



wwPDB EM Map/Model Validation Report ⓘ

Jun 20, 2016 – 02:59 PM EDT

PDB ID : 3JCK
EMDB ID: : EMD-6479
Title : Structure of the yeast 26S proteasome lid sub-complex
Authors : Herzik Jr., M.A.; Dambacher, C.M.; Worden, E.J.; Martin, A.; Lander, G.C.
Deposited on : 2015-12-20
Resolution : 3.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
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) : rb-20027790

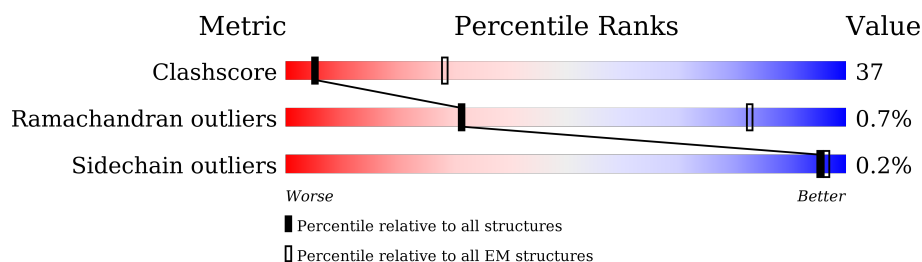
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.




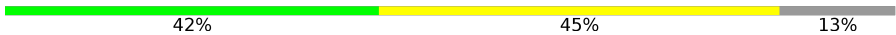
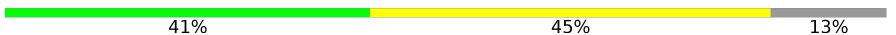



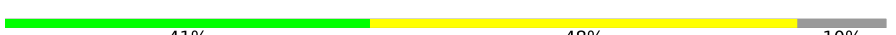
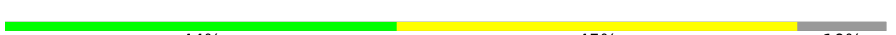



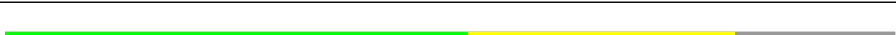

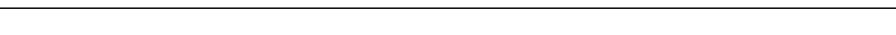
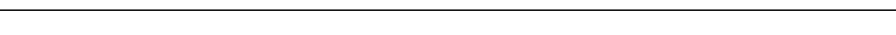
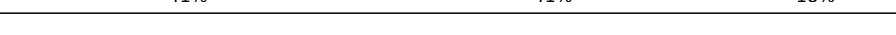

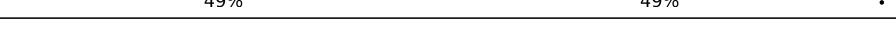







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1-A	438	
1	2-A	438	
1	3-A	438	
1	4-A	438	
1	5-A	438	
2	1-B	445	
2	2-B	445	
2	3-B	445	
2	4-B	445	




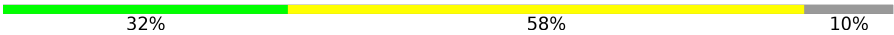
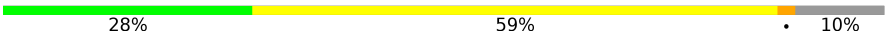
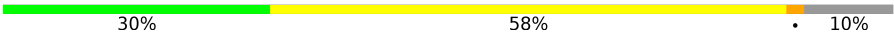
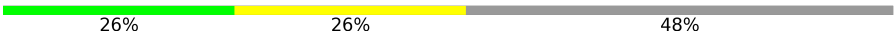

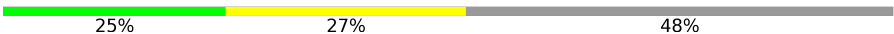


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Mol	Chain	Length	Quality of chain
2	5-B	445	
3	1-C	434	
3	2-C	434	
3	3-C	434	
3	4-C	434	
3	5-C	434	
4	1-D	429	
4	2-D	429	
4	3-D	429	
4	4-D	429	
4	5-D	429	
5	1-E	338	
5	2-E	338	
5	3-E	338	
5	4-E	338	
5	5-E	338	
6	1-F	393	
6	2-F	393	
6	3-F	393	
6	4-F	393	
6	5-F	393	
7	1-G	306	
7	2-G	306	
7	3-G	306	
7	4-G	306	

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Mol	Chain	Length	Quality of chain
7	5-G	306	
8	1-H	274	
8	2-H	274	
8	3-H	274	
8	4-H	274	
8	5-H	274	
9	1-I	89	
9	2-I	89	
9	3-I	89	
9	4-I	89	
9	5-I	89	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 112285 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	397	Total	C	N	O	S	0	0
			3116	1991	528	583	14		
1	2-A	397	Total	C	N	O	S	0	0
			3116	1991	528	583	14		
1	3-A	397	Total	C	N	O	S	0	0
			3116	1991	528	583	14		
1	4-A	397	Total	C	N	O	S	0	0
			3116	1991	528	583	14		
1	5-A	397	Total	C	N	O	S	0	0
			3116	1991	528	583	14		

- Molecule 2 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-B	404	Total	C	N	O	S	0	0
			3323	2118	556	640	9		
2	2-B	404	Total	C	N	O	S	0	0
			3323	2118	556	640	9		
2	3-B	404	Total	C	N	O	S	0	0
			3323	2118	556	640	9		
2	4-B	404	Total	C	N	O	S	0	0
			3323	2118	556	640	9		
2	5-B	404	Total	C	N	O	S	0	0
			3323	2118	556	640	9		

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-C	378	Total	C	N	O	S	0	0
			3060	1959	499	587	15		
3	2-C	378	Total	C	N	O	S	0	0
			3060	1959	499	587	15		
3	3-C	378	Total	C	N	O	S	0	0
			3060	1959	499	587	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	4-C	378	Total	C	N	O	S	0	0
			3060	1959	499	587	15		
3	5-C	378	Total	C	N	O	S	0	0
			3060	1959	499	587	15		

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-D	384	Total	C	N	O	S	0	0
			3084	1975	503	596	10		
4	2-D	384	Total	C	N	O	S	0	0
			3084	1975	503	596	10		
4	3-D	384	Total	C	N	O	S	0	0
			3084	1975	503	596	10		
4	4-D	384	Total	C	N	O	S	0	0
			3084	1975	503	596	10		
4	5-D	384	Total	C	N	O	S	0	0
			3084	1975	503	596	10		

- Molecule 5 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1-E	277	Total	C	N	O	S	0	0
			2224	1414	382	422	6		
5	2-E	277	Total	C	N	O	S	0	0
			2224	1414	382	422	6		
5	3-E	277	Total	C	N	O	S	0	0
			2224	1414	382	422	6		
5	4-E	277	Total	C	N	O	S	0	0
			2224	1414	382	422	6		
5	5-E	277	Total	C	N	O	S	0	0
			2224	1414	382	422	6		

- Molecule 6 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1-F	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		
6	2-F	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		
6	3-F	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	4-F	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		
6	5-F	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

- Molecule 7 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1-G	257	Total	C	N	O	S	0	0
			2036	1285	344	393	14		
7	2-G	257	Total	C	N	O	S	0	0
			2036	1285	344	393	14		
7	3-G	257	Total	C	N	O	S	0	0
			2036	1285	344	393	14		
7	4-G	257	Total	C	N	O	S	0	0
			2036	1285	344	393	14		
7	5-G	257	Total	C	N	O	S	0	0
			2036	1285	344	393	14		

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1-H	246	Total	C	N	O	S	0	0
			2021	1305	321	391	4		
8	2-H	246	Total	C	N	O	S	0	0
			2021	1305	321	391	4		
8	3-H	246	Total	C	N	O	S	0	0
			2021	1305	321	391	4		
8	4-H	246	Total	C	N	O	S	0	0
			2021	1305	321	391	4		
8	5-H	246	Total	C	N	O	S	0	0
			2021	1305	321	391	4		

- Molecule 9 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	1-I	46	Total	C	N	O	0	0
			405	251	62	92		
9	2-I	46	Total	C	N	O	0	0
			405	251	62	92		
9	3-I	46	Total	C	N	O	0	0
			405	251	62	92		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	4-I	46	Total	C	N	O	0	0
			405	251	62	92		
9	5-I	46	Total	C	N	O	0	0
			405	251	62	92		

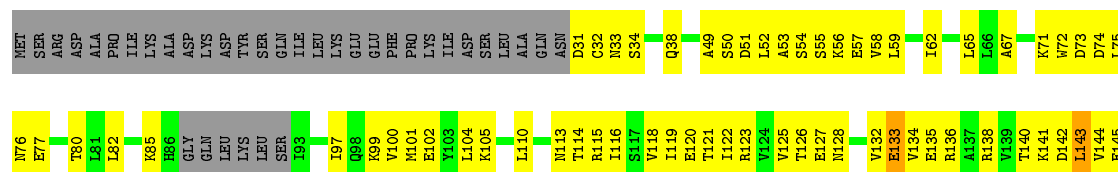
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

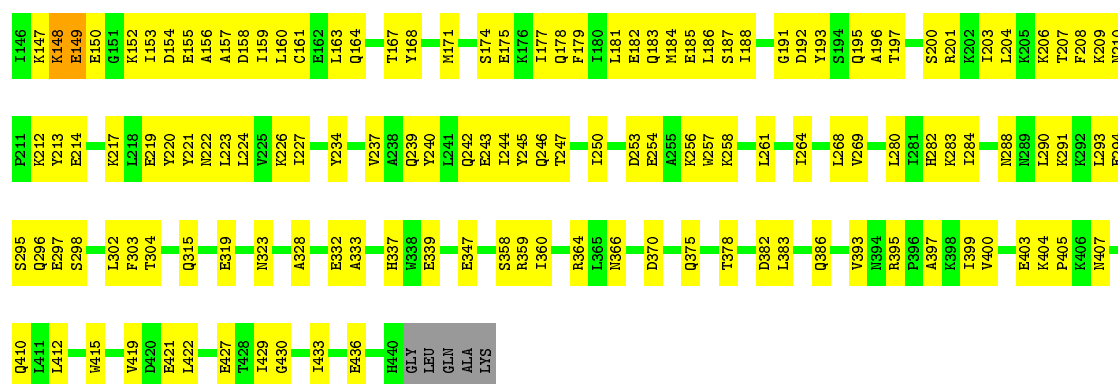
Mol	Chain	Residues	Atoms		AltConf
10	4-G	1	Total	Zn	0
			1	1	
10	1-G	1	Total	Zn	0
			1	1	
10	3-G	1	Total	Zn	0
			1	1	
10	5-G	1	Total	Zn	0
			1	1	
10	2-G	1	Total	Zn	0
			1	1	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	1-B	1	Total	O	0
			1	1	
11	2-B	1	Total	O	0
			1	1	
11	3-B	1	Total	O	0
			1	1	
11	4-B	1	Total	O	0
			1	1	
11	5-B	1	Total	O	0
			1	1	

