WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Jul 8, 2024 – 07:35 am BST

PDB ID	:	7OQY
EMDB ID	:	EMD-13034
Title	:	Cryo-EM structure of the cellular negative regulator TFS4 bound to the archaeal RNA polymerase
Authors	:	Pilotto, S.; Fouqueau, T.; Lukoyanova, N.; Sheppard, C.; Lucas-Staat, S.; Diaz-Santin, L.M.; Matelska, D.; Prangishvili, D.; Cheung, A.C.M.; Werner, F.
Deposited on	:	2021-06-04
Resolution	:	2.61 Å(reported)
Based on initial model	:	7OK0

The following versions of software and data (see references ⓘ) were used in the production of this report:
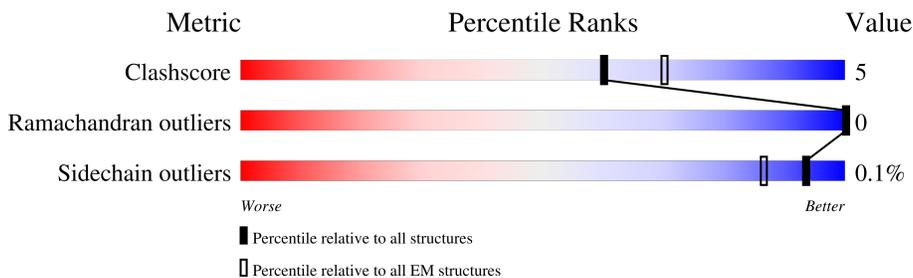
1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.61 Å.

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

Metric	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0.1%

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

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	880	86% · · · · · · · · · · · · · · · 13% ·
2	B	1126	86% · · · · · · · · · · · · · · 12% ·
3	C	393	82% · · · · · · · · · · · · · 15% ·
4	D	264	86% · · · · · · · · · · · · 11% ·
5	E	183	68% / 83% · · · · · · · · · · · 16% ·
6	F	114	91% / 77% · · · · · · · · · 18% ·
7	G	130	80% · · · · · · · · · · · 14% 6%
8	H	84	85% · · · · · · · · · · · 7% 8%

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Mol	Chain	Length	Quality of chain
9	K	89	91% 6%
10	L	90	87% 13%
11	N	66	83% 17%
12	P	48	79% 19%
13	Q	105	34% 7% 59%
14	Y	92	5% 90% 10%

2   Entry composition ⓘ

There are 17 unique types of molecules in this entry. The entry contains 28032 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 DNA-directed RNA polymerase subunit A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	875	Total	C	N	O	S	0	0
			6984	4441	1231	1283	29		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1105	Total	C	N	O	S	0	0
			8718	5524	1532	1629	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ILE	VAL	variant	UNP P11513

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	383	Total	C	N	O	S	0	0
			3024	1900	519	591	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	258	Total	C	N	O	S	0	0
			2039	1304	338	383	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	182	Total	C	N	O	S	0	0
			1421	908	241	267	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	109	Total 856	C 543	N 136	O 174	S 3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase, subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	122	Total 987	C 635	N 155	O 188	S 9	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	125	HIS	-	expression tag	UNP Q4JAY4
G	126	HIS	-	expression tag	UNP Q4JAY4
G	127	HIS	-	expression tag	UNP Q4JAY4
G	128	HIS	-	expression tag	UNP Q4JAY4
G	129	HIS	-	expression tag	UNP Q4JAY4
G	130	HIS	-	expression tag	UNP Q4JAY4

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	77	Total 608	C 393	N 102	O 113	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	86	Total 690	C 441	N 120	O 127	S 2	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	90	Total 707	C 459	N 112	O 134	S 2	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit N.

| Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	66	Total 534	C 339	N 97	O 91	S 7	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	47	Total	C	N	O	S	0	0
			376	241	67	63	5		

- Molecule 13 is a protein called Conserved protein.

| Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	43	Total	C	N	O	S	0	0
			351	221	55	73	2		

- Molecule 14 is a protein called DNA-directed RNA polymerase, subunit M (RpoM-2).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	92	Total	C	N	O	S	0	0
			721	451	131	128	11		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	3	Total	Zn	0
			3	3	
16	B	1	Total	Zn	0
			1	1	
16	N	1	Total	Zn	0
			1	1	
16	P	1	Total	Zn	0
			1	1	
16	Y	2	Total	Zn	0
			2	2	

- Molecule 17 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).
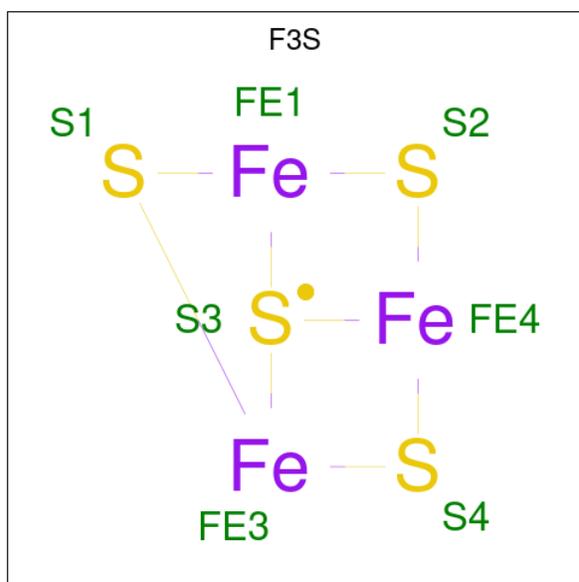
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
17	D	1	7	3	4	0

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-directed RNA polymerase subunit A'

Chain A:
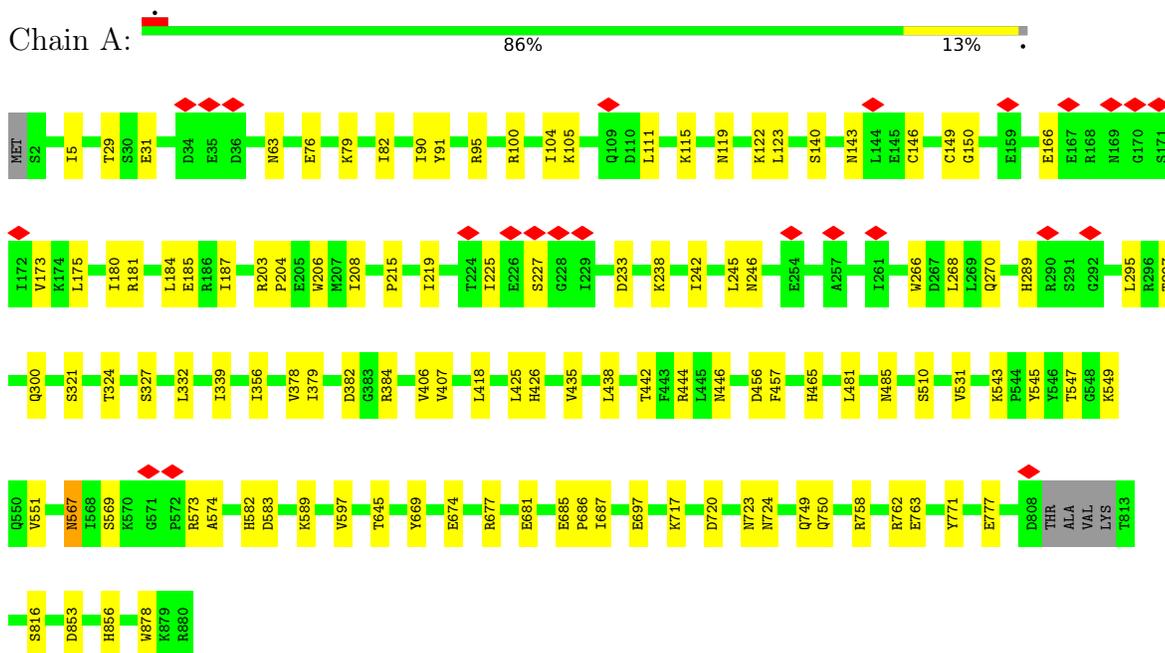
• Molecule 2: DNA-directed RNA polymerase subunit B

