wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 02:01 PM JST

PDB ID	:	5WVI
EMDB ID	:	EMD-6693
Title	:	The resting state of yeast proteasome
Authors	:	Ding, Z.; Cong, Y.
Deposited on	:	2016-12-25
Resolution	:	6.30 Å(reported)

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

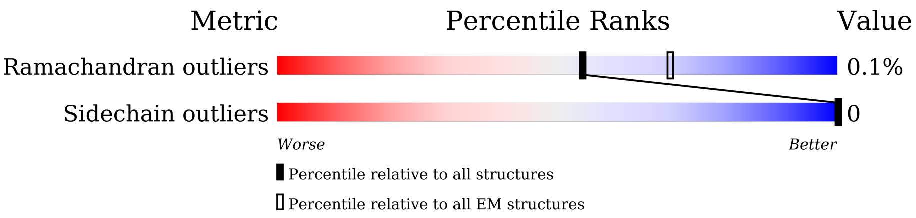
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

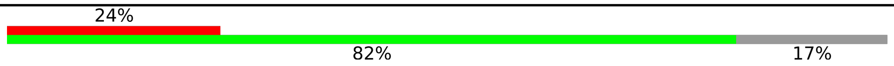
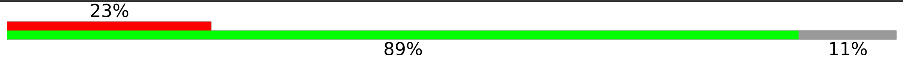
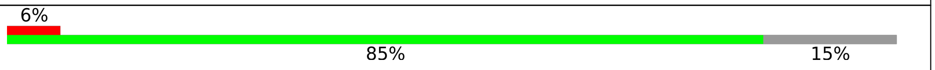
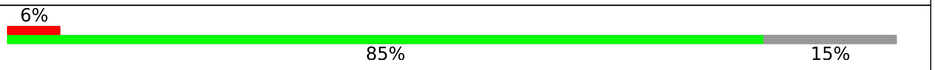
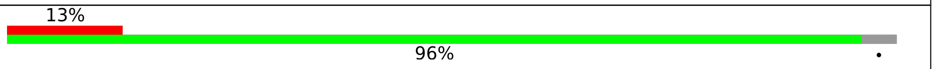
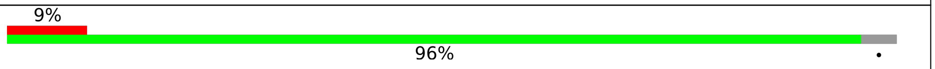
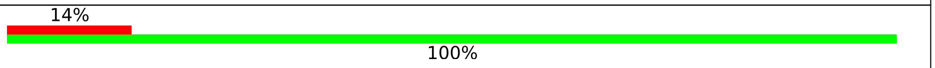
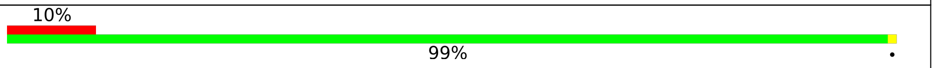
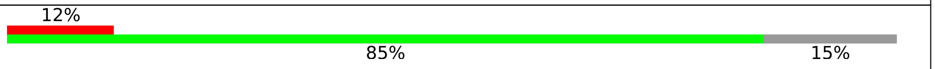
The reported resolution of this entry is 6.30 Å.

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 >=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	I	437	
2	K	428	
3	2	261	
3	i	261	
4	A	252	
4	c	252	
5	3	205	
5	h	205	
6	G	288	

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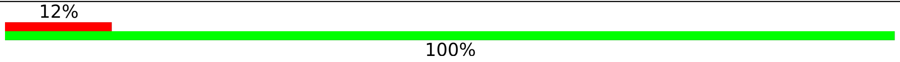
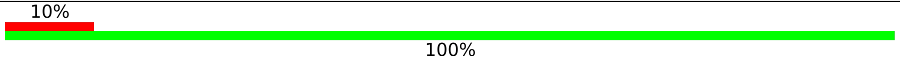
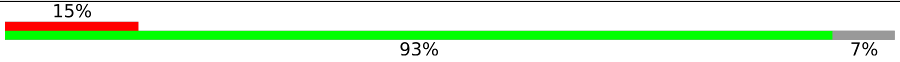
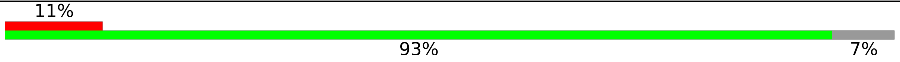
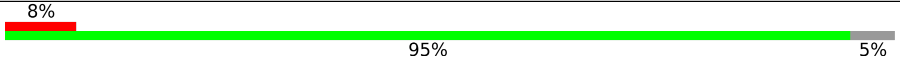
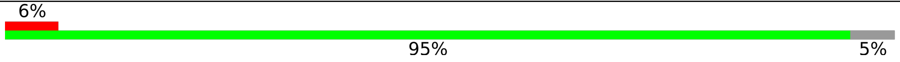
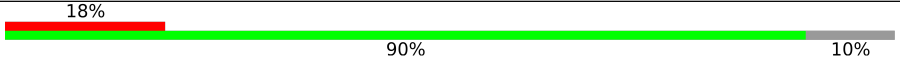
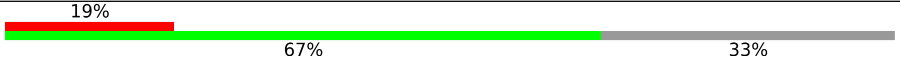
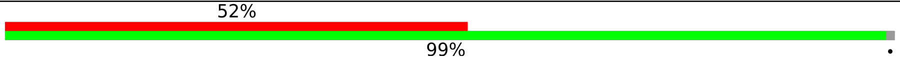
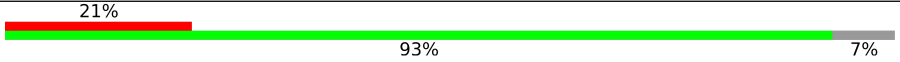
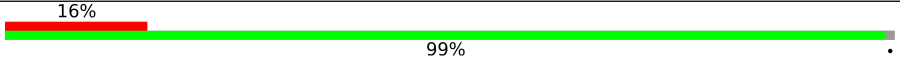
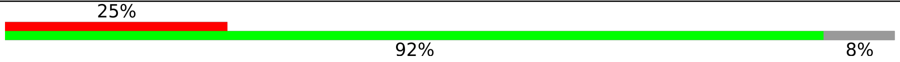
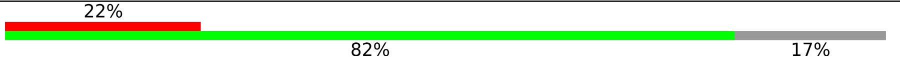
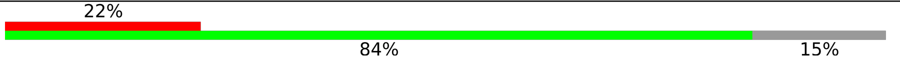
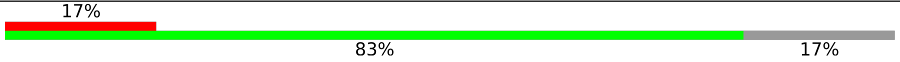
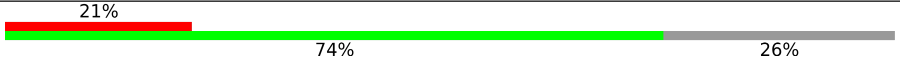
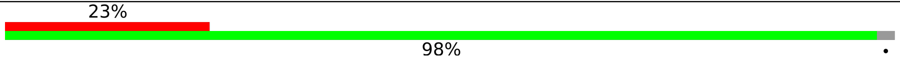
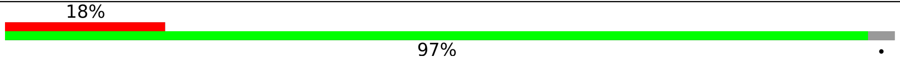
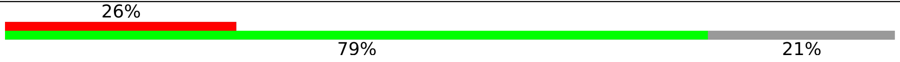
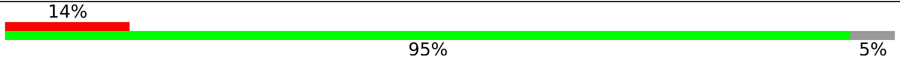
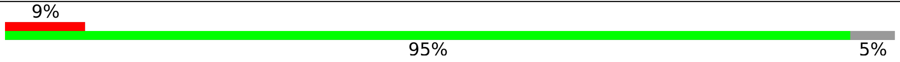
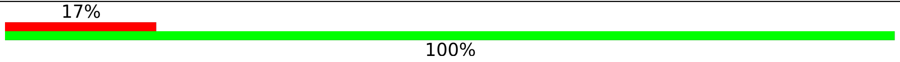
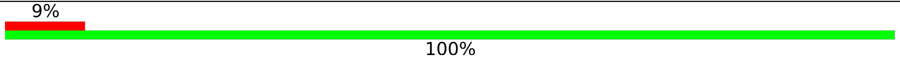
Mol	Chain	Length	Quality of chain
6	k	288	
7	F	234	
7	l	234	
8	E	260	
8	m	260	
9	D	254	
9	n	254	
10	Y	89	
11	N	945	
12	S	523	
13	T	274	
14	R	429	
15	Q	434	
16	J	405	
17	L	437	
18	M	434	
19	U	338	
20	W	268	
21	O	393	
22	P	445	
23	H	467	
24	C	258	
24	d	258	
25	B	250	
25	j	250	

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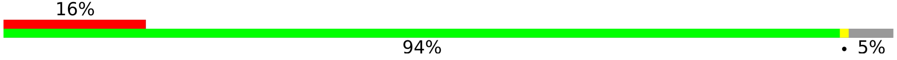
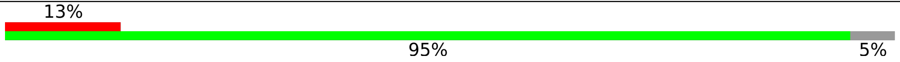
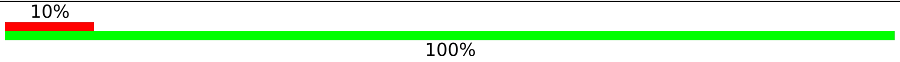
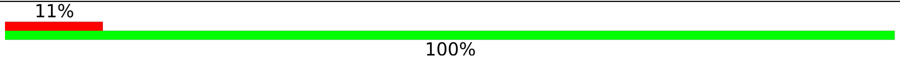
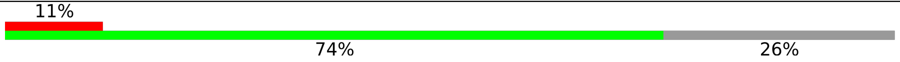
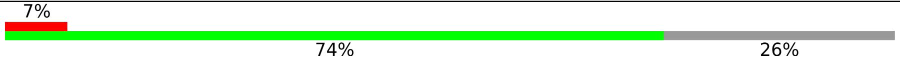
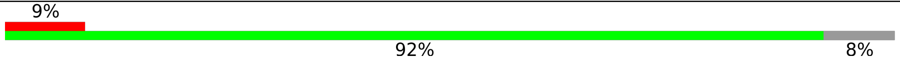
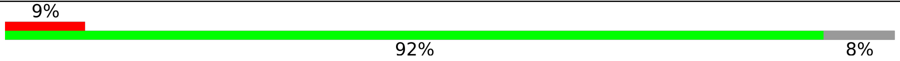
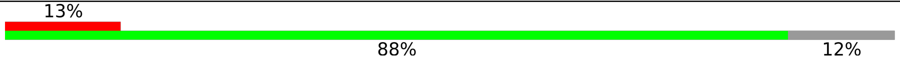
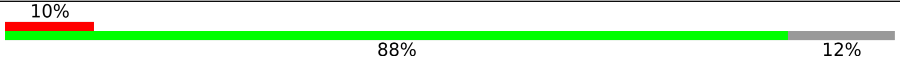
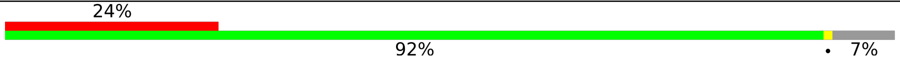
Mol	Chain	Length	Quality of chain
26	1	215	
26	b	215	
27	4	198	
27	g	198	
28	5	287	
28	f	287	
29	6	241	
29	e	241	
30	7	266	
30	a	266	
31	X	156	
32	Z	993	
33	V	306	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 105787 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	362	Total 2822	C 1773	N 471	O 563	S 15	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 6B homolog.

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

- Molecule 3 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	i	222	Total 1684	C 1061	N 293	O 323	S 7	0	0
3	2	222	Total 1684	C 1061	N 293	O 323	S 7	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	243	Total 1921	C 1221	N 322	O 370	S 8	0	0
4	A	243	Total 1921	C 1221	N 322	O 370	S 8	0	0

- Molecule 5 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	204	Total 1581	C 1010	N 258	O 305	S 8	0	0
5	3	204	Total 1581	C 1010	N 258	O 305	S 8	0	0

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	245	Total	C	N	O	S	0	0
			1900	1207	331	358	4		
6	G	245	Total	C	N	O	S	0	0
			1900	1207	331	358	4		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	m	243	Total	C	N	O	S	0	0
			1867	1165	315	380	7		
8	E	243	Total	C	N	O	S	0	0
			1867	1165	315	380	7		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	242	Total	C	N	O	S	0	0
			1899	1186	333	376	4		
9	D	242	Total	C	N	O	S	0	0
			1899	1186	333	376	4		

- Molecule 10 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN2.

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

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	353	Total 2893	C 1857	N 482	O 541	S 13	0	0

- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN12.

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

- Molecule 14 is a protein called 26S proteasome regulatory subunit RPN7.

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

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN6.

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

- Molecule 16 is a protein called 26S protease regulatory subunit 8 homolog.

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

- Molecule 17 is a protein called 26S protease subunit RPT4.

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

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

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

- Molecule 19 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	282	Total	C	N	O	S	0	0
			2257	1429	387	435	6		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN10.

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

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN9.

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

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN5.

