7Y1
Y	192	ALA	-	expression tag	UNP Q8Y7Y1
Y	193	SER	-	expression tag	UNP Q8Y7Y1

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	194	TRP	-	expression tag	UNP Q8Y7Y1
Y	195	SER	-	expression tag	UNP Q8Y7Y1
Y	196	HIS	-	expression tag	UNP Q8Y7Y1
Y	197	PRO	-	expression tag	UNP Q8Y7Y1
Y	198	GLN	-	expression tag	UNP Q8Y7Y1
Y	199	PHE	-	expression tag	UNP Q8Y7Y1
Y	200	GLU	-	expression tag	UNP Q8Y7Y1
Y	201	LYS	-	expression tag	UNP Q8Y7Y1
Z	191	MET	-	expression tag	UNP Q8Y7Y1
Z	192	ALA	-	expression tag	UNP Q8Y7Y1
Z	193	SER	-	expression tag	UNP Q8Y7Y1
Z	194	TRP	-	expression tag	UNP Q8Y7Y1
Z	195	SER	-	expression tag	UNP Q8Y7Y1
Z	196	HIS	-	expression tag	UNP Q8Y7Y1
Z	197	PRO	-	expression tag	UNP Q8Y7Y1
Z	198	GLN	-	expression tag	UNP Q8Y7Y1
Z	199	PHE	-	expression tag	UNP Q8Y7Y1
Z	200	GLU	-	expression tag	UNP Q8Y7Y1
Z	201	LYS	-	expression tag	UNP Q8Y7Y1
a	191	MET	-	expression tag	UNP Q8Y7Y1
a	192	ALA	-	expression tag	UNP Q8Y7Y1
a	193	SER	-	expression tag	UNP Q8Y7Y1
a	194	TRP	-	expression tag	UNP Q8Y7Y1
a	195	SER	-	expression tag	UNP Q8Y7Y1
a	196	HIS	-	expression tag	UNP Q8Y7Y1
a	197	PRO	-	expression tag	UNP Q8Y7Y1
a	198	GLN	-	expression tag	UNP Q8Y7Y1
a	199	PHE	-	expression tag	UNP Q8Y7Y1
a	200	GLU	-	expression tag	UNP Q8Y7Y1
a	201	LYS	-	expression tag	UNP Q8Y7Y1
b	191	MET	-	expression tag	UNP Q8Y7Y1
b	192	ALA	-	expression tag	UNP Q8Y7Y1
b	193	SER	-	expression tag	UNP Q8Y7Y1
b	194	TRP	-	expression tag	UNP Q8Y7Y1
b	195	SER	-	expression tag	UNP Q8Y7Y1
b	196	HIS	-	expression tag	UNP Q8Y7Y1
b	197	PRO	-	expression tag	UNP Q8Y7Y1
b	198	GLN	-	expression tag	UNP Q8Y7Y1
b	199	PHE	-	expression tag	UNP Q8Y7Y1
b	200	GLU	-	expression tag	UNP Q8Y7Y1
b	201	LYS	-	expression tag	UNP Q8Y7Y1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	88	Total O 88 88	0	0
2	B	93	Total O 93 93	0	0
2	C	80	Total O 80 80	0	0
2	D	72	Total O 72 72	0	0
2	E	102	Total O 102 102	0	0
2	F	135	Total O 135 135	0	0
2	G	107	Total O 107 107	0	0
2	H	89	Total O 89 89	0	0
2	I	81	Total O 81 81	0	0
2	J	87	Total O 87 87	0	0
2	K	111	Total O 111 111	0	0
2	L	108	Total O 108 108	0	0
2	M	134	Total O 134 134	0	0
2	N	147	Total O 147 147	0	0
2	O	83	Total O 83 83	0	0
2	P	76	Total O 76 76	0	0
2	Q	100	Total O 100 100	0	0
2	R	99	Total O 99 99	0	0
2	S	124	Total O 124 124	0	0
2	T	157	Total O 157 157	0	0
2	U	93	Total O 93 93	0	0
2	V	106	Total O 106 106	0	0

