wwPDB EM Validation Summary Report (i)

Jun 20, 2024 – 10:36 AM EDT

PDB ID	:	8URQ
EMDB ID	:	EMD-42497
Title	:	Spo11 core complex with gapped DNA
Authors	:	Yu, Y.; Patel, D.J.
Deposited on	:	2023-10-26
Resolution	:	3.30 Å(reported)

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:

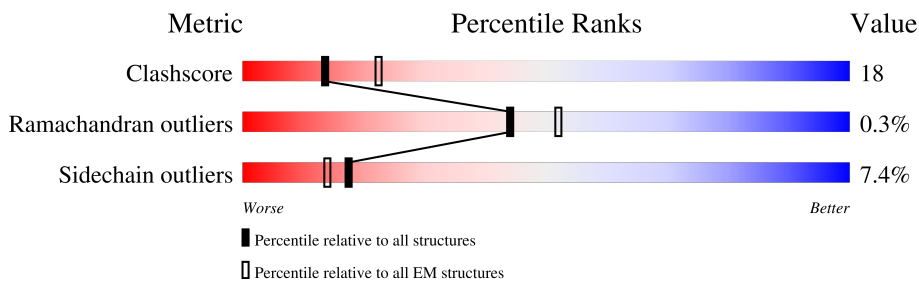|		
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.30 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		18
Ramachandran outliers		0.3%
Sidechain outliers		7.4%

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	F	182	7% / 13% 11% • 73%
2	B	264	• / 53% 29% • 14%
3	A	435	• / 53% 25% • 18%
4	C	397	• / 61% 28% • 10%
5	D	71	18% 25% 56%

2   Entity composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8569 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 Meiotic recombination protein REC104.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	50	Total 407	C 256	N 72	O 76	S 3	0	0

- Molecule 2 is a protein called Meiotic recombination protein REC102.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	227	Total 1845	C 1199	N 300	O 339	S 7	0	0

- Molecule 3 is a protein called Meiosis-specific protein SPO11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	358	Total 2875	C 1847	N 500	O 517	S 11	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ASN	SER	conflict	UNP P23179
A	99	SER	CYS	conflict	UNP P23179
A	204	SER	PRO	conflict	UNP P23179
A	278	ASN	LYS	conflict	UNP P23179
A	372	VAL	ILE	conflict	UNP P23179
A	393	GLY	ARG	conflict	UNP P23179
A	396	LYS	GLU	conflict	UNP P23179
A	399	SER	-	expression tag	UNP P23179
A	400	ARG	-	expression tag	UNP P23179
A	401	HIS	-	expression tag	UNP P23179
A	402	HIS	-	expression tag	UNP P23179
A	403	HIS	-	expression tag	UNP P23179
A	404	HIS	-	expression tag	UNP P23179
A	405	HIS	-	expression tag	UNP P23179
A	406	HIS	-	expression tag	UNP P23179

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Chain	Residue	Modelled	Actual	Comment	Reference
A	407	HIS	-	expression tag	UNP P23179
A	408	HIS	-	expression tag	UNP P23179
A	409	HIS	-	expression tag	UNP P23179
A	410	HIS	-	expression tag	UNP P23179
A	411	GLY	-	expression tag	UNP P23179
A	412	ASP	-	expression tag	UNP P23179
A	413	TYR	-	expression tag	UNP P23179
A	414	LYS	-	expression tag	UNP P23179
A	415	ASP	-	expression tag	UNP P23179
A	416	ASP	-	expression tag	UNP P23179
A	417	ASP	-	expression tag	UNP P23179
A	418	ASP	-	expression tag	UNP P23179
A	419	LYS	-	expression tag	UNP P23179
A	420	ASP	-	expression tag	UNP P23179
A	421	TYR	-	expression tag	UNP P23179
A	422	LYS	-	expression tag	UNP P23179
A	423	ASP	-	expression tag	UNP P23179
A	424	ASP	-	expression tag	UNP P23179
A	425	ASP	-	expression tag	UNP P23179
A	426	ASP	-	expression tag	UNP P23179
A	427	LYS	-	expression tag	UNP P23179
A	428	ASP	-	expression tag	UNP P23179
A	429	TYR	-	expression tag	UNP P23179
A	430	LYS	-	expression tag	UNP P23179
A	431	ASP	-	expression tag	UNP P23179
A	432	ASP	-	expression tag	UNP P23179
A	433	ASP	-	expression tag	UNP P23179
A	434	ASP	-	expression tag	UNP P23179
A	435	LYS	-	expression tag	UNP P23179

- Molecule 4 is a protein called Antiviral protein SKI8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	358	2805	1772	475	543	15	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	THR	ALA	conflict	UNP Q02793

- Molecule 5 is a DNA chain called gapped DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	D	31	636	304	116	185	31	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).
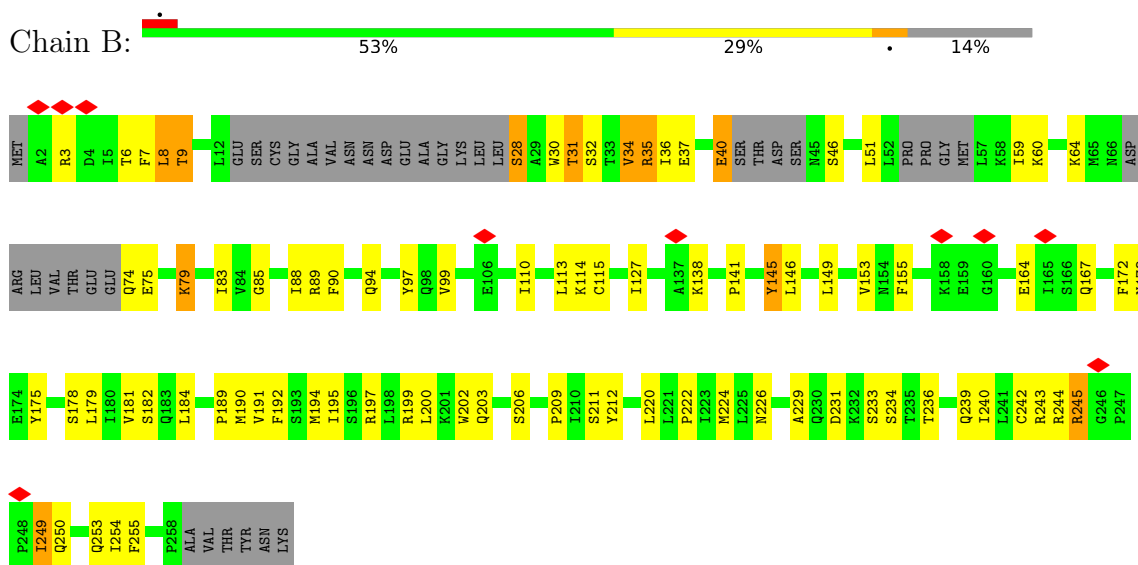
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0