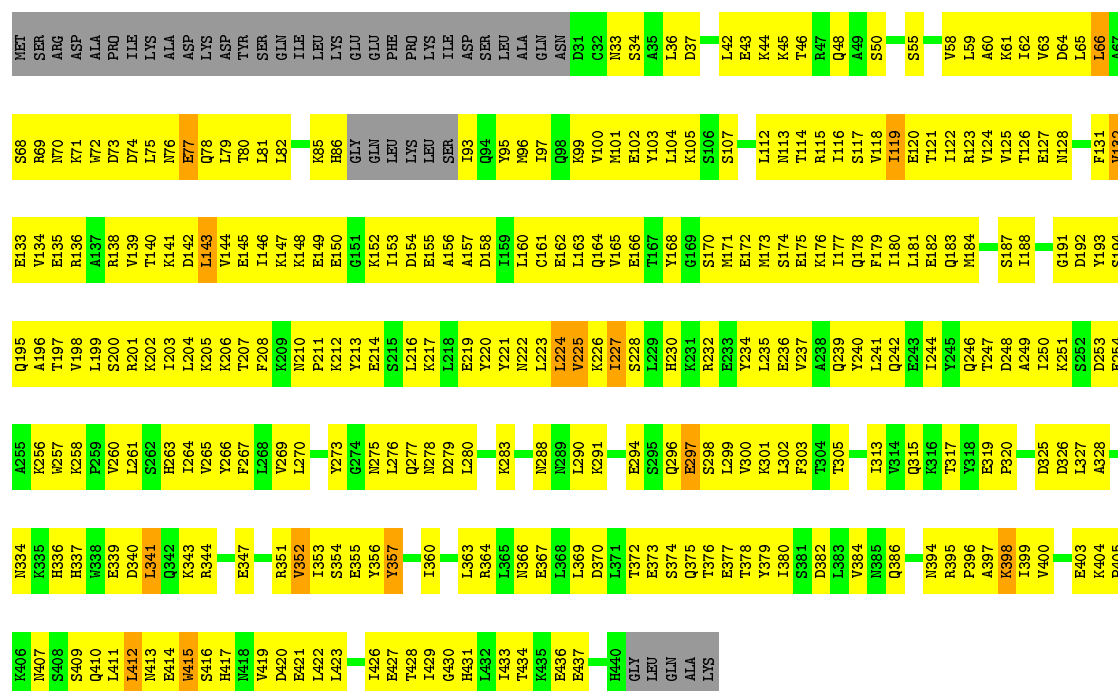




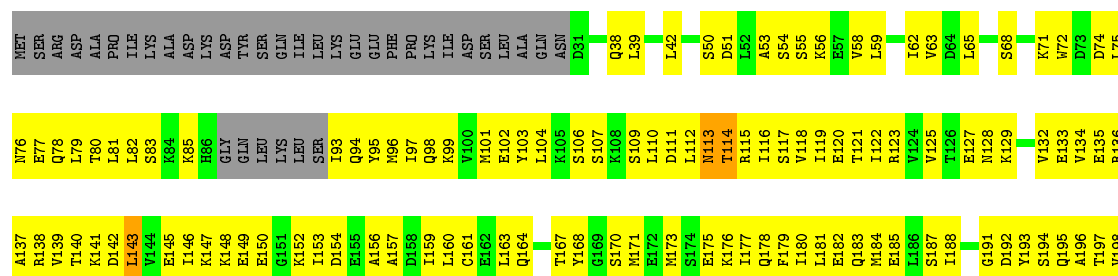
• Molecule 2: 26S proteasome regulatory subunit RPN5

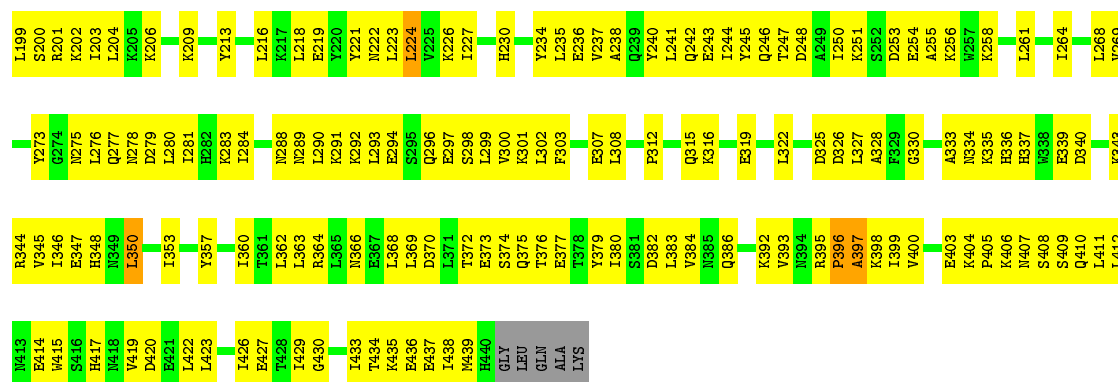
Chain 3-B: 27% 60% 9%



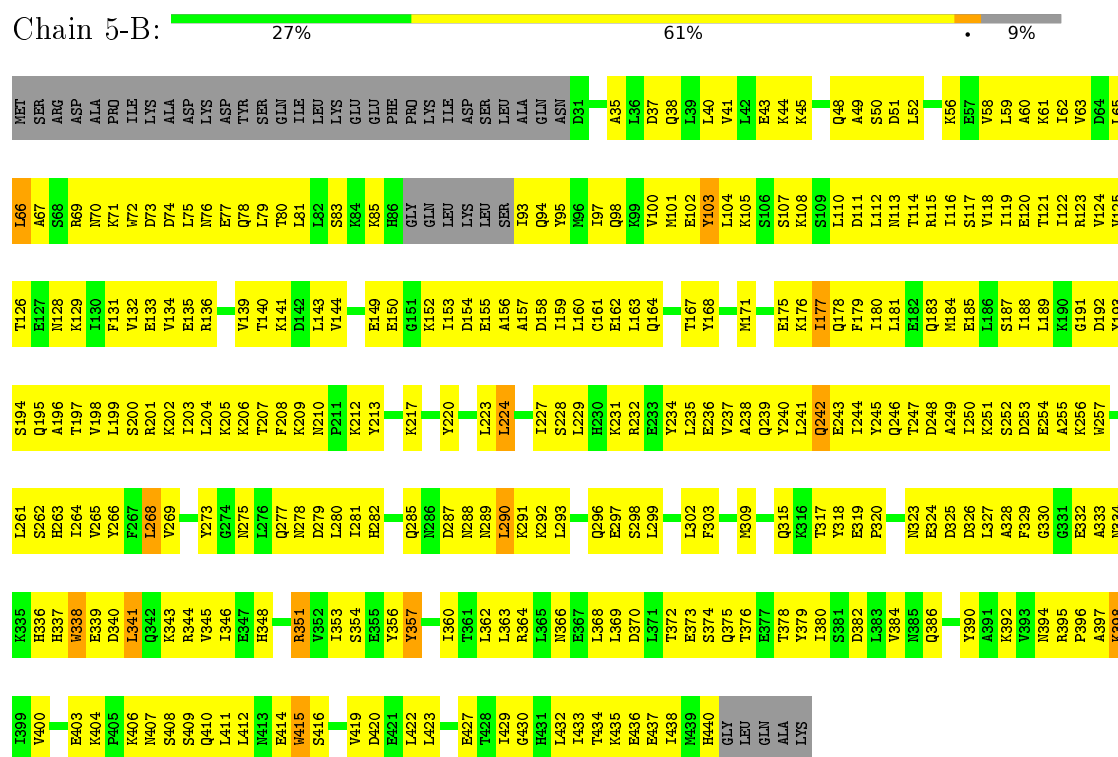
• Molecule 2: 26S proteasome regulatory subunit RPN5

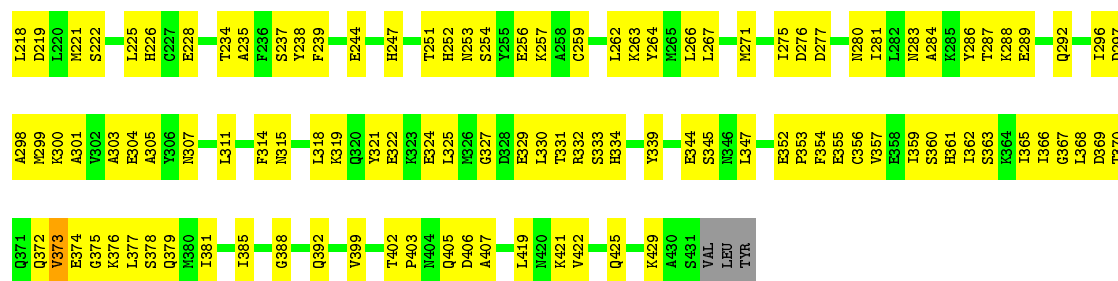
Chain 4-B: 31% 58% 9%





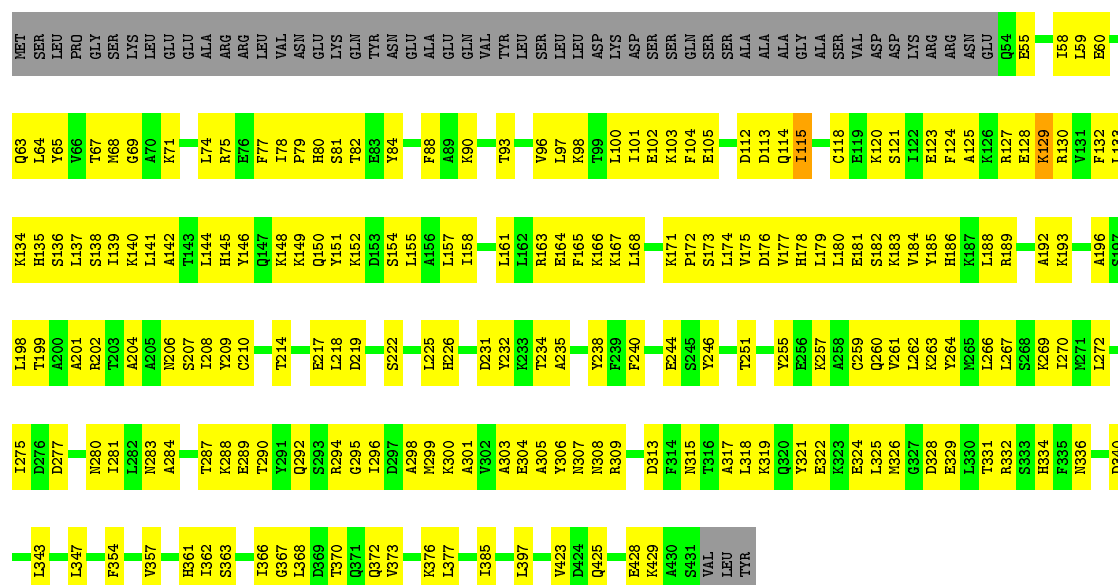
• Molecule 2: 26S proteasome regulatory subunit RPN5