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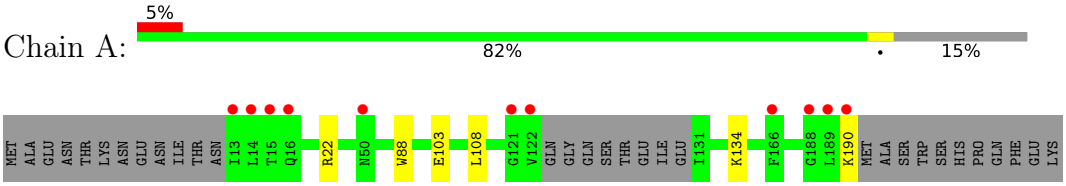
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	W	93	Total O 93 93	0	0
2	X	84	Total O 84 84	0	0
2	Y	90	Total O 90 90	0	0
2	Z	93	Total O 93 93	0	0
2	a	124	Total O 124 124	0	0
2	b	143	Total O 143 143	0	0

3 Residue-property plots (i)

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

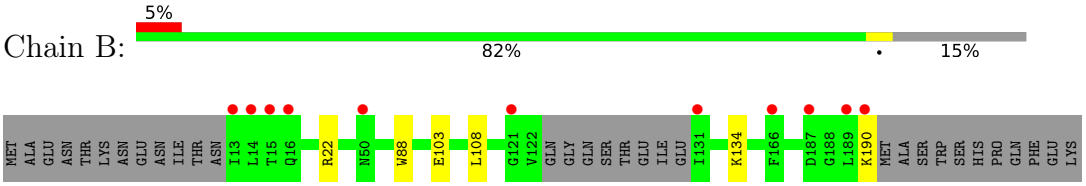
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



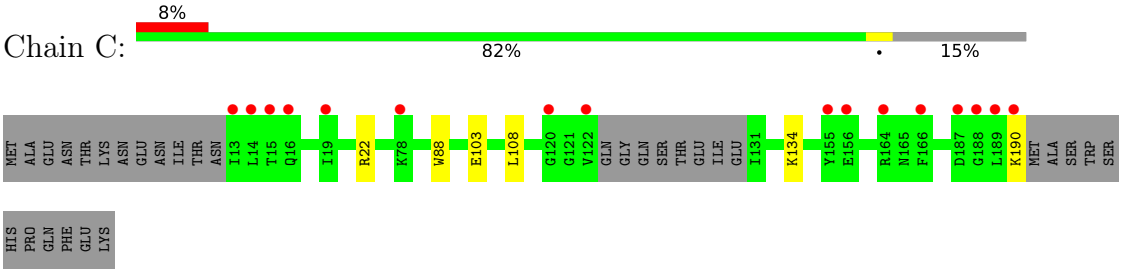
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



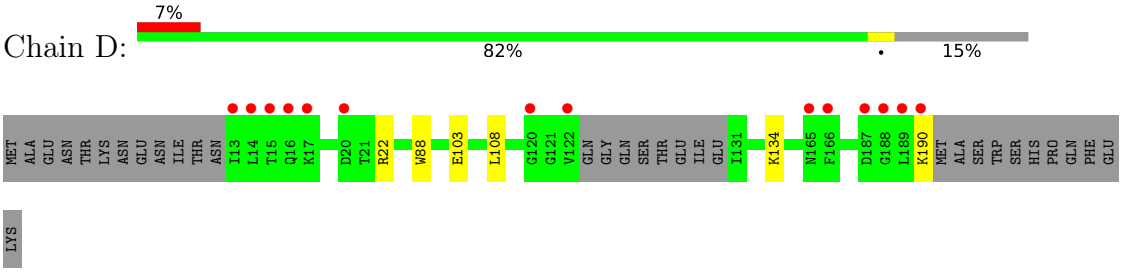
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:



