



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 01:42 AM UTC

PDB ID : 9ZE2 / pdb_00009ze2
EMDB ID : EMD-74089
Title : Cryo-EM structure of the endogenous U2/branchpoint spliceosomal complex (core)
Authors : Liu, S.; Su, T.; Zhou, Z.H.
Deposited on : 2025-11-27
Resolution : 3.26 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

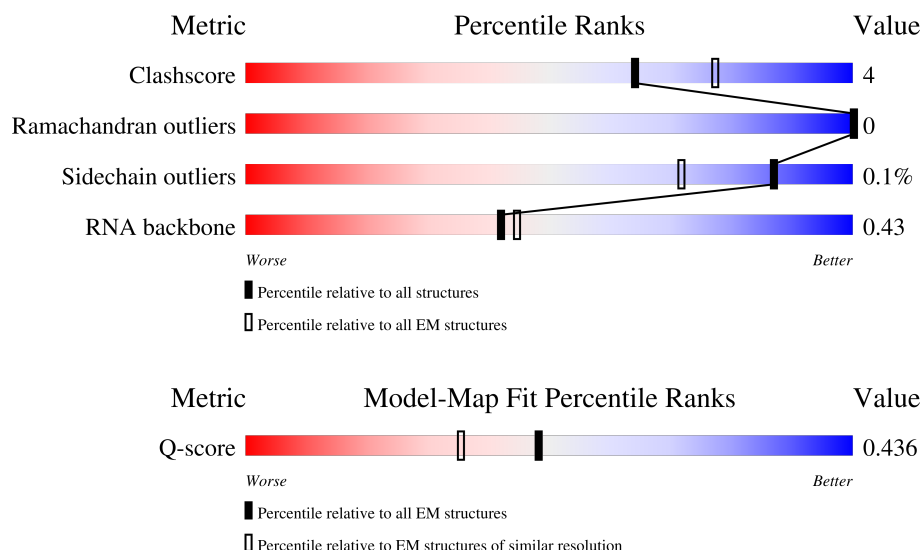
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.26 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.



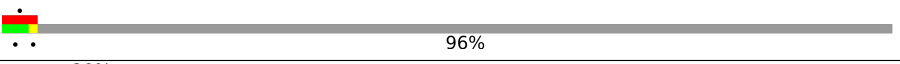






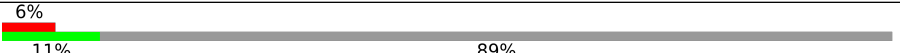

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14557 (2.76 - 3.76)

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 $\leq 5\%$. 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	2	37	<div> <div>38%</div> <div> <div>46%</div> <div>32%</div> <div>16%</div> <div>5%</div> </div> </div>
2	H	110	<div> <div>86%</div> <div>7%</div> <div>6%</div> </div>
3	R	42	<div> <div>50%</div> <div>31%</div> <div>40%</div> <div>5%</div> <div>24%</div> </div>

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Mol	Chain	Length	Quality of chain
4	A	824	
5	B1	1304	
6	B2	895	
7	B3	1217	
8	B4	424	
9	B5	86	
10	B6	125	
11	A2	464	
12	A3	501	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 24516 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	37	Total	C	N	O	P	0	0
			781	352	127	265	37		

- Molecule 2 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	103	Total	C	N	O	S	0	0
			794	490	142	148	14		

- Molecule 3 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	32	Total	C	N	O	P	0	0
			642	289	69	252	32		

- Molecule 4 is a protein called RNA-binding protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	29	Total	C	N	O	S	0	0
			258	161	50	45	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	816	MET	-	expression tag	UNP P52756
A	817	ASP	-	expression tag	UNP P52756
A	818	TYR	-	expression tag	UNP P52756
A	819	LYS	-	expression tag	UNP P52756
A	820	ASP	-	expression tag	UNP P52756
A	821	ASP	-	expression tag	UNP P52756
A	822	ASP	-	expression tag	UNP P52756
A	823	ASP	-	expression tag	UNP P52756
A	824	LYS	-	expression tag	UNP P52756

- Molecule 5 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B1	895	Total	C	N	O	S	0	0
			7142	4581	1225	1295	41		

- Molecule 6 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B2	250	Total	C	N	O	S	0	0
			1960	1260	348	345	7		

- Molecule 7 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B3	1198	Total	C	N	O	S	0	0
			9396	5959	1598	1794	45		

- Molecule 8 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B4	89	Total	C	N	O	S	0	0
			698	446	117	131	4		

- Molecule 9 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B5	75	Total	C	N	O	S	0	0
			616	390	108	113	5		

- Molecule 10 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B6	98	Total	C	N	O	S	0	0
			805	515	144	142	4		

- Molecule 11 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A2	51	Total	C	N	O	S	0	0
			407	252	77	75	3		

- Molecule 12 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A3	123	Total	C	N	O	S	0	0
			1014	646	181	183	4		

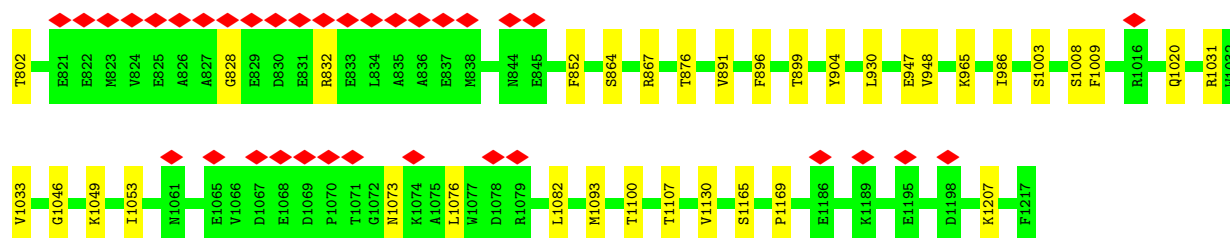
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	H	3	Total	Zn	0
			3	3	

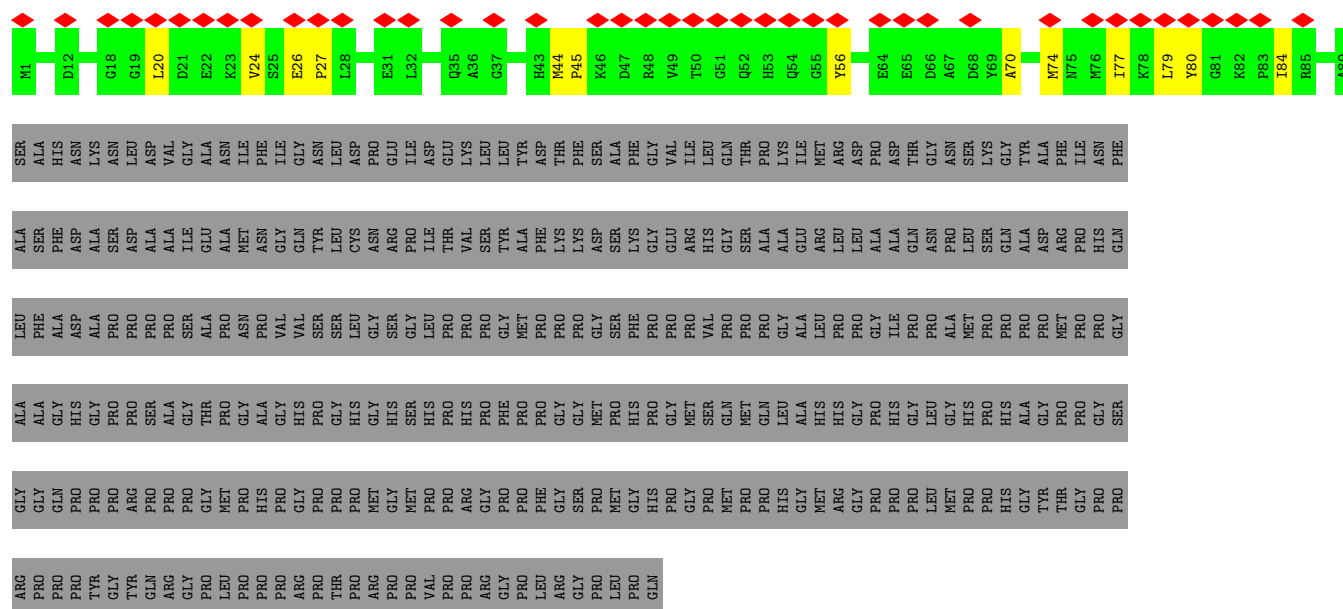
- Molecule 5: Splicing factor 3B subunit 1



