



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 02:46 am GMT

PDB ID : 6GML  
EMDB ID : EMD-0038  
Title : Structure of paused transcription complex Pol II-DSIF-NELF  
Authors : Vos, S.M.; Farnung, L.; Urlaub, H.; Cramer, P.  
Deposited on : 2018-05-27  
Resolution : 3.20 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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>.

---

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

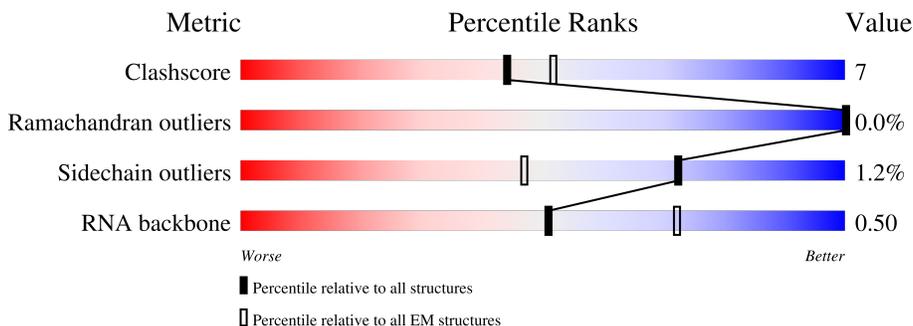
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



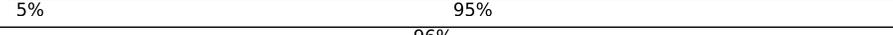
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1970	57% 14% 29%
2	B	1174	75% 19% 5%
3	C	271	82% 13% 5%
4	E	210	80% 19%
5	F	127	52% 13% 35%
6	H	150	74% 25%
7	I	125	72% 21% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	J	67	 88% 10% .
9	K	117	 80% 17% ..
10	L	58	 67% 12% 21%
11	N	48	 27% 63% 12% 25%
12	P	46	 7% 17% 11% . 63%
13	T	48	 19% 83% 8% . 6%
14	U	528	 29% 5% 65%
15	V	577	 73% 82% . 16%
16	W	584	 24% 79% 13% . 8%
17	X	404	 5% 5% 95%
18	Y	121	 96% 83% 13% .
19	Z	1087	 35% 36% 8% 57%
20	D	142	 19% 79% 12% 9%
21	G	172	 13% 81% 19% .

## 2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 44827 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
			Total	C	N	O	S		
1	A	1407	11142	7014	1997	2063	68	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1116	8928	5652	1568	1644	64	0	0

- Molecule 3 is a protein called RNA polymerase II subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2072	1301	353	412	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	209	1721	1089	300	324	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	82	658	418	113	122	5	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	148	1186	750	194	237	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	117	950	587	169	183	11	0	0

- Molecule 8 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	67	533	345	90	92	6	0	0

- Molecule 9 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	115	920	593	152	173	2	0	0

- Molecule 10 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	46	389	241	75	67	6	0	0

- Molecule 11 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	N	36	730	349	131	214	36	0	0

- Molecule 12 is a RNA chain called TAR RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	P	17	361	162	66	116	17	0	0

- Molecule 13 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	T	45	933	443	172	273	45	0	0

- Molecule 14 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	U	183	1410	895	239	269	7	0	0

- Molecule 15 is a protein called Negative elongation factor B,Negative elongation factor B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	V	483	1932	966	483	483	0	0

- Molecule 16 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	W	538	3858	2440	670	728	20	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	7	SER	-	expression tag	UNP Q8IXH7
W	8	ASN	-	expression tag	UNP Q8IXH7
W	9	ALA	-	expression tag	UNP Q8IXH7
W	51	UNK	PHE	conflict	UNP Q8IXH7
W	52	UNK	SER	conflict	UNP Q8IXH7
W	53	UNK	THR	conflict	UNP Q8IXH7
W	54	UNK	ARG	conflict	UNP Q8IXH7
W	55	UNK	ASP	conflict	UNP Q8IXH7
W	56	UNK	TYR	conflict	UNP Q8IXH7
W	57	UNK	ILE	conflict	UNP Q8IXH7
W	58	UNK	MET	conflict	UNP Q8IXH7
W	59	UNK	GLU	conflict	UNP Q8IXH7
W	60	UNK	PRO	conflict	UNP Q8IXH7
W	61	UNK	SER	conflict	UNP Q8IXH7
W	62	UNK	ILE	conflict	UNP Q8IXH7
W	63	UNK	PHE	conflict	UNP Q8IXH7
W	64	UNK	ASN	conflict	UNP Q8IXH7
W	65	UNK	THR	conflict	UNP Q8IXH7
W	66	UNK	LEU	conflict	UNP Q8IXH7
W	67	UNK	LYS	conflict	UNP Q8IXH7
W	68	UNK	ARG	conflict	UNP Q8IXH7
W	69	UNK	TYR	conflict	UNP Q8IXH7
W	70	UNK	PHE	conflict	UNP Q8IXH7
W	71	UNK	GLN	conflict	UNP Q8IXH7
W	72	UNK	ALA	conflict	UNP Q8IXH7

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
W	73	UNK	GLY	conflict	UNP Q8IXH7
W	74	UNK	GLY	conflict	UNP Q8IXH7
W	75	UNK	SER	conflict	UNP Q8IXH7
W	76	UNK	PRO	conflict	UNP Q8IXH7
W	77	UNK	GLU	conflict	UNP Q8IXH7
W	78	UNK	ASN	conflict	UNP Q8IXH7
W	79	UNK	VAL	conflict	UNP Q8IXH7
W	80	UNK	ILE	conflict	UNP Q8IXH7
W	81	UNK	GLN	conflict	UNP Q8IXH7
W	82	UNK	LEU	conflict	UNP Q8IXH7
W	83	UNK	LEU	conflict	UNP Q8IXH7
W	84	UNK	SER	conflict	UNP Q8IXH7
W	85	UNK	GLU	conflict	UNP Q8IXH7
W	86	UNK	ASN	conflict	UNP Q8IXH7
W	87	UNK	TYR	conflict	UNP Q8IXH7
W	88	UNK	THR	conflict	UNP Q8IXH7
W	89	UNK	ALA	conflict	UNP Q8IXH7
W	90	UNK	VAL	conflict	UNP Q8IXH7
W	91	UNK	ALA	conflict	UNP Q8IXH7

- Molecule 17 is a protein called Negative elongation factor E,Negative elongation factor E.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	X	22	110	66	22	22	0	0

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Y	116	911	570	159	173	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	expression tag	UNP P63272
Y	-2	PRO	-	expression tag	UNP P63272
Y	-1	GLY	-	expression tag	UNP P63272
Y	0	SER	-	expression tag	UNP P63272

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Z	470	3770	2400	663	690	17	0	0

- Molecule 20 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	D	129	998	629	170	195	4	0	1

- Molecule 21 is a protein called RNA polymerase II subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	G	171	1305	852	205	240	8	0	0

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

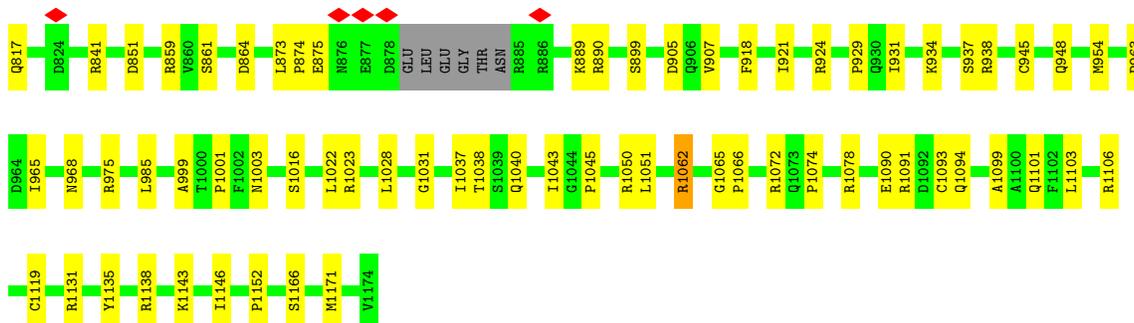
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
22	A	1	1	1	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
23	A	2	2	2	0
23	B	1	1	1	0
23	C	1	1	1	0
23	I	2	2	2	0
23	J	1	1	1	0
23	L	1	1	1	0
23	Y	1	1	1	0

