



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:27 PM BST

PDB ID : 5FJA
EMDB ID: : EMD-3180
Title : Cryo-EM structure of yeast RNA polymerase III at 4.7 Å
Authors : Hoffmann, N.A.; Jakobi, A.J.; Moreno-Morcillo, M.; Glatt, S.; Kosinski, J.;
Hagen, W.J.; Sachse, C.; Muller, C.W.
Deposited on : 2015-10-06
Resolution : 4.65 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

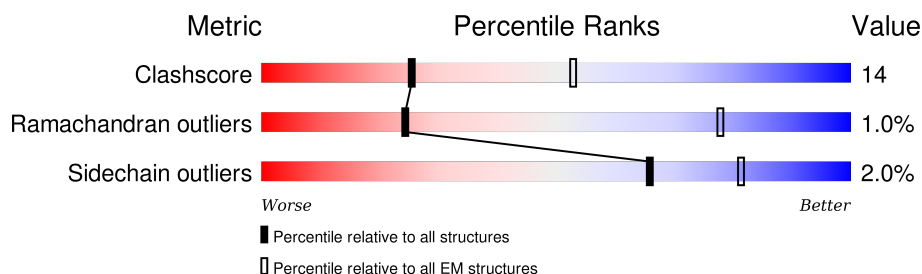
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.65 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1460	68% 27% . .
2	B	1149	68% 28% . .
3	C	335	71% 28% .
4	D	161	46% 27% . 26%
5	E	215	63% 35% .
6	F	155	43% 11% 46%
7	G	212	50% 35% . 14%
8	H	146	71% 25% .
9	I	110	62% 21% . 16%

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Mol	Chain	Length	Quality of chain
10	J	70	<div><div></div><div>76%19%••</div></div>
11	K	142	<div><div></div><div>51%19%•29%</div></div>
12	L	70	<div><div></div><div>41%19%•36%</div></div>
13	M	282	<div><div></div><div>38%19%•42%</div></div>
14	N	422	<div><div></div><div>16%9%•74%</div></div>
15	O	654	<div><div></div><div>55%26%•18%</div></div>
16	P	317	<div><div></div><div>15%12%••72%</div></div>
17	Q	88	<div><div></div><div>48%5%•47%</div></div>

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 38434 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
1	A	1403	Total	C	N	O	S	0	0
			11007	6941	1943	2065	58		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1114	Total	C	N	O	S	0	0
			8788	5558	1516	1654	60		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	335	Total	C	N	O	S	0	0
			2655	1681	454	511	9		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	119	Total	C	N	O	S	0	0
			977	628	156	187	6		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1759	1116	310	321	12		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			671	429	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	182	Total	C	N	O	S	0	0
			1464	961	234	263	6		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	140	Total	C	N	O	S	0	0
			1120	703	188	224	5		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	92	Total	C	N	O	S	0	0
			728	455	117	145	11		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	164	Total	C	N	O	S	0	0
			1338	857	227	253	1		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	110	Total	C	N	O	S	0	0
			845	536	152	154	3		

- Molecule 15 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	539	Total	C	N	O	S	0	0
			4329	2756	741	813	19		

- Molecule 16 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	89	Total	C	N	O	S	0	0
			738	474	115	146	3		

- Molecule 17 is a protein called DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7.

