WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

May 6, 2023 – 12:32 PM EDT

PDB ID	:	8EBT
EMDB ID	:	EMD-27997
Title	:	XPA repositioning Core7 of TFIIH relative to XPC-DNA lesion (Cy5)
Authors	:	Kim, J.; Yang, W.
Deposited on	:	2022-08-31
Resolution	:	3.90 Å(reported)
Based on initial model	:	6RO4

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 3.90 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		2.6%

Worse *Better*

■ Percentile relative to all structures

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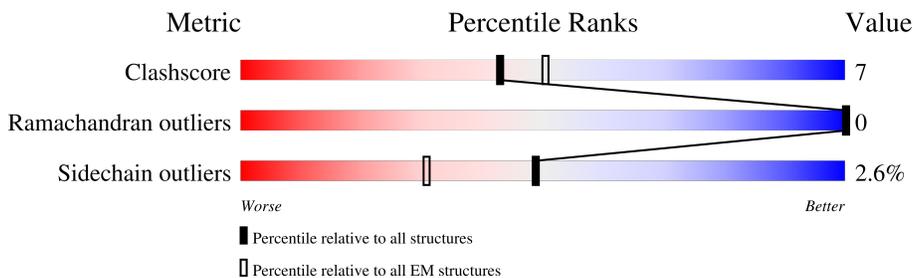
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	603	78% 21% •
2	B	730	74% 18% • 7%
3	C	438	• 36% 8% 56%
4	D	446	• 81% 16% • •
5	E	380	84% 16% •
6	F	284	79% 12% 9%
7	G	66	77% 23%
8	H	274	14% 70% 29% •

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Mol	Chain	Length	Quality of chain
9	J	70	89% 10%
10	K	172	79% 19%
11	L	44	36% 64%
12	M	45	11% 42% 58%

2   Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 27026 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 General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	603	Total 4874	C 3113	N 844	O 888	S 29	0	0

- Molecule 2 is a protein called General transcription and DNA repair factor IIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	677	Total 5457	C 3502	N 948	O 978	S 29	0	0

- Molecule 3 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	191	Total 1547	C 981	N 267	O 290	S 9	0	0

- Molecule 4 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	436	Total 3499	C 2255	N 608	O 623	S 13	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	380	Total 2989	C 1886	N 518	O 558	S 27	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	52	GLY	GLN	conflict	UNP Q13888

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	258	Total	C	N	O	S	0	0
			2034	1301	337	377	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	66	Total	C	N	O	S	0	0
			522	337	82	100	3		

- Molecule 8 is a protein called DNA repair protein complementing XP-C cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	274	Total	C	N	O	S	0	0
			2224	1420	401	395	8		

- Molecule 9 is a protein called Centrin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	70	Total	C	N	O	S	1	0
			573	356	94	121	2		

- Molecule 10 is a protein called DNA repair protein complementing XP-A cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	172	Total	C	N	O	S	0	0
			1450	908	255	273	14		

- Molecule 11 is a DNA chain called DNA (Cy5).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	44	Total	C	N	O	P	0	0
			930	454	170	262	44		

- Molecule 12 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	45	Total	C	N	O	P	0	0
			911	436	158	272	45		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
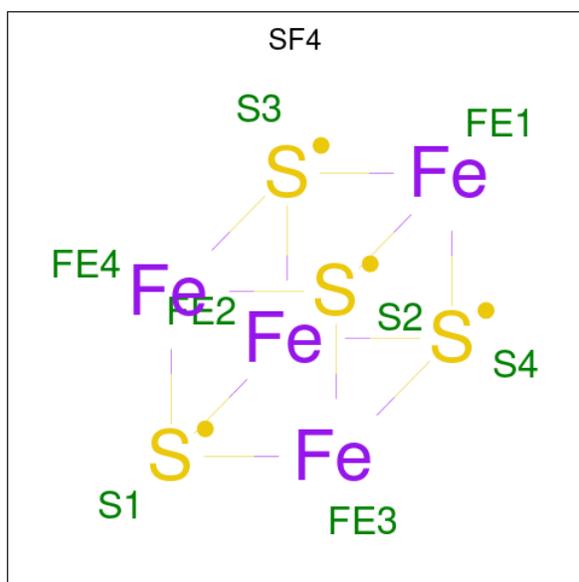
Mol	Chain	Residues	Atoms			AltConf
13	B	1	Total 8	Fe 4	S 4	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	E	3	Total 3	Zn 3	0
14	F	2	Total 2	Zn 2	0
14	K	1	Total 1	Zn 1	0

- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
15	J	2	Total 2	Ca 2	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: General transcription and DNA repair factor IIH helicase subunit XPB

- Molecule 2: General transcription and DNA repair factor IIH helicase subunit XPD

• Molecule 3: General transcription factor IIH subunit 1

Chain C:

36%　　　　8%　　　　　　56%

• Molecule 4: General transcription factor IIH subunit 4

Chain D:

81%　　　　16%

• Molecule 5: General transcription factor IIH subunit 2

Chain E:

84%　　　　16%

• Molecule 6: General transcription factor IIH subunit 3

Chain F:

79%　　　　12%　　　9%

D6 E7 L8 N9 L10 L11 V12 V15 I20 G23 L44 N52 R53 S54 A58 S67 Y71 PRO GLY LYS ASN GLY ARG LEU GLY ASP PHE PHE GLY ASP PRO GLY ASN PRO PRO GLU PHE ASN PRO SER GLY SER LYS D98 E130 K139 V151 N154

M157 K158 S159 R160 I164 S170 L190 C194 L227 L228 W229 P233 D234 Q235 H248 C255 V267 C271 I274 F275 C276 P280 I281 T284 F289

• Molecule 7: General transcription factor IIH subunit 5

Chain G: 77%   23%

V4 L5 V8 L9 C12 D13 Y22 E25 K31 K32 Q36 F44 A47 V50 Q54 T69

• Molecule 8: DNA repair protein complementing XP-C cells

14%

Chain H: 70%   29%   •

P635 T636 A637 I638 G639 L640 Y641 H644 P645 L646 Y647 A648 L649 K650 R651 H652 L653 L654 K655 Y656 E657 A658 I659 Y660 P661 E662 T663 A664 A665 I666 L667 G668 Y669 C670 R671 G672 E673 R678 D679 C680 T683 L684 H685 S686 R687 D688 T689 W690 R695 V696 V697 M706 V707 F710

S711 N712 R713 A714 R715 R718 L719 A720 E721 P722 Q723 L724 R725 E726 E727 N728 D729 L730 G731 T738 P743 P744 V745 A746 V747 D748 G749 K750 V751 P752 R753 G757 N758 V759 Y760 L761 P768 I769 Q773 L774 N775 L776 P777 N778 L779 R784 V791 Q792 A793 F799

