WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 11:37 AM JST

PDB ID	:	7C79
EMDB ID	:	EMD-30296
Title	:	Cryo-EM structure of yeast Ribonuclease MRP
Authors	:	Lan, P.; Wu, J.; Lei, M.
Deposited on	:	2020-05-24
Resolution	:	2.50 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		0.3%
RNA backbone		0.55

Worse ← → *Better*

■ Percentile relative to all structures

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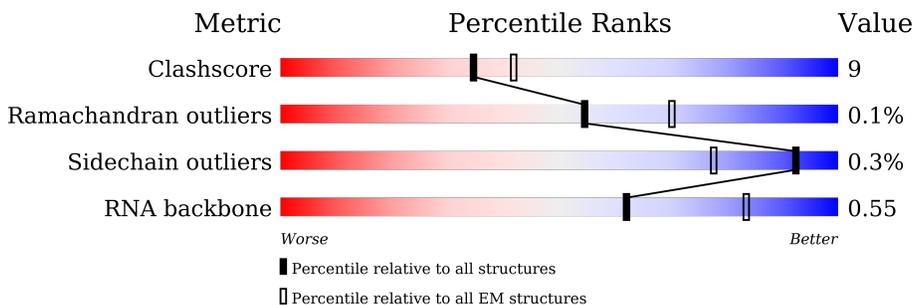
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	340	5% / 41% / 47% / 9% / ·
2	B	875	· / 71% / 19% / 9%
3	C	195	18% / 45% / 33% / · / 22%
4	D	279	5% / 65% / 25% / 10%
5	E	173	72% / 12% / 16%
6	F	158	· / 84% / 15% / ··
7	G	140	77% / 9% / 14%

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Mol	Chain	Length	Quality of chain
8	H	133	5% ▬ 82% 17% .
9	I	293	63% 19% 17%
9	J	293	77% 23%
10	K	198	36% 15% . 47%
11	L	201	51% 14% 35%

2　Entry composition　ⓘ

There are 13 unique types of molecules in this entry. The entry contains 27324 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 Ribonuclease MRP RNA subunit NME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	331	Total 7008	C 3139	N 1204	O 2334	P 331	0	0

- Molecule 2 is a protein called Ribonucleases P/MRP protein subunit POP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	793	Total 6453	C 4085	N 1170	O 1162	S 36	0	0

- Molecule 3 is a protein called Ribonucleases P/MRP protein subunit POP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	152	Total 1246	C 812	N 206	O 219	S 9	0	0

- Molecule 4 is a protein called RNases MRP/P 32.9 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	251	Total 2086	C 1338	N 352	O 386	S 10	0	0

- Molecule 5 is a protein called Ribonuclease P/MRP protein subunit POP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	145	Total 1135	C 716	N 201	O 210	S 8	0	0

- Molecule 6 is a protein called Ribonucleases P/MRP protein subunit POP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	157	Total 1271	C 804	N 222	O 241	S 4	0	0

- Molecule 7 is a protein called Ribonucleases P/MRP protein subunit POP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	121	Total	C	N	O	S	0	0
			960	609	167	182	2		

- Molecule 8 is a protein called Ribonucleases P/MRP protein subunit POP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1079	683	177	215	4		

- Molecule 9 is a protein called Ribonuclease P/MRP protein subunit RPP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	242	Total	C	N	O	S	0	0
			1881	1188	339	345	9		
9	J	292	Total	C	N	O	S	0	0
			2253	1410	412	421	10		

- Molecule 10 is a protein called Ribonuclease MRP protein subunit SNM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	104	Total	C	N	O	S	0	0
			840	527	148	156	9		

- Molecule 11 is a protein called Ribonuclease MRP protein subunit RMP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	131	Total	C	N	O	S	0	0
			1110	711	210	182	7		

