



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:20 PM BST

PDB ID : 5FJ8  
EMDB ID: : EMD-3178  
Title : Cryo-EM structure of yeast RNA polymerase III elongation complex at 3.9 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 : 3.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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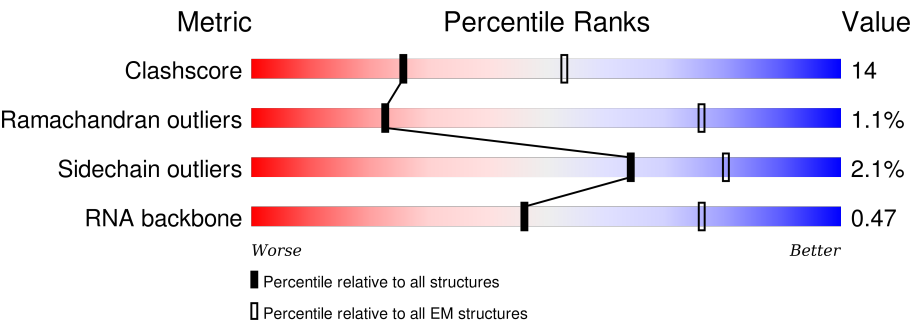
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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.






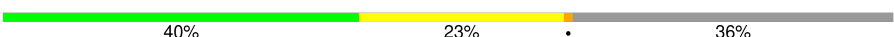
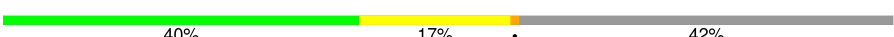





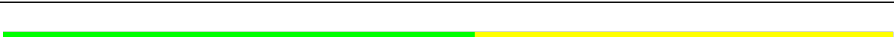
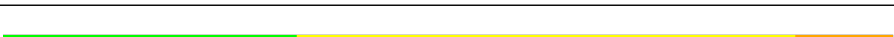
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 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	69% 27% ..
2	B	1149	68% 28% ..
3	C	335	70% 28% .
4	D	161	46% 27% . 26%
5	E	215	62% 35% .
6	F	155	44% 8% . 46%
7	G	212	50% 37% . 10%
8	H	146	73% 23% ..

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Mol	Chain	Length	Quality of chain
9	I	110	
10	J	70	
11	K	142	
12	L	70	
13	M	282	
14	N	422	
15	O	654	
16	P	317	
17	Q	104	
18	R	23	
19	S	15	
20	T	9	

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 39284 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	1422	Total	C	N	O	S	0	0
			11130	7013	1966	2092	59		

- 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 RPABC2.

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	191	Total	C	N	O	S	0	0
			1544	1007	250	281	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	42	Total	C	N	O	S	0	0
			321	204	47	64	6		

- 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	63	Total	C	N	O	0	0
			390	243	73	74		

- Molecule 18 is a DNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	23	Total	C	N	O	P	0	0
			470	224	85	138	23		

- Molecule 19 is a DNA chain called NON-TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	15	Total	C	N	O	P	0	0
			309	148	56	90	15		

- Molecule 20 is a RNA chain called TEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	9	Total	C	N	O	P	0	0
			195	87	39	60	9		

