



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2022 – 09:57 AM EDT

PDB ID : 5VHI
EMDB ID : EMD-8676
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : 2017-04-13
Resolution : 6.80 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:

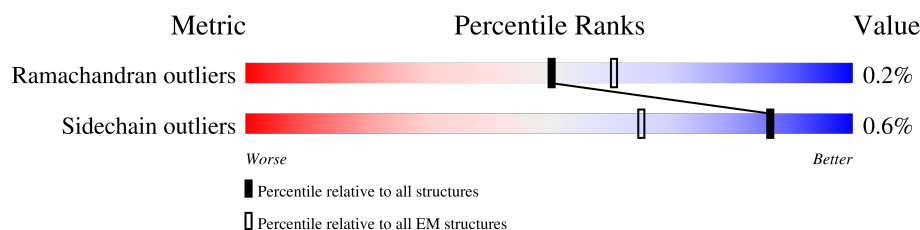
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 6.80 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)
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	A	352	<div> <div>22%</div> <div>91%</div> <div>9%</div> </div>
2	B	341	<div> <div>30%</div> <div>87%</div> <div>13%</div> </div>
3	C	385	<div> <div>38%</div> <div>89%</div> <div>9%</div> </div>
4	D	368	<div> <div>46%</div> <div>92%</div> <div>7%</div> </div>
5	E	379	<div> <div>24%</div> <div>82%</div> <div>18%</div> </div>
6	F	380	<div> <div>20%</div> <div>90%</div> <div>8%</div> </div>
7	U	935	<div> <div>8%</div> <div>90%</div> <div>10%</div> </div>
8	V	488	<div> <div>29%</div> <div>99%</div> <div>.</div> </div>
9	W	456	<div> <div>24%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
10	X	385	<div> <div>44%</div> <div>100%</div> </div>
11	Y	378	<div> <div>7%</div> <div>99%</div> </div>
12	Z	286	<div> <div>10%</div> <div>100%</div> </div>
13	a	374	<div> <div>11%</div> <div>100%</div> </div>
14	b	191	<div> <div>11%</div> <div>100%</div> </div>
15	c	287	<div> <div>12%</div> <div>100%</div> </div>
16	d	257	<div> <div>20%</div> <div>100%</div> </div>
17	G	226	<div> <div>84%</div> <div>100%</div> </div>
18	e	70	<div> <div>41%</div> <div>100%</div> </div>
19	f	848	<div> <div>28%</div> <div>80%</div> <div>19%</div> </div>

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 54640 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 regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	321	Total	C	N	O	S	0	0
			2525	1596	451	463	15		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	298	Total	C	N	O	S	0	0
			2332	1464	400	457	11		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	350	Total	C	N	O	S	0	0
			2757	1728	501	514	14		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	343	Total	C	N	O	S	0	0
			2743	1739	479	516	9		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	311	Total	C	N	O	S	0	0
			2468	1548	445	460	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	351	Total	C	N	O	S	0	0
			2746	1733	476	520	17		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	845	Total	C	N	O	S	0	0
			6568	4169	1118	1236	45		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	488	Total	C	N	O	S	0	0
			3919	2487	695	723	14		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	385	Total	C	N	O	S	0	0
			3048	1939	515	582	12		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	226	Total	C	N	O	S	0	0
			1710	1063	302	334	11		

- Molecule 18 is a protein called 26S proteasome complex subunit SEM1.

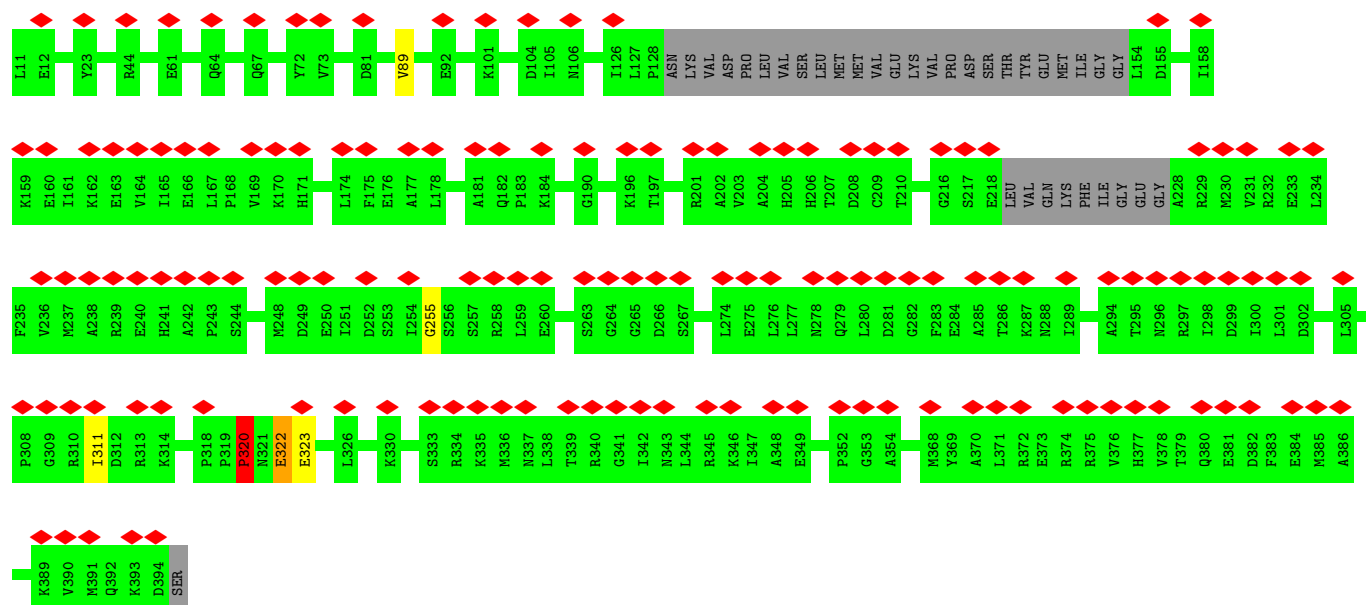
Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	70	Total	C	N	O	S	0	0
			583	357	89	135	2		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	686	Total	C	N	O	S	0	0
			5304	3335	901	1033	35		

