



## Full wwPDB EM Validation Report ⓘ

Aug 11, 2025 – 02:39 PM EDT

PDB ID : 9D35 / pdb\_00009d35  
EMDB ID : EMD-46525  
Title : Proteasome core particle assembly intermediate 5-alpha/3-beta/Ump1 purified from *Saccharomyces cerevisiae*.  
Authors : Chen, X.; Kaur, M.; Roelofs, J.; Walters, K.J.  
Deposited on : 2024-08-09  
Resolution : 3.26 Å(reported)  
Based on initial model : 7LSX

This is a Full wwPDB EM Validation 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.dev126  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

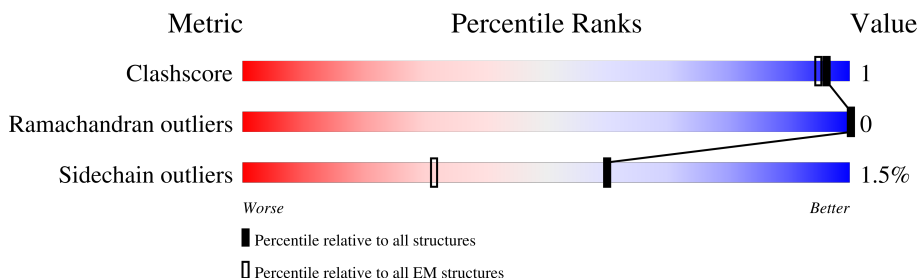
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


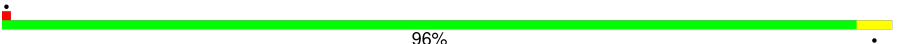






The reported resolution of this entry is 3.26 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	252	
2	B	250	
3	C	258	
4	D	254	
5	G	288	
6	P	200	
7	I	261	
8	J	205	

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Mol	Chain	Length	Quality of chain
9	K	198	 A horizontal bar chart showing the quality of chain K. The bar is primarily green, indicating good quality, with a small red segment at the beginning and a small yellow segment at the end. The text '87%' is centered below the green portion, and '8%' is at the far right end of the bar.

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 29009 atoms, of which 14490 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-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	241	Total	C	H	N	O	S	0	0
			3815	1216	1903	320	368	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	249	Total	C	H	N	O	S	0	0
			3814	1208	1913	314	376	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	232	Total	C	H	N	O	S	0	0
			3599	1137	1803	300	356	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	233	Total	C	H	N	O	S	0	0
			3672	1140	1841	322	365	4		

- Molecule 5 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	237	Total	C	H	N	O	S	0	0
			3692	1175	1845	323	345	4		

- Molecule 6 is a protein called Proteasome maturation factor UMP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	P	78	Total	C	H	N	O	S	0	0
			1281	403	628	118	127	5		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	149	GLY	-	expression tag	UNP P38293
P	150	ARG	-	expression tag	UNP P38293
P	151	ARG	-	expression tag	UNP P38293
P	152	ILE	-	expression tag	UNP P38293
P	153	PRO	-	expression tag	UNP P38293
P	154	GLY	-	expression tag	UNP P38293
P	155	LEU	-	expression tag	UNP P38293
P	156	ILE	-	expression tag	UNP P38293
P	157	ASN	-	expression tag	UNP P38293
P	158	PRO	-	expression tag	UNP P38293
P	159	TRP	-	expression tag	UNP P38293
P	160	LYS	-	expression tag	UNP P38293
P	161	ARG	-	expression tag	UNP P38293
P	162	ARG	-	expression tag	UNP P38293
P	163	TRP	-	expression tag	UNP P38293
P	164	LYS	-	expression tag	UNP P38293
P	165	LYS	-	expression tag	UNP P38293
P	166	ASN	-	expression tag	UNP P38293
P	167	PHE	-	expression tag	UNP P38293
P	168	ILE	-	expression tag	UNP P38293
P	169	ALA	-	expression tag	UNP P38293
P	170	VAL	-	expression tag	UNP P38293
P	171	SER	-	expression tag	UNP P38293
P	172	ALA	-	expression tag	UNP P38293
P	173	ALA	-	expression tag	UNP P38293
P	174	ASN	-	expression tag	UNP P38293
P	175	ARG	-	expression tag	UNP P38293
P	176	PHE	-	expression tag	UNP P38293
P	177	LYS	-	expression tag	UNP P38293
P	178	LYS	-	expression tag	UNP P38293
P	179	ILE	-	expression tag	UNP P38293
P	180	SER	-	expression tag	UNP P38293
P	181	SER	-	expression tag	UNP P38293
P	182	SER	-	expression tag	UNP P38293
P	183	GLY	-	expression tag	UNP P38293
P	184	ALA	-	expression tag	UNP P38293
P	185	LEU	-	expression tag	UNP P38293
P	186	ASP	-	expression tag	UNP P38293
P	187	TYR	-	expression tag	UNP P38293
P	188	ASP	-	expression tag	UNP P38293
P	189	ILE	-	expression tag	UNP P38293
P	190	PRO	-	expression tag	UNP P38293

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Chain	Residue	Modelled	Actual	Comment	Reference
P	191	THR	-	expression tag	UNP P38293
P	192	THR	-	expression tag	UNP P38293
P	193	ALA	-	expression tag	UNP P38293
P	194	SER	-	expression tag	UNP P38293
P	195	GLU	-	expression tag	UNP P38293
P	196	ASN	-	expression tag	UNP P38293
P	197	LEU	-	expression tag	UNP P38293
P	198	TYR	-	expression tag	UNP P38293
P	199	PHE	-	expression tag	UNP P38293
P	200	GLN	-	expression tag	UNP P38293

- Molecule 7 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	218	Total	C	H	N	O	S	0	0
			3277	1037	1630	286	319	5		

- Molecule 8 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	189	Total	C	H	N	O	S	0	0
			2922	944	1457	234	280	7		

- Molecule 9 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K	182	Total	C	H	N	O	S	0	0
			2937	935	1470	247	279	6		



ASP  
ASN  
VAL  
MET  
SER  
SER  
ASP  
ASP  
GLU  
ASN  
ALA  
PRO  
VAL  
ALA  
THR  
ASN  
ALA  
ASN  
ALA  
THR  
THR  
ASP  
GLN  
GLY  
GLY  
ASP  
HIS  
ILE  
LEU  
GLU

● Molecule 6: Proteasome maturation factor UMP1

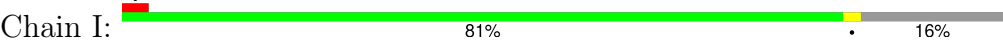


MET  
ASN  
ILE  
VAL  
GLY  
PRO  
GLN  
ASP  
VAL  
THR  
SER  
PHE  
LYS  
GLN  
SER  
VAL  
SER  
THR  
ASP  
GLN  
ASP  
LYS  
SER  
VAL  
LEU  
SER  
LEU  
GLN  
ARG  
ASN  
PHE  
GLN  
GLY  
GLY  
ALA  
VAL  
PRO  
ASN  
LEU  
SER  
THR  
LYS  
ILE  
ASN  
P49  
R50  
H51  
E54  
T126  
GLY  
LEU  
GLN  
ALA  
SER

