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wwPDB EM Validation Summary Report (i)

May 16, 2023 – 04:46 pm BST

PDB ID	:	8C83
EMDB ID	:	EMD-16470
Title	:	Cryo-EM structure of in vitro reconstituted Otu2-bound Ub-40S complex
Authors	:	Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2023-01-18
Resolution	:	3.00 Å(reported)

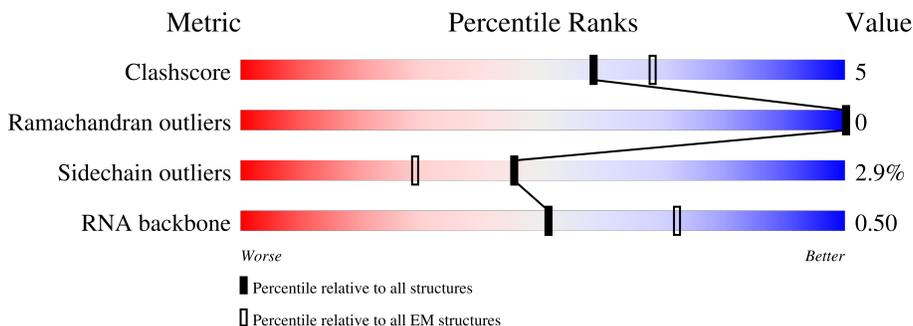The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev50
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)	:	2.32.2

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 3.00 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.
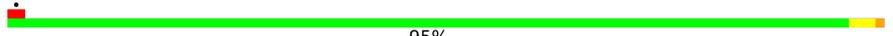
Metric	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.9%
RNA backbone		0.50

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	x	307	8% — 82% · 16%
2	y	76	61% — 100%
3	2	1800	· — 38% 22% 5% 35%
4	P	252	10% — 66% 15% · 18%
5	R	254	· — 65% 19% · 15%
6	S	261	82% 16% ··
7	T	236	79% 17% ·

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Mol	Chain	Length	Quality of chain
8	U	190	80% 16% · ·
9	V	200	74% 20% 6%
10	W	197	80% 13% · 7%
11	X	156	77% 14% 9%
12	Y	151	75% 24% ·
13	a	87	95% · ·
14	b	130	95% · · ·
15	c	145	98% · ·
16	d	135	95% · ·
17	f	82	96% · ·
18	g	63	6% 94% · 5%

2 Entry composition ⓘ

There are 18 unique types of molecules in this entry. The entry contains 45803 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 OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	259	Total 1509	C 917	N 298	O 292	S 2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	178	SER	CYS	engineered mutation	UNP P38747

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	y	76	Total 374	C 222	N 76	O 76	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	19	PRO	SER	conflict	UNP P05759
y	24	GLU	ASP	conflict	UNP P05759
y	28	ALA	SER	conflict	UNP P05759

- Molecule 3 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	1177	Total 25088	C 11220	N 4455	O 8236	P 1177	0	0

- Molecule 4 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	206	Total 1603	C 1030	N 284	O 287	S 2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	216	Total 1626	C 1042	N 287	O 295	S 2	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	258	Total 2056	C 1308	N 387	O 358	S 3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	228	Total 1815	C 1138	N 351	O 323	S 3	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	184	Total 1473	C 946	N 263	O 264	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	187	Total 1476	C 916	N 295	O 263	S 2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	184	Total 1479	C 935	N 285	O 258	S 1	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	142	Total 1142	C 733	N 217	O 189	S 3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	150	Total 1192	C 759	N 224	O 207	S 2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	87	Total 673	C 415	N 125	O 131	S 2	0	0

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	129	Total 1021	C 650	N 188	O 180	S 3	0	0

- Molecule 15 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	144	Total 1121	C 708	N 220	O 191	S 2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	134	Total 1073	C 676	N 208	O 189	0	0

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	f	81	Total 610	C 382	N 110	O 113	S 5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	g	60	Total 472	C 298	N 97	O 76	S 1	0	0

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: OTU domain-containing protein 2

- Molecule 2: Ubiquitin
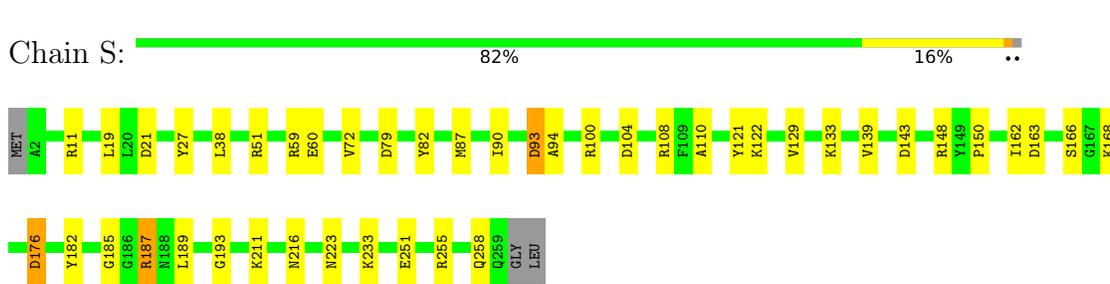

- Molecule 3: 18S ribosomal RNA

C1751 U1752 A1753 A1754 A1755 A1756 G1757 U1758 C1759 G1760 U1761 A1762 A1763 C1764 A1765 A1766 G1767 G1768 U1769 U1770 U1771 C1772 U1775 A1776 G1777 G1778 U1779 G1780 A1781 A1782 C1783 C1784 U1785 G1786 C1787 G1788 G1789 A1790 A1791 G1792 G1793 A1794 U1795 C1796 A1797 U1798 U1799 A

- Molecule 4: 40S ribosomal protein S0-A

Chain P:

10%

66%   15%   ·   18%

MET S2 L3 D8 L9 T10 D13 L16 L17 A20 N28 H32 V37 F38 N39 H46 T53 W54 E55 V58 D72 V73 S77 S78 R79 T80 F81 R84 A90 A91 G94 A95 T103 P104 G105 S106 E117 V123 D129 I133

K134 E135 V139 N140 I141 D148 L149 D150 S153 P161 N164 R165 H168 L172 L176 R183 L184 R185 L188 V189 D190 R191 P194 M198 P199 D200 F203 Y204 R205 D206 P207 GLU GLU VAL GLU GLN GLN VAL ALA GLU GLU ALA THR GLU GLU ALA

GLY GLU GLU GLU ALA LYS GLU VAL THR GLU GLU GLN ALA GLU ALA THR GLU TRP ALA GLU ASN ALA ASP ASN VAL GLU TRP

- Molecule 5: 40S ribosomal protein S2

Chain R:

65%   19%   ·   15%

MET SER ALA PRO GLU ALA GLN GLN GLN LYS ARG GLY GLY PHE GLY GLY ARG ASN ARG GLY ARG PRO ASN ARG ARG GLY PRO ARG ASN THR GLU GLU LYS G34 W35 V36 P37 V38 T39 K40 L41 G42 R43 L44 V45 K49 I53 F57 F66 Q67 I68 D78 K84 P85

Q89 T90 R91 Q94 R97 V101 N108 I115 K116 T117 A118 K119 E120 V121 I125 I139 R140 T146 K157 L169 L170 R174 A180 S181 P182 A183 V184 K185 K186 L187 L188 Q189 E194 D195 V196 Y197 T198 Q199 E208 I218 T221 Y243

S248 A249 GLN LYS LYS ARG PHE

- Molecule 6: 40S ribosomal protein S4-A

Chain S:

82%   16%   ··

MET A2 R11 L19 L20 D21 Y27 L38 R51 R59 E60 V72 D79 Y82 M87 I90 D93 A94 R100 D104 R108 F109 A110 Y121 K122 V129 K133 V139 D143 R148 Y149 P150 I162 D163 S166 G167 K168

D176 Y182 G185 G186 R187 N188 L189 G193 K211 N216 N223 K233 E251 R255 Q258 Q259 GLY LEU

- Molecule 7: 40S ribosomal protein S6-A

Chain T:

79%   17%   ·

M1 K2 Q13 I32 D37 E44 F45 K46 V49 D57 K58 Q59 M63 T71 R72 T78 K79 R87 R88 E91 R92 K93 R94 R98 L106 A107 V108 V114 K115 K116 G117 E118 Q119 R132 P135 N139 N140 I141 R160 T163 K164

G165 T168 Y169 T180 P181 Q182 R191 Q201 R202 K228 ARG ARG ALA SER SER LEU LYS ALA

• Molecule 8: 40S ribosomal protein S7-A

Chain U: 80%   16%   • •

MET SER ALA P4 S10 Q11 E15 L16 E17 V20 F24 V25 E28 N29 S30 S31 L38 I49 A57 F70 Q74 T75 K76 L77 T78 E82 D87 R88 R97 I98 V109 V121 H122 D123 L129 K138 Q150 D163 Y164 I181

S187 GLU THR HIS

• Molecule 9: 40S ribosomal protein S8-B

Chain V: 74%   20%   6%

MET G2 I3 S4 R5 A16 K17 R18 A19 Q20 F21 R22 R25 G30 R31 K37 H44 R56 A57 L58 R59 A79 H84 L90 T95 L96 T97 D105 A106 K123 LYS LYS ASN VAL LYS GLU GLU GLU THR VAL ALA K135 N138 R141 E153

V156 F160 R164 L165 S170 Q175 S176 G177 R178 G181 Y182 I183 L184 L189 L193 L196 T197 A198 K199 LYS

• Molecule 10: 40S ribosomal protein S9-A

Chain W: 80%   13%   •   7%

MET P2 S21 D25 L28 F34 N38 K39 K40 R44 L49 R53 D58 L59 D63 D66 R69 L76 L86 D89 V96 L99 F104 R108 L109 Q110 Q139 S145 R168 V172 R175 G185 GLU ALA ALA

ASP GLU ALA ASP GLU ALA ASP GLU GLU

• Molecule 11: 40S ribosomal protein S11-A

Chain X: 77%   14%   9%

MET SER THR E4 L5 T6 V7 Q8 P17 N22 V25 K26 T27 S28 K29 K43 D55 L63 R67 G73 T78 K79 I84 V85 I86 I94 P95 V125 R129 V139 A145 ALA GLY LYS ALA ASN LYS GLN PHE ALA LYS PHE

• Molecule 12: 40S ribosomal protein S13

Chain Y: 75%   24%   •

MET G2 R3 M4 K27 E31 S32 V33 I34 E35 Q36 I37 V38 Q49 I50 G51 V52 L53 L54 R55 T61 Q62 I71 M72 R73 I74 L75 K76 D87 Y90 L91 I92 K93 R99 L102 E103 R106 K107 D108 K109 E119 S120 R121 T145 L149 V150 N151

• Molecule 13: 40S ribosomal protein S21-A

Chain a:

95%

M1 K5 L11 E42 G43 D66 N81 R87

• Molecule 14: 40S ribosomal protein S22-A

Chain b:

95%

MET I2 K88 L93 L104 S107 M111 D112 Y130

• Molecule 15: 40S ribosomal protein S23-A

Chain c:

98%

MET G2 E60 N79 S145

• Molecule 16: 40S ribosomal protein S24-A

Chain d:

95%

MET S2 R8 D38 E51 K52 D53 Q63 Y94 A134 D135

• Molecule 17: 40S ribosomal protein S27-A

Chain f:

96%

MET V2 L24 L63 K82

• Molecule 18: 40S ribosomal protein S30-A

6%

Chain g:

94%   5%

MET A2 K3 E22 T48 K53 S61 VAL GLN

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31646	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 $(e^-/\text{Å}^2)$	46.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	x	0.29	0/1514	0.58	4/2075 (0.2%)
2	y	0.24	0/373	0.48	0/517
3	2	0.45	0/28062	1.06	142/43713 (0.3%)
4	P	0.31	0/1644	0.75	5/2249 (0.2%)
5	R	0.39	0/1656	0.82	3/2251 (0.1%)
6	S	0.34	0/2097	0.75	4/2823 (0.1%)
7	T	0.30	0/1839	0.61	0/2460
8	U	0.31	0/1498	0.66	2/2019 (0.1%)
9	V	0.32	0/1501	0.78	3/2006 (0.1%)
10	W	0.33	0/1504	0.71	2/2016 (0.1%)
11	X	0.35	0/1168	0.71	2/1575 (0.1%)
12	Y	0.36	0/1215	0.71	1/1638 (0.1%)
13	a	0.39	0/682	0.87	2/921 (0.2%)
14	b	0.36	0/1038	0.72	3/1395 (0.2%)
15	c	0.34	0/1139	0.67	0/1518
16	d	0.38	0/1087	0.81	2/1449 (0.1%)
17	f	0.31	0/620	0.71	1/838 (0.1%)
18	g	0.37	0/480	0.73	0/639
All	All	0.40	0/49117	0.94	176/72102 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P	0	1

There are no bond length outliers.

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	V	105	ASP	CB-CG-OD1	11.16	128.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	85	PRO	CA-N-CD	-10.94	96.19	111.50
9	V	193	LEU	CA-CB-CG	10.56	139.60	115.30
6	S	93	ASP	CB-CG-OD2	9.66	126.99	118.30
3	2	653	C	N1-C2-O2	9.58	124.65	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	P	94	GLY	Peptide

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	x	1509	0	997	0	0
2	y	374	0	163	0	0
3	2	25088	0	12624	138	0
4	P	1603	0	1610	18	0
5	R	1626	0	1715	30	0
6	S	2056	0	2140	23	0
7	T	1815	0	1894	29	0
8	U	1473	0	1555	18	0
9	V	1476	0	1501	25	0
10	W	1479	0	1556	14	0
11	X	1142	0	1209	12	0
12	Y	1192	0	1255	26	0
13	a	673	0	662	0	0
14	b	1021	0	1060	0	0
15	c	1121	0	1196	0	0
16	d	1073	0	1132	0	0
17	f	610	0	633	0	0
18	g	472	0	521	0	0
All	All	45803	0	33423	291	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 5.

