



## wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 12:50 pm GMT

PDB ID : 6RDA  
EMDB ID : EMD-4811  
Title : CryoEM structure of Polytomella F-ATP synthase, Primary rotary state 1, monomer-masked refinement  
Authors : Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.  
Deposited on : 2019-04-12  
Resolution : 3.04 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) : 2.31.3

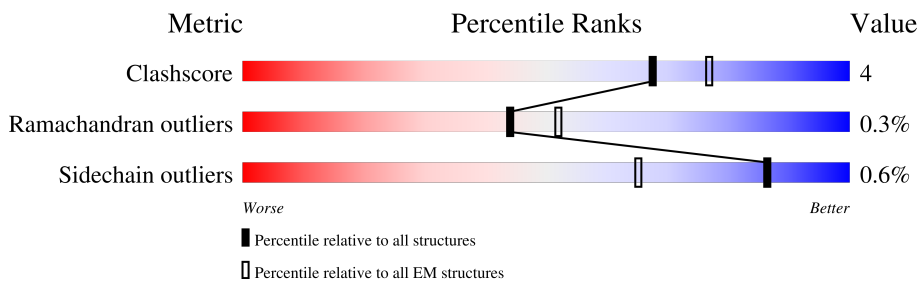
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.04 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	158937	4297
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	0	82	
2	1	618	
3	2	441	
4	3	325	
5	4	294	
6	5	123	
7	6	151	
8	7	190	

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Mol	Chain	Length	Quality of chain
9	8	89	
10	9	97	
11	M	327	
12	P	229	
13	T	562	

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 19856 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	81	607	388	107	110	2	0	0

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	595	4661	2958	798	900	5	0	0

- Molecule 3 is a protein called ASA-2: Polytomella F-ATP synthase associated subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	2	441	3163	2020	532	611	0	0

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	245	1874	1204	299	370	1	0	0

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	290	2177	1385	356	434	2	0	0

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	123	986	640	172	170	4	0	0

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	124	926	599	154	172	1	0	0

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	176	1347	860	227	259	1	0	0

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	8	88	692	456	115	121	0	0

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	97	776	514	124	132	6	0	0

- Molecule 11 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	217	1640	1077	267	288	8	0	0

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit OSCP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	80	646	418	105	120	3	0	0

- Molecule 13 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	T	40	330	215	56	59	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total Zn 1 1	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	AltConf
15	1	2	Total O 2 2	0
15	5	1	Total O 1 1	0
15	6	6	Total O 6 6	0
15	M	21	Total O 21 21	0

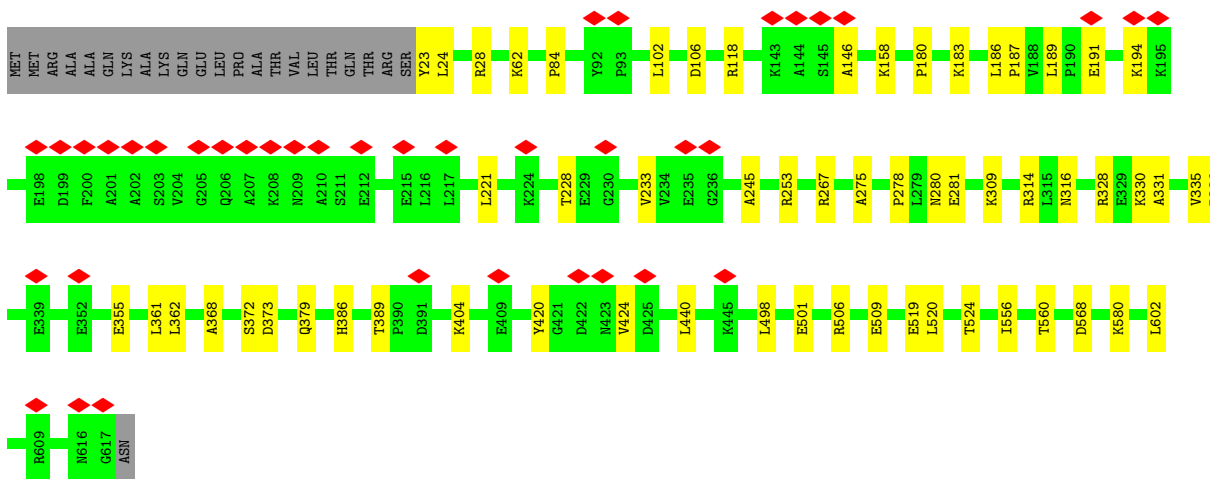
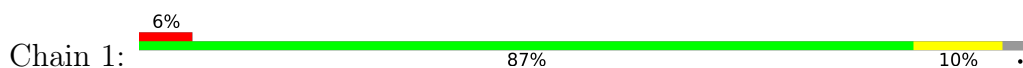
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

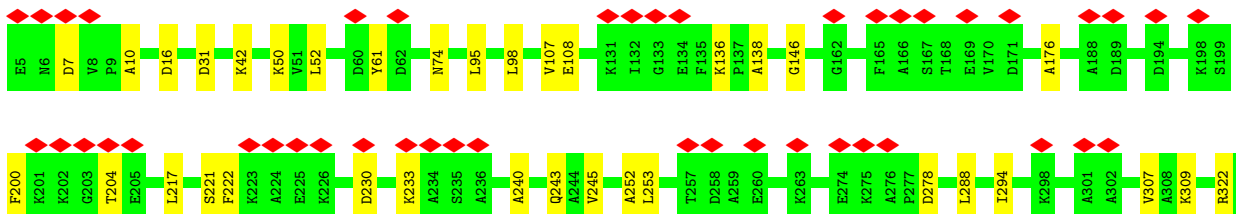
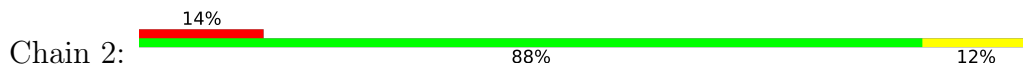
- Molecule 1: ASA-10: Polytomella F-ATP synthase associated subunit 10



- Molecule 2: ATP synthase associated protein ASA1

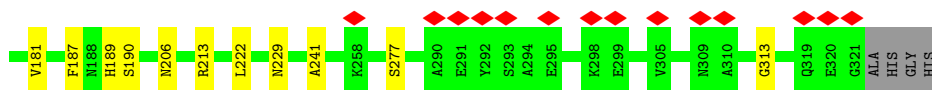
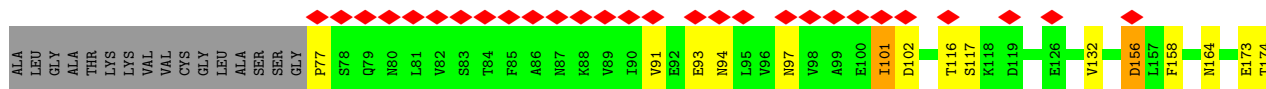
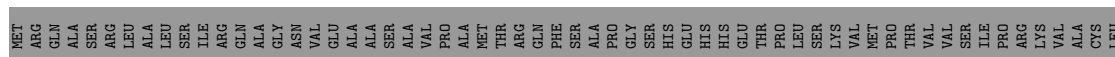


