WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Aug 8, 2023 – 01:44 pm BST

PDB ID	:	8P4D
EMDB ID	:	EMD-17406
Title	:	Structural insights into human co-transcriptional capping - structure 4
Authors	:	Garg, G.; Dienemann, C.; Farnung, L.; Schwarz, J.; Linden, A.; Urlaub, H.; Cramer, P.
Deposited on	:	2023-05-20
Resolution	:	3.60 Å(reported)

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 3.60 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
Clashscore		18
Ramachandran outliers		0.1%
Sidechain outliers		0.7%
RNA backbone		0.43

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
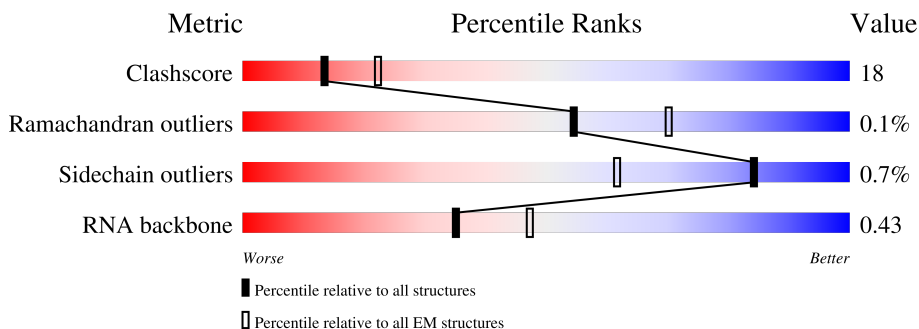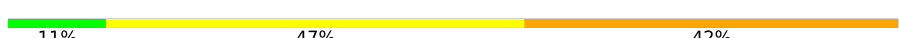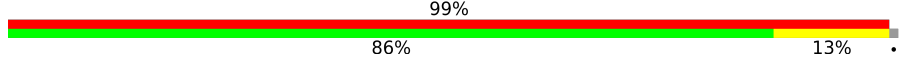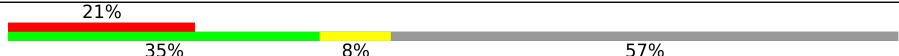
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 >=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	N	32	9% — 78% / 22%
2	T	41	5% — 68% / 29% / •
3	A	1970	48% / 24% / 28%
4	B	1174	• 64% / 32% / •
5	C	275	• 68% / 27% / •
6	E	210	64% / 35% / •
7	F	127	• 47% / 17% / 35%

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Mol	Chain	Length	Quality of chain
8	H	150	61% 38%
9	I	125	64% 30% 6%
10	J	67	75% 25%
11	K	117	68% 31%
12	L	58	52% 28% 21%
13	P	19	11% 47% 42%
14	D	142	61% 27% 11%
15	G	172	61% 38%
16	M	597	35% 30% 24% 44%
17	Y	117	99% 86% 13%
18	Z	1087	21% 35% 8% 57%

2 Entry composition ⓘ

There are 19 unique types of molecules in this entry. The entry contains 40255 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 DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	N	32	652	312	117	191	32	0	0

- Molecule 2 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	T	41	847	403	155	248	41	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1410	11166	7029	2001	2067	69	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	1132	9052	5725	1592	1671	64	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	263	2115	1324	365	420	6	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	209	1720	1089	300	323	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	82	Total 657	C 418	N 113	O 121	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	148	Total 1186	C 750	N 194	O 237	S 5	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	117	Total 949	C 587	N 169	O 182	S 11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

- Molecule 12 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total 388	C 241	N 75	O 66	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	19	Total 410	C 183	N 80	O 128	P 19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	126	Total	C	N	O	S	0	0
			1004	630	170	200	4		

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1333	866	214	245	8		

- Molecule 16 is a protein called mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	333	Total	C	N	O	S	0	0
			2662	1698	460	484	20		

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

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

- Molecule 18 is a protein called Transcription elongation factor SPT5.

| Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	469	Total	C	N	O	S	0	0
			3749	2384	665	684	16		

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol	Chain	Residues	Atoms		AltConf
19	Y	1	Total	Zn	0
			1	1	

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.
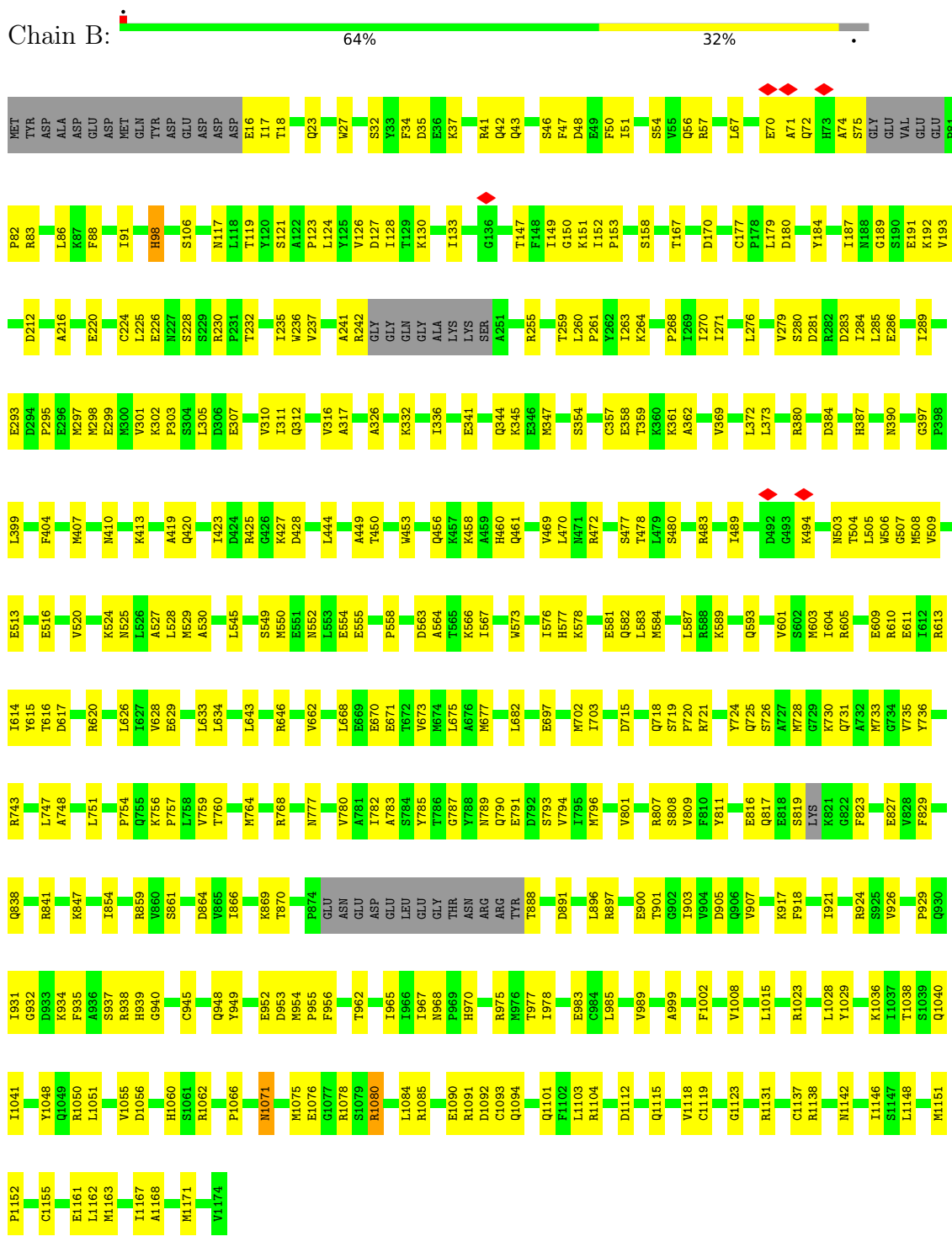
- Molecule 1: DNA (32-MER)
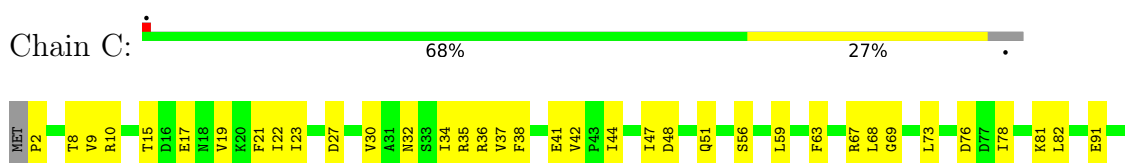
Chain N:
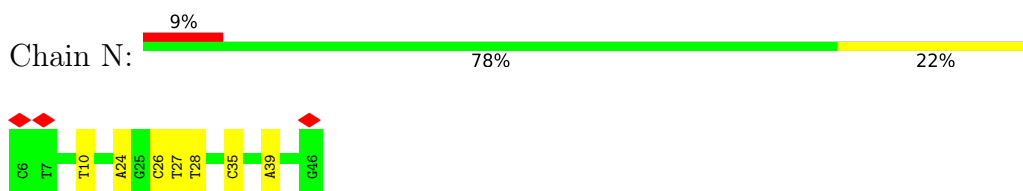
- Molecule 2: DNA (41-MER)

