WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 04:49 PM EST

|		
PDB ID	:	6O7K
EMDB ID	:	EMD-0643
Title	:	30S initiation complex
Authors	:	Frank, J.; Gonzalez Jr., R.L.; kaledhonkar, S.; Fu, Z.; Caban, K.; Li, W.; Chen, B.; Sun, M.
Deposited on	:	2019-03-08
Resolution	:	4.20 Å(reported)
Based on initial model	:	2AVY

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 4.20 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.
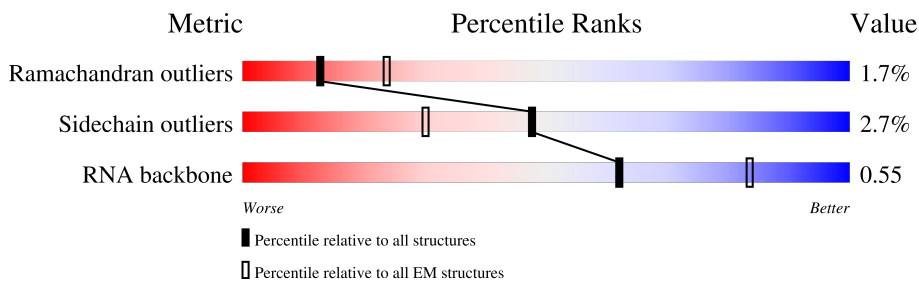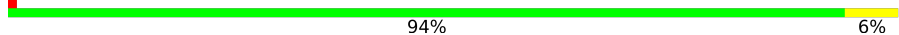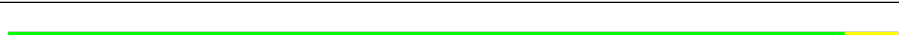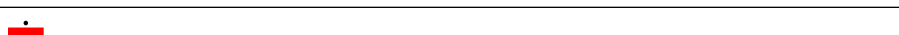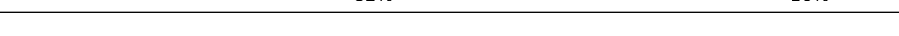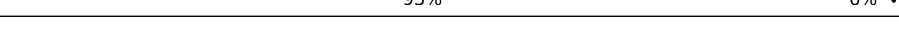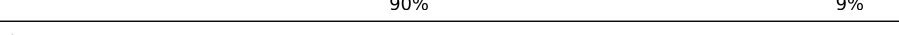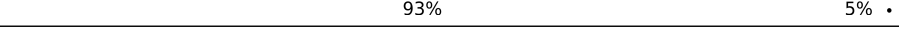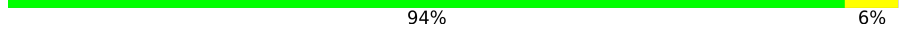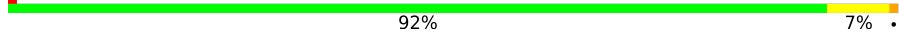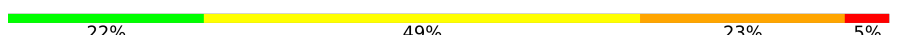

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	5	71	90% 10%
2	f	509	91% 8%
3	g	1539	44% 47% 9%
4	P	80	92% 6%
5	r	98	88% 11%
6	q	117	91% 9%
7	t	123	90% 7%
8	s	114	89% 11%

Continued on next page...

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Mol	Chain	Length	Quality of chain
9	w	100	85% 11%
10	u	88	94% 6%
11	y	82	91% 9%
12	1	55	87% 9%
13	z	79	92% 8%
14	j	218	95%
15	3	85	94% 6%
16	2	51	82% 16%
17	h	206	93% 6%
18	l	205	90% 9%
19	k	150	93% 5%
20	n	100	92% 8%
21	m	151	94% 6%
22	p	129	92% 7%
23	o	127	83% 14%
24	v	77	22% 49% 23% 5%
25	N	6	17% 50% 33%

2 Entry composition ⓘ

There are 25 unique types of molecules in this entry. The entry contains 57748 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 Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	5	71	570	362	103	103	2	0	0

- Molecule 2 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	f	509	3847	2409	675	748	15	0	0

- Molecule 3 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	g	1539	33012	14725	6052	10697	1538	0	0

- Molecule 4 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	80	649	411	121	114	3	0	0

- Molecule 5 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	r	98	787	493	150	143	1	0	0

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	q	117	877	540	174	160	3	0	0

- Molecule 7 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	t	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 8 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	s	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 9 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	w	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 10 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	u	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 11 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	y	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 12 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	1	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 13 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	z	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 14 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	j	218	Total 1705	C 1081	N 305	O 312	S 7	0	0

- Molecule 15 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	85	Total 665	C 411	N 137	O 114	S 3	0	0

- Molecule 16 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	51	Total 426	C 265	N 86	O 74	S 1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	206	Total 1625	C 1028	N 305	O 289	S 3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	205	Total 1643	C 1026	N 315	O 298	S 4	0	0

- Molecule 19 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	k	150	Total 1106	C 687	N 211	O 202	S 6	0	0

- Molecule 20 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	n	100	Total 818	C 515	N 148	O 149	S 6	0	0

- Molecule 21 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 22 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	p	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 23 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	o	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 24 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	77	Total	C	N	O	P	0	0
			1639	732	297	534	76		

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	6	Total	C	N	O	P	0	0
			126	58	24	39	5		

3 Residue-property plots ⓘ
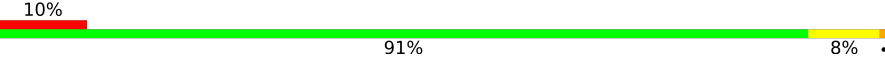
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Translation initiation factor IF-1

Chain 5:

- Molecule 2: Translation initiation factor IF-2

Chain f:
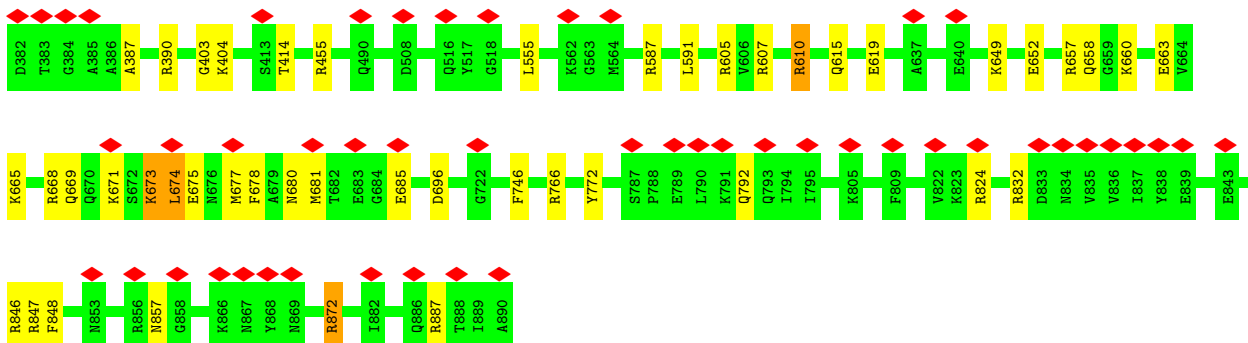
- Molecule 3: 16S ribosomal RNA

