Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 12:50 PM JST

PDB ID	:	6J2C
EMDB ID	:	EMD-9769
Title	:	Yeast proteasome in translocation competent state (C3-a)
Authors	:	Cong, Y.
Deposited on	:	2019-01-01
Resolution	:	7.00 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*
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.

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

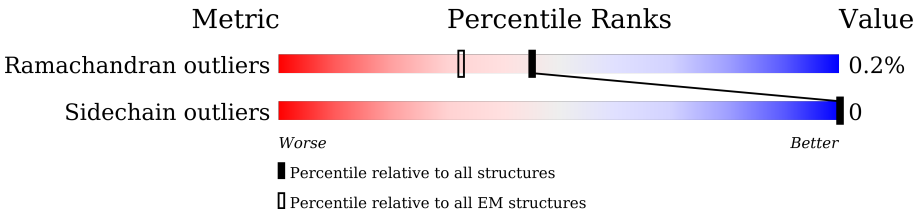
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	1	215	11% 91% 9%
1	b	215	10% 91% 9%
2	2	261	8% 87% 13%
2	i	261	13% 87% 13%
3	3	205	13% 100%
3	h	205	10% 99%
4	4	198	13% 98% .
4	g	198	11% 98% .
5	5	287	9% 74% 26%

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Mol	Chain	Length	Quality of chain
5	f	287	9% 74% 26%
6	6	241	10% 92% 8%
6	e	241	10% 92% 8%
7	7	266	9% 86% 14%
7	a	266	12% 87% 13%
8	A	252	19% 96%
8	c	252	19% 96%
9	B	250	19% 100%
9	j	250	23% 100%
10	C	258	17% 95% 5%
10	d	258	21% 95% 5%
11	D	254	11% 94% 6%
11	n	254	14% 95% 5%
12	E	260	15% 93% 7%
12	m	260	16% 93% 7%
13	F	234	15% 100%
13	l	234	20% 100%
14	G	288	14% 84% 16%
14	k	288	15% 85% 15%
15	H	467	34% 77% 23%
16	I	437	34% 83% 17%
17	J	405	42% 92% 8%
18	K	428	32% 89% 11%
19	L	437	35% 83% 17%
20	M	434	36% 84% 15%

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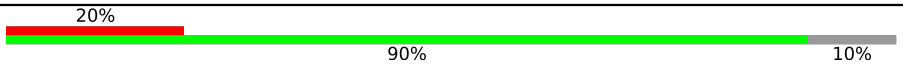
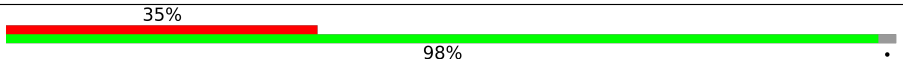
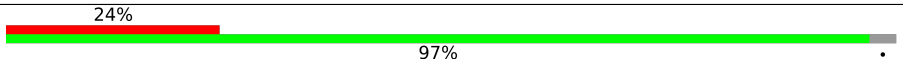
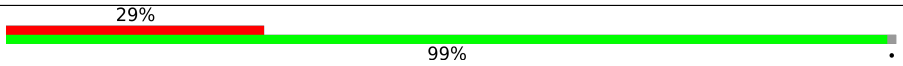
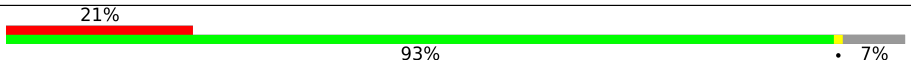
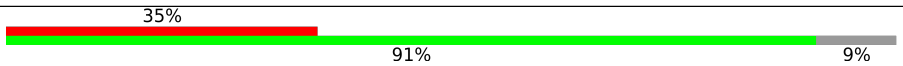
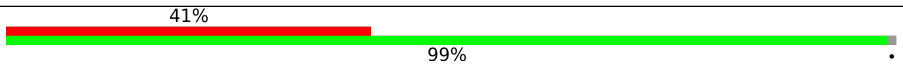
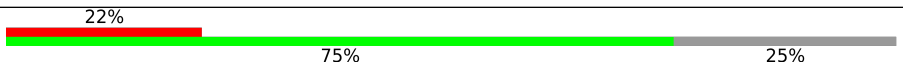
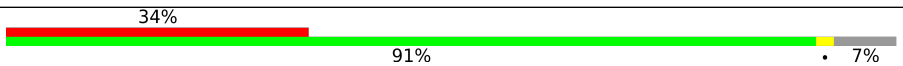
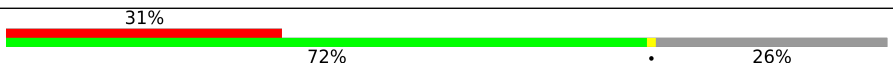
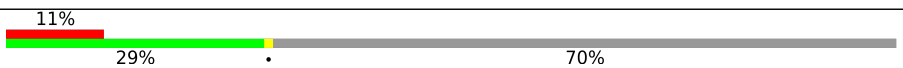
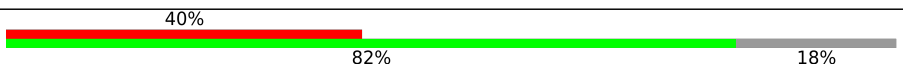
Mol	Chain	Length	Quality of chain
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 106149 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 beta type-1.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
7	a	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
8	c	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
9	j	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
11	n	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
12	m	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		
13	l	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
14	k	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	359	Total	C	N	O	S	0	0
			2792	1755	499	523	15		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	363	Total	C	N	O	S	0	0
			2831	1779	472	565	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

- Molecule 18 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 19 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	361	Total	C	N	O	S	0	0
			2853	1798	507	536	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

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

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

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	255	Total	C	N	O	S	0	0
			2061	1312	352	391	6		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	284	Total	C	N	O	S	0	0
			2236	1405	381	436	14		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

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

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	111	Total	C	N	O	S	0	0
			906	586	148	169	3		

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	27	Total	C	N	O	0	0
			236	143	39	54		

- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

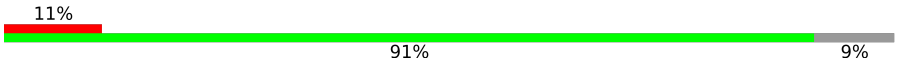
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

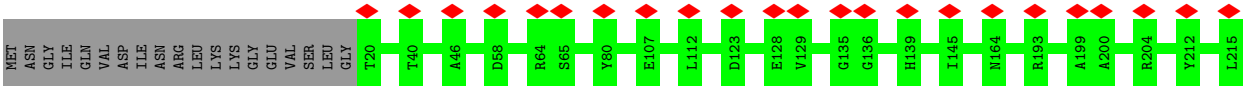
3 Residue-property plots (i)

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 beta type-1

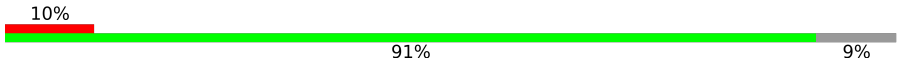
Chain 1:

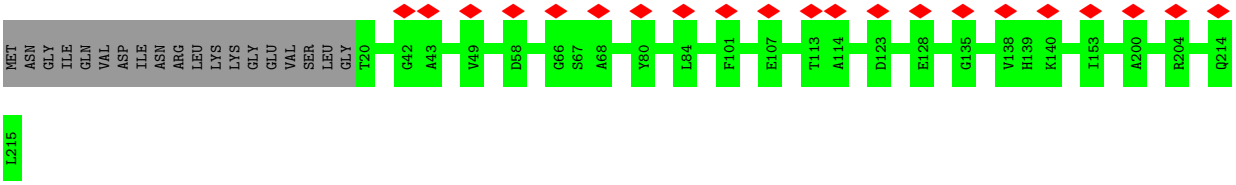




• Molecule 1: Proteasome subunit beta type-1

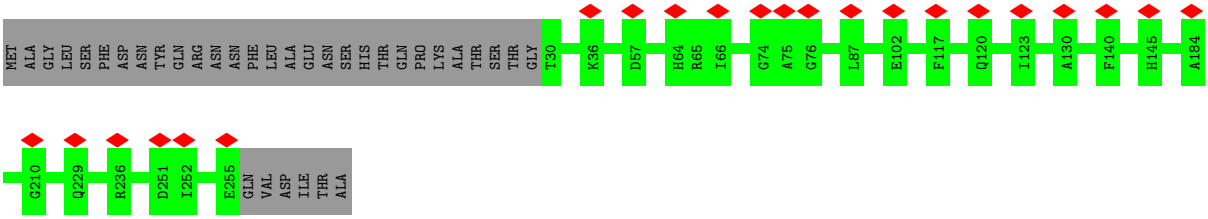
Chain b:





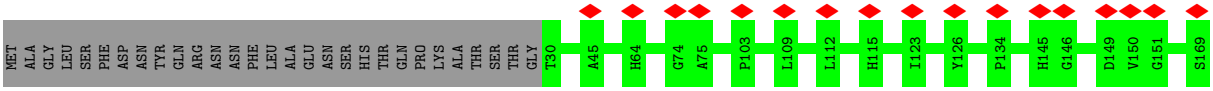
• Molecule 2: Proteasome subunit beta type-2

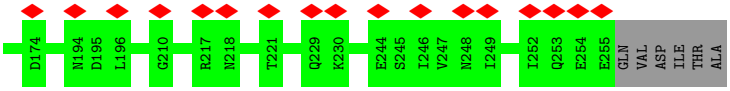
Chain 2:



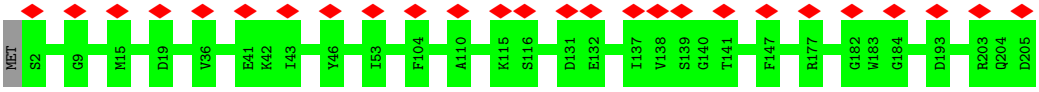
• Molecule 2: Proteasome subunit beta type-2

Chain i:

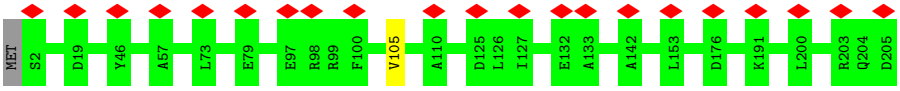




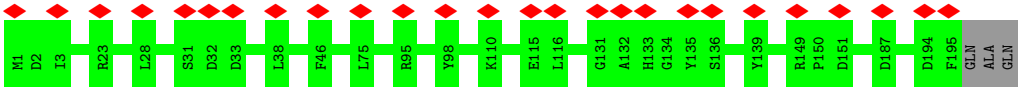
• Molecule 3: Proteasome subunit beta type-3



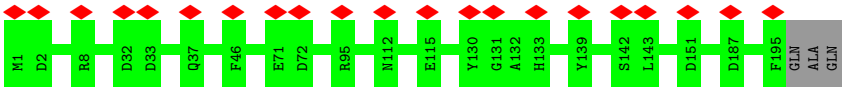
• Molecule 3: Proteasome subunit beta type-3



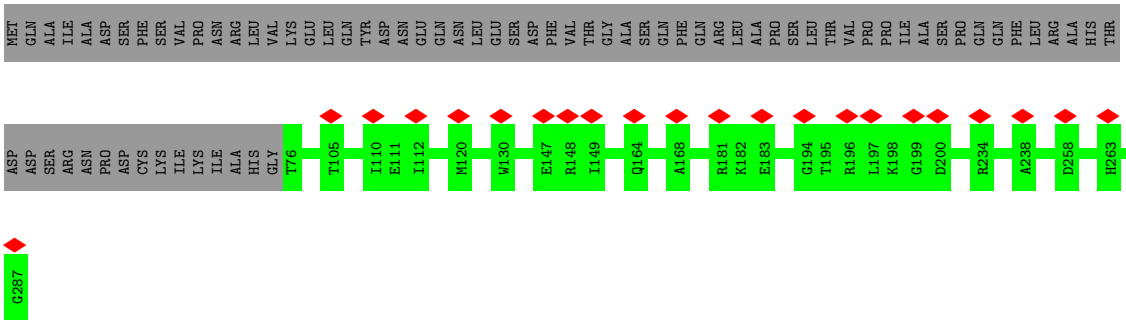
• Molecule 4: Proteasome subunit beta type-4



• Molecule 4: Proteasome subunit beta type-4

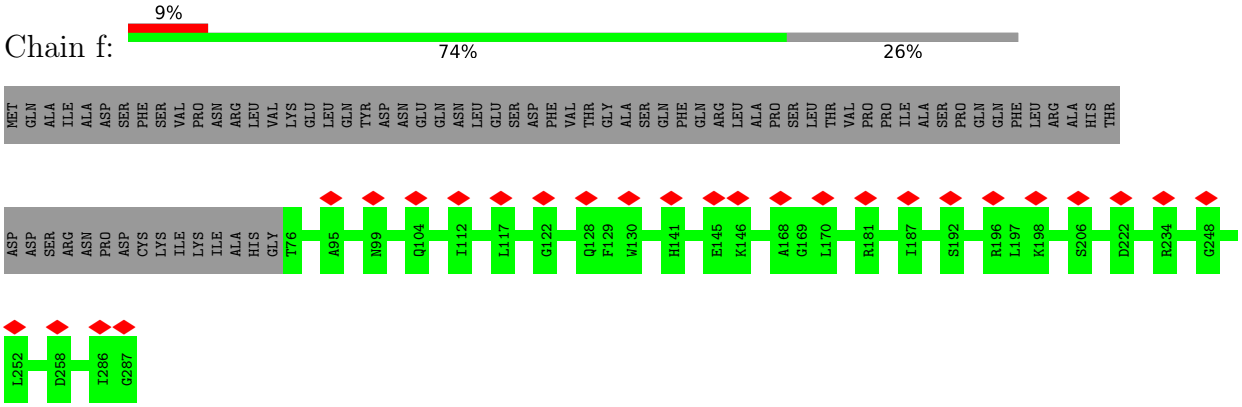


• Molecule 5: Proteasome subunit beta type-5



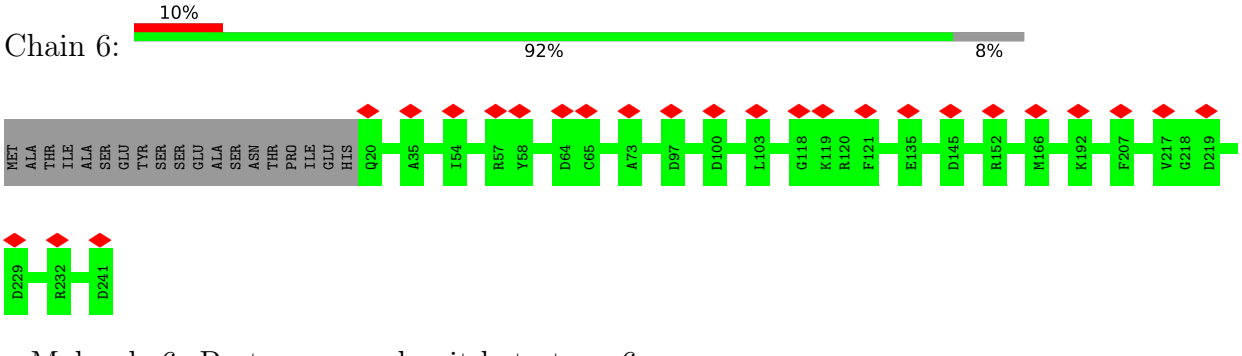
• Molecule 5: Proteasome subunit beta type-5

