



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:28 AM UTC

PDB ID : 8V91 / pdb_00008v91
EMDB ID : EMD-43047
Title : Structure of human AQP4 with a pathogenic autoantibody- rAB 58
Authors : Gupta, M.; Khandelwal, N.K.; Stroud, R.M.
Deposited on : 2023-12-07
Resolution : 2.60 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

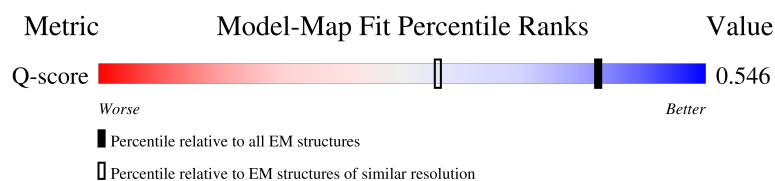
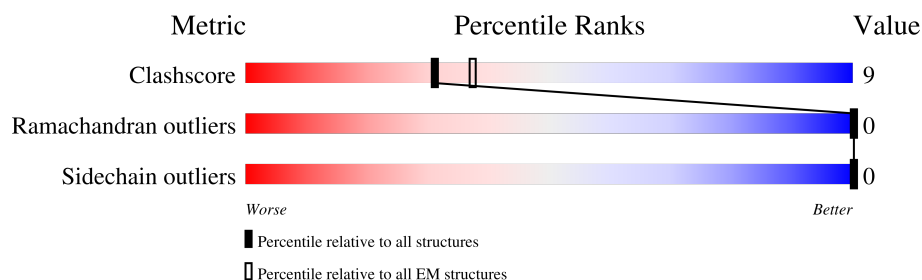
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	323	
1	B	323	
1	C	323	
1	D	323	

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Mol	Chain	Length	Quality of chain
2	I	214	18% 84% 15%
3	J	223	13% 77% 20%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9913 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 Aquaporin-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		
1	B	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		
1	C	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		
1	D	223	Total	C	N	O	S	0	0
			1654	1092	265	284	13		

- Molecule 2 is a protein called rAB 58 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	212	Total	C	N	O	S	0	0
			1626	1021	274	326	5		

- Molecule 3 is a protein called rAB 58 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	216	Total	C	N	O	S	0	0
			1584	997	267	315	5		

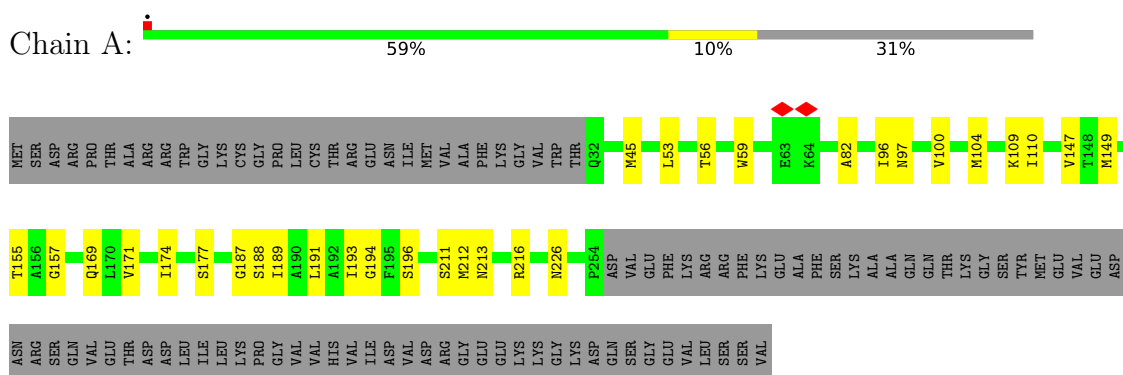
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	21	Total	O	0
			21	21	
4	B	23	Total	O	0
			23	23	
4	C	22	Total	O	0
			22	22	
4	D	21	Total	O	0
			21	21	

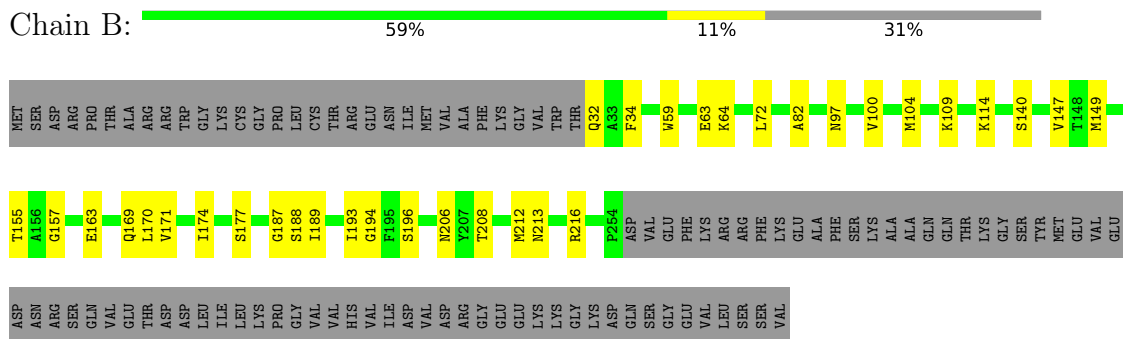
3 Residue-property plots [i](#)

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.

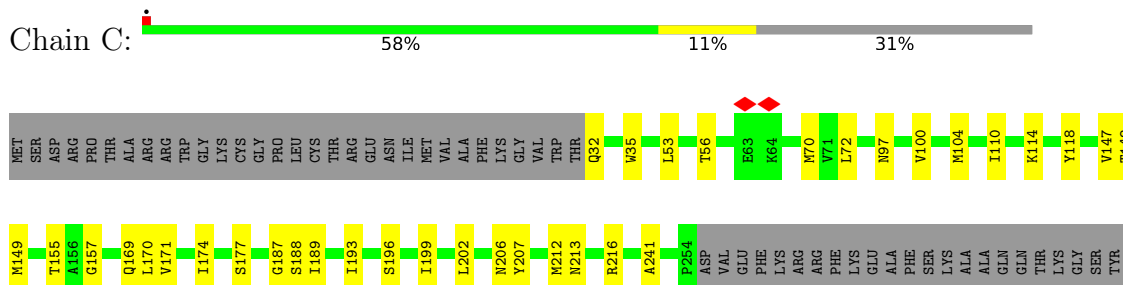
• Molecule 1: Aquaporin-4



• Molecule 1: Aquaporin-4



• Molecule 1: Aquaporin-4



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

• Molecule 1: Aquaporin-4

Chain D:  54% 15% 31%

MET
SER
ARG
PRO
THR
ALA
ARG
GLN
TRP
GLY
LYS
CYS
GLY
PRO
LEU
ILE
CYS
THR
ARG
GLU
ASN
VAL
HIS
MET
VAL
ALA
PHE
LYS
VAL
ASP
VAL
GLY
TRP
THR
Q32
Q33
F34
W35
K36
E41
A44
M45
L53
T56
E63
K64
M70
A82
F88
S92
T96
N97

V100
M104
K109
K114
A126
G146
V147
T148
M153
L154
T155
A156
G157
E163
Q169
L170
V171
I174
S177
K181
G187
S188
I189
I193
G194
F195
S196
T199
G200
H201
L202
I205
N206
T207
T208
S211
M212
N213
R216
P254
VAL

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

GLY
GLU
VAL
LEU
SER
SER
VAL

• Molecule 2: rAB 58 Light Chain

Chain I:  18% 84% 15%

D1
M4
D17
T18
R24
R30
S31
A34
Q37
L47
S76
D81
Q89
H90
Y91
N92
S93
Y96
R107
P113
F116
D122
E123
Q124
L125
K126
S127
G128
T129
A130
S131
L135
F139
R142
E143
A144
K145
V146
Q147
V150
D151

M152
A153
L154
Q155
S156
G157
M158
S159
Q160
V163
S168
K169
ASP
S171
L175
L181
S182
K183
A184
D185
Y186
E187
K188
H189
K190
L201
S202
S203
T206
N210
R211
G212
E213
CYS

• Molecule 3: rAB 58 Heavy Chain

Chain J:  13% 77% 20%

Q1
V12
F29
R30
A33
W36
V37
R38
E46
S52
I70
T71
D73
N74
S75
K76
L86
R87
A88
D89
D90
Y94
A97
D100
Y101
V102
F103
T119
K120
G121
P122
S123
V124
F125
P126
S130
S131
K132
S133
T134
S135
G136
G137
T138
A139
A140

