



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

PDB ID : 1G3I
Title : CRYSTAL STRUCTURE OF THE HSLUV PROTEASE-CHAPERONE COMPLEX
Authors : Sousa, M.C.; Trame, C.B.; Tsuruta, H.; Wilbanks, S.M.; Reddy, V.S.; McKay, D.B.
Deposited on : 2000-10-24
Resolution : 3.41 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

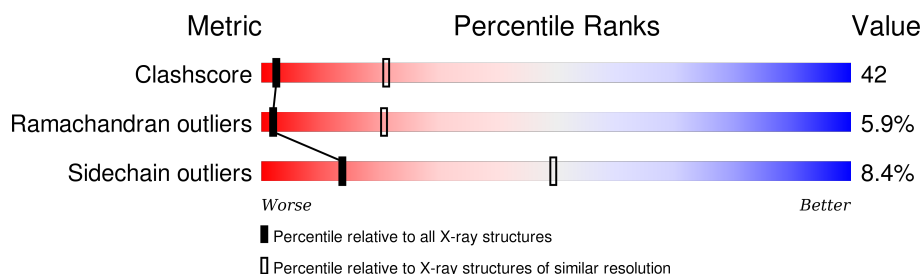
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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))
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	444	<div> <div>29%</div> <div>37%</div> <div>8%</div> <div>27%</div> </div>
1	B	444	<div> <div>27%</div> <div>39%</div> <div>7%</div> <div>27%</div> </div>
1	C	444	<div> <div>26%</div> <div>38%</div> <div>8%</div> <div>28%</div> </div>
1	D	444	<div> <div>26%</div> <div>38%</div> <div>7%</div> <div>28%</div> </div>
1	E	444	<div> <div>25%</div> <div>38%</div> <div>8%</div> <div>29%</div> </div>
1	F	444	<div> <div>25%</div> <div>39%</div> <div>8%</div> <div>28%</div> </div>
1	S	444	<div> <div>29%</div> <div>36%</div> <div>7%</div> <div>29%</div> </div>

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Mol	Chain	Length	Quality of chain
1	T	444	
1	U	444	
1	V	444	
1	W	444	
1	X	444	
2	G	174	
2	H	174	
2	I	174	
2	J	174	
2	K	174	
2	L	174	
2	M	174	
2	N	174	
2	O	174	
2	P	174	
2	Q	174	
2	R	174	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	E	454	-	-	X	-
3	ATP	S	456	-	-	X	-
3	ATP	U	458	-	-	X	-
3	ATP	X	461	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45528 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 HSLU PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2539	1588	454	487	10			
1	B	326	Total	C	N	O	S	0	0	0
			2539	1588	454	487	10			
1	C	319	Total	C	N	O	S	0	0	0
			2484	1554	446	474	10			
1	D	318	Total	C	N	O	S	0	0	0
			2476	1548	445	473	10			
1	E	317	Total	C	N	O	S	0	0	0
			2462	1540	443	469	10			
1	F	320	Total	C	N	O	S	0	0	0
			2495	1560	450	475	10			
1	S	317	Total	C	N	O	S	0	0	0
			2468	1543	444	471	10			
1	T	331	Total	C	N	O	S	0	0	0
			2570	1602	461	497	10			
1	U	322	Total	C	N	O	S	0	0	0
			2503	1562	449	482	10			
1	V	313	Total	C	N	O	S	0	0	0
			2432	1519	436	467	10			
1	W	312	Total	C	N	O	S	0	0	0
			2428	1516	437	465	10			
1	X	322	Total	C	N	O	S	0	0	0
			2500	1562	446	482	10			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

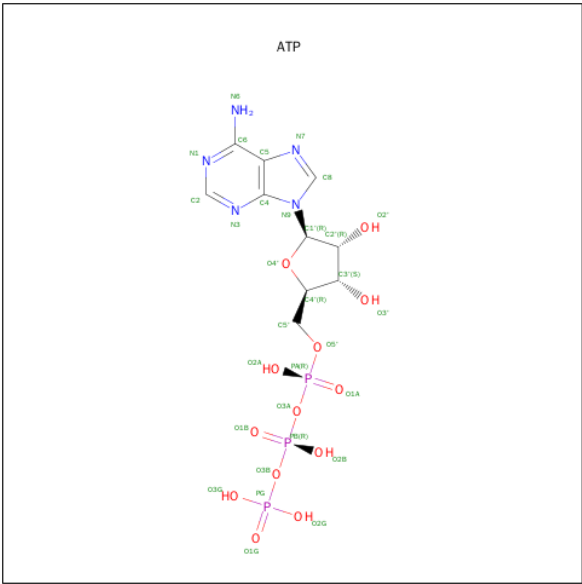
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	173	Total	C	N	O	S	0	0	0
			1280	803	227	246	4			
2	H	173	Total	C	N	O	S	0	0	0
			1280	802	227	247	4			

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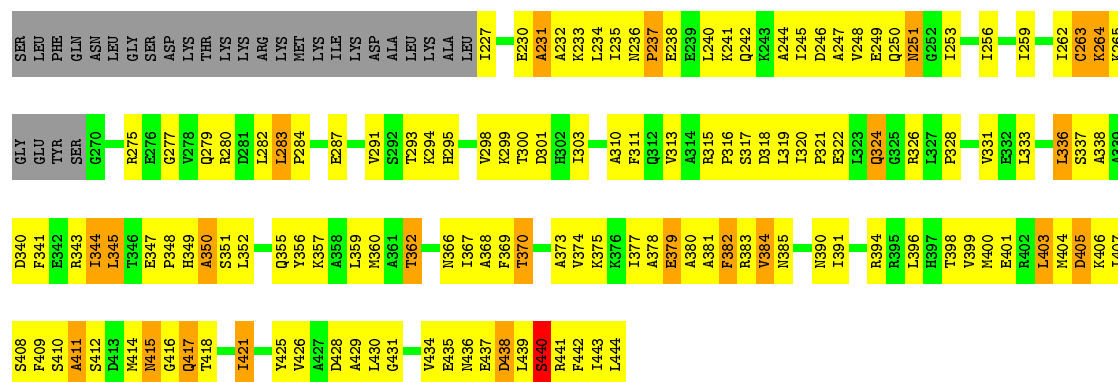
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	173	Total	C	N	O	S	0	0	0
			1292	810	229	249	4			
2	J	173	Total	C	N	O	S	0	0	0
			1280	802	227	247	4			
2	K	173	Total	C	N	O	S	0	0	0
			1280	802	227	247	4			
2	L	173	Total	C	N	O	S	0	0	0
			1294	810	231	249	4			
2	M	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	N	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	O	173	Total	C	N	O	S	0	0	0
			1257	789	225	240	3			
2	P	173	Total	C	N	O	S	0	0	0
			1257	789	225	240	3			
2	Q	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	R	173	Total	C	N	O	S	0	0	0
			1257	789	225	240	3			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



