



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:03 PM UTC

PDB ID : 6KWW / pdb_00006kww
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

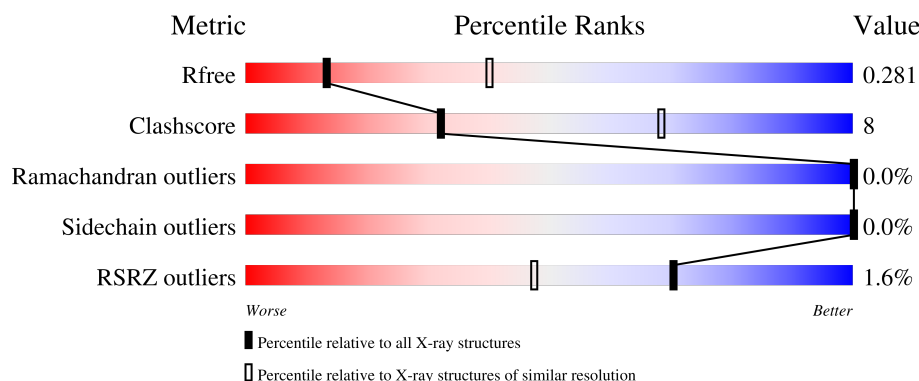
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	
1	B	481	
1	C	481	
1	D	481	
1	E	481	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	481	% 49% 13% 38%
1	G	481	% 45% 15% 40%
1	H	481	% 53% 10% 37%
1	I	481	% 48% 12% 40%
1	J	481	% 49% 14% 37%
1	K	481	% 46% 15% 38%
1	L	481	3% 49% 12% 39%
1	M	481	% 54% 12% 34%
1	N	481	2% 50% 15% 35%
1	O	481	% 52% 10% 37%
1	P	481	% 49% 13% 37%
1	Q	481	% 48% 15% 37%
1	R	481	56% 12% 31%
1	S	481	48% 16% 36%
1	T	481	% 53% 15% 31%
1	U	481	% 57% 12% 31%
1	V	481	% 51% 12% 37%
1	W	481	% 55% 12% 33%
1	X	481	% 52% 13% 34%

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

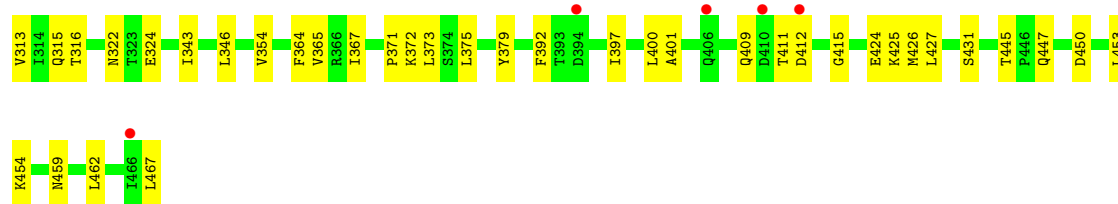
Continued from previous page...

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

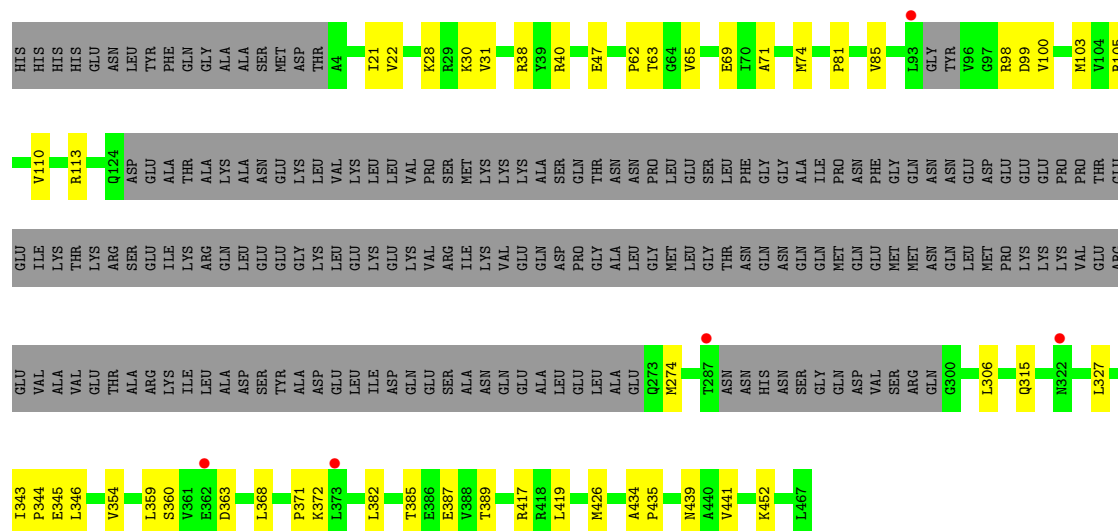
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

- Chain M: 