L141
G142
C143
L144
V145
K146
D147
N158
S159
G160
A161
A171
S175
L178
L181
V184
S189
S190
S191
L192
G193
T194
Q195
T196
V201
N207
T208
K209
V210
D211
K212
K213
V214
E215
P216
LYS
SER
CYS
ASP
LYS
THR
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	323342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	2.848	Depositor
Minimum map value	-1.519	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.55	Depositor
Map size ($\text{\AA}$)	326.928, 326.928, 326.928	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.83400005, 0.83400005, 0.83400005	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	0.11	0/1697	0.31	0/2317
1	B	0.11	0/1697	0.29	0/2317
1	C	0.10	0/1697	0.27	0/2317
1	D	0.11	0/1697	0.30	0/2317
2	I	0.11	0/1663	0.30	0/2260
3	J	0.11	0/1622	0.27	0/2213
All	All	0.11	0/10073	0.29	0/13741

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	1654	0	1692	24	0
1	B	1654	0	1692	25	0
1	C	1654	0	1692	30	0
1	D	1654	0	1692	48	0
2	I	1626	0	1566	30	0
3	J	1584	0	1536	33	0
4	A	21	0	0	0	0
4	B	23	0	0	1	0
4	C	22	0	0	0	0
4	D	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9913	0	9870	174	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 9.

