



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 02:33 AM UTC

PDB ID : 6V4X / pdb_00006v4x
EMDB ID : EMD-21050
Title : Cryo-EM structure of an active human histone pre-mRNA 3'-end processing machinery at 3.2 Angstrom resolution
Authors : Sun, Y.; Zhang, Y.; Walz, T.; Tong, L.
Deposited on : 2019-12-02
Resolution : 3.20 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
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

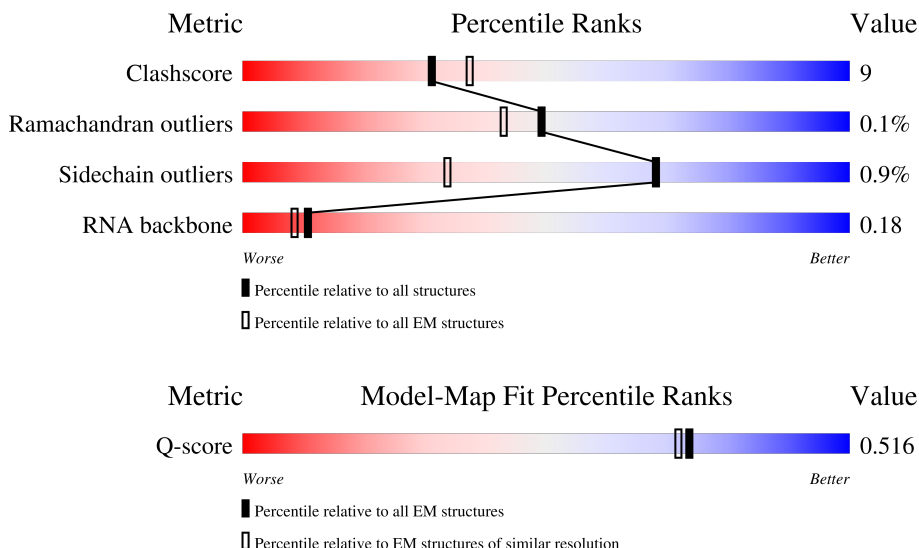
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



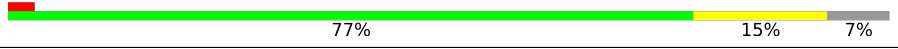
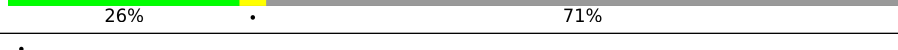
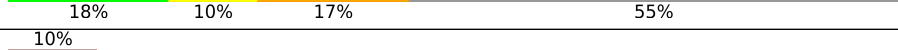
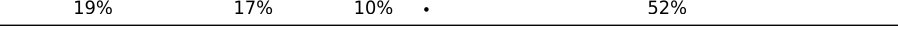
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	A	146	
2	B	95	
3	F	86	

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Mol	Chain	Length	Quality of chain
4	E	92	
5	G	84	
6	C	123	
7	D	259	
8	H	684	
9	I	782	
10	J	1072	
11	Z	60	
12	Y	52	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 16499 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 Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	83	Total	C	N	O	S	0	0
			652	409	115	122	6		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P62318
A	-18	GLY	-	expression tag	UNP P62318
A	-17	SER	-	expression tag	UNP P62318
A	-16	SER	-	expression tag	UNP P62318
A	-15	HIS	-	expression tag	UNP P62318
A	-14	HIS	-	expression tag	UNP P62318
A	-13	HIS	-	expression tag	UNP P62318
A	-12	HIS	-	expression tag	UNP P62318
A	-11	HIS	-	expression tag	UNP P62318
A	-10	HIS	-	expression tag	UNP P62318
A	-9	SER	-	expression tag	UNP P62318
A	-8	SER	-	expression tag	UNP P62318
A	-7	GLY	-	expression tag	UNP P62318
A	-6	LEU	-	expression tag	UNP P62318
A	-5	VAL	-	expression tag	UNP P62318
A	-4	PRO	-	expression tag	UNP P62318
A	-3	ARG	-	expression tag	UNP P62318
A	-2	GLY	-	expression tag	UNP P62318
A	-1	SER	-	expression tag	UNP P62318
A	0	HIS	-	expression tag	UNP P62318

- Molecule 2 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	76	Total	C	N	O	S	0	0
			612	387	111	107	7		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	74	Total	C	N	O	S	0	0
			579	375	95	104	5		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	81	Total	C	N	O	S	0	0
			670	426	119	120	5		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	77	Total	C	N	O	S	0	0
			604	381	110	107	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	77	LEU	-	expression tag	UNP P62308
G	78	GLU	-	expression tag	UNP P62308
G	79	HIS	-	expression tag	UNP P62308
G	80	HIS	-	expression tag	UNP P62308
G	81	HIS	-	expression tag	UNP P62308
G	82	HIS	-	expression tag	UNP P62308
G	83	HIS	-	expression tag	UNP P62308
G	84	HIS	-	expression tag	UNP P62308

- Molecule 6 is a protein called U7 snRNA-associated Sm-like protein LSm10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	114	Total	C	N	O	S	0	0
			911	565	175	169	2		

- Molecule 7 is a protein called U7 snRNA-associated Sm-like protein LSm11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	106	Total	C	N	O	S	0	0
			872	556	170	141	5		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	MET	-	expression tag	UNP P83369
D	-9	HIS	-	expression tag	UNP P83369
D	-8	HIS	-	expression tag	UNP P83369
D	-7	HIS	-	expression tag	UNP P83369
D	-6	HIS	-	expression tag	UNP P83369
D	-5	HIS	-	expression tag	UNP P83369
D	-4	HIS	-	expression tag	UNP P83369
D	-3	SER	-	expression tag	UNP P83369
D	-2	GLY	-	expression tag	UNP P83369
D	-1	GLY	-	expression tag	UNP P83369
D	0	SER	-	expression tag	UNP P83369