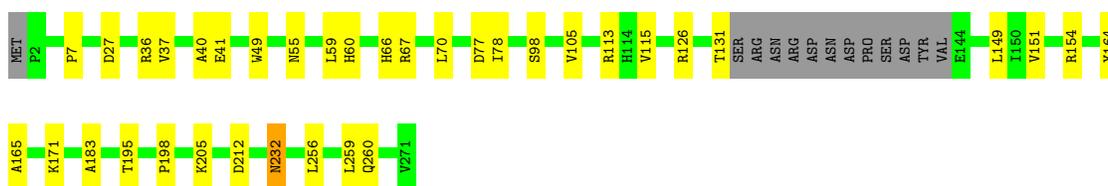






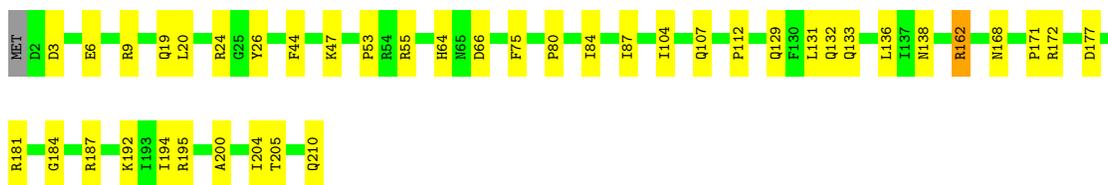
- Molecule 3: RNA polymerase II subunit C

Chain C: 82% 13% 5%



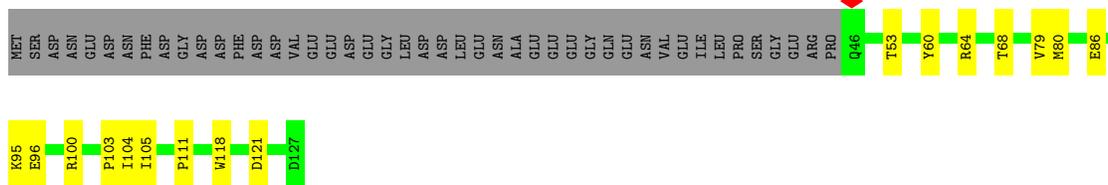
- Molecule 4: RNA polymerase II subunit E

Chain E: 80% 19%



- Molecule 5: RNA polymerase II subunit F

Chain F: 52% 13% 35%



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 74% 25%

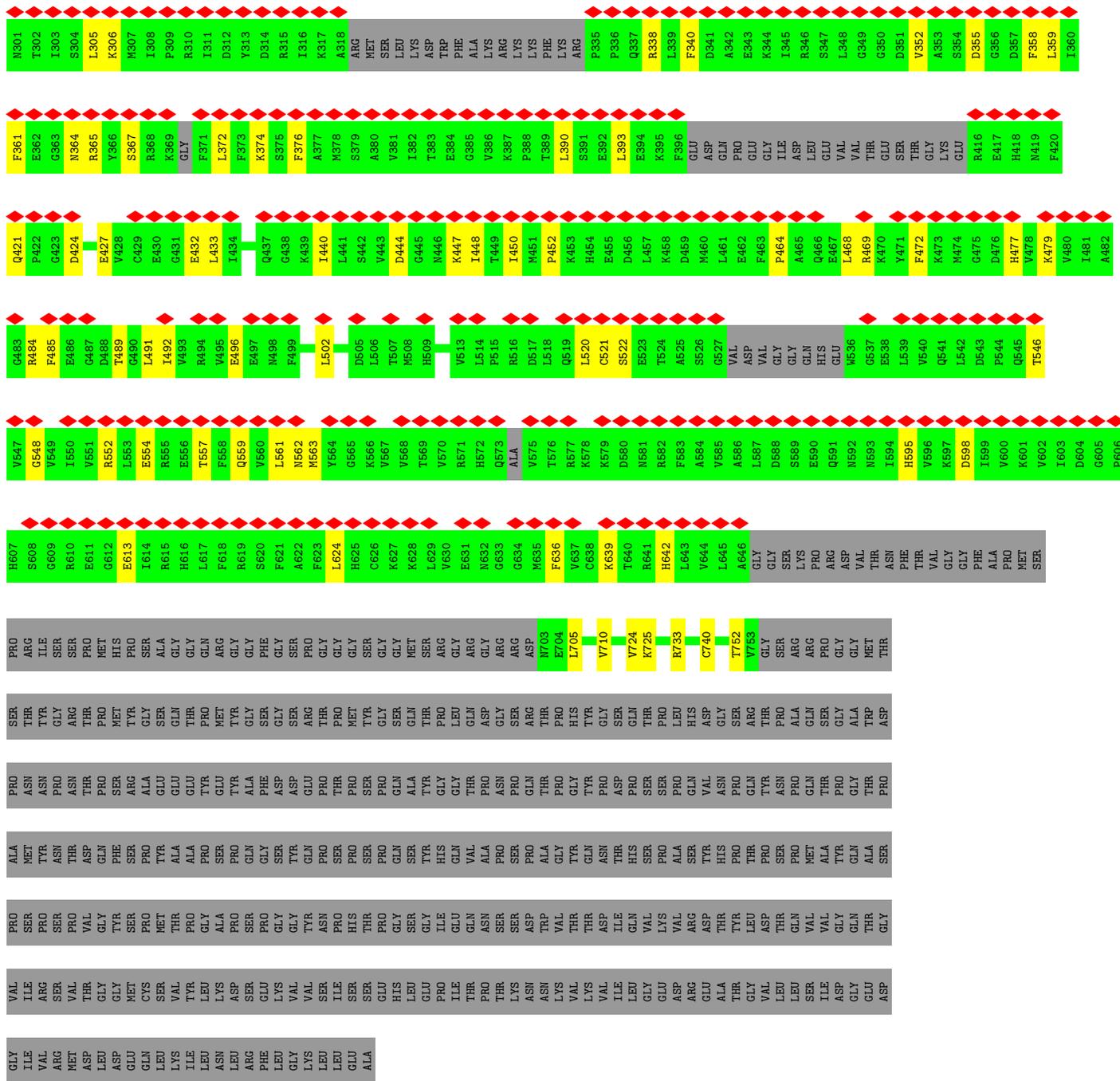




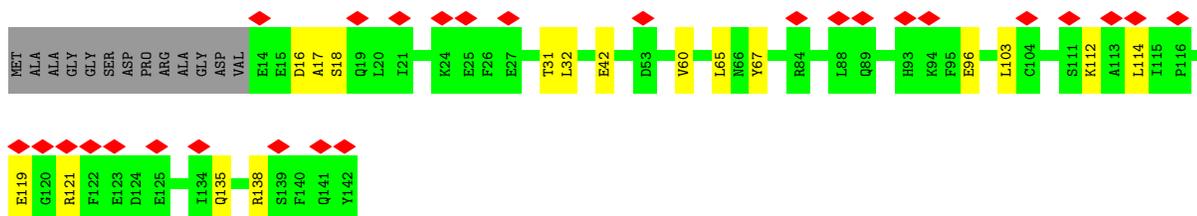
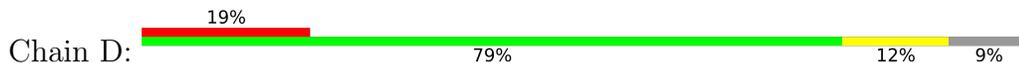