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Mg	0
			1	1	

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	K	1	Total	Zn	0
			1	1	

# 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.
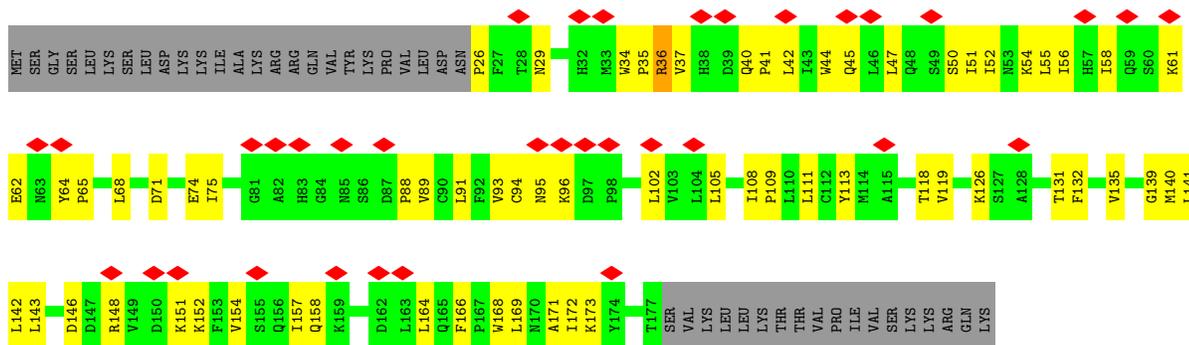
• Molecule 1: Ribonuclease MRP RNA subunit NME1
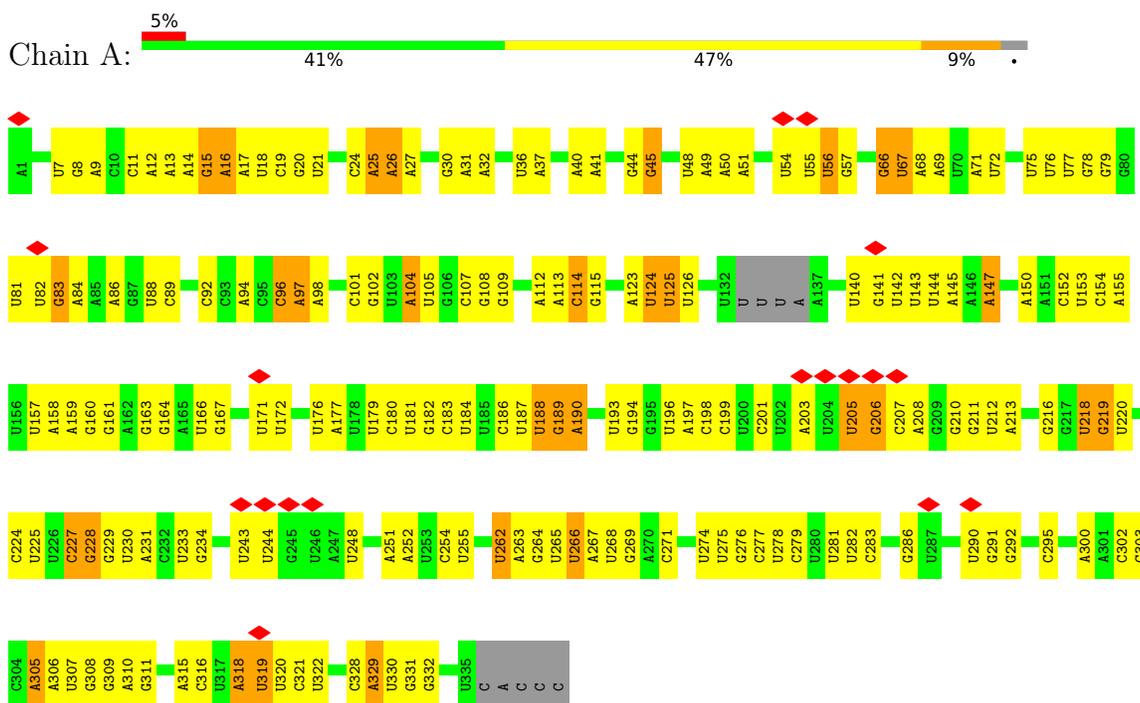
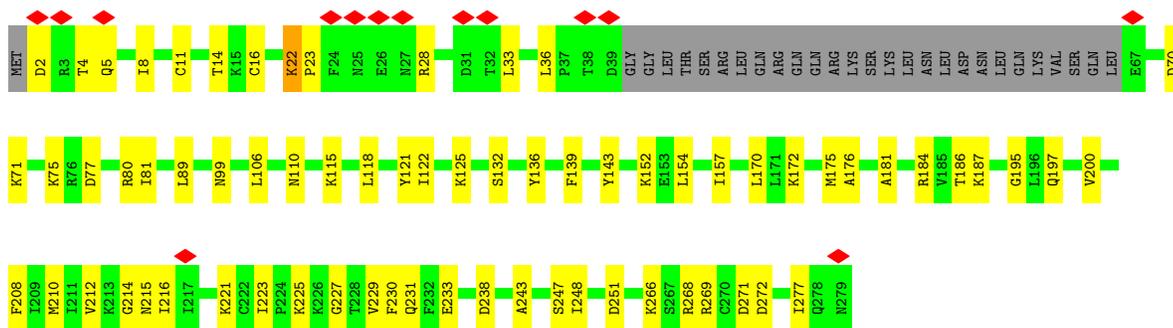• Molecule 2: Ribonucleases P/MRP protein subunit POP1
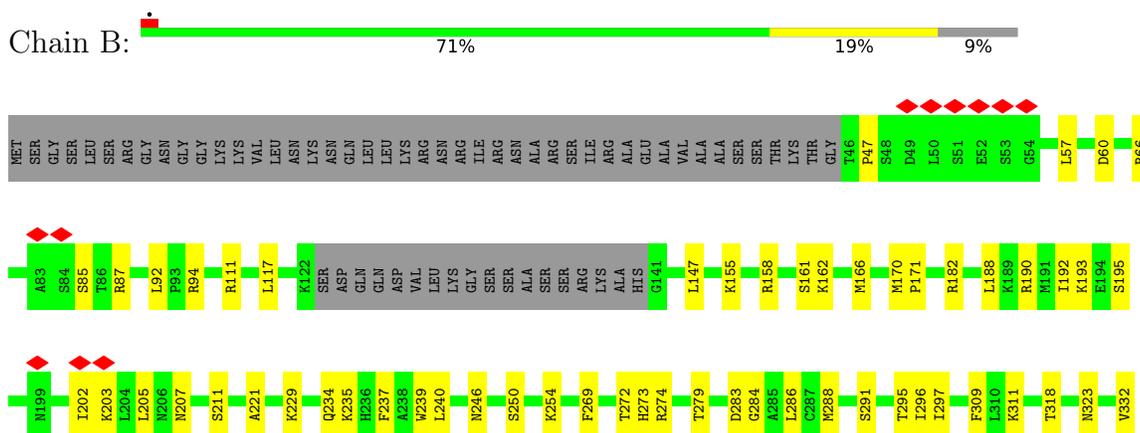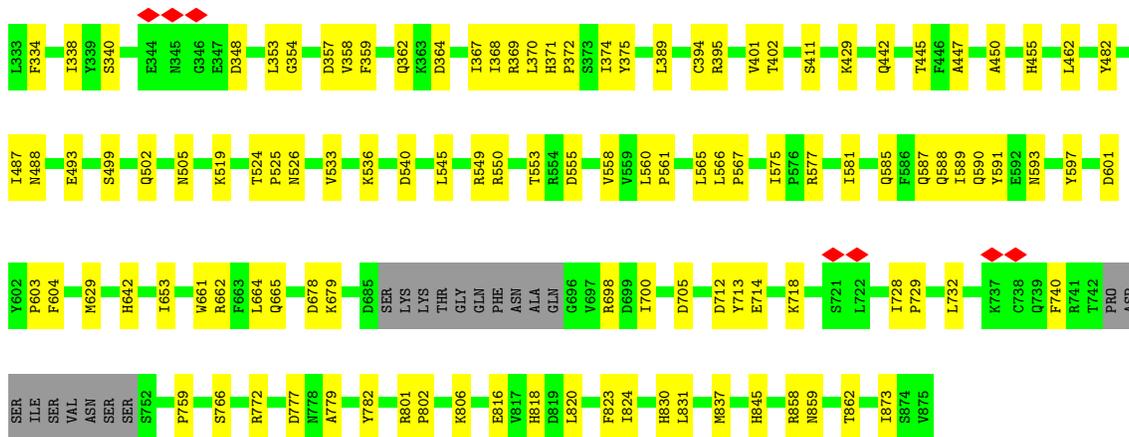
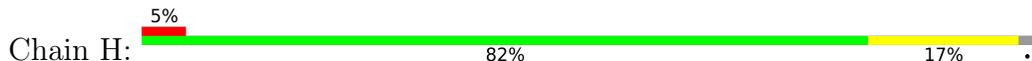• Molecule 3: Ribonucleases P/MRP protein subunit POP3

