



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 02:03 PM JST

PDB ID : 6LMV
EMDB ID : EMD-0921
Title : Cryo-EM structure of the C. elegans CLHM-1
Authors : Demura, K.; Kusakizako, T.; Shihoya, W.; Hiraizumi, M.; Shimada, H.; Yamashita, K.; Nishizawa, T.; Nureki, O.
Deposited on : 2019-12-26
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation 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

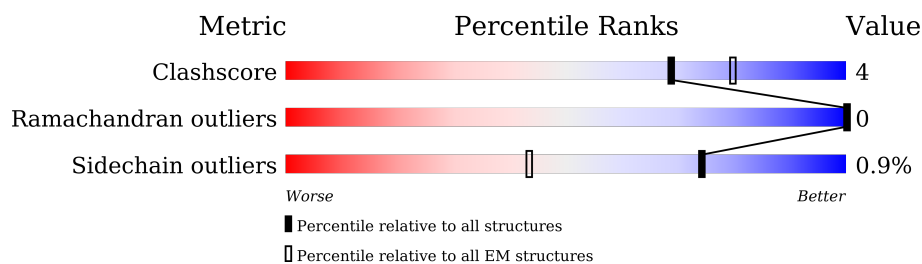
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	337	
1	B	337	
1	C	337	
1	D	337	
1	E	337	
1	F	337	
1	G	337	
1	H	337	

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Mol	Chain	Length	Quality of chain
1	I	337	 A horizontal bar chart showing the quality of chain I. The bar is divided into three segments: a red segment at the beginning, a green segment labeled '65%', a yellow segment labeled '8%', and a grey segment at the end labeled '27%'. A small red dot is visible at the start of the bar.

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 17766 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 Calcium homeostasis modulator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	B	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	C	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	D	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	E	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	F	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	G	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	H	247	Total 1974	C 1282	N 327	O 352	S 13	0	0
1	I	247	Total 1974	C 1282	N 327	O 352	S 13	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	LEU	-	expression tag	UNP Q18593
A	331	GLU	-	expression tag	UNP Q18593
A	332	GLU	-	expression tag	UNP Q18593
A	333	ASN	-	expression tag	UNP Q18593
A	334	LEU	-	expression tag	UNP Q18593
A	335	TYR	-	expression tag	UNP Q18593
A	336	PHE	-	expression tag	UNP Q18593
A	337	GLN	-	expression tag	UNP Q18593
B	330	LEU	-	expression tag	UNP Q18593
B	331	GLU	-	expression tag	UNP Q18593
B	332	GLU	-	expression tag	UNP Q18593
B	333	ASN	-	expression tag	UNP Q18593

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Chain	Residue	Modelled	Actual	Comment	Reference
B	334	LEU	-	expression tag	UNP Q18593
B	335	TYR	-	expression tag	UNP Q18593
B	336	PHE	-	expression tag	UNP Q18593
B	337	GLN	-	expression tag	UNP Q18593
C	330	LEU	-	expression tag	UNP Q18593
C	331	GLU	-	expression tag	UNP Q18593
C	332	GLU	-	expression tag	UNP Q18593
C	333	ASN	-	expression tag	UNP Q18593
C	334	LEU	-	expression tag	UNP Q18593
C	335	TYR	-	expression tag	UNP Q18593
C	336	PHE	-	expression tag	UNP Q18593
C	337	GLN	-	expression tag	UNP Q18593
D	330	LEU	-	expression tag	UNP Q18593
D	331	GLU	-	expression tag	UNP Q18593
D	332	GLU	-	expression tag	UNP Q18593
D	333	ASN	-	expression tag	UNP Q18593
D	334	LEU	-	expression tag	UNP Q18593
D	335	TYR	-	expression tag	UNP Q18593
D	336	PHE	-	expression tag	UNP Q18593
D	337	GLN	-	expression tag	UNP Q18593
E	330	LEU	-	expression tag	UNP Q18593
E	331	GLU	-	expression tag	UNP Q18593
E	332	GLU	-	expression tag	UNP Q18593
E	333	ASN	-	expression tag	UNP Q18593
E	334	LEU	-	expression tag	UNP Q18593
E	335	TYR	-	expression tag	UNP Q18593
E	336	PHE	-	expression tag	UNP Q18593
E	337	GLN	-	expression tag	UNP Q18593
F	330	LEU	-	expression tag	UNP Q18593
F	331	GLU	-	expression tag	UNP Q18593
F	332	GLU	-	expression tag	UNP Q18593
F	333	ASN	-	expression tag	UNP Q18593
F	334	LEU	-	expression tag	UNP Q18593
F	335	TYR	-	expression tag	UNP Q18593
F	336	PHE	-	expression tag	UNP Q18593
F	337	GLN	-	expression tag	UNP Q18593
G	330	LEU	-	expression tag	UNP Q18593
G	331	GLU	-	expression tag	UNP Q18593
G	332	GLU	-	expression tag	UNP Q18593
G	333	ASN	-	expression tag	UNP Q18593
G	334	LEU	-	expression tag	UNP Q18593
G	335	TYR	-	expression tag	UNP Q18593

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Chain	Residue	Modelled	Actual	Comment	Reference
G	336	PHE	-	expression tag	UNP Q18593
G	337	GLN	-	expression tag	UNP Q18593
H	330	LEU	-	expression tag	UNP Q18593
H	331	GLU	-	expression tag	UNP Q18593
H	332	GLU	-	expression tag	UNP Q18593
H	333	ASN	-	expression tag	UNP Q18593
H	334	LEU	-	expression tag	UNP Q18593
H	335	TYR	-	expression tag	UNP Q18593
H	336	PHE	-	expression tag	UNP Q18593
H	337	GLN	-	expression tag	UNP Q18593
I	330	LEU	-	expression tag	UNP Q18593
I	331	GLU	-	expression tag	UNP Q18593
I	332	GLU	-	expression tag	UNP Q18593
I	333	ASN	-	expression tag	UNP Q18593
I	334	LEU	-	expression tag	UNP Q18593
I	335	TYR	-	expression tag	UNP Q18593
I	336	PHE	-	expression tag	UNP Q18593
I	337	GLN	-	expression tag	UNP Q18593

GLY
TYR
ARG
ILE
PRO
GLN
GLN
ASP
LEU
GLN
THR
THR
ILE
ILE
ASP
GLU
THR
LYS
GLY
ASP
LEU
LEU
GLU
ASN
TYR
PHE
GLN

• Molecule 1: Calcium homeostasis modulator protein

Chain D: 

MET
THR
THR
SER
ILE
ASN
SER
VAL
VAL
THR
THR
PHE
GLN
ASN
VAL
PHE
THR
ASN
HIS
GLY
SER
THR
LEU
LEU
ASN
GLY
ILE
LEU
ILE
ALA
THR
VAL
GLY
GLY
GLN
SER
LEU
V39
R40
K41
L42
C48
N76
R89
V90
R91
R94
V107
L119
R130
C138

A143
C146
K147
Y155
D166
N167
P173
C174
I175
C176
V177
P178
N179
A183
E187
Y218
T219
L220
Q222
T263
K264
P274
GLU
VAL
ASN
ASN
PRO
LEU
PHE
PHE
ALA
ARG
LEU
ARG
ILE
ILE
ALA
ALA
GLU
LYS
THR
GLN
THR
MET
Y297
Q301
K307

GLY
TYR
ARG
PRO
GLN
PRO
ASP
LEU
GLN
THR
THR
ILE
ILE
VAL
PHE
THR
ASN
HIS
GLY
SER
THR
LEU
LEU
ASN
GLY
ILE
LEU
ILE
ALA
THR
VAL
GLY
GLY
GLN
SER
LEU

• Molecule 1: Calcium homeostasis modulator protein

Chain E: 

MET
THR
THR
SER
ILE
ASN
SER
VAL
VAL
THR
THR
PHE
GLN
ASN
VAL
PHE
THR
ASN
HIS
GLY
SER
THR
LEU
LEU
ASN
GLY
ILE
LEU
ILE
ALA
THR
VAL
GLY
GLY
GLN
SER
LEU
V39
R40
K41
L42
C48
N76
R89
V90
R91
R94
V107
L124
R130
A143

C146
K147
Y155
D166
N167
P173
C176
V177
P178
N179
A183
E187
Y218
T219
L220
Q222
L248
T263
K264
P274
GLU
VAL
ASN
ASN
PRO
LEU
PHE
PHE
ALA
ARG
LEU
ARG
ILE
ILE
ALA
ALA
GLU
LYS
THR
GLN
GLN
THR
MET
Y297
Q301
K307
GLY