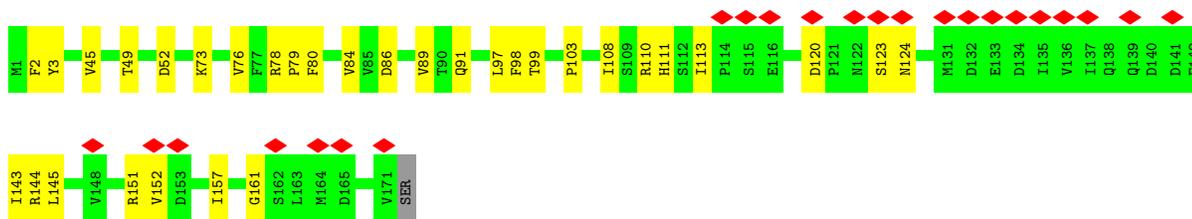


● Molecule 20: RNA polymerase II subunit D



## ● Molecule 21: RNA polymerase II subunit G

Chain G:  13% 81% 19%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	162269	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 ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00596	Depositor
Map size (Å)	314.2912, 314.2912, 314.2912	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2277, 1.2277, 1.2277	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.41	0/11345	0.61	2/15315 (0.0%)
2	B	0.45	1/9105 (0.0%)	0.60	2/12290 (0.0%)
3	C	0.48	0/2115	0.61	0/2873
4	E	0.40	0/1752	0.60	0/2366
5	F	0.40	0/668	0.56	0/901
6	H	0.44	0/1207	0.64	1/1628 (0.1%)
7	I	0.37	0/973	0.53	0/1316
8	J	0.45	0/542	0.56	0/730
9	K	0.43	0/939	0.64	2/1271 (0.2%)
10	L	0.46	0/395	0.59	0/524
11	N	0.61	0/816	0.98	0/1252
12	P	0.50	0/403	1.21	3/625 (0.5%)
13	T	0.65	0/1047	1.01	1/1617 (0.1%)
14	U	0.27	0/1434	0.58	1/1948 (0.1%)
15	V	0.23	0/1772	0.42	0/2201
16	W	0.32	0/3719	0.57	0/5065
18	Y	0.25	0/927	0.46	0/1250
19	Z	0.28	0/3833	0.51	1/5156 (0.0%)
20	D	0.26	0/1012	0.47	0/1366
21	G	0.32	0/1336	0.53	0/1820
All	All	0.40	1/45340 (0.0%)	0.62	13/61514 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	1
16	W	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
21	G	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	94	SER	C-N	-5.76	1.20	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	80	ASP	CB-CG-OD1	7.92	125.43	118.30
14	U	97	LEU	CA-CB-CG	6.36	129.93	115.30
2	B	492	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	486	LEU	CB-CG-CD2	-5.56	101.55	111.00
9	K	79	PRO	C-N-CA	5.50	135.44	121.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1108	HIS	Peptide
1	A	1112	VAL	Peptide
1	A	1467	GLY	Peptide
1	A	412	GLN	Peptide
1	A	910	LYS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11142	0	11291	205	0
2	B	8928	0	8949	172	0
3	C	2072	0	2016	29	0
4	E	1721	0	1737	29	0
5	F	658	0	684	13	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1186	0	1147	30	0
7	I	950	0	880	20	0
8	J	533	0	553	8	0
9	K	920	0	942	15	0
10	L	389	0	395	5	0
11	N	730	0	407	6	0
12	P	361	0	185	9	0
13	T	933	0	509	6	0
14	U	1410	0	1455	22	0
15	V	1932	0	467	5	0
16	W	3858	0	3482	57	0
17	X	110	0	24	0	0
18	Y	911	0	905	12	0
19	Z	3770	0	3836	53	0
20	D	998	0	953	13	0
21	G	1305	0	1267	25	0
22	A	1	0	0	0	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	Y	1	0	0	0	0
All	All	44827	0	42084	599	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 599 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)
16:W:444:GLN:NE2	16:W:488:GLU:OE2	2.05	0.89
18:Y:58:ASP:OD2	19:Z:268:LYS:NZ	2.06	0.89
2:B:83:ARG:HH12	2:B:139:GLN:HB3	1.37	0.87
19:Z:306:LYS:HA	19:Z:372:LEU:O	1.77	0.85
4:E:24:ARG:HH12	4:E:184:GLY:HA3	1.42	0.84

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	1395/1970 (71%)	1299 (93%)	95 (7%)	1 (0%)	51	83
2	B	1102/1174 (94%)	1031 (94%)	71 (6%)	0	100	100
3	C	254/271 (94%)	242 (95%)	12 (5%)	0	100	100
4	E	207/210 (99%)	196 (95%)	11 (5%)	0	100	100
5	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
6	H	146/150 (97%)	138 (94%)	8 (6%)	0	100	100
7	I	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
8	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
9	K	113/117 (97%)	108 (96%)	5 (4%)	0	100	100
10	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
14	U	181/528 (34%)	178 (98%)	3 (2%)	0	100	100
15	V	430/577 (74%)	404 (94%)	26 (6%)	0	100	100
16	W	492/584 (84%)	449 (91%)	42 (8%)	1 (0%)	47	79
18	Y	114/121 (94%)	110 (96%)	4 (4%)	0	100	100
19	Z	454/1087 (42%)	431 (95%)	23 (5%)	0	100	100
20	D	127/142 (89%)	120 (94%)	7 (6%)	0	100	100
21	G	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
All	All	5488/7480 (73%)	5162 (94%)	324 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1108	HIS
16	W	574	PRO

### 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	A	1238/1749 (71%)	1222 (99%)	16 (1%)	69	87
2	B	979/1027 (95%)	963 (98%)	16 (2%)	62	84
3	C	235/248 (95%)	232 (99%)	3 (1%)	69	87
4	E	191/192 (100%)	189 (99%)	2 (1%)	76	90
5	F	71/111 (64%)	71 (100%)	0	100	100
6	H	129/131 (98%)	127 (98%)	2 (2%)	62	84
7	I	105/112 (94%)	102 (97%)	3 (3%)	42	74
8	J	56/56 (100%)	55 (98%)	1 (2%)	59	82
9	K	104/106 (98%)	103 (99%)	1 (1%)	76	90
10	L	43/55 (78%)	42 (98%)	1 (2%)	50	78
14	U	158/451 (35%)	156 (99%)	2 (1%)	69	87
16	W	360/475 (76%)	357 (99%)	3 (1%)	81	93
18	Y	102/105 (97%)	102 (100%)	0	100	100
19	Z	417/940 (44%)	416 (100%)	1 (0%)	93	98
20	D	104/126 (82%)	104 (100%)	0	100	100
21	G	138/153 (90%)	138 (100%)	0	100	100
All	All	4430/6037 (73%)	4379 (99%)	51 (1%)	72	88

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	650	ASN
4	E	162	ARG
16	W	375	ARG
2	B	889	LYS
3	C	55	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	518	HIS
19	Z	642	HIS
2	B	1040	GLN
18	Y	12	HIS
14	U	142	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	P	16/46 (34%)	8 (50%)	1 (6%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	P	31	A
12	P	32	A
12	P	33	C
12	P	34	U
12	P	35	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	P	38	G

## 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 10 ligands modelled in this entry, 10 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	W	2
15	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	419:ARG	C	420:MET	N	7.63
1	W	185:GLN	C	186:GLY	N	4.08
1	W	588:MET	C	589:VAL	N	3.94

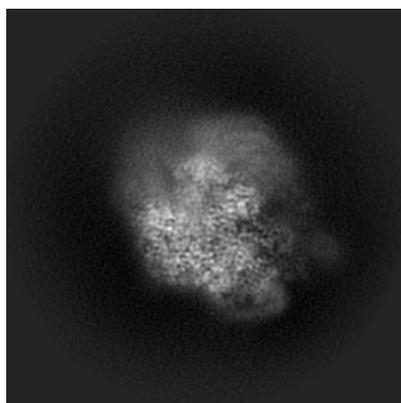
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0038. These allow visual inspection of the internal detail of the map and identification of artifacts.