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: Meiotic recombination protein REC104

• Molecule 2: Meiotic recombination protein REC102

• Molecule 3: Meiosis-specific protein SPO11

F91 P92 L93 N94 H97 L98 S99 T100 H101 Q102 F103 K104 L105 K106 R107 L114 L115 K116 L140 V147 R55 F156 N157 S161 P162 S165 L166 P170 K173 G174 L175 V176 Y177 F180 D183 I184 Y185 D186 N187 I188 LEU THR CYS GLU ASN GLU PRO LYS MET

Q198 K199 Q200 T201 I202 K206 P207 C208 P211 F212 F213 Q214 D215 D216 A217 V218 L221 G222 THR THR SER MET CYS N228 I229 E233 K234 E235 A236 V237 F238 T239 K240 L241 V242 H246 LYS LEU SER THR N251 L254 I255 T256 G257 K258 G259 F260 P261 D262 K270 K271 L272

E273 Q274 Y275 C283 S284 I285 D288 A289 D290 P291 Y292 N299 N304 E305 R306 N307 A308 Y309 M313 A314 R320 I321 T322 Q323 V324 E330 VAL HIS ASN LYS S335 S340 L341 N342 Q343 R344 D345 A349 K350 N351 L352 I353 L356 W361 L368 C375 Q376

K383 K384 A385 E386 M387 N388 D391 Y397 K398 SER ARG HIS HIS HIS HIS HIS HIS HIS HIS HIS GLY ASP TYR LYS ASP ASP ASP LYS ASP TYR LYS ASP ASP ASP LYS ASP ASP ASP LYS ASP TYR LYS ASP ASP ASP LYS

• Molecule 4: Antiviral protein SKI8

Chain C:

61%   28%   10%

MET SER LYS VAL PHE ILE A7 A11 H15 D16 A17 D18 I19 F20 C25 N26 T29 V30 S33 G34 G36 Y37 L38 K39 N43 K44 D47 N48 P51 S55 F59 S63 G64 L65 H66 L71 Q72 E75 ARG ASP ALA F79 V84 A85 T86

T87 S88 Y96 R100 GLU ASP GLU THR LYS K106 F109 D113 K120 K121 H122 S123 W129 S132 N133 ASP ARG LEU LEU S138 L141 K147 G148 W153 F155 F158 ALA ASP GLU SER ASN SER LEU THR LEU N168 W169 T178 V179 M183 S186

Q187 F188 A189 I194 S195 G198 F204 N205 N206 G207 T208 V209 Q210 L214 L220 Y221 N222 F223 E224 S225 Q226 H227 S228 S233 I236 V239 K240 F241 S242 L247 L248 A249 I250 A251 H252 N255 G258 C259 I260 T261 L262 Y263 E264 T265 GLU PHE G268 L274

T278 HIS SER SER GLN ALA SER LEU G286 A289 V294 M295 S296 L297 S298 F299 N300 D301 T305 W311 D312 G313 K314 L315 R316 F317 W318 D319 V320 K321 L329 D335 I336 E337 I338 E339 E340 L343 D346 D350 L363 W367 M371 L375 N376

L379 C380 C381 V382 D385 R386 W390 F391 R392 E393 A394 GLY GLY LYS

• Molecule 5: gapped DNA

Chain D:

18%   25%   56%

DT DA DG DG DC DC DG DT DC DG DG DC DT DA DC DT DA DC DA DA DA DG DT DA DG DC DC DG DA DC DG DG DC DC DG DG DA DT DT A39 G40 C41 G45 A48 T49 C50 C53 T54 DT DA A57 G58 A59 T63 T64 A65 C66

A67 T68 T69 G70 C71

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	548674	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 $(e^-/\text{Å}^2)$	53	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.771	Depositor
Minimum map value	-3.786	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	272.384, 272.384, 272.384	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	F	0.31	0/413	0.58	0/556
2	B	0.26	0/1884	0.51	0/2550
3	A	0.38	0/2926	0.60	0/3945
4	C	0.27	0/2867	0.52	0/3875
5	D	0.42	0/712	0.85	0/1094
All	All	0.33	0/8802	0.59	0/12020

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	407	0	399	40	0
2	B	1845	0	1860	85	0
3	A	2875	0	2930	123	0
4	C	2805	0	2683	70	0
5	D	636	0	352	25	0
6	A	1	0	0	0	0
All	All	8569	0	8224	301	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 18.

The worst 5 of 301 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:F:11:ILE:CG2	2:B:182:SER:HB2	1.70	1.21
1:F:11:ILE:HG22	2:B:182:SER:CB	1.70	1.19
1:F:11:ILE:HG22	2:B:182:SER:HB2	1.22	1.14
2:B:30:TRP:CB	2:B:153:VAL:HA	1.79	1.12
3:A:291:PRO:HG3	3:A:345:ASP:O	1.53	1.07

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	F	48/182 (26%)	46 (96%)	1 (2%)	1 (2%)	7	31
2	B	217/264 (82%)	190 (88%)	27 (12%)	0	100	100
3	A	344/435 (79%)	306 (89%)	36 (10%)	2 (1%)	25	57
4	C	344/397 (87%)	305 (89%)	39 (11%)	0	100	100
All	All	953/1278 (75%)	847 (89%)	103 (11%)	3 (0%)	44	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	98	LEU
3	A	207	PRO
1	F	12	THR

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	F	46/170 (27%)	40 (87%)	6 (13%)	4	17
2	B	212/245 (86%)	197 (93%)	15 (7%)	14	42
3	A	320/398 (80%)	292 (91%)	28 (9%)	10	33
4	C	312/348 (90%)	295 (95%)	17 (5%)	22	53
All	All	890/1161 (77%)	824 (93%)	66 (7%)	17	40

