



# wwPDB EM Validation Summary Report ⓘ

Oct 24, 2022 – 06:24 PM EDT

PDB ID : 7NAN  
EMDB ID : EMD-24275  
Title : Human 20S proteasome core particle  
Authors : Zhao, J.; Makhija, S.; Huang, B.; Cheng, Y.  
Deposited on : 2021-06-22  
Resolution : 2.80 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](mailto: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>.

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

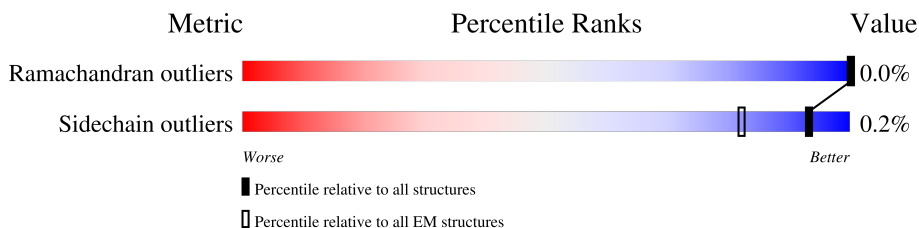
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.80 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.




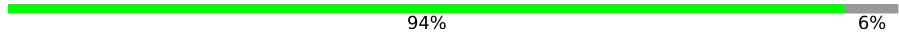
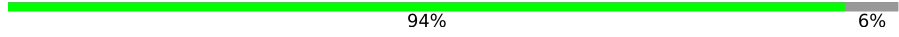
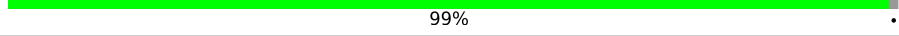
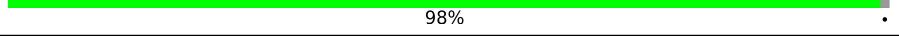


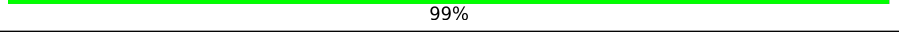
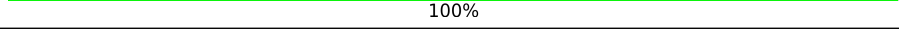
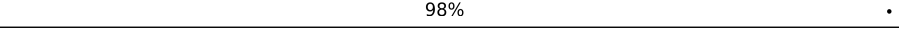
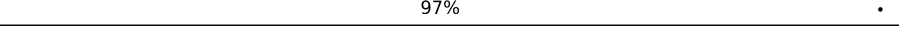
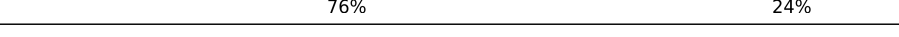

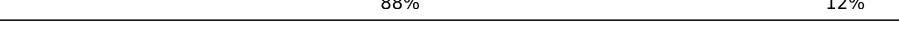


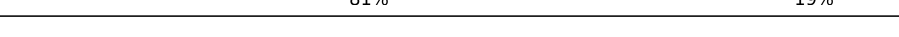

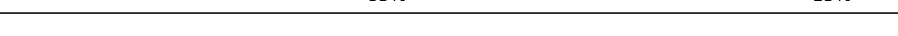
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	234	98% .
1	O	234	98% .
2	B	261	96% .
2	P	261	96% .
3	C	248	95% 5%
3	Q	248	95% 5%
4	D	241	98% .
4	R	241	98% .
5	E	263	90% 10%

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Mol	Chain	Length	Quality of chain
5	S	263	 90% 10%
6	F	255	 94% 6%
6	T	255	 94% 6%
7	G	246	 99% 1%
7	U	246	 98% 2%
8	H	277	 80% 20%
8	V	277	 80% 20%
9	I	205	 99% 1%
9	W	205	 100%
10	J	201	 98% 2%
10	X	201	 97% 3%
11	K	263	 76% 24%
11	Y	263	 76% 24%
12	L	241	 88% 12%
12	Z	241	 88% 12%
13	M	264	 81% 19%
13	a	264	 81% 19%
14	N	239	 85% 15%
14	b	239	 85% 15%

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 46360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	229	Total	C	N	O	S	0	0
			1665	1083	288	288	6		
1	O	229	Total	C	N	O	S	0	0
			1694	1097	296	295	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	250	Total	C	N	O	S	0	0
			1795	1146	322	317	10		
2	P	251	Total	C	N	O	S	0	0
			1850	1177	329	334	10		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	235	Total	C	N	O	S	0	0
			1694	1077	317	295	5		
3	Q	236	Total	C	N	O	S	0	0
			1719	1093	319	302	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	235	Total	C	N	O	S	0	0
			1699	1079	292	317	11		
4	R	235	Total	C	N	O	S	0	0
			1688	1073	292	312	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	238	1794	1134	330	319	11	0	0
5	S	237	1759	1120	329	299	11	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	240	1783	1145	315	313	10	0	0
6	T	239	1784	1144	315	315	10	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	243	1781	1138	308	323	12	0	0
7	U	243	1781	1139	307	323	12	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	222	1604	1020	276	297	11	0	0
8	V	222	1618	1027	275	306	10	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	204	1563	1001	264	279	19	0	0
9	W	204	1559	1000	264	277	18	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	197	1541	996	265	271	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	196	1531	988	264	271	8	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	200	1525	968	273	275	9	0	0
11	Y	200	1522	966	272	275	9	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	213	1604	1025	280	289	10	0	0
12	Z	213	1593	1022	281	280	10	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-4.