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The worst 5 of 291 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)
3:2:1697:G:H1	3:2:1704:U:H3	1.08	0.90
3:2:1688:U:H3	3:2:1713:G:H1	1.28	0.81
3:2:699:U:H3	3:2:739:G:H1	1.26	0.81
3:2:480:G:H1	3:2:508:U:H3	1.40	0.68
8:U:70:PHE:O	8:U:74:GLN:HB2	1.94	0.67

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	x	253/307 (82%)	249 (98%)	4 (2%)	0	100	100
2	y	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
4	P	204/252 (81%)	182 (89%)	22 (11%)	0	100	100
5	R	214/254 (84%)	201 (94%)	13 (6%)	0	100	100
6	S	256/261 (98%)	238 (93%)	18 (7%)	0	100	100
7	T	226/236 (96%)	214 (95%)	12 (5%)	0	100	100
8	U	182/190 (96%)	173 (95%)	9 (5%)	0	100	100
9	V	183/200 (92%)	172 (94%)	11 (6%)	0	100	100
10	W	182/197 (92%)	172 (94%)	10 (6%)	0	100	100
11	X	140/156 (90%)	131 (94%)	9 (6%)	0	100	100
12	Y	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
13	a	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
14	b	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
15	c	142/145 (98%)	131 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	d	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
17	f	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
18	g	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
All	All	2685/2922 (92%)	2521 (94%)	164 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	62/282 (22%)	58 (94%)	4 (6%)	17	50
4	P	170/210 (81%)	167 (98%)	3 (2%)	59	85
5	R	175/205 (85%)	171 (98%)	4 (2%)	50	80
6	S	220/222 (99%)	211 (96%)	9 (4%)	30	67
7	T	189/201 (94%)	185 (98%)	4 (2%)	53	82
8	U	163/170 (96%)	157 (96%)	6 (4%)	34	70
9	V	148/161 (92%)	144 (97%)	4 (3%)	44	77
10	W	156/166 (94%)	152 (97%)	4 (3%)	46	78
11	X	126/137 (92%)	125 (99%)	1 (1%)	81	93
12	Y	127/128 (99%)	124 (98%)	3 (2%)	49	79
13	a	71/74 (96%)	68 (96%)	3 (4%)	30	66
14	b	110/111 (99%)	105 (96%)	5 (4%)	27	64
15	c	119/120 (99%)	117 (98%)	2 (2%)	60	85
16	d	112/113 (99%)	107 (96%)	5 (4%)	27	64
17	f	70/71 (99%)	69 (99%)	1 (1%)	67	88
18	g	50/54 (93%)	49 (98%)	1 (2%)	55	83
All	All	2068/2425 (85%)	2009 (97%)	59 (3%)	45	76

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	123	ASP
16	d	63	GLN
10	W	89	ASP
16	d	53	ASP
14	b	111	MET

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

Mol	Chain	Res	Type
10	W	139	GLN
13	a	7	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	1170/1800 (65%)	319 (27%)	26 (2%)

5 of 319 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	2	A
3	2	4	C
3	2	25	C
3	2	26	A
3	2	34	G

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	555	A
3	2	640	U
3	2	1742	U
3	2	639	U
3	2	705	U

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-16470. 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 ⓘ
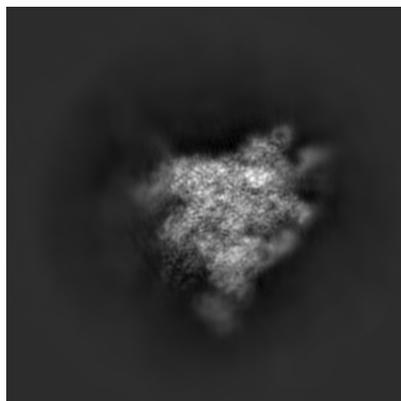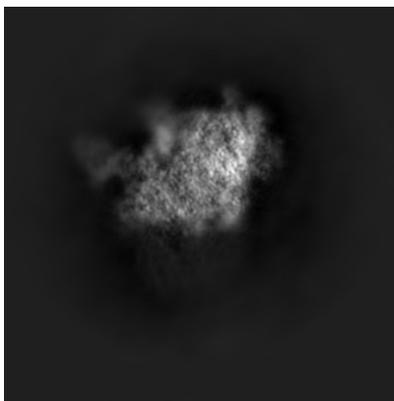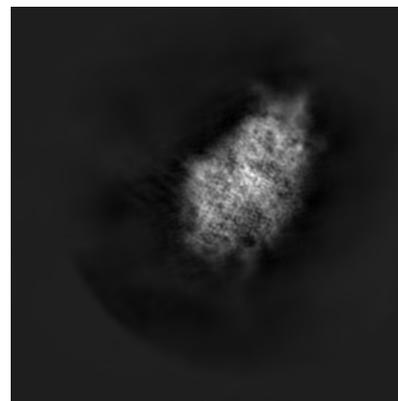
6.1.1   Primary map

| X | Y | Z |

6.1.2   Raw map

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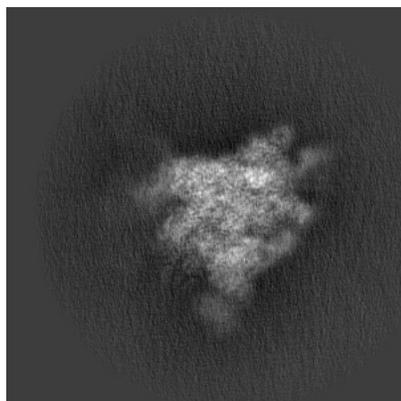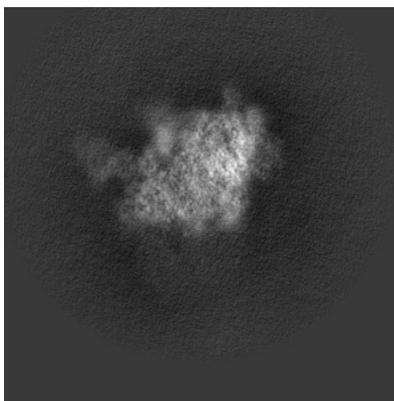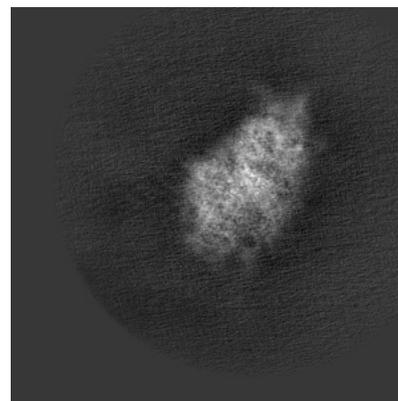
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
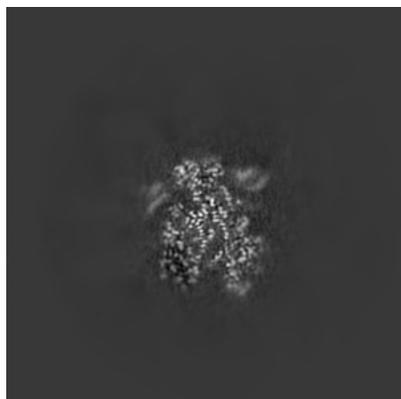
6.2.1   Primary map
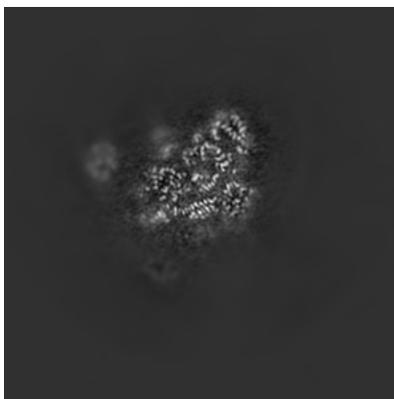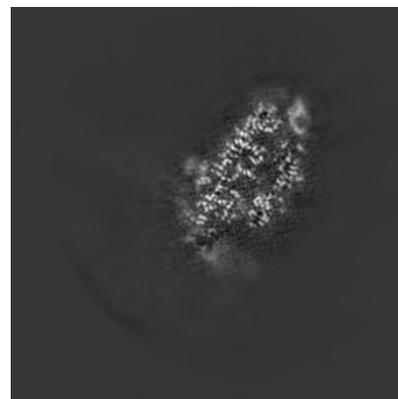
X Index: 180   Y Index: 180   Z Index: 180