TYR
ARG
ILE
PRO
GLN
PRO
ASP
LEU
GLN
THR
THR
ILE
ILE
VAL
PHE
THR
ASN
HIS
GLY
SER
THR
LEU
LEU
ASN
GLY
ILE
LEU
PHE
GLN

• Molecule 1: Calcium homeostasis modulator protein

Chain F: 

MET
THR
THR
SER
ILE
ASN
SER
VAL
VAL
THR
THR
PHE
GLN
ASN
VAL
PHE
THR
ASN
HIS
GLY
SER
THR
LEU
LEU
ASN
GLY
ILE
LEU
ILE
ALA
THR
THR
VAL
VAL
GLY
GLY
GLN
SER
LEU
V39
R40
K41
L42
C48
N76
R89
V90
R91
D92
T93
R94
V107
R130
A143

C146
K147
Y155
D166
P173
C176
V177
P178
N179
A183
E187
Y218
T219
L220
Q222
P274
GLU
VAL
ASN
ASN
PRO
LEU
PHE
PHE
ALA
GLY
ARG
GLN
ARG
LEU
ILE
ALA
ALA
GLU
GLY
LYS
THR
GLN
GLN
THR
MET
Y297
Q301
K307
GLY
TYR
ARG
ILE
PRO
GLN
PRO
ASP

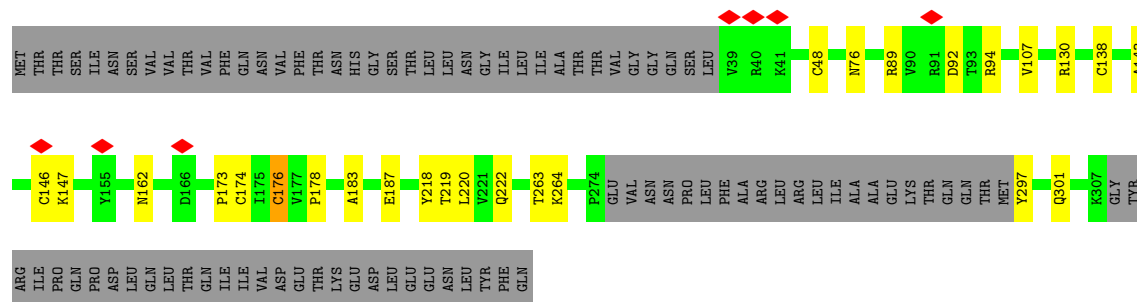
LEU
GLN
LEU
THR
GLN
GLN
ILE
VAL
ASP
THR
THR
GLY
LYS
GLY
ASP
LEU
GLY
GLU
ASN
ASN
THR
TYR
PHE
GLN

• Molecule 1: Calcium homeostasis modulator protein

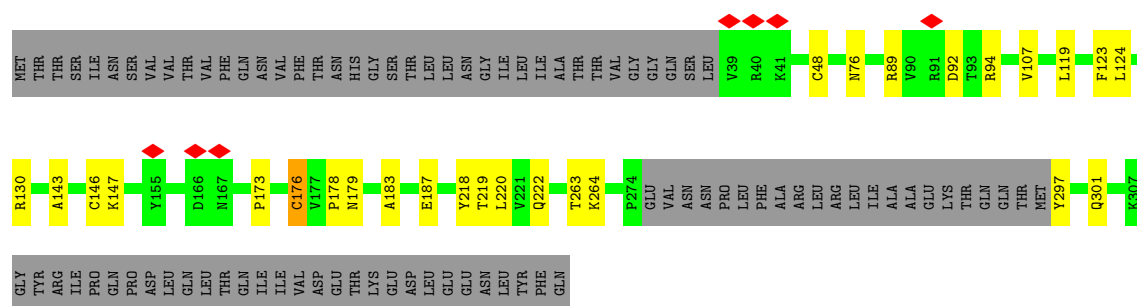
Chain G: 

MET
THR
THR
SER
ILE
ASN
SER
VAL
VAL
THR
THR
PHE
GLN
ASN
VAL
PHE
THR
ASN
HIS
GLY
SER
THR
LEU
LEU
ASN
GLY
ILE
LEU
ILE
ALA
THR
THR
VAL
VAL
GLY
GLY
GLN
SER
LEU
V39
R40
K41
L42
C48
N76
R89
V90
R91
D92
T93
R94
V107
R130
C138

- Molecule 1: Calcium homeostasis modulator protein



- Molecule 1: Calcium homeostasis modulator protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65887	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	258.726, 258.726, 258.726	wwPDB
Map dimensions	178, 178, 178	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.453517, 1.453517, 1.453517	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	0.45	0/2034	0.54	0/2774
1	B	0.45	0/2034	0.54	0/2774
1	C	0.45	0/2034	0.54	0/2774
1	D	0.45	0/2034	0.54	0/2774
1	E	0.45	0/2034	0.54	0/2774
1	F	0.45	0/2034	0.54	0/2774
1	G	0.45	0/2034	0.54	0/2774
1	H	0.45	0/2034	0.54	0/2774
1	I	0.45	0/2034	0.54	0/2774
All	All	0.45	0/18306	0.54	0/24966

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	1974	0	1892	12	0
1	B	1974	0	1892	12	0
1	C	1974	0	1892	15	0
1	D	1974	0	1892	14	0
1	E	1974	0	1892	14	0
1	F	1974	0	1892	12	0
1	G	1974	0	1892	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1974	0	1892	14	0
1	I	1974	0	1892	16	0
All	All	17766	0	17028	123	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.