Chain B:
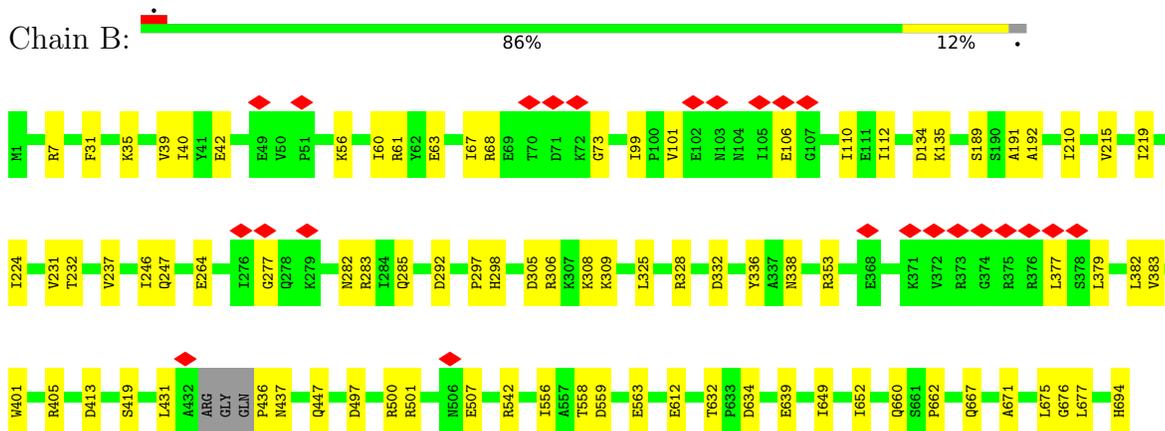
• Molecule 3: DNA-directed RNA polymerase subunit A"

Chain C:
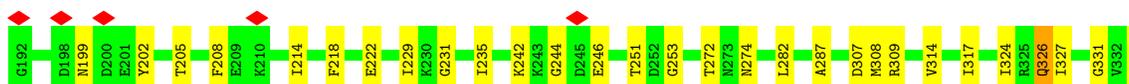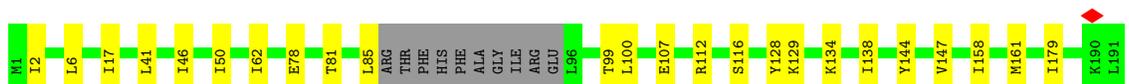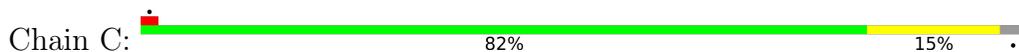
• Molecule 4: DNA-directed RNA polymerase subunit D

Chain D:
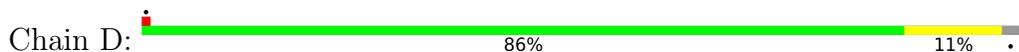
• Molecule 5: DNA-directed RNA polymerase subunit E

Chain E:
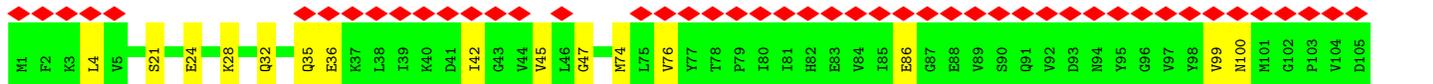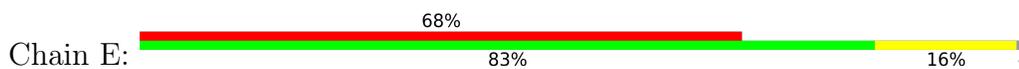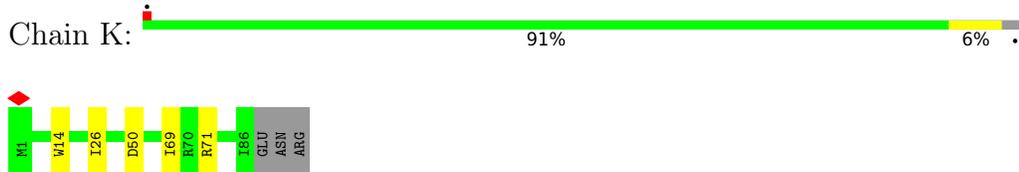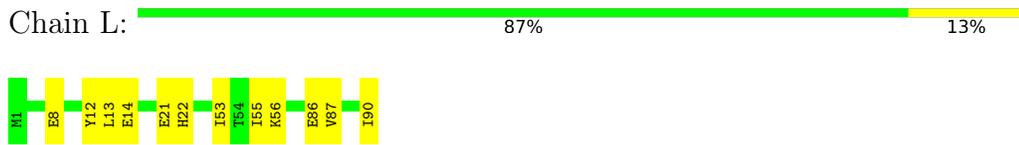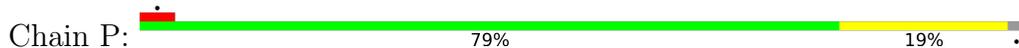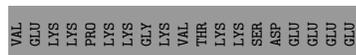

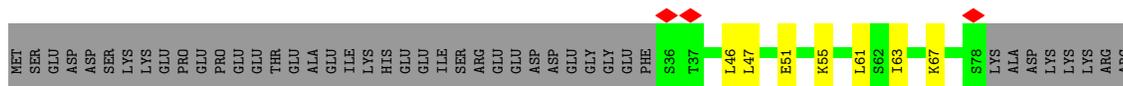• Molecule 6: DNA-directed RNA polymerase, subunit F

Chain F:
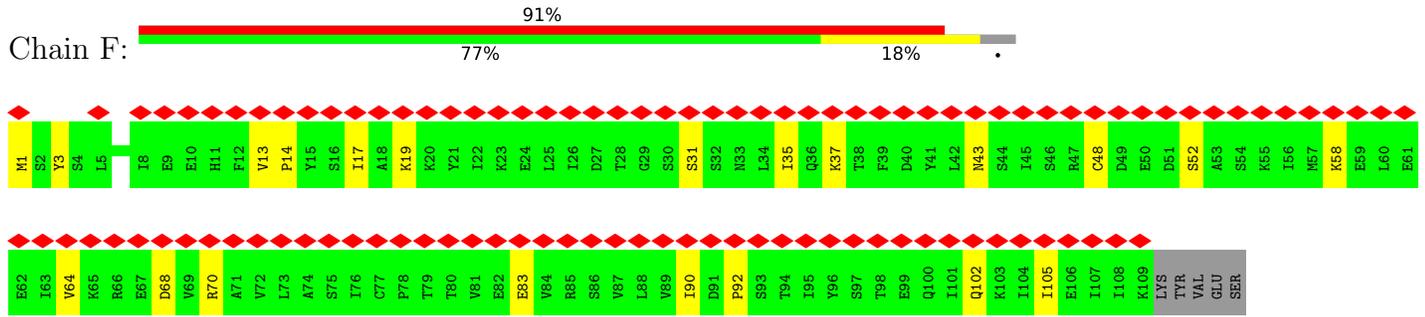
• Molecule 7: DNA-directed RNA polymerase, subunit G

Chain G:
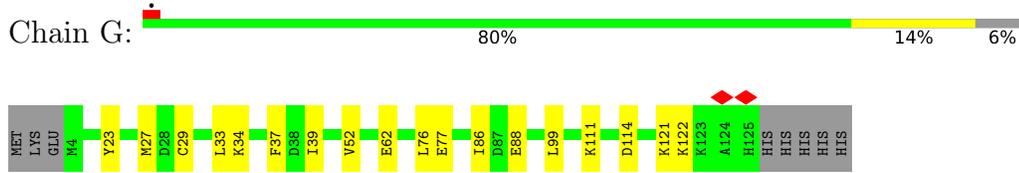
• Molecule 8: DNA-directed RNA polymerase subunit H

Chain H:
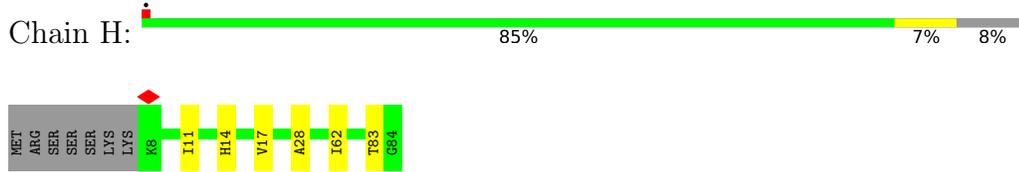
• Molecule 9: DNA-directed RNA polymerase subunit K