- Molecule 3: ASA-2: Polytomella F-ATP synthase associated subunit 2

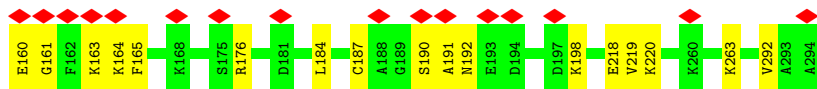
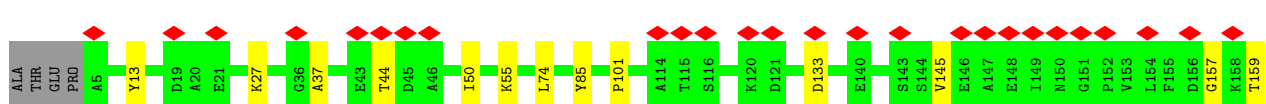
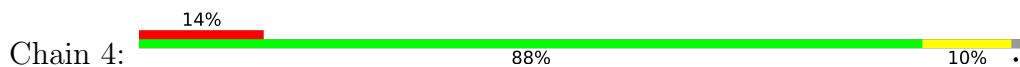




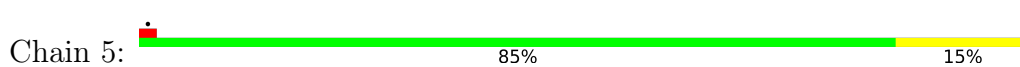
• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein



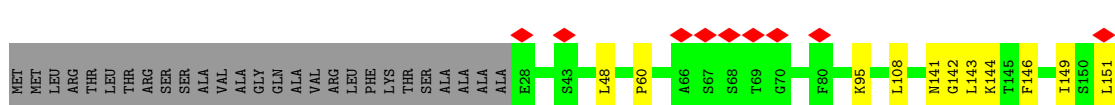
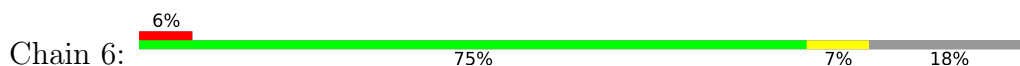
• Molecule 5: Mitochondrial ATP synthase associated protein ASA4



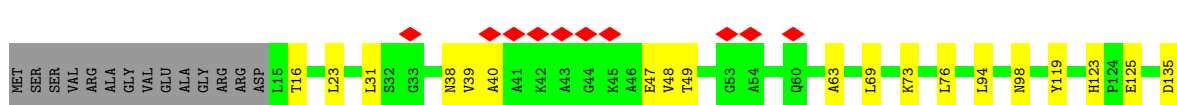
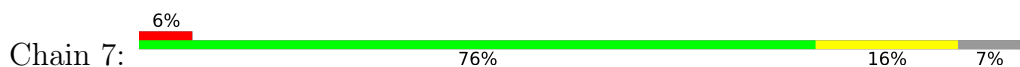
• Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein



• Molecule 7: Mitochondrial ATP synthase subunit ASA6



• Molecule 8: Mitochondrial ATP synthase associated protein ASA7









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	400918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.242	Depositor
Minimum map value	-0.158	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.60	0/628	0.53	0/856
2	1	0.61	0/4750	0.57	0/6434
3	2	0.48	0/3212	0.57	0/4371
4	3	0.57	0/1911	0.56	1/2601 (0.0%)
5	4	0.57	0/2216	0.57	0/3000
6	5	0.79	0/1011	0.67	0/1376
7	6	0.65	0/946	0.61	0/1287
8	7	0.71	0/1374	0.60	0/1865
9	8	0.72	0/715	0.63	0/974
10	9	0.47	0/802	0.58	0/1084
11	M	0.69	0/1683	0.63	0/2295
12	P	0.42	0/653	0.65	0/872
13	T	0.56	0/338	0.64	0/454
All	All	0.60	0/20239	0.59	1/27469 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	1
12	P	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	77	PRO	N-CA-CB	5.87	110.34	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	222	PHE	Peptide
12	P	185	VAL	Peptide

## 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	0	607	0	584	2	0
2	1	4661	0	4695	36	0
3	2	3163	0	3262	29	0
4	3	1874	0	1826	14	0
5	4	2177	0	2169	20	0
6	5	986	0	1021	14	0
7	6	926	0	941	9	0
8	7	1347	0	1345	27	0
9	8	692	0	694	9	0
10	9	776	0	757	5	0
11	M	1640	0	1665	13	0
12	P	646	0	681	7	0
13	T	330	0	342	5	0
14	M	1	0	0	0	0
15	1	2	0	0	0	0
15	5	1	0	0	0	0
15	6	6	0	0	0	0
15	M	21	0	0	1	0
All	All	19856	0	19982	154	0

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

The worst 5 of 154 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)
11:M:223:PRO:O	11:M:227:ILE:HG12	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:123:HIS:HD2	8:7:125:GLU:H	1.35	0.73
2:1:404:LYS:HZ1	6:5:78:GLU:HB3	1.57	0.70
8:7:170:HIS:HD2	8:7:172:ALA:H	1.41	0.68
12:P:156:VAL:HG11	12:P:170:LEU:HD21	1.74	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
2	1	593/618 (96%)	578 (98%)	15 (2%)	0	100	100
3	2	439/441 (100%)	417 (95%)	21 (5%)	1 (0%)	47	80
4	3	243/325 (75%)	231 (95%)	11 (4%)	1 (0%)	34	69
5	4	288/294 (98%)	277 (96%)	11 (4%)	0	100	100
6	5	121/123 (98%)	113 (93%)	7 (6%)	1 (1%)	19	54
7	6	122/151 (81%)	113 (93%)	9 (7%)	0	100	100
8	7	174/190 (92%)	167 (96%)	7 (4%)	0	100	100
9	8	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
10	9	95/97 (98%)	79 (83%)	15 (16%)	1 (1%)	14	47
11	M	213/327 (65%)	204 (96%)	9 (4%)	0	100	100
12	P	78/229 (34%)	71 (91%)	5 (6%)	2 (3%)	5	24
13	T	38/562 (7%)	30 (79%)	7 (18%)	1 (3%)	5	24
All	All	2569/3528 (73%)	2432 (95%)	130 (5%)	7 (0%)	44	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	3	101	ILE
3	2	383	PRO
12	P	186	MET
13	T	56	LYS
10	9	74	GLU