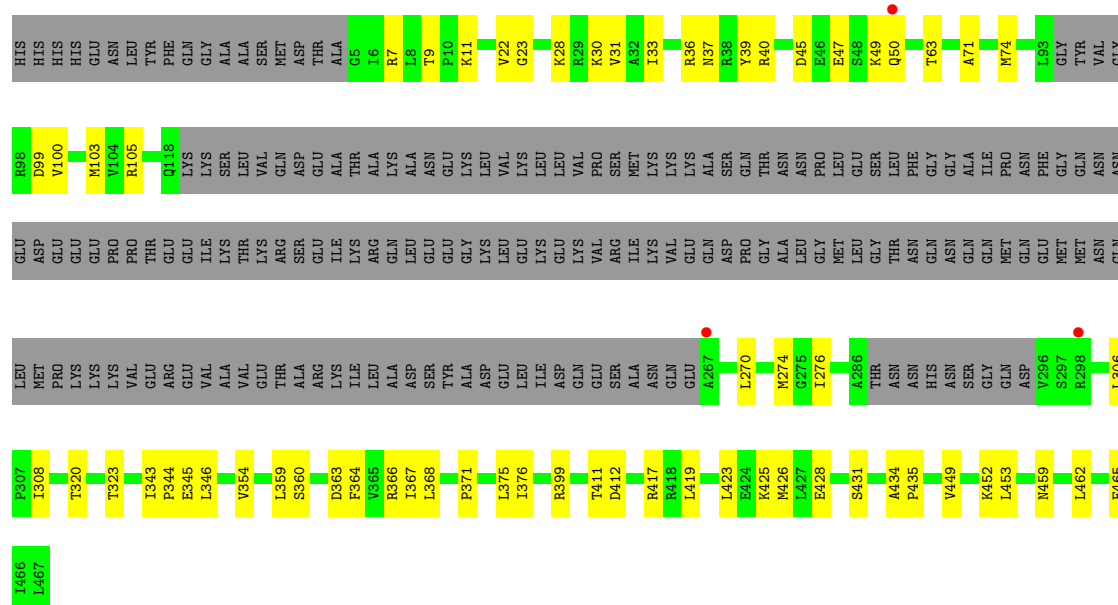
- [illegible]



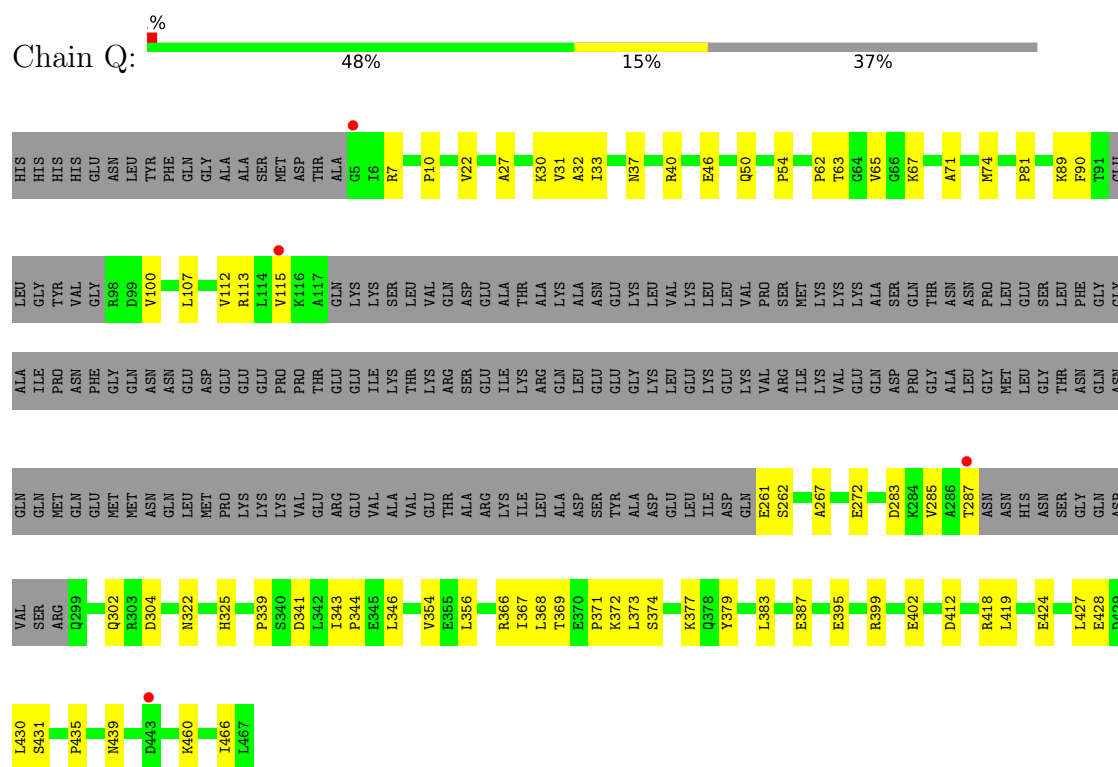
● Molecule 1: ATP-dependent protease ATPase subunit HslU



