



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 05:32 pm BST

PDB ID : 8CR2
EMDB ID : EMD-16802
Title : Homo sapiens Get1/Get2 heterotetramer (a3' deletion variant) in complex with a Get3 dimer
Authors : McDowell, M.A.; Heimes, M.; Wild, K.; Sinning, I.
Deposited on : 2023-03-07
Resolution : 4.20 Å(reported)
Based on initial model : 6SO5

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
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) : 2.39

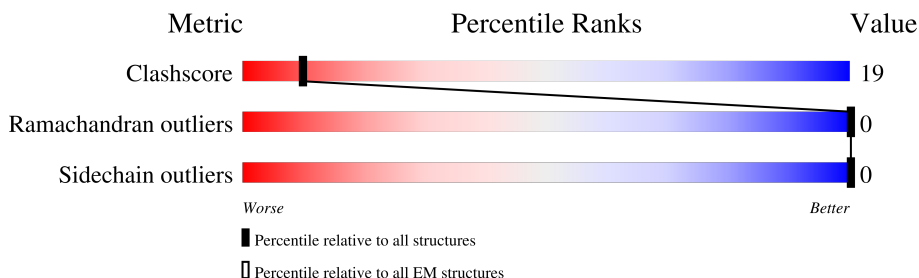
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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 ≥ 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	360	<div> <div>36%</div> <div>47%</div> <div>28%</div> <div>26%</div> </div>
1	B	360	<div> <div>28%</div> <div>45%</div> <div>27%</div> <div>27%</div> </div>
2	C	306	<div> <div>16%</div> <div>13%</div> <div>18%</div> <div>68%</div> </div>
2	D	306	<div> <div>43%</div> <div>45%</div> <div>29%</div> <div>25%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6838 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 ATPase ASNA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	268	Total	C	N	O	S	0	0
			2113	1352	350	397	14		
1	B	262	Total	C	N	O	S	0	0
			2066	1324	342	387	13		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O43681
A	0	ALA	-	expression tag	UNP O43681
A	349	GLY	-	expression tag	UNP O43681
A	350	SER	-	expression tag	UNP O43681
A	351	TRP	-	expression tag	UNP O43681
A	352	SER	-	expression tag	UNP O43681
A	353	HIS	-	expression tag	UNP O43681
A	354	PRO	-	expression tag	UNP O43681
A	355	GLN	-	expression tag	UNP O43681
A	356	PHE	-	expression tag	UNP O43681
A	357	GLU	-	expression tag	UNP O43681
A	358	LYS	-	expression tag	UNP O43681
B	-1	GLY	-	expression tag	UNP O43681
B	0	ALA	-	expression tag	UNP O43681
B	349	GLY	-	expression tag	UNP O43681
B	350	SER	-	expression tag	UNP O43681
B	351	TRP	-	expression tag	UNP O43681
B	352	SER	-	expression tag	UNP O43681
B	353	HIS	-	expression tag	UNP O43681
B	354	PRO	-	expression tag	UNP O43681
B	355	GLN	-	expression tag	UNP O43681
B	356	PHE	-	expression tag	UNP O43681
B	357	GLU	-	expression tag	UNP O43681
B	358	LYS	-	expression tag	UNP O43681

- Molecule 2 is a protein called Guided entry of tail-anchored proteins factor CAMLG, Guided

entry of tail-anchored proteins factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	97	Total	C	N	O	S	0	0
			802	515	138	142	7		
2	D	228	Total	C	N	O	S	0	0
			1856	1228	303	308	17		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	185	MET	-	initiating methionine	UNP P49069
C	242	GLY	-	linker	UNP P49069
C	243	GLY	-	linker	UNP P49069
C	244	GLY	-	linker	UNP P49069
C	245	GLY	-	linker	UNP P49069
C	297	GLY	-	linker	UNP P49069
C	298	SER	-	linker	UNP P49069
C	299	GLY	-	linker	UNP P49069
C	300	SER	-	linker	UNP P49069
C	301	GLU	-	linker	UNP P49069
C	302	ASN	-	linker	UNP P49069
C	303	LEU	-	linker	UNP P49069
C	304	TYR	-	linker	UNP P49069
C	305	PHE	-	linker	UNP P49069
C	306	GLN	-	linker	UNP P49069
C	307	SER	-	linker	UNP P49069
C	308	GLY	-	linker	UNP P49069
C	309	SER	-	linker	UNP P49069
C	310	GLY	-	linker	UNP P49069
C	311	SER	-	linker	UNP P49069
C	1175	GLY	-	expression tag	UNP O00258
C	1176	SER	-	expression tag	UNP O00258
C	1177	GLY	-	expression tag	UNP O00258
C	1178	SER	-	expression tag	UNP O00258
C	1179	LEU	-	expression tag	UNP O00258
C	1180	GLU	-	expression tag	UNP O00258
C	1181	VAL	-	expression tag	UNP O00258
C	1182	LEU	-	expression tag	UNP O00258
C	1183	PHE	-	expression tag	UNP O00258
C	1184	GLN	-	expression tag	UNP O00258
D	185	MET	-	initiating methionine	UNP P49069
D	242	GLY	-	linker	UNP P49069
D	243	GLY	-	linker	UNP P49069
D	244	GLY	-	linker	UNP P49069

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Chain	Residue	Modelled	Actual	Comment	Reference
D	245	GLY	-	linker	UNP P49069
D	297	GLY	-	linker	UNP P49069
D	298	SER	-	linker	UNP P49069
D	299	GLY	-	linker	UNP P49069
D	300	SER	-	linker	UNP P49069
D	301	GLU	-	linker	UNP P49069
D	302	ASN	-	linker	UNP P49069
D	303	LEU	-	linker	UNP P49069
D	304	TYR	-	linker	UNP P49069
D	305	PHE	-	linker	UNP P49069
D	306	GLN	-	linker	UNP P49069
D	307	SER	-	linker	UNP P49069
D	308	GLY	-	linker	UNP P49069
D	309	SER	-	linker	UNP P49069
D	310	GLY	-	linker	UNP P49069
D	311	SER	-	linker	UNP P49069
D	1175	GLY	-	expression tag	UNP O00258
D	1176	SER	-	expression tag	UNP O00258
D	1177	GLY	-	expression tag	UNP O00258
D	1178	SER	-	expression tag	UNP O00258
D	1179	LEU	-	expression tag	UNP O00258
D	1180	GLU	-	expression tag	UNP O00258
D	1181	VAL	-	expression tag	UNP O00258
D	1182	LEU	-	expression tag	UNP O00258
D	1183	PHE	-	expression tag	UNP O00258
D	1184	GLN	-	expression tag	UNP O00258

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	

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.