THR  
MET  
VAL  
GLY  
SER  
ASN  
ASP  
VAL  
THR  
HIS  
SER  
LYS  
ILE  
GLN  
LYS  
GLN  
LEU  
GLY  
ILE  
GLY  
ARG  
CYS  
THR  
ILE  
ASN  
PRO  
TRP  
LYS  
ARG  
TRP  
LYS  
PHE  
ILE  
ALA  
VAL  
SER  
ASN  
ARG  
PHE  
LYS  
LYS  
ILE  
SER  
SER  
SER  
GLY  
ALA  
LEU  
ASP  
TYR  
ASP  
ILE  
PRO  
THR

THR  
ALA  
SER  
GLU  
ASN  
LEU  
TYR  
PHE  
GLN

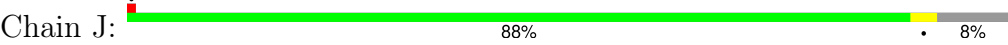
● Molecule 7: Proteasome subunit beta type-2



MET  
A2  
F6  
Y9  
S49  
THR  
GLN  
GLY  
PRO  
ILE  
VAL  
ALA  
ASP  
LYS  
ASN  
CYS  
A61  
I188  
I192  
W193  
N194  
D195  
L196  
G197  
S198  
G199  
S200  
N201  
V202  
L220  
THR  
PRO  
ASN  
VAL  
ARG  
GLU  
GLY  
LYS  
LYS  
SER  
TYR  
LYS  
PHE  
PRO  
ARG  
GLY  
T238  
V247  
ASN  
ILE  
CYS  
ASP

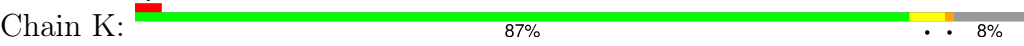
ILE  
GLN  
GLU  
GLN  
VAL  
ASP  
ILE  
THR  
ALA

● Molecule 8: Proteasome subunit beta type-3



MET  
SER  
ASP  
P4  
G9  
G10  
I11  
V21  
A22  
T23  
L27  
ARG  
LEU  
GLY  
SER  
GLN  
SER  
LEU  
GLY  
V36  
S37  
A110  
L163  
V186  
L200  
LYS  
MET  
ARG  
GLN  
ASP

● Molecule 9: Proteasome subunit beta type-4



M1  
I4  
K19  
ALA  
VAL  
THR  
ARG  
GLY  
ILE  
SER  
VAL  
LEU  
LYS  
ASP  
SER  
ASP  
D33  
S94  
R95  
L128  
P129  
Y135  
L144  
D145  
Y148  
L161  
C164  
R171  
D175  
F195  
GLN  
ALA  
GLN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	78759	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	14.367	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.339	Depositor
Recommended contour level	3	Depositor
Map size (Å)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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	0.75	0/1950	1.29	0/2640
2	B	0.79	0/1937	1.28	0/2623
3	C	0.71	0/1824	1.25	0/2471
4	D	0.71	0/1857	1.34	0/2513
5	G	0.74	0/1886	1.29	0/2546
6	P	0.78	0/666	1.31	0/899
7	I	0.76	0/1676	1.38	0/2272
8	J	0.78	0/1494	1.25	0/2019
9	K	0.74	0/1494	1.23	0/2012
All	All	0.75	0/14784	1.29	0/19995

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	A	1912	1903	1902	4	0
2	B	1901	1913	1910	5	0
3	C	1796	1803	1798	0	0
4	D	1831	1841	1840	3	0
5	G	1847	1845	1844	1	0
6	P	653	628	628	3	0
7	I	1647	1630	1628	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	1465	1457	1456	5	0
9	K	1467	1470	1469	3	0
All	All	14519	14490	14475	23	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 1.

All (23) 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)
1:A:17:THR:HG22	1:A:27:GLN:HB2	1.84	0.59
6:P:51:HIS:HB3	6:P:54:GLU:HB2	1.92	0.52
6:P:51:HIS:CD2	7:I:6:PHE:CD1	3.01	0.48
7:I:188:ILE:HG21	7:I:202:VAL:HG22	1.96	0.48
5:G:43:ASN:O	5:G:44:ASP:OD1	2.34	0.45
8:J:23:ILE:HD11	8:J:110:ALA:CB	2.47	0.44
9:K:129:PRO:HB3	9:K:148:TYR:CZ	2.52	0.44
4:D:108:TYR:C	4:D:108:TYR:CD1	2.95	0.44
9:K:144:LEU:HD11	9:K:164:CYS:SG	2.58	0.44
2:B:212:ALA:O	2:B:213:ILE:HG23	2.16	0.44
6:P:51:HIS:HA	7:I:9:TYR:CZ	2.52	0.44
8:J:27:LEU:HD11	8:J:186:VAL:HG22	1.99	0.43
1:A:130:GLN:HG2	2:B:127:VAL:HG13	1.99	0.43
8:J:21:VAL:HG12	8:J:22:ALA:N	2.34	0.43
9:K:94:SER:O	9:K:95:ARG:C	2.62	0.42
8:J:21:VAL:HG11	8:J:110:ALA:HB1	2.02	0.42
4:D:192:VAL:HG11	4:D:232:TYR:CD2	2.55	0.41
2:B:70:ASP:O	2:B:214:ILE:HG21	2.21	0.41
4:D:192:VAL:HG11	4:D:232:TYR:CE2	2.54	0.41
2:B:232:GLY:O	2:B:233:PRO:C	2.63	0.41
8:J:11:ILE:HD12	8:J:11:ILE:C	2.46	0.41
1:A:17:THR:HG22	1:A:27:GLN:CB	2.50	0.41
1:A:130:GLN:HG2	2:B:127:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	239/252 (95%)	232 (97%)	7 (3%)	0	100	100
2	B	247/250 (99%)	232 (94%)	15 (6%)	0	100	100
3	C	230/258 (89%)	220 (96%)	10 (4%)	0	100	100
4	D	231/254 (91%)	218 (94%)	13 (6%)	0	100	100
5	G	235/288 (82%)	225 (96%)	10 (4%)	0	100	100
6	P	76/200 (38%)	73 (96%)	3 (4%)	0	100	100
7	I	212/261 (81%)	206 (97%)	6 (3%)	0	100	100
8	J	185/205 (90%)	171 (92%)	14 (8%)	0	100	100
9	K	178/198 (90%)	169 (95%)	9 (5%)	0	100	100
All	All	1833/2166 (85%)	1746 (95%)	87 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	207/210 (99%)	204 (99%)	3 (1%)	62	77
2	B	207/209 (99%)	203 (98%)	4 (2%)	52	71
3	C	190/216 (88%)	186 (98%)	4 (2%)	48	69
4	D	207/226 (92%)	206 (100%)	1 (0%)	86	90
5	G	196/239 (82%)	193 (98%)	3 (2%)	60	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	P	74/180 (41%)	74 (100%)	0	100	100
7	I	175/214 (82%)	172 (98%)	3 (2%)	56	73
8	J	159/173 (92%)	157 (99%)	2 (1%)	65	78
9	K	162/175 (93%)	158 (98%)	4 (2%)	42	65
All	All	1577/1842 (86%)	1553 (98%)	24 (2%)	60	75

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	242	GLU
1	A	244	ARG
2	B	7	PHE
2	B	122	THR
2	B	157	PHE
2	B	213	ILE
3	C	20	TYR
3	C	123	THR
3	C	227	GLN
3	C	228	LYS
4	D	172	ARG
5	G	23	GLN
5	G	57	LYS
5	G	138	PHE
7	I	6	PHE
7	I	192	ILE
7	I	200	SER
8	J	11	ILE
8	J	163	LEU
9	K	4	ILE
9	K	128	LEU
9	K	144	LEU
9	K	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	240	ASN
2	B	20	GLN

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Mol	Chain	Res	Type
2	B	94	HIS
2	B	123	GLN
2	B	139	HIS
3	C	96	GLN
3	C	221	ASN
3	C	227	GLN
4	D	55	GLN
5	G	12	ASN
5	G	43	ASN
5	G	183	HIS
7	I	95	HIS
7	I	138	HIS
8	J	48	HIS
8	J	72	ASN
9	K	101	ASN

### 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 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](#)

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46525. These allow visual inspection of the internal detail of the map and identification of artifacts.

