



## wwPDB EM Validation Summary Report ⓘ

Jun 29, 2024 – 10:12 am BST

PDB ID : 8QPA  
EMDB ID : EMD-18546  
Title : Cryo-EM Structure of Pre-B+5'ssLNG Complex (core part)  
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.  
Deposited on : 2023-10-01  
Resolution : 3.70 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:

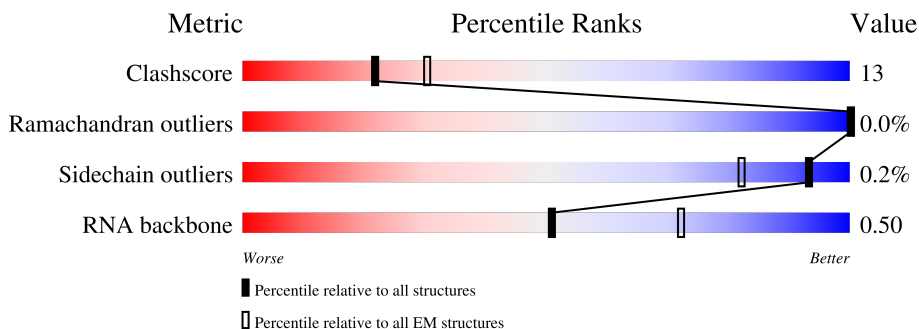
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (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 3.70 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	B	2136	99%
2	G	820	6% 10% 5% 85%
3	J	683	8% 25% 88%
4	L	499	25% 51% 24% 25%
5	F	522	6% 6% 88%
6	N	941	22% 39% 10% 51%
7	A	2335	8% 58% 27% 16%

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Mol	Chain	Length	Quality of chain
8	U	565	
9	S	800	
10	C	972	
11	M	128	
12	D	142	
13	5	117	
14	z	18	
15	7	793	
16	4	144	
17	6	106	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 43455 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 U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	22	158	97	28	32	1	0	0

- Molecule 2 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	122	1077	673	205	197	2	0	0

- Molecule 3 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	85	678	416	139	120	3	0	0

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	376	2874	1788	524	550	12	0	0

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	61	488	297	97	93	1	0	0

- Molecule 6 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	457	3095	1902	591	595	7	0	0

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	1971	16383	10554	2858	2901	70	0	0

- Molecule 8 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	U	456	3749	2427	635	673	14	0	0

- Molecule 9 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	148	1167	727	216	222	2	0	0

- Molecule 10 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	836	6592	4211	1110	1238	33	0	0

- Molecule 11 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	124	962	608	171	178	5	0	0

- Molecule 12 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	141	1170	751	194	215	10	0	0

- Molecule 13 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	5	79	1660	744	275	562	79	0	0

- Molecule 14 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	z	18	384	172	69	125	18	0	0

- Molecule 15 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	7	81	650	405	115	128	2	0	0

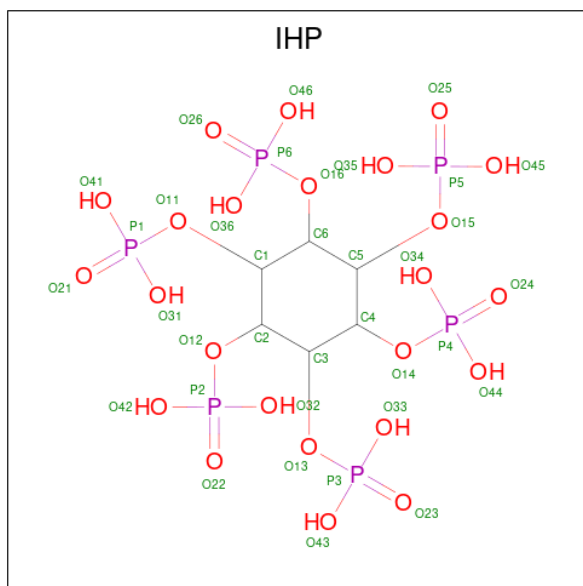
- Molecule 16 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	4	62	1322	590	233	437	62	0	0

- Molecule 17 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	6	47	1010	453	194	317	46	0	0

- Molecule 18 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	A	1	36	6	24	6	0

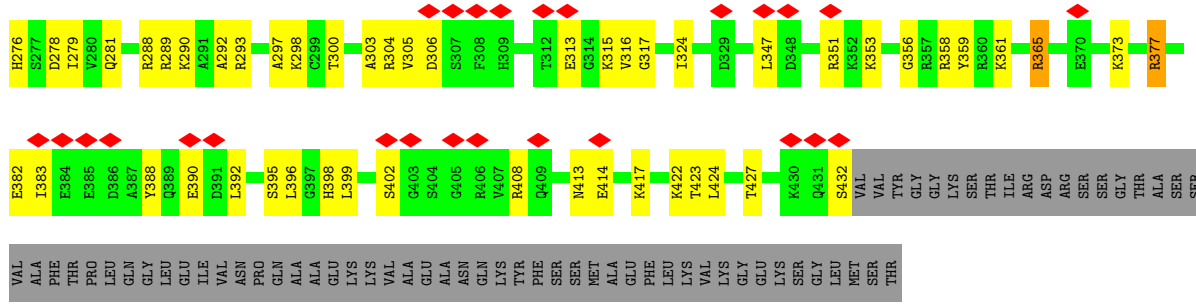




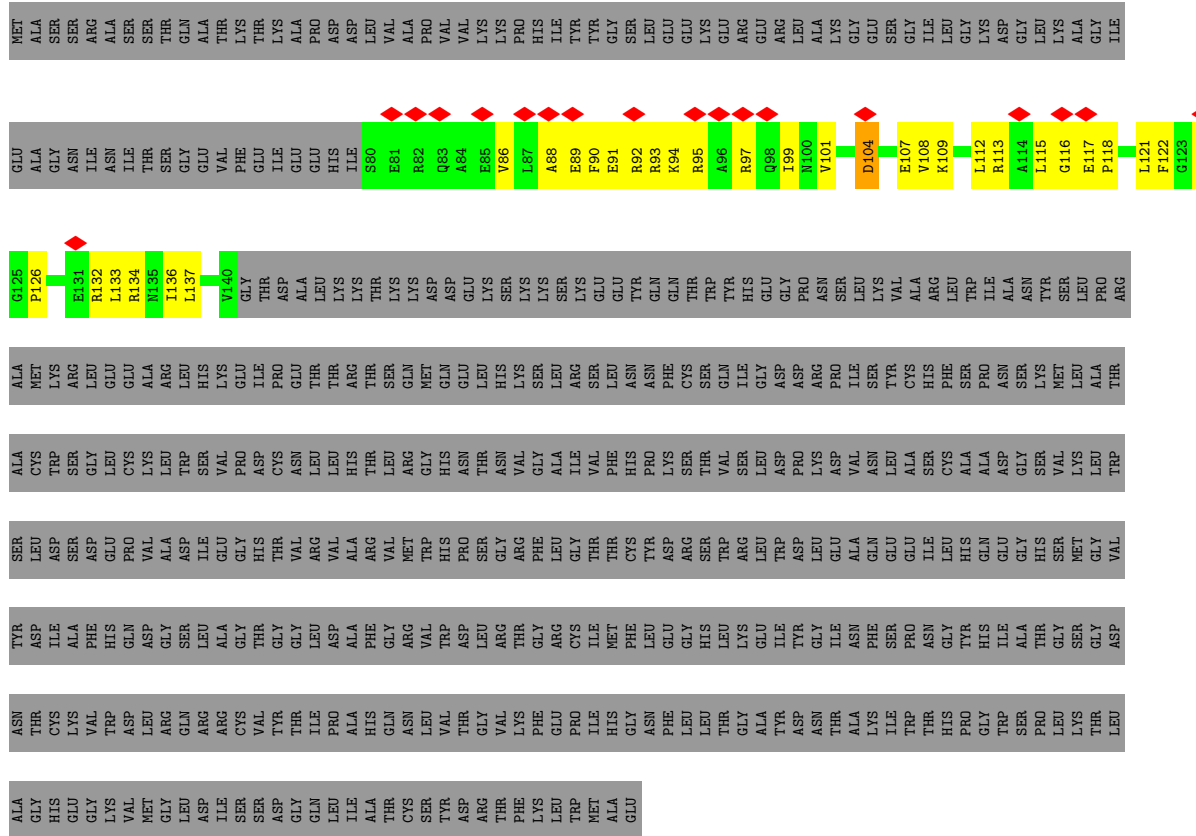




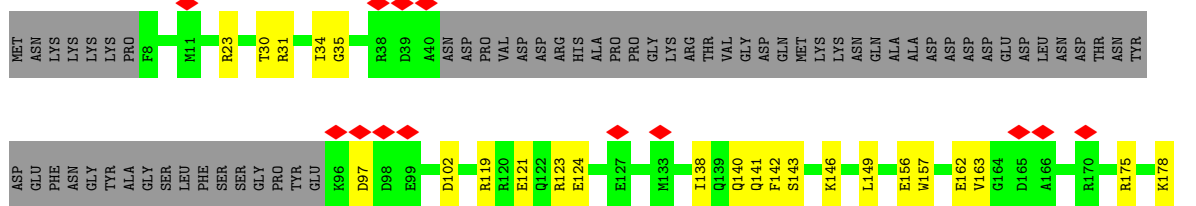
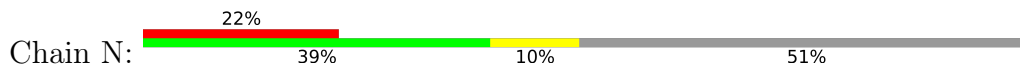


