



## wwPDB EM Validation Summary Report ⓘ

Apr 4, 2022 – 01:09 pm BST

PDB ID : 7QO3  
EMDB ID : EMD-14082  
Title : Structure of the 26S proteasome-Ubp6 complex in the si state (Core Particle and Lid)  
Authors : Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsassser, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.  
Deposited on : 2021-12-23  
Resolution : 6.10 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.

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

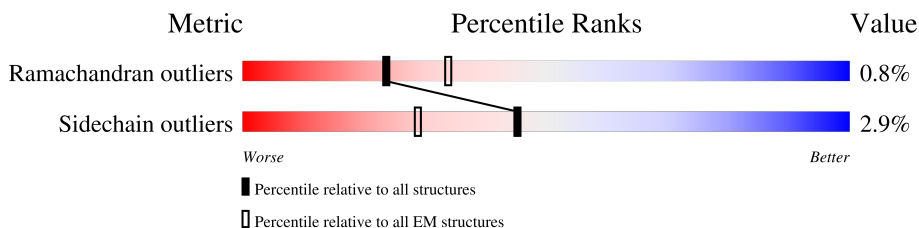
EMDB validation analysis : 0.0.0.dev97  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.10 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	A	252	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">92% . .</p>
1	a	252	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">92% . .</p>
2	B	250	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">95% 5%</p>
2	b	250	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 96%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">96% 95% 5%</p>
3	C	258	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">91% . 5%</p>
3	c	258	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">92% 91% . 5%</p>
4	D	254	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">88% . 7%</p>
4	d	254	<div style="display: flex; align-items: center;"> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">91% 80% 11% . 7%</p>
5	E	260	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 90%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">90% . . 6%</p>

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Mol	Chain	Length	Quality of chain
5	e	260	90% 90% 6%
6	F	234	8% 92% 5%
6	f	234	94% 92% 5%
7	G	288	6% 79% 5% 16%
7	g	288	80% 79% 5% 16%
8	1	215	5% 82% 8% 9%
8	h	215	19% 82% 9% 9%
9	2	261	5% 74% 10% 13%
9	i	261	16% 74% 10% 13%
10	3	205	7% 89% 10%
10	j	205	18% 89% 10%
11	4	198	5% 88% 10%
11	k	198	11% 88% 10%
12	5	287	66% 7% 26%
12	l	287	22% 66% 7% 26%
13	6	241	86% 8%
13	m	241	21% 86% 8%
14	7	266	7% 83% 14%
14	n	266	15% 83% 14%
15	W	268	23% 71% 26%
16	V	306	25% 88% 6% 6%
17	T	274	52% 93% 6%
18	X	156	78% 77% 19%
19	Y	89	70% 89% 10%
20	Z	993	91% 80% 8% 9%

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Mol	Chain	Length	Quality of chain
21	N	945	
22	S	523	
23	P	445	
24	Q	434	
25	R	429	
26	U	338	
27	O	393	

## 2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 90281 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		
4	D	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		
5	E	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	3	204	1581	1010	258	305	8	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	195	1561	992	264	299	6	0	0
11	4	195	1561	992	264	299	6	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	212	1644	1045	280	312	7	0	0
12	5	212	1644	1045	280	312	7	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	222	1757	1115	303	335	4	0	0
13	6	222	1757	1115	303	335	4	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	229	1790	1133	306	344	7	0	0
14	7	229	1790	1133	306	344	7	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	W	197	1534	962	269	300	3	0	0

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	V	289	2274	1425	389	446	14	0	0

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	266	2192	1405	349	432	6	0	0

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	127	1032	664	169	195	4	0	0

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Y	89	731	447	119	164	1	0	0

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Z	906	7005	4416	1150	1409	30	0	0

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	832	6418	4078	1077	1238	25	0	0

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	475	3894	2488	653	738	15	0	0

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	440	3608	2297	604	697	10	0	0

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	434	3499	2225	577	681	16	0	0

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	405	3258	2077	535	636	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	290	2306	1454	392	453	7	0	0

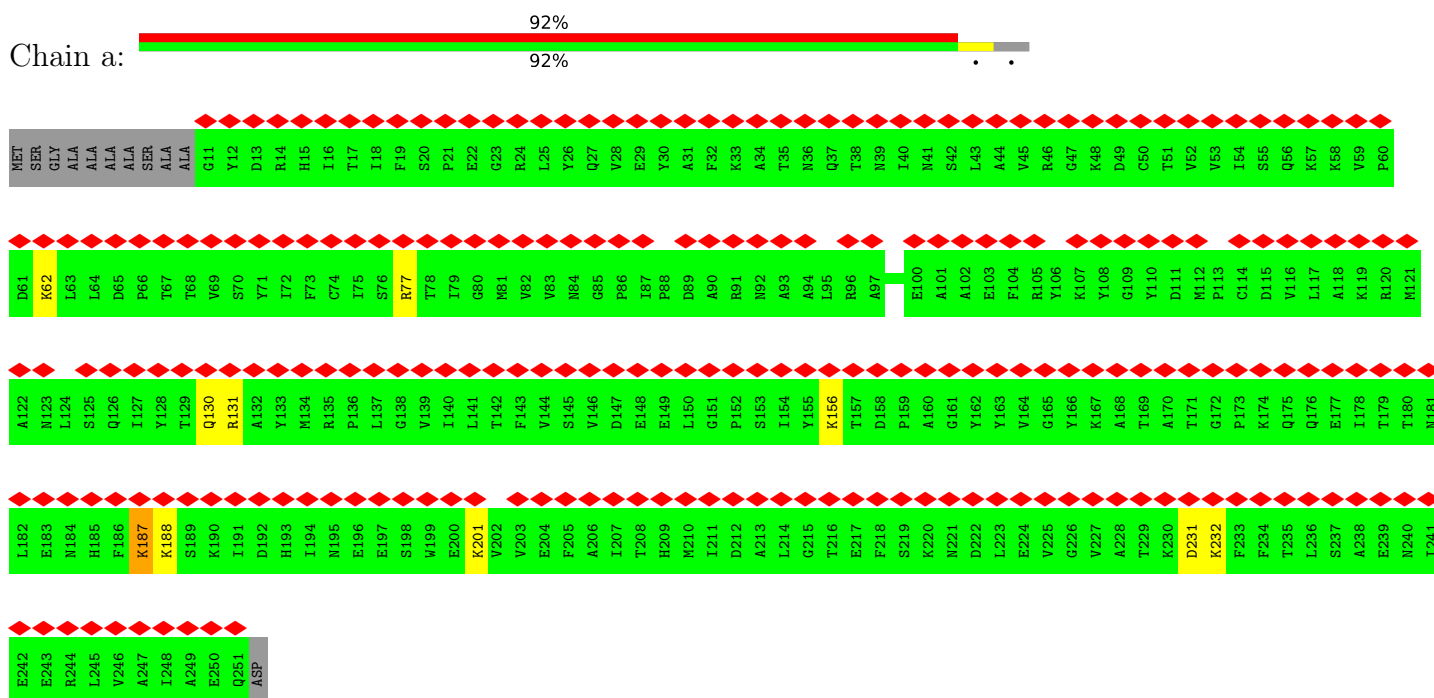
- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	O	388	3186	2051	519	608	8	0	0

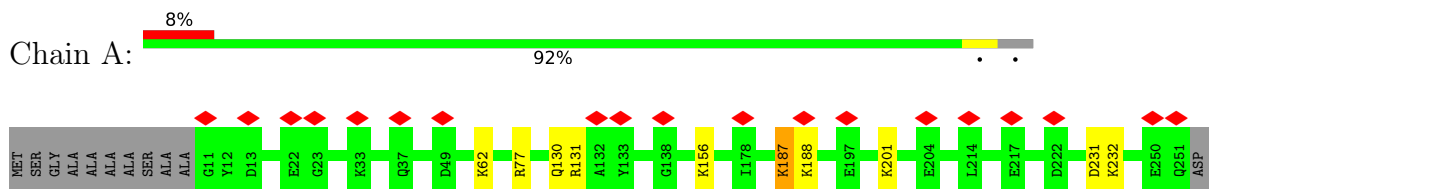
### 3 Residue-property plots

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.

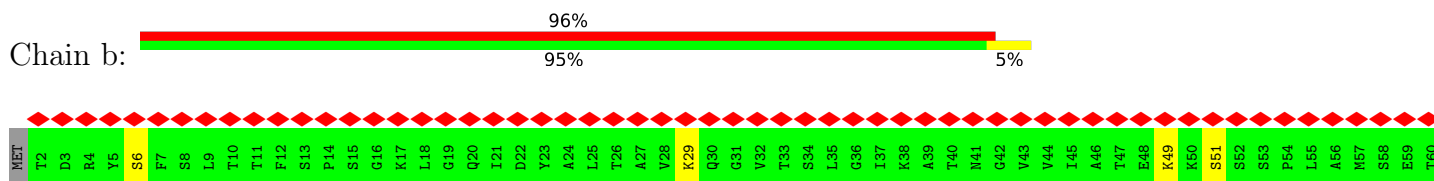
- Molecule 1: Proteasome subunit alpha type-1

