



wwPDB EM Validation Summary Report

Mar 11, 2024 – 12:43 pm GMT


PDB ID : 8P0X
EMDB ID : EMD-17341
Title : Structure of the human Commander complex Retriever Subcomplex
Authors : Kumpula, E.P.; Laulumaa, S.; Huiskonen, J.T.
Deposited on : 2023-05-11
Resolution : 7.50 Å(reported)
Based on initial model : .

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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

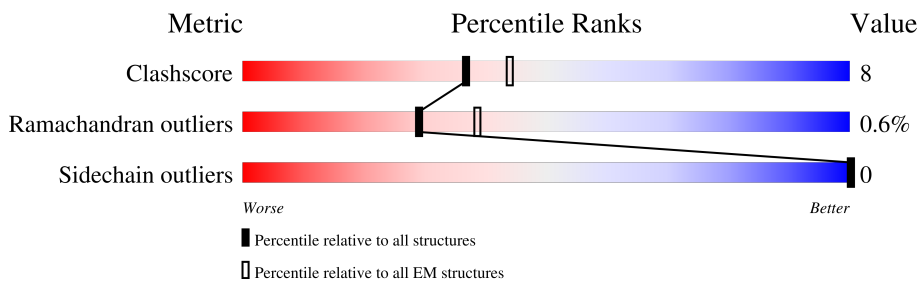
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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 ≥ 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	K	631	
2	L	627	
3	N	182	
4	O	963	
5	P	297	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9322 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 Coiled-coil domain-containing protein 93.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	K	186	933	560	186	187	0	0

- Molecule 2 is a protein called Coiled-coil domain-containing protein 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	L	294	1478	889	294	295	0	0

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	N	182	914	549	182	183	0	0

- Molecule 4 is a protein called VPS35 endosomal protein-sorting factor-like.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	O	891	4496	2713	891	892	0	0

- Molecule 5 is a protein called Vacuolar protein sorting-associated protein 26C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	P	297	1501	906	297	298	0	0

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

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

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

A561
R623
V624
R625
E626
A627

- Molecule 3: Vacuolar protein sorting-associated protein 29

Chain N: 7% 79% 21%

H1
H10
I11
P19
K23
G29
T37
L40
L52
A53
G54
W59
R60
G61
D62
P70
K73
V74
V75
I82
G83
L84
G87
H88
Q89
W90
T91
I110
L111
I112
S113
G114
H115
E120
E125
M126
K127
F128
M131
P132
A135
T136
G137

M140
L142
I146
T147
P148
I155
Q156
A157
V160
V164
Y165
Q166
G169
D170
K173
V174
E175
E178
P182

- Molecule 4: VPS35 endosomal protein-sorting factor-like

Chain O: 10% 85% 8% 7%

M1
A2
V3
F17
R21
L27
E28
P37
I37
THR THR
VAL VAL
THR THR
GLU GLU
SER SER
LYS LYS
THR THR
LYS LYS
VAL VAL
ASN ASN
ARG ARG
LYS LYS
GLY GLY
SER SER
THR THR
SER SER
SER SER
SER SER
SER SER
SER SER
SER SER
SER SER
SER SER
VAL VAL
VAL VAL
VAL VAL
PRO PRO
LEU LEU
SER SER
SER SER
VAL VAL
ASP ASP
GLY GLY
THR THR
ASP ASP
PRO PRO
LEU LEU
SER SER
MET MET
PHE PHE
ALA ALA
ALA ALA
THR THR

ALA ASP
PRO PRO
ALA ALA
LEU LEU
ALA ALA
ALA ALA
ALA ALA
MET MET
ASP ASP
SER SER
SER SER
ARG ARG
ARG ARG
LYS LYS
ASP ASP
ASP ASP
ASN ASN
SER SER
VAL VAL
V110
G111
S112
T131
E132
K133
L134
S135
I136
M137
L138
F139
M140
G141
S142
E143
K144
G145
K146
A147
G148
T149
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S152
L152
A153
M154
S155
E156
K157
V158
R159
T160
R161
L162

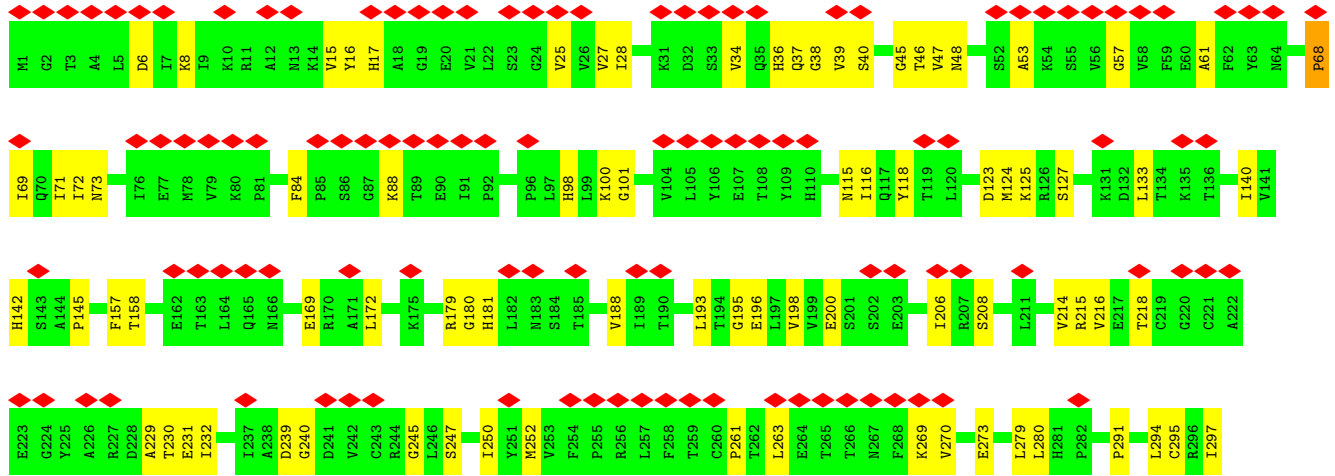
E163
E164
L165
D166
D167
F168
E169
E170
G171
S172
Q173
K174
E175
L176
L177
M178
L179
A198
Q203
Q213
S219
D236
V245
Y246
E247
R248
I249
F250
V254
D255
S256
R257
S258
V259
L260
P261
D262
H263
F264
S265
P266
E267
N268
A269
N270
D271
T272
A273
K274
E275
T276
C277