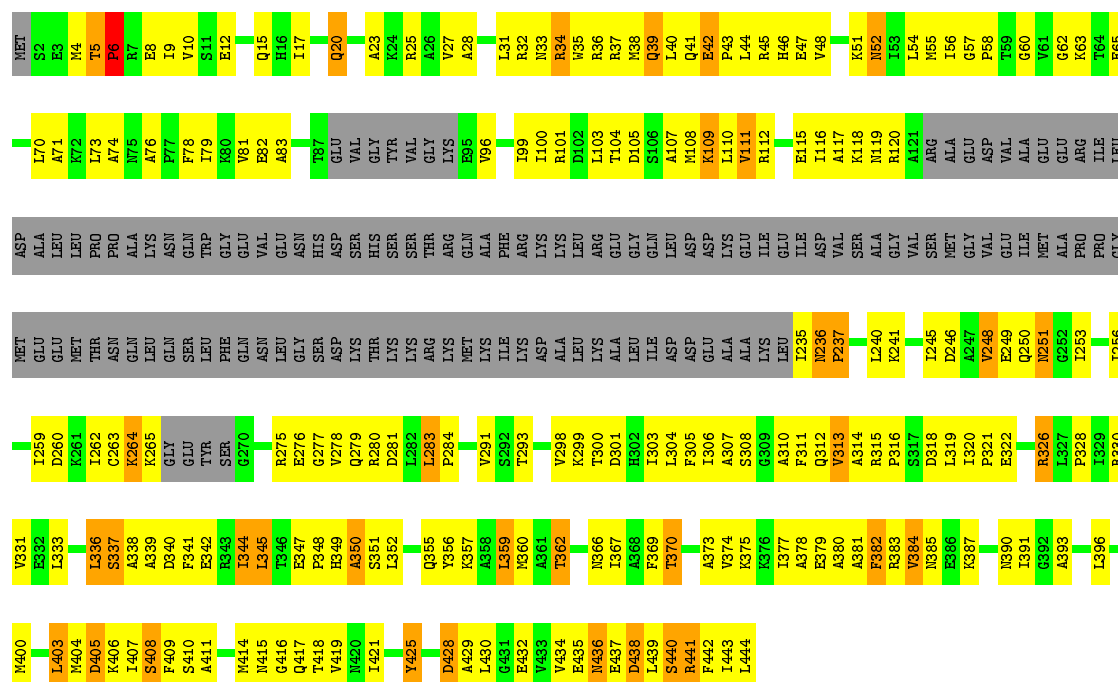
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	F	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	S	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	T	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	U	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	V	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	W	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	X	1	Total 31	C 10	N 5	O 13	P 3	0	0



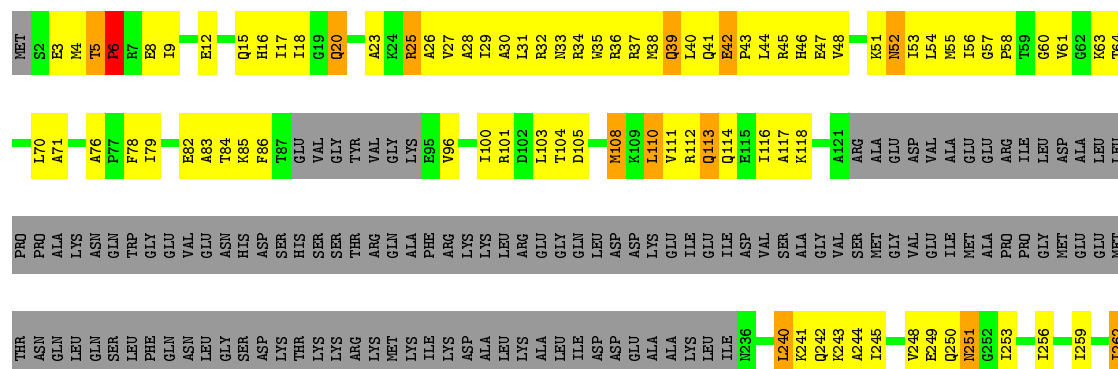
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