Chain A:

36% 47% 28% 26%

GLY
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ALA
GLY
VAL
ALA
ALA
TRP
GLY
VAL
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GLU
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PRO
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VAL
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P23
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T27
L28
S29
N30
L31
L32
E33
Q34
R35
S36
L37
K38
W39
L40
F41
V42
G43
G44
K45
P46
G47
V48
G49
K50
T51
T52
C53
S56
L57
A58
V59
Q60

L61
S62
K63
G64
R65
E66
S67
T71
S72
T73
D74
P75
A76
H77
N78
S80
D81
A82
F83
D84
K85
K86
F87
S88
K89
T92
K93
Y94
K95
G96
N99
K98
L100
F101
A102
M103
I104
I105
D106
P107
S108
L109
V110
A111
A112
G113
L114
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L398
L399
L400

LEU
SER
MET
GLN
LYS
MET
MET
GLN
ALA
ALA
SER
SER
PHE
P140
G141
I142
D143
E144
A145
Y1

Chain B:

28%

45%

27%

27%

GLY
ALA
MET
ALA
ALA
GLY
VAL
ALA
GLY
TRP
GLY
VAL
GLU
ALA
GLU
GLU
PHE
GLU
ASP
ALA
PRO
ASP
VAL
P23
L24
E25
P26
T27
L28
I31
I32
E33
Q34
R35
W39
I40
Q44
G47
C55
S56
V59
Q60
L61
R65
E66
S67
I70
I71
S72
H77



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224354	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 ($e^-/\text{\AA}^2$)	53.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.027	Depositor
Minimum map value	-1.396	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	284.16, 284.16, 284.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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	A	0.28	0/2154	0.59	1/2911 (0.0%)
1	B	0.29	0/2107	0.62	1/2848 (0.0%)
2	C	0.30	0/815	0.75	1/1091 (0.1%)
2	D	0.29	0/1899	0.68	1/2563 (0.0%)
All	All	0.29	0/6975	0.64	4/9413 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1067	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	323	HIS	CA-C-N	5.44	129.17	117.20
1	B	84	ASP	CB-CG-OD2	5.26	123.03	118.30
2	D	1116	MET	CB-CG-SD	5.25	128.16	112.40

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	2113	0	2145	74	0
1	B	2066	0	2100	70	0
2	C	802	0	833	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1856	0	1904	77	0
3	B	1	0	0	0	0
All	All	6838	0	6982	264	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 19.

The worst 5 of 264 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:B:83:PHE:O	1:B:84:ASP:OD1	1.91	0.87
1:B:168:ALA:HB1	1:B:169:PRO:HD2	1.56	0.86
1:B:309:LEU:HD12	2:C:1070:ALA:HA	1.59	0.85
2:D:1036:SER:HA	2:D:1039:LEU:HB2	1.57	0.84
2:C:1088:THR:HA	2:C:1091:LYS:HE2	1.60	0.82

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	A	262/360 (73%)	242 (92%)	20 (8%)	0	100	100
1	B	256/360 (71%)	238 (93%)	18 (7%)	0	100	100
2	C	95/306 (31%)	92 (97%)	3 (3%)	0	100	100
2	D	220/306 (72%)	213 (97%)	7 (3%)	0	100	100
All	All	833/1332 (62%)	785 (94%)	48 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/313 (77%)	241 (100%)	0	100	100
1	B	236/313 (75%)	236 (100%)	0	100	100
2	C	87/262 (33%)	87 (100%)	0	100	100
2	D	199/262 (76%)	199 (100%)	0	100	100
All	All	763/1150 (66%)	763 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	B	299	GLN
2	D	1096	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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

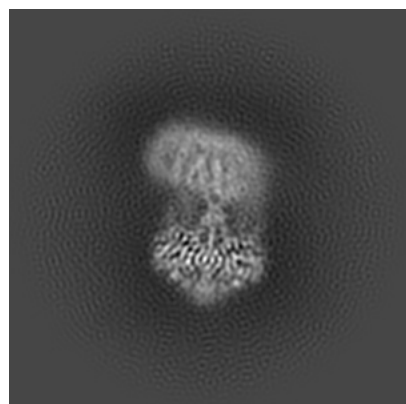
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16802. These allow visual inspection of the internal detail of the map and identification of artifacts.

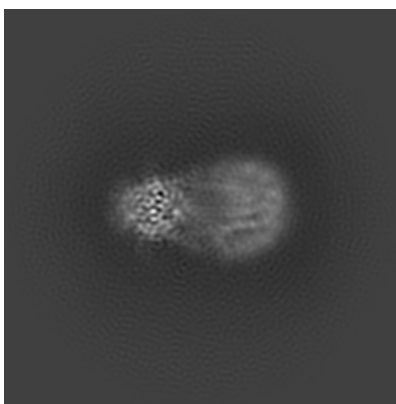
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