Chain T:
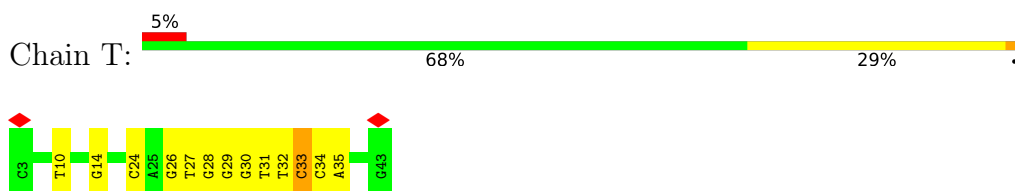
- Molecule 3: DNA-directed RNA polymerase II subunit RPB1

Chain A:
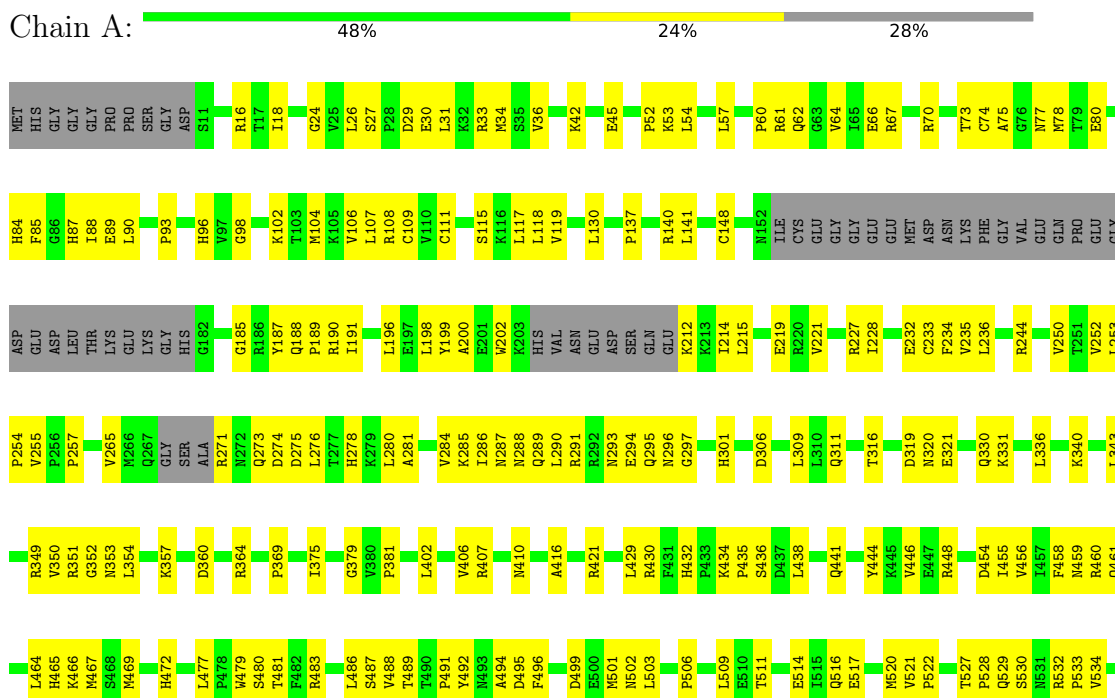
● Molecule 4: DNA-directed RNA polymerase subunit beta

Chain B:

64%					32%

● Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C:

68%					27%

L103 D104 V105 V115 L120 N123 S124 N134 R135 D136 ASN ASP PRO SER ASP TYR VAL E144 Q145 D146 D147 I148 L149 I150 V151 E158 L161 A165 K175 P178 A183 F184 E185 D189 N190 A191 T195 V196 D221 R228 F229 Y230 Y231 N232 V233 E234

L239 R240 P241 E242 T243 I244 V245 G251 K254 L259 Q260 V271 LEU THR ILE ASN

• Molecule 6: DNA-directed RNA polymerase II subunit E

Chain E:

64%   35%

MET D2 Y8 R9 K12 I13 R14 M18 R24 T29 E32 T36 E39 F44 K47 R52 P53 R54 D57 L58 T59 V60 L61 H64 N65 D66 D67 P68 T69 D70 Q71 M72 F73 V74 P80 I84 I87 Y90 C91 Q92 R93 M94 Q95

E96 E97 N98 I99 T100 R101 A102 L103 I104 V105 V106 Q107 Q108 T111 A114 S117 D120 M121 I126 L127 F130 L135 L136 V149 T152 V156 R162 P171 R172 I173 Y182 F183 K192 I193 I194 T199 A200 G201 R202 Y203 I204 R207 L208 V209

Q210

• Molecule 7: DNA-directed RNA polymerase II subunit F

Chain F:

47%   17%   35%

MET SER ASP ASN GLU ASP ASN PHE ASP ASP GLY ASP ASP PHE ASP ASP VAL GLU GLU GLU GLY LEU ASP LEU GLU ASN GLU GLU GLY GLN GLU ASN VAL GLU ILE LEU PRO SER GLY GLU ARG PRO Q46 R51 T58 R62 V65 R69 I73 C76

A77 P78 V79 M80 V81 E82 L83 E84 G85 P89 K95 P103 I104 I105 I106 R107 G119 V120 D121 E122 D127
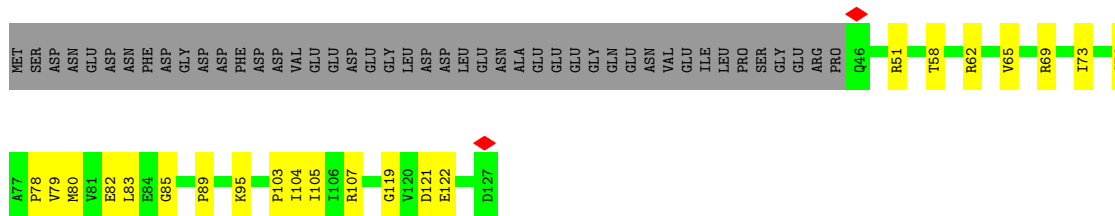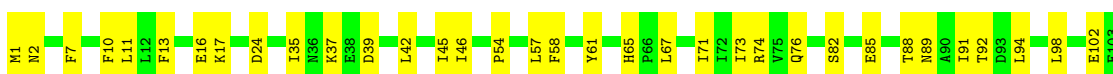
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

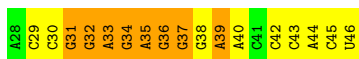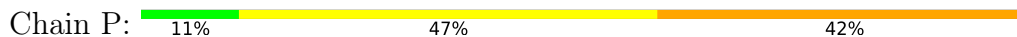Chain H:

61%   38%

MET A2 G3 I4 L5 F6 E7 F10 D11 V12 I15 D16 D23 R24 V25 S26 R27 L28 H29 C30 E31 S32 L39 I40 N44 K55 V59 I60 T63 L64 Y65 E66 D67 G68 D71 Y75 N76 P77 D80 R84 A85 D86 Q87 F88 E89 Y90 V91 M92

Y93 G94 K95 V96 Y97 E100 E103 T106 E107 R111 L112 S113 A114 V115 V116 L121 L122 M123 R124 L125 D128 A129 N130 N131 F135 L144 M145 K146 A149 PHE
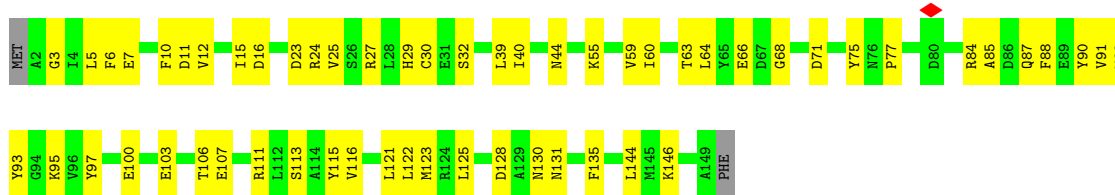
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:

64%   30%   6%

MET GLU PRO ASP GLY THR TYR GLU P9 G10 F11 V12 G13 I14 R15 L35 N50 S51 C52 I53 Y54 V55 N56 E64 L65 I68 D71 Q74 T77 L78 P79 R80 T81 E82 D83 H84 P85 C86 Q87 K88 K92 V95 F96 F97 H100 R109 V113 C114

T115 A116 H121 R122 W123 T124 E125

• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 75% 25%

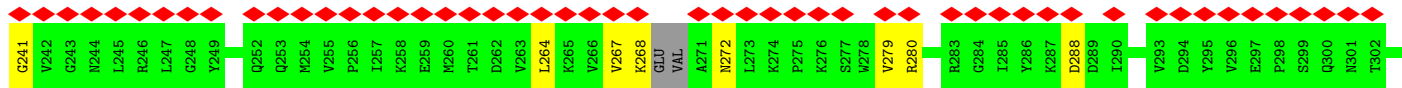M1 I2 I3 R6 T9 C10 I13 W18 L35 L40 K41 R42 Y43 C44 C45 L49 L50 A51 D54 L55 I56 L65 E66 K67

• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 68% 31% .