Chain K:

• Molecule 10: DNA-directed RNA polymerase subunit L

Chain L:

• Molecule 11: DNA-directed RNA polymerase subunit N

Chain N:
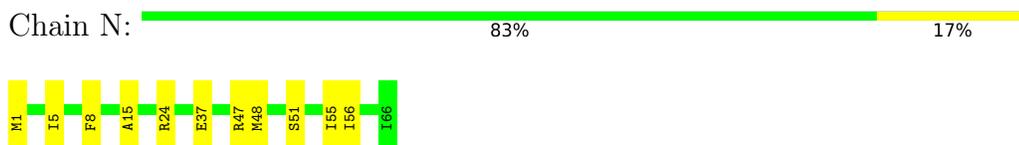
• Molecule 12: DNA-directed RNA polymerase subunit P

Chain P:

MET A2 R5 C6 C9 W10 K11 E12 L13 K19 C26 P27 Y28 A47 I48

• Molecule 13: Conserved protein

Chain Q:

34% 7% 59%

MET SER GLU ASP ASP SER LYS LYS GLU PRO GLU GLU PRO GLU GLU THR GLU ALA GLU ILE LYS HIS GLU GLU ILE SER ARG GLU GLU ASP ASP GLU GLY GLY GLU PHE S36 T37 L46 L47 E51 K55 L61 S62 I63 K67 S78 LYS ALA ASP LYS LYS ARG ARG

VAL GLU LYS LYS PRO LYS GLY LYS VAL THR LYS LYS SER ASP GLU GLU GLU GLU

• Molecule 14: DNA-directed RNA polymerase, subunit M (RpoM-2)

Chain Y:

5% 90% 10%

M1 K6 H28 D29 E42 K45 A49 I54 I60 N75 K76 K77 Y81 R82 V89 I92
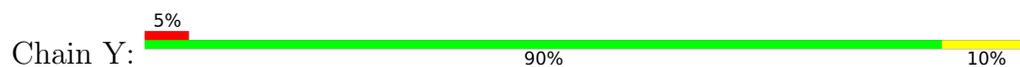
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	350682	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 $(e^-/Å^2)$	45.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	51.285	Depositor
Minimum map value	-35.128	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.2	Depositor
Map size (Å)	360.22, 360.22, 360.22	wwPDB
Map dimensions	332, 332, 332	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	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, F3S, 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	0.25	0/7132	0.50	0/9642
2	B	0.25	0/8877	0.50	0/12003
3	C	0.25	0/3049	0.49	0/4096
4	D	0.25	0/2072	0.49	0/2798
5	E	0.24	0/1443	0.49	0/1944
6	F	0.23	0/866	0.43	0/1172
7	G	0.25	0/1002	0.45	0/1337
8	H	0.25	0/621	0.47	0/840
9	K	0.24	0/697	0.48	0/938
10	L	0.26	0/716	0.44	0/964
11	N	0.26	0/545	0.54	0/735
12	P	0.25	0/382	0.56	0/510
13	Q	0.23	0/354	0.43	0/475
14	Y	0.25	0/730	0.51	0/973
All	All	0.25	0/28486	0.49	0/38427

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 ⓘ

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6984	0	7060	72	0
2	B	8718	0	8860	78	0
3	C	3024	0	3151	38	0
4	D	2039	0	2102	19	0
5	E	1421	0	1457	19	0
6	F	856	0	869	14	0
7	G	987	0	999	9	0
8	H	608	0	631	4	0
9	K	690	0	745	3	0
10	L	707	0	751	8	0
11	N	534	0	545	7	0
12	P	376	0	399	9	0
13	Q	351	0	352	4	0
14	Y	721	0	747	7	0
15	A	1	0	0	0	0
16	A	3	0	0	0	0
16	B	1	0	0	0	0
16	N	1	0	0	0	0
16	P	1	0	0	0	0
16	Y	2	0	0	0	0
17	D	7	0	0	1	0
All	All	28032	0	28668	269	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 269 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)
1:A:438:LEU:HB2	1:A:444:ARG:HH21	1.39	0.88
2:B:1060:CYS:HB2	2:B:1078:CYS:SG	2.25	0.75
1:A:29:THR:HG22	1:A:31:GLU:H	1.52	0.74
2:B:61:ARG:NH1	2:B:63:GLU:OE2	2.22	0.73
12:P:12:GLU:HG2	12:P:13:LEU:H	1.55	0.72

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	871/880 (99%)	843 (97%)	28 (3%)	0	100	100
2	B	1099/1126 (98%)	1063 (97%)	36 (3%)	0	100	100
3	C	379/393 (96%)	373 (98%)	6 (2%)	0	100	100
4	D	254/264 (96%)	251 (99%)	3 (1%)	0	100	100
5	E	180/183 (98%)	173 (96%)	7 (4%)	0	100	100
6	F	107/114 (94%)	102 (95%)	5 (5%)	0	100	100
7	G	120/130 (92%)	117 (98%)	3 (2%)	0	100	100
8	H	75/84 (89%)	74 (99%)	1 (1%)	0	100	100
9	K	84/89 (94%)	79 (94%)	5 (6%)	0	100	100
10	L	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
11	N	64/66 (97%)	62 (97%)	2 (3%)	0	100	100
12	P	45/48 (94%)	41 (91%)	4 (9%)	0	100	100
13	Q	41/105 (39%)	41 (100%)	0	0	100	100
14	Y	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3497/3664 (95%)	3395 (97%)	102 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	763/768 (99%)	762 (100%)	1 (0%)	93	98
2	B	951/972 (98%)	951 (100%)	0	100	100
3	C	339/348 (97%)	338 (100%)	1 (0%)	92	97
4	D	233/239 (98%)	233 (100%)	0	100	100
5	E	154/157 (98%)	154 (100%)	0	100	100
6	F	100/109 (92%)	100 (100%)	0	100	100
7	G	112/121 (93%)	112 (100%)	0	100	100
8	H	67/75 (89%)	67 (100%)	0	100	100
9	K	78/81 (96%)	78 (100%)	0	100	100
10	L	78/78 (100%)	78 (100%)	0	100	100
11	N	60/60 (100%)	60 (100%)	0	100	100
12	P	41/43 (95%)	41 (100%)	0	100	100
13	Q	41/98 (42%)	41 (100%)	0	100	100
14	Y	82/82 (100%)	82 (100%)	0	100	100
All	All	3099/3231 (96%)	3097 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	567	ASN
3	C	326	GLN

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

Mol	Chain	Res	Type
1	A	426	HIS
3	C	375	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
17	F3S	D	301	4	0,9,9	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	F3S	D	301	4	-	-	0/3/3/3