6.2.2   Raw map
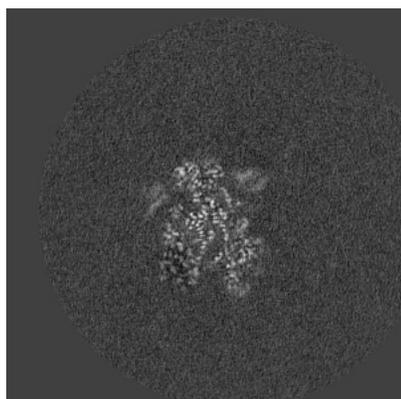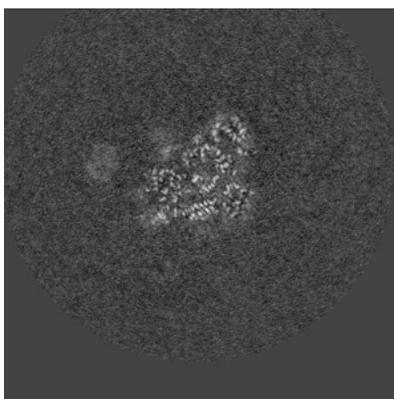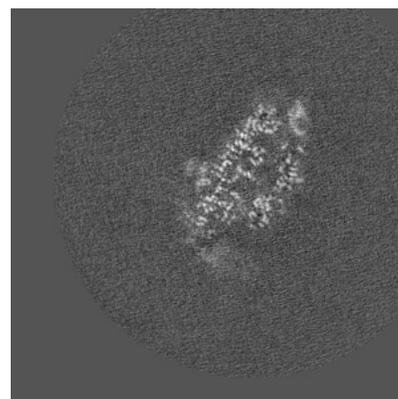
X Index: 180   Y Index: 180   Z Index: 180

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
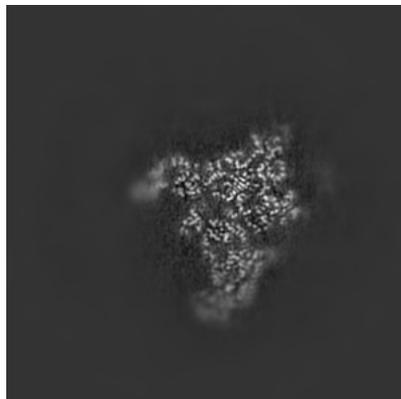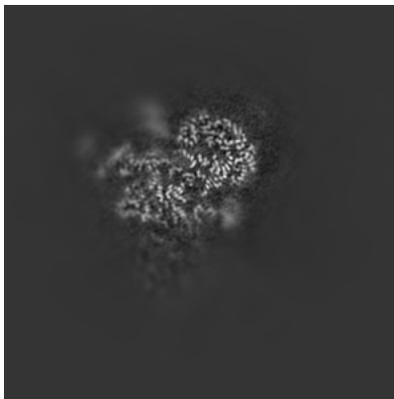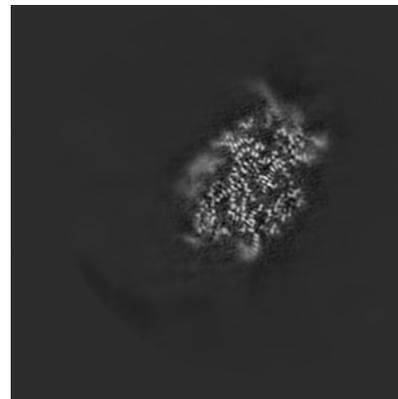
X Index: 213   Y Index: 207   Z Index: 207

6.3.2 Raw map
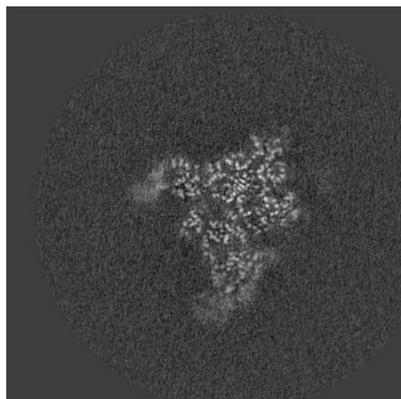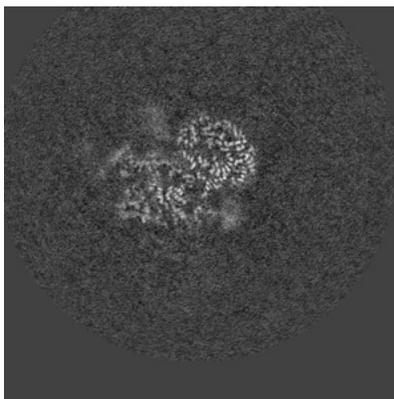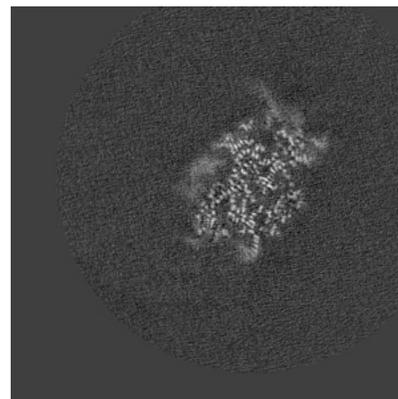
X Index: 213   Y Index: 207   Z Index: 207

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
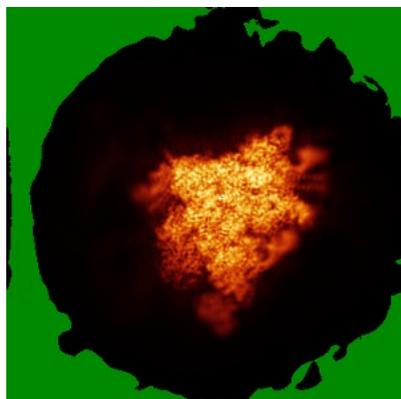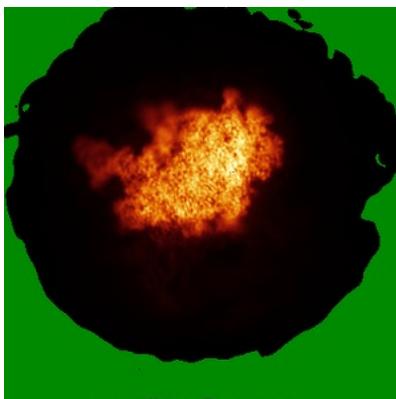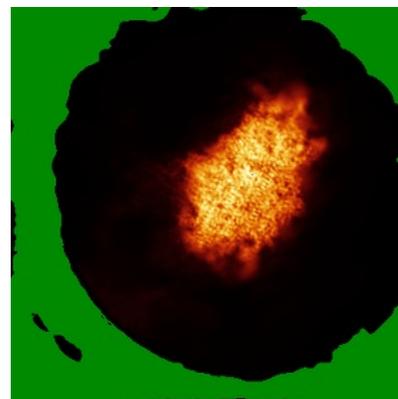
| X | Y | Z |