G810 Y811 I812 V813 C814 E815 E816 F817 R818 L821 W825 E828 W848 K849 K853 L856 K862 R863 G866 E895 R898 S903 W904 N907 R908 E909 D910 K927 A931 F935 P936 L940

• Molecule 9: Centrin-2

Chain J: 89%   10%   •

K103 I106 D114 D115 D116 E117 T118 G119 F162 L163 R164 I165 K168 Y172

• Molecule 10: DNA repair protein complementing XP-A cells

Chain K: 79%   19%   •

Y102 V103 I104 E107 E111 L117 L123 P124 D131 A132 D131 A132 K135 H136 K137 L138 F164 I165 K168 N169 P170 Q174 W175 G176 D177 M178 K179 L180 Y181 L182 Q185 E212 K213 M214 K215 Q216 F219 K222 V223 R227 R228 Y246 K259 E271 K272

M273

• Molecule 11: DNA (Cy5)

Chain L: 36%   64%

A1 G2 G3 T4 A5 G6 T7 C10 A11 G12 C13 T14 G15 A16 T17 T18 G19 C20 G21 G24 A25 G26 G33 A34 C35 G36 T37 G38 C39 G40 A41 T42 A43 T44

• Molecule 12: DNA

Chain M:

11%

42%　58%

A12 T13 A14 G21 T22 C23 T24 A25 T26 T27 A28 T32 C33 A34 G35 C36 G37 C38 C42 A43 T46 G47 T48 G49 A50 A53 C54 C55 T56

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	54.1	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	319.872, 319.872, 319.872	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	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: SF4, VM6, CA, 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	A	0.24	0/4977	0.40	0/6723
2	B	0.24	0/5578	0.41	0/7551
3	C	0.23	0/1575	0.35	0/2125
4	D	0.24	0/3581	0.37	0/4851
5	E	0.24	0/3057	0.39	0/4136
6	F	0.24	0/2070	0.36	0/2803
7	G	0.24	0/528	0.41	0/713
8	H	0.23	0/2275	0.39	0/3064
9	J	0.24	0/577	0.37	0/762
10	K	0.23	0/1478	0.39	0/1974
11	L	0.53	0/1001	0.91	0/1543
12	M	0.54	0/1018	0.94	0/1566
All	All	0.27	0/27715	0.46	0/37811

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	A	4874	0	4912	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5457	0	5499	86	0
3	C	1547	0	1561	20	0
4	D	3499	0	3541	44	0
5	E	2989	0	2950	36	0
6	F	2034	0	2050	21	0
7	G	522	0	531	13	0
8	H	2224	0	2239	52	0
9	J	573	0	555	6	0
10	K	1450	0	1434	24	0
11	L	930	0	485	24	0
12	M	911	0	509	22	0
13	B	8	0	0	0	0
14	E	3	0	0	0	0
14	F	2	0	0	0	0
14	K	1	0	0	0	0
15	J	2	0	0	0	0
All	All	27026	0	26266	380	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 380 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)
8:H:649:LEU:HD11	8:H:673:GLU:HB3	1.66	0.78
8:H:758:ASN:HD21	8:H:792:GLN:HB2	1.50	0.77
11:L:14:DT:H2'	11:L:15:DG:C8	2.25	0.71
2:B:353:SER:HB2	2:B:356:ALA:HB3	1.73	0.71
2:B:258:ARG:HE	2:B:393:ASP:HA	1.56	0.70

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	597/603 (99%)	544 (91%)	53 (9%)	0	100	100
2	B	673/730 (92%)	647 (96%)	26 (4%)	0	100	100
3	C	187/438 (43%)	179 (96%)	8 (4%)	0	100	100
4	D	432/446 (97%)	428 (99%)	4 (1%)	0	100	100
5	E	378/380 (100%)	369 (98%)	9 (2%)	0	100	100
6	F	254/284 (89%)	249 (98%)	5 (2%)	0	100	100
7	G	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
8	H	268/274 (98%)	262 (98%)	6 (2%)	0	100	100
9	J	69/70 (99%)	69 (100%)	0	0	100	100
10	K	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
All	All	3092/3463 (89%)	2969 (96%)	123 (4%)	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	535/535 (100%)	518 (97%)	17 (3%)	39	63
2	B	591/636 (93%)	575 (97%)	16 (3%)	44	67
3	C	175/389 (45%)	169 (97%)	6 (3%)	37	62
4	D	379/384 (99%)	372 (98%)	7 (2%)	59	77
5	E	338/338 (100%)	332 (98%)	6 (2%)	59	77
6	F	230/250 (92%)	228 (99%)	2 (1%)	78	87
7	G	59/59 (100%)	59 (100%)	0	100	100
8	H	231/231 (100%)	221 (96%)	10 (4%)	29	57
9	J	61/63 (97%)	59 (97%)	2 (3%)	38	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	162/162 (100%)	155 (96%)	7 (4%)	29	57
All	All	2761/3047 (91%)	2688 (97%)	73 (3%)	49	68

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	671	ARG
10	K	227	ARG
8	H	711	SER
9	J	168	LYS
2	B	397	LEU

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

Mol	Chain	Res	Type
3	C	501	GLN
6	F	52	ASN

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 9 ligands modelled in this entry, 8 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	$\#|Z| > 2$
13	SF4	B	1000	2	0,12,12	-	-	-		

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
13	SF4	B	1000	2	-	-	0/6/5/5

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   ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	866:GLY	C	889:GLY	N	33.59
1	H	915:LYS	C	926:GLU	N	19.41
1	A	645:ARG	C	655:TYR	N	13.35
1	A	208:GLU	C	267:THR	N	6.37

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-27997. 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 ⓘ
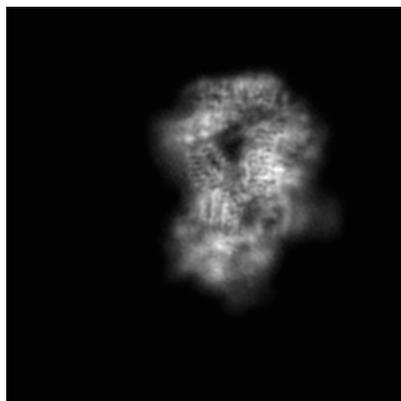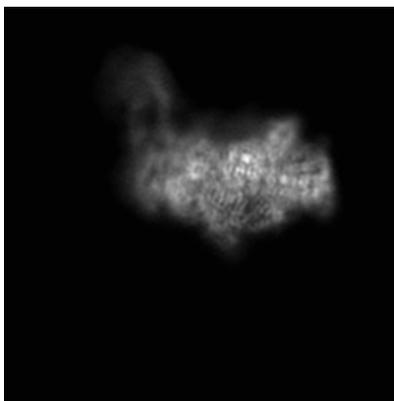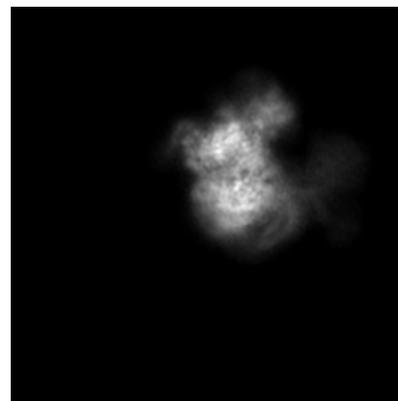
6.1.1 Primary map