Chain f:



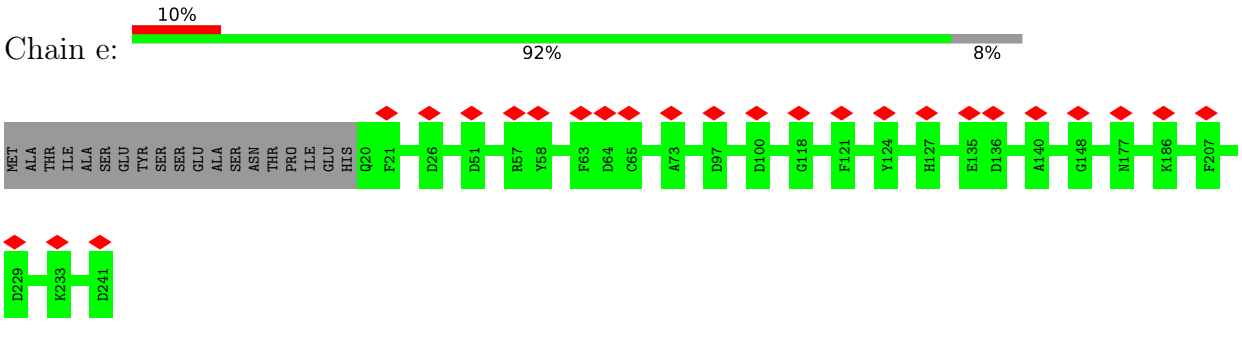
• Molecule 6: Proteasome subunit beta type-6

Chain 6:



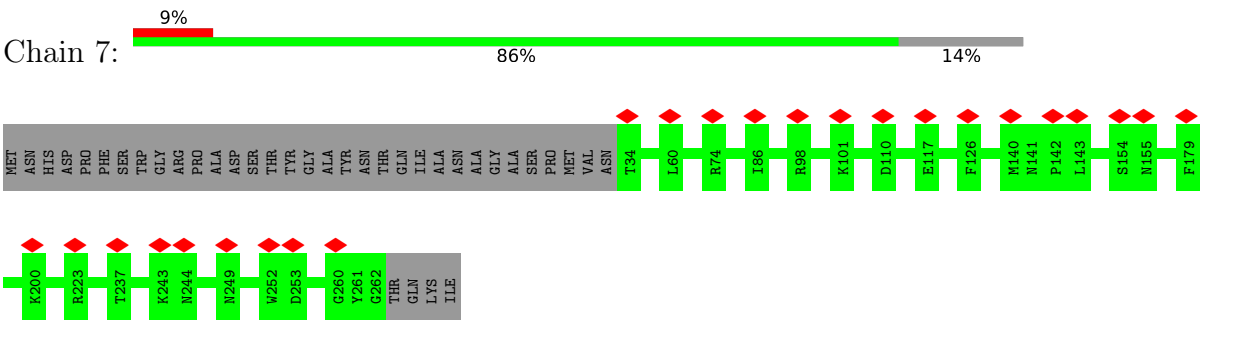
• Molecule 6: Proteasome subunit beta type-6

Chain e:



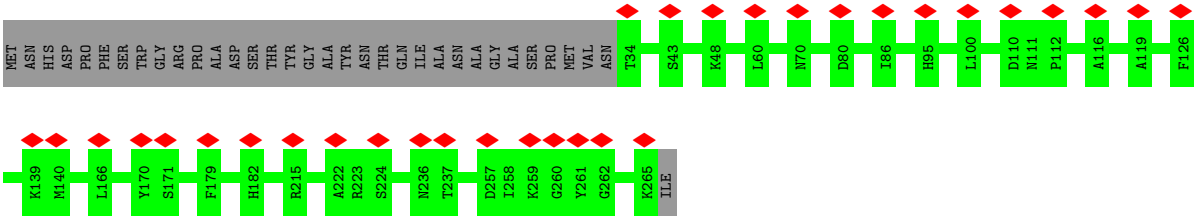
• Molecule 7: Proteasome subunit beta type-7

Chain 7:

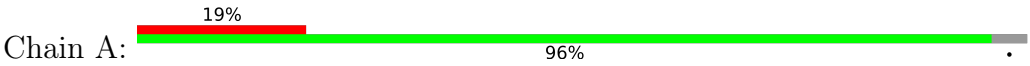


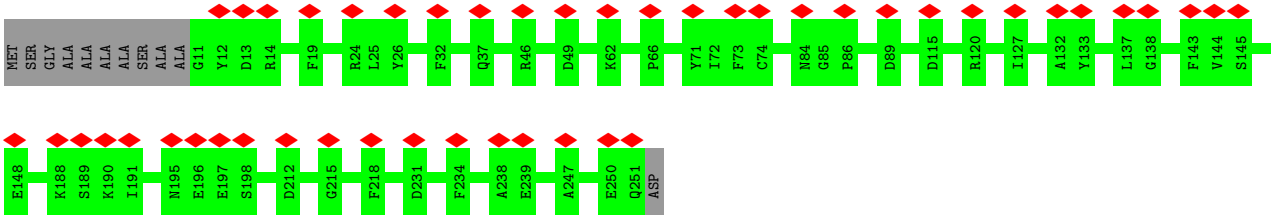
• Molecule 7: Proteasome subunit beta type-7

Chain a:

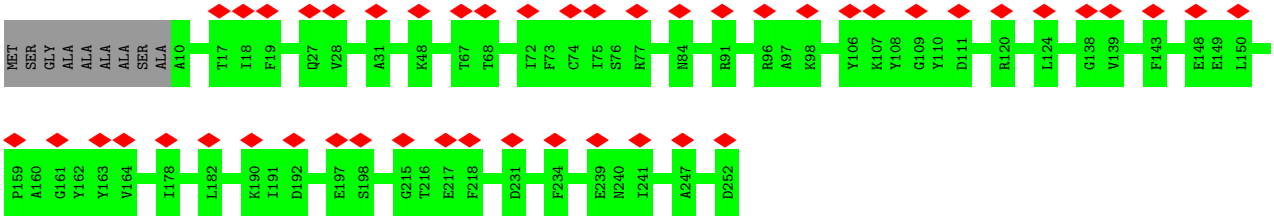


• Molecule 8: Proteasome subunit alpha type-1

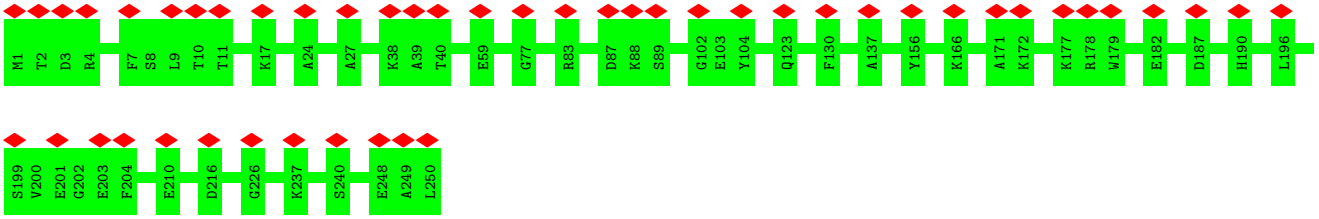




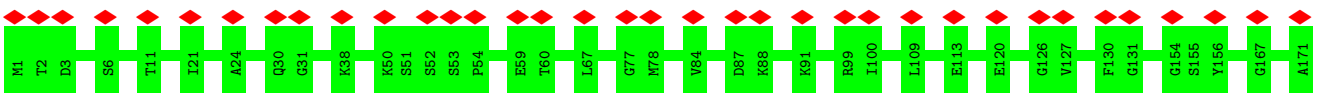
• Molecule 8: Proteasome subunit alpha type-1

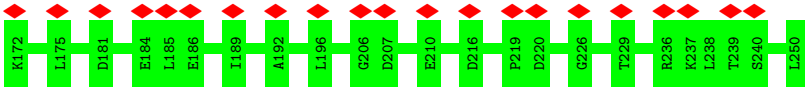


• Molecule 9: Proteasome subunit alpha type-2

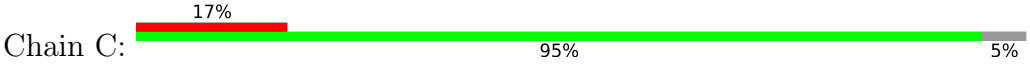


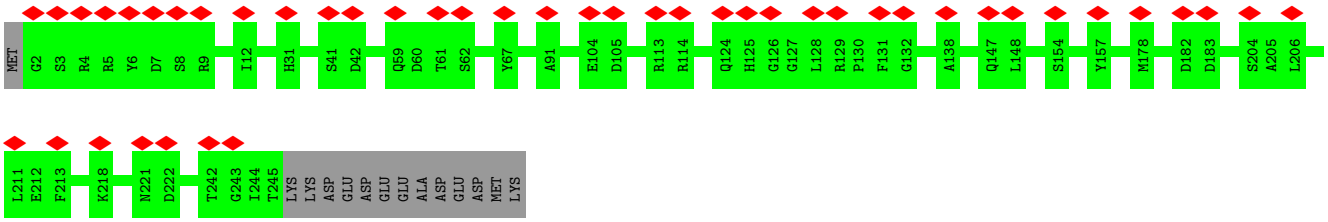
• Molecule 9: Proteasome subunit alpha type-2



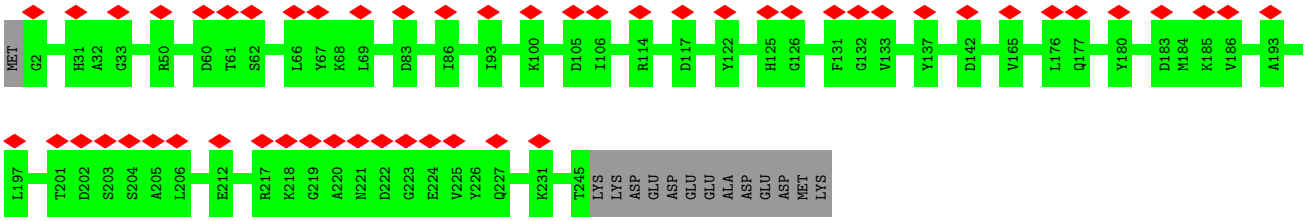


• Molecule 10: Proteasome subunit alpha type-3

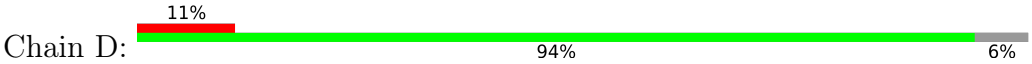


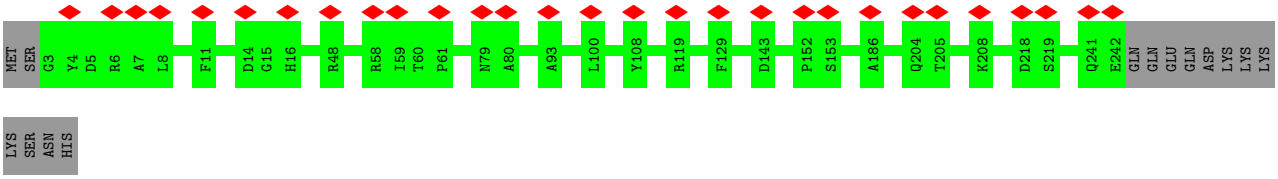


• Molecule 10: Proteasome subunit alpha type-3

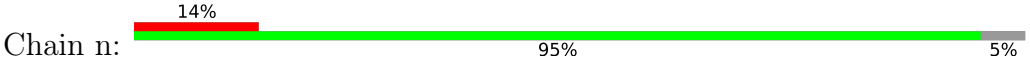


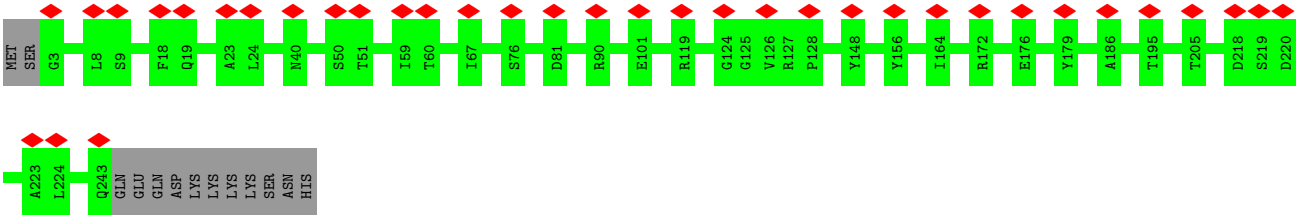
• Molecule 11: Proteasome subunit alpha type-4



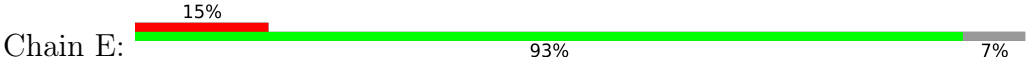


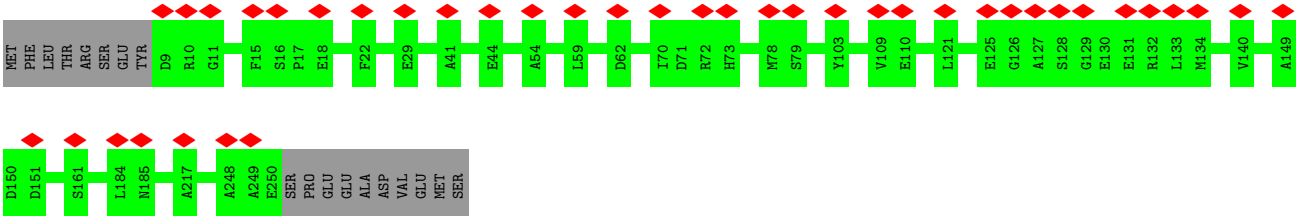
• Molecule 11: Proteasome subunit alpha type-4



