WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Jun 1, 2024 – 07:46 AM EDT

PDB ID	:	7UBN
EMDB ID	:	EMD-26439
Title	:	Transcription antitermination complex: NusA-containing "engaged" Qlambda-loading complex
Authors	:	Yin, Z.; Ebright, R.H.
Deposited on	:	2022-03-15
Resolution	:	3.36 Å(reported)
Based on initial models	:	1LB2, 5LM9, 5LM7, 4YLN

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 3.36 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		7
Ramachandran outliers		0
Sidechain outliers		4.9%
RNA backbone		0.61

Worse   *Better*

▌ Percentile relative to all structures

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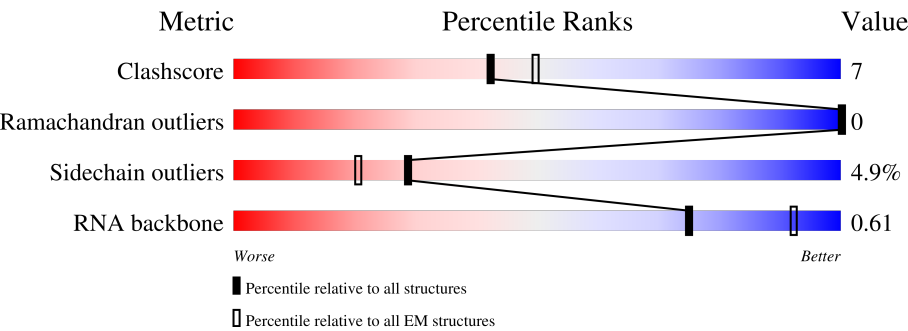
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1	61	• 56% 31% 13%
2	2	61	• 64% 21% 15%
3	A	329	5% 59% 11% 30%
3	B	329	32% 66% 22% • 11%
4	C	1342	15% 81% 18% •
5	D	1430	16% 76% 16% 7%
6	E	91	52% 69% 11% • 18%

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Mol	Chain	Length	Quality of chain
7	F	627	31% / 40% / 15% / · / 44%
8	N	515	55% / 46% / 20% / 34%
9	Q	207	8% / 79% / 19% / ·
10	R	11	9% / 73% / 18% / 9%

2　Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 35069 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 DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	53	Total	C	N	O	P	0	0
			1096	525	195	323	53		

- Molecule 2 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	52	Total	C	N	O	P	0	0
			1052	506	184	310	52		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		
3	B	294	Total	C	N	O	S	0	0
			2274	1420	400	447	7		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	1339	Total	C	N	O	S	0	0
			10556	6620	1840	2053	43		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	1327	Total	C	N	O	S	0	0
			10319	6484	1839	1947	49		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1409	GLU	-	expression tag	UNP P0A8T7
D	1410	ARG	-	expression tag	UNP P0A8T7
D	1411	ARG	-	expression tag	UNP P0A8T7
D	1412	ALA	-	expression tag	UNP P0A8T7
D	1413	SER	-	expression tag	UNP P0A8T7
D	1414	GLU	-	expression tag	UNP P0A8T7
D	1415	ASN	-	expression tag	UNP P0A8T7
D	1416	LEU	-	expression tag	UNP P0A8T7
D	1417	TYR	-	expression tag	UNP P0A8T7
D	1418	PHE	-	expression tag	UNP P0A8T7
D	1419	GLN	-	expression tag	UNP P0A8T7
D	1420	GLY	-	expression tag	UNP P0A8T7
D	1421	HIS	-	expression tag	UNP P0A8T7
D	1422	HIS	-	expression tag	UNP P0A8T7
D	1423	HIS	-	expression tag	UNP P0A8T7
D	1424	HIS	-	expression tag	UNP P0A8T7
D	1425	HIS	-	expression tag	UNP P0A8T7
D	1426	HIS	-	expression tag	UNP P0A8T7
D	1427	HIS	-	expression tag	UNP P0A8T7
D	1428	HIS	-	expression tag	UNP P0A8T7
D	1429	HIS	-	expression tag	UNP P0A8T7
D	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	75	600	365	114	120	1	0	0

- Molecule 7 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	353	2900	1823	521	539	17	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	MET	-	expression tag	UNP Q0P6L9
F	-12	GLY	-	expression tag	UNP Q0P6L9
F	-11	SER	-	expression tag	UNP Q0P6L9
F	-10	SER	-	expression tag	UNP Q0P6L9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP Q0P6L9
F	-8	HIS	-	expression tag	UNP Q0P6L9
F	-7	HIS	-	expression tag	UNP Q0P6L9
F	-6	HIS	-	expression tag	UNP Q0P6L9
F	-5	HIS	-	expression tag	UNP Q0P6L9
F	-4	HIS	-	expression tag	UNP Q0P6L9
F	-3	SER	-	expression tag	UNP Q0P6L9
F	-2	SER	-	expression tag	UNP Q0P6L9
F	-1	GLY	-	expression tag	UNP Q0P6L9
F	0	HIS	-	expression tag	UNP Q0P6L9

- Molecule 8 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	340	2674	1662	481	522	9	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-19	MET	-	expression tag	UNP C3SSN7
N	-18	GLY	-	expression tag	UNP C3SSN7
N	-17	SER	-	expression tag	UNP C3SSN7
N	-16	SER	-	expression tag	UNP C3SSN7
N	-15	HIS	-	expression tag	UNP C3SSN7
N	-14	HIS	-	expression tag	UNP C3SSN7
N	-13	HIS	-	expression tag	UNP C3SSN7
N	-12	HIS	-	expression tag	UNP C3SSN7
N	-11	HIS	-	expression tag	UNP C3SSN7
N	-10	HIS	-	expression tag	UNP C3SSN7
N	-9	SER	-	expression tag	UNP C3SSN7
N	-8	SER	-	expression tag	UNP C3SSN7
N	-7	GLY	-	expression tag	UNP C3SSN7
N	-6	LEU	-	expression tag	UNP C3SSN7
N	-5	VAL	-	expression tag	UNP C3SSN7
N	-4	PRO	-	expression tag	UNP C3SSN7
N	-3	ARG	-	expression tag	UNP C3SSN7
N	-2	GLY	-	expression tag	UNP C3SSN7
N	-1	SER	-	expression tag	UNP C3SSN7
N	0	HIS	-	expression tag	UNP C3SSN7

- Molecule 9 is a protein called Antitermination protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	207	Total 1567	C 972	N 287	O 291	S 17	0	0

- Molecule 10 is a RNA chain called RNA (5'-R(*UP*GP*GP*GP*AP*GP*AP*GP*GP*UP *A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	11	Total 241	C 108	N 49	O 74	P 10	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	D	2	Total 2	Zn 2	0
11	Q	1	Total 1	Zn 1	0

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

Mol	Chain	Residues	Atoms		AltConf
12	D	1	Total 1	Mg 1	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: DNA (53-MER)
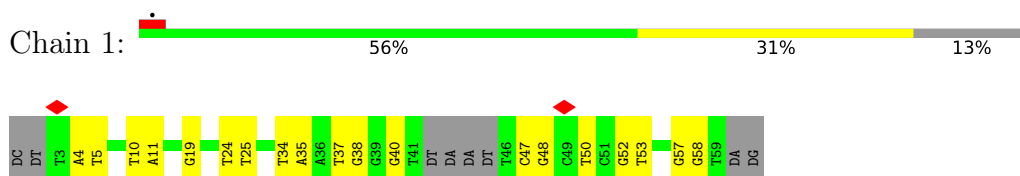
Chain 1:

• Molecule 2: DNA (52-MER)
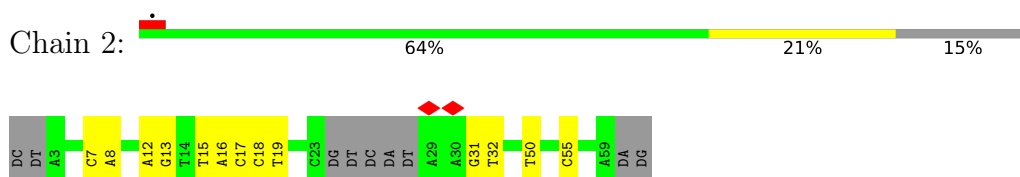
Chain 2:

• Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain A:

• Molecule 3: DNA-directed RNA polymerase subunit alpha

Chain B:

• Molecule 4: DNA-directed RNA polymerase subunit beta

Chain C:

15%

81%

18%
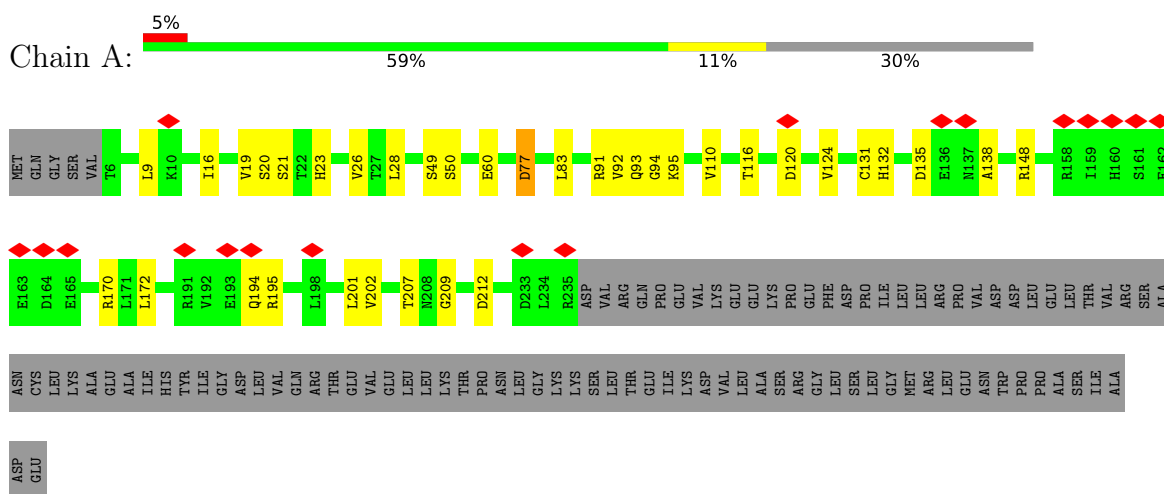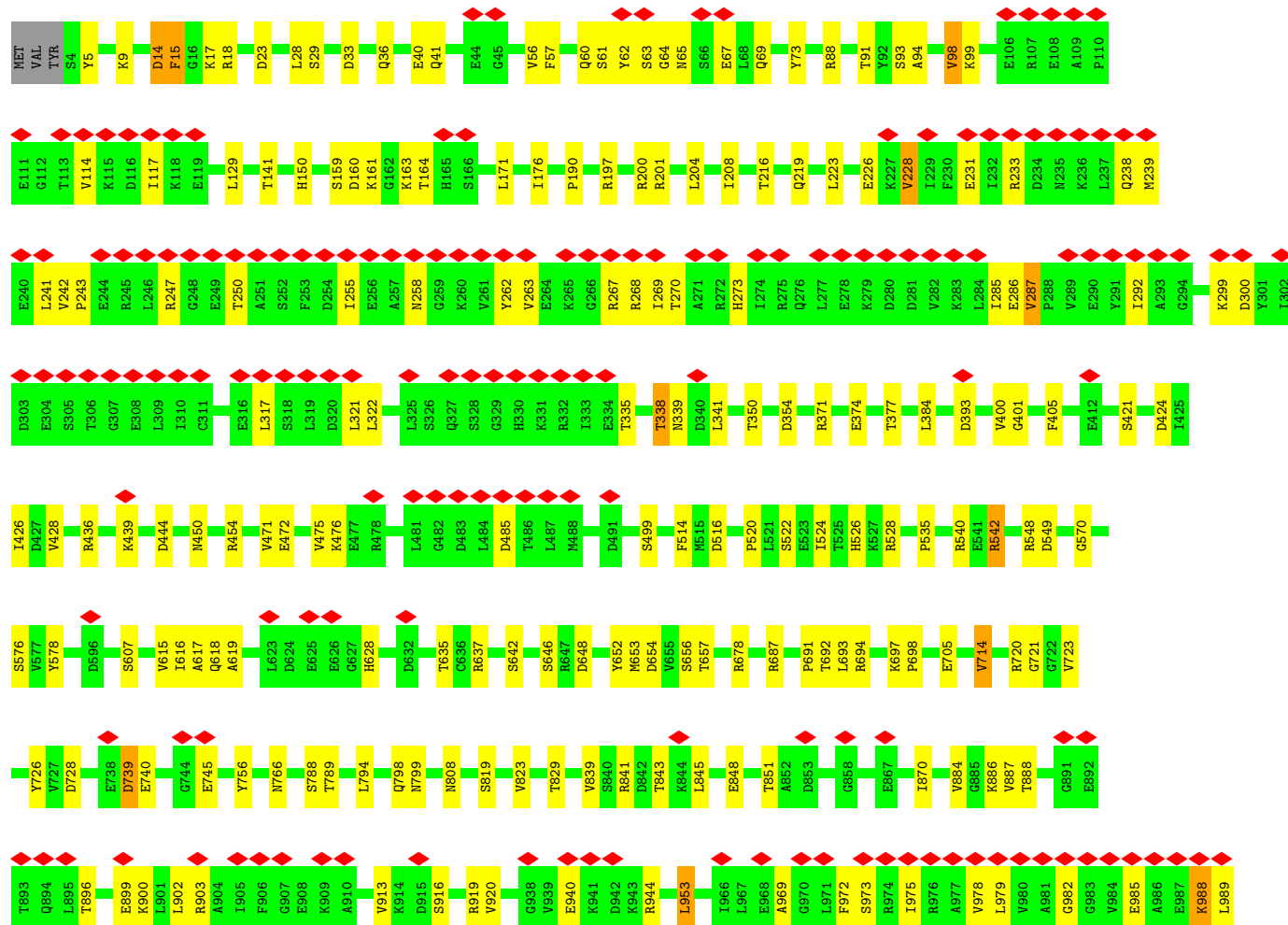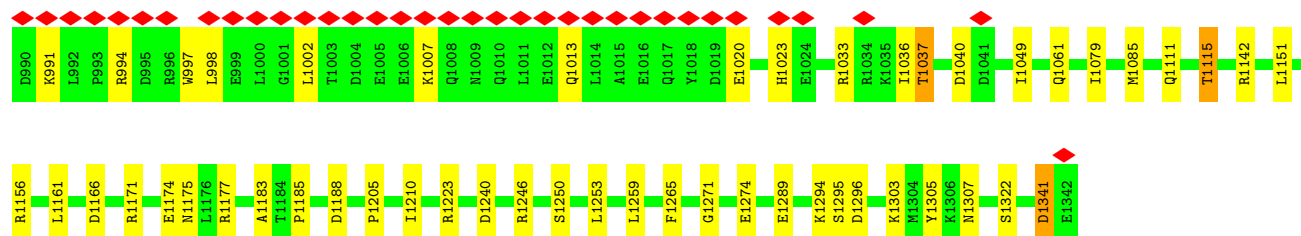
• Molecule 5: DNA-directed RNA polymerase subunit beta'

• Molecule 6: DNA-directed RNA polymerase subunit omega

Chain E:

• Molecule 7: RNA polymerase sigma factor RpoD
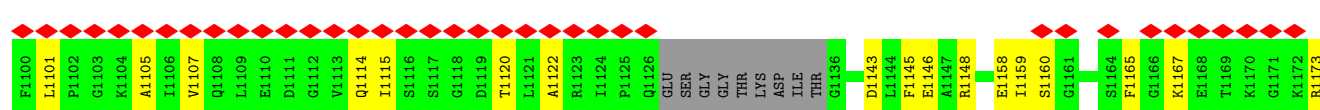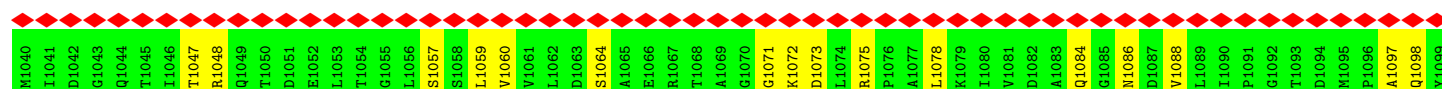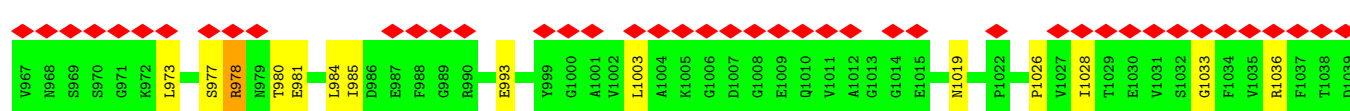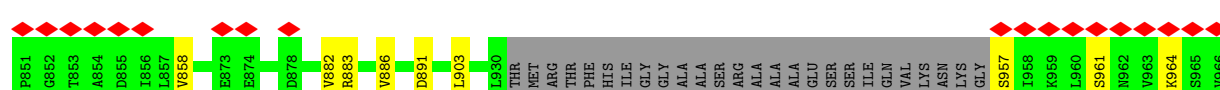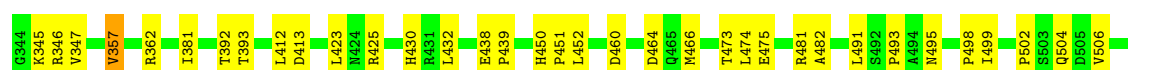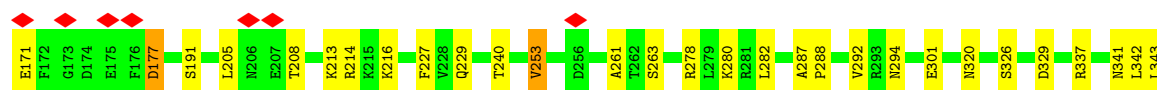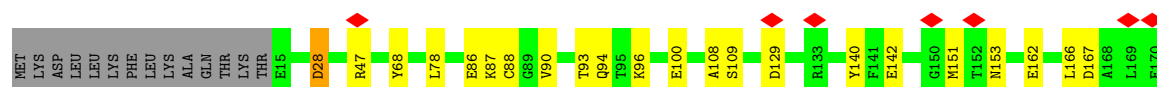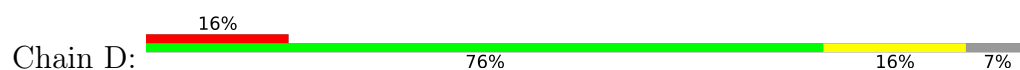
Chain F:

• Molecule 8: Transcription termination/antitermination protein NusA
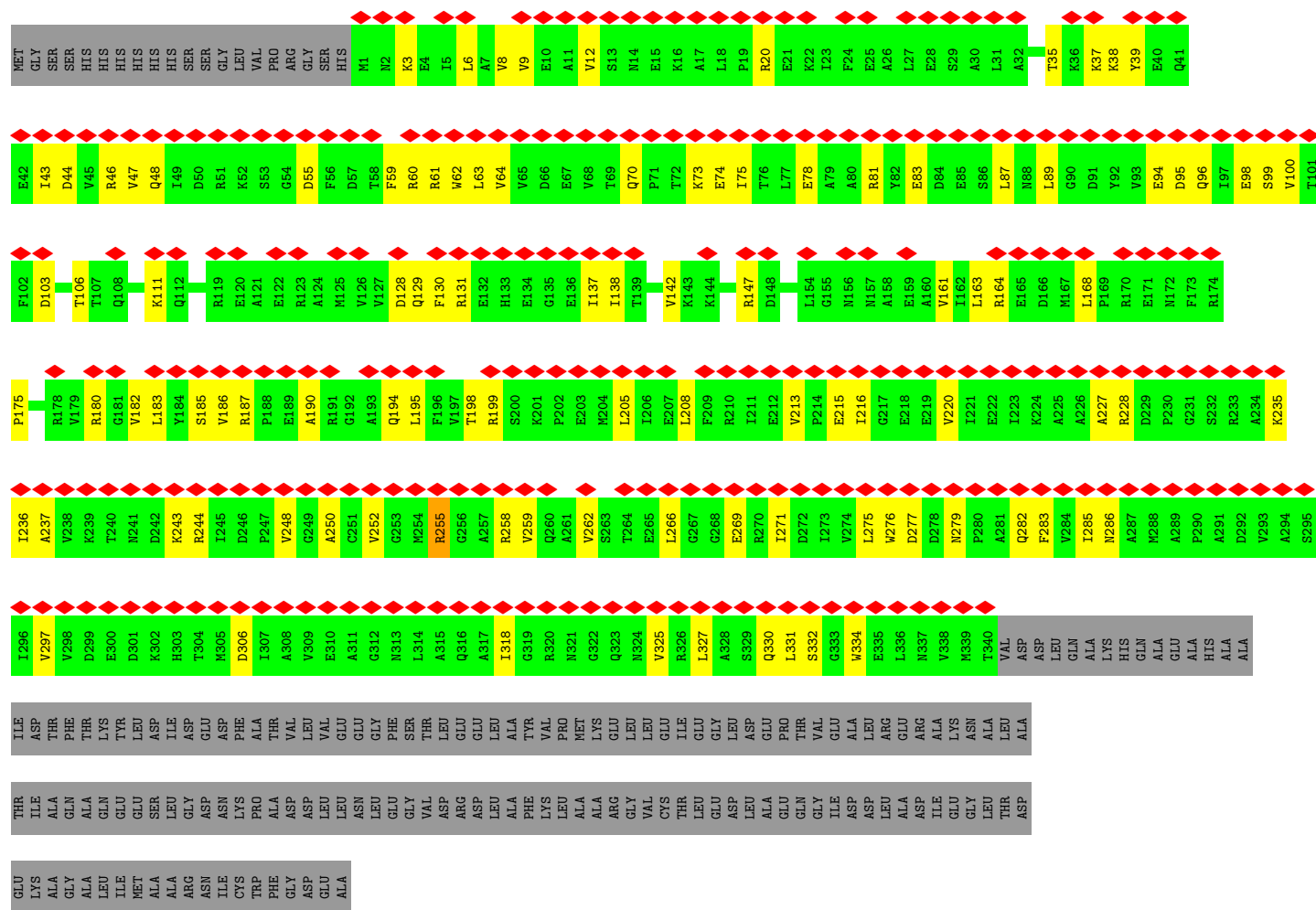
Chain N:

• Molecule 9: Antitermination protein
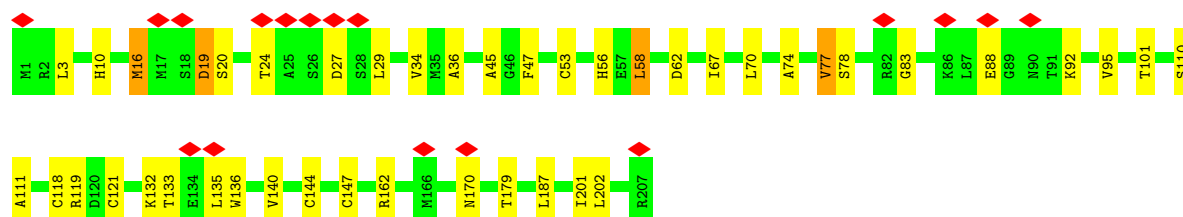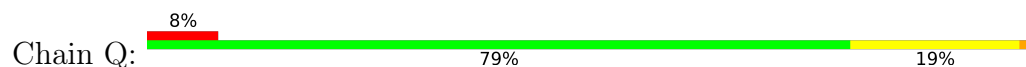
Chain Q:

• Molecule 10: RNA (5'-R(*UP*GP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3')

Chain R:

9%

73%   18%   9%

U1 G2 G3 G8 A11
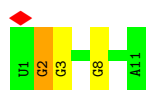
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.1	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0402	Depositor
Map size (Å)	262.144, 262.144, 262.144	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.024, 1.024, 1.024	Depositor

5   Model quality (i)

5.1   Standard geometry (i)

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

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	1	0.64	0/1228	1.06	0/1894
2	2	0.74	0/1176	1.02	0/1806
3	A	0.32	0/1808	0.48	0/2450
3	B	0.30	0/2300	0.57	0/3116
4	C	0.37	0/10724	0.52	0/14468
5	D	0.36	0/10476	0.53	0/14146
6	E	0.29	0/602	0.49	0/810
7	F	0.29	0/2936	0.54	0/3935
8	N	0.31	0/2708	0.62	0/3659
9	Q	0.32	0/1595	0.55	0/2147
10	R	0.81	0/271	1.07	0/423
All	All	0.38	0/35824	0.60	0/48854

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	1096	0	605	15	0
2	2	1052	0	590	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1786	0	1813	18	0
3	B	2274	0	2329	48	0
4	C	10556	0	10566	141	0
5	D	10319	0	10530	124	0
6	E	600	0	607	10	0
7	F	2900	0	2956	65	0
8	N	2674	0	2705	64	0
9	Q	1567	0	1572	38	0
10	R	241	0	120	3	0
11	D	2	0	0	0	0
11	Q	1	0	0	0	0
12	D	1	0	0	0	0
All	All	35069	0	34393	496	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 7.

