



## Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 09:27 AM 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 Full wwPDB EM Validation 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:

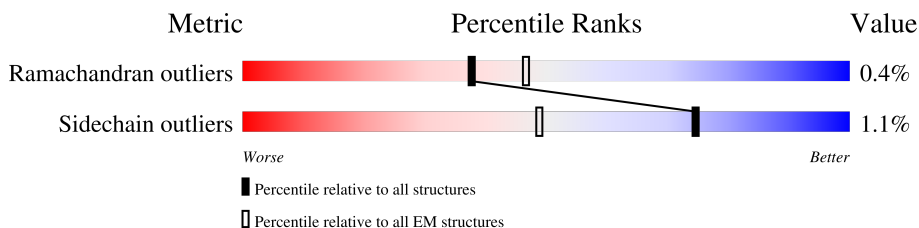
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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	154571	4023
Sidechain outliers	154315	3826

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	
2	V	480	
3	W	456	
4	X	380	
5	Y	378	
6	Z	286	
7	a	373	
8	b	191	
9	c	287	

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

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

## 2 Entry composition [i](#)

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
			Total	C	N	O	S		
1	U	806	6287	3990	1075	1178	44	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
8	b	191	1458	910	261	279	8	0	0

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

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

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

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

- Molecule 11 is a protein called Sem1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
30	s	213	1641	1036	282	313	10	0	0

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

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

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

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

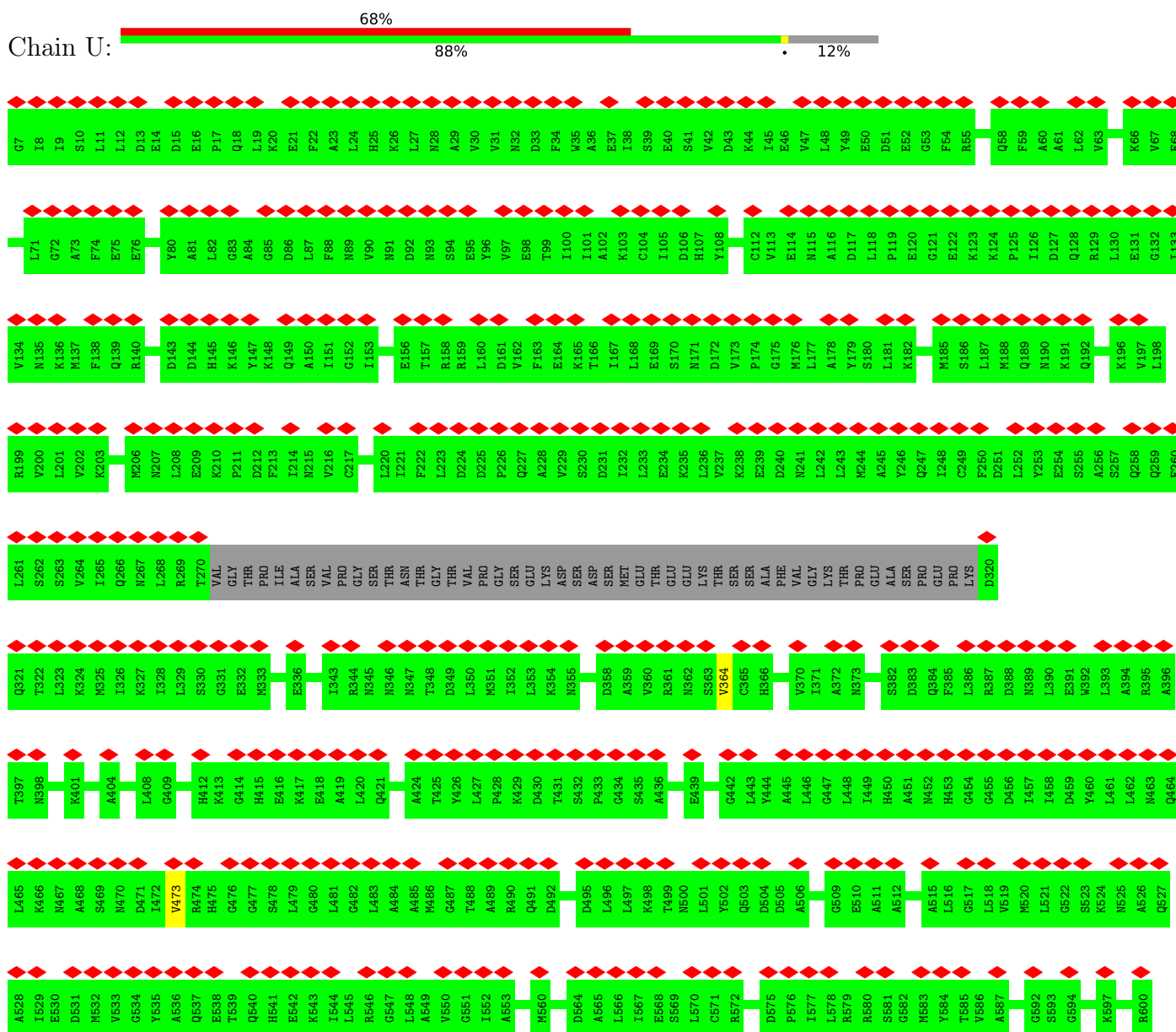
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

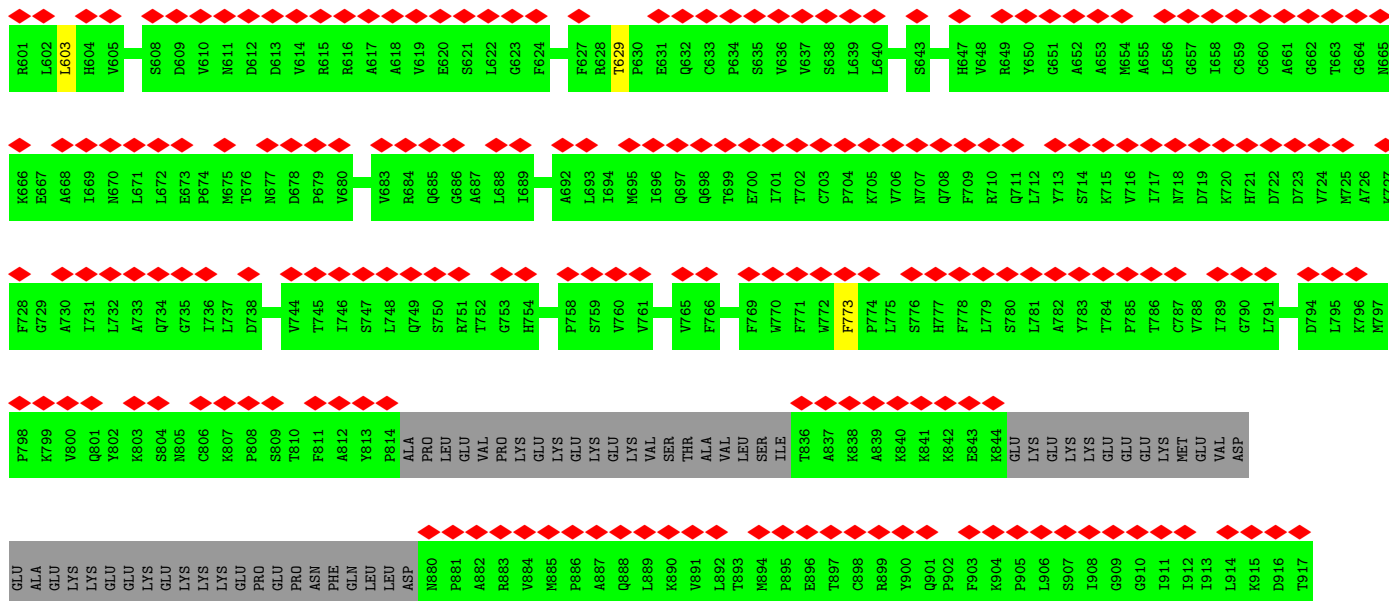
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
33	c	1	1	1	0

### 3 Residue-property plots

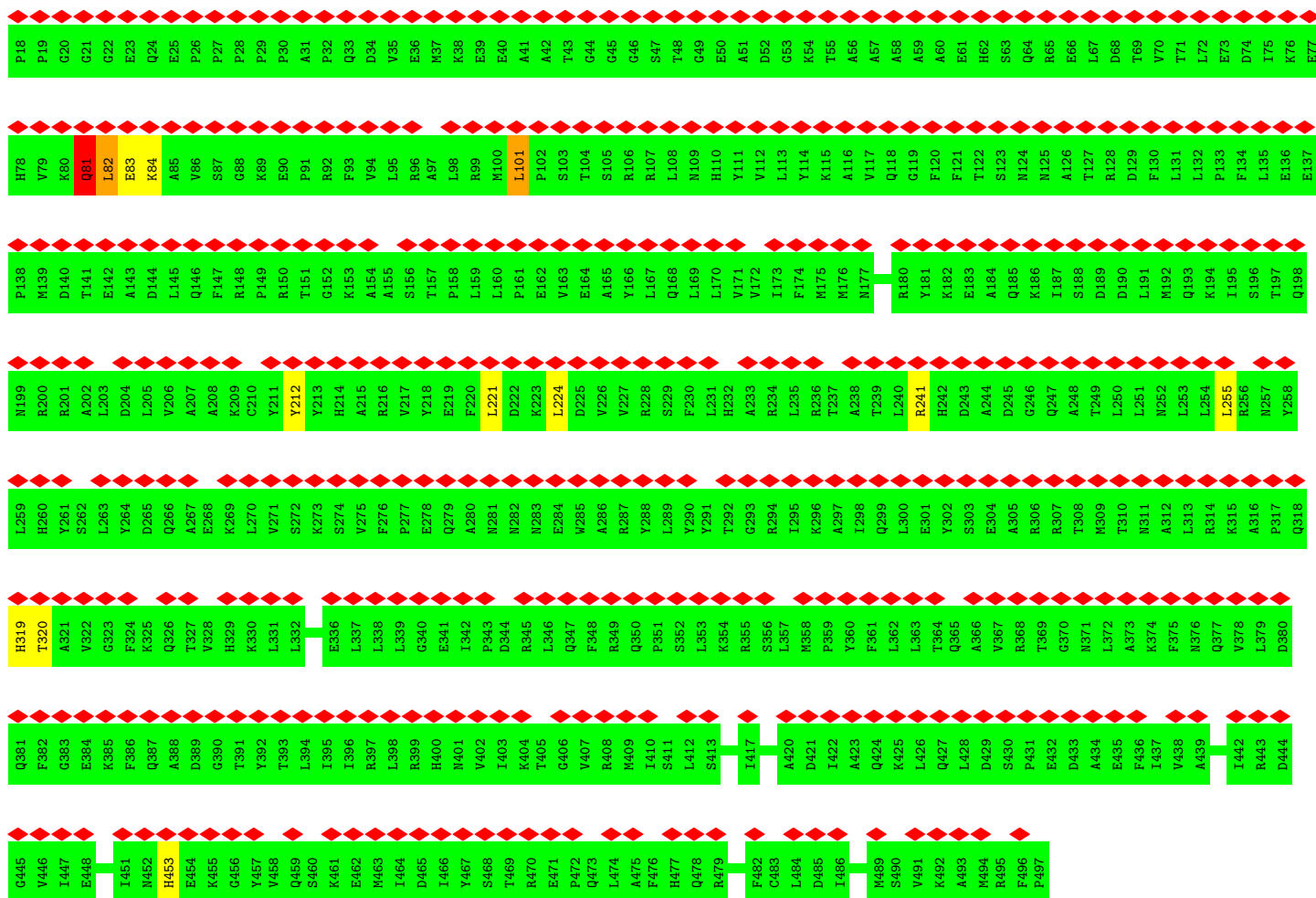
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

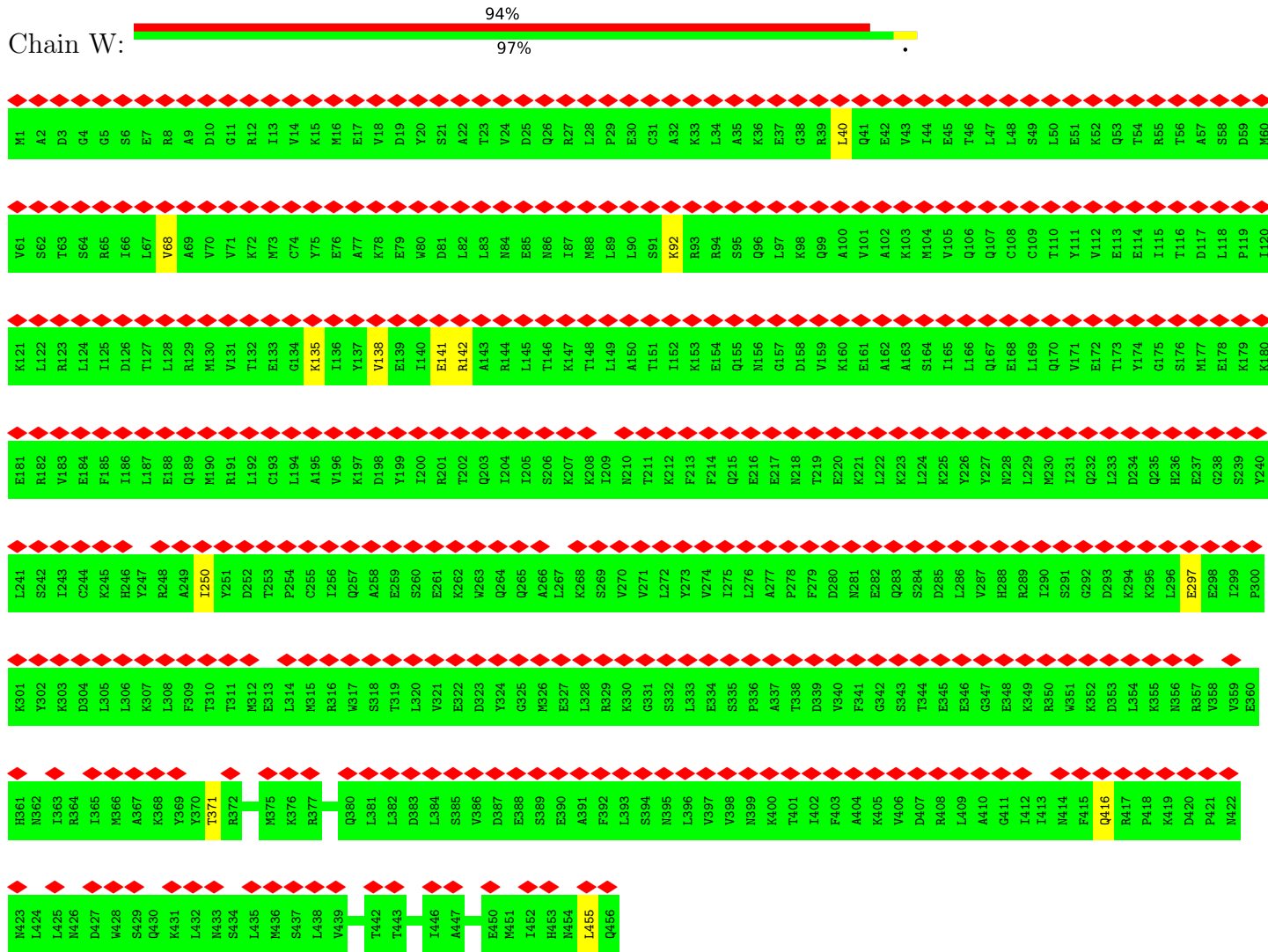




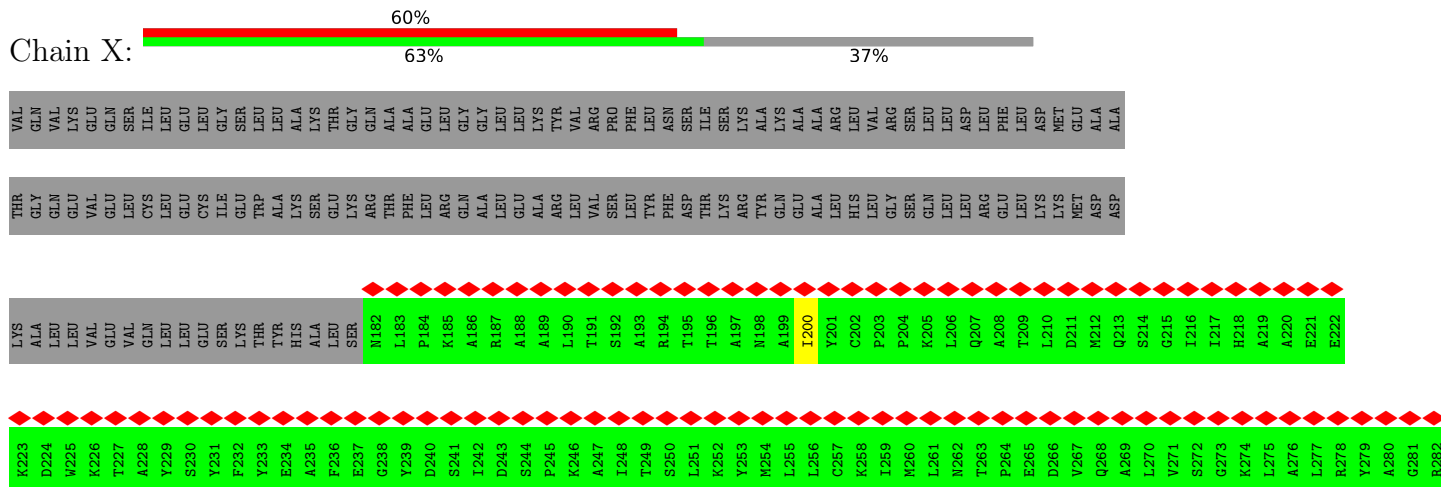
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



