



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 05:30 AM UTC

PDB ID : 5MPE / pdb_00005mpe
EMDB ID : EMD-3535
Title : 26S proteasome in presence of ATP (s2)
Authors : Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.;
Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on : 2016-12-16
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

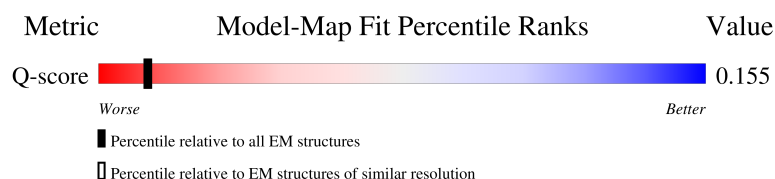
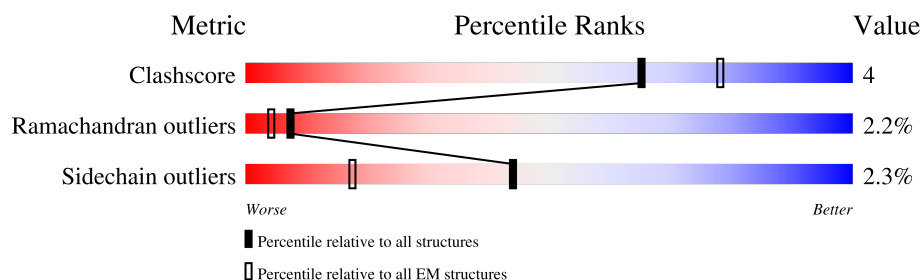
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	W	268	
2	V	306	
3	T	274	
4	X	156	

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Mol	Chain	Length	Quality of chain
5	Y	89	
6	Z	993	
7	N	945	
8	S	523	
9	P	445	
10	Q	434	
11	R	429	
12	U	338	
13	O	393	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 40974 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 RPN10.

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

- Molecule 2 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	289	Total	C	N	O	S	0	0
			2274	1425	389	446	14		

- Molecule 3 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN13.

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

- Molecule 5 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Y	51	Total	C	N	O	0	0
			435	264	69	102		

- Molecule 6 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

- Molecule 7 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	890	Total	C	N	O	S	0	0
			6882	4373	1156	1325	28		

- Molecule 8 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 9 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

- Molecule 10 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN7.

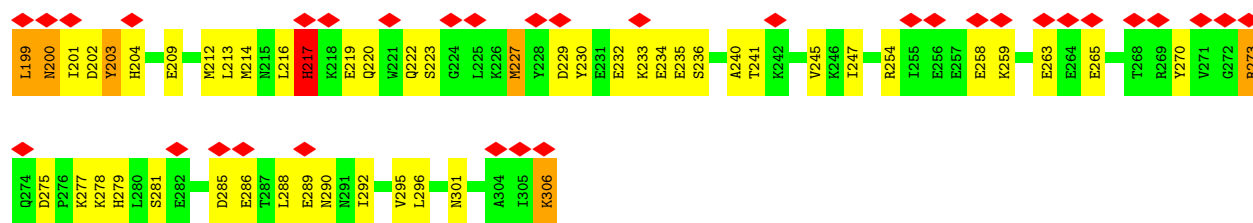
Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	381	Total	C	N	O	S	0	0
			3060	1955	502	593	10		

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN8.

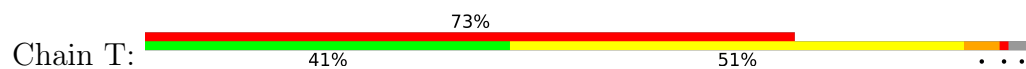
Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	298	Total	C	N	O	S	0	0
			2373	1496	404	466	7		

- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN9.

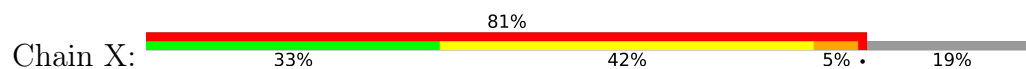
Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		



• Molecule 3: 26S proteasome regulatory subunit RPN12



• Molecule 4: 26S proteasome regulatory subunit RPN13

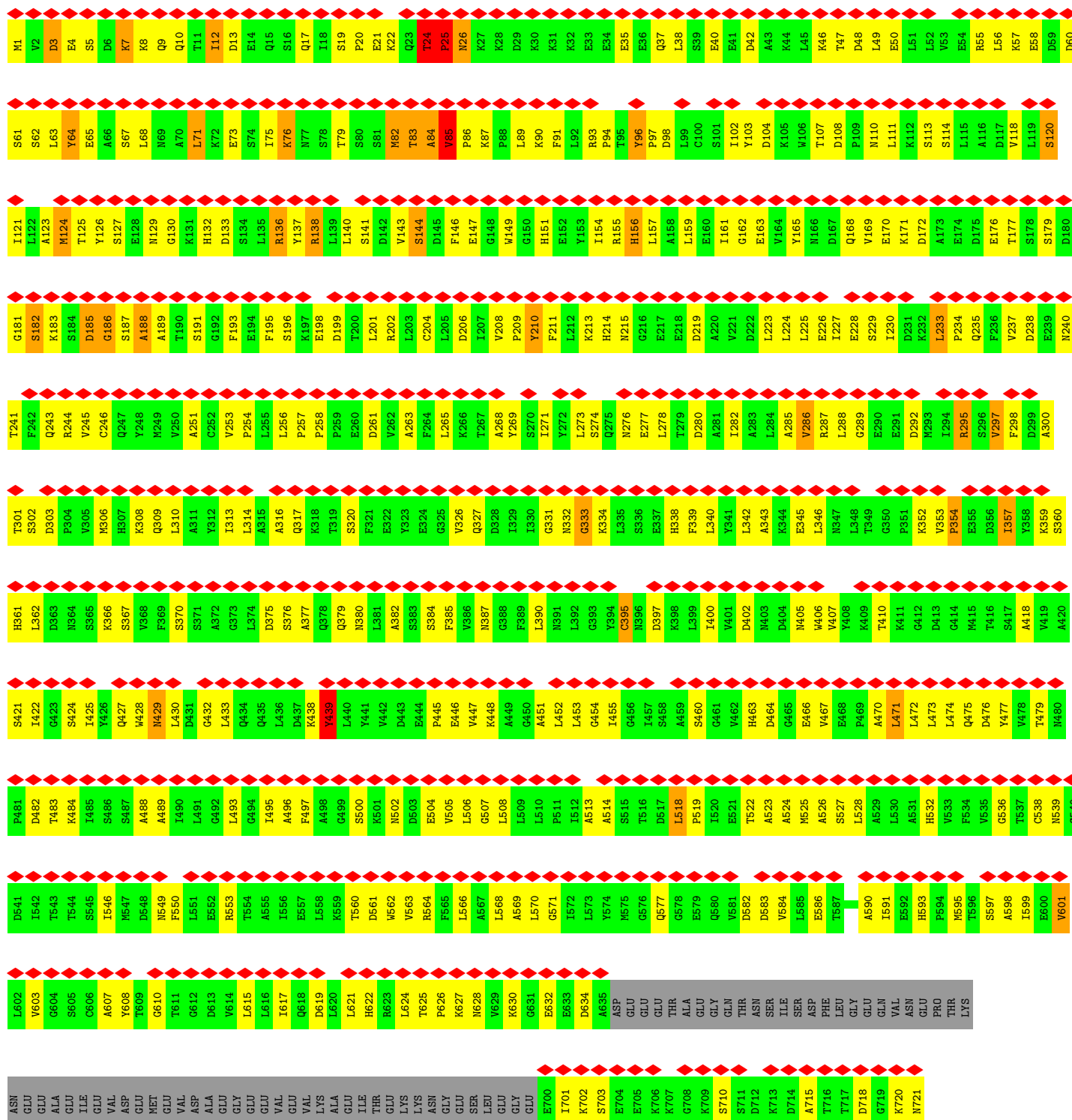
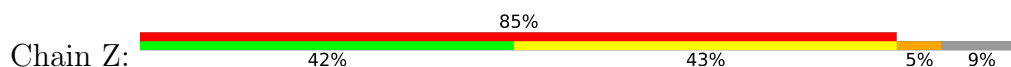


