



## wwPDB EM Validation Summary Report ⓘ

Jun 4, 2023 – 08:09 am BST

PDB ID : 8BVW  
EMDB ID : EMD-16274  
Title : RNA polymerase II pre-initiation complex with the distal +1 nucleosome (PIC-Nuc18W)  
Authors : Abril-Garrido, J.; Dienemann, C.; Grabbe, F.; Velychko, T.; Lidschreiber, M.; Wang, H.; Cramer, P.  
Deposited on : 2022-12-20  
Resolution : 4.00 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:

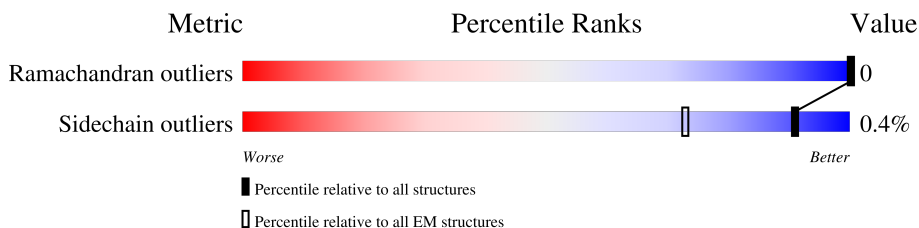
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

# 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 4.00 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	0	772	78% (green), 22% (grey)
2	1	760	94% (green), 6% (grey)
3	2	548	48% (green), 52% (grey)
4	3	462	91% (green), 9% (grey)
5	4	395	88% (green), 12% (grey)
6	5	308	85% (green), 15% (grey)
7	6	71	97% (green), 3% (grey)
8	7	309	11% (red), 68% (green), 31% (grey)
9	8	346	7% (red), 86% (green), 14% (grey)









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Mol	Chain	Length	Quality of chain
10	9	323	18% 88% 11%
11	A	1970	72% 28%
12	B	1174	97%
13	C	275	93% 7%
14	D	142	90% 10%
15	E	210	98%
16	F	127	62% 38%
17	G	172	98%
18	H	150	99%
19	I	125	91% 9%
20	J	67	94%
21	K	117	98%
22	L	58	76% 24%
23	M	316	79% 20%
24	N	218	5% 90% 5% 6%
25	O	339	53% 47%
26	Q	517	26% 73%
27	R	249	89% 11%
28	T	218	5% 90% 6%
29	U	376	30% 70%
30	V	109	89% 9%
31	W	439	46% 54%
32	X	291	59% 41%
33	Y	8	100%
34	Z	19	100%

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Mol	Chain	Length	Quality of chain
35	a	136	 71% 29%
35	e	136	 72% 28%
36	b	103	 80% 20%
36	f	103	 78% 22%
37	c	130	 84% 16%
37	g	130	 82% 18%
38	d	126	 77% 23%
38	h	126	 75% 25%

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 84783 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 General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

- Molecule 2 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 3 is a protein called General transcription factor IIIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	265	Total	C	N	O	S	0	0
			2167	1382	378	395	12		

- Molecule 4 is a protein called General transcription factor IIIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	421	Total	C	N	O	S	0	0
			3337	2154	584	586	13		

- Molecule 5 is a protein called General transcription factor IIIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	347	Total	C	N	O	S	0	0
			2732	1726	471	508	27		

- Molecule 6 is a protein called General transcription factor IIIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	263	Total	C	N	O	S	0	0
			2066	1323	344	380	19		

- Molecule 7 is a protein called General transcription factor IIIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	69	548	352	88	105	3	0	0

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	212	1724	1083	297	332	12	0	0

- Molecule 9 is a protein called Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	299	2378	1535	406	426	11	0	0

- Molecule 10 is a protein called Cyclin-H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	287	2334	1493	402	422	17	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	A	1423	11274	7092	2016	2094	72	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	TYR	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	THR	deletion	UNP A0A7M4DUC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP A0A7M4DUC2
A	?	-	PRO	deletion	UNP A0A7M4DUC2
A	?	-	SER	deletion	UNP A0A7M4DUC2

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	B	1136	9076	5739	1597	1676	64	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C	257	2059	1294	351	408	6	0	0

- Molecule 14 is a protein called RNA polymerase II subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	D	128	1050	656	178	212	4	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit E.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	79	636	406	108	117	5	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	171	1351	875	219	249	8	0	0

- Molecule 18 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		
18	H	148	1186	750	194	237	5	0	0

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	114	928	571	166	180	11	0	0

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	64	507	328	86	87	6	0	0

- Molecule 21 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 22 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	L	44	373	231	72	64	6	0	0

- Molecule 23 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	M	252	1953	1224	346	366	17	0	0

- Molecule 24 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	N	206	4213	1998	774	1236	205	0	0

- Molecule 25 is a protein called TATA-box-binding protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	179	Total	C	N	O	S	0	0
			1422	923	251	241	7		

- Molecule 26 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 27 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 28 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	206	Total	C	N	O	P	0	0
			4227	2002	788	1232	205		

- Molecule 29 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 30 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 31 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	202	Total	C	N	O	S	0	0
			1659	1042	299	307	11		

- Molecule 32 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	171	1403	895	243	261	4	0	0

- Molecule 33 is a protein called Unassigned peptide, likely XPB.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Y	8	40	24	8	8	0	0

- Molecule 34 is a protein called Unassigned peptide, likely TFIIE-beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	Z	19	95	57	19	19	0	0

- Molecule 35 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	a	97	802	506	155	138	3	0	0
35	e	98	811	512	157	139	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	103	ALA	GLY	engineered mutation	UNP P84233
e	103	ALA	GLY	engineered mutation	UNP P84233

- Molecule 36 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	b	82	653	412	127	113	1	0	0
36	f	80	638	401	125	111	1	0	0

- Molecule 37 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	c	109	843	531	167	145	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
37	g	106	818	516	160	142	0	0

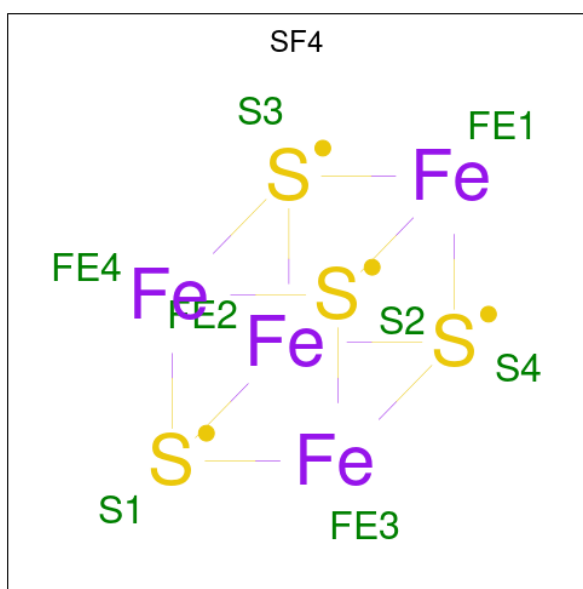
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	100	ARG	GLY	engineered mutation	UNP P06897
g	100	ARG	GLY	engineered mutation	UNP P06897

- Molecule 38 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	d	97	766	480	142	142	2	0	0
38	h	95	744	468	134	140	2	0	0

- Molecule 39 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
39	1	1	8	4	4	0

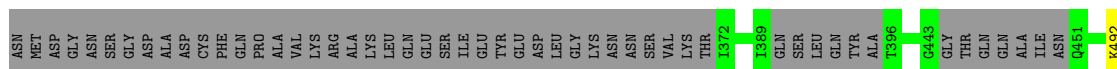
- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
40	4	3	Total 3	Zn 3	0
40	5	2	Total 2	Zn 2	0
40	7	2	Total 2	Zn 2	0
40	A	2	Total 2	Zn 2	0
40	B	1	Total 1	Zn 1	0
40	C	1	Total 1	Zn 1	0
40	I	2	Total 2	Zn 2	0
40	J	1	Total 1	Zn 1	0
40	L	1	Total 1	Zn 1	0
40	M	1	Total 1	Zn 1	0
40	W	1	Total 1	Zn 1	0

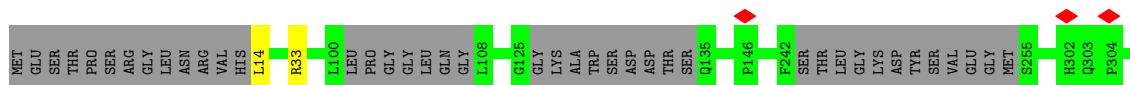
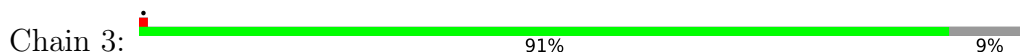
- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

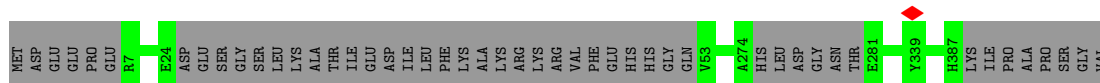
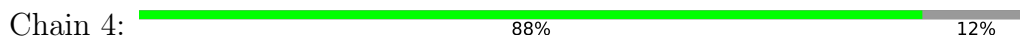