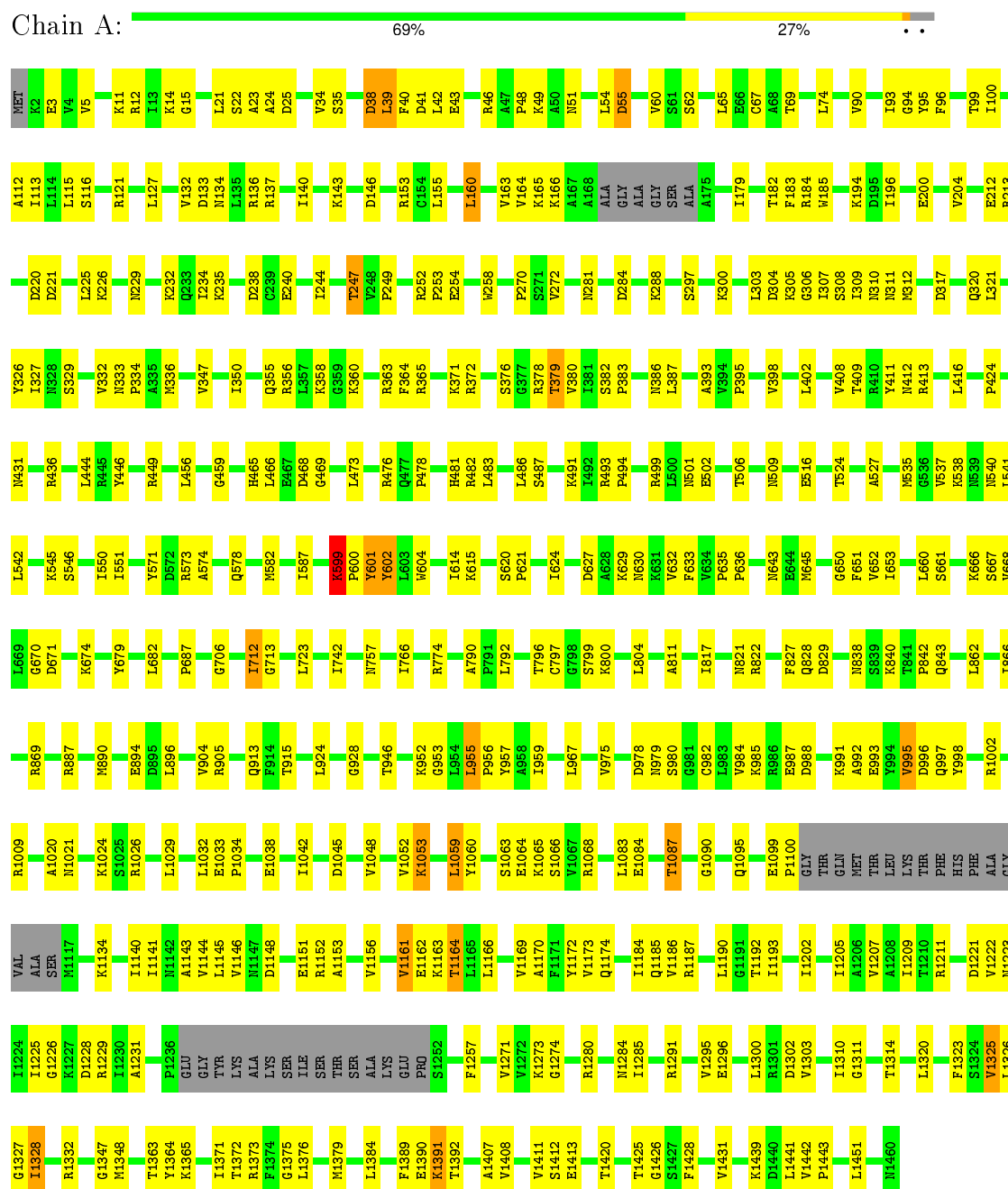
- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