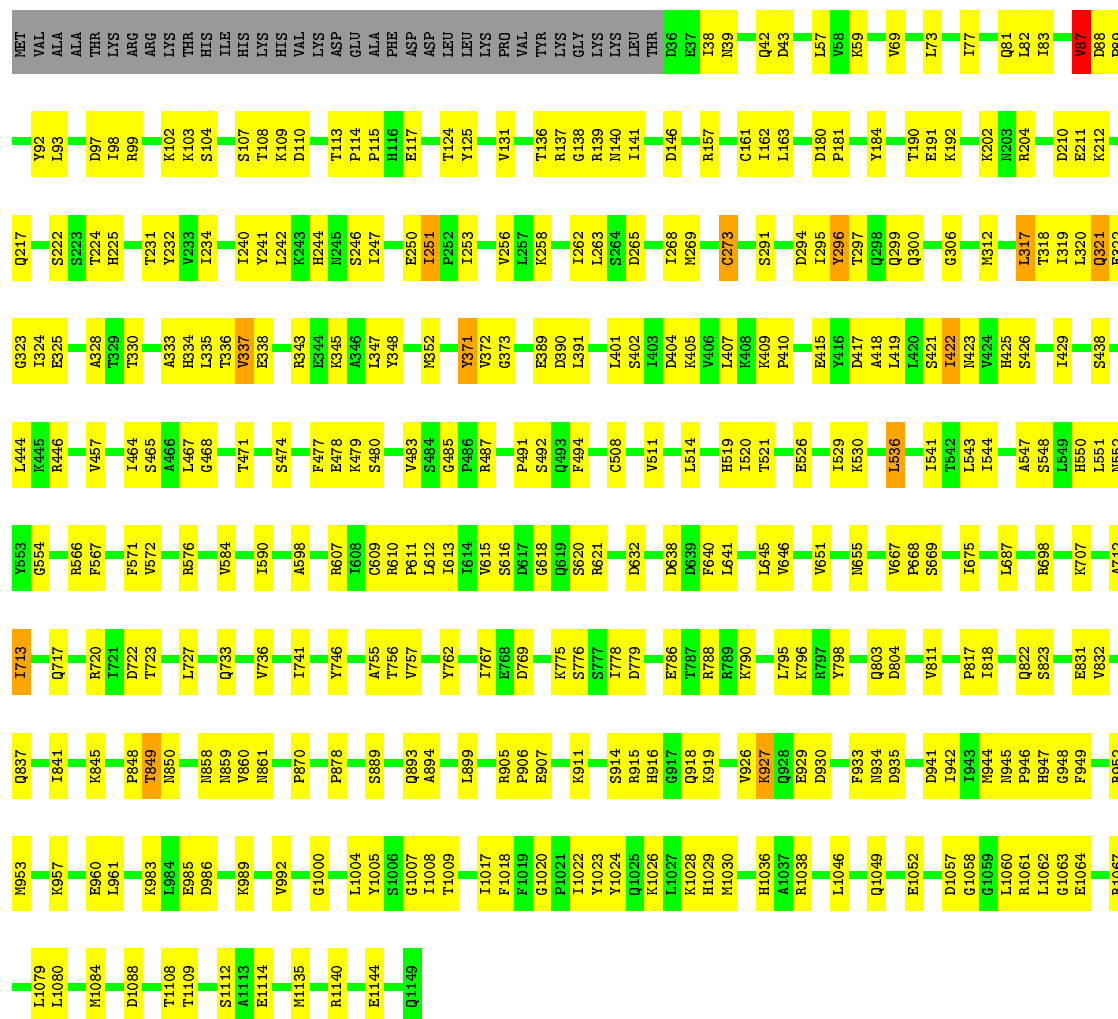
Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	47	Total	C	N	O	0	0
			310	195	57	58		

- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

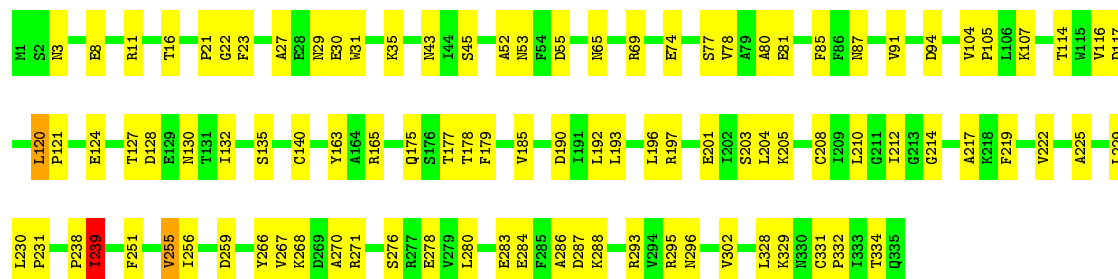
• Molecule 2: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2

Chain B:  68% 28% ..

