W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report ⓘ

Feb 19, 2024 – 03:04 PM JST

PDB ID	:	8WIF
EMDB ID	:	EMD-37565
Title	:	Cryo- EM structure of Mycobacterium smegmatis 30S ribosomal subunit (body 2) of 70S ribosome and RafH.
Authors	:	Kumar, N.; Sharma, S.; Kaushal, P.S.
Deposited on	:	2023-09-24
Resolution	:	2.90 Å(reported)
Based on initial model	:	8WHX

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 2.90 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.

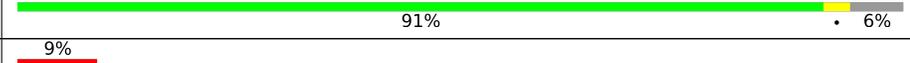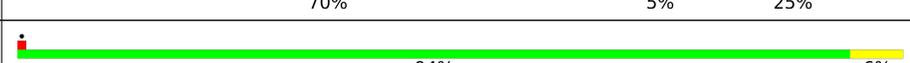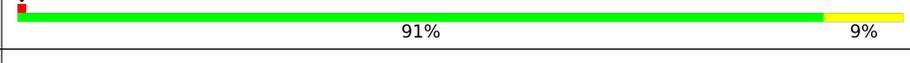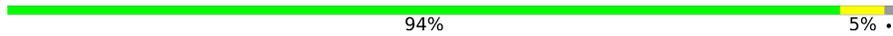| Metric	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.0%
Sidechain outliers		8.9%
RNA backbone		0.60

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
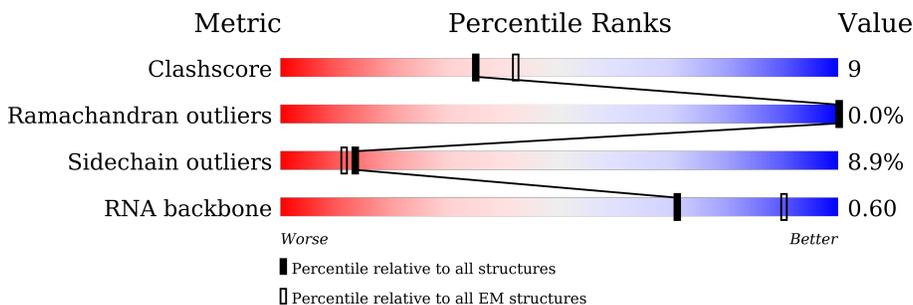
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	1528	81% 18% •
2	v	33	91% • 6%
3	d	275	9% 70% 5% 25%
4	e	201	94% 6%
5	f	214	5% 74% 5% 21%
6	g	96	91% 9%
7	h	156	86% 12% •

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Mol	Chain	Length	Quality of chain
8	i	132	94% 5%
9	j	150	77% 7% 16%
10	k	101	26% 92% 5%
11	l	138	77% 7% 17%
12	m	124	92% 6%
13	n	124	83% 10% 6%
14	o	101	29% 92% 7%
15	p	89	93% 6%
16	q	156	67% 5% 28%
17	r	98	88% 8%
18	s	84	76% 23%
19	t	93	78% 10% 12%
20	u	86	94% 5%
21	c	277	55% 76% 6% 18%
22	x	75	7% 12% 85%
23	w	264	44% 52%

2 Entry composition ⓘ

There are 23 unique types of molecules in this entry. The entry contains 52783 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1517	Total 32561	C 14503	N 5949	O 10592	P 1517	0	0

- Molecule 2 is a protein called 30S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	31	Total 271	C 166	N 69	O 35	S 1	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	207	Total 1656	C 1034	N 321	O 297	S 4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	200	Total 1641	C 1028	N 316	O 295	S 2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	170	Total 1236	C 778	N 232	O 222	S 4	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	96	Total 771	C 486	N 138	O 145	S 2	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	153	Total	C	N	O	S	0	0
			1207	751	235	219	2		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	131	Total	C	N	O	S	0	0
			1010	633	189	187	1		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	j	126	Total	C	N	O	0	0
			994	630	194	170		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	98	Total	C	N	O	S	0	0
			784	493	145	143	3		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	115	Total	C	N	O	S	0	0
			855	528	170	156	1		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 14 is a protein called 30S ribosomal protein S14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	o	100	Total	C	N	O	S	0	0
			819	497	183	138	1		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	p	88	Total	C	N	O	0	0
			720	449	147	124		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	q	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 18 is a protein called 30S ribosomal protein S18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	s	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	85	Total	C	N	O	0	0
			660	402	139	119		

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	228	Total 1793	C 1132	N 322	O 330	S 9	0	0

- Molecule 22 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	x	11	Total 94	C 59	N 21	O 14	0	0

- Molecule 23 is a protein called Ribosome hibernation promotion factor RafH.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	w	126	Total 1004	C 609	N 214	O 180	S 1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	259	HIS	-	expression tag	UNP A0QZ86
w	260	HIS	-	expression tag	UNP A0QZ86
w	261	HIS	-	expression tag	UNP A0QZ86
w	262	HIS	-	expression tag	UNP A0QZ86
w	263	HIS	-	expression tag	UNP A0QZ86
w	264	HIS	-	expression tag	UNP A0QZ86

3   Residue-property plots ⓘ

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: 16S rRNA
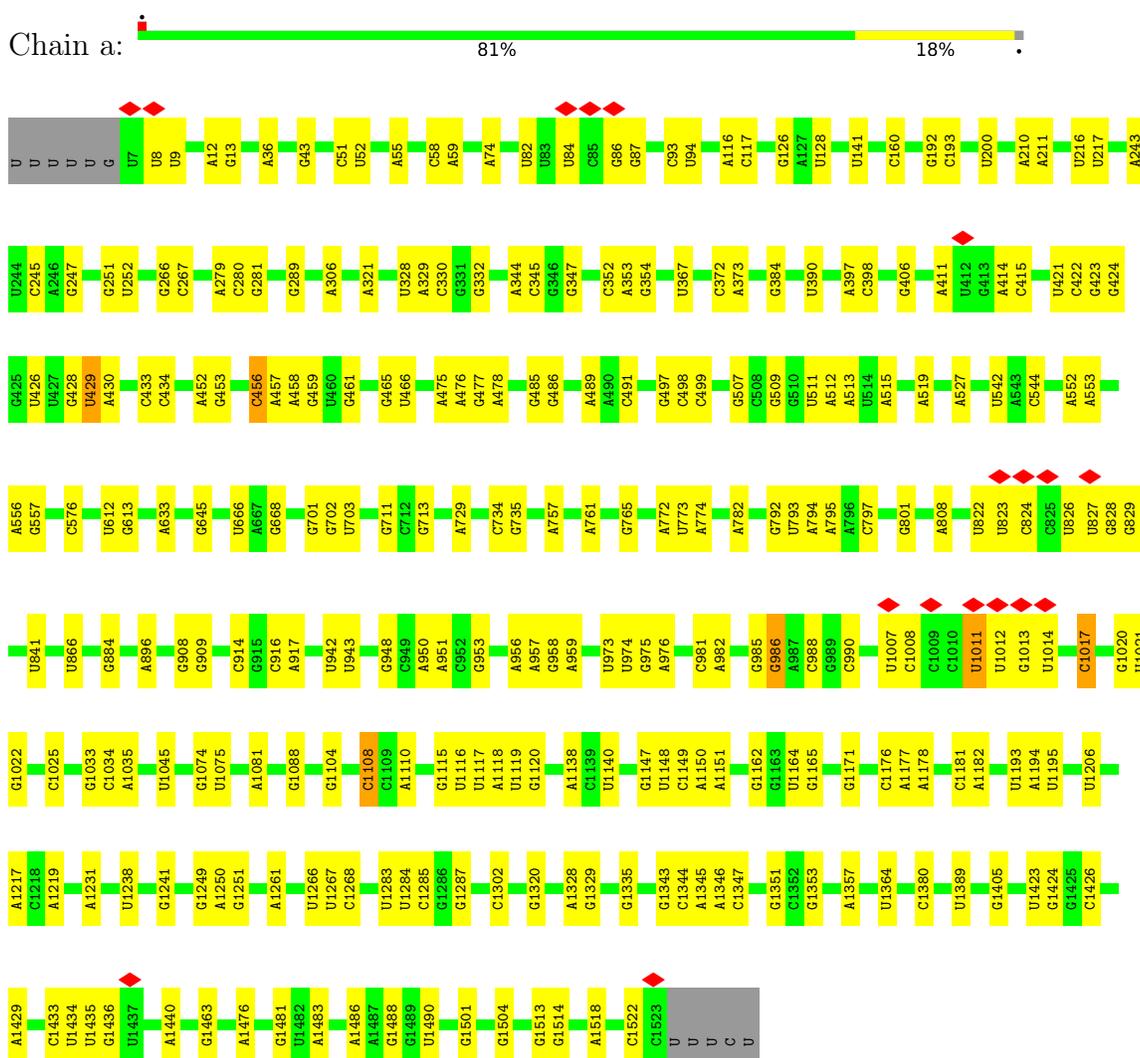
- Molecule 2: 30S ribosomal protein S22

