



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2022 – 08:58 AM EDT

PDB ID : 5VFT
EMDB ID : EMD-8667
Title : Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome
Authors : Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.
Deposited on : 2017-04-09
Resolution : 7.00 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:

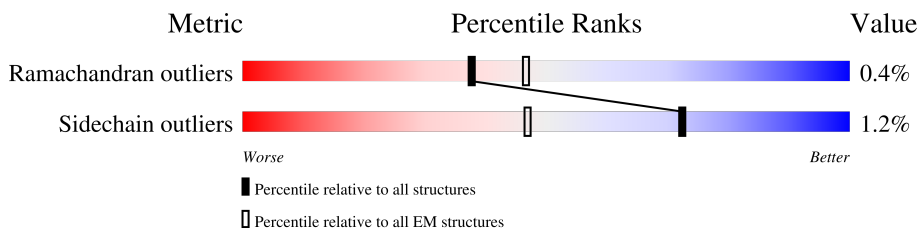
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 7.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	U	911	
2	V	480	
3	W	456	
4	X	380	
5	Y	378	
6	Z	286	
7	a	373	
8	b	191	
9	c	287	

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Mol	Chain	Length	Quality of chain
10	d	257	77% 98%
11	e	70	26% 34% 66%
12	A	361	53% 98%
13	B	341	59% 97%
14	C	384	57% 96%
15	D	380	65% 97%
16	E	353	61% 99%
17	F	377	53% 93%
18	G	240	20% 99%
18	g	240	14% 100%
19	H	232	22% 99%
19	h	232	19% 100%
20	I	250	28% 99%
20	i	250	26% 99%
21	J	243	21% 97%
21	j	243	20% 98%
22	K	234	18% 95%
22	k	234	15% 95%
23	L	238	14% 98%
23	l	238	12% 100%
24	M	245	15% 97%
24	m	245	17% 97%
25	N	191	14% 100%
25	n	191	9% 99%
26	O	220	15% 100%

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Mol	Chain	Length	Quality of chain
26	o	220	12% 100%
27	P	204	11% 100%
27	p	204	11% 100%
28	Q	199	8% 98%
28	q	199	7% 98%
29	R	201	. 100%
29	r	201	8% 100%
30	S	213	9% 100%
30	s	213	10% 100%
31	T	215	7% 99%
31	t	215	9% 100%
32	f	908	30% 73% 24%

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 96994 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	U	806	6287	3990	1075	1178	44	0	0

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V	480	3852	2444	684	710	14	0	0

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	W	236	1940	1237	331	361	11	0	0

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	81	647	414	107	124	2	0	0

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	Y	378	3115	1987	533	578	17	0	0

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Z	286	2281	1457	392	427	5	0	0

- Molecule 7 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 13, isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	a	373	2993	1910	509	559	15	0	0

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	c	287	2260	1430	389	422	19	0	0

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d	257	2116	1371	346	390	9	0	0

- Molecule 11 is a protein called sem1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e	24	197	121	34	40	2	0	0

- Molecule 12 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A	361	2835	1788	501	528	18	0	0

- Molecule 13 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	B	341	2662	1671	453	526	12	0	0

- Molecule 14 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	C	384	3015	1894	540	564	17	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	D	380	3040	1923	524	580	13	0	0

- Molecule 16 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	E	353	2790	1755	494	525	16	0	0

- Molecule 17 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	F	366	2863	1802	496	549	16	0	0

- Molecule 18 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	G	240	1825	1160	304	348	13	0	0
18	g	240	1826	1160	305	348	13	0	0

- Molecule 19 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	H	232	1708	1081	289	333	5	0	0
19	h	232	1708	1081	289	333	5	0	0

- Molecule 20 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
20	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 21 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
21	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
22	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 23 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
23	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
24	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 25 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	n	191	1430	893	245	280	12	0	0

- Molecule 26 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	O	220	1643	1033	280	318	12	0	0
26	o	220	1643	1033	280	318	12	0	0

- Molecule 27 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	P	204	1585	1010	262	294	19	0	0
27	p	204	1585	1010	262	294	19	0	0

- Molecule 28 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Q	199	1570	1006	265	290	9	0	0
28	q	199	1570	1006	265	290	9	0	0

- Molecule 29 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	R	201	1548	974	273	292	9	0	0
29	r	201	1548	974	273	292	9	0	0

- Molecule 30 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	S	213	1641	1036	282	313	10	0	0
30	s	213	1641	1036	282	313	10	0	0

- Molecule 31 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	T	215	1667	1052	285	318	12	0	0
31	t	215	1667	1052	285	318	12	0	0

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	689	5319	3343	904	1037	35	0	0

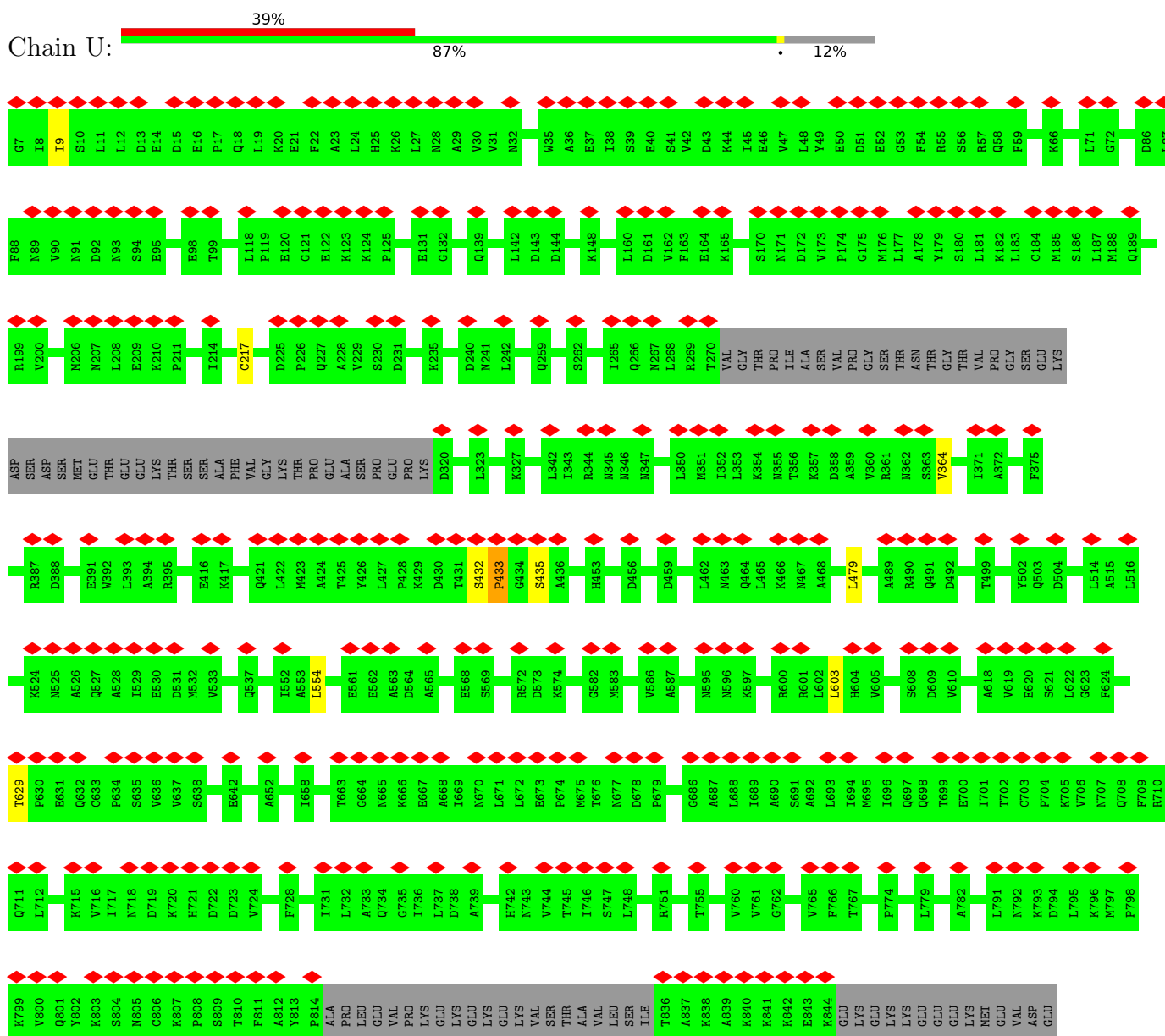
- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

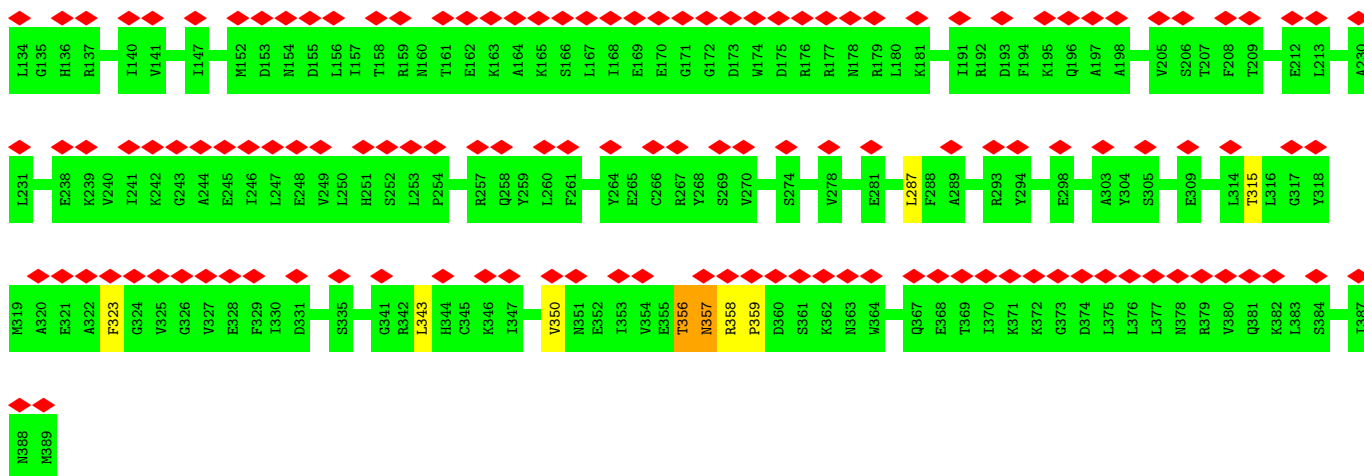
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
33	c	1	1	1	0

3 Residue-property plots

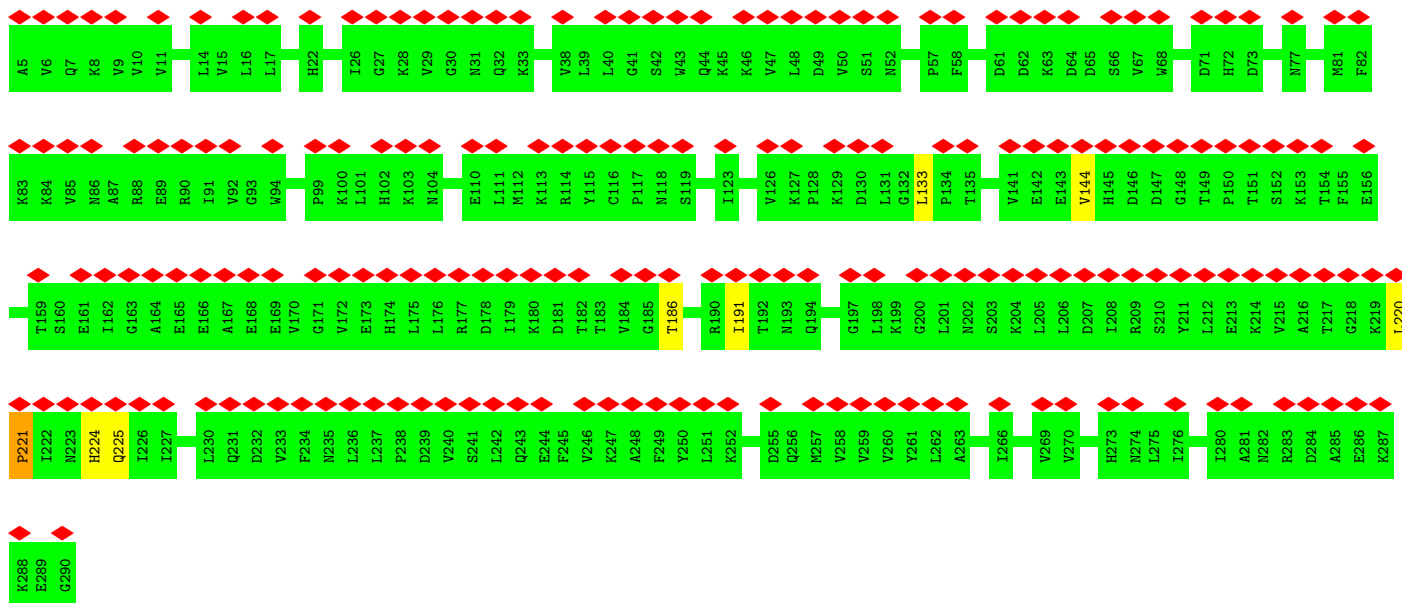
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