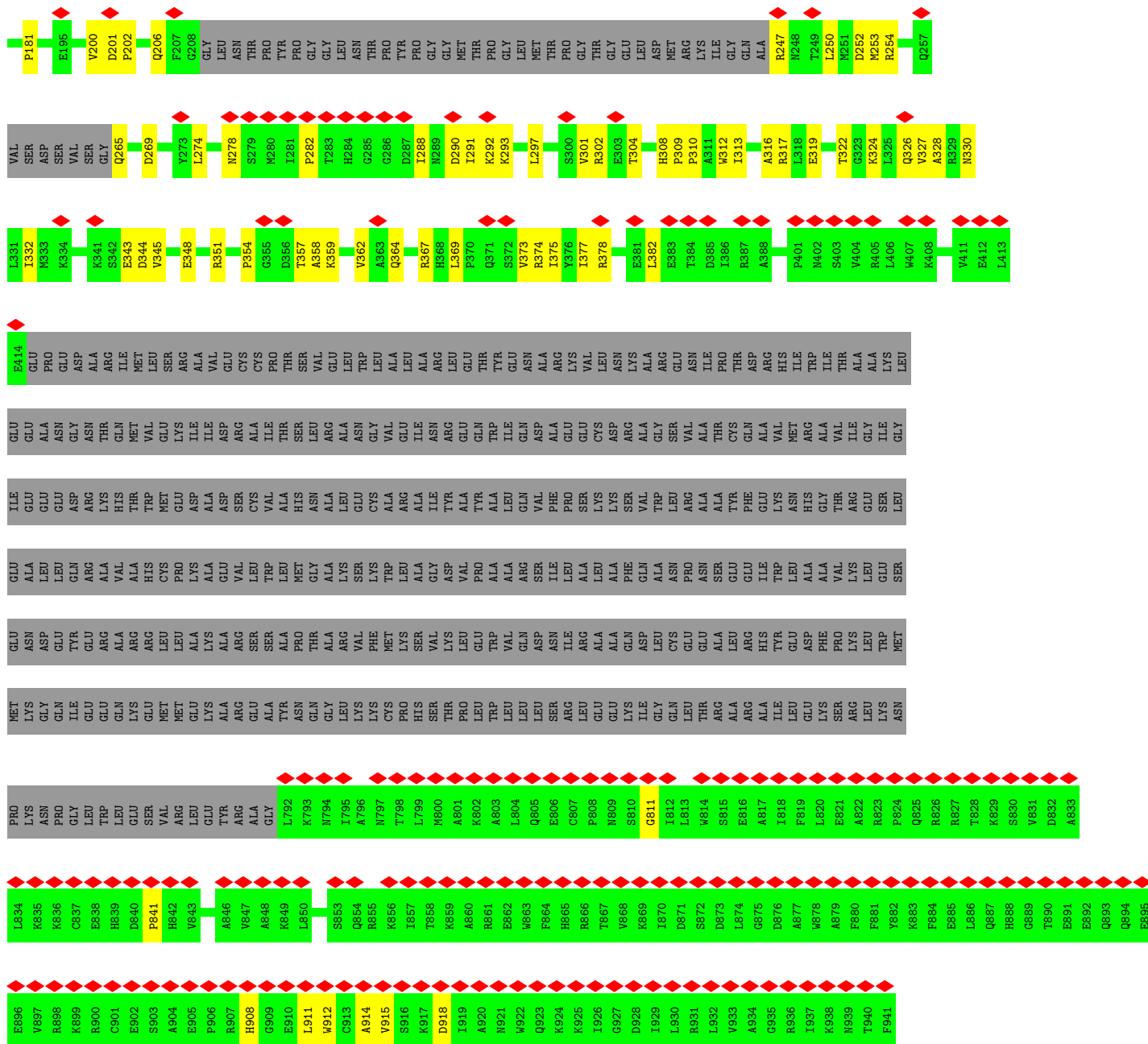


• Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp4

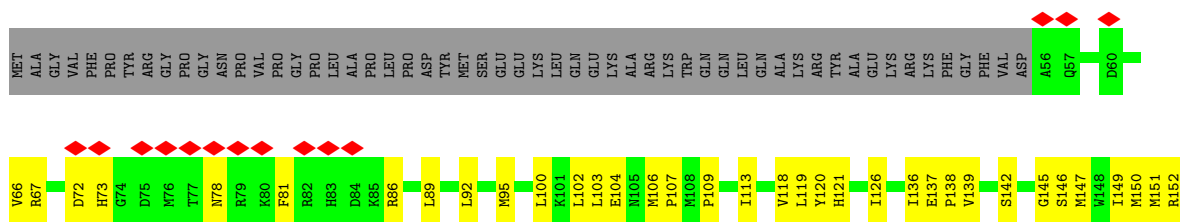


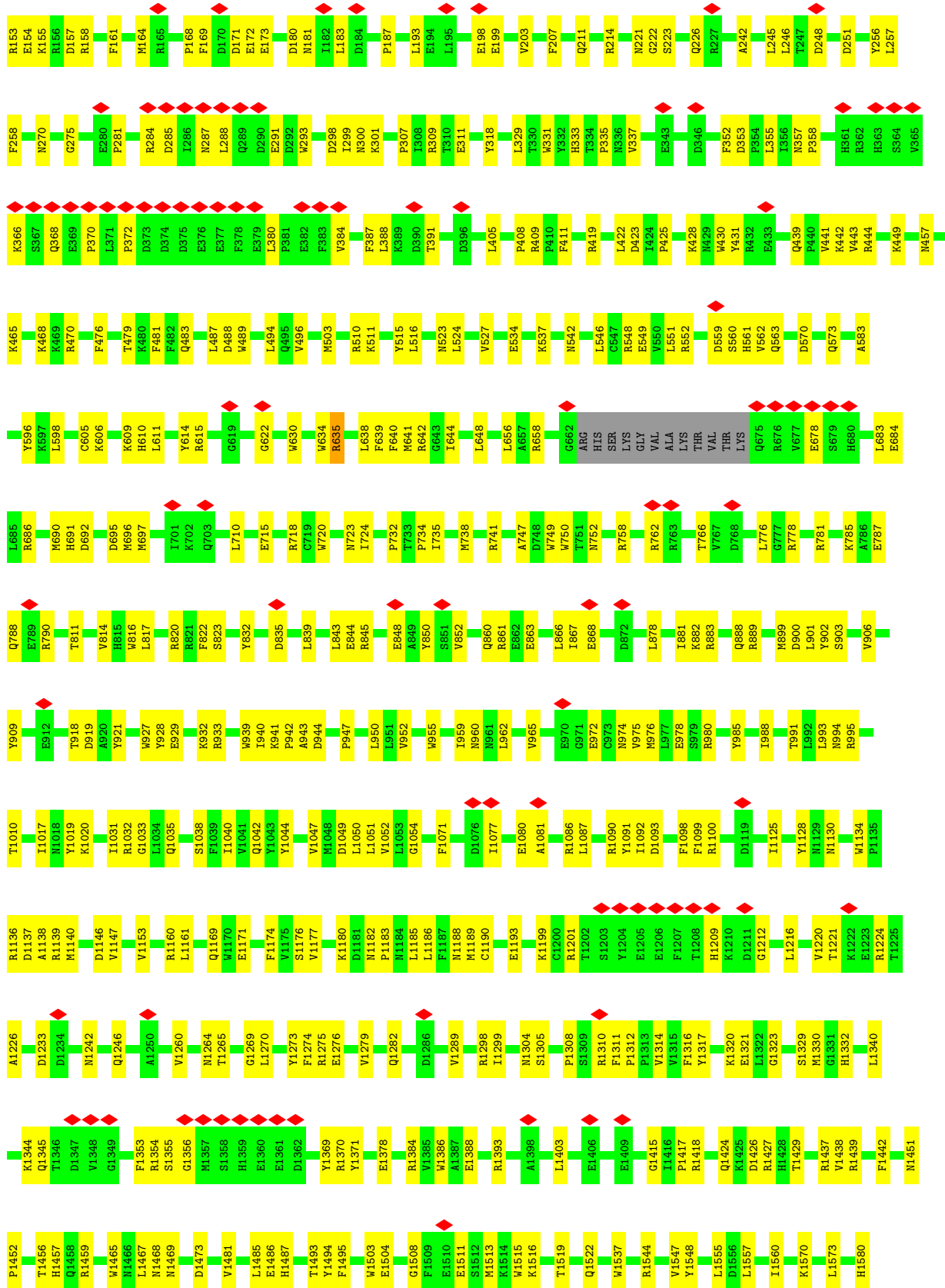
• Molecule 6: Pre-mRNA-processing factor 6