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

- Molecule 23 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	H	370	Total	C	N	O	S	0	0
			2889	1815	515	543	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	245	Total	C	N	O	S	0	0
			1913	1207	323	380	3		
24	d	245	Total	C	N	O	S	0	0
			1913	1207	323	380	3		

- Molecule 25 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 26 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
26	b	205	Total	C	N	O	S	0	0
			1574	995	261	311	7		

- Molecule 27 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
27	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

- Molecule 28 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
28	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 29 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
29	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 30 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
30	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

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

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

- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Z	813	6289	3995	1029	1236	29	0	0

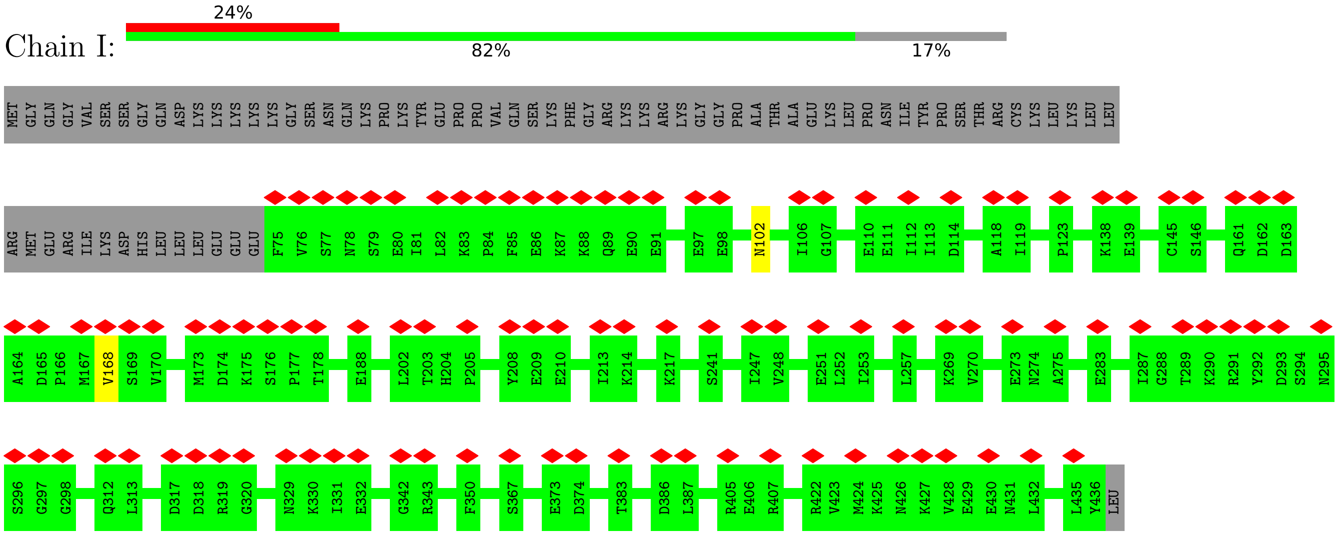
- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

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

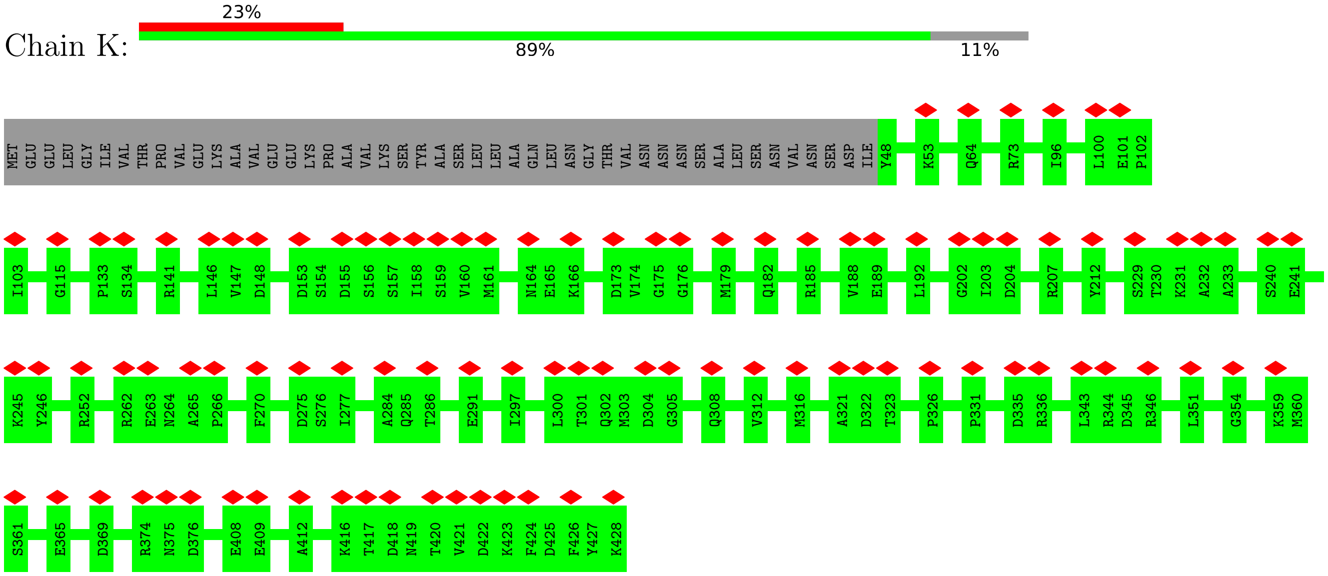
3 Residue-property plots

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: 26S protease regulatory subunit 4 homolog

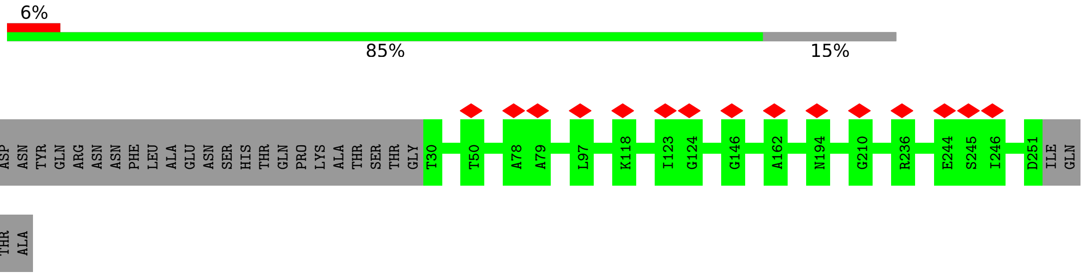


- Molecule 2: 26S protease regulatory subunit 6B homolog



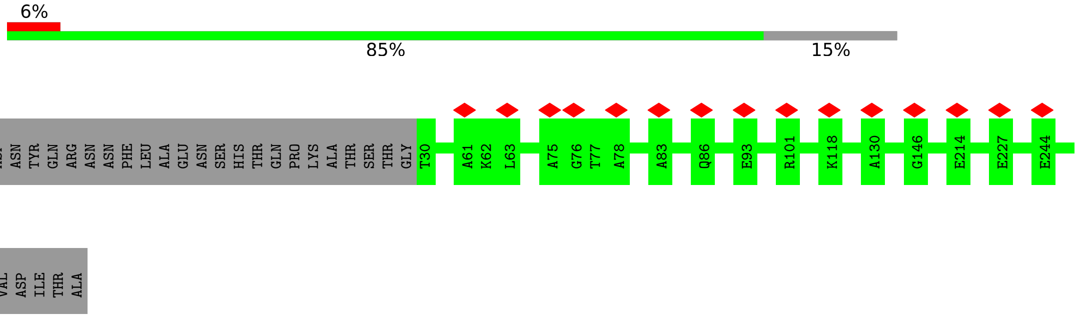
- Molecule 3: Proteasome subunit beta type-2

Chain i:



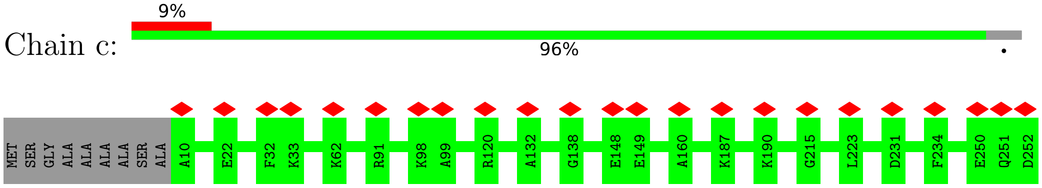
- Molecule 3: Proteasome subunit beta type-2

Chain 2:



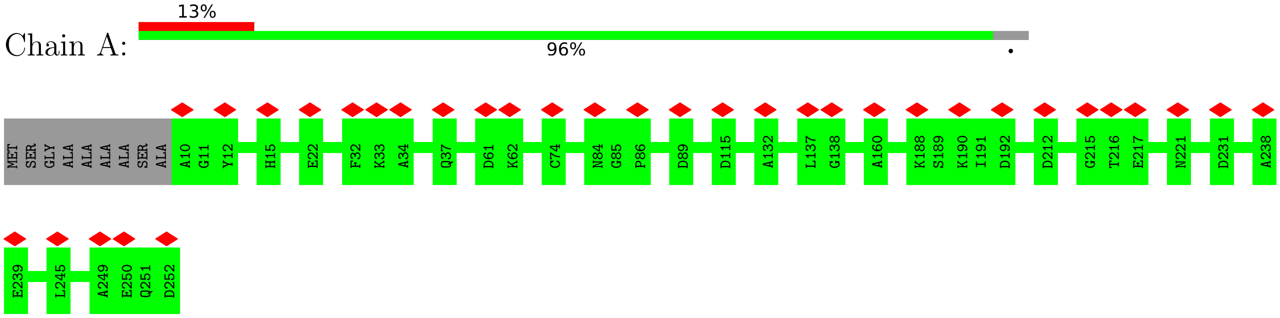
- Molecule 4: Proteasome subunit alpha type-1

Chain c:



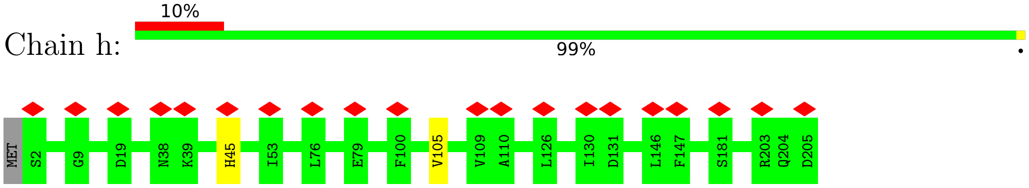
- Molecule 4: Proteasome subunit alpha type-1

Chain A:



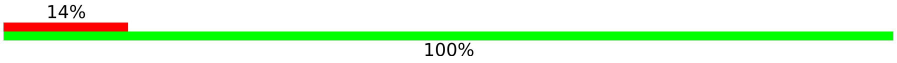
- Molecule 5: Proteasome subunit beta type-3

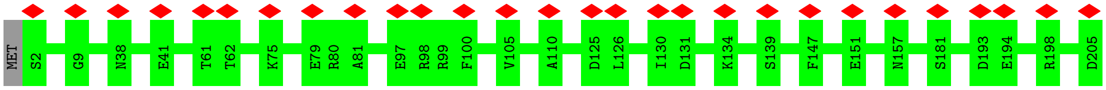
Chain h:



- Molecule 5: Proteasome subunit beta type-3

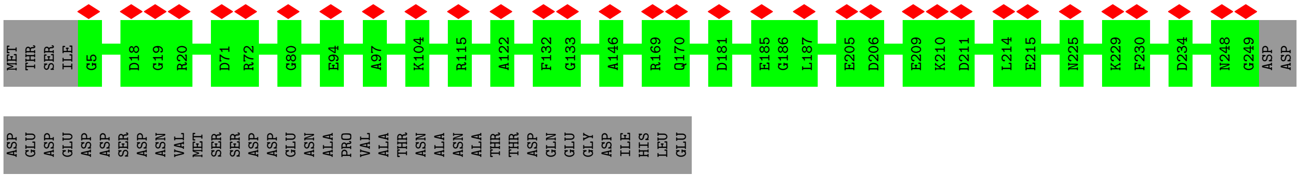
Chain 3:





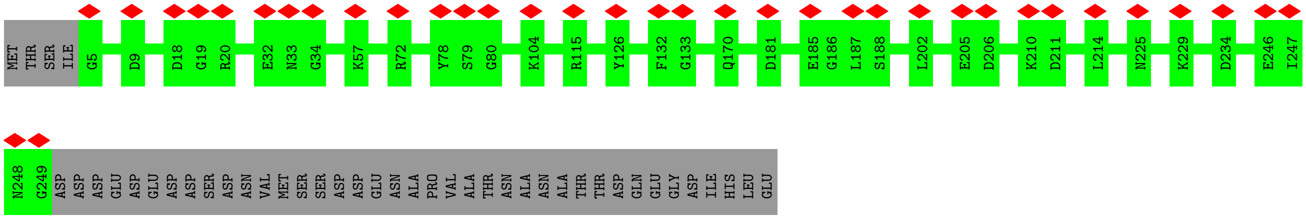
- Molecule 6: Probable proteasome subunit alpha type-7

Chain k:



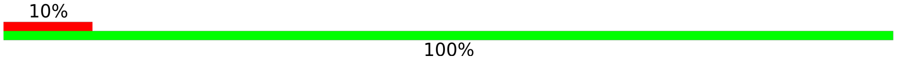
- Molecule 6: Probable proteasome subunit alpha type-7

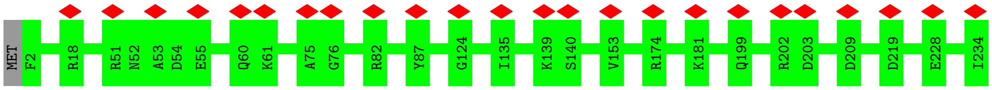
Chain G:



- Molecule 7: Proteasome subunit alpha type-6

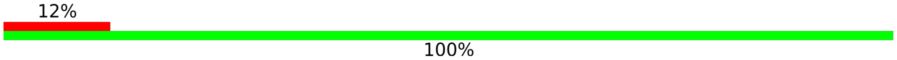
Chain l:

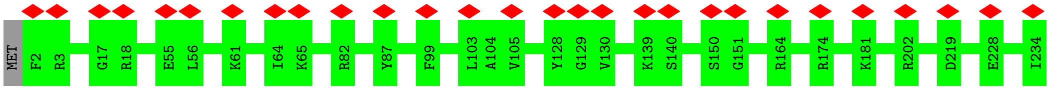




- Molecule 7: Proteasome subunit alpha type-6

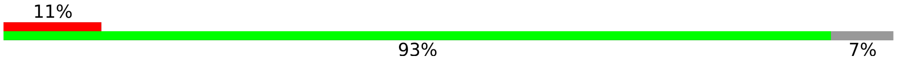
Chain F:

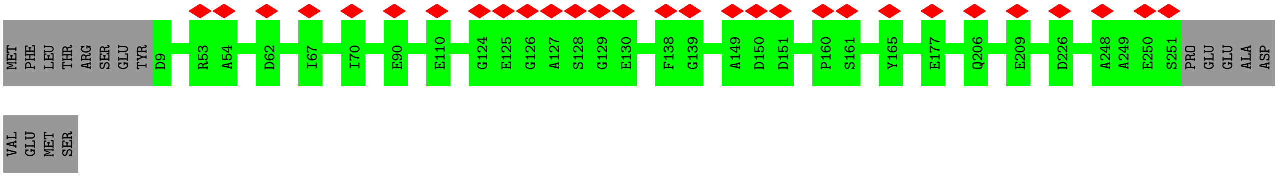




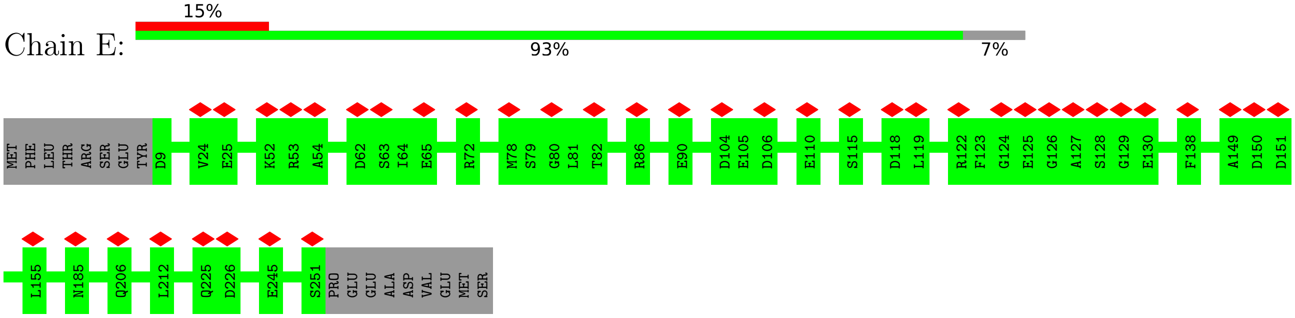
- Molecule 8: Proteasome subunit alpha type-5

Chain m:

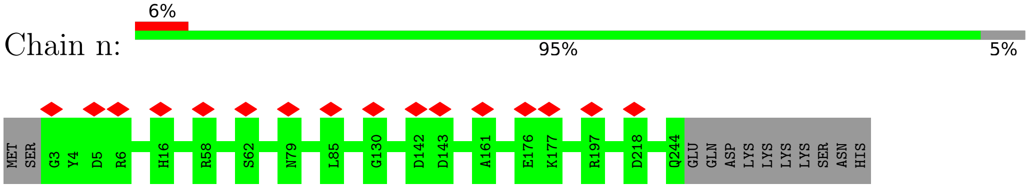




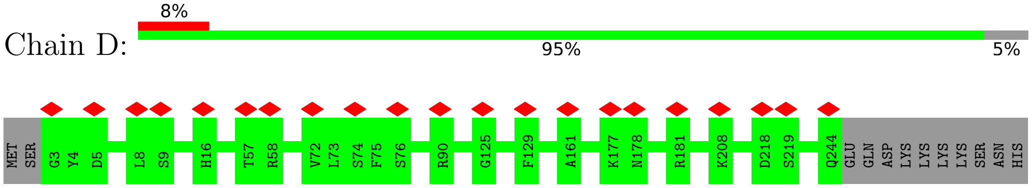
- Molecule 8: Proteasome subunit alpha type-5