The worst 5 of 496 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)
9:Q:53:CYS:HA	9:Q:58:LEU:HD11	1.44	0.98
7:F:290:LEU:HD21	7:F:336:GLU:OE1	1.67	0.95
5:D:78:LEU:HD21	9:Q:56:HIS:NE2	1.87	0.90
9:Q:58:LEU:HD12	9:Q:58:LEU:O	1.82	0.79
9:Q:53:CYS:HA	9:Q:58:LEU:CD1	2.15	0.77

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	
3	A	228/329 (69%)	223 (98%)	5 (2%)	0	100	100
3	B	290/329 (88%)	273 (94%)	17 (6%)	0	100	100
4	C	1337/1342 (100%)	1269 (95%)	68 (5%)	0	100	100
5	D	1321/1430 (92%)	1253 (95%)	68 (5%)	0	100	100
6	E	73/91 (80%)	71 (97%)	2 (3%)	0	100	100
7	F	345/627 (55%)	325 (94%)	20 (6%)	0	100	100
8	N	339/515 (66%)	318 (94%)	21 (6%)	0	100	100
9	Q	205/207 (99%)	191 (93%)	14 (7%)	0	100	100
All	All	4138/4870 (85%)	3923 (95%)	215 (5%)	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	
3	A	198/286 (69%)	191 (96%)	7 (4%)	36	66
3	B	254/286 (89%)	242 (95%)	12 (5%)	26	58
4	C	1153/1157 (100%)	1109 (96%)	44 (4%)	33	63
5	D	1110/1189 (93%)	1049 (94%)	61 (6%)	21	53
6	E	65/75 (87%)	61 (94%)	4 (6%)	18	49
7	F	310/552 (56%)	284 (92%)	26 (8%)	11	37
8	N	288/426 (68%)	280 (97%)	8 (3%)	43	71
9	Q	164/164 (100%)	154 (94%)	10 (6%)	18	50
All	All	3542/4135 (86%)	3370 (95%)	172 (5%)	29	57

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	1145	PHE
7	F	357	GLN

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Mol	Chain	Res	Type
5	D	1226	VAL
7	F	147	GLN
7	F	552	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	1259	GLN
7	F	409	ASN
7	F	265	GLN
7	F	342	GLN
8	N	112	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	R	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	R	2	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 ⓘ

Of 4 ligands modelled in this entry, 4 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-26439. 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 ⓘ
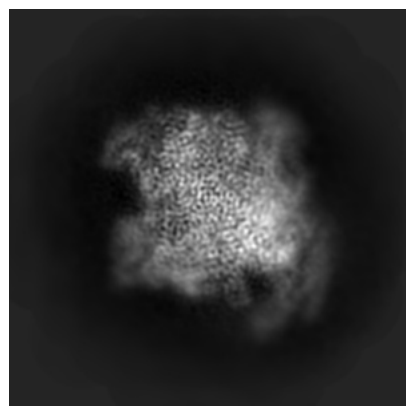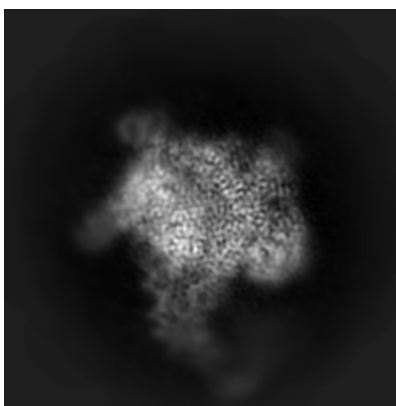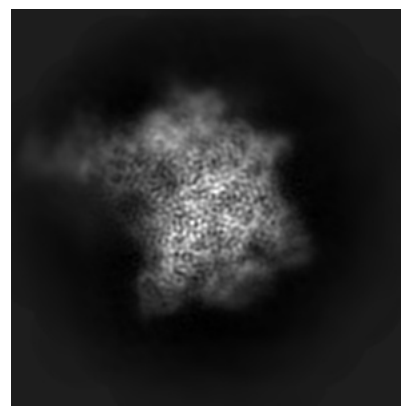
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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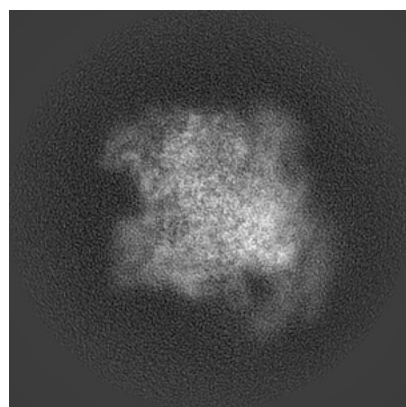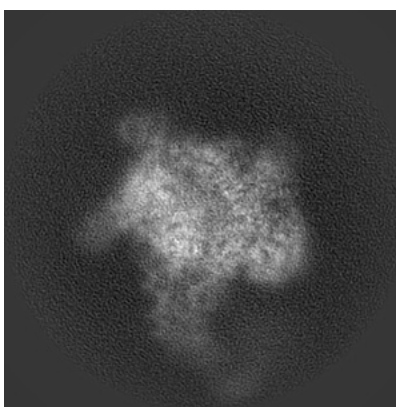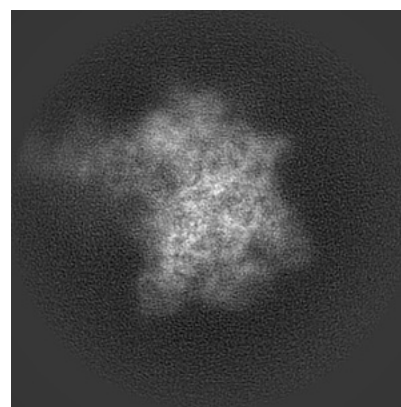
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
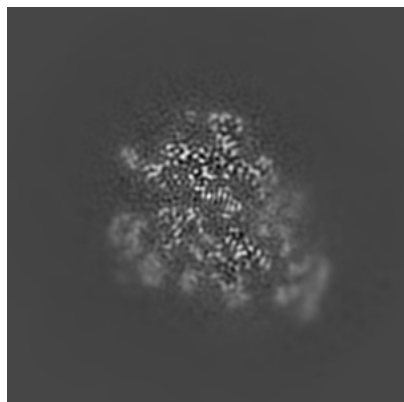
6.2.1   Primary map
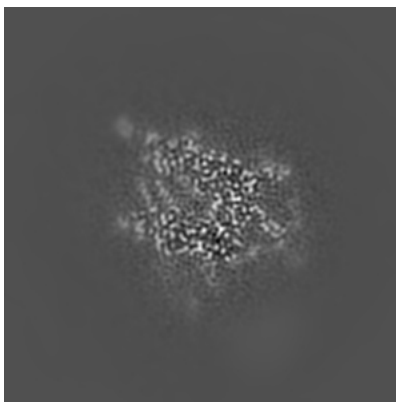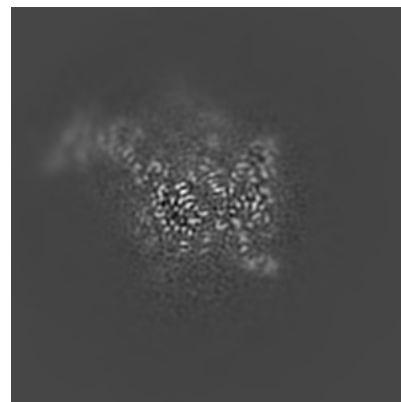
| X Index: 128 | Y Index: 128 | Z Index: 128 |