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

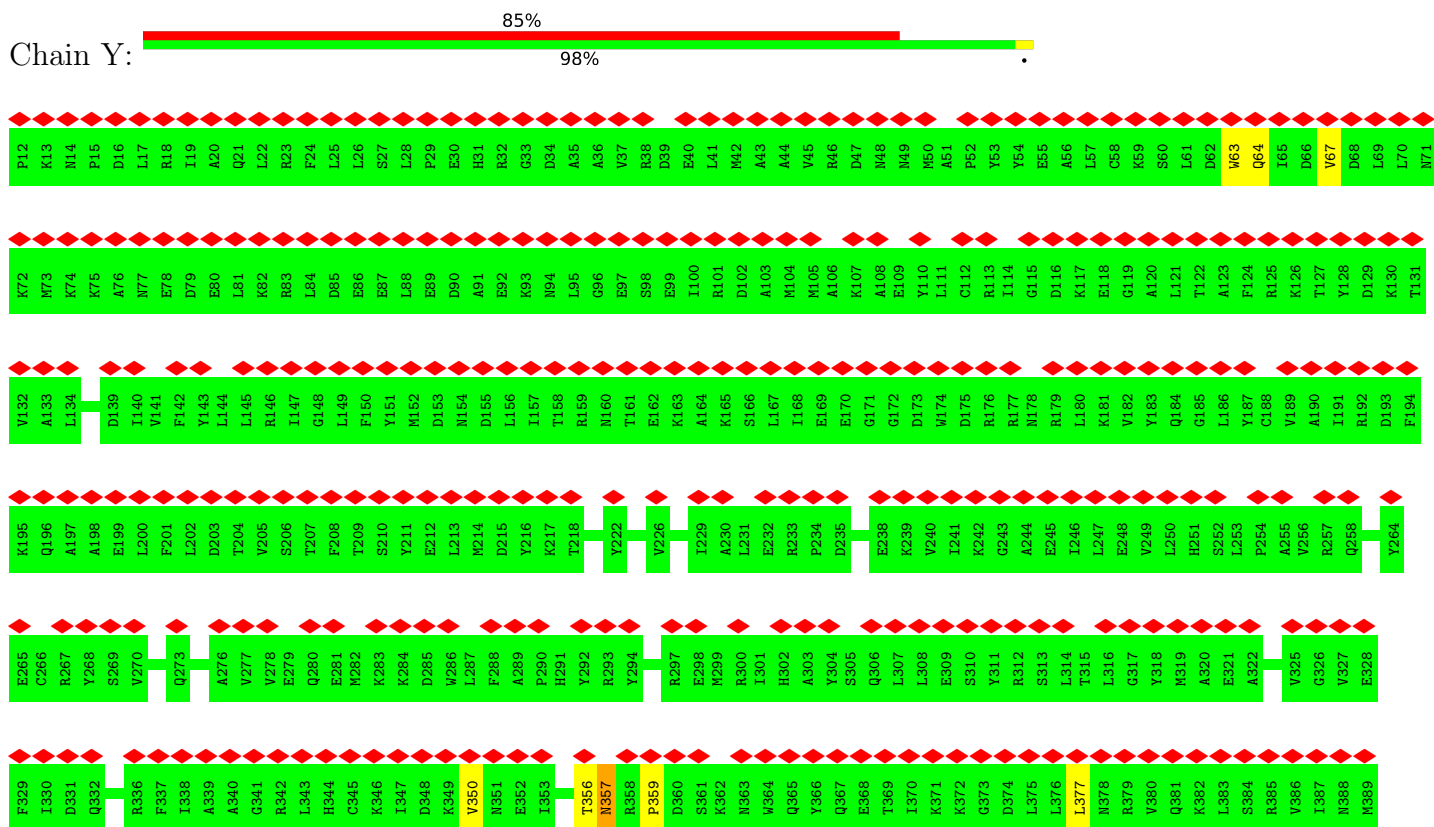


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

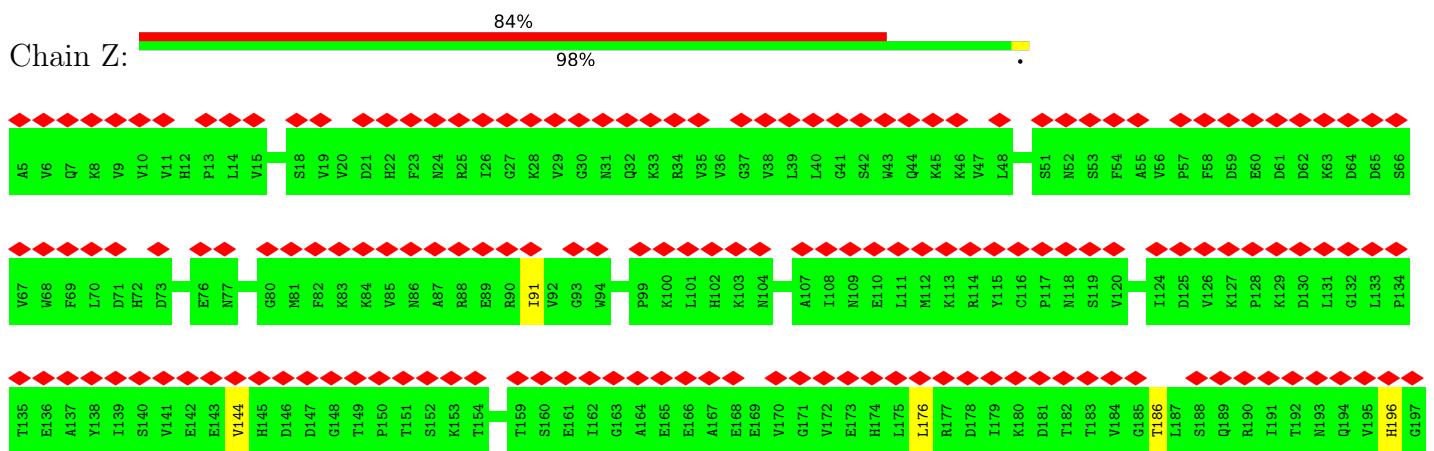


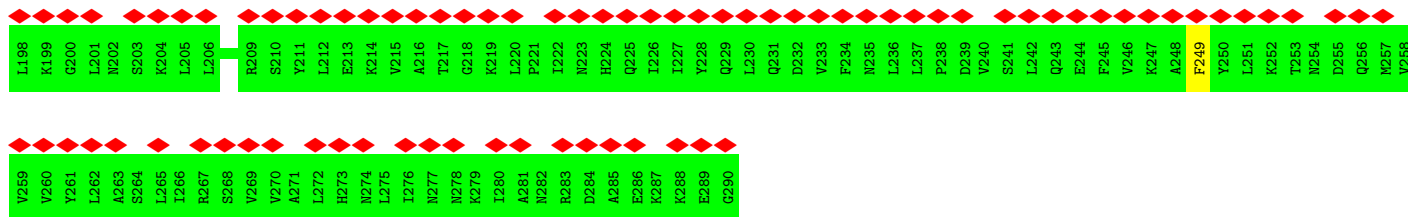


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

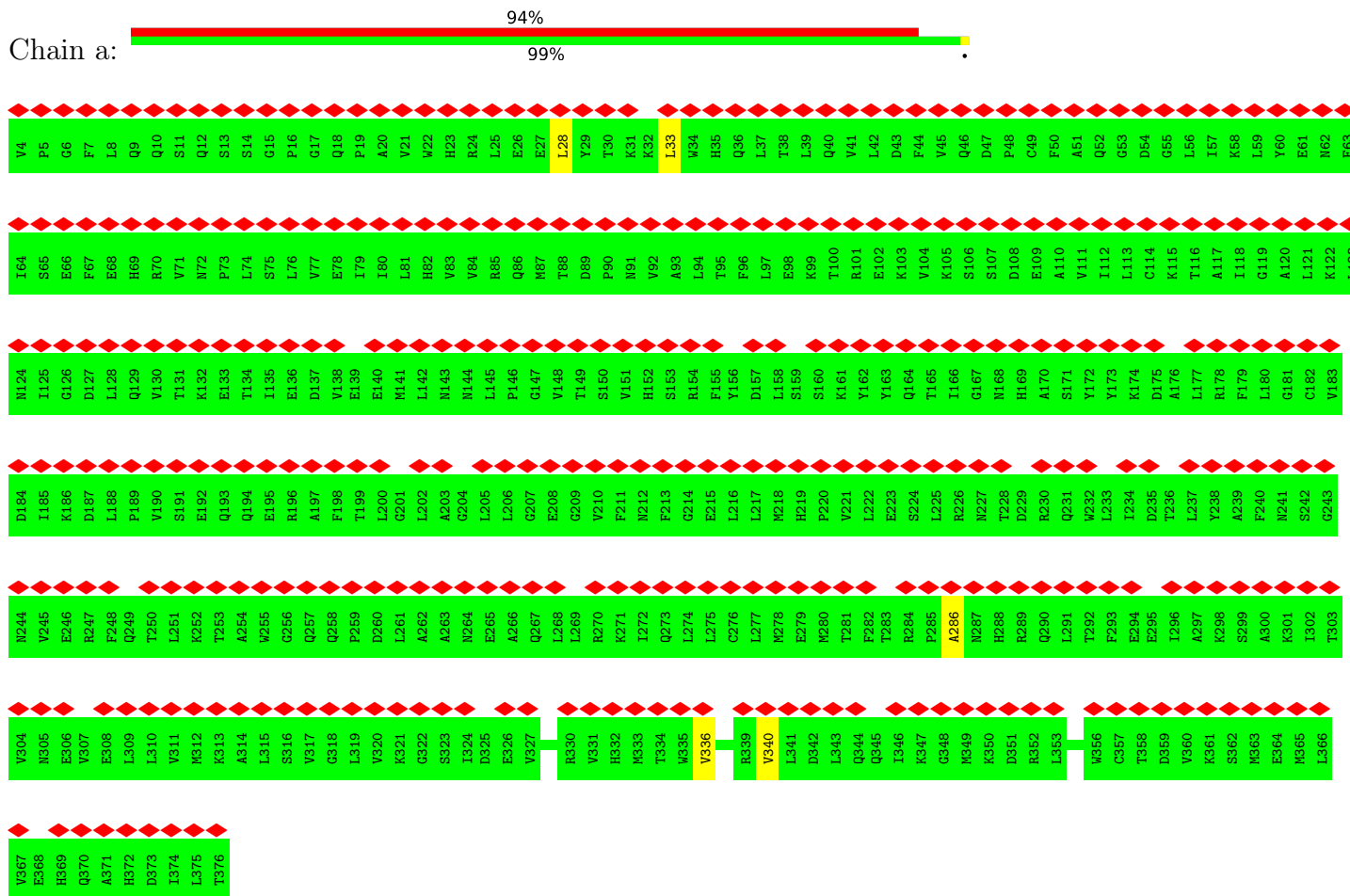


• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

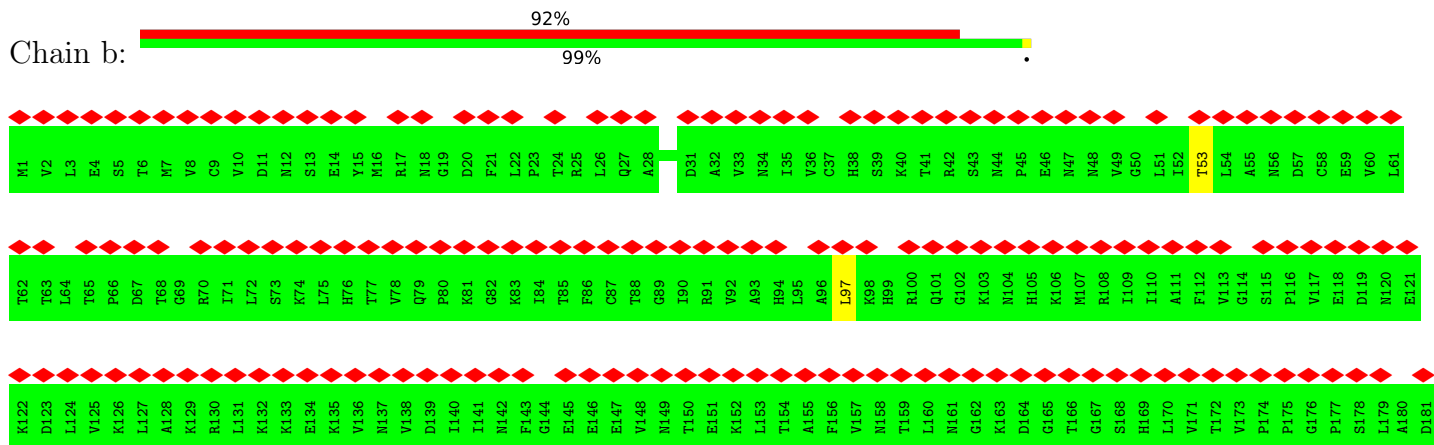


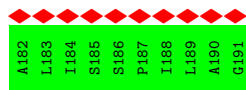


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