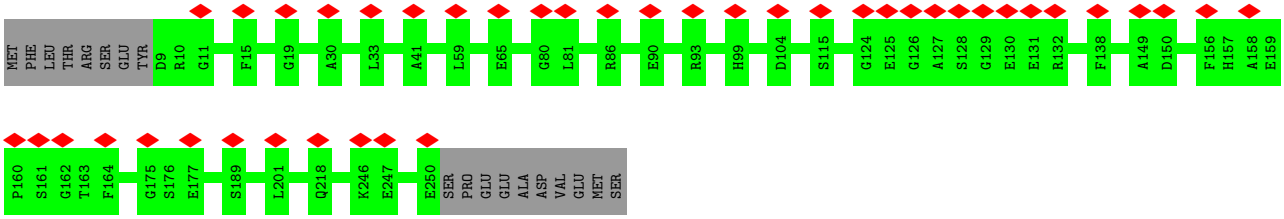


• Molecule 12: Proteasome subunit alpha type-5

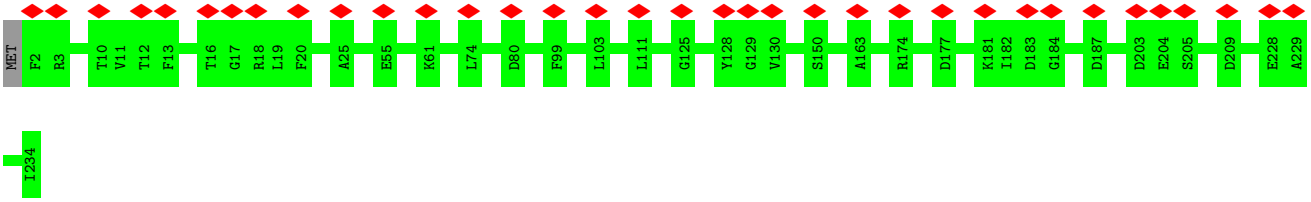




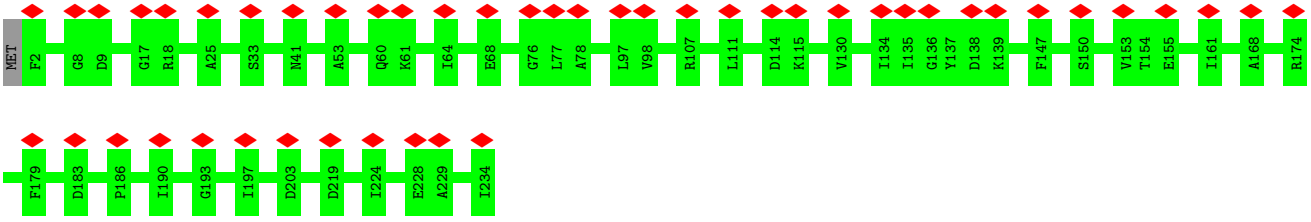
• Molecule 12: Proteasome subunit alpha type-5



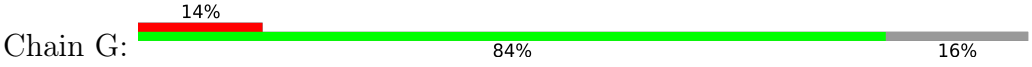
• Molecule 13: Proteasome subunit alpha type-6

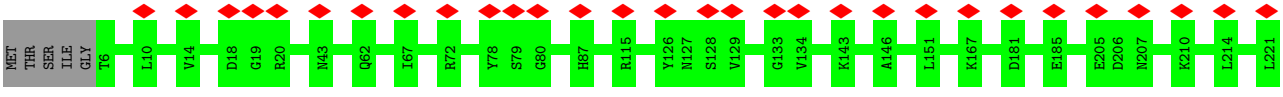


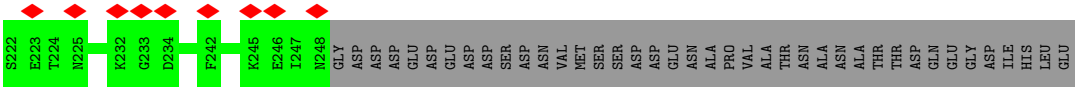
• Molecule 13: Proteasome subunit alpha type-6



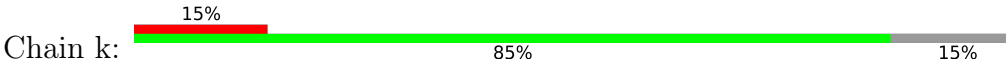
• Molecule 14: Probable proteasome subunit alpha type-7

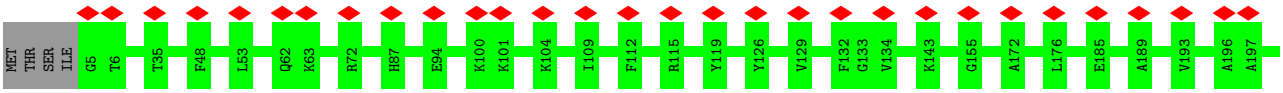


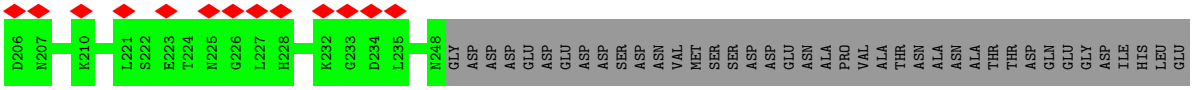




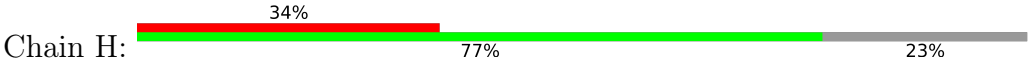
• Molecule 14: Probable proteasome subunit alpha type-7

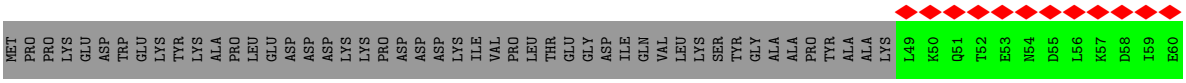


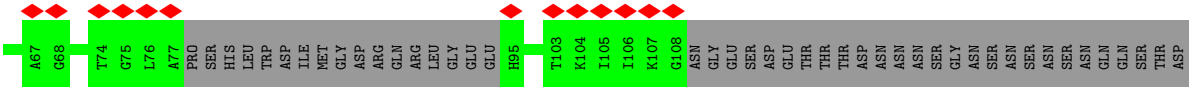


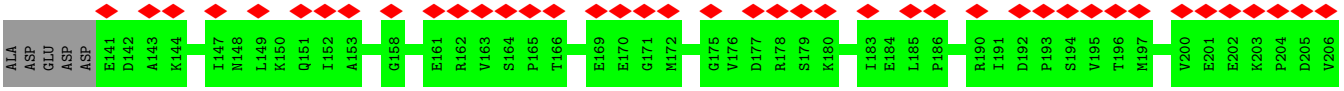


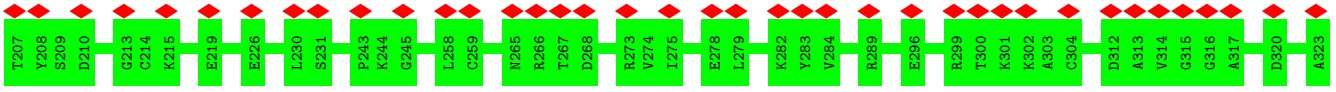
• Molecule 15: 26S protease regulatory subunit 7 homolog

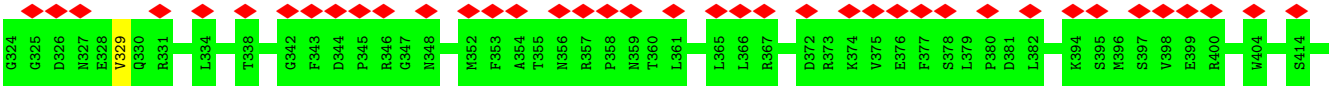


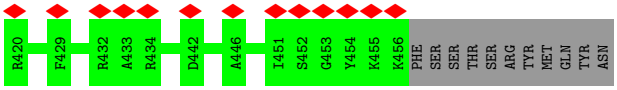




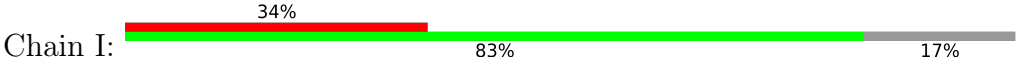


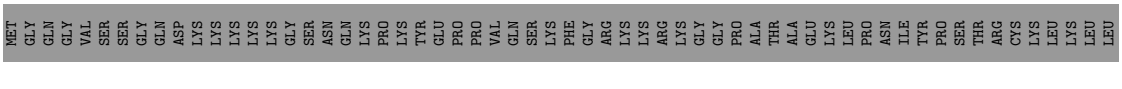


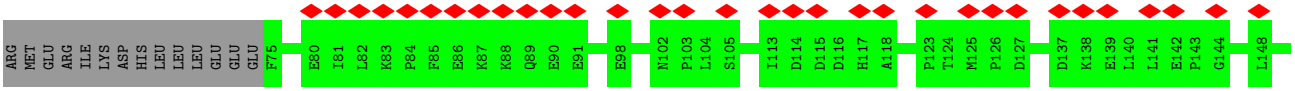


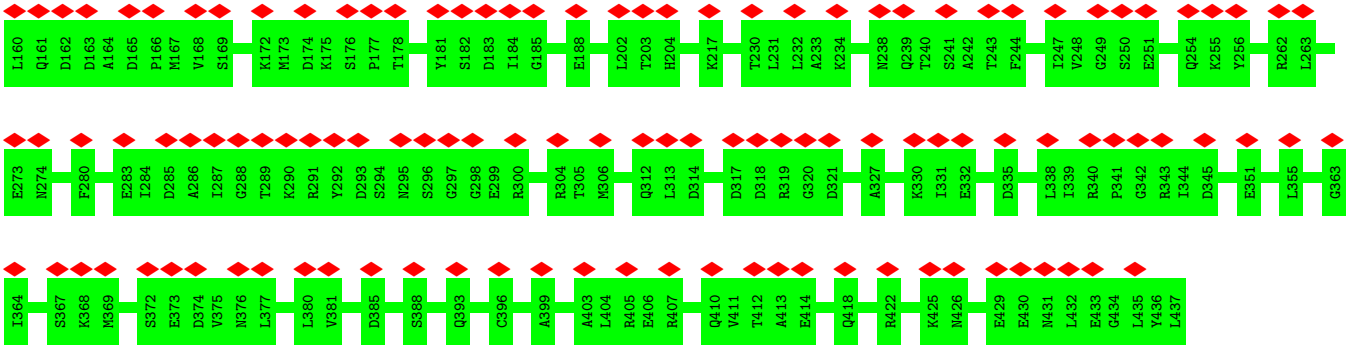


• Molecule 16: 26S protease regulatory subunit 4 homolog



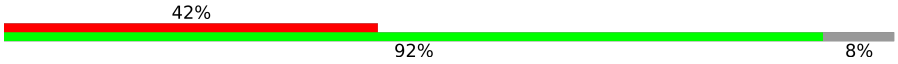


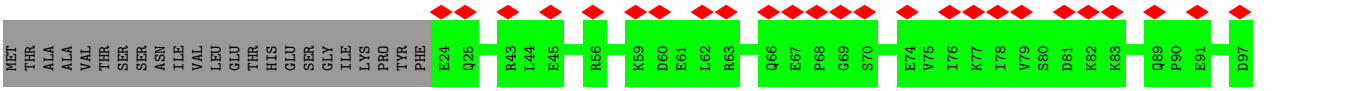


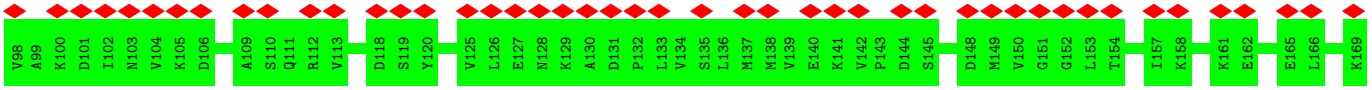


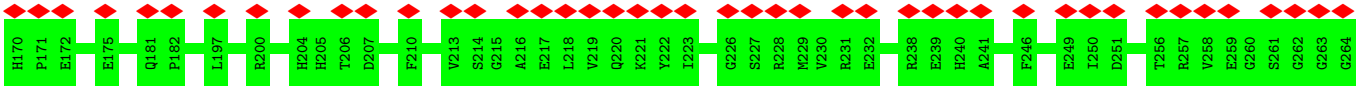
• Molecule 17: 26S protease regulatory subunit 8 homolog

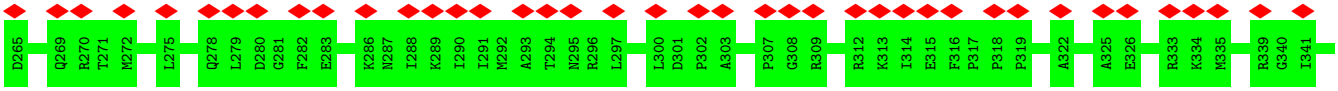
Chain J:

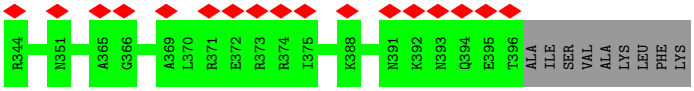






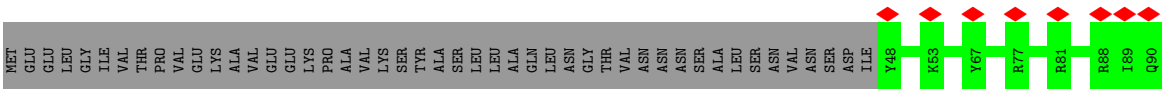


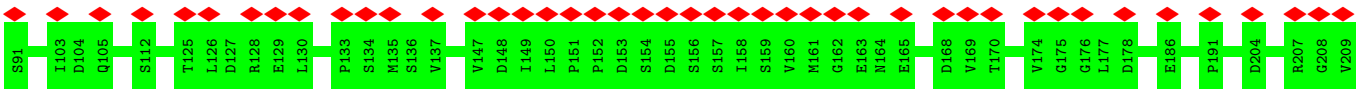


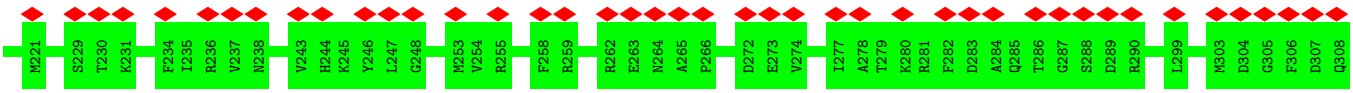


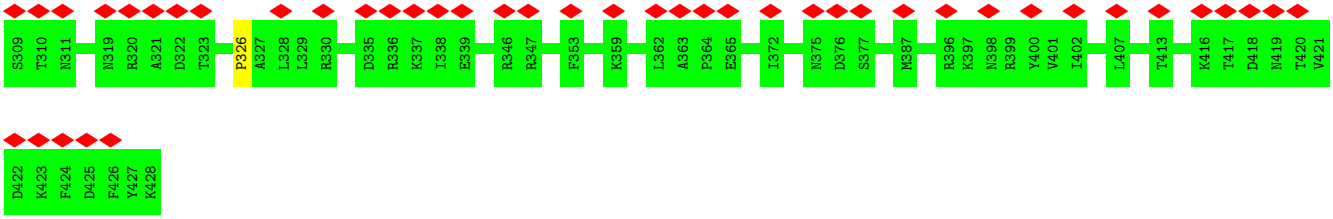
• Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K:

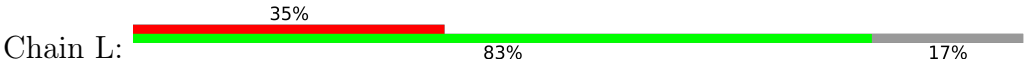


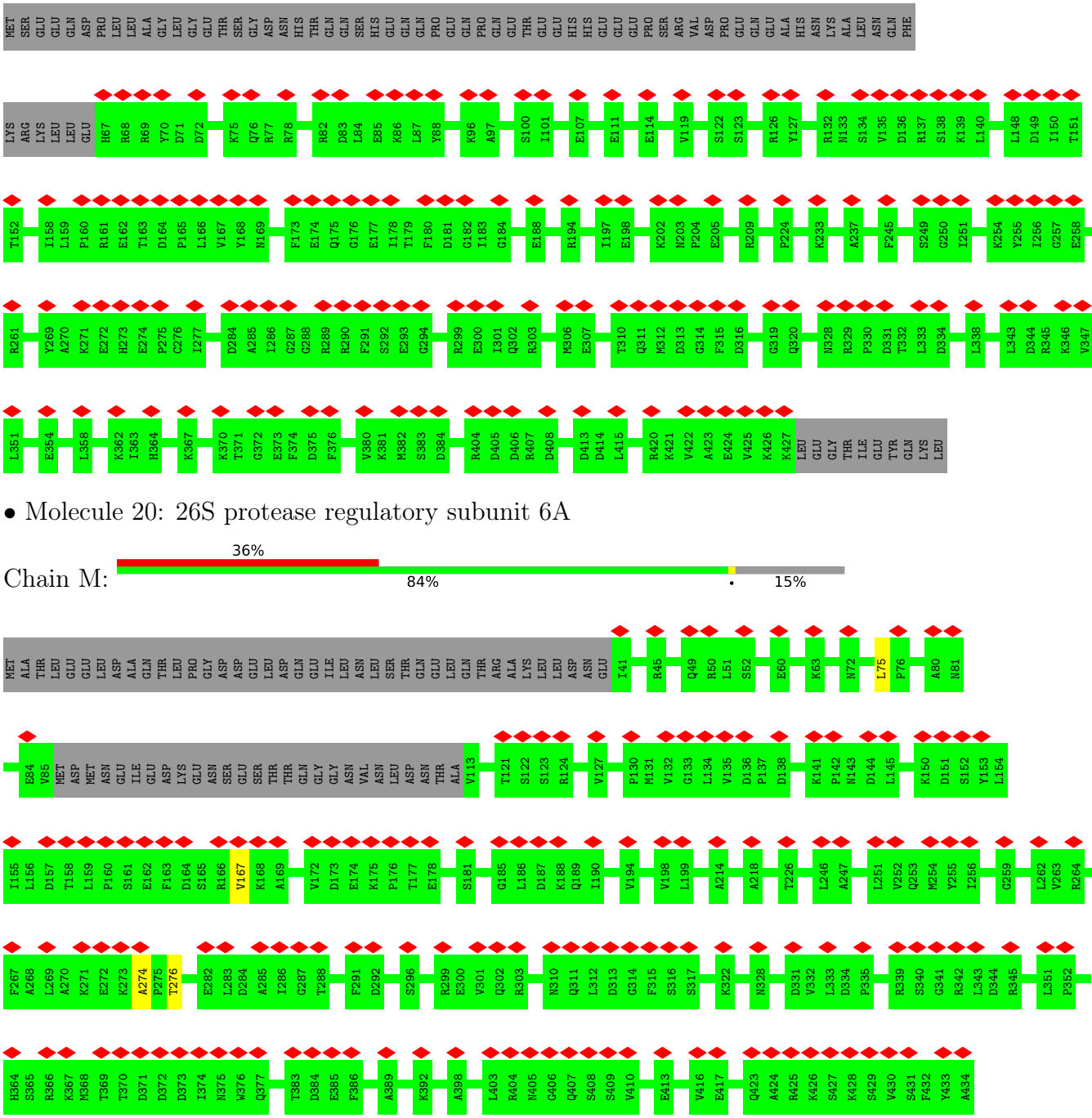






• Molecule 19: 26S protease subunit RPT4

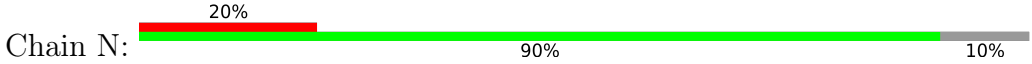


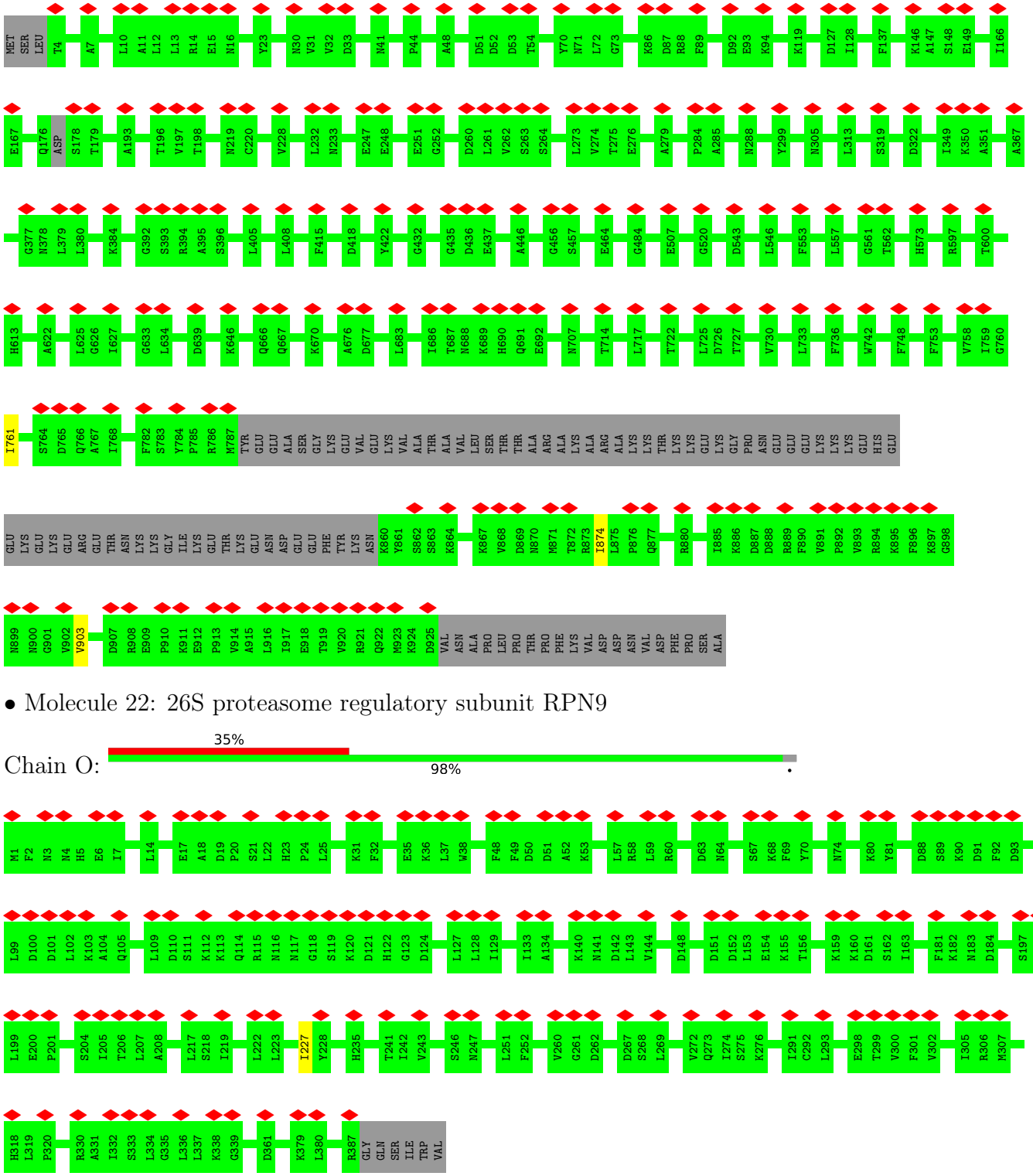


• Molecule 20: 26S protease regulatory subunit 6A

• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain N:



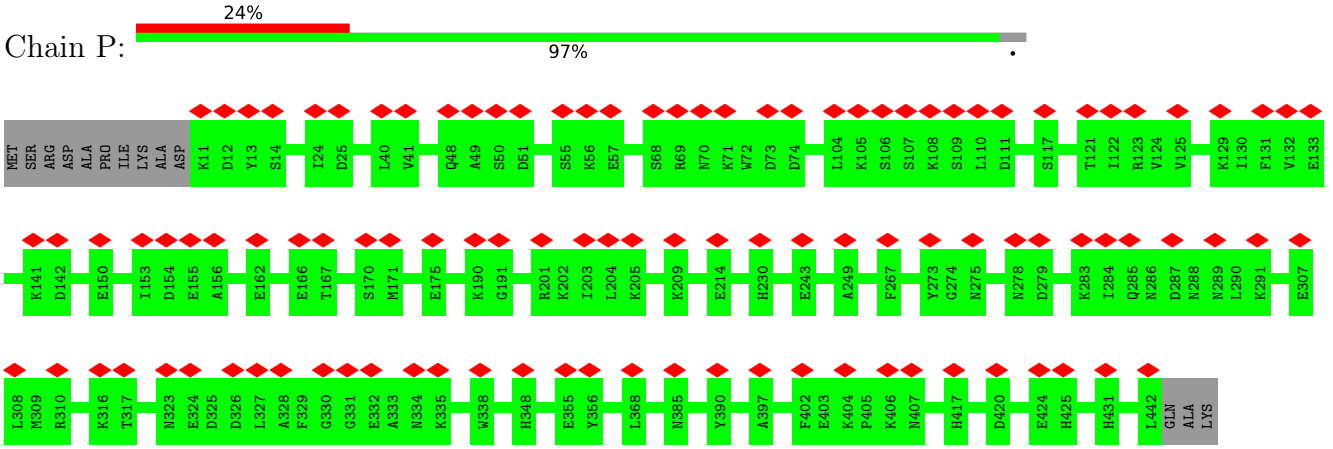


• Molecule 22: 26S proteasome regulatory subunit RPN9

Chain O:

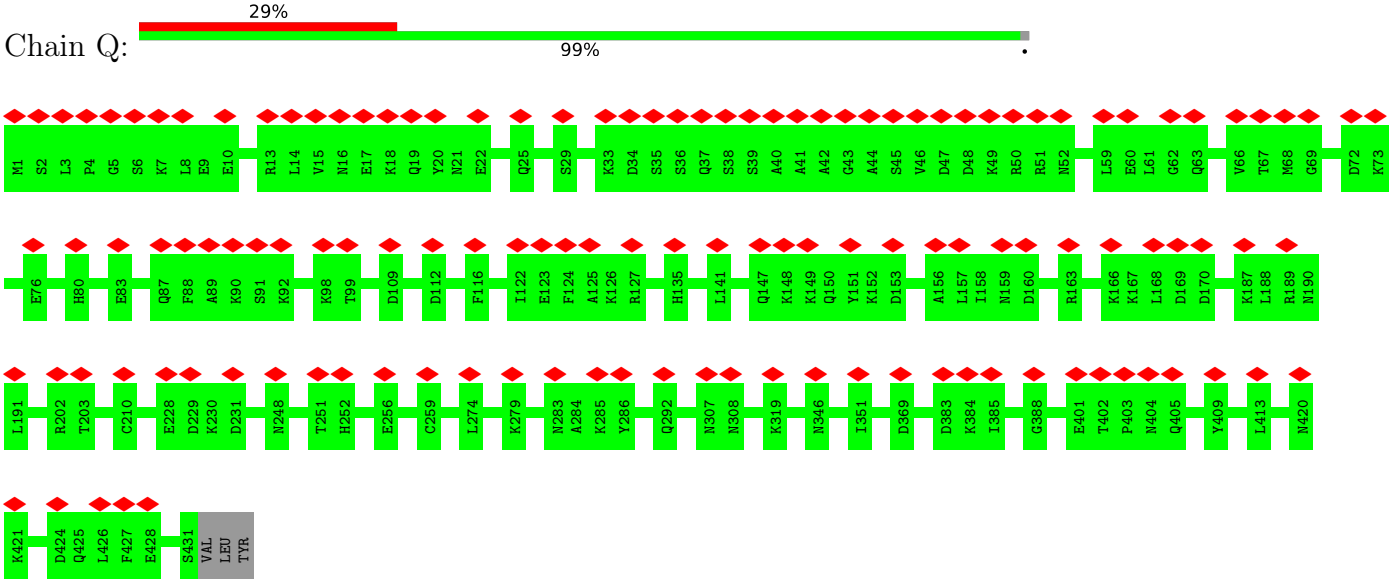
• Molecule 23: 26S proteasome regulatory subunit RPN5