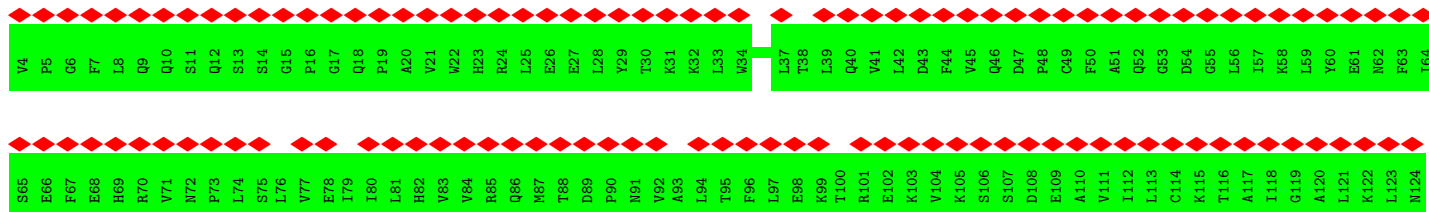
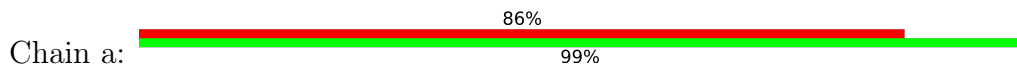


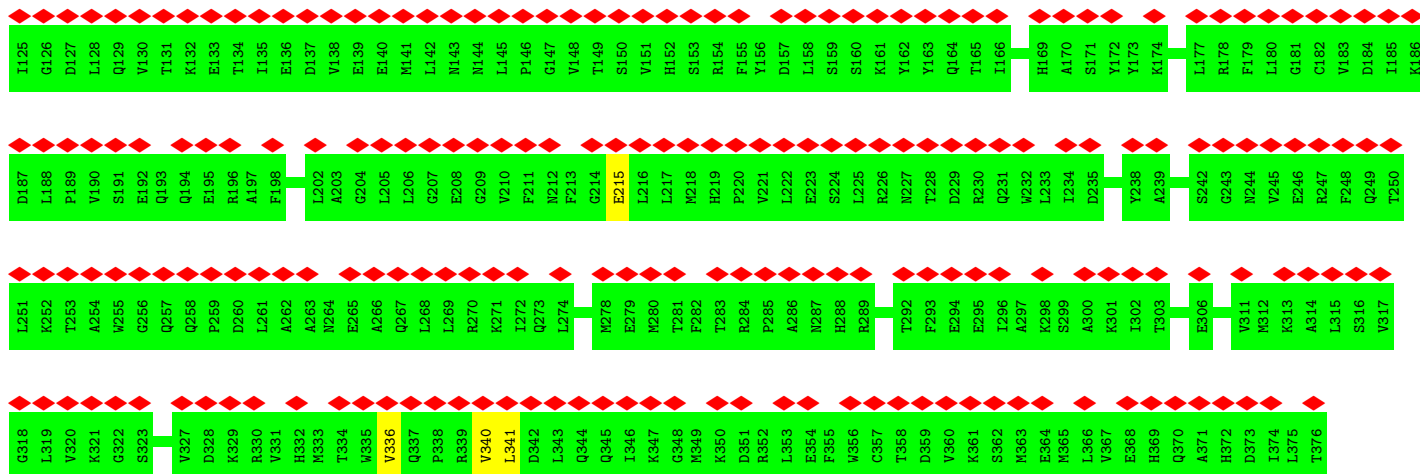


• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

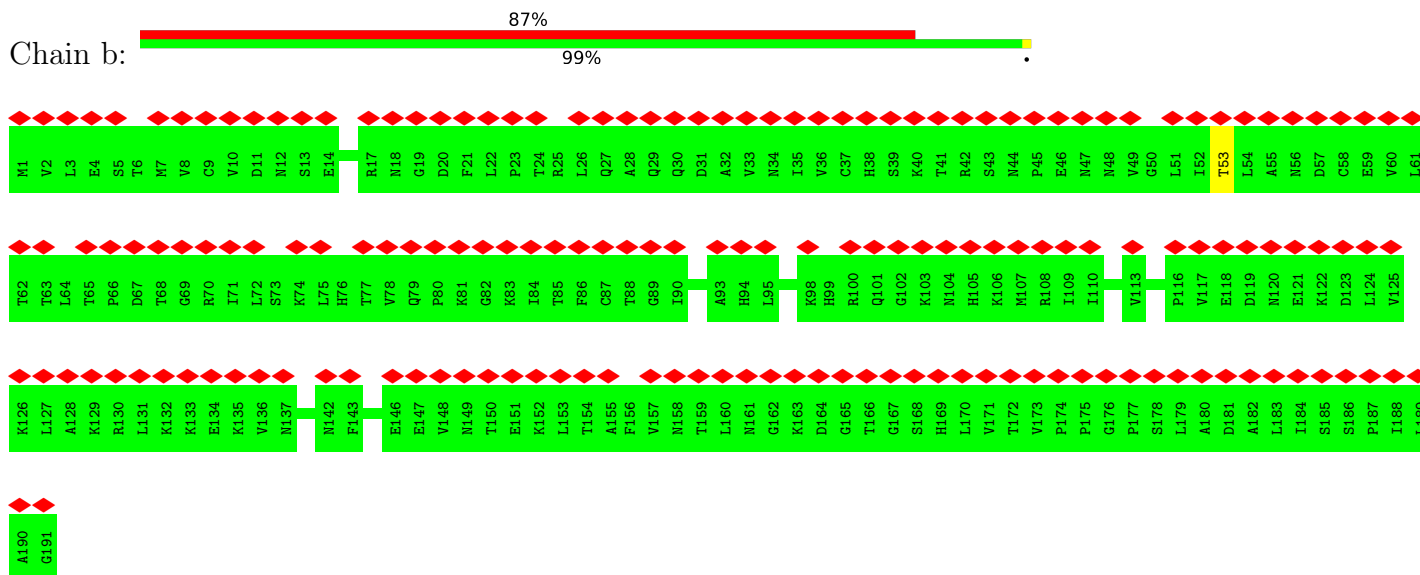


• Molecule 7: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 13, isoform CRA_a