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	188	PHE
4	C	221	TYR
4	C	379	LEU
3	A	52	PHE
3	A	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	144	GLN
3	A	342	ASN
4	C	43	ASN
3	A	14	GLN
1	F	20	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 1 ligands modelled in this entry, 1 is 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-42497. 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 ⓘ
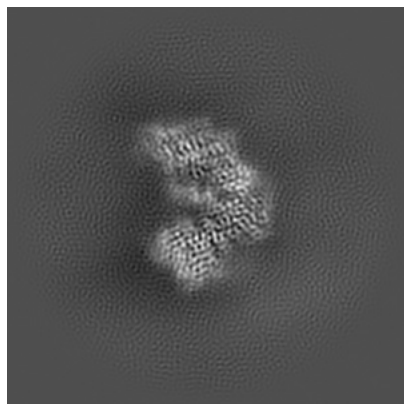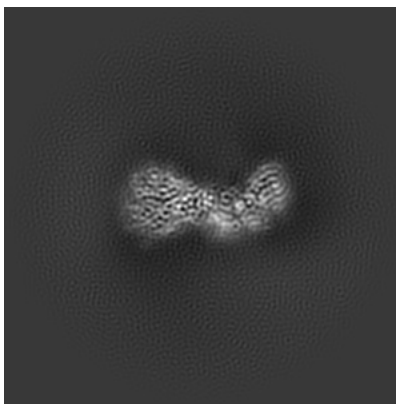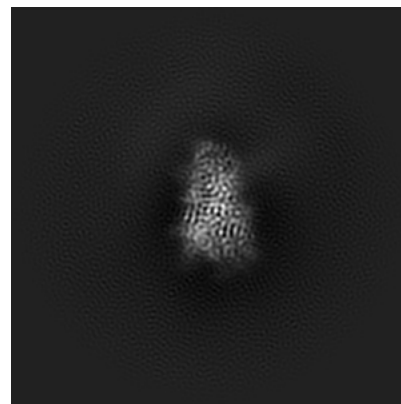
6.1.1   Primary map

X	Y	Z

6.1.2   Raw map

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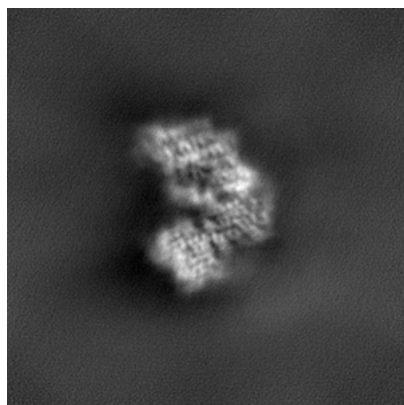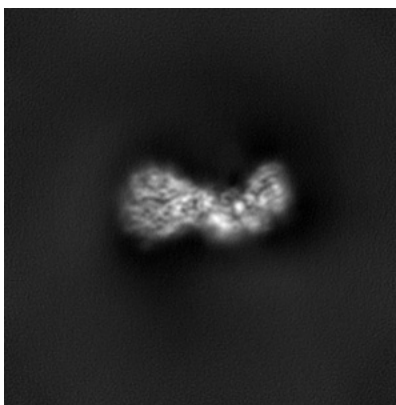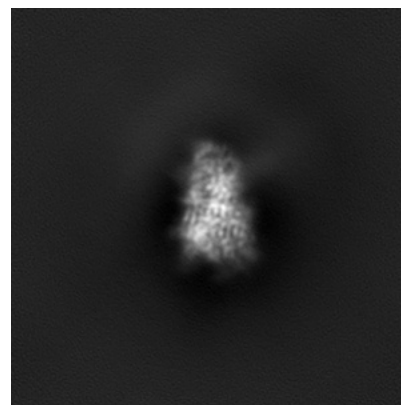
The images above show the map projected vin three orthogonal directions.

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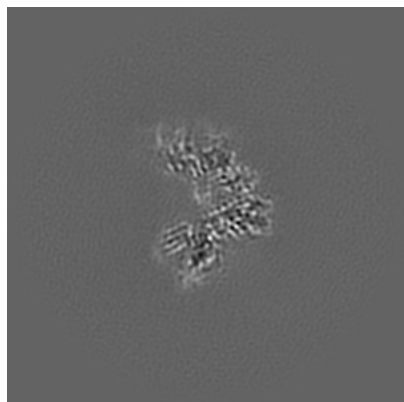
6.2.1 Primary map
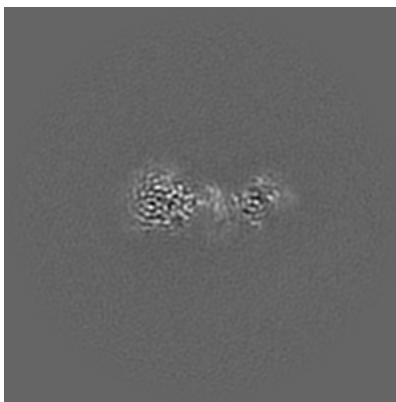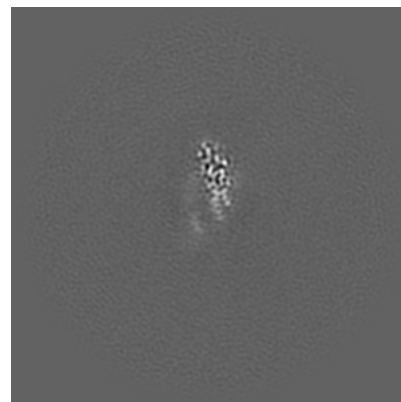
| X Index: 128 | Y Index: 128 | Z Index: 128 |