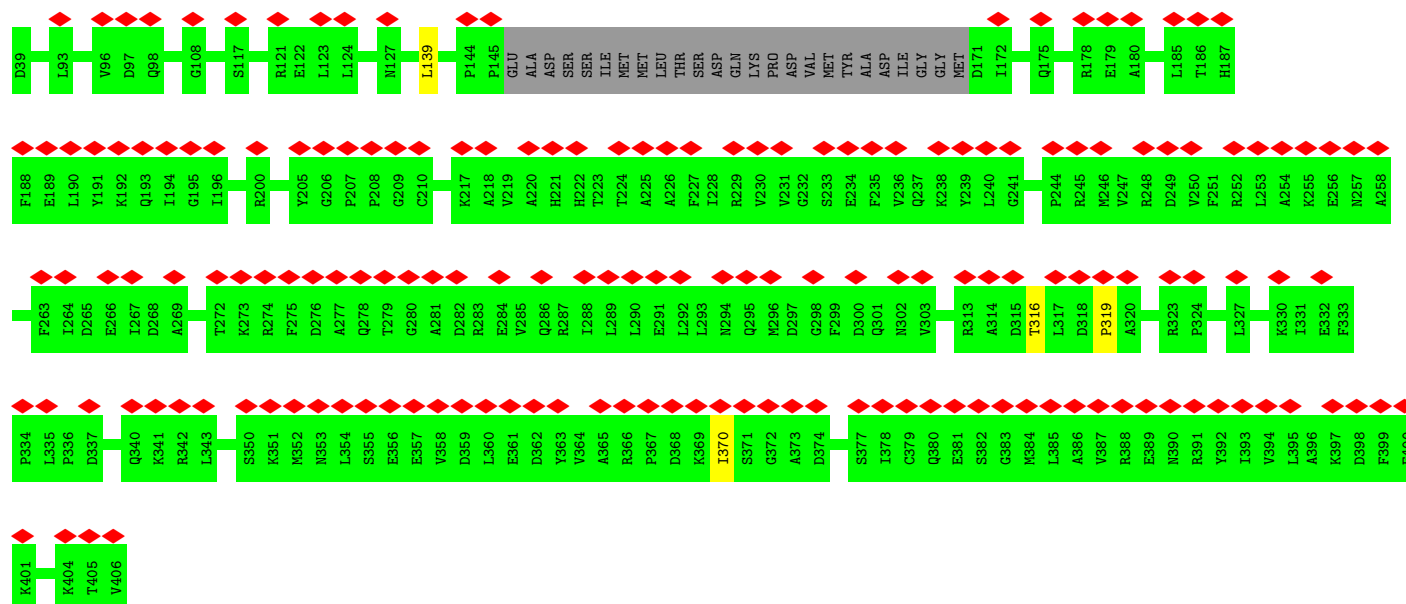
- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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



• Molecule 4: 26S proteasome regulatory subunit 6B

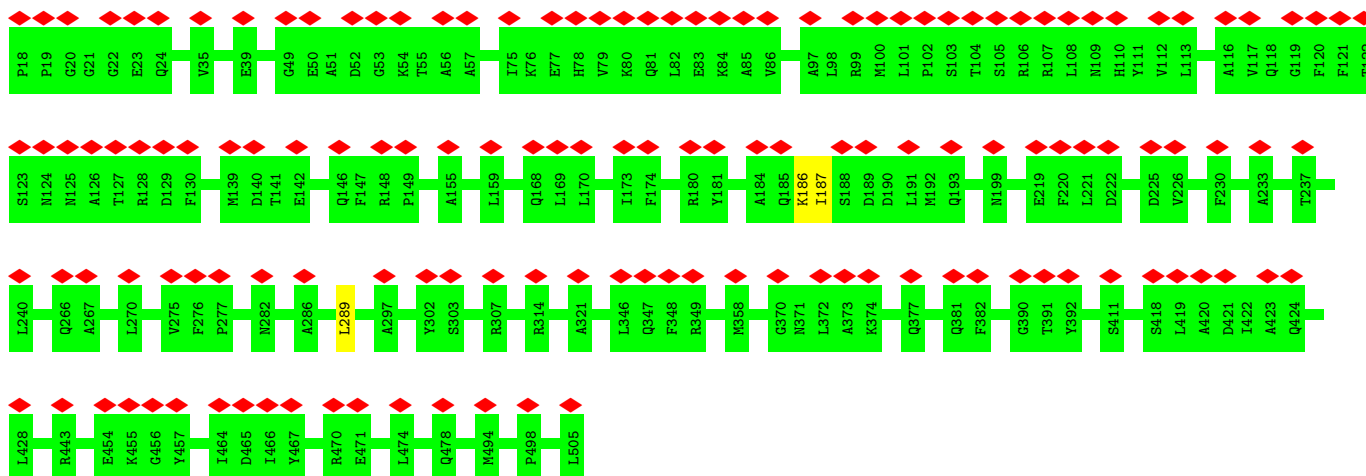
Chain D: 46% 92% 7%



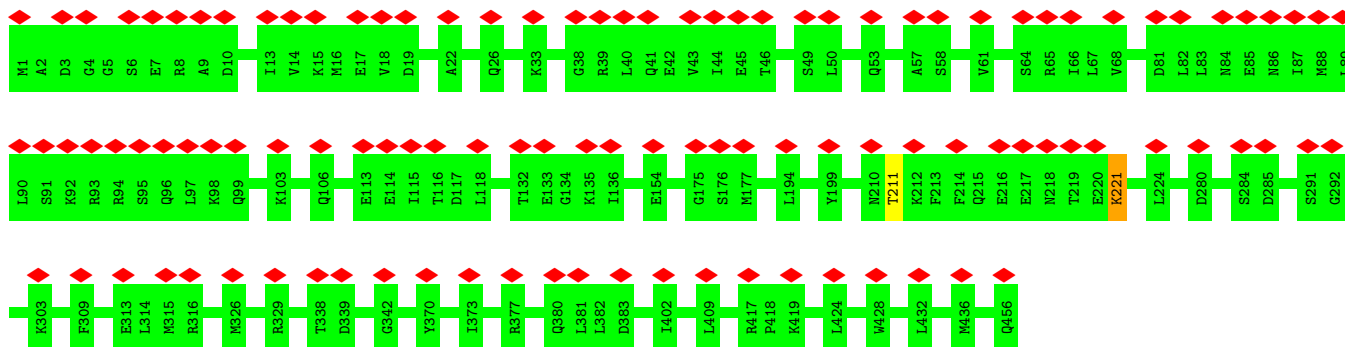
• Molecule 5: 26S proteasome regulatory subunit 10B

