wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 05:10 AM JST

PDB ID	:	6KWW
Title	:	HslU from Staphylococcus aureus
Authors	:	Ha, N.-C.; Jeong, S.
Deposited on	:	2019-09-09
Resolution	:	3.00 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:

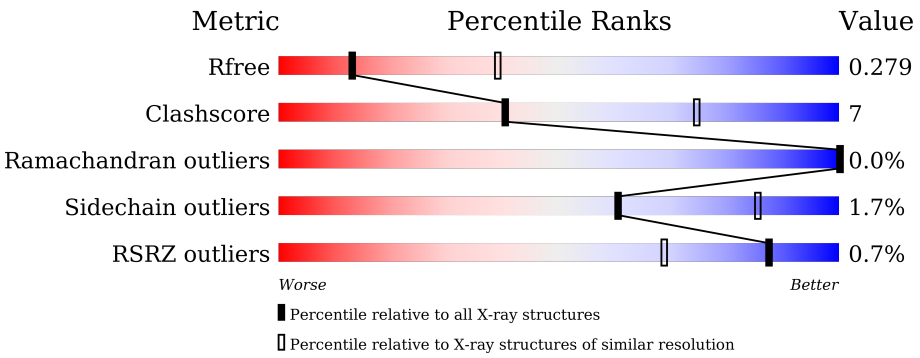
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	481	.% 50% 14% 36%
1	B	481	.% 47% 13% • 39%
1	C	481	52% 9% 38%
1	D	481	.% 44% 17% 38%
1	E	481	50% 10% 39%
1	F	481	50% 11% 38%

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Mol	Chain	Length	Quality of chain
1	G	481	45% 14% 40%
1	H	481	54% 9% 37%
1	I	481	49% 11% 40%
1	J	481	.% 49% 13% • 37%
1	K	481	47% 14% 38%
1	L	481	.% 50% 11% 39%
1	M	481	54% 11% 34%
1	N	481	51% 13% 35%
1	O	481	.% 53% 9% • 37%
1	P	481	50% 12% • 37%
1	Q	481	48% 15% • 37%
1	R	481	.% 57% 12% 31%
1	S	481	.% 48% 16% 36%
1	T	481	.% 54% 14% • 31%
1	U	481	57% 12% 31%
1	V	481	50% 12% 37%
1	W	481	.% 56% 11% 33%
1	X	481	53% 12% 34%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 57793 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 protease ATPase subunit HslU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	M	317	2493	1576	424	486	7	0	0	0
			Total	C	N	O	S			
1	N	311	2449	1550	421	471	7	0	0	0
			Total	C	N	O	S			
1	O	302	2375	1507	407	454	7	0	0	0
			Total	C	N	O	S			
1	P	302	2381	1509	408	457	7	0	0	0
			Total	C	N	O	S			
1	Q	303	2384	1508	407	462	7	0	0	0
			Total	C	N	O	S			
1	R	330	2594	1640	443	504	7	0	0	0
			Total	C	N	O	S			
1	S	309	2431	1537	416	471	7	0	0	0
			Total	C	N	O	S			
1	T	330	2595	1641	446	501	7	0	0	0
			Total	C	N	O	S			
1	U	332	2606	1644	444	511	7	0	0	0
			Total	C	N	O	S			
1	V	301	2377	1503	406	461	7	0	0	0
			Total	C	N	O	S			
1	W	323	2547	1608	438	494	7	0	0	0
			Total	C	N	O	S			
1	X	316	2492	1571	429	485	7	0	0	0
			Total	C	N	O	S			
1	A	307	2425	1535	412	471	7	0	0	0
			Total	C	N	O	S			
1	B	292	2299	1458	391	443	7	0	0	0
			Total	C	N	O	S			
1	C	296	2337	1481	401	448	7	0	0	0
			Total	C	N	O	S			
1	D	296	2329	1478	397	447	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	292	2300	1458	394	441	7	0	0	0
			Total	C	N	O	S			
1	F	298	2348	1488	403	450	7	0	0	0
			Total	C	N	O	S			
1	G	287	2266	1437	389	433	7	0	0	0
			Total	C	N	O	S			
1	H	304	2396	1517	411	461	7	0	0	0
			Total	C	N	O	S			
1	I	291	2297	1457	390	443	7	0	0	0
			Total	C	N	O	S			
1	J	305	2404	1521	412	464	7	0	0	0
			Total	C	N	O	S			
1	K	297	2341	1485	398	451	7	0	0	0
			Total	C	N	O	S			
1	L	295	2327	1477	394	449	7	0	0	0

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-13	HIS	-	expression tag	UNP P63796
M	-12	HIS	-	expression tag	UNP P63796
M	-11	HIS	-	expression tag	UNP P63796
M	-10	HIS	-	expression tag	UNP P63796
M	-9	GLU	-	expression tag	UNP P63796
M	-8	ASN	-	expression tag	UNP P63796
M	-7	LEU	-	expression tag	UNP P63796
M	-6	TYR	-	expression tag	UNP P63796
M	-5	PHE	-	expression tag	UNP P63796
M	-4	GLN	-	expression tag	UNP P63796
M	-3	GLY	-	expression tag	UNP P63796
M	-2	ALA	-	expression tag	UNP P63796
M	-1	ALA	-	expression tag	UNP P63796
M	0	SER	-	expression tag	UNP P63796
N	-13	HIS	-	expression tag	UNP P63796
N	-12	HIS	-	expression tag	UNP P63796
N	-11	HIS	-	expression tag	UNP P63796
N	-10	HIS	-	expression tag	UNP P63796
N	-9	GLU	-	expression tag	UNP P63796
N	-8	ASN	-	expression tag	UNP P63796
N	-7	LEU	-	expression tag	UNP P63796
N	-6	TYR	-	expression tag	UNP P63796
N	-5	PHE	-	expression tag	UNP P63796

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-4	GLN	-	expression tag	UNP P63796
N	-3	GLY	-	expression tag	UNP P63796
N	-2	ALA	-	expression tag	UNP P63796
N	-1	ALA	-	expression tag	UNP P63796
N	0	SER	-	expression tag	UNP P63796
O	-13	HIS	-	expression tag	UNP P63796
O	-12	HIS	-	expression tag	UNP P63796
O	-11	HIS	-	expression tag	UNP P63796
O	-10	HIS	-	expression tag	UNP P63796
O	-9	GLU	-	expression tag	UNP P63796
O	-8	ASN	-	expression tag	UNP P63796
O	-7	LEU	-	expression tag	UNP P63796
O	-6	TYR	-	expression tag	UNP P63796
O	-5	PHE	-	expression tag	UNP P63796
O	-4	GLN	-	expression tag	UNP P63796
O	-3	GLY	-	expression tag	UNP P63796
O	-2	ALA	-	expression tag	UNP P63796
O	-1	ALA	-	expression tag	UNP P63796
O	0	SER	-	expression tag	UNP P63796
P	-13	HIS	-	expression tag	UNP P63796
P	-12	HIS	-	expression tag	UNP P63796
P	-11	HIS	-	expression tag	UNP P63796
P	-10	HIS	-	expression tag	UNP P63796
P	-9	GLU	-	expression tag	UNP P63796
P	-8	ASN	-	expression tag	UNP P63796
P	-7	LEU	-	expression tag	UNP P63796
P	-6	TYR	-	expression tag	UNP P63796
P	-5	PHE	-	expression tag	UNP P63796
P	-4	GLN	-	expression tag	UNP P63796
P	-3	GLY	-	expression tag	UNP P63796
P	-2	ALA	-	expression tag	UNP P63796
P	-1	ALA	-	expression tag	UNP P63796
P	0	SER	-	expression tag	UNP P63796
Q	-13	HIS	-	expression tag	UNP P63796
Q	-12	HIS	-	expression tag	UNP P63796
Q	-11	HIS	-	expression tag	UNP P63796
Q	-10	HIS	-	expression tag	UNP P63796
Q	-9	GLU	-	expression tag	UNP P63796
Q	-8	ASN	-	expression tag	UNP P63796
Q	-7	LEU	-	expression tag	UNP P63796
Q	-6	TYR	-	expression tag	UNP P63796
Q	-5	PHE	-	expression tag	UNP P63796

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-4	GLN	-	expression tag	UNP P63796
Q	-3	GLY	-	expression tag	UNP P63796
Q	-2	ALA	-	expression tag	UNP P63796
Q	-1	ALA	-	expression tag	UNP P63796
Q	0	SER	-	expression tag	UNP P63796
R	-13	HIS	-	expression tag	UNP P63796
R	-12	HIS	-	expression tag	UNP P63796
R	-11	HIS	-	expression tag	UNP P63796
R	-10	HIS	-	expression tag	UNP P63796
R	-9	GLU	-	expression tag	UNP P63796
R	-8	ASN	-	expression tag	UNP P63796
R	-7	LEU	-	expression tag	UNP P63796
R	-6	TYR	-	expression tag	UNP P63796
R	-5	PHE	-	expression tag	UNP P63796
R	-4	GLN	-	expression tag	UNP P63796
R	-3	GLY	-	expression tag	UNP P63796
R	-2	ALA	-	expression tag	UNP P63796
R	-1	ALA	-	expression tag	UNP P63796
R	0	SER	-	expression tag	UNP P63796
S	-13	HIS	-	expression tag	UNP P63796
S	-12	HIS	-	expression tag	UNP P63796
S	-11	HIS	-	expression tag	UNP P63796
S	-10	HIS	-	expression tag	UNP P63796
S	-9	GLU	-	expression tag	UNP P63796
S	-8	ASN	-	expression tag	UNP P63796
S	-7	LEU	-	expression tag	UNP P63796
S	-6	TYR	-	expression tag	UNP P63796
S	-5	PHE	-	expression tag	UNP P63796
S	-4	GLN	-	expression tag	UNP P63796
S	-3	GLY	-	expression tag	UNP P63796
S	-2	ALA	-	expression tag	UNP P63796
S	-1	ALA	-	expression tag	UNP P63796
S	0	SER	-	expression tag	UNP P63796
T	-13	HIS	-	expression tag	UNP P63796
T	-12	HIS	-	expression tag	UNP P63796
T	-11	HIS	-	expression tag	UNP P63796
T	-10	HIS	-	expression tag	UNP P63796
T	-9	GLU	-	expression tag	UNP P63796
T	-8	ASN	-	expression tag	UNP P63796
T	-7	LEU	-	expression tag	UNP P63796
T	-6	TYR	-	expression tag	UNP P63796
T	-5	PHE	-	expression tag	UNP P63796