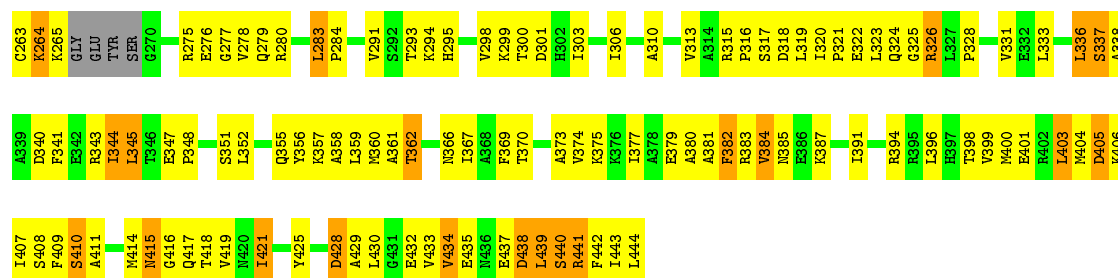
Chain C: 26% 38% 8% 28%



• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

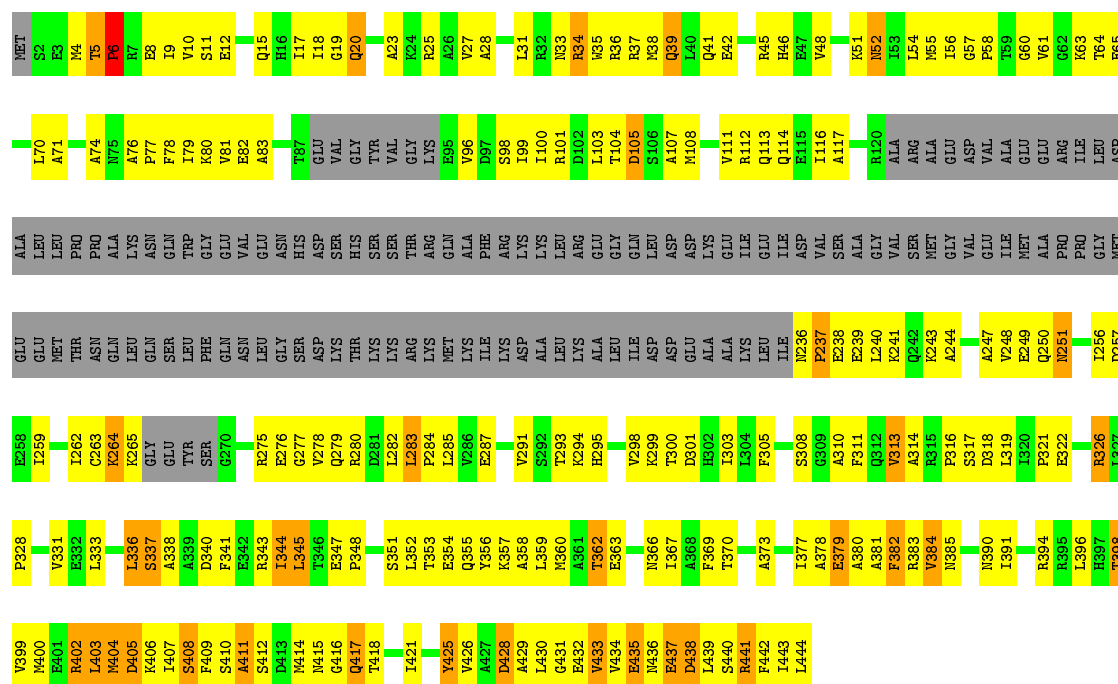
Chain D: 26% 38% 7% 28%





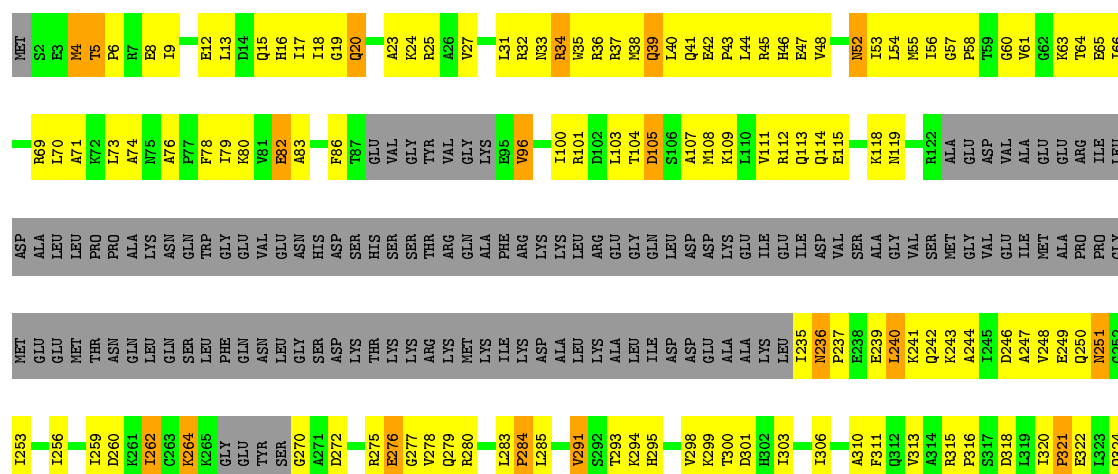
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

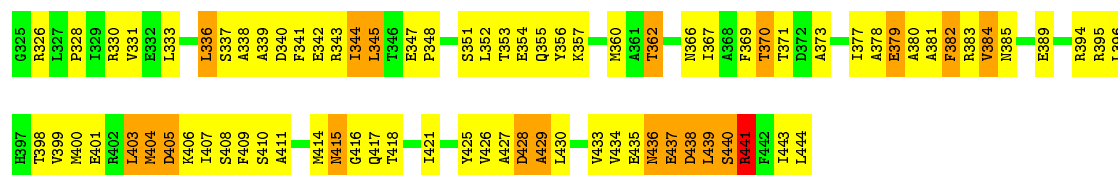
Chain E: 25% 38% 8% 29%



• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

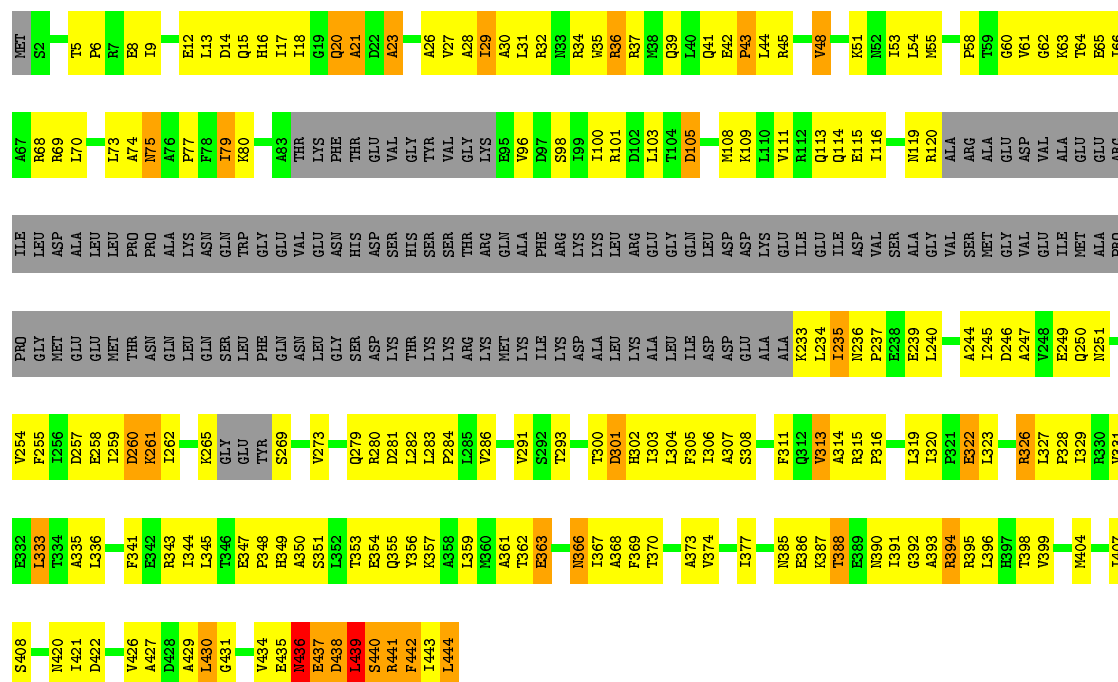
Chain F: 25% 39% 8% 28%





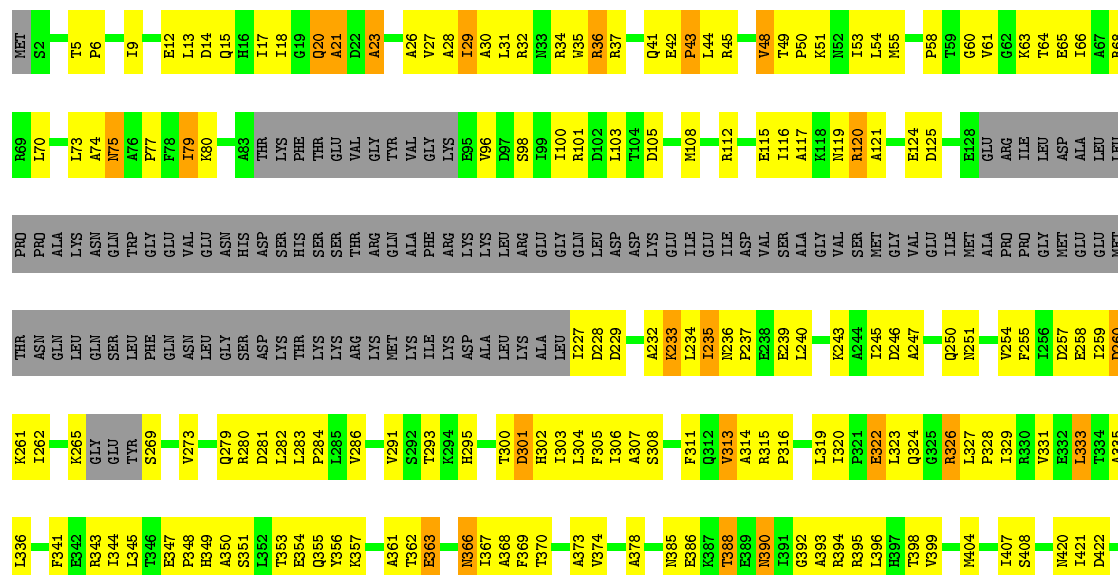
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