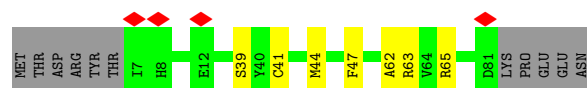
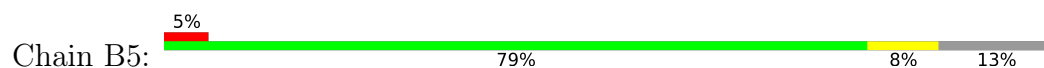
GLY	THR	ARG	GLY	LEU	LYS	THR	MET
THR	THR	ASP	SER	LYS	HIS	GLU	ALA
PRO	THR	THR	GLU	VAL	ARG	LEU	LYS
ALA	PRO	PRO	THR	ASN	ARG	ASP	ILE
MET	GLY	GLY	PRO	VAL	THR	GLU	ALA
ASN	HIS	HIS	GLY	GLY	MET	ASP	LYS
MET	GLY	GLY	ALA	ALA	ILE	ASP	THR
ALA	SER	SER	THR	ALA	ILE	ASP	HIS
MET	GLY	GLY	PRO	ALA	ILE	ASP	GLU
THR	TRP	TRP	PRO	ALA	SER	TYR	ASP
PRO	ALA	ALA	SER	GLN	GLU	SER	ILE
PRO	GLU	GLU	LYS	PRO	ARG	SER	GLU
GLY	THR	THR	ILE	PRO	LEU	SER	ALA
HIS	PRO	PRO	TRP	SER	ASP	THR	GLN
ILE	ARG	ARG	ASP	LYS	PRO	SER	ILE
MET	THR	THR	PRO	ARG	PHE	LEU	ARG
SER	ASP	ASP	THR	LYS	ALA	GLU	ILE
	ARG	GLY	PRO	ARG	ASP	GLY	ILE
	GLY	GLY	SER	ARG	GLY	GLN	GLY
	GLY	GLY	HIS	TRP	GLY	LYS	GLY
	ASP	ASP	THR	GLN	THR	LYS	LYS
	SER	ILE	ALA	THR	PRO	PRO	LYS
	ILE	GLU	GLY	ALA	ASP	TYR	ALA
	GLU	GLU	ALA	ASP	PRO	HIS	LEU
	THR	THR	ALA	GLN	ALA	ASP	ALA
	PRO	PRO	ALA	GLN	LYS	ALA	LEU
	PRO	PRO	THR	THR	MET	PRO	ASP
	PRO	PRO	GLY	GLY	THR	GLU	GLU
	GLY	GLY	ARG	ALA	THR	LEU	VAL
	ALA	ALA	GLY	THR	THR	ASN	GLY
	ALA	ALA	ASP	PRO	TYR	PHE	TYR
	SER	SER	ASP	PRO	GLU	ALA	GLY
	LYS	LYS	THR	LYS	GLN	GLU	GLY
	ARG	ARG	PRO	LYS	ARG	HIS	GLY
	LYS	LYS	GLY	ALA	ILE	SER	ASP
	E391	SER	HIS	SEU	VAL	ARG	ASP
	I392	ARG	ALA	SER	THR	PRO	ARG
	D393	TRP	THR	TRP	GLU	LYS	PRO
	E394	ASP	PRO	ASP	HIS	PHE	TYR
	R395	GLU	GLY	GLN	THR	ALA	GLY
	M396	THR	GLY	GLU	THR	GLY	GLY
	R397	PRO	GLY	THR	LYS	ASN	GLY
	R397	ALA	GLY	PRO	THR	LEU	VAL
	P398	SER	ALA	PRO	GLU	ASN	GLY
	L399	GLN	THR	GLY	GLU	ASP	LEU
	S400	MET	SER	HIS	ARG	ILE	ASP
	D401	GLY	SER	THR	GLU	THR	THR
	E402	GLY	ALA	PRO	ILE	GLN	GLN
	E403	SER	ARG	SEU	ARG	ASP	GLY
	L404	THR	LYS	LEU	GLN	PRO	ARG
	D405	PRO	ASN	ARG	GLN	LYS	PHE
	A406	VAL	TRP	TRP	LEU	ILE	ALA
	M407	THR	ASP	GLU	ALA	GLY	GLY
	F408	THR	GLU	THR	LYS	ASP	TYR
	F409	GLY	THR	PRO	ALA	ARG	GLY
	E410	LYS	PRO	GLY	LYS	THR	THR
	G411	THR	PRO	GLY	ALA	ASP	ILE
	Y412	THR	THR	ARG	LYS	GLU	ILE
	K413	PRO	THR	ALA	GLY	TYR	ALA
	V414	ILE	GLU	LYS	GLY	LYS	ALA
	P416	ALA	GLU	ALA	GLY	GLY	ALA
	P417	ALA	THR	ALA	GLY	GLY	ALA
	P418	ALA	GLU	LYS	GLY	GLY	ALA
	A419	ALA	LYS	LYS	GLY	LYS	ALA
	A420	ALA	LYS	LYS	GLY	LYS	ALA



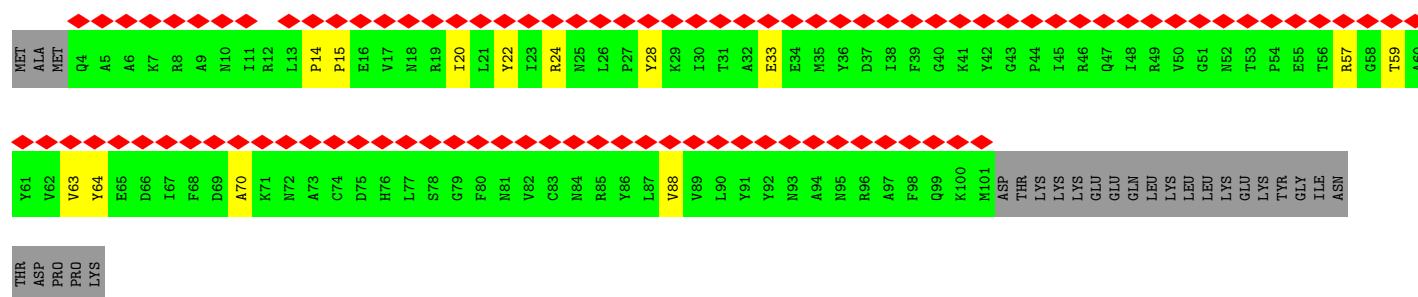
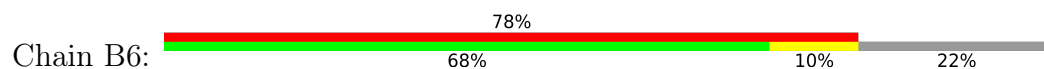
• Molecule 8: Splicing factor 3B subunit 4



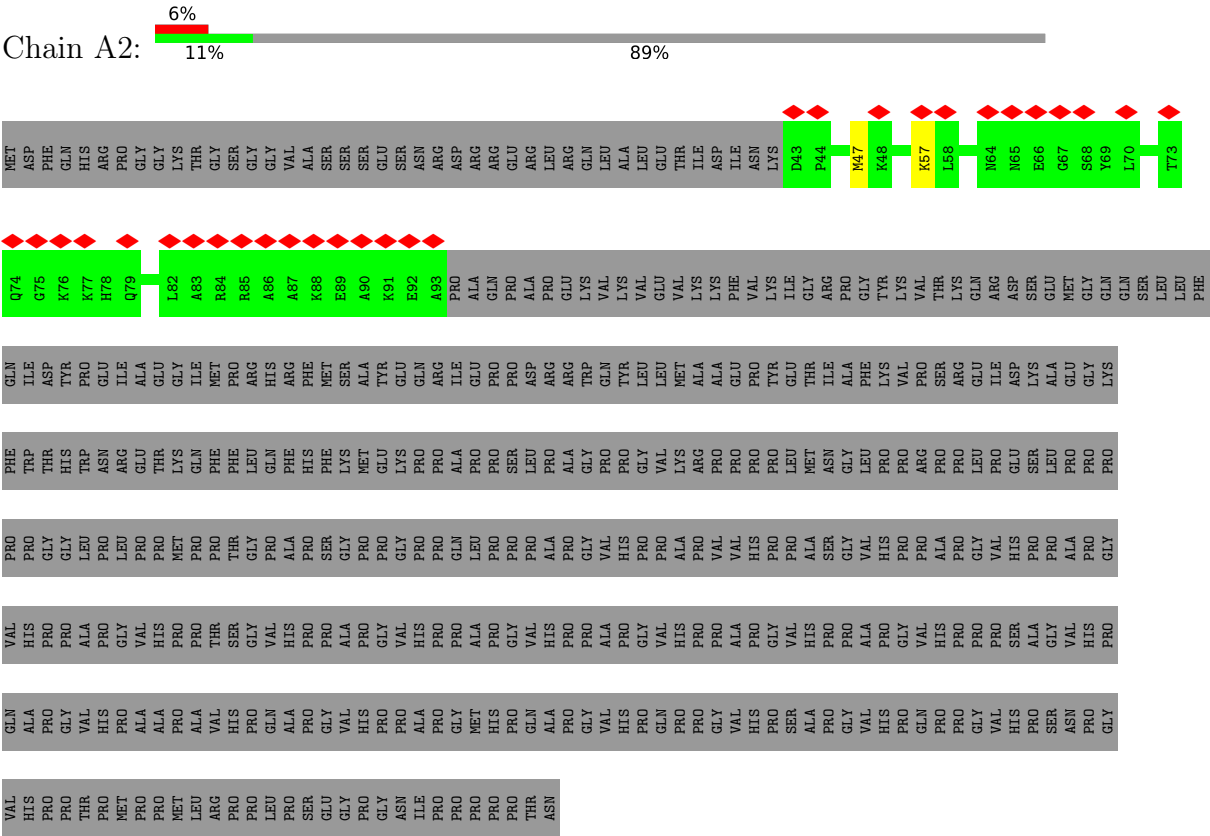
• Molecule 9: Splicing factor 3B subunit 5



