



## wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 06:46 pm GMT

PDB ID : 5FUR  
EMDB ID : EMD-3305  
Title : Structure of human TFIID-IIA bound to core promoter DNA  
Authors : Louder, R.K.; He, Y.; Lopez-Blanco, J.R.; Fang, J.; Chacon, P.; Nogales, E.  
Deposited on : 2016-01-29  
Resolution : 8.50 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.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

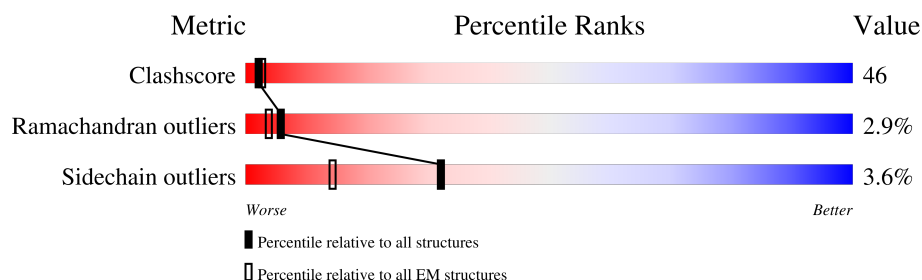
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	339	
2	B	43	
3	C	47	
4	D	97	
5	E	89	
6	F	93	
7	G	1893	
8	H	349	

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Mol	Chain	Length	Quality of chain
9	I	1199	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>11%33%31%12%24%</div></div>
10	J	677	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>22%8%68%</div></div>
10	K	677	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>18%8%71%</div></div>
11	L	310	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%91%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21485 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 TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	180	Total	C	N	O	S	0	0
			1429	927	252	243	7		

- Molecule 2 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	43	Total	C	N	O	S	0	0
			356	228	56	70	2		

- Molecule 3 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	47	Total	C	N	O	S	0	0
			393	250	70	71	2		

- Molecule 4 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	97	Total	C	N	O	S	0	0
			793	502	140	149	2		

- Molecule 5 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	80	Total	C	N	O	P	0	0
			1654	778	320	476	80		

- Molecule 6 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	P	0	0
			1626	770	292	484	80		

- Molecule 7 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	406	Total	C	N	O	P	S	0	0
			3290	2090	580	596	2	22		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	178	VAL	-	insertion	UNP P21675
G	179	SER	-	insertion	UNP P21675
G	180	GLU	-	insertion	UNP P21675
G	181	ASN	-	insertion	UNP P21675
G	182	GLY	-	insertion	UNP P21675
G	183	GLU	-	insertion	UNP P21675
G	184	GLY	-	insertion	UNP P21675
G	185	ILE	-	insertion	UNP P21675
G	186	ILE	-	insertion	UNP P21675
G	187	LEU	-	insertion	UNP P21675
G	188	PRO	-	insertion	UNP P21675
G	189	SER	-	insertion	UNP P21675
G	190	ILE	-	insertion	UNP P21675
G	191	ILE	-	insertion	UNP P21675
G	192	ALA	-	insertion	UNP P21675
G	193	PRO	-	insertion	UNP P21675
G	194	SER	-	insertion	UNP P21675
G	195	SER	-	insertion	UNP P21675
G	196	LEU	-	insertion	UNP P21675
G	197	ALA	-	insertion	UNP P21675
G	198	SER	-	insertion	UNP P21675

- Molecule 8 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S	0	0
			998	638	184	172	4		

- Molecule 9 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	914	Total	C	N	O	S	0	2
			7404	4761	1251	1336	56		

- Molecule 10 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	220	Total	C	N	O	S	0	0
			1741	1106	306	318	11		
10	K	198	Total	C	N	O	S	0	0
			1582	1006	276	290	10		

- Molecule 11 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	27	Total	C	N	O	S	0	1
			219	134	46	38	1		

