



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 06:08 am GMT

PDB ID : 5GAP  
EMDB ID : EMD-8014  
Title : Body region of the U4/U6.U5 tri-snRNP  
Authors : Nguyen, T.H.D.; Galej, W.P.; Oubridge, C.; Bai, X.C.; Newman, A.; Scheres, S.; Nagai, K.  
Deposited on : 2015-12-15  
Resolution : 3.60 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](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev43
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)	:	2.31.2

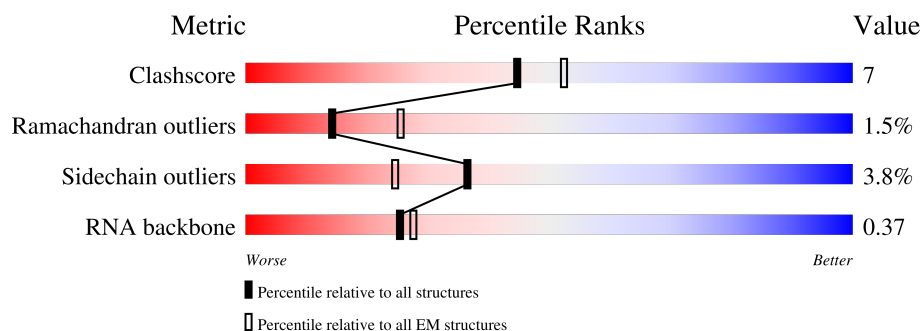
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	V	67	
2	W	112	
3	U	214	
4	x	82	
5	A	2413	
6	H	465	
7	J	899	

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Mol	Chain	Length	Quality of chain
8	D	143	
9	F	494	
10	G	469	
11	K	126	
12	B	2163	

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31576 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 U4 snRNA, 5' region, nucleotides 1-67.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	67	Total	C	N	O	P	0	0
			1426	637	247	475	67		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	56	Total	C	N	O	P	0	0
			1190	533	210	391	56		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	20	Total	C	N	O	P	0	0
			414	186	64	144	20		

- Molecule 4 is a protein called unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	x	82	Total	C	N	O	0	0
			410	246	82	82		

- Molecule 5 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1349	Total	C	N	O	S	0	0
			11066	7094	1901	2031	40		

- Molecule 6 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	357	Total	C	N	O	S	0	0
			2789	1743	501	532	13		

- Molecule 7 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	729	Total	C	N	O	S	0	0
			5822	3726	992	1079	25		

- Molecule 8 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	140	Total	C	N	O	S	0	0
			1151	728	200	212	11		

- Molecule 9 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	415	Total	C	N	O	S	0	0
			3218	2052	575	580	11		

- Molecule 10 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	318	Total	C	N	O	S	0	0
			2632	1659	469	488	16		

- Molecule 11 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	124	Total	C	N	O	S	0	0
			936	597	161	174	4		

- Molecule 12 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	71	Total	C	N	O	S	0	0
			522	326	89	106	1		

### 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.

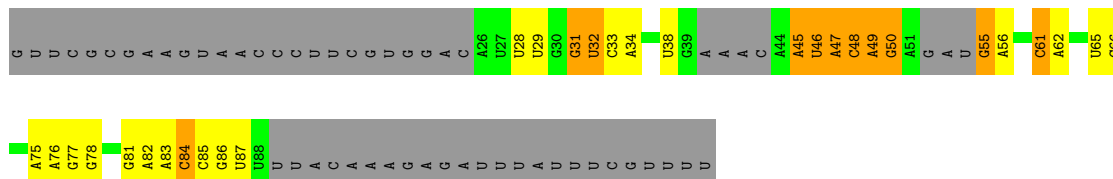
- Molecule 1: U4 snRNA, 5' region, nucleotides 1-67

Chain V: 



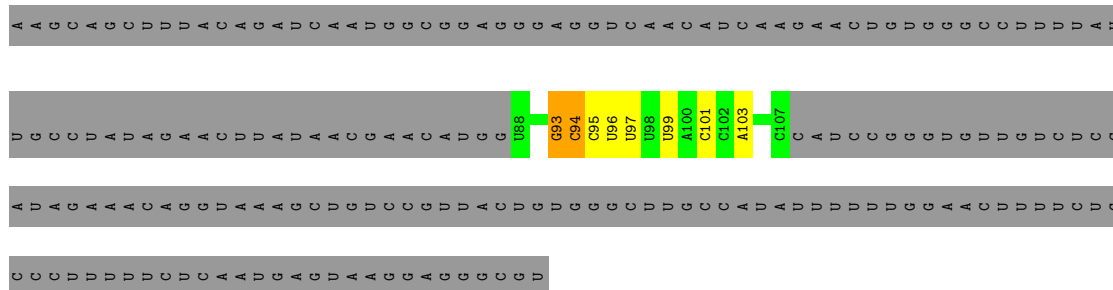
- Molecule 2: U6 snRNA

Chain W: 



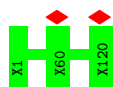
- Molecule 3: U5 snRNA

Chain U: 

