



## Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 08:16 PM UTC

PDB ID : 9D3I / pdb\_00009d3i  
EMDB ID : EMD-46535  
Title : Proteasome core particle assembly intermediate 5-alpha/4-beta/Ump1 purified from *Saccharomyces cerevisiae*.  
Authors : Chen, X.; Kaur, M.; Roelofs, J.; Walters, K.J.  
Deposited on : 2024-08-10  
Resolution : 3.11 Å (reported)  
Based on initial models : 4V7O, 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:

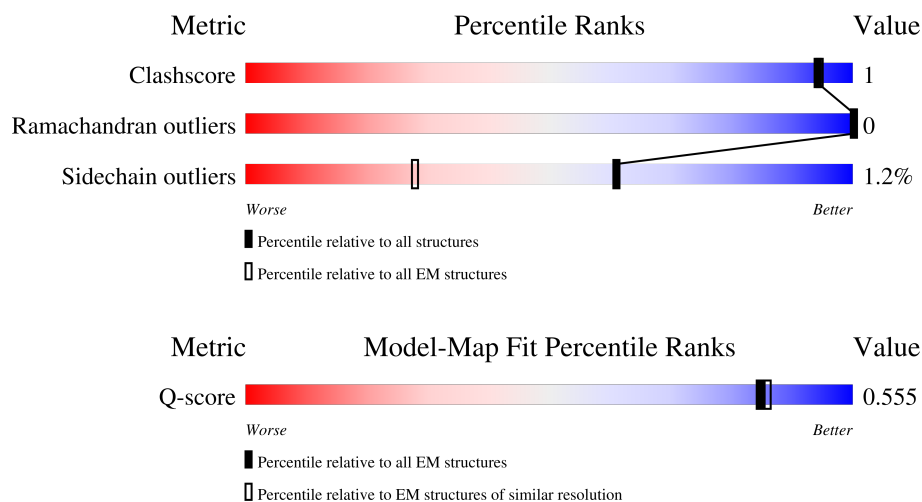
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.11 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.








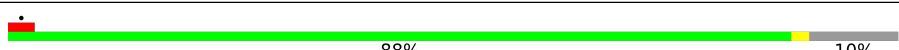
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 ( 2.61 - 3.61 )

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	 94%
2	B	250	 94% 5%
3	C	258	 88% 10%
4	D	254	 88% 9%

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Mol	Chain	Length	Quality of chain
5	G	288	
6	P	200	
7	H	215	
8	I	261	
9	J	205	
10	K	198	

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 31326 atoms, of which 15653 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	242	Total	C	H	N	O	S	0	0
			3822	1218	1906	321	369	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	247	Total	C	H	N	O	S	0	0
			3799	1206	1907	312	371	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	233	Total	C	H	N	O	S	0	0
			3625	1148	1812	301	361	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	232	Total	C	H	N	O	S	0	0
			3665	1138	1838	321	364	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	235	Total	C	H	N	O	S	0	0
			3664	1167	1834	320	339	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	P	87	Total	C	H	N	O	S	0	0
			1439	451	710	132	141	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-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	146	Total	C	H	N	O	S	0	0
			2274	730	1133	187	217	7		

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	214	Total	C	H	N	O	S	0	0
			3229	1022	1609	281	312	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	189	Total	C	H	N	O	S	0	0
			2928	944	1462	236	279	7		

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	179	Total	C	H	N	O	S	0	0
			2881	916	1442	243	274	6		



ASN  
ALA  
PRO  
VAL  
ALA  
THR  
ASN  
ALA  
THR  
THR  
THR  
GLN  
GLY  
ILE  
HIS  
LEU  
GLU

• Molecule 6: Proteasome maturation factor UMP1

Chain P:  40% 56%

MET ASN ILE VAL PRO GLN ASP THR PHE SER LYS MET THR VAL SER THR ASP GLN LYS SER VAL LEU SER SER ALA VAL PRO SER LEU PRO ASP THR ARG GLN GLN GLY GLY ALA VAL PRO LEU SER SER D49 N82 D95 F96 I109 E114 G115 S116

I117 G125 LEU GLN ASP D137 G145 L146 GLY ILE GLY ARG ARG ILE PRO GLY LEU ILE ASP ASN PRO TRP ARG LYS LYS PHE ASN PHE VAL VAL SER ALA ALA ASN ARG PHE LYS ILE SER SER SER SER GLY ALA LEU ASP

ILE PRO THR THR ALA SER GLU ASN LEU TYR PHE GLN


• Molecule 7: Proteasome subunit beta type-1

Chain H:  5% 68% 32%

MET ASN GLY ILE VAL ASP ILE ASN ARG LEU LYS GLY VAL LEU GLY THR S2 D10 L14 GLY ALA ASP SER ARG THR THR GLY ALA TYR ILE ASN ARG VAL ASP K33 G47 Y87 E88 N89 LYS ASP ASN LEU THR ALA G96 D104

P114 L115 G116 G117 H120 G128 SER GLY THR PHE ILE Y135 S160 GLN ALA ILE LYS TRP ASP GLY SER SER GLY VAL I173 Y189 PRO ASP GLU TYR GLN LEU


• Molecule 8: Proteasome subunit beta type-2

Chain I:  79% 18%

MET A2 T30 K36 G40 V41 S49 THR GLN GLY PRO ILE VAL ALA ASP LYS ASN CYS A61 A79 L94 S137 W193 ASN ASP LEU GLY SER G199 V204 T221 PRO ASN VAL ARG GLU LYS LYS SER TYR LYS PHE PRO ARG GLY T238 E244


V247 ILE ASN ILE CYS ASP ILE GLN GLU GLN VAL ASP ILE THR ALA

• Molecule 9: Proteasome subunit beta type-3

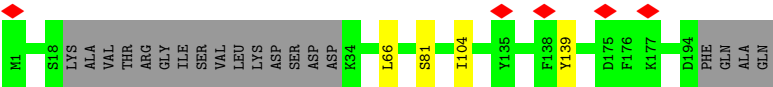
Chain J:  86% 6% 8%

MET SER ASP PRO S5 S6 V21 L27 G30 S31 GLN SER LEU VAL GLY VAL SER ASN K39 Y46 T71 Y74 E78 D125 L126 I127 R177 L180 W183 V186 L200 LYS MET ARG GLN ASP

