WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Mar 19, 2024 – 04:40 PM JST

PDB ID	:	6A5T
EMDB ID	:	EMD-6984
Title	:	RNA polymerase II elongation complex stalled at SHL(-1) of the nucleosome
Authors	:	Kujirai, T.; Ehara, H.; Fujino, Y.; Shirouzu, M.; Sekine, S.; Kurumizaka, H.
Deposited on	:	2018-06-25
Resolution	:	6.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:
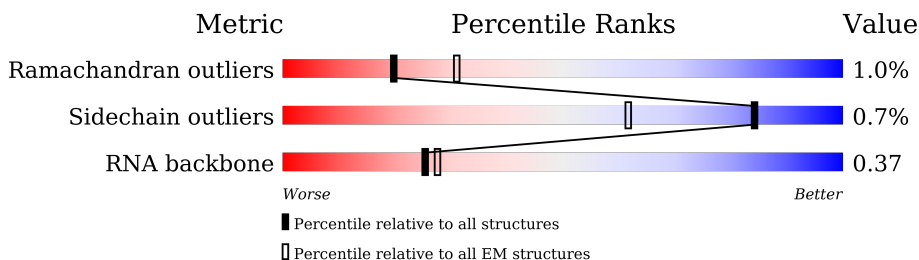
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.70 Å.

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

Metric	Percentile Ranks	Value
Ramachandran outliers		1.0%
Sidechain outliers		0.7%
RNA backbone		0.37

Worse　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
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 >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1743	20% / 78% · 19%
2	B	1227	29% / 92% · 5%
3	C	304	14% / 85% · 13%
4	D	186	84% / 83% · 16%
5	E	214	9% / 96% ·
6	F	155	14% / 54% · 46%
7	G	171	100% / 98% ·
8	H	145	14% / 91% · 8%

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Mol	Chain	Length	Quality of chain
9	I	115	74% / 94%
10	J	72	11% / 89% 8%
11	K	118	22% / 94%
12	L	72	18% / 61% 38%
13	P	11	9% / 64% 18% 18%
14	T	198	7% / 59% 5% 36%
15	N	198	8% / 58% 41%
16	a	139	42% / 68% 30%
16	e	139	22% / 68% 30%
17	b	106	37% / 74% 25%
17	f	106	27% / 73% 26%
18	c	133	31% / 77% 23%
18	g	133	71% / 78% 21%
19	d	129	28% / 72% 26%
19	h	129	58% / 69% 29%

2 Entry composition ⓘ

There are 21 unique types of molecules in this entry. The entry contains 42343 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1408	Total 11095	C 6997	N 1935	O 2093	S 70	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	156	Total 1210	C 753	N 210	O 245	S 2	0	0

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

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

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

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

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

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

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

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

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

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

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

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

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

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

- Molecule 13 is a RNA chain called RNA (5'-R(P*GP*GP*UP*GP*UP*CP*UP*UP*GP*G P*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	11	Total 238	C 105	N 41	O 81	P 11	0	0

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	126	Total 2567	C 1217	N 481	O 744	P 125	0	0

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	117	Total 2409	C 1140	N 444	O 708	P 117	0	0

- Molecule 16 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	97	Total 797	C 503	N 155	O 137	S 2	0	0
16	e	97	Total 796	C 501	N 155	O 138	S 2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	80	Total 638	C 401	N 125	O 111	S 1	0	0
17	f	78	Total 619	C 391	N 120	O 107	S 1	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	103	Total	C	N	O	0	0
			796	502	155	139		
18	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
19	h	91	Total	C	N	O	S	0	0
			708	447	125	134	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3   Residue-property plots ⓘ

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

• Molecule 1: DNA-directed RNA polymerase subunit
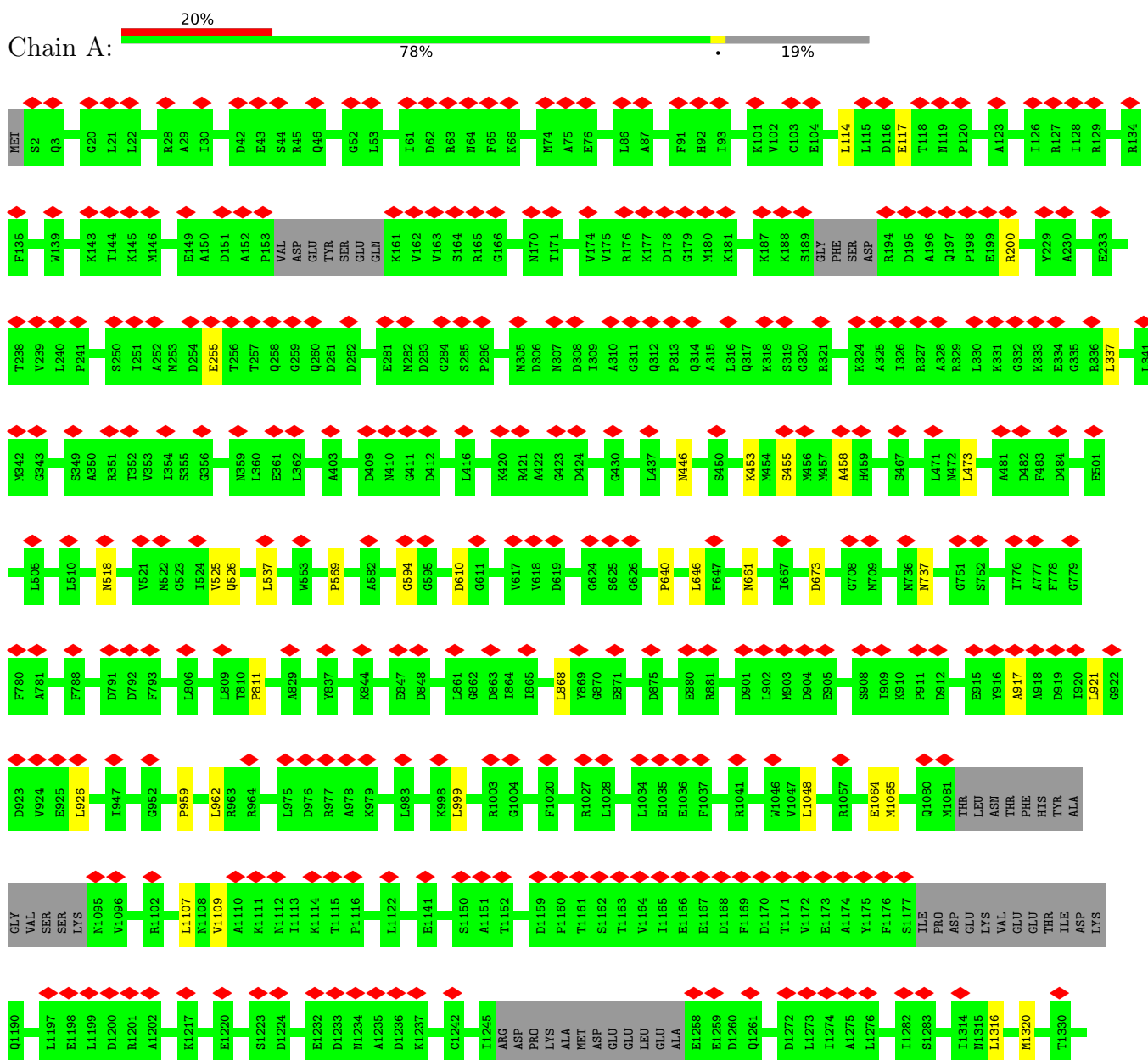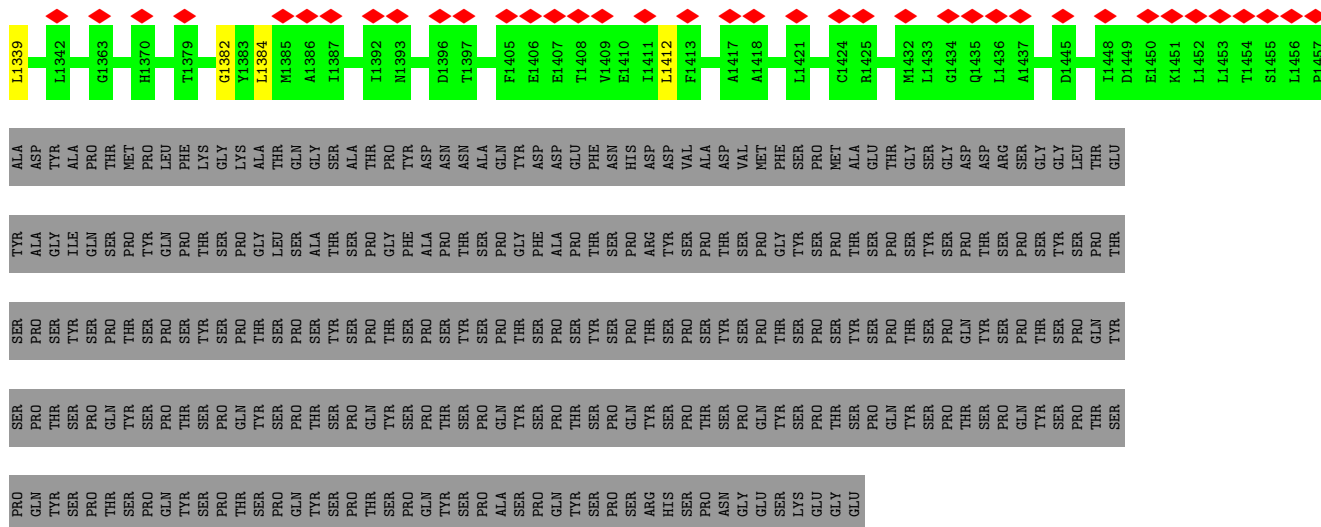
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:

29%

92%

• 5%
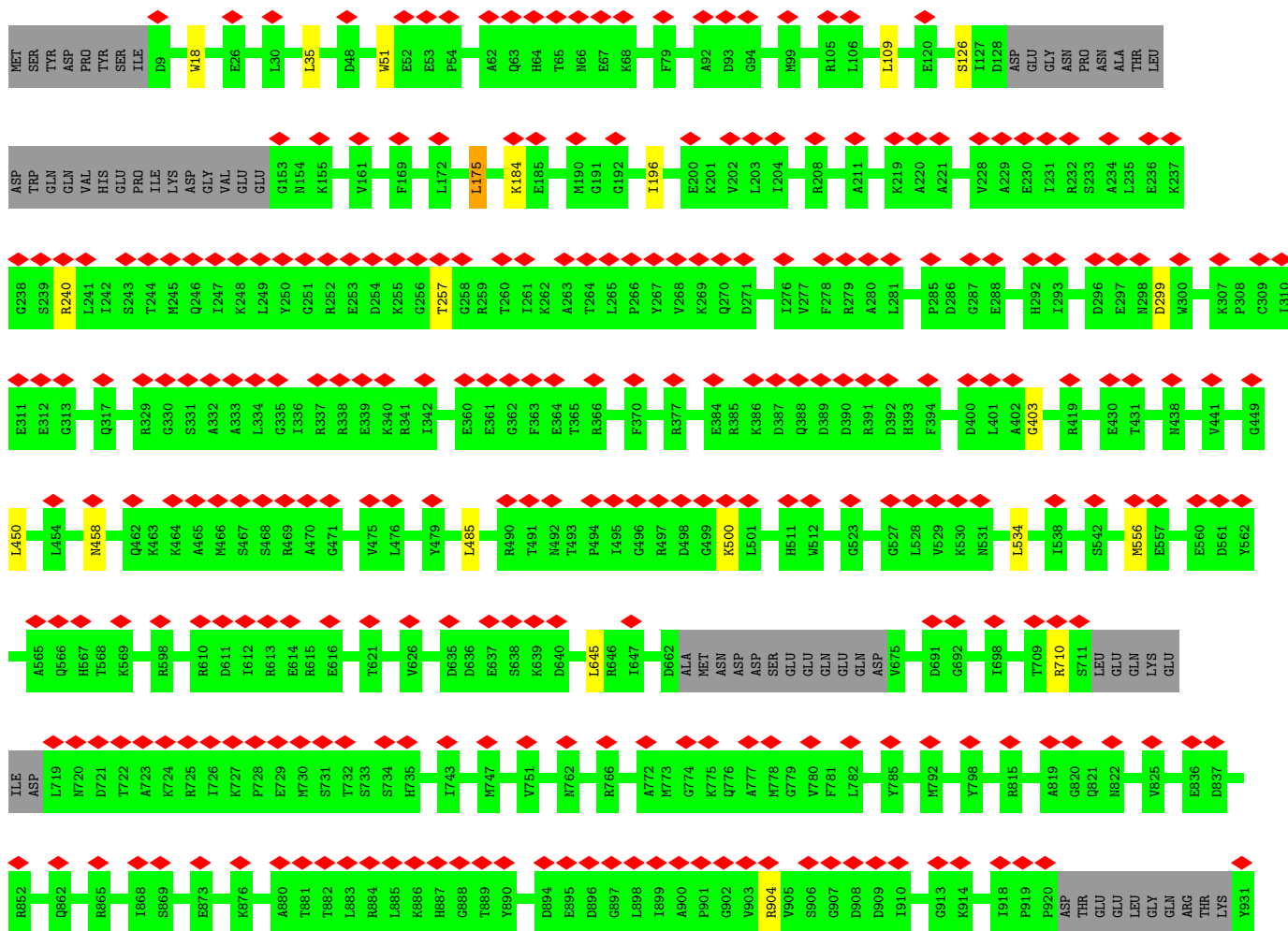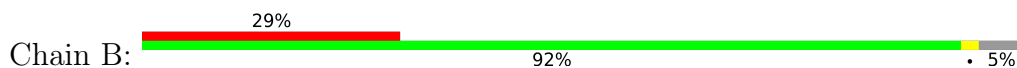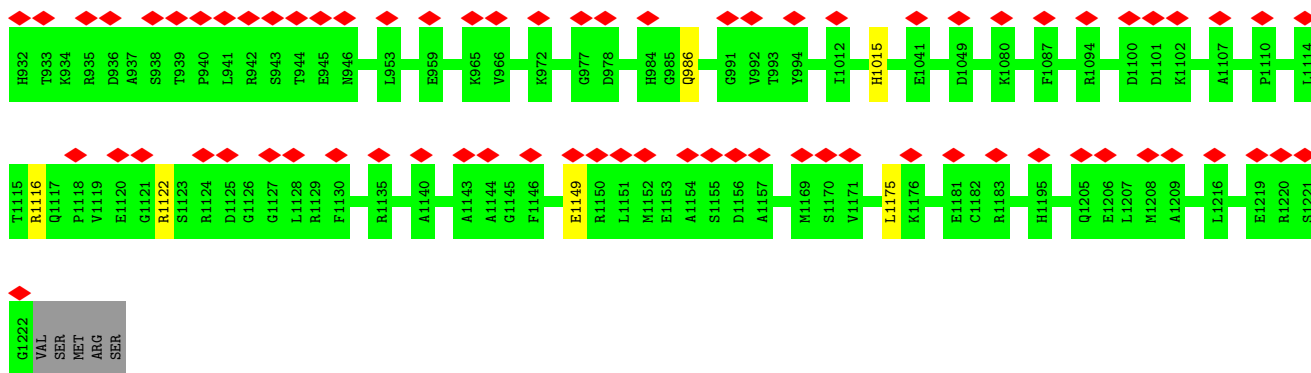
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

Chain C:
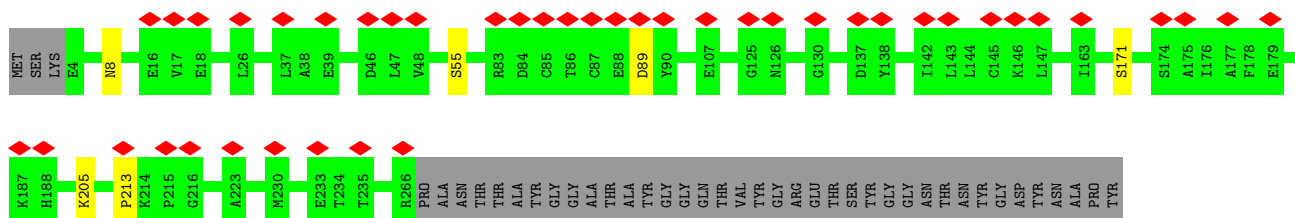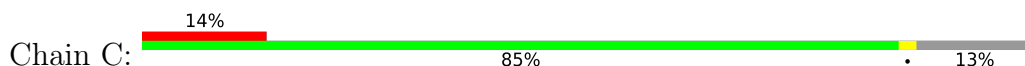
• Molecule 4: RNA polymerase II subunit B32