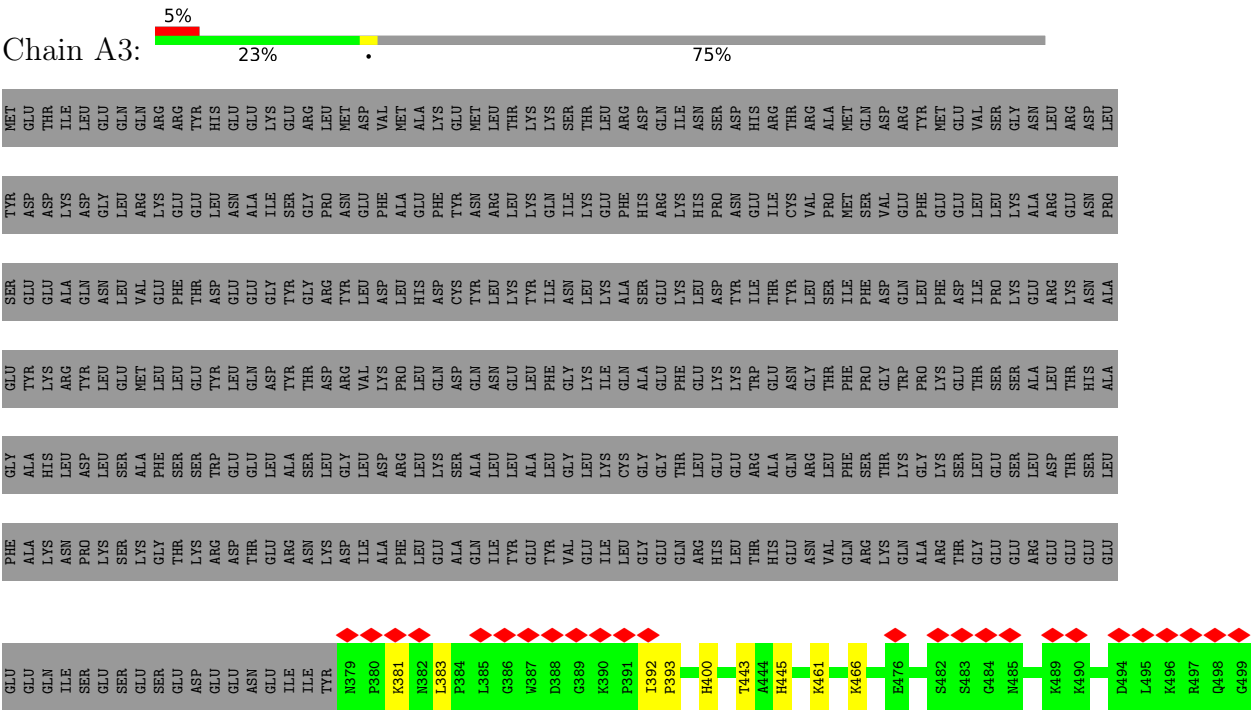
• Molecule 10: Splicing factor 3B subunit 6



● Molecule 11: Splicing factor 3A subunit 2



● Molecule 12: Splicing factor 3A subunit 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.200	Depositor
Minimum map value	-2.717	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.72	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2	0.17	0/625	0.33	0/972
2	H	0.09	0/807	0.28	0/1082
3	R	0.25	0/706	0.44	0/1089
4	A	0.07	0/261	0.16	0/342
5	B1	0.10	0/7284	0.26	0/9868
6	B2	0.18	0/2017	0.30	0/2735
7	B3	0.09	0/9590	0.28	0/13015
8	B4	0.08	0/713	0.26	0/964
9	B5	0.08	0/634	0.20	0/857
10	B6	0.07	0/823	0.21	0/1114
11	A2	0.06	0/415	0.16	0/555
12	A3	0.08	0/1045	0.25	0/1416
All	All	0.11	0/24920	0.28	0/34009

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	2	781	0	398	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	794	0	775	5	0
3	R	642	0	324	7	0
4	A	258	0	251	7	0
5	B1	7142	0	7319	62	0
6	B2	1960	0	1911	15	0
7	B3	9396	0	9309	79	0
8	B4	698	0	694	8	0
9	B5	616	0	579	6	0
10	B6	805	0	802	7	0
11	A2	407	0	397	1	0
12	A3	1014	0	974	9	0
13	H	3	0	0	0	0
All	All	24516	0	23733	198	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 4.

The worst 5 of 198 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)
5:B1:460:PRO:HD3	5:B1:467:LEU:HD11	1.65	0.79
5:B1:731:LEU:HD22	5:B1:750:ILE:HD13	1.70	0.74
5:B1:1017:LEU:HD21	5:B1:1042:ILE:HG21	1.69	0.73
5:B1:501:LEU:HD21	5:B1:535:ILE:HG12	1.75	0.67
7:B3:704:VAL:HG11	7:B3:754:ILE:HG22	1.75	0.67

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	101/110 (92%)	95 (94%)	6 (6%)	0	100	100
4	A	25/824 (3%)	25 (100%)	0	0	100	100
5	B1	891/1304 (68%)	866 (97%)	25 (3%)	0	100	100
6	B2	246/895 (28%)	233 (95%)	13 (5%)	0	100	100
7	B3	1192/1217 (98%)	1140 (96%)	52 (4%)	0	100	100
8	B4	87/424 (20%)	83 (95%)	4 (5%)	0	100	100
9	B5	73/86 (85%)	70 (96%)	3 (4%)	0	100	100
10	B6	96/125 (77%)	93 (97%)	3 (3%)	0	100	100
11	A2	49/464 (11%)	48 (98%)	1 (2%)	0	100	100
12	A3	121/501 (24%)	118 (98%)	3 (2%)	0	100	100
All	All	2881/5950 (48%)	2771 (96%)	110 (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	
2	H	89/95 (94%)	89 (100%)	0	100	100
4	A	24/704 (3%)	24 (100%)	0	100	100
5	B1	775/1104 (70%)	774 (100%)	1 (0%)	88	89
6	B2	201/776 (26%)	200 (100%)	1 (0%)	81	82
7	B3	1037/1051 (99%)	1036 (100%)	1 (0%)	88	89
8	B4	74/336 (22%)	74 (100%)	0	100	100
9	B5	66/77 (86%)	66 (100%)	0	100	100
10	B6	84/109 (77%)	84 (100%)	0	100	100
11	A2	42/382 (11%)	42 (100%)	0	100	100
12	A3	106/446 (24%)	106 (100%)	0	100	100
All	All	2498/5080 (49%)	2495 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B1	817	HIS
6	B2	609	LEU
7	B3	667	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
7	B3	104	GLN
7	B3	206	GLN
12	A3	448	ASN
7	B3	164	ASN
7	B3	422	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	36/37 (97%)	7 (19%)	1 (2%)
3	R	31/42 (73%)	14 (45%)	0
All	All	67/79 (84%)	21 (31%)	1 (1%)

5 of 21 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	30	A
1	2	31	G
1	2	44	PSU
1	2	45	C
1	2	46	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	44	PSU

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	PSU	2	43	1,3	18,21,22	0.99	1 (5%)	21,30,33	1.13	2 (9%)
1	PSU	2	34	1,3	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
1	OMC	2	47	1	19,22,23	0.52	0	25,31,34	1.03	2 (8%)
1	PSU	2	58	1	18,21,22	1.12	1 (5%)	21,30,33	1.74	4 (19%)
1	PSU	2	39	1	18,21,22	1.14	1 (5%)	21,30,33	1.91	5 (23%)
1	OMC	2	40	1,3	19,22,23	0.48	0	25,31,34	0.65	0
1	PSU	2	44	1,3	18,21,22	0.88	1 (5%)	21,30,33	0.96	1 (4%)
1	PSU	2	41	1	18,21,22	1.13	1 (5%)	21,30,33	1.84	4 (19%)
1	PSU	2	37	1	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
1	PSU	2	54	1	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
1	OMC	2	61	1	19,22,23	0.49	0	25,31,34	0.73	0