Y296
V296
E297
N304
L307
S308
S313
P317
I323
G327
D328
H349
L350
K351
Q367
G370
S386
P389
L390
Y391
P392
I402
A437
E456
S457
L472
A475
E507
C514
T534
V553
F557
E567
L570
F593

Q597
P600
M643
S655
V688
E689
S660
R661
S662
F709
I710
P713
L738
A741
S750
P753
N760
K764
D788
G793
V794
L795
F796
L797
L801
N813
S814
D815
L827
A830
L849
Y850
G851
G852
D853
S854
R855
A858
T877

D881
S942
M947
T951
E952
L953
A954
L955
R956
L957
P958
L959
Q960
T961
R962
T963

- Molecule 5: Vacuolar protein sorting-associated protein 26C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13000	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 ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.301	Depositor
Minimum map value	-0.154	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	473.984, 473.984, 473.984	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	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	K	0.39	0/934	0.52	0/1305
2	L	0.38	0/1485	0.55	0/2075
3	N	0.44	0/921	0.84	0/1285
4	O	0.40	0/4529	0.61	2/6346 (0.0%)
5	P	0.31	0/1516	0.61	0/2122
All	All	0.39	0/9385	0.62	2/13133 (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	N	0	1
4	O	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	852	GLY	N-CA-C	-5.10	100.36	113.10
4	O	851	GLY	N-CA-C	-5.01	100.58	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	112	ILE	Peptide
4	O	788	ASP	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	K	933	0	416	2	0
2	L	1478	0	726	5	0
3	N	914	0	446	19	0
4	O	4496	0	2156	44	0
5	P	1501	0	735	50	0
All	All	9322	0	4479	115	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 8.

The worst 5 of 115 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)
5:P:200:GLU:HA	5:P:245:GLY:H	1.29	0.95
4:O:947:MET:O	4:O:951:THR:N	2.23	0.71
4:O:153:ALA:O	4:O:157:LYS:N	2.23	0.71
3:N:110:ILE:HA	3:N:128:PHE:O	1.92	0.70
3:N:120:GLU:N	3:N:131:ASN:O	2.18	0.70

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	K	184/631 (29%)	183 (100%)	1 (0%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	290/627 (46%)	288 (99%)	2 (1%)	0	100	100
3	N	180/182 (99%)	150 (83%)	23 (13%)	7 (4%)	3	23
4	O	887/963 (92%)	848 (96%)	37 (4%)	2 (0%)	47	81
5	P	295/297 (99%)	278 (94%)	15 (5%)	2 (1%)	22	63
All	All	1836/2700 (68%)	1747 (95%)	78 (4%)	11 (1%)	29	66

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	62	ASP
3	N	70	PRO
3	N	126	ASN
3	N	142	LEU
4	O	534	THR

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	K	2/563 (0%)	2 (100%)	0	100	100
2	L	9/538 (2%)	9 (100%)	0	100	100
3	N	8/160 (5%)	8 (100%)	0	100	100
4	O	35/867 (4%)	35 (100%)	0	100	100
5	P	16/266 (6%)	16 (100%)	0	100	100
All	All	70/2394 (3%)	70 (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. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

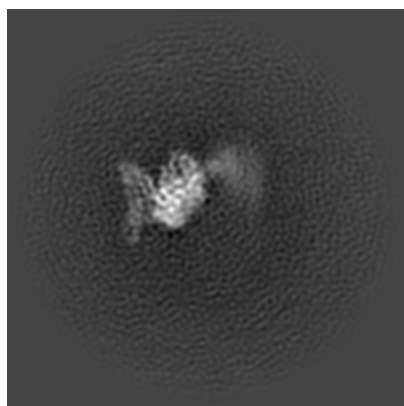
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17341. These allow visual inspection of the internal detail of the map and identification of artifacts.

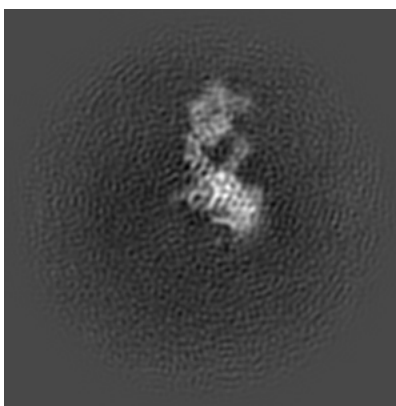
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

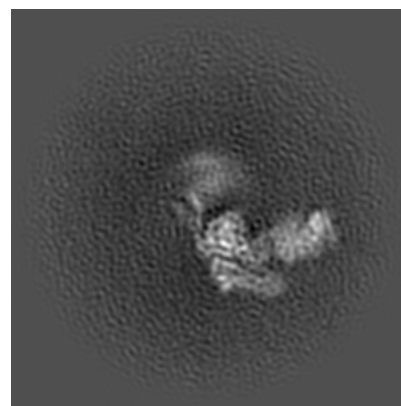
6.1.1 Primary map



X

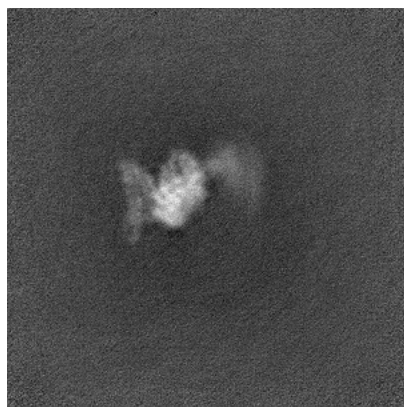


Y

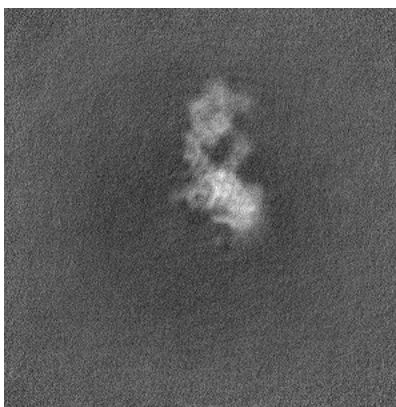


Z

6.1.2 Raw map



X



Y

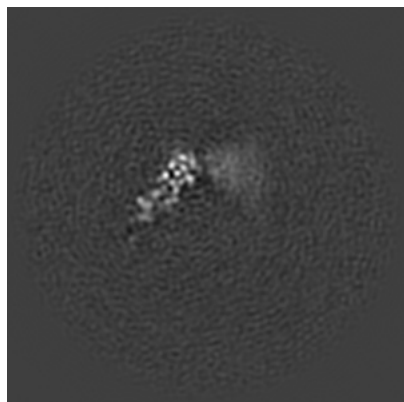


Z

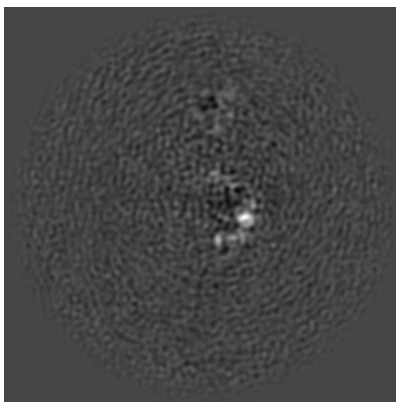
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