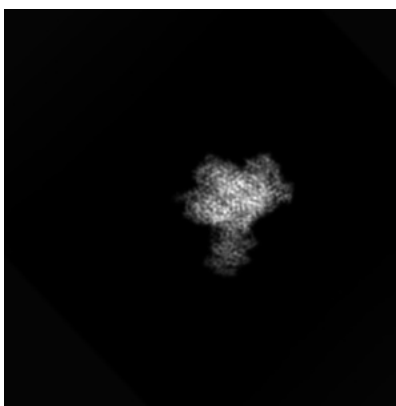
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

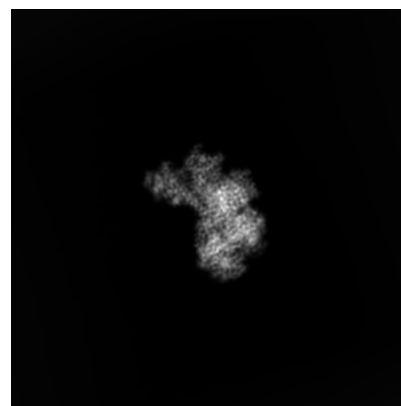
#### 6.1.1 Primary map



X

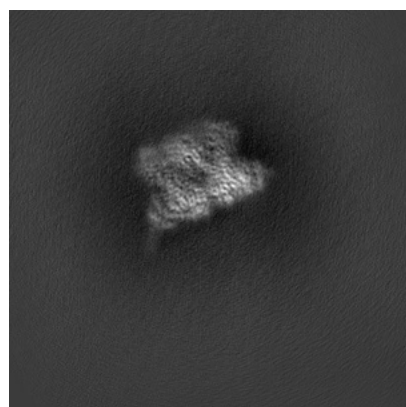


Y

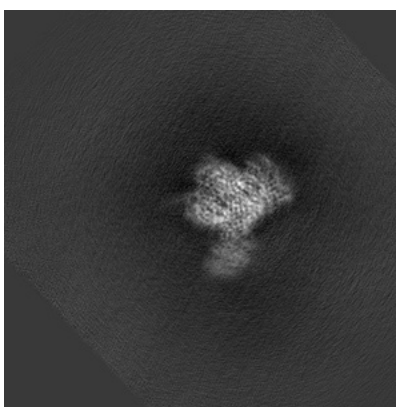


Z

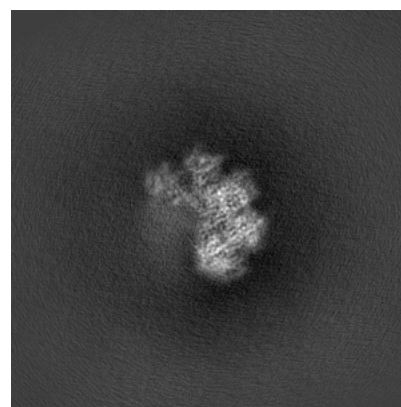
#### 6.1.2 Raw map



X



Y

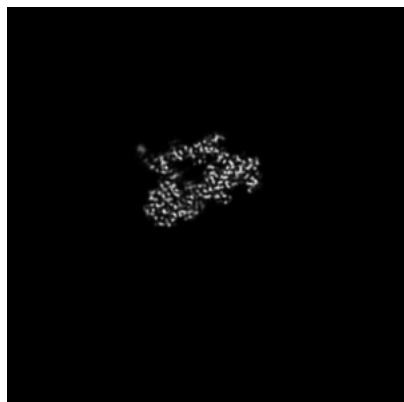


Z

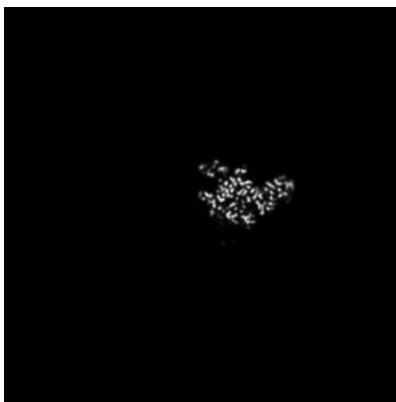
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

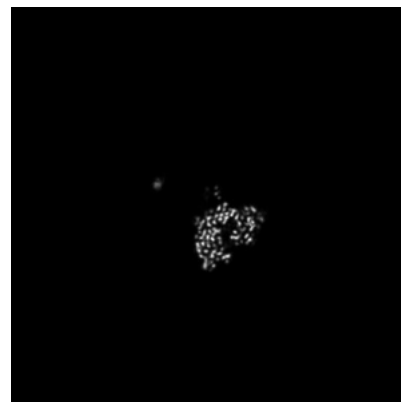
### 6.2.1 Primary map



X Index: 170

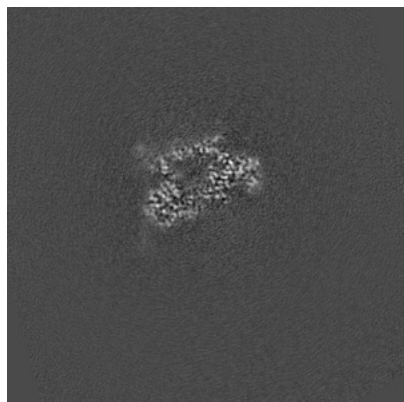


Y Index: 170

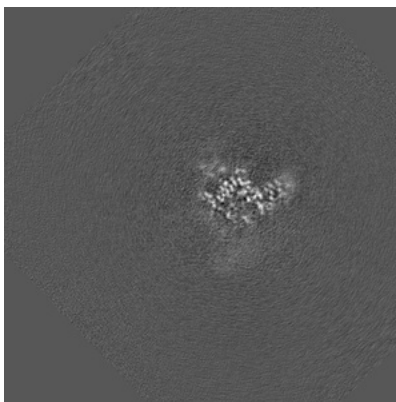


Z Index: 170

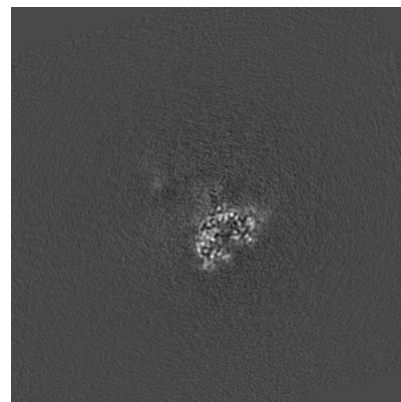
### 6.2.2 Raw map



X Index: 170



Y Index: 170

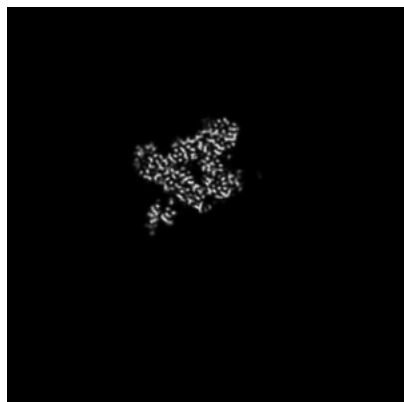


Z Index: 170

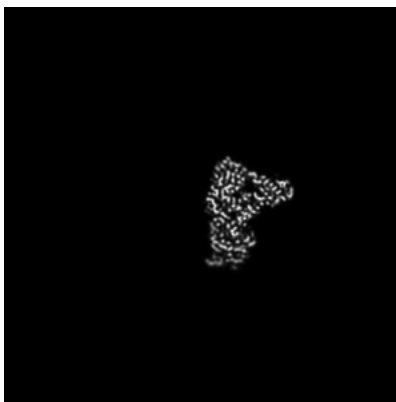
The images above show central slices of the map in three orthogonal directions.