All (174) 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:D:32:GLN:HB3	1:D:35:TRP:CD1	1.71	1.25
1:D:32:GLN:N	1:D:35:TRP:HE1	1.54	1.04
3:J:86:LEU:HD23	3:J:90:ASP:OD2	1.66	0.93
1:D:32:GLN:O	1:D:35:TRP:CD1	2.22	0.92
1:D:32:GLN:HB3	1:D:35:TRP:HD1	1.06	0.88
1:D:32:GLN:O	1:D:35:TRP:NE1	2.09	0.85
1:B:59:TRP:CD1	1:C:206:ASN:HD22	1.94	0.85
1:C:114:LYS:HE3	1:C:118:TYR:CZ	2.15	0.81
1:D:97:ASN:HB3	1:D:100:VAL:HG22	1.63	0.80
1:D:32:GLN:CB	1:D:35:TRP:CD1	2.60	0.79
1:C:97:ASN:HB3	1:C:100:VAL:HG22	1.66	0.77
2:I:17:ASP:OD1	2:I:18:THR:N	2.20	0.75
1:A:147:VAL:HG12	1:A:149:MET:HE3	1.70	0.74
1:C:114:LYS:NZ	1:C:118:TYR:OH	2.19	0.73
1:B:97:ASN:HB3	1:B:100:VAL:HG22	1.69	0.72
3:J:86:LEU:CD2	3:J:90:ASP:OD2	2.37	0.72
1:B:147:VAL:HG12	1:B:149:MET:HE3	1.70	0.71
1:B:163:GLU:OE2	1:B:208:THR:OG1	2.09	0.70
1:D:32:GLN:CB	1:D:35:TRP:HD1	1.95	0.69
1:D:155:THR:HG22	1:D:157:GLY:H	1.59	0.68
3:J:90:ASP:OD1	3:J:90:ASP:O	2.13	0.67
1:C:155:THR:HG22	1:C:157:GLY:H	1.60	0.67
1:B:155:THR:HG22	1:B:157:GLY:H	1.60	0.65
2:I:190:LYS:HA	2:I:211:ARG:HD2	1.81	0.62
1:A:155:THR:HG22	1:A:157:GLY:H	1.65	0.62
1:A:45:MET:HE2	1:A:96:ILE:O	2.00	0.61
3:J:73:ASP:OD2	3:J:76:LYS:NZ	2.27	0.61
3:J:124:VAL:HG11	3:J:201:VAL:HG21	1.82	0.61
1:D:32:GLN:CA	1:D:35:TRP:HE1	2.14	0.60
3:J:196:THR:HG23	3:J:213:LYS:HE3	1.83	0.60
2:I:113:PRO:HB3	2:I:139:PHE:HB3	1.83	0.60
1:A:104:MET:HB3	1:A:109:LYS:HB2	1.84	0.60
1:C:114:LYS:CE	1:C:118:TYR:CZ	2.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:90:ASP:OD1	3:J:94:TYR:OH	2.20	0.60
1:D:32:GLN:N	1:D:35:TRP:NE1	2.38	0.59
3:J:119:THR:HB	3:J:178:LEU:HD11	1.83	0.59
2:I:150:VAL:HG21	2:I:155:GLN:HE21	1.69	0.58
1:A:59:TRP:CD1	1:B:206:ASN:HD22	2.20	0.58
1:A:45:MET:CE	1:A:96:ILE:O	2.51	0.58
2:I:30:ARG:HG3	2:I:31:SER:N	2.19	0.57
2:I:30:ARG:HG3	2:I:31:SER:H	1.68	0.57
2:I:34:ALA:HB3	2:I:89:GLN:HB3	1.87	0.57
1:D:199:ILE:HA	1:D:202:LEU:HB2	1.87	0.57
1:B:174:ILE:HG12	1:B:193:ILE:HD13	1.87	0.56
1:B:63:GLU:HG3	3:J:101:TYR:HD2	1.70	0.56
1:C:104:MET:HB2	1:C:110:ILE:HG12	1.87	0.56
1:A:169:GLN:OE1	1:A:196:SER:OG	2.25	0.55
1:A:174:ILE:HG12	1:A:193:ILE:HD13	1.88	0.55
3:J:29:PHE:O	3:J:72:ARG:NH2	2.39	0.55
1:A:45:MET:CE	1:A:96:ILE:C	2.80	0.55
1:C:174:ILE:HG12	1:C:193:ILE:HD13	1.90	0.54
1:D:70:MET:HE1	1:D:205:ILE:HG21	1.88	0.54
1:A:187:GLY:HA3	1:D:188:SER:HB2	1.90	0.54
1:D:45:MET:HE2	1:D:126:ALA:HB2	1.89	0.54
1:D:174:ILE:HG12	1:D:193:ILE:HD13	1.90	0.54
1:A:188:SER:HB2	1:B:187:GLY:HA3	1.89	0.54
1:D:32:GLN:CA	1:D:35:TRP:NE1	2.71	0.54
1:D:148:THR:HG21	1:D:211:SER:HB2	1.90	0.53
1:B:188:SER:HB2	1:C:187:GLY:HA3	1.89	0.53
1:C:188:SER:HB2	1:D:187:GLY:HA3	1.89	0.53
1:A:177:SER:HB3	1:A:189:ILE:HG23	1.90	0.53
2:I:163:VAL:HG22	2:I:175:LEU:HG	1.91	0.52
1:B:104:MET:HB3	1:B:109:LYS:HB2	1.90	0.52
1:D:41:GLU:HG2	1:D:92:SER:OG	2.09	0.52
3:J:147:ASP:HA	3:J:178:LEU:HB3	1.92	0.52
1:C:147:VAL:HG12	1:C:149:MET:HE3	1.92	0.52
1:D:169:GLN:OE1	1:D:196:SER:OG	2.27	0.52
1:B:169:GLN:OE1	1:B:196:SER:OG	2.25	0.52
1:C:213:ASN:HB3	1:C:216:ARG:HB3	1.91	0.52
3:J:134:THR:HA	3:J:139:ALA:HB2	1.92	0.51
1:D:181:LYS:NZ	1:D:254:PRO:O	2.42	0.51
1:C:114:LYS:NZ	1:C:118:TYR:CZ	2.79	0.51
1:D:200:GLY:HA3	1:D:212:MET:HE1	1.94	0.51
2:I:160:GLN:HA	2:I:160:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:SER:HB3	1:C:189:ILE:HG23	1.92	0.50
1:D:104:MET:HB3	1:D:109:LYS:HB2	1.93	0.50
1:B:82:ALA:HB2	1:B:194:GLY:HA3	1.94	0.50
1:B:213:ASN:HB3	1:B:216:ARG:HB3	1.94	0.50
2:I:89:GLN:HE21	2:I:96:TYR:HB3	1.75	0.50
2:I:124:GLN:HE22	2:I:131:SER:HB2	1.76	0.50
1:C:169:GLN:OE1	1:C:196:SER:OG	2.26	0.49
1:B:72:LEU:HD13	1:C:70:MET:HB3	1.94	0.49
3:J:30:ARG:HG2	3:J:74:ASN:HB3	1.94	0.49
1:A:82:ALA:HB2	1:A:194:GLY:HA3	1.95	0.49
1:B:170:LEU:HD22	1:B:212:MET:HE2	1.94	0.49
1:C:114:LYS:NZ	1:C:118:TYR:CE1	2.80	0.49
1:D:163:GLU:OE2	1:D:208:THR:OG1	2.23	0.49
3:J:171:ALA:HB2	3:J:181:LEU:HD23	1.95	0.48
2:I:90:HIS:CE1	2:I:92:ASN:HB3	2.48	0.48
1:D:32:GLN:HB3	1:D:35:TRP:NE1	2.24	0.48
1:D:32:GLN:C	1:D:35:TRP:NE1	2.71	0.48
1:B:140:SER:OG	4:B:401:HOH:O	2.19	0.47
1:C:114:LYS:CE	1:C:118:TYR:OH	2.62	0.47
1:D:213:ASN:HB3	1:D:216:ARG:HB3	1.96	0.47
2:I:37:GLN:HB2	2:I:47:LEU:HD11	1.95	0.47
1:B:177:SER:HB3	1:B:189:ILE:HG23	1.95	0.47
1:D:32:GLN:C	1:D:35:TRP:CD1	2.91	0.47
1:A:97:ASN:HB3	1:A:100:VAL:HG22	1.96	0.47
1:C:114:LYS:CE	1:C:118:TYR:CE1	2.98	0.47
1:D:34:PHE:HE1	1:D:114:LYS:HD3	1.80	0.47
1:D:63:GLU:OE1	1:D:64:LYS:HB2	2.15	0.47
1:D:146:GLY:O	1:D:216:ARG:NH2	2.33	0.47
1:D:70:MET:HE1	1:D:205:ILE:CG2	2.43	0.47
2:I:124:GLN:HG3	3:J:125:PHE:CE2	2.50	0.47
1:A:213:ASN:HB3	1:A:216:ARG:HB3	1.97	0.47
1:B:149:MET:HA	1:B:149:MET:HE2	1.96	0.47
1:A:100:VAL:HG12	1:A:171:VAL:HG22	1.97	0.46
1:A:149:MET:HE2	1:A:149:MET:HA	1.98	0.46
1:C:114:LYS:HE3	1:C:118:TYR:CE1	2.51	0.46
1:D:100:VAL:HG12	1:D:171:VAL:HG22	1.97	0.46
3:J:158:ASN:HB2	3:J:161:ALA:HB3	1.97	0.46
1:D:63:GLU:OE1	1:D:64:LYS:CB	2.64	0.46
1:D:53:LEU:O	1:D:56:THR:HG22	2.16	0.45
2:I:4:MET:HE3	2:I:4:MET:HB3	1.81	0.45
1:C:100:VAL:O	1:C:104:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:HE3	1:A:96:ILE:C	2.42	0.45
2:I:90:HIS:HE1	2:I:92:ASN:HB3	1.82	0.45
2:I:116:PHE:HZ	3:J:138:THR:HG23	1.82	0.45
2:I:124:GLN:HG3	3:J:125:PHE:CZ	2.52	0.45
3:J:38:ARG:NE	3:J:46:GLU:OE1	2.50	0.45
1:A:211:SER:C	1:A:212:MET:HG2	2.41	0.45
1:D:35:TRP:CZ3	1:D:36:LYS:HG3	2.52	0.45
2:I:142:ARG:HH11	2:I:142:ARG:HG3	1.82	0.45
3:J:126:PRO:HA	3:J:143:CYS:HA	1.98	0.44
1:A:53:LEU:O	1:A:56:THR:HG22	2.17	0.44
1:C:148:THR:O	1:C:149:MET:HE2	2.17	0.44
1:C:170:LEU:HD22	1:C:212:MET:HE2	1.99	0.44
2:I:91:TYR:CD2	3:J:101:TYR:HB3	2.52	0.44
3:J:52:SER:O	3:J:72:ARG:NH1	2.49	0.44
1:B:100:VAL:O	1:B:104:MET:HG2	2.18	0.43
1:D:44:ALA:HB2	1:D:88:PHE:CD2	2.53	0.43
2:I:107:ARG:HH11	2:I:107:ARG:HG2	1.82	0.43
1:B:34:PHE:CE1	1:B:114:LYS:HD3	2.52	0.43
1:D:96:ILE:O	1:D:96:ILE:HG22	2.18	0.43
2:I:210:ASN:HB2	2:I:213:GLU:HB2	2.00	0.43
1:A:100:VAL:O	1:A:104:MET:HG2	2.18	0.43
1:C:53:LEU:O	1:C:56:THR:HG22	2.19	0.43
2:I:135:LEU:HD22	3:J:184:VAL:HG11	2.01	0.43
1:D:70:MET:HE1	1:D:205:ILE:CB	2.49	0.43
1:C:199:ILE:HA	1:C:202:LEU:HD12	2.01	0.43
3:J:124:VAL:HG12	3:J:145:VAL:HG12	2.00	0.43
1:A:104:MET:HB2	1:A:110:ILE:HG12	2.01	0.43
1:B:64:LYS:HG3	2:I:91:TYR:HE2	1.83	0.43
1:D:100:VAL:O	1:D:104:MET:HG2	2.18	0.43
1:C:110:ILE:HB	1:C:114:LYS:HG2	2.00	0.42
2:I:18:THR:OG1	2:I:76:SER:O	2.33	0.42
1:C:32:GLN:OE1	1:C:35:TRP:NE1	2.51	0.42
3:J:36:TRP:HD1	3:J:70:ILE:HD12	1.84	0.42
3:J:97:ALA:HB1	3:J:103:PHE:HB3	2.02	0.42
3:J:141:LEU:HD13	3:J:214:VAL:HG11	2.01	0.42
2:I:142:ARG:HG3	2:I:142:ARG:NH1	2.34	0.42
3:J:33:ALA:CB	3:J:100:ASP:OD1	2.67	0.42
1:D:177:SER:HB3	1:D:189:ILE:HG23	2.00	0.42
1:D:45:MET:O	1:D:45:MET:HE3	2.20	0.42
1:D:82:ALA:HB2	1:D:194:GLY:HA3	2.01	0.42
1:B:100:VAL:HG12	1:B:171:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:24:ARG:HE	2:I:24:ARG:HB3	1.68	0.42
2:I:90:HIS:CE1	2:I:93:SER:H	2.38	0.42
1:B:59:TRP:HZ2	1:C:207:TYR:CE1	2.38	0.42
3:J:12:VAL:HG11	3:J:86:LEU:HD13	2.01	0.41
1:B:32:GLN:HG2	1:B:34:PHE:H	1.85	0.41
3:J:33:ALA:HB3	3:J:100:ASP:OD1	2.19	0.41
1:C:171:VAL:HG21	1:C:241:ALA:HA	2.02	0.41
1:A:191:LEU:HD12	1:A:191:LEU:HA	1.89	0.41
3:J:134:THR:O	3:J:189:SER:OG	2.27	0.41
3:J:73:ASP:OD1	3:J:75:SER:OG	2.29	0.41
1:D:70:MET:HE1	1:D:205:ILE:HB	2.02	0.41
1:D:32:GLN:CA	1:D:35:TRP:CD1	3.03	0.40
1:D:206:ASN:OD1	1:D:206:ASN:N	2.54	0.40
1:C:72:LEU:HD12	1:D:202:LEU:HD22	2.03	0.40
1:A:226:ASN:OD1	1:A:226:ASN:C	2.65	0.40
2:I:91:TYR:HA	2:I:96:TYR:CD1	2.56	0.40
2:I:107:ARG:HG2	2:I:107:ARG:NH1	2.37	0.40
3:J:120:LYS:HA	3:J:120:LYS:HD3	1.83	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	221/323 (68%)	212 (96%)	9 (4%)	0	100	100
1	B	221/323 (68%)	215 (97%)	6 (3%)	0	100	100
1	C	221/323 (68%)	216 (98%)	5 (2%)	0	100	100
1	D	221/323 (68%)	216 (98%)	5 (2%)	0	100	100
2	I	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
3	J	214/223 (96%)	210 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1306/1729 (76%)	1270 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/261 (67%)	174 (100%)	0	100	100
1	B	174/261 (67%)	174 (100%)	0	100	100
1	C	174/261 (67%)	174 (100%)	0	100	100
1	D	174/261 (67%)	174 (100%)	0	100	100
2	I	182/187 (97%)	182 (100%)	0	100	100
3	J	174/183 (95%)	174 (100%)	0	100	100
All	All	1052/1414 (74%)	1052 (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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	229	ASN
1	C	229	ASN
1	D	122	GLN
2	I	3	GLN
2	I	79	GLN
2	I	89	GLN
2	I	138	ASN
2	I	199	GLN
3	J	35	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 [i](#)

There are no chain breaks in this entry.