### 3 Residue-property plots

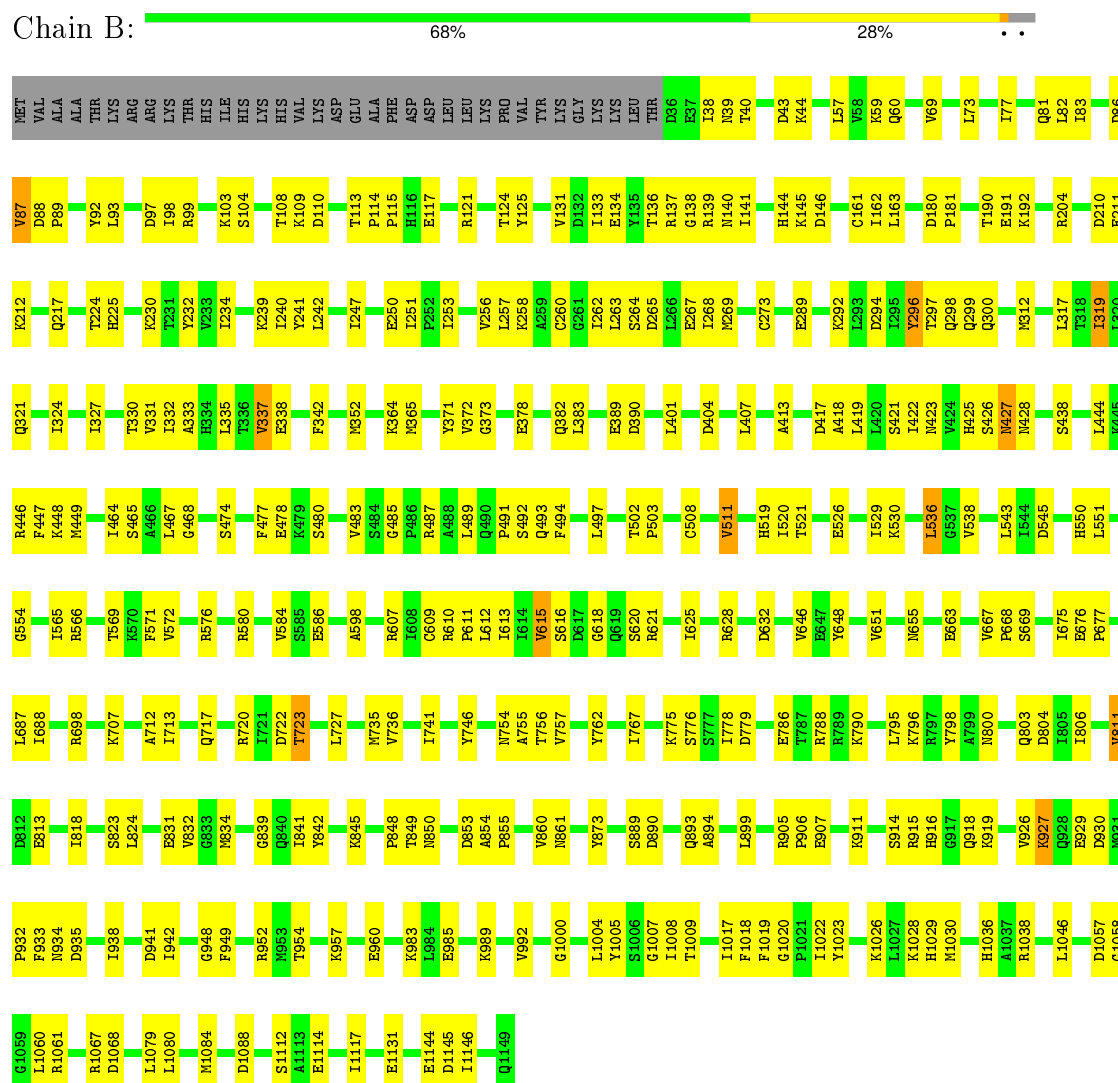
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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 III SUBUNIT RPC1