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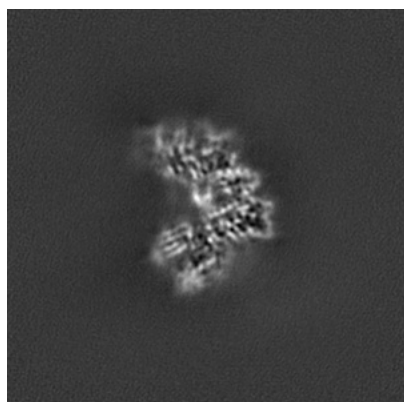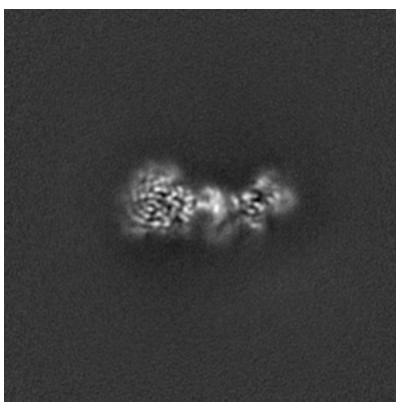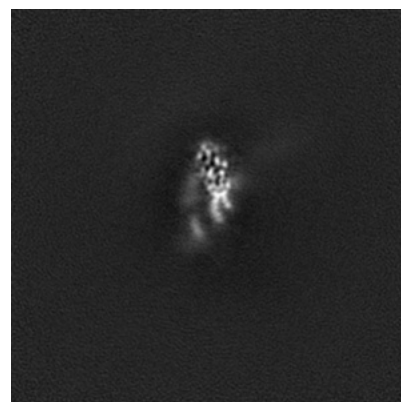
| X Index: 128 | Y Index: 128 | Z Index: 128 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
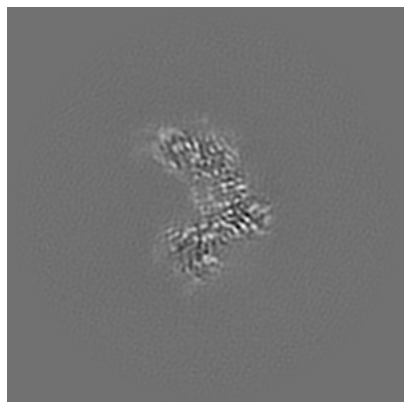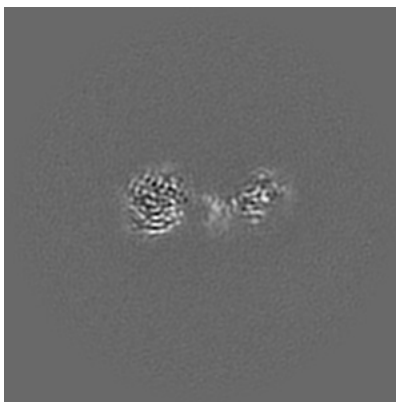
X Index: 132   Y Index: 121   Z Index: 107
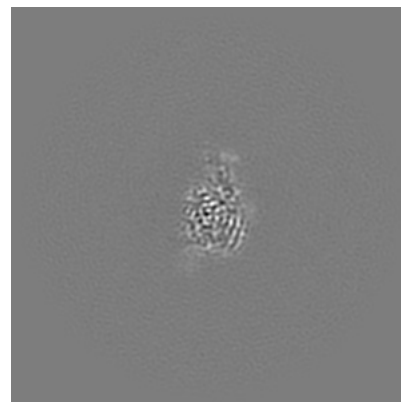
6.3.2 Raw map
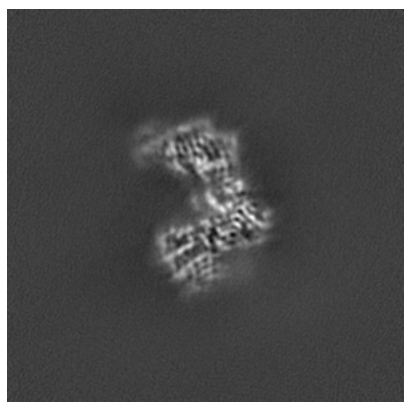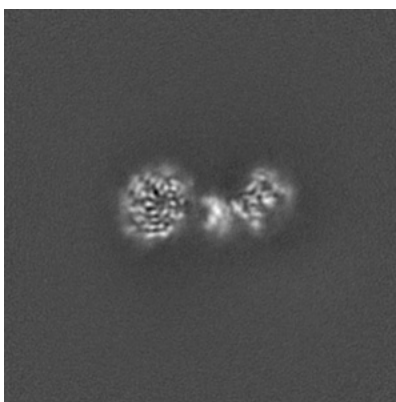
X Index: 135   Y Index: 120   Z Index: 107
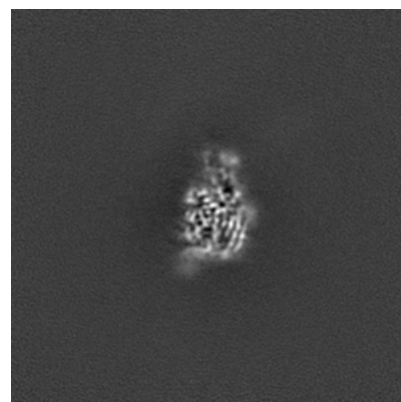
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
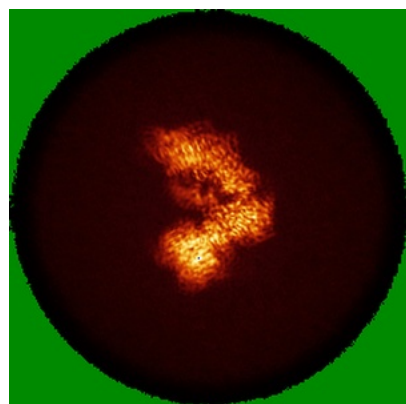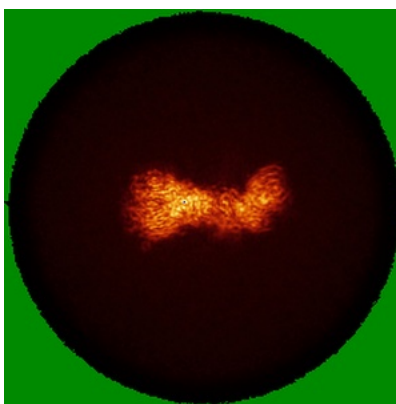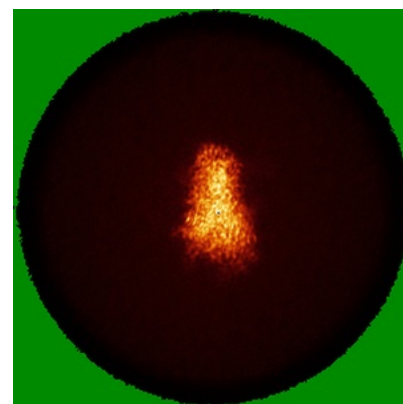
| X | Y | Z |