M1 N2 F7 F10 L11 L12 F13 E16 K17 D24 I35 N36 K37 E38 D39 L42 I45 I46 P54 L57 F58 Y61 H65 P66 L67 I71 I72 I73 R74 V75 Q76 S82 E85 T88 N89 A90 I91 T92 D93 L94 L98 E102 E103

R104 F105 G115 ILE GLU
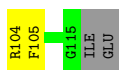
• Molecule 12: RNA polymerase II subunit K

Chain L: 52% 28% 21%

MET ASP THR GLN LYS ASP VAL GLN PRO PRO LYS GLN Q13 E27 I28 K29 I34 R35 C36 R37 E38 Y41 R42 I43 M44 Y45 K46 K47 R51 L52 V53 V54 A57 R58
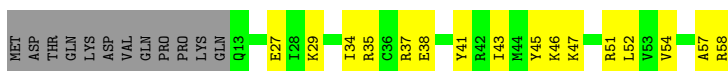
• Molecule 13: RNA (5'-R(P*AP*CP*CP*GP*GP*AP*GP*AP*GP*GP*GP*AP*AP*CP*CP*CP*AP*CP*U)-3')

Chain P: 11% 47% 42%

A28 C29 C30 G31 G32 A33 G34 A35 G36 G37 G38 A39 A40 C41 C42 C43 A44 C45 U46

• Molecule 14: RNA polymerase II subunit D

Chain D: 61% 27% . 11%

MET ALA ALA GLY SER ASP PRO ARG ALA GLY ASP VAL E14 T31 L32 L33 N34 S35 E36 V37 H38 M39 L40 L41 N48 D53 V60 F61 Y67 T68 A69 R70 F71 S72 R73 R84 L87 L92 H93 K94 F95 E96 L97 A98 C99 L100 A101 N102 L103 C104 P105

A108 K112 A113 L114 L118 E119 G120 R121 L127 L131 Q135 R138 S139 PHE GLN TYR
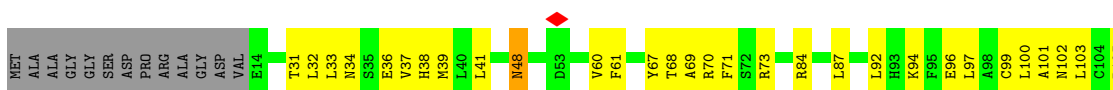
• Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G: 61% 38% ..

• Molecule 16: mRNA-capping enzyme

Chain M:

35%

30%   24%   •   44%

• Molecule 17: Transcription elongation factor SPT4

Chain Y:

99%

86%   13%   •

I61 A62 M63 M64 S65 P66 E67 D68 S69 W70 V71 S72 K73 W74 Q75 R76 V77 S78 N79 F80 K81 P82 G83 V84 Y85 A86 V87 S88 V89 T90 G91 R92 L93 P94 Q95 G96 I97 V98 R99 E100 L101 K102 S103 R104 G105 V106 A107 Y108 K109 S110 R111 D112 T113 A114 I115 K116 T117
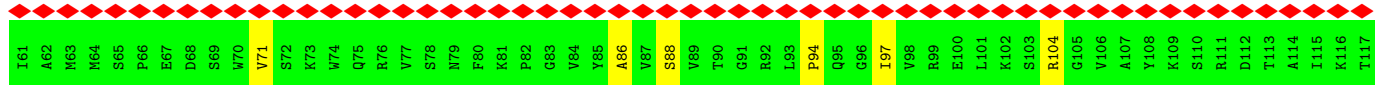
• Molecule 18: Transcription elongation factor SPT5

Chain Z:

21%
35% 8% 57%

MET SER ASP SER GLU ASP SER ASN PHE SER GLU GLU GLU ASP SER GLU ARG SER SER ASP SER GLY GLU GLU ALA GLU VAL ASP GLU ARG SER ALA ALA GLY SER GLU LYS GLU GLU GLU PRO GLU ASP GLU GLU GLU GLU GLU GLU GLU TYR ASP GLU GLU GLU GLU

GLU ASP ASP ARG PRO PRO LYS LYS PRO ARG HIS GLY GLY PHE ILE LEU ASP ASP GLU ALA ASP VAL ASP ASP GLU GLU ASP TYR GLU ASP GLU ASP GLN TRP GLU ASP GLY ALA ASP GLU GLU GLU ILE GLU ALA SER ASN ILE ASP ASN VAL VAL LEU ASP ASP ARG SER

GLY ALA ARG ARG LEU GLN ASN LEU TRP ARG ASP GLN ARG GLU GLU GLU LEU GLY GLU GLU TYR TYR MET LYS LYS TYR ALA LYS SER VAL GLY THR VAL TYR GLY SER GLY SER ASP GLU LEU SER ASP ASP ILE THR GLN GLN LEU LEU PRO GLY VAL LYS **D176 P177 N178 L179 W180**

T181 V182 K183 C184 K185 I186 G187 E188 E189 R190 A191 T192 A193 I194 S195 L196 M197 R198 K199 F200 I201 A202 Y203 Q204 F205 T206 D207 T208 P209 L210 Q211 I212 K213 S214 V215 V216 A217 P218 E219 H220 V221 K222 G223 Y224 I225 Y226 V227 E228 A229 Y230 K231 Q232 T233 H234 V235 K236 Q237 A238 I239 E240

G241 V242 G243 N244 L245 R246 L247 G248 Y249 Q252 Q253 M254 V255 P256 I257 K258 E259 M260 T261 D262 V263 L264 K265 V266 V267 K268 GLU VAL A271 N272 L273 K274 P275 K276 S277 W278 V279 R280 R283 G284 I285 Y286 K287 D288 D289 I290 V293 D294 Y295 V296 E297 P298 S299 Q300 N301 T302

K306 R310 I311 D312 I316 K317 A318 ARG MET SER LEU LYS ASP TRP PHE ALA LYS ARG LYS LYS PHE LYS ARG P335 P336 Q337 R338 L339 G349 G350 D351 V352 A353 S354 D355 G356 D357 F358 L359 I360 F361 R365 Y366 S367 R368 K369 G370 F371 L372 T383 E384 G385 V386 K387 P388

THR LEU SER GLU LEU GLU LYS PHE GLU ASP GLN PRO GLU GLY ILE ASP LEU GLU VAL VAL THR GLU SER THR GLY LYS GLU R416 E417 H418 N419 F420 G423 D424 N425 E430 G431 E432 L433 I434 N435 V443 D444 G445 N446 **K447 I448 T449** I450 E455 D456 L457 K458 D459 P464

A465 Q466 E467 L468 R469 K470 Y471 F472 K473 M474 H477 V478 K479 A482 G483 R484 F485 E486 G487 D488 T489 I492 V493 E496 E497 N498 F499 L502 F503 S504 D505 L506 T507 M508 L511 L514 P515 R516 D517 LEU GLN LEU CYS SER GLU THR ALA S526 V530 G531 E535

W536 G537 E538 D543 P544 Q545 R552 R555 Q559 V560 M563 Y564 G565 K566 V567 V568 T569 V570 R571 H572 Q573 R577 K578 K579 D580 N581 R582 F583 A584 V585 A586 L587 E590 Q591 H595 V596 K597 D598 I599 P606 H607 S608 G609 R610 E611 R615 F618 R619 S620

F621 A622 F623 L624 H625 C626 K627 K628 L629 V630 E631 N632 G633 G634 M635 R641 L645 A646 GLY GLY SER LYS PRO ARG ASP VAL THR ASN PHE THR VAL GLY GLY PHE ALA PRO MET SER PRO ARG ILE SER SER PRO MET HIS PRO SER ALA GLY SER GLY GLN ARG GLY GLY PHE GLY SER

PRO GLY GLY SER GLY GLY MET SER ARG ARG GLY ARG ARG ASP N703 E704 L705 V710 S713 I721 V724 K725 D726 A727 E735 L736 H737 S738 T752 V753 GLY SER ARG ARG PRO GLY GLY MET THR THR TYR GLY ARG THR PRO MET TYR GLY SER GLN THR

PRO MET TYR SER GLY GLY SER ARG THR PRO MET TYR GLY SER PRO GLN THR PRO HIS TYR GLY SER GLN THR PRO LEU HIS ASP GLY SER ARG THR PRO HIS TYR GLY SER ARG THR PRO ALA GLN SER GLY ALA TRP ASP PRO ASN ASN PRO ASN THR PRO SER ARG GLY GLY GLU GLU GLU

TYR GLU TYR ALA PHE ASP ASP GLU PRO THR PRO MET TYR GLY SER PRO GLN ALA TYR GLY GLN SER ASN PRO GLN TYR ASN PRO ALA MET TYR ASN THR ASP PHE SER PRO TYR ALA ALA

PRO SER PRO GLN GLY SER TYR GLN PRO SER PRO SER PRO GLN SER TYR HIS GLN VAL ALA PRO SER PRO ALA GLY TYR GLN ASN THR HIS SER PRO ALA SER TYR HIS PRO THR PRO SER PRO MET ALA TYR GLN ALA SER PRO SER PRO SER PRO VAL GLY TYR SER PRO MET THR PRO

