wwPDB EM Validation Summary Report (i)

Feb 26, 2024 – 07:25 AM EST

PDB ID	:	6WUB
EMDB ID	:	EMD-21909
Title	:	30S subunit (head) of 70S Ribosome Enterococcus faecalis MultiBody refinement
Authors	:	Jogl, G.; Khayat, R.
Deposited on	:	2020-05-04
Resolution	:	3.20 Å(reported)
Based on initial models	:	4YBB, 5LI0

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 3.20 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.
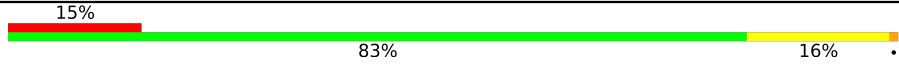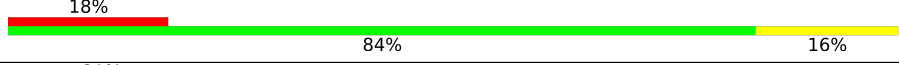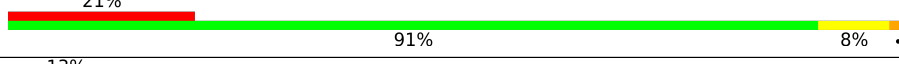
Metric	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		17.0%
RNA backbone		0.46

Worse   *Better*

▌ Percentile relative to all structures

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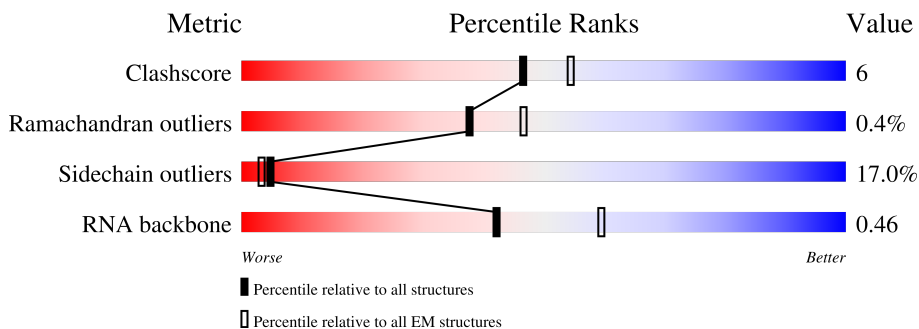
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1548	· 57% 15% · 28%
2	d	201	20% 83% 17%
3	e	163	16% 87% 12% ·
4	f	97	35% 88% 12%
5	h	131	7% 85% 15%
6	k	117	40% 88% 12%
7	l	136	10% 79% 20% ·

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Mol	Chain	Length	Quality of chain
8	o	88	15% 83% 16%
9	p	89	6% 88% 12%
10	q	83	18% 84% 16%
11	r	66	21% 91% 8%
12	t	82	13% 88% 12%

2   Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 33949 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	1121	Total	C	N	O	P	0	0
			24077	10736	4434	7786	1121		

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	201	Total	C	N	O	S	0	0
			1620	1016	303	297	4		

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	163	Total	C	N	O	S	0	0
			1204	759	222	221	2		

- Molecule 4 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	97	Total	C	N	O	S	0	0
			795	501	137	154	3		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	117	Total	C	N	O	S	0	0
			863	533	165	161	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	l	136	1065	661	214	188	2	0	0

- Molecule 8 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	o	88	741	455	152	133	1	0	0

- Molecule 9 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	p	89	708	448	131	127	2	0	0

- Molecule 10 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	q	83	681	427	127	124	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	r	66	537	343	99	94	1	0	0

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	t	82	617	377	120	118	2	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: 16S rRNA

• Molecule 2: 30S ribosomal protein S4

Chain d:
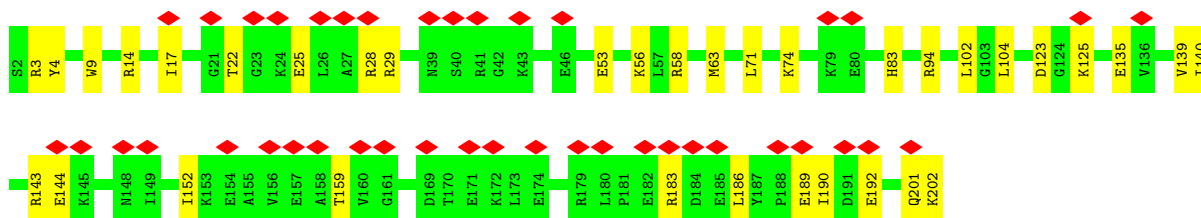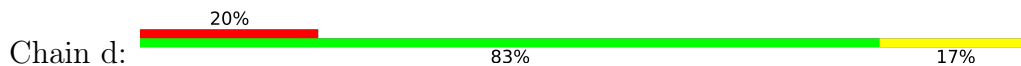
• Molecule 3: 30S ribosomal protein S5

Chain e:
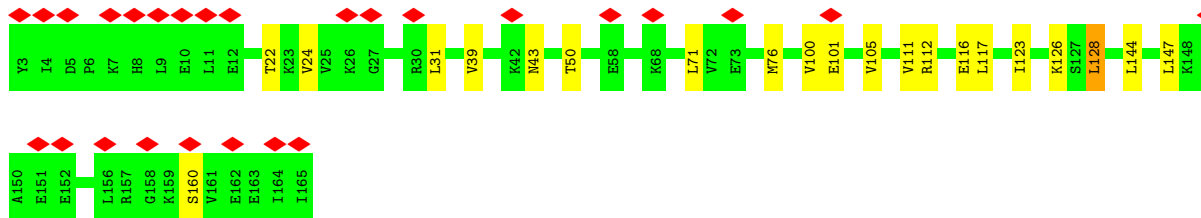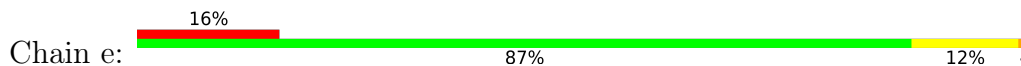
• Molecule 4: 30S ribosomal protein S6
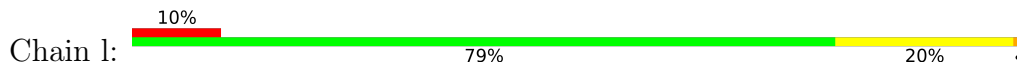
Chain f:
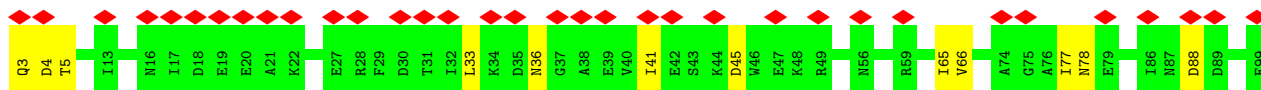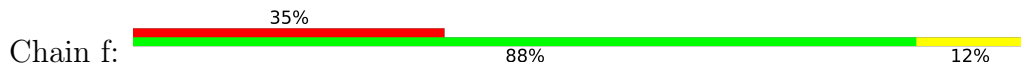
• Molecule 5: 30S ribosomal protein S8