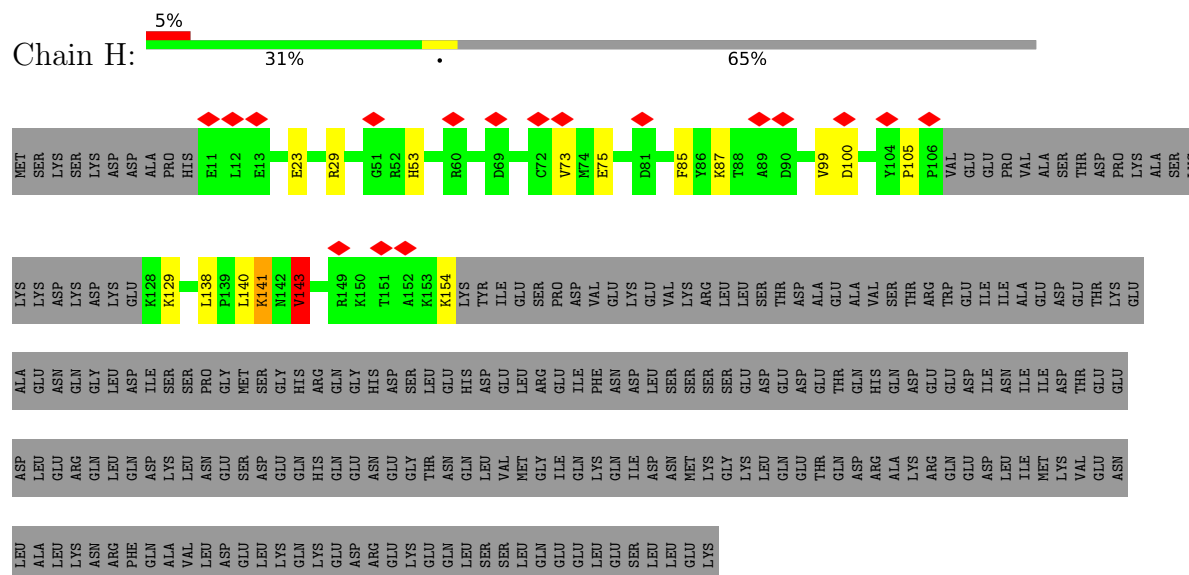




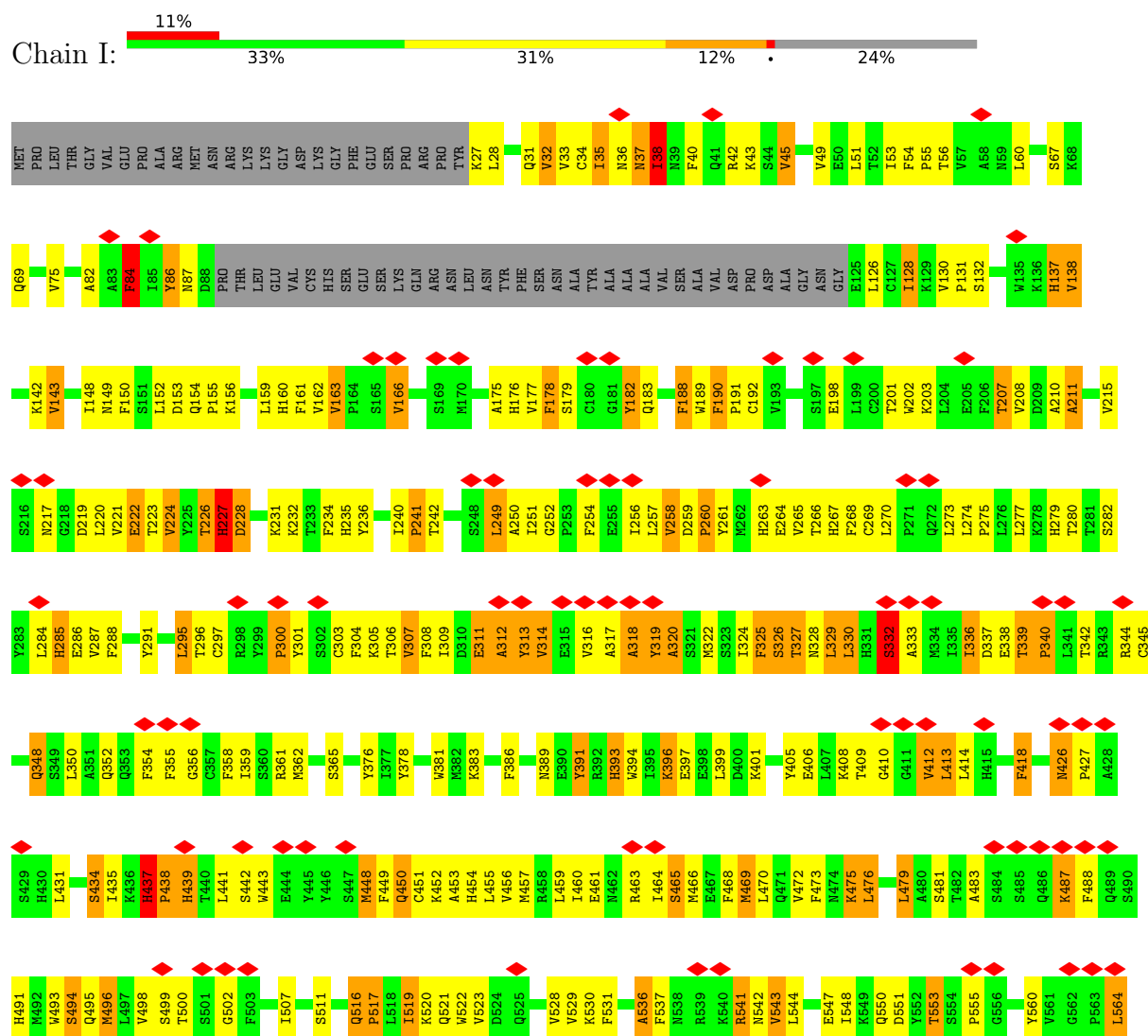


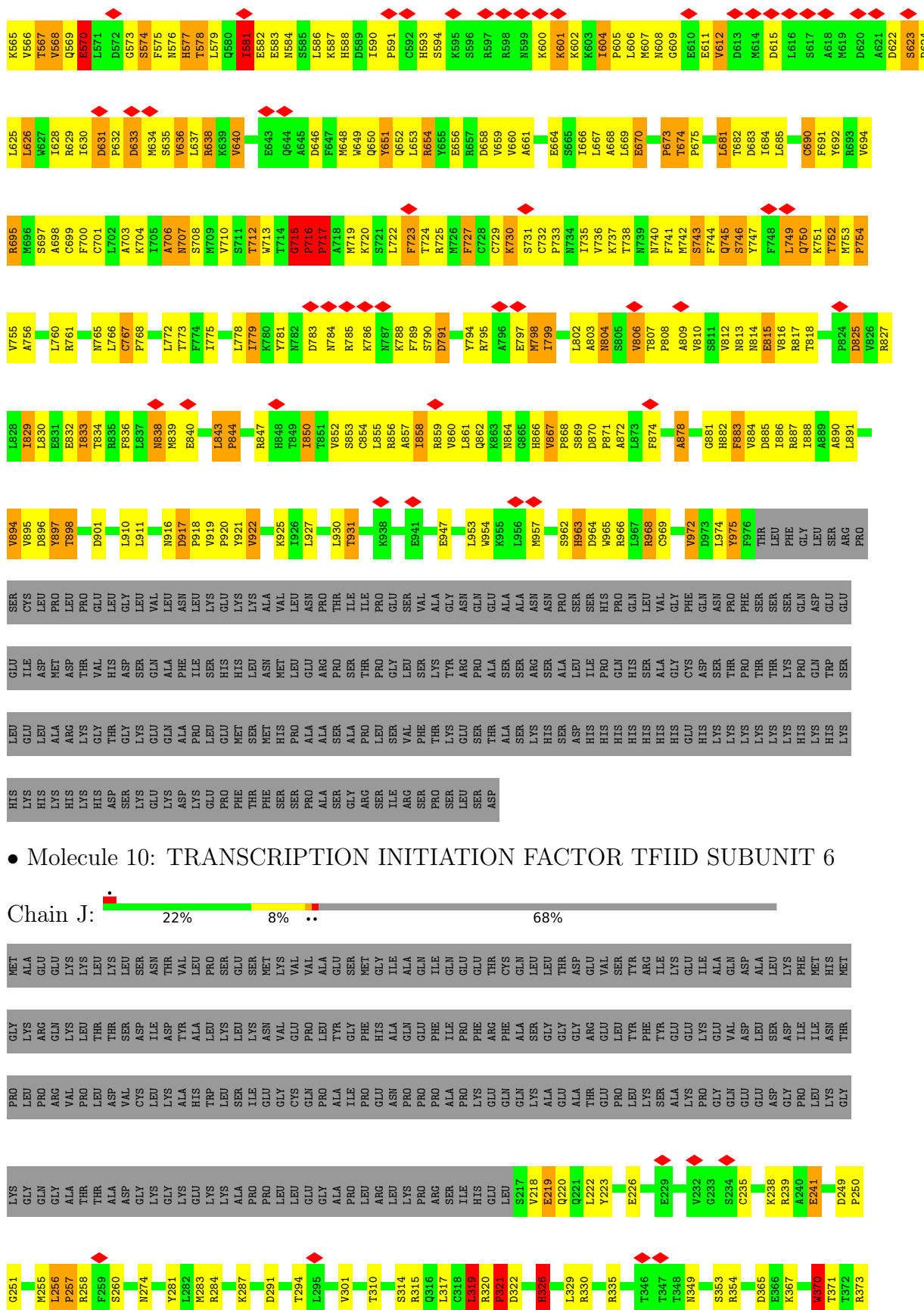


• Molecule 8: TRANSCRIPTION INITIATION FACTOR TFIIID SUBUNIT 7

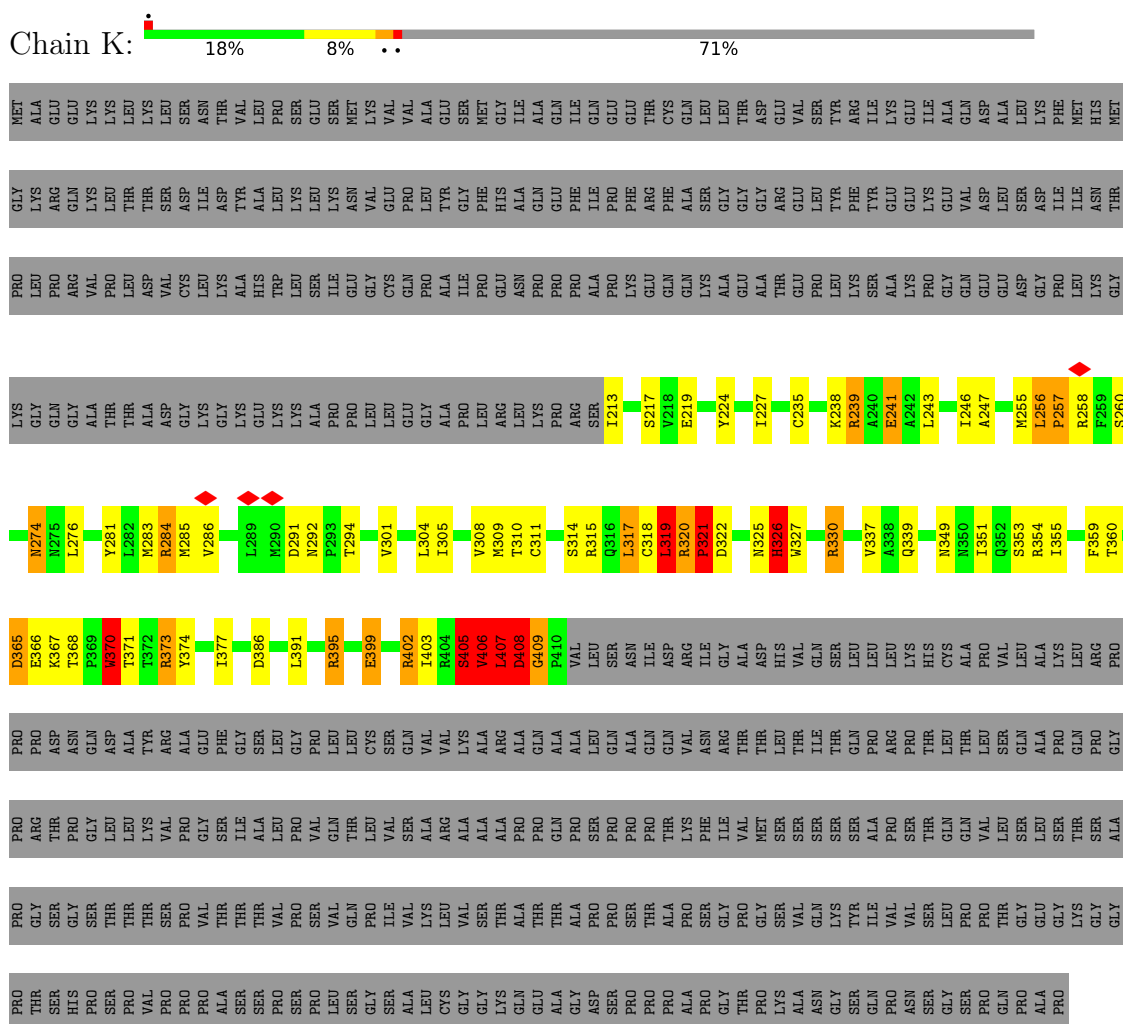


• Molecule 9: TRANSCRIPTION INITIATION FACTOR TFIIID SUBUNIT 2

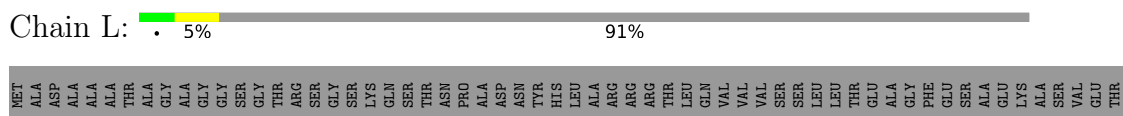




● Molecule 10: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 6



- Molecule 11: TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 8



LYS	ASP	R184	LEU
LYS	GLU	D185	THR
SER	GLN	R186	GLU
LEU	THR	E187	LEU
SER	ASP	R188	THR
	THR		GLN
	GLU	R192	SER
	ASN	F193	SER
	LEU	M194	TYR
	ALA	A195	THR
	LEU	K196	GLU
	ILE	T197	ILE
	SER	G198	GLY
	MET	GLU	ARG
	GLU	GLN	LEU
	ASP	SER	ALA
	SER	LEU	LYS
	GLY	PHE	SER
	ALA	LYS	TYR
	GLU	ASP	GLU
	LYS	ASP	THR
	GLU	VAL	THR
	ASN	SER	ALA
	THR	THR	ARG
	SER	PHE	THR
	VAL	PRO	GLN
	LEU	LEU	PRO
	GLN	ILE	THR
	GLN	ALA	LEU
	ASN	ALA	SER
	PRO	ARG	ASP
	SER	PRO	ILE
	LEU	PHE	VAL
	SER	THR	VAL
	GLY	ILE	THR
	SER	PRO	LEU
	ASN	THR	VAL
	GLY	THR	GLU
	GLU	ALA	GLY
	GLU	LEU	PHE
	ASN	LEU	ASN
	ILE	PRO	VAL
	ILE	SER	ASP
	ASP	GLU	THR
	ASN	LEU	LEU
	PRO	GLU	PRO
	TYR	MET	ALA
	LEU	GLN	ALA
	ARG	GLN	TYR
	PRO	MET	ALA
	VAL	GLU	LYS
	LYS	GLU	ARG
	LYS	THR	SER
	PRO	ASP	ARG
	LYS	SER	MET
	ILE	SER	VAL
	ARG	GLU	THR
	ARG	GLN	ILE

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22050	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37879	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.049	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	506.88, 506.88, 506.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, SEP