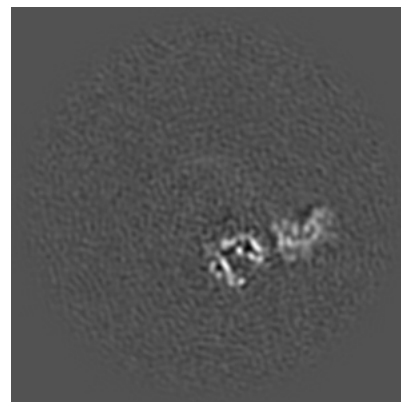
6.2.1 Primary map



X Index: 280



Y Index: 280

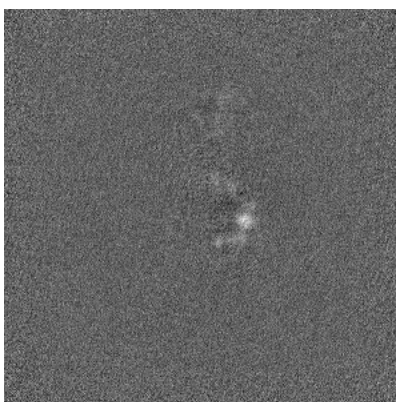


Z Index: 280

6.2.2 Raw map



X Index: 280



Y Index: 280

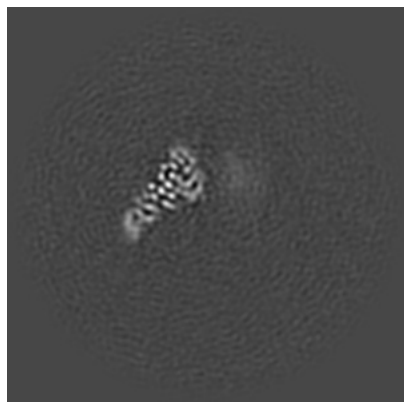


Z Index: 280

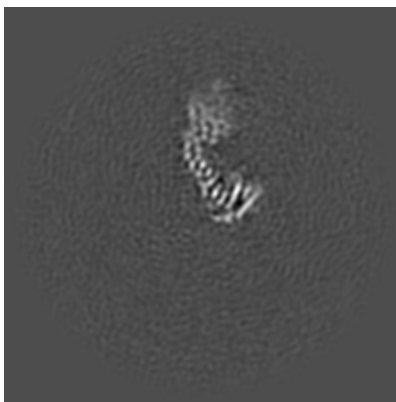
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

