



Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 01:32 PM EST

PDB ID : 7UN6
EMDB ID : EMD-26614
Title : Complex of UBE2O with NAP1L1
Authors : Yip, M.C.J.; Sedor, S.F.; Shao, S.
Deposited on : 2022-04-09
Resolution : 3.30 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

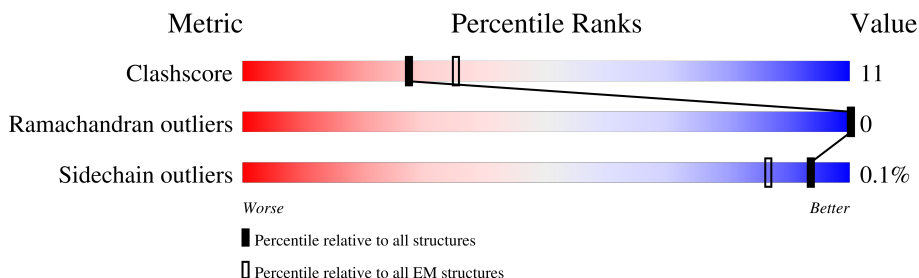
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	A	1342	<div> <div>14%</div> <div>37%</div> <div>12%</div> <div>52%</div> </div>
2	B	416	<div> <div>8%</div> <div>44%</div> <div>14%</div> <div>42%</div> </div>
2	C	416	<div> <div>8%</div> <div>45%</div> <div>11%</div> <div>45%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9042 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 (E3-independent) E2 ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	648	Total	C	N	O	S	0	0
			5186	3322	892	945	27		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-49	MET	-	initiating methionine	UNP Q9C0C9
A	-48	ALA	-	expression tag	UNP Q9C0C9
A	-47	SER	-	expression tag	UNP Q9C0C9
A	-46	TRP	-	expression tag	UNP Q9C0C9
A	-45	SER	-	expression tag	UNP Q9C0C9
A	-44	HIS	-	expression tag	UNP Q9C0C9
A	-43	PRO	-	expression tag	UNP Q9C0C9
A	-42	GLN	-	expression tag	UNP Q9C0C9
A	-41	PHE	-	expression tag	UNP Q9C0C9
A	-40	GLU	-	expression tag	UNP Q9C0C9
A	-39	LYS	-	expression tag	UNP Q9C0C9
A	-38	GLY	-	expression tag	UNP Q9C0C9
A	-37	ALA	-	expression tag	UNP Q9C0C9
A	-36	TRP	-	expression tag	UNP Q9C0C9
A	-35	SER	-	expression tag	UNP Q9C0C9
A	-34	HIS	-	expression tag	UNP Q9C0C9
A	-33	PRO	-	expression tag	UNP Q9C0C9
A	-32	GLN	-	expression tag	UNP Q9C0C9
A	-31	PHE	-	expression tag	UNP Q9C0C9
A	-30	GLU	-	expression tag	UNP Q9C0C9
A	-29	LYS	-	expression tag	UNP Q9C0C9
A	-28	GLY	-	expression tag	UNP Q9C0C9
A	-27	SER	-	expression tag	UNP Q9C0C9
A	-26	TRP	-	expression tag	UNP Q9C0C9
A	-25	SER	-	expression tag	UNP Q9C0C9
A	-24	HIS	-	expression tag	UNP Q9C0C9
A	-23	PRO	-	expression tag	UNP Q9C0C9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLN	-	expression tag	UNP Q9C0C9
A	-21	PHE	-	expression tag	UNP Q9C0C9
A	-20	GLU	-	expression tag	UNP Q9C0C9
A	-19	LYS	-	expression tag	UNP Q9C0C9
A	-18	GLY	-	expression tag	UNP Q9C0C9
A	-17	PRO	-	expression tag	UNP Q9C0C9
A	-16	ALA	-	expression tag	UNP Q9C0C9
A	-15	GLY	-	expression tag	UNP Q9C0C9
A	-14	SER	-	expression tag	UNP Q9C0C9
A	-13	GLU	-	expression tag	UNP Q9C0C9
A	-12	ASN	-	expression tag	UNP Q9C0C9
A	-11	LEU	-	expression tag	UNP Q9C0C9
A	-10	TYR	-	expression tag	UNP Q9C0C9
A	-9	PHE	-	expression tag	UNP Q9C0C9
A	-8	GLN	-	expression tag	UNP Q9C0C9
A	-7	GLY	-	expression tag	UNP Q9C0C9
A	-6	SER	-	expression tag	UNP Q9C0C9
A	-5	GLY	-	expression tag	UNP Q9C0C9
A	-4	ILE	-	expression tag	UNP Q9C0C9
A	-3	ARG	-	expression tag	UNP Q9C0C9
A	-2	ASP	-	expression tag	UNP Q9C0C9
A	-1	ARG	-	expression tag	UNP Q9C0C9
A	0	THR	-	expression tag	UNP Q9C0C9
A	1040	LYS	CYS	conflict	UNP Q9C0C9

- Molecule 2 is a protein called Nucleosome assembly protein 1-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	240	Total	C	N	O	S	0	0
			1965	1265	326	367	7		
2	C	230	Total	C	N	O	S	0	0
			1891	1221	315	348	7		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	initiating methionine	UNP P55209
B	-23	ASP	-	expression tag	UNP P55209
B	-22	TYR	-	expression tag	UNP P55209
B	-21	LYS	-	expression tag	UNP P55209
B	-20	ASP	-	expression tag	UNP P55209
B	-19	HIS	-	expression tag	UNP P55209

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	ASP	-	expression tag	UNP P55209
B	-17	GLY	-	expression tag	UNP P55209
B	-16	ASP	-	expression tag	UNP P55209
B	-15	TYR	-	expression tag	UNP P55209
B	-14	LYS	-	expression tag	UNP P55209
B	-13	ASP	-	expression tag	UNP P55209
B	-12	HIS	-	expression tag	UNP P55209
B	-11	ASP	-	expression tag	UNP P55209
B	-10	ILE	-	expression tag	UNP P55209
B	-9	ASP	-	expression tag	UNP P55209
B	-8	TYR	-	expression tag	UNP P55209
B	-7	LYS	-	expression tag	UNP P55209
B	-6	ASP	-	expression tag	UNP P55209
B	-5	ASP	-	expression tag	UNP P55209
B	-4	ASP	-	expression tag	UNP P55209
B	-3	ASP	-	expression tag	UNP P55209
B	-2	LYS	-	expression tag	UNP P55209
B	-1	ALA	-	expression tag	UNP P55209
B	0	GLY	-	expression tag	UNP P55209
B	1	SER	-	expression tag	UNP P55209
C	-24	MET	-	initiating methionine	UNP P55209
C	-23	ASP	-	expression tag	UNP P55209
C	-22	TYR	-	expression tag	UNP P55209
C	-21	LYS	-	expression tag	UNP P55209
C	-20	ASP	-	expression tag	UNP P55209
C	-19	HIS	-	expression tag	UNP P55209
C	-18	ASP	-	expression tag	UNP P55209
C	-17	GLY	-	expression tag	UNP P55209
C	-16	ASP	-	expression tag	UNP P55209
C	-15	TYR	-	expression tag	UNP P55209
C	-14	LYS	-	expression tag	UNP P55209
C	-13	ASP	-	expression tag	UNP P55209
C	-12	HIS	-	expression tag	UNP P55209
C	-11	ASP	-	expression tag	UNP P55209
C	-10	ILE	-	expression tag	UNP P55209
C	-9	ASP	-	expression tag	UNP P55209
C	-8	TYR	-	expression tag	UNP P55209
C	-7	LYS	-	expression tag	UNP P55209
C	-6	ASP	-	expression tag	UNP P55209
C	-5	ASP	-	expression tag	UNP P55209
C	-4	ASP	-	expression tag	UNP P55209
C	-3	ASP	-	expression tag	UNP P55209

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	LYS	-	expression tag	UNP P55209
C	-1	ALA	-	expression tag	UNP P55209
C	0	GLY	-	expression tag	UNP P55209
C	1	SER	-	expression tag	UNP P55209