● Molecule 7: Pre-mRNA-processing-splicing factor 8



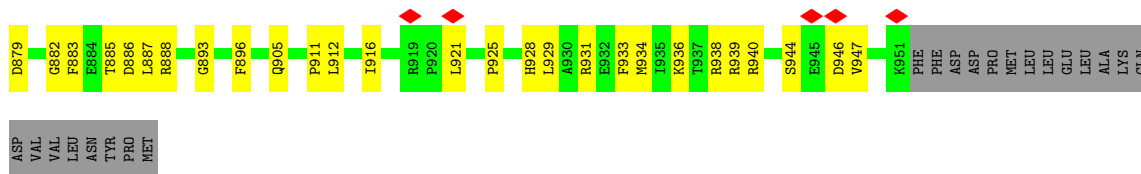




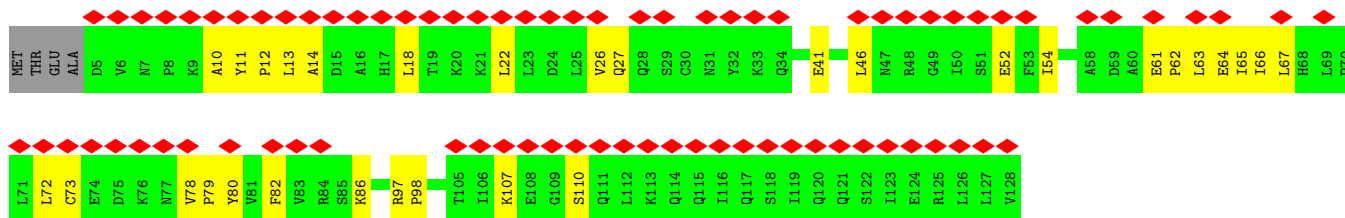
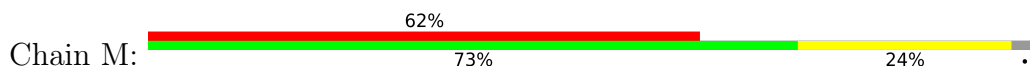




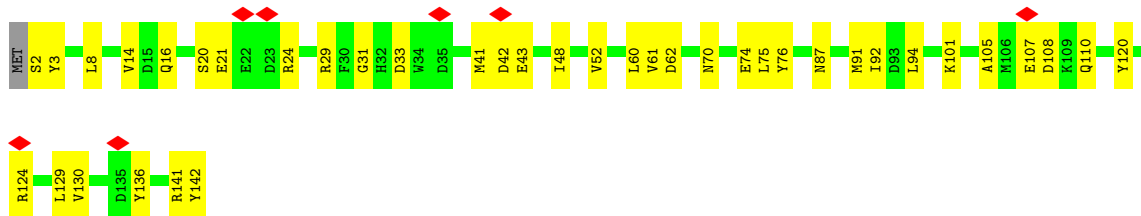




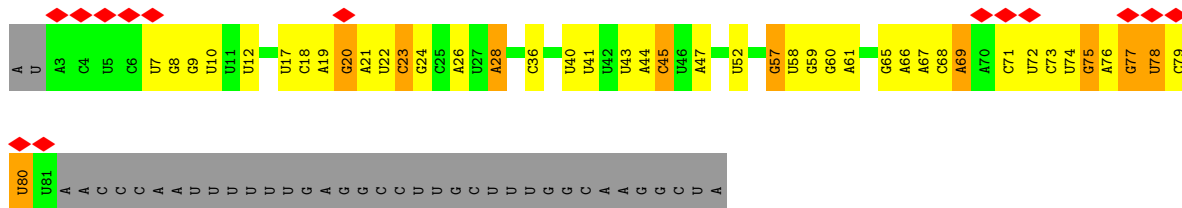
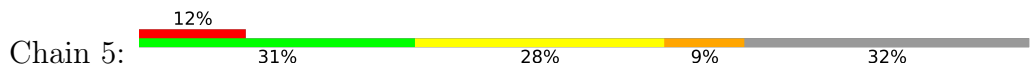
• Molecule 11: NHP2-like protein 1, N-terminally processed



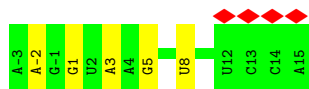
• Molecule 12: Thioredoxin-like protein 4A



• Molecule 13: U5 snRNA



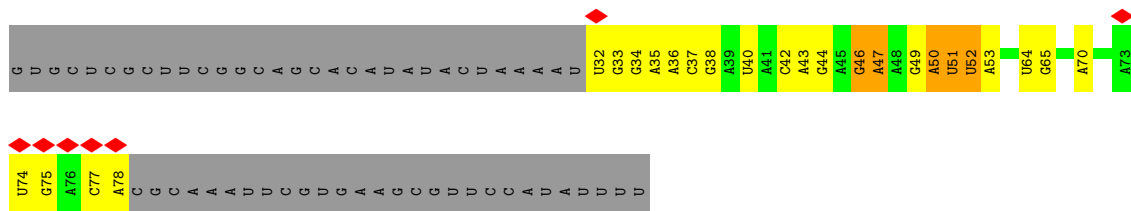
• Molecule 14: 5'ss oligo



• Molecule 15: Splicing factor 3A subunit 1







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136333	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.031	Depositor
Map size ( $\text{\AA}$ )	556.8, 556.8, 556.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.16, 1.16, 1.16	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: IHP

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	B	0.23	0/158	0.60	0/209
2	G	0.24	0/1096	0.55	0/1455
3	J	0.26	0/685	0.57	0/911
4	L	0.25	0/2912	0.49	0/3924
5	F	0.27	0/491	0.66	0/657
6	N	0.24	0/3136	0.51	0/4273
7	A	0.26	0/16830	0.50	0/22831
8	U	0.25	0/3845	0.48	0/5208
9	S	0.23	0/1175	0.51	0/1571
10	C	0.26	0/6739	0.49	0/9151
11	M	0.24	0/974	0.50	0/1316
12	D	0.26	0/1199	0.48	0/1620
13	5	0.20	0/1850	0.77	0/2875
14	z	0.20	0/429	0.74	0/666
15	7	0.25	0/659	0.53	0/884
16	4	0.20	0/1477	0.69	0/2300
17	6	0.20	0/1133	0.71	0/1766
All	All	0.25	0/44788	0.53	0/61617

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	B	158	0	166	9	0
2	G	1077	0	1066	28	0
3	J	678	0	711	24	0
4	L	2874	0	2856	94	0
5	F	488	0	499	29	0
6	N	3095	0	2612	81	0
7	A	16383	0	16318	484	0
8	U	3749	0	3769	111	0
9	S	1167	0	1182	23	0
10	C	6592	0	6615	185	0
11	M	962	0	1012	29	0
12	D	1170	0	1141	28	0
13	5	1660	0	842	25	0
14	z	384	0	194	0	0
15	7	650	0	655	18	0
16	4	1322	0	666	28	0
17	6	1010	0	512	17	0
18	A	36	0	6	0	0
All	All	43455	0	40822	1060	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 13.

The worst 5 of 1060 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)
6:N:378:ARG:O	6:N:382:LEU:HB2	1.72	0.89
7:A:752:ASN:HD22	8:U:462:PHE:HB3	1.39	0.88
7:A:942:PRO:HG2	7:A:1042:GLN:HE22	1.40	0.87
8:U:460:ASN:HD21	8:U:465:GLU:HG2	1.45	0.81
17:6:42:C:H2'	17:6:43:A:C8	2.16	0.80

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	
1	B	20/2136 (1%)	20 (100%)	0	0	100	100
2	G	118/820 (14%)	117 (99%)	1 (1%)	0	100	100
3	J	83/683 (12%)	83 (100%)	0	0	100	100
4	L	372/499 (74%)	364 (98%)	8 (2%)	0	100	100
5	F	59/522 (11%)	56 (95%)	3 (5%)	0	100	100
6	N	447/941 (48%)	433 (97%)	14 (3%)	0	100	100
7	A	1965/2335 (84%)	1899 (97%)	65 (3%)	1 (0%)	51	83
8	U	454/565 (80%)	435 (96%)	19 (4%)	0	100	100
9	S	138/800 (17%)	138 (100%)	0	0	100	100
10	C	834/972 (86%)	803 (96%)	31 (4%)	0	100	100
11	M	122/128 (95%)	118 (97%)	4 (3%)	0	100	100
12	D	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
15	7	79/793 (10%)	78 (99%)	1 (1%)	0	100	100
All	All	4830/11336 (43%)	4675 (97%)	154 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	172	GLU

### 5.3.2 Protein sidechains [i](#)

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	B	17/1908 (1%)	17 (100%)	0	100	100
2	G	113/721 (16%)	113 (100%)	0	100	100
3	J	70/599 (12%)	70 (100%)	0	100	100
4	L	299/424 (70%)	296 (99%)	3 (1%)	76	86
5	F	52/442 (12%)	51 (98%)	1 (2%)	57	76
6	N	233/792 (29%)	233 (100%)	0	100	100
7	A	1786/2108 (85%)	1783 (100%)	3 (0%)	93	97
8	U	418/511 (82%)	417 (100%)	1 (0%)	93	97
9	S	121/681 (18%)	121 (100%)	0	100	100
10	C	738/866 (85%)	738 (100%)	0	100	100
11	M	108/111 (97%)	108 (100%)	0	100	100
12	D	129/130 (99%)	129 (100%)	0	100	100
15	7	71/709 (10%)	71 (100%)	0	100	100
All	All	4155/10002 (42%)	4147 (100%)	8 (0%)	93	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	270	MET
7	A	1641	ARG
7	A	409	ARG
5	F	104	ASP
7	A	635	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
8	U	460	ASN
10	C	238	ASN
10	C	306	ASN
9	S	291	ASN
7	A	1583	GLN

### 5.3.3 RNA [i](#)



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	5	78/117 (66%)	25 (32%)	2 (2%)
14	z	17/18 (94%)	5 (29%)	0
16	4	61/144 (42%)	17 (27%)	0
17	6	46/106 (43%)	10 (21%)	3 (6%)
All	All	202/385 (52%)	57 (28%)	5 (2%)

5 of 57 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	5	8	G
13	5	9	G
13	5	10	U
13	5	20	G
13	5	21	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	5	77	G
13	5	78	U
17	6	46	G
17	6	51	U
17	6	77	C

## 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](#)

1 ligand is 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	$\# Z  > 2$
18	IHP	A	2401	-	36,36,36	0.73	0	54,60,60	1.05	2 (3%)

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
18	IHP	A	2401	-	-	3/30/54/54	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
18	A	2401	IHP	O14-C4-C5	2.20	113.88	108.69
18	A	2401	IHP	C3-C2-C1	2.03	114.86	110.41

There are no chirality outliers.