### 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	0	63/64 (98%)	63 (100%)	0	100	100
2	1	493/512 (96%)	492 (100%)	1 (0%)	93	98
3	2	312/312 (100%)	310 (99%)	2 (1%)	86	94
4	3	195/258 (76%)	193 (99%)	2 (1%)	76	91
5	4	220/223 (99%)	217 (99%)	3 (1%)	67	86
6	5	107/107 (100%)	106 (99%)	1 (1%)	78	91
7	6	96/115 (84%)	95 (99%)	1 (1%)	76	91
8	7	140/150 (93%)	139 (99%)	1 (1%)	84	93
9	8	71/72 (99%)	71 (100%)	0	100	100
10	9	79/79 (100%)	79 (100%)	0	100	100
11	M	178/272 (65%)	177 (99%)	1 (1%)	86	94
12	P	73/196 (37%)	73 (100%)	0	100	100
13	T	36/448 (8%)	36 (100%)	0	100	100
All	All	2063/2808 (74%)	2051 (99%)	12 (1%)	86	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4	198	LYS
6	5	113	VAL
11	M	199	LYS
7	6	146	PHE
4	3	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
11	M	108	ASN
11	M	163	ASN
13	T	64	GLN
3	2	243	GLN
3	2	177	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.



## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

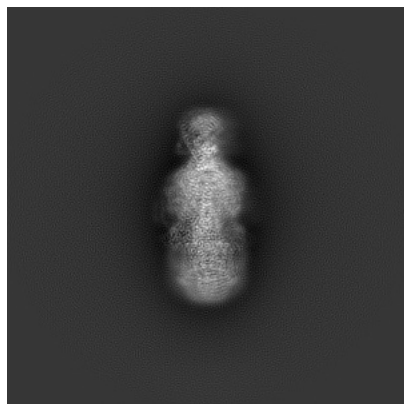
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4811. These allow visual inspection of the internal detail of the map and identification of artifacts.

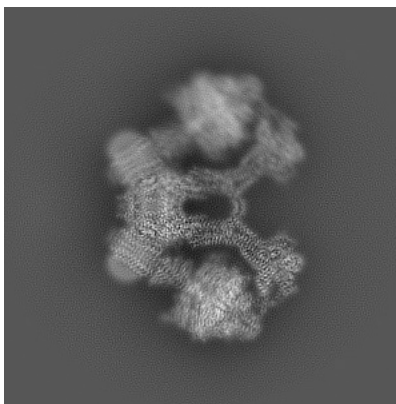
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

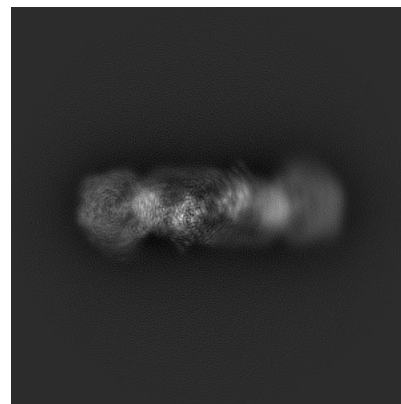
#### 6.1.1 Primary map



X

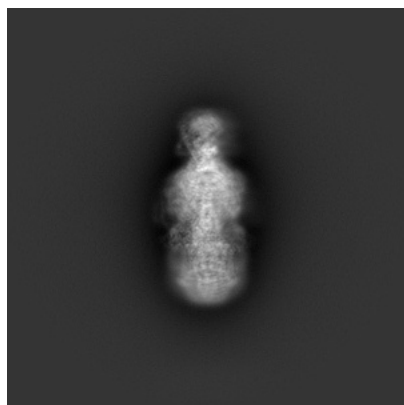


Y

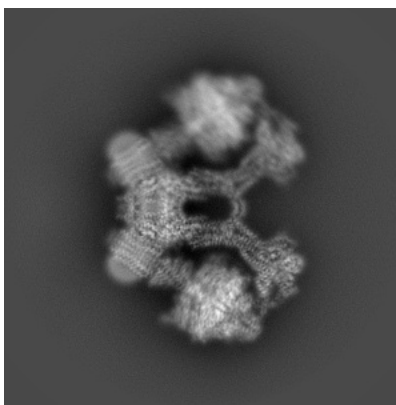


Z

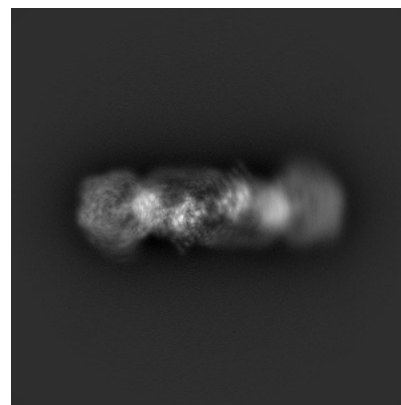
#### 6.1.2 Raw map



X



Y



Z

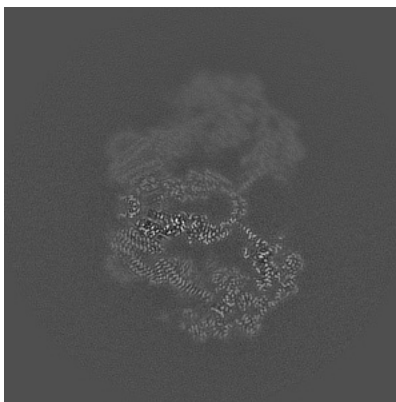
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