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-4	GLN	-	expression tag	UNP P63796
T	-3	GLY	-	expression tag	UNP P63796
T	-2	ALA	-	expression tag	UNP P63796
T	-1	ALA	-	expression tag	UNP P63796
T	0	SER	-	expression tag	UNP P63796
U	-13	HIS	-	expression tag	UNP P63796
U	-12	HIS	-	expression tag	UNP P63796
U	-11	HIS	-	expression tag	UNP P63796
U	-10	HIS	-	expression tag	UNP P63796
U	-9	GLU	-	expression tag	UNP P63796
U	-8	ASN	-	expression tag	UNP P63796
U	-7	LEU	-	expression tag	UNP P63796
U	-6	TYR	-	expression tag	UNP P63796
U	-5	PHE	-	expression tag	UNP P63796
U	-4	GLN	-	expression tag	UNP P63796
U	-3	GLY	-	expression tag	UNP P63796
U	-2	ALA	-	expression tag	UNP P63796
U	-1	ALA	-	expression tag	UNP P63796
U	0	SER	-	expression tag	UNP P63796
V	-13	HIS	-	expression tag	UNP P63796
V	-12	HIS	-	expression tag	UNP P63796
V	-11	HIS	-	expression tag	UNP P63796
V	-10	HIS	-	expression tag	UNP P63796
V	-9	GLU	-	expression tag	UNP P63796
V	-8	ASN	-	expression tag	UNP P63796
V	-7	LEU	-	expression tag	UNP P63796
V	-6	TYR	-	expression tag	UNP P63796
V	-5	PHE	-	expression tag	UNP P63796
V	-4	GLN	-	expression tag	UNP P63796
V	-3	GLY	-	expression tag	UNP P63796
V	-2	ALA	-	expression tag	UNP P63796
V	-1	ALA	-	expression tag	UNP P63796
V	0	SER	-	expression tag	UNP P63796
W	-13	HIS	-	expression tag	UNP P63796
W	-12	HIS	-	expression tag	UNP P63796
W	-11	HIS	-	expression tag	UNP P63796
W	-10	HIS	-	expression tag	UNP P63796
W	-9	GLU	-	expression tag	UNP P63796
W	-8	ASN	-	expression tag	UNP P63796
W	-7	LEU	-	expression tag	UNP P63796
W	-6	TYR	-	expression tag	UNP P63796
W	-5	PHE	-	expression tag	UNP P63796

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-4	GLN	-	expression tag	UNP P63796
W	-3	GLY	-	expression tag	UNP P63796
W	-2	ALA	-	expression tag	UNP P63796
W	-1	ALA	-	expression tag	UNP P63796
W	0	SER	-	expression tag	UNP P63796
X	-13	HIS	-	expression tag	UNP P63796
X	-12	HIS	-	expression tag	UNP P63796
X	-11	HIS	-	expression tag	UNP P63796
X	-10	HIS	-	expression tag	UNP P63796
X	-9	GLU	-	expression tag	UNP P63796
X	-8	ASN	-	expression tag	UNP P63796
X	-7	LEU	-	expression tag	UNP P63796
X	-6	TYR	-	expression tag	UNP P63796
X	-5	PHE	-	expression tag	UNP P63796
X	-4	GLN	-	expression tag	UNP P63796
X	-3	GLY	-	expression tag	UNP P63796
X	-2	ALA	-	expression tag	UNP P63796
X	-1	ALA	-	expression tag	UNP P63796
X	0	SER	-	expression tag	UNP P63796
A	-13	HIS	-	expression tag	UNP P63796
A	-12	HIS	-	expression tag	UNP P63796
A	-11	HIS	-	expression tag	UNP P63796
A	-10	HIS	-	expression tag	UNP P63796
A	-9	GLU	-	expression tag	UNP P63796
A	-8	ASN	-	expression tag	UNP P63796
A	-7	LEU	-	expression tag	UNP P63796
A	-6	TYR	-	expression tag	UNP P63796
A	-5	PHE	-	expression tag	UNP P63796
A	-4	GLN	-	expression tag	UNP P63796
A	-3	GLY	-	expression tag	UNP P63796
A	-2	ALA	-	expression tag	UNP P63796
A	-1	ALA	-	expression tag	UNP P63796
A	0	SER	-	expression tag	UNP P63796
B	-13	HIS	-	expression tag	UNP P63796
B	-12	HIS	-	expression tag	UNP P63796
B	-11	HIS	-	expression tag	UNP P63796
B	-10	HIS	-	expression tag	UNP P63796
B	-9	GLU	-	expression tag	UNP P63796
B	-8	ASN	-	expression tag	UNP P63796
B	-7	LEU	-	expression tag	UNP P63796
B	-6	TYR	-	expression tag	UNP P63796
B	-5	PHE	-	expression tag	UNP P63796

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLN	-	expression tag	UNP P63796
B	-3	GLY	-	expression tag	UNP P63796
B	-2	ALA	-	expression tag	UNP P63796
B	-1	ALA	-	expression tag	UNP P63796
B	0	SER	-	expression tag	UNP P63796
C	-13	HIS	-	expression tag	UNP P63796
C	-12	HIS	-	expression tag	UNP P63796
C	-11	HIS	-	expression tag	UNP P63796
C	-10	HIS	-	expression tag	UNP P63796
C	-9	GLU	-	expression tag	UNP P63796
C	-8	ASN	-	expression tag	UNP P63796
C	-7	LEU	-	expression tag	UNP P63796
C	-6	TYR	-	expression tag	UNP P63796
C	-5	PHE	-	expression tag	UNP P63796
C	-4	GLN	-	expression tag	UNP P63796
C	-3	GLY	-	expression tag	UNP P63796
C	-2	ALA	-	expression tag	UNP P63796
C	-1	ALA	-	expression tag	UNP P63796
C	0	SER	-	expression tag	UNP P63796
D	-13	HIS	-	expression tag	UNP P63796
D	-12	HIS	-	expression tag	UNP P63796
D	-11	HIS	-	expression tag	UNP P63796
D	-10	HIS	-	expression tag	UNP P63796
D	-9	GLU	-	expression tag	UNP P63796
D	-8	ASN	-	expression tag	UNP P63796
D	-7	LEU	-	expression tag	UNP P63796
D	-6	TYR	-	expression tag	UNP P63796
D	-5	PHE	-	expression tag	UNP P63796
D	-4	GLN	-	expression tag	UNP P63796
D	-3	GLY	-	expression tag	UNP P63796
D	-2	ALA	-	expression tag	UNP P63796
D	-1	ALA	-	expression tag	UNP P63796
D	0	SER	-	expression tag	UNP P63796
E	-13	HIS	-	expression tag	UNP P63796
E	-12	HIS	-	expression tag	UNP P63796
E	-11	HIS	-	expression tag	UNP P63796
E	-10	HIS	-	expression tag	UNP P63796
E	-9	GLU	-	expression tag	UNP P63796
E	-8	ASN	-	expression tag	UNP P63796
E	-7	LEU	-	expression tag	UNP P63796
E	-6	TYR	-	expression tag	UNP P63796
E	-5	PHE	-	expression tag	UNP P63796

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLN	-	expression tag	UNP P63796
E	-3	GLY	-	expression tag	UNP P63796
E	-2	ALA	-	expression tag	UNP P63796
E	-1	ALA	-	expression tag	UNP P63796
E	0	SER	-	expression tag	UNP P63796
F	-13	HIS	-	expression tag	UNP P63796
F	-12	HIS	-	expression tag	UNP P63796
F	-11	HIS	-	expression tag	UNP P63796
F	-10	HIS	-	expression tag	UNP P63796
F	-9	GLU	-	expression tag	UNP P63796
F	-8	ASN	-	expression tag	UNP P63796
F	-7	LEU	-	expression tag	UNP P63796
F	-6	TYR	-	expression tag	UNP P63796
F	-5	PHE	-	expression tag	UNP P63796
F	-4	GLN	-	expression tag	UNP P63796
F	-3	GLY	-	expression tag	UNP P63796
F	-2	ALA	-	expression tag	UNP P63796
F	-1	ALA	-	expression tag	UNP P63796
F	0	SER	-	expression tag	UNP P63796
G	-13	HIS	-	expression tag	UNP P63796
G	-12	HIS	-	expression tag	UNP P63796
G	-11	HIS	-	expression tag	UNP P63796
G	-10	HIS	-	expression tag	UNP P63796
G	-9	GLU	-	expression tag	UNP P63796
G	-8	ASN	-	expression tag	UNP P63796
G	-7	LEU	-	expression tag	UNP P63796
G	-6	TYR	-	expression tag	UNP P63796
G	-5	PHE	-	expression tag	UNP P63796
G	-4	GLN	-	expression tag	UNP P63796
G	-3	GLY	-	expression tag	UNP P63796
G	-2	ALA	-	expression tag	UNP P63796
G	-1	ALA	-	expression tag	UNP P63796
G	0	SER	-	expression tag	UNP P63796
H	-13	HIS	-	expression tag	UNP P63796
H	-12	HIS	-	expression tag	UNP P63796
H	-11	HIS	-	expression tag	UNP P63796
H	-10	HIS	-	expression tag	UNP P63796
H	-9	GLU	-	expression tag	UNP P63796
H	-8	ASN	-	expression tag	UNP P63796
H	-7	LEU	-	expression tag	UNP P63796
H	-6	TYR	-	expression tag	UNP P63796
H	-5	PHE	-	expression tag	UNP P63796

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	GLN	-	expression tag	UNP P63796
H	-3	GLY	-	expression tag	UNP P63796
H	-2	ALA	-	expression tag	UNP P63796
H	-1	ALA	-	expression tag	UNP P63796
H	0	SER	-	expression tag	UNP P63796
I	-13	HIS	-	expression tag	UNP P63796
I	-12	HIS	-	expression tag	UNP P63796
I	-11	HIS	-	expression tag	UNP P63796
I	-10	HIS	-	expression tag	UNP P63796
I	-9	GLU	-	expression tag	UNP P63796
I	-8	ASN	-	expression tag	UNP P63796
I	-7	LEU	-	expression tag	UNP P63796
I	-6	TYR	-	expression tag	UNP P63796
I	-5	PHE	-	expression tag	UNP P63796
I	-4	GLN	-	expression tag	UNP P63796
I	-3	GLY	-	expression tag	UNP P63796
I	-2	ALA	-	expression tag	UNP P63796
I	-1	ALA	-	expression tag	UNP P63796
I	0	SER	-	expression tag	UNP P63796
J	-13	HIS	-	expression tag	UNP P63796
J	-12	HIS	-	expression tag	UNP P63796
J	-11	HIS	-	expression tag	UNP P63796
J	-10	HIS	-	expression tag	UNP P63796
J	-9	GLU	-	expression tag	UNP P63796
J	-8	ASN	-	expression tag	UNP P63796
J	-7	LEU	-	expression tag	UNP P63796
J	-6	TYR	-	expression tag	UNP P63796
J	-5	PHE	-	expression tag	UNP P63796
J	-4	GLN	-	expression tag	UNP P63796
J	-3	GLY	-	expression tag	UNP P63796
J	-2	ALA	-	expression tag	UNP P63796
J	-1	ALA	-	expression tag	UNP P63796
J	0	SER	-	expression tag	UNP P63796
K	-13	HIS	-	expression tag	UNP P63796
K	-12	HIS	-	expression tag	UNP P63796
K	-11	HIS	-	expression tag	UNP P63796
K	-10	HIS	-	expression tag	UNP P63796
K	-9	GLU	-	expression tag	UNP P63796
K	-8	ASN	-	expression tag	UNP P63796
K	-7	LEU	-	expression tag	UNP P63796
K	-6	TYR	-	expression tag	UNP P63796
K	-5	PHE	-	expression tag	UNP P63796