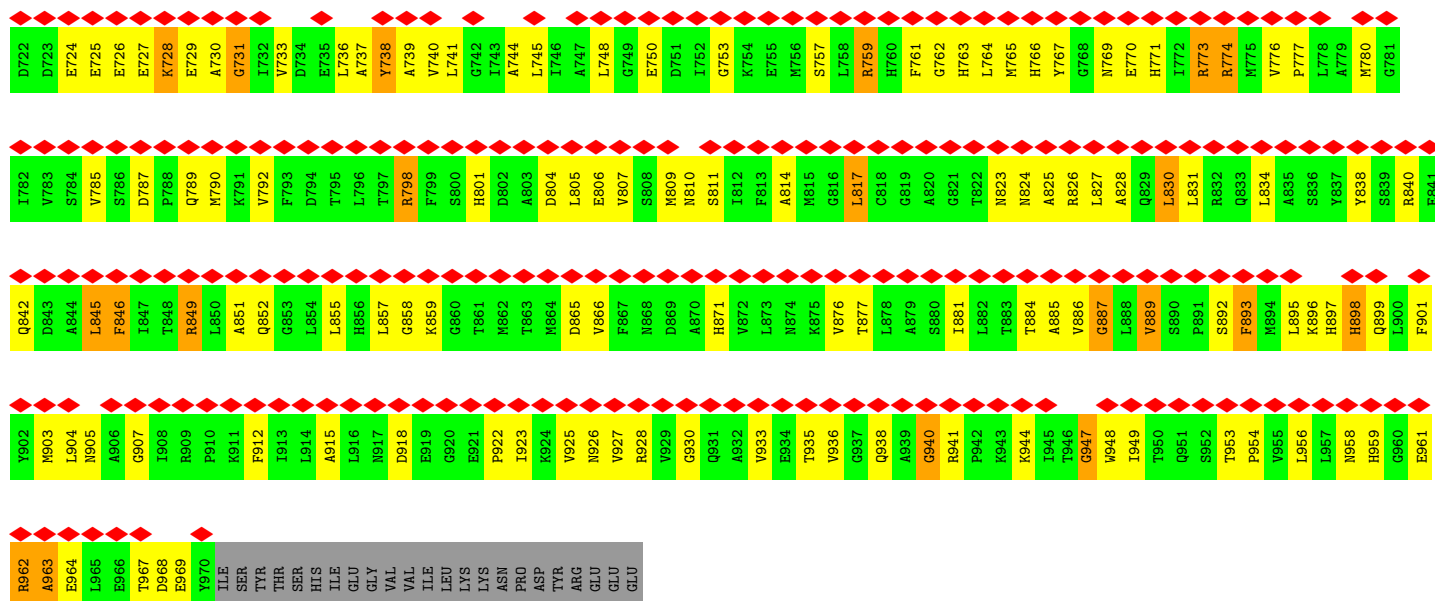
• Molecule 5: 26S proteasome complex subunit SEM1



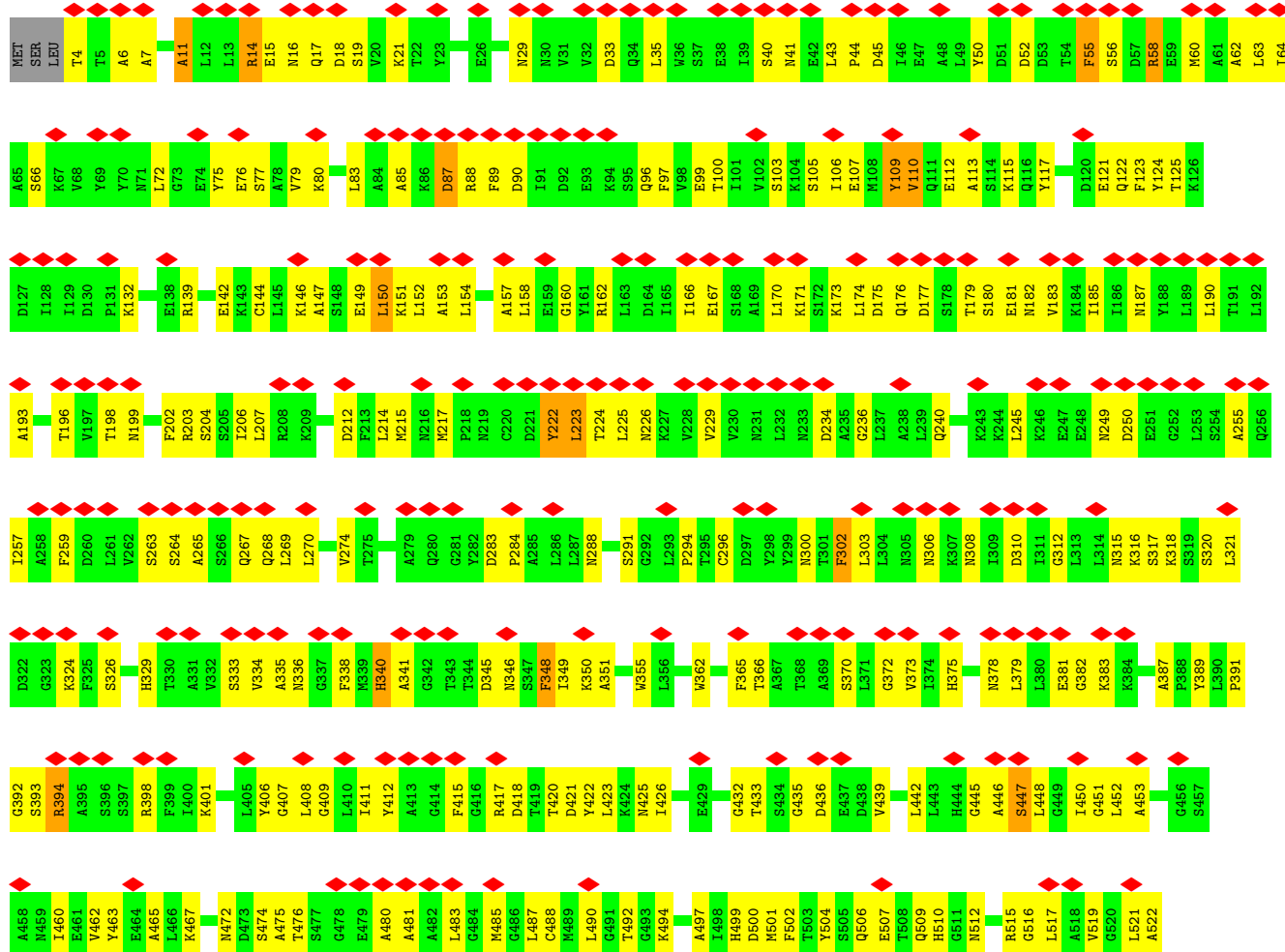
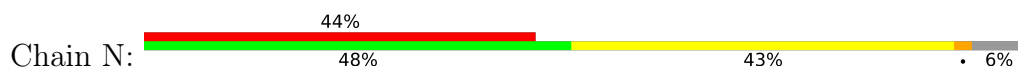


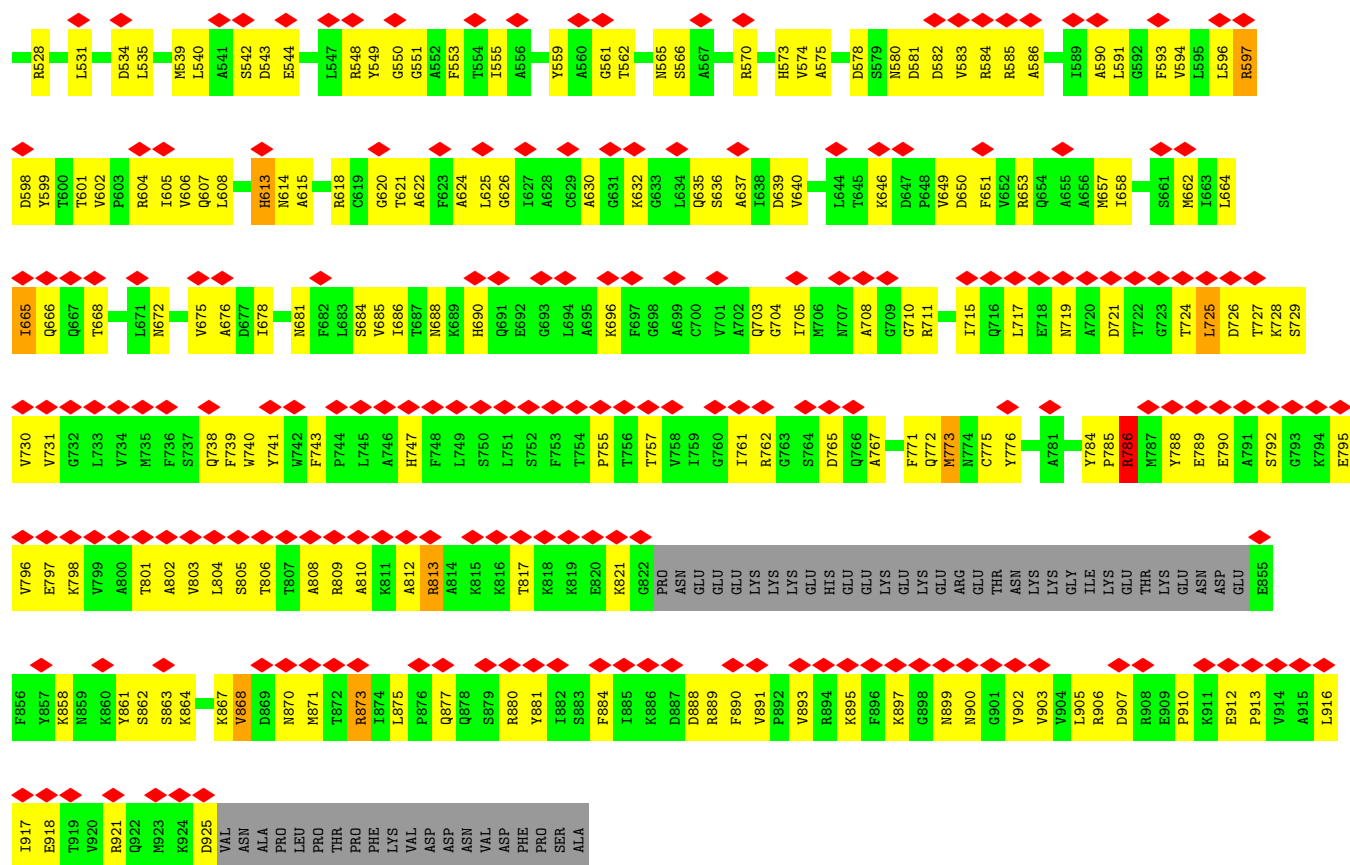
● Molecule 6: 26S proteasome regulatory subunit RPN1



