



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 05:04 PM UTC

PDB ID : 4CR4 / pdb_00004cr4
EMDB ID : EMD-2596
Title : Deep classification of a large cryo-EM dataset defines the conformational landscape of the 26S proteasome
Authors : Unverdorben, P.; Beck, F.; Sledz, P.; Schweitzer, A.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Foerster, F.
Deposited on : 2014-02-25
Resolution : 8.80 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
MolProbity : 4-5-2 with Phenix2.0
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

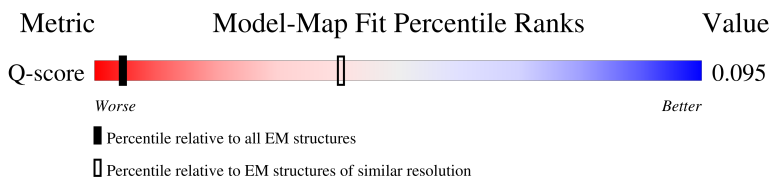
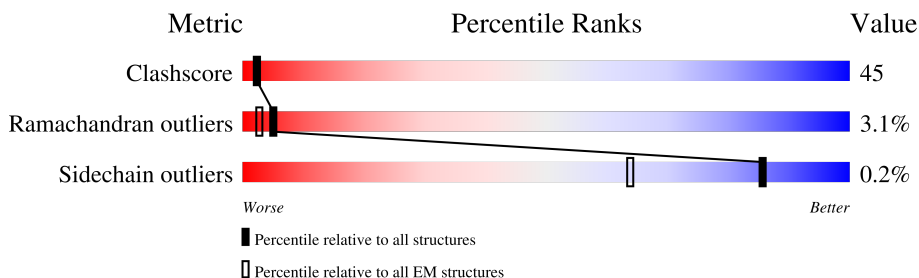
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	265 (8.30 - 9.30)

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	1	215	
2	2	261	
3	3	205	
4	4	198	

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Mol	Chain	Length	Quality of chain
5	5	287	
6	6	241	
7	7	266	
8	A	252	
9	B	250	
10	C	258	
11	D	254	
12	E	260	
13	F	234	
14	G	288	
15	H	467	
16	I	437	
17	J	405	
18	K	428	
19	L	437	
20	M	434	
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	

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Mol	Chain	Length	Quality of chain
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 80139 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 COMPONENT PRE3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

- Molecule 2 is a protein called PROTEASOME COMPONENT PUP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	223	Total	C	N	O	S	0	0
			1692	1067	294	324	7		

- Molecule 3 is a protein called PROTEASOME COMPONENT PUP3.

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

- Molecule 4 is a protein called PROTEASOME COMPONENT C11.

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

- Molecule 5 is a protein called PROTEASOME COMPONENT PRE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1646	1045	282	312	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	33	ARG	LYS	SEE REMARK 999	UNP P30656

- Molecule 6 is a protein called PROTEASOME COMPONENT C5.

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

- Molecule 7 is a protein called PROTEASOME COMPONENT PRE4.

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

- Molecule 8 is a protein called PROTEASOME COMPONENT C7-ALPHA.

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

- Molecule 9 is a protein called PROTEASOME COMPONENT Y7.

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

- Molecule 10 is a protein called PROTEASOME COMPONENT Y13.

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

- Molecule 11 is a protein called PROTEASOME COMPONENT PRE6.

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

- Molecule 12 is a protein called PROTEASOME COMPONENT PUP2.

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

- Molecule 13 is a protein called PROTEASOME COMPONENT PRE5.

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

- Molecule 14 is a protein called PROTEASOME COMPONENT C1.

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

- Molecule 15 is a protein called 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG.

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

- Molecule 16 is a protein called 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG.

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

- Molecule 17 is a protein called 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG.

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

- Molecule 18 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG.

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

- Molecule 19 is a protein called 26S PROTEASE SUBUNIT RPT4.

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

- Molecule 20 is a protein called 26S PROTEASE REGULATORY SUBUNIT 6A.

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

- Molecule 21 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN2.

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

- Molecule 22 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN9.

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

- Molecule 23 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	415	Total	C	N	O	S	0	0
			3401	2166	571	655	9		

- Molecule 24 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN6.

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

- Molecule 25 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN7.

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

- Molecule 26 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN3.

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

- Molecule 27 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN12.

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

- Molecule 28 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN8.

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

- Molecule 29 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	247	Total	C	N	O	S	0	0
			1942	1225	328	376	13		

- Molecule 30 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN10.

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

- Molecule 31 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN13.

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

- Molecule 32 is a protein called 26S PROTEASOME COMPLEX SUBUNIT SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	19	Total	C	N	O	0	0
			168	101	30	37		

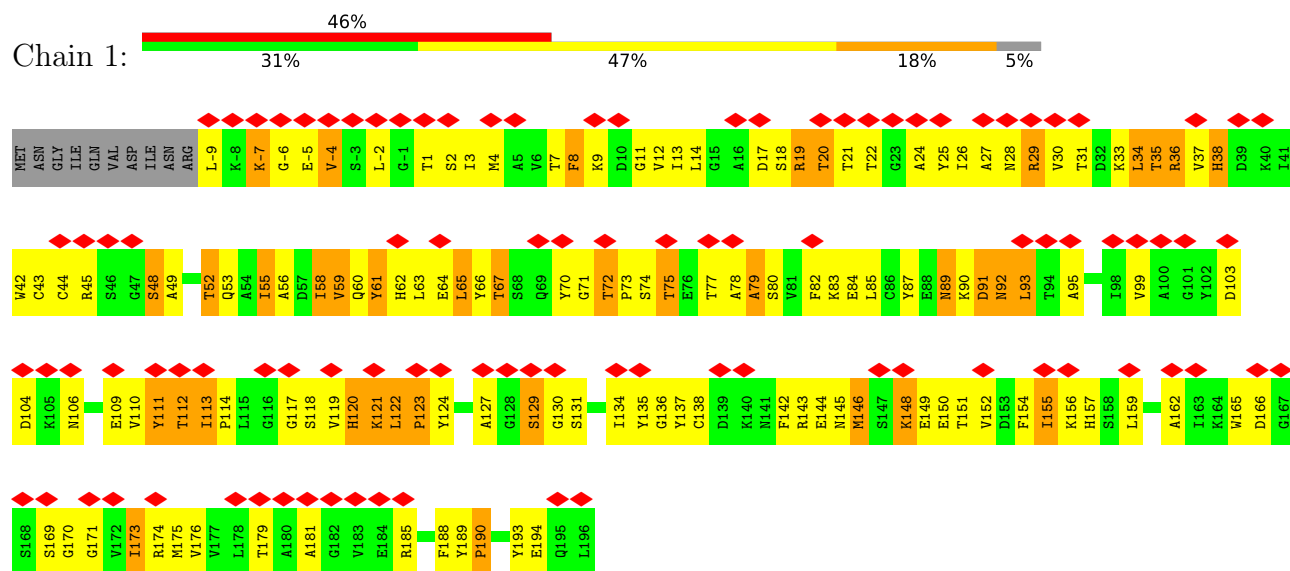
- Molecule 33 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN1.

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

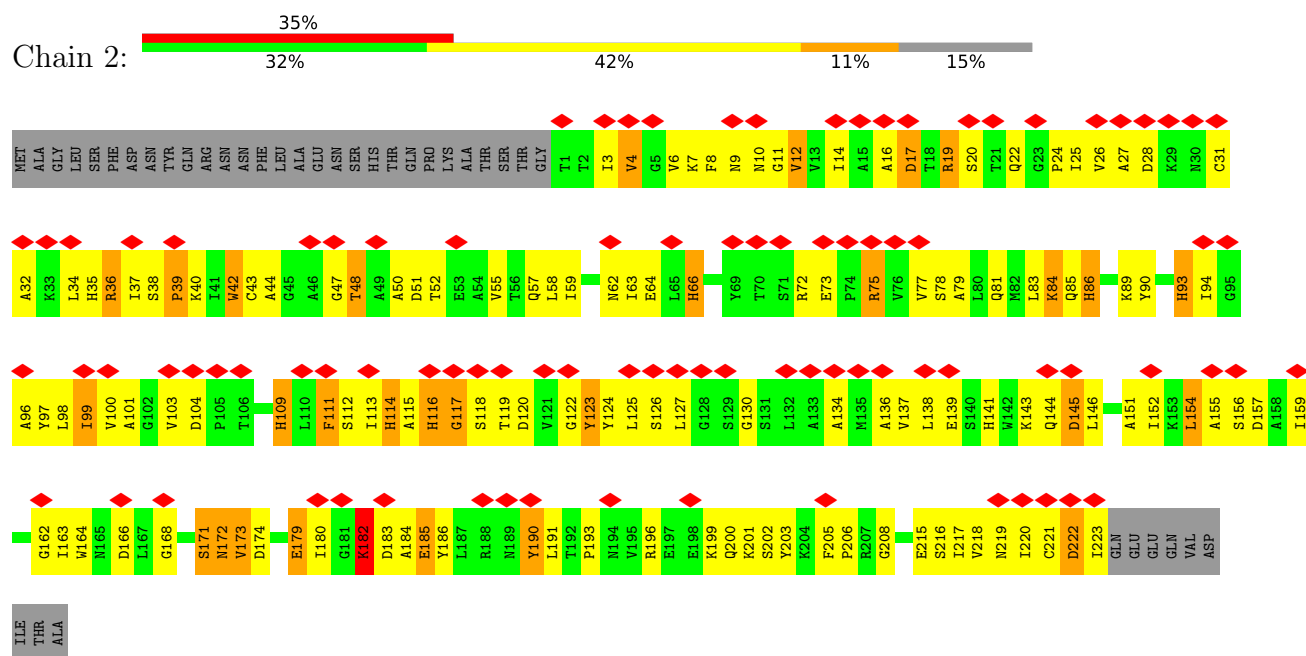
3 Residue-property plots

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.