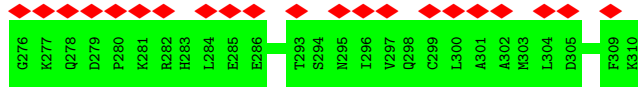


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

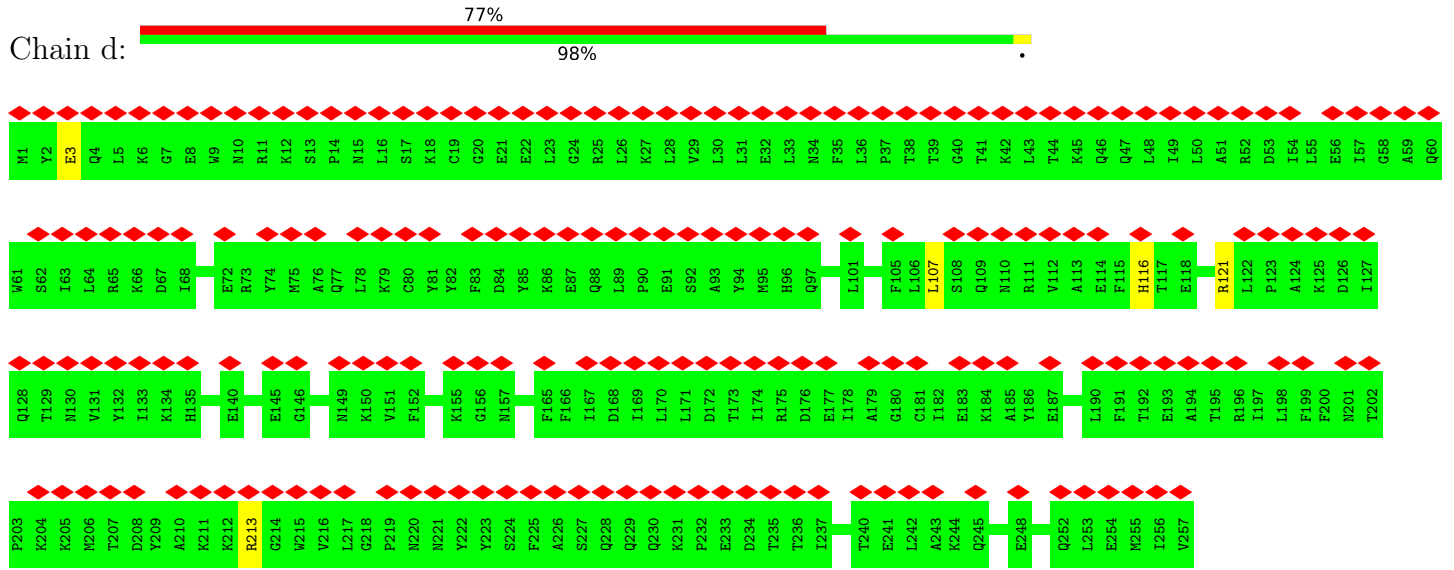


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

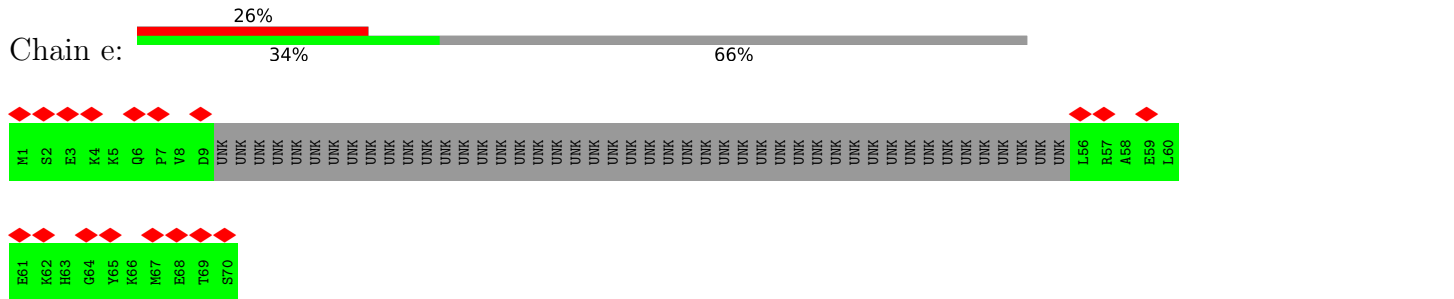




• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 11: sem1

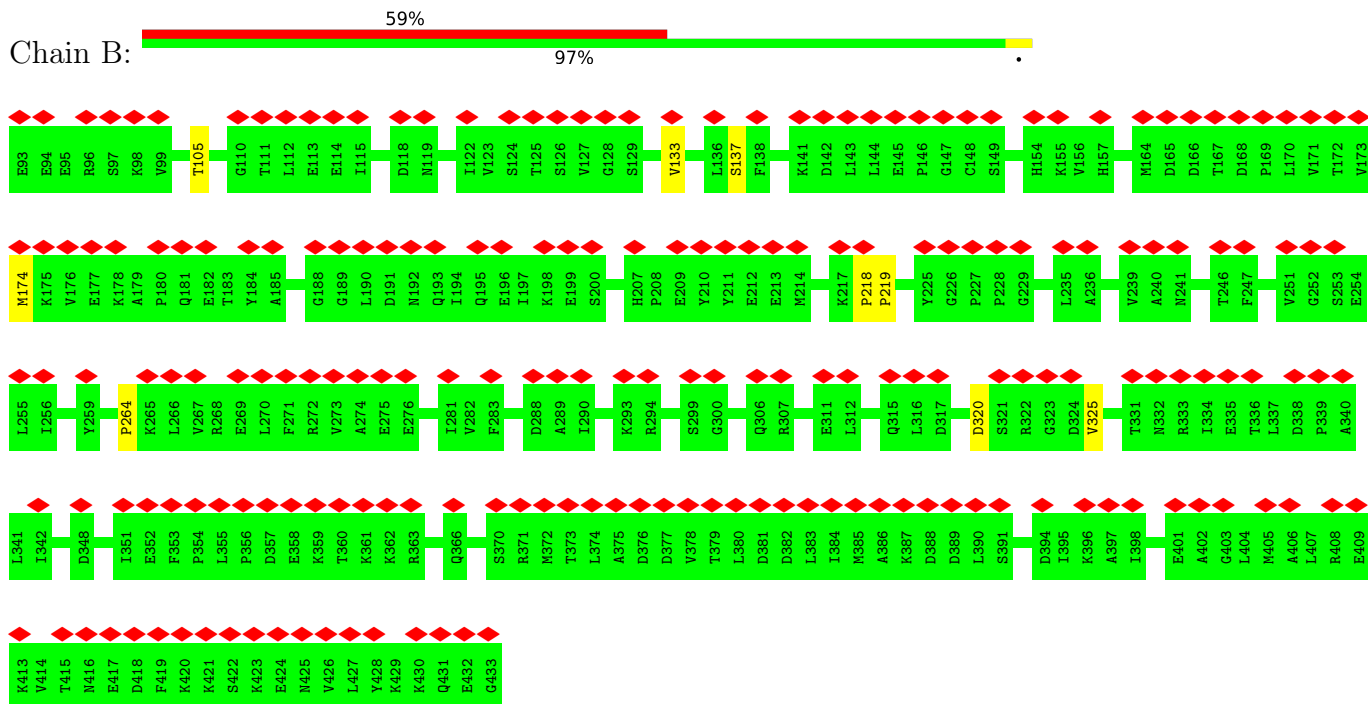


• Molecule 12: 26S proteasome regulatory subunit 7

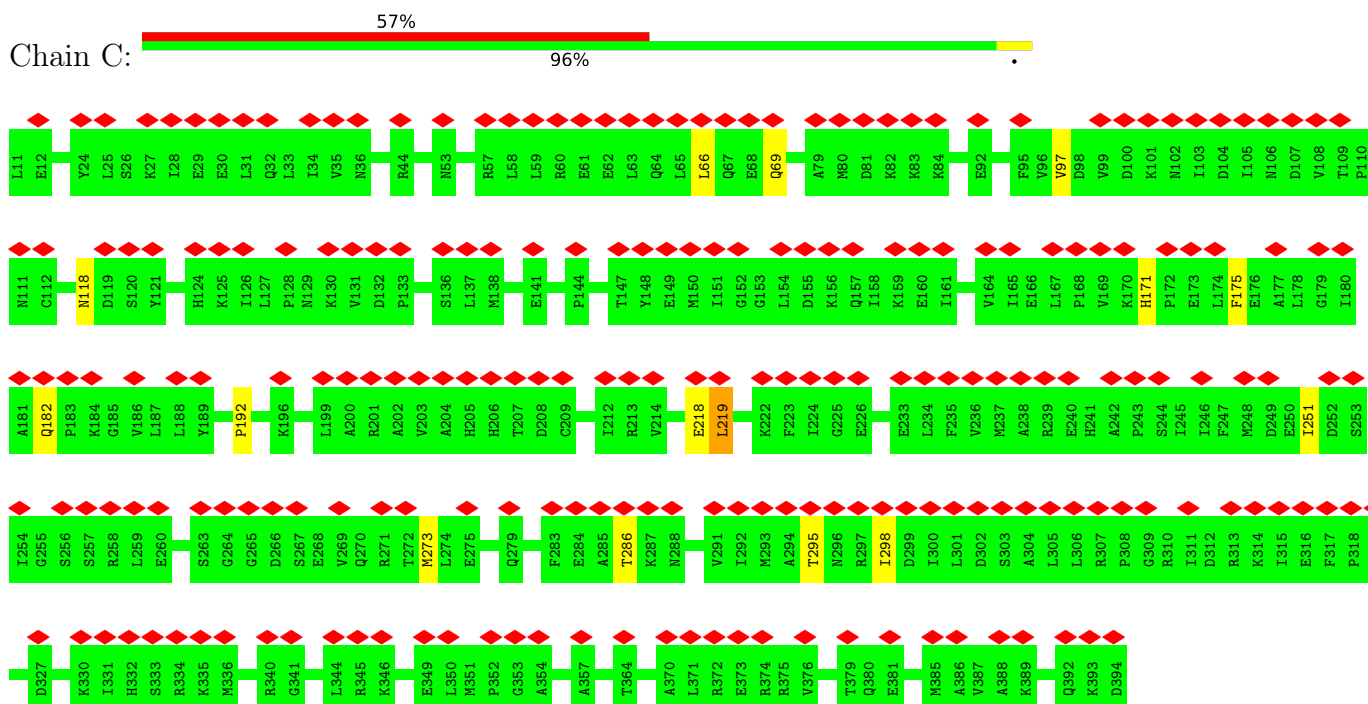




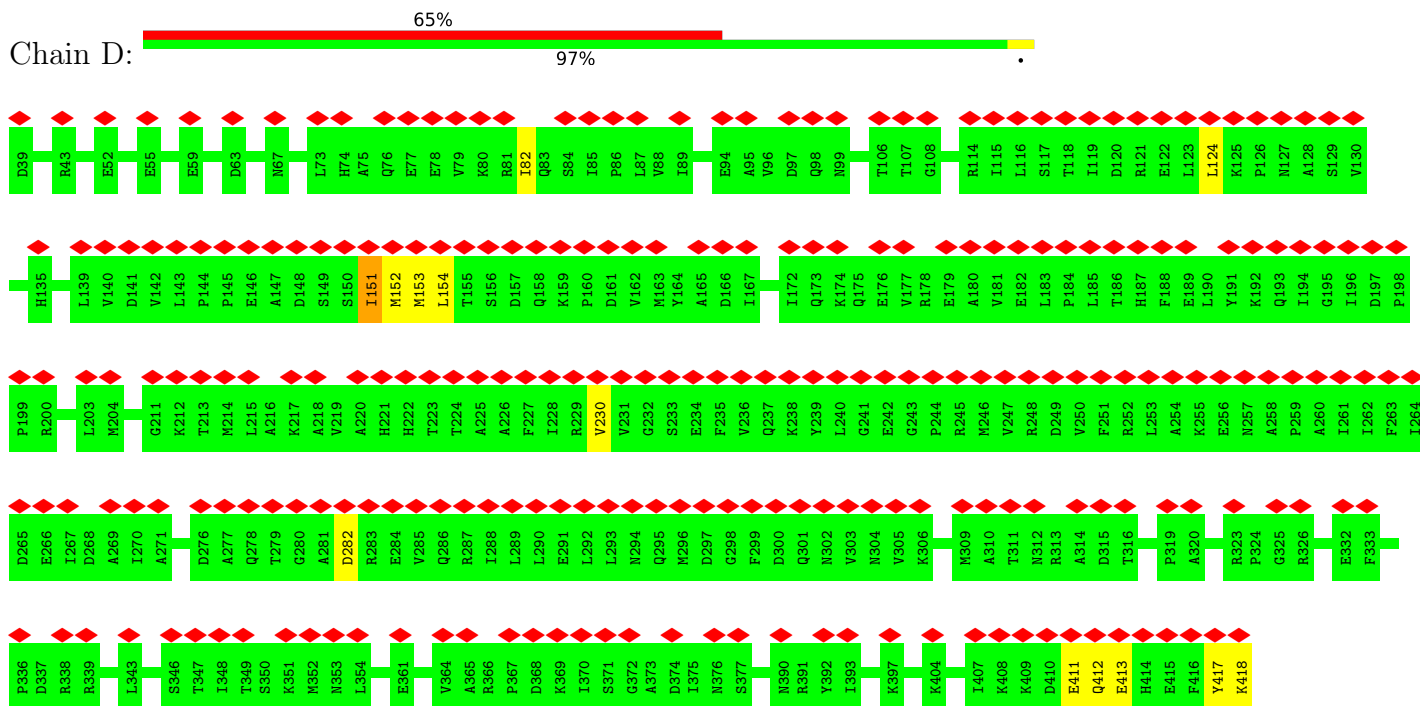
• Molecule 13: 26S proteasome regulatory subunit 4



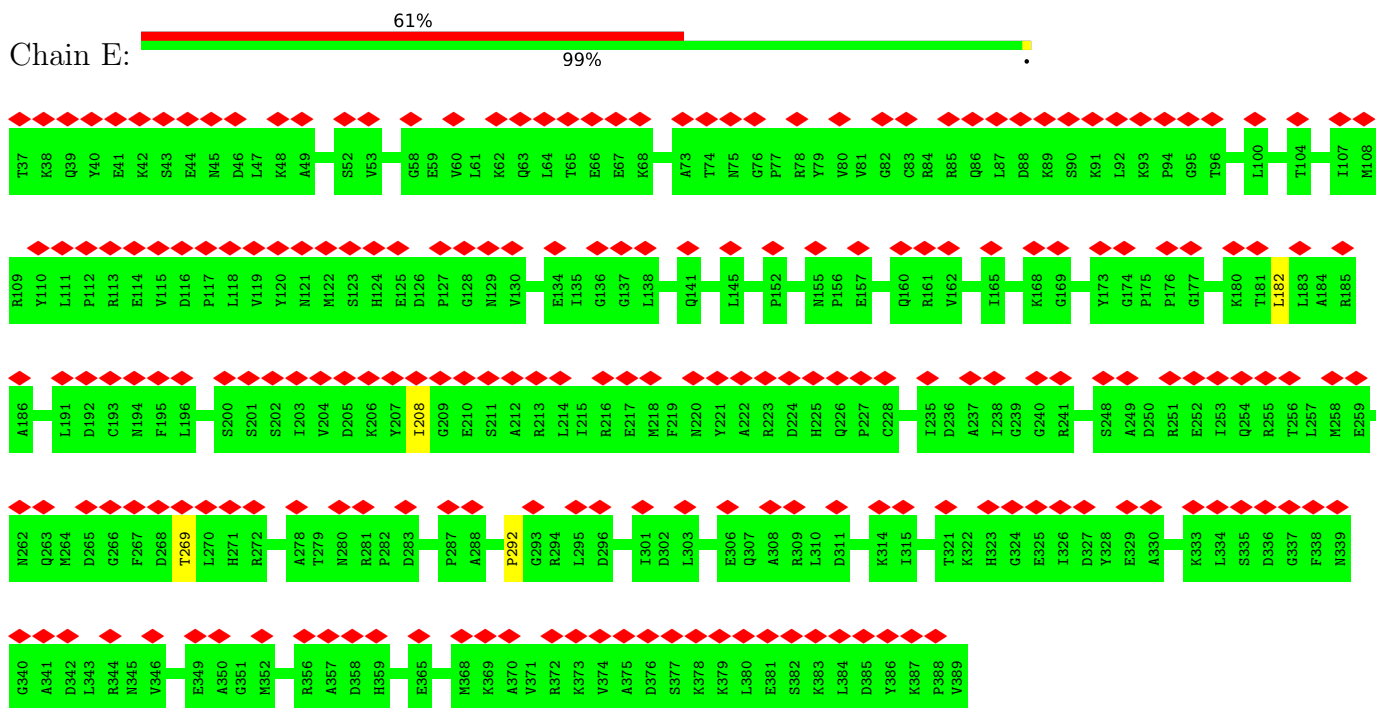
• Molecule 14: 26S proteasome regulatory subunit 8



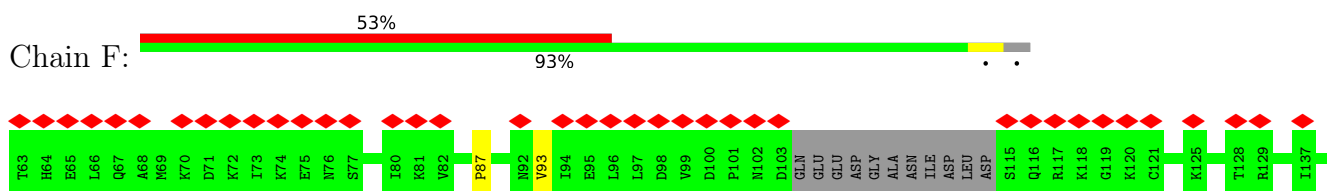
• Molecule 15: 26S proteasome regulatory subunit 6B