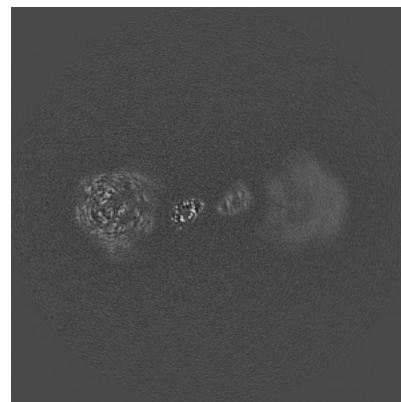
### 6.2.1 Primary map



X Index: 240

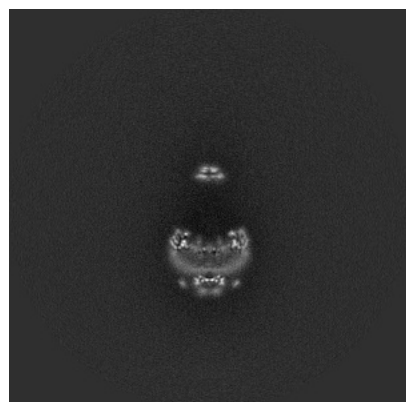


Y Index: 240

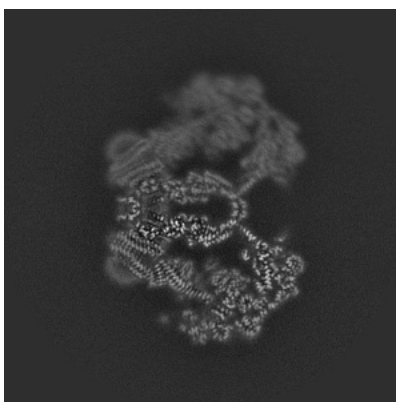


Z Index: 240

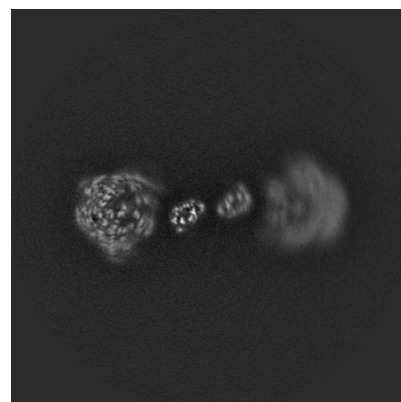
### 6.2.2 Raw map



X Index: 240



Y Index: 240

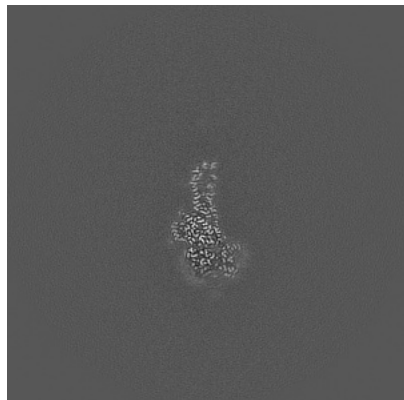


Z Index: 240

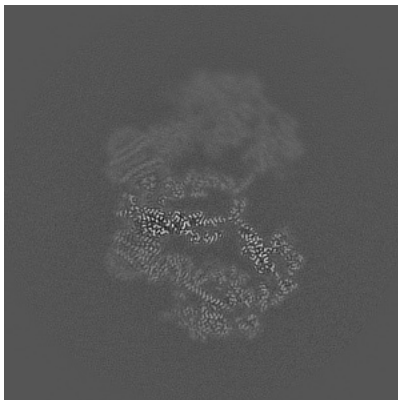
The images above show central slices of the map in three orthogonal directions.