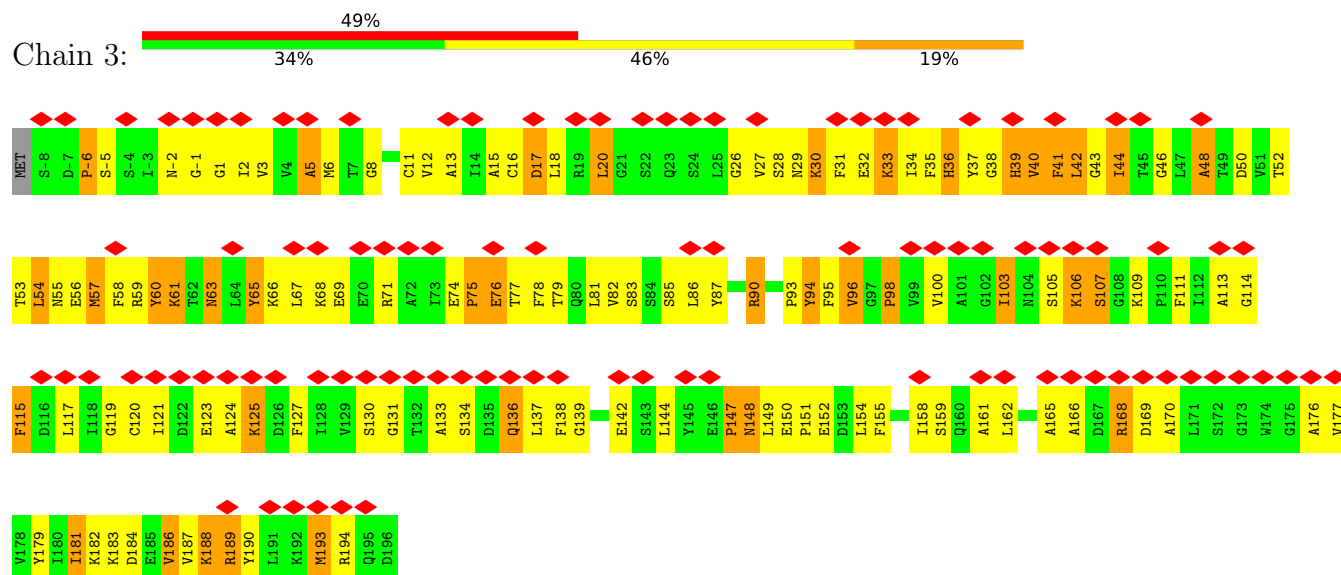
• Molecule 1: PROTEASOME COMPONENT PRE3



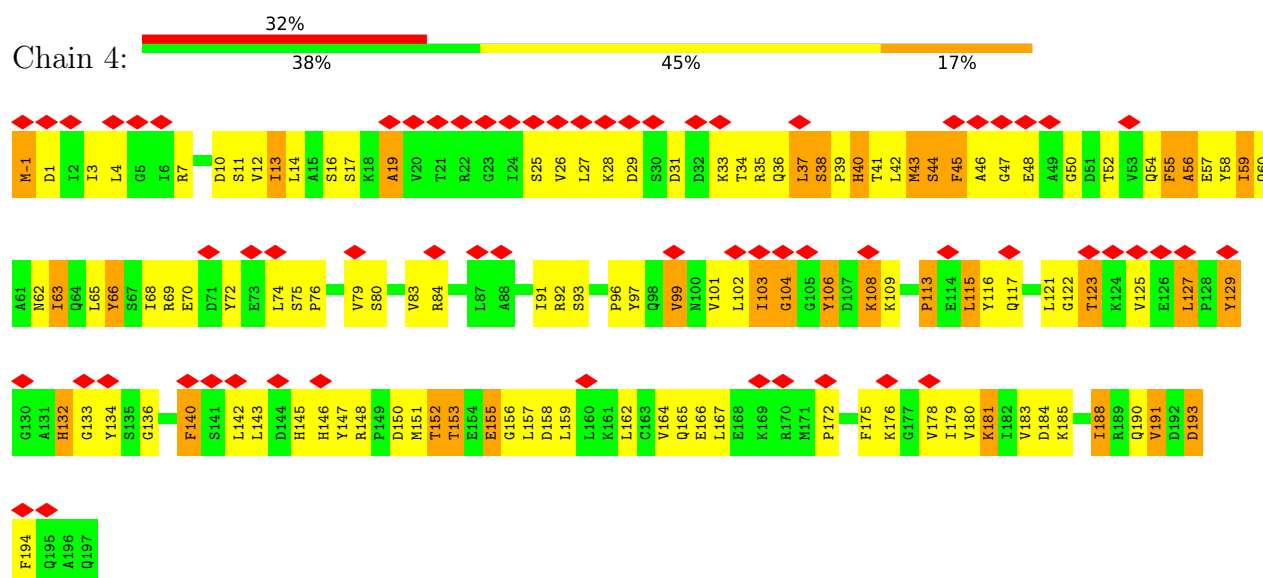
• Molecule 2: PROTEASOME COMPONENT PUP1



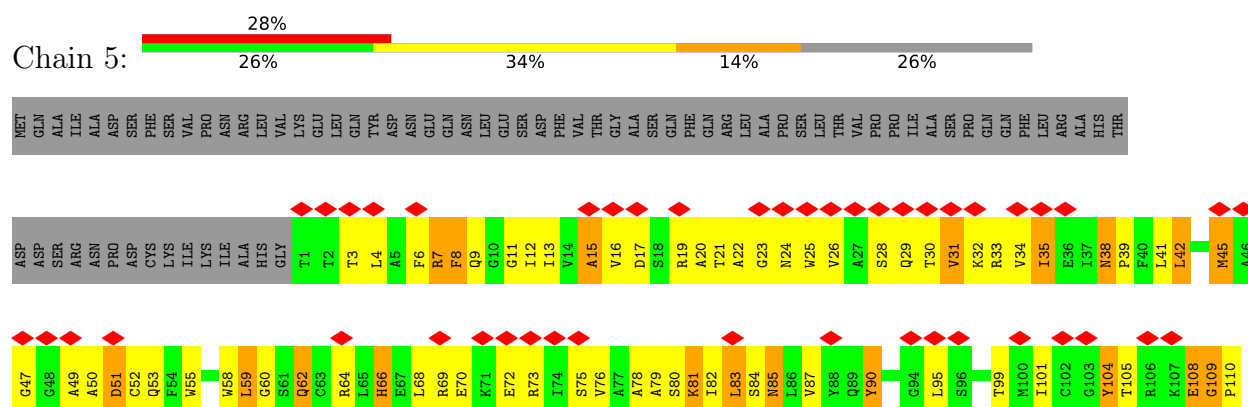
• Molecule 3: PROTEASOME COMPONENT PUP3

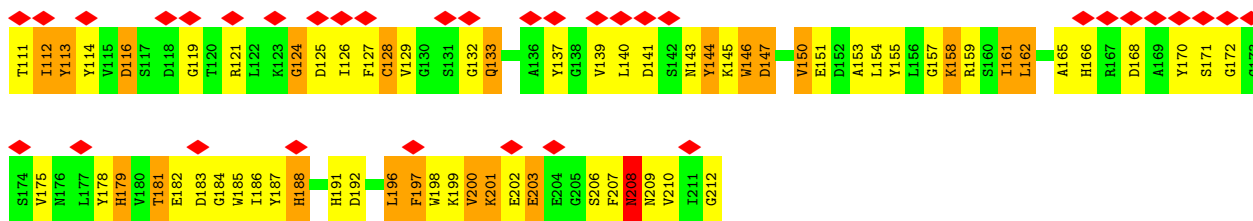


• Molecule 4: PROTEASOME COMPONENT C11

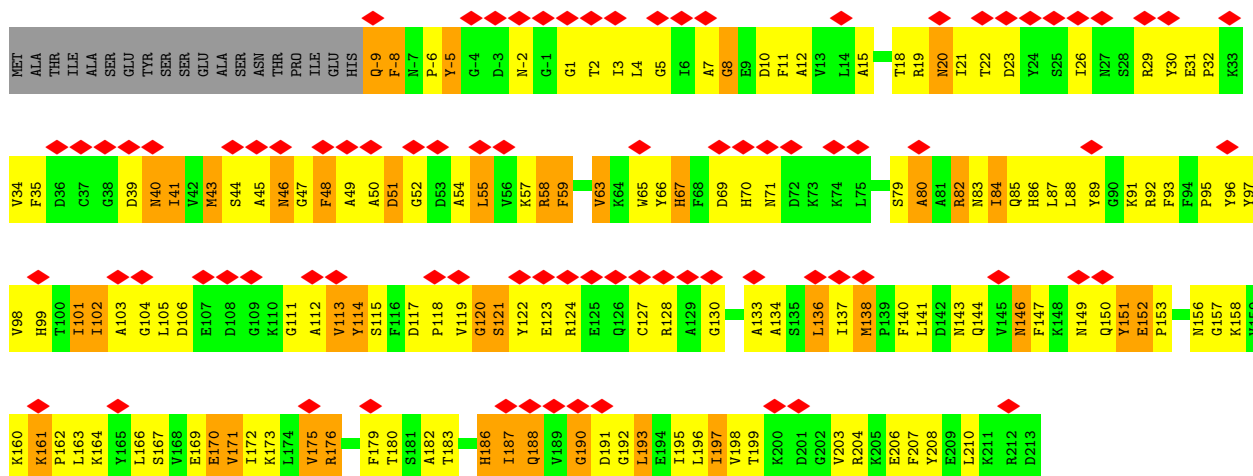


• Molecule 5: PROTEASOME COMPONENT PRE2

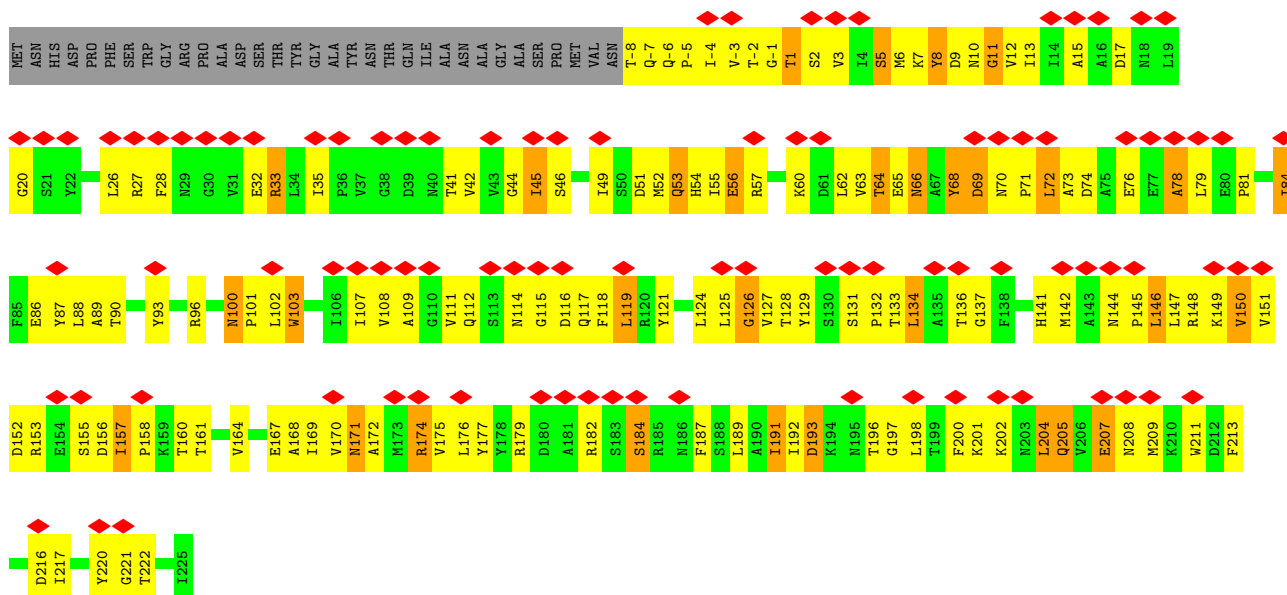




• Molecule 6: PROTEASOME COMPONENT C5

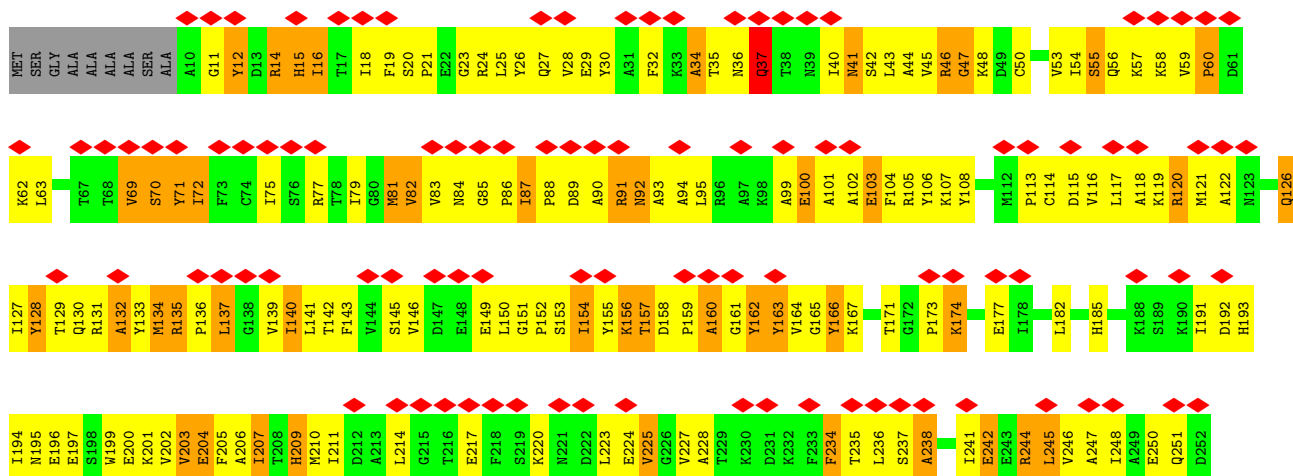


• Molecule 7: PROTEASOME COMPONENT PRE4

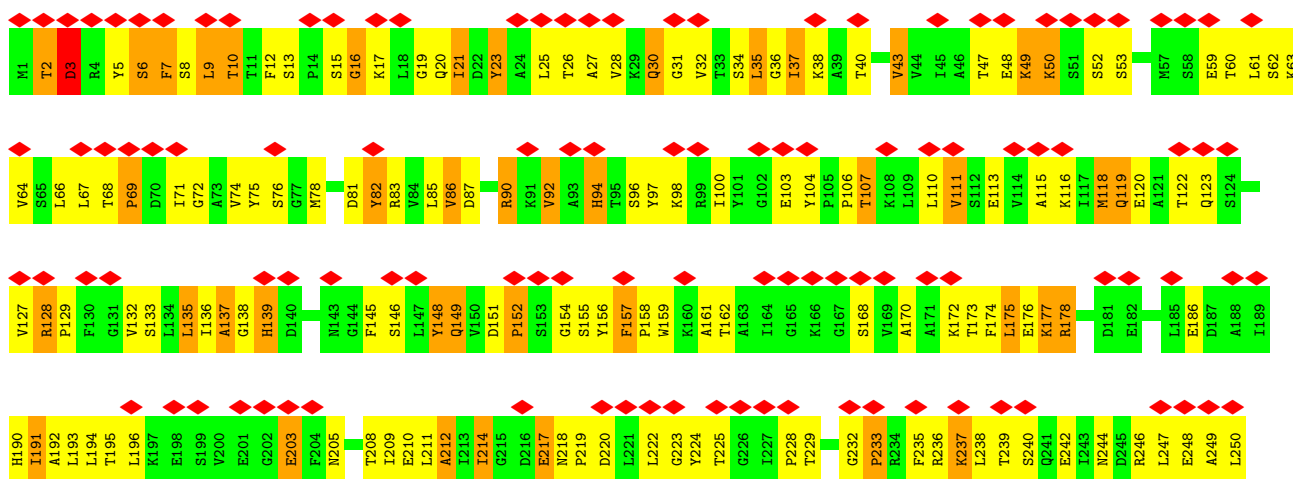
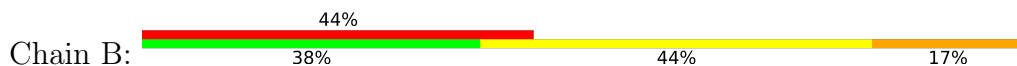


• Molecule 8: PROTEASOME COMPONENT C7-ALPHA

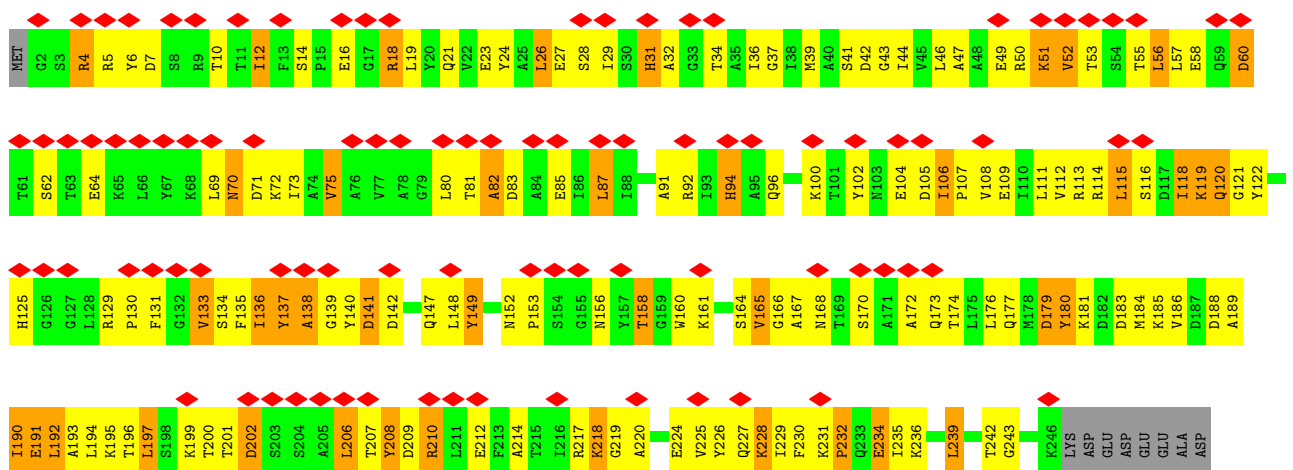
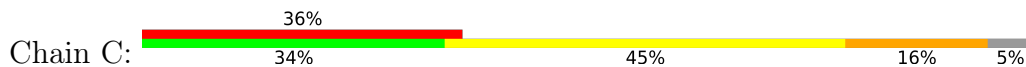