Chain h:
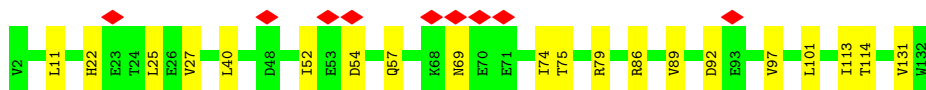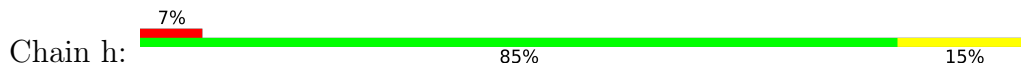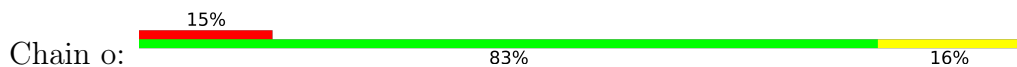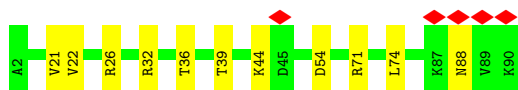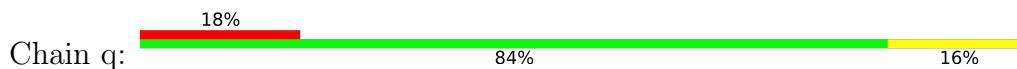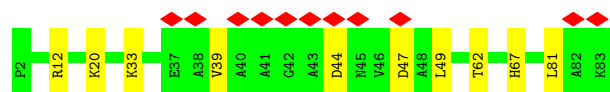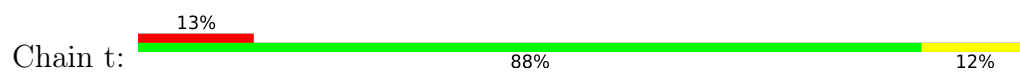

• Molecule 6: 30S ribosomal protein S11

Chain k:

K13 K14 N15 I16 E17 S18 G19 V20 T30 I31 V32 M33 I34 T35 D36 T37 H38 G39 N40 A41 S45 S49 S55 K56 T59 P60 F61 A62 M65 E68 A69 A70 T71 A74 M75 E76 H77 G78 L79 K80 T81 V82 D83 V84 T85 V86 K87 G88 S91 G92 R93

E94 A95 A96 I97 R98 S99 L100 Q101 A102 T103 G104 L105 E106 V107 T108 A109 I110 R111 N119 R126 V129
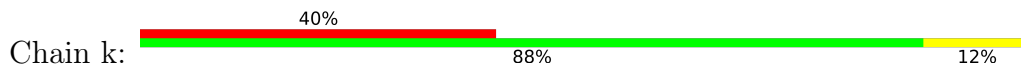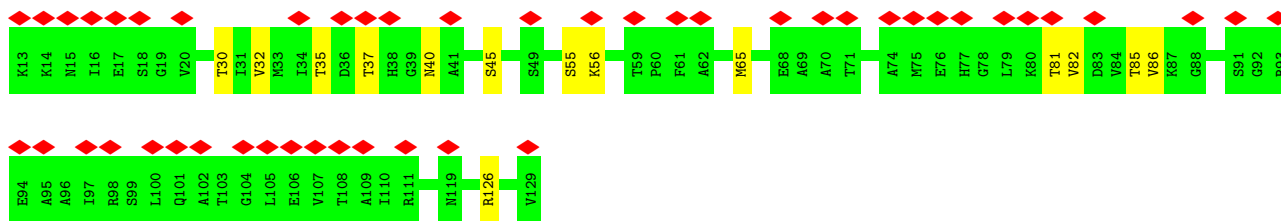
- Molecule 7: 30S ribosomal protein S12

Chain l:

10%

79%   20%   •

P2 K10 K13 E17 K18 S19 D20 L24 N25 Y28 N29 K32 K33 T34 Q35 T36 N37 Q42 K43 R44 R49 T54 K57 R63 K64 N72 T77 I80 Q88 E89 V92 D102 L103 V106 I110 V111 D116 T117 D122

K129 K136 A137
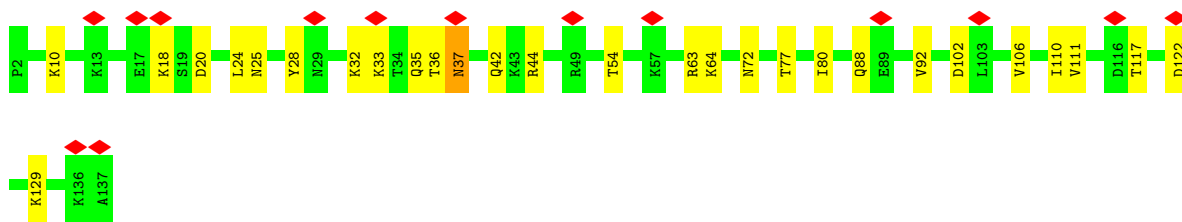
- Molecule 8: 30S ribosomal protein S15

