



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 03:29 PM JST

PDB ID : 5XON  
EMDB ID : EMD-6747  
Title : RNA Polymerase II elongation complex bound with Spt4/5 and TFIIS  
Authors : Ehara, H.; Yokoyama, T.; Shigematsu, H.; Shirouzu, M.; Sekine, S.  
Deposited on : 2017-05-29  
Resolution : 3.83 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

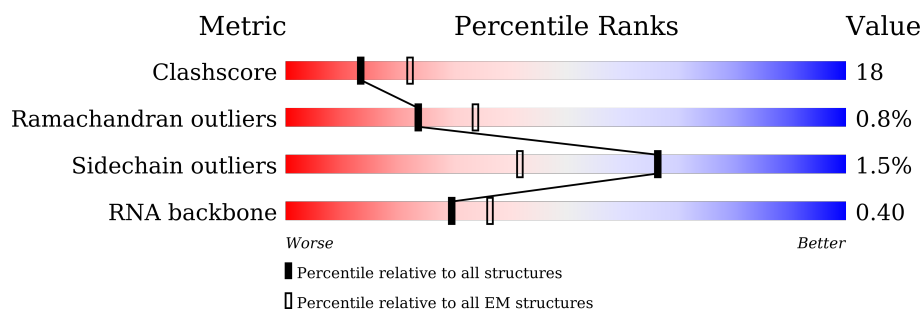
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.83 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.





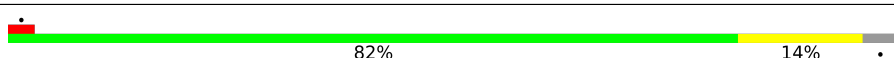
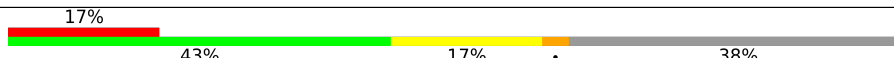



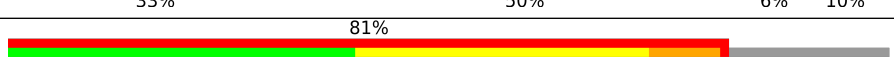
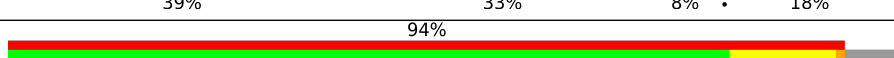

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	A	1743	
2	B	1227	
3	C	304	
4	D	186	
5	E	214	
6	F	155	
7	G	171	

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Mol	Chain	Length	Quality of chain
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	30	
14	T	48	
15	N	48	
16	U	190	
17	V	108	
18	W	612	

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 38369 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 DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1427	Total	C	N	O	S	0	0
			11239	7089	1958	2122	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1161	Total	C	N	O	S	0	0
			9261	5835	1636	1732	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MET	-	see sequence details	UNP C4QY79
I	2	ALA	-	see sequence details	UNP C4QY79
I	3	SER	MET	see sequence details	UNP C4QY79
I	4	PHE	THR	see sequence details	UNP C4QY79
I	5	ARG	ASN	see sequence details	UNP C4QY79
I	6	PHE	VAL	see sequence details	UNP C4QY79
I	7	CYS	ASN	see sequence details	UNP C4QY79
I	8	LEU	SER	see sequence details	UNP C4QY79
I	9	GLU	LEU	see sequence details	UNP C4QY79
I	10	CYS	SER	see sequence details	UNP C4QY79

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit, found in RNA polymerase complexes I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	67	ILE	SER	see sequence details	UNP C4QWA8
L	68	GLN	LYS	see sequence details	UNP C4QWA8
L	70	ASP	LEU	see sequence details	UNP C4QWA8
L	71	ALA	THR	see sequence details	UNP C4QWA8
L	72	ARG	THR	see sequence details	UNP C4QWA8

- Molecule 13 is a RNA chain called RNA (30-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			338	151	55	116	16		

- Molecule 14 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	48	Total	C	N	O	P	0	0
			975	463	179	285	48		

- Molecule 15 is a DNA chain called DNA (48-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	43	Total	C	N	O	P	0	0
			889	422	163	261	43		

- Molecule 16 is a protein called General transcription elongation factor TFIIS.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	155	Total	C	N	O	S	0	0
			1239	774	223	232	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	96	GLY	-	expression tag	UNP C4R2R6
U	97	PRO	-	expression tag	UNP C4R2R6
U	98	GLY	-	expression tag	UNP C4R2R6
U	266	ALA	ASP	conflict	UNP C4R2R6
U	267	ALA	GLU	conflict	UNP C4R2R6

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	expression tag	UNP C4R0E6

- Molecule 18 is a protein called Protein that forms a complex with Spt4p.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	329	Total	C	N	O	S	0	0
			2667	1698	483	485	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	204	GLY	-	expression tag	UNP C4R370
W	205	PRO	-	expression tag	UNP C4R370

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
19	C	1	Total 1	Zn 1	0
19	I	2	Total 2	Zn 2	0
19	J	1	Total 1	Zn 1	0
19	L	1	Total 1	Zn 1	0
19	U	1	Total 1	Zn 1	0
19	V	1	Total 1	Zn 1	0

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total 1	Mg 1	0



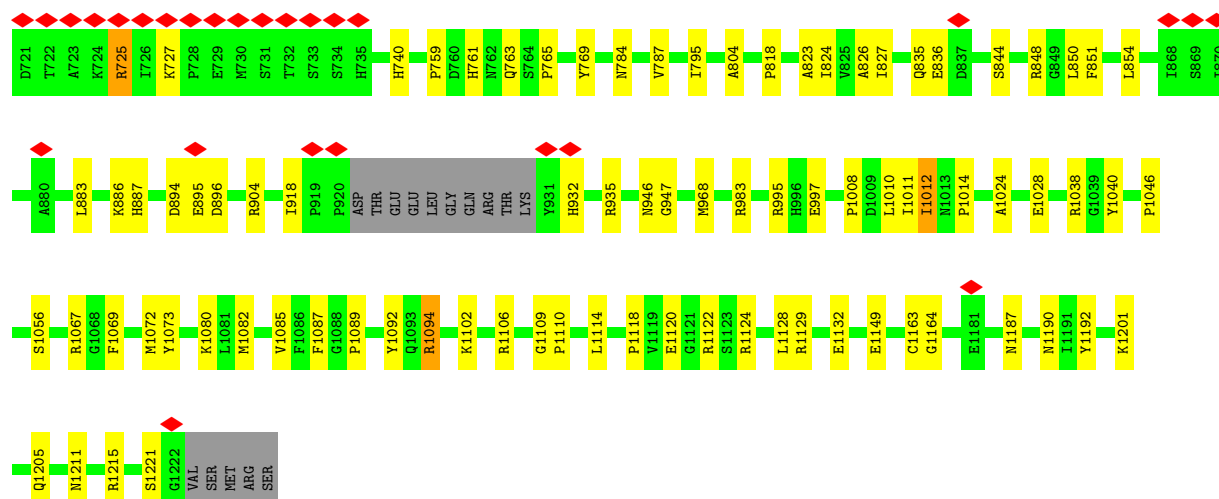
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