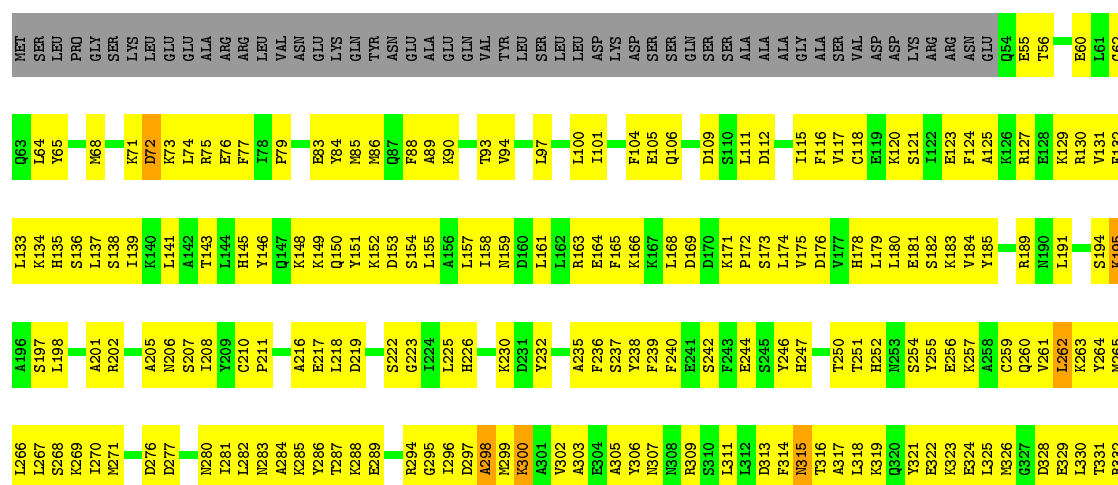
• Molecule 3: 26S proteasome regulatory subunit RPN6

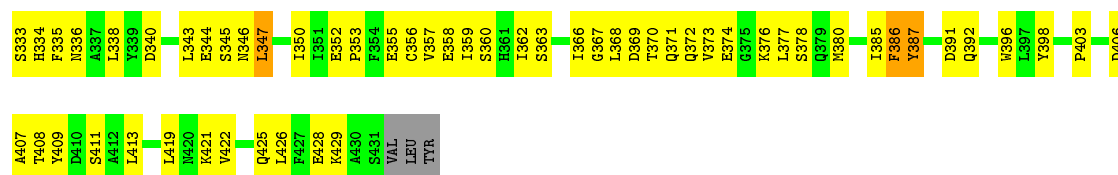
Chain 2-C: 41% 45% 13%



• Molecule 3: 26S proteasome regulatory subunit RPN6

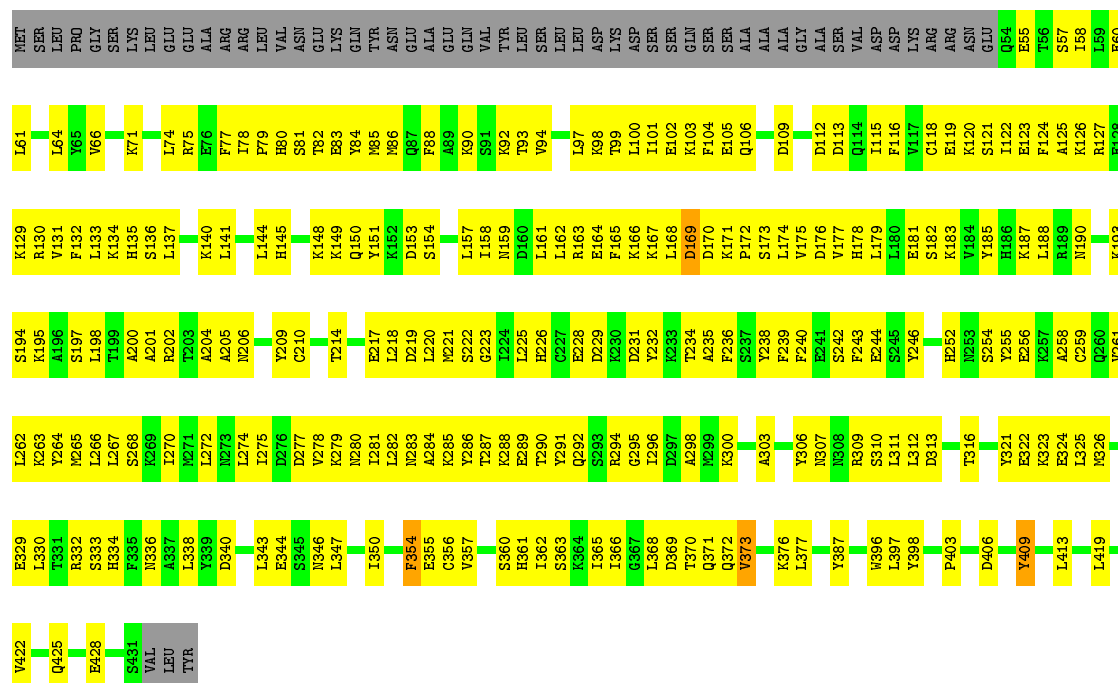
Chain 3-C: 31% 54% 13%





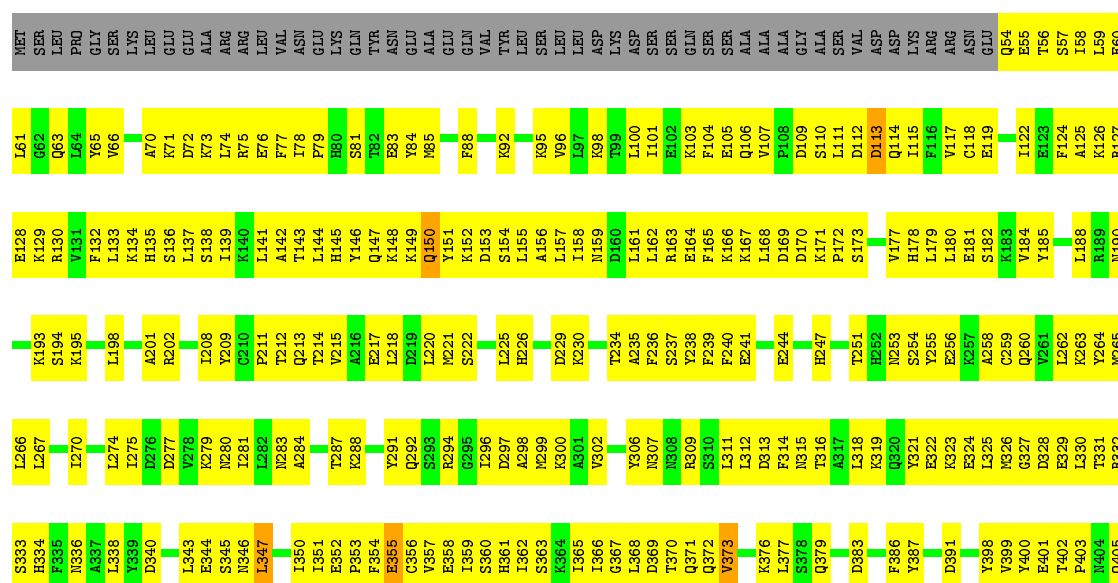
• Molecule 3: 26S proteasome regulatory subunit RPN6