Chain o:

15%

83%   16%   •

A2 R7 I12 K13 H18 E19 T22 P25 I29 D35 N40 R44 R54 G55 L56 L67 I75 Q76 R79 E80 L81 I82 Q83 R84 L87 R88 R89

- Molecule 9: 30S ribosomal protein S16

Chain p:

6%

88%   12%

A2 V21 V22 R26 R32 T36 T39 K44 D45 D54 R71 L74 K87 N88 V89 K90
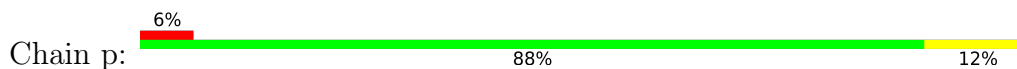
- Molecule 10: 30S ribosomal protein S17

Chain q:

18%

84%   16%

E4 V10 R14 K19 M20 D21 V28 E29 T30 K31 K32 R40 M41 K42 D51 E52 N53 N54 T55 A56 K57 V62 L78 L79 E80 V81 V82 E83 E84 A85 V86

- Molecule 11: 30S ribosomal protein S18

Chain r:

21%

91%   8%   •

K13 A18 A19 N20 H21 I22 E23 Y24 I25 D26 Y27 K28 D29 T30 E31 E39 R40 I63 K64 R65 S76 D77 E78
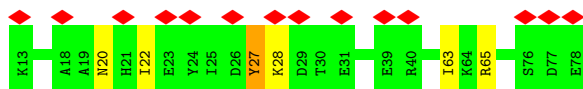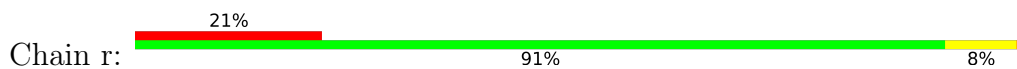
- Molecule 12: 30S ribosomal protein S20

Chain t:

13%

88%

12%

P2 R12 K20 K33 E37 A38 V39 A40 A41 G42 A43 D44 N45 V46 D47 A48 L49 T62 H67 L81 A82 K83

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	335675	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 $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.068	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	482.68, 482.68, 482.68	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.097, 1.097, 1.097	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	a	1.07	1/26962 (0.0%)	1.08	49/42059 (0.1%)
2	d	0.44	0/1650	0.58	0/2217
3	e	0.41	0/1217	0.56	1/1641 (0.1%)
4	f	0.38	0/807	0.52	0/1087
5	h	0.48	0/1054	0.57	0/1417
6	k	0.34	0/878	0.56	0/1185
7	l	0.49	0/1082	0.61	0/1453
8	o	0.44	0/751	0.58	1/1001 (0.1%)
9	p	0.54	0/720	0.58	0/966
10	q	0.47	0/689	0.58	0/920
11	r	0.44	0/544	0.54	0/728
12	t	0.39	0/620	0.54	0/829
All	All	0.94	1/36974 (0.0%)	0.98	51/55503 (0.1%)

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.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	h	0	1
7	l	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	183	G	N9-C4	-5.25	1.33	1.38

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	35	G	O5'-P-OP1	-12.49	94.45	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	183	G	N3-C4-N9	-8.13	121.12	126.00
1	a	183	G	N3-C4-C5	7.65	132.43	128.60
1	a	255	U	O4'-C1'-N1	7.57	114.25	108.20
1	a	488	C	C6-N1-C2	7.45	123.28	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	h	22	HIS	Peptide
7	l	37	ASN	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	a	24077	0	12112	0	0
2	d	1620	0	1641	0	0
3	e	1204	0	1280	0	0
4	f	795	0	789	0	0
5	h	1041	0	1092	0	0
6	k	863	0	882	0	0
7	l	1065	0	1133	0	0
8	o	741	0	756	0	0
9	p	708	0	746	0	0
10	q	681	0	719	0	0
11	r	537	0	572	0	0
12	t	617	0	648	0	0
All	All	33949	0	22370	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 6.

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	d	199/201 (99%)	168 (84%)	29 (15%)	2 (1%)	15	54
3	e	161/163 (99%)	146 (91%)	15 (9%)	0	100	100
4	f	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
5	h	129/131 (98%)	115 (89%)	14 (11%)	0	100	100
6	k	115/117 (98%)	94 (82%)	21 (18%)	0	100	100
7	l	134/136 (98%)	110 (82%)	24 (18%)	0	100	100
8	o	86/88 (98%)	74 (86%)	11 (13%)	1 (1%)	13	49
9	p	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
10	q	81/83 (98%)	69 (85%)	12 (15%)	0	100	100
11	r	64/66 (97%)	52 (81%)	11 (17%)	1 (2%)	9	43
12	t	80/82 (98%)	76 (95%)	3 (4%)	1 (1%)	12	47
All	All	1231/1253 (98%)	1061 (86%)	165 (13%)	5 (0%)	38	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	t	67	HIS
2	d	144	GLU
2	d	4	TYR
8	o	25	PRO
11	r	27	TYR

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	d	175/175 (100%)	142 (81%)	33 (19%)	1	8
3	e	126/126 (100%)	105 (83%)	21 (17%)	2	10
4	f	86/86 (100%)	74 (86%)	12 (14%)	3	16
5	h	112/112 (100%)	93 (83%)	19 (17%)	2	10
6	k	91/91 (100%)	77 (85%)	14 (15%)	2	13
7	l	118/118 (100%)	90 (76%)	28 (24%)	1	3
8	o	78/78 (100%)	64 (82%)	14 (18%)	2	9
9	p	79/79 (100%)	68 (86%)	11 (14%)	3	16
10	q	76/76 (100%)	63 (83%)	13 (17%)	2	10
11	r	57/57 (100%)	51 (90%)	6 (10%)	7	28
12	t	63/63 (100%)	54 (86%)	9 (14%)	3	15
All	All	1061/1061 (100%)	881 (83%)	180 (17%)	5	10

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	l	72	ASN
9	p	26	ARG
7	l	92	VAL
8	o	22	THR
9	p	74	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
8	o	83	GLN
10	q	34	HIS
12	t	45	ASN
9	p	72	ASN
5	h	57	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1117/1548 (72%)	217 (19%)	0