GLY ALA PRO SER PRO GLY GLY TYR ASN PRO HIS THR PRO GLY SER GLY ILE GLU GLN GLN ASN SER SER ASP TRP VAL THR THR ASP ILE GLN VAL LYS VAL ARG ASP THR TYR LEU ASP THR GLN VAL VAL GLY GLN THR GLY VAL ILE ARG SER VAL THR GLY GLY MET CYS SER VAL TYR

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

LEU ASN LEU ARG PHE LEU GLY LYS LEU LEU GLU ALA

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73948	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 $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0181	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	N	0.62	0/729	1.01	0/1119
2	T	0.66	0/950	1.00	1/1466 (0.1%)
3	A	0.26	0/11369	0.54	0/15347
4	B	0.27	0/9232	0.54	0/12462
5	C	0.26	0/2158	0.50	0/2931
6	E	0.26	0/1751	0.57	0/2366
7	F	0.26	0/667	0.56	0/901
8	H	0.27	0/1207	0.54	0/1628
9	I	0.27	0/972	0.57	0/1316
10	J	0.26	0/542	0.49	0/730
11	K	0.27	0/939	0.49	0/1271
12	L	0.28	0/394	0.72	0/524
13	P	0.25	0/459	0.68	0/714
14	D	0.25	0/1017	0.51	0/1368
15	G	0.28	0/1364	0.54	0/1853
16	M	0.52	0/2717	0.69	2/3659 (0.1%)
17	Y	0.25	0/927	0.46	0/1250
18	Z	0.47	0/3815	0.59	4/5136 (0.1%)
All	All	0.33	0/41209	0.58	7/56041 (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
3	A	0	2
4	B	0	1
6	E	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Z	450	ILE	N-CA-C	-6.22	94.20	111.00
18	Z	449	THR	N-CA-C	-6.12	94.46	111.00
16	M	362	TYR	CB-CA-C	6.10	122.60	110.40
18	Z	423	GLY	N-CA-C	5.54	126.96	113.10
18	Z	447	LYS	N-CA-C	-5.37	96.49	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	538	VAL	Peptide
3	A	539	GLN	Peptide
4	B	98	HIS	Peptide
6	E	57	ASP	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	N	652	0	363	26	0
2	T	847	0	464	35	0
3	A	11166	0	11320	368	0
4	B	9052	0	9081	345	0
5	C	2115	0	2061	62	0
6	E	1720	0	1737	52	0
7	F	657	0	684	18	0
8	H	1186	0	1147	44	0
9	I	949	0	887	23	0
10	J	533	0	557	14	0
11	K	920	0	942	27	0
12	L	388	0	397	24	0
13	P	410	0	209	45	0
14	D	1004	0	980	34	0
15	G	1333	0	1321	76	0
16	M	2662	0	2650	327	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Y	911	0	905	12	0
18	Z	3749	0	3804	175	0
19	Y	1	0	0	0	0
All	All	40255	0	39509	1435	0

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

The worst 5 of 1435 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)
4:B:859:ARG:HG3	18:Z:737:HIS:CG	1.32	1.62
16:M:278:LYS:HG3	16:M:551:ASN:CB	1.19	1.62
16:M:419:CYS:HA	16:M:559:PHE:CE1	1.24	1.62
16:M:462:PRO:CA	16:M:465:ASN:HB2	1.27	1.61
4:B:859:ARG:HG3	18:Z:737:HIS:CD2	1.34	1.57

There are no symmetry-related clashes.

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	
3	A	1398/1970 (71%)	1315 (94%)	82 (6%)	1 (0%)	51	83
4	B	1122/1174 (96%)	1061 (95%)	61 (5%)	0	100	100
5	C	259/275 (94%)	246 (95%)	13 (5%)	0	100	100
6	E	207/210 (99%)	198 (96%)	8 (4%)	1 (0%)	29	68
7	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
8	H	146/150 (97%)	137 (94%)	9 (6%)	0	100	100
9	I	115/125 (92%)	104 (90%)	11 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	44/58 (76%)	37 (84%)	7 (16%)	0	100	100
14	D	124/142 (87%)	120 (97%)	4 (3%)	0	100	100
15	G	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
16	M	326/597 (55%)	312 (96%)	14 (4%)	0	100	100
17	Y	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
18	Z	457/1087 (42%)	440 (96%)	16 (4%)	1 (0%)	47	79
All	All	4739/6388 (74%)	4495 (95%)	241 (5%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	57	ASP
18	Z	497	GLU
3	A	911	PRO

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	
3	A	1241/1749 (71%)	1240 (100%)	1 (0%)	93	98
4	B	992/1027 (97%)	987 (100%)	5 (0%)	88	95
5	C	240/252 (95%)	239 (100%)	1 (0%)	91	97
6	E	191/192 (100%)	190 (100%)	1 (0%)	88	95
7	F	71/111 (64%)	71 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	105/112 (94%)	104 (99%)	1 (1%)	76	88
10	J	56/56 (100%)	56 (100%)	0	100	100
11	K	104/106 (98%)	103 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	43/55 (78%)	43 (100%)	0	100	100
14	D	109/126 (86%)	108 (99%)	1 (1%)	78	90
15	G	146/153 (95%)	145 (99%)	1 (1%)	84	93
16	M	294/534 (55%)	278 (95%)	16 (5%)	22	57
17	Y	102/103 (99%)	102 (100%)	0	100	100
18	Z	412/940 (44%)	411 (100%)	1 (0%)	93	98
All	All	4235/5647 (75%)	4206 (99%)	29 (1%)	84	93

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	M	244	VAL
16	M	463	SER
16	M	329	PHE
16	M	416	PHE
16	M	293	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
16	M	280	ASN
17	Y	12	HIS
18	Z	703	ASN
18	Z	272	ASN
16	M	547	ASN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	18/19 (94%)	10 (55%)	3 (16%)

5 of 10 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	29	C
13	P	30	C
13	P	31	G
13	P	32	G

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Mol	Chain	Res	Type
13	P	33	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	P	36	G
13	P	37	G
13	P	38	G

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

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 1 ligands modelled in this entry, 1 is 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	M	2
1	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	14:DT	O3'	24:DA	P	38.25
1	M	465:ASN	C	466:SER	N	4.87
1	M	464:LEU	C	465:ASN	N	3.20

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-17406. 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 ⓘ
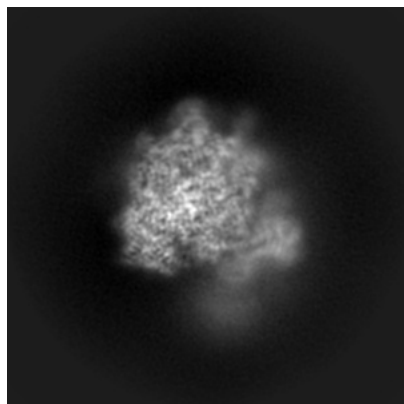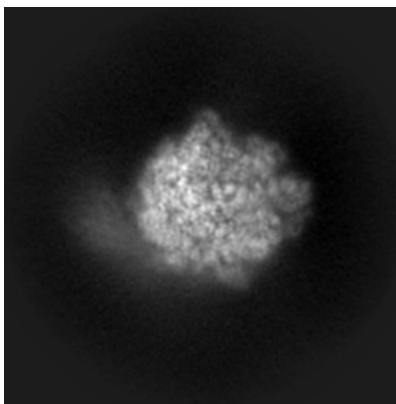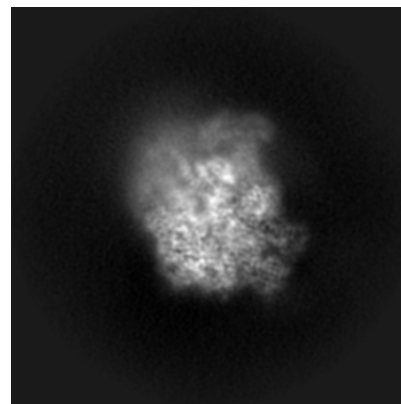
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

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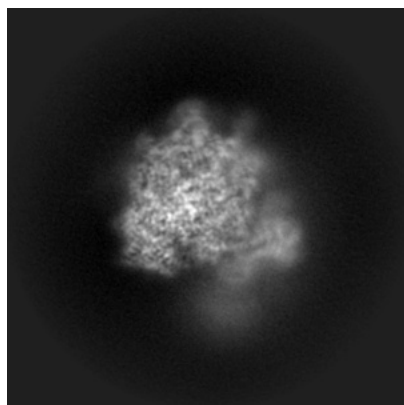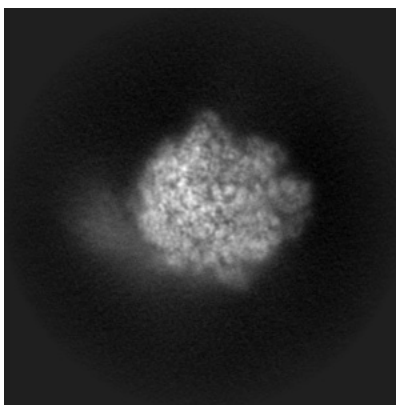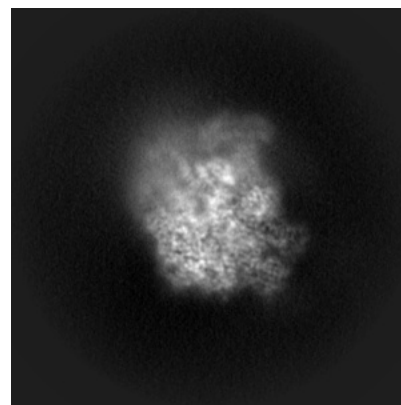
The images above show the map projected in three orthogonal directions.