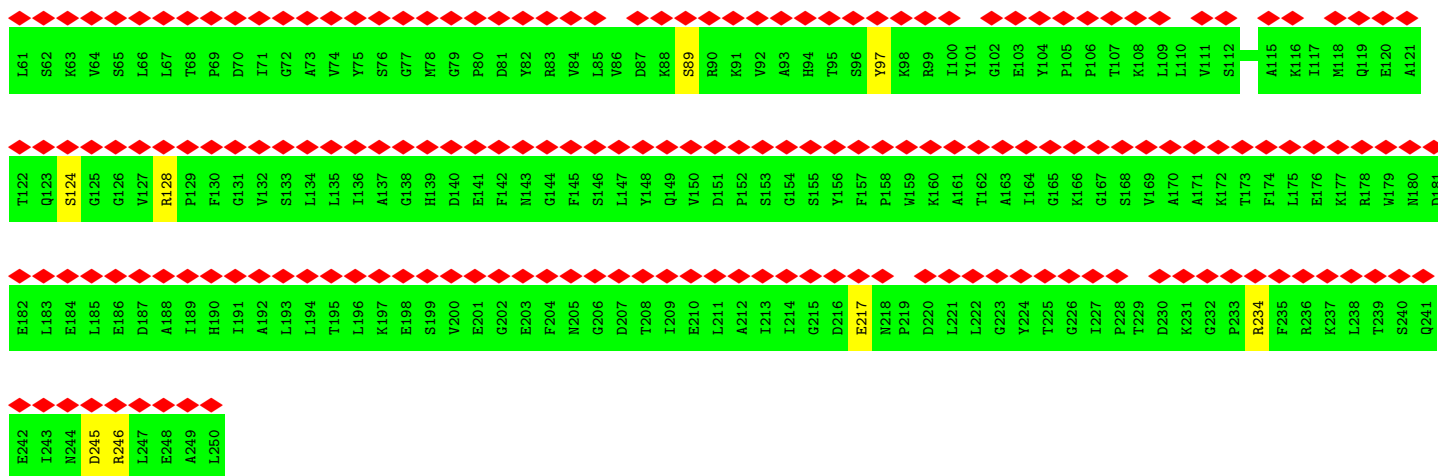


- Molecule 1: Proteasome subunit alpha type-1

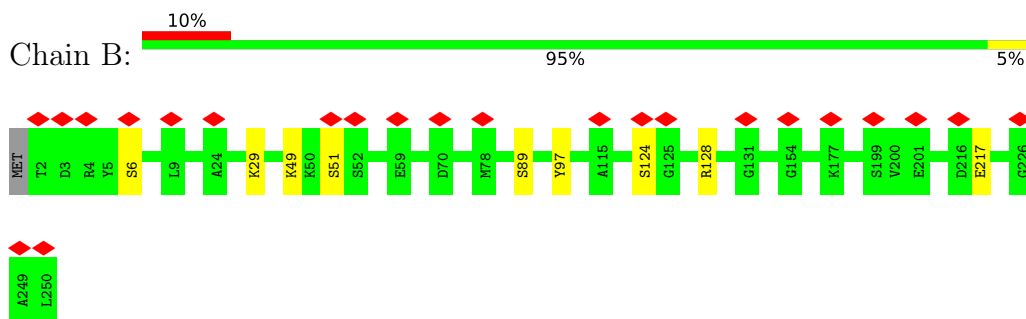


- Molecule 2: Proteasome subunit alpha type-2

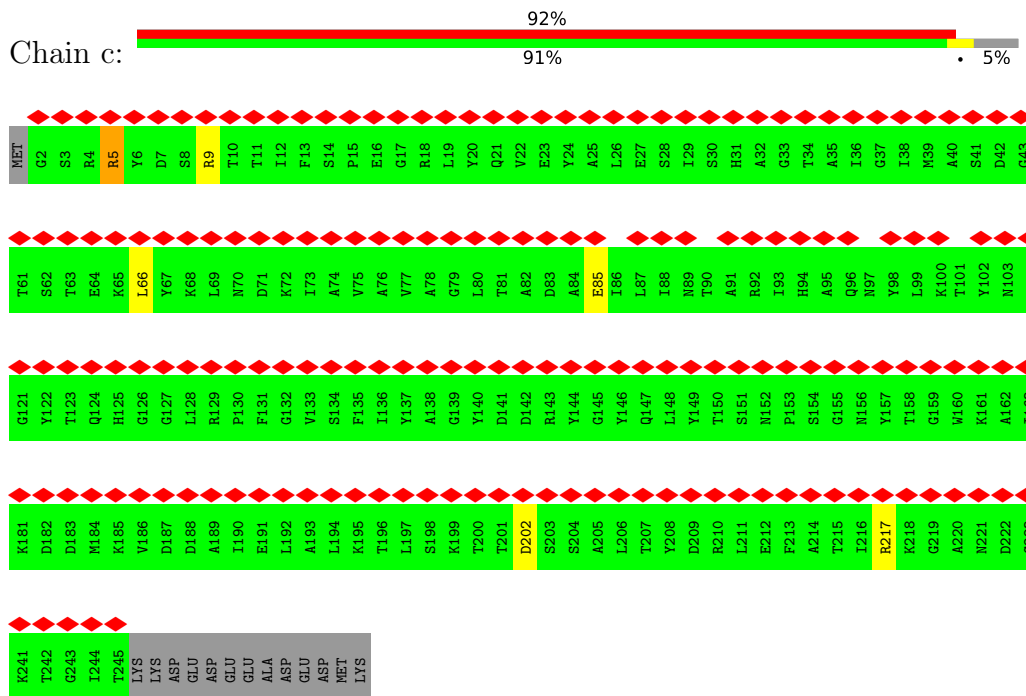




• Molecule 2: Proteasome subunit alpha type-2

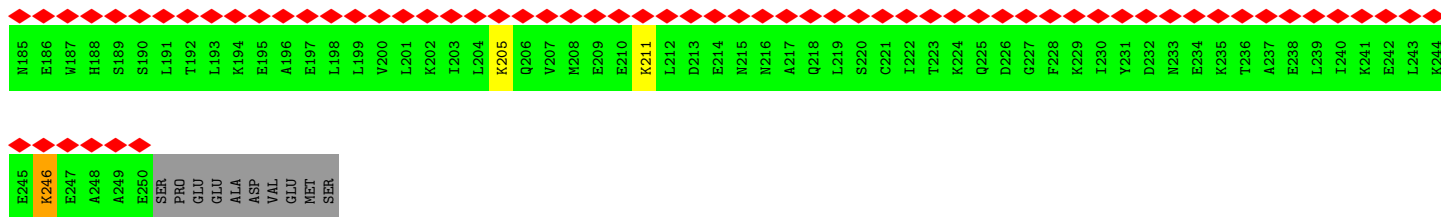


• Molecule 3: Proteasome subunit alpha type-3

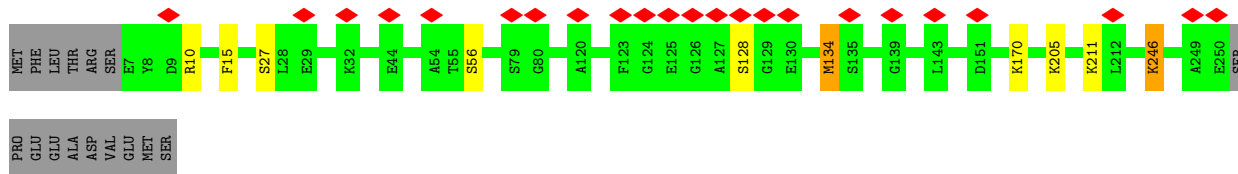
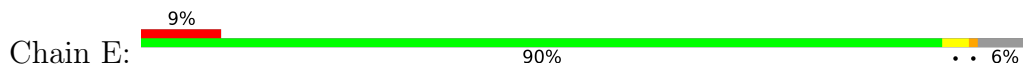


• Molecule 3: Proteasome subunit alpha type-3

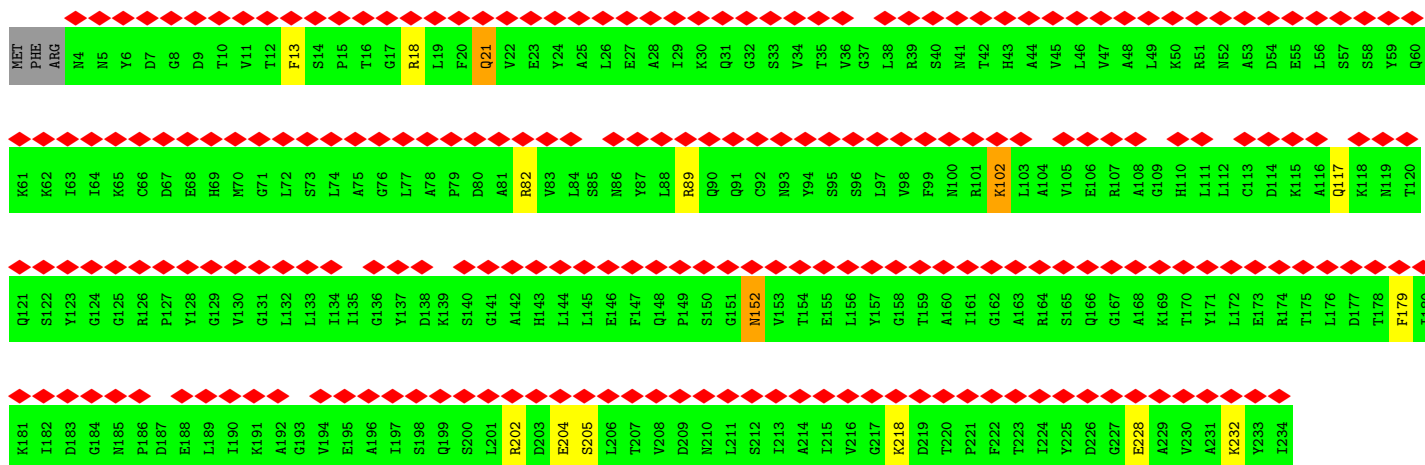
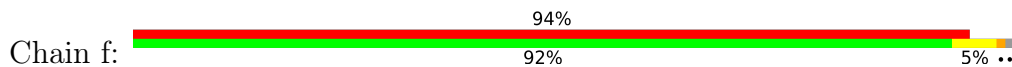




• Molecule 5: Proteasome subunit alpha type-5



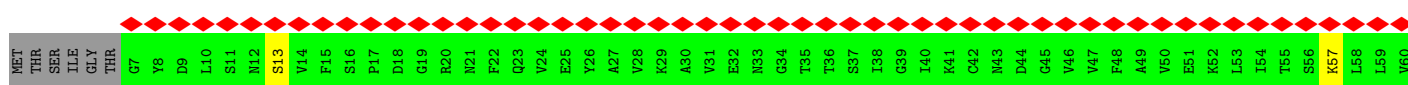
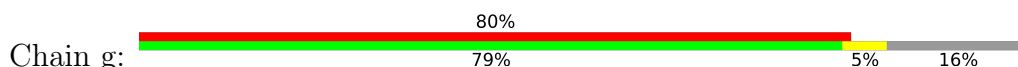
• Molecule 6: Proteasome subunit alpha type-6

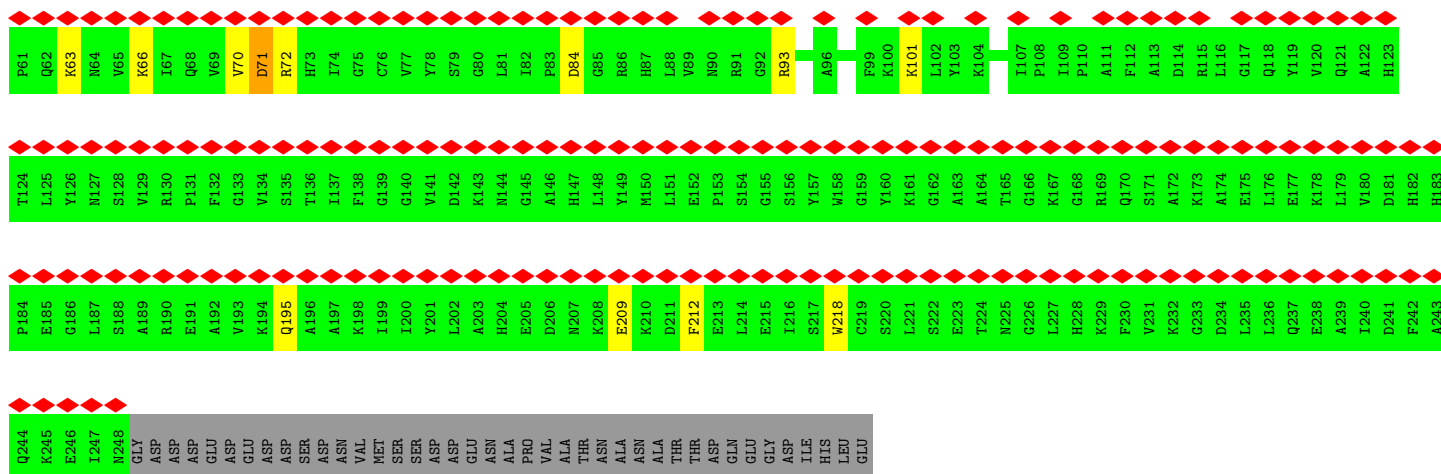


• Molecule 6: Proteasome subunit alpha type-6

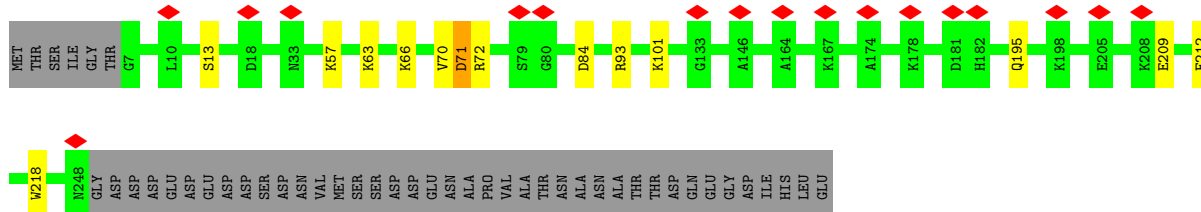
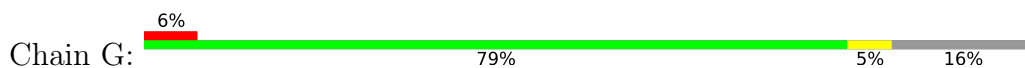


• Molecule 7: Probable proteasome subunit alpha type-7

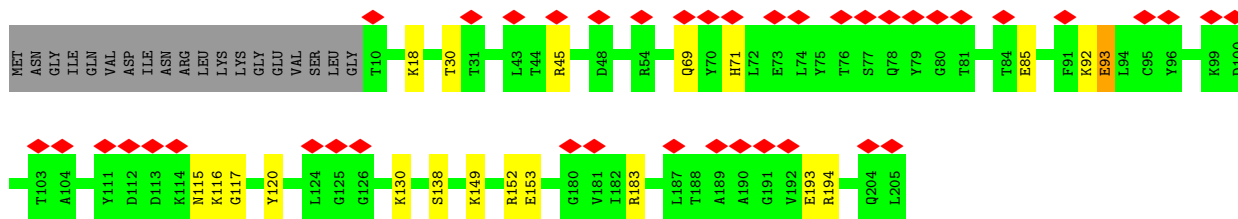
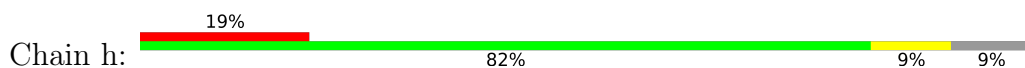




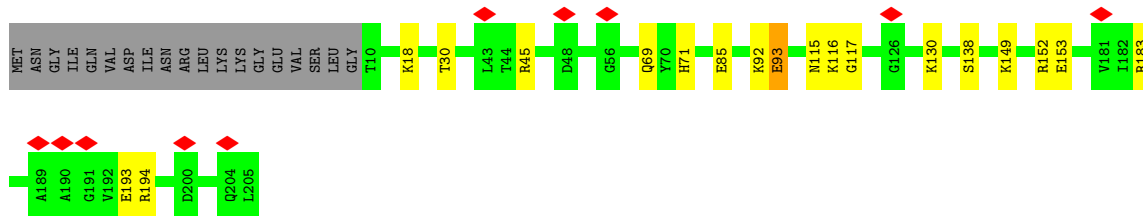
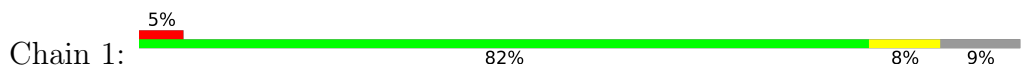
• Molecule 7: Probable proteasome subunit alpha type-7



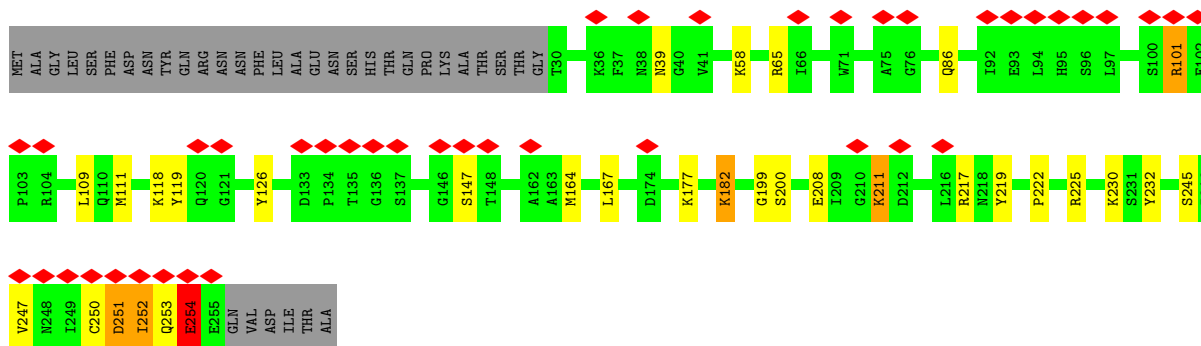
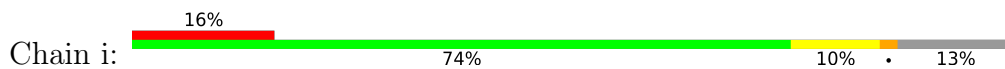
• Molecule 8: Proteasome subunit beta type-1



