wwPDB EM Validation Summary Report (i)

May 13, 2024 – 08:52 pm BST

PDB ID	:	6TPS
EMDB ID	:	EMD-10544
Title	:	early intermediate RNA Polymerase I Pre-initiation complex - eiPIC
Authors	:	Pilsl, M.; Engel, C.
Deposited on	:	2019-12-14
Resolution	:	3.54 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:

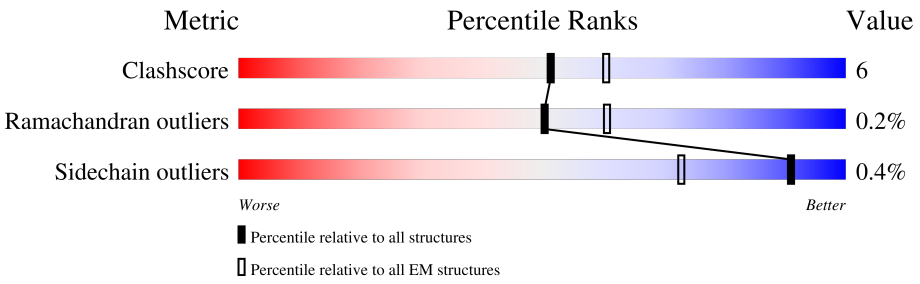
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.54 Å.

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



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

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%

Mol	Chain	Length	Quality of chain
1	A	1664	78% 11% 11%
2	B	1203	85% 13% .
3	C	335	80% 11% 9%
4	D	137	36% 6% 58%
5	E	215	84% 15% .
6	F	155	58% 6% 35%
7	G	326	50% 9% 41%
8	H	146	73% 17% 10%
9	I	125	48% 10% 42%

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Mol	Chain	Length	Quality of chain
10	J	70	81% 17%
11	K	142	61% 11% 29%
12	L	70	51% 10% 39%
13	M	415	20% 5% 75%
14	N	233	52% 10% 38%
15	O	627	64% 10% 26%
16	P	636	70% 22% 6%
17	Q	514	68% 21% 10%
18	R	507	50% 14% 36%
19	S	27	78% 22%
20	T	27	74% 26%
21	U	12	100%
22	V	12	83% 17%

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 50070 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1475	11659	7364	2029	2205	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1177	9350	5913	1639	1747	51	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	305	2423	1539	416	460	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	58	459	289	78	92	0	0

- Molecule 5 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		
5	E	212	1735	1102	306	316	11	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	F	100	823	522	144	154	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	193	1520	982	259	274	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
			Total	C	N	O	S		
8	H	131	1052	664	176	208	4	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	73	542	340	91	107	4	0	0

- Molecule 10 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		
10	J	69	569	362	101	100	6	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	101	793	496	130	162	5	0	0

- Molecule 12 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		
12	L	43	340	211	66	59	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	105	833	528	138	167	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	145	1151	735	188	224	4	0	0

- Molecule 15 is a protein called RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	463	3811	2473	623	694	21	0	0

- Molecule 16 is a protein called RNA polymerase I-specific transcription initiation factor RRN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	595	4840	3080	823	927	10	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	44	ARG	-	expression tag	UNP P32786
P	45	PRO	-	expression tag	UNP P32786
P	46	VAL	-	expression tag	UNP P32786
P	47	ASP	-	expression tag	UNP P32786
P	48	ASP	-	expression tag	UNP P32786
P	49	THR	-	expression tag	UNP P32786
P	50	LEU	-	expression tag	UNP P32786
P	51	ALA	-	expression tag	UNP P32786
P	52	GLU	-	expression tag	UNP P32786
P	53	ASP	-	expression tag	UNP P32786
P	54	ALA	-	expression tag	UNP P32786
P	55	LEU	-	expression tag	UNP P32786
P	56	ASP	-	expression tag	UNP P32786
P	57	LEU	-	expression tag	UNP P32786
P	58	HIS	-	expression tag	UNP P32786
P	59	ILE	-	expression tag	UNP P32786
P	60	VAL	-	expression tag	UNP P32786
P	61	VAL	-	expression tag	UNP P32786
P	62	LYS	-	expression tag	UNP P32786
P	63	SER	-	expression tag	UNP P32786
P	64	LEU	-	expression tag	UNP P32786
P	65	LEU	-	expression tag	UNP P32786
P	66	CYS	-	expression tag	UNP P32786