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	0.52	0/1455	0.69	0/1958
2	B	0.34	0/360	0.53	0/487
3	C	0.40	0/402	0.83	1/539 (0.2%)
4	D	0.35	0/803	0.73	2/1088 (0.2%)
5	E	3.85	16/1806 (0.9%)	1.89	49/2658 (1.8%)
6	F	3.55	15/1764 (0.9%)	2.11	46/2582 (1.8%)
7	G	0.41	0/3349	0.55	0/4506
8	H	0.42	0/1017	0.59	1/1370 (0.1%)
9	I	0.84	8/7587 (0.1%)	0.82	5/10278 (0.0%)
10	J	0.74	0/1773	1.42	26/2408 (1.1%)
10	K	0.75	0/1612	1.38	21/2188 (1.0%)
11	L	0.61	1/220 (0.5%)	1.10	0/292
All	All	1.61	40/22148 (0.2%)	1.16	151/30354 (0.5%)

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	E	0	2
7	G	0	1
9	I	0	235
10	J	2	16
10	K	1	12
All	All	3	266

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	43	DC	O3'-P	49.26	2.20	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	44	DG	O3'-P	48.90	2.19	1.61
5	E	62	DC	O3'-P	48.41	2.19	1.61
5	E	59	DA	O3'-P	46.14	2.16	1.61
6	F	105	DA	O3'-P	46.09	2.16	1.61

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	145	DC	O5'-P-OP2	-41.73	60.62	110.70
9	I	437	HIS	C-N-CD	-27.62	59.83	120.60
5	E	17	DG	P-O3'-C3'	-27.17	87.10	119.70
6	F	145	DC	P-O5'-C5'	-24.28	82.05	120.90
6	F	156	DG	O5'-P-OP1	-23.00	83.11	110.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	J	326	HIS	CA
10	J	411	VAL	CA
10	K	326	HIS	CA

5 of 266 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	DA	Sidechain
5	E	7	DC	Sidechain
7	G	1104	LEU	Peptide
9	I	32	VAL	Mainchain
9	I	33	VAL	Mainchain

## 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	1429	0	1521	49	0
2	B	356	0	360	7	0
3	C	393	0	380	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	793	0	801	39	0
5	E	1654	0	958	423	0
6	F	1626	0	962	396	0
7	G	3290	0	3276	61	0
8	H	998	0	1055	6	0
9	I	7404	0	7381	897	0
10	J	1741	0	1782	103	0
10	K	1582	0	1612	40	0
11	L	219	0	222	130	0
All	All	21485	0	20310	1916	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 46.

The worst 5 of 1916 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)
9:I:84:PHE:HZ	9:I:126:LEU:CG	1.10	1.64
5:E:70:DC:C5'	7:G:875:ARG:NH1	1.68	1.53
9:I:566:VAL:HB	9:I:579:LEU:CD1	1.36	1.51
9:I:309:ILE:CG2	9:I:312:ALA:HB2	1.42	1.48
9:I:84:PHE:CZ	9:I:126:LEU:CG	1.96	1.47

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	178/339 (52%)	175 (98%)	3 (2%)	0	100	100
2	B	41/43 (95%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
4	D	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	12	47
7	G	398/1893 (21%)	391 (98%)	7 (2%)	0	100	100
8	H	119/349 (34%)	117 (98%)	2 (2%)	0	100	100
9	I	910/1199 (76%)	753 (83%)	122 (13%)	35 (4%)	2	19
10	J	218/677 (32%)	185 (85%)	17 (8%)	16 (7%)	1	10
10	K	196/677 (29%)	163 (83%)	20 (10%)	13 (7%)	1	12
11	L	25/310 (8%)	25 (100%)	0	0	100	100
All	All	2225/5631 (40%)	1979 (89%)	181 (8%)	65 (3%)	6	23

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	84	VAL
9	I	222	GLU
9	I	413	LEU
9	I	438	PRO
9	I	577	HIS

### 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	155/293 (53%)	152 (98%)	3 (2%)	52	69
2	B	42/42 (100%)	41 (98%)	1 (2%)	44	62
3	C	42/42 (100%)	41 (98%)	1 (2%)	44	62
4	D	89/89 (100%)	87 (98%)	2 (2%)	47	65
7	G	355/1680 (21%)	331 (93%)	24 (7%)	13	34
8	H	113/322 (35%)	104 (92%)	9 (8%)	10	29
9	I	832/1083 (77%)	830 (100%)	2 (0%)	92	94
10	J	194/574 (34%)	177 (91%)	17 (9%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	176/574 (31%)	162 (92%)	14 (8%)	10	29
11	L	22/270 (8%)	22 (100%)	0	100	100
All	All	2020/4969 (41%)	1947 (96%)	73 (4%)	32	50

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	415	ILE
10	K	399	GLU
10	K	219	GLU
10	K	319	LEU
7	G	943	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	343	HIS
10	K	254	GLN
9	I	838	ASN
10	K	220	GLN
9	I	542	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SEP	G	1105	7	8,9,10	1.62	1 (12%)	8,12,14	1.08	1 (12%)
7	TPO	G	1106	7	8,10,11	1.13	0	10,14,16	1.61	1 (10%)

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
7	SEP	G	1105	7	-	3/5/8/10	-
7	TPO	G	1106	7	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1105	SEP	P-O1P	3.51	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1106	TPO	P-OG1-CB	-4.54	109.50	123.21
7	G	1105	SEP	OG-P-O1P	2.17	112.57	106.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1105	SEP	CB-OG-P-O2P
7	G	1105	SEP	CB-OG-P-O3P
7	G	1105	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	F	68
5	E	65
9	I	1

The worst 5 of 134 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	158:DC	O3'	159:DC	P	4.06
1	E	2:DG	O3'	3:DG	P	3.41
1	F	159:DC	O3'	160:DT	P	3.14
1	E	1:DA	O3'	2:DG	P	2.67
1	F	142:DC	O3'	143:DC	P	2.56

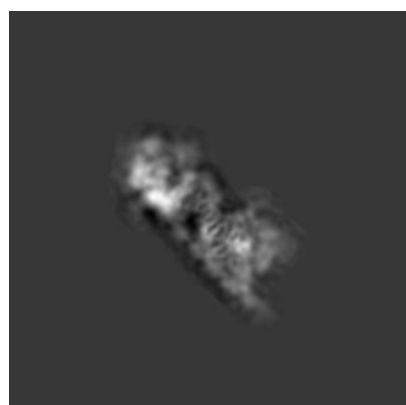
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3305. 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](#)

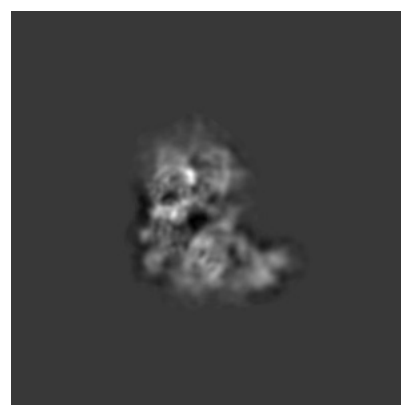
#### 6.1.1 Primary map



X



Y



Z

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

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

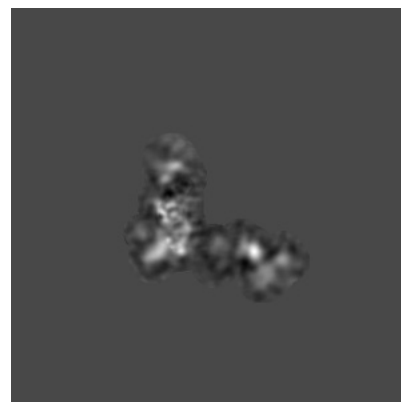
#### 6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