Chain g:

G1438 A1441 G1442 C1443 U1444 U1445 A1446 A1447 C1448 C1449 G1453 G1457 C1460 G1461 C1462 U1463 U1464 A1465 C1466 C1467 A1468 C1469 U1470 U1471 U1472 G1473 U1474 U1477 U1478 C1479 A1480 U1481 G1482 A1483 C1484 U1485 U1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497 C1501 A1502 A1503 G1504 G1505 U1506 C1509

C1510 G1516 G1517 A1518 A1519 C1520 C1521 C1524 G1529 G1530 A1531 U1532 C1533 A1534 C1535 C1536 U1537 C1538 C1539 U1540

- Molecule 4: 30S ribosomal protein S17

Chain P:　　　　　　　　　　　　　　92%　　　　　　　　　　　6%

K3 I4 R5 F27 H30 R39 N49 S67 V82
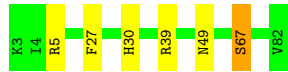
- Molecule 5: 30S ribosomal protein S10

Chain r:　　　　　　　　　　　　　　88%　　　　　　　　　　　11%

R5 I6 R9 V36 R37 R45 V57 N58 K59 D60 A61 R62 R72 D75 R89 L102
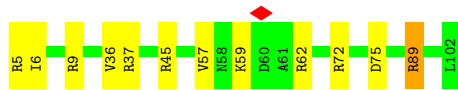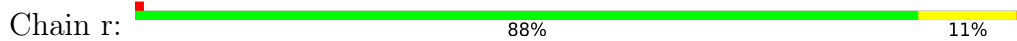
- Molecule 6: 30S ribosomal protein S11

Chain q:　　　　　　　　　　　　　　91%　　　　　　　　　　　9%

R12 K13 Q14 H21 R36 R52 P88 R97 C120 R121 R126 R127 V128
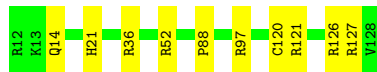
- Molecule 7: 30S ribosomal protein S12

Chain t:　　　　　　　　　　　　　　90%　　　　　　　　　　　7%

A1 R8 R11 A12 R13 E24 A25 R30 C33 T34 R35 A47 R53 R98 L101 R109 R113 A123
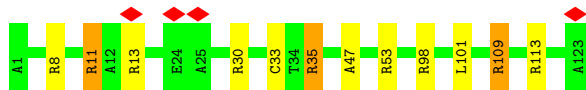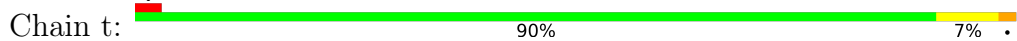
- Molecule 8: 30S ribosomal protein S13

Chain s:　　　　　　　　　　　　　　89%　　　　　　　　　　　11%

A1 R2 P9 V24 R56 E65 R69 R70 L82 R86 R89 R97 R100 R112 K113 P114
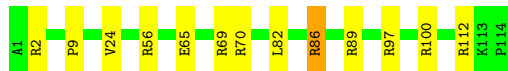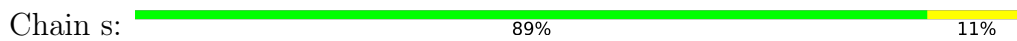
- Molecule 9: 30S ribosomal protein S14

Chain w:　　　　　　　　　　　　　　85%　　　　　　　　　　　11%

A1 R8 R12 F20 A35 SER ASP GLU GLU R41 R53 R59 Q60 R61 N62 R63 R69 R75 R90 W101
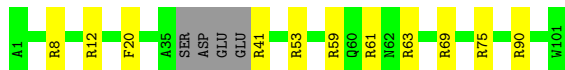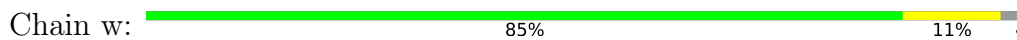
• Molecule 10: 30S ribosomal protein S15

Chain u:

94%   6%

S1 R16 N19 R63 R71 R76 R88

• Molecule 11: 30S ribosomal protein S16

Chain y:

91%   9%

M1 R31 R35 A43 E47 R56 R70 N79 K80 A81 A82

• Molecule 12: 30S ribosomal protein S18

Chain 1:

87%   9%

E19 R42 R47 Y50 Q51 R52 R56 R60 R72 H73

• Molecule 13: 30S ribosomal protein S19

Chain z:

92%   8%

R2 S3 L4 R36 R54 E64 R77 R80

• Molecule 14: 30S ribosomal protein S2

Chain j:

95%

M8 Q18 T19 R20 Y21 W22 F31 M48 L67 Q88 R94 F125 R136 T137 R138 G148 D152 S225

• Molecule 15: 30S ribosomal protein S20

Chain 3:

94%   6%

N2 R17 R24 R28 R59 R73 A86

• Molecule 16: 30S ribosomal protein S21

Chain 2:

82%   16%

• Molecule 17: 30S ribosomal protein S3

Chain h:
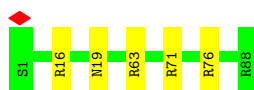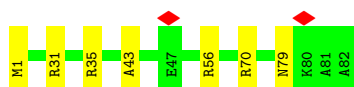

• Molecule 18: 30S ribosomal protein S4

Chain l:

• Molecule 19: 30S ribosomal protein S5

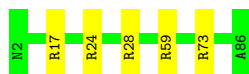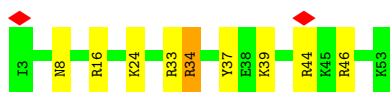Chain k:

• Molecule 20: 30S ribosomal protein S6
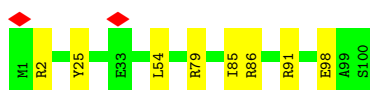
Chain n:

• Molecule 21: 30S ribosomal protein S7
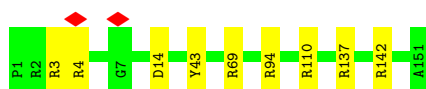
Chain m:

• Molecule 22: 30S ribosomal protein S8
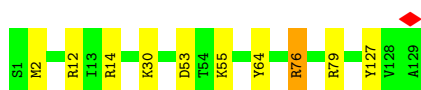
Chain p:

• Molecule 23: 30S ribosomal protein S9

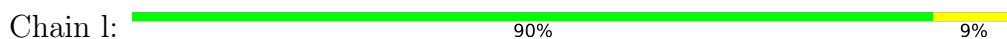Chain o:

83% 14%

N3 Y6 R10 R11 R17 K26 R40 E41 R44 D55 M56 V57 M87 D90 R94 R98 F102 R105 R108 R118 R121 R122 R123 R129
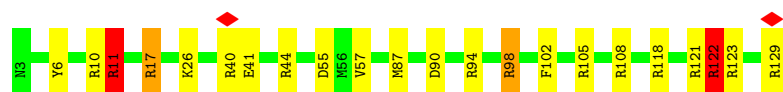
• Molecule 24: tRNA

Chain v:

22% 49% 23% 5%

C1 G2 C3 G4 G5 G6 G7 U8 G9 G10 A14 G15 C16 C17 U18 G19 G20 U21 A22 G23 C24 U25 C26 C29 G30 G31 G32 C33 U34 C35 A36 U37 C40 C41 C42 G43 A47 U48 C49 G50 U51 C52 G53 G54 U55 U56 C57 A58 A59 A60 U61 C62 C63 G64 G65 C66

C67 C68 C69 C70 G71 C72 A73 A74 C75 C76 A77
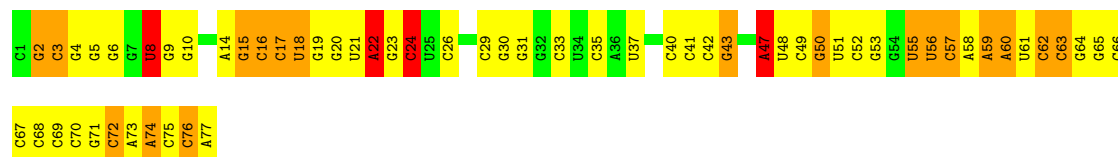
• Molecule 25: mRNA

Chain N:

17% 50% 33%

A13 A14 U15 A16 U17 G18

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86367	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	5	0.70	0/580	1.14	5/782 (0.6%)
2	f	0.66	0/3895	1.01	17/5264 (0.3%)
3	g	1.07	1/36963 (0.0%)	1.45	759/57662 (1.3%)
4	P	0.69	0/658	1.10	4/881 (0.5%)
5	r	0.67	0/797	1.15	7/1077 (0.6%)
6	q	0.68	0/893	1.09	5/1205 (0.4%)
7	t	0.69	0/969	1.21	12/1300 (0.9%)
8	s	0.68	0/893	1.21	10/1193 (0.8%)
9	w	0.69	0/785	1.29	12/1043 (1.2%)
10	u	0.69	0/722	1.13	5/964 (0.5%)
11	y	0.70	0/659	1.13	3/884 (0.3%)
12	1	0.73	0/463	1.34	8/621 (1.3%)
13	z	0.68	0/653	1.14	6/877 (0.7%)
14	j	0.67	0/1736	1.01	5/2338 (0.2%)
15	3	0.67	0/671	1.09	5/888 (0.6%)
16	2	0.78	0/431	1.33	4/570 (0.7%)
17	h	0.68	0/1652	1.07	11/2225 (0.5%)
18	l	0.71	0/1665	1.15	13/2227 (0.6%)
19	k	0.67	0/1119	1.06	5/1504 (0.3%)
20	n	0.69	0/836	1.12	7/1128 (0.6%)
21	m	0.70	0/1196	1.16	12/1602 (0.7%)
22	p	0.67	0/989	1.08	7/1326 (0.5%)
23	o	0.73	0/1034	1.37	23/1375 (1.7%)
24	v	1.21	2/1831 (0.1%)	1.74	70/2853 (2.5%)
25	N	1.37	0/141	2.23	8/218 (3.7%)
All	All	0.95	3/62231 (0.0%)	1.36	1023/92007 (1.1%)

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.

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Mol	Chain	#Chirality outliers	#Planarity outliers

Mol	Chain	#Chirality outliers	#Planarity outliers
2	f	0	3
3	g	0	108
4	P	0	1
5	r	0	1
6	q	0	2
7	t	0	2
8	s	0	3
11	y	0	1
12	1	0	2
14	j	0	1
16	2	0	3
17	h	0	3
18	l	0	5
19	k	0	4
21	m	0	1
22	p	0	2
23	o	0	4
24	v	0	15
25	N	0	2
All	All	0	163

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	v	22	A	N9-C4	-7.46	1.33	1.37
24	v	22	A	C3'-C2'	5.83	1.59	1.52
3	g	1228	C	P-O5'	-5.20	1.54	1.59

The worst 5 of 1023 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	v	56	U	P-O3'-C3'	16.86	139.93	119.70
25	N	14	A	P-O3'-C3'	13.63	136.06	119.70
3	g	325	A	P-O3'-C3'	10.67	132.50	119.70
3	g	1201	A	P-O3'-C3'	10.60	132.42	119.70
24	v	24	C	C6-N1-C2	-10.25	116.20	120.30

There are no chirality outliers.

5 of 163 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	f	607	ARG	Sidechain
2	f	610	ARG	Sidechain
2	f	772	TYR	Sidechain
3	g	3	A	Sidechain
3	g	42	G	Sidechain

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	5	570	0	598	0	0
2	f	3847	0	3896	0	0
3	g	33012	0	16618	0	0
4	P	649	0	691	0	0
5	r	787	0	828	0	0
6	q	877	0	887	0	0
7	t	955	0	1018	0	0
8	s	884	0	944	0	0
9	w	774	0	827	0	0
10	u	714	0	737	0	0
11	y	649	0	666	0	0
12	1	456	0	478	0	0
13	z	638	0	665	0	0
14	j	1705	0	1732	0	0
15	3	665	0	714	0	0
16	2	426	0	449	0	0
17	h	1625	0	1699	0	0
18	l	1643	0	1710	0	0
19	k	1106	0	1148	0	0
20	n	818	0	808	0	0
21	m	1182	0	1240	0	0
22	p	979	0	1034	0	0
23	o	1022	0	1070	0	0
24	v	1639	0	837	0	0
25	N	126	0	66	0	0
All	All	57748	0	41360	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	5	69/71 (97%)	64 (93%)	4 (6%)	1 (1%)	11	47
2	f	507/509 (100%)	465 (92%)	33 (6%)	9 (2%)	8	42
4	P	78/80 (98%)	69 (88%)	8 (10%)	1 (1%)	12	48
5	r	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	2	22
6	q	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	17	56
7	t	121/123 (98%)	111 (92%)	7 (6%)	3 (2%)	5	35
8	s	112/114 (98%)	106 (95%)	5 (4%)	1 (1%)	17	56
9	w	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
10	u	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
11	y	80/82 (98%)	73 (91%)	4 (5%)	3 (4%)	3	27
12	1	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
13	z	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
14	j	216/218 (99%)	200 (93%)	12 (6%)	4 (2%)	8	41
15	3	83/85 (98%)	82 (99%)	1 (1%)	0	100	100
16	2	49/51 (96%)	37 (76%)	9 (18%)	3 (6%)	1	20
17	h	204/206 (99%)	196 (96%)	6 (3%)	2 (1%)	15	54
18	l	203/205 (99%)	190 (94%)	10 (5%)	3 (2%)	10	46
19	k	148/150 (99%)	136 (92%)	8 (5%)	4 (3%)	5	34
20	n	98/100 (98%)	92 (94%)	3 (3%)	3 (3%)	4	31
21	m	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
22	p	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	o	125/127 (98%)	114 (91%)	6 (5%)	5 (4%)	3	26
All	All	2888/2938 (98%)	2671 (92%)	169 (6%)	48 (2%)	13	44