5 of 217 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	G
1	a	5	A
1	a	6	G
1	a	13	A
1	a	19	G

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-21909. 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 |
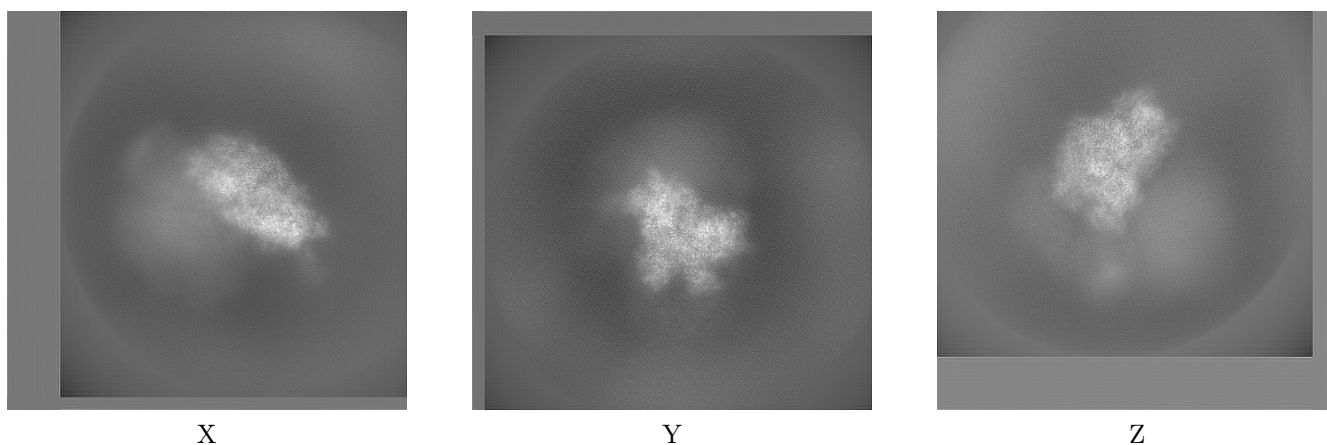
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 220 | Y Index: 220 | Z Index: 220 |
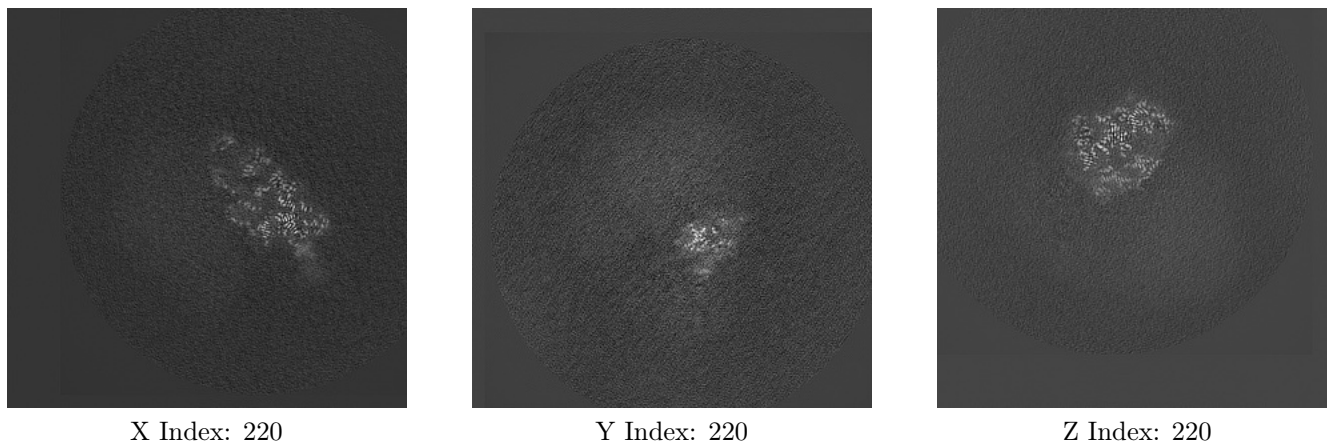
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
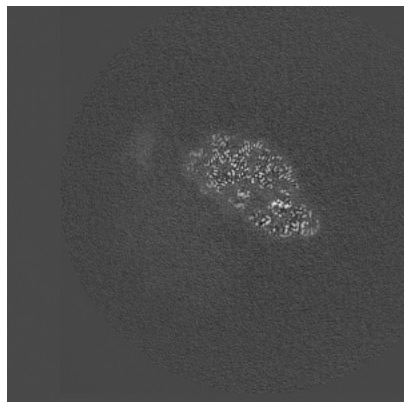
6.3.1 Primary map
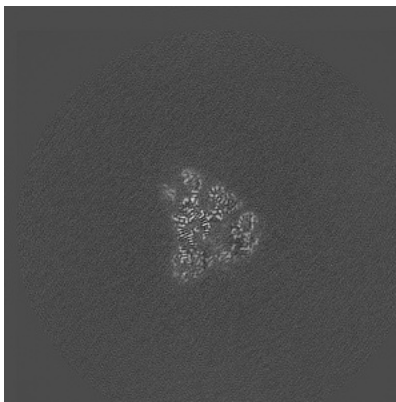
| X Index: 196 | Y Index: 297 | Z Index: 206 |
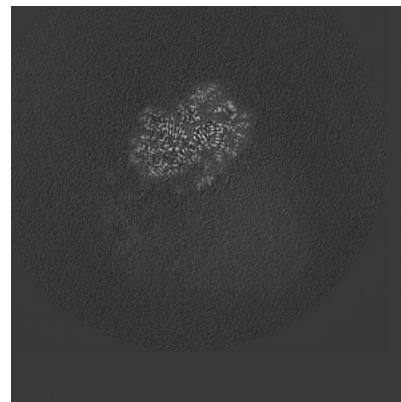
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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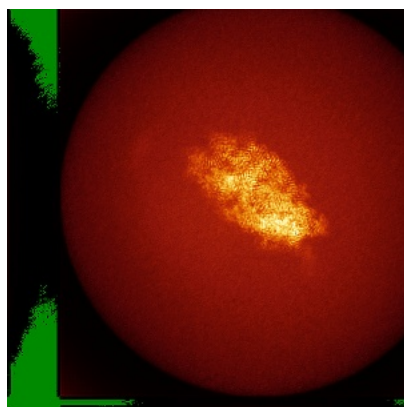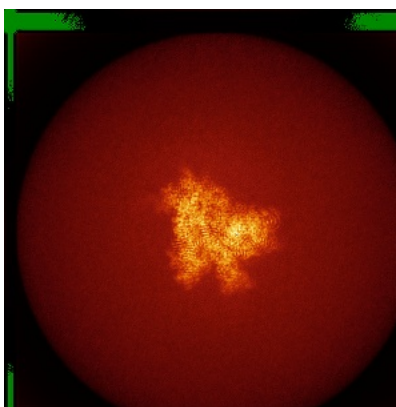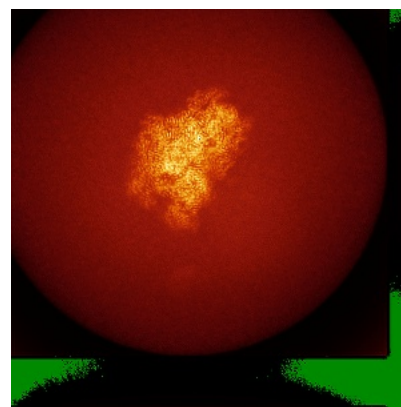
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5   Orthogonal surface views (i)

