



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 02:14 PM JST

PDB ID : 5WVK
EMDB ID : EMD-6694
Title : Yeast proteasome-ADP-AlFx
Authors : Ding, Z.; Cong, Y.
Deposited on : 2016-12-25
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

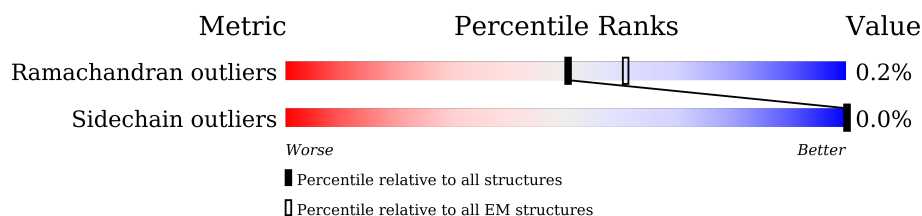
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	b	215	
2	2	261	
2	i	261	
3	3	205	
3	h	205	
4	4	198	
4	g	198	
5	5	287	

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Mol	Chain	Length	Quality of chain
5	f	287	
6	6	241	
6	e	241	
7	7	266	
7	a	266	
8	A	252	
8	c	252	
9	B	250	
9	j	250	
10	C	258	
10	d	258	
11	D	254	
11	n	254	
12	E	260	
12	m	260	
13	F	234	
13	l	234	
14	G	288	
14	k	288	
15	H	467	
16	I	437	
17	J	405	
18	K	428	
19	L	437	
20	M	434	

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

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 105261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	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 Ubiquitin carboxyl-terminal hydrolase RPN11.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	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		

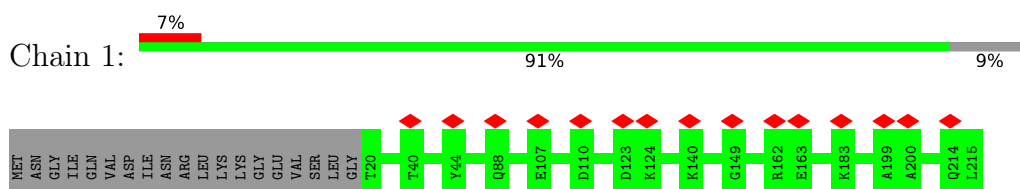
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

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

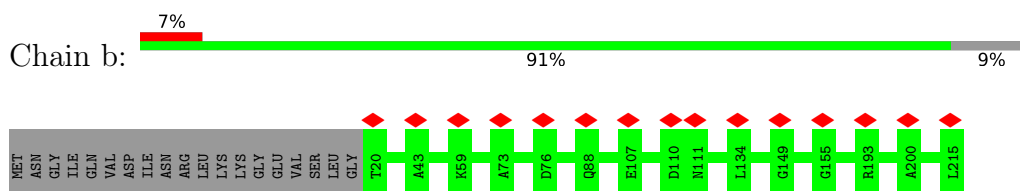
3 Residue-property plots [i](#)

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

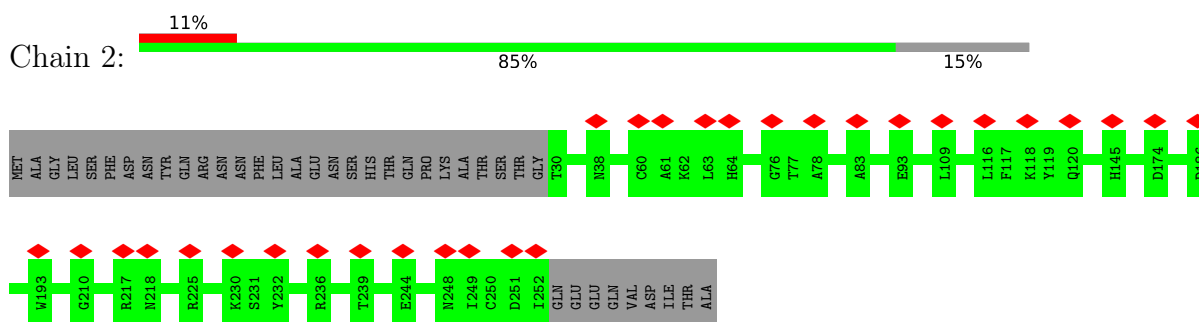
- Molecule 1: Proteasome subunit beta type-1



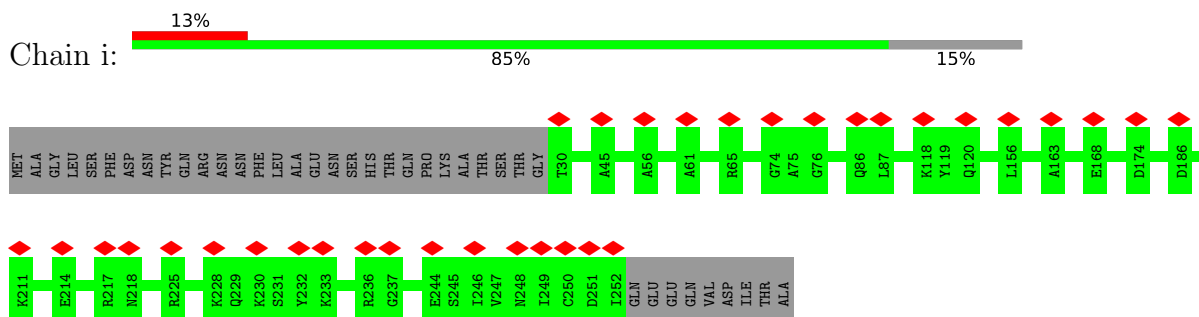
- Molecule 1: Proteasome subunit beta type-1



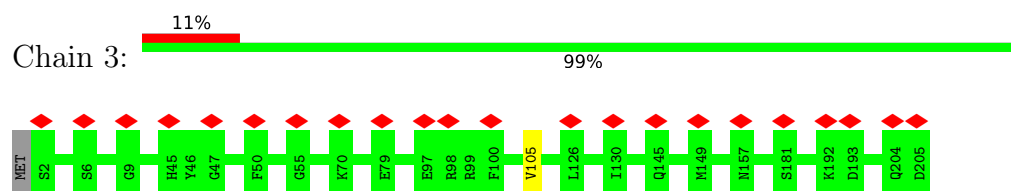
- Molecule 2: Proteasome subunit beta type-2



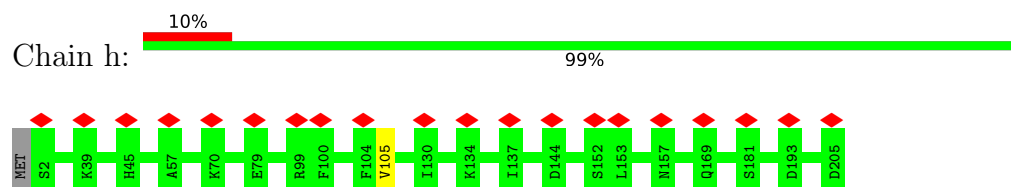
- Molecule 2: Proteasome subunit beta type-2



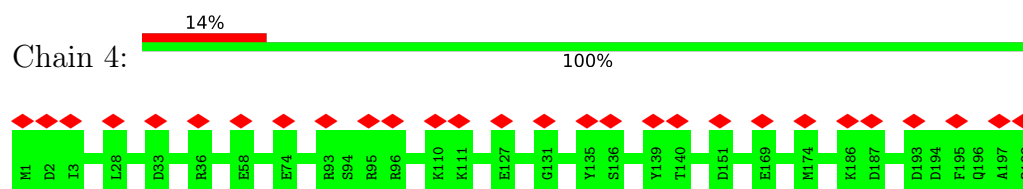
- Molecule 3: Proteasome subunit beta type-3



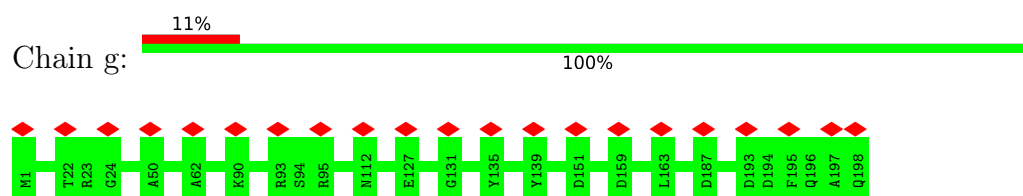
- Molecule 3: Proteasome subunit beta type-3



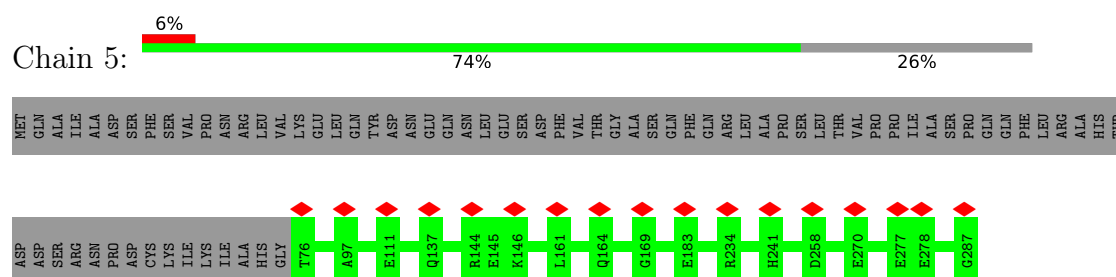
- Molecule 4: Proteasome subunit beta type-4



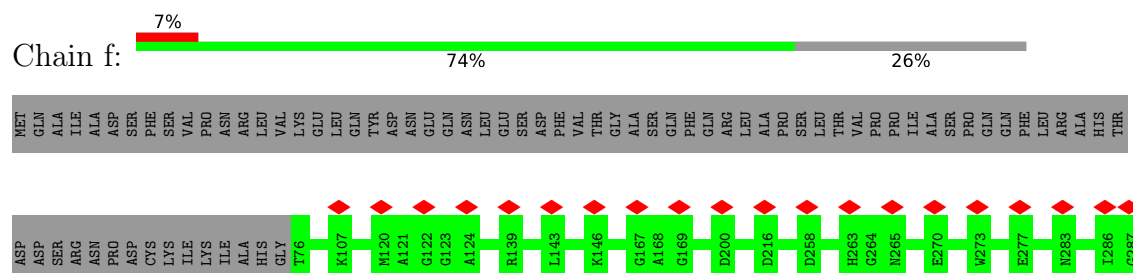
- Molecule 4: Proteasome subunit beta type-4



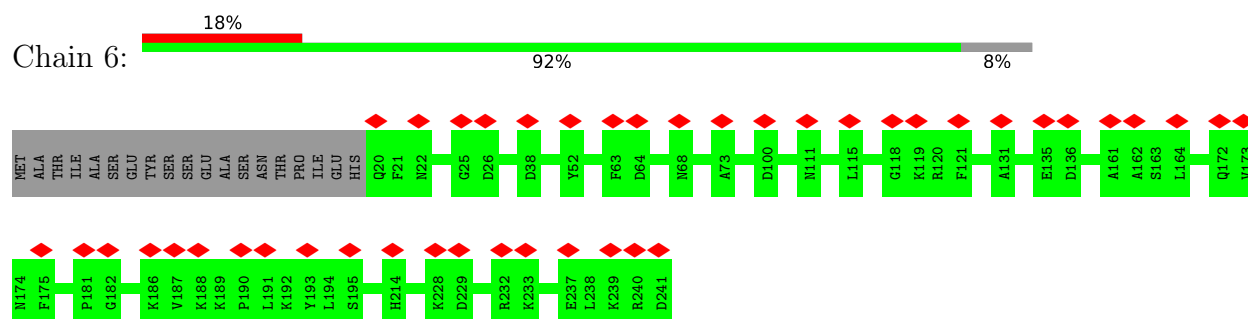
- Molecule 5: Proteasome subunit beta type-5