6.4.2 Raw map

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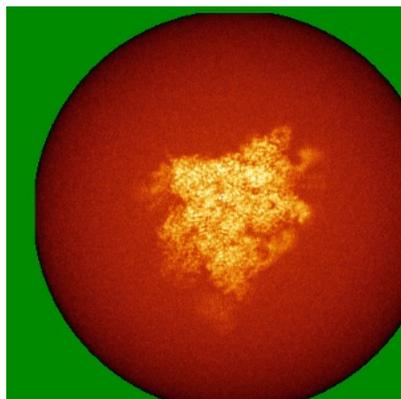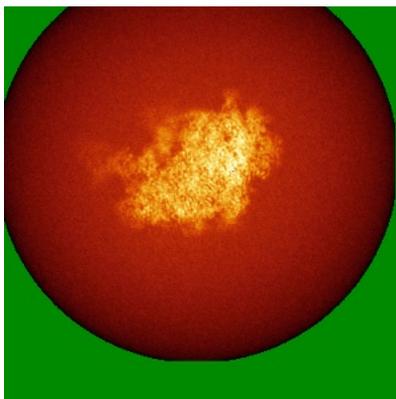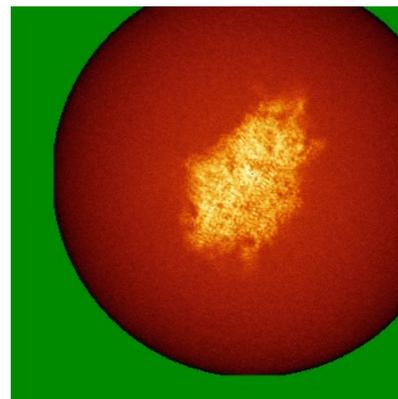
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
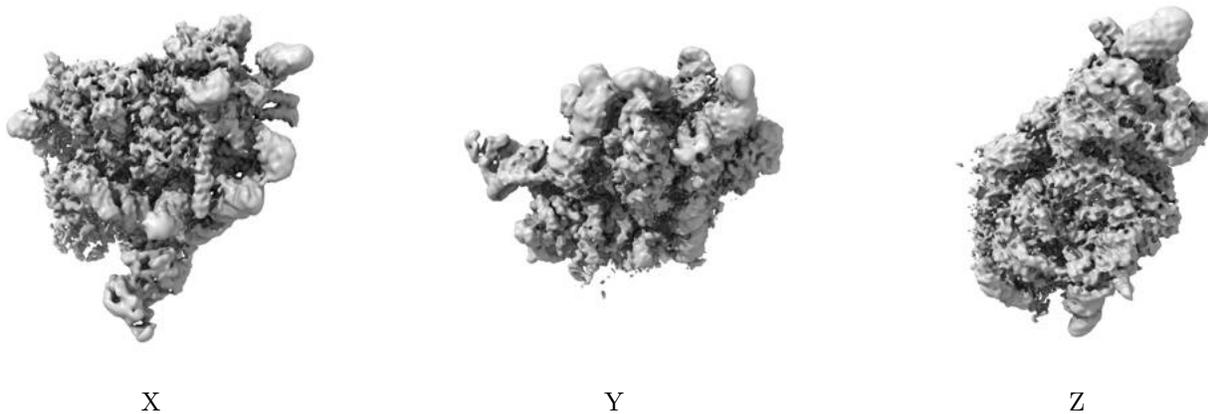
The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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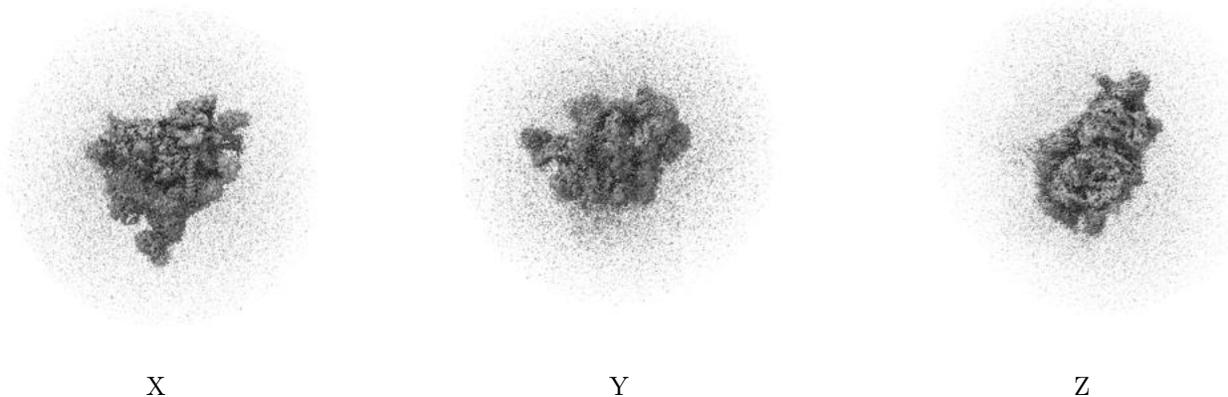
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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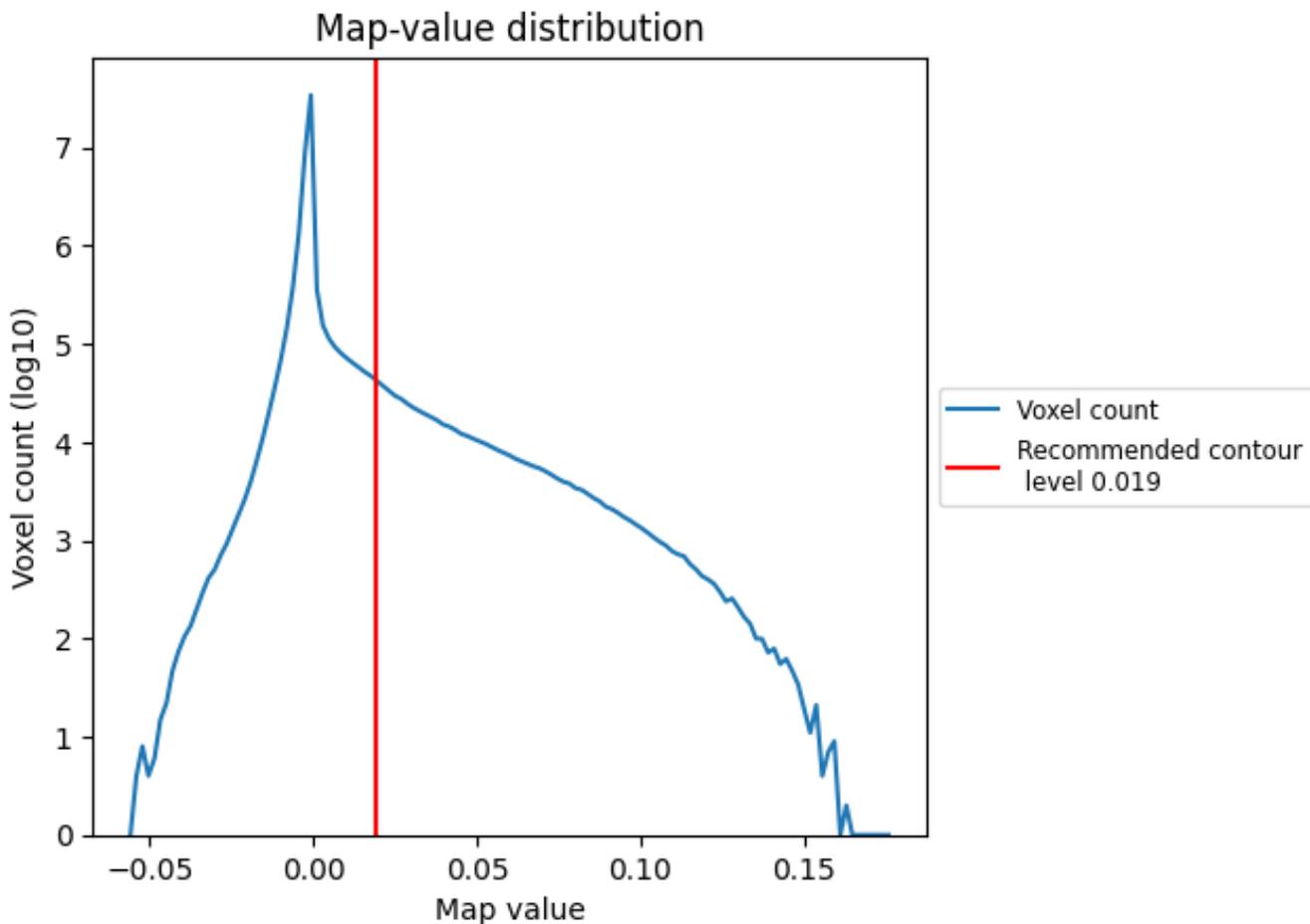
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
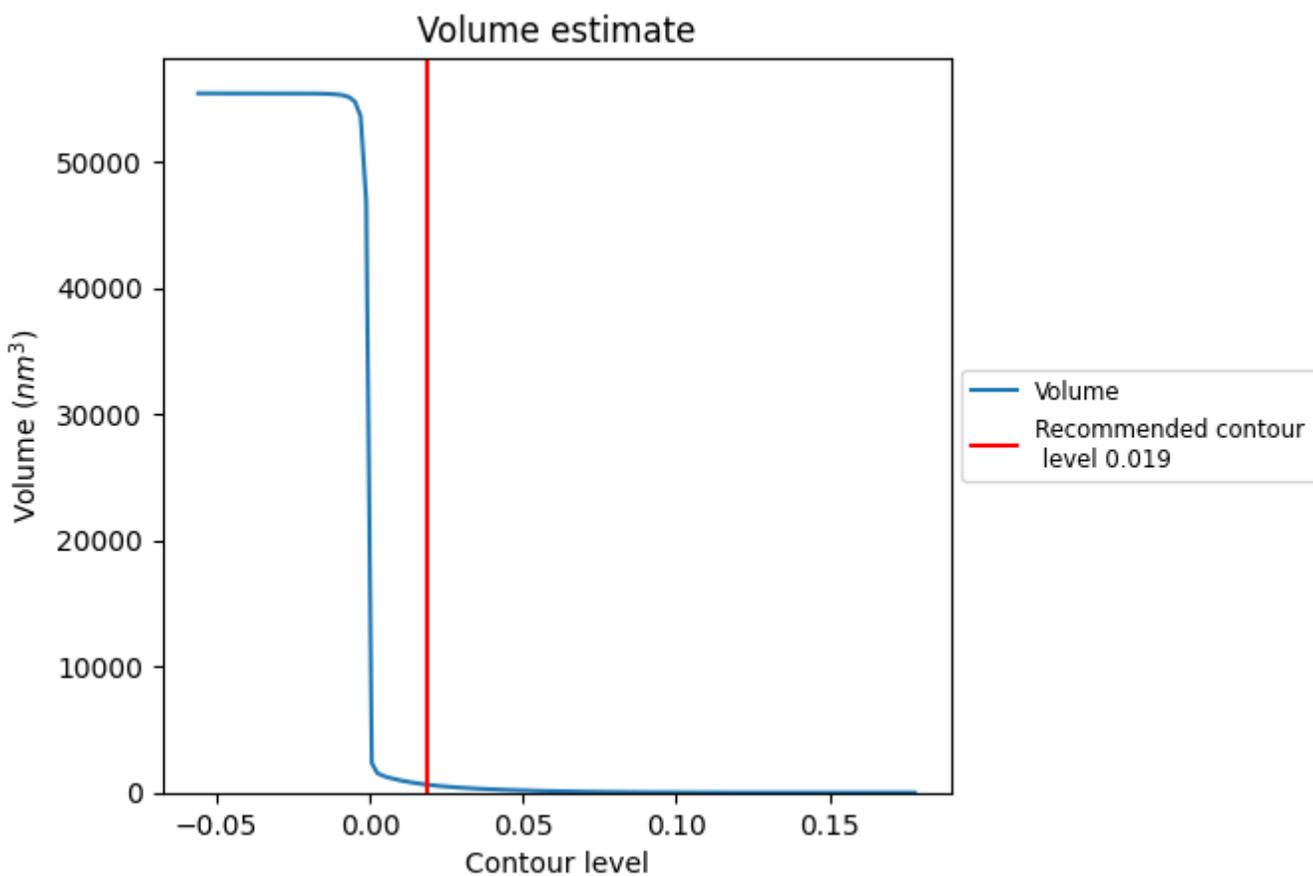
The volume at the recommended contour level is 624 nm^3; this corresponds to an approximate mass of 564 kDa.