6.4.2 Raw map

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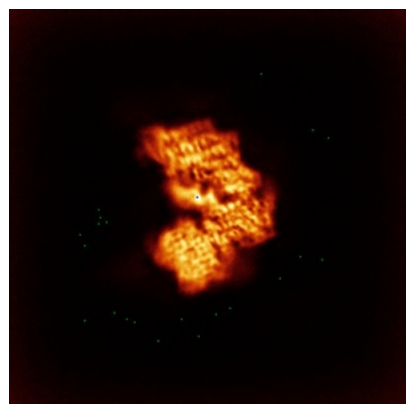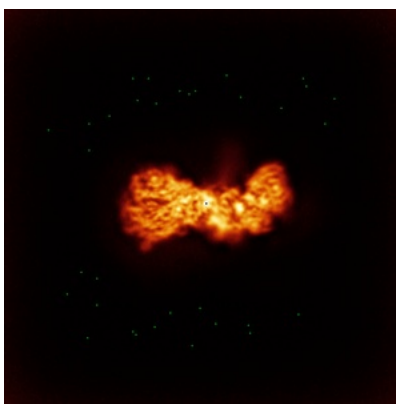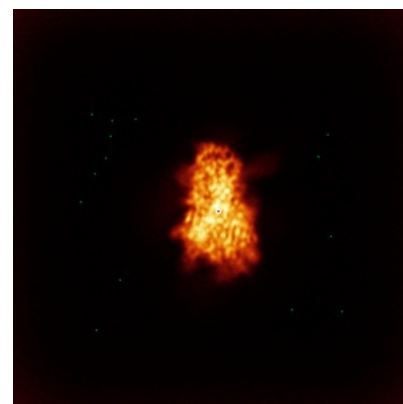
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.28. 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
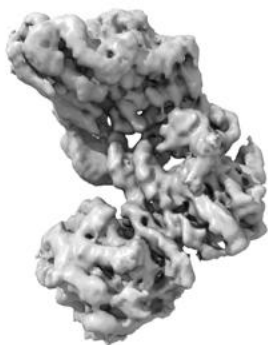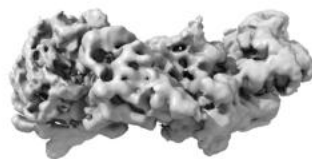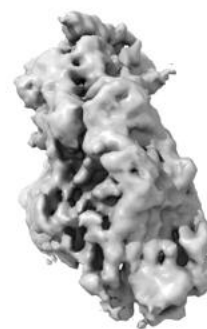
X   Y   Z

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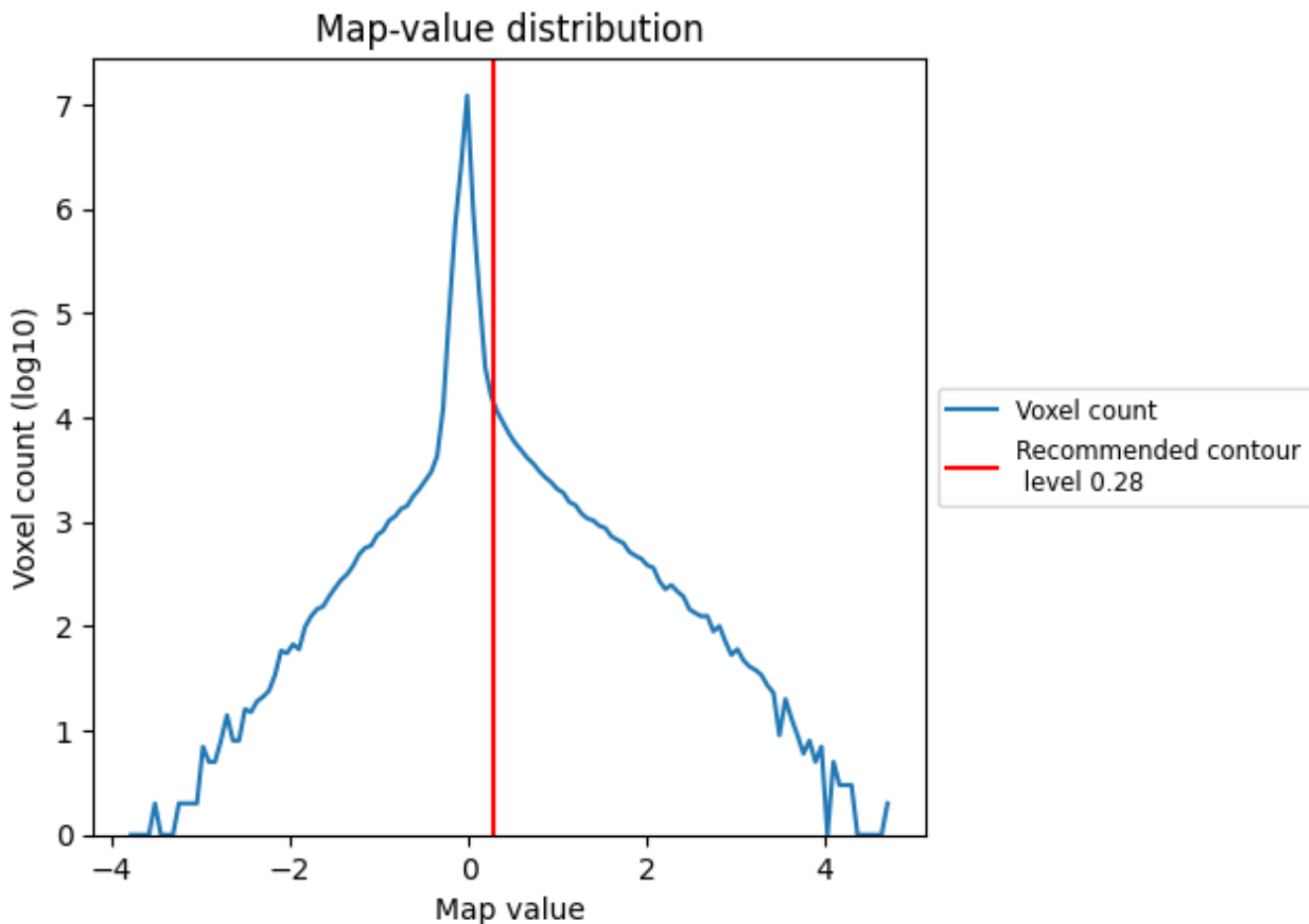
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
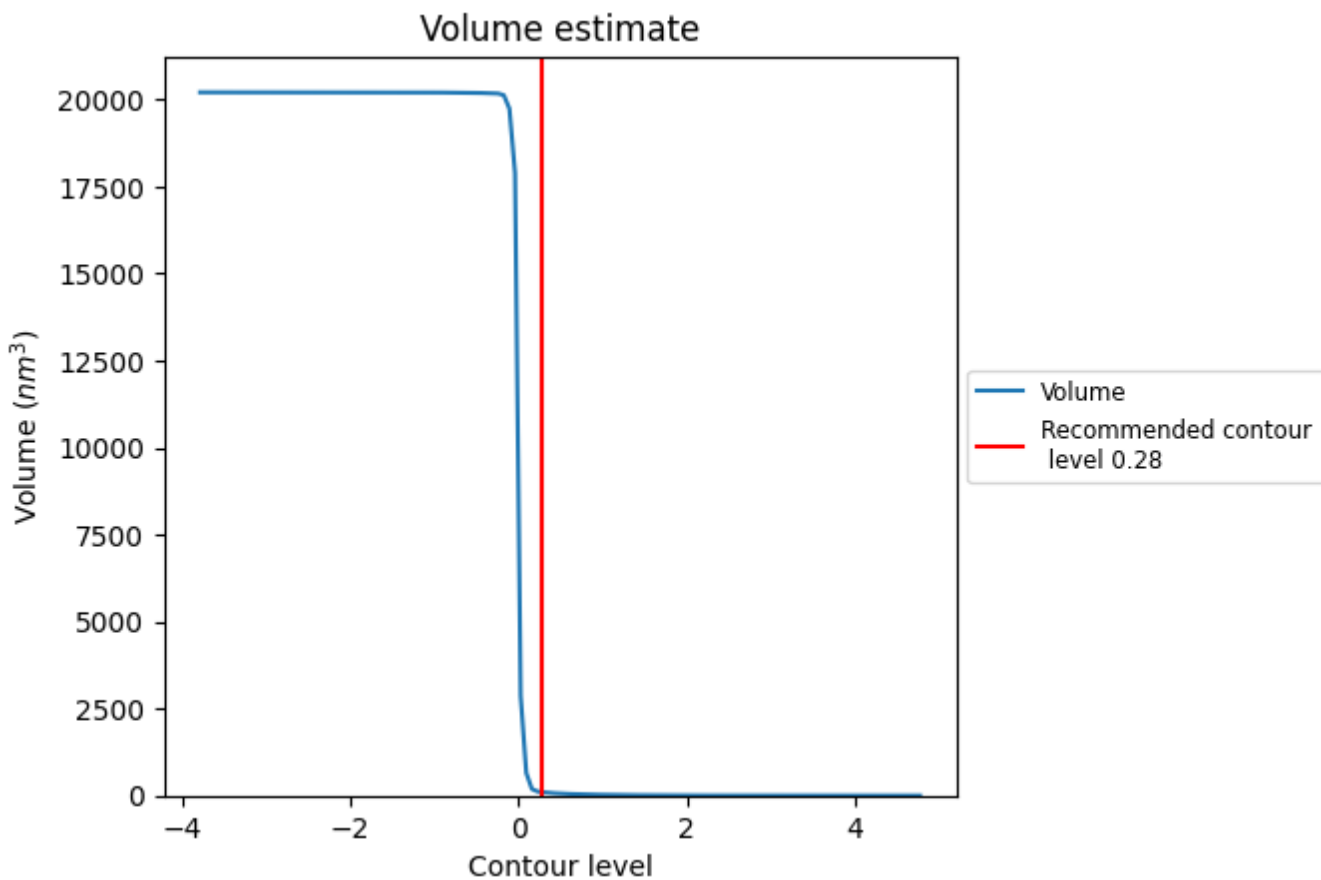
The volume at the recommended contour level is 99 nm^3; this corresponds to an approximate mass of 90 kDa.