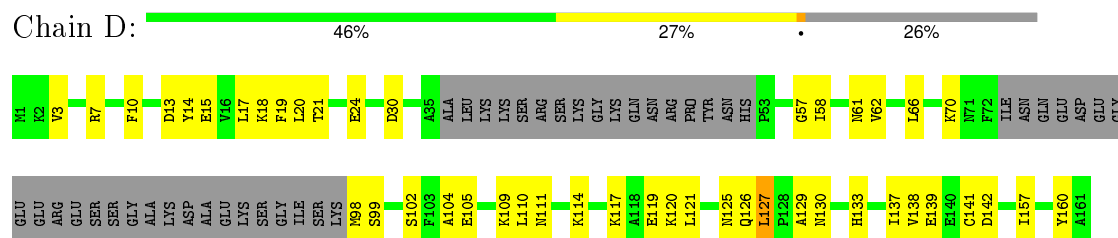


● Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

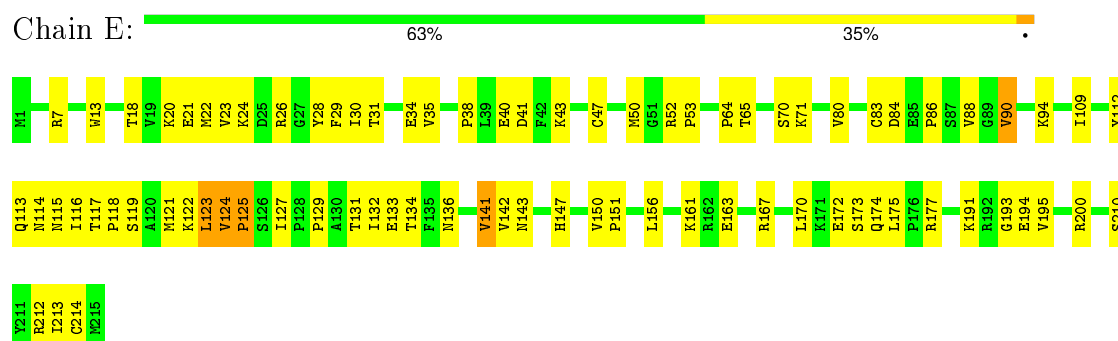
Chain C: 71% 28%



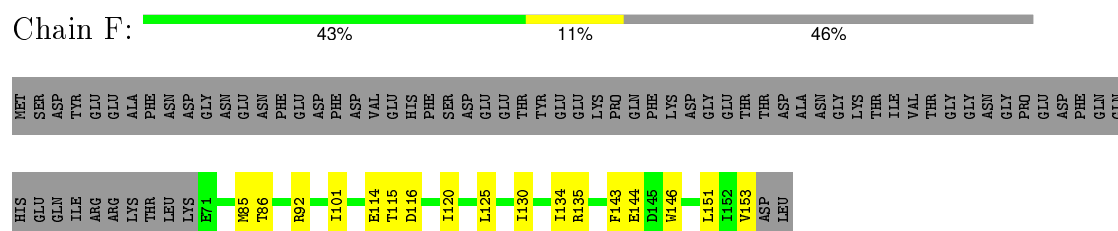
- Molecule 4: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9