All (3) torsion outliers are listed below:

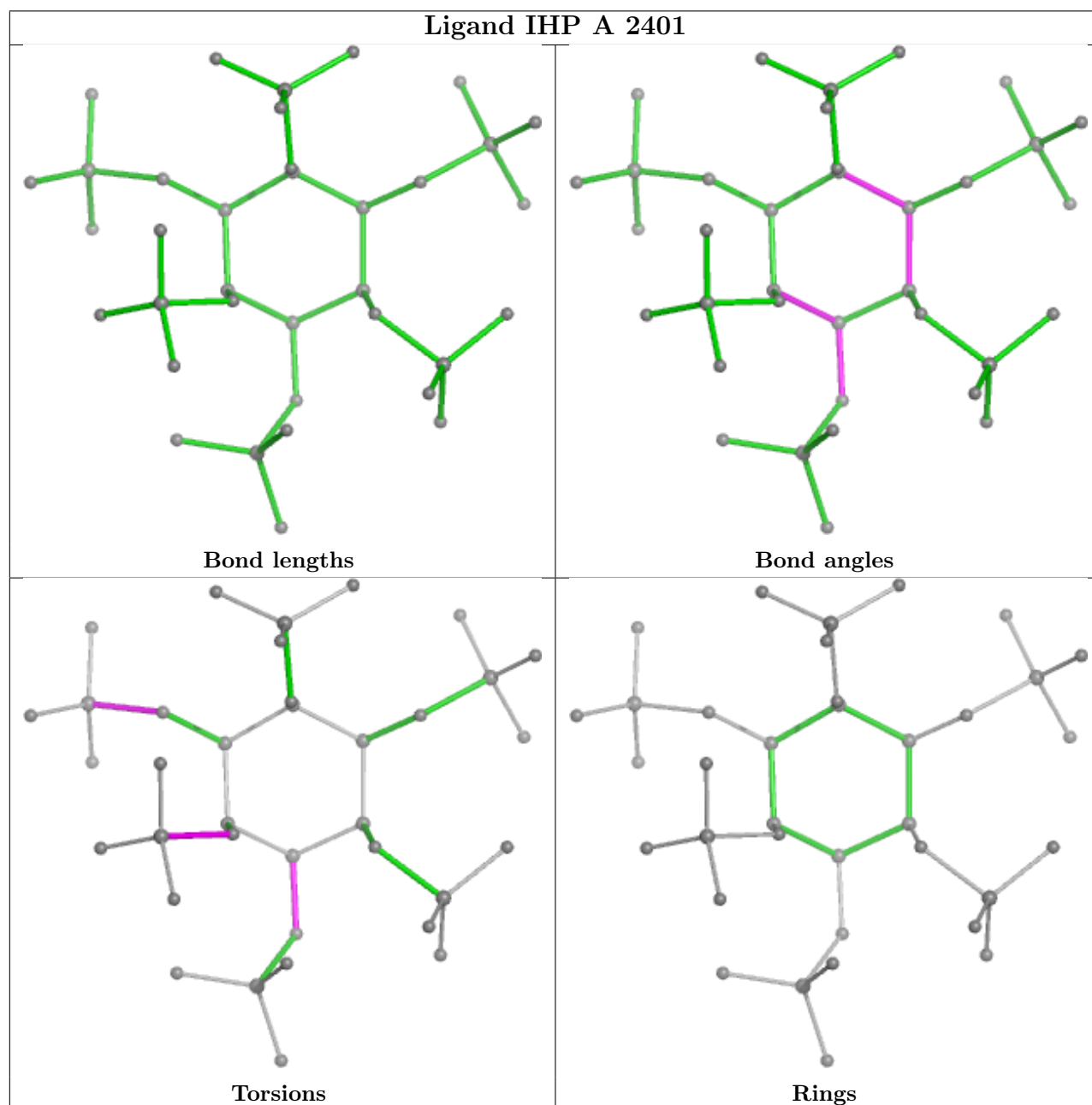
Mol	Chain	Res	Type	Atoms
18	A	2401	IHP	C5-C4-O14-P4
18	A	2401	IHP	C5-O15-P5-O25
18	A	2401	IHP	C6-O16-P6-O36

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

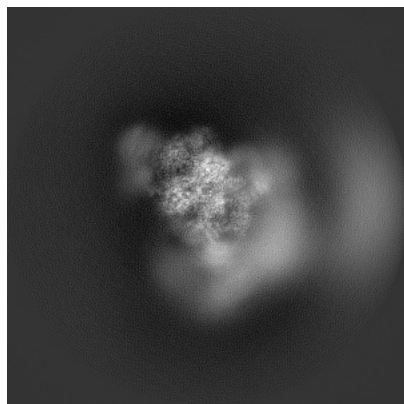
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18546. These allow visual inspection of the internal detail of the map and identification of artifacts.

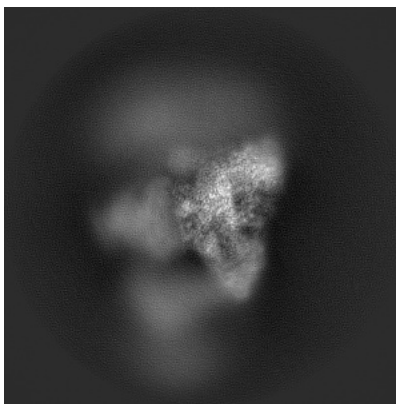
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

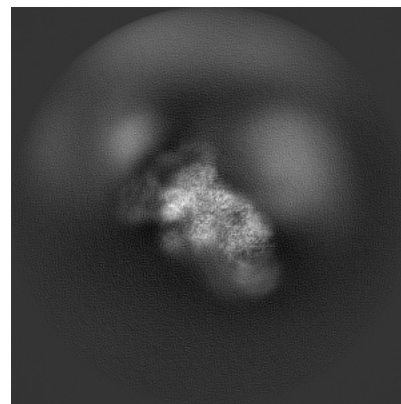
#### 6.1.1 Primary map



X

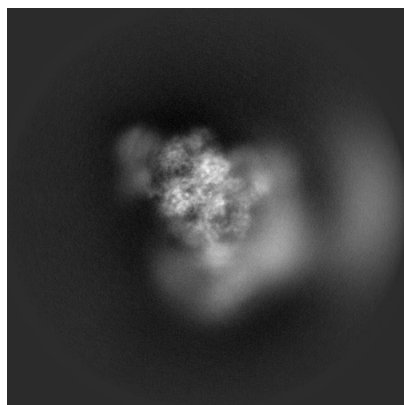


Y

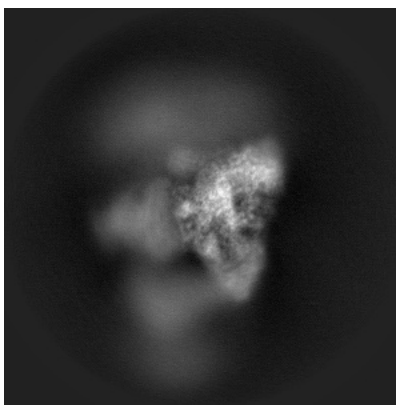


Z

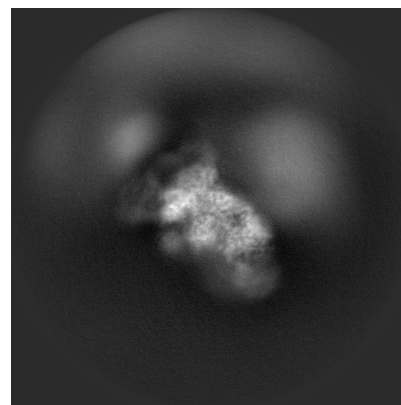
#### 6.1.2 Raw map



X



Y

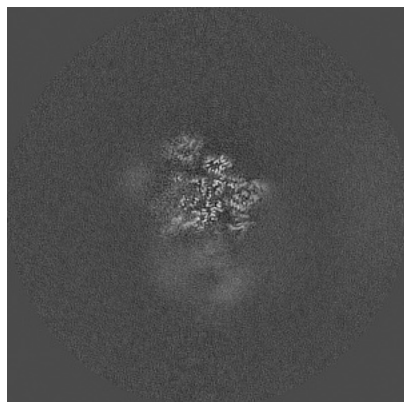


Z

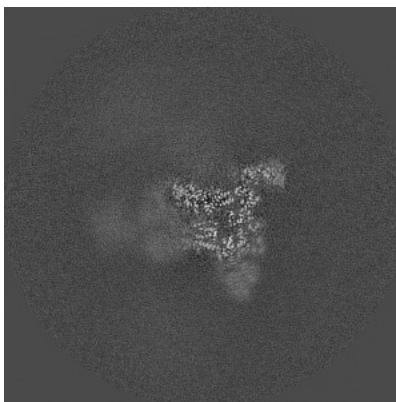
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