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
1	PSU	2	43	1,3	-	1/7/25/26	0/2/2/2
1	PSU	2	34	1,3	-	0/7/25/26	0/2/2/2
1	OMC	2	47	1	-	6/9/27/28	0/2/2/2
1	PSU	2	58	1	-	2/7/25/26	0/2/2/2
1	PSU	2	39	1	-	0/7/25/26	0/2/2/2
1	OMC	2	40	1,3	-	0/9/27/28	0/2/2/2
1	PSU	2	44	1,3	-	3/7/25/26	0/2/2/2
1	PSU	2	41	1	-	0/7/25/26	0/2/2/2
1	PSU	2	37	1	-	0/7/25/26	0/2/2/2
1	PSU	2	54	1	-	0/7/25/26	0/2/2/2
1	OMC	2	61	1	-	0/9/27/28	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	58	PSU	C6-C5	3.86	1.39	1.35
1	2	34	PSU	C6-C5	3.85	1.39	1.35
1	2	39	PSU	C6-C5	3.79	1.39	1.35
1	2	41	PSU	C6-C5	3.77	1.39	1.35
1	2	37	PSU	C6-C5	3.76	1.39	1.35

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	54	PSU	C4-N3-C2	-4.84	119.70	126.37
1	2	37	PSU	C4-N3-C2	-4.81	119.74	126.37
1	2	54	PSU	N1-C2-N3	4.74	120.17	115.17
1	2	39	PSU	N1-C2-N3	4.74	120.16	115.17
1	2	39	PSU	C4-N3-C2	-4.71	119.89	126.37

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	58	PSU	O4'-C1'-C5-C4
1	2	58	PSU	O4'-C1'-C5-C6
1	2	44	PSU	O4'-C4'-C5'-O5'
1	2	47	OMC	C4'-C5'-O5'-P
1	2	47	OMC	O4'-C1'-N1-C6

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	43	PSU	1	0
1	2	47	OMC	2	0
1	2	58	PSU	1	0
1	2	40	OMC	1	0
1	2	44	PSU	4	0
1	2	41	PSU	3	0
1	2	54	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

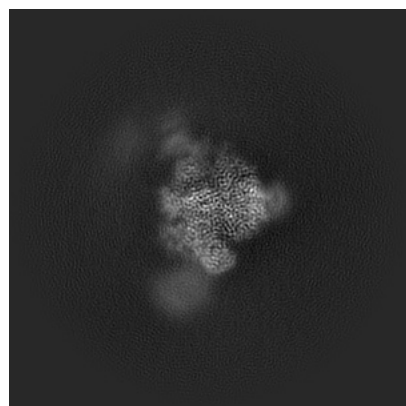
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74089. These allow visual inspection of the internal detail of the map and identification of artifacts.

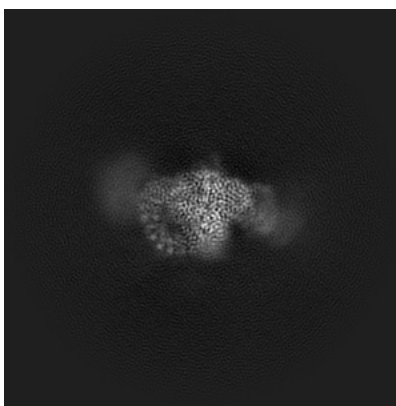
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

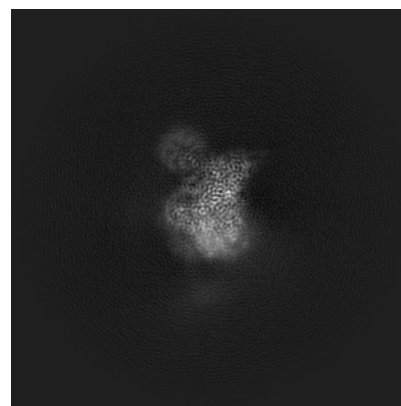
6.1.1 Primary map



X

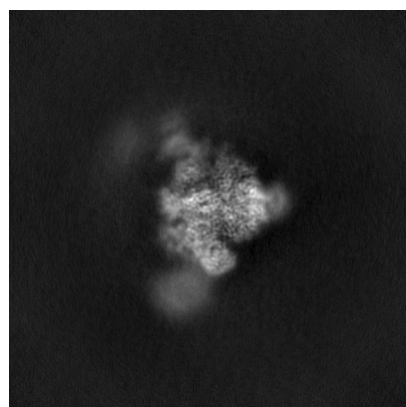


Y

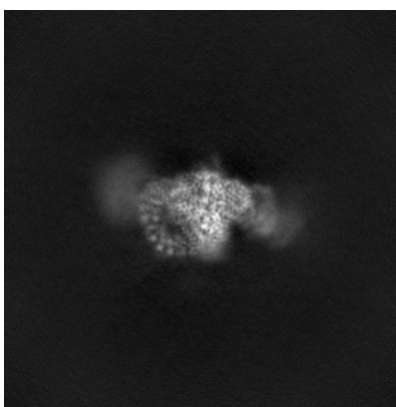


Z

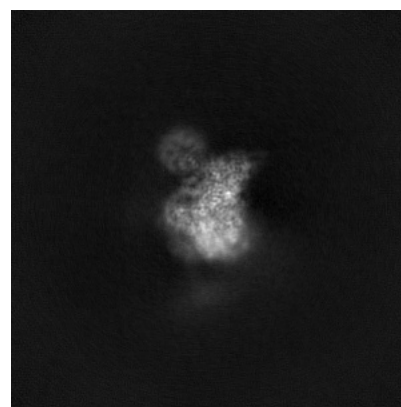
6.1.2 Raw map



X



Y

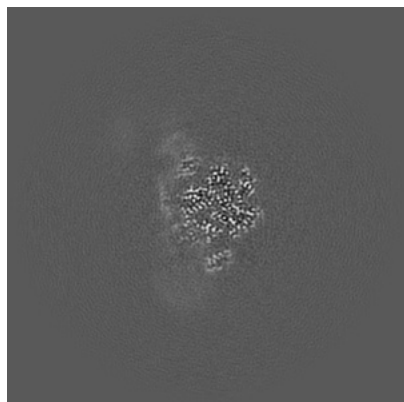


Z

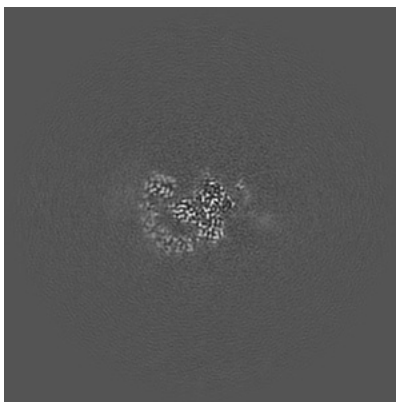
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