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	D	301	F3S	1	0

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-13034. 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
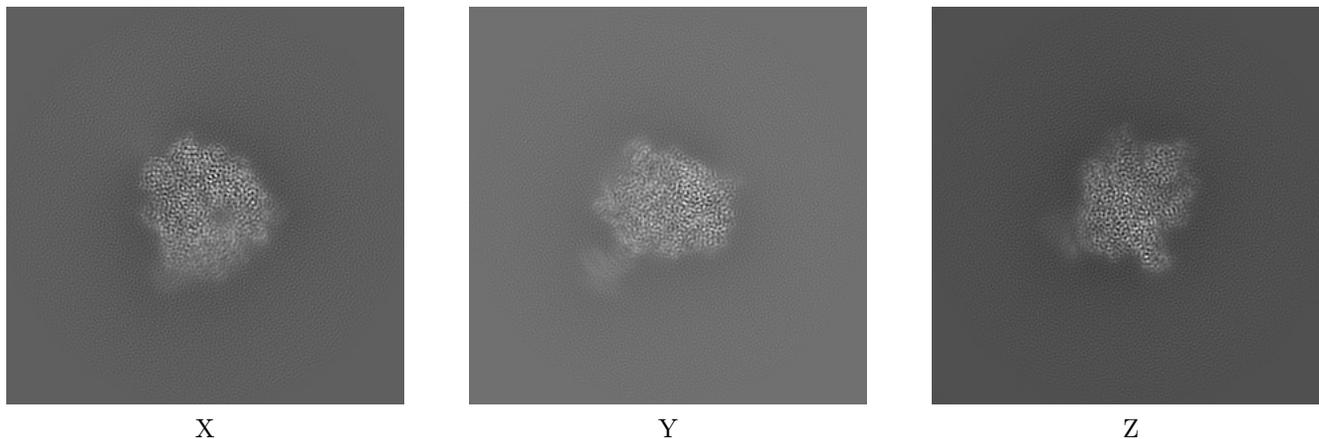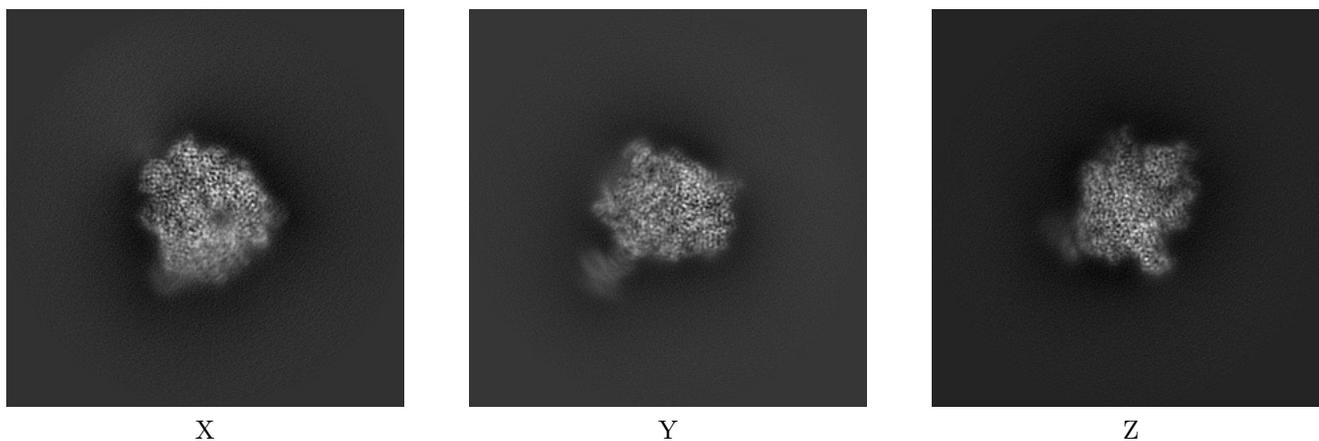
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
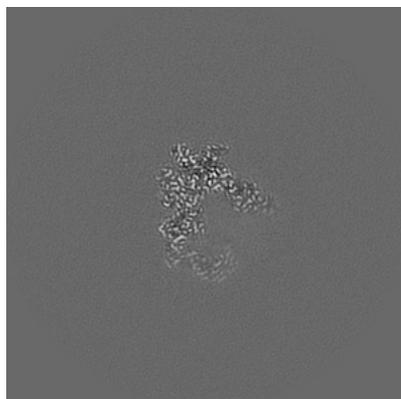
6.2.1 Primary map
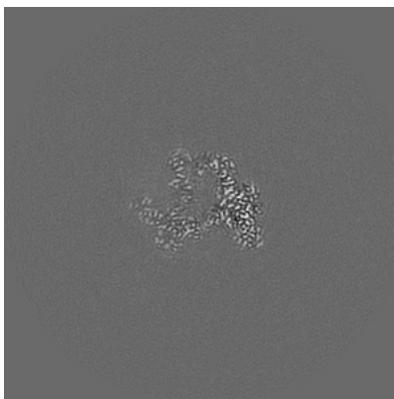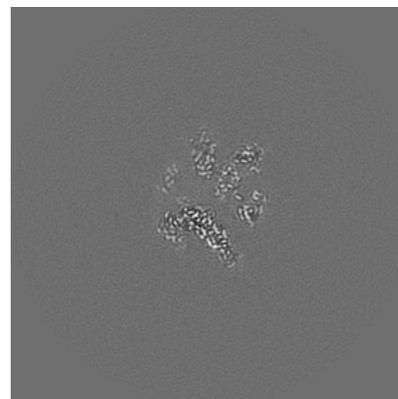
X Index: 166   Y Index: 166   Z Index: 166

6.2.2 Raw map
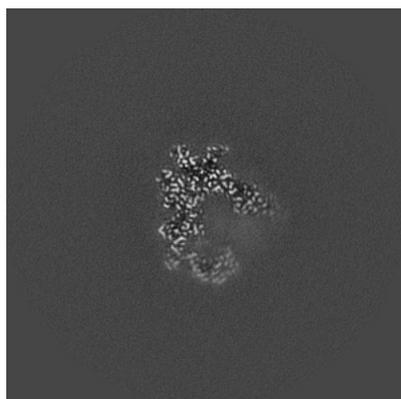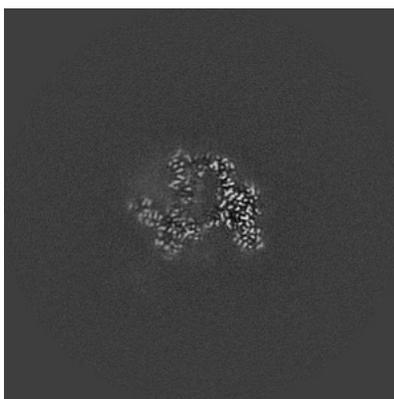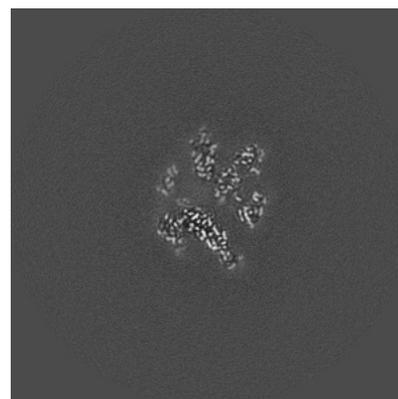
X Index: 166   Y Index: 166   Z Index: 166