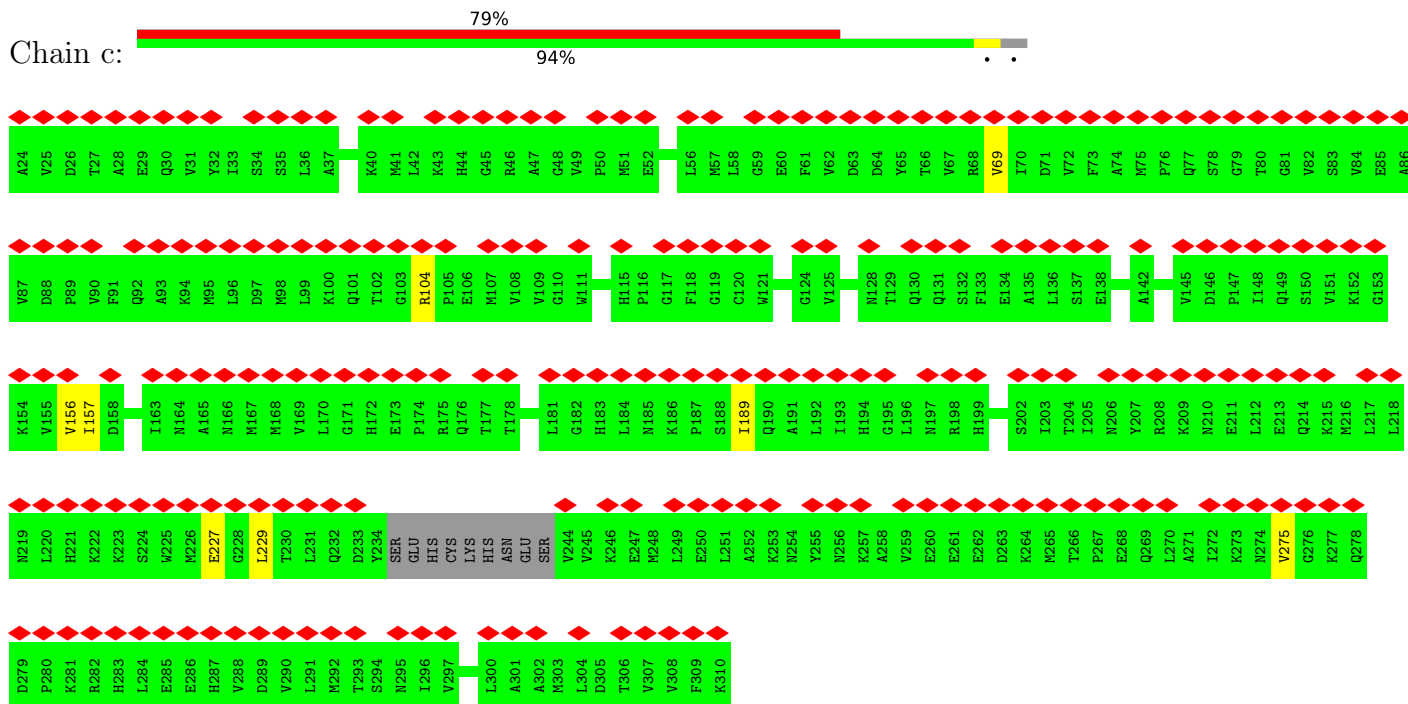


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

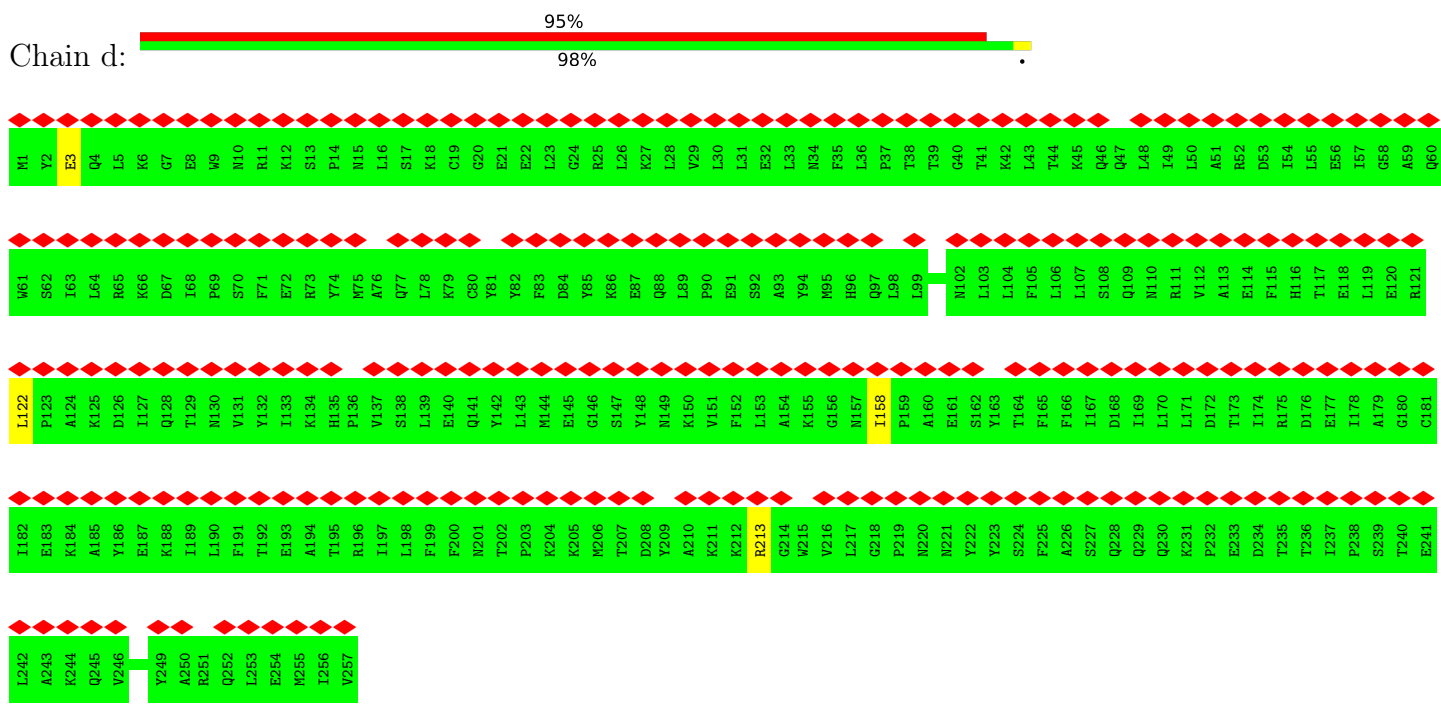




• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14



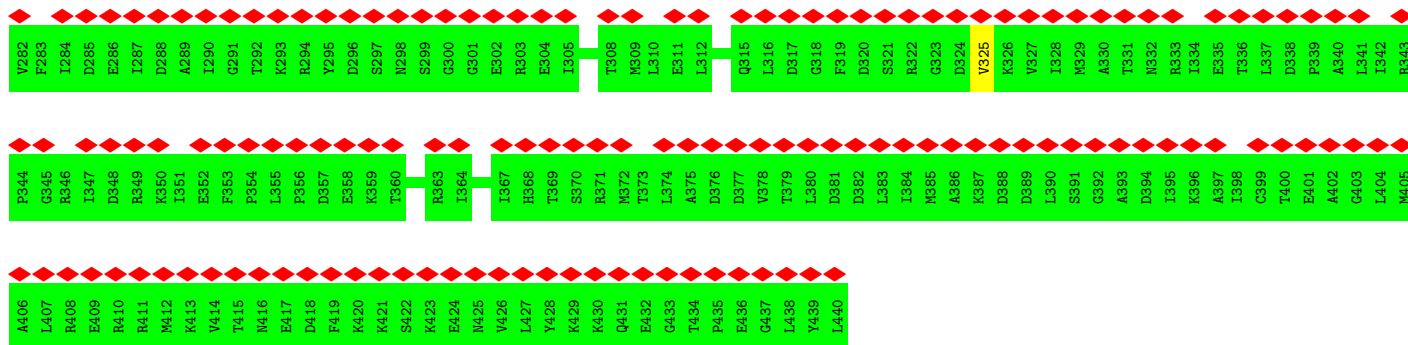
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



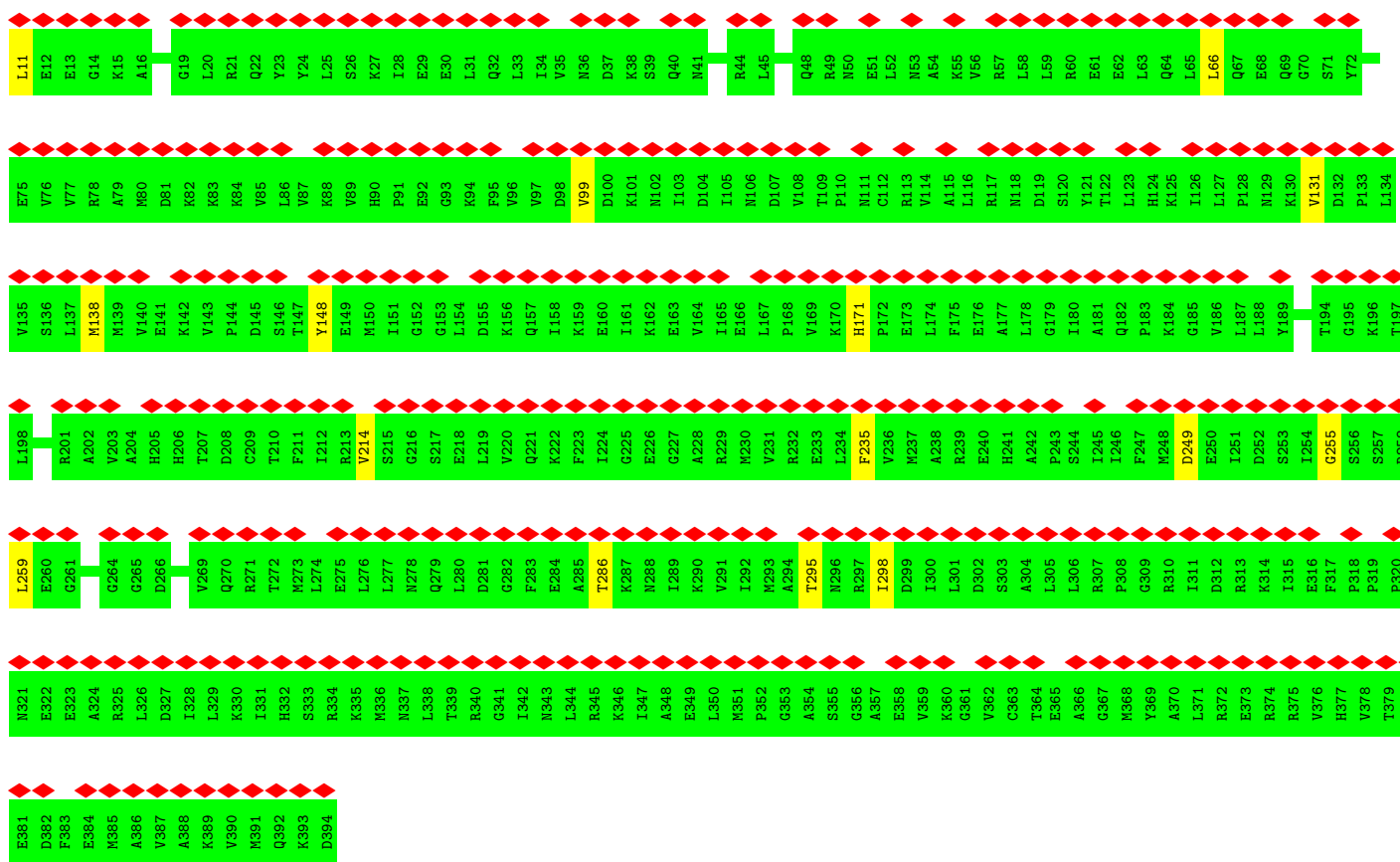
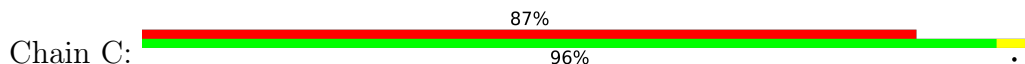
• Molecule 11: Sem1



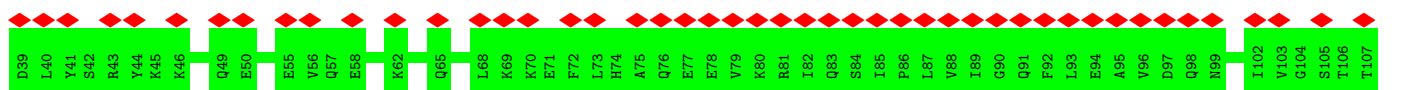
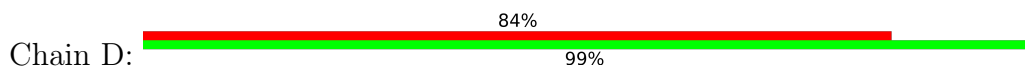