X	Y	Z

6.1.2 Raw map

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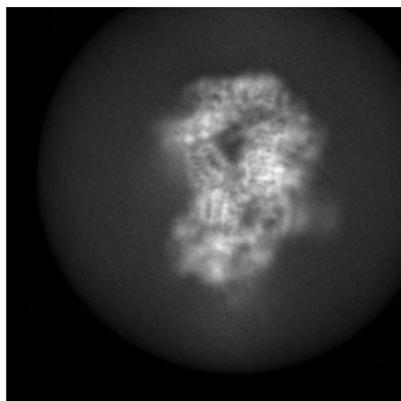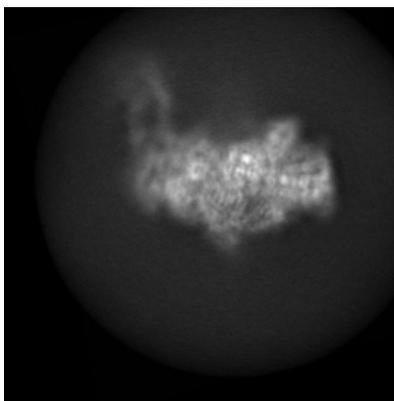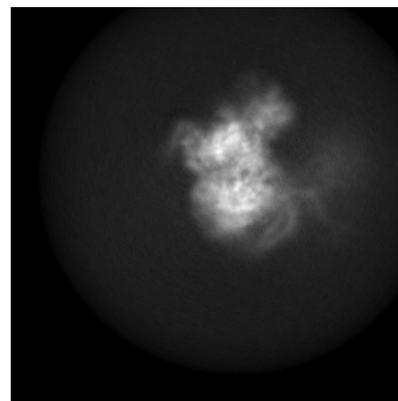
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
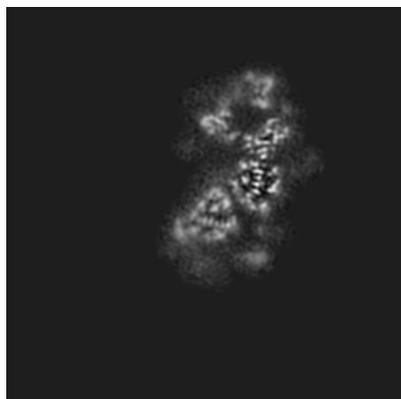
6.2.1 Primary map
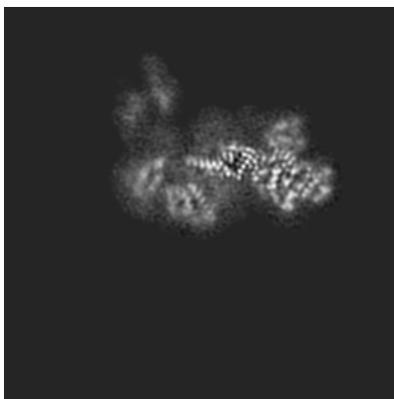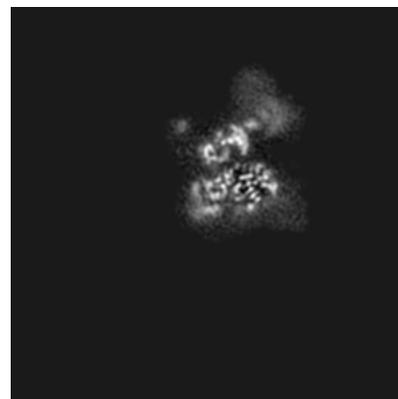
| X Index: 192 | Y Index: 192 | Z Index: 192 |

6.2.2 Raw map
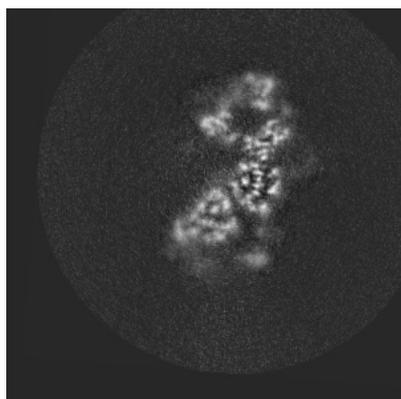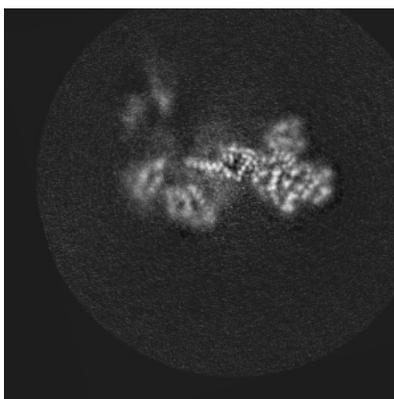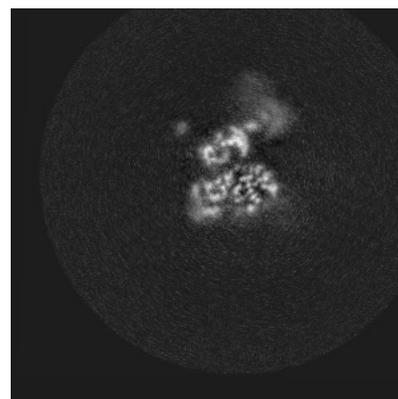
| X Index: 192 | Y Index: 192 | Z Index: 192 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
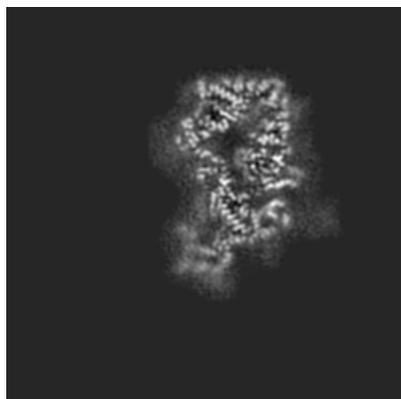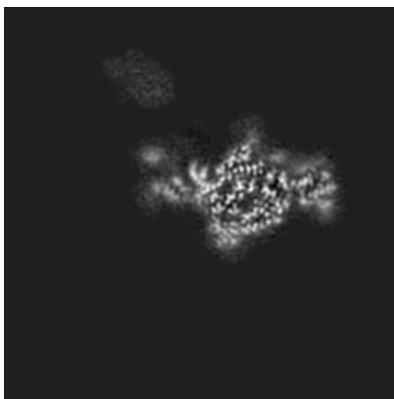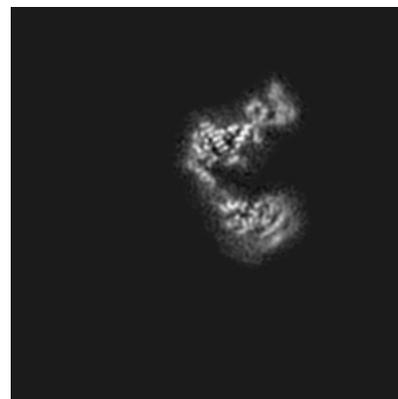
X Index: 218	Y Index: 253	Z Index: 259