TYR
ASP
PRO
LYS
LYS
ASP
GLN
ASN
PRO
ALA
GLU
CYS
LYS
GLN
GLN

● Molecule 2: Nucleosome assembly protein 1-like 1



MET
ASP
TYR
LYS
ASP
HIS
ASP
GLY
ASP
TYR
LYS
ASP
HIS
ASP
ILE
ASP
TYR
LYS
ASP
GLN
GLU
CYS
LYS
GLN
GLN

ARG
GLN
LEU
THR
VAL
GLN
MET
MET
GLN
ASN
PRO
GLN
ILE
LEU
ALA
ALA
LEU
GLN
GLU
ARG
LEU
ASP
GLY
GLY
VAL
GLU
THR
PRO
THR
GLY
ALA
TYR
ILE
GLU
SER
LEU
PRO
LYS
ASP
ARG
Y73
R77
L81
F95
V99
Y106
L109
Y110
Q111
P112
L113
F114
D115
K116
R117
F118
E119

A123
I124
Y125
E126
PRO
THR
GLU
GLU
CYS
TRP
LYS
PRO
ASP
GLU
ASP
GLU
ILE
SER
GLU
LEU
LYS
LYS
ALA
ILE
GLU
ASP
GLU
LYS
ASP
PRO
LYS
G186
I167
F170
V171
L172
D173
V185
I192
L193
L196

I199
K200
V201
F212
V213
L214
F218
E219
Y223
L229
T230
K231
T232
Y233
E238
D243
D248
C258
Q259
I260
L270
K271
T272
I273
K274
K275
K276
Q277
K278
K279
K280
G281
R282
G283
T284
V285
R286
T287
V288
T289
K290
S293
R294
D295
F300
V306
PRO
GLU

SER
GLY
ASP
LEU
ASP
ASP
D315
D323
R331
I335
P336
F337
S338
Y339
L340
I347
E348
D349
ASP
ASP
ASP
TYR
ASP
GLU
GLU
GLY
GLU
GLU
ALA
ASP
GLU
GLU
GLY
GLU
GLU
GLY
ASP
GLU
GLU
ASN
ASP
PRO
ASP
TYR
ASP
PRO
LYS
LYS
ASP
GLN
ASN
PRO
ALA
GLU

CYS
LYS
GLN
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	447881	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 ($e^-/\text{\AA}^2$)	57.4	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.778	Depositor
Minimum map value	-4.532	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	280.5, 280.5, 280.5	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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	0.29	0/5306	0.51	0/7190
2	B	0.28	0/2012	0.48	0/2713
2	C	0.28	0/1935	0.48	0/2607
All	All	0.29	0/9253	0.50	0/12510

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	5186	0	5168	121	0
2	B	1965	0	1938	50	0
2	C	1891	0	1872	36	0
All	All	9042	0	8978	195	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 11.