• Molecule 9: PROTEASOME COMPONENT Y7

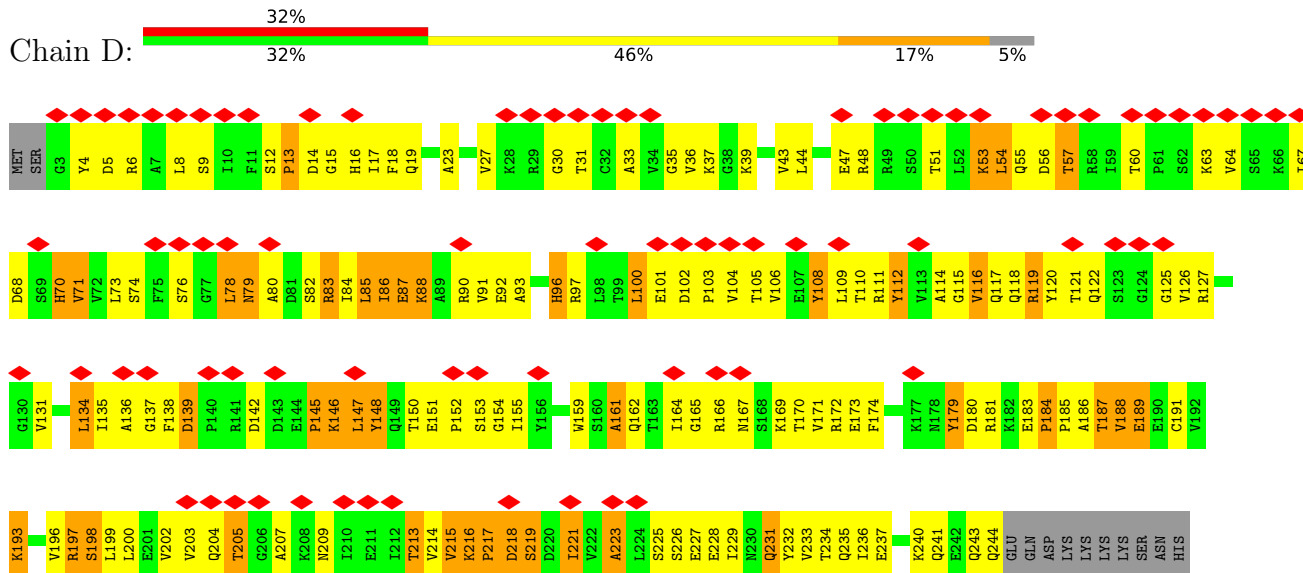


• Molecule 10: PROTEASOME COMPONENT Y13

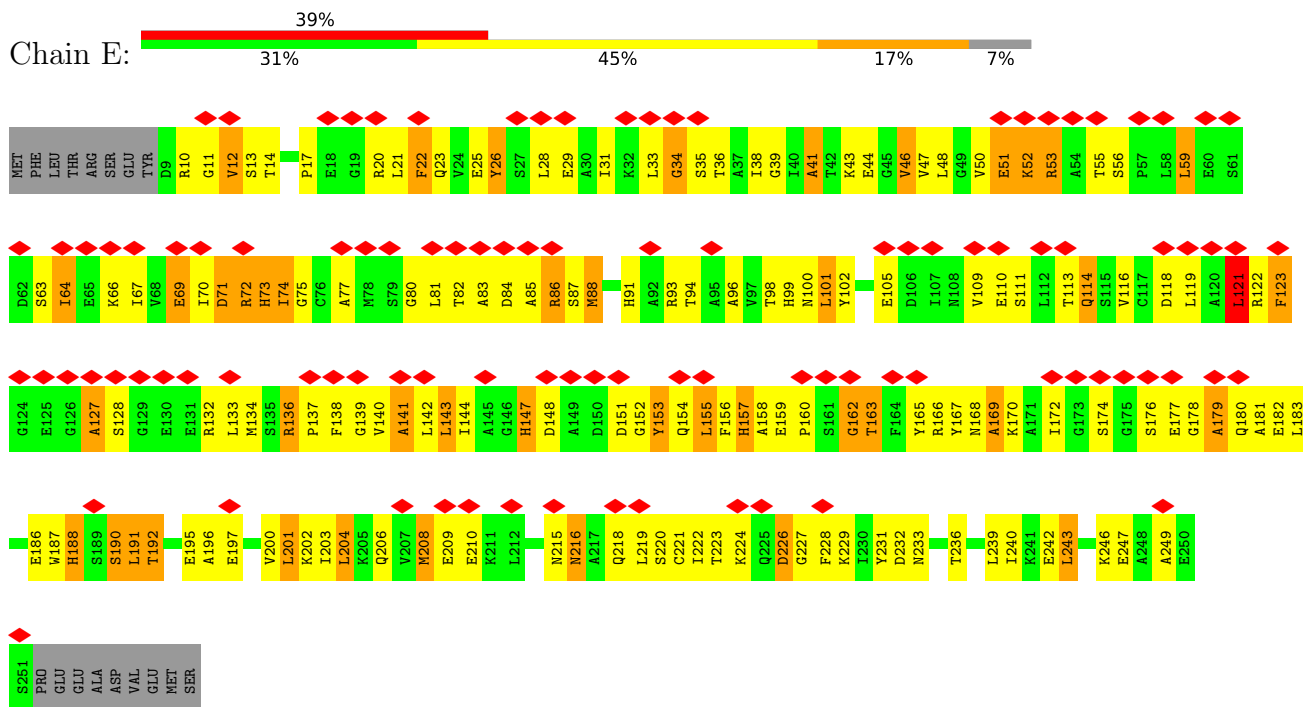


GLU
ASP
MET
LYS

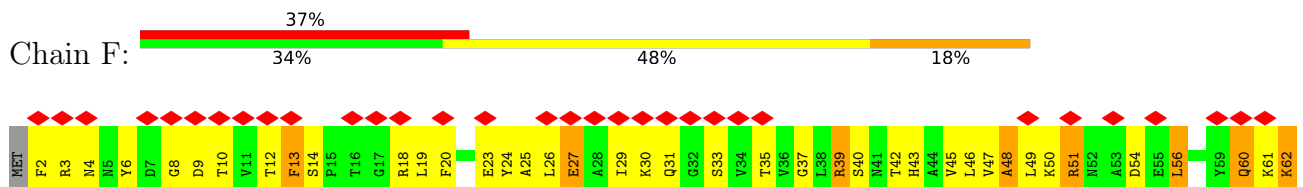
• Molecule 11: PROTEASOME COMPONENT PRE6



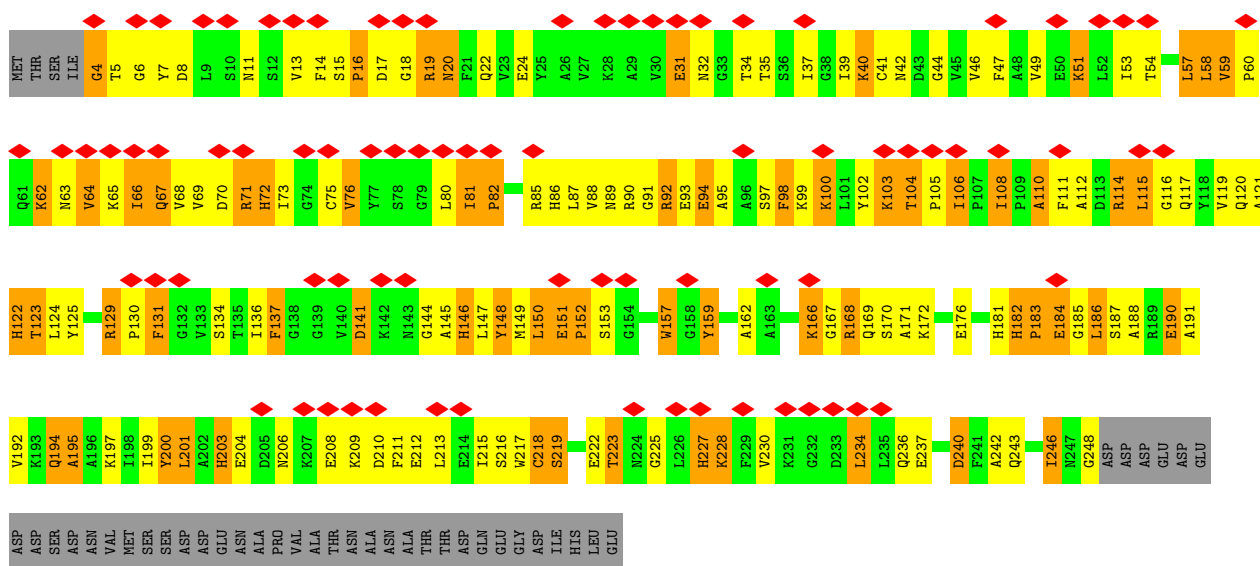
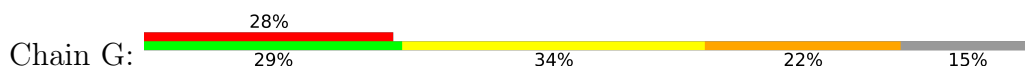
• Molecule 12: PROTEASOME COMPONENT PUP2



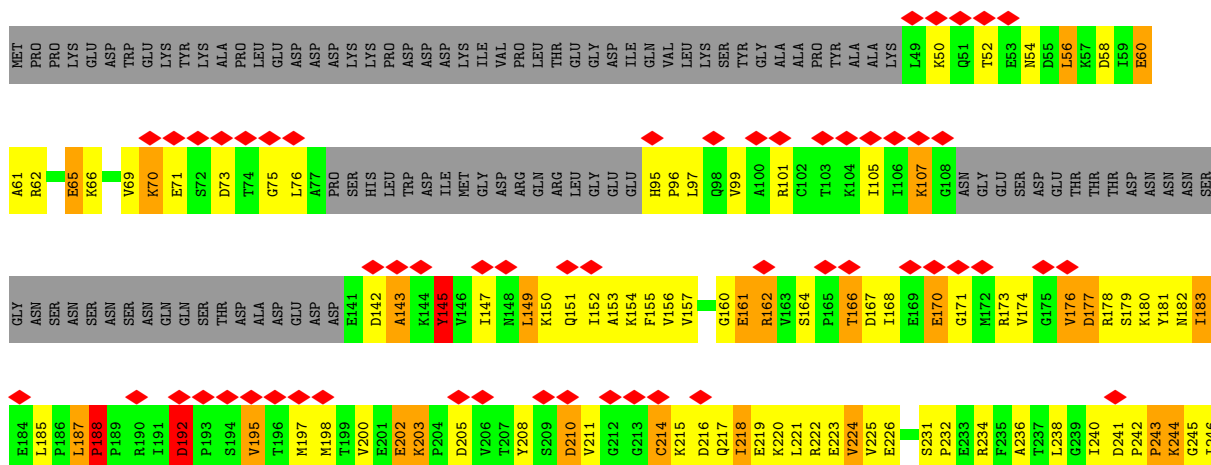
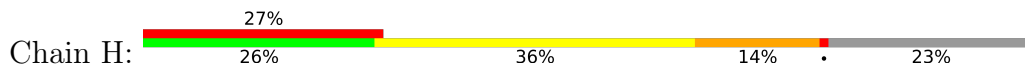
• Molecule 13: PROTEASOME COMPONENT PRE5

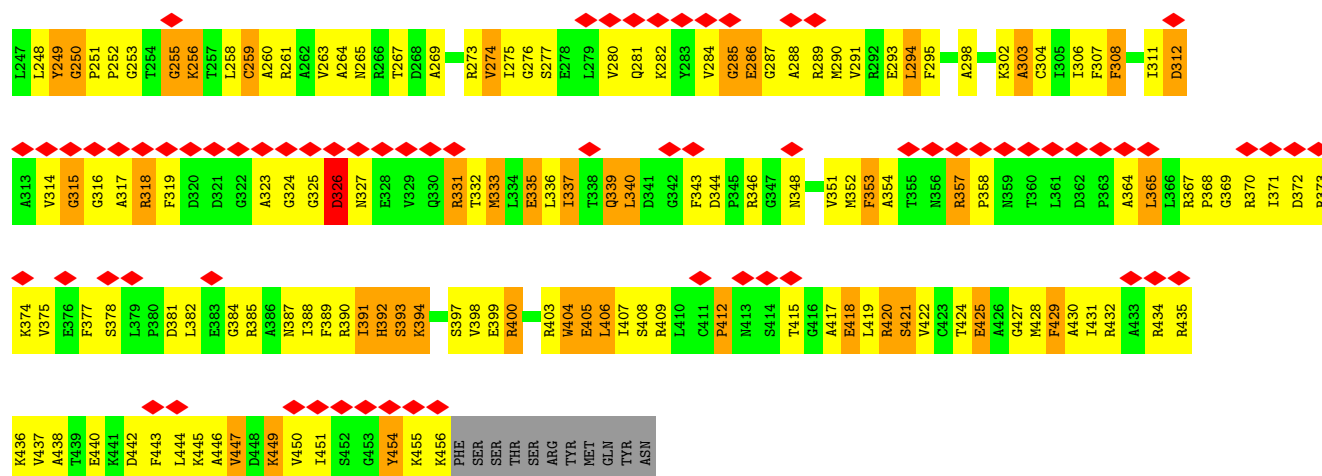


- Molecule 14: PROTEASOME COMPONENT C1

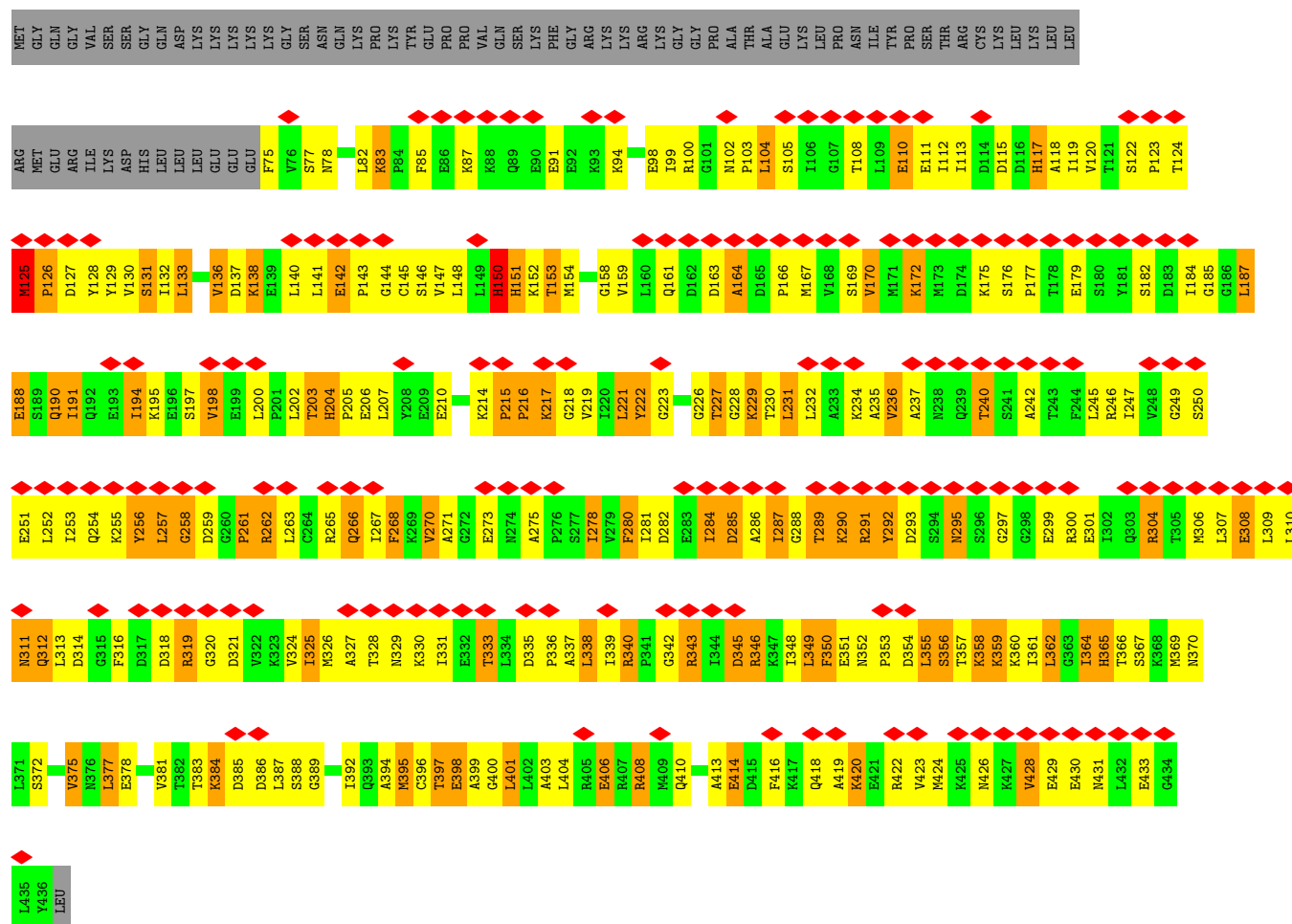
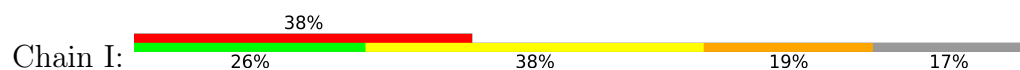