Chain D:
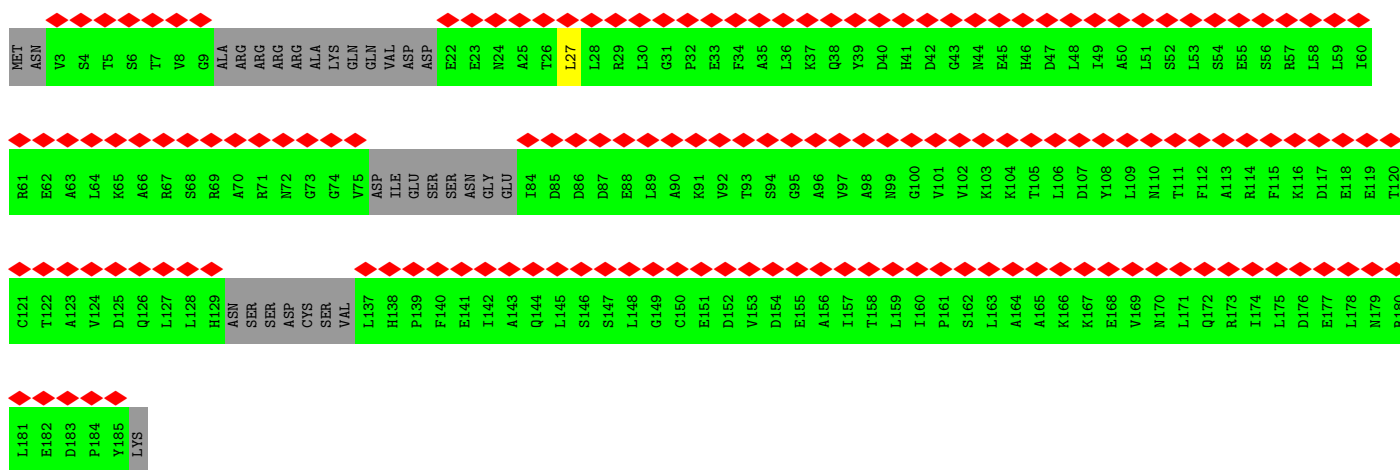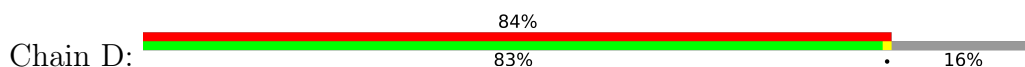
• Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III

Chain E:
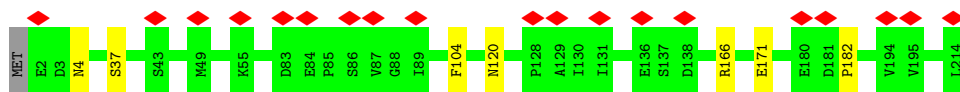
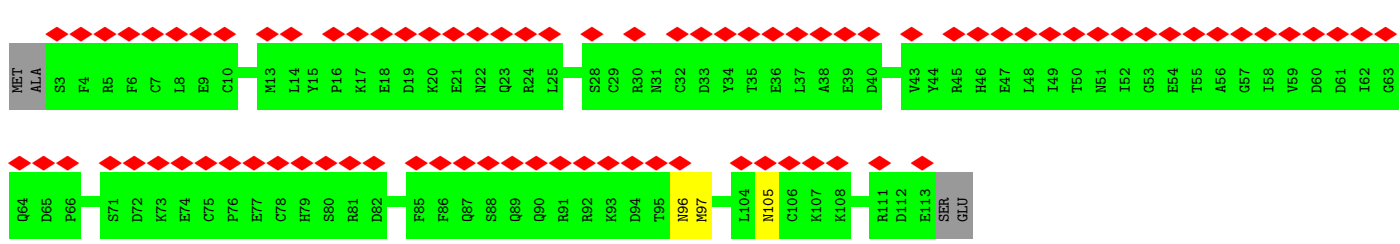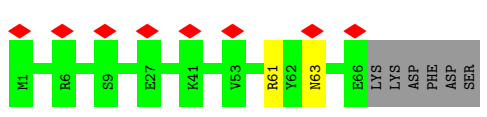• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

Chain F:

14%

54% · 46%

MET SER GLU ASP GLU ALA PHE ASN GLU GLN THR GLU ASN PHE GLU ASN PHE GLU ASP GLU HIS PHE SER ASP ASP ASN PHE GLU ASP ARG SER THR GLN PRO GLU ASP TYR ALA VAL GLY VAL THR ALA ASP GLY ARG GLN GLN ILE ILE ASN GLY ASP GLY ILE GLN GLU VAL ASN GLY THR

ILE LYS ALA HIS ARG LYS SER ARG ASN LYS E71 L72 A73 I74 L75 L85 R90 R97 P106 V107 L108 V109 D110 I111 E112 G113 E114 T115 D116 K129 V153 D154 ASN
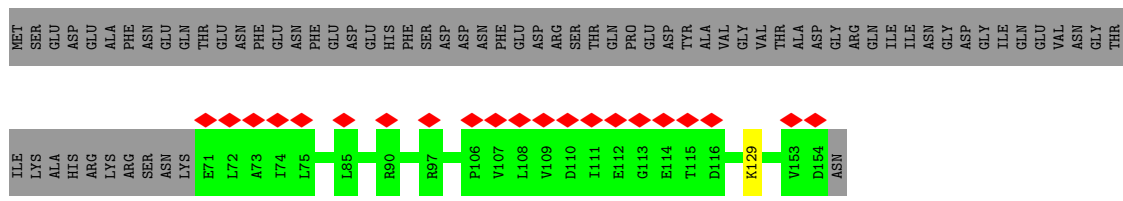
• Molecule 7: RNA polymerase II subunit

Chain G:

100%

98% ·

M1 F2 F3 L4 K5 D6 L7 S8 L9 I10 L11 T12 L13 H14 P15 S16 Y17 F18 G19 P20 Q21 M22 N23 Q24 Y25 L26 R27 E28 K29 L30 L31 T32 D33 V34 E35 G36 T37 C38 T39 G40 Q41 F42 G43 Y44 I45 V46 T47 V48 L49 D50 G51 M52 N53 I54 D55 V56 G57 K58 G59 R60

I61 I62 P63 G64 S65 G66 S67 A68 E69 F70 E71 V72 K73 Y74 R75 A76 V77 V78 W79 K80 P81 F82 K83 G84 E85 V86 V87 D88 A89 I90 V91 S92 N93 V94 S95 P96 I97 G98 F99 F100 A101 D102 V103 G104 P105 L106 N107 V108 F109 V110 S111 T112 R113 L114 L115 P116 D117 N118 L119 V120

Y121 N122 P123 S124 N125 S126 P127 P128 A129 Y130 M131 S132 N133 D134 E135 L136 I137 T138 K139 G140 S141 V143 K142 V143 R144 L145 K146 V147 V148 G149 T150 R151 T152 D153 V154 N155 E156 I157 Y158 A159 I160 G161 S162 I163 K164 E165 D166 F167 L168 G169 A170 I171

• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

14%

91% · 8%

MET SER S3 G18 T32 K37 D41 E45 L65 ASP GLY GLU ASP GLU SER ALA ASN PHE SER K76 K82 P83 T84 D85 F97 Y101 E104 E105 G106 D107 E108 D109 K110 G118 M122 K129 L134 N138 R145
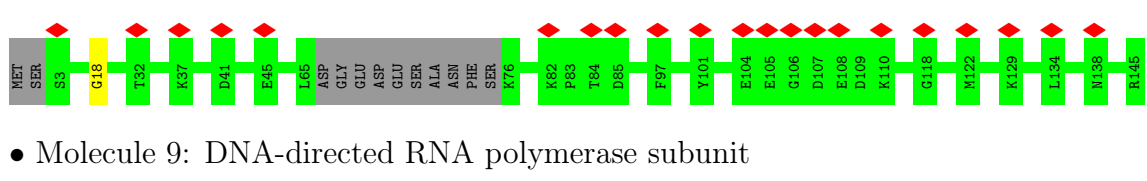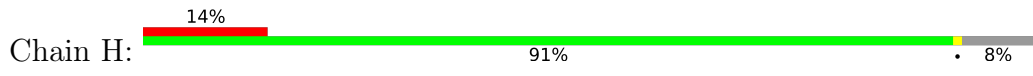
• Molecule 9: DNA-directed RNA polymerase subunit

Chain I:

74%

94% · ·

MET ALA S3 F4 R5 F6 C7 L8 E9 C10 M13 L14 Y15 P16 K17 E18 D19 K20 E21 N22 Q23 R24 L25 S28 C29 R30 N31 C32 D33 Y34 T35 E36 L37 A38 E39 D40 V43 Y44 R45 H46 E47 L48 I49 T50 N51 I52 G53 E54 T55 A56 G57 I58 V59 D60 D61 I62 G63

Q64 D65 P66 S71 D72 K73 E74 C75 P76 E77 C78 H79 S80 R81 D82 F85 F86 Q87 S88 Q89 Q90 R91 R92 K93 D94 T95 N96 M97 L104 N105 C106 K107 K108 R111 D112 E113 SER GLU

• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J:

11%

89% · 8%

M1 R6 S9 E27 K41 V53 R61 Y62 N63 E66 LYS LYS ASP PHE ASP SER

• Molecule 11: RNA polymerase II subunit B12.5

Chain K:

22%

94%

M1 N2 A3 P4 D5 R6 F7 E8 L9 F10 I11 L12 P13 D14 D15 V16 L19 S25 A43 R47 A51 F58 E64 A69 N70 E79 L98 N113 PHE SER LEU ASN ASP

• Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L:

18%

61%   38%

MET SER ARG GLU GLY PHE VAL ALA PRO SER GLY THR ASP LEU ALA ALA ALA SER GLY VAL ALA PRO ASN LYS HIS TYR G28 G34 L42 N43 K44 S45 D46 P47 V48 R62 T63 K64 R65 F69 D70 A71 R72