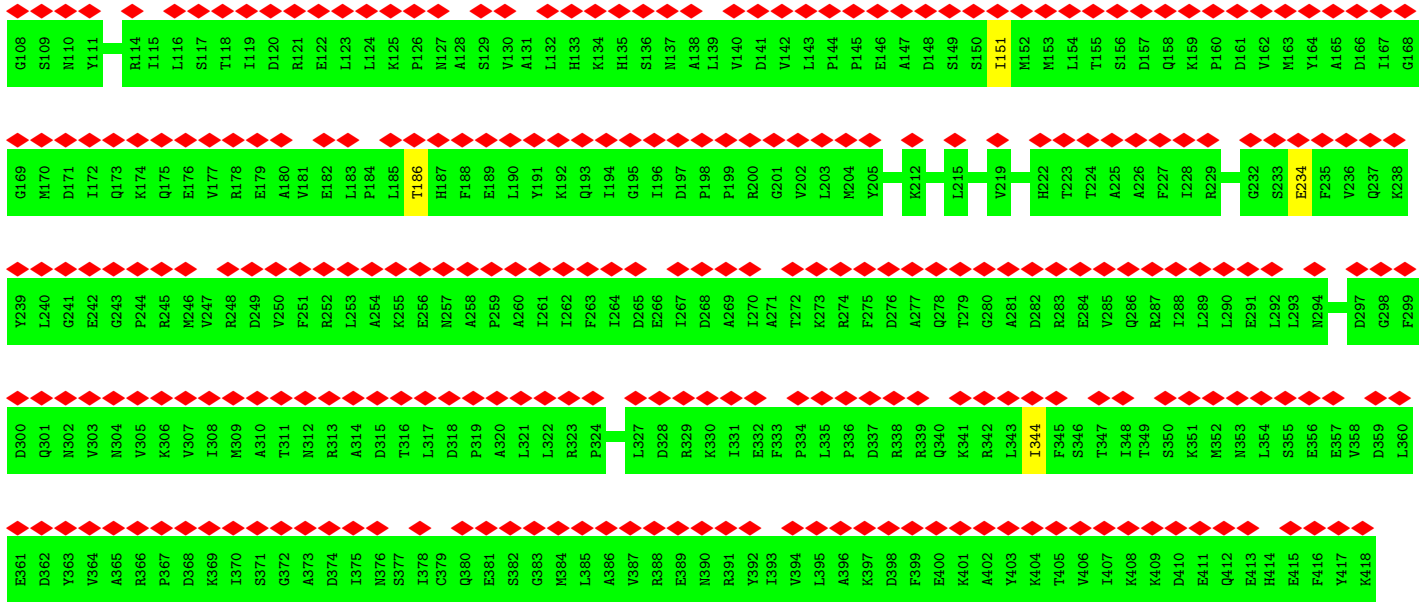


• Molecule 14: 26S protease regulatory subunit 8



• Molecule 15: 26S protease regulatory subunit 6B



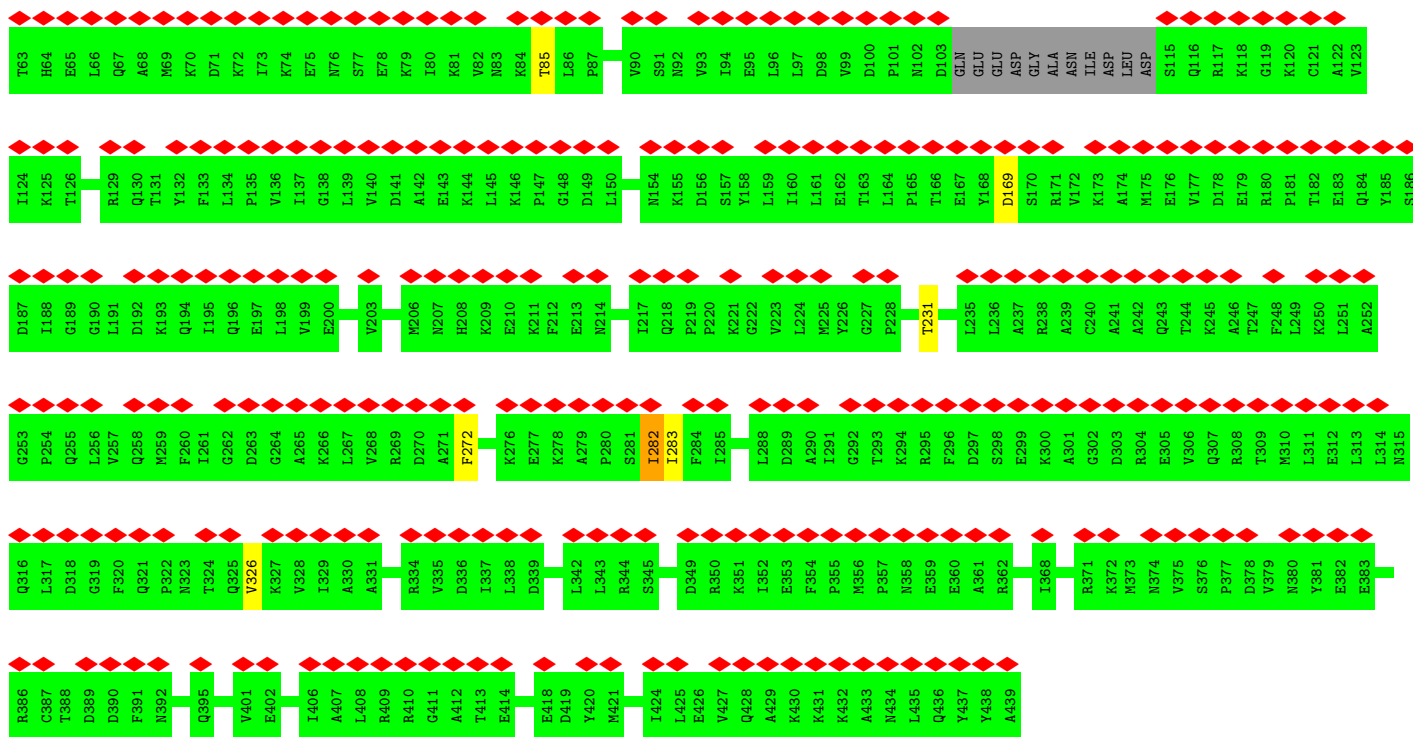


• Molecule 16: 26S protease regulatory subunit 10B

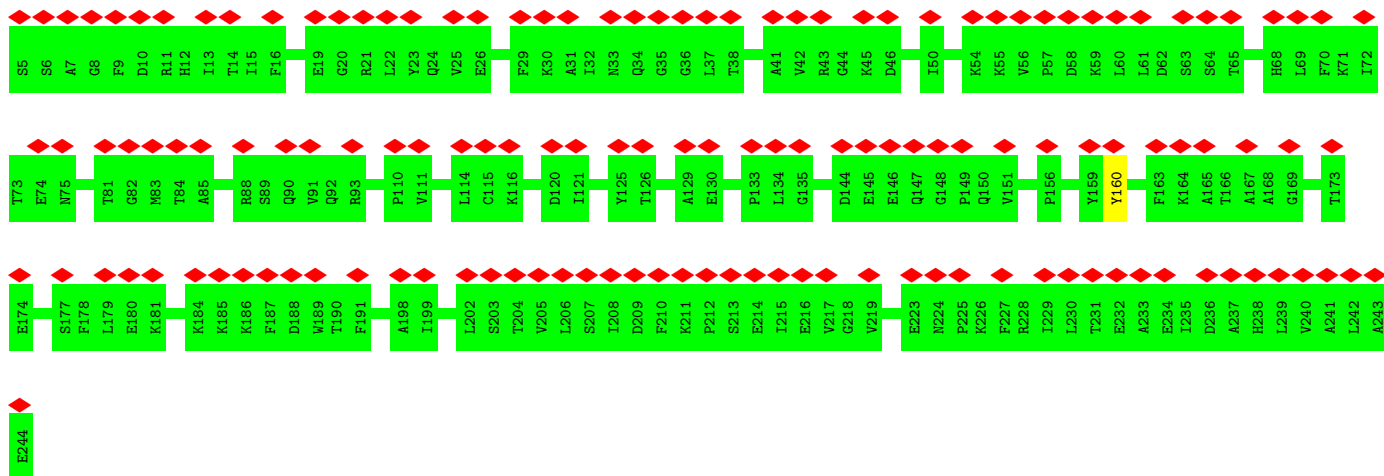


• Molecule 17: 26S protease regulatory subunit 6A

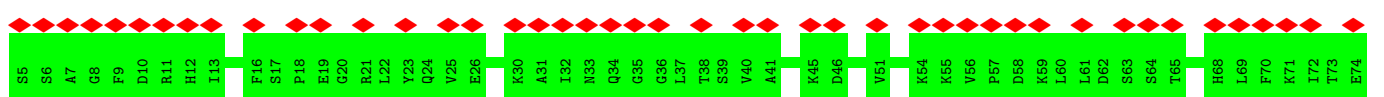


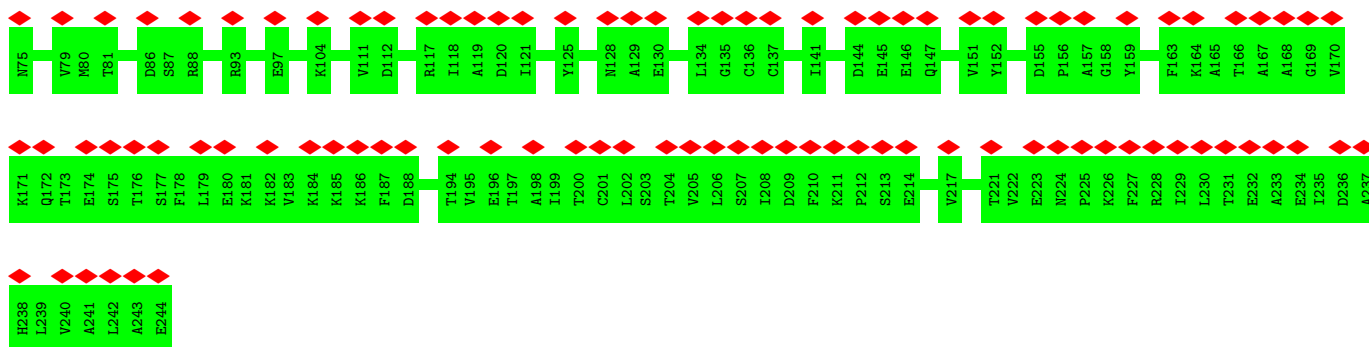


• Molecule 18: Proteasome subunit alpha type-6

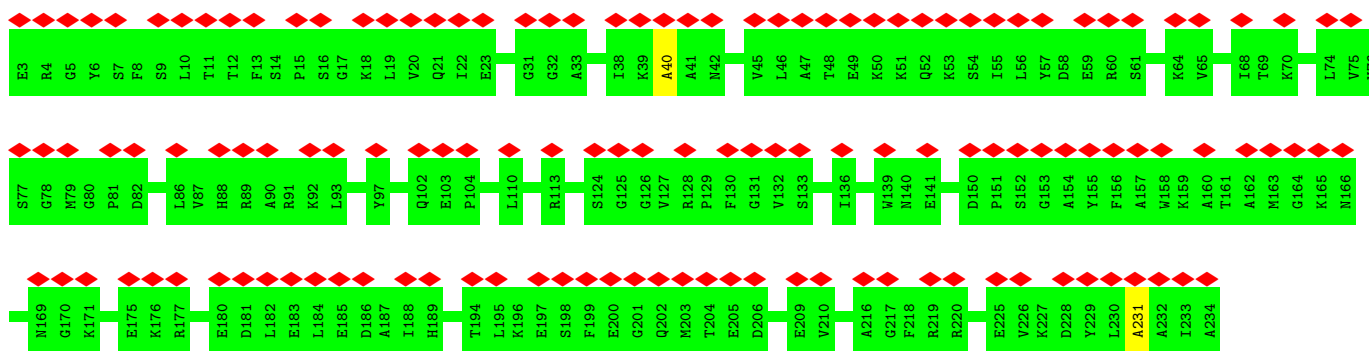


• Molecule 18: Proteasome subunit alpha type-6

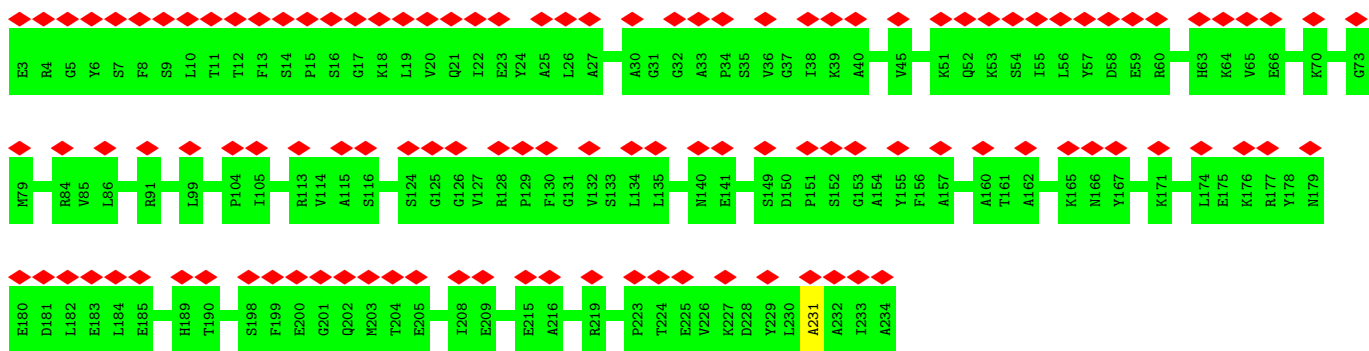




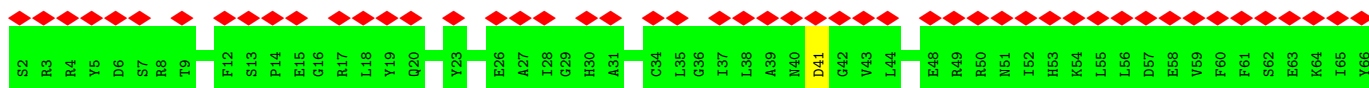
• Molecule 19: Proteasome subunit alpha type-2

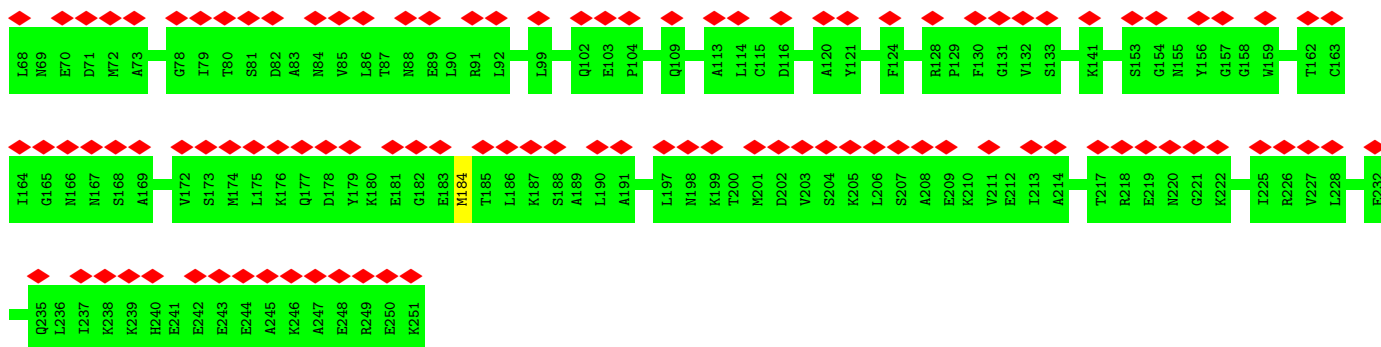


• Molecule 19: Proteasome subunit alpha type-2

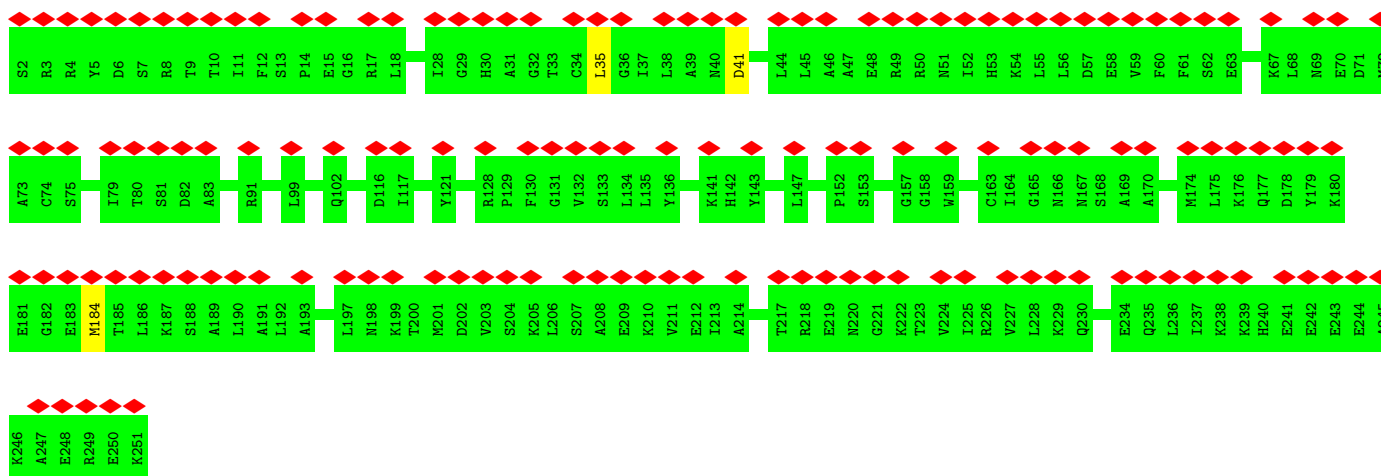


• Molecule 20: Proteasome subunit alpha type-4

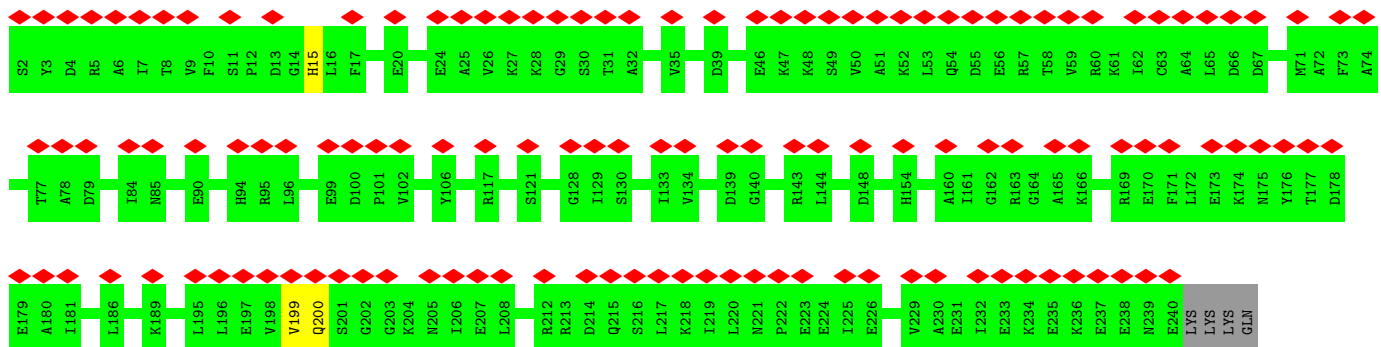




• Molecule 20: Proteasome subunit alpha type-4

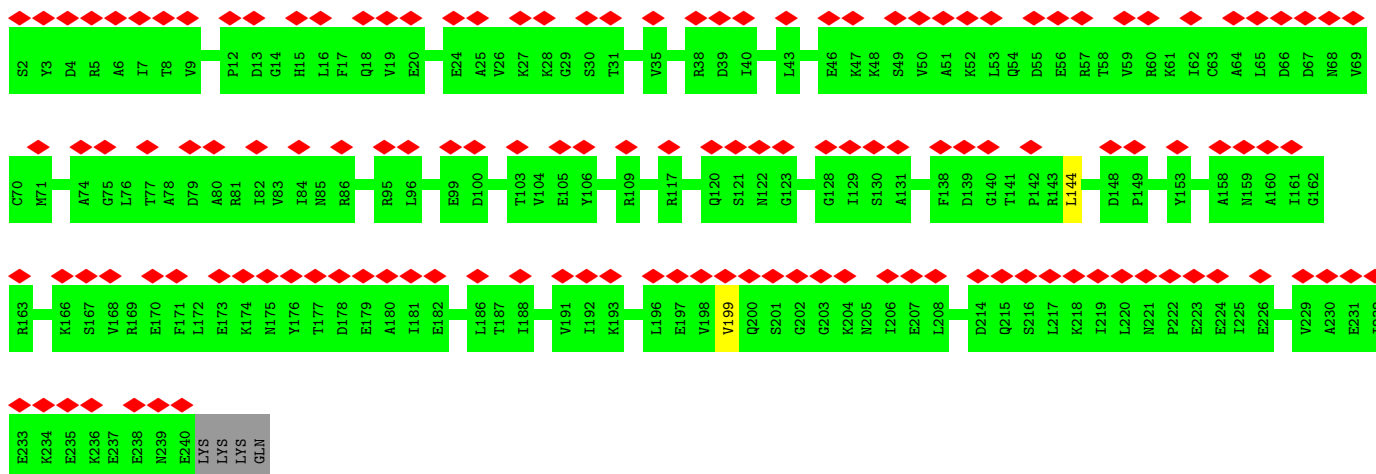


• Molecule 21: Proteasome subunit alpha type-7

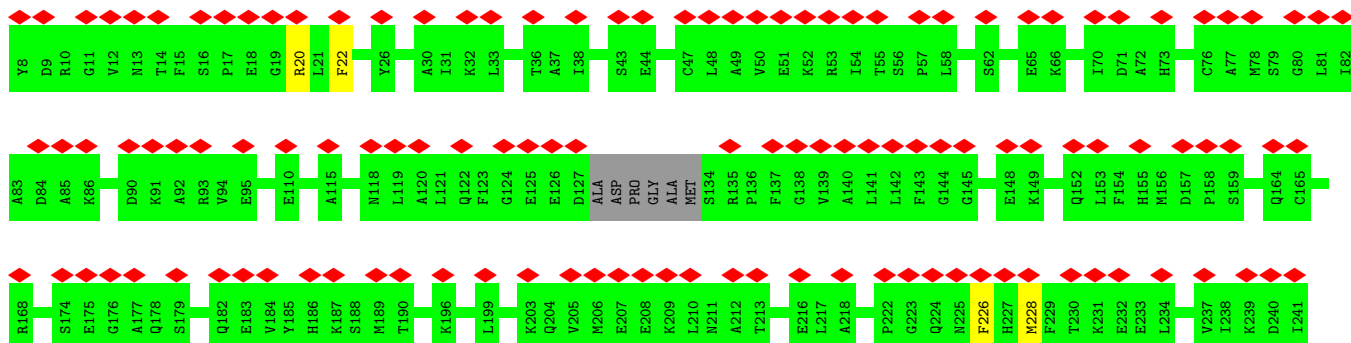


• Molecule 21: Proteasome subunit alpha type-7

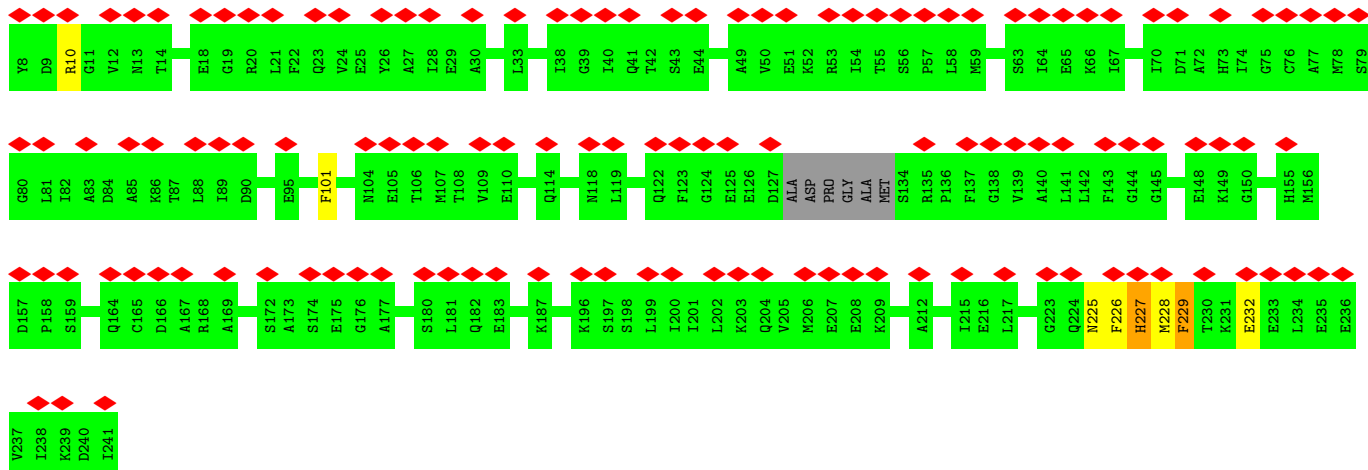
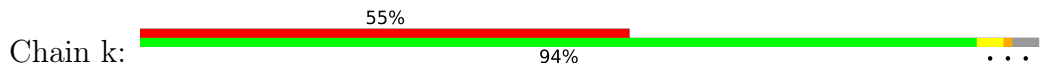




