



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:08 AM UTC

PDB ID : 9SZT / pdb_00009szt
EMDB ID : EMD-52193
Title : Co-chaperone Bag1-bound human 26S proteasome in SBAG1.2 state
Authors : Cheng, T.C.; Sakata, E.; Muntaner, J.; Maestro-Lopez, M.; Cuellar, J.; Valpuesta, J.M.
Deposited on : 2025-10-15
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

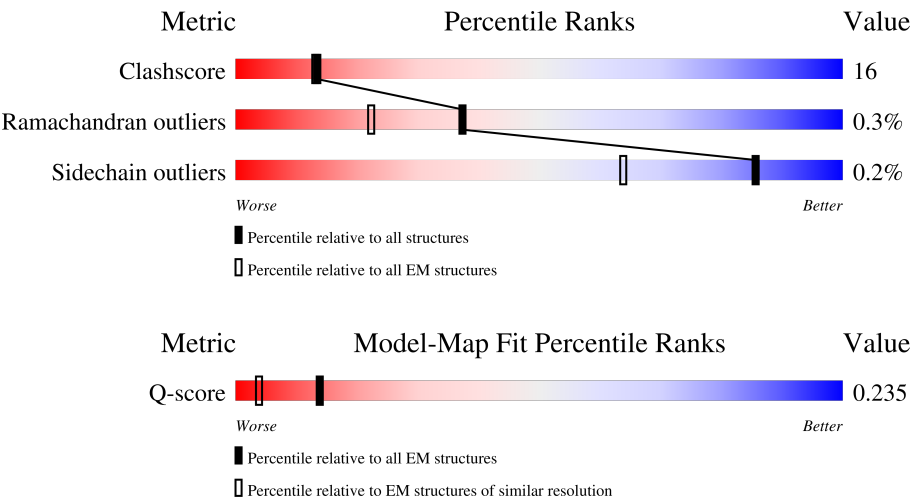
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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.



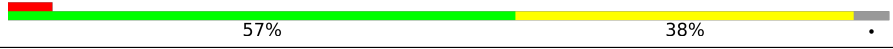
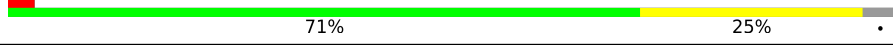
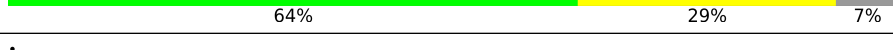
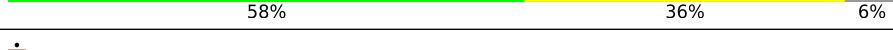
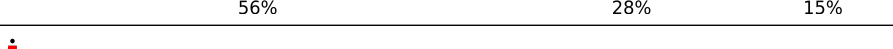
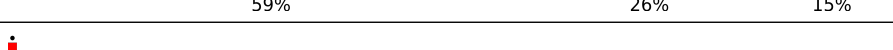
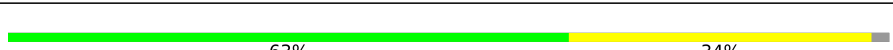
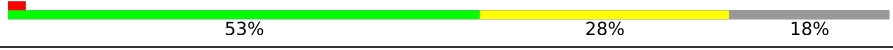
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	246	65%30%.
1	g	246	65%34%.
2	H	234	59%37%..
2	h	234	69%30%.

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Mol	Chain	Length	Quality of chain
3	I	261	
3	i	261	
4	J	248	
4	j	248	
5	L	269	
5	l	269	
6	M	255	
6	m	255	
7	N	239	
7	n	239	
8	O	277	
8	o	277	
9	P	205	
9	p	205	
10	Q	201	
10	q	201	
11	R	263	
11	r	263	
12	S	241	
12	s	241	
13	T	264	
13	t	264	
14	K	241	
14	k	241	
15	f	908	

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Mol	Chain	Length	Quality of chain
16	x	230	
17	a	376	
18	b	377	
19	c	310	
20	d	350	
21	e	70	
22	U	953	
23	V	534	
24	X	422	
25	Y	389	
26	Z	324	
27	W	456	
28	A	433	
29	B	440	
30	C	398	
31	D	418	
32	E	403	
33	F	439	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 104201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	237	Total	C	N	O	S	0	0
			1841	1168	307	353	13		
1	g	243	Total	C	N	O	S	0	0
			1885	1194	316	362	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	226	Total	C	N	O	S	0	0
			1749	1116	297	330	6		
2	h	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	247	Total	C	N	O	S	0	0
			1933	1222	330	372	9		
3	i	250	Total	C	N	O	S	0	0
			1971	1245	339	377	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	237	Total	C	N	O	S	0	0
			1869	1171	332	361	5		
4	j	238	Total	C	N	O	S	0	0
			1878	1178	333	362	5		

- Molecule 5 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		
5	l	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	238	Total	C	N	O	S	0	0
			1862	1180	318	353	11		
6	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	203	Total	C	N	O	S	0	0
			1521	954	259	296	12		
7	n	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		
8	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
9	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	196	Total	C	N	O	S	0	0
			1571	1006	267	289	9		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
11	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
12	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		
13	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 14 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	k	234	Total	C	N	O	S	0	0
			1789	1125	295	358	11		
14	K	222	Total	C	N	O	S	0	0
			1694	1066	280	338	10		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	823	Total	C	N	O	S	0	0
			6292	3963	1077	1208	44		

- Molecule 16 is a protein called BAG family molecular chaperone regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	x	85	Total	C	N	O	S	0	0
			635	397	110	125	3		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	373	Total	C	N	O	S	0	0
			2969	1887	510	557	15		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	287	Total	C	N	O	S	0	0
			2224	1398	388	419	19		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	252	Total	C	N	O	S	0	0
			2063	1338	335	382	8		

- Molecule 21 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	e	50	Total	C	N	O	0	0
			407	244	63	100		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	859	Total	C	N	O	S	0	0
			6648	4199	1136	1269	44		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	444	Total	C	N	O	S	0	0
			3600	2289	645	653	13		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total	C	N	O	S	0	0
			3002	1912	509	569	12		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	380	Total	C	N	O	S	0	0
			3021	1904	530	570	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total	C	N	O	S	0	0
			2248	1427	392	424	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	444	Total	C	N	O	S	0	0
			3570	2250	616	680	24		

- Molecule 28 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	403	Total	C	N	O	S	0	0
			3119	1958	548	596	17		

- Molecule 29 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	400	Total	C	N	O	S	0	0
			3060	1918	527	601	14		

- Molecule 30 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	C	368	Total	C	N	O	S	0	0
			2839	1766	518	537	18		

- Molecule 31 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D	372	Total	C	N	O	S	0	0
			2893	1818	504	560	11		

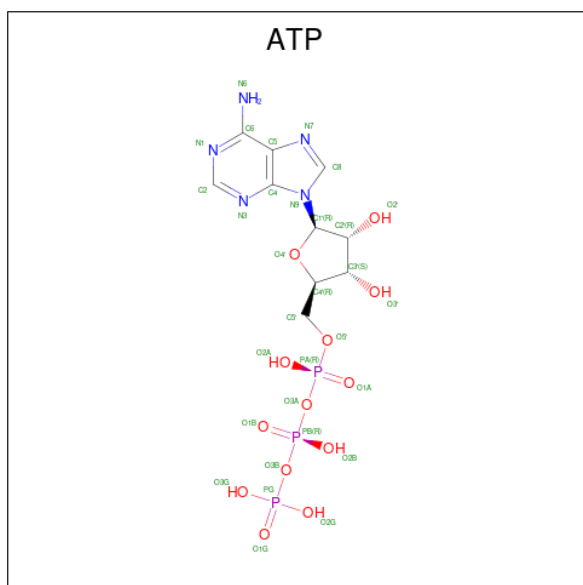
- Molecule 32 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	E	370	Total	C	N	O	S	0	0
			2929	1843	518	552	16		

- Molecule 33 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	F	355	Total	C	N	O	S	0	0
			2699	1700	464	518	17		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

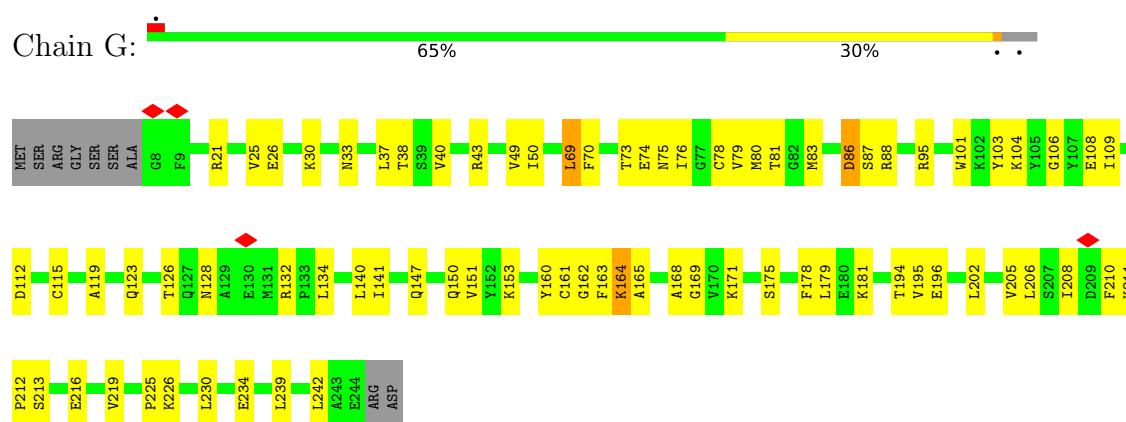
- # ADP

Mol	Chain	Residues	Atoms					AltConf
35	B	1	Total 27	C 10	N 5	O 10	P 2	0
35	C	1	Total 27	C 10	N 5	O 10	P 2	0
35	D	1	Total 27	C 10	N 5	O 10	P 2	0
35	E	1	Total 27	C 10	N 5	O 10	P 2	0
35	F	1	Total 27	C 10	N 5	O 10	P 2	0

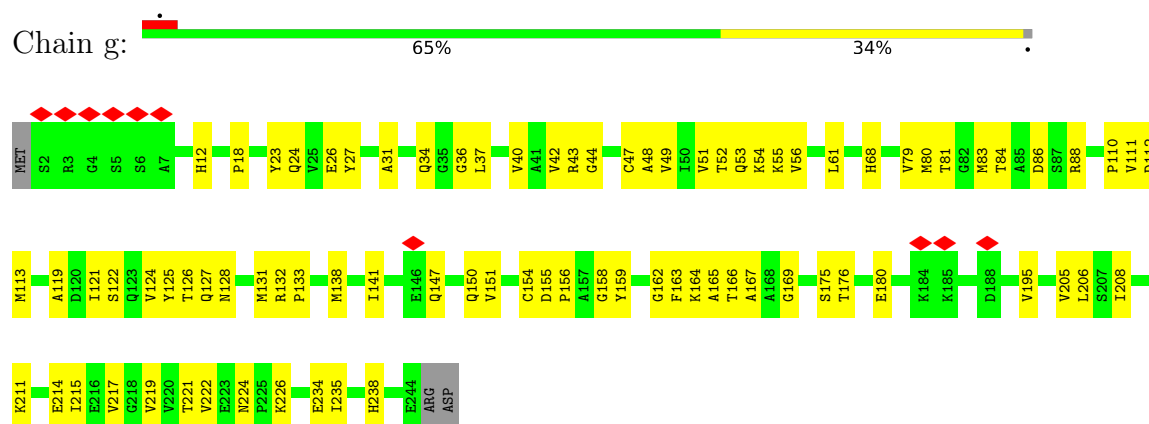
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

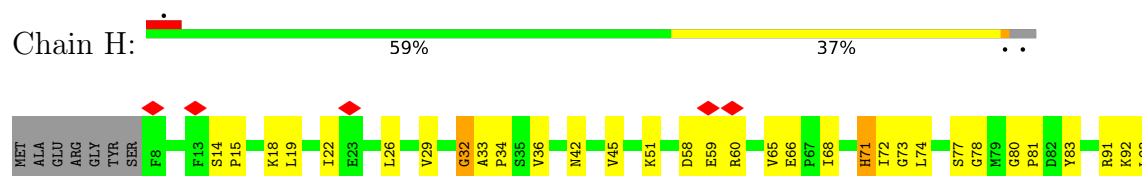
• Molecule 1: Proteasome subunit alpha type-6

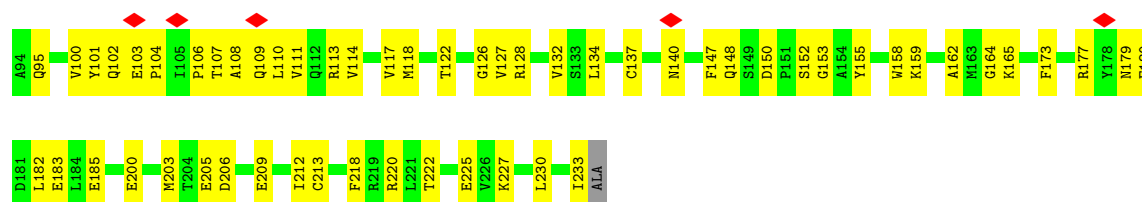


• Molecule 1: Proteasome subunit alpha type-6

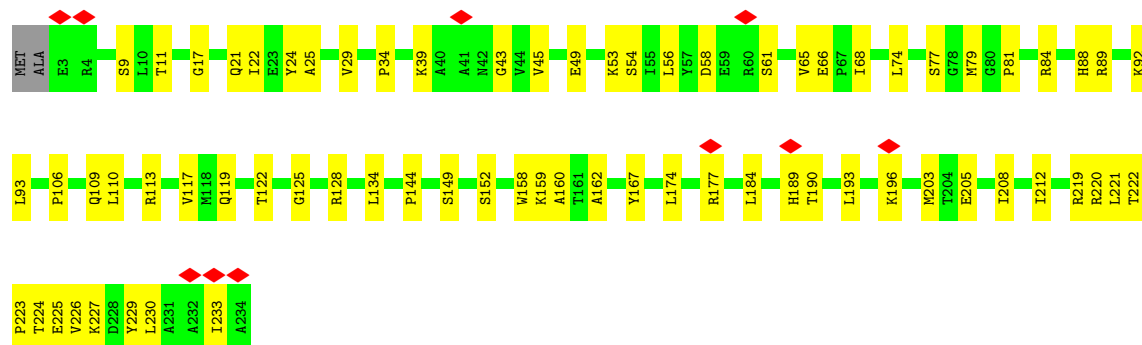


• Molecule 2: Proteasome subunit alpha type-2

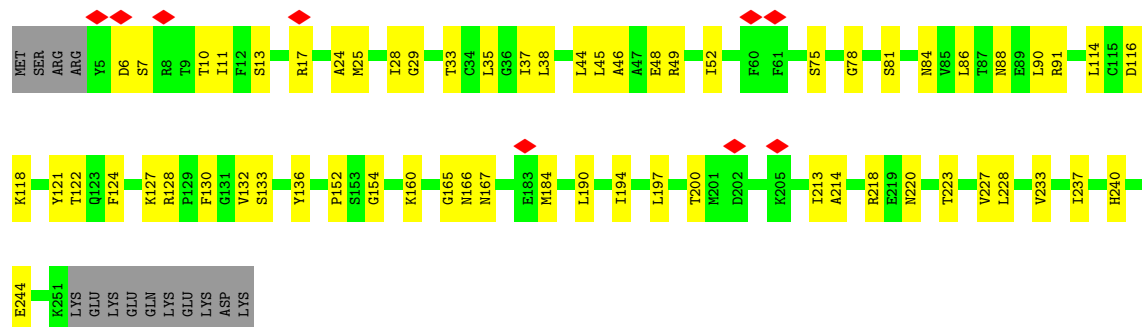




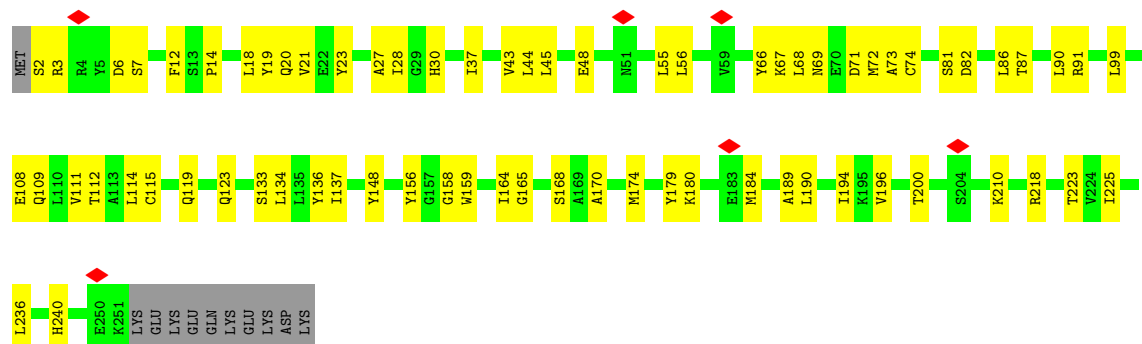
• Molecule 2: Proteasome subunit alpha type-2



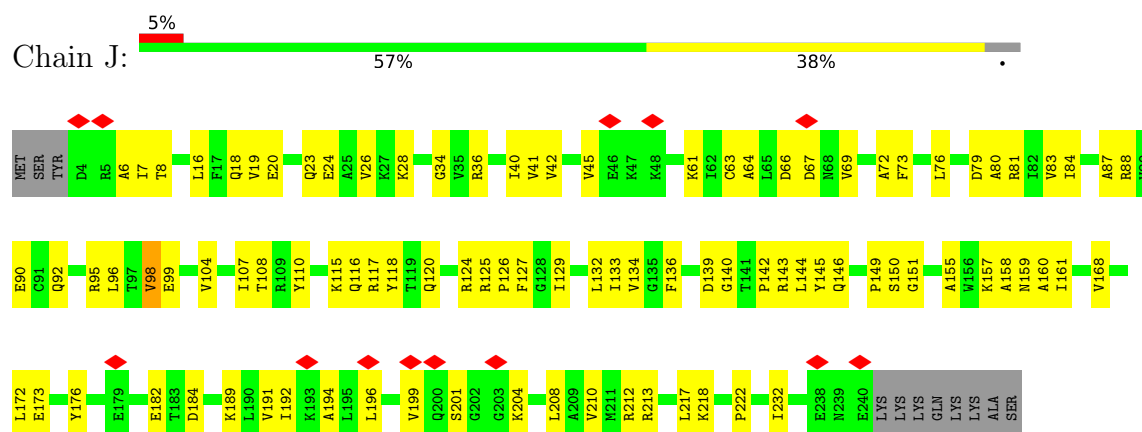
• Molecule 3: Proteasome subunit alpha type-4



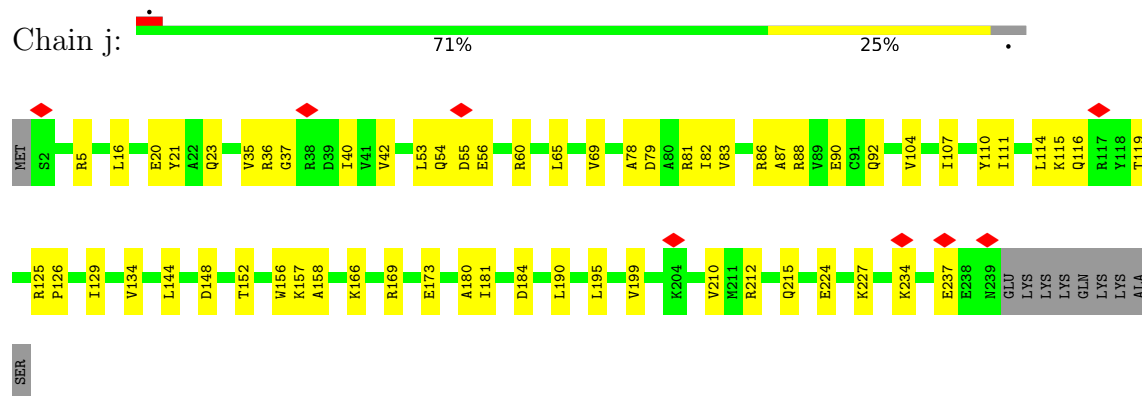
• Molecule 3: Proteasome subunit alpha type-4



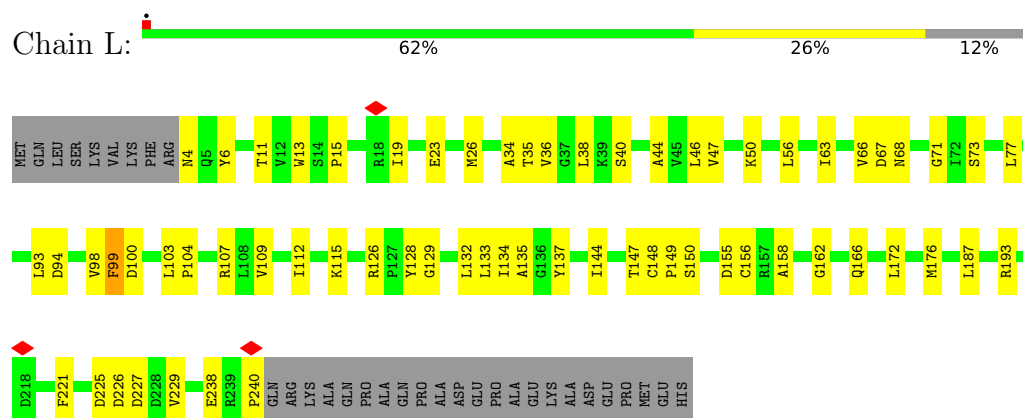
- Molecule 4: Proteasome subunit alpha type-7



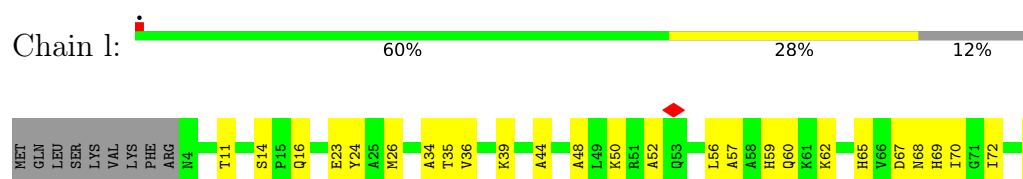
- Molecule 4: Proteasome subunit alpha type-7