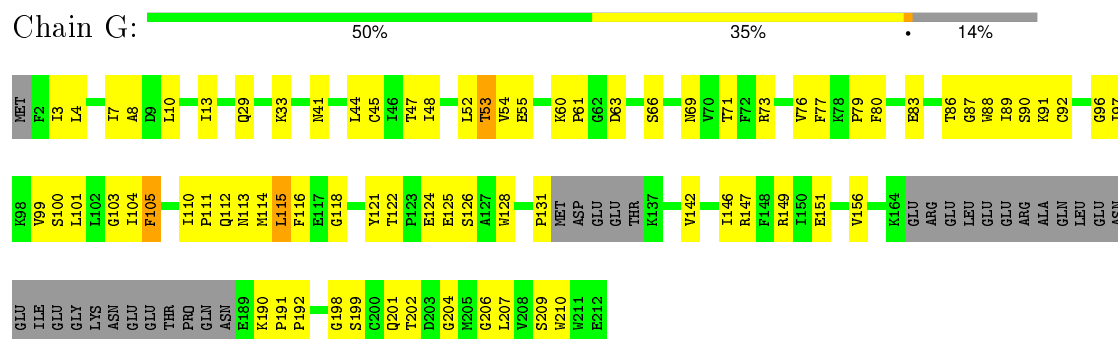
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



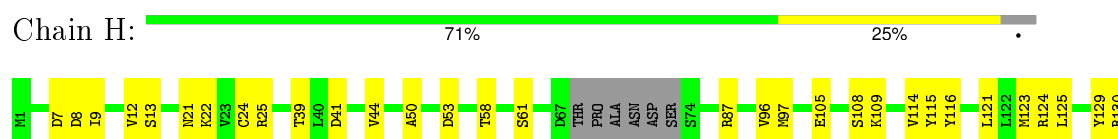
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

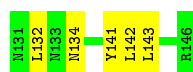


- Molecule 7: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC8

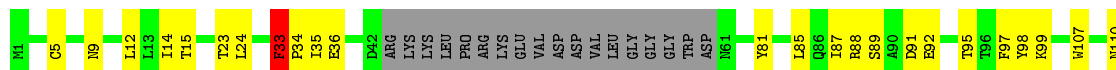


- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3





- Molecule 9: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC10



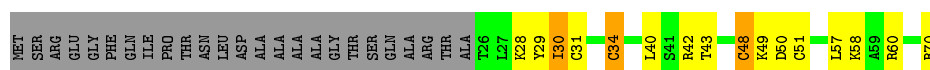
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



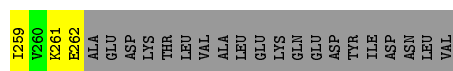
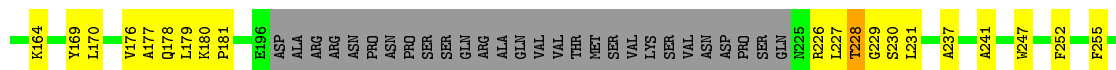
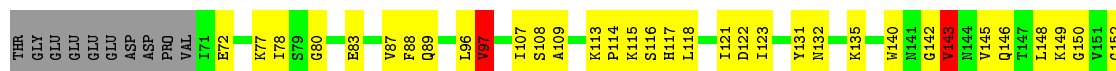
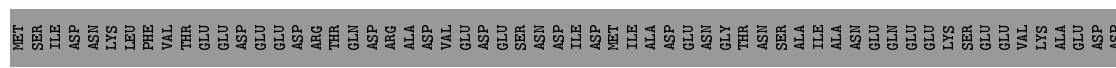
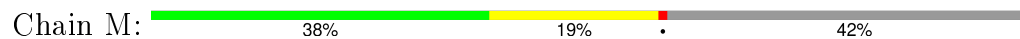
- Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2



- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

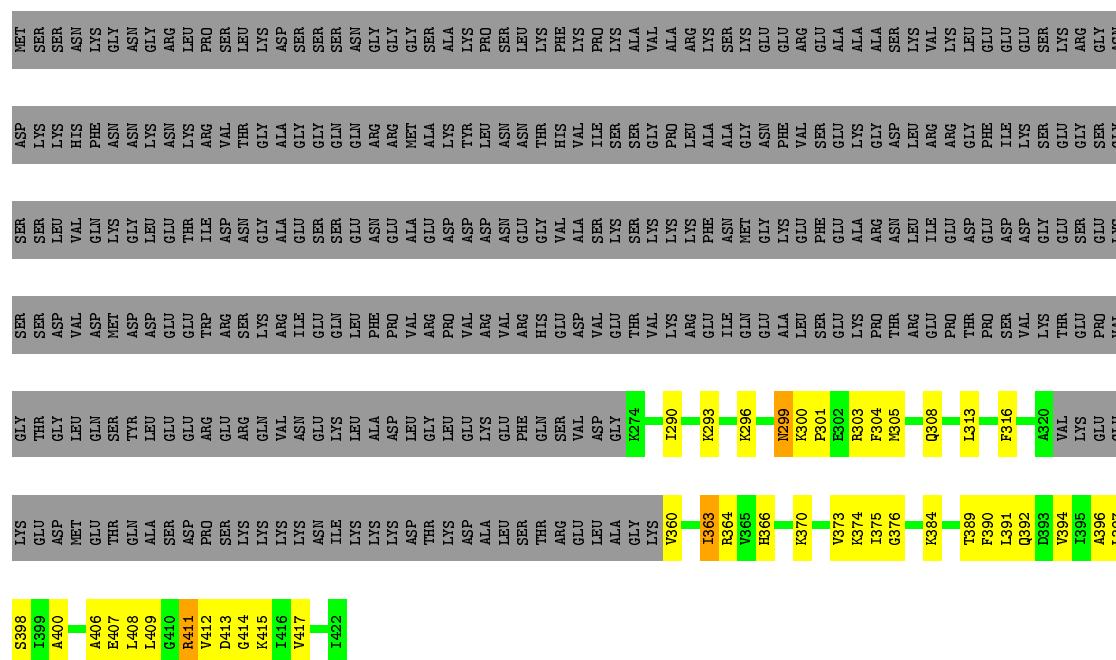


- Molecule 13: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC5



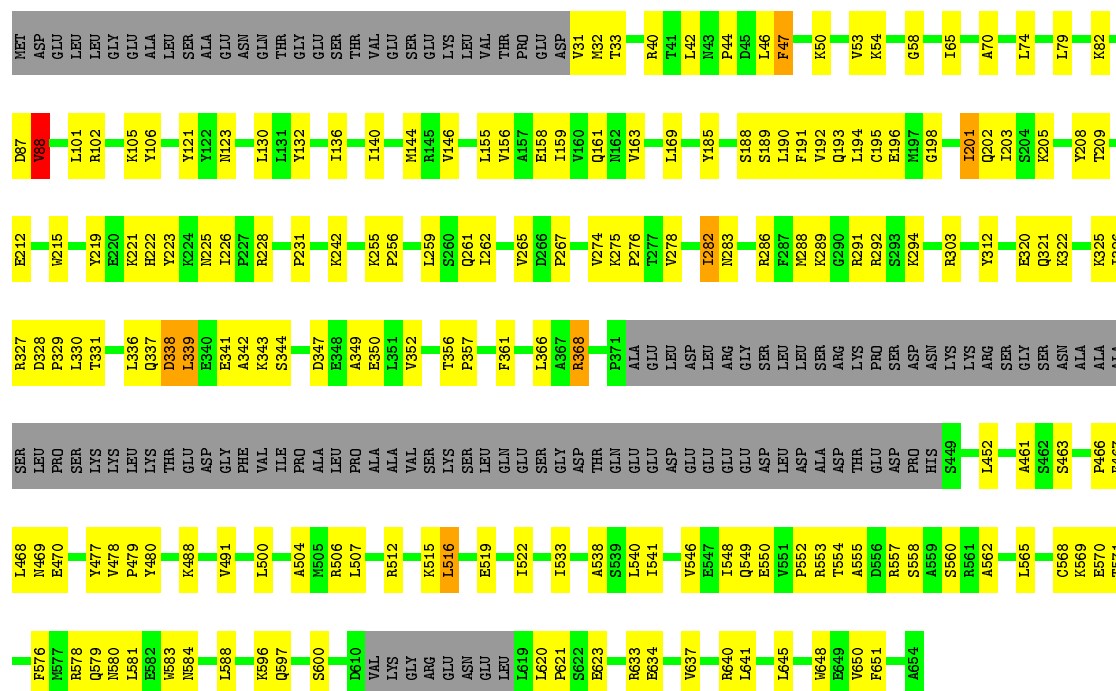
- Molecule 14: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4