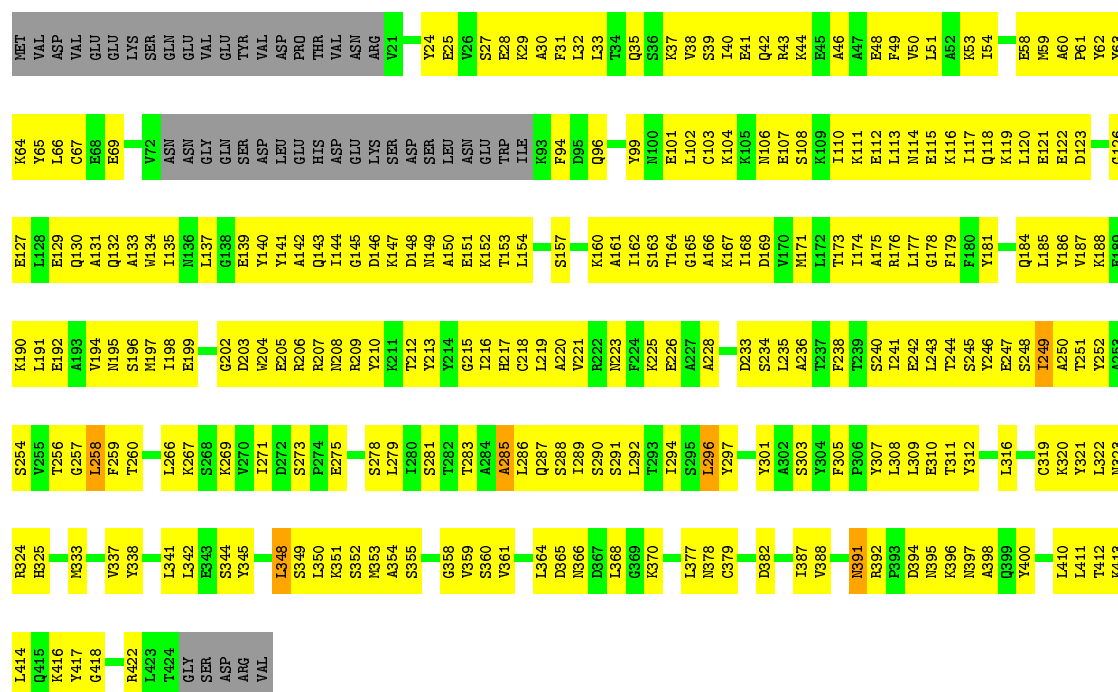
Chain 4-C: 34% 53% 13%



• Molecule 3: 26S proteasome regulatory subunit RPN6

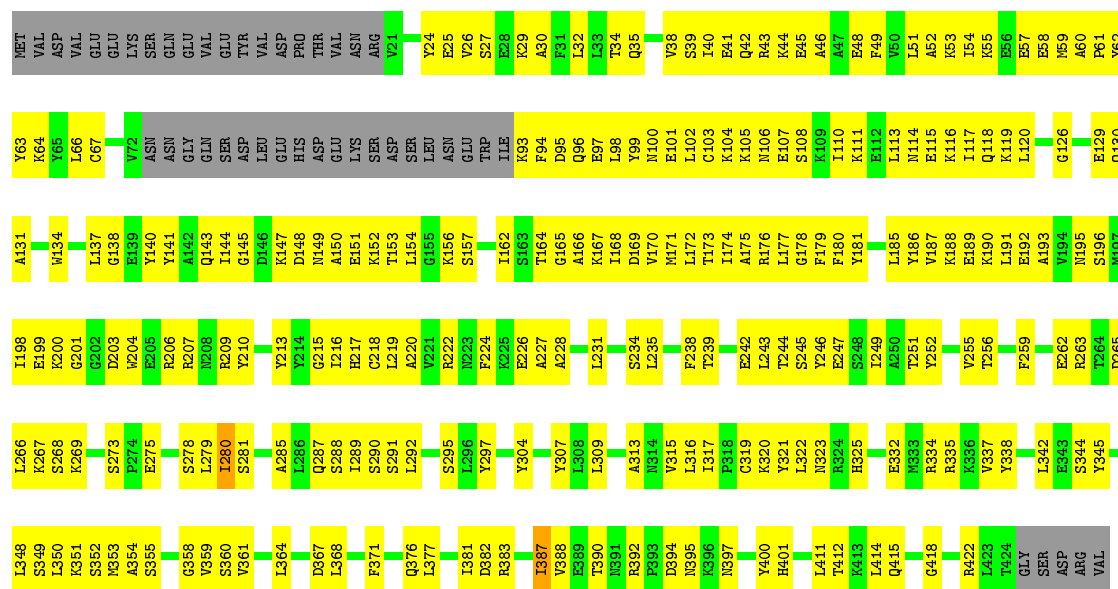
Chain 5-C: 29% 57% 13%





• Molecule 4: 26S proteasome regulatory subunit RPN7

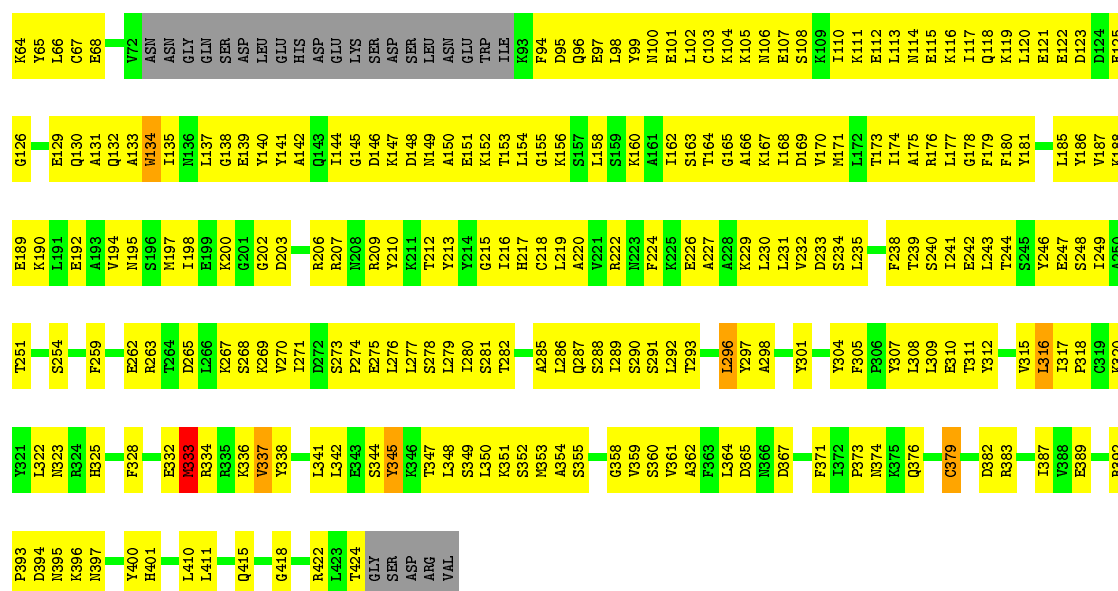
Chain 4-D: 36% 53% 10%



• Molecule 4: 26S proteasome regulatory subunit RPN7

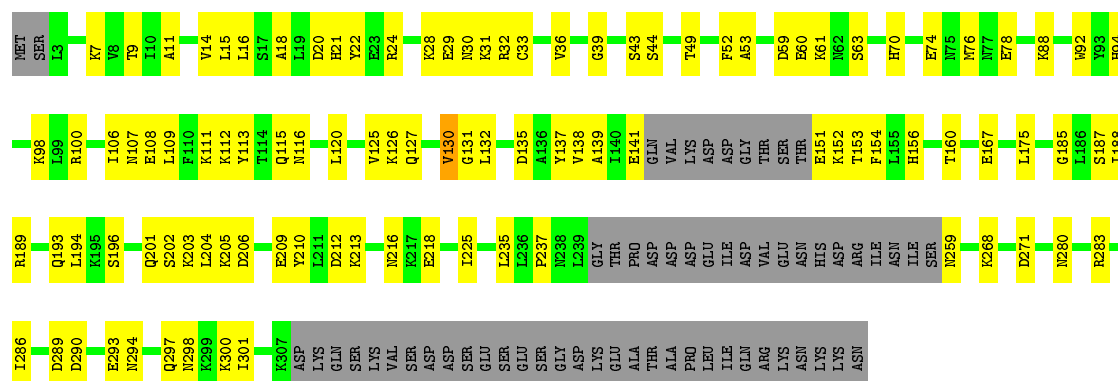
Chain 5-D: 28% 60% 10%





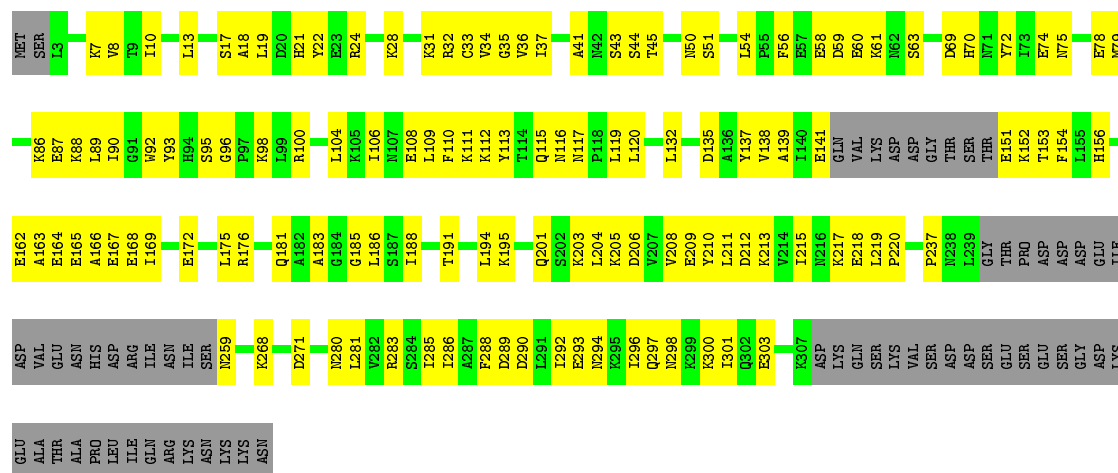
• Molecule 5: 26S proteasome regulatory subunit RPN8

Chain 1-E: 52% 30% 18%

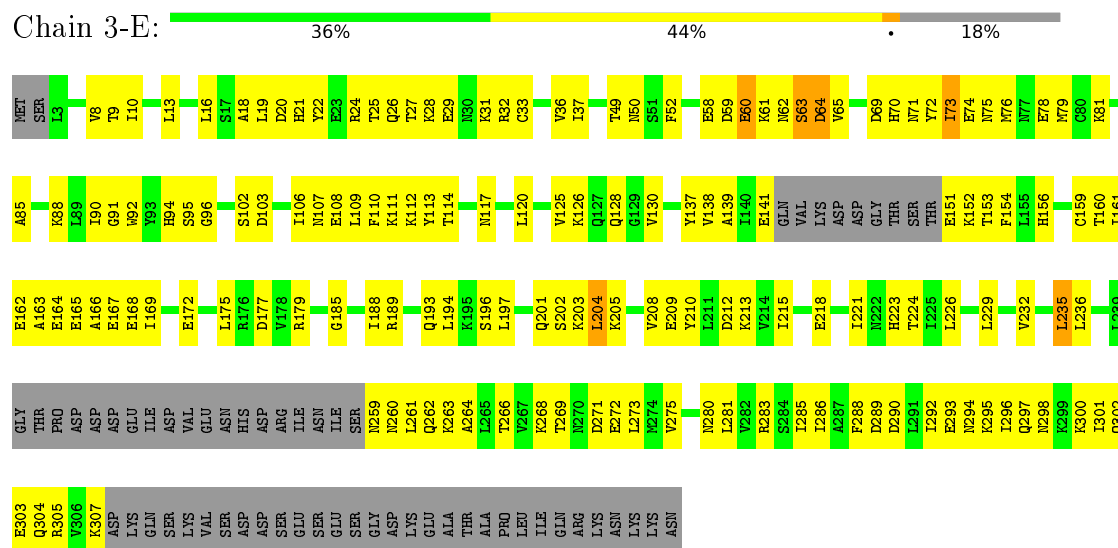


• Molecule 5: 26S proteasome regulatory subunit RPN8

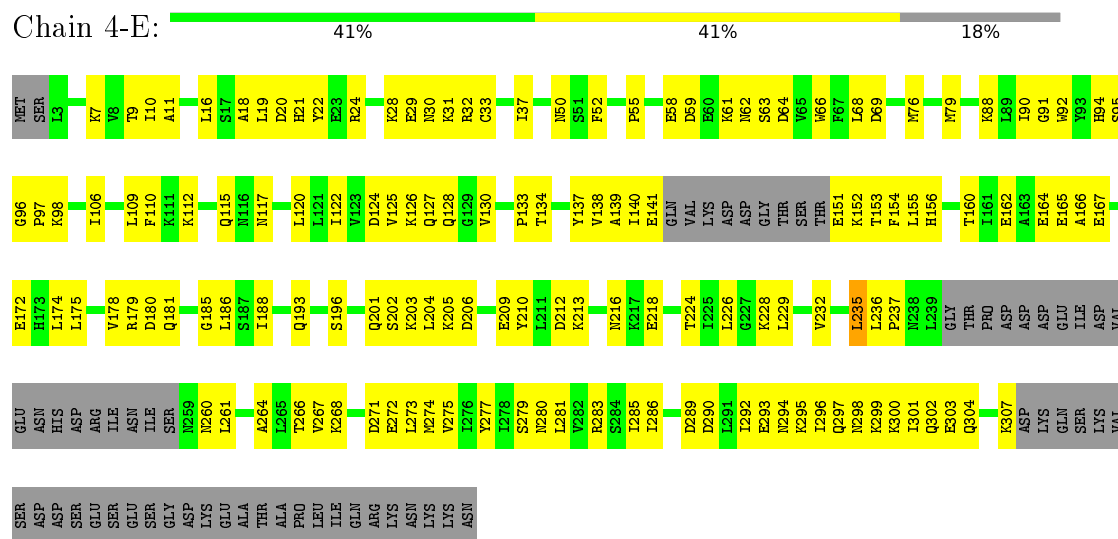
Chain 2-E: 44% 38% 18%



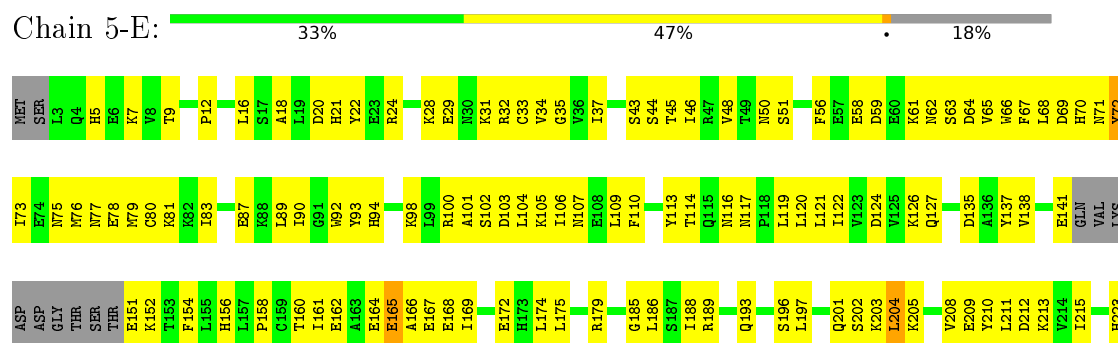
- Molecule 5: 26S proteasome regulatory subunit RPN8

