wwPDB EM Validation Summary Report (i)

Oct 28, 2024 – 02:47 pm GMT

PDB ID	:	7AST
EMDB ID	:	EMD-11904
Title	:	Apo Human RNA Polymerase III
Authors	:	Ramsay, E.P.; Abascal-Palacios, G.; Daiss, J.L.; King, H.; Gouge, J.; Pilsl, M.; Beuron, F.; Morris, E.; Gunkel, P.; Engel, C.; Vannini, A.
Deposited on	:	2020-10-28
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

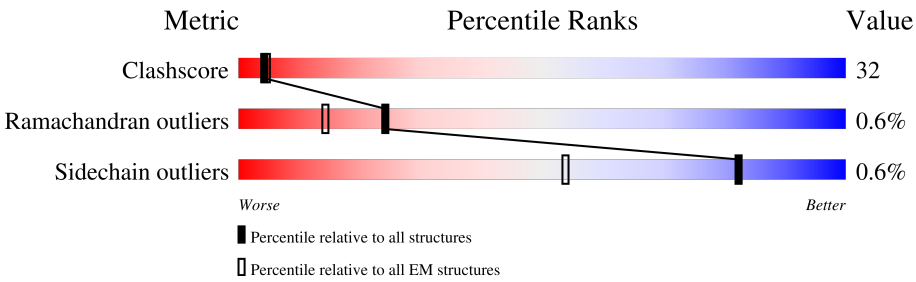
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	1390	5%, 43%, 44%, •, 11%
2	A	108	19%, 15%, •, 66%
3	B	67	43%, 52%, •
4	C	58	33%, 41%, 5%, 21%
5	D	150	•, 23%, 53%, •, •, 19%
6	E	127	6%, 24%, 39%, •, 36%
7	F	210	•, 47%, 51%, •
8	G	133	40%, 35%, 25%

Continued on next page...

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Mol	Chain	Length	Quality of chain
9	H	346	38% 55% 5%
10	I	148	31% 36% 48% 16%
11	J	204	19% 45% 42% 12%
12	K	708	8% 10% 81%
13	L	398	7% 13% 79%
14	M	1133	43% 53%
15	Z	316	5% 12% 8% 80%
16	X	534	30% 53% 29% 18%
17	Y	36	47% 72% 28%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 34518 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	1238	9385	5928	1643	1746	68	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	37	288	179	55	49	5	0	0

- Molecule 3 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		
3	B	64	507	328	86	87	6	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 5 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		
5	D	121	972	627	160	179	6	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	81	649	414	111	119	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	209	1715	1083	300	324	8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	100	794	493	142	152	7	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	329	2635	1663	472	489	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	125	1008	631	175	199	3	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	179	1442	938	226	271	7	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	137	1119	718	192	204	5	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	82	620	397	104	115	4	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	1114	8811	5581	1540	1621	69	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Z	63	518	337	78	99	4	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	X	440	3487	2193	607	665	22	0	0

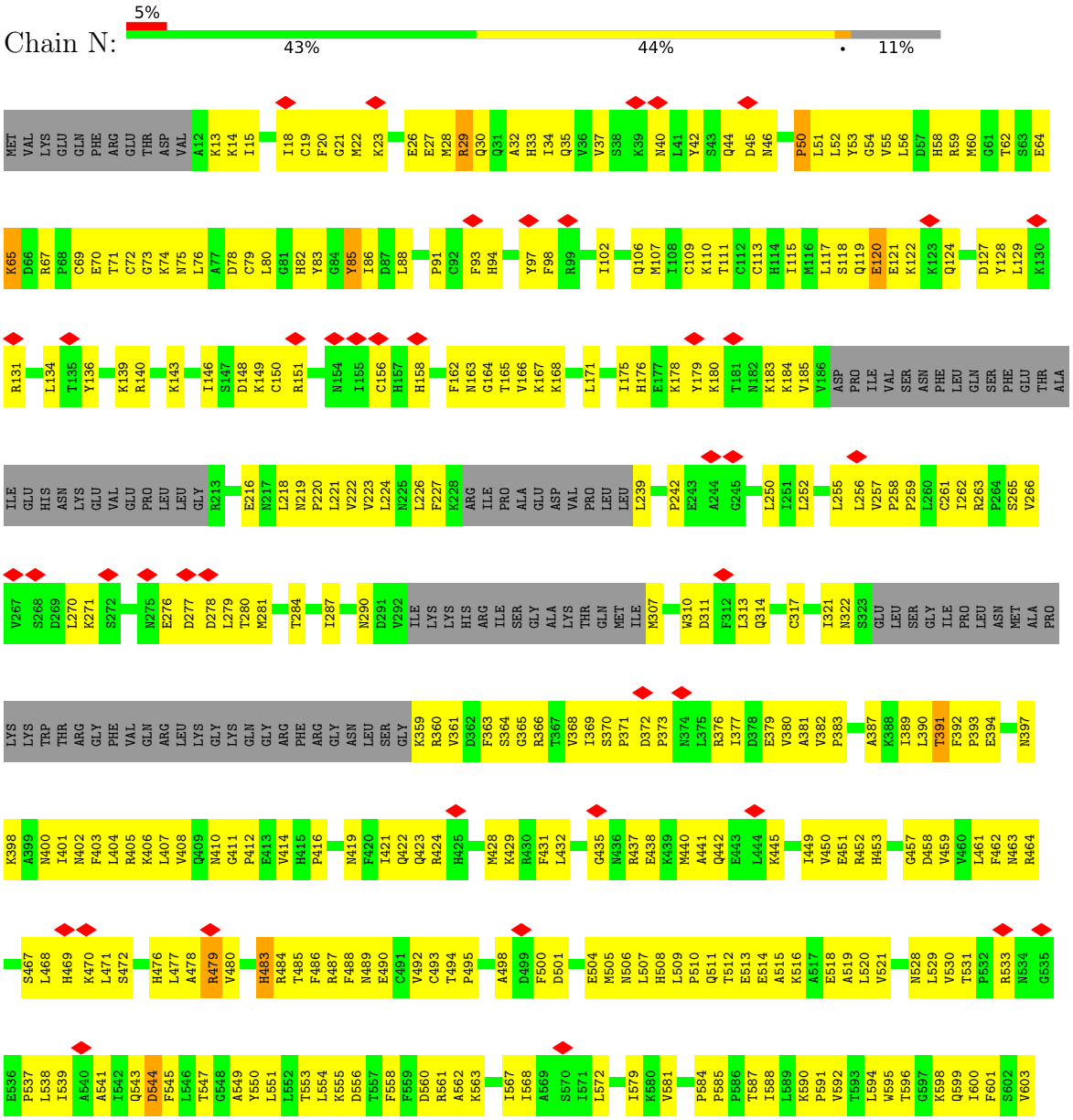
- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7-beta.

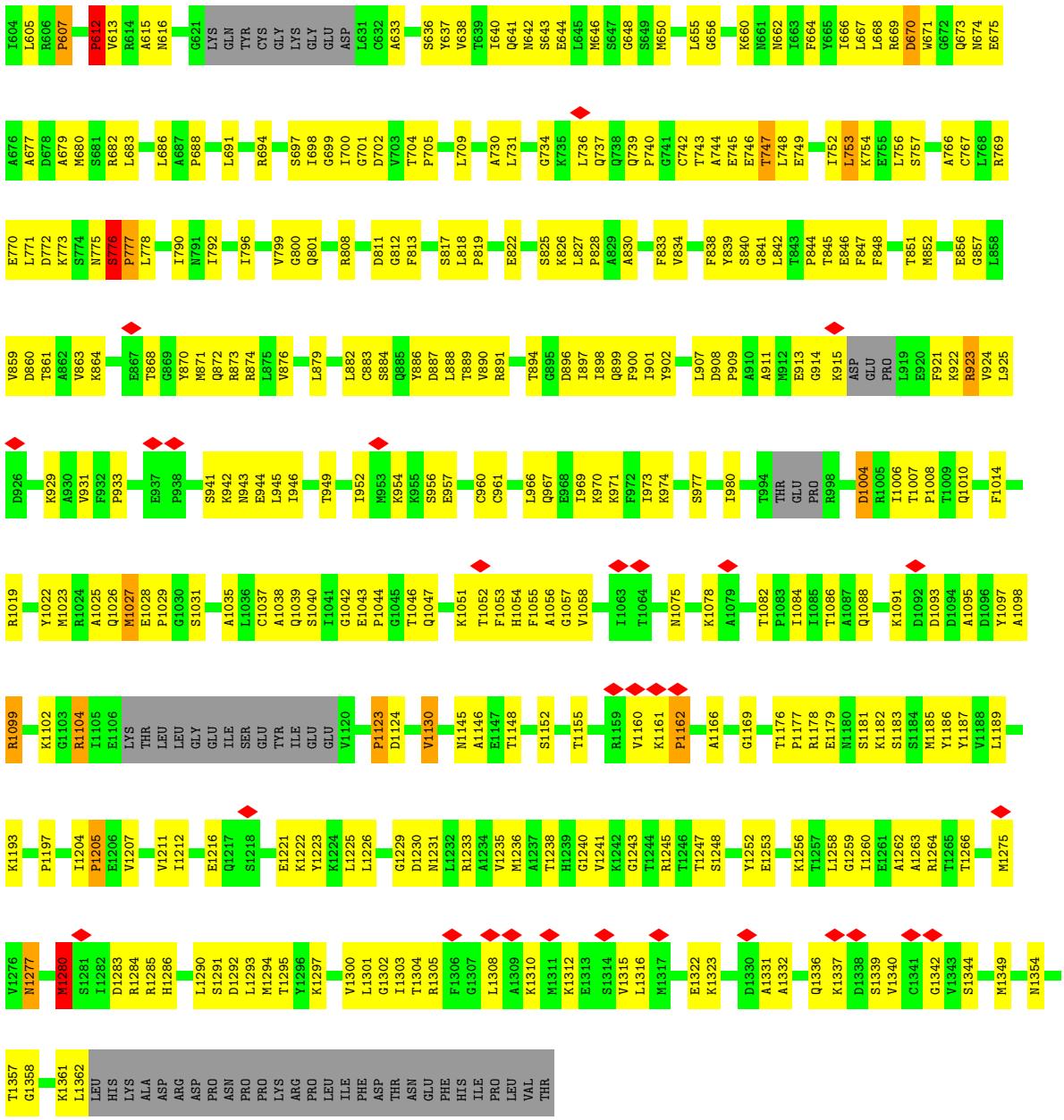
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Y	36	180	108	36	36	0	0

3 Residue-property plots (i)

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.