All (123) 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:F:143:ALA:O	1:F:147:LYS:NZ	2.34	0.61
1:A:143:ALA:O	1:A:147:LYS:NZ	2.34	0.61
1:C:143:ALA:O	1:C:147:LYS:NZ	2.34	0.61
1:D:143:ALA:O	1:D:147:LYS:NZ	2.34	0.61
1:I:143:ALA:O	1:I:147:LYS:NZ	2.34	0.61
1:B:143:ALA:O	1:B:147:LYS:NZ	2.34	0.60
1:E:143:ALA:O	1:E:147:LYS:NZ	2.34	0.60
1:H:143:ALA:O	1:H:147:LYS:NZ	2.34	0.60
1:G:143:ALA:O	1:G:147:LYS:NZ	2.34	0.60
1:F:130:ARG:NH1	1:F:187:GLU:OE1	2.38	0.57
1:E:130:ARG:NH1	1:E:187:GLU:OE1	2.38	0.56
1:I:130:ARG:NH1	1:I:187:GLU:OE1	2.38	0.56
1:G:130:ARG:NH1	1:G:187:GLU:OE1	2.38	0.56
1:H:130:ARG:NH1	1:H:187:GLU:OE1	2.38	0.56
1:F:146:CYS:SG	1:F:147:LYS:NZ	2.77	0.56
1:C:130:ARG:NH1	1:C:187:GLU:OE1	2.38	0.56
1:G:146:CYS:SG	1:G:147:LYS:NZ	2.77	0.56
1:E:146:CYS:SG	1:E:147:LYS:NZ	2.77	0.55
1:D:130:ARG:NH1	1:D:187:GLU:OE1	2.38	0.55
1:A:130:ARG:NH1	1:A:187:GLU:OE1	2.38	0.55
1:B:130:ARG:NH1	1:B:187:GLU:OE1	2.38	0.55
1:H:146:CYS:SG	1:H:147:LYS:NZ	2.77	0.55
1:D:146:CYS:SG	1:D:147:LYS:NZ	2.76	0.54
1:I:146:CYS:SG	1:I:147:LYS:NZ	2.77	0.53
1:C:146:CYS:SG	1:C:147:LYS:NZ	2.77	0.53
1:A:146:CYS:SG	1:A:147:LYS:NZ	2.77	0.52
1:B:146:CYS:SG	1:B:147:LYS:NZ	2.76	0.52
1:B:219:THR:OG1	1:B:220:LEU:N	2.45	0.49
1:E:219:THR:OG1	1:E:220:LEU:N	2.45	0.49
1:D:219:THR:OG1	1:D:220:LEU:N	2.45	0.49
1:C:219:THR:OG1	1:C:220:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PRO:HG2	1:B:183:ALA:HB2	1.95	0.49
1:C:178:PRO:HG2	1:C:183:ALA:HB2	1.95	0.49
1:A:178:PRO:HG2	1:A:183:ALA:HB2	1.95	0.48
1:D:178:PRO:HG2	1:D:183:ALA:HB2	1.95	0.48
1:G:219:THR:OG1	1:G:220:LEU:N	2.45	0.48
1:I:219:THR:OG1	1:I:220:LEU:N	2.45	0.48
1:A:219:THR:OG1	1:A:220:LEU:N	2.45	0.48
1:H:219:THR:OG1	1:H:220:LEU:N	2.45	0.48
1:I:178:PRO:HG2	1:I:183:ALA:HB2	1.95	0.48
1:F:219:THR:OG1	1:F:220:LEU:N	2.45	0.48
1:F:178:PRO:HG2	1:F:183:ALA:HB2	1.95	0.48
1:G:178:PRO:HG2	1:G:183:ALA:HB2	1.95	0.48
1:H:178:PRO:HG2	1:H:183:ALA:HB2	1.95	0.47
1:B:138:CYS:HB3	1:B:174:CYS:HB3	1.71	0.47
1:E:178:PRO:HG2	1:E:183:ALA:HB2	1.95	0.47
1:D:138:CYS:HB3	1:D:174:CYS:HB3	1.71	0.47
1:C:76:ASN:HD22	1:C:107:VAL:HG13	1.80	0.47
1:H:76:ASN:HD22	1:H:107:VAL:HG13	1.80	0.47
1:D:76:ASN:HD22	1:D:107:VAL:HG13	1.80	0.47
1:E:76:ASN:HD22	1:E:107:VAL:HG13	1.80	0.47
1:G:76:ASN:HD22	1:G:107:VAL:HG13	1.80	0.47
1:A:76:ASN:HD22	1:A:107:VAL:HG13	1.80	0.47
1:I:76:ASN:HD22	1:I:107:VAL:HG13	1.80	0.47
1:F:76:ASN:HD22	1:F:107:VAL:HG13	1.80	0.46
1:B:76:ASN:HD22	1:B:107:VAL:HG13	1.80	0.46
1:C:138:CYS:HB3	1:C:174:CYS:HB3	1.71	0.46
1:G:138:CYS:HB3	1:G:174:CYS:HB3	1.71	0.46
1:G:297:TYR:N	1:G:301:GLN:OE1	2.49	0.46
1:H:297:TYR:N	1:H:301:GLN:OE1	2.49	0.46
1:I:297:TYR:N	1:I:301:GLN:OE1	2.49	0.46
1:A:138:CYS:HB3	1:A:174:CYS:HB3	1.71	0.46
1:C:218:TYR:HB3	1:C:222:GLN:HB3	1.98	0.46
1:F:297:TYR:N	1:F:301:GLN:OE1	2.49	0.46
1:G:218:TYR:HB3	1:G:222:GLN:HB3	1.99	0.46
1:E:218:TYR:HB3	1:E:222:GLN:HB3	1.98	0.45
1:E:297:TYR:N	1:E:301:GLN:OE1	2.49	0.45
1:A:297:TYR:N	1:A:301:GLN:OE1	2.49	0.45
1:A:218:TYR:HB3	1:A:222:GLN:HB3	1.98	0.45
1:B:297:TYR:N	1:B:301:GLN:OE1	2.49	0.45
1:C:297:TYR:N	1:C:301:GLN:OE1	2.49	0.45
1:D:297:TYR:N	1:D:301:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:TYR:HB3	1:I:222:GLN:HB3	1.98	0.45
1:D:218:TYR:HB3	1:D:222:GLN:HB3	1.99	0.44
1:H:218:TYR:HB3	1:H:222:GLN:HB3	1.98	0.44
1:F:218:TYR:HB3	1:F:222:GLN:HB3	1.98	0.44
1:B:218:TYR:HB3	1:B:222:GLN:HB3	1.98	0.44
1:C:124:LEU:HD12	1:C:124:LEU:HA	1.89	0.43
1:H:138:CYS:HB3	1:H:174:CYS:HB3	1.71	0.42
1:E:179:ASN:O	1:E:183:ALA:N	2.50	0.42
1:E:124:LEU:HD12	1:E:124:LEU:HA	1.89	0.42
1:G:263:THR:OG1	1:G:264:LYS:N	2.53	0.42
1:A:173:PRO:HA	1:A:176:CYS:HB2	2.02	0.42
1:B:173:PRO:HA	1:B:176:CYS:HB2	2.02	0.42
1:D:179:ASN:O	1:D:183:ALA:N	2.50	0.42
1:E:89:ARG:HB3	1:E:94:ARG:HE	1.85	0.42
1:C:173:PRO:HA	1:C:176:CYS:HB2	2.02	0.42
1:I:89:ARG:HB3	1:I:94:ARG:HE	1.85	0.42
1:E:263:THR:OG1	1:E:264:LYS:N	2.53	0.41
1:H:89:ARG:HB3	1:H:94:ARG:HE	1.85	0.41
1:I:173:PRO:HA	1:I:176:CYS:HB2	2.02	0.41
1:D:263:THR:OG1	1:D:264:LYS:N	2.53	0.41
1:H:173:PRO:HA	1:H:176:CYS:HB2	2.02	0.41
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.94	0.41
1:F:92:ASP:OD1	1:F:92:ASP:N	2.54	0.41
1:F:179:ASN:O	1:F:183:ALA:N	2.50	0.41
1:I:179:ASN:O	1:I:183:ALA:N	2.50	0.41
1:I:263:THR:OG1	1:I:264:LYS:N	2.53	0.41
1:C:89:ARG:HB3	1:C:94:ARG:HE	1.85	0.41
1:D:173:PRO:HA	1:D:176:CYS:HB2	2.02	0.41
1:H:263:THR:OG1	1:H:264:LYS:N	2.53	0.41
1:B:89:ARG:HB3	1:B:94:ARG:HE	1.85	0.41
1:D:89:ARG:HB3	1:D:94:ARG:HE	1.85	0.41
1:F:173:PRO:HA	1:F:176:CYS:HB2	2.02	0.41
1:G:92:ASP:OD1	1:G:92:ASP:N	2.54	0.41
1:H:92:ASP:OD1	1:H:92:ASP:N	2.54	0.41
1:C:263:THR:OG1	1:C:264:LYS:N	2.53	0.41
1:I:92:ASP:OD1	1:I:92:ASP:N	2.54	0.41
1:A:263:THR:OG1	1:A:264:LYS:N	2.53	0.41
1:I:119:LEU:HD23	1:I:119:LEU:HA	1.94	0.41
1:I:124:LEU:HD12	1:I:124:LEU:HA	1.89	0.41
1:B:162:ASN:HD22	1:B:162:ASN:HA	1.72	0.41
1:D:119:LEU:HD23	1:D:119:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:PRO:HA	1:E:176:CYS:HB2	2.02	0.41
1:F:89:ARG:HB3	1:F:94:ARG:HE	1.85	0.41
1:G:173:PRO:HA	1:G:176:CYS:HB2	2.02	0.41
1:G:179:ASN:O	1:G:183:ALA:N	2.50	0.41
1:C:179:ASN:O	1:C:183:ALA:N	2.50	0.41
1:H:162:ASN:HD22	1:H:162:ASN:HA	1.72	0.40
1:A:89:ARG:HB3	1:A:94:ARG:HE	1.85	0.40
1:E:248:LEU:HD23	1:E:248:LEU:HA	1.91	0.40
1:G:89:ARG:HB3	1:G:94:ARG:HE	1.85	0.40
1:I:123:PHE:HD1	1:I:123:PHE:HA	1.76	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	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	B	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	C	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	D	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	E	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	F	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	G	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	H	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
1	I	243/337 (72%)	228 (94%)	15 (6%)	0	100	100
All	All	2187/3033 (72%)	2052 (94%)	135 (6%)	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	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	B	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	C	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	D	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	E	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	F	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	G	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	H	212/299 (71%)	210 (99%)	2 (1%)	75	87
1	I	212/299 (71%)	210 (99%)	2 (1%)	75	87
All	All	1908/2691 (71%)	1890 (99%)	18 (1%)	74	87

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	CYS
1	A	176	CYS
1	B	48	CYS
1	B	176	CYS
1	C	48	CYS
1	C	176	CYS
1	D	48	CYS
1	D	176	CYS
1	E	48	CYS
1	E	176	CYS
1	F	48	CYS
1	F	176	CYS
1	G	48	CYS
1	G	176	CYS
1	H	48	CYS
1	H	176	CYS
1	I	48	CYS
1	I	176	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	162	ASN
1	B	84	HIS
1	B	162	ASN
1	C	84	HIS
1	C	162	ASN
1	D	84	HIS
1	D	162	ASN
1	E	84	HIS
1	E	162	ASN
1	F	84	HIS
1	F	162	ASN
1	G	84	HIS
1	G	162	ASN
1	H	84	HIS
1	H	162	ASN
1	I	162	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

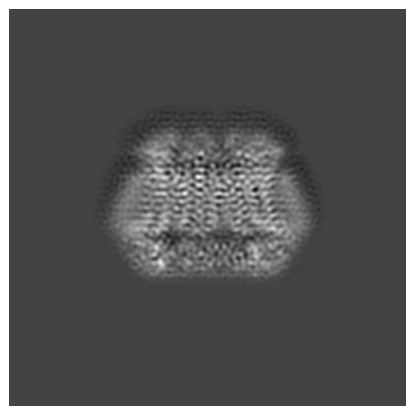
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0921. These allow visual inspection of the internal detail of the map and identification of artifacts.