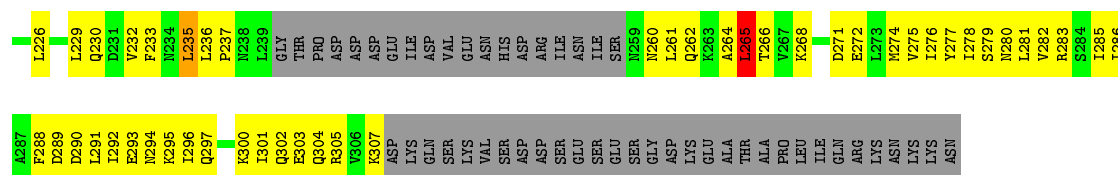


- Molecule 5: 26S proteasome regulatory subunit RPN8



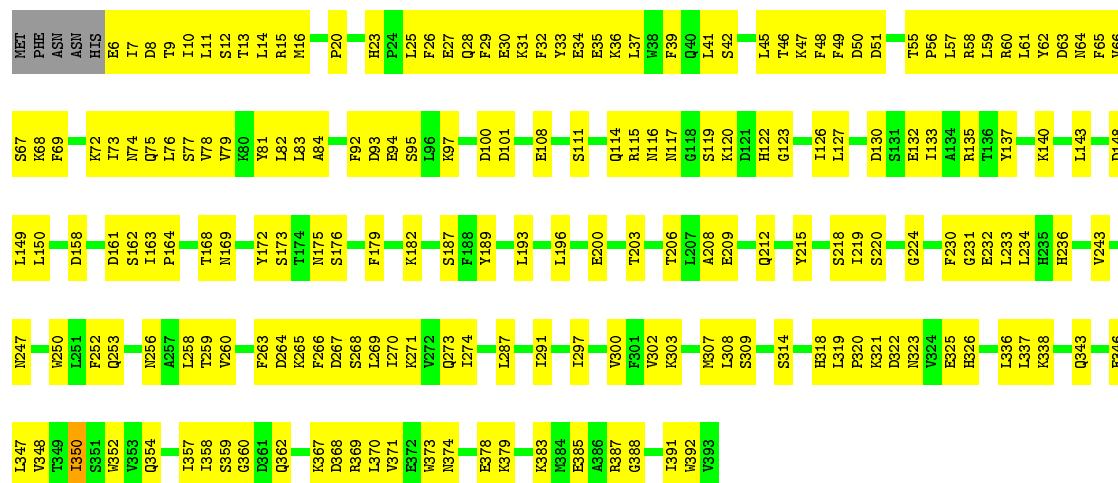
- Molecule 5: 26S proteasome regulatory subunit RPN8





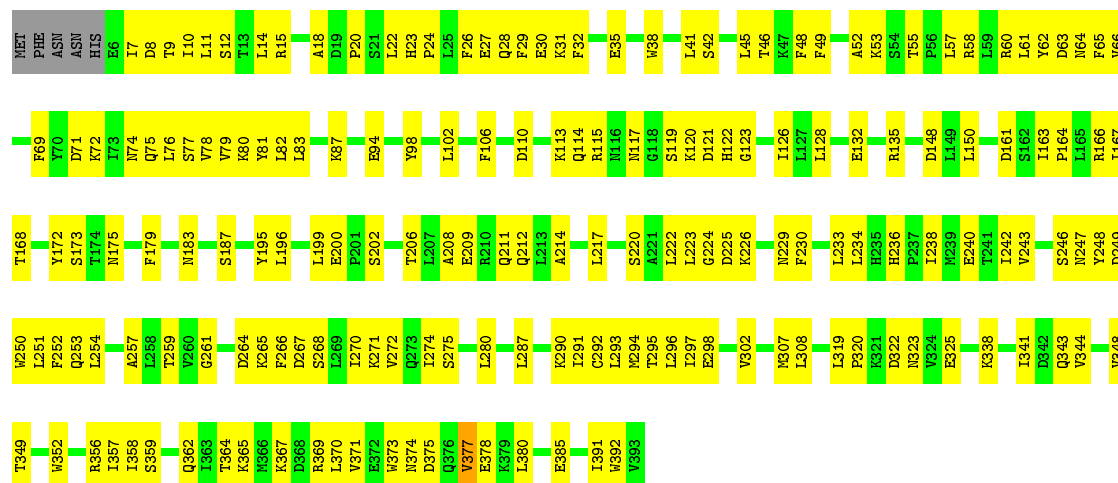
• Molecule 6: 26S proteasome regulatory subunit RPN9

Chain 1-F: 49% 49%



• Molecule 6: 26S proteasome regulatory subunit RPN9

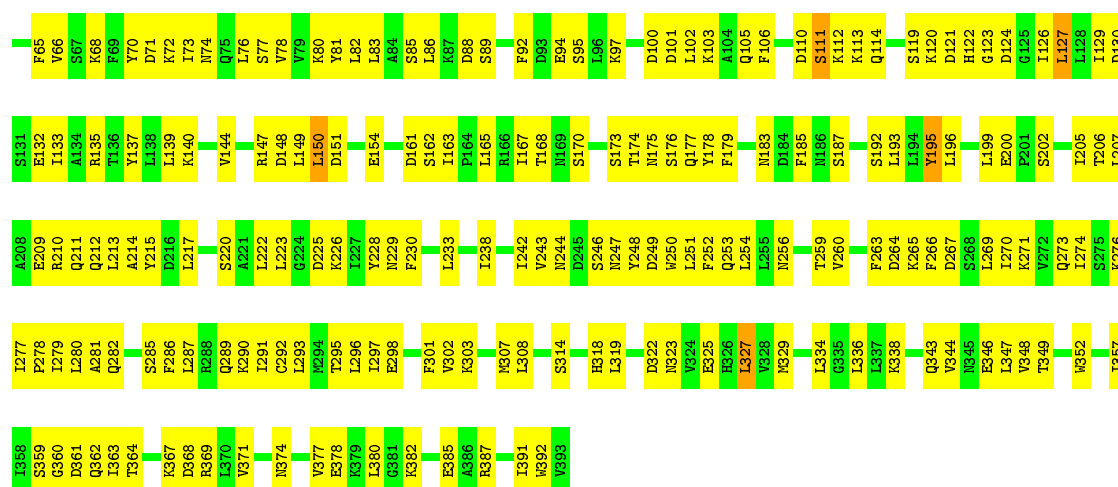
Chain 2-F: 53% 46%



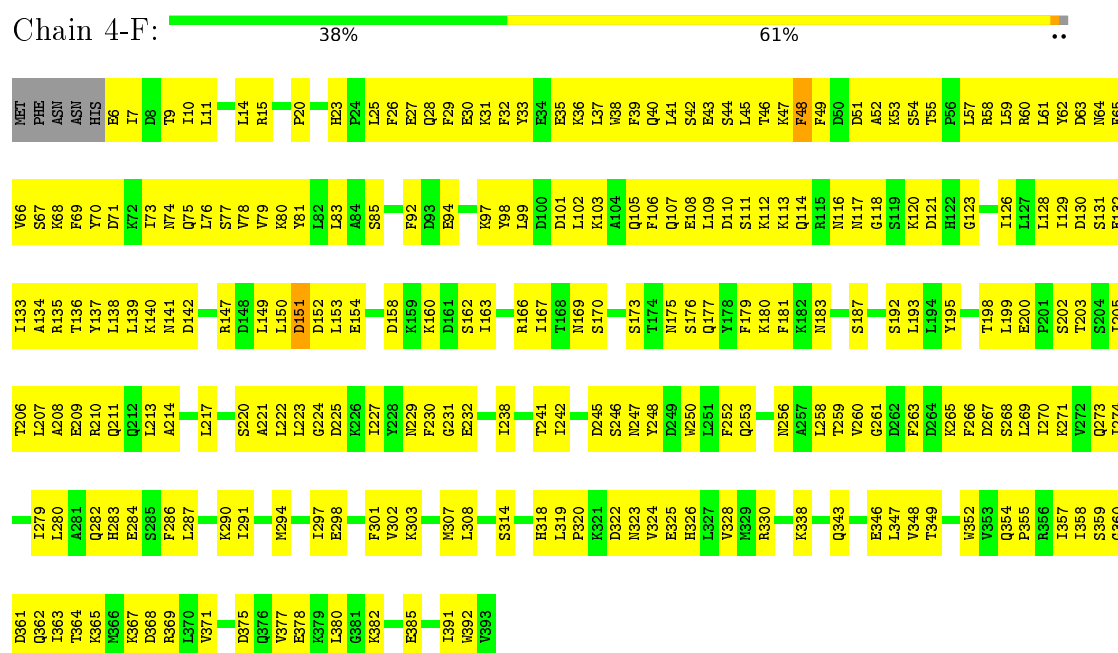
• Molecule 6: 26S proteasome regulatory subunit RPN9