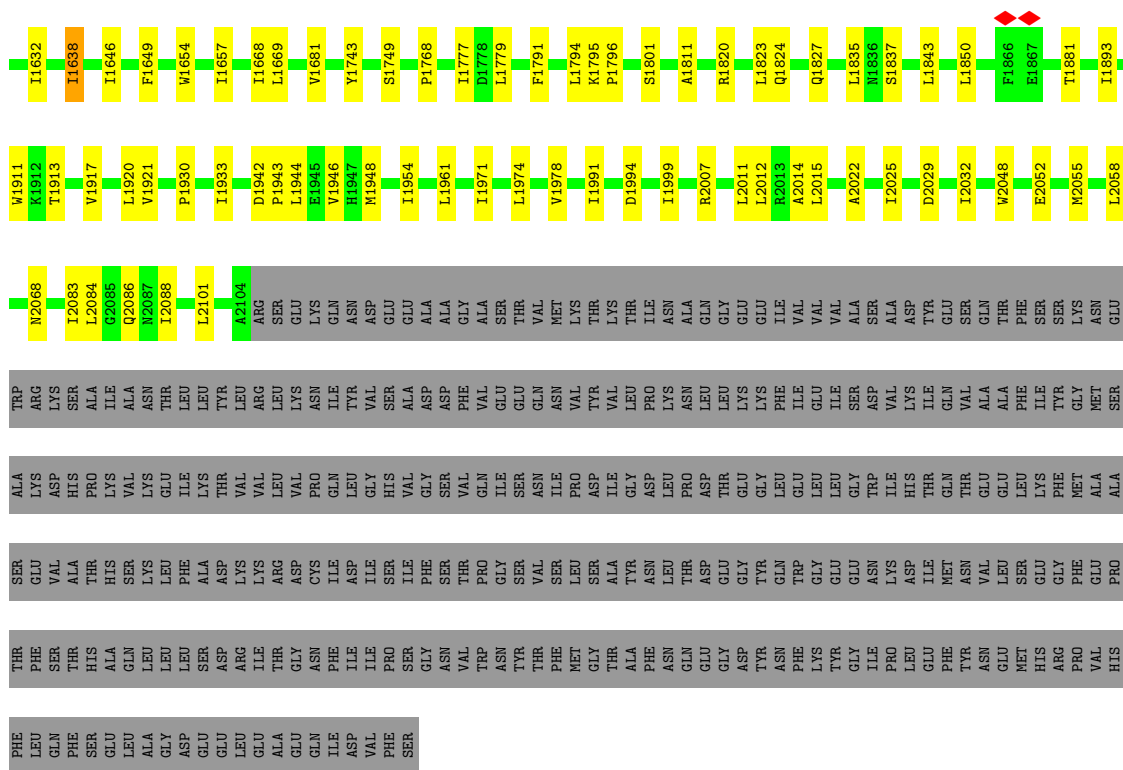


- Molecule 4: unknown protein

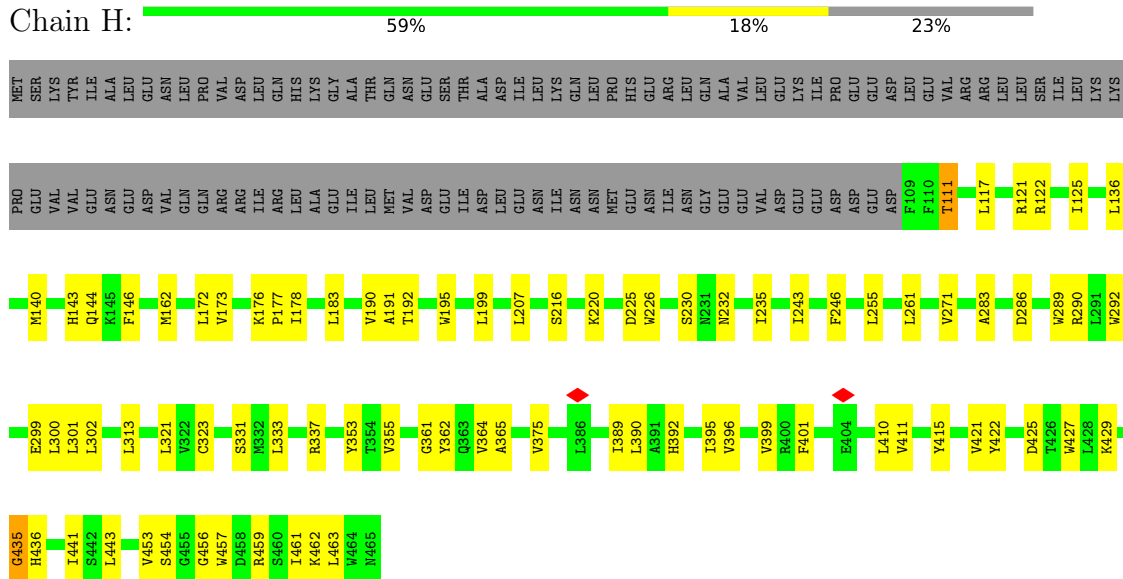
Chain x: 



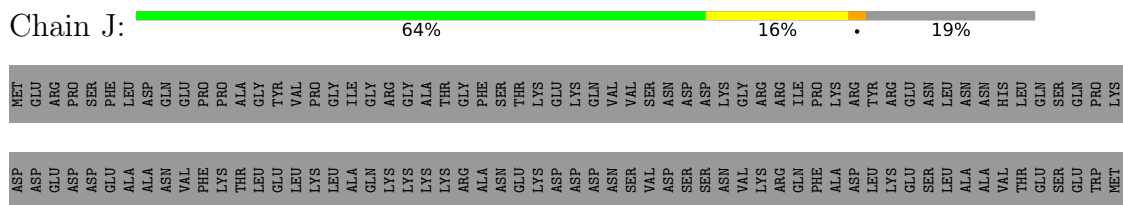
[illegible]



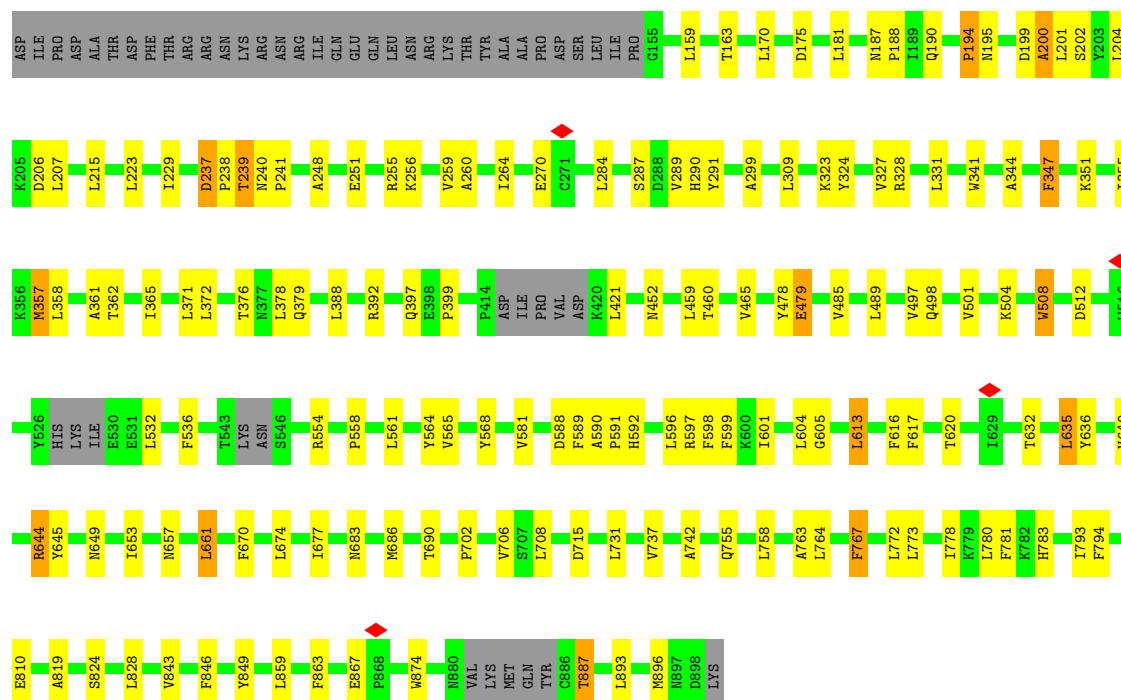
- Molecule 6: U4/U6 small nuclear ribonucleoprotein PRP4



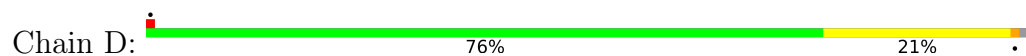
- Molecule 7: Pre-mRNA-splicing factor 6