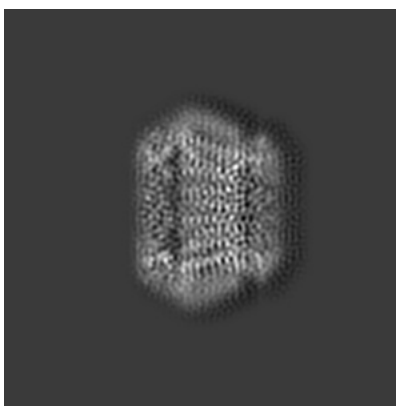
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

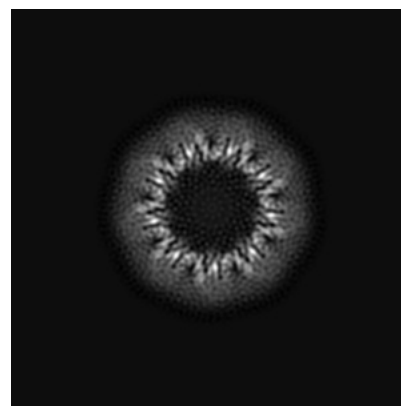
6.1.1 Primary map



X

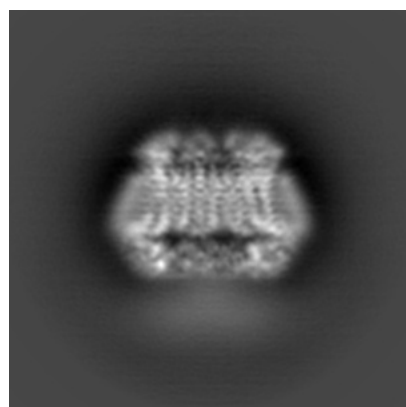


Y

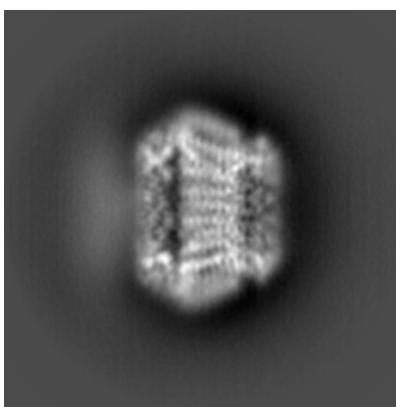


Z

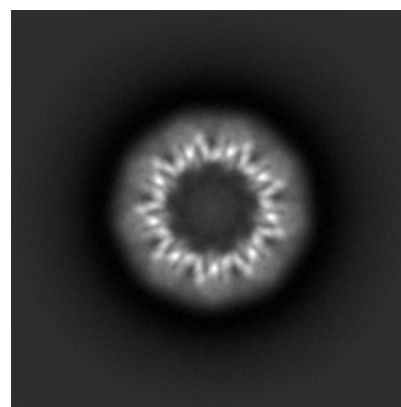
6.1.2 Raw map



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: 89

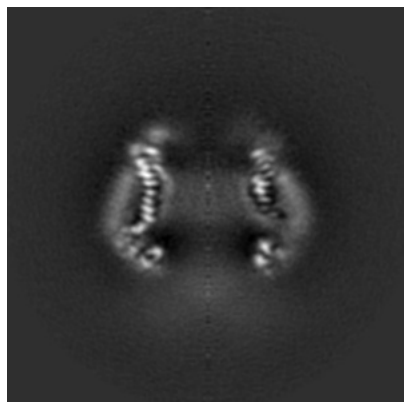


Y Index: 89

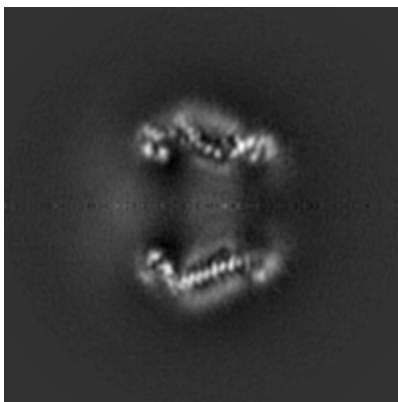


Z Index: 89

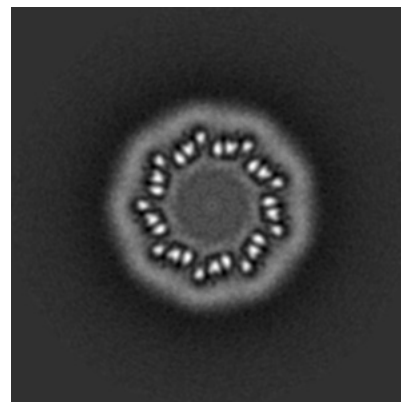
6.2.2 Raw map



X Index: 89



Y Index: 89

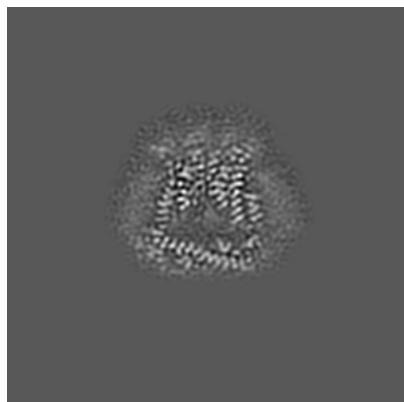


Z Index: 89

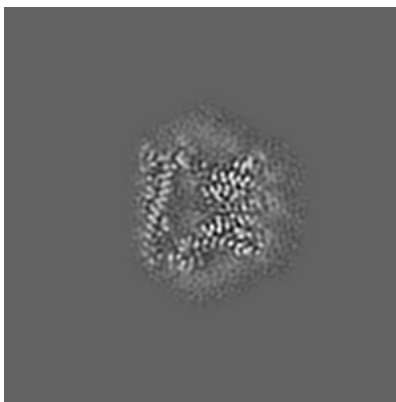
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