● Molecule 15: 26S PROTEASE REGULATORY SUBUNIT 7 HOMOLOG



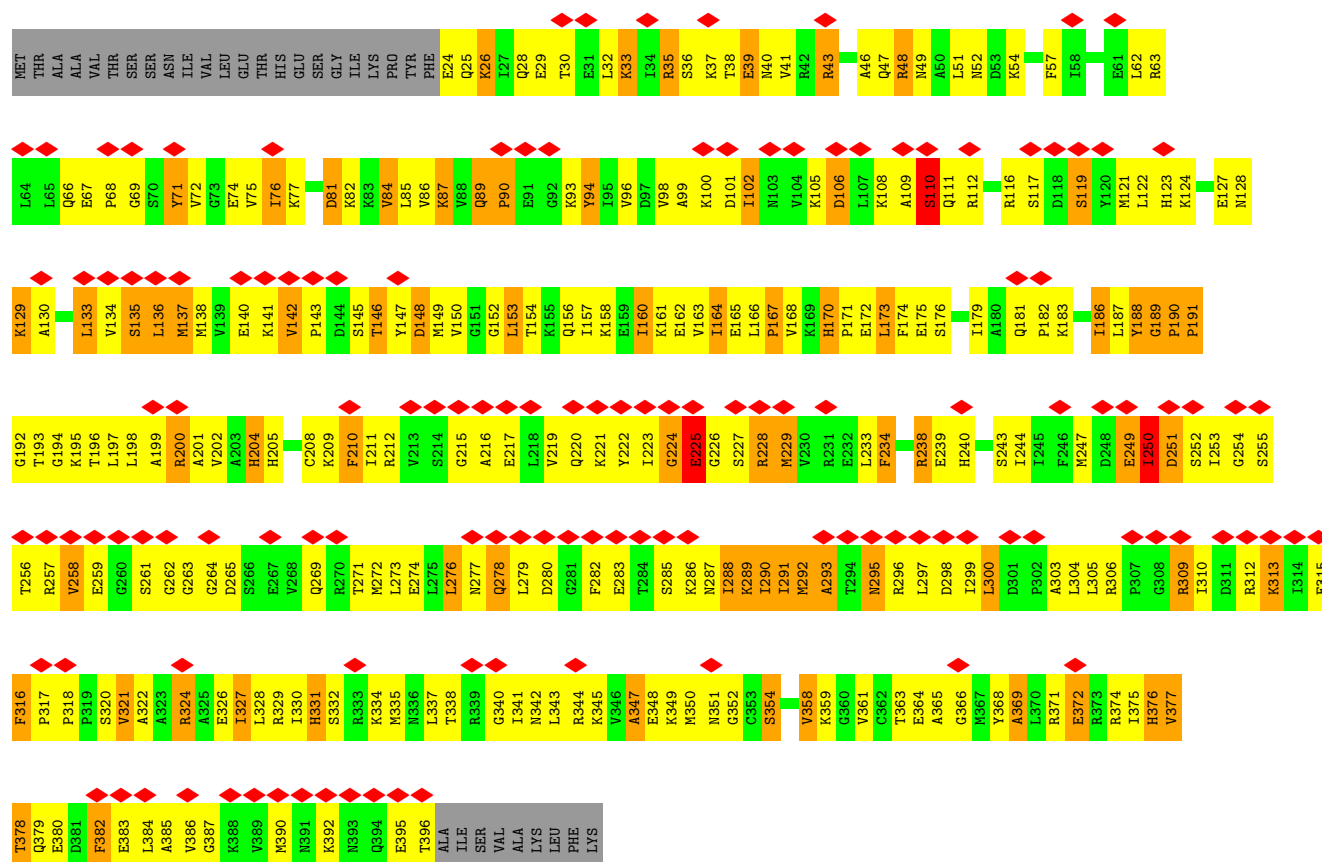


• Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

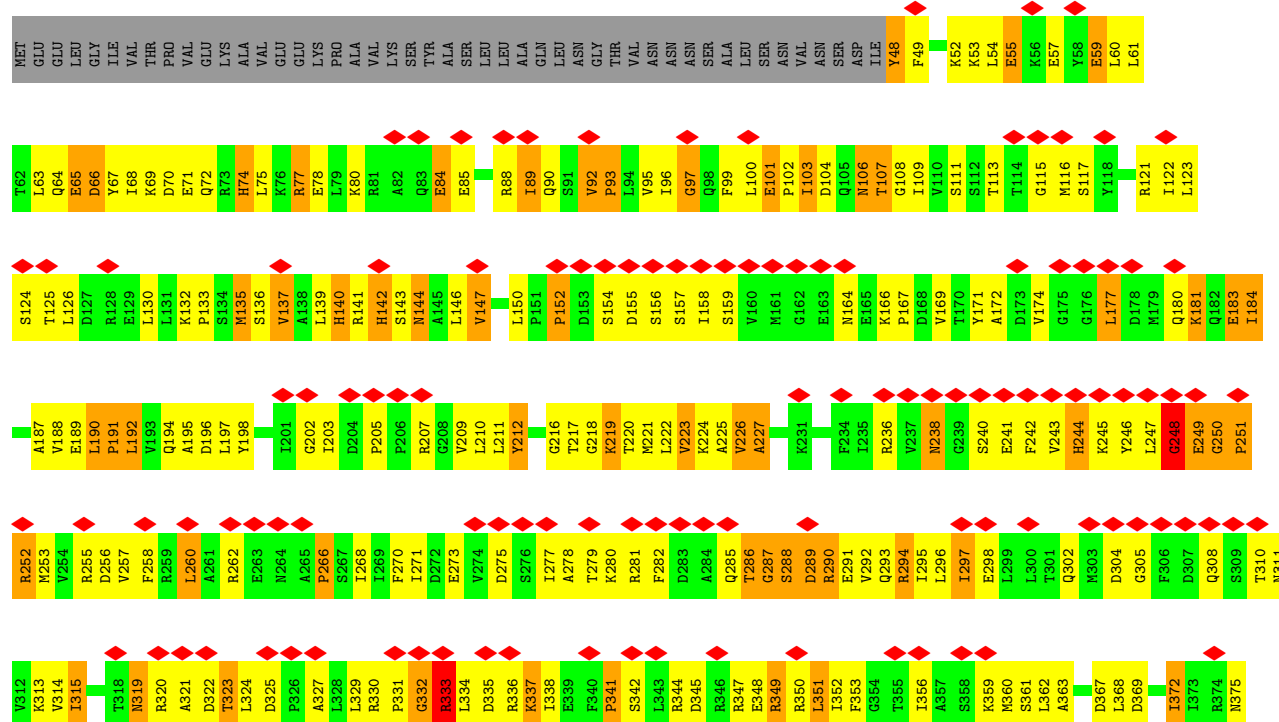


• Molecule 17: 26S PROTEASE REGULATORY SUBUNIT 8 HOMOLOG

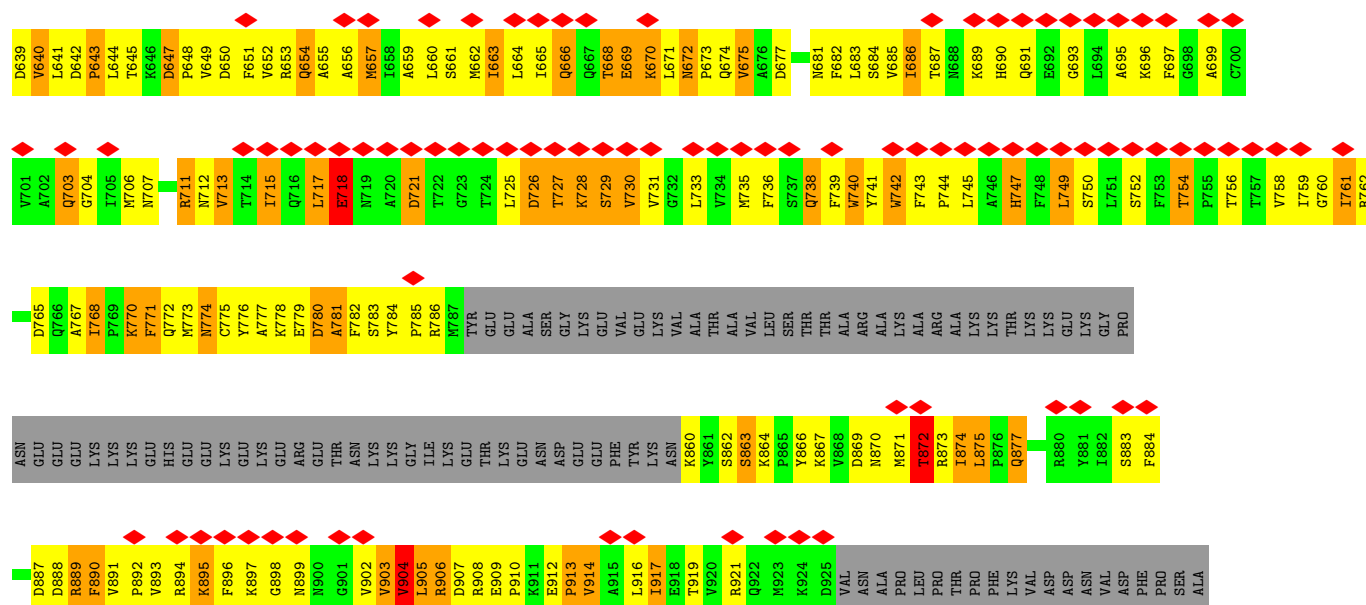


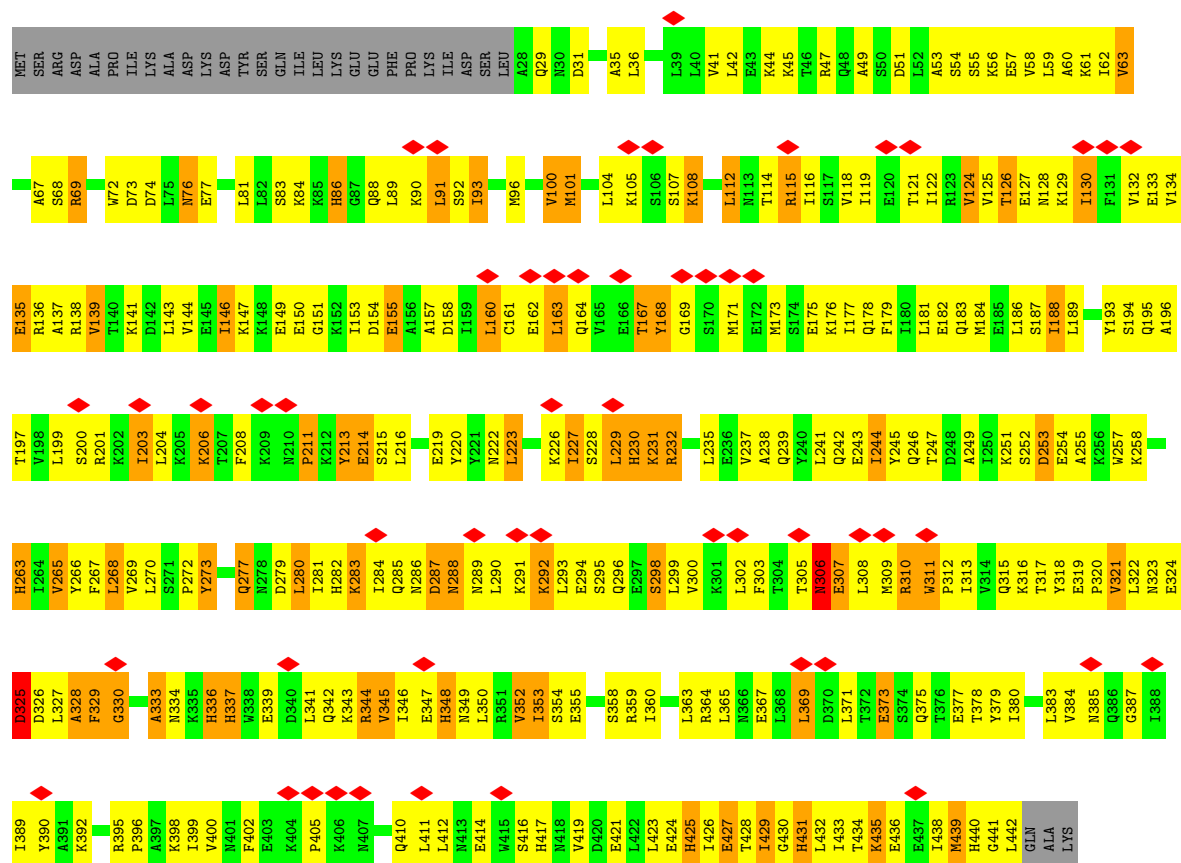


• Molecule 18: 26S PROTEASE REGULATORY SUBUNIT 6B HOMOLOG

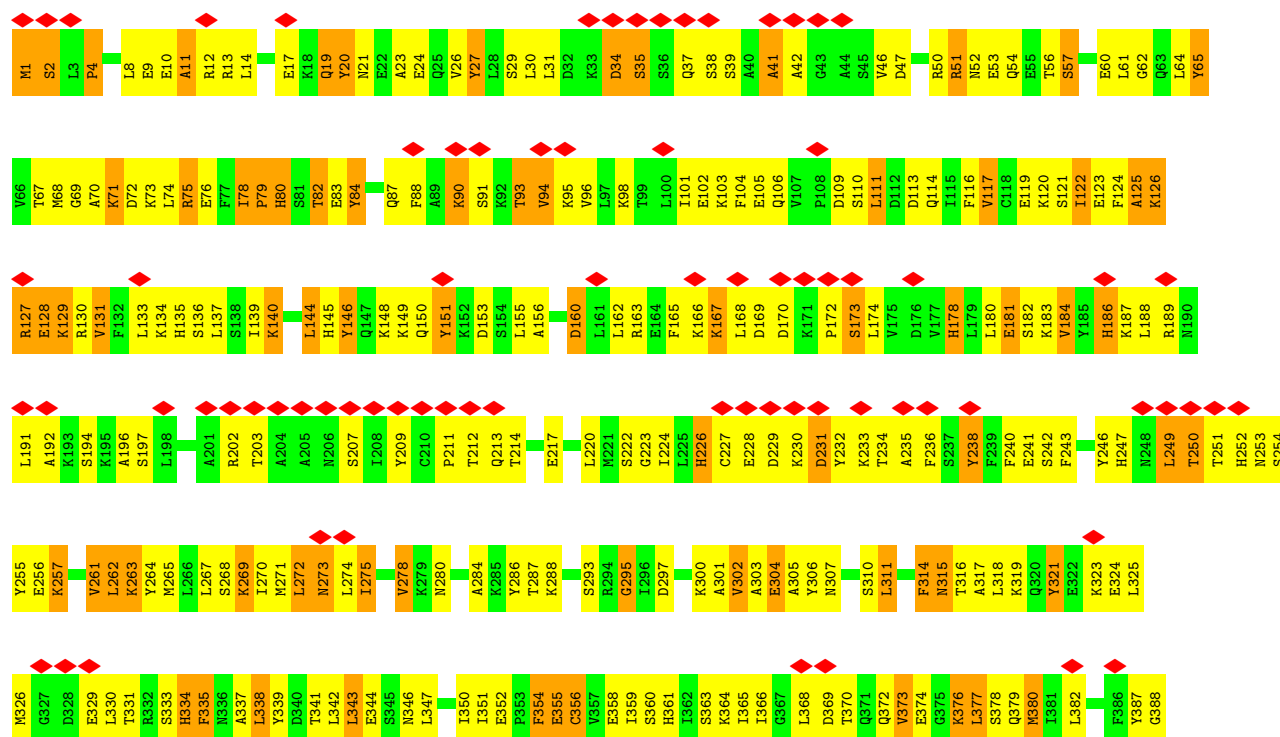


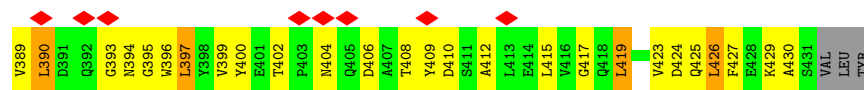




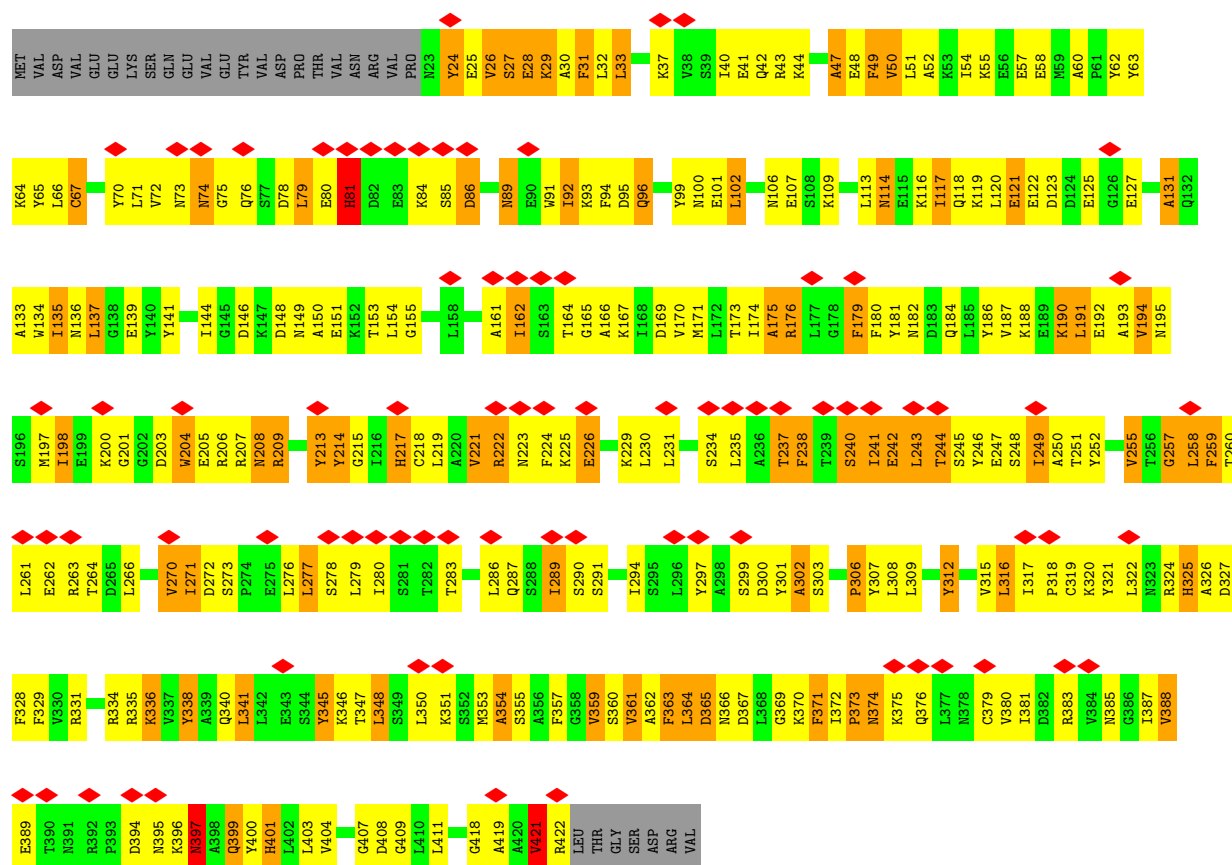