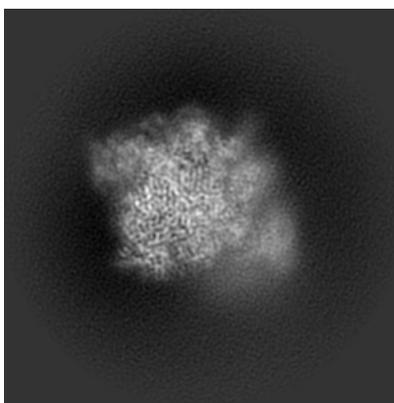
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

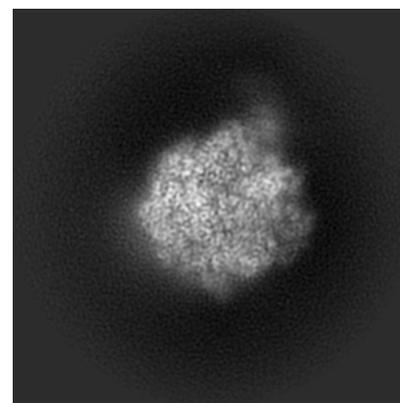
#### 6.1.1 Primary map



X

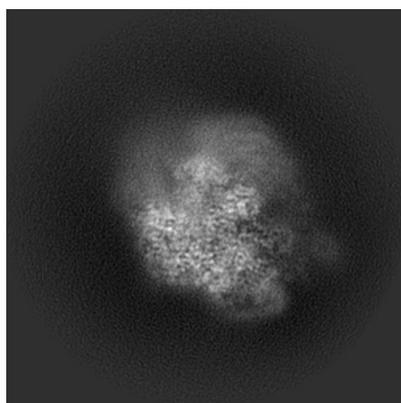


Y

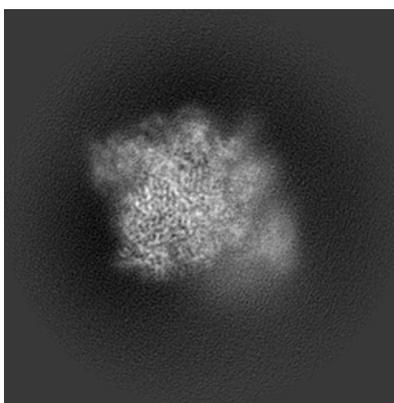


Z

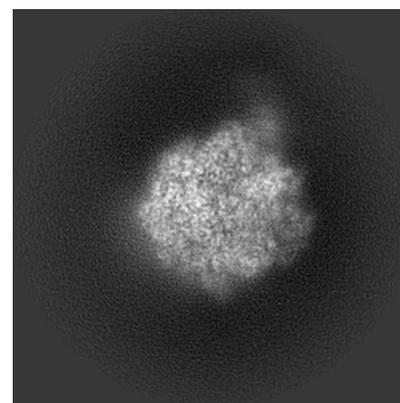
#### 6.1.2 Raw map



X



Y

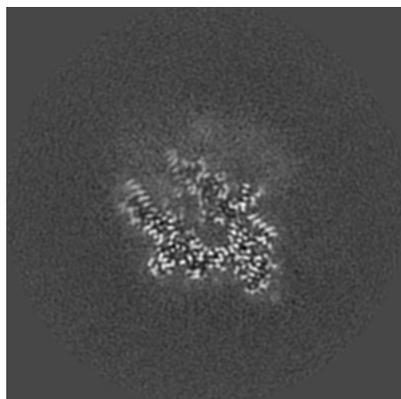


Z

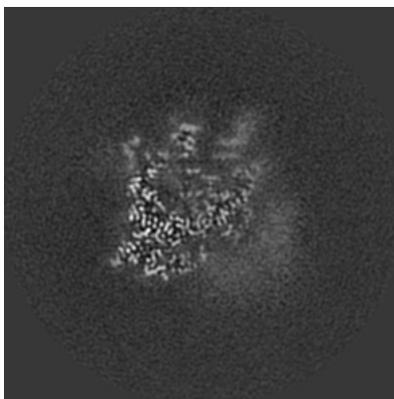
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

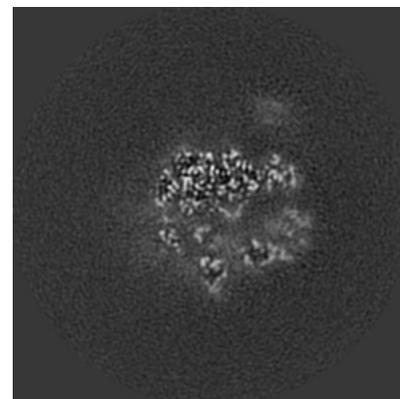
### 6.2.1 Primary map



X Index: 128

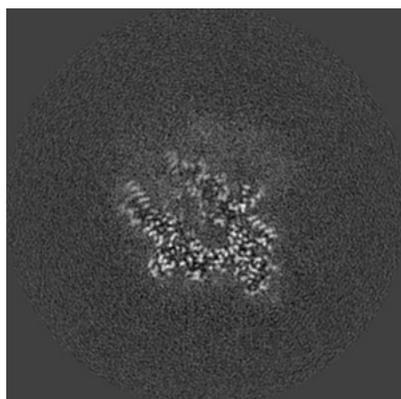


Y Index: 128

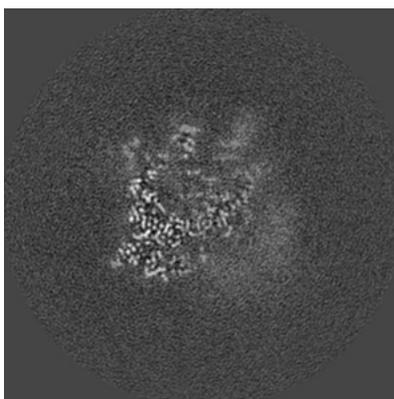


Z Index: 128

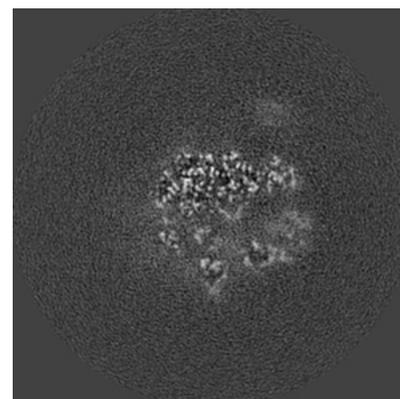
### 6.2.2 Raw map



X Index: 128



Y Index: 128

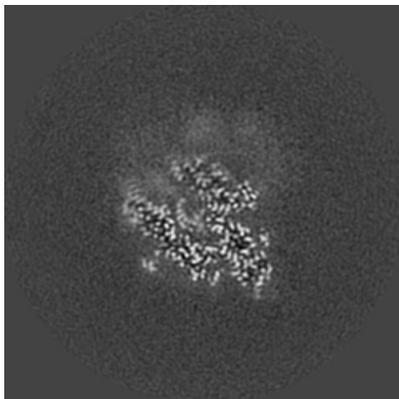


Z Index: 128

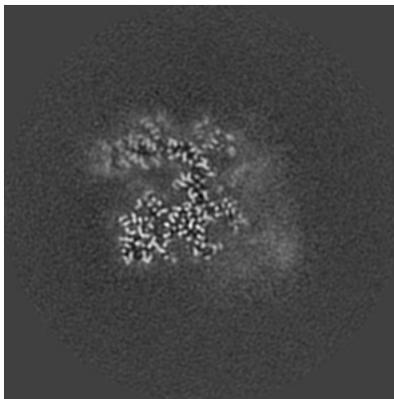
The images above show central slices of the map in three orthogonal directions.