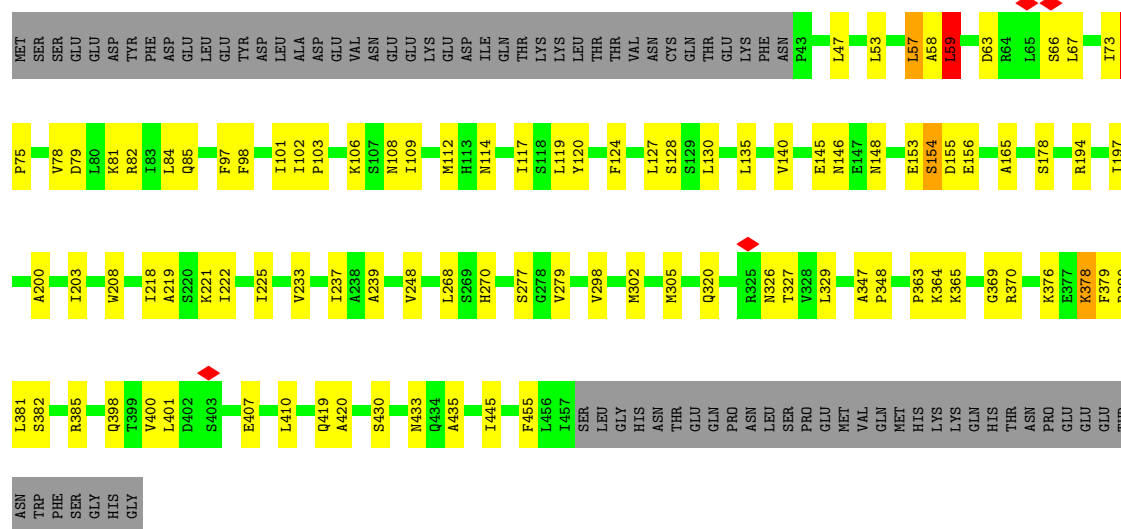




• Molecule 8: Spliceosomal protein DIB1



• Molecule 9: Pre-mRNA-processing factor 31



• Molecule 10: U4/U6 small nuclear ribonucleoprotein PRP3





TYR	GLU	GLU	GLY	GLY	LEU	GLY	LEU	ASN	TYR
LEU	LYS	ILE	TYR	TYR	PRO	LEU	LEU	GLY	GLY
ASP	TYR	LEU	ASN	LEU	LEU	LEU	VAL	LEU	VAL
ALA	PRO	THR	ASN	ARG	ARG	ARG	ILE	ILE	ARG
ASP	PHE	LEU	ALA	THR	PHE	ALA	ASP	ALA	ASP
LYS	ASP	THR	THR	THR	GLU	THR	SER	SER	THR
GLU	LYS	ASP	THR	THR	GLU	THR	HIS	HIS	SER
LEU	LEU	SER	ALA	ALA	HIS	THR	PRO	PRO	GLY
GLU	GLU	GLN	MET	MET	THR	THR	GLY	GLY	HIS
PHE	SER	LEU	ASP	ASP	SER	SER	VAL	VAL	GLY
GLU	TRP	ALA	LEU	LEU	SER	SER	SER	SER	ILE
ILE	TRP	GLN	ALA	ALA	GLY	PHE	PHE	PHE	SER
ASN	LEU	VAL	GLN	GLN	SER	SER	VAL	VAL	VAL
VAL	VAL	ALA	MET	MET	VAL	THR	THR	THR	PHE
LYS	LEU	ALA	ILE	ILE	PHE	ILE	ILE	ILE	THR
	GLY	PHE	ILE	GLN	GLY	GLN	SER	SER	GLN
	GLU	VAL	GLN	GLY	VAL	VAL	PHE	PHE	ASN
	VAL	ASN	VAL	VAL	ASN	ASN	ASN	ASN	LEU
	SER	ASN	TYR	VAL	ASN	THR	VAL	VAL	VAL
	LYS	TYR	PRO	TRP	LEU	SER	SER	SER	GLU
	GLU	ASN	ASP	ASP	LEU	LEU	THR	THR	THR
	LEU	VAL	VAL	ASP	GLN	LEU	SER	SER	LEU
	TYR	GLU	ASN	ASN	ALA	ALA	ASN	ASN	ASN
	ALA	LEU	PRO	PRO	TYR	THR	THR	THR	ASP
	ILE	THR	ILE	ARG	PHE	SER	SER	SER	ASP
	LYS	THR	GLN	GLN	LEU	ARG	THR	THR	VAL
	VAL	LEU	ILE	ILE	LEU	ILE	LYS	SER	LEU
	THR	ASN	PRO	PRO	GLU	ASN	ASN	ASN	SER
	LEU	ASN	HIS	HIS	LEU	MET	MET	MET	SER
	ASN	SER	PHE	PHE	PRO	LEU	ASN	ASN	PHE
	LYS	ASP	ASN	ASN	VAL	TYR	GLU	GLU	ILE
	GLU	SER	ASN	ASN	LYS	ASP	VAL	VAL	GLY
	THR	LEU	LYS	LYS	PHE	ASP	VAL	VAL	ASP
	GLN	ILE	ILE	ILE	GLN	SER	PHE	PHE	ASP
	GLN	SER	LEU	LEU	ASN	THR	SER	THR	THR
	GLN	GLY	GLU	GLU	ASP	ALA	THR	GLU	ALA
	TYR	VAL	THR	LYS	LEU	VAL	GLU	GLU	GLU
	GLU	LEU	LYS	LYS	LYS	LYS	GLY	GLY	VAL
	PHE	GLN	GLY	GLY	ASP	ILE	THR	THR	THR
	ASP	ILE	ILE	ILE	LEU	LEU	VAL	VAL	ALA
	THR	THR	THR	VAL	GLU	GLU	VAL	VAL	GLU
	PRO	ILE	VAL	VAL	ASN	VAL	PRO	PRO	VAL
	THR	THR	VAL	GLU	GLU	THR	VAL	VAL	GLY
	SER	GLN	THR	LYS	VAL	ASP	GLY	GLY	GLY
	GLY	LYS	THR	GLY	PRO	LEU	ARG	ASP	GLY
	LYS	ARG	VAL	VAL	ILE	ILE	THR	GLY	ASP
	ASN	ASN	ASP	ASP	ASN	ASN	ASN	ASN	ASP
	HIS	VAL	ILE	ILE	ASN	ARG	GLU	GLU	GLU
	LEU	THR	THR	ALA	VAL	VAL	ALA	ALA	THR
	THR	ILE	GLU	GLU	VAL	VAL	LEU	LEU	GLU
	TRP	CYS	ASP	ASP	ASP	VAL	VAL	VAL	ILE
	CYS	GLN	GLY	GLY	ILE	GLY	THR	THR	THR
	VAL	THR	THR	THR	THR	THR	THR	THR	THR
	GLY	VAL	GLU	GLU	GLU	GLU	GLY	GLY	LYS
	ASP	THR	ASP	ASP	ASN	ASN	ASN	ASN	ASN
	SER	SER	SER	SER	ASN	ASN	ASN	ASN	ASN
	THR	THR	THR	THR	THR	THR	THR	THR	THR
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
	THR	THR	THR	THR	THR	THR	THR	THR	THR
	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
	ILE	ILE	ILE	ILE	ILE</				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.326	Depositor
Minimum map value	-0.232	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.43, 1.43, 1.43	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	V	0.36	0/1593	0.79	1/2480 (0.0%)
2	W	0.38	0/1328	0.84	2/2061 (0.1%)
3	U	0.32	0/459	0.76	0/710
5	A	0.42	1/11327 (0.0%)	0.73	2/15348 (0.0%)
6	H	0.38	0/2845	0.71	0/3843
7	J	0.44	0/5934	0.80	2/8039 (0.0%)
8	D	0.42	0/1172	0.75	1/1578 (0.1%)
9	F	0.43	0/3273	0.80	2/4413 (0.0%)
10	G	0.41	0/2687	0.69	0/3611
11	K	0.45	0/949	0.81	0/1292
12	B	0.42	0/529	0.69	0/716
All	All	0.42	1/32096 (0.0%)	0.76	10/44091 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	3
9	F	0	1
12	B	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	825	SER	CB-OG	5.40	1.49	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	613	LEU	CA-CB-CG	7.12	131.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	979	SER	C-N-CD	-6.95	105.32	120.60
1	V	17	A	C2'-C3'-O3'	6.90	124.74	113.70
2	W	55	G	C2'-C3'-O3'	5.73	122.87	113.70
9	F	74	LEU	CA-CB-CG	5.58	128.14	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1278	VAL	Peptide
5	A	1994	ASP	Peptide
5	A	979	SER	Peptide
12	B	423	ILE	Peptide
9	F	154	SER	Peptide