Chain C:

18%

45% 33% 22%

• Molecule 4: RNases MRP/P 32.9 kDa subunit

Chain D:

5%

65% 25% 10%

• Molecule 5: Ribonuclease P/MRP protein subunit POP5

Chain E:

72% 12% 16%

GLY ARG GLU ASN GLU ASN GLU ASN GLU ASP

• Molecule 6: Ribonucleases P/MRP protein subunit POP6

Chain F:
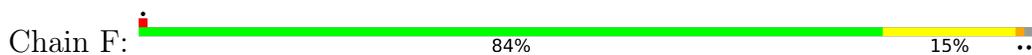
• Molecule 7: Ribonucleases P/MRP protein subunit POP7

Chain G:
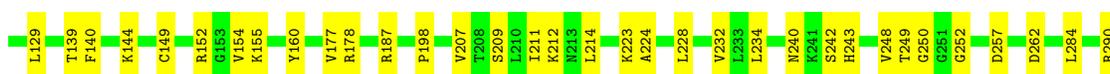

• Molecule 8: Ribonucleases P/MRP protein subunit POP8

Chain H:

• Molecule 9: Ribonuclease P/MRP protein subunit RPP1

Chain I:

• Molecule 9: Ribonuclease P/MRP protein subunit RPP1

Chain J:

• Molecule 10: Ribonuclease MRP protein subunit SNM1

Chain K:

36% 15% • 47%

M1 Y9 R12 R15 Y18 N19 H22 V23 L24 P25 T26 R30 S33 G34 L35 H41 V44 L51 P52 E53 Q54 L55 K56 K59 F60 C61 S62 H63 C64 V67 P70 N71 PHE ASN ALA SER LEU GLN LEU THR THR ASN THR GLN G85

L90 E93 K99 K100 C101 I102 Q103 L114 F115 E116 W117 LYS SER GLU PHE VAL VAL PRO THR PHE GLY GLN ASP VAL VAL SER PRO MET ILE ASN SER THR SER SER GLY LYS VAL SER TYR ALA VAL LYS LYS PRO GLN LYS SER LYS THR SER THR GLY LYS GLU ARG SER LYS LYS

ARG LYS LEU ASN SER LEU THR ASN LEU LEU SER LYS ARG ASN GLN GLU LYS LYS MET GLU LYS LYS LYS SER SER LEU LEU GLU SER PHE MET LYS SER

• Molecule 11: Ribonuclease MRP protein subunit RMP1

Chain L:

51% 14% 35%

MET ASP E3 L11 E14 R24 A32 E40 R43 L51 F52 S53 S54 R55 R56 K60 R61 L62 K69 R72 L73 L74 L78 I93 A94 L95 G96 Q97 F98 V99 T100 L101 L109 A110 N111 V112 Y116 L119 E126 R129 L133 ILE

LYS ASN LEU PRO ARG THR LYS ALA LYS SER VAL VAL ASN ASP VAL GLU GLU LEU GLY GLU ILE ILE ASP GLU ILE GLY ASN ASN VAL GLN GLU ASN GLU LEU VAL ILE THR SER ILE PRO LYS PRO LEU THR GLU ASN CYS LYS LYS LYS LYS LYS ARG LYS LYS LYS ASN LYS SER

ALA ILE ASP GLY ILE PHE GLY

4   Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1232761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	A	0.14	0/7828	0.72	0/12182
2	B	0.24	0/6593	0.40	0/8887
3	C	0.27	0/1281	0.54	0/1744
4	D	0.25	0/2123	0.41	0/2851
5	E	0.23	0/1148	0.38	0/1542
6	F	0.23	0/1289	0.41	0/1733
7	G	0.23	0/972	0.41	0/1305
8	H	0.25	0/1101	0.43	0/1488
9	I	0.23	0/1908	0.42	0/2577
9	J	0.23	0/2283	0.41	0/3080
10	K	0.25	0/856	0.47	0/1145
11	L	0.23	0/1132	0.43	0/1523
All	All	0.22	0/28514	0.53	0/40057

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
10	K	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	K	22	HIS	Peptide

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Mol	Chain	Res	Type	Group
10	K	99	LYS	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7008	0	3534	111	0
2	B	6453	0	6530	115	0
3	C	1246	0	1261	50	0
4	D	2086	0	2132	53	0
5	E	1135	0	1199	15	0
6	F	1271	0	1305	17	0
7	G	960	0	1005	8	0
8	H	1079	0	1037	12	0
9	I	1881	0	1975	34	0
9	J	2253	0	2344	43	0
10	K	840	0	830	24	0
11	L	1110	0	1138	21	0
12	A	1	0	0	0	0
13	K	1	0	0	0	0
All	All	27324	0	24290	447	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 447 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:C:151:LYS:HA	3:C:154:VAL:HG12	1.59	0.84
8:H:91:VAL:HG12	8:H:93:SER:H	1.44	0.83
2:B:587:GLN:O	2:B:597:TYR:OH	1.97	0.81
2:B:353:LEU:HG	2:B:374:ILE:HD11	1.63	0.80
2:B:729:PRO:HD3	2:B:759:PRO:HB2	1.61	0.80