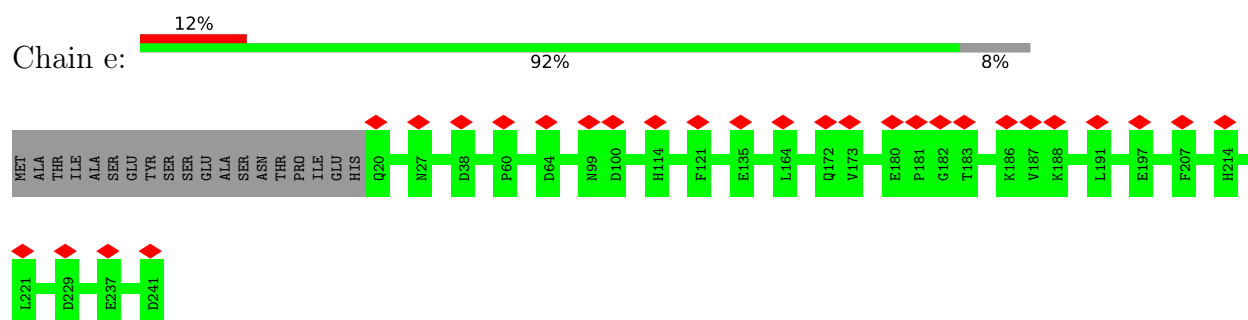
- Molecule 5: Proteasome subunit beta type-5



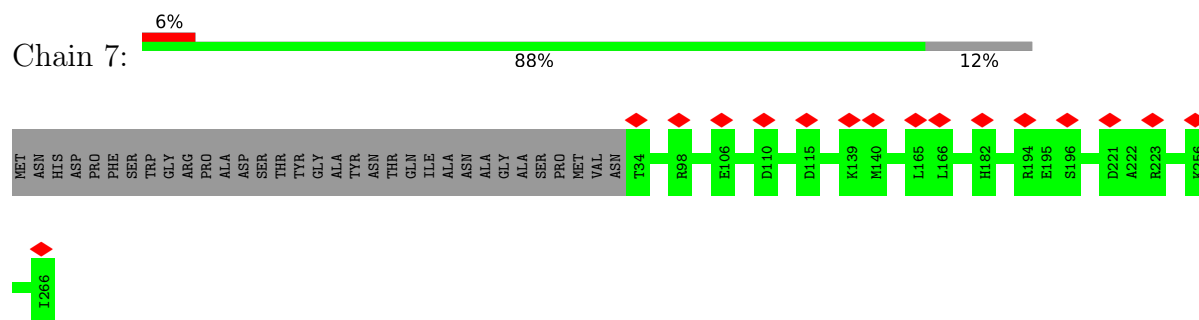
- Molecule 6: Proteasome subunit beta type-6



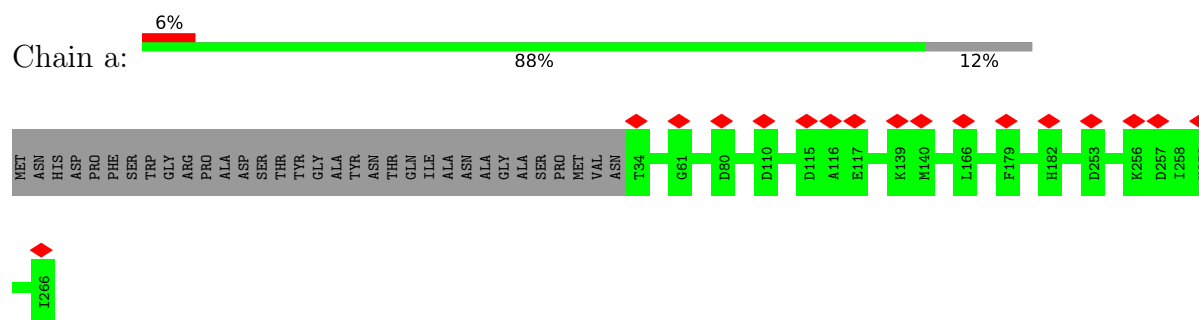
- Molecule 6: Proteasome subunit beta type-6



- Molecule 7: Proteasome subunit beta type-7

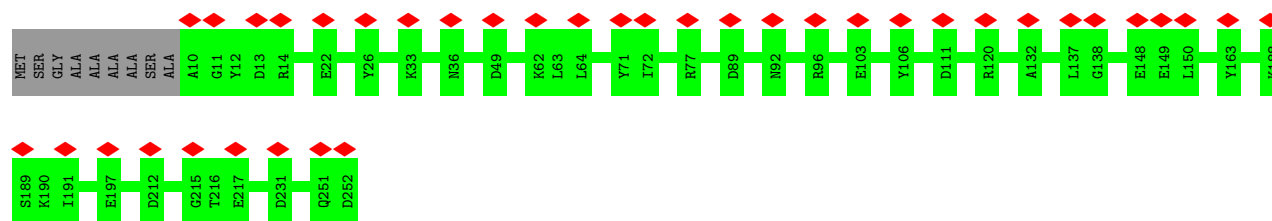


- Molecule 7: Proteasome subunit beta type-7

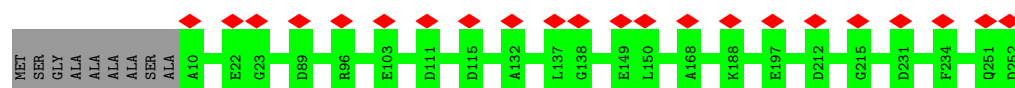


- Molecule 8: Proteasome subunit alpha type-1

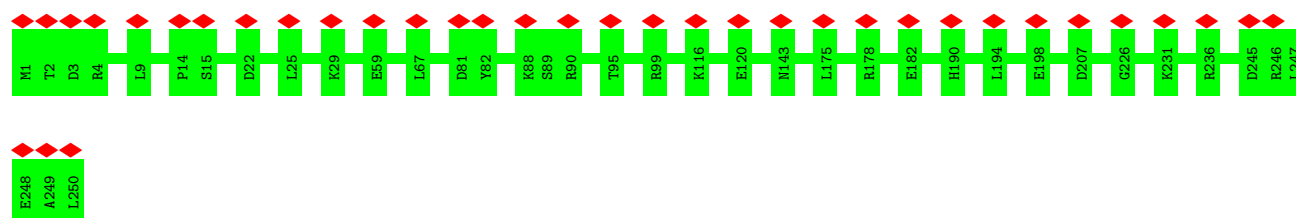




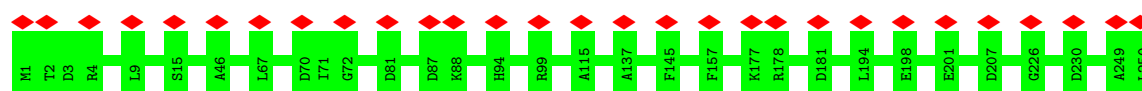
• Molecule 8: Proteasome subunit alpha type-1



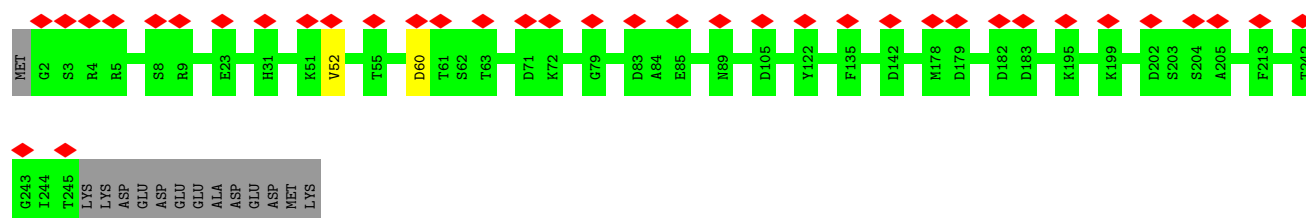
• Molecule 9: Proteasome subunit alpha type-2



• Molecule 9: Proteasome subunit alpha type-2

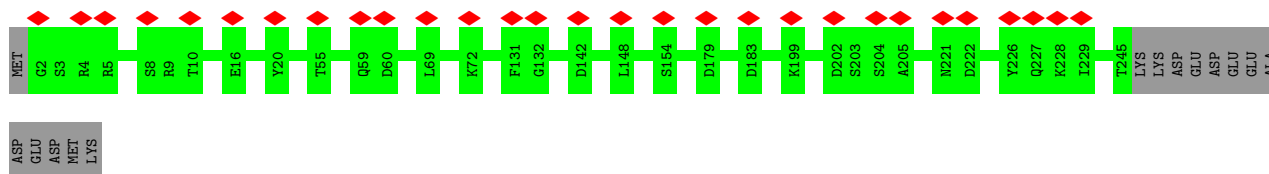


• Molecule 10: Proteasome subunit alpha type-3



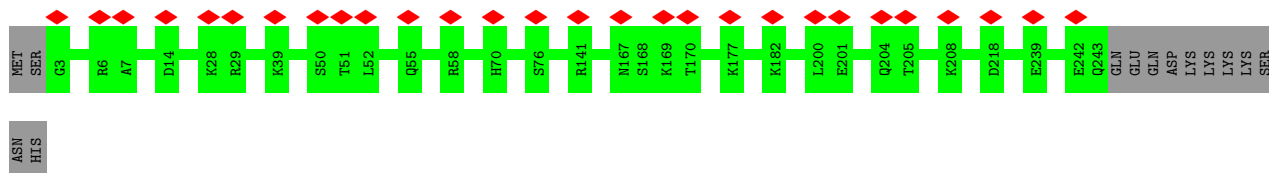
• Molecule 10: Proteasome subunit alpha type-3





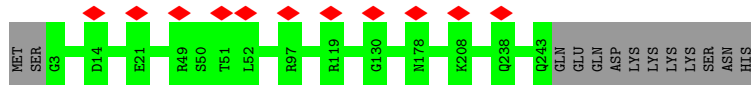
- Molecule 11: Proteasome subunit alpha type-4

Chain D:



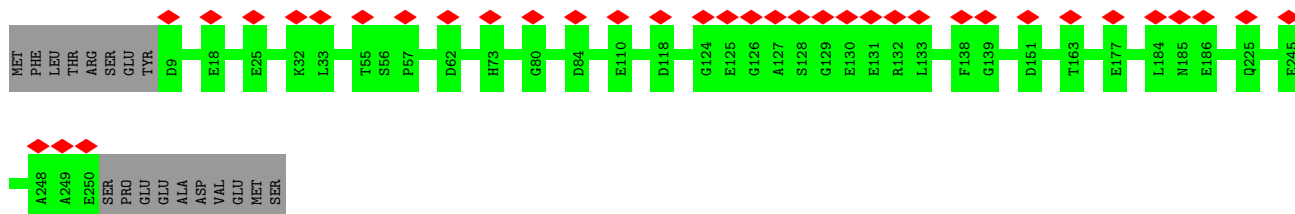
- Molecule 11: Proteasome subunit alpha type-4

Chain n:



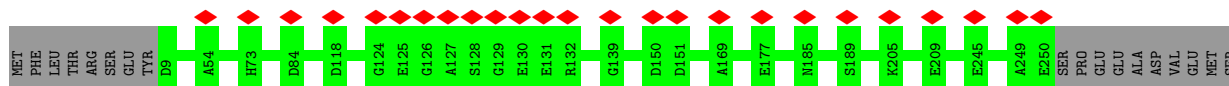
- Molecule 12: Proteasome subunit alpha type-5

Chain E:



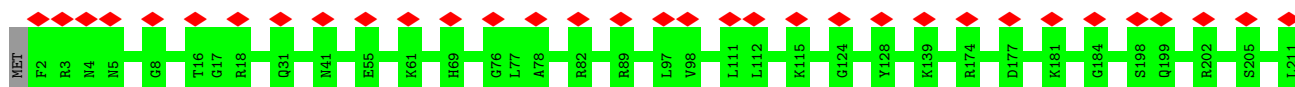
- Molecule 12: Proteasome subunit alpha type-5