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
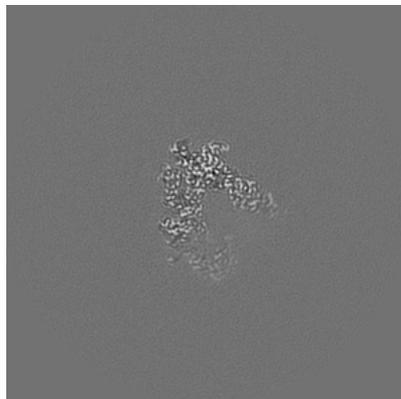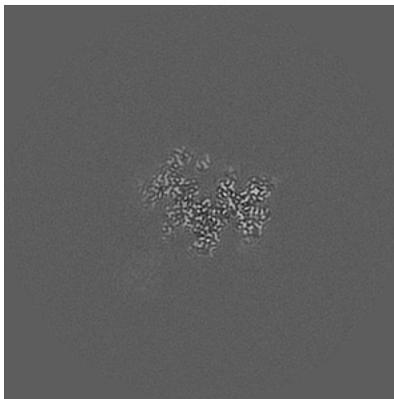
| X Index: 164 | Y Index: 152 | Z Index: 181 |
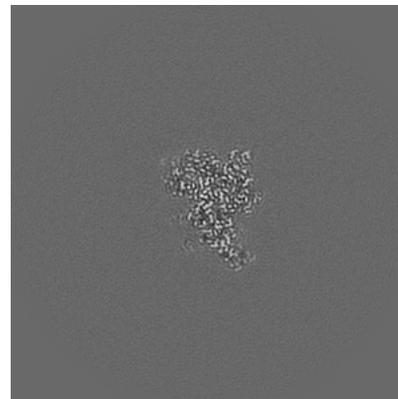
6.3.2 Raw map
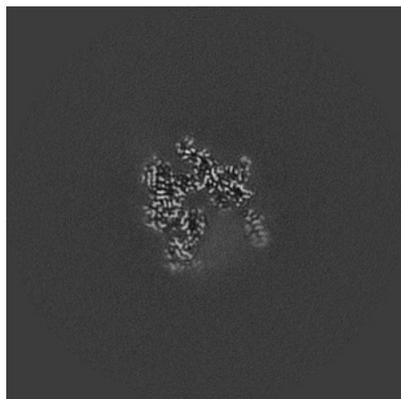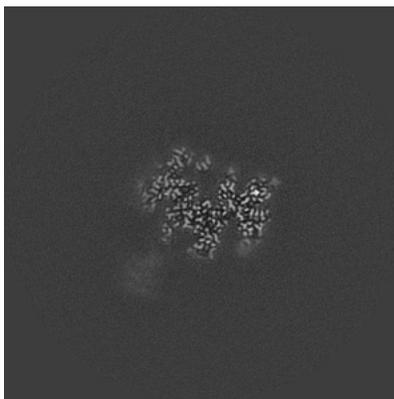
| X Index: 178 | Y Index: 152 | Z Index: 179 |
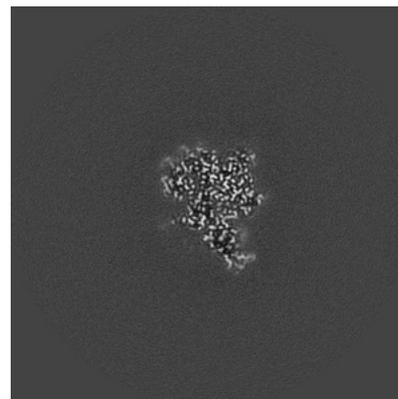
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
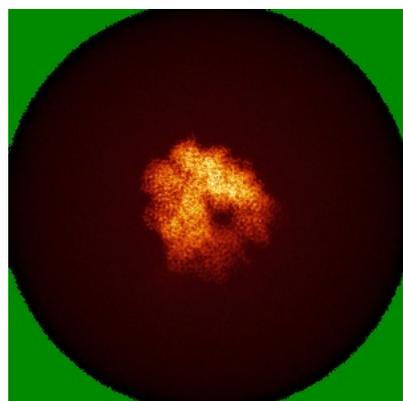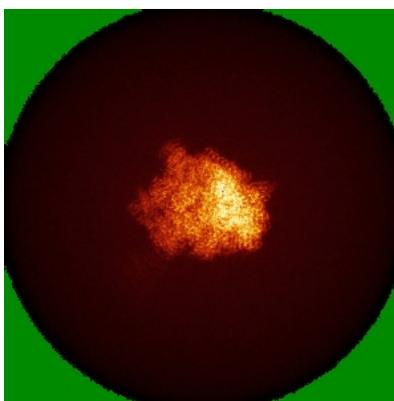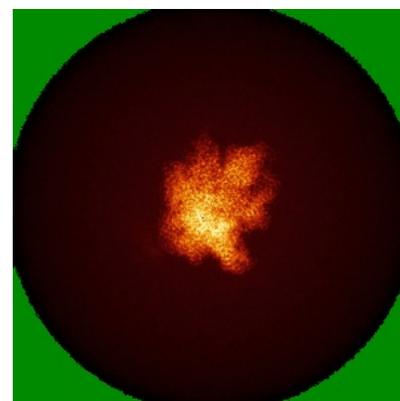
X	Y	Z

6.4.2 Raw map

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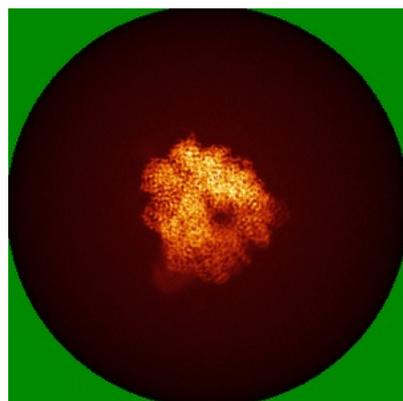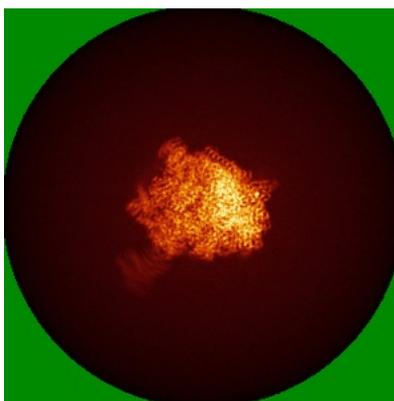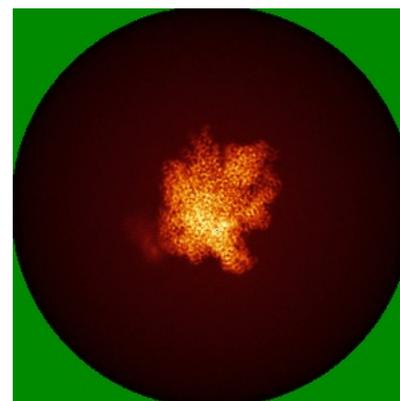
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.
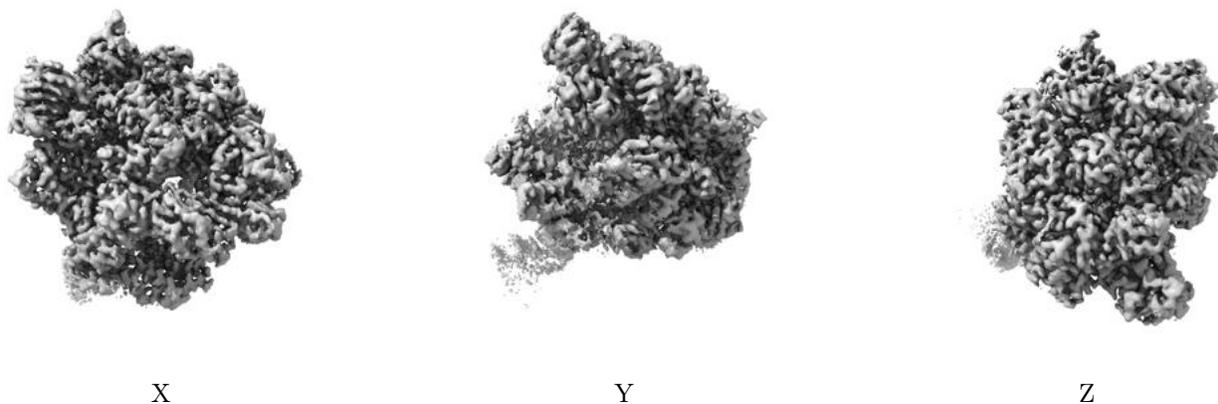
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z
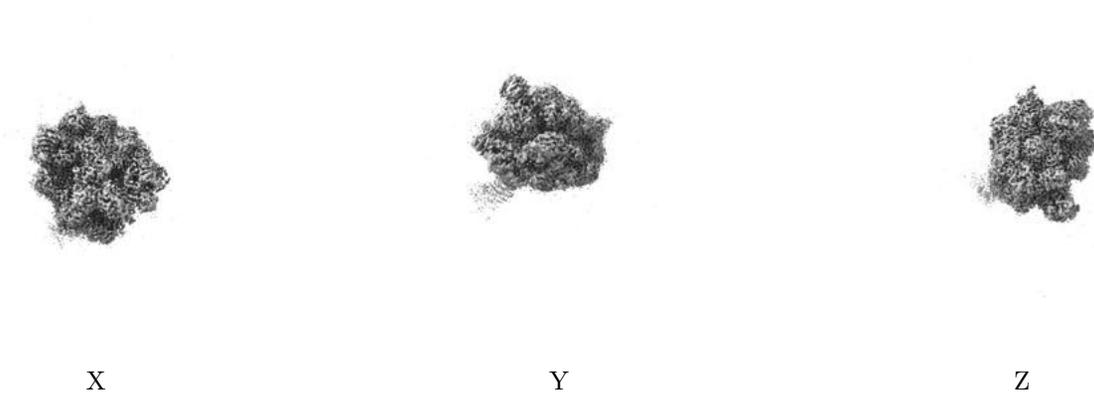
The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