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	B	785/875 (90%)	730 (93%)	54 (7%)	1 (0%)	51	73
3	C	150/195 (77%)	129 (86%)	21 (14%)	0	100	100
4	D	247/279 (88%)	240 (97%)	7 (3%)	0	100	100
5	E	143/173 (83%)	138 (96%)	5 (4%)	0	100	100
6	F	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
7	G	117/140 (84%)	114 (97%)	3 (3%)	0	100	100
8	H	129/133 (97%)	124 (96%)	5 (4%)	0	100	100
9	I	240/293 (82%)	221 (92%)	18 (8%)	1 (0%)	34	54
9	J	290/293 (99%)	277 (96%)	13 (4%)	0	100	100
10	K	100/198 (50%)	89 (89%)	10 (10%)	1 (1%)	15	28
11	L	129/201 (64%)	126 (98%)	3 (2%)	0	100	100
All	All	2485/2938 (85%)	2340 (94%)	142 (6%)	3 (0%)	54	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	593	ASN
10	K	23	VAL
9	I	138	PRO

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	B	718/785 (92%)	716 (100%)	2 (0%)	92	97	
3	C	144/185 (78%)	143 (99%)	1 (1%)	84	94	
4	D	235/261 (90%)	234 (100%)	1 (0%)	91	97	
5	E	133/160 (83%)	133 (100%)	0	100	100	
6	F	148/149 (99%)	147 (99%)	1 (1%)	84	94	
7	G	110/127 (87%)	110 (100%)	0	100	100	
8	H	122/123 (99%)	122 (100%)	0	100	100	
9	I	216/258 (84%)	216 (100%)	0	100	100	
9	J	257/258 (100%)	256 (100%)	1 (0%)	91	97	
10	K	95/184 (52%)	95 (100%)	0	100	100	
11	L	118/182 (65%)	117 (99%)	1 (1%)	81	93	
All	All	2296/2672 (86%)	2289 (100%)	7 (0%)	92	97	

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	22	LYS
6	F	132	ARG
11	L	62	LEU
9	J	144	LYS
3	C	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	83	HIS
9	J	48	ASN
4	D	197	GLN
8	H	71	HIS
4	D	99	ASN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	329/340 (96%)	79 (24%)	13 (3%)

5 of 79 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	A
1	A	25	A
1	A	26	A
1	A	30	G
1	A	36	U

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	104	A
1	A	143	U
1	A	318	A
1	A	205	U
1	A	227	C