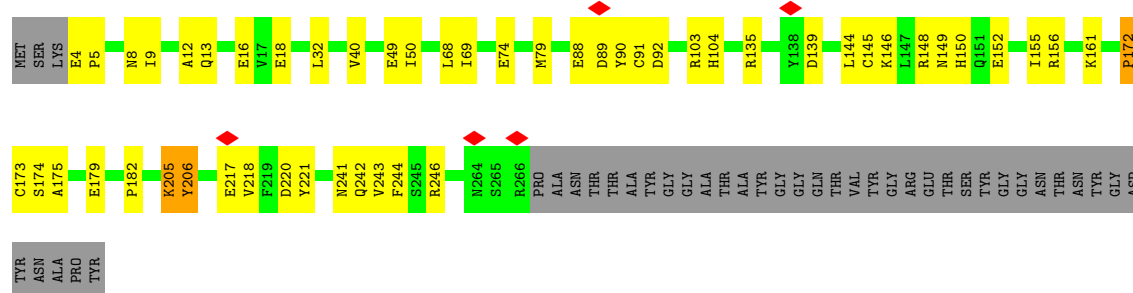
- Molecule 1: DNA-directed RNA polymerase subunit



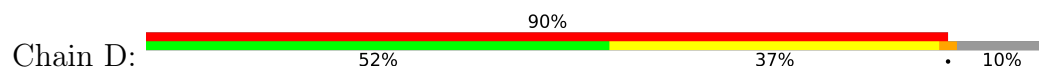




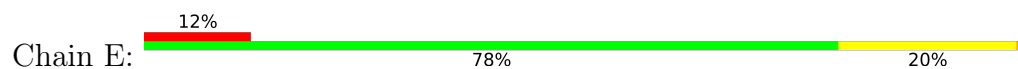
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core

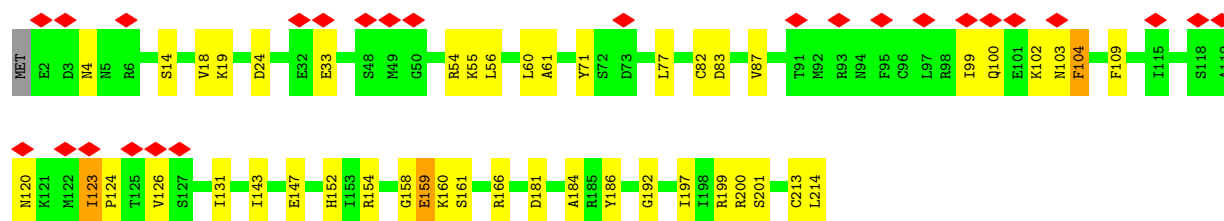


- Molecule 4: RNA polymerase II subunit B32



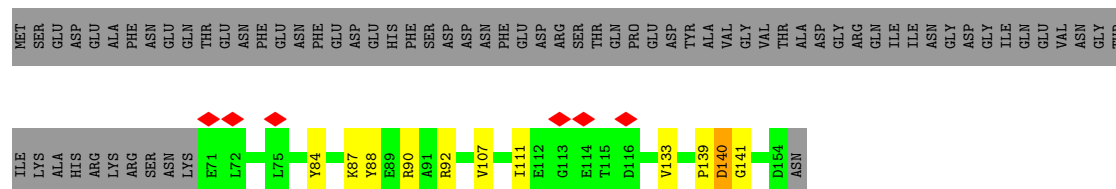
- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III





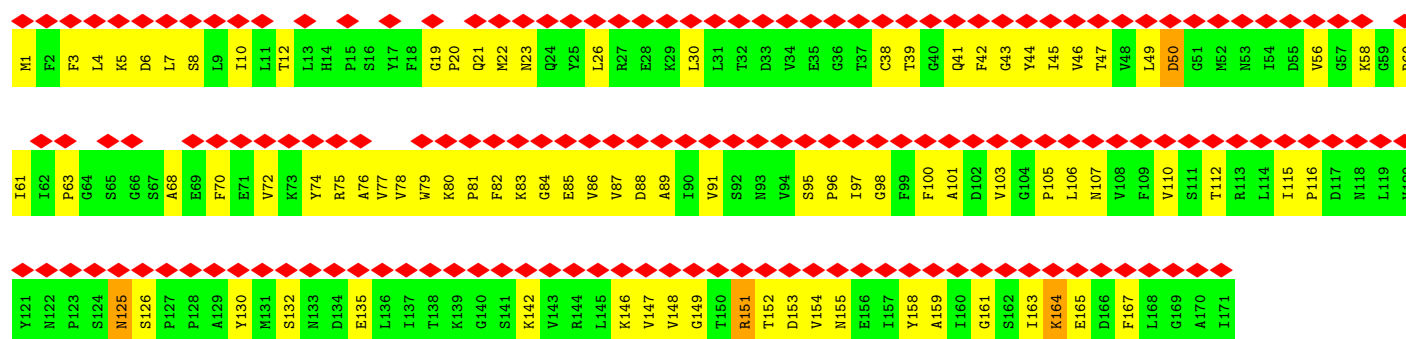
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F:



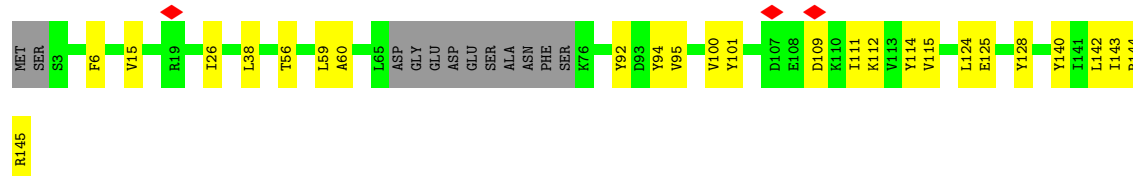
- Molecule 7: RNA polymerase II subunit

Chain G:



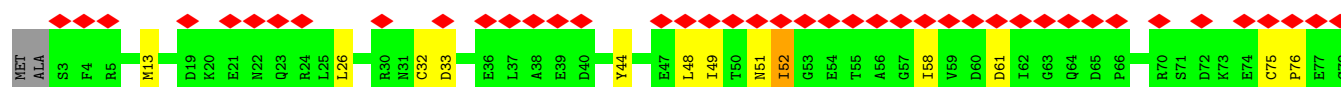
- Molecule 8: RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III

Chain H:



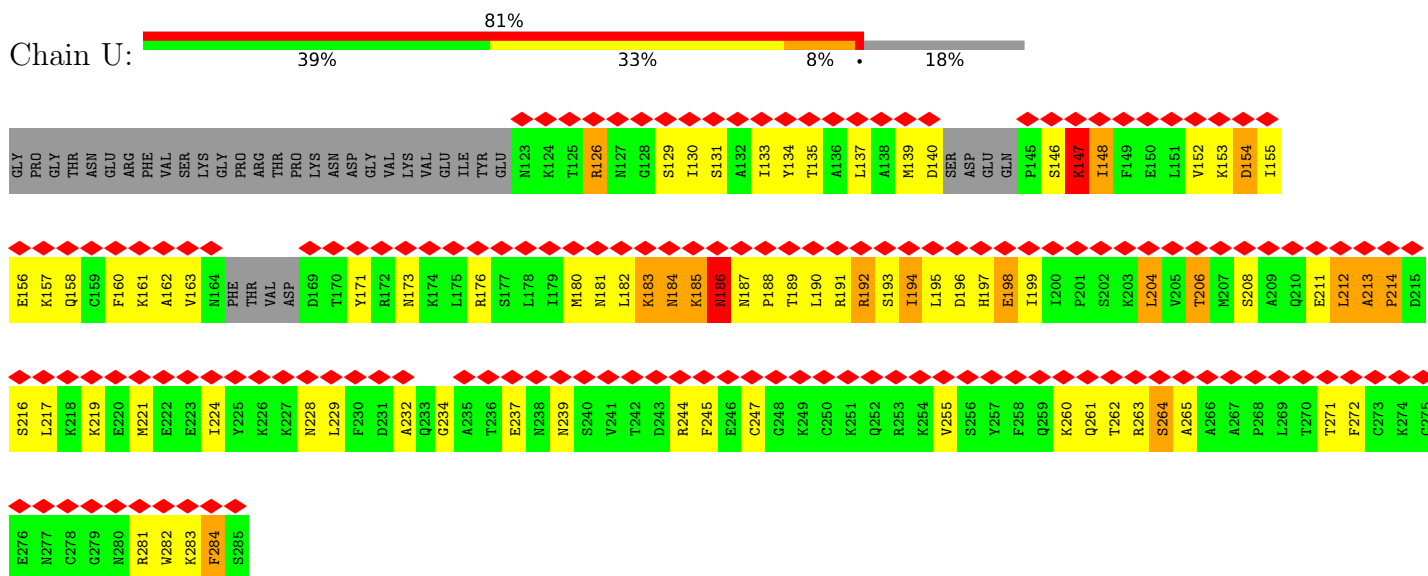
- Molecule 9: DNA-directed RNA polymerase subunit

Chain I:

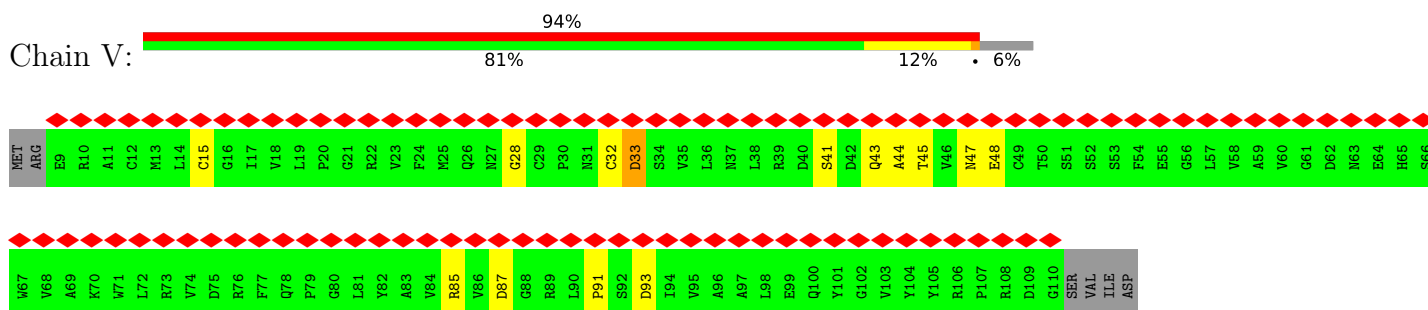




- Molecule 16: General transcription elongation factor TFIIS



- Molecule 17: Transcription elongation factor SPT4



- Molecule 18: Protein that forms a complex with Spt4p





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	682749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.503	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0666	Depositor
Map size ( $\text{\AA}$ )	275.94, 275.94, 275.94	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.533, 1.533, 1.533	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.26	0/11449	0.69	42/15474 (0.3%)
2	B	0.26	0/9441	0.62	28/12732 (0.2%)
3	C	0.25	0/2139	0.50	2/2895 (0.1%)
4	D	0.31	0/1326	0.54	3/1788 (0.2%)
5	E	0.25	0/1772	0.56	1/2385 (0.0%)
6	F	0.24	0/687	0.52	1/931 (0.1%)
7	G	0.33	0/1353	0.60	4/1837 (0.2%)
8	H	0.25	0/1069	0.45	0/1444
9	I	0.22	0/934	0.40	0/1257
10	J	0.25	0/554	0.44	0/742
11	K	0.26	0/953	0.44	0/1291
12	L	0.25	0/365	0.70	2/484 (0.4%)
13	P	0.28	0/376	0.85	0/583
14	T	0.99	9/1092 (0.8%)	1.22	3/1680 (0.2%)
15	N	0.89	10/996 (1.0%)	1.21	6/1535 (0.4%)
16	U	0.29	0/1255	0.71	7/1677 (0.4%)
17	V	0.46	0/808	0.60	0/1097
18	W	0.40	0/2713	0.61	5/3646 (0.1%)
All	All	0.35	19/39282 (0.0%)	0.67	104/53478 (0.2%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	-6	DC	C3'-O3'	-6.37	1.35	1.44
15	N	2	DT	C1'-N1	6.00	1.57	1.49
15	N	-24	DC	C1'-N1	5.26	1.56	1.49
15	N	-19	DC	C1'-N1	5.24	1.56	1.49
15	N	-25	DC	C1'-N1	5.24	1.56	1.49

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ALA	CB-CA-C	16.63	135.04	110.10
2	B	221	ALA	N-CA-CB	-14.50	89.80	110.10
2	B	167	SER	CB-CA-C	14.38	137.42	110.10
1	A	47	ARG	C-N-CD	-13.03	91.93	120.60
1	A	861	LEU	CB-CA-C	-12.61	86.24	110.20