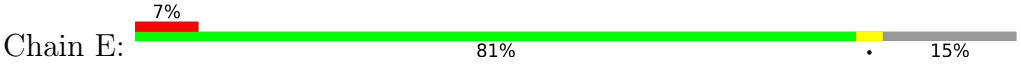
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

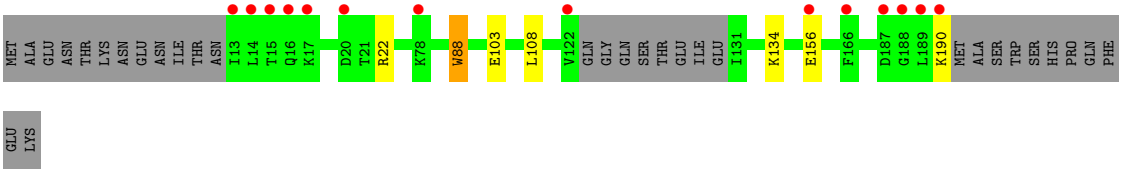
Chain D:



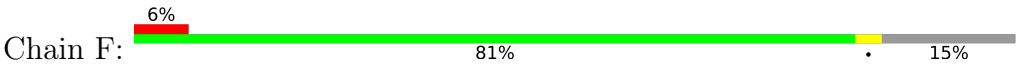
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

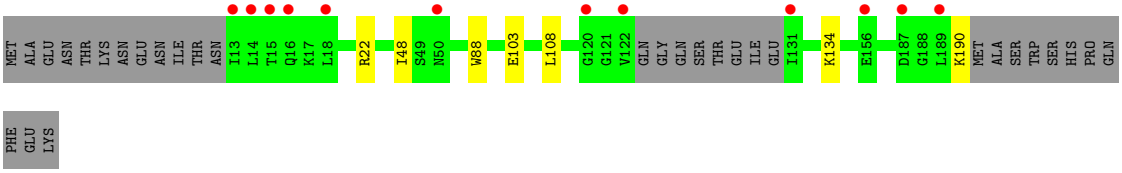
Chain E:



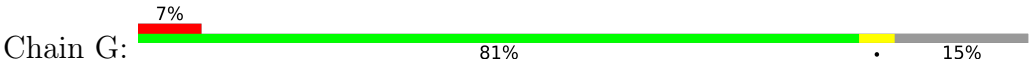


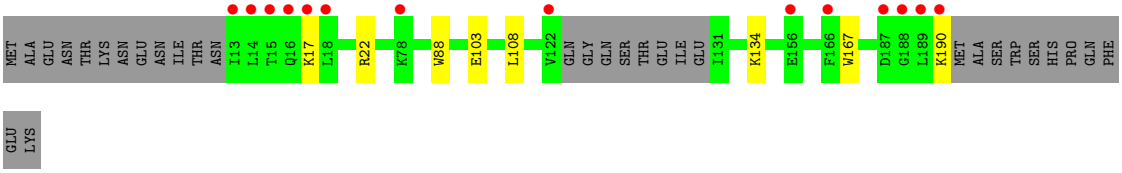
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



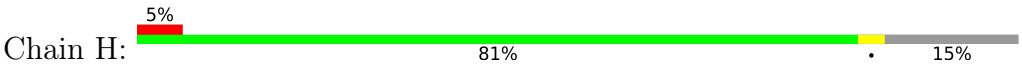


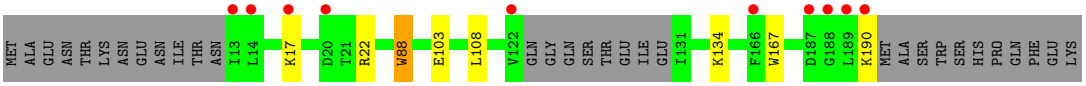
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