• Molecule 22: Proteasome subunit alpha type-5



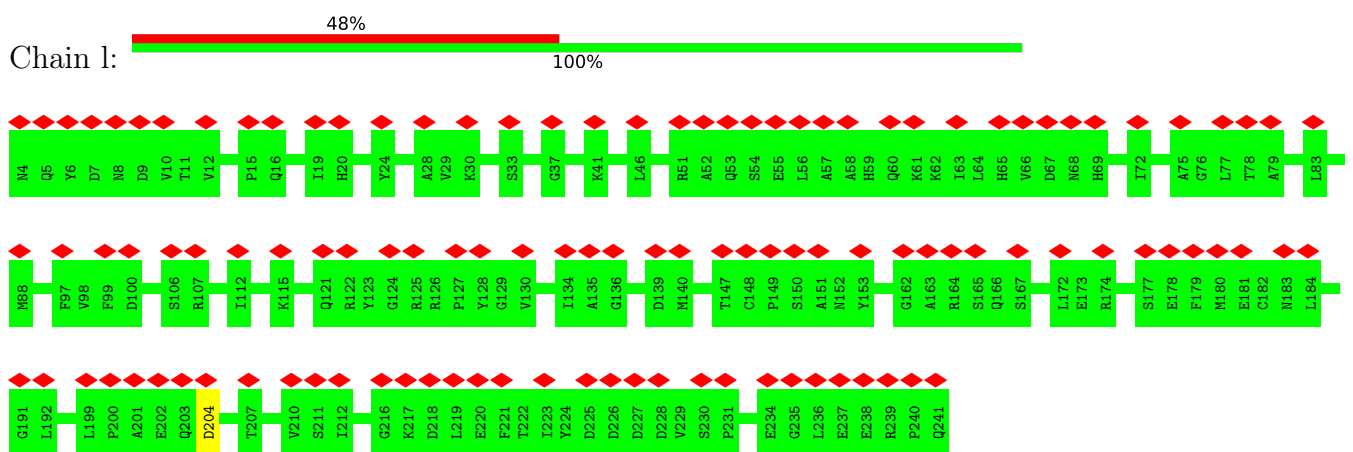
• Molecule 22: Proteasome subunit alpha type-5



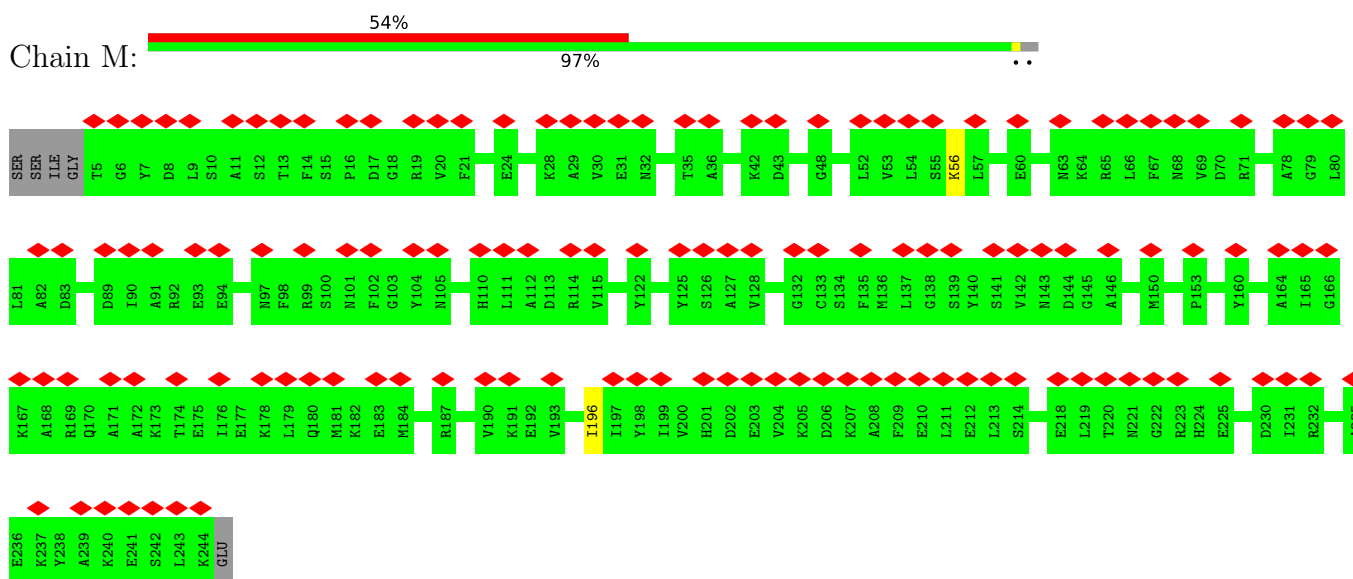
• Molecule 23: Proteasome subunit alpha type-1



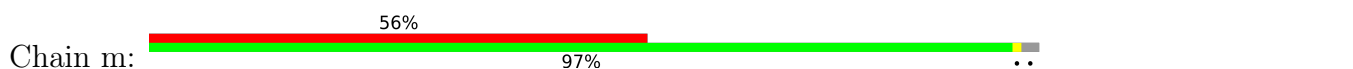
• Molecule 23: Proteasome subunit alpha type-1



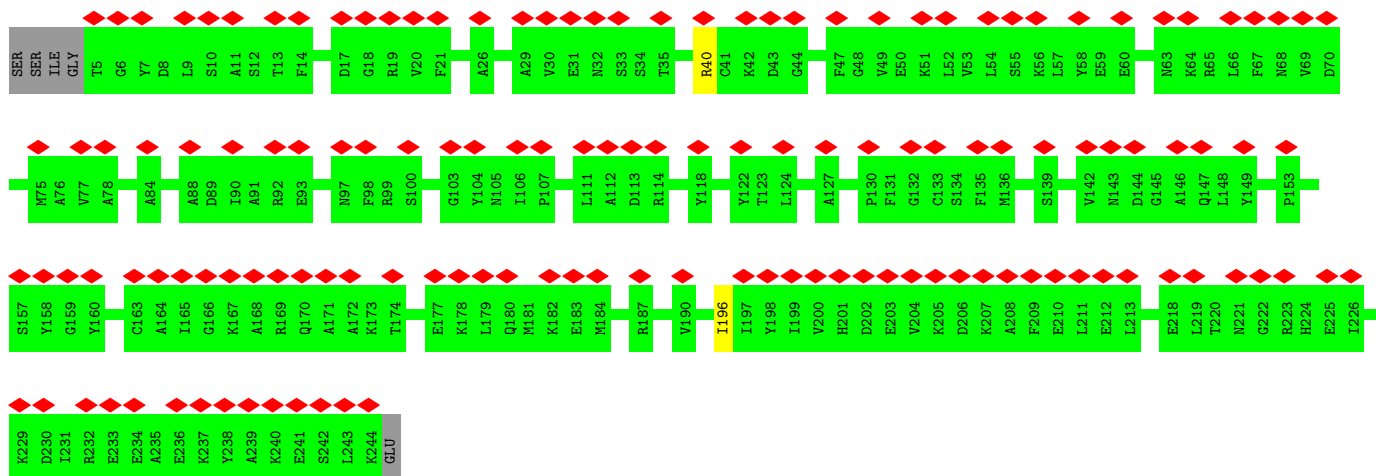
• Molecule 24: Proteasome subunit alpha type-3



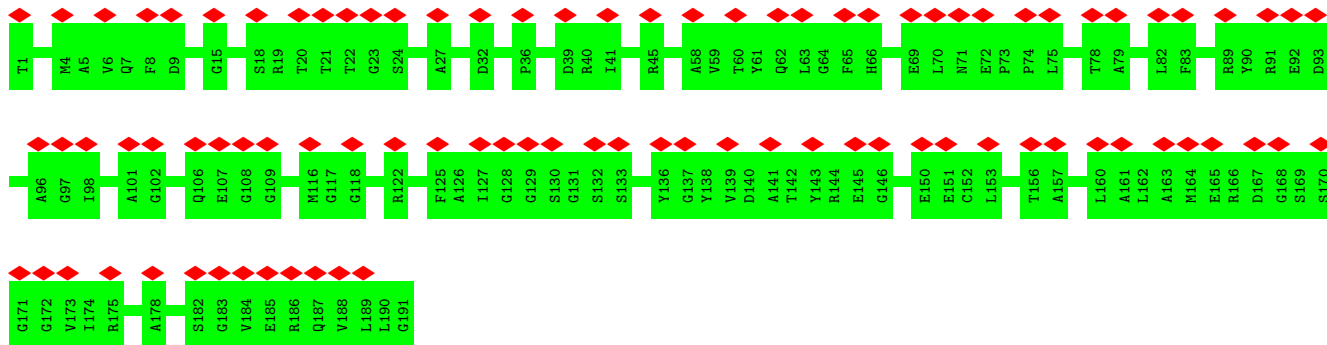
• Molecule 24: Proteasome subunit alpha type-3



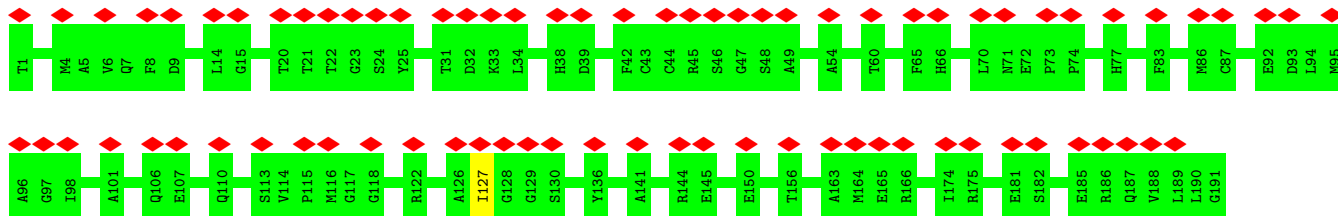




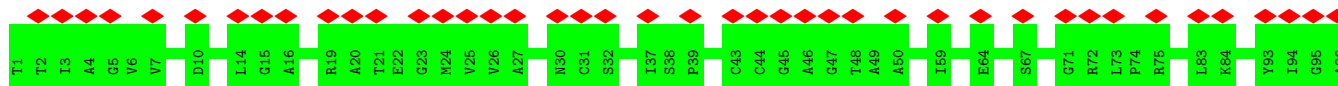
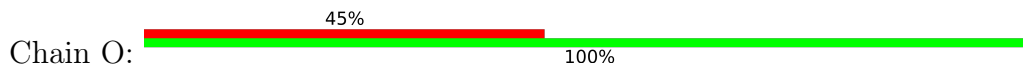
• Molecule 25: Proteasome subunit beta type-6

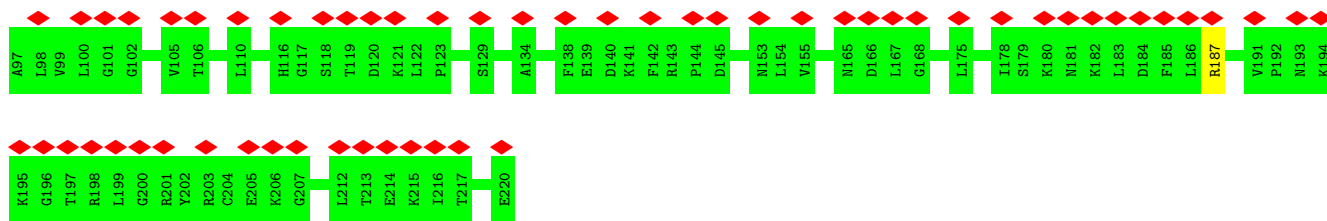


• Molecule 25: Proteasome subunit beta type-6

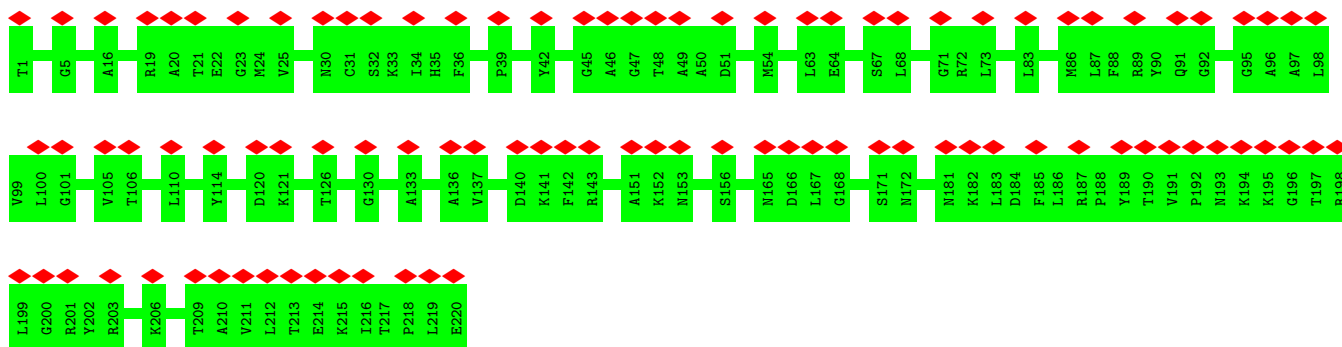
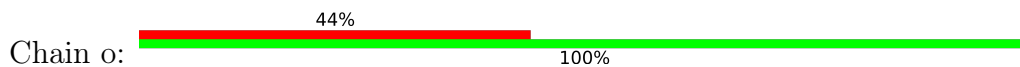


• Molecule 26: Proteasome subunit beta type-7

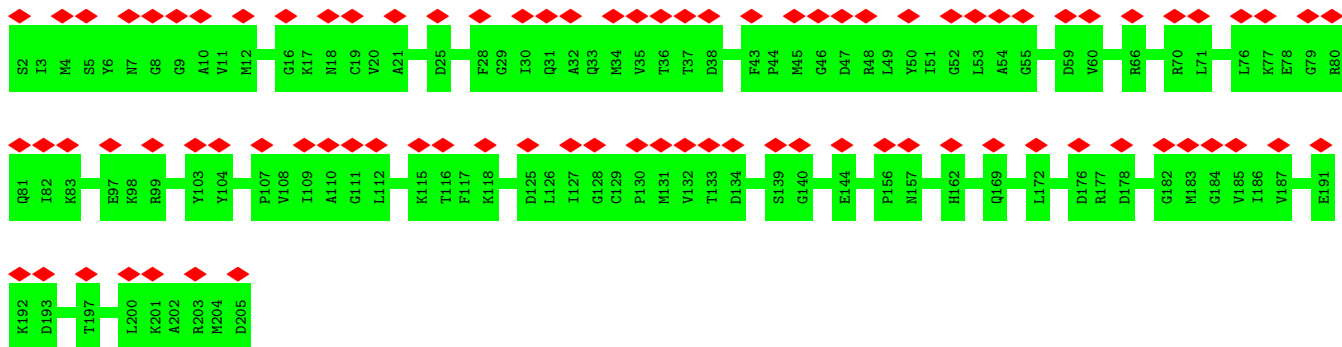
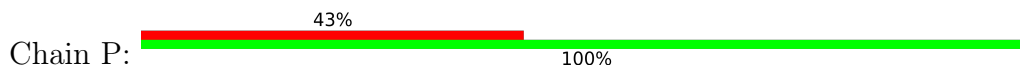




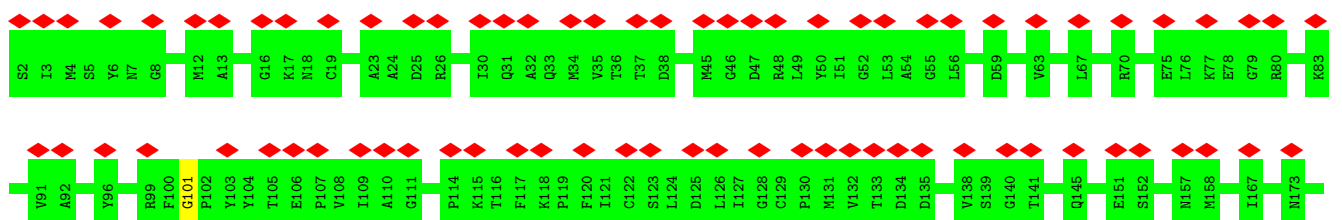
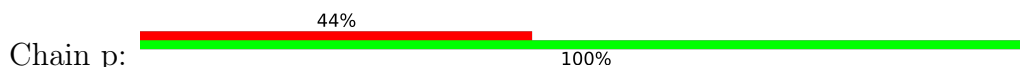
• Molecule 26: Proteasome subunit beta type-7

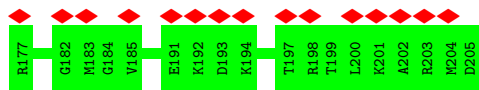


• Molecule 27: Proteasome subunit beta type-3

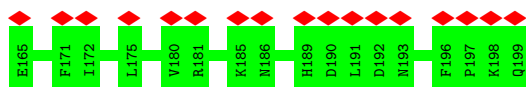
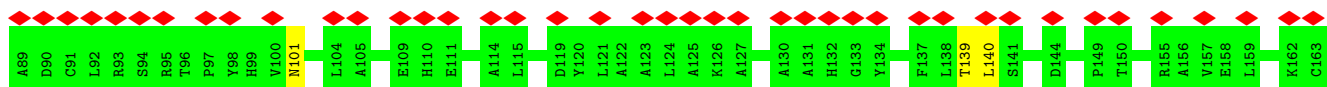
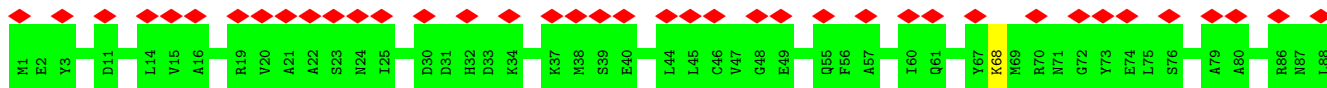


