



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 03:19 PM EDT

PDB ID : 5VFU  
EMDB ID : EMD-8668  
Title : Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome  
Authors : Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.  
Deposited on : 2017-04-09  
Resolution : 5.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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>.

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

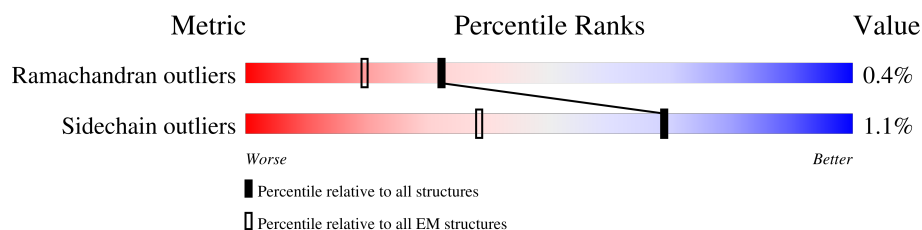
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 5.80 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	911	<div> <div>68%</div> <div>88%</div> <div>12%</div> </div>
2	V	480	<div> <div>91%</div> <div>97%</div> </div>
3	W	456	<div> <div>94%</div> <div>97%</div> </div>
4	X	380	<div> <div>60%</div> <div>63%</div> <div>37%</div> </div>
5	Y	378	<div> <div>85%</div> <div>98%</div> </div>
6	Z	286	<div> <div>84%</div> <div>98%</div> </div>
7	a	373	<div> <div>94%</div> <div>99%</div> </div>
8	b	191	<div> <div>92%</div> <div>99%</div> </div>
9	c	287	<div> <div>79%</div> <div>94%</div> </div>

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Mol	Chain	Length	Quality of chain
10	d	257	<div>95%</div> <div>98%</div>
11	e	70	<div>54%</div> <div>53%</div> <div>43%</div>
12	A	361	<div>77%</div> <div>98%</div>
13	B	348	<div>87%</div> <div>96%</div>
14	C	384	<div>87%</div> <div>96%</div>
15	D	380	<div>84%</div> <div>99%</div>
16	E	353	<div>81%</div> <div>99%</div>
17	F	377	<div>76%</div> <div>95%</div>
18	G	240	<div>58%</div> <div>100%</div>
18	g	240	<div>58%</div> <div>100%</div>
19	H	232	<div>57%</div> <div>99%</div>
19	h	232	<div>50%</div> <div>100%</div>
20	I	250	<div>62%</div> <div>99%</div>
20	i	250	<div>58%</div> <div>99%</div>
21	J	243	<div>53%</div> <div>97%</div>
21	j	243	<div>57%</div> <div>98%</div>
22	K	234	<div>52%</div> <div>96%</div>
22	k	234	<div>55%</div> <div>94%</div>
23	L	238	<div>50%</div> <div>98%</div>
23	l	238	<div>48%</div> <div>100%</div>
24	M	245	<div>54%</div> <div>97%</div>
24	m	245	<div>56%</div> <div>97%</div>
25	N	191	<div>47%</div> <div>100%</div>
25	n	191	<div>40%</div> <div>99%</div>
26	O	220	<div>45%</div> <div>100%</div>

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Mol	Chain	Length	Quality of chain
26	o	220	<div>44%</div> <div>100%</div>
27	P	204	<div>43%</div> <div>100%</div>
27	p	204	<div>44%</div> <div>100%</div>
28	Q	199	<div>49%</div> <div>98%</div>
28	q	199	<div>41%</div> <div>98%</div>
29	R	201	<div>37%</div> <div>100%</div>
29	r	201	<div>38%</div> <div>100%</div>
30	S	213	<div>44%</div> <div>100%</div>
30	s	213	<div>43%</div> <div>100%</div>
31	T	215	<div>32%</div> <div>99%</div>
31	t	215	<div>33%</div> <div>100%</div>
32	f	908	<div>71%</div> <div>73%</div> <div>24%</div>

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 100133 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 non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	373	Total	C	N	O	S	0	0
			2993	1910	509	559	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	13	SER	ASN	conflict	UNP Q9UNM6

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 11 is a protein called Sem1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	361	Total	C	N	O	S	0	0
			2834	1788	500	528	18		

- Molecule 13 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	348	Total	C	N	O	S	0	0
			2717	1708	460	537	12		

- Molecule 14 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

- Molecule 15 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 16 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

- Molecule 17 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 18 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	G	240	Total	C	N	O	S	0	0
			1825	1160	304	348	13		
18	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 19 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
19	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 20 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
20	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 21 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
21	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
22	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 23 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
23	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
24	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 25 is a protein called Proteasome subunit beta type-6.



Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
25	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 26 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
26	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 27 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
27	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 28 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
28	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 29 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
29	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 30 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
30	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 31 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
31	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	689	Total	C	N	O	S	0	0
			5319	3343	904	1037	35		

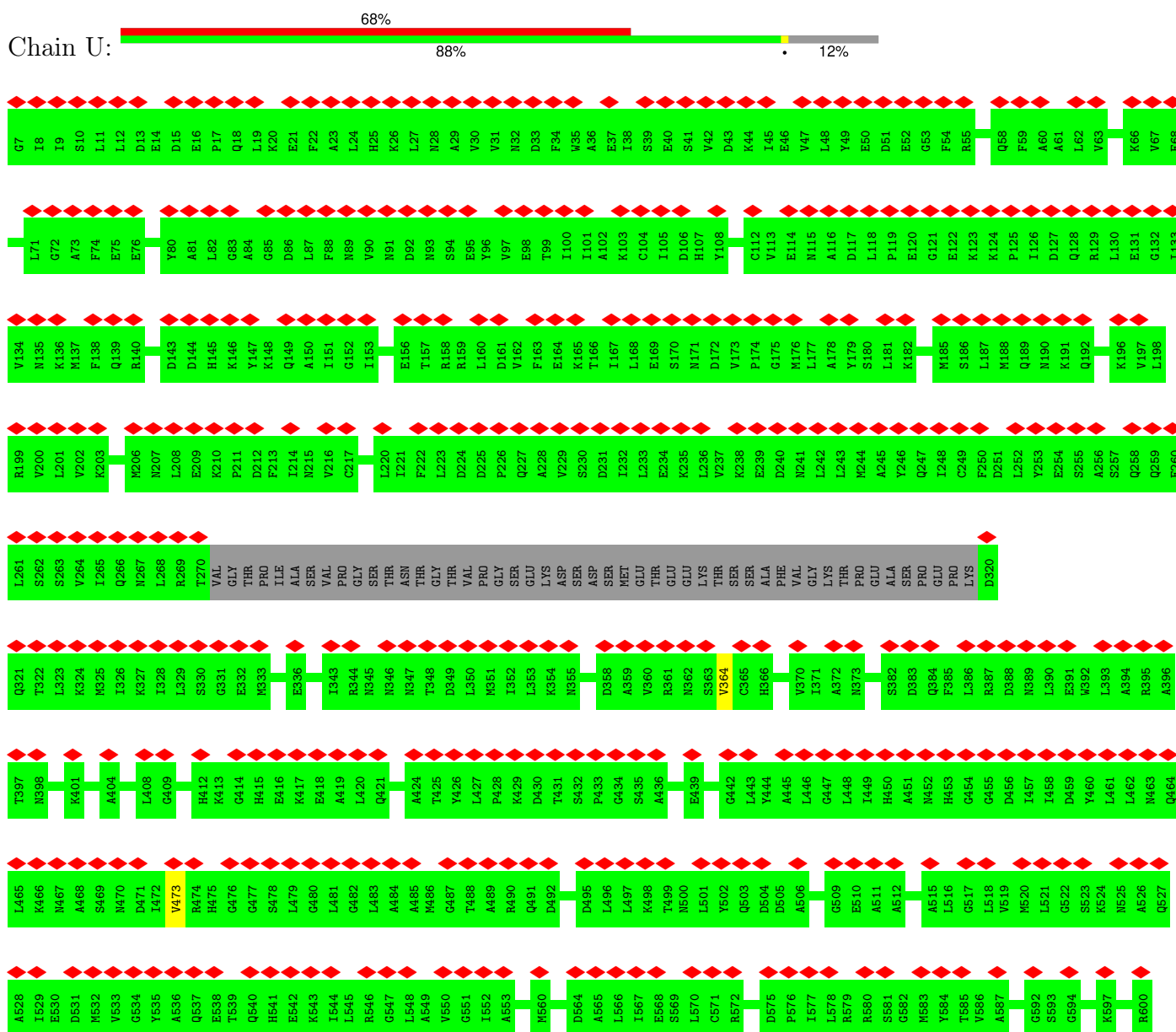
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

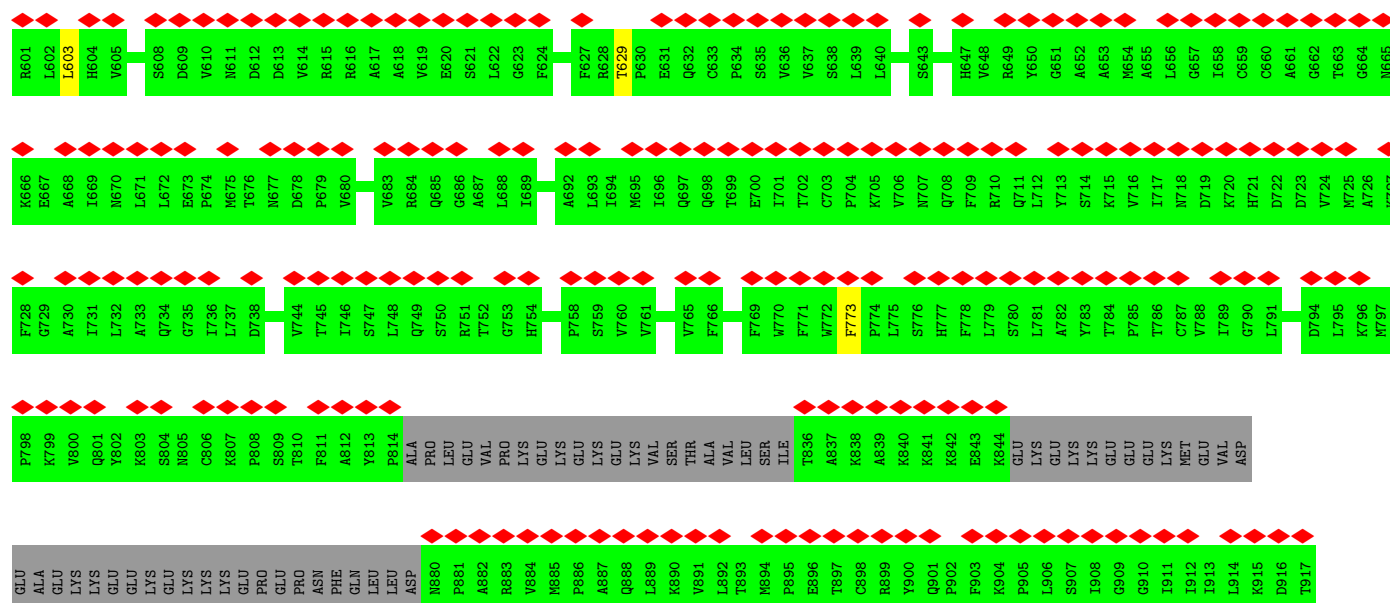
Mol	Chain	Residues	Atoms		AltConf
33	c	1	Total	Zn	0
			1	1	

### 3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

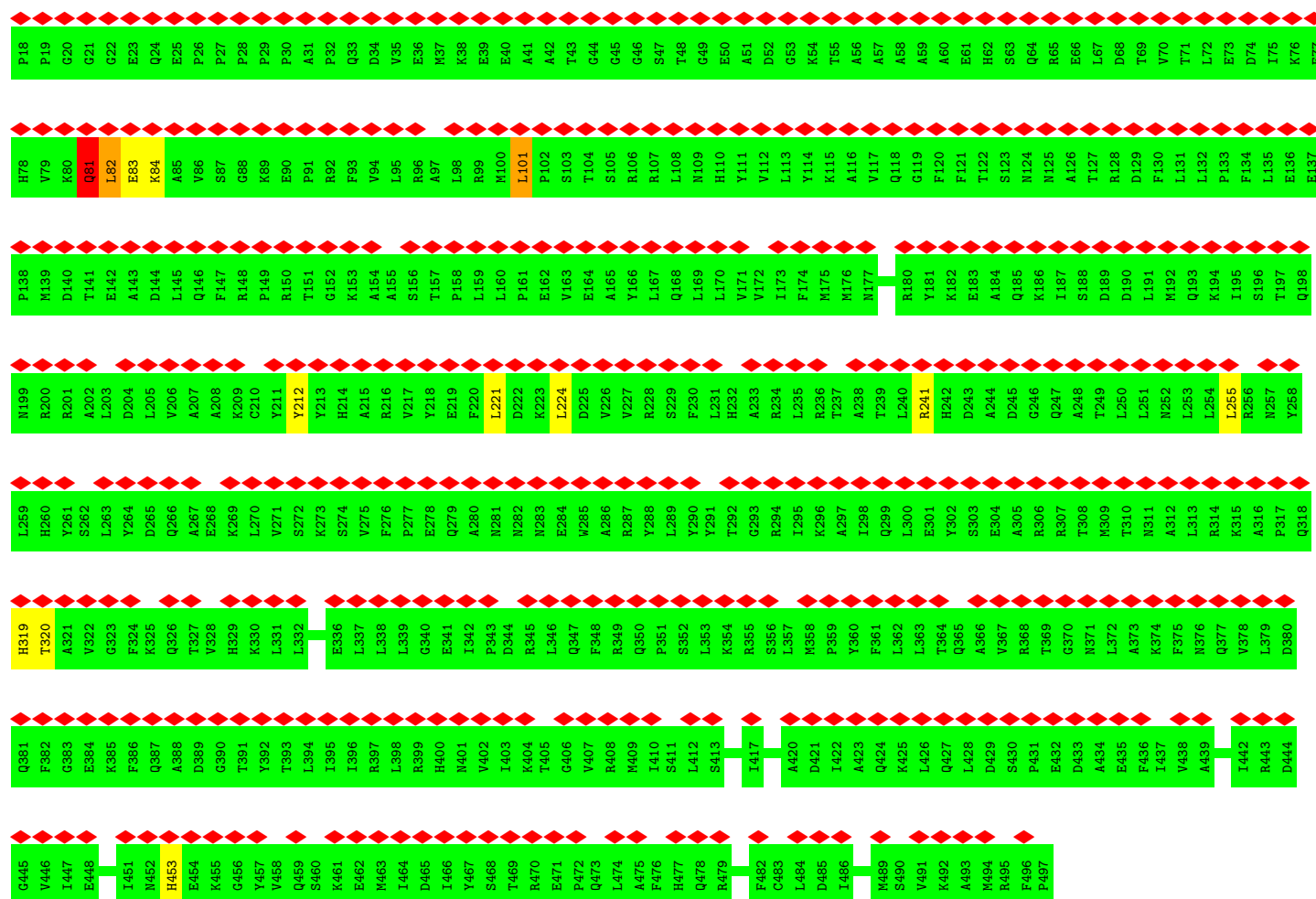
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1