MET G2 R11 G32 LYS

• Molecule 3: 30S ribosomal protein S3

Chain d:

9%

70% 5% 25%

MET G2 R21 T44 G45 L46 E47 R48 R60 D61 R62 R71 I74 V75 I76 G77 R78 R79 G80 T81 E82 A83 D84 R85 A88 D89 K92 L93 T94 G95 K96 Q97 V98 K106 S110 R126 M133 R134 K147 M162 T191 D206 I207 V208 GLY

GLY LYS ARG GLU LEU ALA ALA ALA ALA PRO ALA SER ASP ARG PRO ARG ARG GLU ARG PRO SER GLY THR THR ARG PRO ARG ARG SER GLY SER ALA GLY THR THR ALA THR SER THR GLU GLY ALA GLY ARG ALA ALA THR SER ASP ALA PRO ALA ALA GLY THR ALA ALA ALA GLU ALA PRO

ALA GLU SER THR GLU SER

• Molecule 4: 30S ribosomal protein S4

Chain e:

94% 6%

MET A2 T5 K80 R99 Q111 D126 Y135 D136 D139 V140 K141 R154 G158 E159 R160 E171 L190 K201

• Molecule 5: 30S ribosomal protein S5

Chain f:

5%

74% 5% 21%

MET ALA GLU GLN ALA GLY ALA GLY SER ALA GLN ASP ASN ARG GLY GLY ARG GLY ARG ARG ASP ASP ARG GLY GLY ARG GLY ARG ASP GLY GLY ASP LYS SER N35 V41 K51 T59 D66 G67 K68 F96 F97 S104 M120 H146 S152 R174 K196

A197 R198 R199 E200 S201 E202 A203 L204 ALA ALA ALA ALA ALA ARG GLU GLY GLY SER ALA

• Molecule 6: 30S ribosomal protein S6

Chain g:

91% 9%

M1 V8 E16 F26 G35 D38 K39 R46 D64 V65 H96

• Molecule 7: 30S ribosomal protein S7

Chain h:

86% 12%

MET P2 R10 P11 L12 T24 Q49 T56 D57 T61 L66 T84 Y85 D94 S108 R112 D126 S134 V135 K136 R137 D140 Y154 ARG TRP

• Molecule 8: 30S ribosomal protein S8

Chain i: 94% 5%

MET T2 D9 L27 T51 S73 N93 R96 D115 W132
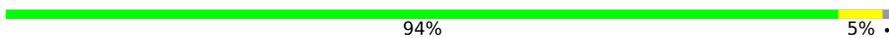
• Molecule 9: 30S ribosomal protein S9

Chain j: 77% 7% 16%

MET THR ASP VAL THR GLU THR GLU VAL VAL THR GLU SER ALA GLU PRO ARG GLU PRO VAL ILE ILE ASP ARG P25 K33 R40 F48 L55 Y58 S93 R105 E113 R126 K134 Y147 S148 K149 R150

• Molecule 10: 30S ribosomal protein S10

Chain k: 26% 92% 5%

MET ALA GLY Q4 K5 I6 H15 E27 R31 T32 G33 A34 S35 V36 V37 E45 K57 L77 D78 P79 T80 P81 K82 T83 V84 D85 A86 L87 M88 R89 I90 D91 L92 Q101
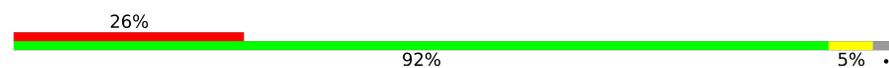
• Molecule 11: 30S ribosomal protein S11

Chain l: 77% 7% 17%

MET ALA GLN ALA LYS LYS GLY GLY THR ALA ALA LYS LYS GLY GLN LYS LYS THR ARG ARG ARG GLU GLU LYS K23 T35 F36 N37 N38 T39 V91 D92 V93 S100 T118 P132 R137 VAL
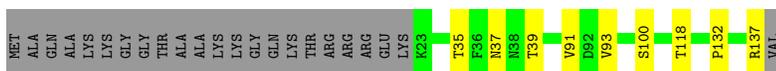
• Molecule 12: 30S ribosomal protein S12

Chain m: 92% 6%

MET P2 R36 E62 V63 T64 Q75 L90 T104 R110 E122 K123 SER
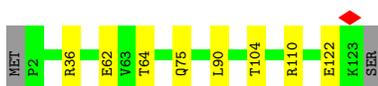
• Molecule 13: 30S ribosomal protein S13

Chain n: 83% 10% 6%

MET A2 D8 R11 M15 E32 M43 K46 T49 Q75 A76 D77 I78 R79 R80 E83 L90 R91 I117 ALA GLY LYS LYS LYS ALA ARG

• Molecule 14: 30S ribosomal protein S14A

Chain o: 29% 92% 7%

MET A2 E15 Q18 R19 Y20 A21 E22 R23 R24 A25 E26 L27 K28 R29 T30 I31 R32 D33 P34 A35 S36 S37 P38 E39 R40 R41 A42 A43 V45 S46 A47 R50 D54 S55 K76 W101
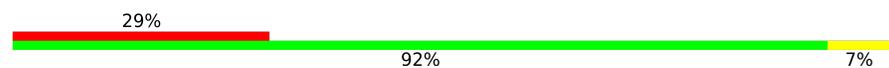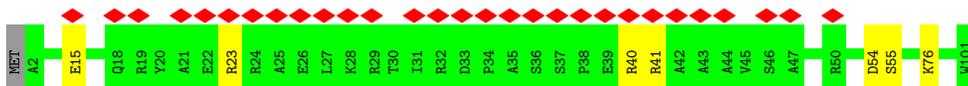
• Molecule 15: 30S ribosomal protein S15

Chain p:

93%   6%

MET A2 E6 K44 V70 E83 R89

• Molecule 16: 30S ribosomal protein S16

Chain q:

67%   5%   28%

MET A2 R9 R14 R39 Y40 H41 L48 S53 L86 P87 G88 A89 E90 G91 E97 P98 K99 E112 A113 E114 SER GLY THR THR ALA ALA THR THR PRO LYS LYS LYS LYS ALA PRO LYS LYS ASP GLU ALA ALA GLU ALA PRO ALA GLU ALA ALA GLU ALA

PRO ALA GLU ALA ALA ASP ALA ALA SER GLU SER

• Molecule 17: 30S ribosomal protein S17

Chain r:

88%   8%

MET ALA ASP Q4 K5 K31 E64 N65 G66 E67 D72 M77 E95 K96 A97 LYS

• Molecule 18: 30S ribosomal protein S18B

Chain s:

76%   23%

MET ALA LYS SER ASN LYS ARG PRO ALA PRO GLU LYS PRO VAL LYS T17 R18 K25 K26 S81 SER THR ARG

• Molecule 19: 30S ribosomal protein S19

Chain t:

78%   10%   12%

MET P2 H14 L15 E24 K25 N26 T27 K28 W34 T39 K56 T79 H83 ILE LYS ASP ASP ARG LYS SER LYS ARG ARG

• Molecule 20: 30S ribosomal protein S20

Chain u:

94%   5%

MET A2 R33 D40 D43 K44 D45 L86

• Molecule 21: 30S ribosomal protein S2

Chain c:

55%

76%   6%   18%

M1 A2 V3 V4 T5 M6 K7 Q8 L9 L10 D11 S12 G13 A14 H15 F16 G17 H18 Q19 W23 K28 R29 F30 I31 F32 T33 D34 R35 N36 G37 I38 Y39 I40 I41 D42 L43 Q44 Q45 T46 L47 T48 Y49 I50 D51 K52 A53 Y54 E55 F56 V57 K58 E59 T60 V61 A62 H63 G64 G65

T66 V67 L68 F69 K74 Q77 E78 S79 I80 A81 E82 E83 A84 T85 R86 V87 G88 M89 P90 Y91 V92 N93 Q94 F104 H108 K109 R110 L111 Q112 R113 L114 K115 E116 L117 E118 A119 M120 E121 Q122 T123 G124 G125 F126 E127 G128 R129 T130 K131 K132 E133 I134 L135 M136 L137 T138 R139

E140 K141 N142 K143 L144 E145 R146 S147 L148 G149 G150 I151 R152 D153 M154 Q155 K156 V157 P158 S159 V164 D165 R177 K178 L179 G180 I181 P182 L187 D192 P193 D194 V195 V196 D197 Y198 D205 A206 I207 R208 S209 L212 L213 T214 K215 V216 I217 A218 S219 A220 V221 A222 E223 C224

L225 Q226 A227 R228 ALA GLY GLN GLY SER GLY GLU LYS PRO ALA GLY ALA GLU PRO LEU ALA GLU TRP GLU GLN GLU LEU LEU ALA ALA THR ALA GLY ALA ALA ASP ALA SER ALA GLU ALA GLY ALA ALA PRO GLU SER SER THR ASP ALA SER

• Molecule 22: 50S ribosomal protein L31

Chain x:

7%

12% · 85%

MET LYS THR GLY ILE HIS PRO GLU TYR VAL ASP THR THR VAL GLN CYS GLY CYS GLY HIS SER PHE THR THR ARG SER THR LYS GLN SER GLY THR ILE VAL VAL GLU VAL CYS SER GLN CYS HIS PRO PHE TYR THR GLY LYS GLN LYS ILE LEU ASP SER GLY GLY G56 R57 R60 F61

E62 G66 LYS ARG ASN LYS ALA ALA ALA ASP LYS
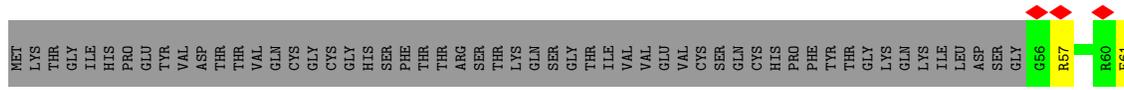
• Molecule 23: Ribosome hibernation promotion factor RafH

Chain w:

•

44% · 52%

M1 D2 T7 R27 T41 R66 R75 R84 L85 R86 I92 A107 G108 R109 R119 Y123 R126 PRO PRO GLU ARG ARG ILE ILE ARG LYS SER PHE SER MET VAL PRO CYS THR VAL ASP GLU ALA ALA LEU GLU MET GLU MET LEU ASP TYR

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

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

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion3.1.4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.34	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.236	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	0.74	0/36444	0.81	18/56866 (0.0%)
2	v	0.26	0/271	0.67	0/348
3	d	0.33	0/1680	0.57	0/2256
4	e	0.36	0/1672	0.59	1/2251 (0.0%)
5	f	0.30	0/1252	0.53	0/1691
6	g	0.38	0/782	0.59	0/1059
7	h	0.32	0/1225	0.57	0/1653
8	i	0.41	0/1025	0.57	0/1385
9	j	0.33	0/1012	0.62	1/1362 (0.1%)
10	k	0.31	0/798	0.59	0/1081
11	l	0.36	0/873	0.58	0/1180
12	m	0.38	0/969	0.59	0/1294
13	n	0.32	0/942	0.67	0/1260
14	o	0.32	0/830	0.64	0/1106
15	p	0.37	0/729	0.58	0/977
16	q	0.38	0/908	0.58	0/1226
17	r	0.39	0/759	0.60	0/1016
18	s	0.37	0/518	0.58	0/693
19	t	0.35	0/680	0.57	0/915
20	u	0.34	0/663	0.55	0/882
21	c	0.28	0/1822	0.53	0/2457
22	x	0.29	0/95	0.71	0/123
23	w	0.32	0/1023	0.61	0/1381
All	All	0.63	0/56972	0.75	20/84462 (0.0%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1017	C	N3-C2-O2	-8.07	116.25	121.90
1	a	1206	U	C2-N1-C1'	7.12	126.24	117.70
1	a	1017	C	N1-C2-O2	6.77	122.96	118.90
1	a	1011	U	C2-N1-C1'	6.20	125.14	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	986	G	N3-C4-N9	-5.91	122.45	126.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	32561	0	16386	0	0
2	v	271	0	329	0	0
3	d	1656	0	1704	0	0
4	e	1641	0	1668	0	0
5	f	1236	0	1303	0	0
6	g	771	0	797	0	0
7	h	1207	0	1259	0	0
8	i	1010	0	1046	0	0
9	j	994	0	1050	0	0
10	k	784	0	816	0	0
11	l	855	0	863	0	0
12	m	958	0	1045	0	0
13	n	935	0	986	0	0
14	o	819	0	866	0	0
15	p	720	0	760	0	0
16	q	891	0	935	0	0
17	r	748	0	795	0	0
18	s	513	0	540	0	0
19	t	662	0	677	0	0
20	u	660	0	712	0	0
21	c	1793	0	1839	0	0
22	x	94	0	95	0	0
23	w	1004	0	991	0	0
All	All	52783	0	37462	0	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.

There are no clashes within the asymmetric unit.

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	
2	v	29/33 (88%)	29 (100%)	0	0	100	100
3	d	205/275 (74%)	196 (96%)	9 (4%)	0	100	100
4	e	198/201 (98%)	184 (93%)	14 (7%)	0	100	100
5	f	168/214 (78%)	160 (95%)	8 (5%)	0	100	100
6	g	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
7	h	151/156 (97%)	147 (97%)	4 (3%)	0	100	100
8	i	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
9	j	124/150 (83%)	117 (94%)	7 (6%)	0	100	100
10	k	96/101 (95%)	92 (96%)	3 (3%)	1 (1%)	15	45
11	l	113/138 (82%)	106 (94%)	7 (6%)	0	100	100
12	m	120/124 (97%)	111 (92%)	9 (8%)	0	100	100
13	n	114/124 (92%)	109 (96%)	5 (4%)	0	100	100
14	o	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	p	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	q	111/156 (71%)	106 (96%)	5 (4%)	0	100	100
17	r	92/98 (94%)	88 (96%)	4 (4%)	0	100	100
18	s	63/84 (75%)	60 (95%)	3 (5%)	0	100	100
19	t	80/93 (86%)	76 (95%)	4 (5%)	0	100	100
20	u	83/86 (96%)	83 (100%)	0	0	100	100
21	c	226/277 (82%)	210 (93%)	16 (7%)	0	100	100
22	x	9/75 (12%)	9 (100%)	0	0	100	100
23	w	124/264 (47%)	120 (97%)	4 (3%)	0	100	100
All	All	2513/3067 (82%)	2398 (95%)	114 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	k	57	LYS

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	
2	v	29/31 (94%)	28 (97%)	1 (3%)	37	71
3	d	170/212 (80%)	156 (92%)	14 (8%)	11	32
4	e	175/176 (99%)	164 (94%)	11 (6%)	18	46
5	f	124/147 (84%)	113 (91%)	11 (9%)	9	29
6	g	85/85 (100%)	76 (89%)	9 (11%)	6	20
7	h	129/132 (98%)	110 (85%)	19 (15%)	3	9
8	i	107/108 (99%)	100 (94%)	7 (6%)	17	45
9	j	102/125 (82%)	92 (90%)	10 (10%)	8	24
10	k	89/90 (99%)	85 (96%)	4 (4%)	27	61
11	l	89/105 (85%)	80 (90%)	9 (10%)	7	23
12	m	103/105 (98%)	95 (92%)	8 (8%)	12	34
13	n	99/104 (95%)	86 (87%)	13 (13%)	4	12
14	o	85/86 (99%)	78 (92%)	7 (8%)	11	32
15	p	76/77 (99%)	71 (93%)	5 (7%)	16	44
16	q	92/118 (78%)	84 (91%)	8 (9%)	10	30
17	r	80/83 (96%)	72 (90%)	8 (10%)	7	23
18	s	55/72 (76%)	54 (98%)	1 (2%)	59	85
19	t	73/84 (87%)	64 (88%)	9 (12%)	4	14
20	u	69/70 (99%)	65 (94%)	4 (6%)	20	50
21	c	191/218 (88%)	173 (91%)	18 (9%)	8	26
22	x	8/63 (13%)	6 (75%)	2 (25%)	0	2
23	w	98/215 (46%)	87 (89%)	11 (11%)	6	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2128/2506 (85%)	1939 (91%)	189 (9%)	13 29