All (195) 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)
2:C:233:TYR:OH	2:C:323:ASP:OD1	1.88	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:SER:OG	2:C:248:ASP:OD2	1.95	0.83
1:A:171:ILE:HD12	1:A:553:THR:HG22	1.64	0.79
1:A:221:ILE:HD11	1:A:279:LEU:HD12	1.65	0.79
1:A:997:TYR:OH	1:A:1029:LEU:O	1.98	0.78
1:A:1031:PRO:HB2	1:A:1081:GLU:HB3	1.66	0.77
2:B:110:TYR:O	2:B:113:LEU:N	2.17	0.76
2:B:231:LYS:NZ	2:B:255:CYS:SG	2.60	0.75
1:A:70:TYR:OH	1:A:129:GLU:OE1	2.08	0.71
1:A:958:VAL:HG12	1:A:962:MET:HE1	1.73	0.70
1:A:656:THR:N	1:A:681:VAL:O	2.24	0.70
1:A:345:ALA:O	1:A:347:ARG:NH2	2.25	0.69
1:A:171:ILE:CD1	1:A:553:THR:HG22	2.22	0.69
2:B:238:GLU:N	2:B:238:GLU:OE1	2.26	0.69
2:C:212:PHE:CE2	2:C:214:LEU:HD11	2.28	0.68
2:C:201:VAL:HG23	2:C:335:ILE:HD13	1.76	0.67
1:A:152:VAL:HG13	1:A:576:VAL:HB	1.76	0.67
1:A:341:CYS:O	1:A:680:GLN:NE2	2.29	0.66
1:A:167:ILE:HA	1:A:655:THR:HG21	1.77	0.66
1:A:1028:ARG:NH1	1:A:1031:PRO:O	2.29	0.66
1:A:222:LEU:HD23	1:A:296:VAL:HG22	1.78	0.65
1:A:154:ARG:NH1	1:A:576:VAL:HG22	2.12	0.65
2:B:196:LEU:HD21	2:B:199:ILE:CG1	2.26	0.65
2:B:117:ARG:NH2	2:B:335:ILE:O	2.30	0.64
2:C:201:VAL:HG21	2:C:331:ARG:HG2	1.79	0.63
1:A:606:VAL:O	1:A:608:GLN:NE2	2.32	0.63
2:C:117:ARG:NH1	2:C:338:SER:OG	2.32	0.62
2:B:212:PHE:CE2	2:B:214:LEU:HD11	2.32	0.62
2:C:229:LEU:HD11	2:C:258:CYS:SG	2.40	0.61
2:B:335:ILE:HG23	2:B:336:PRO:HD3	1.83	0.61
1:A:175:VAL:HG21	1:A:355:TYR:CD2	2.36	0.60
1:A:958:VAL:HG12	1:A:962:MET:CE	2.31	0.60
1:A:290:SER:HB2	2:B:347:ILE:HD11	1.83	0.59
1:A:569:ARG:NH2	1:A:571:ASN:OD1	2.35	0.59
1:A:1123:PHE:O	1:A:1127:ILE:HD12	2.03	0.59
1:A:168:ASP:OD1	1:A:169:VAL:N	2.36	0.58
2:C:167:ILE:HG21	2:C:170:PHE:HD1	1.68	0.58
1:A:144:ASP:OD2	1:A:553:THR:HG23	2.02	0.58
1:A:592:ASP:OD1	1:A:593:LYS:N	2.36	0.58
2:B:330:LEU:O	2:B:335:ILE:HG22	2.04	0.57
1:A:985:PHE:HB2	1:A:1006:ILE:HG23	1.86	0.57
1:A:994:ARG:NH2	1:A:1253:ASP:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:NE2	2:C:336:PRO:O	2.34	0.56
1:A:59:LEU:H	1:A:59:LEU:HD23	1.71	0.56
1:A:303:GLU:OE1	1:A:329:THR:HG22	2.06	0.56
2:B:198:ASP:OD1	2:B:199:ILE:N	2.39	0.55
1:A:680:GLN:H	1:A:692:VAL:HG11	1.71	0.55
1:A:213:VAL:O	1:A:213:VAL:HG23	2.05	0.55
1:A:1081:GLU:OE2	1:A:1084:PHE:CE2	2.59	0.55
1:A:693:VAL:O	1:A:693:VAL:HG23	2.07	0.55
1:A:1035:ASP:OD1	1:A:1036:ASN:N	2.39	0.54
1:A:603:VAL:HG13	1:A:634:ILE:CD1	2.38	0.54
1:A:1254:ILE:HG22	1:A:1254:ILE:O	2.07	0.54
2:B:340:LEU:O	2:B:346:ALA:N	2.39	0.54
2:B:190:GLU:O	2:B:194:LYS:HG3	2.08	0.54
2:C:196:LEU:HD21	2:C:199:ILE:CG1	2.38	0.54
2:B:343:THR:HG22	2:B:343:THR:O	2.08	0.53
2:C:231:LYS:NZ	2:C:300:PHE:O	2.40	0.53
1:A:960:LYS:O	1:A:964:LEU:HD23	2.09	0.53
1:A:222:LEU:CD2	1:A:296:VAL:HG22	2.38	0.53
2:B:196:LEU:HD21	2:B:199:ILE:HG13	1.90	0.53
2:B:184:MET:SD	2:B:326:ILE:HD13	2.49	0.52
2:C:167:ILE:HG21	2:C:170:PHE:CD1	2.44	0.52
2:C:119:GLU:O	2:C:123:ALA:N	2.42	0.52
2:C:214:LEU:HD12	2:C:214:LEU:H	1.74	0.52
2:C:171:TRP:CG	2:C:196:LEU:HD22	2.44	0.52
2:C:270:LEU:HD23	2:C:293:SER:HA	1.92	0.52
1:A:680:GLN:O	1:A:692:VAL:HG21	2.10	0.52
2:C:201:VAL:HG23	2:C:335:ILE:CD1	2.39	0.52
1:A:578:HIS:ND1	1:A:1087:ASP:OD2	2.40	0.51
1:A:1032:ASN:HD21	1:A:1072:ILE:HG23	1.74	0.51
2:B:178:VAL:HG22	2:B:348:GLU:HG2	1.91	0.51
1:A:174:ALA:HB3	1:A:550:THR:HG22	1.93	0.50
1:A:648:HIS:ND1	1:A:650:ASP:O	2.44	0.50
1:A:655:THR:O	1:A:656:THR:HG22	2.12	0.50
2:B:339:VAL:HB	2:C:81:LEU:CD2	2.41	0.50
2:B:236:ARG:HD2	2:B:253:MET:HE2	1.94	0.50
2:B:231:LYS:NZ	2:B:323:ASP:OD2	2.43	0.50
1:A:175:VAL:HG21	1:A:355:TYR:HD2	1.76	0.50
2:B:101:ASP:OD1	2:B:104:ARG:NH2	2.41	0.50
1:A:1116:VAL:HG22	1:A:1131:PHE:CD2	2.46	0.49
1:A:167:ILE:HD11	1:A:558:MET:HB2	1.93	0.49
2:B:306:VAL:HG13	2:B:312:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:ILE:HG12	2:B:223:TYR:CG	2.47	0.49
1:A:953:LYS:O	1:A:956:SER:OG	2.28	0.49
1:A:1142:ILE:HG21	1:A:1273:LEU:HD13	1.94	0.49
1:A:178:ILE:HD12	1:A:545:ALA:HB1	1.94	0.49
1:A:292:PHE:CE1	2:B:347:ILE:HG22	2.48	0.49
1:A:147:VAL:O	1:A:169:VAL:HG21	2.14	0.48
2:B:196:LEU:HD21	2:B:199:ILE:HD11	1.94	0.48
1:A:1036:ASN:OD1	1:A:1037:GLY:N	2.46	0.48
1:A:290:SER:CB	2:B:347:ILE:HD11	2.43	0.48
1:A:292:PHE:CZ	2:B:347:ILE:HG22	2.48	0.48
1:A:931:VAL:HG13	1:A:977:THR:HG23	1.95	0.48
2:B:233:TYR:OH	2:B:323:ASP:OD1	2.13	0.48
1:A:147:VAL:CG1	1:A:166:VAL:HG21	2.44	0.48
1:A:1028:ARG:O	1:A:1107:ARG:NH2	2.43	0.48
1:A:1030:ASN:ND2	1:A:1032:ASN:OD1	2.47	0.48
1:A:175:VAL:HG21	1:A:355:TYR:CE2	2.49	0.47
2:B:334:ILE:O	2:B:338:SER:N	2.47	0.47
1:A:692:VAL:HG13	1:A:694:TRP:CD1	2.49	0.47
2:B:120:ILE:HD11	2:C:81:LEU:HD12	1.97	0.47
1:A:1031:PRO:CB	1:A:1081:GLU:HB3	2.42	0.47
2:B:201:VAL:HG13	2:B:201:VAL:O	2.15	0.47
1:A:587:GLY:HA2	1:A:684:VAL:HG11	1.97	0.46
2:B:174:VAL:HG11	2:B:334:ILE:HG23	1.96	0.46
2:C:231:LYS:O	2:C:231:LYS:HG3	2.16	0.46
1:A:1269:ILE:HA	1:A:1272:VAL:HG22	1.98	0.46
2:B:178:VAL:HG21	2:B:334:ILE:HD11	1.97	0.46
1:A:1044:LEU:HD23	1:A:1046:THR:HG23	1.98	0.46
2:B:339:VAL:HB	2:C:81:LEU:HD22	1.98	0.46
2:B:93:ALA:HB1	2:B:237:SER:O	2.15	0.46
2:C:171:TRP:CB	2:C:196:LEU:HD22	2.46	0.46
1:A:66:VAL:HG22	1:A:77:GLY:O	2.16	0.46
1:A:590:VAL:O	1:A:605:GLY:N	2.49	0.46
1:A:989:ILE:HG23	1:A:1069:GLN:OE1	2.15	0.46
1:A:931:VAL:HG12	1:A:932:LEU:N	2.31	0.46
2:C:171:TRP:CE3	2:C:199:ILE:HD12	2.51	0.45
1:A:1001:LEU:N	1:A:1112:MET:SD	2.89	0.45
1:A:622:PHE:CE2	1:A:633:LEU:HD13	2.51	0.45
2:B:192:ILE:HD11	2:B:223:TYR:CD1	2.52	0.45
2:B:212:PHE:HE2	2:B:214:LEU:HD11	1.79	0.45
2:C:106:TYR:CD1	2:C:109:LEU:HD12	2.52	0.45
1:A:202:ASP:OD1	1:A:338:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:PHE:HE2	1:A:688:SER:HG	1.64	0.45
1:A:1074:VAL:HG22	1:A:1075:ASN:H	1.82	0.45
1:A:156:MET:N	1:A:572:ASP:O	2.43	0.44
1:A:196:TRP:CD1	1:A:299:VAL:HG11	2.53	0.44
1:A:603:VAL:HG22	1:A:634:ILE:HD11	1.98	0.44
1:A:59:LEU:HD21	1:A:137:GLU:HB3	2.00	0.44
1:A:147:VAL:HG13	1:A:166:VAL:HG21	1.99	0.44
1:A:1043:LEU:HD12	1:A:1044:LEU:N	2.33	0.44
2:B:202:LYS:HE2	2:B:215:GLU:OE2	2.18	0.44
1:A:1112:MET:O	1:A:1116:VAL:HG23	2.18	0.44
1:A:82:ILE:HG13	1:A:82:ILE:O	2.17	0.44
1:A:149:PRO:HB2	1:A:656:THR:HG21	1.99	0.44
1:A:215:ASP:OD1	1:A:216:LEU:N	2.51	0.44
1:A:974:MET:SD	1:A:1123:PHE:HE1	2.41	0.44
2:C:192:ILE:HG12	2:C:223:TYR:CG	2.52	0.44
2:B:82:LYS:HZ3	2:C:340:LEU:HD23	1.82	0.43
1:A:347:ARG:NE	1:A:351:GLU:OE2	2.52	0.43
1:A:1074:VAL:HG22	1:A:1075:ASN:N	2.34	0.43
2:C:117:ARG:NH2	2:C:335:ILE:O	2.47	0.43
1:A:151:ASP:O	1:A:166:VAL:HG23	2.18	0.43
1:A:282:VAL:HG23	1:A:282:VAL:O	2.18	0.43
1:A:187:VAL:HG12	1:A:188:ASN:N	2.34	0.43
1:A:678:VAL:O	1:A:694:TRP:N	2.49	0.43
1:A:1006:ILE:HD12	1:A:1019:PHE:CZ	2.54	0.43
2:B:196:LEU:HD21	2:B:199:ILE:CD1	2.48	0.43
2:B:199:ILE:HG12	2:B:216:PHE:CD1	2.53	0.43
2:C:95:PHE:O	2:C:99:VAL:HG23	2.18	0.43
1:A:590:VAL:HB	1:A:645:ILE:CG2	2.48	0.43
2:C:179:ASP:N	2:C:348:GLU:OE1	2.50	0.43
1:A:221:ILE:O	1:A:221:ILE:HG23	2.19	0.42
1:A:1127:ILE:HD12	1:A:1127:ILE:H	1.83	0.42
1:A:1265:PHE:O	1:A:1269:ILE:HG22	2.19	0.42
2:B:267:ASN:OD1	2:B:268:VAL:N	2.52	0.42
1:A:988:LEU:HD12	1:A:1003:LEU:HD21	2.01	0.42
1:A:65:LEU:CD1	1:A:349:LEU:HD22	2.49	0.42
1:A:203:TYR:HE1	1:A:212:LYS:HZ3	1.67	0.42
1:A:929:PHE:CZ	1:A:962:MET:HG3	2.55	0.42
1:A:1254:ILE:O	1:A:1254:ILE:CG2	2.67	0.42
2:B:106:TYR:CD2	2:B:109:LEU:HD12	2.54	0.42
1:A:166:VAL:HG22	1:A:557:VAL:HG22	2.01	0.42
2:B:166:GLY:O	2:C:77:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ILE:HG21	2:B:170:PHE:HD2	1.85	0.42
2:C:218:PHE:O	2:C:219:GLU:C	2.58	0.42
1:A:306:VAL:HG12	1:A:307:THR:N	2.35	0.42
1:A:1030:ASN:CG	1:A:1031:PRO:HD2	2.40	0.42
1:A:606:VAL:HG11	1:A:688:SER:OG	2.20	0.41
1:A:1105:LEU:O	1:A:1108:VAL:HG12	2.20	0.41
1:A:997:TYR:HE2	1:A:1077:PRO:HB3	1.85	0.41
2:B:120:ILE:HD11	2:C:81:LEU:HB2	2.02	0.41
2:B:221:ASN:OD1	2:B:224:PHE:N	2.50	0.41
1:A:178:ILE:HD12	1:A:545:ALA:CB	2.50	0.41
1:A:177:LEU:HD11	1:A:544:VAL:HG21	2.02	0.41
1:A:706:HIS:O	1:A:707:LEU:HD22	2.21	0.41
1:A:1019:PHE:CE1	1:A:1064:VAL:HG11	2.56	0.41
2:B:192:ILE:HG12	2:B:223:TYR:CD1	2.56	0.41
2:B:335:ILE:CG2	2:B:336:PRO:HD3	2.48	0.41
1:A:622:PHE:CD1	1:A:688:SER:HB2	2.56	0.41
2:C:110:TYR:O	2:C:113:LEU:N	2.54	0.40
1:A:221:ILE:HD12	1:A:230:CYS:O	2.21	0.40
1:A:1075:ASN:ND2	1:A:1255:GLY:O	2.47	0.40
1:A:79:VAL:HA	1:A:123:ARG:O	2.21	0.40
1:A:1040:LYS:HD2	1:A:1046:THR:HB	2.04	0.40
1:A:1139:VAL:HA	1:A:1273:LEU:HD11	2.04	0.40
1:A:1142:ILE:HA	1:A:1145:TRP:HD1	1.86	0.40
2:C:111:GLN:NE2	2:C:115:ASP:OD1	2.55	0.40
2:C:185:VAL:HG22	2:C:193:LEU:HD23	2.03	0.40
1:A:221:ILE:CD1	1:A:279:LEU:HD12	2.46	0.40
1:A:690:VAL:HG12	1:A:702:ILE:O	2.22	0.40
2:C:111:GLN:HB3	2:C:112:PRO:HD3	2.02	0.40
1:A:619:VAL:HG11	1:A:645:ILE:HD13	2.03	0.40
2:B:171:TRP:CE3	2:B:199:ILE:HD12	2.57	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	630/1342 (47%)	586 (93%)	44 (7%)	0	100	100
2	B	236/416 (57%)	231 (98%)	5 (2%)	0	100	100
2	C	224/416 (54%)	218 (97%)	6 (3%)	0	100	100
All	All	1090/2174 (50%)	1035 (95%)	55 (5%)	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	583/1146 (51%)	582 (100%)	1 (0%)	93	97
2	B	217/377 (58%)	217 (100%)	0	100	100
2	C	208/377 (55%)	208 (100%)	0	100	100
All	All	1008/1900 (53%)	1007 (100%)	1 (0%)	93	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	959	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	680	GLN
1	A	1030	ASN