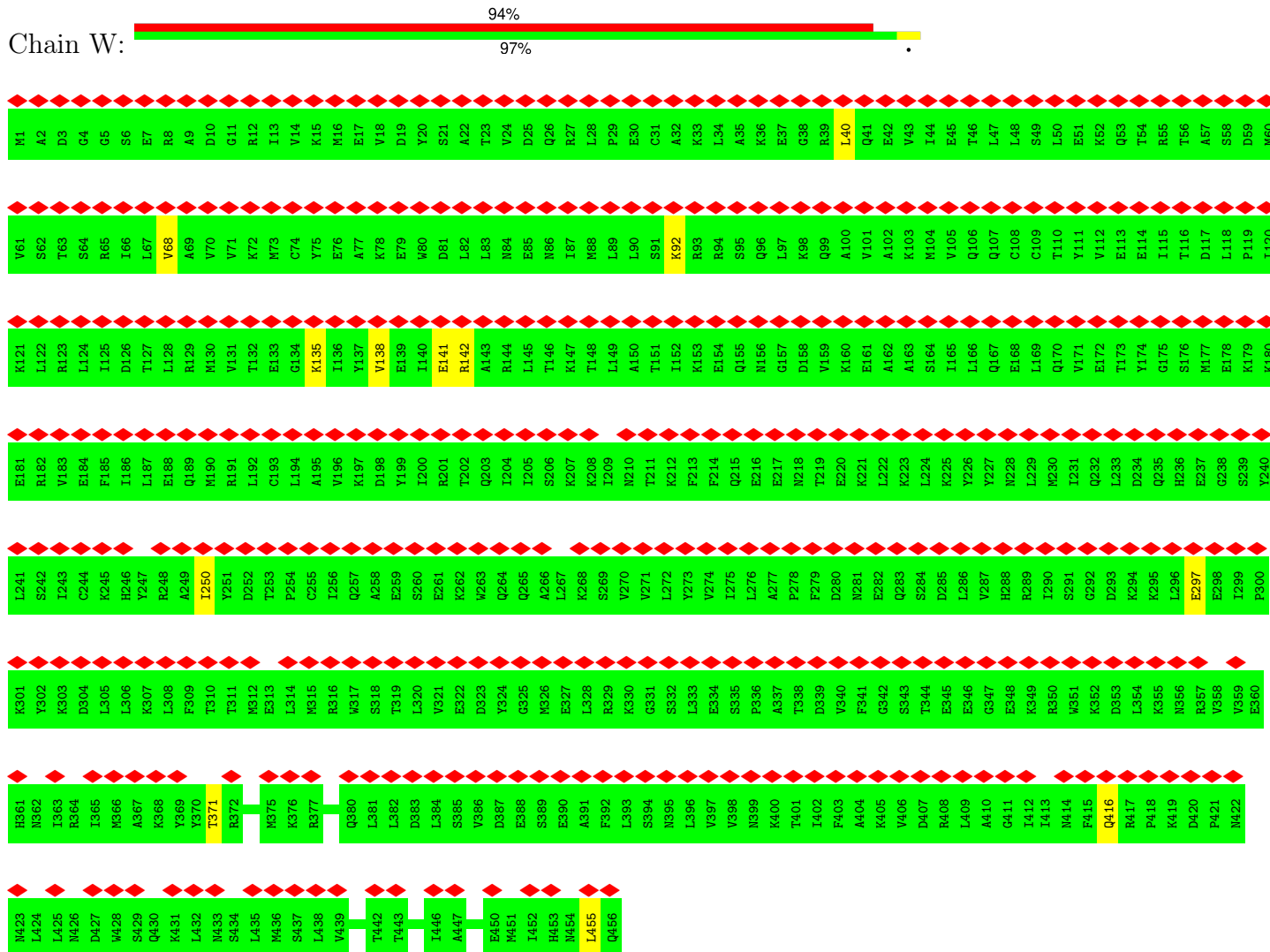


• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

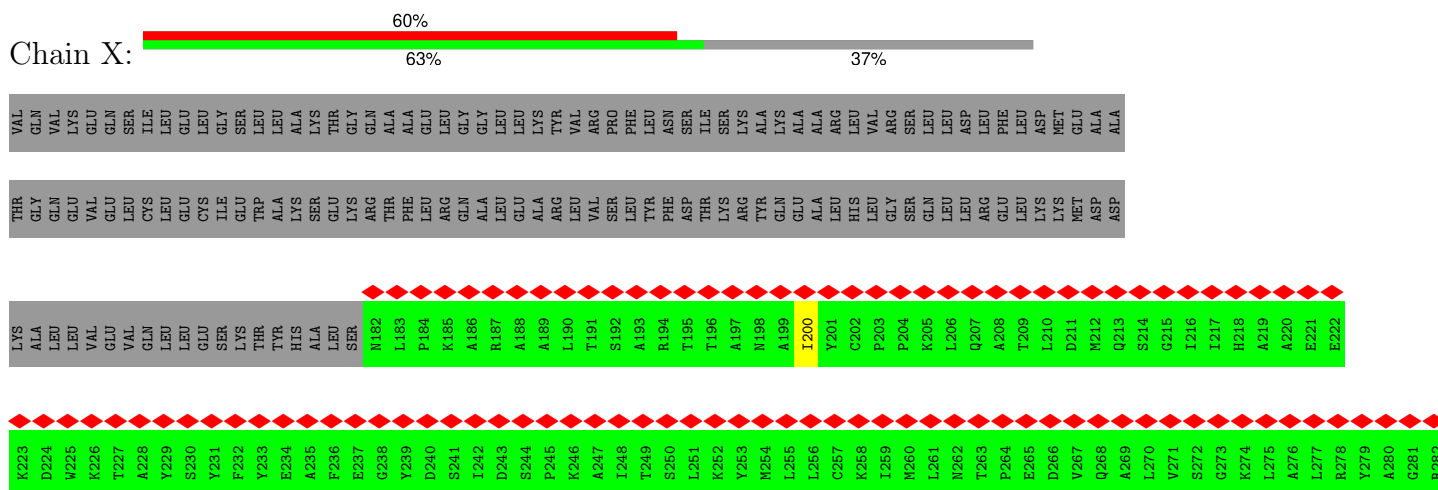
Chain V: 91% 97%

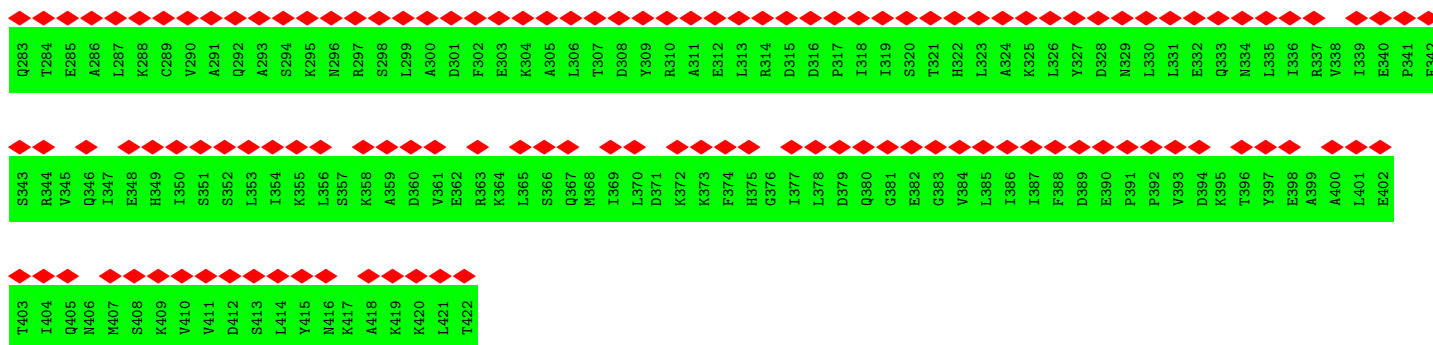


• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

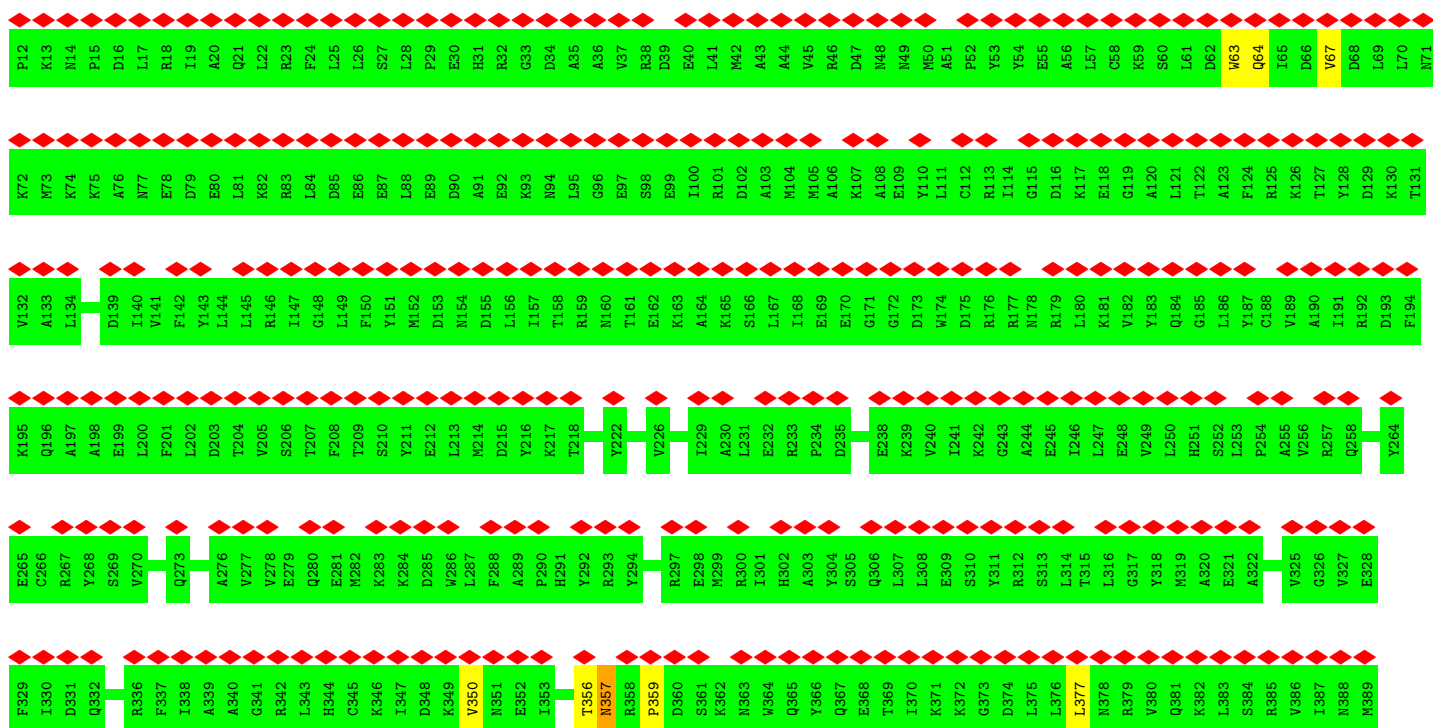
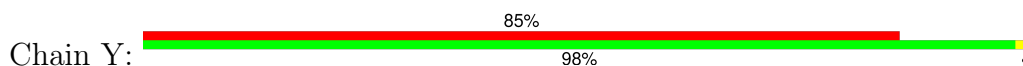


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

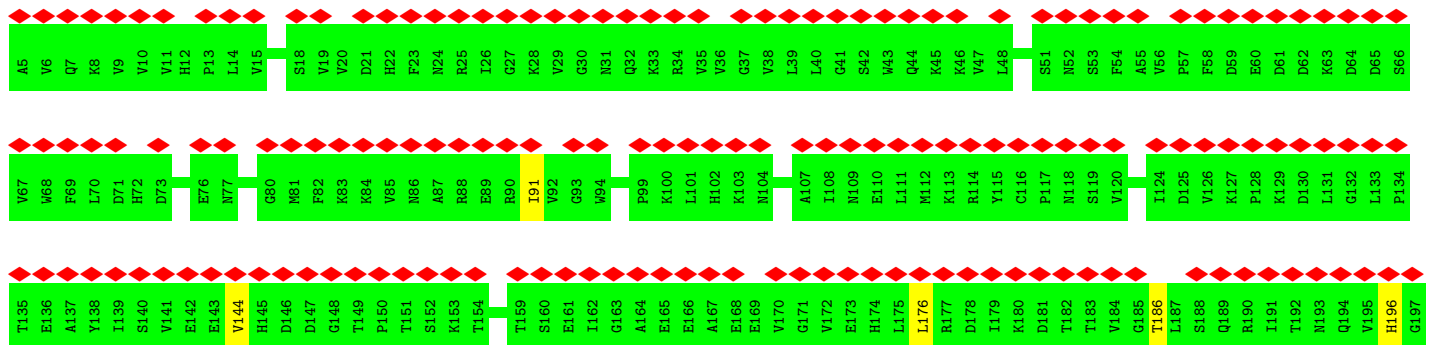
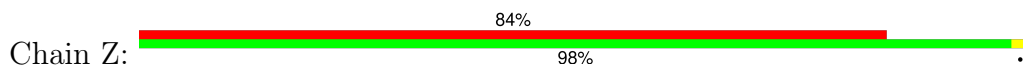


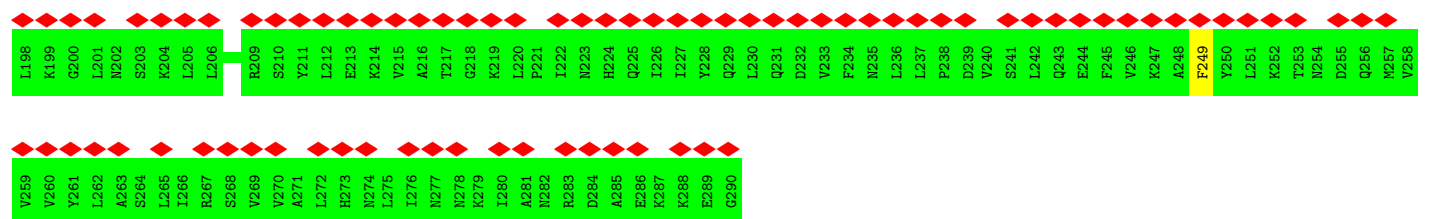


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6



• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

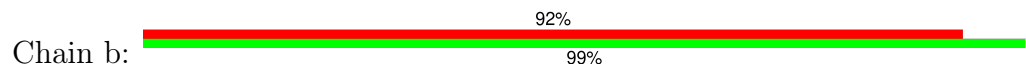


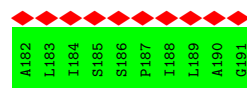


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

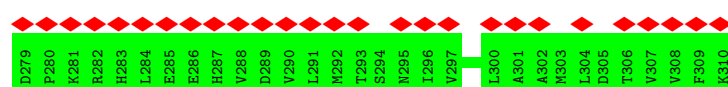
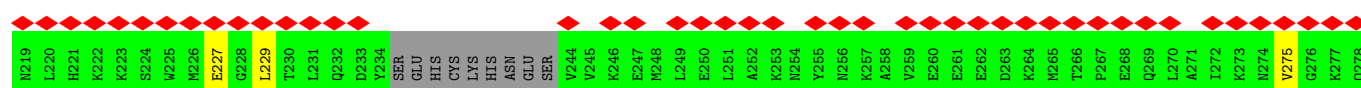
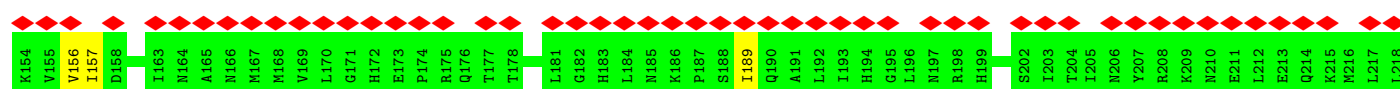
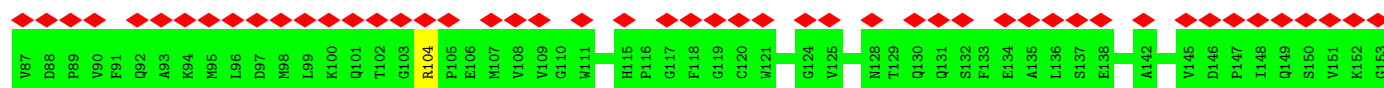
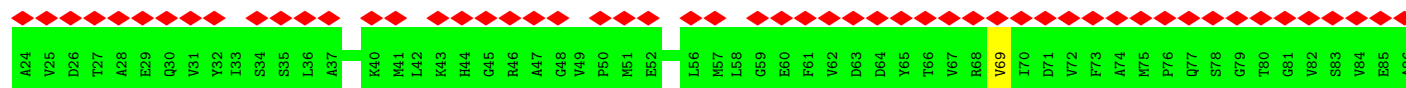
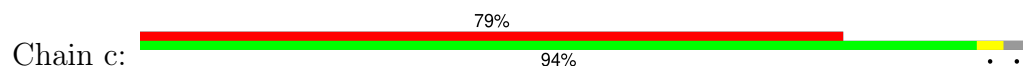


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

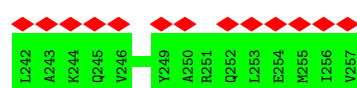
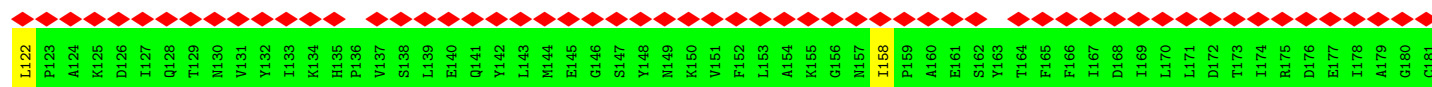
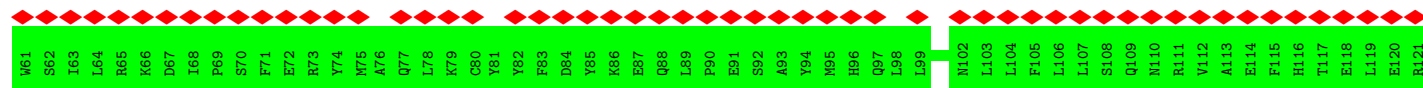
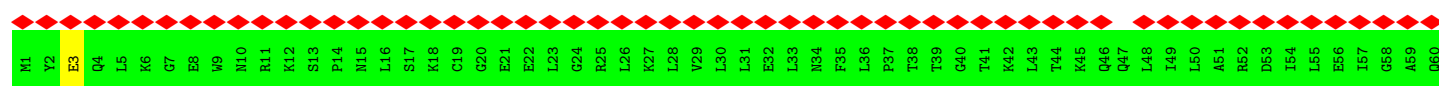




• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

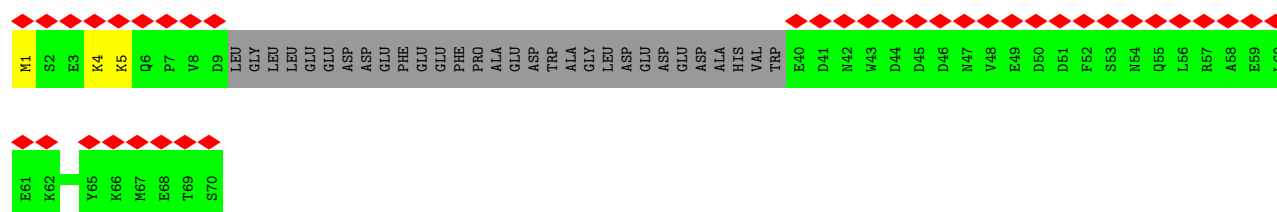


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

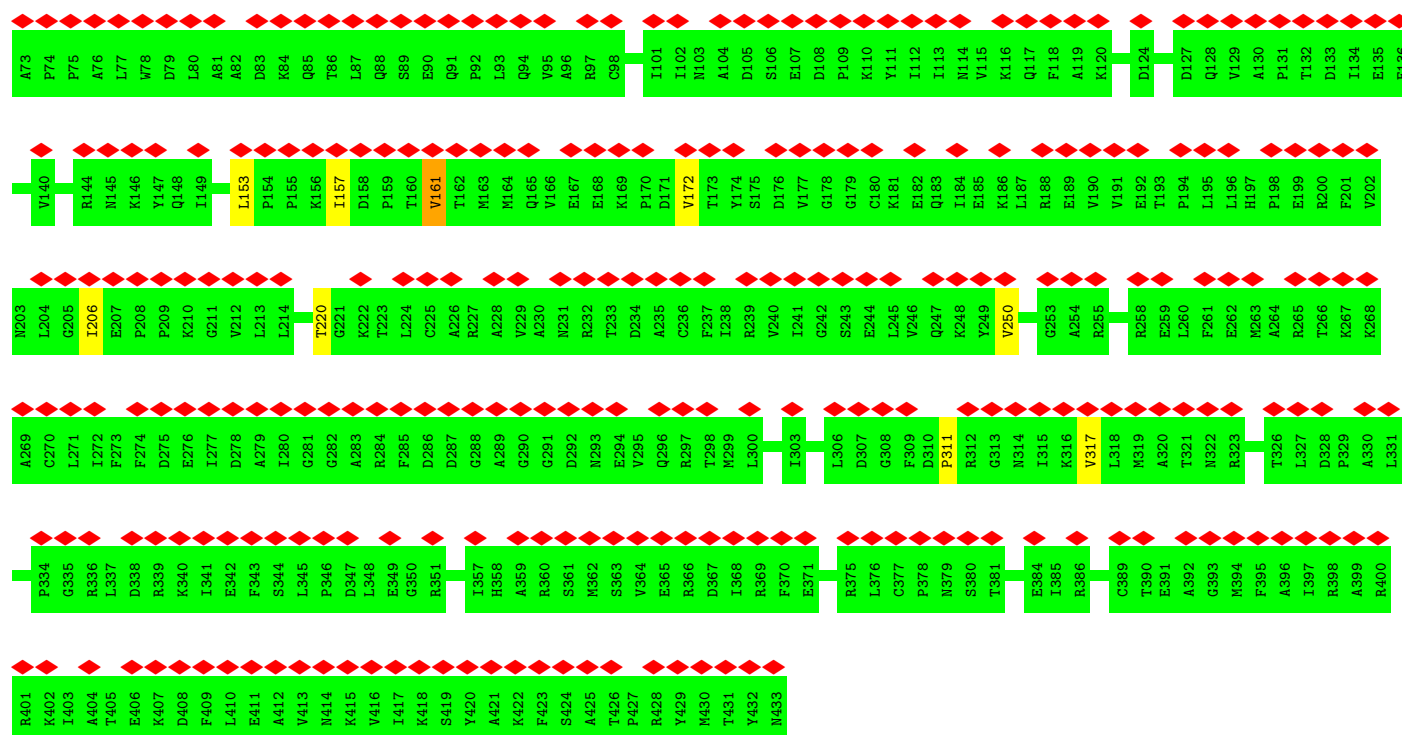
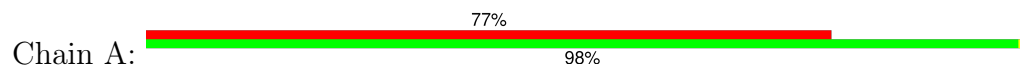