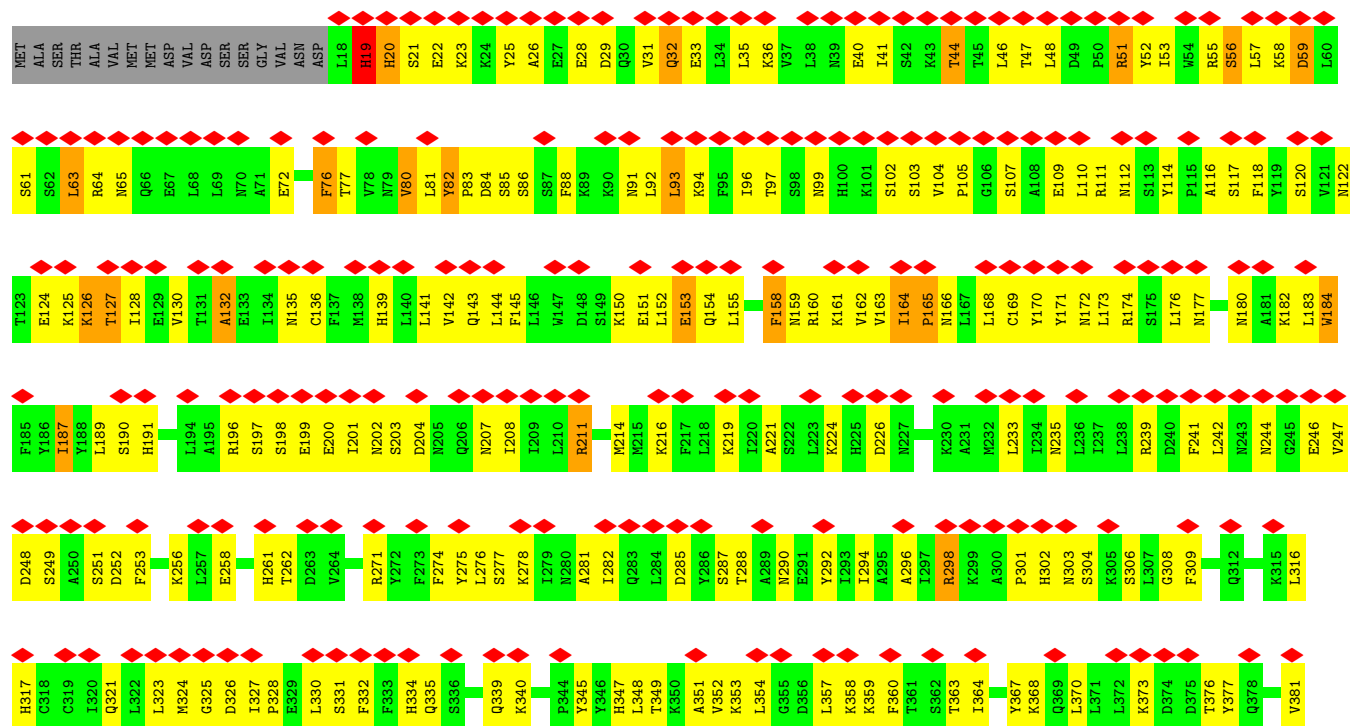


• Molecule 7: 26S proteasome regulatory subunit RPN2



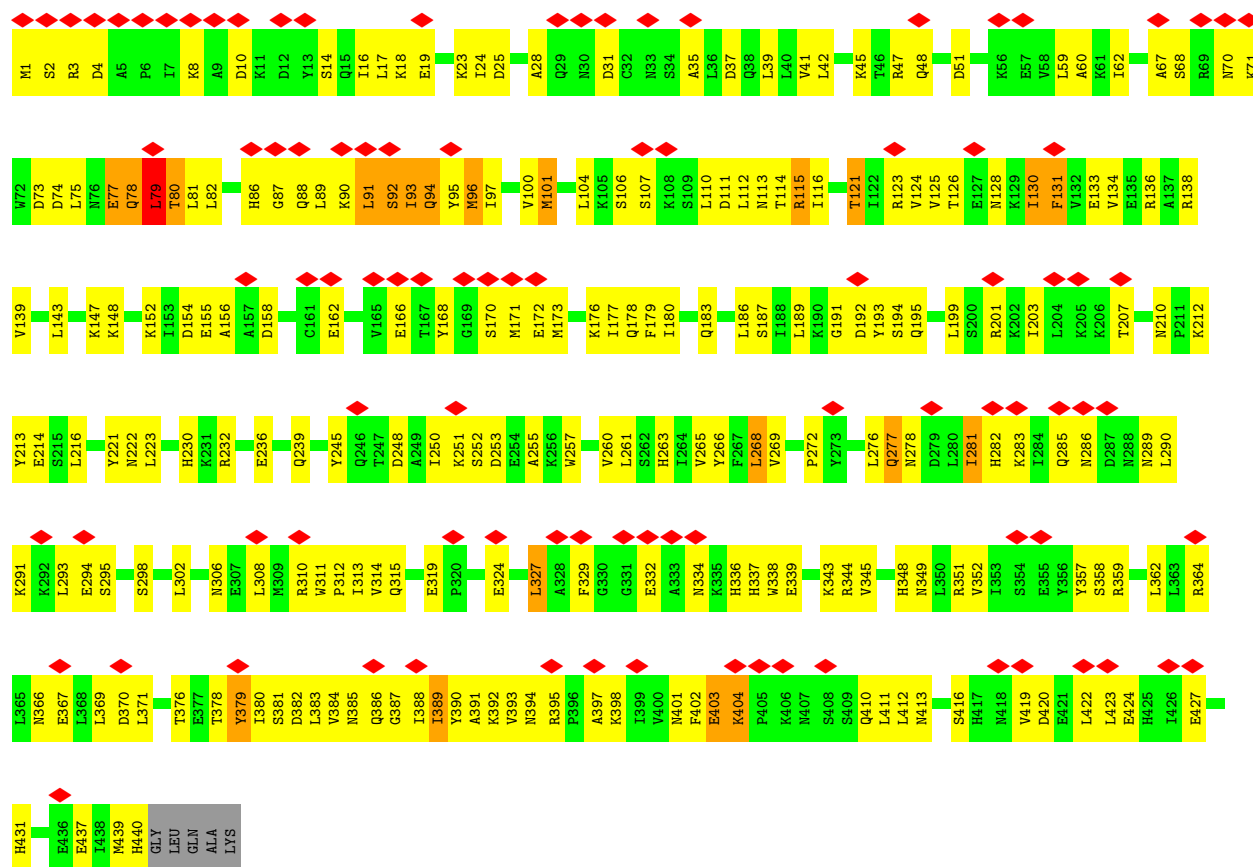


• Molecule 8: 26S proteasome regulatory subunit RPN3

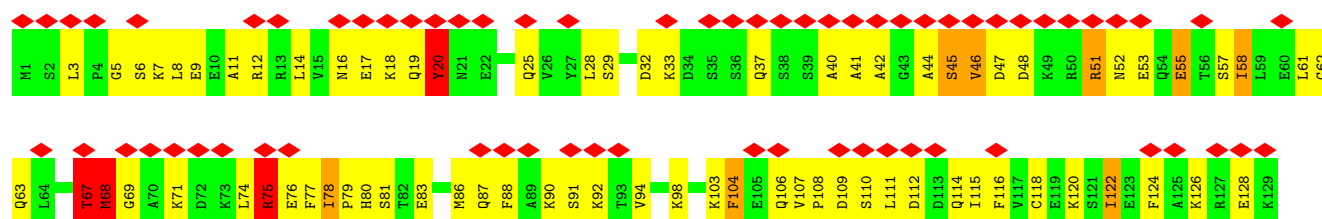
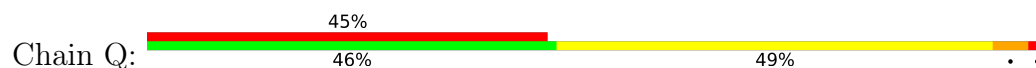