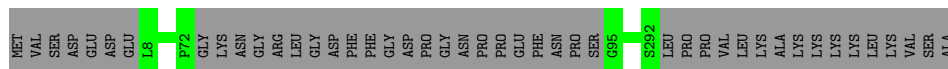
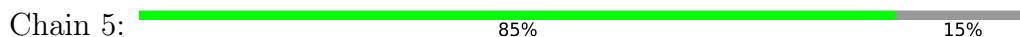
- Molecule 4: General transcription factor IIH subunit 4



- Molecule 5: General transcription factor IIH subunit 2



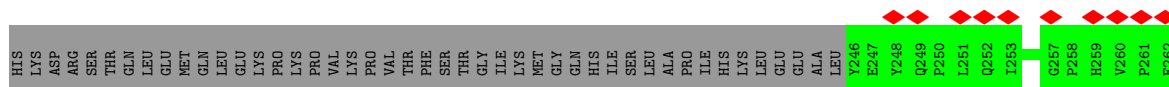
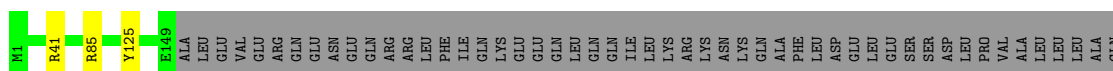
- Molecule 6: General transcription factor IIH subunit 3



- Molecule 7: General transcription factor IIH subunit 5



- Molecule 8: CDK-activating kinase assembly factor MAT1









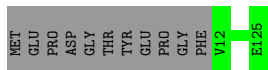
- Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  99%



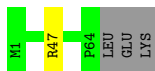
- Molecule 19: DNA-directed RNA polymerase II subunit RPB9

Chain I:  91%



- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  94%



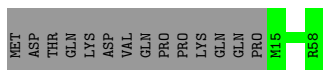
- Molecule 21: DNA-directed RNA polymerase II subunit RPB11-a

Chain K:  98%




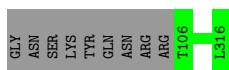
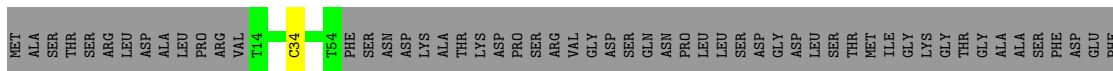
- Molecule 22: RNA polymerase II subunit K

Chain L:  76%




- Molecule 23: Transcription initiation factor IIB

Chain M:  79%

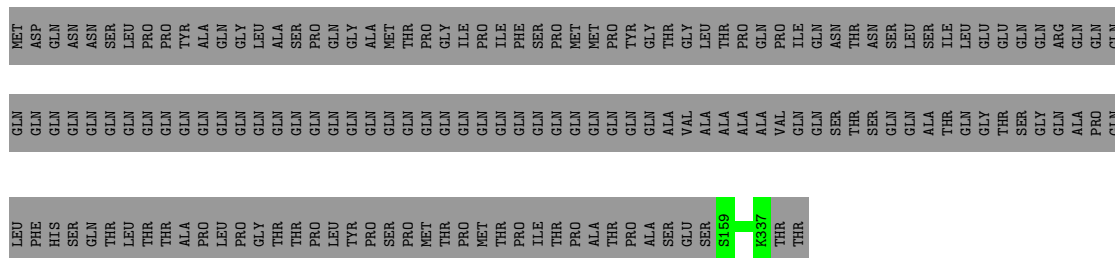


- Molecule 24: Non-template DNA

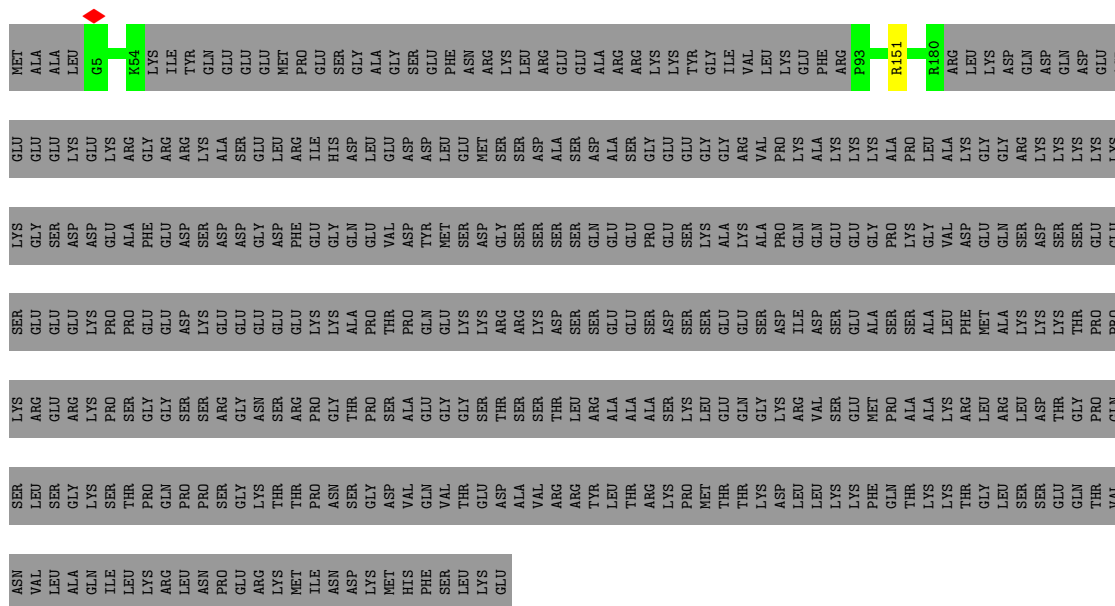
Chain N:  5%



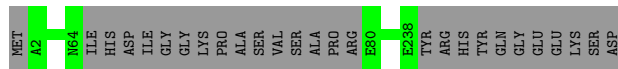
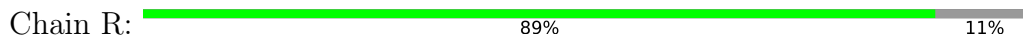
• Molecule 25: TATA-box-binding protein



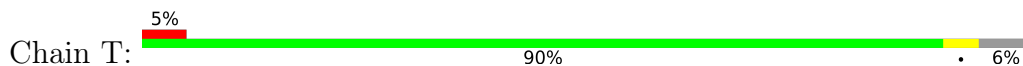
• Molecule 26: General transcription factor IIF subunit 1



• Molecule 27: General transcription factor IIF subunit 2



• Molecule 28: Template DNA





MET ASP PRO SER LEU ARG GLU ARG GLU LEU PHE LYS LYS ARG SER ALA LEU MET GLN SER THR PRO VAL VAL ARG LYS ARG SER SER ALA PRO ALA SER GLN ARG GLU SER SER SER SER SER SER LYS LYS LYS LYS LYS THR LYS VAL VAL GLU HIS GLY SER SER SER GLY SER VAL LYS LYS THR THR LYS VAL GLU HIS HIS ASN GLY SER SER SER SER GLY SER SER ASP HIS ASP ASP ASP ASP ASP ASN ASN GLY

SER PHE ASN LEU LYS LYS LEU SER GLY SER SER SER G72 G72 1242 1242 SER SER MET GLN SER THR PRO VAL VAL LYS LYS LYS VAL ALA ALA PRO ILE SER SER GLN ARG ARG GLU SER SER SER SER SER SER SER SER SER LYS LYS LYS LYS ARG ARG PHE LYS LYS THR THR LYS VAL VAL GLU HIS HIS ASN GLY SER SER SER SER GLY SER SER ASP HIS ASP ASP ASP ASN ASN GLY

SER SER LYS

- Molecule 33: Unassigned peptide, likely XPB

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: Unassigned peptide, likely TFIIE-beta

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 35: Histone H3.2

Chain a:  71% 29%


MET ALA ARG THR LYS LYS THR ALA ARG LYS THR GLY LYS PRO ARG LYS GLN LEU ALA THR LYS LYS ALA ALA ARG LYS SER SER ALA PRO ALA THR GLY GLY VAL LYS LYS P39 H40 H35 ALA

- Molecule 35: Histone H3.2

Chain e:  72% 28%


MET ALA ARG THR LYS LYS THR ALA ARG LYS THR GLY LYS PRO ARG LYS GLN LEU ALA THR LYS LYS ALA ALA ARG LYS SER SER ALA PRO ALA THR GLY GLY VAL LYS LYS K38 P39 H35 ALA

- Molecule 36: Histone H4

Chain b:  80% 20%

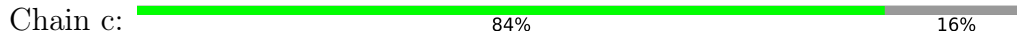
MET SER GLY ARG GLY LYS GLY LYS LEU LEU GLY LYS GLY LYS GLY ALA ALA LYS ARG HIS ARG LYS W22 G103