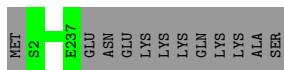
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	215	1635	1038	288	297	12	0	0
13	a	214	1624	1033	288	291	12	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	202	1485	935	258	281	11	0	0
14	b	202	1470	929	257	272	12	0	0

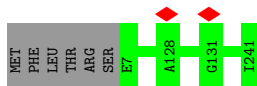


Chain Q:  95% 5%



- Molecule 4: Proteasome subunit alpha type-5

Chain D:  98%




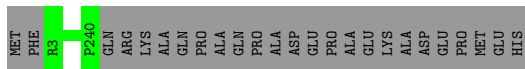
- Molecule 4: Proteasome subunit alpha type-5

Chain R:  98%




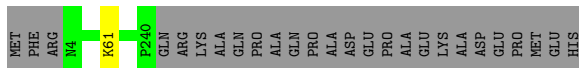
- Molecule 5: Proteasome subunit alpha type-1

Chain E:  90% 10%



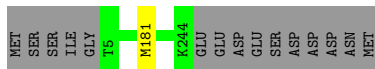
- Molecule 5: Proteasome subunit alpha type-1

Chain S:  90% 10%



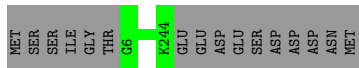
- Molecule 6: Proteasome subunit alpha type-3

Chain F:  94% 6%



- Molecule 6: Proteasome subunit alpha type-3

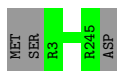
Chain T:  94% 6%



- Molecule 7: Proteasome subunit alpha type-6



Chain G:  99%




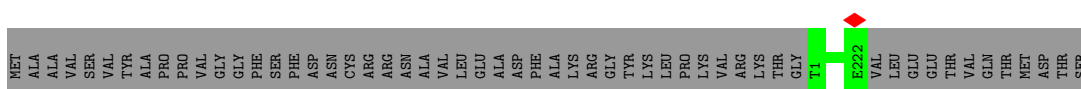
- Molecule 7: Proteasome subunit alpha type-6

Chain U:  98%




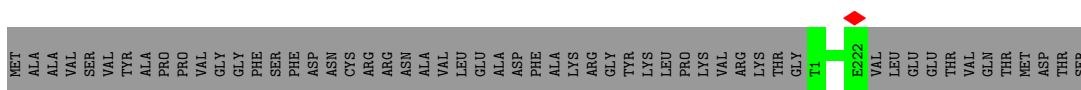
- Molecule 8: Proteasome subunit beta type-7

Chain H:  80%



- Molecule 8: Proteasome subunit beta type-7

Chain V:  80%



- Molecule 9: Proteasome subunit beta type-3

Chain I:  99%



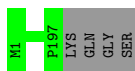
- Molecule 9: Proteasome subunit beta type-3

Chain W:  100%



- Molecule 10: Proteasome subunit beta type-2

Chain J:  98%




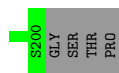
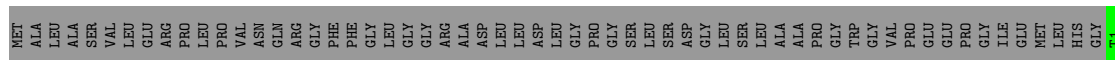
- Molecule 10: Proteasome subunit beta type-2

Chain X:  97%




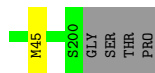
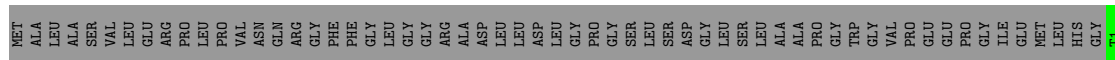
- Molecule 11: Proteasome subunit beta type-5

Chain K:  76% 24%




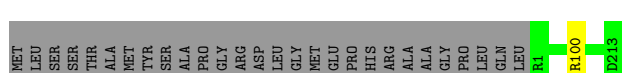
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  76% 24%




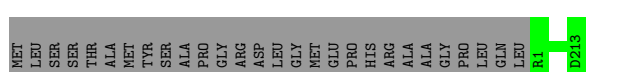
- Molecule 12: Proteasome subunit beta type-1

Chain L:  88% 12%




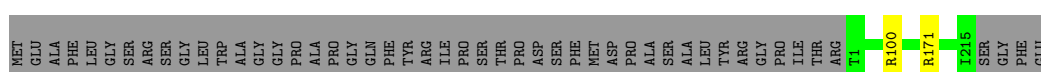
- Molecule 12: Proteasome subunit beta type-1

Chain Z:  88% 12%




- Molecule 13: Proteasome subunit beta type-4

Chain M:  81% 19%



- Molecule 13: Proteasome subunit beta type-4

Chain a:  81% 19%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	499629	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	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	30.094	Depositor
Minimum map value	-13.549	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	388.992, 388.992, 388.992	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.47	0/1704	0.53	0/2322
1	O	0.48	0/1733	0.53	0/2358
2	B	0.42	0/1824	0.53	0/2482
2	P	0.43	0/1879	0.53	0/2550
3	C	0.44	0/1719	0.56	0/2341
3	Q	0.43	0/1745	0.58	0/2375
4	D	0.42	0/1725	0.51	0/2342
4	R	0.41	0/1714	0.51	0/2327
5	E	0.44	0/1829	0.58	0/2484
5	S	0.43	0/1794	0.57	0/2436
6	F	0.46	0/1818	0.55	0/2461
6	T	0.46	0/1819	0.55	0/2462
7	G	0.46	0/1813	0.51	0/2464
7	U	0.45	0/1813	0.51	0/2464
8	H	0.48	0/1631	0.59	0/2217
8	V	0.48	0/1645	0.57	0/2235
9	I	0.50	0/1592	0.56	0/2149
9	W	0.50	0/1588	0.55	0/2144
10	J	0.50	0/1574	0.56	0/2134
10	X	0.52	0/1563	0.57	0/2119
11	K	0.53	0/1556	0.60	0/2104
11	Y	0.51	0/1553	0.61	1/2102 (0.0%)
12	L	0.49	0/1634	0.57	0/2206
12	Z	0.48	0/1623	0.56	0/2192
13	M	0.52	0/1668	0.62	1/2263 (0.0%)
13	a	0.50	0/1657	0.60	0/2248
14	N	0.50	0/1511	0.54	0/2049
14	b	0.51	0/1496	0.54	0/2029
All	All	0.47	0/47220	0.56	2/64059 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	45	MET	C-N-CA	6.95	139.06	121.70
13	M	171	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	227/234 (97%)	226 (100%)	1 (0%)	0	100	100
1	O	227/234 (97%)	227 (100%)	0	0	100	100
2	B	248/261 (95%)	245 (99%)	3 (1%)	0	100	100
2	P	249/261 (95%)	246 (99%)	3 (1%)	0	100	100
3	C	233/248 (94%)	229 (98%)	4 (2%)	0	100	100
3	Q	234/248 (94%)	229 (98%)	5 (2%)	0	100	100
4	D	233/241 (97%)	227 (97%)	6 (3%)	0	100	100
4	R	233/241 (97%)	227 (97%)	6 (3%)	0	100	100
5	E	236/263 (90%)	232 (98%)	4 (2%)	0	100	100
5	S	235/263 (89%)	228 (97%)	6 (3%)	1 (0%)	34	66
6	F	238/255 (93%)	236 (99%)	2 (1%)	0	100	100
6	T	237/255 (93%)	232 (98%)	5 (2%)	0	100	100
7	G	241/246 (98%)	235 (98%)	6 (2%)	0	100	100
7	U	241/246 (98%)	236 (98%)	5 (2%)	0	100	100
8	H	220/277 (79%)	213 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/277 (79%)	215 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	194/201 (96%)	190 (98%)	4 (2%)	0	100	100
11	K	198/263 (75%)	193 (98%)	5 (2%)	0	100	100
11	Y	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
12	L	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
12	Z	211/241 (88%)	209 (99%)	2 (1%)	0	100	100
13	M	213/264 (81%)	207 (97%)	6 (3%)	0	100	100
13	a	212/264 (80%)	205 (97%)	7 (3%)	0	100	100
14	N	200/239 (84%)	197 (98%)	3 (2%)	0	100	100
14	b	200/239 (84%)	199 (100%)	1 (0%)	0	100	100
All	All	6188/6876 (90%)	6067 (98%)	120 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	S	61	LYS