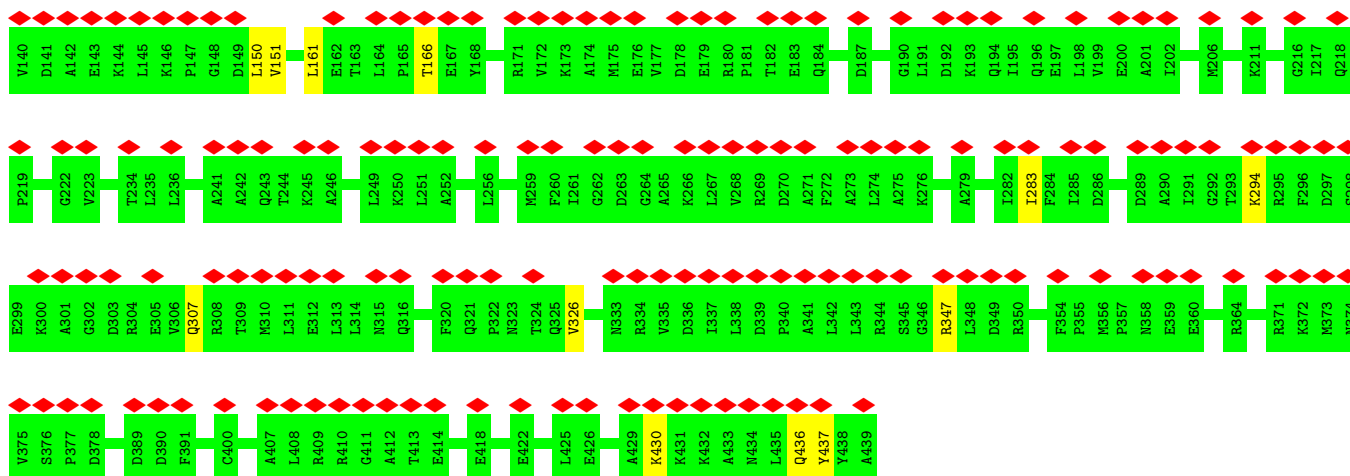


• Molecule 16: 26S proteasome regulatory subunit 10B

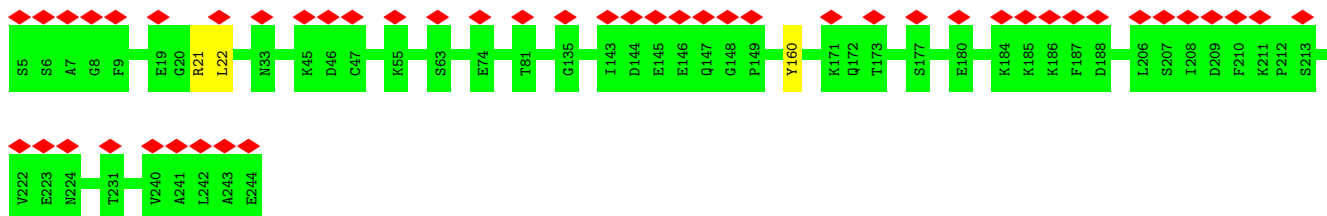


• Molecule 17: 26S proteasome regulatory subunit 6A

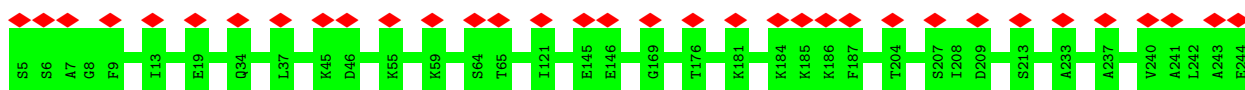




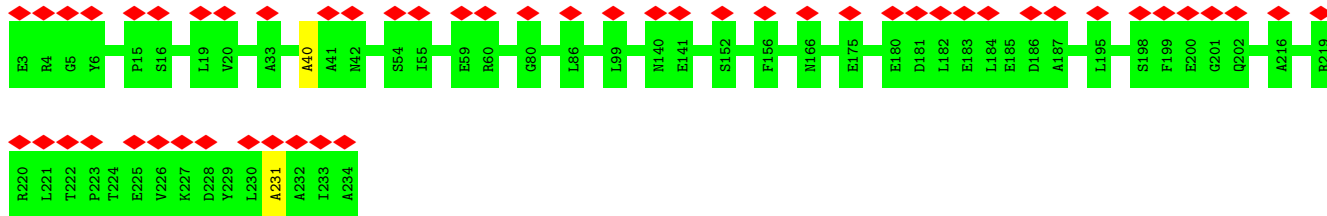
• Molecule 18: Proteasome subunit alpha type-6



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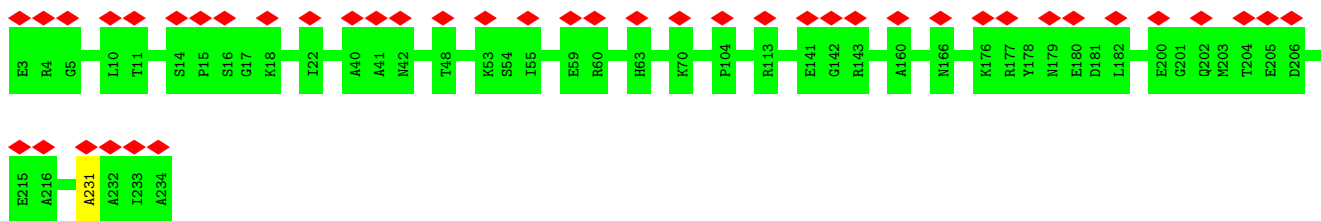


• Molecule 19: Proteasome subunit alpha type-2

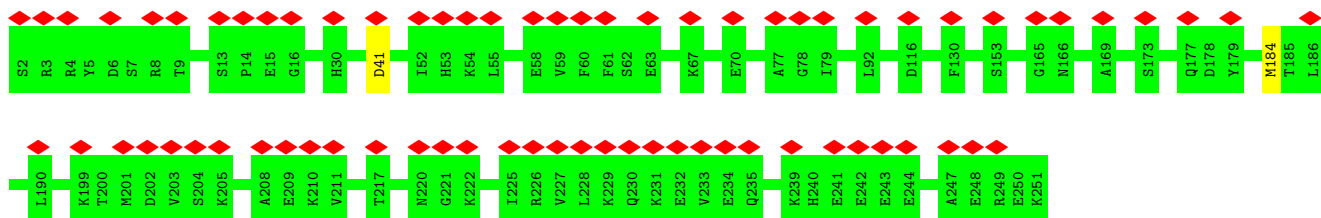


• Molecule 19: Proteasome subunit alpha type-2

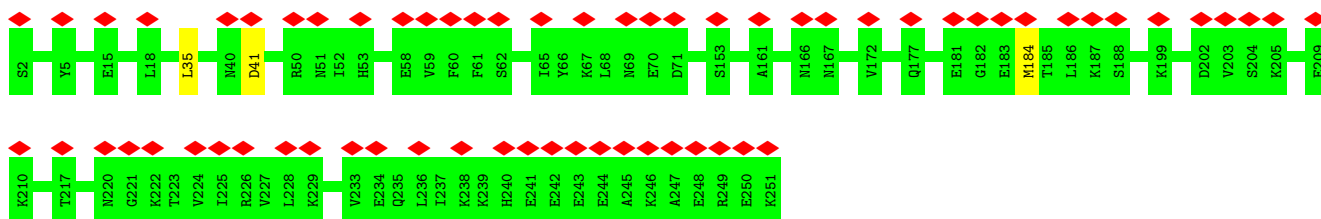




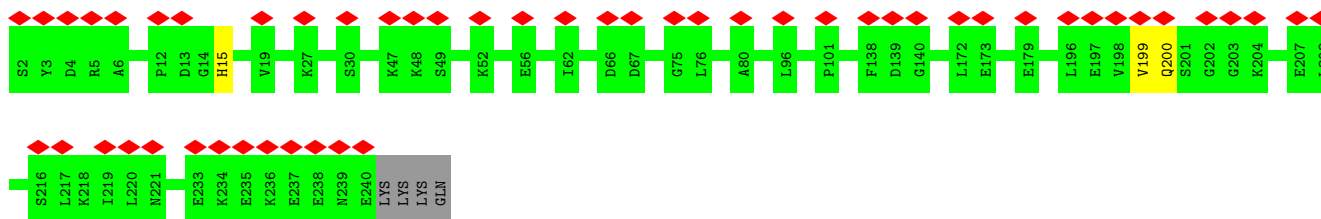
• Molecule 20: Proteasome subunit alpha type-4



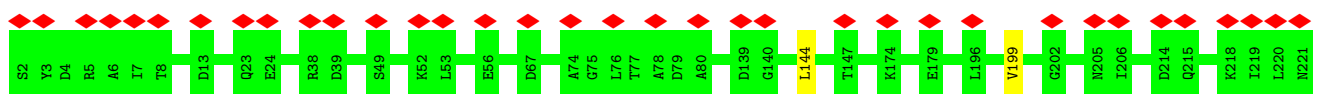
• Molecule 20: Proteasome subunit alpha type-4

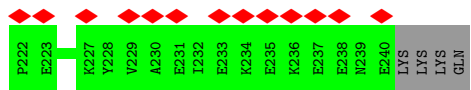


• Molecule 21: Proteasome subunit alpha type-7

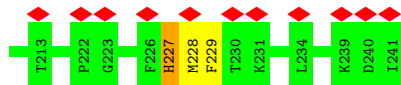
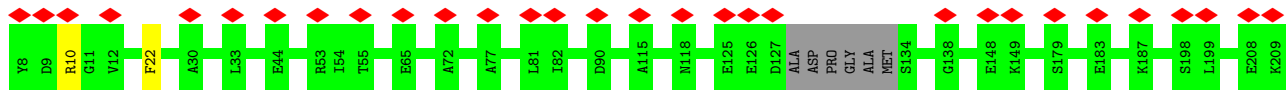


• Molecule 21: Proteasome subunit alpha type-7

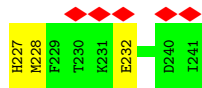
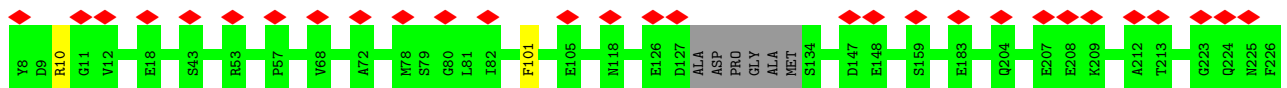




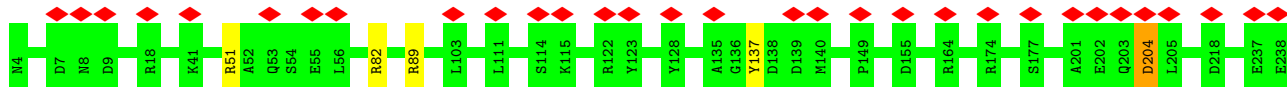
• Molecule 22: Proteasome subunit alpha type-5



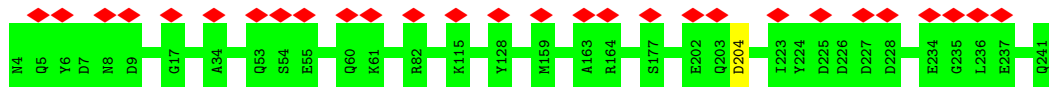
• Molecule 22: Proteasome subunit alpha type-5