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

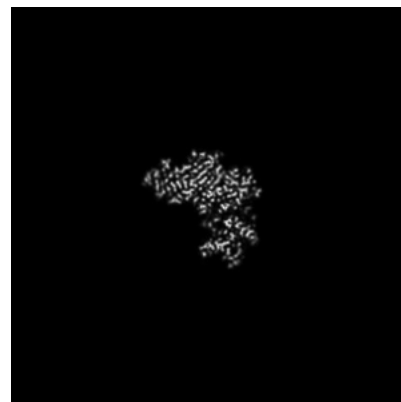
### 6.3.1 Primary map



X Index: 183

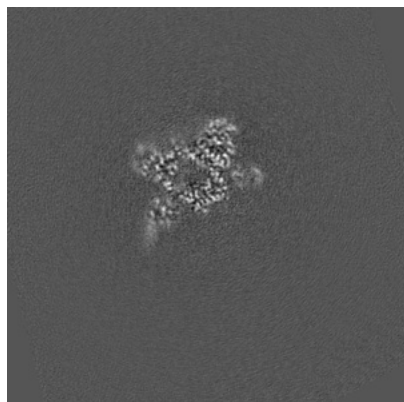


Y Index: 184

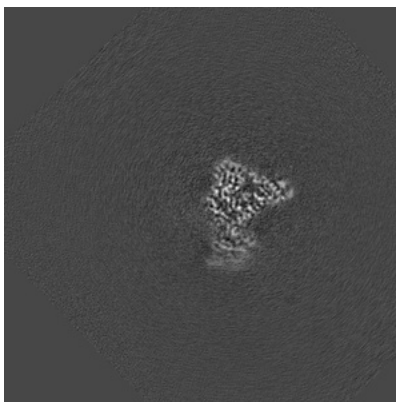


Z Index: 190

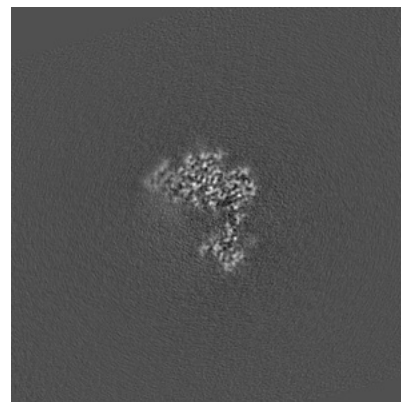
### 6.3.2 Raw map



X Index: 179



Y Index: 184

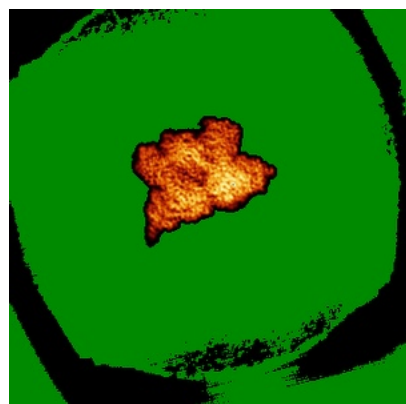


Z Index: 195

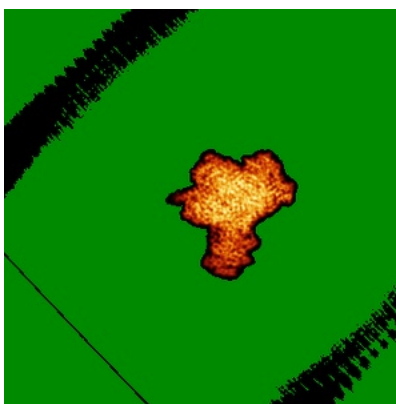
The images above show the largest variance slices of the map in three orthogonal directions.

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

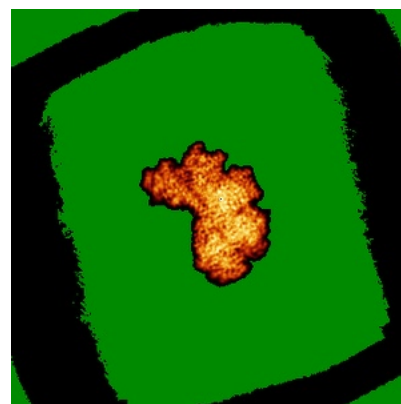
### 6.4.1 Primary map



X

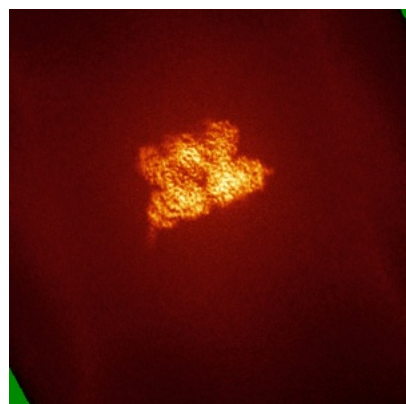


Y

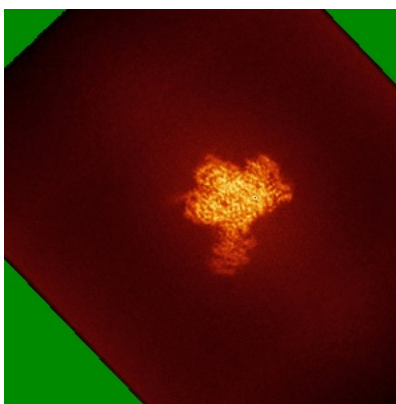


Z

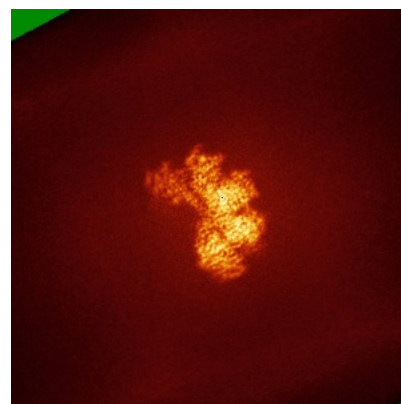
### 6.4.2 Raw map



X



Y

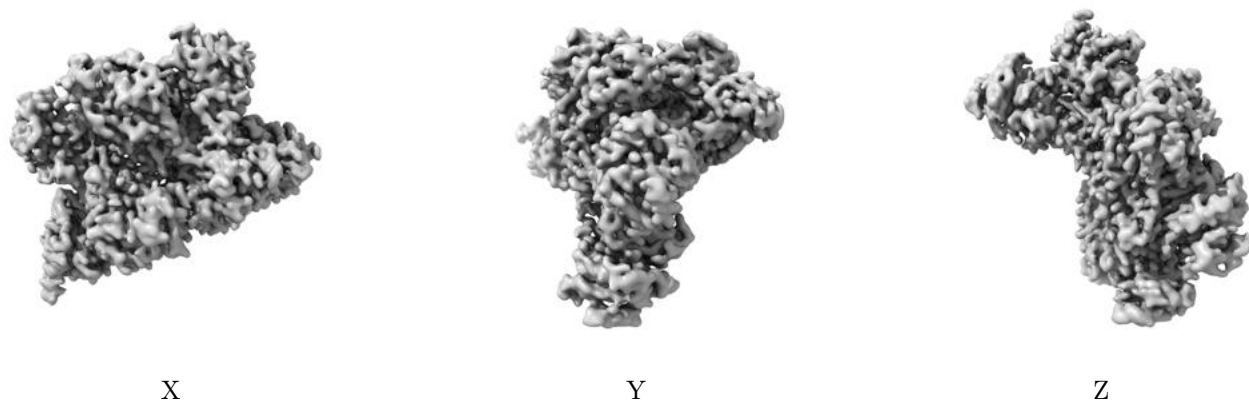


Z

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.