6.2   Central slices   ⓘ
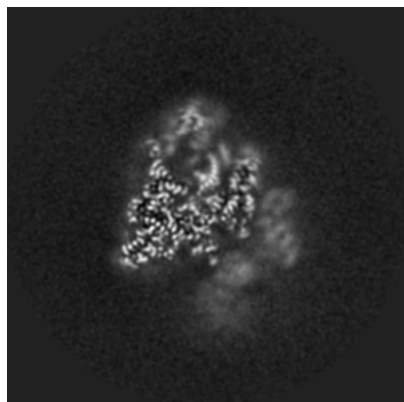
6.2.1   Primary map
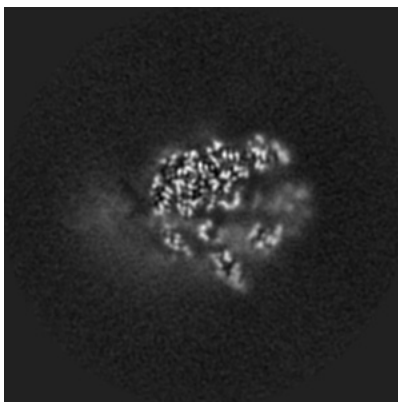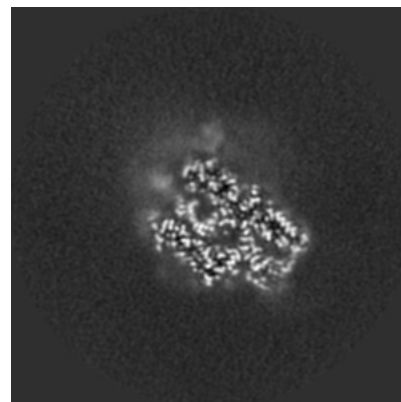
X Index: 150   Y Index: 150   Z Index: 150

6.2.2   Raw map
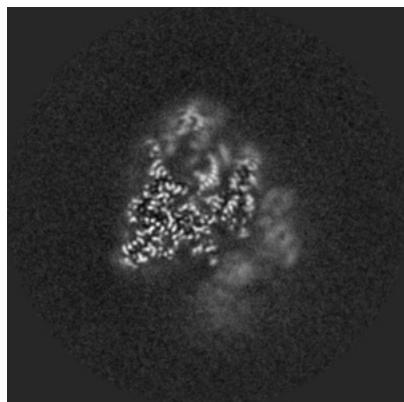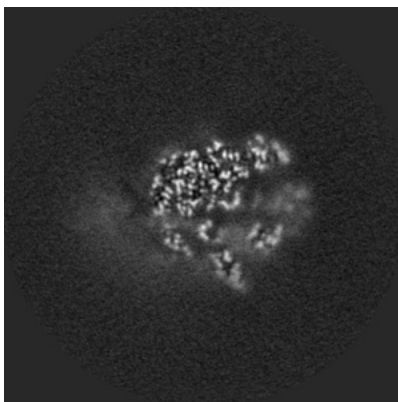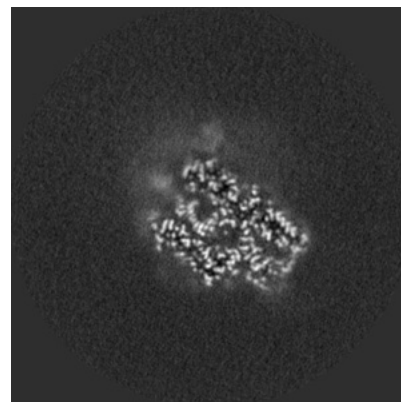
X Index: 150   Y Index: 150   Z Index: 150

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
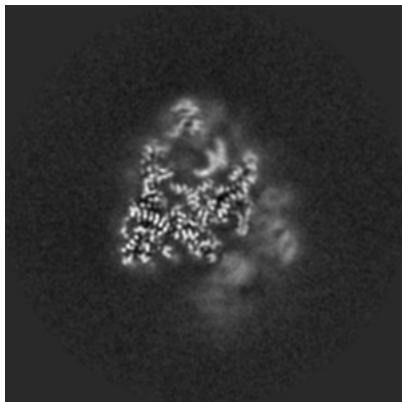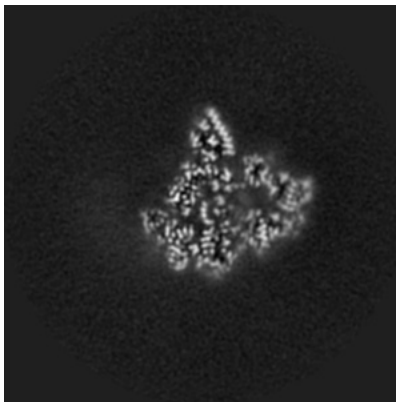
| X Index: 153 | Y Index: 134 | Z Index: 135 |
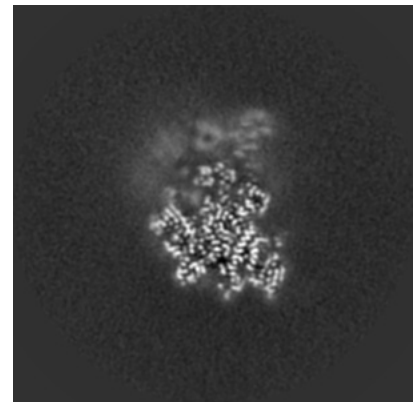
6.3.2 Raw map
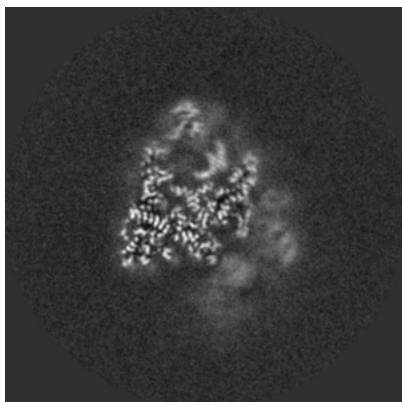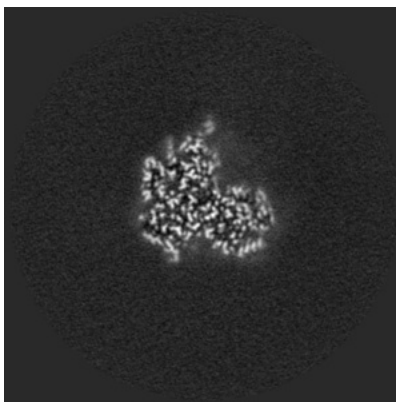
| X Index: 153 | Y Index: 110 | Z Index: 135 |
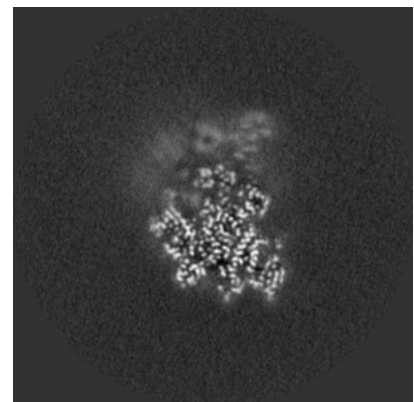
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1   Primary map
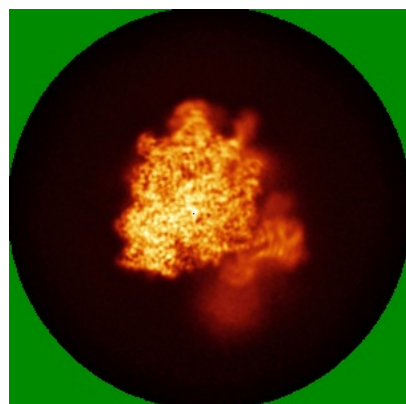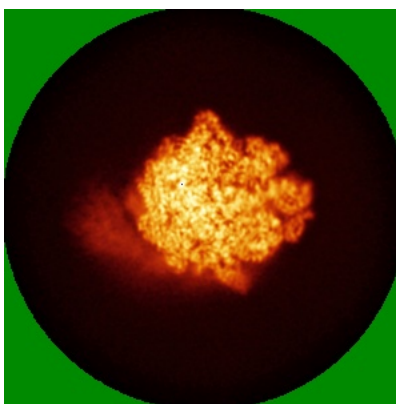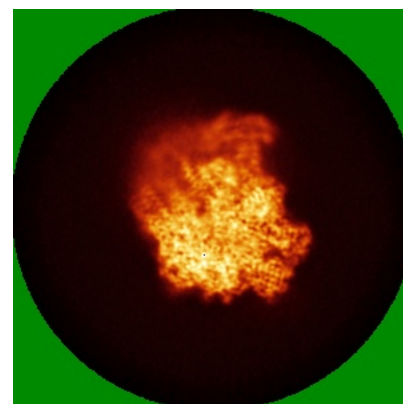
X	Y	Z