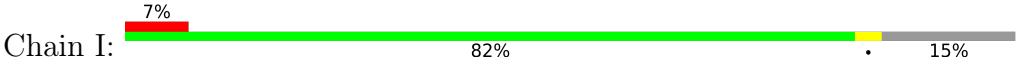


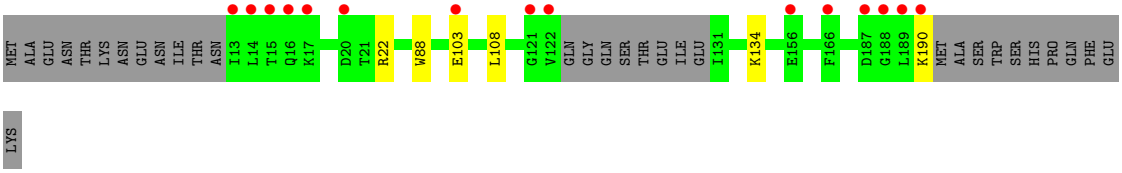
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



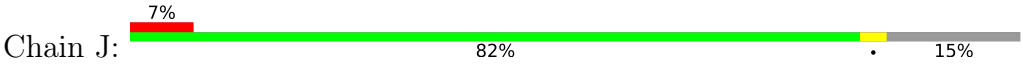


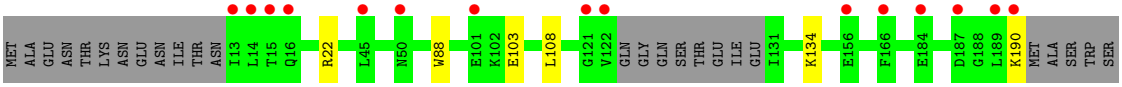
• Molecule 1: ATP-dependent Clp protease proteolytic subunit





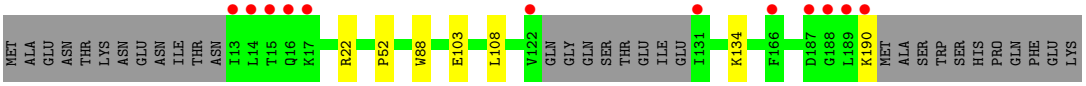
• Molecule 1: ATP-dependent Clp protease proteolytic subunit





• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:

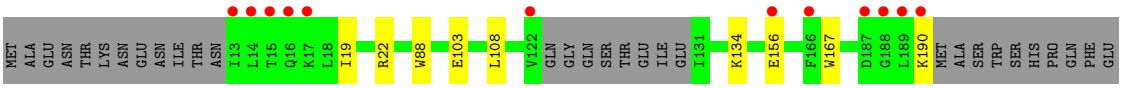


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:

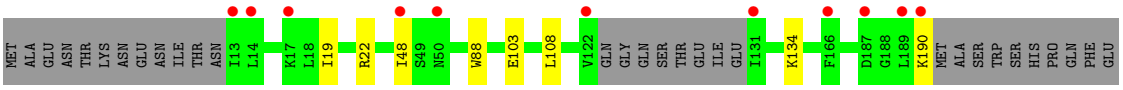
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:



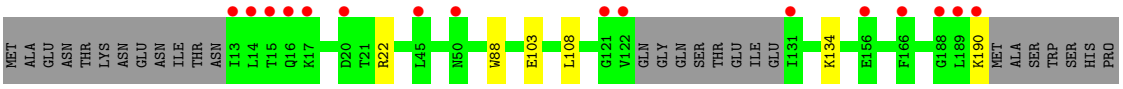
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O:

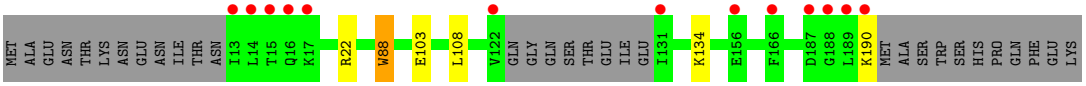


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain P:

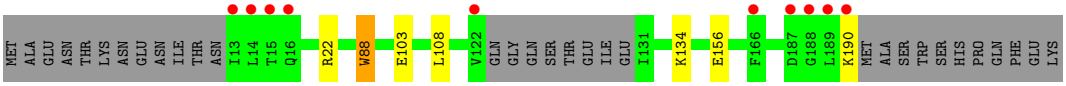
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Q:



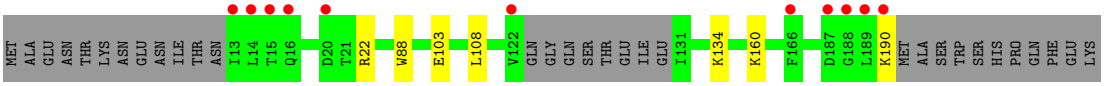
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain R:



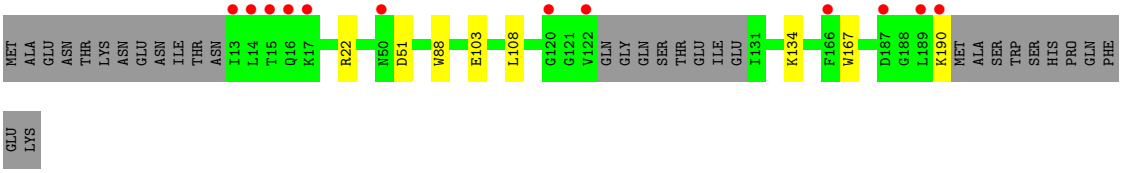
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain S:



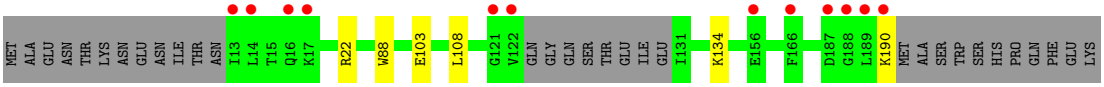
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain T:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain U:

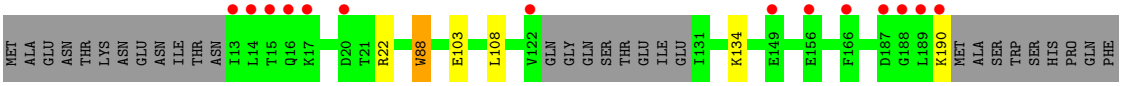


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain V:

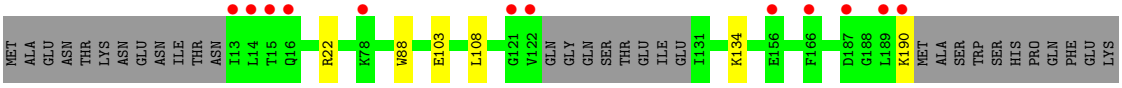
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain W:



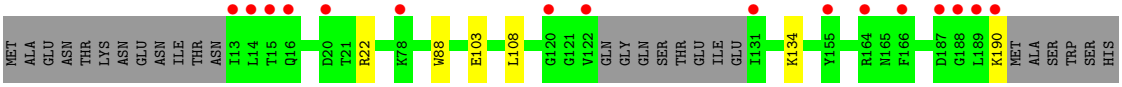
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain X:



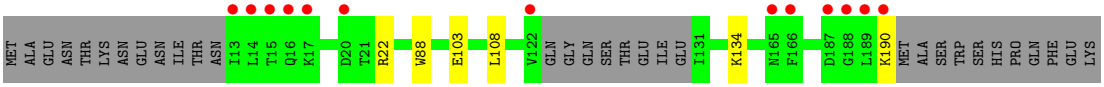
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



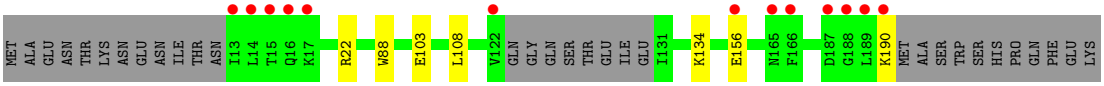
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