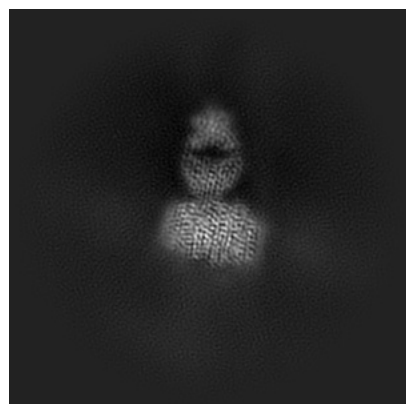
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43047. These allow visual inspection of the internal detail of the map and identification of artifacts.

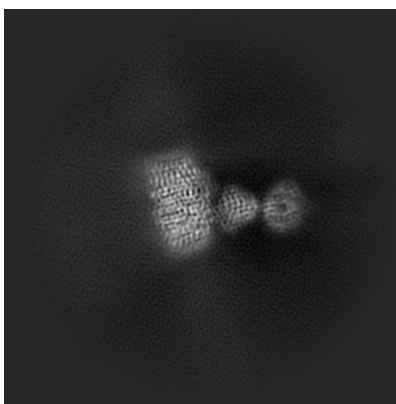
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

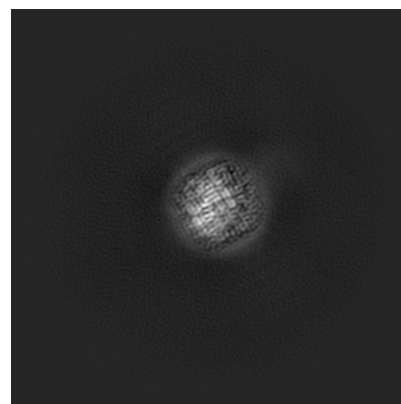
6.1.1 Primary map



X

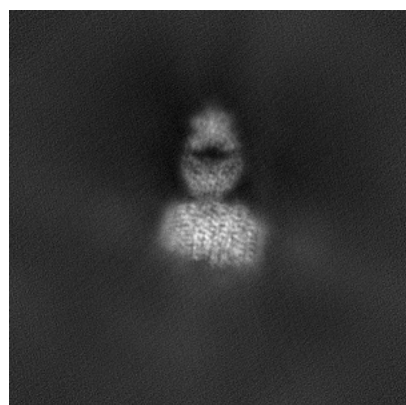


Y

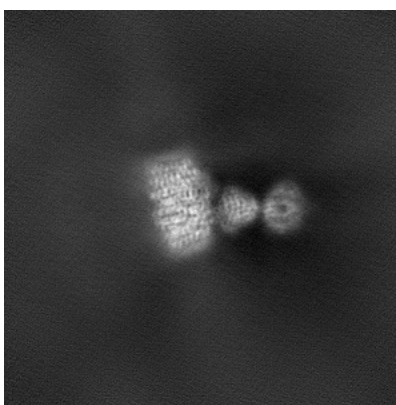


Z

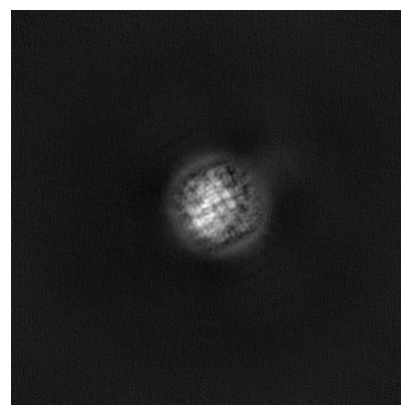
6.1.2 Raw map



X



Y

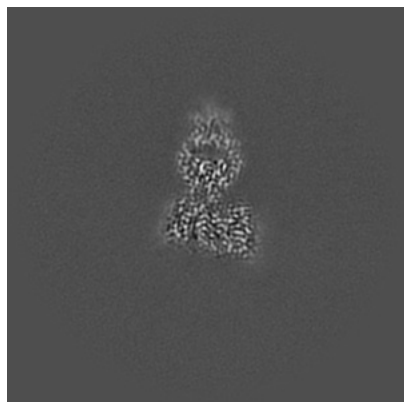


Z

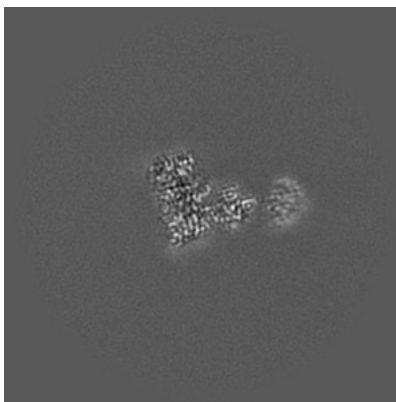
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

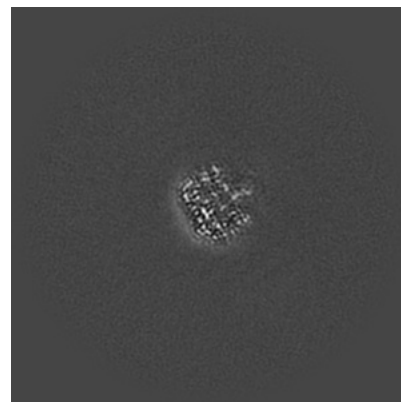
6.2.1 Primary map



X Index: 196

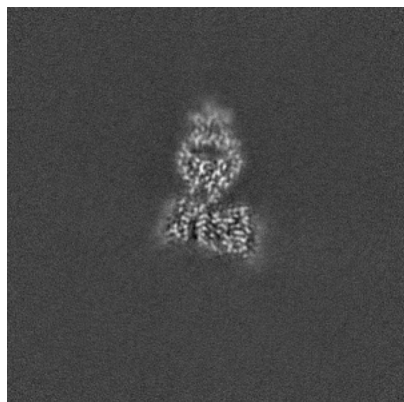


Y Index: 196

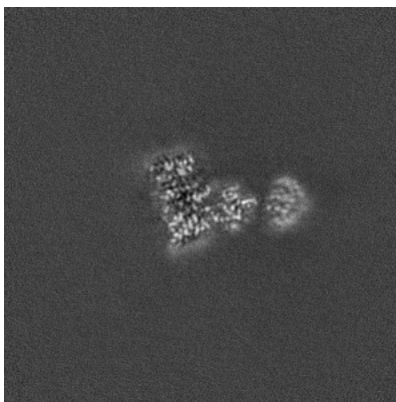


Z Index: 196

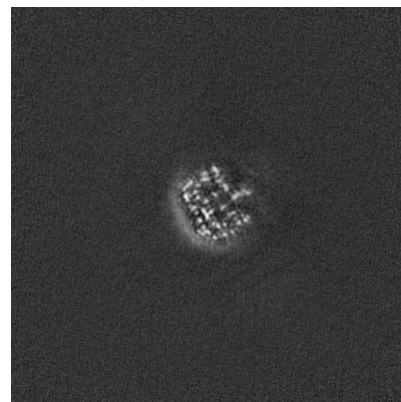
6.2.2 Raw map



X Index: 196



Y Index: 196

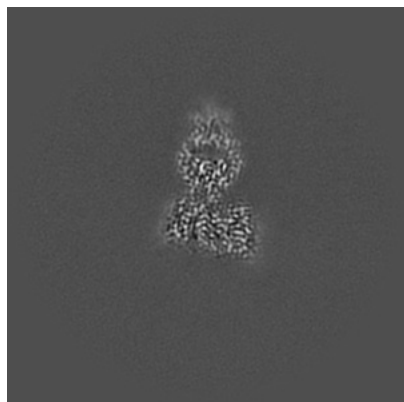


Z Index: 196

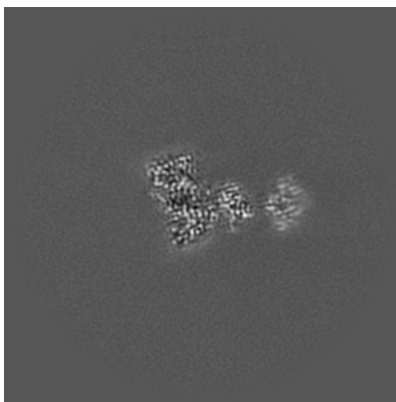
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