6.4.2   Raw map

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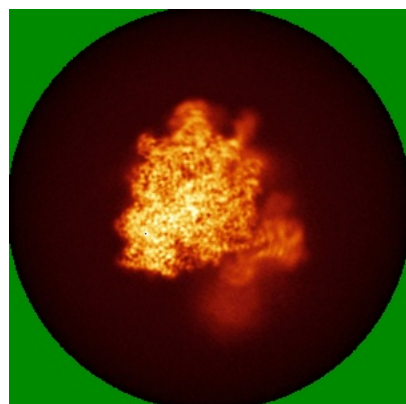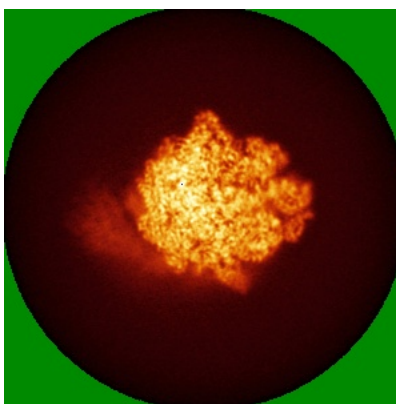
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0181. 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 ⓘ

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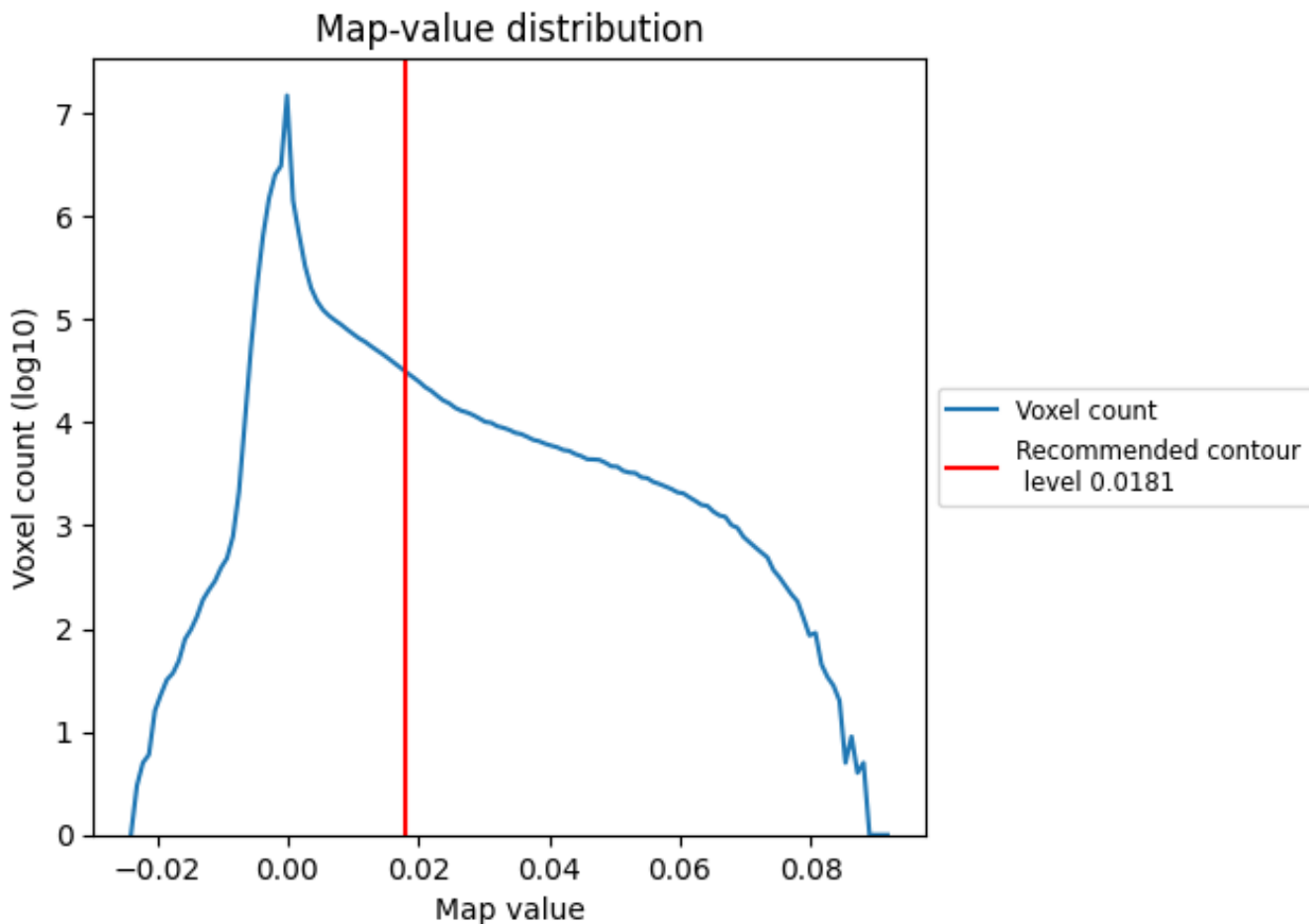
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
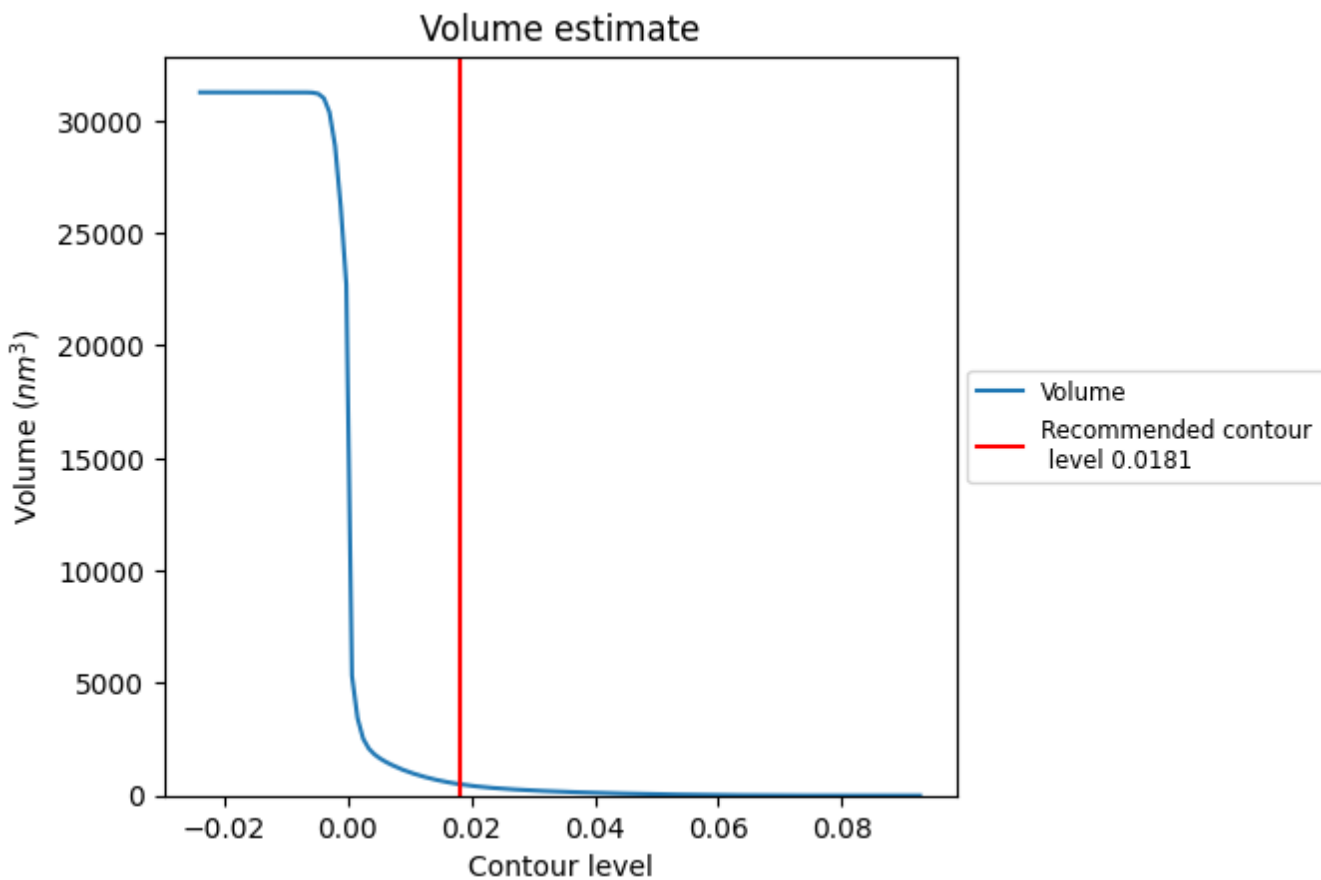
The volume at the recommended contour level is 505 nm^3; this corresponds to an approximate mass of 457 kDa.