Chain E: 24% 82% 18%

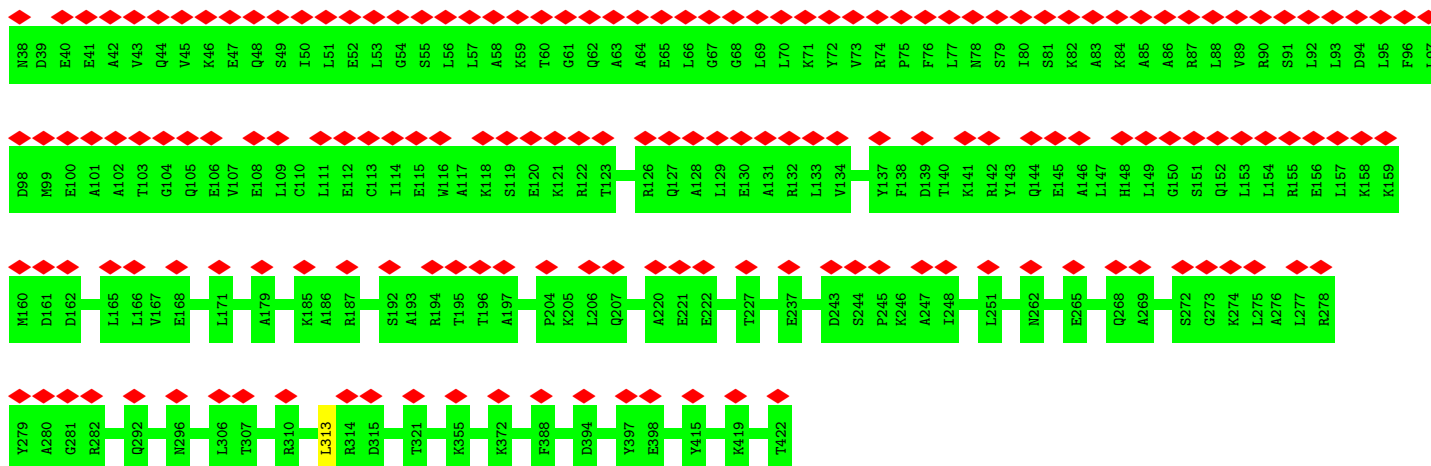
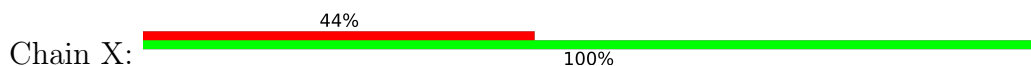




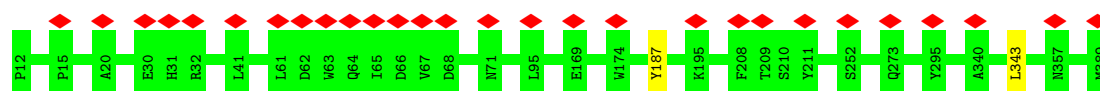
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12



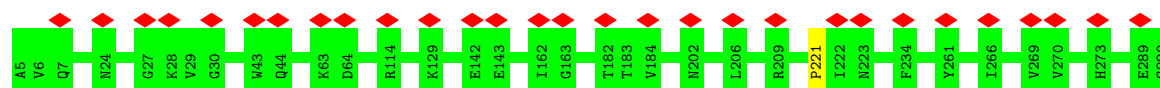
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11



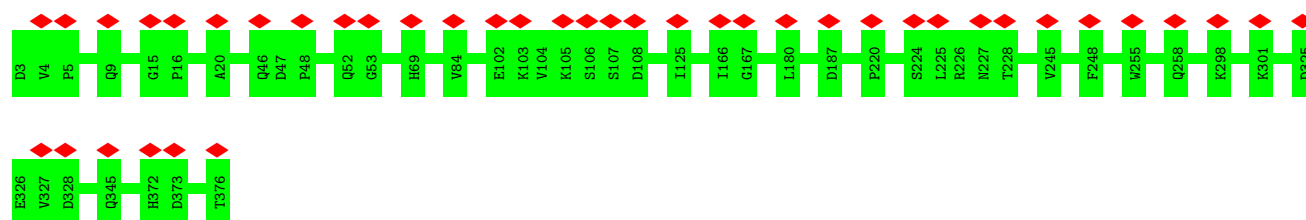
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 6



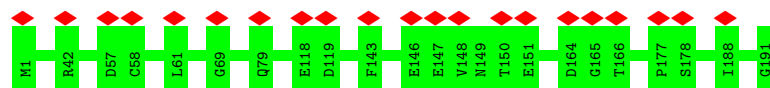
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 7



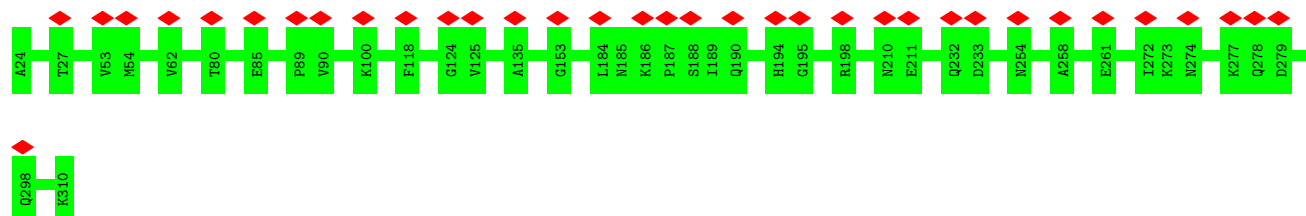
- Molecule 13: 26S proteasome non-ATPase regulatory subunit 13



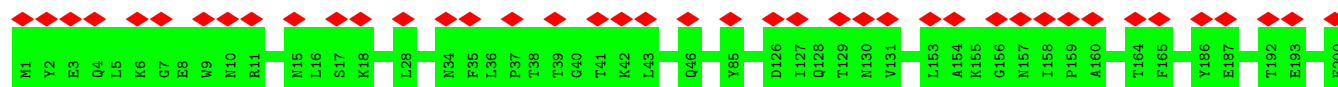
- Molecule 14: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 15: 26S proteasome non-ATPase regulatory subunit 14