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	f	674	LEU
2	f	685	GLU
5	r	57	VAL
7	t	33	CYS
16	2	39	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	
1	5	62/62 (100%)	60 (97%)	2 (3%)	39	62
2	f	409/409 (100%)	384 (94%)	25 (6%)	18	46
4	P	74/74 (100%)	72 (97%)	2 (3%)	44	66
5	r	86/86 (100%)	85 (99%)	1 (1%)	71	83
6	q	90/90 (100%)	87 (97%)	3 (3%)	38	61
7	t	103/103 (100%)	102 (99%)	1 (1%)	76	86
8	s	92/92 (100%)	88 (96%)	4 (4%)	29	55
9	w	79/83 (95%)	78 (99%)	1 (1%)	69	82
10	u	76/76 (100%)	75 (99%)	1 (1%)	69	82
11	y	65/65 (100%)	64 (98%)	1 (2%)	65	80
12	1	48/48 (100%)	47 (98%)	1 (2%)	53	71
13	z	70/70 (100%)	68 (97%)	2 (3%)	42	64
14	j	180/180 (100%)	176 (98%)	4 (2%)	52	70
15	3	65/65 (100%)	65 (100%)	0	100	100
16	2	44/44 (100%)	43 (98%)	1 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	h	170/170 (100%)	168 (99%)	2 (1%)	71	83
18	l	172/172 (100%)	168 (98%)	4 (2%)	50	70
19	k	113/113 (100%)	112 (99%)	1 (1%)	78	87
20	n	87/87 (100%)	87 (100%)	0	100	100
21	m	124/124 (100%)	123 (99%)	1 (1%)	81	89
22	p	104/104 (100%)	100 (96%)	4 (4%)	33	58
23	o	105/105 (100%)	101 (96%)	4 (4%)	33	58
All	All	2418/2422 (100%)	2353 (97%)	65 (3%)	48	66

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	p	2	MET
22	p	53	ASP
2	f	696	ASP
2	f	681	MET
22	p	55	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	v	76/77 (98%)	26 (34%)	0
25	N	5/6 (83%)	5 (100%)	2 (40%)
3	g	1538/1539 (99%)	202 (13%)	0
All	All	1619/1622 (99%)	233 (14%)	2 (0%)

5 of 233 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	g	4	U
3	g	5	U
3	g	9	G
3	g	31	G
3	g	32	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	N	14	A
25	N	16	A

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-0643. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

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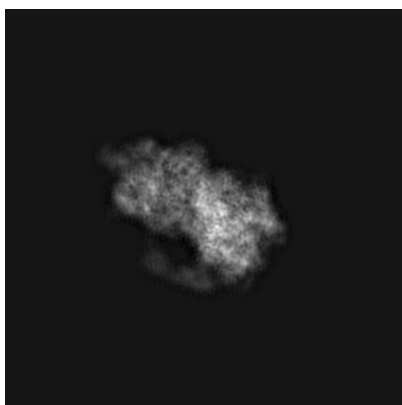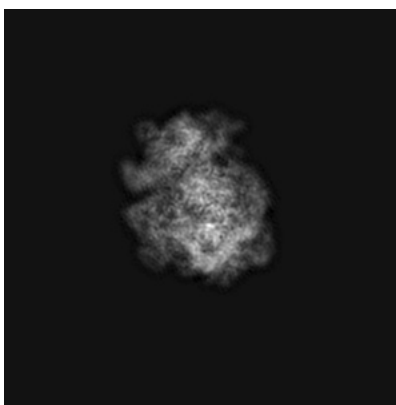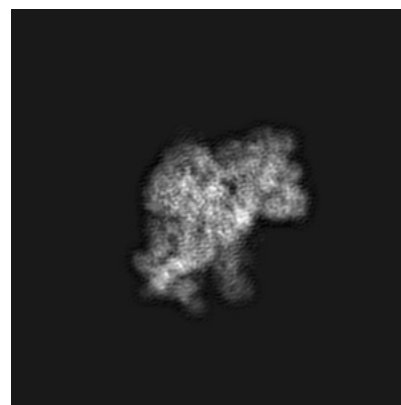
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map
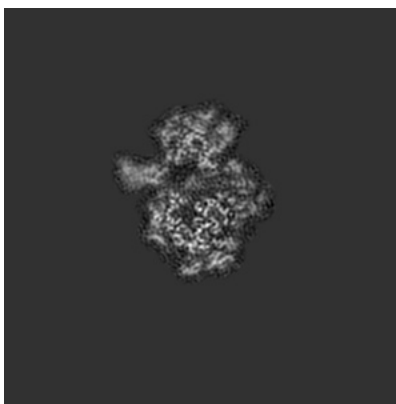
X Index: 128   Y Index: 128   Z Index: 128
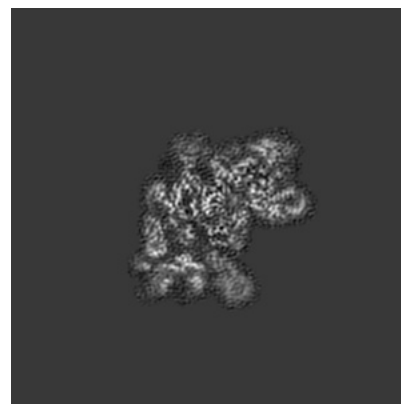
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
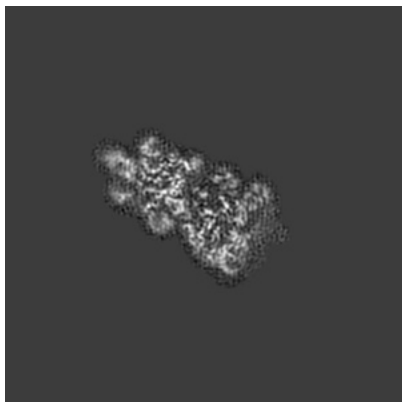
6.3.1   Primary map
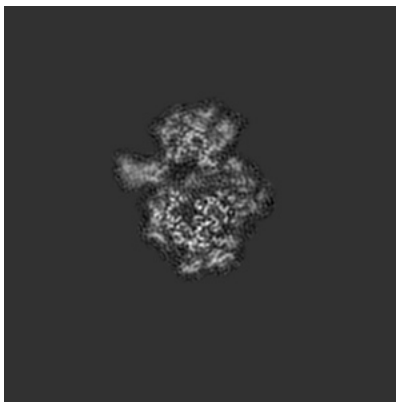
| X Index: 112 | Y Index: 128 | Z Index: 124 |
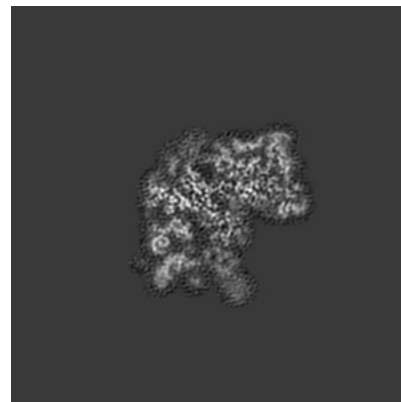
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views ⓘ