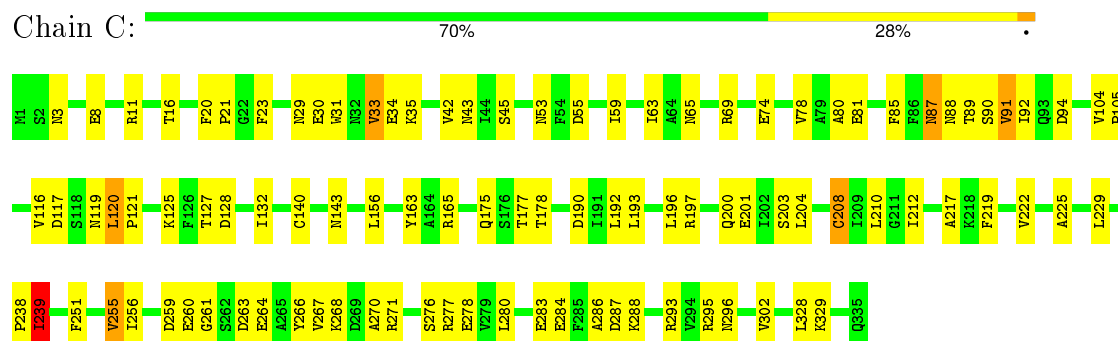




• Molecule 2: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC2



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

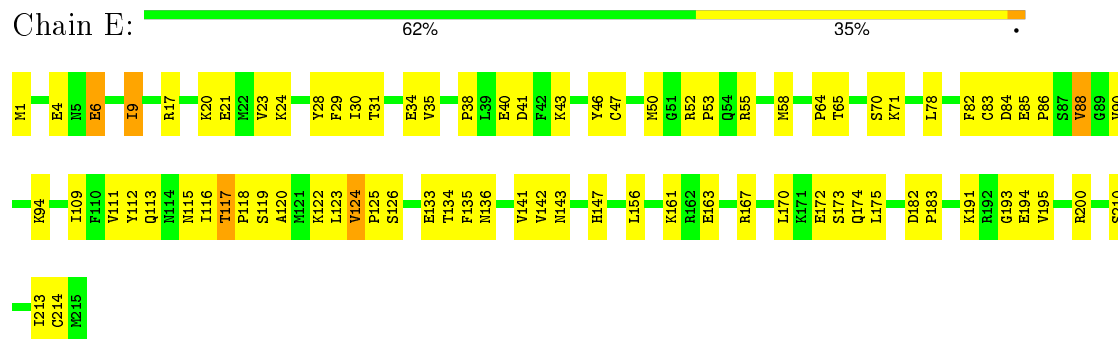


• Molecule 4: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC9

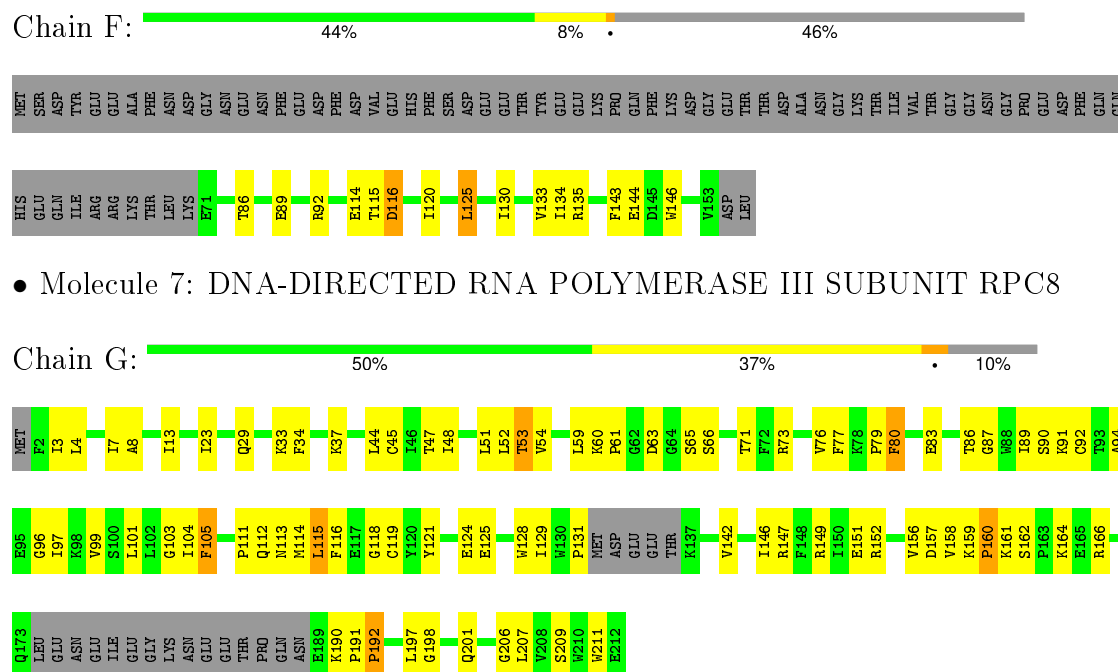




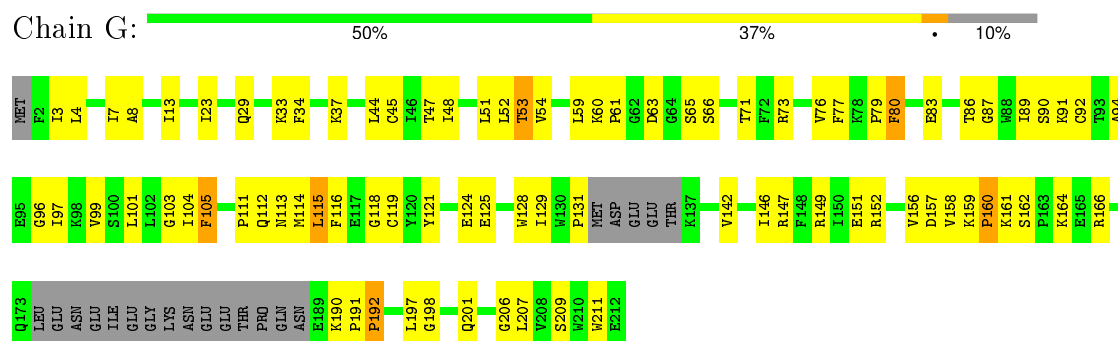
- Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