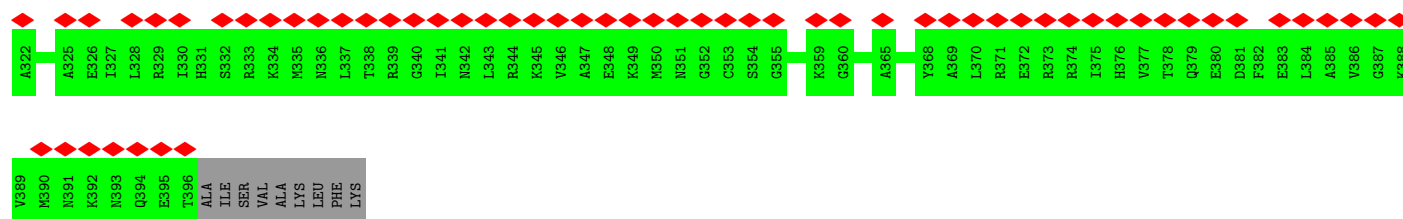
Chain m:



- Molecule 13: Proteasome subunit alpha type-6

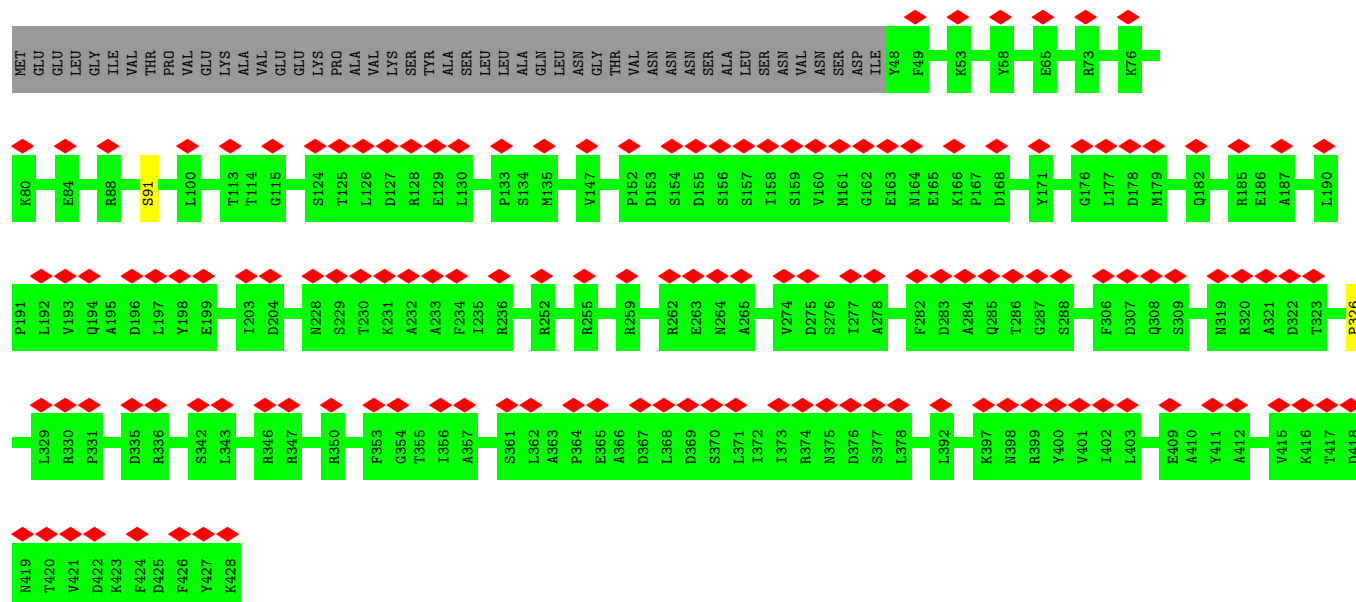
Chain F:





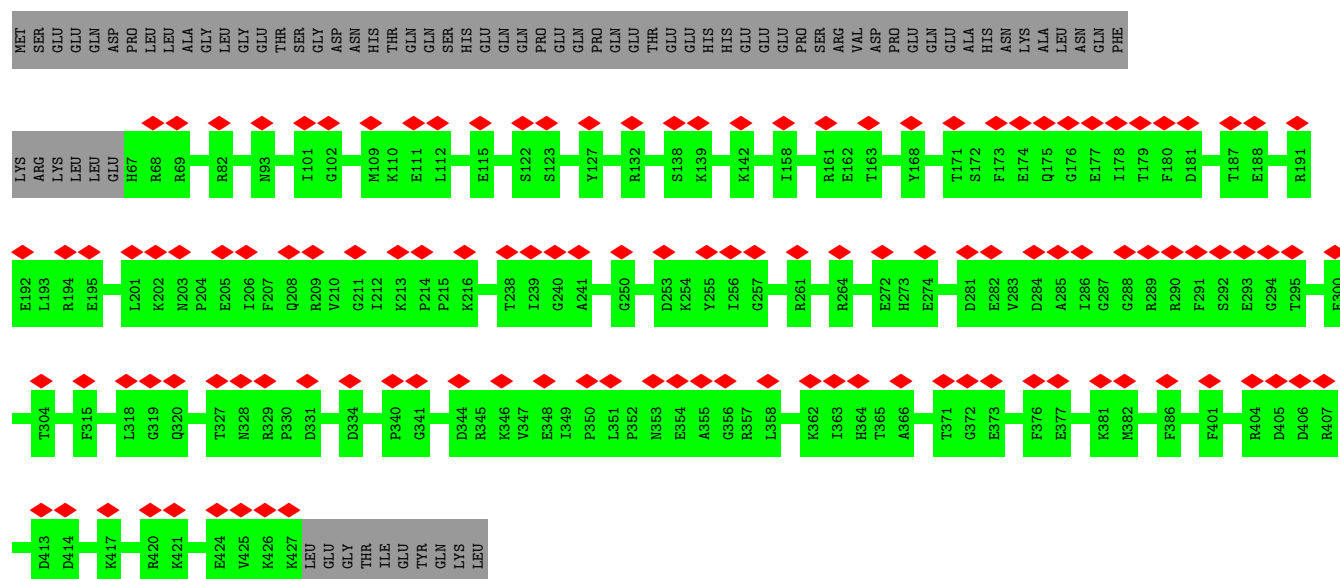
- Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K: 33% 89% 11%

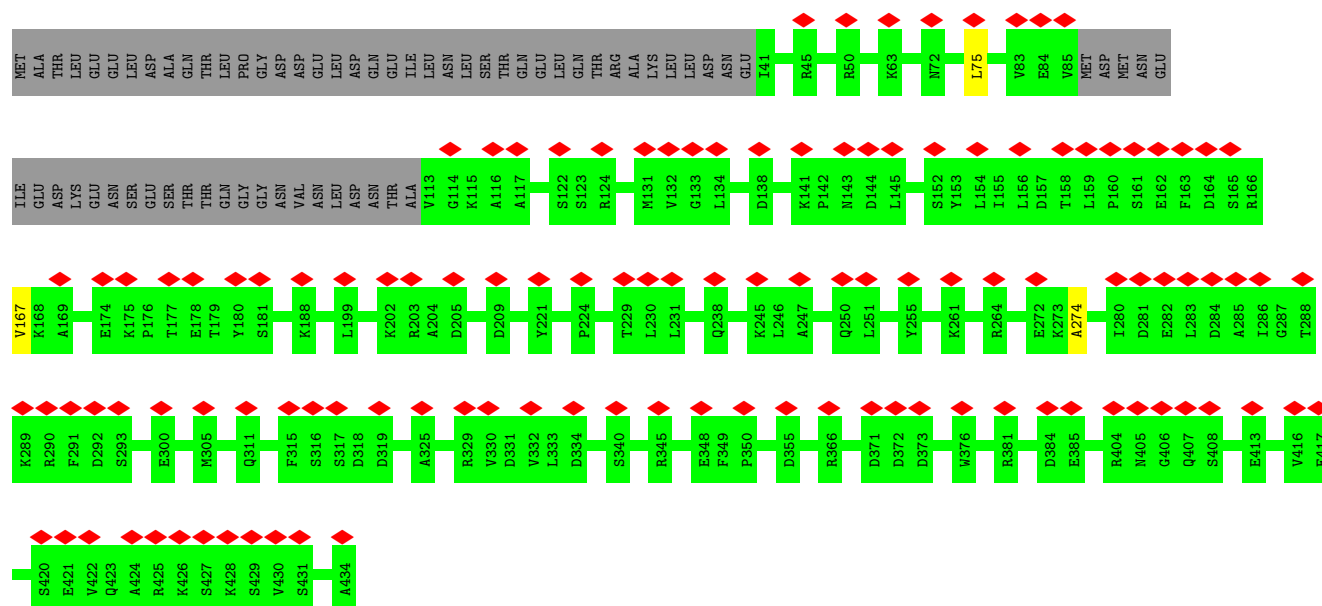
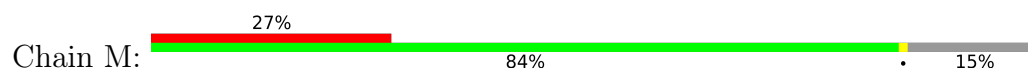


- Molecule 19: 26S protease subunit RPT4

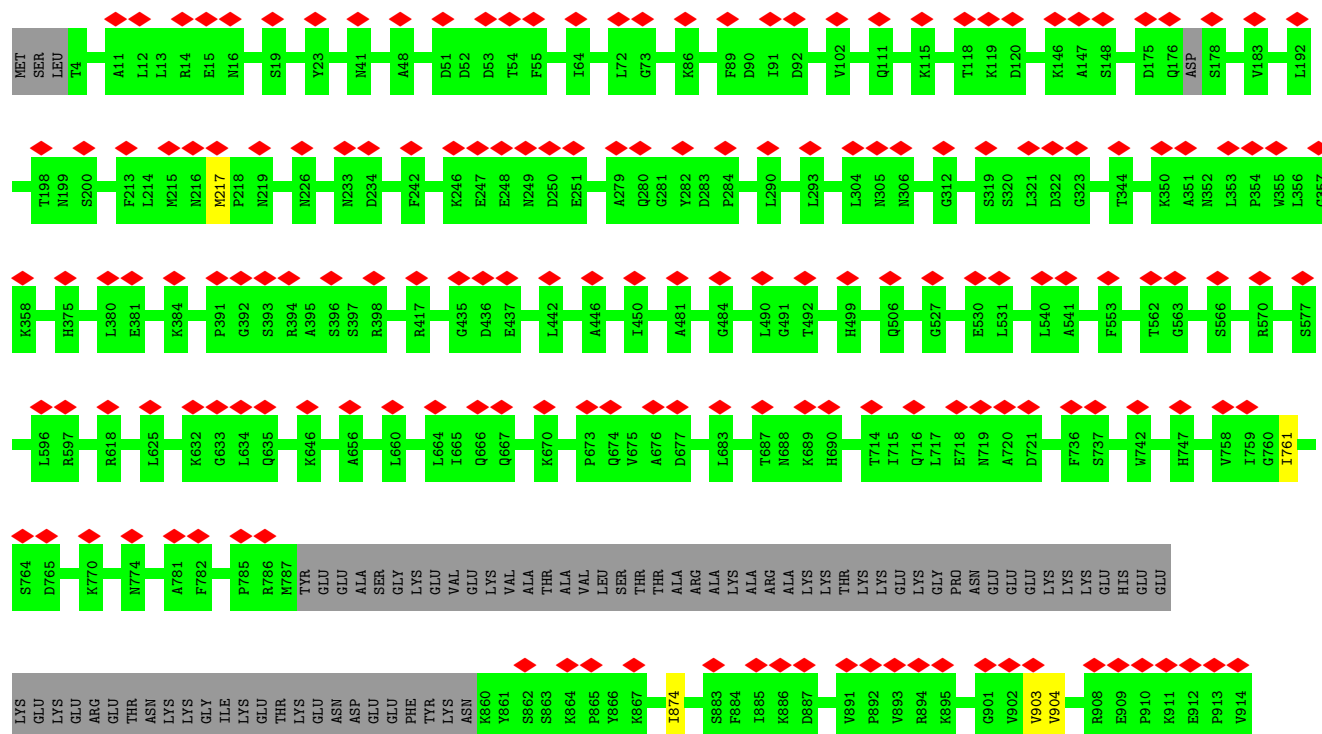
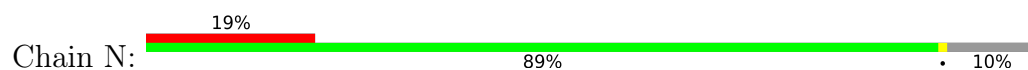
Chain L: 28% 83% 17%