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)
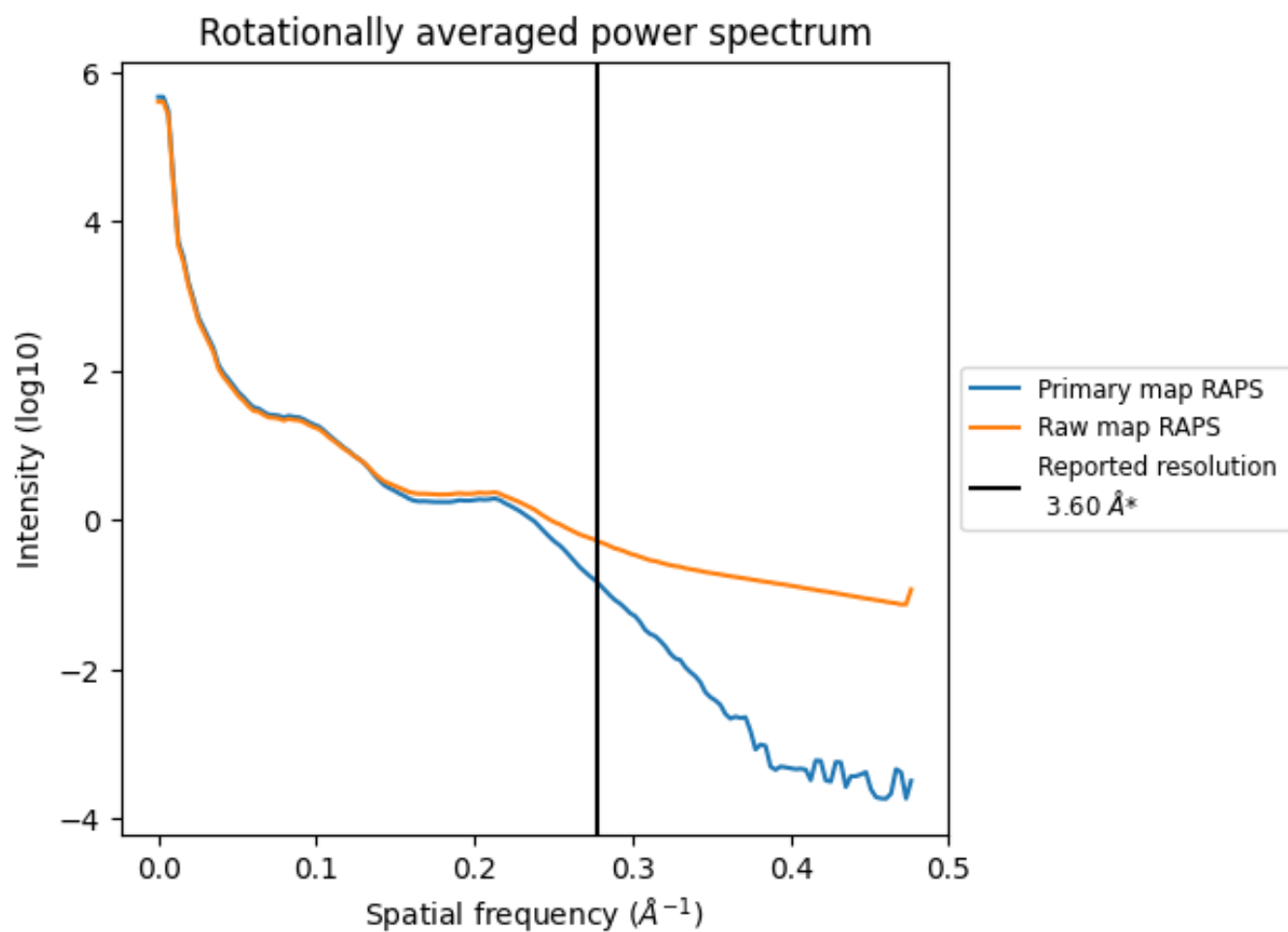
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 ⓘ
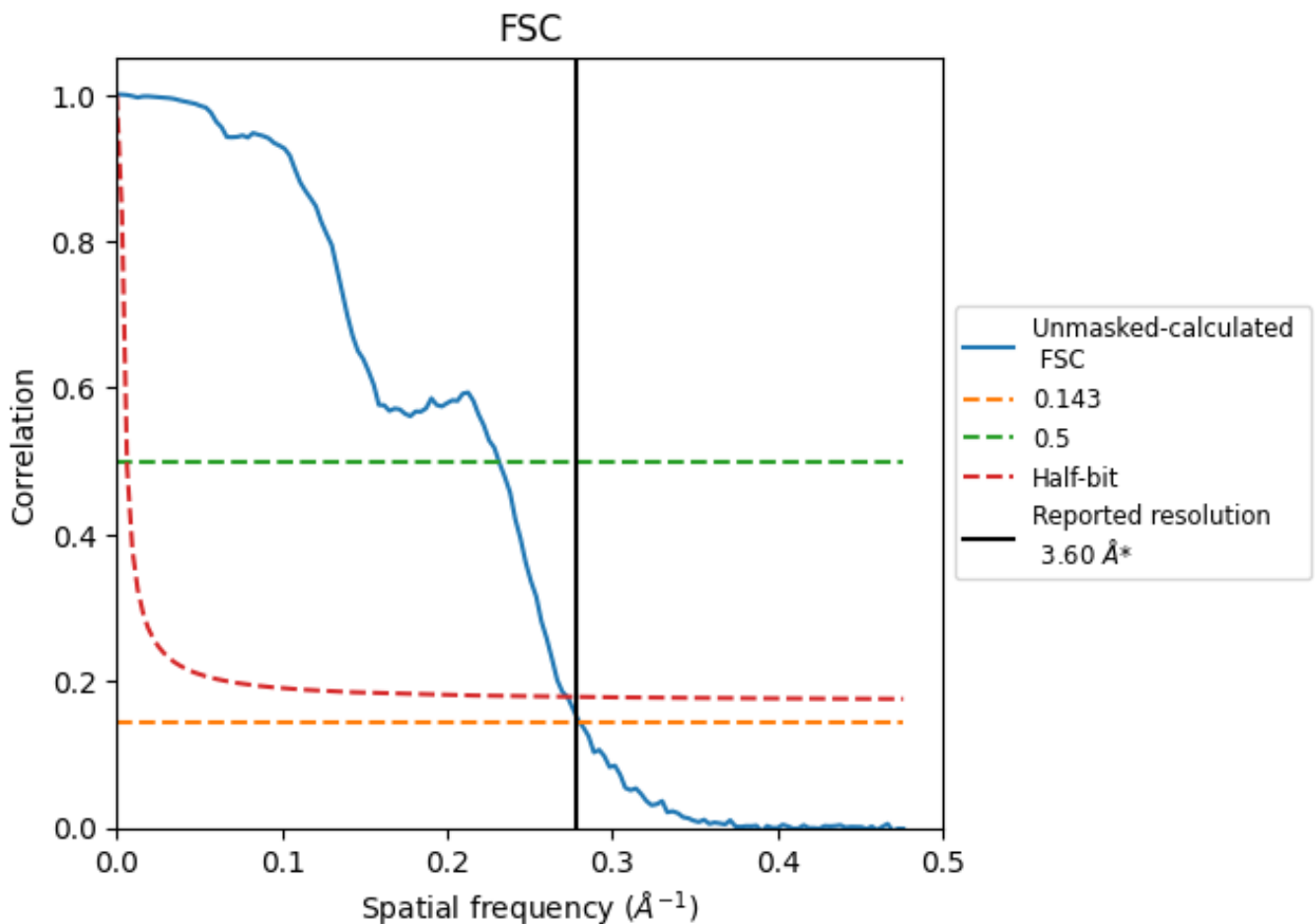
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.32	3.67

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

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-17406 and PDB model 8P4D. Per-residue inclusion information can be found in section 3 on page 7.