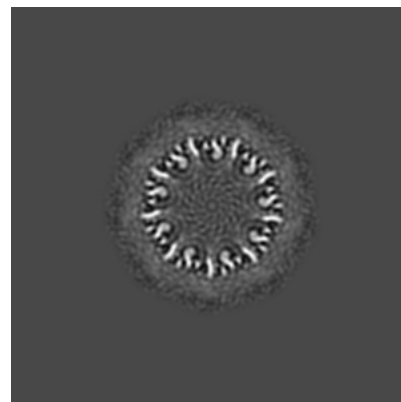
6.3.1 Primary map



X Index: 66

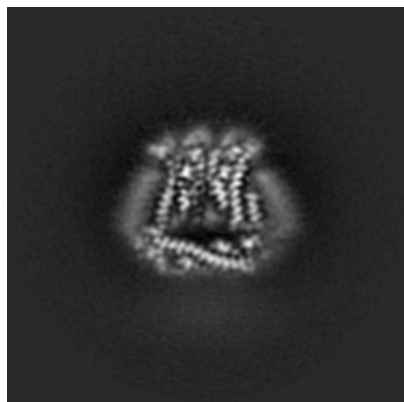


Y Index: 66

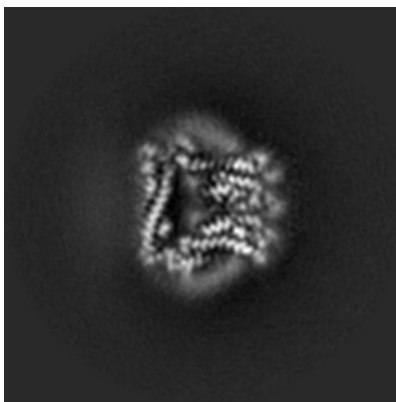


Z Index: 103

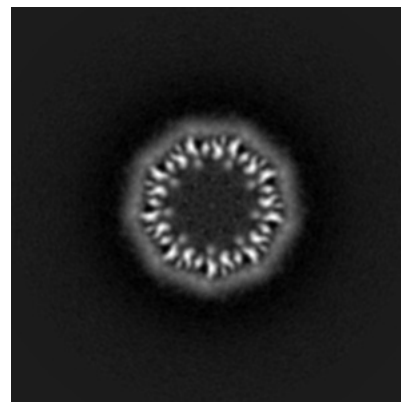
6.3.2 Raw map



X Index: 66



Y Index: 67

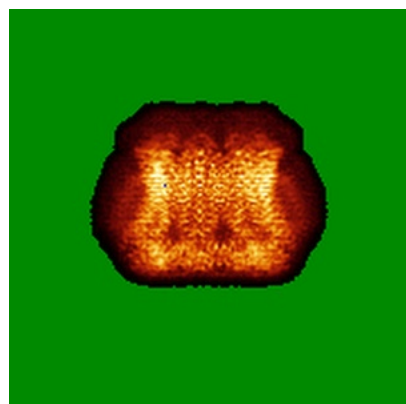


Z Index: 103

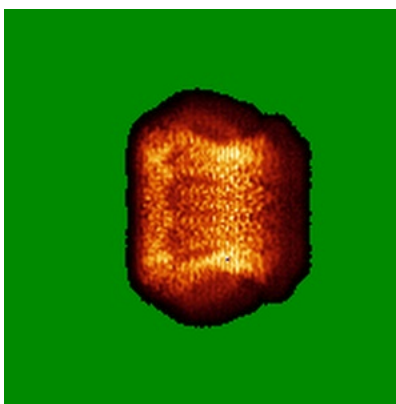
The images above show the largest variance slices of the map in three orthogonal directions.

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

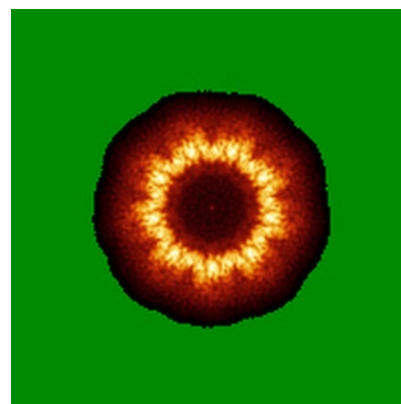
6.4.1 Primary map



X

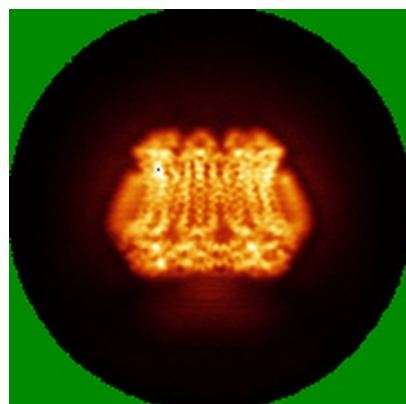


Y

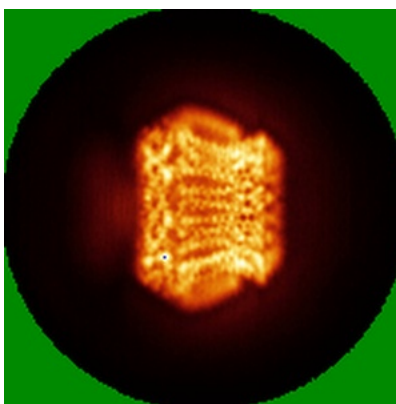


Z

6.4.2 Raw map



X



Y

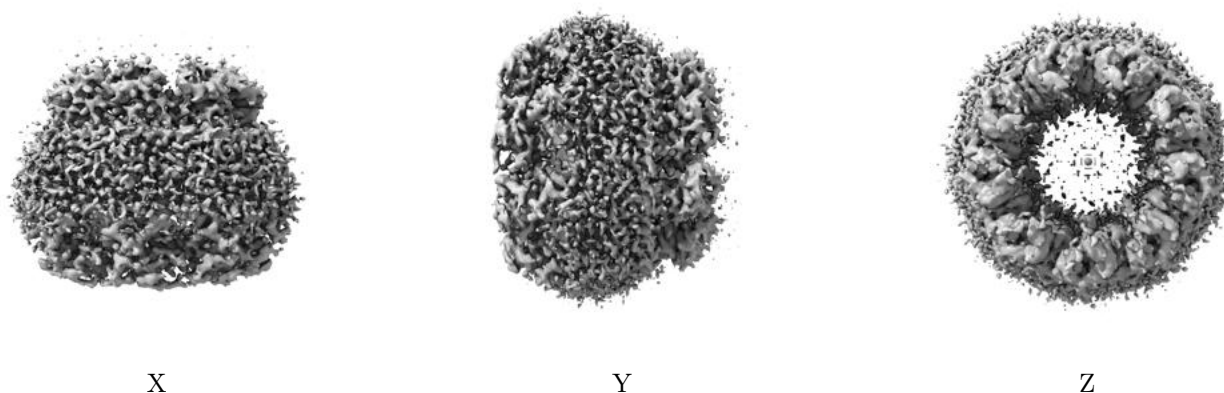


Z

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.

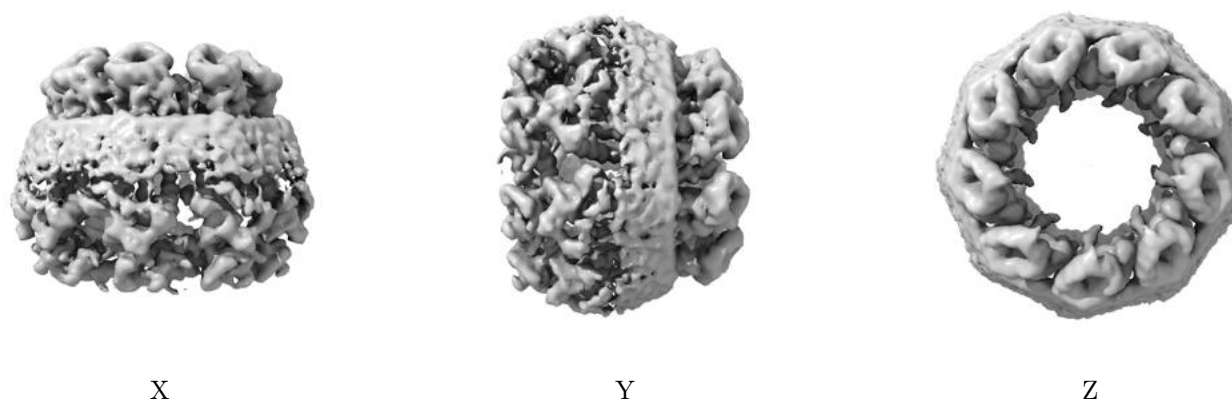
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. 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.

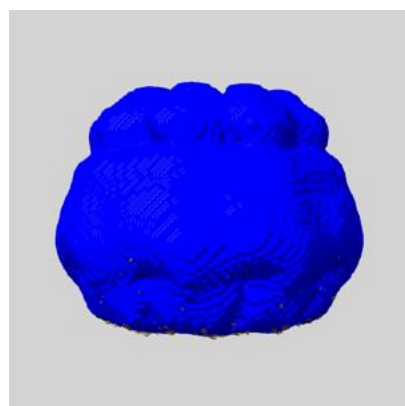
6.6 Mask visualisation [i](#)

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

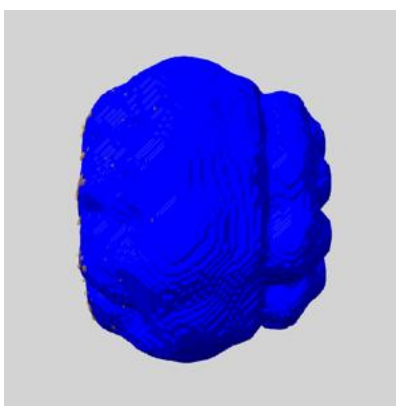
A mask typically either:

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

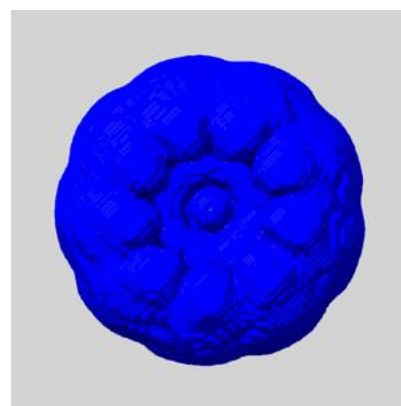
6.6.1 emd_0921_msk_1.map [i](#)