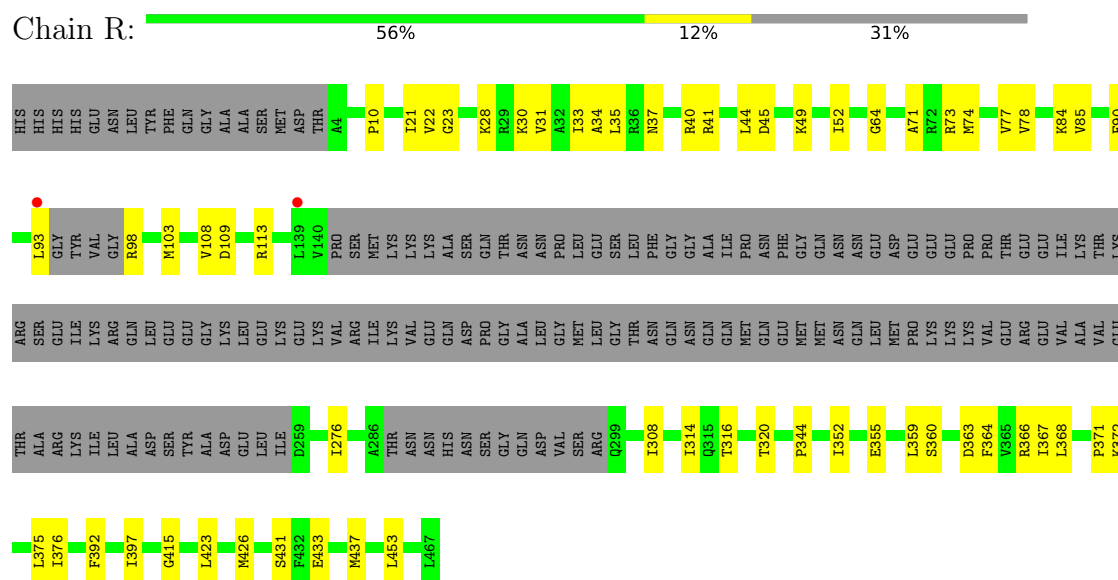
● Molecule 1: ATP-dependent protease ATPase subunit HslU



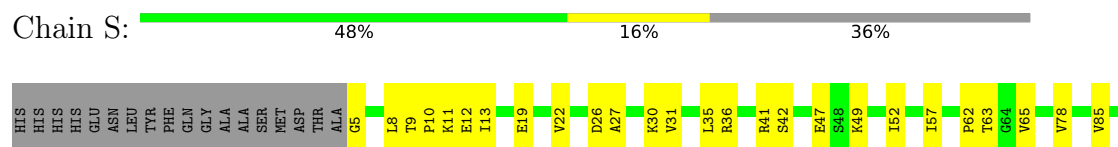
● Molecule 1: ATP-dependent protease ATPase subunit HslU