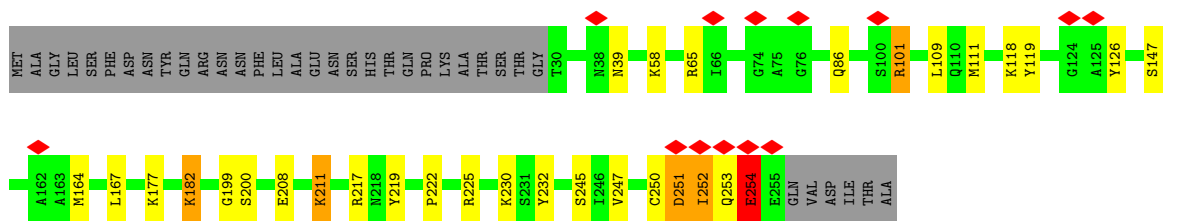
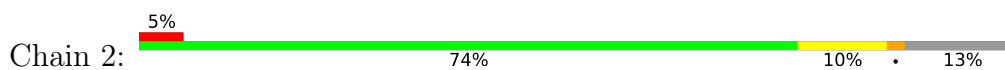
• Molecule 8: Proteasome subunit beta type-1



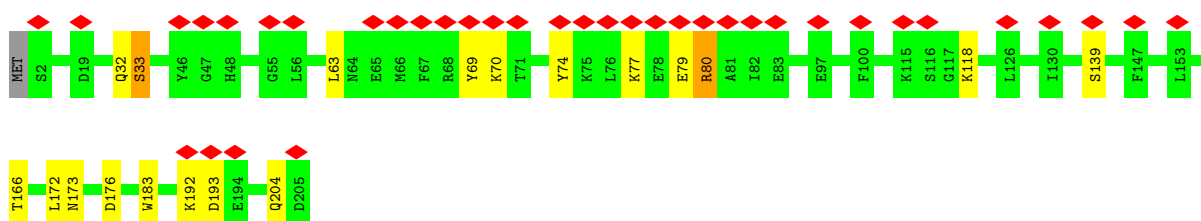
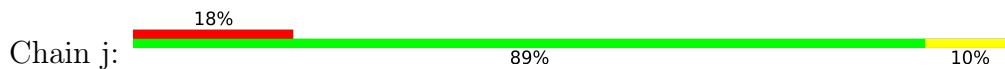
• Molecule 9: Proteasome subunit beta type-2



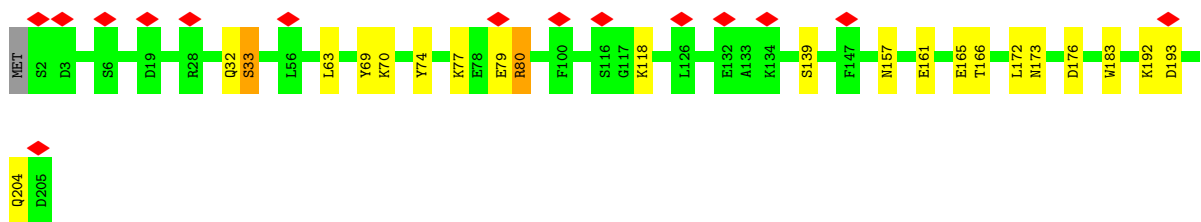
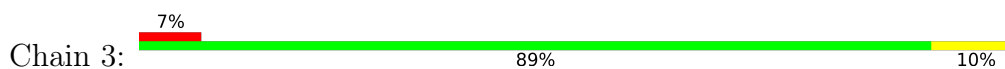
• Molecule 9: Proteasome subunit beta type-2



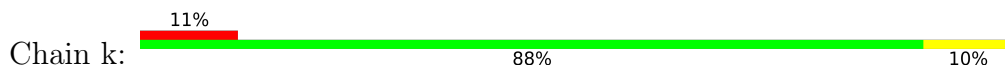
• Molecule 10: Proteasome subunit beta type-3

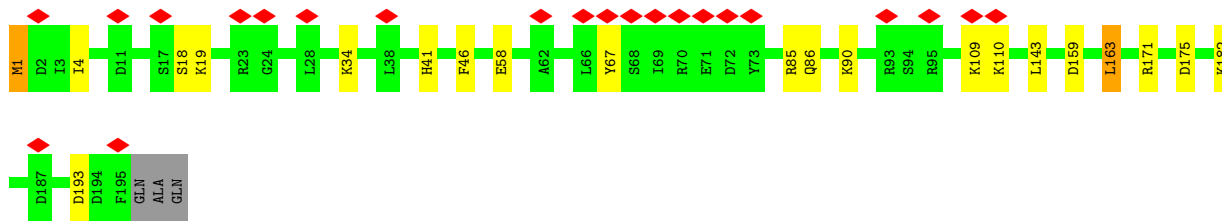


• Molecule 10: Proteasome subunit beta type-3

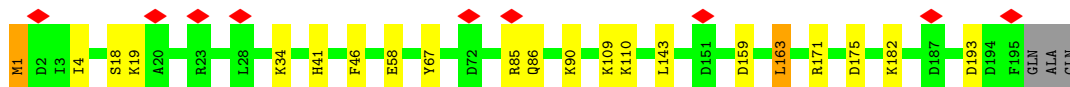
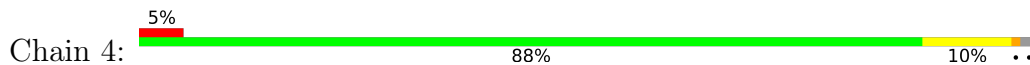


• Molecule 11: Proteasome subunit beta type-4

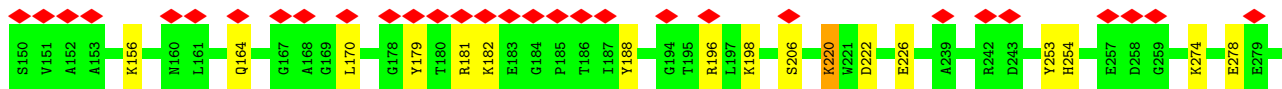
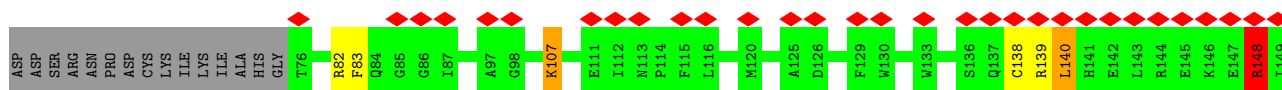




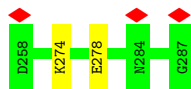
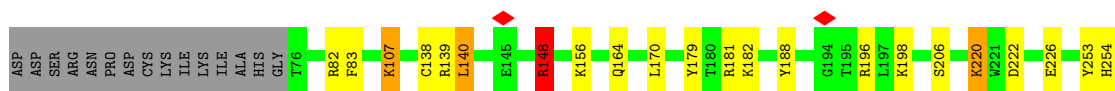
• Molecule 11: Proteasome subunit beta type-4



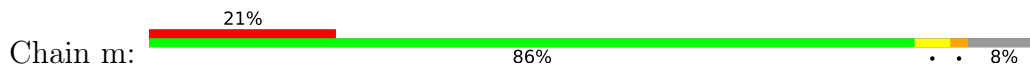
• Molecule 12: Proteasome subunit beta type-5



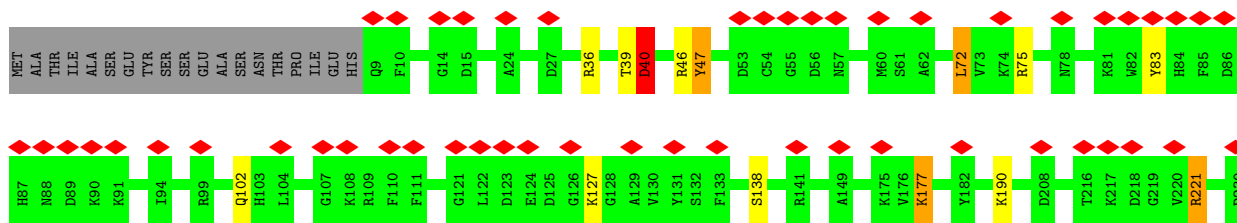
• Molecule 12: Proteasome subunit beta type-5



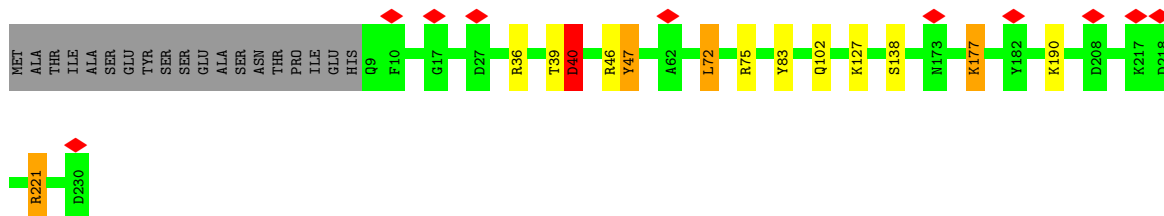
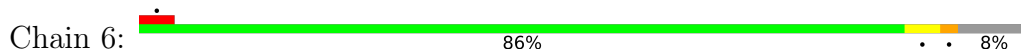
• Molecule 13: Proteasome subunit beta type-6



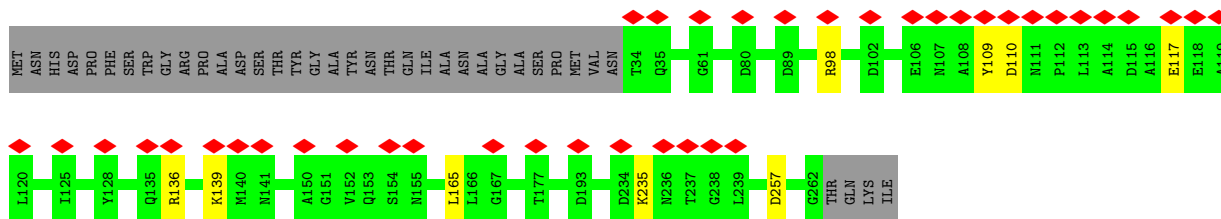
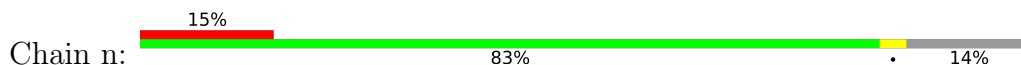




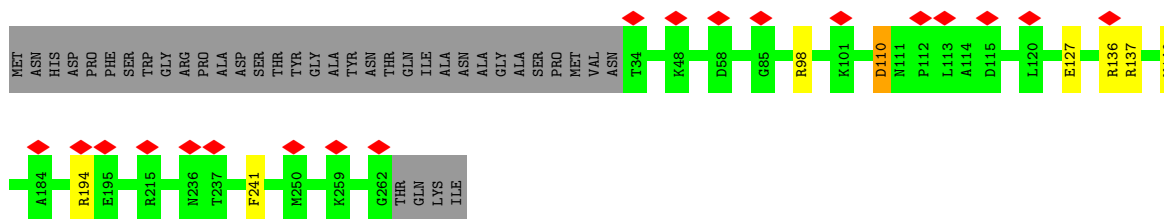
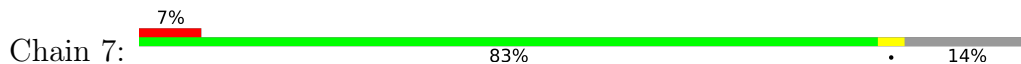
• Molecule 13: Proteasome subunit beta type-6



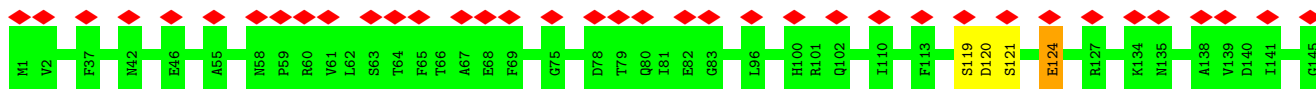
• Molecule 14: Proteasome subunit beta type-7