X



Y

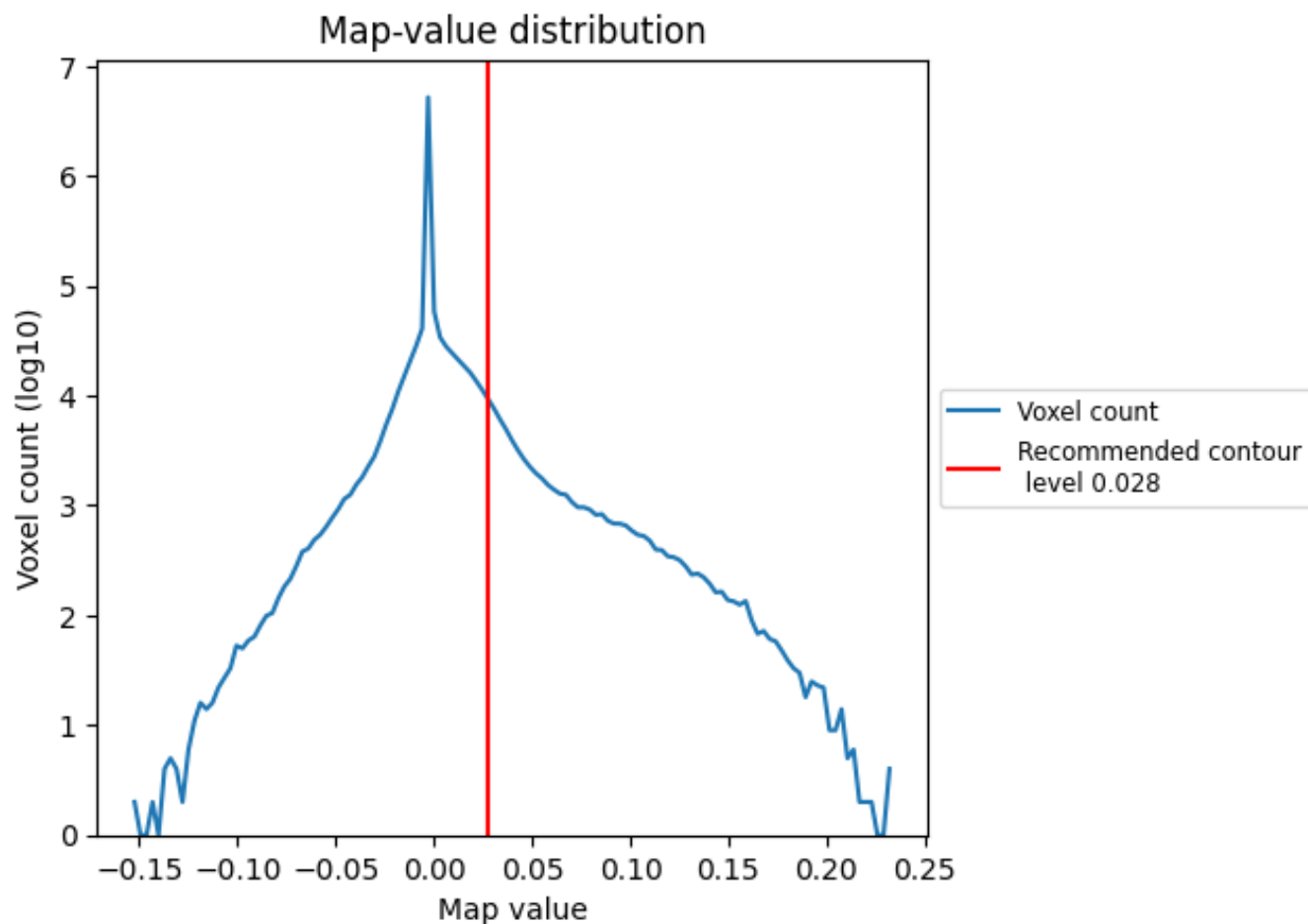


Z

7 Map analysis [i](#)

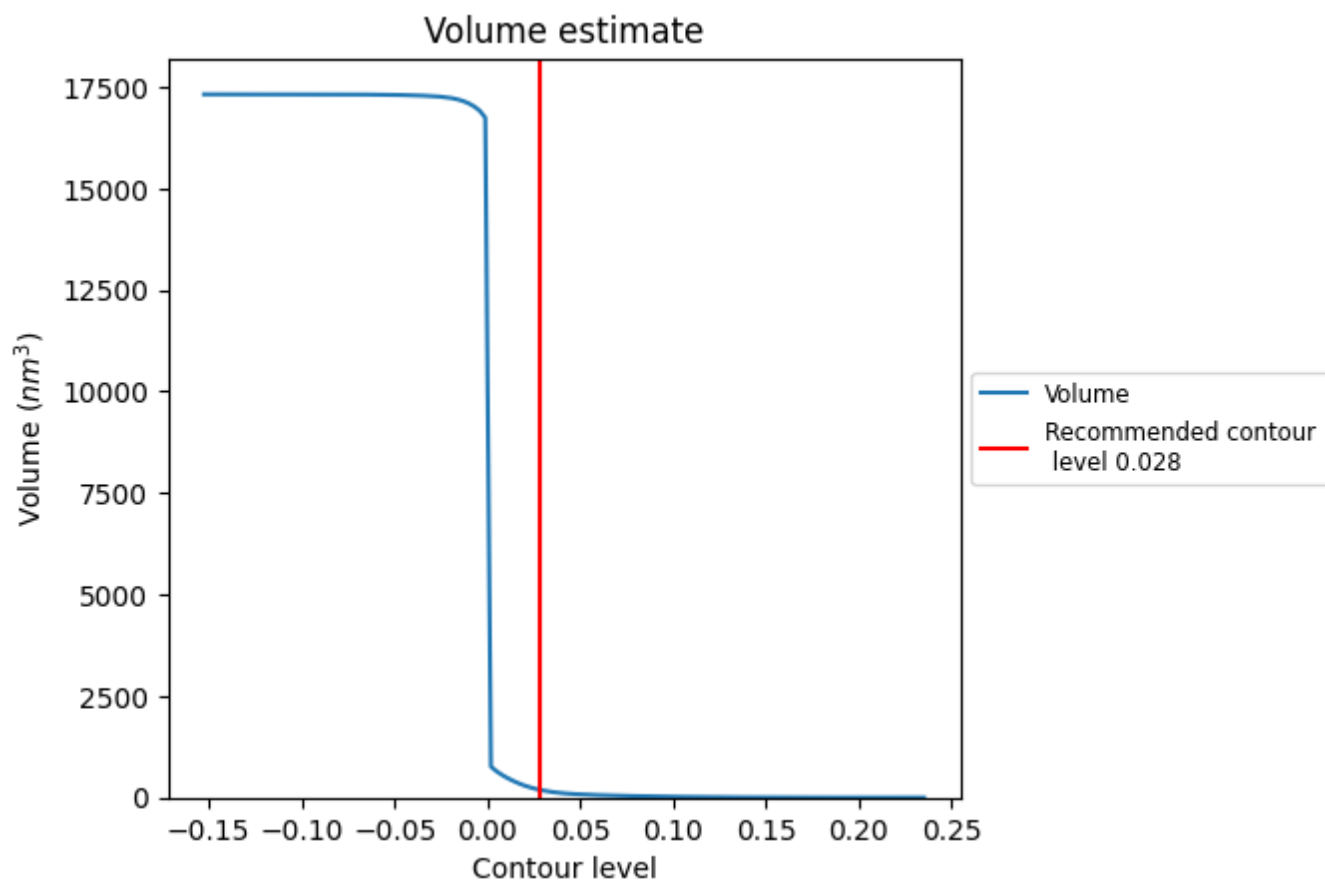
This section contains the results of statistical analysis of the map.

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.