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

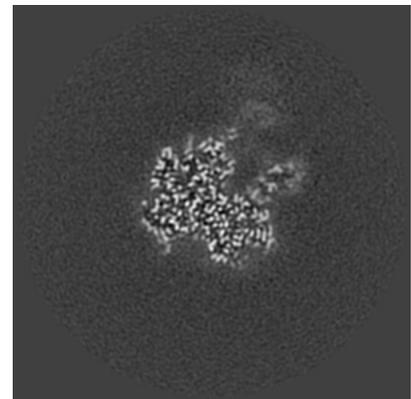
### 6.3.1 Primary map



X Index: 124

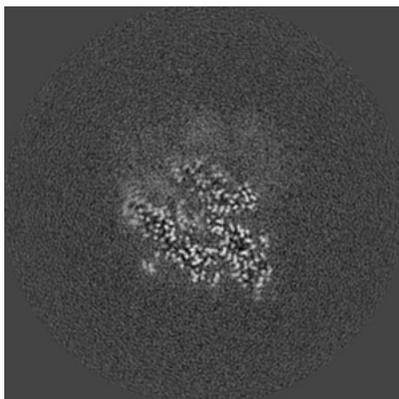


Y Index: 139

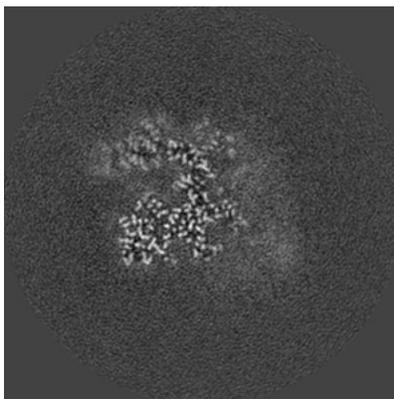


Z Index: 93

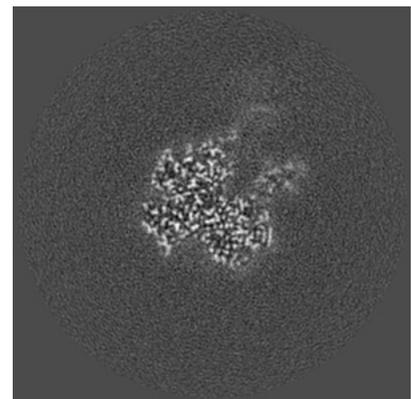
### 6.3.2 Raw map



X Index: 124



Y Index: 139

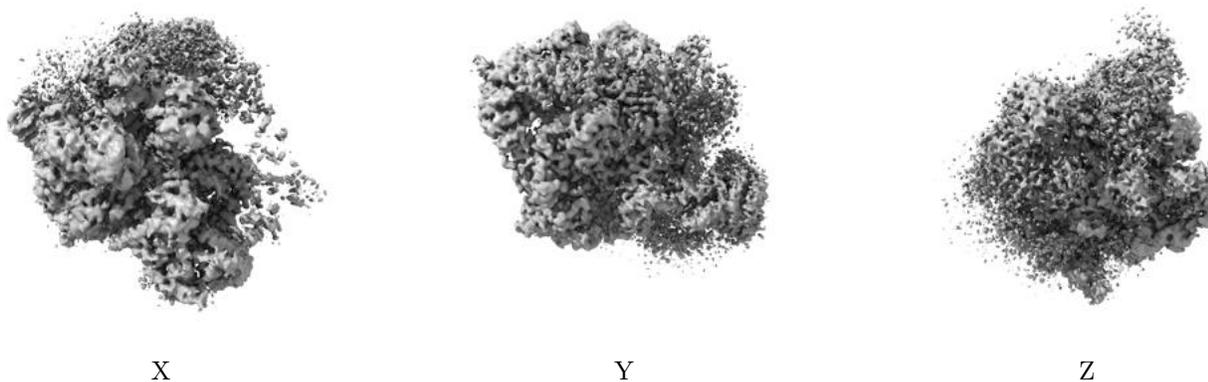


Z Index: 94

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

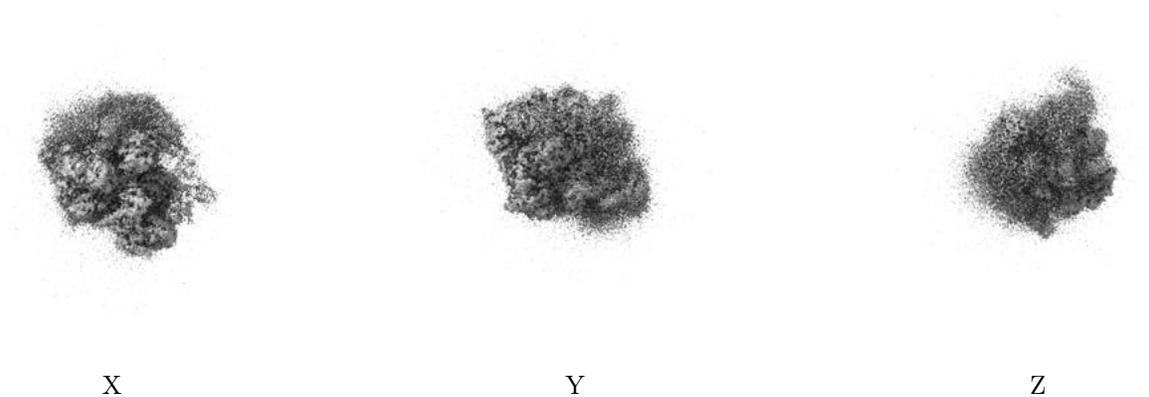
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00596. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

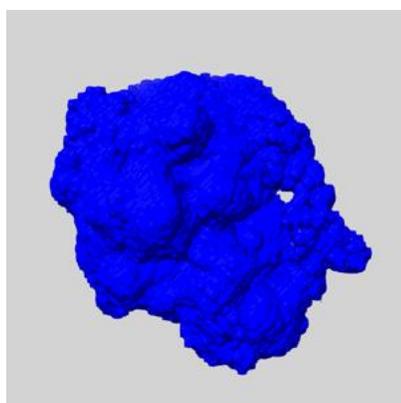
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

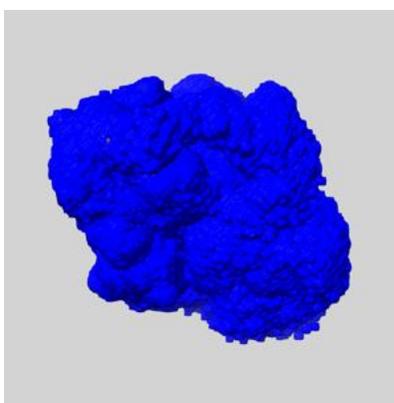
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

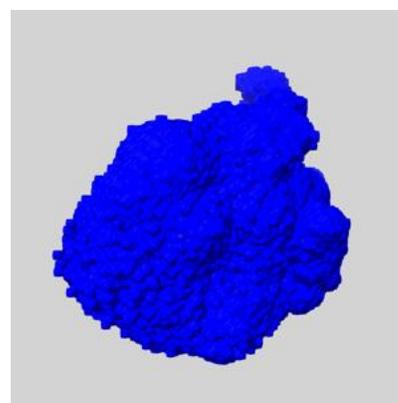
### 6.5.1 emd\_0038\_msk\_1.map [i](#)