• Molecule 13: RNA (5'-R(P*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*G)-3')

Chain P:

9%

64%   18%   18%

G0 G1 U2 G3 U4 G10

• Molecule 14: DNA (198-MER)

Chain T:

7%

59%   5%   36%

A-72 T-47 T-26 C-21 C-18 C-10 A-9 C8 A17 A23 A32 C33 A34 C35 A38 C44 C45 A46 G47 G48 C49 A50 C51 G52 A53 DG DA DC DA DG DA DA DA DA DA DA DC DA DC DG DA DA DA DC DG

DC DC DA DC DA DC DC DA DA DA DC DA DC DA DC DA DC DA DA DC DA DC DA DA DG DA DG DC DT DA DT DT DG DA DC DT DG DA DC DT DA DA DG

• Molecule 15: DNA (198-MER)

Chain N:

8%

58%   41%

DG DC DT DT DA DC DG DT DC DA DG DT DT DT DG DG DC DA DC DT DC DT DT DT DG DT DG DT DT DG DG DC DT DC DT DG DG DT DG DT DT DG DG DT DC DC DC DT DT DT DC DG DT DG

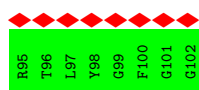DT DT DT DT DT DT DC DT DG DT DC T-53 C-52 G-51 T-50 G-49 C-48 C-47 T-46 G-45 G-44 T-43 G-42 DT DC DT DG DG DG DT DG T-32 G12 A43 T44 T45 T72

• Molecule 16: Histone H3.3

Chain a:

42%

68%   30%

GLY SER HIS MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO SER THR GLY GLY VAL LYS LYS P38 H39 R40 Y41 R42 P43 G44 T45 V46 A47 L48 R49 E50 I51 R52 R53 Y54 Q55 K56

• Molecule 16: Histone H3.3

Chain e:

• Molecule 17: Histone H4

Chain b:

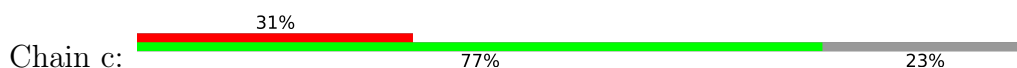• Molecule 17: Histone H4

Chain f:

• Molecule 18: Histone H2A type 1-B/E

Chain c:

• Molecule 18: Histone H2A type 1-B/E

Chain g:

71%

78% · 21%

GLY SER HIS MET SER GLY ARG GLY LYS GLN GLY GLY LYS ALA ARG ALA LYS A14 K15 T16 R17 S18 S19 R20 A21 G22 L23 Q24 F25 P26 V30 H31 R32 L33 L34 R35 K36 G37 N38 Y39 S40 E41 R42 A45 G46 A47 P48 V49 L55 E56 Y57 L58 T59 A60 E61 I62 L63

E64 L65 A66 G67 N68 A69 A70 R71 D72 N73 K74 K75 T76 R77 I78 I79 P80 R81 H82 L83 Q84 L85 A86 I87 R88 N89 D90 E91 E92 L93 N94 K95 L96 L97 G98 R99 V100 T101 I102 A103 Q104 G105 G106 V107 L108 P109 N110 I111 Q112 A113 V114 L115 L116 P117 K118 LYS THR GLU SER HIS

HIS LYS ALA LYS GLY LYS

• Molecule 19: Histone H2B type 1-J

Chain d:

28%

72% · 26%

GLY SER HIS MET PRO GLU PRO ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS ALA GLN LYS LYS ASP GLY LYS LYS ARG LYS R28 S29 R30 K31 E32 Q44 P47 D48 T49 F67 E68 R69 I70 R76 L77 A78 H79 K82 V95

L98 L99 P100 G101 V108 S109 E110 G111 T112 K113 A114 V115 T116 K117 Y118 T119 S120 A121 K122

• Molecule 19: Histone H2B type 1-J

Chain h:

58%

69% · 29%

GLY SER HIS MET PRO GLU PRO ALA LYS SER ALA PRO ALA PRO LYS LYS GLY SER LYS LYS ALA VAL THR LYS ALA GLN LYS LYS ASP GLY LYS LYS ARG LYS ARG SER ARG K31 E32 S33 Y34 S35 I36 Y37 V38 Y39 K40 V41 L42 K43 Q44 V45 H46 P47 D48 T49 Q50 I51 S52 S53

K54 A55 M56 G57 I58 M59 N60 S61 N64 D65 E68 R69 I70 R76 H79 Y80 N81 K82 R83 S84 T85 I86 T87 E90 I91 A94 V95 R96 L97 L98 L99 P100 G101 E102 L103 A104 K105 H106 A107 V108 S109 E110 G111 T112 K113 A114 V115 T116 K117 Y118 T119 S120 A121 LYS

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	0.69	0/11299	0.72	13/15266 (0.1%)
2	B	0.75	0/9441	0.75	9/12732 (0.1%)
3	C	0.73	0/2139	0.73	1/2895 (0.0%)
4	D	0.31	0/1221	0.53	0/1648
5	E	0.69	0/1772	0.69	0/2385
6	F	0.66	0/687	0.65	0/931
7	G	0.34	0/1353	0.59	1/1837 (0.1%)
8	H	0.77	0/1069	0.69	0/1444
9	I	0.43	0/934	0.58	0/1257
10	J	0.90	0/554	0.81	0/742
11	K	0.68	0/953	0.68	1/1291 (0.1%)
12	L	0.62	0/365	0.66	0/484
13	P	1.19	3/265 (1.1%)	1.29	2/412 (0.5%)
14	T	1.15	8/2880 (0.3%)	1.05	3/4438 (0.1%)
15	N	1.07	2/2701 (0.1%)	1.02	0/4168
16	a	0.42	0/809	0.62	0/1085
16	e	0.46	0/807	0.57	0/1081
17	b	0.44	0/645	0.64	0/862
17	f	0.42	0/626	0.61	0/837
18	c	0.40	0/806	0.58	0/1089
18	g	0.36	0/820	0.55	0/1107
19	d	0.45	0/757	0.56	0/1015
19	h	0.41	0/719	0.57	0/968
All	All	0.73	13/43622 (0.0%)	0.76	30/59974 (0.1%)

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	1
2	B	0	2
3	C	0	1
4	D	0	1
7	G	0	1
10	J	0	1
16	a	0	2
16	e	0	1
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	38	DA	C1'-N9	-8.74	1.35	1.47
14	T	17	DA	C1'-N9	-8.37	1.35	1.47
14	T	32	DA	C1'-N9	-7.42	1.36	1.47
15	N	-49	DG	C1'-N9	-6.74	1.37	1.47
13	P	10	G	C1'-N9	-6.70	1.37	1.46

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	473	LEU	CA-CB-CG	-9.82	92.71	115.30
2	B	556	MET	C-N-CA	-8.42	100.65	121.70
2	B	485	LEU	CA-CB-CG	-7.86	97.22	115.30
14	T	-26	DT	O4'-C4'-C3'	-6.95	101.72	104.50
7	G	106	LEU	CA-CB-CG	6.75	130.83	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	VAL	Peptide
2	B	126	SER	Peptide
2	B	175	LEU	Peptide
3	C	89	ASP	Peptide
4	D	27	LEU	Peptide

5.2   Too-close contacts   ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1396/1743 (80%)	1138 (82%)	235 (17%)	23 (2%)	9	44
2	B	1151/1227 (94%)	925 (80%)	216 (19%)	10 (1%)	17	57
3	C	261/304 (86%)	207 (79%)	51 (20%)	3 (1%)	14	52
4	D	148/186 (80%)	136 (92%)	12 (8%)	0	100	100
5	E	211/214 (99%)	175 (83%)	32 (15%)	4 (2%)	8	38
6	F	82/155 (53%)	73 (89%)	9 (11%)	0	100	100
7	G	169/171 (99%)	154 (91%)	15 (9%)	0	100	100
8	H	129/145 (89%)	104 (81%)	24 (19%)	1 (1%)	19	60
9	I	109/115 (95%)	88 (81%)	19 (17%)	2 (2%)	8	40
10	J	64/72 (89%)	53 (83%)	10 (16%)	1 (2%)	9	44
11	K	111/118 (94%)	100 (90%)	10 (9%)	1 (1%)	17	57
12	L	43/72 (60%)	31 (72%)	12 (28%)	0	100	100
16	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
16	e	95/139 (68%)	86 (90%)	9 (10%)	0	100	100
17	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
17	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100
18	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
18	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
19	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
19	h	89/129 (69%)	87 (98%)	2 (2%)	0	100	100
All	All	4604/5536 (83%)	3862 (84%)	697 (15%)	45 (1%)	20	54