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Chain	Residue	Modelled	Actual	Comment	Reference
P	67	ASP	-	expression tag	UNP P32786
P	68	THR	-	expression tag	UNP P32786

- Molecule 17 is a protein called RNA polymerase I-specific transcription initiation factor RRN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	461	3839	2473	658	688	20	0	0

- Molecule 18 is a protein called RNA polymerase I-specific transcription initiation factor RRN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	325	2725	1763	479	472	11	0	0

- Molecule 19 is a DNA chain called NTS-DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	S	27	567	270	135	135	27	0	0

- Molecule 20 is a DNA chain called TS-DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	T	27	539	269	55	188	27	0	0

- Molecule 21 is a DNA chain called DNA foreign.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	U	12	264	120	60	72	12	0	0

- Molecule 22 is a DNA chain called DNA foreign.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	V	12	228	108	36	72	12	0	0

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

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

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

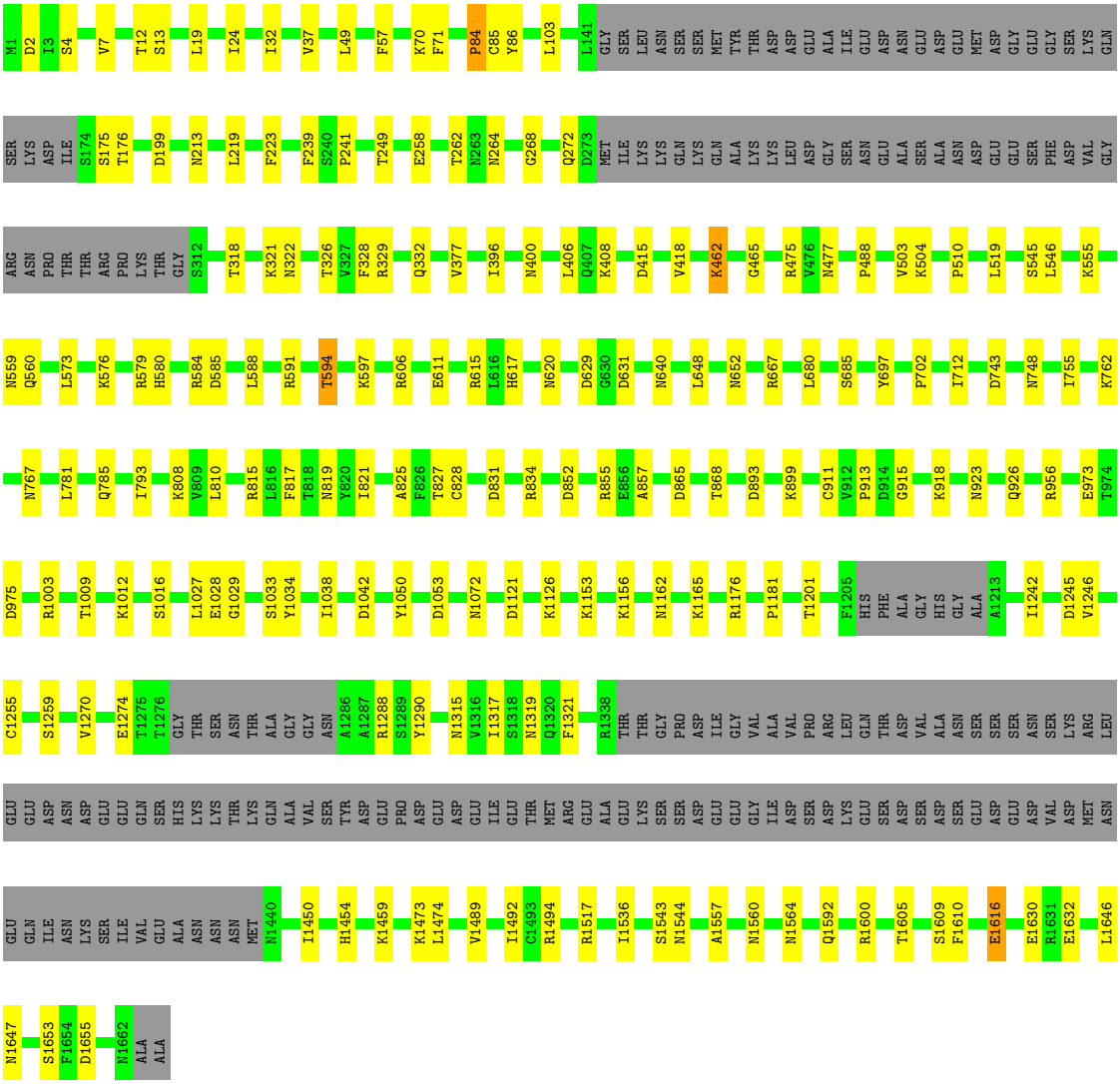
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
24	A	1	1	1	0