• Molecule 24: 26S PROTEASOME REGULATORY SUBUNIT RPN6

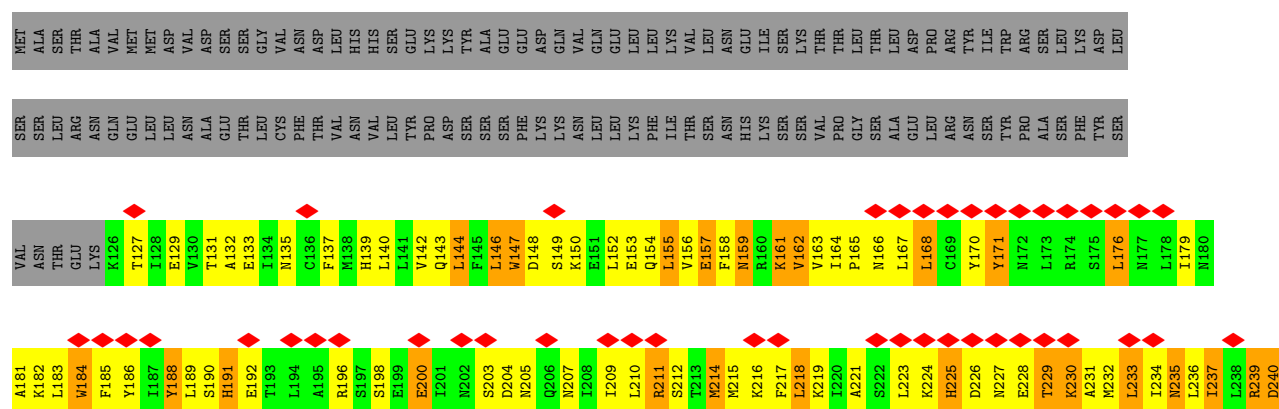
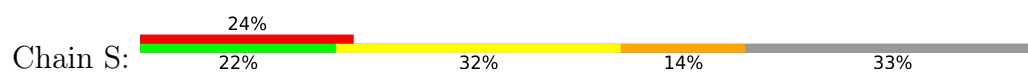




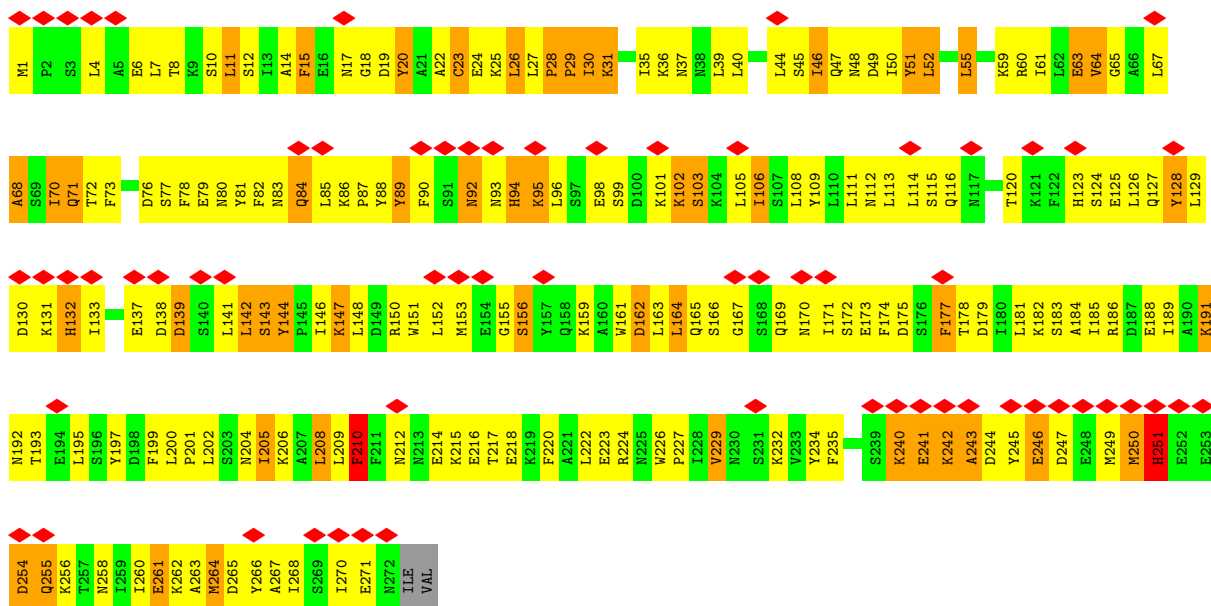
• Molecule 25: 26S PROTEASOME REGULATORY SUBUNIT RPN7



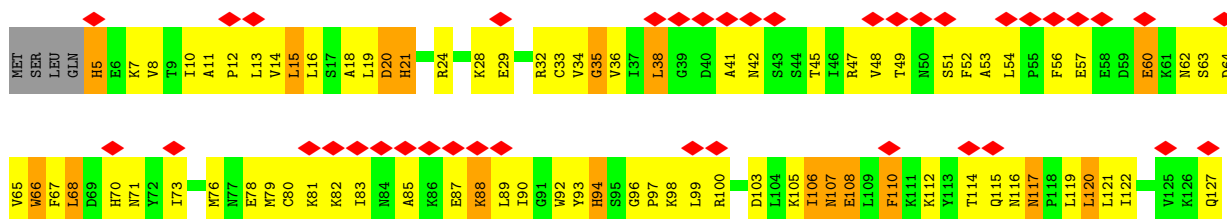
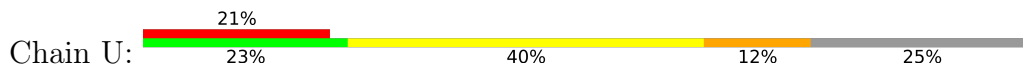
• Molecule 26: 26S PROTEASOME REGULATORY SUBUNIT RPN3

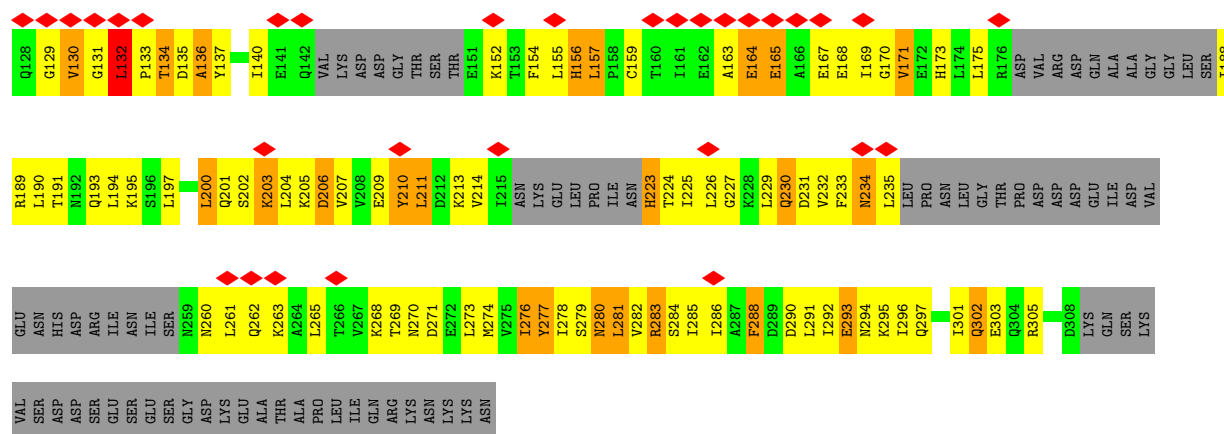


• Molecule 27: 26S PROTEASOME REGULATORY SUBUNIT RPN12

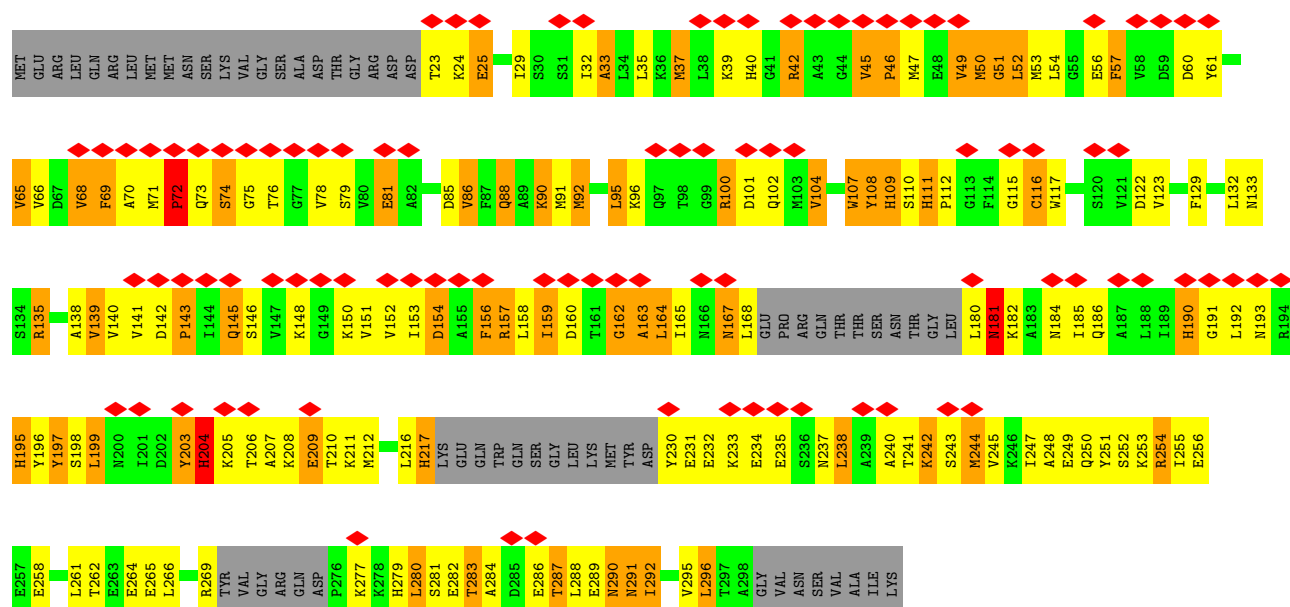
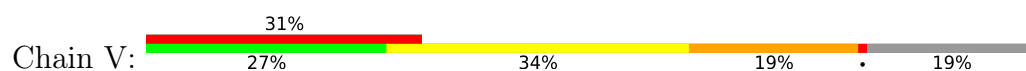