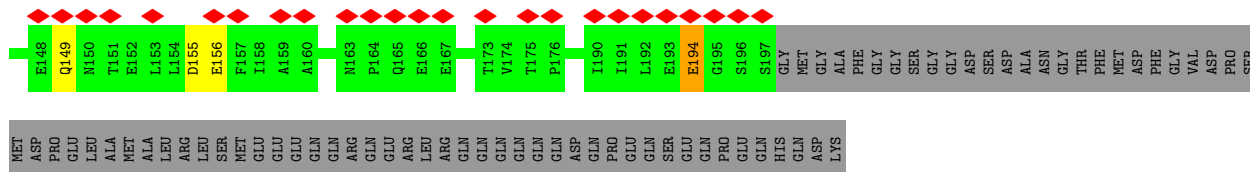


• Molecule 14: Proteasome subunit beta type-7

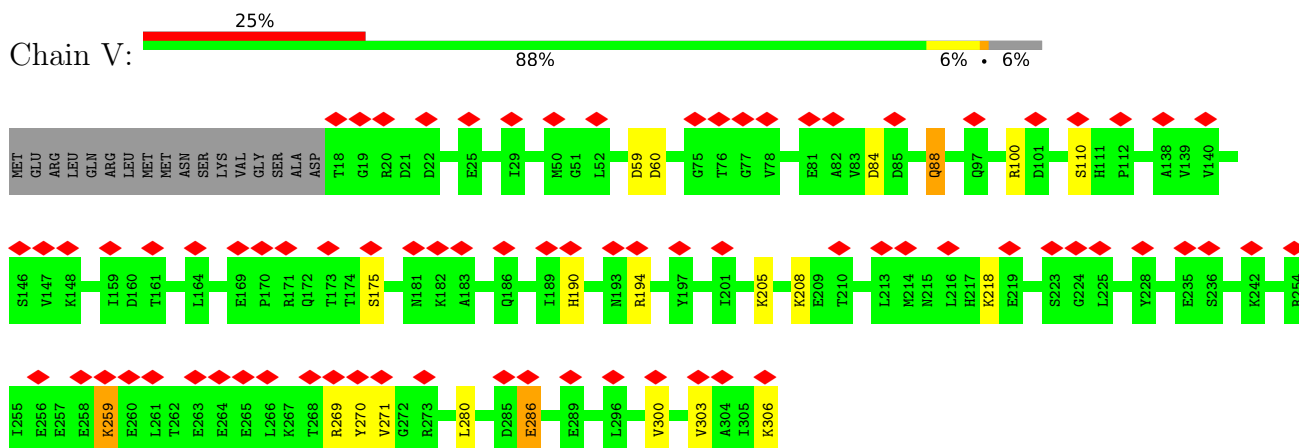


• Molecule 15: 26S proteasome regulatory subunit RPN10

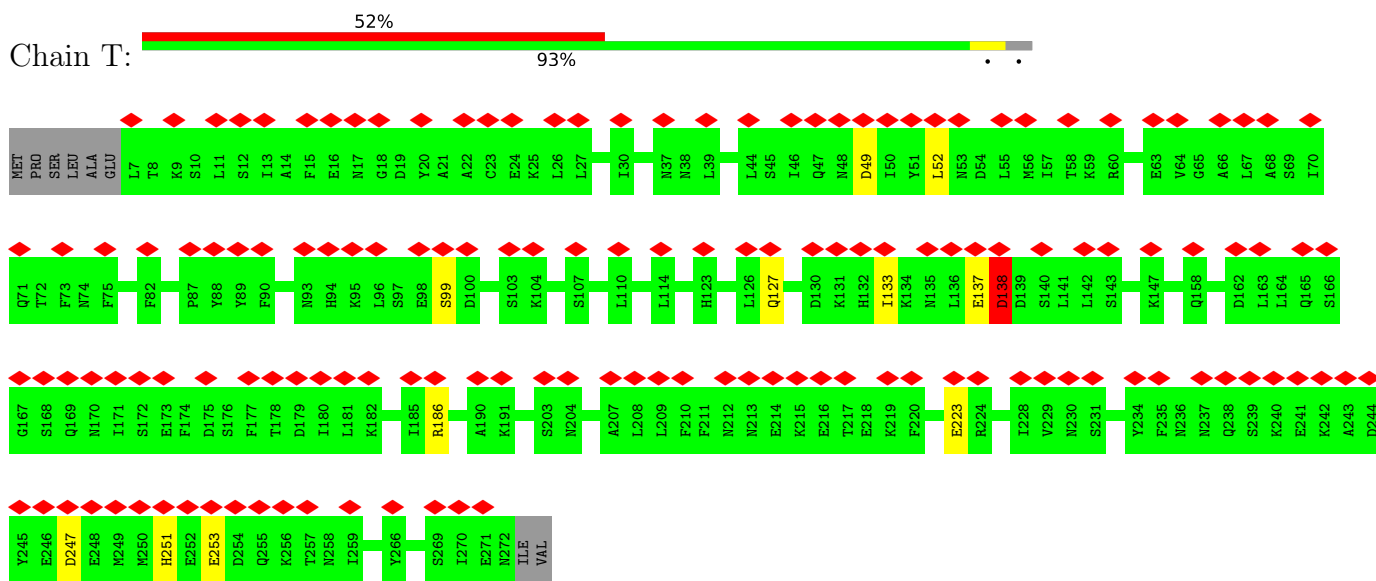




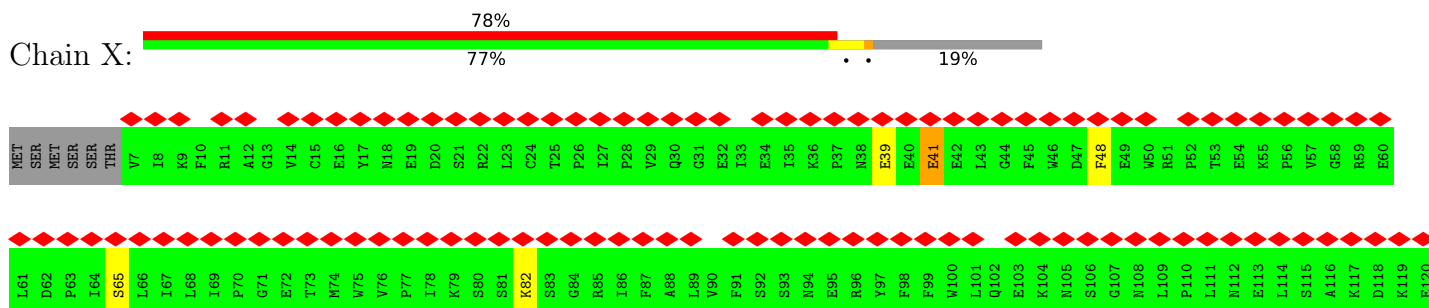
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

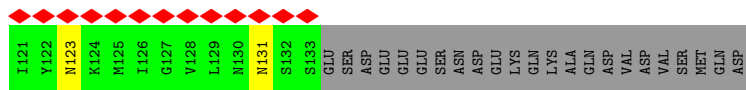


• Molecule 17: 26S proteasome regulatory subunit RPN12

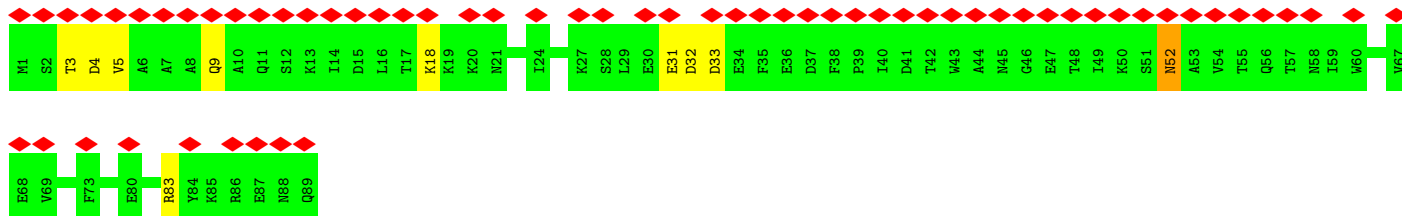
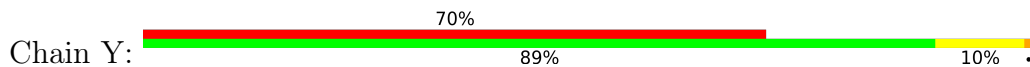


• Molecule 18: 26S proteasome regulatory subunit RPN13

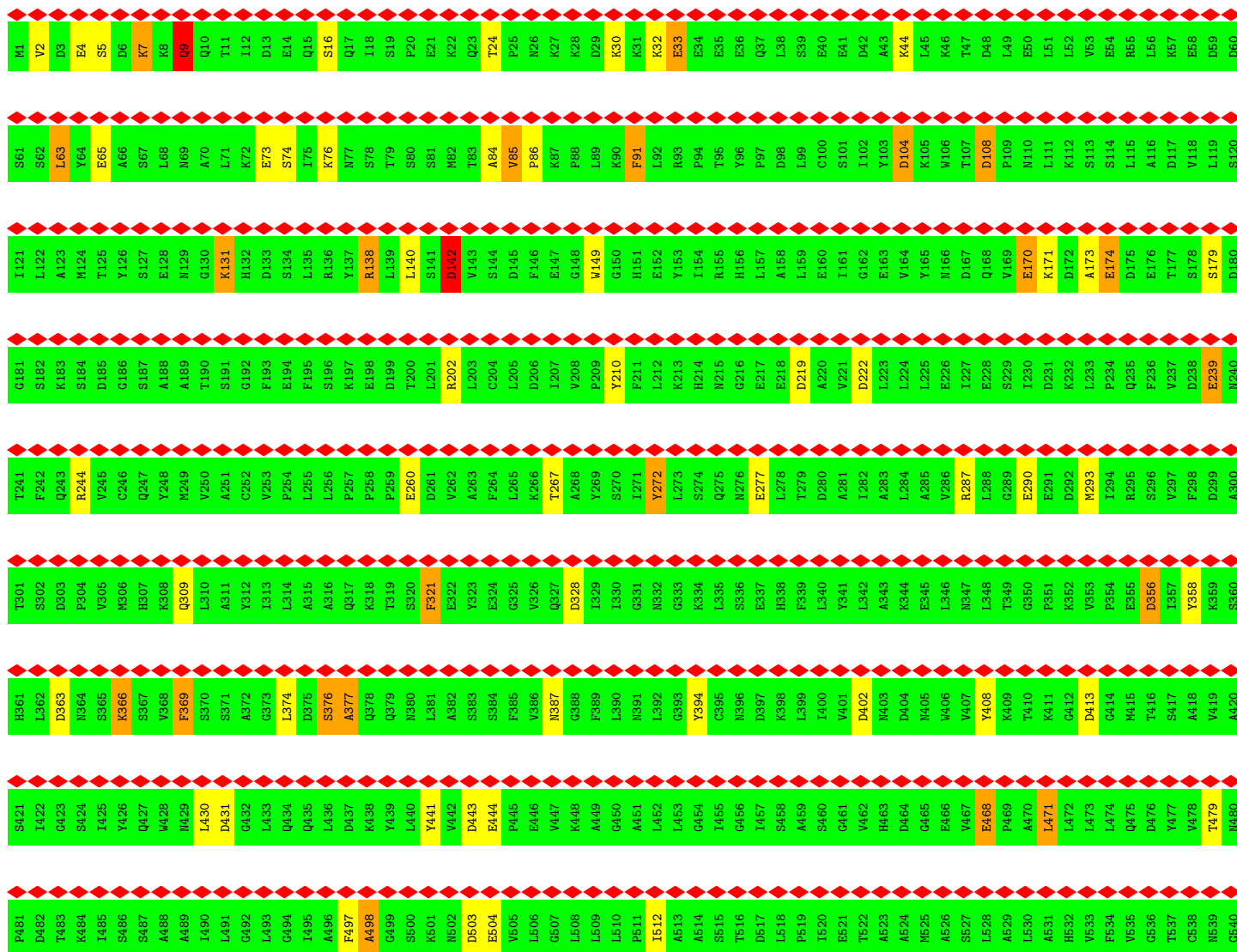
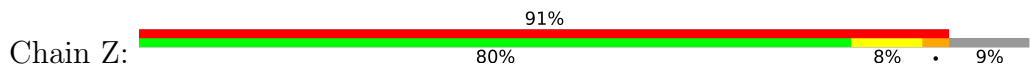