- Molecule 8 is a protein called Cleavage and polyadenylation specificity factor subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	499	Total	C	N	O	S	0	0
			3980	2534	682	735	29		

- Molecule 9 is a protein called Cleavage and polyadenylation specificity factor subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	510	Total	C	N	O	S	0	0
			4055	2580	692	760	23		

- Molecule 10 is a protein called Symplekin.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	311	Total	C	N	O	S	0	0
			2461	1569	422	457	13		

- Molecule 11 is a RNA chain called U7 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	27	Total	C	N	O	P	0	0
			564	253	88	196	27		

- Molecule 12 is a RNA chain called modified H2a pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	P	0	0
			537	241	102	169	25		

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

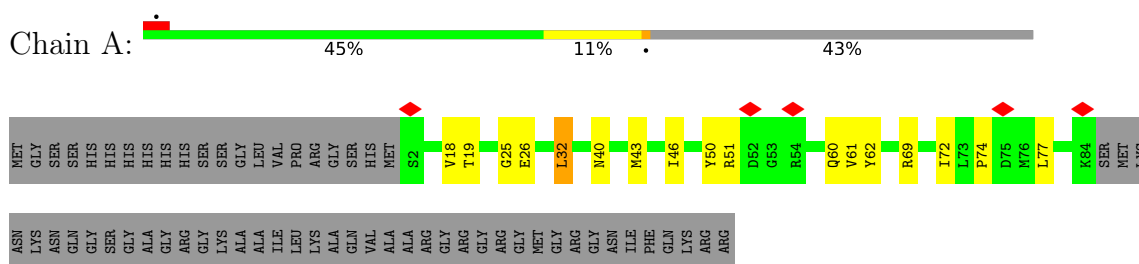
depositor).

Mol	Chain	Residues	Atoms		AltConf
13	H	2	Total	Zn	0
			2	2	

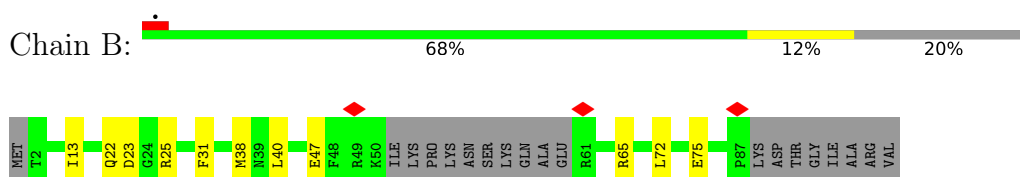
3 Residue-property plots [i](#)

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.

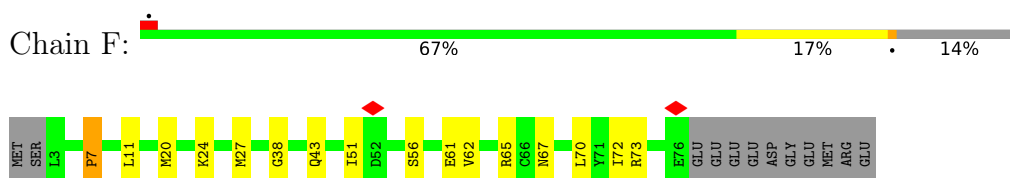
- Molecule 1: Small nuclear ribonucleoprotein Sm D3



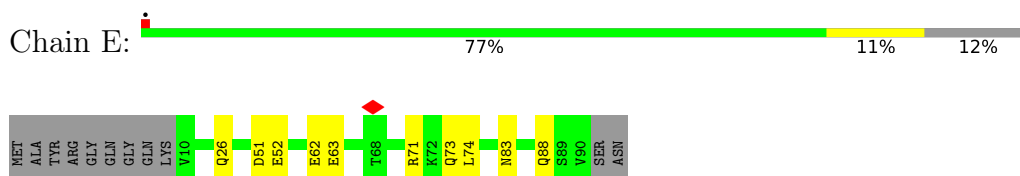
- Molecule 2: Small nuclear ribonucleoprotein-associated proteins B and B'



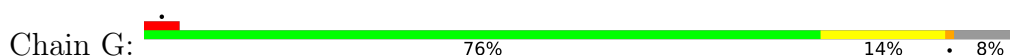
- Molecule 3: Small nuclear ribonucleoprotein F

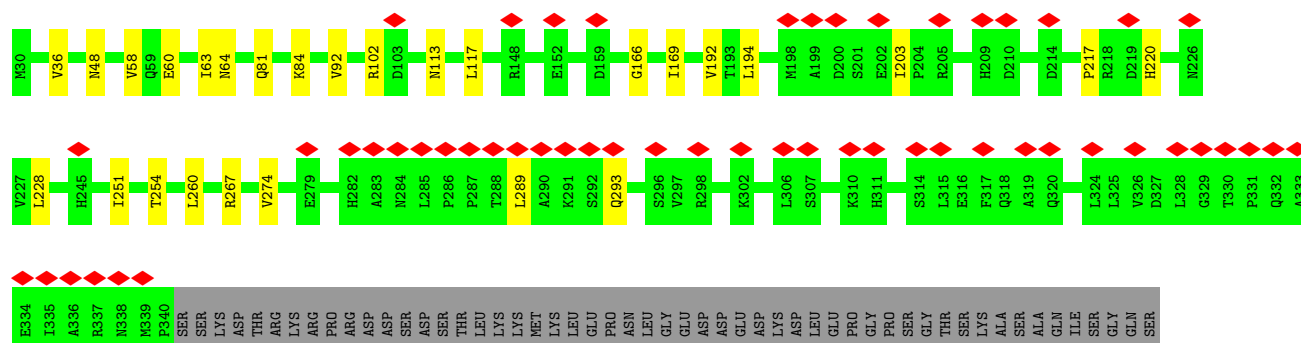


- Molecule 4: Small nuclear ribonucleoprotein E



- Molecule 5: Small nuclear ribonucleoprotein G







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	325282	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 ($e^-/\text{\AA}^2$)	70, 73	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.158	Depositor
Minimum map value	-0.106	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0243	Depositor
Map size ($\text{\AA}$)	357.38, 357.38, 357.38	wwPDB
Map dimensions	334, 334, 334	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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