- Molecule 28: 26S PROTEASOME REGULATORY SUBUNIT RPN8

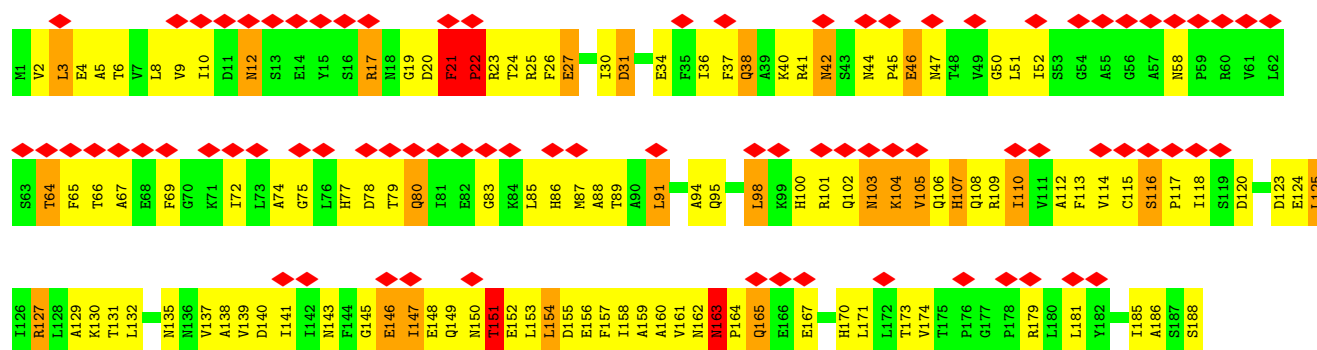
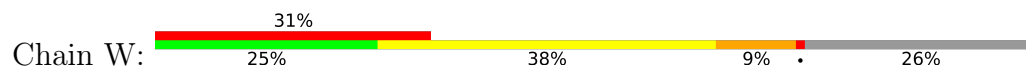


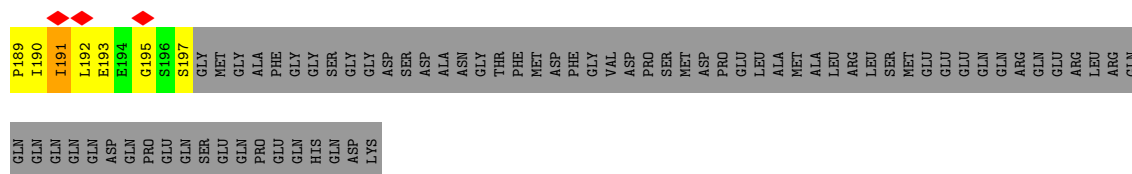


• Molecule 29: 26S PROTEASOME REGULATORY SUBUNIT RPN11

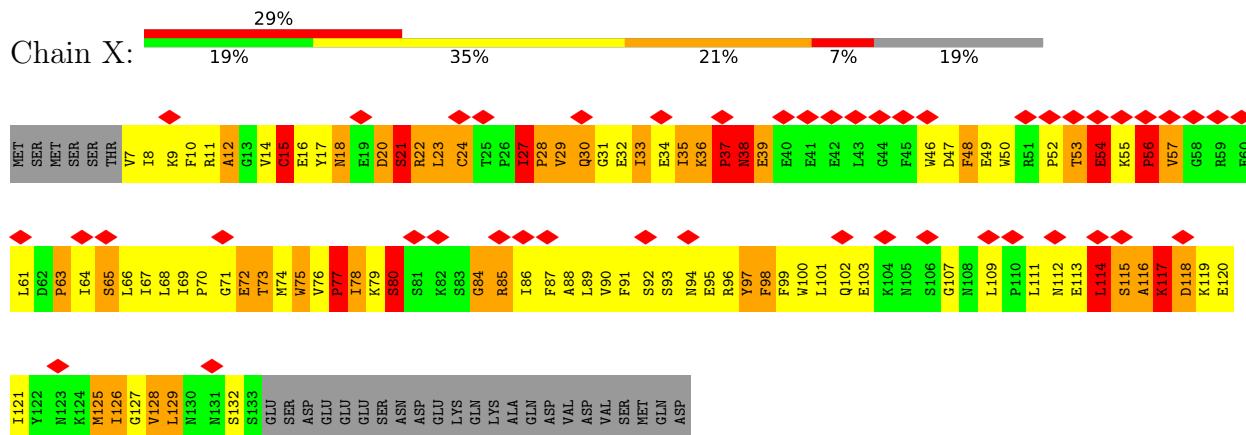


• Molecule 30: 26S PROTEASOME REGULATORY SUBUNIT RPN10

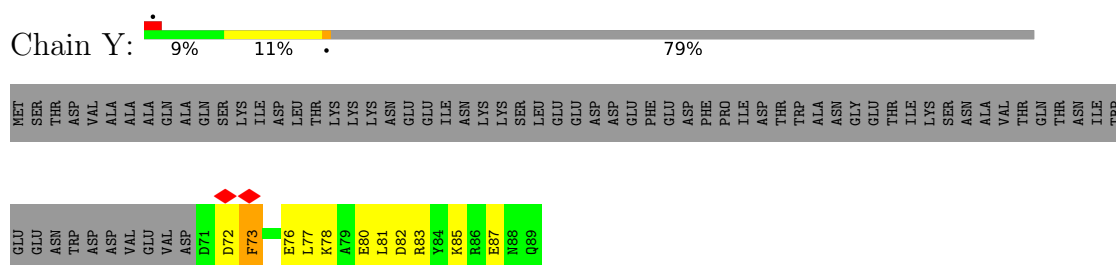




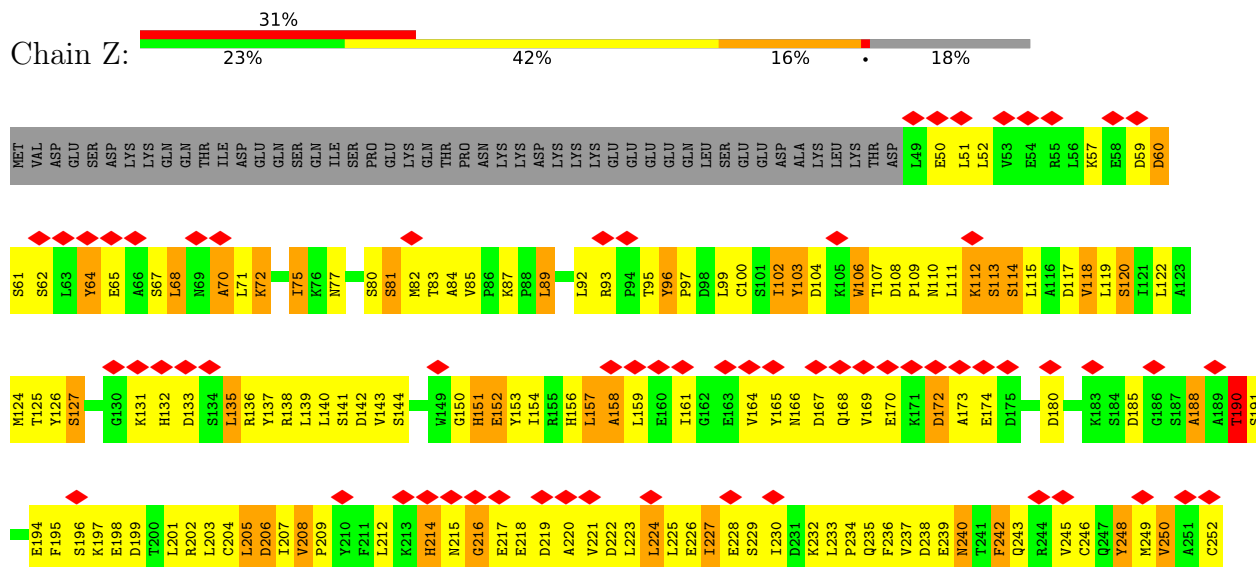
• Molecule 31: 26S PROTEASOME REGULATORY SUBUNIT RPN13



• Molecule 32: 26S PROTEASOME COMPLEX SUBUNIT SEM1



• Molecule 33: 26S PROTEASOME REGULATORY SUBUNIT RPN1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	560000	Depositor
Resolution determination method	Not provided	
CTF correction method	MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	5.177	Depositor
Minimum map value	-3.208	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.149	Depositor
Recommended contour level	0.81	Depositor
Map size ($\text{\AA}$)	557.2, 557.2, 557.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.99, 1.99, 1.99	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	1.94	46/1605 (2.9%)	2.03	77/2171 (3.5%)
2	2	1.98	61/1723 (3.5%)	2.02	81/2337 (3.5%)
3	3	1.84	52/1611 (3.2%)	1.96	80/2174 (3.7%)
4	4	1.85	42/1613 (2.6%)	1.96	86/2173 (4.0%)
5	5	1.94	57/1683 (3.4%)	2.09	92/2277 (4.0%)
6	6	1.90	66/1795 (3.7%)	2.02	77/2420 (3.2%)
7	7	1.82	43/1855 (2.3%)	2.02	95/2514 (3.8%)
8	A	1.89	65/1959 (3.3%)	1.98	90/2652 (3.4%)
9	B	1.85	48/1952 (2.5%)	2.04	116/2642 (4.4%)
10	C	1.90	56/1943 (2.9%)	1.92	82/2629 (3.1%)
11	D	1.87	64/1928 (3.3%)	2.05	91/2610 (3.5%)
12	E	1.99	65/1892 (3.4%)	2.09	92/2549 (3.6%)
13	F	1.98	63/1823 (3.5%)	2.10	100/2463 (4.1%)
14	G	2.09	76/1940 (3.9%)	2.06	99/2619 (3.8%)
15	H	1.91	62/2830 (2.2%)	2.10	144/3805 (3.8%)
16	I	1.93	103/2859 (3.6%)	2.11	162/3853 (4.2%)
17	J	1.97	99/2964 (3.3%)	2.12	176/3981 (4.4%)
18	K	1.84	84/3061 (2.7%)	2.08	170/4129 (4.1%)
19	L	1.86	71/2895 (2.5%)	2.03	135/3892 (3.5%)
20	M	1.94	87/2903 (3.0%)	2.11	173/3909 (4.4%)
21	N	1.87	200/6670 (3.0%)	2.15	414/9023 (4.6%)
22	O	1.79	94/3243 (2.9%)	2.07	190/4374 (4.3%)
23	P	1.87	113/3452 (3.3%)	2.12	195/4657 (4.2%)
24	Q	1.82	87/3527 (2.5%)	2.13	200/4748 (4.2%)
25	R	1.80	84/3272 (2.6%)	2.02	174/4412 (3.9%)
26	S	2.09	85/2945 (2.9%)	2.18	182/3976 (4.6%)
27	T	1.83	72/2279 (3.2%)	2.09	121/3077 (3.9%)
28	U	1.81	68/2087 (3.3%)	2.10	122/2811 (4.3%)
29	V	2.19	68/1969 (3.5%)	2.14	97/2652 (3.7%)
30	W	1.58	24/1557 (1.5%)	1.84	50/2111 (2.4%)
31	X	1.57	16/1058 (1.5%)	1.93	47/1432 (3.3%)
32	Y	1.76	3/169 (1.8%)	1.94	5/223 (2.2%)
33	Z	1.88	193/6403 (3.0%)	2.11	358/8686 (4.1%)
All	All	1.89	2417/81465 (3.0%)	2.07	4373/109981 (4.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
2	2	0	1
9	B	0	1
14	G	0	1
15	H	0	7
16	I	0	1
17	J	0	4
18	K	0	2
19	L	0	4
20	M	0	2
21	N	0	1
22	O	0	2
23	P	0	2
24	Q	0	1
25	R	0	2
26	S	0	1
27	T	0	1
28	U	0	1
29	V	0	1
30	W	0	6
31	X	0	4
33	Z	0	7
All	All	0	53

The worst 5 of 2417 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	285	GLY	C-N	45.89	1.98	1.33
26	S	257	LEU	CA-C	42.25	2.10	1.52
29	V	290	ASN	C-N	39.38	1.83	1.33
26	S	257	LEU	N-CA	-30.00	1.06	1.46
20	M	257	GLY	C-N	25.90	1.69	1.33

The worst 5 of 4373 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V	291	ASN	O-C-N	26.64	149.51	122.07
15	H	285	GLY	CA-C-N	-17.70	87.74	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	285	GLY	C-N-CA	-17.70	87.74	121.54
15	H	187	LEU	C-N-CD	-17.57	52.98	125.00
29	V	291	ASN	CA-C-N	-15.29	99.51	120.46

There are no chirality outliers.

5 of 53 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	-2	LEU	Peptide
2	2	202	SER	Peptide
9	B	9	LEU	Peptide
14	G	246	ILE	Peptide
15	H	101	ARG	Peptide

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	1	1576	0	1554	150	0
2	2	1692	0	1698	97	0
3	3	1581	0	1573	104	0
4	4	1585	0	1590	80	0
5	5	1646	0	1595	141	0
6	6	1757	0	1711	130	0
7	7	1824	0	1832	158	0
8	A	1921	0	1910	225	0
9	B	1915	0	1929	138	0
10	C	1913	0	1914	148	0
11	D	1899	0	1908	134	0
12	E	1867	0	1841	165	0
13	F	1795	0	1796	205	0
14	G	1900	0	1889	218	0
15	H	2792	0	2875	269	0
16	I	2822	0	2869	278	0
17	J	2928	0	3056	284	0
18	K	3019	0	3082	335	0
19	L	2853	0	2925	334	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	M	2866	0	2937	306	0
21	N	6562	0	6624	574	0
22	O	3182	0	3207	546	0
23	P	3401	0	3483	353	0
24	Q	3471	0	3491	313	0
25	R	3218	0	3216	394	0
26	S	2893	0	2937	264	0
27	T	2235	0	2207	208	0
28	U	2061	0	2114	269	0
29	V	1942	0	1948	263	0
30	W	1534	0	1542	143	0
31	X	1032	0	1015	252	0
32	Y	168	0	153	6	0
33	Z	6289	0	6233	692	0
All	All	80139	0	80654	7171	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 45.