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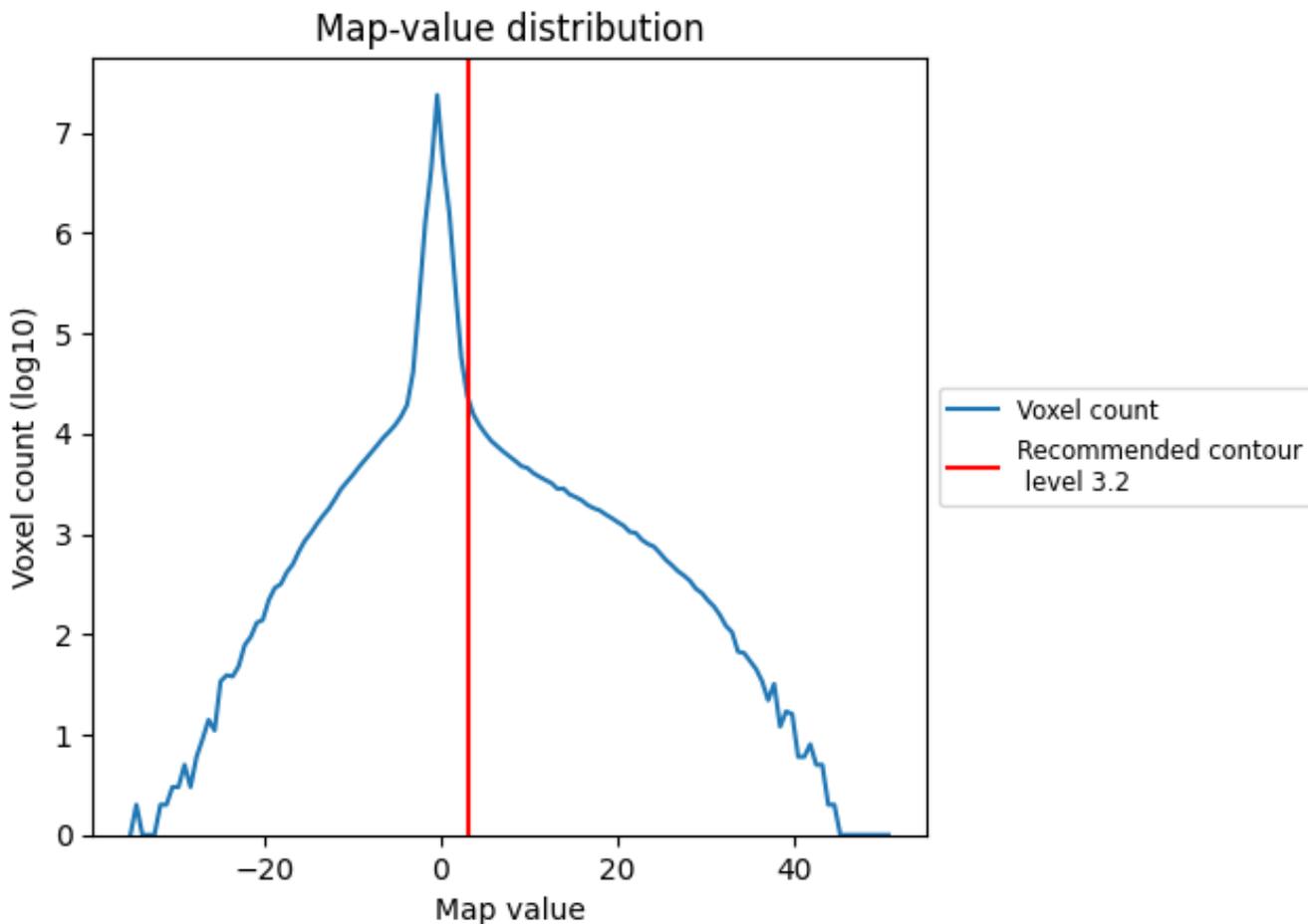
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate (i)
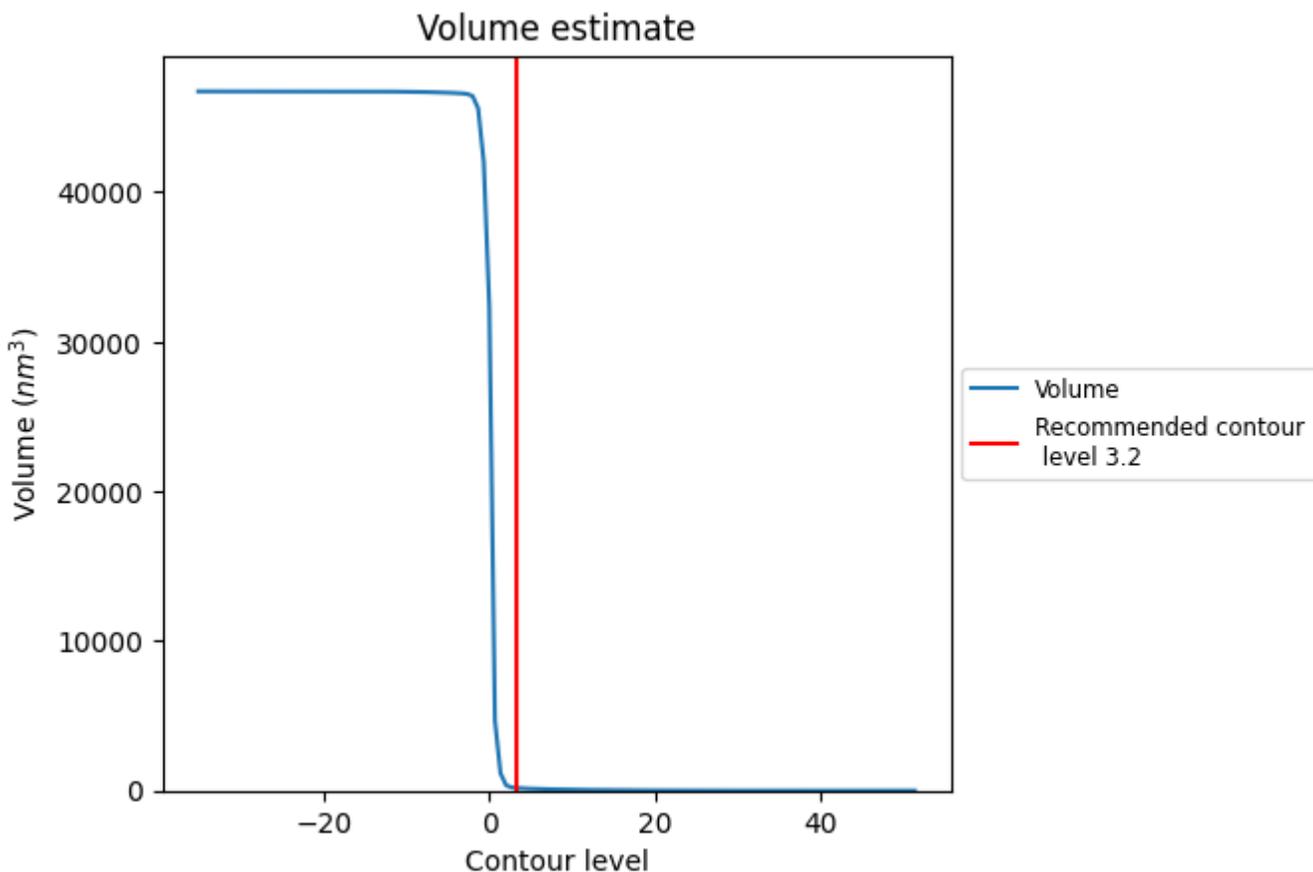
Volume estimate