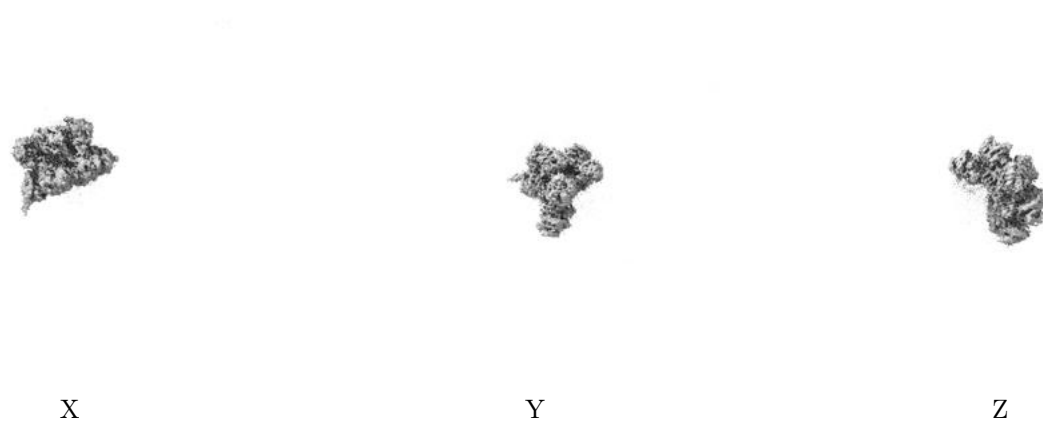
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

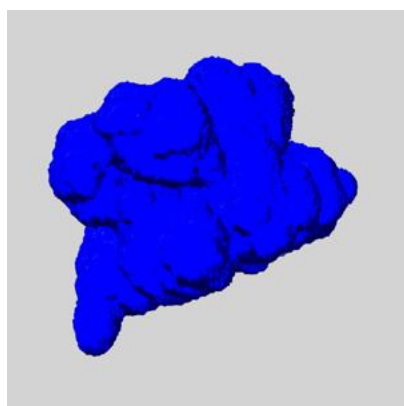
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

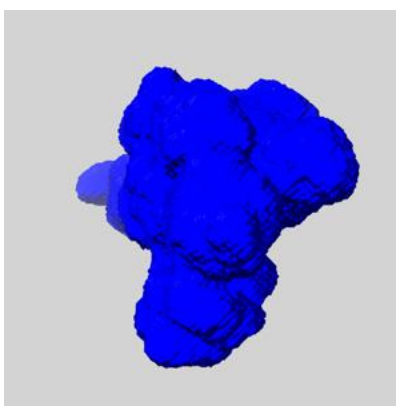
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

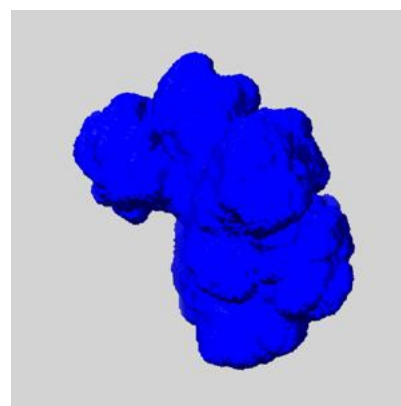
### 6.6.1 emd\_46525\_msk\_1.map [i](#)