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

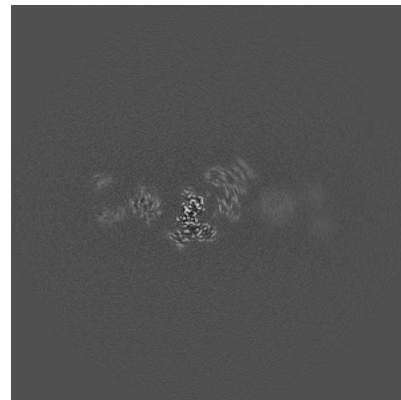
### 6.3.1 Primary map



X Index: 216

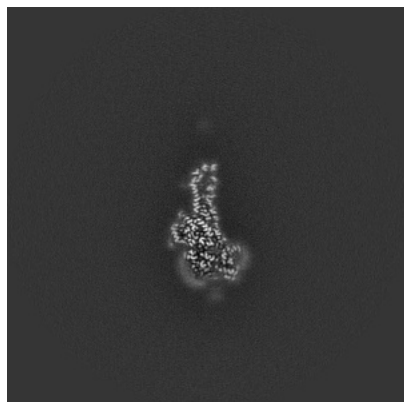


Y Index: 235

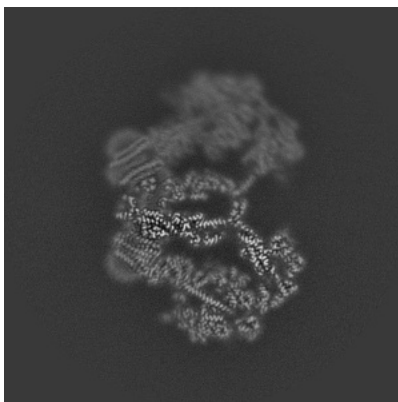


Z Index: 206

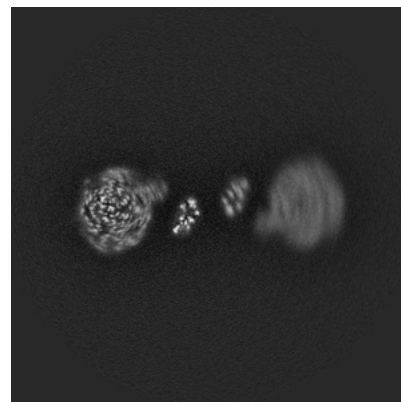
### 6.3.2 Raw map



X Index: 216



Y Index: 235

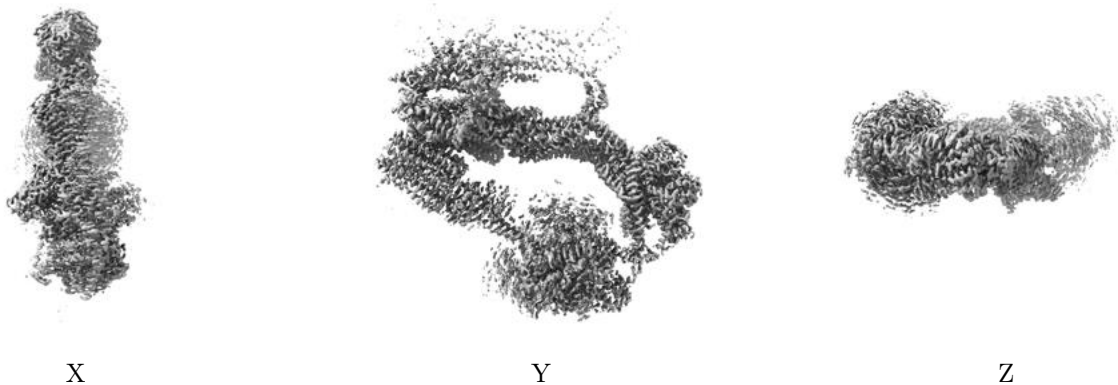


Z Index: 262

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

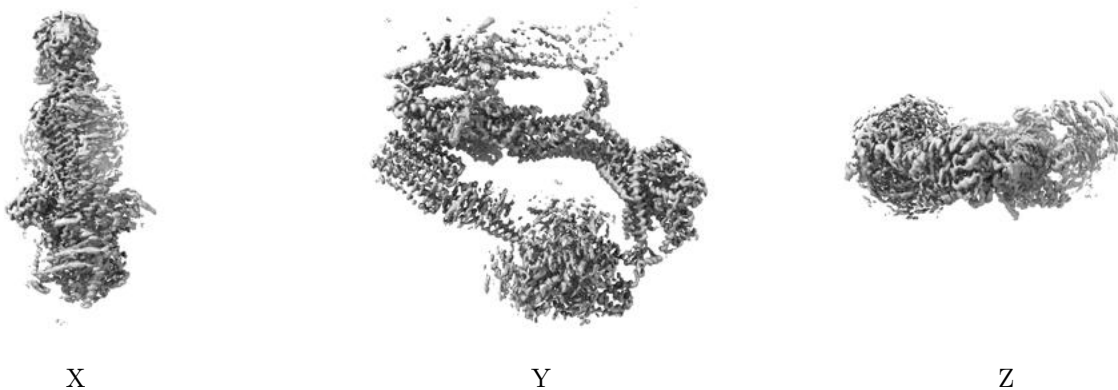
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

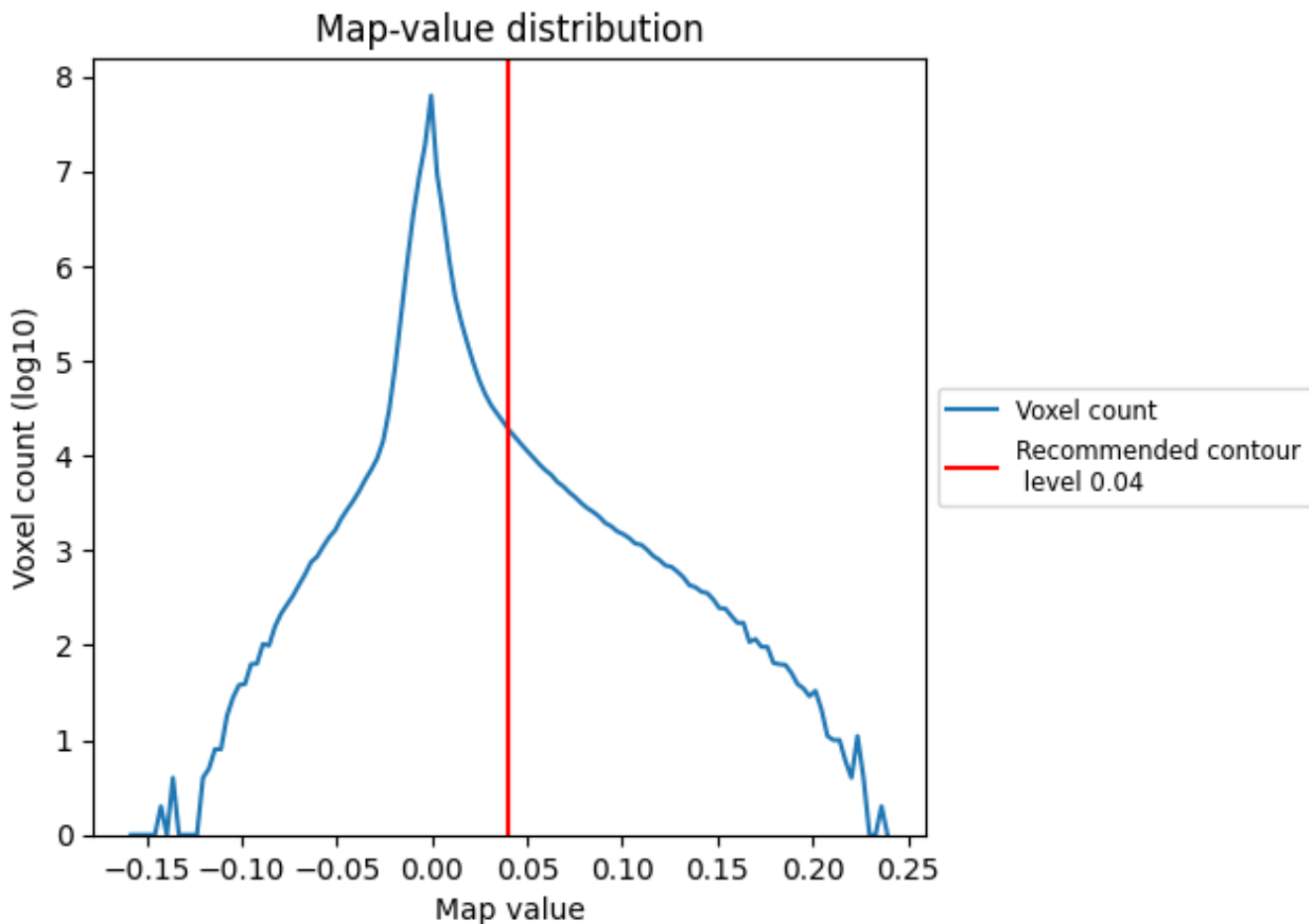
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