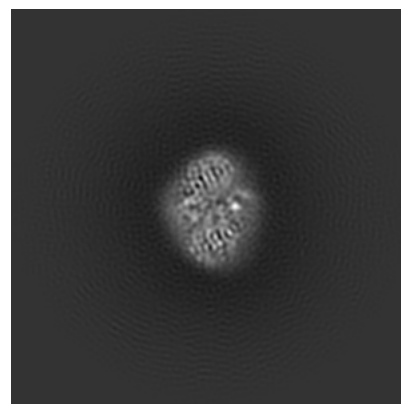
6.1.1 Primary map



X

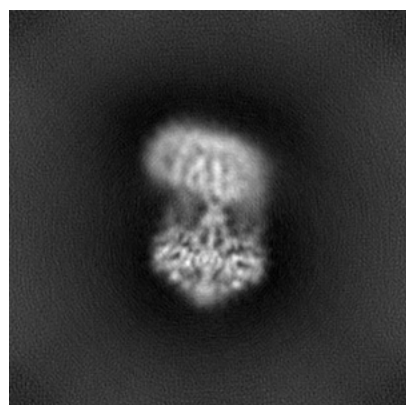


Y

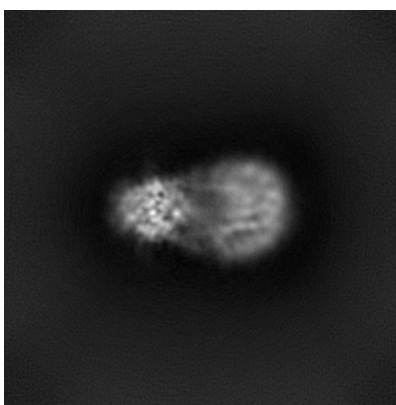


Z

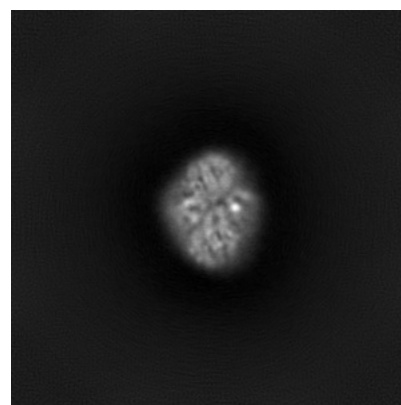
6.1.2 Raw map



X



Y

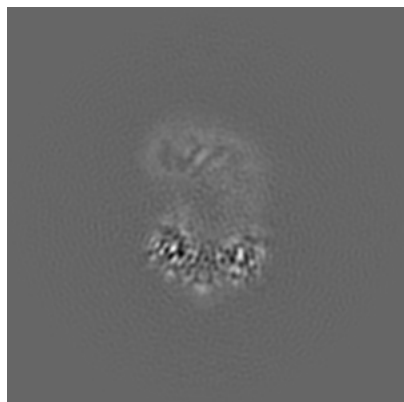


Z

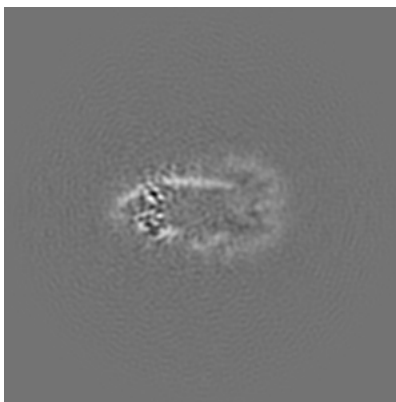
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

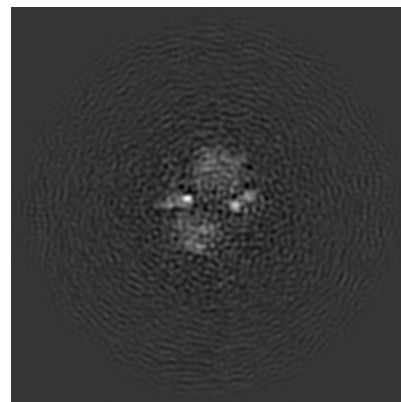
6.2.1 Primary map



X Index: 128

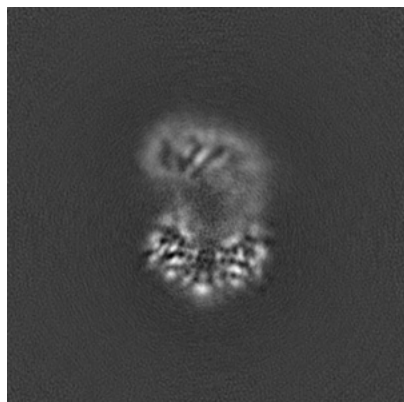


Y Index: 128

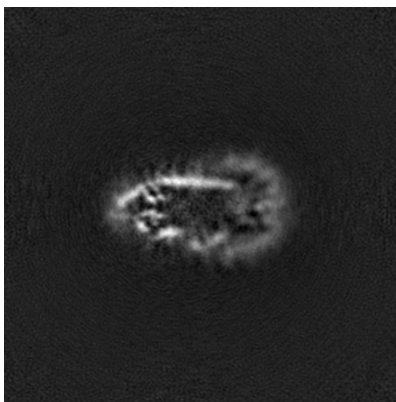


Z Index: 128

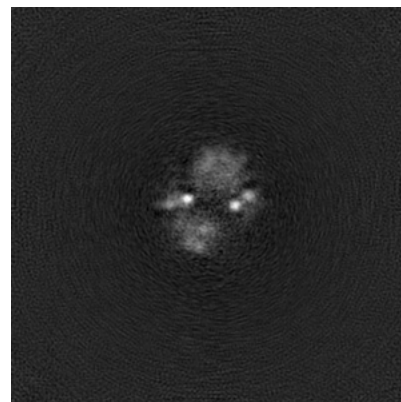
6.2.2 Raw map



X Index: 128



Y Index: 128

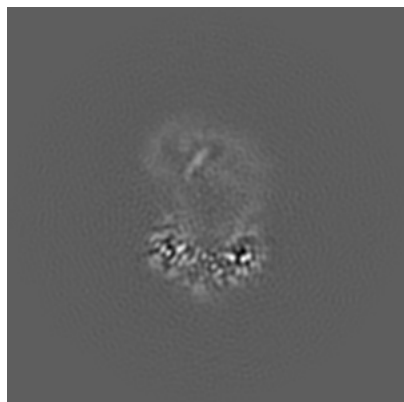


Z Index: 128

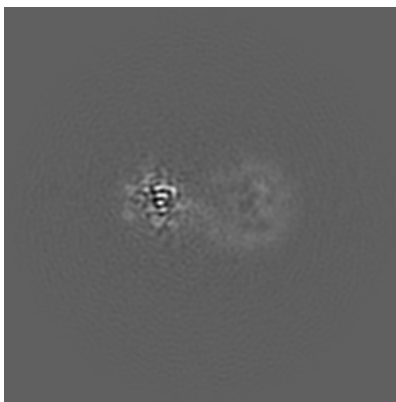
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