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	0/660	0.56	0/889
2	B	0.26	0/620	0.49	0/826
3	F	0.29	0/591	0.60	1/799 (0.1%)
4	E	0.28	0/678	0.54	0/910
5	G	0.25	0/613	0.49	0/821
6	C	0.27	0/923	0.60	0/1246
7	D	0.29	0/888	0.61	0/1192
8	H	0.29	0/4068	0.58	2/5498 (0.0%)
9	I	0.31	0/4135	0.64	3/5596 (0.1%)
10	J	0.19	0/2497	0.44	0/3385
11	Z	0.34	0/627	0.51	0/972
12	Y	0.42	2/602 (0.3%)	0.75	4/936 (0.4%)
All	All	0.28	2/16902 (0.0%)	0.58	10/23070 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Y	46	G	O3'-P	5.84	1.70	1.61
12	Y	48	A	O3'-P	5.40	1.69	1.61

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Y	48	A	P-O3'-C3'	12.69	139.23	120.20
8	H	507	ALA	N-CA-C	11.21	123.25	111.14
12	Y	48	A	OP1-P-O3'	-8.90	81.30	108.00
12	Y	47	U	P-O3'-C3'	-8.21	107.88	120.20
12	Y	48	A	OP2-P-O3'	7.94	131.83	108.00

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	A	652	0	670	20	0
2	B	612	0	634	8	0
3	F	579	0	590	12	0
4	E	670	0	696	9	0
5	G	604	0	621	19	0
6	C	911	0	923	17	0
7	D	872	0	907	23	0
8	H	3980	0	3947	79	0
9	I	4055	0	4080	104	0
10	J	2461	0	2566	17	0
11	Z	564	0	285	23	0
12	Y	537	0	271	10	0
13	H	2	0	0	0	0
All	All	16499	0	16190	285	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 9.

The worst 5 of 285 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:TYR:HB3	5:G:70:LEU:HD21	1.27	1.10
8:H:471:ALA:HB1	9:I:604:HIS:O	1.59	1.00
9:I:194:ARG:NH2	9:I:557:LYS:HB3	1.79	0.98
1:A:62:TYR:HB3	5:G:70:LEU:CD2	1.93	0.97
8:H:465:LYS:NZ	9:I:166:GLY:HA2	1.90	0.86

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	81/146 (56%)	78 (96%)	3 (4%)	0	100	100
2	B	72/95 (76%)	68 (94%)	4 (6%)	0	100	100
3	F	72/86 (84%)	70 (97%)	2 (3%)	0	100	100
4	E	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
5	G	75/84 (89%)	75 (100%)	0	0	100	100
6	C	112/123 (91%)	100 (89%)	12 (11%)	0	100	100
7	D	100/259 (39%)	93 (93%)	7 (7%)	0	100	100
8	H	495/684 (72%)	469 (95%)	25 (5%)	1 (0%)	43	73
9	I	504/782 (64%)	457 (91%)	47 (9%)	0	100	100
10	J	309/1072 (29%)	303 (98%)	6 (2%)	0	100	100
All	All	1899/3423 (56%)	1790 (94%)	108 (6%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	267	PRO

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	73/118 (62%)	71 (97%)	2 (3%)	39	68
2	B	69/85 (81%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	63/74 (85%)	63 (100%)	0	100	100
4	E	76/84 (90%)	76 (100%)	0	100	100
5	G	67/74 (90%)	66 (98%)	1 (2%)	57	76
6	C	101/110 (92%)	100 (99%)	1 (1%)	68	80
7	D	95/206 (46%)	95 (100%)	0	100	100
8	H	435/602 (72%)	429 (99%)	6 (1%)	59	77
9	I	455/695 (66%)	449 (99%)	6 (1%)	61	78
10	J	278/946 (29%)	278 (100%)	0	100	100
All	All	1712/2994 (57%)	1696 (99%)	16 (1%)	68	81

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	628	LEU
9	I	602	GLU
8	H	466	VAL
9	I	327	LEU
8	H	357	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	64	ASN
10	J	113	ASN
10	J	304	HIS
8	H	187	HIS
8	H	183	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	Z	26/60 (43%)	13 (50%)	2 (7%)
12	Y	24/52 (46%)	11 (45%)	1 (4%)
All	All	50/112 (44%)	24 (48%)	3 (6%)

5 of 24 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	Z	7	U
11	Z	8	A
11	Z	12	C
11	Z	16	U
11	Z	20	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	Z	7	U
11	Z	26	G
12	Y	48	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

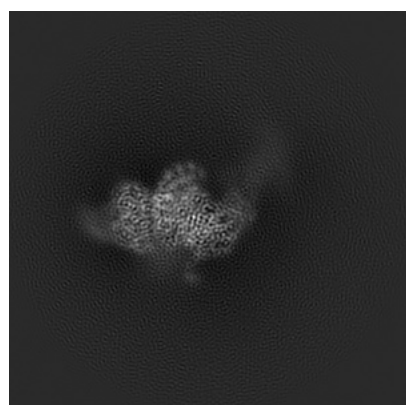
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21050. These allow visual inspection of the internal detail of the map and identification of artifacts.