5.3.3 RNA ⓘ

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.

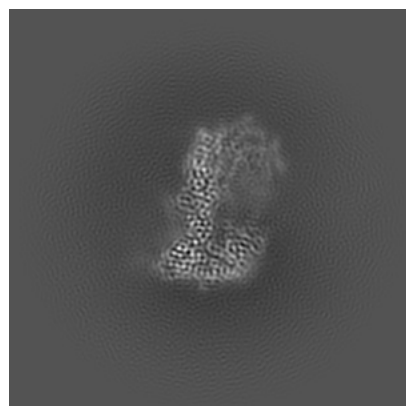
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26614. These allow visual inspection of the internal detail of the map and identification of artifacts.

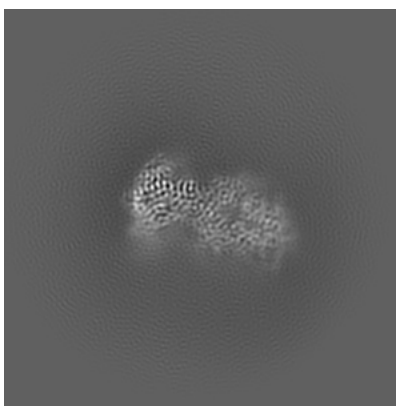
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

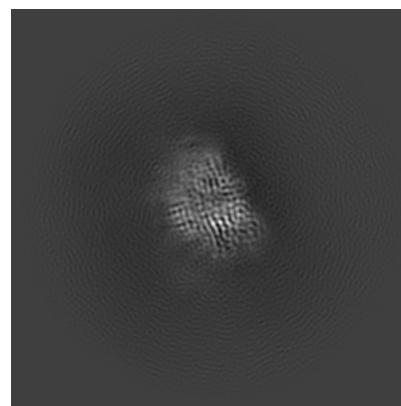
6.1.1 Primary map



X

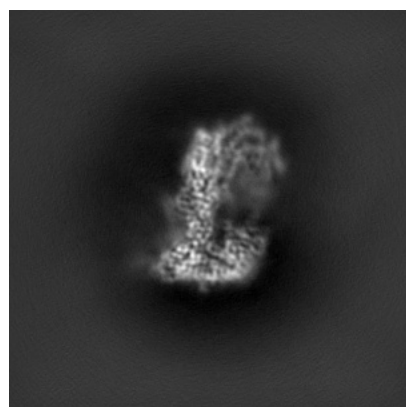


Y

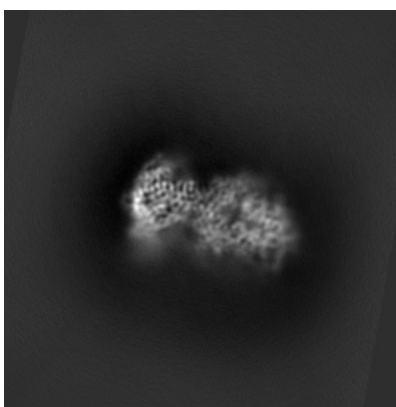


Z

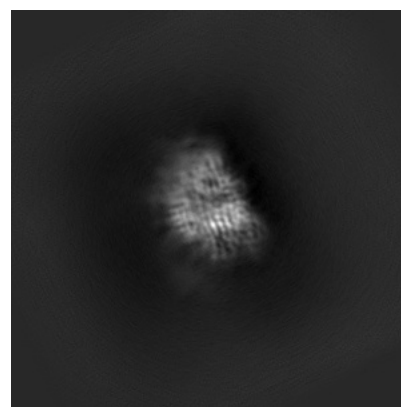
6.1.2 Raw map



X



Y

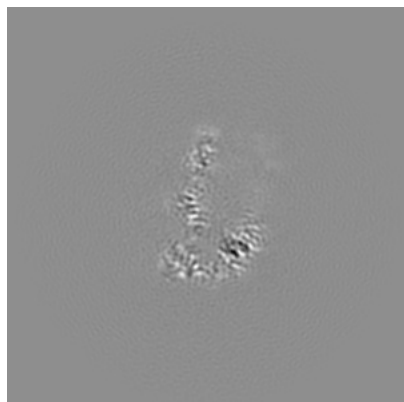


Z

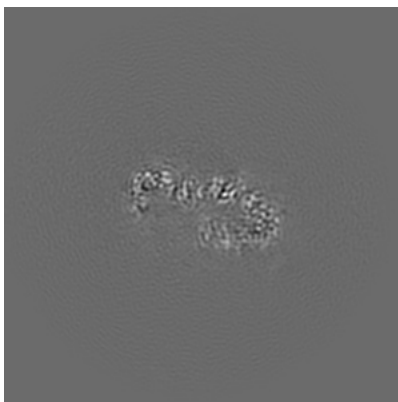
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