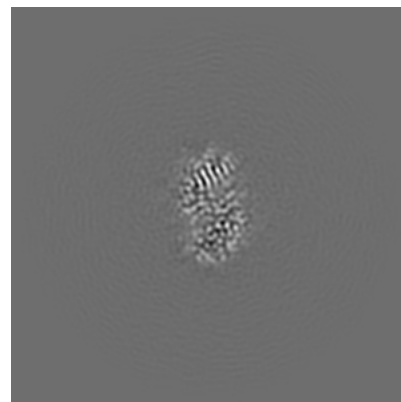
6.3.1 Primary map



X Index: 126

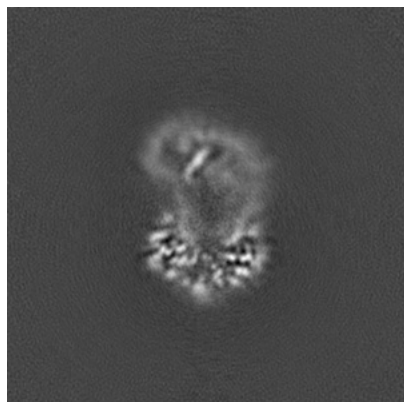


Y Index: 112

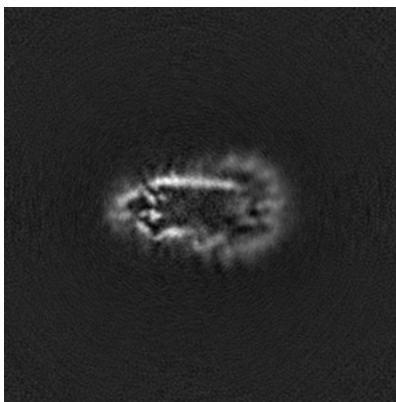


Z Index: 96

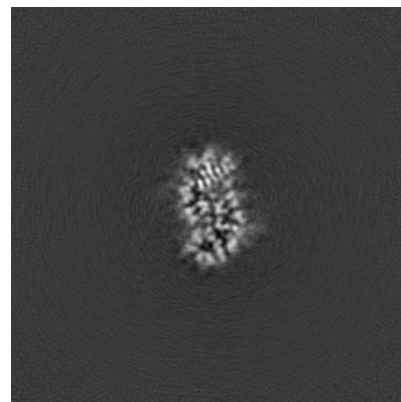
6.3.2 Raw map



X Index: 126



Y Index: 129

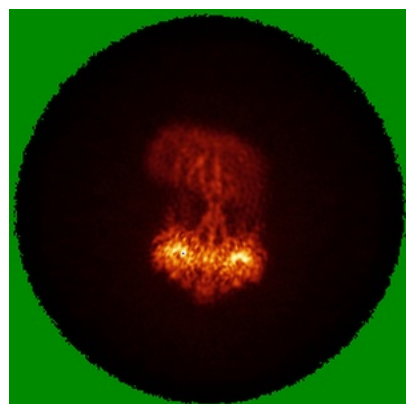


Z Index: 95

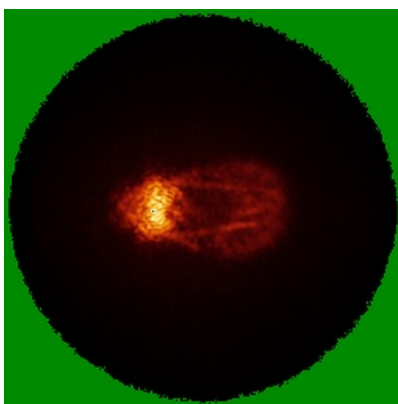
The images above show the largest variance slices of the map in three orthogonal directions.

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

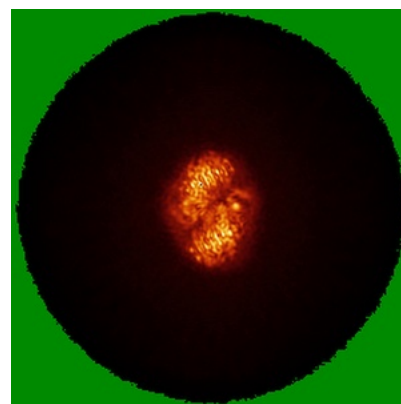
6.4.1 Primary map



X

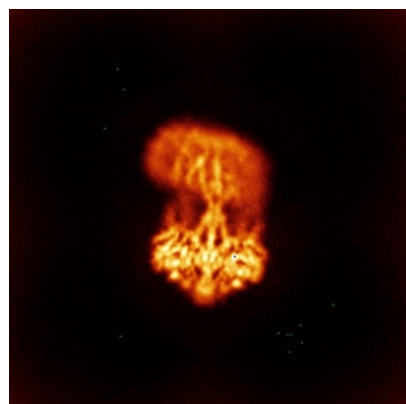


Y

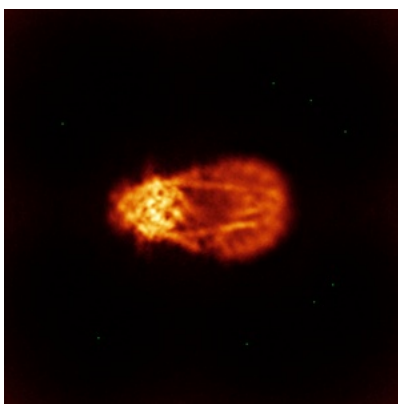


Z

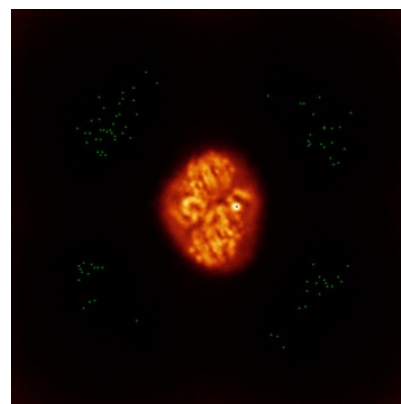
6.4.2 Raw map



X



Y

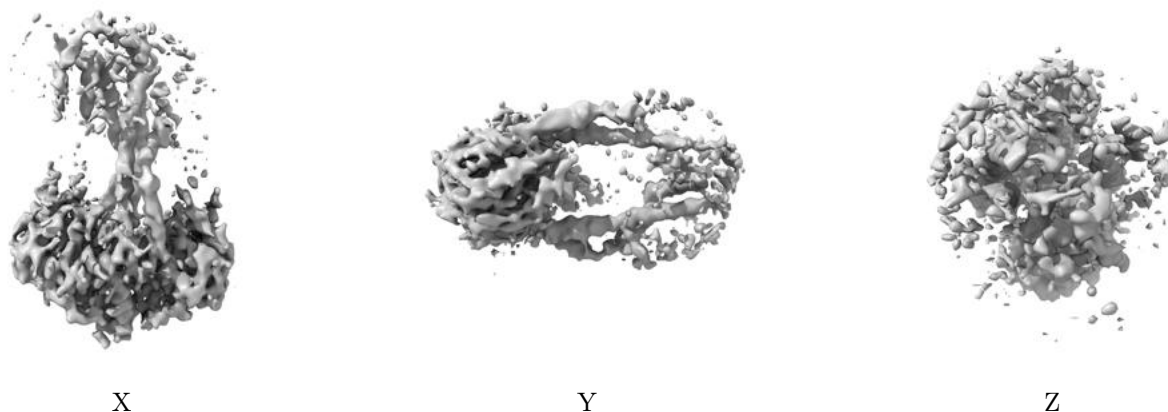


Z

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.

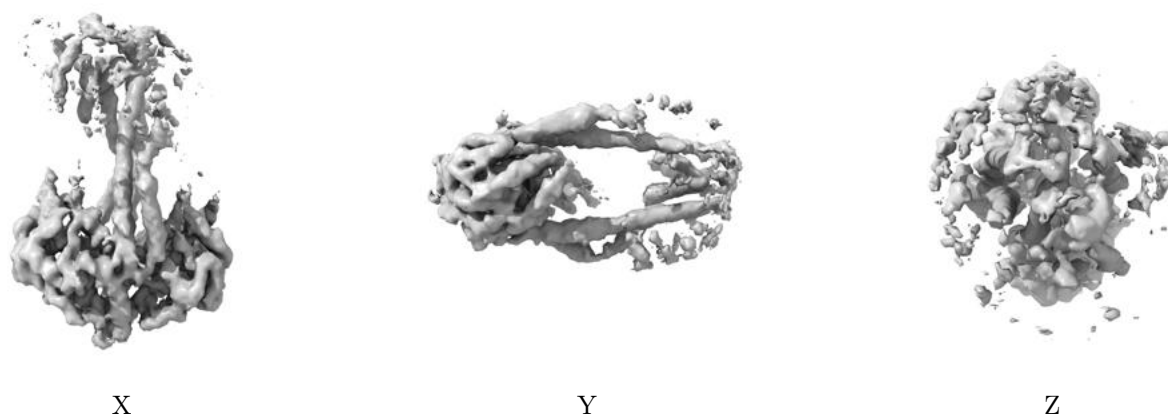
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.21. 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.