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU

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Mol	Chain	Res	Type
1	A	453	LYS
1	A	537	LEU
2	B	257	THR
2	B	1015	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	1223/1528 (80%)	1219 (100%)	4 (0%)	92	94
2	B	1016/1077 (94%)	1009 (99%)	7 (1%)	84	90
3	C	236/264 (89%)	235 (100%)	1 (0%)	91	94
4	D	133/160 (83%)	133 (100%)	0	100	100
5	E	196/197 (100%)	193 (98%)	3 (2%)	65	80
6	F	75/137 (55%)	74 (99%)	1 (1%)	69	82
7	G	148/148 (100%)	147 (99%)	1 (1%)	84	90
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	105 (99%)	1 (1%)	78	87
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	46	66
16	a	83/112 (74%)	82 (99%)	1 (1%)	71	83
16	e	82/112 (73%)	80 (98%)	2 (2%)	49	69
17	b	65/81 (80%)	63 (97%)	2 (3%)	40	62
17	f	63/81 (78%)	62 (98%)	1 (2%)	62	79
18	c	82/102 (80%)	82 (100%)	0	100	100
18	g	83/102 (81%)	82 (99%)	1 (1%)	71	83
19	d	81/107 (76%)	79 (98%)	2 (2%)	47	68
19	h	77/107 (72%)	75 (97%)	2 (3%)	46	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4071/4785 (85%)	4041 (99%)	30 (1%)	84 90

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	166	ARG
18	g	71	ARG
9	I	105	ASN
19	h	76	ARG
16	e	53	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	8	ASN
5	E	112	GLN
18	g	112	GLN
4	D	46	HIS
4	D	179	ASN

5.3.3   RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	10/11 (90%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	1	G
13	P	4	U

There are no RNA pucker outliers to report.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-6984. 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 ⓘ

6.1.1   Primary map

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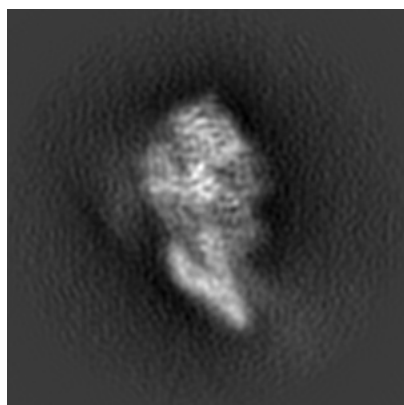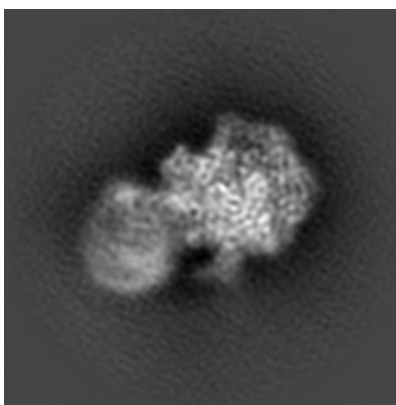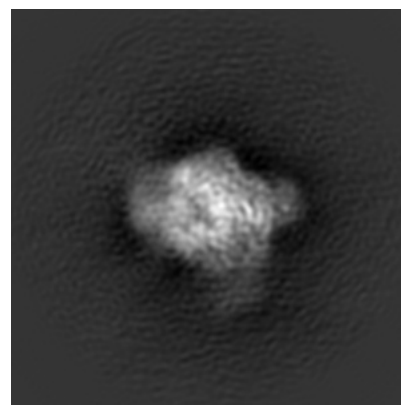
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
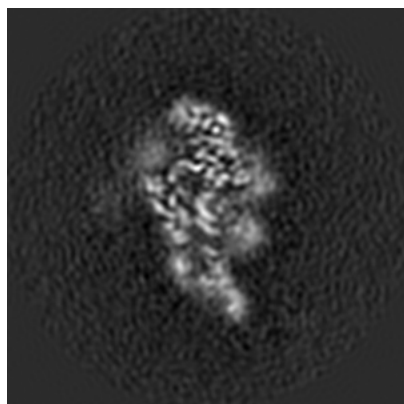
6.2.1   Primary map
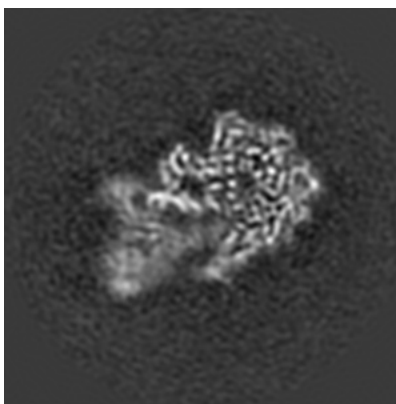
X Index: 120   Y Index: 120   Z Index: 120
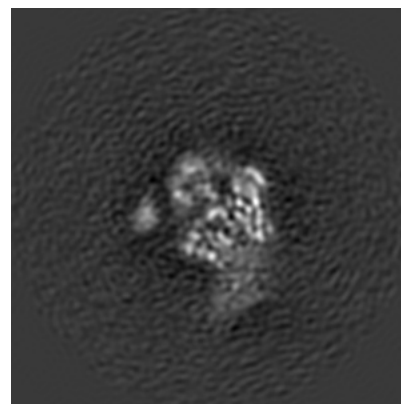
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map
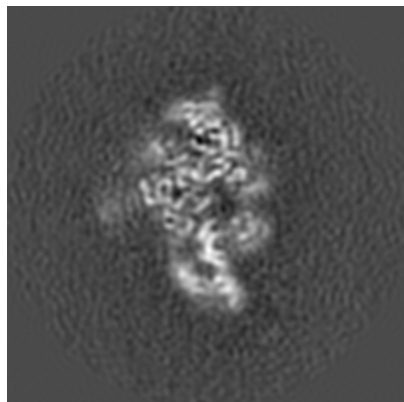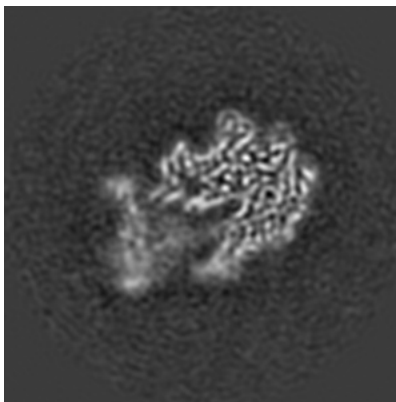
| X Index: 126 | Y Index: 116 | Z Index: 131 |
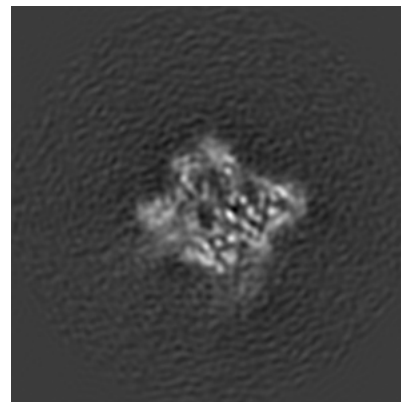
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

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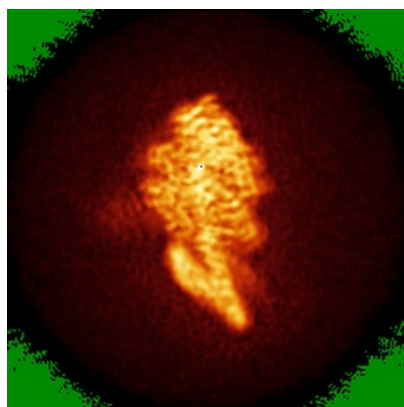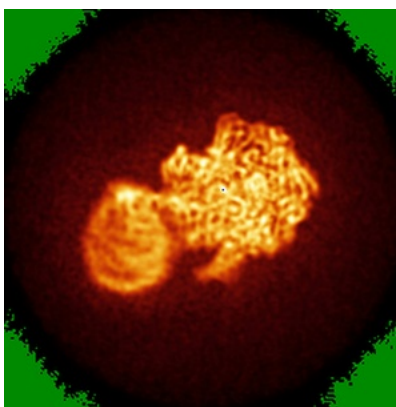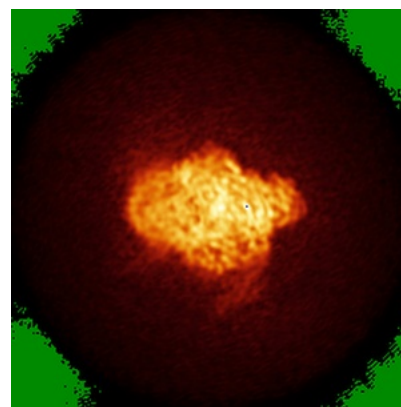
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
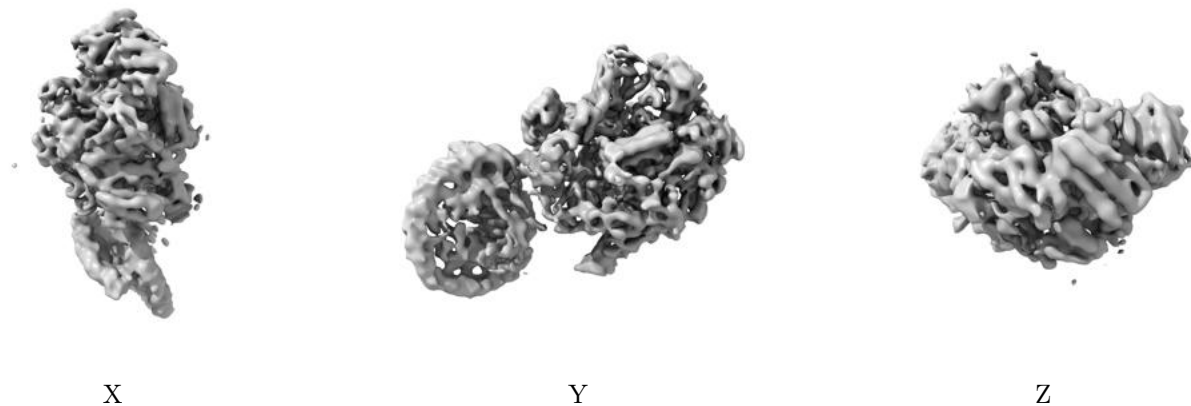
The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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