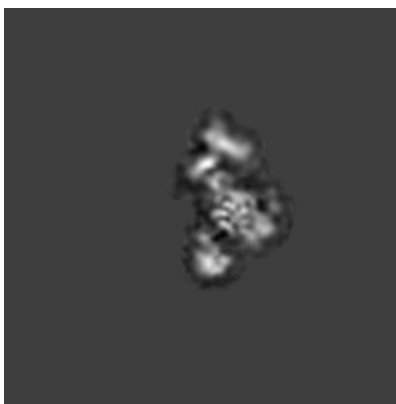
The images above show central slices of the map in three orthogonal directions.

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

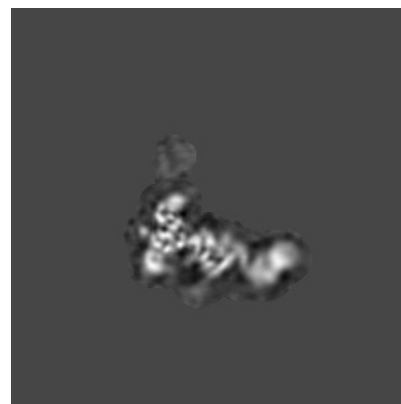
### 6.3.1 Primary map



X Index: 166



Y Index: 147



Z Index: 206

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

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

### 6.4.1 Primary map



X



Y

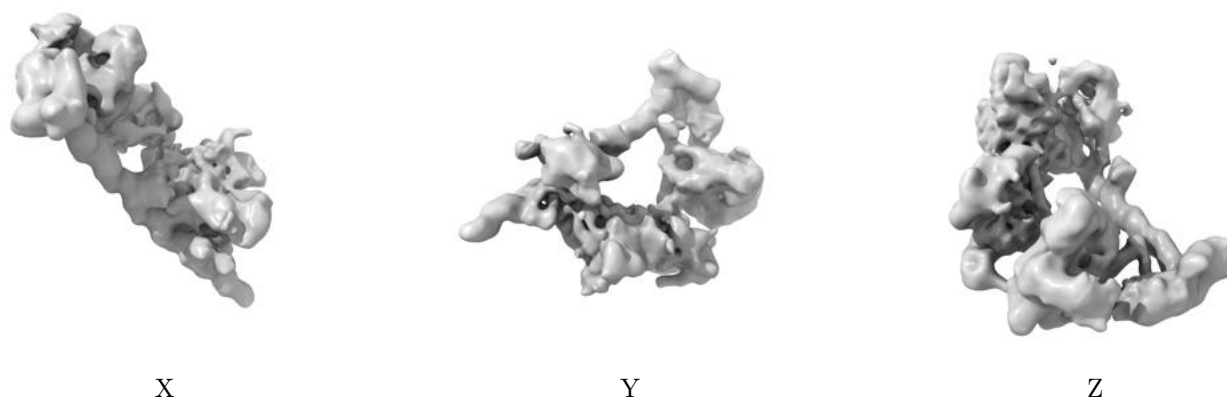


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

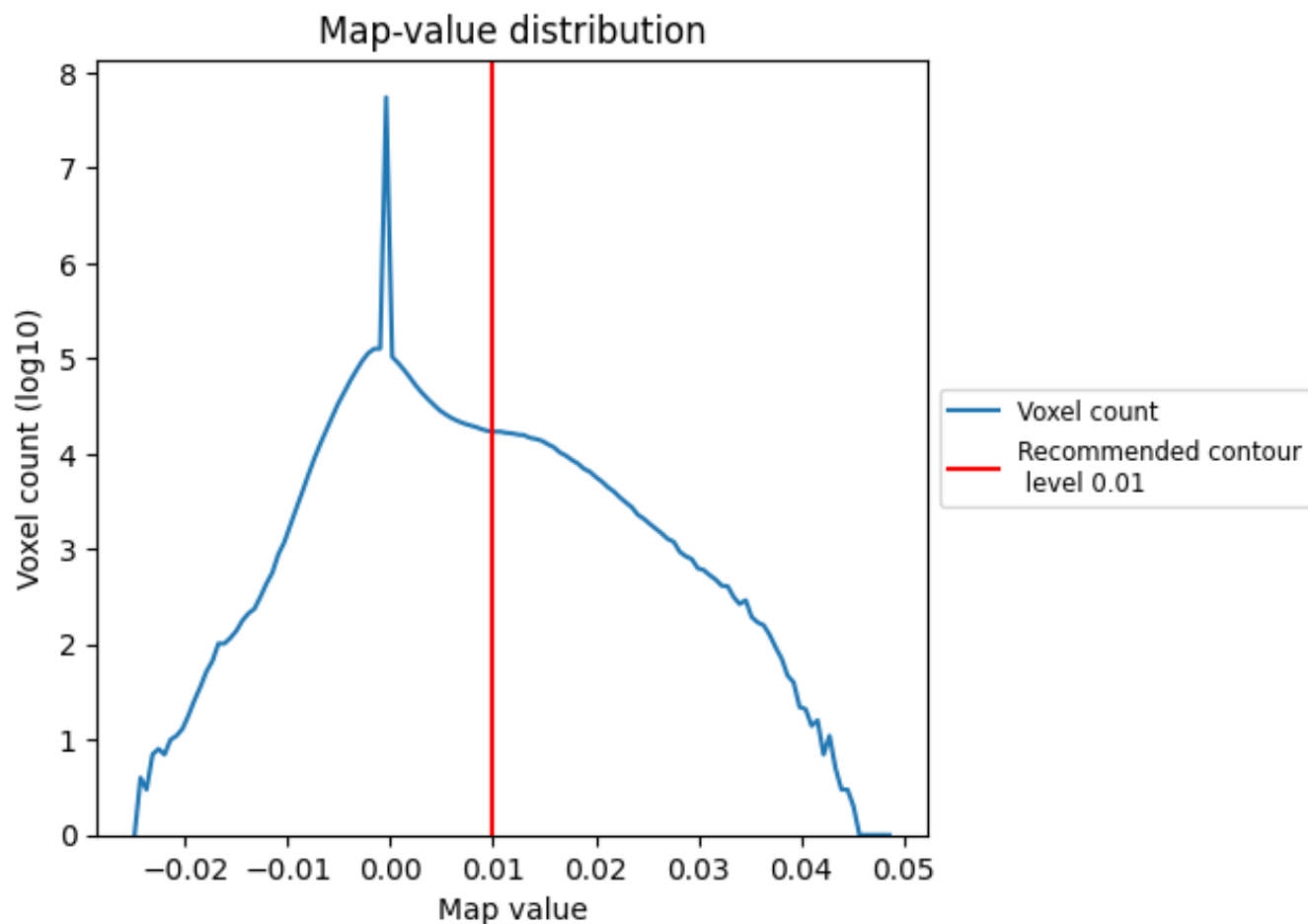
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