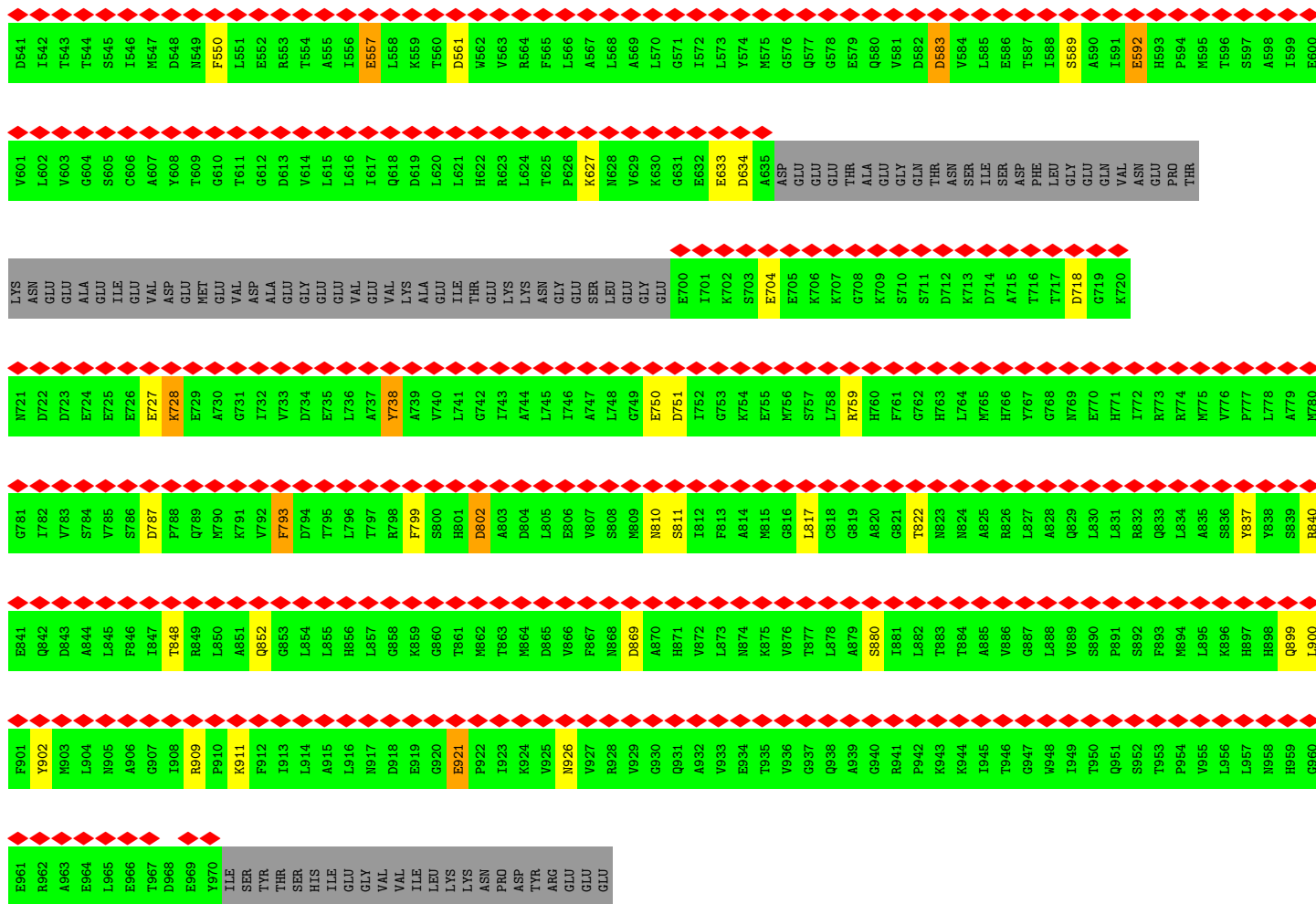


• Molecule 19: 26S proteasome complex subunit SEM1

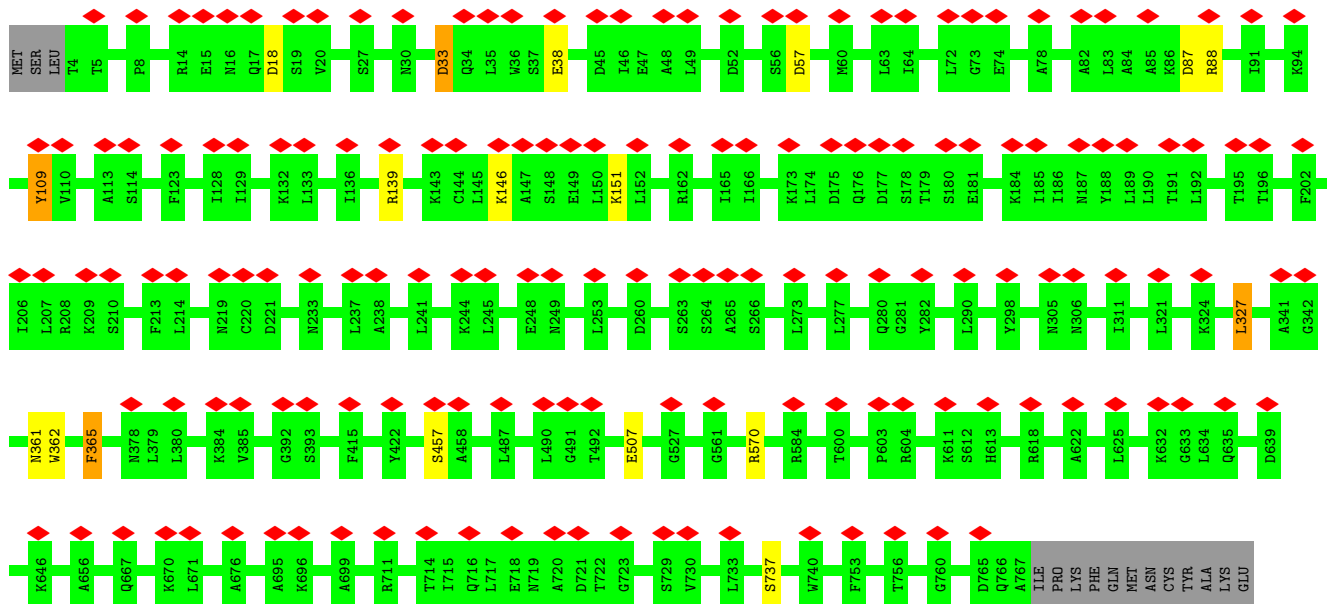
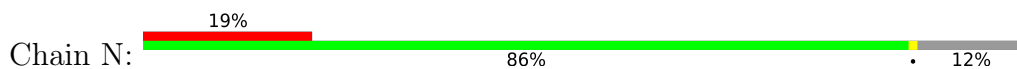


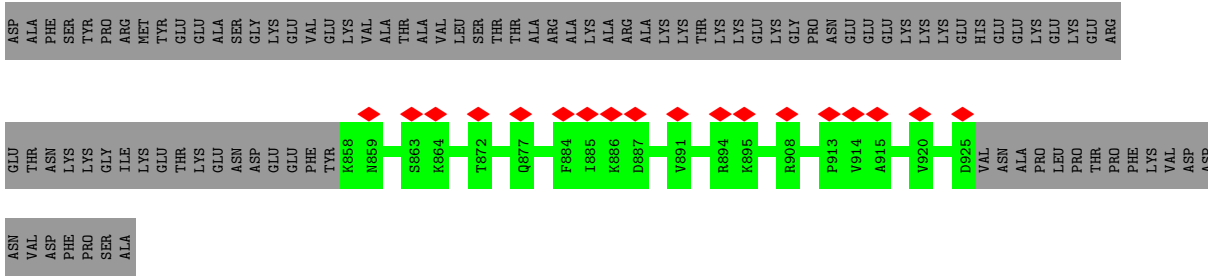
• Molecule 20: 26S proteasome regulatory subunit RPN1



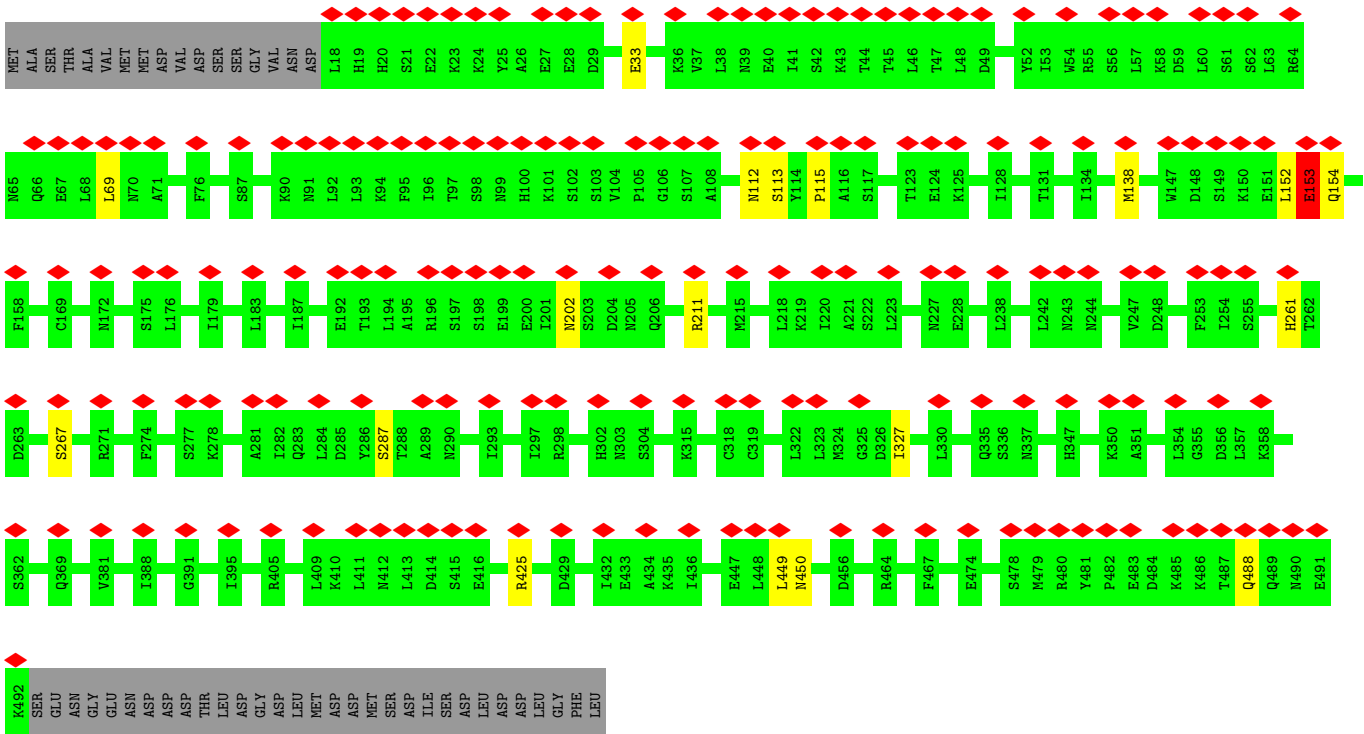
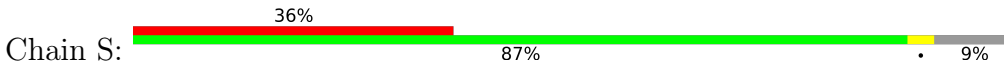


• Molecule 21: 26S proteasome regulatory subunit RPN2

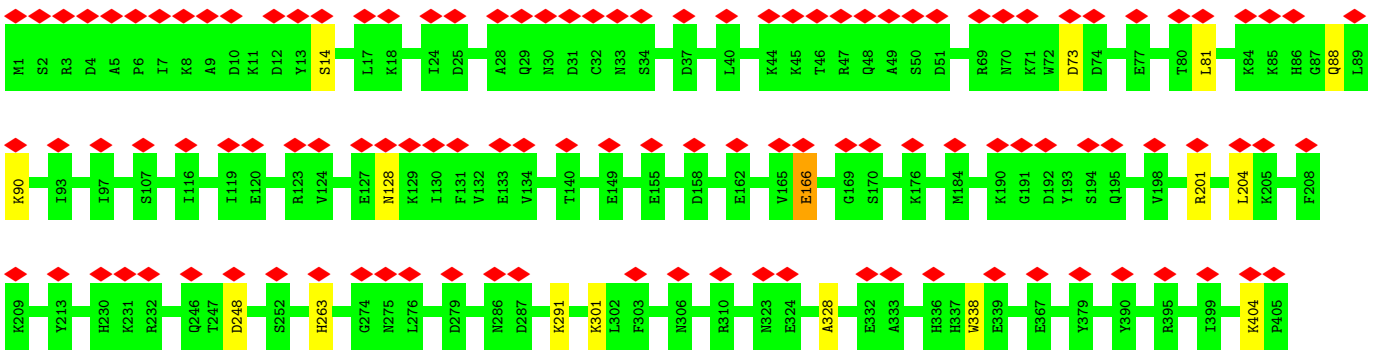
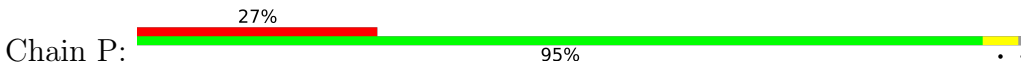


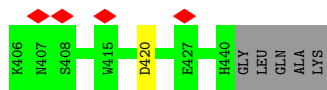


• Molecule 22: 26S proteasome regulatory subunit RPN3

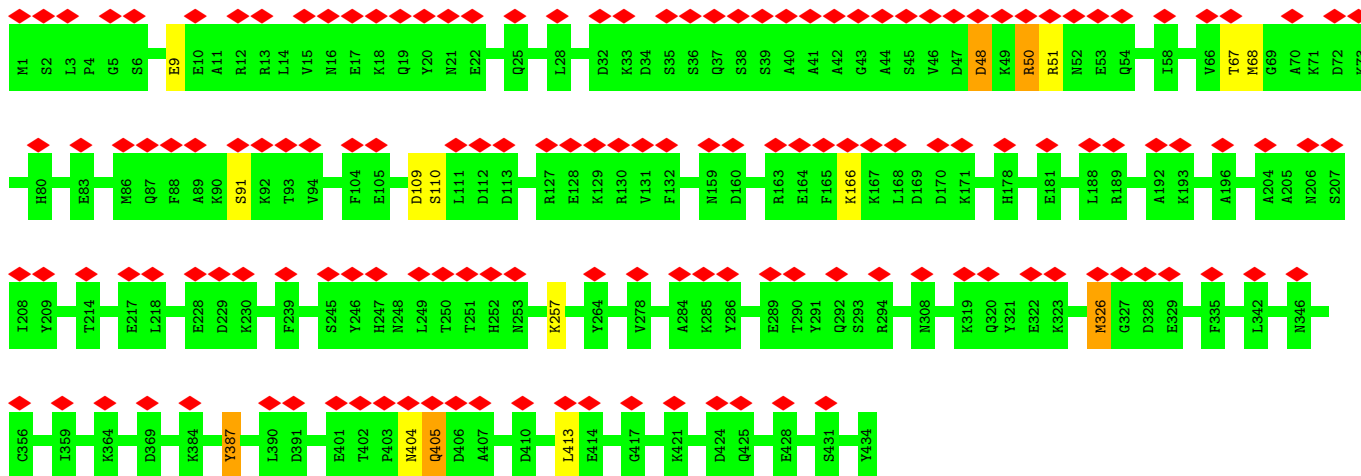


• Molecule 23: 26S proteasome regulatory subunit RPN5

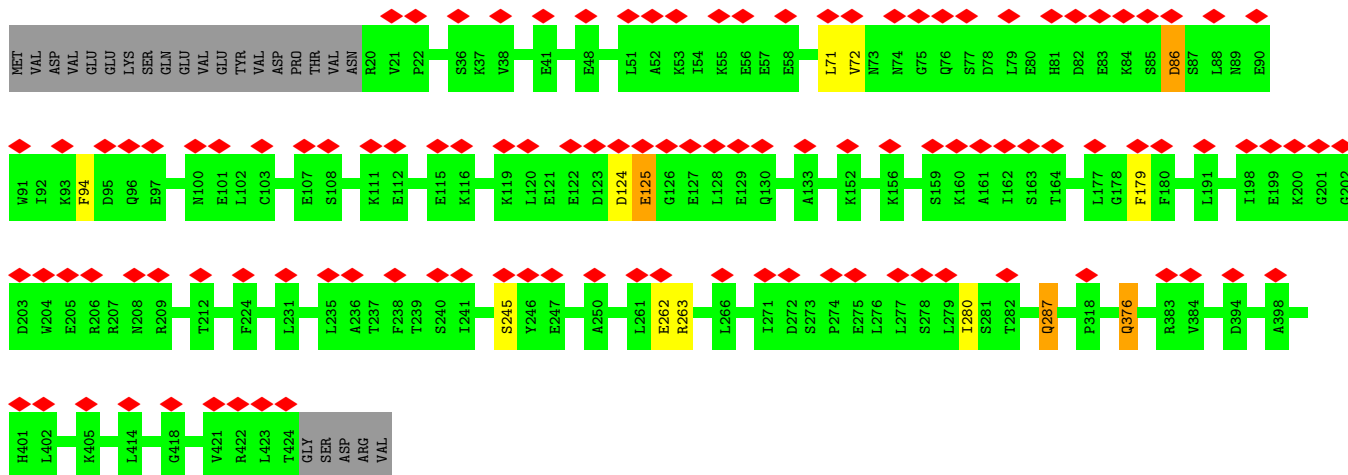
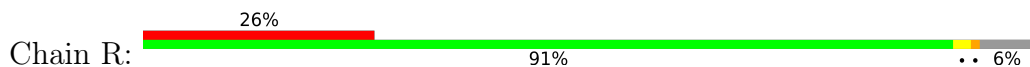