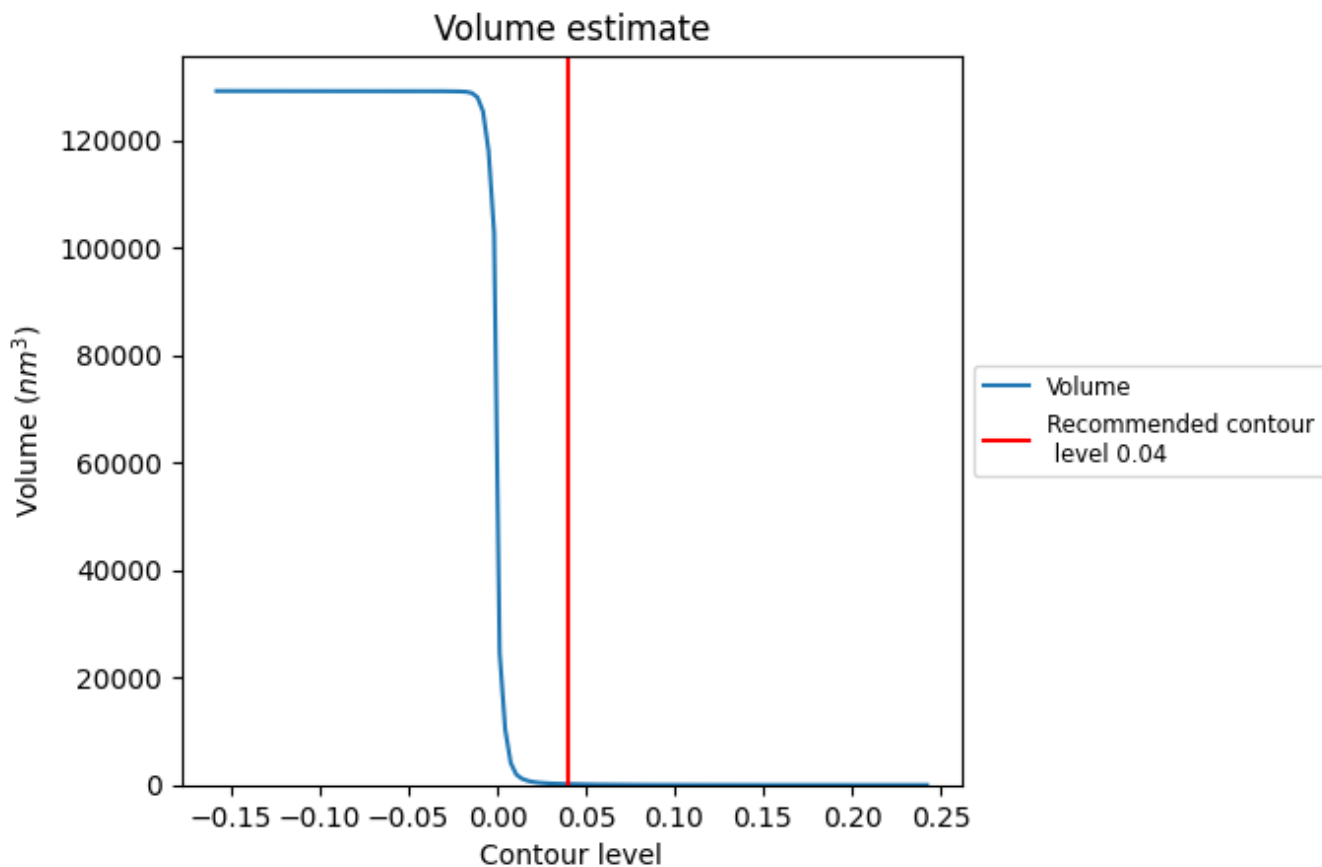
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

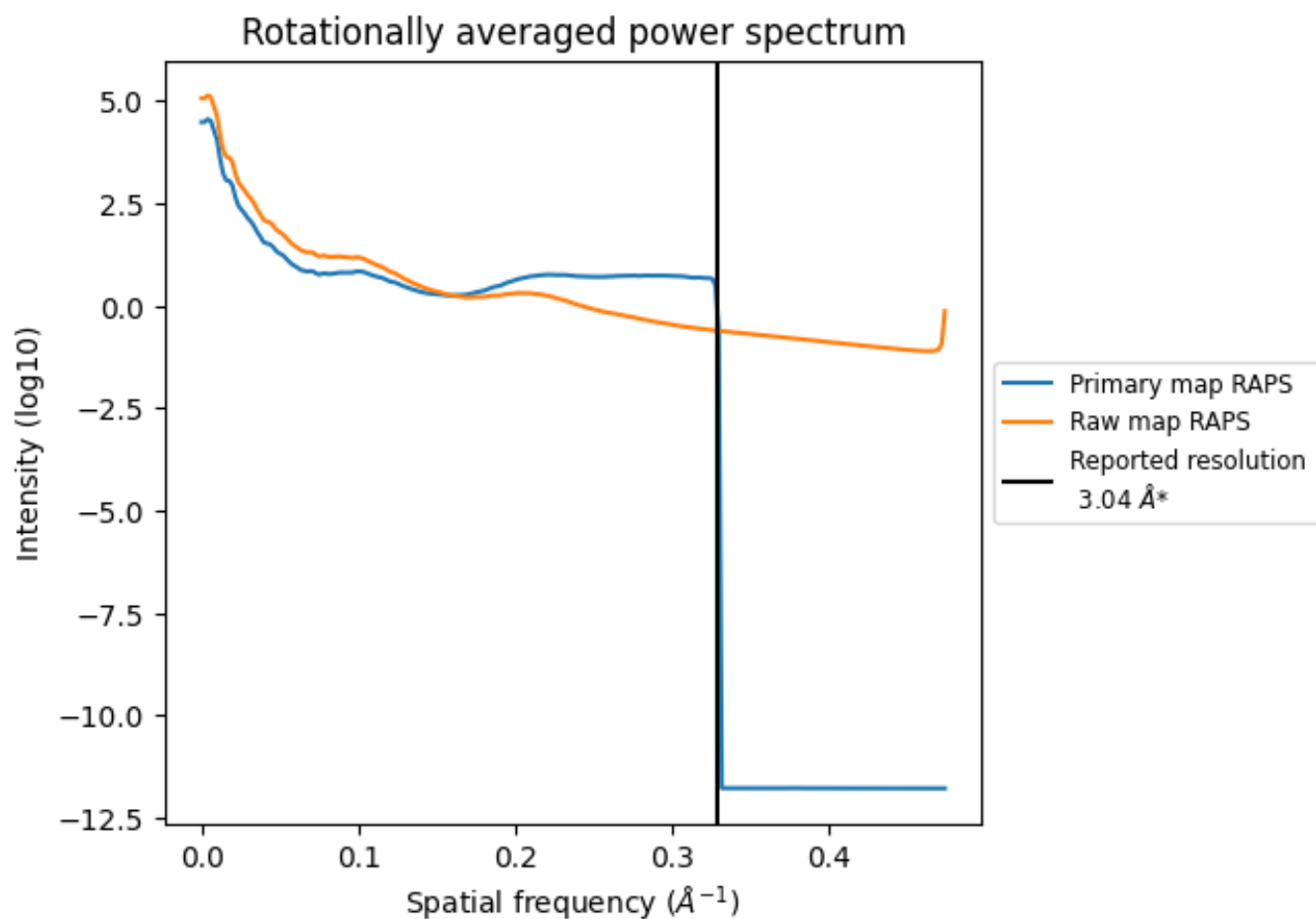
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165  $\text{nm}^3$ ; this corresponds to an approximate mass of 149 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](#)