7   Map analysis ⓘ

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

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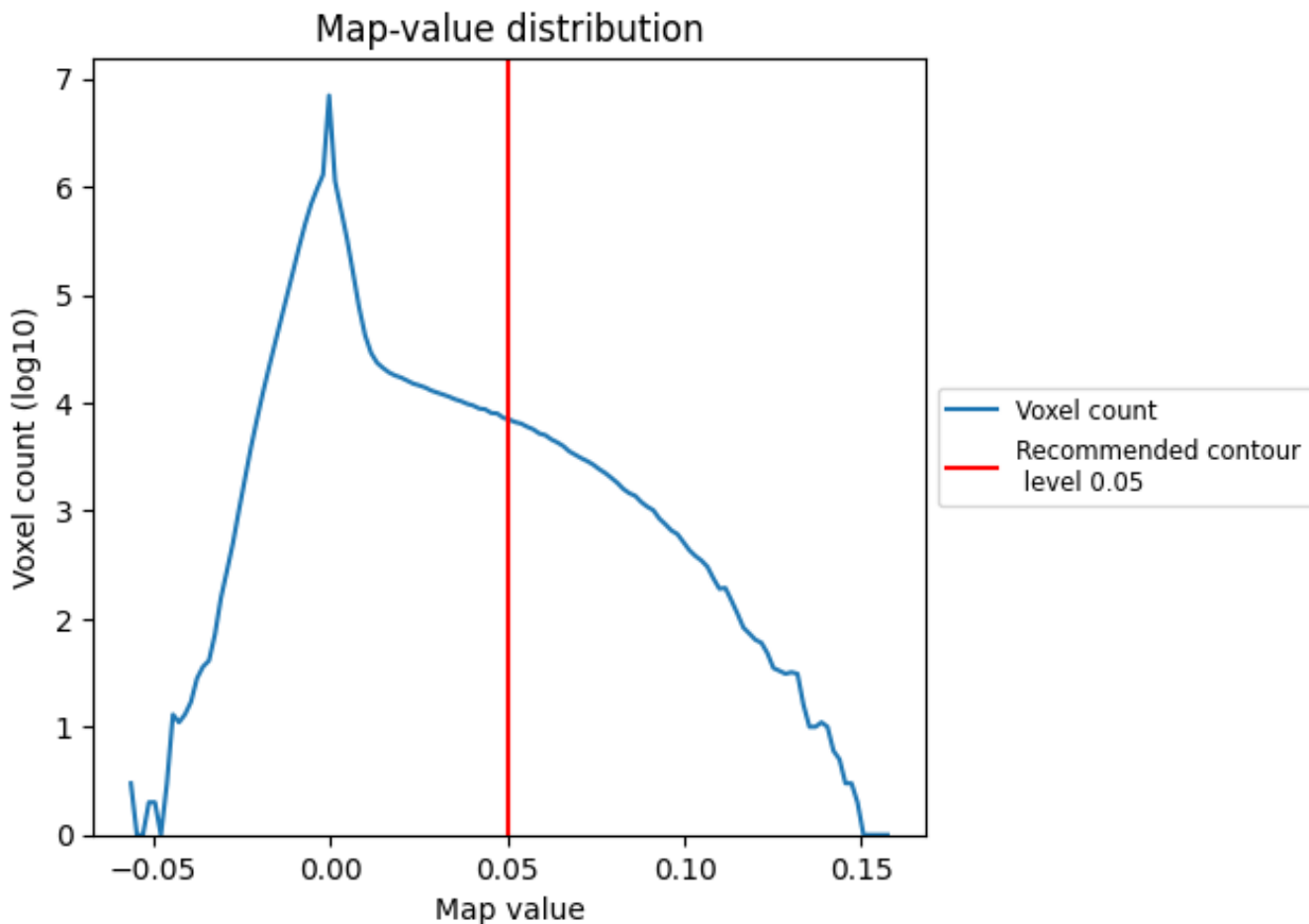
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
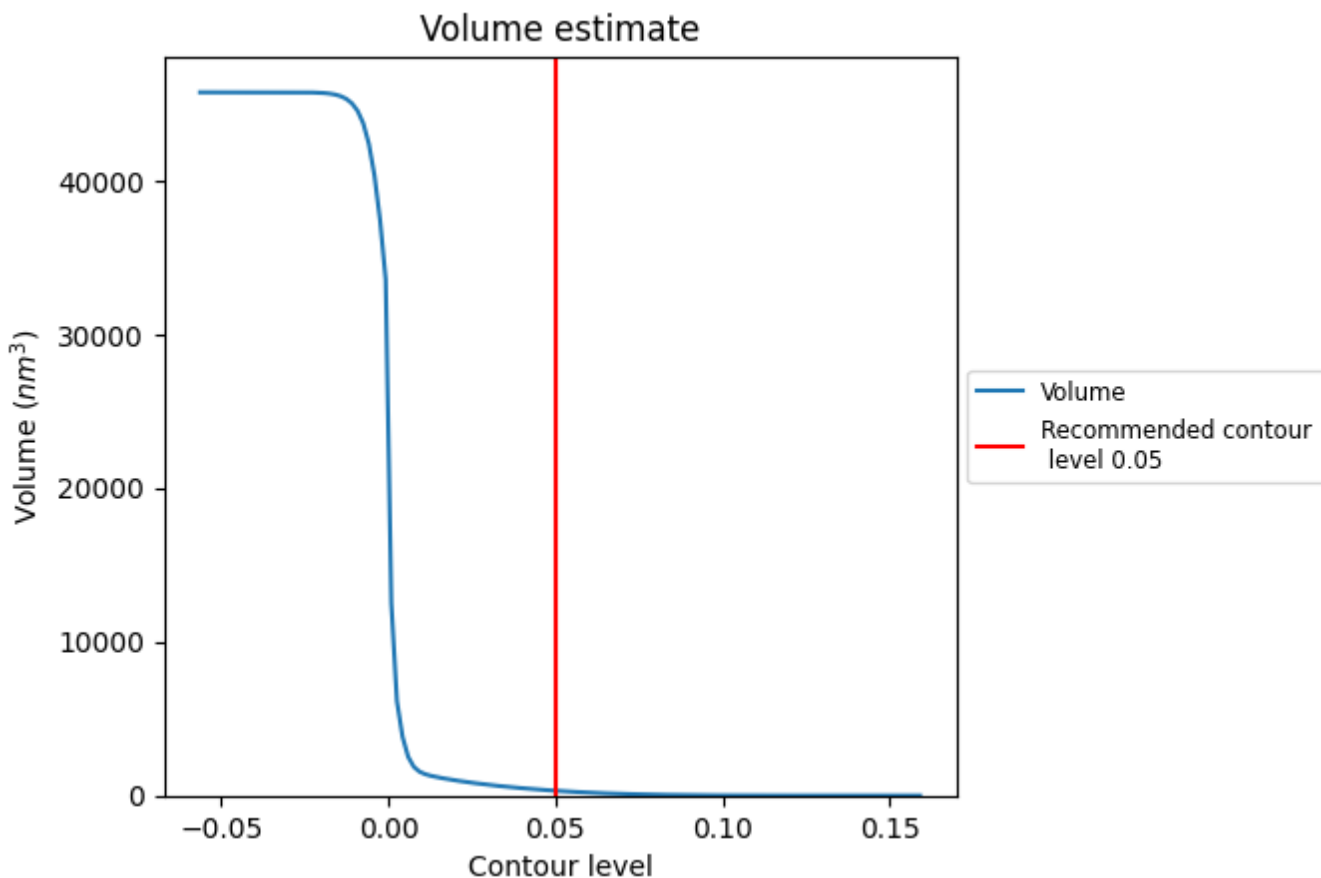
The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 285 kDa.