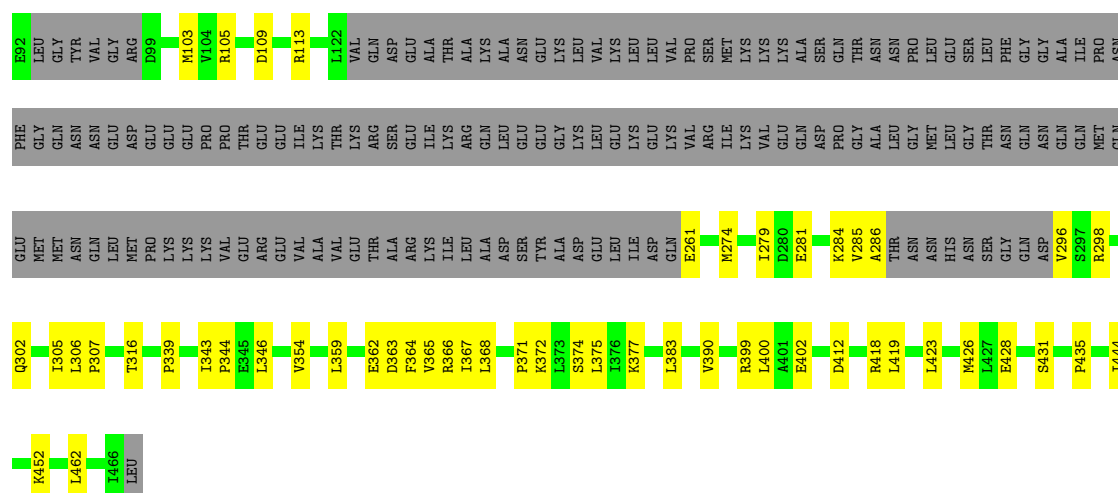


• Molecule 1: ATP-dependent protease ATPase subunit HslU

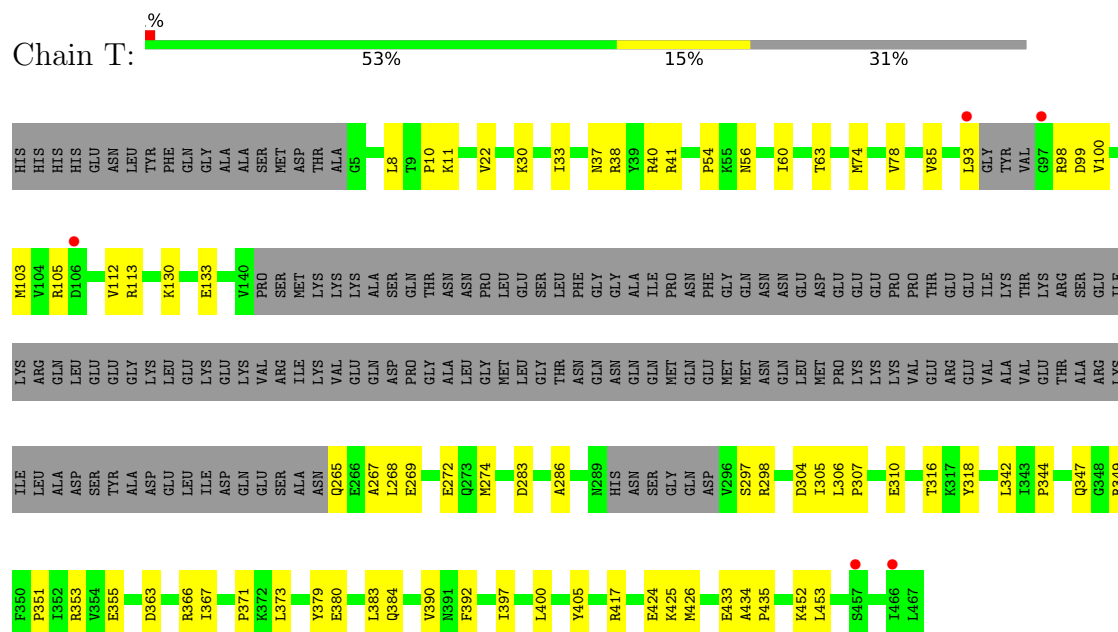


• Molecule 1: ATP-dependent protease ATPase subunit HslU

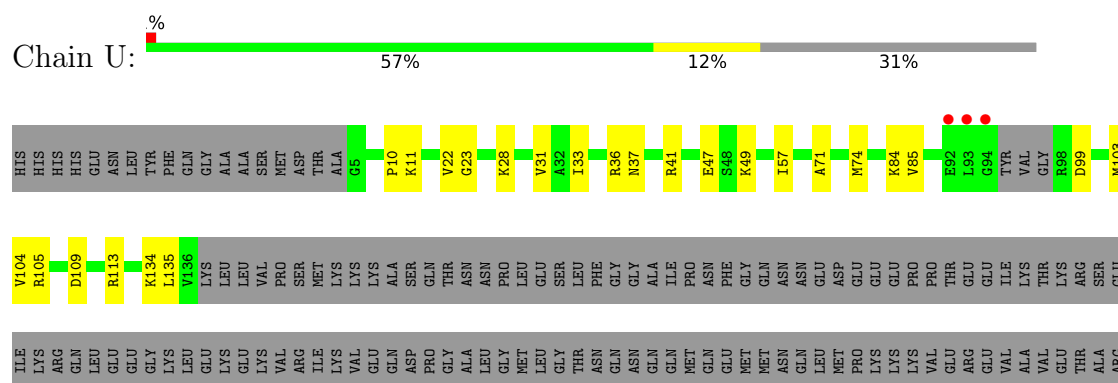




● Molecule 1: ATP-dependent protease ATPase subunit HslU



● Molecule 1: ATP-dependent protease ATPase subunit HslU

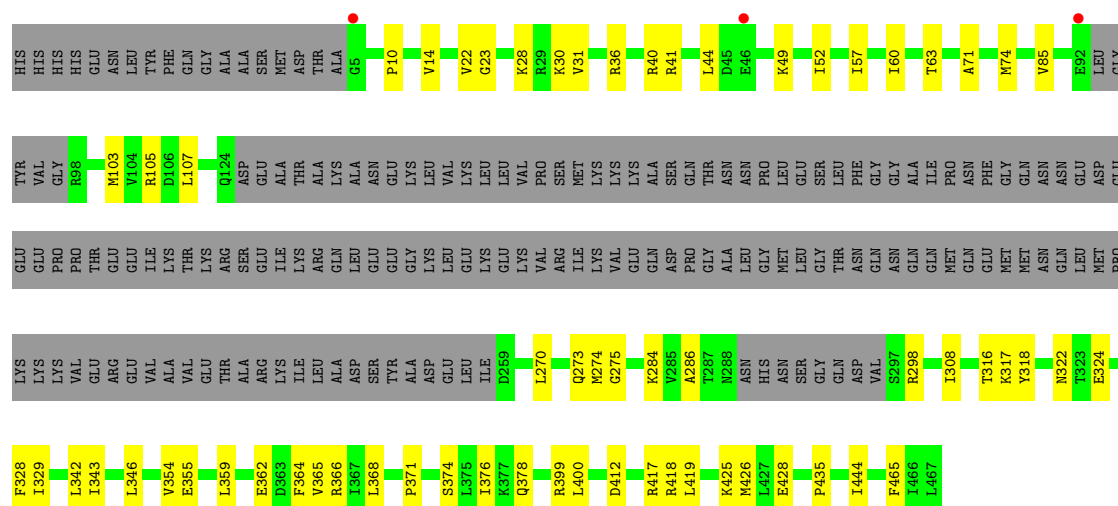


- Molecule 1: ATP-dependent protease ATPase subunit HslU

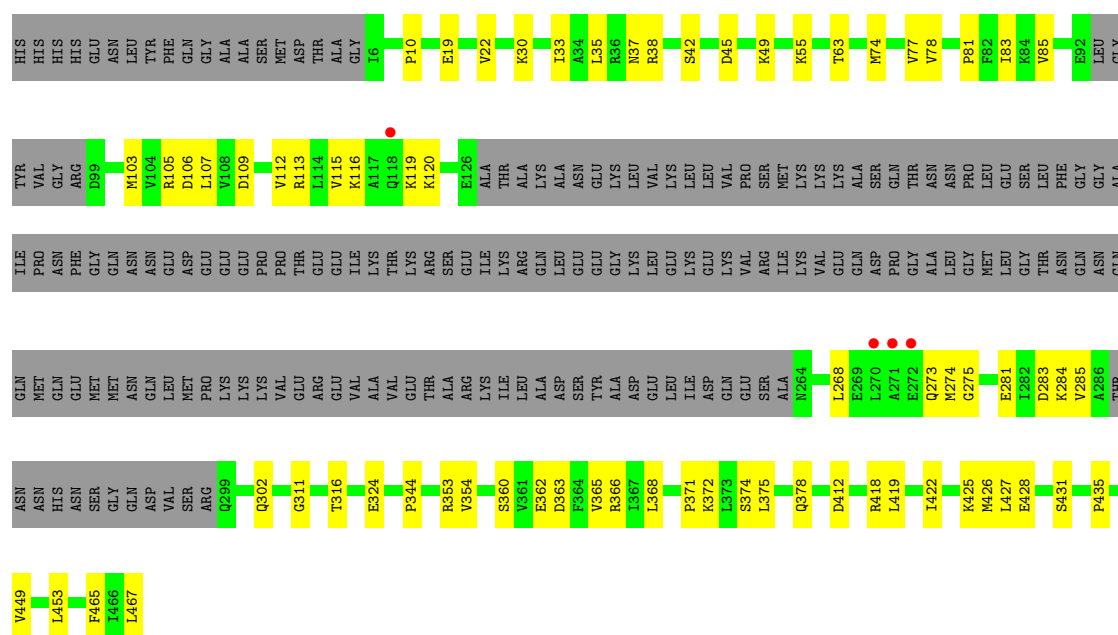
- Molecule 1: ATP-dependent protease ATPase subunit HslU