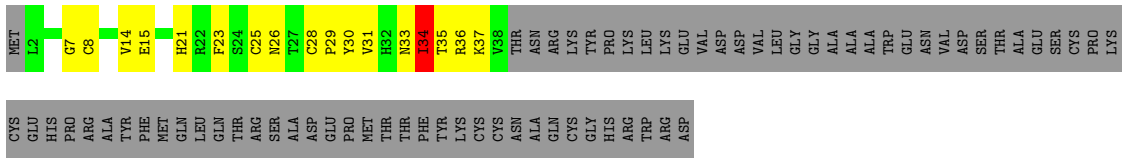
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1





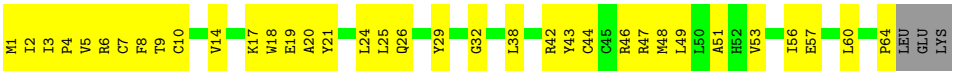
• Molecule 2: DNA-directed RNA polymerase III subunit RPC10

Chain A: 19% 15% 66%



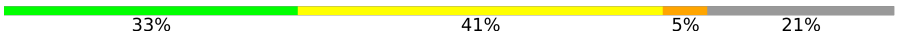
• Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC5

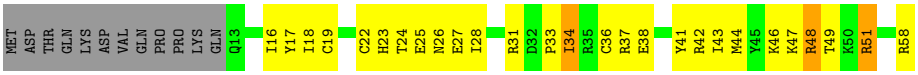
Chain B: 43% 52%



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC4

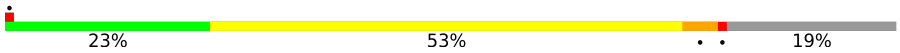
Chain C:

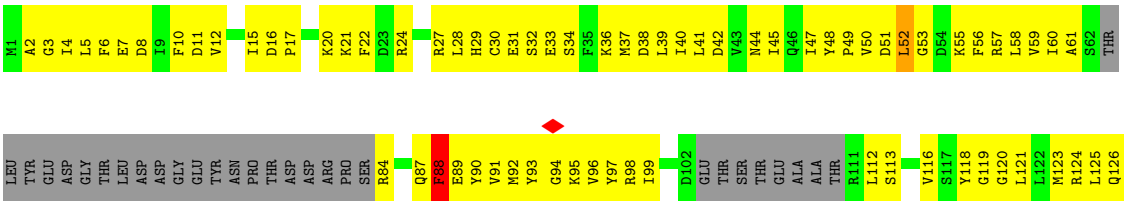


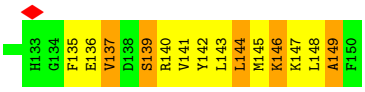


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain D:

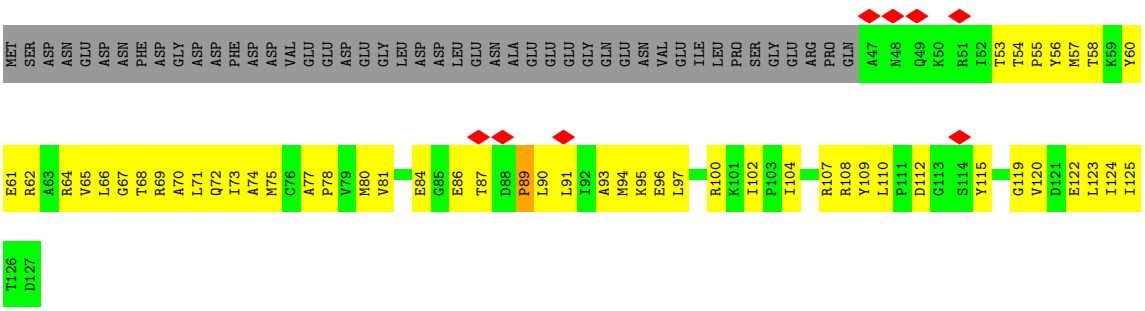






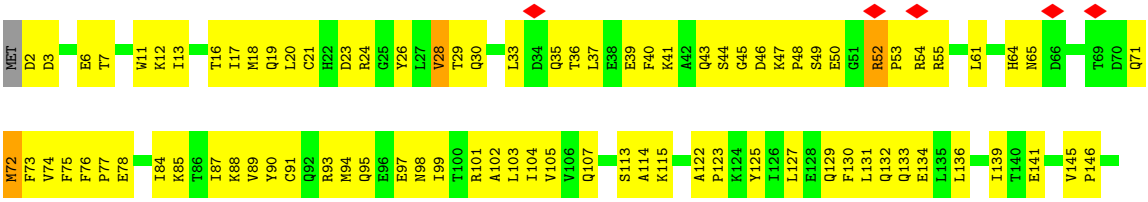
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

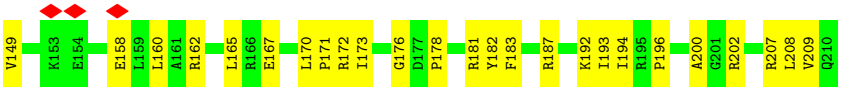
Chain E:



• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

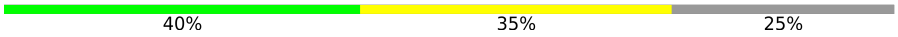
Chain F:

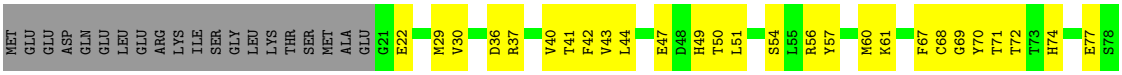




• Molecule 8: DNA-directed RNA polymerases I and III subunit RPAC2

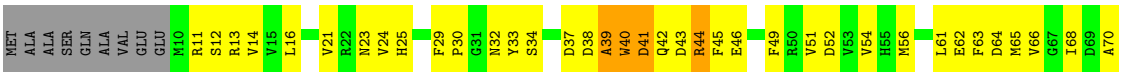
Chain G:

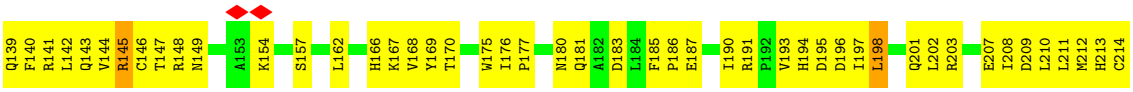


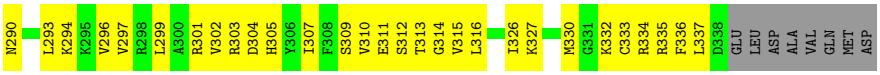


• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC1

Chain H:

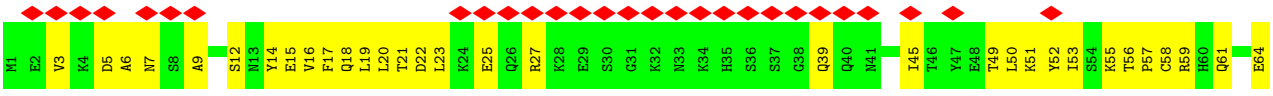


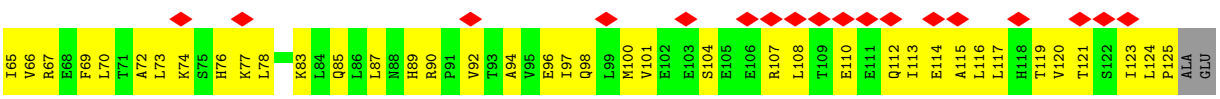




• Molecule 10: DNA-directed RNA polymerase III subunit RPC9

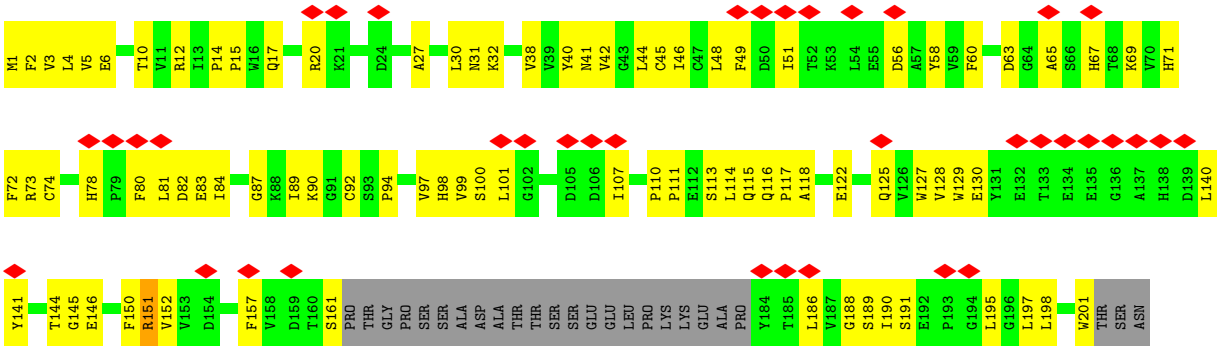
Chain I:





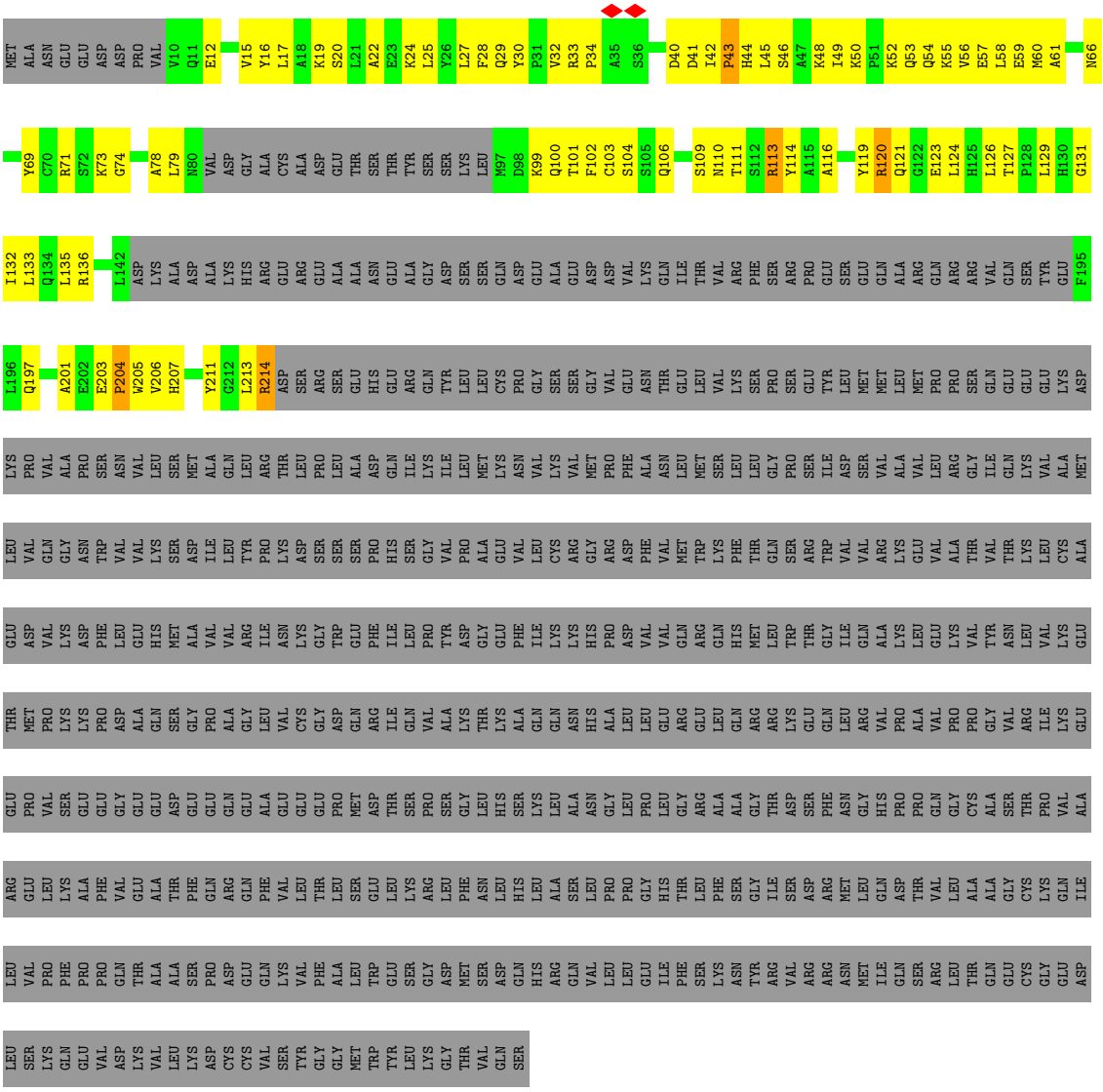
• Molecule 11: DNA-directed RNA polymerase III subunit RPC8

Chain J: 19% 45% 42% 12%



• Molecule 12: DNA-directed RNA polymerase III subunit RPC5

Chain K: 8% 10% • 81%



• Molecule 13: DNA-directed RNA polymerase III subunit RPC4

Chain L: 7% 13% 79%

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

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

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

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

LYS THR PRO GLY LEU PRO LYS ASP VAL SER VAL ALA GLU LEU LEU ARG GLU LEU SER L260 T261 K262 E263 L266 L267 F268 L269 Q270 L271 P272 L275 P276 G277 GLN PRO PRO THR GLN ASP ILE LYS PRO ILE LYS THR GLU VAL GLN GLY GLU ASP GLY GLN VAL VAL LEU ILE LYS

GLN GLU LYS ASP ARG GLU ALA LYS LEU ALA GLU ASN ALA CYS THR LEU ALA ASP LEU THR GLU GLY GLN V326 G327 L330 I331 R332 R336 V337 Q338 L339 L340 L341 G342 K343 V344 T345 L346 D347 V348 T349 A353 C354 S355 F356 L357 Q358 E359 L360 V361 S362 V363 G364 L365 G366 D367

S368 R369 T370 G371 E372 M373 T374 V375 L376 G377 H378 V379 K380 H381 K382 L383 V384 C385 S386 P387 D388 F389 GLU SER LEU LEU ASP HIS LYS HIS ARG

- Molecule 14: DNA-directed RNA polymerase III subunit RPC2

Chain M: 43% 53%

MET ASP VAL LEU ALA GLU GLU PHE GLY ASN LEU THR PRO GLU GLN LEU ALA ALA PRO I20 P21 E24 E25 K26 W27 R28 L29 L30 P31 A32 F33 L34 K35 V36 K37 G38 L39 Q42 H43 I44 F47 N48 Y49 N52 K56 K57 I58 M59 E63 T66 S67 D68 A69

D70 W73 Y74 L75 K76 I80 Y81 V82 G83 L84 P85 D86 V87 E88 E89 S90 V93 T94 R95 P96 V97 S98 P99 H100 E101 C102 R105 T108 Y109 S110 A111 P112 I113 T114 I117 E118 Y119 T120 S123 Q124 R125 I126 I127 R128 L131 P132 I133 G134 R135 M136 P137 I138

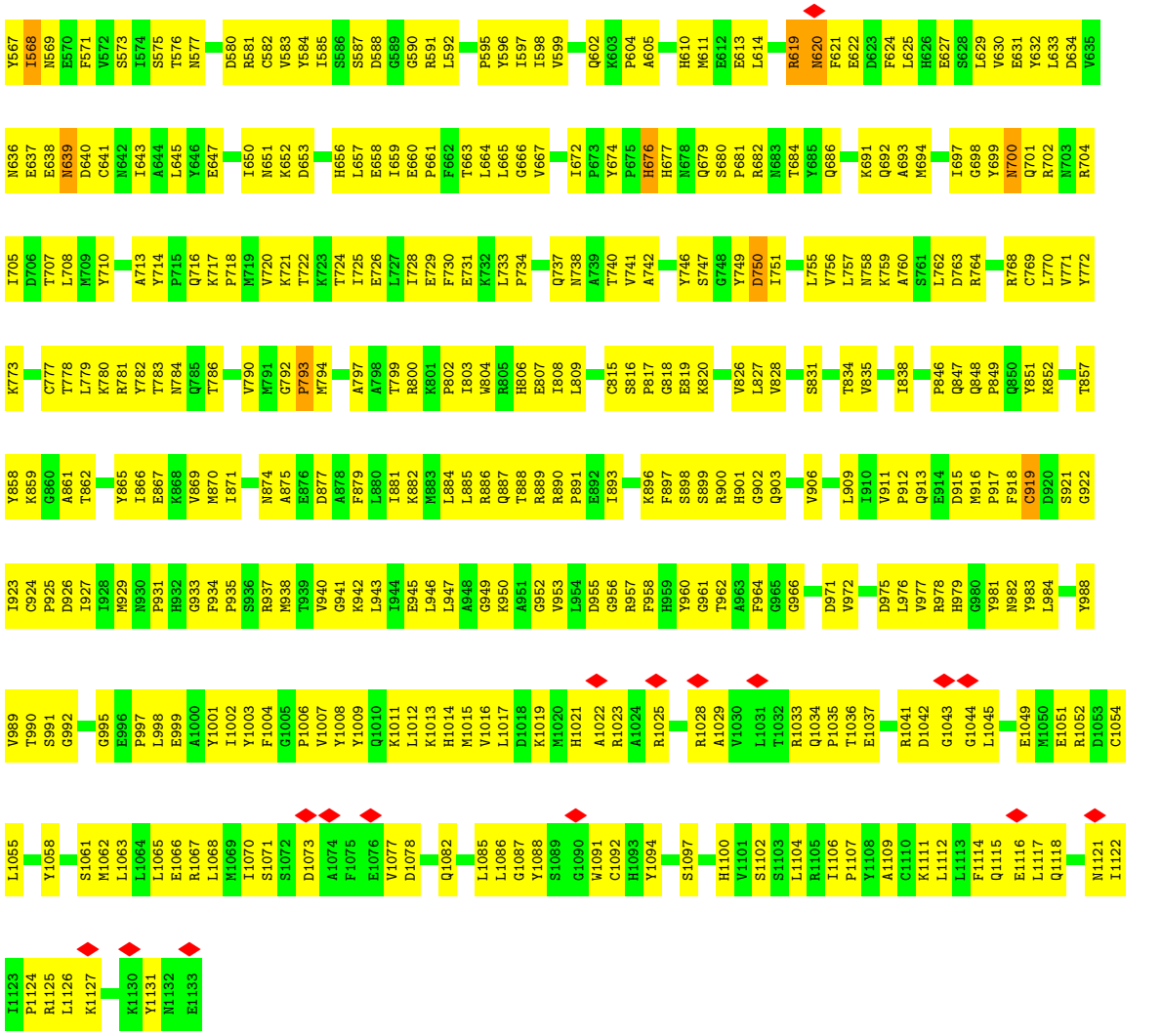
M139 L140 R141 C145 V146 L147 F155 N159 E160 C161 P162 L163 D164 G167 Y168 F169 I170 V171 K172 E175 I178 N187 R188 I189 E192 R195 K196 V199 T204 S205 S206 T207 H208 E209 S212 R213 T214 N215 M216 A217 V218 K219 R222 F223 Y224 L225 R226