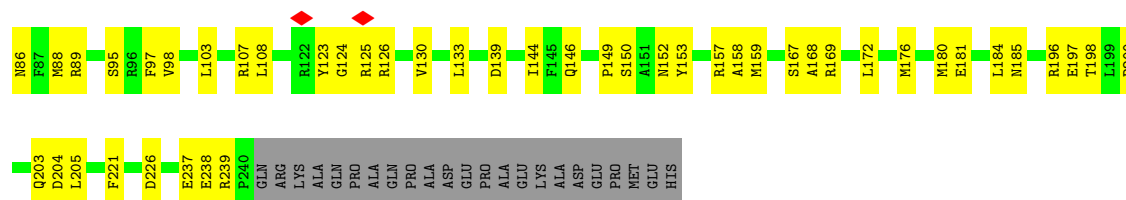


- Molecule 5: Isoform Long of Proteasome subunit alpha type-1

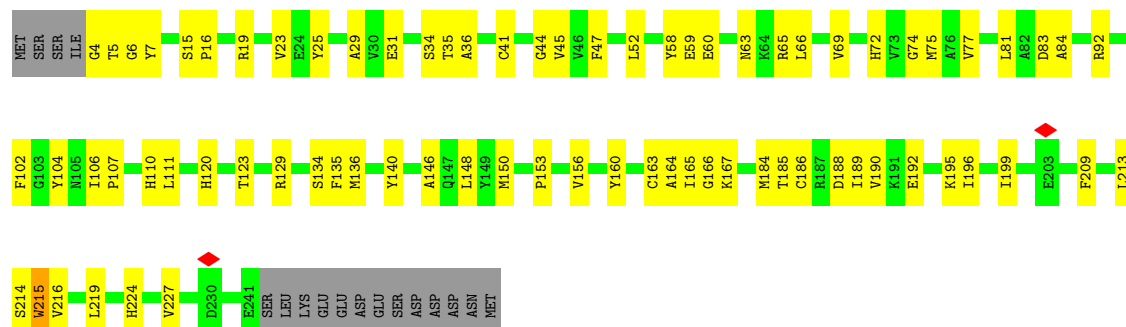


- Molecule 5: Isoform Long of Proteasome subunit alpha type-1

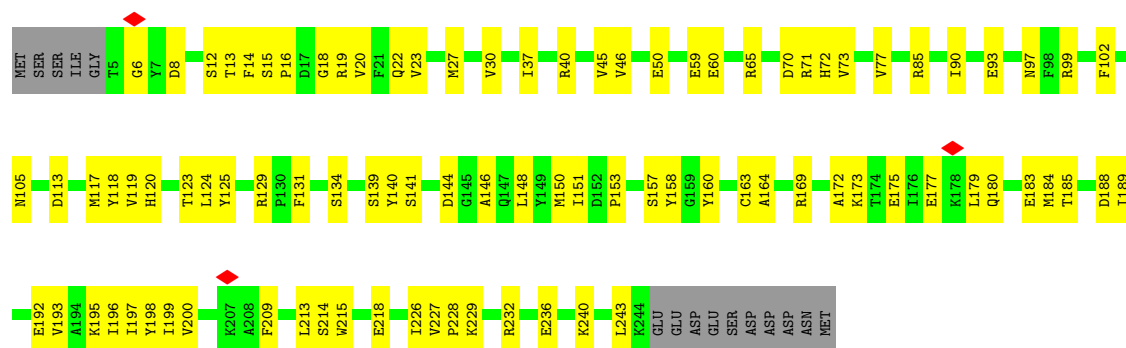




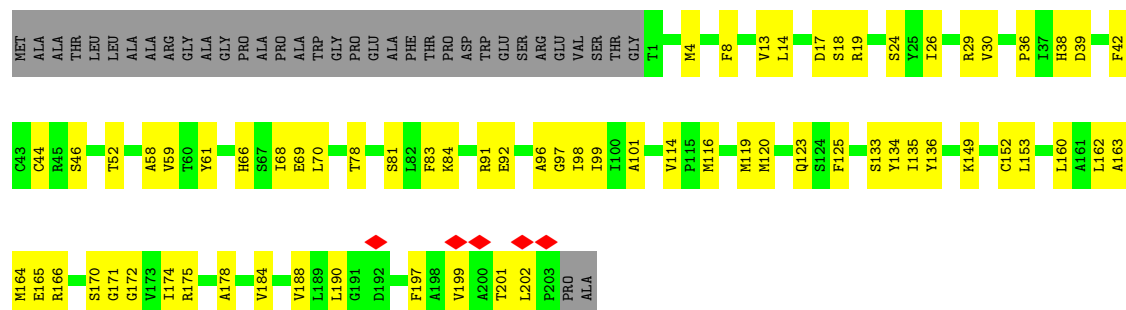
• Molecule 6: Proteasome subunit alpha type-3



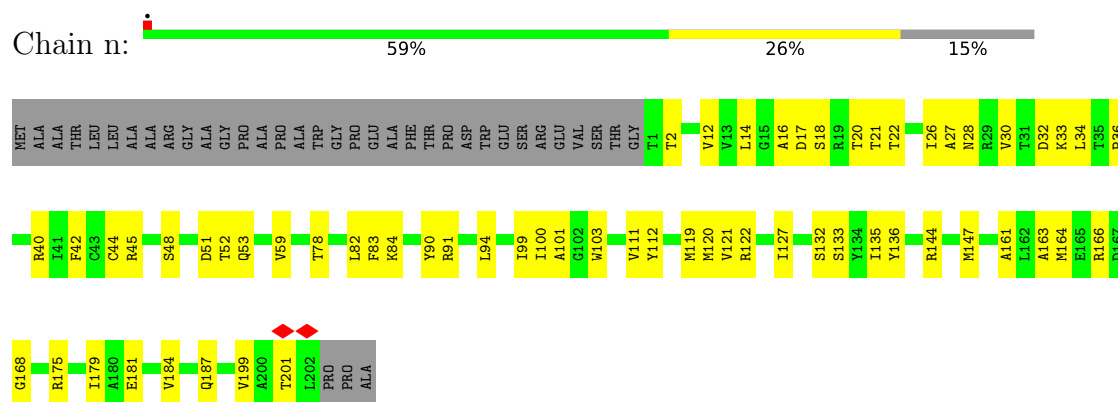
• Molecule 6: Proteasome subunit alpha type-3



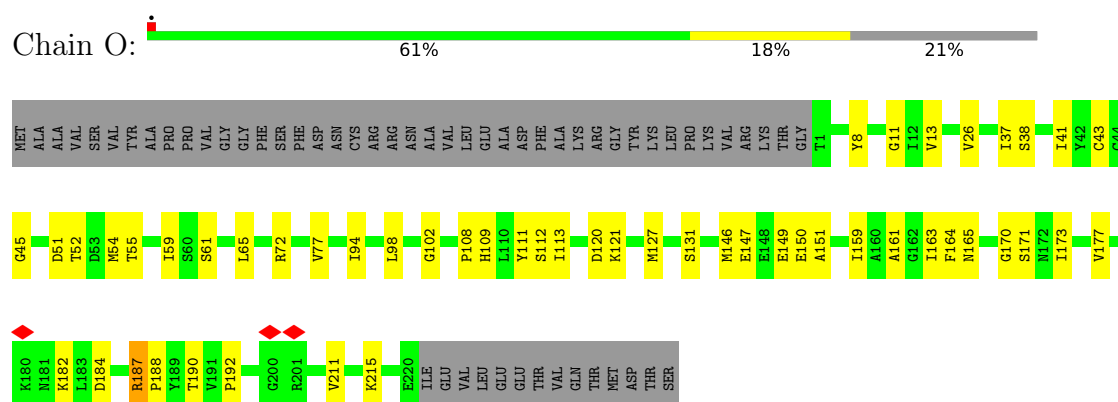
• Molecule 7: Proteasome subunit beta type-6



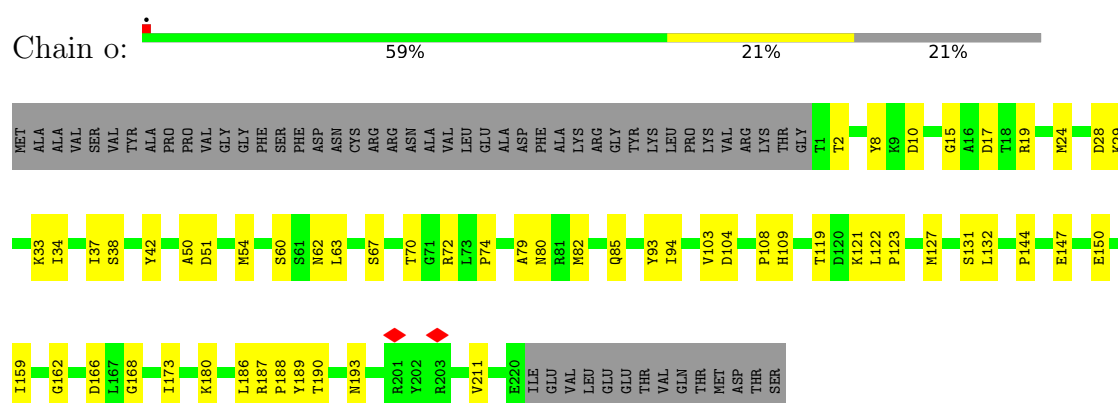
- Molecule 7: Proteasome subunit beta type-6



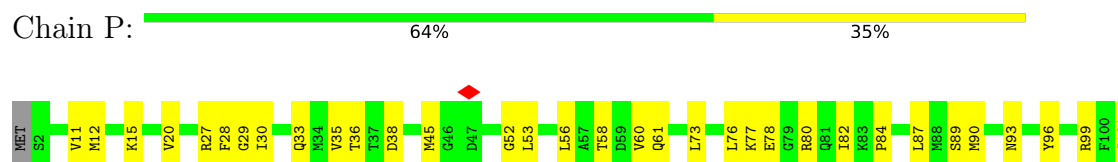
- Molecule 8: Proteasome subunit beta type-7

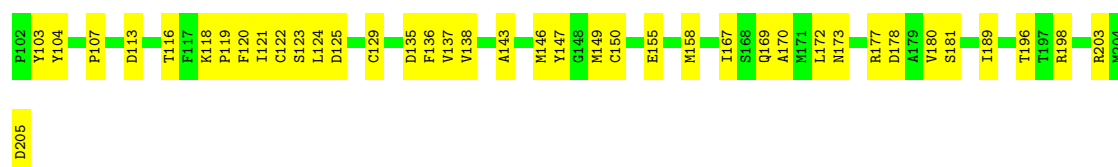


- Molecule 8: Proteasome subunit beta type-7

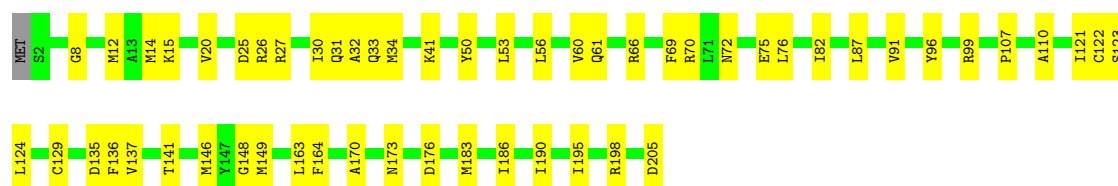


- Molecule 9: Proteasome subunit beta type-3

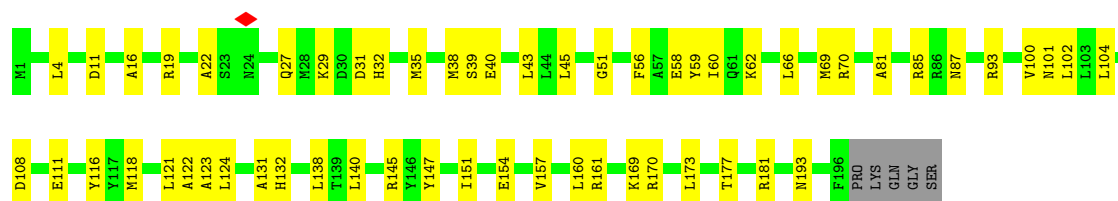




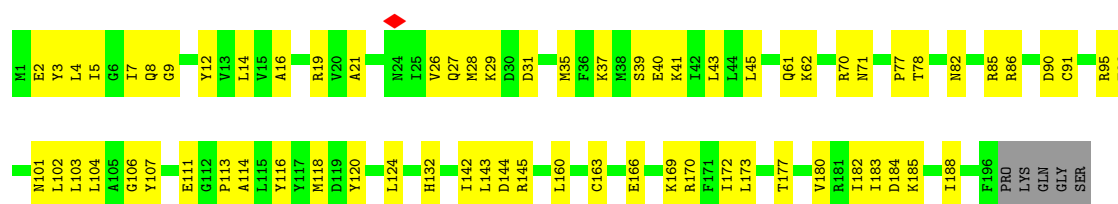
• Molecule 9: Proteasome subunit beta type-3



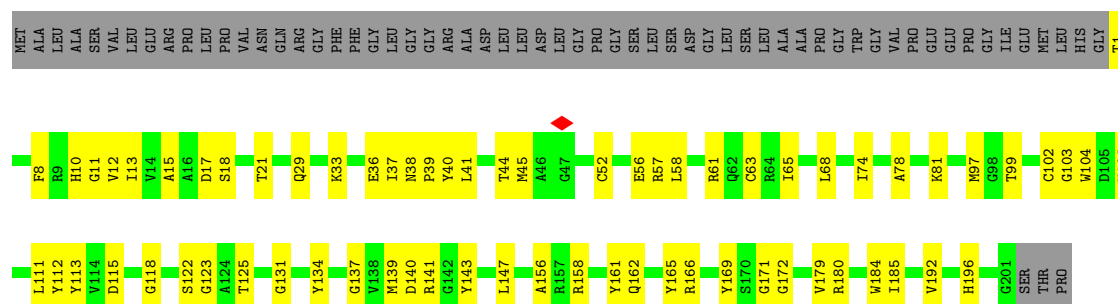
• Molecule 10: Proteasome subunit beta type-2



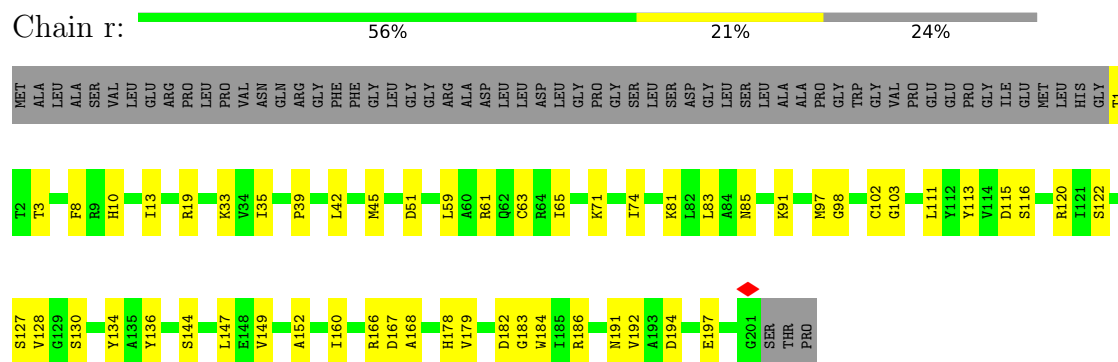
• Molecule 10: Proteasome subunit beta type-2



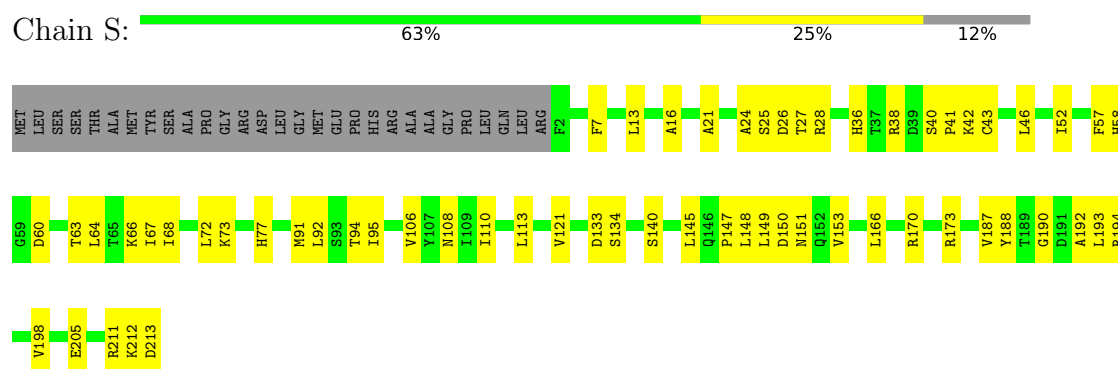
• Molecule 11: Proteasome subunit beta type-5



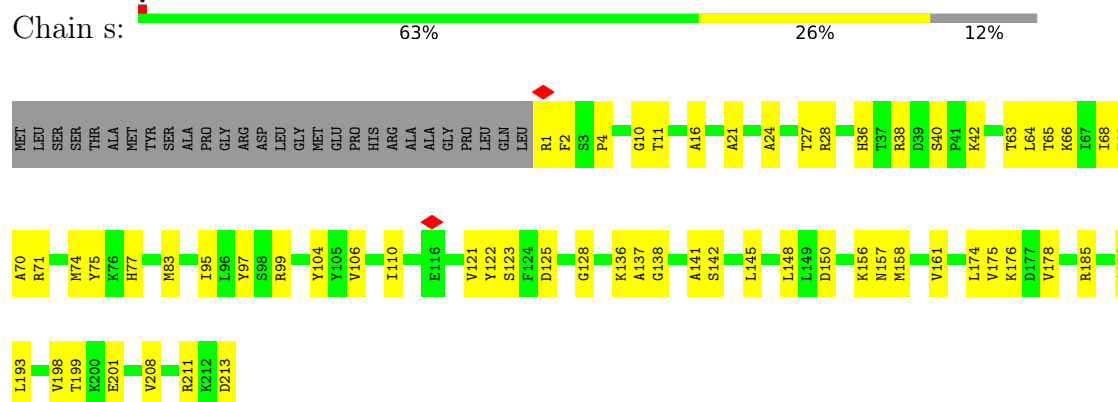
- Molecule 11: Proteasome subunit beta type-5



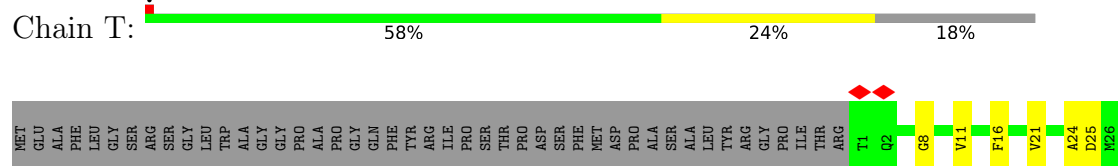
- Molecule 12: Proteasome subunit beta type-1

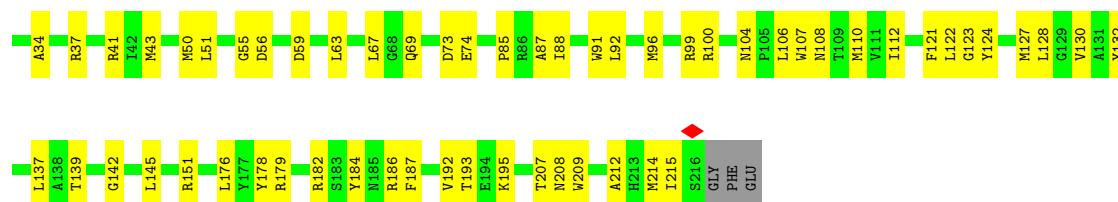


- Molecule 12: Proteasome subunit beta type-1

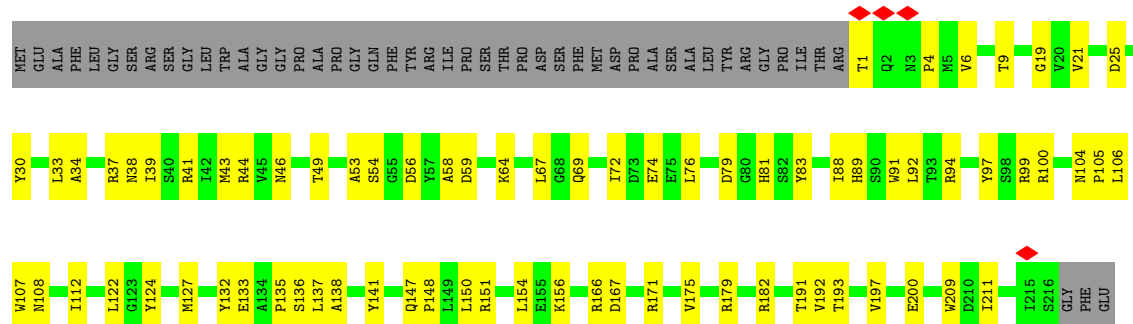


- Molecule 13: Proteasome subunit beta type-4

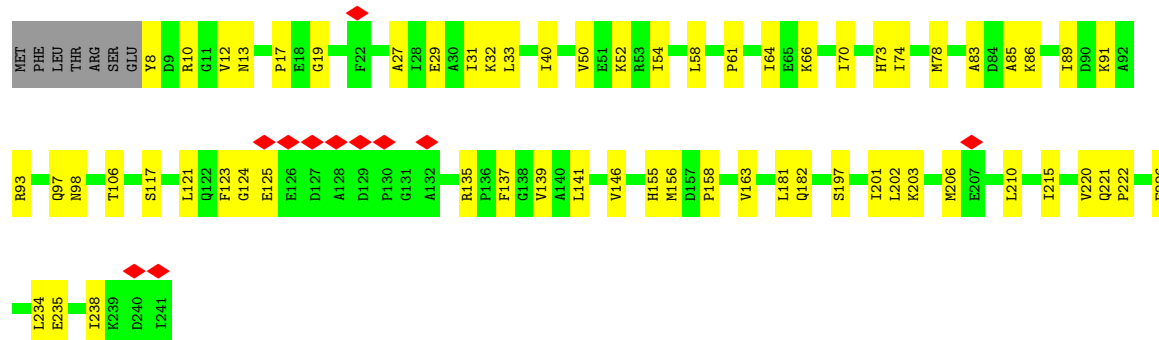




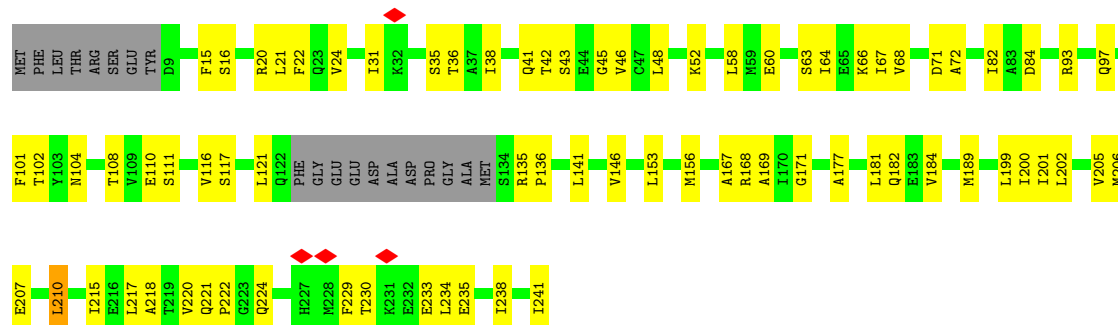
• Molecule 13: Proteasome subunit beta type-4