• Molecule 11: Sem1

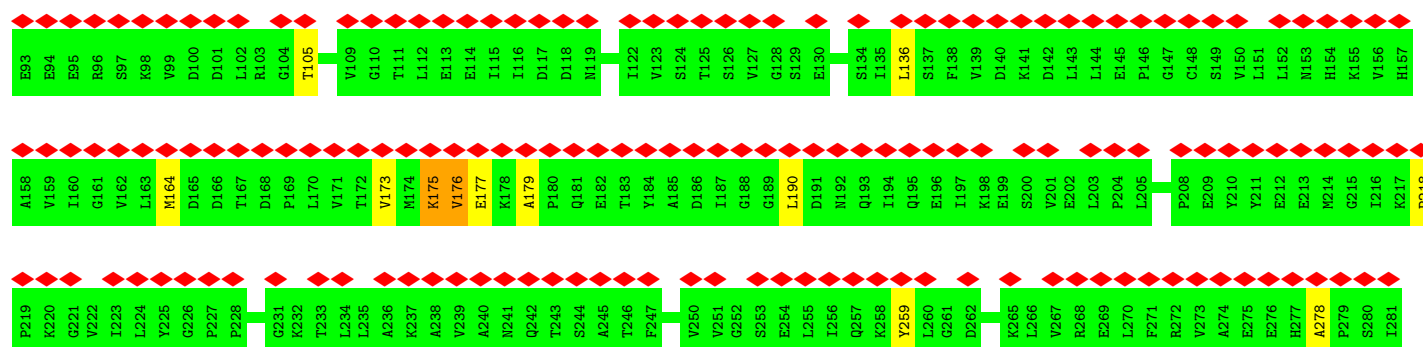
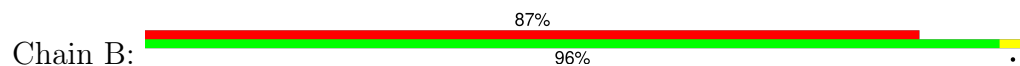


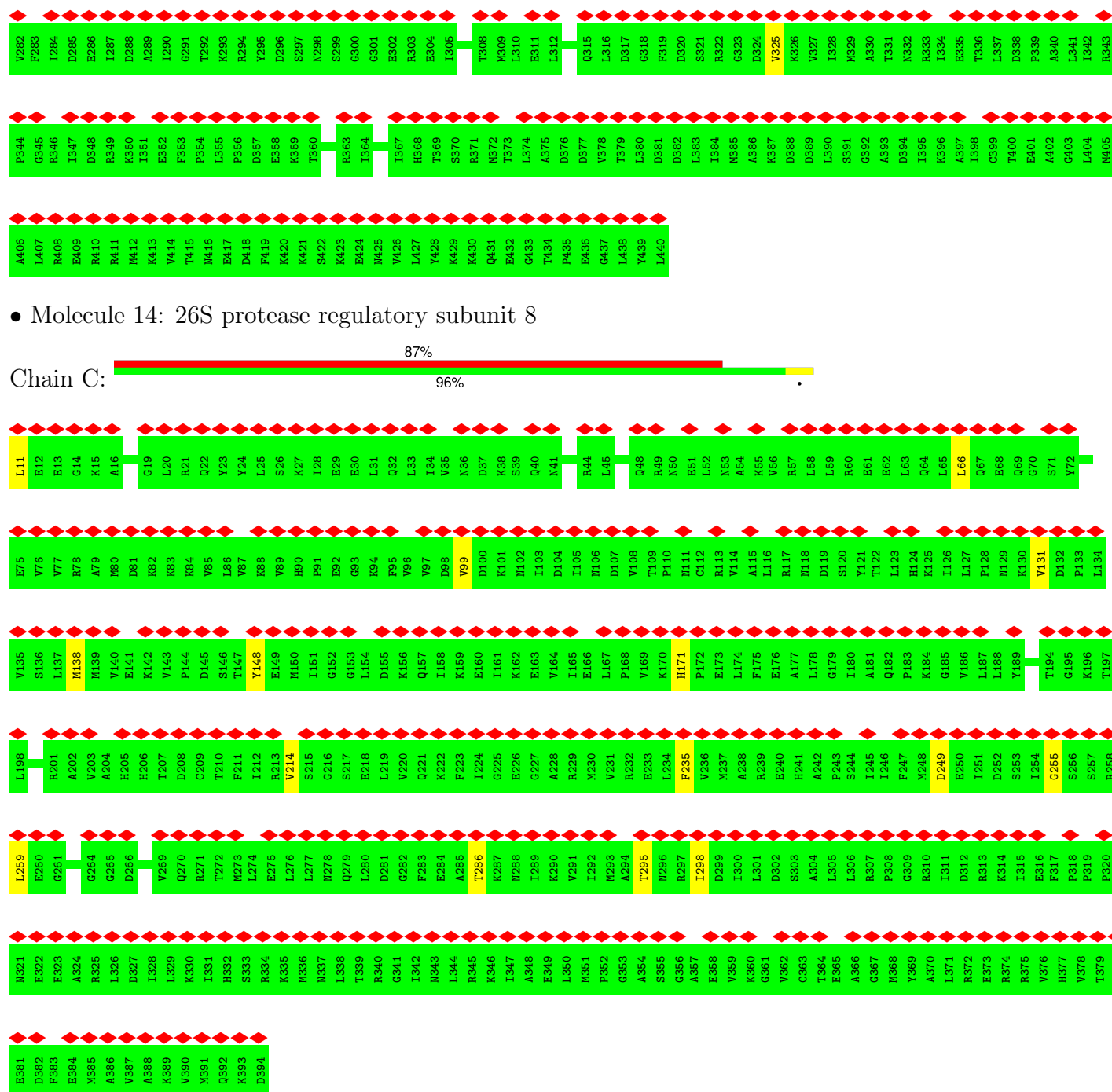


• Molecule 12: 26S protease regulatory subunit 7



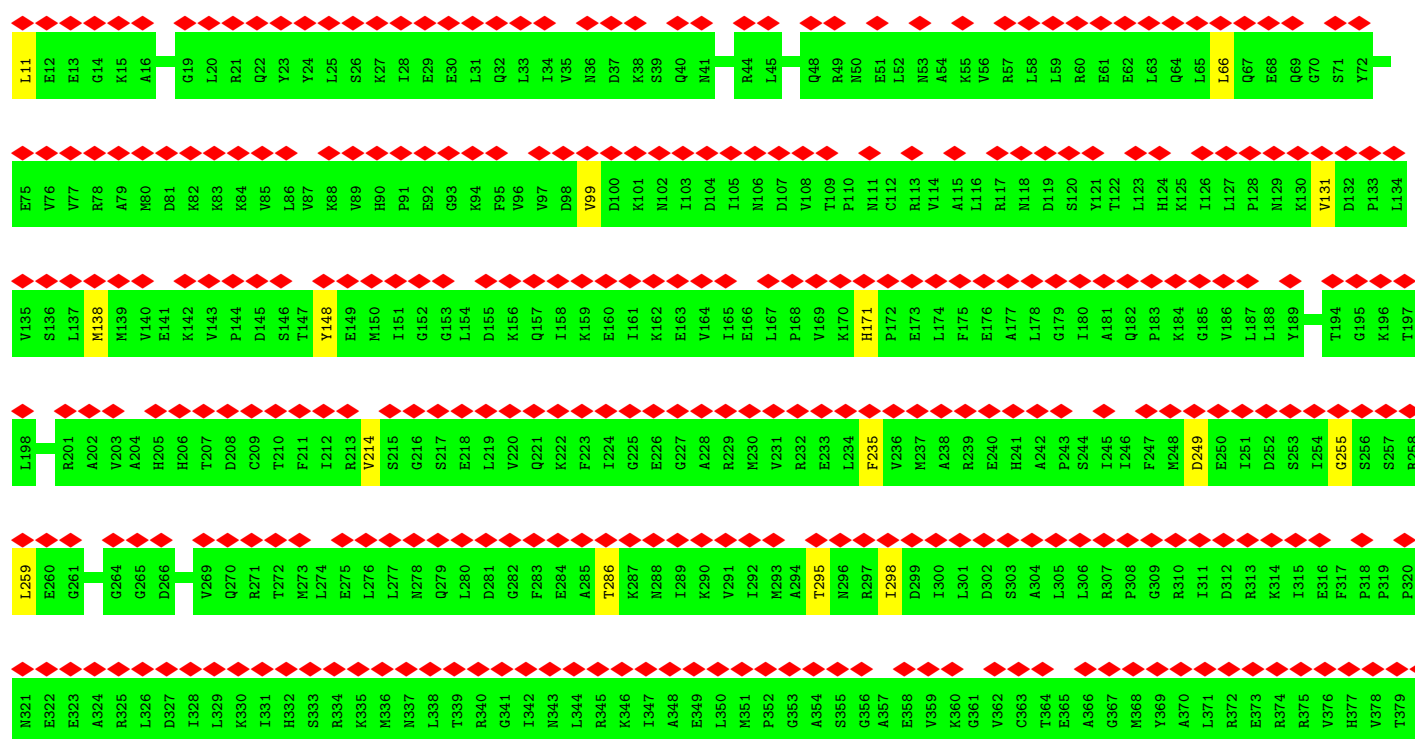
• Molecule 13: 26S protease regulatory subunit 4





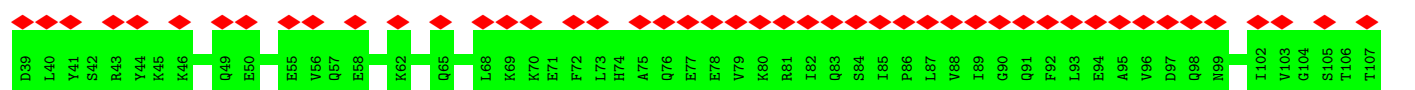
• Molecule 14: 26S protease regulatory subunit 8

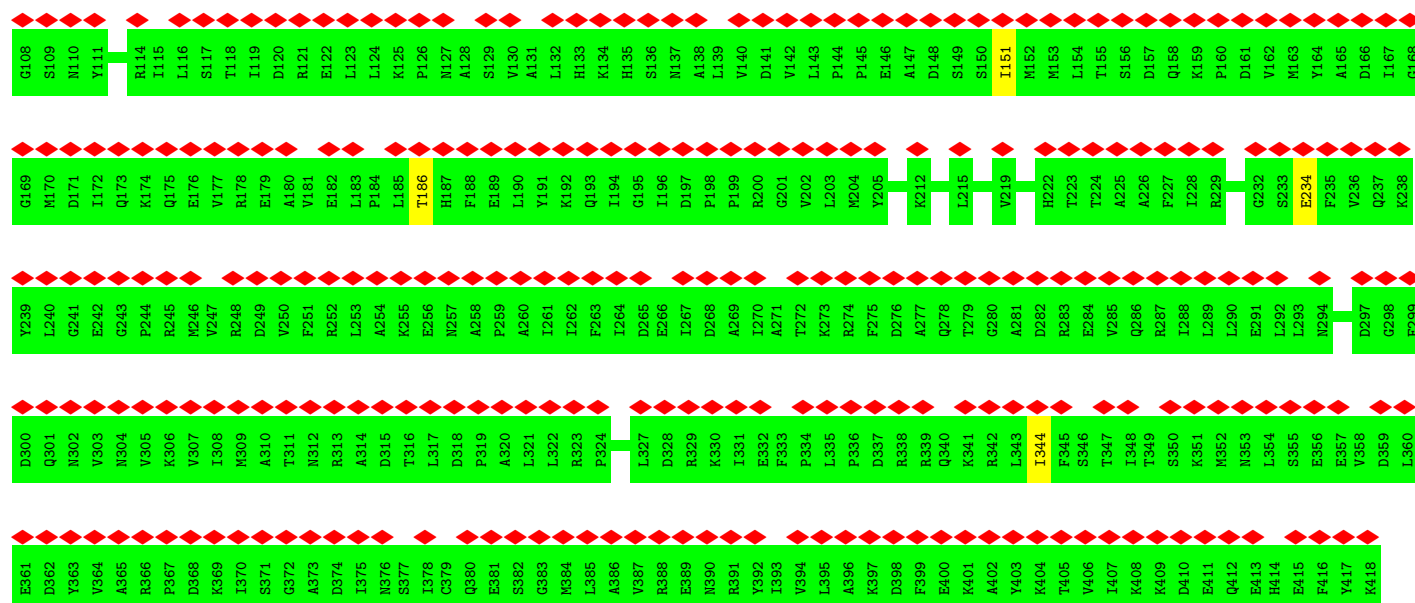
Chain C:



• Molecule 15: 26S protease regulatory subunit 6B

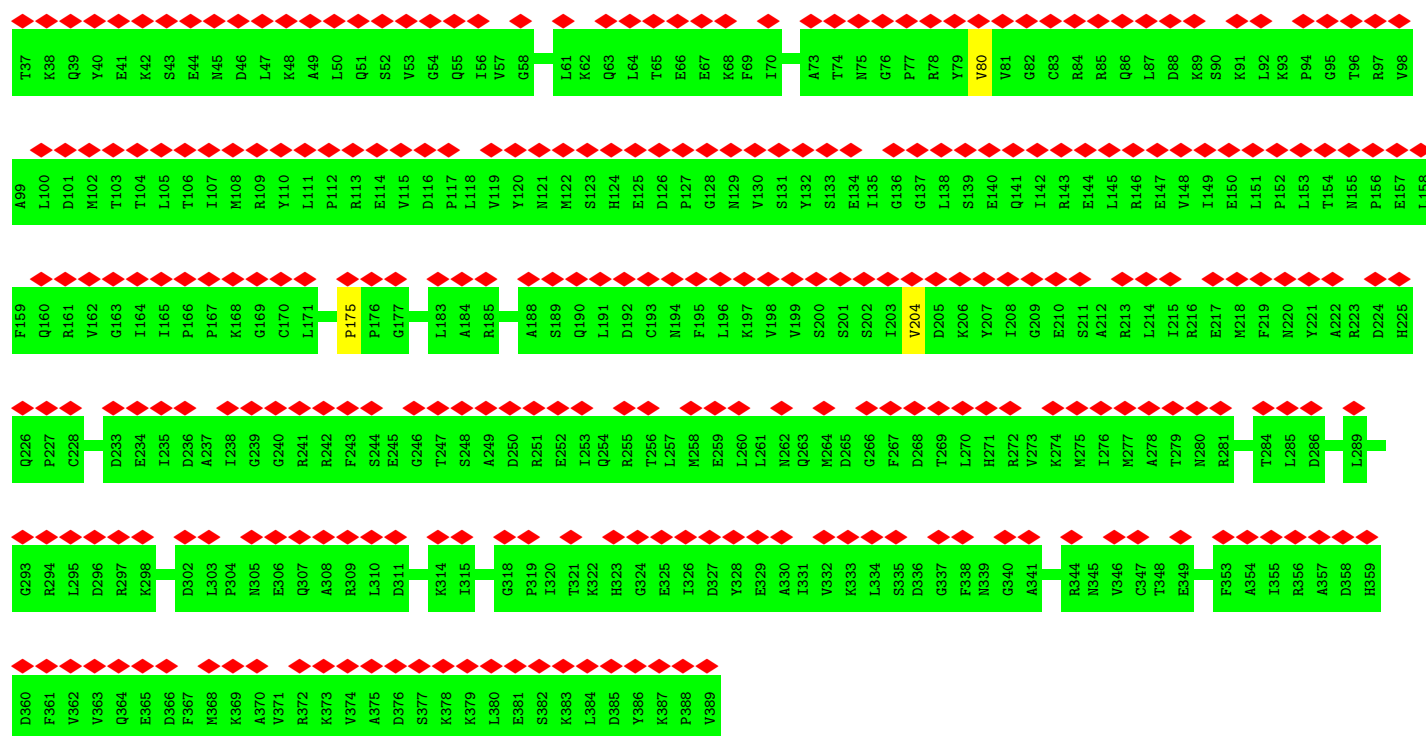
Chain D:





• Molecule 16: 26S protease regulatory subunit 10B

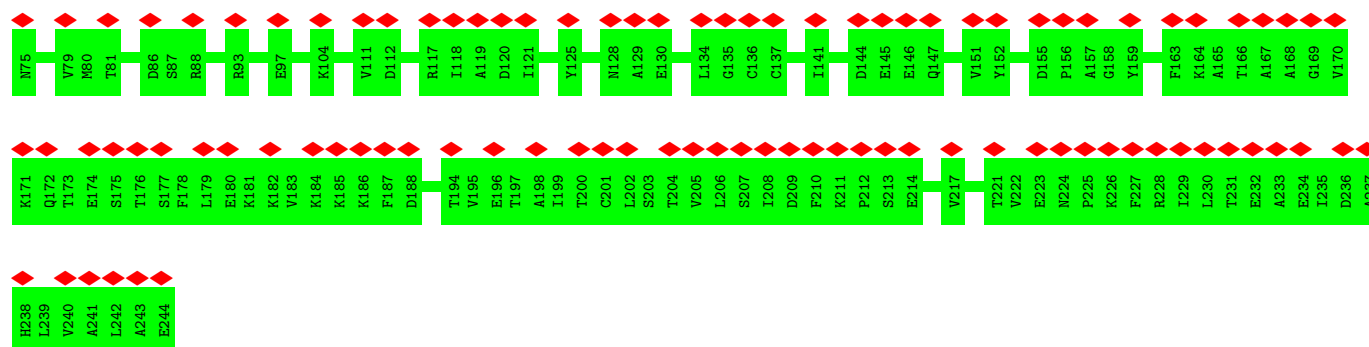
Chain E: 81% 99%



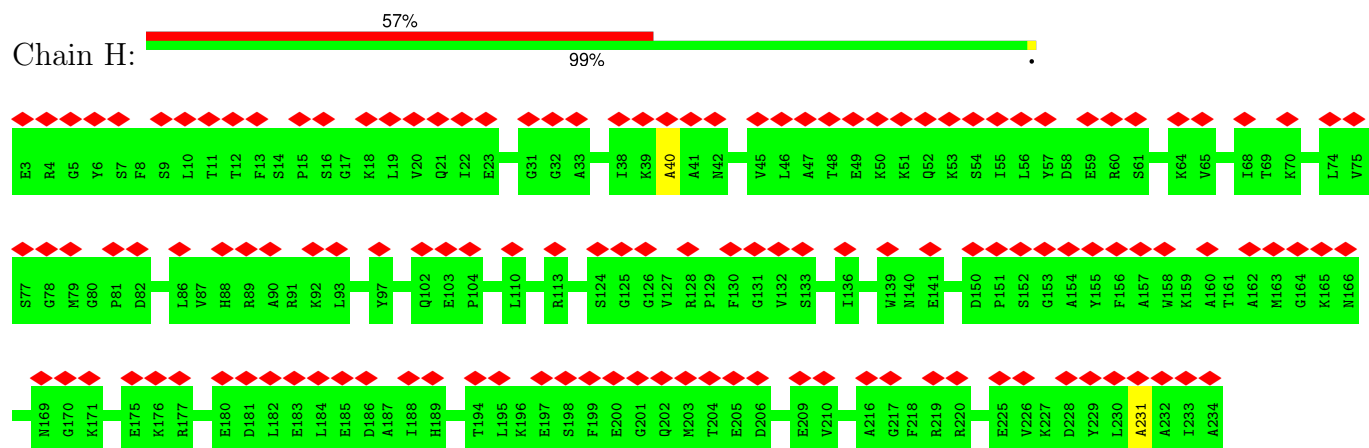
• Molecule 17: 26S protease regulatory subunit 6A

Chain F: 76% 95%

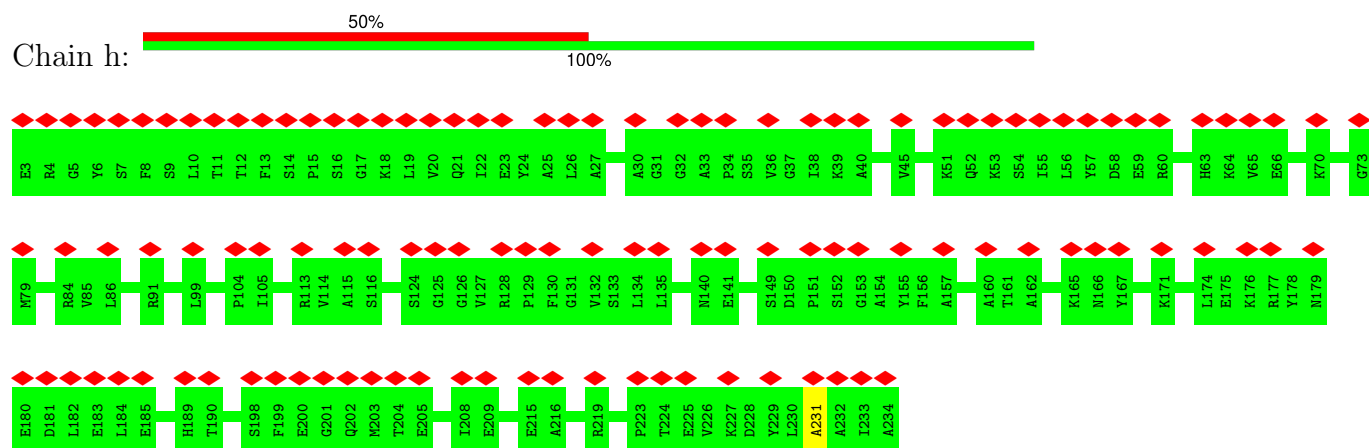




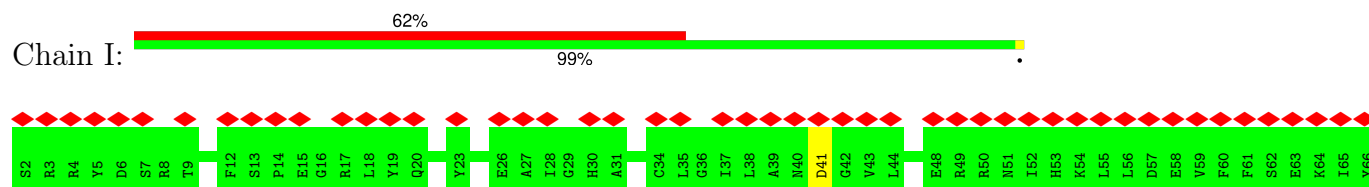
• Molecule 19: Proteasome subunit alpha type-2

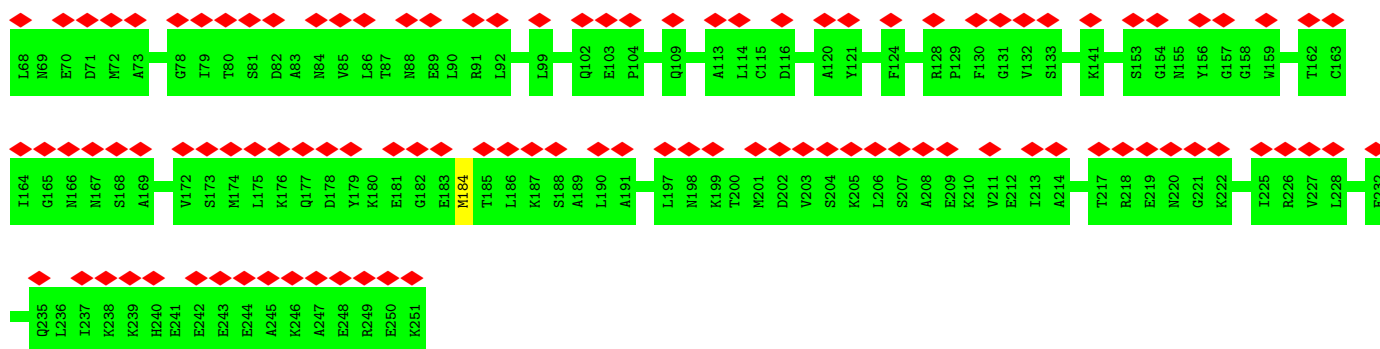


• Molecule 19: Proteasome subunit alpha type-2



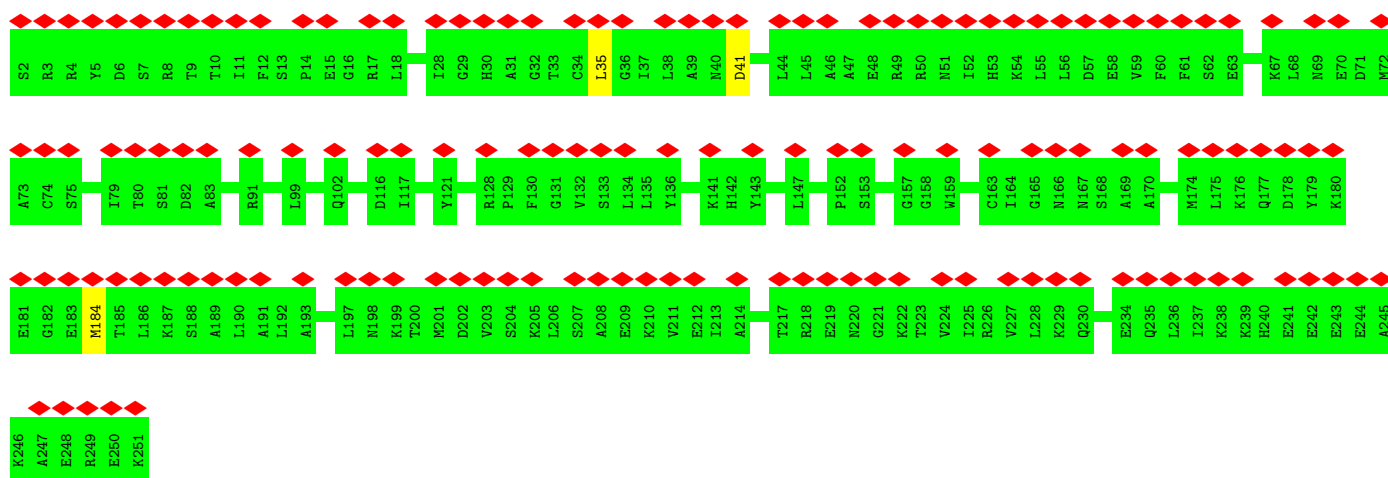
• Molecule 20: Proteasome subunit alpha type-4





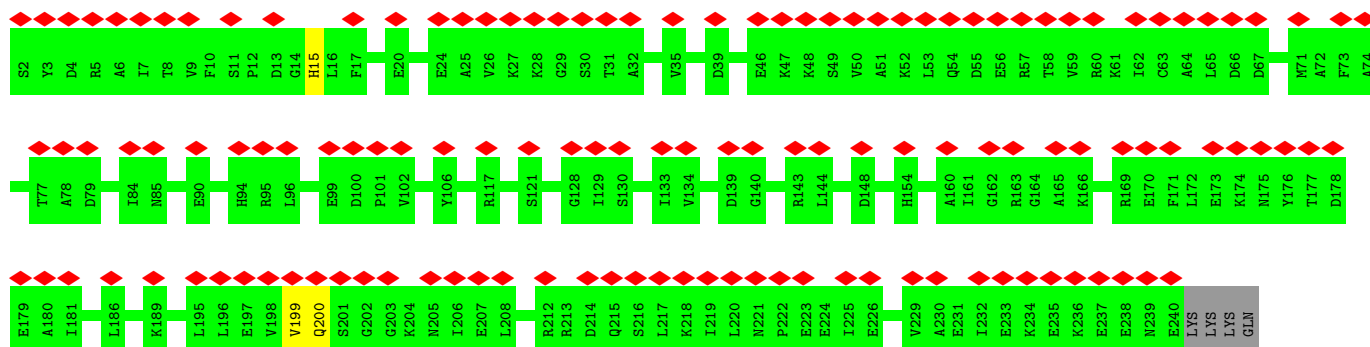
• Molecule 20: Proteasome subunit alpha type-4

Chain i: 58% 99%



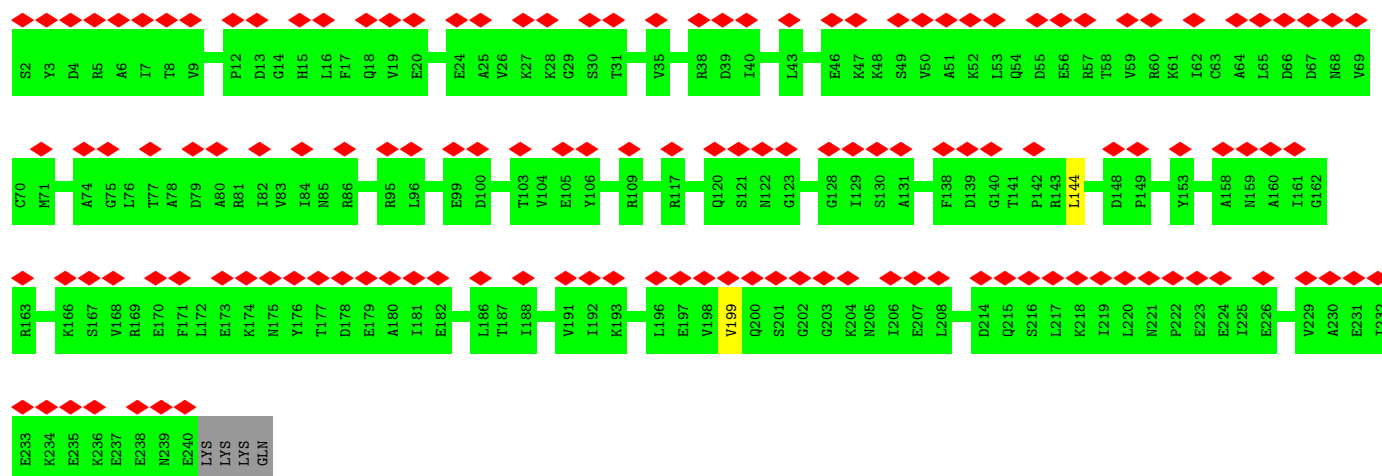
• Molecule 21: Proteasome subunit alpha type-7

Chain J: 53% 97%

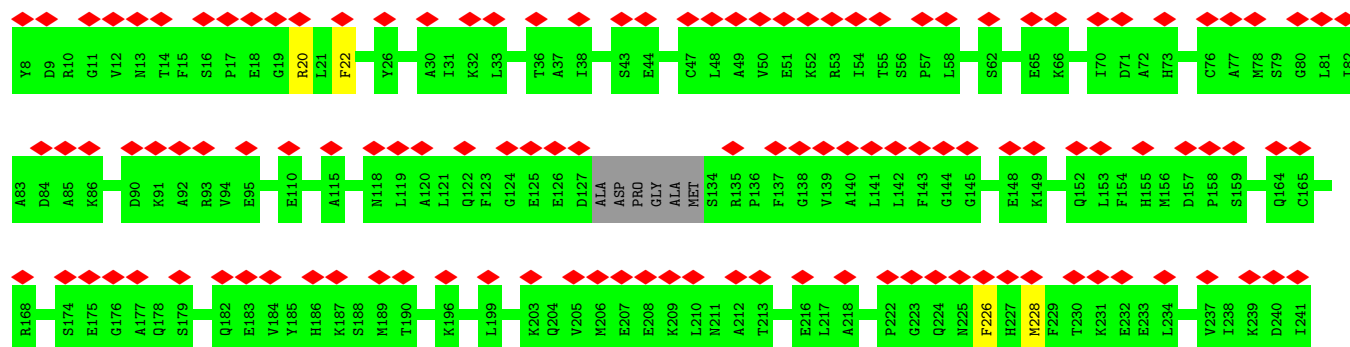


• Molecule 21: Proteasome subunit alpha type-7

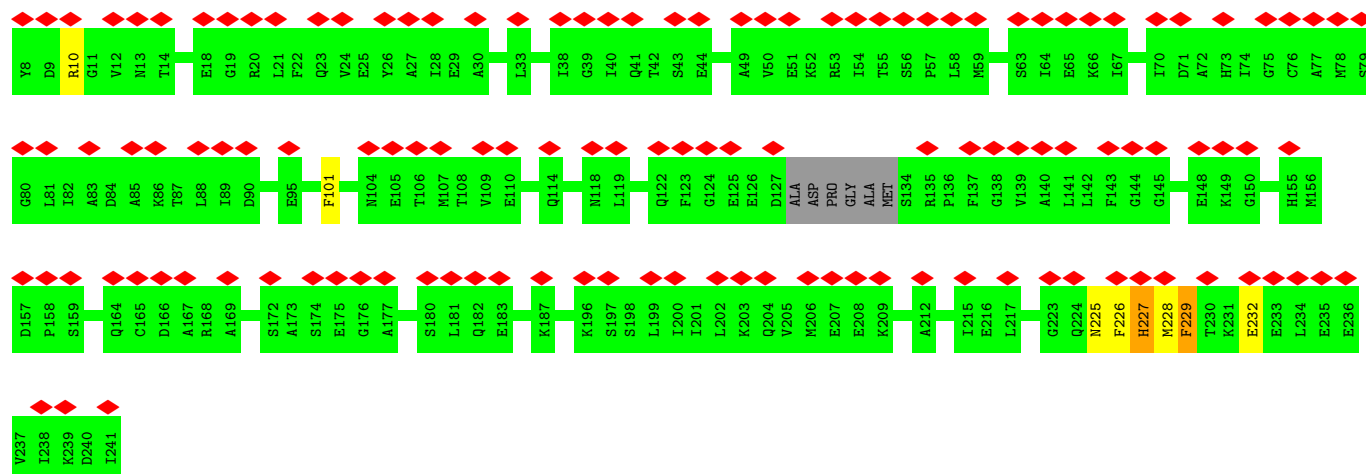
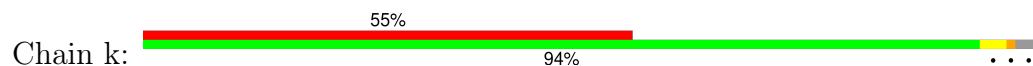
Chain j: 57% 98%