• Molecule 10: Proteasome subunit beta type-4

Chain K:  88% 10%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81760	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	16.225	Depositor
Minimum map value	-0.110	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.363	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	0.72	0/1954	1.30	0/2645
2	B	0.75	0/1929	1.28	0/2611
3	C	0.72	0/1842	1.28	0/2495
4	D	0.73	0/1853	1.32	0/2508
5	G	0.73	0/1869	1.26	0/2523
6	P	0.80	0/742	1.33	0/998
7	H	0.70	0/1160	1.20	0/1563
8	I	0.77	0/1648	1.32	0/2233
9	J	0.75	0/1494	1.30	0/2017
10	K	0.74	0/1465	1.29	0/1974
All	All	0.74	0/15956	1.29	0/21567

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	1916	1906	1905	4	0
2	B	1892	1907	1906	7	0
3	C	1813	1812	1811	4	0
4	D	1827	1838	1837	7	0
5	G	1830	1834	1831	3	0
6	P	729	710	707	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	1141	1133	1128	0	0
8	I	1620	1609	1605	5	0
9	J	1466	1462	1460	5	0
10	K	1439	1442	1443	1	0
All	All	15673	15653	15633	37	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 (37) 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)
4:D:203:VAL:HG21	4:D:210:ILE:CG2	2.27	0.65
1:A:127:ILE:HD11	6:P:109:ILE:HB	1.81	0.62
6:P:117:ILE:HD11	8:I:94:LEU:HD13	1.81	0.62
4:D:199:LEU:O	4:D:203:VAL:HG22	2.00	0.61
6:P:116:SER:C	6:P:117:ILE:HD13	2.26	0.60
9:J:74:TYR:CE2	9:J:78:GLU:OE2	2.59	0.55
4:D:203:VAL:O	4:D:203:VAL:HG23	2.08	0.54
8:I:36:LYS:HA	8:I:41:VAL:HA	1.89	0.54
6:P:117:ILE:HD11	8:I:94:LEU:CD1	2.38	0.53
8:I:79:ALA:HB3	9:J:127:ILE:HD12	1.91	0.53
4:D:203:VAL:HG21	4:D:210:ILE:HG23	1.92	0.51
2:B:74:VAL:HG13	2:B:135:LEU:HD12	1.93	0.50
5:G:200:ILE:HG21	5:G:214:LEU:HD13	1.92	0.50
2:B:64:VAL:HG11	2:B:212:ALA:HB3	1.94	0.50
4:D:47:GLU:HG3	4:D:203:VAL:HG12	1.93	0.49
2:B:21:ILE:HD11	2:B:122:THR:HG21	1.95	0.48
2:B:111:VAL:HG22	2:B:136:ILE:HD12	1.94	0.48
2:B:111:VAL:HG22	2:B:136:ILE:HB	1.95	0.48
3:C:123:THR:HG22	3:C:123:THR:O	2.14	0.48
1:A:28:VAL:HG21	1:A:129:THR:HG23	1.97	0.46
3:C:22:VAL:CG2	3:C:123:THR:HG23	2.45	0.45
5:G:109:ILE:HB	5:G:110:PRO:HD3	1.98	0.45
2:B:21:ILE:HD11	2:B:122:THR:CG2	2.47	0.44
8:I:40:GLY:HA2	8:I:137:SER:HB3	2.01	0.43
4:D:171:VAL:HG13	4:D:198:SER:HB3	2.01	0.43
1:A:128:TYR:CD1	1:A:128:TYR:N	2.88	0.42
1:A:129:THR:HG22	1:A:129:THR:O	2.19	0.42
3:C:15:PRO:HB3	3:C:19:LEU:HD22	2.00	0.42
6:P:95:ASP:O	6:P:96:PHE:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:70:VAL:HG11	5:G:112:PHE:CZ	2.55	0.42
4:D:207:ALA:HB1	4:D:229:ILE:HG22	2.01	0.42
9:J:46:TYR:HB3	9:J:71:THR:HG21	2.03	0.41
3:C:22:VAL:HG21	3:C:123:THR:HG21	2.01	0.41
2:B:91:LYS:HE3	6:P:117:ILE:HD12	2.02	0.41
10:K:81:SER:HA	10:K:104:ILE:HD13	2.03	0.40
9:J:27:LEU:HG	9:J:186:VAL:HG23	2.03	0.40
9:J:27:LEU:HD21	9:J:186:VAL:CG2	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	240/252 (95%)	234 (98%)	6 (2%)	0	100	100
2	B	245/250 (98%)	241 (98%)	4 (2%)	0	100	100
3	C	231/258 (90%)	227 (98%)	4 (2%)	0	100	100
4	D	230/254 (91%)	222 (96%)	8 (4%)	0	100	100
5	G	233/288 (81%)	229 (98%)	4 (2%)	0	100	100
6	P	83/200 (42%)	79 (95%)	4 (5%)	0	100	100
7	H	136/215 (63%)	132 (97%)	4 (3%)	0	100	100
8	I	206/261 (79%)	198 (96%)	8 (4%)	0	100	100
9	J	185/205 (90%)	176 (95%)	9 (5%)	0	100	100
10	K	175/198 (88%)	164 (94%)	11 (6%)	0	100	100
All	All	1964/2381 (82%)	1902 (97%)	62 (3%)	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%)	205 (99%)	2 (1%)	68	77
2	B	206/209 (99%)	202 (98%)	4 (2%)	50	71
3	C	193/216 (89%)	191 (99%)	2 (1%)	68	77
4	D	207/226 (92%)	207 (100%)	0	100	100
5	G	193/239 (81%)	193 (100%)	0	100	100
6	P	83/180 (46%)	80 (96%)	3 (4%)	31	59
7	H	123/178 (69%)	123 (100%)	0	100	100
8	I	172/214 (80%)	169 (98%)	3 (2%)	53	72
9	J	158/173 (91%)	153 (97%)	5 (3%)	34	61
10	K	159/175 (91%)	157 (99%)	2 (1%)	61	75
All	All	1701/2020 (84%)	1680 (99%)	21 (1%)	61	76

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	TYR
1	A	244	ARG
2	B	6	SER
2	B	10	THR
2	B	132	VAL
2	B	210	GLU
3	C	16	GLU
3	C	19	LEU
6	P	82	MET
6	P	114	GLU
6	P	117	ILE
8	I	30	THR
8	I	204	VAL
8	I	247	VAL
9	J	21	VAL
9	J	125	ASP

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Mol	Chain	Res	Type
9	J	126	LEU
9	J	177	ARG
9	J	183	TRP
10	K	66	LEU
10	K	139	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	221	ASN
1	A	240	ASN
2	B	123	GLN
2	B	149	GLN
3	C	96	GLN
4	D	94	GLN
5	G	182	HIS
7	H	53	GLN
7	H	120	HIS
8	I	64	HIS
8	I	120	GLN
8	I	138	HIS
9	J	45	HIS
9	J	72	ASN
10	K	61	GLN
10	K	65	GLN
10	K	86	GLN
10	K	101	ASN
10	K	118	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 [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.