- Molecule 36: Histone H4

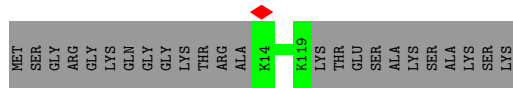
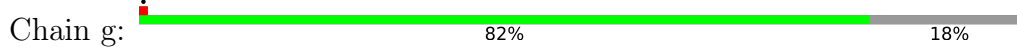
Chain f:  78% 22%

MET SER GLY ARG GLY LYS GLY LYS LEU LEU GLY LYS GLY LYS GLY ALA ALA LYS ARG HIS ARG LYS VAL LEU R24 G103

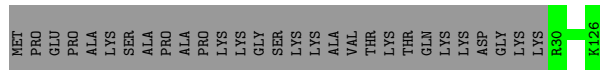
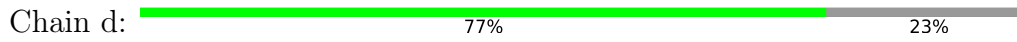
- Molecule 37: Histone H2A type 1



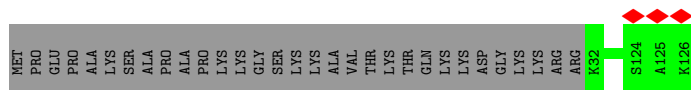
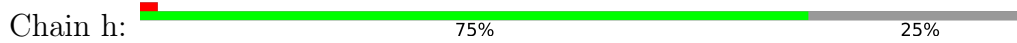
● Molecule 37: Histone H2A type 1



● Molecule 38: Histone H2B 1.1



● Molecule 38: Histone H2B 1.1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188832	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 ( $e^-/\text{\AA}^2$ )	41.58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	44.013	Depositor
Minimum map value	-19.392	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size ( $\text{\AA}$ )	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.05, 1.05, 1.05	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 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	0	0.27	0/4994	0.53	0/6745
2	1	0.26	0/5875	0.56	0/7955
3	2	0.25	0/2210	0.49	0/2975
4	3	0.26	0/3411	0.54	0/4622
5	4	0.26	0/2793	0.54	0/3780
6	5	0.26	0/2103	0.50	0/2846
7	6	0.26	0/554	0.55	0/747
8	7	0.26	0/1756	0.53	0/2367
9	8	0.25	0/2437	0.54	0/3306
10	9	0.26	0/2384	0.54	0/3220
11	A	0.39	0/11479	0.60	0/15496
12	B	0.49	0/9257	0.64	0/12493
13	C	0.52	0/2102	0.62	0/2857
14	D	0.25	0/1064	0.51	0/1428
15	E	0.34	0/1752	0.57	0/2366
16	F	0.45	0/646	0.64	0/871
17	G	0.32	0/1382	0.56	0/1874
18	H	0.49	0/1207	0.65	0/1628
19	I	0.37	0/949	0.59	0/1284
20	J	0.60	0/516	0.67	0/696
21	K	0.44	0/939	0.59	0/1271
22	L	0.48	0/378	0.71	0/500
23	M	0.34	0/1983	0.59	1/2679 (0.0%)
24	N	0.65	0/4724	1.10	12/7288 (0.2%)
25	O	0.30	0/1448	0.58	0/1948
26	Q	0.27	0/1167	0.56	0/1576
27	R	0.29	0/1817	0.53	0/2445
28	T	0.62	0/4744	1.06	9/7322 (0.1%)
29	U	0.25	0/945	0.53	0/1274
30	V	0.26	0/816	0.57	0/1105
31	W	0.25	0/1686	0.55	0/2266
32	X	0.26	0/1427	0.51	0/1916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	a	0.25	0/814	0.53	0/1092
35	e	0.24	0/823	0.53	0/1104
36	b	0.24	0/660	0.56	0/883
36	f	0.24	0/645	0.59	0/862
37	c	0.24	0/853	0.53	0/1149
37	g	0.25	0/828	0.53	0/1117
38	d	0.24	0/777	0.49	0/1041
38	h	0.26	0/755	0.46	0/1013
All	All	0.39	0/87100	0.65	22/119407 (0.0%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	11	DG	O4'-C1'-N9	8.01	113.61	108.00
24	N	11	DG	C1'-O4'-C4'	-7.21	102.89	110.10
24	N	97	DC	O4'-C1'-N1	6.55	112.59	108.00
28	T	-140	DT	O4'-C1'-N1	6.38	112.47	108.00
28	T	-68	DG	O4'-C1'-N9	6.38	112.47	108.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	0	601/772 (78%)	581 (97%)	20 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	710/760 (93%)	679 (96%)	31 (4%)	0	100	100
3	2	253/548 (46%)	246 (97%)	7 (3%)	0	100	100
4	3	413/462 (89%)	398 (96%)	15 (4%)	0	100	100
5	4	341/395 (86%)	330 (97%)	11 (3%)	0	100	100
6	5	259/308 (84%)	245 (95%)	14 (5%)	0	100	100
7	6	67/71 (94%)	66 (98%)	1 (2%)	0	100	100
8	7	208/309 (67%)	191 (92%)	17 (8%)	0	100	100
9	8	297/346 (86%)	286 (96%)	11 (4%)	0	100	100
10	9	285/323 (88%)	278 (98%)	7 (2%)	0	100	100
11	A	1413/1970 (72%)	1375 (97%)	38 (3%)	0	100	100
12	B	1130/1174 (96%)	1093 (97%)	37 (3%)	0	100	100
13	C	253/275 (92%)	246 (97%)	7 (3%)	0	100	100
14	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
15	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
16	F	77/127 (61%)	76 (99%)	1 (1%)	0	100	100
17	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
18	H	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
19	I	112/125 (90%)	104 (93%)	8 (7%)	0	100	100
20	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
22	L	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
23	M	248/316 (78%)	239 (96%)	9 (4%)	0	100	100
25	O	177/339 (52%)	175 (99%)	2 (1%)	0	100	100
26	Q	134/517 (26%)	129 (96%)	5 (4%)	0	100	100
27	R	218/249 (88%)	214 (98%)	4 (2%)	0	100	100
29	U	109/376 (29%)	107 (98%)	2 (2%)	0	100	100
30	V	97/109 (89%)	92 (95%)	5 (5%)	0	100	100
31	W	198/439 (45%)	196 (99%)	2 (1%)	0	100	100
32	X	169/291 (58%)	161 (95%)	8 (5%)	0	100	100
35	a	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
35	e	96/136 (71%)	95 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	b	80/103 (78%)	80 (100%)	0	0	100	100
36	f	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
37	c	107/130 (82%)	105 (98%)	2 (2%)	0	100	100
37	g	104/130 (80%)	102 (98%)	2 (2%)	0	100	100
38	d	95/126 (75%)	94 (99%)	1 (1%)	0	100	100
38	h	93/126 (74%)	91 (98%)	2 (2%)	0	100	100
All	All	9382/12507 (75%)	9090 (97%)	292 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	0	536/678 (79%)	531 (99%)	5 (1%)	78	88
2	1	624/664 (94%)	622 (100%)	2 (0%)	92	95
3	2	241/484 (50%)	240 (100%)	1 (0%)	91	94
4	3	351/399 (88%)	349 (99%)	2 (1%)	86	92
5	4	311/352 (88%)	311 (100%)	0	100	100
6	5	234/272 (86%)	234 (100%)	0	100	100
7	6	62/64 (97%)	62 (100%)	0	100	100
8	7	194/283 (69%)	191 (98%)	3 (2%)	65	80
9	8	259/299 (87%)	258 (100%)	1 (0%)	91	94
10	9	259/296 (88%)	257 (99%)	2 (1%)	81	89
11	A	1254/1749 (72%)	1252 (100%)	2 (0%)	93	96
12	B	994/1027 (97%)	991 (100%)	3 (0%)	92	95
13	C	234/252 (93%)	233 (100%)	1 (0%)	91	94
14	D	118/126 (94%)	118 (100%)	0	100	100
15	E	191/192 (100%)	188 (98%)	3 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	F	69/111 (62%)	69 (100%)	0	100	100
17	G	152/153 (99%)	149 (98%)	3 (2%)	55	73
18	H	129/131 (98%)	129 (100%)	0	100	100
19	I	103/112 (92%)	103 (100%)	0	100	100
20	J	53/56 (95%)	52 (98%)	1 (2%)	57	75
21	K	104/106 (98%)	104 (100%)	0	100	100
22	L	41/55 (74%)	41 (100%)	0	100	100
23	M	215/268 (80%)	215 (100%)	0	100	100
25	O	154/293 (53%)	154 (100%)	0	100	100
26	Q	121/448 (27%)	120 (99%)	1 (1%)	81	89
27	R	196/218 (90%)	196 (100%)	0	100	100
29	U	105/324 (32%)	105 (100%)	0	100	100
30	V	90/98 (92%)	88 (98%)	2 (2%)	52	71
31	W	182/373 (49%)	181 (100%)	1 (0%)	88	93
32	X	154/261 (59%)	154 (100%)	0	100	100
35	a	85/111 (77%)	85 (100%)	0	100	100
35	e	86/111 (78%)	86 (100%)	0	100	100
36	b	67/79 (85%)	67 (100%)	0	100	100
36	f	65/79 (82%)	65 (100%)	0	100	100
37	c	86/101 (85%)	86 (100%)	0	100	100
37	g	84/101 (83%)	84 (100%)	0	100	100
38	d	83/106 (78%)	83 (100%)	0	100	100
38	h	81/106 (76%)	81 (100%)	0	100	100
All	All	8367/10938 (76%)	8334 (100%)	33 (0%)	91	94

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	J	47	ARG
26	Q	151	ARG
31	W	56	ARG
8	7	125	TYR
8	7	85	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
12	B	941	GLN
19	I	100	HIS
6	5	258	HIS
8	7	24	ASN
9	8	71	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
39	SF4	1	1000	2	0,12,12	-	-	-		

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
39	SF4	1	1000	2	-	-	0/6/5/5

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.