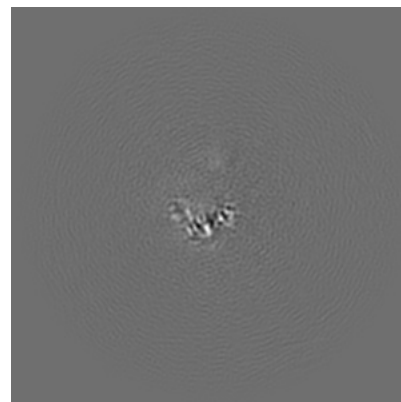
6.2.1 Primary map



X Index: 170

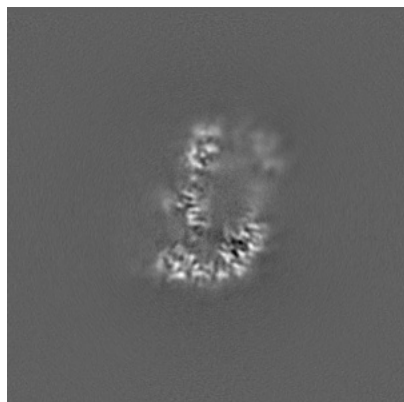


Y Index: 170

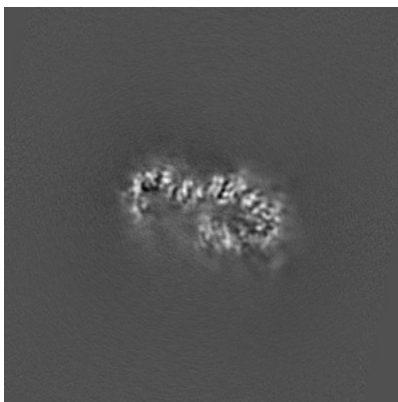


Z Index: 170

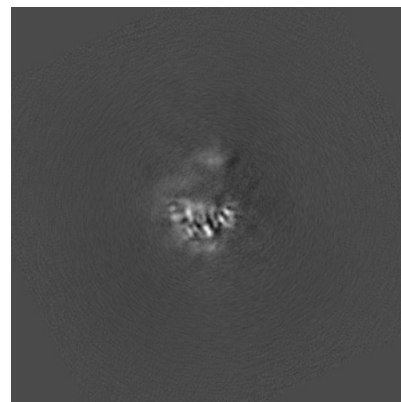
6.2.2 Raw map



X Index: 170



Y Index: 170

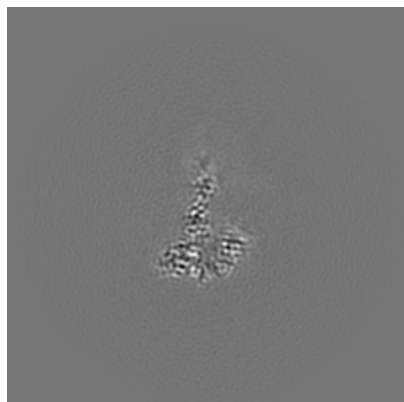


Z Index: 170

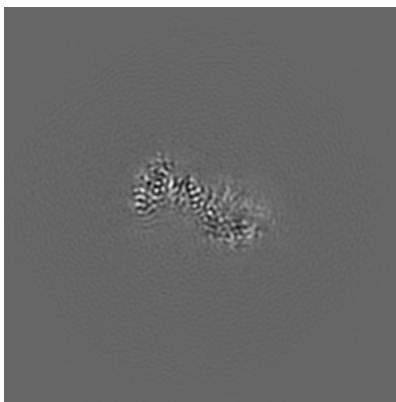
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