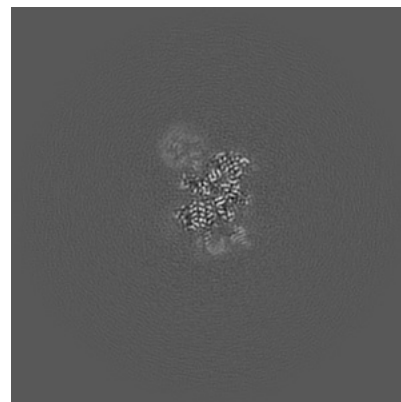
6.2.1 Primary map



X Index: 192

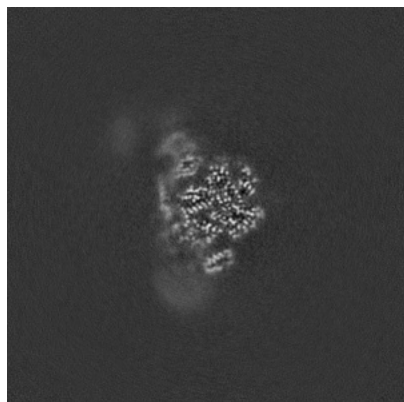


Y Index: 192

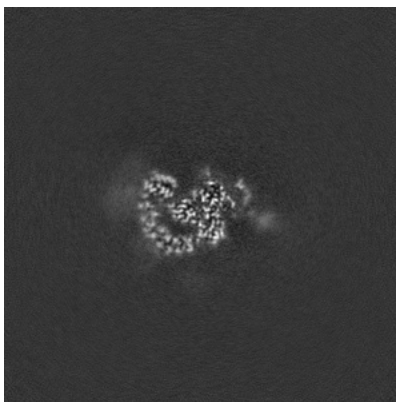


Z Index: 192

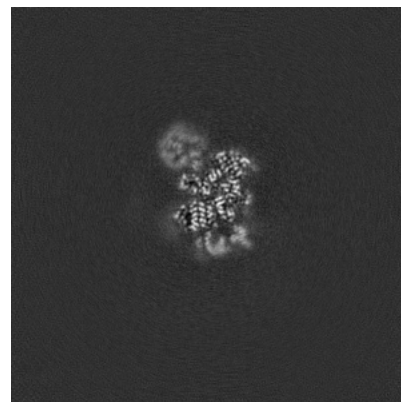
6.2.2 Raw map



X Index: 192



Y Index: 192

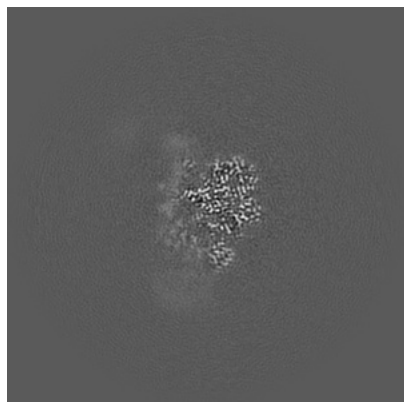


Z Index: 192

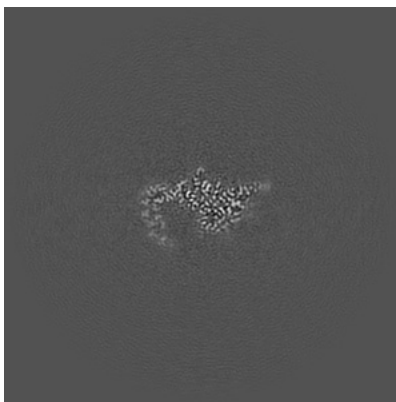
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

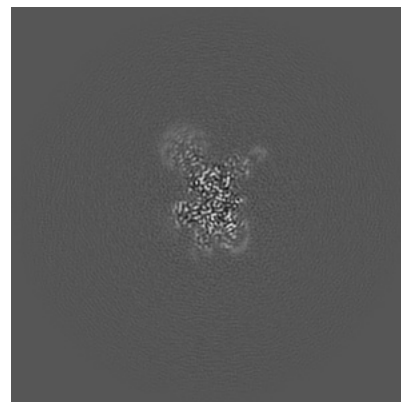
6.3.1 Primary map



X Index: 199

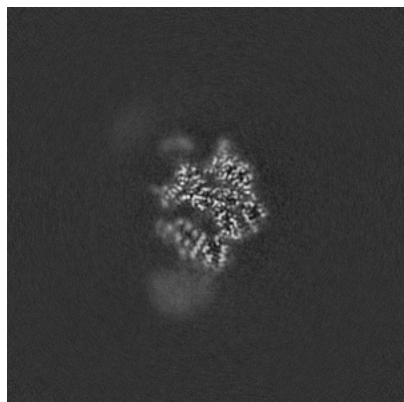


Y Index: 207

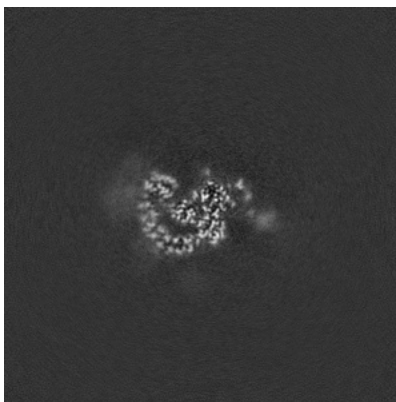


Z Index: 201

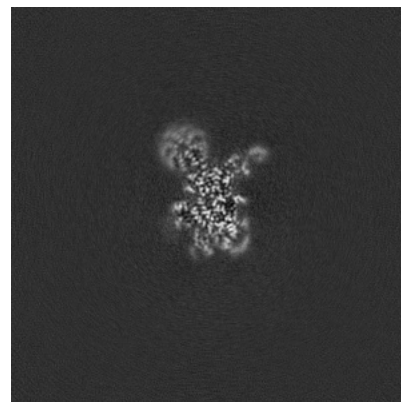
6.3.2 Raw map



X Index: 209



Y Index: 191

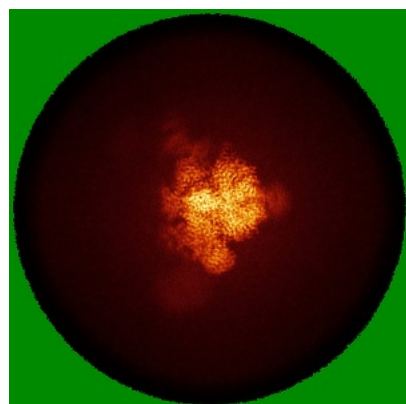


Z Index: 202

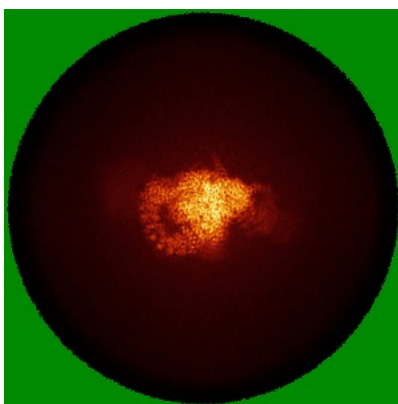
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

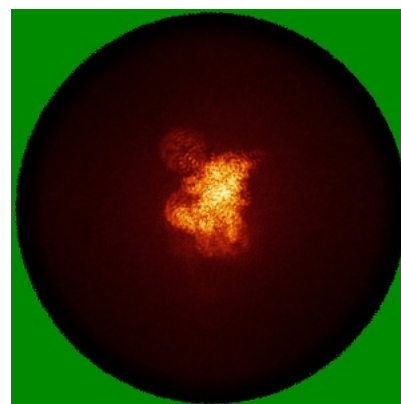
6.4.1 Primary map



X

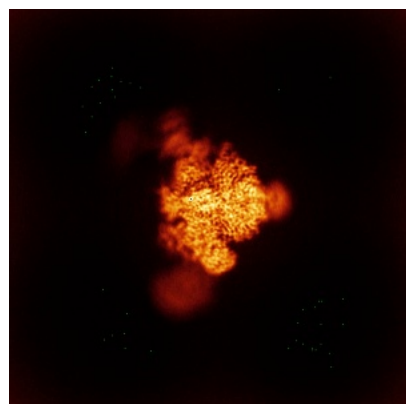


Y

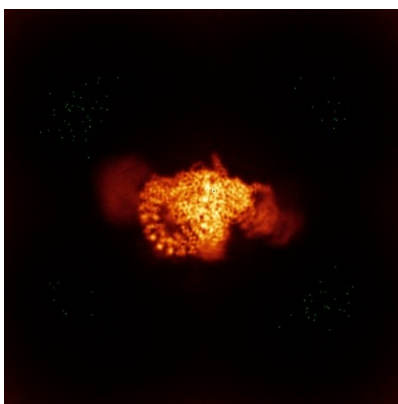


Z

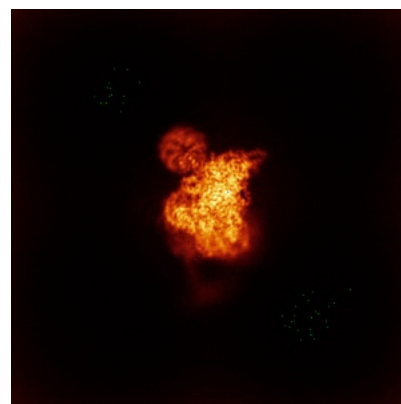
6.4.2 Raw map



X



Y

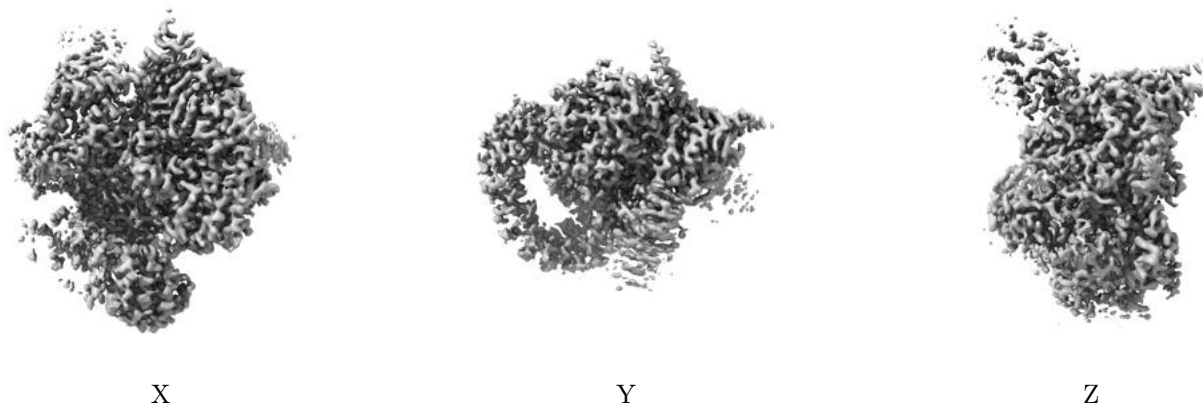


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.72. 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



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.