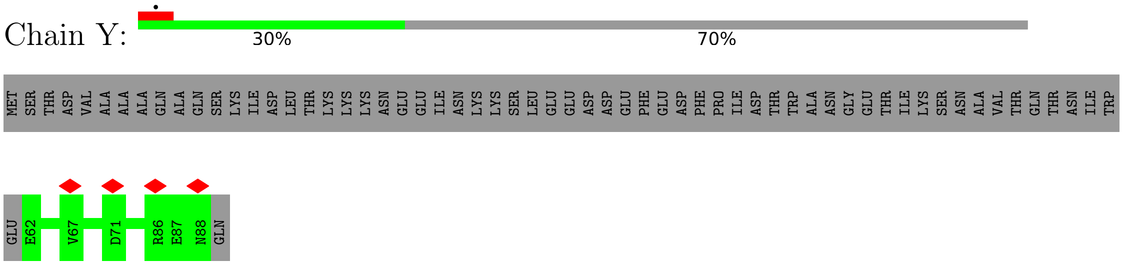
- Molecule 9: Proteasome subunit alpha type-4



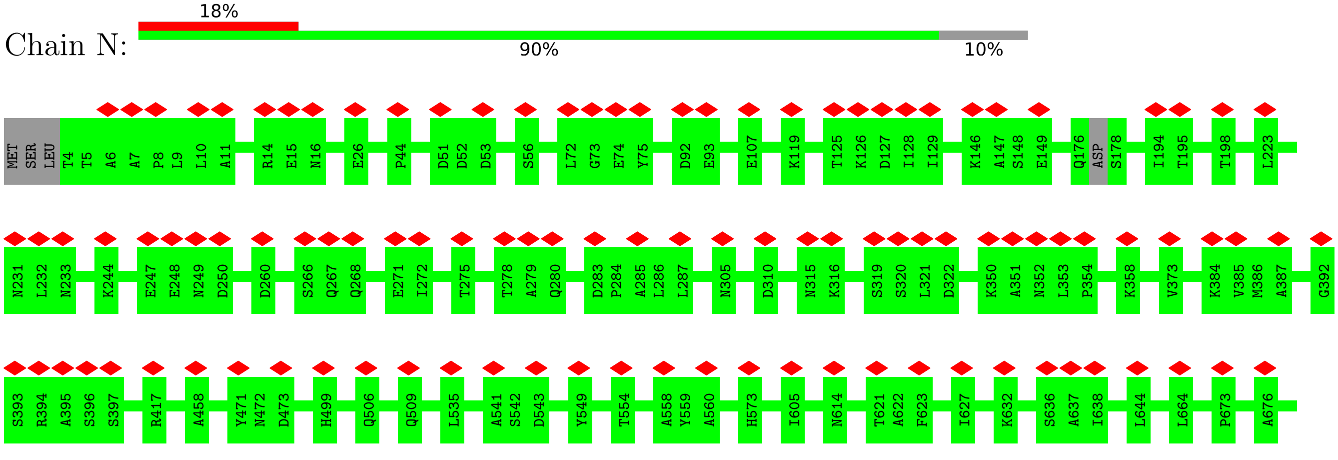
- Molecule 9: Proteasome subunit alpha type-4

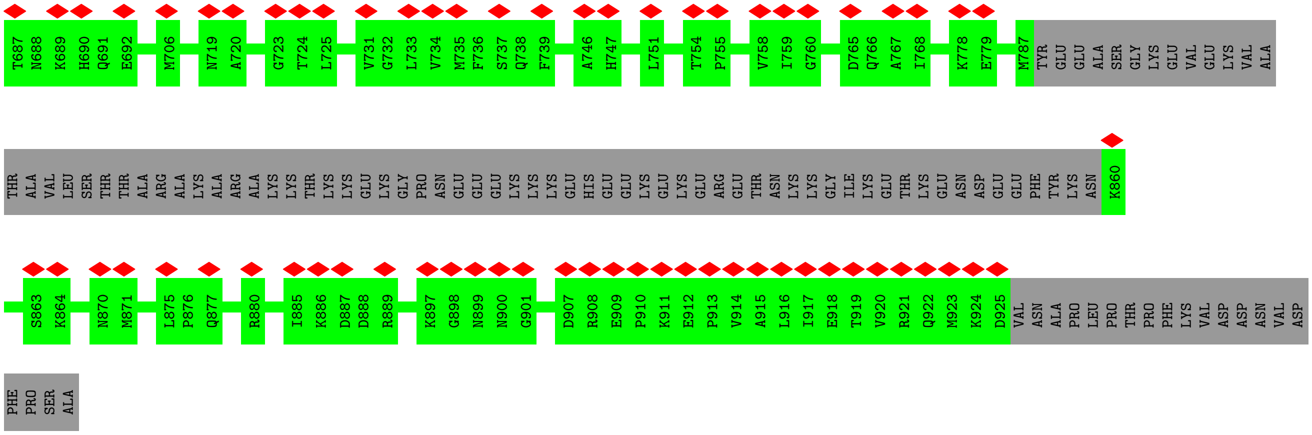


- Molecule 10: 26S proteasome complex subunit SEM1



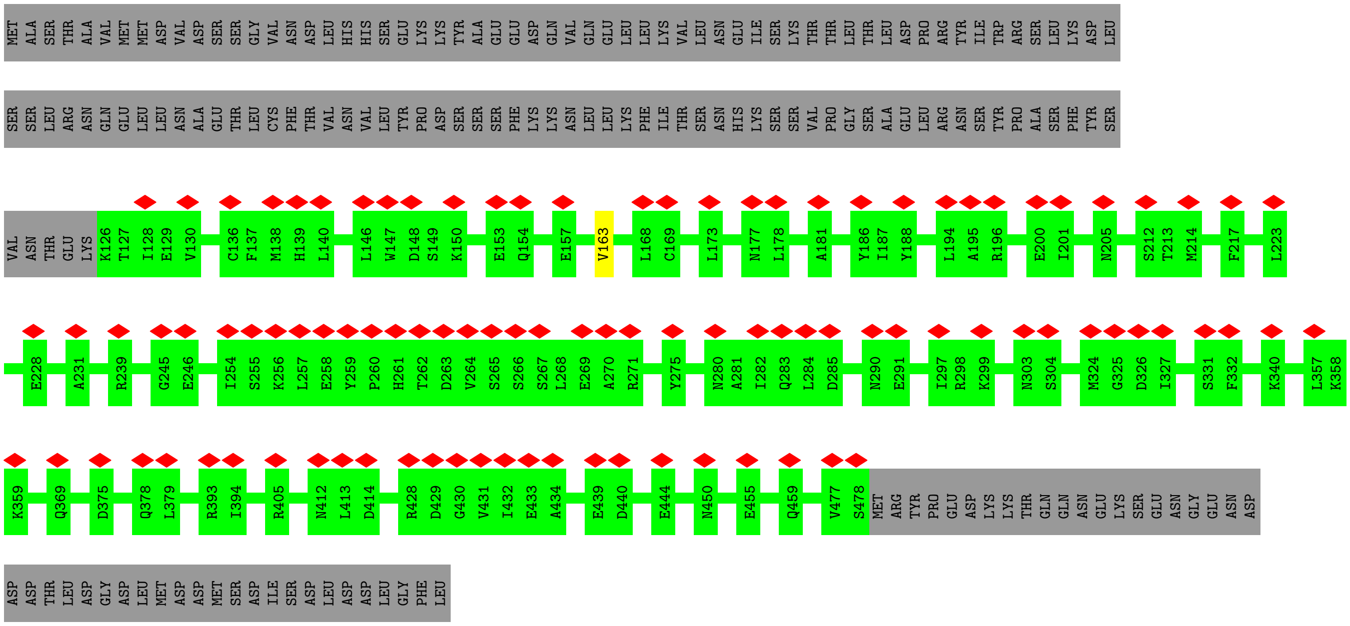
- Molecule 11: 26S proteasome regulatory subunit RPN2





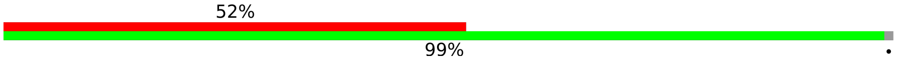
- Molecule 12: 26S proteasome regulatory subunit RPN3

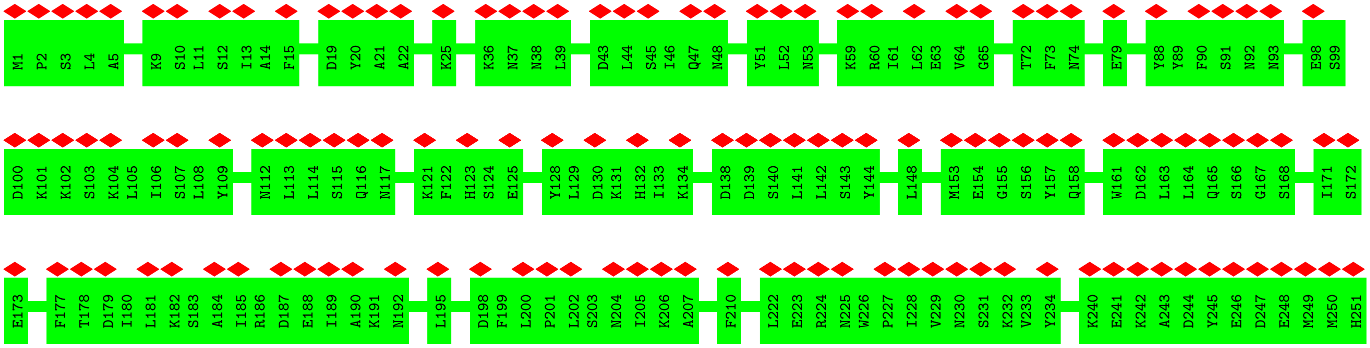
Chain S:

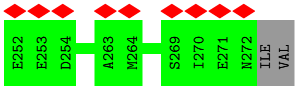


- Molecule 13: 26S proteasome regulatory subunit RPN12

Chain T:

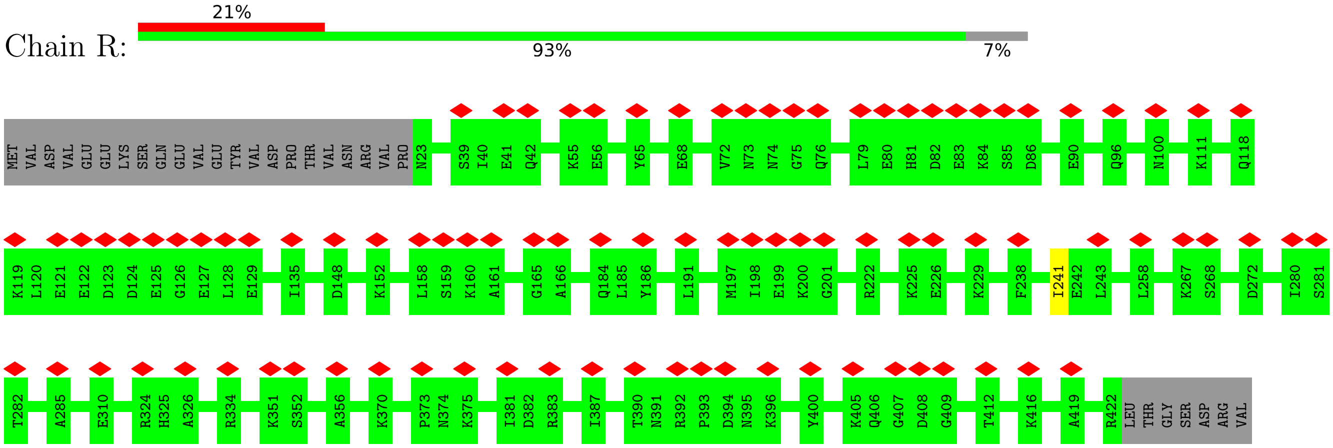






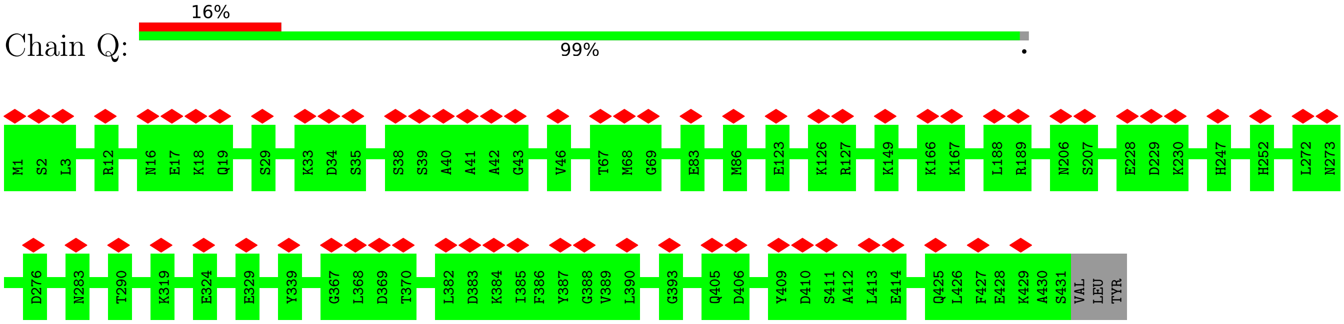
- Molecule 14: 26S proteasome regulatory subunit RPN7

Chain R:



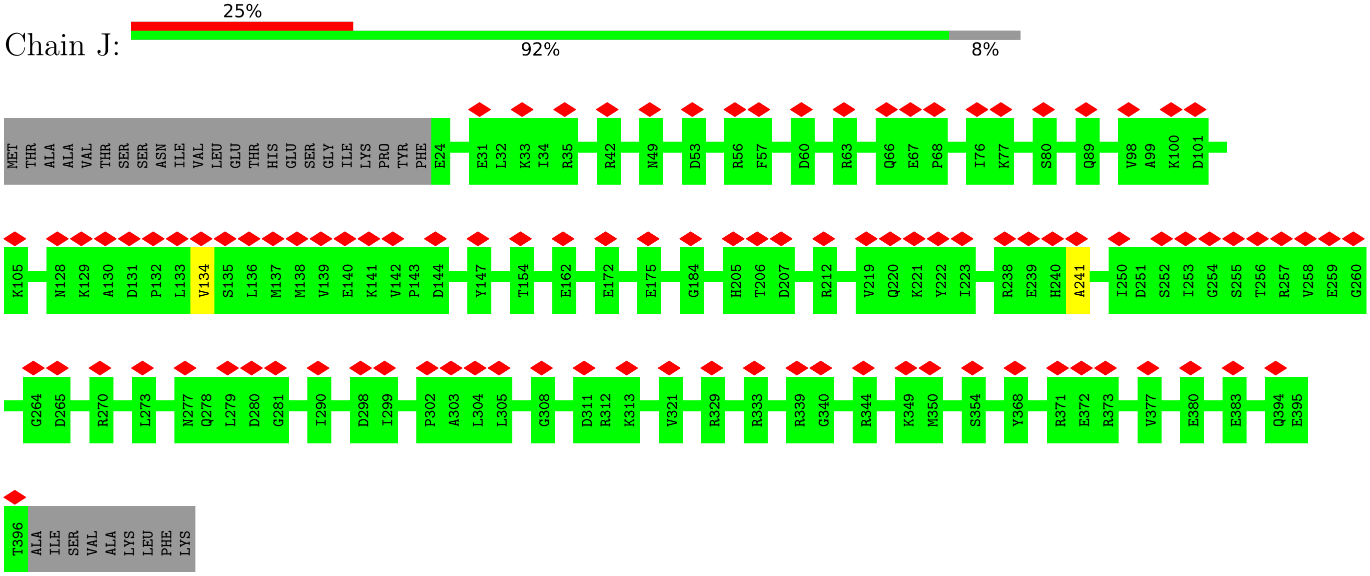
- Molecule 15: 26S proteasome regulatory subunit RPN6