6.5.1   Primary map

| X | Y | Z |
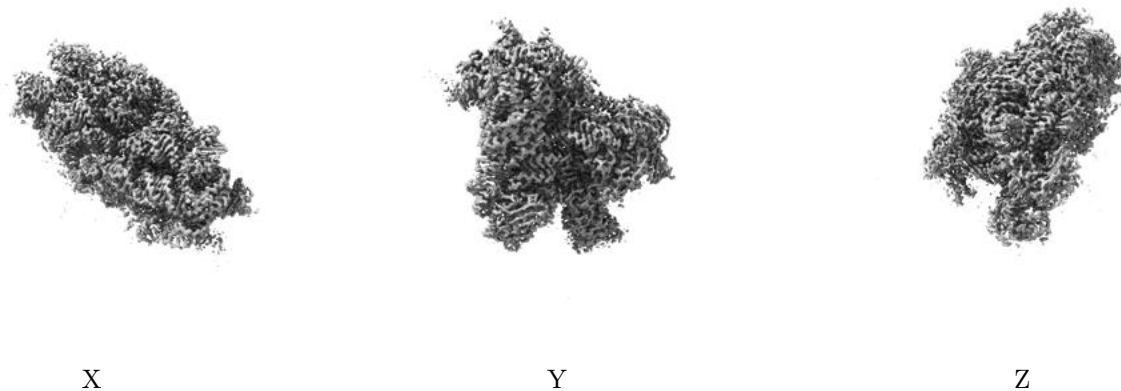
The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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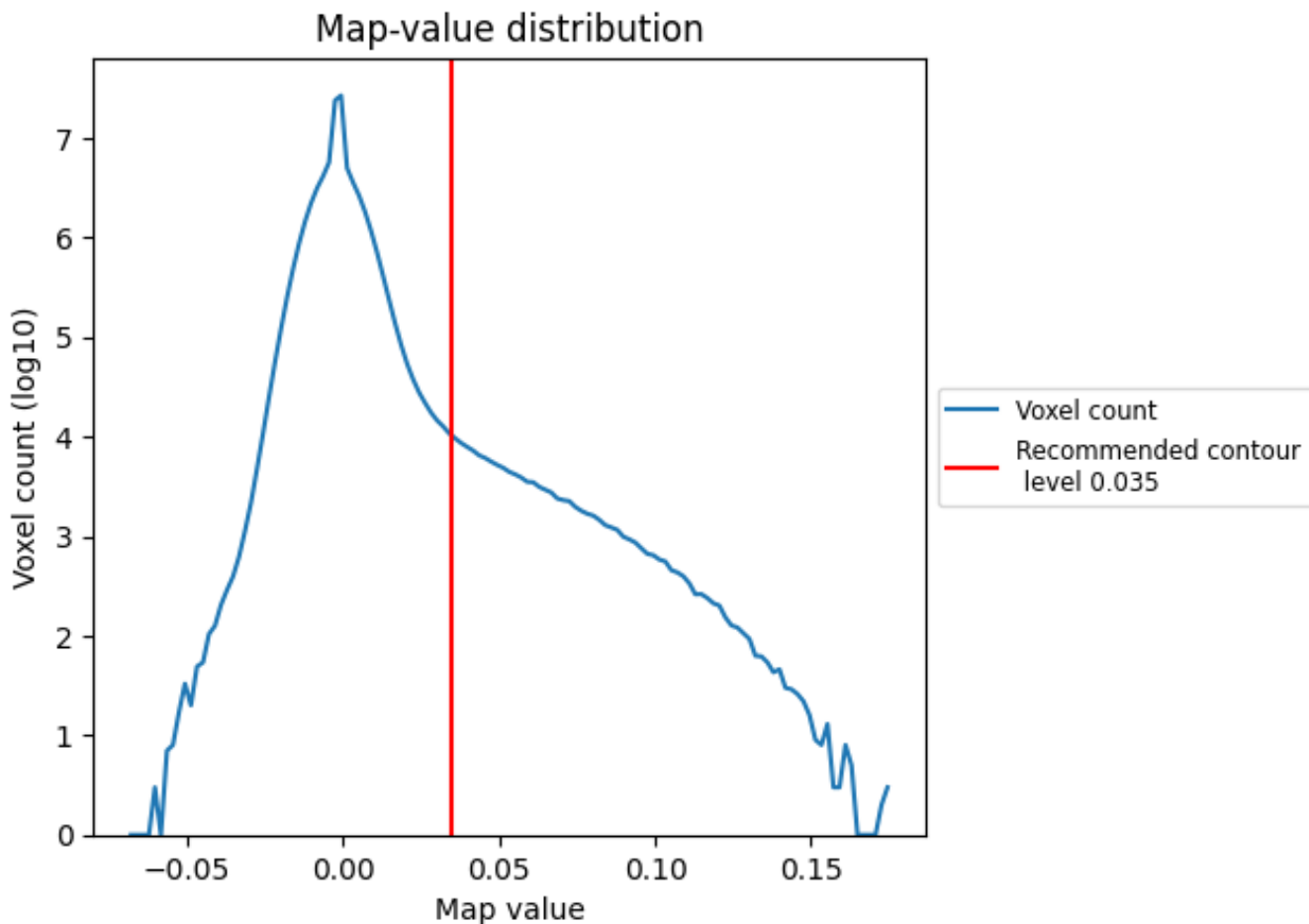
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
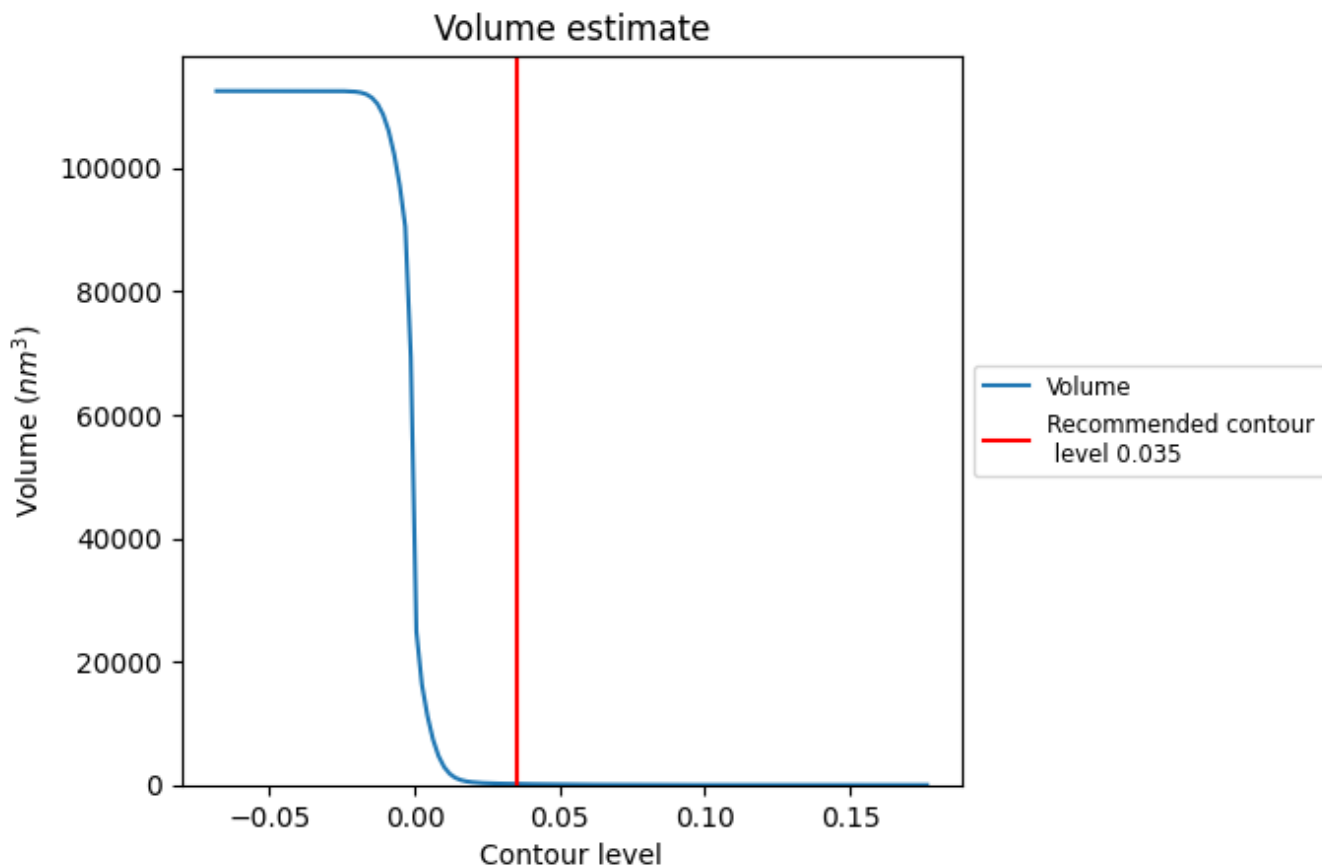
The volume at the recommended contour level is 163 nm^3; this corresponds to an approximate mass of 148 kDa.