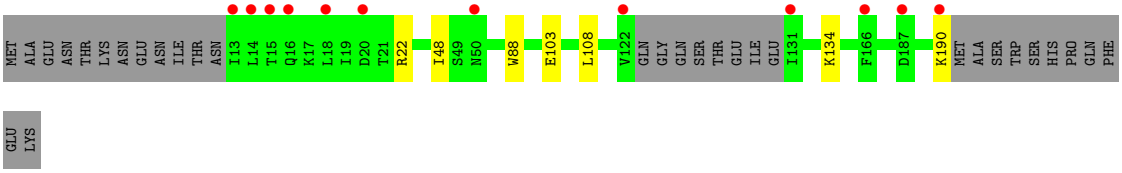
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:


MET
ALA
GLU
ASN
THR
LYS
ASN
GLU
ASN
ILE
THR
ASN
I13
L14
T15
Q16
K17
L18
I19
D20
T21
R22
I48
S49
N50
W88
E103
L108
V122
GLN
GLY
GLN
SER
THR
GLU
ILE
GLU
I131
K134
F166
D187
K190
MET
ALA
SER
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	140.95Å 109.06Å 196.26Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 15.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.00) 99.7 (15.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.192 , 0.213 0.192 , 0.213	Depositor DCC
R_{free} test set	19880 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40559	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0334e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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	0.40	0/1363	0.49	0/1841
1	B	0.40	0/1363	0.49	0/1841
1	C	0.40	0/1363	0.49	0/1841
1	D	0.40	0/1363	0.48	0/1841
1	E	0.41	1/1363 (0.1%)	0.49	0/1841
1	F	0.41	0/1363	0.49	0/1841
1	G	0.40	1/1363 (0.1%)	0.49	0/1841
1	H	0.41	2/1363 (0.1%)	0.49	0/1841
1	I	0.40	0/1363	0.48	0/1841
1	J	0.40	0/1363	0.49	0/1841
1	K	0.40	0/1363	0.49	0/1841
1	L	0.40	0/1363	0.49	0/1841
1	M	0.41	1/1363 (0.1%)	0.49	0/1841
1	N	0.41	0/1363	0.49	0/1841
1	O	0.40	0/1363	0.49	0/1841
1	P	0.40	1/1363 (0.1%)	0.49	0/1841
1	Q	0.41	1/1363 (0.1%)	0.49	0/1841
1	R	0.40	1/1363 (0.1%)	0.49	0/1841
1	S	0.41	0/1363	0.49	0/1841
1	T	0.41	1/1363 (0.1%)	0.49	0/1841
1	U	0.40	0/1363	0.49	0/1841
1	V	0.41	0/1363	0.49	0/1841
1	W	0.41	1/1363 (0.1%)	0.49	0/1841
1	X	0.40	0/1363	0.48	0/1841
1	Y	0.41	0/1363	0.48	0/1841
1	Z	0.40	0/1363	0.48	0/1841
1	a	0.41	0/1363	0.49	0/1841
1	b	0.41	0/1363	0.49	0/1841
All	All	0.40	10/38164 (0.0%)	0.49	0/51548

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	88	TRP	CD2-CE2	5.07	1.47	1.41
1	Q	88	TRP	CD2-CE2	5.05	1.47	1.41
1	M	167	TRP	CD2-CE2	5.04	1.47	1.41
1	H	167	TRP	CD2-CE2	5.03	1.47	1.41
1	P	88	TRP	CD2-CE2	5.03	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	B	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	C	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	D	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	E	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	F	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	G	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	H	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	I	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	J	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	K	166/201 (83%)	162 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	M	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	N	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	O	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	P	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	Q	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	R	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	S	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	T	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	U	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	V	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	W	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	X	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	Y	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	Z	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	a	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
1	b	166/201 (83%)	162 (98%)	4 (2%)	0	100	100
All	All	4648/5628 (83%)	4536 (98%)	112 (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	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	B	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	C	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	D	147/175 (84%)	141 (96%)	6 (4%)	30	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	F	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	G	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	H	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	I	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	J	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	K	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	L	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	M	147/175 (84%)	140 (95%)	7 (5%)	25	22
1	N	147/175 (84%)	140 (95%)	7 (5%)	25	22
1	O	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	P	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	Q	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	R	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	S	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	T	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	U	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	V	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	W	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	X	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	Y	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	Z	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	a	147/175 (84%)	141 (96%)	6 (4%)	30	28
1	b	147/175 (84%)	141 (96%)	6 (4%)	30	28
All	All	4116/4900 (84%)	3946 (96%)	170 (4%)	30	28