- Molecule 1: ATP-dependent protease ATPase subunit HslU

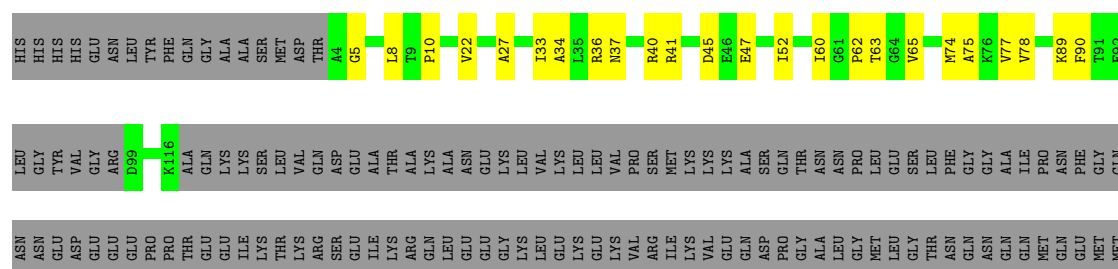




• Molecule 1: ATP-dependent protease ATPase subunit HslU

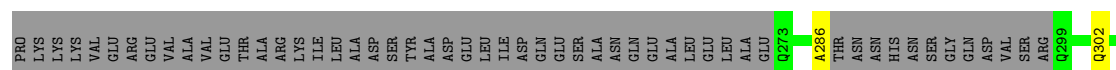
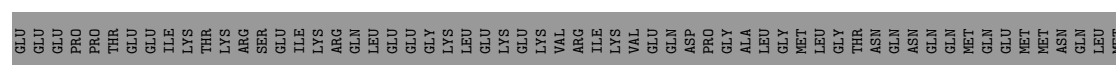
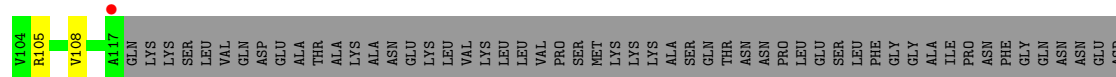


• Molecule 1: ATP-dependent protease ATPase subunit HslU

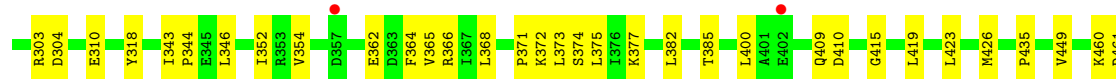
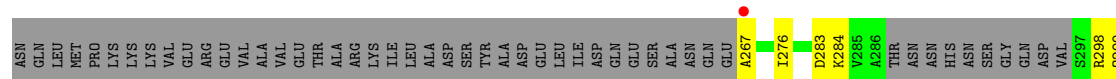
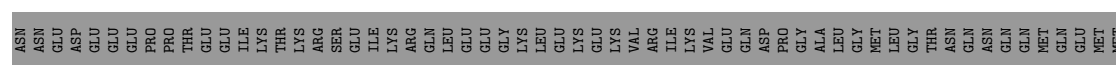
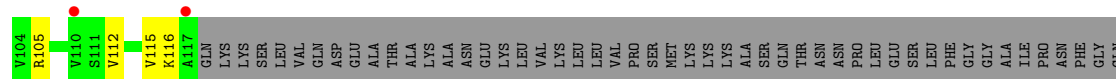
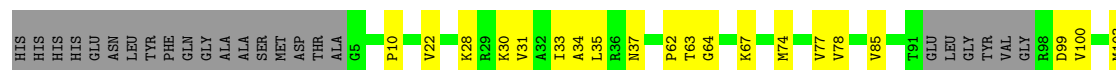