### 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	A	151/191 (79%)	151 (100%)	0	100	100
1	O	158/191 (83%)	158 (100%)	0	100	100
2	B	159/221 (72%)	159 (100%)	0	100	100
2	P	173/221 (78%)	173 (100%)	0	100	100
3	C	149/211 (71%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	156/211 (74%)	156 (100%)	0	100	100
4	D	167/203 (82%)	167 (100%)	0	100	100
4	R	162/203 (80%)	162 (100%)	0	100	100
5	E	179/224 (80%)	179 (100%)	0	100	100
5	S	169/224 (75%)	169 (100%)	0	100	100
6	F	166/212 (78%)	165 (99%)	1 (1%)	86	96
6	T	168/212 (79%)	168 (100%)	0	100	100
7	G	174/210 (83%)	174 (100%)	0	100	100
7	U	171/210 (81%)	170 (99%)	1 (1%)	86	96
8	H	164/228 (72%)	164 (100%)	0	100	100
8	V	167/228 (73%)	167 (100%)	0	100	100
9	I	164/174 (94%)	163 (99%)	1 (1%)	86	96
9	W	162/174 (93%)	162 (100%)	0	100	100
10	J	156/171 (91%)	156 (100%)	0	100	100
10	X	155/171 (91%)	154 (99%)	1 (1%)	86	96
11	K	146/202 (72%)	146 (100%)	0	100	100
11	Y	144/202 (71%)	144 (100%)	0	100	100
12	L	163/199 (82%)	162 (99%)	1 (1%)	86	96
12	Z	160/199 (80%)	160 (100%)	0	100	100
13	M	164/215 (76%)	163 (99%)	1 (1%)	86	96
13	a	161/215 (75%)	160 (99%)	1 (1%)	86	96
14	N	148/181 (82%)	148 (100%)	0	100	100
14	b	143/181 (79%)	143 (100%)	0	100	100
All	All	4499/5684 (79%)	4492 (100%)	7 (0%)	93	98

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	100	ARG
7	U	131	MET
13	a	100	ARG
10	X	62	LYS
12	L	100	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	110	GLN
4	R	204	GLN
13	a	2	GLN
5	E	21	GLN
2	B	20	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

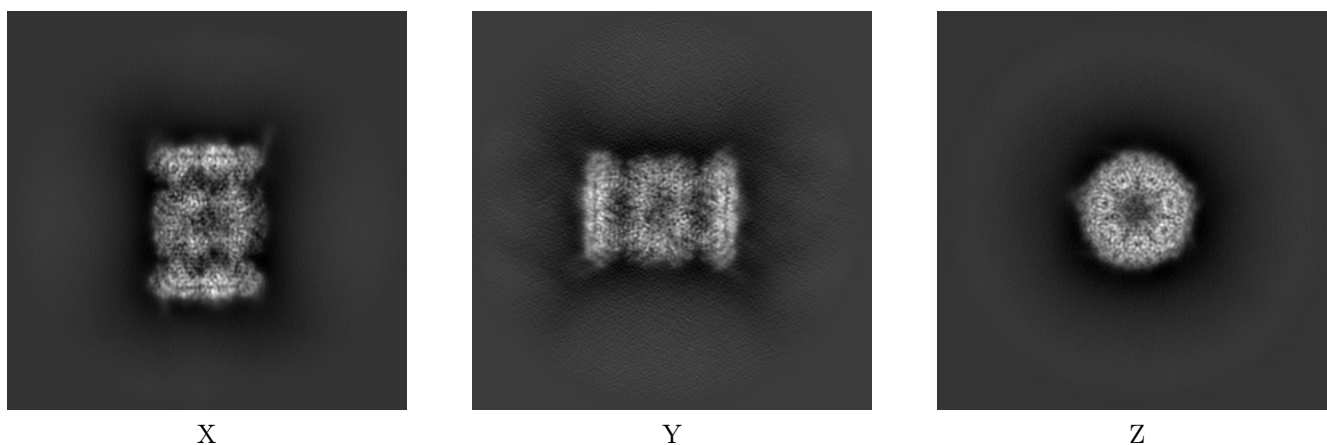
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24275. 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](#)