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	n	91	ARG
17	r	95	GLU
14	o	41	ARG
16	q	39	ARG
19	t	34	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
23	w	95	HIS
19	t	22	GLN
14	o	49	GLN
11	l	47	GLN
15	p	18	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1516/1528 (99%)	271 (17%)	0

5 of 271 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	U
1	a	9	U
1	a	12	A
1	a	13	G
1	a	36	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation   ⓘ

This section contains visualisations of the EMDB entry EMD-37565. 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   ⓘ
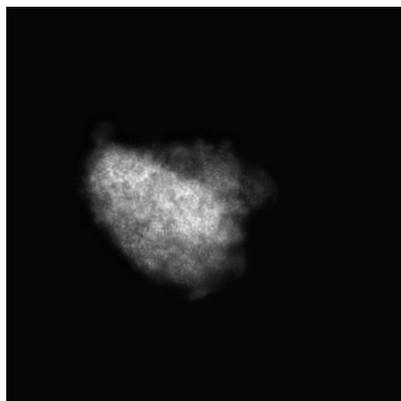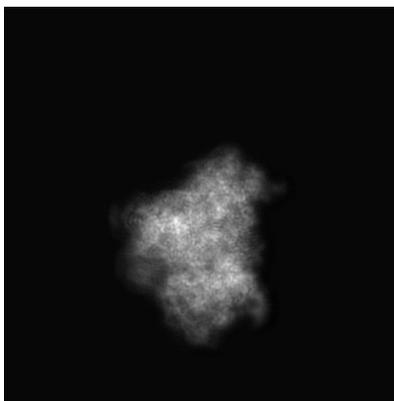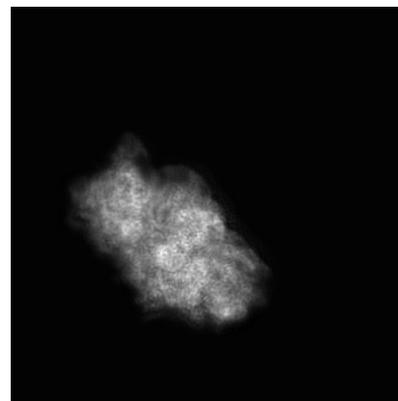
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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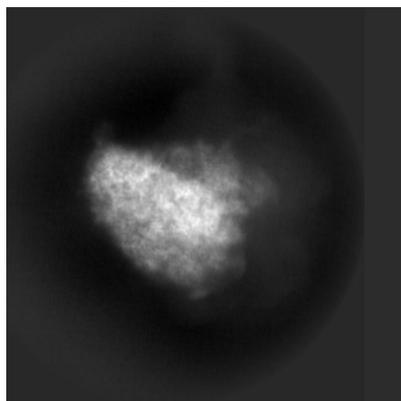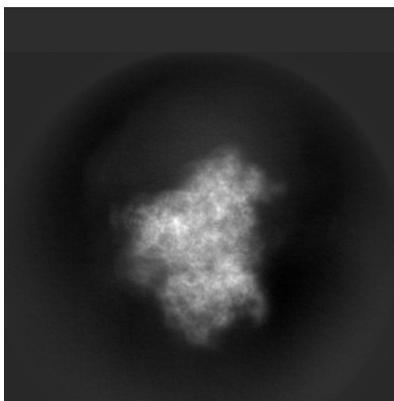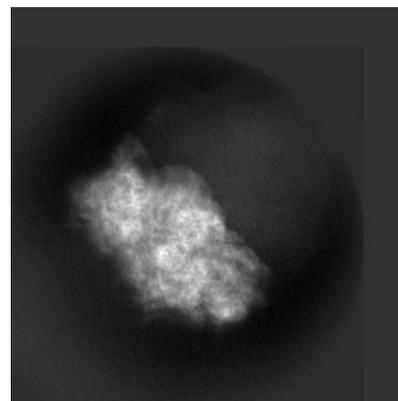
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
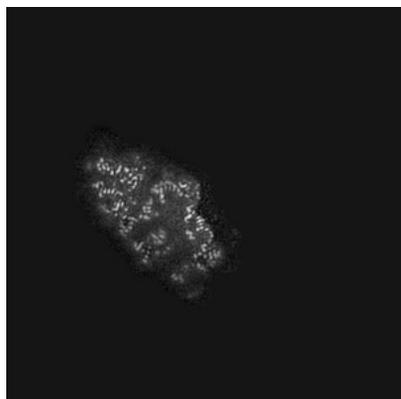
6.2.1 Primary map
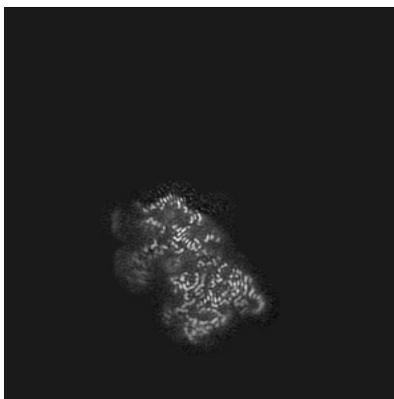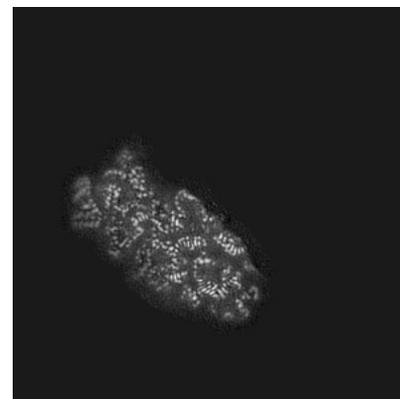
| X Index: 190 | Y Index: 190 | Z Index: 190 |