The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 166 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 ⓘ
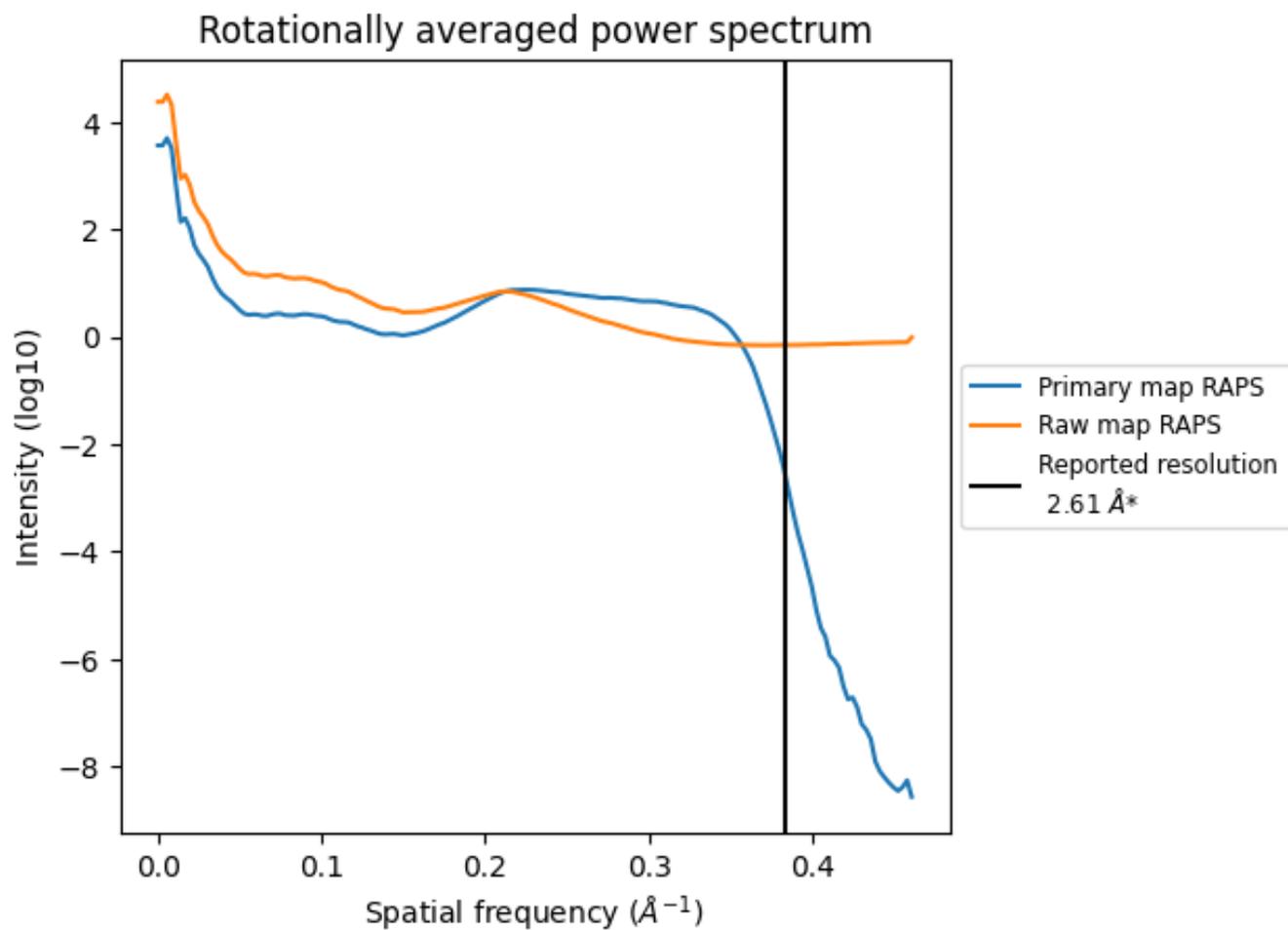
*Reported resolution corresponds to spatial frequency of 0.383 Å^{-1}

8   Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1   FSC ⓘ
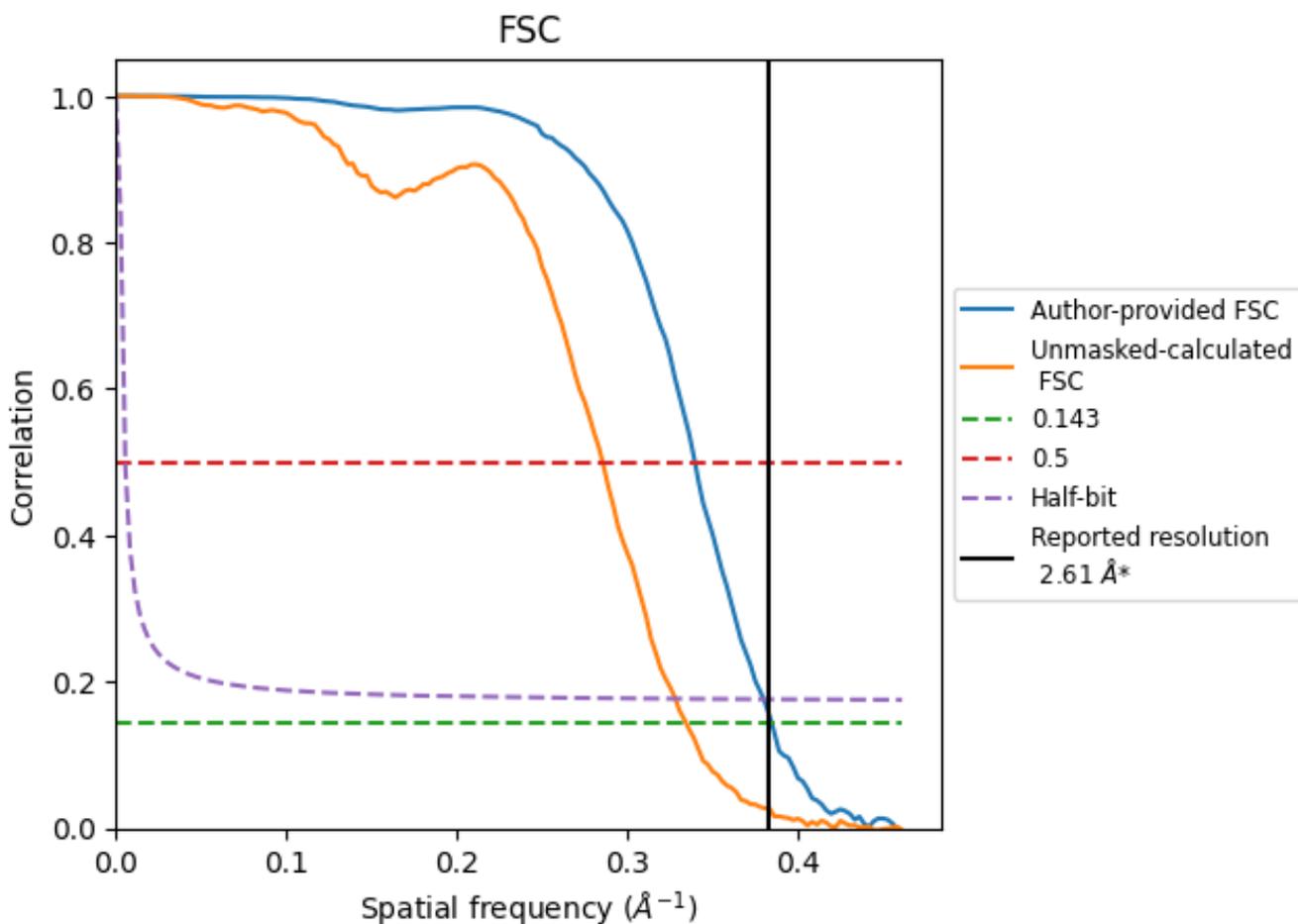
*Reported resolution corresponds to spatial frequency of 0.383 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	2.60	2.95	2.63
Unmasked-calculated*	2.99	3.51	3.05

*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 2.99 differs from the reported value 2.61 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-13034 and PDB model 7OQY. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ