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. 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. 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 I subunit RPA190

Chain A: 78% 11% 11%



- Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B: 85% 13%

MET SER LYS VAL ILE LYS PRO PRO GLY GLN ALA ARG T13 E20 R24 K66 E70 D75 S81 GLU ASP GLU ILE SER N87 N93 S96 P107 V113 A116 V121 S126 S132 Y133 K136 L137 L138 E154 V155 R156 M164 S167

N168 R169 N173 E200 K201 L202 R210 I218 R219 P220 S221 F222 R225 G233 D242 T247 N248 V249 R261 E268 R286 G291 I292 E307 R311 S341 Q344 D369 R372 M373 L374 L375 R379 S383 P391 K414 E415 K416

Y420 Q427 V428 R429 N433 D442 K443 R444 R448 R452 E455 N456 S459 T467 G468 M469 S474 G475 S482 G483 A488 N492 P530 L565 H575 H598 E625 P638 N673 H686 S698 I699 D708 T725 V731

R736 Q748 V752 D763 N767 G768 I776 D782 A786 S792 R796 L811 H824 K839 D856 T873 E878 D890 N893 K894 F895 Q896 E897 R906 R909 S918 S919 R920 S928 I934 D935 S939 E940 H975

S981 T991 D994 A1003 M1013 L1022 D1025 I1026 Y1032 Q1045 V1046 R1047 R1063 K1064 R1065 H1066 G1067 G1068 I1069 E1075 H1082 S1085 F1086 L1087 L1088 Q1089 D1097 Y1098 T1099 V1103 I1110 R1119 I1120 C1127 D1137 K1140 L1141 LEU THR LYS SER

GLU ASP GLY GLU LYS I1151 N1171 A1177 F1180 N1199 V1200 E1201 P1202 K1203

- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 80% 11% 9%

MET SER ASN ILE VAL GLY ILE GLU TYR ASN ARG VAL THR ASN THR THR SER THR ASP PHE PRO GLY PHE SER LYS ASP ALA GLU ASN GLU W31 R50 N53 R69 A80 N88 E95 R100 V104 V116 K125 D128 E129 N130 T131 K139 R142

K154 Y157 A160 H161 Q175 I191 L192 K195 L196 R197 E201 H207 C208 P253 T274 N301 G306 A307 M308 T309 K316 E326 N330 Q335

- Molecule 4: DNA-directed RNA polymerase I subunit RPA14

Chain D: 36% 6% 58%

MET MET LYS GLY SER ARG ARG THR GLY ASN ASN T12 T25 Q26 L27 P28 E48 ASN ILE ILE ASP SER THR THR MET ASN THR ILE SER GLY ASN ALA ALA ASP ALA ASP ALA ALA ALA VAL ALA ASN THR SER LEU ASN ILE ASP T80 K90 R94 D95 L99 P100 PRO

ALA GLN ASP PHE SER ALA ALA PRO ILE GLN VAL SER THR THR GLU LYS LYS GLU THR SER ILE GLY VAL SER ALA THR GLY GLY LYS LYS THR THR PHE ALA ASP GLU

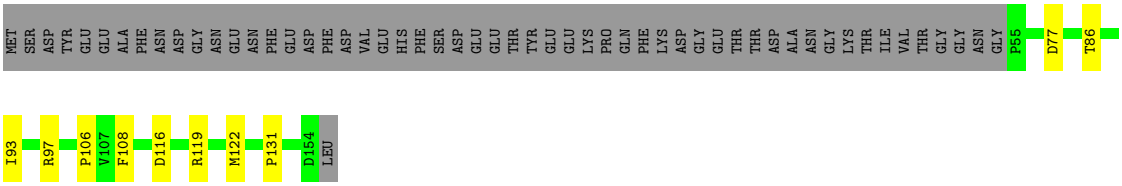
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 84% 15%