Chain S: 29% 36% 7% 29%



• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

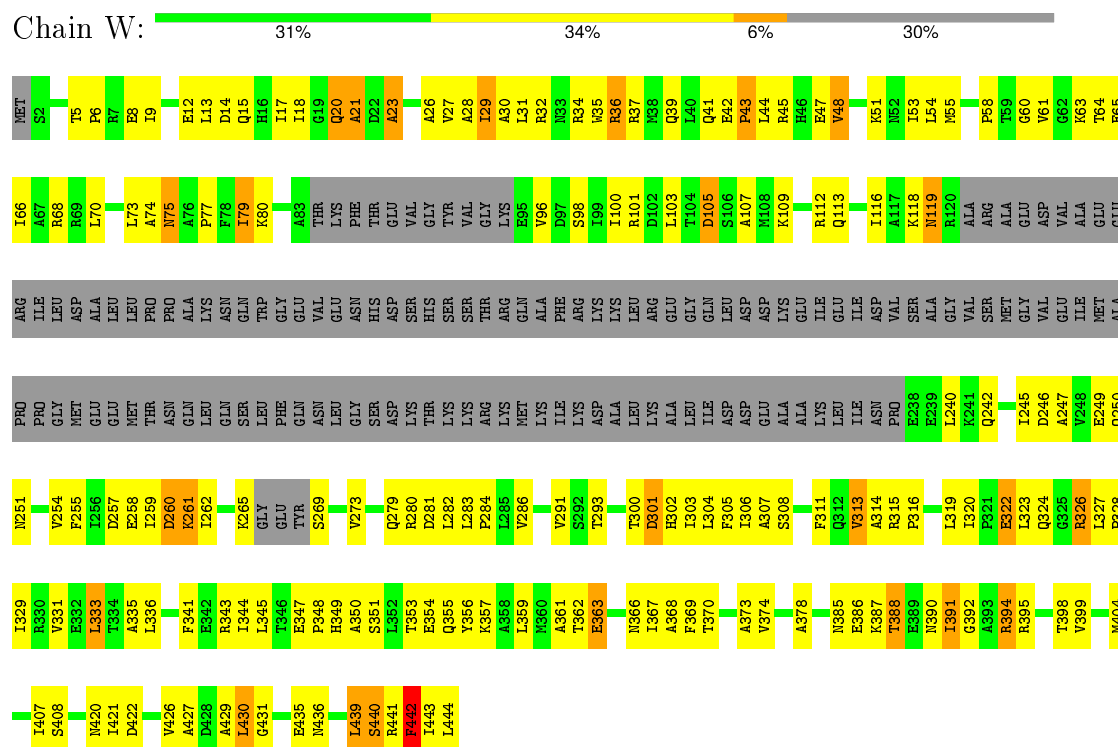
Chain T: 31% 37% 6% 25%



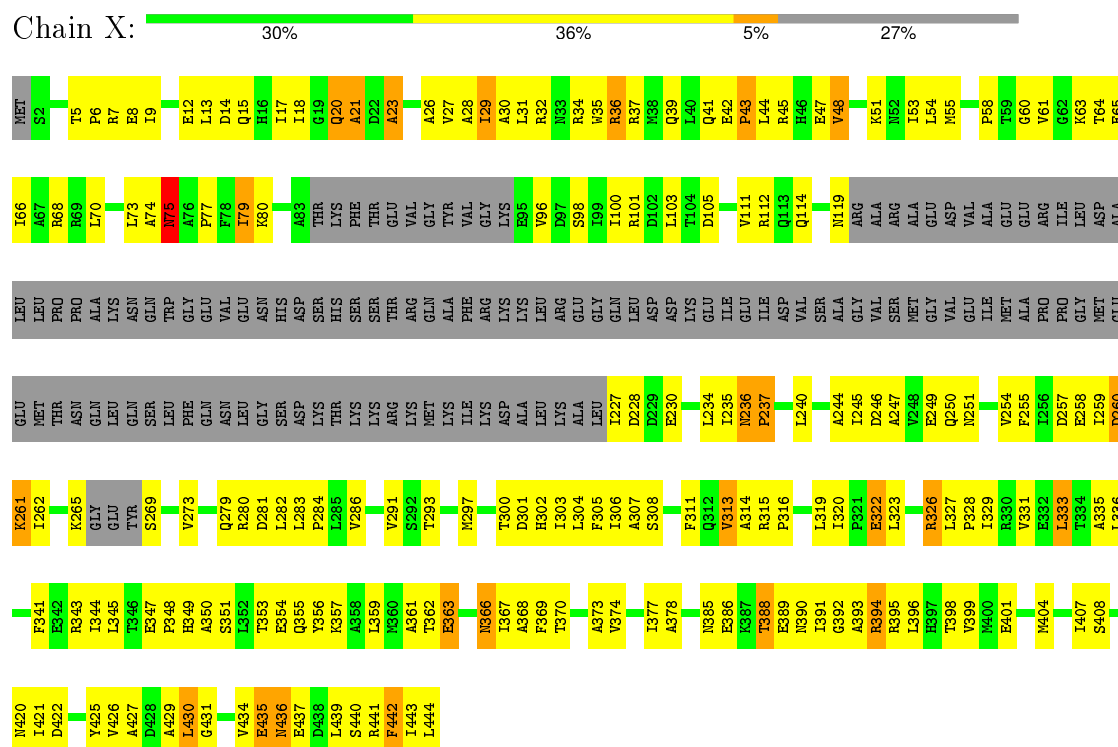
E432	E347	S269	GLN	ASN	A74	MET
E435	P348	V273	LEU	THR	N75	S2
N436	E349		LEU	GLN	A76	T5
E437	S351	Q279	PHE	GLY	P77	P6
D438	E352	A280	ASN	VAL	A78	
L439	T353	D281	LEU	ASN	I79	I9
S440	E354	D282	GLY	ASN	K80	
R441	Q355	D283	LEU	HIS	A83	E12
Y356	Q357	D284	ASP	ASP	L83	L13
K357		L285	LYS	THR	L84	D14
		V286	THR	GLN	L85	
A361			LYS	LYS	PHE	I17
T362	E363	V291	LYS	THR	LYS	I18
E368		S292	ARG	THR	GLU	G19
T370		T293	LYS	ARG	VAL	Q20
			LYS	GLN	GLY	A21
N366		N297	MET	ALA	THR	D22
T367			LYS	ALA	VAL	A23
A368		T300	ILE	PHE	GLY	
T370		D301	LYS	ARG	LYS	A26
		H302	ASP	LVS	E95	V27
A373		I303	ALA	LVS	N96	A28
Y374		L304	LEU	LEU	D97	I29
		F305	LYS	ARG	S98	A30
T377		A306	ALA	GLU	I99	L31
A378		A307	LEU	GLY	I100	R32
		S308	ILE	GLN	R101	N33
			D228	LEU	D102	R34
N385		F311	ASP	ASP	L103	S35
E386		Q312	A232	ASP	T104	R36
T387		R313	R233	LYS	D105	R37
N389		A314	L234	GLU		
I390		R315	I235	ILE	L110	Q41
T391		P316	N236	GLU	V111	E42
G392			P237	ILE	R112	P43
A393				ASP	Q113	L44
R394		L319	L240	VAL	Q114	R45
R395		I320	Q242	SER		
		E322	Q241	ALA	N119	V48
T398		L323	D246	VAL	R120	
V399		Q324	A247	SER	ALA	K51
E401		G325		MET	ARG	R52
		R326	Q250	GLY	GLU	L54
		L327	N251	VAL	ASP	M55
N404		P328	L254	GLU	VAL	
		I329	V255	ILE	ALA	
T407		R330	T255	MET	GLU	P58
S408		V331	I256	ALA	GLU	T59
		E332	D257	ARG	ARG	G60
N420		L333	E258	PRO	ILE	V61
T421		T334	I259	GLY	LEU	G62
D422		A335	D260	MET	ASP	K63
		L336	K261	GLU	ALA	T64
V426			I262	GLU	LEU	E65
A427		F341		MET	LEU	I66
D428		I344	K265	THR	PRO	A67
A429		L345	GLY	ASN	PRO	R68
L430		T446	THR	GLN	LYS	
C431			T272	LEU	ALA	T72