• Molecule 27: Proteasome subunit beta type-3

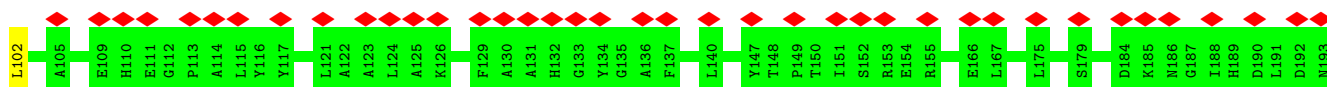
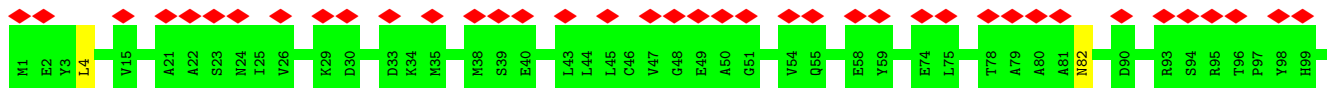
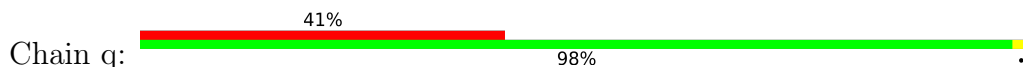




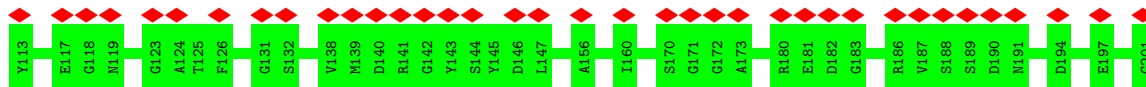
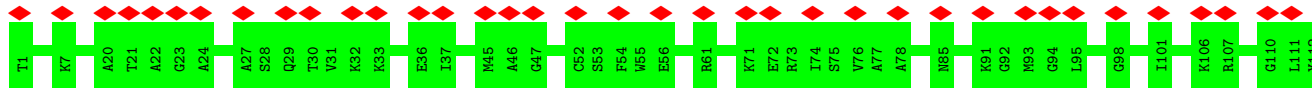
- Molecule 28: Proteasome subunit beta type-2



- Molecule 28: Proteasome subunit beta type-2

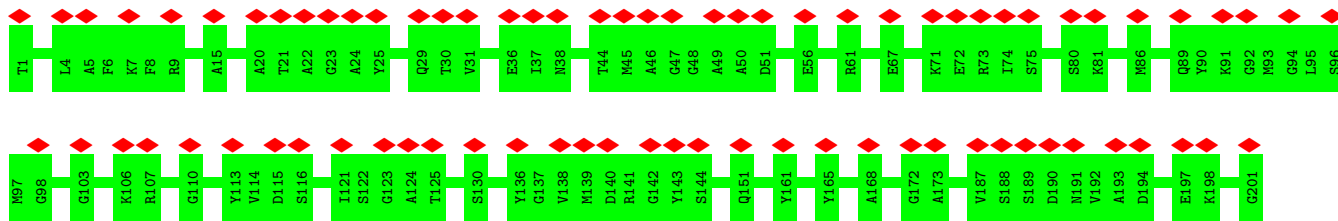


- Molecule 29: Proteasome subunit beta type-5

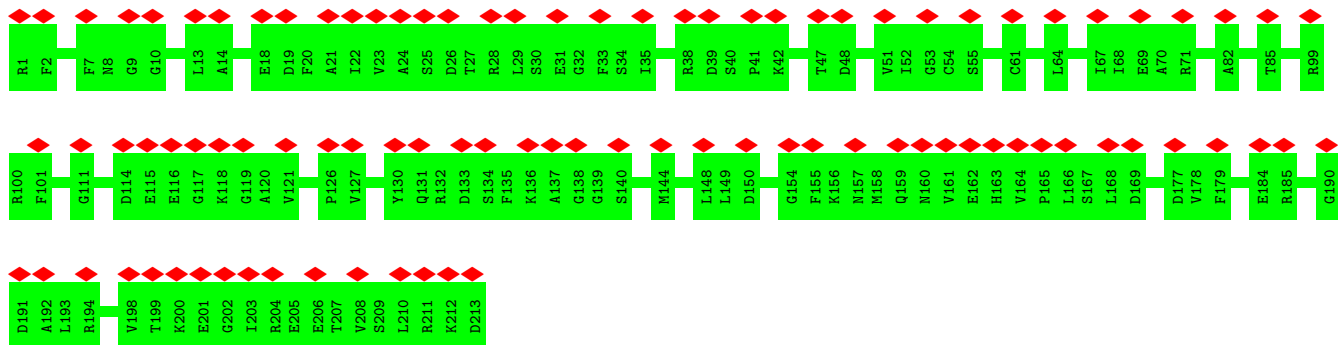
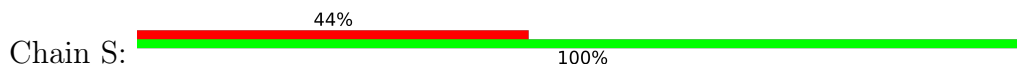


- Molecule 29: Proteasome subunit beta type-5

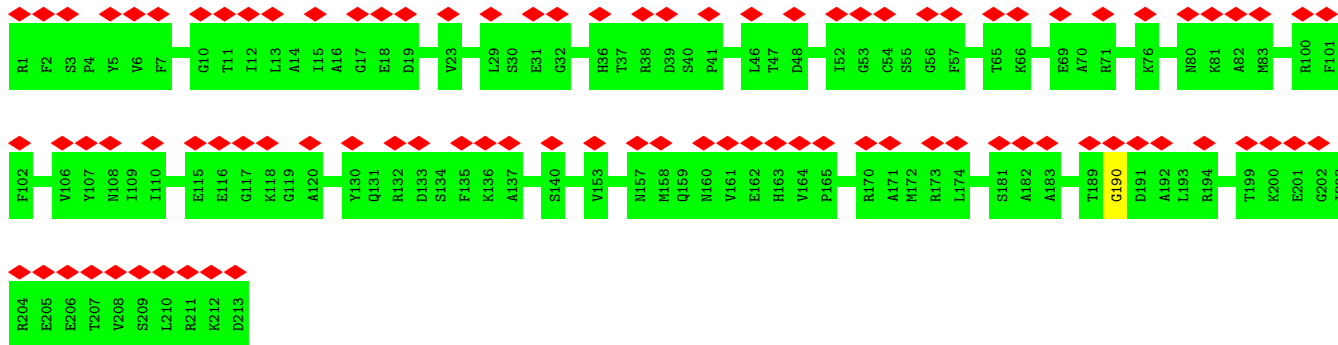
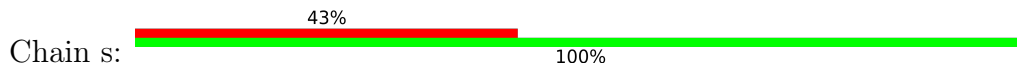




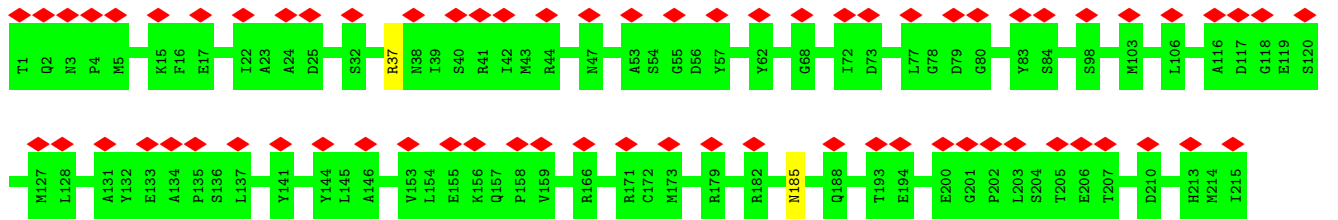
• Molecule 30: Proteasome subunit beta type-1



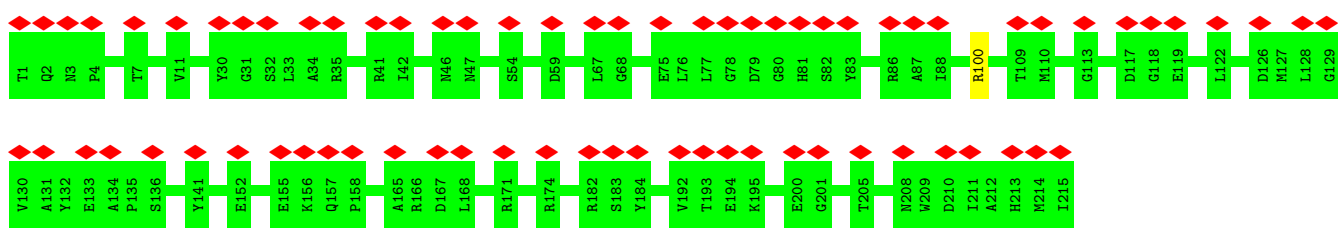
• Molecule 30: Proteasome subunit beta type-1



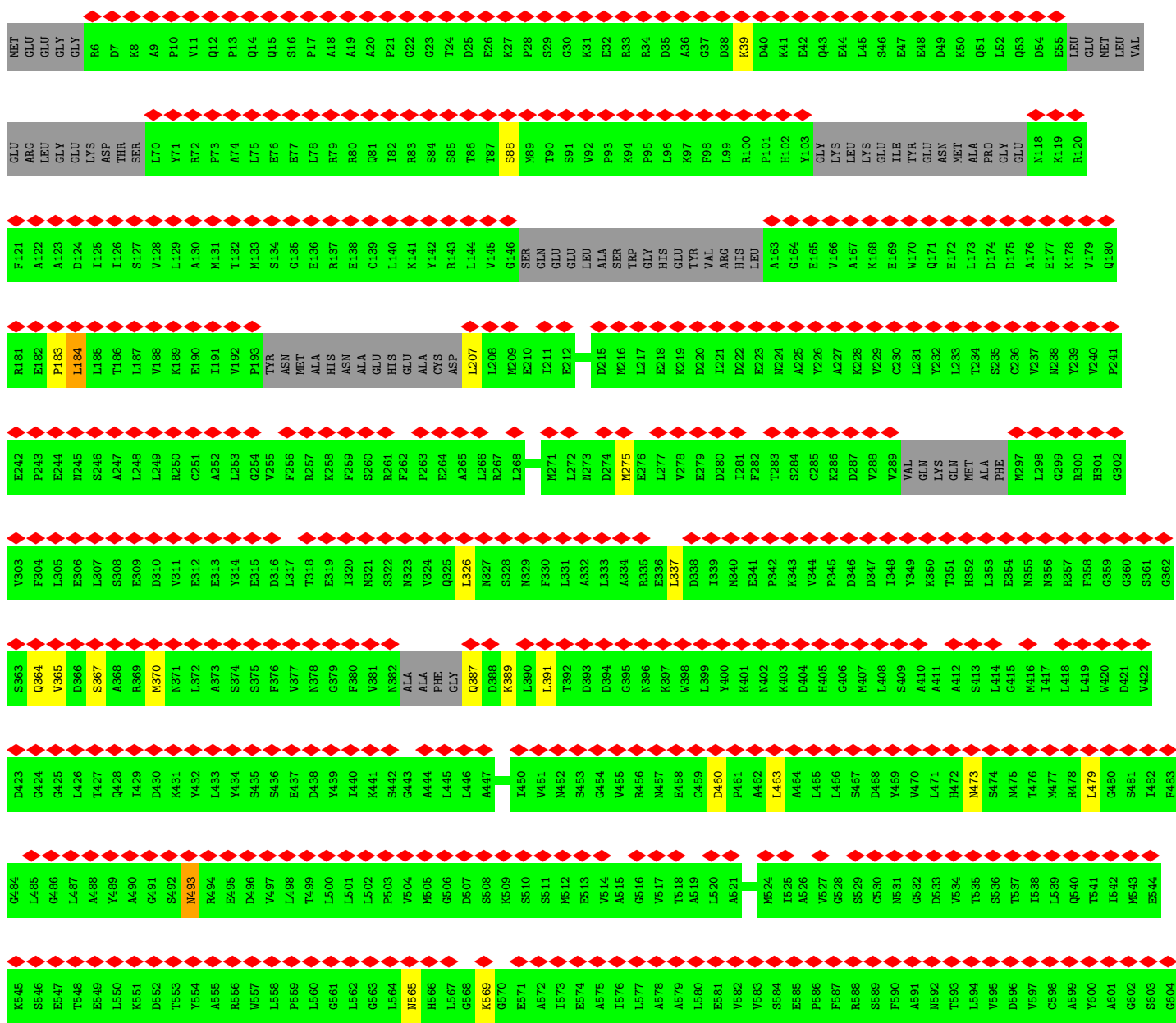
• Molecule 31: Proteasome subunit beta type-4



• Molecule 31: Proteasome subunit beta type-4



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





## 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 i

### 5.1 Standard geometry i

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

All (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
20	I	41	ASP	CB-CG-OD1	5.55	123.29	118.30
23	L	204	ASP	C-N-CA	5.50	135.46	121.70
21	j	144	LEU	CA-CB-CG	5.37	127.64	115.30
20	I	184	MET	C-N-CA	5.36	135.10	121.70
3	W	92	LYS	C-N-CA	5.28	134.89	121.70
3	W	40	LEU	CA-CB-CG	5.05	126.91	115.30
20	i	184	MET	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	311	PRO	Peptide
13	B	278	ALA	Peptide
14	C	171	HIS	Peptide
14	C	255	GLY	Peptide
18	G	160	TYR	Peptide
19	H	231	ALA	Peptide
19	H	40	ALA	Peptide
21	J	15	HIS	Peptide
21	J	199	VAL	Peptide
22	K	226	PHE	Peptide
23	L	137	TYR	Peptide

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Mol	Chain	Res	Type	Group
23	L	204	ASP	Peptide
24	M	56	LYS	Peptide
26	O	187	ARG	Peptide
28	Q	101	ASN	Peptide
28	Q	139	THR	Peptide
2	V	101	LEU	Peptide
2	V	319	HIS	Peptide
2	V	81	GLN	Peptide
3	W	416	GLN	Peptide
5	Y	356	THR	Peptide
5	Y	63	TRP	Peptide
7	a	286	ALA	Peptide
10	d	3	GLU	Peptide
11	e	1	MET	Peptide
21	j	199	VAL	Peptide
22	k	10	ARG	Peptide
22	k	226	PHE	Peptide
22	k	232	GLU	Peptide
23	l	204	ASP	Peptide
27	p	101	GLY	Peptide
28	q	102	LEU	Peptide
30	s	190	GLY	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%)	51	85
2	V	478/480 (100%)	413 (86%)	59 (12%)	6 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	W	454/456 (100%)	406 (89%)	45 (10%)	3 (1%)	22	62
4	X	239/380 (63%)	213 (89%)	26 (11%)	0	100	100
5	Y	376/378 (100%)	333 (89%)	38 (10%)	5 (1%)	12	48
6	Z	284/286 (99%)	253 (89%)	30 (11%)	1 (0%)	34	72
7	a	371/373 (100%)	331 (89%)	38 (10%)	2 (0%)	29	69
8	b	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
9	c	274/287 (96%)	242 (88%)	28 (10%)	4 (2%)	10	45
10	d	255/257 (99%)	227 (89%)	27 (11%)	1 (0%)	34	72
11	e	36/70 (51%)	30 (83%)	6 (17%)	0	100	100
12	A	359/361 (99%)	312 (87%)	43 (12%)	4 (1%)	14	51
13	B	346/348 (99%)	295 (85%)	46 (13%)	5 (1%)	11	46
14	C	382/384 (100%)	339 (89%)	41 (11%)	2 (0%)	29	69
15	D	378/380 (100%)	333 (88%)	44 (12%)	1 (0%)	41	76
16	E	351/353 (99%)	321 (92%)	29 (8%)	1 (0%)	41	76
17	F	362/377 (96%)	322 (89%)	38 (10%)	2 (1%)	25	66
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%)	34	72
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%)	12	48
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	13	49
All	All	12761/13430 (95%)	11639 (91%)	1072 (8%)	50 (0%)	38	72

All (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
3	W	135	LYS
5	Y	64	GLN
5	Y	350	VAL
12	A	161	VAL
22	k	229	PHE
32	f	337	LEU
32	f	364	GLN
32	f	367	SER
32	f	665	GLU
2	V	81	GLN
3	W	138	VAL
5	Y	357	ASN
5	Y	359	PRO
9	c	157	ILE