MET ASP GLN E4 N5 E6 K20 E21 E34 D48 Q54 N63 S77 C83 D84 S87 V88 V97 N115 I116 L123 H146 V150 D159 R177 I178 Q179 R180 A185 L190 K191 R192 G193 E194 S210 Y211 R212 I213 C214 M215

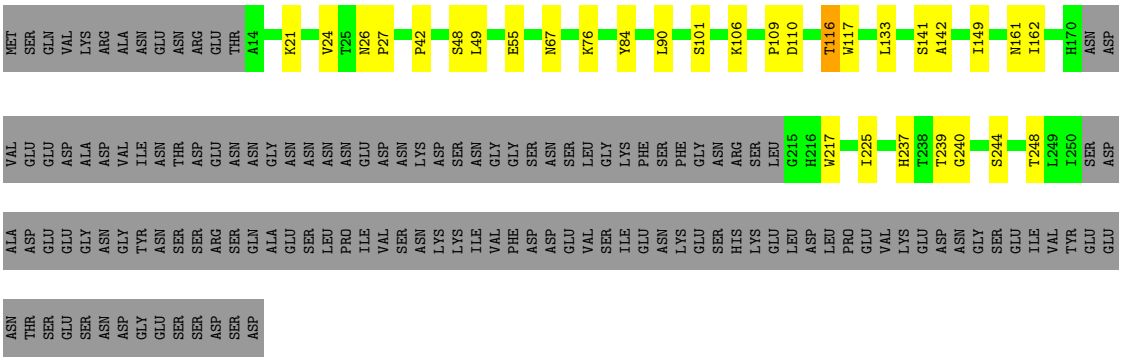
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 58% 6% 35%



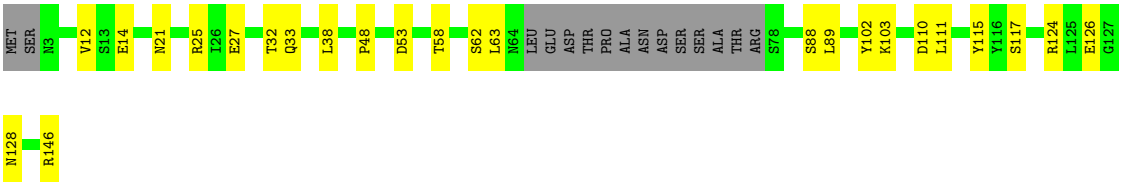
• Molecule 7: DNA-directed RNA polymerase I subunit RPA43

Chain G:



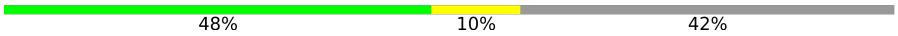
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

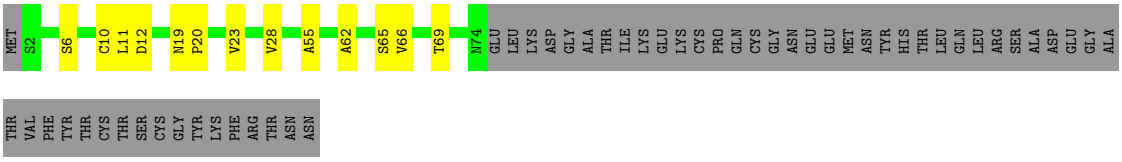
Chain H:



• Molecule 9: DNA-directed RNA polymerase I subunit RPA12

Chain I:



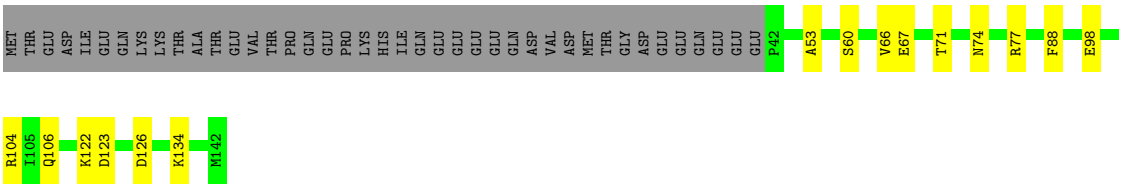


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 61% 11% 29%

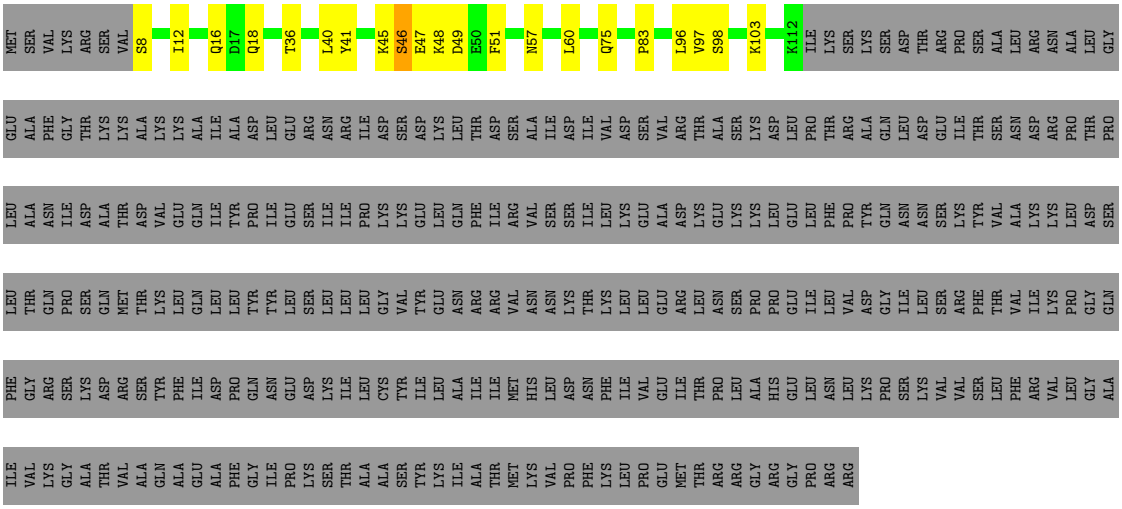


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 51% 10% 39%

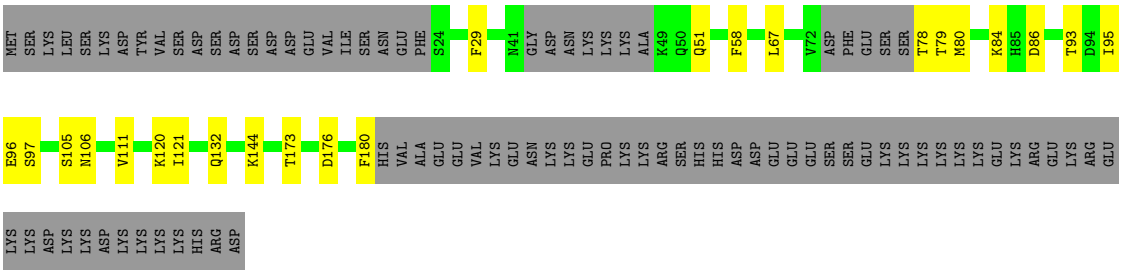
• Molecule 13: DNA-directed RNA polymerase I subunit RPA49

Chain M: 20% 5% 75%



• Molecule 14: DNA-directed RNA polymerase I subunit RPA34

Chain N: 52% 10% 38%



• Molecule 15: RNA polymerase I-specific transcription initiation factor RRN3

Chain O: 64% 10% 26%

MET MET ALA PHE GLU ASN THR SER LYS ARG PRO PRO GLN ASP PHE VAL ALA PRO ILE ASP GLN LYS LYS ARG LYS VAL GLN PHE SER ASP SER THR GLY LEU VAL THR LEU GLN PRO GLU GLU ILE LYS ASP GLU VAL PHE S48 L80 R87 D90 N103 F122 W125

P130 H131 T132 L133 I147 P148 K149 I166 N200 K201 N202 S213 R219 L225 G226 F227 S239 I240 D241 L248 ASP GLU LEU ASP ASP VAL ASP ASP ASP ASP LEU GLU ASP ASP ASP LEU ASP ASP ASP SER GLY ASP ASP

ASP GLU ASN CYS GLY ASN SER ASN GLU GLU LEU ARG SER GLY ALA ALA ASP GLY SER GLN SER ASP SER GLU ASP MET ASP ILE ILE GLU GLY MET ASP GLY THR GLU GLU TYR ASN VAL GLU LEU THR GLN G324 D333 N362 T363 L364 T365 T366 T378 R379 S380 I381 Q382 Y383