• Molecule 14: Proteasome subunit alpha type-5

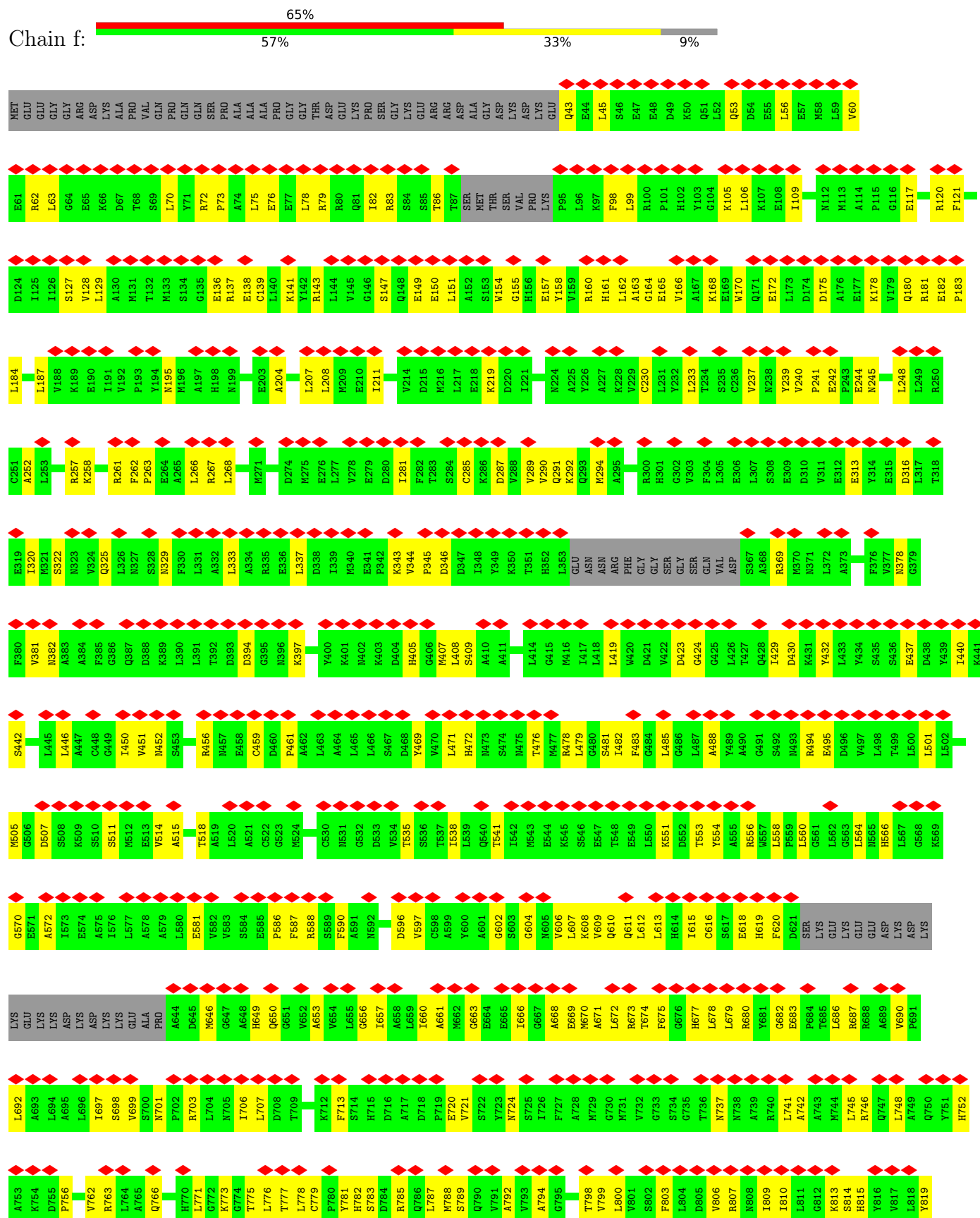


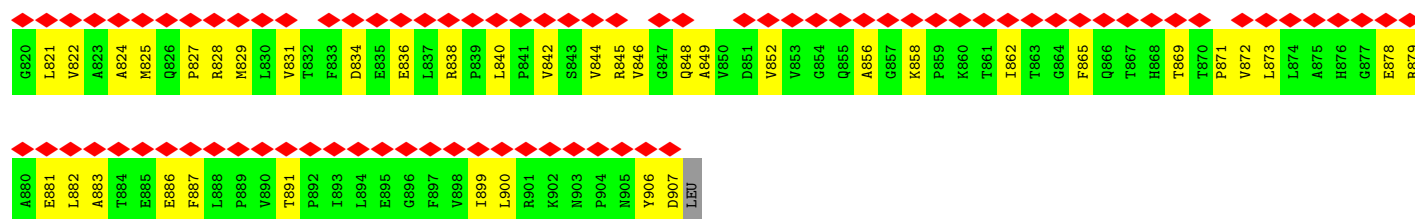
• Molecule 14: Proteasome subunit alpha type-5



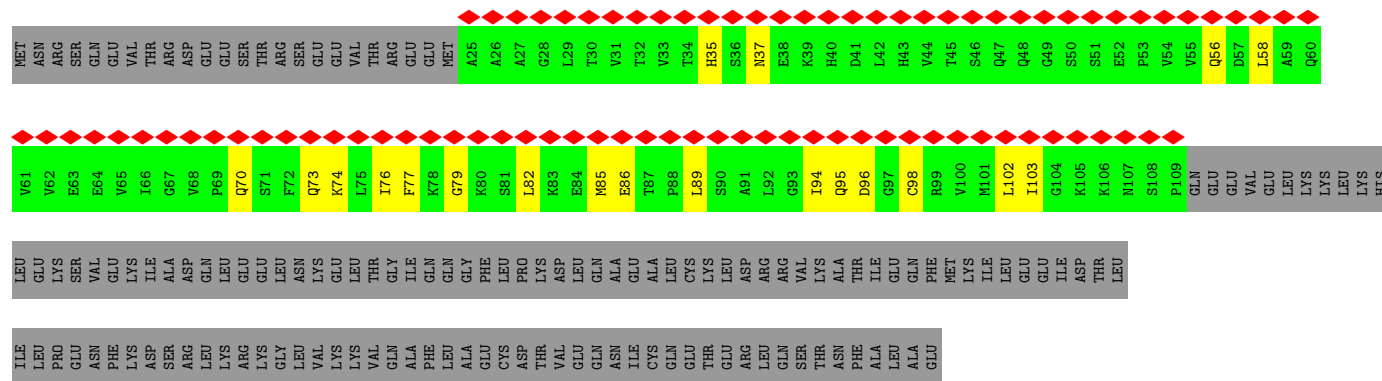
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 2

Chain f:

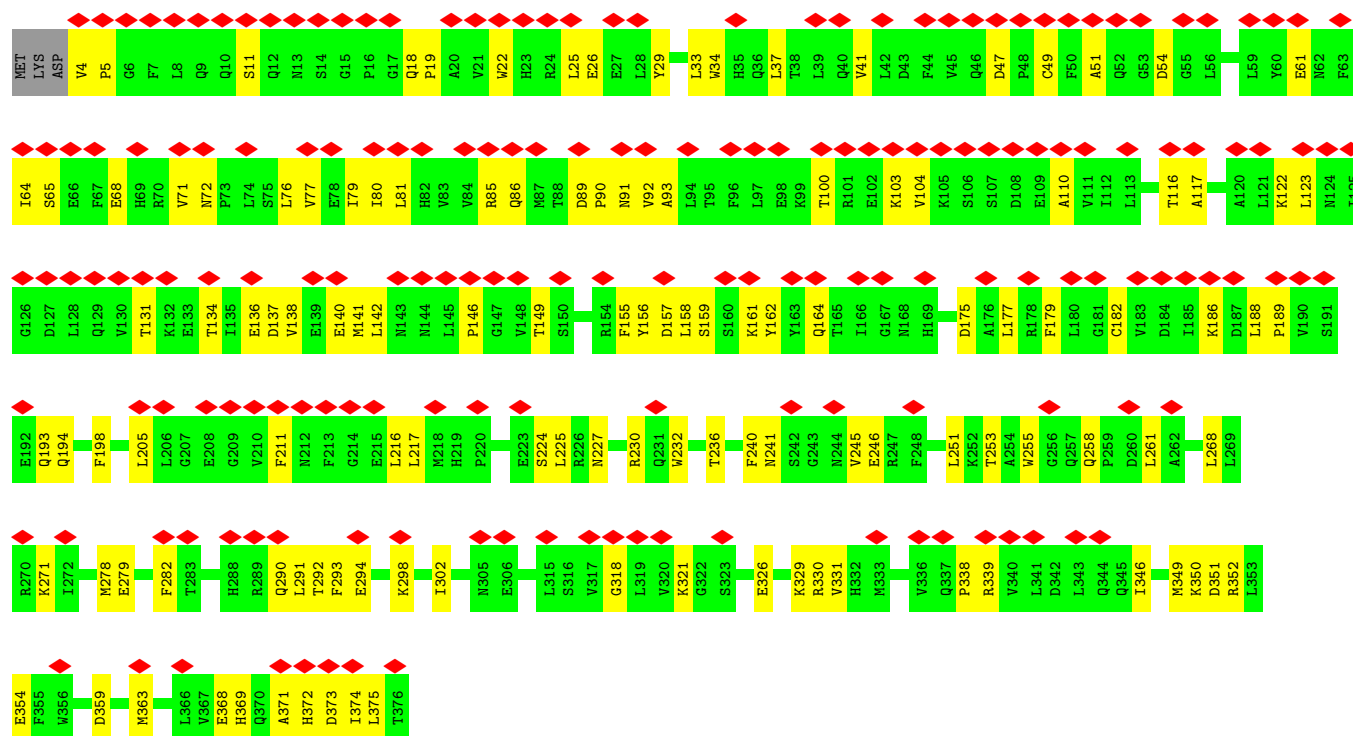




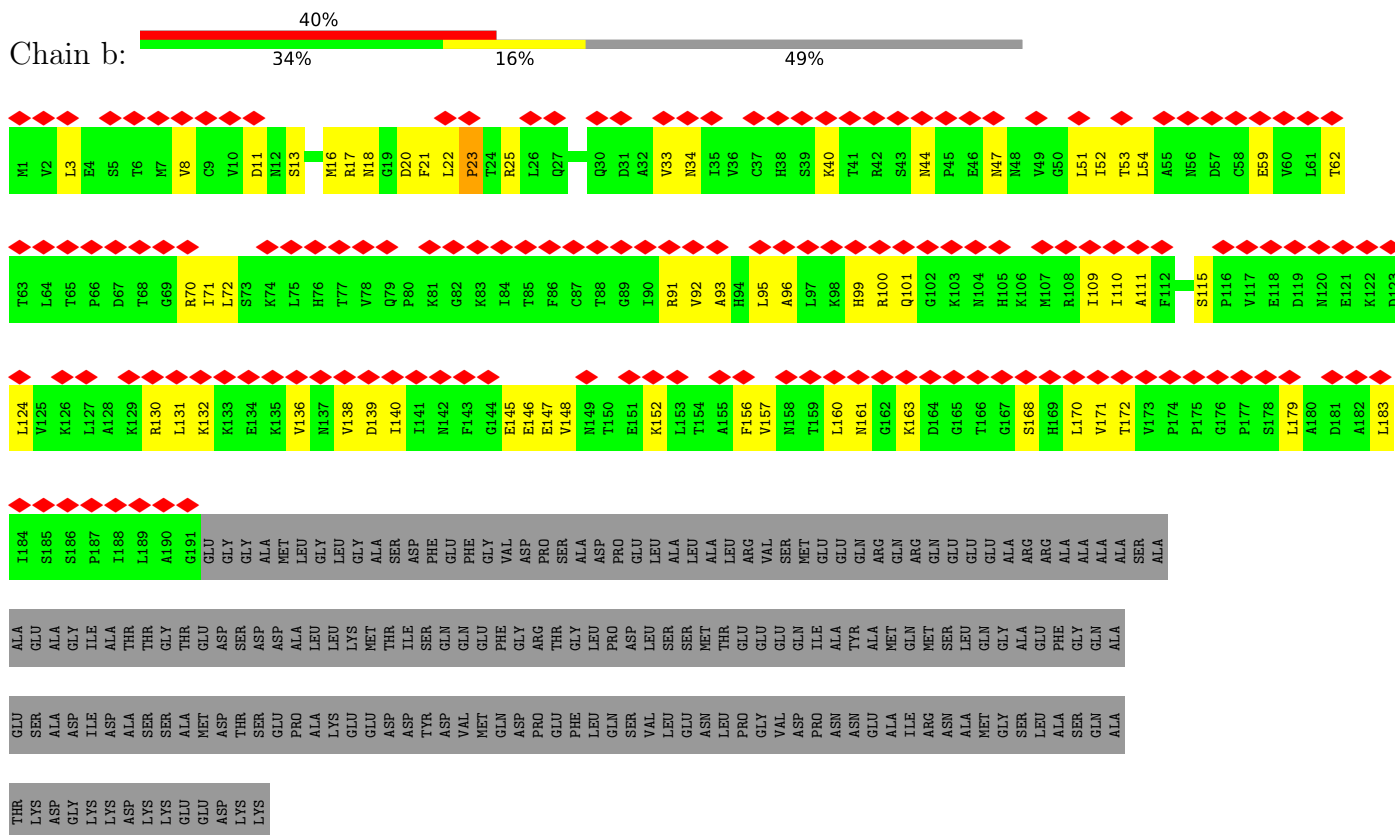
• Molecule 16: BAG family molecular chaperone regulator 1



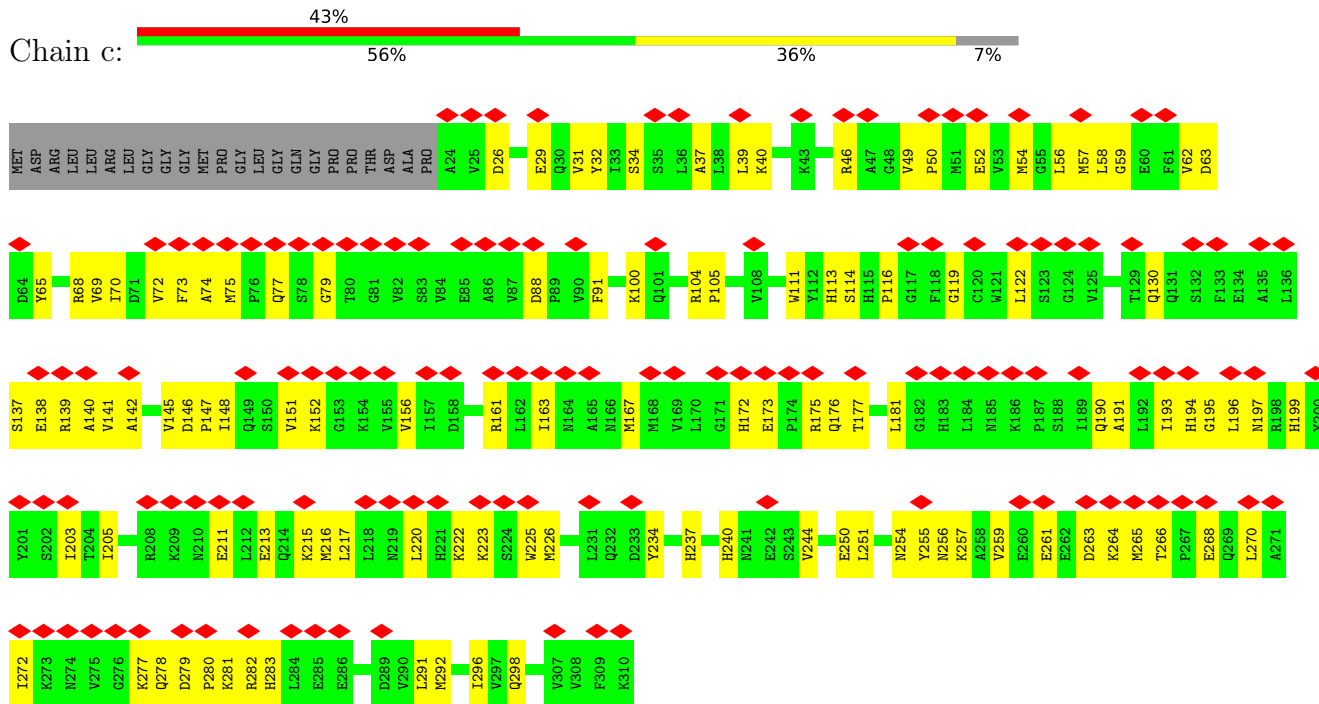
• Molecule 17: 26S proteasome non-ATPase regulatory subunit 13