Chain 3-F: 39% 59%

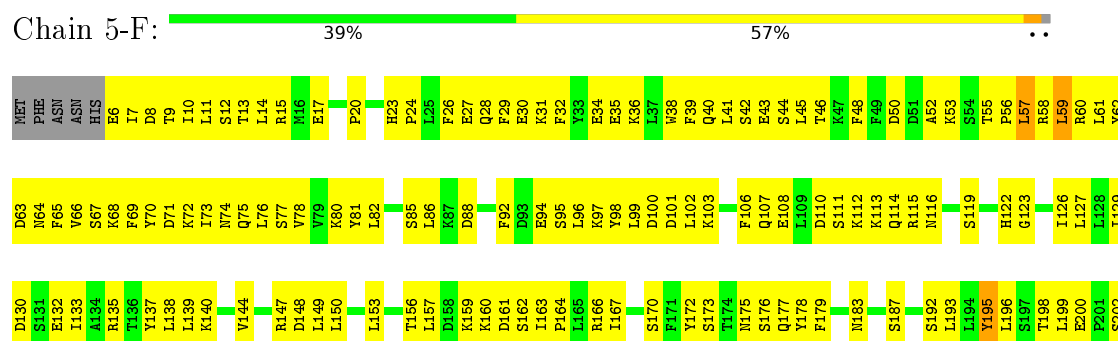


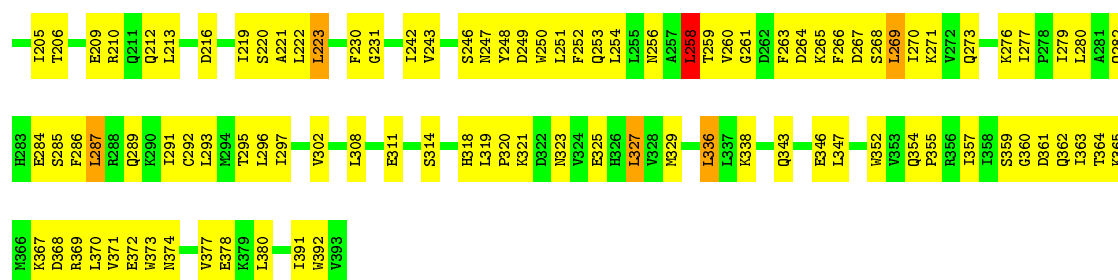


- Molecule 6: 26S proteasome regulatory subunit RPN9



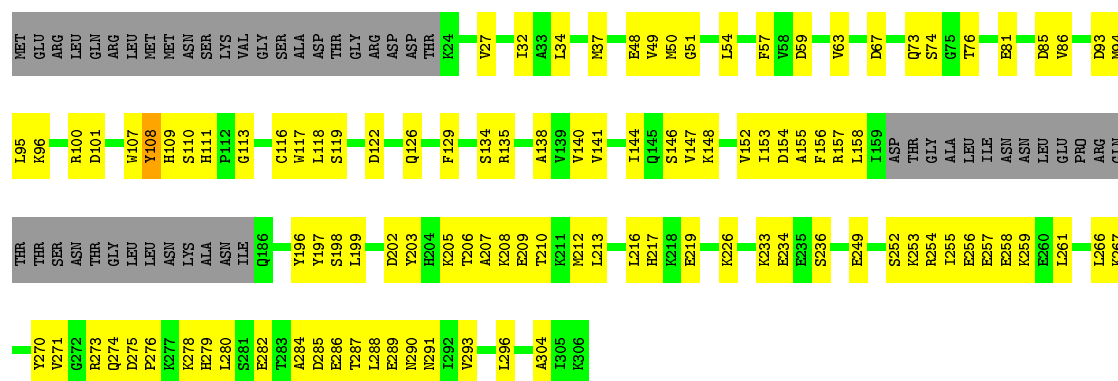
- Molecule 6: 26S proteasome regulatory subunit RPN9





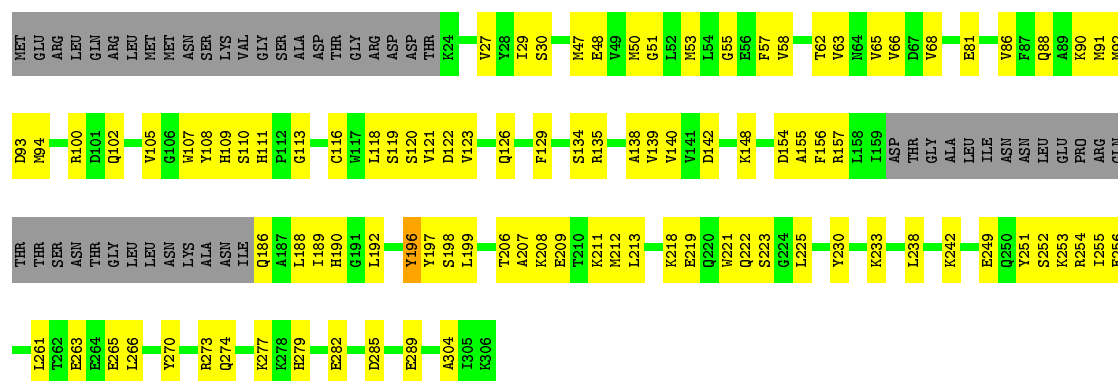
• Molecule 7: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain 1-G: 49% 35% 16%



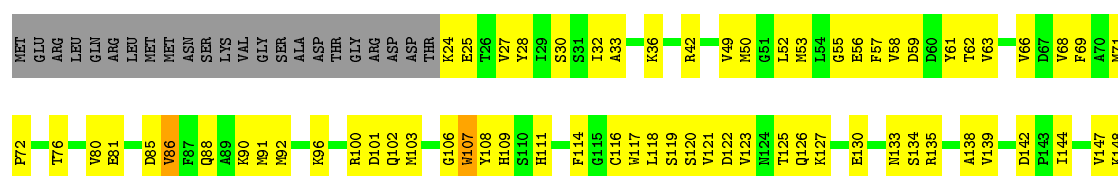
• Molecule 7: Ubiquitin carboxyl-terminal hydrolase RPN11

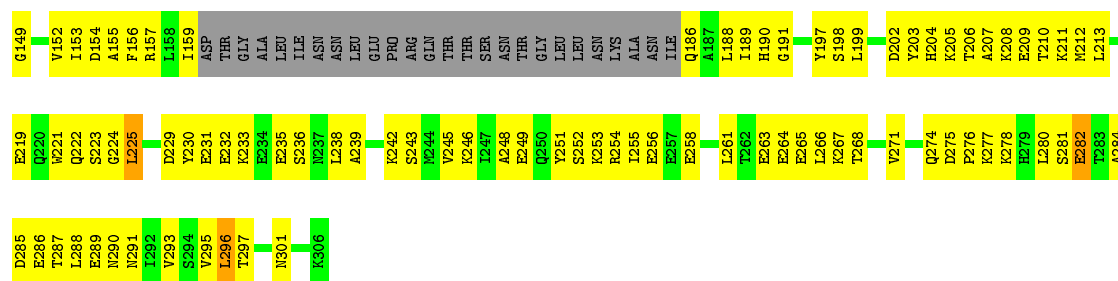
Chain 2-G: 52% 32% 16%



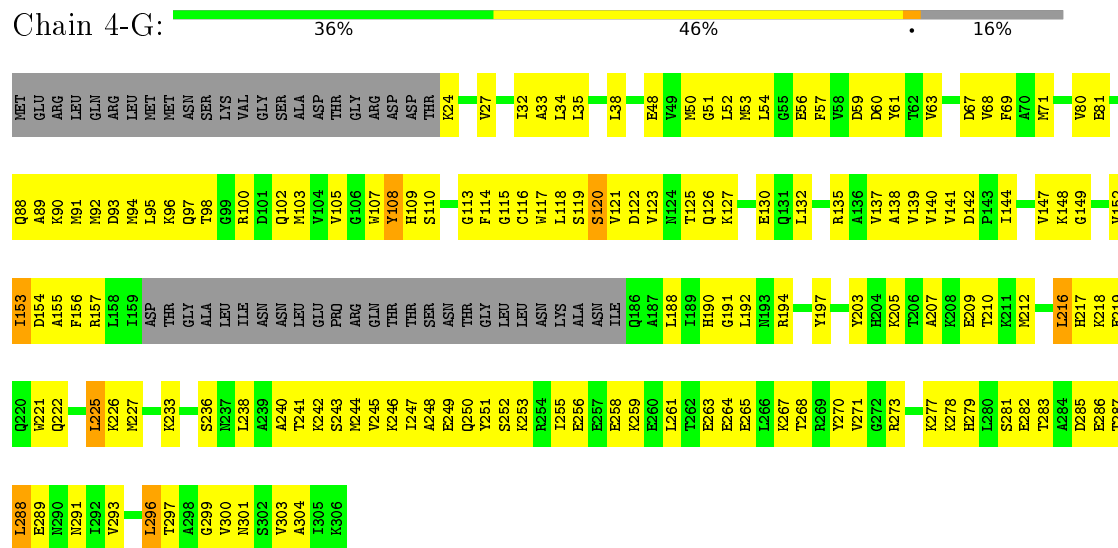
• Molecule 7: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain 3-G: 34% 48% 16%

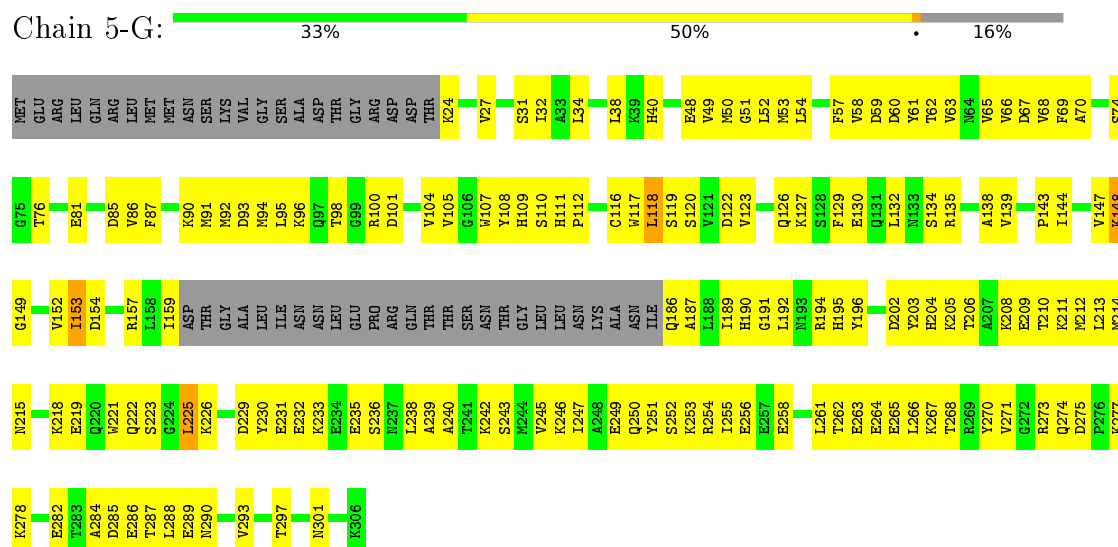




• Molecule 7: Ubiquitin carboxyl-terminal hydrolase RPN11

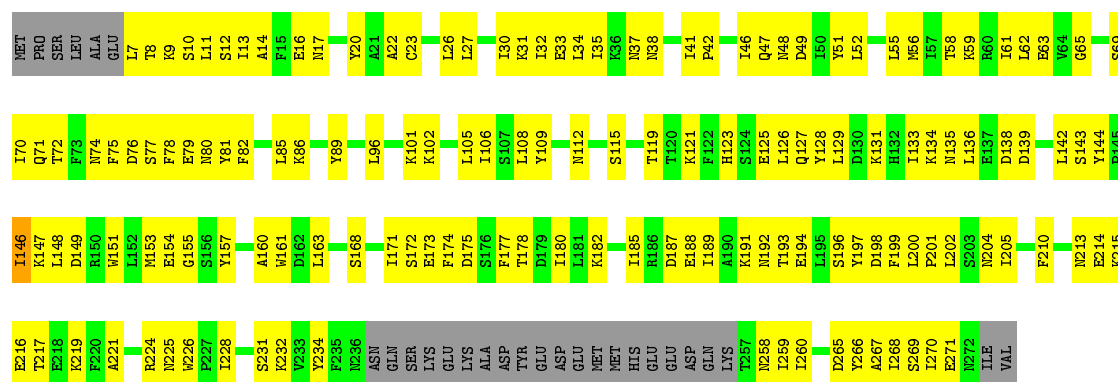


• Molecule 7: Ubiquitin carboxyl-terminal hydrolase RPN11



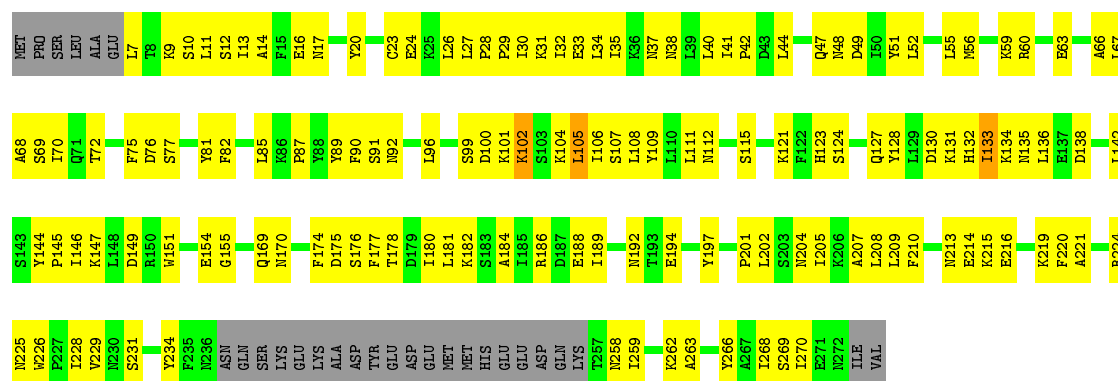
• Molecule 8: 26S proteasome regulatory subunit RPN12