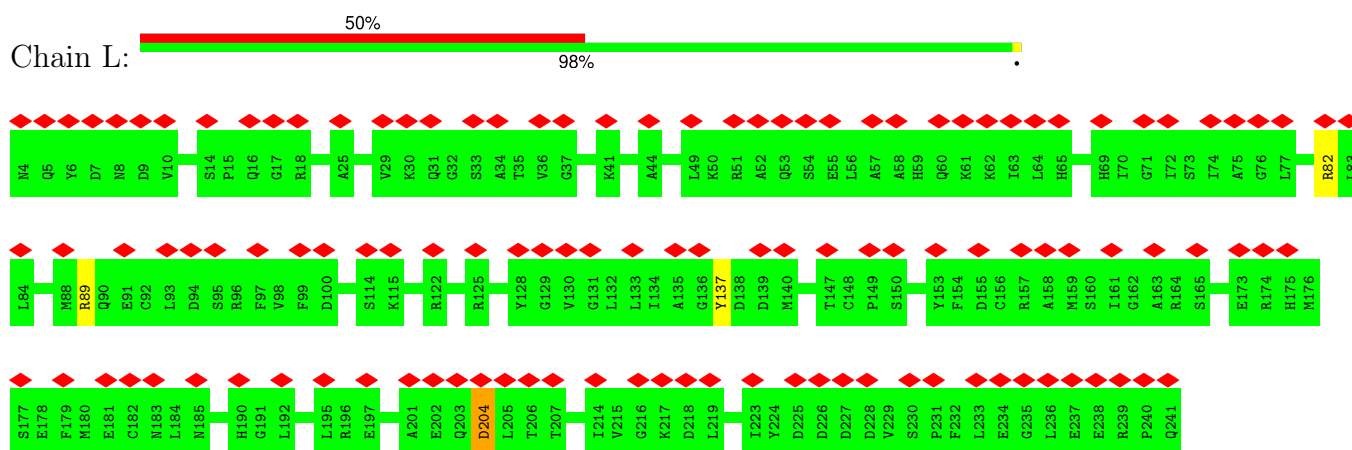
• Molecule 22: Proteasome subunit alpha type-5



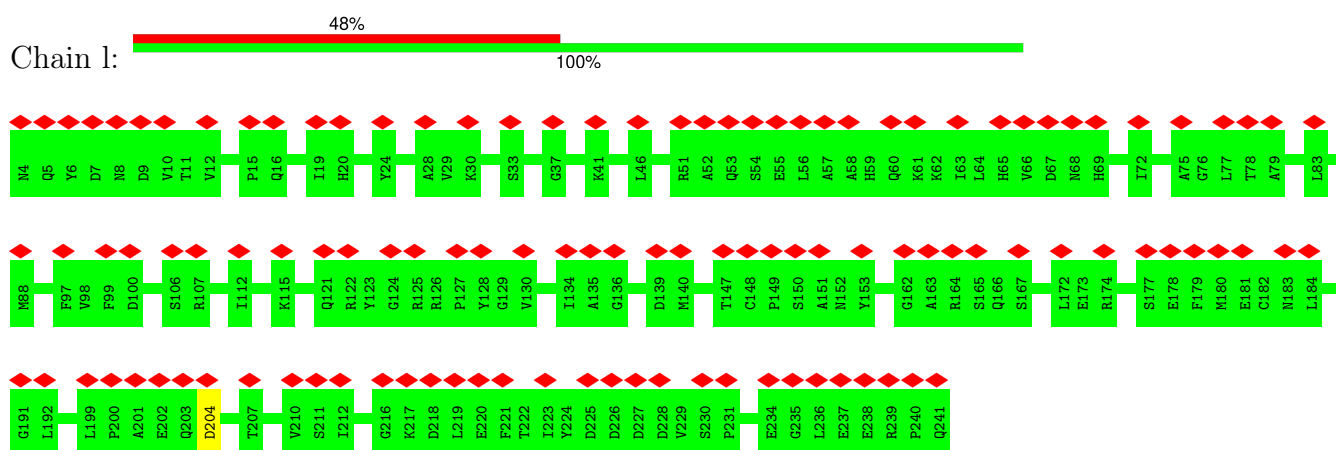
• Molecule 22: Proteasome subunit alpha type-5



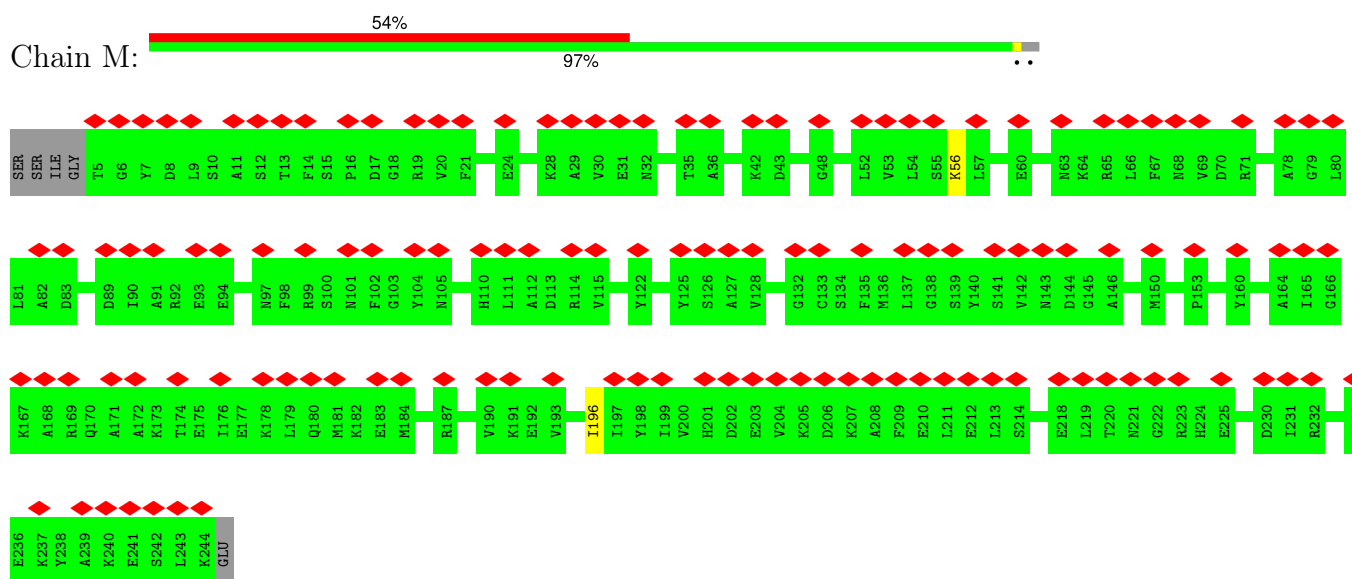
• Molecule 23: Proteasome subunit alpha type-1



• Molecule 23: Proteasome subunit alpha type-1



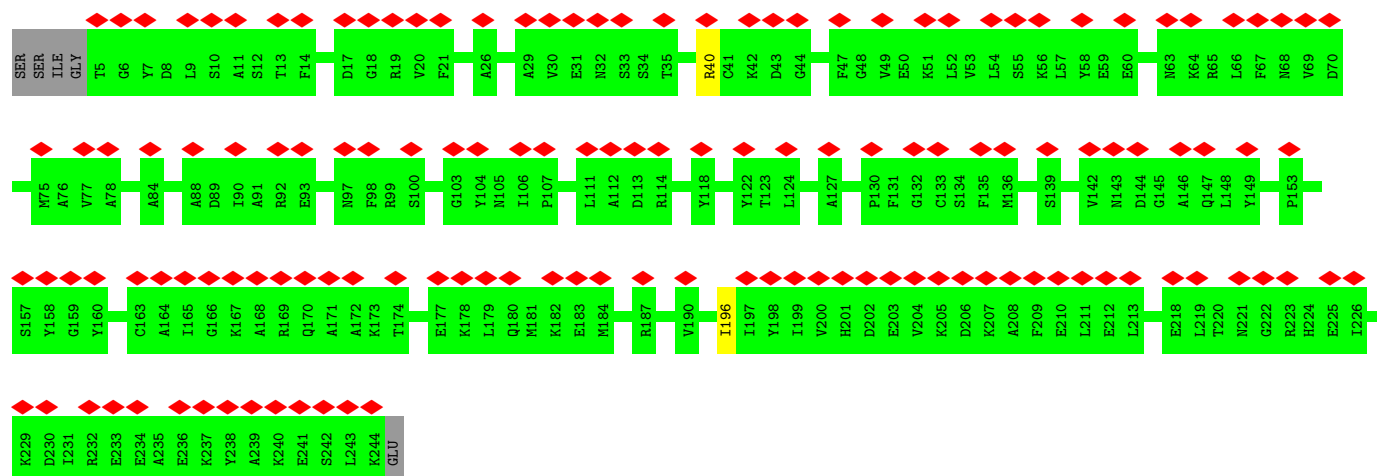
• Molecule 24: Proteasome subunit alpha type-3



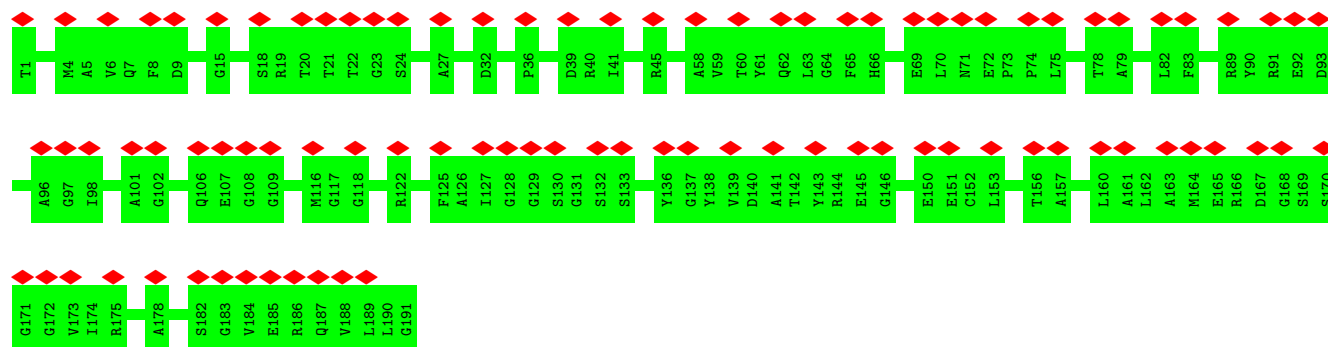
• Molecule 24: Proteasome subunit alpha type-3



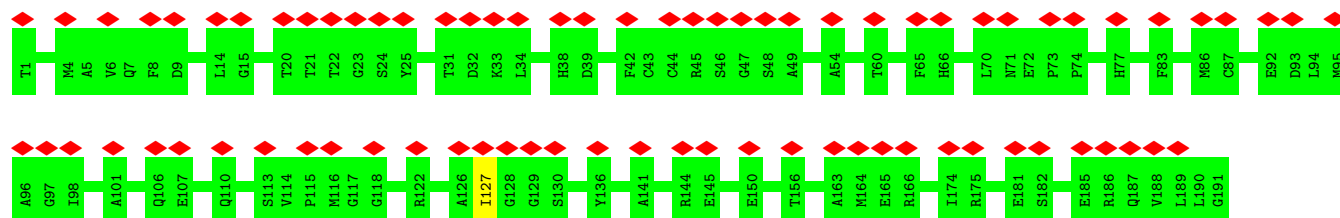
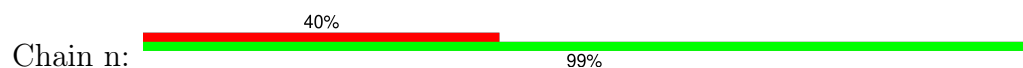




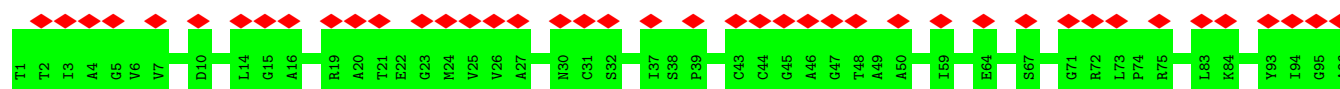
• Molecule 25: Proteasome subunit beta type-6

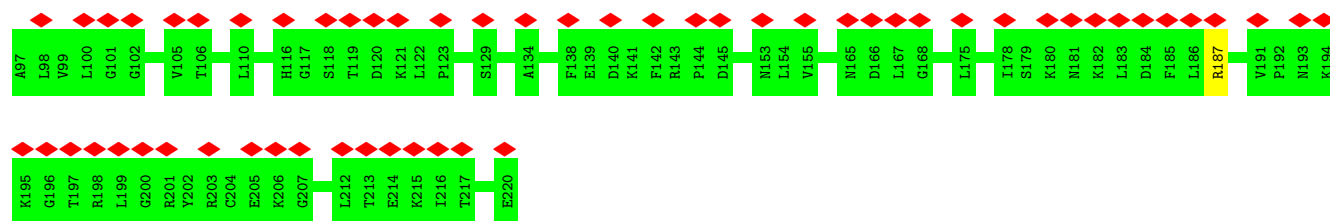


• Molecule 25: Proteasome subunit beta type-6

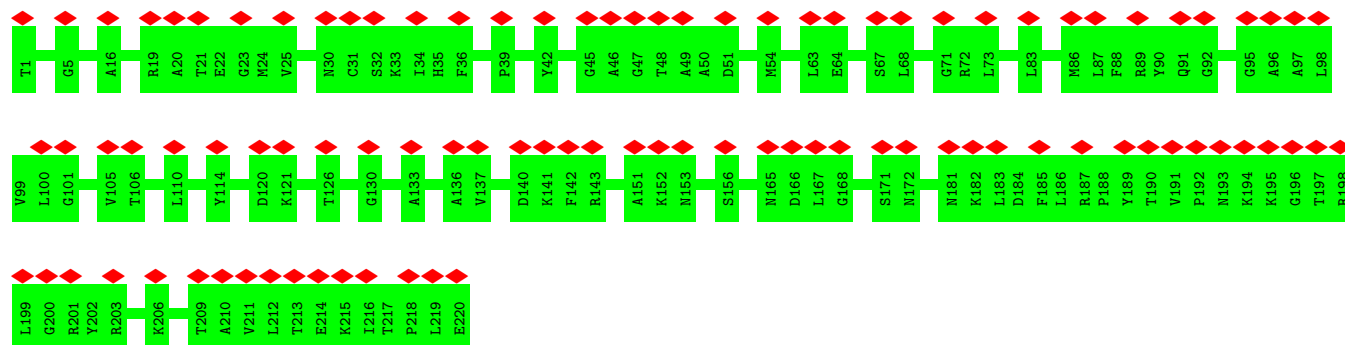
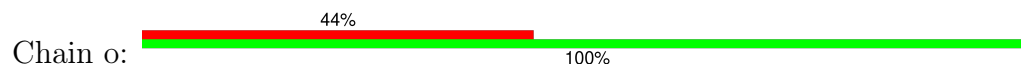


• Molecule 26: Proteasome subunit beta type-7

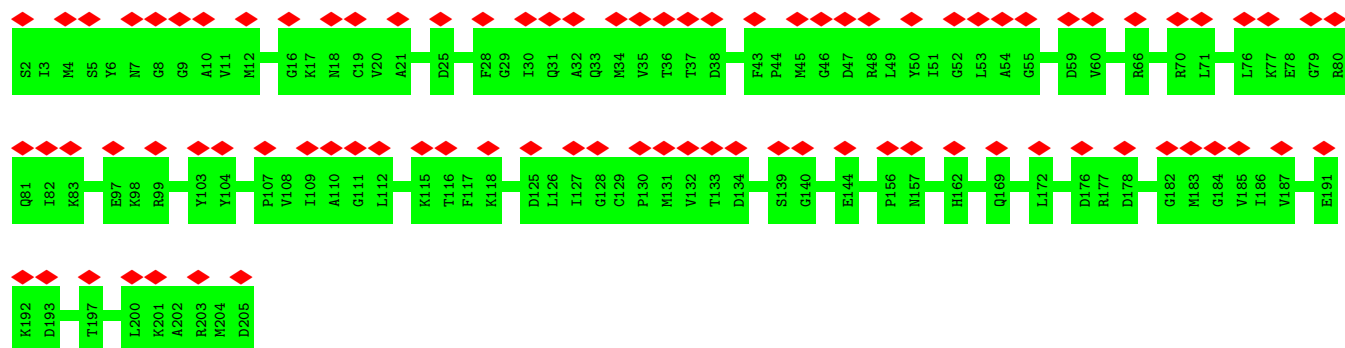
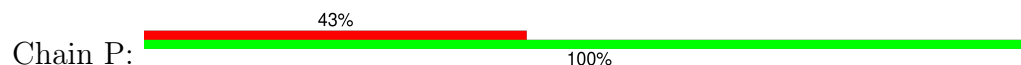




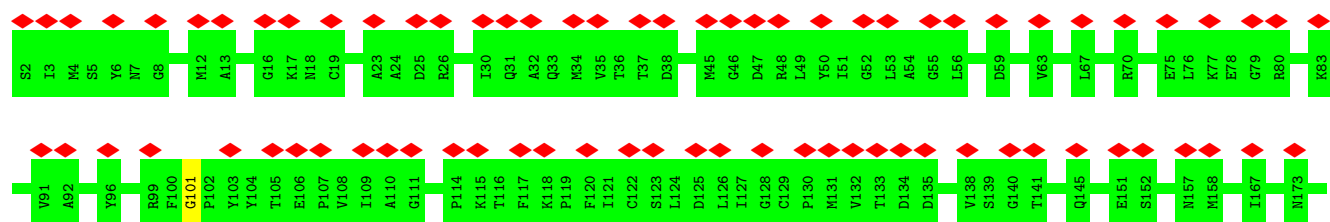
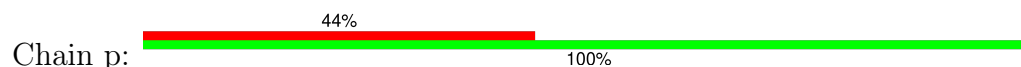
• Molecule 26: Proteasome subunit beta type-7