H227 N228 T229 L230 S231 E232 D233 I234 P235 I236 V237 I238 I239 F240 K241 A242 M243 G244 V245 E246 S247 D248 Q249 E250 I251 V252 Q253 M254 I255 G266 L269 Q273 K274 I277 F278 T279 Q280 M281 Q282 A283 L284 K285 Y286 I287 Q288 N289 K290 V291 R292 R293 Q294 R295 M296 G299 G300

P301 K302 K303 T304 K305 I306 E307 E308 A309 R310 E311 L312 S315 L318 T319 H320 V321 P322 V323 K324 F328 R329 I333 A336 V337 R340 R341 L344 A345 Q346 G347 D348 N349 K350 D355 Y356 N359 K360 R361 L364 A365 G366 Q367 L368 L369 S370 L371 L372 F373 E374

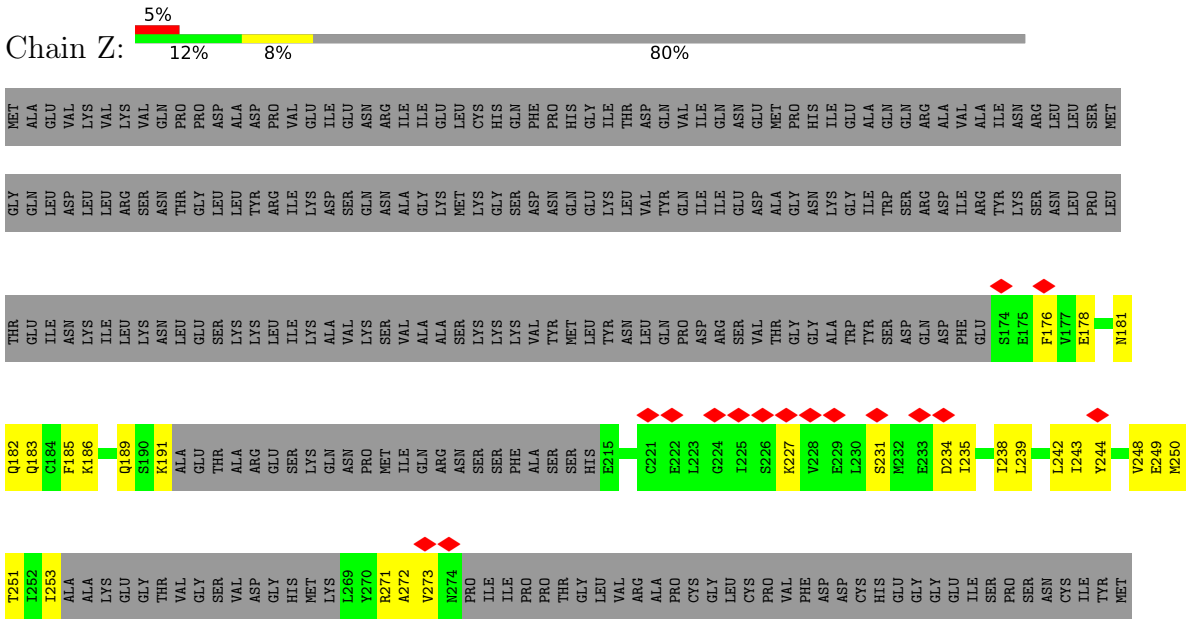
D375 L376 F377 F380 N381 S382 E383 M384 K385 A388 V391 I392 P393 K394 Q395 R396 Q399 F400 D401 V402 H405 M406 R407 Q408 D409 Q410 I411 T412 N413 V416 N417 W424 S425 L426 K430 T437 L440 S441 R442 Y445 M451 R454 I455 E460 P473

S474 Q475 W476 G477 M478 L479 K494 N495 L496 A497 L498 M499 T500 H501 I502 T503 T504 D505 D508 I511 V512 K513 L514 A515 S516 N517 L518 E521 L525 L526 C527 G528 E529 E530 L531 F537 L538 V539 F540 L541 N542 G543 N544 I545 L546 G547 V548 I549 R550 V556 R563



- Molecule 15: DNA-directed RNA polymerase III subunit RPC6

Chain Z:



THR GLU TRP LEU GLU PHE
• Molecule 16: DNA-directed RNA polymerase III subunit RPC3
Chain X:
30%
53%
29%
18%
MET THR GLN A4 E5 S10 L11 L12 L13 Q14 E15 E22 K23 I24 H27 L28 I29 R30 Q34 P35 V38 I39 A40 H41 D42 T43 G44 T45 S46 L47 D48 K52 V56 L57 V58 Q59 H60 N61 L62 V63 S64 Y65 Q66 V67 H68 K69 R70 G71 V72 V73 E74 Y75 E76
A77 Q78 C79 S80 R81 V82 L83 R84 M85 L86 R87 Y88 P89 R90 Y91 I92 K96 T97 L98 Y99 S100 D101 T102 I106 E109 L110 L111 L112 N113 G114 K115 L116 T117 M118 V122 V125 R128 L129 T130 E131 T132 M133 E134 D135 G136 K137 T138 M139 D140 E143 V144 T154
H155 F156 C160 P161 S162 V163 PRO THR THR GLU ASN SER ASP PRO GLY PRO PRO PRO PRO ALA PRO THR LEU VAL ILE ASN GLU LYS ASP MET TYR LEU VAL PRO LYS LEU SER LEU ILE GLY LYS GLY LYS ARG ARG ARG SER SER ASP GLU ASP ALA ALA GLY GLU PRO LYS ALA LYS
ARG PRO LYS TYR THR THR ASP ASN LYS GLU PRO ILE PRO ASP D231 G232 I233 Y234 W235 Q236 A237 N238 L239 F242 H243 R247 I251 A254 V255 A256 N257 R258 M259 D260 Q261 T262 S263 S264 E265 I266 V267 R268 T269 M270 L271 R272 M273 S274 E275 I276 T277 T278 S279 S280 S281 A282
P283 F284 T285 Q286 P287 L288 S289 S290 N291 E292 I293 F294 R295 S296 L297 P298 V299 G300 Y301 N302 I303 S304 K305 Q306 D309 Q310 Y311 L312 T313 A316 P319 L320 E321 F322 Y323 G324 K325 S326 G327 D328 S329 G330 G331 G332 M333 Y334 V335 I336 N337 L338 H339 K340 A341 L345 E351
V354 Q355 E356 R357 F358 G359 S360 R361 C362 A363 R364 I365 L368 Q371 K372 K373 H374 I375 E376 Q377 K378 Q379 V380 E381 D382 F383 A384 M385 I386 P387 A388 K389 E390 A391 K392 D393 M394 L395 Y396 K397 M398 F403 MET SER LEU GLN GLU ILE PRO LYS THR PRO ASP HIS ALA PRO
SER ARG THR PHE TYR LEU TYR THR V426 L429 S430 R433 M434 L435 L436 H437 R438 K441 S442 I443 I447 E448 R449 R450 Q451 F452 E453 T454 K455 E456 M457 K458 R459 L460 L461 E462 K463 S464 Q465 R466 V467 E468 A469 I470 I471 A472 S473 M474 Q475 A476 T477 G478 A479 E480 E481 A482
Q483 L484 Q485 E486 I487 E488 E489 M490 I491 T492 A493 P494 E495 R496 Q497 Q498 L499 E500 T501 L502 I514 Q515 V516 I520 L523 E524 S525 Y526 I527 E528 C529 T530 M531 K532 ARG GLN
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7-beta
Chain Y:
47%
72%
28%
X-15 X-14 X-13 X-12 X-11 X-10 X-9 X-8 X-7 X-6 X-5 X-2 X-1 X0 X1 X2 X9 X10 X11 X17 X18 X19 X20

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25369	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 ($e^-/Å^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.365	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	383.40002, 383.40002, 383.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1.06	8/9535 (0.1%)	0.63	11/12862 (0.1%)
2	A	0.33	0/294	0.71	0/396
3	B	0.45	0/516	0.67	0/696
4	C	0.31	0/394	0.69	0/524
5	D	2.96	7/988 (0.7%)	0.89	5/1323 (0.4%)
6	E	0.31	0/659	0.62	0/891
7	F	0.27	0/1745	0.55	2/2358 (0.1%)
8	G	0.39	0/808	0.54	0/1090
9	H	0.35	0/2689	0.62	1/3644 (0.0%)
10	I	0.24	0/1021	0.51	0/1377
11	J	0.28	0/1481	0.54	0/2013
12	K	0.27	0/1146	0.55	0/1549
13	L	0.26	0/626	0.62	0/842
14	M	0.36	0/8982	0.63	1/12118 (0.0%)
15	Z	0.25	0/523	0.53	0/701
16	X	0.24	0/3534	0.46	0/4766
All	All	0.79	15/34941 (0.0%)	0.61	20/47150 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	16
2	A	0	1
3	B	0	1
4	C	0	1
5	D	0	5
6	E	0	1
7	F	0	2
9	H	0	7
12	K	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
13	L	0	4
14	M	0	16
16	X	0	1
All	All	0	58