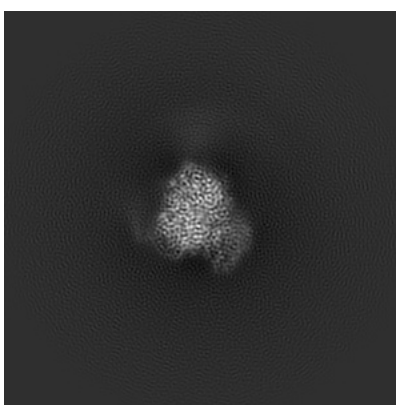
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

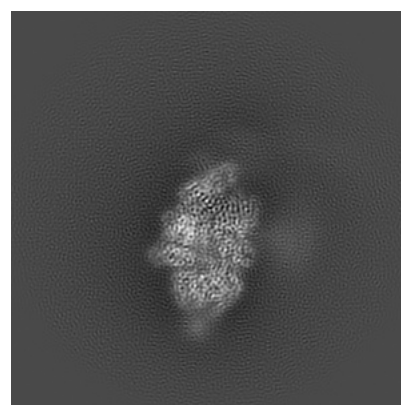
6.1.1 Primary map



X



Y

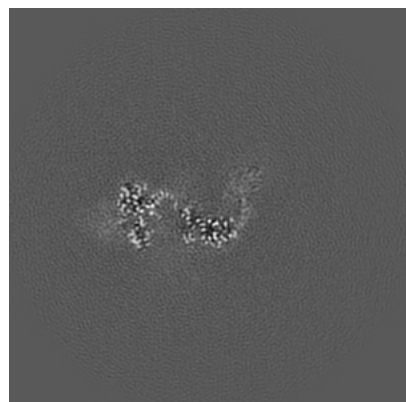


Z

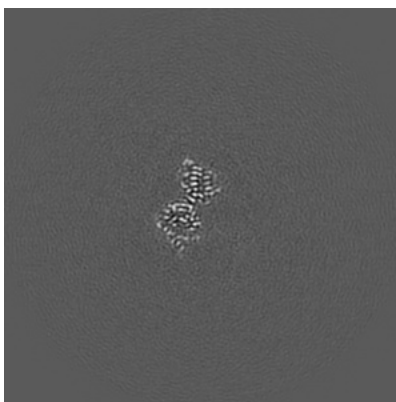
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

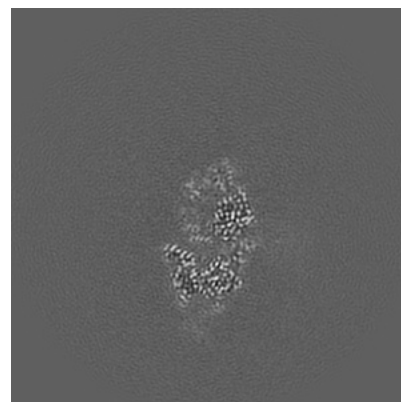
6.2.1 Primary map



X Index: 167



Y Index: 167

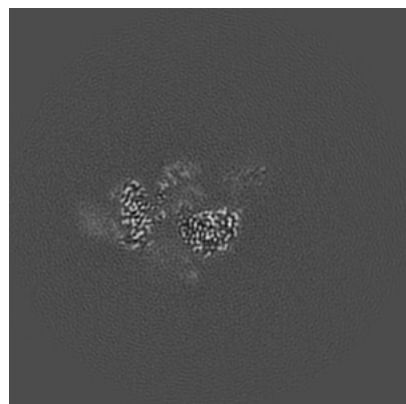


Z Index: 167

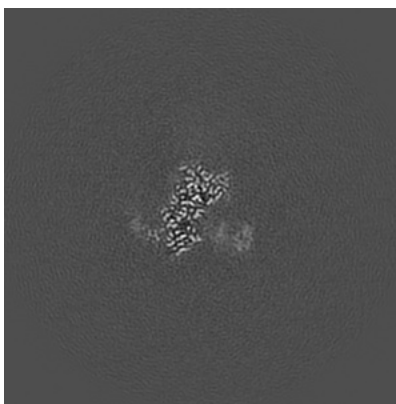
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

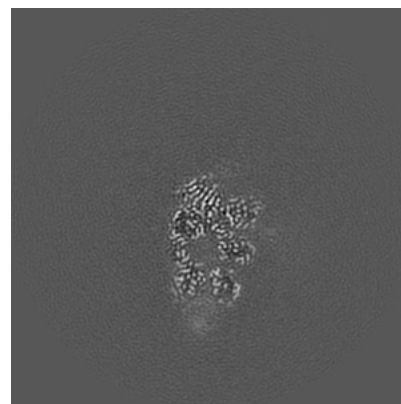
6.3.1 Primary map



X Index: 153



Y Index: 153

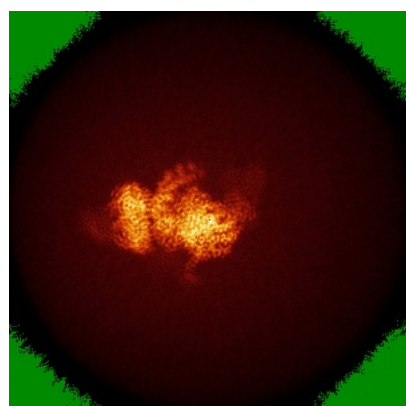


Z Index: 153

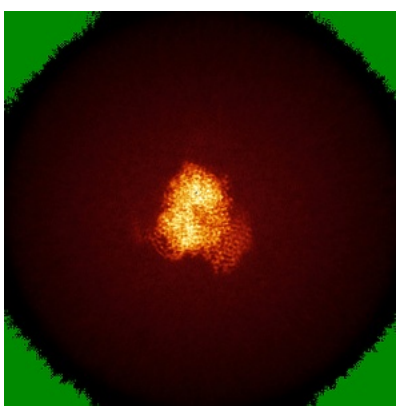
The images above show the largest variance slices of the map in three orthogonal directions.