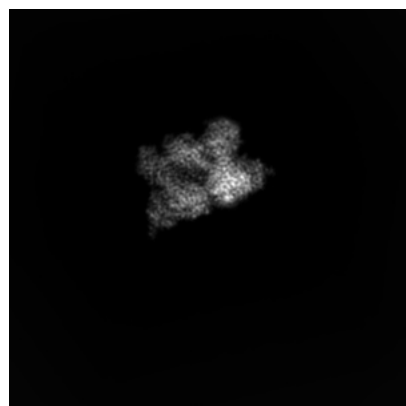
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46535. These allow visual inspection of the internal detail of the map and identification of artifacts.

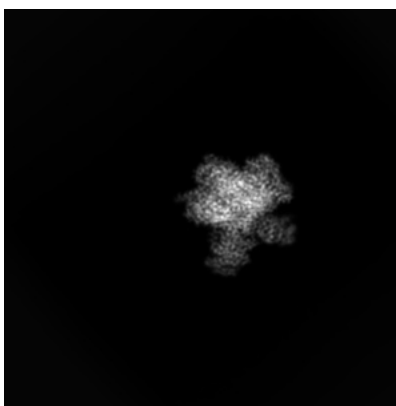
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

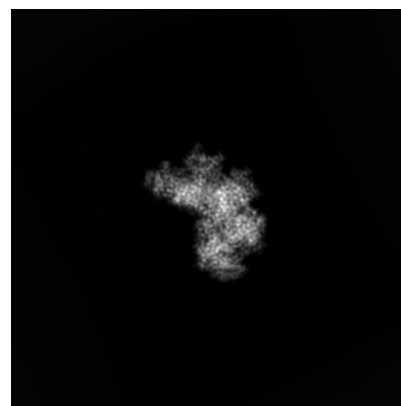
#### 6.1.1 Primary map



X

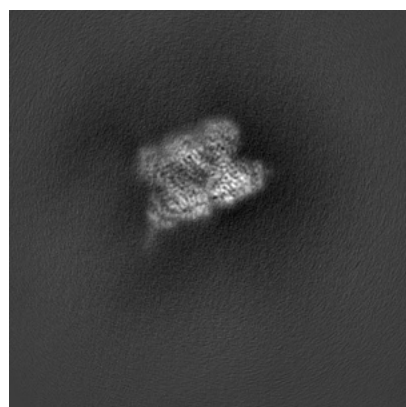


Y

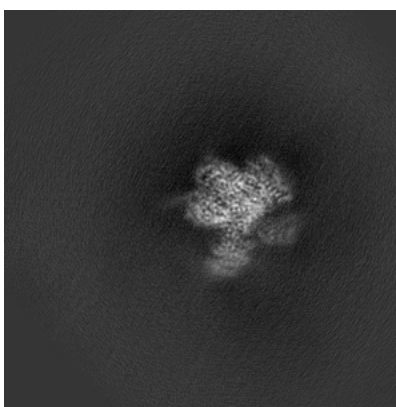


Z

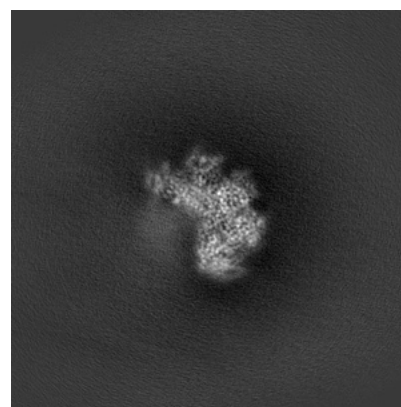
#### 6.1.2 Raw map



X



Y



Z

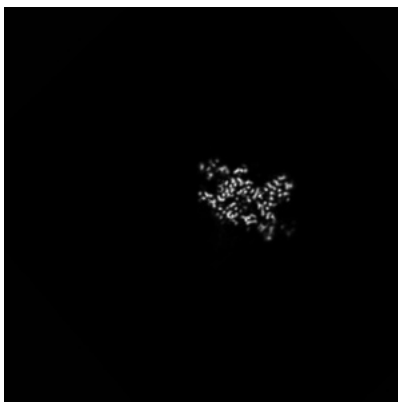
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 170