6.2.2 Raw map
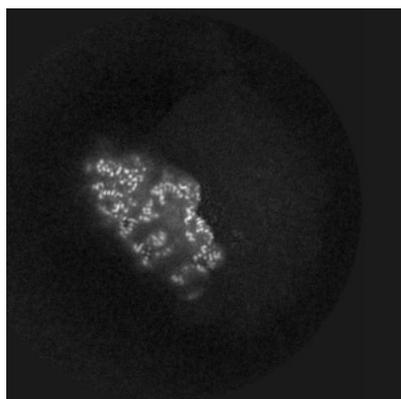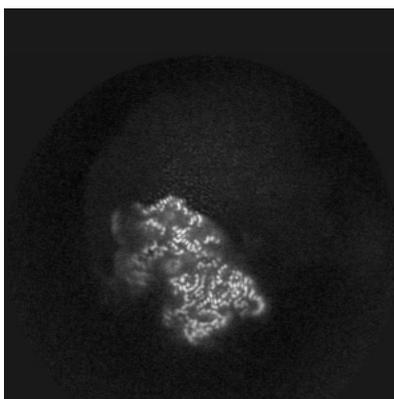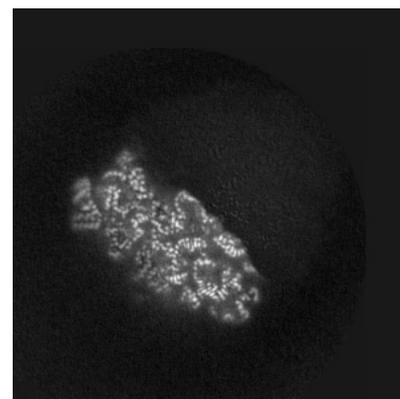
| X Index: 190 | Y Index: 190 | Z Index: 190 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
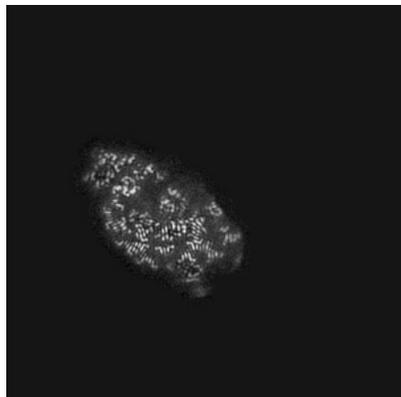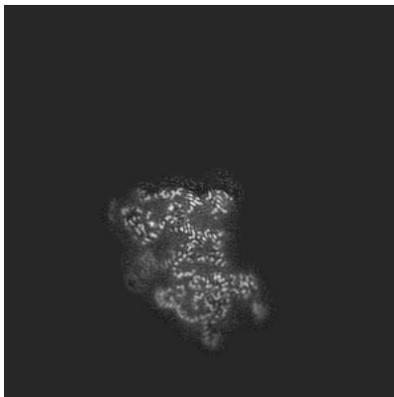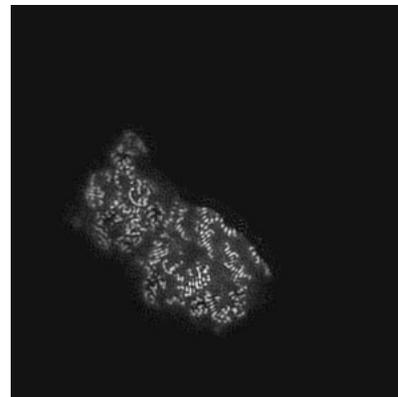
X Index: 171	Y Index: 174	Z Index: 205

6.3.2 Raw map
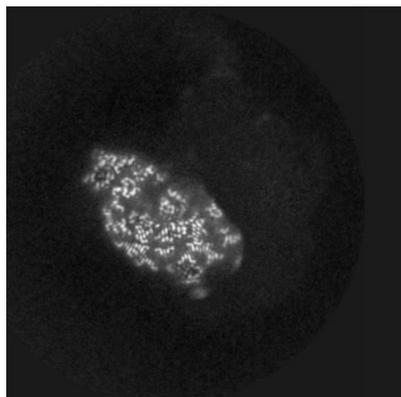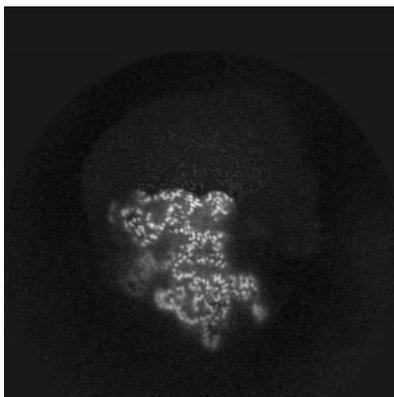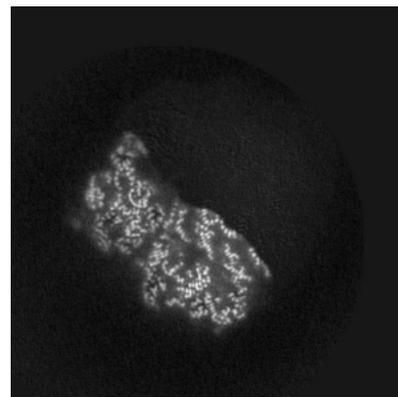
X Index: 171	Y Index: 174	Z Index: 205

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
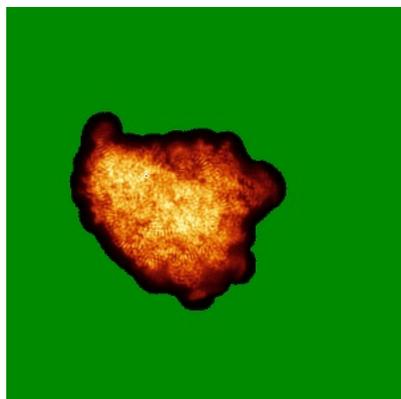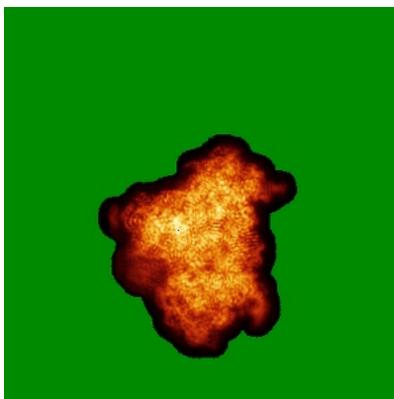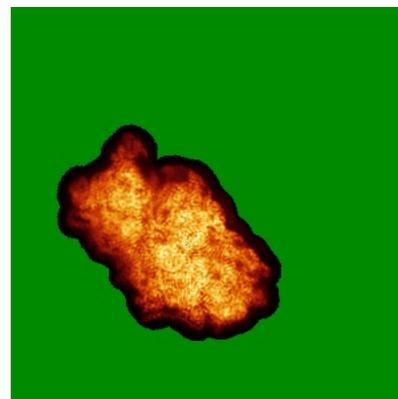
| X | Y | Z |

6.4.2 Raw map

| X | Y | Z |
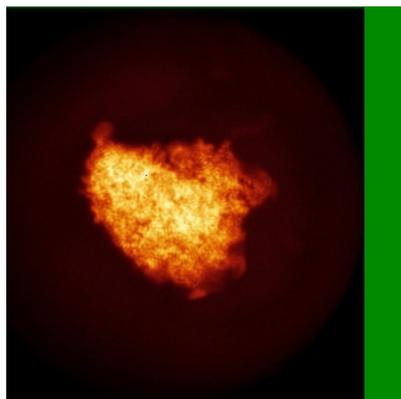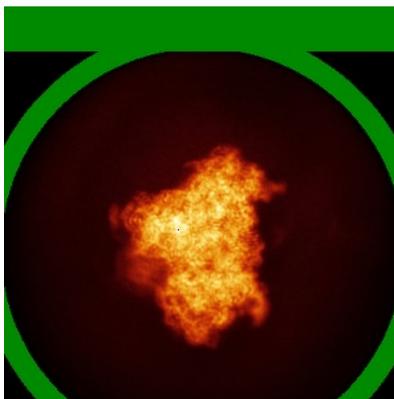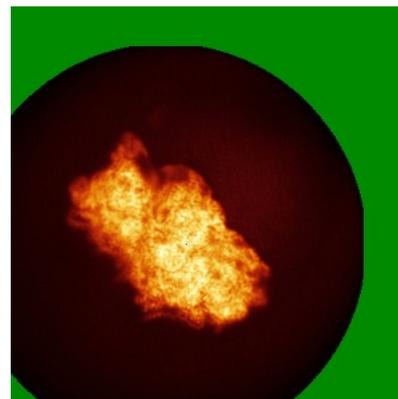
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.045. 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