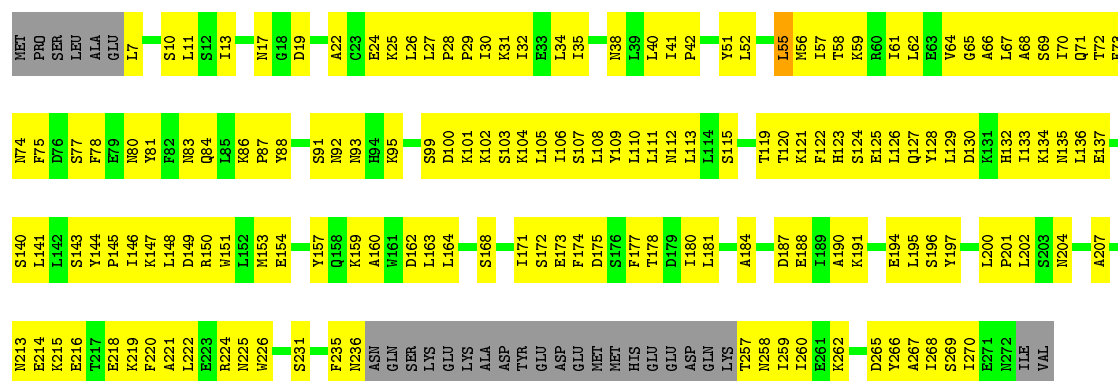
• Molecule 8: 26S proteasome regulatory subunit RPN12

Chain 2-H: 39% 49% 10%



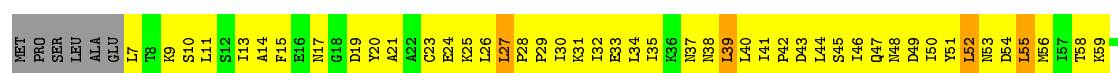
• Molecule 8: 26S proteasome regulatory subunit RPN12

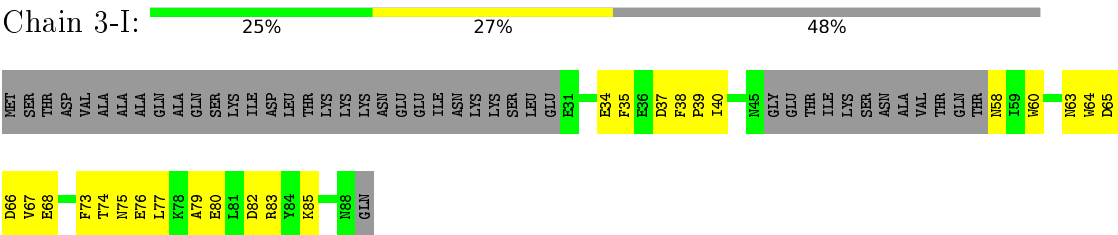
Chain 3-H: 32% 58% 10%



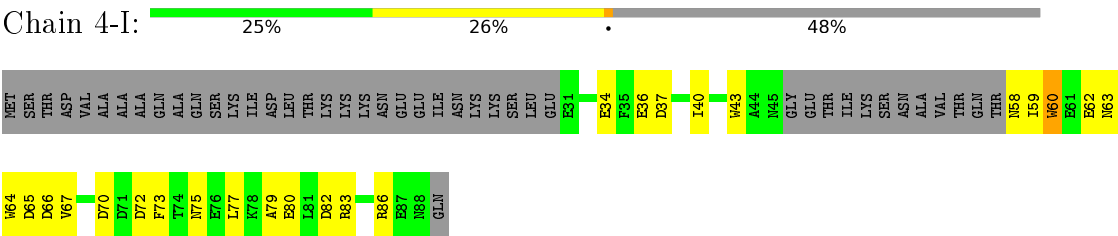
• Molecule 8: 26S proteasome regulatory subunit RPN12

Chain 4-H: 28% 59% 10%

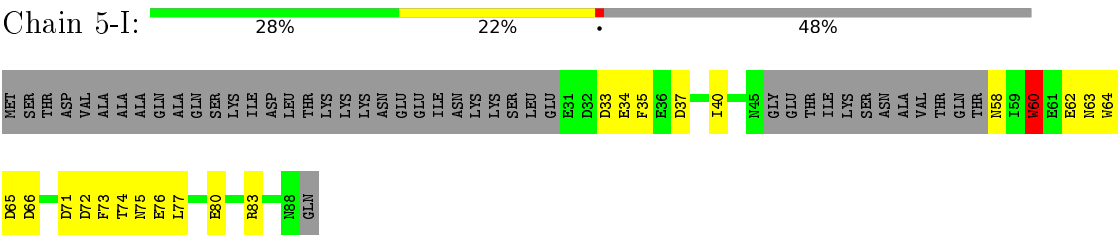




• Molecule 9: 26S proteasome complex subunit SEM1



• Molecule 9: 26S proteasome complex subunit SEM1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	109396	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	whole micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.8	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1-A	0.52	0/2945	0.60	0/3976
1	2-A	0.45	0/2945	0.56	0/3976
1	3-A	0.89	0/2945	0.80	6/3976 (0.2%)
1	4-A	0.74	0/2945	0.73	1/3976 (0.0%)
1	5-A	0.90	1/2945 (0.0%)	0.82	5/3976 (0.1%)
2	1-B	0.55	0/3373	0.65	1/4550 (0.0%)
2	2-B	0.49	0/3373	0.59	1/4550 (0.0%)
2	3-B	1.00	5/3373 (0.1%)	0.87	8/4550 (0.2%)
2	4-B	0.83	1/3373 (0.0%)	0.78	4/4550 (0.1%)
2	5-B	1.00	5/3373 (0.1%)	0.87	8/4550 (0.2%)
3	1-C	0.47	0/3113	0.60	0/4193
3	2-C	0.42	0/3113	0.56	0/4193
3	3-C	0.81	3/3113 (0.1%)	0.79	4/4193 (0.1%)
3	4-C	0.68	2/3113 (0.1%)	0.70	0/4193
3	5-C	0.82	5/3113 (0.2%)	0.80	3/4193 (0.1%)
4	1-D	0.58	0/3135	0.59	0/4227
4	2-D	0.50	0/3135	0.57	1/4227 (0.0%)
4	3-D	1.00	2/3135 (0.1%)	0.84	7/4227 (0.2%)
4	4-D	0.82	1/3135 (0.0%)	0.72	1/4227 (0.0%)
4	5-D	0.97	3/3135 (0.1%)	0.83	3/4227 (0.1%)
5	1-E	0.53	0/2254	0.61	1/3042 (0.0%)
5	2-E	0.47	0/2254	0.60	1/3042 (0.0%)
5	3-E	0.89	0/2254	0.87	5/3042 (0.2%)
5	4-E	0.74	0/2254	0.73	1/3042 (0.0%)
5	5-E	0.94	1/2254 (0.0%)	0.85	4/3042 (0.1%)
6	1-F	0.53	0/3247	0.60	0/4380
6	2-F	0.48	0/3247	0.55	0/4380
6	3-F	0.93	1/3247 (0.0%)	0.84	5/4380 (0.1%)
6	4-F	0.77	0/3247	0.73	0/4380
6	5-F	0.92	1/3247 (0.0%)	0.82	7/4380 (0.2%)
7	1-G	0.56	0/2069	0.63	0/2786
7	2-G	0.51	0/2069	0.58	0/2786

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	3-G	1.00	1/2069 (0.0%)	0.85	4/2786 (0.1%)
7	4-G	0.83	0/2069	0.75	2/2786 (0.1%)
7	5-G	0.98	0/2069	0.85	1/2786 (0.0%)
8	1-H	0.45	0/2061	0.56	0/2785
8	2-H	0.40	0/2061	0.56	2/2785 (0.1%)
8	3-H	0.73	0/2061	0.74	1/2785 (0.0%)
8	4-H	0.61	0/2061	0.69	2/2785 (0.1%)
8	5-H	0.73	0/2061	0.74	2/2785 (0.1%)
9	1-I	0.47	0/414	0.49	0/562
9	2-I	0.44	0/414	0.46	0/562
9	3-I	0.84	0/414	0.81	0/562
9	4-I	0.72	0/414	0.64	0/562
9	5-I	0.84	0/414	0.71	1/562 (0.2%)
All	All	0.74	32/113055 (0.0%)	0.72	92/152505 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	4-A	0	1
3	4-C	0	1
3	5-C	0	1
4	5-D	0	1
7	1-G	0	1
7	4-G	0	1
All	All	0	6

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3-C	409	TYR	CD1-CE1	-6.84	1.29	1.39
2	5-B	415	TRP	CB-CG	-5.97	1.39	1.50
3	5-C	409	TYR	CD1-CE1	-5.92	1.30	1.39
5	5-E	72	TYR	CD1-CE1	-5.91	1.30	1.39
7	3-G	107	TRP	CB-CG	-5.65	1.40	1.50