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 ⓘ
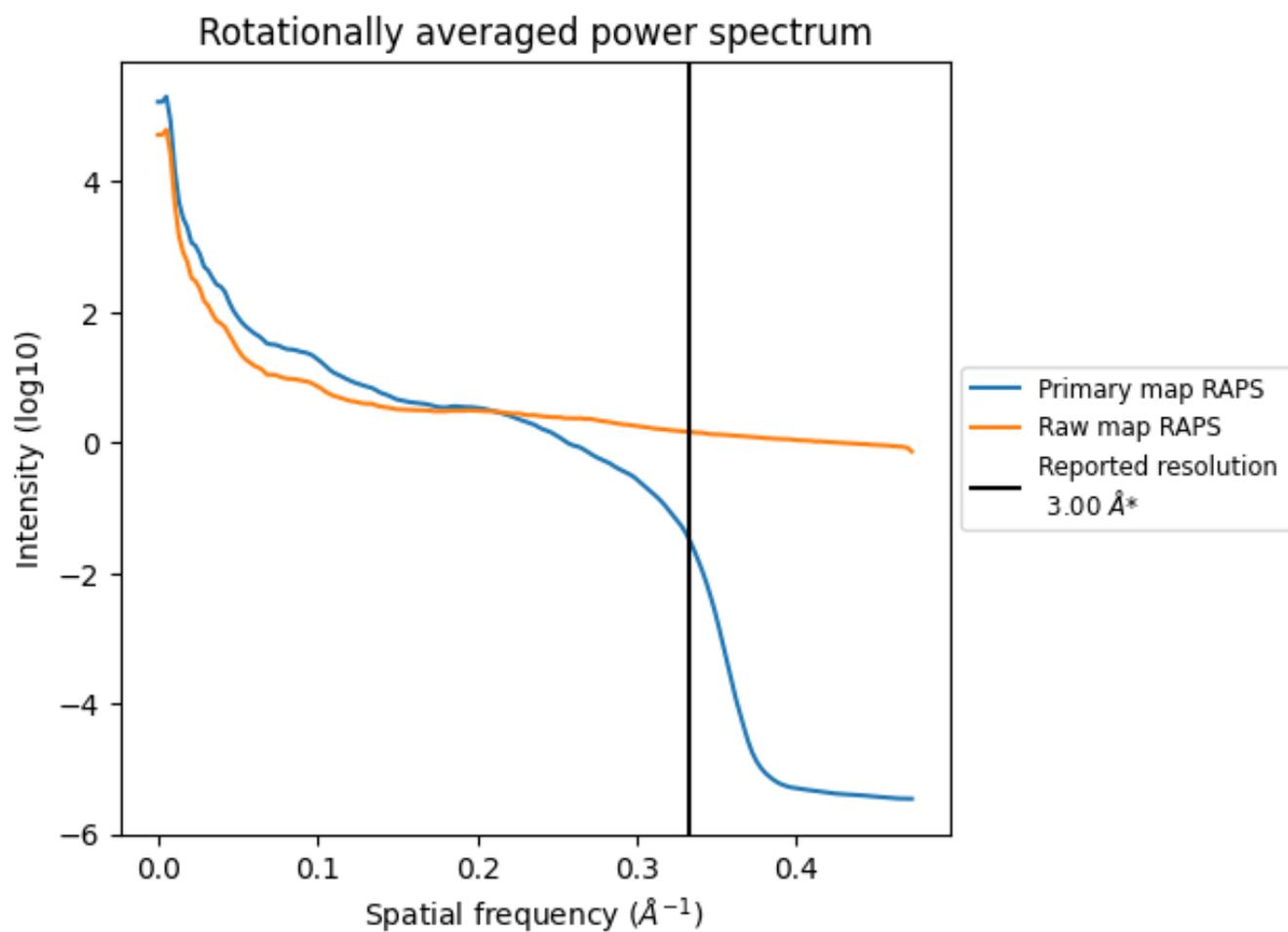
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 ⓘ
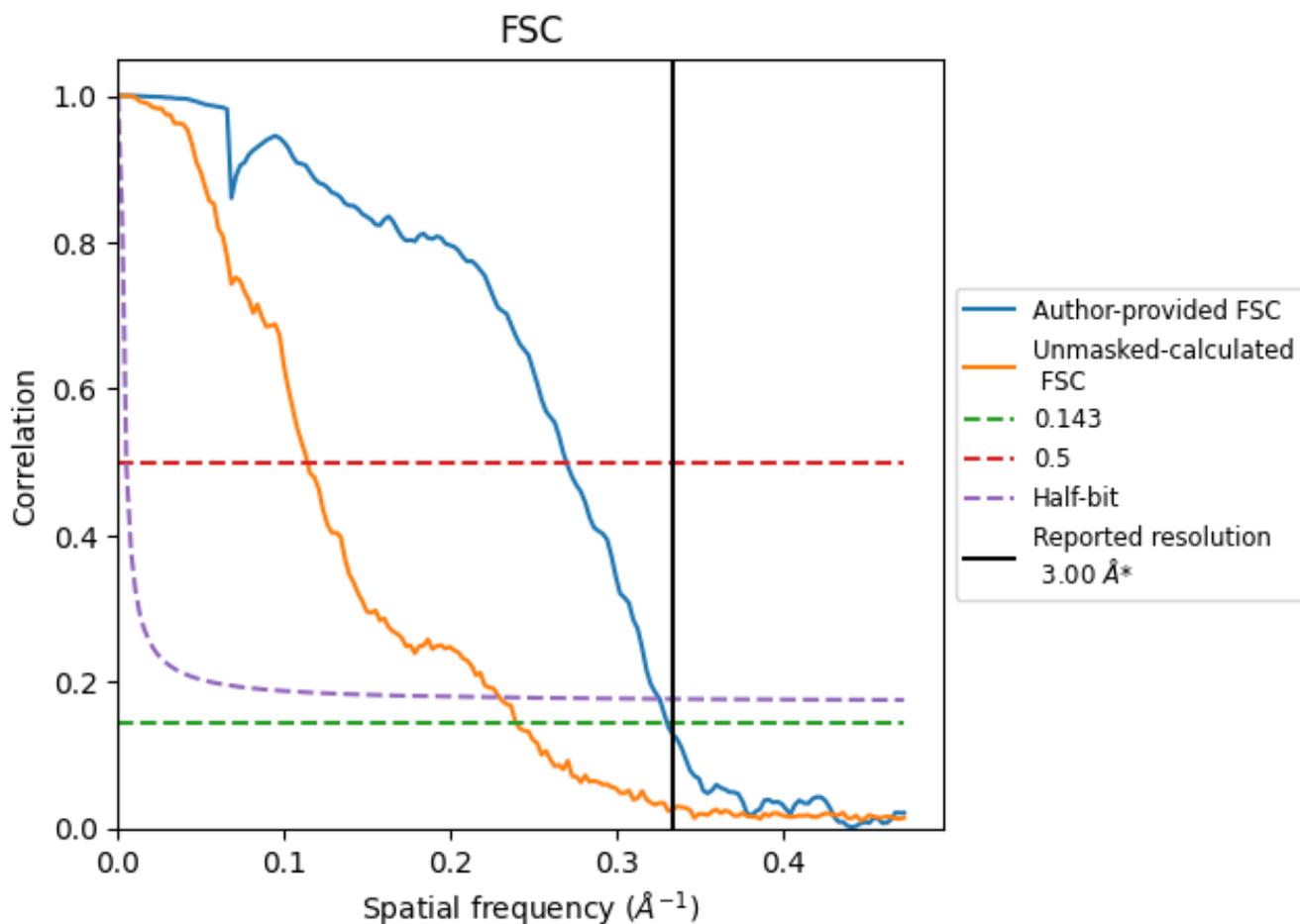
*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.71	3.07
Unmasked-calculated*	4.18	8.80	4.36