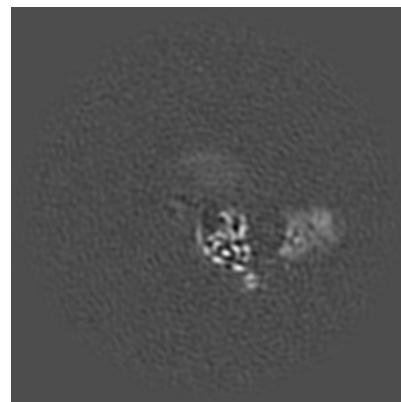
6.3.1 Primary map



X Index: 299

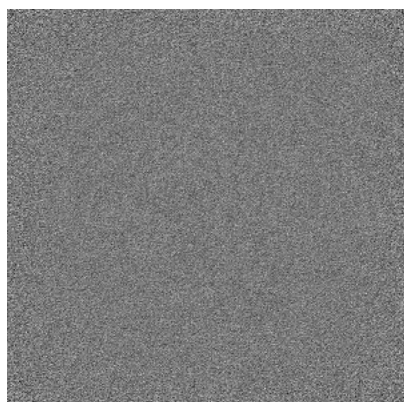


Y Index: 230

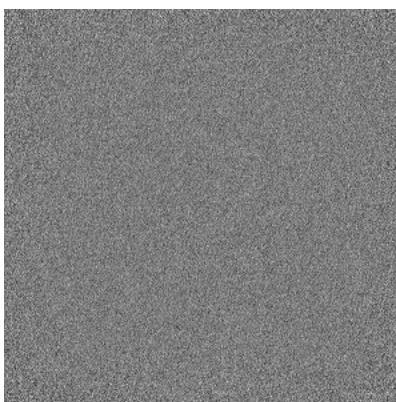


Z Index: 304

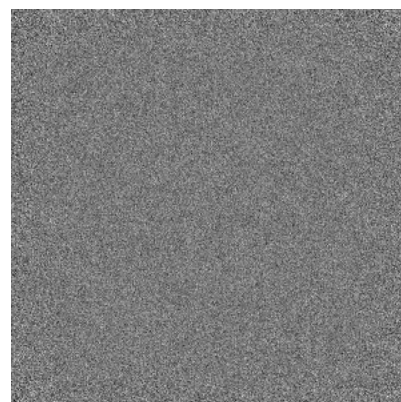
6.3.2 Raw map



X Index: 0



Y Index: 0

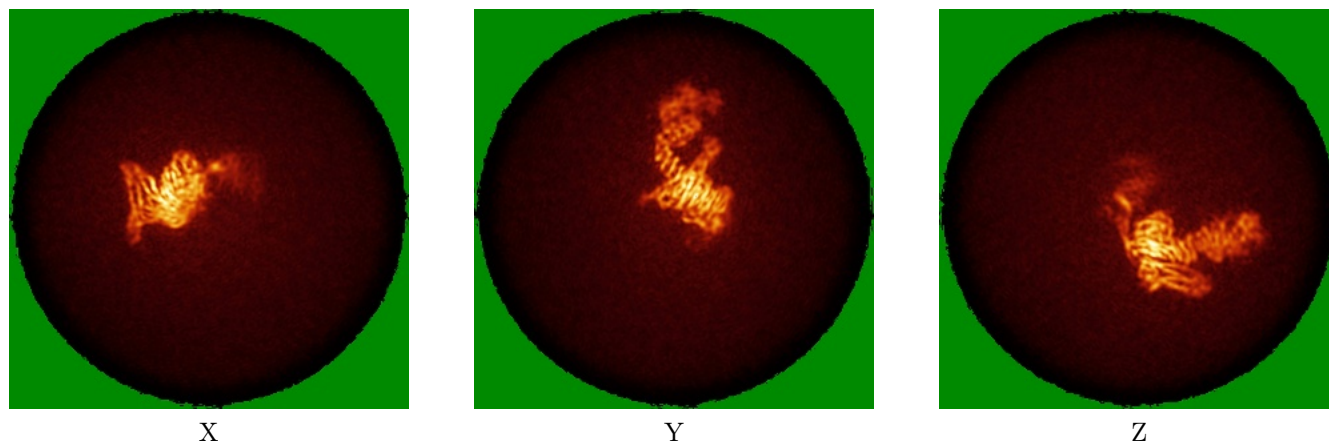


Z Index: 0

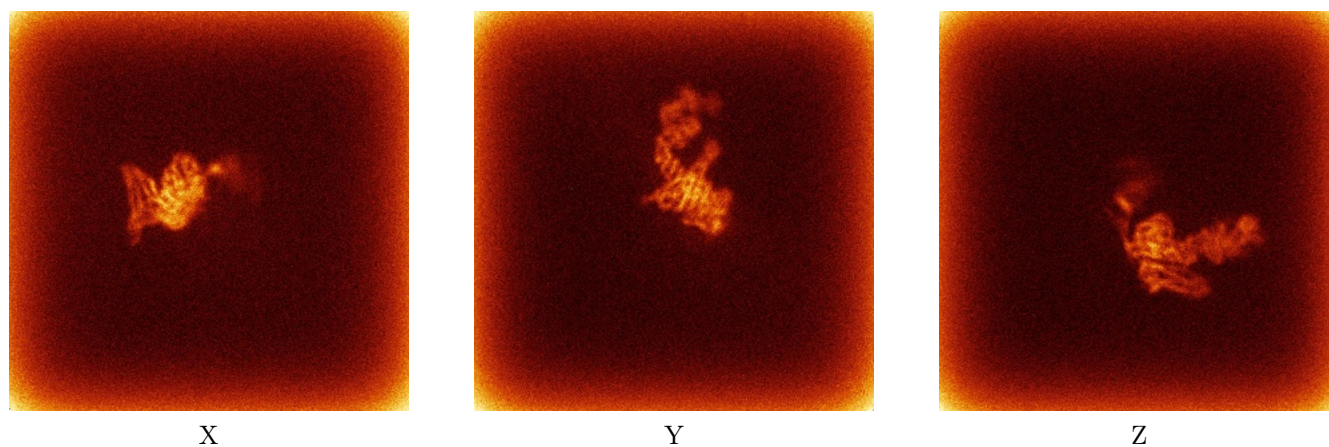
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

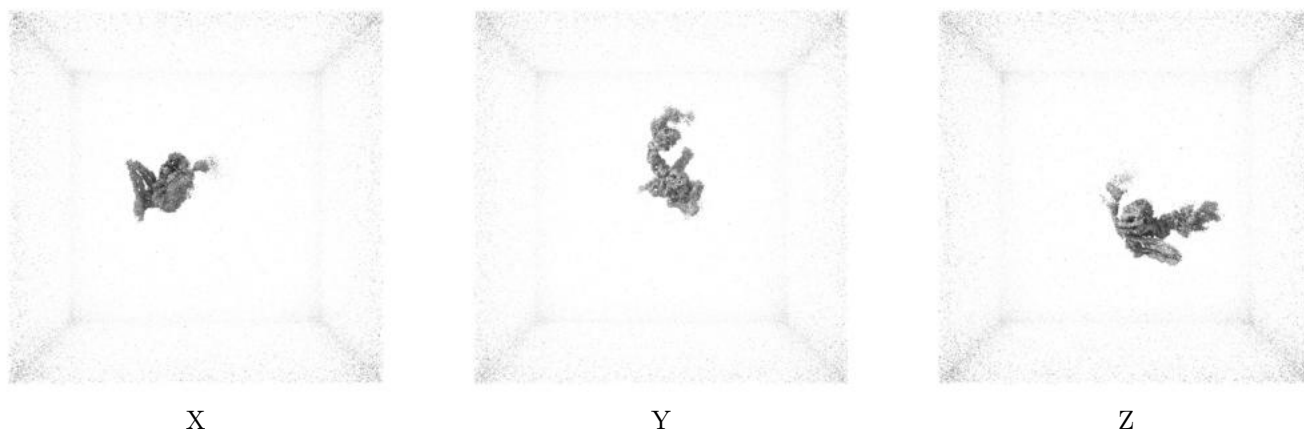
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

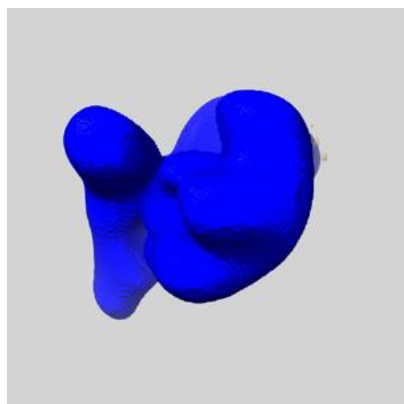
6.6 Mask visualisation [i](#)

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

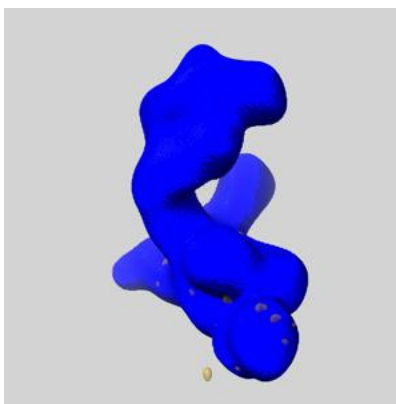
A mask typically either:

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

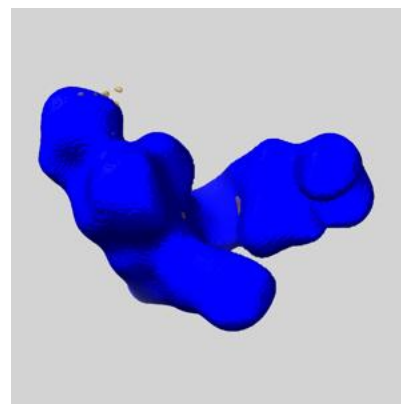
6.6.1 emd_17341_msk_1.map [i](#)



X



Y

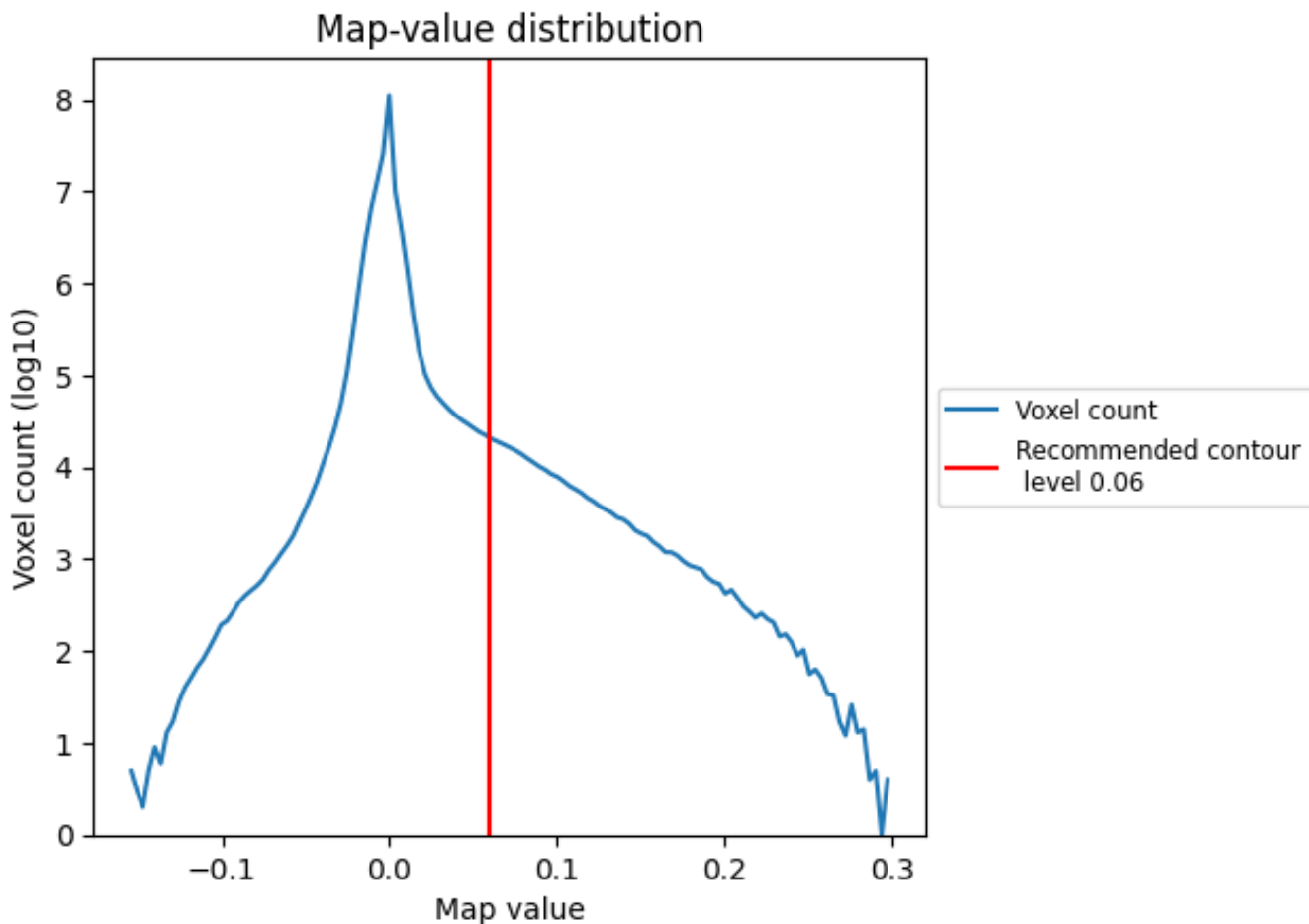


Z

7 Map analysis [i](#)

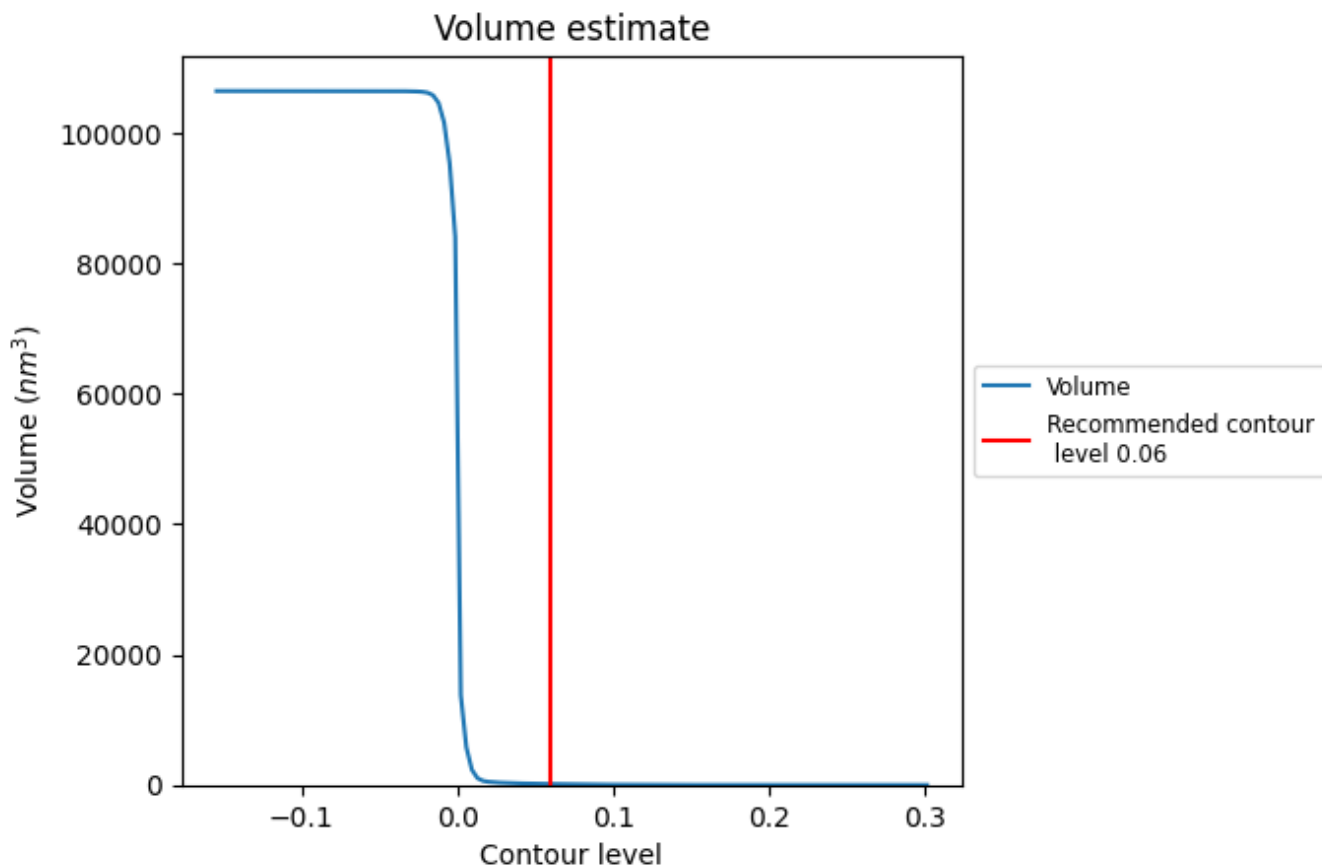
This section contains the results of statistical analysis of the map.