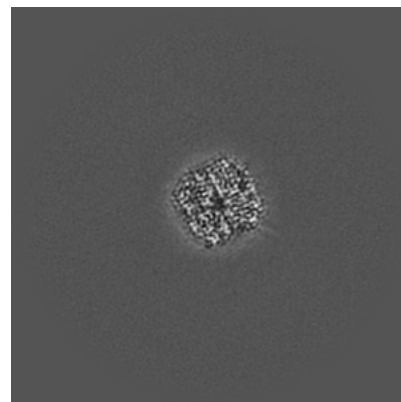
6.3.1 Primary map



X Index: 196

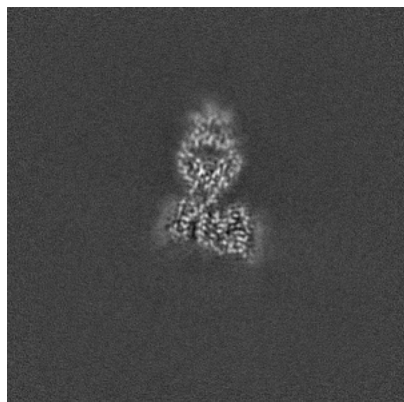


Y Index: 199

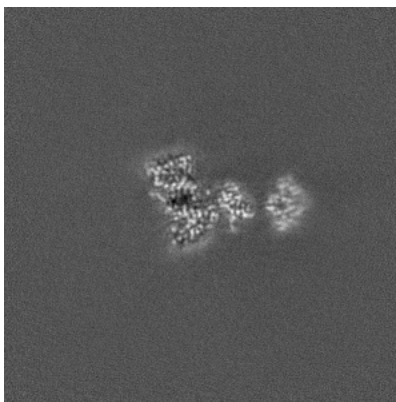


Z Index: 177

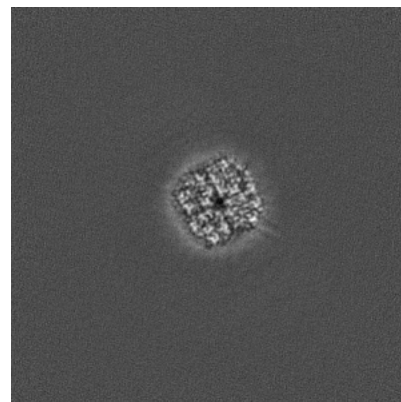
6.3.2 Raw map



X Index: 195



Y Index: 199

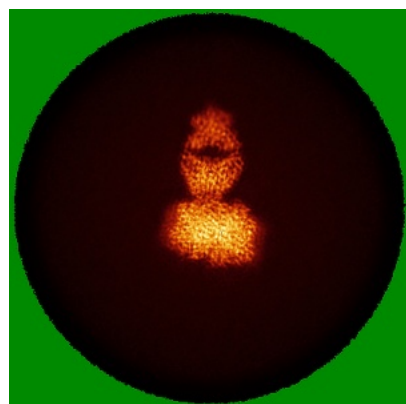


Z Index: 177

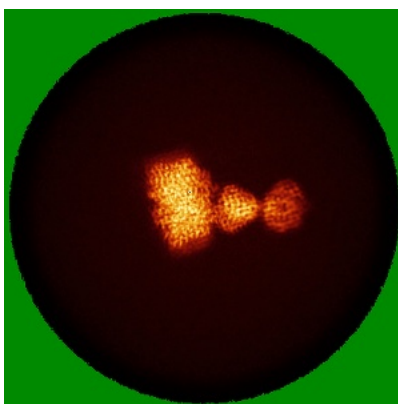
The images above show the largest variance slices of the map in three orthogonal directions.

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

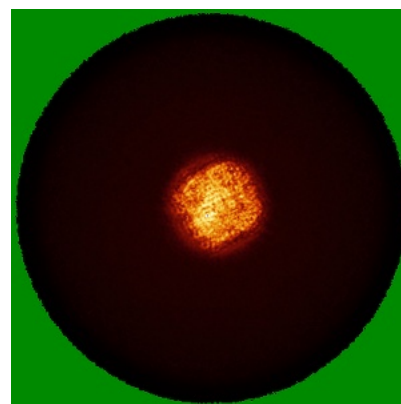
6.4.1 Primary map



X

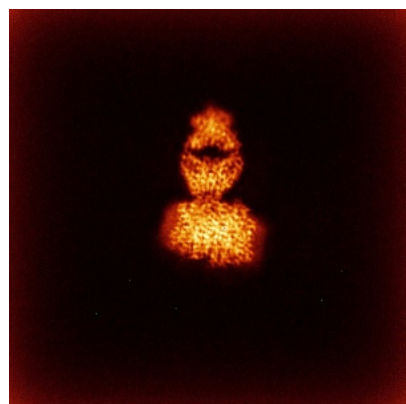


Y

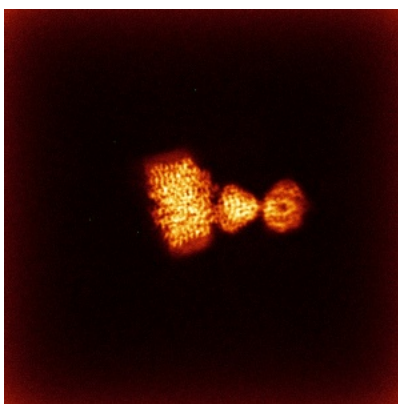


Z

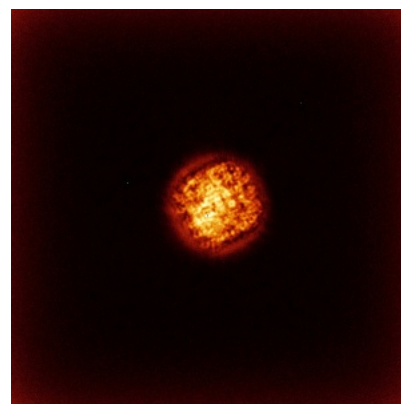
6.4.2 Raw map



X



Y

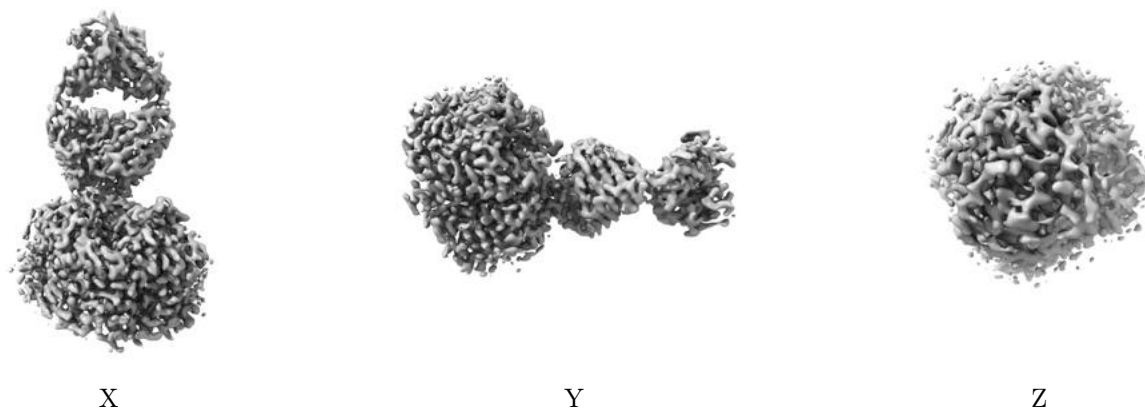


Z

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.