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	11239	0	11263	452	0
2	B	9261	0	9267	204	0
3	C	2098	0	2058	32	0
4	D	1314	0	1314	153	0
5	E	1740	0	1754	28	0
6	F	677	0	693	11	0
7	G	1324	0	1342	222	0
8	H	1052	0	1050	15	0
9	I	917	0	865	30	0
10	J	545	0	560	9	0
11	K	932	0	944	9	0
12	L	359	0	360	16	0
13	P	338	0	169	25	0
14	T	975	0	538	43	0
15	N	889	0	487	35	0
16	U	1239	0	1263	264	0
17	V	792	0	757	7	0
18	W	2667	0	2712	250	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
19	U	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	V	1	0	0	0	0
20	A	1	0	0	0	0
All	All	38369	0	37396	1359	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 1359 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:1363:GLY:CA	16:U:282:TRP:HA	1.30	1.62
7:G:100:PHE:HZ	18:W:698:PHE:CE1	1.21	1.54
7:G:100:PHE:CZ	18:W:698:PHE:CE1	1.94	1.53
16:U:133:ILE:HG21	16:U:155:ILE:CG2	1.38	1.49
1:A:1232:GLU:HG3	16:U:180:MET:CB	1.43	1.48

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	A	1417/1743 (81%)	1235 (87%)	169 (12%)	13 (1%)	17	53
2	B	1151/1227 (94%)	987 (86%)	159 (14%)	5 (0%)	34	70
3	C	261/304 (86%)	231 (88%)	27 (10%)	3 (1%)	14	50
4	D	162/186 (87%)	141 (87%)	20 (12%)	1 (1%)	25	62
5	E	211/214 (99%)	190 (90%)	19 (9%)	2 (1%)	17	53
6	F	82/155 (53%)	70 (85%)	12 (15%)	0	100	100
7	G	169/171 (99%)	150 (89%)	19 (11%)	0	100	100
8	H	129/145 (89%)	111 (86%)	18 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	109/115 (95%)	93 (85%)	14 (13%)	2 (2%)	8	40
10	J	64/72 (89%)	62 (97%)	2 (3%)	0	100	100
11	K	111/118 (94%)	99 (89%)	12 (11%)	0	100	100
12	L	43/72 (60%)	37 (86%)	6 (14%)	0	100	100
16	U	149/190 (78%)	120 (80%)	24 (16%)	5 (3%)	3	30
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	317/612 (52%)	288 (91%)	26 (8%)	3 (1%)	17	53
All	All	4475/5432 (82%)	3911 (87%)	530 (12%)	34 (1%)	24	56

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	48	PRO
1	A	743	ASN
1	A	1085	THR
2	B	62	ALA

### 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	1238/1528 (81%)	1222 (99%)	16 (1%)	69	82
2	B	1016/1077 (94%)	1008 (99%)	8 (1%)	81	89
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	95
4	D	143/160 (89%)	142 (99%)	1 (1%)	84	91
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	81
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	145 (98%)	3 (2%)	55	74
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	103 (97%)	3 (3%)	43	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	46	69
16	U	139/171 (81%)	127 (91%)	12 (9%)	10	39
17	V	86/92 (94%)	85 (99%)	1 (1%)	71	84
18	W	290/548 (53%)	279 (96%)	11 (4%)	33	60
All	All	3995/4792 (83%)	3935 (98%)	60 (2%)	66	81

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	166	ARG
18	W	777	ARG
12	L	62	ARG
18	W	685	PHE
18	W	809	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	13	GLN
5	E	100	GLN
18	W	682	ASN
3	C	150	HIS
4	D	46	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/30 (50%)	7 (46%)	1 (6%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	C
13	P	-3	U
13	P	-2	U
13	P	0	U

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Mol	Chain	Res	Type
13	P	1	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	P	-1	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](#)

Of 11 ligands modelled in this entry, 11 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 [i](#)

There are no chain breaks in this entry.

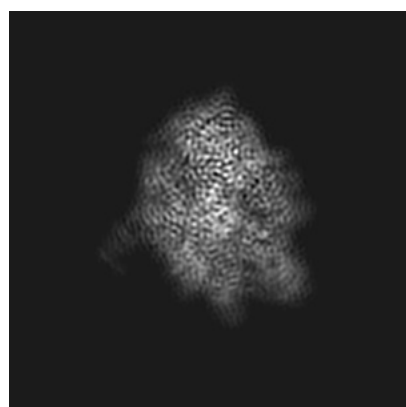
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6747. These allow visual inspection of the internal detail of the map and identification of artifacts.

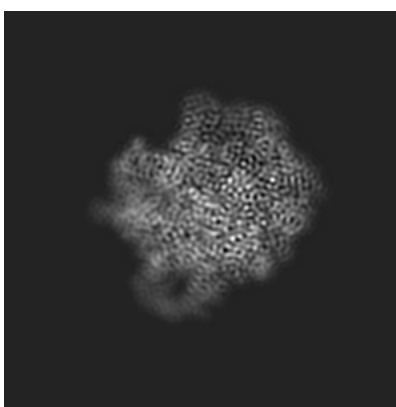
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

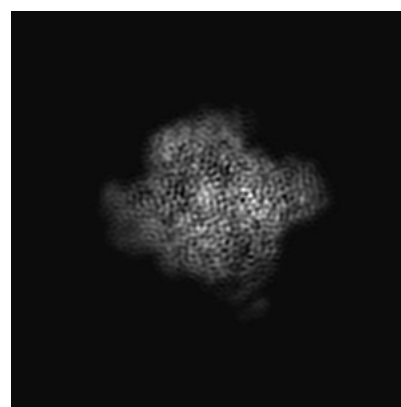
#### 6.1.1 Primary map



X



Y

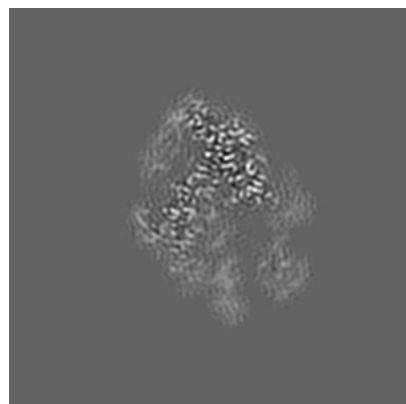


Z

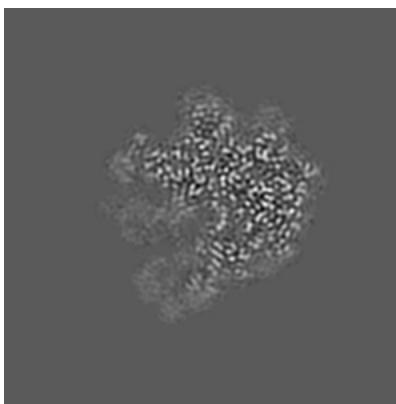
The images above show the map projected in three orthogonal directions.