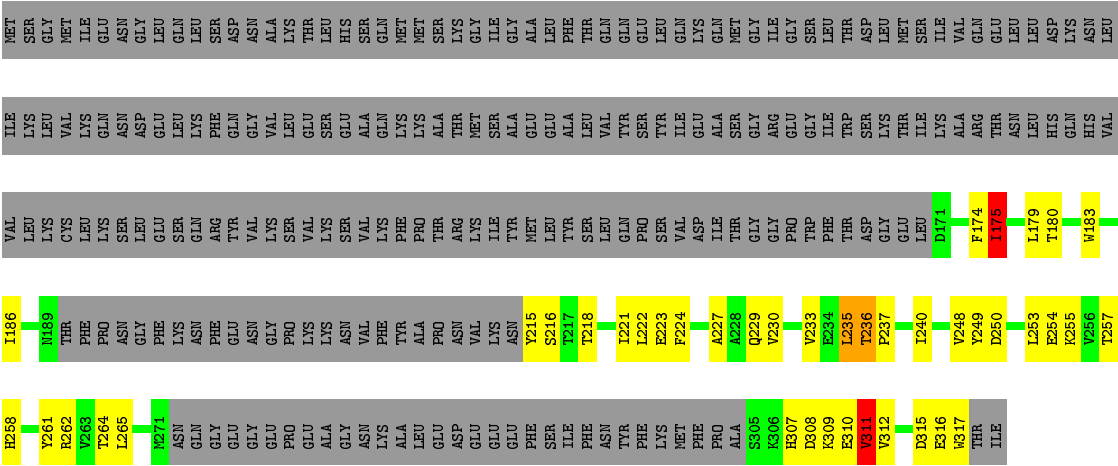
Chain N: 



• Molecule 15: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3

Chain O: 





● Molecule 17: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4K X 4K)	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 >2	RMSZ	# Z >2
1	A	0.22	0/11202	0.45	0/15130
10	J	0.21	0/558	0.43	0/750
11	K	0.22	0/803	0.44	0/1083
12	L	0.22	0/360	0.46	0/478
13	M	0.24	0/1369	0.45	0/1851
14	N	0.23	0/855	0.54	0/1149
15	O	0.22	0/4394	0.49	1/5928 (0.0%)
16	P	0.25	0/750	0.49	0/1017
17	Q	0.25	0/219	0.41	0/294
2	B	0.21	0/8943	0.44	0/12068
3	C	0.23	0/2711	0.44	1/3676 (0.0%)
4	D	0.23	0/991	0.50	0/1328
5	E	0.22	0/1795	0.43	0/2416
6	F	0.21	0/683	0.41	0/923
7	G	0.22	0/1503	0.49	0/2040
8	H	0.21	0/1138	0.43	0/1540
9	I	0.22	0/745	0.48	1/1007 (0.1%)
All	All	0.22	0/39019	0.46	3/52678 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	468	LEU	CA-CB-CG	5.47	127.89	115.30
3	C	120	LEU	CA-CB-CG	5.10	127.03	115.30
9	I	33	PHE	C-N-CD	-5.02	109.55	120.60

There are no chirality outliers.

There are no planarity outliers.

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	A	11007	0	11137	321	0
2	B	8788	0	8902	250	0
3	C	2655	0	2628	71	0
4	D	977	0	983	37	0
5	E	1759	0	1788	57	0
6	F	671	0	692	12	0
7	G	1464	0	1466	51	0
8	H	1120	0	1089	30	0
9	I	728	0	672	26	0
10	J	549	0	560	10	0
11	K	792	0	790	29	0
12	L	358	0	381	15	0
13	M	1338	0	1307	47	0
14	N	845	0	891	37	0
15	O	4329	0	4497	145	0
16	P	738	0	719	35	0
17	Q	310	0	248	7	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	I	1	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
All	All	38434	0	38750	1046	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 14.