| X | Y | Z |

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 ⓘ

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

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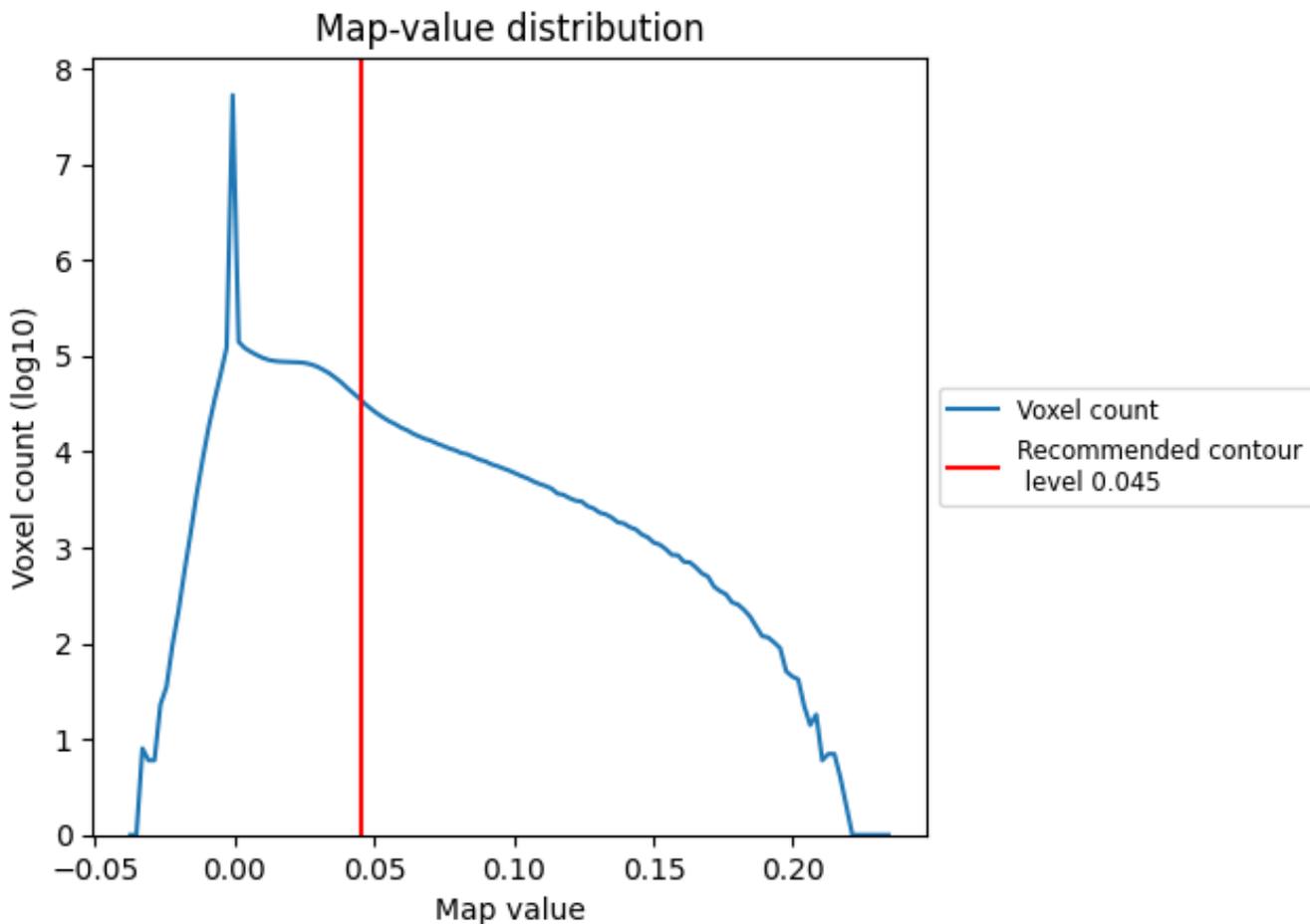
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
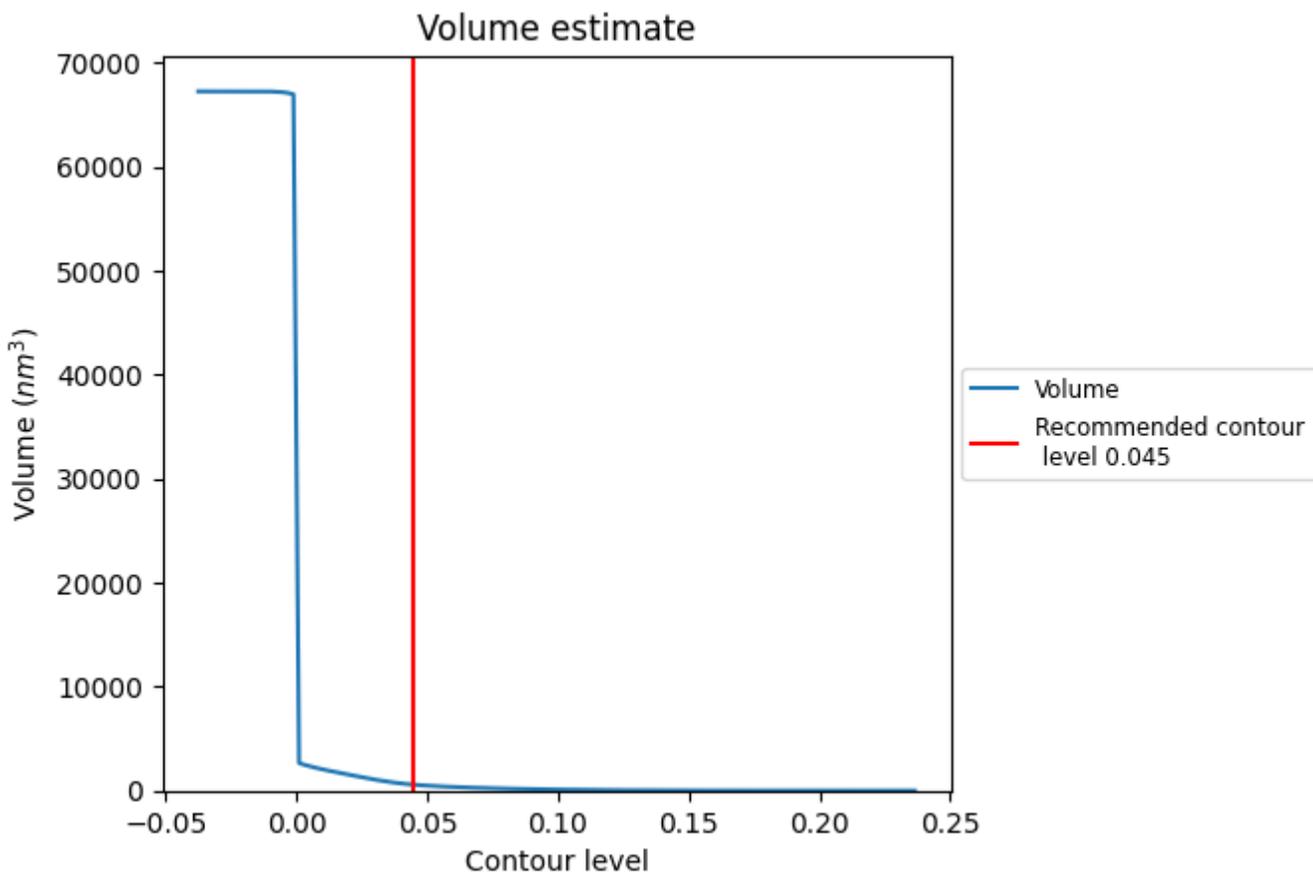
The volume at the recommended contour level is 570 nm^3; this corresponds to an approximate mass of 515 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3   Rotationally averaged power spectrum (i)
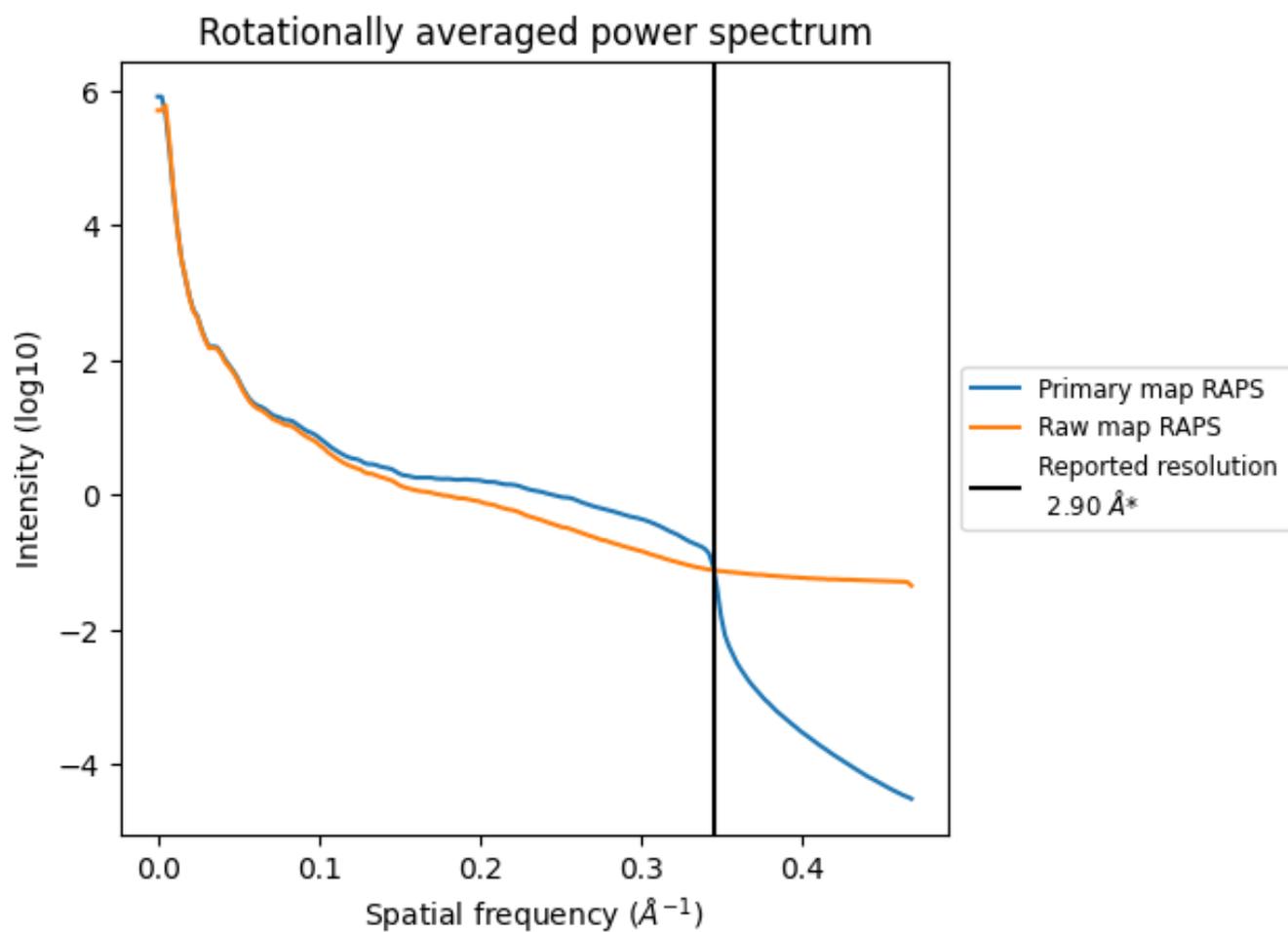
*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
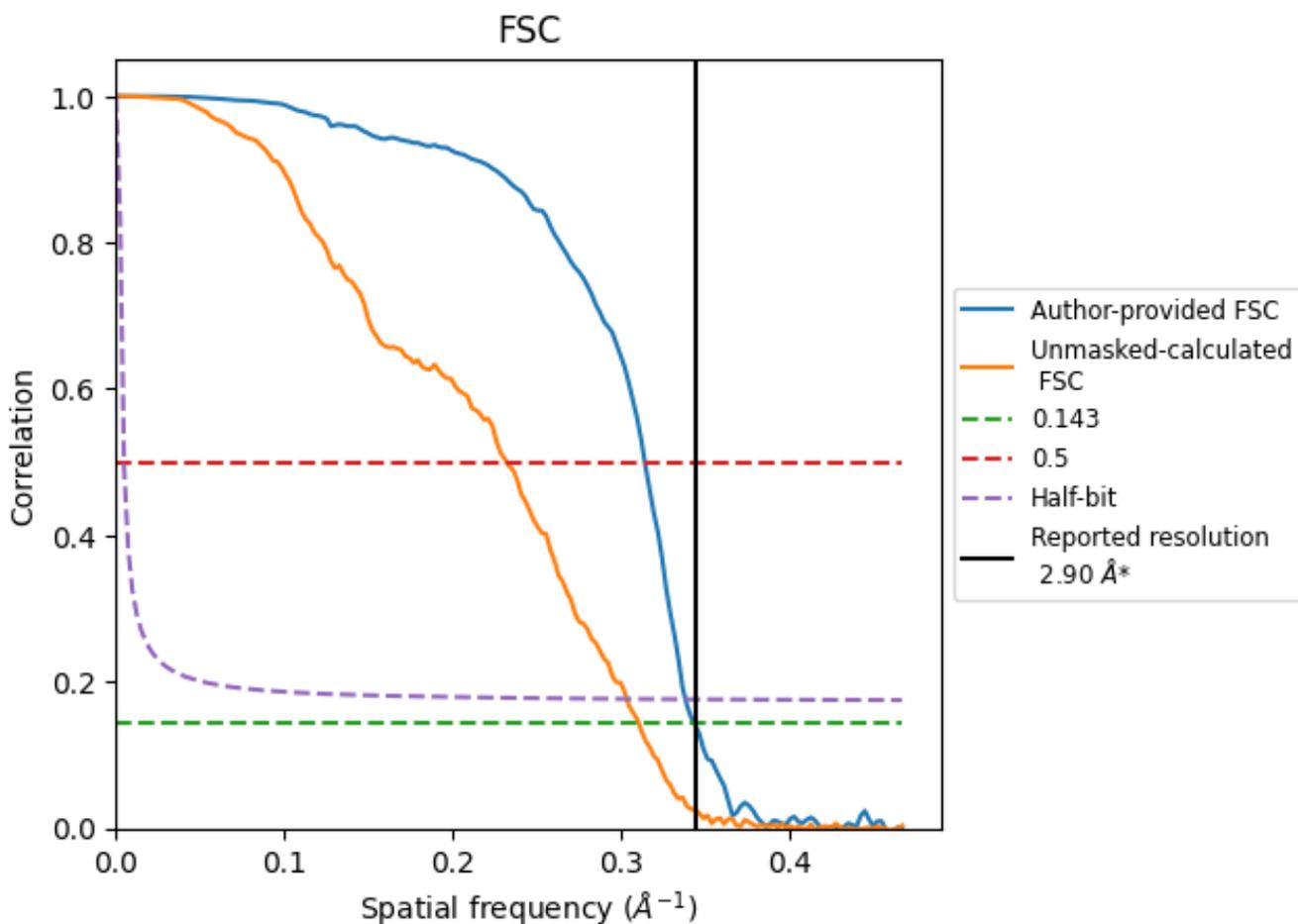
*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.18	2.95
Unmasked-calculated*	3.22	4.30	3.29