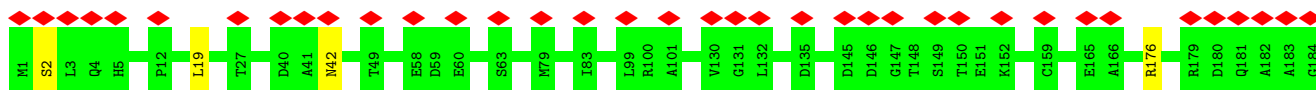
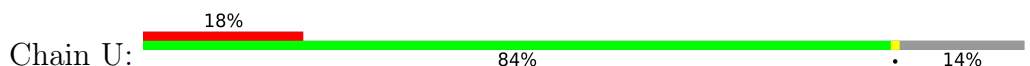
• Molecule 24: 26S proteasome regulatory subunit RPN6

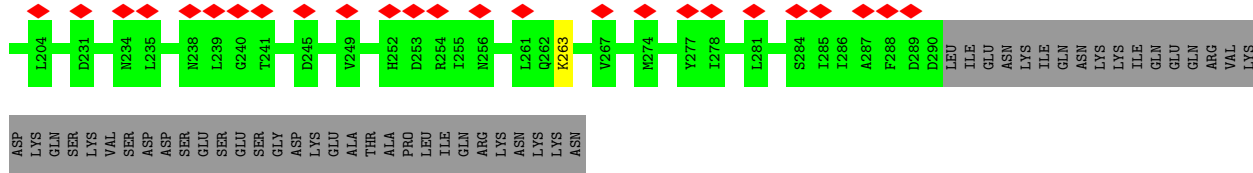


• Molecule 25: 26S proteasome regulatory subunit RPN7

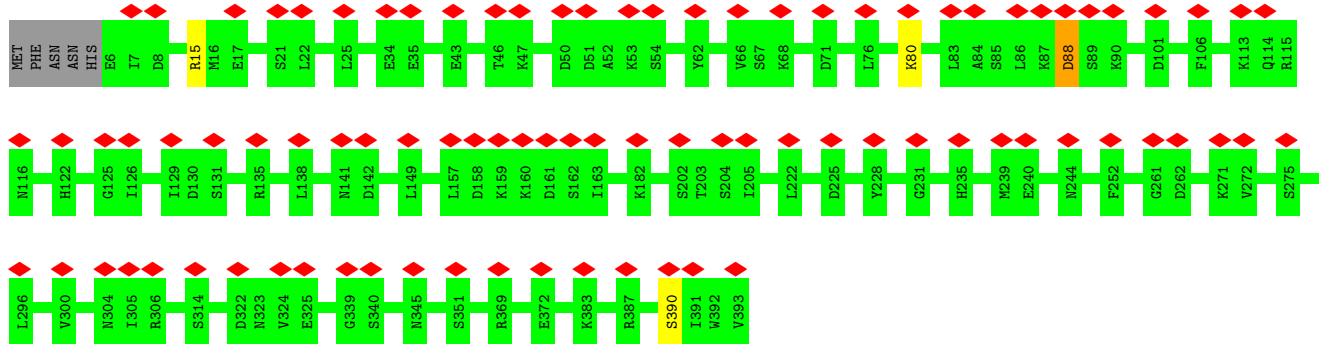


• Molecule 26: 26S proteasome regulatory subunit RPN8





• Molecule 27: 26S proteasome regulatory subunit RPN9



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	25.065	Depositor
Minimum map value	-11.917	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.815	Depositor
Recommended contour level	5.4	Depositor
Map size (Å)	588.0, 588.0, 588.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.1, 2.1, 2.1	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.62	2/1945 (0.1%)	1.00	9/2634 (0.3%)
1	a	0.62	2/1945 (0.1%)	1.00	8/2634 (0.3%)
2	B	0.57	0/1944	0.91	3/2632 (0.1%)
2	b	0.57	0/1944	0.91	3/2632 (0.1%)
3	C	0.52	0/1934	0.91	8/2618 (0.3%)
3	c	0.52	0/1934	0.91	8/2618 (0.3%)
4	D	0.61	3/1879 (0.2%)	0.88	5/2546 (0.2%)
4	d	0.56	0/1879	1.14	16/2546 (0.6%)
5	E	0.68	2/1908 (0.1%)	0.99	9/2571 (0.4%)
5	e	0.68	2/1908 (0.1%)	0.99	9/2571 (0.4%)
6	F	0.69	4/1800 (0.2%)	0.93	5/2433 (0.2%)
6	f	0.69	4/1800 (0.2%)	0.93	5/2433 (0.2%)
7	G	0.59	1/1925 (0.1%)	0.95	5/2599 (0.2%)
7	g	0.59	1/1925 (0.1%)	0.95	5/2599 (0.2%)
8	1	0.81	3/1541 (0.2%)	1.10	13/2087 (0.6%)
8	h	0.81	4/1541 (0.3%)	1.10	13/2087 (0.6%)
9	2	0.93	9/1750 (0.5%)	1.21	17/2373 (0.7%)
9	i	0.93	9/1750 (0.5%)	1.21	17/2373 (0.7%)
10	3	0.90	8/1611 (0.5%)	1.05	10/2174 (0.5%)
10	j	0.90	8/1611 (0.5%)	1.05	10/2174 (0.5%)
11	4	0.92	7/1589 (0.4%)	1.22	19/2142 (0.9%)
11	k	0.92	7/1589 (0.4%)	1.22	19/2142 (0.9%)
12	5	0.79	4/1681 (0.2%)	1.21	19/2274 (0.8%)
12	l	0.79	4/1681 (0.2%)	1.21	19/2274 (0.8%)
13	6	0.91	6/1795 (0.3%)	1.17	14/2420 (0.6%)
13	m	0.91	6/1795 (0.3%)	1.17	14/2420 (0.6%)
14	7	0.48	0/1821	0.92	5/2470 (0.2%)
14	n	0.50	0/1821	0.93	7/2470 (0.3%)
15	W	0.48	0/1557	0.82	3/2111 (0.1%)
16	V	0.69	4/2309 (0.2%)	1.21	18/3115 (0.6%)
17	T	0.45	0/2235	0.87	7/3017 (0.2%)
18	X	0.52	1/1058 (0.1%)	0.93	5/1432 (0.3%)
19	Y	0.45	0/741	0.96	5/1000 (0.5%)
20	Z	0.66	2/7122 (0.0%)	1.27	77/9645 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
21	N	0.45	0/6521	0.80	11/8824 (0.1%)
22	S	0.46	0/3966	0.81	4/5355 (0.1%)
23	P	0.45	0/3663	0.82	7/4940 (0.1%)
24	Q	0.42	0/3556	0.82	7/4787 (0.1%)
25	R	0.44	0/3313	0.84	9/4469 (0.2%)
26	U	0.54	1/2340 (0.0%)	0.83	3/3168 (0.1%)
27	O	0.47	2/3247 (0.1%)	0.88	6/4380 (0.1%)
All	All	0.64	106/91874 (0.1%)	1.00	456/124189 (0.4%)

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
4	d	0	8
5	E	0	1
5	e	0	1
6	F	0	3
6	f	0	3
7	G	0	2
7	g	0	2
8	l	0	1
8	h	0	1
9	2	0	3
9	i	0	3
12	5	0	1
12	l	0	1
15	W	0	2
16	V	0	4
17	T	0	6
18	X	0	3
19	Y	0	3
20	Z	0	41
21	N	0	2
22	S	0	2
23	P	0	3
24	Q	0	4
25	R	0	1
All	All	0	101

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	211	LYS	CB-CG	-12.88	1.17	1.52
5	E	211	LYS	CB-CG	-12.87	1.17	1.52
4	D	11	PHE	CD2-CE2	-10.90	1.17	1.39
8	1	69	GLN	CD-NE2	-10.26	1.07	1.32
8	h	69	GLN	CD-NE2	-10.25	1.07	1.32

The worst 5 of 456 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	259	LYS	CG-CD-CE	21.63	176.79	111.90
20	Z	33	GLU	OE1-CD-OE2	-17.74	102.02	123.30
20	Z	366	LYS	CG-CD-CE	16.98	162.82	111.90
27	O	88	ASP	CB-CG-OD1	15.90	132.62	118.30
1	a	201	LYS	CD-CE-NZ	-15.85	75.25	111.70

There are no chirality outliers.

5 of 101 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	d	100	LEU	Peptide
4	d	151	GLU	Sidechain
4	d	18	PHE	Sidechain
4	d	203	VAL	Peptide
4	d	218	ASP	Sidechain

## 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	A	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
1	a	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
2	B	247/250 (99%)	237 (96%)	9 (4%)	1 (0%)	34	72
2	b	247/250 (99%)	237 (96%)	9 (4%)	1 (0%)	34	72
3	C	242/258 (94%)	229 (95%)	13 (5%)	0	100	100
3	c	242/258 (94%)	229 (95%)	13 (5%)	0	100	100
4	D	234/254 (92%)	218 (93%)	11 (5%)	5 (2%)	7	36
4	d	234/254 (92%)	215 (92%)	14 (6%)	5 (2%)	7	36
5	E	242/260 (93%)	228 (94%)	13 (5%)	1 (0%)	34	72
5	e	242/260 (93%)	228 (94%)	13 (5%)	1 (0%)	34	72
6	F	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	34	72
6	f	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	34	72
7	G	240/288 (83%)	234 (98%)	5 (2%)	1 (0%)	34	72
7	g	240/288 (83%)	234 (98%)	5 (2%)	1 (0%)	34	72
8	1	194/215 (90%)	182 (94%)	10 (5%)	2 (1%)	15	54
8	h	194/215 (90%)	182 (94%)	10 (5%)	2 (1%)	15	54
9	2	224/261 (86%)	209 (93%)	11 (5%)	4 (2%)	8	40
9	i	224/261 (86%)	209 (93%)	11 (5%)	4 (2%)	8	40
10	3	202/205 (98%)	186 (92%)	14 (7%)	2 (1%)	15	54
10	j	202/205 (98%)	186 (92%)	14 (7%)	2 (1%)	15	54
11	4	193/198 (98%)	182 (94%)	11 (6%)	0	100	100
11	k	193/198 (98%)	182 (94%)	11 (6%)	0	100	100
12	5	210/287 (73%)	201 (96%)	8 (4%)	1 (0%)	29	69
12	l	210/287 (73%)	201 (96%)	8 (4%)	1 (0%)	29	69
13	6	220/241 (91%)	207 (94%)	11 (5%)	2 (1%)	17	56
13	m	220/241 (91%)	207 (94%)	11 (5%)	2 (1%)	17	56
14	7	227/266 (85%)	199 (88%)	27 (12%)	1 (0%)	34	72
14	n	227/266 (85%)	211 (93%)	16 (7%)	0	100	100
15	W	195/268 (73%)	181 (93%)	13 (7%)	1 (0%)	29	69
16	V	287/306 (94%)	258 (90%)	26 (9%)	3 (1%)	15	54
17	T	264/274 (96%)	240 (91%)	23 (9%)	1 (0%)	34	72
18	X	125/156 (80%)	112 (90%)	12 (10%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	87/89 (98%)	76 (87%)	8 (9%)	3 (3%)	3	26
20	Z	902/993 (91%)	817 (91%)	70 (8%)	15 (2%)	9	42
21	N	828/945 (88%)	789 (95%)	36 (4%)	3 (0%)	34	72
22	S	473/523 (90%)	438 (93%)	26 (6%)	9 (2%)	8	38
23	P	438/445 (98%)	417 (95%)	19 (4%)	2 (0%)	29	69
24	Q	432/434 (100%)	400 (93%)	26 (6%)	6 (1%)	11	46
25	R	403/429 (94%)	383 (95%)	17 (4%)	3 (1%)	22	62
26	U	288/338 (85%)	274 (95%)	13 (4%)	1 (0%)	41	76
27	O	386/393 (98%)	376 (97%)	10 (3%)	0	100	100
All	All	11394/12531 (91%)	10688 (94%)	617 (5%)	89 (1%)	24	60