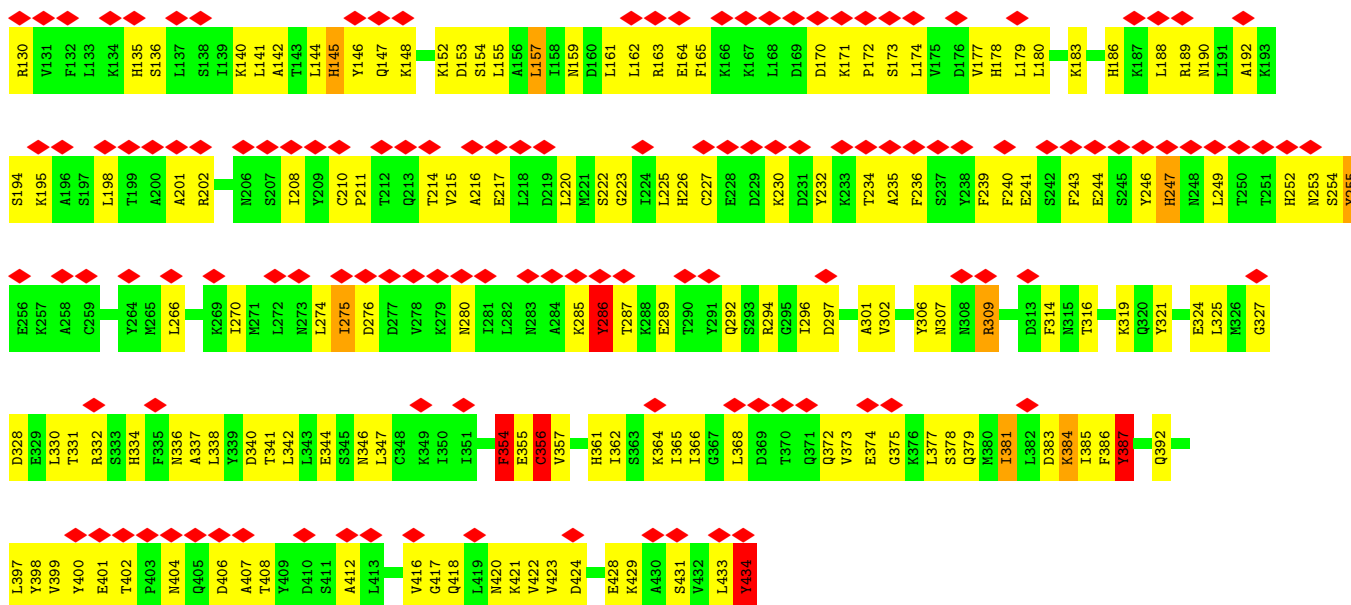


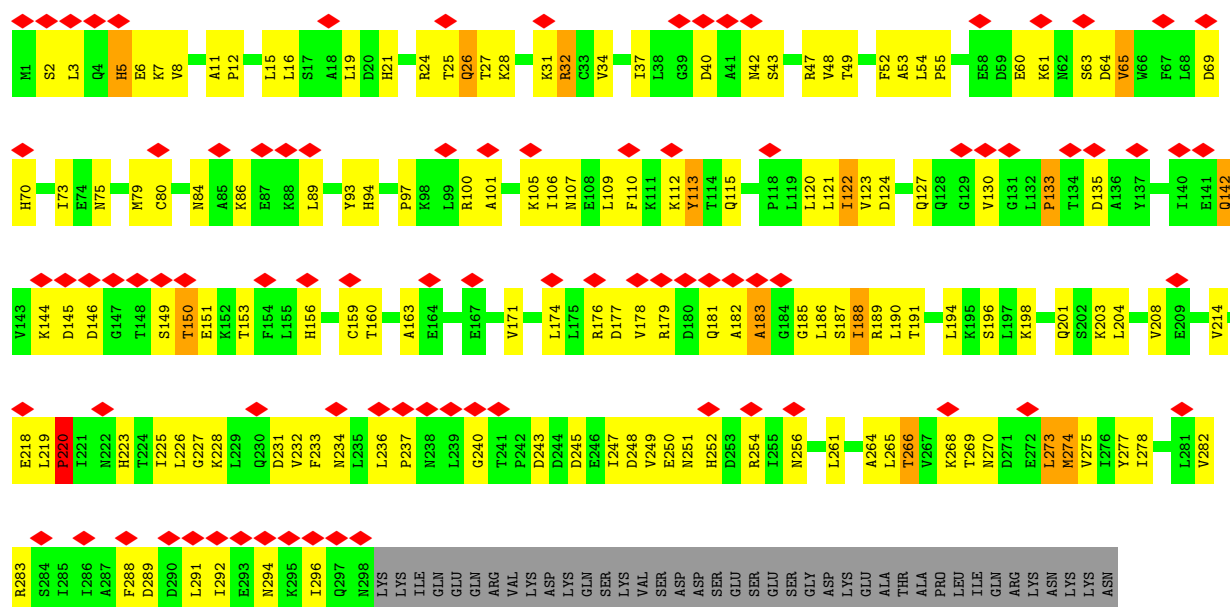
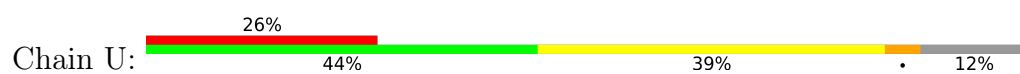
• Molecule 9: 26S proteasome regulatory subunit RPN5



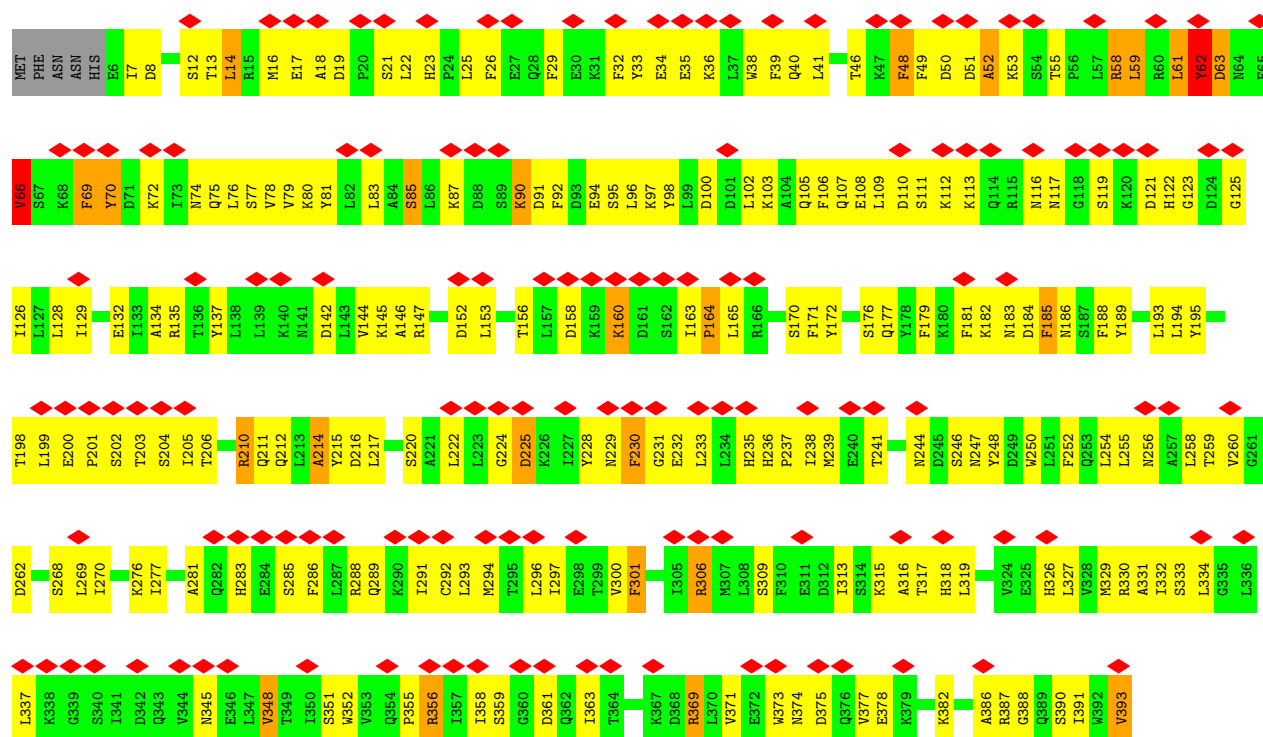
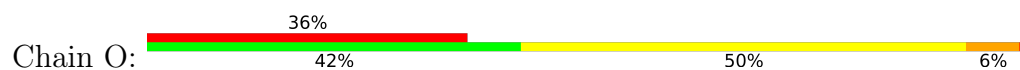
• Molecule 10: 26S proteasome regulatory subunit RPN6