- Molecule 1: ATP-dependent protease ATPase subunit HslU

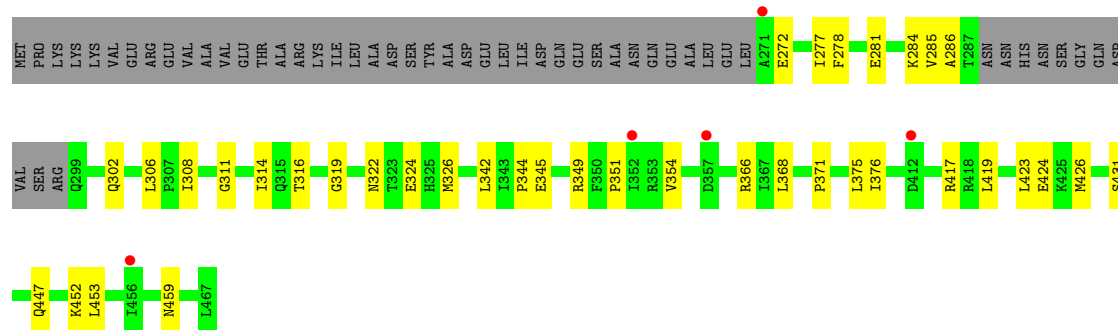


- Molecule 1: ATP-dependent protease ATPase subunit HslU

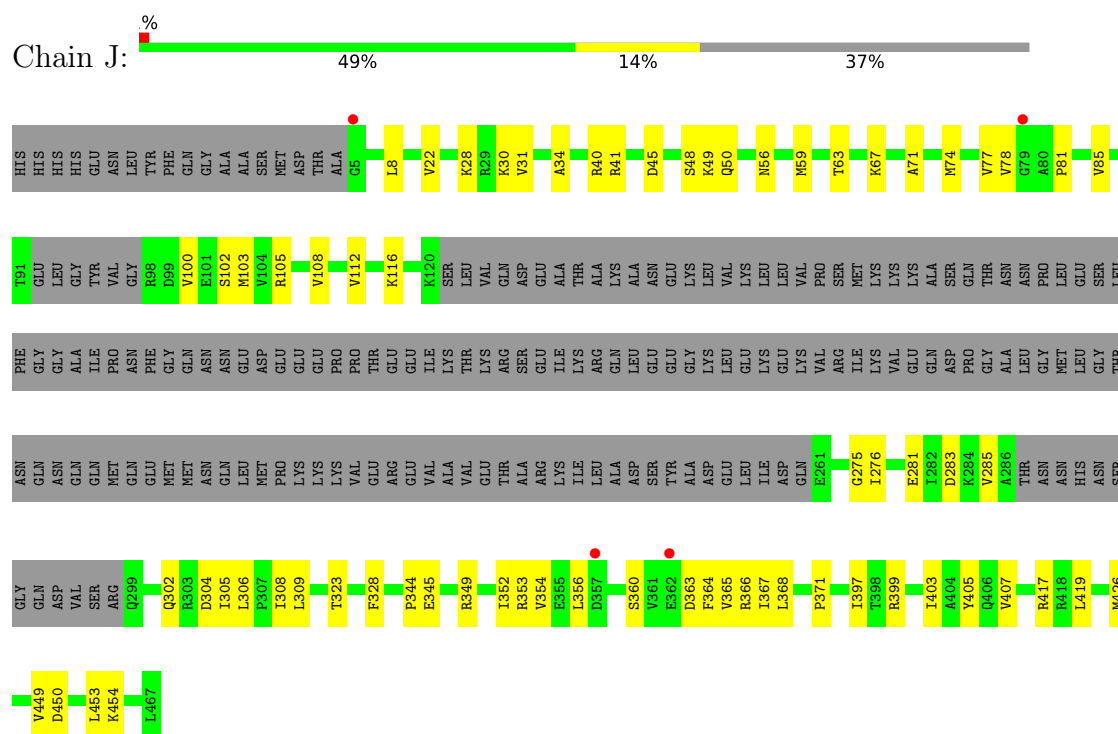


- Molecule 1: ATP-dependent protease ATPase subunit HslU

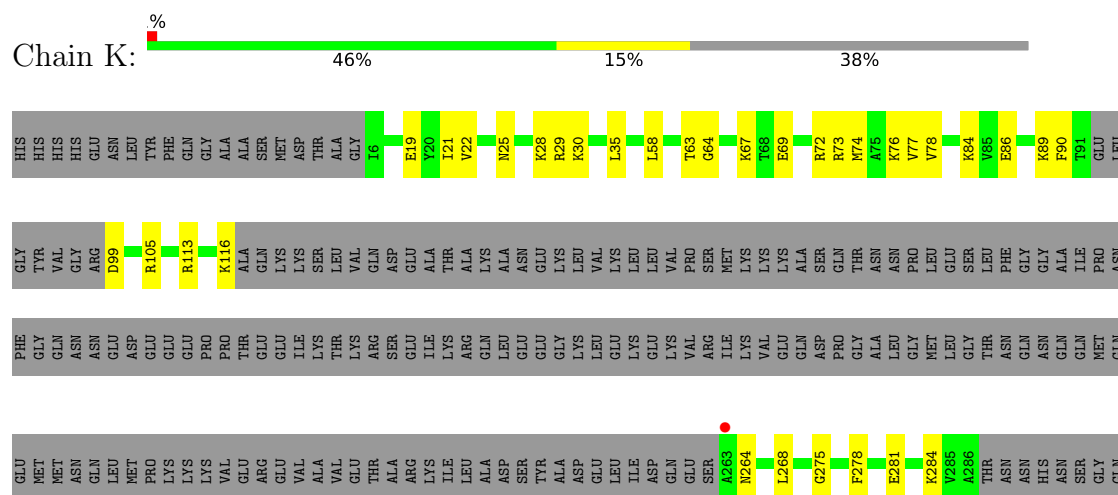


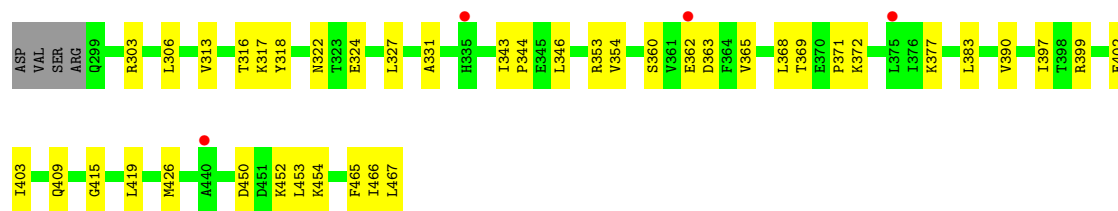


- Molecule 1: ATP-dependent protease ATPase subunit HslU

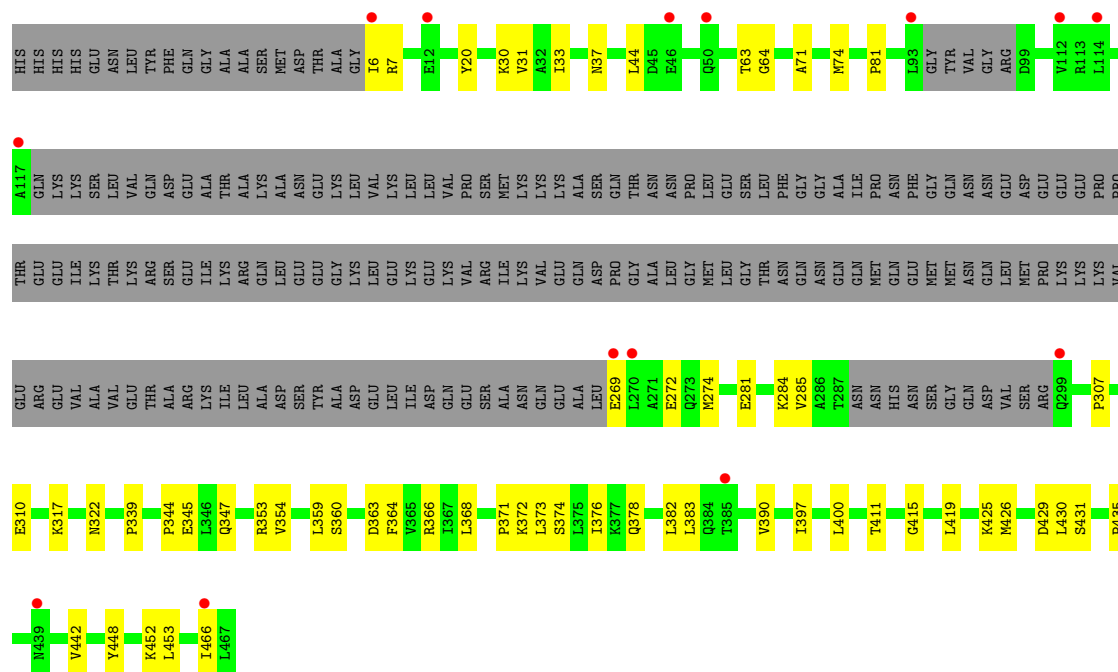


- Molecule 1: ATP-dependent protease ATPase subunit HslU





● Molecule 1: ATP-dependent protease ATPase subunit HslU



4 Data and refinement statistics

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) 90.5 (36.37-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 0.236 , 0.281	Depositor DCC
R_{free} test set	2010 reflections (0.86%)	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 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.10	0/2452	0.28	0/3307
1	B	0.10	0/2326	0.28	0/3138
1	C	0.10	0/2364	0.30	0/3186
1	D	0.11	0/2356	0.30	0/3179
1	E	0.11	0/2327	0.30	0/3138
1	F	0.10	0/2375	0.30	0/3203
1	G	0.11	0/2293	0.30	0/3094
1	H	0.10	0/2423	0.28	0/3267