• Molecule 23: Proteasome subunit alpha type-1

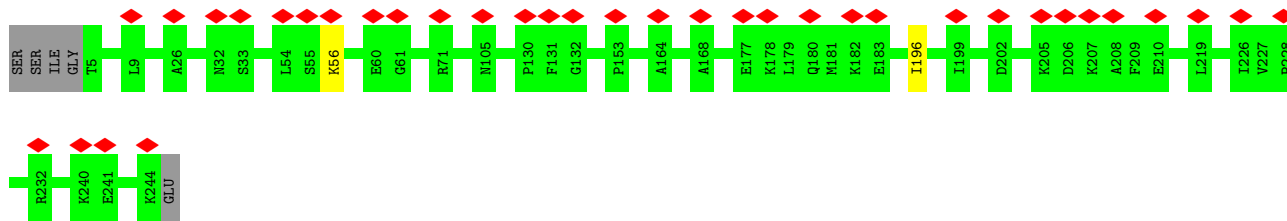


• Molecule 23: Proteasome subunit alpha type-1

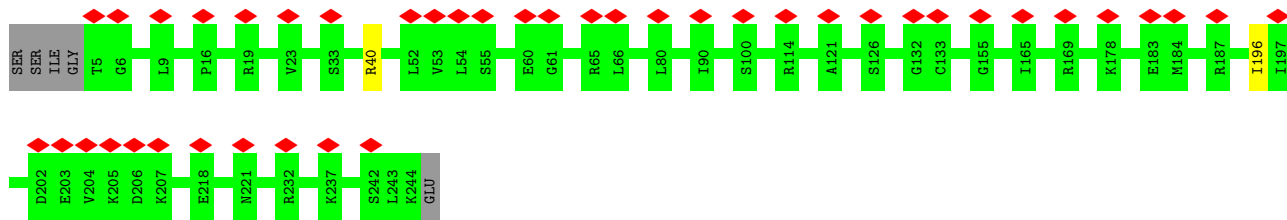


• Molecule 24: Proteasome subunit alpha type-3

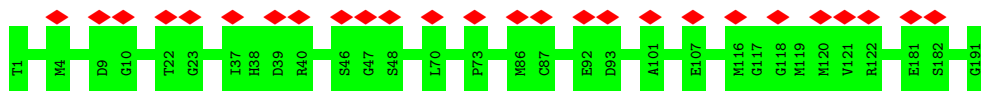




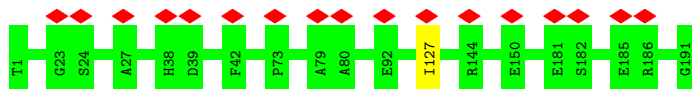
• Molecule 24: Proteasome subunit alpha type-3



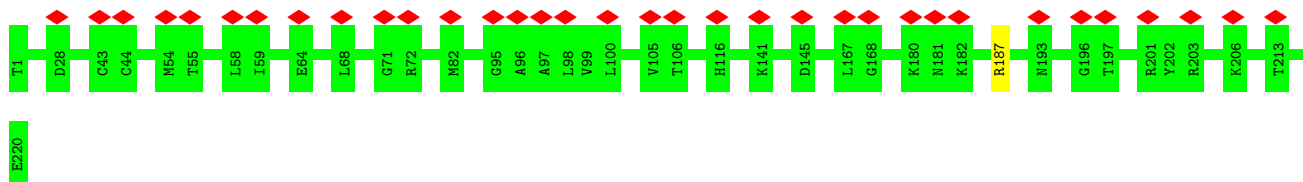
• Molecule 25: Proteasome subunit beta type-6



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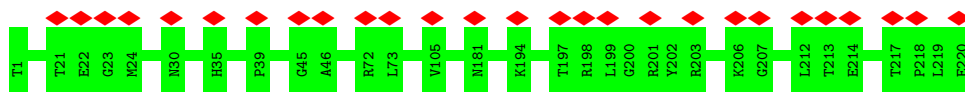


• Molecule 26: Proteasome subunit beta type-7

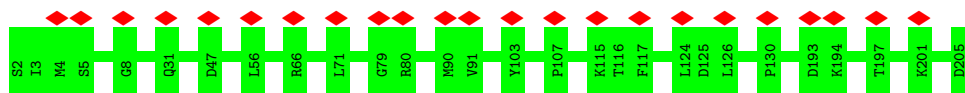


• Molecule 26: Proteasome subunit beta type-7

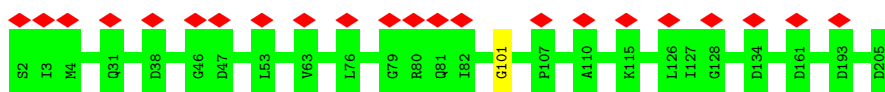




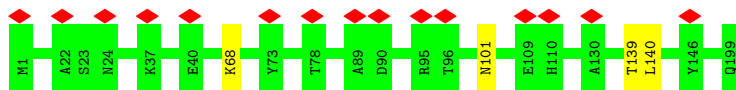
- Molecule 27: Proteasome subunit beta type-3



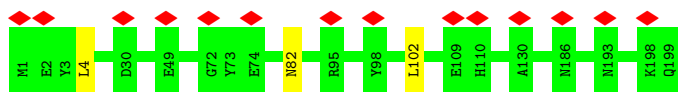
- Molecule 27: Proteasome subunit beta type-3



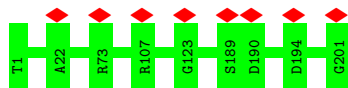
- Molecule 28: Proteasome subunit beta type-2



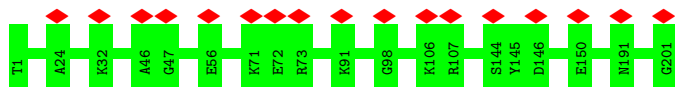
- Molecule 28: Proteasome subunit beta type-2



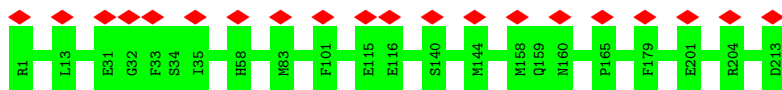
- Molecule 29: Proteasome subunit beta type-5



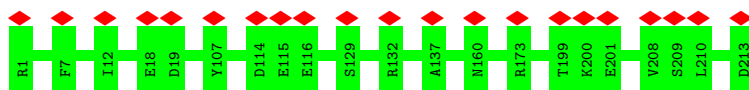
- Molecule 29: Proteasome subunit beta type-5



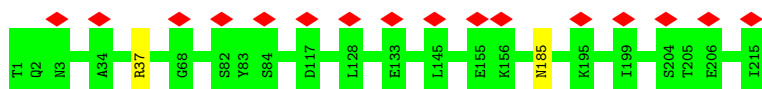
- Molecule 30: Proteasome subunit beta type-1



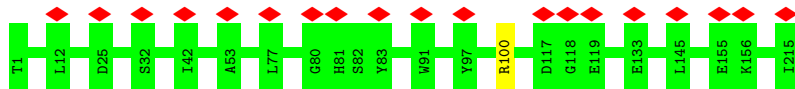
• Molecule 30: Proteasome subunit beta type-1



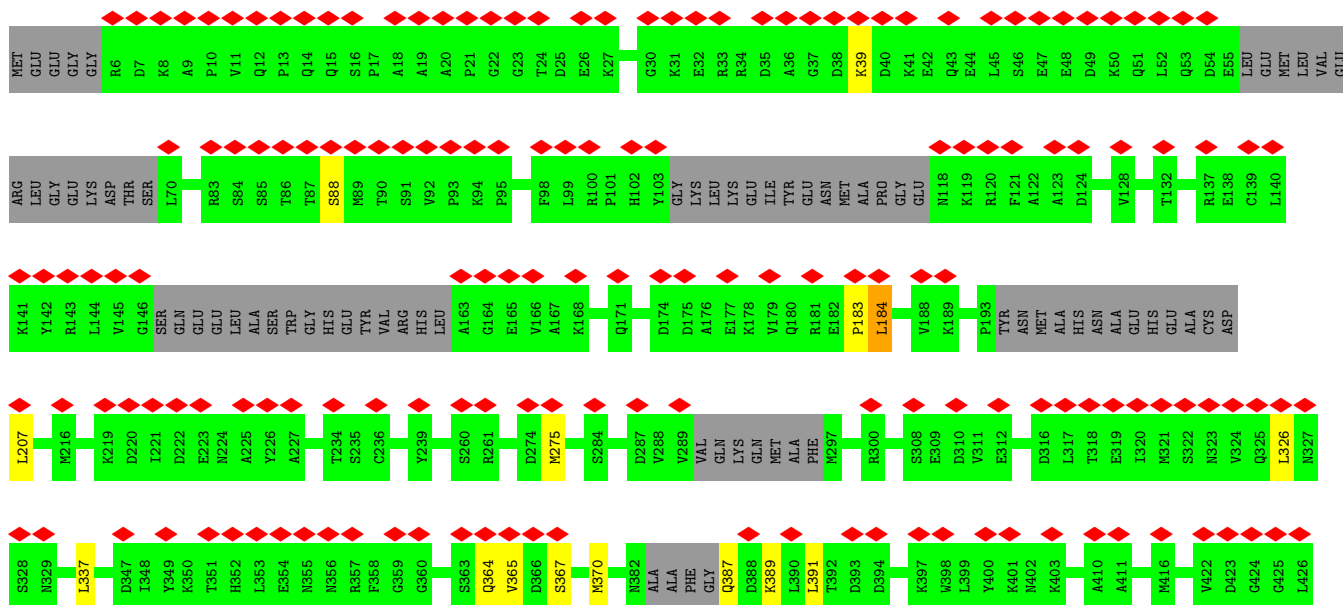
• Molecule 31: Proteasome subunit beta type-4