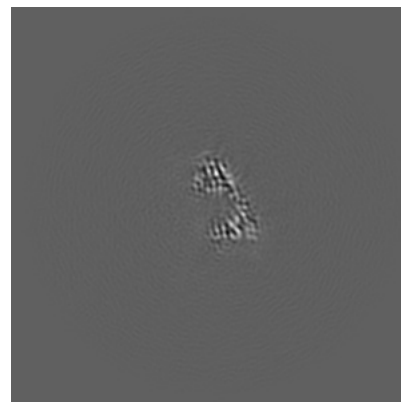
6.3.1 Primary map



X Index: 184

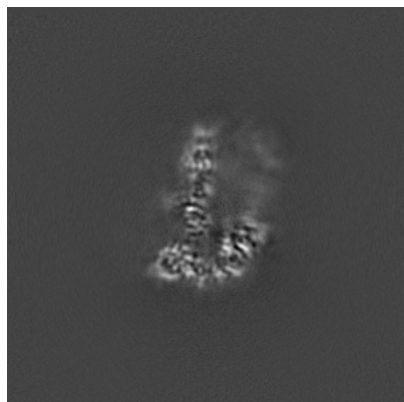


Y Index: 158

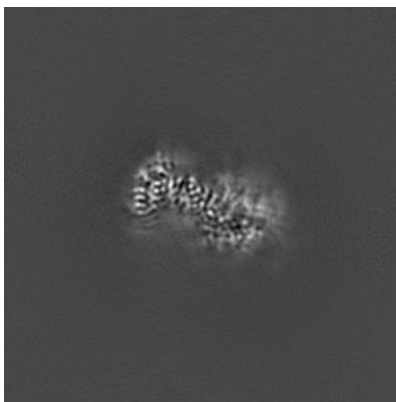


Z Index: 136

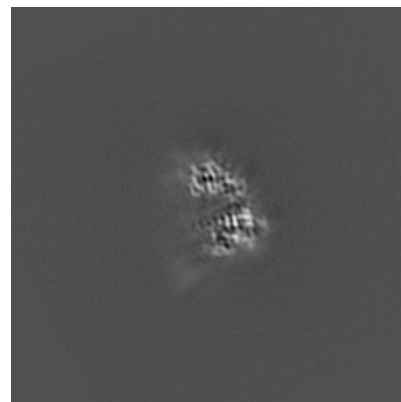
6.3.2 Raw map



X Index: 173



Y Index: 158

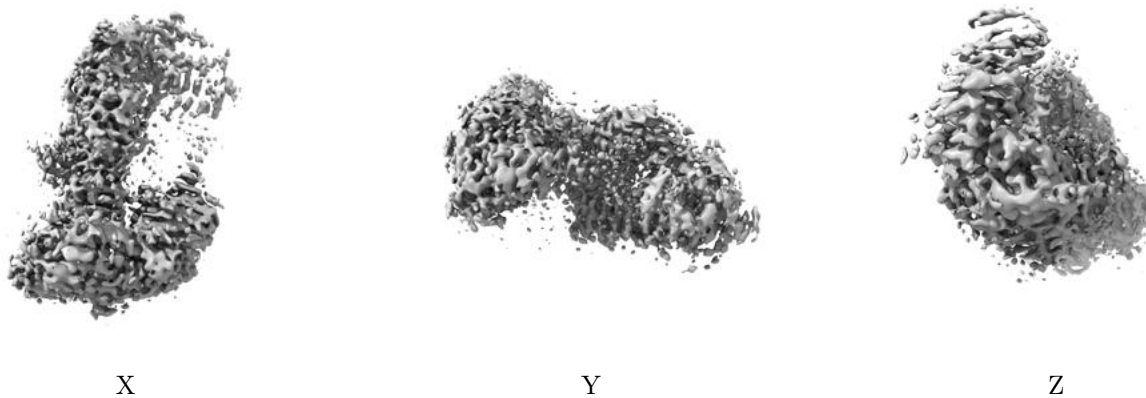


Z Index: 130

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

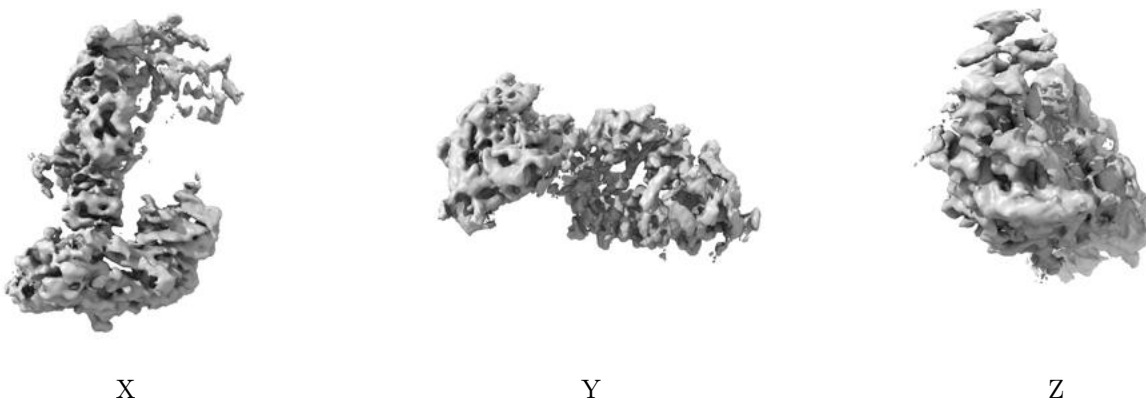
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

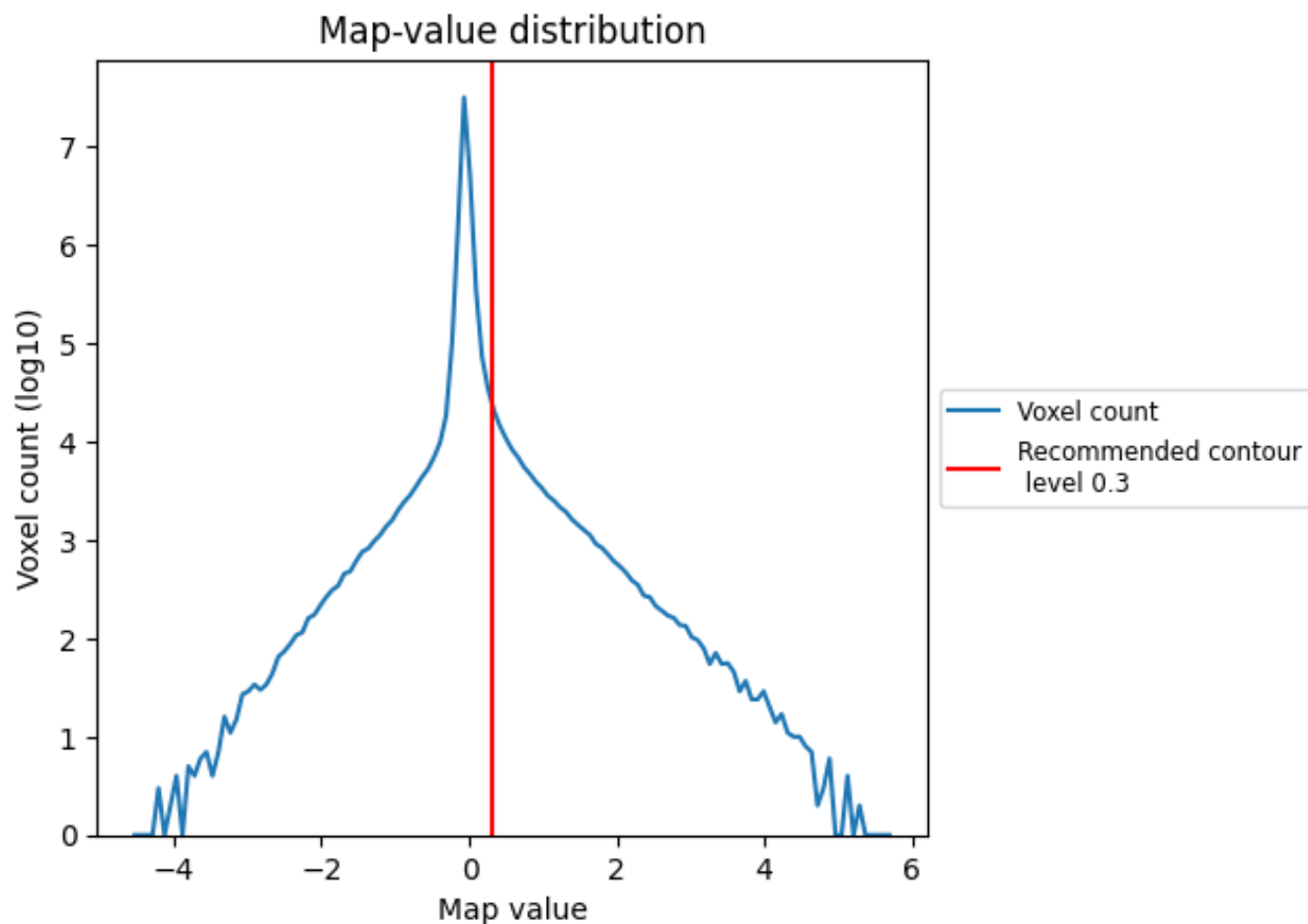
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

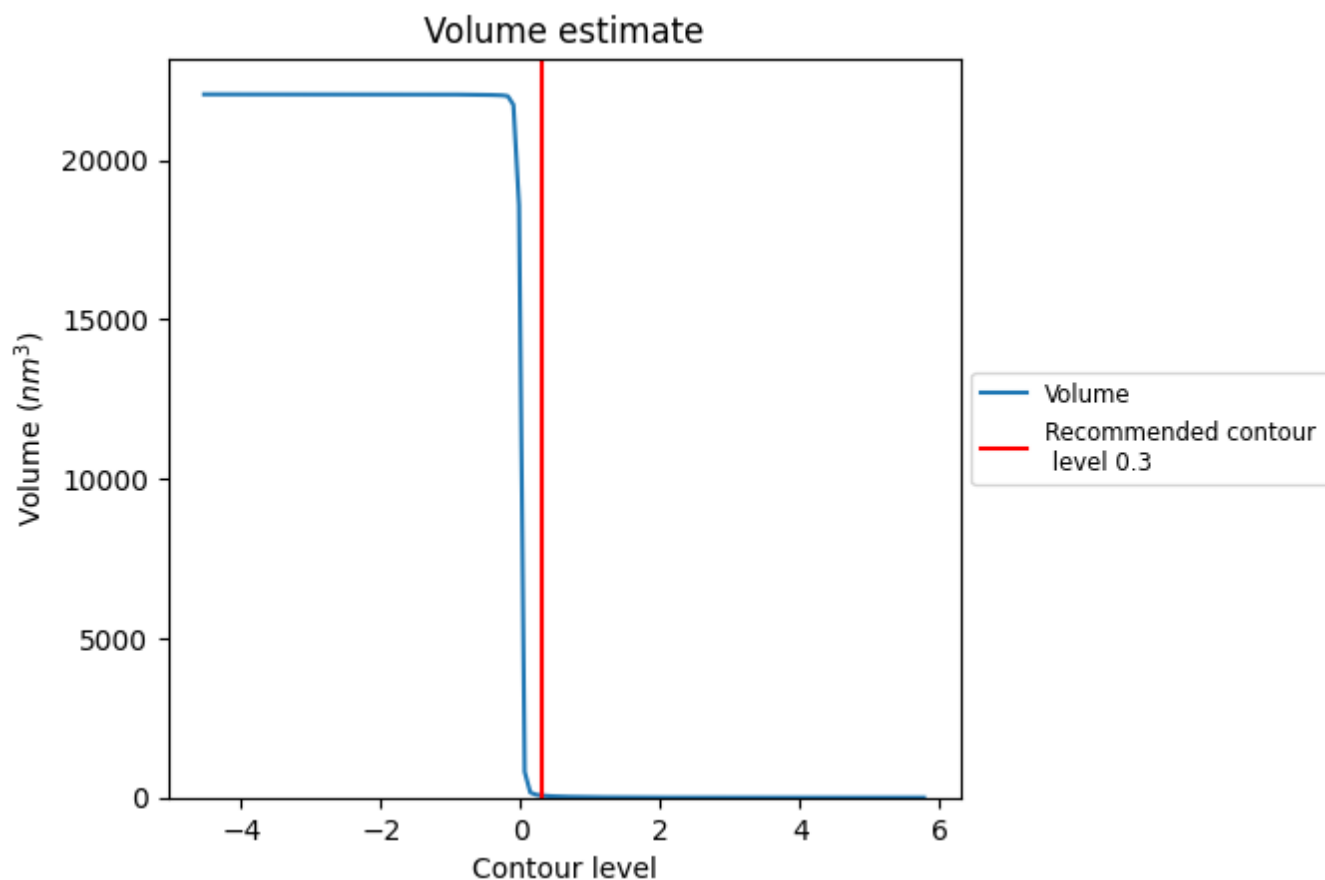
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