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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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-30296. 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 |
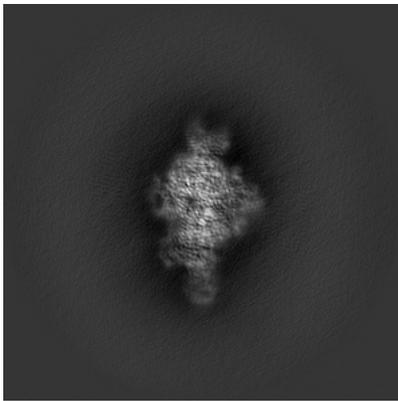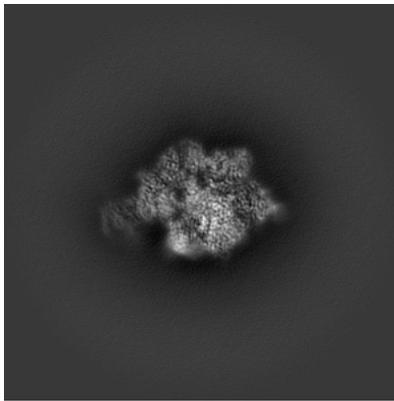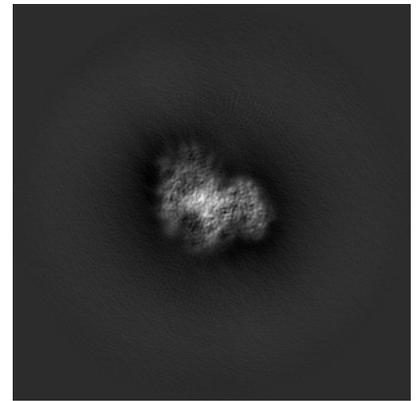
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
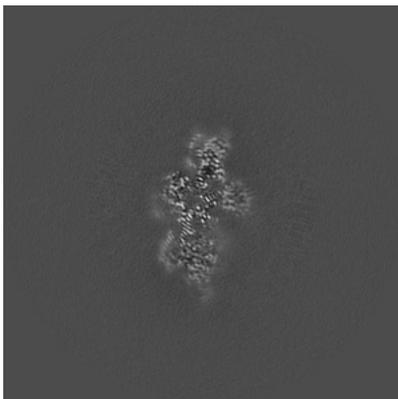
6.2.1   Primary map
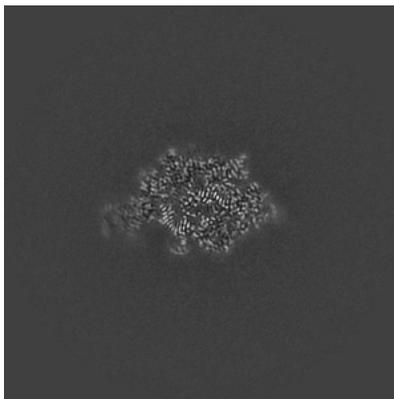
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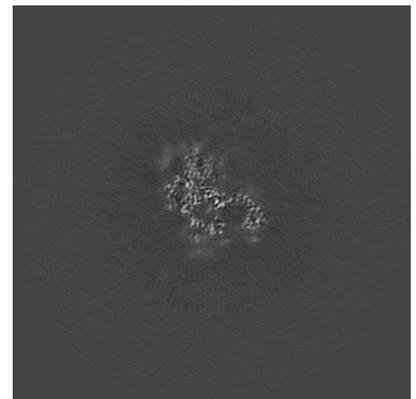
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
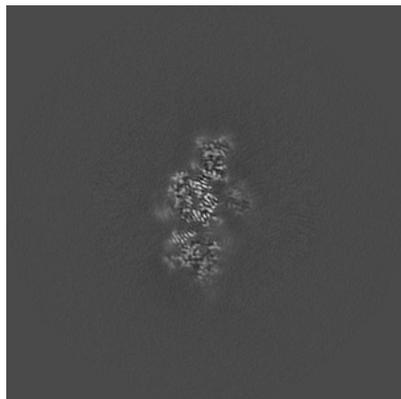
6.3.1 Primary map
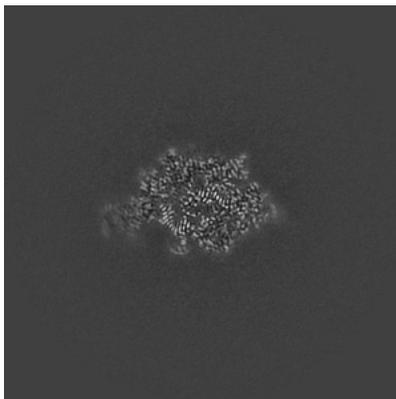
| X Index: 195 | Y Index: 192 | Z Index: 203 |
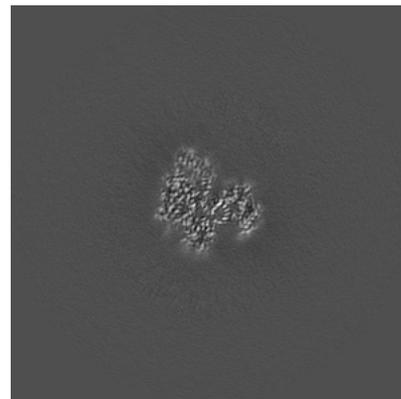
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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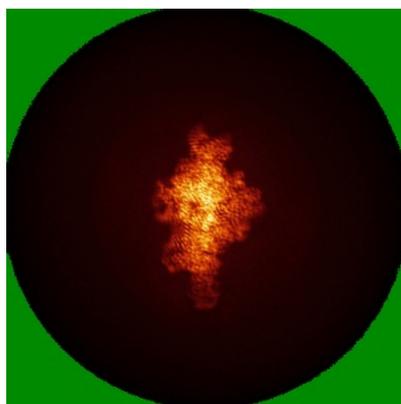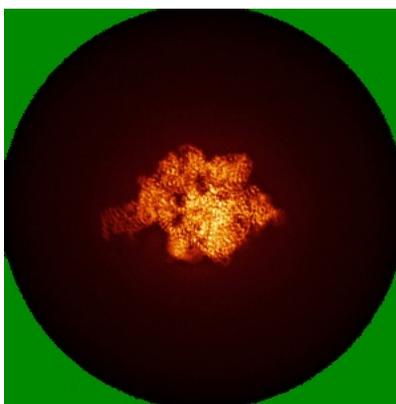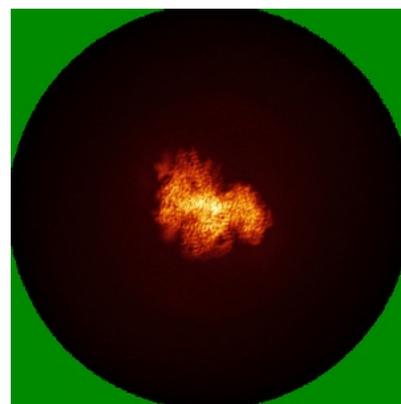
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
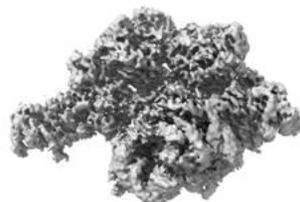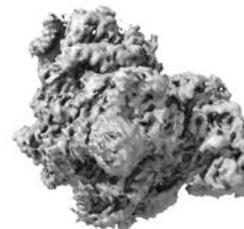
The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.
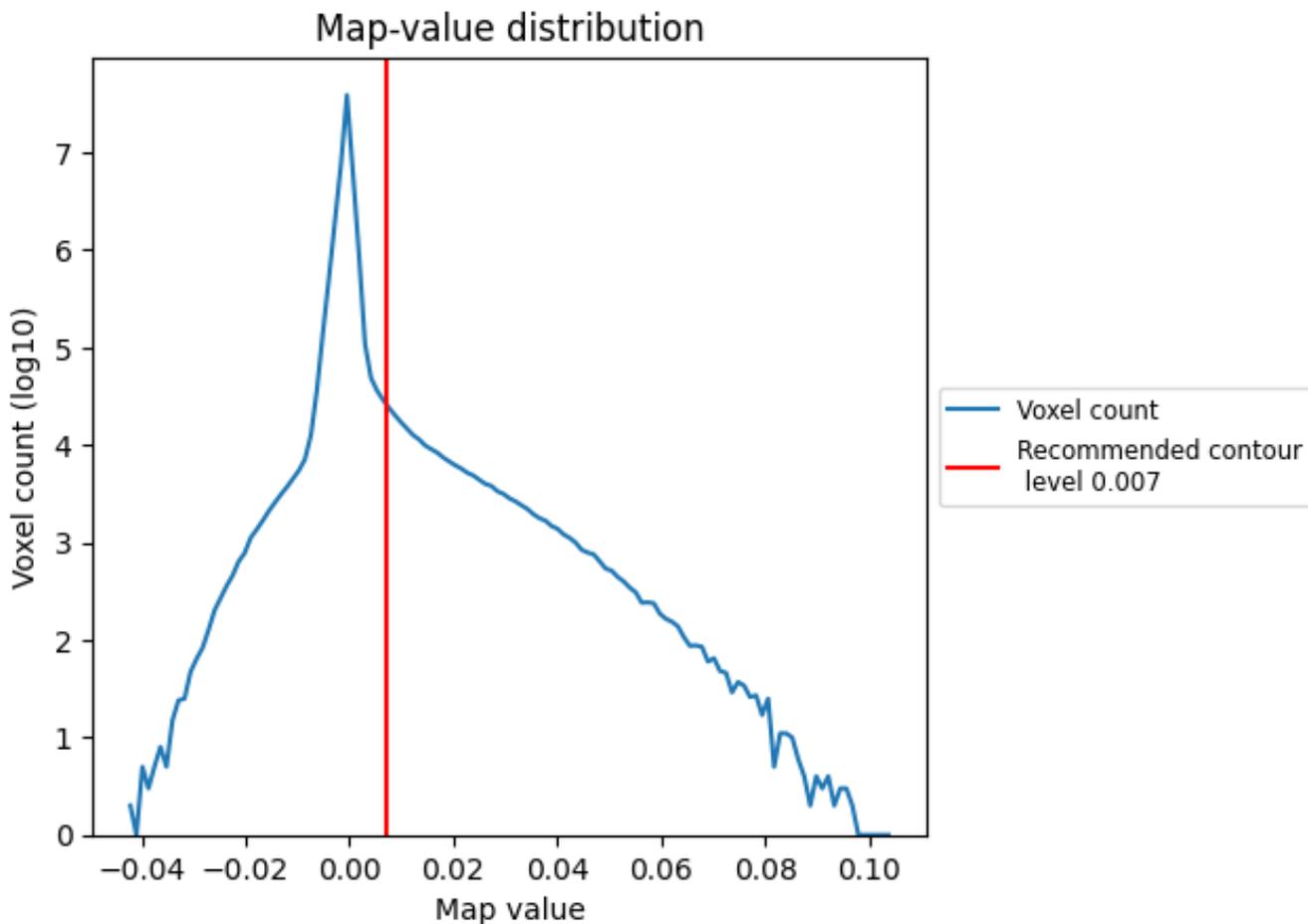
6.6 Mask visualisation (i)