## 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	V	1426	0	716	22	0
2	W	1190	0	603	14	0
3	U	414	0	213	4	0
4	x	410	0	89	0	0
5	A	11066	0	11078	138	0
6	H	2789	0	2725	53	0
7	J	5822	0	5792	103	0
8	D	1151	0	1138	17	0
9	F	3218	0	3297	53	0
10	G	2632	0	2599	27	0
11	K	936	0	987	24	0
12	B	522	0	506	5	0
All	All	31576	0	29743	413	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 413 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:A:1578:ALA:HB1	5:A:1602:PRO:HB3	1.40	1.02
5:A:1275:MET:HE2	5:A:1281:ASN:ND2	1.92	0.84
10:G:272:VAL:HG12	10:G:280:VAL:HG21	1.59	0.81
5:A:1067:ASN:HB2	5:A:1083:THR:HG21	1.64	0.80
7:J:199:ASP:O	7:J:201:LEU:N	2.14	0.79

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	
5	A	1343/2413 (56%)	1226 (91%)	104 (8%)	13 (1%)	15	55
6	H	355/465 (76%)	301 (85%)	48 (14%)	6 (2%)	9	45
7	J	719/899 (80%)	650 (90%)	56 (8%)	13 (2%)	8	43
8	D	138/143 (96%)	126 (91%)	11 (8%)	1 (1%)	22	61
9	F	413/494 (84%)	364 (88%)	38 (9%)	11 (3%)	5	35
10	G	316/469 (67%)	283 (90%)	32 (10%)	1 (0%)	41	75
11	K	122/126 (97%)	111 (91%)	9 (7%)	2 (2%)	9	46
12	B	69/2163 (3%)	57 (83%)	8 (12%)	4 (6%)	1	18
All	All	3475/7172 (48%)	3118 (90%)	306 (9%)	51 (2%)	14	47

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	1093	LYS
5	A	1278	VAL
5	A	2088	ILE
6	H	362	TYR
7	J	479	GLU



### 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	
5	A	1216/2182 (56%)	1194 (98%)	22 (2%)	59	81
6	H	305/410 (74%)	290 (95%)	15 (5%)	25	59
7	J	627/813 (77%)	600 (96%)	27 (4%)	29	63
8	D	129/132 (98%)	121 (94%)	8 (6%)	18	53
9	F	346/445 (78%)	324 (94%)	22 (6%)	17	52
10	G	289/436 (66%)	283 (98%)	6 (2%)	53	78
11	K	102/104 (98%)	90 (88%)	12 (12%)	5	28
12	B	56/1955 (3%)	52 (93%)	4 (7%)	14	48
All	All	3070/6477 (47%)	2954 (96%)	116 (4%)	36	66

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	J	657	ASN
11	K	113	GLN
8	D	139	HIS
11	K	93	VAL
10	G	395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
7	J	397	GLN
7	J	578	GLN
10	G	300	GLN
7	J	537	GLN
7	J	673	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	66/67 (98%)	29 (43%)	6 (9%)
2	W	54/112 (48%)	20 (37%)	9 (16%)
3	U	19/214 (8%)	8 (42%)	1 (5%)
All	All	139/393 (35%)	57 (41%)	16 (11%)

5 of 57 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	V	2	U
1	V	11	A
1	V	18	A
1	V	19	U
1	V	20	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	W	84	C
2	W	83	A
2	W	45	A
2	W	75	A
2	W	32	U

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	x	1
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	62:UNK	C	101:UNK	N	54.04
1	A	1860:VAL	C	1861:THR	N	4.50

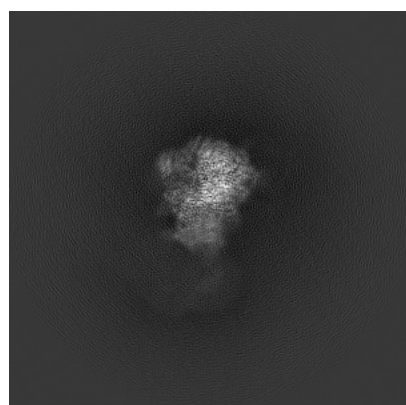
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8014. These allow visual inspection of the internal detail of the map and identification of artifacts.

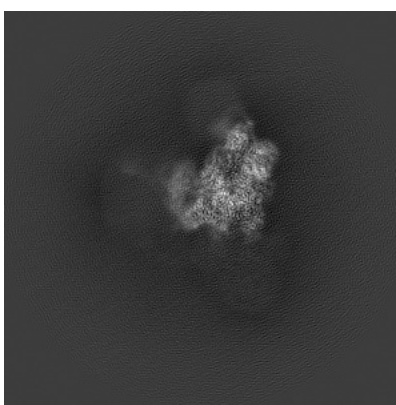
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

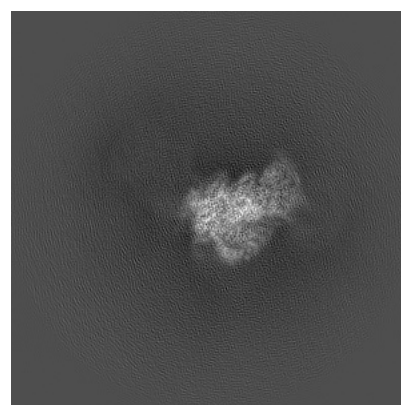
#### 6.1.1 Primary map



X



Y

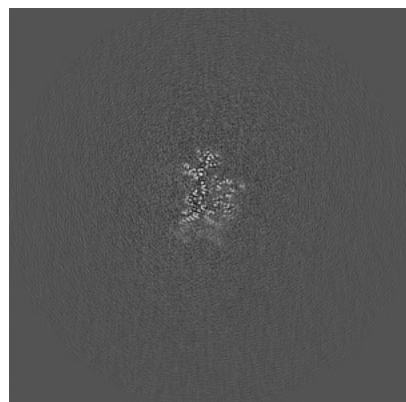


Z

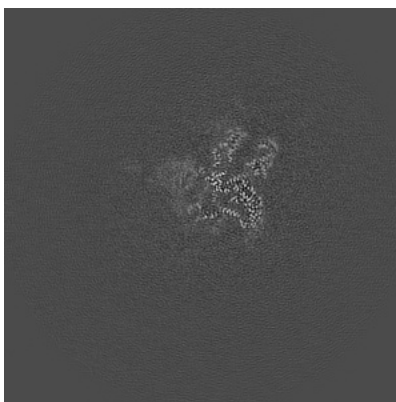
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