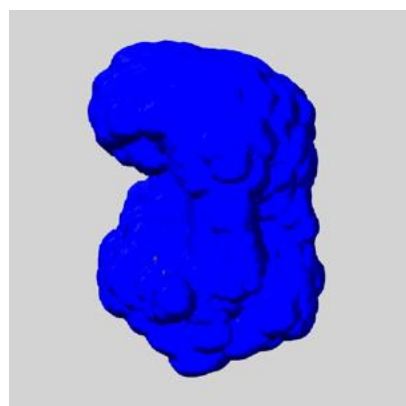
6.6 Mask visualisation [i](#)

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

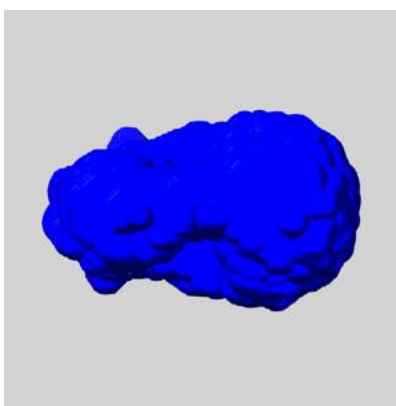
A mask typically either:

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

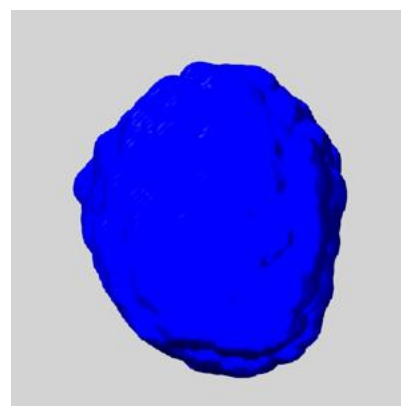
6.6.1 emd_16802_msk_1.map [i](#)