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 ⓘ
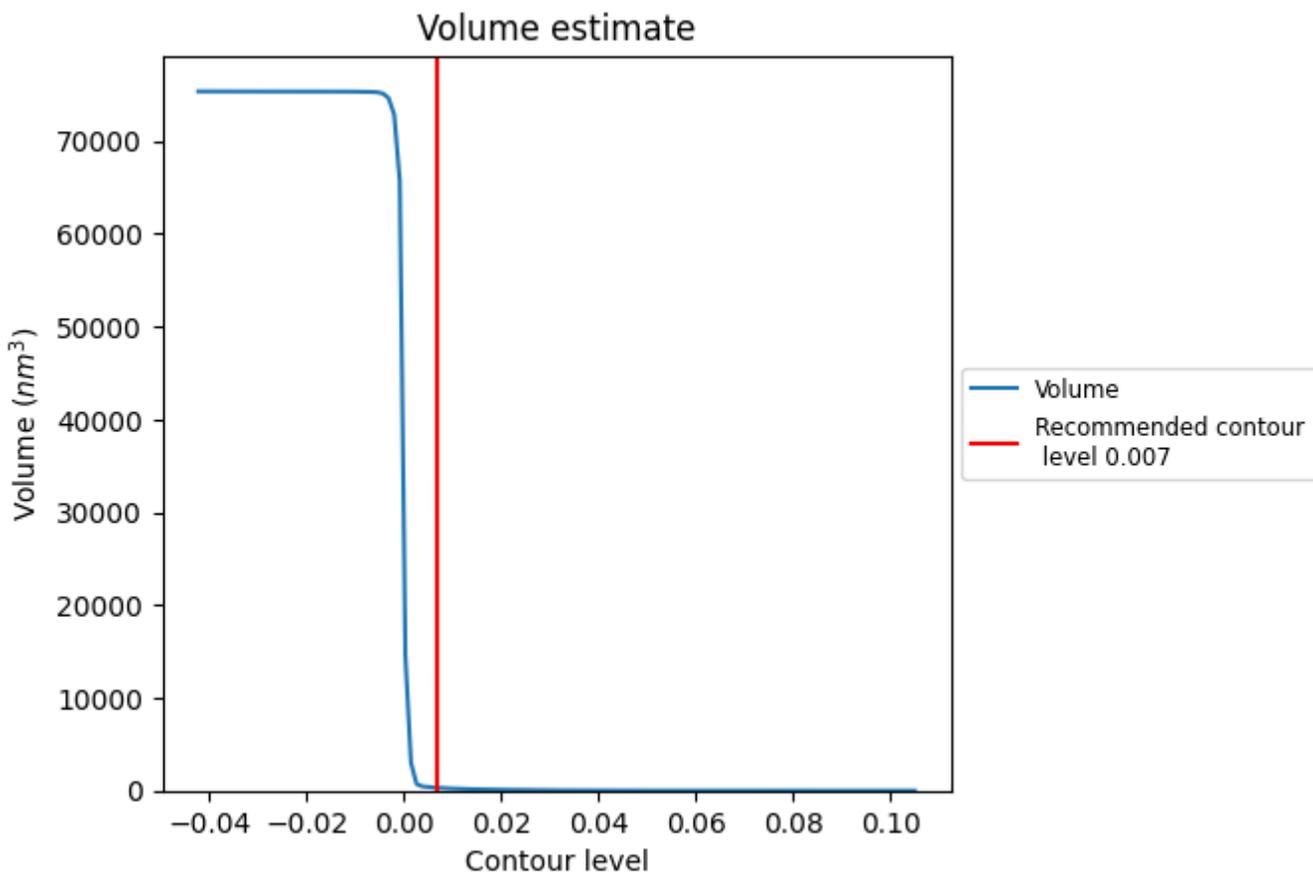
The volume at the recommended contour level is 302 nm^3; this corresponds to an approximate mass of 273 kDa.