Chain P:



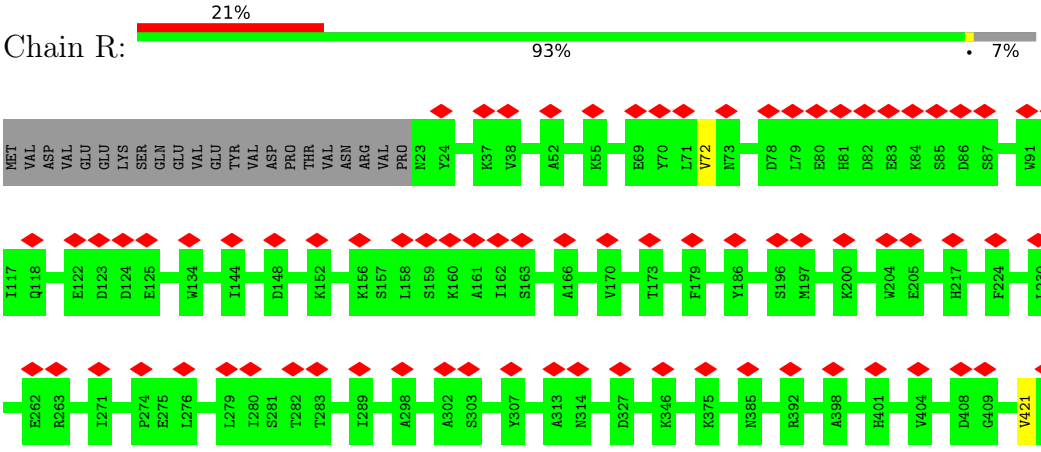
• Molecule 24: 26S proteasome regulatory subunit RPN6

Chain Q:



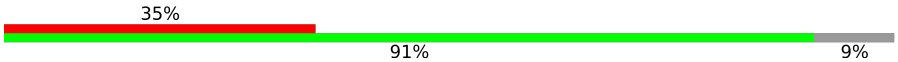
• Molecule 25: 26S proteasome regulatory subunit RPN7

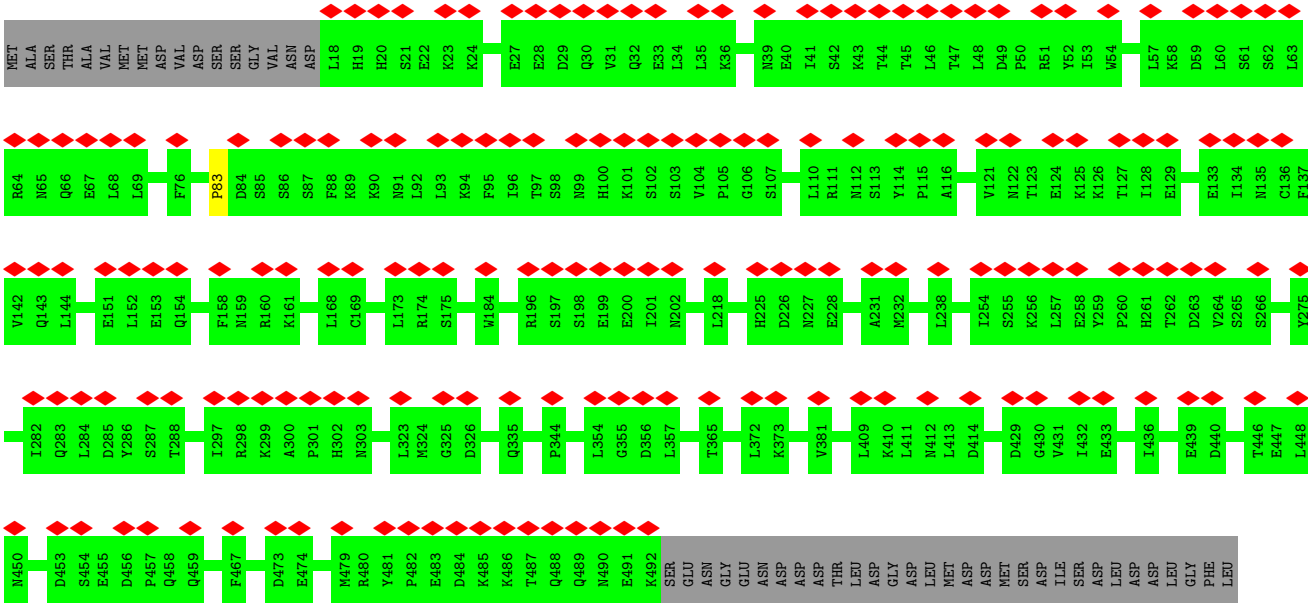
Chain R:



• Molecule 26: 26S proteasome regulatory subunit RPN3

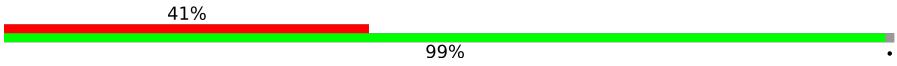
Chain S:

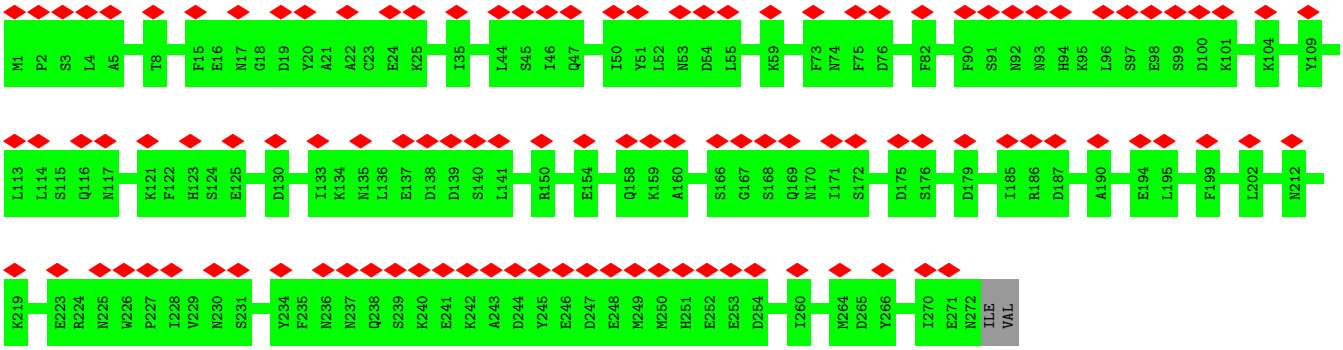




• Molecule 27: 26S proteasome regulatory subunit RPN12

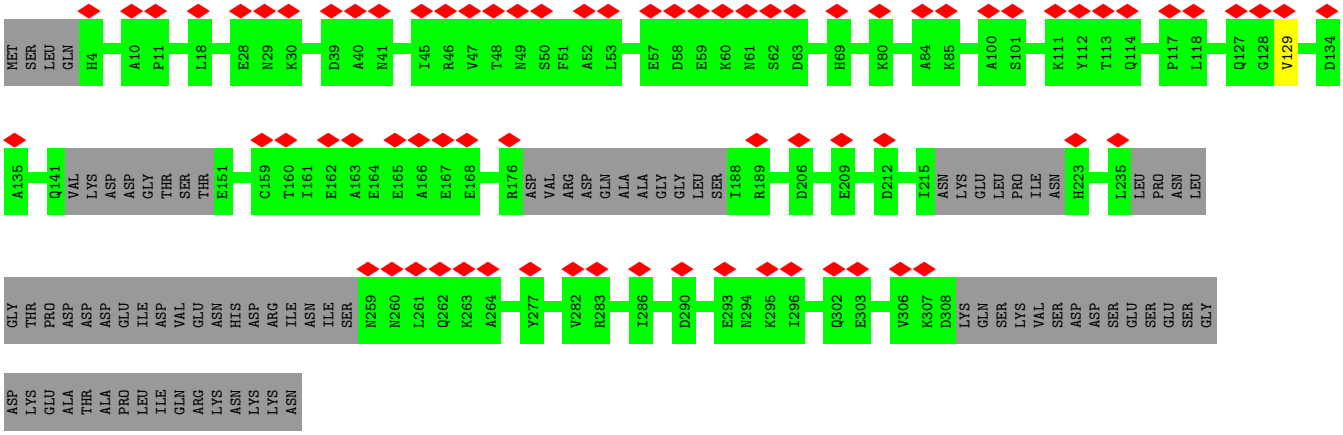
Chain T:





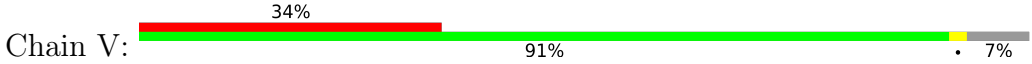
• Molecule 28: 26S proteasome regulatory subunit RPN8

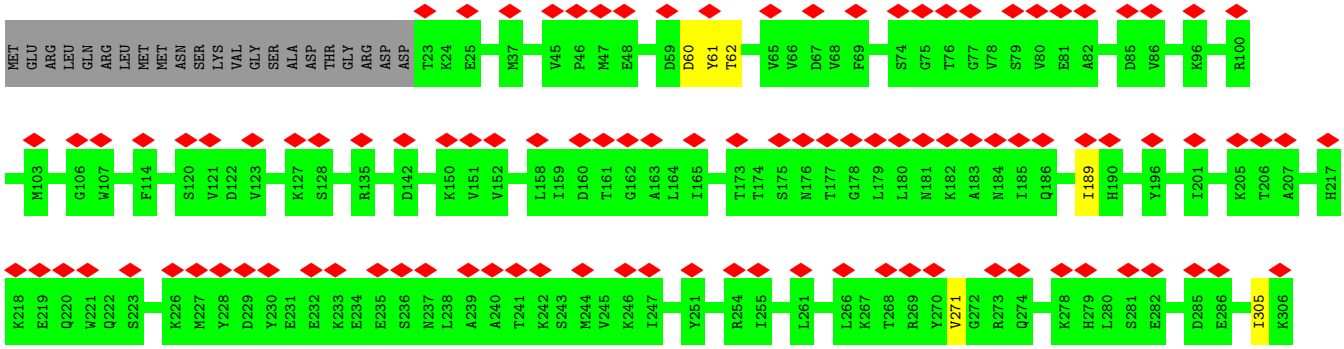
Chain U:



• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

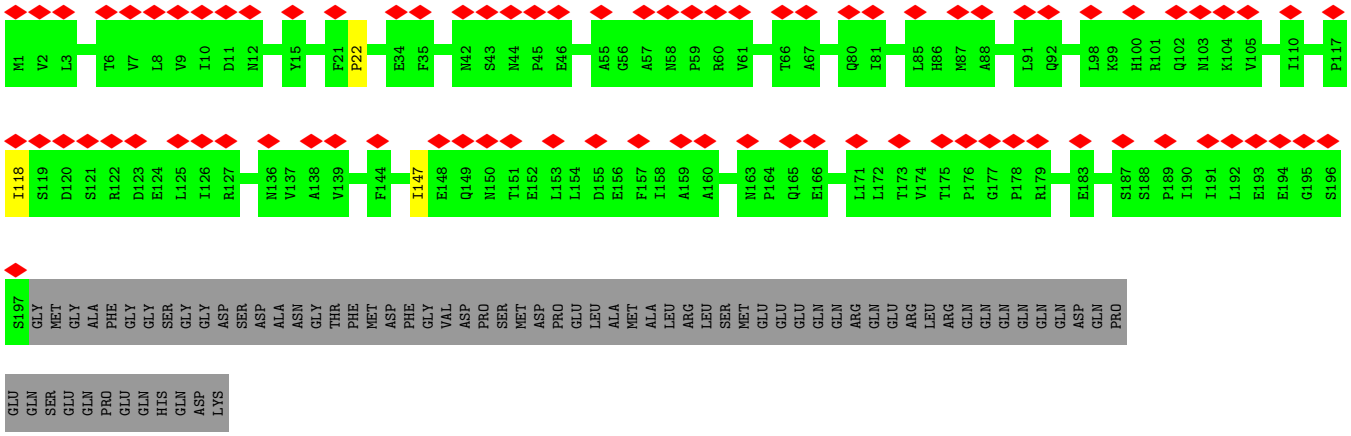
Chain V:





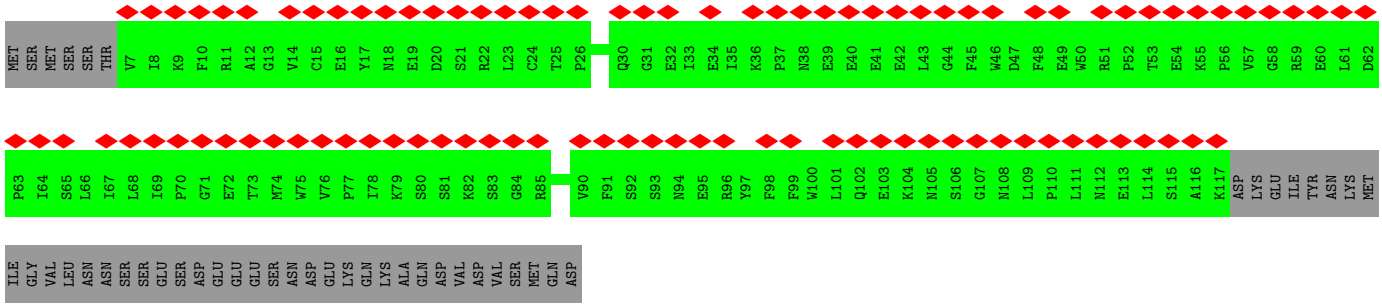
• Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W:



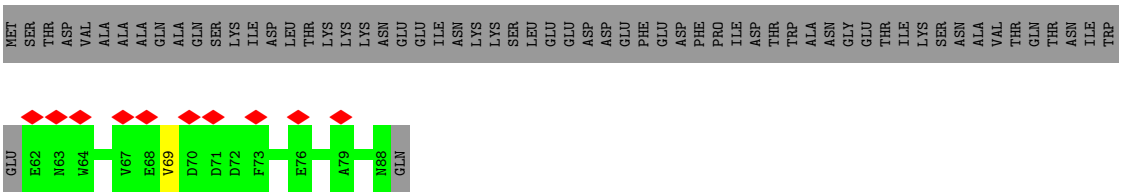
• Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X:



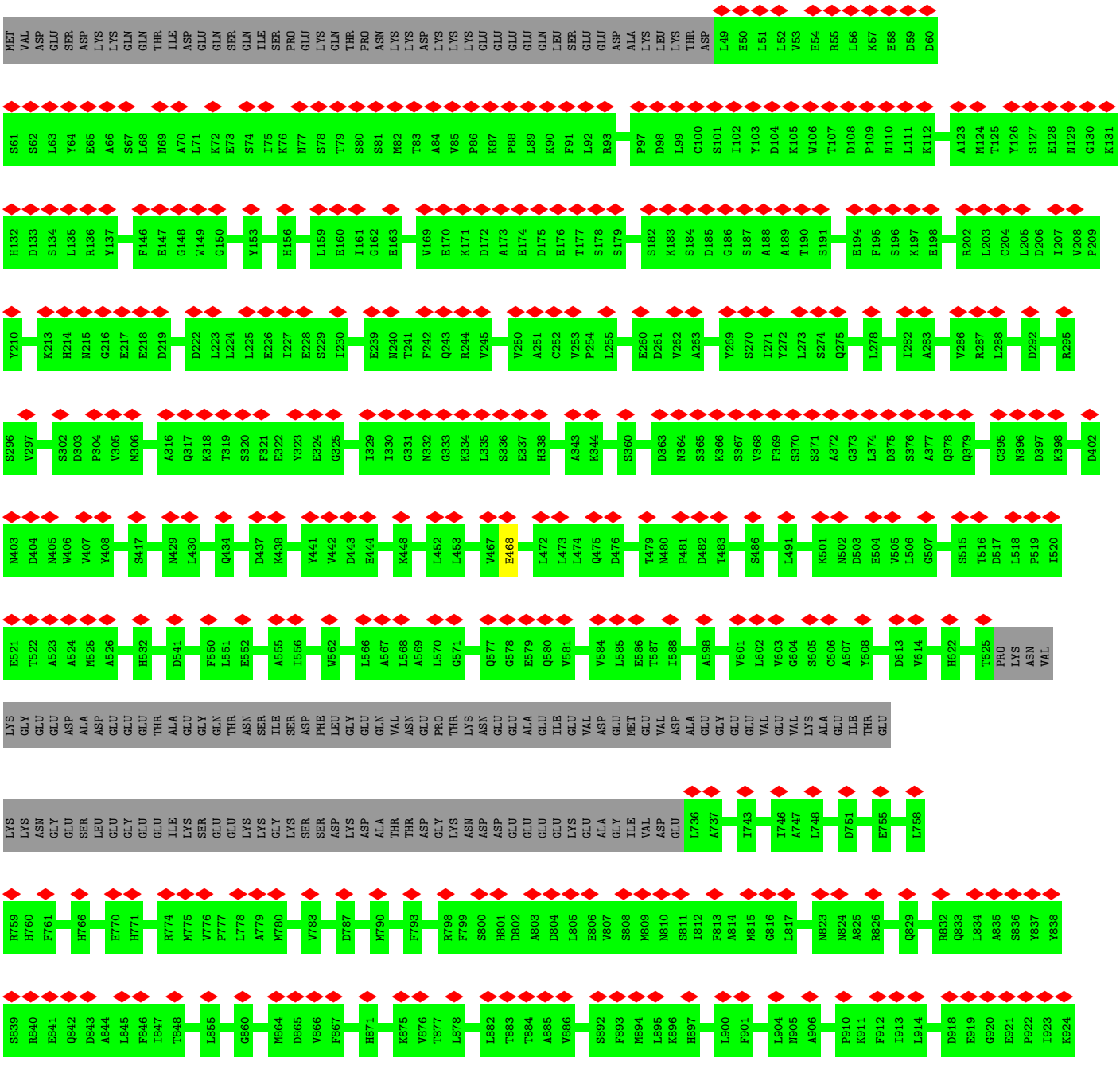
• Molecule 32: 26S proteasome complex subunit SEM1

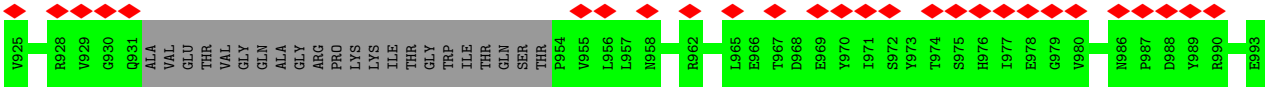
Chain Y:



• Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z:




V925
R928
V929
G930
Q931
ALA
VAL
GLU
THR
VAL
GLY
GLN
ALA
GLY
ARG
PRO
LYS
LYS
ILE
THR
GLY
TRP
ILE
THR
GLN
SER
THR
P954
V955
L956
L957
N958
R962
L965
E966
T967
D968
E969
Y970
I971
S972
Y973
T974
S975
H976
I977
E978
G979
V980
N986
P987
D988
Y989
R990
E993

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8320	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 ($e^-/Å^2$)	38	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	2.100	Depositor
Minimum map value	-1.052	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.657	Depositor
Map size (Å)	474.47998, 474.47998, 474.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.23	0/1541	0.41	0/2087
1	b	0.23	0/1541	0.41	0/2087
2	2	0.23	0/1750	0.40	0/2373
2	i	0.23	0/1750	0.42	0/2373
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.41	0/2174
4	4	0.23	0/1589	0.38	0/2142
4	g	0.23	0/1589	0.39	0/2142
5	5	0.23	0/1681	0.39	0/2274
5	f	0.23	0/1681	0.40	0/2274
6	6	0.24	0/1795	0.39	0/2420
6	e	0.24	0/1795	0.39	0/2420
7	7	0.24	0/1821	0.41	0/2470
7	a	0.24	0/1846	0.42	0/2503
8	A	0.23	0/1945	0.38	0/2634
8	c	0.23	0/1959	0.39	0/2652
9	B	0.24	0/1952	0.41	0/2642
9	j	0.24	0/1952	0.40	0/2642
10	C	0.23	0/1934	0.40	0/2618
10	d	0.23	0/1934	0.40	0/2618
11	D	0.23	0/1910	0.39	0/2586
11	n	0.23	0/1919	0.40	0/2598
12	E	0.23	0/1886	0.40	0/2541
12	m	0.23	0/1886	0.40	0/2541
13	F	0.24	0/1823	0.41	0/2463
13	l	0.24	0/1823	0.40	0/2463
14	G	0.23	0/1932	0.38	0/2609
14	k	0.23	0/1936	0.39	0/2614
15	H	0.24	0/2831	0.41	0/3808
16	I	0.24	0/2869	0.41	0/3867
17	J	0.23	0/2964	0.40	0/3981
18	K	0.23	0/3062	0.39	0/4132
19	L	0.24	0/2896	0.39	0/3895
20	M	0.31	1/2903 (0.0%)	0.41	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
21	N	0.24	0/6670	0.39	0/9023
22	O	0.23	0/3243	0.39	0/4374
23	P	0.22	0/3599	0.36	0/4854
24	Q	0.23	0/3527	0.38	0/4748
25	R	0.23	0/3272	0.39	0/4412
26	S	0.23	0/3966	0.37	0/5355
27	T	0.24	0/2279	0.40	0/3077
28	U	0.23	0/2087	0.37	0/2811
29	V	0.23	0/2271	0.44	0/3064
30	W	0.25	0/1557	0.42	0/2111
31	X	0.23	0/931	0.41	0/1262
32	Y	0.22	0/239	0.40	0/322
33	Z	0.26	1/6404 (0.0%)	0.40	0/8686
All	All	0.24	2/107962 (0.0%)	0.40	0/145825

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	M	75	LEU	C-N	9.87	1.53	1.34
33	Z	468	GLU	C-N	9.19	1.51	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	194/215 (90%)	189 (97%)	5 (3%)	0	100	100
1	b	194/215 (90%)	189 (97%)	5 (3%)	0	100	100
2	2	224/261 (86%)	218 (97%)	6 (3%)	0	100	100
2	i	224/261 (86%)	220 (98%)	4 (2%)	0	100	100
3	3	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
3	h	202/205 (98%)	189 (94%)	12 (6%)	1 (0%)	25	64
4	4	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
4	g	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
5	5	210/287 (73%)	208 (99%)	2 (1%)	0	100	100
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
6	6	220/241 (91%)	215 (98%)	5 (2%)	0	100	100
6	e	220/241 (91%)	213 (97%)	7 (3%)	0	100	100
7	7	227/266 (85%)	218 (96%)	9 (4%)	0	100	100
7	a	230/266 (86%)	223 (97%)	7 (3%)	0	100	100
8	A	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
9	j	248/250 (99%)	238 (96%)	10 (4%)	0	100	100
10	C	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
10	d	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
11	D	238/254 (94%)	228 (96%)	10 (4%)	0	100	100
11	n	239/254 (94%)	231 (97%)	8 (3%)	0	100	100
12	E	240/260 (92%)	229 (95%)	11 (5%)	0	100	100
12	m	240/260 (92%)	233 (97%)	7 (3%)	0	100	100
13	F	231/234 (99%)	220 (95%)	11 (5%)	0	100	100
13	l	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
14	G	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
14	k	242/288 (84%)	237 (98%)	5 (2%)	0	100	100
15	H	353/467 (76%)	311 (88%)	41 (12%)	1 (0%)	37	73
16	I	361/437 (83%)	334 (92%)	27 (8%)	0	100	100
17	J	371/405 (92%)	350 (94%)	21 (6%)	0	100	100
18	K	379/428 (89%)	343 (90%)	35 (9%)	1 (0%)	37	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	L	359/437 (82%)	335 (93%)	24 (7%)	0	100 100
20	M	363/434 (84%)	336 (93%)	24 (7%)	3 (1%)	16 55
21	N	843/945 (89%)	793 (94%)	47 (6%)	3 (0%)	30 68
22	O	385/393 (98%)	348 (90%)	36 (9%)	1 (0%)	37 73
23	P	430/445 (97%)	390 (91%)	40 (9%)	0	100 100
24	Q	429/434 (99%)	398 (93%)	31 (7%)	0	100 100
25	R	398/429 (93%)	357 (90%)	38 (10%)	3 (1%)	16 55
26	S	473/523 (90%)	451 (95%)	21 (4%)	1 (0%)	44 78
27	T	270/274 (98%)	239 (88%)	31 (12%)	0	100 100
28	U	245/338 (72%)	240 (98%)	4 (2%)	1 (0%)	30 68
29	V	282/306 (92%)	243 (86%)	33 (12%)	6 (2%)	5 30
30	W	195/268 (73%)	174 (89%)	18 (9%)	3 (2%)	8 40
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100 100
32	Y	25/89 (28%)	18 (72%)	6 (24%)	1 (4%)	2 18
33	Z	807/993 (81%)	743 (92%)	64 (8%)	0	100 100
All	All	13382/15139 (88%)	12602 (94%)	755 (6%)	25 (0%)	45 78

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	H	329	VAL
29	V	61	TYR
3	h	105	VAL
20	M	274	ALA
29	V	62	THR
21	N	874	ILE
21	N	903	VAL
28	U	129	VAL
29	V	60	ASP
32	Y	69	VAL
20	M	276	THR
21	N	761	ILE
25	R	241	ILE
25	R	421	VAL
29	V	189	ILE
29	V	305	ILE
30	W	147	ILE

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Mol	Chain	Res	Type
30	W	22	PRO
18	K	326	PRO
25	R	72	VAL
20	M	167	VAL
26	S	83	PRO
29	V	271	VAL
22	O	227	ILE
30	W	118	ILE

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	1	162/178 (91%)	162 (100%)	0	100	100
1	b	162/178 (91%)	162 (100%)	0	100	100
2	2	185/214 (86%)	185 (100%)	0	100	100
2	i	185/214 (86%)	185 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	173/175 (99%)	173 (100%)	0	100	100
4	g	173/175 (99%)	173 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
5	f	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	195/224 (87%)	195 (100%)	0	100	100
7	a	198/224 (88%)	198 (100%)	0	100	100
8	A	206/210 (98%)	206 (100%)	0	100	100
8	c	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	212/226 (94%)	212 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	201 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	320/385 (83%)	320 (100%)	0	100	100
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	308/377 (82%)	308 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	447/489 (91%)	447 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	249/268 (93%)	249 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	101/144 (70%)	101 (100%)	0	100	100
32	Y	26/81 (32%)	26 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	11628/13054 (89%)	11628 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	214	GLN
2	2	64	HIS
2	2	95	HIS
2	2	114	GLN
3	3	89	GLN
3	3	145	GLN
3	3	169	GLN
3	3	204	GLN
5	5	104	GLN
5	5	128	GLN
5	5	254	HIS
5	5	283	ASN
6	6	55	ASN
6	6	113	GLN
7	7	107	ASN
1	b	81	HIS
2	i	51	GLN
4	g	65	GLN
4	g	86	GLN
4	g	147	HIS
4	g	191	GLN
5	f	104	GLN
5	f	208	GLN
6	e	89	ASN
6	e	113	GLN
6	e	171	ASN
7	a	95	HIS
7	a	145	ASN
9	B	20	GLN
9	B	30	GLN
9	B	119	GLN
10	C	120	GLN
10	C	227	GLN
11	D	79	ASN
11	D	122	GLN
11	D	149	GLN
11	D	178	ASN
13	F	4	ASN
13	F	43	HIS

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Mol	Chain	Res	Type
13	F	117	GLN
13	F	143	HIS
14	G	182	HIS
8	c	92	ASN
8	c	126	GLN
10	d	94	HIS
10	d	120	GLN
11	n	19	GLN
11	n	118	GLN
11	n	162	GLN
12	m	147	HIS
13	l	93	ASN
13	l	117	GLN
14	k	12	ASN
14	k	121	GLN
14	k	127	ASN
14	k	183	HIS
15	H	54	ASN
15	H	182	ASN
15	H	281	GLN
15	H	359	ASN
15	H	413	ASN
17	J	66	GLN
17	J	181	GLN
17	J	240	HIS
18	K	72	GLN
21	N	34	GLN
21	N	375	HIS
21	N	747	HIS
22	O	4	ASN
22	O	235	HIS
22	O	354	GLN
23	P	30	ASN
23	P	263	HIS
23	P	286	ASN
23	P	418	ASN
24	Q	19	GLN
24	Q	114	GLN
24	Q	226	HIS
25	R	399	GLN
26	S	227	ASN
26	S	283	GLN

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Mol	Chain	Res	Type
26	S	311	GLN
26	S	321	GLN
26	S	334	HIS
27	T	92	ASN
28	U	127	GLN
28	U	280	ASN
29	V	111	HIS
29	V	145	GLN
29	V	195	HIS
29	V	204	HIS
29	V	250	GLN
29	V	279	HIS
30	W	18	ASN
30	W	42	ASN
30	W	92	GLN
31	X	38	ASN
31	X	94	ASN
33	Z	327	GLN
33	Z	361	HIS
33	Z	379	GLN
33	Z	475	GLN
33	Z	801	HIS
33	Z	829	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

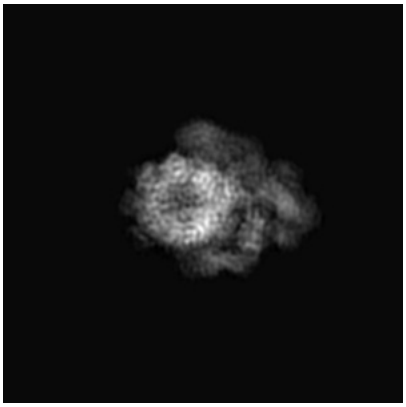
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9769. These allow visual inspection of the internal detail of the map and identification of artifacts.