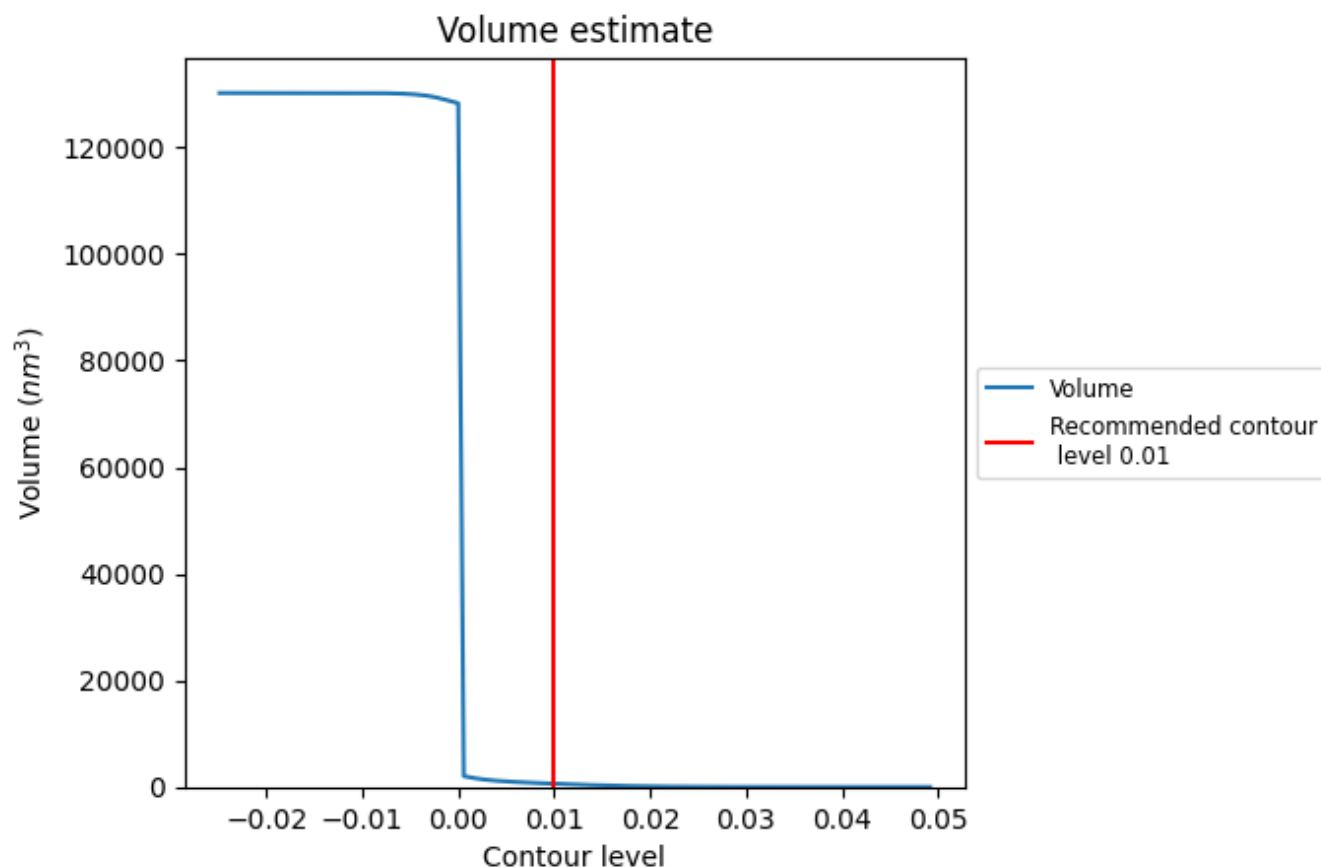
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

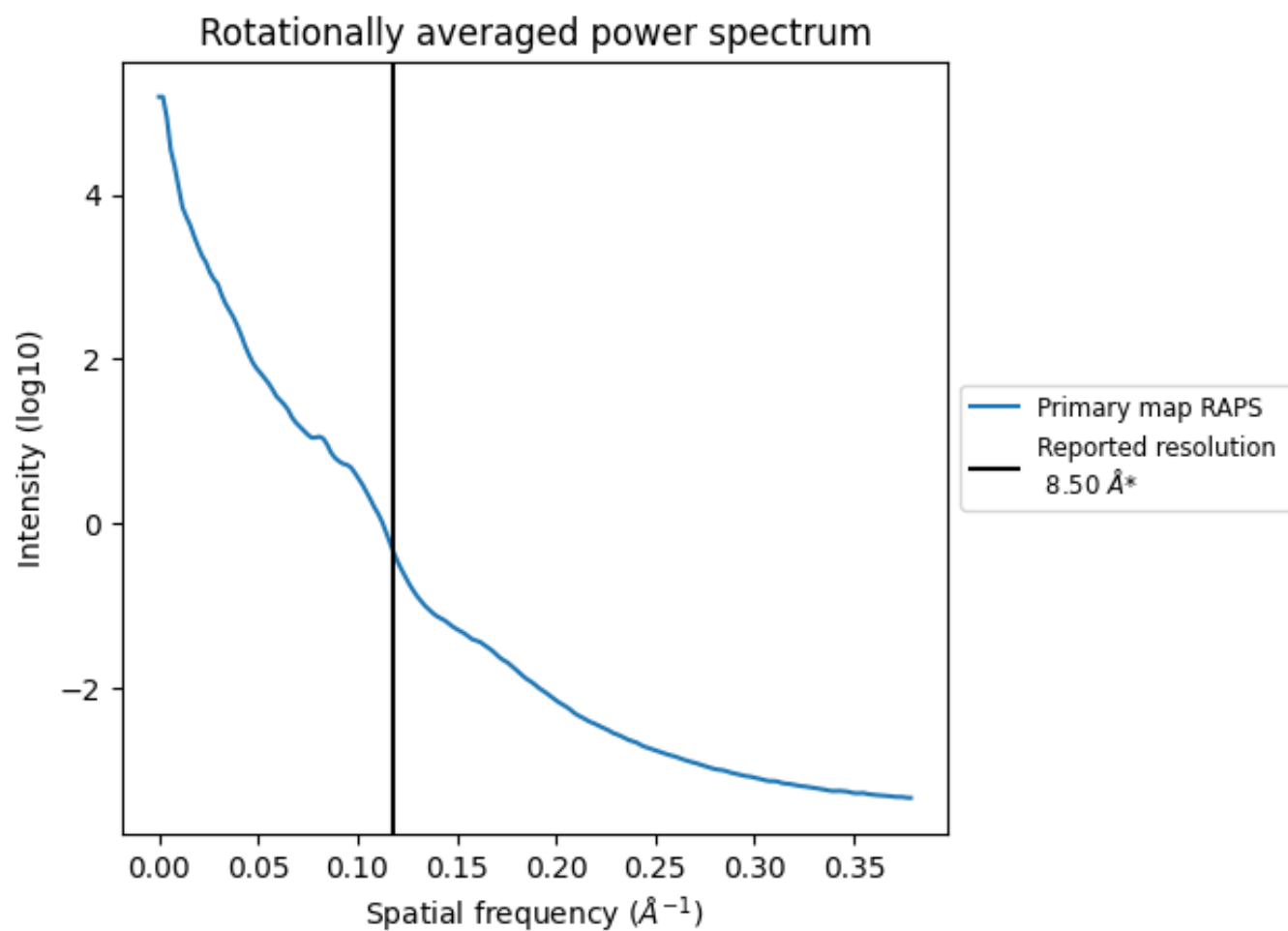
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 613  $\text{nm}^3$ ; this corresponds to an approximate mass of 553 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 ⓘ