6.3.2 Raw map
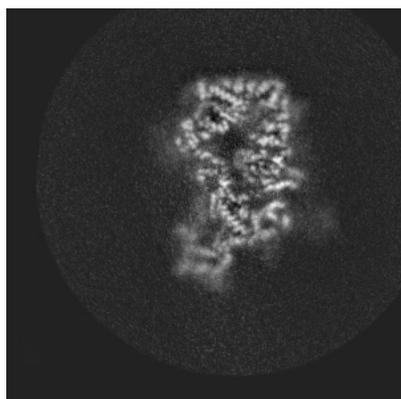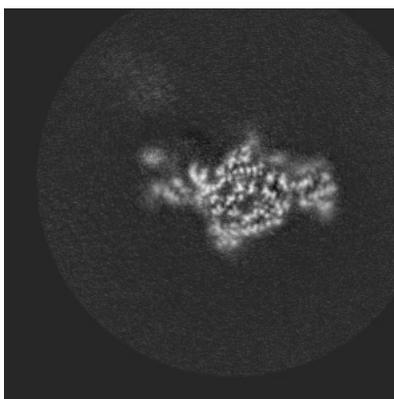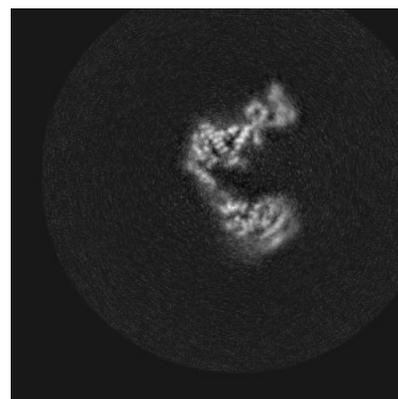
X Index: 218	Y Index: 253	Z Index: 259

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
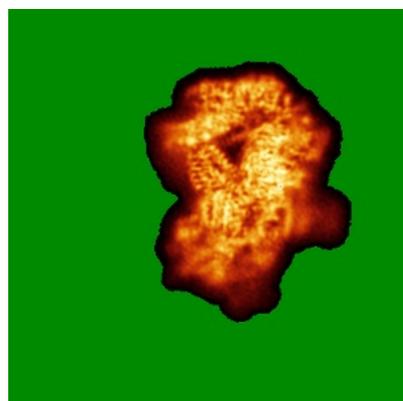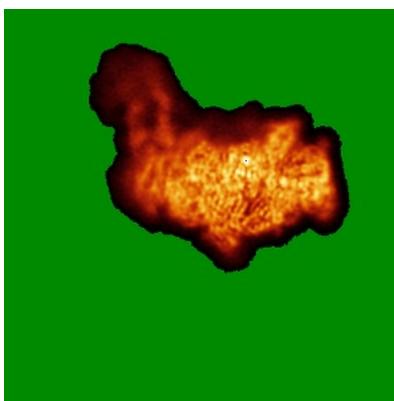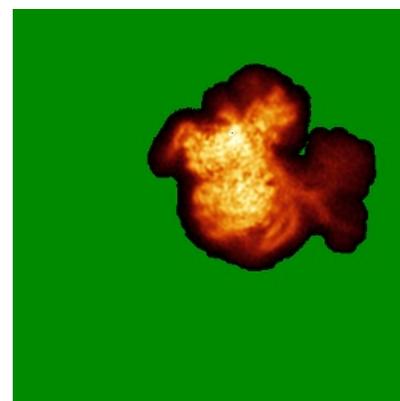
| X | Y | Z |