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

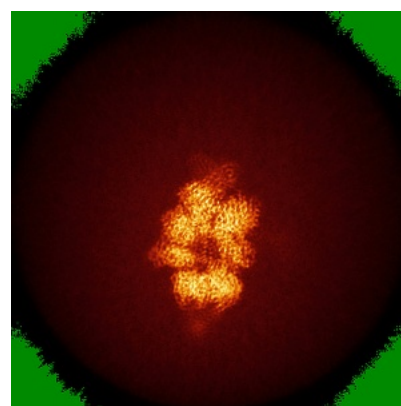
6.4.1 Primary map



X



Y



Z

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 0.0243. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

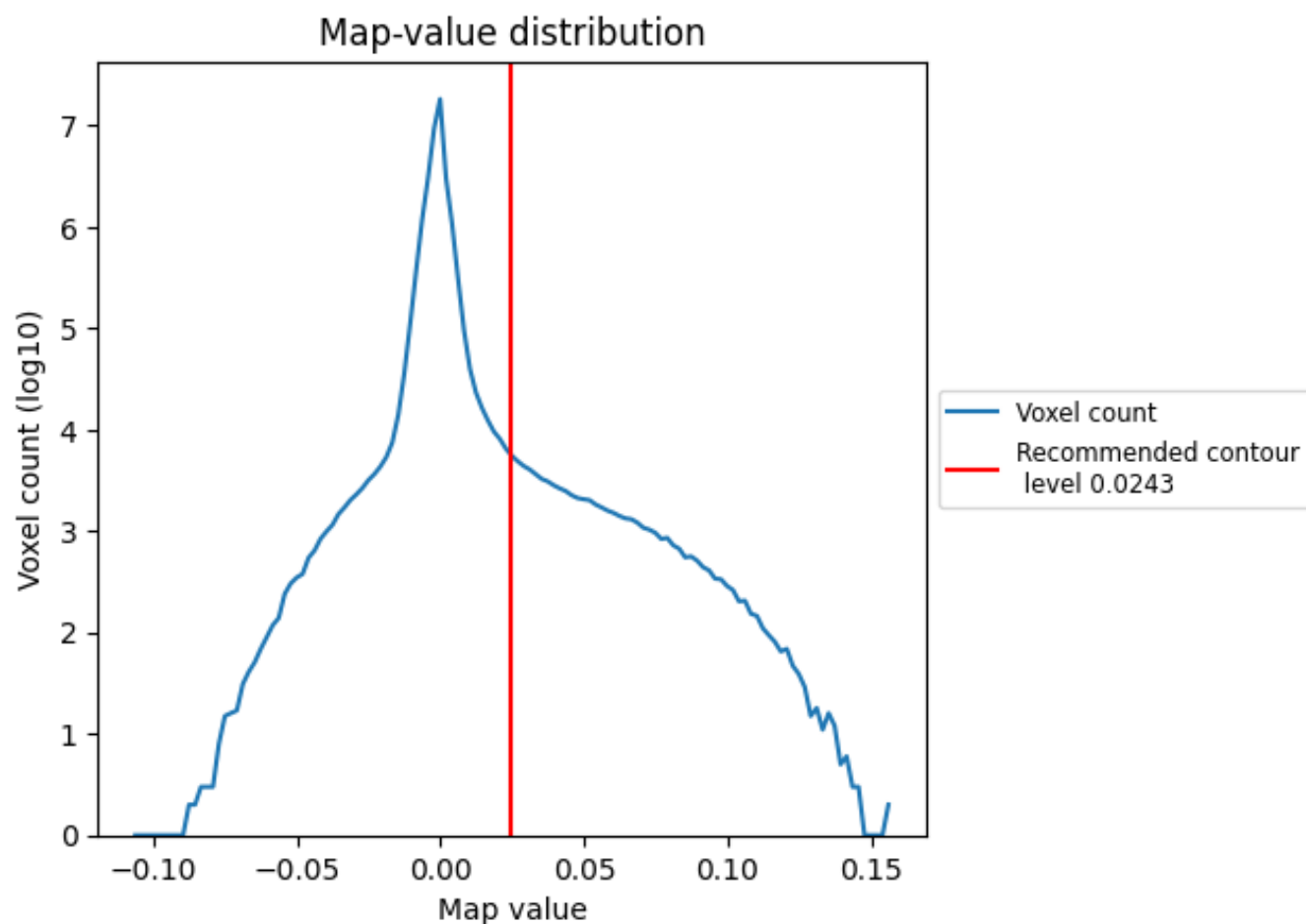
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