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   ⓘ
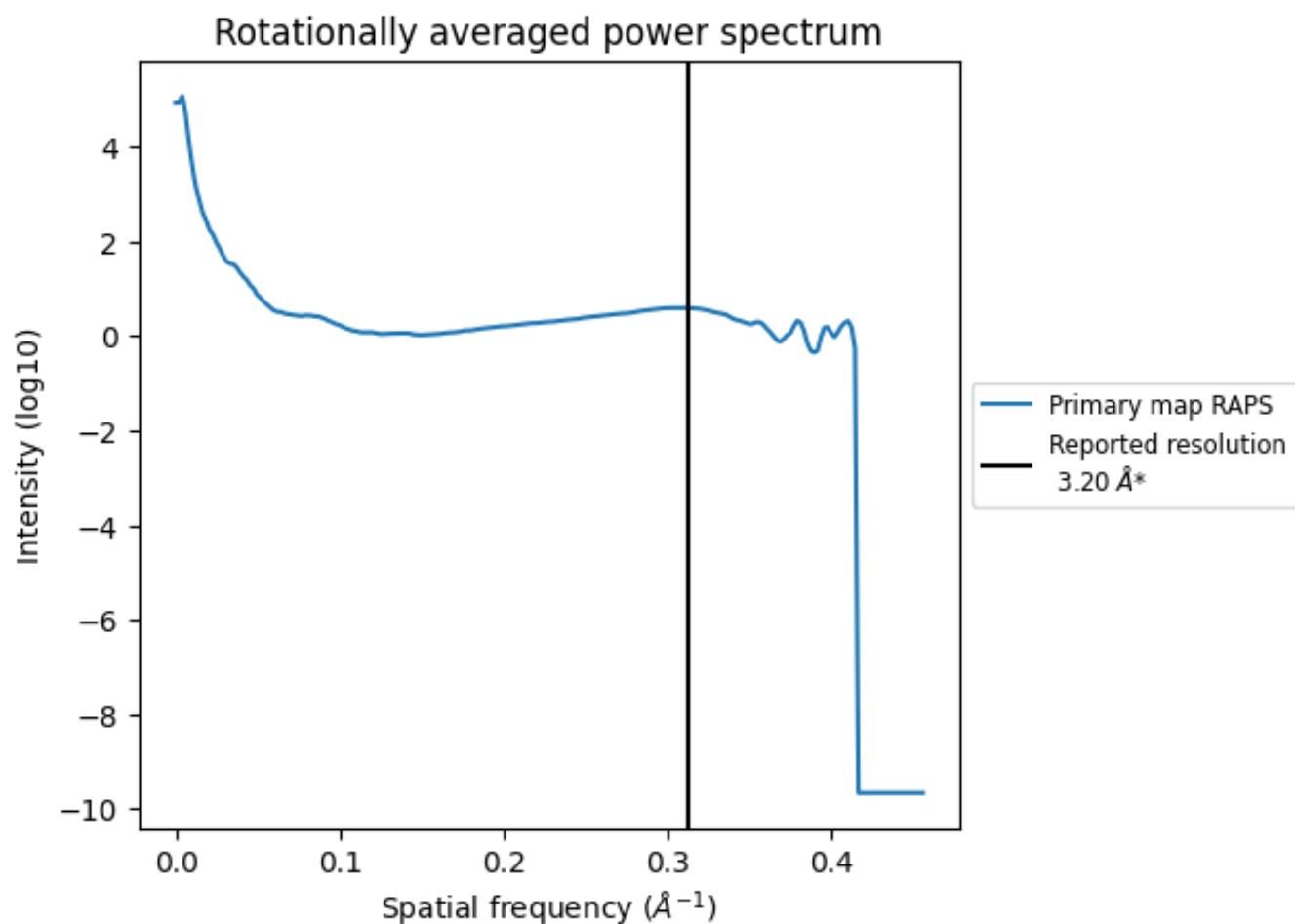
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-21909 and PDB model 6WUB. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