• Molecule 18: 26S proteasome non-ATPase regulatory subunit 4

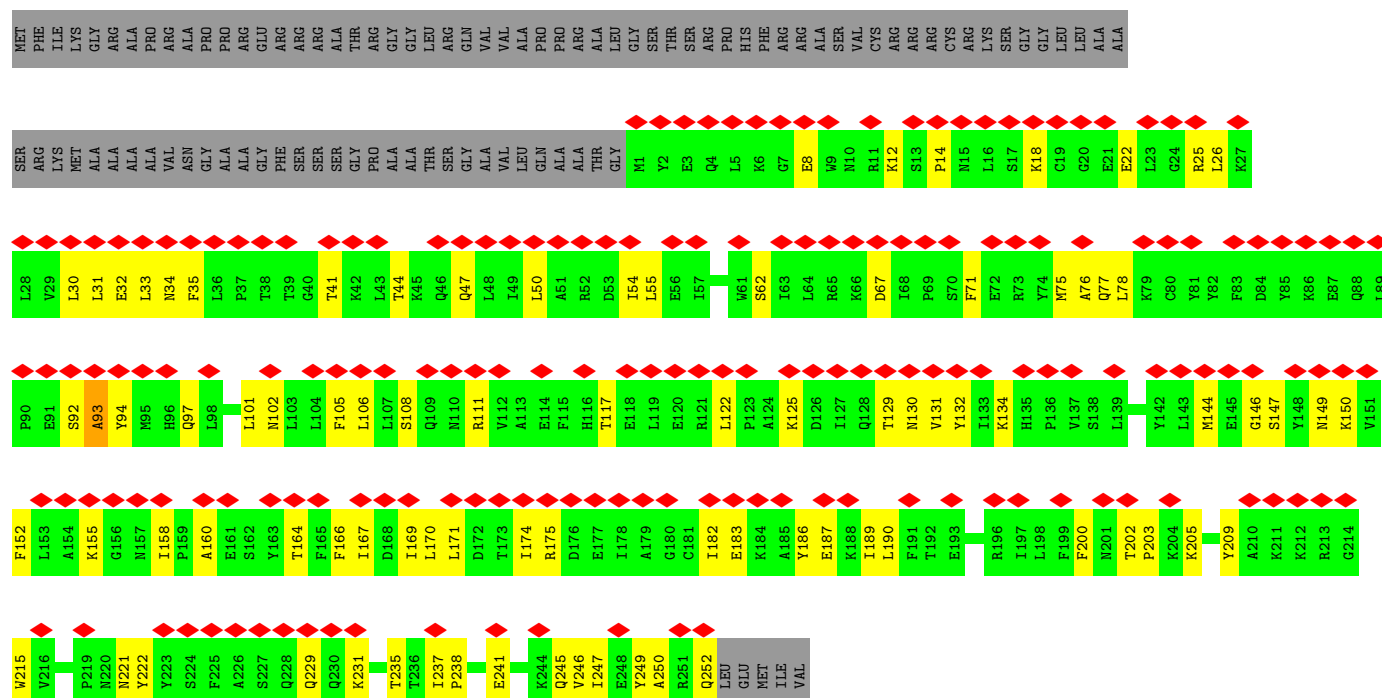


- Molecule 19: 26S proteasome non-ATPase regulatory subunit 14

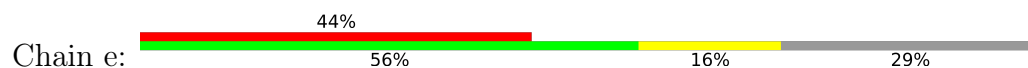


- Molecule 20: 26S proteasome non-ATPase regulatory subunit 8

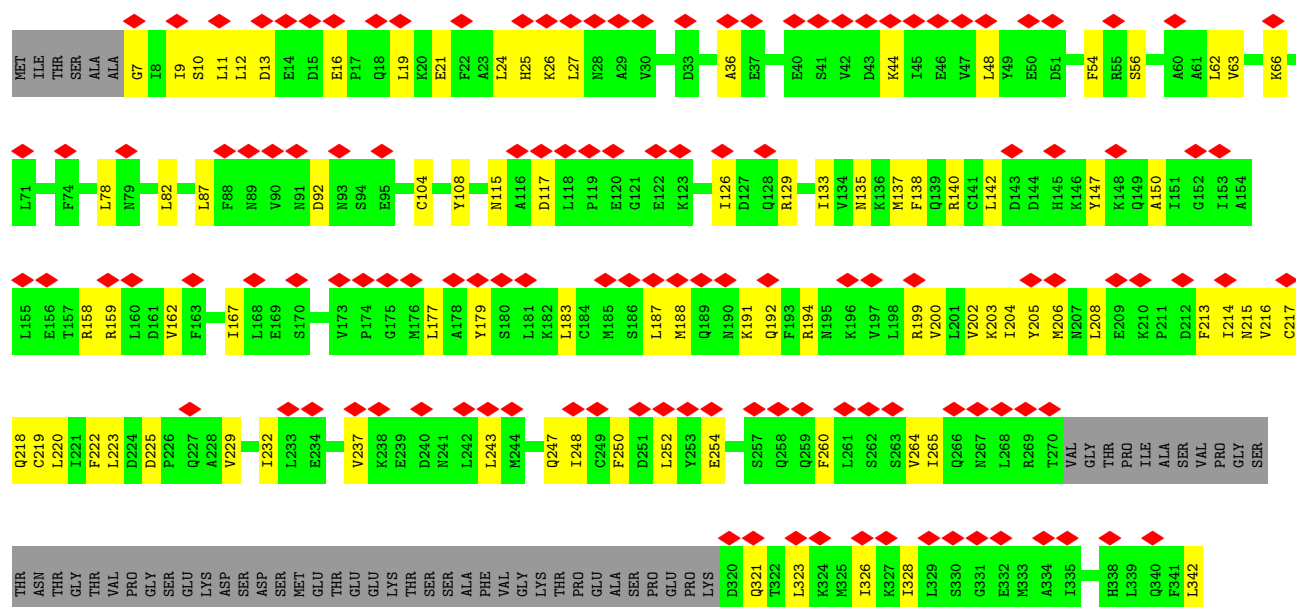


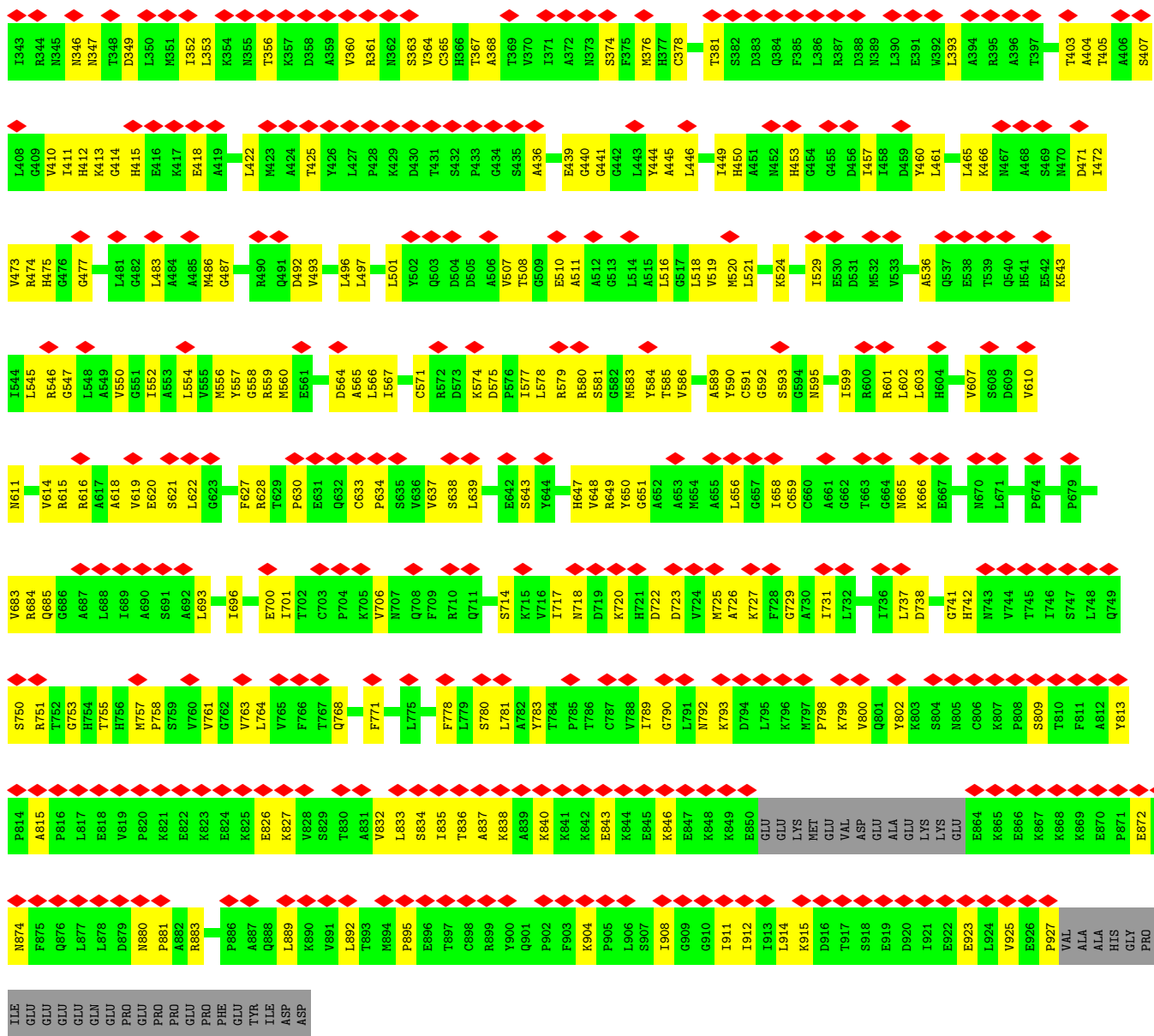


• Molecule 21: 26S proteasome complex subunit SEM1

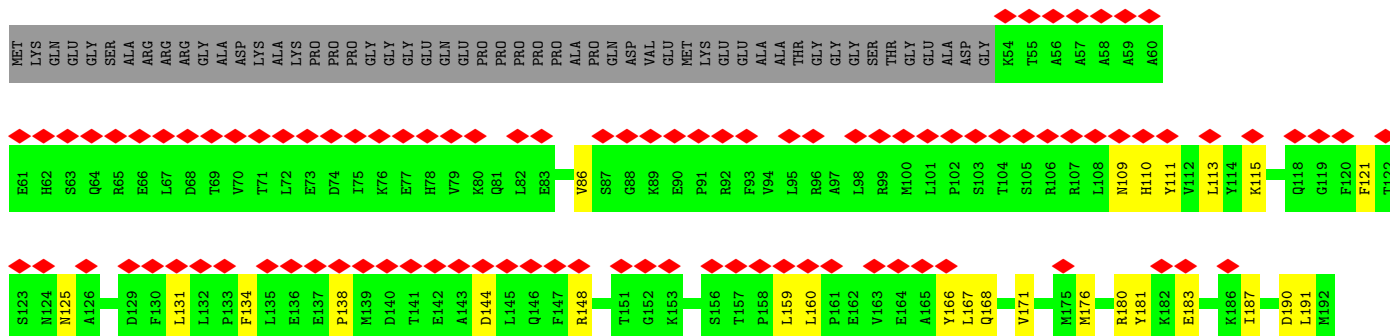
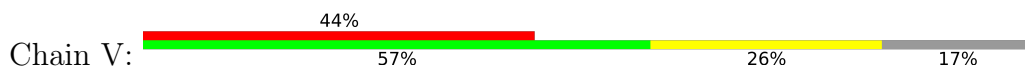


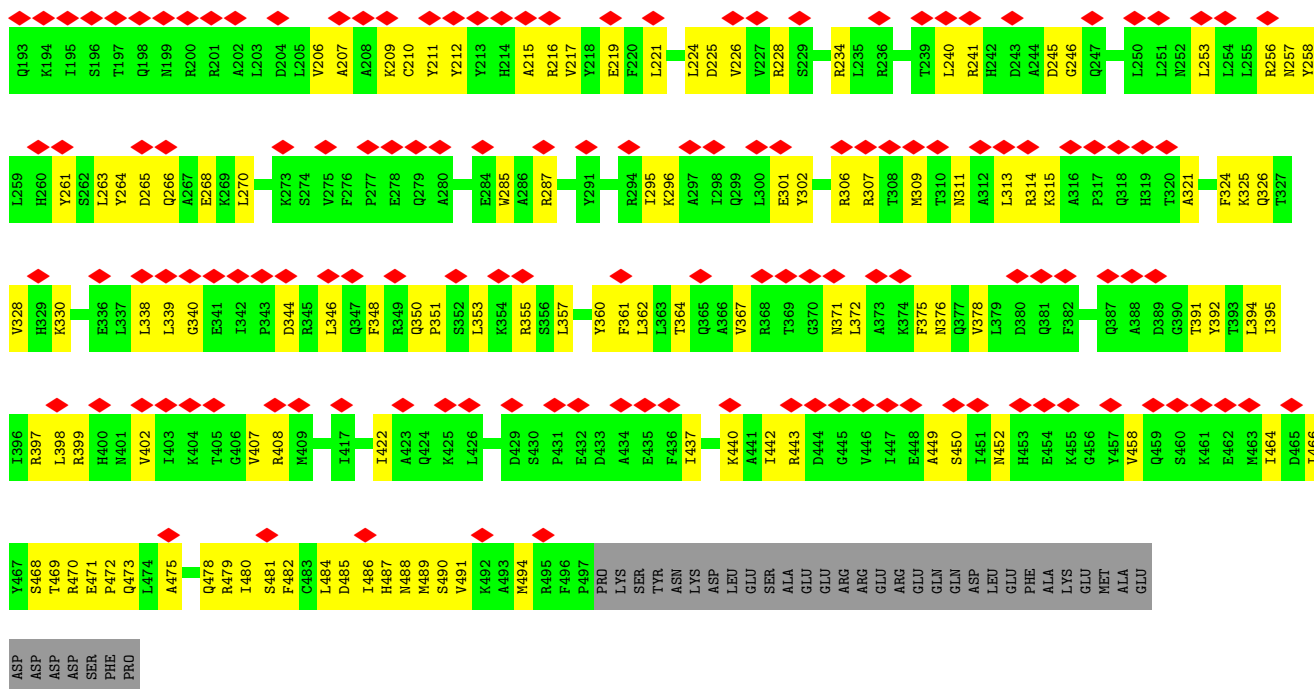
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1