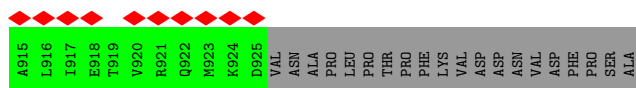


- Molecule 20: 26S protease regulatory subunit 6A

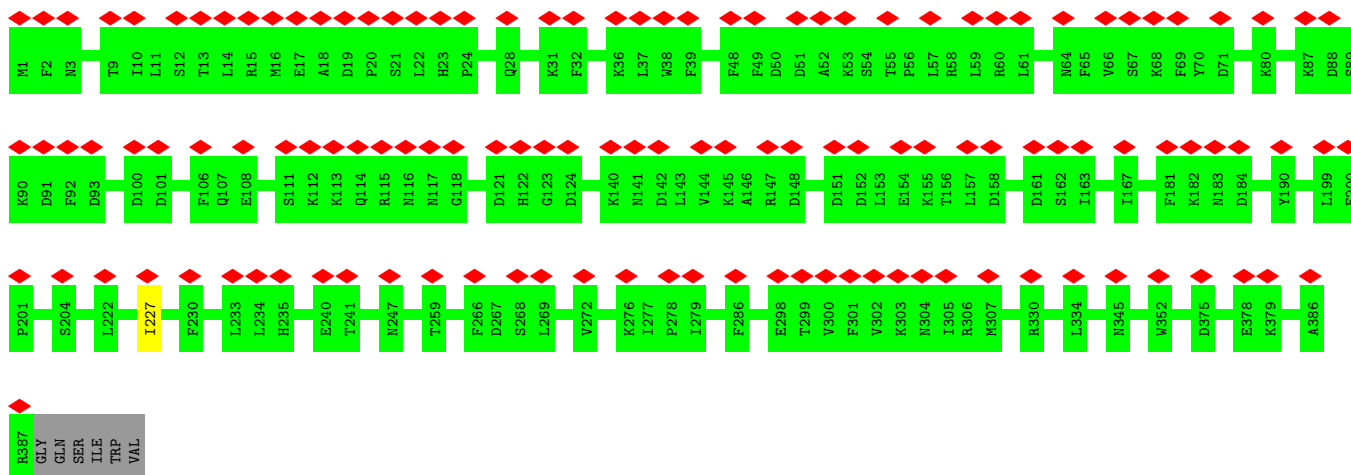


- Molecule 21: 26S proteasome regulatory subunit RPN2

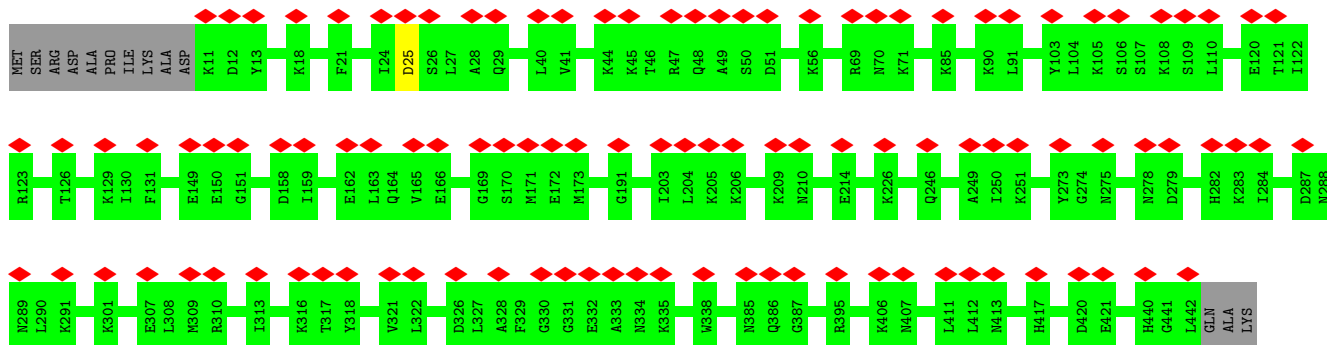




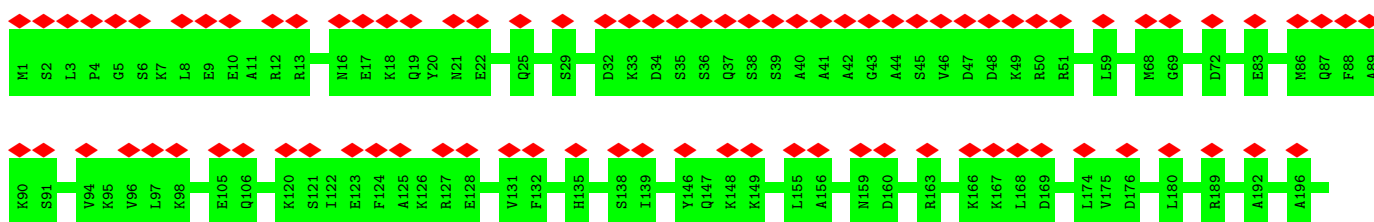
• Molecule 22: 26S proteasome regulatory subunit RPN9

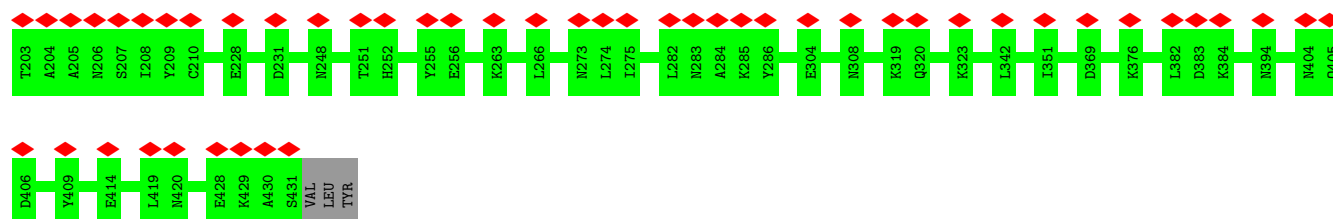


• Molecule 23: 26S proteasome regulatory subunit RPN5



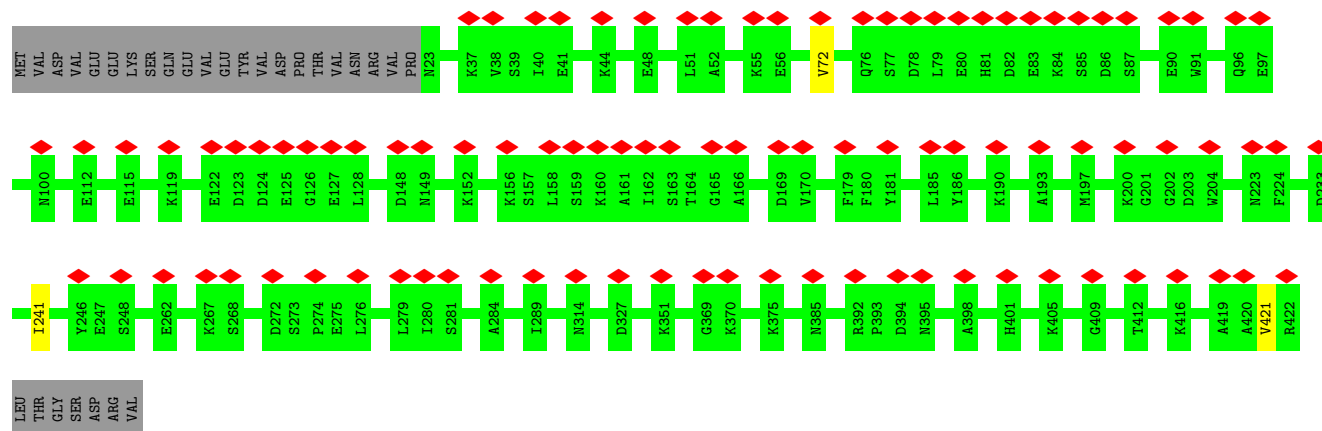
• Molecule 24: 26S proteasome regulatory subunit RPN6





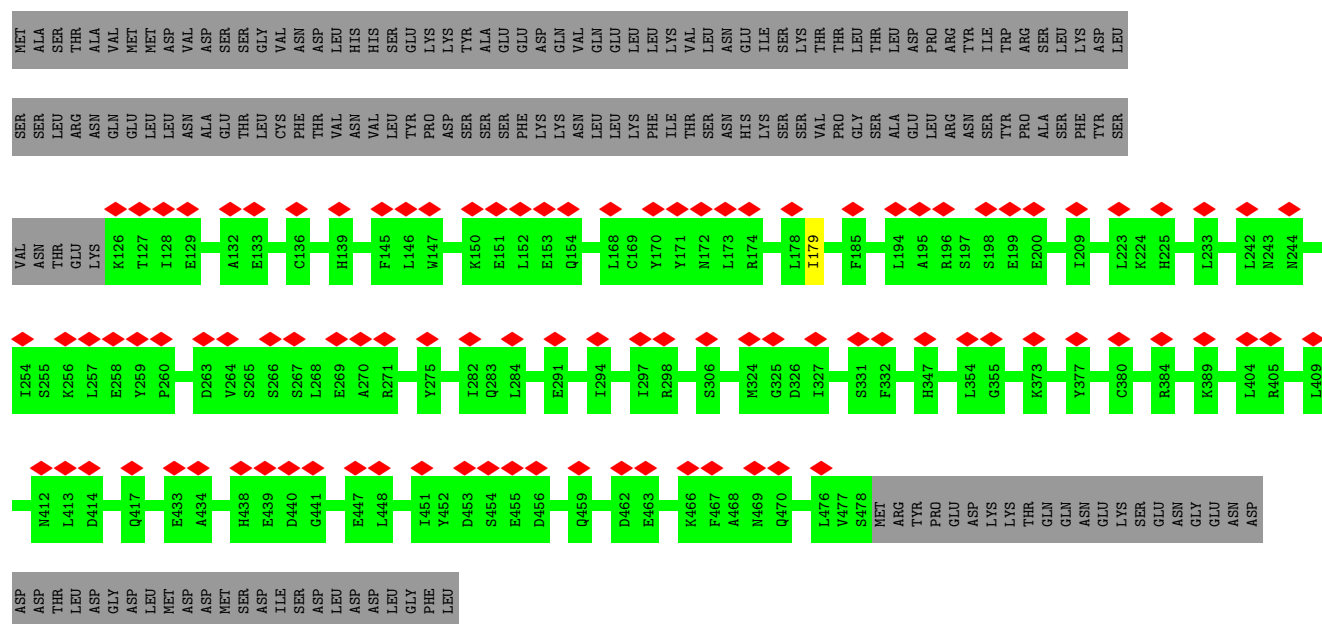
• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R: 23% 93% 7%



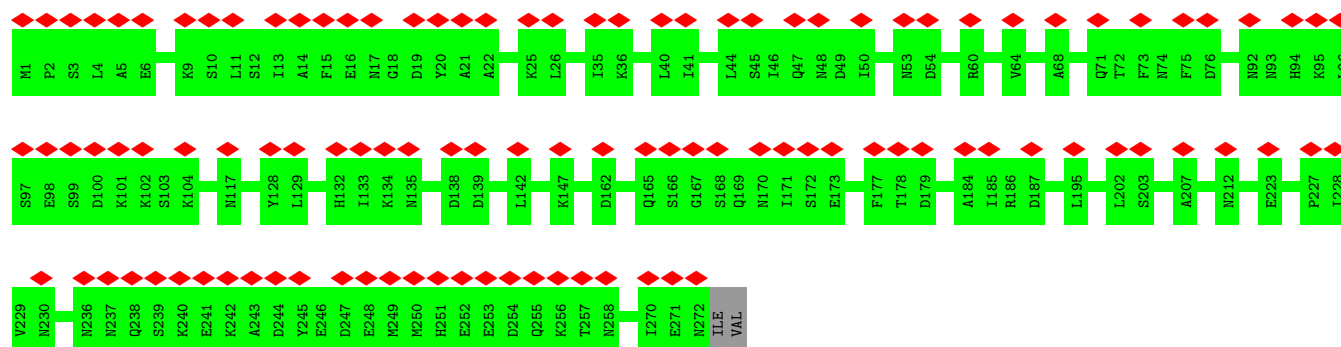
• Molecule 26: 26S proteasome regulatory subunit RPN3