The worst 5 of 7171 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)
23:P:427:GLU:HA	29:V:230:TYR:CE1	1.27	1.67
22:O:185:PHE:CE2	22:O:223:LEU:HD13	1.30	1.66
22:O:310:PHE:HZ	22:O:341:ILE:CG2	1.04	1.62
12:E:12:VAL:HG12	12:E:123:PHE:CE2	1.37	1.60
33:Z:233:LEU:HD22	33:Z:268:ALA:CB	1.32	1.59

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	1	203/215 (94%)	189 (93%)	12 (6%)	2 (1%)	12	49
2	2	221/261 (85%)	209 (95%)	9 (4%)	3 (1%)	9	40
3	3	202/205 (98%)	179 (89%)	14 (7%)	9 (4%)	2	17
4	4	196/198 (99%)	178 (91%)	15 (8%)	3 (2%)	8	40
5	5	210/287 (73%)	199 (95%)	8 (4%)	3 (1%)	9	40
6	6	220/241 (91%)	207 (94%)	9 (4%)	4 (2%)	6	34
7	7	231/266 (87%)	208 (90%)	18 (8%)	5 (2%)	5	29
8	A	241/252 (96%)	222 (92%)	16 (7%)	3 (1%)	10	44
9	B	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	16	54
10	C	243/258 (94%)	229 (94%)	13 (5%)	1 (0%)	30	67
11	D	240/254 (94%)	222 (92%)	15 (6%)	3 (1%)	9	42
12	E	241/260 (93%)	224 (93%)	11 (5%)	6 (2%)	4	26
13	F	231/234 (99%)	216 (94%)	13 (6%)	2 (1%)	14	51
14	G	243/288 (84%)	224 (92%)	17 (7%)	2 (1%)	16	54
15	H	351/467 (75%)	297 (85%)	37 (10%)	17 (5%)	2	16
16	I	358/437 (82%)	322 (90%)	28 (8%)	8 (2%)	5	29
17	J	371/405 (92%)	336 (91%)	24 (6%)	11 (3%)	3	23
18	K	377/428 (88%)	343 (91%)	23 (6%)	11 (3%)	3	23
19	L	357/437 (82%)	320 (90%)	28 (8%)	9 (2%)	4	26
20	M	363/434 (84%)	331 (91%)	22 (6%)	10 (3%)	4	24
21	N	843/945 (89%)	772 (92%)	45 (5%)	26 (3%)	3	22
22	O	385/393 (98%)	332 (86%)	26 (7%)	27 (7%)	1	11
23	P	413/445 (93%)	377 (91%)	19 (5%)	17 (4%)	2	18
24	Q	429/434 (99%)	398 (93%)	20 (5%)	11 (3%)	4	25
25	R	398/429 (93%)	351 (88%)	36 (9%)	11 (3%)	4	24
26	S	351/523 (67%)	318 (91%)	19 (5%)	14 (4%)	2	18
27	T	270/274 (98%)	233 (86%)	25 (9%)	12 (4%)	2	17
28	U	245/338 (72%)	237 (97%)	5 (2%)	3 (1%)	10	44
29	V	239/306 (78%)	214 (90%)	15 (6%)	10 (4%)	2	17
30	W	195/268 (73%)	171 (88%)	12 (6%)	12 (6%)	1	13
31	X	125/156 (80%)	83 (66%)	18 (14%)	24 (19%)	0	2
32	Y	17/89 (19%)	17 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Z	807/993 (81%)	714 (88%)	59 (7%)	34 (4%)	2	17
All	All	10064/11670 (86%)	9107 (90%)	642 (6%)	315 (3%)	5	22

5 of 315 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	196	ARG
3	3	194	ARG
5	5	31	VAL
7	7	209	MET
10	C	224	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	169/178 (95%)	169 (100%)	0	100	100
2	2	182/214 (85%)	182 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
10	C	204/216 (94%)	204 (100%)	0	100	100
11	D	214/226 (95%)	214 (100%)	0	100	100
12	E	199/215 (93%)	199 (100%)	0	100	100
13	F	192/193 (100%)	191 (100%)	1 (0%)	81	83
14	G	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	300 (99%)	3 (1%)	68	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	I	319/385 (83%)	317 (99%)	2 (1%)	78	83
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	308/377 (82%)	307 (100%)	1 (0%)	86	86
20	M	315/375 (84%)	314 (100%)	1 (0%)	86	86
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	388/415 (94%)	384 (99%)	4 (1%)	68	78
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	350 (100%)	1 (0%)	86	86
26	S	330/489 (68%)	329 (100%)	1 (0%)	86	86
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	217/268 (81%)	217 (100%)	0	100	100
30	W	171/230 (74%)	169 (99%)	2 (1%)	63	75
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	8816/10146 (87%)	8800 (100%)	16 (0%)	85	87

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	W	21	PHE
26	S	416	GLU
23	P	244	ILE
25	R	397	ASN
20	M	433	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 207 such sidechains are listed below:

Mol	Chain	Res	Type
22	O	289	GLN
25	R	323	ASN
33	Z	766	HIS

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Mol	Chain	Res	Type
23	P	239	GLN
24	Q	54	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
15	H	2
29	V	2
20	M	2
16	I	1
18	K	1
19	L	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	252:LEU	C	253:ILE	N	3.25
1	H	279:LEU	C	280:VAL	N	2.88
1	K	242:PHE	C	243:VAL	N	2.46
1	L	251:ILE	C	252:VAL	N	2.09
1	H	285:GLY	C	286:GLU	N	1.97

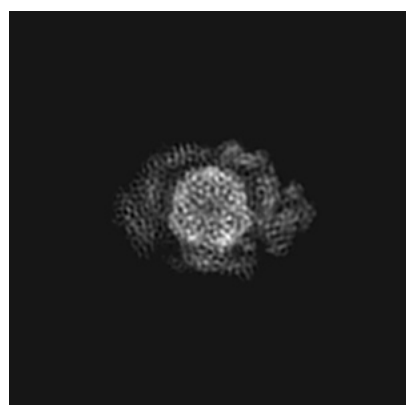
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2596. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

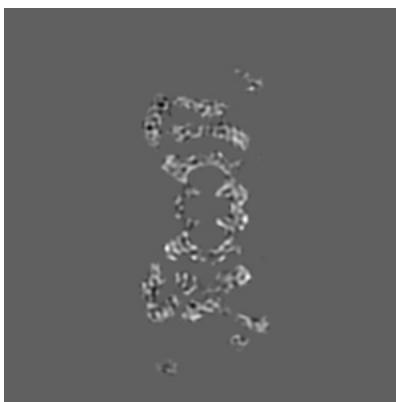
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140



Z Index: 140

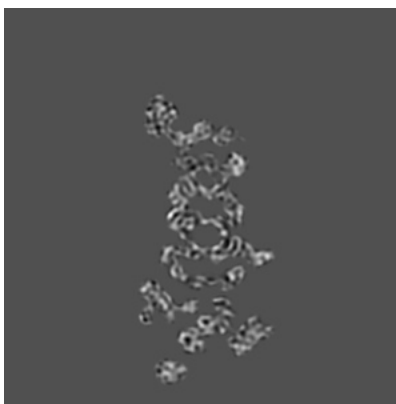
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 93



Y Index: 149

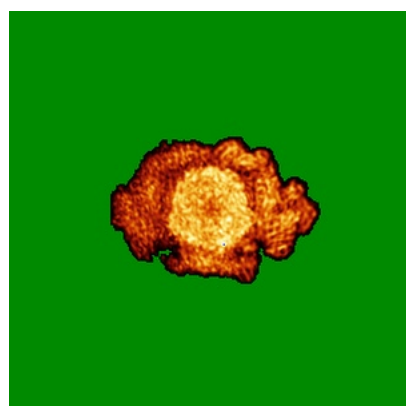


Z Index: 134

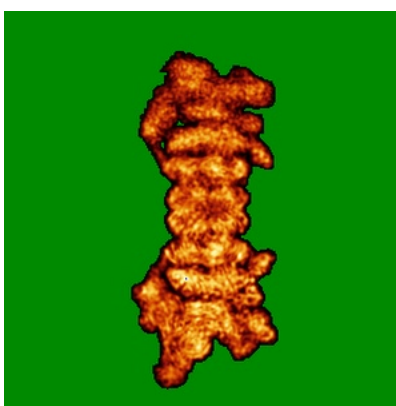
The images above show the largest variance slices of the map in three orthogonal directions.

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

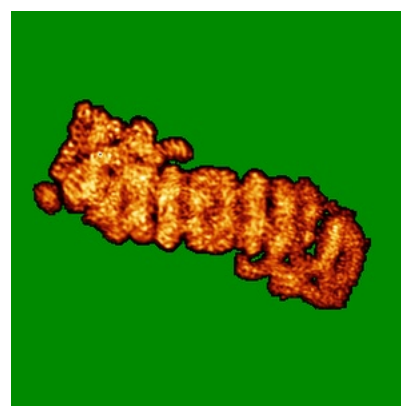
6.4.1 Primary map



X



Y

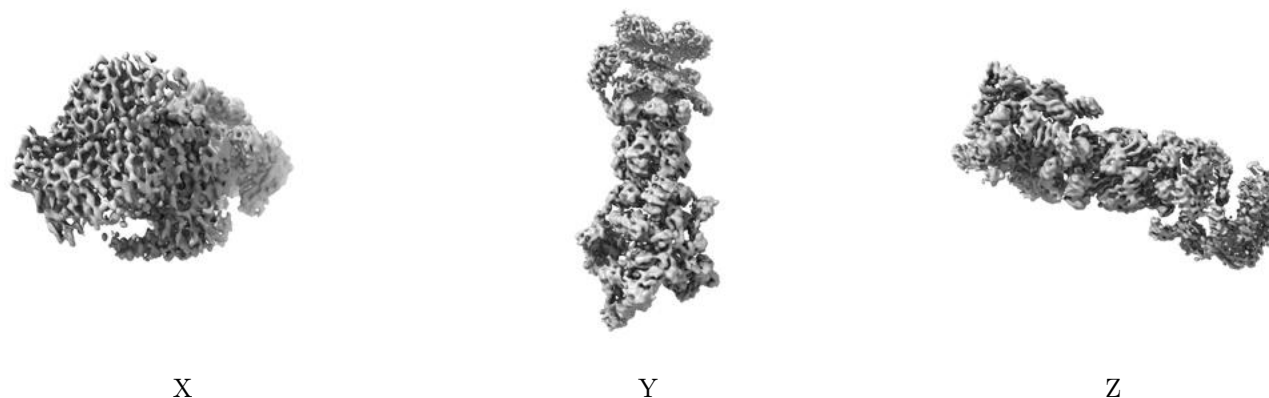


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.81. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

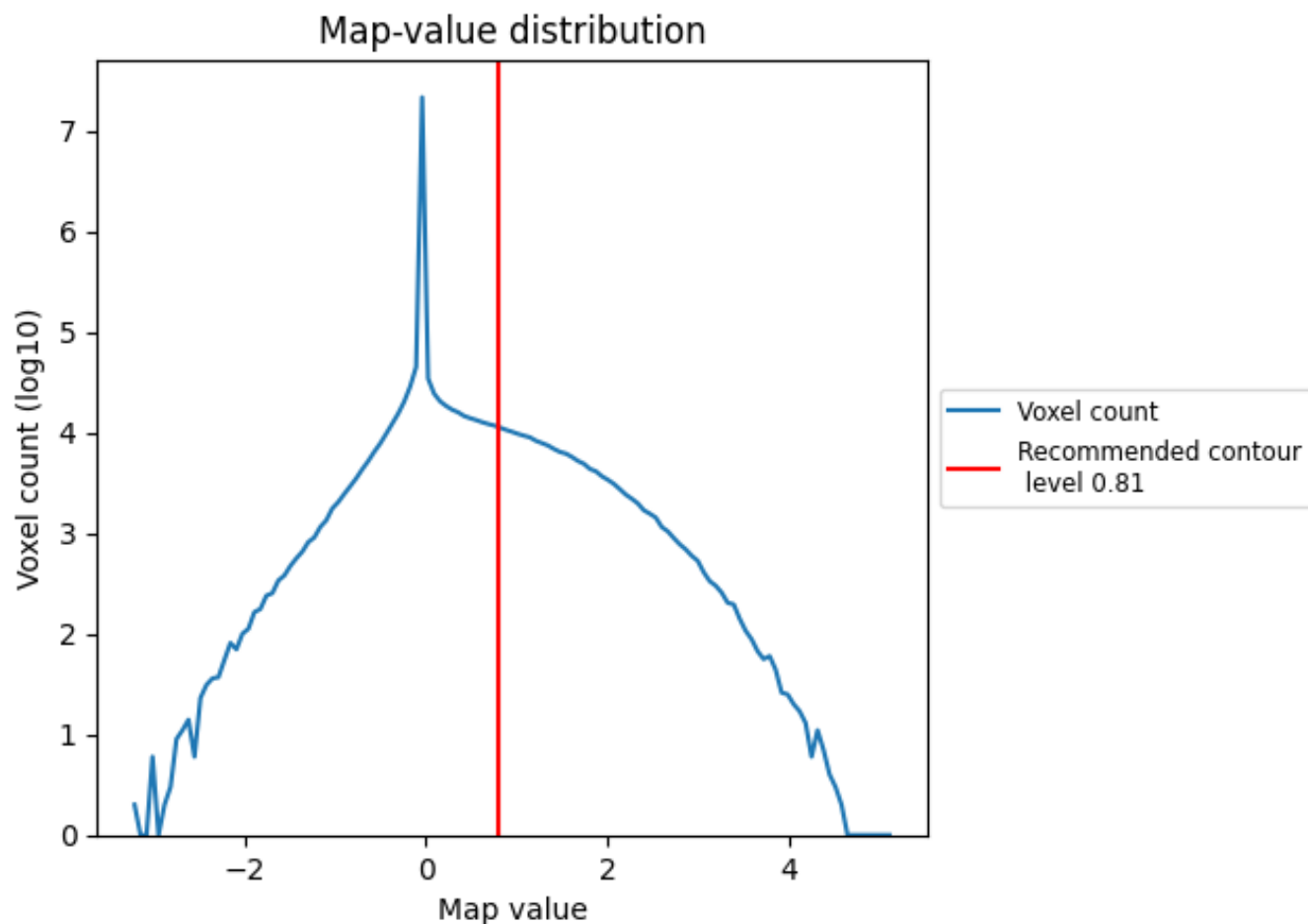
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

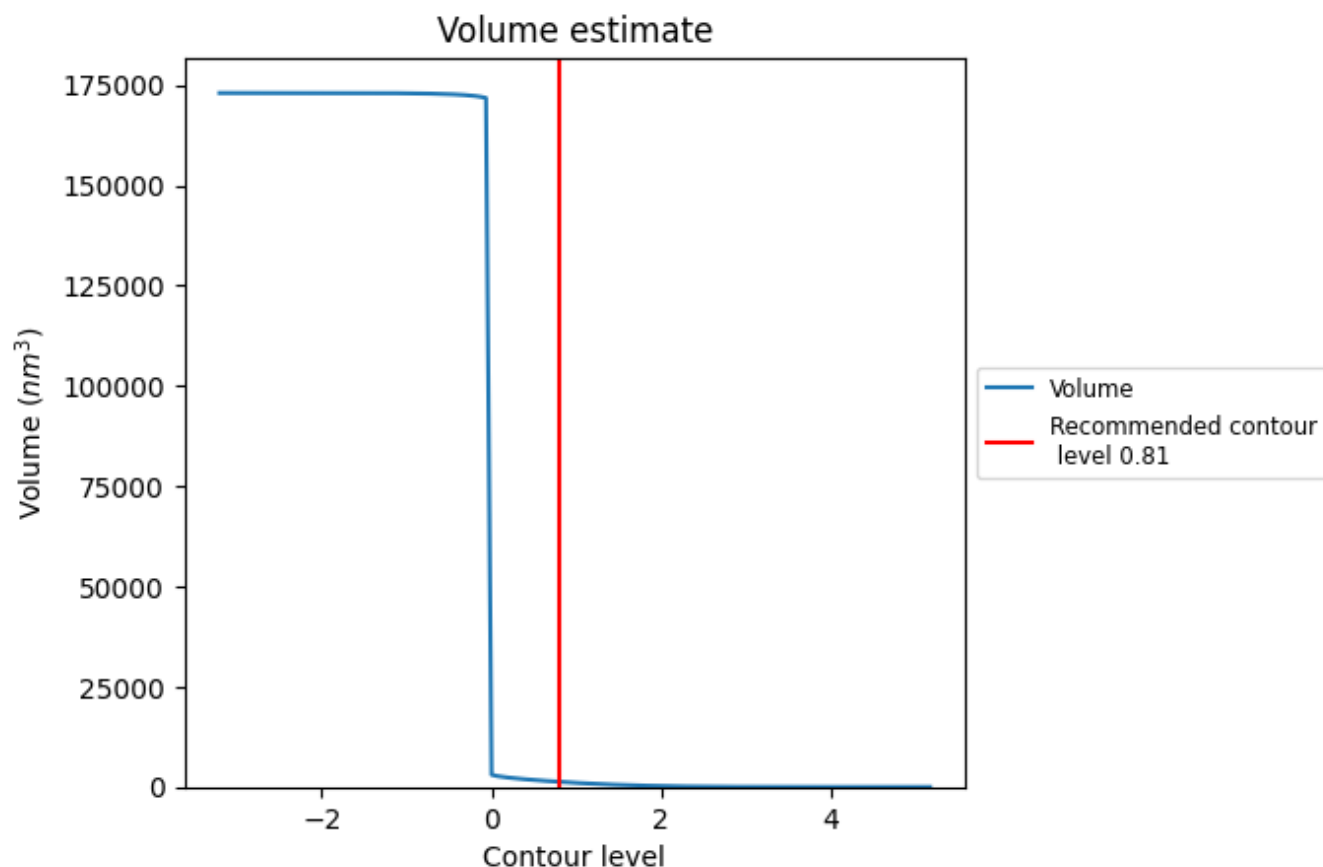
This section contains the results of statistical analysis of the map.