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	143	LEU	CA-CB-CG	8.14	134.02	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-B	290	LEU	CB-CG-CD2	-7.81	97.72	111.00
5	2-E	132	LEU	CA-CB-CG	7.25	131.99	115.30
1	3-A	323	LEU	CA-CB-CG	-6.99	99.22	115.30
2	3-B	224	LEU	CA-CB-CG	-6.97	99.26	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	1-G	108	TYR	Peptide
1	4-A	261	HIS	Peptide
3	4-C	354	PHE	Peptide
7	4-G	108	TYR	Peptide
3	5-C	354	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3116	0	2979	236	0
1	2-A	3116	0	2977	172	0
1	3-A	3116	0	2977	228	0
1	4-A	3116	0	2980	232	0
1	5-A	3116	0	2979	296	0
2	1-B	3323	0	3398	321	0
2	2-B	3323	0	3398	196	0
2	3-B	3323	0	3398	316	0
2	4-B	3323	0	3398	295	0
2	5-B	3323	0	3398	400	0
3	1-C	3060	0	3091	179	0
3	2-C	3060	0	3091	198	0
3	3-C	3060	0	3091	286	0
3	4-C	3060	0	3091	291	0
3	5-C	3060	0	3091	326	0
4	1-D	3084	0	3112	196	0
4	2-D	3084	0	3112	173	0
4	3-D	3084	0	3112	273	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4-D	3084	0	3112	222	0
4	5-D	3084	0	3112	285	0
5	1-E	2224	0	2290	104	0
5	2-E	2224	0	2290	114	0
5	3-E	2224	0	2290	178	0
5	4-E	2224	0	2290	152	0
5	5-E	2224	0	2290	186	0
6	1-F	3186	0	3213	184	0
6	2-F	3186	0	3213	144	0
6	3-F	3186	0	3213	256	0
6	4-F	3186	0	3213	275	0
6	5-F	3186	0	3213	271	0
7	1-G	2036	0	2038	106	0
7	2-G	2036	0	2038	90	0
7	3-G	2036	0	2038	163	0
7	4-G	2036	0	2038	148	0
7	5-G	2036	0	2038	167	0
8	1-H	2021	0	2013	139	0
8	2-H	2021	0	2013	124	0
8	3-H	2021	0	2013	157	0
8	4-H	2021	0	2013	236	0
8	5-H	2021	0	2013	184	0
9	1-I	405	0	333	31	0
9	2-I	405	0	333	23	0
9	3-I	405	0	333	35	0
9	4-I	405	0	333	31	0
9	5-I	405	0	333	25	0
10	1-G	1	0	0	0	0
10	2-G	1	0	0	0	0
10	3-G	1	0	0	0	0
10	4-G	1	0	0	0	0
10	5-G	1	0	0	0	0
11	1-B	1	0	0	0	0
11	2-B	1	0	0	1	0
11	3-B	1	0	0	1	0
11	4-B	1	0	0	1	0
11	5-B	1	0	0	1	0
All	All	112285	0	112332	8245	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 37.

The worst 5 of 8245 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)
3:C:74:LEU:HD22	3:C:104:PHE:CE1	1.21	1.67
1:A:163:VAL:CG1	1:A:167:LEU:HD21	1.29	1.55
2:B:141:LYS:HD2	2:B:179:PHE:CD1	1.37	1.55
3:C:74:LEU:CD2	3:C:104:PHE:CE1	1.90	1.52
2:B:141:LYS:CD	2:B:179:PHE:CD1	1.99	1.44

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 PDB entries followed by that with respect to all EM entries.

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	1-A	350/438 (80%)	316 (90%)	33 (9%)	1 (0%)	46	84
1	2-A	350/438 (80%)	306 (87%)	38 (11%)	6 (2%)	11	54
1	3-A	350/438 (80%)	305 (87%)	44 (13%)	1 (0%)	46	84
1	4-A	350/438 (80%)	308 (88%)	40 (11%)	2 (1%)	30	75
1	5-A	350/438 (80%)	310 (89%)	37 (11%)	3 (1%)	21	68
2	1-B	400/445 (90%)	353 (88%)	45 (11%)	2 (0%)	34	78
2	2-B	400/445 (90%)	348 (87%)	49 (12%)	3 (1%)	24	70
2	3-B	400/445 (90%)	355 (89%)	41 (10%)	4 (1%)	19	66
2	4-B	400/445 (90%)	333 (83%)	64 (16%)	3 (1%)	24	70
2	5-B	400/445 (90%)	349 (87%)	48 (12%)	3 (1%)	24	70
3	1-C	376/434 (87%)	344 (92%)	29 (8%)	3 (1%)	24	70
3	2-C	376/434 (87%)	323 (86%)	50 (13%)	3 (1%)	24	70
3	3-C	376/434 (87%)	323 (86%)	48 (13%)	5 (1%)	15	60
3	4-C	376/434 (87%)	333 (89%)	42 (11%)	1 (0%)	46	84
3	5-C	376/434 (87%)	325 (86%)	49 (13%)	2 (0%)	34	78
4	1-D	380/429 (89%)	337 (89%)	41 (11%)	2 (0%)	34	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2-D	380/429 (89%)	341 (90%)	37 (10%)	2 (0%)	34	78
4	3-D	380/429 (89%)	334 (88%)	45 (12%)	1 (0%)	46	84
4	4-D	380/429 (89%)	337 (89%)	42 (11%)	1 (0%)	46	84
4	5-D	380/429 (89%)	342 (90%)	33 (9%)	5 (1%)	15	60
5	1-E	271/338 (80%)	243 (90%)	27 (10%)	1 (0%)	39	81
5	2-E	271/338 (80%)	247 (91%)	24 (9%)	0	100	100
5	3-E	271/338 (80%)	245 (90%)	23 (8%)	3 (1%)	17	63
5	4-E	271/338 (80%)	243 (90%)	27 (10%)	1 (0%)	39	81
5	5-E	271/338 (80%)	247 (91%)	22 (8%)	2 (1%)	26	72
6	1-F	386/393 (98%)	352 (91%)	33 (8%)	1 (0%)	46	84
6	2-F	386/393 (98%)	352 (91%)	33 (8%)	1 (0%)	46	84
6	3-F	386/393 (98%)	348 (90%)	37 (10%)	1 (0%)	46	84
6	4-F	386/393 (98%)	349 (90%)	36 (9%)	1 (0%)	46	84
6	5-F	386/393 (98%)	341 (88%)	42 (11%)	3 (1%)	24	70
7	1-G	253/306 (83%)	234 (92%)	19 (8%)	0	100	100
7	2-G	253/306 (83%)	227 (90%)	26 (10%)	0	100	100
7	3-G	253/306 (83%)	227 (90%)	23 (9%)	3 (1%)	16	61
7	4-G	253/306 (83%)	225 (89%)	23 (9%)	5 (2%)	9	51
7	5-G	253/306 (83%)	225 (89%)	26 (10%)	2 (1%)	24	70
8	1-H	242/274 (88%)	213 (88%)	27 (11%)	2 (1%)	24	70
8	2-H	242/274 (88%)	218 (90%)	21 (9%)	3 (1%)	16	61
8	3-H	242/274 (88%)	210 (87%)	31 (13%)	1 (0%)	39	81
8	4-H	242/274 (88%)	213 (88%)	25 (10%)	4 (2%)	11	54
8	5-H	242/274 (88%)	218 (90%)	22 (9%)	2 (1%)	24	70
9	1-I	42/89 (47%)	38 (90%)	4 (10%)	0	100	100
9	2-I	42/89 (47%)	35 (83%)	7 (17%)	0	100	100
9	3-I	42/89 (47%)	38 (90%)	4 (10%)	0	100	100
9	4-I	42/89 (47%)	37 (88%)	5 (12%)	0	100	100
9	5-I	42/89 (47%)	38 (90%)	4 (10%)	0	100	100
All	All	13500/15730 (86%)	11985 (89%)	1426 (11%)	89 (1%)	31	72

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	451	ILE
2	1-B	132	VAL
5	3-E	64	ASP
2	4-B	396	PRO
8	4-H	198	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 PDB entries followed by that with respect to all EM entries.

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	1-A	329/367 (90%)	328 (100%)	1 (0%)	94	99
1	2-A	329/367 (90%)	329 (100%)	0	100	100
1	3-A	329/367 (90%)	329 (100%)	0	100	100
1	4-A	329/367 (90%)	329 (100%)	0	100	100
1	5-A	329/367 (90%)	328 (100%)	1 (0%)	94	99
2	1-B	380/415 (92%)	375 (99%)	5 (1%)	76	91
2	2-B	380/415 (92%)	380 (100%)	0	100	100
2	3-B	380/415 (92%)	379 (100%)	1 (0%)	94	99
2	4-B	380/415 (92%)	380 (100%)	0	100	100
2	5-B	380/415 (92%)	379 (100%)	1 (0%)	94	99
3	1-C	343/391 (88%)	343 (100%)	0	100	100
3	2-C	343/391 (88%)	343 (100%)	0	100	100
3	3-C	343/391 (88%)	343 (100%)	0	100	100
3	4-C	343/391 (88%)	342 (100%)	1 (0%)	94	99
3	5-C	343/391 (88%)	342 (100%)	1 (0%)	94	99
4	1-D	336/379 (89%)	336 (100%)	0	100	100
4	2-D	336/379 (89%)	336 (100%)	0	100	100
4	3-D	336/379 (89%)	334 (99%)	2 (1%)	90	97
4	4-D	336/379 (89%)	336 (100%)	0	100	100
4	5-D	336/379 (89%)	336 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1-E	252/308 (82%)	252 (100%)	0	100	100
5	2-E	252/308 (82%)	252 (100%)	0	100	100
5	3-E	252/308 (82%)	252 (100%)	0	100	100
5	4-E	252/308 (82%)	252 (100%)	0	100	100
5	5-E	252/308 (82%)	252 (100%)	0	100	100
6	1-F	363/368 (99%)	363 (100%)	0	100	100
6	2-F	363/368 (99%)	363 (100%)	0	100	100
6	3-F	363/368 (99%)	363 (100%)	0	100	100
6	4-F	363/368 (99%)	362 (100%)	1 (0%)	94	99
6	5-F	363/368 (99%)	363 (100%)	0	100	100
7	1-G	226/268 (84%)	226 (100%)	0	100	100
7	2-G	226/268 (84%)	225 (100%)	1 (0%)	93	98
7	3-G	226/268 (84%)	226 (100%)	0	100	100
7	4-G	226/268 (84%)	226 (100%)	0	100	100
7	5-G	226/268 (84%)	224 (99%)	2 (1%)	84	94
8	1-H	230/256 (90%)	230 (100%)	0	100	100
8	2-H	230/256 (90%)	230 (100%)	0	100	100
8	3-H	230/256 (90%)	230 (100%)	0	100	100
8	4-H	230/256 (90%)	229 (100%)	1 (0%)	93	98
8	5-H	230/256 (90%)	229 (100%)	1 (0%)	93	98
9	1-I	44/81 (54%)	44 (100%)	0	100	100
9	2-I	44/81 (54%)	44 (100%)	0	100	100
9	3-I	44/81 (54%)	43 (98%)	1 (2%)	58	85
9	4-I	44/81 (54%)	43 (98%)	1 (2%)	58	85
9	5-I	44/81 (54%)	43 (98%)	1 (2%)	58	85
All	All	12515/14165 (88%)	12493 (100%)	22 (0%)	95	99

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	3-D	249	ILE
6	4-F	48	PHE
8	5-H	175	ASP

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Mol	Chain	Res	Type
9	3-I	60	TRP
3	4-C	169	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
1	3-A	280	ASN
6	3-F	256	ASN
5	5-E	94	HIS
2	3-B	195	GLN
4	3-D	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.