X



Y

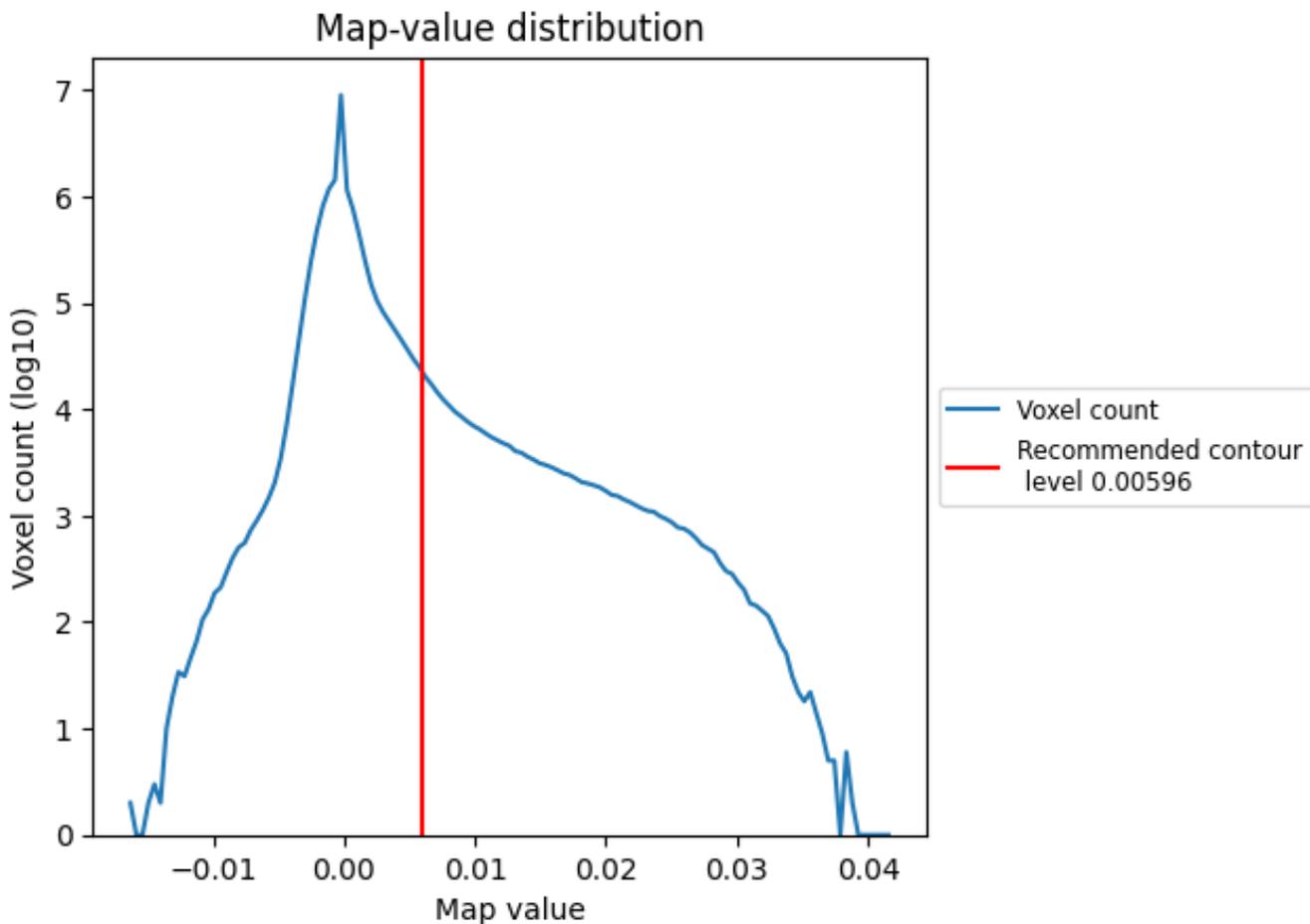


Z

## 7 Map analysis [i](#)

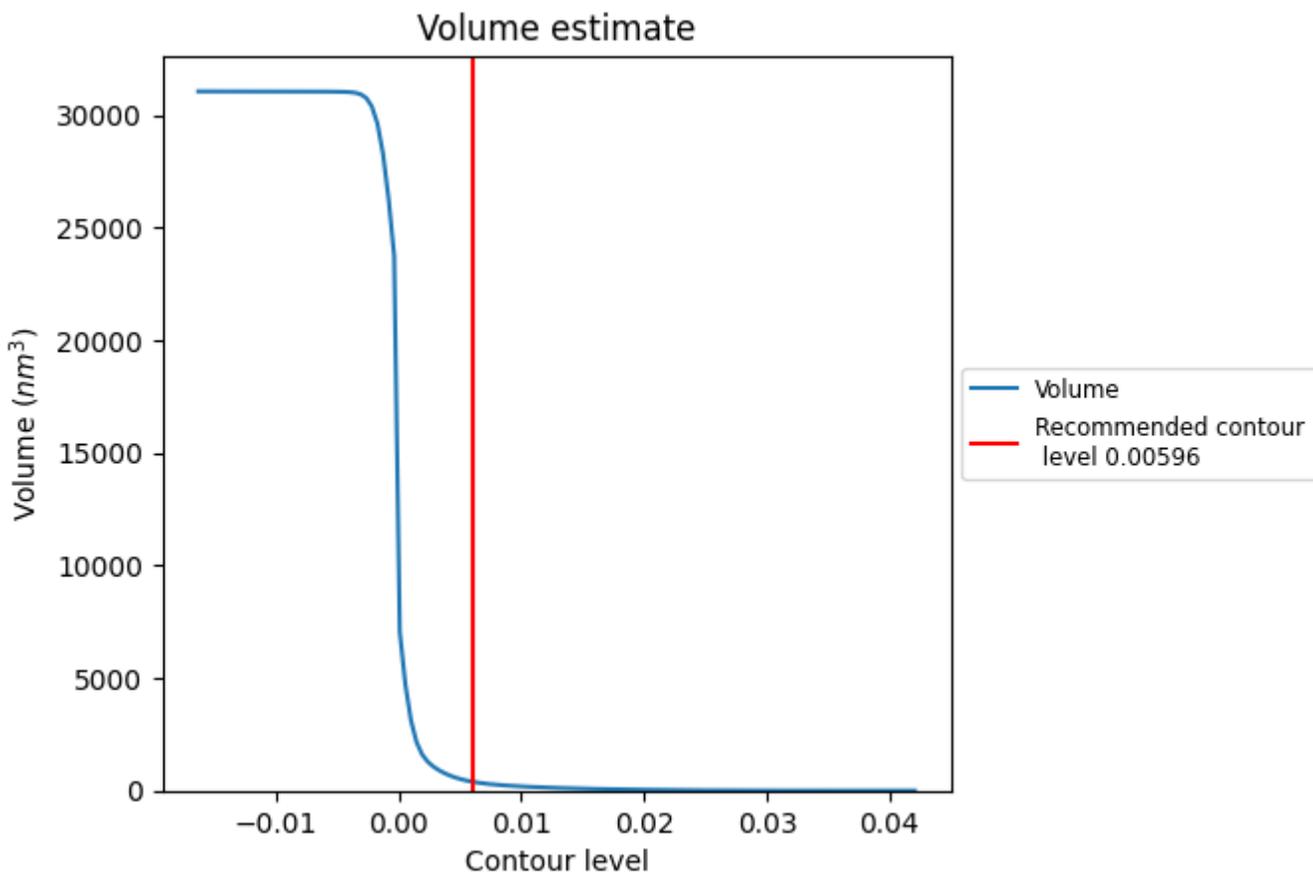
This section contains the results of statistical analysis of the map.

### 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.

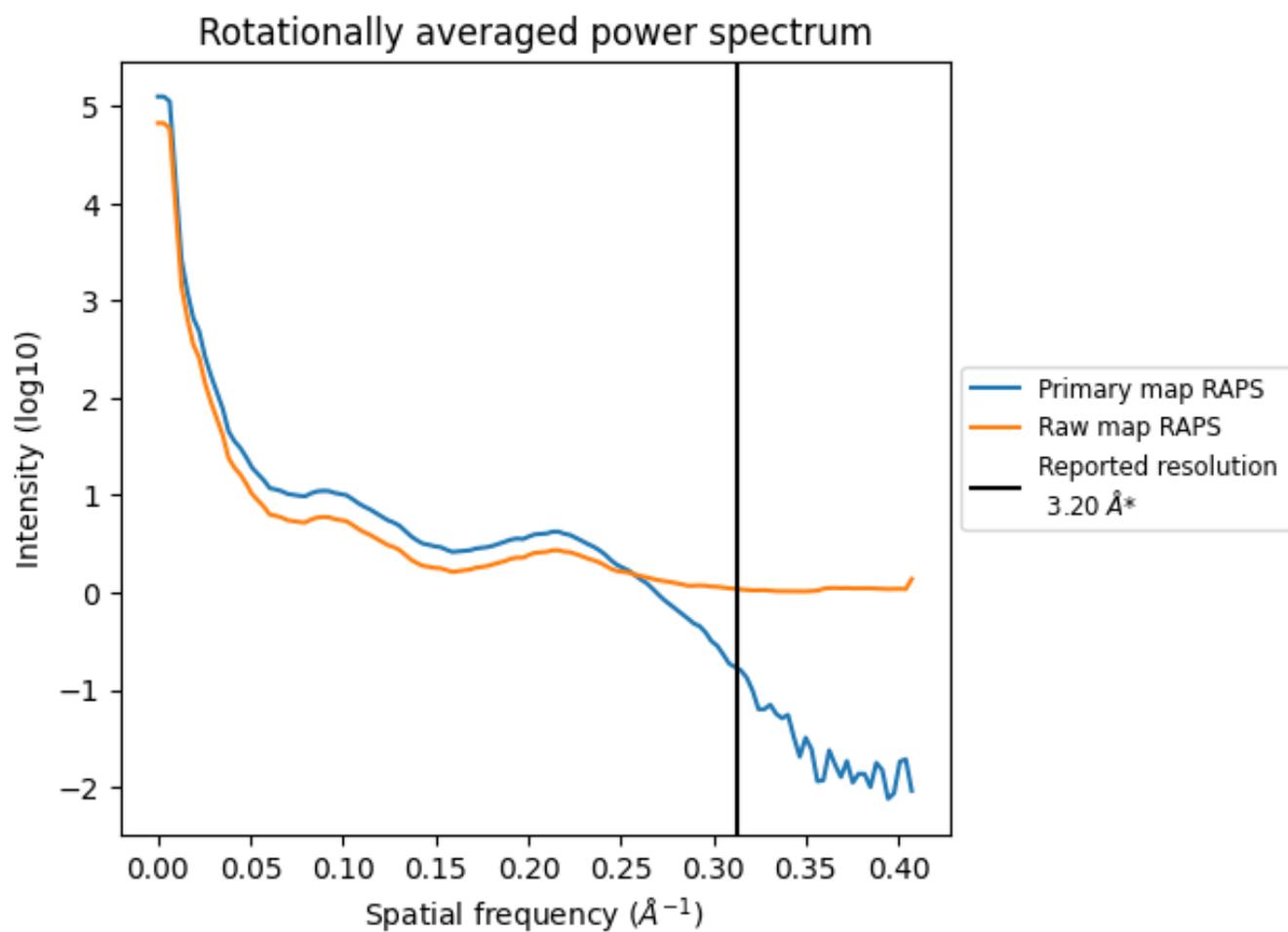
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 400 nm<sup>3</sup>; this corresponds to an approximate mass of 362 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