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Mol	Chain	Res	Type
9	c	227	GLU
13	B	175	LYS
13	B	176	VAL
14	C	214	VAL
22	k	227	HIS
32	f	183	PRO
32	f	365	VAL
7	a	340	VAL
12	A	206	ILE
12	A	317	VAL
13	B	218	PRO
15	D	151	ILE
32	f	184	LEU
32	f	326	LEU
5	Y	67	VAL
9	c	156	VAL
14	C	298	ILE
17	F	282	ILE
2	V	241	ARG
6	Z	144	VAL
21	J	200	GLN
22	k	225	ASN
10	d	213	ARG
2	V	101	LEU
7	a	336	VAL
9	c	189	ILE
13	B	179	ALA
13	B	325	VAL
12	A	172	VAL
17	F	326	VAL
16	E	175	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	685/779 (88%)	681 (99%)	4 (1%)	86	92
2	V	414/414 (100%)	406 (98%)	8 (2%)	57	75
3	W	416/416 (100%)	410 (99%)	6 (1%)	67	80
4	X	208/327 (64%)	207 (100%)	1 (0%)	88	93
5	Y	334/334 (100%)	332 (99%)	2 (1%)	86	92
6	Z	257/257 (100%)	252 (98%)	5 (2%)	57	75
7	a	333/333 (100%)	331 (99%)	2 (1%)	86	92
8	b	167/167 (100%)	165 (99%)	2 (1%)	71	83
9	c	243/252 (96%)	240 (99%)	3 (1%)	71	83
10	d	231/231 (100%)	229 (99%)	2 (1%)	78	87
11	e	38/63 (60%)	36 (95%)	2 (5%)	22	47
12	A	308/308 (100%)	303 (98%)	5 (2%)	62	79
13	B	304/304 (100%)	295 (97%)	9 (3%)	41	63
14	C	332/332 (100%)	321 (97%)	11 (3%)	38	61
15	D	333/333 (100%)	330 (99%)	3 (1%)	78	87
16	E	308/308 (100%)	306 (99%)	2 (1%)	86	92
17	F	312/321 (97%)	306 (98%)	6 (2%)	57	75
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%)	62	79
22	k	186/196 (95%)	182 (98%)	4 (2%)	52	71
23	L	198/204 (97%)	196 (99%)	2 (1%)	76	86
23	l	198/204 (97%)	198 (100%)	0	100	100
24	M	192/202 (95%)	191 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	m	192/202 (95%)	190 (99%)	2 (1%)	76	86
25	N	148/148 (100%)	148 (100%)	0	100	100
25	n	148/148 (100%)	147 (99%)	1 (1%)	84	90
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%)	71	83
28	q	164/170 (96%)	163 (99%)	1 (1%)	86	92
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%)	73	84
31	t	175/178 (98%)	174 (99%)	1 (1%)	86	92
32	f	580/763 (76%)	559 (96%)	21 (4%)	35	59
All	All	10684/11438 (93%)	10571 (99%)	113 (1%)	74	84

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	473	VAL
1	U	603	LEU
1	U	629	THR
1	U	773	PHE
2	V	81	GLN
2	V	82	LEU
2	V	212	TYR
2	V	221	LEU
2	V	224	LEU
2	V	255	LEU
2	V	320	THR
2	V	453	HIS
3	W	141	GLU
3	W	142	ARG
3	W	250	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	W	297	GLU
3	W	371	THR
3	W	455	LEU
4	X	200	ILE
5	Y	357	ASN
5	Y	377	LEU
6	Z	91	ILE
6	Z	176	LEU
6	Z	186	THR
6	Z	196	HIS
6	Z	249	PHE
7	a	28	LEU
7	a	33	LEU
8	b	53	THR
8	b	97	LEU
9	c	69	VAL
9	c	229	LEU
9	c	275	VAL
10	d	122	LEU
10	d	158	ILE
11	e	4	LYS
11	e	5	LYS
12	A	153	LEU
12	A	157	ILE
12	A	161	VAL
12	A	220	THR
12	A	250	VAL
13	B	105	THR
13	B	136	LEU
13	B	164	MET
13	B	173	VAL
13	B	175	LYS
13	B	176	VAL
13	B	177	GLU
13	B	190	LEU
13	B	259	TYR
14	C	11	LEU
14	C	66	LEU
14	C	99	VAL
14	C	131	VAL
14	C	138	MET
14	C	148	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	C	235	PHE
14	C	249	ASP
14	C	259	LEU
14	C	286	THR
14	C	295	THR
15	D	186	THR
15	D	234	GLU
15	D	344	ILE
16	E	80	VAL
16	E	204	VAL
17	F	85	THR
17	F	169	ASP
17	F	231	THR
17	F	272	PHE
17	F	282	ILE
17	F	283	ILE
22	K	20	ARG
22	K	22	PHE
22	K	228	MET
23	L	82	ARG
23	L	89	ARG
24	M	196	ILE
28	Q	68	LYS
28	Q	140	LEU
31	T	37	ARG
31	T	185	ASN
22	k	101	PHE
22	k	227	HIS
22	k	228	MET
22	k	229	PHE
24	m	40	ARG
24	m	196	ILE
25	n	127	ILE
28	q	82	ASN
31	t	100	ARG
32	f	39	LYS
32	f	88	SER
32	f	184	LEU
32	f	207	LEU
32	f	275	MET
32	f	370	MET
32	f	387	GLN

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Mol	Chain	Res	Type
32	f	389	LYS
32	f	391	LEU
32	f	460	ASP
32	f	463	LEU
32	f	473	ASN
32	f	479	LEU
32	f	493	ASN
32	f	565	ASN
32	f	569	LYS
32	f	639	LYS
32	f	641	GLU
32	f	662	MET
32	f	788	MET
32	f	797	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	70	HIS
1	U	107	HIS
1	U	145	HIS
1	U	149	GLN
1	U	258	GLN
1	U	345	ASN
1	U	389	ASN
1	U	438	GLN
1	U	453	HIS
1	U	475	HIS
1	U	698	GLN
1	U	734	GLN
1	U	777	HIS
2	V	81	GLN
2	V	279	GLN
2	V	281	ASN
2	V	299	GLN
2	V	401	ASN
2	V	427	GLN
2	V	477	HIS
2	V	487	HIS
3	W	235	GLN
3	W	246	HIS
3	W	426	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	W	444	HIS
4	X	207	GLN
4	X	262	ASN
4	X	406	ASN
5	Y	302	HIS
5	Y	363	ASN
5	Y	365	GLN
5	Y	378	ASN
6	Z	102	HIS
6	Z	194	GLN
6	Z	224	HIS
7	a	23	HIS
7	a	249	GLN
7	a	257	GLN
7	a	290	GLN
7	a	337	GLN
8	b	76	HIS
8	b	142	ASN
9	c	30	GLN
9	c	115	HIS
9	c	199	HIS
9	c	219	ASN
9	c	283	HIS
10	d	109	GLN
12	A	304	ASN
12	A	305	GLN
12	A	314	ASN
13	B	154	HIS
13	B	241	ASN
13	B	431	GLN
14	C	205	HIS
14	C	241	HIS
15	D	187	HIS
15	D	302	ASN
15	D	376	ASN
15	D	412	GLN
15	D	414	HIS
16	E	190	GLN
16	E	220	ASN
16	E	316	HIS
17	F	255	GLN
17	F	323	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	F	325	GLN
17	F	395	GLN
19	H	119	GLN
19	H	166	ASN
20	I	53	HIS
20	I	95	GLN
20	I	119	GLN
20	I	155	ASN
22	K	214	ASN
22	K	224	GLN
22	K	227	HIS
23	L	59	HIS
23	L	166	GLN
25	N	28	ASN
25	N	154	GLN
26	O	193	ASN
27	P	93	ASN
28	Q	82	ASN
28	Q	101	ASN
31	T	185	ASN
20	i	53	HIS
20	i	95	GLN
20	i	119	GLN
20	i	240	HIS
22	k	114	GLN
22	k	214	ASN
23	l	152	ASN
25	n	154	GLN
26	o	165	ASN
27	p	93	ASN
27	p	169	GLN
28	q	101	ASN
30	s	163	HIS
31	t	81	HIS
32	f	387	GLN
32	f	452	ASN
32	f	473	ASN
32	f	493	ASN
32	f	540	GLN
32	f	752	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

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.

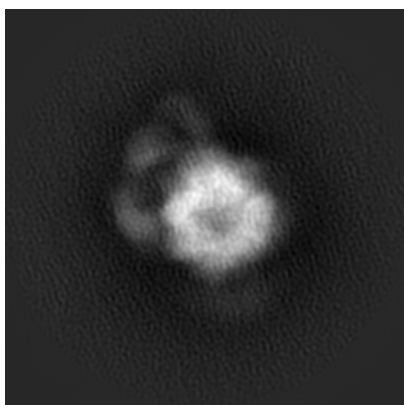
## 6 Map visualisation [i](#)

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](#)

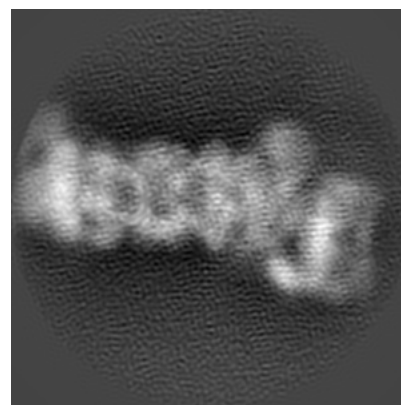
#### 6.1.1 Primary map



X



Y

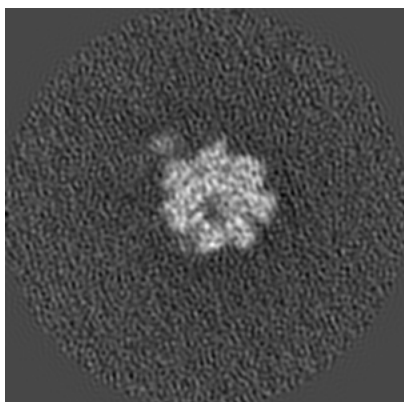


Z

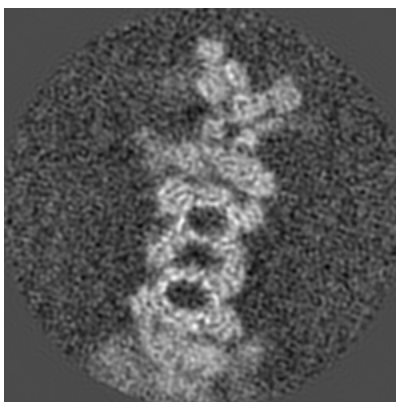
The images above show the map projected in three orthogonal directions.

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

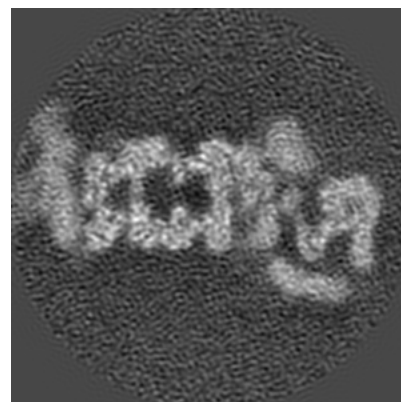
#### 6.2.1 Primary map



X Index: 280



Y Index: 280

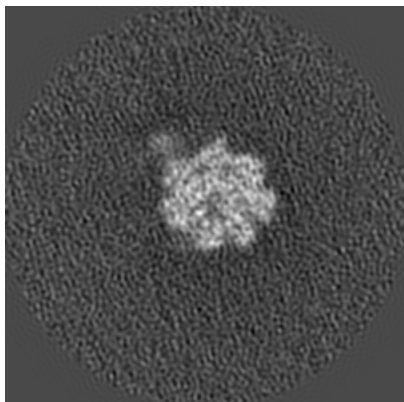


Z Index: 280

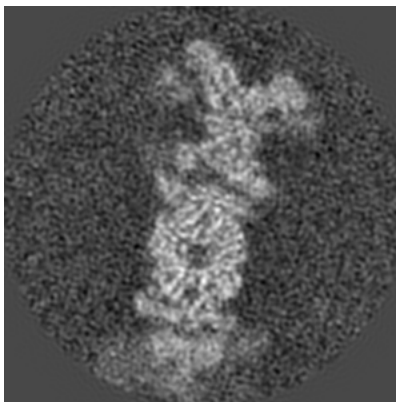
The images above show central slices of the map in three orthogonal directions.

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

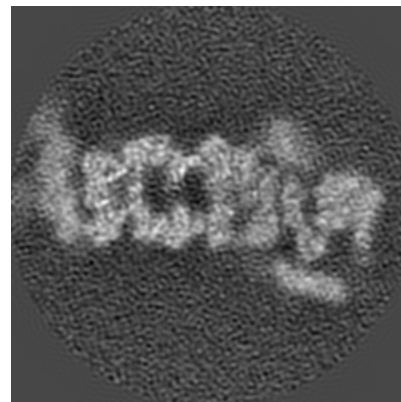
### 6.3.1 Primary map



X Index: 282



Y Index: 264

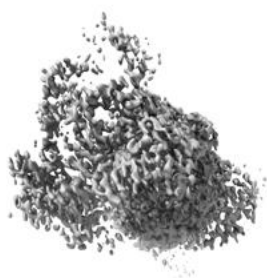


Z Index: 286

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

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

### 6.4.1 Primary map



X



Y



Z

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.



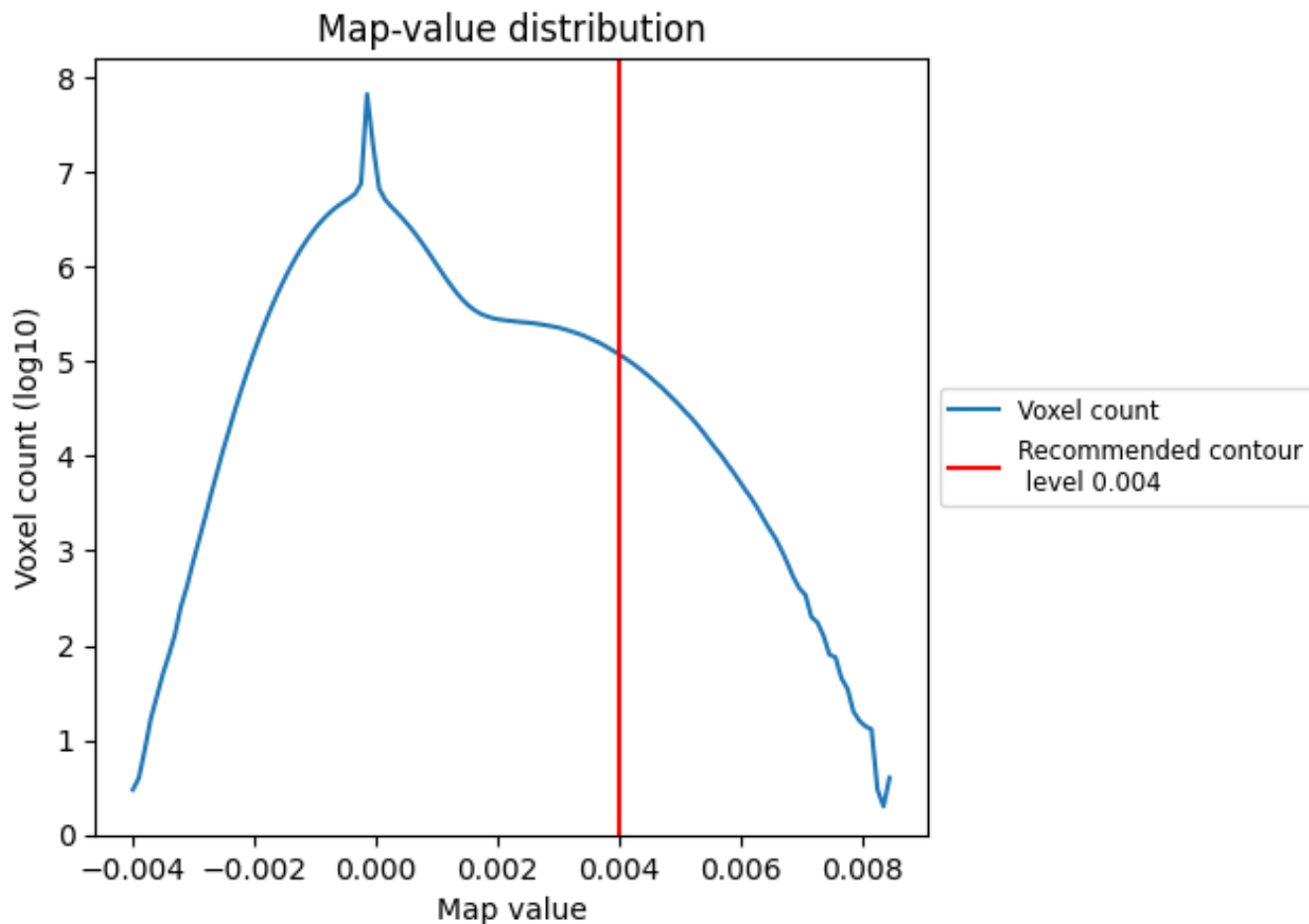
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