X



Y

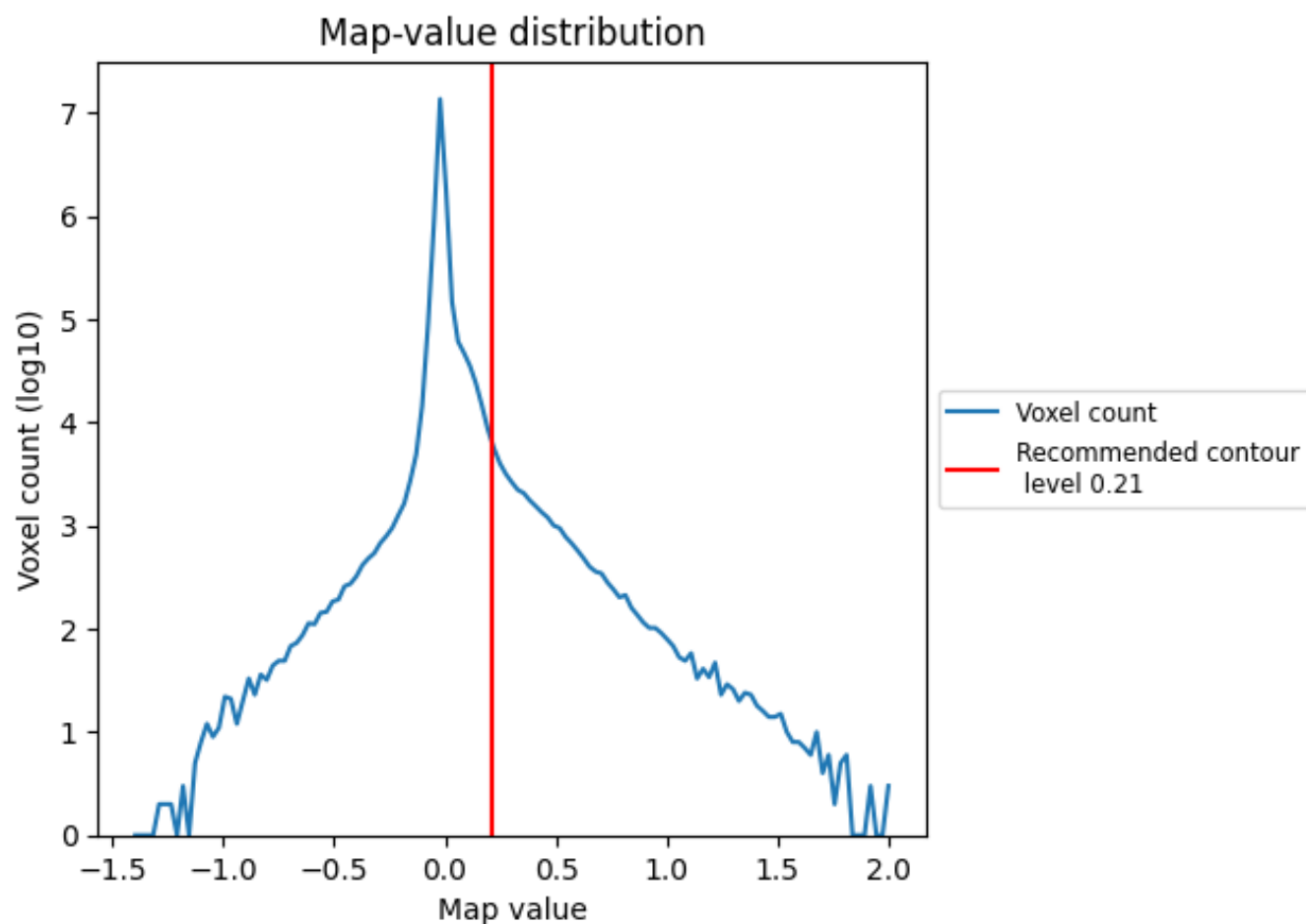


Z

7 Map analysis [i](#)

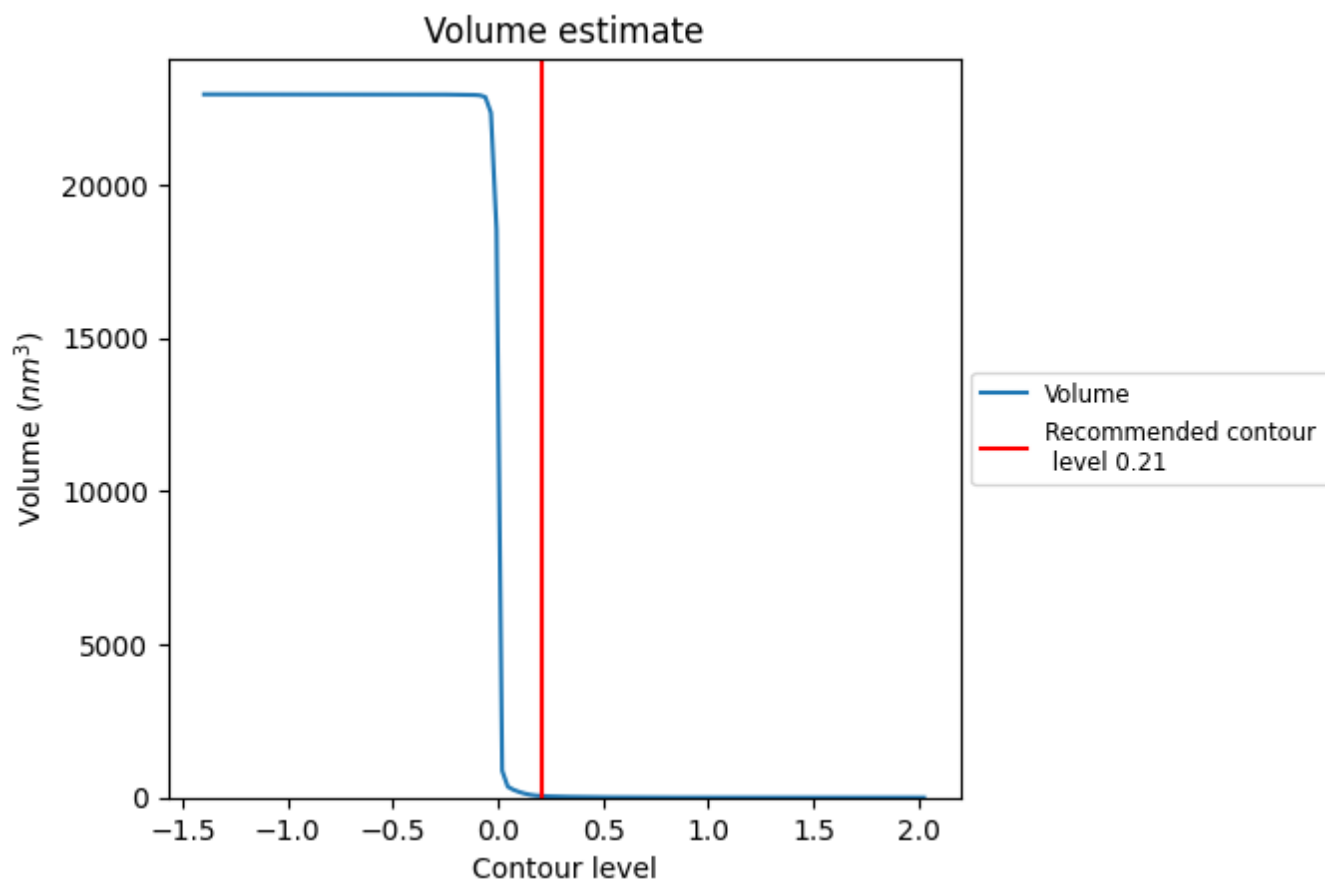
This section contains the results of statistical analysis of the map.

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.

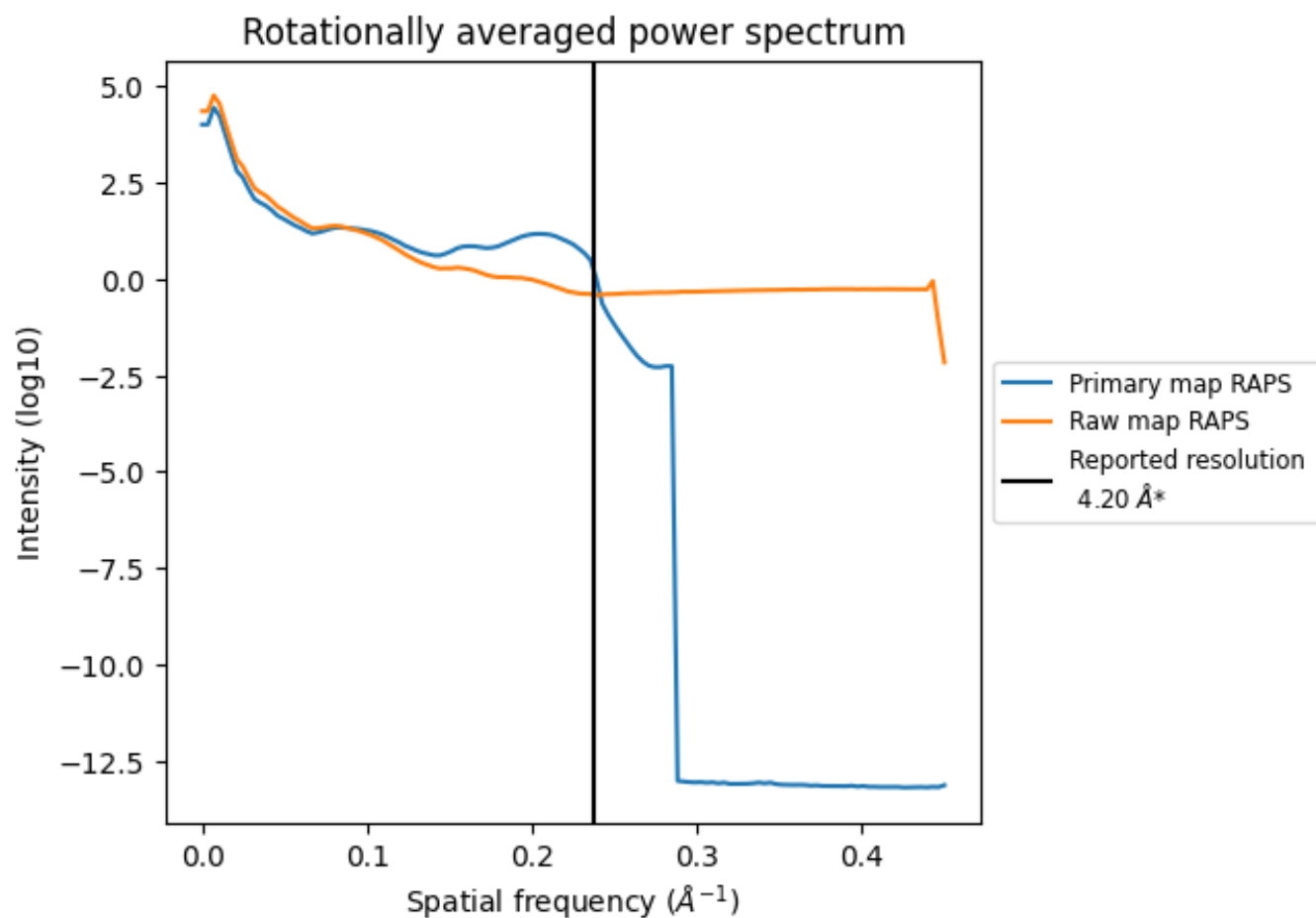
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm^3 ; this corresponds to an approximate mass of 45 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 ⓘ