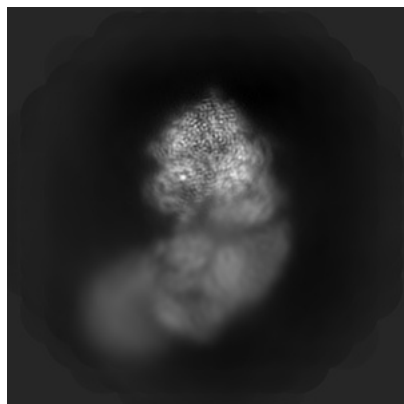
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16274. These allow visual inspection of the internal detail of the map and identification of artifacts.

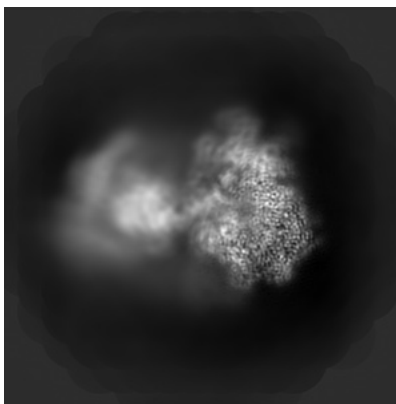
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

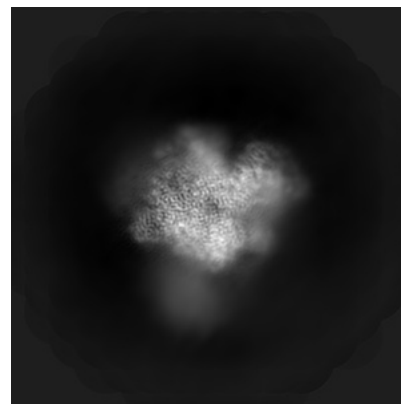
#### 6.1.1 Primary map



X

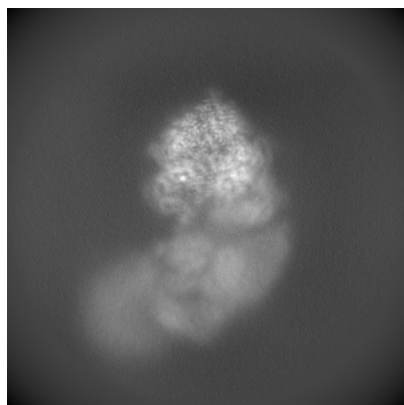


Y

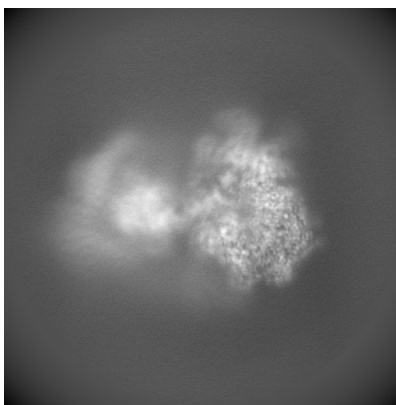


Z

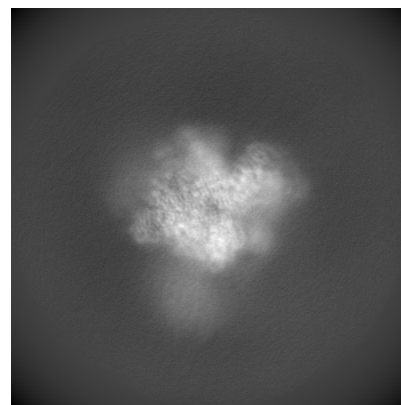
#### 6.1.2 Raw map



X



Y

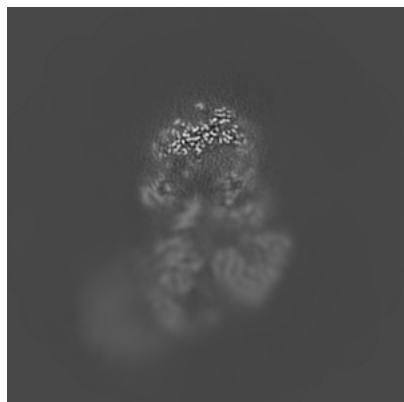


Z

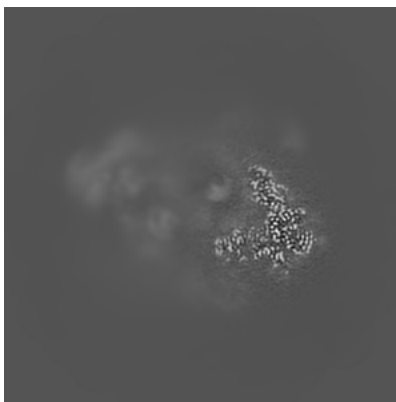
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

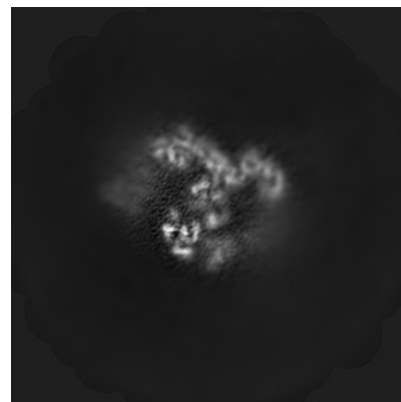
### 6.2.1 Primary map



X Index: 200

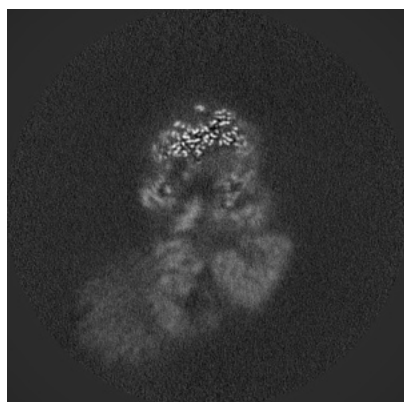


Y Index: 200

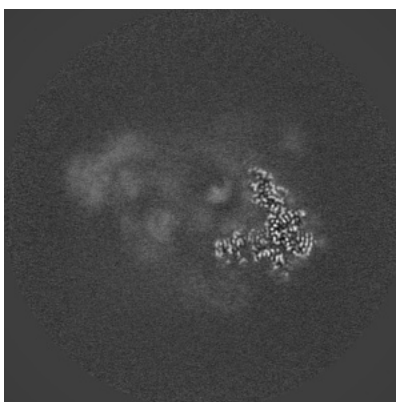


Z Index: 200

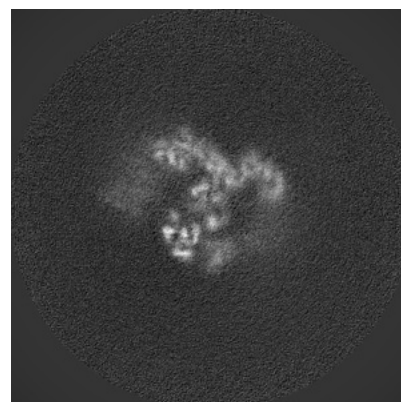
### 6.2.2 Raw map



X Index: 200



Y Index: 200

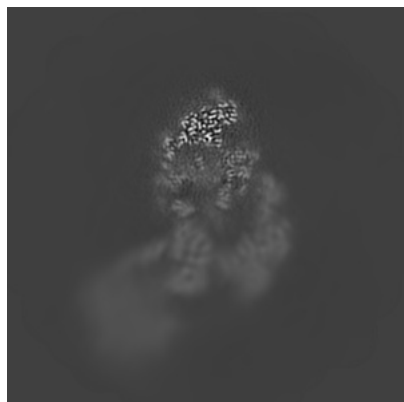


Z Index: 200

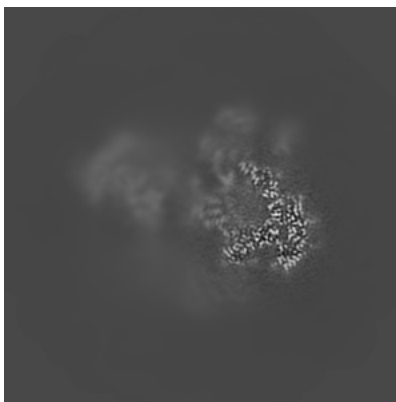
The images above show central slices of the map in three orthogonal directions.