- Molecule 16: 26S proteasome non-ATPase regulatory subunit 8





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10891	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 ($e^-/\text{\AA}^2$)	50	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	0.015	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	250.88, 250.88, 250.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.21	0/2567	0.40	0/3462
2	B	0.20	0/2362	0.39	0/3182
3	C	0.26	0/2790	0.44	2/3748 (0.1%)
4	D	0.21	0/2787	0.39	0/3763
5	E	0.20	0/2499	0.37	0/3350
6	F	0.21	0/2781	0.42	1/3745 (0.0%)
7	U	0.20	0/6684	0.37	0/9043
8	V	0.22	0/3997	0.44	0/5399
9	W	0.21	0/3750	0.40	1/5039 (0.0%)
10	X	0.20	0/3092	0.35	0/4168
11	Y	0.20	0/3173	0.35	0/4273
12	Z	0.20	0/2324	0.37	0/3150
13	a	0.21	0/3061	0.37	0/4144
14	b	0.21	0/1478	0.37	0/2001
15	c	0.20	0/2302	0.35	0/3110
16	d	0.21	0/2162	0.38	0/2919
17	G	0.19	0/1735	0.33	0/2343
18	e	0.21	0/596	0.36	0/805
19	f	0.22	0/5377	0.43	1/7248 (0.0%)
All	All	0.21	0/55517	0.39	5/74892 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	320	PRO	CA-N-CD	-7.46	101.05	111.50
19	f	407	MET	N-CA-C	-6.27	94.06	111.00
6	F	164	LEU	C-N-CD	-5.61	108.25	120.60
3	C	255	GLY	N-CA-C	5.32	126.40	113.10
9	W	221	LYS	N-CA-C	-5.10	97.23	111.00

There are no chirality outliers.

There are no planarity outliers.

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	A	315/352 (90%)	285 (90%)	30 (10%)	0	100	100
2	B	290/341 (85%)	263 (91%)	27 (9%)	0	100	100
3	C	344/385 (89%)	324 (94%)	17 (5%)	3 (1%)	17	57
4	D	339/368 (92%)	321 (95%)	17 (5%)	1 (0%)	41	77
5	E	303/379 (80%)	283 (93%)	19 (6%)	1 (0%)	41	77
6	F	345/380 (91%)	316 (92%)	25 (7%)	4 (1%)	13	50
7	U	837/935 (90%)	791 (94%)	46 (6%)	0	100	100
8	V	484/488 (99%)	419 (87%)	65 (13%)	0	100	100
9	W	452/456 (99%)	411 (91%)	40 (9%)	1 (0%)	47	81
10	X	383/385 (100%)	364 (95%)	18 (5%)	1 (0%)	41	77
11	Y	376/378 (100%)	348 (93%)	28 (7%)	0	100	100
12	Z	284/286 (99%)	256 (90%)	27 (10%)	1 (0%)	34	72
13	a	372/374 (100%)	349 (94%)	23 (6%)	0	100	100
14	b	189/191 (99%)	171 (90%)	18 (10%)	0	100	100
15	c	285/287 (99%)	262 (92%)	23 (8%)	0	100	100
16	d	255/257 (99%)	236 (92%)	19 (8%)	0	100	100
17	G	224/226 (99%)	224 (100%)	0	0	100	100
18	e	68/70 (97%)	62 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	f	664/848 (78%)	600 (90%)	62 (9%)	2 (0%)	41	77
All	All	6809/7386 (92%)	6285 (92%)	510 (8%)	14 (0%)	50	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	320	PRO
3	C	322	GLU
3	C	323	GLU
5	E	295	LEU
10	X	313	LEU

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	A	274/300 (91%)	272 (99%)	2 (1%)	84	90
2	B	262/298 (88%)	260 (99%)	2 (1%)	81	89
3	C	302/333 (91%)	298 (99%)	4 (1%)	69	82
4	D	300/321 (94%)	297 (99%)	3 (1%)	76	86
5	E	270/333 (81%)	269 (100%)	1 (0%)	91	94
6	F	302/326 (93%)	298 (99%)	4 (1%)	69	82
7	U	717/798 (90%)	711 (99%)	6 (1%)	81	89
8	V	422/422 (100%)	419 (99%)	3 (1%)	84	90
9	W	416/416 (100%)	415 (100%)	1 (0%)	93	96
10	X	331/331 (100%)	331 (100%)	0	100	100
11	Y	334/334 (100%)	332 (99%)	2 (1%)	86	92
12	Z	257/257 (100%)	257 (100%)	0	100	100
13	a	334/334 (100%)	334 (100%)	0	100	100
14	b	167/167 (100%)	167 (100%)	0	100	100
15	c	252/252 (100%)	252 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	d	231/231 (100%)	231 (100%)	0	100	100
17	G	180/180 (100%)	180 (100%)	0	100	100
18	e	63/63 (100%)	63 (100%)	0	100	100
19	f	579/714 (81%)	572 (99%)	7 (1%)	71	83
All	All	5993/6410 (94%)	5958 (99%)	35 (1%)	86	92

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	f	86	THR
19	f	192	VAL
19	f	460	ASP
6	F	86	LEU
5	E	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
9	W	257	GLN
19	f	750	GLN
12	Z	102	HIS
19	f	592	ASN
16	d	141	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	V	1
9	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	237:THR	C	238:ALA	N	3.31
1	W	205:ILE	C	206:SER	N	3.16

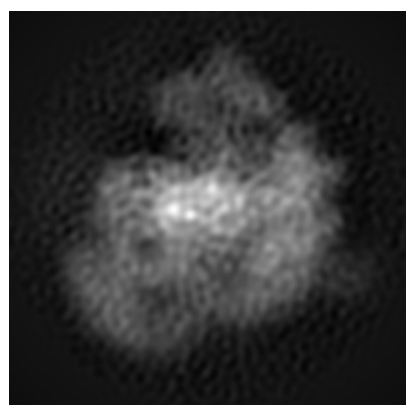
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8676. These allow visual inspection of the internal detail of the map and identification of artifacts.