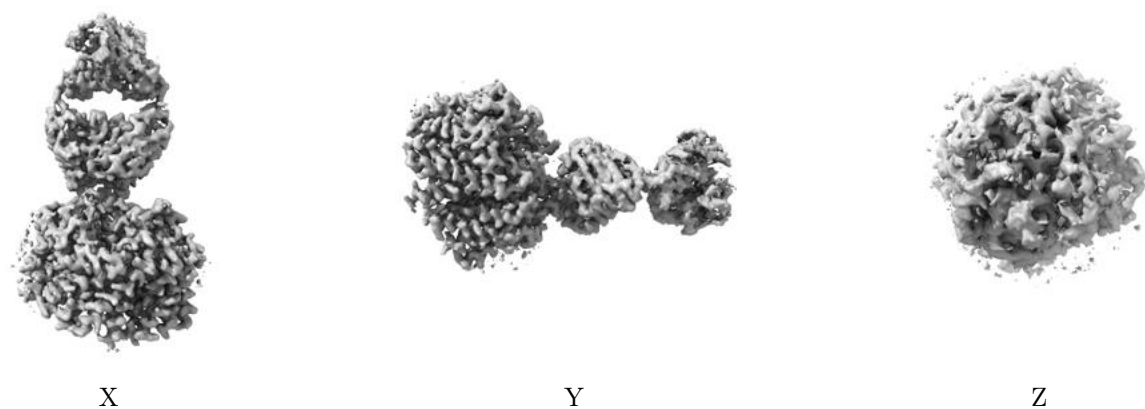
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

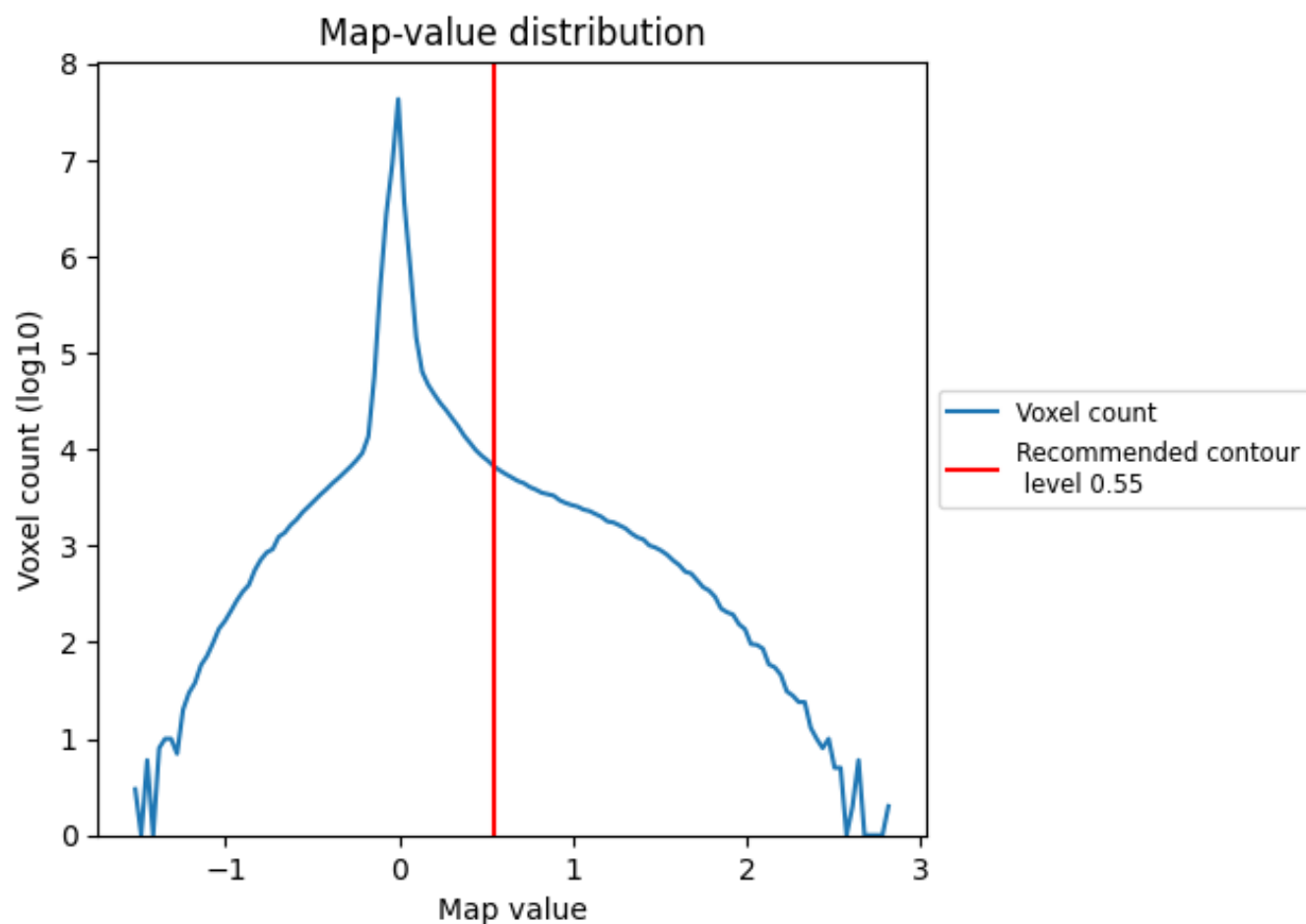
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

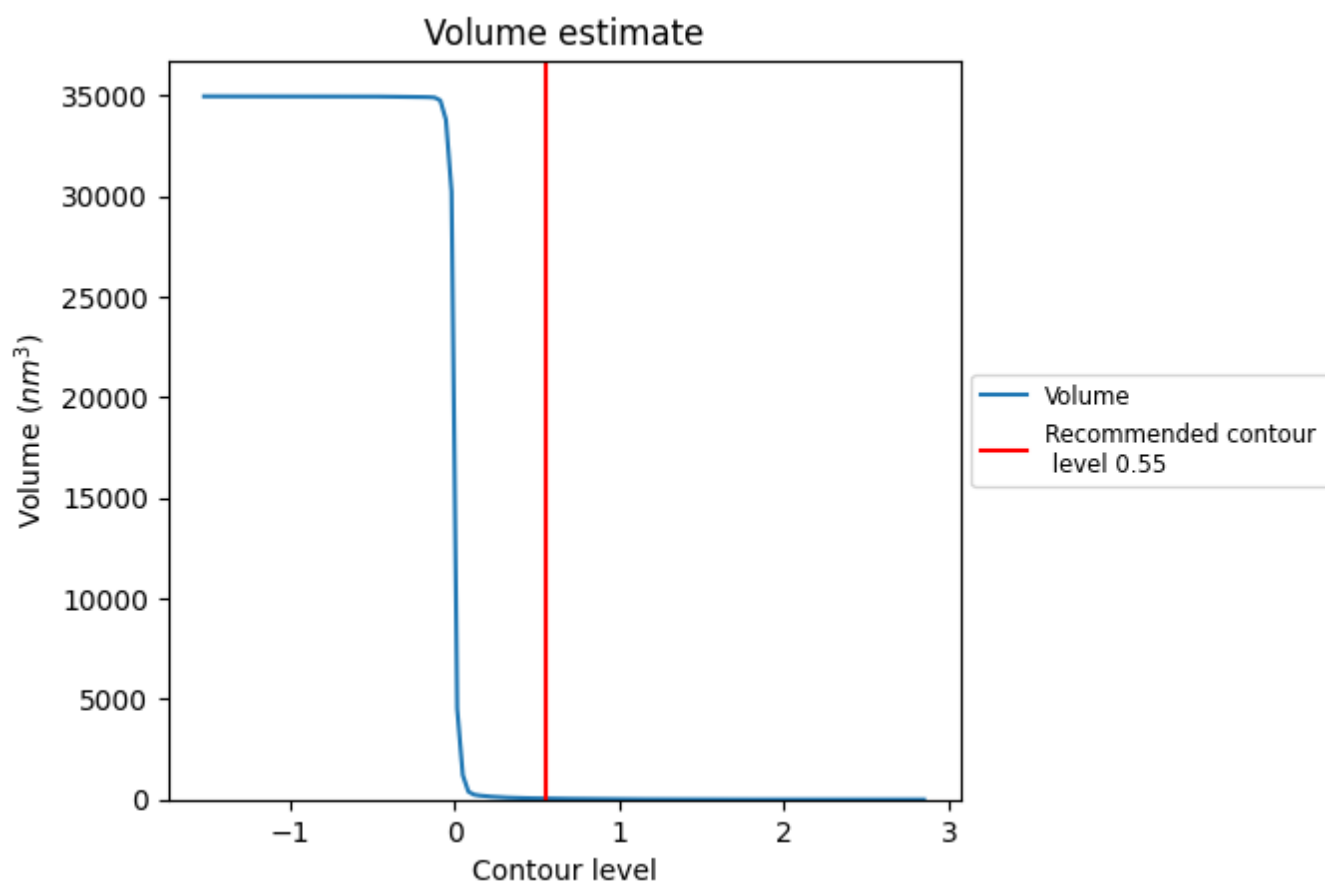
This section contains the results of statistical analysis of the map.

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.