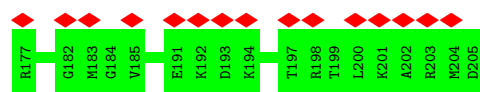


• Molecule 27: Proteasome subunit beta type-3

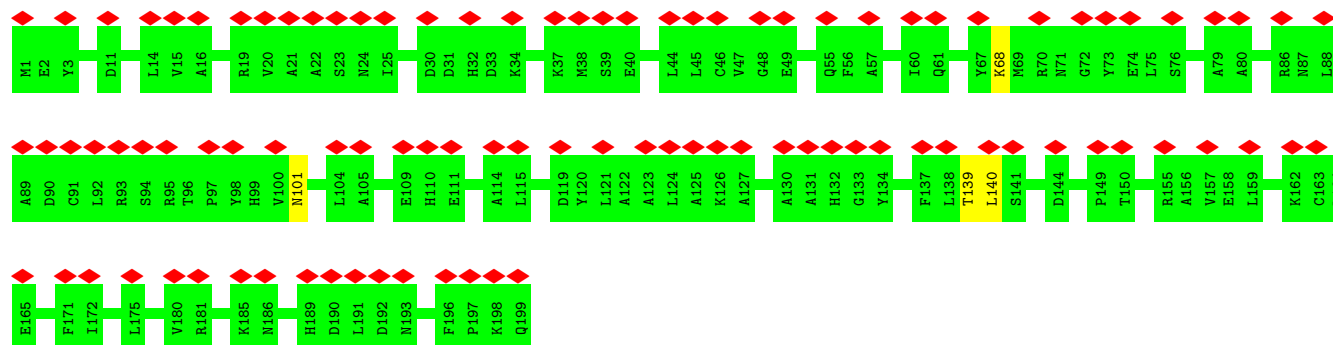


• Molecule 27: Proteasome subunit beta type-3

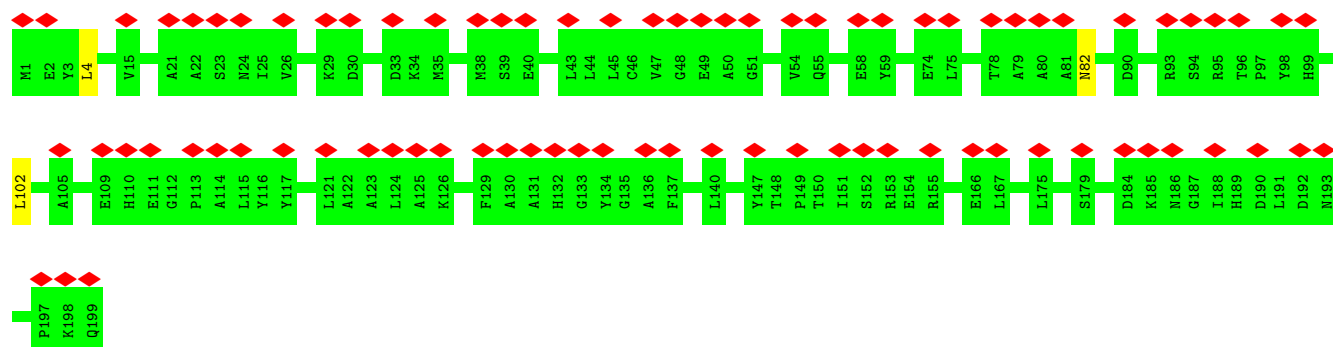
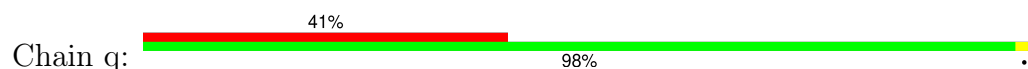




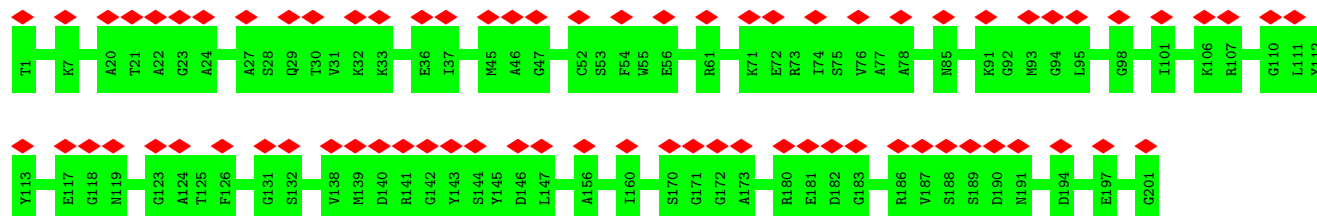
• Molecule 28: Proteasome subunit beta type-2



• Molecule 28: Proteasome subunit beta type-2

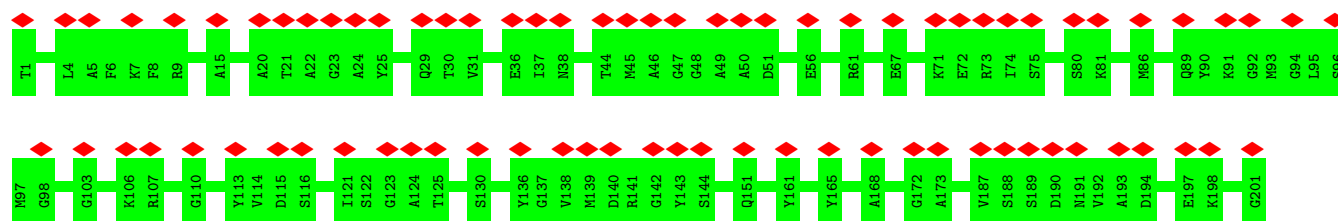


• Molecule 29: Proteasome subunit beta type-5

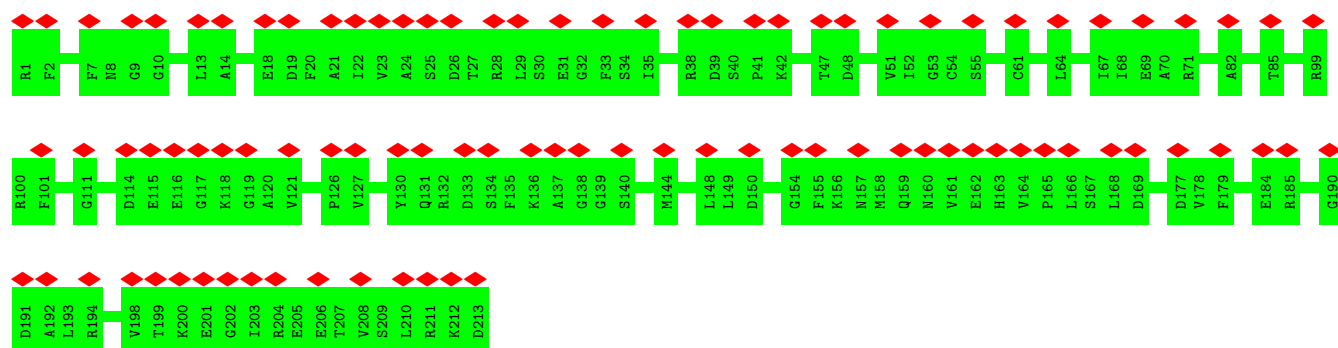


• Molecule 29: Proteasome subunit beta type-5

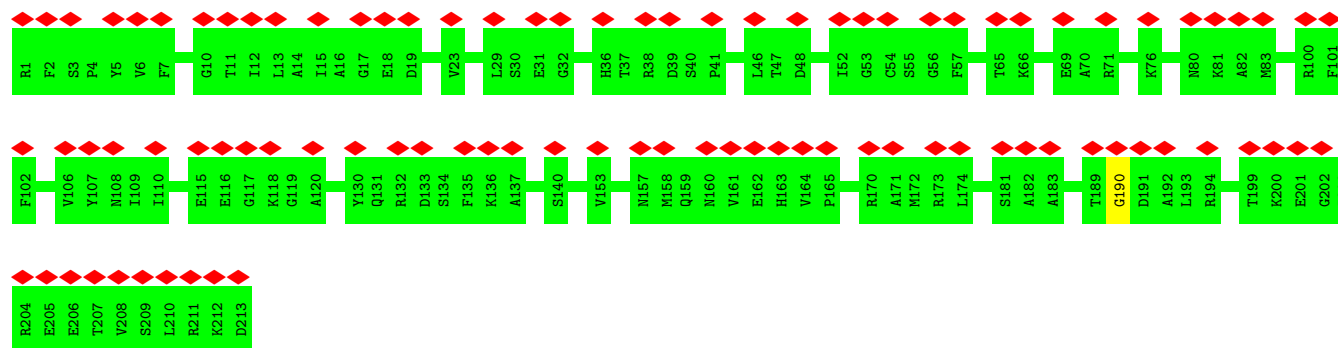
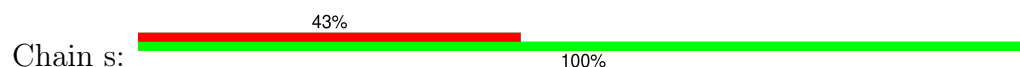




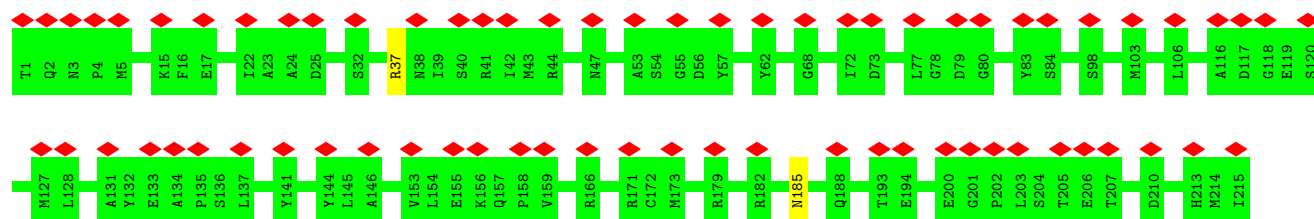
- Molecule 30: Proteasome subunit beta type-1



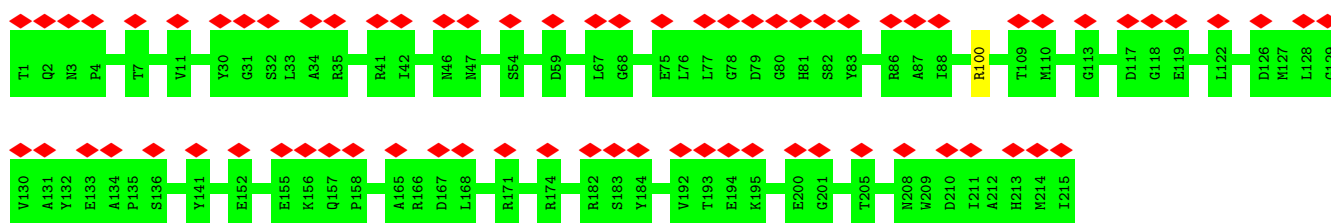
- Molecule 30: Proteasome subunit beta type-1



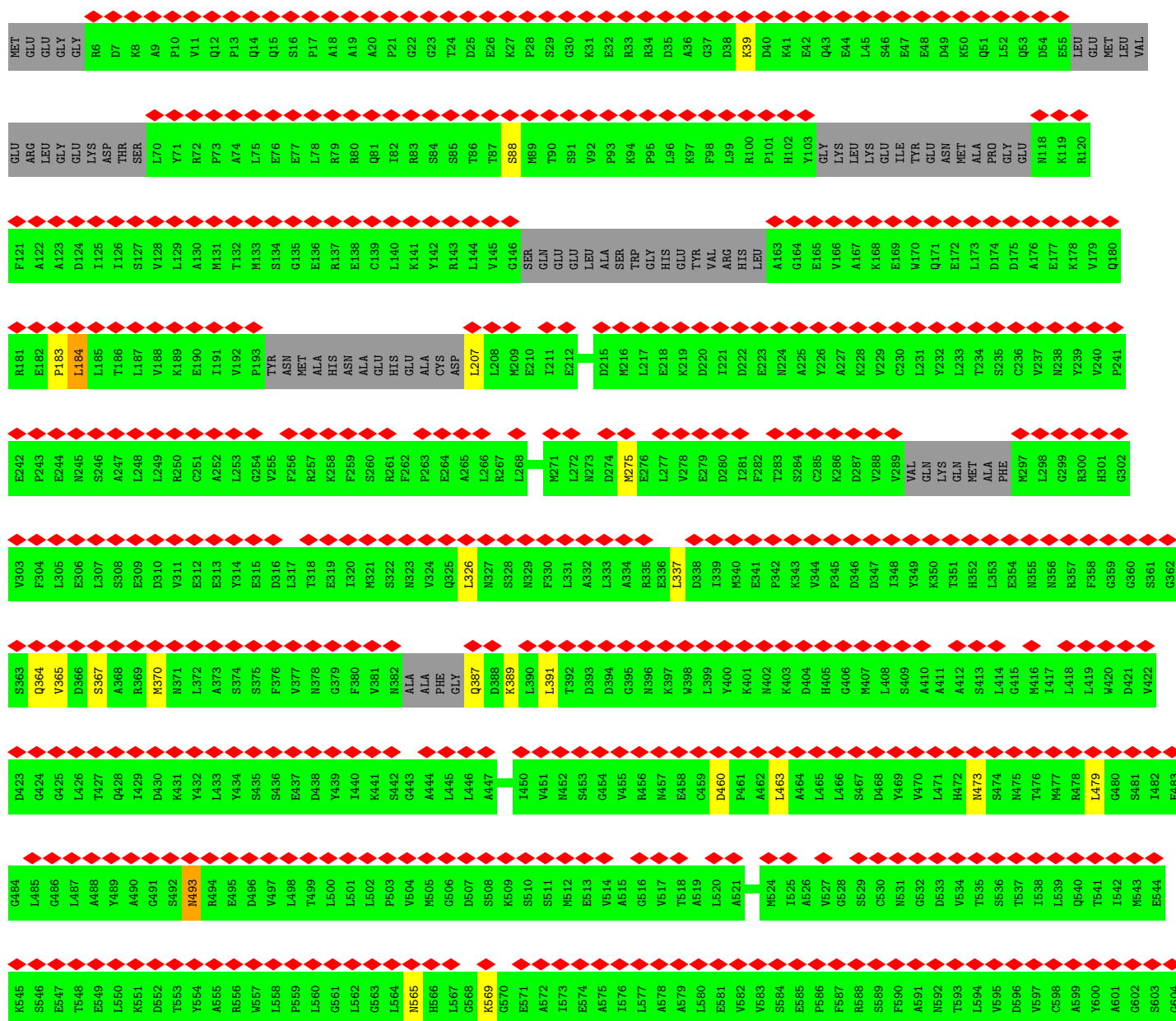
- Molecule 31: Proteasome subunit beta type-4



- Molecule 31: Proteasome subunit beta type-4



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23567	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	U	0.23	0/6396	0.41	0/8646
2	V	0.25	0/3929	0.49	0/5309
3	W	0.24	0/3751	0.46	2/5042 (0.0%)
4	X	0.23	0/1936	0.43	0/2614
5	Y	0.24	0/3173	0.45	0/4273
6	Z	0.24	0/2324	0.49	0/3150
7	a	0.23	0/3051	0.43	0/4130
8	b	0.25	0/1478	0.44	0/2001
9	c	0.28	1/2226 (0.0%)	0.48	0/3007
10	d	0.25	0/2162	0.50	0/2919
11	e	0.24	0/338	0.47	0/450
12	A	0.25	0/2885	0.48	0/3897
13	B	0.26	0/2757	0.55	0/3724
14	C	0.26	0/3054	0.48	0/4107
15	D	0.24	0/3090	0.46	0/4168
16	E	0.24	0/2835	0.44	0/3821
17	F	0.25	0/2903	0.48	0/3912
18	G	0.36	0/1858	0.59	0/2521
18	g	0.33	0/1859	0.58	0/2523
19	H	0.37	0/1743	0.59	0/2372
19	h	0.35	0/1743	0.59	1/2372 (0.0%)
20	I	0.36	0/1942	0.62	2/2628 (0.1%)
20	i	0.34	0/1942	0.63	3/2628 (0.1%)
21	J	0.38	0/1728	0.60	0/2358
21	j	0.34	0/1728	0.57	1/2358 (0.0%)
22	K	0.35	0/1747	0.59	0/2364
22	k	0.33	0/1747	0.60	0/2364
23	L	0.37	0/1885	0.59	1/2552 (0.0%)
23	l	0.33	0/1885	0.58	0/2552
24	M	0.38	0/1891	0.58	0/2552
24	m	0.34	0/1891	0.57	0/2552
25	N	0.35	0/1454	0.53	0/1967



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
25	n	0.35	0/1454	0.55	0/1967
26	O	0.34	0/1670	0.53	0/2265
26	o	0.34	0/1670	0.53	0/2265
27	P	0.35	0/1614	0.53	0/2177
27	p	0.34	0/1614	0.53	0/2177
28	Q	0.38	0/1603	0.60	0/2174
28	q	0.40	0/1603	0.65	1/2174 (0.0%)
29	R	0.38	0/1579	0.52	0/2134
29	r	0.36	0/1579	0.51	0/2134
30	S	0.35	0/1671	0.54	0/2253
30	s	0.34	0/1671	0.55	0/2253
31	T	0.37	0/1700	0.55	0/2305
31	t	0.36	0/1700	0.53	0/2305
32	f	0.32	0/5393	0.68	1/7271 (0.0%)
All	All	0.31	1/101852 (0.0%)	0.53	12/137687 (0.0%)

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
2	V	0	3
3	W	0	1
5	Y	0	2
7	a	0	1
10	d	0	1
11	e	0	1
12	A	0	1
13	B	0	1
14	C	0	2
18	G	0	1
19	H	0	2
21	J	0	2
21	j	0	1
22	K	0	1
22	k	0	3
23	L	0	2
23	l	0	1
24	M	0	1
26	O	0	1
27	p	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	Q	0	2
28	q	0	1
30	s	0	1
All	All	0	33