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 ⓘ
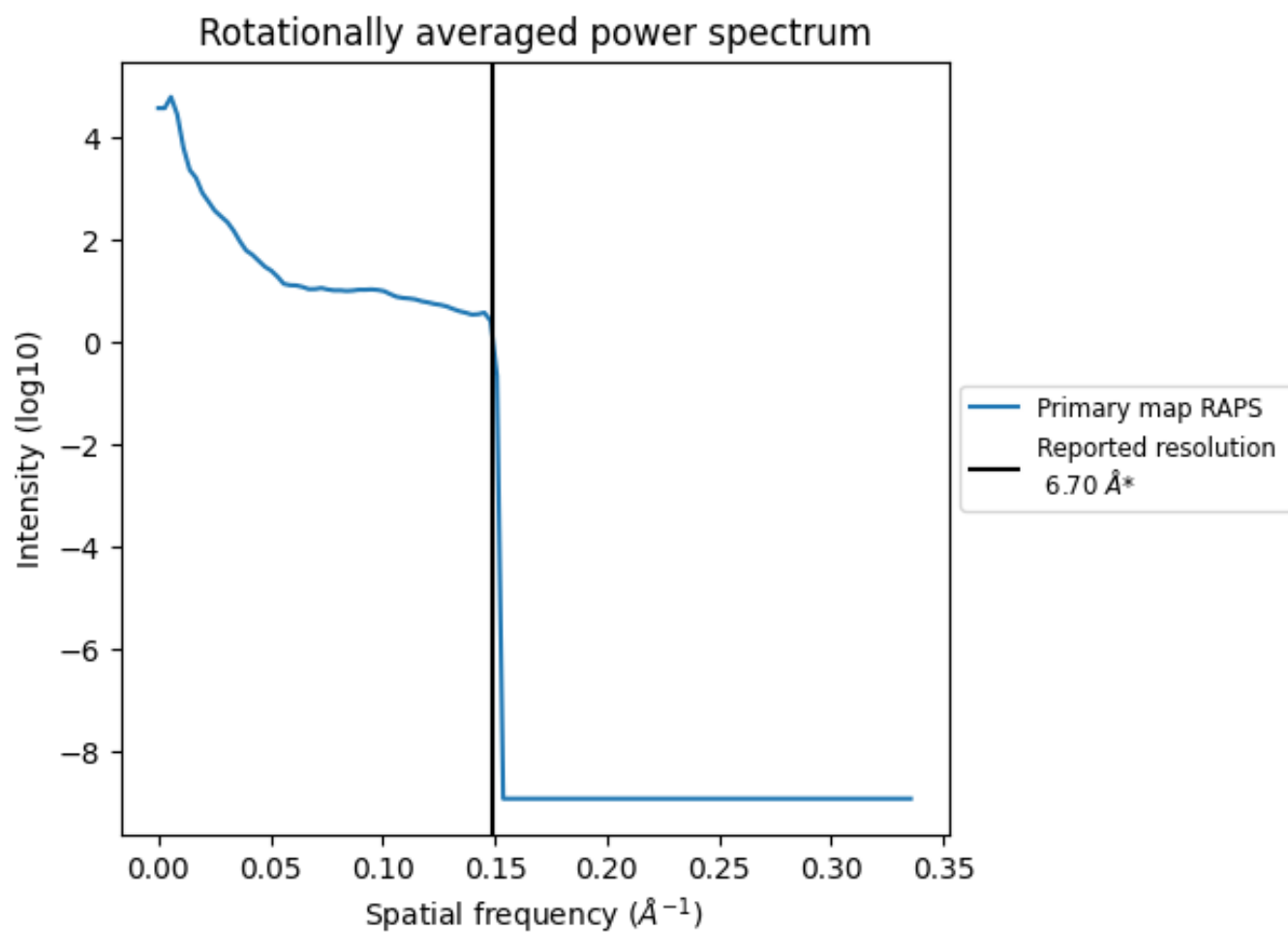
*Reported resolution corresponds to spatial frequency of 0.149 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
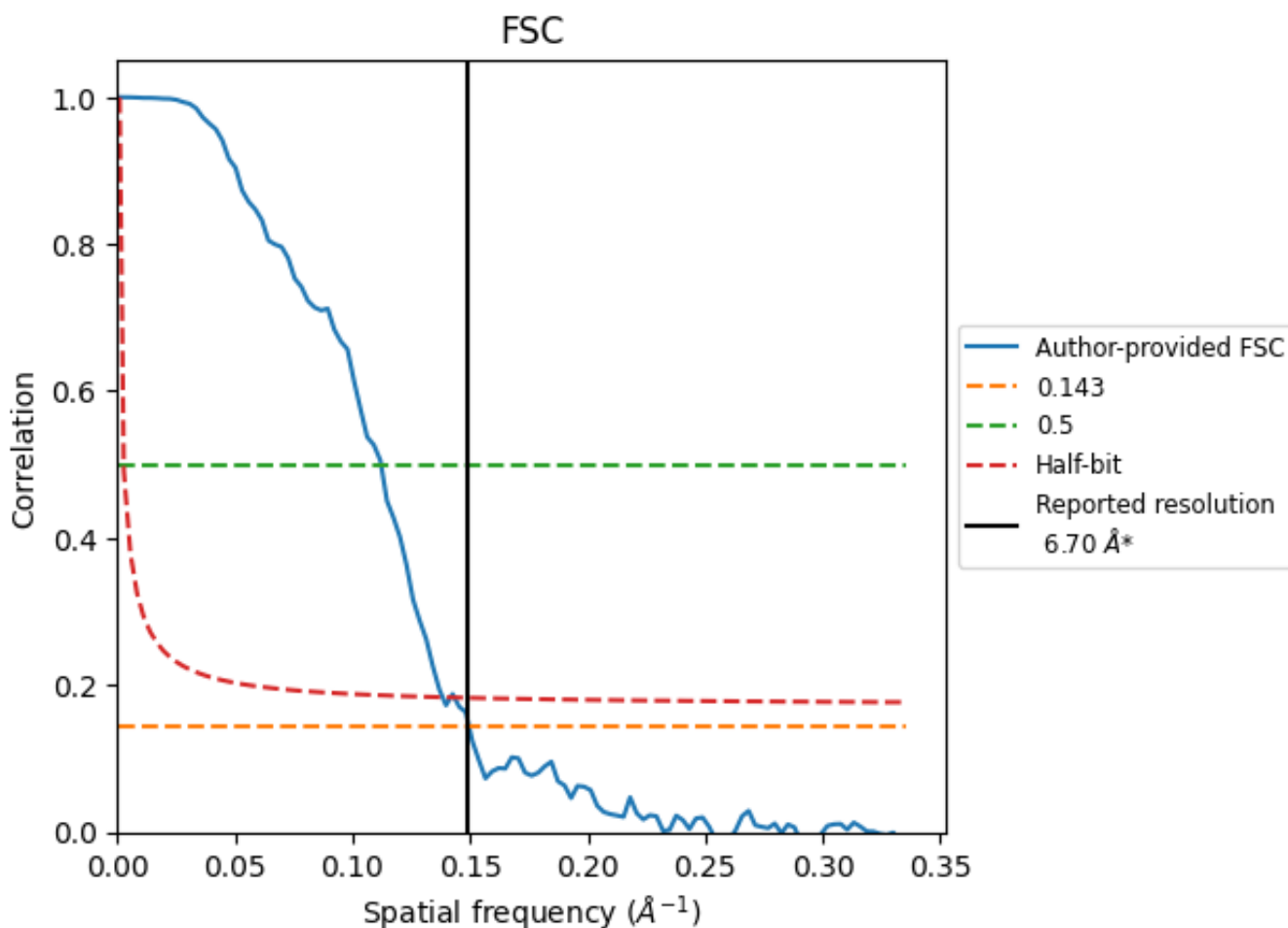
*Reported resolution corresponds to spatial frequency of 0.149 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	6.68	8.92	7.23
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-6984 and PDB model 6A5T. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlay (i)