Chain S: 19% 67% 33%

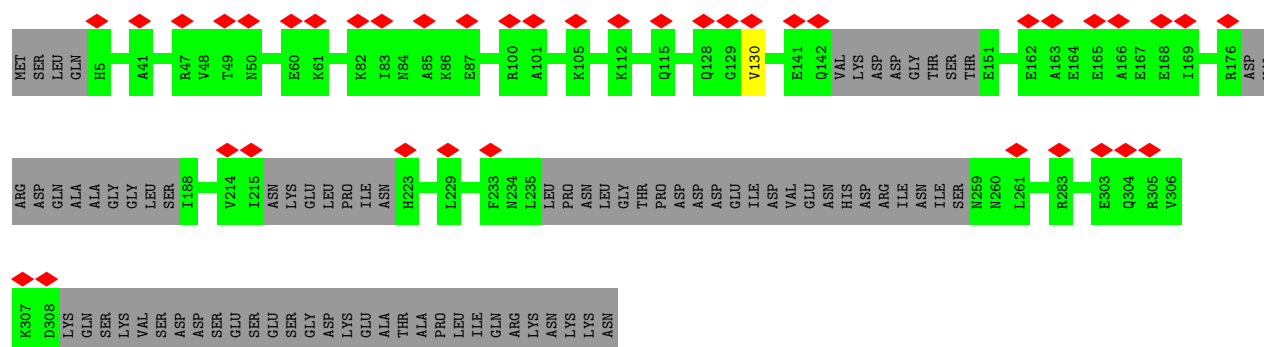
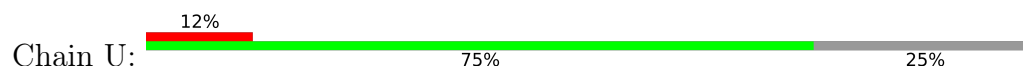


• Molecule 27: 26S proteasome regulatory subunit RPN12

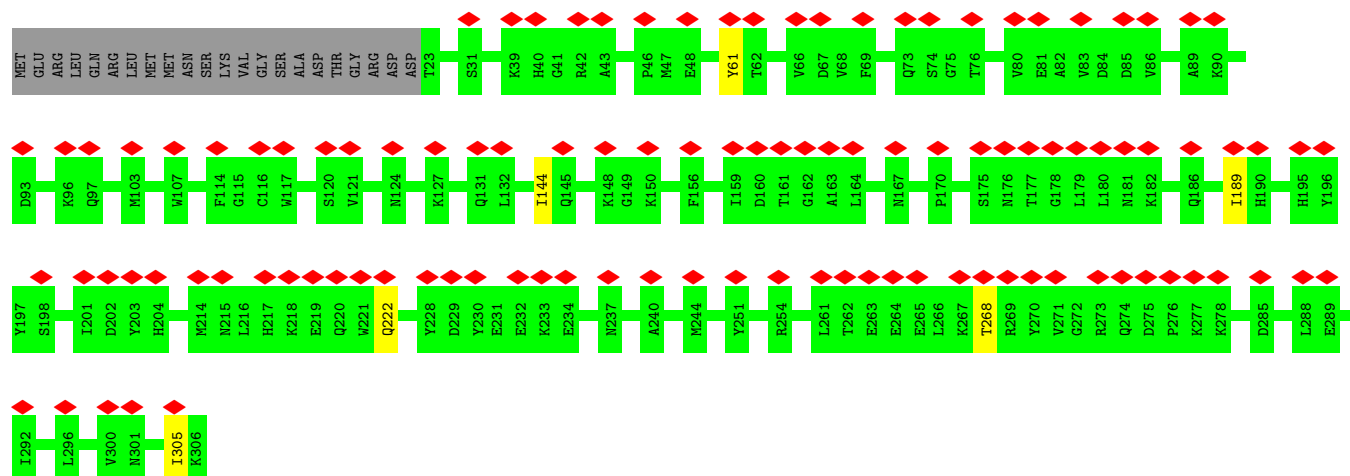
Chain T: 40% 99% 1%



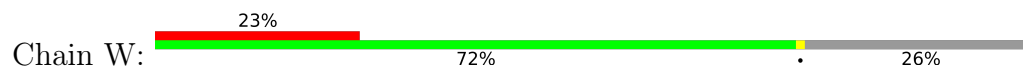
• Molecule 28: 26S proteasome regulatory subunit RPN8

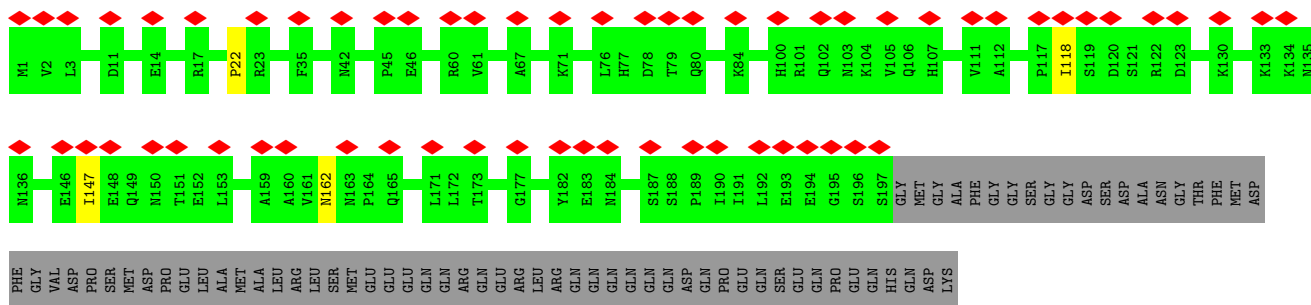


• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

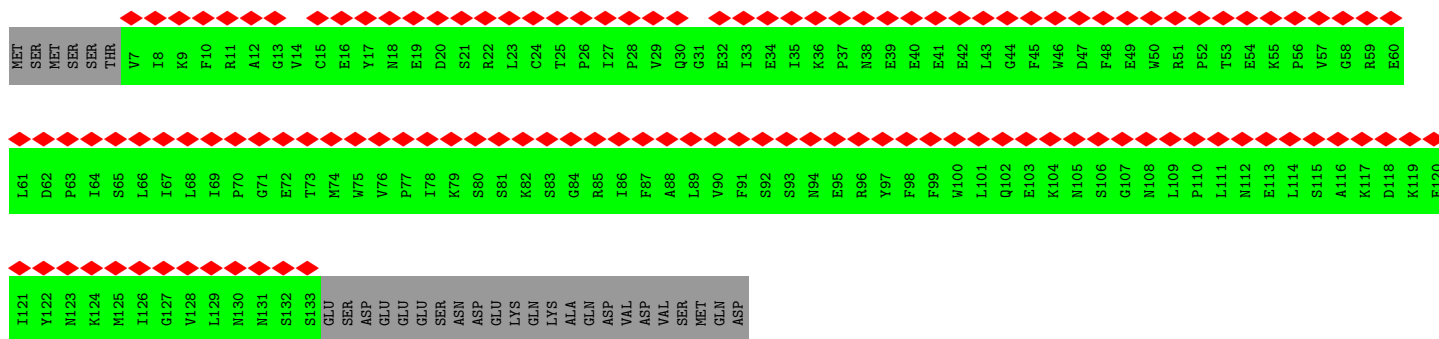
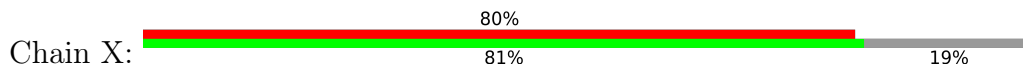


• Molecule 30: 26S proteasome regulatory subunit RPN10

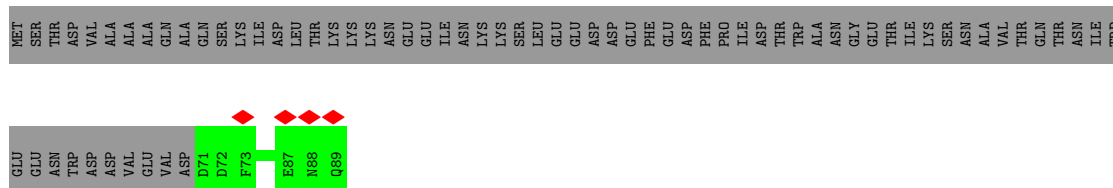




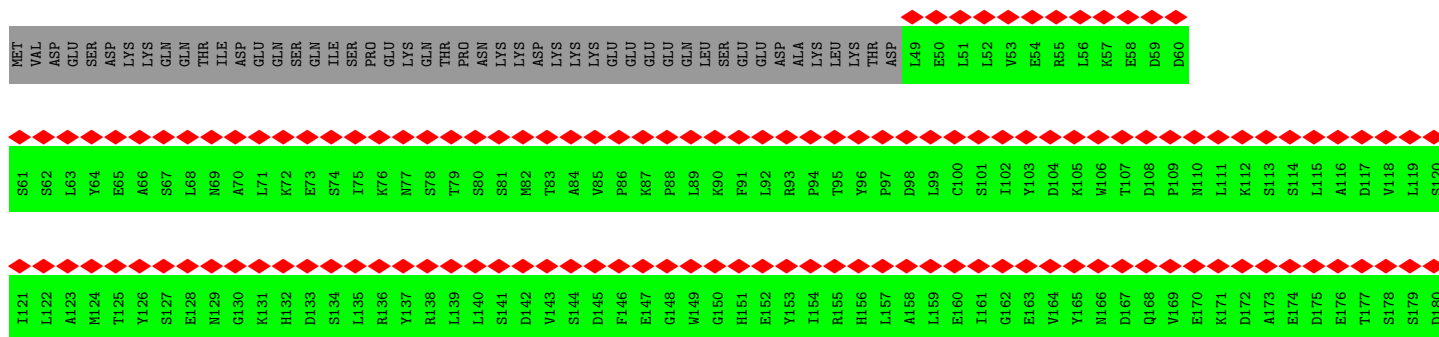
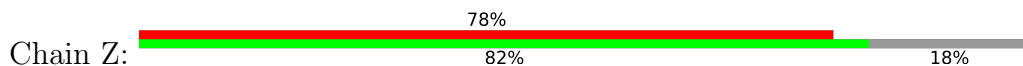
• Molecule 31: 26S proteasome regulatory subunit RPN13



• 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, Not provided	
Number of particles used	178576	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.666	Depositor
Minimum map value	-0.738	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.543	Depositor
Map size (Å)	474.47998, 474.47998, 474.47998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.23	0/1541	0.41	0/2087
1	b	0.23	0/1541	0.42	0/2087
2	2	0.23	0/1723	0.41	0/2337
2	i	0.23	0/1723	0.41	0/2337
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.41	0/2174
4	4	0.23	0/1613	0.39	0/2173
4	g	0.23	0/1613	0.40	0/2173
5	5	0.23	0/1681	0.40	0/2274
5	f	0.23	0/1681	0.41	0/2274
6	6	0.24	0/1795	0.40	0/2420
6	e	0.24	0/1795	0.39	0/2420
7	7	0.23	0/1855	0.41	0/2514
7	a	0.23	0/1855	0.42	0/2514
8	A	0.24	0/1959	0.40	0/2652
8	c	0.23	0/1959	0.39	0/2652
9	B	0.24	0/1952	0.40	0/2642
9	j	0.25	0/1952	0.40	0/2642
10	C	0.23	0/1934	0.43	0/2618
10	d	0.23	0/1934	0.41	0/2618
11	D	0.23	0/1919	0.39	0/2598
11	n	0.23	0/1919	0.40	0/2598
12	E	0.23	0/1886	0.41	0/2541
12	m	0.23	0/1886	0.39	0/2541
13	F	0.24	0/1823	0.42	0/2463
13	l	0.24	0/1823	0.42	0/2463
14	G	0.23	0/1936	0.39	0/2614
14	k	0.24	0/1936	0.39	0/2614
15	H	0.23	0/2831	0.41	0/3808
16	I	0.34	1/2860 (0.0%)	0.43	1/3856 (0.0%)
17	J	0.23	0/2964	0.40	0/3981
18	K	0.25	0/3062	0.42	0/4132
19	L	0.24	0/2896	0.39	0/3895
20	M	0.35	2/2903 (0.1%)	0.41	0/3909