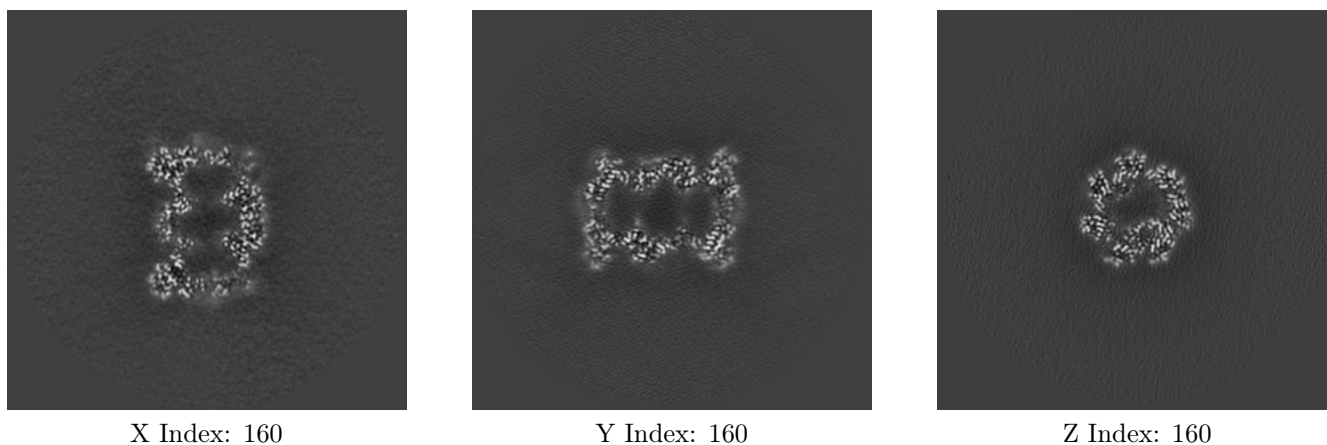
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

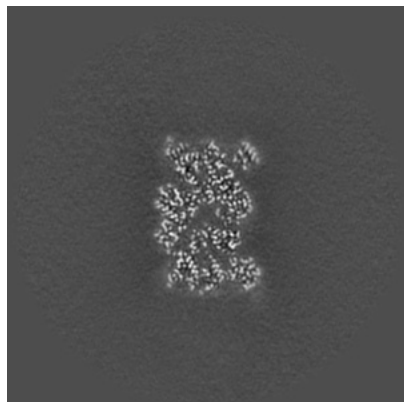
#### 6.2.1 Primary map



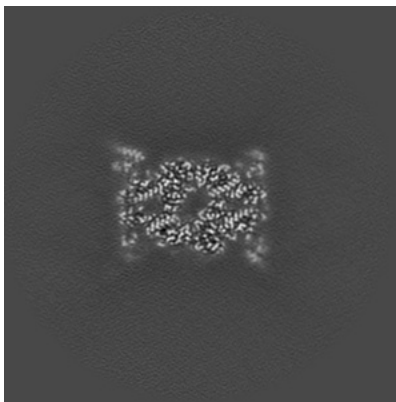
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

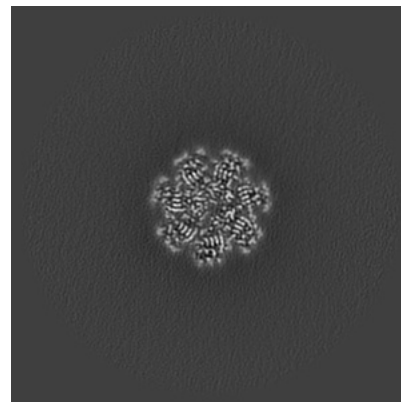
### 6.3.1 Primary map



X Index: 180



Y Index: 179

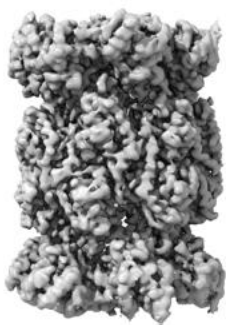


Z Index: 197

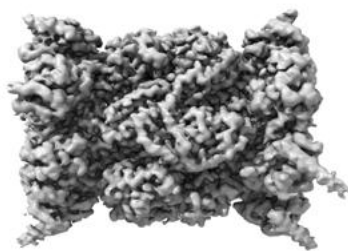
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

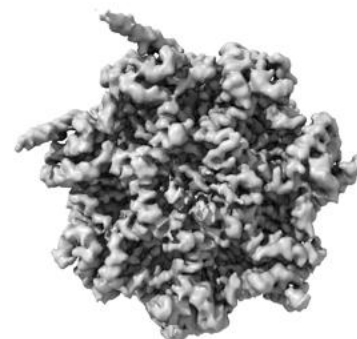
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