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	29	ARG	CB-CG	64.17	3.25	1.52
5	D	146	LYS	CD-CE	63.43	3.09	1.51
1	N	85	TYR	CD2-CE2	39.90	1.99	1.39
1	N	85	TYR	CD1-CE1	38.31	1.96	1.39
5	D	88	PHE	CE1-CZ	30.63	1.95	1.37

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	146	LYS	CG-CD-CE	9.84	141.41	111.90
1	N	29	ARG	CA-CB-CG	9.73	134.80	113.40
1	N	391	THR	C-N-CA	9.00	144.21	121.70
1	N	29	ARG	CB-CG-CD	8.77	134.41	111.60
5	D	146	LYS	CD-CE-NZ	8.33	130.87	111.70

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	120	GLU	Peptide
1	N	480	VAL	Peptide
1	N	483	HIS	Peptide
1	N	563	LYS	Peptide
1	N	572	LEU	Peptide

5.2 Too-close contacts (i)

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	9385	0	9273	666	0
2	A	288	0	279	24	0
3	B	507	0	525	52	0
4	C	388	0	395	34	0
5	D	972	0	959	154	0
6	E	649	0	678	59	0
7	F	1715	0	1733	98	0
8	G	794	0	780	49	0
9	H	2635	0	2620	201	0
10	I	1008	0	1035	72	0
11	J	1442	0	1396	77	0
12	K	1119	0	1109	83	0
13	L	620	0	660	62	0
14	M	8811	0	8937	653	0
15	Z	518	0	525	25	0
16	X	3487	0	3523	134	0
17	Y	180	0	41	5	0
All	All	34518	0	34468	2177	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 32.

The worst 5 of 2177 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)
1:N:85:TYR:CZ	1:N:85:TYR:CE2	1.75	1.70
1:N:85:TYR:CZ	1:N:85:TYR:CE1	1.75	1.60
5:D:88:PHE:CE1	5:D:88:PHE:CZ	1.95	1.54
1:N:85:TYR:CE1	1:N:85:TYR:CD1	1.96	1.53
5:D:88:PHE:CZ	5:D:88:PHE:CE2	1.95	1.53

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	1220/1390 (88%)	948 (78%)	258 (21%)	14 (1%)	12	45
2	A	35/108 (32%)	23 (66%)	11 (31%)	1 (3%)	3	27
3	B	62/67 (92%)	54 (87%)	8 (13%)	0	100	100
4	C	44/58 (76%)	32 (73%)	11 (25%)	1 (2%)	5	32
5	D	115/150 (77%)	77 (67%)	38 (33%)	0	100	100
6	E	79/127 (62%)	56 (71%)	22 (28%)	1 (1%)	10	42
7	F	207/210 (99%)	182 (88%)	24 (12%)	1 (0%)	25	61
8	G	98/133 (74%)	71 (72%)	27 (28%)	0	100	100
9	H	327/346 (94%)	246 (75%)	80 (24%)	1 (0%)	37	71
10	I	123/148 (83%)	113 (92%)	10 (8%)	0	100	100
11	J	175/204 (86%)	138 (79%)	37 (21%)	0	100	100
12	K	131/708 (18%)	92 (70%)	38 (29%)	1 (1%)	16	53
13	L	78/398 (20%)	60 (77%)	17 (22%)	1 (1%)	10	42
14	M	1112/1133 (98%)	831 (75%)	276 (25%)	5 (0%)	30	66
15	Z	57/316 (18%)	50 (88%)	7 (12%)	0	100	100
16	X	434/534 (81%)	405 (93%)	29 (7%)	0	100	100
All	All	4297/6030 (71%)	3378 (79%)	893 (21%)	26 (1%)	24	58

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	607	PRO
1	N	612	PRO
1	N	777	PRO
1	N	1162	PRO
1	N	1205	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	983/1212 (81%)	976 (99%)	7 (1%)	81	86
2	A	33/94 (35%)	33 (100%)	0	100	100
3	B	53/56 (95%)	53 (100%)	0	100	100
4	C	43/55 (78%)	41 (95%)	2 (5%)	22	45
5	D	103/131 (79%)	102 (99%)	1 (1%)	73	81
6	E	70/111 (63%)	70 (100%)	0	100	100
7	F	191/192 (100%)	191 (100%)	0	100	100
8	G	89/119 (75%)	89 (100%)	0	100	100
9	H	289/302 (96%)	285 (99%)	4 (1%)	62	75
10	I	117/136 (86%)	117 (100%)	0	100	100
11	J	160/181 (88%)	158 (99%)	2 (1%)	65	77
12	K	122/622 (20%)	120 (98%)	2 (2%)	58	74
13	L	72/347 (21%)	72 (100%)	0	100	100
14	M	973/988 (98%)	971 (100%)	2 (0%)	92	93
15	Z	60/280 (21%)	60 (100%)	0	100	100
16	X	386/476 (81%)	383 (99%)	3 (1%)	79	84
All	All	3744/5302 (71%)	3721 (99%)	23 (1%)	82	88

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	71	HIS
12	K	214	ARG
12	K	120	ARG
14	M	128	ARG
1	N	1284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	1034	GLN
14	M	1115	GLN
16	X	497	GLN
9	H	180	ASN
9	H	32	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

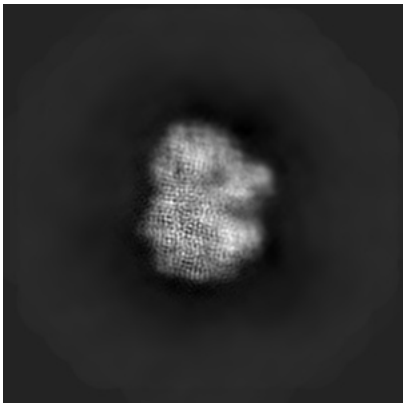
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11904. These allow visual inspection of the internal detail of the map and identification of artifacts.

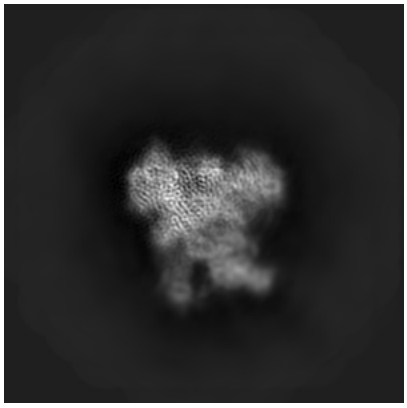
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

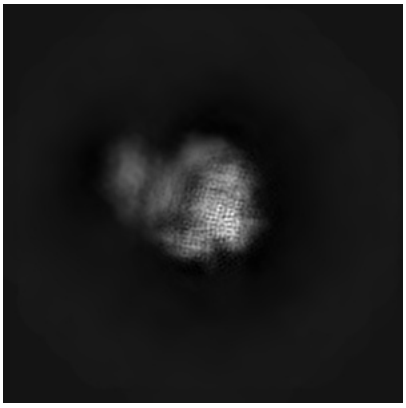
6.1.1 Primary map



X



Y

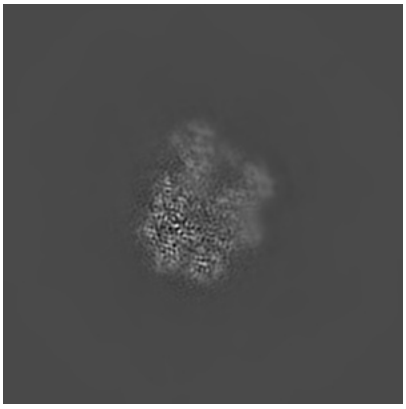


Z

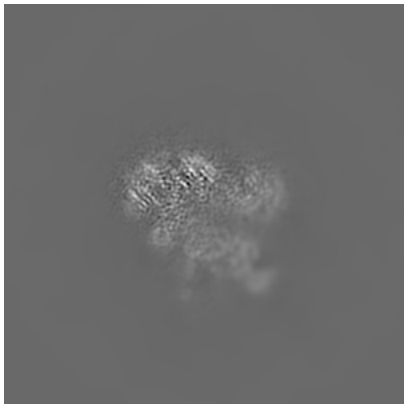
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

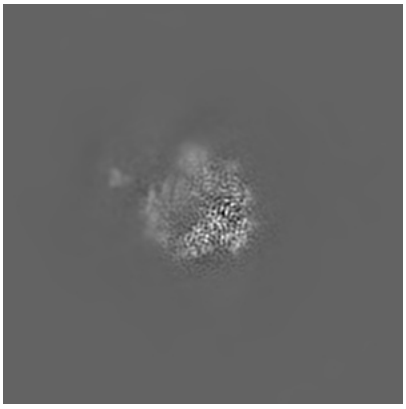
6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180

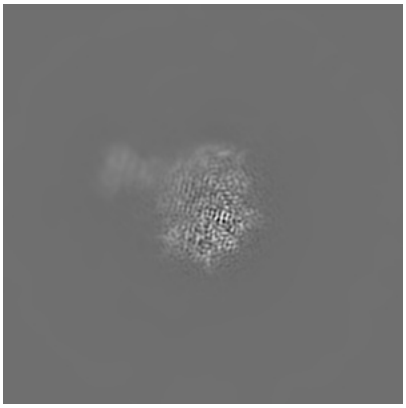
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 202

Y Index: 157

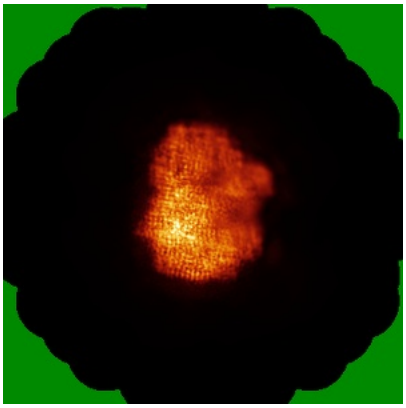


Z Index: 150

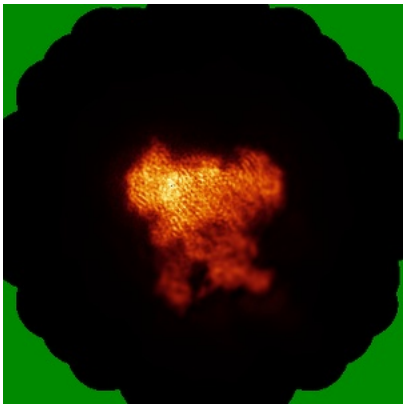
The images above show the largest variance slices of the map in three orthogonal directions.