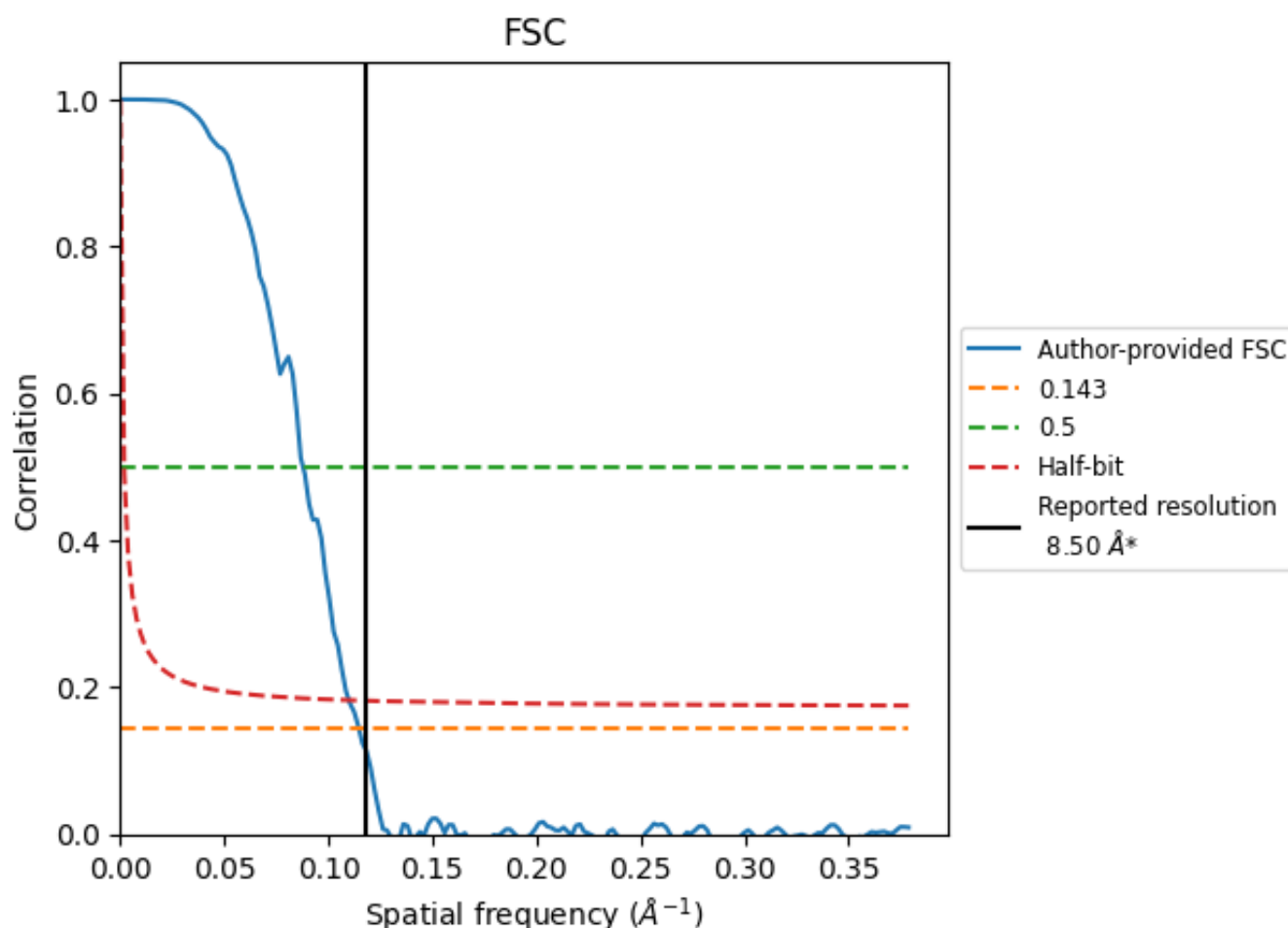


\*Reported resolution corresponds to spatial frequency of 0.118 Å<sup>-1</sup>

## 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 0.118 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

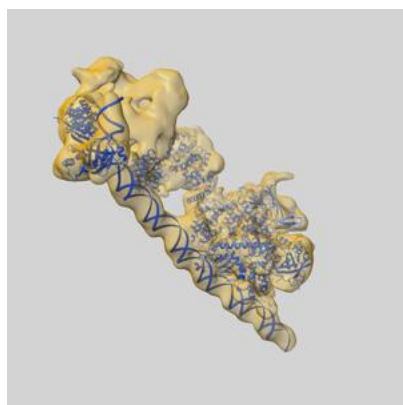
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	8.71	11.38	9.10
Unmasked-calculated*	-	-	-

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

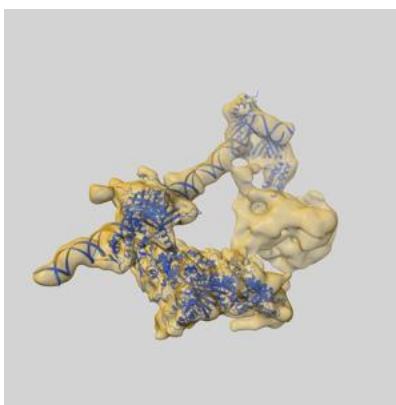
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3305 and PDB model 5FUR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