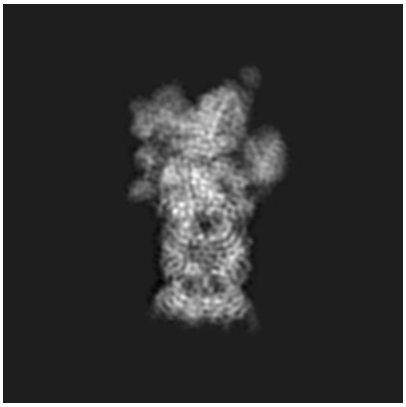
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

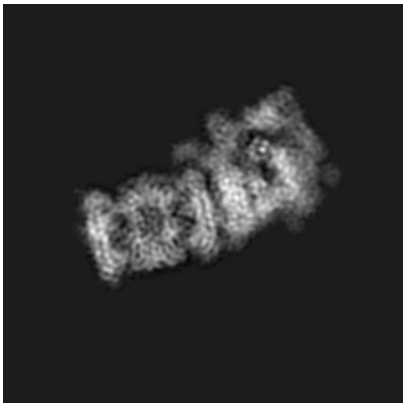
6.1.1 Primary map



X



Y



Z

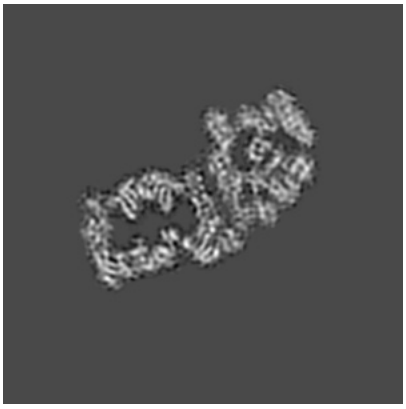
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 180

Y Index: 180

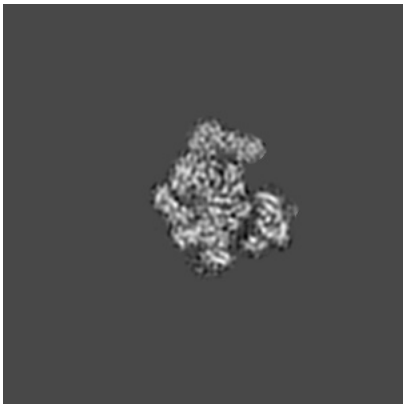


Z Index: 180

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

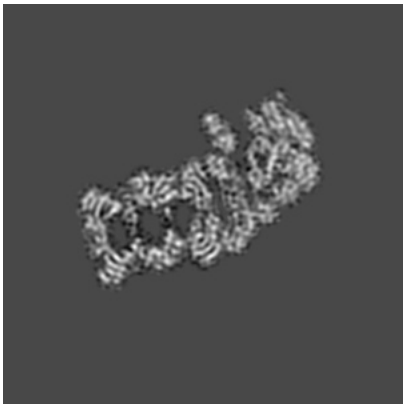
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 204

Y Index: 183

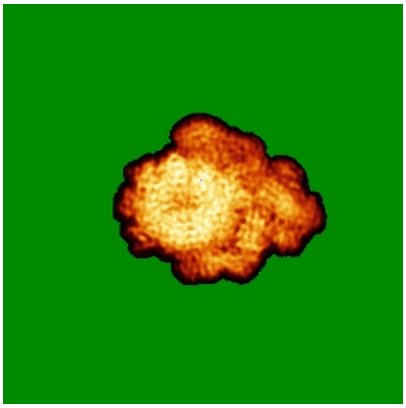


Z Index: 187

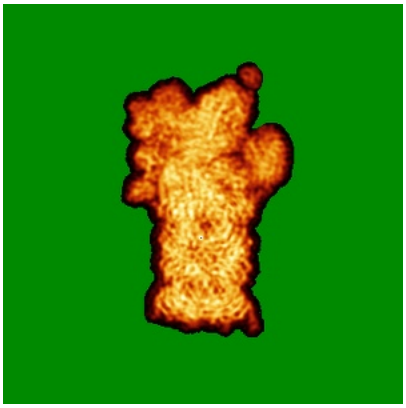
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

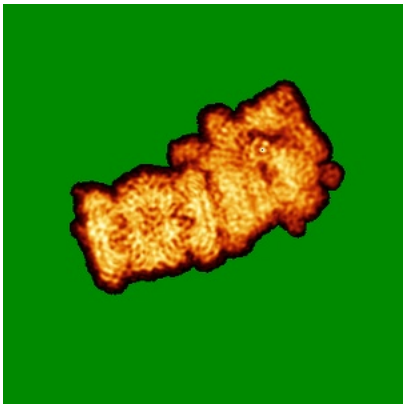
6.4.1 Primary map



X



Y

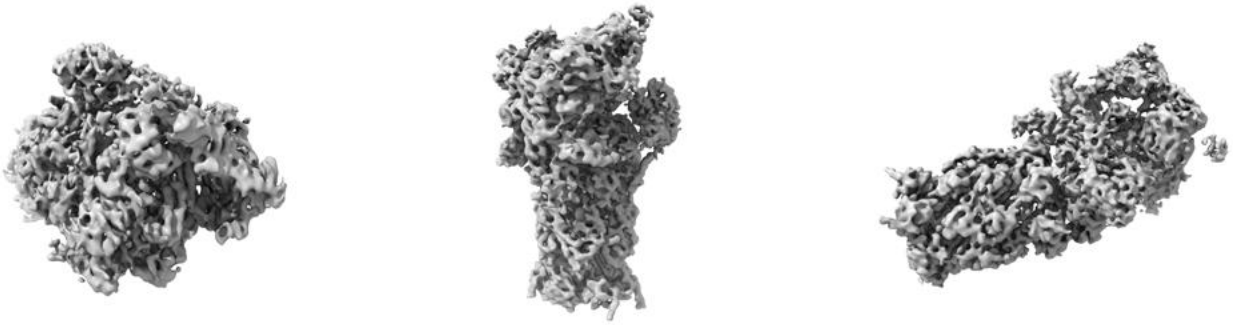


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.657. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

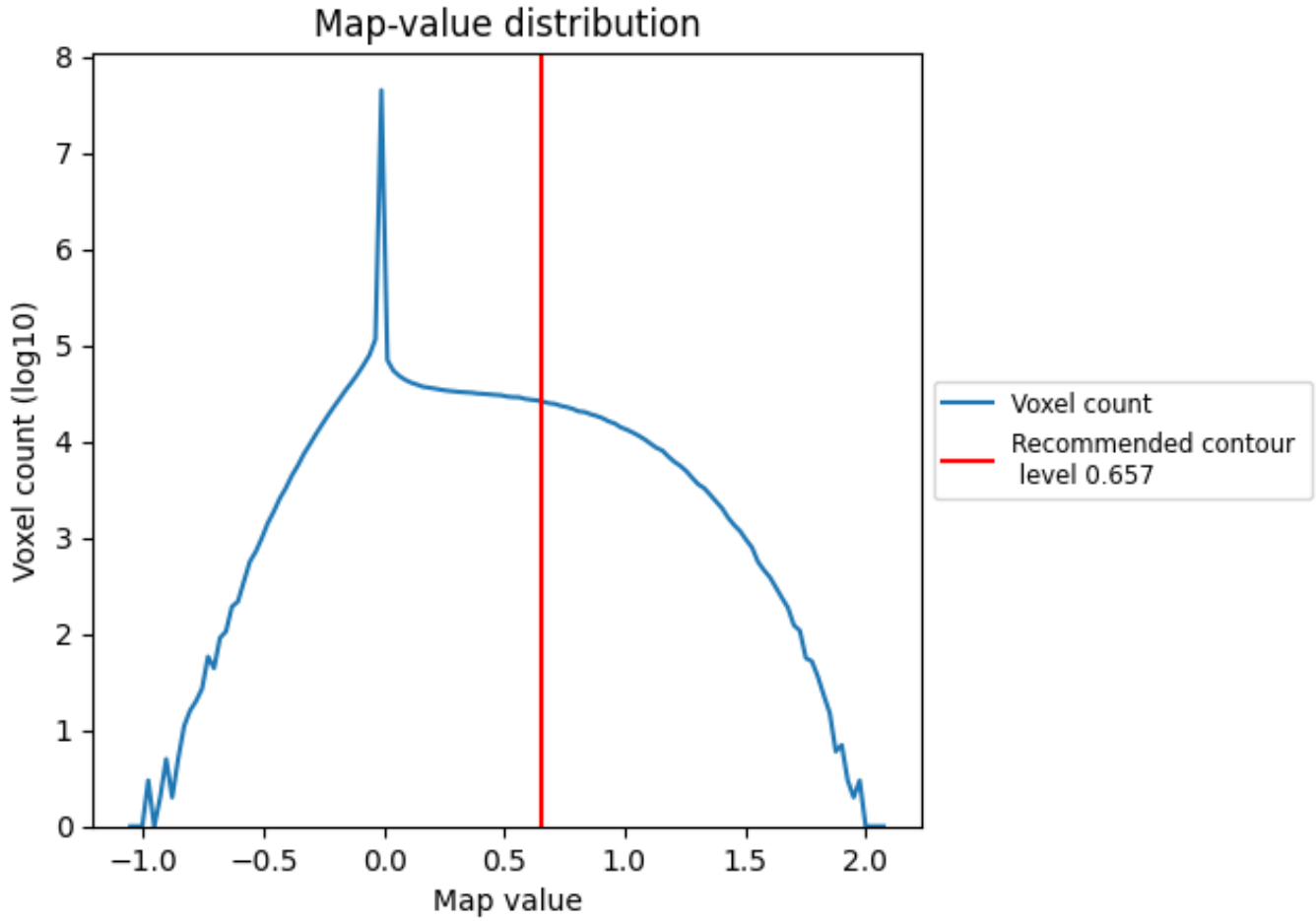
6.6 Mask visualisation (i)

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

7 Map analysis

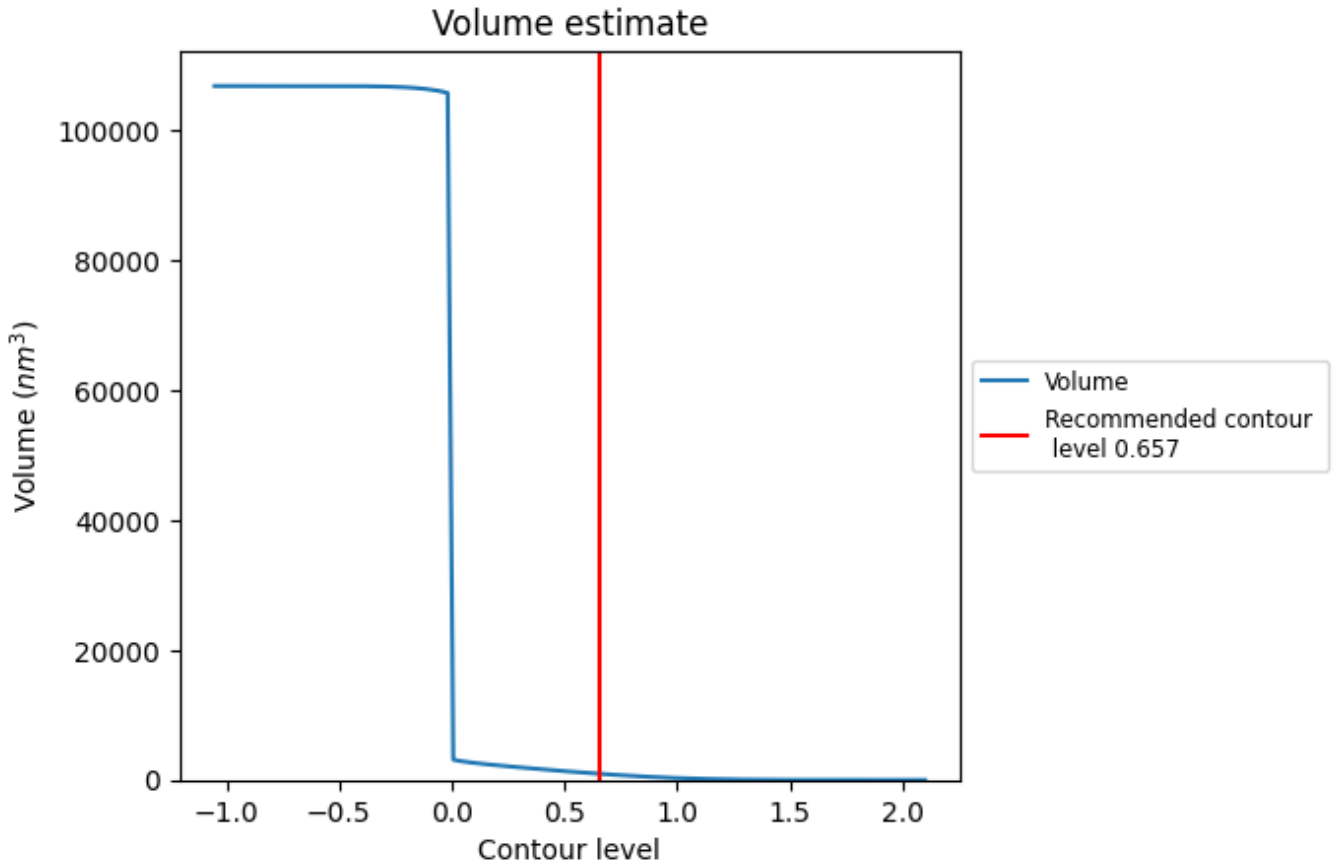
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