• Molecule 13: 26S proteasome regulatory subunit RPN9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	193337	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.092	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	W	2.27	60/1557 (3.9%)	2.38	94/2111 (4.5%)
2	V	2.12	65/2309 (2.8%)	2.25	127/3115 (4.1%)
3	T	2.15	79/2235 (3.5%)	2.46	152/3017 (5.0%)
4	X	2.31	47/1058 (4.4%)	2.34	68/1432 (4.7%)
5	Y	2.27	18/438 (4.1%)	2.17	19/583 (3.3%)
6	Z	2.18	245/7122 (3.4%)	2.41	450/9645 (4.7%)
7	N	2.19	251/6994 (3.6%)	2.33	403/9455 (4.3%)
8	S	2.30	151/3966 (3.8%)	2.47	306/5355 (5.7%)
9	P	2.25	127/3663 (3.5%)	2.32	211/4940 (4.3%)
10	Q	2.20	120/3556 (3.4%)	2.43	234/4787 (4.9%)
11	R	2.33	106/3110 (3.4%)	2.41	186/4193 (4.4%)
12	U	2.17	89/2407 (3.7%)	2.36	137/3258 (4.2%)
13	O	2.17	113/3247 (3.5%)	2.33	179/4380 (4.1%)
All	All	2.21	1471/41662 (3.5%)	2.38	2566/56271 (4.6%)

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	W	0	2
2	V	0	7
3	T	0	9
4	X	0	7
5	Y	0	1
6	Z	0	19
7	N	0	13
8	S	0	10
9	P	0	5
10	Q	0	11
11	R	0	18
12	U	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	O	0	13
All	All	0	118

The worst 5 of 1471 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	99	TYR	CZ-OH	31.69	2.04	1.38
9	P	78	GLN	C-N	30.09	1.75	1.33
11	R	99	TYR	CE1-CZ	29.61	2.09	1.38
8	S	59	ASP	CA-CB	-27.78	1.10	1.53
8	S	127	THR	CA-CB	27.40	1.98	1.53

The worst 5 of 2566 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	99	TYR	CE1-CZ-OH	-22.86	51.30	119.90
13	O	62	TYR	CB-CA-C	-20.12	78.61	110.81
10	Q	77	PHE	CA-C-N	17.63	131.34	120.24
10	Q	77	PHE	C-N-CA	17.63	131.34	120.24
9	P	78	GLN	O-C-N	-17.38	99.48	122.59

There are no chirality outliers.

5 of 118 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	100	ARG	Sidechain
2	V	156	PHE	Sidechain
2	V	20	ARG	Sidechain
1	W	15	TYR	Sidechain
1	W	21	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1534	0	1542	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	2274	0	2273	25	0
3	T	2192	0	2161	7	0
4	X	1032	0	1017	4	0
5	Y	435	0	393	10	0
6	Z	7005	0	6932	75	0
7	N	6882	0	6959	25	0
8	S	3894	0	3938	23	0
9	P	3608	0	3693	21	0
10	Q	3499	0	3524	25	0
11	R	3060	0	3083	51	0
12	U	2373	0	2403	17	0
13	O	3186	0	3213	58	0
All	All	40974	0	41131	328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 328 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:78:GLN:C	9:P:79:LEU:N	1.75	1.41
11:R:99:TYR:CE1	11:R:99:TYR:CZ	2.09	1.39
8:S:127:THR:CB	8:S:127:THR:CA	1.98	1.37
11:R:99:TYR:CE1	11:R:99:TYR:OH	1.79	1.32
9:P:212:LYS:O	9:P:213:TYR:CD1	1.92	1.22

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	195/268 (73%)	179 (92%)	12 (6%)	4 (2%)	5	30
2	V	287/306 (94%)	263 (92%)	18 (6%)	6 (2%)	5	30
3	T	264/274 (96%)	236 (89%)	21 (8%)	7 (3%)	4	25
4	X	125/156 (80%)	107 (86%)	12 (10%)	6 (5%)	2	16
5	Y	47/89 (53%)	43 (92%)	3 (6%)	1 (2%)	5	30
6	Z	902/993 (91%)	820 (91%)	55 (6%)	27 (3%)	3	22
7	N	886/945 (94%)	849 (96%)	30 (3%)	7 (1%)	16	53
8	S	473/523 (90%)	436 (92%)	24 (5%)	13 (3%)	4	25
9	P	438/445 (98%)	408 (93%)	22 (5%)	8 (2%)	6	33
10	Q	432/434 (100%)	388 (90%)	26 (6%)	18 (4%)	2	17
11	R	377/429 (88%)	352 (93%)	17 (4%)	8 (2%)	5	30
12	U	296/338 (88%)	280 (95%)	11 (4%)	5 (2%)	7	35
13	O	386/393 (98%)	368 (95%)	16 (4%)	2 (0%)	24	63
All	All	5108/5593 (91%)	4729 (93%)	267 (5%)	112 (2%)	7	29

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	200	ASN
3	T	92	ASN
3	T	96	LEU
3	T	173	GLU
4	X	116	ALA

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	W	171/230 (74%)	165 (96%)	6 (4%)	32	53
2	V	253/268 (94%)	248 (98%)	5 (2%)	48	65
3	T	249/256 (97%)	243 (98%)	6 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	116/144 (81%)	114 (98%)	2 (2%)	53	67
5	Y	50/81 (62%)	49 (98%)	1 (2%)	48	65
6	Z	773/850 (91%)	754 (98%)	19 (2%)	42	62
7	N	745/797 (94%)	731 (98%)	14 (2%)	50	66
8	S	447/489 (91%)	440 (98%)	7 (2%)	55	69
9	P	412/415 (99%)	404 (98%)	8 (2%)	50	66
10	Q	391/391 (100%)	382 (98%)	9 (2%)	44	63
11	R	333/379 (88%)	322 (97%)	11 (3%)	33	55
12	U	271/308 (88%)	266 (98%)	5 (2%)	51	67
13	O	363/368 (99%)	353 (97%)	10 (3%)	38	59
All	All	4574/4976 (92%)	4471 (98%)	103 (2%)	44	63

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	S	105	PRO
10	Q	173	SER
13	O	153	LEU
8	S	487	THR
9	P	308	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
7	N	719	ASN
12	U	201	GLN
8	S	458	GLN
12	U	192	ASN
13	O	177	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	78:GLN	C	79:LEU	N	1.75

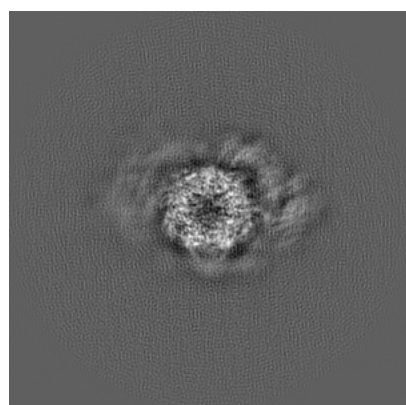
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3535. These allow visual inspection of the internal detail of the map and identification of artifacts.

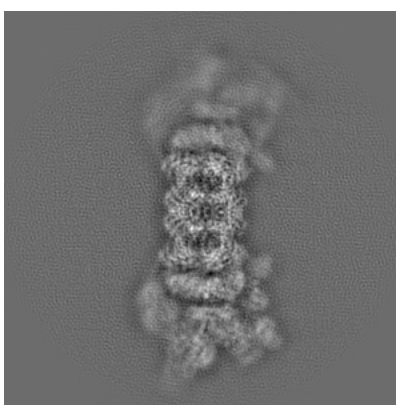
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

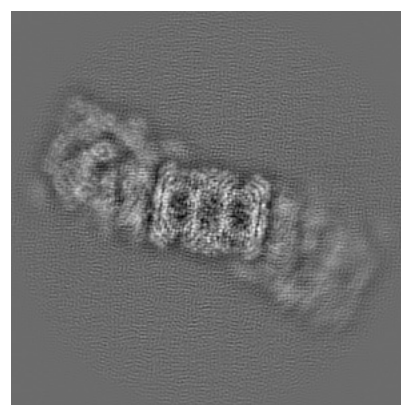
6.1.1 Primary map



X



Y

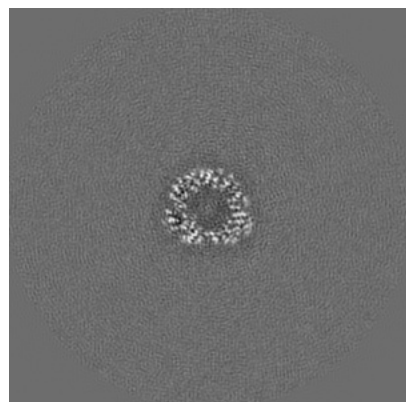


Z

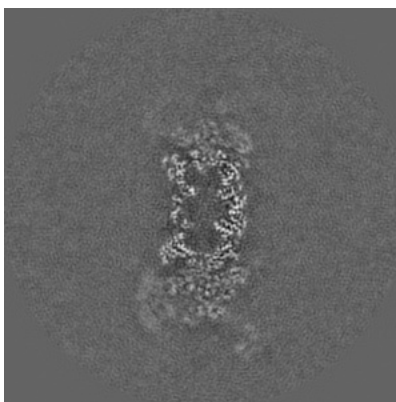
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