6.2.2   Raw map
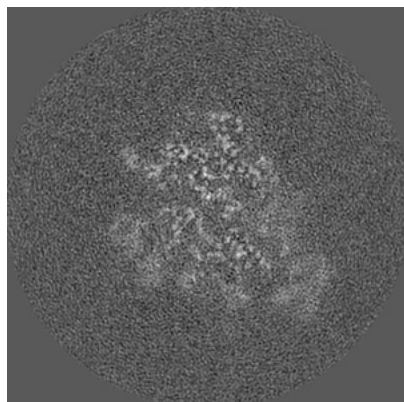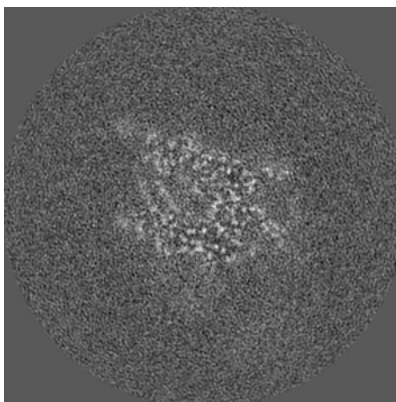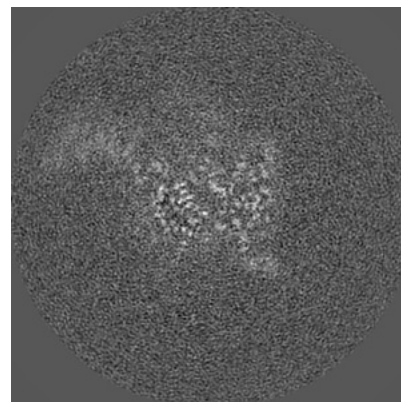
| X Index: 128 | Y Index: 128 | Z Index: 128 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
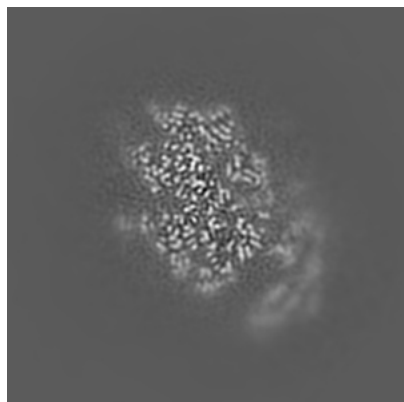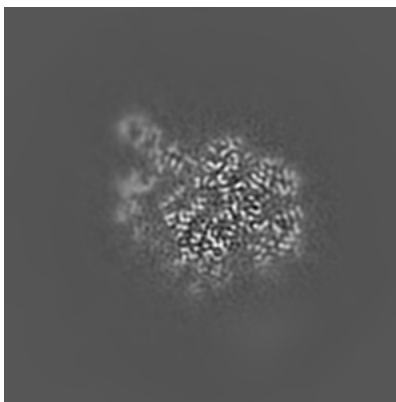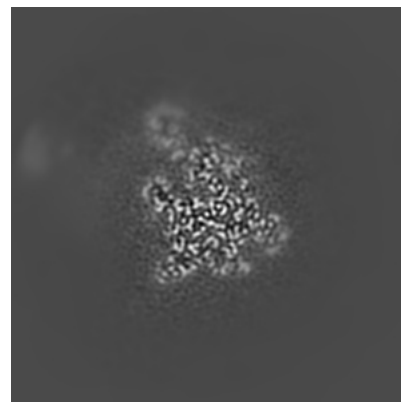
| X Index: 116 | Y Index: 117 | Z Index: 147 |

6.3.2 Raw map
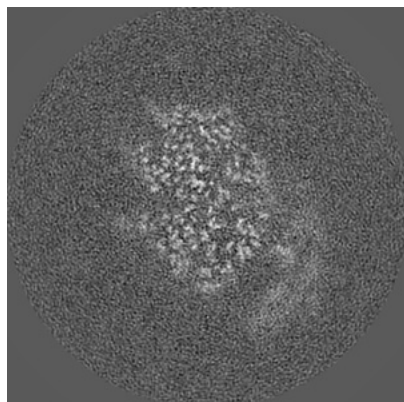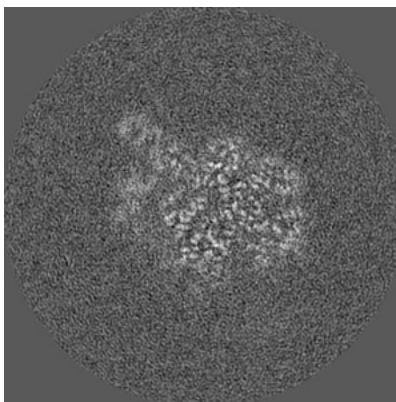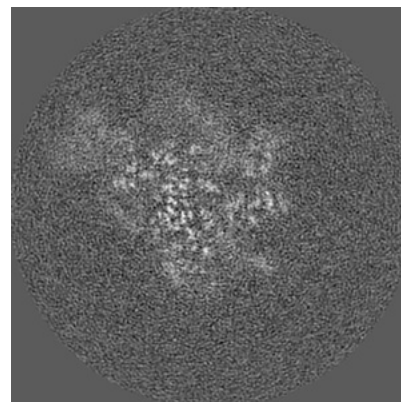
| X Index: 116 | Y Index: 117 | Z Index: 122 |

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
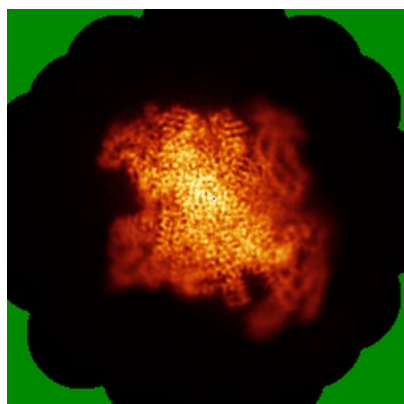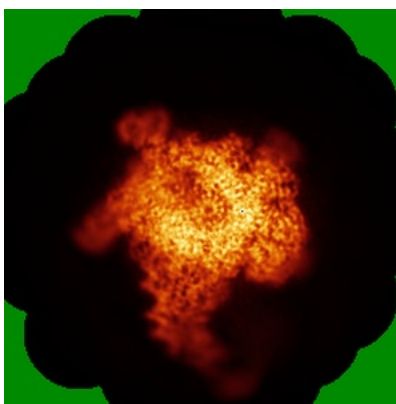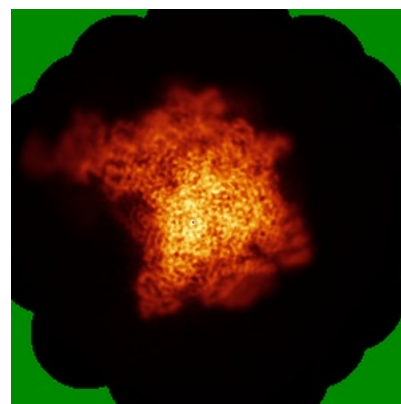
X   Y   Z