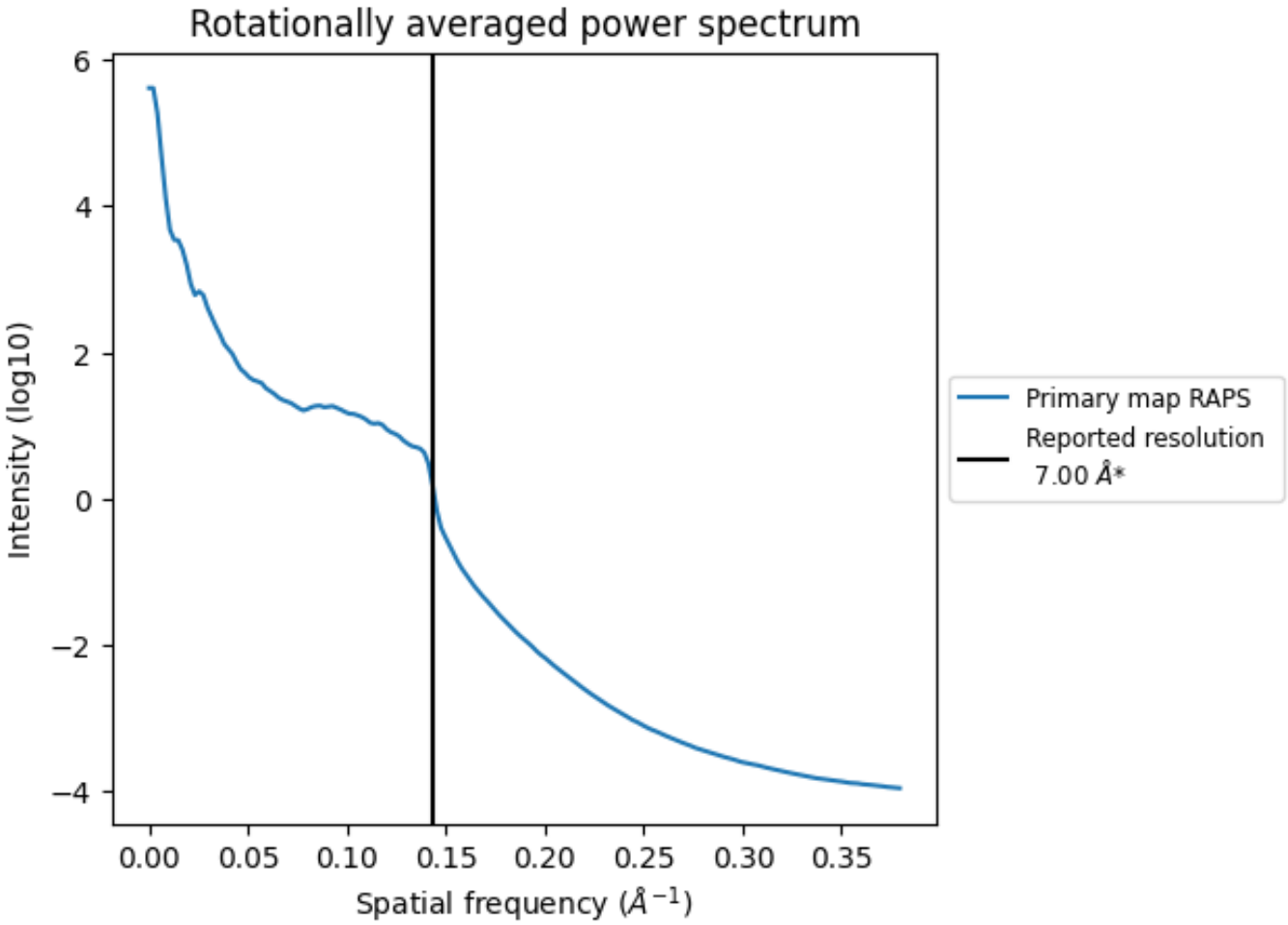
7.2 Volume estimate



The volume at the recommended contour level is 945 nm^3; this corresponds to an approximate mass of 854 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 0.143 Å^{-1}

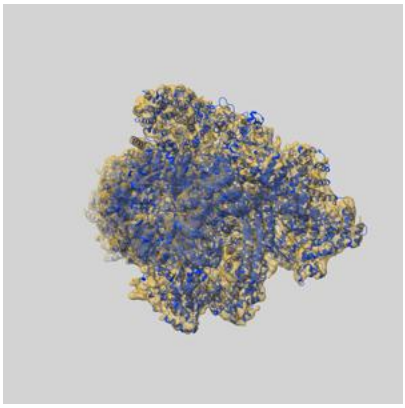
8 Fourier-Shell correlation (i)

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

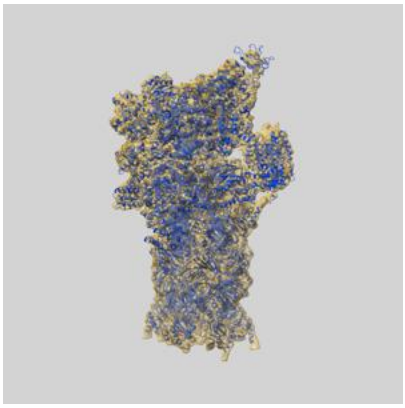
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9769 and PDB model 6J2C. Per-residue inclusion information can be found in section 3 on page 11.

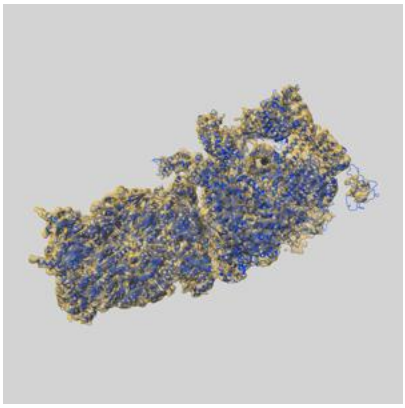
9.1 Map-model overlay



X



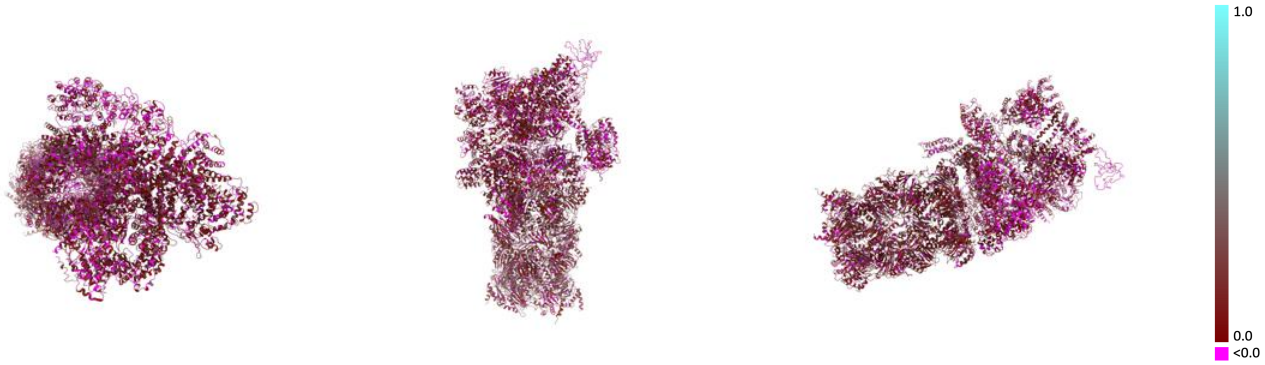
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.657 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.

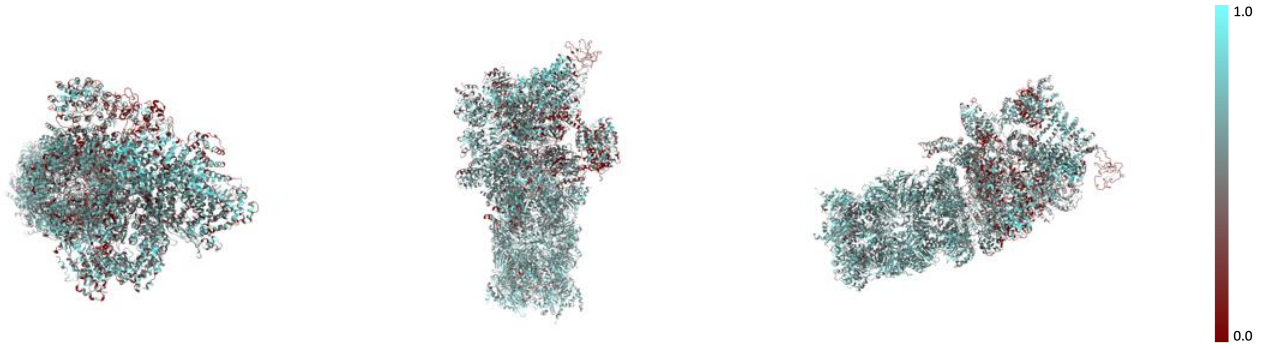
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

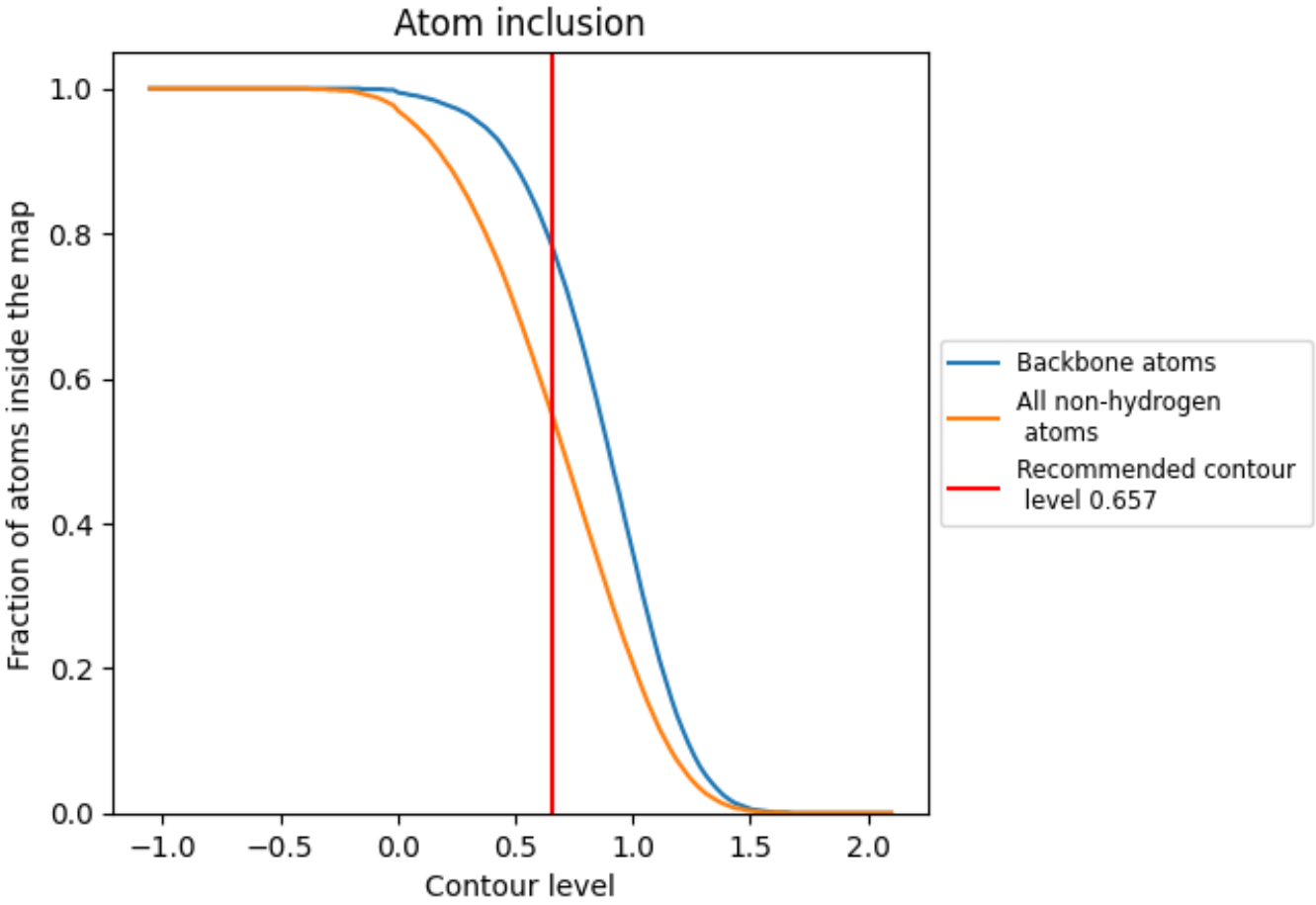
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.657).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 55% 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 (0.657) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5500	0.1170
1	0.6150	0.1440
2	0.6270	0.1540
3	0.6060	0.1300
4	0.5990	0.1350
5	0.6350	0.1470
6	0.6360	0.1430
7	0.6370	0.1480
A	0.5770	0.1440
B	0.5670	0.1330
C	0.5880	0.1410
D	0.6060	0.1390
E	0.5910	0.1500
F	0.6130	0.1320
G	0.6190	0.1440
H	0.4720	0.0780
I	0.4640	0.0960
J	0.4290	0.0980
K	0.4830	0.1140
L	0.4620	0.0930
M	0.4680	0.0860
N	0.6170	0.1120
O	0.5060	0.0970
P	0.5600	0.1200
Q	0.5280	0.1140
R	0.5700	0.1160
S	0.4880	0.1050
T	0.4600	0.0960
U	0.5300	0.1090
V	0.4920	0.0890
W	0.4660	0.0720
X	0.1230	-0.0200
Y	0.4960	0.0870
Z	0.4280	0.0620
a	0.6030	0.1490

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Chain	Atom inclusion	Q-score
b	0.6210	0.1380
c	0.6240	0.1380
d	0.5990	0.1270
e	0.6270	0.1470
f	0.6400	0.1500
g	0.6240	0.1490
h	0.6200	0.1400
i	0.6100	0.1430
j	0.5920	0.1300
k	0.6400	0.1400
l	0.6410	0.1380
m	0.6130	0.1370
n	0.6180	0.1390