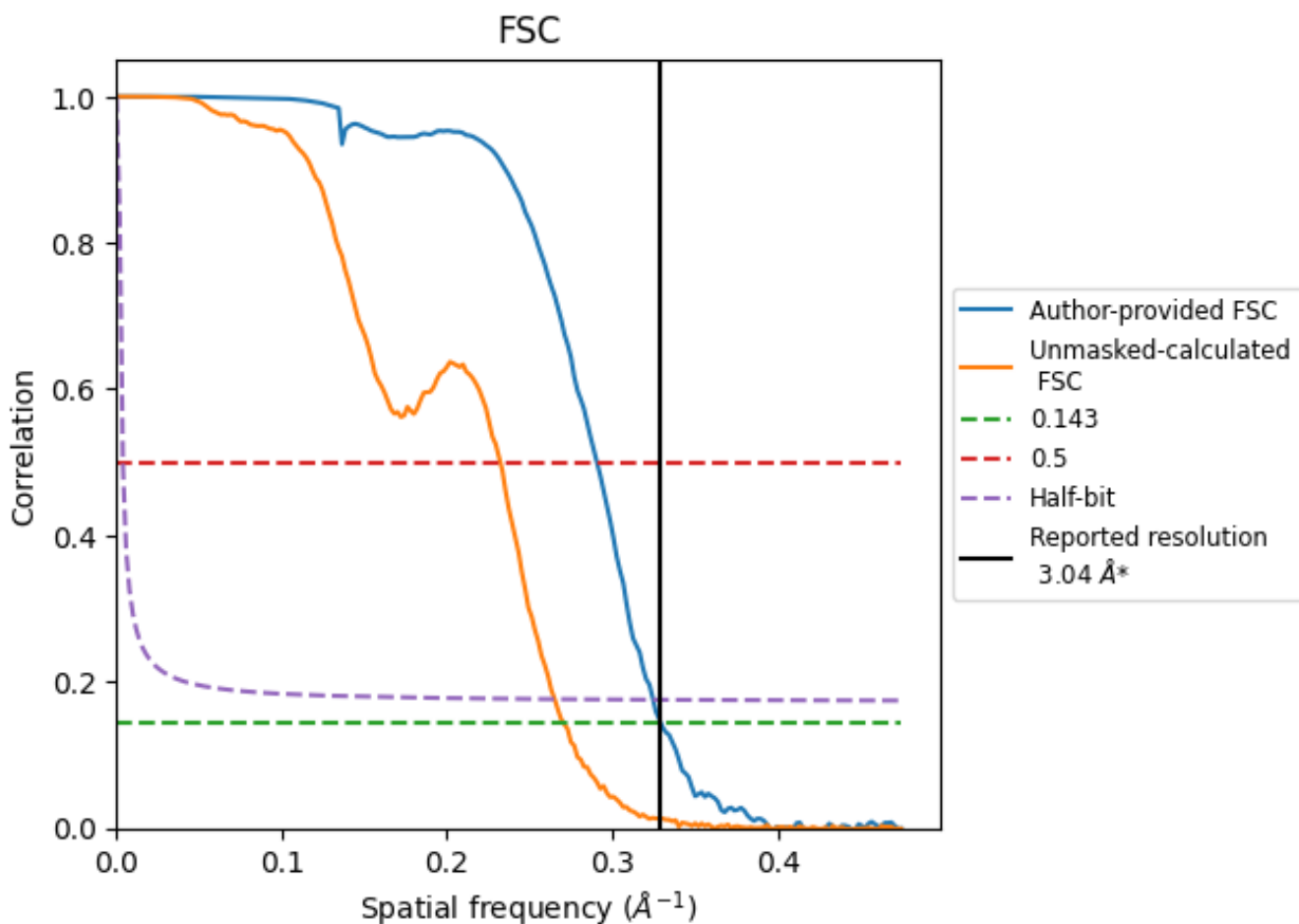
\*Reported resolution corresponds to spatial frequency of 0.329 Å<sup>-1</sup>



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

## 8.2 Resolution estimates [i](#)

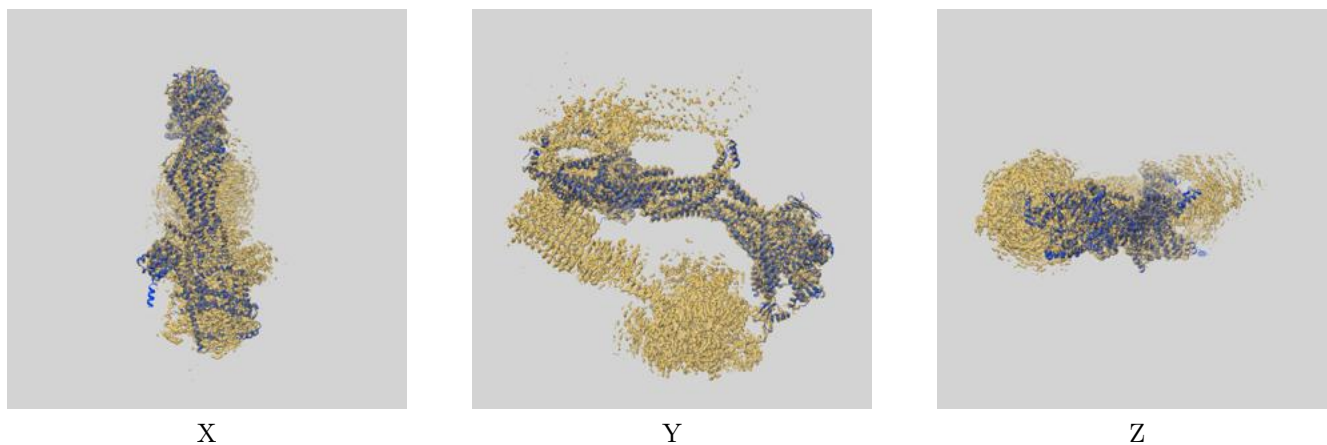
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.03	3.44	3.08
Unmasked-calculated*	3.70	4.30	3.77

\*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 3.70 differs from the reported value 3.04 by more than 10 %

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

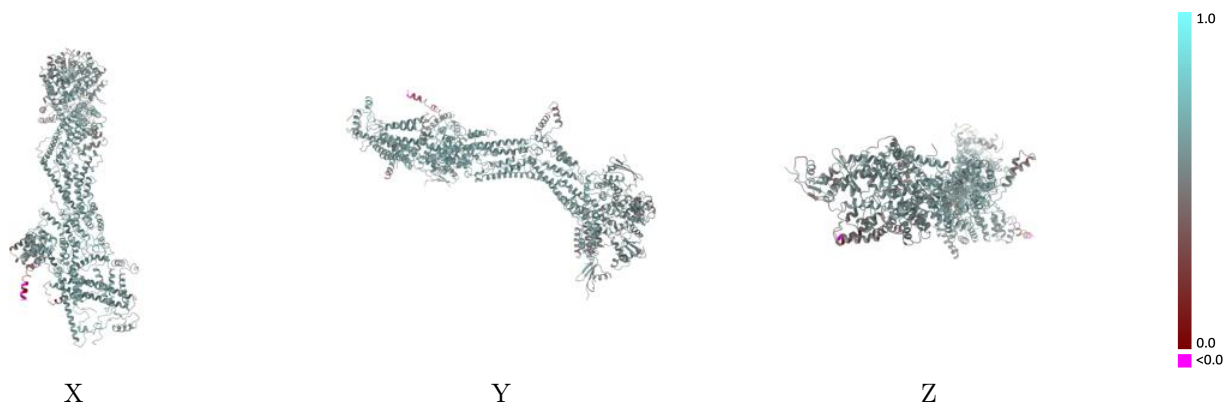
This section contains information regarding the fit between EMDB map EMD-4811 and PDB model 6RDA. Per-residue inclusion information can be found in section 3 on page 7.