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 ⓘ
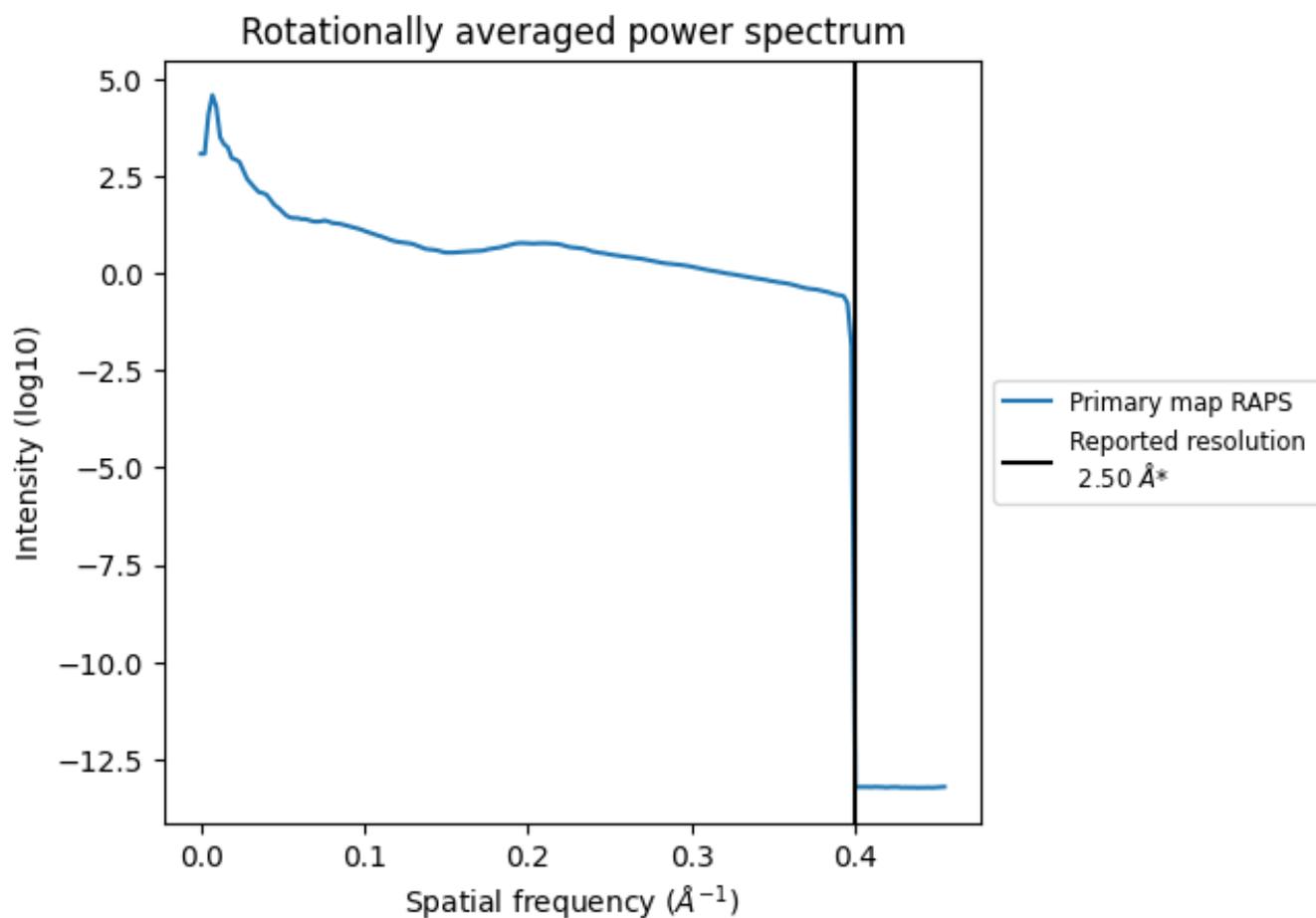
*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}
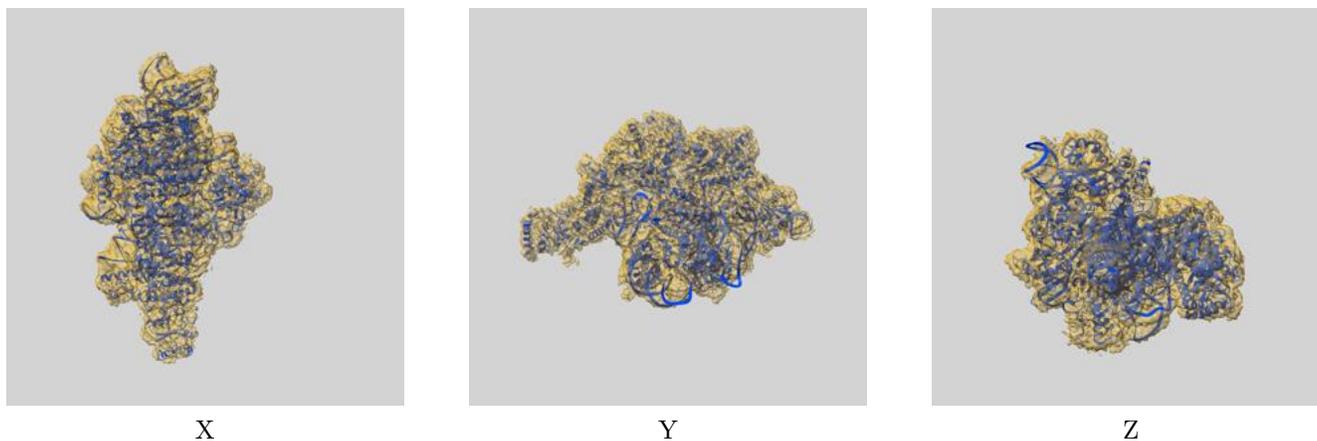
8 Fourier-Shell correlation (i)

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-30296 and PDB model 7C79. 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 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model (i)