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.

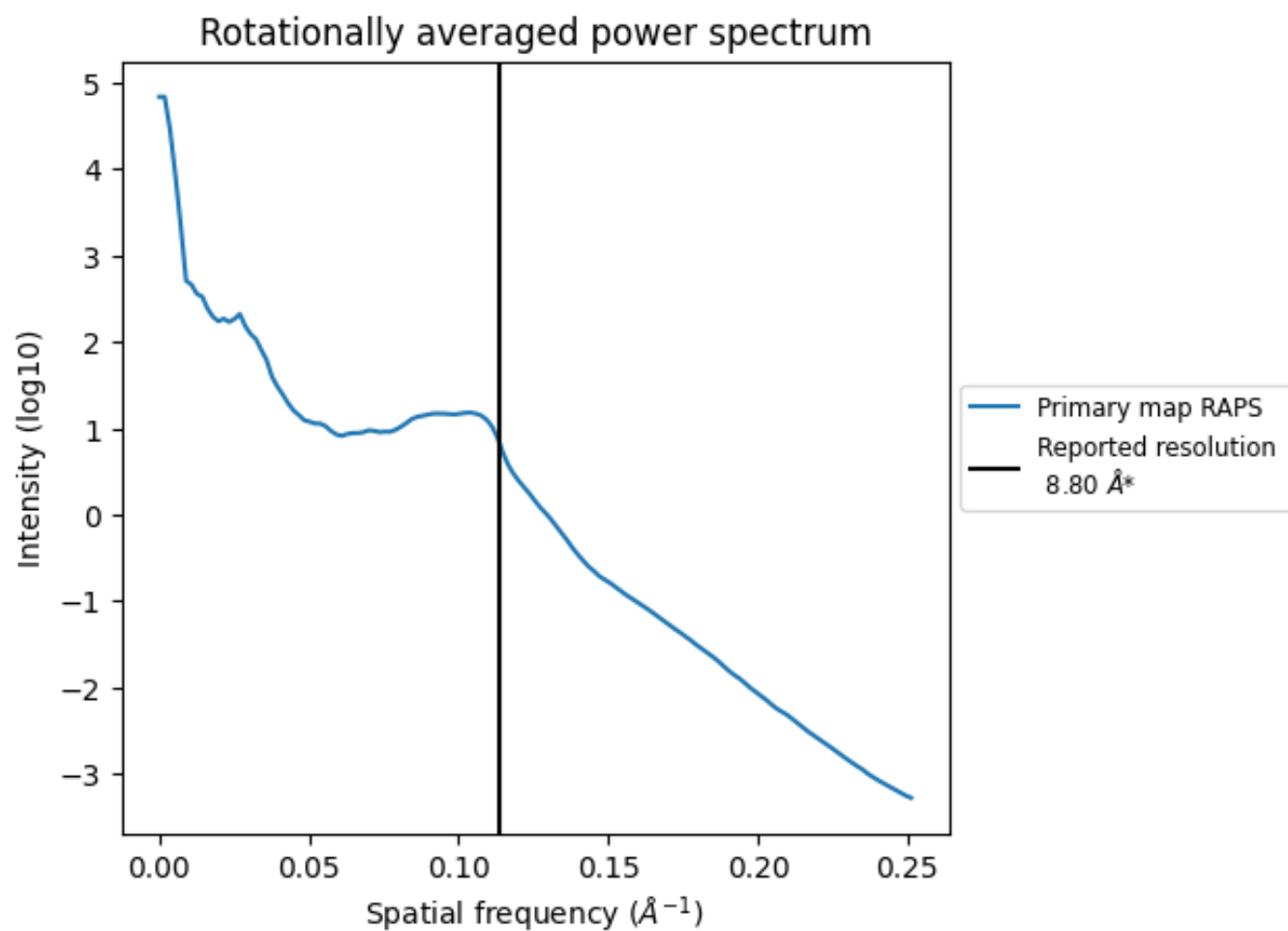
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1269 nm³; this corresponds to an approximate mass of 1146 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 0.114 Å⁻¹

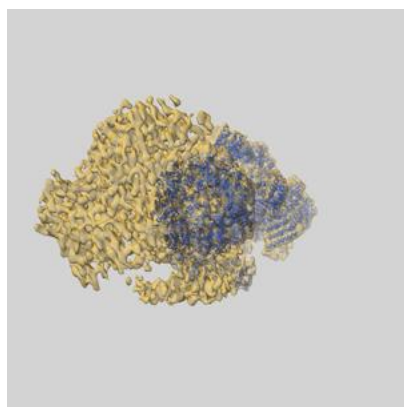
8 Fourier-Shell correlation

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

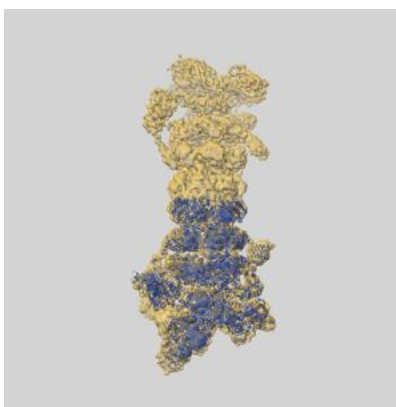
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2596 and PDB model 4CR4. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

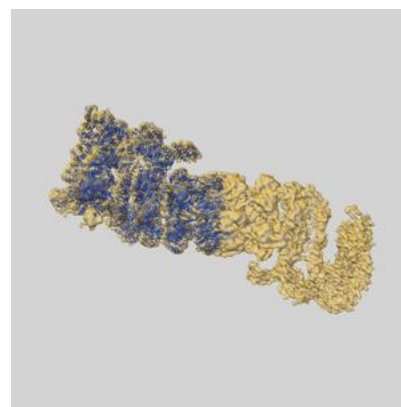
9.1 Map-model overlay [i](#)



X



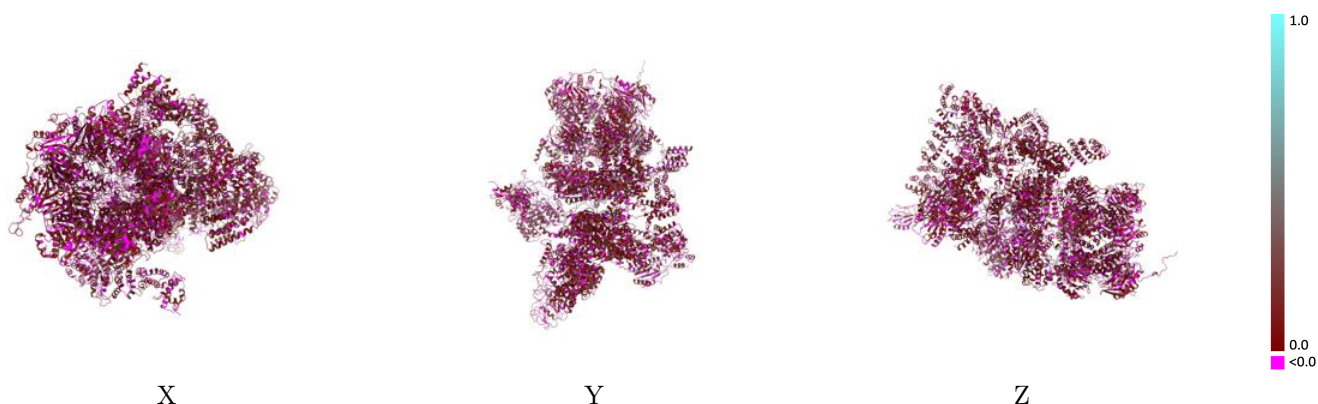
Y



Z

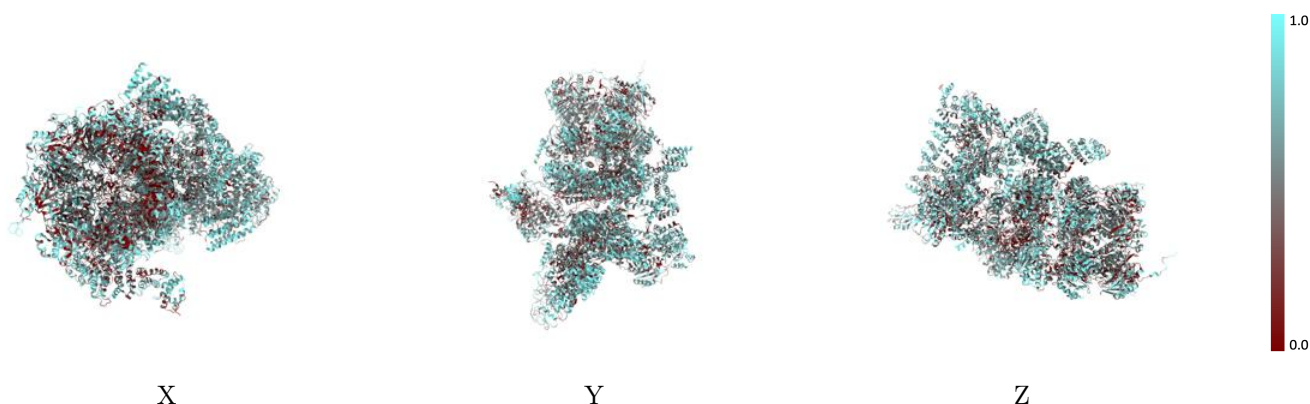
The images above show the 3D surface view of the map at the recommended contour level 0.81 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



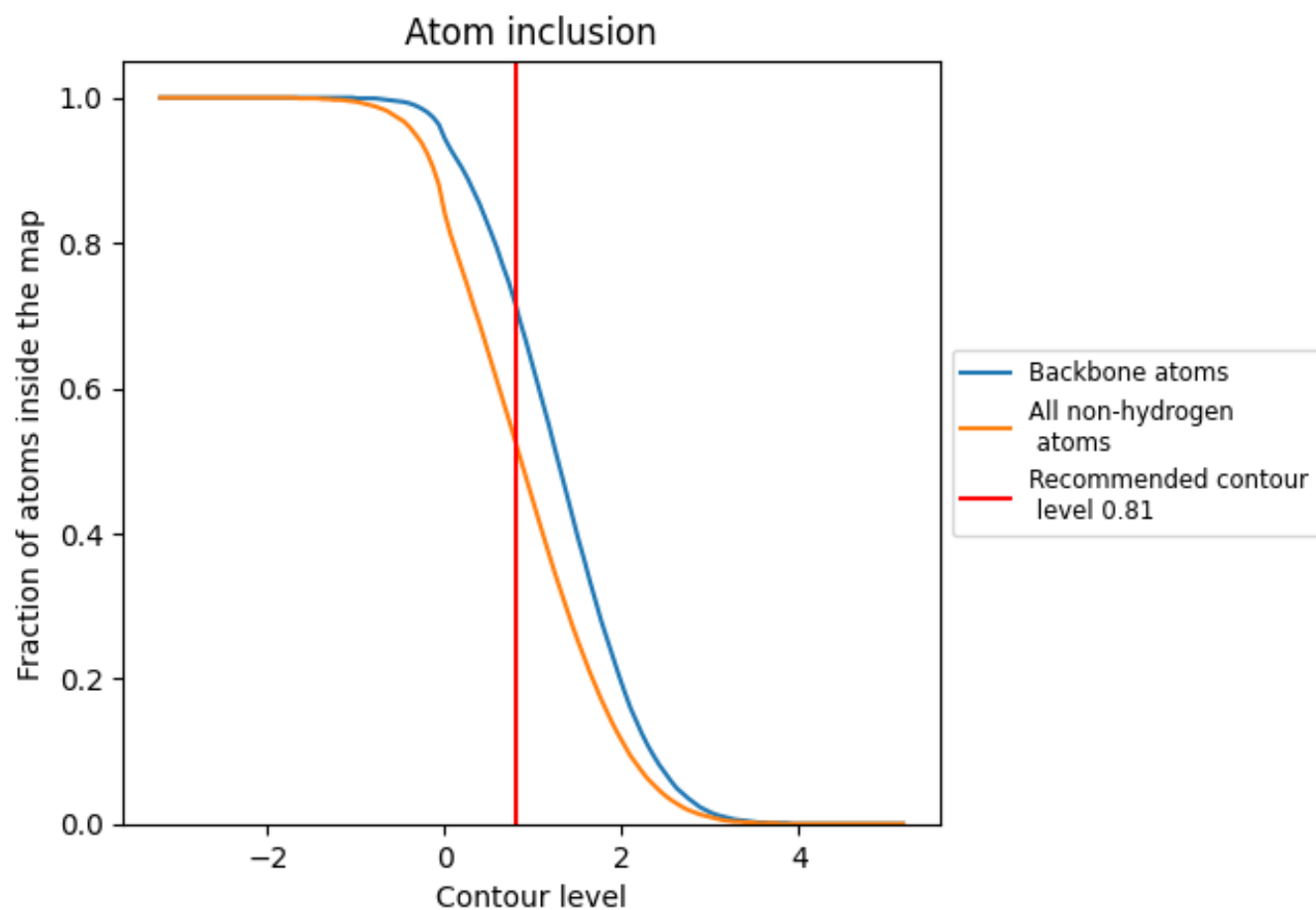
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.81).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 52% 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 (0.81) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5220	 0.0950
1	 0.4600	 0.0620
2	 0.4860	 0.0940
3	 0.4220	 0.0820
4	 0.5320	 0.0980
5	 0.5260	 0.0990
6	 0.5070	 0.0980
7	 0.4880	 0.0750
A	 0.4790	 0.1150
B	 0.4390	 0.0940
C	 0.4990	 0.0930
D	 0.4990	 0.1020
E	 0.4870	 0.0970
F	 0.5000	 0.0860
G	 0.5300	 0.0960
H	 0.5230	 0.0860
I	 0.4190	 0.0790
J	 0.4720	 0.0910
K	 0.4440	 0.1040
L	 0.5170	 0.0990
M	 0.4580	 0.0890
N	 0.5620	 0.1060
O	 0.6040	 0.0960
P	 0.6550	 0.1040
Q	 0.6180	 0.1110
R	 0.6140	 0.1040
S	 0.4910	 0.0920
T	 0.6140	 0.1080
U	 0.5270	 0.1130
V	 0.4650	 0.0920
W	 0.4620	 0.0690
X	 0.5660	 0.0510
Y	 0.6990	 0.1450
Z	 0.5370	 0.0900