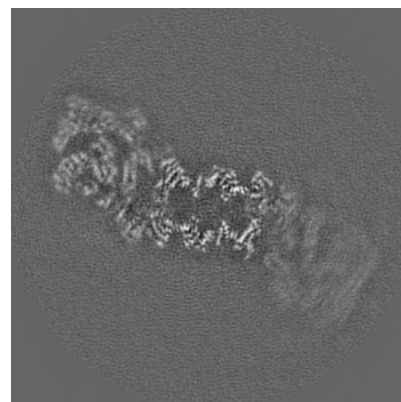
6.2.1 Primary map



X Index: 192



Y Index: 192

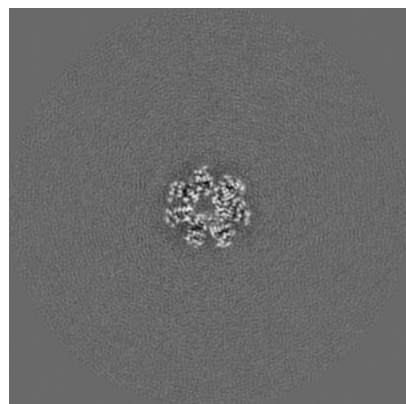


Z Index: 192

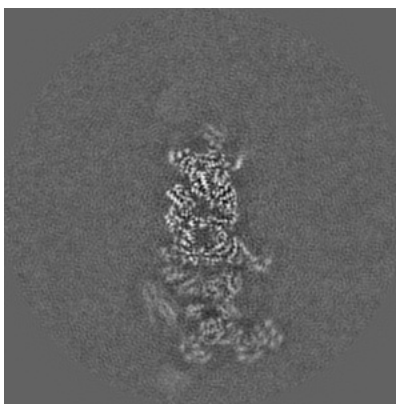
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

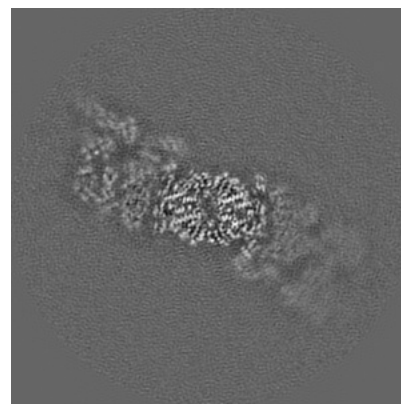
6.3.1 Primary map



X Index: 206



Y Index: 210

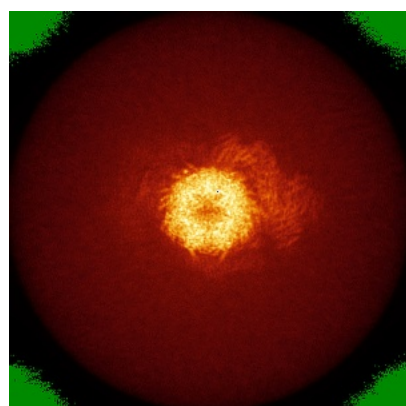


Z Index: 210

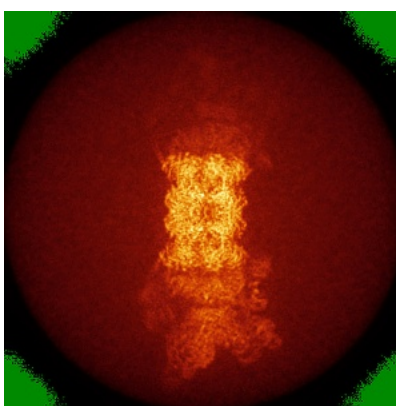
The images above show the largest variance slices of the map in three orthogonal directions.

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

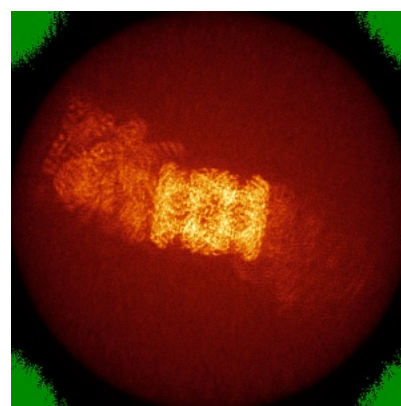
6.4.1 Primary map



X



Y

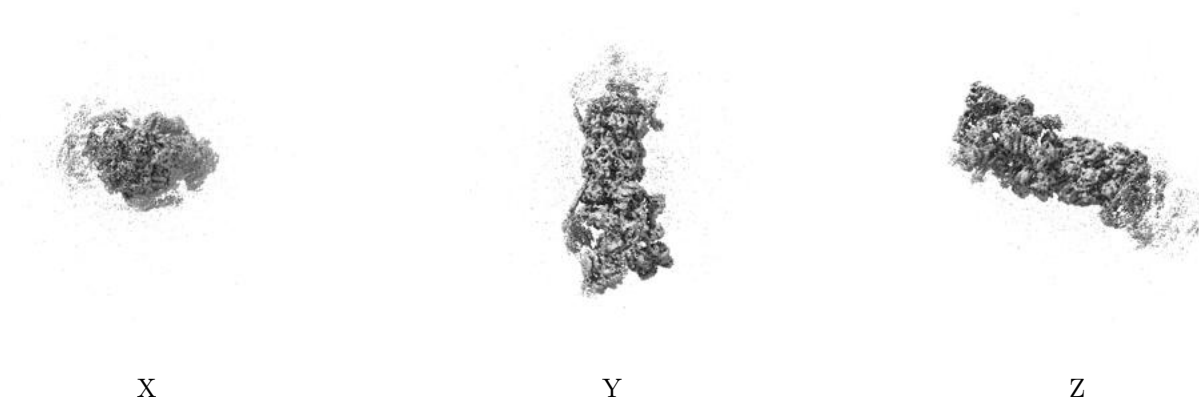


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

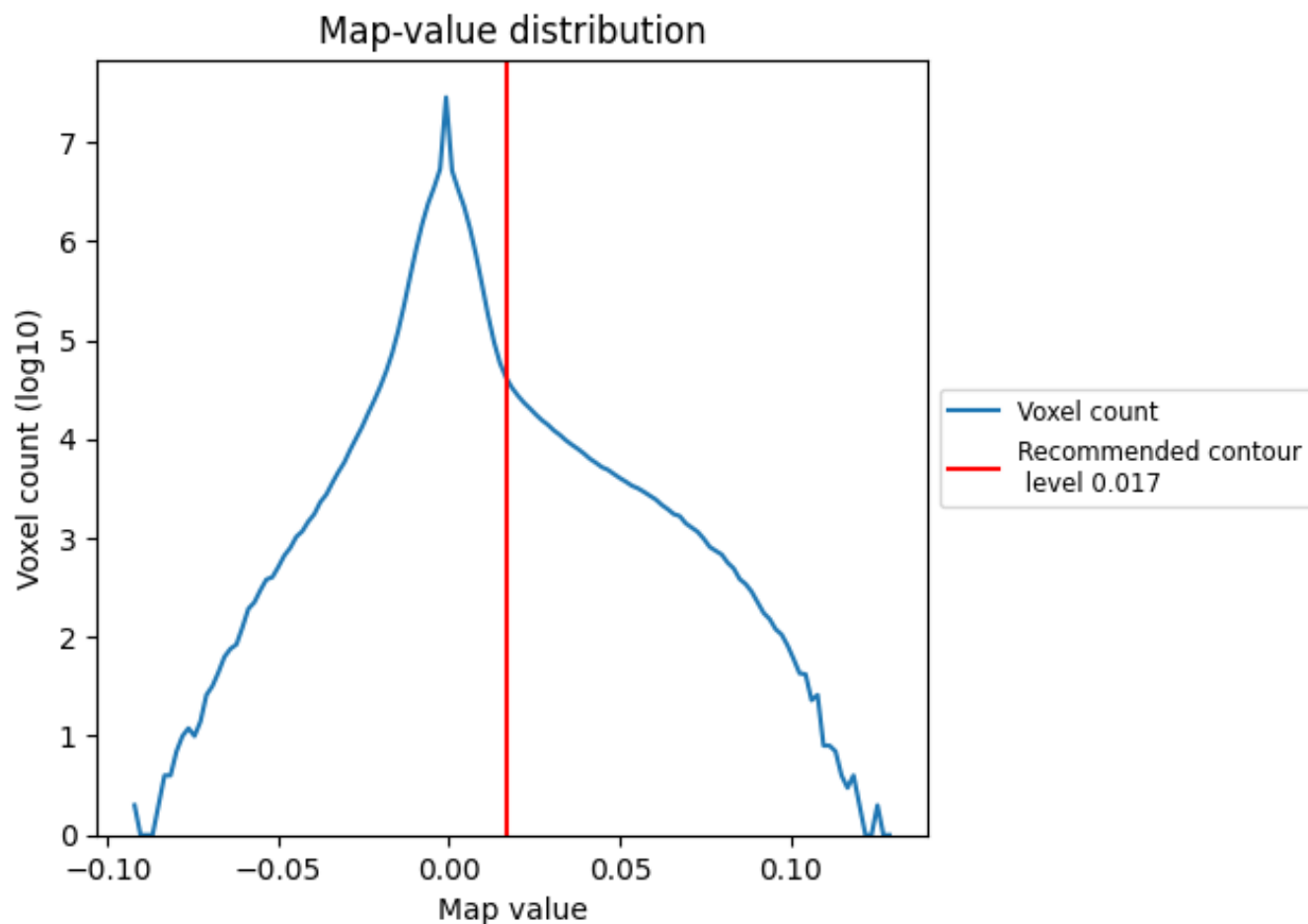
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