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

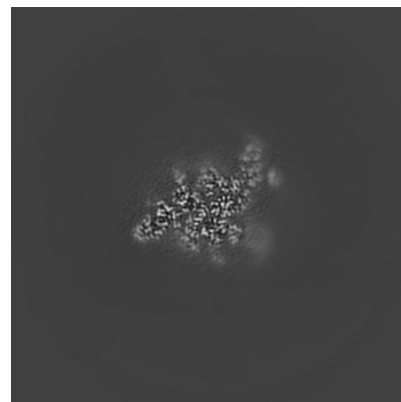
### 6.3.1 Primary map



X Index: 183

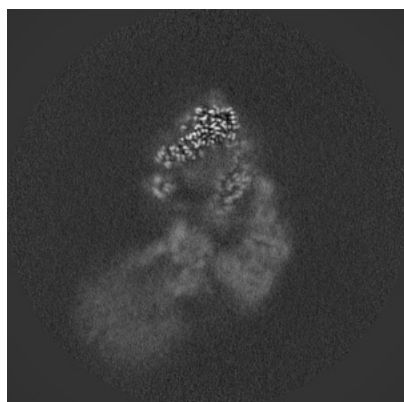


Y Index: 213

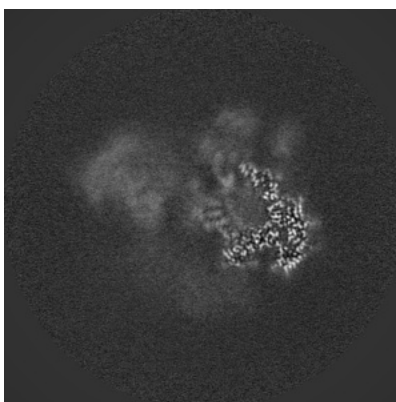


Z Index: 265

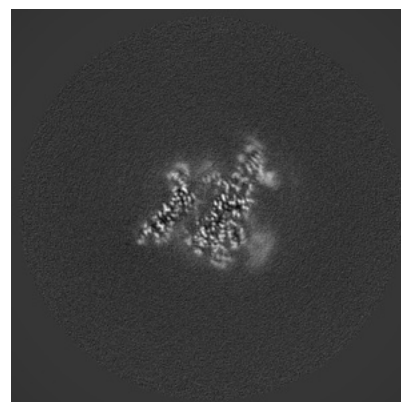
### 6.3.2 Raw map



X Index: 190



Y Index: 213



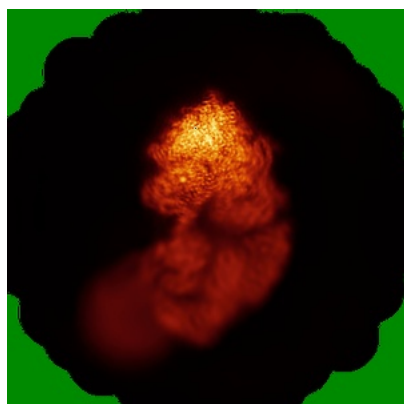
Z Index: 260

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

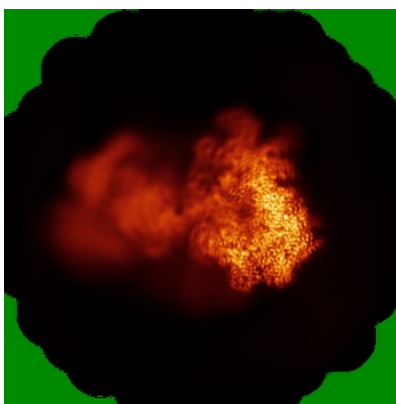


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

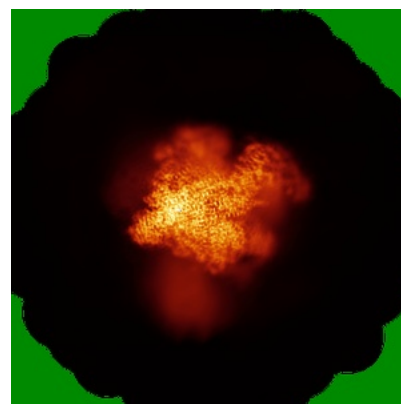
### 6.4.1 Primary map



X

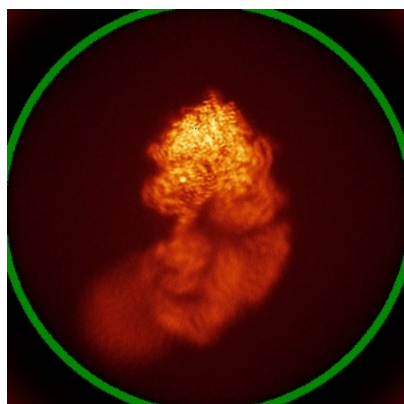


Y

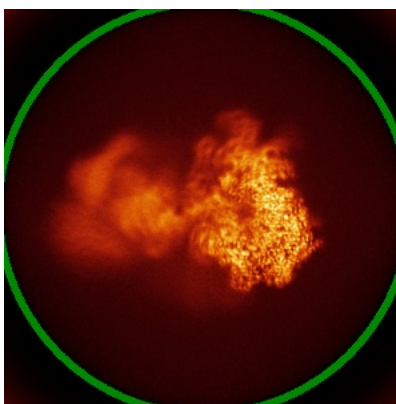


Z

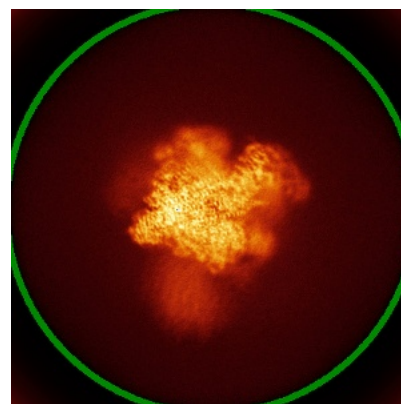
### 6.4.2 Raw map



X



Y

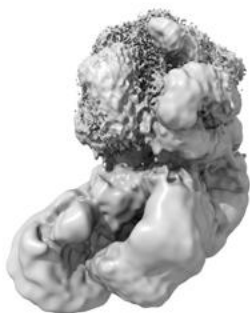


Z

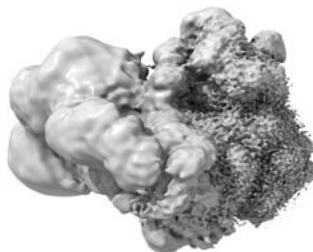
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

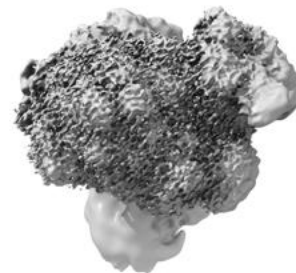
### 6.5.1 Primary map



X



Y



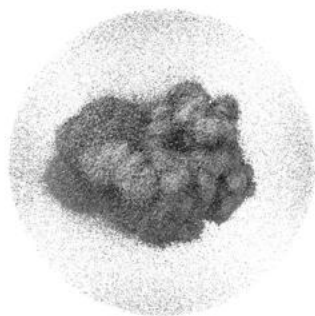
Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

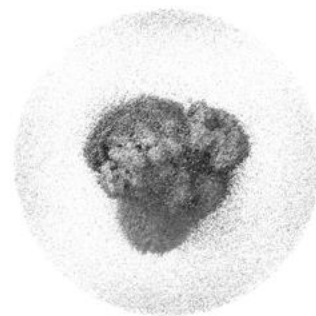
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

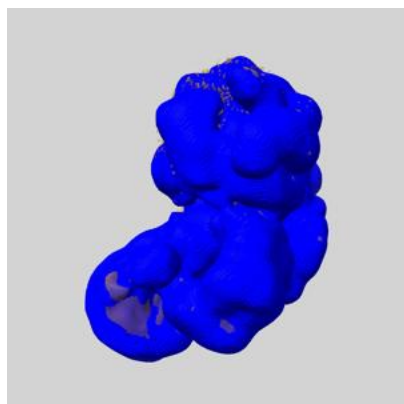
## 6.6 Mask visualisation [i](#)

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

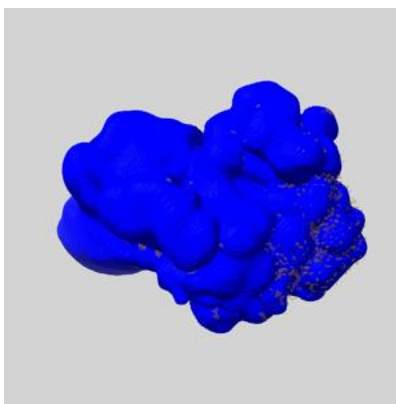
A mask typically either:

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

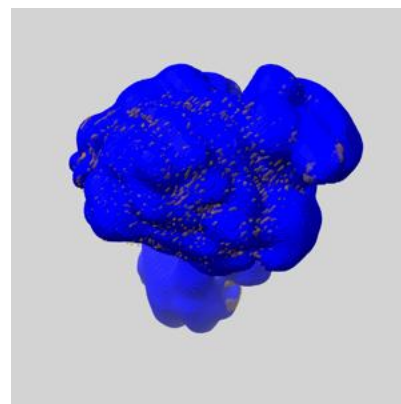
### 6.6.1 emd\_16274\_msk\_1.map [i](#)



X



Y

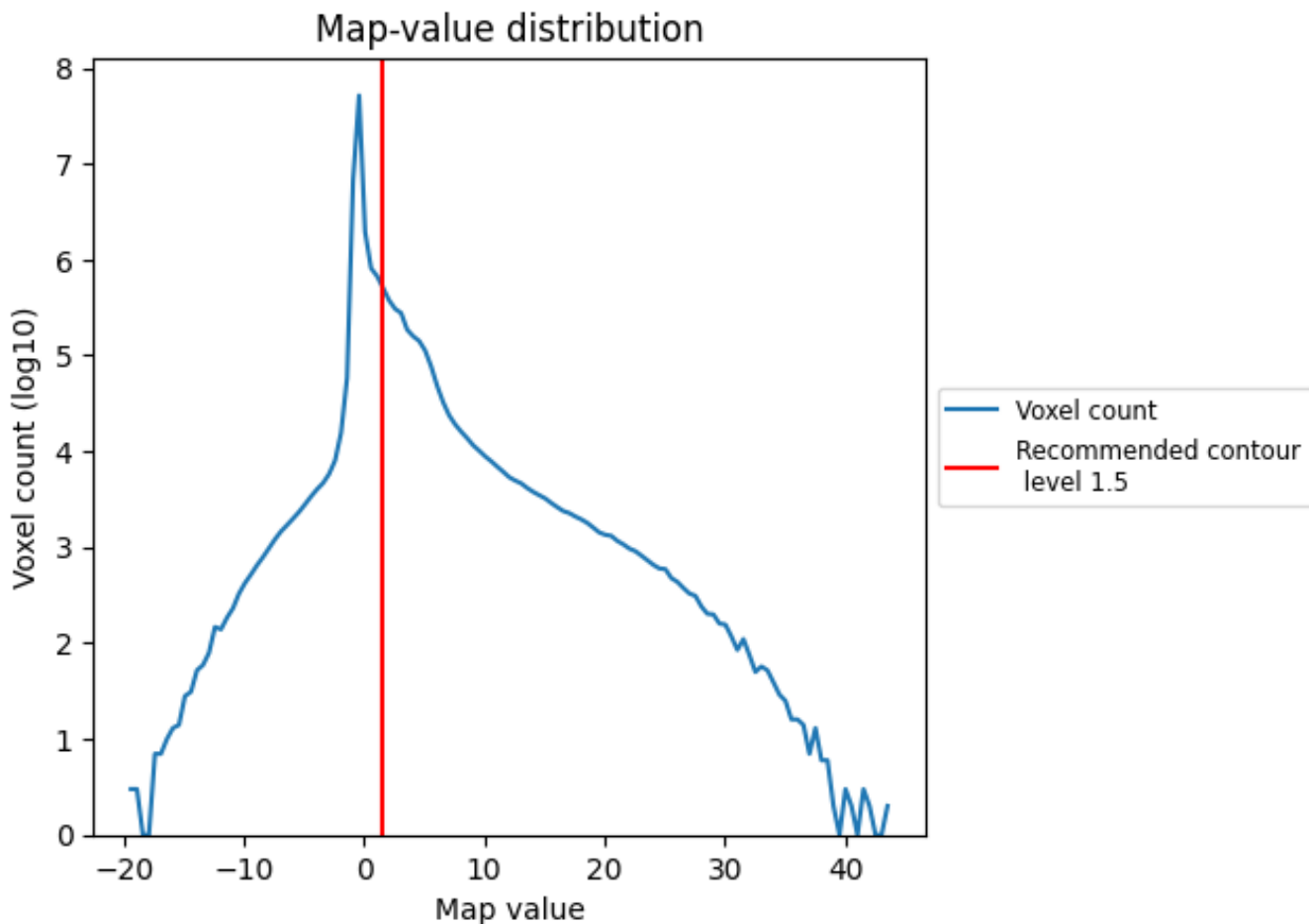


Z

## 7 Map analysis [i](#)

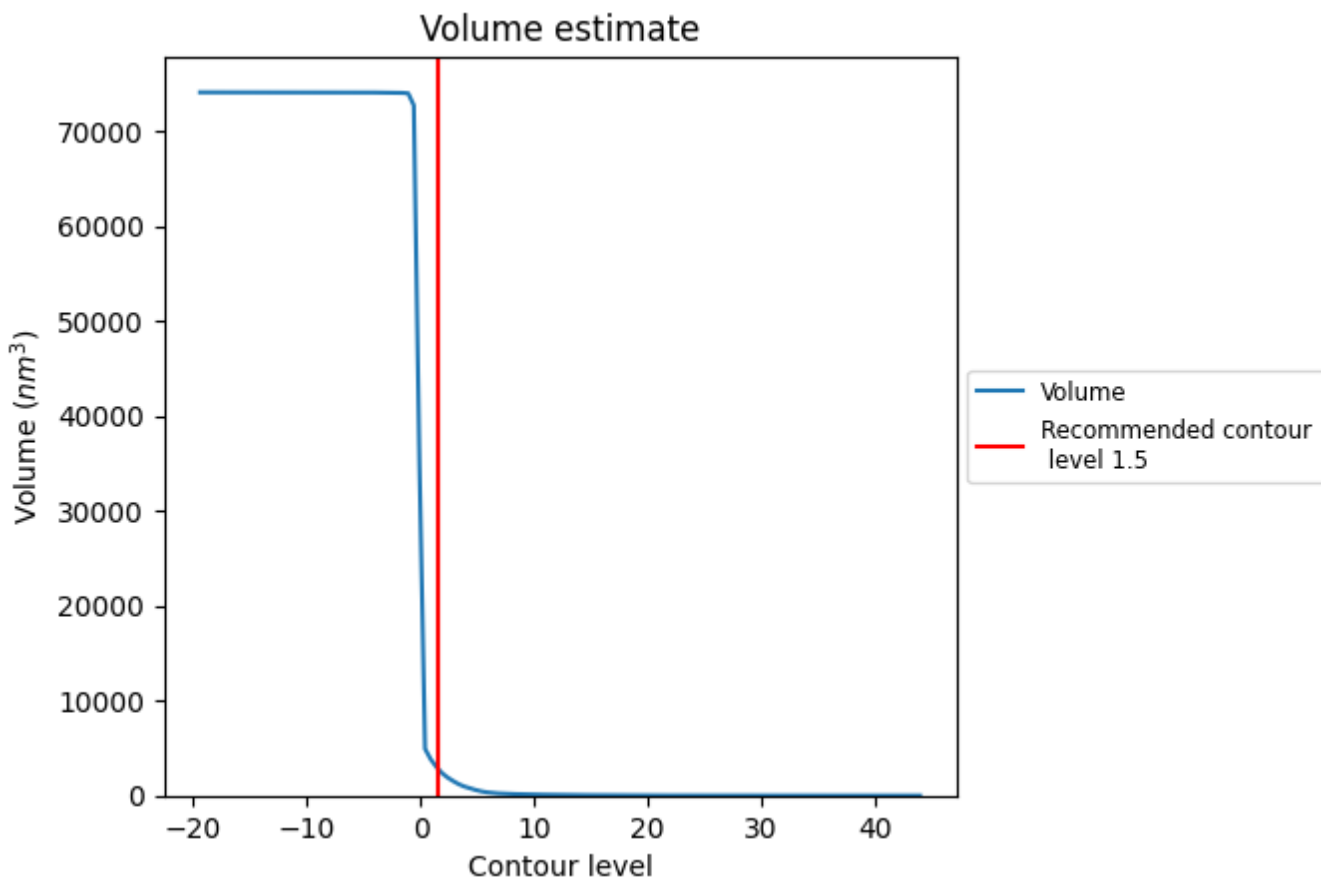
This section contains the results of statistical analysis of the map.