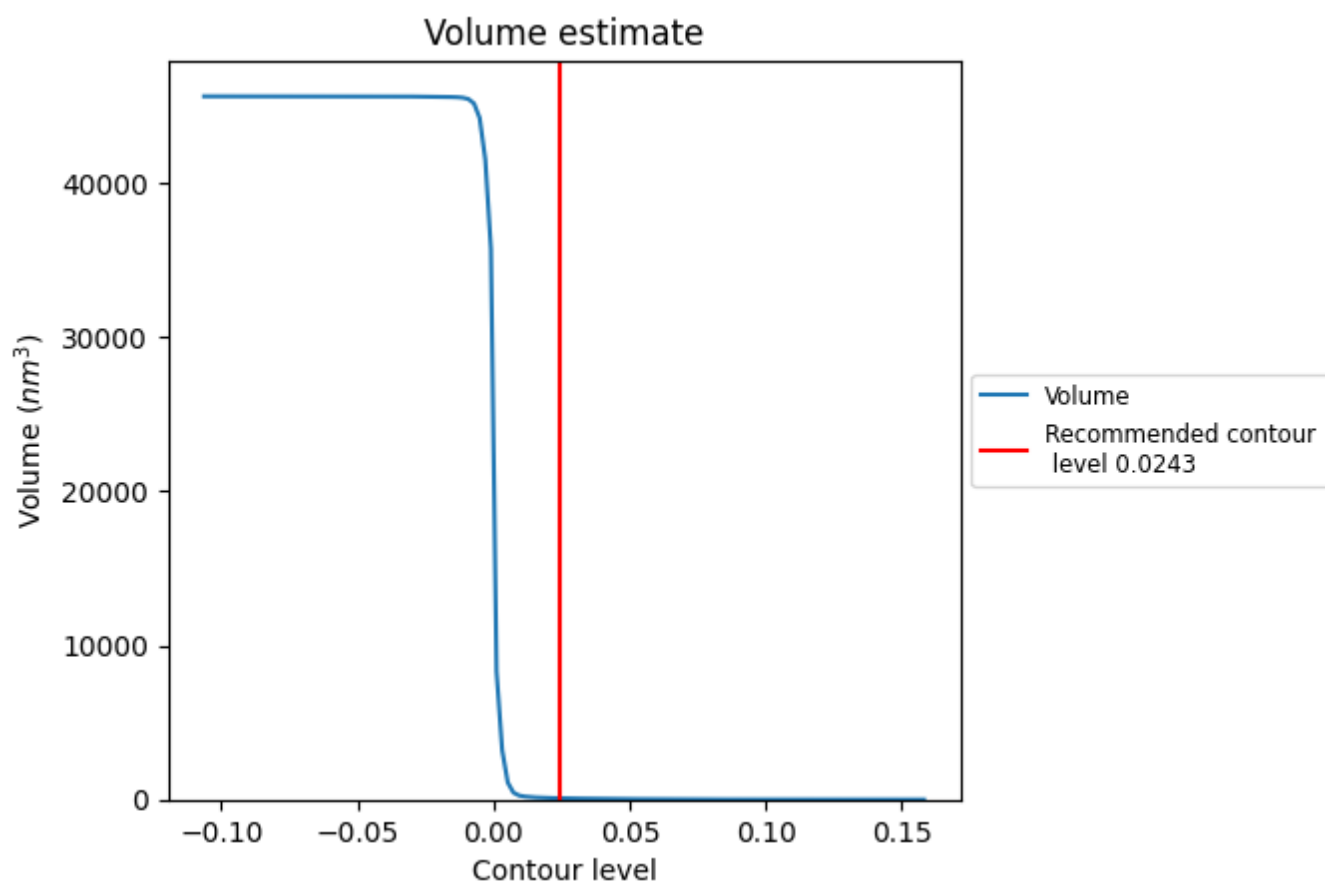
This section contains the results of statistical analysis of the map.

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.

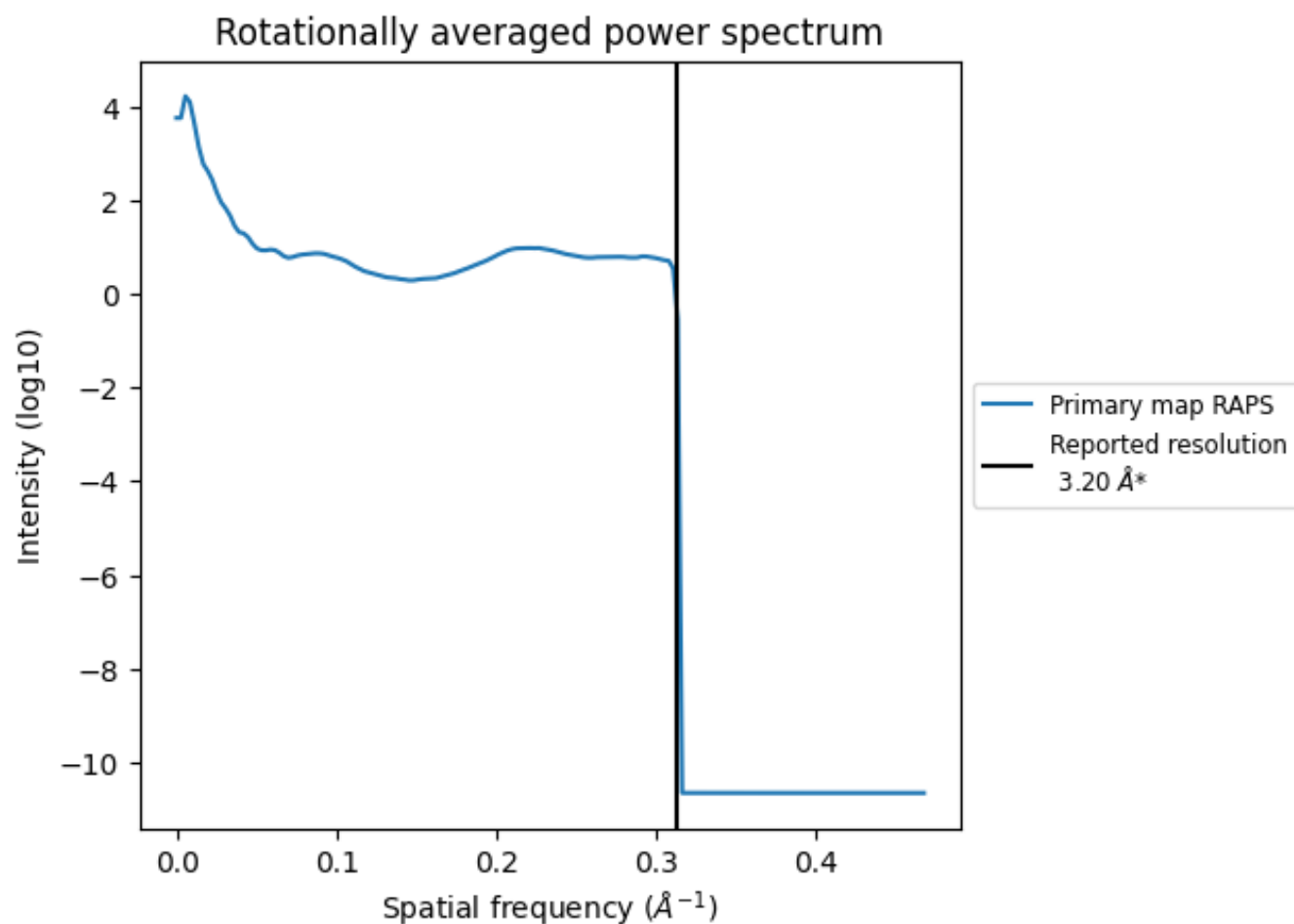
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm³; this corresponds to an approximate mass of 78 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 0.312 Å⁻¹