6.4.1   Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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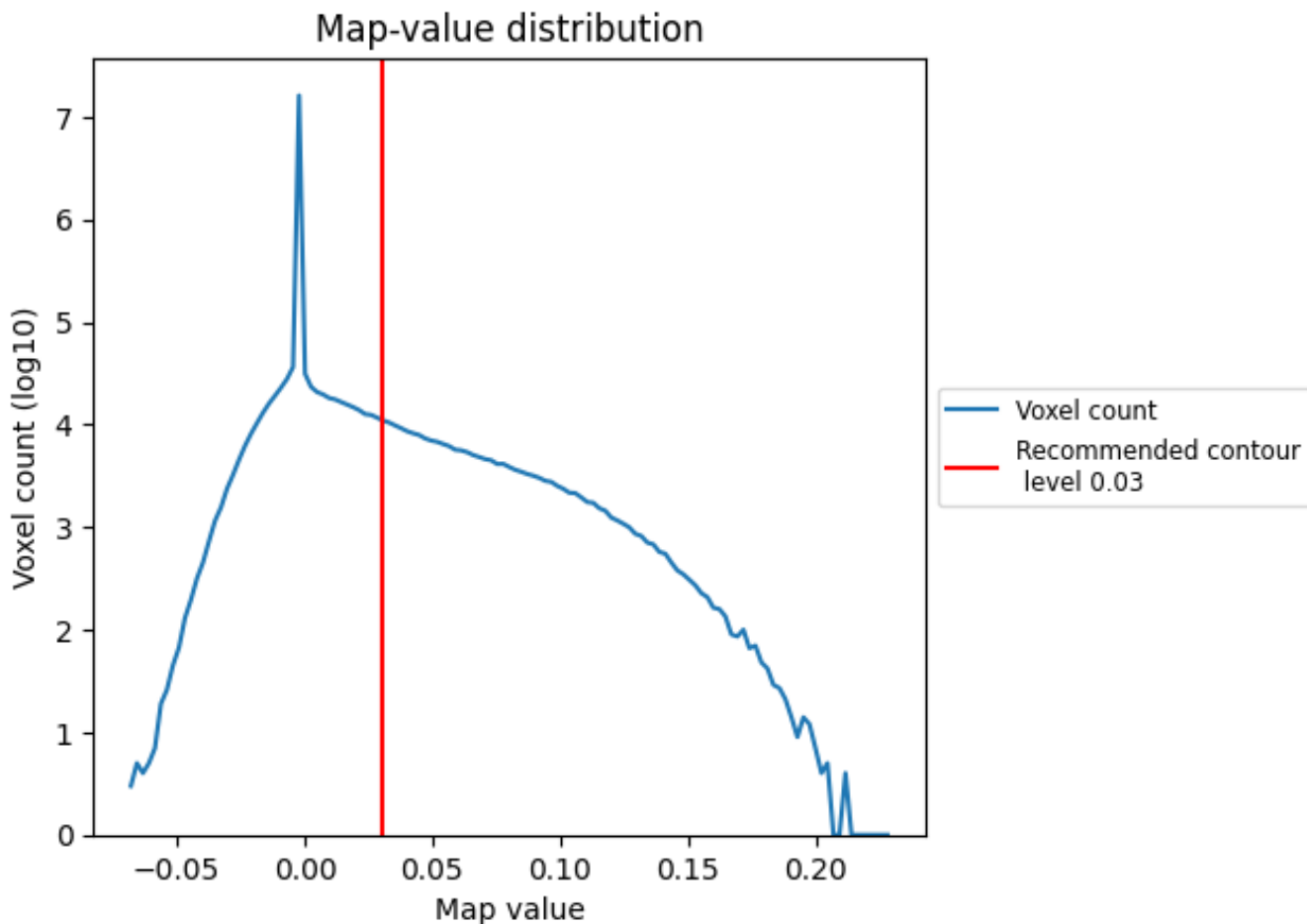
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
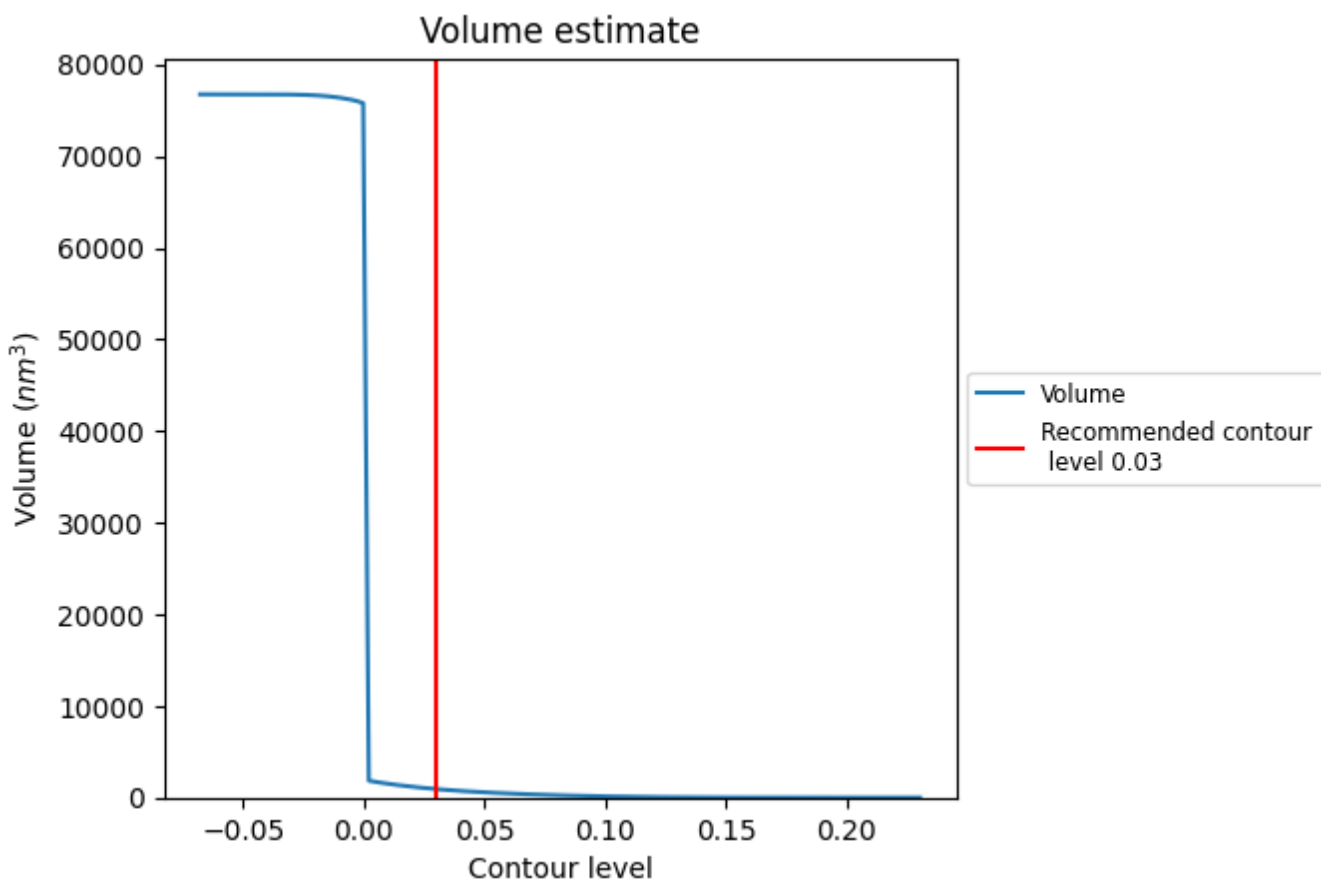
The volume at the recommended contour level is 925 nm^3; this corresponds to an approximate mass of 836 kDa.