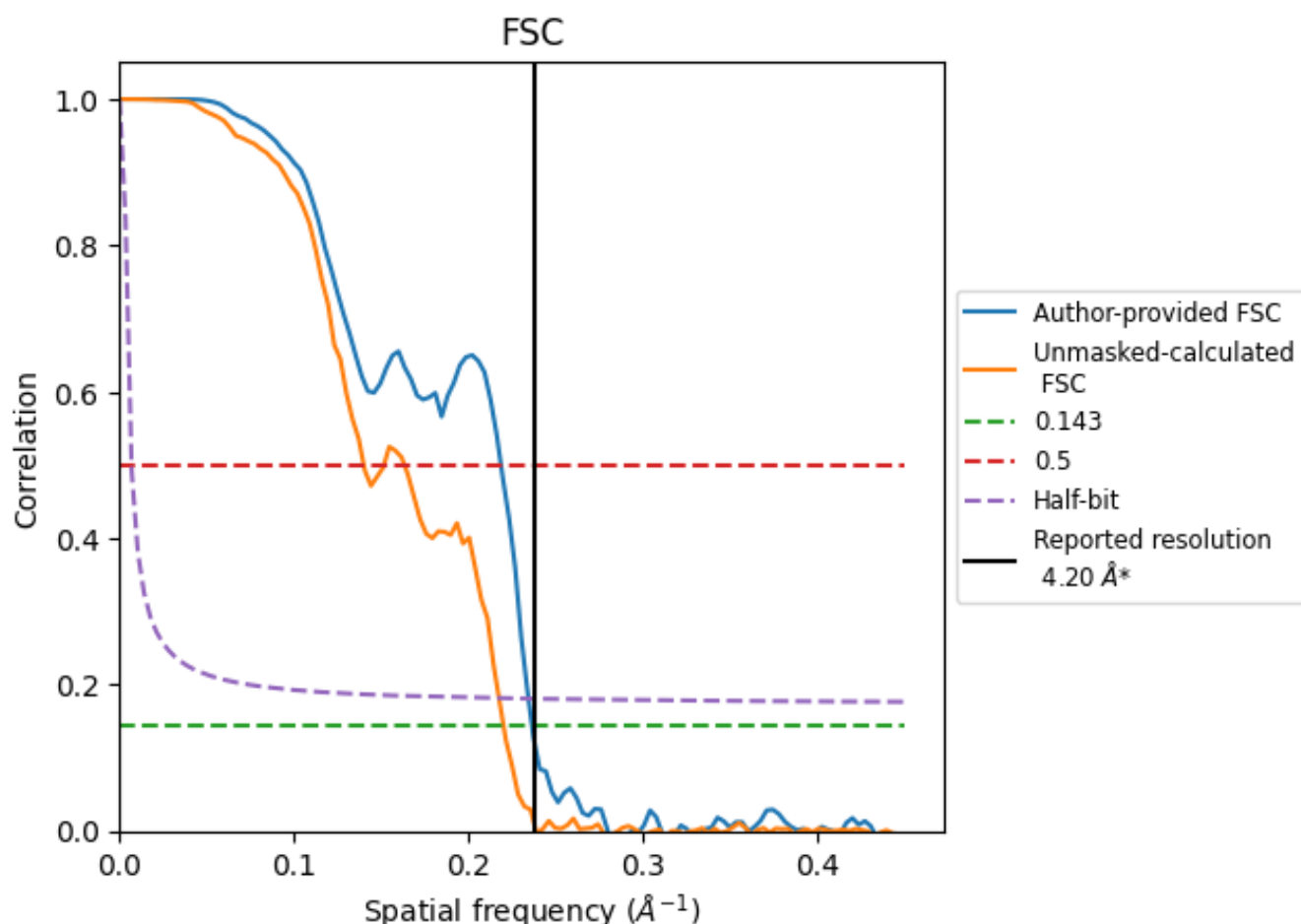


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

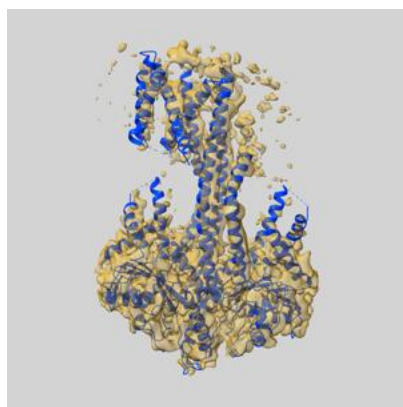
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.22	4.57	4.26
Unmasked-calculated*	4.54	7.14	4.59

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

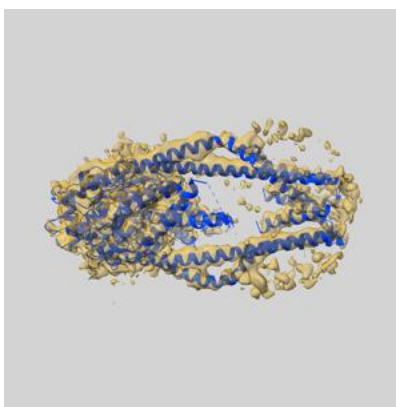
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16802 and PDB model 8CR2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

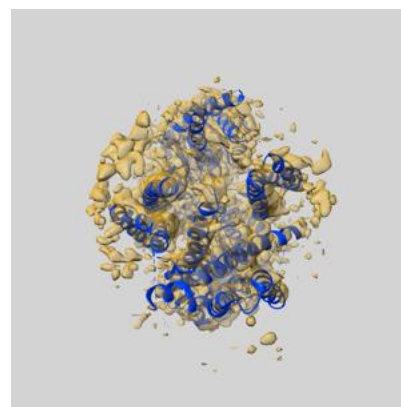
9.1 Map-model overlay [i](#)