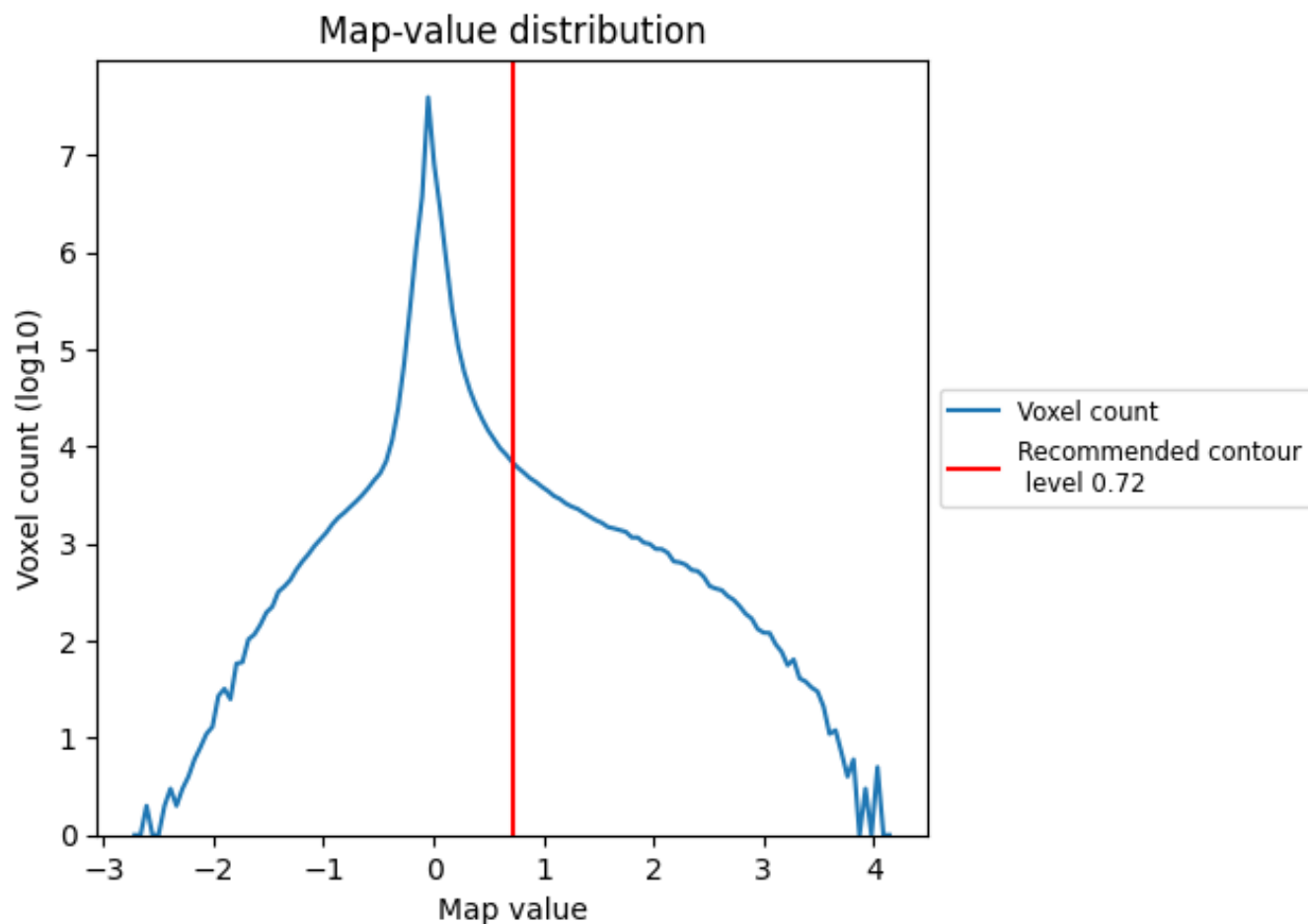
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

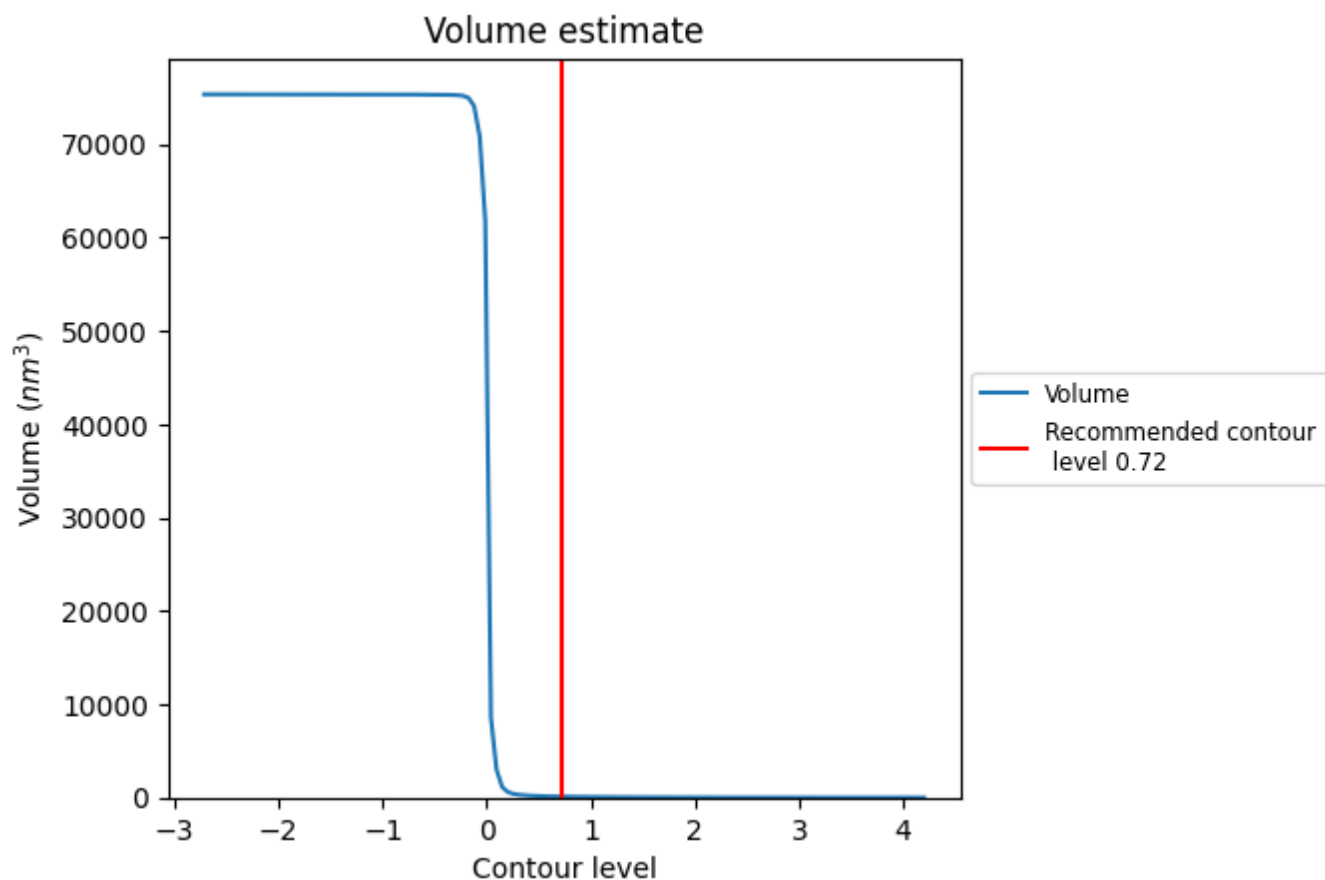
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