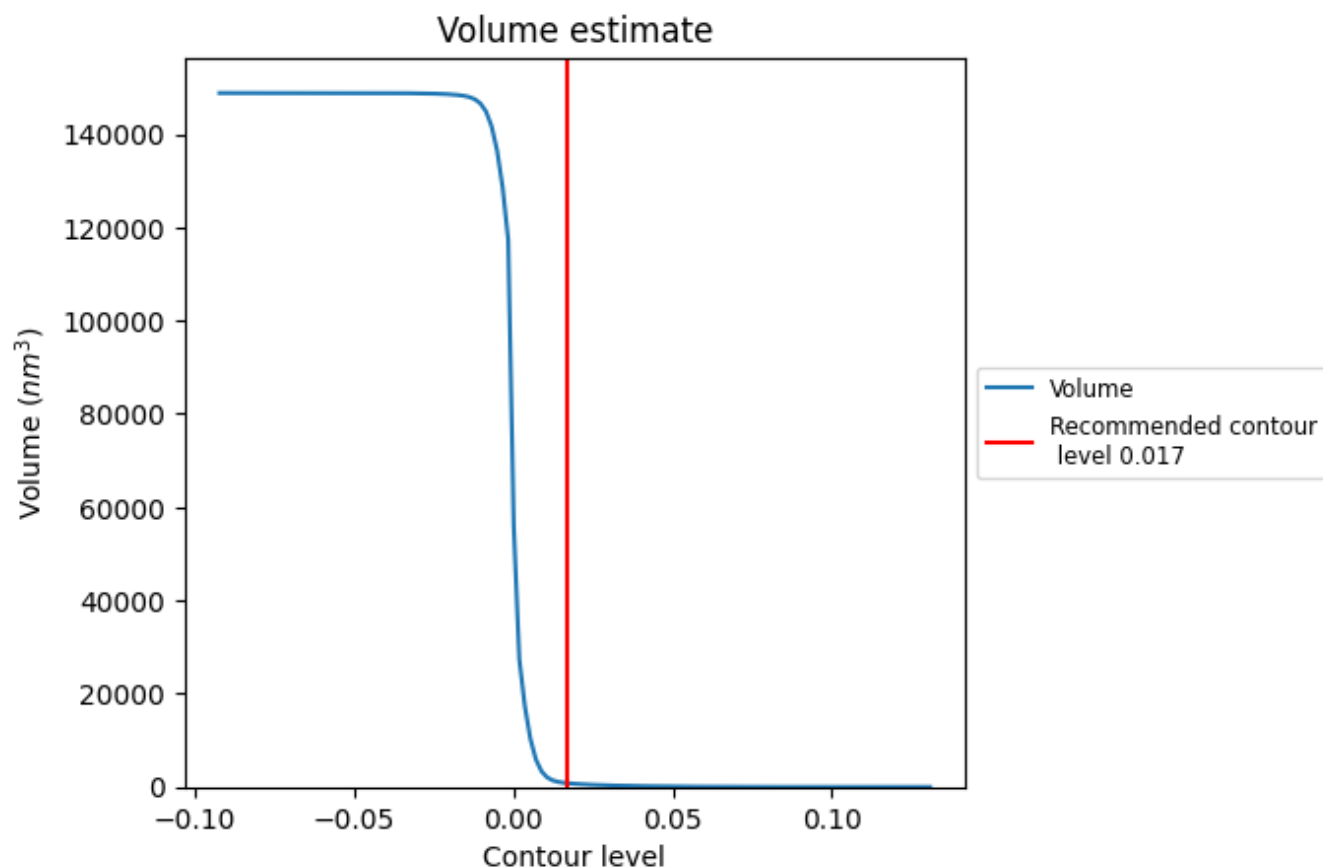
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

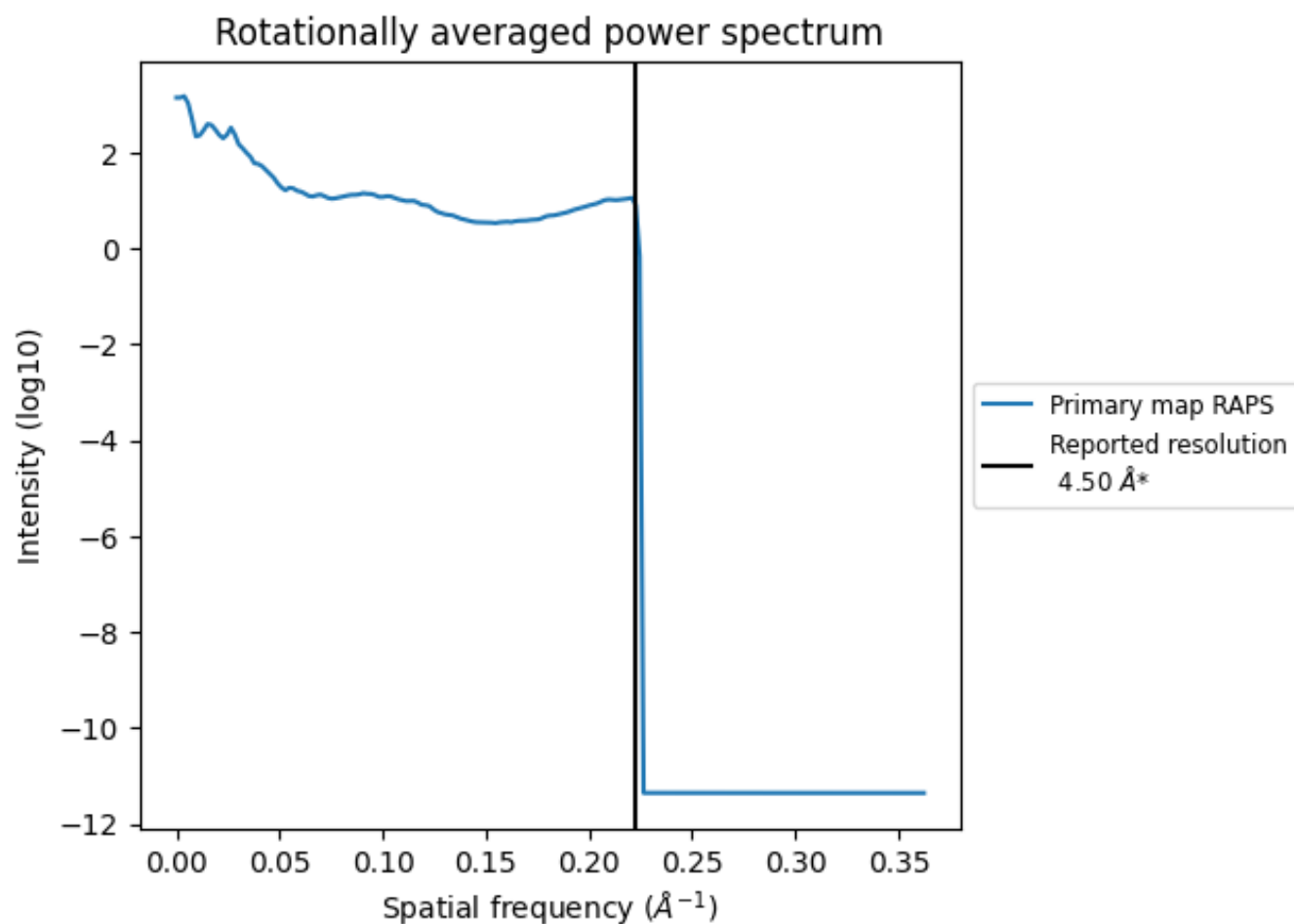
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 813 nm³; this corresponds to an approximate mass of 734 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 0.222 Å⁻¹