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.

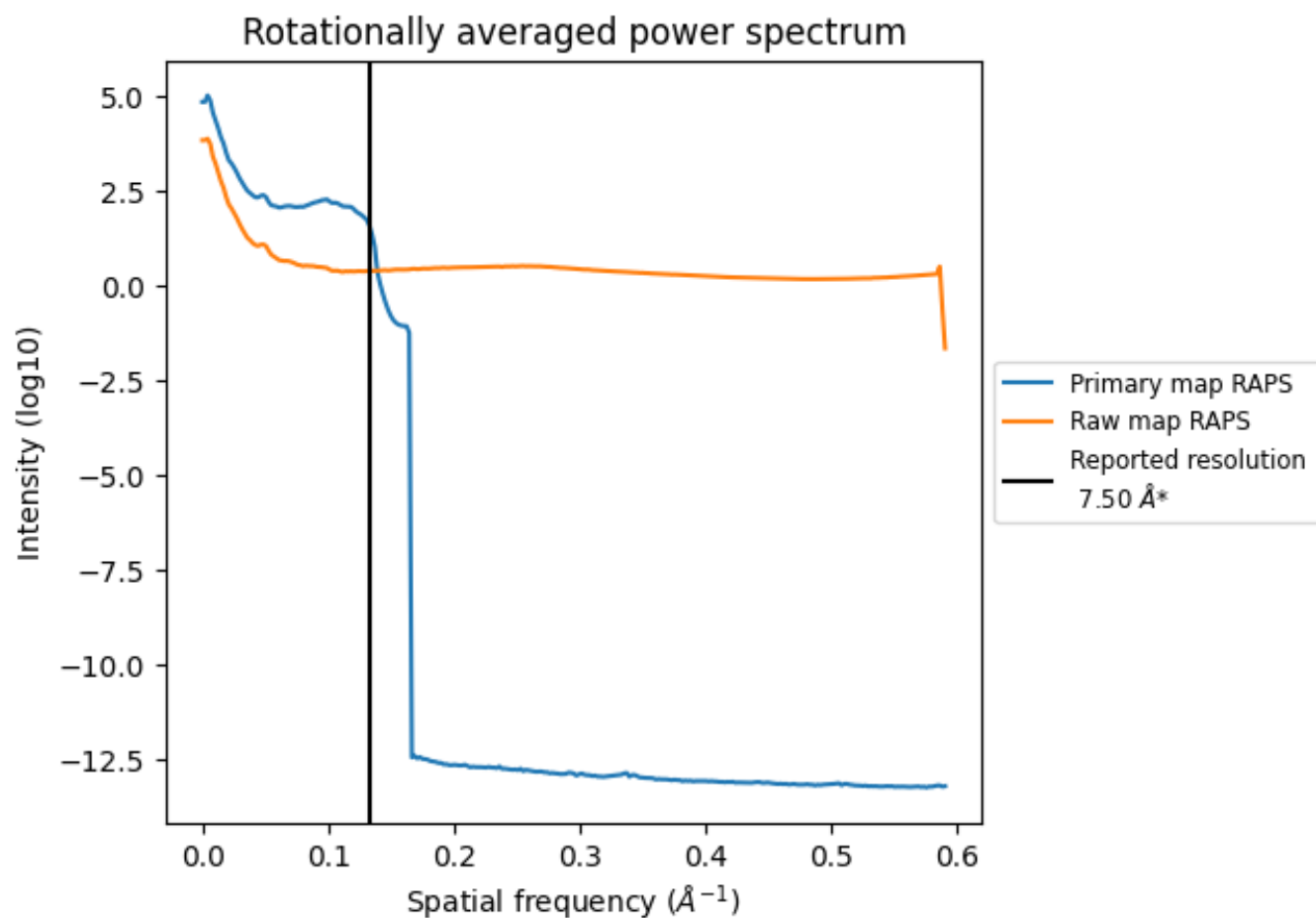
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 145 nm³; this corresponds to an approximate mass of 131 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](#)