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	N	0.25	1/6670 (0.0%)	0.39	0/9023
22	O	0.23	0/3243	0.41	0/4374
23	P	0.23	0/3599	0.37	0/4854
24	Q	0.23	0/3527	0.38	0/4748
25	R	0.23	0/3272	0.38	0/4412
26	S	0.23	0/2945	0.39	0/3976
27	T	0.23	0/2279	0.40	0/3077
28	U	0.23	0/2087	0.37	0/2811
29	V	0.24	0/2271	0.49	0/3064
30	W	0.25	0/1557	0.43	0/2111
31	X	0.26	0/1058	0.43	0/1432
32	Y	0.22	0/169	0.30	0/223
33	Z	0.25	1/6404 (0.0%)	0.41	1/8686 (0.0%)
All	All	0.24	5/107053 (0.0%)	0.40	2/144586 (0.0%)

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
15	H	0	1
16	I	0	1
29	V	0	3
30	W	0	1
33	Z	0	1
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	102	ASN	C-N	13.06	1.59	1.34
20	M	274	ALA	C-N	10.62	1.54	1.34
20	M	75	LEU	C-N	9.21	1.51	1.34
21	N	217	MET	C-N	7.33	1.48	1.34
33	Z	468	GLU	C-N	6.91	1.47	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	432	LEU	CA-CB-CG	5.89	128.84	115.30
33	Z	558	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	H	185	LEU	Peptide
16	I	254	GLN	Peptide
29	V	222	GLN	Peptide
29	V	268	THR	Peptide
29	V	61	TYR	Peptide
30	W	162	ASN	Peptide
33	Z	255	LEU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	194/215 (90%)	186 (96%)	8 (4%)	0	100	100
1	b	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
2	2	221/261 (85%)	208 (94%)	13 (6%)	0	100	100
2	i	221/261 (85%)	209 (95%)	12 (5%)	0	100	100
3	3	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	29	68
3	h	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	29	68
4	4	196/198 (99%)	183 (93%)	13 (7%)	0	100	100
4	g	196/198 (99%)	186 (95%)	10 (5%)	0	100	100
5	5	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
5	f	210/287 (73%)	198 (94%)	12 (6%)	0	100	100
6	6	220/241 (91%)	211 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	e	220/241 (91%)	206 (94%)	14 (6%)	0	100	100
7	7	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
7	a	231/266 (87%)	218 (94%)	13 (6%)	0	100	100
8	A	241/252 (96%)	230 (95%)	11 (5%)	0	100	100
8	c	241/252 (96%)	229 (95%)	12 (5%)	0	100	100
9	B	248/250 (99%)	237 (96%)	11 (4%)	0	100	100
9	j	248/250 (99%)	235 (95%)	13 (5%)	0	100	100
10	C	242/258 (94%)	224 (93%)	16 (7%)	2 (1%)	19	60
10	d	242/258 (94%)	228 (94%)	14 (6%)	0	100	100
11	D	239/254 (94%)	230 (96%)	9 (4%)	0	100	100
11	n	239/254 (94%)	224 (94%)	15 (6%)	0	100	100
12	E	240/260 (92%)	230 (96%)	10 (4%)	0	100	100
12	m	240/260 (92%)	231 (96%)	9 (4%)	0	100	100
13	F	231/234 (99%)	220 (95%)	11 (5%)	0	100	100
13	l	231/234 (99%)	221 (96%)	10 (4%)	0	100	100
14	G	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
14	k	242/288 (84%)	232 (96%)	10 (4%)	0	100	100
15	H	353/467 (76%)	321 (91%)	32 (9%)	0	100	100
16	I	360/437 (82%)	334 (93%)	25 (7%)	1 (0%)	41	76
17	J	371/405 (92%)	351 (95%)	20 (5%)	0	100	100
18	K	379/428 (89%)	345 (91%)	33 (9%)	1 (0%)	41	76
19	L	359/437 (82%)	334 (93%)	25 (7%)	0	100	100
20	M	363/434 (84%)	343 (94%)	19 (5%)	1 (0%)	41	76
21	N	843/945 (89%)	796 (94%)	43 (5%)	4 (0%)	29	68
22	O	385/393 (98%)	339 (88%)	45 (12%)	1 (0%)	41	76
23	P	430/445 (97%)	387 (90%)	42 (10%)	1 (0%)	47	80
24	Q	429/434 (99%)	400 (93%)	29 (7%)	0	100	100
25	R	398/429 (93%)	366 (92%)	29 (7%)	3 (1%)	19	60
26	S	351/523 (67%)	320 (91%)	30 (8%)	1 (0%)	41	76
27	T	270/274 (98%)	244 (90%)	26 (10%)	0	100	100
28	U	245/338 (72%)	237 (97%)	7 (3%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	V	282/306 (92%)	242 (86%)	37 (13%)	3 (1%)	14	52
30	W	195/268 (73%)	170 (87%)	22 (11%)	3 (2%)	10	46
31	X	125/156 (80%)	100 (80%)	25 (20%)	0	100	100
32	Y	17/89 (19%)	17 (100%)	0	0	100	100
33	Z	807/993 (81%)	736 (91%)	71 (9%)	0	100	100
All	All	13276/15139 (88%)	12380 (93%)	872 (7%)	24 (0%)	50	80

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	C	52	VAL
16	I	255	LYS
21	N	874	ILE
28	U	130	VAL
3	3	105	VAL
21	N	903	VAL
30	W	22	PRO
21	N	761	ILE
25	R	241	ILE
25	R	421	VAL
29	V	189	ILE
29	V	305	ILE
30	W	147	ILE
10	C	60	ASP
18	K	326	PRO
23	P	25	ASP
29	V	144	ILE
3	h	105	VAL
20	M	167	VAL
25	R	72	VAL
26	S	179	ILE
21	N	904	VAL
22	O	227	ILE
30	W	118	ILE

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	1	162/178 (91%)	162 (100%)	0	100	100
1	b	162/178 (91%)	162 (100%)	0	100	100
2	2	182/214 (85%)	182 (100%)	0	100	100
2	i	182/214 (85%)	182 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
4	g	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100
5	f	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
7	a	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
8	c	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	j	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	201 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	319/385 (83%)	319 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	333 (100%)	1 (0%)	92	95
19	L	308/377 (82%)	308 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	330/489 (68%)	330 (100%)	0	100	100
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	249/268 (93%)	249 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	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	11522/13054 (88%)	11521 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	K	91	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	81	HIS
2	2	51	GLN
2	2	120	GLN
4	4	37	GLN
4	4	86	GLN
4	4	112	ASN
4	4	133	HIS
6	6	55	ASN

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Mol	Chain	Res	Type
6	6	216	GLN
7	7	145	ASN
7	7	182	HIS
7	7	249	ASN
2	i	194	ASN
3	h	48	HIS
3	h	169	GLN
4	g	37	GLN
4	g	55	GLN
4	g	146	HIS
5	f	208	GLN
6	e	48	ASN
6	e	214	HIS
6	e	216	GLN
7	a	59	ASN
7	a	182	HIS
9	B	119	GLN
10	C	59	GLN
10	C	120	GLN
10	C	156	ASN
11	D	55	GLN
11	D	118	GLN
11	D	162	GLN
12	E	180	GLN
13	F	210	ASN
14	G	23	GLN
14	G	90	ASN
8	c	37	GLN
8	c	84	ASN
8	c	126	GLN
8	c	251	GLN
10	d	120	GLN
11	n	55	GLN
11	n	167	ASN
12	m	100	ASN
14	k	23	GLN
14	k	228	HIS
15	H	182	ASN
15	H	265	ASN
15	H	330	GLN
16	I	78	ASN
16	I	254	GLN

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Mol	Chain	Res	Type
17	J	52	ASN
18	K	144	ASN
19	L	133	ASN
19	L	320	GLN
19	L	364	HIS
20	M	74	GLN
21	N	17	GLN
21	N	240	GLN
21	N	256	GLN
21	N	329	HIS
21	N	690	HIS
21	N	703	GLN
21	N	712	ASN
21	N	716	GLN
21	N	766	GLN
21	N	922	GLN
22	O	105	GLN
22	O	354	GLN
23	P	195	GLN
23	P	277	GLN
23	P	401	ASN
23	P	440	HIS
24	Q	186	HIS
24	Q	260	GLN
24	Q	334	HIS
25	R	184	GLN
26	S	337	ASN
27	T	132	HIS
28	U	71	ASN
28	U	84	ASN
28	U	156	HIS
28	U	270	ASN
29	V	111	HIS
29	V	166	ASN
29	V	167	ASN
29	V	290	ASN
30	W	44	ASN
30	W	170	HIS
33	Z	332	ASN
33	Z	475	GLN
33	Z	810	ASN
33	Z	833	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

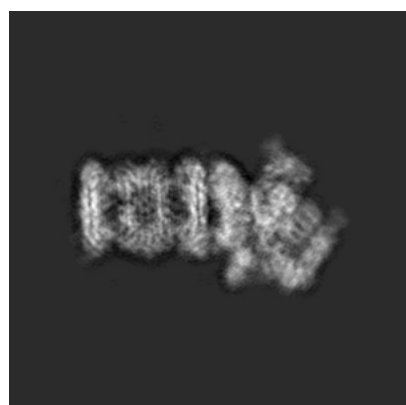
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6694. These allow visual inspection of the internal detail of the map and identification of artifacts.

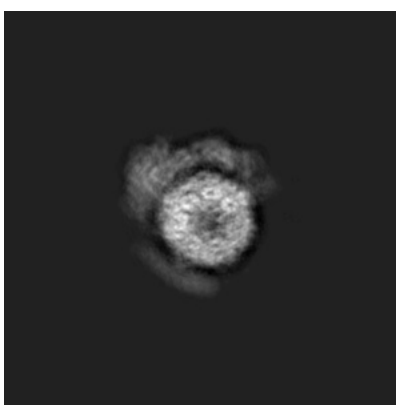
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

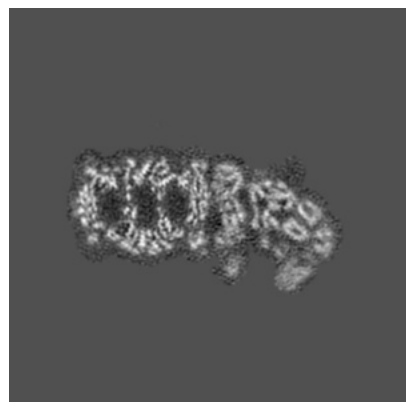


Z

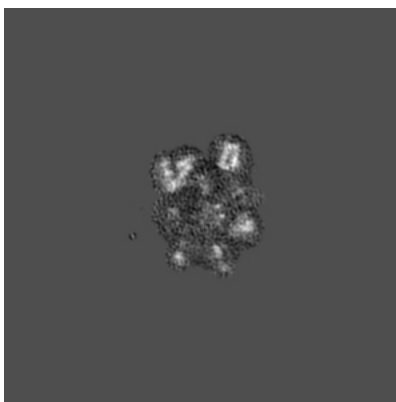
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