Chain Q:



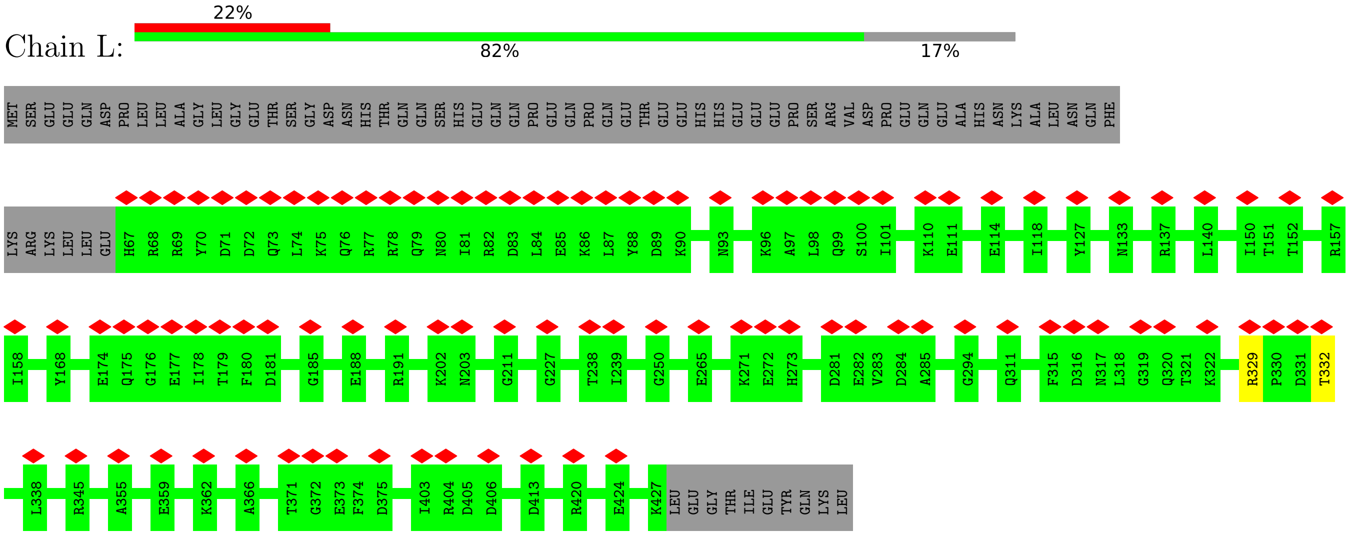
- Molecule 16: 26S protease regulatory subunit 8 homolog

Chain J:



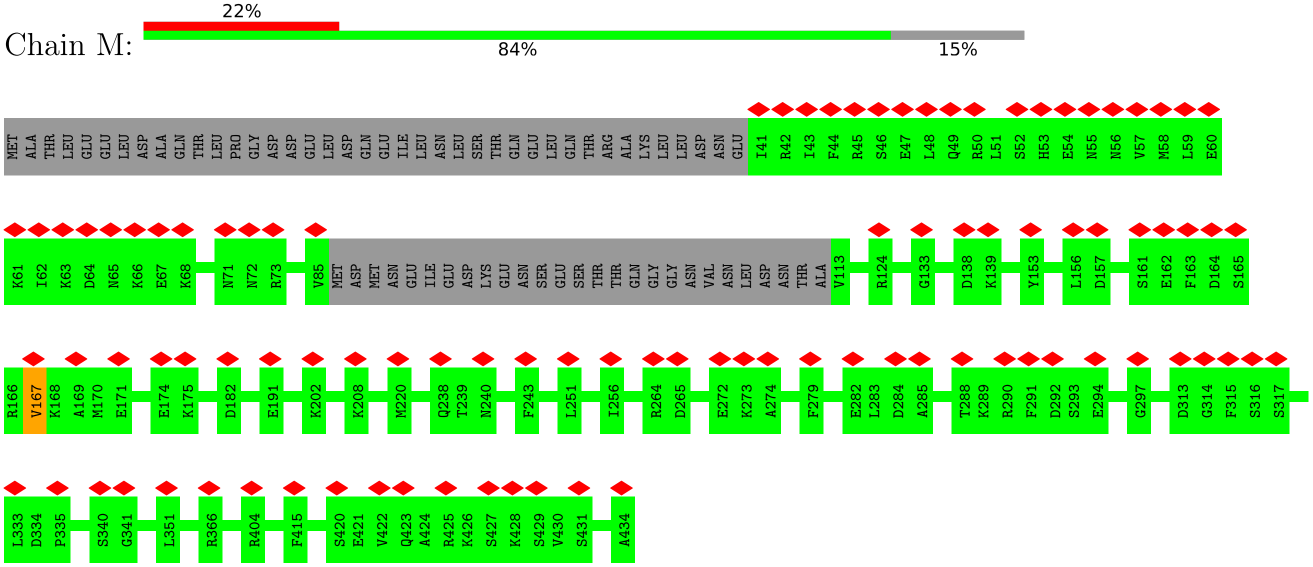
- Molecule 17: 26S protease subunit RPT4

Chain L:



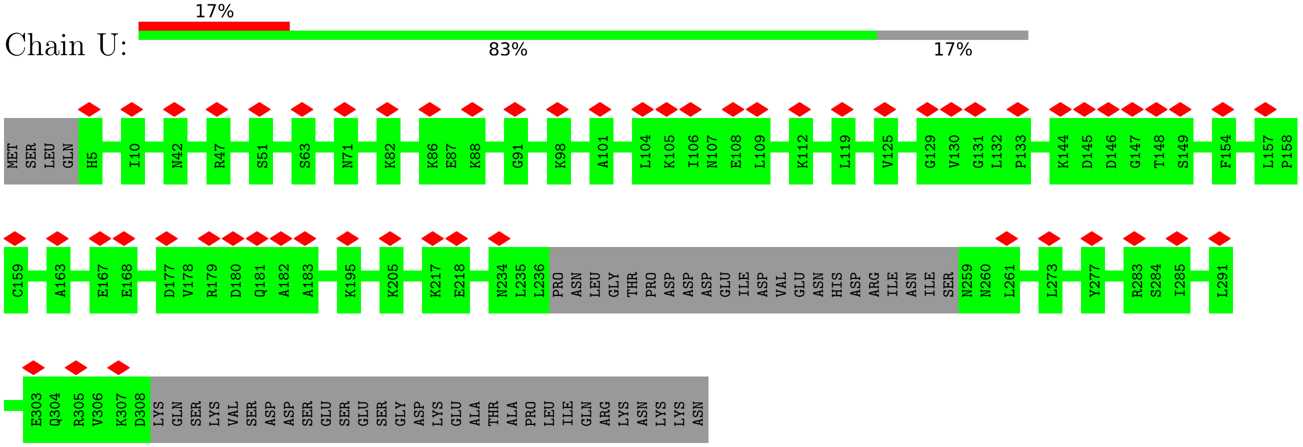
- Molecule 18: 26S protease regulatory subunit 6A

Chain M:

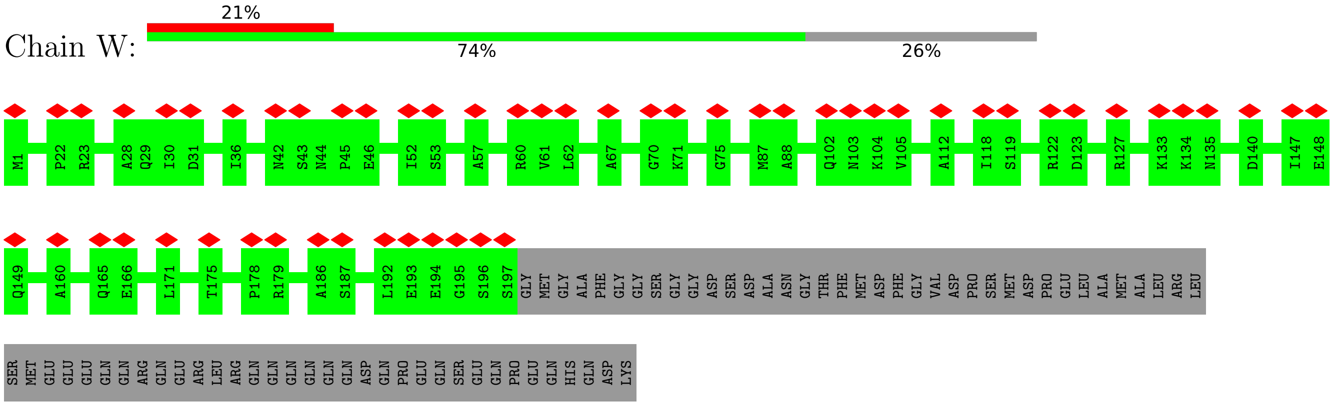


- Molecule 19: 26S proteasome regulatory subunit RPN8

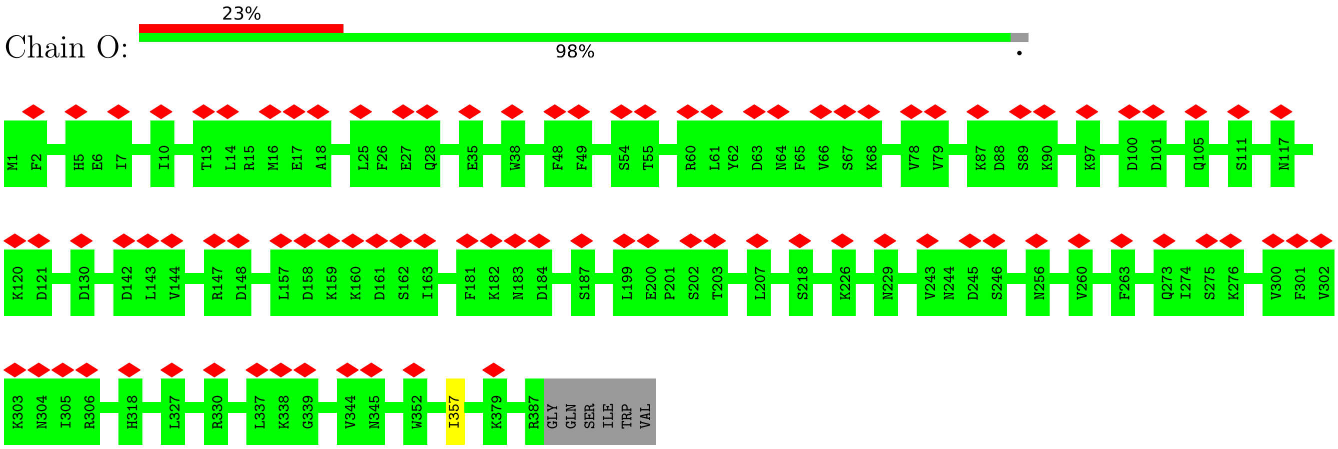
Chain U:



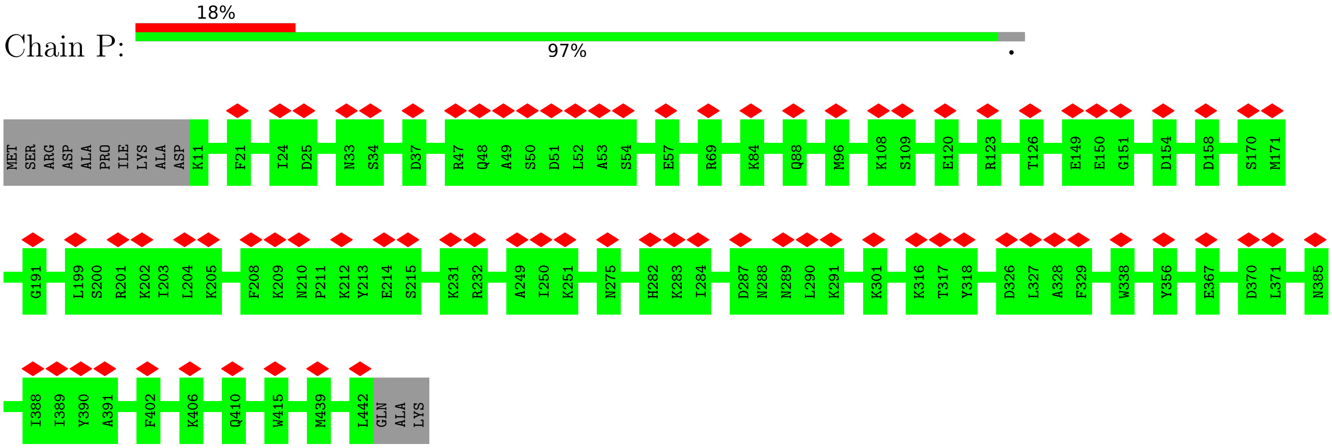
- Molecule 20: 26S proteasome regulatory subunit RPN10



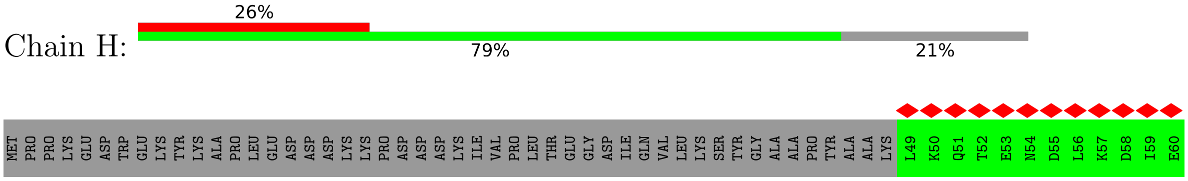
- Molecule 21: 26S proteasome regulatory subunit RPN9

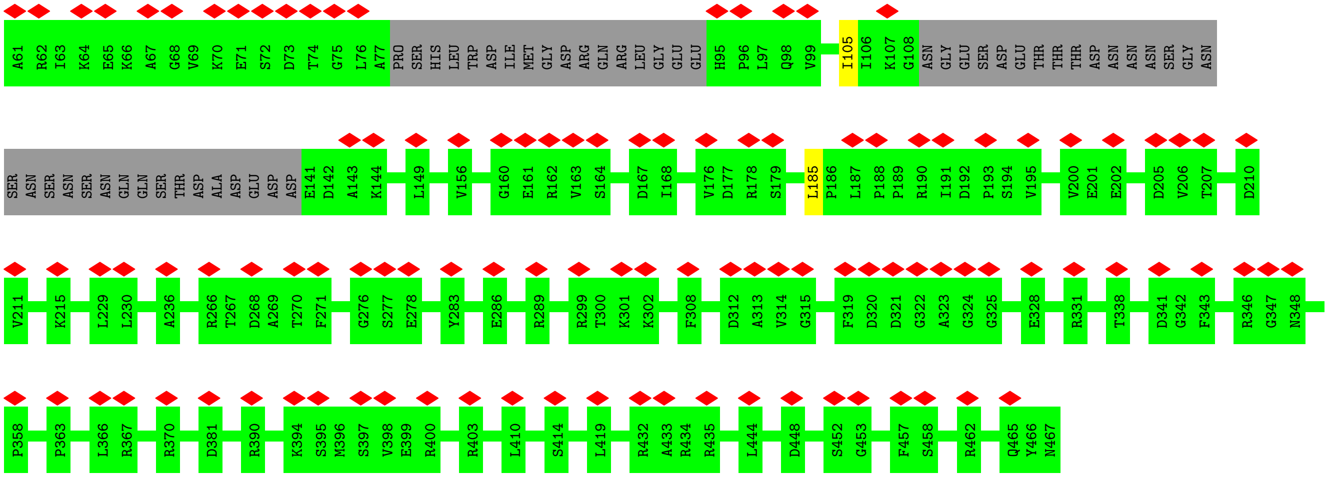


- Molecule 22: 26S proteasome regulatory subunit RPN5

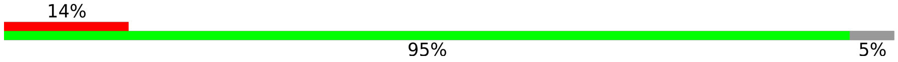


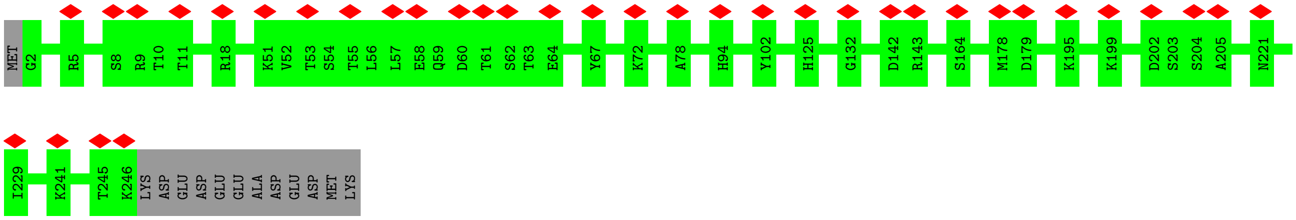
- Molecule 23: 26S protease regulatory subunit 7 homolog