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

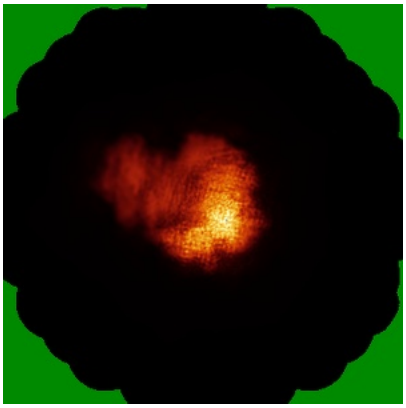
6.4.1 Primary map



X



Y

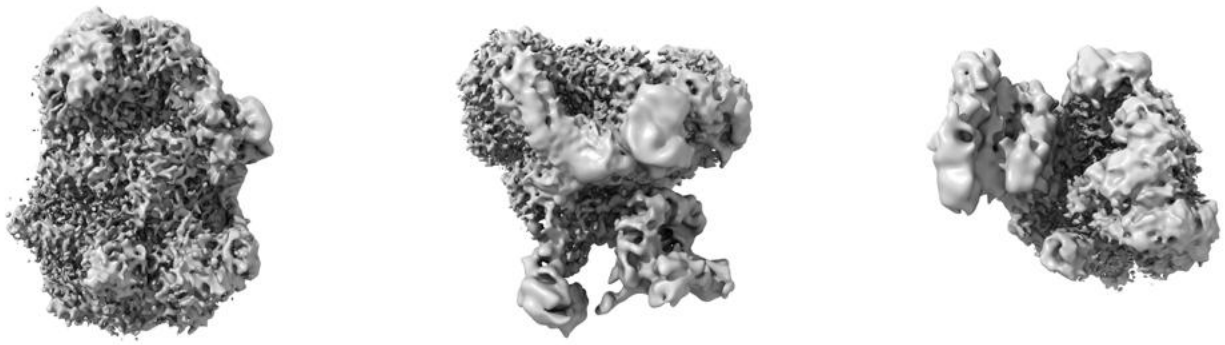


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

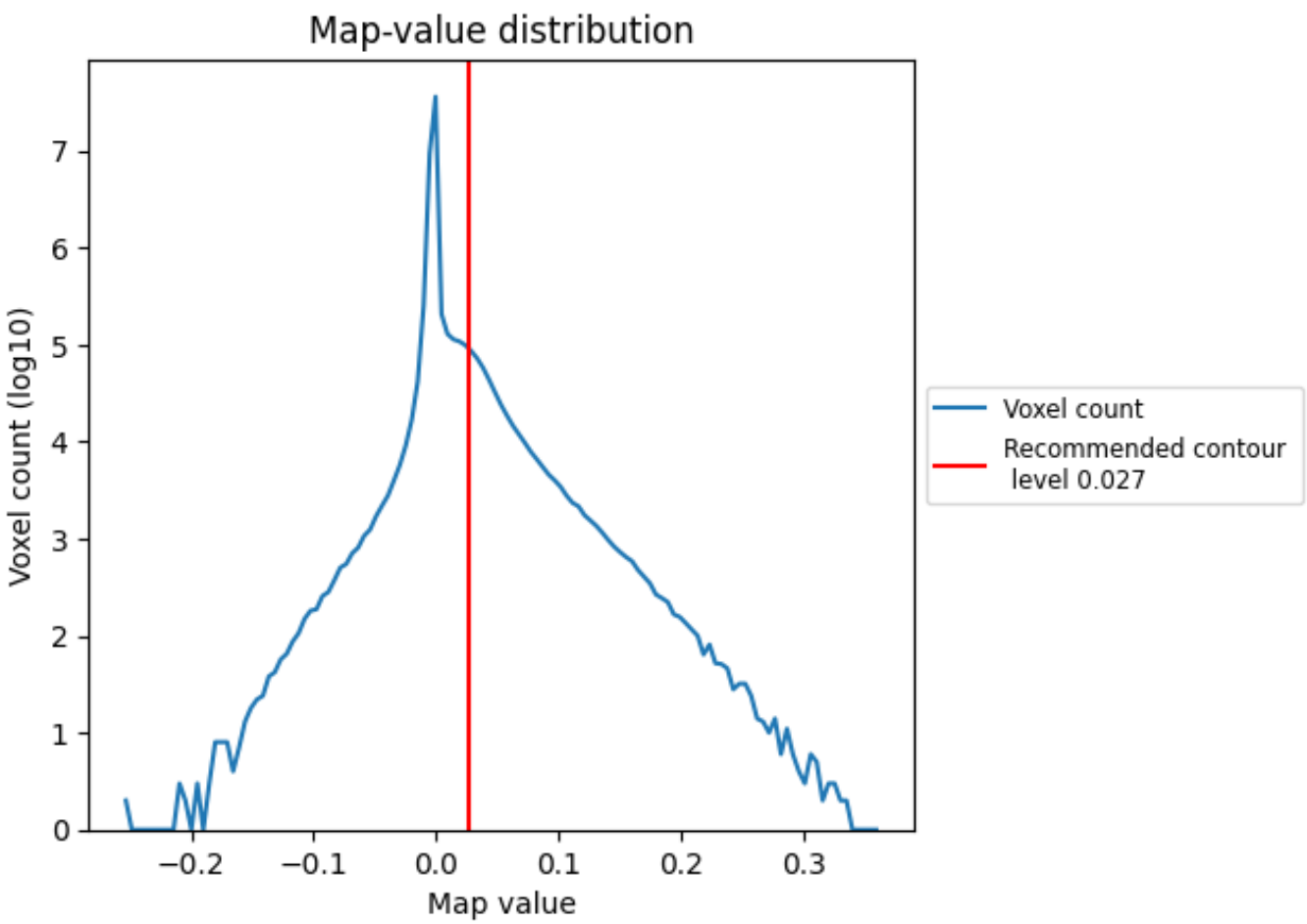
6.6 Mask visualisation (i)

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

7 Map analysis (i)

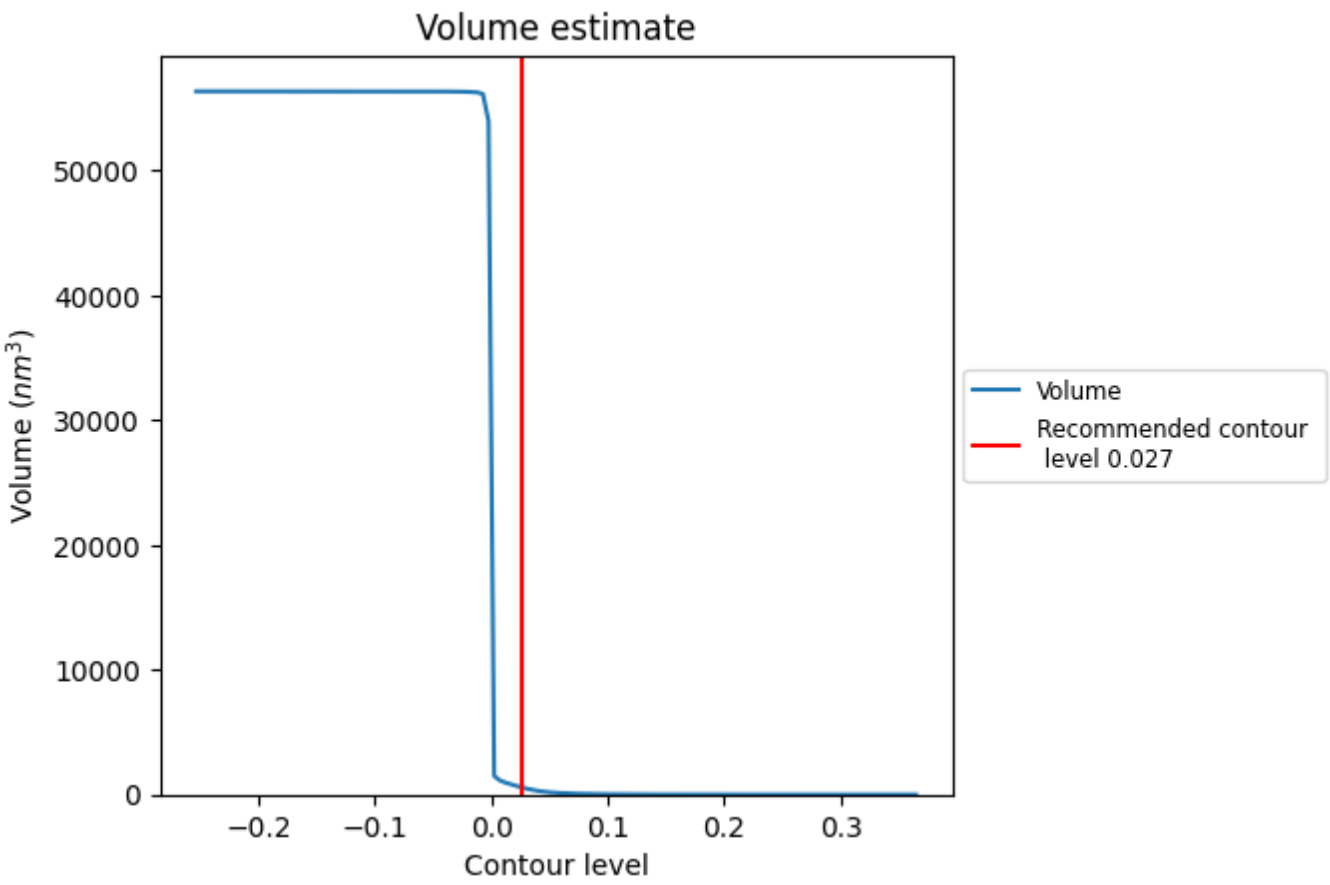
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