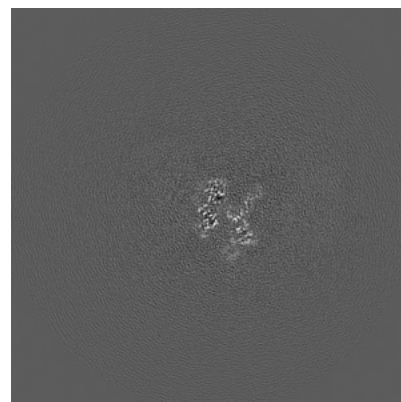
#### 6.2.1 Primary map



X Index: 190



Y Index: 190

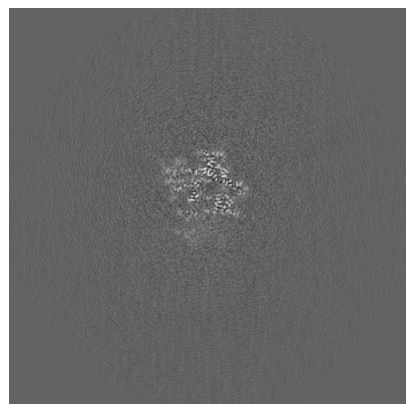


Z Index: 190

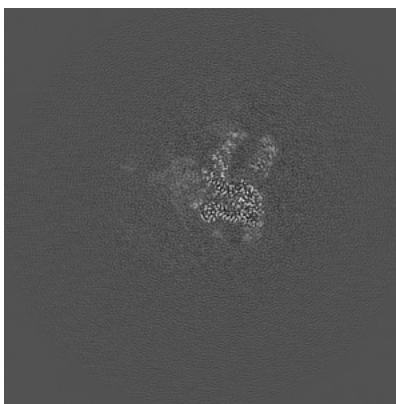
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices ⓘ

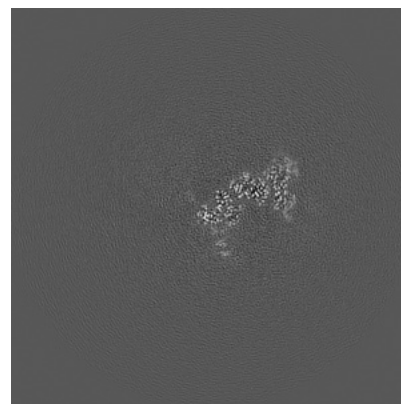
### 6.3.1 Primary map



X Index: 197



Y Index: 186

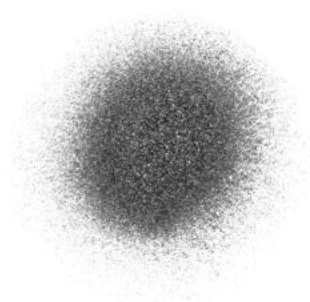


Z Index: 221

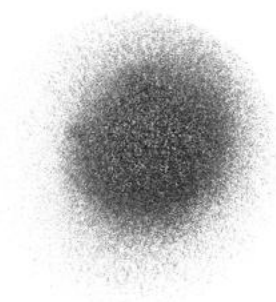
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views ⓘ

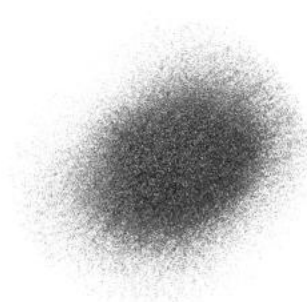
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

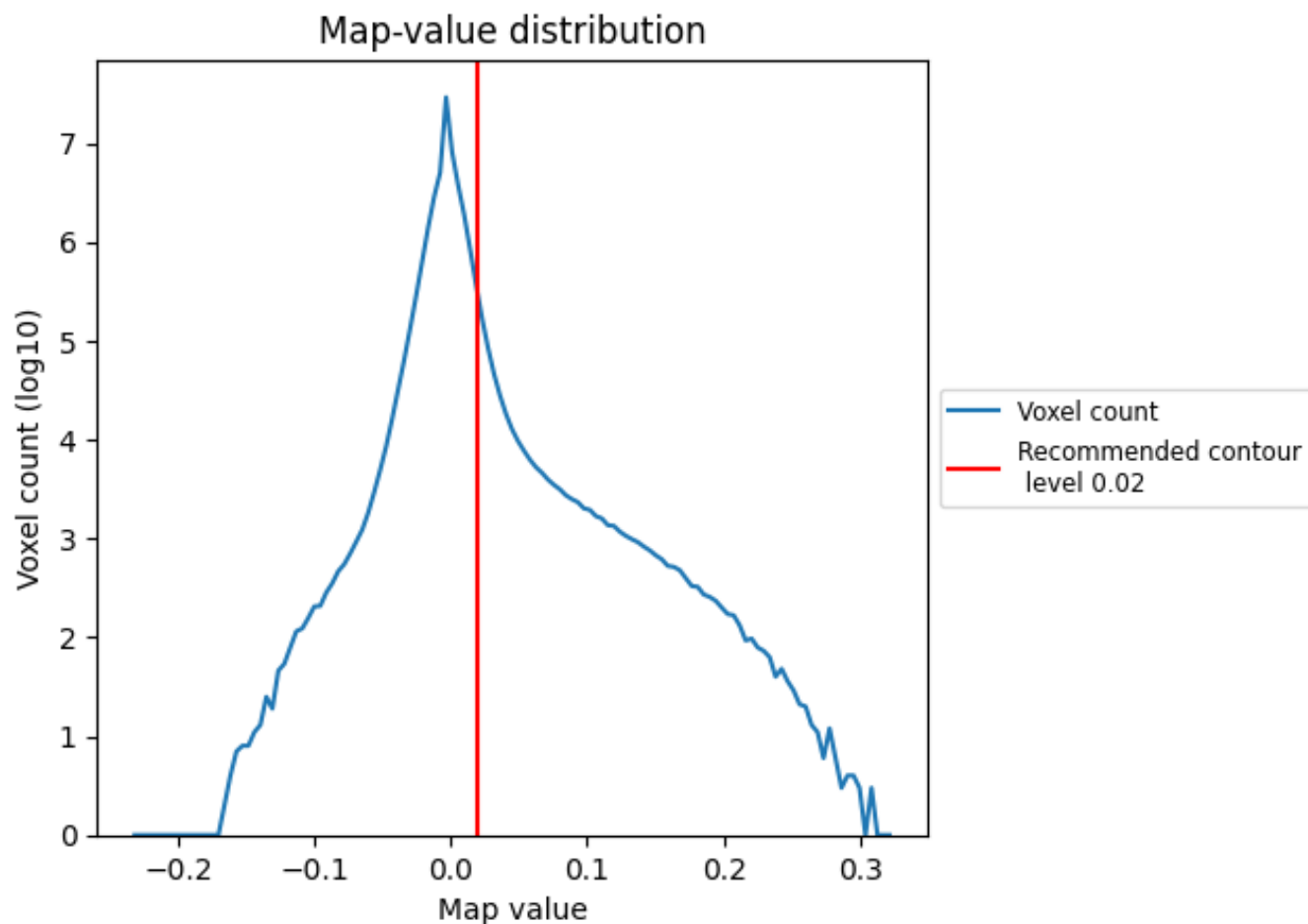
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