6.4.2 Raw map

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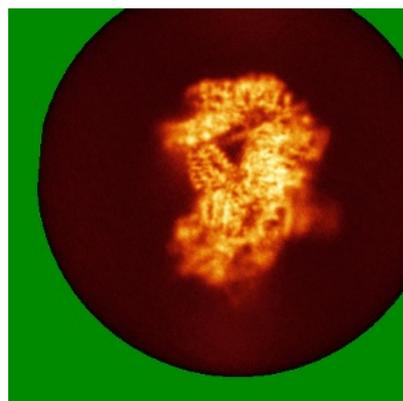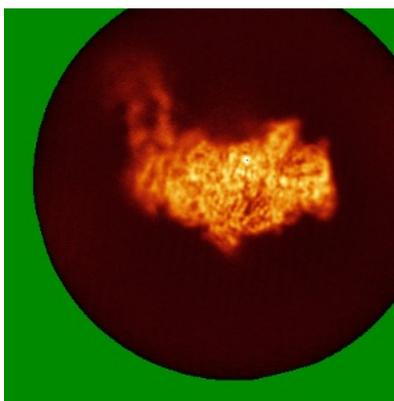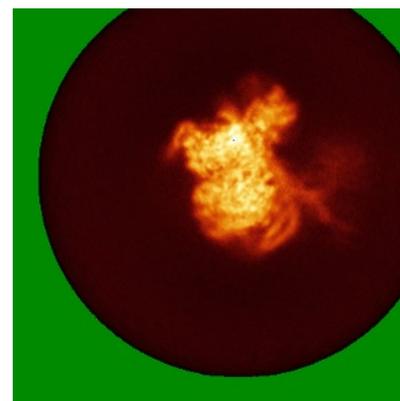
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.005. 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
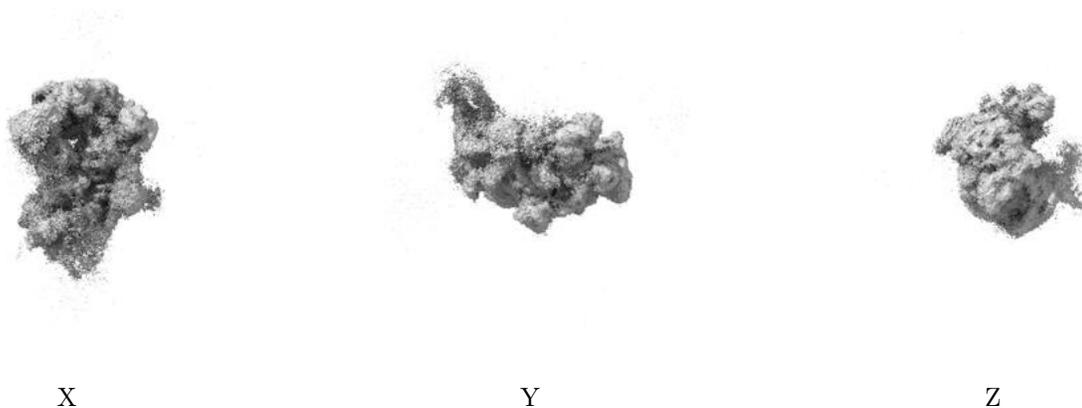