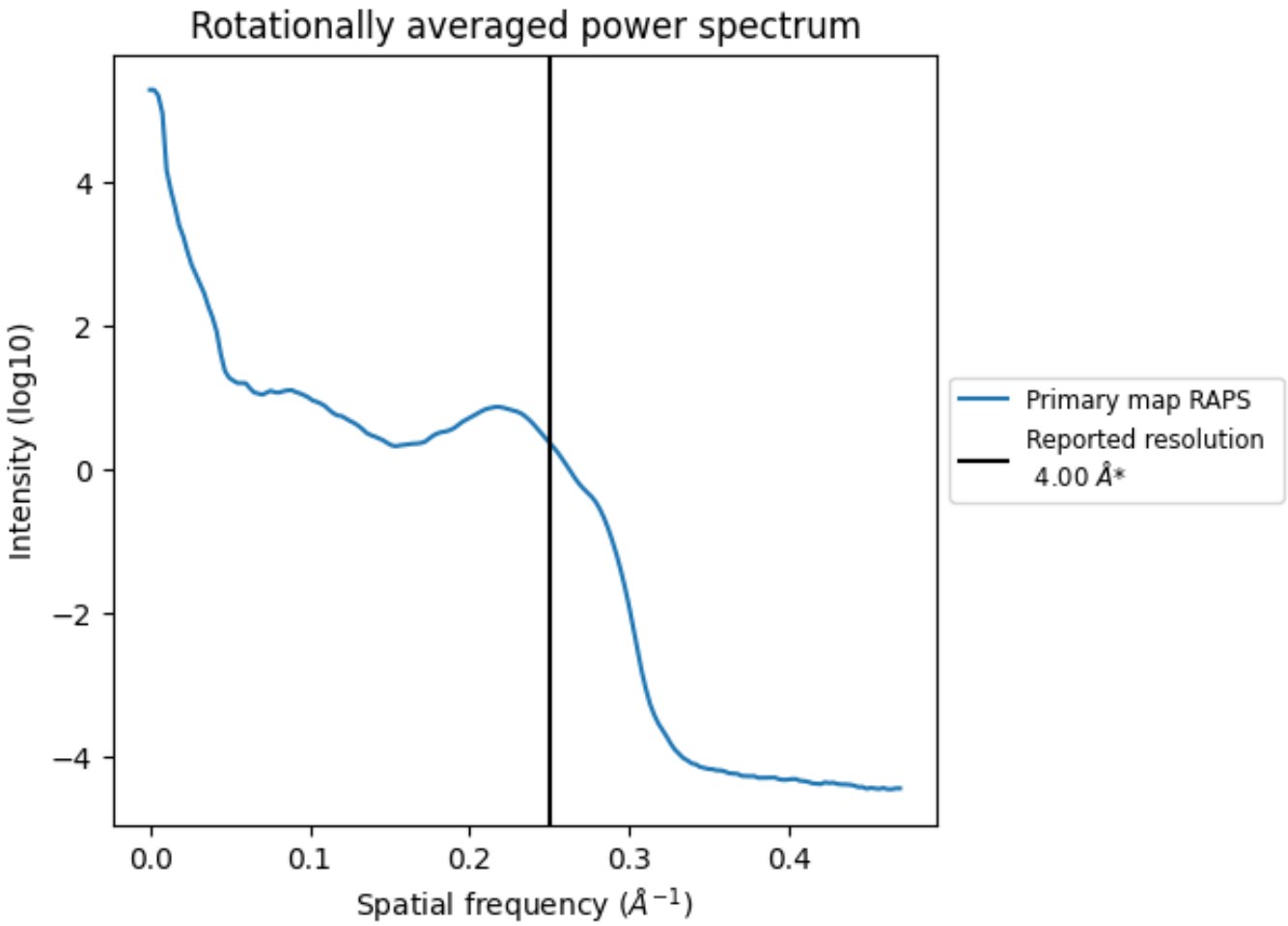
7.2 Volume estimate (i)



The volume at the recommended contour level is 555 nm^3; this corresponds to an approximate mass of 501 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)

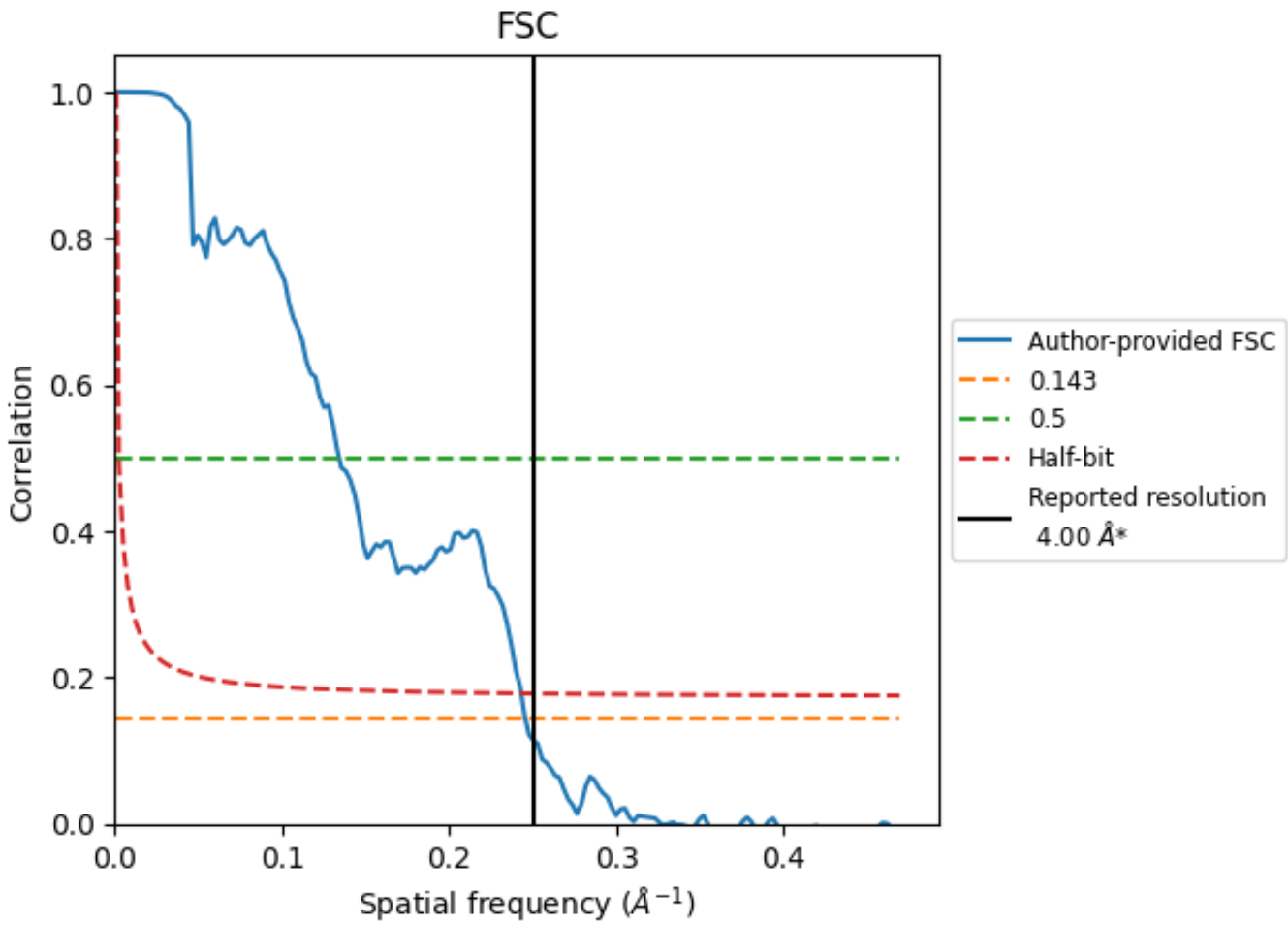


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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^{-1}

8.2 Resolution estimates (i)

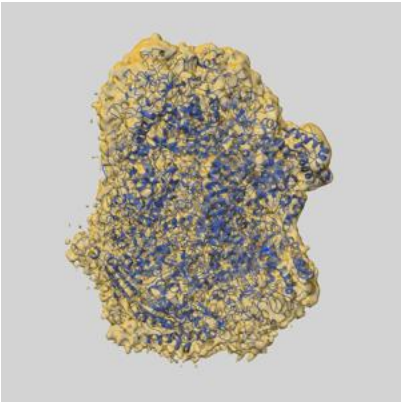
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.07	7.45	4.11
Unmasked-calculated*	-	-	-

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

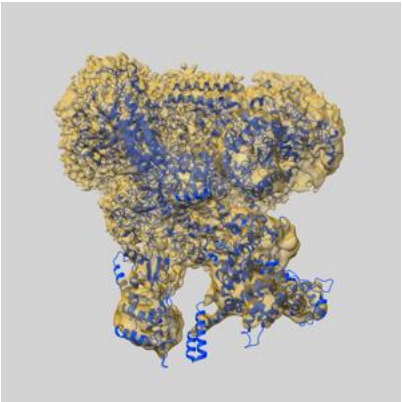
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11904 and PDB model 7AST. Per-residue inclusion information can be found in section 3 on page 7.