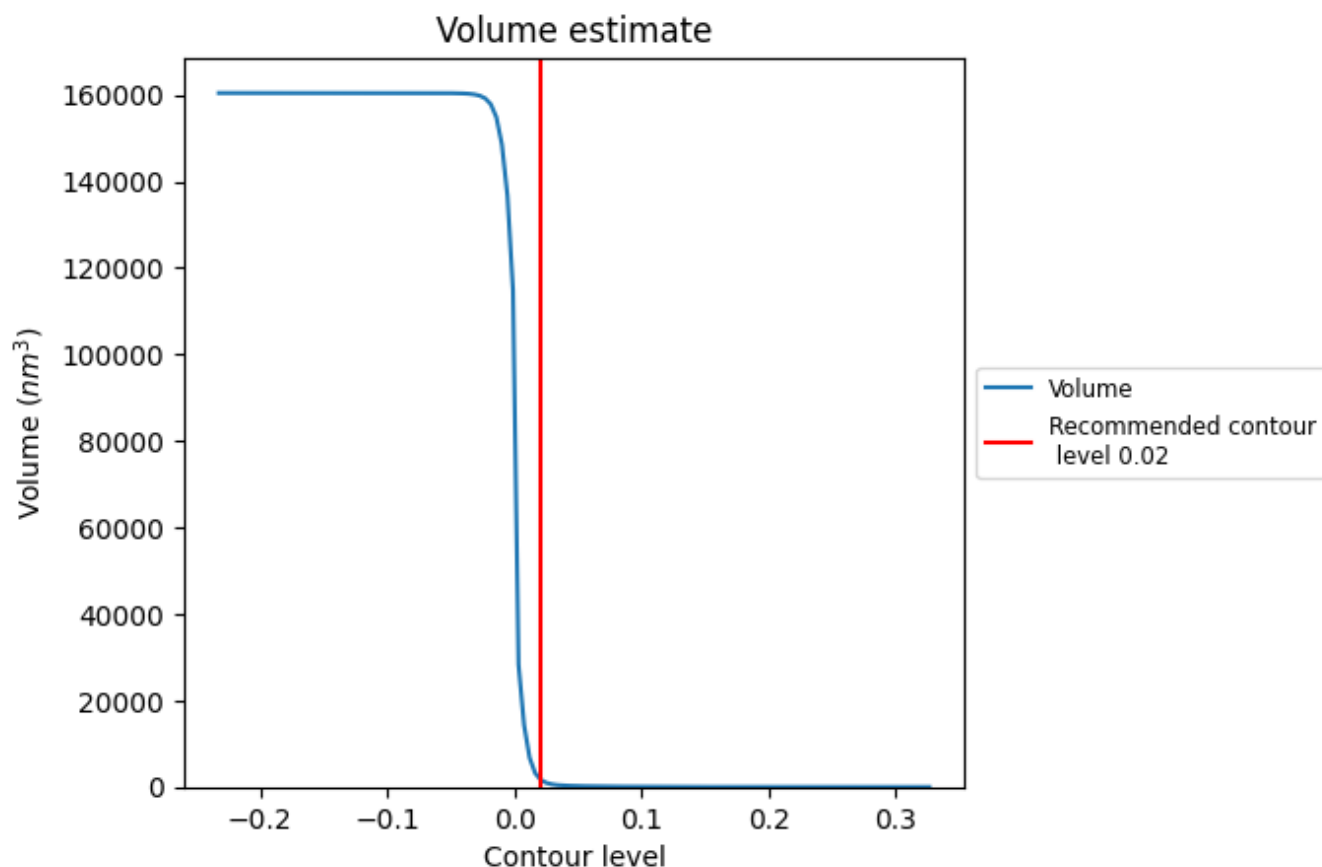
This section contains the results of statistical analysis of the map.

### 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](#)

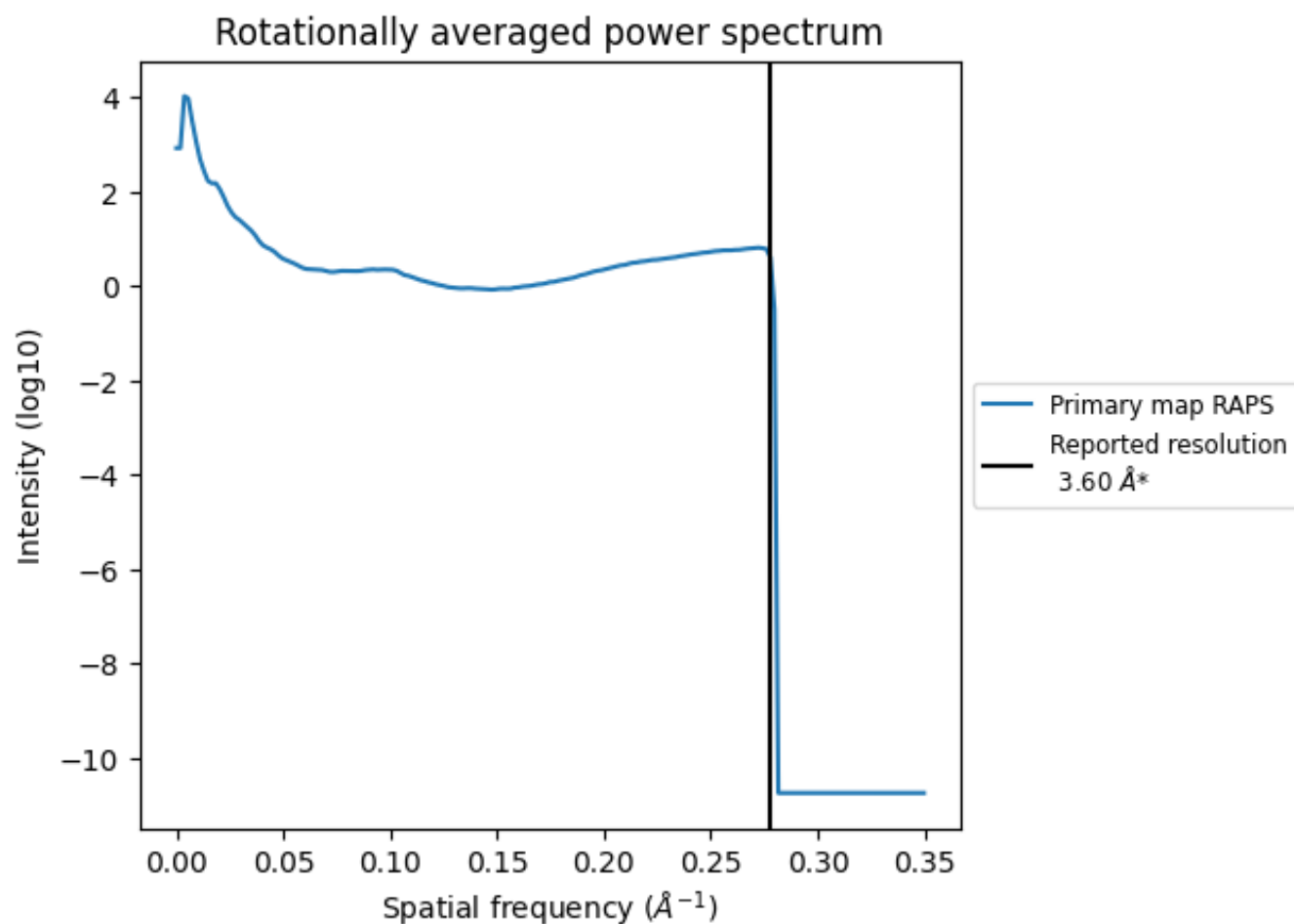


The volume at the recommended contour level is 1921  $\text{nm}^3$ ; this corresponds to an approximate mass of 1735 kDa.