*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 4.18 differs from the reported value 3.0 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-16470 and PDB model 8C83. Per-residue inclusion information can be found in section 3 on page 7.

## 9.1   Map-model overlay ⓘ

| X | Y | Z |
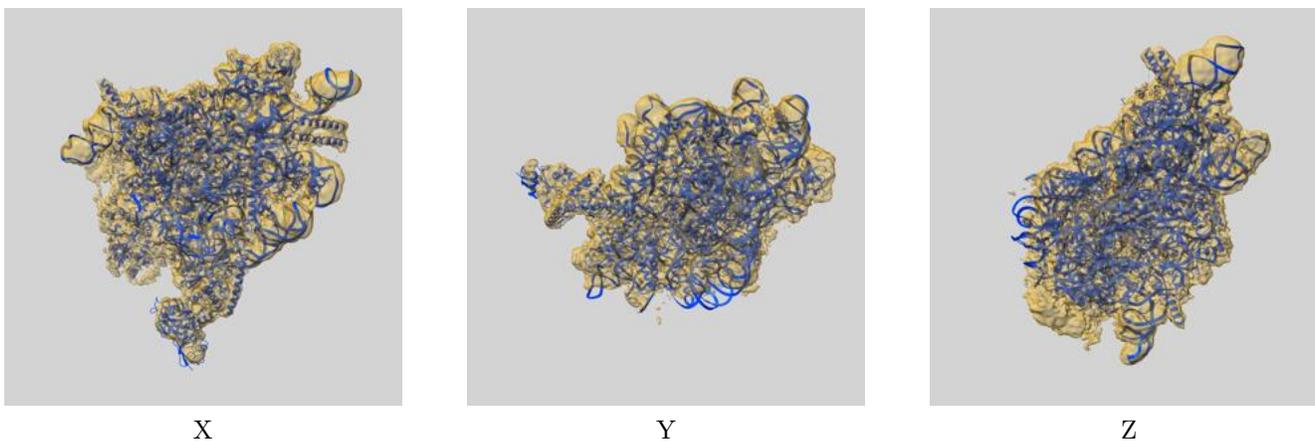
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2　Q-score mapped to coordinate model ⓘ