### 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.

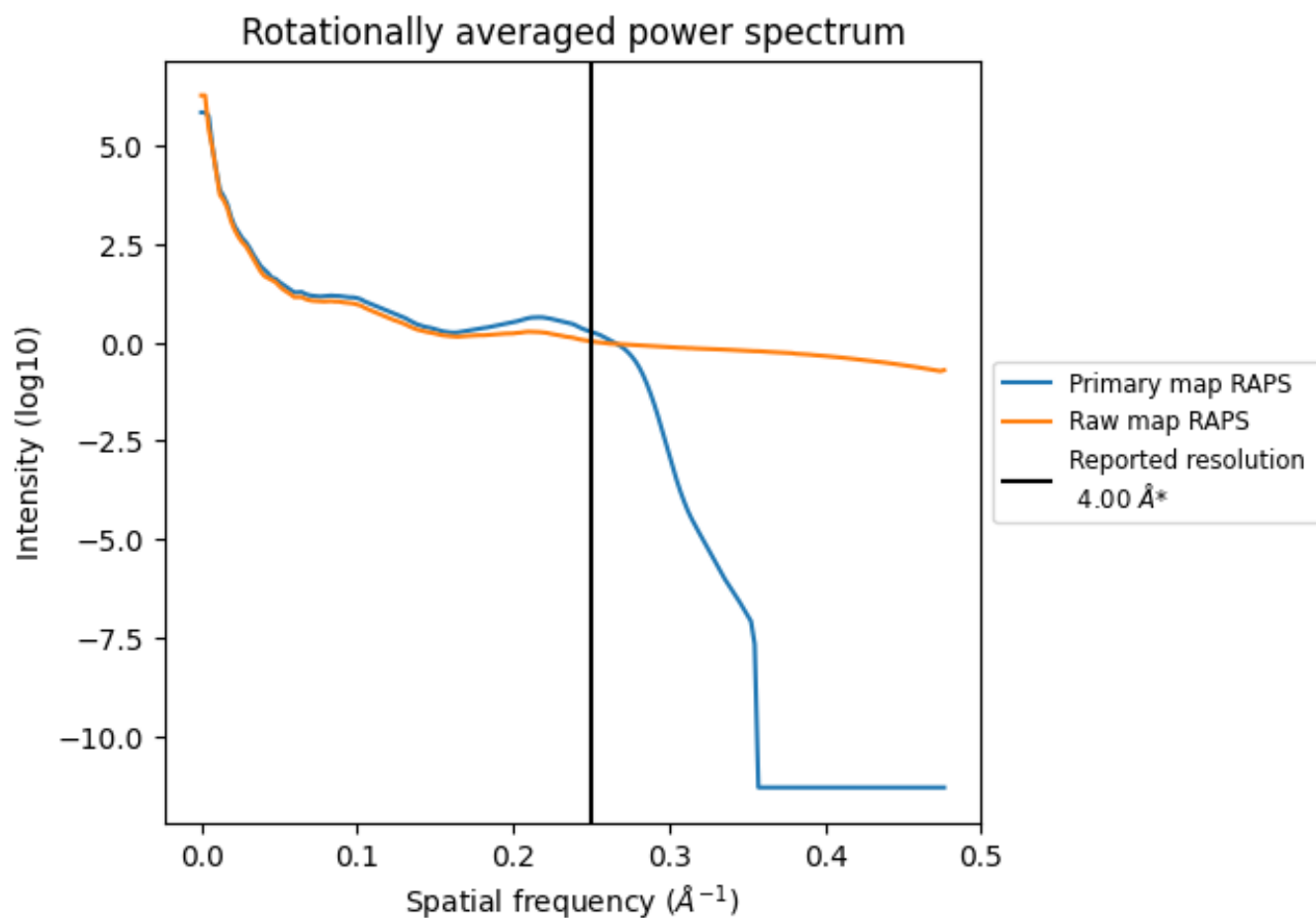
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2912  $\text{nm}^3$ ; this corresponds to an approximate mass of 2631 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](#)

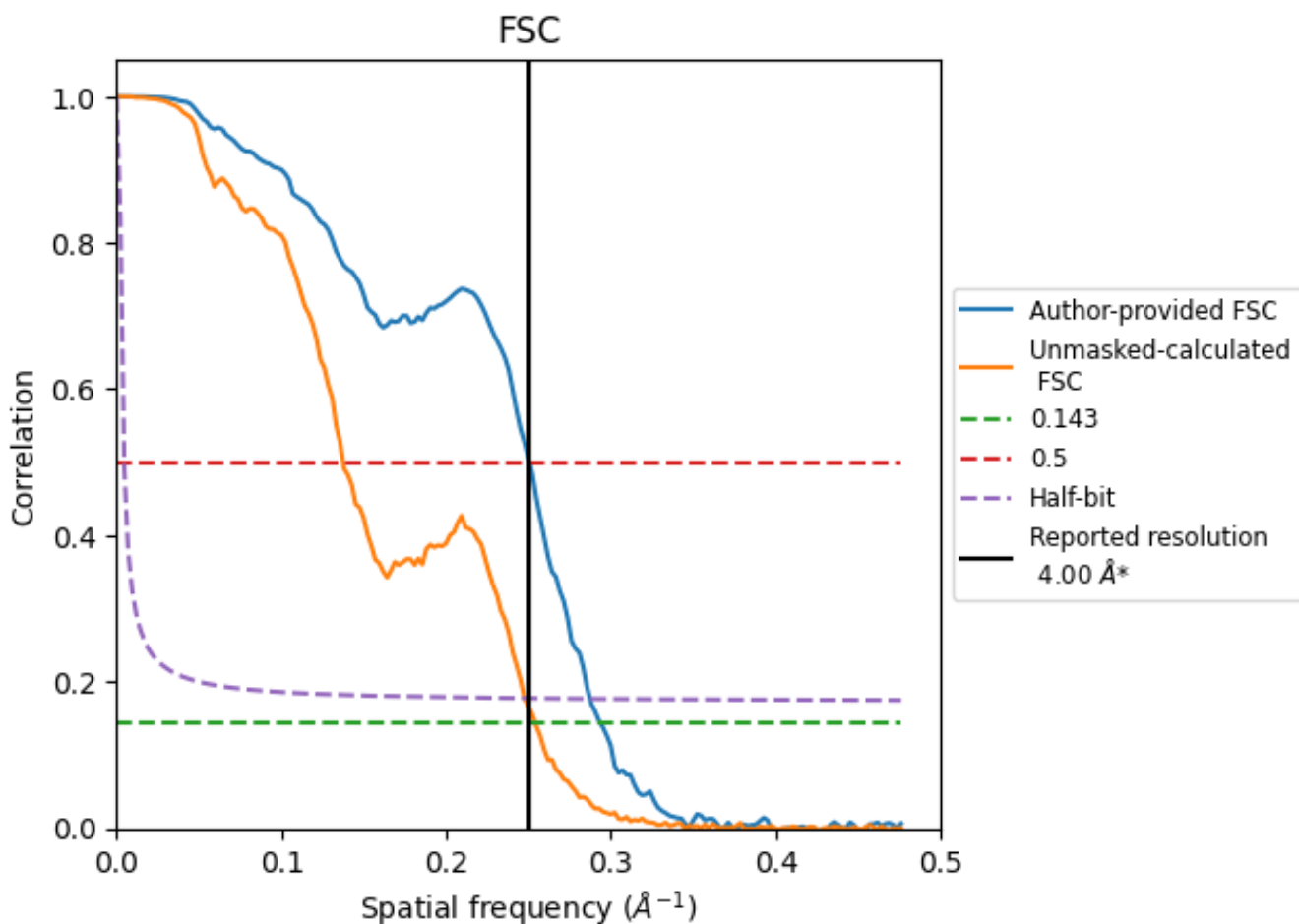


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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 0.250 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	4.00	-	-
Author-provided FSC curve	3.40	3.99	3.48
Unmasked-calculated*	3.93	7.27	4.04

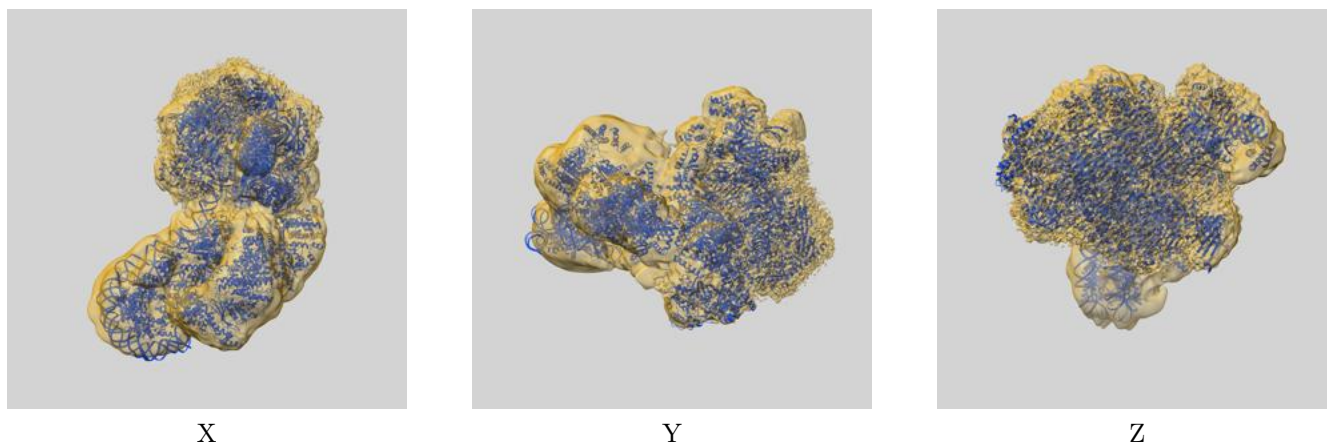
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 4.0 by more than 10 %