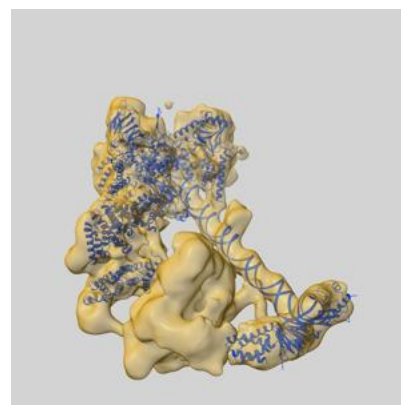
### 9.1 Map-model overlay [i](#)



X



Y



Z

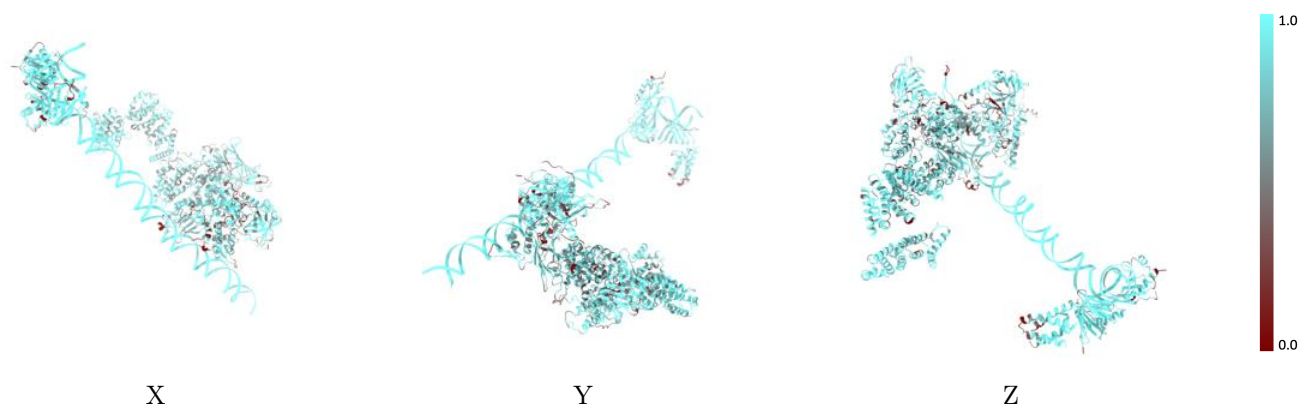
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



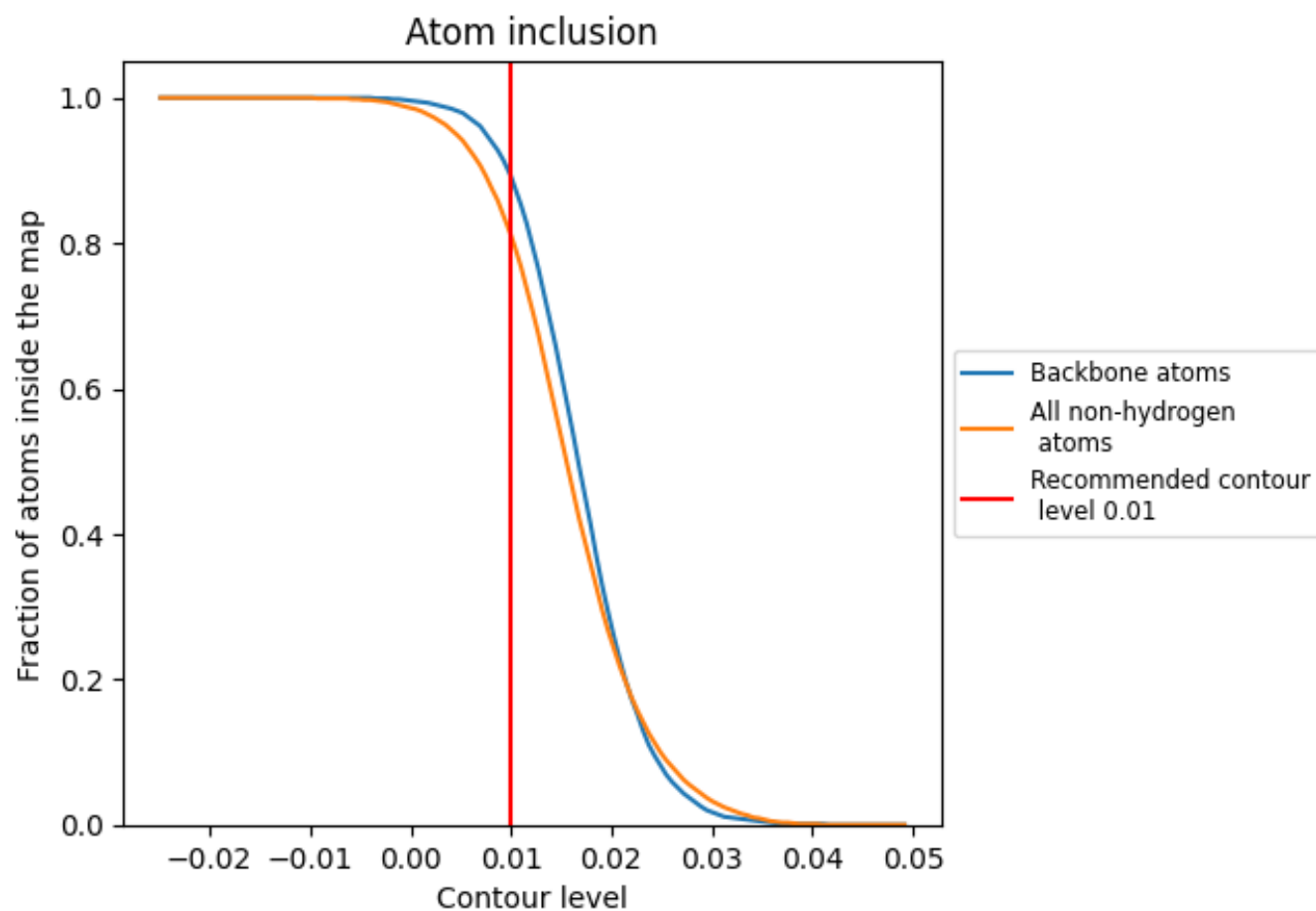
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8110	<div></div> 0.1040
A	<div></div> 0.8630	<div></div> 0.0790
B	<div></div> 0.8140	<div></div> 0.1020
C	<div></div> 0.9480	<div></div> 0.0800
D	<div></div> 0.8450	<div></div> 0.0560
E	<div></div> 0.9300	<div></div> 0.1260
F	<div></div> 0.9510	<div></div> 0.1200
G	<div></div> 0.7140	<div></div> 0.1040
H	<div></div> 0.8030	<div></div> 0.1020
I	<div></div> 0.7510	<div></div> 0.0980
J	<div></div> 0.8300	<div></div> 0.1180
K	<div></div> 0.9010	<div></div> 0.1170
L	<div></div> 0.8890	<div></div> 0.1510

1.0

0.0

<0.0