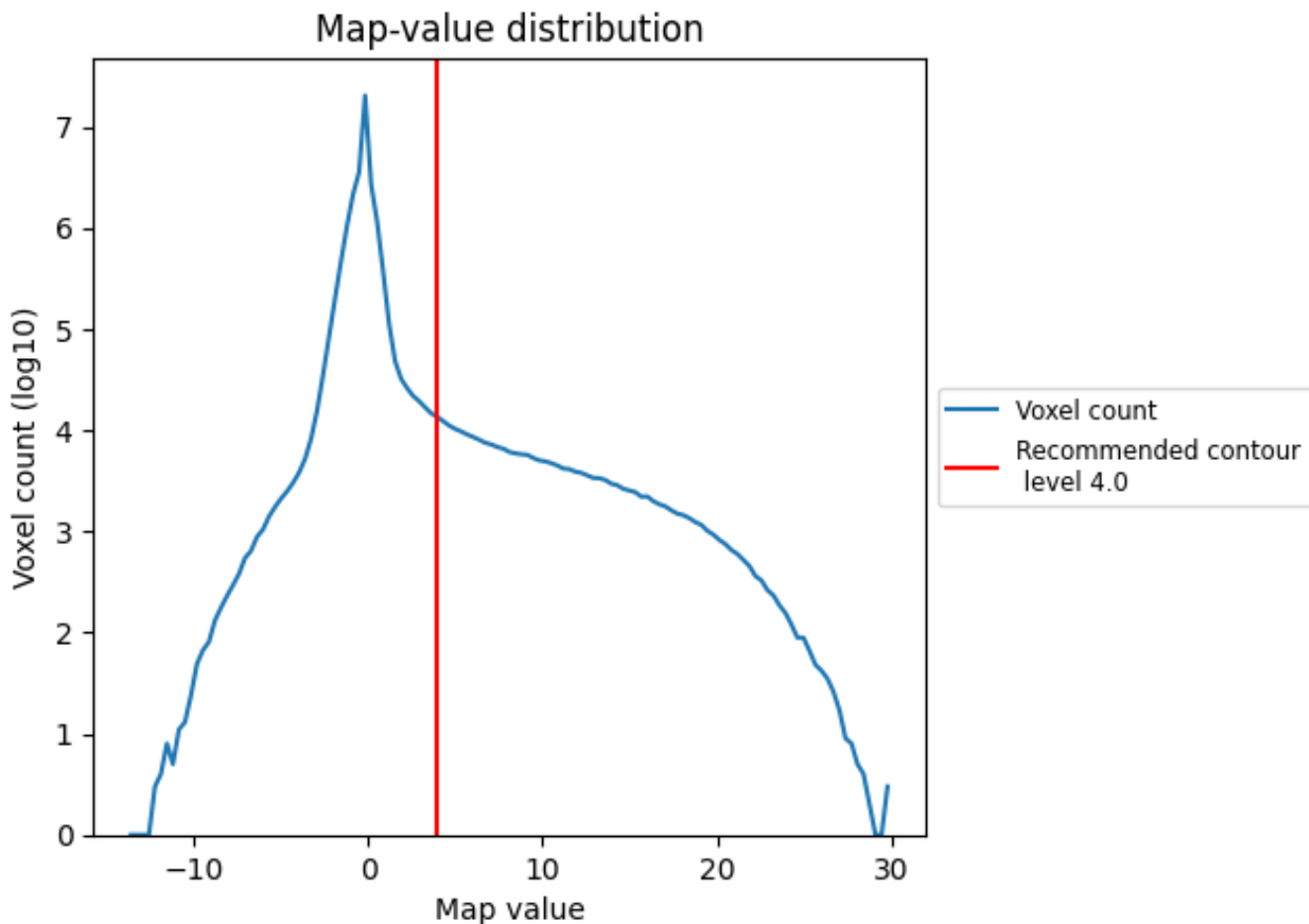
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

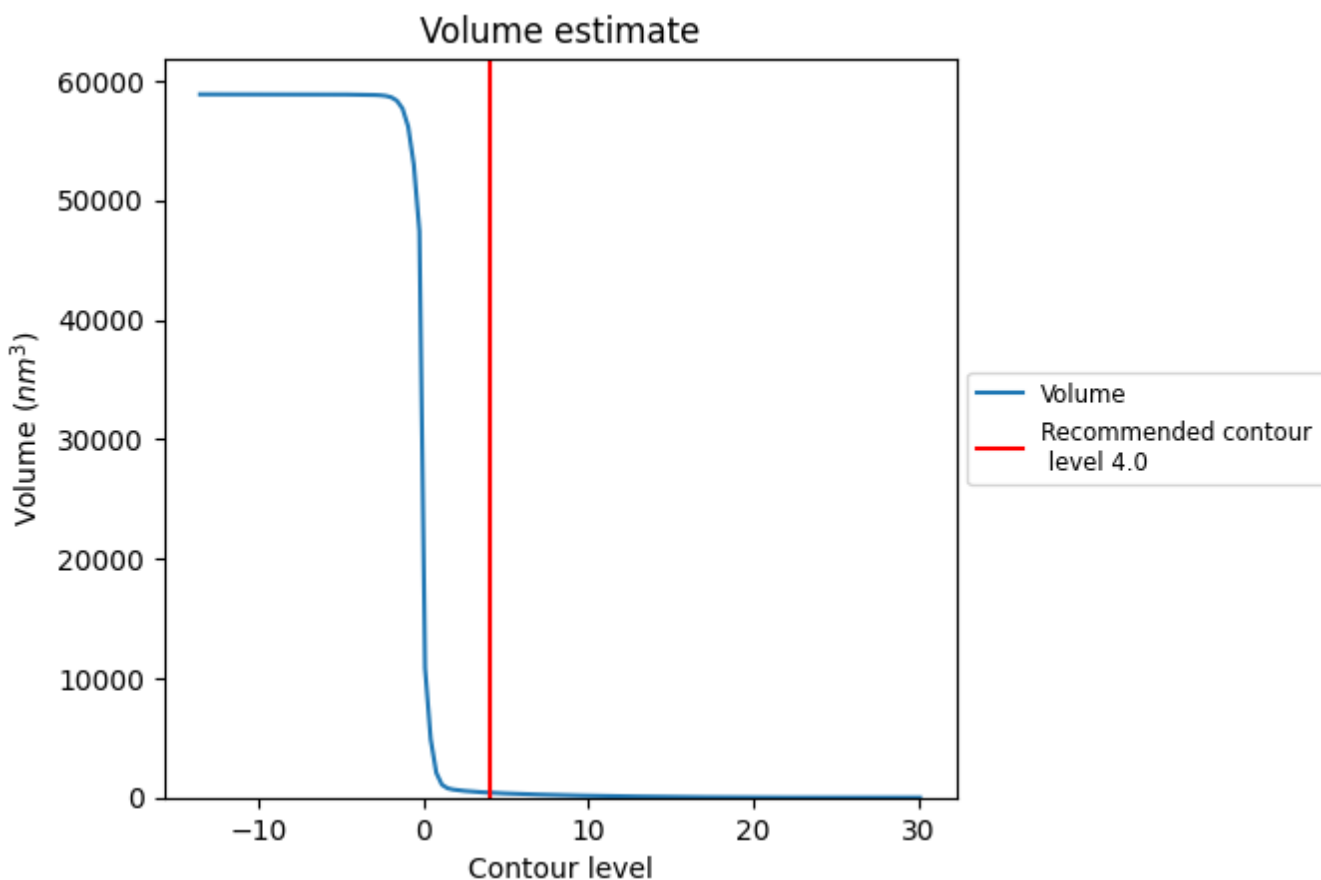
This section contains the results of statistical analysis of the map.