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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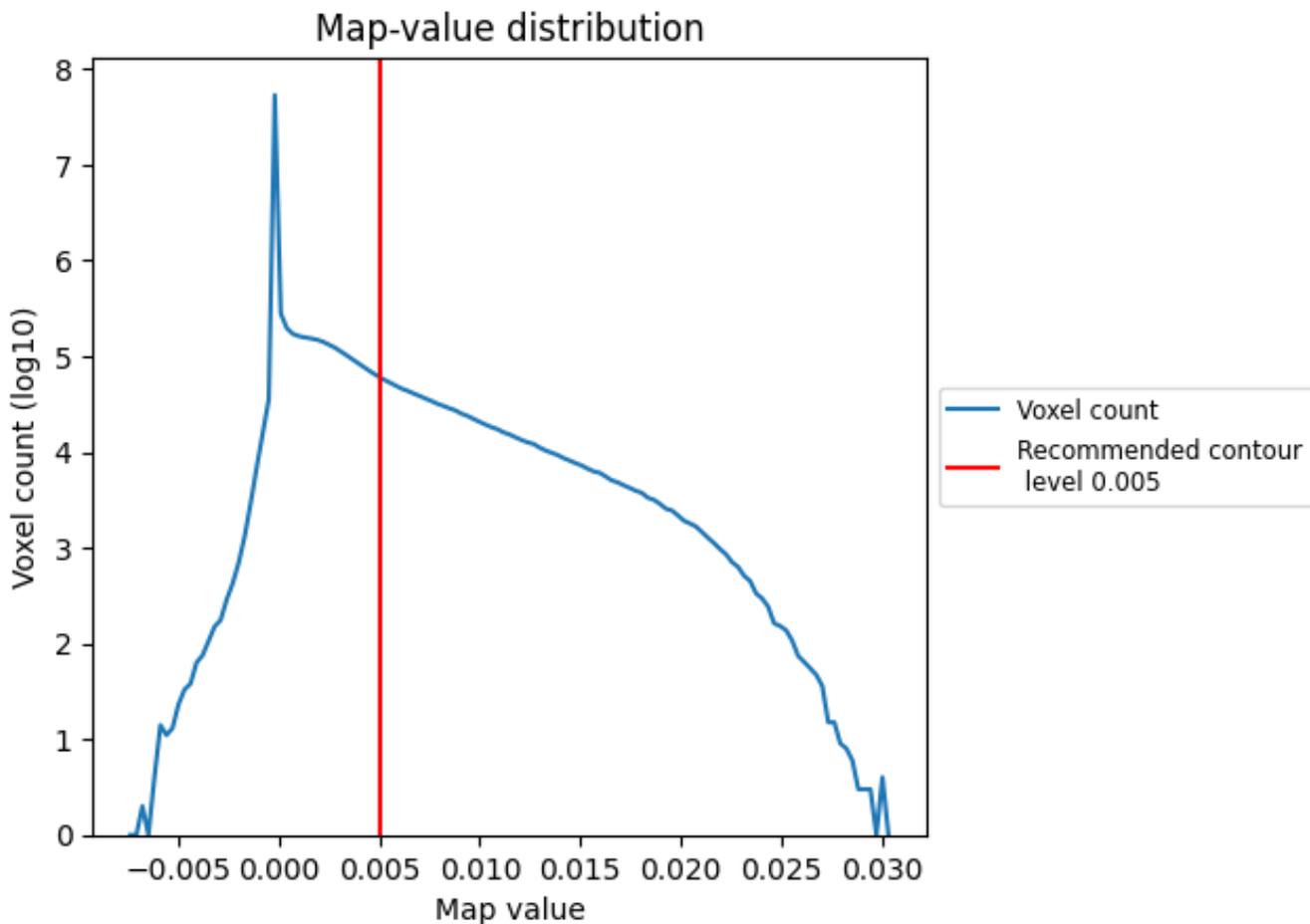
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
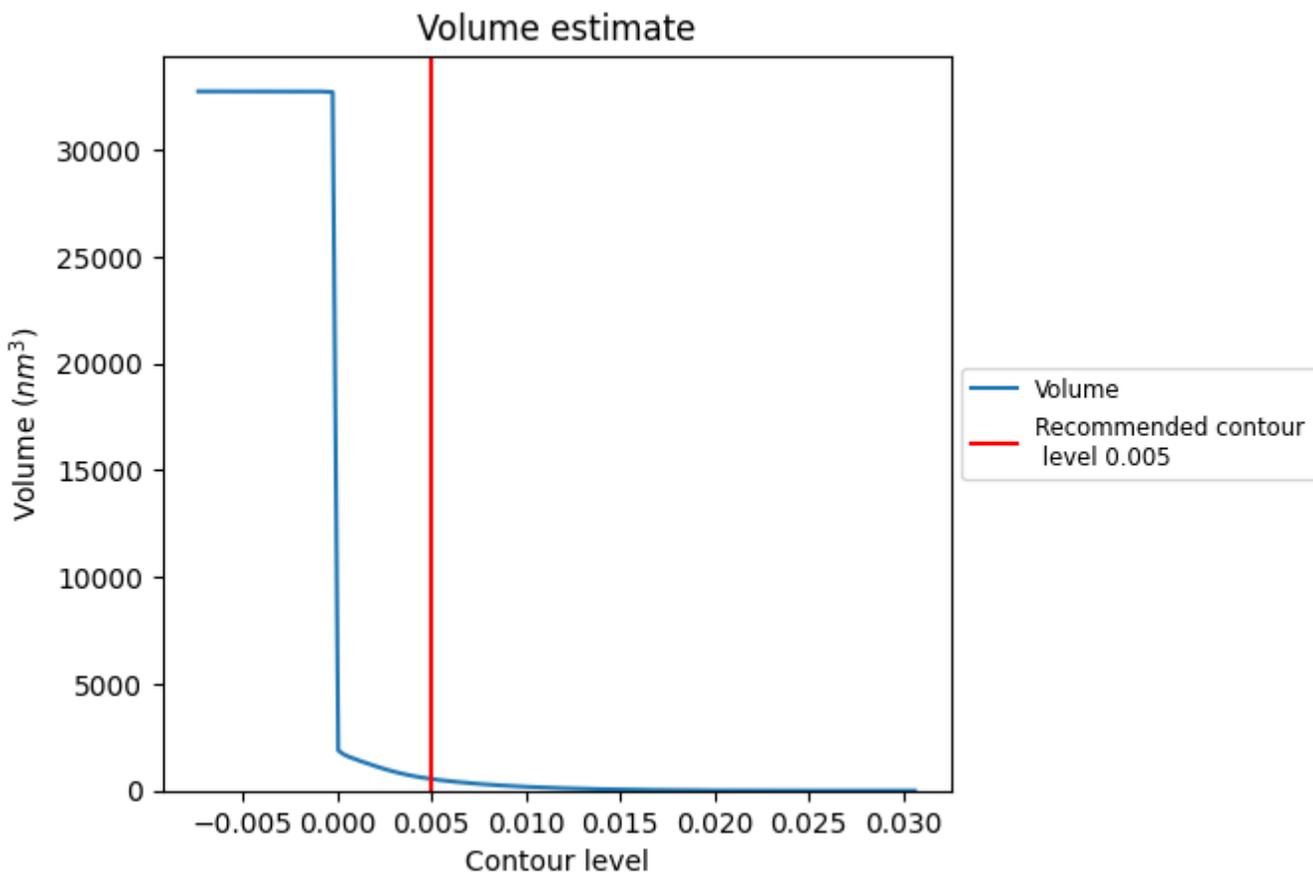
The volume at the recommended contour level is 546 nm^3; this corresponds to an approximate mass of 493 kDa.