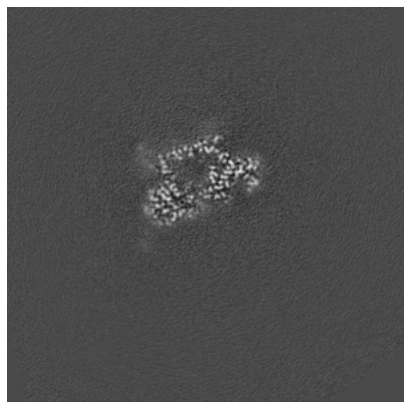


Y Index: 170

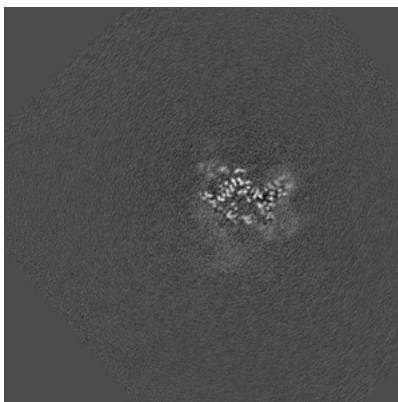


Z Index: 170

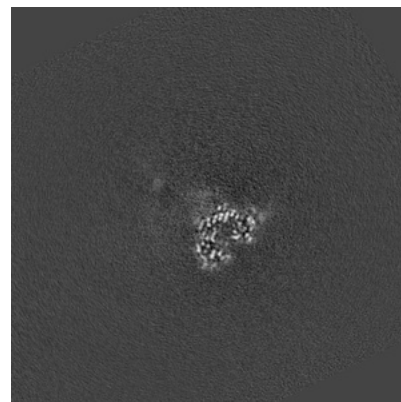
### 6.2.2 Raw map



X Index: 170



Y Index: 170

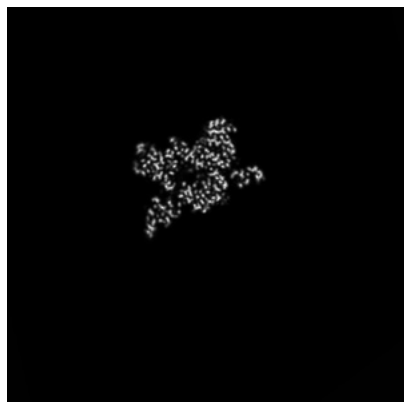


Z Index: 170

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

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

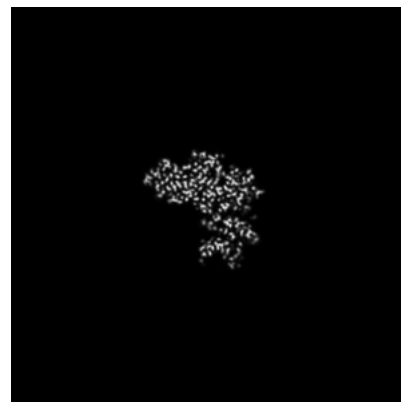
### 6.3.1 Primary map



X Index: 178

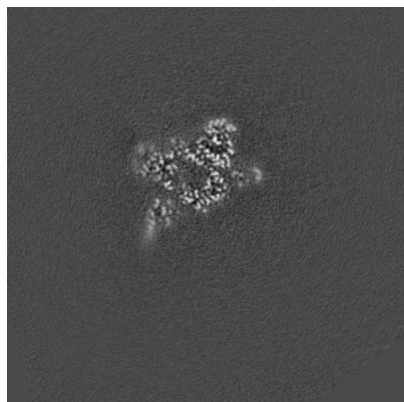


Y Index: 185

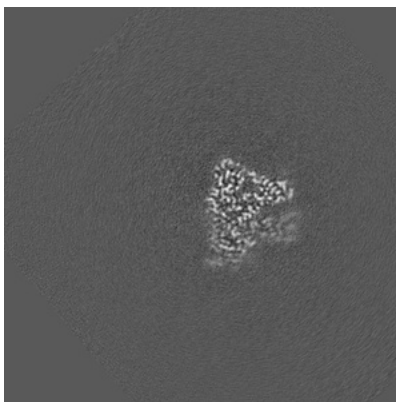


Z Index: 190

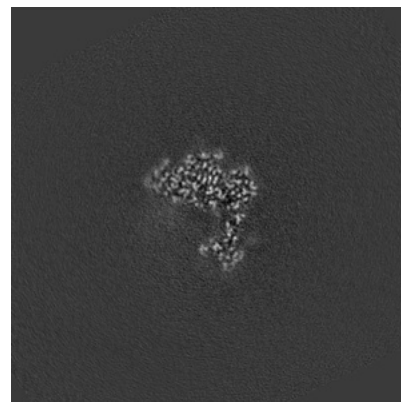
### 6.3.2 Raw map



X Index: 179



Y Index: 184

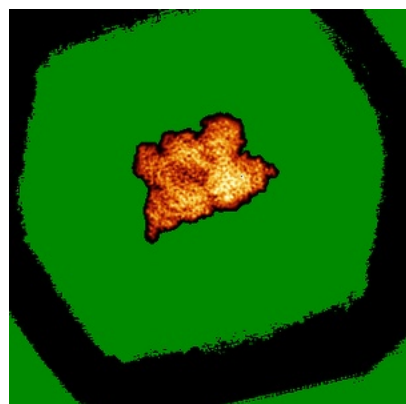


Z Index: 195

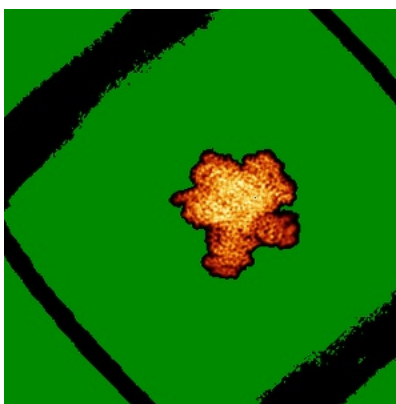
The images above show the largest variance slices of the map in three orthogonal directions.