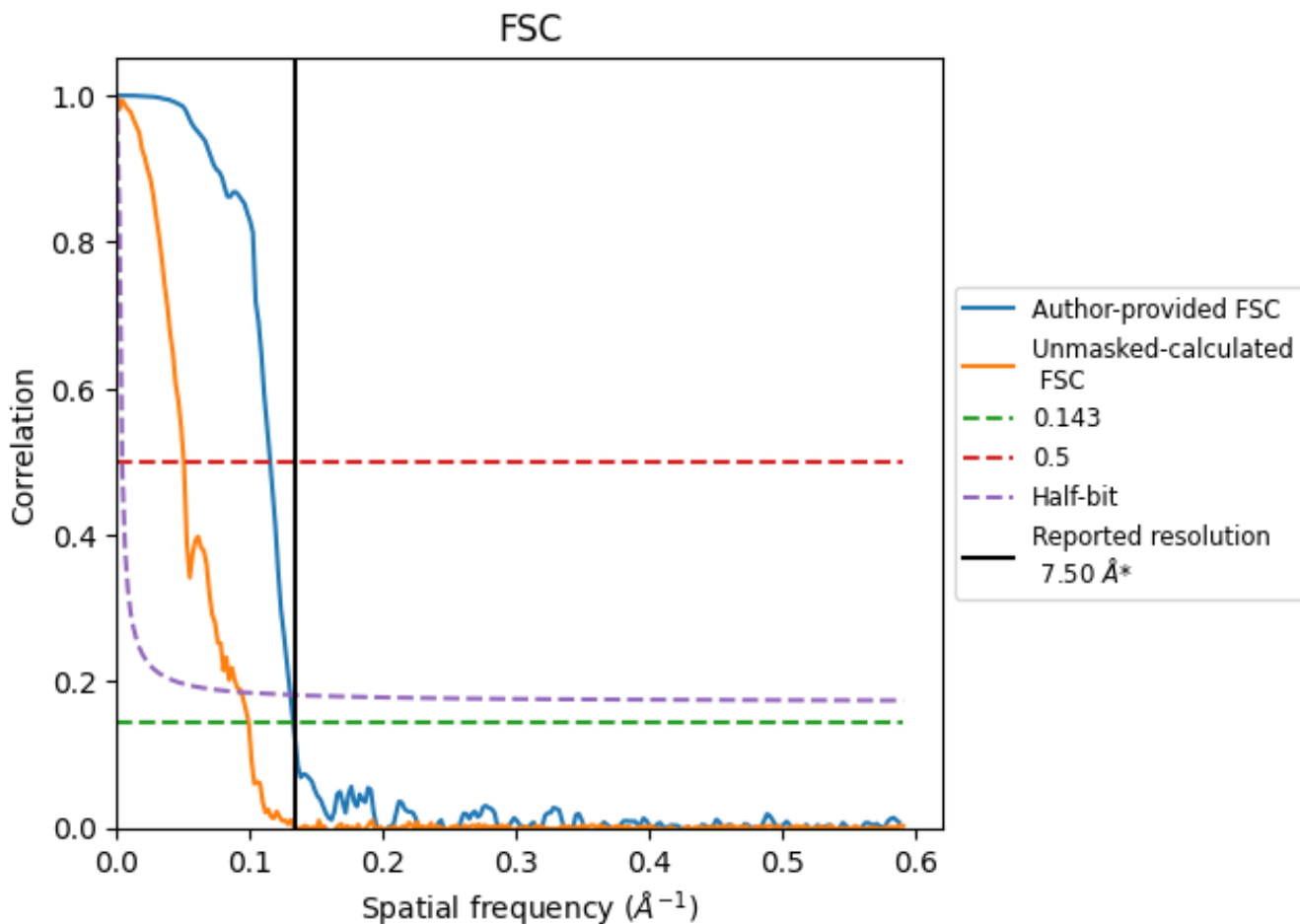


*Reported resolution corresponds to spatial frequency of 0.133 Å⁻¹

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 0.133 Å⁻¹

8.2 Resolution estimates [i](#)

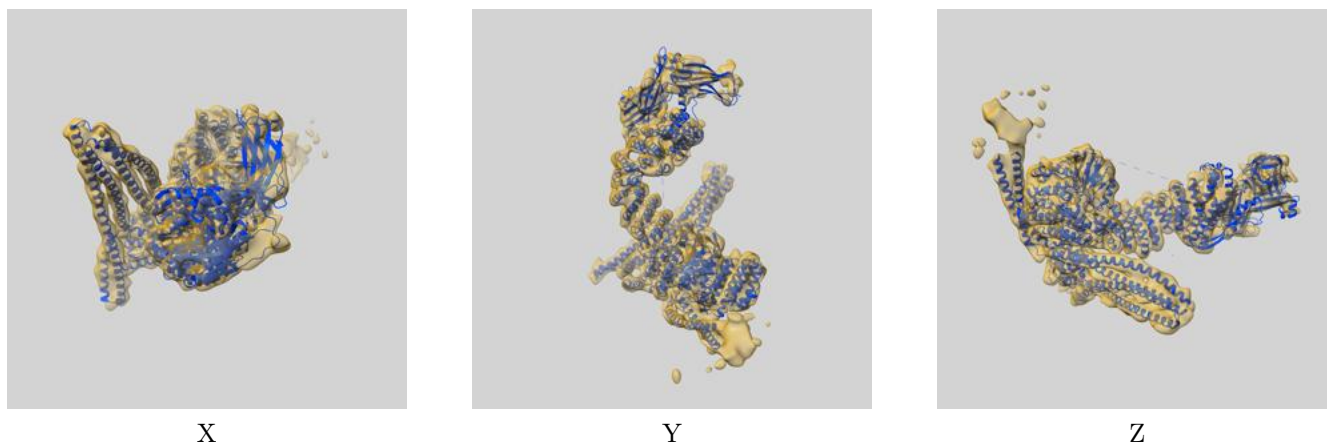
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.50	-	-
Author-provided FSC curve	7.54	8.67	7.66
Unmasked-calculated*	10.08	19.84	10.70

*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 10.08 differs from the reported value 7.5 by more than 10 %

9 Map-model fit [i](#)

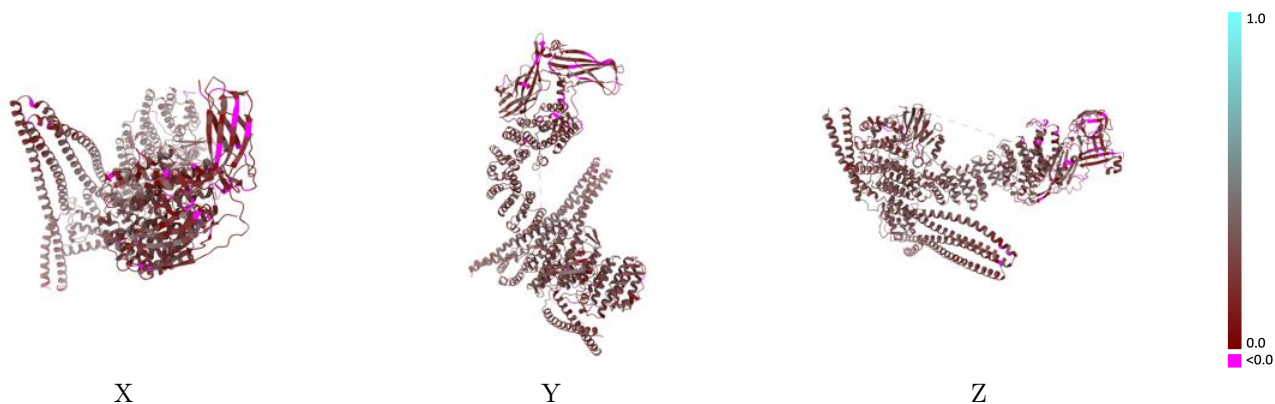
This section contains information regarding the fit between EMDB map EMD-17341 and PDB model 8P0X. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