I421	E332	D257	PRO	ILE	A67	MET
D422	I333	E258	GLY	GLY	R68	S2
	T334	I259	MET	ASP	R69	
Y425	A335	D260	GLU	ALA	L70	T5
Y426	I336	K261	GLU	LEU		R6
A427		I262	MET	LEU	L73	R7
D428	F341		THR	PRO	A74	E8
A429		K265	ASN	ASN	N75	I9
L430	I344	GLY	GLN	ALA	A76	E12
G431	L345	GLU	LEU	LYS	P77	L13
E432	T346	TVR	GLN	ASN	F78	D14
V433	E347	S269	SER	GLN	I79	Q15
V434	F348		LEU	THR	R80	
A435	R349	V273	PHE	GLY		H16
N436	A350		GLN	GLU	A83	I17
A437	S351	Q279	ASN	VAL	THR	I18
D438	L352	R280	LEU	GLU	LYS	G19
L439	T353	D281	GLY	ASN	PHE	Q20
S440	E354	L282	SER	HIS	THR	A21
R441	Q355	L283	ASP	ASP	GLU	D22
F442	V356	P284	LYS	SER	VAL	A23
I443	K357	L285	THR	HIS	GLY	
L444		V286	LYS	SER	TVR	A26
	A361		LYS	SER	VAL	V27
	T362	V291	ARG	THR	GLY	A28
	E363	S292	LYS	ARG	LYS	I29
		T293	MET	GLN	E95	A30
	N366		LYS	ALA	V96	L31
	I367	M297	ILE	PHE	D97	R32
	A368		LYS	ARG	S98	R33
	F369	T300	ASP	LYS	I99	R34
	T370	D301	ALA	LYS	I100	M35
		H302	LEU	LEU	R101	R36
	A373	I303	LYS	ARG	D102	R37
	V374	L304	ALA	GLU	L103	M38
		F305	LEU	GLY	T104	Q39
		I306	ILE	GLN	D105	L40
	I377	A307	ASP	LEU	S106	Q41
	A378	S308	ASP	ASP	A107	E42
	N395		GLU	LYS	M108	P43
	E396	F311	ALA	LYS	K109	L44
	K397	Q312	ALA	GLU	L110	R45
	T398	V313	LYS	LEU	V111	
	E399	R314	LEU	GLU	R112	V48
	N390	P315	ILE	ILE		
	I391	R316	N236	ASP	E115	K51
	G392		P237	VAL		M52
	A395	L319	E238	SER	K118	I53
	R394	I320	E239	ALA	N119	L54
	R395	P321		GLY	ARG	M55
		E322	A244	VAL	ALA	
	L323	Q324	I245	ARG	S58	P58
	G325	I324		NET	ALA	T59
	R326	Q325	E249	GLY	GLU	G60
		L327	M251	VAL	ASP	V61
	P328	I329	V254	ILE	VAL	G62
	I329		V255	NET	ALA	K63
	R330		F256	GLU	GLU	T64
		N231	T258	ALA	GLU	E65
				TVR	V92	I66

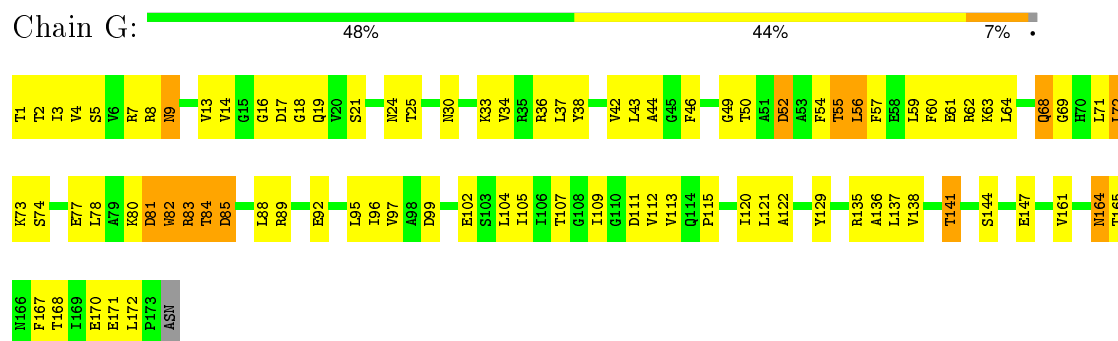
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



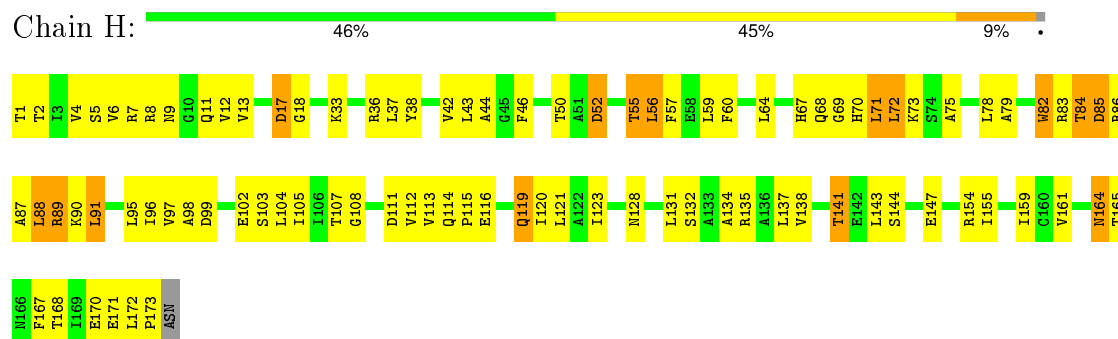
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