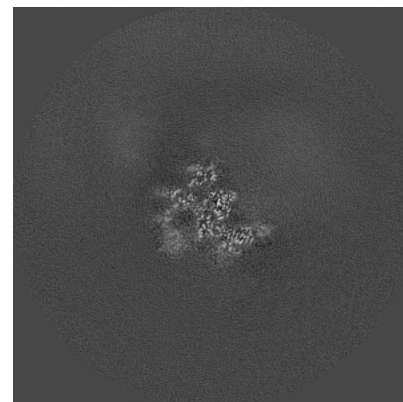
### 6.2.1 Primary map



X Index: 240

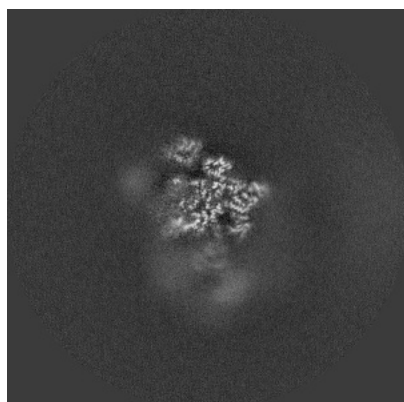


Y Index: 240

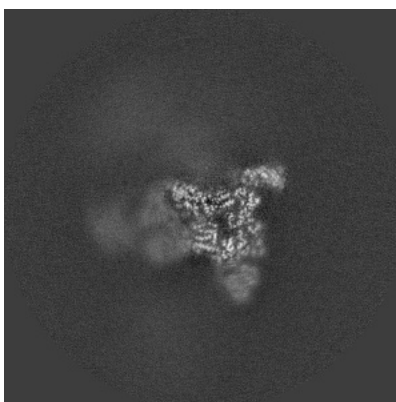


Z Index: 240

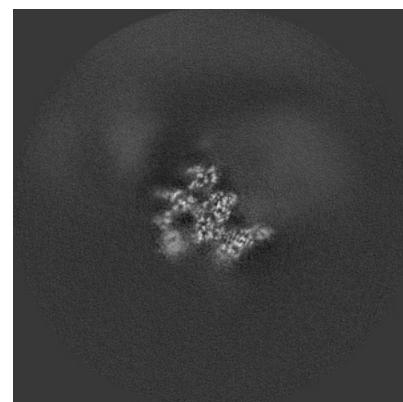
### 6.2.2 Raw map



X Index: 240



Y Index: 240

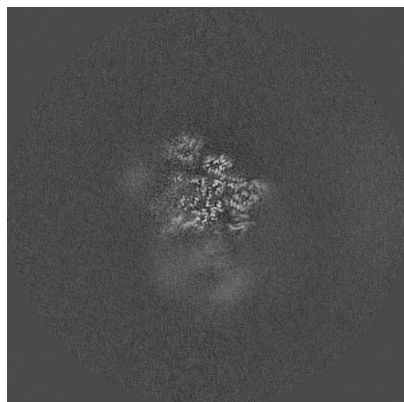


Z Index: 240

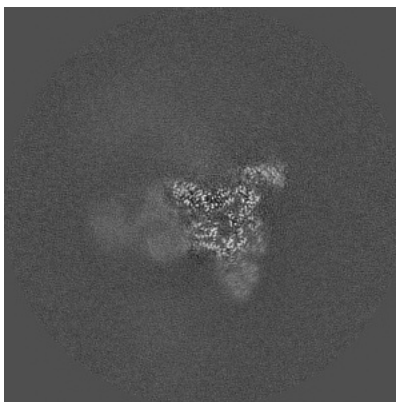
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

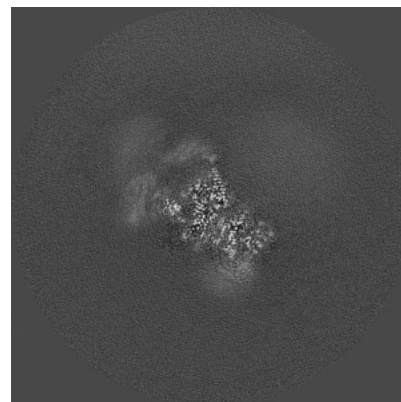
### 6.3.1 Primary map



X Index: 240

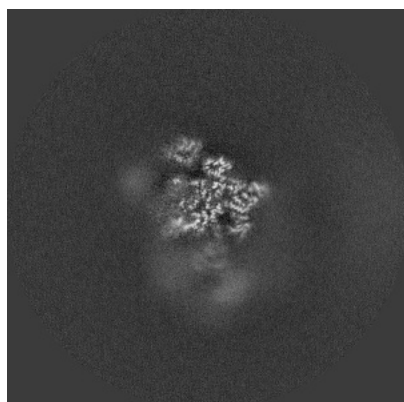


Y Index: 241

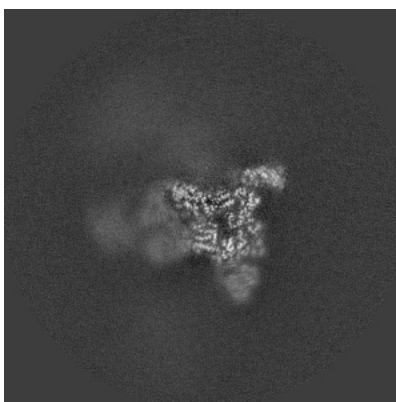


Z Index: 270

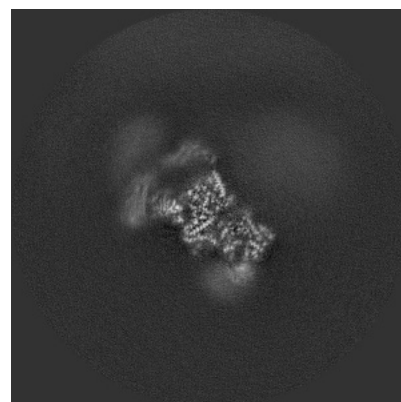
### 6.3.2 Raw map



X Index: 240



Y Index: 240



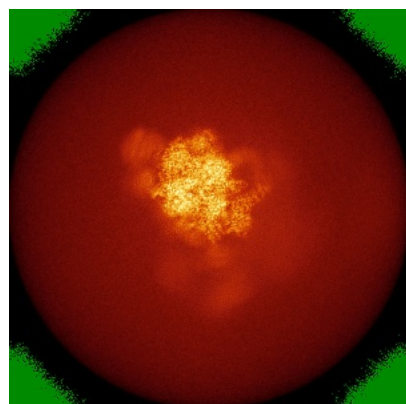
Z Index: 272

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

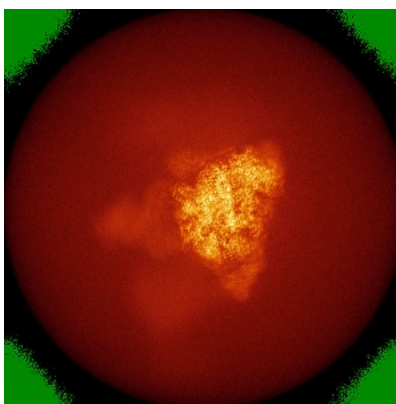


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

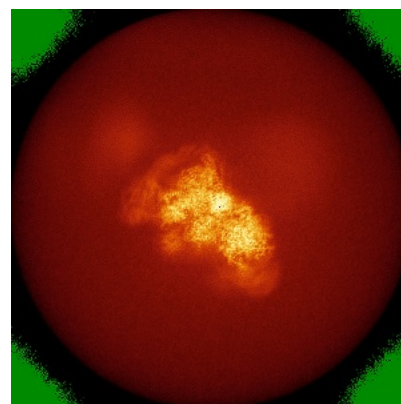
### 6.4.1 Primary map



X

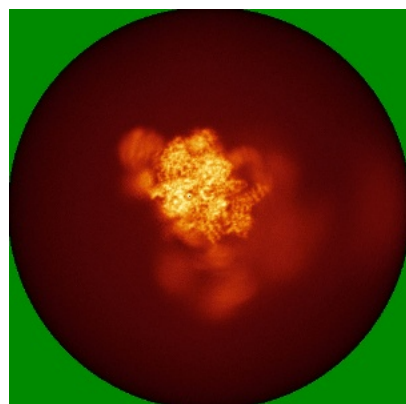


Y

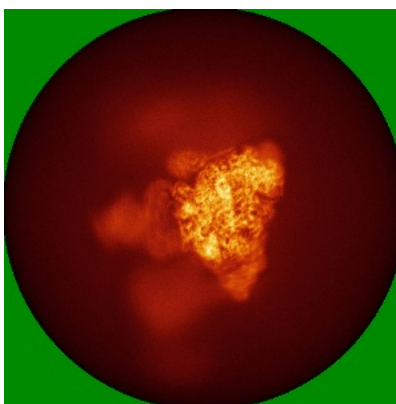


Z

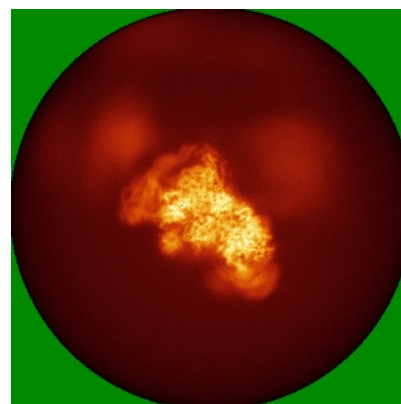
### 6.4.2 Raw map



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.