### 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.

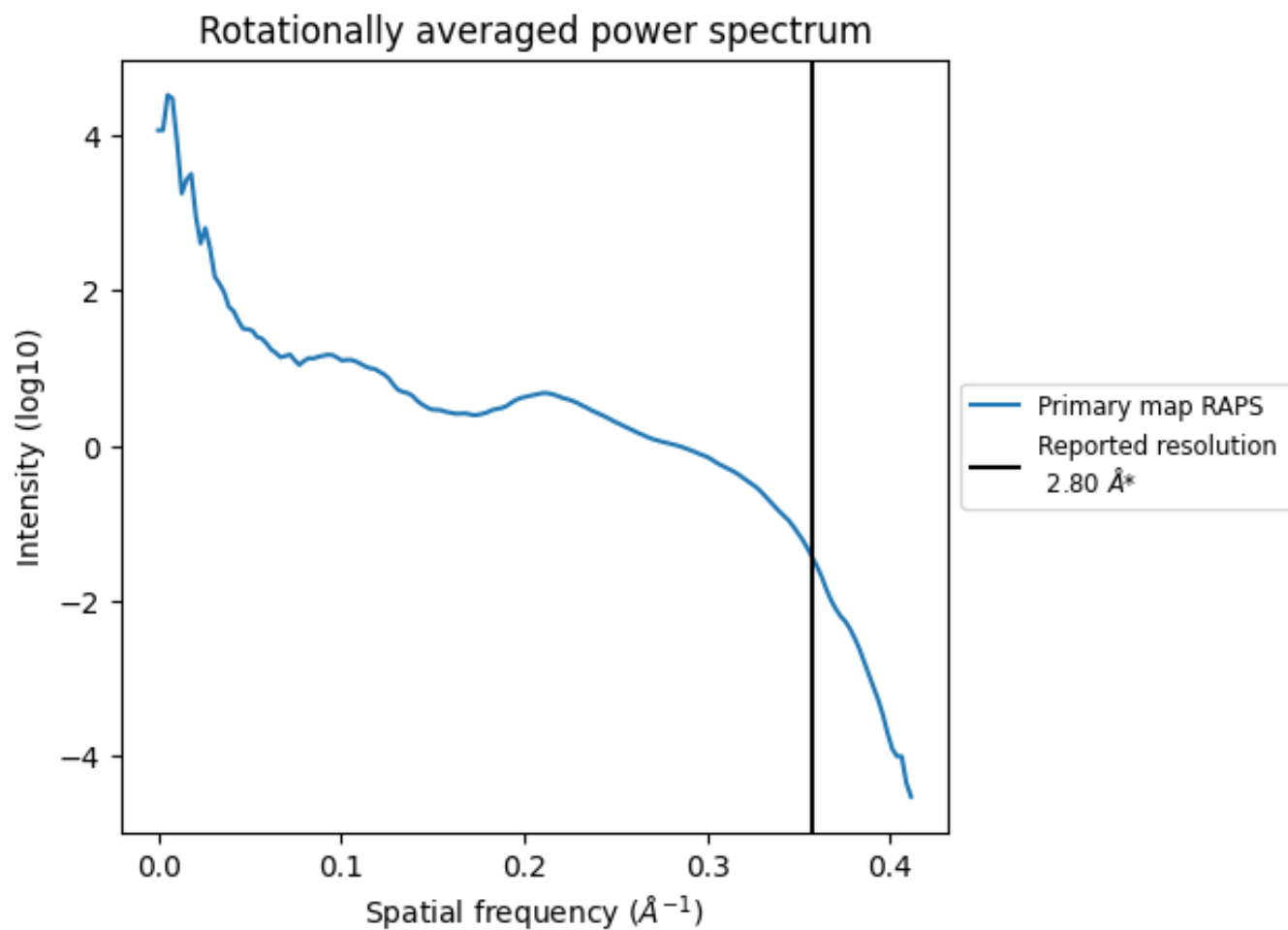
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 408 nm<sup>3</sup>; this corresponds to an approximate mass of 369 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](#)