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	124	SER
4	d	101	GLU
4	d	204	GLN
5	e	128	SER
6	f	205	SER

### 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	203 (98%)	3 (2%)	65	80
1	a	206/210 (98%)	203 (98%)	3 (2%)	65	80
2	B	208/209 (100%)	200 (96%)	8 (4%)	33	57
2	b	208/209 (100%)	200 (96%)	8 (4%)	33	57
3	C	203/216 (94%)	200 (98%)	3 (2%)	65	80
3	c	203/216 (94%)	200 (98%)	3 (2%)	65	80
4	D	209/226 (92%)	205 (98%)	4 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	209/226 (92%)	196 (94%)	13 (6%)	18	43
5	E	200/215 (93%)	196 (98%)	4 (2%)	55	74
5	e	200/215 (93%)	196 (98%)	4 (2%)	55	74
6	F	190/193 (98%)	183 (96%)	7 (4%)	34	58
6	f	190/193 (98%)	183 (96%)	7 (4%)	34	58
7	G	200/239 (84%)	193 (96%)	7 (4%)	36	59
7	g	200/239 (84%)	193 (96%)	7 (4%)	36	59
8	l	162/178 (91%)	155 (96%)	7 (4%)	29	53
8	h	162/178 (91%)	155 (96%)	7 (4%)	29	53
9	2	185/214 (86%)	174 (94%)	11 (6%)	19	45
9	i	185/214 (86%)	174 (94%)	11 (6%)	19	45
10	3	172/173 (99%)	162 (94%)	10 (6%)	20	45
10	j	172/173 (99%)	162 (94%)	10 (6%)	20	45
11	4	173/175 (99%)	164 (95%)	9 (5%)	23	48
11	k	173/175 (99%)	164 (95%)	9 (5%)	23	48
12	5	169/235 (72%)	158 (94%)	11 (6%)	17	42
12	l	169/235 (72%)	158 (94%)	11 (6%)	17	42
13	6	185/201 (92%)	178 (96%)	7 (4%)	33	57
13	m	185/201 (92%)	178 (96%)	7 (4%)	33	57
14	7	195/224 (87%)	192 (98%)	3 (2%)	65	80
14	n	195/224 (87%)	192 (98%)	3 (2%)	65	80
15	W	171/230 (74%)	167 (98%)	4 (2%)	50	70
16	V	253/268 (94%)	249 (98%)	4 (2%)	62	79
17	T	249/256 (97%)	247 (99%)	2 (1%)	81	89
18	X	116/144 (81%)	114 (98%)	2 (2%)	60	78
19	Y	81/81 (100%)	78 (96%)	3 (4%)	34	58
20	Z	773/850 (91%)	736 (95%)	37 (5%)	25	51
21	N	698/797 (88%)	689 (99%)	9 (1%)	69	82
22	S	447/489 (91%)	441 (99%)	6 (1%)	69	82
23	P	412/415 (99%)	404 (98%)	8 (2%)	57	75
24	Q	391/391 (100%)	386 (99%)	5 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	R	356/379 (94%)	348 (98%)	8 (2%)	52	71
26	U	263/308 (85%)	261 (99%)	2 (1%)	81	89
27	O	363/368 (99%)	361 (99%)	2 (1%)	86	92
All	All	9887/10792 (92%)	9598 (97%)	289 (3%)	45	64

5 of 289 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	Z	402	ASP
26	U	176	ARG
20	Z	589	SER
22	S	261	HIS
13	m	83	TYR

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

Mol	Chain	Res	Type
25	R	184	GLN
25	R	287	GLN
26	U	252	HIS
11	4	65	GLN
10	3	72	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



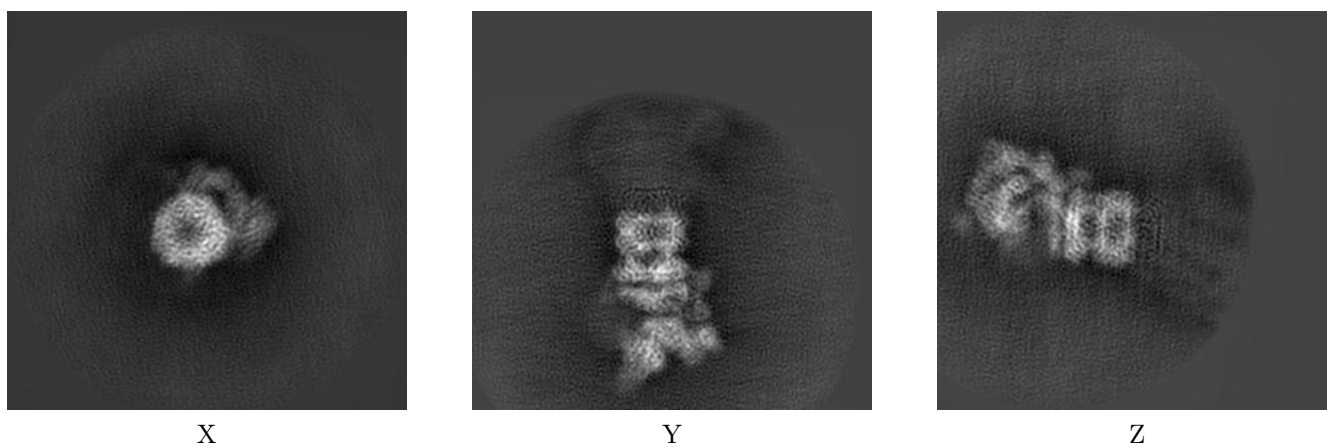
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14082. 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](#)

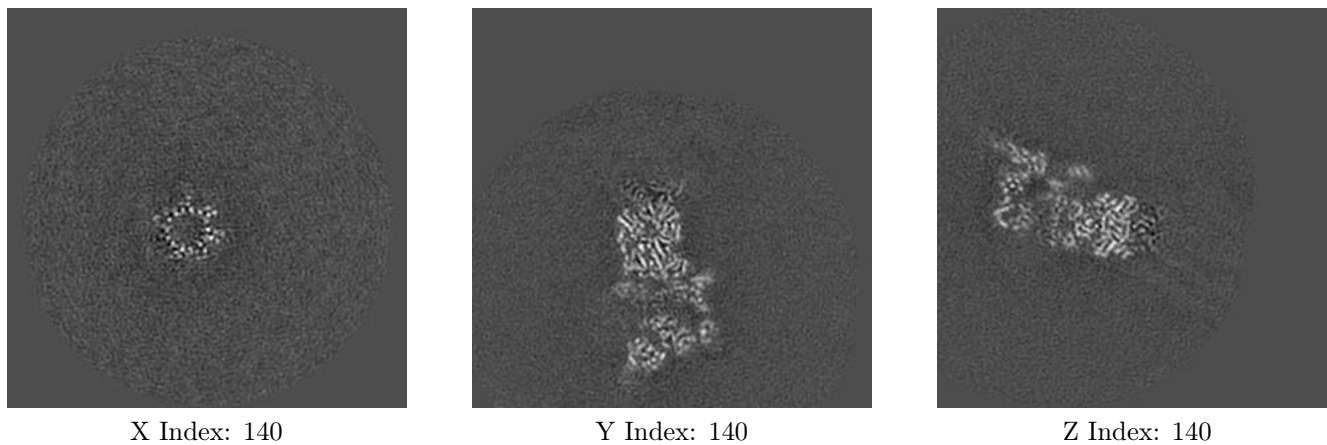
#### 6.1.1 Primary map



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

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

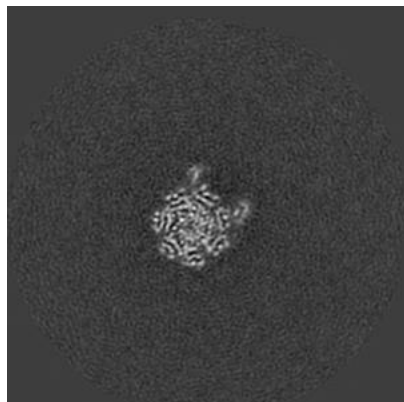
#### 6.2.1 Primary map



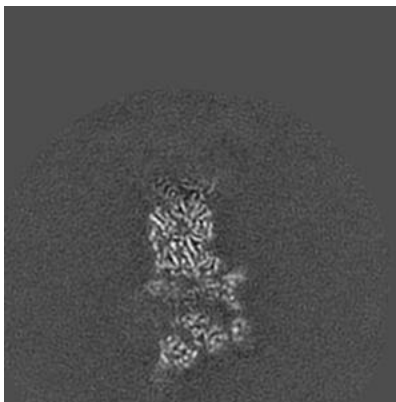
The images above show central slices of the map in three orthogonal directions.

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

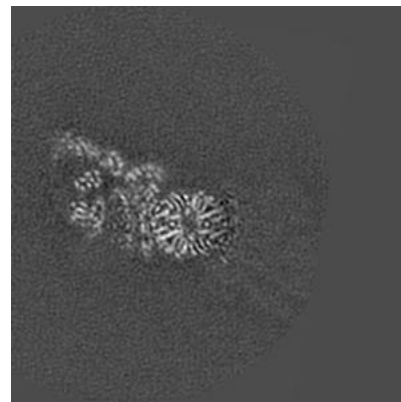
### 6.3.1 Primary map



X Index: 97



Y Index: 140



Z Index: 136

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

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

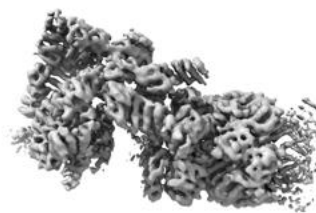
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

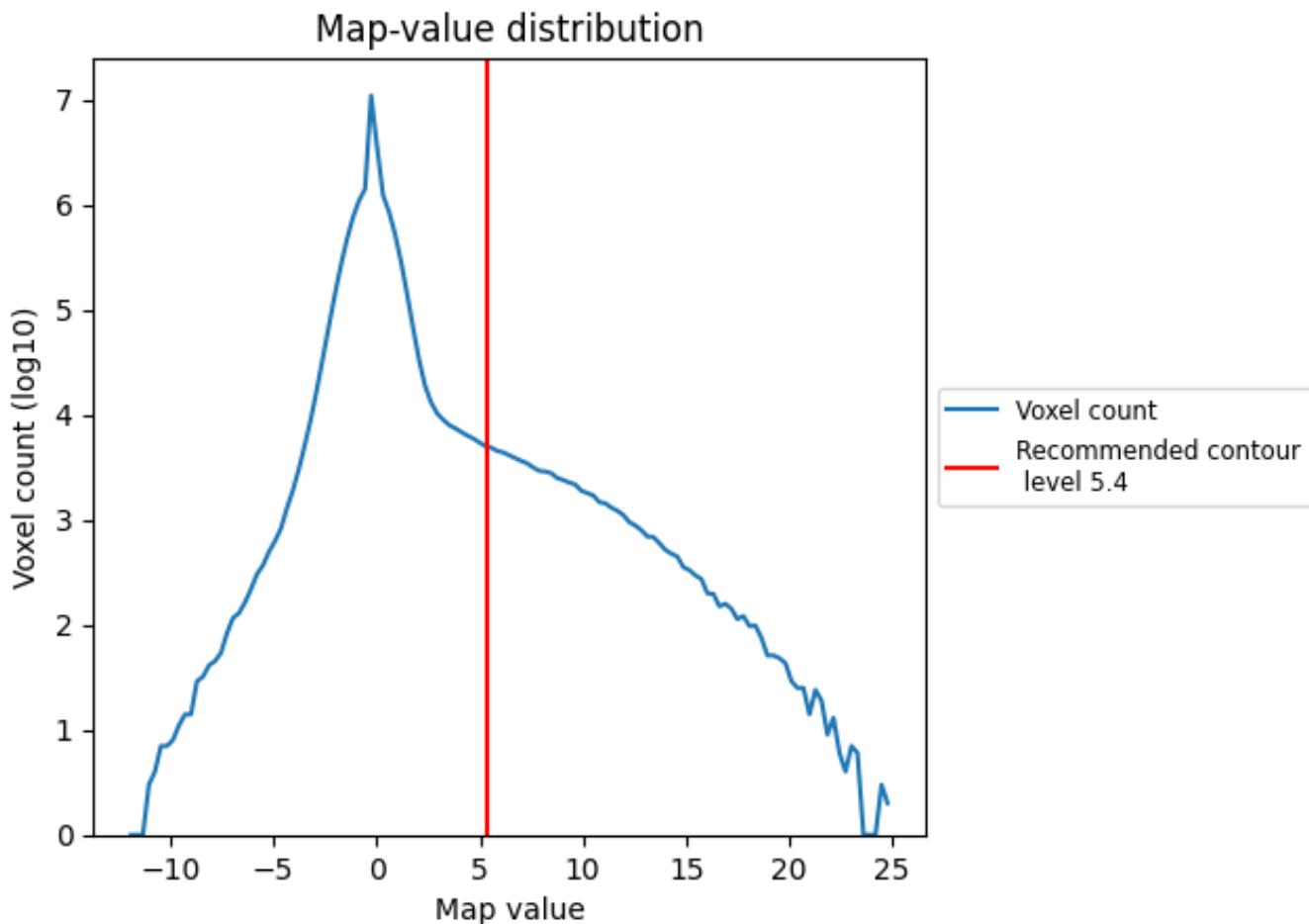
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