X



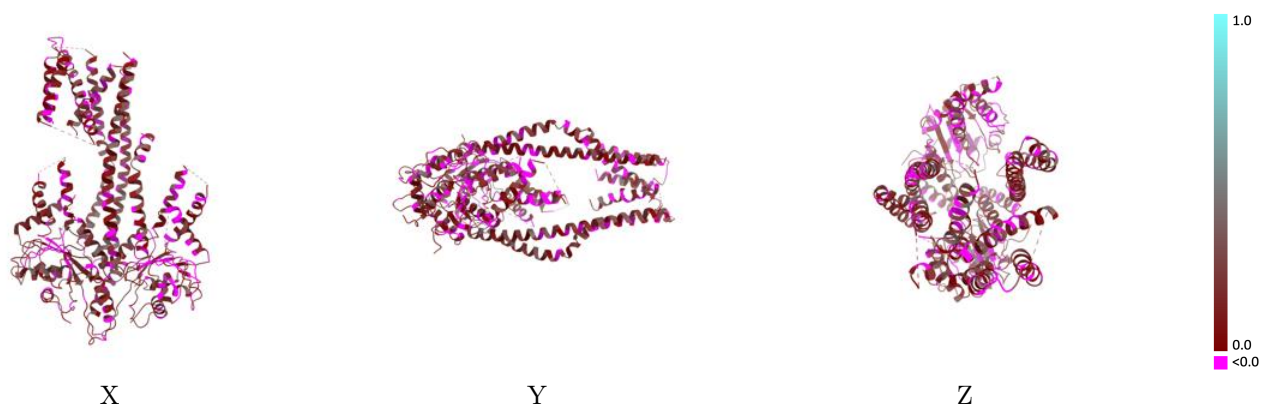
Y



Z

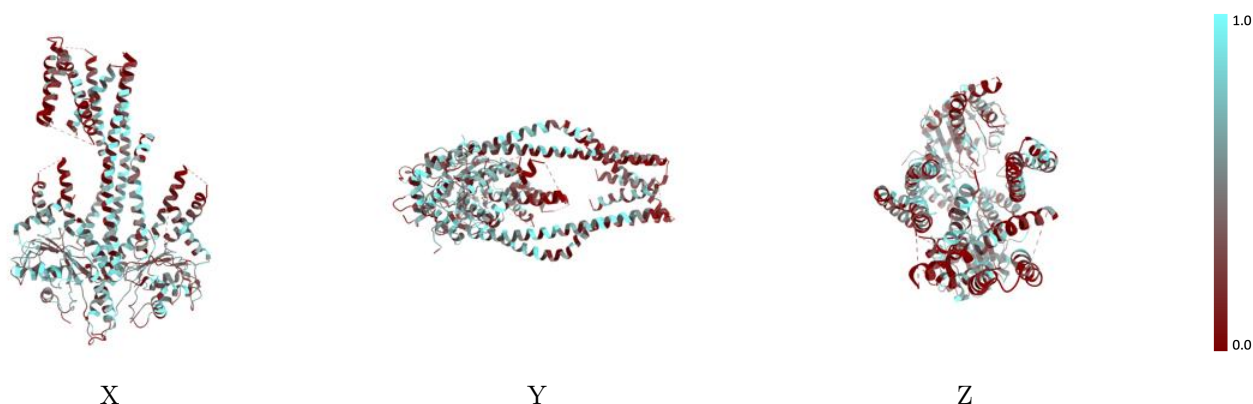
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



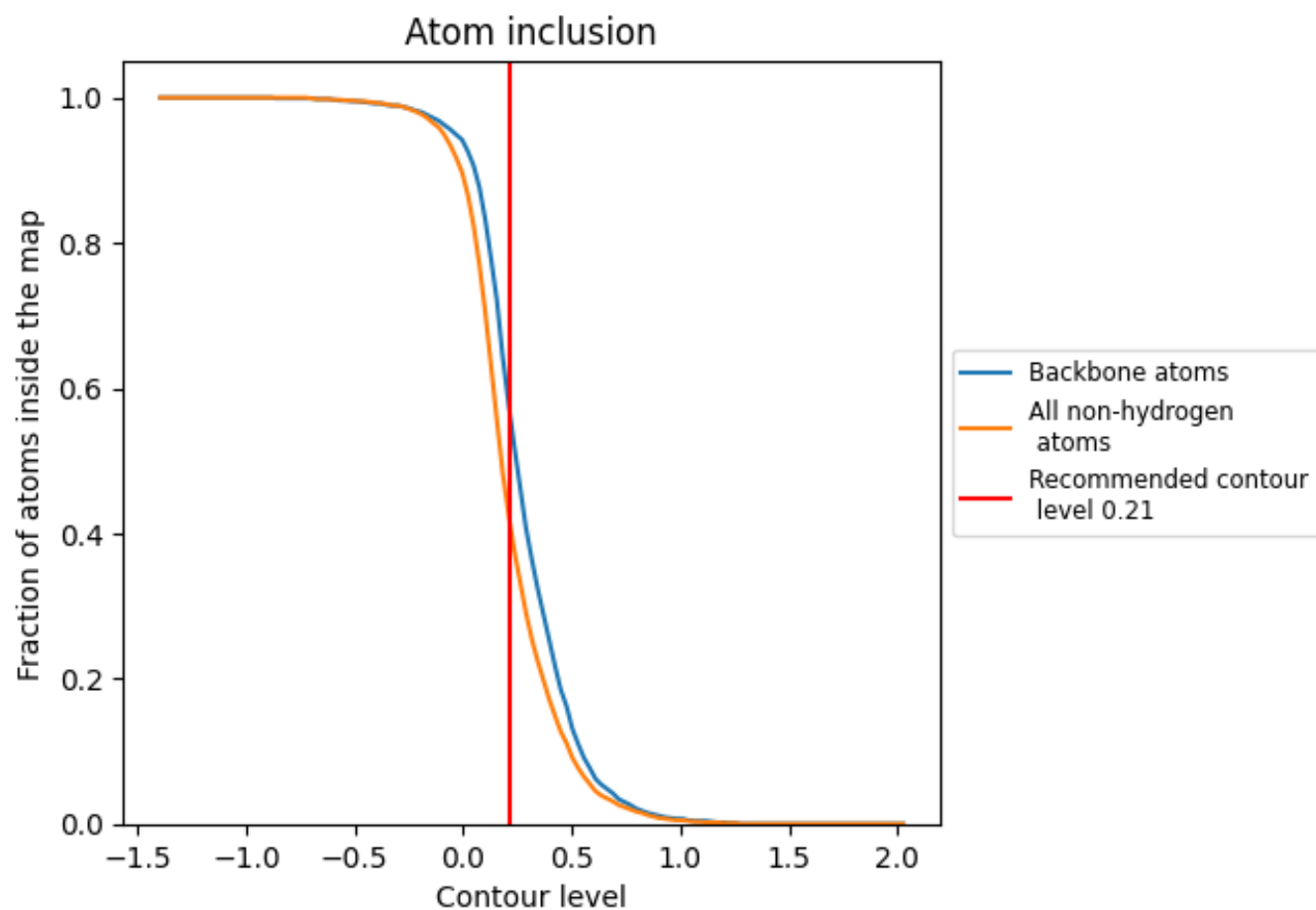
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.21).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 42% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4230	<div></div> 0.1080
A	<div></div> 0.4340	<div></div> 0.0820
B	<div></div> 0.4800	<div></div> 0.1240
C	<div></div> 0.4040	<div></div> 0.1090
D	<div></div> 0.3540	<div></div> 0.1210