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

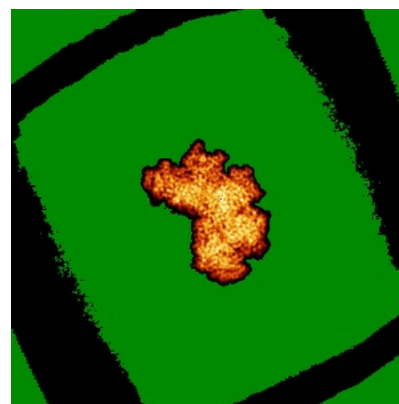
### 6.4.1 Primary map



X

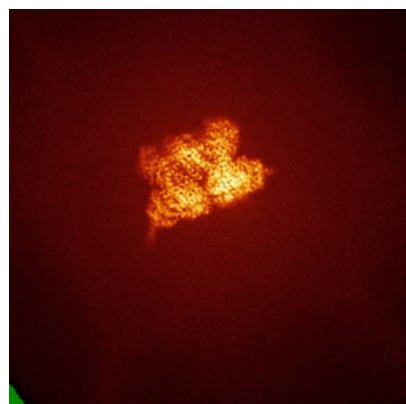


Y

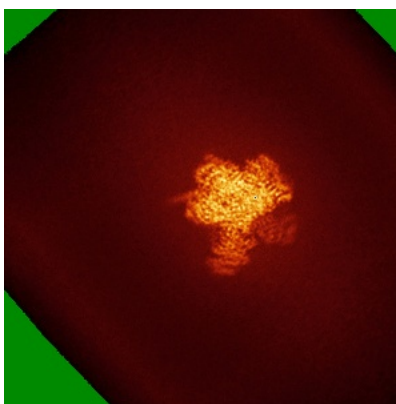


Z

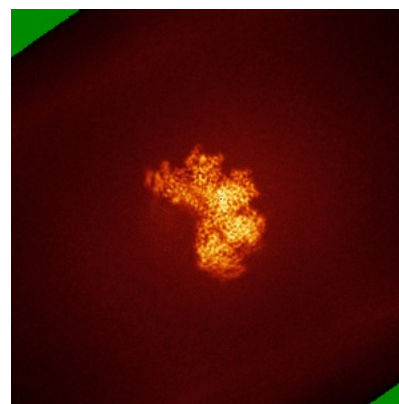
### 6.4.2 Raw map



X



Y

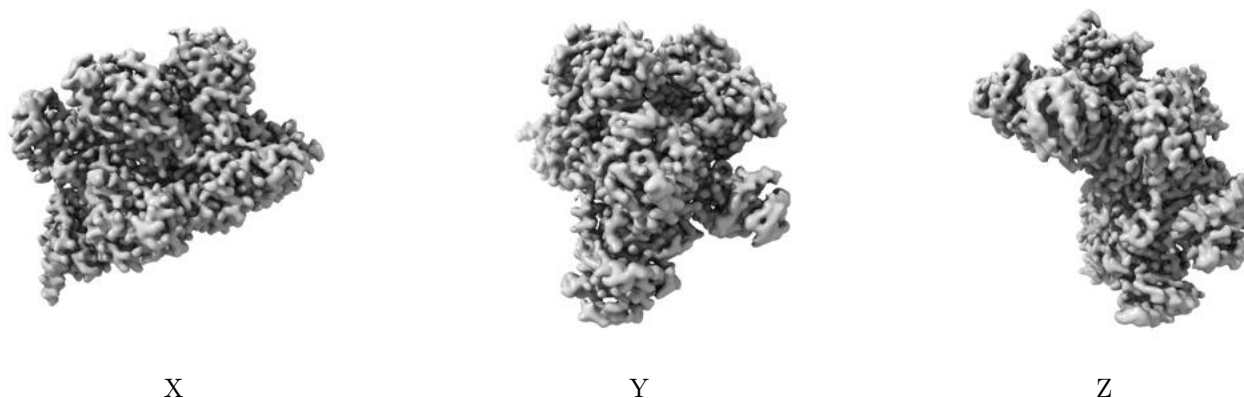


Z

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.

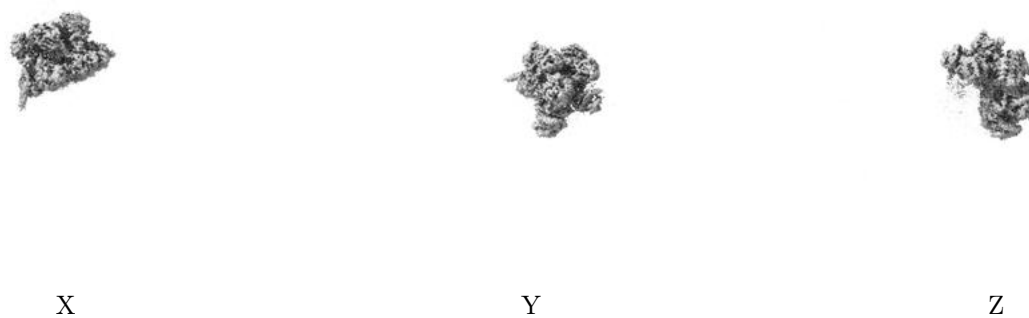
## 6.5 Orthogonal surface views [i](#)

### 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.

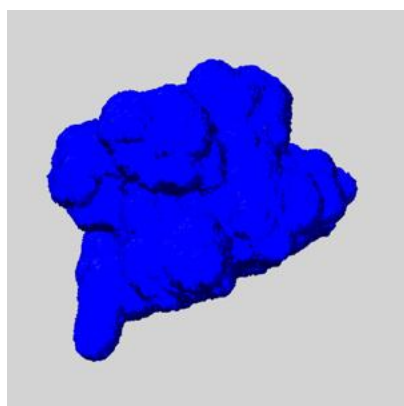
## 6.6 Mask visualisation [i](#)

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

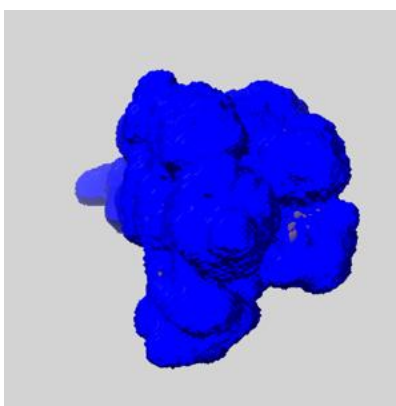
A mask typically either:

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

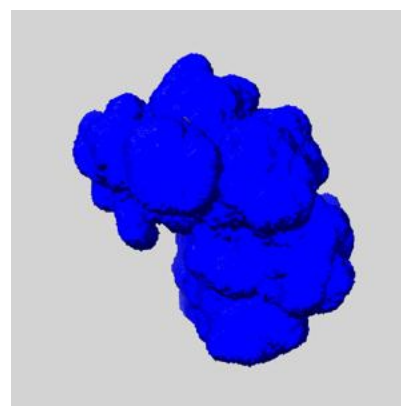
### 6.6.1 emd\_46535\_msk\_1.map [i](#)