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 ⓘ
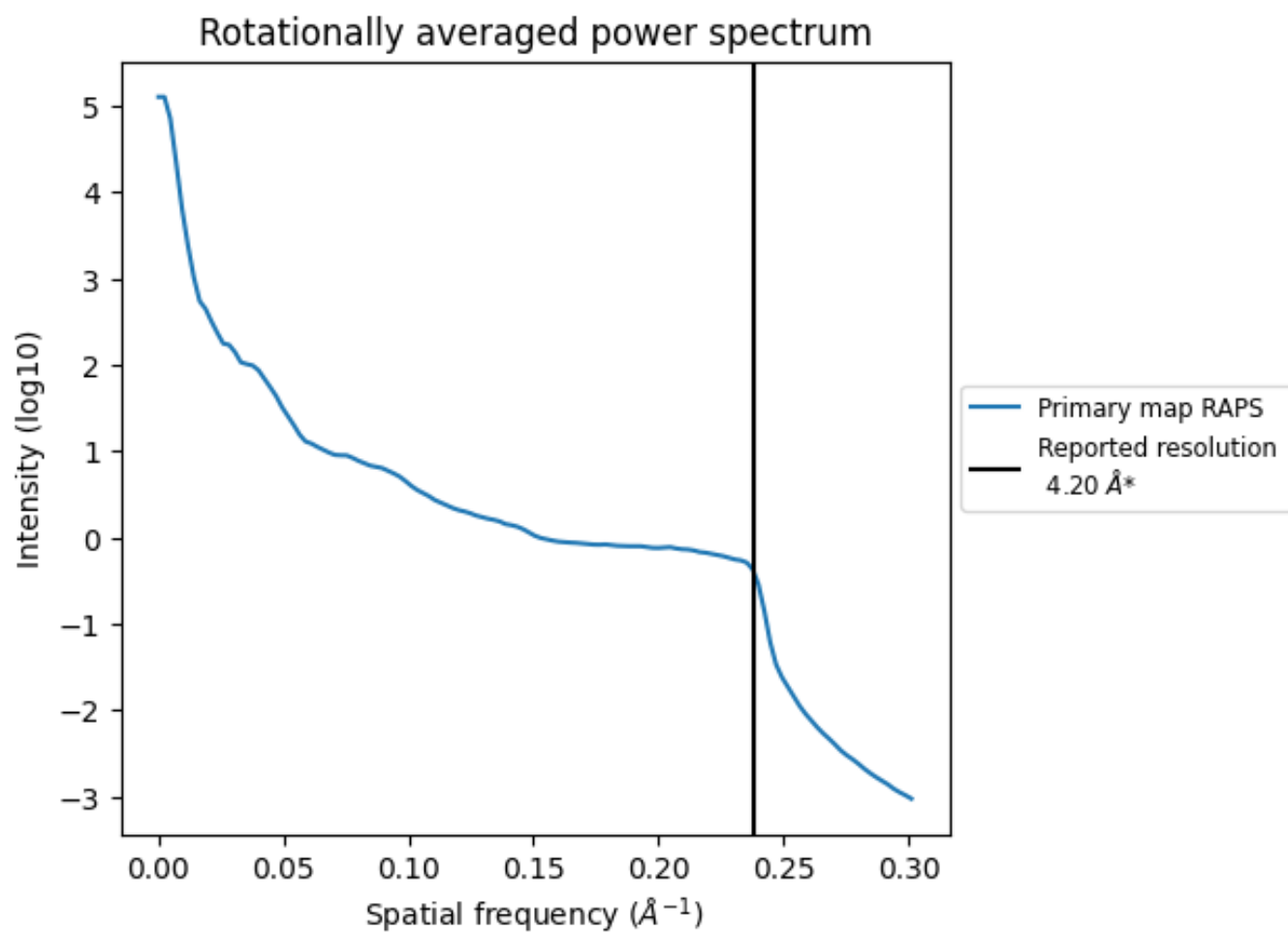
*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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)
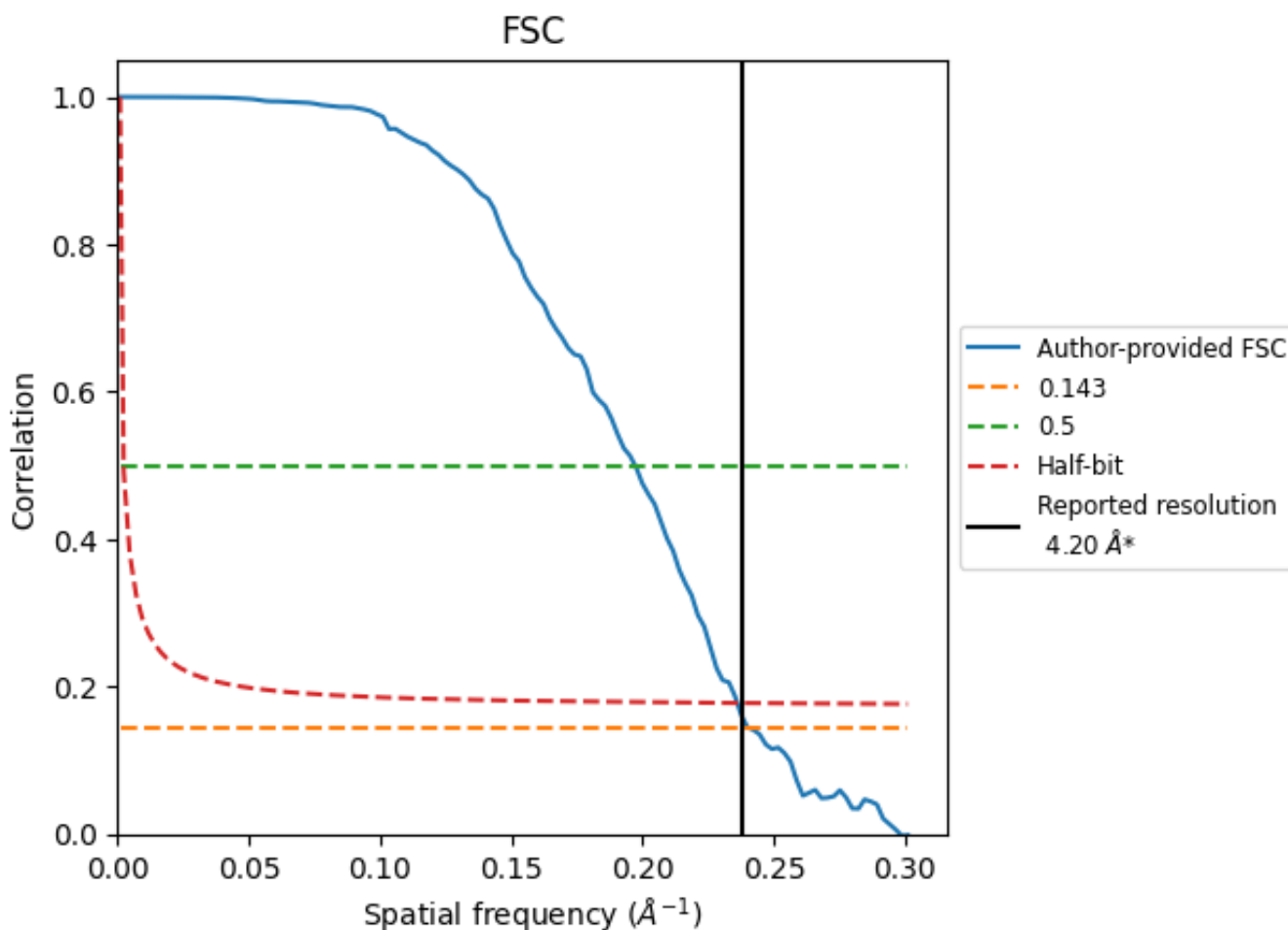
*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.15	5.07	4.23
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0643 and PDB model 6O7K. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay (i)