1	I	0.10	0/2324	0.29	0/3136
1	J	0.10	0/2431	0.28	0/3277
1	K	0.10	0/2368	0.29	0/3197
1	L	0.10	0/2354	0.28	0/3177
1	M	0.10	0/2520	0.28	0/3399
1	N	0.10	0/2476	0.29	0/3338
1	O	0.11	0/2402	0.32	0/3239
1	P	0.11	0/2408	0.30	0/3248
1	Q	0.11	0/2411	0.30	0/3253
1	R	0.10	0/2621	0.29	0/3534
1	S	0.11	0/2458	0.31	0/3315
1	T	0.10	0/2622	0.28	0/3535
1	U	0.10	0/2633	0.29	0/3551
1	V	0.10	0/2402	0.29	0/3236
1	W	0.10	0/2574	0.29	0/3471
1	X	0.10	0/2519	0.29	0/3396
All	All	0.10	0/58439	0.29	0/78814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2425	0	2503	45	0
1	B	2299	0	2376	40	0
1	C	2337	0	2423	36	0
1	D	2329	0	2415	63	0
1	E	2300	0	2381	38	0
1	F	2348	0	2434	44	0
1	G	2266	0	2347	49	0
1	H	2396	0	2482	34	0
1	I	2297	0	2375	41	0
1	J	2404	0	2486	48	0
1	K	2341	0	2420	45	0
1	L	2327	0	2408	38	0
1	M	2493	0	2572	38	0
1	N	2449	0	2540	48	0
1	O	2375	0	2472	33	0
1	P	2381	0	2468	44	0
1	Q	2384	0	2459	51	0
1	R	2594	0	2687	40	0
1	S	2431	0	2511	52	0
1	T	2595	0	2697	51	0
1	U	2606	0	2685	41	0
1	V	2377	0	2451	36	0
1	W	2547	0	2633	42	0
1	X	2492	0	2568	46	0
All	All	57793	0	59793	938	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 8.