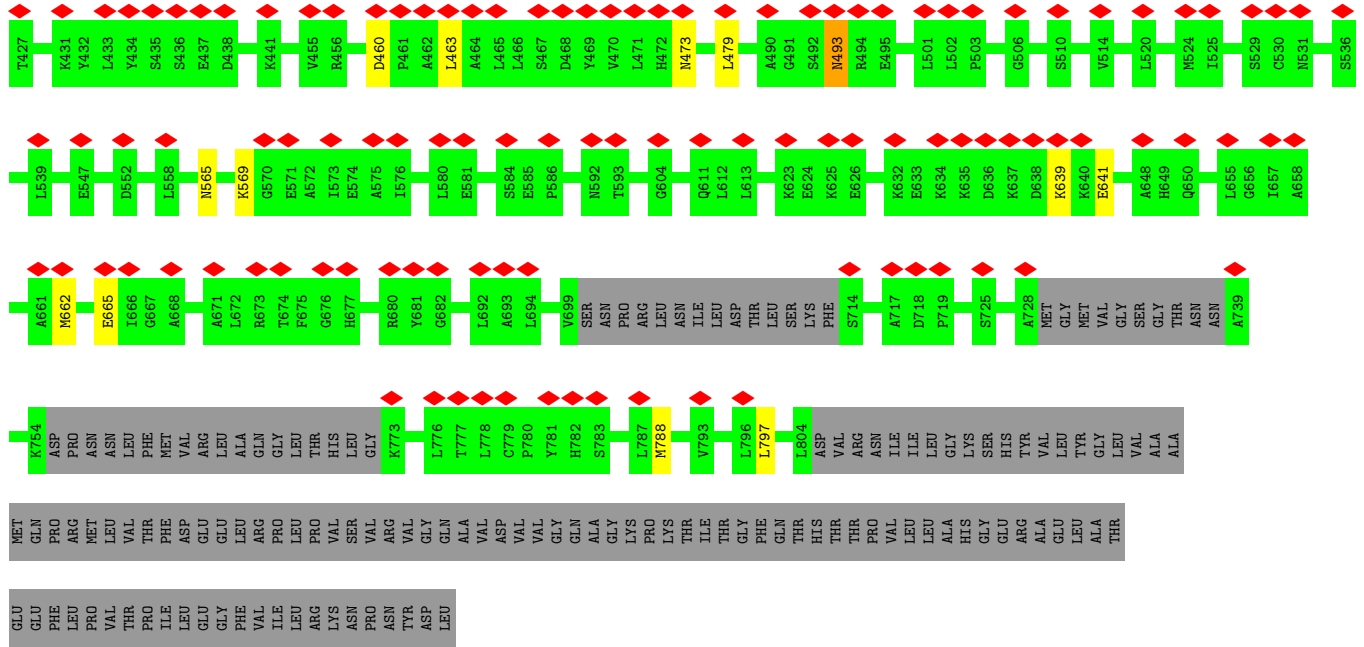


• Molecule 31: Proteasome subunit beta type-4



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15536	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	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	0.008	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	U	0.24	0/6396	0.42	0/8646
2	V	0.25	0/3929	0.46	0/5309
3	W	0.24	0/1975	0.46	0/2659
4	X	0.22	0/655	0.40	0/877
5	Y	0.23	0/3173	0.44	1/4273 (0.0%)
6	Z	0.23	0/2324	0.51	1/3150 (0.0%)
7	a	0.24	0/3051	0.45	0/4130
8	b	0.25	0/1478	0.43	0/2001
9	c	0.25	0/2302	0.51	0/3110
10	d	0.26	0/2162	0.51	0/2919
11	e	0.24	0/198	0.52	0/258
12	A	0.27	0/2886	0.53	0/3899
13	B	0.27	0/2700	0.55	0/3645
14	C	0.25	0/3054	0.49	0/4107
15	D	0.26	0/3090	0.52	0/4168
16	E	0.25	0/2835	0.48	0/3821
17	F	0.26	0/2903	0.54	0/3912
18	G	0.36	0/1858	0.58	0/2521
18	g	0.33	0/1859	0.58	0/2523
19	H	0.37	0/1743	0.60	0/2372
19	h	0.35	0/1743	0.59	1/2372 (0.0%)
20	I	0.36	0/1942	0.62	2/2628 (0.1%)
20	i	0.34	0/1942	0.63	3/2628 (0.1%)
21	J	0.38	0/1728	0.60	0/2358
21	j	0.34	0/1728	0.57	1/2358 (0.0%)
22	K	0.35	0/1747	0.61	0/2364
22	k	0.34	0/1747	0.63	1/2364 (0.0%)
23	L	0.37	0/1885	0.59	1/2552 (0.0%)
23	l	0.33	0/1885	0.58	0/2552
24	M	0.38	0/1891	0.58	0/2552
24	m	0.34	0/1891	0.57	0/2552
25	N	0.35	0/1454	0.53	0/1967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	n	0.35	0/1454	0.55	0/1967
26	O	0.34	0/1670	0.53	0/2265
26	o	0.34	0/1670	0.53	0/2265
27	P	0.35	0/1614	0.53	0/2177
27	p	0.35	0/1614	0.53	0/2177
28	Q	0.38	0/1603	0.60	0/2174
28	q	0.40	0/1603	0.65	1/2174 (0.0%)
29	R	0.38	0/1579	0.52	0/2134
29	r	0.36	0/1579	0.51	0/2134
30	S	0.35	0/1671	0.54	0/2253
30	s	0.33	0/1671	0.53	0/2253
31	T	0.37	0/1700	0.55	0/2305
31	t	0.36	0/1700	0.53	0/2305
32	f	0.31	0/5393	0.68	1/7271 (0.0%)
All	All	0.31	0/98675	0.54	13/133401 (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
1	U	0	3
2	V	0	4
5	Y	0	2
6	Z	0	1
9	c	0	1
10	d	0	1
12	A	0	1
13	B	0	2
14	C	0	1
15	D	0	1
16	E	0	1
17	F	0	2
18	G	0	1
19	H	0	2
21	J	0	2
21	j	0	1
22	K	0	1
22	k	0	3
23	L	0	2
23	l	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	M	0	1
26	O	0	1
27	p	0	1
28	Q	0	2
28	q	0	1
All	All	0	39

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	220	LEU	C-N-CD	-11.96	94.29	120.60
20	i	35	LEU	CA-CB-CG	6.83	131.01	115.30
28	q	4	LEU	CB-CG-CD2	5.70	120.69	111.00
19	h	231	ALA	C-N-CA	5.69	135.93	121.70
20	i	41	ASP	CB-CG-OD1	5.68	123.41	118.30

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	U	432	SER	Peptide
1	U	433	PRO	Peptide
1	U	435	SER	Peptide
2	V	54	LYS	Peptide
2	V	57	ALA	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	U	798/911 (88%)	729 (91%)	67 (8%)	2 (0%)	41	77
2	V	478/480 (100%)	412 (86%)	60 (13%)	6 (1%)	12	48
3	W	234/456 (51%)	213 (91%)	21 (9%)	0	100	100
4	X	79/380 (21%)	75 (95%)	4 (5%)	0	100	100
5	Y	376/378 (100%)	331 (88%)	36 (10%)	9 (2%)	6	33
6	Z	284/286 (99%)	252 (89%)	30 (11%)	2 (1%)	22	63
7	a	371/373 (100%)	340 (92%)	28 (8%)	3 (1%)	19	60
8	b	189/191 (99%)	178 (94%)	11 (6%)	0	100	100
9	c	285/287 (99%)	241 (85%)	39 (14%)	5 (2%)	8	40
10	d	255/257 (99%)	220 (86%)	33 (13%)	2 (1%)	19	60
11	e	20/70 (29%)	16 (80%)	4 (20%)	0	100	100
12	A	359/361 (99%)	303 (84%)	54 (15%)	2 (1%)	25	66
13	B	339/341 (99%)	298 (88%)	38 (11%)	3 (1%)	17	57
14	C	382/384 (100%)	318 (83%)	60 (16%)	4 (1%)	15	54
15	D	378/380 (100%)	325 (86%)	51 (14%)	2 (0%)	29	69
16	E	351/353 (99%)	299 (85%)	51 (14%)	1 (0%)	41	77
17	F	362/377 (96%)	315 (87%)	45 (12%)	2 (1%)	25	66
18	G	238/240 (99%)	223 (94%)	15 (6%)	0	100	100
18	g	238/240 (99%)	226 (95%)	12 (5%)	0	100	100
19	H	230/232 (99%)	213 (93%)	17 (7%)	0	100	100
19	h	230/232 (99%)	214 (93%)	16 (7%)	0	100	100
20	I	248/250 (99%)	236 (95%)	12 (5%)	0	100	100
20	i	248/250 (99%)	228 (92%)	20 (8%)	0	100	100
21	J	237/243 (98%)	215 (91%)	21 (9%)	1 (0%)	34	72
21	j	237/243 (98%)	222 (94%)	15 (6%)	0	100	100
22	K	224/234 (96%)	204 (91%)	19 (8%)	1 (0%)	34	72
22	k	224/234 (96%)	203 (91%)	21 (9%)	0	100	100
23	L	236/238 (99%)	222 (94%)	14 (6%)	0	100	100
23	l	236/238 (99%)	222 (94%)	14 (6%)	0	100	100
24	M	238/245 (97%)	221 (93%)	17 (7%)	0	100	100
24	m	238/245 (97%)	220 (92%)	18 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	N	189/191 (99%)	179 (95%)	10 (5%)	0	100	100
25	n	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
26	O	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
26	o	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
27	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
27	p	202/204 (99%)	186 (92%)	16 (8%)	0	100	100
28	Q	197/199 (99%)	179 (91%)	18 (9%)	0	100	100
28	q	197/199 (99%)	177 (90%)	20 (10%)	0	100	100
29	R	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
29	r	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
30	S	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
30	s	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
31	T	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
31	t	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	13	50
All	All	12369/13423 (92%)	11219 (91%)	1097 (9%)	53 (0%)	38	72

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	364	VAL
2	V	58	ALA
2	V	81	GLN
2	V	193	GLN
2	V	197	THR

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	U	685/779 (88%)	679 (99%)	6 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	414/414 (100%)	402 (97%)	12 (3%)	42	64
3	W	218/416 (52%)	215 (99%)	3 (1%)	67	80
4	X	74/327 (23%)	74 (100%)	0	100	100
5	Y	334/334 (100%)	326 (98%)	8 (2%)	49	69
6	Z	257/257 (100%)	252 (98%)	5 (2%)	57	75
7	a	333/333 (100%)	332 (100%)	1 (0%)	92	95
8	b	167/167 (100%)	166 (99%)	1 (1%)	86	92
9	c	252/252 (100%)	249 (99%)	3 (1%)	71	83
10	d	231/231 (100%)	229 (99%)	2 (1%)	78	87
11	e	22/22 (100%)	22 (100%)	0	100	100
12	A	308/308 (100%)	303 (98%)	5 (2%)	62	79
13	B	298/298 (100%)	294 (99%)	4 (1%)	69	81
14	C	332/332 (100%)	321 (97%)	11 (3%)	38	61
15	D	333/333 (100%)	322 (97%)	11 (3%)	38	61
16	E	308/308 (100%)	306 (99%)	2 (1%)	86	92
17	F	312/321 (97%)	302 (97%)	10 (3%)	39	61
18	G	192/205 (94%)	190 (99%)	2 (1%)	76	86
18	g	193/205 (94%)	193 (100%)	0	100	100
19	H	164/190 (86%)	164 (100%)	0	100	100
19	h	164/190 (86%)	164 (100%)	0	100	100
20	I	193/210 (92%)	193 (100%)	0	100	100
20	i	193/210 (92%)	193 (100%)	0	100	100
21	J	152/207 (73%)	152 (100%)	0	100	100
21	j	152/207 (73%)	152 (100%)	0	100	100
22	K	186/196 (95%)	182 (98%)	4 (2%)	52	71
22	k	186/196 (95%)	185 (100%)	1 (0%)	88	93
23	L	198/204 (97%)	195 (98%)	3 (2%)	65	80
23	l	198/204 (97%)	198 (100%)	0	100	100
24	M	192/202 (95%)	191 (100%)	1 (0%)	88	93
24	m	192/202 (95%)	190 (99%)	2 (1%)	76	86
25	N	148/148 (100%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	n	148/148 (100%)	147 (99%)	1 (1%)	84	90
26	O	177/181 (98%)	177 (100%)	0	100	100
26	o	177/181 (98%)	177 (100%)	0	100	100
27	P	172/173 (99%)	172 (100%)	0	100	100
27	p	172/173 (99%)	172 (100%)	0	100	100
28	Q	164/170 (96%)	162 (99%)	2 (1%)	71	83
28	q	164/170 (96%)	163 (99%)	1 (1%)	86	92
29	R	153/156 (98%)	153 (100%)	0	100	100
29	r	153/156 (98%)	153 (100%)	0	100	100
30	S	174/178 (98%)	174 (100%)	0	100	100
30	s	174/178 (98%)	174 (100%)	0	100	100
31	T	175/178 (98%)	173 (99%)	2 (1%)	73	84
31	t	175/178 (98%)	174 (99%)	1 (1%)	86	92
32	f	580/763 (76%)	559 (96%)	21 (4%)	35	59
All	All	10339/11391 (91%)	10214 (99%)	125 (1%)	72	83

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	C	219	LEU
32	f	387	GLN
15	D	418	LYS
32	f	370	MET
32	f	565	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
19	H	119	GLN
20	i	53	HIS
20	I	53	HIS
25	N	154	GLN
22	k	114	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

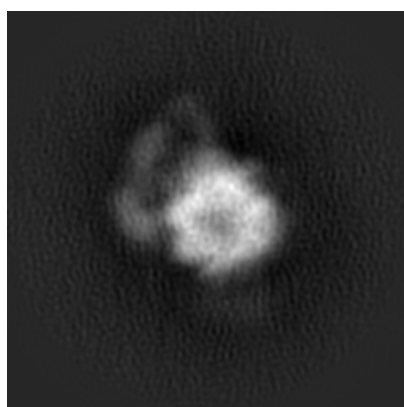
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8667. These allow visual inspection of the internal detail of the map and identification of artifacts.

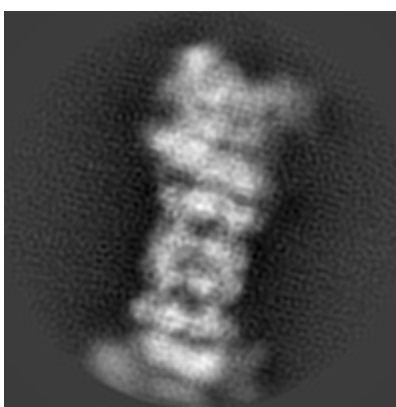
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

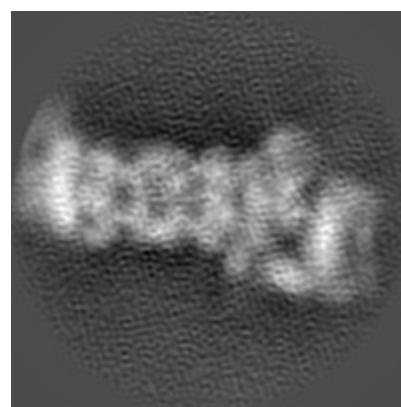
6.1.1 Primary map



X



Y

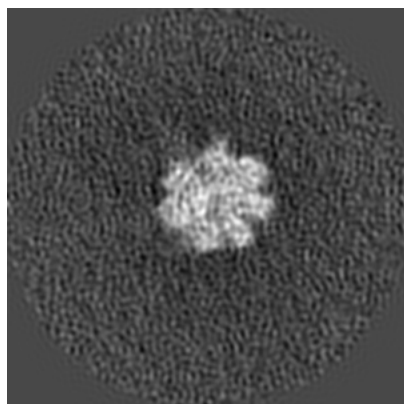


Z

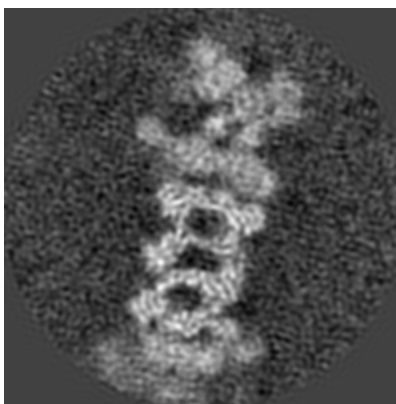
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 280