X



Y

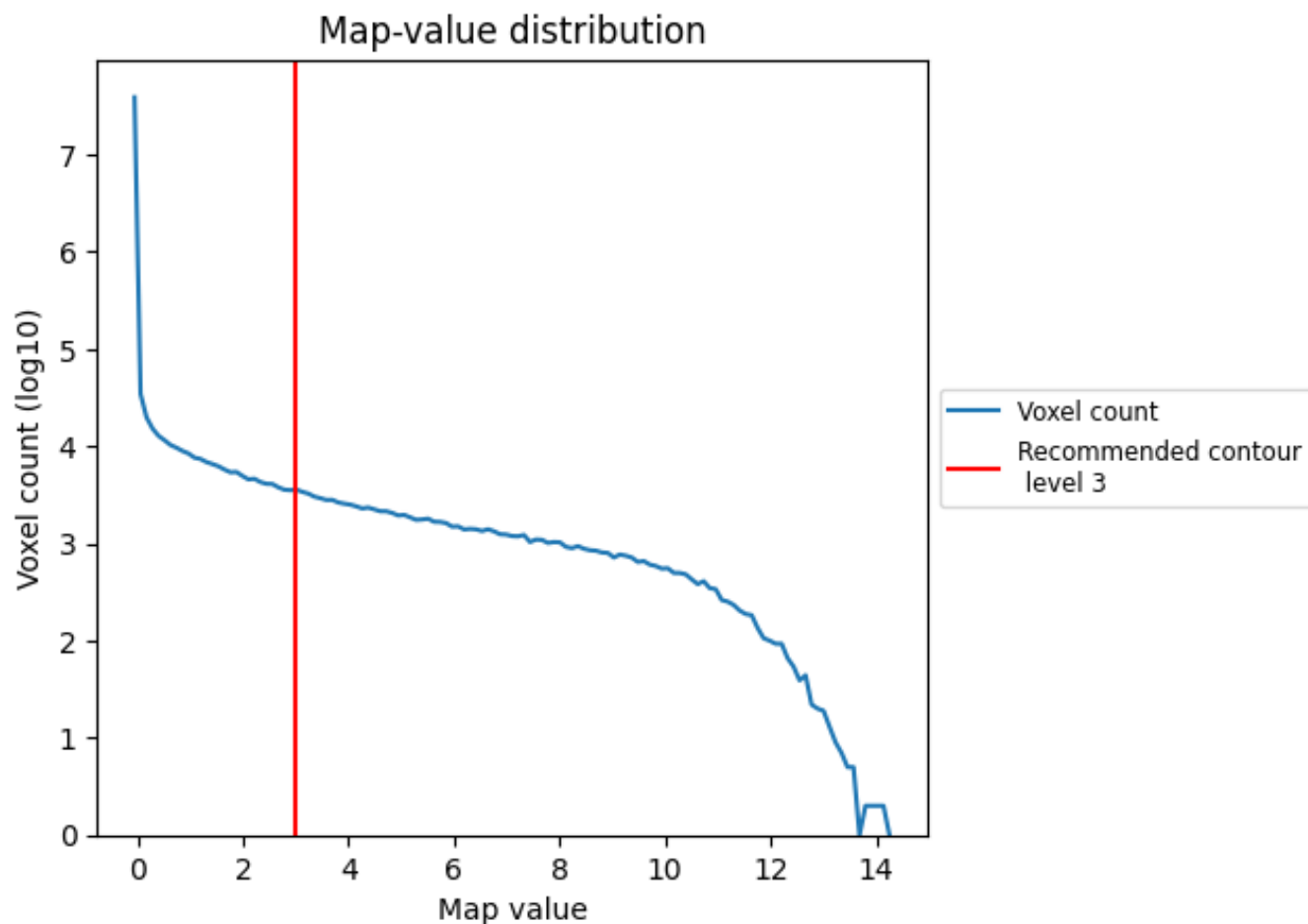


Z

## 7 Map analysis [i](#)

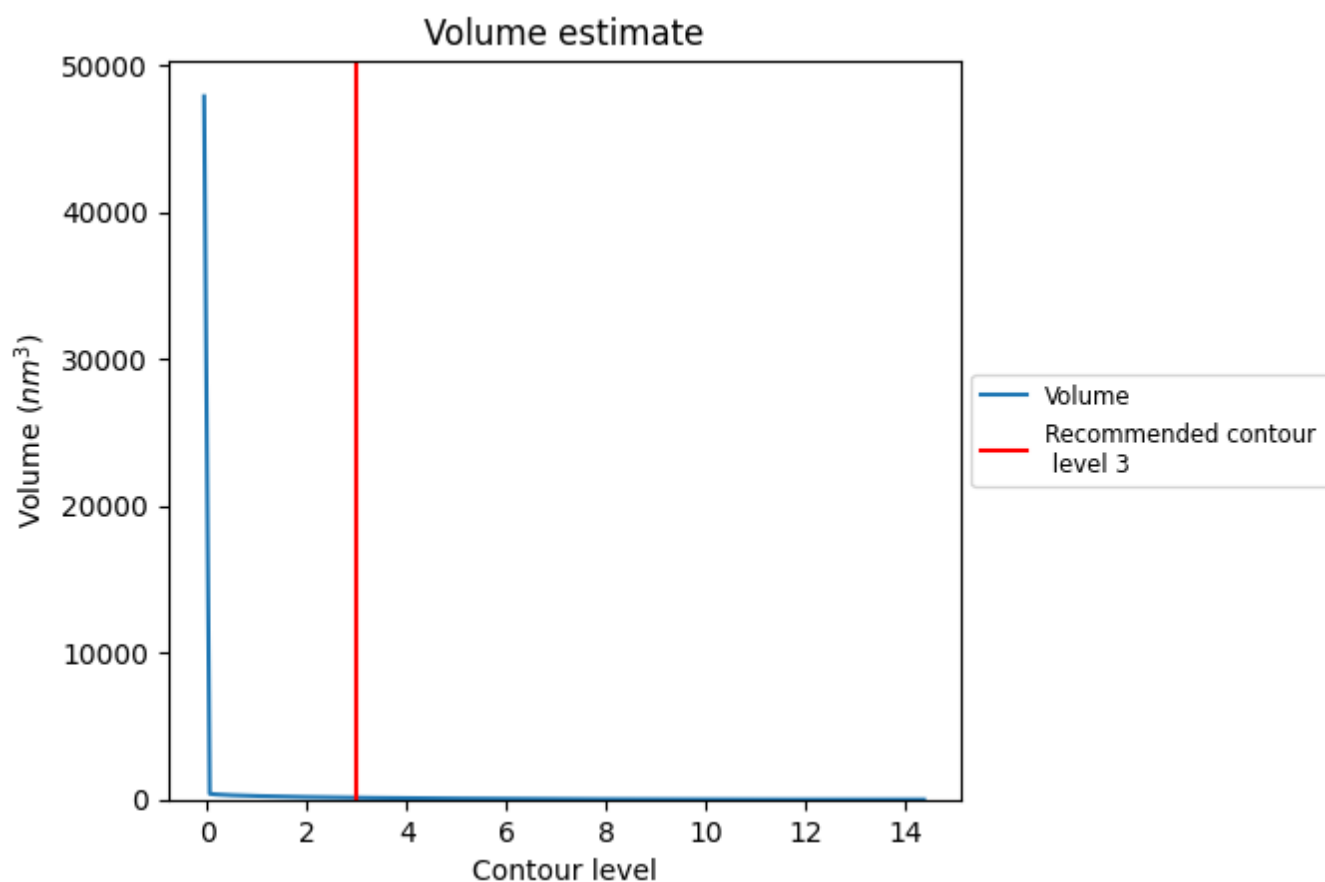
This section contains the results of statistical analysis of the map.

### 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.

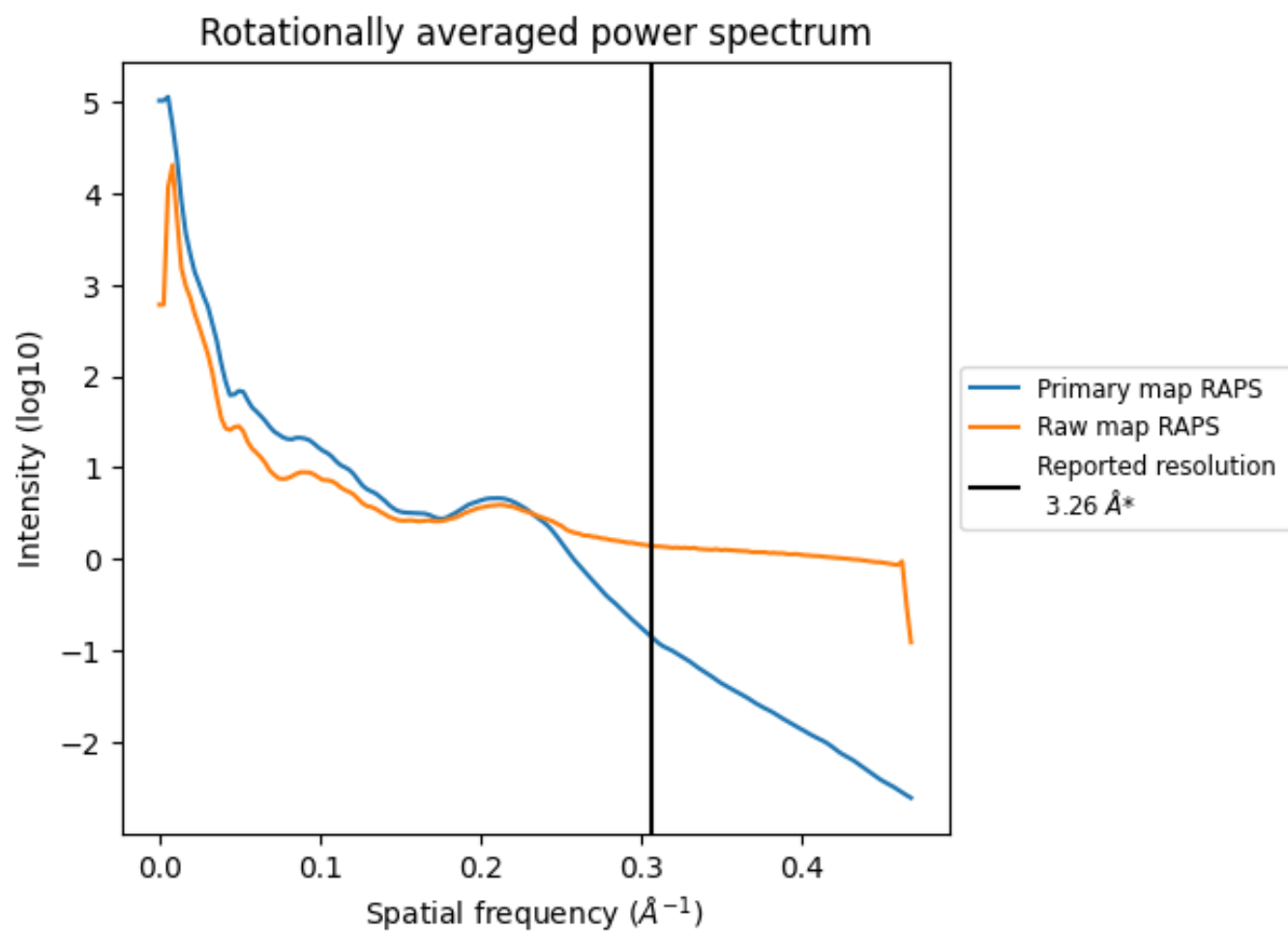
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 127 nm<sup>3</sup>; this corresponds to an approximate mass of 115 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 ⓘ