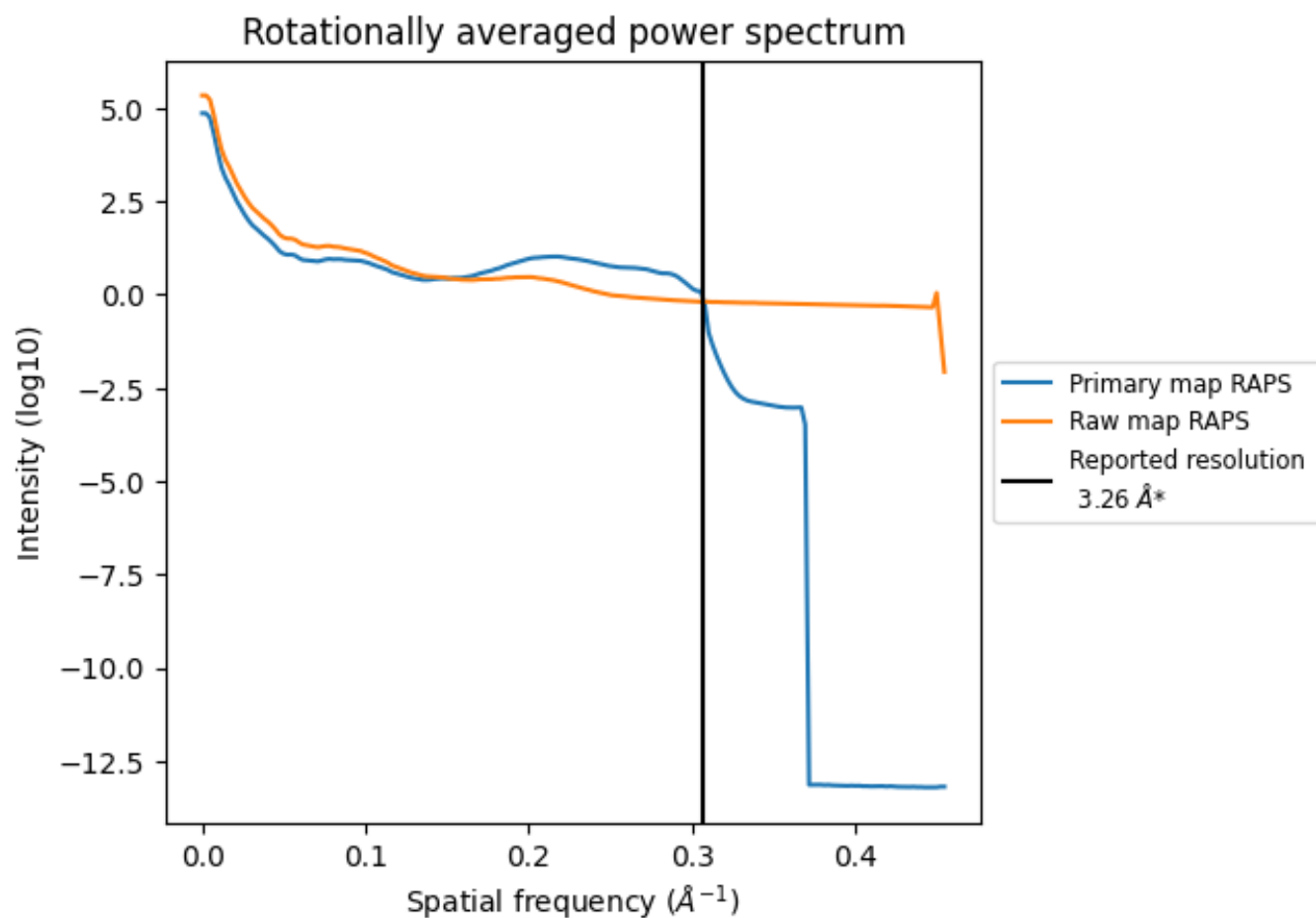
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 88 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 ⓘ

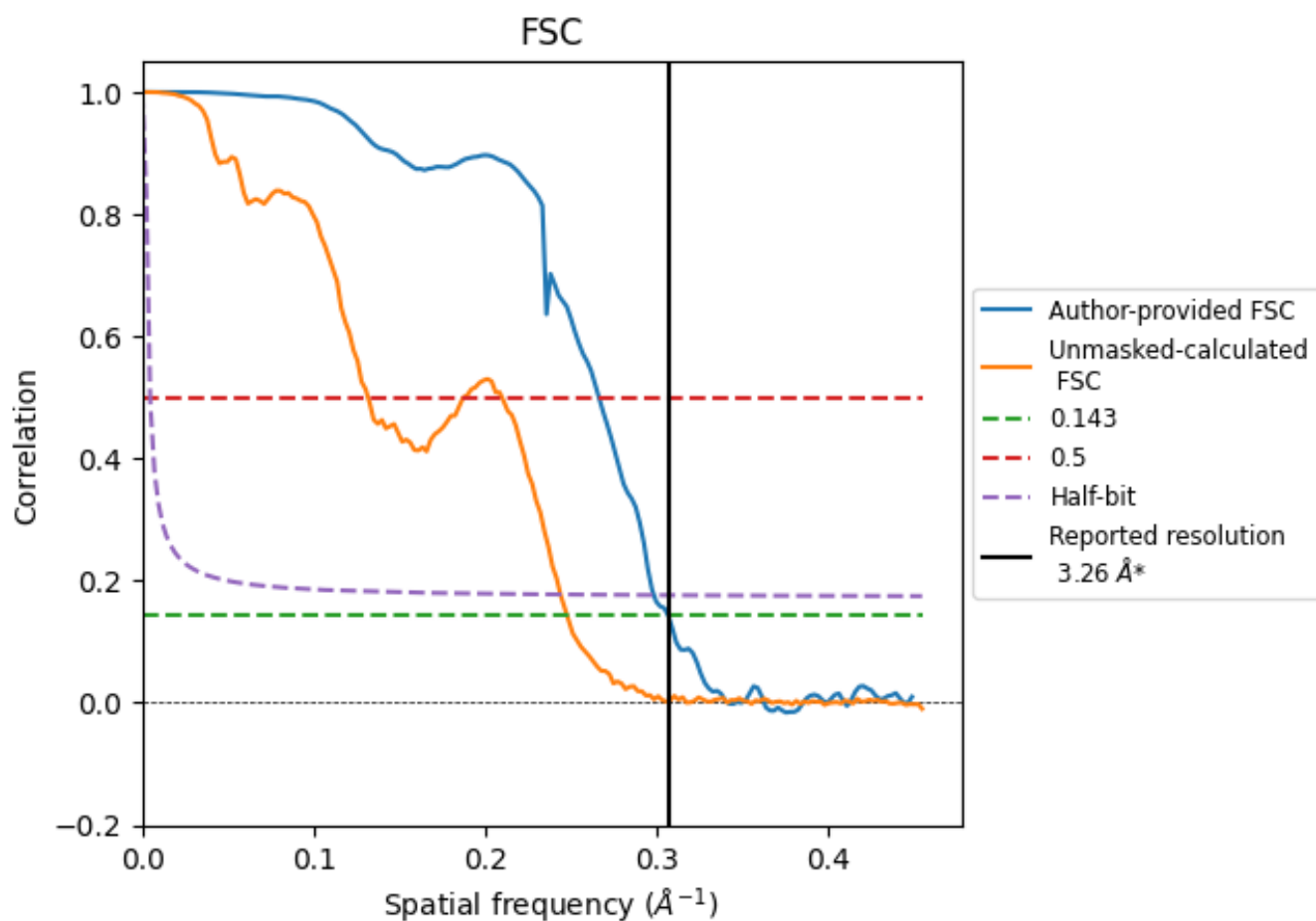


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 0.307 \AA^{-1}

8.2 Resolution estimates [i](#)

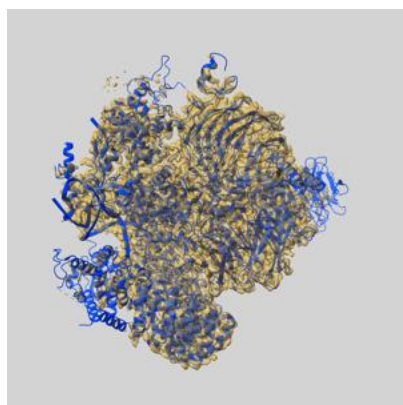
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	3.26	3.76	3.35
Unmasked-calculated*	4.04	7.60	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.26 by more than 10 %

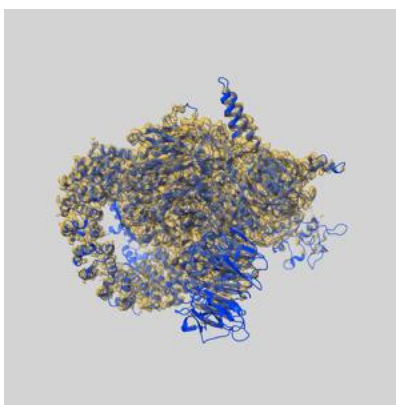
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74089 and PDB model 9ZE2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