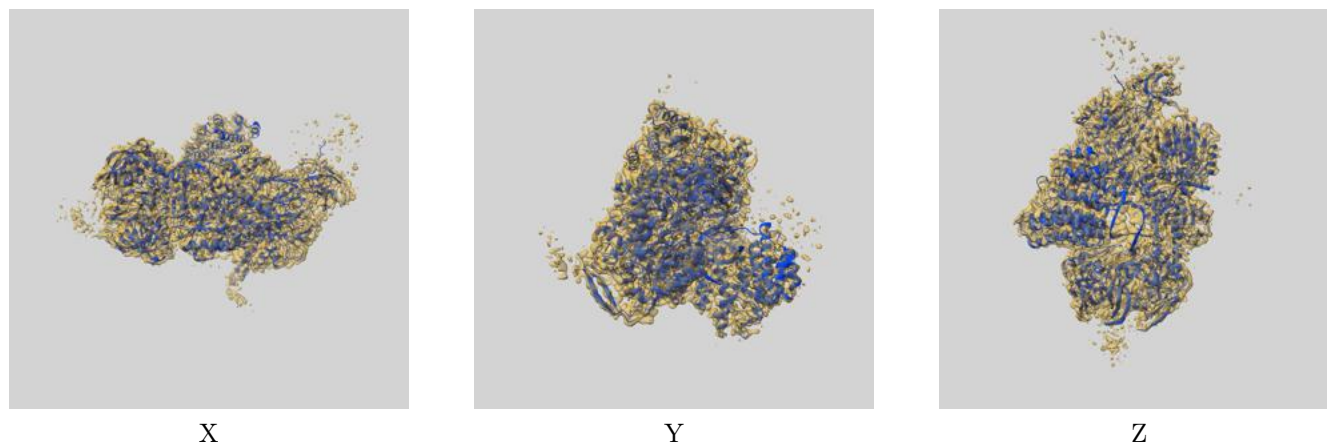
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

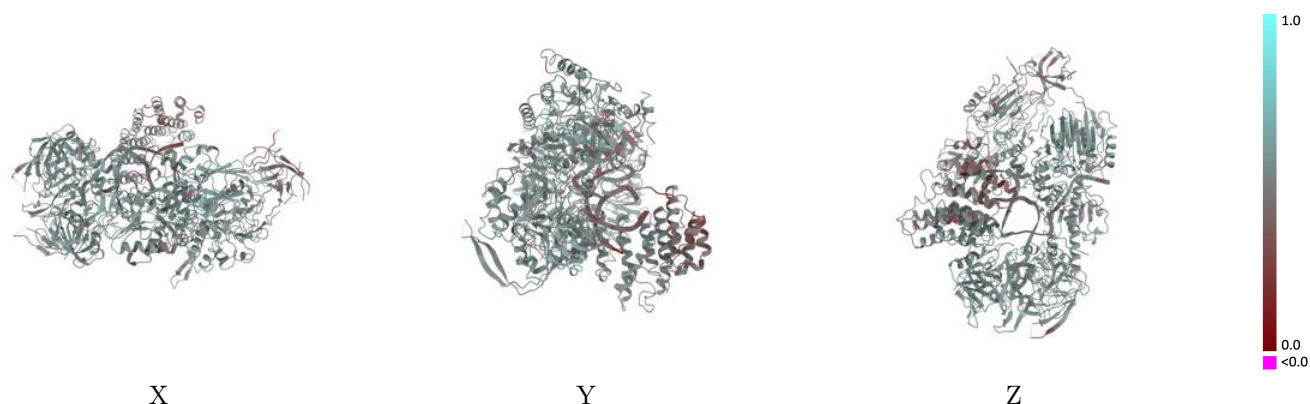
This section contains information regarding the fit between EMDB map EMD-21050 and PDB model 6V4X. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