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   ⓘ
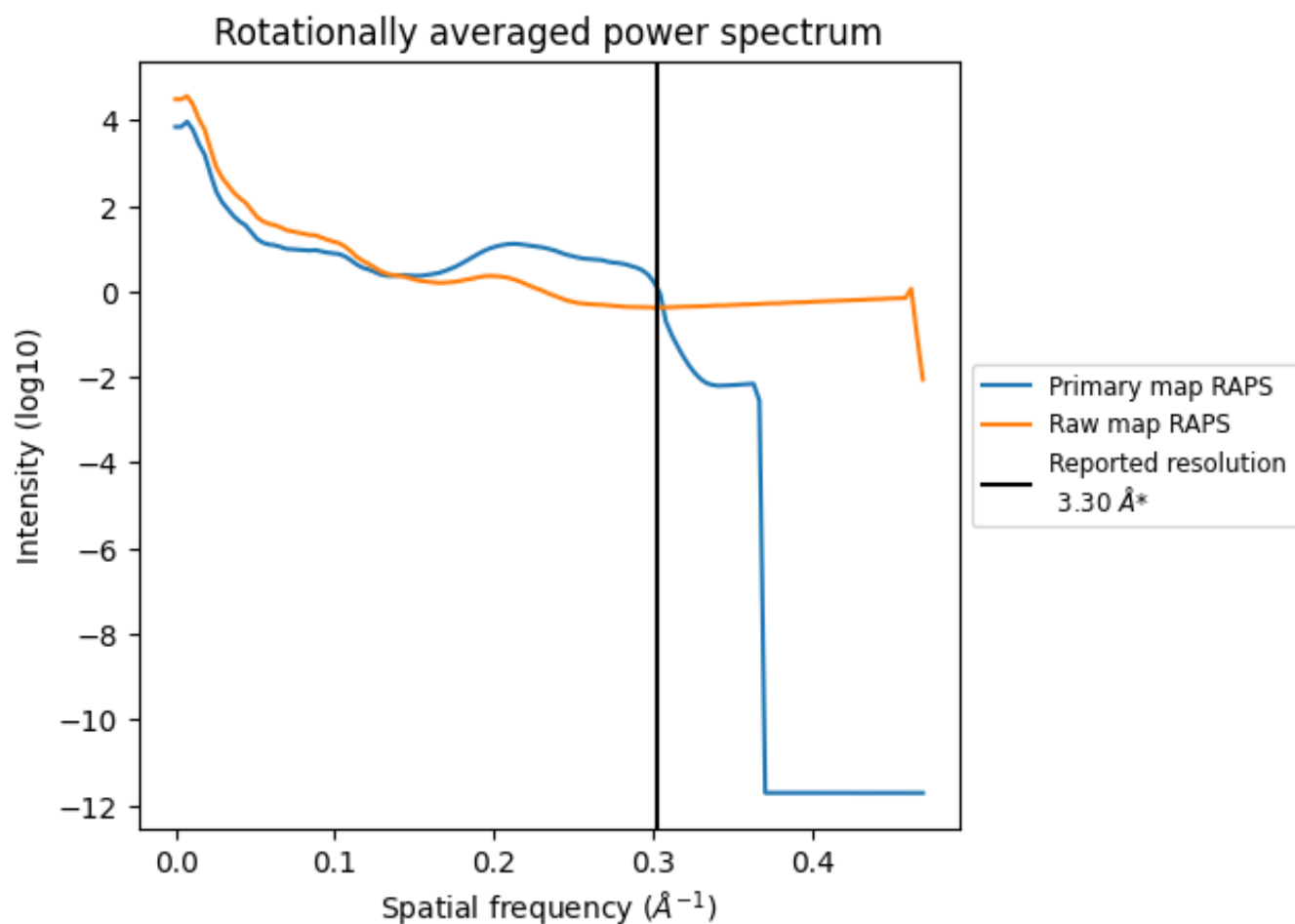
*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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)
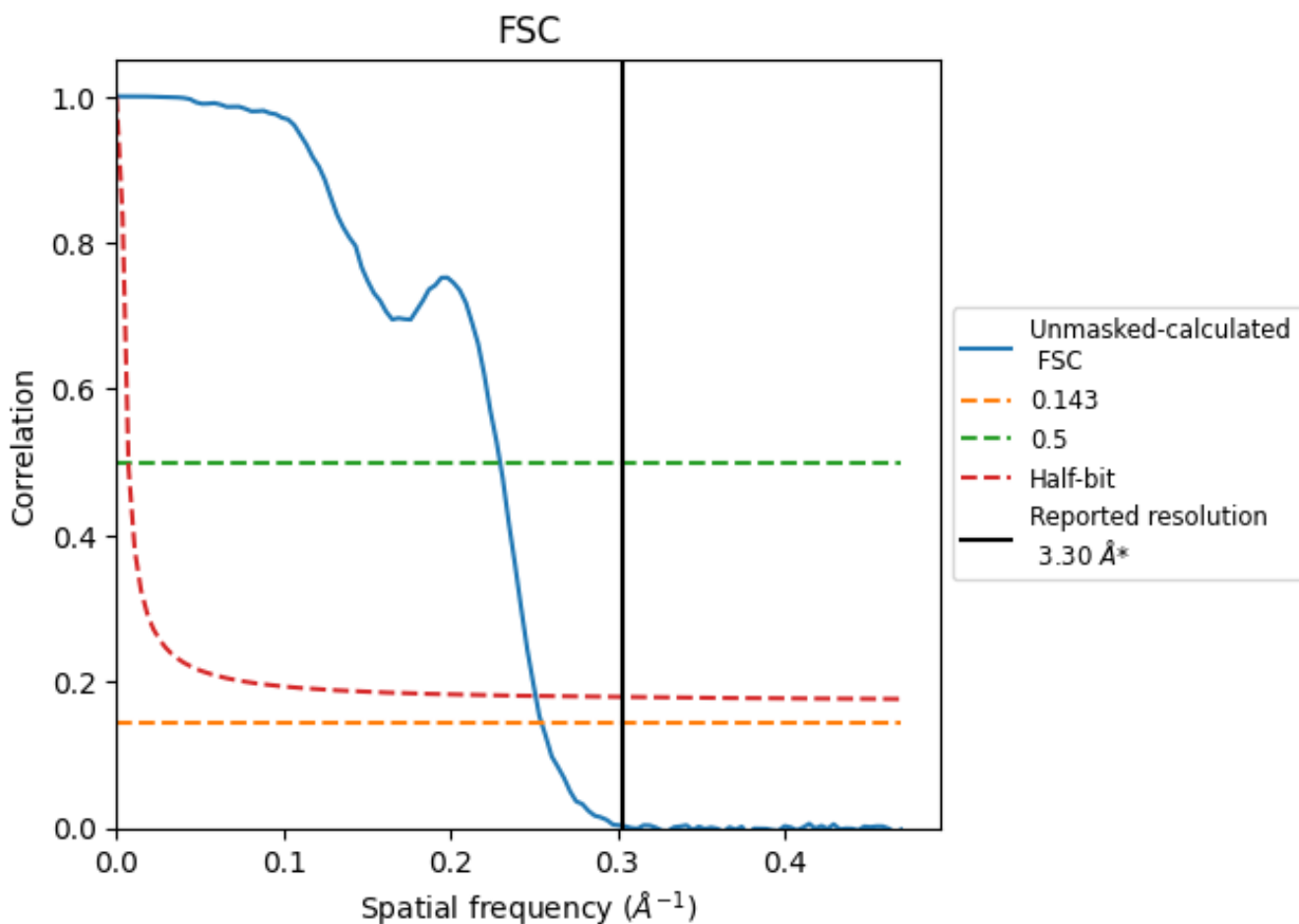
*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	4.35	3.98