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 ⓘ

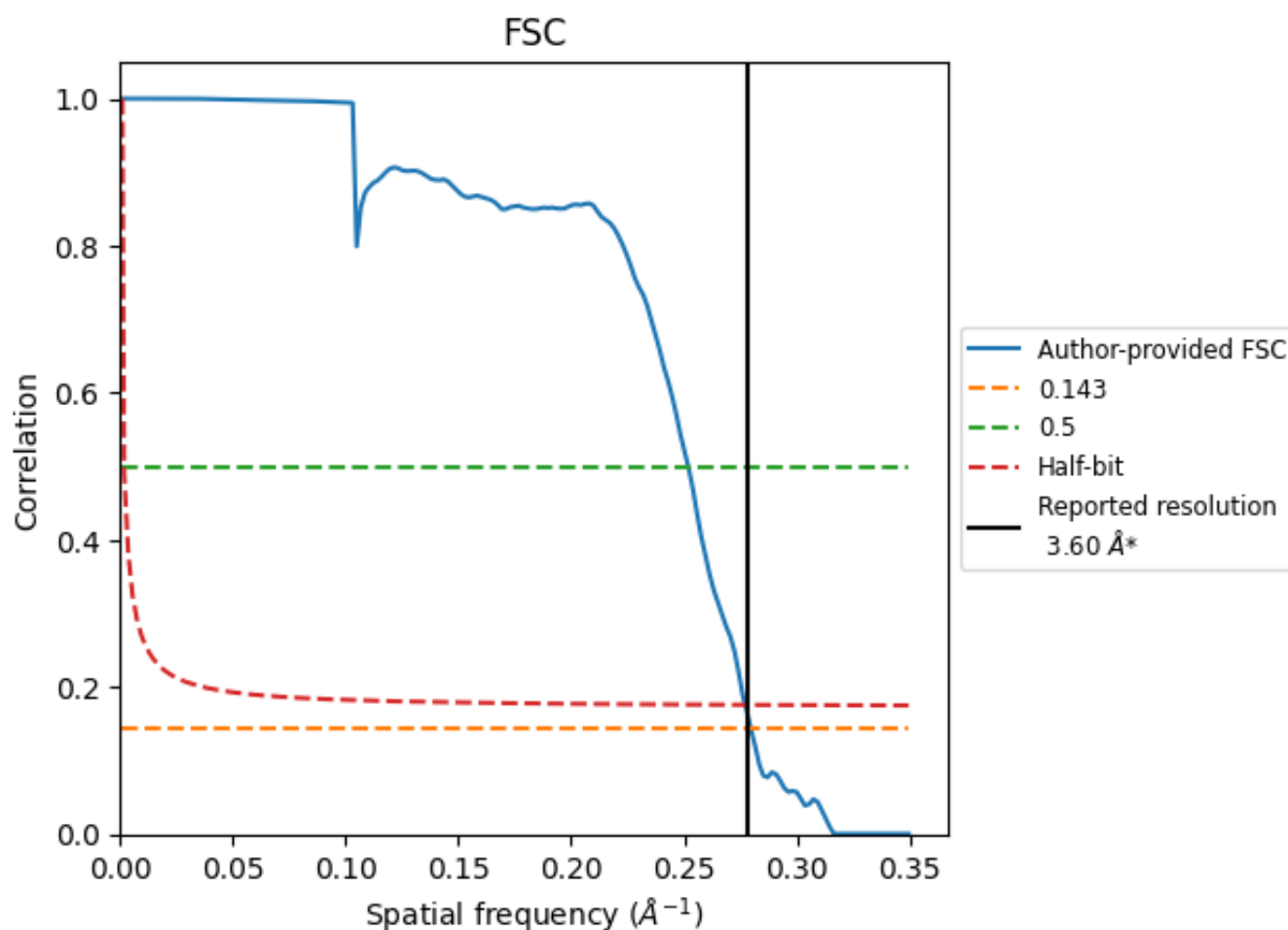


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

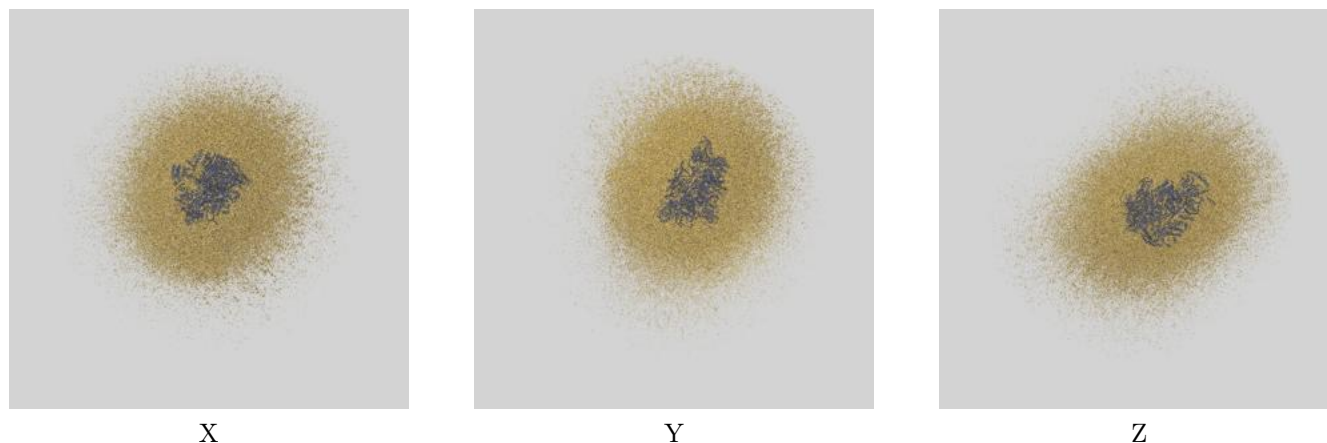
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.97	3.61
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

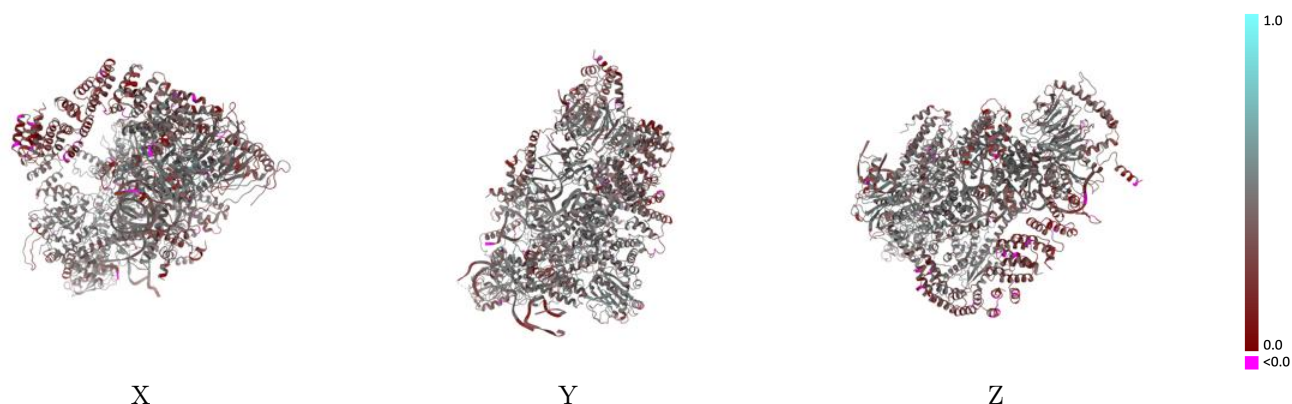
This section contains information regarding the fit between EMDB map EMD-8014 and PDB model 5GAP. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