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

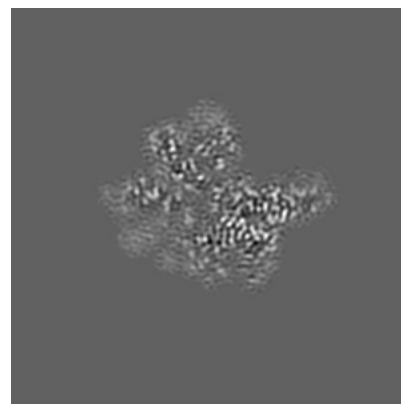
#### 6.2.1 Primary map



X Index: 90



Y Index: 90



Z Index: 90

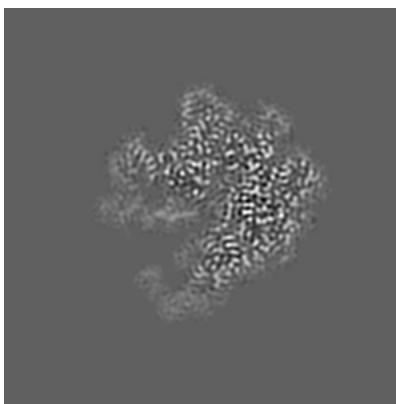
The images above show central slices of the map in three orthogonal directions.

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

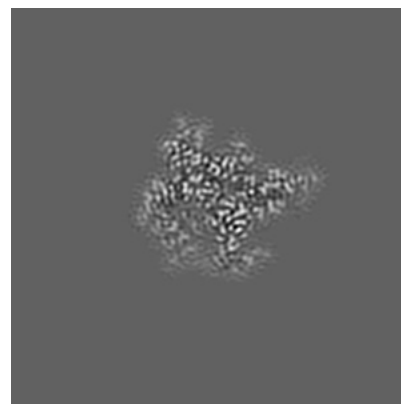
### 6.3.1 Primary map



X Index: 107



Y Index: 93



Z Index: 105

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0666. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



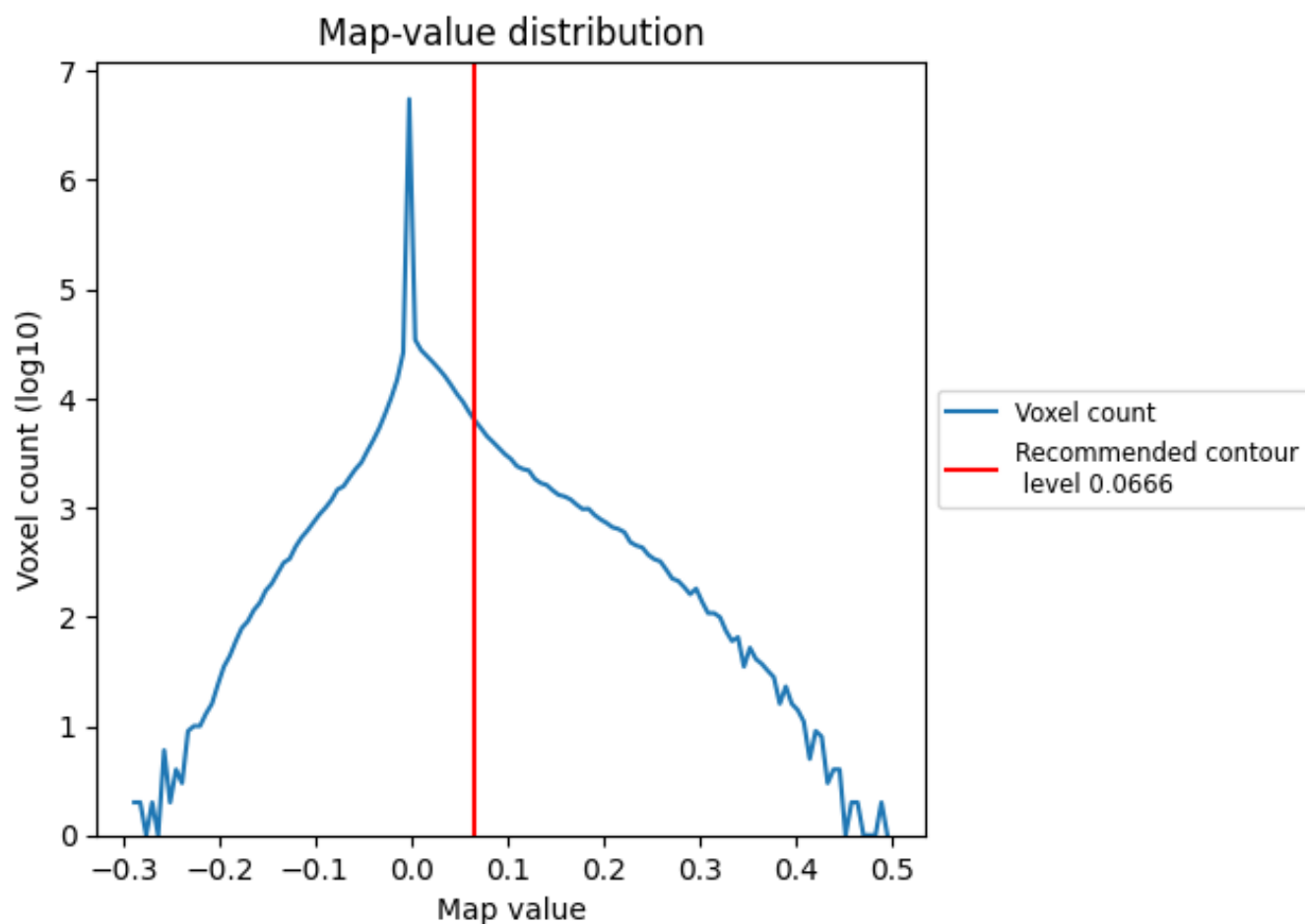
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