*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 3.93 differs from the reported value 3.3 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42497 and PDB model 8URQ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)

| X | Y | Z |
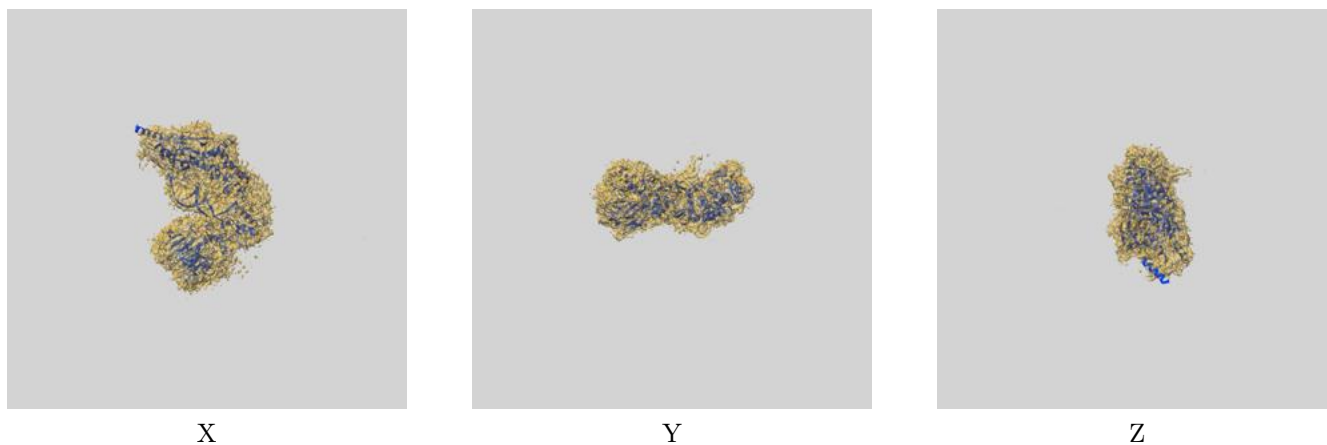
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
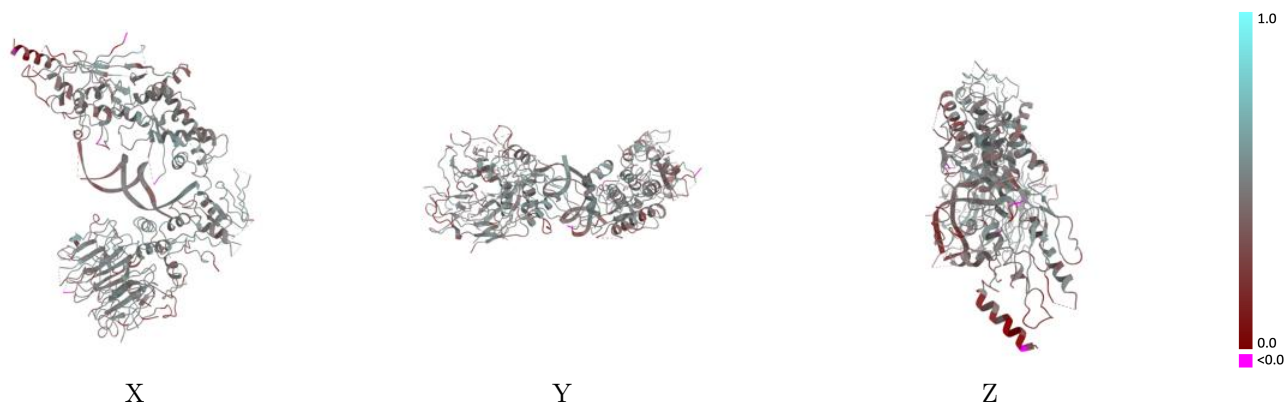
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
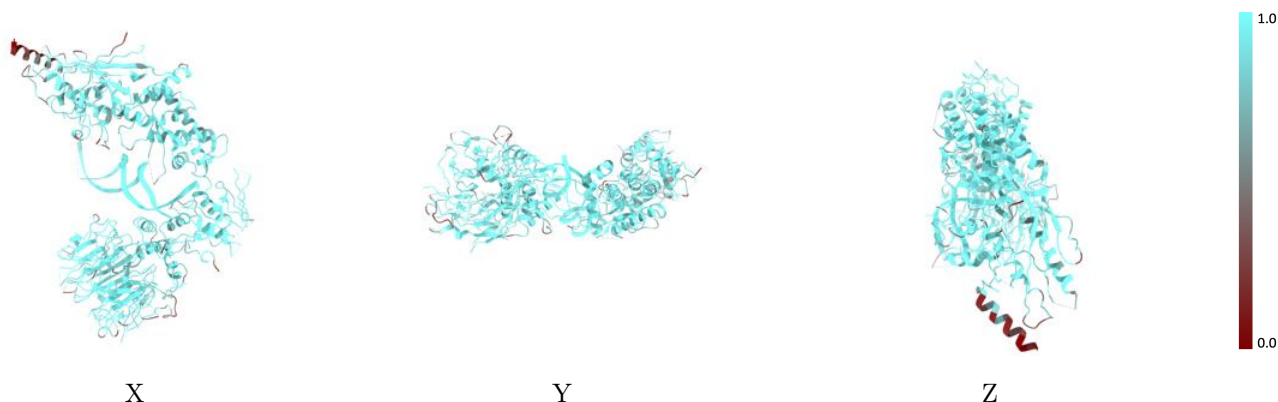
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.28).