L400 E412 K416 I428 A431 K432 K433 L434 S435 R436 T437 Q438 I439 I440 S444 N451 E460 V461 R469 Q478 I483 R487 F506 Q507 K513 L517 F528 A532 Y539 I543 R551 LEU ARG GLY ILE ILE GLY LYS ALA ASP

SER ASP LYS LYS GLU ASN SER ALA GLN ALA ASN THR THR SER SER SER TRP SER LEU ALA T581 D595 P596 L597 F598 L599 Y609 S614 GLU ALA SER GLY GLU TYR GLU SER ASP GLY SER ASP ASP

• Molecule 16: RNA polymerase I-specific transcription initiation factor RRN6

Chain P: 70% 22% • 6%

R44 P45 V46 T49 L50 A51 V61 K62 S63 L64 N180 R181 L182 D183 S184 Q185 E201 L219 N228 N232 V233 T234 L238 H239 S240 I247 A250 S253 R256 R257 S258 N259 I264 R273 V277 V284 V302 V303 D304 F305 ALA PHE ASN

PRO TRP ASP LEU GLN Q314 F315 A316 I317 K321 I326 I329 N332 N335 ASN ASN LYS ARG LYS LEU Q342 L347 H348 G349 T350 I351 F352 D353 P354 E355 R362 I363 E364 W365 I372 D376 R377 S378 K379 M380 V393 V394 Q395 S400 R403 K411

L416 R419 E420 I421 I422 I423 E428 S429 N430 R434 S437 W438 D441 L442 D443 T448 L449 S470 M471 K474 R475 K485 A486 N487 L488 F489 Q490 S491 L492 I500 P505 I511 LEU THR LEU ASP HIS ILE ASP ASP GLU SER ARG ARG GLU GLU ASP ALA

ASP GLU ASN F531 K540 S544 A551 L552 S553 N554 S558 GLU PRO ASN LYS GLN GLU THR PRO I567 I568 V569 D570 H571 R584 S588 I589 L592 V593 S594 Q595 I596 K597 L598 K599 E600 R601 S605 Q608 K621 Y622 L623 L626 R629 L630 S631 I632 A633

T634 N635 L638 L650 S653 L654 L662 N665 I672 P673 L678 Q681 Y685 Y686 T692 F693 I694 K698 L699 L702 D707 D712 Q720 S726 A729 L732 T733 K734 E735 I736 R746 K749 E754 Q757 N758 Q769