The worst 5 of 938 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
1:E:71:ALA:HA	1:E:74:MET:HE3	1.65	0.79
1:F:100:VAL:HG21	1:F:304:ASP:HB3	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	36	70
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%)	18	53
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
1	Q	295/481 (61%)	283 (96%)	12 (4%)	0	100	100
1	R	322/481 (67%)	313 (97%)	9 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	273 (100%)	0	100	100
1	B	258/421 (61%)	258 (100%)	0	100	100
1	C	262/421 (62%)	262 (100%)	0	100	100
1	D	261/421 (62%)	261 (100%)	0	100	100
1	E	258/421 (61%)	258 (100%)	0	100	100
1	F	263/421 (62%)	262 (100%)	1 (0%)	84	90
1	G	255/421 (61%)	255 (100%)	0	100	100
1	H	268/421 (64%)	268 (100%)	0	100	100
1	I	259/421 (62%)	259 (100%)	0	100	100
1	J	269/421 (64%)	269 (100%)	0	100	100
1	K	263/421 (62%)	263 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	262/421 (62%)	262 (100%)	0	100	100
1	M	279/421 (66%)	279 (100%)	0	100	100
1	N	274/421 (65%)	274 (100%)	0	100	100
1	O	267/421 (63%)	267 (100%)	0	100	100
1	P	267/421 (63%)	267 (100%)	0	100	100
1	Q	267/421 (63%)	267 (100%)	0	100	100
1	R	290/421 (69%)	290 (100%)	0	100	100
1	S	273/421 (65%)	273 (100%)	0	100	100
1	T	291/421 (69%)	291 (100%)	0	100	100
1	U	291/421 (69%)	291 (100%)	0	100	100
1	V	266/421 (63%)	266 (100%)	0	100	100
1	W	285/421 (68%)	285 (100%)	0	100	100
1	X	280/421 (66%)	280 (100%)	0	100	100
All	All	6481/10104 (64%)	6480 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	462	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	50	GLN
1	J	335	HIS
1	L	325	HIS
1	T	335	HIS
1	T	25	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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, 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%)	0.23	4 (1%) 75 53	34, 56, 81, 91	0
1	B	292/481 (60%)	0.15	4 (1%) 73 51	31, 53, 79, 94	0
1	C	296/481 (61%)	0.01	4 (1%) 73 51	25, 47, 76, 92	0
1	D	296/481 (61%)	0.12	6 (2%) 65 41	24, 48, 75, 90	0
1	E	292/481 (60%)	0.09	7 (2%) 59 36	25, 45, 65, 78	0
1	F	298/481 (61%)	0.12	5 (1%) 69 45	27, 54, 77, 89	0
1	G	287/481 (59%)	-0.00	5 (1%) 69 45	29, 46, 71, 94	0
1	H	304/481 (63%)	0.19	6 (1%) 65 41	28, 53, 74, 88	0
1	I	291/481 (60%)	0.23	5 (1%) 69 45	34, 57, 81, 103	0
1	J	305/481 (63%)	0.22	4 (1%) 75 53	33, 54, 82, 97	0
1	K	297/481 (61%)	0.22	5 (1%) 69 45	29, 57, 81, 92	0
1	L	295/481 (61%)	0.27	14 (4%) 36 19	29, 54, 80, 94	0
1	M	317/481 (65%)	0.03	5 (1%) 70 47	22, 48, 71, 80	0
1	N	311/481 (64%)	0.10	11 (3%) 47 27	24, 49, 72, 107	0
1	O	302/481 (62%)	-0.03	5 (1%) 69 45	19, 41, 65, 84	0
1	P	302/481 (62%)	-0.06	3 (0%) 79 59	18, 38, 68, 87	0
1	Q	303/481 (62%)	-0.05	4 (1%) 75 53	19, 40, 68, 94	0
1	R	330/481 (68%)	-0.07	2 (0%) 85 69	19, 45, 70, 86	0
1	S	309/481 (64%)	0.04	0 100 100	21, 43, 71, 88	0
1	T	330/481 (68%)	0.02	5 (1%) 72 49	25, 49, 74, 96	0
1	U	332/481 (69%)	0.03	5 (1%) 72 49	29, 46, 68, 88	0
1	V	301/481 (62%)	-0.01	4 (1%) 75 53	22, 44, 74, 103	0
1	W	323/481 (67%)	-0.05	3 (0%) 81 61	20, 40, 71, 90	0
1	X	316/481 (65%)	-0.06	3 (0%) 81 61	15, 42, 75, 94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	7336/11544 (63%)	0.07	119 (1%)	70 47	15, 48, 76, 107	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	94	GLY	4.4
1	D	460	LYS	4.4
1	C	412	ASP	4.3
1	N	263	ALA	3.9
1	H	263	ALA	3.8

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.