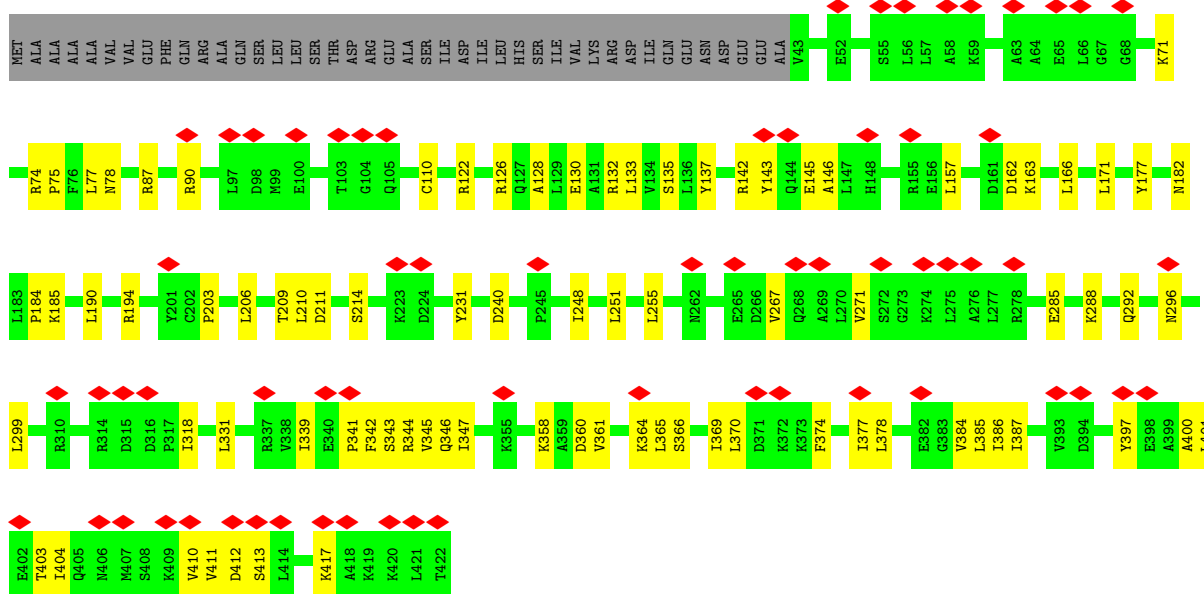


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 3

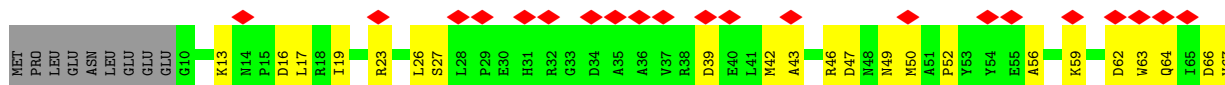


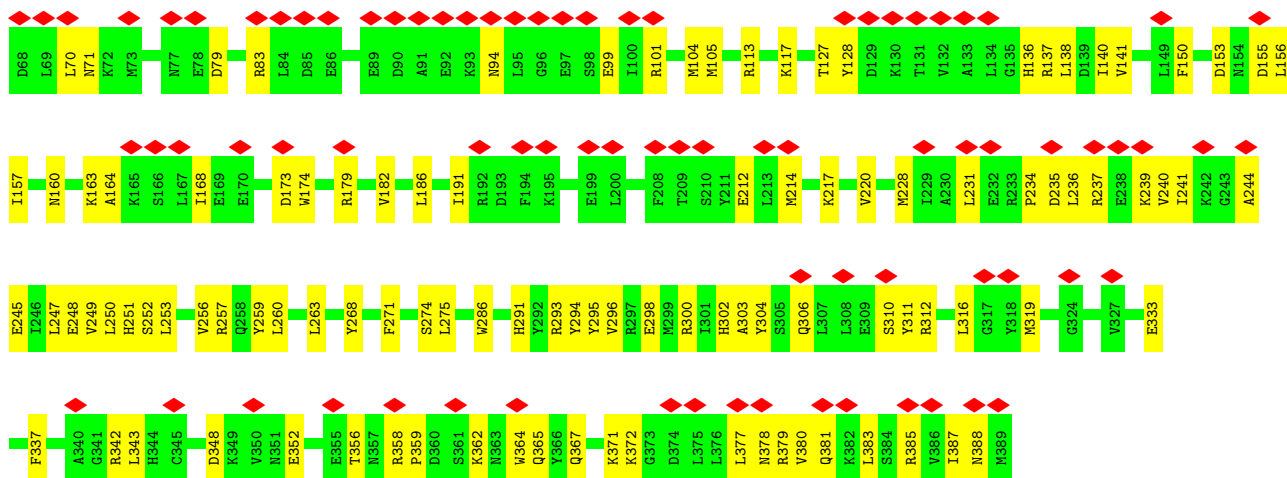


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

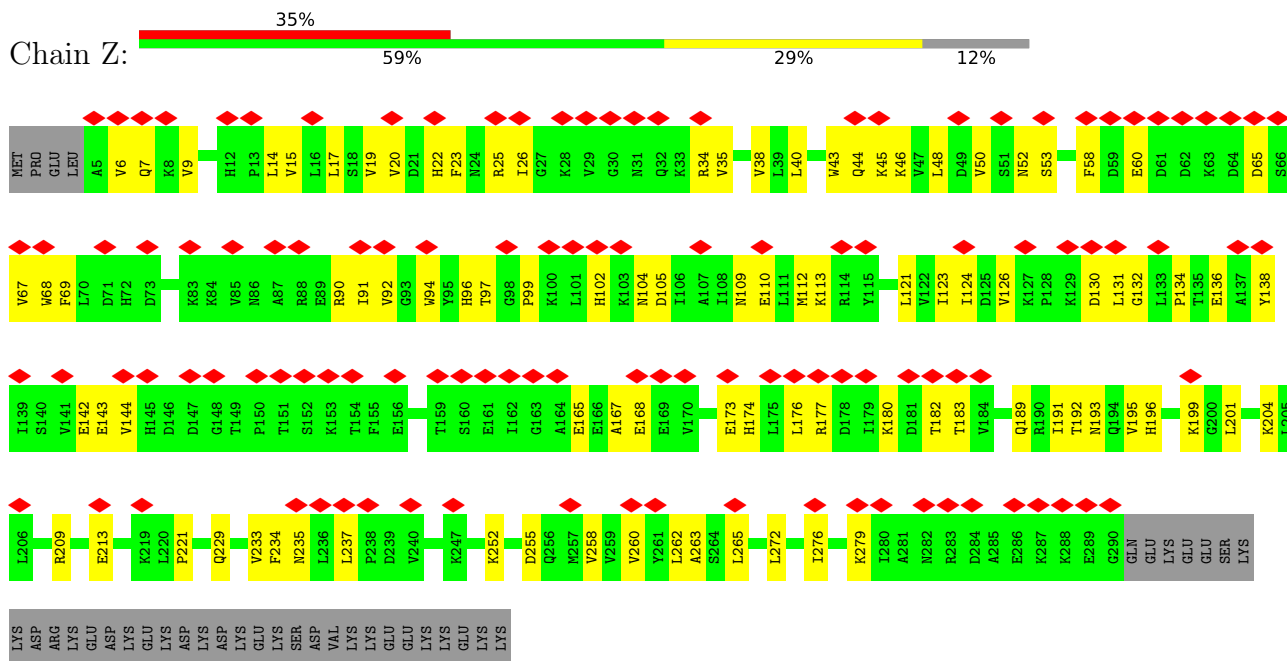


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

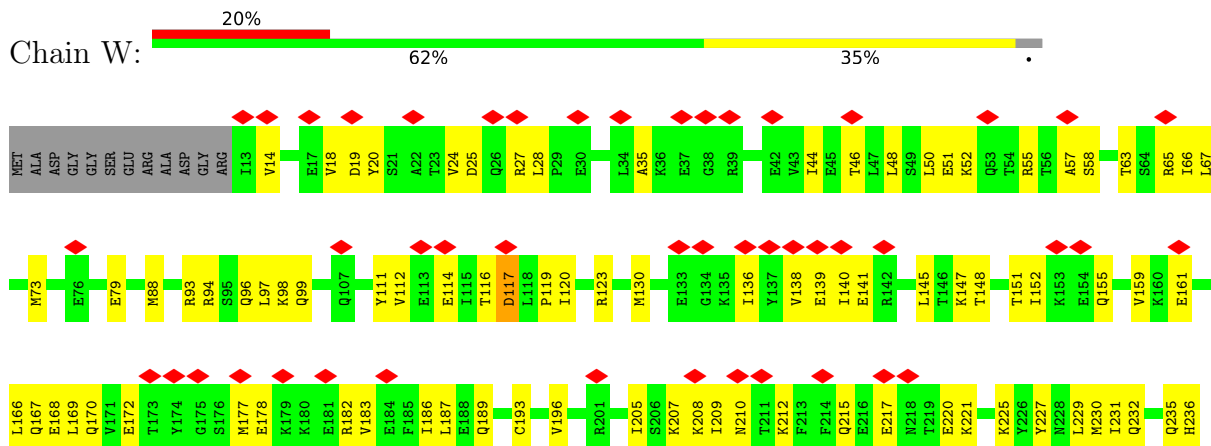


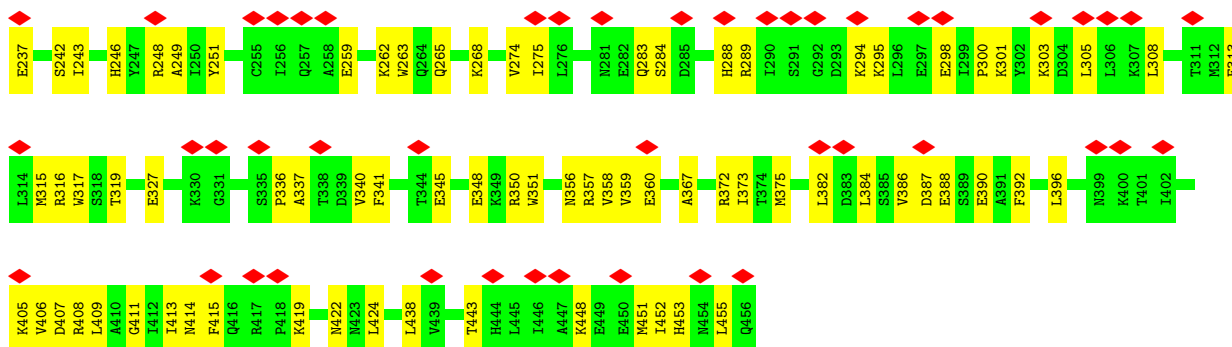


• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

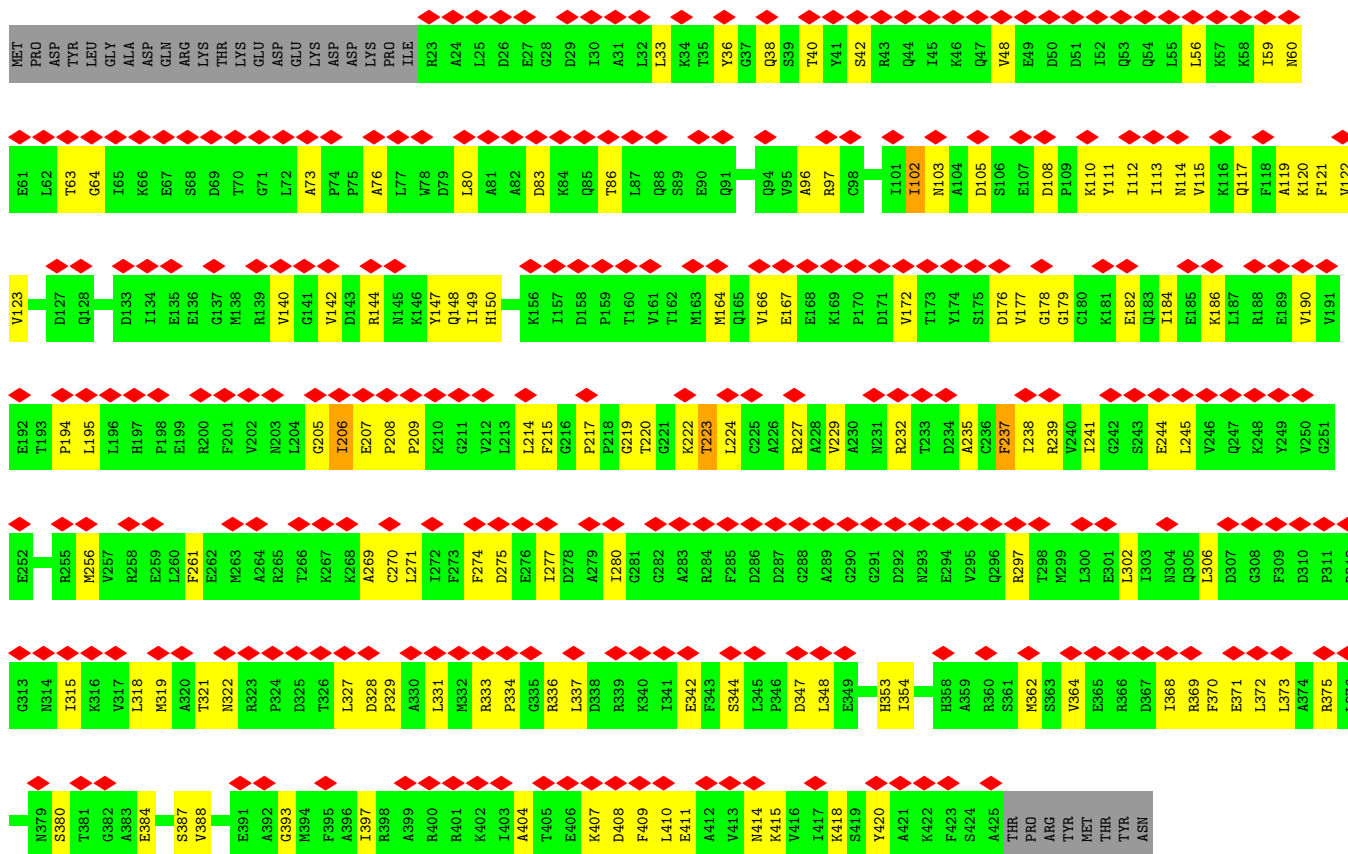


• Molecule 27: 26S proteasome non-ATPase regulatory subunit 12

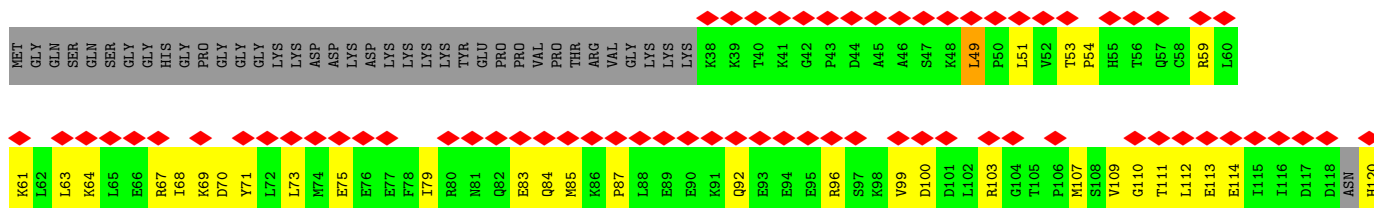


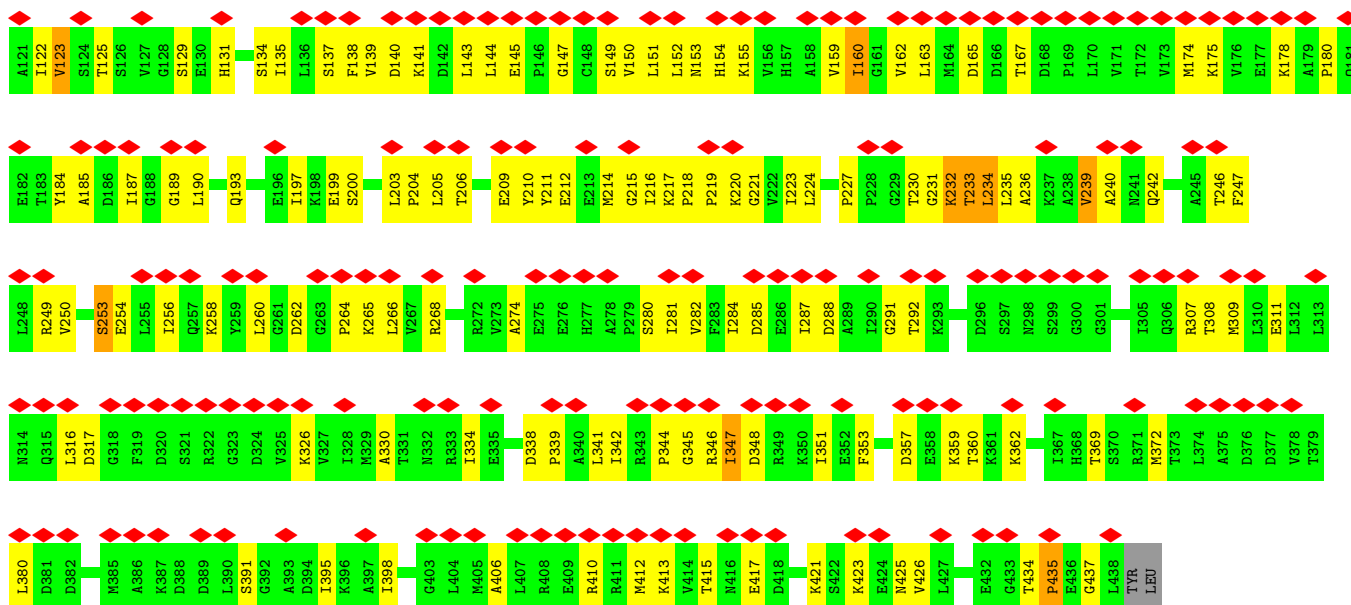


• Molecule 28: 26S protease regulatory subunit 7

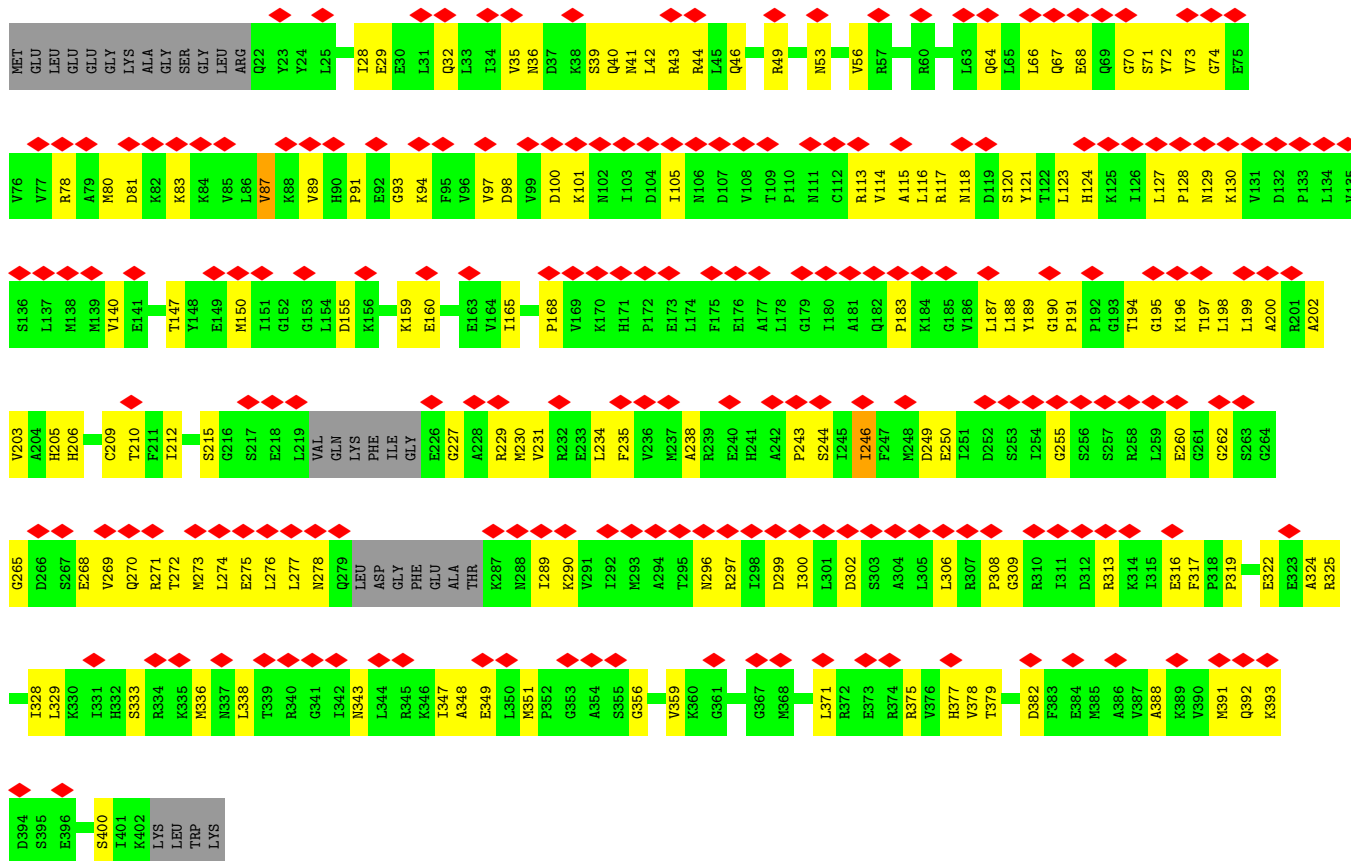


• Molecule 29: 26S protease regulatory subunit 4

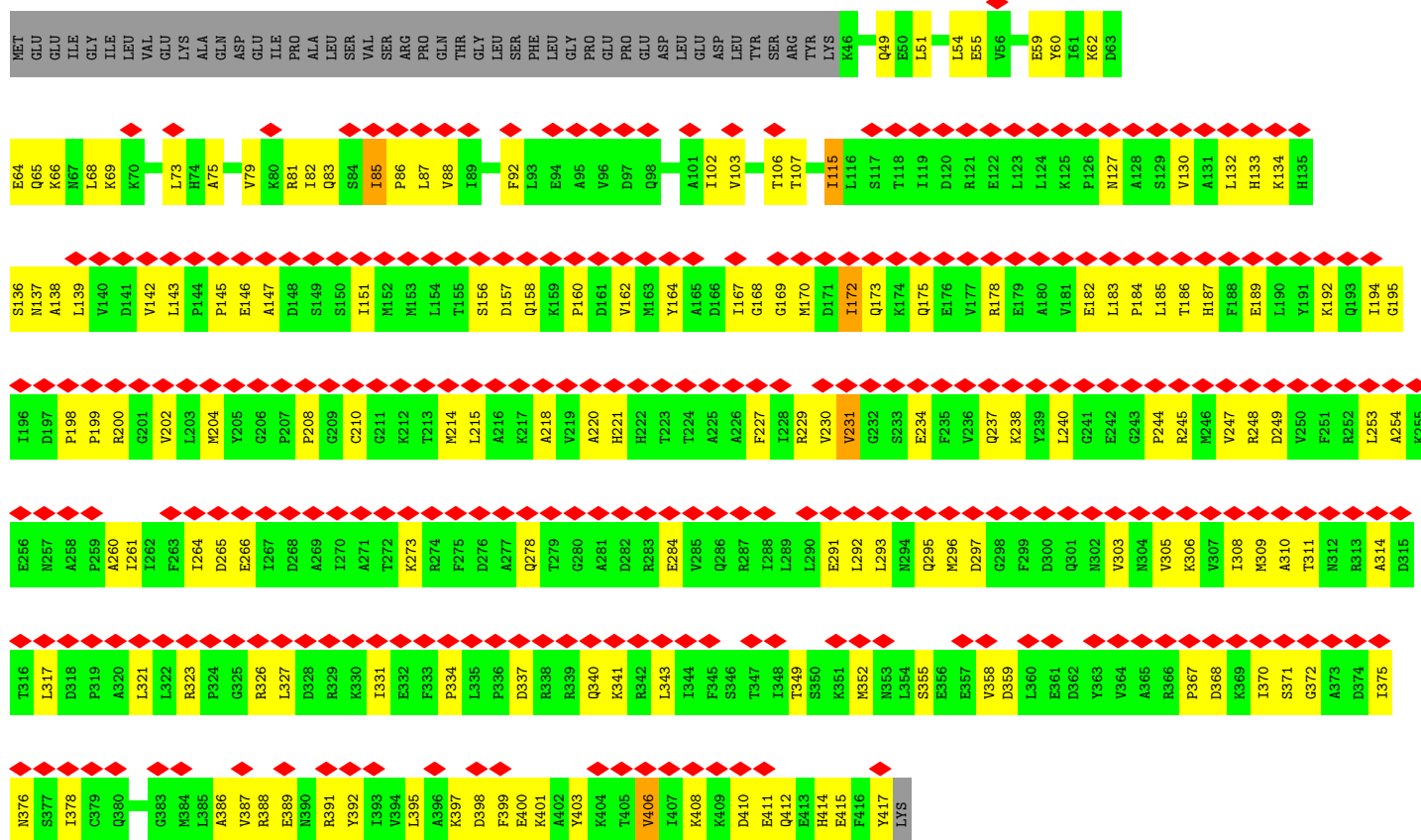




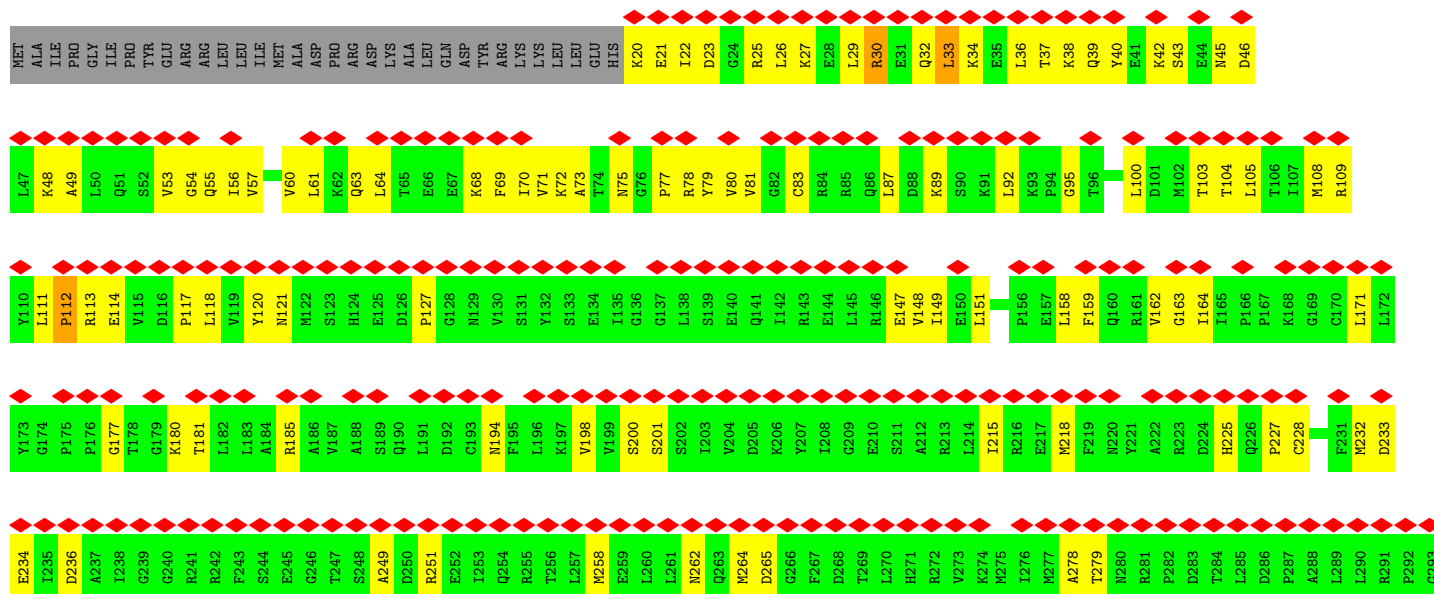
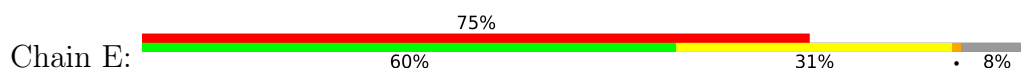
- Molecule 30: Isoform 2 of 26S proteasome regulatory subunit 8



- Molecule 31: 26S protease regulatory subunit 6B

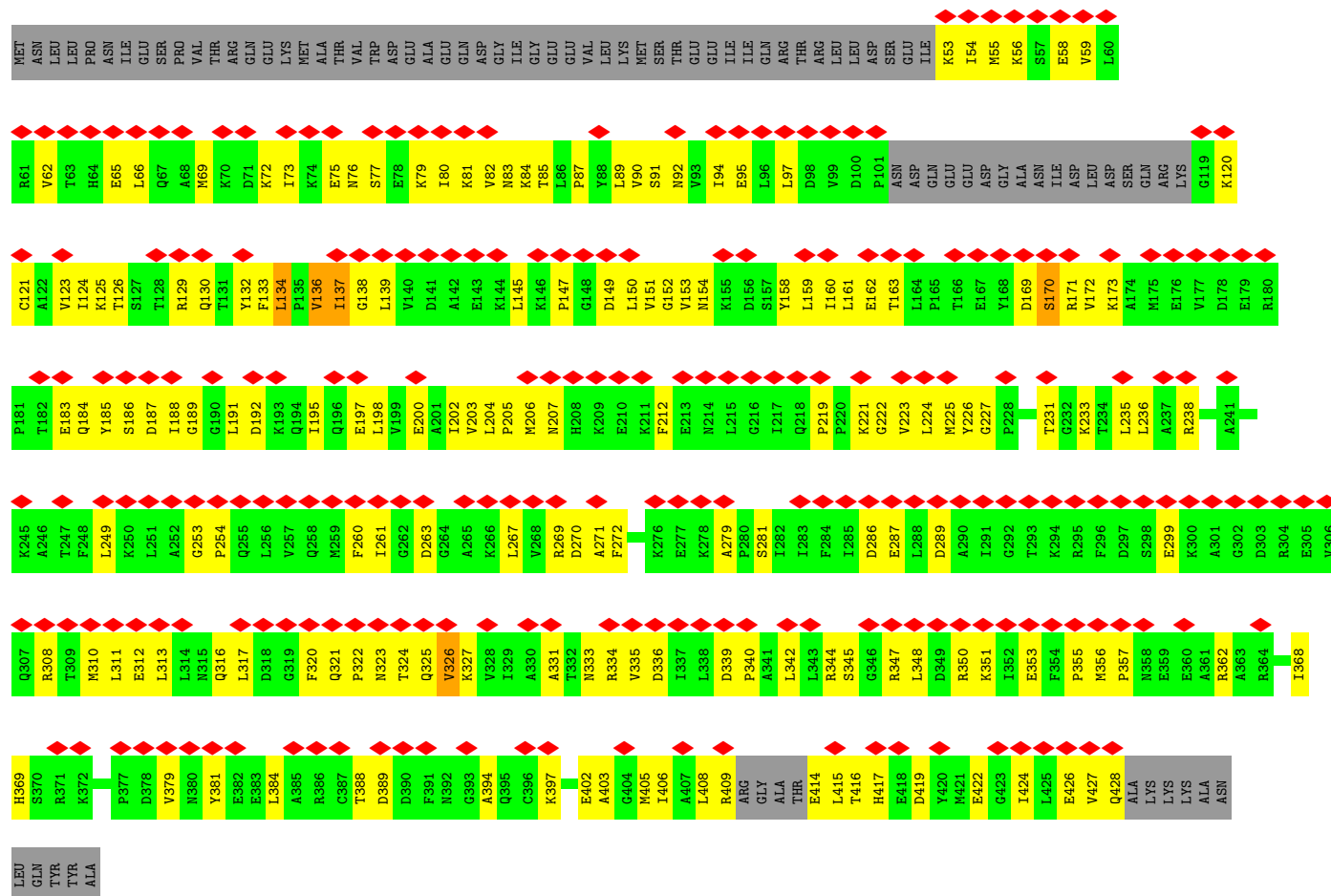
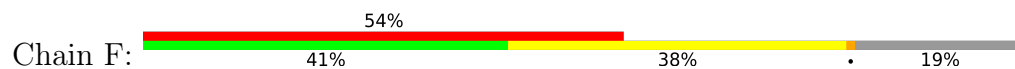


• Molecule 32: 26S proteasome regulatory subunit 10B





• Molecule 33: 26S protease regulatory subunit 6A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16466	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.168	Depositor
Minimum map value	-1.072	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	423.99002, 423.99002, 423.99002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4133, 1.4133, 1.4133	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP

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	G	0.10	0/1873	0.31	0/2533
1	g	0.11	0/1918	0.33	0/2592
2	H	0.13	0/1784	0.36	0/2416
2	h	0.10	0/1852	0.30	0/2507
3	I	0.10	0/1962	0.29	0/2644
3	i	0.11	0/2001	0.32	0/2694
4	J	0.12	0/1894	0.37	0/2555
4	j	0.10	0/1904	0.28	0/2569
5	L	0.11	0/1899	0.29	0/2567
5	l	0.10	0/1899	0.29	0/2567
6	M	0.12	0/1897	0.32	0/2555
6	m	0.12	0/1916	0.32	0/2580
7	N	0.10	0/1548	0.26	0/2097
7	n	0.10	0/1540	0.29	0/2085
8	O	0.11	0/1686	0.30	0/2282
8	o	0.11	0/1686	0.28	0/2282
9	P	0.10	0/1620	0.29	0/2184
9	p	0.11	0/1620	0.28	0/2184
10	Q	0.12	0/1603	0.33	0/2168
10	q	0.11	0/1603	0.30	0/2168
11	R	0.09	0/1590	0.26	0/2147
11	r	0.10	0/1590	0.25	0/2147
12	S	0.12	0/1673	0.34	0/2254
12	s	0.11	0/1684	0.30	0/2268
13	T	0.09	0/1720	0.25	0/2328
13	t	0.10	0/1720	0.28	0/2328
14	K	0.10	0/1718	0.31	0/2319
14	k	0.09	0/1817	0.26	0/2455
15	f	0.11	0/6385	0.32	0/8637
16	x	0.07	0/643	0.26	0/868
17	a	0.10	0/3023	0.30	0/4093
18	b	0.10	0/1478	0.34	0/2001

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	c	0.11	0/2260	0.37	0/3052
20	d	0.10	0/2109	0.32	0/2851
21	e	0.08	0/415	0.31	0/563
22	U	0.10	0/6750	0.30	0/9116
23	V	0.10	0/3667	0.27	0/4951
24	X	0.09	0/3045	0.26	0/4104
25	Y	0.11	0/3063	0.31	0/4123
26	Z	0.10	0/2286	0.31	0/3099
27	W	0.11	0/3610	0.33	0/4853
28	A	0.12	0/3165	0.34	0/4273
29	B	0.15	0/3100	0.47	2/4189 (0.0%)
30	C	0.12	0/2865	0.37	0/3851
31	D	0.16	0/2932	0.43	1/3962 (0.0%)
32	E	0.16	0/2974	0.41	1/4006 (0.0%)
33	F	0.15	0/2731	0.40	0/3688
All	All	0.11	0/105718	0.32	4/142755 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	233	THR	N-CA-C	-13.79	95.88	113.12
29	B	234	LEU	N-CA-C	-9.59	100.68	112.38
32	E	344	ARG	CB-CG-CD	5.67	124.34	111.30
31	D	186	THR	CB-CA-C	-5.53	110.18	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1841	0	1848	56	0
1	g	1885	0	1891	66	0
2	H	1749	0	1750	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	h	1813	0	1806	56	0
3	I	1933	0	1947	49	0
3	i	1971	0	1992	66	0
4	J	1869	0	1891	76	0
4	j	1878	0	1899	52	0
5	L	1864	0	1852	48	0
5	l	1864	0	1852	66	0
6	M	1862	0	1842	59	0
6	m	1881	0	1868	71	0
7	N	1521	0	1494	53	0
7	n	1514	0	1487	55	0
8	O	1659	0	1681	39	0
8	o	1659	0	1681	41	0
9	P	1591	0	1609	72	0
9	p	1591	0	1609	46	0
10	Q	1571	0	1573	70	0
10	q	1571	0	1573	60	0
11	R	1559	0	1523	53	0
11	r	1559	0	1523	46	0
12	S	1643	0	1640	49	0
12	s	1654	0	1656	47	0
13	T	1687	0	1666	48	0
13	t	1687	0	1666	67	0
14	K	1694	0	1691	57	0
14	k	1789	0	1773	53	0
15	f	6292	0	6314	236	0
16	x	635	0	652	16	0
17	a	2969	0	2984	88	0
18	b	1458	0	1505	52	0
19	c	2224	0	2240	103	0
20	d	2063	0	2078	71	0
21	e	407	0	312	15	0
22	U	6648	0	6715	256	0
23	V	3600	0	3668	121	0
24	X	3002	0	3106	68	0
25	Y	3021	0	3022	104	0
26	Z	2248	0	2277	96	0
27	W	3570	0	3696	128	0
28	A	3119	0	3162	105	0
29	B	3060	0	3090	156	0
30	C	2839	0	2942	153	0
31	D	2893	0	2913	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	E	2929	0	2994	168	0
33	F	2699	0	2743	208	0
34	A	31	0	12	1	0
35	B	27	0	12	5	0
35	C	27	0	12	6	0
35	D	27	0	12	4	0
35	E	27	0	12	1	0
35	F	27	0	12	4	0
All	All	104201	0	104768	3369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 3369 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:607:VAL:HB	31:D:68:LEU:CD2	1.37	1.50
22:U:607:VAL:CB	31:D:68:LEU:HD21	1.40	1.48
30:C:56:VAL:CG2	31:D:79:VAL:HG21	1.51	1.40
30:C:56:VAL:HG21	31:D:79:VAL:CG2	1.57	1.30
6:M:41:CYS:SG	6:M:189:ILE:CB	2.32	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	235/246 (96%)	217 (92%)	17 (7%)	1 (0%)	30	62
1	g	241/246 (98%)	229 (95%)	12 (5%)	0	100	100
2	H	224/234 (96%)	197 (88%)	26 (12%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
3	I	245/261 (94%)	232 (95%)	13 (5%)	0	100	100
3	i	248/261 (95%)	241 (97%)	7 (3%)	0	100	100
4	J	235/248 (95%)	205 (87%)	27 (12%)	3 (1%)	9	39
4	j	236/248 (95%)	228 (97%)	8 (3%)	0	100	100
5	L	235/269 (87%)	226 (96%)	8 (3%)	1 (0%)	30	62
5	l	235/269 (87%)	229 (97%)	6 (3%)	0	100	100
6	M	236/255 (92%)	220 (93%)	15 (6%)	1 (0%)	30	62
6	m	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
7	N	201/239 (84%)	197 (98%)	4 (2%)	0	100	100
7	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
8	O	218/277 (79%)	212 (97%)	5 (2%)	1 (0%)	24	57
8	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
9	P	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	Q	194/201 (96%)	189 (97%)	5 (3%)	0	100	100
10	q	194/201 (96%)	191 (98%)	3 (2%)	0	100	100
11	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
11	r	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
12	S	210/241 (87%)	205 (98%)	5 (2%)	0	100	100
12	s	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
13	T	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
13	t	214/264 (81%)	209 (98%)	5 (2%)	0	100	100
14	K	218/241 (90%)	207 (95%)	11 (5%)	0	100	100
14	k	232/241 (96%)	223 (96%)	9 (4%)	0	100	100
15	f	815/908 (90%)	780 (96%)	35 (4%)	0	100	100
16	x	83/230 (36%)	81 (98%)	2 (2%)	0	100	100
17	a	371/376 (99%)	347 (94%)	24 (6%)	0	100	100
18	b	189/377 (50%)	177 (94%)	11 (6%)	1 (0%)	24	57
19	c	285/310 (92%)	254 (89%)	31 (11%)	0	100	100
20	d	250/350 (71%)	211 (84%)	38 (15%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
22	U	853/953 (90%)	801 (94%)	52 (6%)	0	100	100
23	V	442/534 (83%)	427 (97%)	15 (3%)	0	100	100
24	X	378/422 (90%)	366 (97%)	11 (3%)	1 (0%)	36	67
25	Y	378/389 (97%)	346 (92%)	31 (8%)	1 (0%)	36	67
26	Z	284/324 (88%)	256 (90%)	27 (10%)	1 (0%)	30	62
27	W	442/456 (97%)	417 (94%)	23 (5%)	2 (0%)	24	57
28	A	401/433 (93%)	351 (88%)	45 (11%)	5 (1%)	10	41
29	B	398/440 (90%)	338 (85%)	55 (14%)	5 (1%)	9	39
30	C	362/398 (91%)	315 (87%)	44 (12%)	3 (1%)	16	49
31	D	370/418 (88%)	308 (83%)	57 (15%)	5 (1%)	9	38
32	E	368/403 (91%)	340 (92%)	27 (7%)	1 (0%)	36	67
33	F	349/439 (80%)	309 (88%)	35 (10%)	5 (1%)	9	38
All	All	13230/15118 (88%)	12367 (94%)	824 (6%)	39 (0%)	37	67