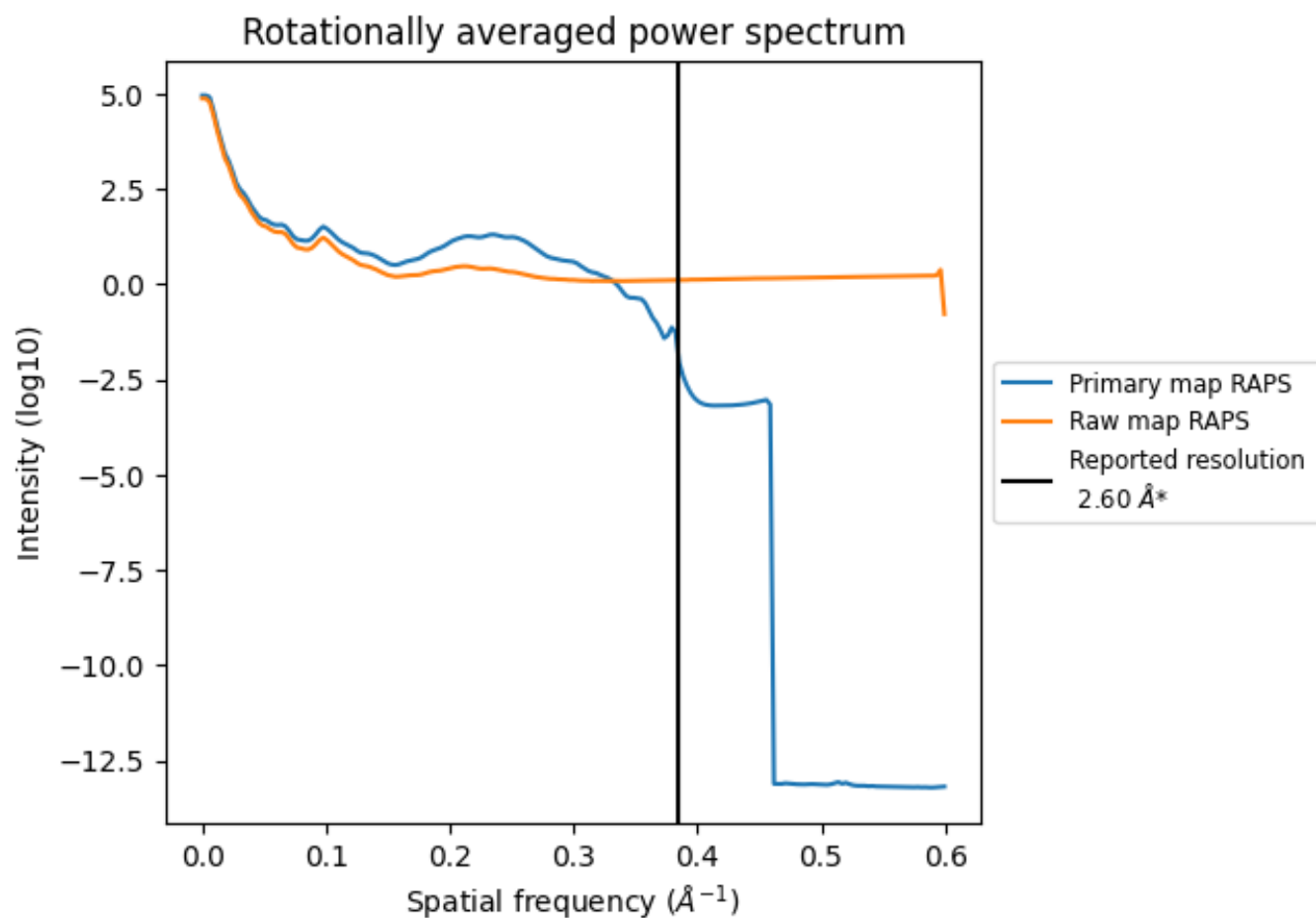
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 52 nm³; this corresponds to an approximate mass of 47 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 ⓘ

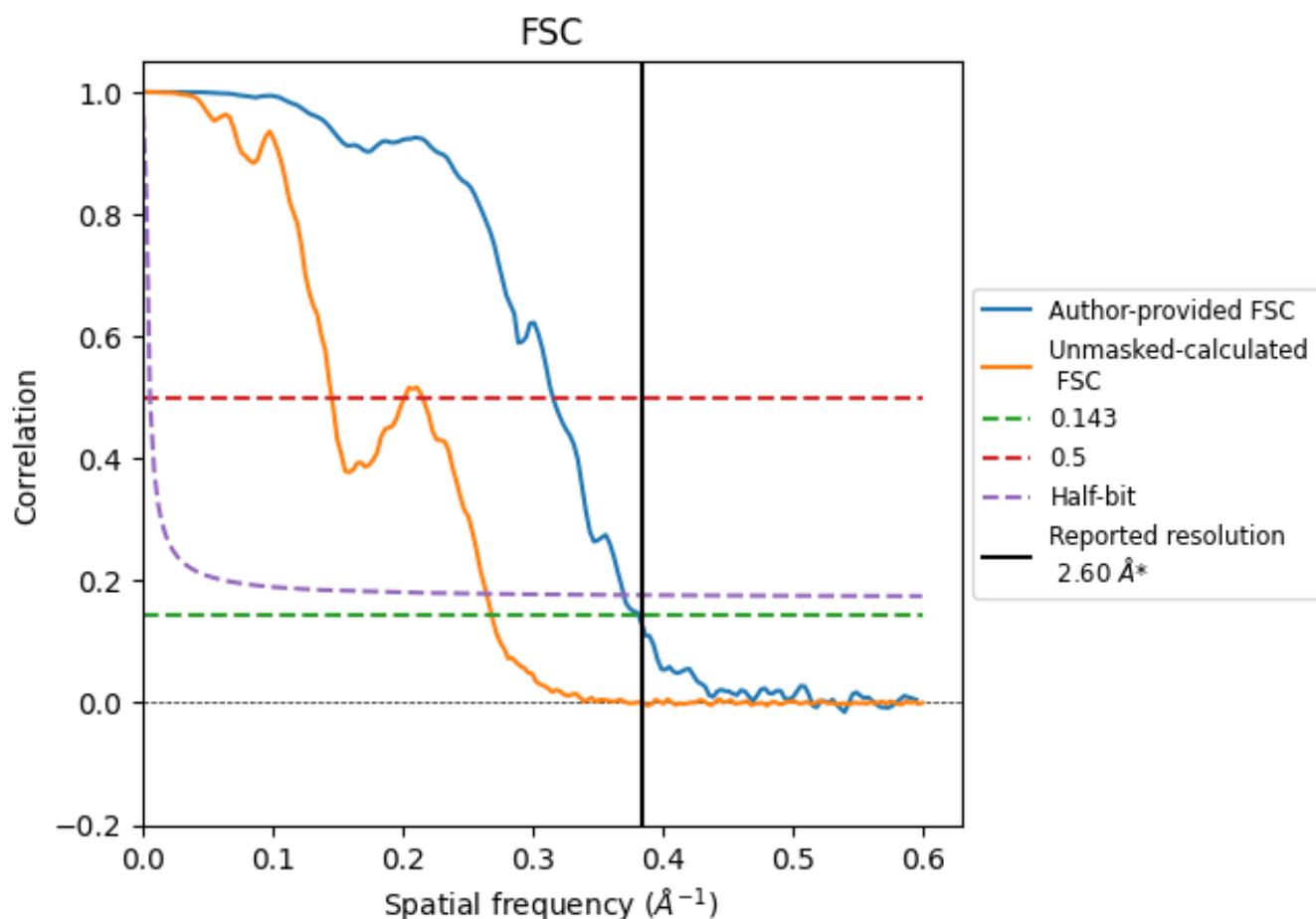


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 $0.385 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

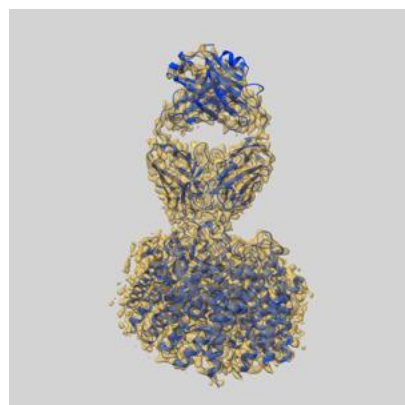
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	3.17	2.70
Unmasked-calculated*	3.72	6.86	3.78

*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 3.72 differs from the reported value 2.6 by more than 10 %