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	c	104	ARG	C-N	6.63	1.46	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	i	35	LEU	CA-CB-CG	6.85	131.05	115.30
19	h	231	ALA	C-N-CA	5.71	135.96	121.70
28	q	4	LEU	CB-CG-CD2	5.69	120.67	111.00
20	i	41	ASP	CB-CG-OD1	5.61	123.35	118.30
32	f	493	ASN	N-CA-C	-5.58	95.92	111.00

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	101	LEU	Peptide
2	V	319	HIS	Peptide
2	V	81	GLN	Peptide
3	W	416	GLN	Peptide
5	Y	63	TRP	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	U	798/911 (88%)	735 (92%)	62 (8%)	1 (0%)	48	83
2	V	478/480 (100%)	413 (86%)	59 (12%)	6 (1%)	10	42
3	W	454/456 (100%)	406 (89%)	45 (10%)	3 (1%)	19	57
4	X	239/380 (63%)	213 (89%)	26 (11%)	0	100	100
5	Y	376/378 (100%)	333 (89%)	38 (10%)	5 (1%)	10	42
6	Z	284/286 (99%)	253 (89%)	30 (11%)	1 (0%)	30	69
7	a	371/373 (100%)	331 (89%)	38 (10%)	2 (0%)	25	65
8	b	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
9	c	274/287 (96%)	242 (88%)	28 (10%)	4 (2%)	8	40
10	d	255/257 (99%)	227 (89%)	27 (11%)	1 (0%)	30	69
11	e	36/70 (51%)	30 (83%)	6 (17%)	0	100	100
12	A	359/361 (99%)	312 (87%)	43 (12%)	4 (1%)	12	46
13	B	346/348 (99%)	295 (85%)	46 (13%)	5 (1%)	9	40
14	C	382/384 (100%)	339 (89%)	41 (11%)	2 (0%)	25	65
15	D	378/380 (100%)	333 (88%)	44 (12%)	1 (0%)	37	73
16	E	351/353 (99%)	321 (92%)	29 (8%)	1 (0%)	37	73
17	F	362/377 (96%)	322 (89%)	38 (10%)	2 (1%)	22	61
18	G	238/240 (99%)	224 (94%)	14 (6%)	0	100	100
18	g	238/240 (99%)	226 (95%)	12 (5%)	0	100	100
19	H	230/232 (99%)	213 (93%)	17 (7%)	0	100	100
19	h	230/232 (99%)	215 (94%)	15 (6%)	0	100	100
20	I	248/250 (99%)	236 (95%)	12 (5%)	0	100	100
20	i	248/250 (99%)	228 (92%)	20 (8%)	0	100	100
21	J	237/243 (98%)	216 (91%)	20 (8%)	1 (0%)	30	69
21	j	237/243 (98%)	222 (94%)	15 (6%)	0	100	100
22	K	224/234 (96%)	205 (92%)	19 (8%)	0	100	100
22	k	224/234 (96%)	203 (91%)	18 (8%)	3 (1%)	10	42
23	L	236/238 (99%)	224 (95%)	12 (5%)	0	100	100
23	l	236/238 (99%)	222 (94%)	14 (6%)	0	100	100
24	M	238/245 (97%)	221 (93%)	17 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	m	238/245 (97%)	220 (92%)	18 (8%)	0	100	100
25	N	189/191 (99%)	179 (95%)	10 (5%)	0	100	100
25	n	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
26	O	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
26	o	218/220 (99%)	211 (97%)	7 (3%)	0	100	100
27	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
27	p	202/204 (99%)	186 (92%)	16 (8%)	0	100	100
28	Q	197/199 (99%)	179 (91%)	18 (9%)	0	100	100
28	q	197/199 (99%)	177 (90%)	20 (10%)	0	100	100
29	R	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
29	r	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
30	S	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
30	s	211/213 (99%)	201 (95%)	10 (5%)	0	100	100
31	T	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
31	t	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	11	44
All	All	12761/13430 (95%)	11639 (91%)	1072 (8%)	50 (0%)	32	69

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	364	VAL
2	V	82	LEU
2	V	83	GLU
2	V	84	LYS
3	W	68	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 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	U	685/779 (88%)	681 (99%)	4 (1%)	84	88
2	V	414/414 (100%)	406 (98%)	8 (2%)	52	69
3	W	416/416 (100%)	410 (99%)	6 (1%)	62	75
4	X	208/327 (64%)	207 (100%)	1 (0%)	86	89
5	Y	334/334 (100%)	332 (99%)	2 (1%)	84	88
6	Z	257/257 (100%)	252 (98%)	5 (2%)	52	69
7	a	333/333 (100%)	331 (99%)	2 (1%)	84	88
8	b	167/167 (100%)	165 (99%)	2 (1%)	67	78
9	c	243/252 (96%)	240 (99%)	3 (1%)	67	78
10	d	231/231 (100%)	229 (99%)	2 (1%)	75	83
11	e	38/63 (60%)	36 (95%)	2 (5%)	19	40
12	A	308/308 (100%)	303 (98%)	5 (2%)	58	73
13	B	304/304 (100%)	295 (97%)	9 (3%)	36	55
14	C	332/332 (100%)	321 (97%)	11 (3%)	33	52
15	D	333/333 (100%)	330 (99%)	3 (1%)	75	83
16	E	308/308 (100%)	306 (99%)	2 (1%)	84	88
17	F	312/321 (97%)	306 (98%)	6 (2%)	52	69
18	G	192/205 (94%)	192 (100%)	0	100	100
18	g	193/205 (94%)	193 (100%)	0	100	100
19	H	164/190 (86%)	164 (100%)	0	100	100
19	h	164/190 (86%)	164 (100%)	0	100	100
20	I	193/210 (92%)	193 (100%)	0	100	100
20	i	193/210 (92%)	193 (100%)	0	100	100
21	J	152/207 (73%)	152 (100%)	0	100	100
21	j	152/207 (73%)	152 (100%)	0	100	100
22	K	186/196 (95%)	183 (98%)	3 (2%)	58	73
22	k	186/196 (95%)	182 (98%)	4 (2%)	47	65
23	L	198/204 (97%)	196 (99%)	2 (1%)	73	82
23	l	198/204 (97%)	198 (100%)	0	100	100
24	M	192/202 (95%)	191 (100%)	1 (0%)	86	89
24	m	192/202 (95%)	190 (99%)	2 (1%)	73	82
25	N	148/148 (100%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	n	148/148 (100%)	147 (99%)	1 (1%)	81	87
26	O	177/181 (98%)	177 (100%)	0	100	100
26	o	177/181 (98%)	177 (100%)	0	100	100
27	P	172/173 (99%)	172 (100%)	0	100	100
27	p	172/173 (99%)	172 (100%)	0	100	100
28	Q	164/170 (96%)	162 (99%)	2 (1%)	67	78
28	q	164/170 (96%)	163 (99%)	1 (1%)	84	88
29	R	153/156 (98%)	153 (100%)	0	100	100
29	r	153/156 (98%)	153 (100%)	0	100	100
30	S	174/178 (98%)	174 (100%)	0	100	100
30	s	174/178 (98%)	174 (100%)	0	100	100
31	T	175/178 (98%)	173 (99%)	2 (1%)	70	80
31	t	175/178 (98%)	174 (99%)	1 (1%)	84	88
32	f	580/763 (76%)	559 (96%)	21 (4%)	30	50
All	All	10684/11438 (93%)	10571 (99%)	113 (1%)	69	80

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	C	235	PHE
32	f	662	MET
17	F	282	ILE
32	f	641	GLU
32	f	389	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
15	D	302	ASN
20	I	95	GLN
31	t	81	HIS
15	D	412	GLN
17	F	323	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.

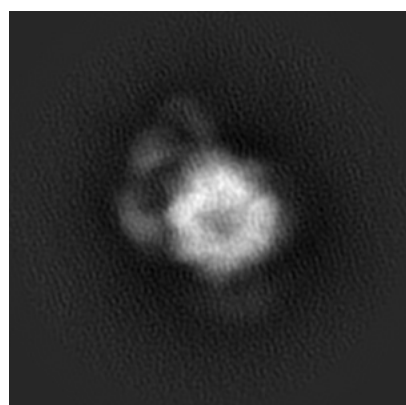
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8668. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

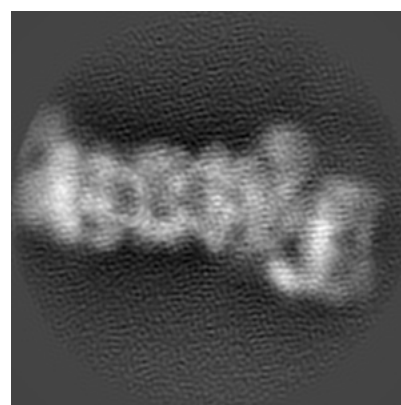
#### 6.1.1 Primary map



X



Y

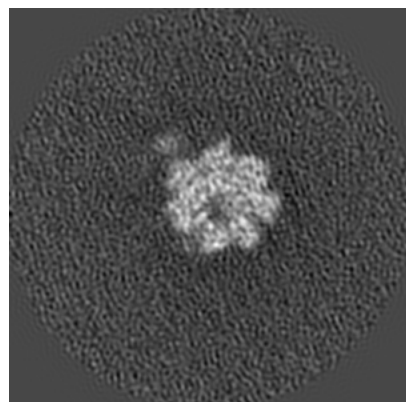


Z

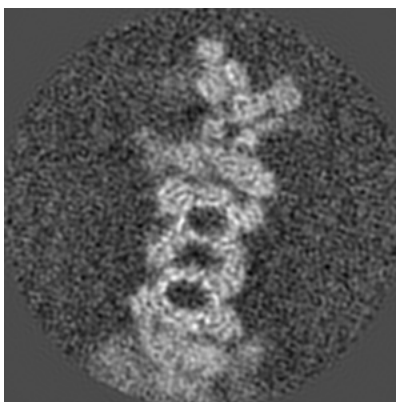
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

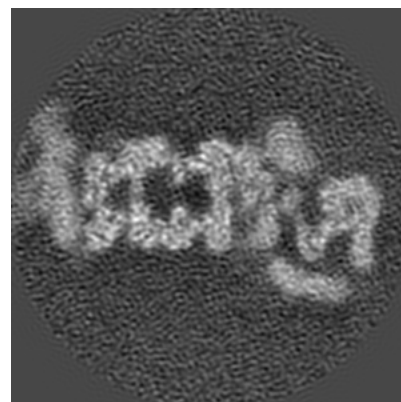
#### 6.2.1 Primary map



X Index: 280



Y Index: 280



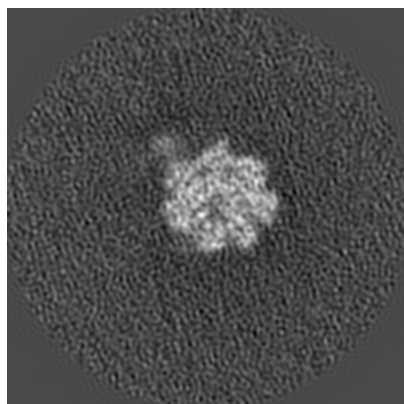
Z Index: 280



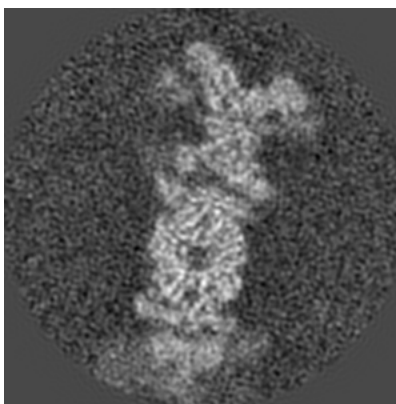
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

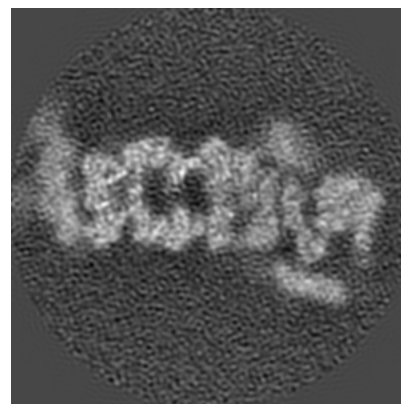
### 6.3.1 Primary map



X Index: 282



Y Index: 264

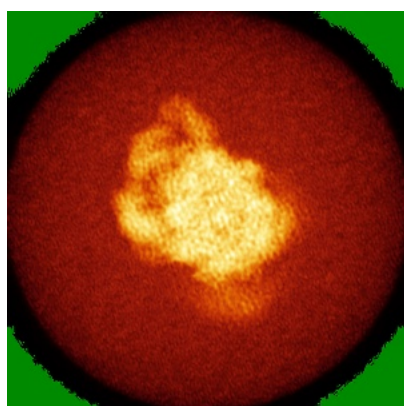


Z Index: 286

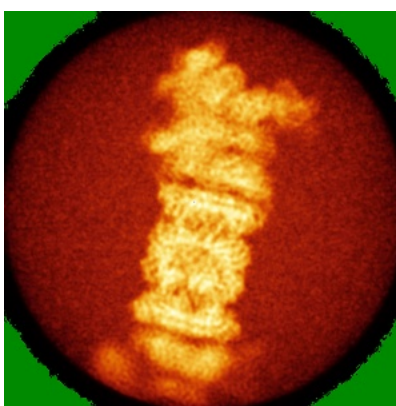
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

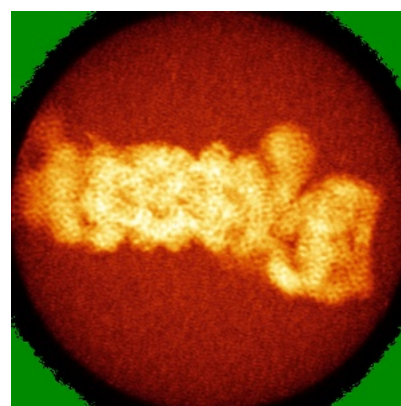
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

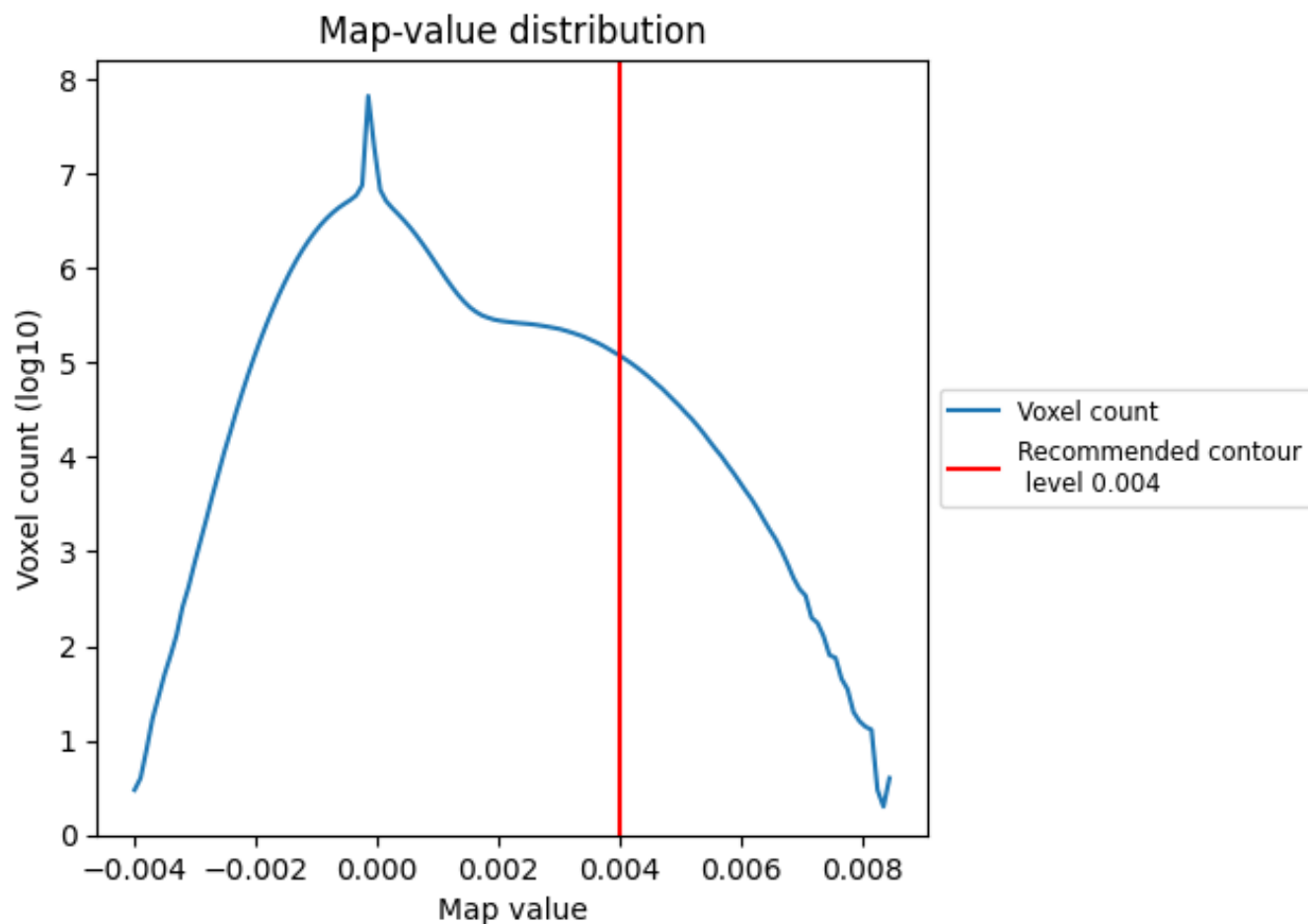
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