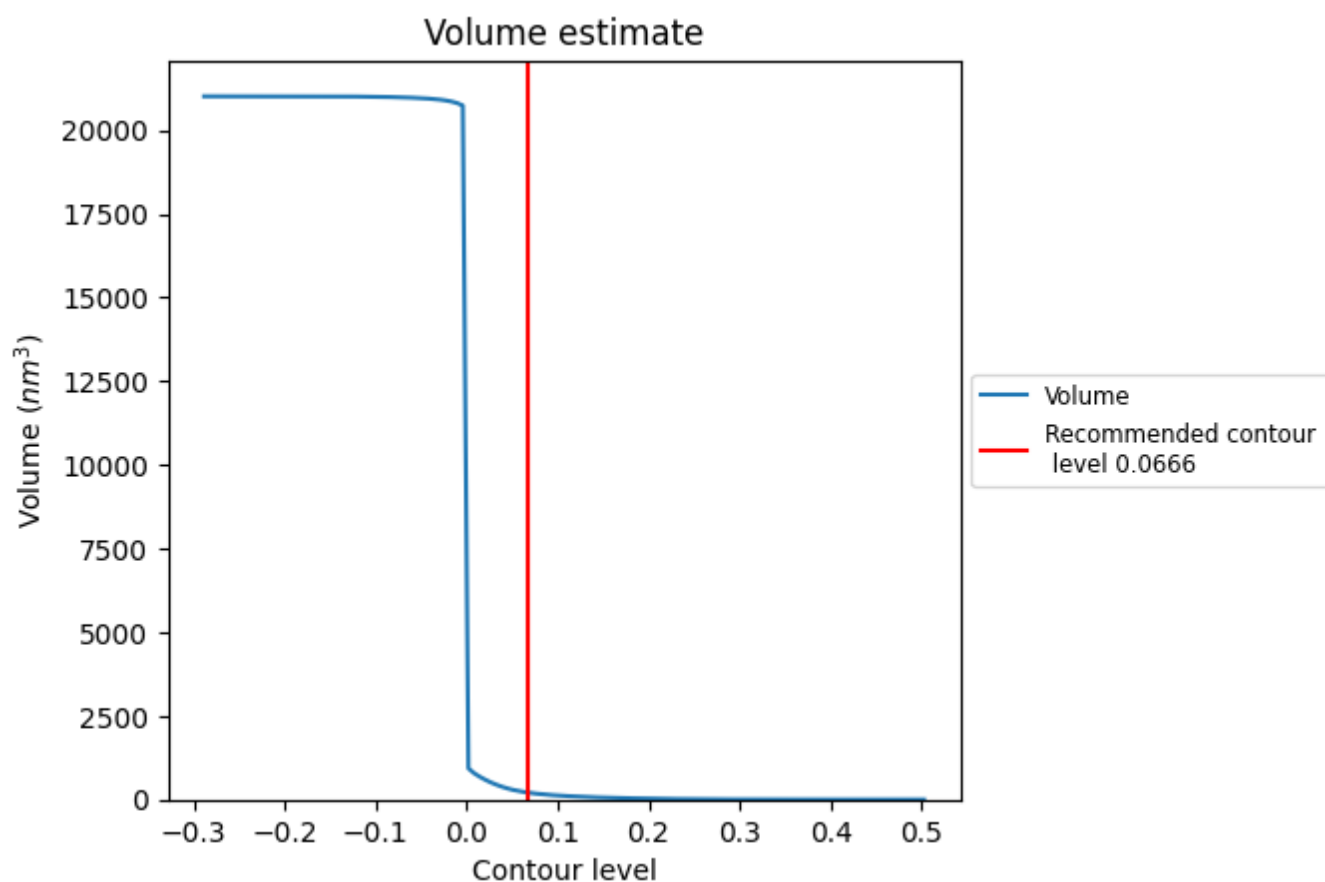
This section contains the results of statistical analysis of the map.

### 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.

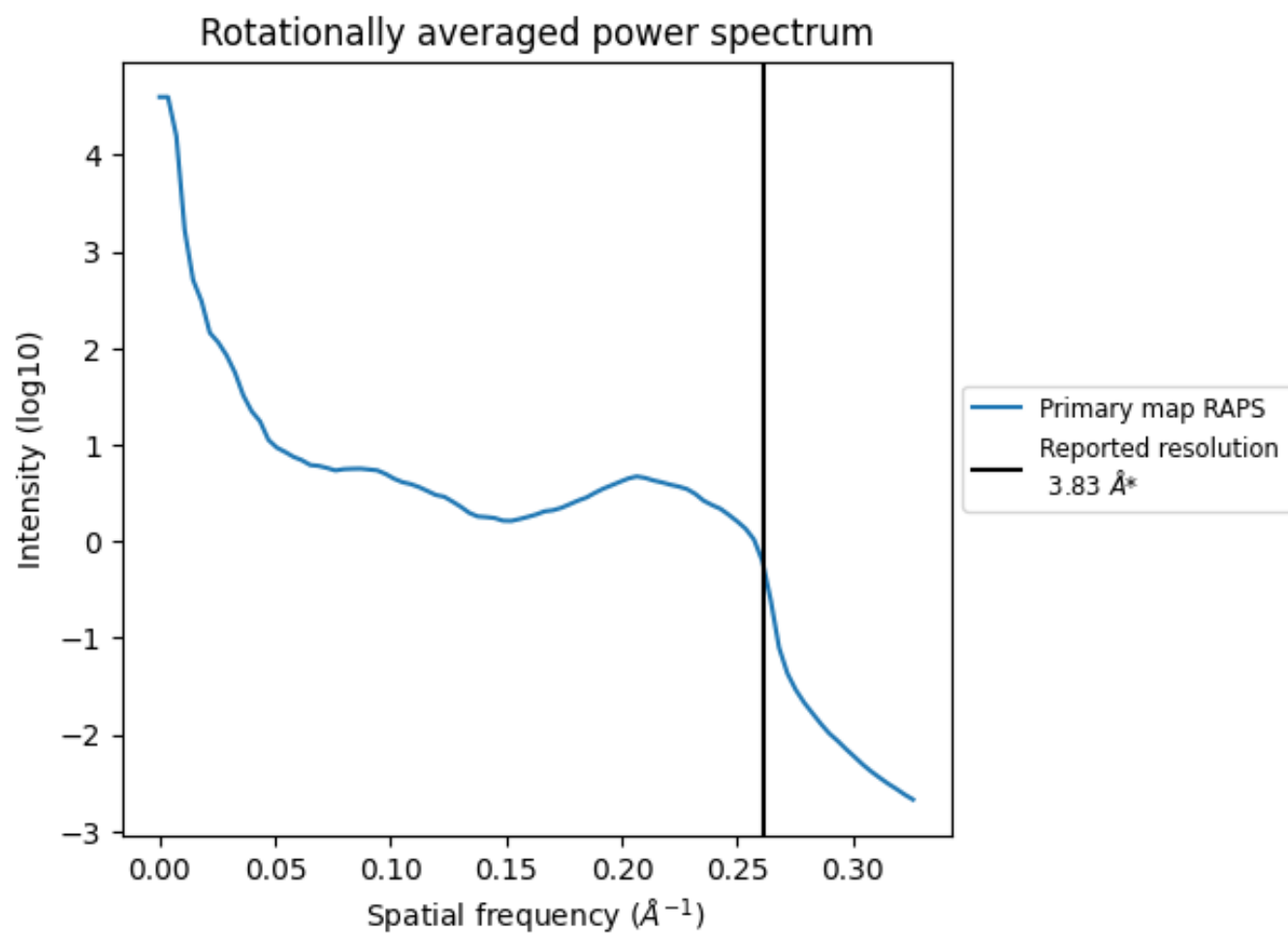
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm<sup>3</sup>; this corresponds to an approximate mass of 191 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 ⓘ