Y Index: 280

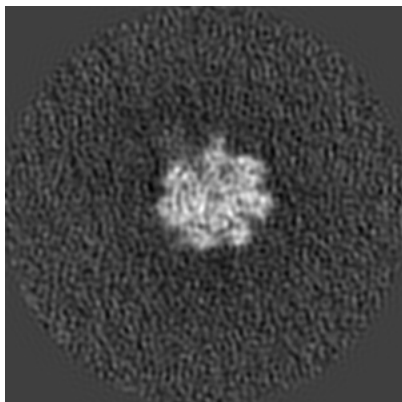


Z Index: 280

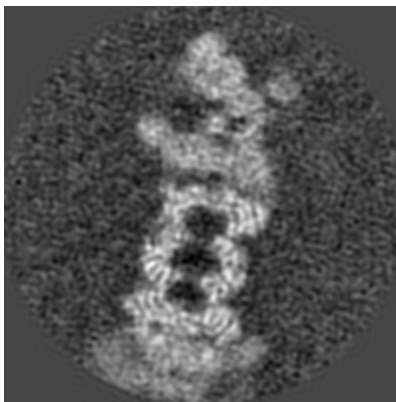
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

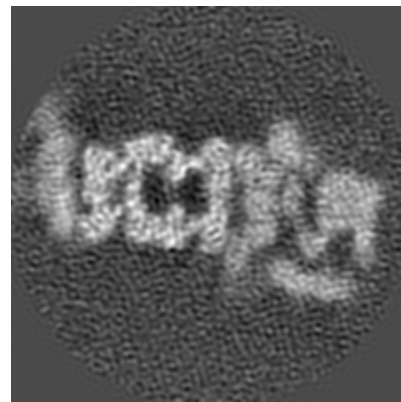
6.3.1 Primary map



X Index: 283



Y Index: 290

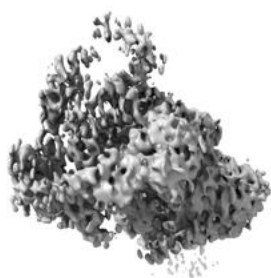


Z Index: 283

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 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

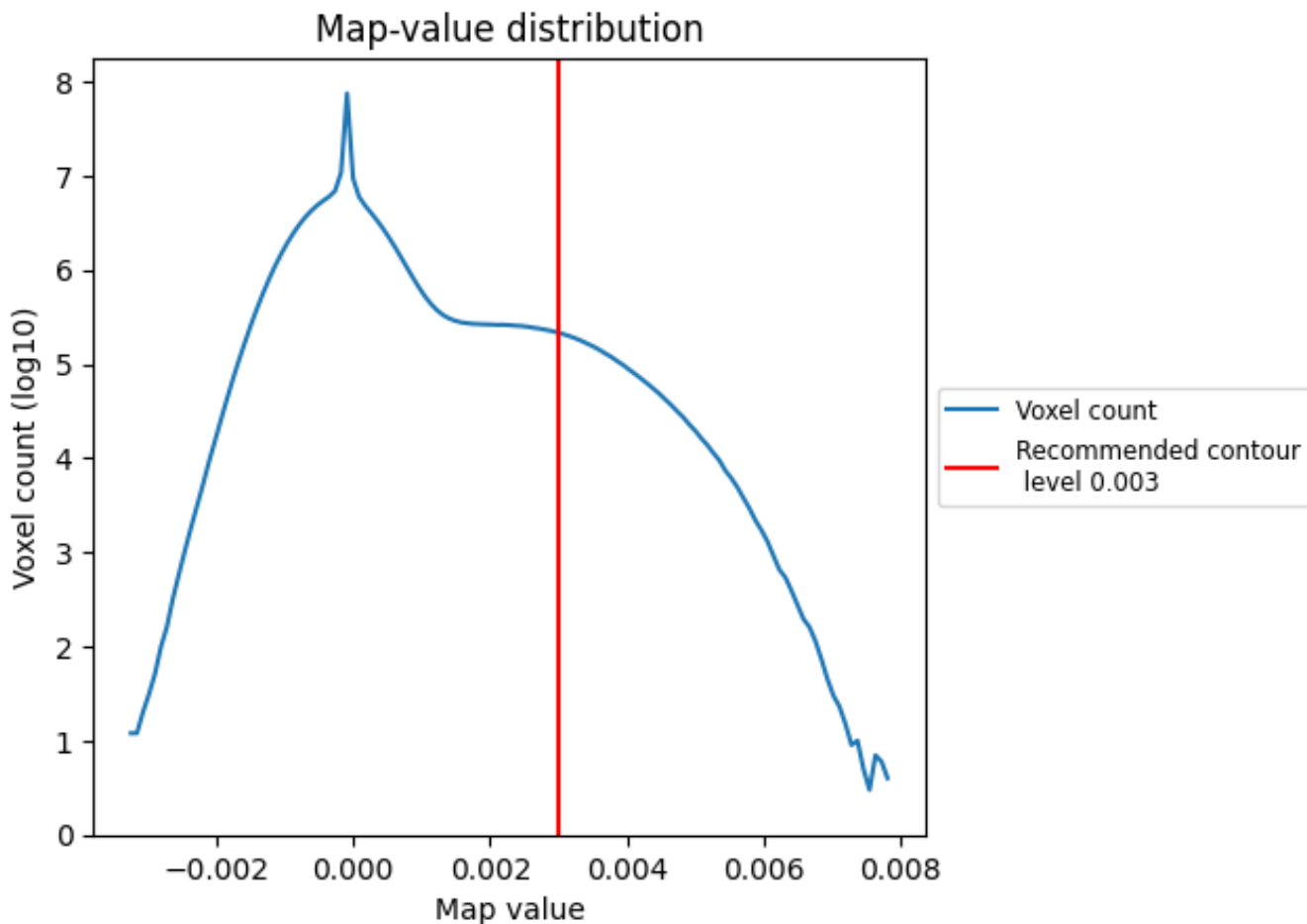
6.5 Mask visualisation

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

7 Map analysis [i](#)

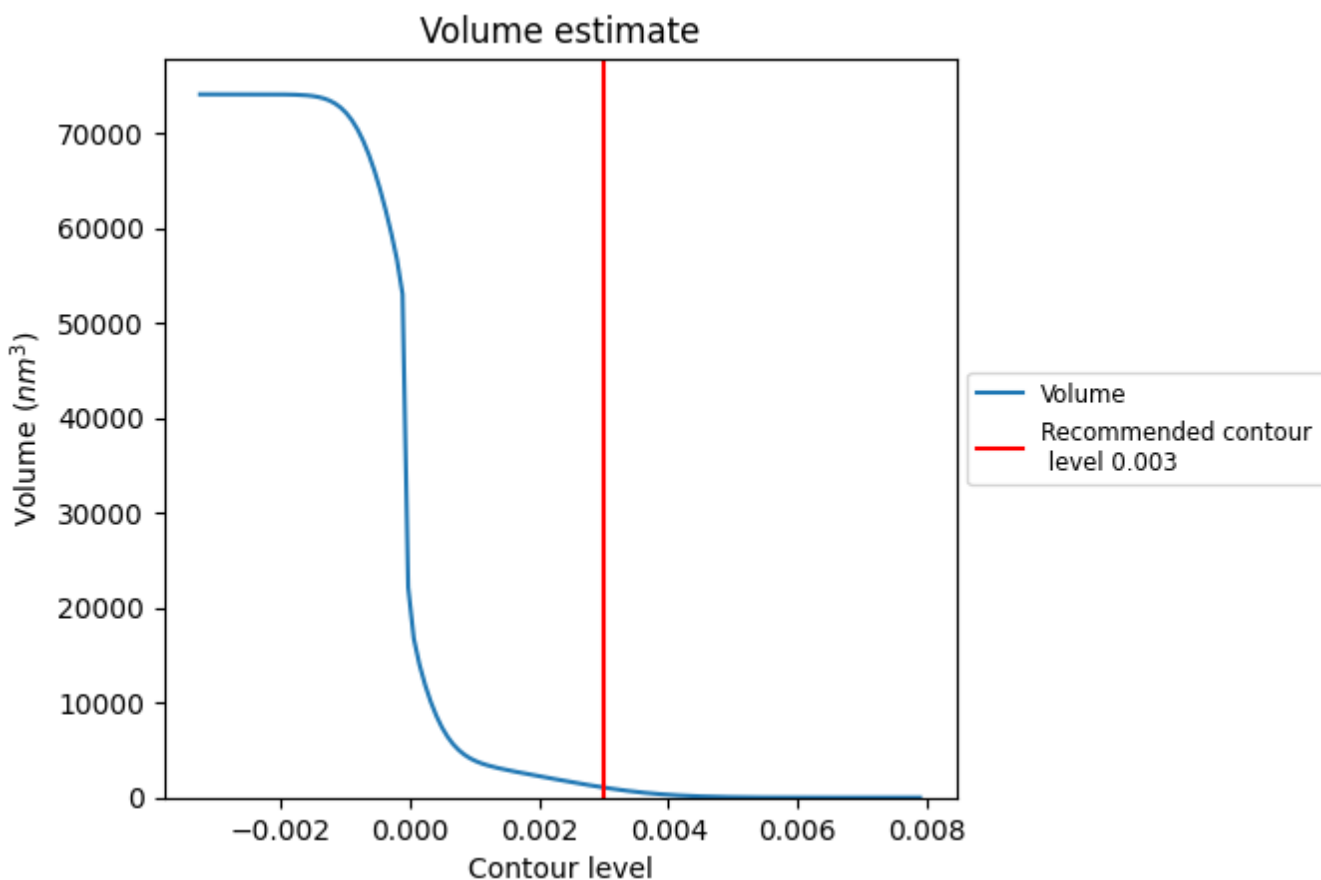
This section contains the results of statistical analysis of the map.

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.

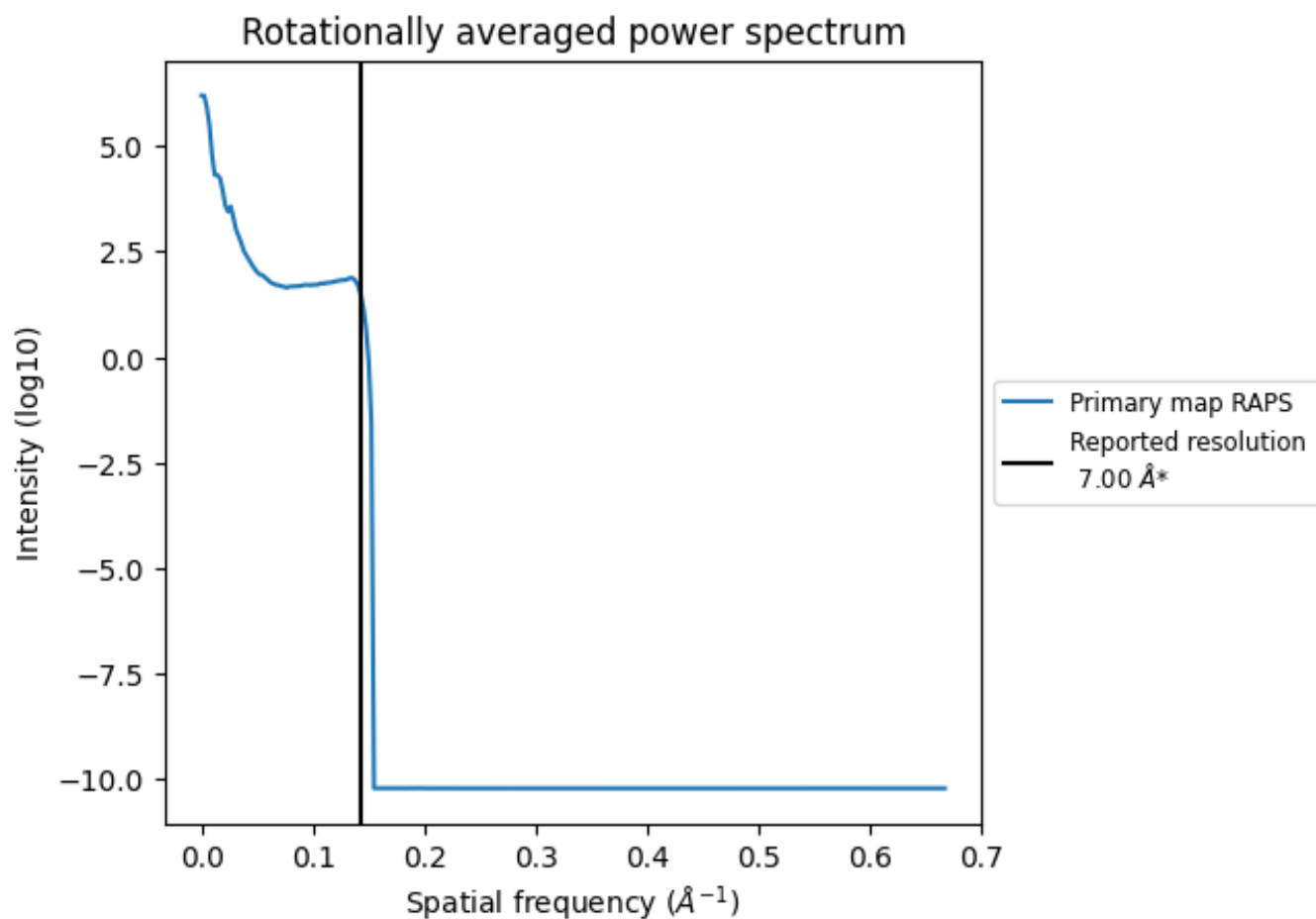
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1064 nm³; this corresponds to an approximate mass of 961 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