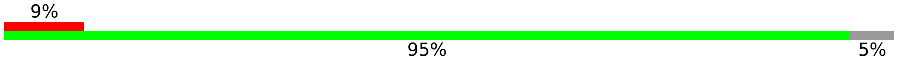


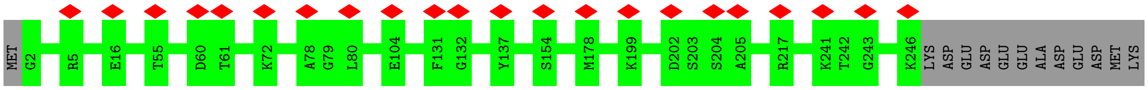
- Molecule 24: Proteasome subunit alpha type-3

Chain C:


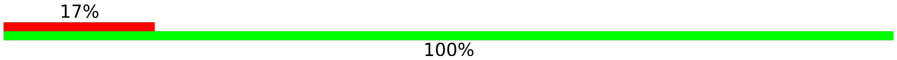


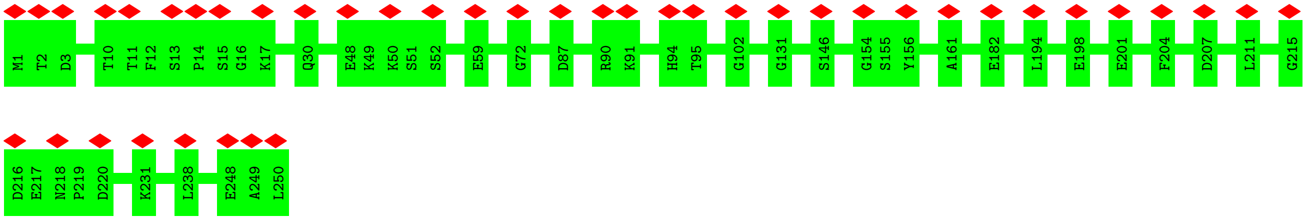
- Molecule 24: Proteasome subunit alpha type-3

Chain d:


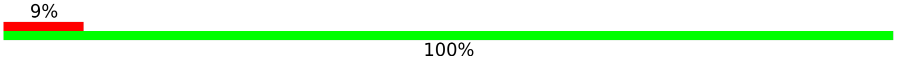


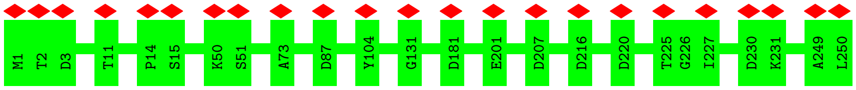
- Molecule 25: Proteasome subunit alpha type-2

Chain B:


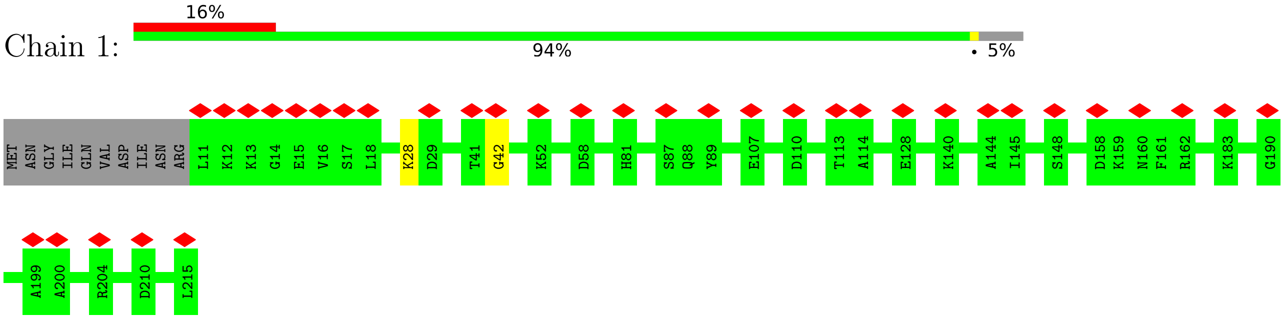


- Molecule 25: Proteasome subunit alpha type-2

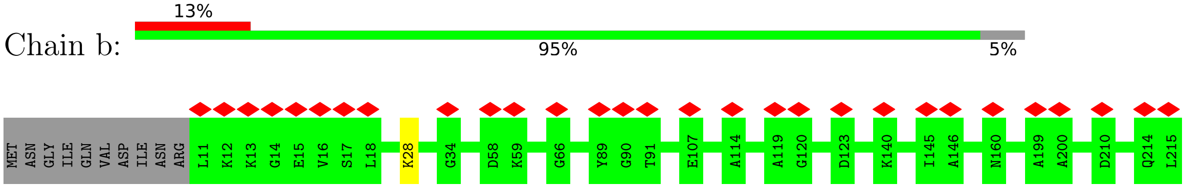
Chain j:




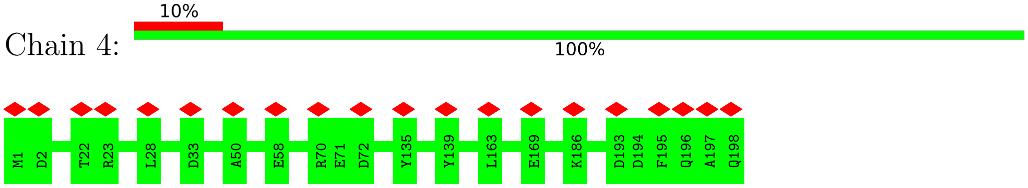
- Molecule 26: Proteasome subunit beta type-1



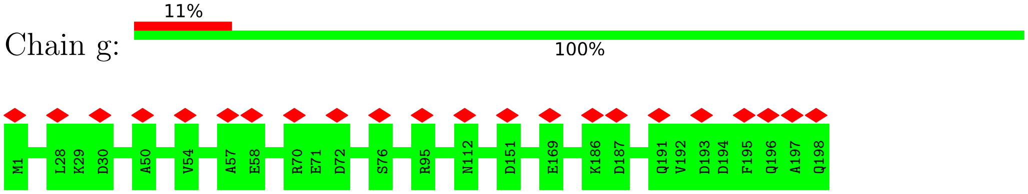
- Molecule 26: Proteasome subunit beta type-1



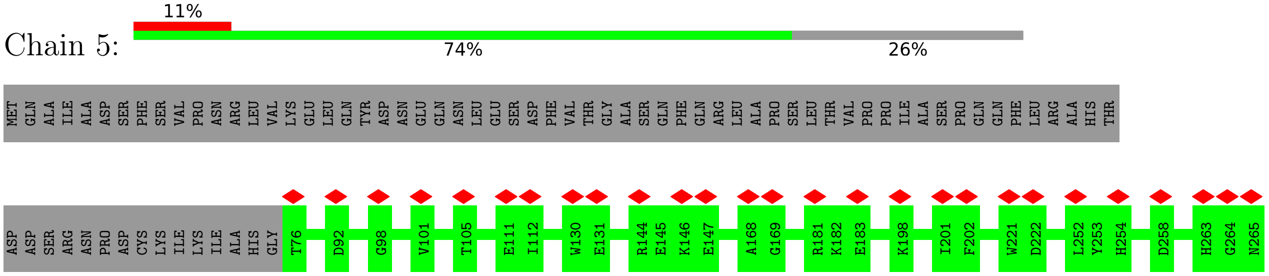
- Molecule 27: Proteasome subunit beta type-4

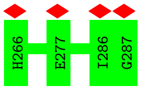


- Molecule 27: Proteasome subunit beta type-4

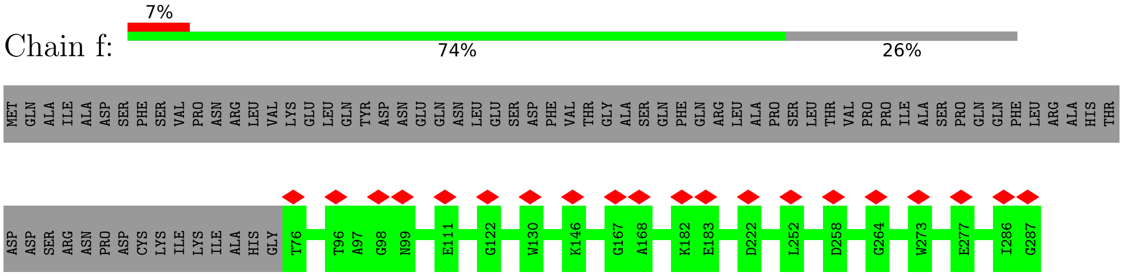


- Molecule 28: Proteasome subunit beta type-5

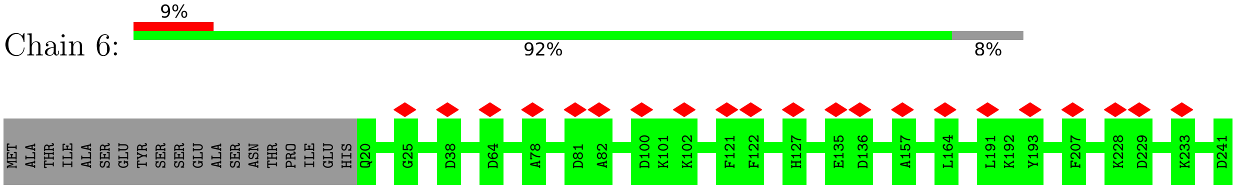




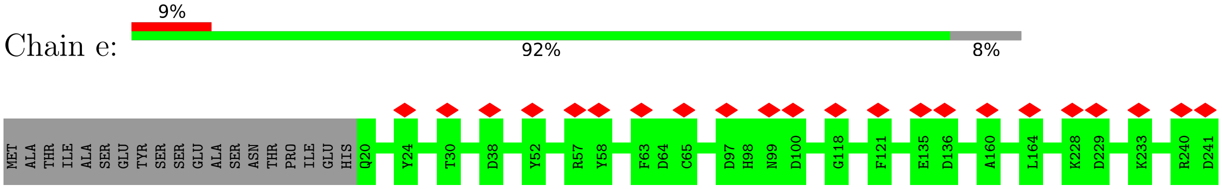
- Molecule 28: Proteasome subunit beta type-5



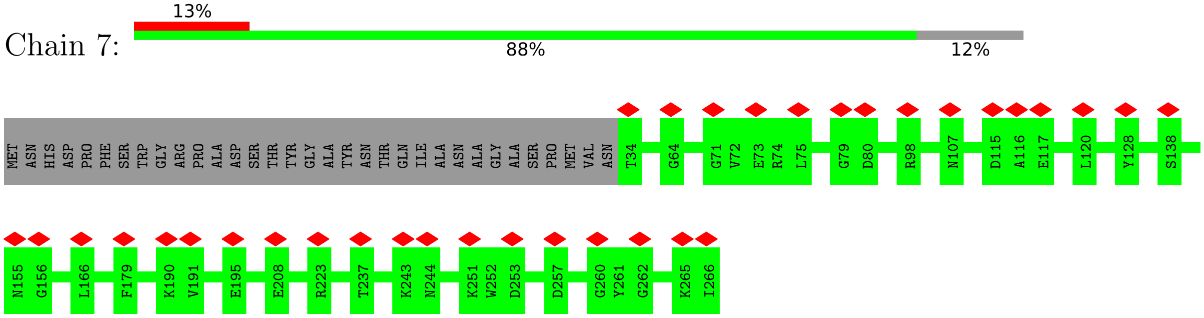
- Molecule 29: Proteasome subunit beta type-6



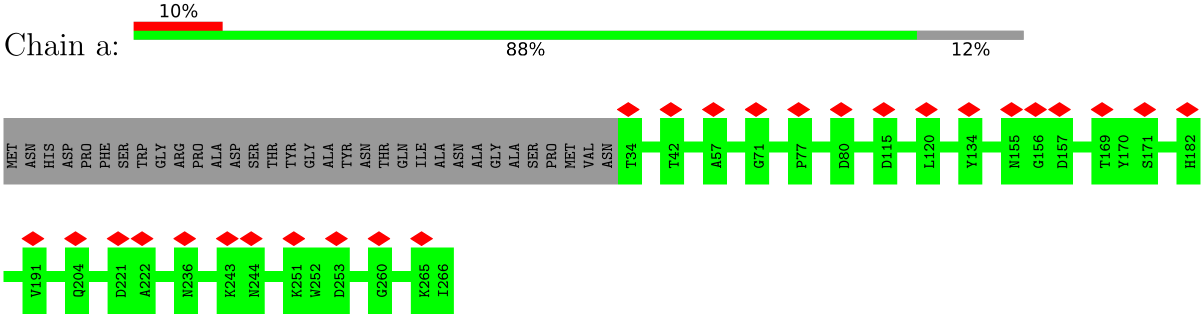
- Molecule 29: Proteasome subunit beta type-6



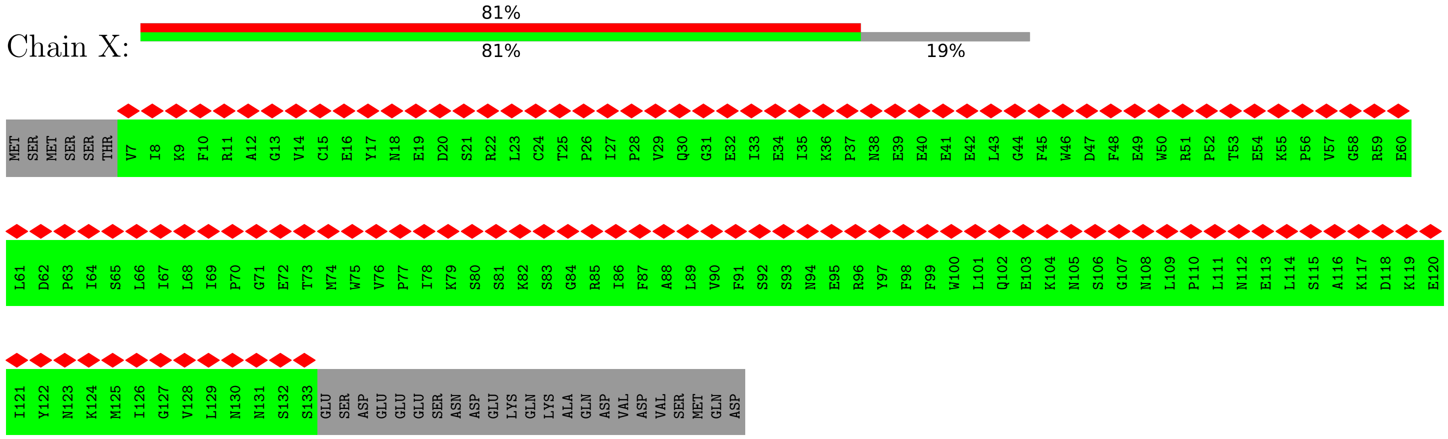
- Molecule 30: Proteasome subunit beta type-7