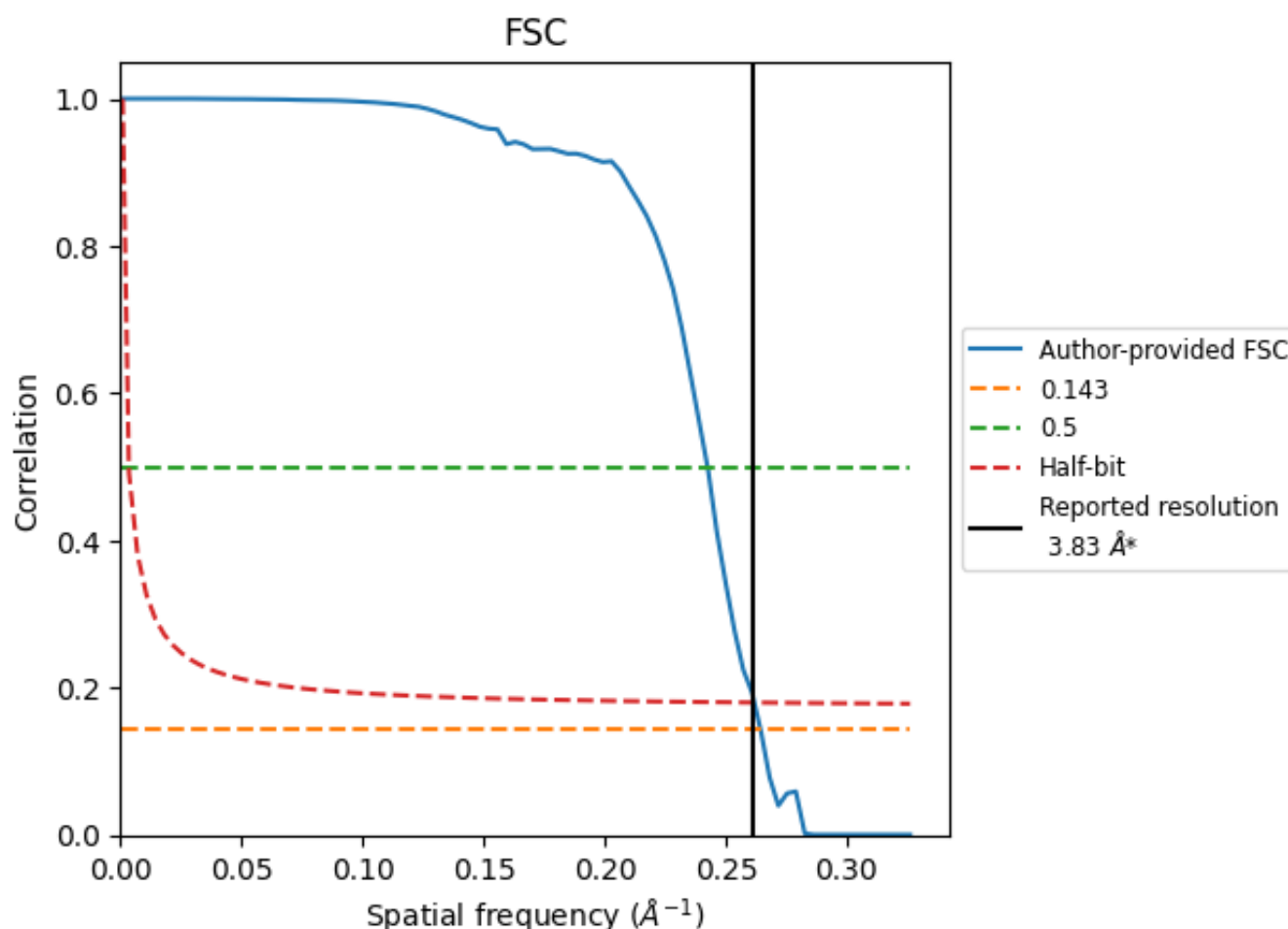


\*Reported resolution corresponds to spatial frequency of 0.261 Å<sup>-1</sup>

## 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 0.261 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

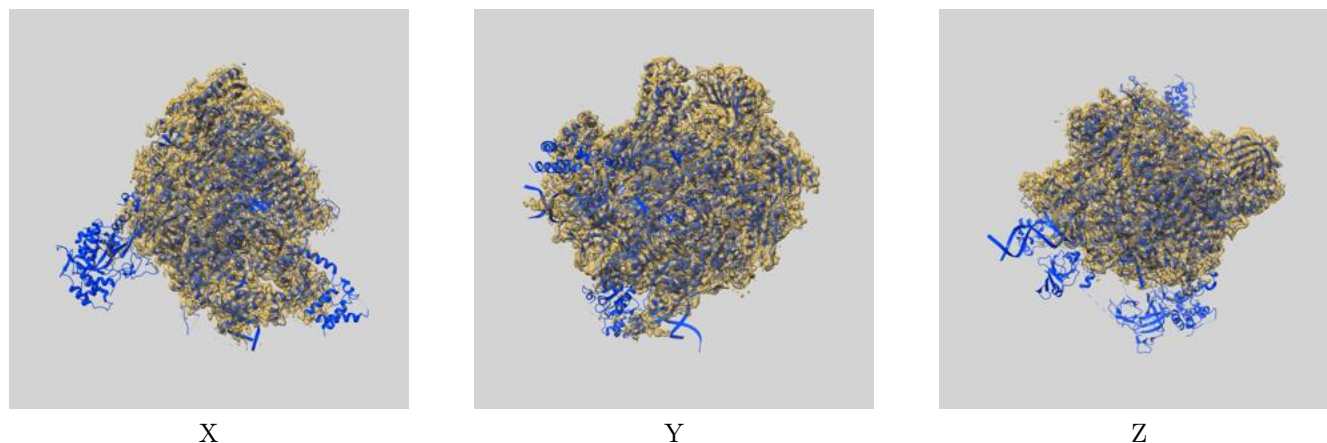
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	3.78	4.12	3.82
Unmasked-calculated*	-	-	-

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

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

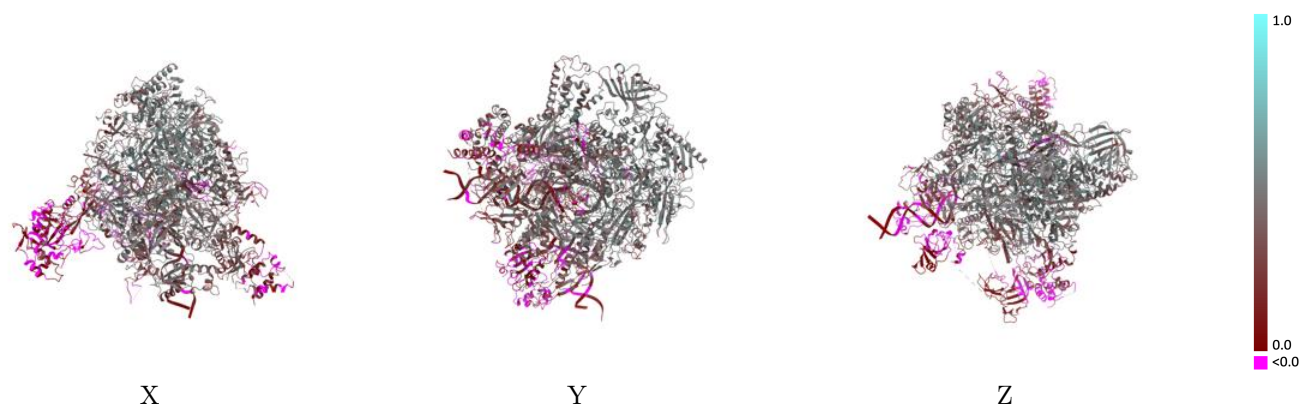
This section contains information regarding the fit between EMDB map EMD-6747 and PDB model 5XON. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