| X | Y | Z |
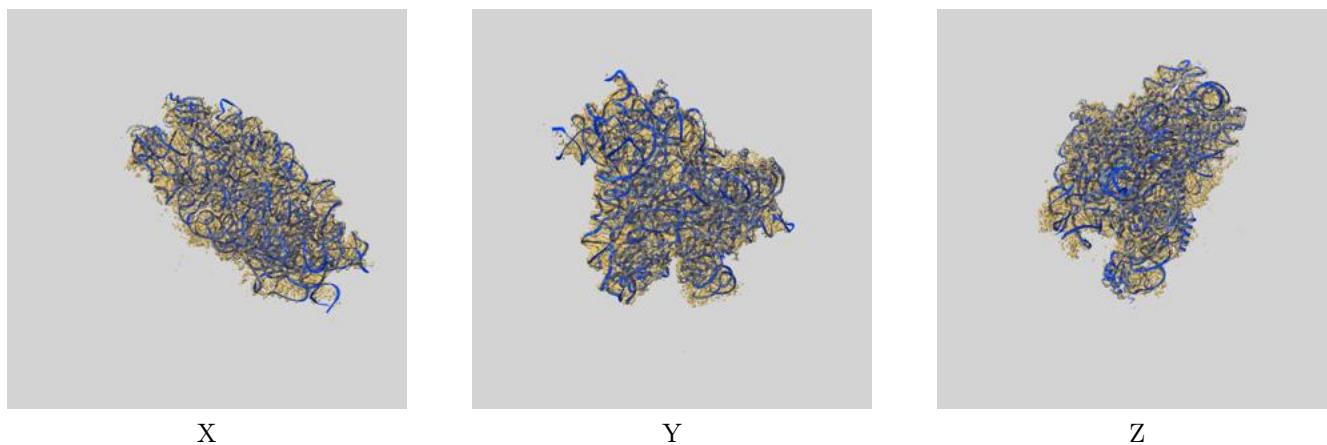
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
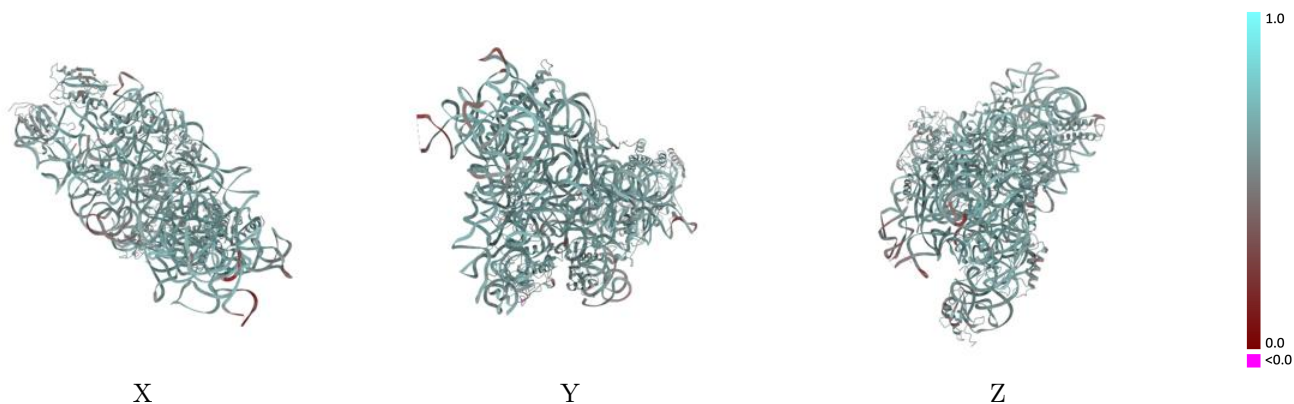
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
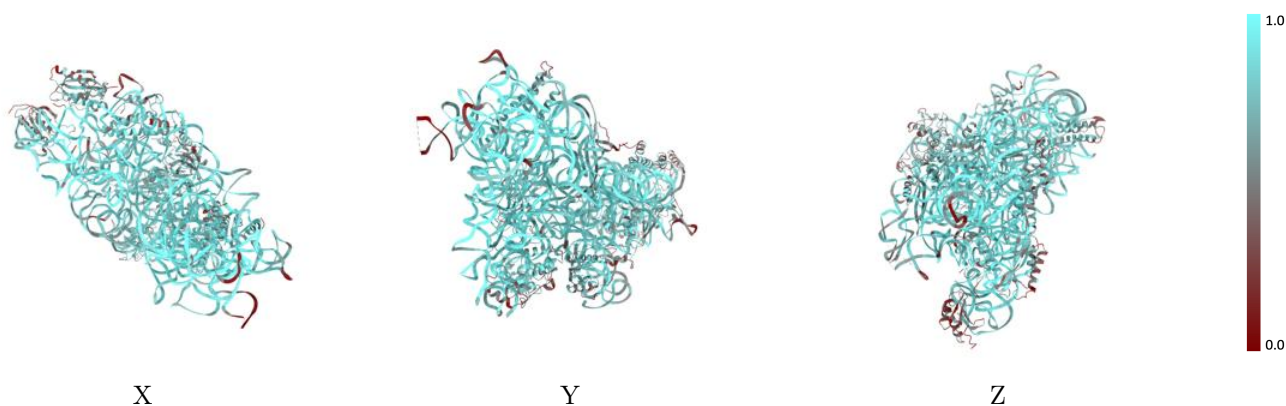
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion ⓘ