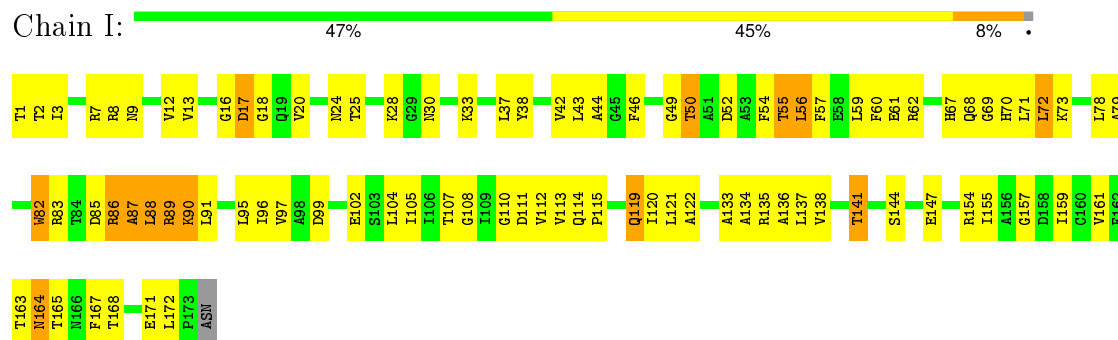
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV



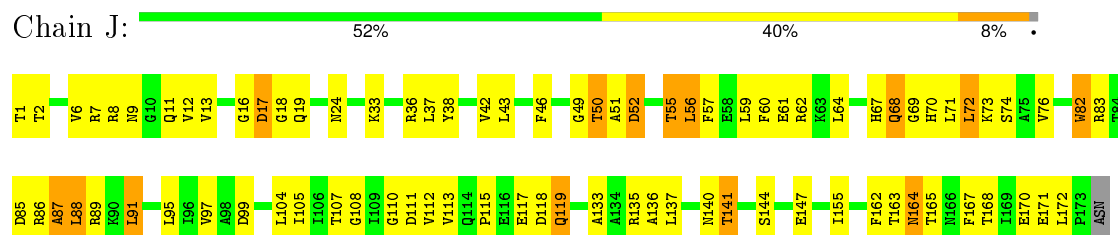
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



- Molecule 2: ATP-DEPENDENT PROTEASE HSLV

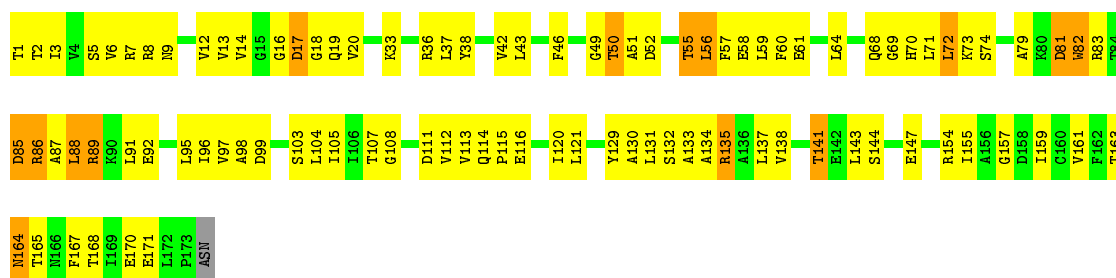


- Molecule 2: ATP-DEPENDENT PROTEASE HSLV



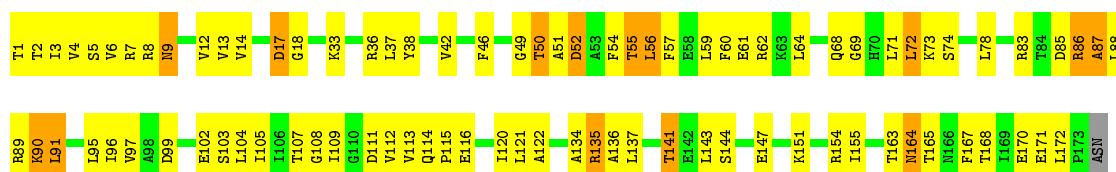
- Molecule 2: ATP-DEPENDENT PROTEASE HSLV





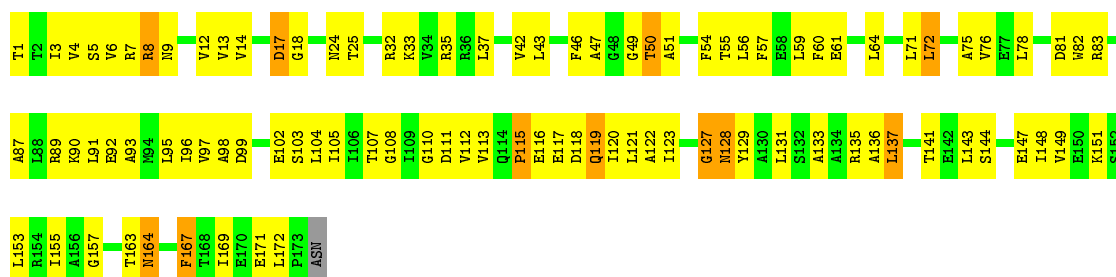
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain L: 49% 42% 8%



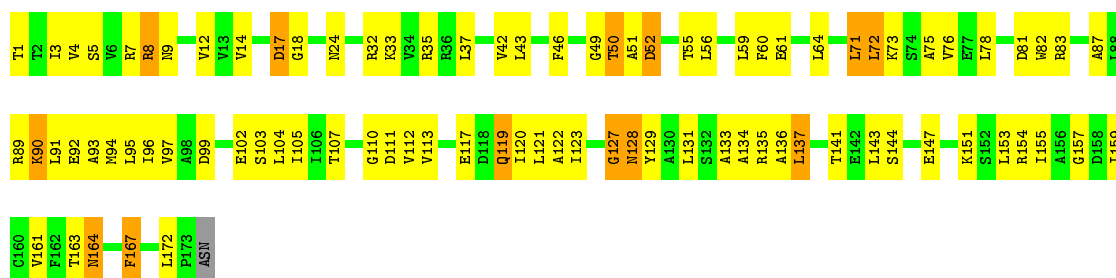
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M: 44% 49% 6%