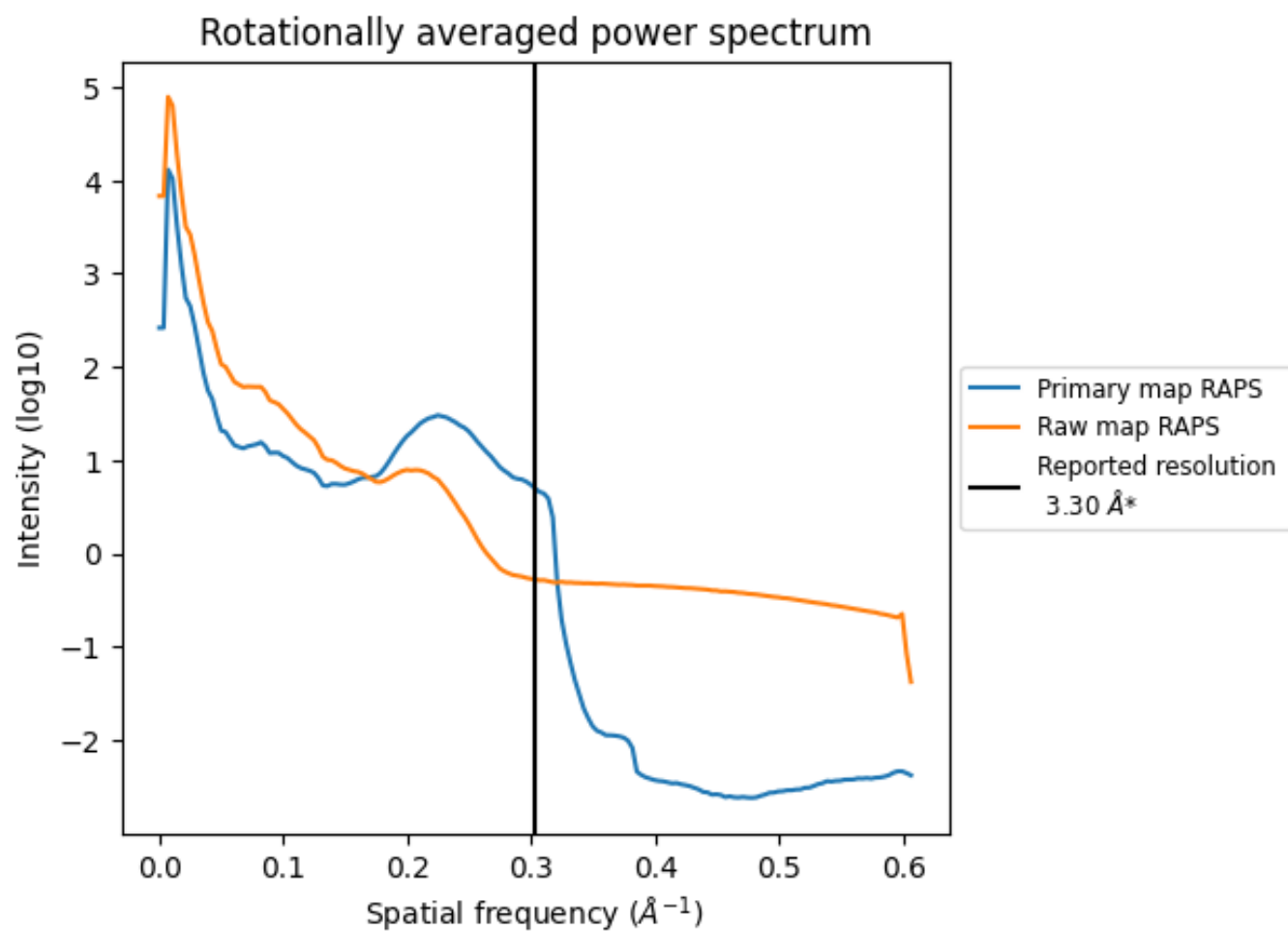
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 65 nm³; this corresponds to an approximate mass of 58 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 ⓘ

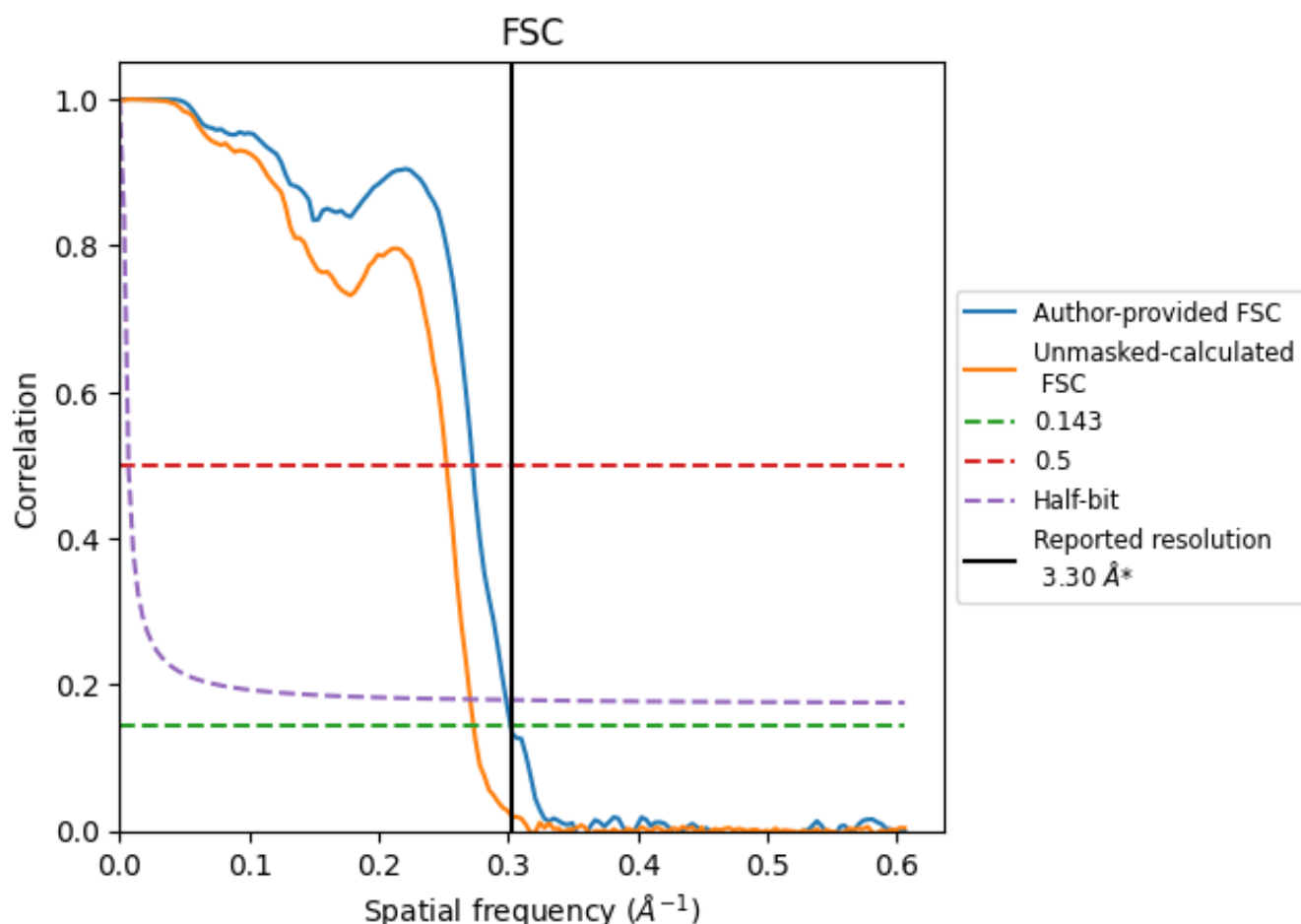


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

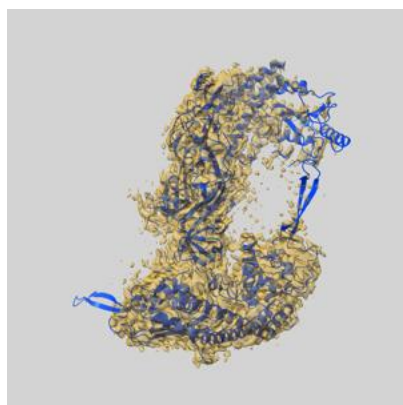
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.67	3.35
Unmasked-calculated*	3.66	3.96	3.69