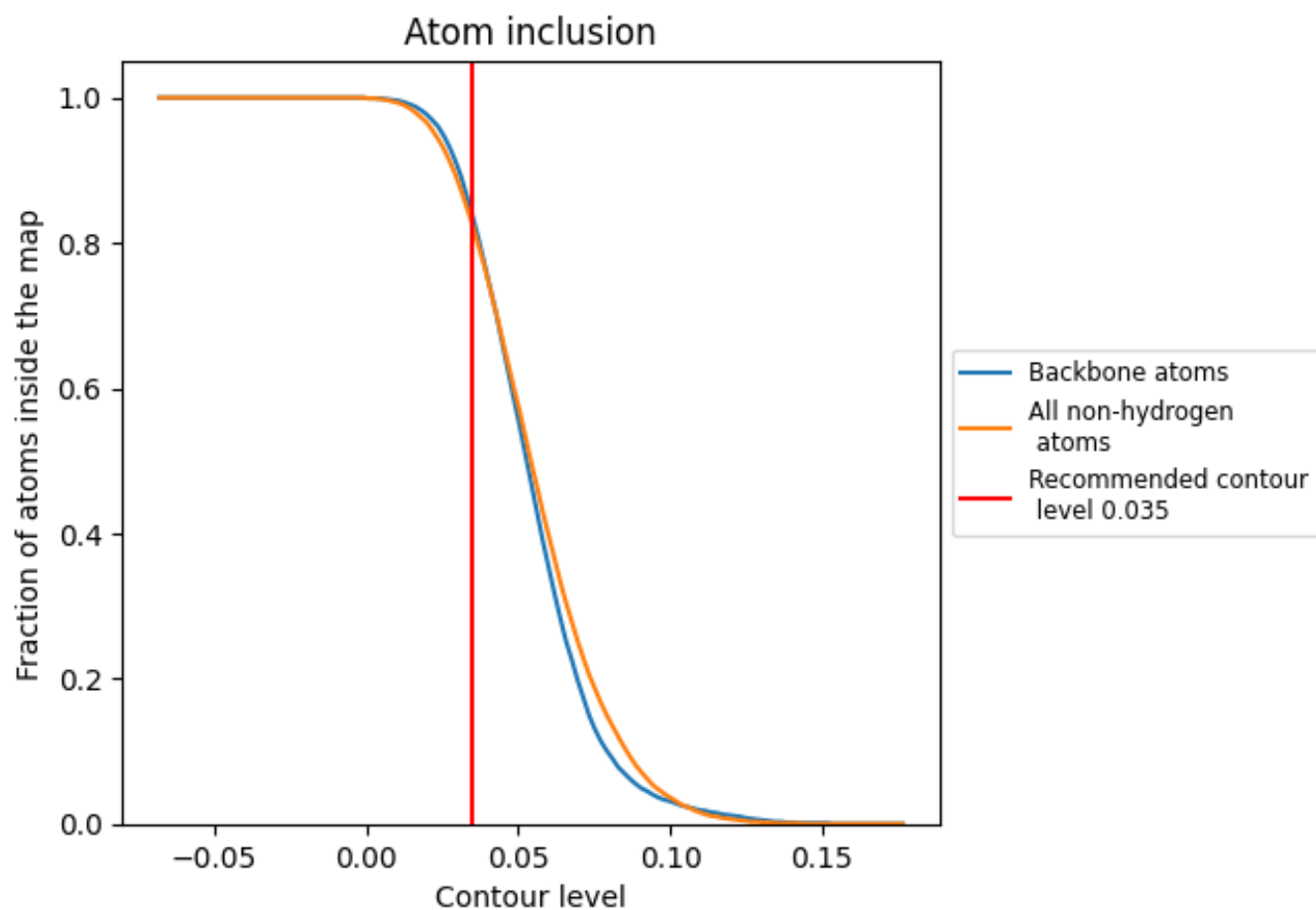
At the recommended contour level, 84% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.6030
a	0.8850	0.6100
d	0.6590	0.5690
e	0.6620	0.5850
f	0.5390	0.5640
h	0.7370	0.6090
k	0.4850	0.5400
l	0.7420	0.5810
o	0.6930	0.5820
p	0.7970	0.6130
q	0.6770	0.5990
r	0.6670	0.5930
t	0.7390	0.6050

1.0

0.0
<0.0