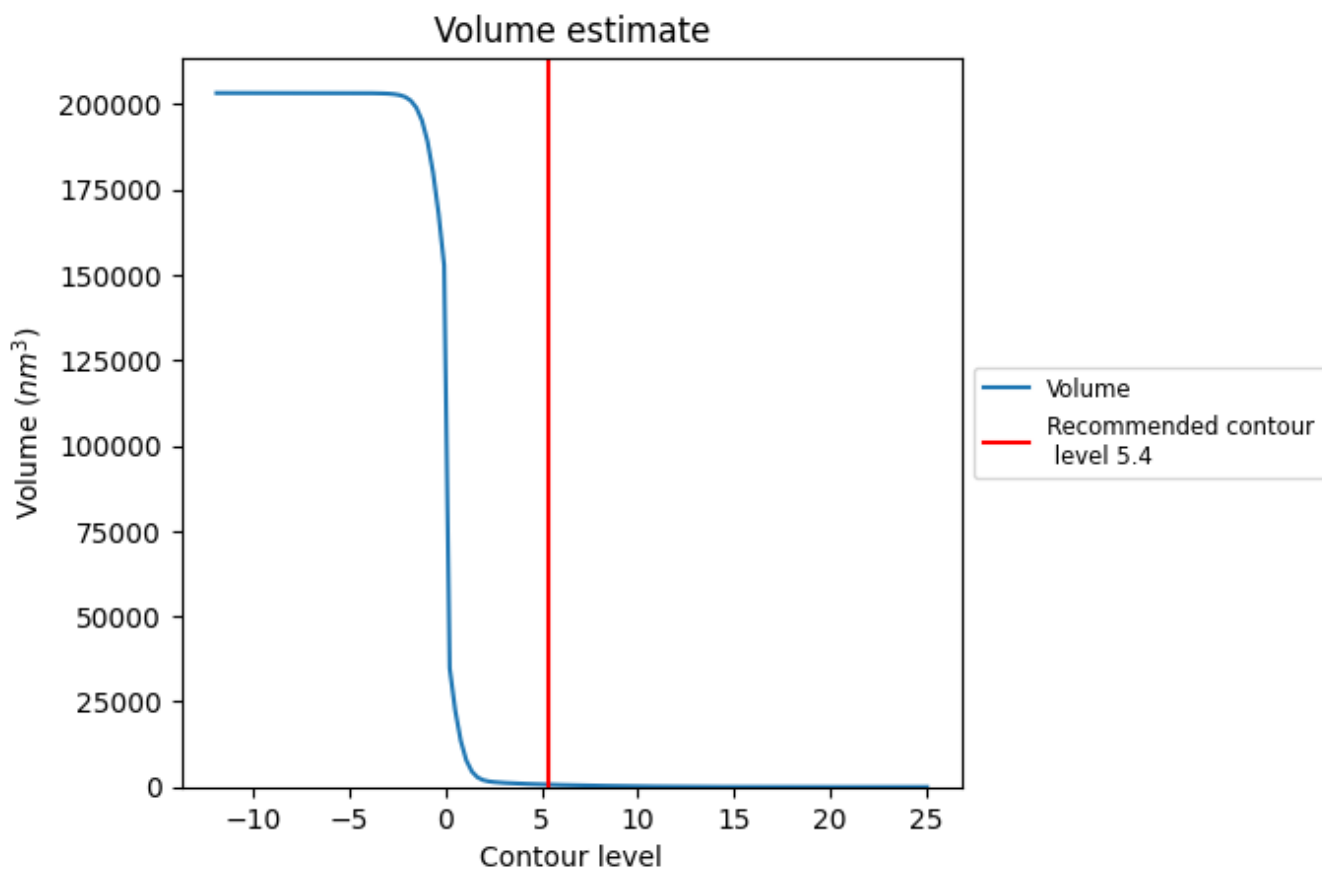
This section contains the results of statistical analysis of the map.

### 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.

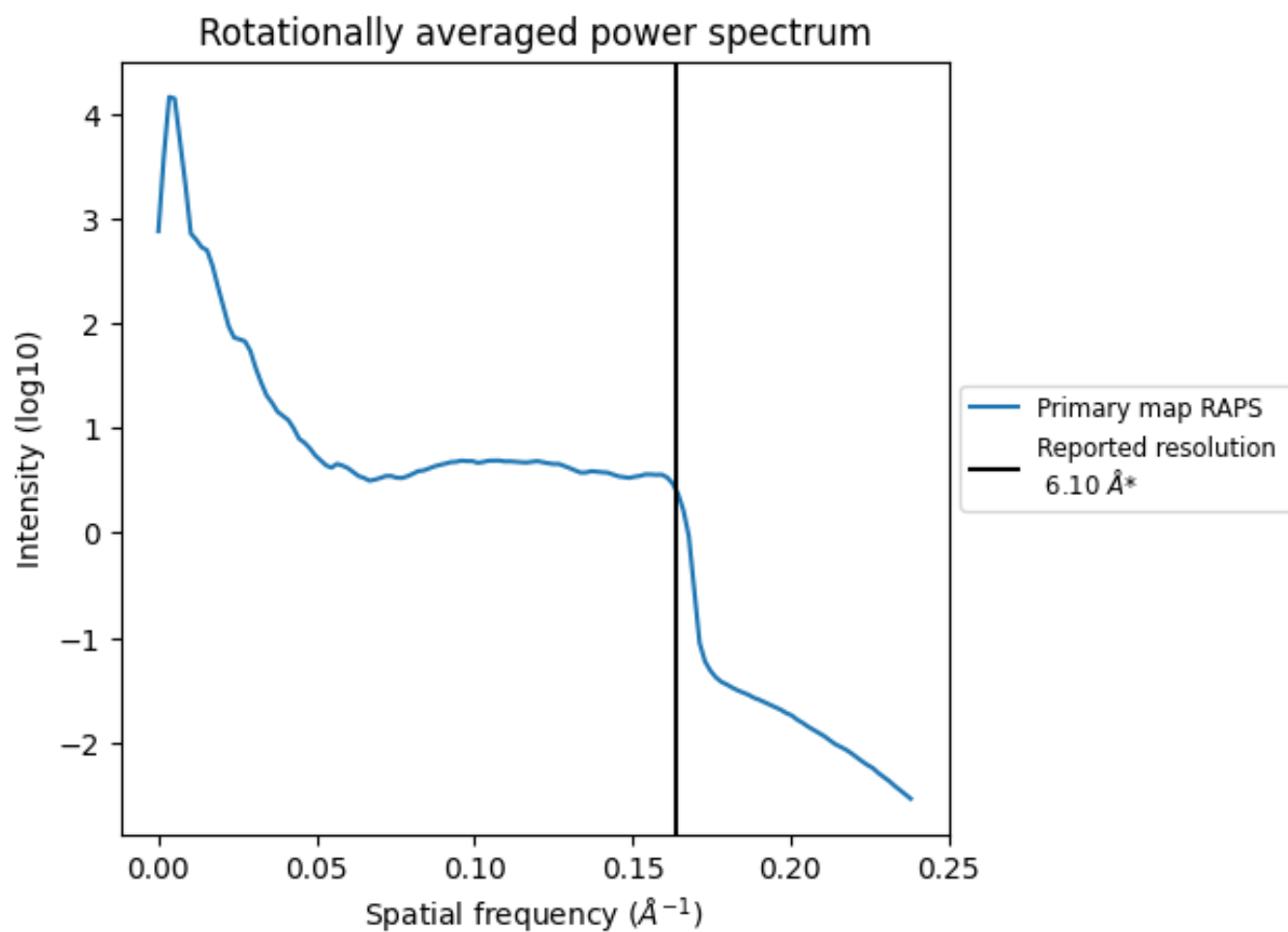
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 678 nm<sup>3</sup>; this corresponds to an approximate mass of 613 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 0.164 Å<sup>-1</sup>

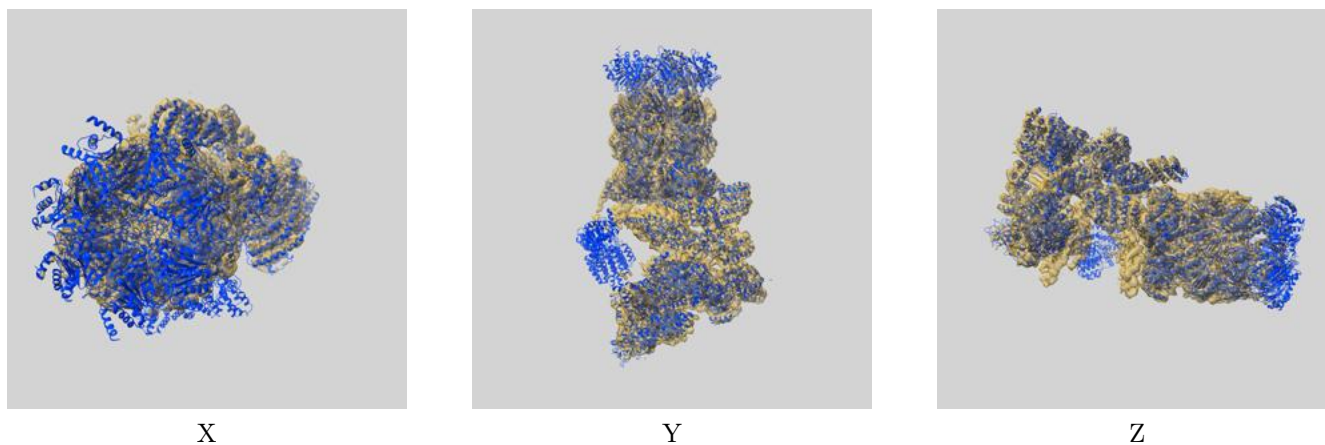
## 8 Fourier-Shell correlation

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-14082 and PDB model 7QO3. Per-residue inclusion information can be found in section 3 on page 10.

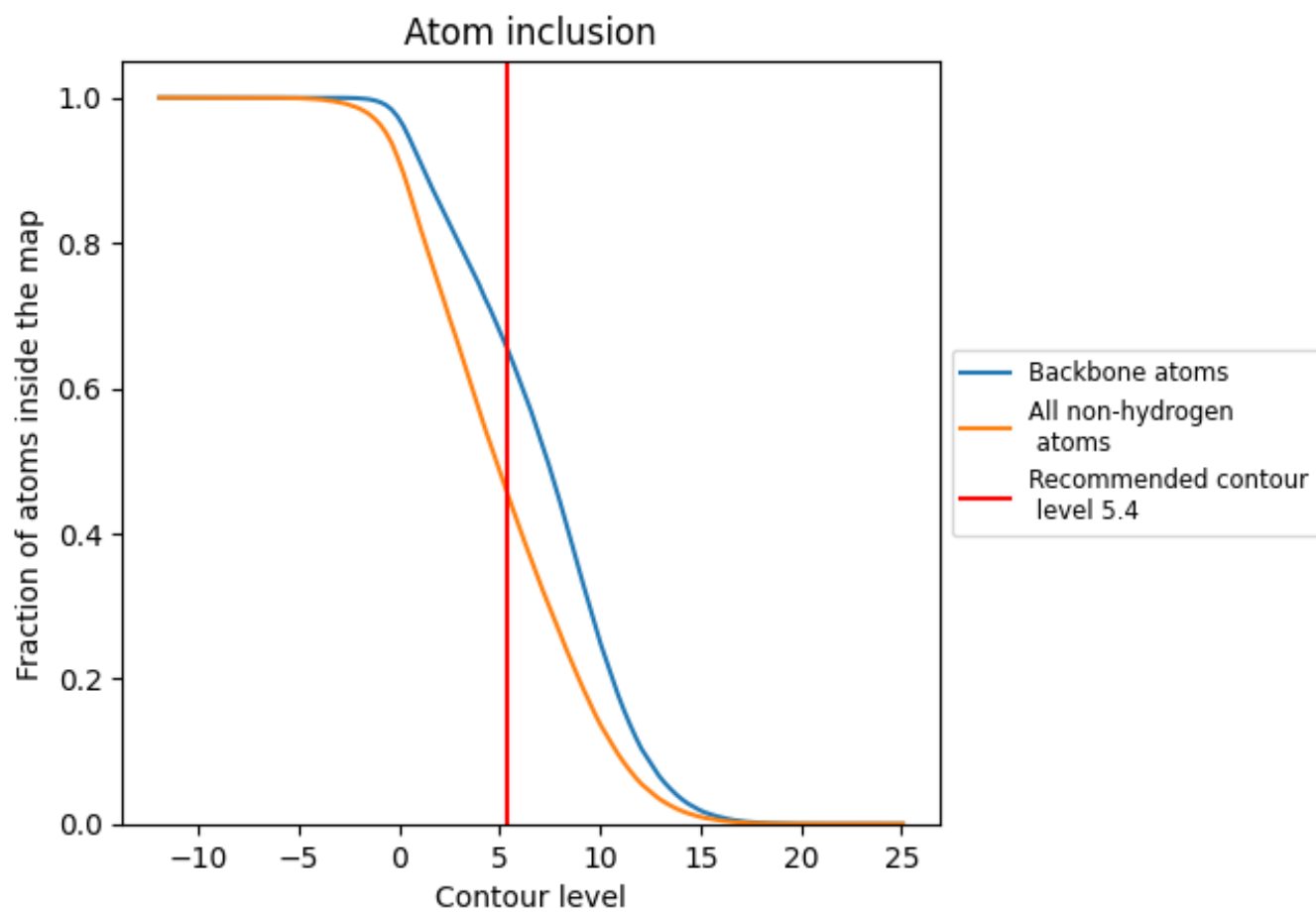
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 5.4 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 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 45% of all non-hydrogen atoms, are inside the map.