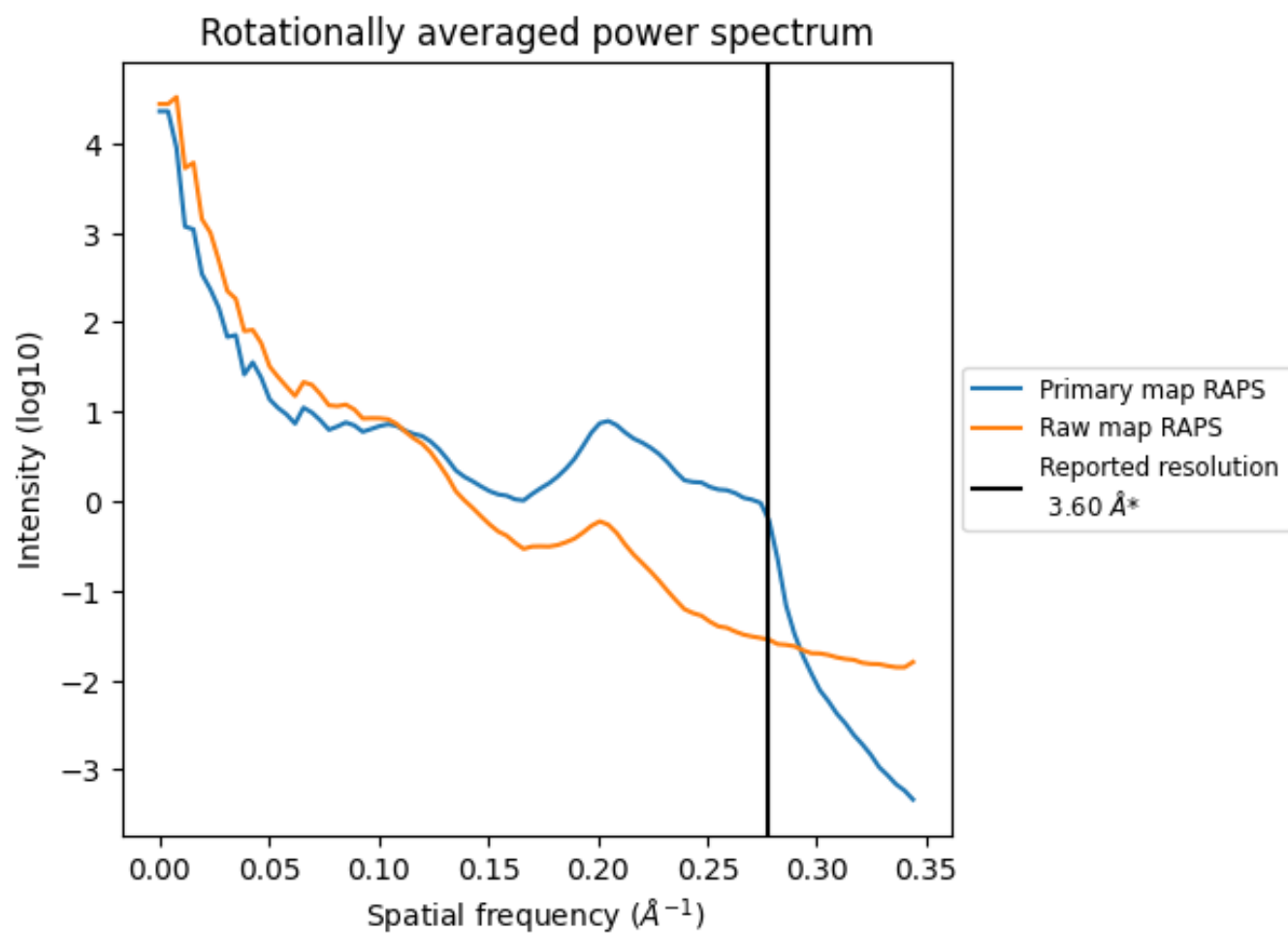
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 193 nm³; this corresponds to an approximate mass of 174 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 ⓘ

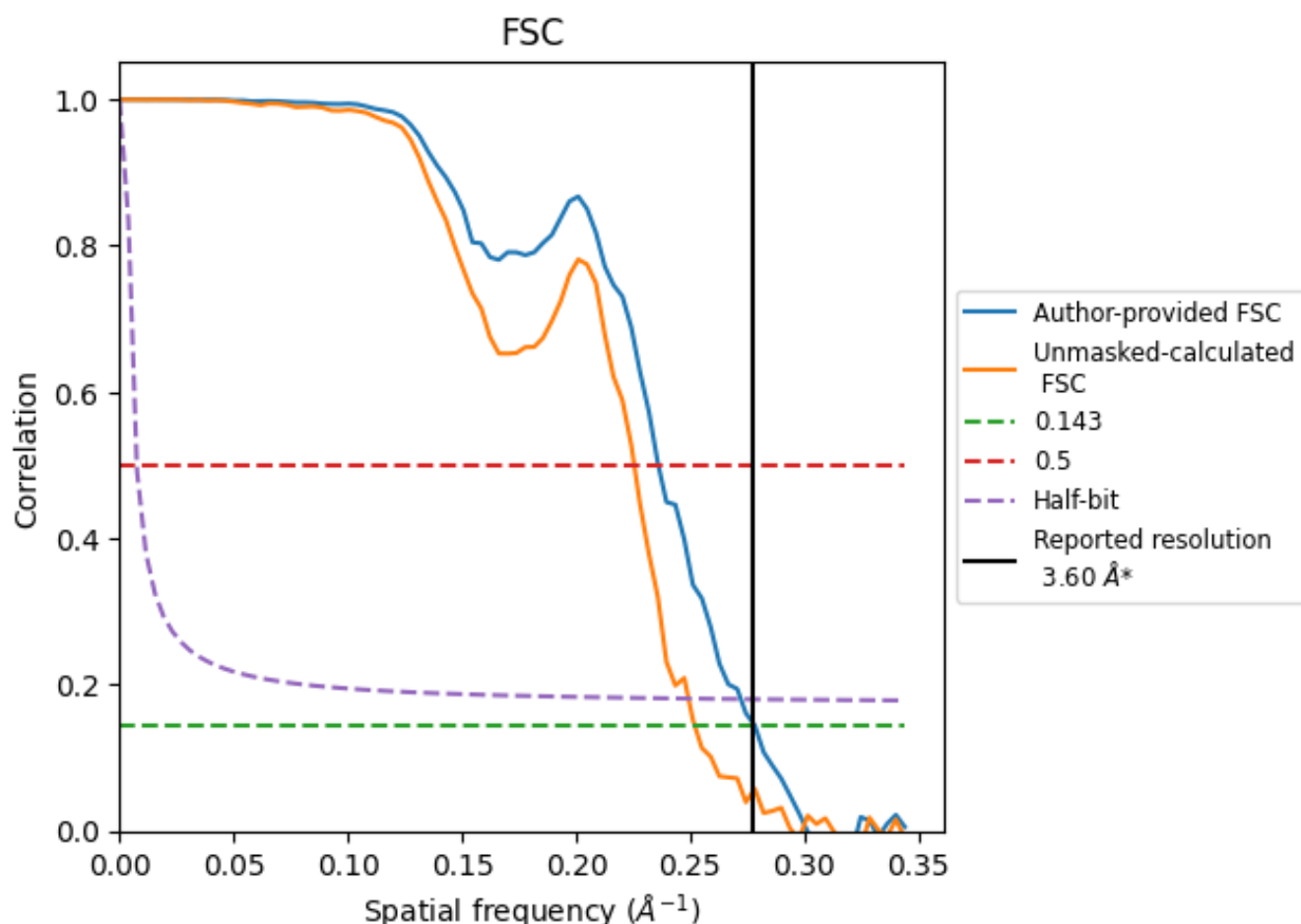


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

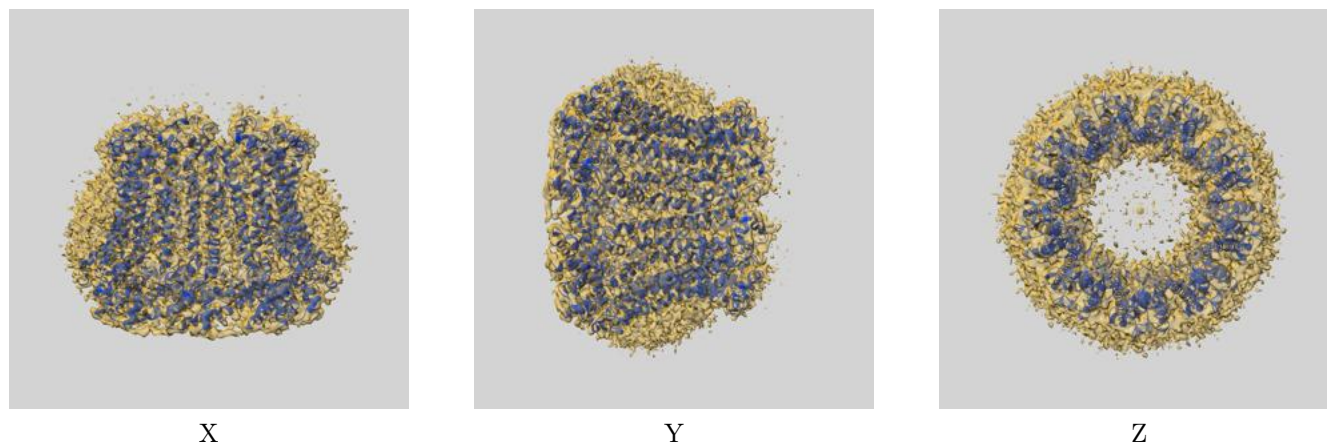
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.24	3.67
Unmasked-calculated*	3.97	4.43	4.01