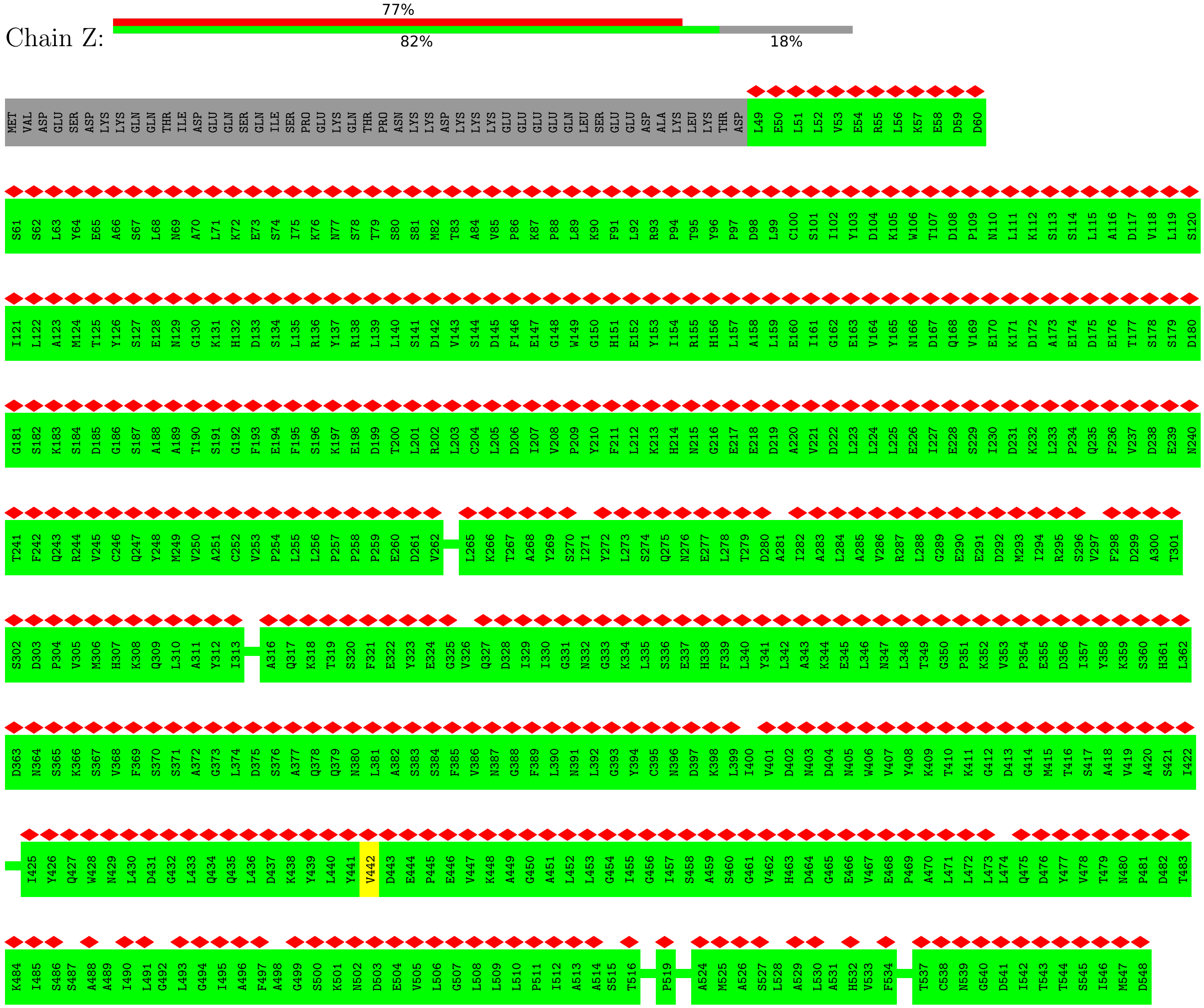
- Molecule 30: Proteasome subunit beta type-7

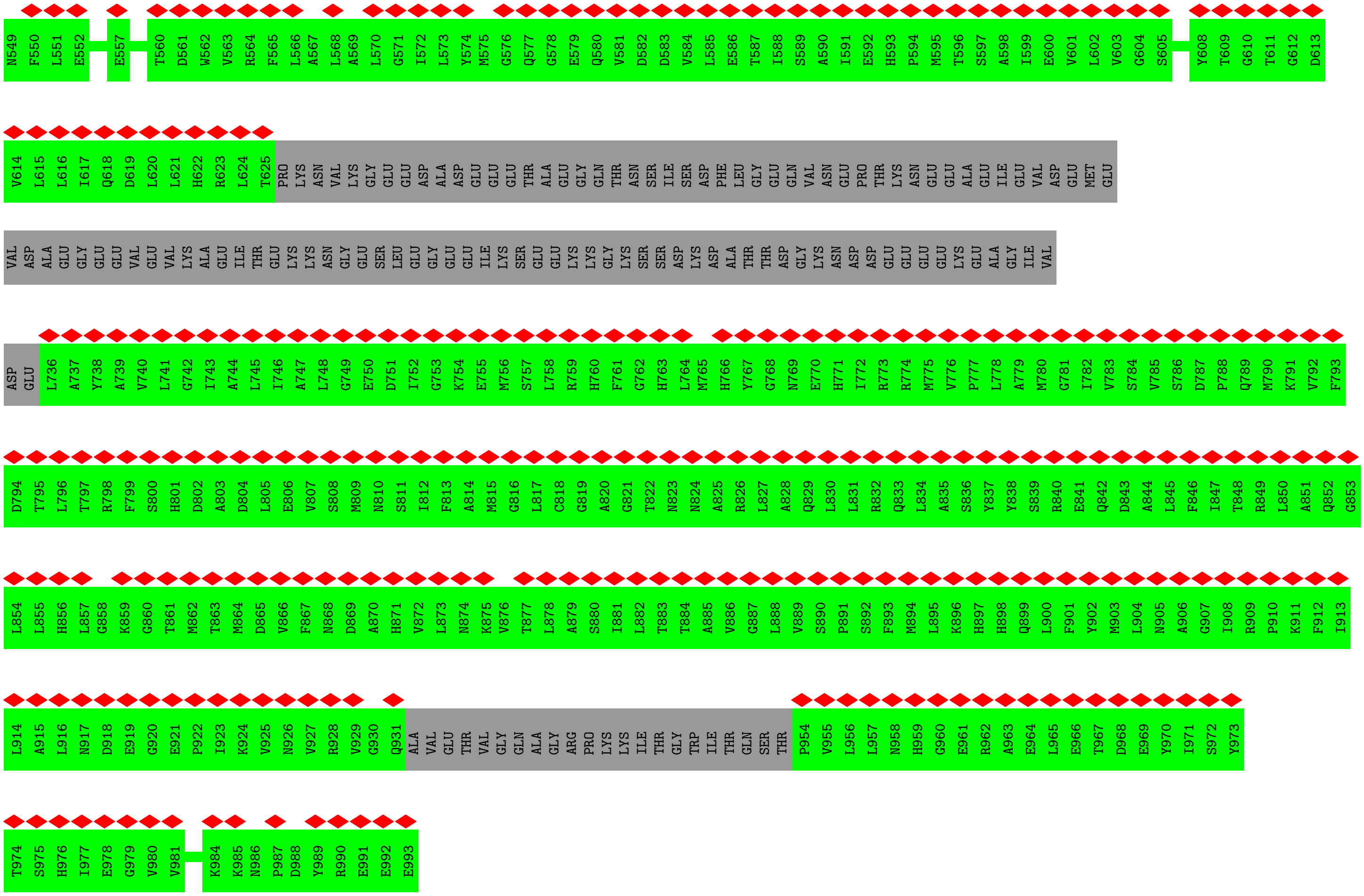


- Molecule 31: 26S proteasome regulatory subunit RPN13



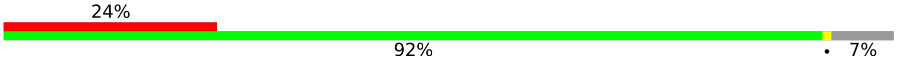
- Molecule 32: 26S proteasome regulatory subunit RPN1

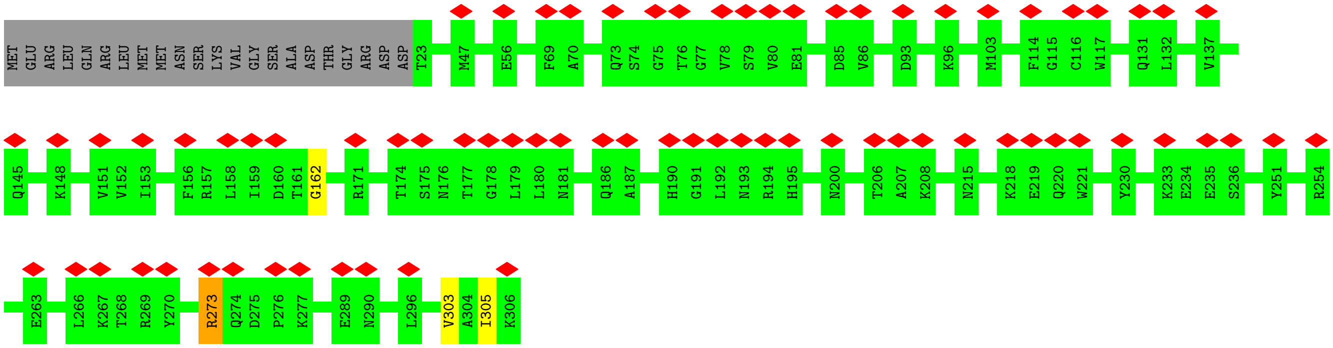




- Molecule 33: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26000	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 ($e^-/\text{Å}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.237	Depositor
Minimum map value	-1.142	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.755	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	I	0.24	0/2860	0.44	0/3856
2	K	0.24	0/3062	0.42	0/4132
3	2	0.23	0/1715	0.41	0/2326
3	i	0.23	0/1715	0.42	0/2326
4	A	0.24	0/1959	0.39	0/2652
4	c	0.24	0/1959	0.39	0/2652
5	3	0.24	0/1611	0.41	0/2174
5	h	0.25	0/1611	0.42	0/2174
6	G	0.24	0/1940	0.38	0/2619
6	k	0.24	0/1940	0.39	0/2619
7	F	0.23	0/1823	0.42	0/2463
7	l	0.23	0/1823	0.41	0/2463
8	E	0.23	0/1892	0.40	0/2549
8	m	0.23	0/1892	0.40	0/2549
9	D	0.23	0/1928	0.41	0/2610
9	n	0.23	0/1928	0.40	0/2610
10	Y	0.21	0/239	0.32	0/322
11	N	0.24	0/6670	0.39	0/9023
12	S	0.23	0/2945	0.37	0/3976
13	T	0.23	0/2279	0.38	0/3077
14	R	0.23	0/3272	0.38	0/4412
15	Q	0.23	0/3527	0.37	0/4748
16	J	0.33	1/2964 (0.0%)	0.40	0/3981
17	L	0.28	1/2896 (0.0%)	0.40	0/3895
18	M	0.23	0/2903	0.41	0/3909
19	U	0.23	0/2287	0.40	0/3087
20	W	0.24	0/1557	0.40	0/2111
21	O	0.23	0/3243	0.38	0/4374
22	P	0.22	0/3599	0.38	0/4854
23	H	0.35	1/2931 (0.0%)	0.46	0/3941
24	C	0.23	0/1943	0.40	0/2629
24	d	0.23	0/1943	0.41	0/2629
25	B	0.24	0/1952	0.41	0/2642
25	j	0.24	0/1952	0.42	0/2642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
26	1	0.23	0/1605	0.44	0/2171
26	b	0.23	0/1603	0.43	0/2168
27	4	0.23	0/1613	0.39	0/2173
27	g	0.23	0/1613	0.41	0/2173
28	5	0.24	0/1681	0.41	0/2274
28	f	0.23	0/1681	0.41	0/2274
29	6	0.24	0/1795	0.40	0/2420
29	e	0.24	0/1795	0.40	0/2420
30	7	0.24	0/1855	0.41	0/2514
30	a	0.24	0/1855	0.42	0/2514
31	X	0.23	0/1058	0.40	0/1432
32	Z	0.23	0/6403	0.41	0/8686
33	V	0.24	0/2271	0.47	0/3064
All	All	0.24	3/107588 (0.0%)	0.40	0/145309

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1
5	h	0	1
18	M	0	1
26	1	0	1
33	V	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	185	LEU	C-N	12.79	1.58	1.34
16	J	241	ALA	C-N	12.54	1.58	1.34
17	L	329	ARG	C-N	8.34	1.50	1.34

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	42	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	I	102	ASN	Peptide
18	M	167	VAL	Peptide
33	V	162	GLY	Peptide
5	h	45	HIS	Peptide

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	I	360/437 (82%)	315 (88%)	44 (12%)	1 (0%)	41	76
2	K	379/428 (89%)	326 (86%)	53 (14%)	0	100	100
3	2	220/261 (84%)	210 (96%)	10 (4%)	0	100	100
3	i	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
4	A	241/252 (96%)	228 (95%)	13 (5%)	0	100	100
4	c	241/252 (96%)	227 (94%)	14 (6%)	0	100	100
5	3	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
5	h	202/205 (98%)	188 (93%)	13 (6%)	1 (0%)	29	69
6	G	243/288 (84%)	235 (97%)	8 (3%)	0	100	100
6	k	243/288 (84%)	233 (96%)	10 (4%)	0	100	100
7	F	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
7	l	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
8	E	241/260 (93%)	226 (94%)	15 (6%)	0	100	100
8	m	241/260 (93%)	227 (94%)	14 (6%)	0	100	100
9	D	240/254 (94%)	222 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	n	240/254 (94%)	226 (94%)	14 (6%)	0	100	100
10	Y	25/89 (28%)	23 (92%)	2 (8%)	0	100	100
11	N	843/945 (89%)	786 (93%)	57 (7%)	0	100	100
12	S	351/523 (67%)	313 (89%)	37 (10%)	1 (0%)	41	76
13	T	270/274 (98%)	231 (86%)	39 (14%)	0	100	100
14	R	398/429 (93%)	357 (90%)	40 (10%)	1 (0%)	41	76
15	Q	429/434 (99%)	393 (92%)	36 (8%)	0	100	100
16	J	371/405 (92%)	335 (90%)	35 (9%)	1 (0%)	41	76
17	L	359/437 (82%)	320 (89%)	38 (11%)	1 (0%)	41	76
18	M	363/434 (84%)	331 (91%)	31 (8%)	1 (0%)	41	76
19	U	278/338 (82%)	260 (94%)	18 (6%)	0	100	100
20	W	195/268 (73%)	182 (93%)	13 (7%)	0	100	100
21	O	385/393 (98%)	341 (89%)	43 (11%)	1 (0%)	41	76
22	P	430/445 (97%)	386 (90%)	44 (10%)	0	100	100
23	H	364/467 (78%)	311 (85%)	52 (14%)	1 (0%)	41	76
24	C	243/258 (94%)	228 (94%)	15 (6%)	0	100	100
24	d	243/258 (94%)	227 (93%)	16 (7%)	0	100	100
25	B	248/250 (99%)	234 (94%)	14 (6%)	0	100	100
25	j	248/250 (99%)	232 (94%)	16 (6%)	0	100	100
26	1	203/215 (94%)	185 (91%)	17 (8%)	1 (0%)	29	69
26	b	203/215 (94%)	184 (91%)	18 (9%)	1 (0%)	29	69
27	4	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
27	g	196/198 (99%)	182 (93%)	14 (7%)	0	100	100
28	5	210/287 (73%)	200 (95%)	10 (5%)	0	100	100
28	f	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
29	6	220/241 (91%)	204 (93%)	16 (7%)	0	100	100
29	e	220/241 (91%)	205 (93%)	15 (7%)	0	100	100
30	7	231/266 (87%)	215 (93%)	16 (7%)	0	100	100
30	a	231/266 (87%)	216 (94%)	15 (6%)	0	100	100
31	X	125/156 (80%)	113 (90%)	12 (10%)	0	100	100
32	Z	807/993 (81%)	716 (89%)	90 (11%)	1 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	V	282/306 (92%)	234 (83%)	45 (16%)	3 (1%)	14	52
All	All	13352/15139 (88%)	12232 (92%)	1105 (8%)	15 (0%)	54	85