X



Y

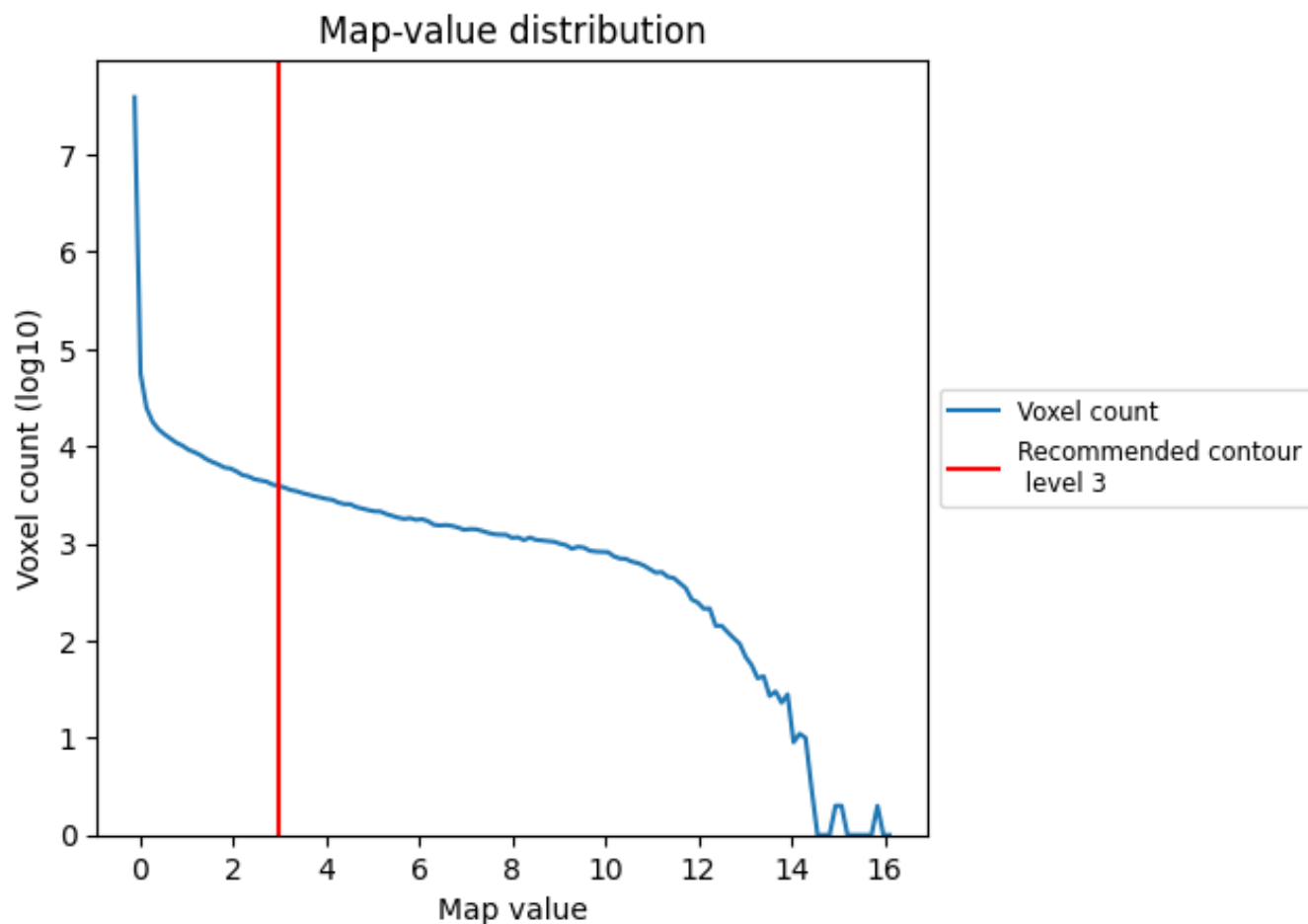


Z

## 7 Map analysis [i](#)

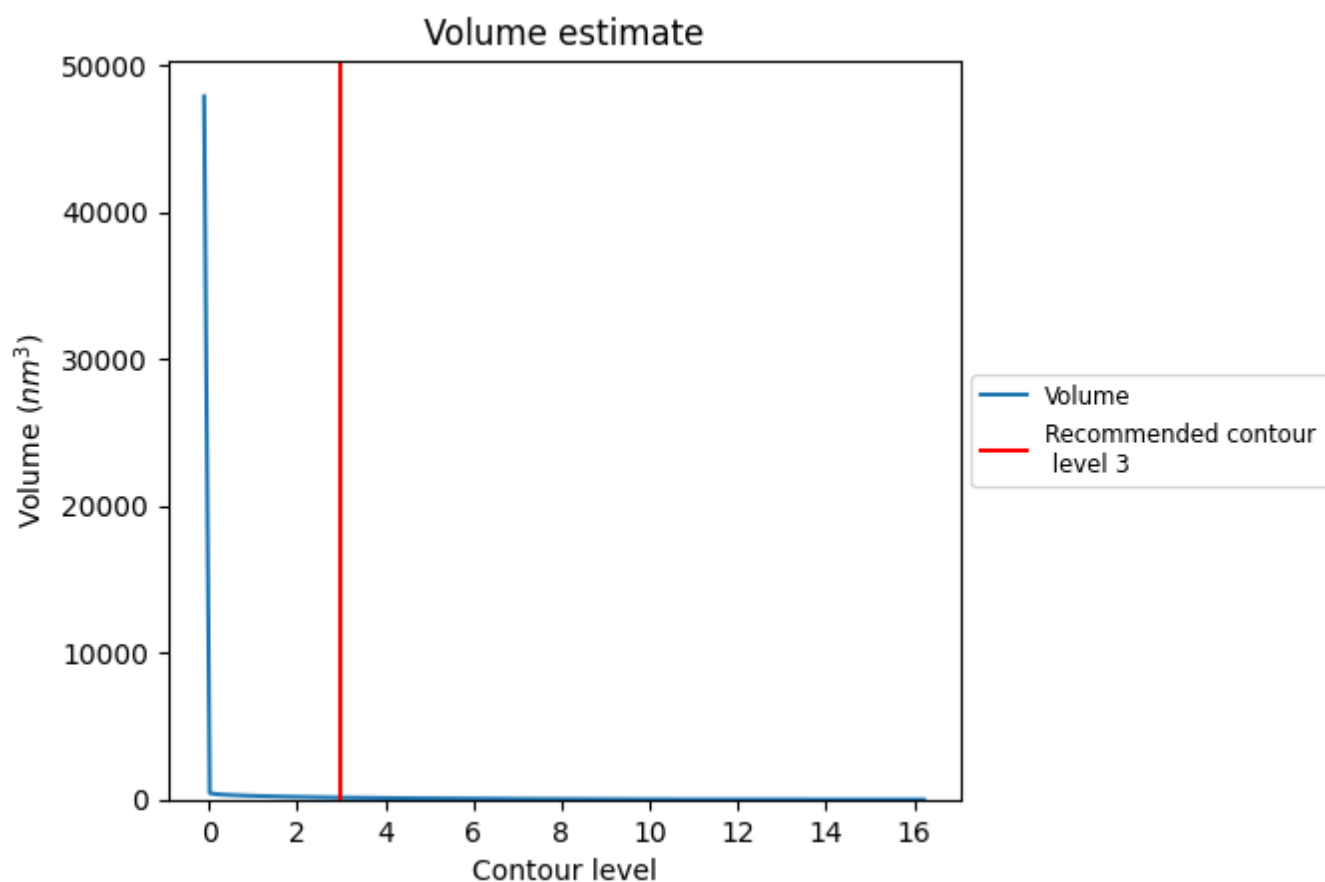
This section contains the results of statistical analysis of the map.