The worst 5 of 1046 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:599:LYS:HG2	1:A:600:PRO:CD	1.32	1.57
1:A:599:LYS:CG	1:A:600:PRO:HD2	1.25	1.56
1:A:599:LYS:CG	1:A:600:PRO:CD	1.99	1.11
1:A:599:LYS:HG3	1:A:600:PRO:HD2	1.47	0.93
3:C:251:PHE:HB3	3:C:255:VAL:HG11	1.51	0.92

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	
1	A	1393/1460 (95%)	1147 (82%)	233 (17%)	13 (1%)	21	67
2	B	1112/1149 (97%)	943 (85%)	160 (14%)	9 (1%)	24	69
3	C	333/335 (99%)	282 (85%)	47 (14%)	4 (1%)	16	62
4	D	113/161 (70%)	80 (71%)	33 (29%)	0	100	100
5	E	213/215 (99%)	170 (80%)	41 (19%)	2 (1%)	21	67
6	F	81/155 (52%)	74 (91%)	7 (9%)	0	100	100
7	G	176/212 (83%)	149 (85%)	25 (14%)	2 (1%)	17	64
8	H	136/146 (93%)	117 (86%)	19 (14%)	0	100	100
9	I	88/110 (80%)	75 (85%)	13 (15%)	0	100	100
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	13	58
11	K	99/142 (70%)	83 (84%)	15 (15%)	1 (1%)	19	65
12	L	43/70 (61%)	33 (77%)	10 (23%)	0	100	100
13	M	160/282 (57%)	138 (86%)	18 (11%)	4 (2%)	7	47
14	N	106/422 (25%)	80 (76%)	24 (23%)	2 (2%)	10	53
15	O	533/654 (82%)	436 (82%)	93 (17%)	4 (1%)	24	69
16	P	83/317 (26%)	54 (65%)	26 (31%)	3 (4%)	4	40
17	Q	26/88 (30%)	22 (85%)	3 (12%)	1 (4%)	4	38
All	All	4760/5988 (80%)	3936 (83%)	778 (16%)	46 (1%)	24	65

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ILE
1	A	587	ILE

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Mol	Chain	Res	Type
1	A	603	LEU
1	A	632	VAL
1	A	1371	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1217/1257 (97%)	1193 (98%)	24 (2%)	63	86
2	B	975/1006 (97%)	959 (98%)	16 (2%)	70	88
3	C	296/296 (100%)	293 (99%)	3 (1%)	82	91
4	D	110/145 (76%)	109 (99%)	1 (1%)	84	92
5	E	197/197 (100%)	193 (98%)	4 (2%)	63	86
6	F	73/137 (53%)	72 (99%)	1 (1%)	74	89
7	G	162/190 (85%)	157 (97%)	5 (3%)	47	78
8	H	123/128 (96%)	120 (98%)	3 (2%)	57	83
9	I	83/98 (85%)	82 (99%)	1 (1%)	78	90
10	J	62/65 (95%)	60 (97%)	2 (3%)	46	77
11	K	91/130 (70%)	90 (99%)	1 (1%)	80	91
12	L	40/57 (70%)	37 (92%)	3 (8%)	17	55
13	M	142/249 (57%)	138 (97%)	4 (3%)	51	79
14	N	92/360 (26%)	90 (98%)	2 (2%)	60	84
15	O	495/593 (84%)	485 (98%)	10 (2%)	63	86
16	P	86/285 (30%)	81 (94%)	5 (6%)	25	63
17	Q	24/56 (43%)	24 (100%)	0	100	100
All	All	4268/5249 (81%)	4183 (98%)	85 (2%)	66	86

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	818	ILE
5	E	141	VAL
15	O	339	LEU
2	B	849	THR
4	D	127	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	ASN
1	A	625	ASN
15	O	337	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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](#)

There are no chain breaks in this entry.