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



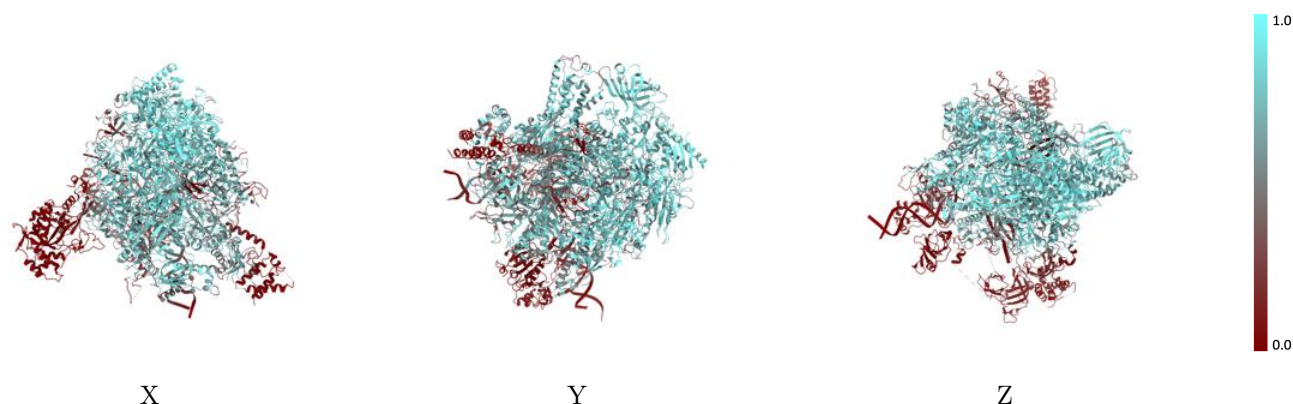
The images above show the 3D surface view of the map at the recommended contour level 0.0666 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

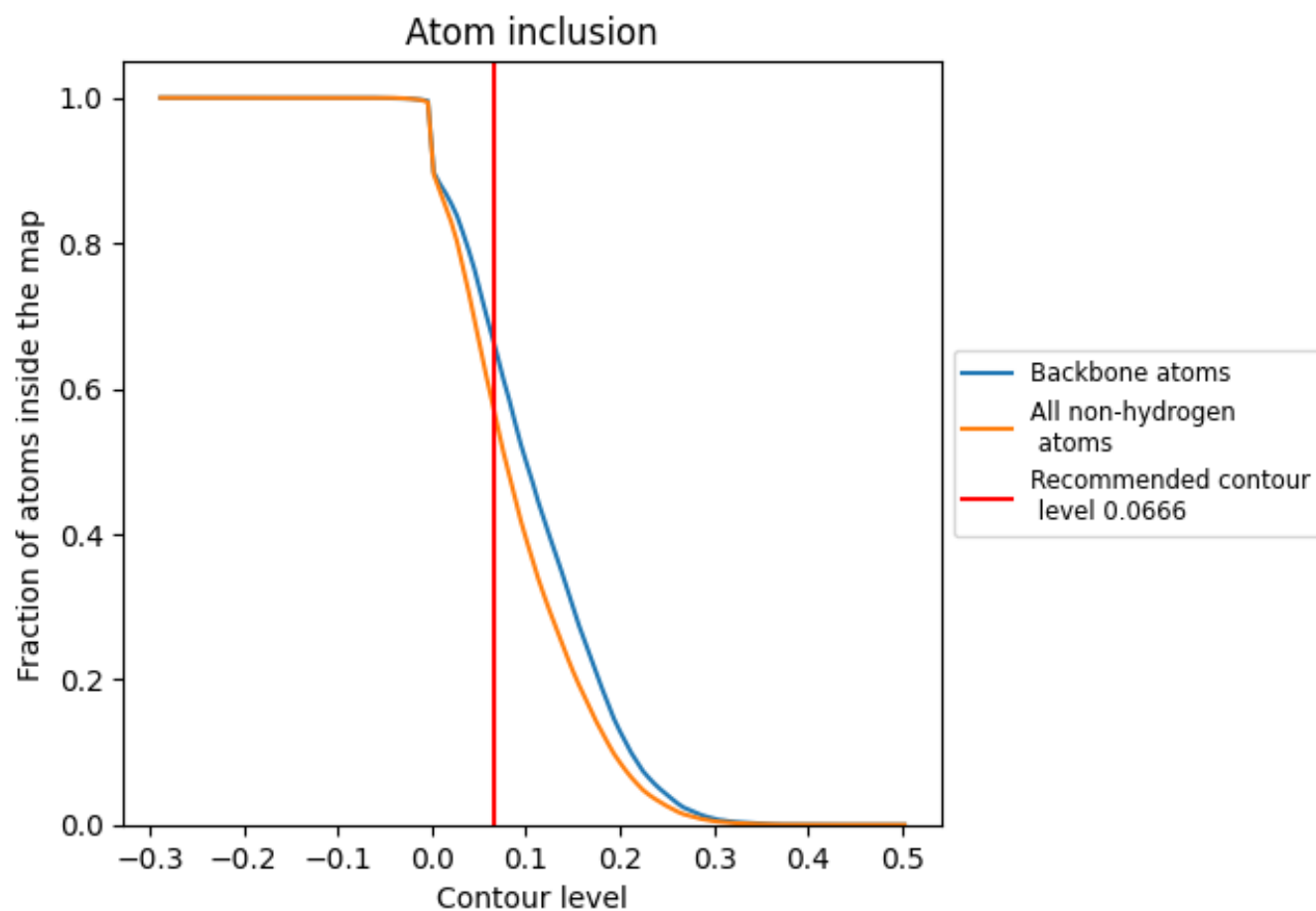
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0666).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 57% 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 (0.0666) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5680	 0.3360
A	 0.7109	 0.4260
B	 0.7301	 0.4330
C	 0.7911	 0.4560
D	 0.0016	 -0.0280
E	 0.7047	 0.4120
F	 0.7523	 0.4670
G	 0.0752	 0.0730
H	 0.7863	 0.4550
I	 0.3281	 0.1860
J	 0.8094	 0.4670
K	 0.7847	 0.4540
L	 0.6063	 0.3260
N	 0.2576	 0.0980
P	 0.5473	 0.3630
T	 0.3867	 0.1670
U	 0.0337	 0.0710
V	 0.0039	 0.0070
W	 0.0709	 0.0530