| X | Y | Z |
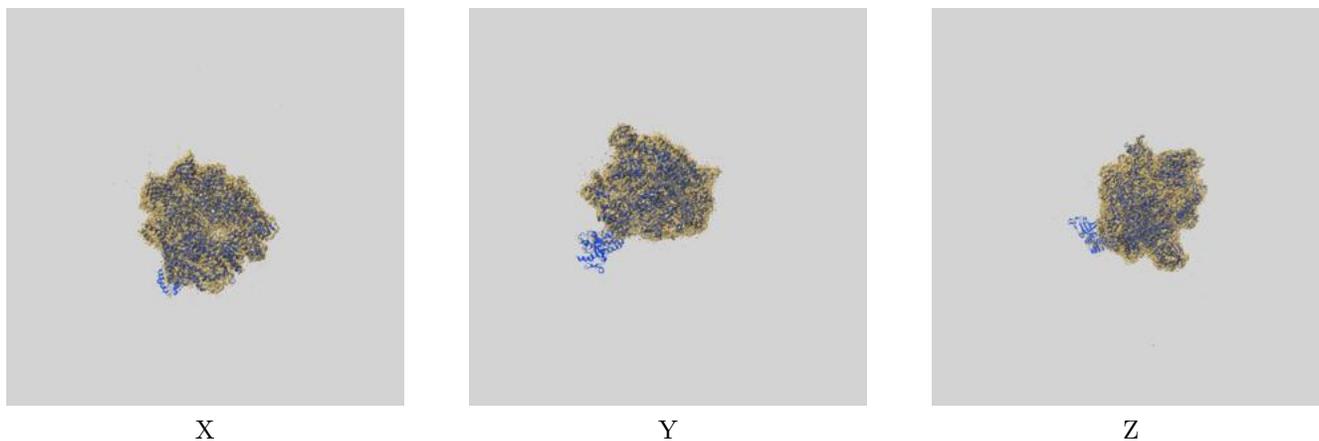
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X   Y   Z
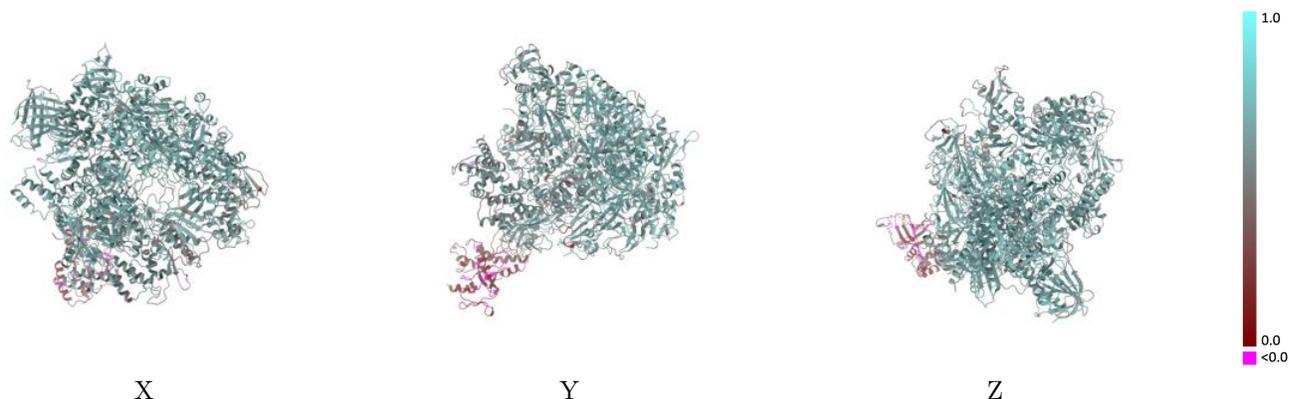
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
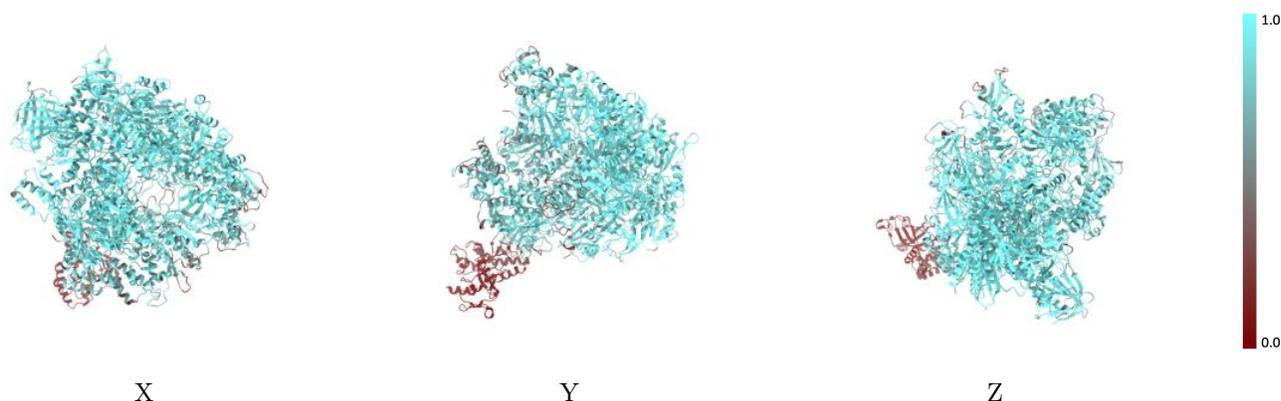
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.2).

9.4　Atom inclusion ⓘ
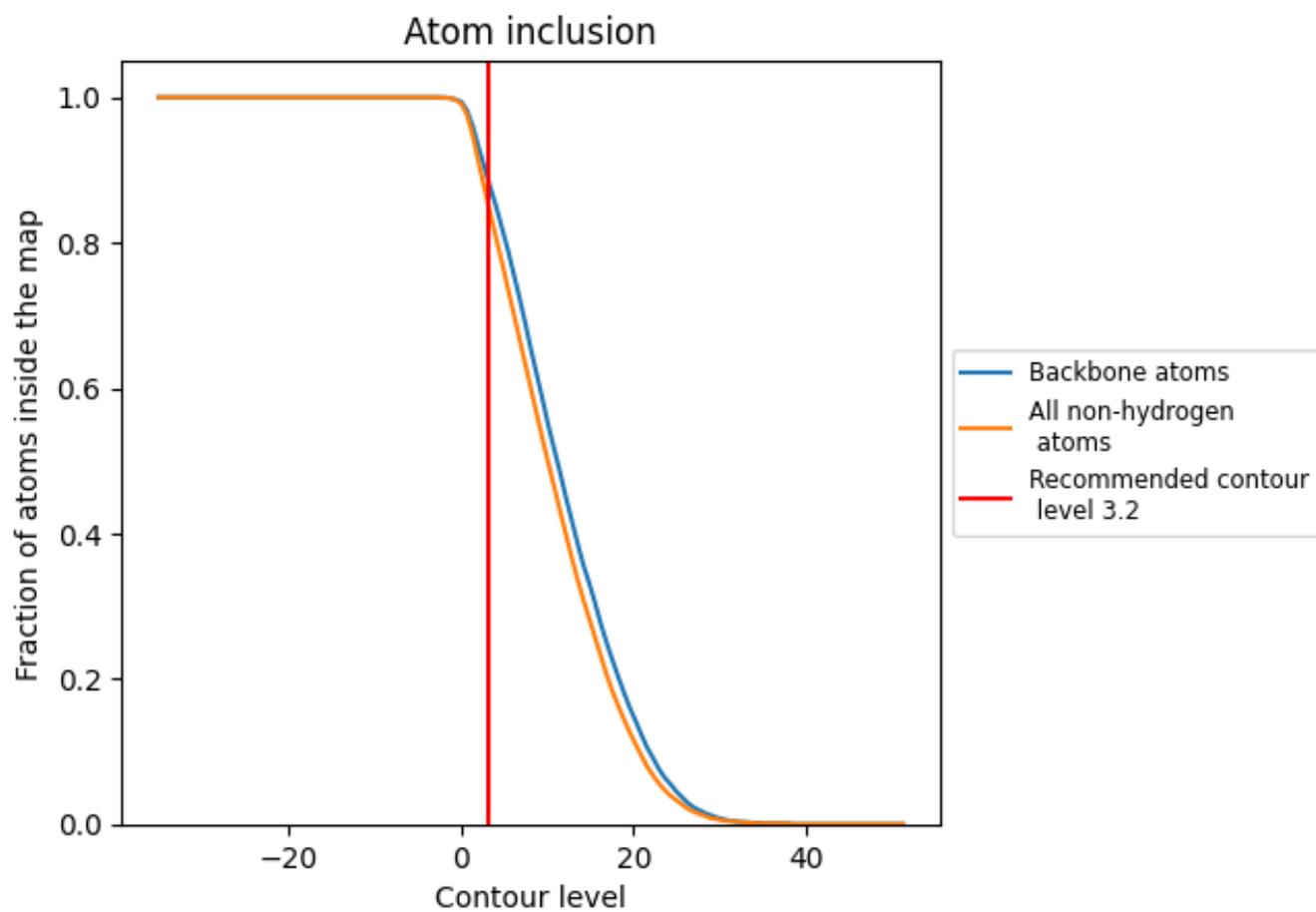
At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8480	0.5860
A	0.8960	0.6070
B	0.9140	0.6230
C	0.8840	0.6030
D	0.9480	0.6350
E	0.2860	0.2820
F	0.0810	0.2010
G	0.8880	0.6100
H	0.9300	0.6320
K	0.9010	0.6120
L	0.9520	0.6350
N	0.9690	0.6500
P	0.8710	0.5630
Q	0.8000	0.5710
Y	0.8310	0.5970

1.0

0.0
<0.0