### 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](#)

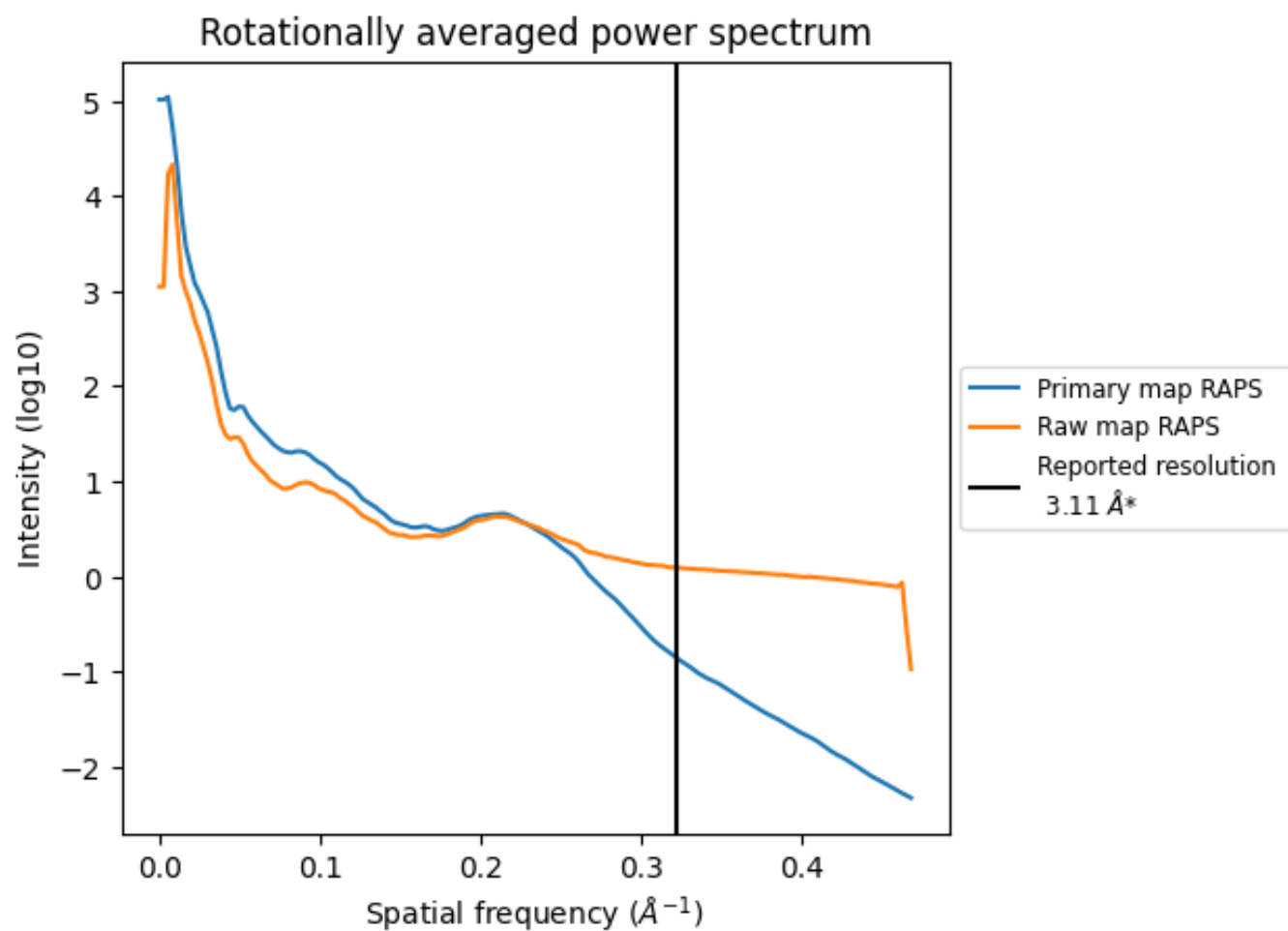


The volume at the recommended contour level is 134  $\text{nm}^3$ ; this corresponds to an approximate mass of 121 kDa.

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 ⓘ

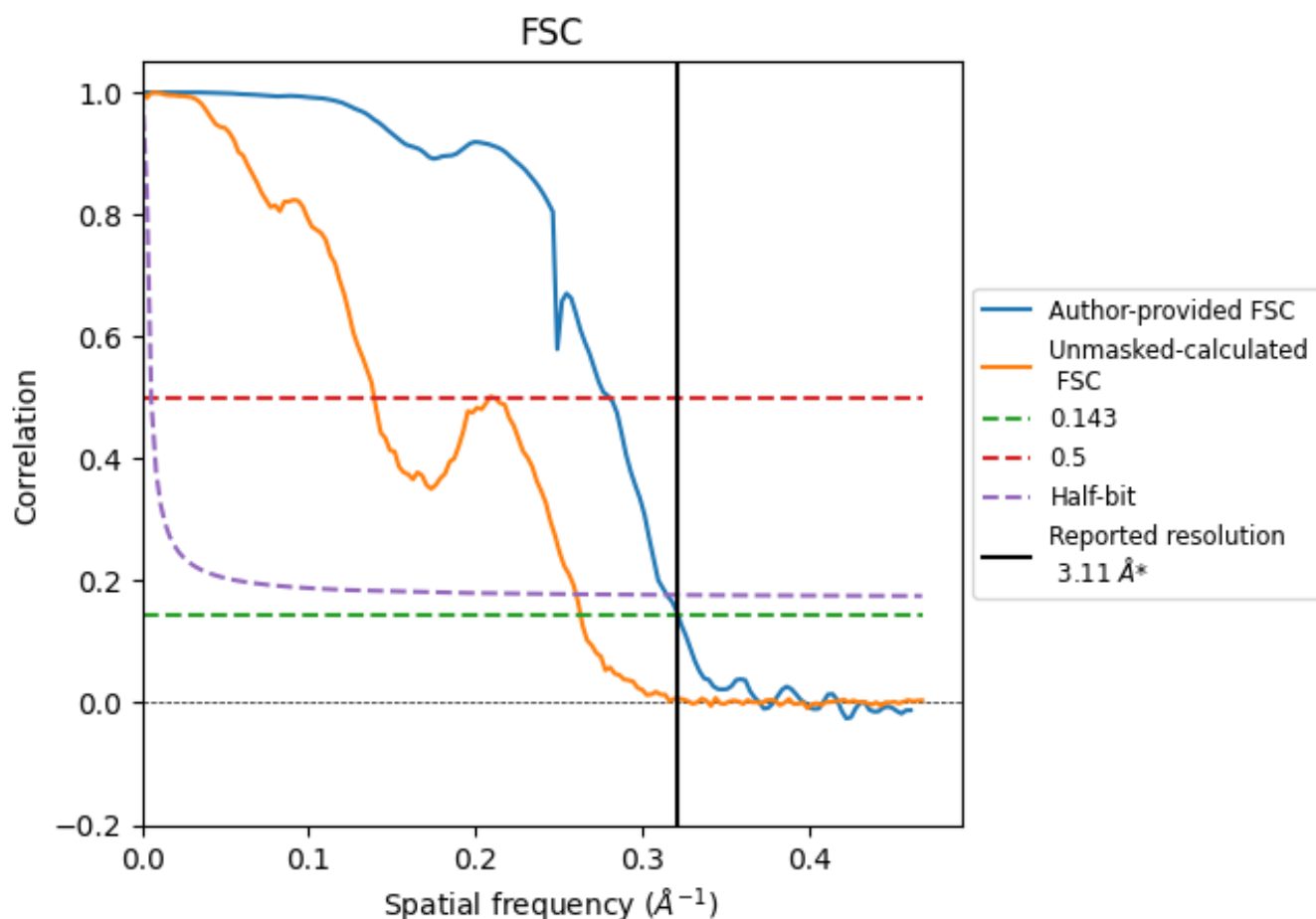


\*Reported resolution corresponds to spatial frequency of  $0.322 \text{ \AA}^{-1}$