6.4.2 Raw map

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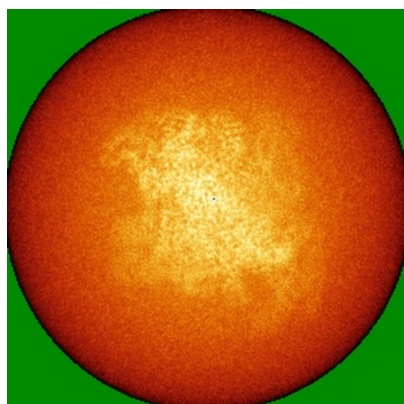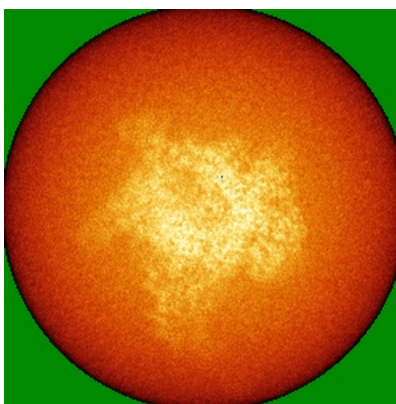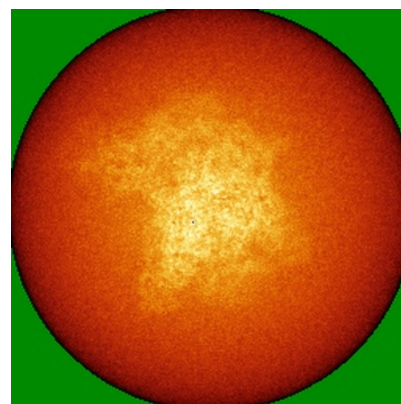
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0402. 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
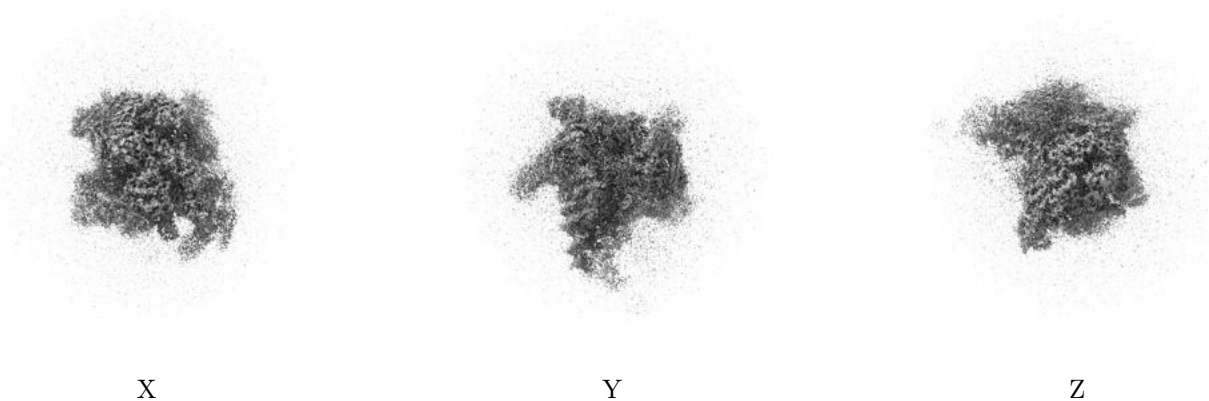
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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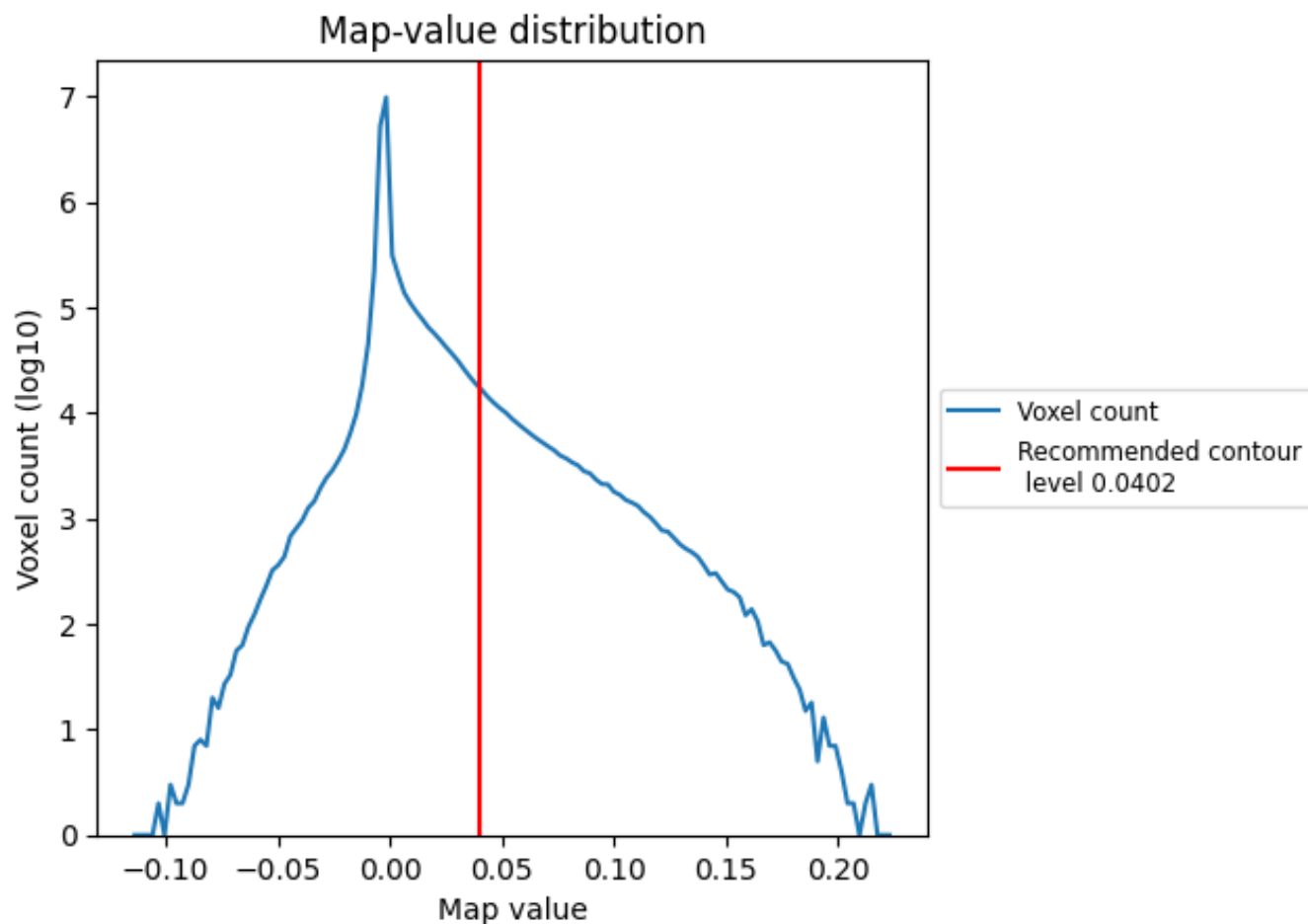
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
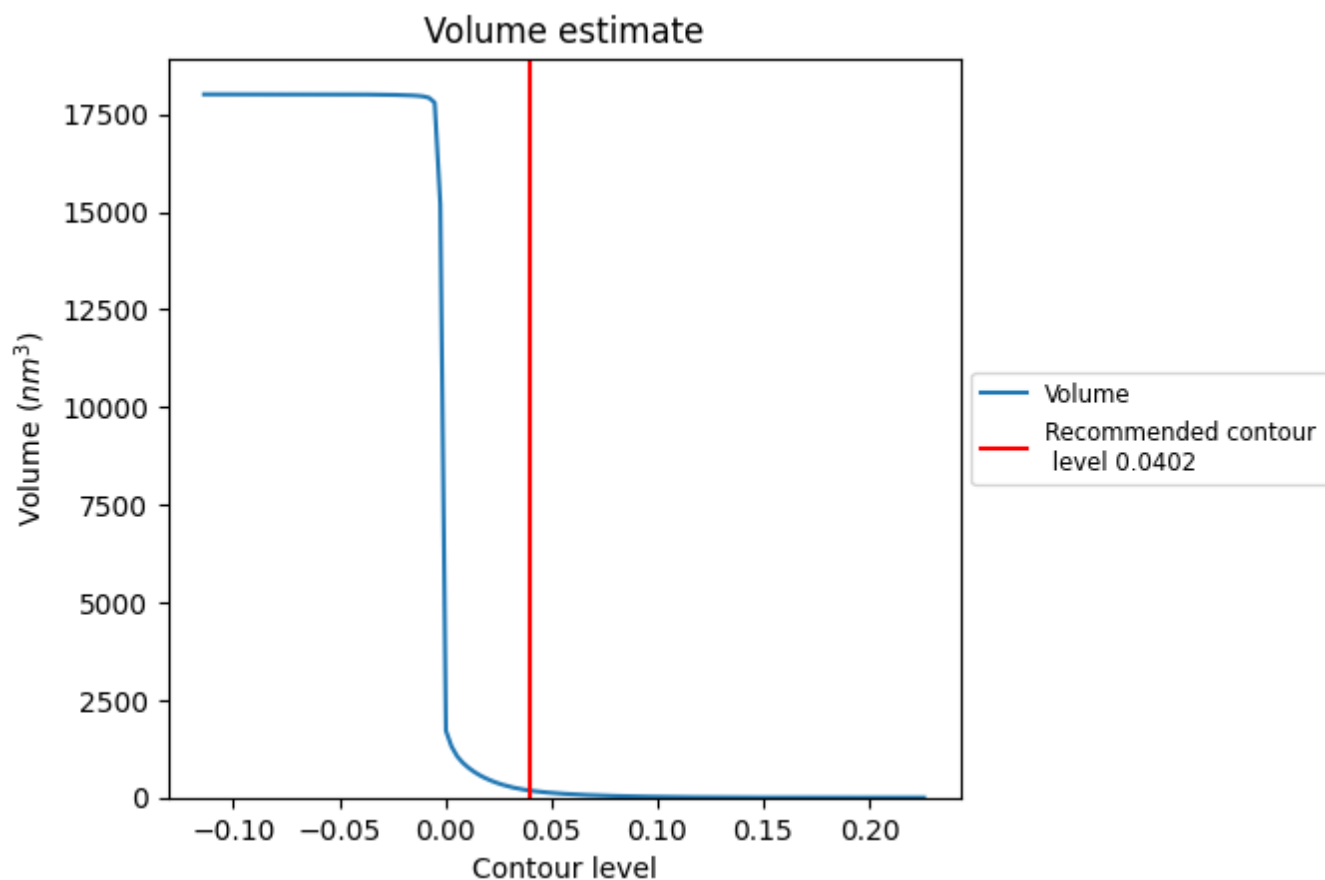
The volume at the recommended contour level is 178 nm^3; this corresponds to an approximate mass of 161 kDa.