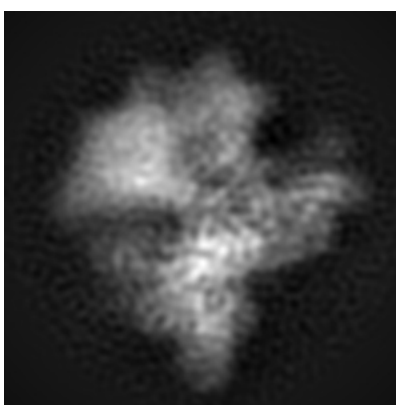
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

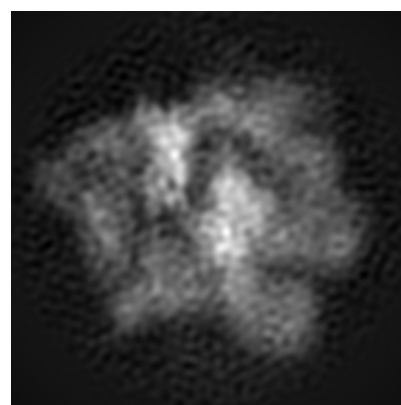
6.1.1 Primary map



X



Y

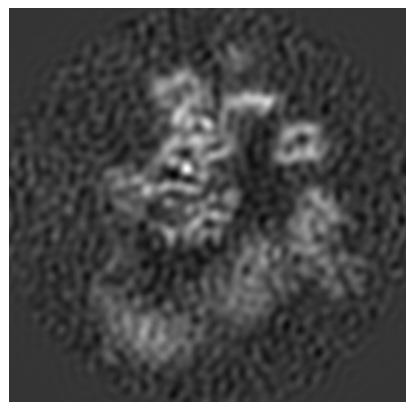


Z

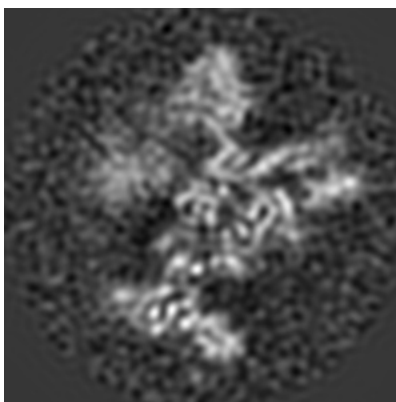
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

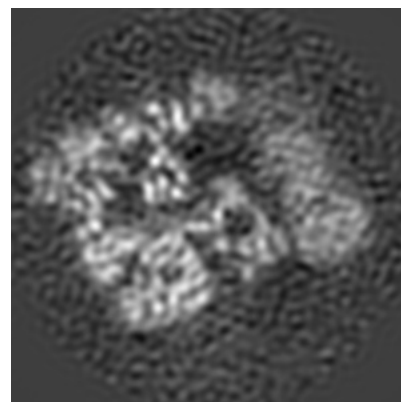
6.2.1 Primary map



X Index: 128



Y Index: 128

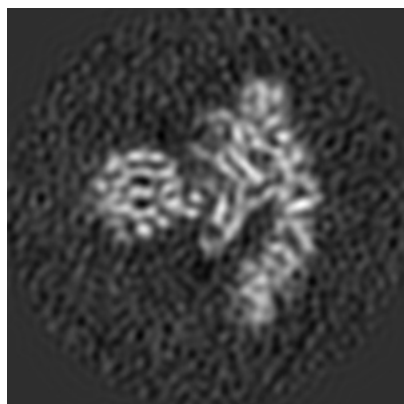


Z Index: 128

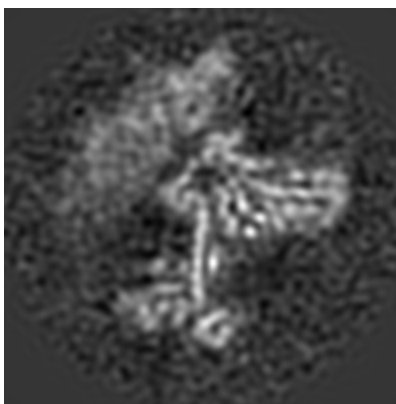
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

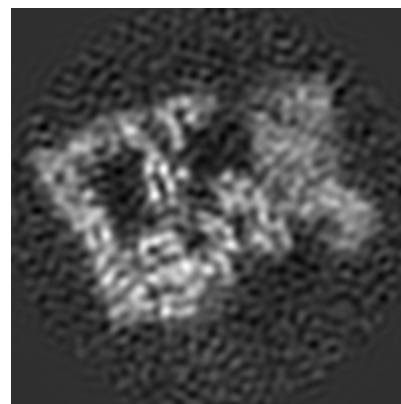
6.3.1 Primary map



X Index: 106



Y Index: 115

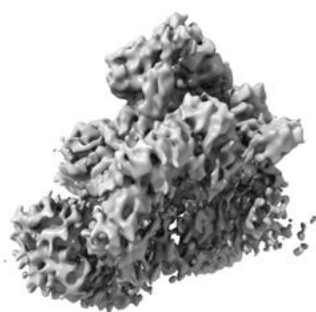


Z Index: 139

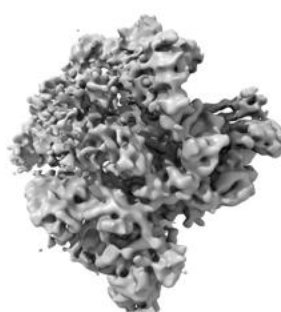
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

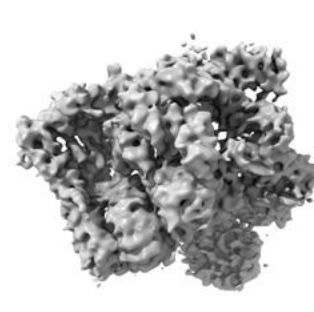
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