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 ⓘ
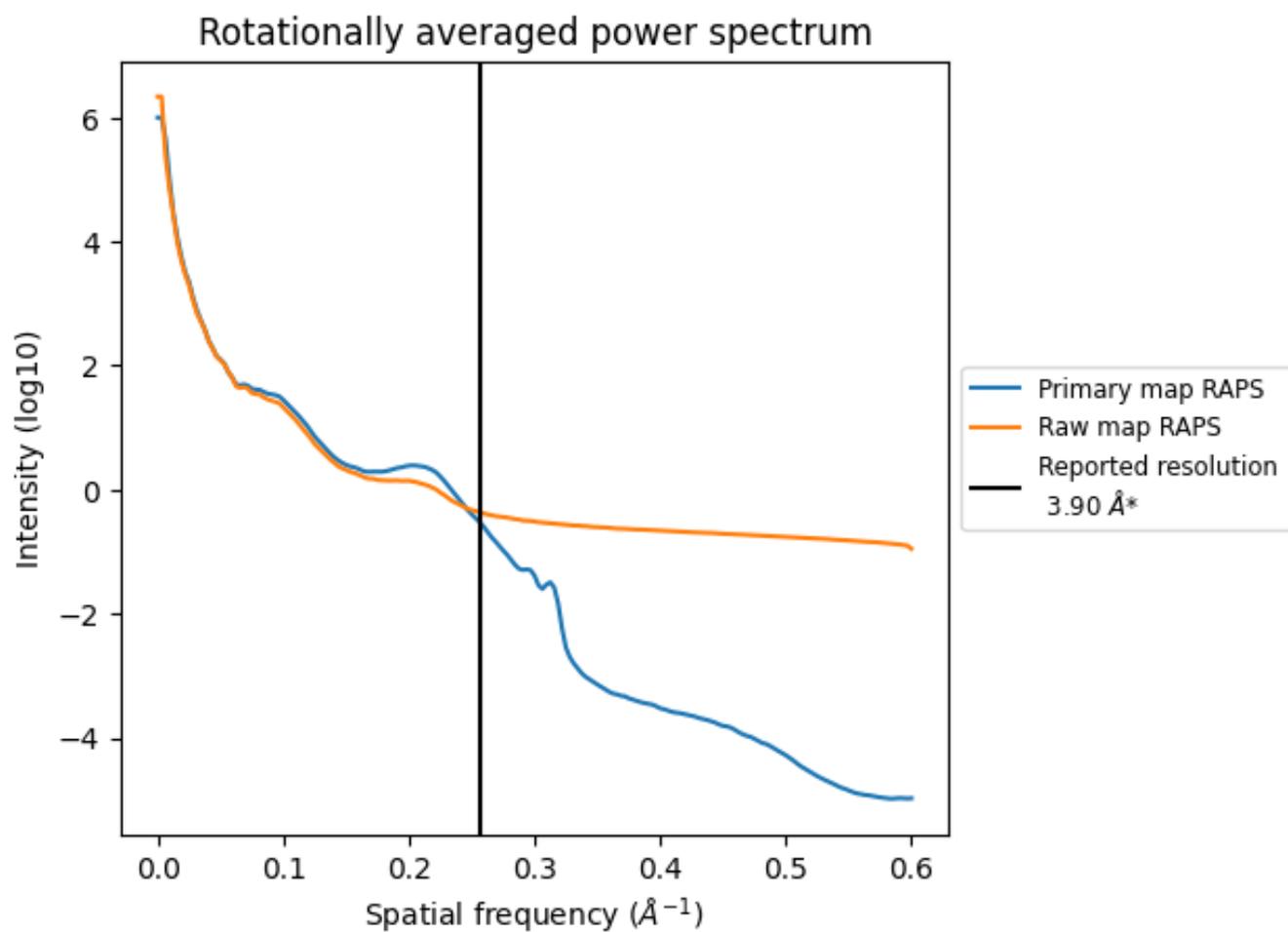
*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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)
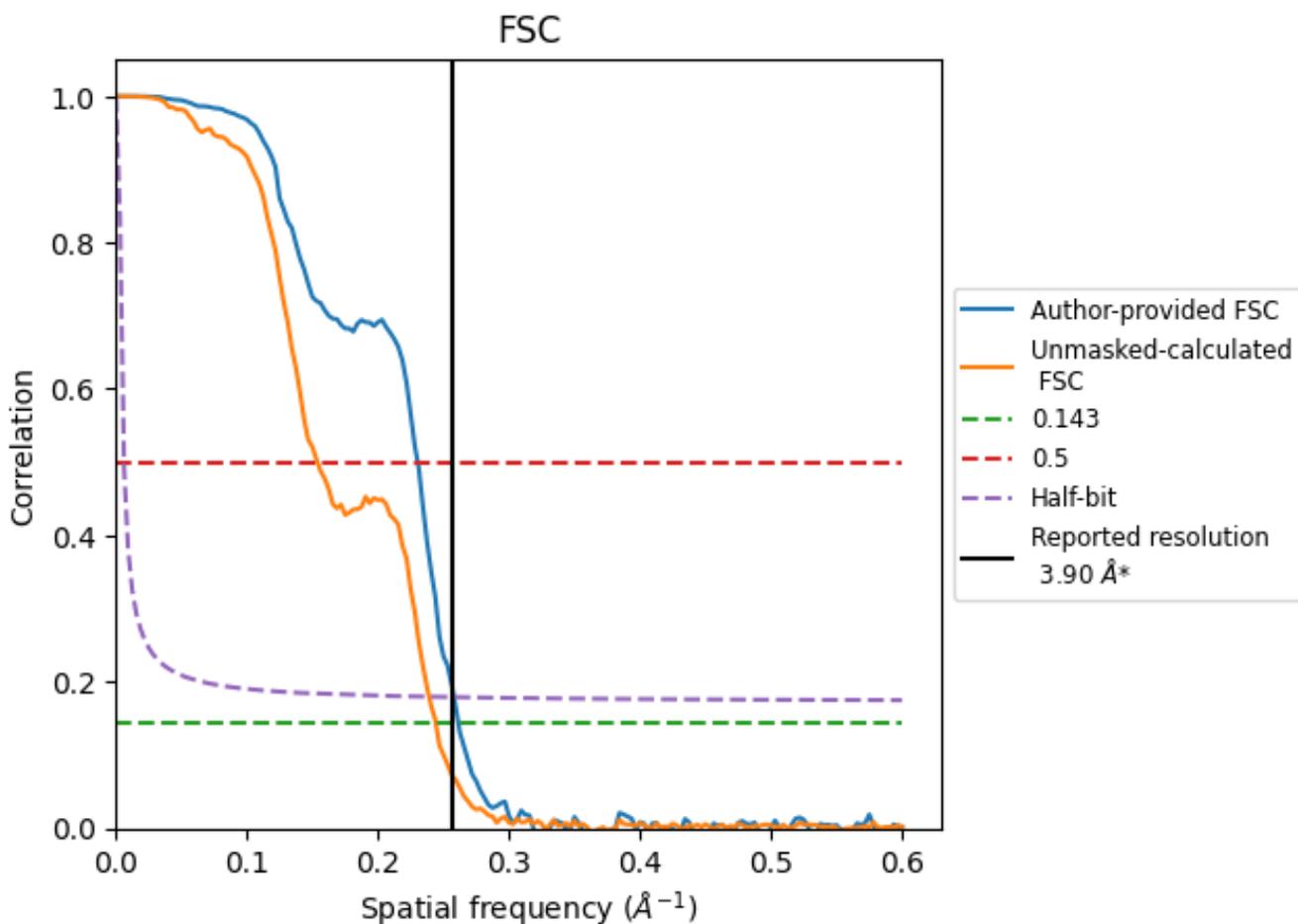
*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.82	4.34	3.87
Unmasked-calculated*	4.09	6.50	4.18