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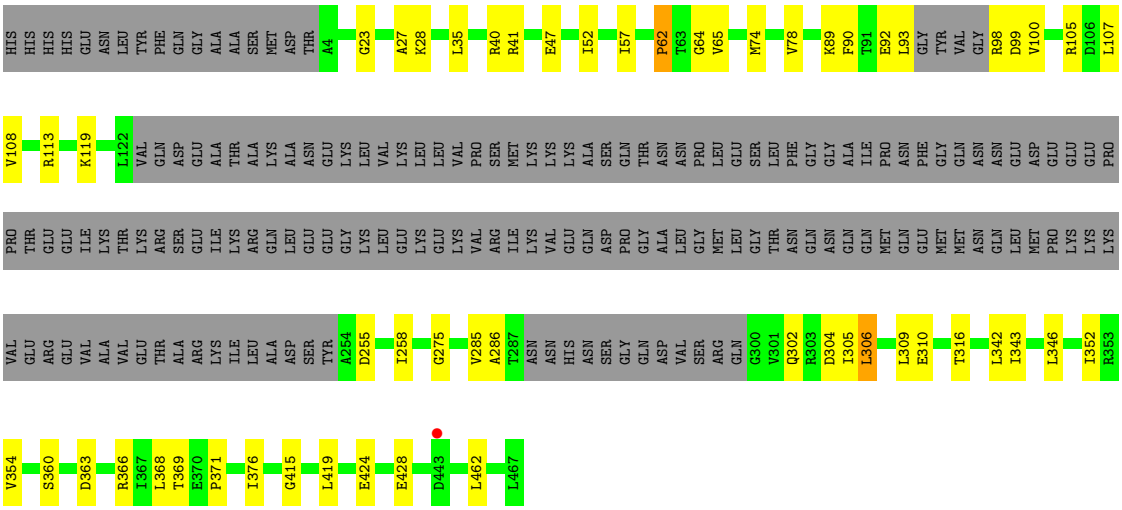
Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	GLN	-	expression tag	UNP P63796
K	-3	GLY	-	expression tag	UNP P63796
K	-2	ALA	-	expression tag	UNP P63796
K	-1	ALA	-	expression tag	UNP P63796
K	0	SER	-	expression tag	UNP P63796
L	-13	HIS	-	expression tag	UNP P63796
L	-12	HIS	-	expression tag	UNP P63796
L	-11	HIS	-	expression tag	UNP P63796
L	-10	HIS	-	expression tag	UNP P63796
L	-9	GLU	-	expression tag	UNP P63796
L	-8	ASN	-	expression tag	UNP P63796
L	-7	LEU	-	expression tag	UNP P63796
L	-6	TYR	-	expression tag	UNP P63796
L	-5	PHE	-	expression tag	UNP P63796
L	-4	GLN	-	expression tag	UNP P63796
L	-3	GLY	-	expression tag	UNP P63796
L	-2	ALA	-	expression tag	UNP P63796
L	-1	ALA	-	expression tag	UNP P63796
L	0	SER	-	expression tag	UNP P63796

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.

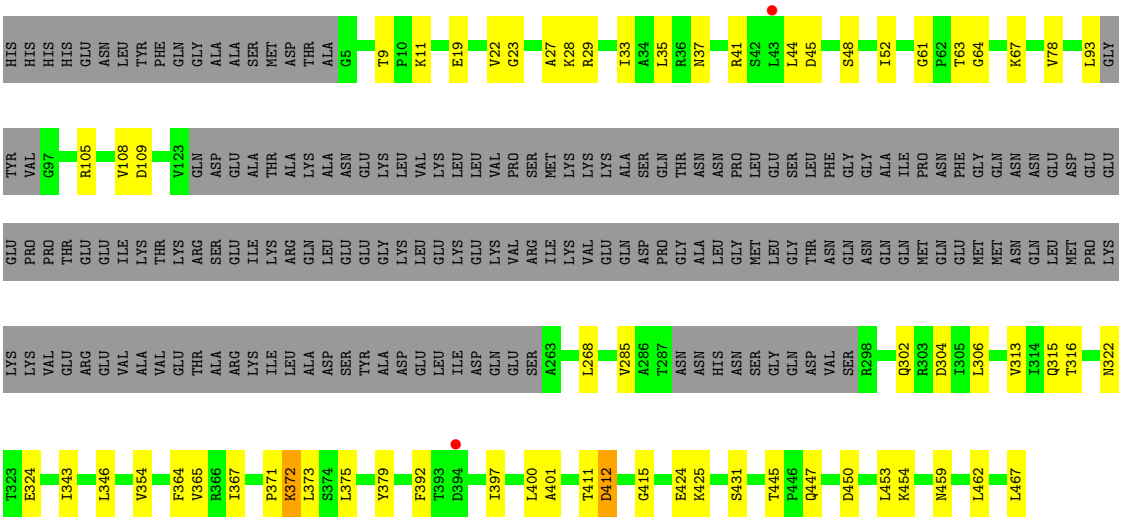
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain M: 54% 11% 34%



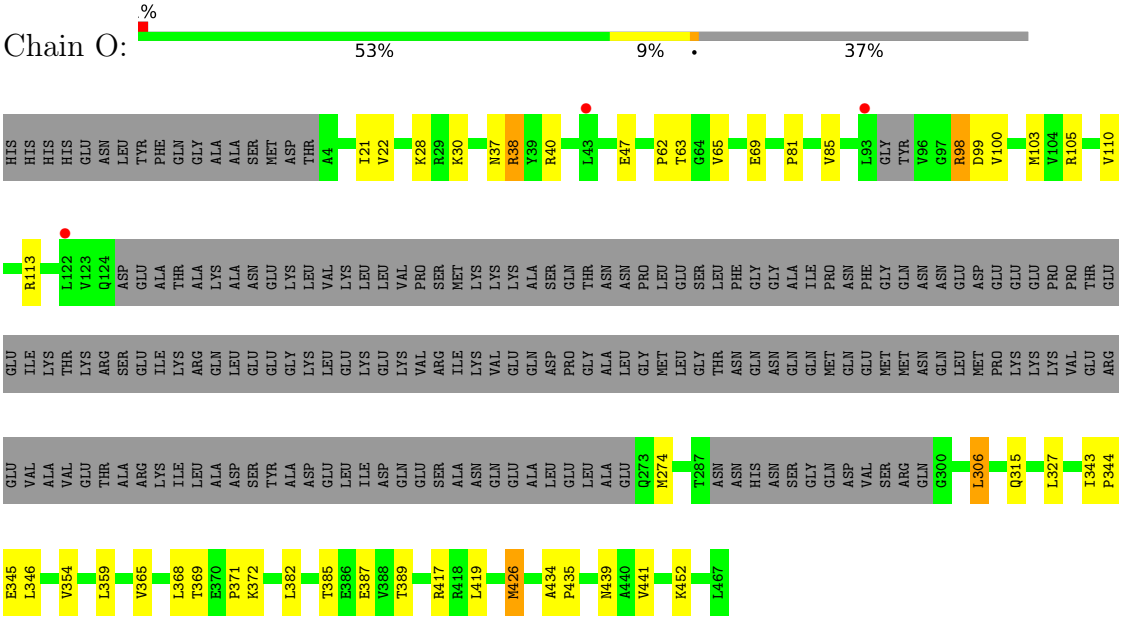
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain N: 51% 13% 35%



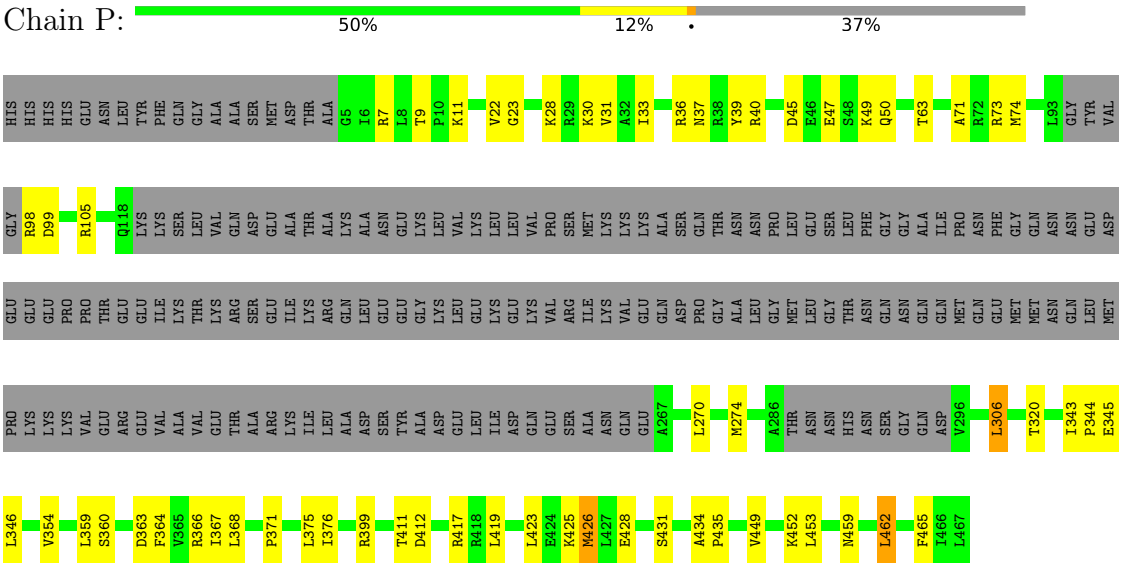
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain O:



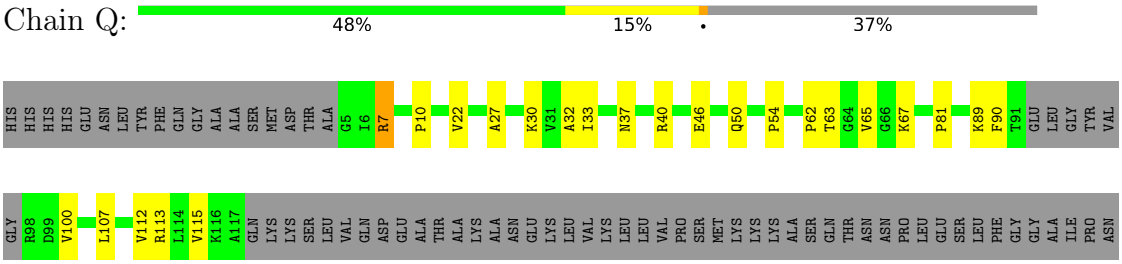
• Molecule 1: ATP-dependent protease ATPase subunit HslU

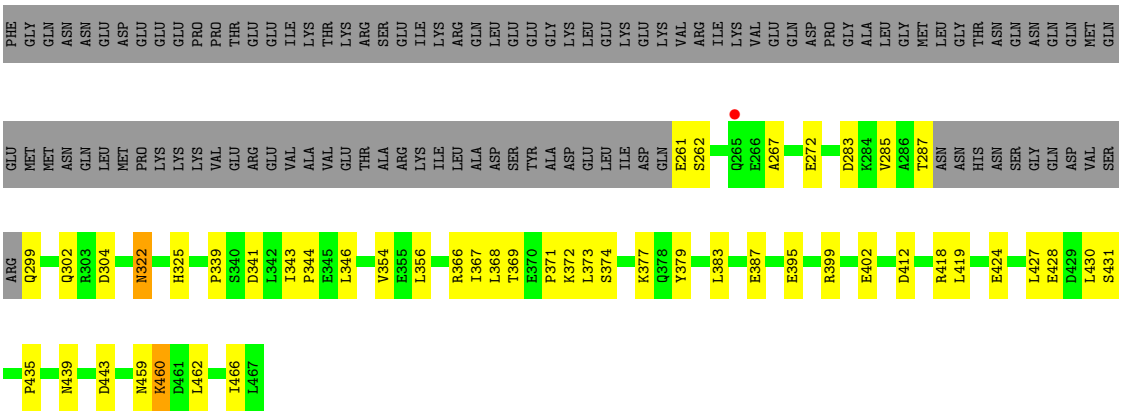
Chain P:



• Molecule 1: ATP-dependent protease ATPase subunit HslU

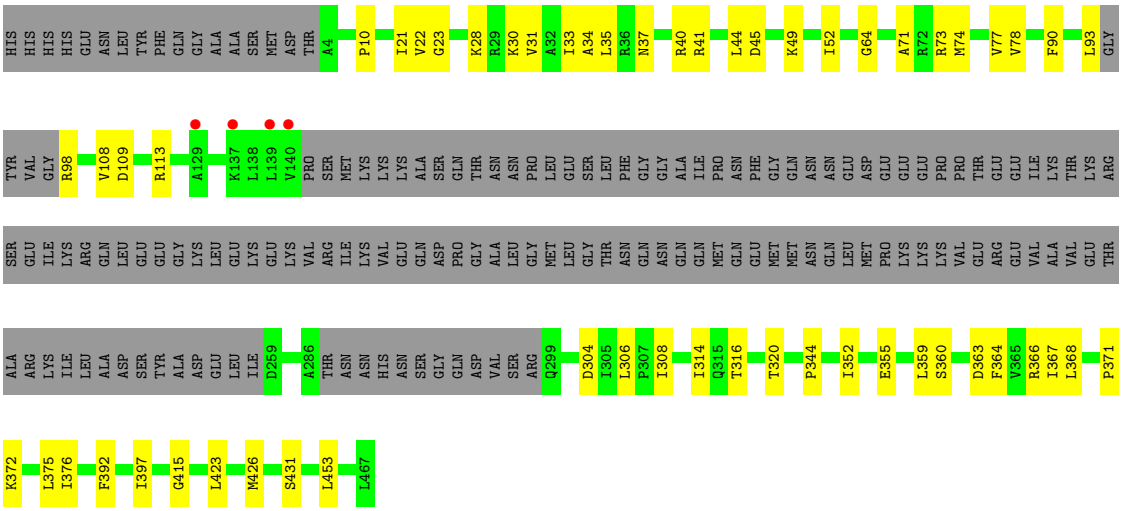
Chain Q:





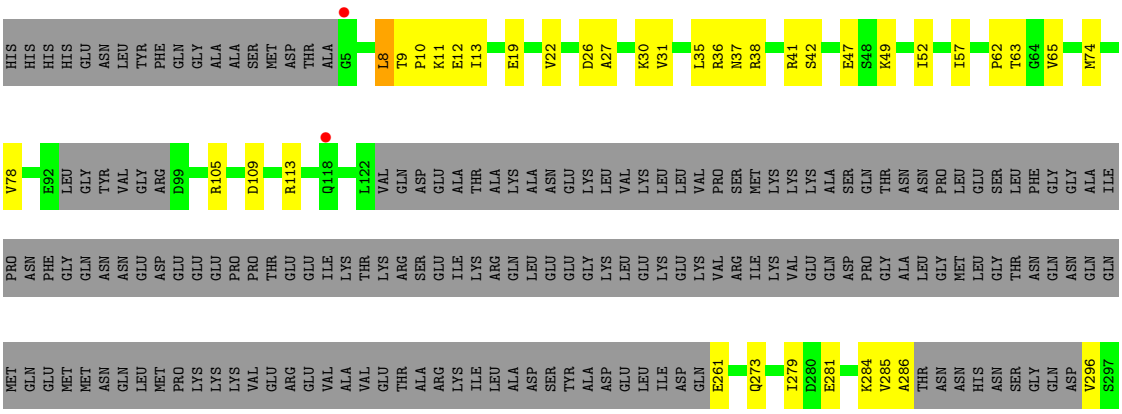
• Molecule 1: ATP-dependent protease ATPase subunit HslU

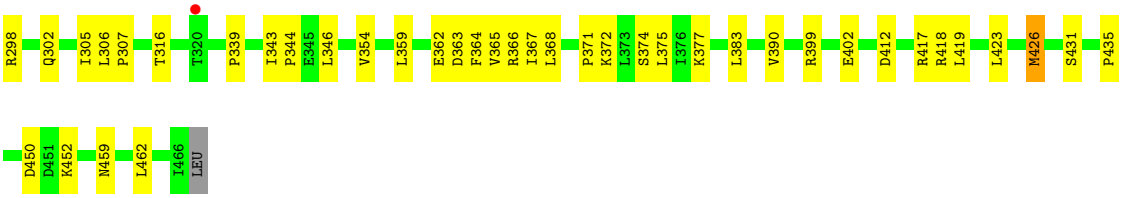
Chain R:



• Molecule 1: ATP-dependent protease ATPase subunit HslU

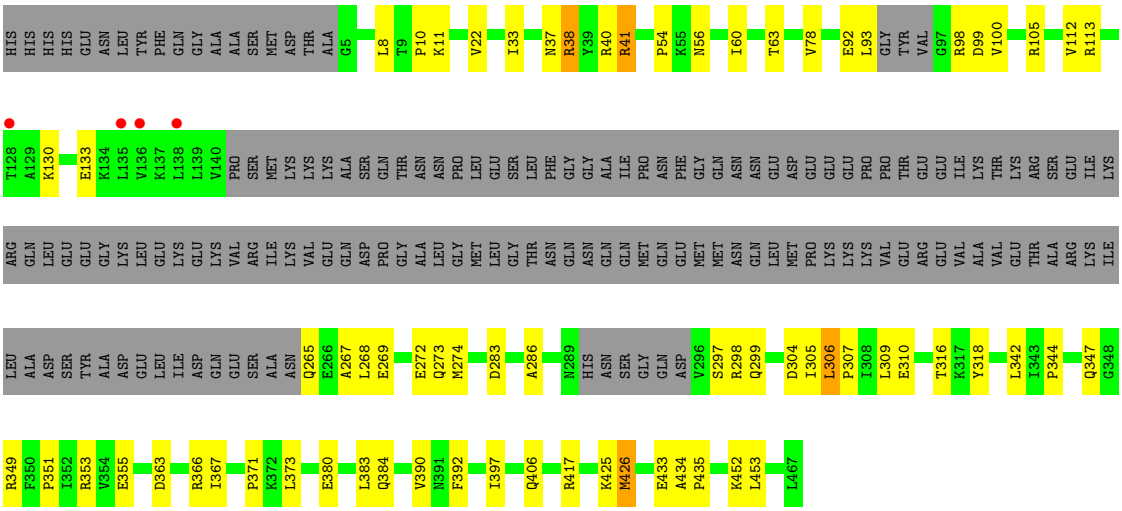
Chain S:





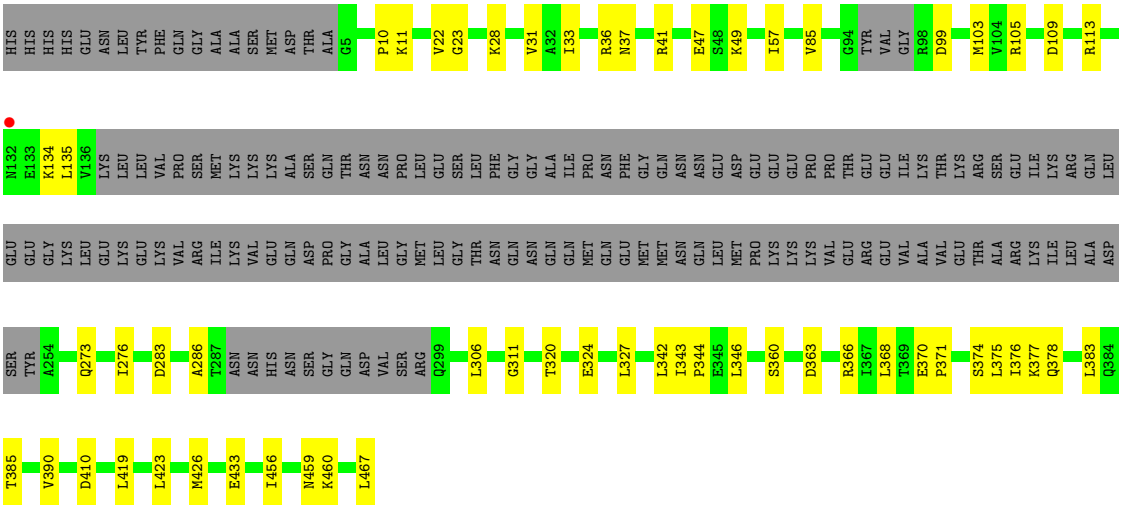
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain T:



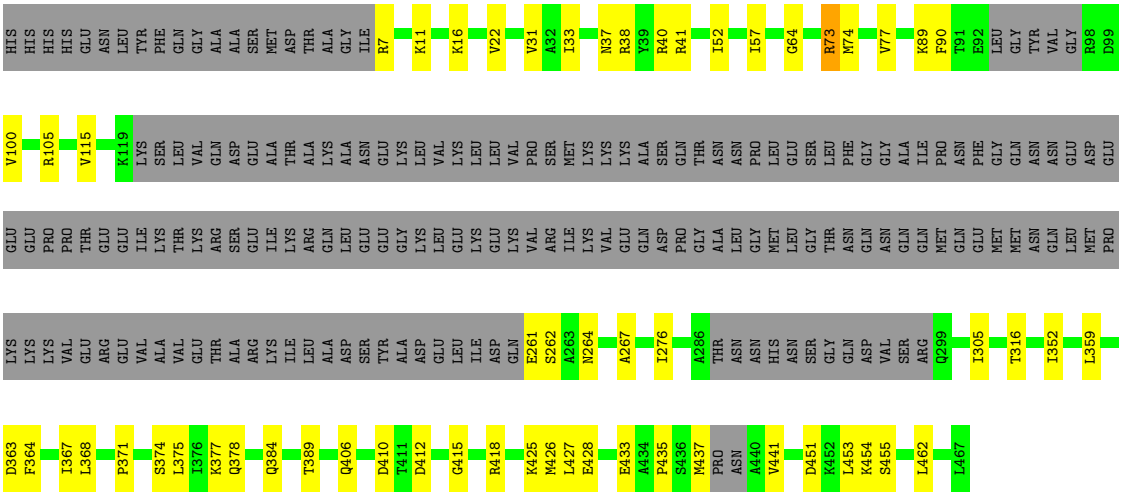
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain U:



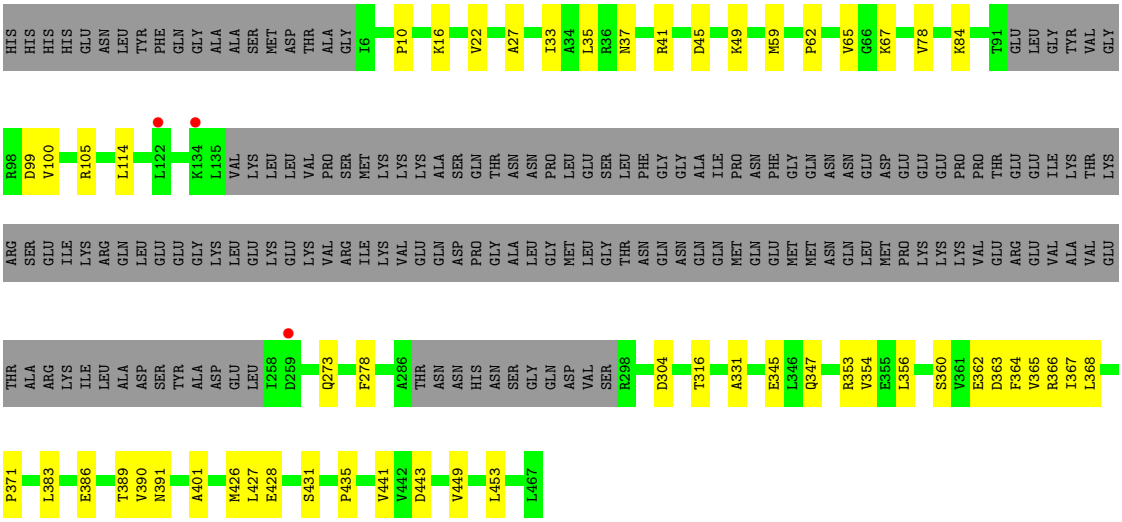
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain V:



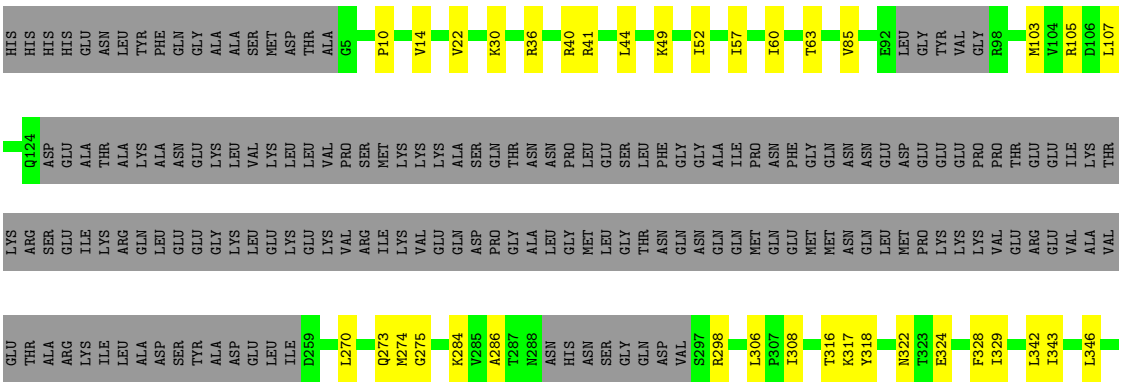
• Molecule 1: ATP-dependent protease ATPase subunit HslU

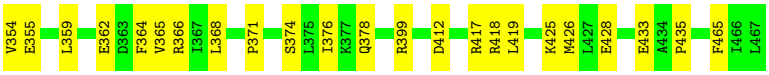
Chain W:



• Molecule 1: ATP-dependent protease ATPase subunit HslU

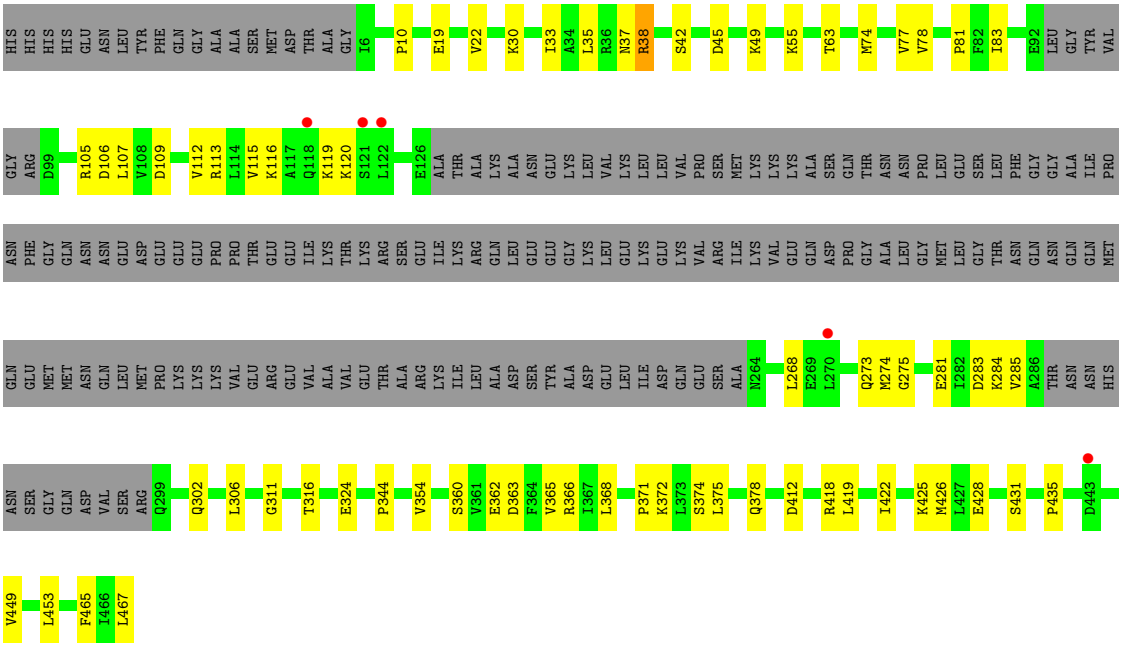
Chain X:





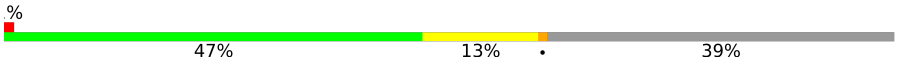
• Molecule 1: ATP-dependent protease ATPase subunit HslU

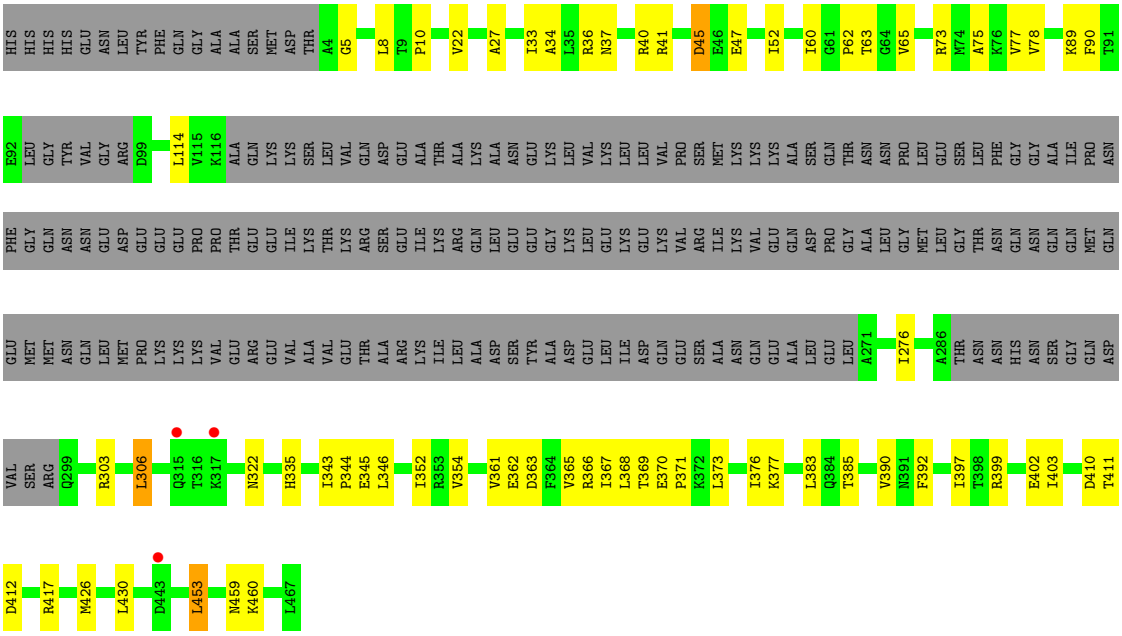
Chain A:



• Molecule 1: ATP-dependent protease ATPase subunit HslU

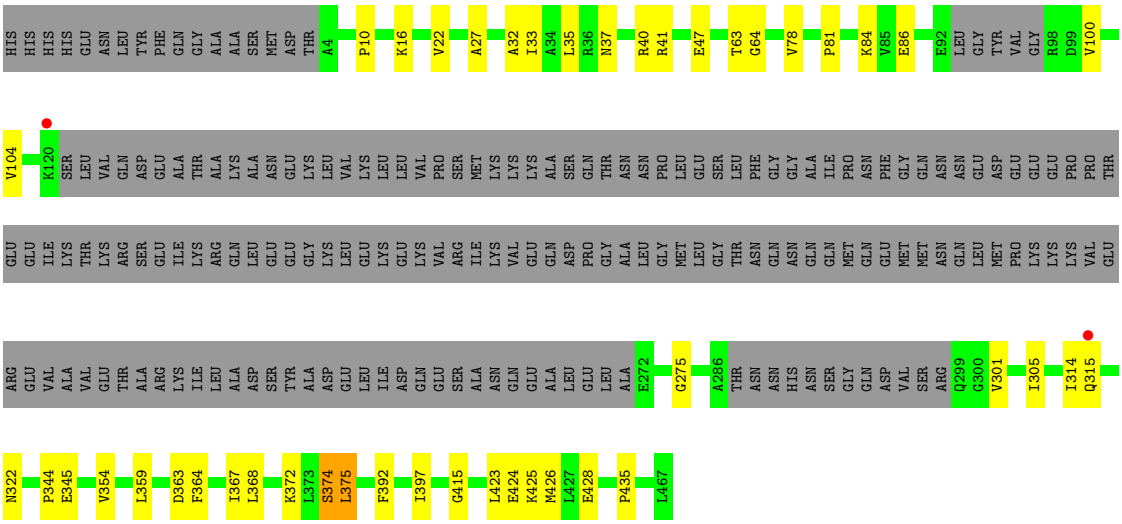
Chain B:





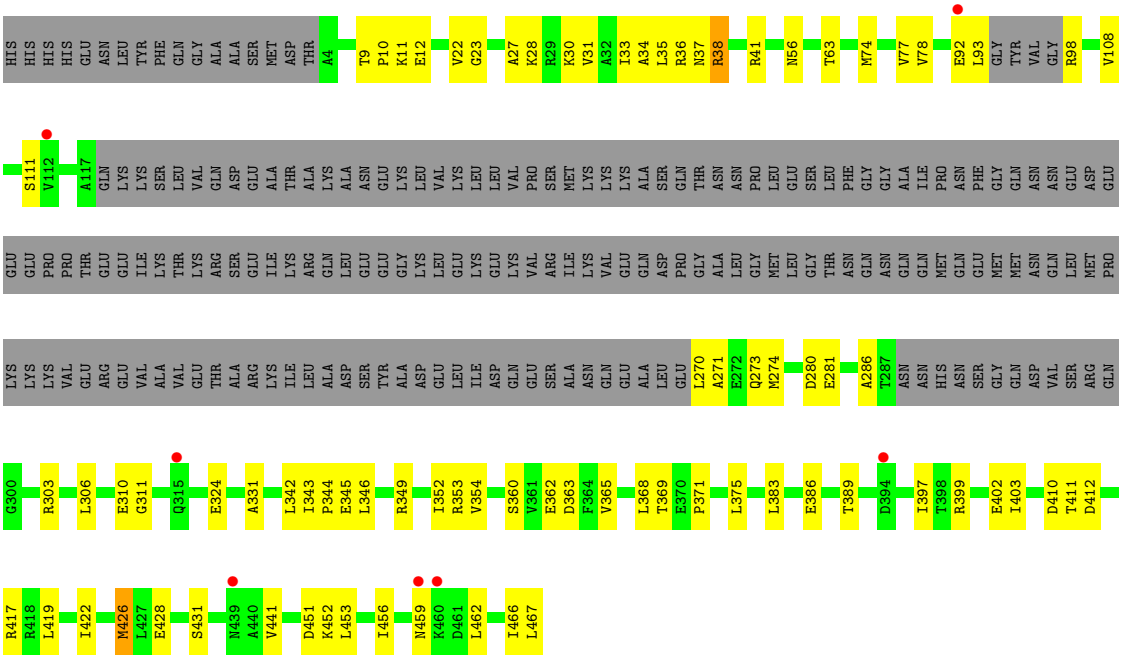
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain C: 52% 9% 38%



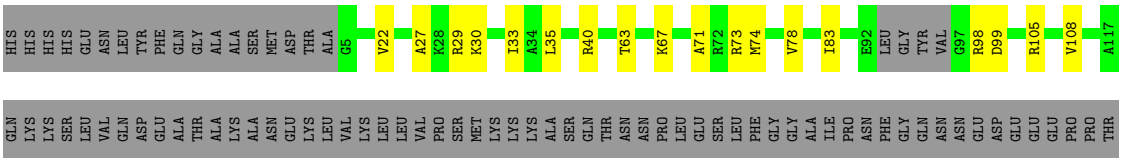
- Molecule 1: ATP-dependent protease ATPase subunit HslU

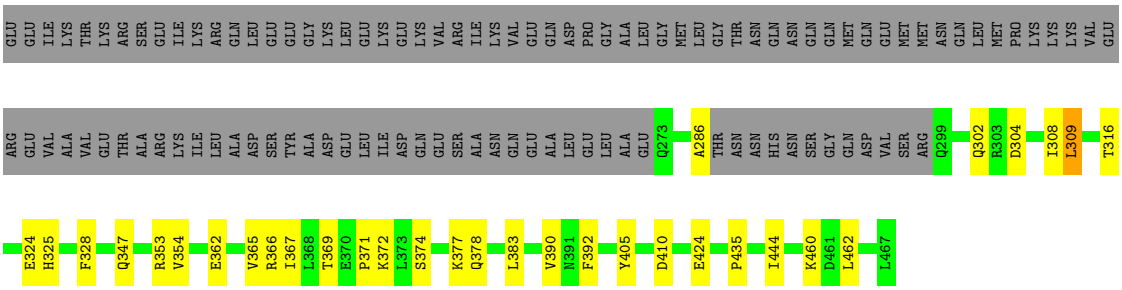
Chain D: % 44% 17% 38%



- Molecule 1: ATP-dependent protease ATPase subunit HslU

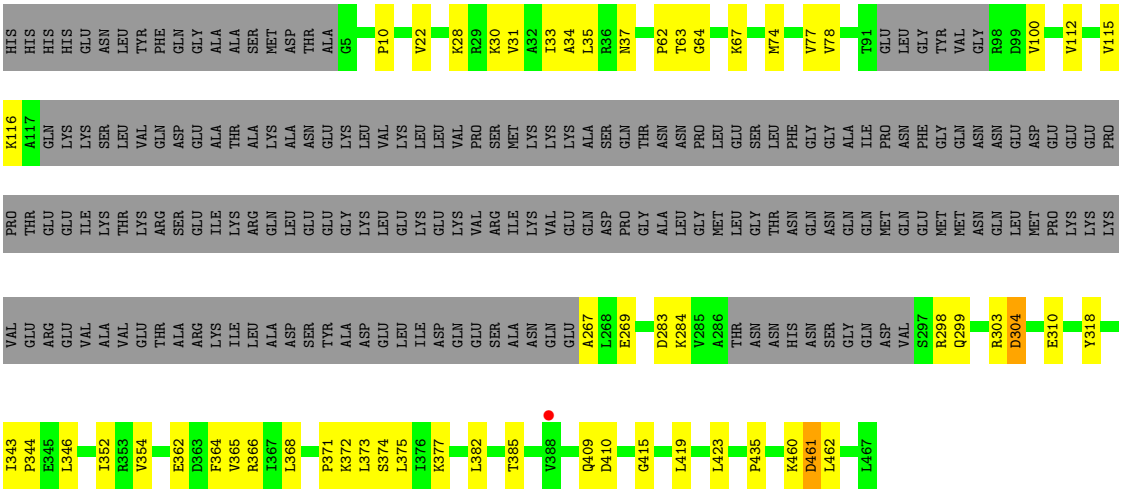
Chain E: 50% 10% 39%





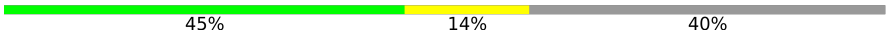
• Molecule 1: ATP-dependent protease ATPase subunit HslU

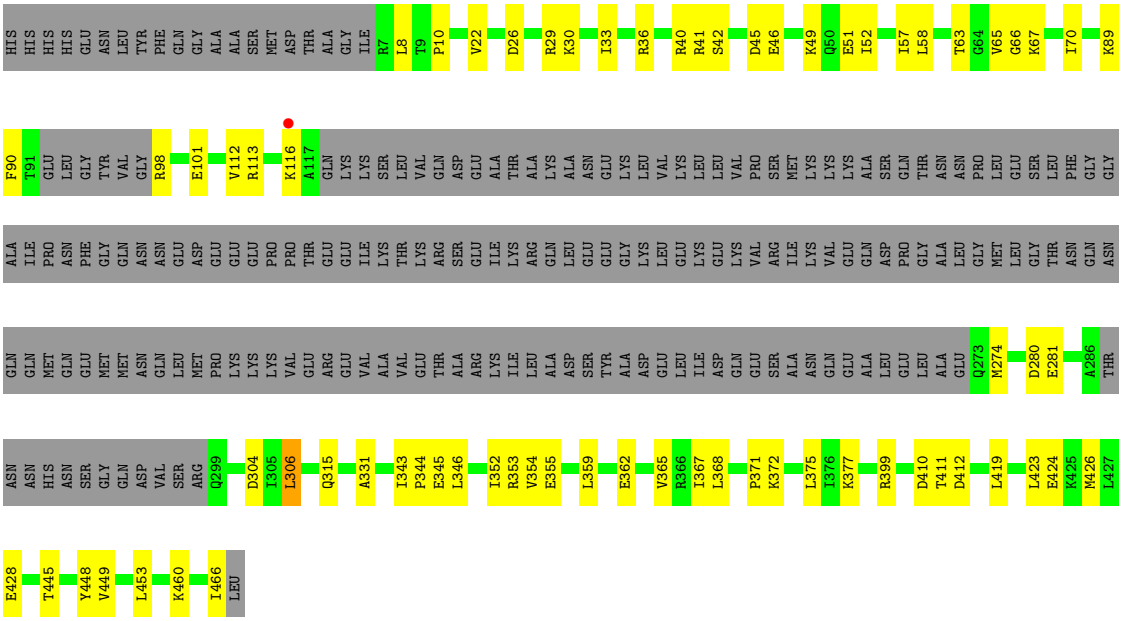
Chain F:



• Molecule 1: ATP-dependent protease ATPase subunit HslU

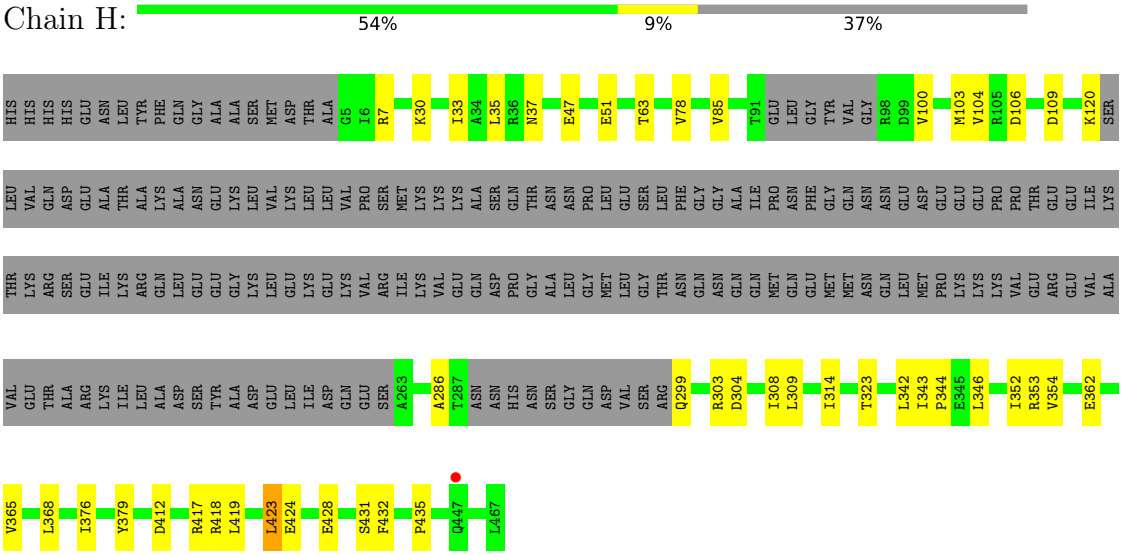
Chain G:





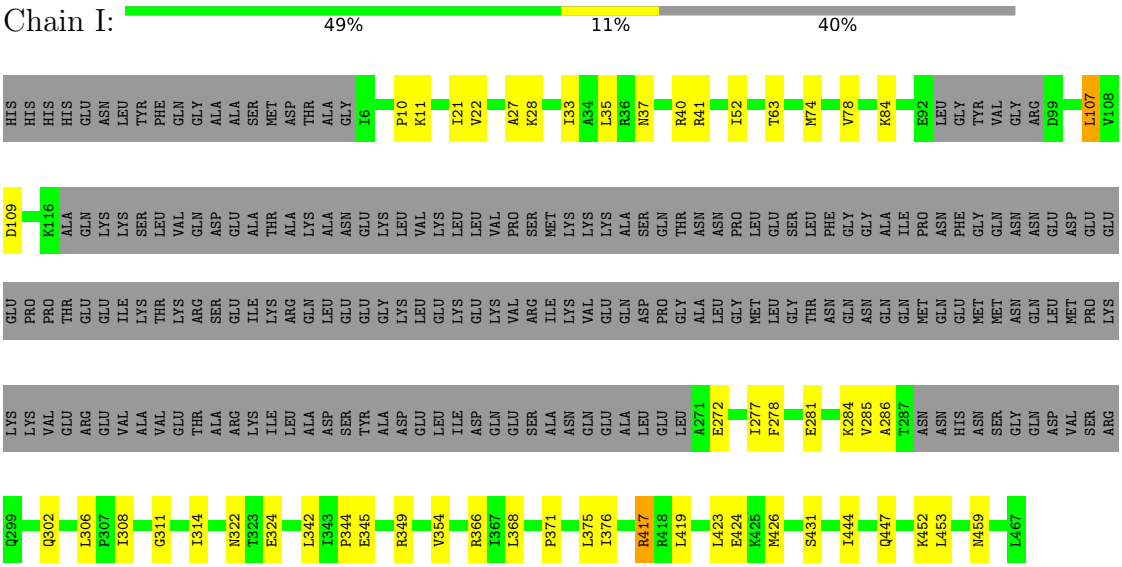
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain H:



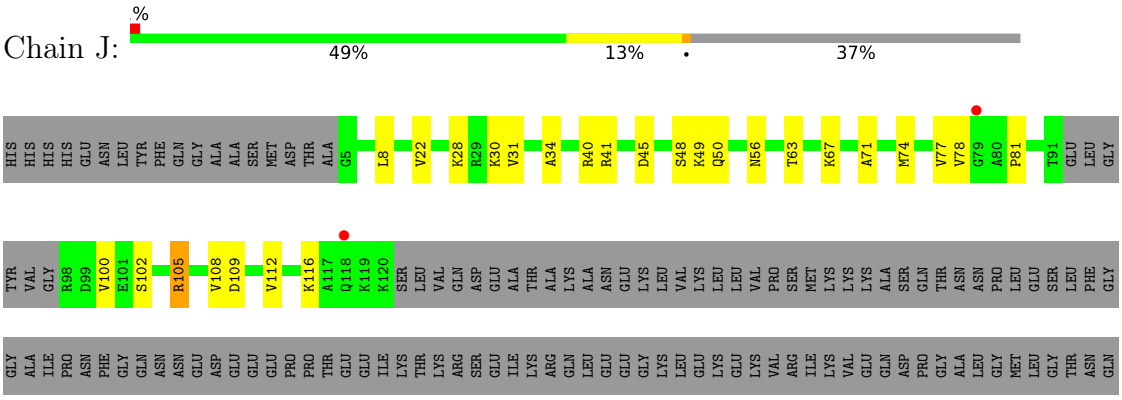
• Molecule 1: ATP-dependent protease ATPase subunit HslU

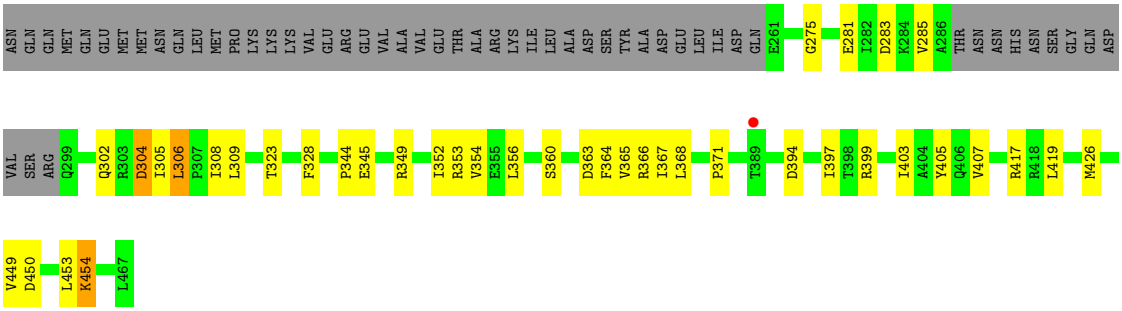
Chain I:



• Molecule 1: ATP-dependent protease ATPase subunit HslU

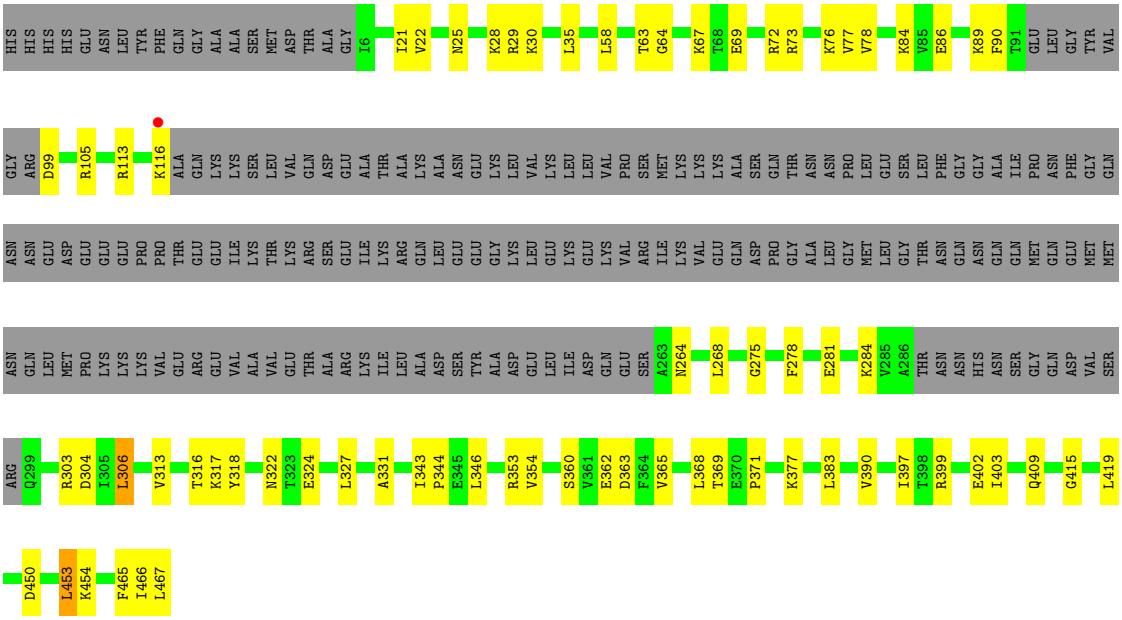
Chain J:





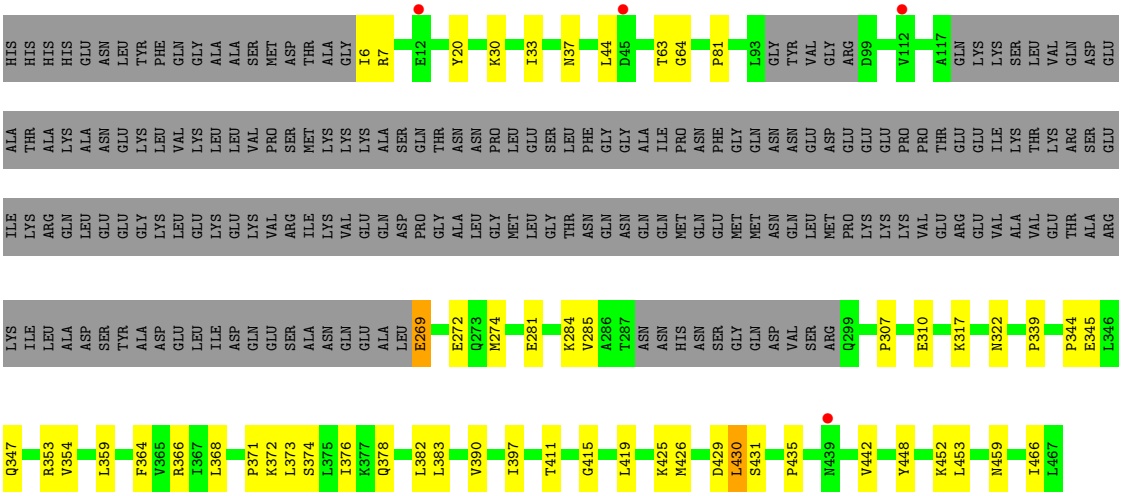
• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain K:



• Molecule 1: ATP-dependent protease ATPase subunit HslU

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	146.62Å 189.60Å 215.81Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	36.37 – 3.00 36.37 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (36.37-3.00) 90.6 (36.37-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.235 , 0.279 0.235 , 0.279	Depositor DCC
R_{free} test set	2010 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	57793	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.12% 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 (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	0.23	0/2452	0.40	0/3307
1	B	0.23	0/2326	0.41	0/3138
1	C	0.24	0/2364	0.41	0/3186
1	D	0.24	0/2356	0.41	0/3179
1	E	0.24	0/2327	0.42	0/3138
1	F	0.23	0/2375	0.42	0/3203
1	G	0.24	0/2293	0.43	0/3094
1	H	0.24	0/2423	0.41	0/3267
1	I	0.24	0/2324	0.42	0/3136
1	J	0.24	0/2431	0.41	0/3277
1	K	0.24	0/2368	0.41	0/3197
1	L	0.24	0/2354	0.41	0/3177
1	M	0.24	0/2520	0.41	0/3399
1	N	0.24	0/2476	0.40	0/3338
1	O	0.24	0/2402	0.41	0/3239
1	P	0.24	0/2408	0.40	0/3248
1	Q	0.24	0/2411	0.42	0/3253
1	R	0.24	0/2621	0.41	0/3534
1	S	0.24	0/2458	0.43	1/3315 (0.0%)
1	T	0.24	0/2622	0.41	0/3535
1	U	0.24	0/2633	0.41	0/3551
1	V	0.24	0/2402	0.41	0/3236
1	W	0.24	0/2574	0.41	0/3471
1	X	0.24	0/2519	0.41	0/3396
All	All	0.24	0/58439	0.41	1/78814 (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	S	8	LEU	C-N-CA	5.56	135.59	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2425	0	2503	41	0
1	B	2299	0	2376	39	0
1	C	2337	0	2423	32	0
1	D	2329	0	2415	56	0
1	E	2300	0	2381	33	0
1	F	2348	0	2434	38	0
1	G	2266	0	2347	47	0
1	H	2396	0	2482	30	0
1	I	2297	0	2375	36	0
1	J	2404	0	2486	44	0
1	K	2341	0	2420	42	0
1	L	2327	0	2408	34	0
1	M	2493	0	2572	33	0
1	N	2449	0	2540	40	0
1	O	2375	0	2472	31	0
1	P	2381	0	2468	41	0
1	Q	2384	0	2459	49	0
1	R	2594	0	2687	35	0
1	S	2431	0	2511	47	0
1	T	2595	0	2697	44	0
1	U	2606	0	2685	37	0
1	V	2377	0	2451	33	0
1	W	2547	0	2633	36	0
1	X	2492	0	2568	40	0
All	All	57793	0	59793	842	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 7.

The worst 5 of 842 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:38:ARG:NH1	1:A:273:GLN:O	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:VAL:HG21	1:F:304:ASP:HB3	1.65	0.78
1:H:100:VAL:HG21	1:H:304:ASP:HB3	1.66	0.77
1:G:30:LYS:HD2	1:G:354:VAL:HB	1.66	0.76
1:W:431:SER:HB2	1:X:40:ARG:HH12	1.51	0.76

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	299/481 (62%)	290 (97%)	9 (3%)	0	100	100
1	B	284/481 (59%)	271 (95%)	13 (5%)	0	100	100
1	C	288/481 (60%)	272 (94%)	16 (6%)	0	100	100
1	D	288/481 (60%)	279 (97%)	9 (3%)	0	100	100
1	E	284/481 (59%)	273 (96%)	11 (4%)	0	100	100
1	F	290/481 (60%)	282 (97%)	7 (2%)	1 (0%)	41	76
1	G	279/481 (58%)	268 (96%)	11 (4%)	0	100	100
1	H	296/481 (62%)	284 (96%)	12 (4%)	0	100	100
1	I	283/481 (59%)	273 (96%)	10 (4%)	0	100	100
1	J	297/481 (62%)	290 (98%)	7 (2%)	0	100	100
1	K	289/481 (60%)	275 (95%)	14 (5%)	0	100	100
1	L	287/481 (60%)	278 (97%)	7 (2%)	2 (1%)	22	60
1	M	309/481 (64%)	301 (97%)	8 (3%)	0	100	100
1	N	303/481 (63%)	297 (98%)	6 (2%)	0	100	100
1	O	294/481 (61%)	279 (95%)	15 (5%)	0	100	100
1	P	294/481 (61%)	285 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	295/481 (61%)	283 (96%)	12 (4%)	0	100	100
1	R	322/481 (67%)	313 (97%)	9 (3%)	0	100	100
1	S	301/481 (63%)	290 (96%)	11 (4%)	0	100	100
1	T	322/481 (67%)	312 (97%)	10 (3%)	0	100	100
1	U	324/481 (67%)	314 (97%)	10 (3%)	0	100	100
1	V	291/481 (60%)	283 (97%)	8 (3%)	0	100	100
1	W	315/481 (66%)	305 (97%)	10 (3%)	0	100	100
1	X	308/481 (64%)	302 (98%)	6 (2%)	0	100	100
All	All	7142/11544 (62%)	6899 (97%)	240 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	310	GLU
1	L	411	THR
1	L	285	VAL

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	273/421 (65%)	270 (99%)	3 (1%)	73	90
1	B	258/421 (61%)	248 (96%)	10 (4%)	32	69
1	C	262/421 (62%)	258 (98%)	4 (2%)	65	87
1	D	261/421 (62%)	257 (98%)	4 (2%)	65	87
1	E	258/421 (61%)	254 (98%)	4 (2%)	62	86
1	F	263/421 (62%)	260 (99%)	3 (1%)	73	90
1	G	255/421 (61%)	251 (98%)	4 (2%)	62	86
1	H	268/421 (64%)	264 (98%)	4 (2%)	65	87
1	I	259/421 (62%)	256 (99%)	3 (1%)	71	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	269/421 (64%)	263 (98%)	6 (2%)	52	81
1	K	263/421 (62%)	260 (99%)	3 (1%)	73	90
1	L	262/421 (62%)	258 (98%)	4 (2%)	65	87
1	M	279/421 (66%)	275 (99%)	4 (1%)	67	88
1	N	274/421 (65%)	269 (98%)	5 (2%)	59	85
1	O	267/421 (63%)	262 (98%)	5 (2%)	57	84
1	P	267/421 (63%)	262 (98%)	5 (2%)	57	84
1	Q	267/421 (63%)	260 (97%)	7 (3%)	46	78
1	R	290/421 (69%)	288 (99%)	2 (1%)	84	94
1	S	273/421 (65%)	265 (97%)	8 (3%)	42	76
1	T	291/421 (69%)	282 (97%)	9 (3%)	40	75
1	U	291/421 (69%)	287 (99%)	4 (1%)	67	88
1	V	266/421 (63%)	259 (97%)	7 (3%)	46	78
1	W	285/421 (68%)	284 (100%)	1 (0%)	91	97
1	X	280/421 (66%)	277 (99%)	3 (1%)	73	90
All	All	6481/10104 (64%)	6369 (98%)	112 (2%)	60	85

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	306	LEU
1	L	430	LEU
1	B	453	LEU
1	L	426	MET
1	J	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	50	GLN
1	O	315	GLN

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	307/481 (63%)	-0.21	5 (1%)	72	44	34, 56, 81, 91	0
1	B	292/481 (60%)	-0.28	3 (1%)	82	59	31, 53, 79, 94	0
1	C	296/481 (61%)	-0.40	2 (0%)	87	69	25, 47, 76, 92	0
1	D	296/481 (61%)	-0.29	7 (2%)	59	30	24, 48, 75, 90	0
1	E	292/481 (60%)	-0.38	0	100	100	25, 45, 65, 78	0
1	F	298/481 (61%)	-0.35	1 (0%)	94	84	27, 54, 77, 89	0
1	G	287/481 (59%)	-0.43	1 (0%)	94	84	29, 46, 71, 94	0
1	H	304/481 (63%)	-0.29	1 (0%)	94	84	28, 53, 74, 88	0
1	I	291/481 (60%)	-0.28	0	100	100	34, 57, 81, 103	0
1	J	305/481 (63%)	-0.26	3 (0%)	82	59	33, 54, 82, 97	0
1	K	297/481 (61%)	-0.35	1 (0%)	94	84	29, 57, 81, 92	0
1	L	295/481 (61%)	-0.25	4 (1%)	75	49	29, 54, 80, 94	0
1	M	317/481 (65%)	-0.38	1 (0%)	94	84	22, 48, 71, 80	0
1	N	311/481 (64%)	-0.33	2 (0%)	89	72	24, 49, 72, 107	0
1	O	302/481 (62%)	-0.44	3 (0%)	82	59	19, 41, 65, 84	0
1	P	302/481 (62%)	-0.46	0	100	100	18, 38, 68, 87	0
1	Q	303/481 (62%)	-0.43	1 (0%)	94	84	19, 40, 68, 94	0
1	R	330/481 (68%)	-0.35	4 (1%)	79	54	19, 45, 70, 86	0
1	S	309/481 (64%)	-0.42	3 (0%)	82	59	21, 43, 71, 88	0
1	T	330/481 (68%)	-0.23	4 (1%)	79	54	25, 49, 74, 96	0
1	U	332/481 (69%)	-0.36	1 (0%)	94	84	29, 46, 68, 88	0
1	V	301/481 (62%)	-0.44	0	100	100	22, 44, 74, 103	0
1	W	323/481 (67%)	-0.38	3 (0%)	84	63	20, 40, 71, 90	0
1	X	316/481 (65%)	-0.41	0	100	100	15, 42, 75, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	7336/11544 (63%)	-0.35	50 (0%)	87	69	15, 48, 76, 107	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	43	LEU	3.7
1	W	259	ASP	3.4
1	A	121	SER	3.4
1	T	136	VAL	3.3
1	K	116	LYS	3.1

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.