*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 3.66 differs from the reported value 3.3 by more than 10 %

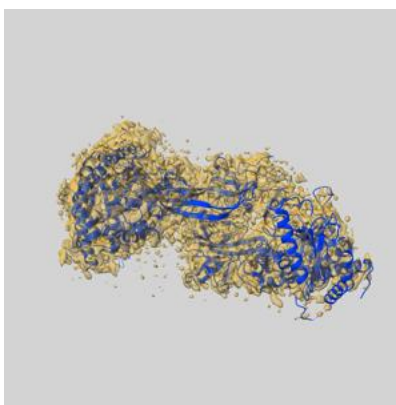
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26614 and PDB model 7UN6. Per-residue inclusion information can be found in section [3](#) on page [7](#).

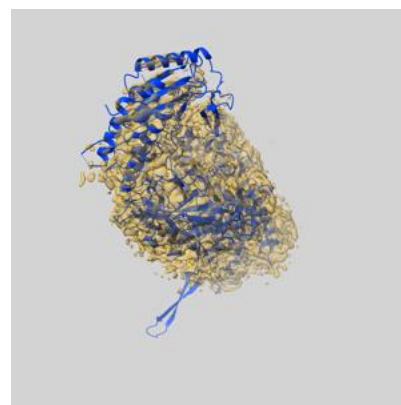
9.1 Map-model overlay [i](#)



X



Y



Z

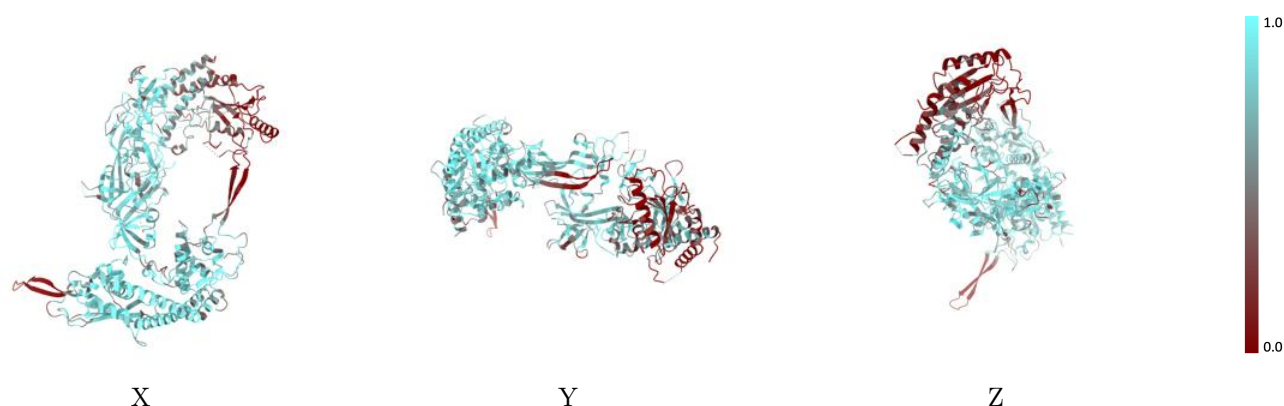
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



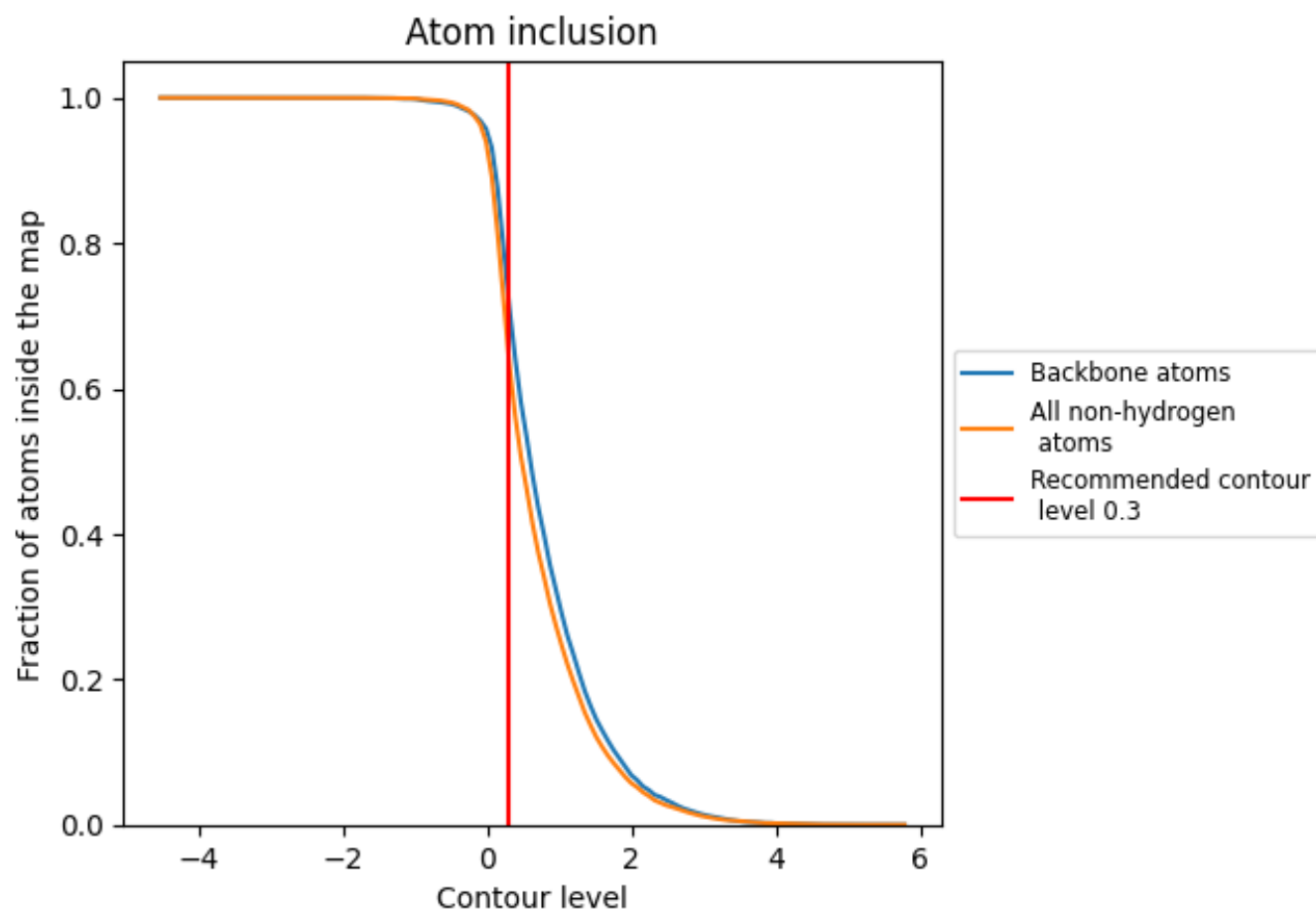
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6359	<div></div> 0.3620
A	<div></div> 0.5897	<div></div> 0.3600
B	<div></div> 0.6908	<div></div> 0.3610
C	<div></div> 0.7048	<div></div> 0.3670