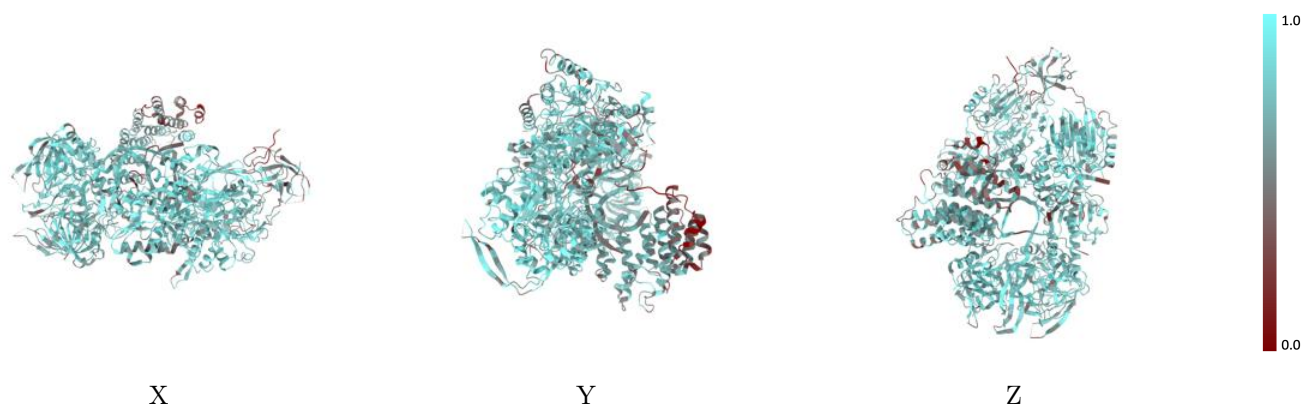
The images above show the 3D surface view of the map at the recommended contour level 0.0243 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



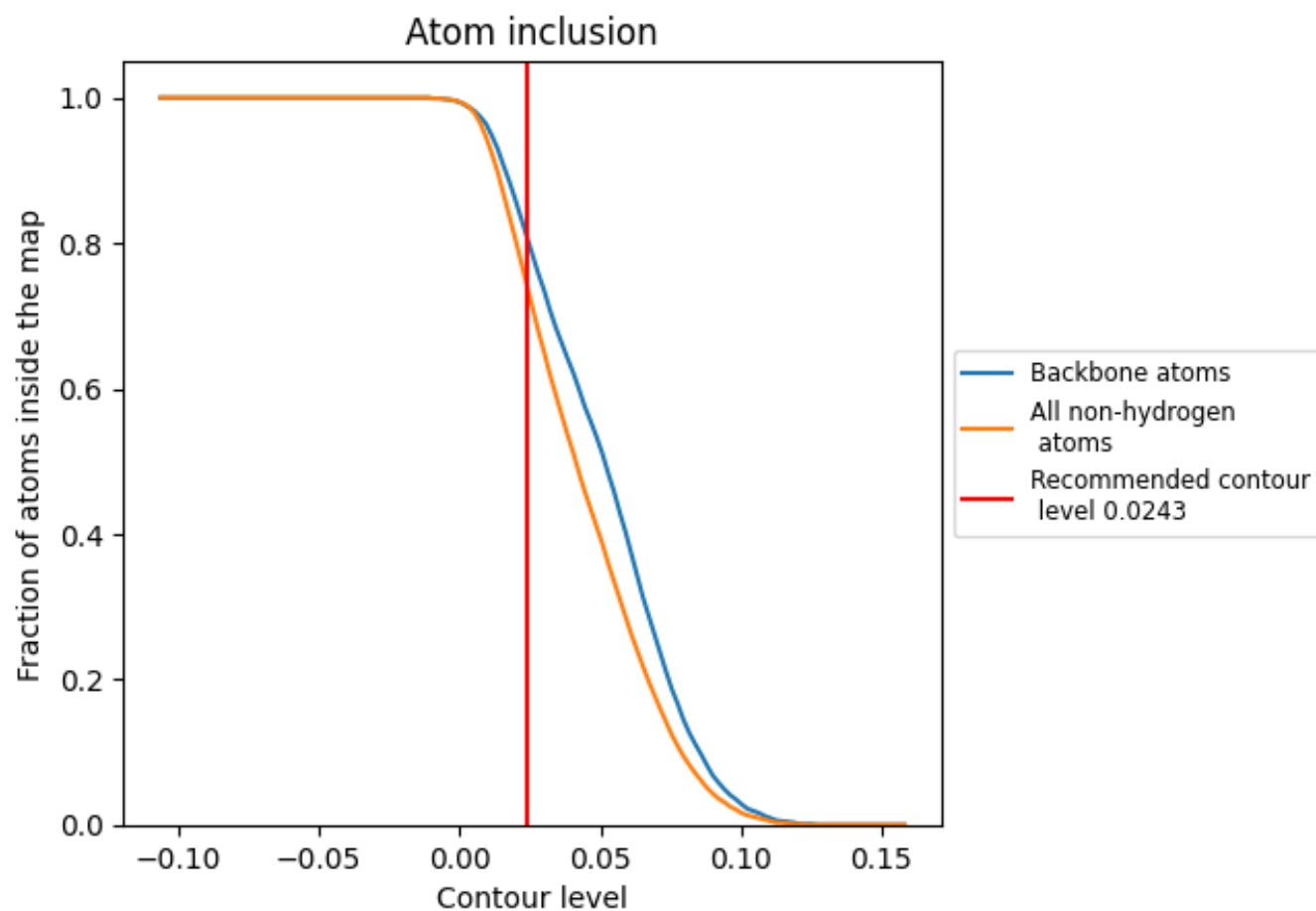
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0243).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.0243) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7360	0.5160
A	0.7420	0.5300
B	0.7520	0.5350
C	0.7760	0.5310
D	0.7800	0.5130
E	0.7720	0.5430
F	0.7840	0.5400
G	0.7420	0.5410
H	0.7520	0.5290
I	0.7520	0.5200
J	0.6370	0.4800
Y	0.6630	0.4560
Z	0.7470	0.4820

1.0

0.0

<0.0