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

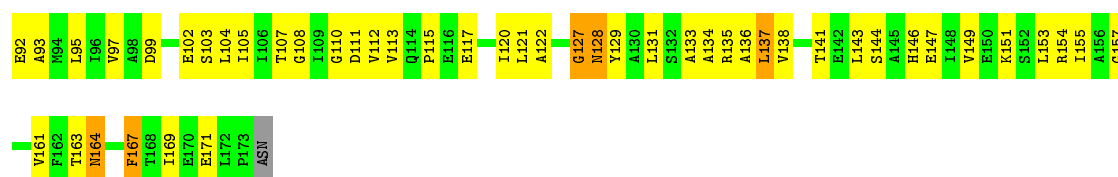
Chain N: 49% 43% 7%



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

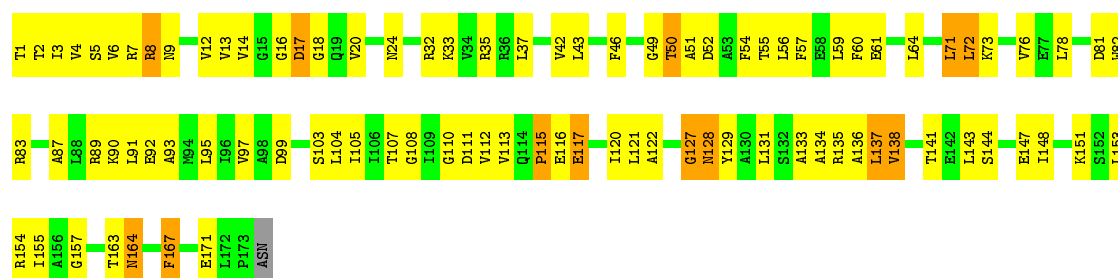
Chain O: 49% 45% 5%





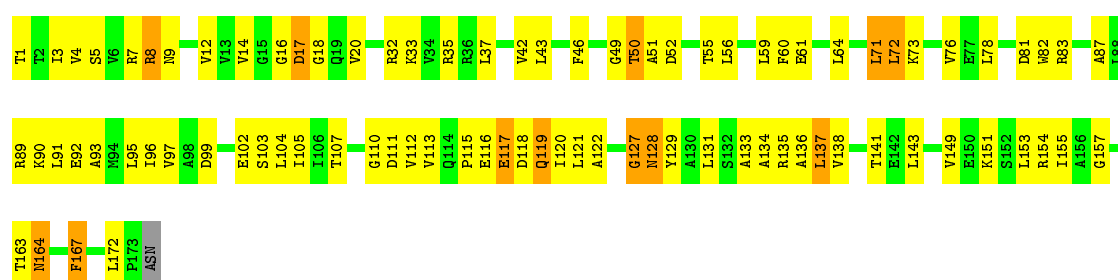
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain P: 47% 45% 7%



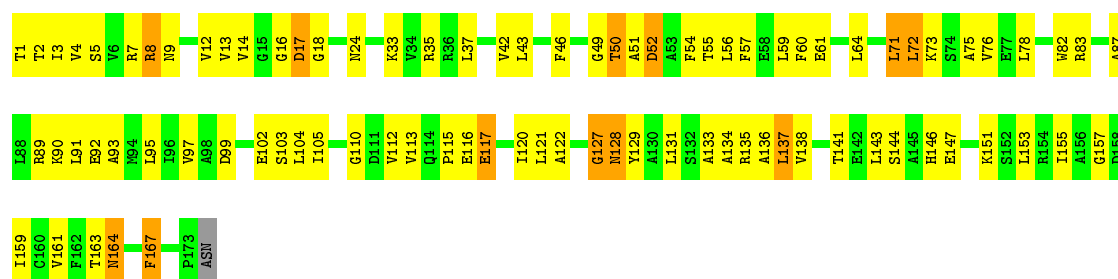
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain Q: 49% 43% 7%



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain R: 49% 43% 7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	209.22Å 220.58Å 241.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.08 – 3.41	Depositor
% Data completeness (in resolution range)	(Not available) (30.08-3.41)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	45528	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	0.65	1/2566 (0.0%)	0.81	0/3458
1	B	0.62	0/2566	0.81	2/3458 (0.1%)
1	C	0.55	0/2511	0.78	1/3384 (0.0%)
1	D	0.64	1/2503 (0.0%)	0.82	1/3373 (0.0%)
1	E	0.67	0/2489	0.83	2/3354 (0.1%)
1	F	0.64	0/2522	0.79	0/3398
1	S	0.31	0/2494	0.55	0/3360
1	T	0.31	0/2596	0.56	0/3499
1	U	0.30	0/2529	0.55	0/3408
1	V	0.30	0/2458	0.55	0/3313
1	W	0.30	0/2453	0.55	0/3304
1	X	0.31	0/2526	0.55	0/3405
2	G	0.55	0/1294	0.76	0/1753
2	H	0.55	0/1294	0.78	0/1754
2	I	0.50	0/1306	0.73	0/1767
2	J	0.50	0/1294	0.75	0/1754
2	K	0.52	0/1294	0.74	0/1754
2	L	0.55	0/1308	0.77	0/1770
2	M	0.41	0/1275	0.66	0/1732
2	N	0.39	0/1275	0.65	0/1732
2	O	0.35	0/1271	0.62	0/1727
2	P	0.37	0/1271	0.63	0/1727
2	Q	0.45	0/1275	0.65	0/1732
2	R	0.40	0/1271	0.63	0/1727
All	All	0.49	2/45641 (0.0%)	0.70	6/61643 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	CYS	CB-SG	-8.39	1.68	1.82
1	D	263	CYS	CB-SG	-5.66	1.72	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	283	LEU	CA-CB-CG	-7.04	99.10	115.30
1	C	283	LEU	CA-CB-CG	-6.71	99.88	115.30
1	E	431	GLY	N-CA-C	6.00	128.10	113.10
1	B	283	LEU	CA-CB-CG	-5.45	102.76	115.30
1	D	283	LEU	CA-CB-CG	-5.20	103.34	115.30

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	2539	0	2606	238	0
1	B	2539	0	2606	245	0
1	C	2484	0	2552	237	0
1	D	2476	0	2541	237	0
1	E	2462	0	2521	241	0
1	F	2495	0	2565	257	0
1	S	2468	0	2540	242	0
1	T	2570	0	2628	223	0
1	U	2503	0	2564	225	0
1	V	2432	0	2492	216	0
1	W	2428	0	2492	218	0
1	X	2500	0	2562	237	1
2	G	1280	0	1275	107	0
2	H	1280	0	1270	115	0
2	I	1292	0	1296	110	0
2	J	1280	0	1270	101	0
2	K	1280	0	1270	111	0
2	L	1294	0	1296	101	0
2	M	1261	0	1240	106	0
2	N	1261	0	1240	104	0
2	O	1257	0	1234	98	0
2	P	1257	0	1234	98	0
2	Q	1261	0	1240	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1257	0	1234	93	0
3	A	31	0	12	2	0
3	B	31	0	12	5	0
3	C	31	0	12	5	0
3	D	31	0	12	4	0
3	E	31	0	12	9	0
3	F	31	0	12	8	0
3	S	31	0	12	14	0
3	T	31	0	12	3	0
3	U	31	0	12	12	0
3	V	31	0	12	3	0
3	W	31	0	12	8	0
3	X	31	0	12	9	0
All	All	45528	0	45912	3804	1

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 42.