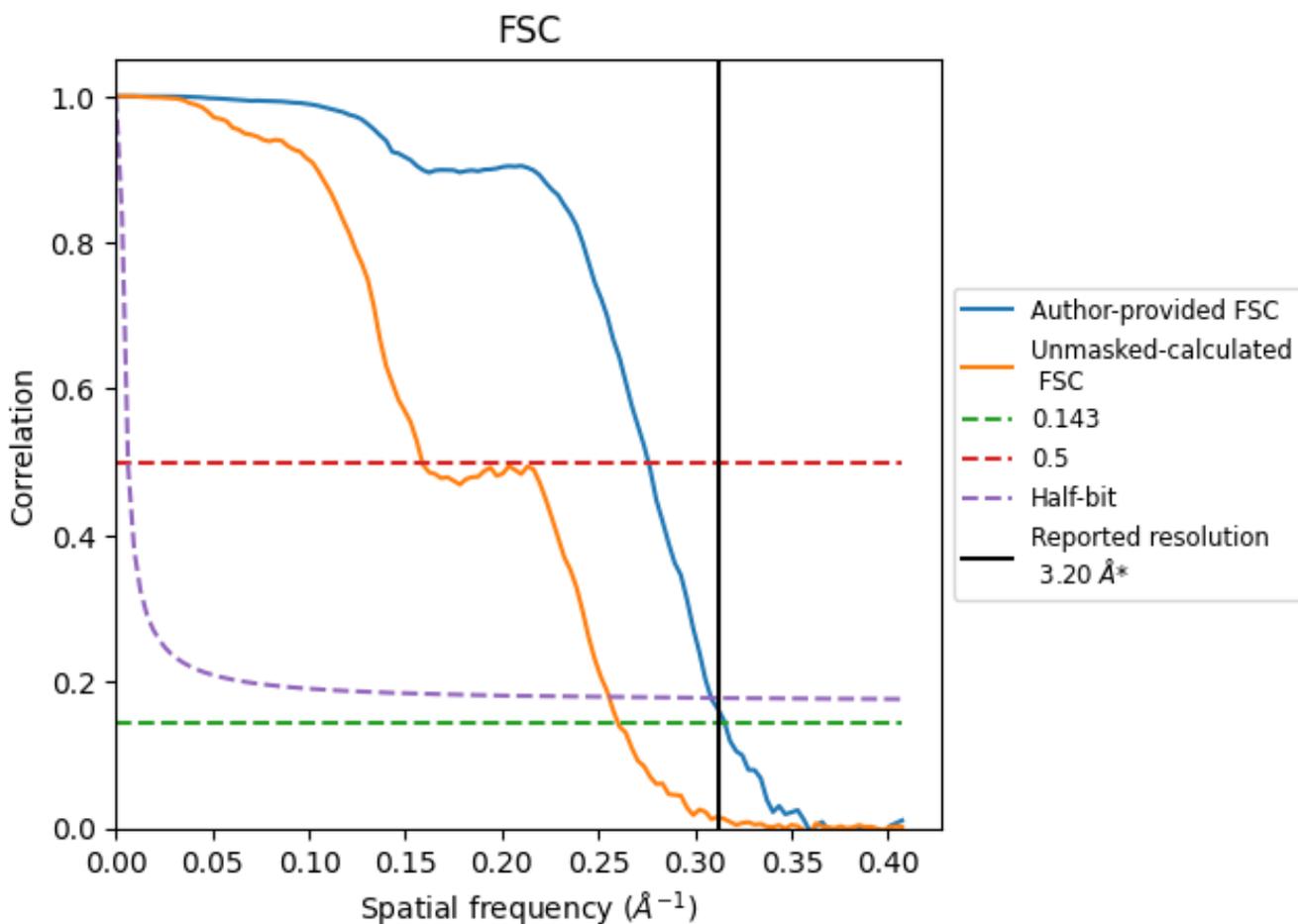


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

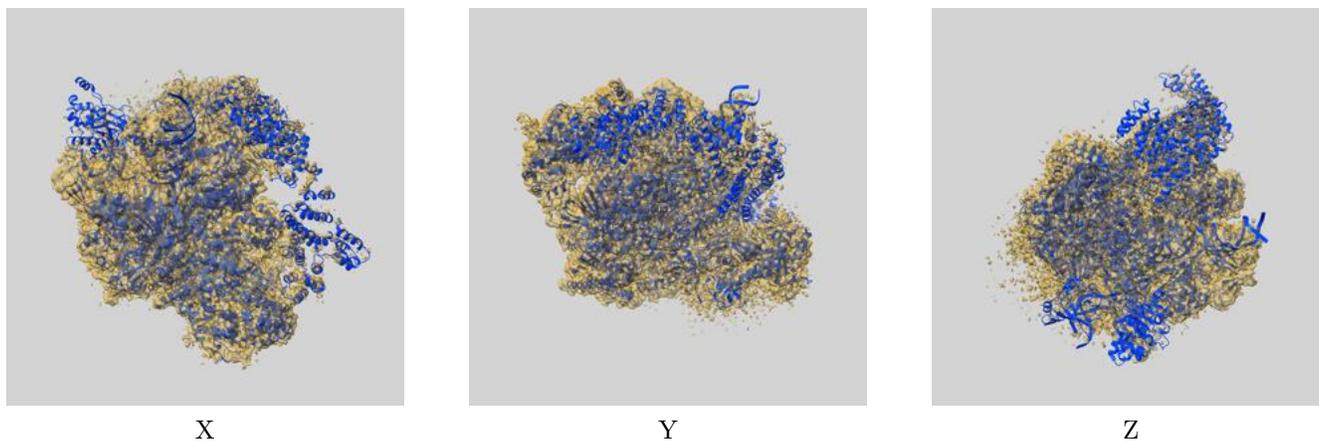
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.62	3.24
Unmasked-calculated*	3.84	6.30	3.91

\*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 3.84 differs from the reported value 3.2 by more than 10 %