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	190	LYS
1	X	108	LEU
1	T	108	LEU
1	V	103	GLU
1	Y	134	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	180	ASN
1	V	16	GLN
1	U	180	ASN
1	W	16	GLN
1	L	63	HIS

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	170/201 (84%)	0.14	11 (6%)	18	18	19, 30, 67, 111	0
1	B	170/201 (84%)	0.19	11 (6%)	18	18	23, 35, 71, 116	0
1	C	170/201 (84%)	0.31	16 (9%)	8	8	24, 36, 74, 121	0
1	D	170/201 (84%)	0.43	14 (8%)	11	11	23, 36, 74, 118	0
1	E	170/201 (84%)	0.19	14 (8%)	11	11	16, 27, 66, 111	0
1	F	170/201 (84%)	0.11	12 (7%)	16	15	15, 25, 60, 102	0
1	G	170/201 (84%)	0.12	14 (8%)	11	11	16, 27, 65, 107	0
1	H	170/201 (84%)	0.17	10 (5%)	22	21	17, 29, 63, 106	0
1	I	170/201 (84%)	0.37	15 (8%)	10	9	22, 34, 69, 112	0
1	J	170/201 (84%)	0.27	15 (8%)	10	9	25, 36, 67, 114	0
1	K	170/201 (84%)	0.27	12 (7%)	16	15	22, 32, 72, 114	0
1	L	170/201 (84%)	0.16	12 (7%)	16	15	18, 30, 66, 112	0
1	M	170/201 (84%)	0.13	12 (7%)	16	15	13, 23, 62, 108	0
1	N	170/201 (84%)	0.08	11 (6%)	18	18	13, 23, 55, 101	0
1	O	170/201 (84%)	0.25	16 (9%)	8	8	21, 33, 67, 114	0
1	P	170/201 (84%)	0.24	11 (6%)	18	18	23, 35, 70, 114	0
1	Q	170/201 (84%)	0.19	13 (7%)	13	13	20, 31, 69, 112	0
1	R	170/201 (84%)	0.10	10 (5%)	22	21	18, 28, 66, 110	0
1	S	170/201 (84%)	0.12	11 (6%)	18	18	13, 23, 65, 109	0
1	T	170/201 (84%)	0.03	12 (7%)	16	15	13, 23, 50, 100	0
1	U	170/201 (84%)	0.16	12 (7%)	16	15	17, 28, 63, 108	0
1	V	170/201 (84%)	0.13	15 (8%)	10	9	16, 27, 65, 109	0
1	W	170/201 (84%)	0.20	14 (8%)	11	11	17, 28, 65, 110	0
1	X	170/201 (84%)	0.17	12 (7%)	16	15	21, 33, 68, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	Y	170/201 (84%)	0.33	16 (9%)	8 8	21, 32, 69, 116	0
1	Z	170/201 (84%)	0.21	13 (7%)	13 13	21, 32, 70, 114	0
1	a	170/201 (84%)	0.12	13 (7%)	13 13	15, 24, 65, 107	0
1	b	170/201 (84%)	0.10	12 (7%)	16 15	14, 23, 59, 102	0
All	All	4760/5628 (84%)	0.19	359 (7%)	14 13	13, 30, 73, 121	0

The worst 5 of 359 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	14	LEU	14.8
1	I	14	LEU	13.7
1	K	13	ILE	13.2
1	J	14	LEU	12.3
1	Q	188	GLY	11.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.