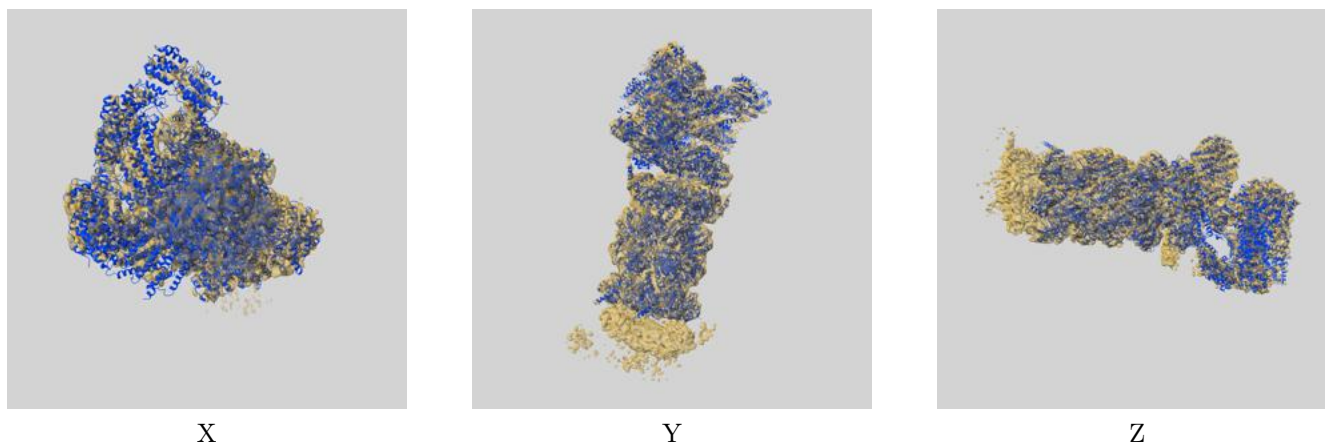
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

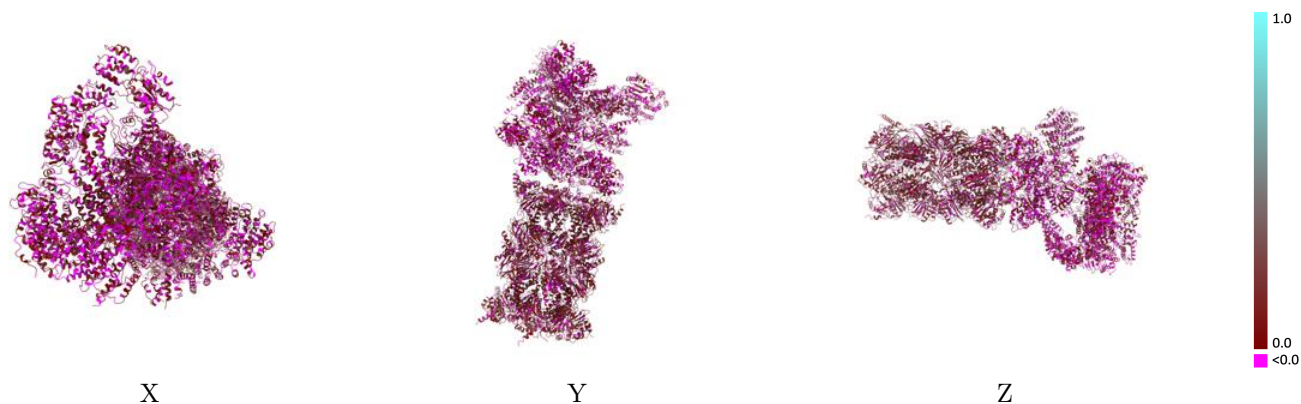
This section contains information regarding the fit between EMDB map EMD-8667 and PDB model 5VFT. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



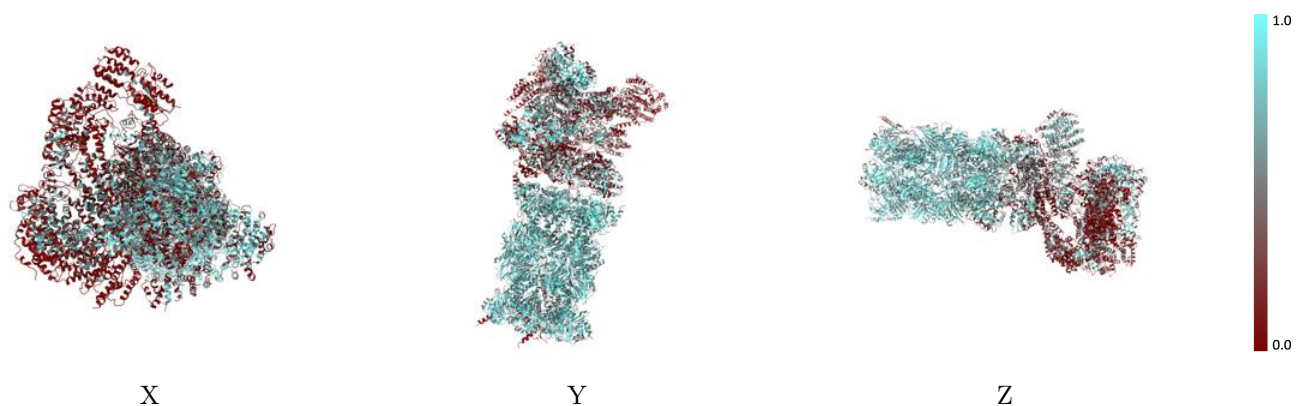
The images above show the 3D surface view of the map at the recommended contour level 0.003 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



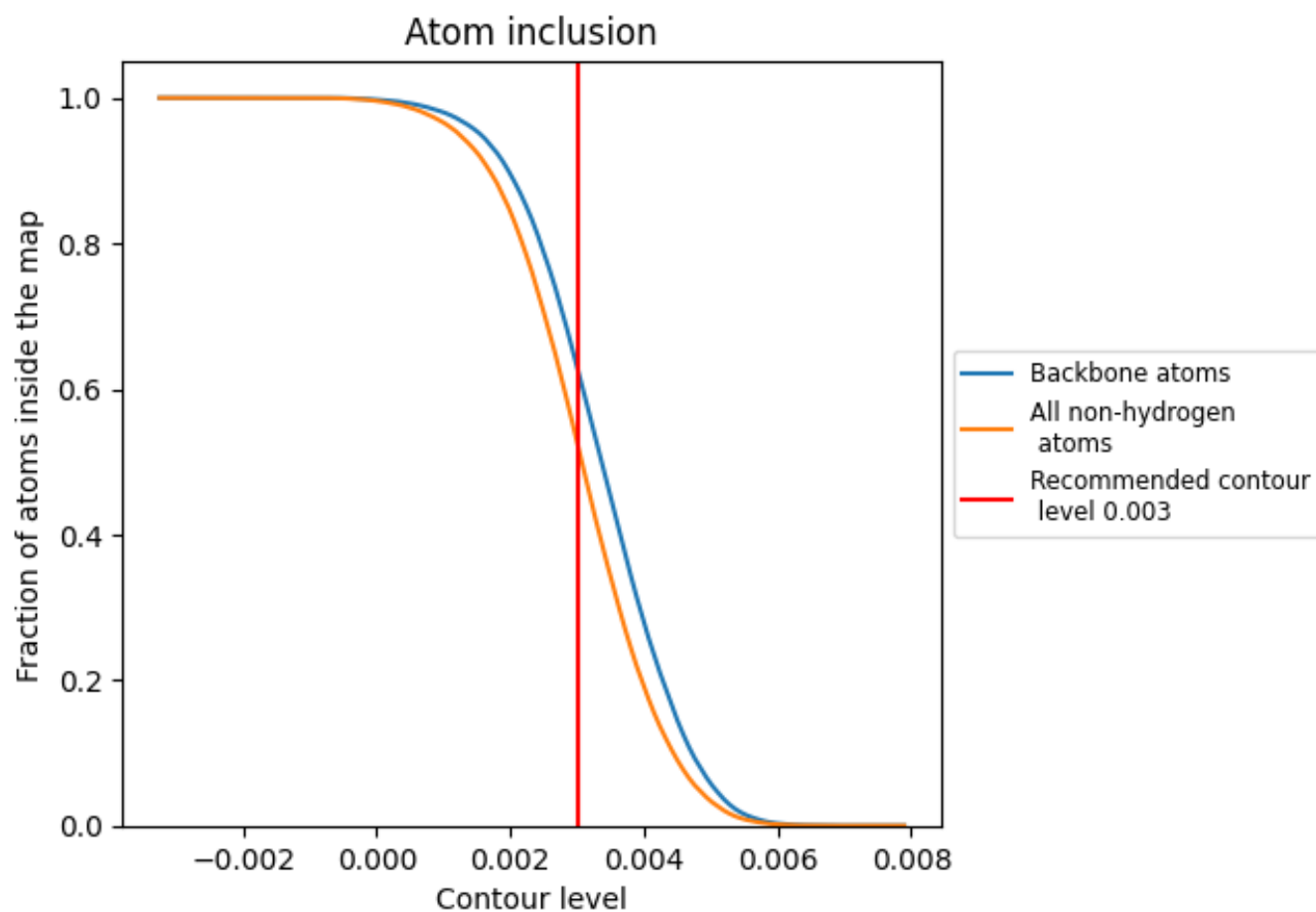
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.003).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5273	 0.0860
A	 0.4110	 0.0520
B	 0.3575	 0.0310
C	 0.3819	 0.0460
D	 0.3210	 0.0300
E	 0.3464	 0.0490
F	 0.3879	 0.0470
G	 0.6552	 0.1240
H	 0.6353	 0.1190
I	 0.6126	 0.1090
J	 0.6855	 0.1340
K	 0.6841	 0.1080
L	 0.7250	 0.1150
M	 0.7017	 0.1220
N	 0.7353	 0.1150
O	 0.7107	 0.1090
P	 0.7426	 0.1080
Q	 0.7375	 0.1360
R	 0.7750	 0.1420
S	 0.7414	 0.1350
T	 0.7505	 0.1290
U	 0.5029	 0.0500
V	 0.2901	 0.0350
W	 0.2096	 0.0430
X	 0.2215	 0.0750
Y	 0.3365	 0.0310
Z	 0.2681	 0.0460
a	 0.1388	 0.0500
b	 0.1346	 0.0560
c	 0.3499	 0.0820
d	 0.2235	 0.0360
e	 0.2474	 0.0240
f	 0.5169	 0.0680
g	 0.7344	 0.1350
h	 0.6776	 0.1260



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Chain	Atom inclusion	Q-score
i	 0.6041	 0.1370
j	 0.7053	 0.1300
k	 0.7069	 0.1280
l	 0.7216	 0.1160
m	 0.6901	 0.1180
n	 0.7561	 0.1400
o	 0.7206	 0.1440
p	 0.7311	 0.1080
q	 0.7700	 0.1410
r	 0.7684	 0.1310
s	 0.7427	 0.1220
t	 0.7770	 0.1290