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	164	LYS
6	M	104	TYR
29	B	256	ILE
29	B	435	PRO
30	C	87	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	G	201/210 (96%)	199 (99%)	2 (1%)	68	75
1	g	206/210 (98%)	206 (100%)	0	100	100
2	H	184/191 (96%)	183 (100%)	1 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	h	190/191 (100%)	190 (100%)	0	100	100
3	I	205/221 (93%)	205 (100%)	0	100	100
3	i	210/221 (95%)	210 (100%)	0	100	100
4	J	201/211 (95%)	201 (100%)	0	100	100
4	j	202/211 (96%)	202 (100%)	0	100	100
5	L	203/230 (88%)	201 (99%)	2 (1%)	68	75
5	l	203/230 (88%)	203 (100%)	0	100	100
6	M	195/212 (92%)	193 (99%)	2 (1%)	68	75
6	m	198/212 (93%)	198 (100%)	0	100	100
7	N	158/181 (87%)	158 (100%)	0	100	100
7	n	157/181 (87%)	157 (100%)	0	100	100
8	O	181/228 (79%)	181 (100%)	0	100	100
8	o	181/228 (79%)	181 (100%)	0	100	100
9	P	173/174 (99%)	173 (100%)	0	100	100
9	p	173/174 (99%)	173 (100%)	0	100	100
10	Q	167/171 (98%)	167 (100%)	0	100	100
10	q	167/171 (98%)	167 (100%)	0	100	100
11	R	156/202 (77%)	156 (100%)	0	100	100
11	r	156/202 (77%)	156 (100%)	0	100	100
12	S	177/199 (89%)	177 (100%)	0	100	100
12	s	178/199 (89%)	178 (100%)	0	100	100
13	T	179/215 (83%)	179 (100%)	0	100	100
13	t	179/215 (83%)	179 (100%)	0	100	100
14	K	187/203 (92%)	185 (99%)	2 (1%)	65	74
14	k	196/203 (97%)	196 (100%)	0	100	100
15	f	682/763 (89%)	682 (100%)	0	100	100
16	x	73/207 (35%)	73 (100%)	0	100	100
17	a	329/336 (98%)	329 (100%)	0	100	100
18	b	167/312 (54%)	167 (100%)	0	100	100
19	c	247/268 (92%)	247 (100%)	0	100	100
20	d	224/294 (76%)	224 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	e	42/63 (67%)	42 (100%)	0	100	100
22	U	727/816 (89%)	727 (100%)	0	100	100
23	V	388/460 (84%)	388 (100%)	0	100	100
24	X	326/362 (90%)	326 (100%)	0	100	100
25	Y	320/344 (93%)	320 (100%)	0	100	100
26	Z	252/295 (85%)	252 (100%)	0	100	100
27	W	402/416 (97%)	402 (100%)	0	100	100
28	A	338/372 (91%)	334 (99%)	4 (1%)	63	73
29	B	333/385 (86%)	325 (98%)	8 (2%)	43	64
30	C	313/346 (90%)	313 (100%)	0	100	100
31	D	312/366 (85%)	309 (99%)	3 (1%)	68	75
32	E	323/353 (92%)	321 (99%)	2 (1%)	78	79
33	F	290/379 (76%)	289 (100%)	1 (0%)	86	83
All	All	11251/12833 (88%)	11224 (100%)	27 (0%)	85	85

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	B	123	VAL
29	B	232	LYS
32	E	30	ARG
29	B	210	TYR
29	B	239	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
29	B	181	GLN
30	C	206	HIS
33	F	130	GLN
12	s	157	ASN
12	s	151	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
35	ADP	D	501	-	28,29,29	1.43	5 (17%)	43,45,45	1.91	8 (18%)
35	ADP	F	501	-	28,29,29	1.43	5 (17%)	43,45,45	1.87	8 (18%)
35	ADP	B	501	-	28,29,29	1.45	5 (17%)	43,45,45	1.85	9 (20%)
35	ADP	E	501	-	28,29,29	1.26	3 (10%)	43,45,45	1.79	7 (16%)
34	ATP	A	501	-	32,33,33	0.26	0	48,52,52	0.31	0
35	ADP	C	501	-	28,29,29	1.48	5 (17%)	43,45,45	1.89	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ADP	D	501	-	-	4/16/32/32	0/3/3/3
35	ADP	F	501	-	-	3/16/32/32	0/3/3/3
35	ADP	B	501	-	-	3/16/32/32	0/3/3/3
35	ADP	E	501	-	-	2/16/32/32	0/3/3/3
34	ATP	A	501	-	-	6/22/38/38	0/3/3/3
35	ADP	C	501	-	-	1/16/32/32	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	501	ADP	C5-C4	4.83	1.47	1.39
35	C	501	ADP	C5-C4	4.81	1.47	1.39
35	B	501	ADP	C5-C4	4.77	1.47	1.39
35	D	501	ADP	C5-C4	4.74	1.47	1.39
35	E	501	ADP	C5-C4	4.03	1.46	1.39

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	501	ADP	C5-C4-N3	-6.40	117.91	126.72
35	F	501	ADP	C5-C4-N3	-6.23	118.14	126.72
35	D	501	ADP	C5-C4-N3	-6.13	118.28	126.72
35	C	501	ADP	C5-C4-N3	-6.00	118.46	126.72
35	B	501	ADP	C5-C4-N3	-5.84	118.67	126.72

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	501	ADP	C5'-O5'-PA-O1A
35	B	501	ADP	C5'-O5'-PA-O2A
35	D	501	ADP	C2'-C1'-N9-C8
35	E	501	ADP	C5'-O5'-PA-O2A
35	E	501	ADP	C5'-O5'-PA-O3A

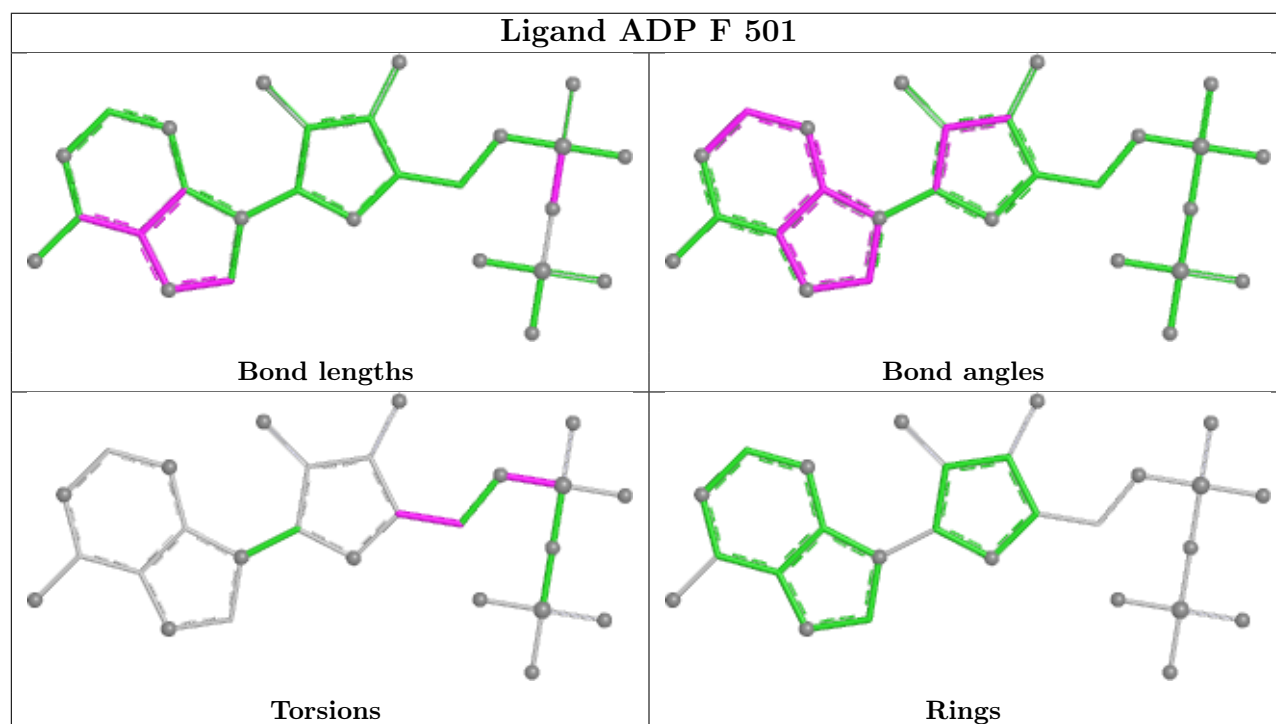
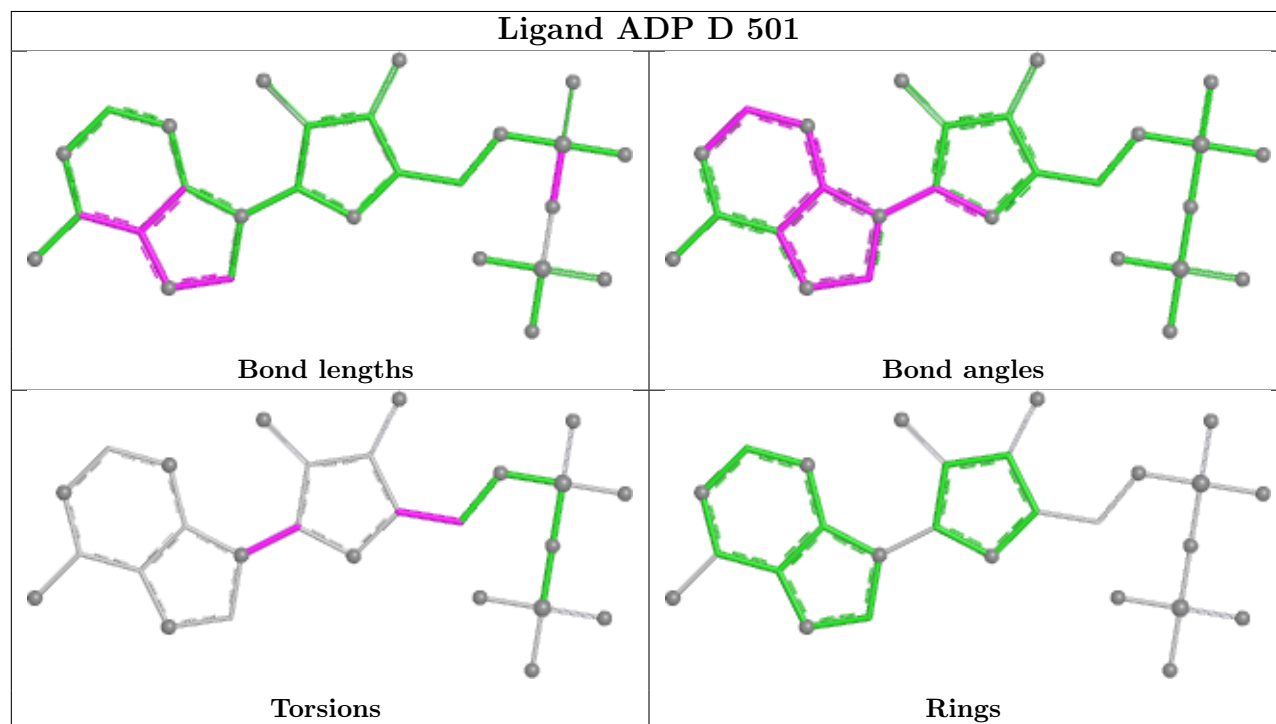
There are no ring outliers.

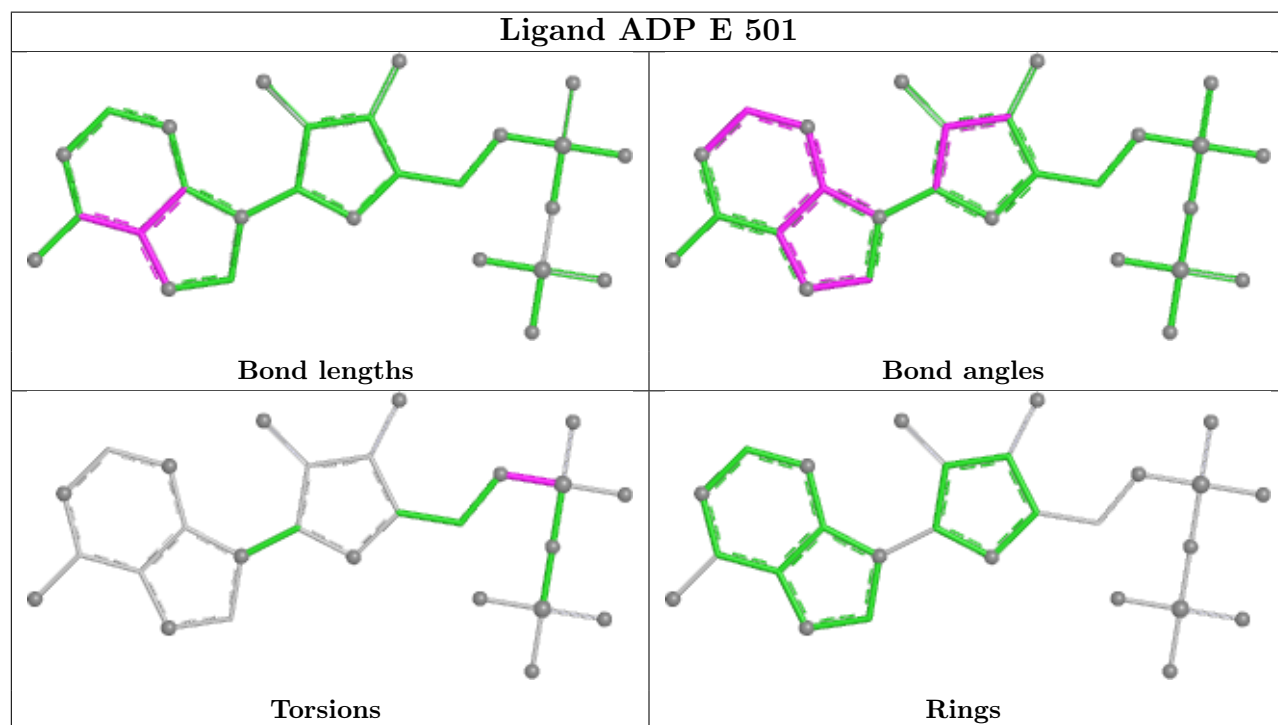
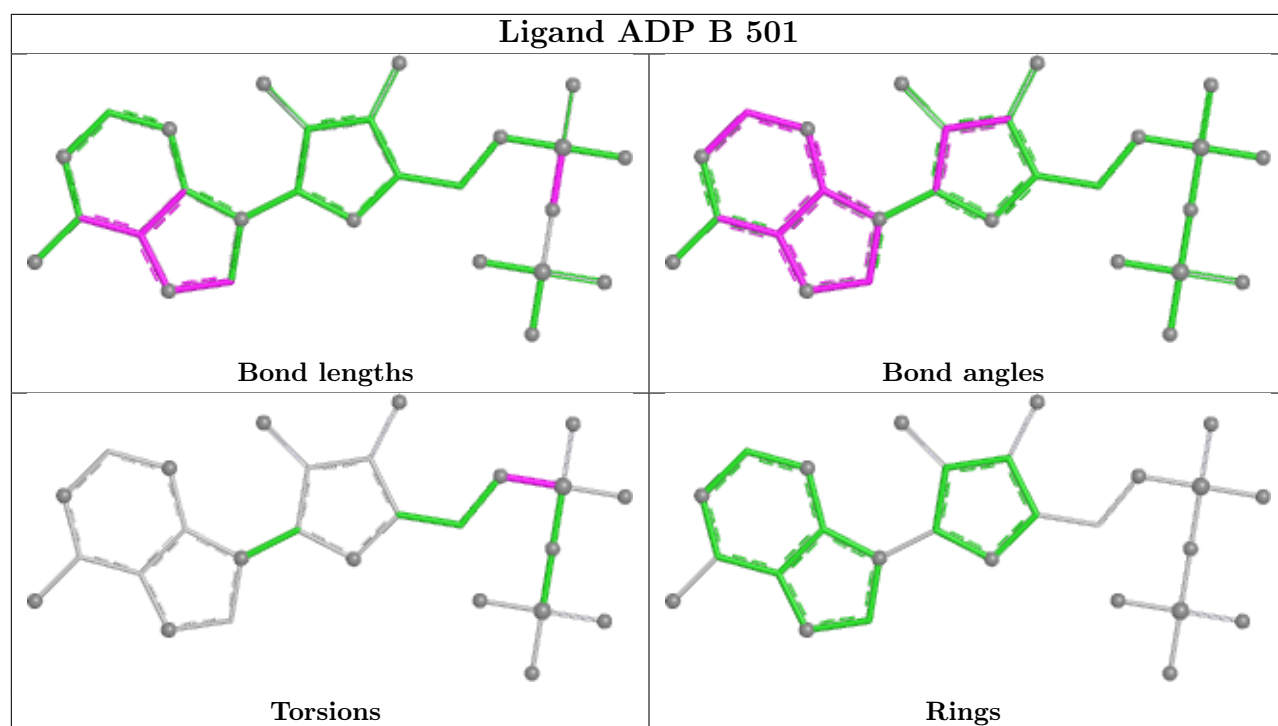
6 monomers are involved in 21 short contacts:

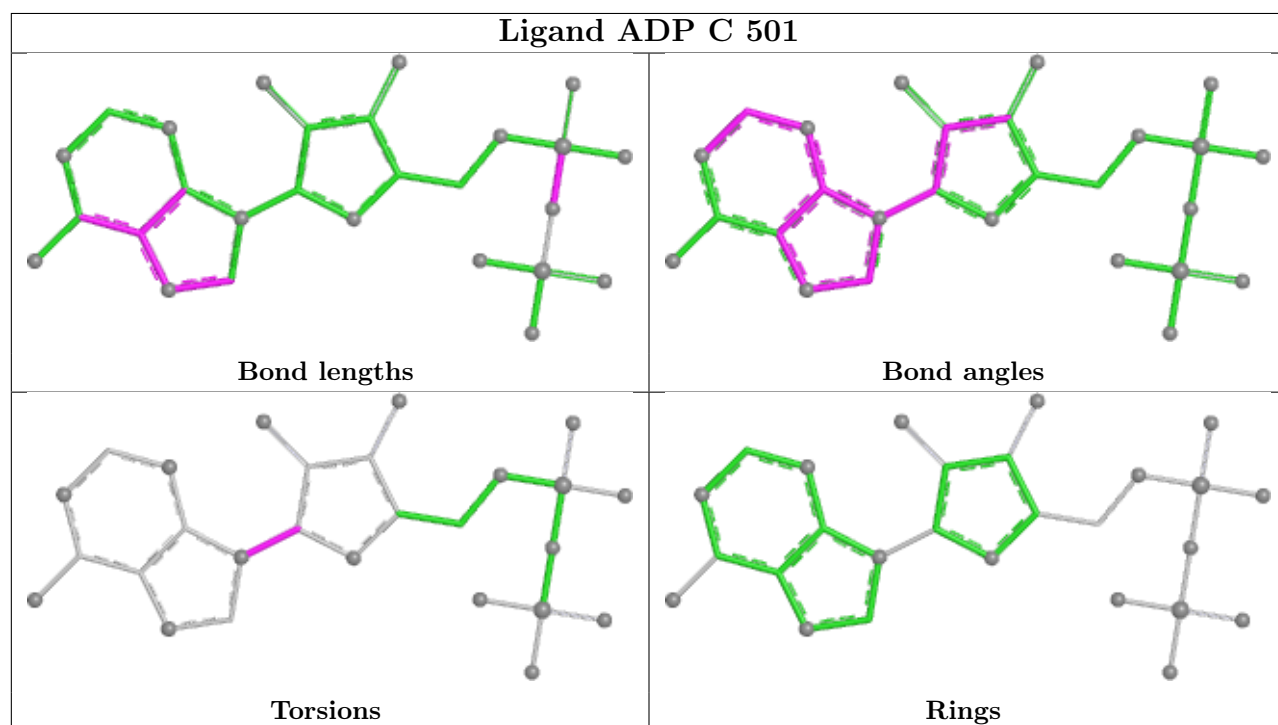
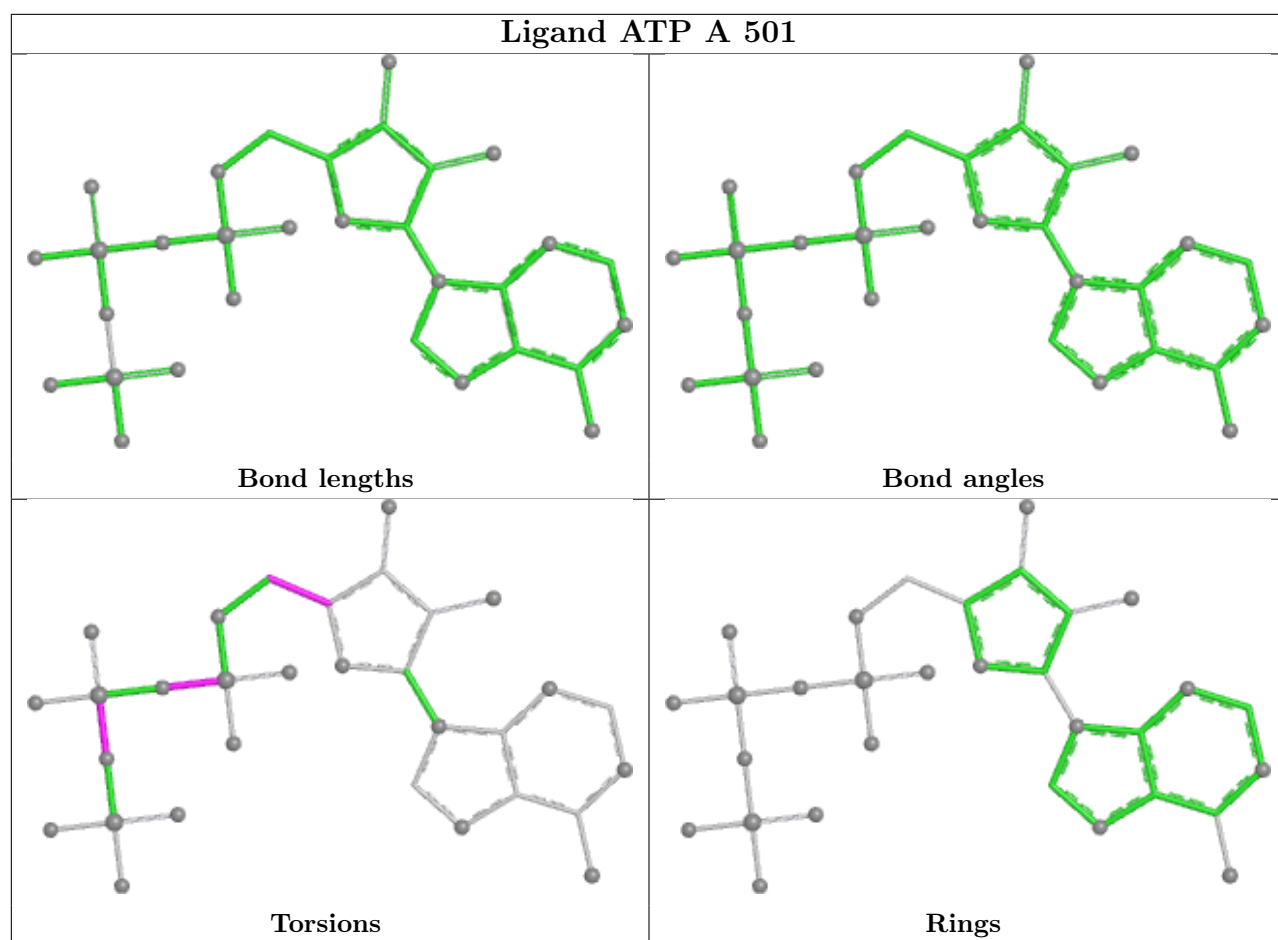
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	D	501	ADP	4	0
35	F	501	ADP	4	0
35	B	501	ADP	5	0
35	E	501	ADP	1	0
34	A	501	ATP	1	0
35	C	501	ADP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

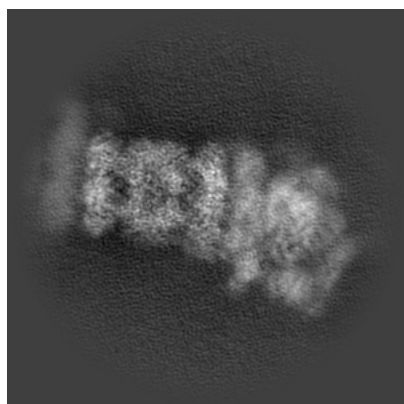
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52193. These allow visual inspection of the internal detail of the map and identification of artifacts.

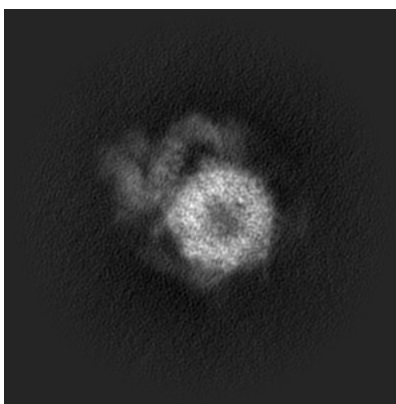
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

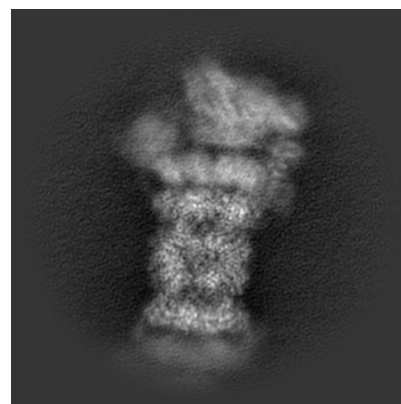
6.1.1 Primary map



X

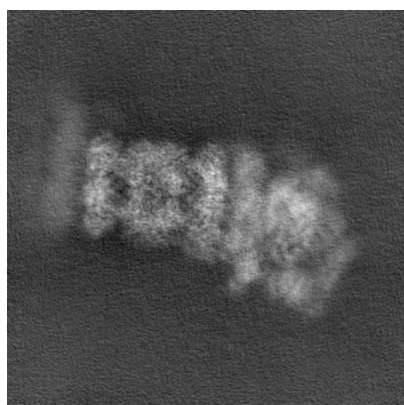


Y

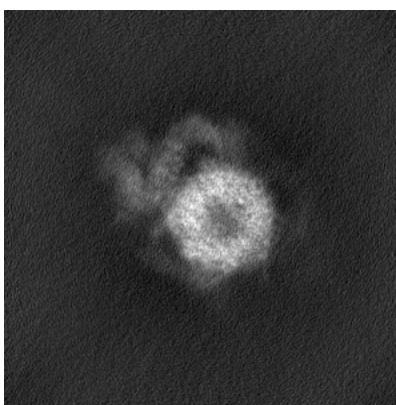


Z

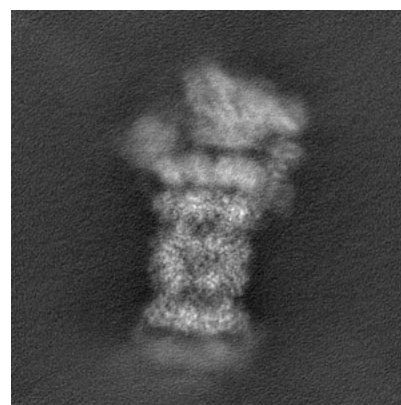
6.1.2 Raw map



X



Y

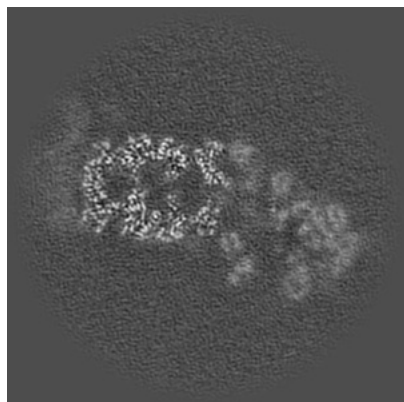


Z

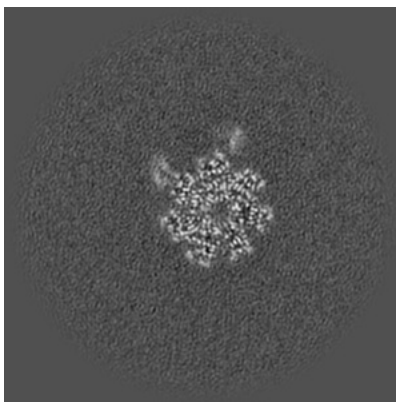
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

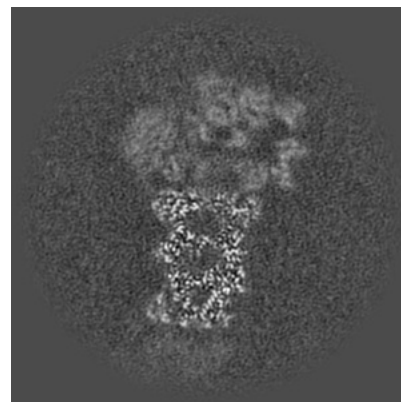
6.2.1 Primary map



X Index: 150

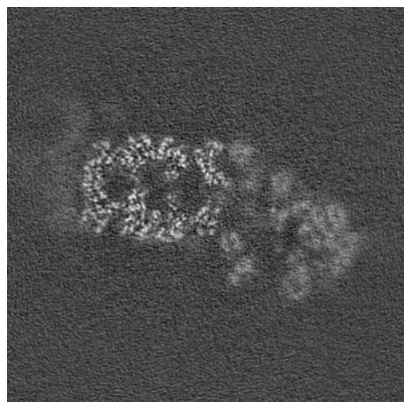


Y Index: 150

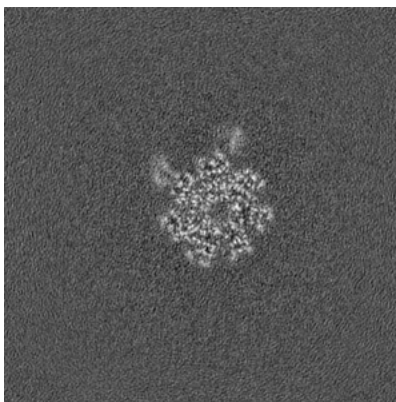


Z Index: 150

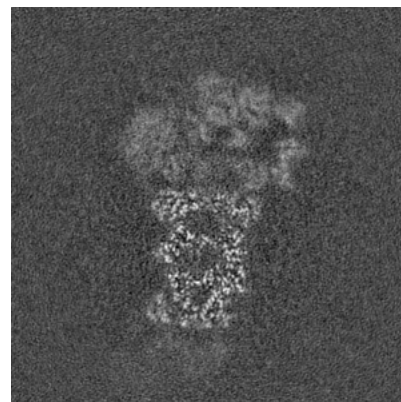
6.2.2 Raw map



X Index: 150



Y Index: 150

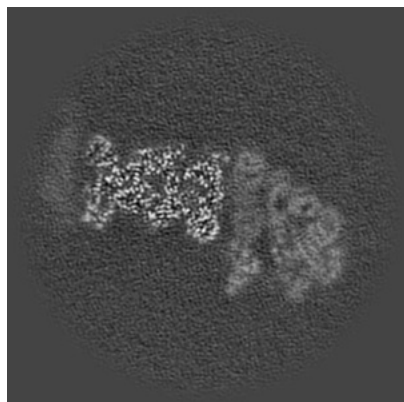


Z Index: 150

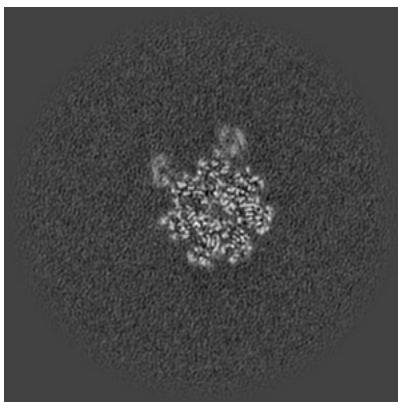
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

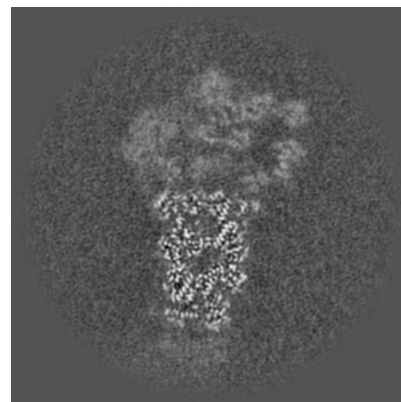
6.3.1 Primary map



X Index: 161

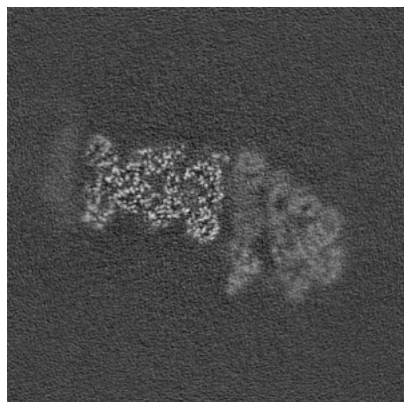


Y Index: 152

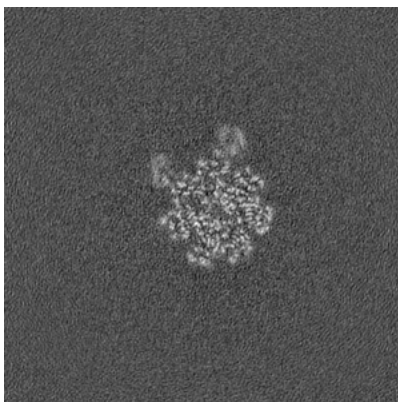


Z Index: 147

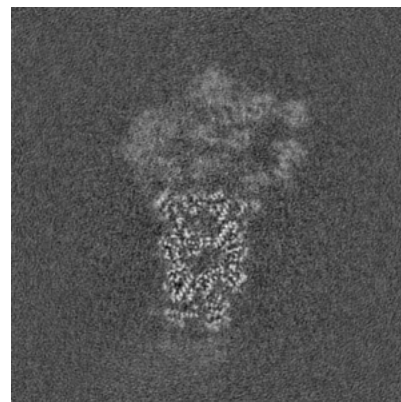
6.3.2 Raw map



X Index: 161



Y Index: 152

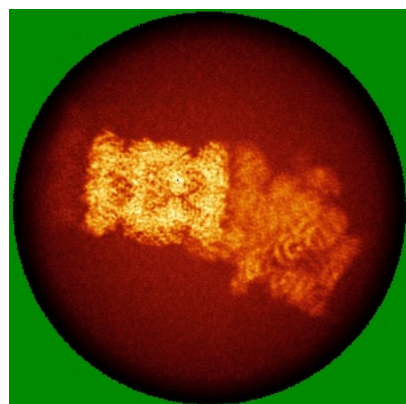


Z Index: 147

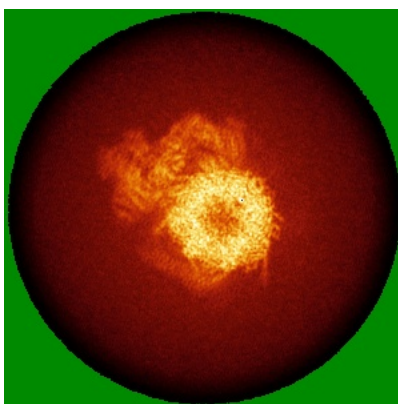
The images above show the largest variance slices of the map in three orthogonal directions.

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

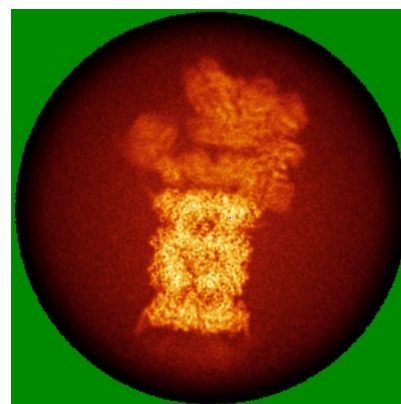
6.4.1 Primary map



X

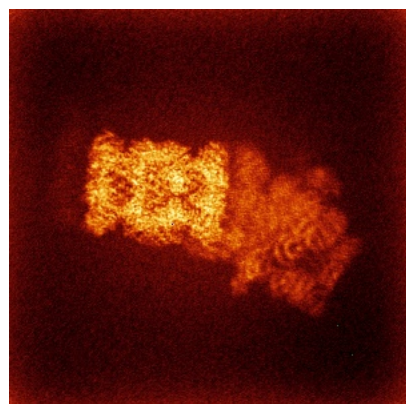


Y

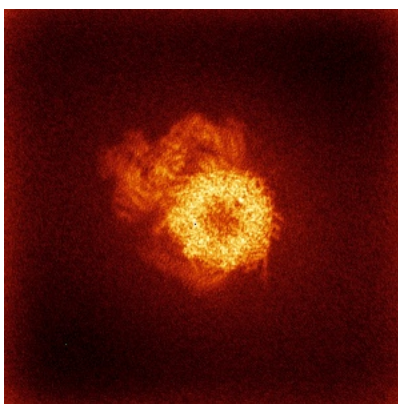


Z

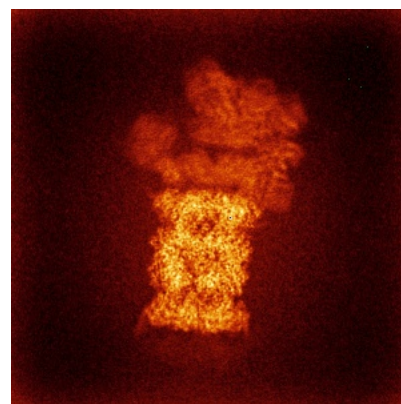
6.4.2 Raw map



X



Y

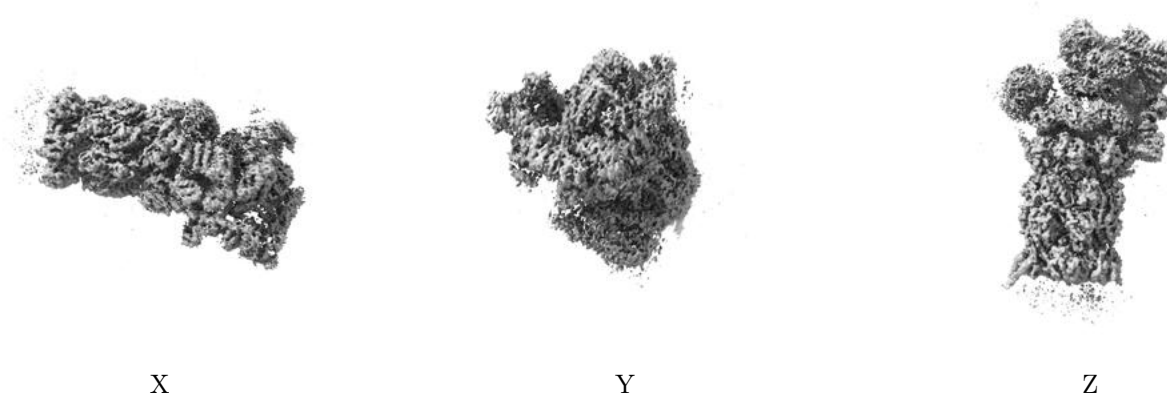


Z

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

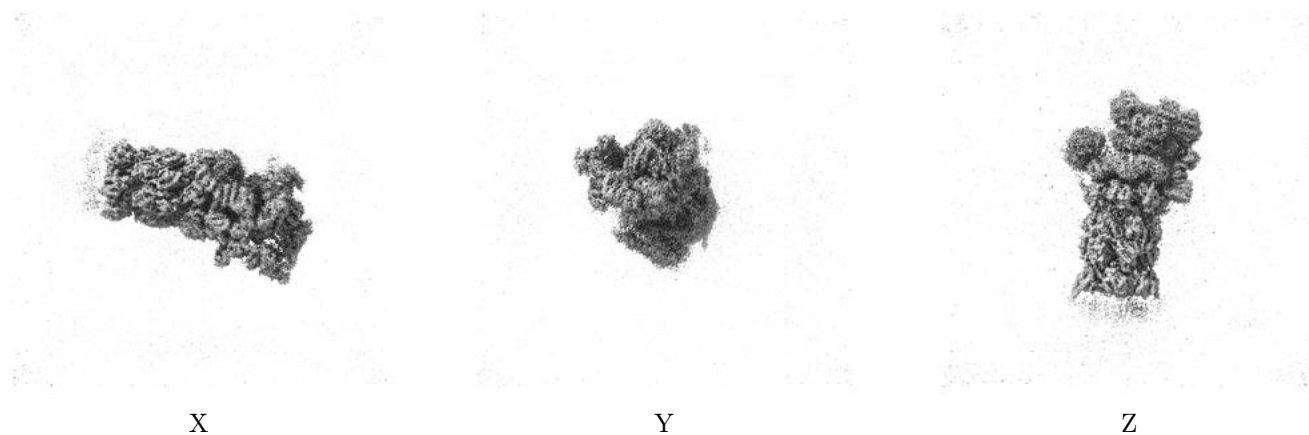
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