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 ⓘ
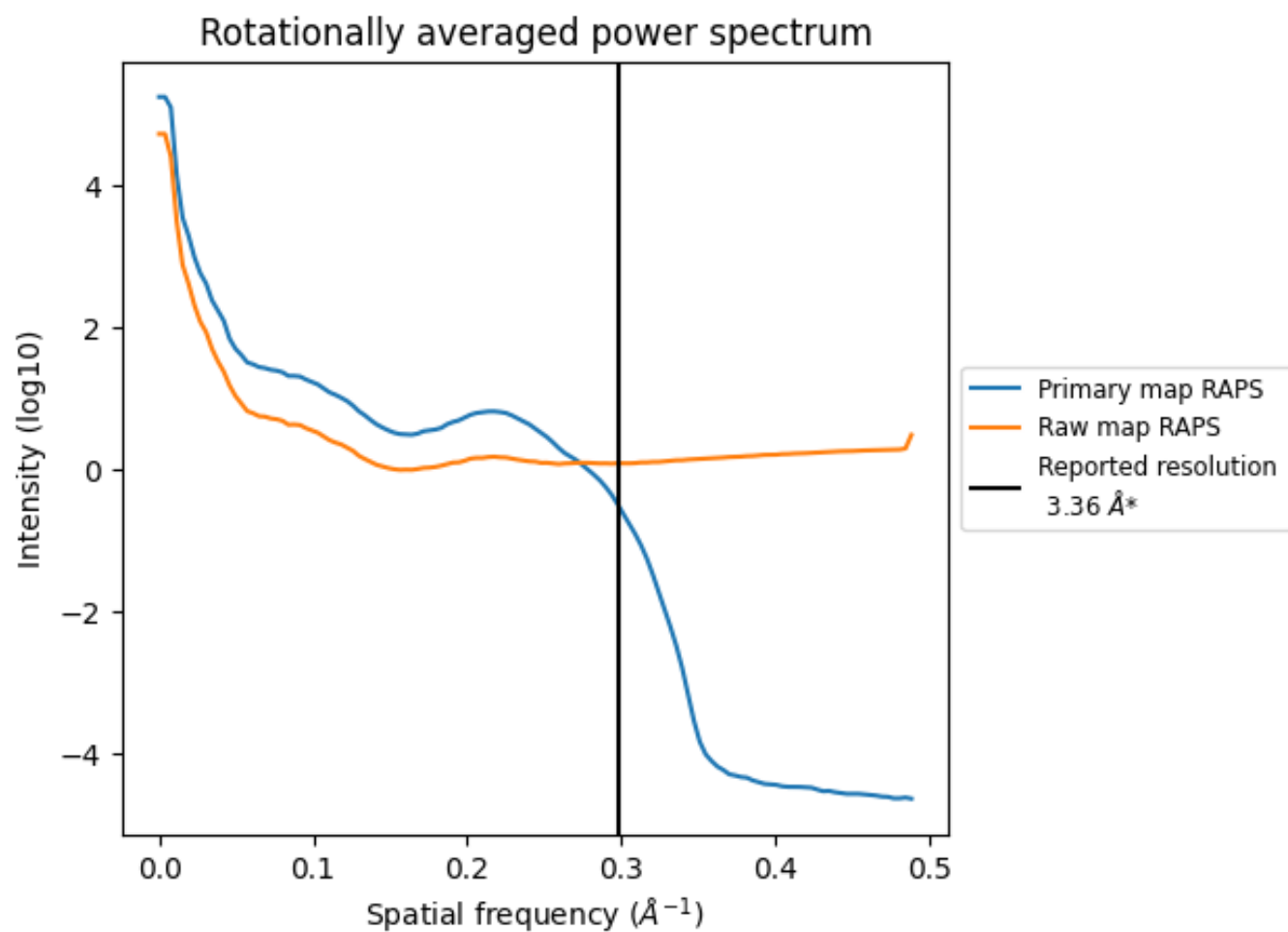
*Reported resolution corresponds to spatial frequency of 0.298 Å^{-1}

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)
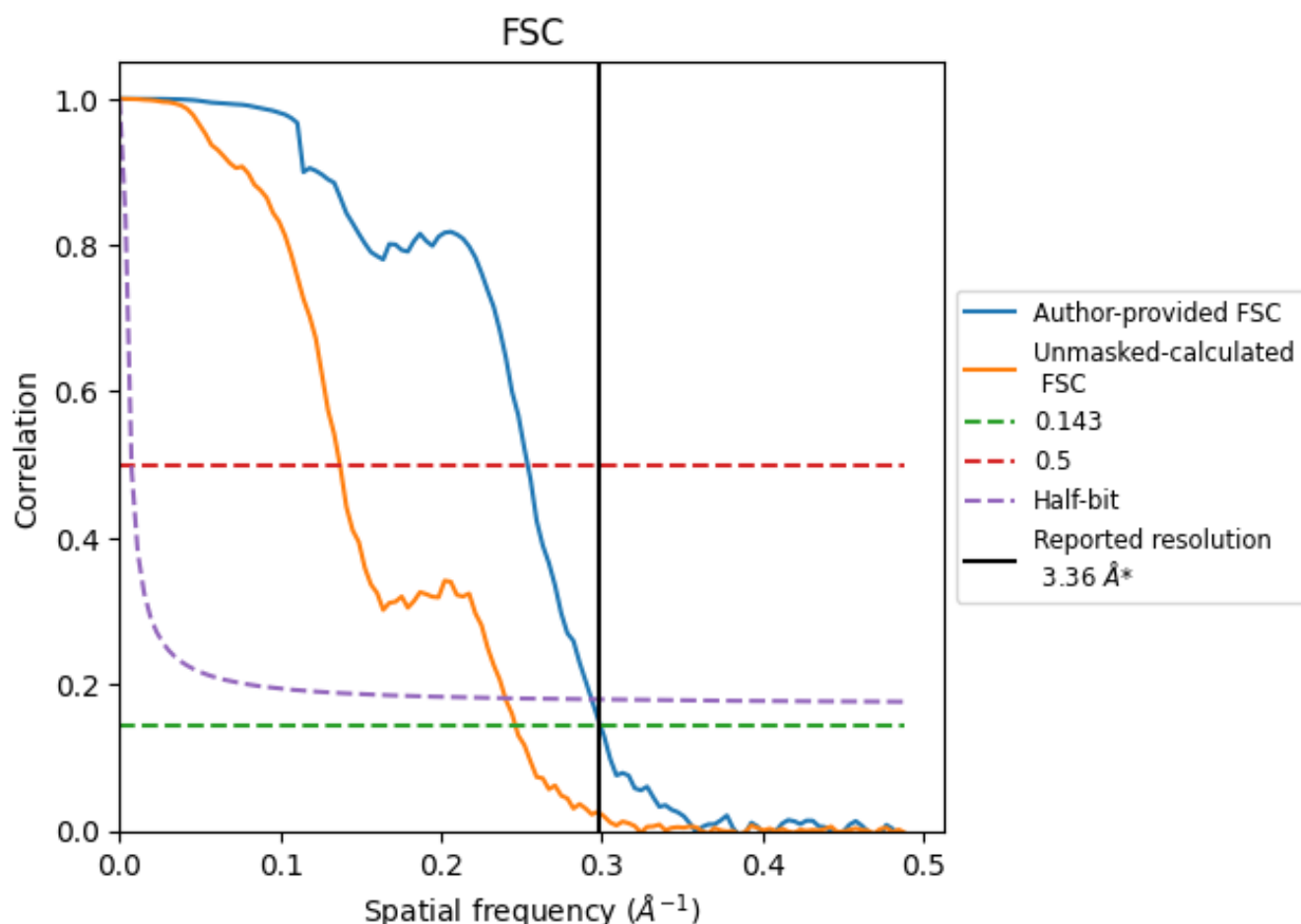
*Reported resolution corresponds to spatial frequency of 0.298 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.34	3.94	3.41
Unmasked-calculated*	4.06	7.29	4.17