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	L	332	THR
5	h	105	VAL
14	R	241	ILE
33	V	305	ILE
16	J	134	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	319/385 (83%)	319 (100%)	0	100	100
2	K	334/374 (89%)	334 (100%)	0	100	100
3	2	181/214 (85%)	181 (100%)	0	100	100
3	i	181/214 (85%)	181 (100%)	0	100	100
4	A	207/210 (99%)	207 (100%)	0	100	100
4	c	207/210 (99%)	207 (100%)	0	100	100
5	3	172/173 (99%)	172 (100%)	0	100	100
5	h	172/173 (99%)	172 (100%)	0	100	100
6	G	201/239 (84%)	201 (100%)	0	100	100
6	k	201/239 (84%)	201 (100%)	0	100	100
7	F	192/193 (100%)	192 (100%)	0	100	100
7	l	192/193 (100%)	192 (100%)	0	100	100
8	E	199/215 (93%)	199 (100%)	0	100	100
8	m	199/215 (93%)	199 (100%)	0	100	100
9	D	214/226 (95%)	214 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	n	214/226 (95%)	214 (100%)	0	100	100
10	Y	26/81 (32%)	26 (100%)	0	100	100
11	N	713/797 (90%)	713 (100%)	0	100	100
12	S	330/489 (68%)	330 (100%)	0	100	100
13	T	254/256 (99%)	254 (100%)	0	100	100
14	R	351/379 (93%)	351 (100%)	0	100	100
15	Q	388/391 (99%)	388 (100%)	0	100	100
16	J	325/352 (92%)	325 (100%)	0	100	100
17	L	308/377 (82%)	308 (100%)	0	100	100
18	M	315/375 (84%)	315 (100%)	0	100	100
19	U	256/308 (83%)	256 (100%)	0	100	100
20	W	171/230 (74%)	171 (100%)	0	100	100
21	O	363/368 (99%)	363 (100%)	0	100	100
22	P	405/415 (98%)	405 (100%)	0	100	100
23	H	314/399 (79%)	314 (100%)	0	100	100
24	C	204/216 (94%)	204 (100%)	0	100	100
24	d	204/216 (94%)	204 (100%)	0	100	100
25	B	209/209 (100%)	209 (100%)	0	100	100
25	j	209/209 (100%)	209 (100%)	0	100	100
26	1	169/178 (95%)	169 (100%)	0	100	100
26	b	168/178 (94%)	168 (100%)	0	100	100
27	4	175/175 (100%)	175 (100%)	0	100	100
27	g	175/175 (100%)	175 (100%)	0	100	100
28	5	169/235 (72%)	169 (100%)	0	100	100
28	f	169/235 (72%)	169 (100%)	0	100	100
29	6	185/201 (92%)	185 (100%)	0	100	100
29	e	185/201 (92%)	185 (100%)	0	100	100
30	7	199/224 (89%)	199 (100%)	0	100	100
30	a	199/224 (89%)	199 (100%)	0	100	100
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Z	692/850 (81%)	692 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	V	249/268 (93%)	249 (100%)	0	100	100
All	All	11580/13054 (89%)	11580 (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. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
30	a	36	GLN
29	e	89	ASN
14	R	397	ASN
14	R	378	ASN
29	e	171	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

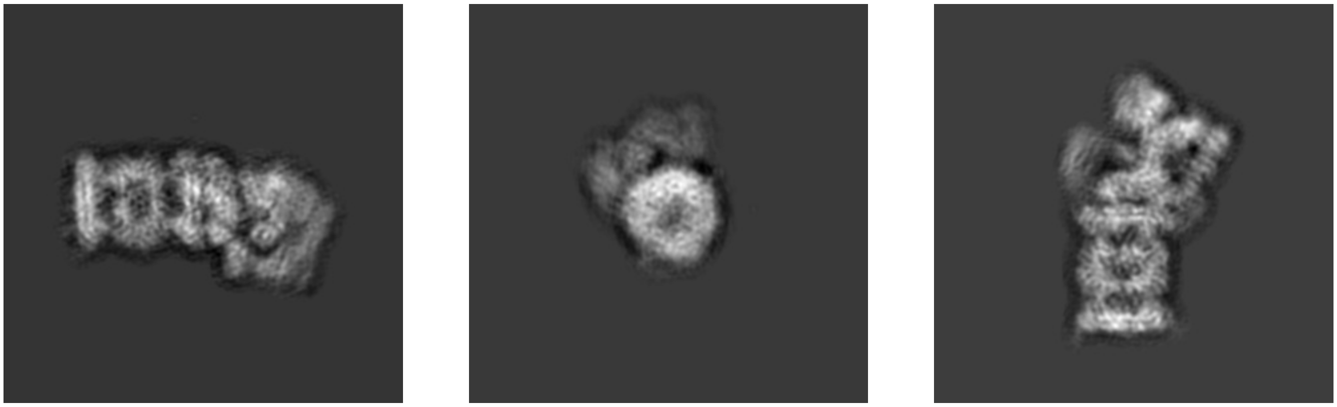
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-6693. 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

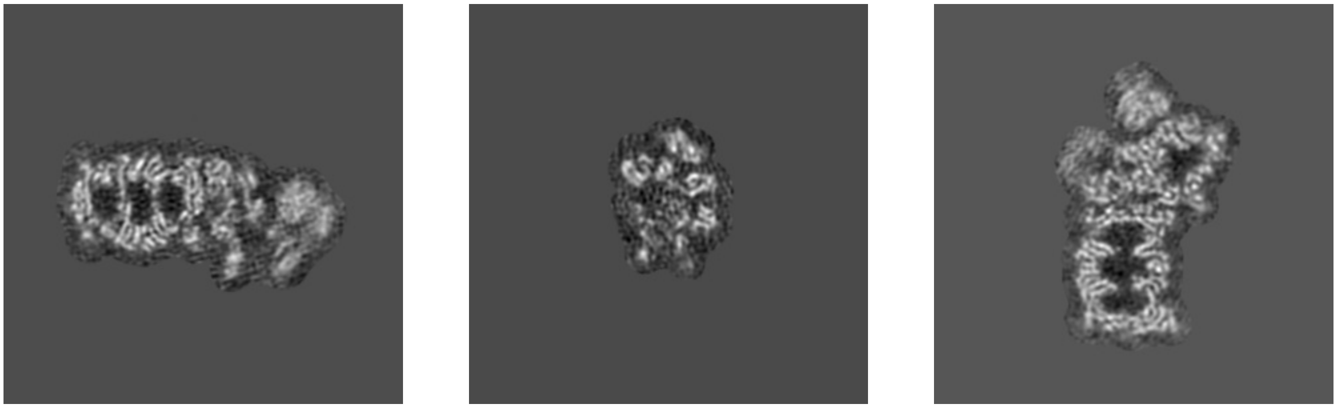


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

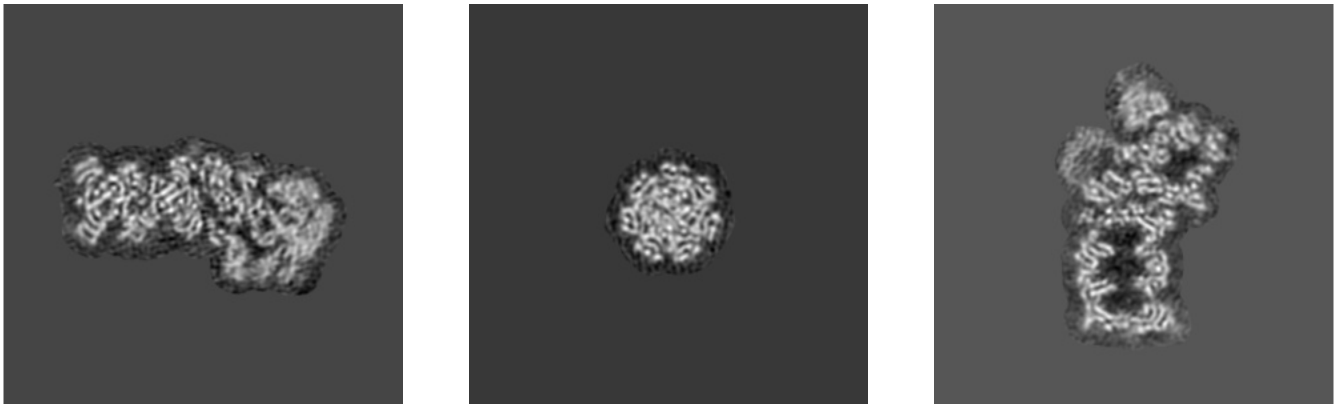


X Index: 180 Y Index: 180 Z Index: 180

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

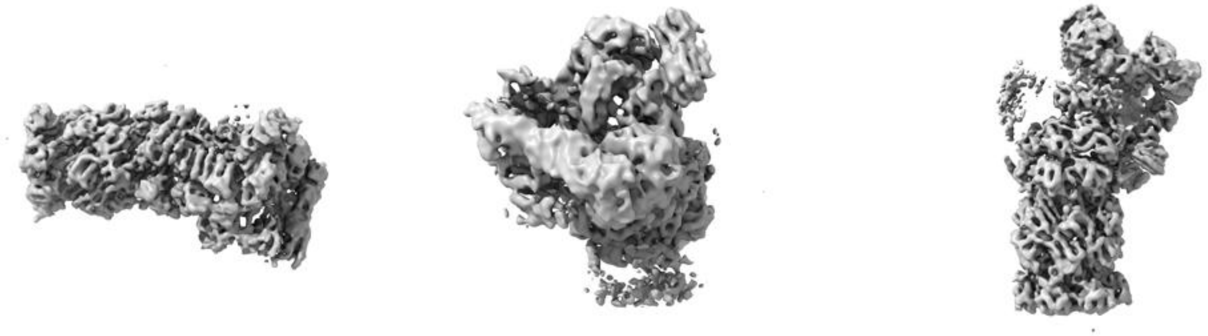


X Index: 192 Y Index: 77 Z Index: 182

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.755. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

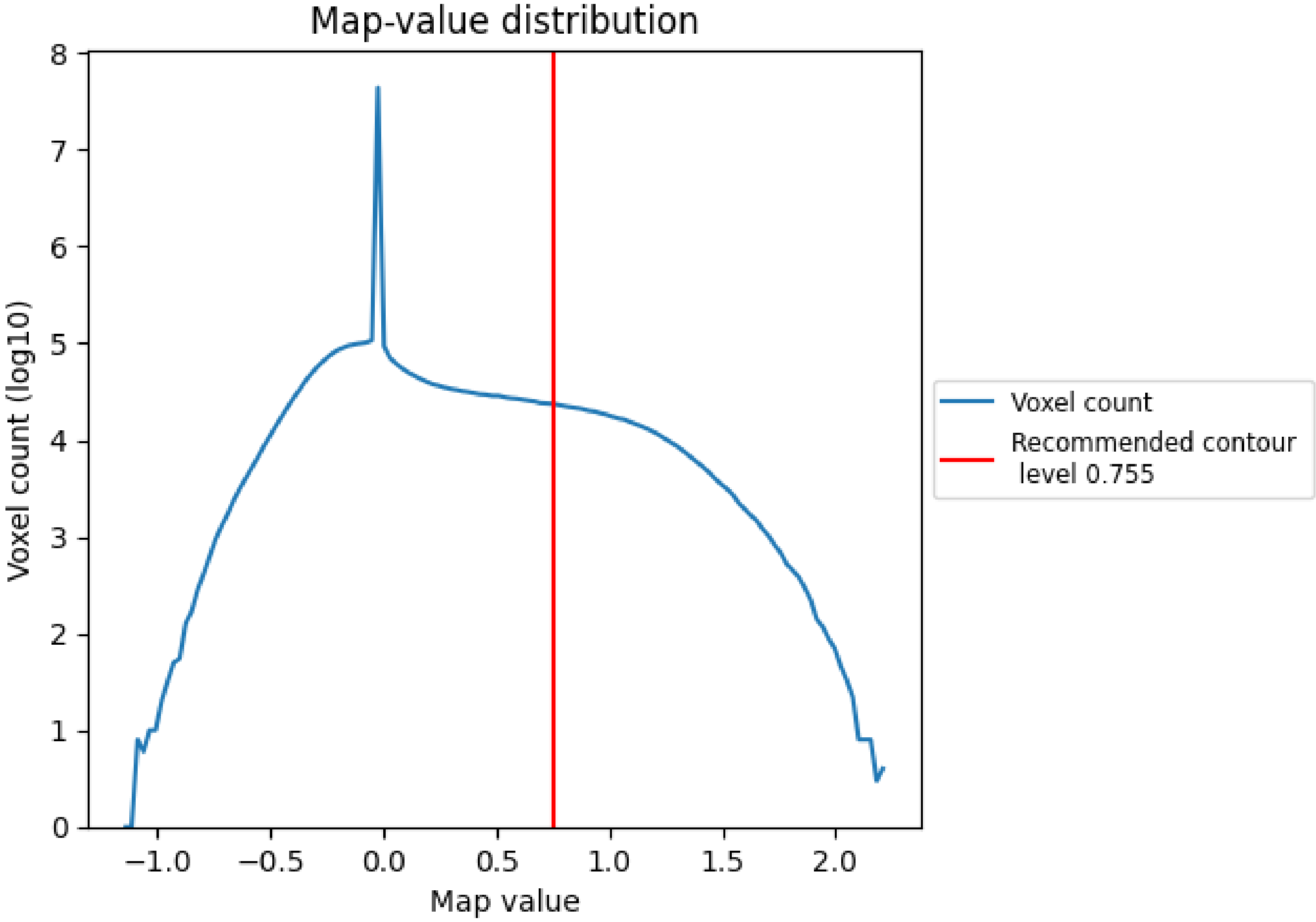
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

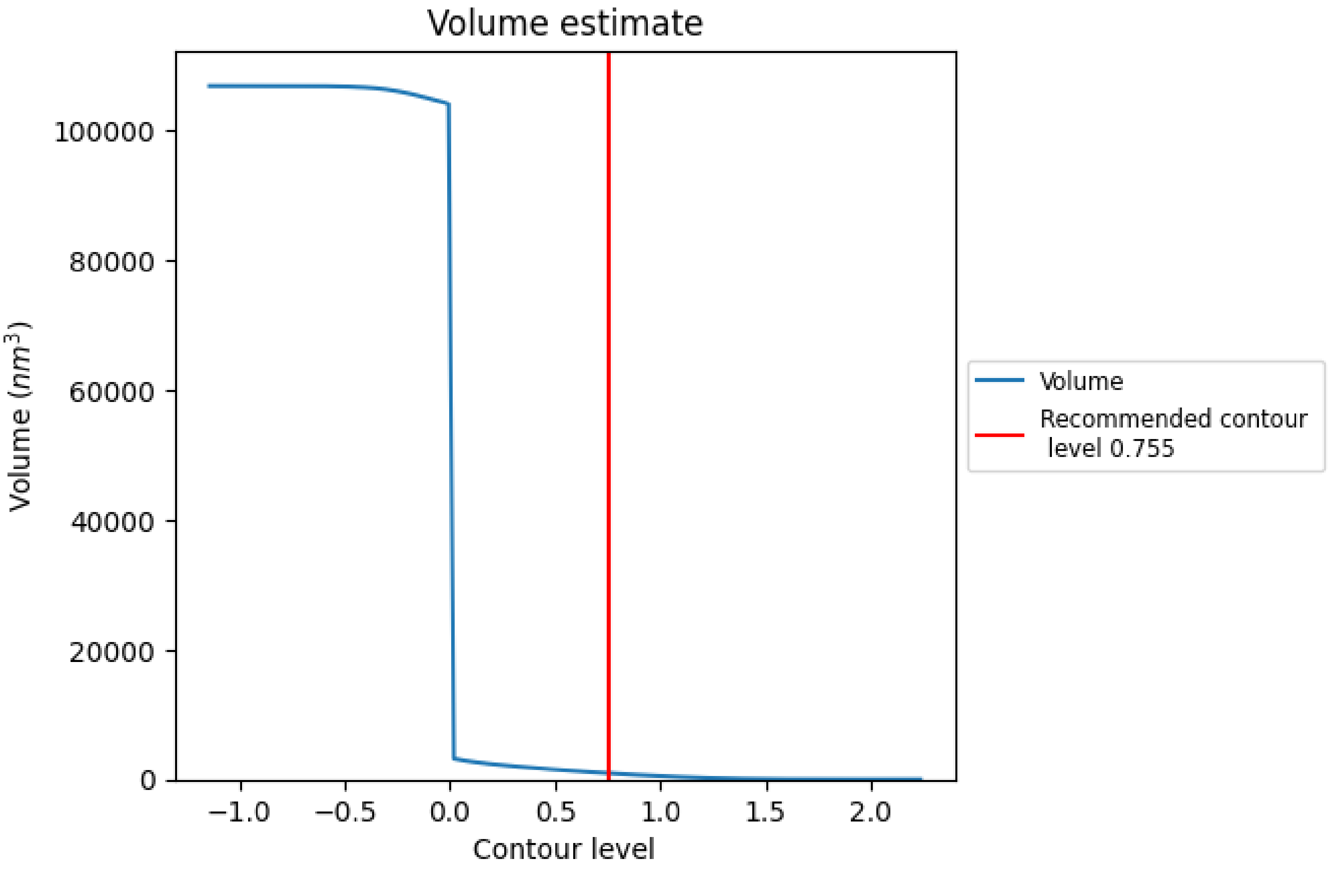
This section contains the results of statistical analysis of the map.