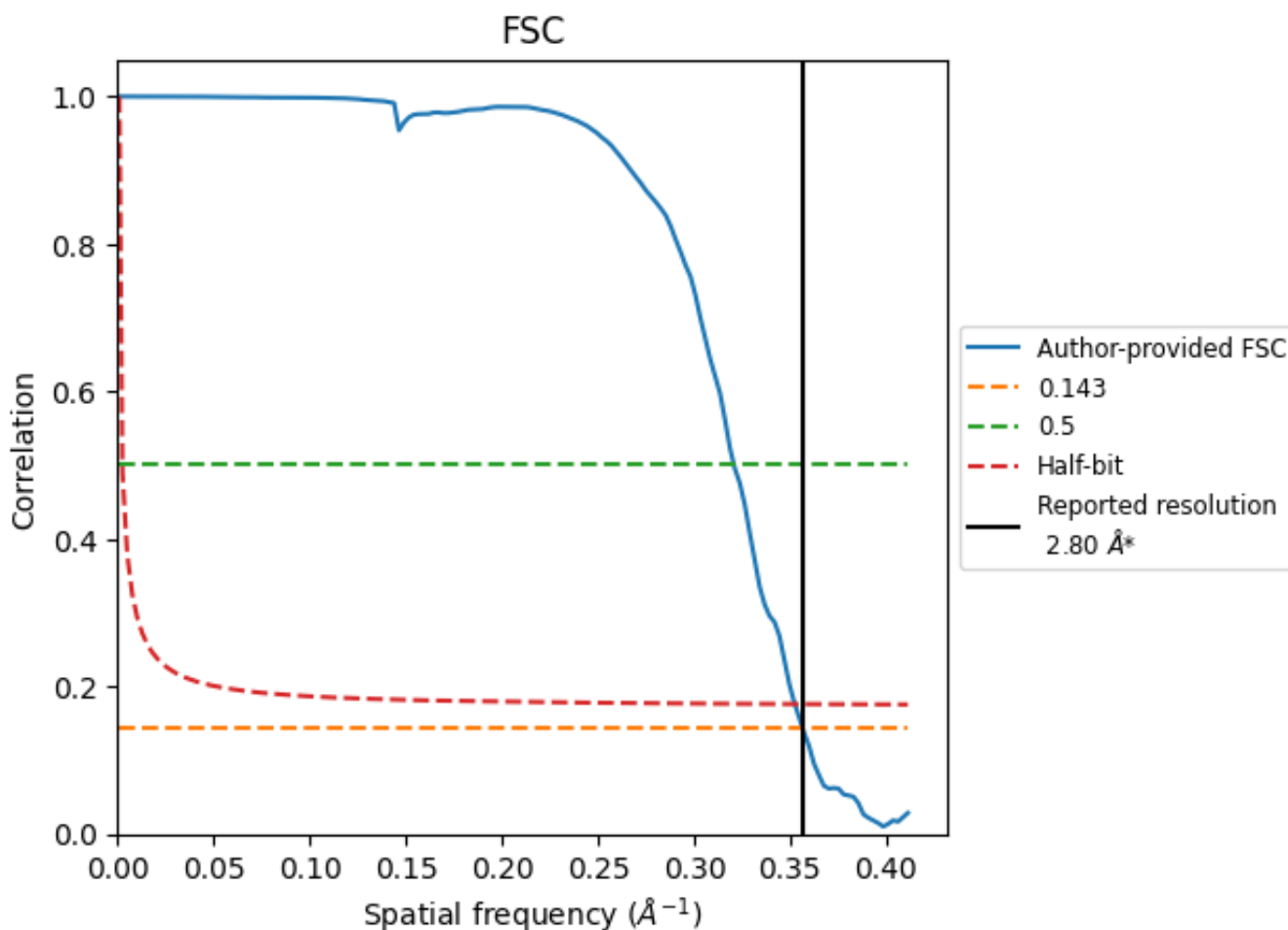


\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

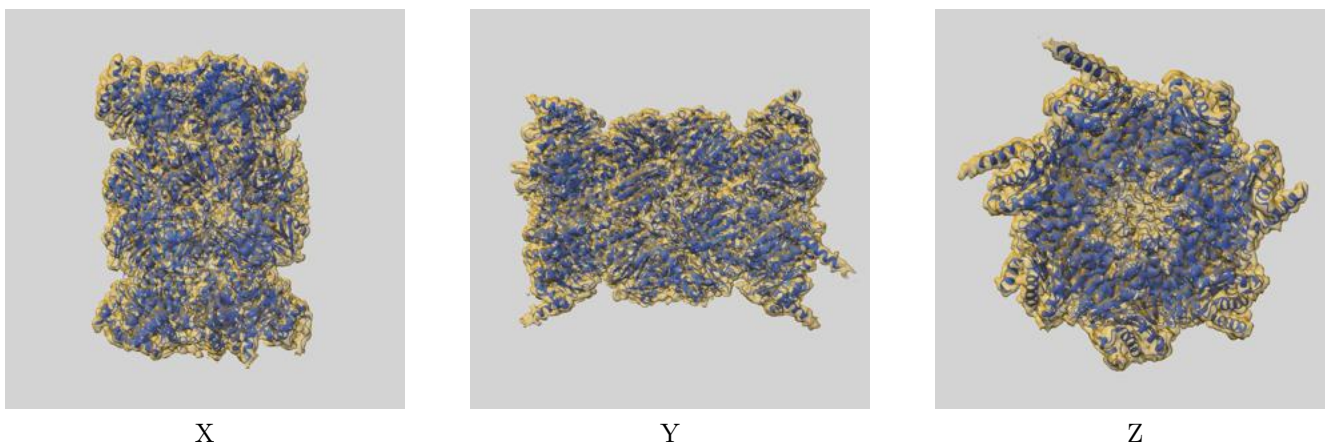
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.12	2.84
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

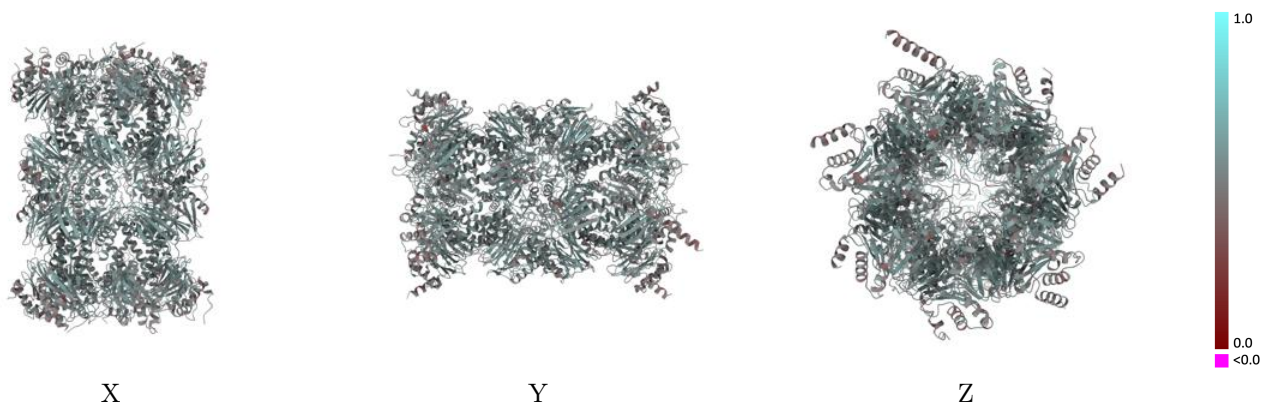
This section contains information regarding the fit between EMDB map EMD-24275 and PDB model 7NAN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