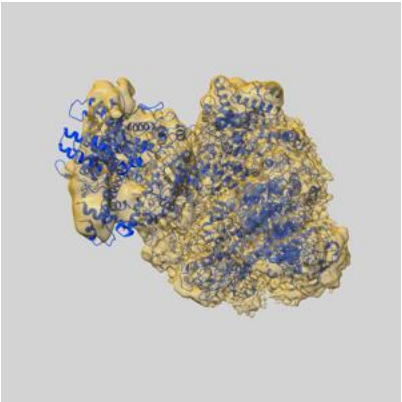
9.1 Map-model overlay (i)



X



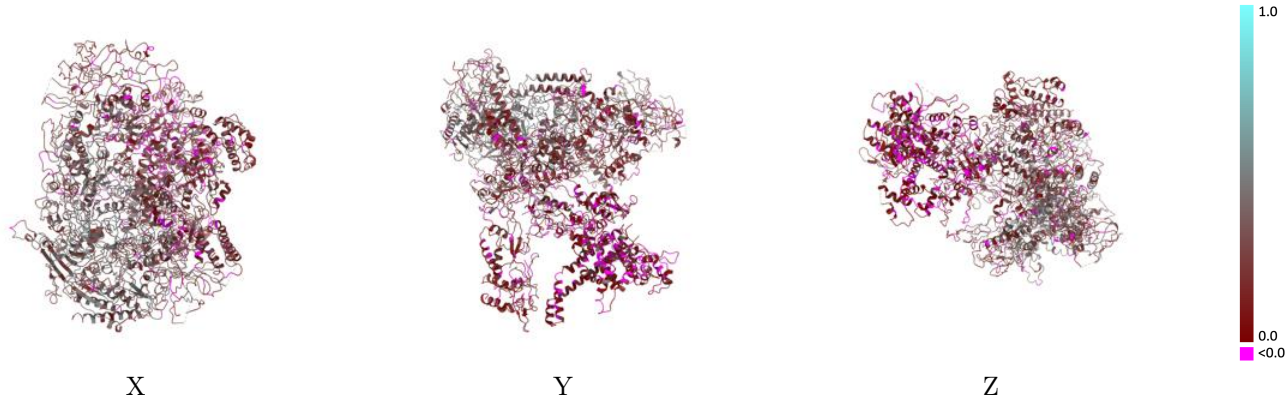
Y



Z

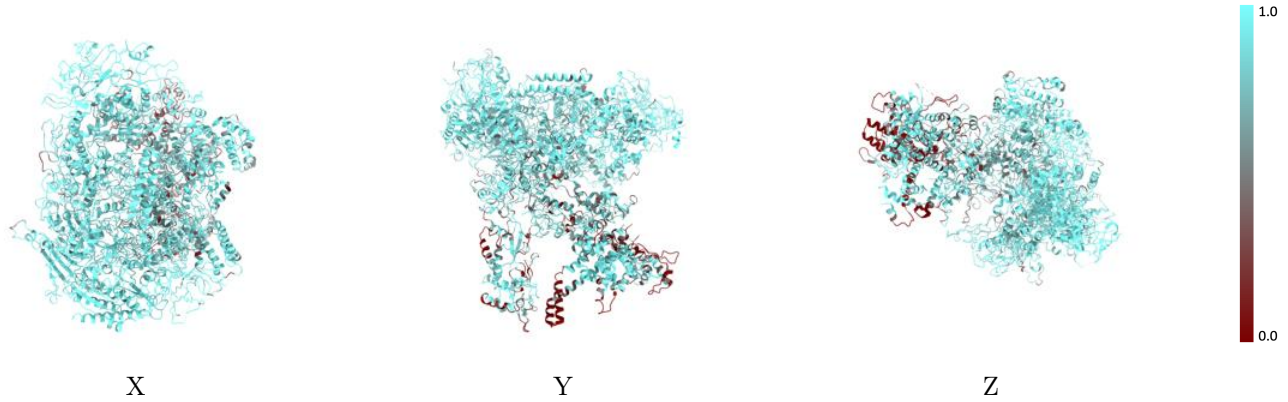
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



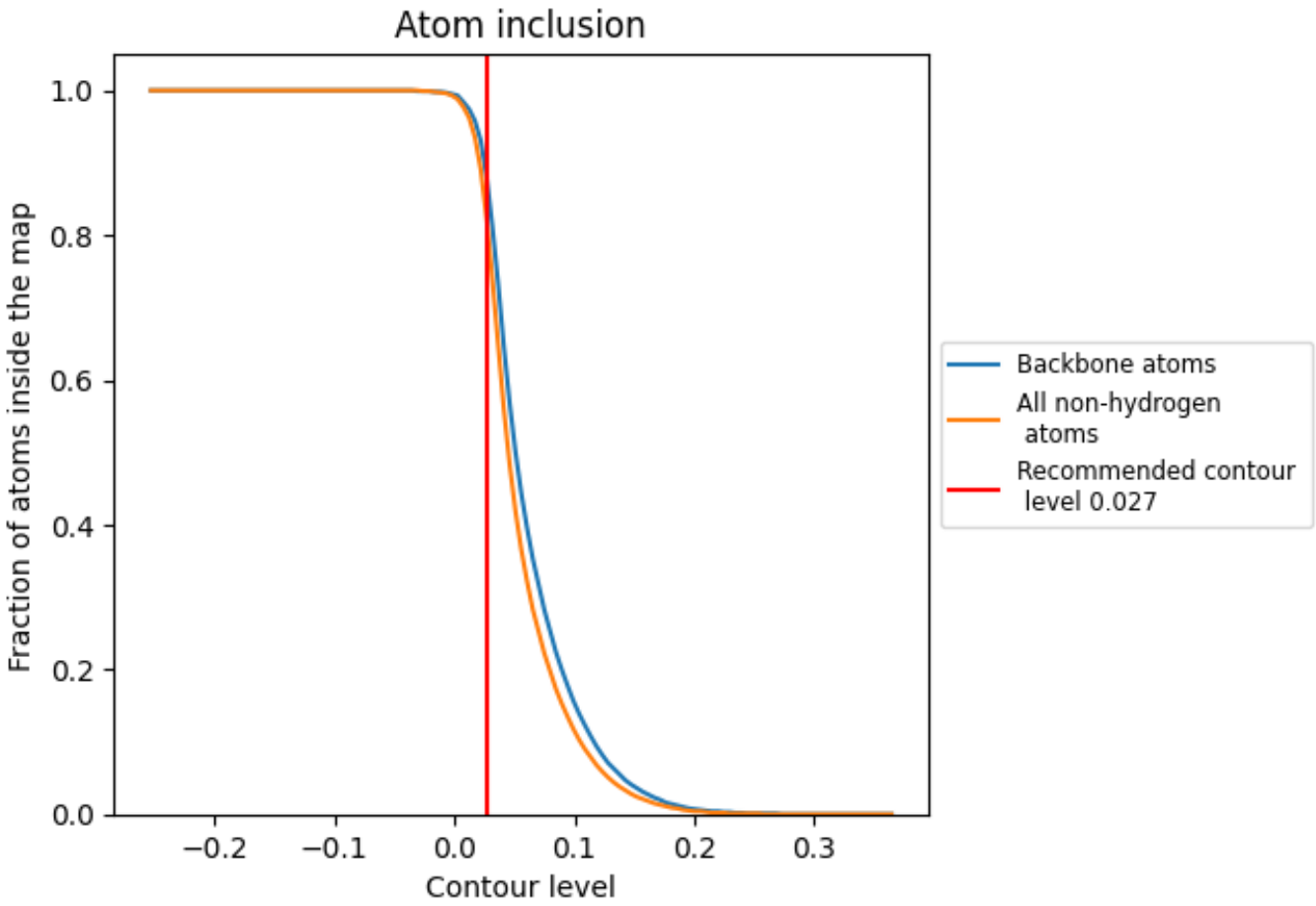
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.027).

9.4 Atom inclusion (i)



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 (i)

The table lists the average atom inclusion at the recommended contour level (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8200	0.2400
A	0.9960	0.2280
B	0.9190	0.3890
C	0.9270	0.2890
D	0.8980	0.2860
E	0.8180	0.2110
F	0.8750	0.1970
G	0.9240	0.3620
H	0.9170	0.3520
I	0.5670	0.1330
J	0.6800	0.1370
K	0.9380	0.2130
L	0.9480	0.2860
M	0.8720	0.3090
N	0.8270	0.2280
X	0.5860	0.0820
Y	0.5280	0.0640
Z	0.7230	0.0750