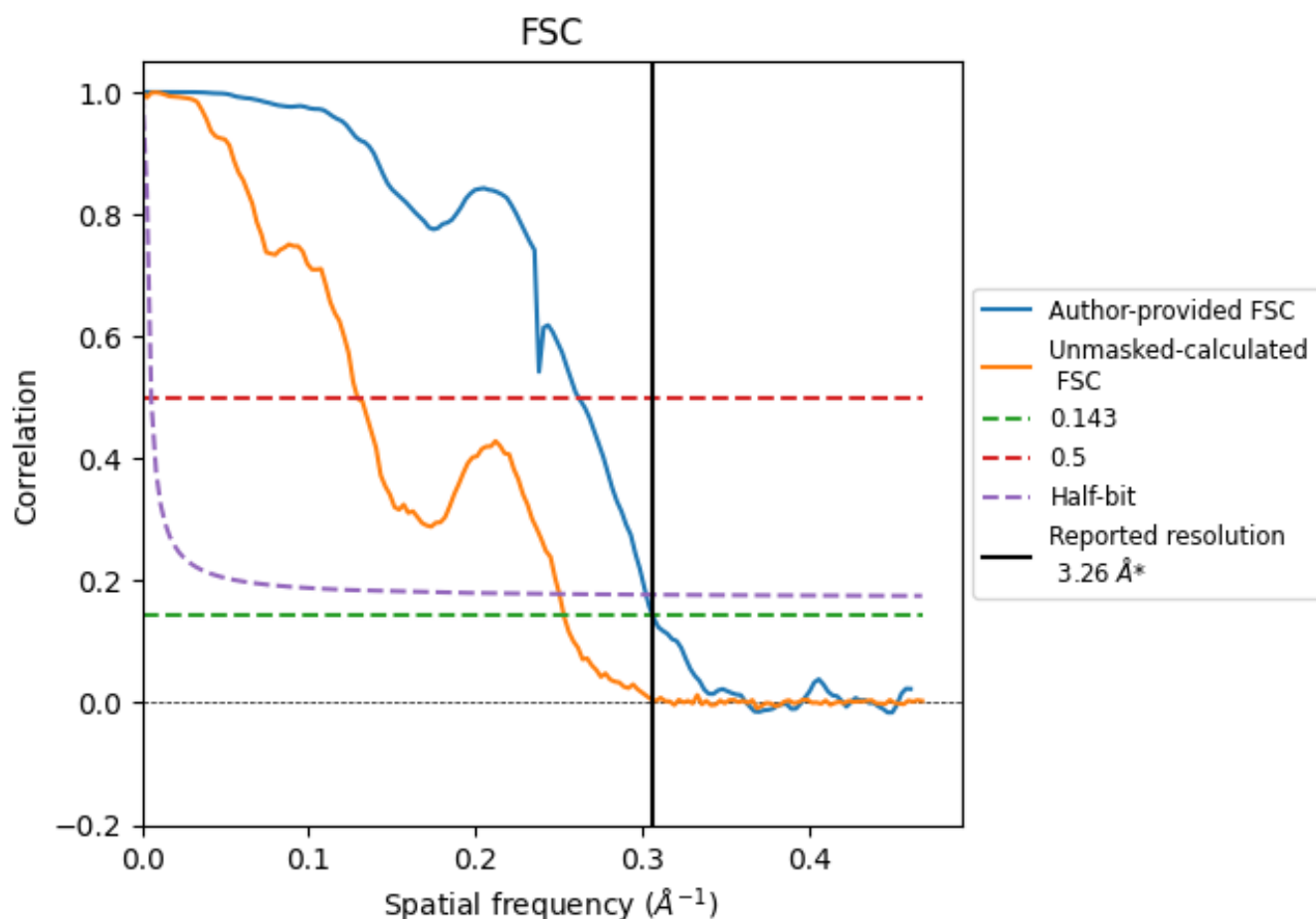


\*Reported resolution corresponds to spatial frequency of 0.307 Å<sup>-1</sup>

## 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 0.307  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

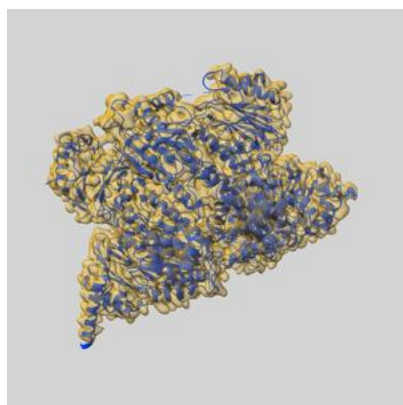
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.82	3.31
Unmasked-calculated*	3.95	7.74	3.99

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.26 by more than 10 %

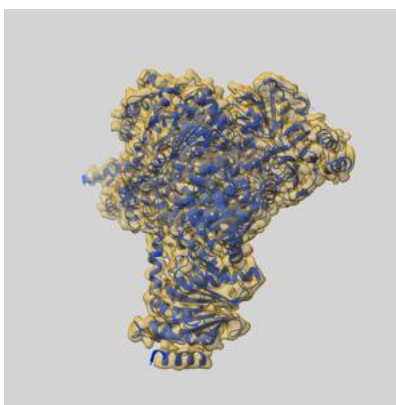
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46525 and PDB model 9D35. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

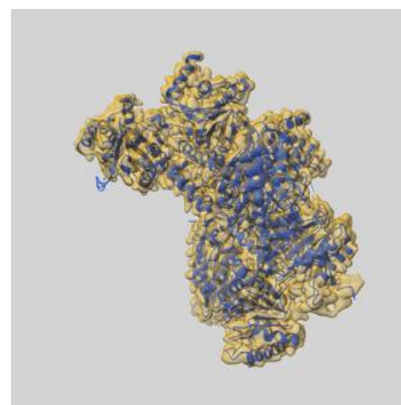
### 9.1 Map-model overlay [i](#)