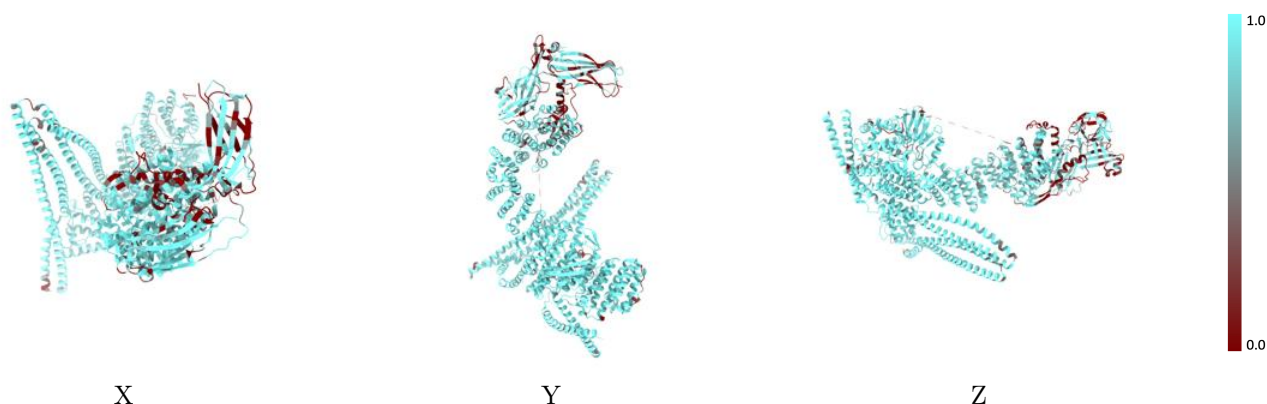
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



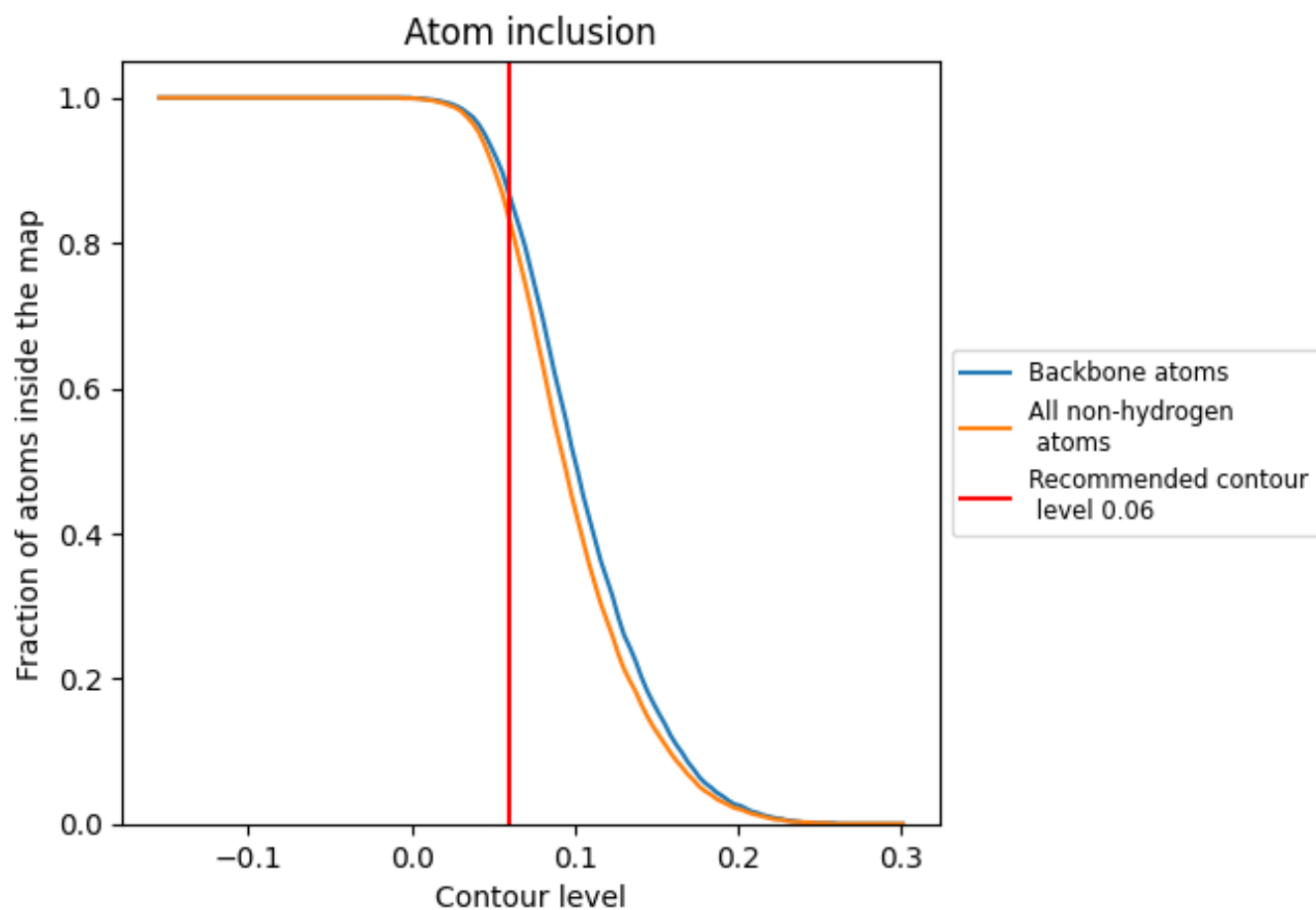
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).













9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.2570
K	 0.9530	 0.2730
L	 0.9280	 0.2890
N	 0.8830	 0.2570
O	 0.8500	 0.2740
P	 0.5800	 0.1640