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

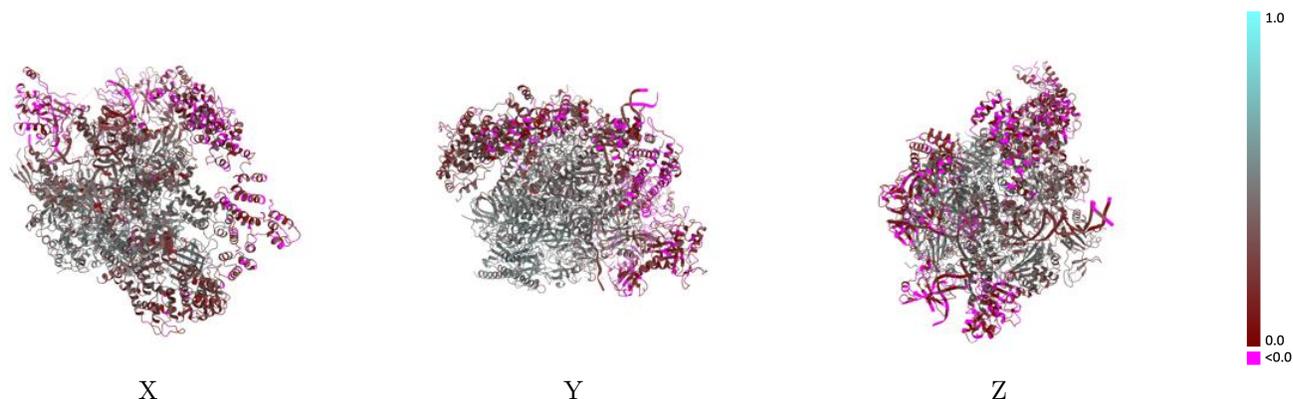
This section contains information regarding the fit between EMDB map EMD-0038 and PDB model 6GML. Per-residue inclusion information can be found in section [3](#) on page [9](#).

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



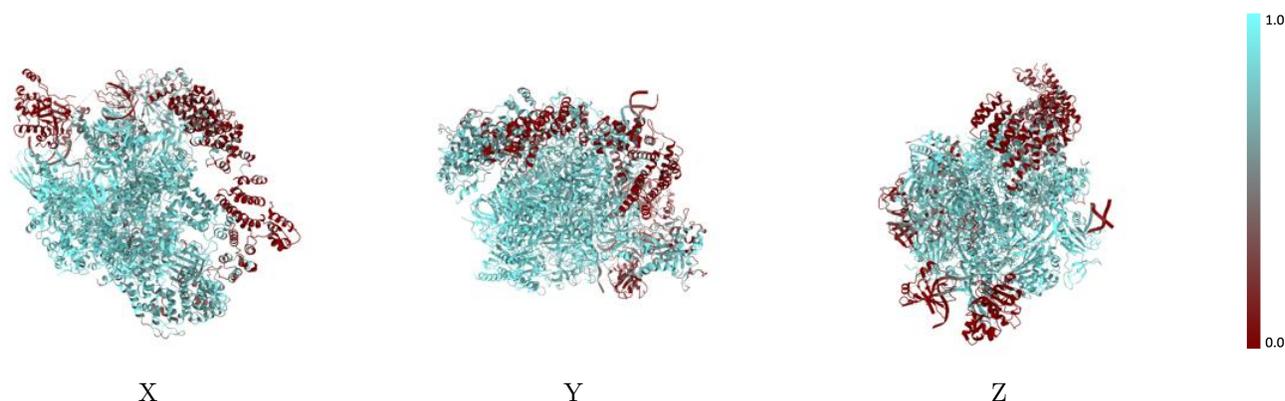
The images above show the 3D surface view of the map at the recommended contour level 0.00596 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



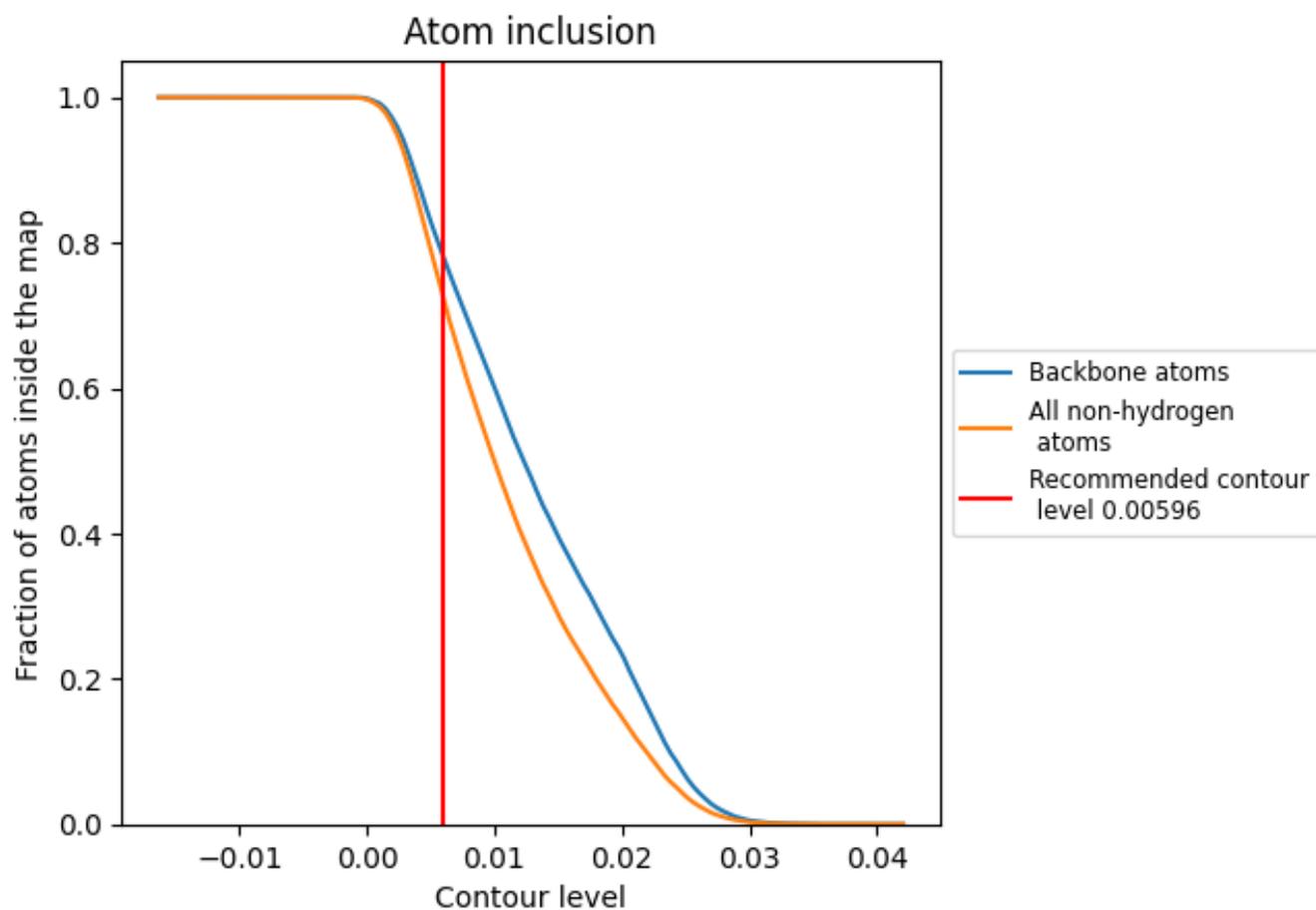
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00596).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.00596) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7258	 0.3400
A	 0.8634	 0.4160
B	 0.9000	 0.4560
C	 0.9321	 0.4940
D	 0.6416	 0.1410
E	 0.8429	 0.3590
F	 0.8670	 0.4310
G	 0.7073	 0.2060
H	 0.8904	 0.4620
I	 0.8743	 0.3860
J	 0.9213	 0.4940
K	 0.9320	 0.5010
L	 0.8820	 0.4270
N	 0.5822	 0.1630
P	 0.8033	 0.2980
T	 0.7181	 0.2310
U	 0.7116	 0.2660
V	 0.1325	 0.1000
W	 0.6354	 0.2640
X	 0.1455	 0.0280
Y	 0.0022	 0.0200
Z	 0.1865	 0.0840