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

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27997 and PDB model 8EBT. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)

| X | Y | Z |
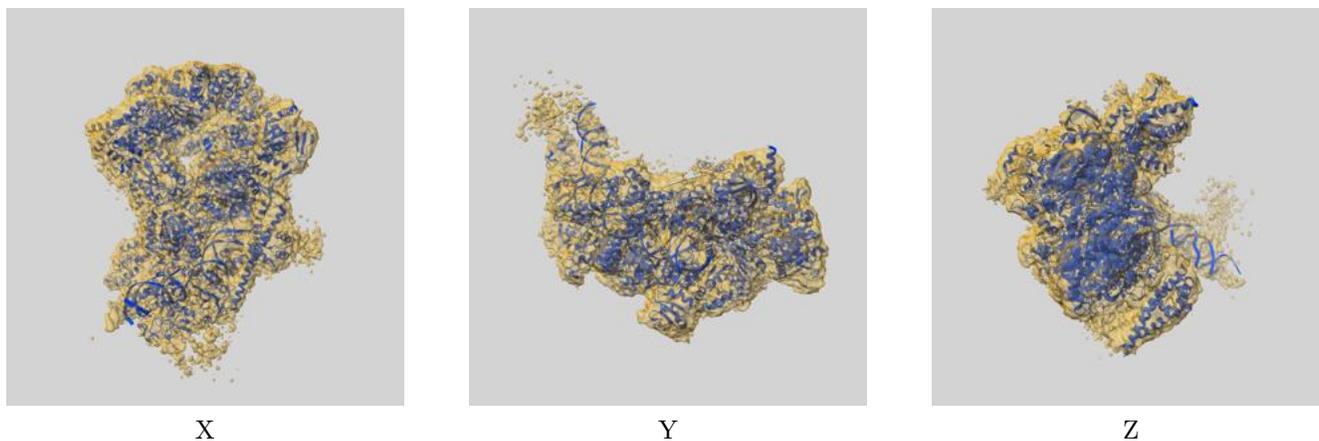
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ
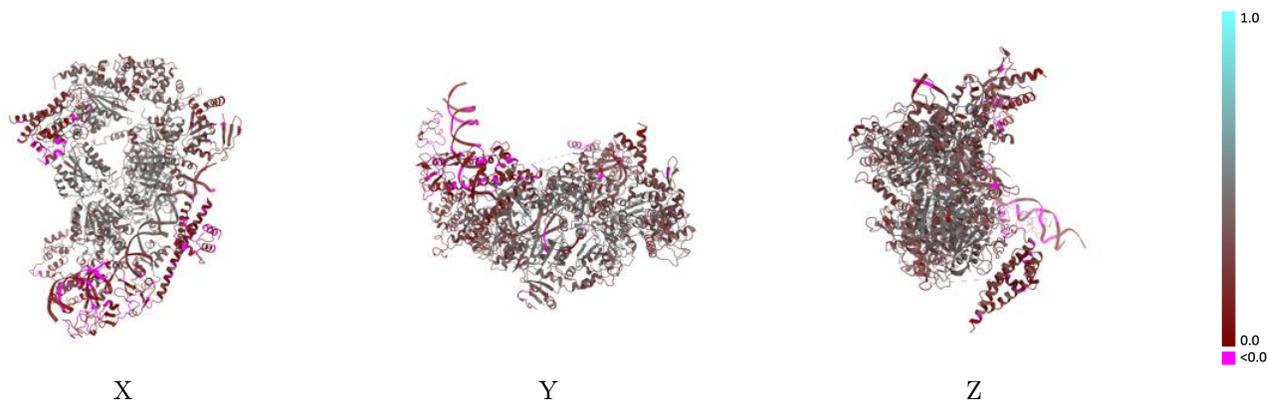
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
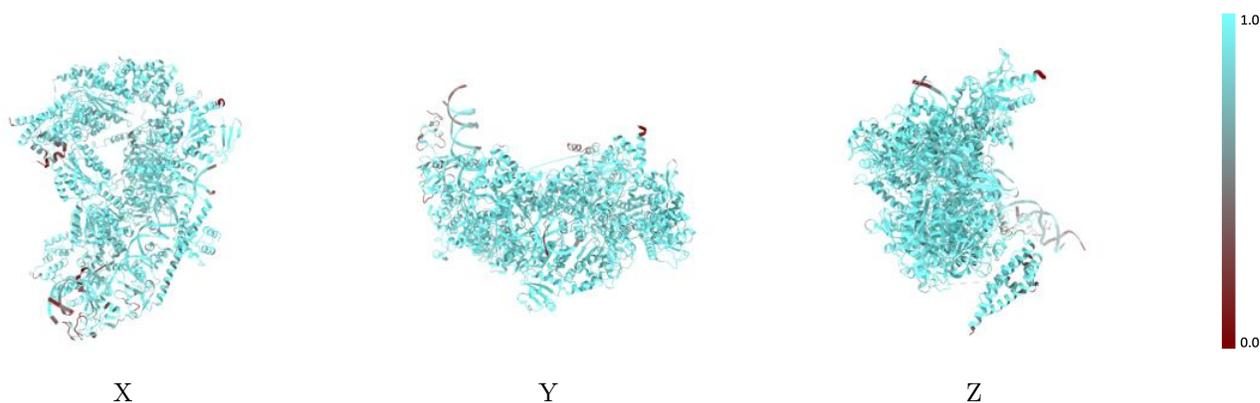
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4   Atom inclusion ⓘ
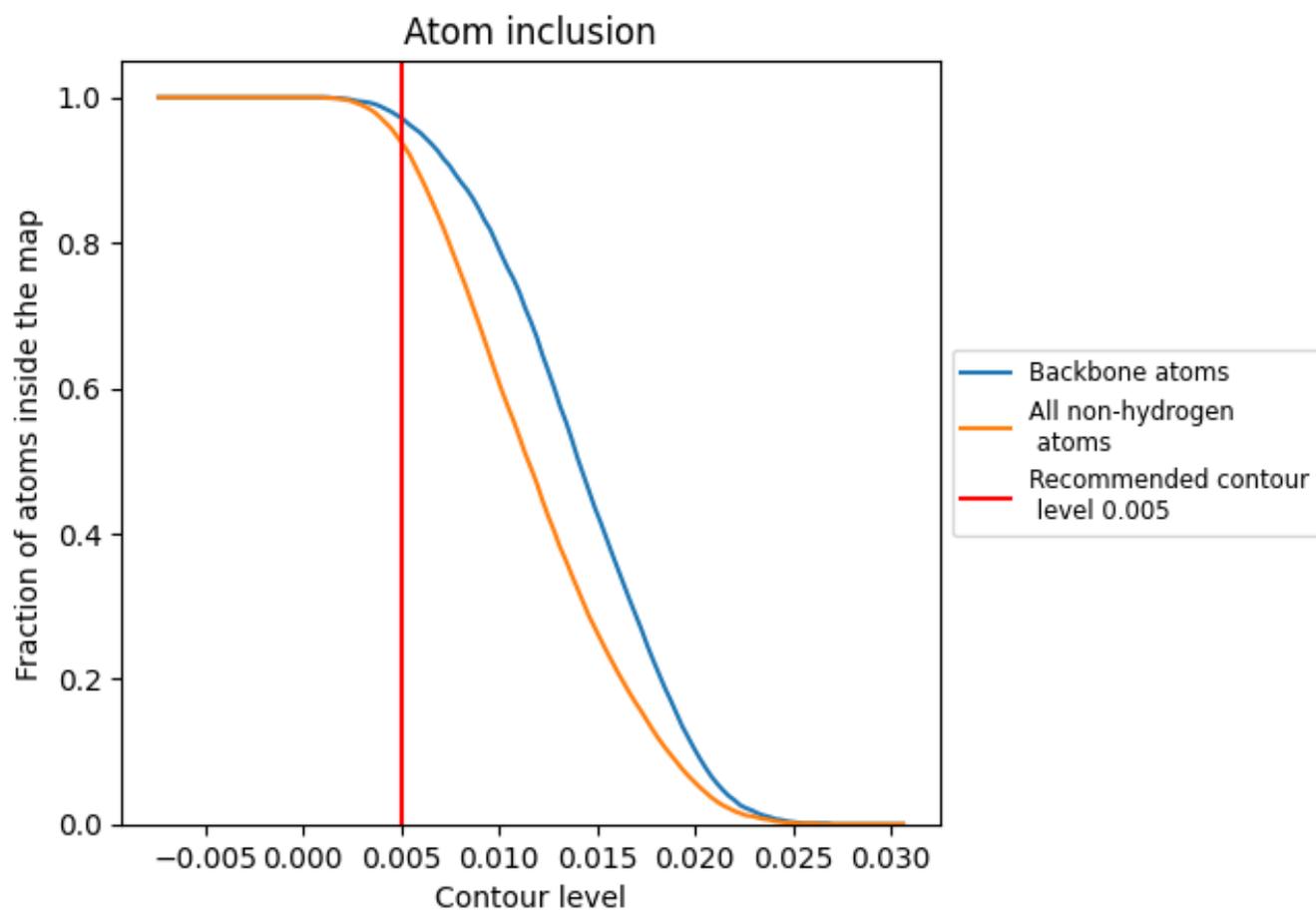
At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary   ⓘ

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.3040
A	0.9820	0.3980
B	0.9730	0.3110
C	0.8570	0.1780
D	0.9610	0.3340
E	0.9640	0.3710
F	0.9730	0.3900
G	0.9620	0.3230
H	0.7940	0.1130
J	0.9280	0.0820
K	0.9440	0.2690
L	0.8800	0.2060
M	0.8070	0.2000

1.0

0.0

<0.0