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

## 8.2 Resolution estimates [i](#)

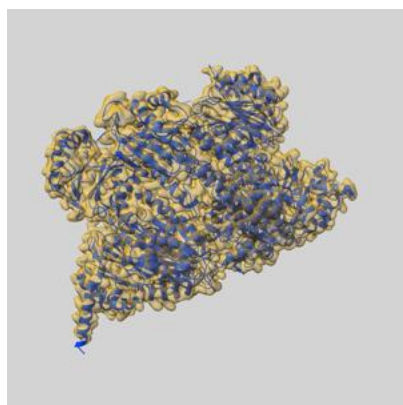
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.57	3.17
Unmasked-calculated*	3.80	7.18	3.84

\*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 3.80 differs from the reported value 3.11 by more than 10 %

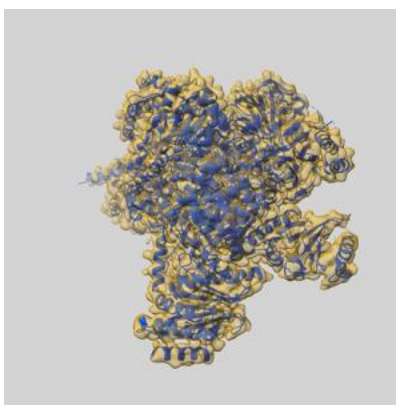
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46535 and PDB model 9D3I. Per-residue inclusion information can be found in section 3 on page 7.

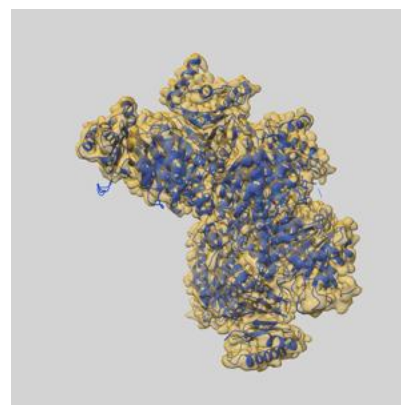
### 9.1 Map-model overlay [i](#)



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](#)



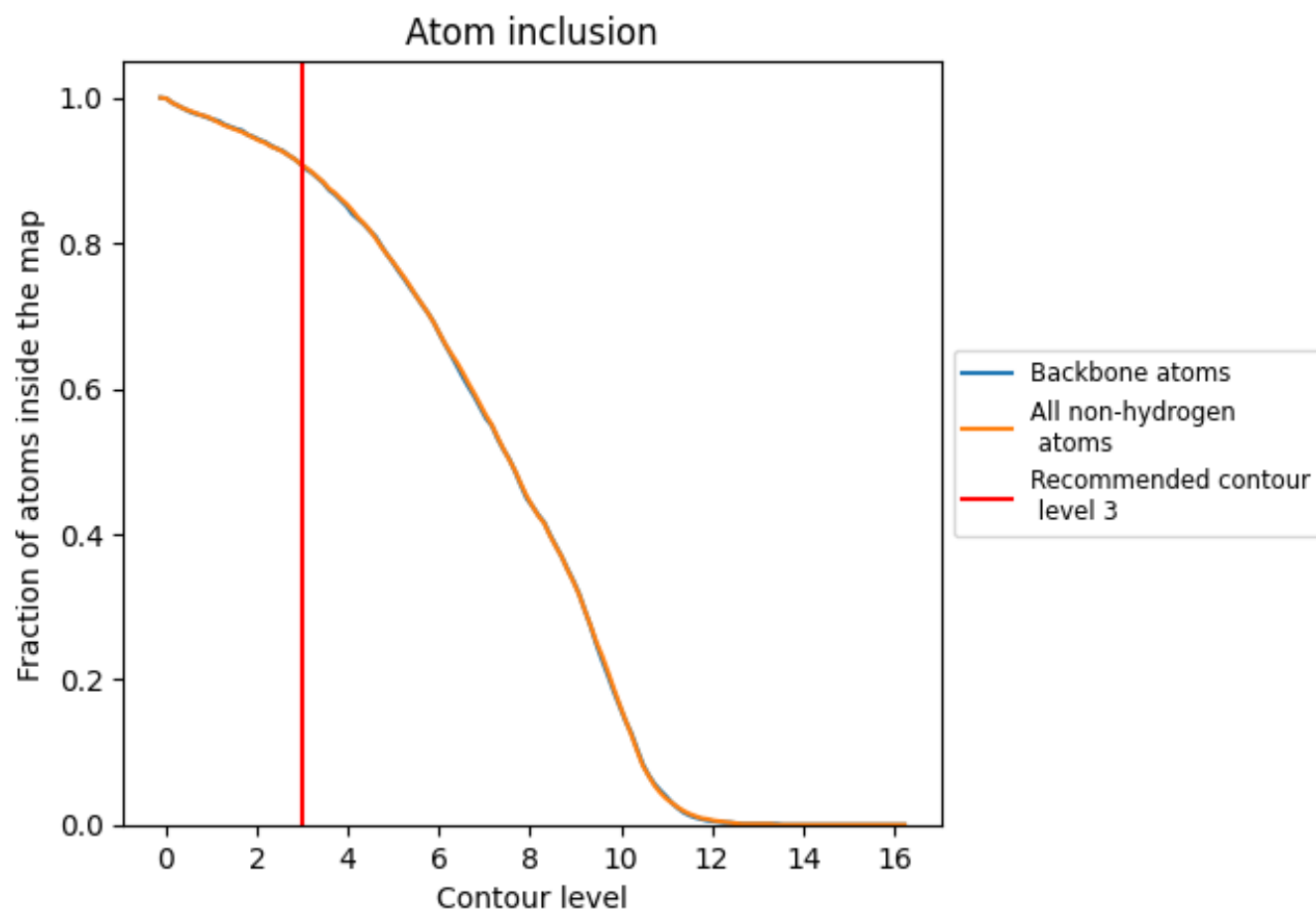
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 91% 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> 0.9070	<div></div> 0.5550
A	<div></div> 0.9550	<div></div> 0.5980
B	<div></div> 0.9480	<div></div> 0.5920
C	<div></div> 0.9400	<div></div> 0.5810
D	<div></div> 0.9080	<div></div> 0.5520
G	<div></div> 0.8400	<div></div> 0.4970
H	<div></div> 0.7840	<div></div> 0.4480
I	<div></div> 0.9340	<div></div> 0.5810
J	<div></div> 0.9300	<div></div> 0.5700
K	<div></div> 0.8870	<div></div> 0.5370
P	<div></div> 0.9210	<div></div> 0.5560