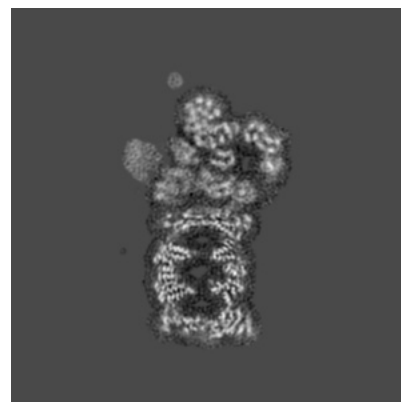
6.2.1 Primary map



X Index: 180



Y Index: 180

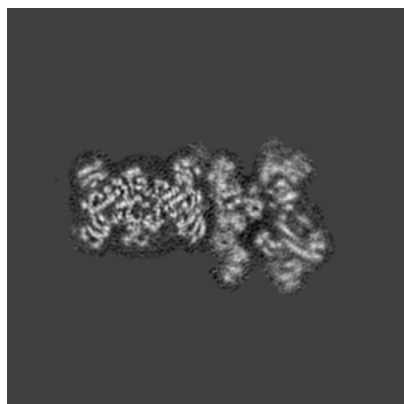


Z Index: 180

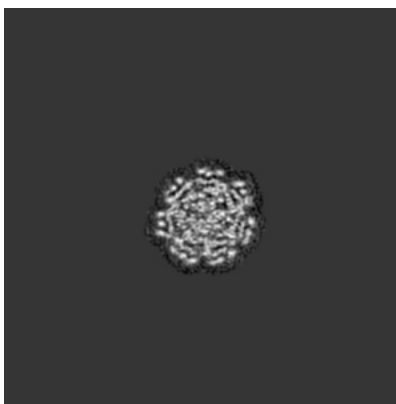
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

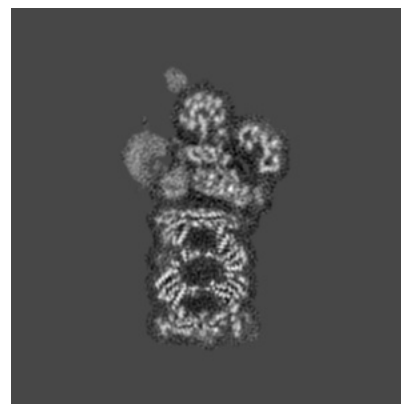
6.3.1 Primary map



X Index: 192



Y Index: 77



Z Index: 173

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.543. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

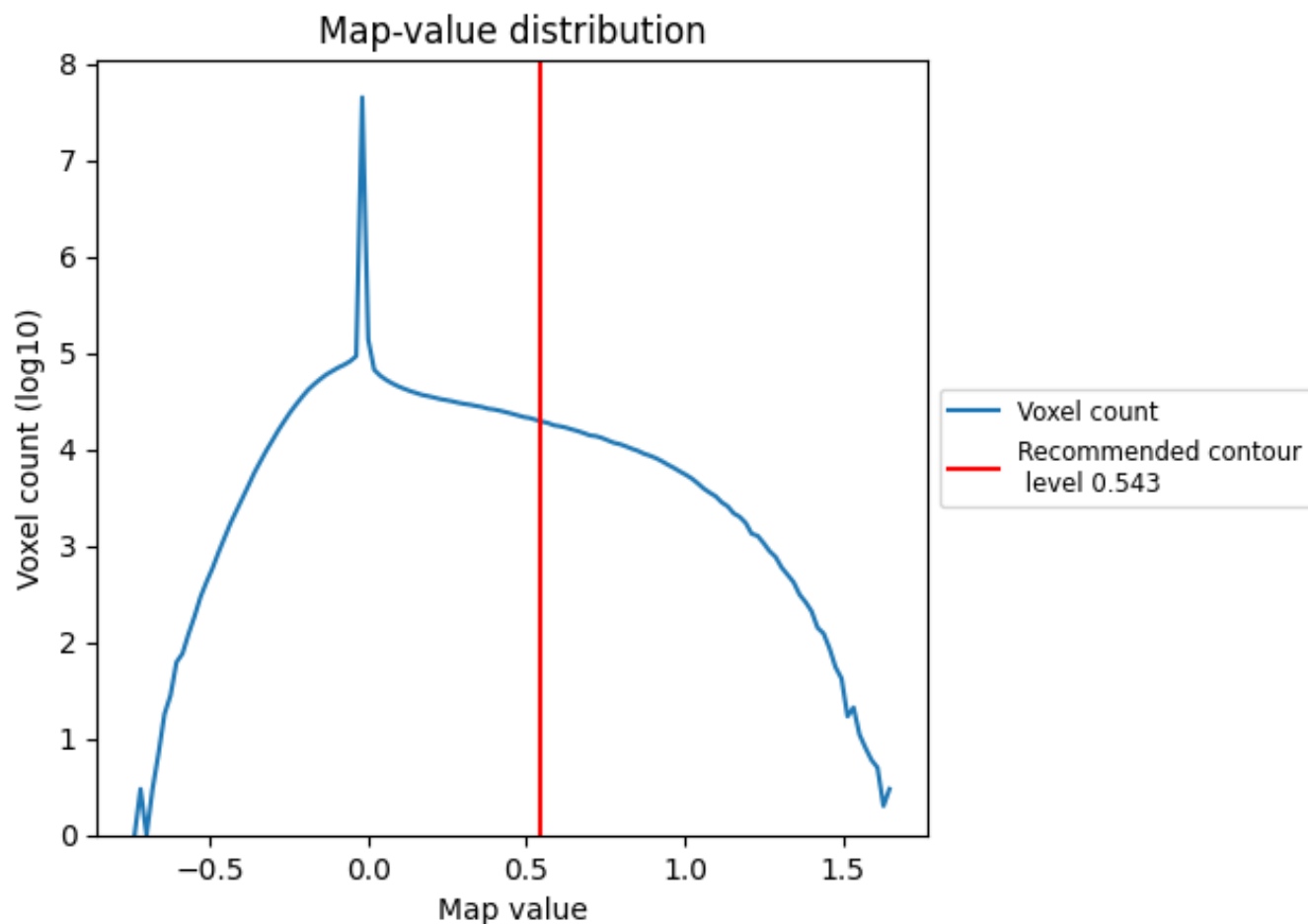
6.5 Mask visualisation

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

7 Map analysis [i](#)

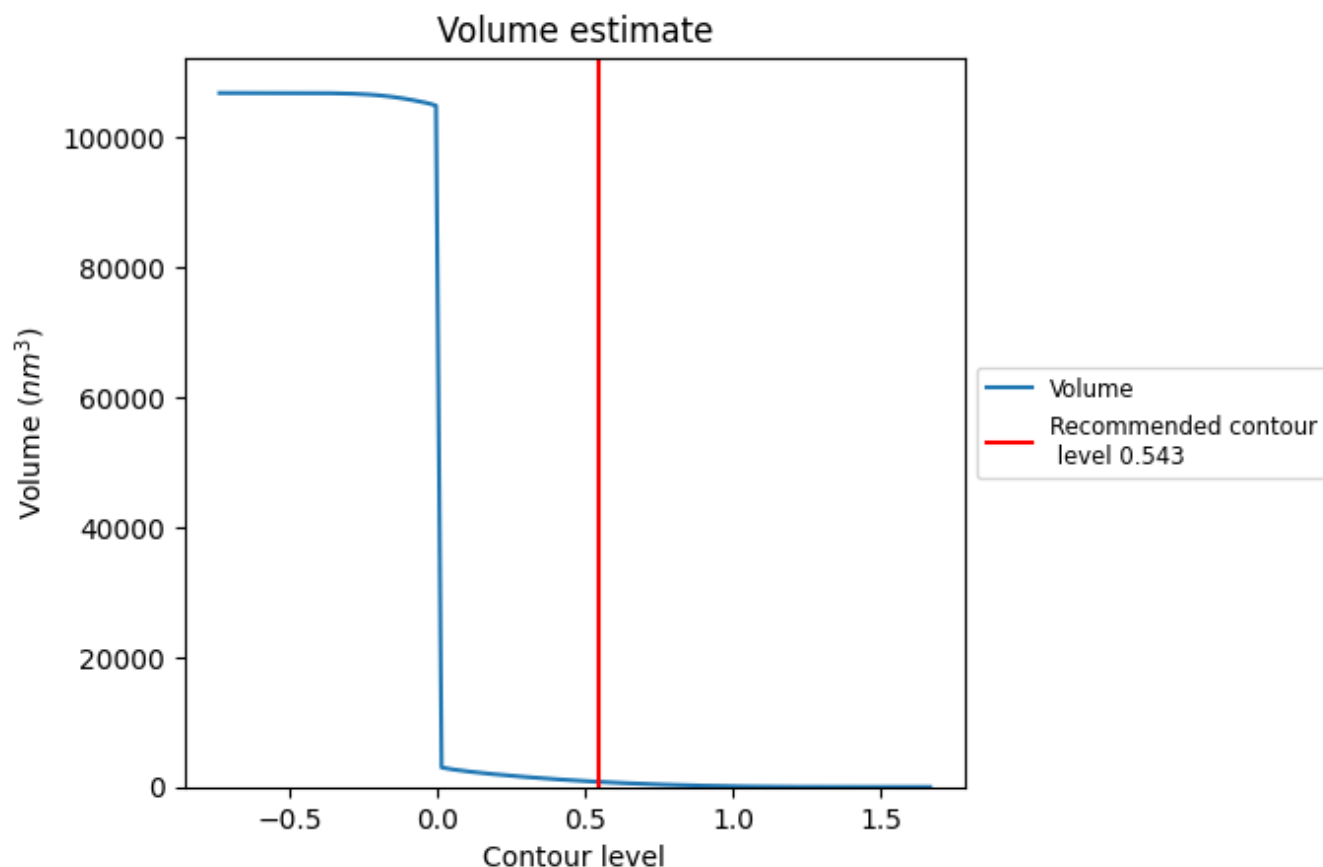
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

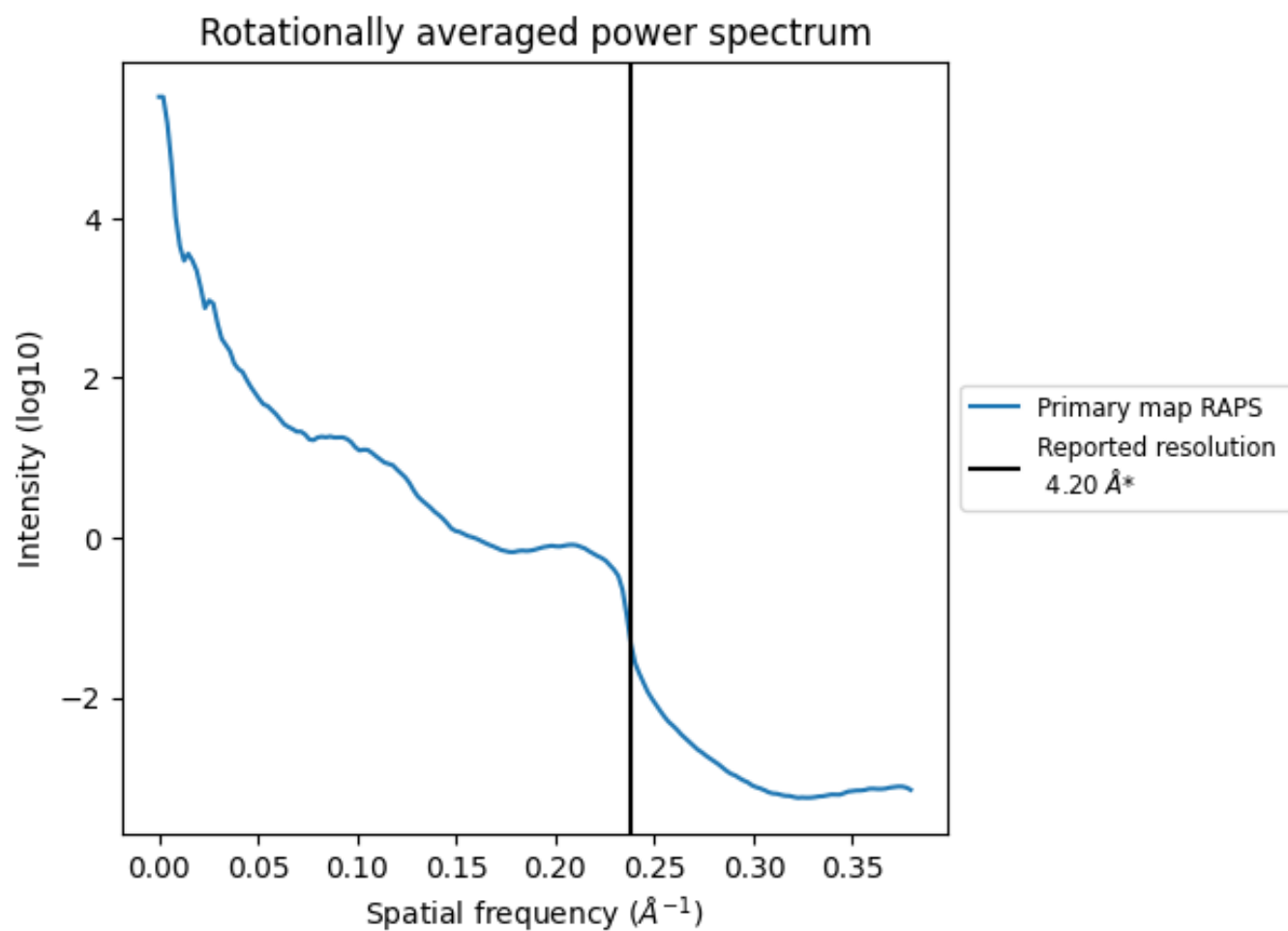
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 792 nm^3 ; this corresponds to an approximate mass of 715 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 0.238 Å⁻¹