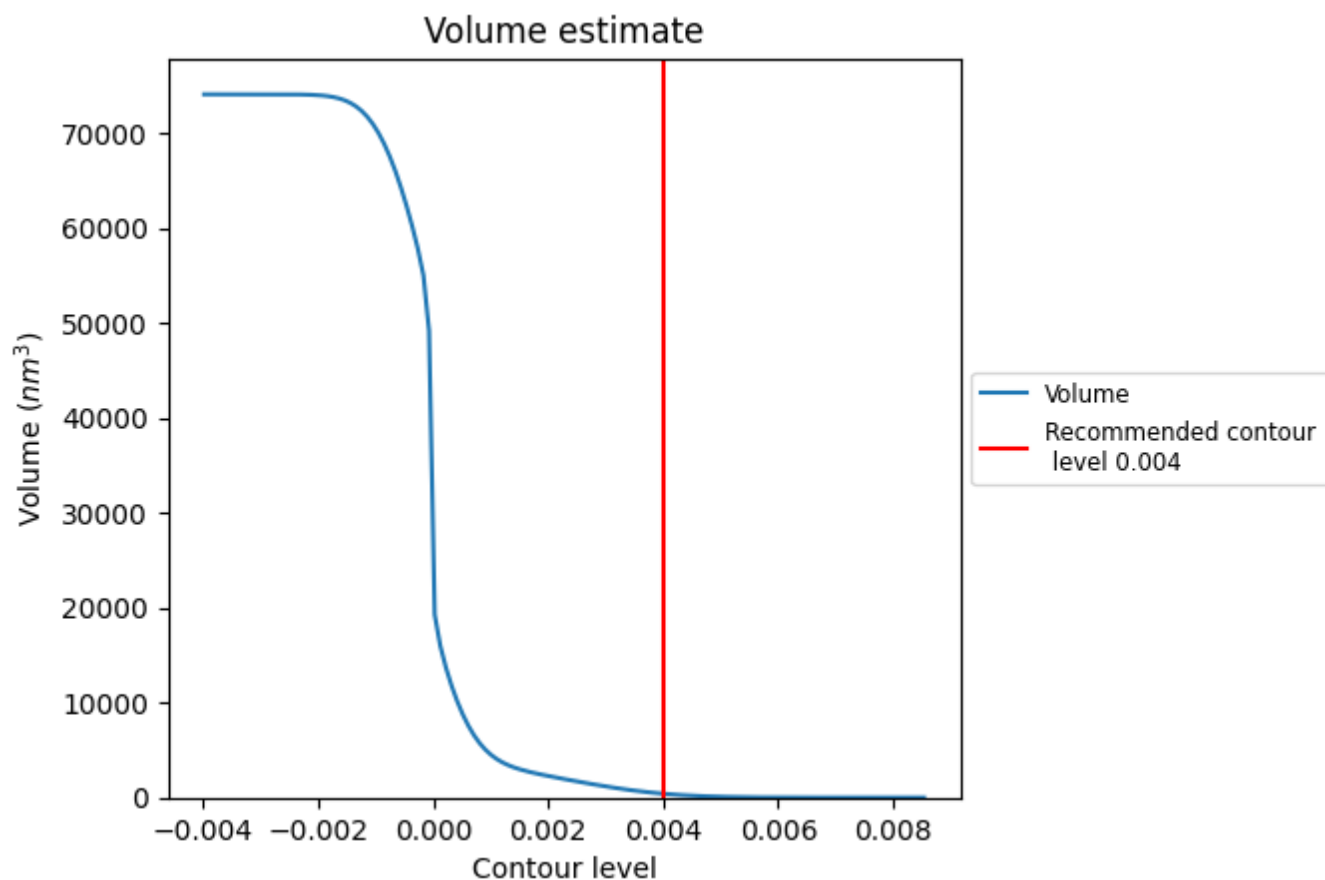
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

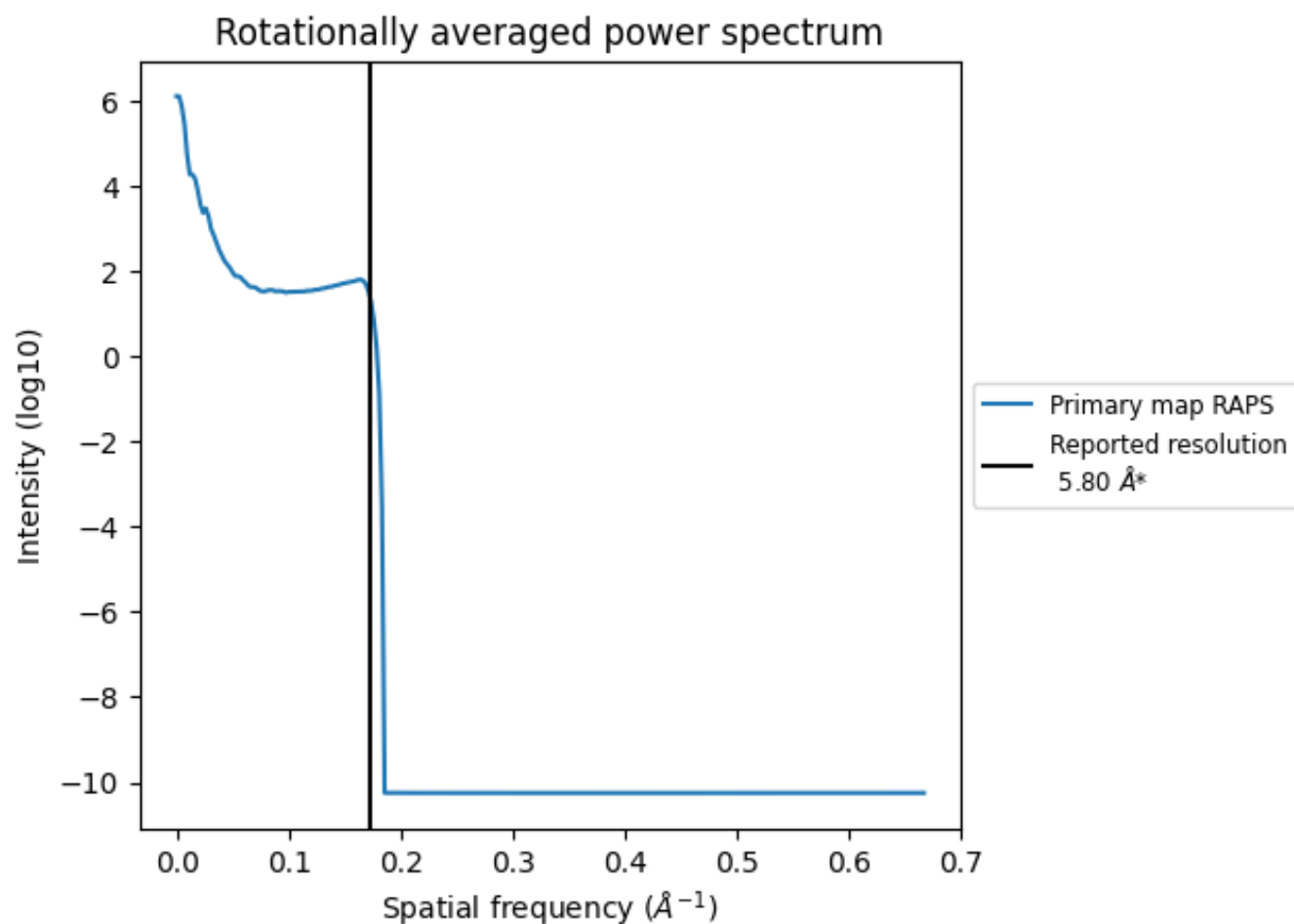
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 405 nm<sup>3</sup>; this corresponds to an approximate mass of 366 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.172  $\text{\AA}^{-1}$

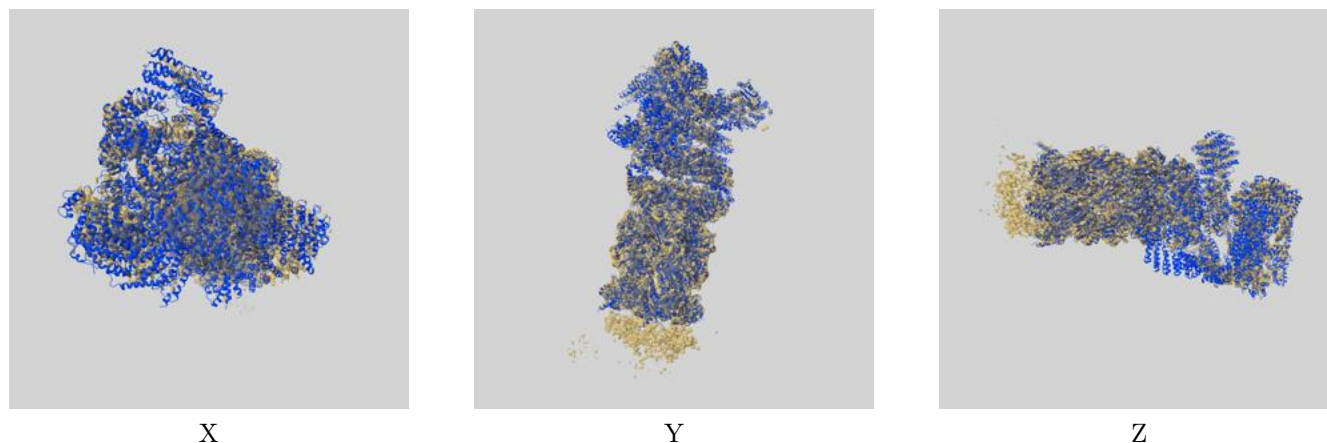
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

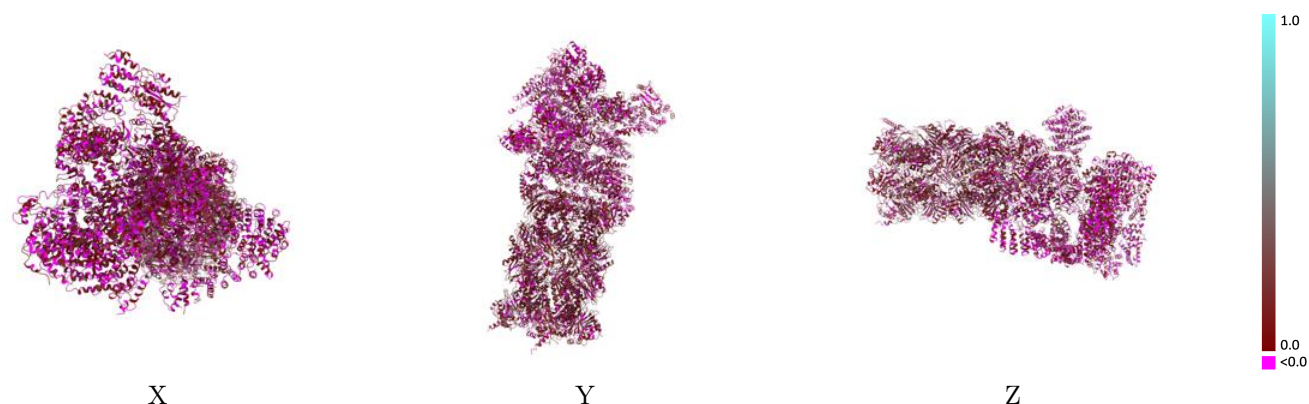
This section contains information regarding the fit between EMDB map EMD-8668 and PDB model 5VFU. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



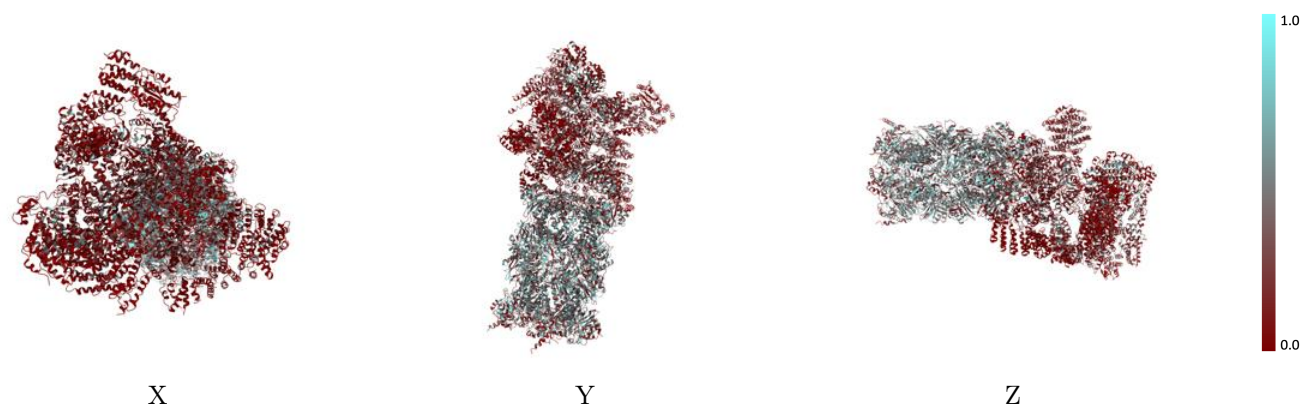
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

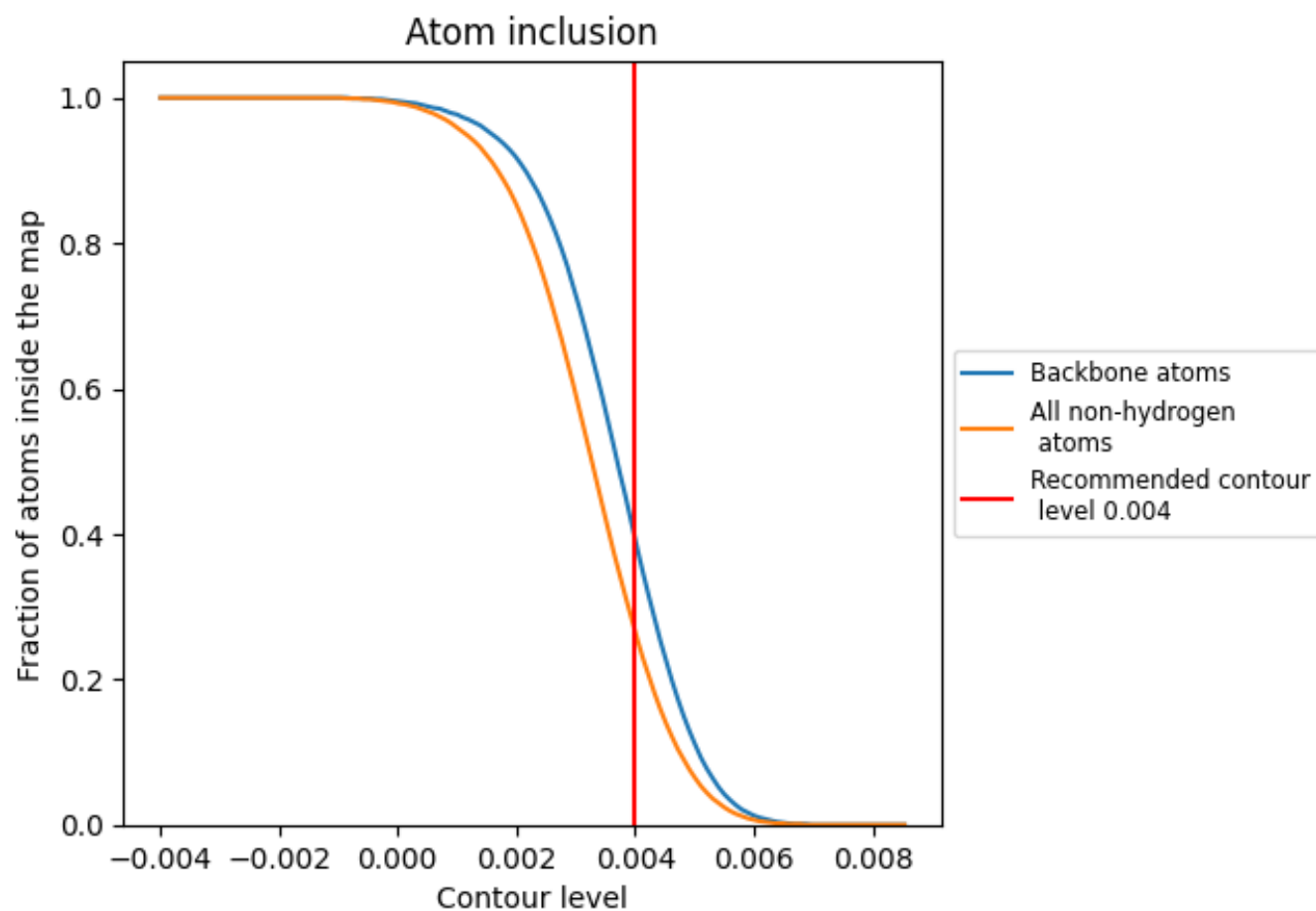
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 39% of all backbone atoms, 27% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

























The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2660	 0.0980
A	 0.2200	 0.0990
B	 0.1390	 0.0780
C	 0.1390	 0.0700
D	 0.1580	 0.0620
E	 0.1750	 0.0740
F	 0.1900	 0.0820
G	 0.3340	 0.1230
H	 0.3590	 0.1240
I	 0.3240	 0.1260
J	 0.3840	 0.1400
K	 0.3600	 0.1350
L	 0.4080	 0.1320
M	 0.3730	 0.1270
N	 0.4330	 0.1320
O	 0.4280	 0.1470
P	 0.4560	 0.1280
Q	 0.4330	 0.1480
R	 0.4850	 0.1440
S	 0.4390	 0.1460
T	 0.4970	 0.1530
U	 0.2190	 0.0670
V	 0.1150	 0.0620
W	 0.0590	 0.0590
X	 0.0580	 0.0180
Y	 0.1650	 0.0630
Z	 0.1760	 0.0760
a	 0.0840	 0.0600
b	 0.0790	 0.0550
c	 0.2020	 0.0920
d	 0.0790	 0.0290
e	 0.0610	 0.0310
f	 0.0640	 0.0400
g	 0.3650	 0.1320
h	 0.3980	 0.1420



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Chain	Atom inclusion	Q-score
i	 0.3310	 0.1280
j	 0.3490	 0.1290
k	 0.3650	 0.1410
l	 0.4020	 0.1280
m	 0.3610	 0.1150
n	 0.4620	 0.1440
o	 0.4440	 0.1520
p	 0.4520	 0.1350
q	 0.4460	 0.1370
r	 0.4670	 0.1380
s	 0.4490	 0.1400
t	 0.4980	 0.1630