The worst 5 of 3804 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:F:264:LYS:NZ	1:F:279:GLN:HE22	1.38	1.21
2:Q:7:ARG:HD2	2:Q:119:GLN:OE1	1.44	1.17
1:E:264:LYS:NZ	1:E:279:GLN:HE22	1.42	1.15
2:N:7:ARG:HD2	2:N:119:GLN:HE21	1.09	1.15
1:A:264:LYS:NZ	1:A:279:GLN:HE22	1.45	1.12

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:7:ARG:NH2	1:X:7:ARG:NH2[2_765]	2.08	0.12

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	318/444 (72%)	244 (77%)	57 (18%)	17 (5%)	2	23
1	B	318/444 (72%)	241 (76%)	58 (18%)	19 (6%)	2	20
1	C	311/444 (70%)	234 (75%)	60 (19%)	17 (6%)	2	22
1	D	310/444 (70%)	235 (76%)	56 (18%)	19 (6%)	2	19
1	E	309/444 (70%)	238 (77%)	51 (16%)	20 (6%)	1	18
1	F	312/444 (70%)	240 (77%)	54 (17%)	18 (6%)	2	21
1	S	309/444 (70%)	227 (74%)	57 (18%)	25 (8%)	1	13
1	T	323/444 (73%)	236 (73%)	63 (20%)	24 (7%)	1	15
1	U	314/444 (71%)	237 (76%)	54 (17%)	23 (7%)	1	15
1	V	305/444 (69%)	228 (75%)	54 (18%)	23 (8%)	1	14
1	W	304/444 (68%)	223 (73%)	57 (19%)	24 (8%)	1	13
1	X	314/444 (71%)	235 (75%)	56 (18%)	23 (7%)	1	15
2	G	171/174 (98%)	141 (82%)	28 (16%)	2 (1%)	16	60
2	H	171/174 (98%)	139 (81%)	26 (15%)	6 (4%)	4	36
2	I	171/174 (98%)	136 (80%)	30 (18%)	5 (3%)	6	41
2	J	171/174 (98%)	136 (80%)	28 (16%)	7 (4%)	3	32
2	K	171/174 (98%)	138 (81%)	26 (15%)	7 (4%)	3	32
2	L	171/174 (98%)	137 (80%)	27 (16%)	7 (4%)	3	32
2	M	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	2	23
2	N	171/174 (98%)	129 (75%)	34 (20%)	8 (5%)	3	28
2	O	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	2	23
2	P	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	2	23
2	Q	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	2	23
2	R	171/174 (98%)	128 (75%)	33 (19%)	10 (6%)	2	21
All	All	5799/7416 (78%)	4418 (76%)	1041 (18%)	340 (6%)	2	21

5 of 340 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	235	ILE

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Mol	Chain	Res	Type
1	A	417	GLN
1	A	436	ASN
1	A	438	ASP

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	274/373 (74%)	244 (89%)	30 (11%)	8	36
1	B	274/373 (74%)	248 (90%)	26 (10%)	11	43
1	C	268/373 (72%)	231 (86%)	37 (14%)	4	24
1	D	267/373 (72%)	237 (89%)	30 (11%)	7	33
1	E	264/373 (71%)	232 (88%)	32 (12%)	6	29
1	F	269/373 (72%)	242 (90%)	27 (10%)	9	40
1	S	267/373 (72%)	246 (92%)	21 (8%)	15	52
1	T	276/373 (74%)	258 (94%)	18 (6%)	21	62
1	U	270/373 (72%)	250 (93%)	20 (7%)	17	56
1	V	263/373 (70%)	246 (94%)	17 (6%)	21	62
1	W	262/373 (70%)	246 (94%)	16 (6%)	23	63
1	X	270/373 (72%)	252 (93%)	18 (7%)	20	61
2	G	130/140 (93%)	115 (88%)	15 (12%)	7	32
2	H	130/140 (93%)	115 (88%)	15 (12%)	7	32
2	I	133/140 (95%)	119 (90%)	14 (10%)	8	38
2	J	130/140 (93%)	118 (91%)	12 (9%)	11	44
2	K	130/140 (93%)	118 (91%)	12 (9%)	11	44
2	L	133/140 (95%)	123 (92%)	10 (8%)	17	55
2	M	125/140 (89%)	121 (97%)	4 (3%)	46	80
2	N	125/140 (89%)	119 (95%)	6 (5%)	31	71
2	O	124/140 (89%)	120 (97%)	4 (3%)	46	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	124/140 (89%)	119 (96%)	5 (4%)	38	75
2	Q	125/140 (89%)	121 (97%)	4 (3%)	46	80
2	R	124/140 (89%)	119 (96%)	5 (4%)	38	75
All	All	4757/6156 (77%)	4359 (92%)	398 (8%)	14	49

5 of 398 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	437	GLU
2	I	135	ARG
1	W	246	ASP
2	G	68	GLN
2	H	82	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	24	ASN
2	M	164	ASN
1	W	385	ASN
2	H	164	ASN
2	J	164	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	450	-	24,33,33	0.78	0	31,52,52	1.11	2 (6%)
3	ATP	B	451	-	24,33,33	0.72	0	31,52,52	1.25	4 (12%)
3	ATP	C	452	-	24,33,33	0.69	0	31,52,52	1.54	5 (16%)
3	ATP	D	453	-	24,33,33	0.67	0	31,52,52	1.36	4 (12%)
3	ATP	E	454	-	24,33,33	0.78	0	31,52,52	1.37	3 (9%)
3	ATP	F	455	-	24,33,33	0.76	0	31,52,52	1.15	2 (6%)
3	ATP	S	456	-	24,33,33	0.58	0	31,52,52	0.90	1 (3%)
3	ATP	T	457	-	24,33,33	0.63	0	31,52,52	0.88	1 (3%)
3	ATP	U	458	-	24,33,33	0.57	0	31,52,52	0.89	1 (3%)
3	ATP	V	459	-	24,33,33	0.58	0	31,52,52	0.86	1 (3%)
3	ATP	W	460	-	24,33,33	0.62	0	31,52,52	0.91	1 (3%)
3	ATP	X	461	-	24,33,33	0.59	0	31,52,52	0.88	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	450	-	-	0/18/38/38	0/3/3/3
3	ATP	B	451	-	-	0/18/38/38	0/3/3/3
3	ATP	C	452	-	-	0/18/38/38	0/3/3/3
3	ATP	D	453	-	-	0/18/38/38	0/3/3/3
3	ATP	E	454	-	-	0/18/38/38	0/3/3/3
3	ATP	F	455	-	-	0/18/38/38	0/3/3/3
3	ATP	S	456	-	-	0/18/38/38	0/3/3/3
3	ATP	T	457	-	-	0/18/38/38	0/3/3/3
3	ATP	U	458	-	-	0/18/38/38	0/3/3/3
3	ATP	V	459	-	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	W	460	-	-	0/18/38/38	0/3/3/3
3	ATP	X	461	-	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	454	ATP	C2'-C1'-N9	-4.74	107.05	114.29
3	C	452	ATP	PA-O3A-PB	-4.28	120.71	132.73
3	D	453	ATP	C2'-C1'-N9	-3.32	109.23	114.29
3	C	452	ATP	C2'-C1'-N9	-2.86	109.92	114.29
3	F	455	ATP	C2'-C1'-N9	-2.56	110.38	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	ATP	2	0
3	B	451	ATP	5	0
3	C	452	ATP	5	0
3	D	453	ATP	4	0
3	E	454	ATP	9	0
3	F	455	ATP	8	0
3	S	456	ATP	14	0
3	T	457	ATP	3	0
3	U	458	ATP	12	0
3	V	459	ATP	3	0
3	W	460	ATP	8	0
3	X	461	ATP	9	0

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.