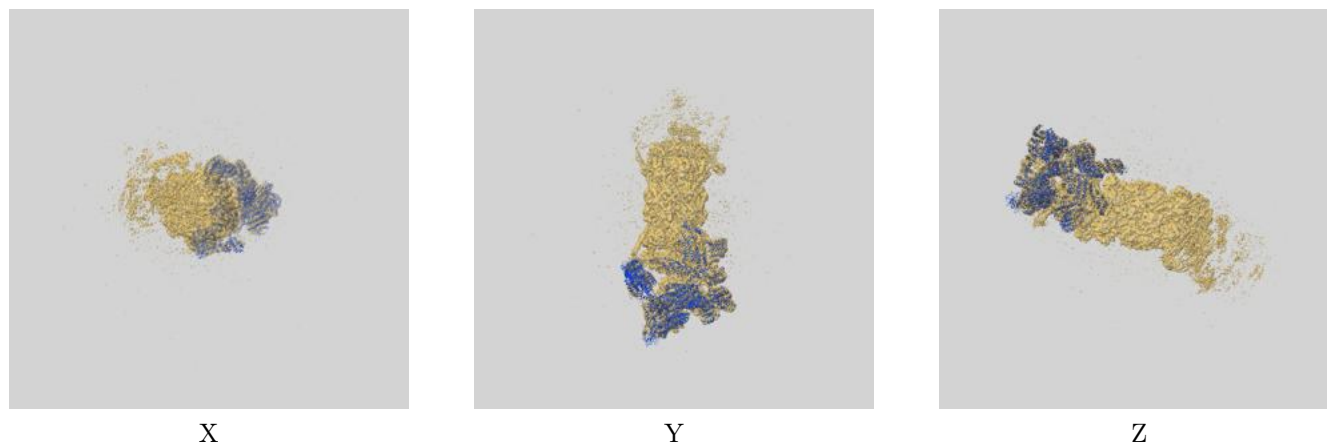
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

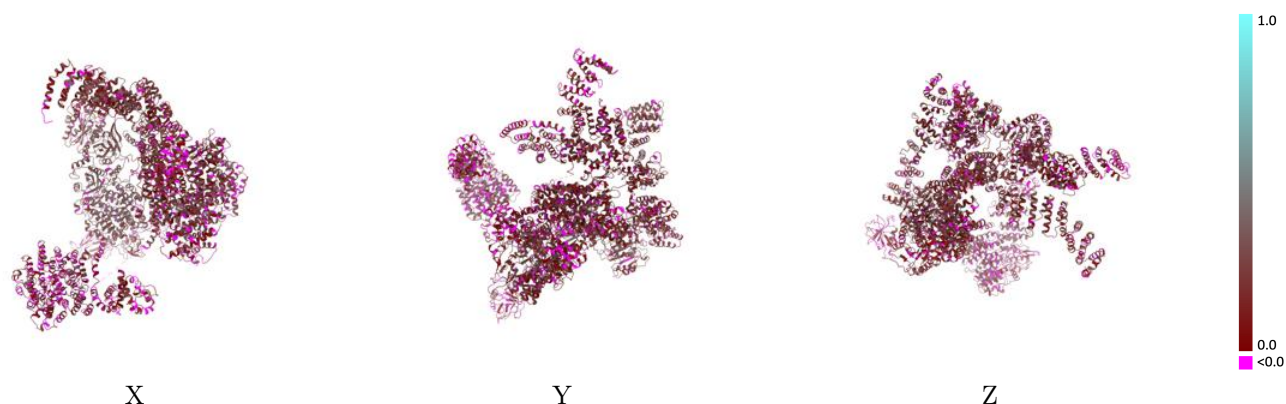
This section contains information regarding the fit between EMDB map EMD-3535 and PDB model 5MPE. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



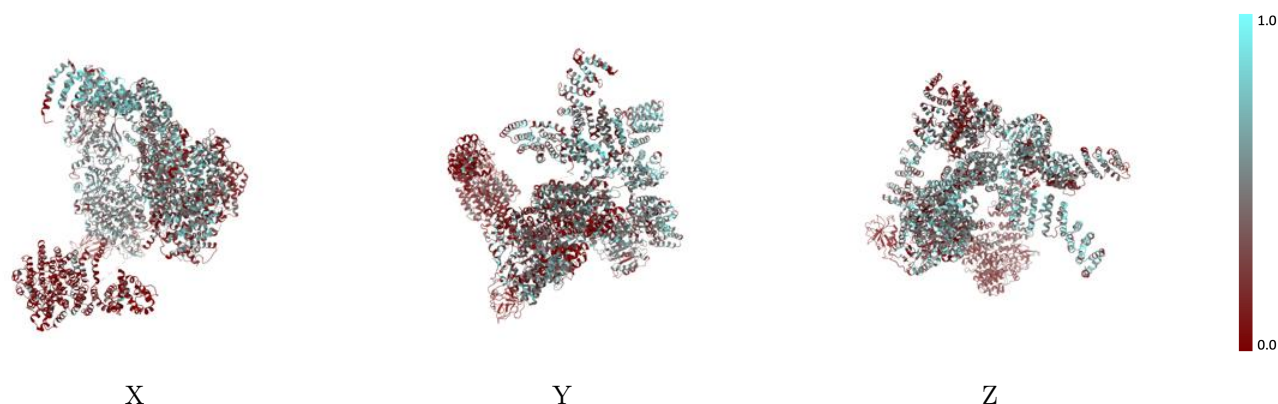
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



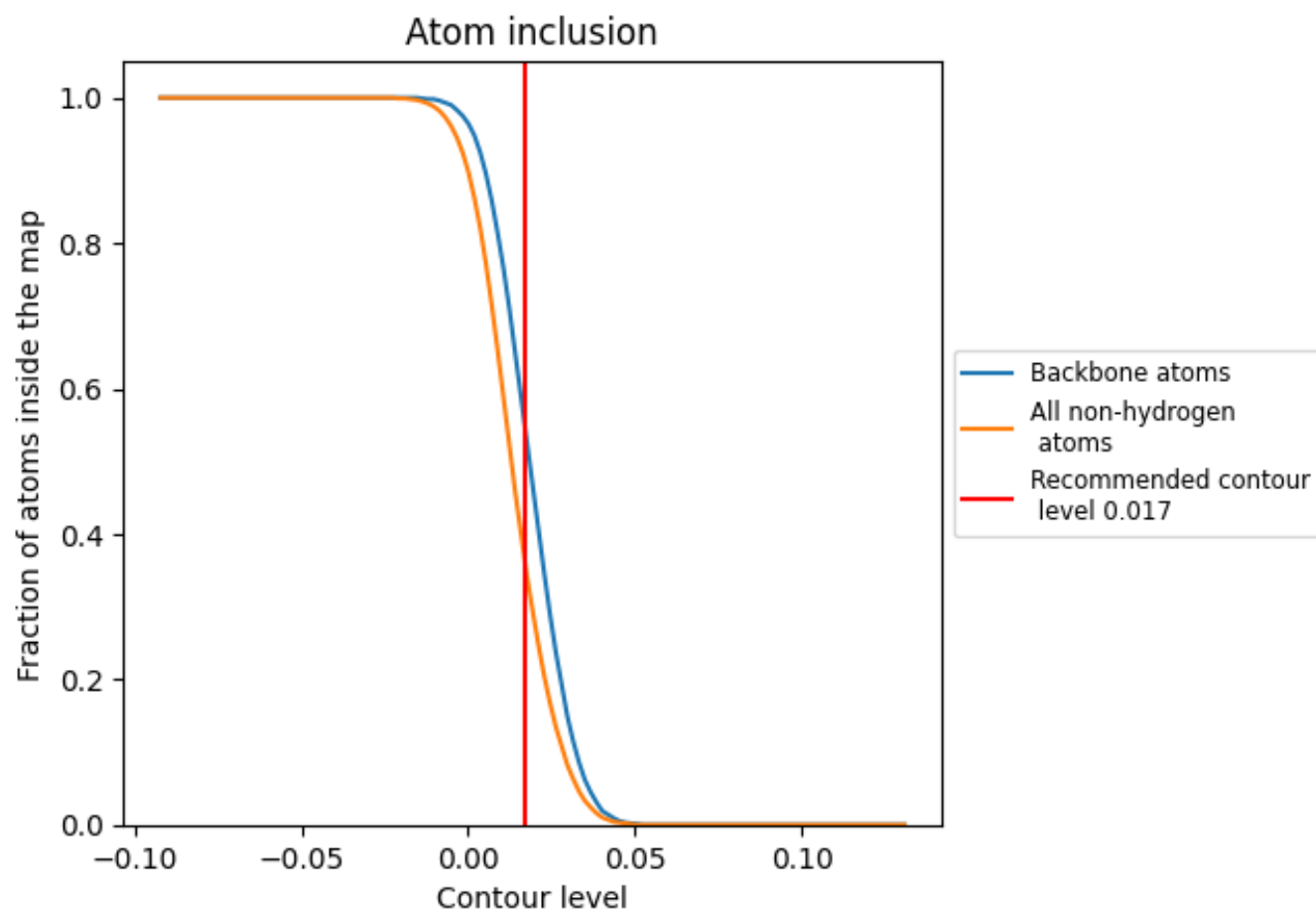
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 36% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3630	 0.1550
N	 0.4280	 0.1860
O	 0.4690	 0.1680
P	 0.5630	 0.1960
Q	 0.4330	 0.1430
R	 0.4580	 0.1670
S	 0.3410	 0.1390
T	 0.2140	 0.1130
U	 0.4780	 0.2160
V	 0.4870	 0.2080
W	 0.3990	 0.1820
X	 0.0170	 0.0660
Y	 0.2810	 0.1360
Z	 0.0980	 0.0930