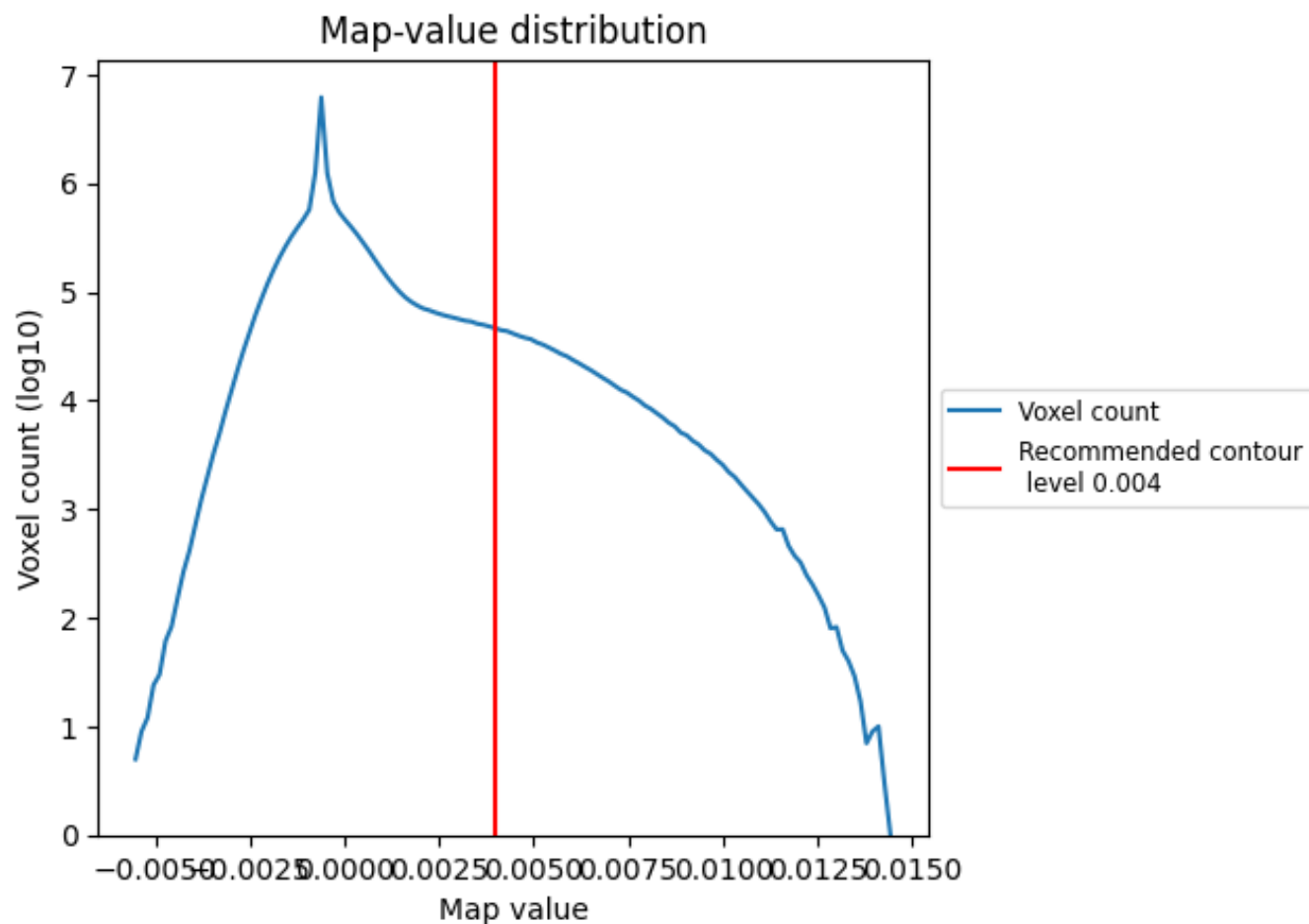
6.5 Mask visualisation

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

7 Map analysis [i](#)

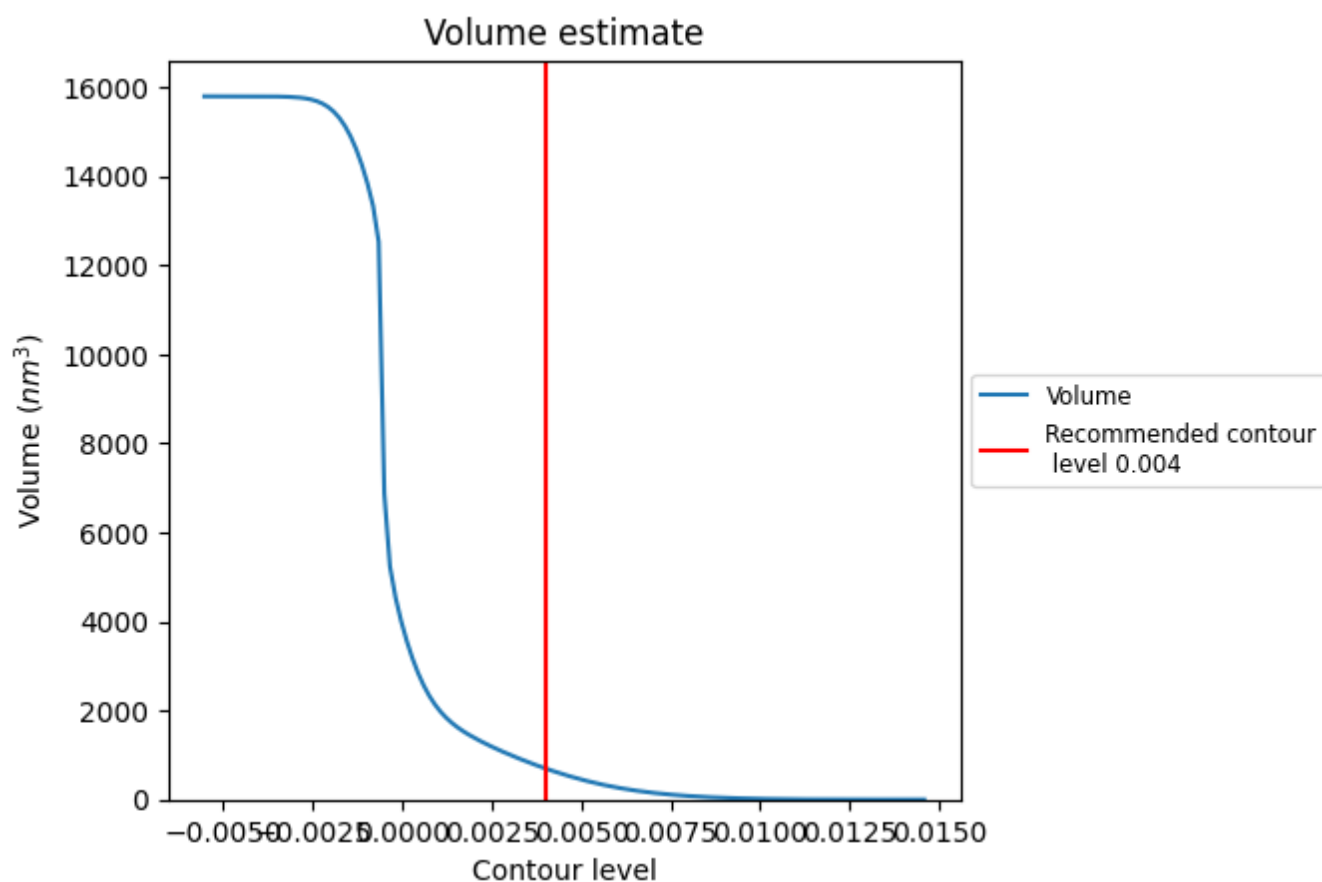
This section contains the results of statistical analysis of the map.