D779

• Molecule 17: RNA polymerase I-specific transcription initiation factor RRN7

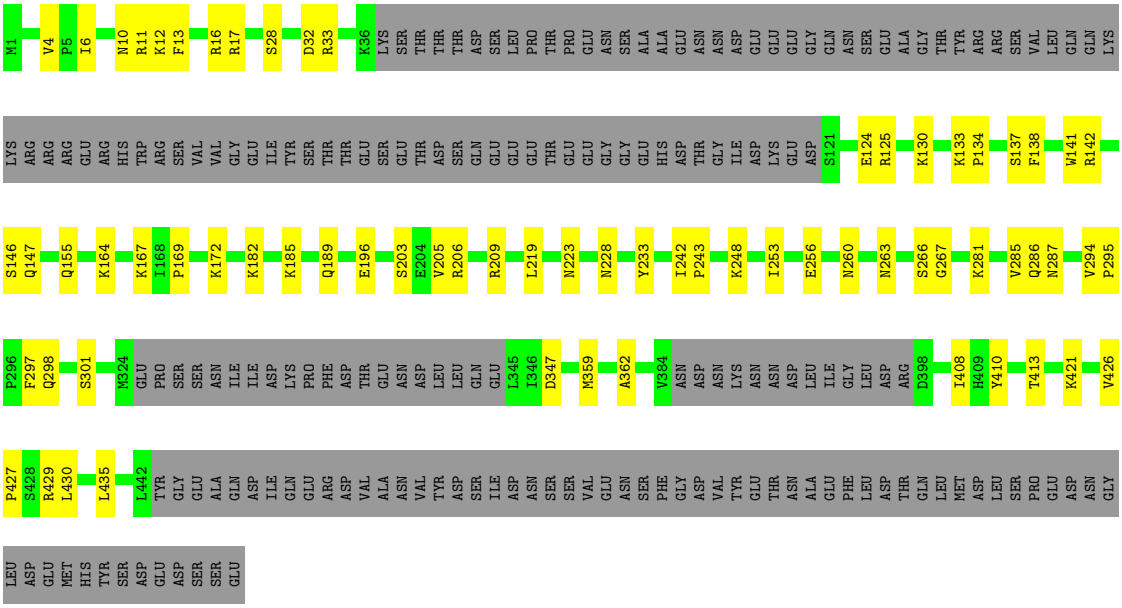
Chain Q: 68% 21% 10%

MET SER T3 F4 I9 C10 N14 C15 P16 W20 I23 R27 Q30 E36 G37 D38 D44 E45 ASP ASP LEU ASN GLY LEU GLY ALA GLY VAL ILE T57 L62 T63 T64 F70 N77 Q85 S88 H89 K90 K93 K94 L95 L112 I120

R124 F125 A133 I136 T143 I144 N145 D146 L154 I164 S169 L174 P175 T178 I182 F193 Q194 Y211 V212 S213 I214 L215 E216 G217 S218 I219 Q225 L226 Y227 N228 K229 L232 I237 H238 F239 N244 S248 C249 Q250 K255 L256 V257

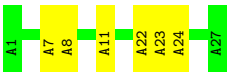
• Molecule 18: RNA polymerase I-specific transcription initiation factor RRN11

Chain R:



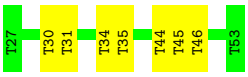
• Molecule 19: NTS-DNA (27-MER)

Chain S:



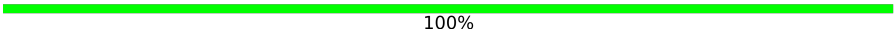
• Molecule 20: TS-DNA (27-MER)

Chain T:



• Molecule 21: DNA foreign

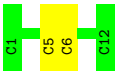
Chain U:



There are no outlier residues recorded for this chain.

• Molecule 22: DNA foreign

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.51	0/11873	0.57	1/16035 (0.0%)
2	B	0.55	1/9557 (0.0%)	0.58	0/12918
3	C	0.50	0/2475	0.55	0/3354
4	D	0.35	0/465	0.62	1/630 (0.2%)
5	E	0.44	0/1771	0.52	0/2383
6	F	0.52	0/838	0.53	0/1129
7	G	0.39	0/1558	0.54	0/2120
8	H	0.50	0/1070	0.59	1/1449 (0.1%)
9	I	0.36	0/548	0.56	0/740
10	J	0.59	0/578	0.55	0/775
11	K	0.47	0/804	0.53	0/1083
12	L	0.48	0/342	0.63	0/454
13	M	0.32	0/849	0.51	0/1140
14	N	0.33	0/1172	0.52	0/1580
15	O	0.36	0/3897	0.52	0/5268
16	P	0.33	0/4939	0.61	1/6689 (0.0%)
17	Q	0.34	0/3928	0.60	3/5302 (0.1%)
18	R	0.38	0/2789	0.57	0/3755
19	S	0.66	0/647	0.87	0/995
20	T	0.71	0/592	1.34	0/912
21	U	0.68	0/299	0.89	0/464
22	V	0.65	0/251	0.85	0/380
All	All	0.47	1/51242 (0.0%)	0.59	7/69555 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
3	C	0	1
13	M	0	1
16	P	0	6
17	Q	0	7
18	R	0	4
All	All	0	25

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	VAL	C-N	-5.99	1.20	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	15	CYS	C-N-CD	-11.98	94.24	120.60
17	Q	15	CYS	C-N-CA	7.41	153.10	122.00
17	Q	154	LEU	CA-CB-CG	5.47	127.88	115.30
16	P	654	LEU	CA-CB-CG	5.46	127.86	115.30
4	D	95	ASP	CB-CG-OD2	5.34	123.11	118.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1616	GLU	Peptide
1	A	57	PHE	Peptide
1	A	84	PRO	Peptide
2	B	116	ALA	Peptide
2	B	893	ASN	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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11659	0	11753	121	0
2	B	9350	0	9241	106	0
3	C	2423	0	2412	26	0
4	D	459	0	462	5	0
5	E	1735	0	1764	17	0
6	F	823	0	841	8	0
7	G	1520	0	1529	22	0
8	H	1052	0	1021	13	0
9	I	542	0	557	9	0
10	J	569	0	586	9	0
11	K	793	0	790	9	0
12	L	340	0	362	5	0
13	M	833	0	826	16	0
14	N	1151	0	1169	19	0
15	O	3811	0	3804	36	0
16	P	4840	0	4773	99	0
17	Q	3839	0	3861	70	0
18	R	2725	0	2798	43	0
19	S	567	0	298	4	0
20	T	539	0	324	6	0
21	U	264	0	133	0	0
22	V	228	0	133	1	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	Q	1	0	0	0	0
24	A	1	0	0	0	0
All	All	50070	0	49437	576	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 6.