| X | Y | Z |
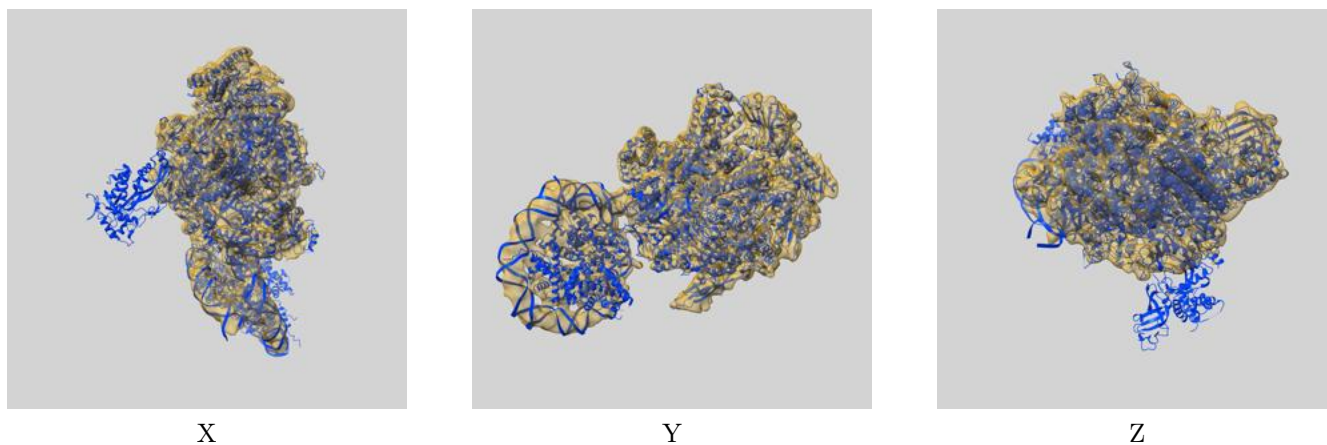
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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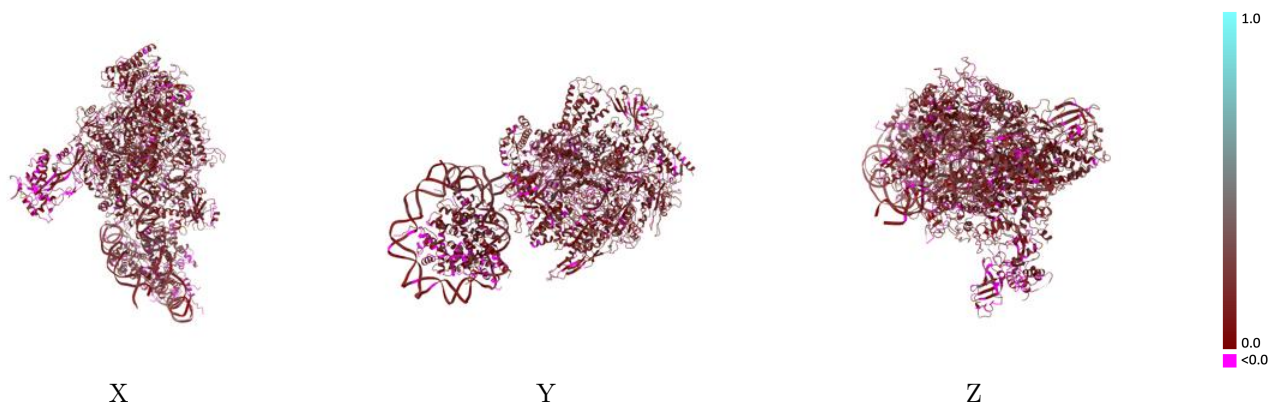
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
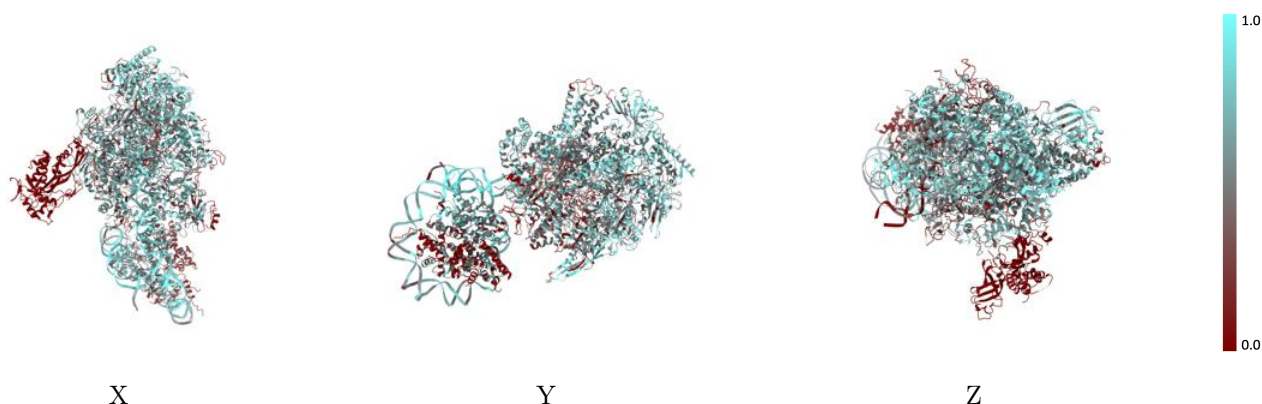
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ
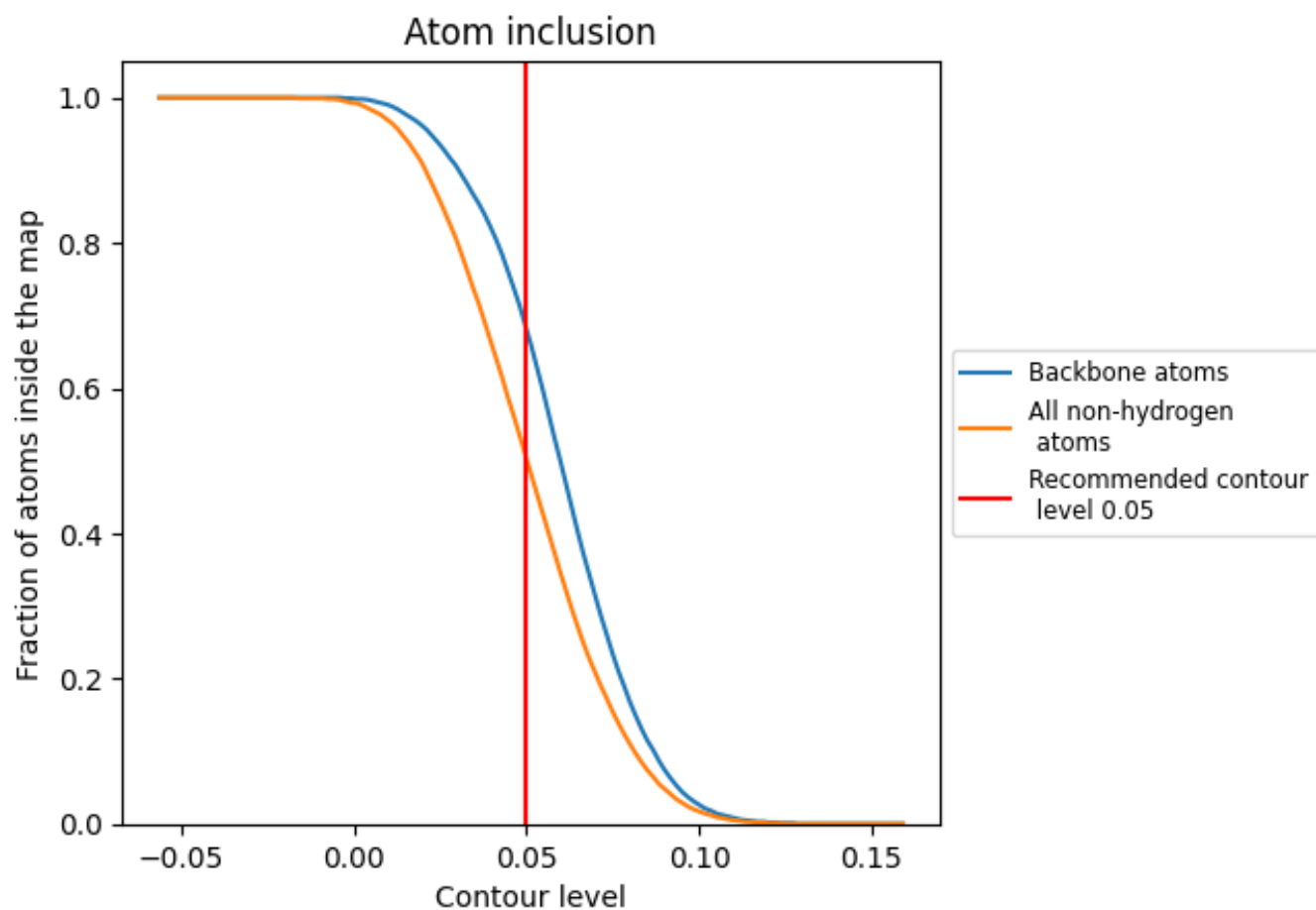
At the recommended contour level, 68% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5040	0.1510
A	0.5390	0.1690
B	0.5180	0.1550
C	0.6280	0.1720
D	0.0000	0.0570
E	0.6570	0.1860
F	0.5500	0.1750
G	0.0050	0.0860
H	0.6490	0.1830
I	0.1850	0.1170
J	0.6280	0.1500
K	0.5930	0.1590
L	0.5320	0.1590
N	0.6700	0.1590
P	0.7230	0.2080
T	0.6850	0.1680
a	0.3040	0.0760
b	0.4080	0.0940
c	0.4990	0.1320
d	0.4790	0.1380
e	0.5330	0.1320
f	0.5010	0.1310
g	0.0830	0.0610
h	0.1860	0.1010

1.0

0.0
<0.0