*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 4.06 differs from the reported value 3.36 by more than 10 %
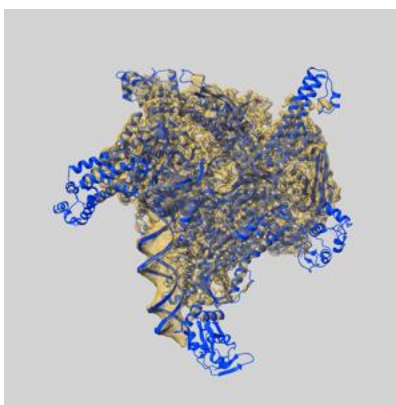
9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-26439 and PDB model 7UBN. Per-residue inclusion information can be found in section 3 on page 8.
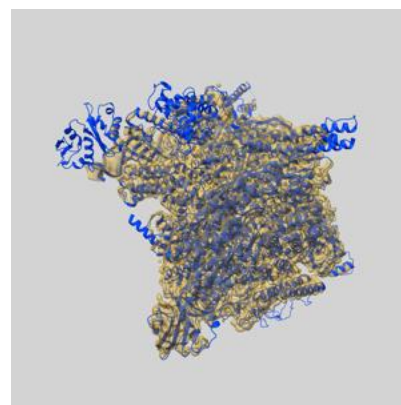
9.1   Map-model overlay ⓘ
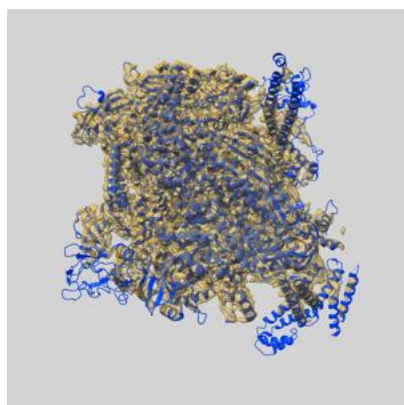
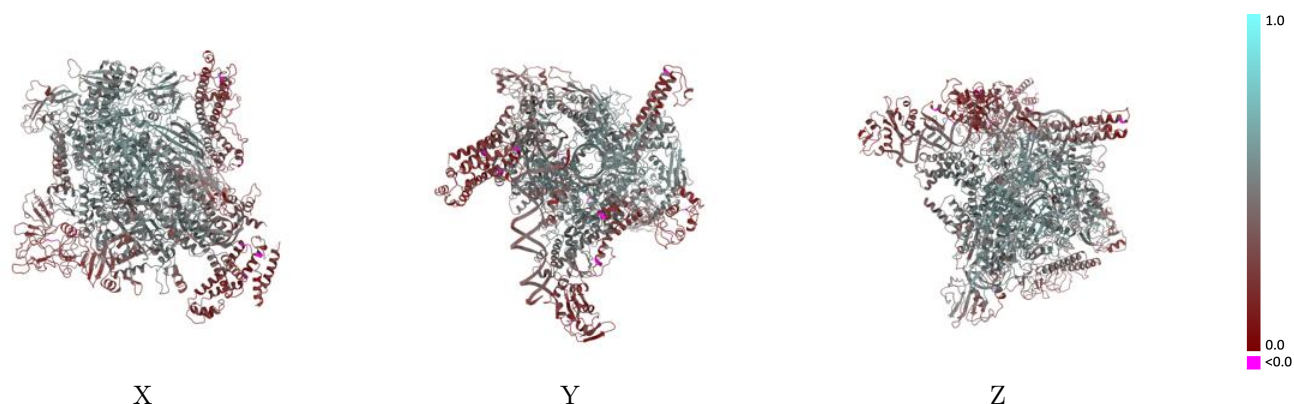X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0402 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
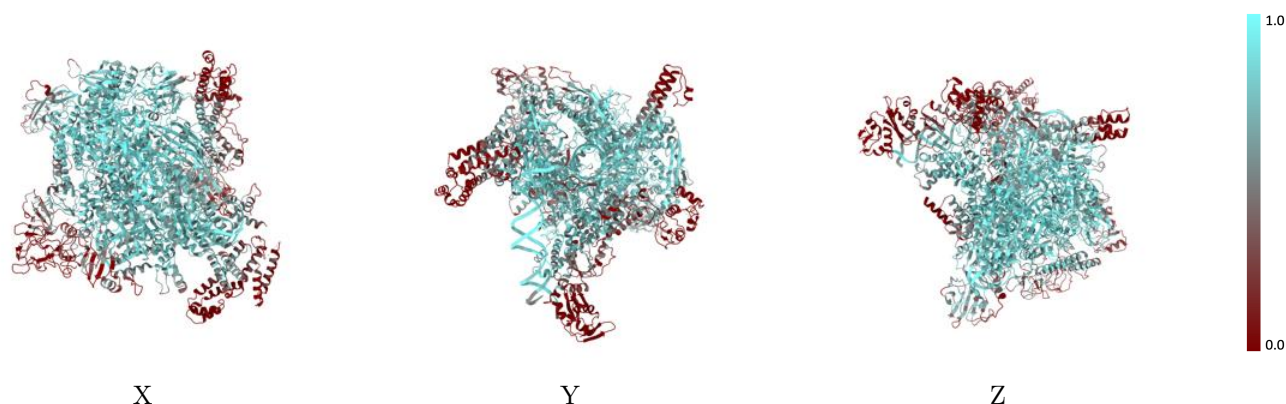
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0402).

9.4   Atom inclusion ⓘ
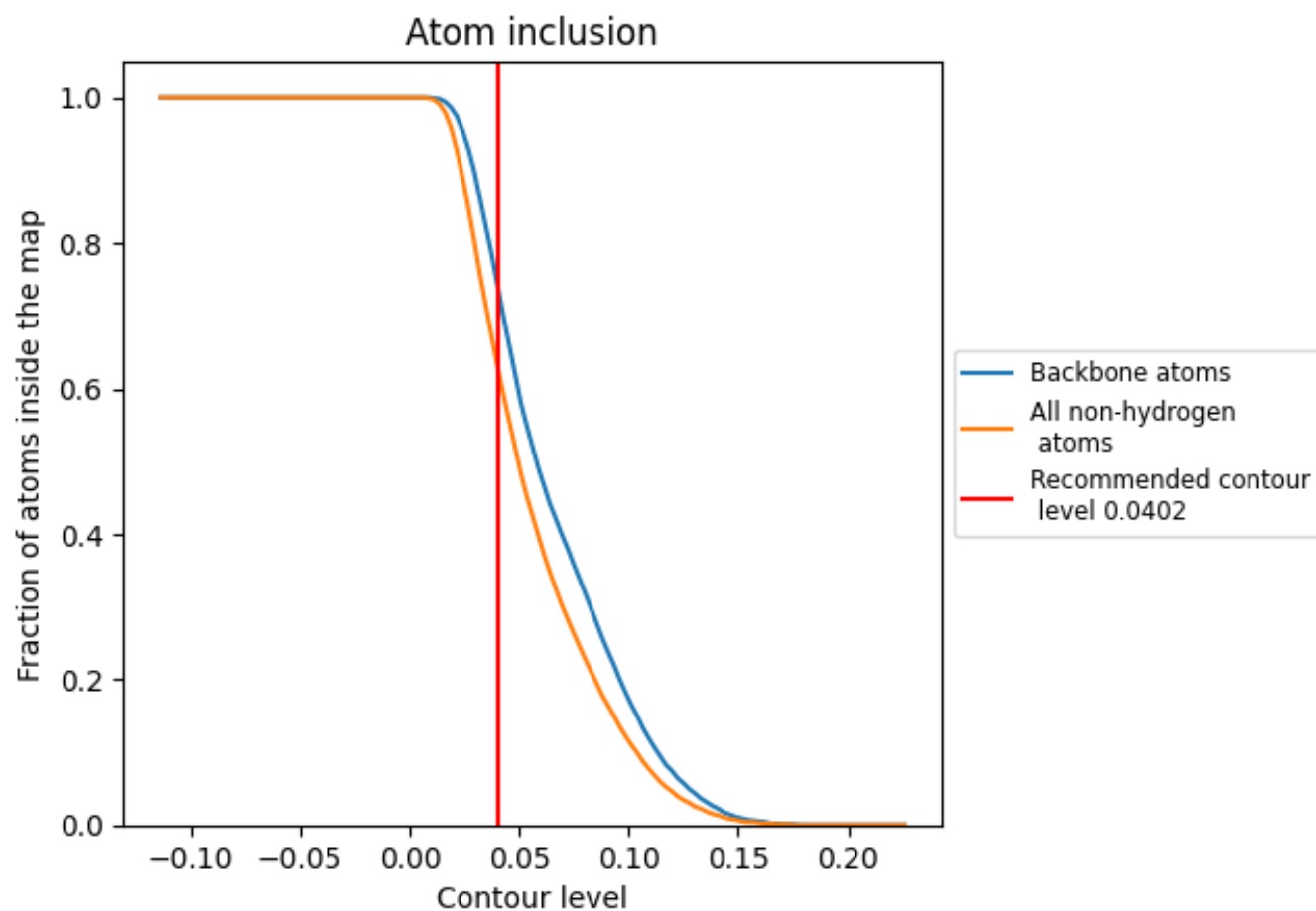
At the recommended contour level, 74% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0402) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6280	0.4350
1	0.8310	0.3920
2	0.8310	0.3920
A	0.7300	0.5090
B	0.4840	0.3860
C	0.7190	0.4820
D	0.6990	0.4720
E	0.3030	0.4660
F	0.3670	0.2890
N	0.1550	0.2560
Q	0.7180	0.4610
R	0.9210	0.5500

1.0

0.0
<0.0