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



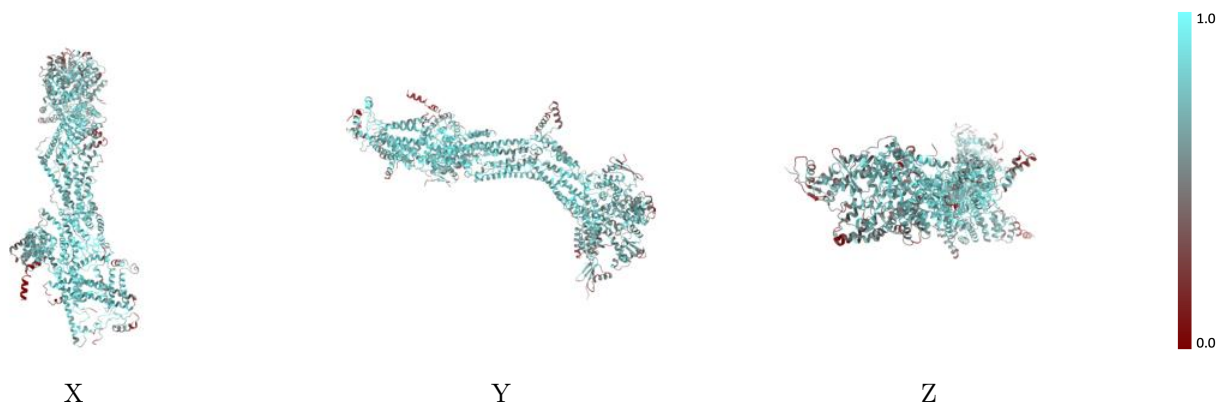
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



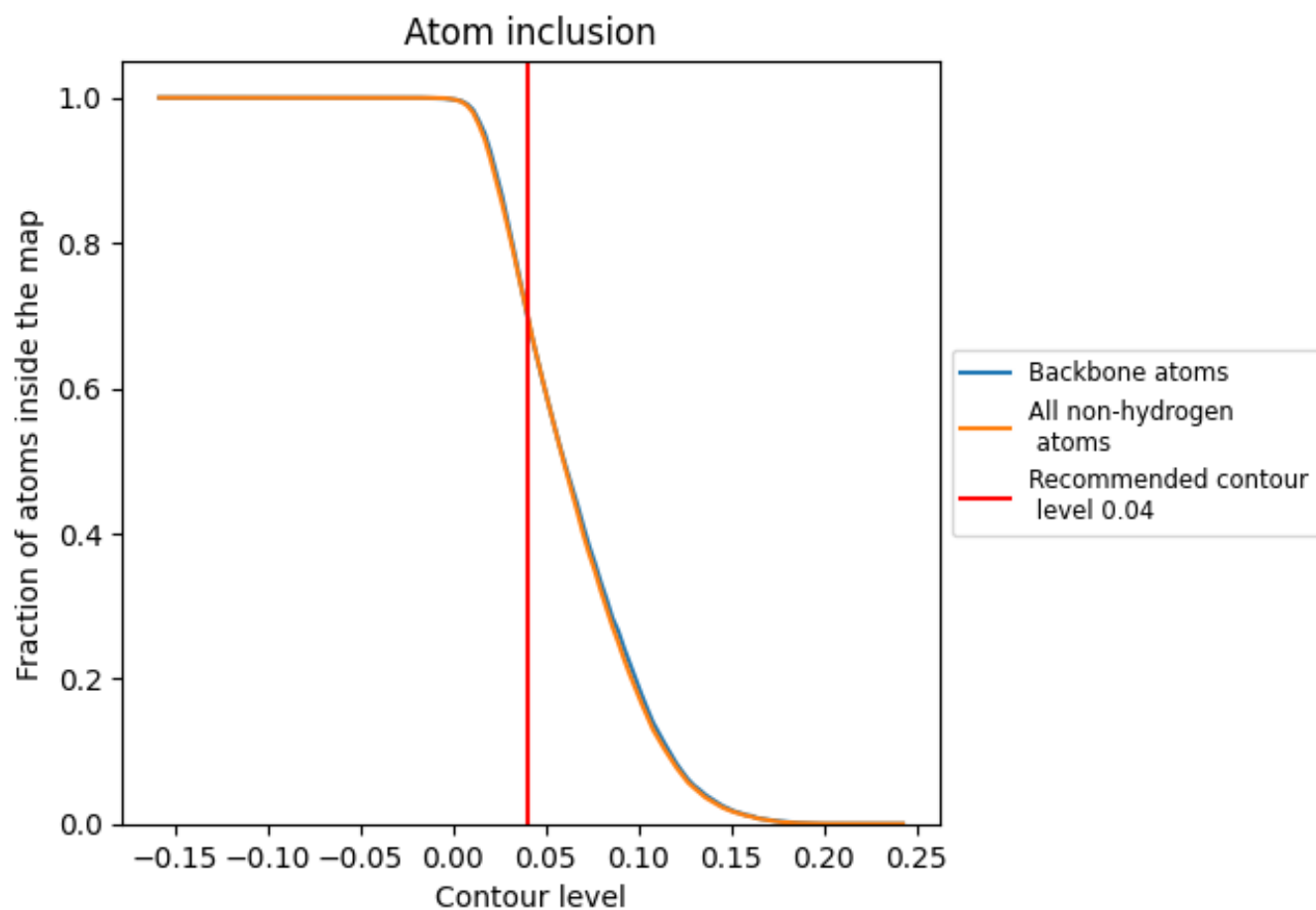
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).





























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7034	 0.5600
0	 0.7504	 0.5820
1	 0.7476	 0.5810
2	 0.6456	 0.5380
3	 0.6427	 0.5240
4	 0.6628	 0.5420
5	 0.8363	 0.6040
6	 0.7547	 0.5820
7	 0.7678	 0.5760
8	 0.7994	 0.5910
9	 0.5916	 0.5240
M	 0.7622	 0.5810
P	 0.5023	 0.5000
T	 0.7015	 0.5520