9.1   Map-model overlay ⓘ
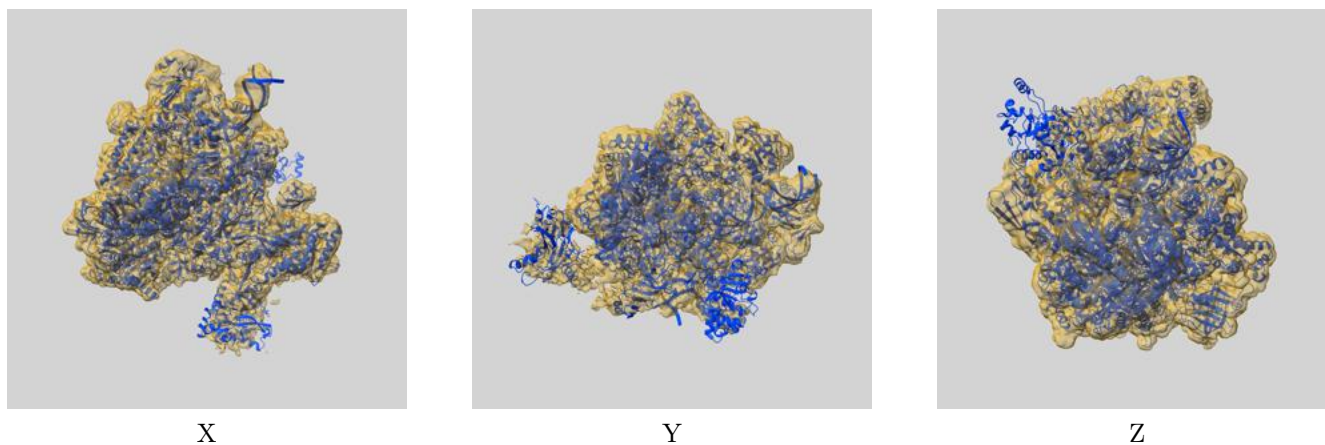
X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 0.0181 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
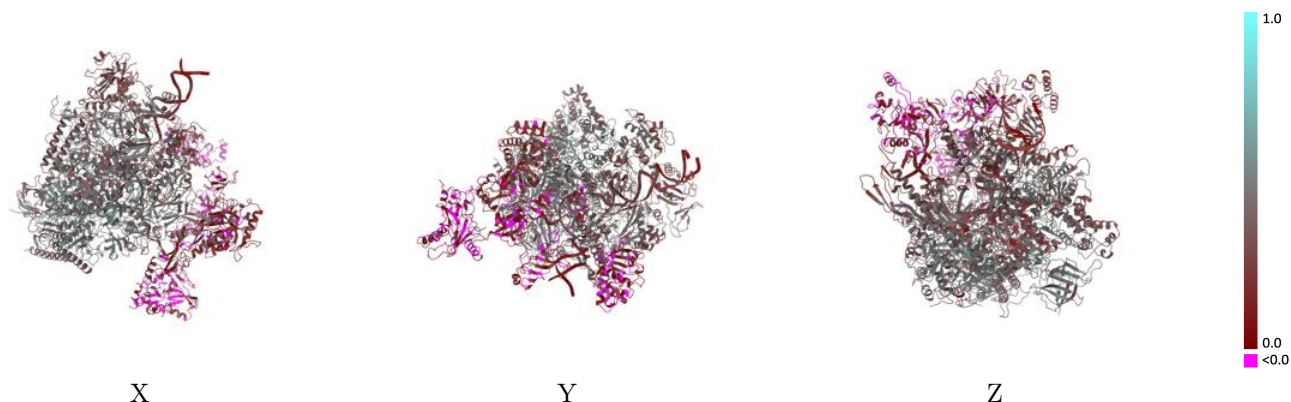
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
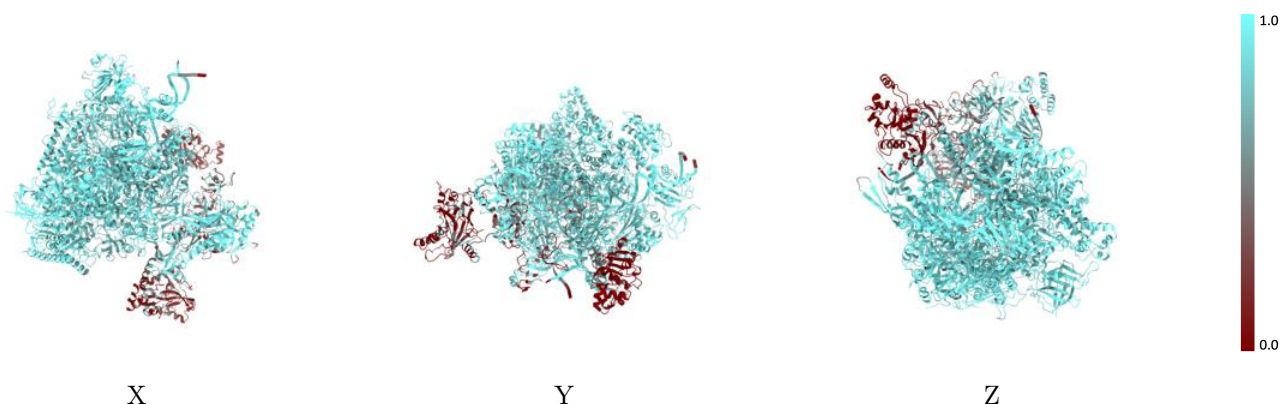
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0181).

9.4   Atom inclusion ⓘ
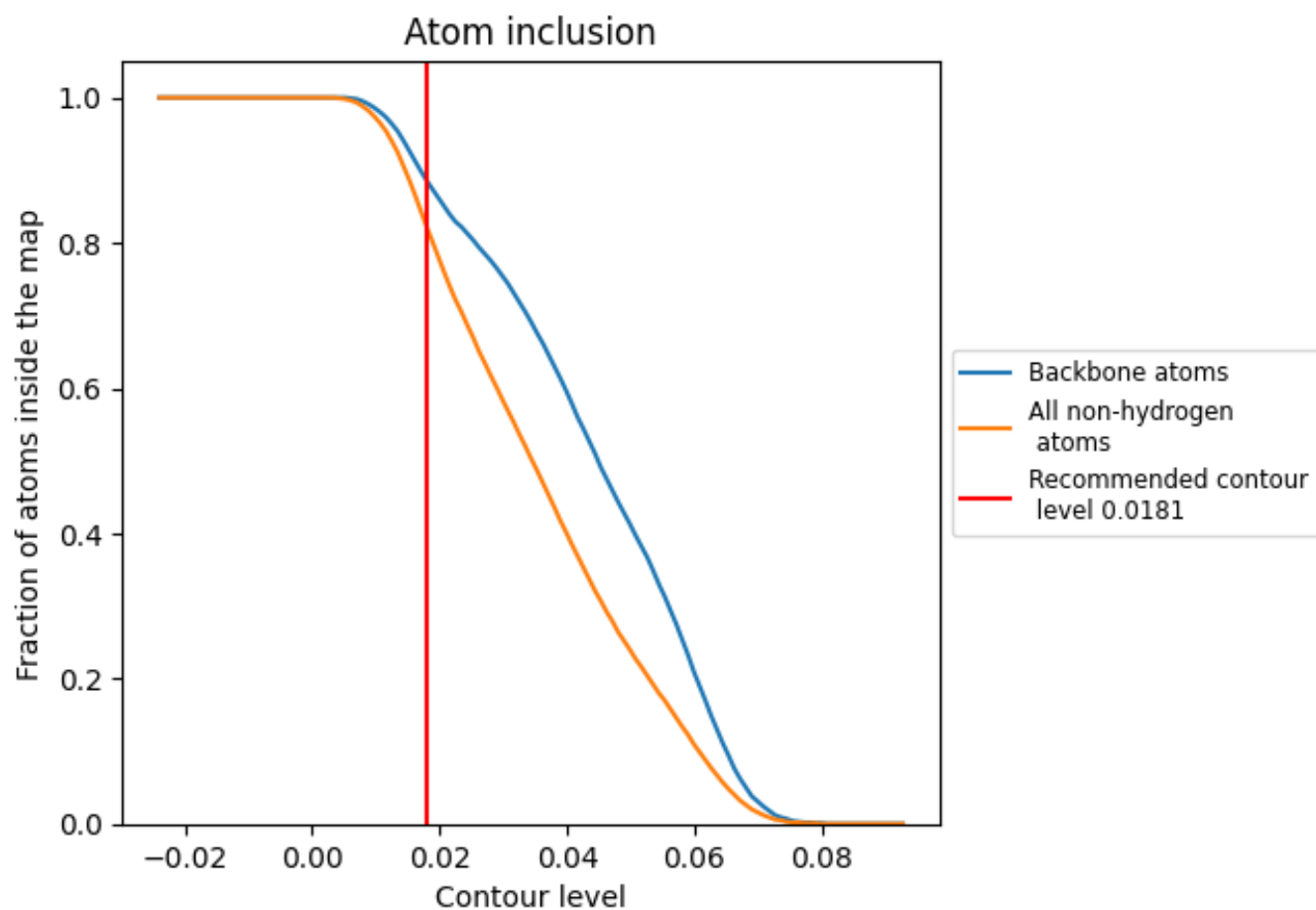
At the recommended contour level, 88% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0181) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8190	0.3480
A	0.9240	0.4200
B	0.9280	0.4340
C	0.9260	0.4450
D	0.8840	0.2200
E	0.9380	0.3970
F	0.9040	0.4420
G	0.8820	0.2590
H	0.9470	0.4460
I	0.9360	0.3720
J	0.9210	0.4590
K	0.9300	0.4520
L	0.9520	0.4120
M	0.3480	0.0840
N	0.8330	0.1810
P	0.9190	0.3280
T	0.9040	0.2520
Y	0.0020	0.0600
Z	0.4510	0.1220

1.0

0.0
<0.0