X   Y   Z
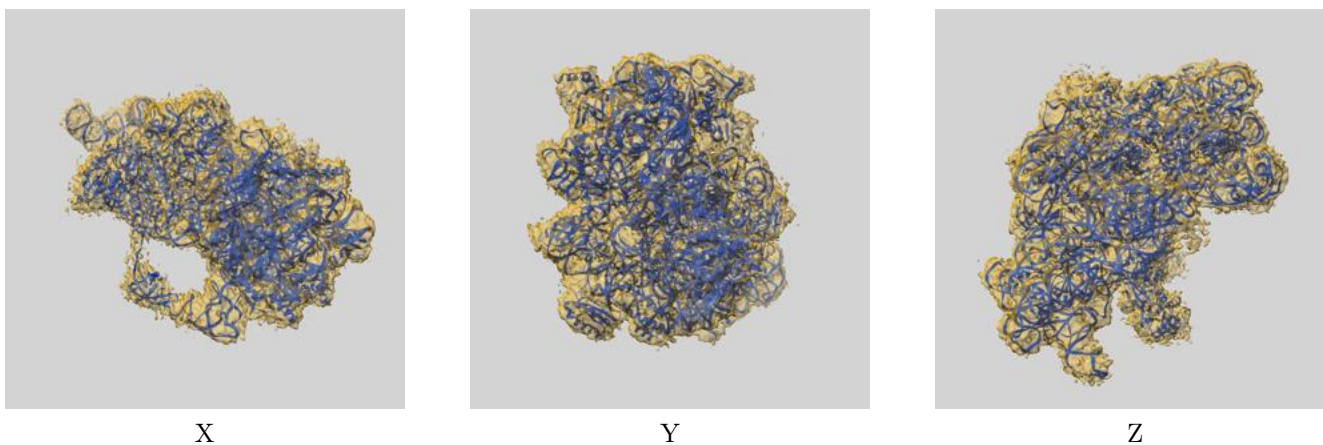
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
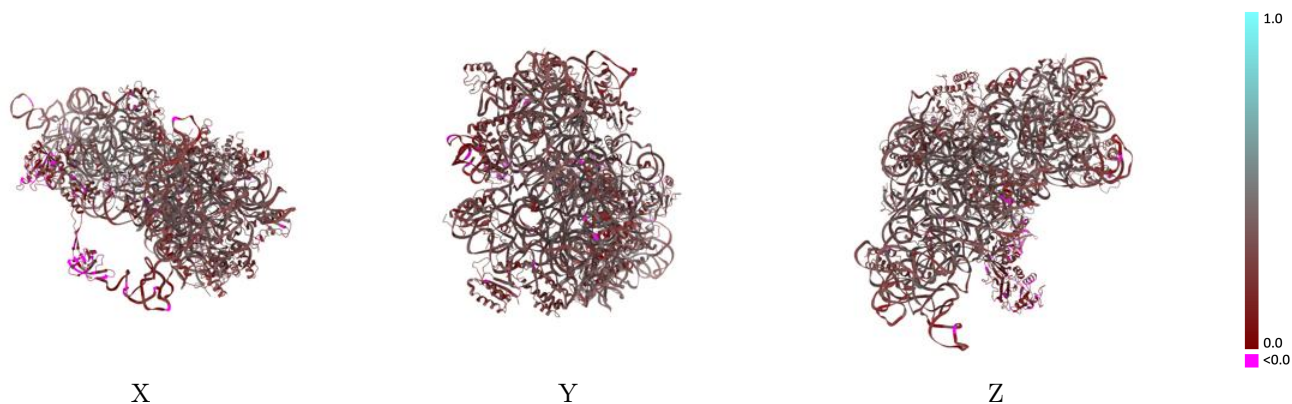
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
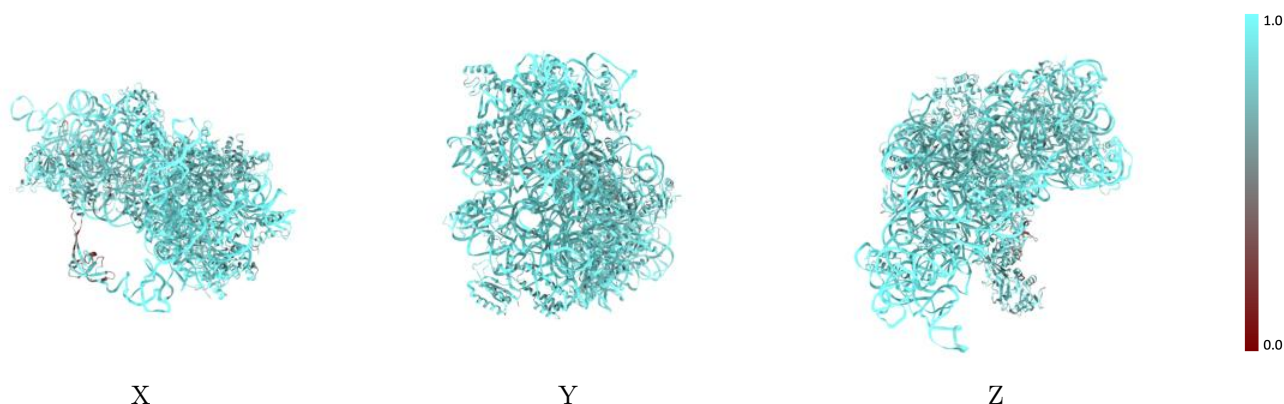
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion ⓘ
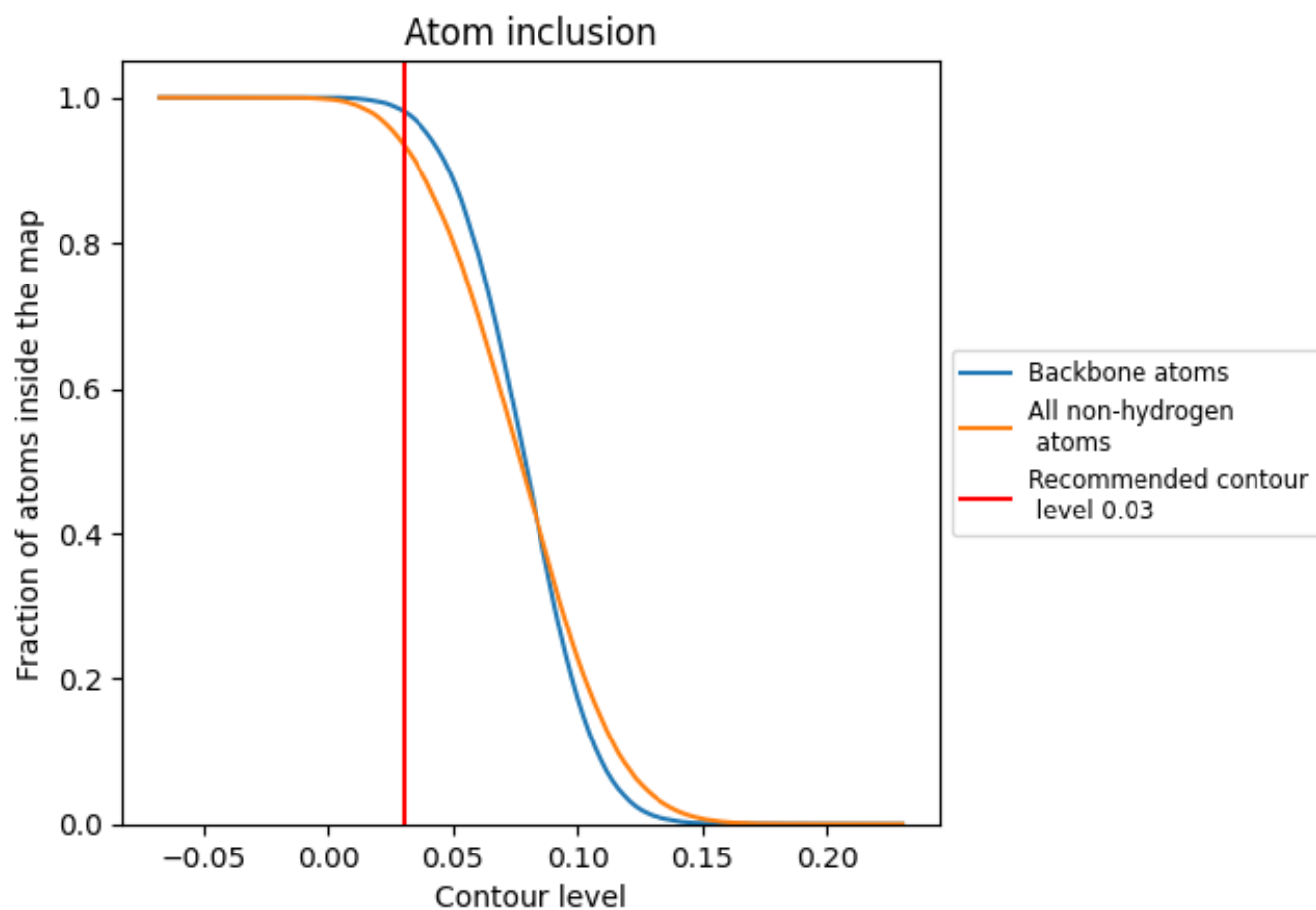
At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9359	0.3060
1	0.8719	0.2680
2	0.8305	0.2120
3	0.9015	0.2790
5	0.7909	0.2650
N	0.9603	0.3340
P	0.8878	0.3280
f	0.7614	0.1710
g	0.9925	0.3370
h	0.8835	0.3220
j	0.8246	0.2530
k	0.8681	0.3330
l	0.8742	0.2830
m	0.8507	0.2690
n	0.8507	0.2380
o	0.8876	0.2880
p	0.8646	0.3180
q	0.8781	0.2790
r	0.8622	0.2870
s	0.8908	0.2510
t	0.8588	0.3610
u	0.8710	0.2660
v	0.9664	0.1950
w	0.8896	0.3000
y	0.8868	0.3290
z	0.9116	0.2640

1.0

0.0
<0.0