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

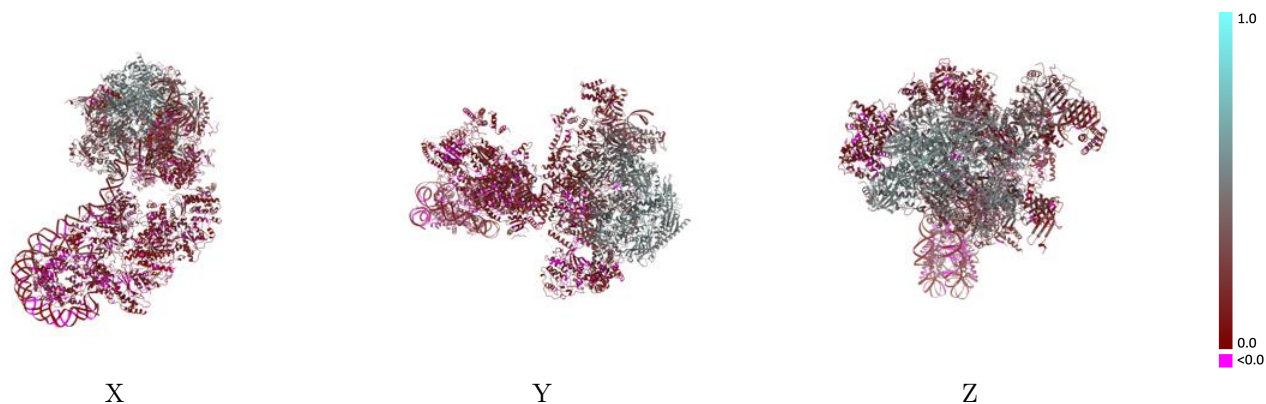
This section contains information regarding the fit between EMDB map EMD-16274 and PDB model 8BVW. Per-residue inclusion information can be found in section 3 on page 13.

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



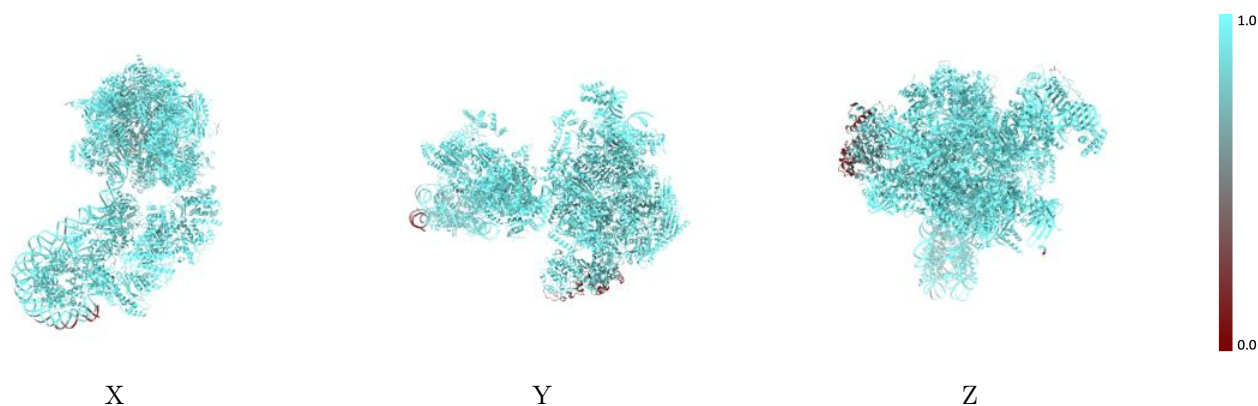
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



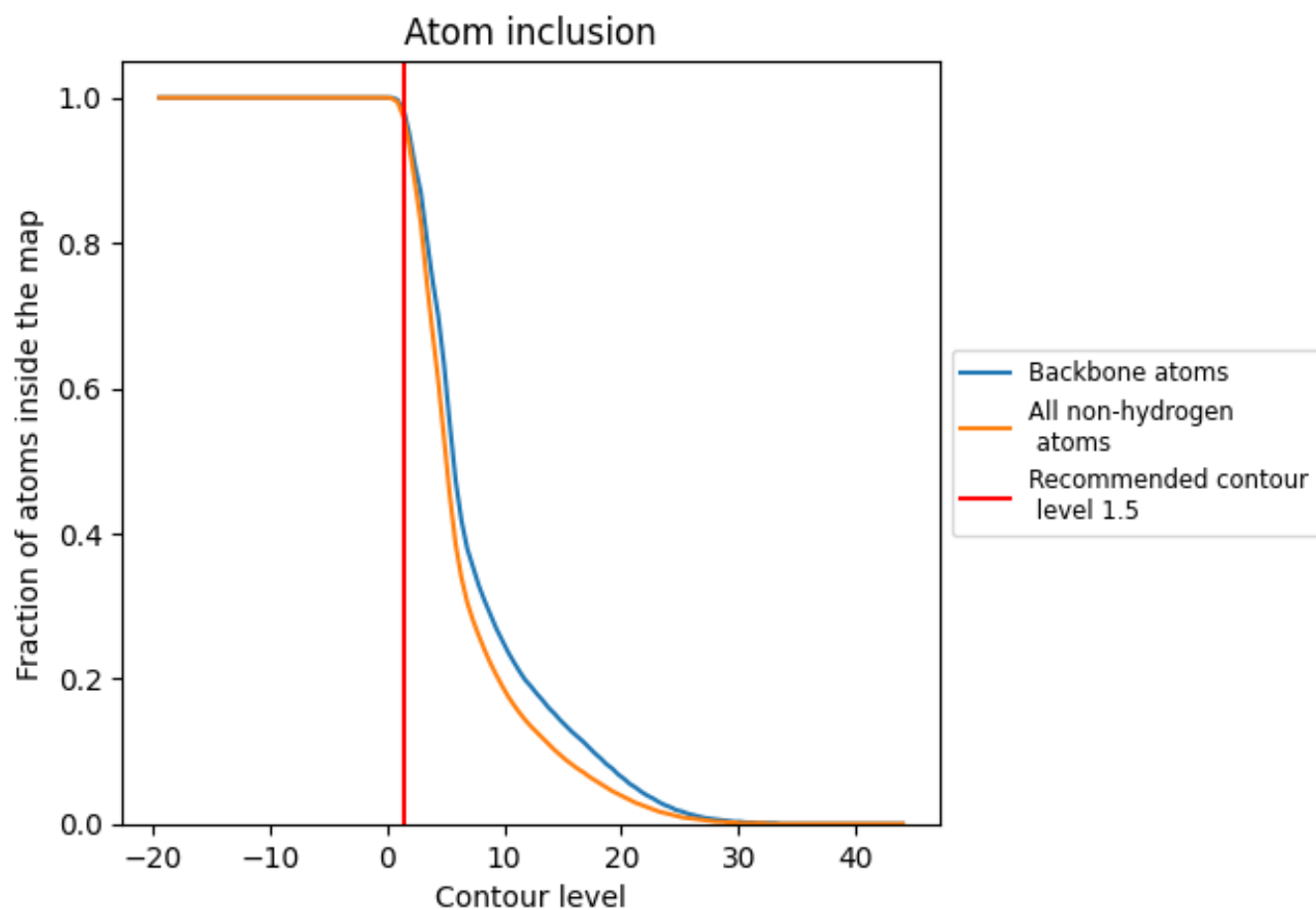
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.2340
0	 0.9990	 0.1090
1	 1.0000	 0.1240
2	 0.9970	 0.0750
3	 0.9910	 0.0850
4	 0.9970	 0.1070
5	 0.9990	 0.0820
6	 1.0000	 0.1000
7	 0.8290	 0.1100
8	 0.8600	 0.0850
9	 0.6860	 0.1290
A	 0.9900	 0.4010
B	 0.9940	 0.4740
C	 0.9960	 0.5080
D	 0.9960	 0.1830
E	 0.9920	 0.3460
F	 0.9950	 0.4830
G	 0.9980	 0.2590
H	 0.9930	 0.4830
I	 0.9970	 0.3870
J	 1.0000	 0.5280
K	 0.9950	 0.5110
L	 0.9970	 0.4690
M	 0.9870	 0.3920
N	 0.9230	 0.1080
O	 0.9950	 0.2900
Q	 0.9780	 0.2450
R	 0.9930	 0.2160
T	 0.9130	 0.1080
U	 0.9860	 0.1570
V	 1.0000	 0.1780
W	 0.9900	 0.1360
X	 0.9960	 0.1540
Y	 1.0000	 0.0750
Z	 1.0000	 0.0600



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Chain	Atom inclusion	Q-score
a	 0.9820	 0.0580
b	 1.0000	 0.0440
c	 0.9950	 0.0220
d	 1.0000	 0.0450
e	 0.9830	 0.0430
f	 1.0000	 0.0550
g	 0.9840	 0.0480
h	 0.9750	 0.0810