9.4   Atom inclusion ⓘ
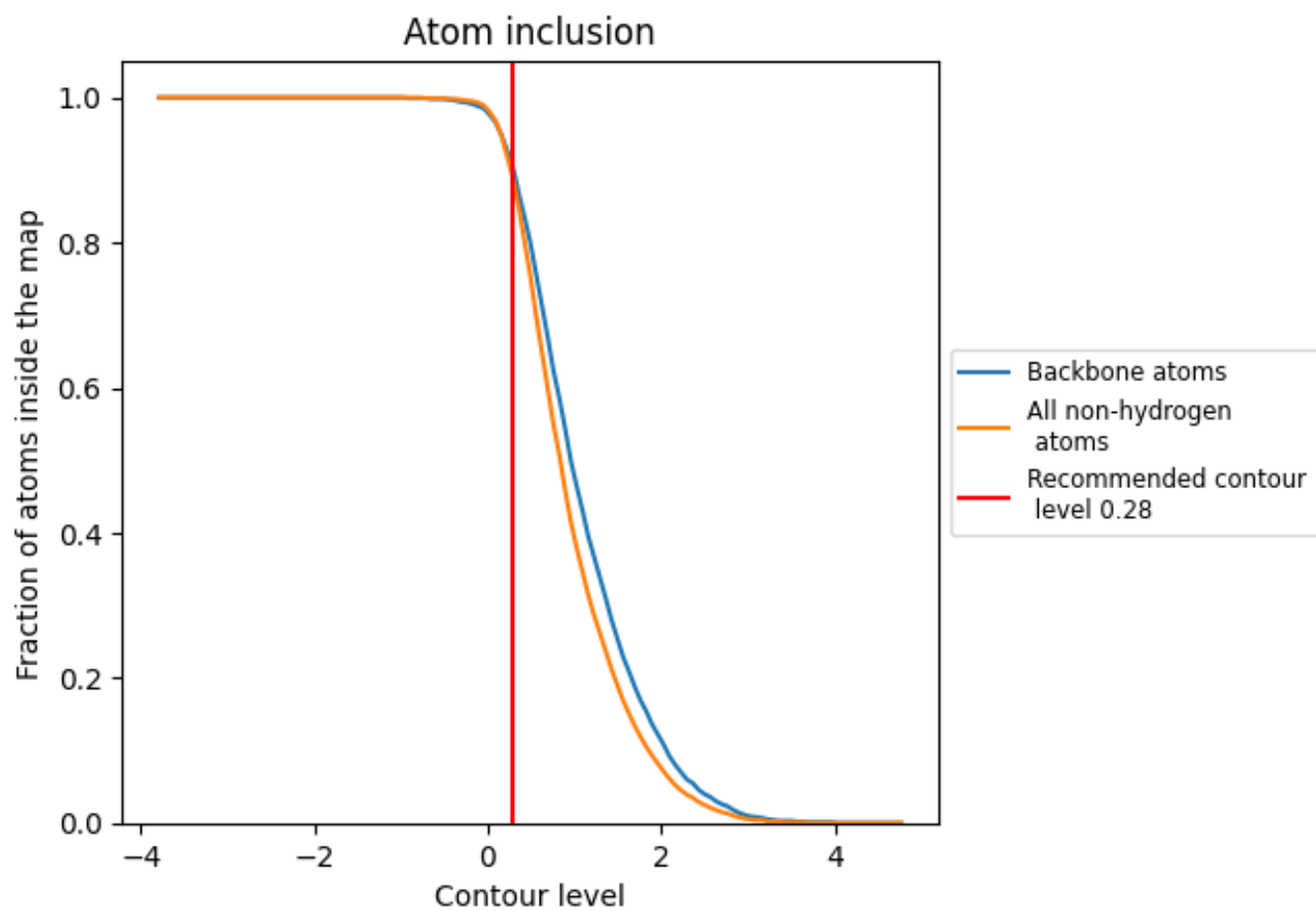
At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.4420
A	0.9090	0.4640
B	0.8870	0.4360
C	0.8930	0.4430
D	0.9830	0.4110
F	0.7130	0.3540

1.0

0.0
<0.0