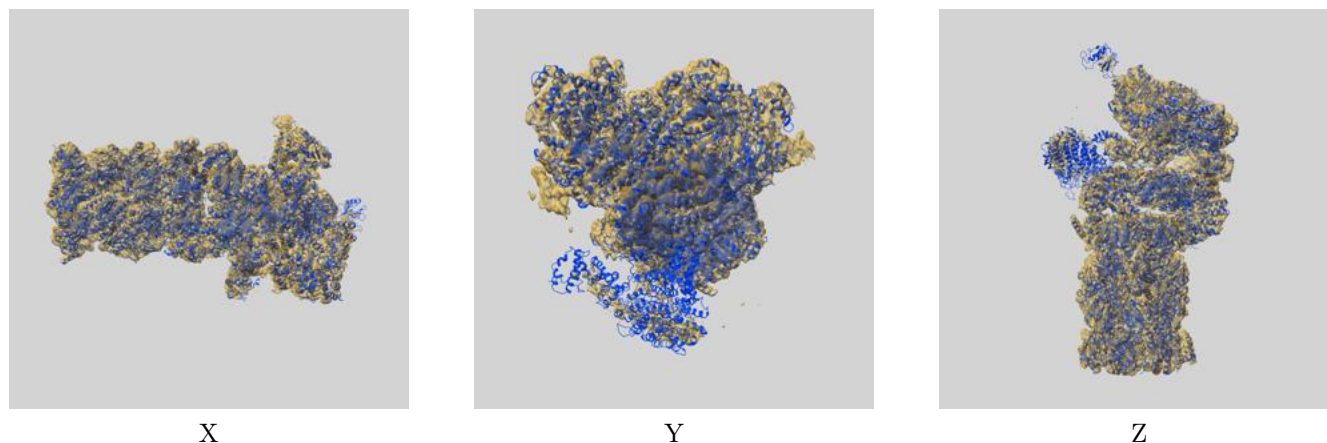
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

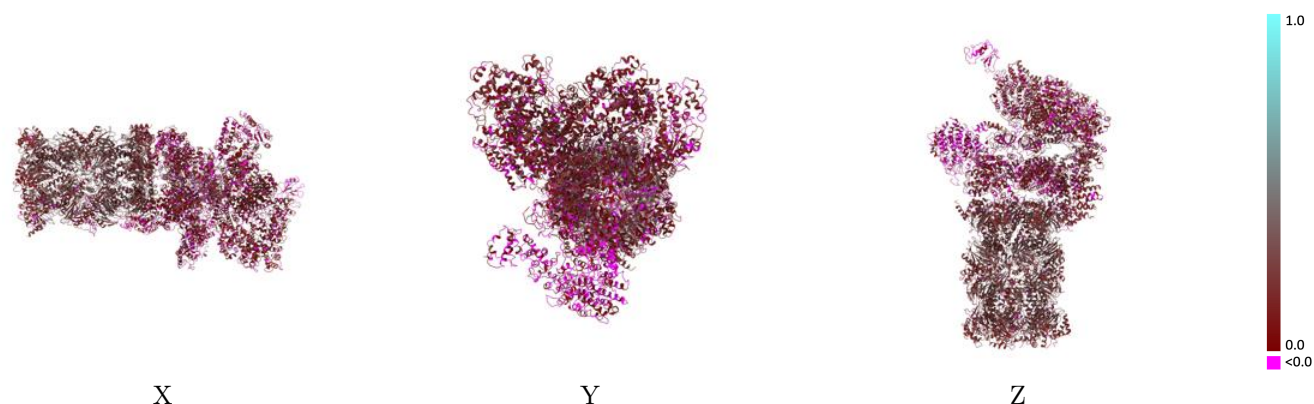
This section contains information regarding the fit between EMDB map EMD-6694 and PDB model 5WVK. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



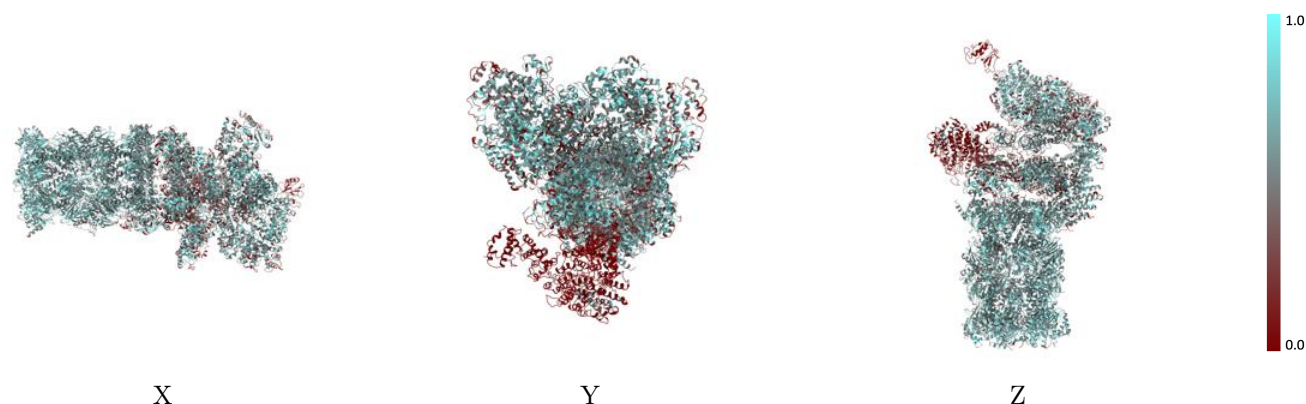
The images above show the 3D surface view of the map at the recommended contour level 0.543 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



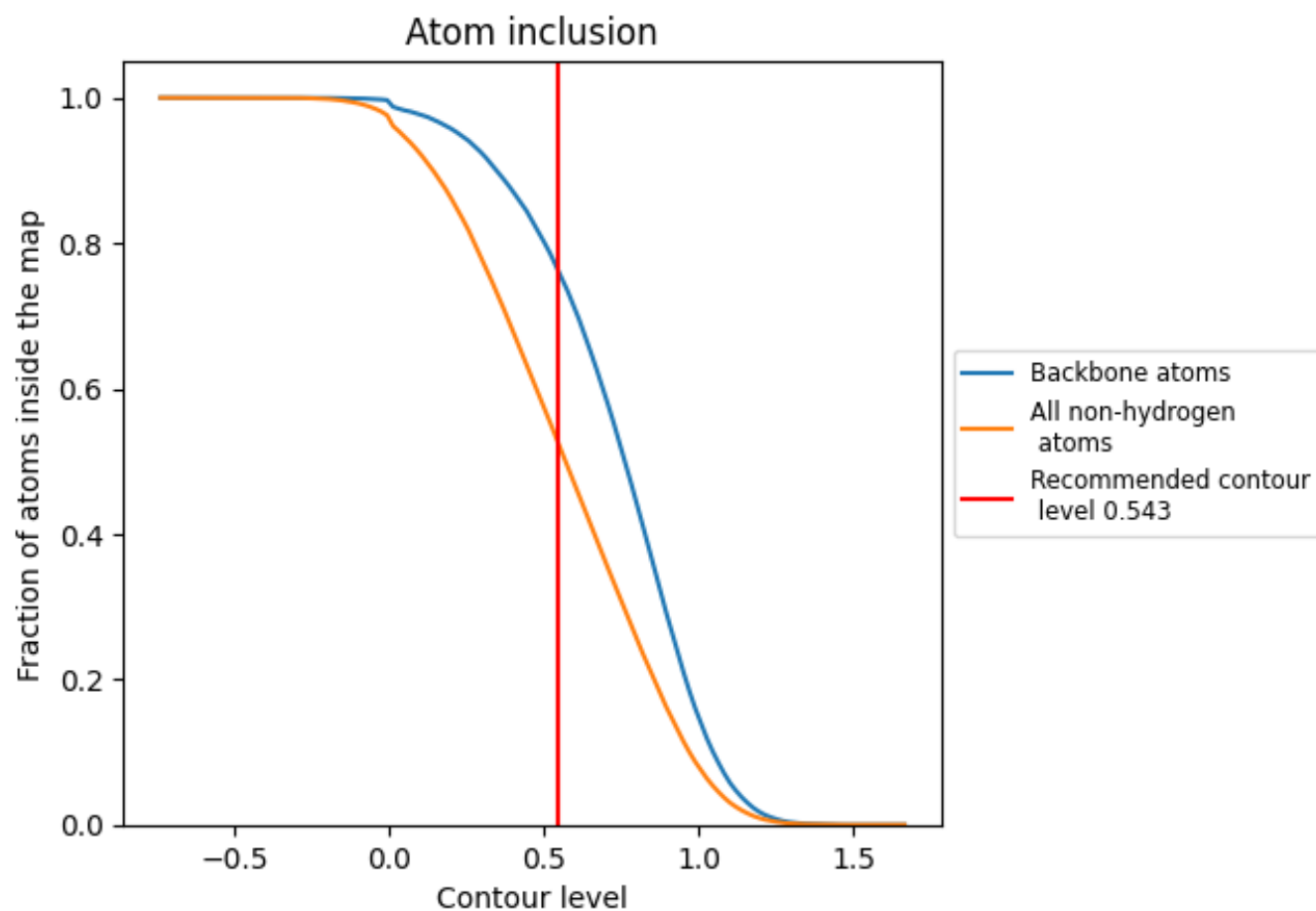
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.543).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 53% 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 (0.543) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5293	 0.1690
1	 0.6543	 0.2880
2	 0.6191	 0.2380
3	 0.6189	 0.2580
4	 0.6089	 0.2530
5	 0.6321	 0.2570
6	 0.5801	 0.2350
7	 0.6323	 0.2730
A	 0.5995	 0.2470
B	 0.5947	 0.2350
C	 0.5963	 0.2100
D	 0.6142	 0.2250
E	 0.6077	 0.2210
F	 0.6077	 0.2210
G	 0.6190	 0.2380
H	 0.4705	 0.1010
I	 0.2985	 0.1050
J	 0.3153	 0.1100
K	 0.4834	 0.1280
L	 0.4955	 0.1090
M	 0.5343	 0.1160
N	 0.5853	 0.1410
O	 0.5112	 0.1140
P	 0.5455	 0.1280
Q	 0.5453	 0.1160
R	 0.5784	 0.1210
S	 0.5383	 0.1170
T	 0.4645	 0.1310
U	 0.5923	 0.1770
V	 0.4649	 0.1180
W	 0.5476	 0.1080
X	 0.0207	 -0.0290
Y	 0.5521	 0.1430
Z	 0.0496	 0.0070
a	 0.6475	 0.2620



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Chain	Atom inclusion	Q-score
b	 0.6489	 0.2850
c	 0.6430	 0.2330
d	 0.6409	 0.2160
e	 0.6138	 0.2250
f	 0.6364	 0.2320
g	 0.6276	 0.2620
h	 0.6073	 0.2550
i	 0.5975	 0.2350
j	 0.6403	 0.2250
k	 0.6608	 0.2330
l	 0.6600	 0.2140
m	 0.6318	 0.2110
n	 0.6596	 0.2240