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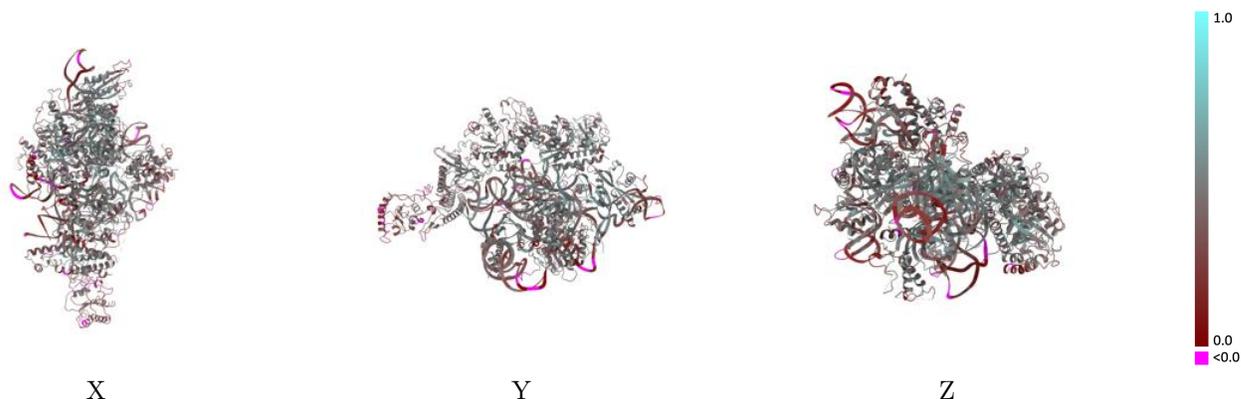
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
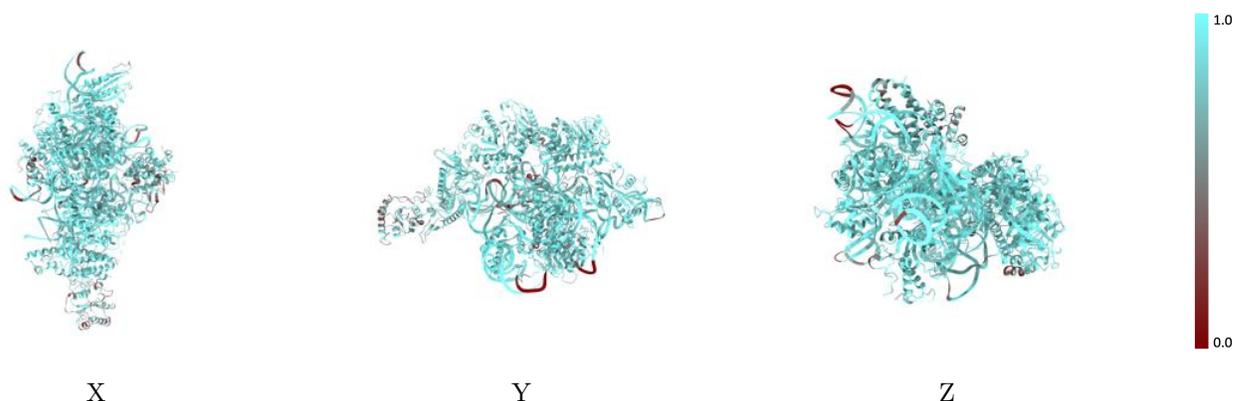
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4   Atom inclusion ⓘ
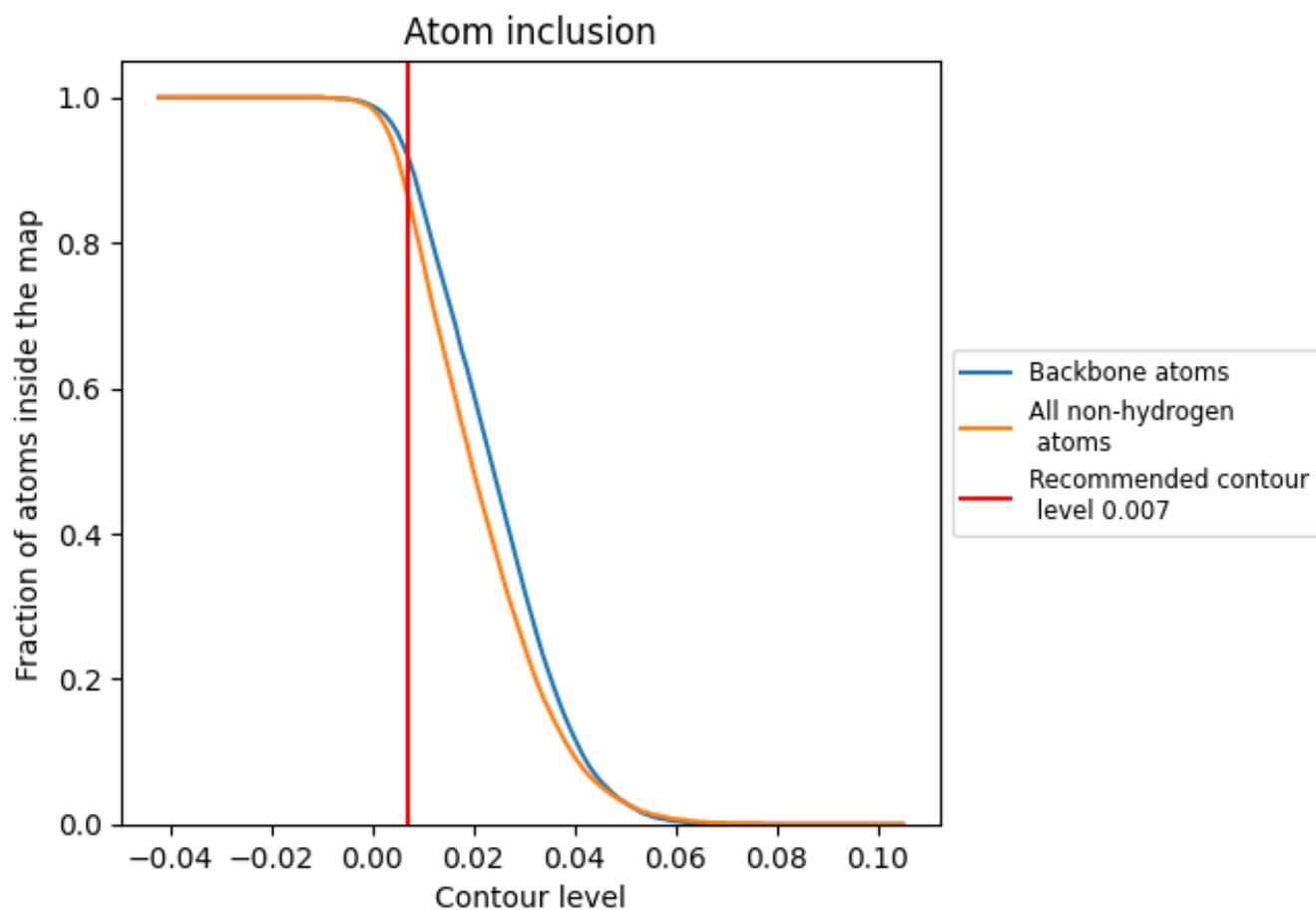
At the recommended contour level, 92% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.4020
A	0.8770	0.3610
B	0.8920	0.4380
C	0.6030	0.2430
D	0.8220	0.4020
E	0.9120	0.4620
F	0.9020	0.4350
G	0.9200	0.4830
H	0.8080	0.3590
I	0.8980	0.4570
J	0.8900	0.4140
K	0.8480	0.3720
L	0.8390	0.3970

1.0

0.0
<0.0