*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 3.22 differs from the reported value 2.9 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37565 and PDB model 8WIF. Per-residue inclusion information can be found in section 3 on page 8.

## 9.1 Map-model overlay (i)

X   Y   Z
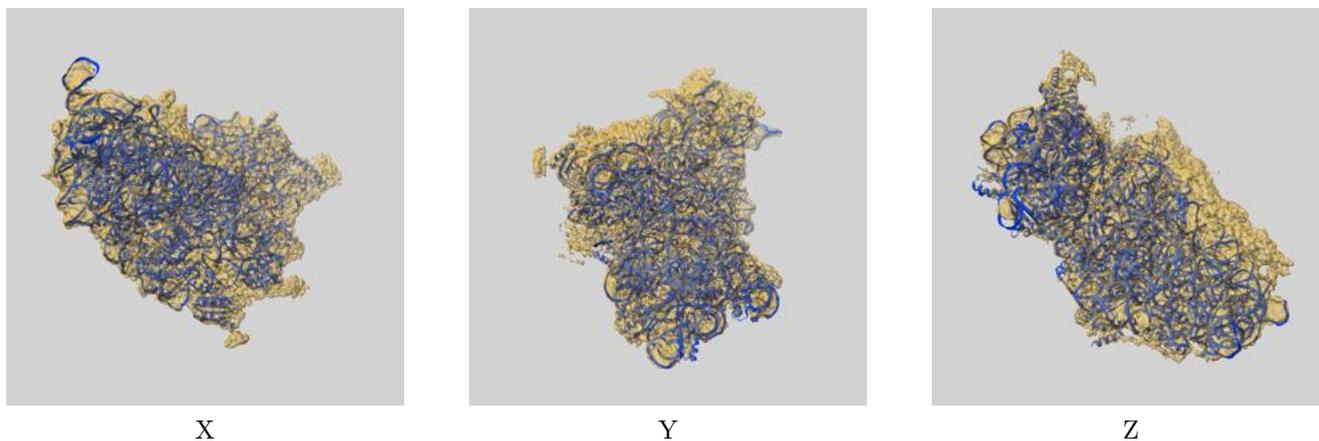
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ
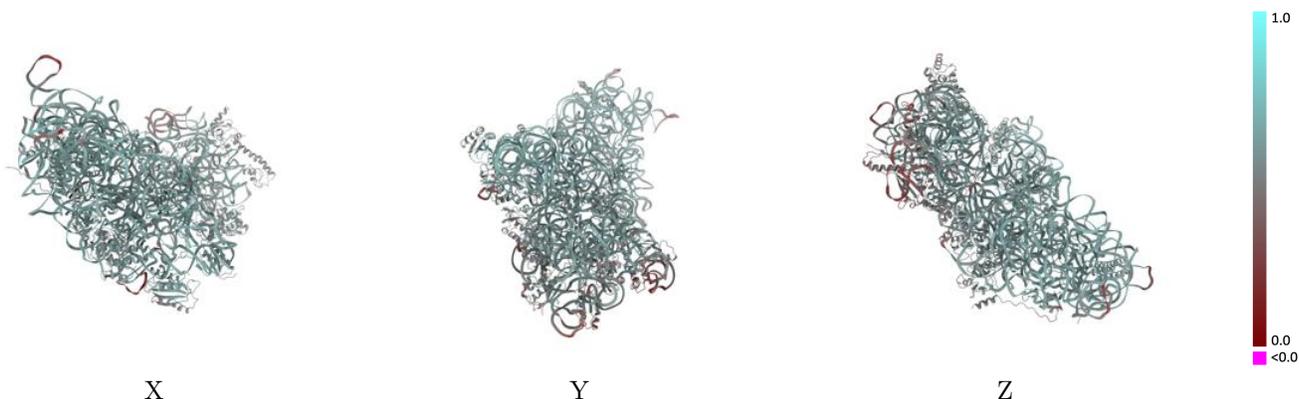