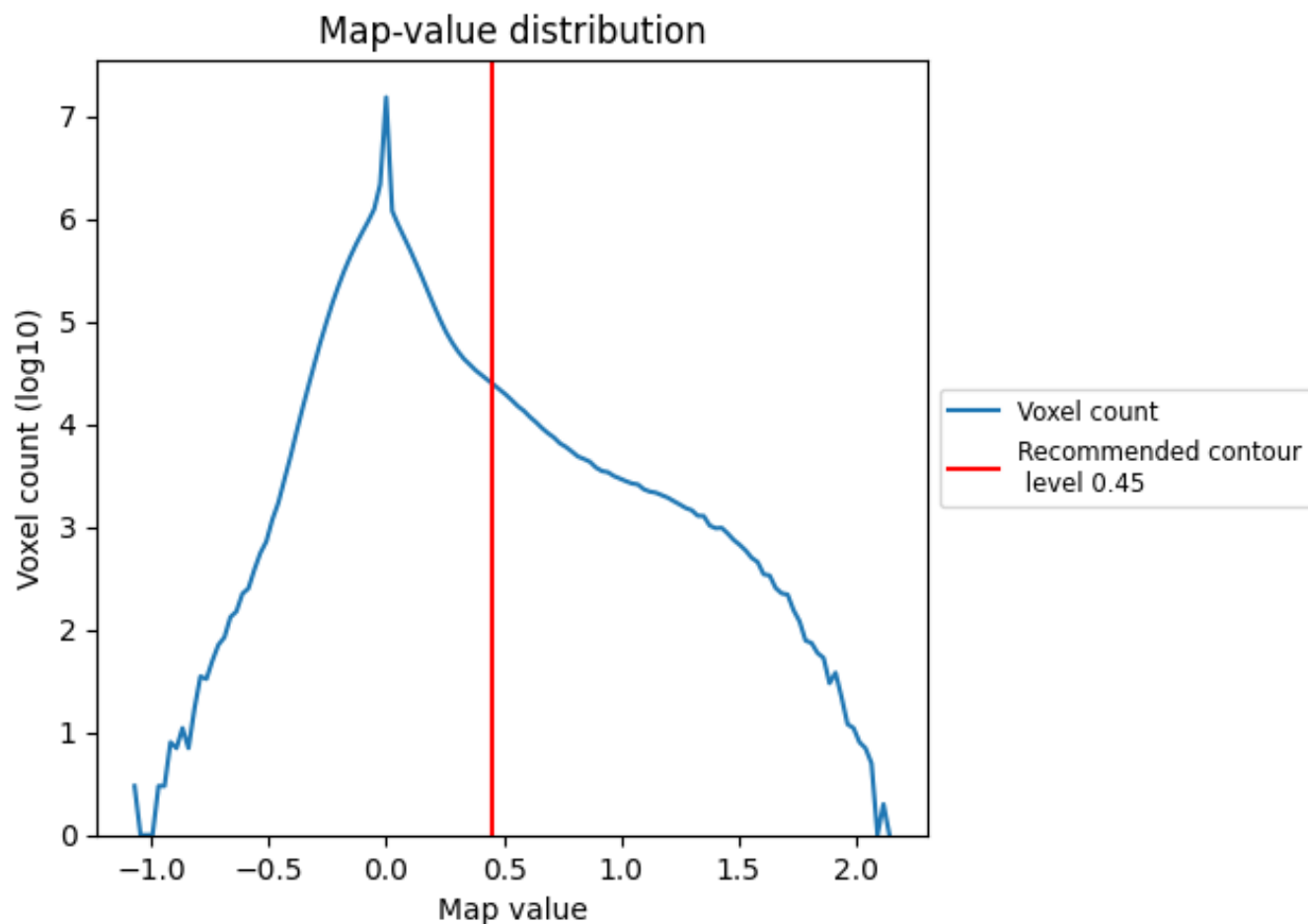
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

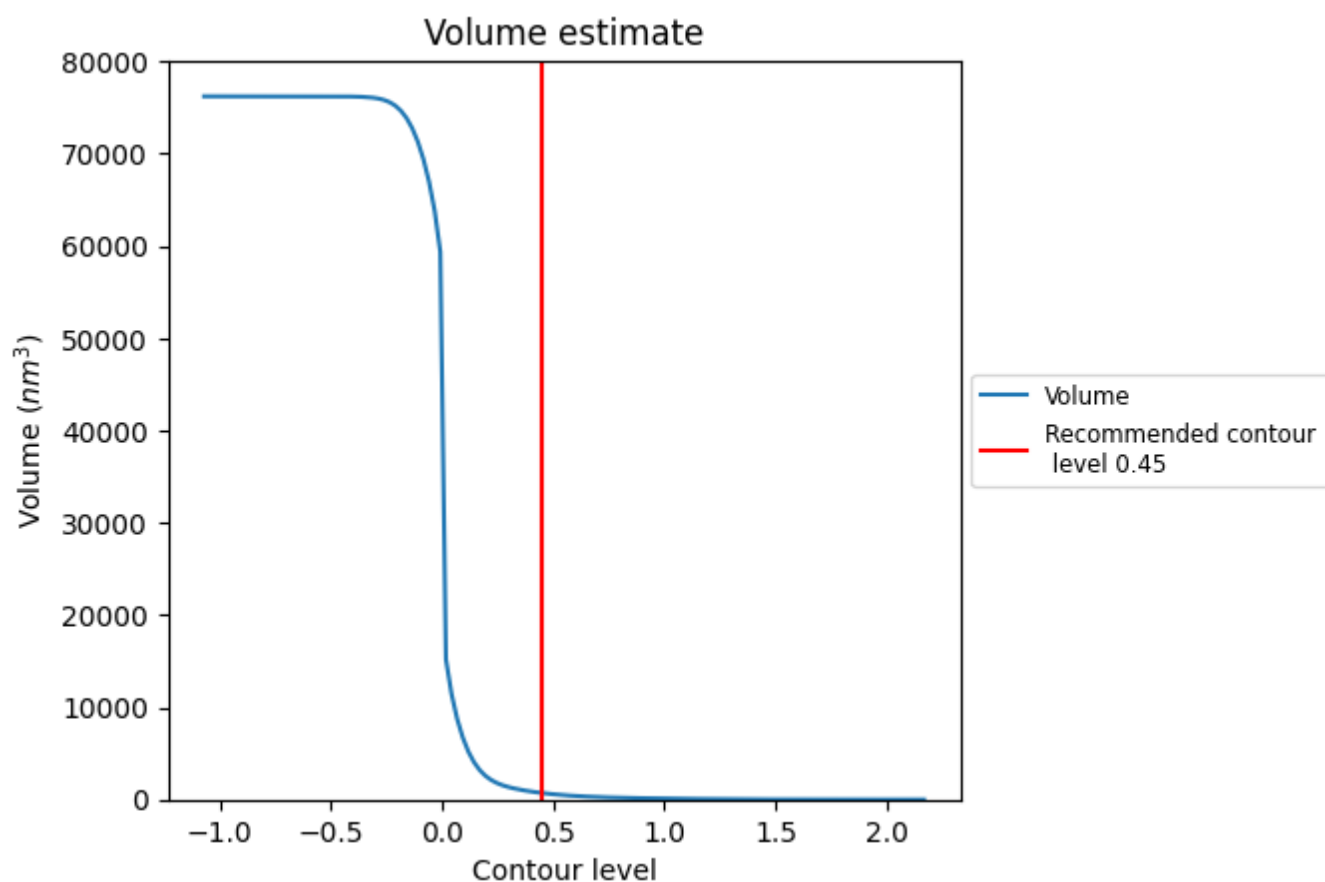
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

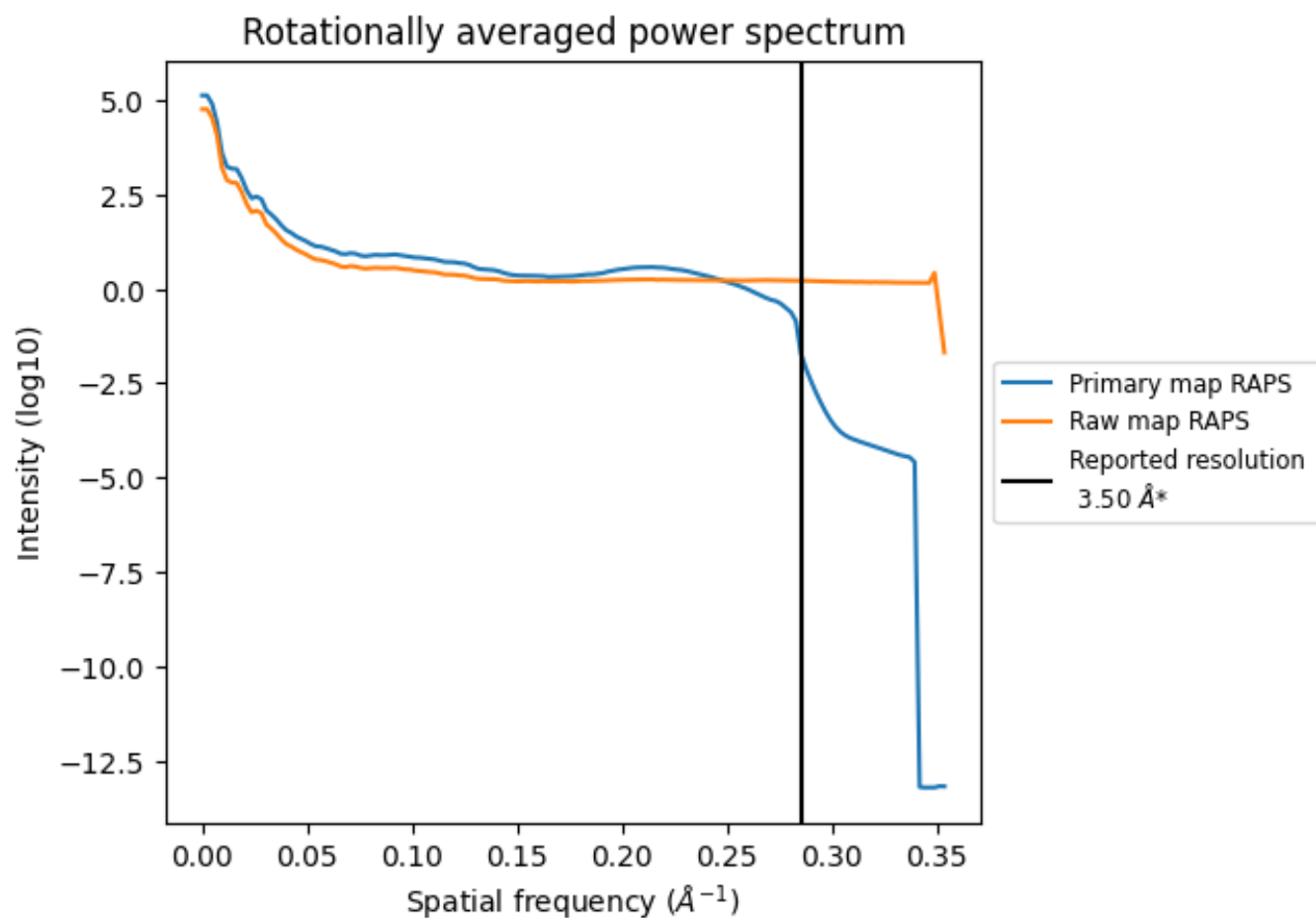
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 707 nm³; this corresponds to an approximate mass of 639 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 ⓘ

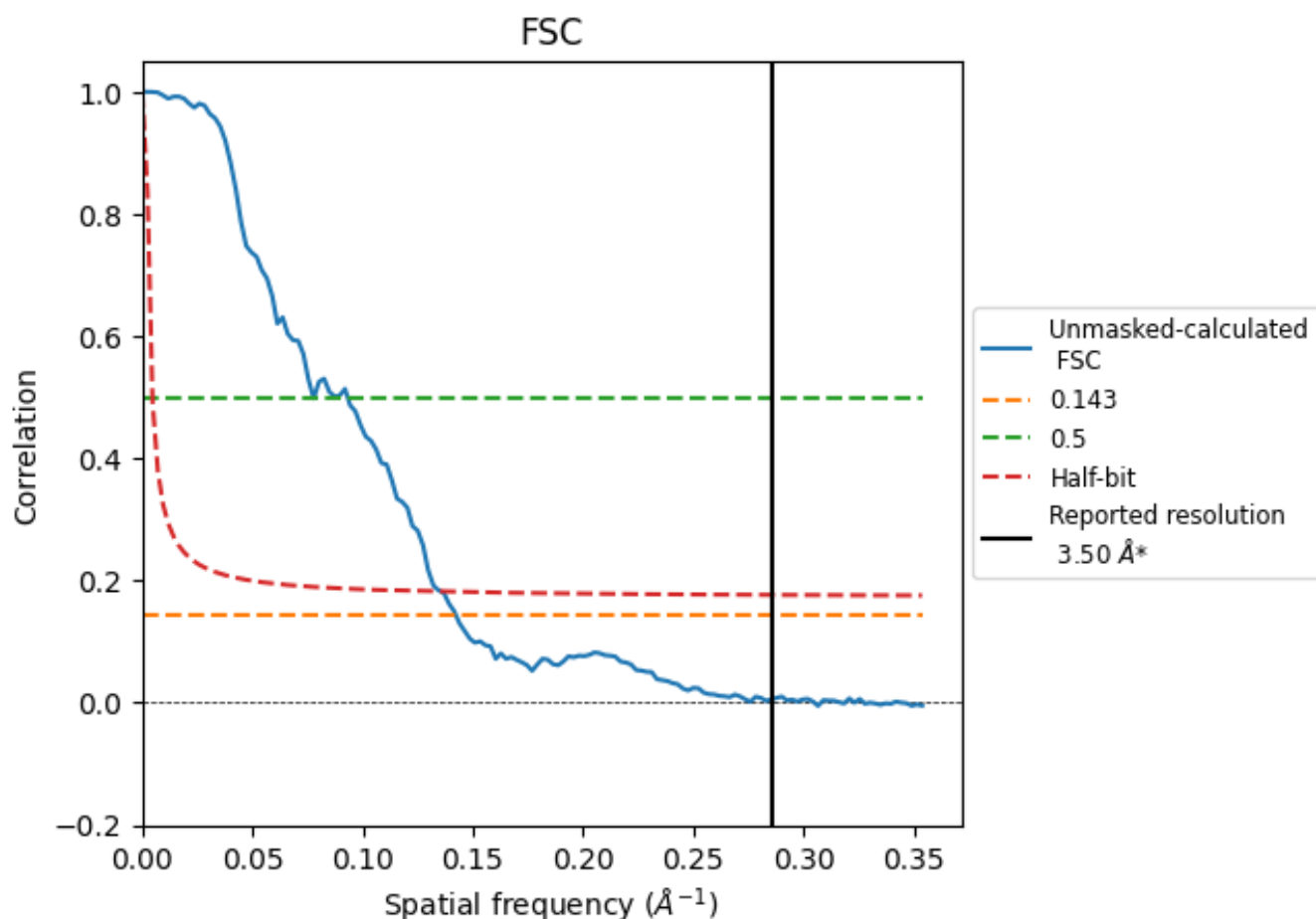


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

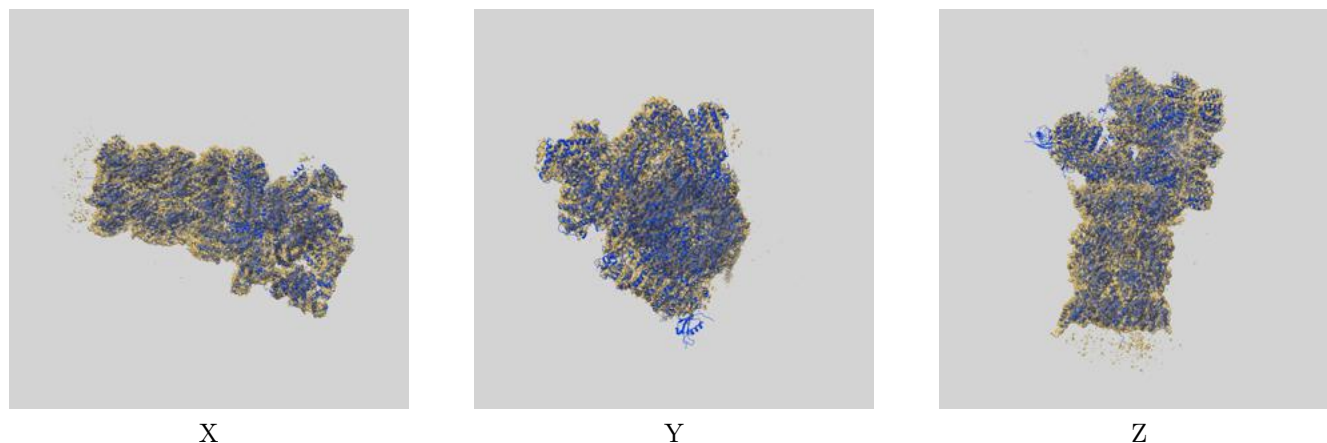
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.03	12.87	7.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.03 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52193 and PDB model 9SZT. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



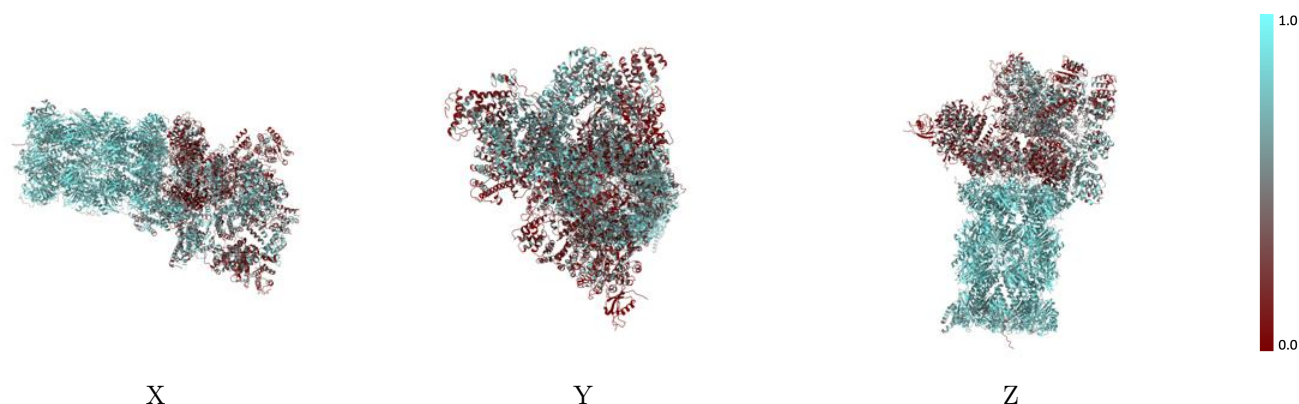
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



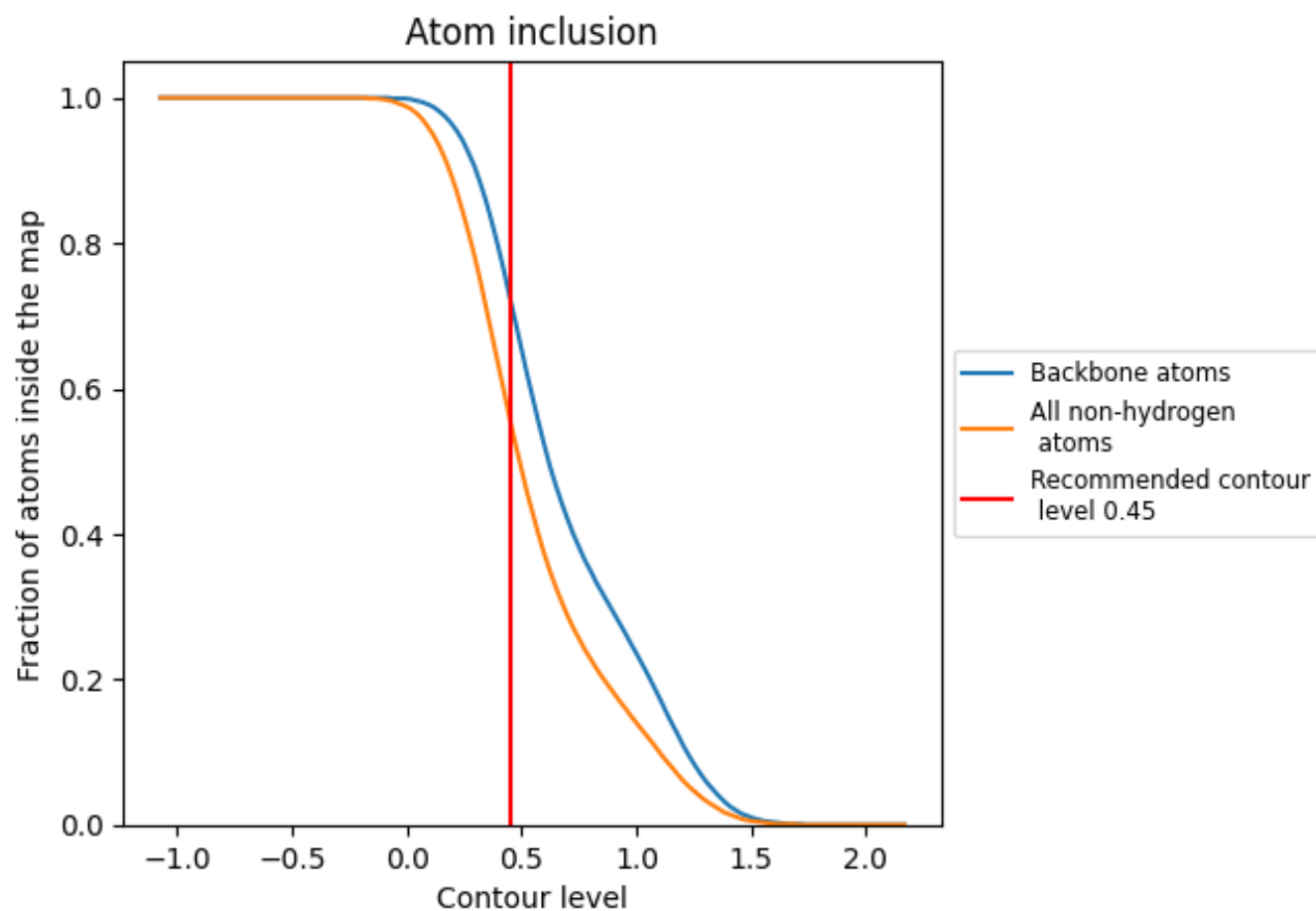
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 56% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5570	 0.2350
A	 0.2980	 0.0840
B	 0.3190	 0.1180
C	 0.3690	 0.1320
D	 0.2030	 0.0980
E	 0.1840	 0.0510
F	 0.2960	 0.0730
G	 0.7780	 0.3830
H	 0.7570	 0.3640
I	 0.7510	 0.3740
J	 0.7170	 0.3310
K	 0.7590	 0.3660
L	 0.7840	 0.3940
M	 0.7840	 0.3810
N	 0.8060	 0.4150
O	 0.8250	 0.4180
P	 0.8230	 0.4260
Q	 0.8100	 0.4220
R	 0.8460	 0.4250
S	 0.8230	 0.4230
T	 0.8230	 0.4130
U	 0.4040	 0.0960
V	 0.3840	 0.1090
W	 0.5770	 0.1670
X	 0.6090	 0.2250
Y	 0.5590	 0.1520
Z	 0.4550	 0.1190
a	 0.4260	 0.1070
b	 0.2220	 0.0580
c	 0.4300	 0.1110
d	 0.2790	 0.0810
e	 0.3250	 0.0810
f	 0.2620	 0.0800
g	 0.7170	 0.3410
h	 0.7160	 0.3360



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Chain	Atom inclusion	Q-score
i	 0.7170	 0.3190
j	 0.7230	 0.3350
k	 0.7280	 0.3430
l	 0.7600	 0.3540
m	 0.7480	 0.3470
n	 0.8120	 0.4110
o	 0.7990	 0.3970
p	 0.8010	 0.4040
q	 0.8140	 0.4100
r	 0.8340	 0.4190
s	 0.8010	 0.4060
t	 0.8020	 0.4110
x	 0.0030	 0.0290