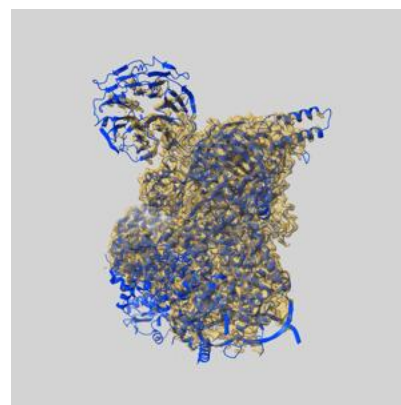
9.1 Map-model overlay [i](#)



X



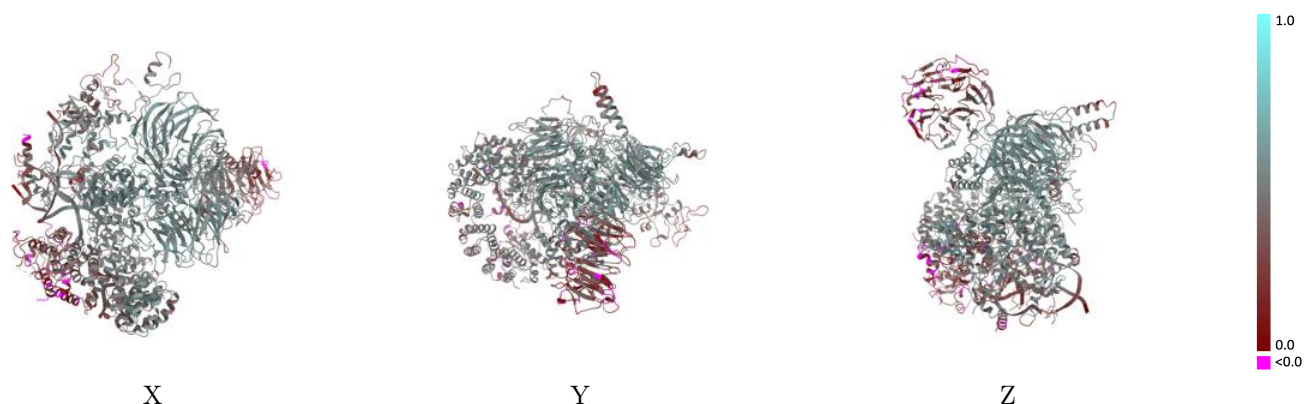
Y



Z

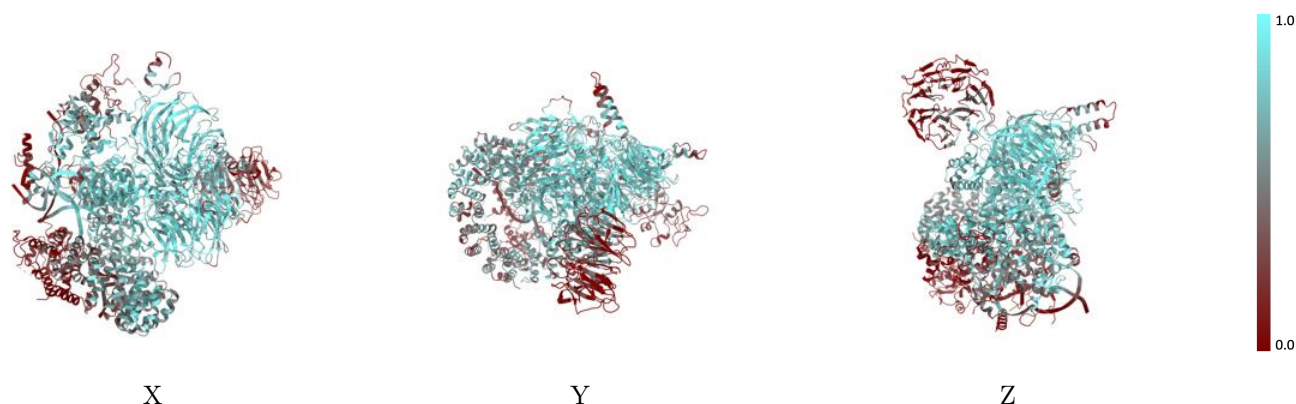
The images above show the 3D surface view of the map at the recommended contour level 0.72 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



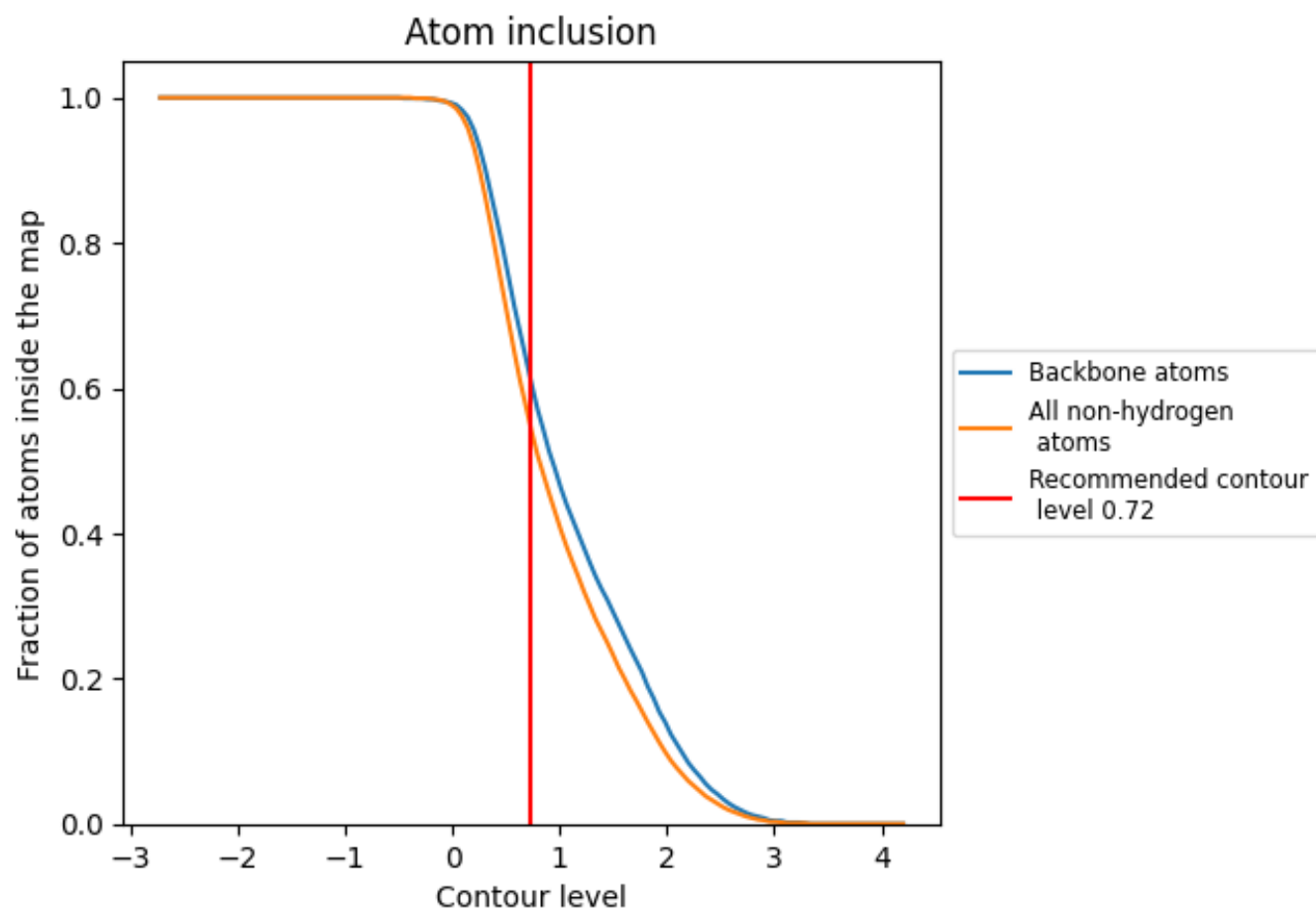
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.72).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 55% 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 (0.72) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.4360
2	 0.5220	 0.4110
A	 0.0000	 0.1220
A2	 0.3880	 0.4180
A3	 0.6090	 0.4740
B1	 0.5600	 0.4410
B2	 0.4490	 0.4020
B3	 0.6190	 0.4610
B4	 0.4130	 0.4020
B5	 0.8110	 0.5500
B6	 0.0100	 0.1870
H	 0.7910	 0.5300
R	 0.3630	 0.3600