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
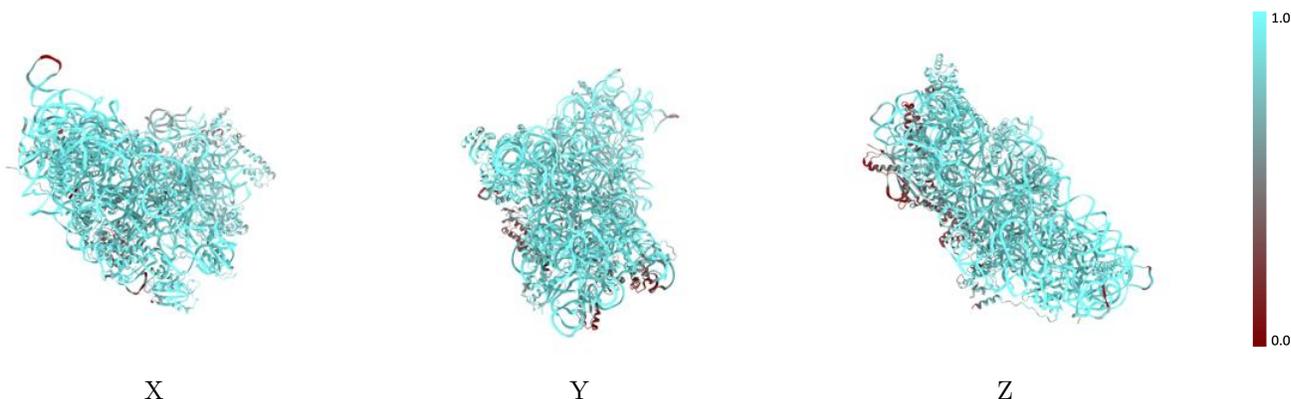
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion ⓘ
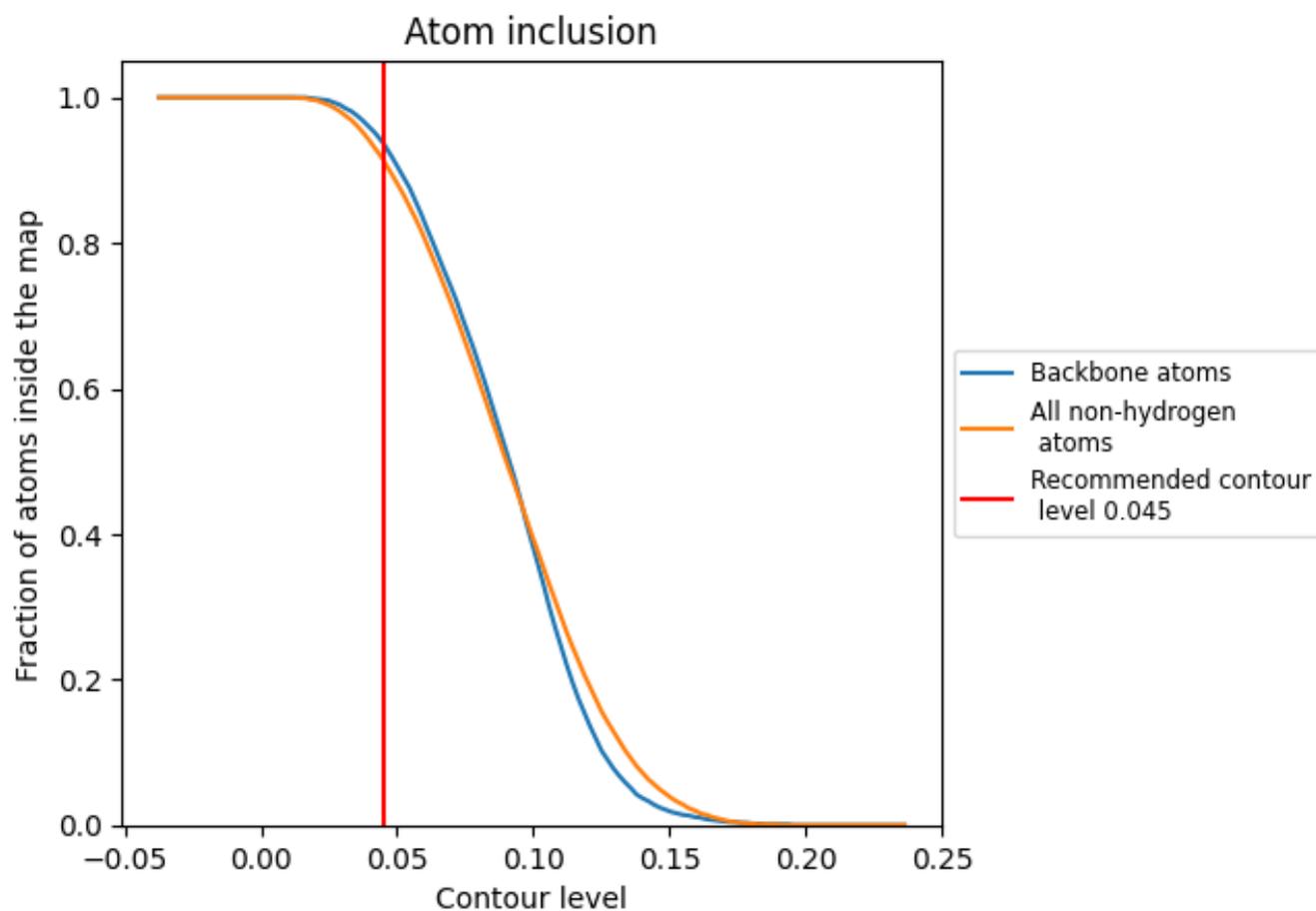
At the recommended contour level, 94% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.5640
a	0.9750	0.5780
c	0.2960	0.4670
d	0.7340	0.5040
e	0.8800	0.5530
f	0.7940	0.5600
g	0.8800	0.5530
h	0.8990	0.5370
i	0.9560	0.5860
j	0.8690	0.5190
k	0.6410	0.5020
l	0.9300	0.5670
m	0.9420	0.5900
n	0.8870	0.5210
o	0.6550	0.4790
p	0.9410	0.5760
q	0.8970	0.5670
r	0.9310	0.5850
s	0.9070	0.5490
t	0.8880	0.5410
u	0.9630	0.5810
v	0.9880	0.5840
w	0.9170	0.5640
x	0.5060	0.4720

1.0

0.0
<0.0