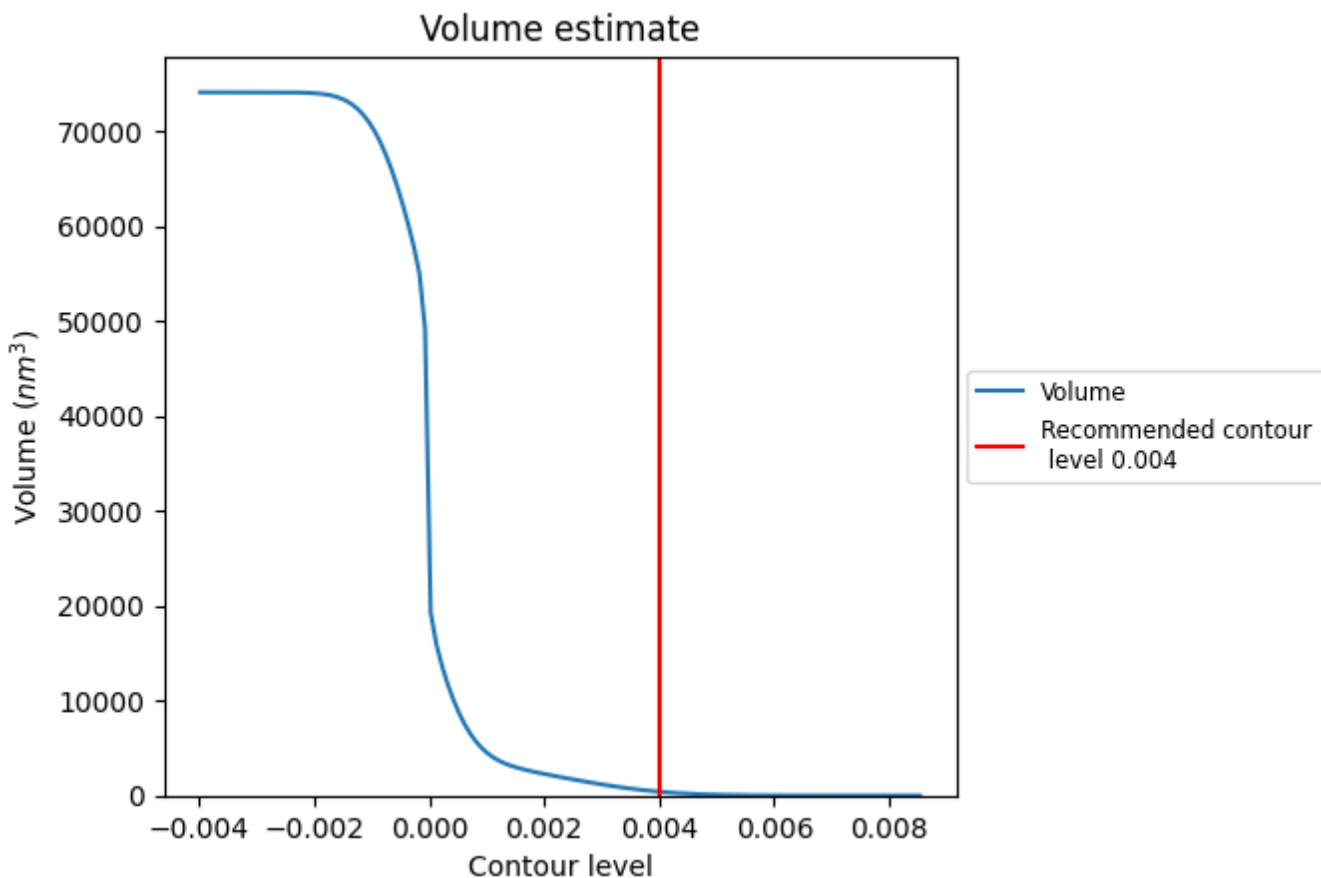
This section contains the results of statistical analysis of the map.

### 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.

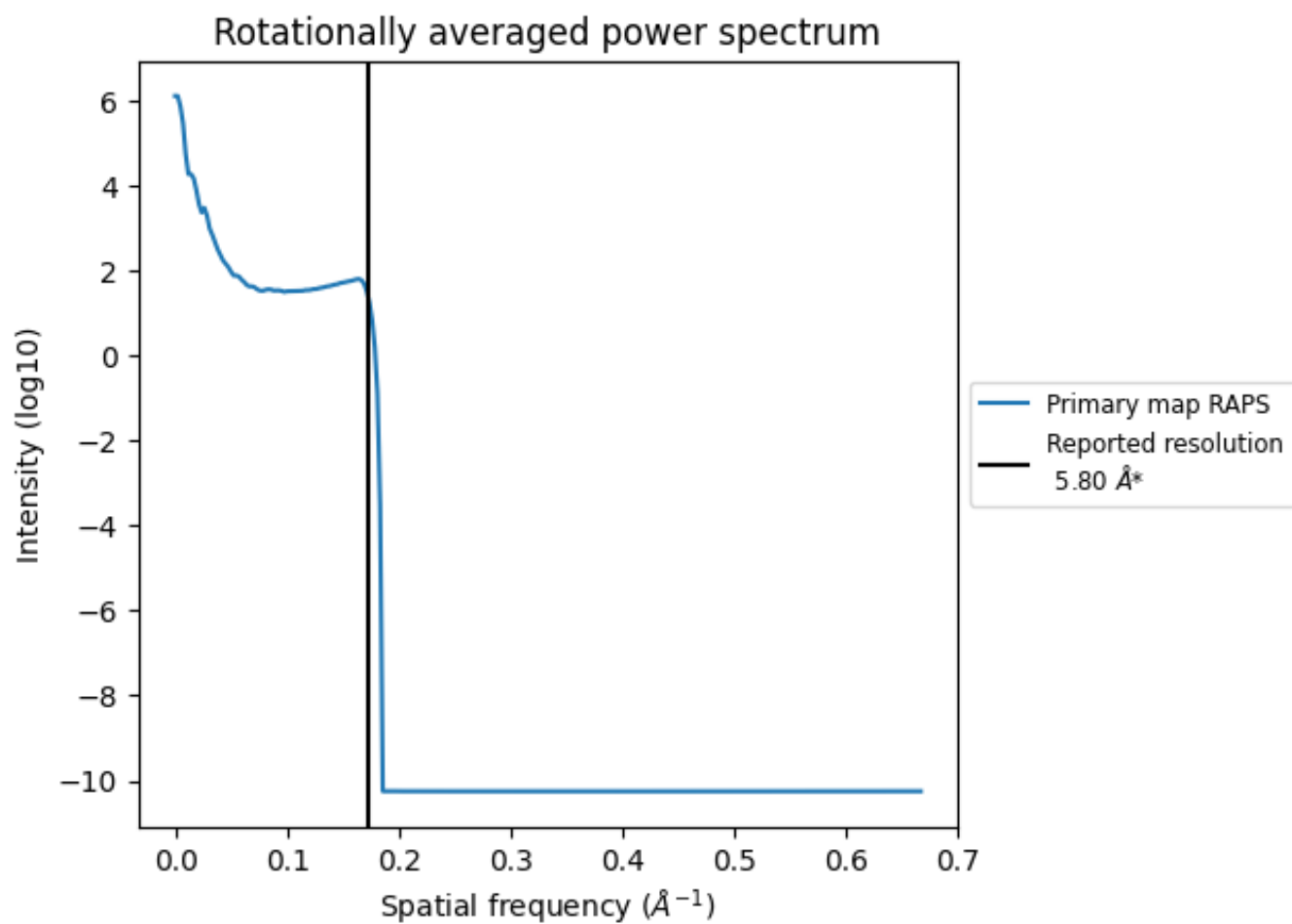
## 7.2 Volume estimate [i](#)



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 i



\*Reported resolution corresponds to spatial frequency of 0.172 Å<sup>-1</sup>

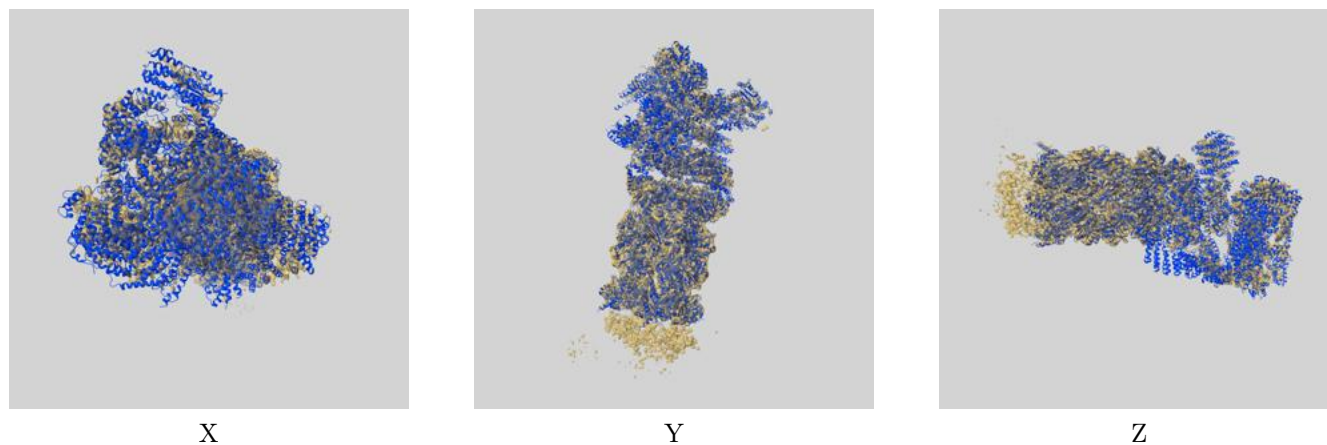
## 8 Fourier-Shell correlation

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

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

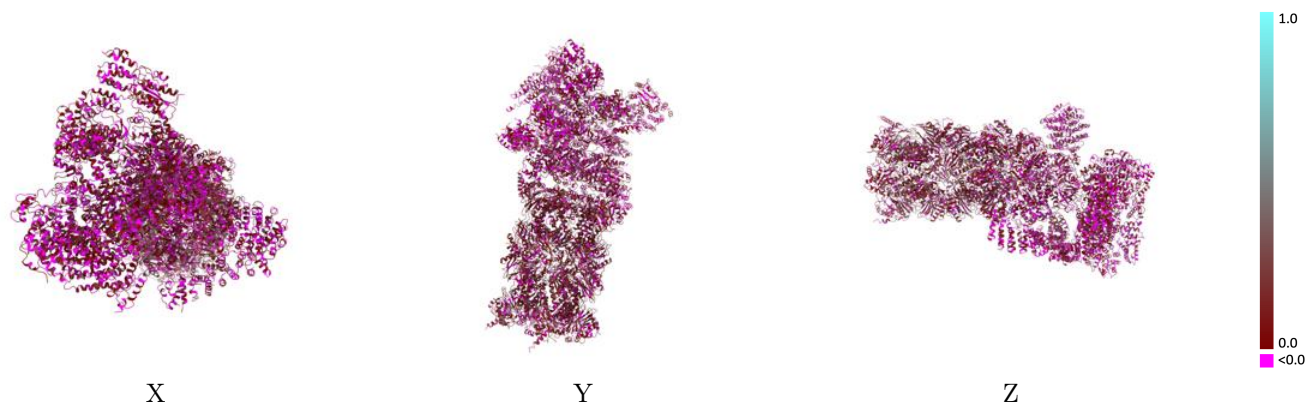
This section contains information regarding the fit between EMDB map EMD-8668 and PDB model 5VFU. Per-residue inclusion information can be found in section 3 on page 11.

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



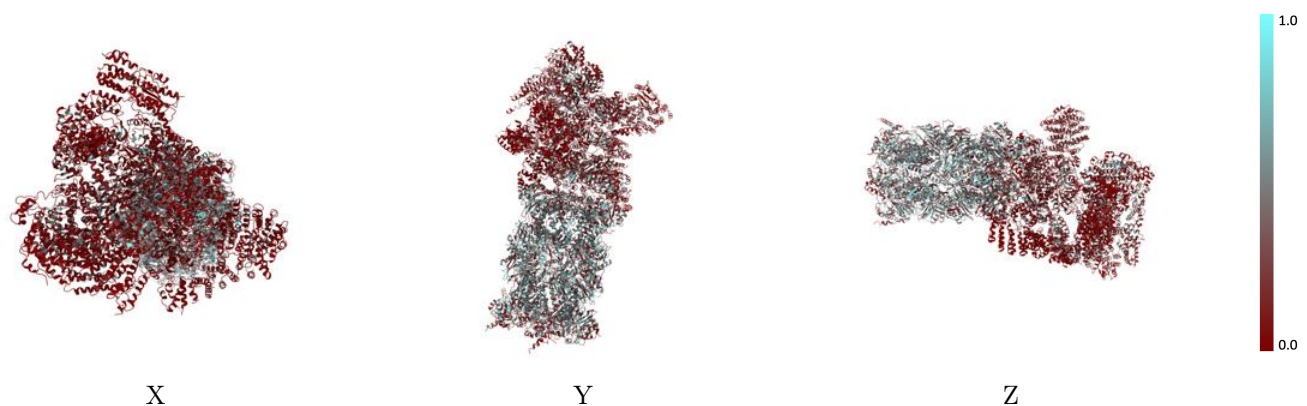
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



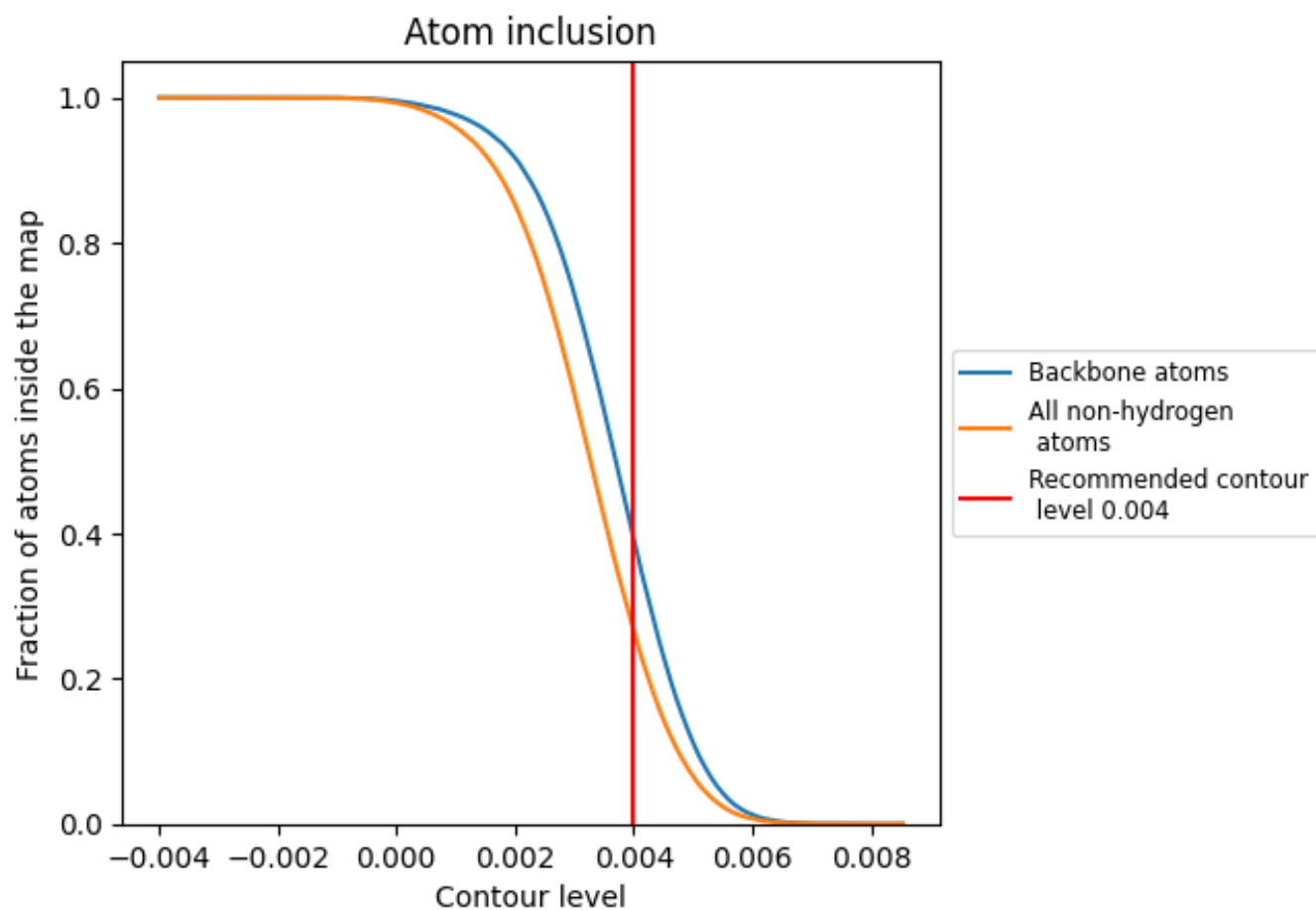
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.2657	0.0980
A	0.2199	0.0990
B	0.1392	0.0780
C	0.1391	0.0700
D	0.1580	0.0620
E	0.1749	0.0740
F	0.1897	0.0820
G	0.3343	0.1230
H	0.3594	0.1240
I	0.3244	0.1260
J	0.3836	0.1400
K	0.3605	0.1350
L	0.4079	0.1320
M	0.3726	0.1270
N	0.4328	0.1320
O	0.4281	0.1470
P	0.4557	0.1280
Q	0.4326	0.1480
R	0.4853	0.1440
S	0.4386	0.1460
T	0.4966	0.1530
U	0.2193	0.0670
V	0.1151	0.0620
W	0.0592	0.0590
X	0.0577	0.0180
Y	0.1646	0.0630
Z	0.1761	0.0760
a	0.0835	0.0600
b	0.0791	0.0550
c	0.2015	0.0920
d	0.0785	0.0290
e	0.0606	0.0310
f	0.0637	0.0400
g	0.3653	0.1320
h	0.3975	0.1420



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Chain	Atom inclusion	Q-score
i	 0.3314	 0.1280
j	 0.3487	 0.1290
k	 0.3652	 0.1410
l	 0.4023	 0.1280
m	 0.3610	 0.1150
n	 0.4621	 0.1440
o	 0.4442	 0.1520
p	 0.4519	 0.1350
q	 0.4456	 0.1370
r	 0.4673	 0.1380
s	 0.4492	 0.1400
t	 0.4978	 0.1630