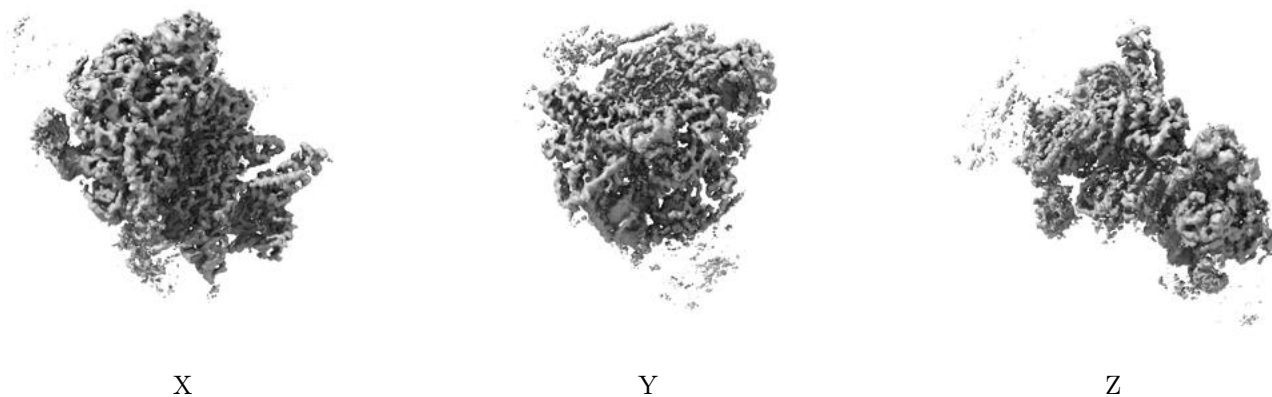
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.031. 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](#)

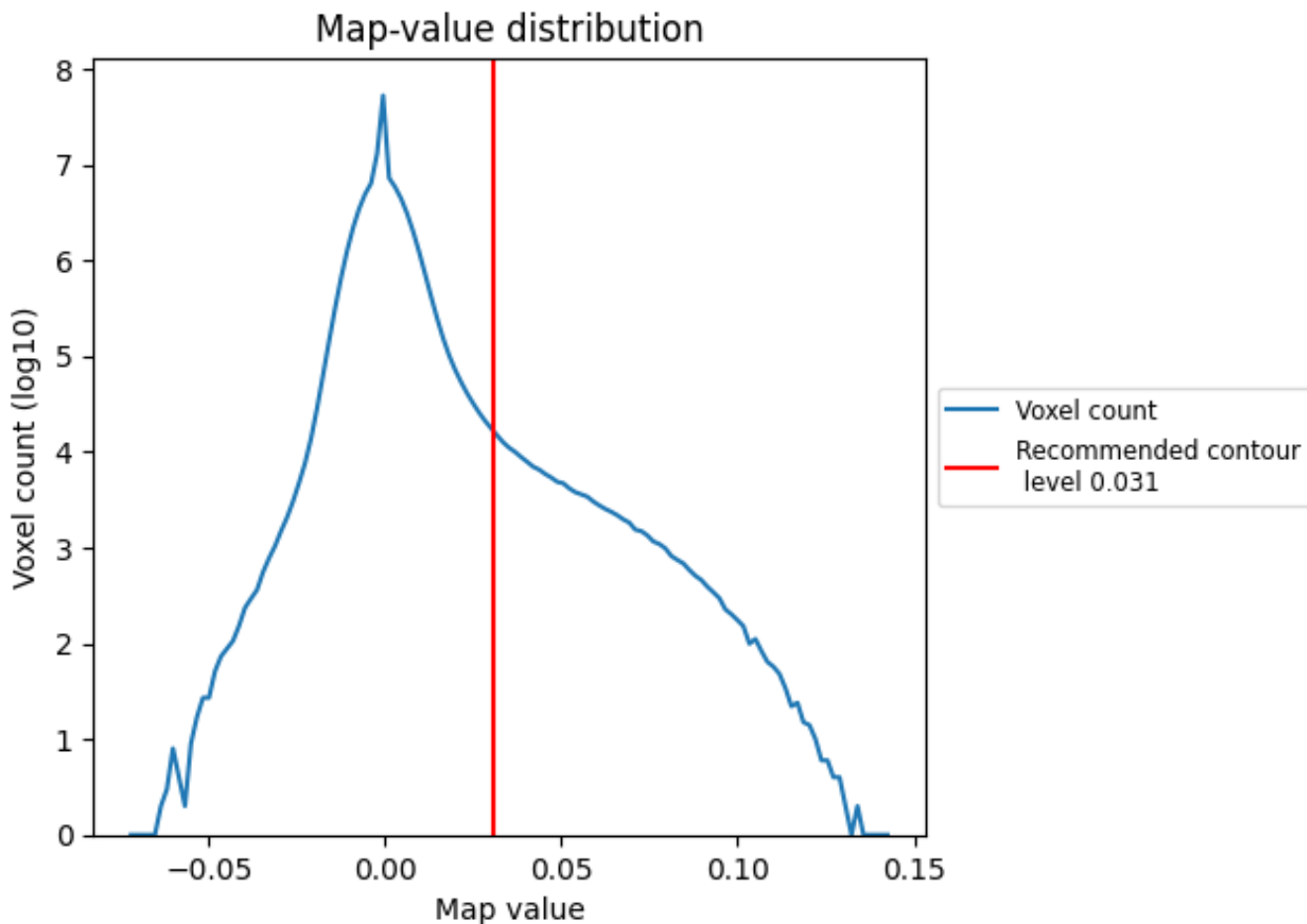
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

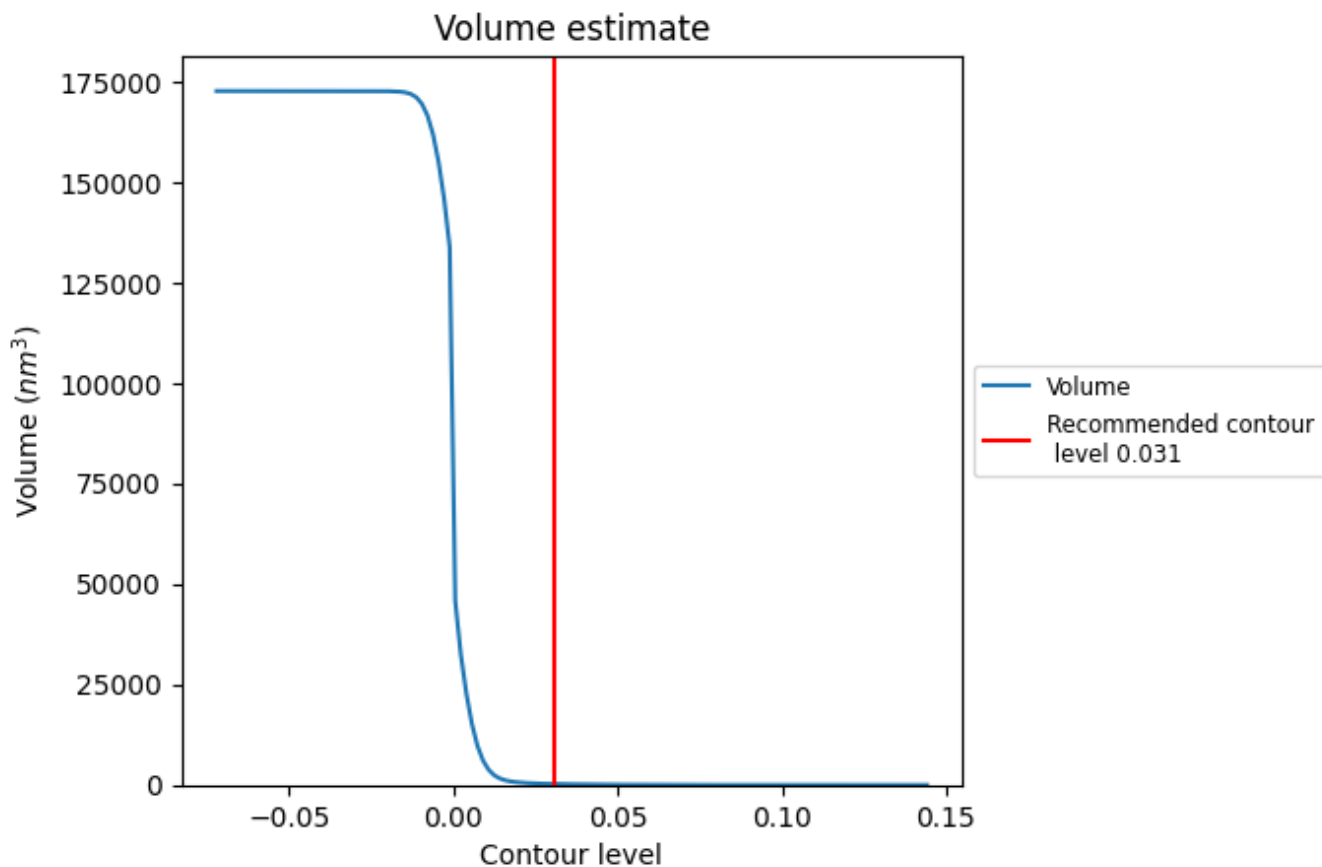
This section contains the results of statistical analysis of the map.