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.

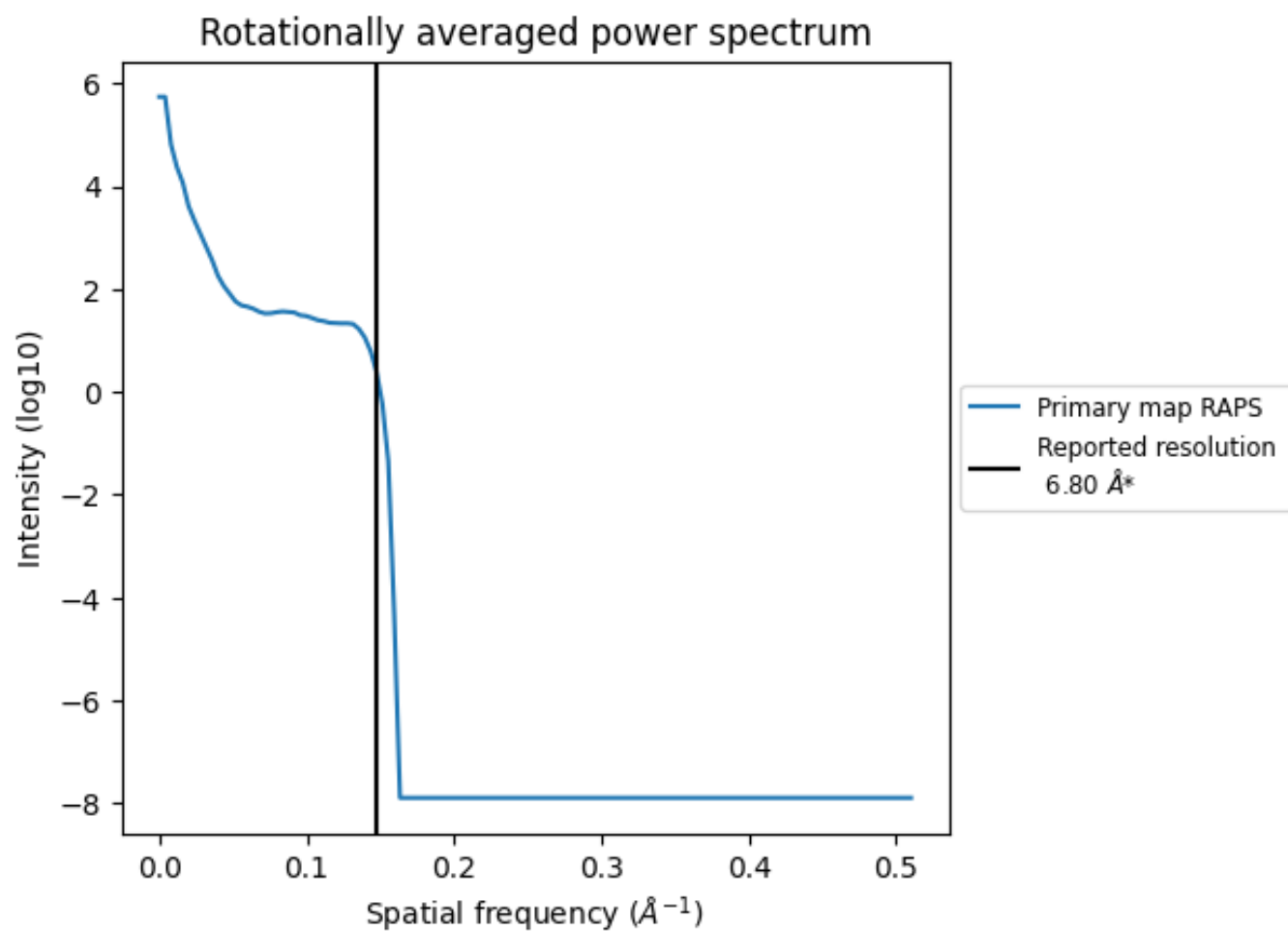
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 632 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 0.147 Å⁻¹

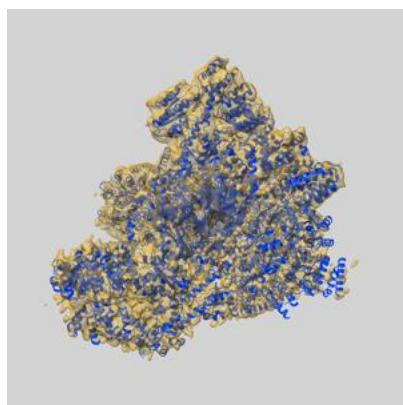
8 Fourier-Shell correlation

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

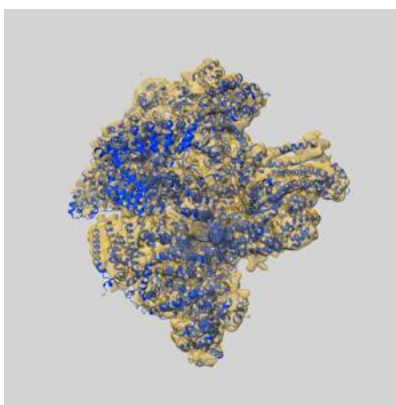
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8676 and PDB model 5VHI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

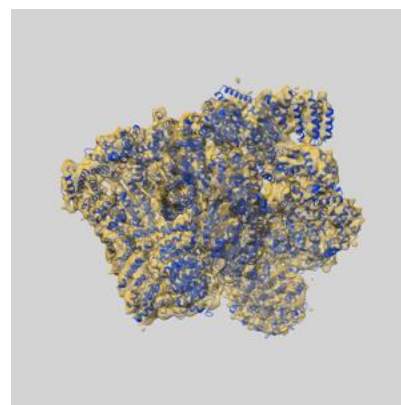
9.1 Map-model overlay [i](#)