The worst 5 of 576 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:A:239:PHE:H	1:A:264:ASN:HD21	1.45	0.65
16:P:584:ARG:HH12	16:P:588:SER:HB3	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:THR:HG23	2:B:469:ASN:H	1.61	0.65
16:P:228:ASN:ND2	16:P:232:ASN:OD1	2.30	0.64
18:R:427:PRO:HD2	18:R:430:LEU:HB2	1.79	0.64

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1463/1664 (88%)	1339 (92%)	120 (8%)	4 (0%)	41	75
2	B	1171/1203 (97%)	1083 (92%)	85 (7%)	3 (0%)	41	75
3	C	303/335 (90%)	281 (93%)	22 (7%)	0	100	100
4	D	54/137 (39%)	52 (96%)	2 (4%)	0	100	100
5	E	210/215 (98%)	193 (92%)	17 (8%)	0	100	100
6	F	98/155 (63%)	93 (95%)	5 (5%)	0	100	100
7	G	189/326 (58%)	172 (91%)	17 (9%)	0	100	100
8	H	127/146 (87%)	115 (91%)	12 (9%)	0	100	100
9	I	71/125 (57%)	63 (89%)	8 (11%)	0	100	100
10	J	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	41/70 (59%)	35 (85%)	6 (15%)	0	100	100
13	M	103/415 (25%)	89 (86%)	14 (14%)	0	100	100
14	N	139/233 (60%)	121 (87%)	18 (13%)	0	100	100
15	O	457/627 (73%)	431 (94%)	26 (6%)	0	100	100
16	P	583/636 (92%)	515 (88%)	68 (12%)	0	100	100
17	Q	451/514 (88%)	402 (89%)	47 (10%)	2 (0%)	34	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	317/507 (62%)	273 (86%)	44 (14%)	0	100	100
All	All	5943/7520 (79%)	5414 (91%)	520 (9%)	9 (0%)	50	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	1028	GLU
1	A	85	CYS
2	B	1119	ARG
1	A	462	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1304/1465 (89%)	1303 (100%)	1 (0%)	93	98
2	B	1030/1053 (98%)	1026 (100%)	4 (0%)	91	97
3	C	269/296 (91%)	267 (99%)	2 (1%)	84	93
4	D	55/116 (47%)	55 (100%)	0	100	100
5	E	194/197 (98%)	192 (99%)	2 (1%)	76	89
6	F	90/137 (66%)	90 (100%)	0	100	100
7	G	170/291 (58%)	169 (99%)	1 (1%)	86	94
8	H	115/128 (90%)	113 (98%)	2 (2%)	60	83
9	I	65/110 (59%)	65 (100%)	0	100	100
10	J	64/65 (98%)	64 (100%)	0	100	100
11	K	91/130 (70%)	90 (99%)	1 (1%)	73	88
12	L	38/57 (67%)	38 (100%)	0	100	100
13	M	95/371 (26%)	95 (100%)	0	100	100
14	N	135/220 (61%)	134 (99%)	1 (1%)	84	93
15	O	427/576 (74%)	425 (100%)	2 (0%)	88	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	551/590 (93%)	548 (100%)	3 (0%)	88	95
17	Q	430/476 (90%)	428 (100%)	2 (0%)	88	95
18	R	308/474 (65%)	305 (99%)	3 (1%)	76	89
All	All	5431/6752 (80%)	5407 (100%)	24 (0%)	91	97

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	219	ARG
16	P	419	ARG
16	P	321	LYS
16	P	475	ARG
3	C	309	THR

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

Mol	Chain	Res	Type
3	C	323	ASN
18	R	189	GLN
8	H	139	ASN
17	Q	507	ASN
17	Q	85	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	P	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	68:THR	C	169:GLN	N	23.31
1	B	121:VAL	C	122:TYR	N	1.20

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10544. 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)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

This section was not generated.