### 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.

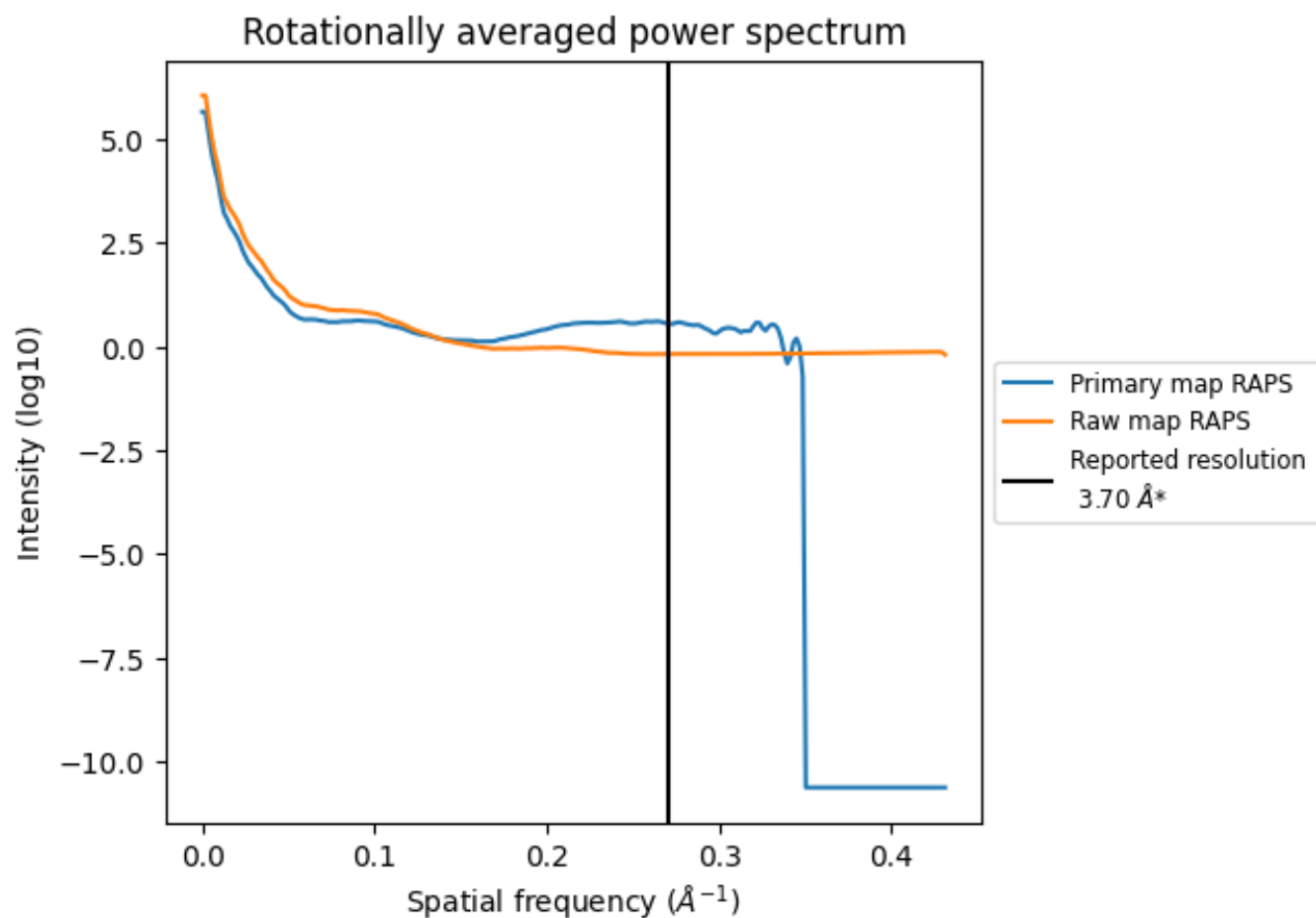
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm<sup>3</sup>; this corresponds to an approximate mass of 215 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 [i](#)

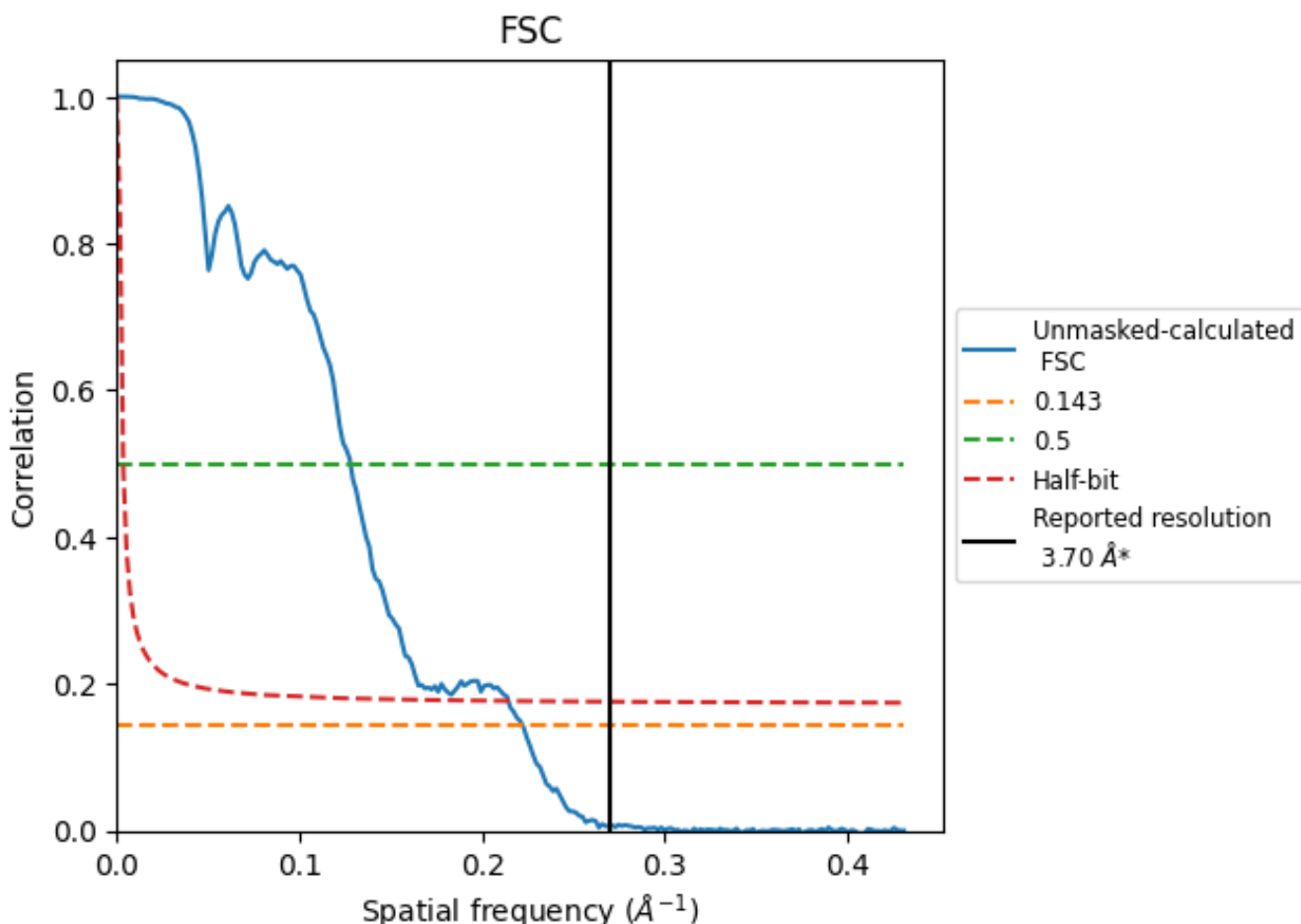


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

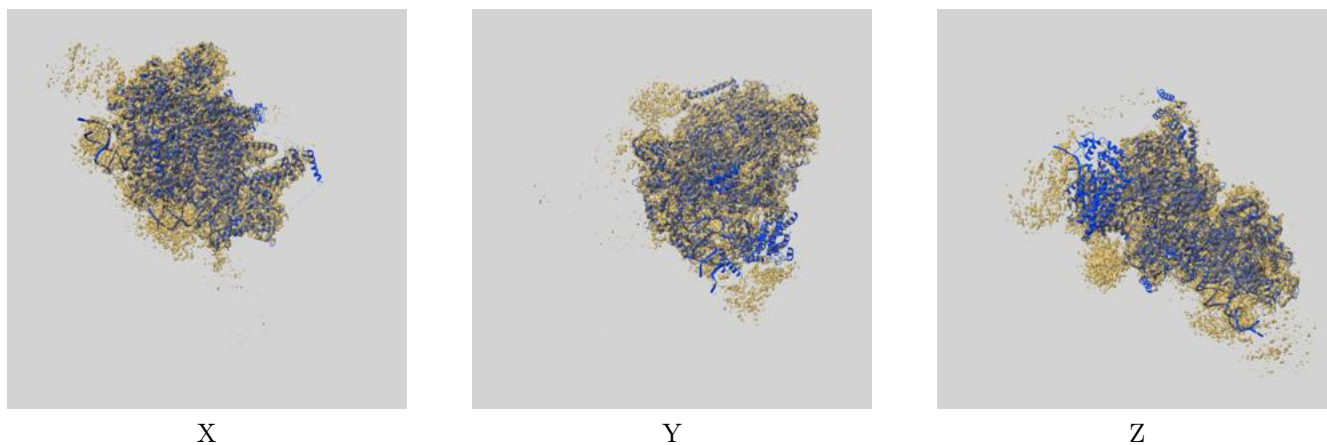
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	7.81	4.66