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.

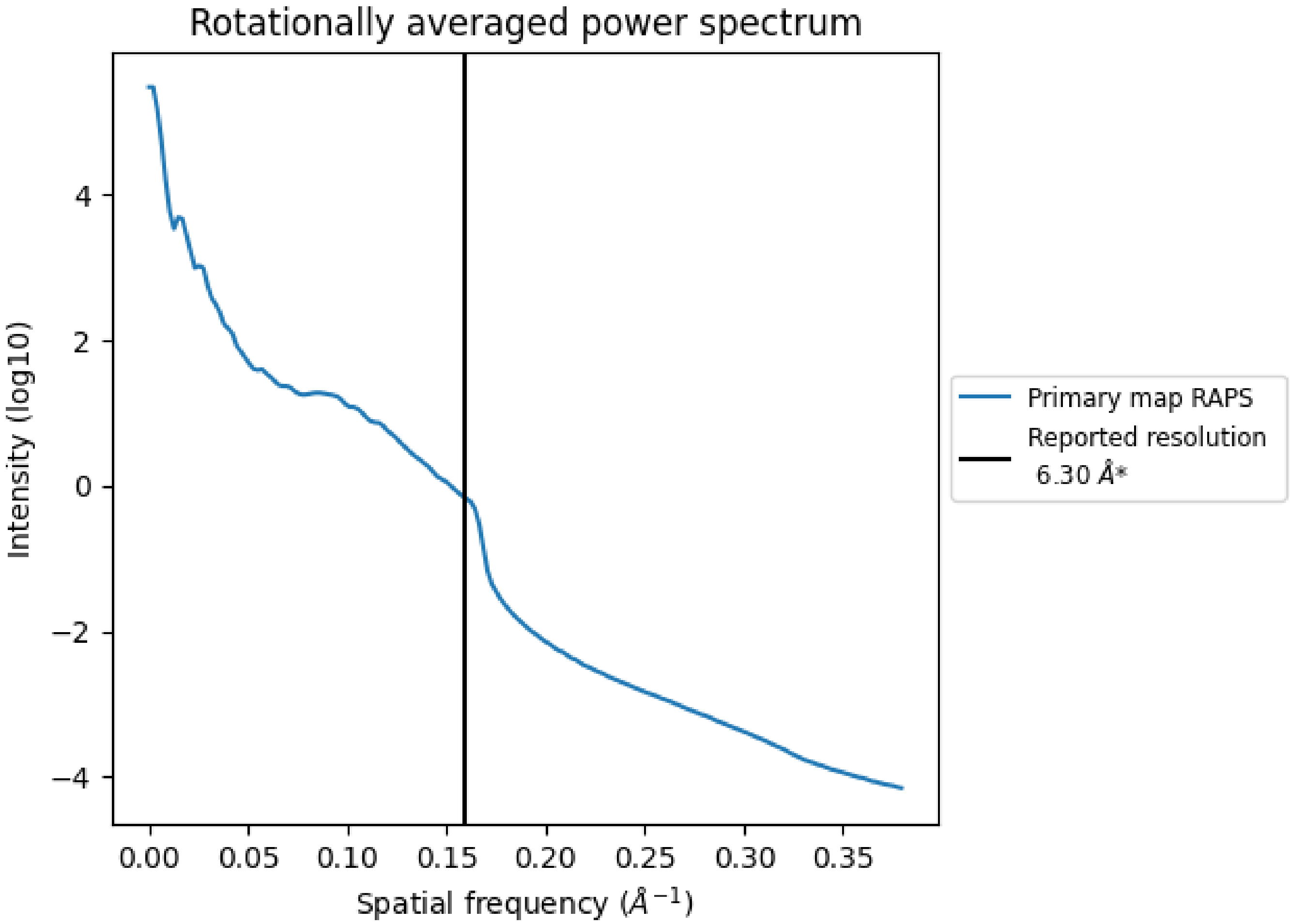
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 959 nm^3; this corresponds to an approximate mass of 866 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.159 Å^{-1}

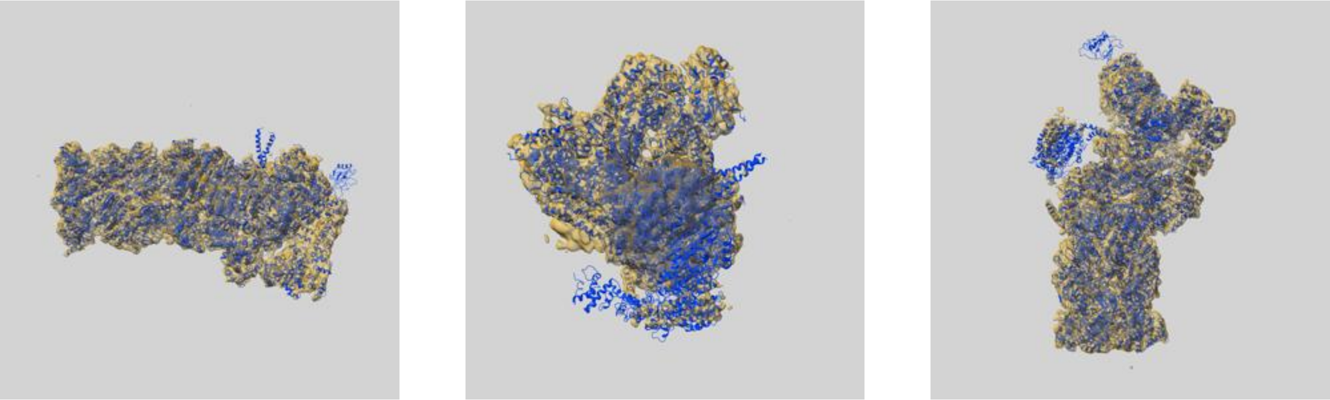
8 Fourier-Shell correlation ⓘ

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-6693 and PDB model 5WVI. Per-residue inclusion information can be found in section 3 on page 11.

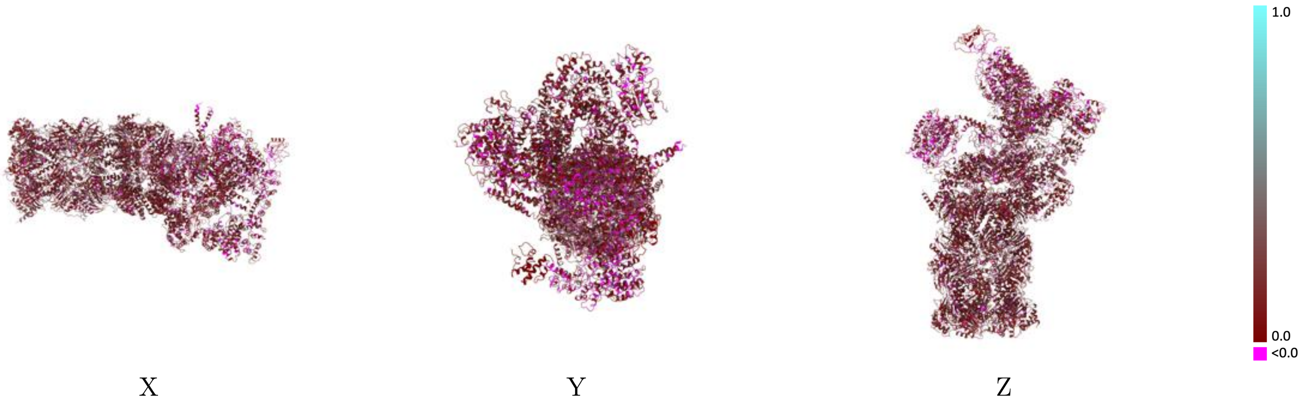
9.1 Map-model overlay ⓘ



X Y Z

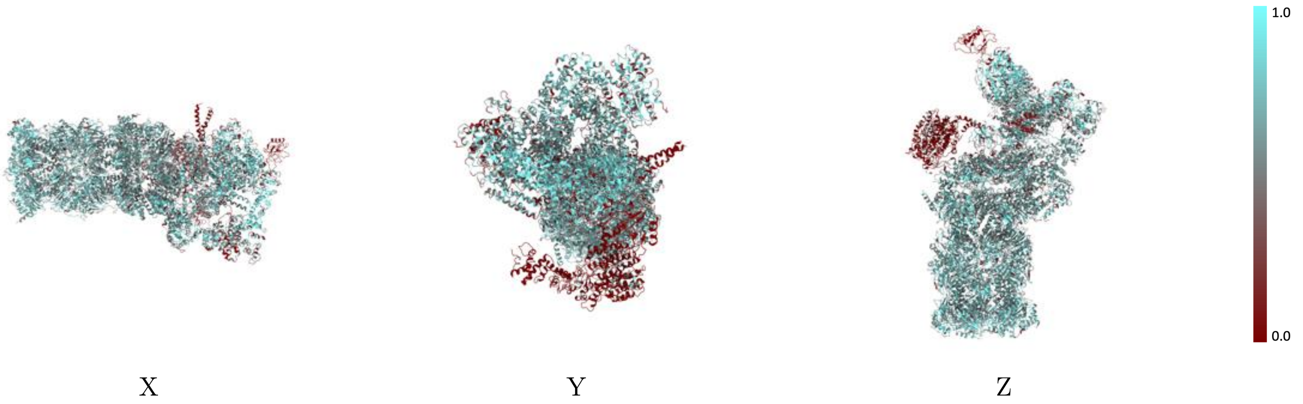
The images above show the 3D surface view of the map at the recommended contour level 0.755 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



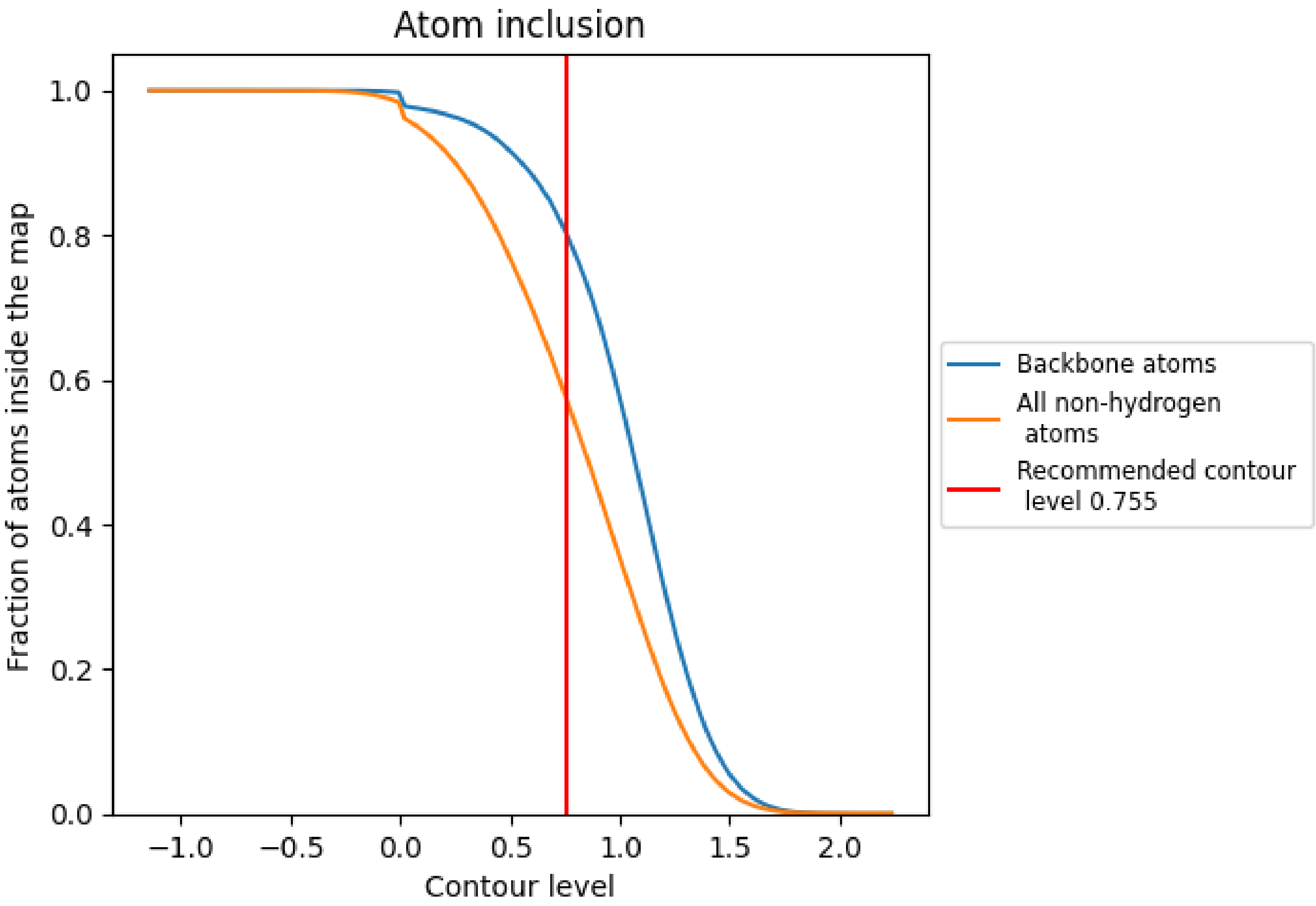
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.755).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 57% 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 (0.755) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5748	0.1400
1	0.6150	0.1510
2	0.6522	0.1760
3	0.6420	0.1510
4	0.6488	0.1670
5	0.6426	0.1550
6	0.6458	0.1600
7	0.6290	0.1730
A	0.6069	0.1720
B	0.5830	0.1580
C	0.6191	0.1490
D	0.6505	0.1610
E	0.6188	0.1520
F	0.6276	0.1530
G	0.6112	0.1600
H	0.5323	0.1330
I	0.5359	0.1430
J	0.5497	0.1370
K	0.5556	0.1460
L	0.5418	0.1380
M	0.5482	0.1460
N	0.6806	0.1050
O	0.6004	0.1270
P	0.5956	0.1430
Q	0.6192	0.1520
R	0.6012	0.1280
S	0.5632	0.1330
T	0.3939	0.1160
U	0.6130	0.1370
V	0.5800	0.1280
W	0.6058	0.1200
X	0.0000	0.0040
Y	0.5826	0.1600
Z	0.0598	0.0640
a	0.6346	0.1700

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Chain	Atom inclusion	Q-score
b	0.6300	0.1500
c	0.6812	0.1640
d	0.6784	0.1490
e	0.6684	0.1670
f	0.6681	0.1560
g	0.6534	0.1580
h	0.6710	0.1500
i	0.6715	0.1860
j	0.6743	0.1650
k	0.6658	0.1550
l	0.6720	0.1540
m	0.6672	0.1530
n	0.6877	0.1530