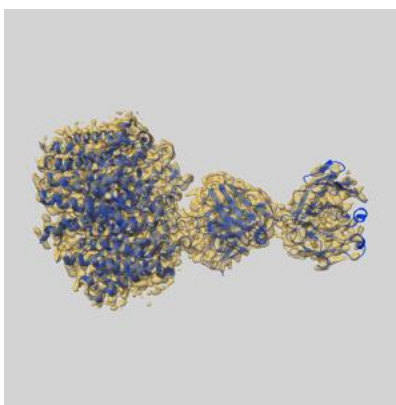
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43047 and PDB model 8V91. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

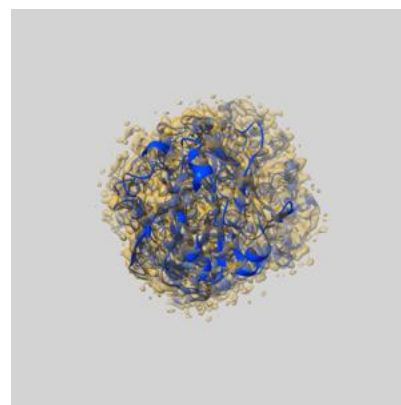
9.1 Map-model overlay [i](#)



X



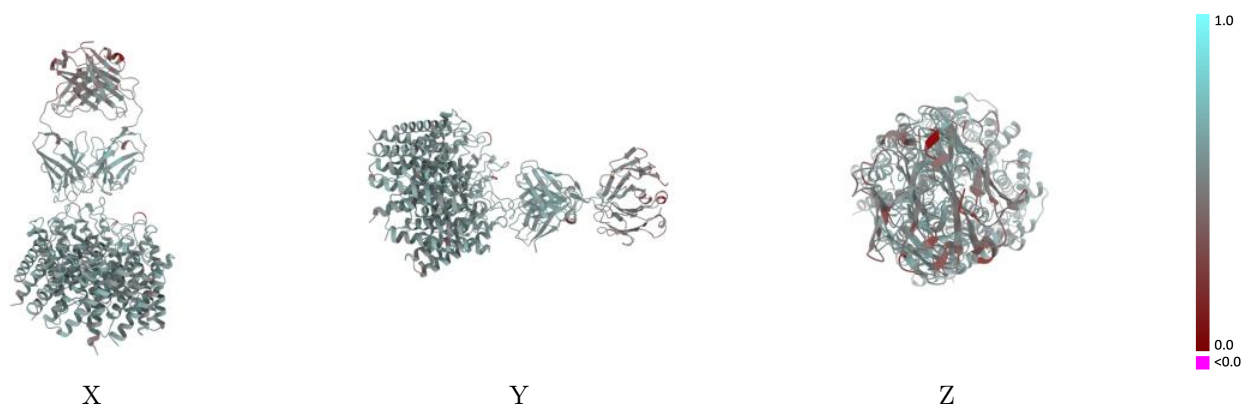
Y



Z

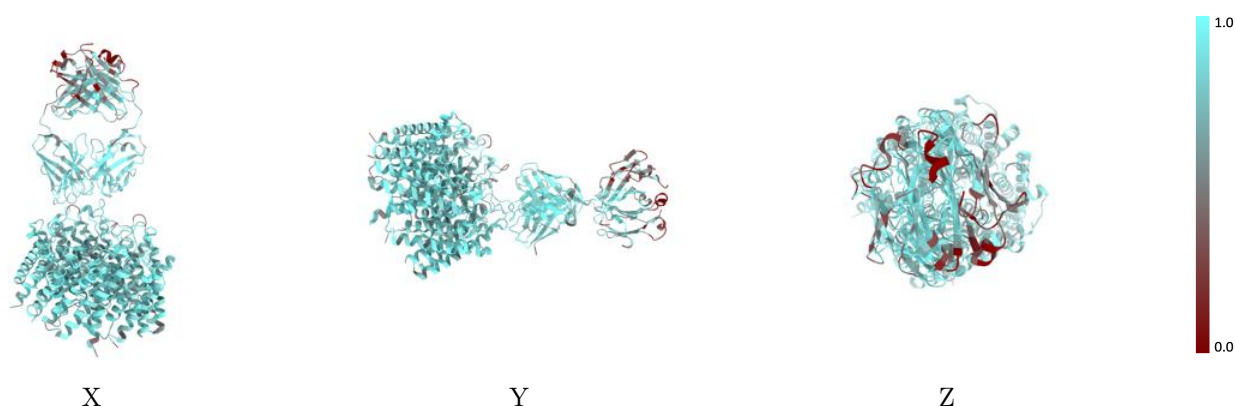
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



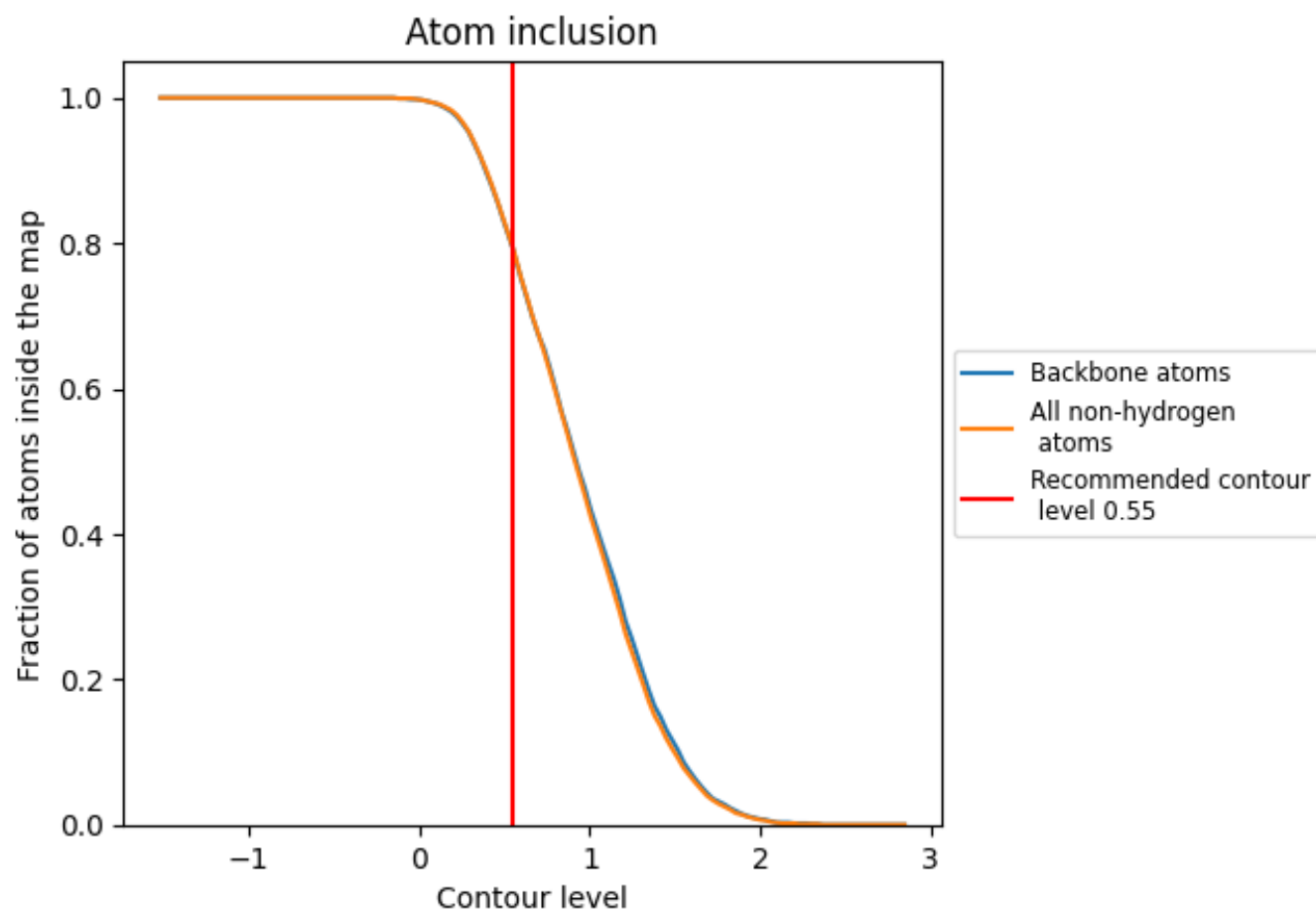
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 79% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.5460
A	0.8300	0.5630
B	0.8500	0.5670
C	0.8450	0.5660
D	0.8270	0.5610
I	0.6860	0.5100
J	0.7330	0.5060

1.0

0.0

<0.0