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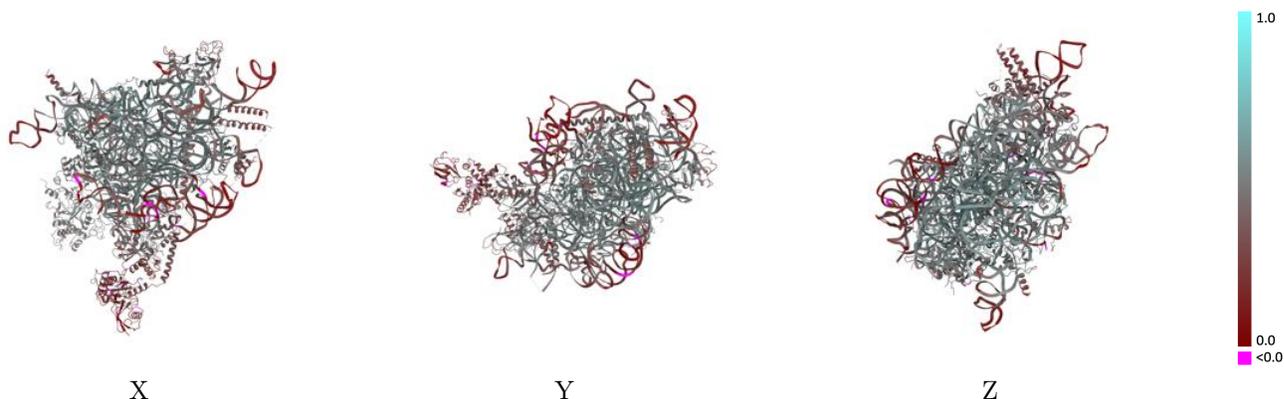
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X　　　　　　　　　　　Y　　　　　　　　　　　Z
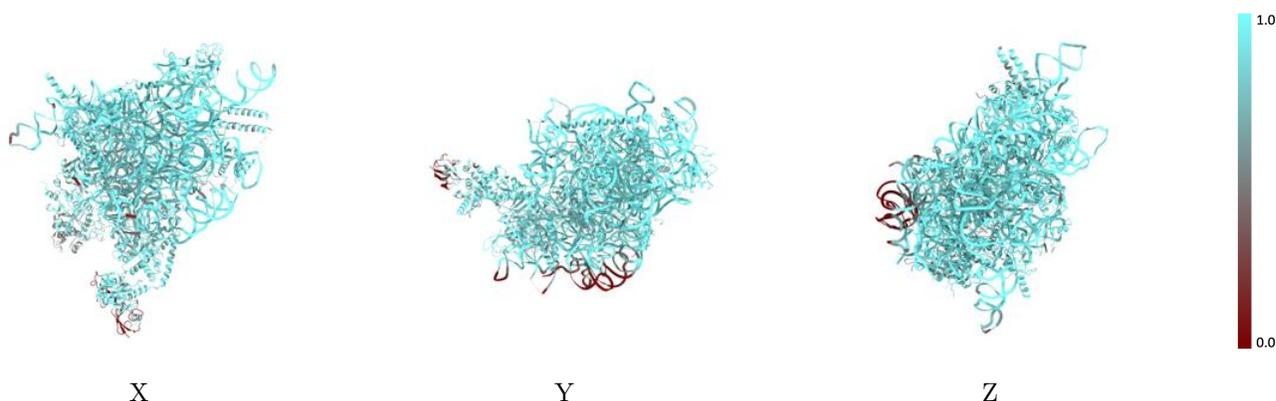
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4　Atom inclusion ⓘ
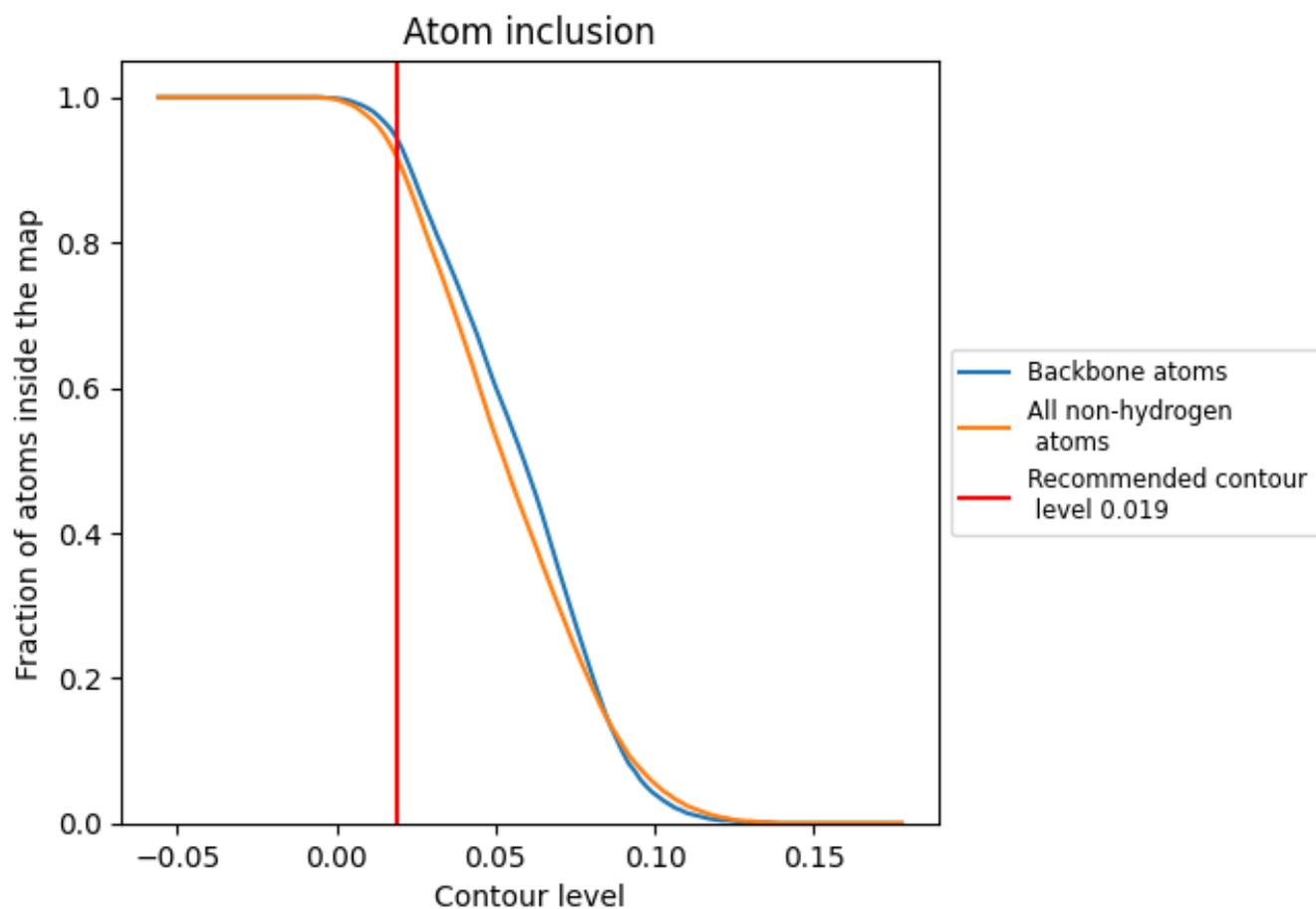
At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9180	0.4410
2	0.9220	0.4290
P	0.7100	0.4460
R	0.9300	0.4900
S	0.9690	0.5140
T	0.9600	0.4410
U	0.9310	0.3960
V	0.9750	0.4910
W	0.9570	0.4980
X	0.9520	0.5270
Y	0.9130	0.4180
a	0.9110	0.4770
b	0.9740	0.5300
c	0.9800	0.5270
d	0.9460	0.4810
f	0.9700	0.4580
g	0.9190	0.4420
x	0.8130	0.2800
y	0.3960	0.1370

1.0

0.0
<0.0