X



Y



Z

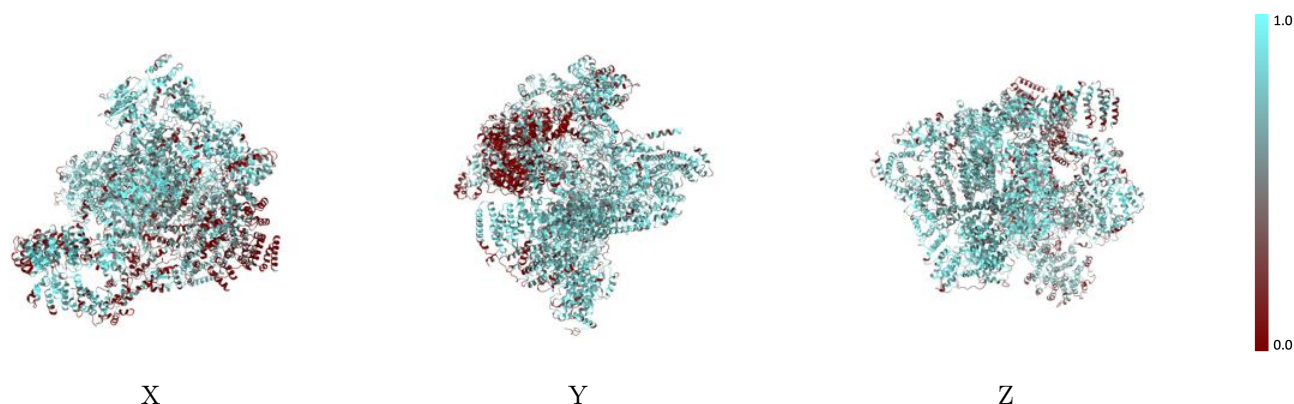
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



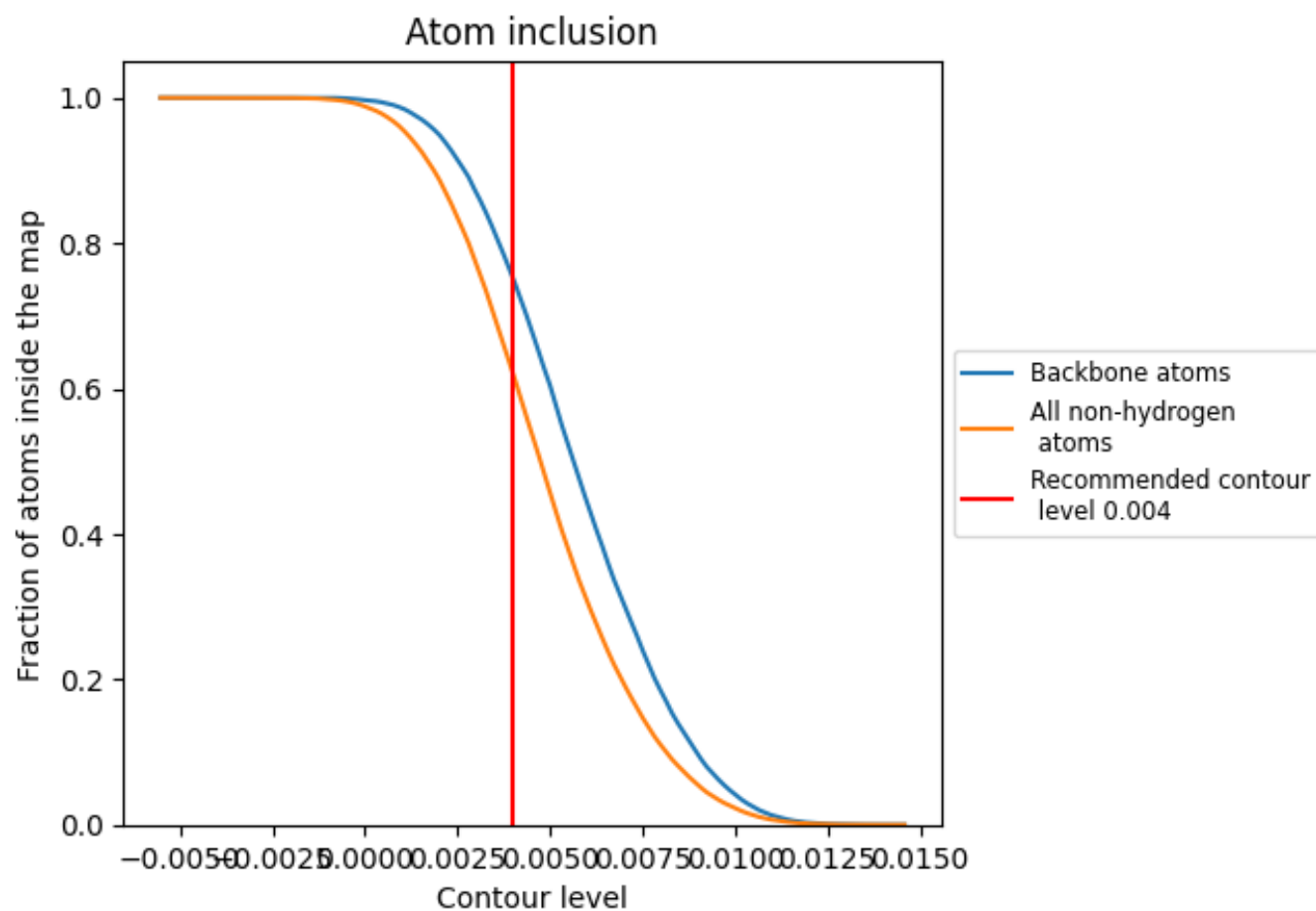
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 62% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6214	 0.0990
A	 0.6434	 0.0840
B	 0.5526	 0.0660
C	 0.4835	 0.0670
D	 0.4348	 0.0610
E	 0.5997	 0.0810
F	 0.6746	 0.0940
G	 0.1647	 0.0280
U	 0.7754	 0.1400
V	 0.6067	 0.1070
W	 0.6449	 0.1100
X	 0.4718	 0.1030
Y	 0.7684	 0.1300
Z	 0.7159	 0.1330
a	 0.7308	 0.1330
b	 0.7481	 0.1270
c	 0.6909	 0.1340
d	 0.6614	 0.1290
e	 0.4835	 0.0680
f	 0.5746	 0.0410