\*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 4.50 differs from the reported value 3.7 by more than 10 %

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

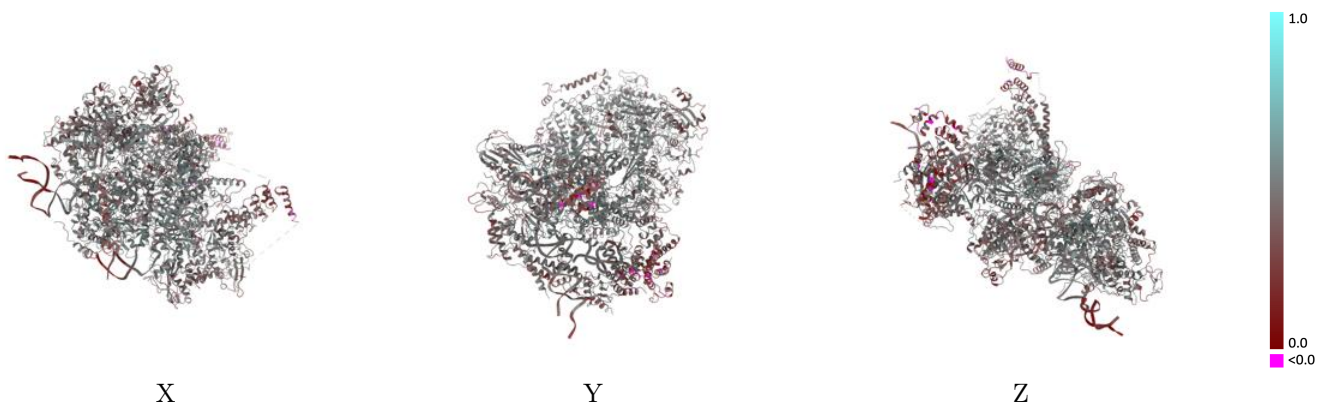
This section contains information regarding the fit between EMDB map EMD-18546 and PDB model 8QPA. Per-residue inclusion information can be found in section 3 on page 7.

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



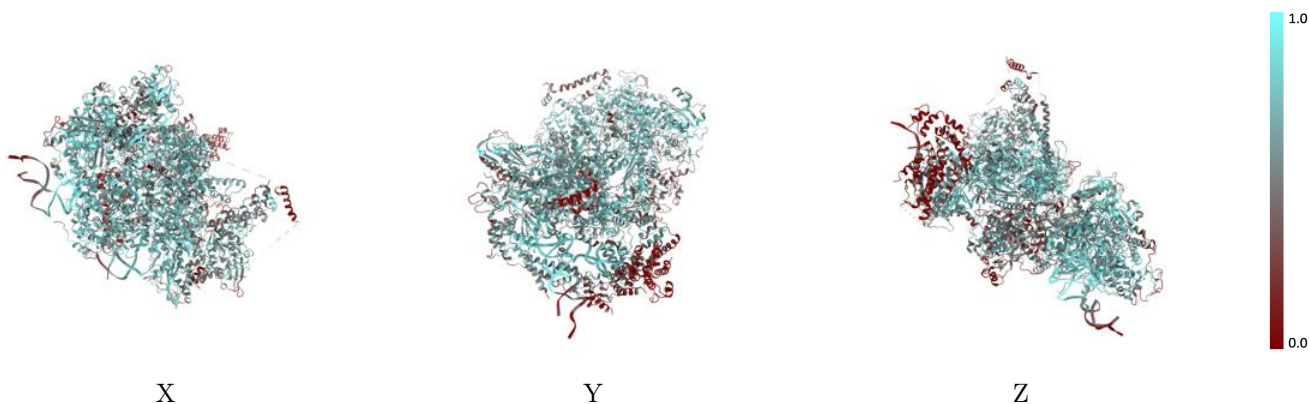
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



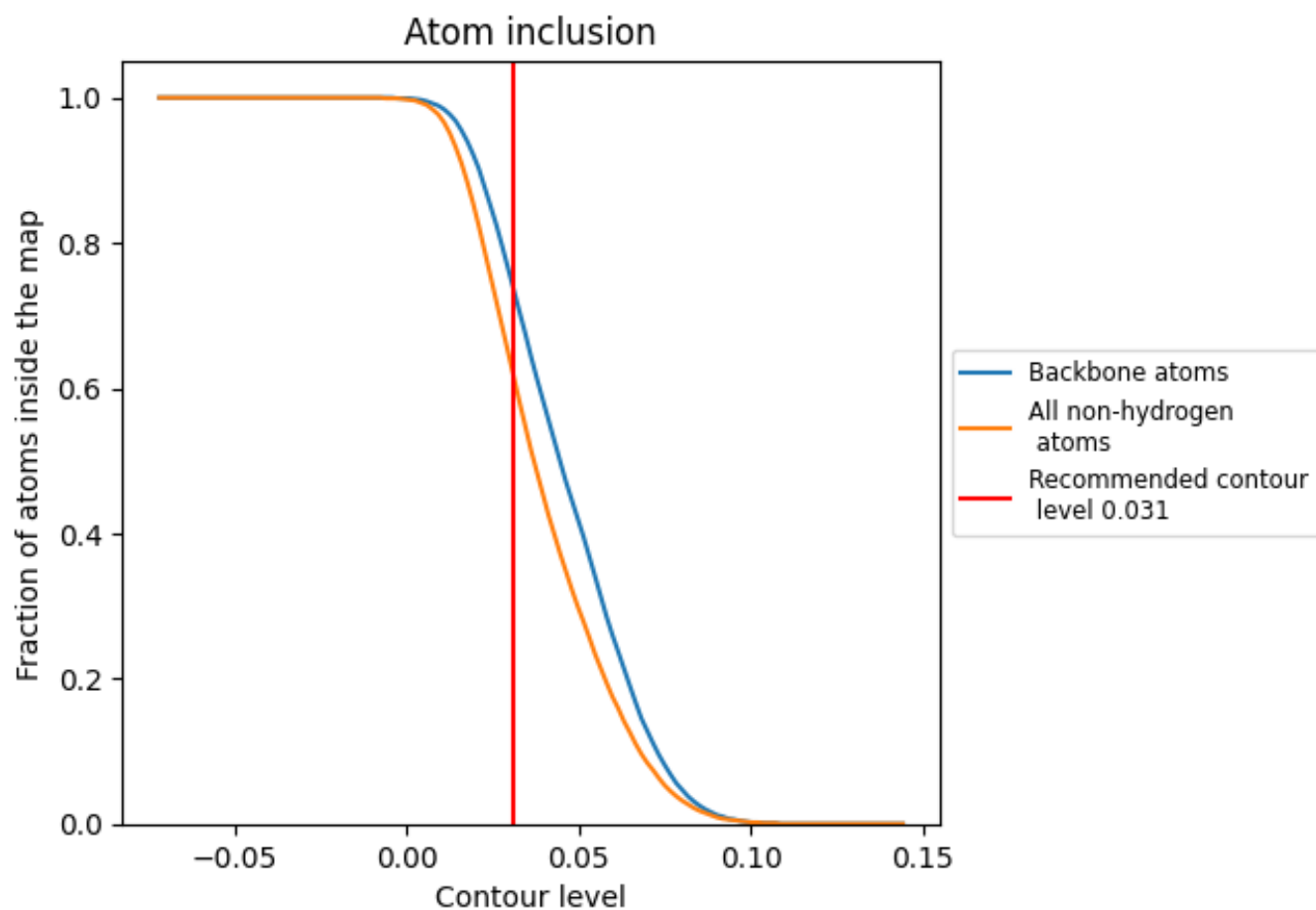
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.031).

## 9.4 Atom inclusion [i](#)







































At the recommended contour level, 74% of all backbone atoms, 62% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6150	 0.4390
4	 0.8200	 0.4640
5	 0.7390	 0.3960
6	 0.6960	 0.3970
7	 0.5510	 0.4130
A	 0.6920	 0.4740
B	 0.4360	 0.4480
C	 0.7080	 0.4540
D	 0.7260	 0.5050
F	 0.5080	 0.3480
G	 0.4550	 0.3950
J	 0.6530	 0.4490
L	 0.5240	 0.4130
M	 0.3140	 0.4010
N	 0.4730	 0.3870
S	 0.3720	 0.3700
U	 0.3380	 0.3960
z	 0.6740	 0.3540