X



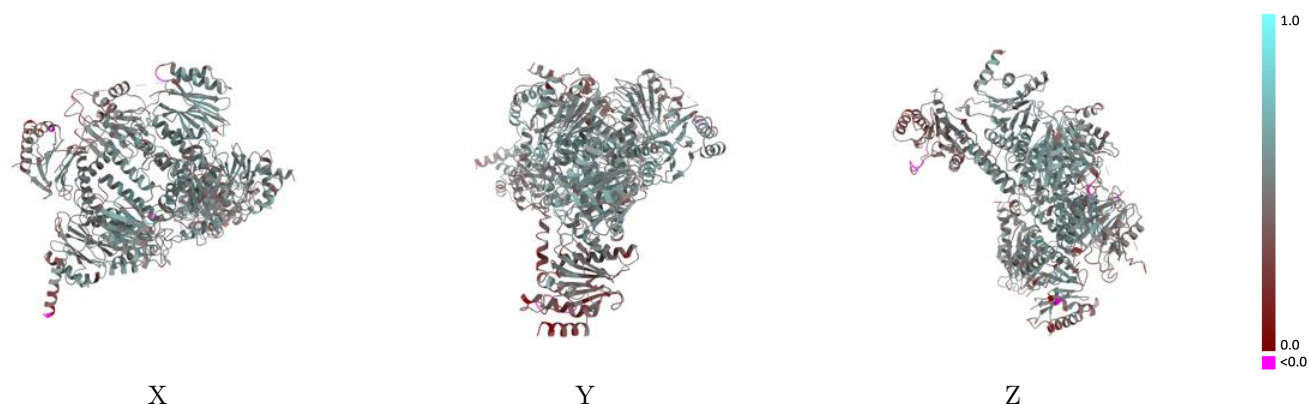
Y



Z

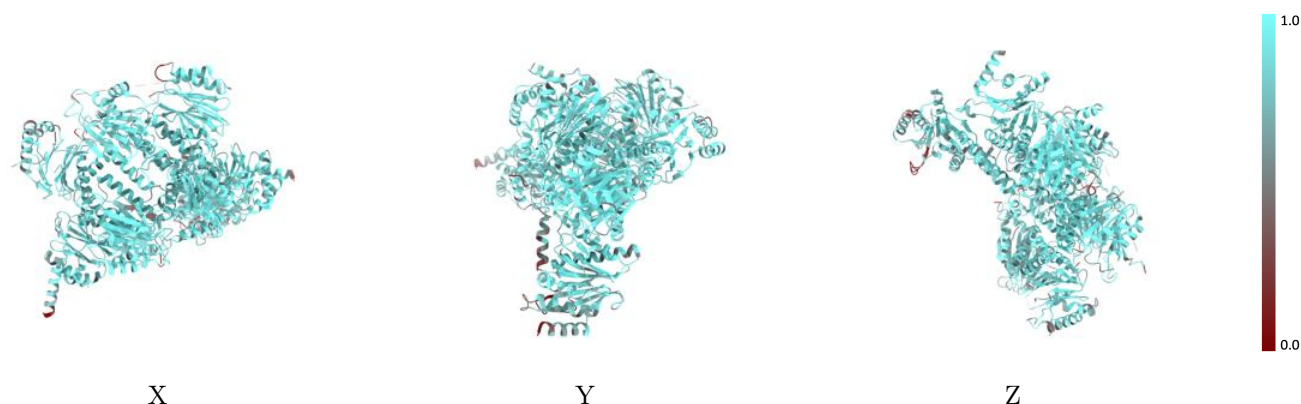
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



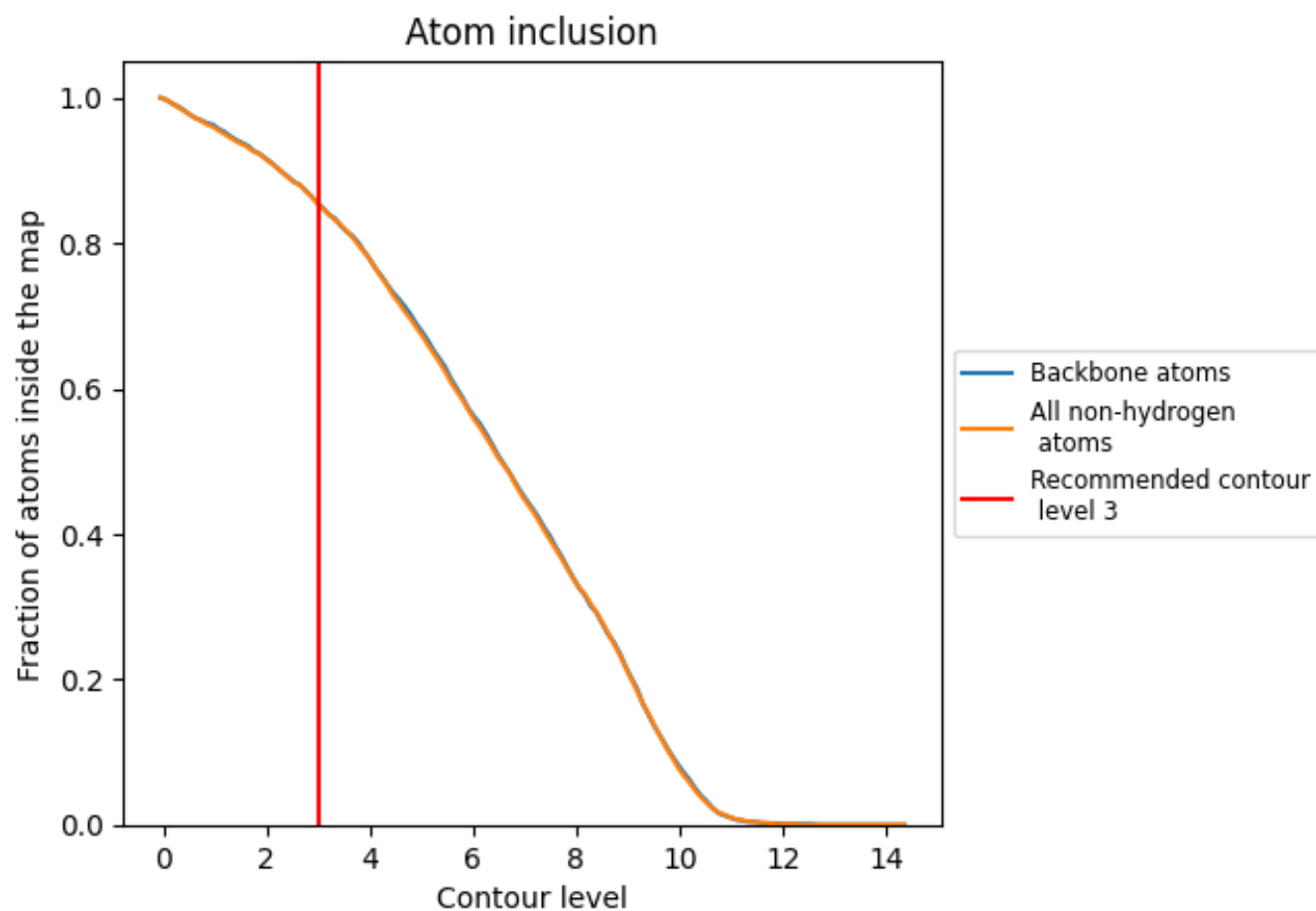
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8530	<div><div></div></div> 0.4780
A	<div><div></div></div> 0.9030	<div><div></div></div> 0.5210
B	<div><div></div></div> 0.8870	<div><div></div></div> 0.4990
C	<div><div></div></div> 0.9100	<div><div></div></div> 0.5080
D	<div><div></div></div> 0.8350	<div><div></div></div> 0.4640
G	<div><div></div></div> 0.7340	<div><div></div></div> 0.3530
I	<div><div></div></div> 0.8930	<div><div></div></div> 0.5190
J	<div><div></div></div> 0.8930	<div><div></div></div> 0.4900
K	<div><div></div></div> 0.8380	<div><div></div></div> 0.4610
P	<div><div></div></div> 0.8820	<div><div></div></div> 0.5070

1.0

0.0

<0.0