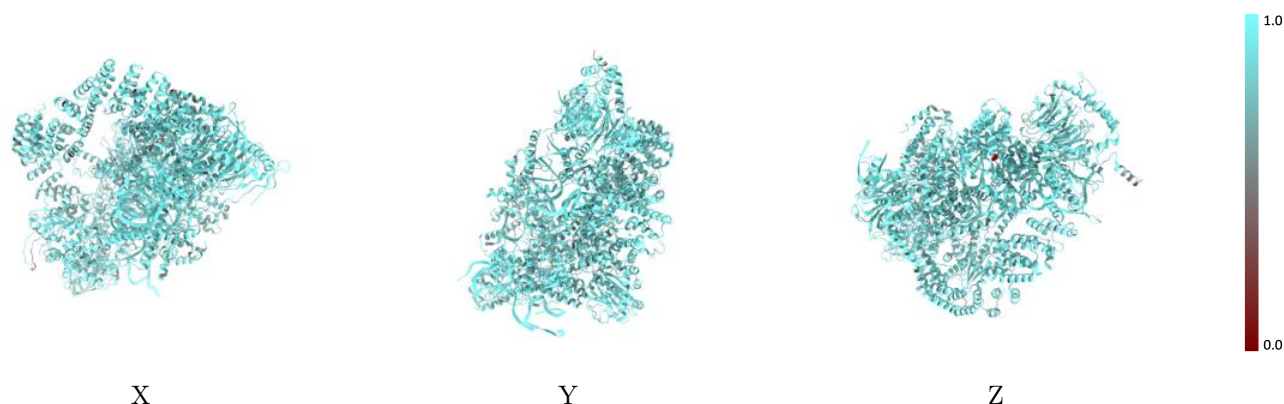
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



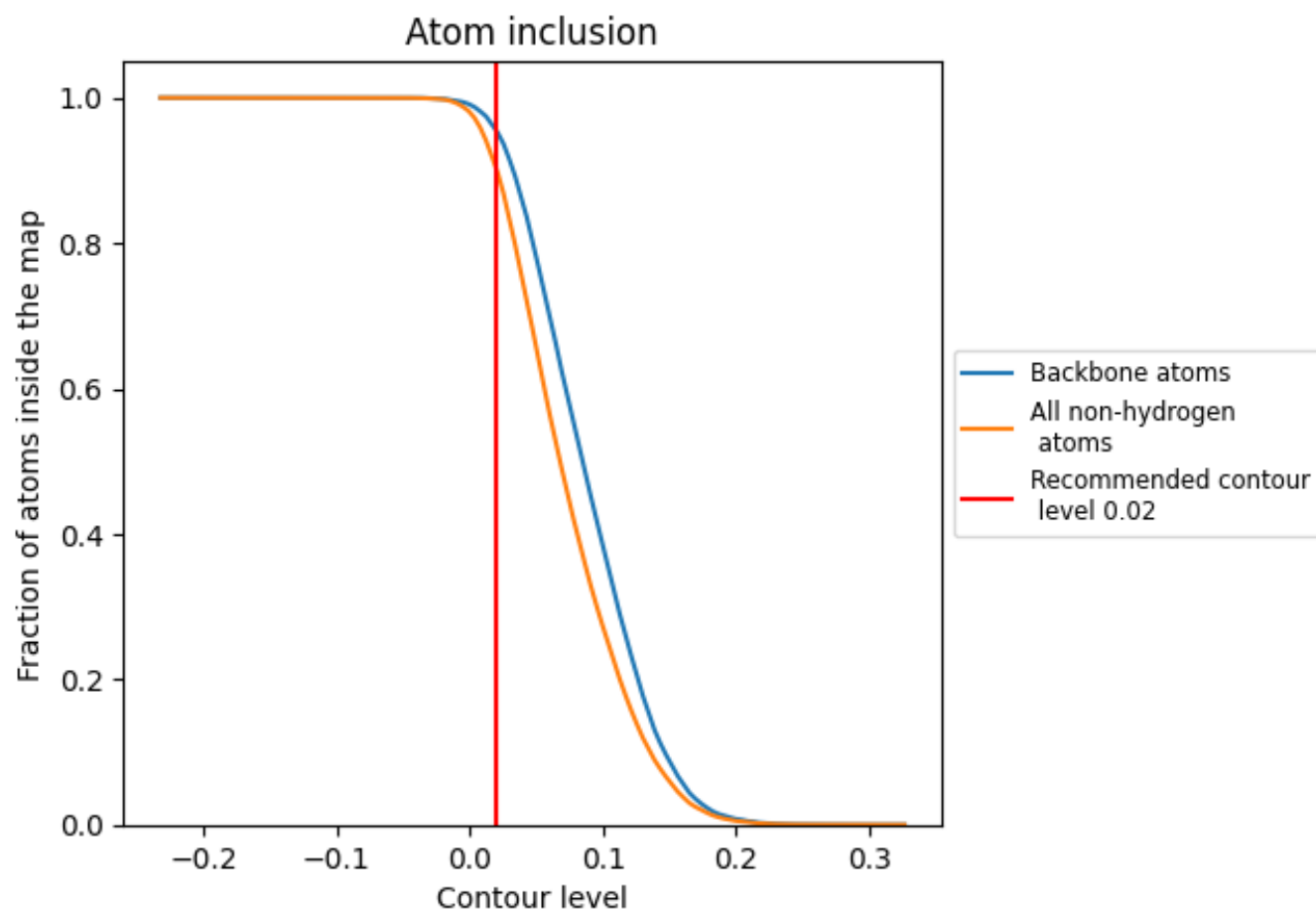
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9015	<div><div></div></div> 0.3970
A	<div><div></div></div> 0.9039	<div><div></div></div> 0.4340
B	<div><div></div></div> 0.8192	<div><div></div></div> 0.3180
D	<div><div></div></div> 0.8951	<div><div></div></div> 0.4260
F	<div><div></div></div> 0.8993	<div><div></div></div> 0.4110
G	<div><div></div></div> 0.8874	<div><div></div></div> 0.3770
H	<div><div></div></div> 0.8954	<div><div></div></div> 0.4080
J	<div><div></div></div> 0.8807	<div><div></div></div> 0.3130
K	<div><div></div></div> 0.9134	<div><div></div></div> 0.4670
U	<div><div></div></div> 0.9251	<div><div></div></div> 0.2810
V	<div><div></div></div> 0.9670	<div><div></div></div> 0.4390
W	<div><div></div></div> 0.9639	<div><div></div></div> 0.3760
x	<div><div></div></div> 0.9390	<div><div></div></div> 0.4020

1.0

0.0

<0.0