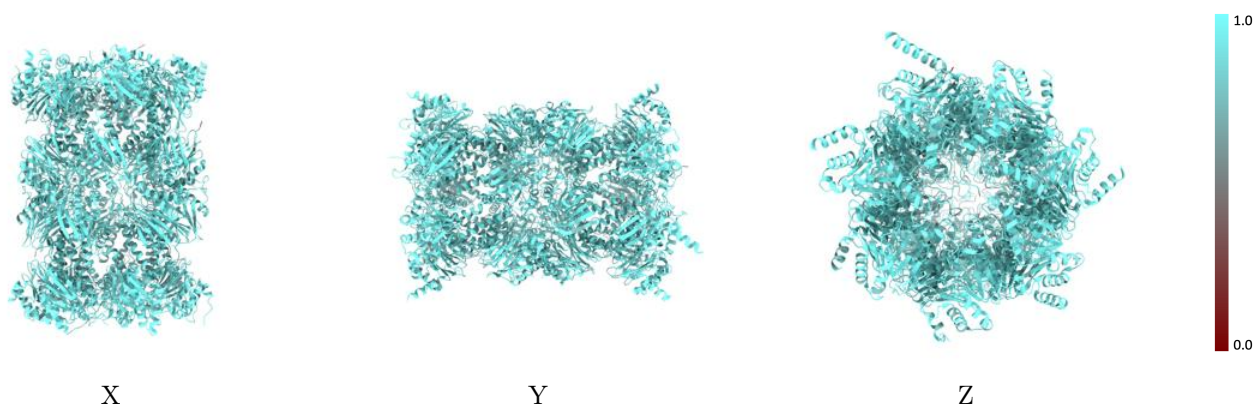
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



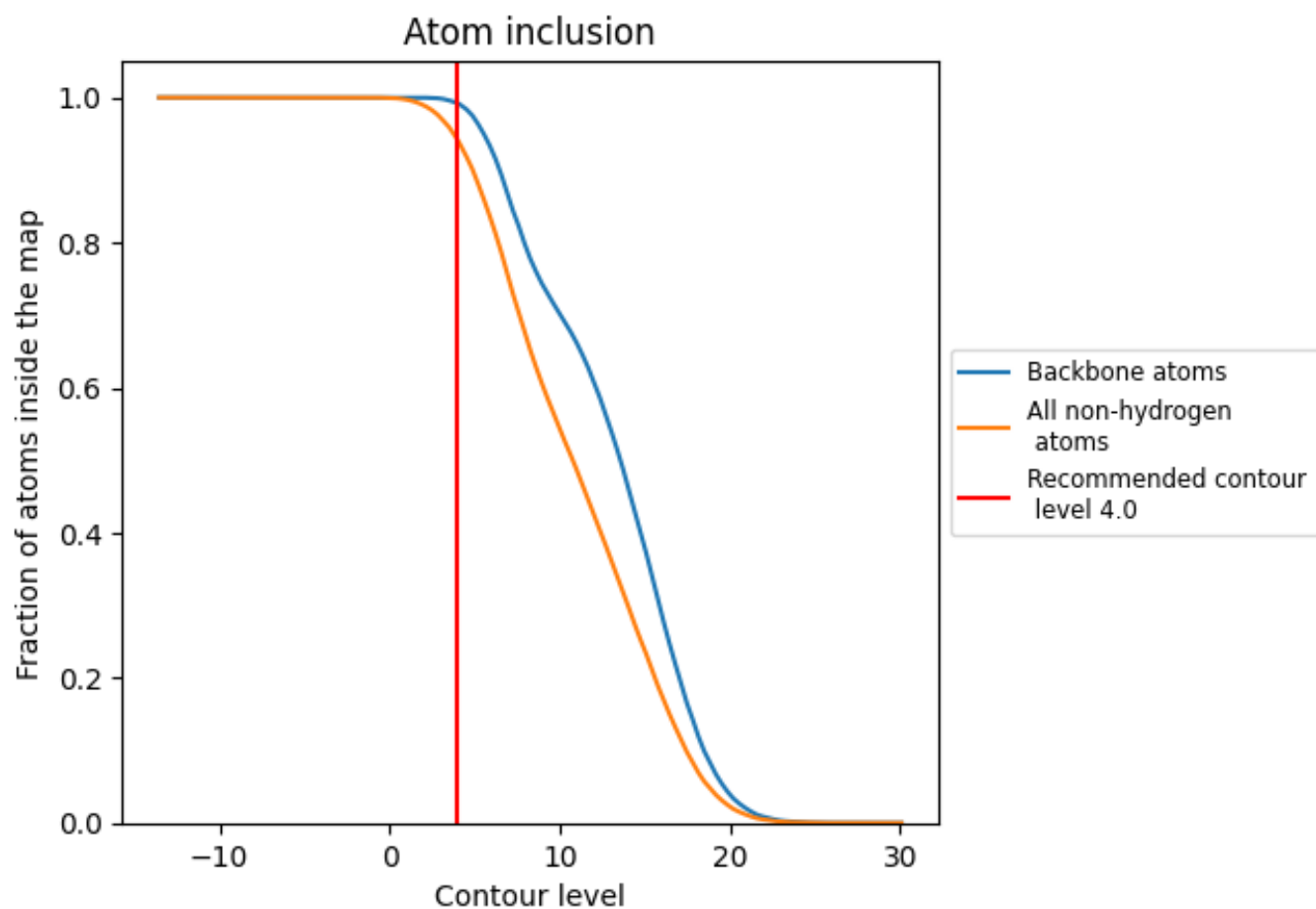
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.0).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9415	 0.5310
A	 0.9546	 0.5270
B	 0.9431	 0.5210
C	 0.9484	 0.5120
D	 0.9168	 0.5180
E	 0.9389	 0.5190
F	 0.9449	 0.5180
G	 0.9417	 0.5200
H	 0.9424	 0.5380
I	 0.9329	 0.5430
J	 0.9382	 0.5430
K	 0.9525	 0.5500
L	 0.9395	 0.5410
M	 0.9465	 0.5420
N	 0.9394	 0.5490
O	 0.9511	 0.5290
P	 0.9283	 0.5160
Q	 0.9426	 0.5140
R	 0.9169	 0.5160
S	 0.9499	 0.5240
T	 0.9438	 0.5200
U	 0.9452	 0.5200
V	 0.9379	 0.5350
W	 0.9405	 0.5490
X	 0.9385	 0.5510
Y	 0.9511	 0.5420
Z	 0.9365	 0.5430
a	 0.9512	 0.5520
b	 0.9534	 0.5500