*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 3.97 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

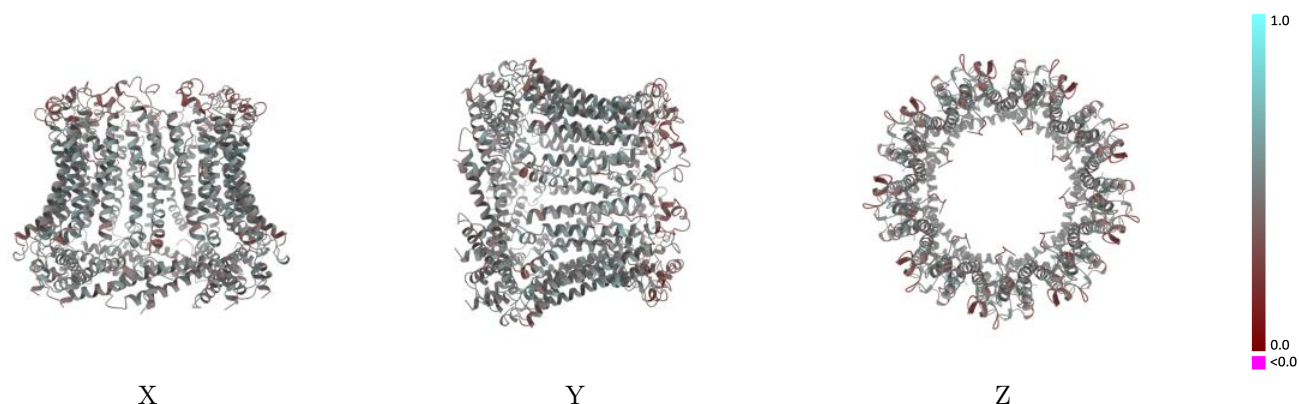
This section contains information regarding the fit between EMDB map EMD-0921 and PDB model 6LMV. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



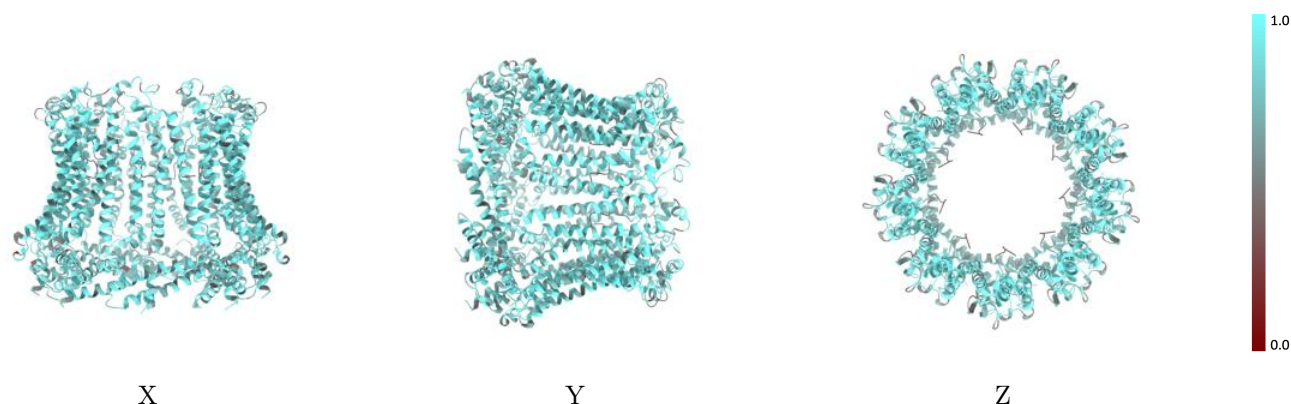
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



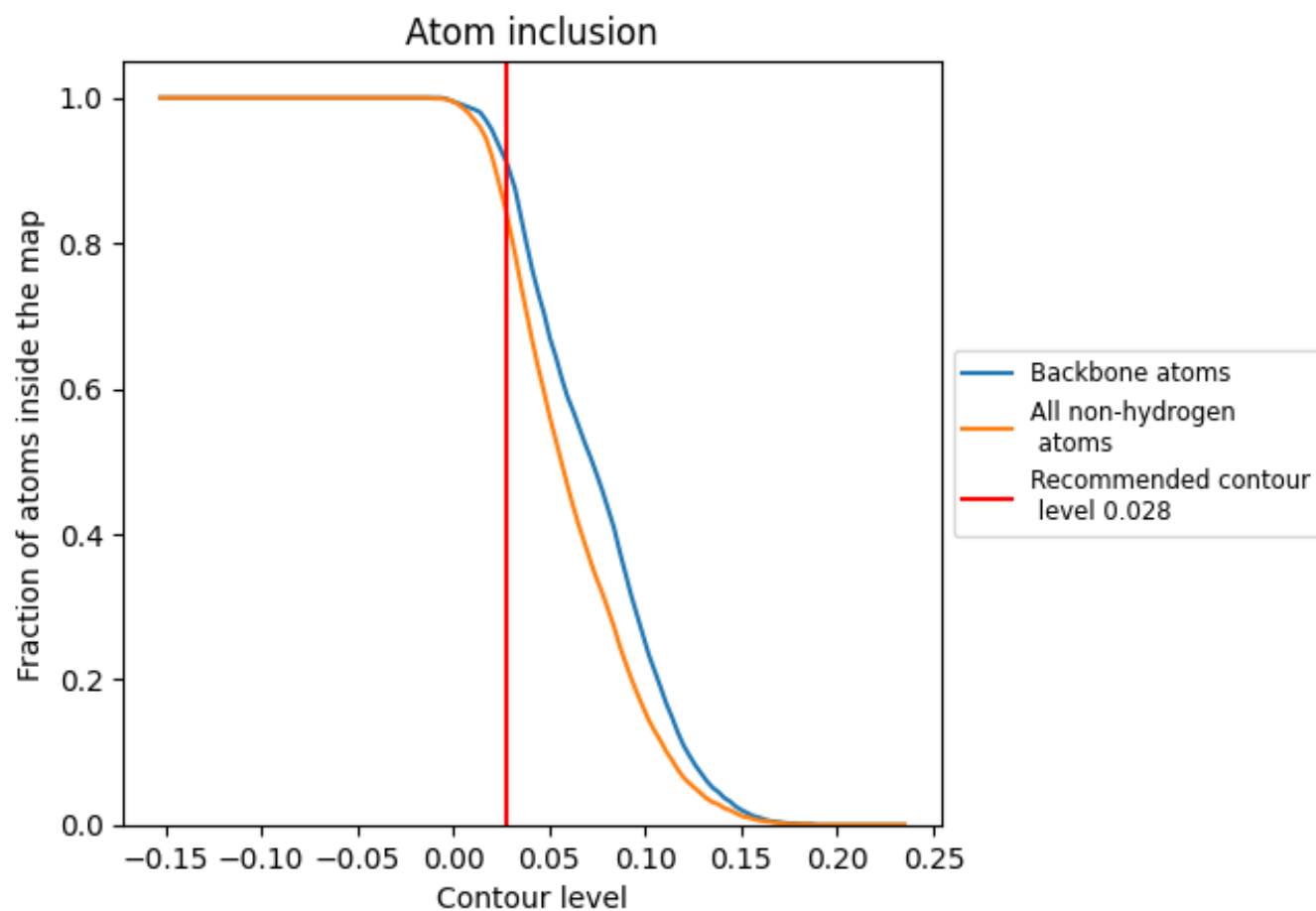
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8390	<div><div></div></div> 0.4670
A	<div><div></div></div> 0.8350	<div><div></div></div> 0.4690
B	<div><div></div></div> 0.8390	<div><div></div></div> 0.4670
C	<div><div></div></div> 0.8430	<div><div></div></div> 0.4670
D	<div><div></div></div> 0.8370	<div><div></div></div> 0.4690
E	<div><div></div></div> 0.8380	<div><div></div></div> 0.4660
F	<div><div></div></div> 0.8430	<div><div></div></div> 0.4700
G	<div><div></div></div> 0.8390	<div><div></div></div> 0.4670
H	<div><div></div></div> 0.8380	<div><div></div></div> 0.4660
I	<div><div></div></div> 0.8380	<div><div></div></div> 0.4650

1.0

0.0

<0.0