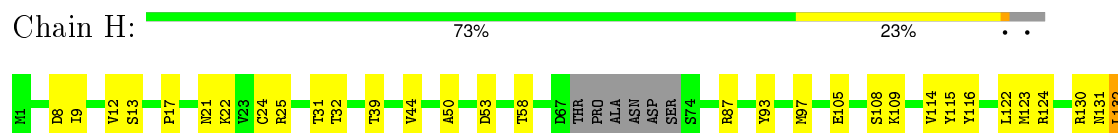
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2



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

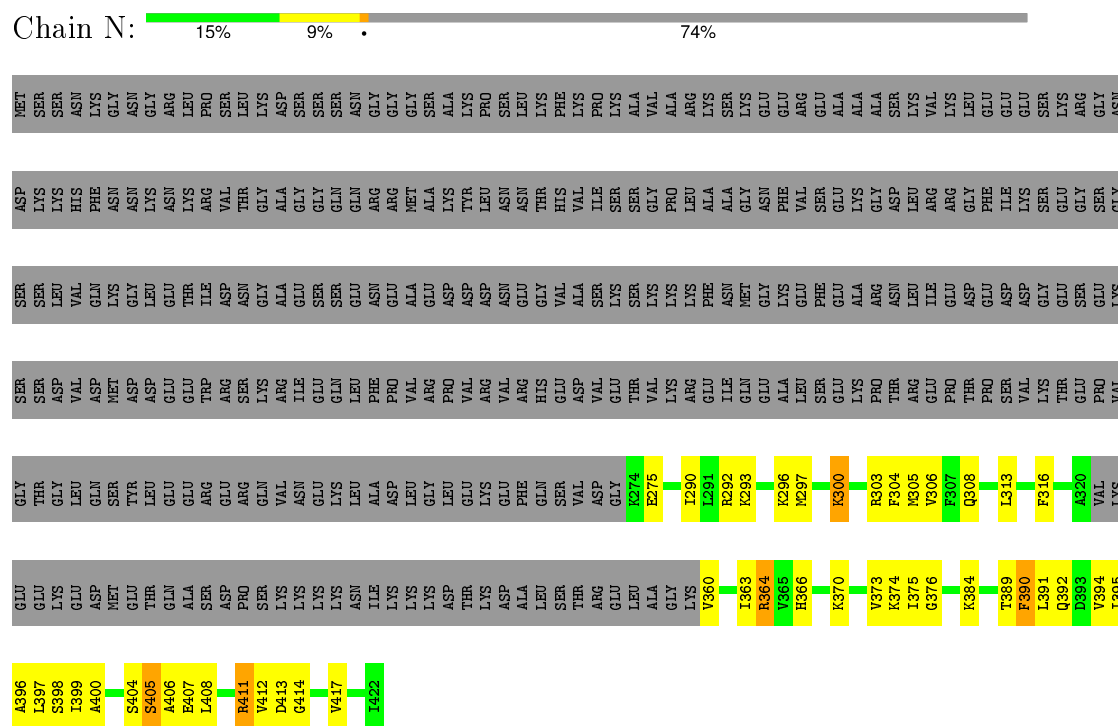


- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

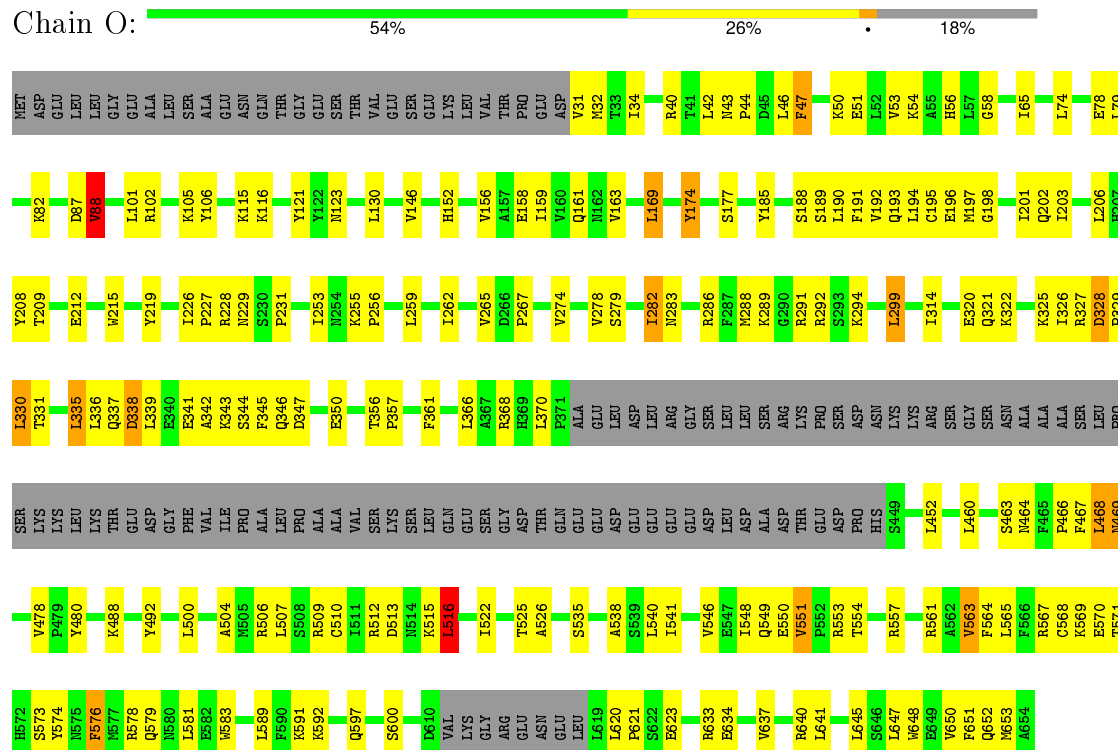




• Molecule 14: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC4

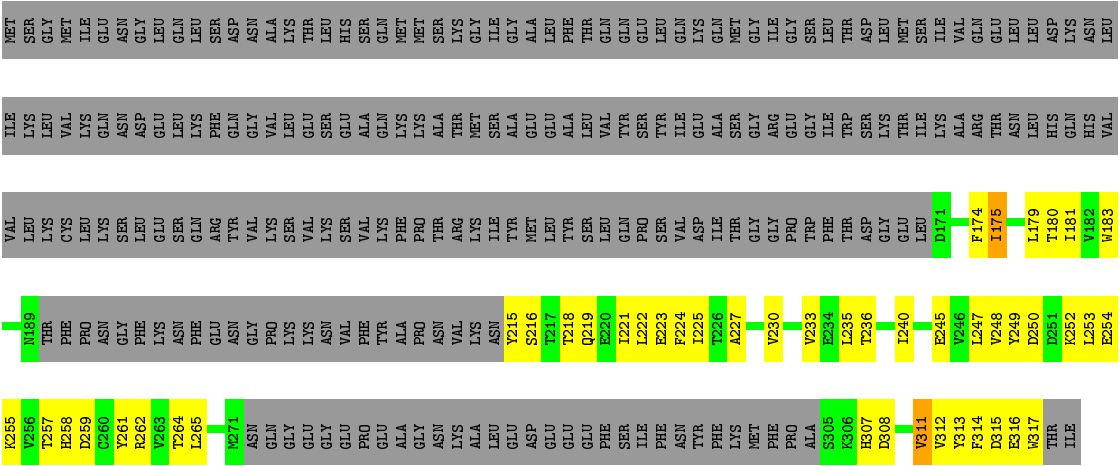


• Molecule 15: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC3



• Molecule 16: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC6

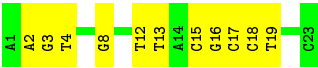




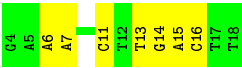
• Molecule 17: DNA-DIRECTED RNA POLYMERASE III SUBUNIT RPC7



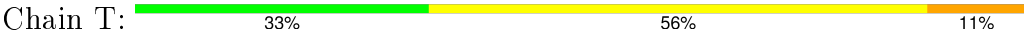
• Molecule 18: RNA



• Molecule 19: NON-TEMPLATE DNA



• Molecule 20: TEMPLATE DNA



## 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 ( $e^-/\text{\AA}^2$ )	45	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	0/11328	0.47	0/15303
10	J	0.21	0/558	0.45	0/750
11	K	0.22	0/803	0.43	0/1083
12	L	0.24	0/360	0.49	0/478
13	M	0.23	0/1369	0.46	0/1851
14	N	0.26	0/855	0.56	0/1149
15	O	0.23	0/4394	0.50	1/5928 (0.0%)
16	P	0.28	0/750	0.53	0/1017
17	Q	0.27	0/219	0.44	0/294
18	R	0.47	0/526	0.89	0/809
19	S	0.51	0/346	0.94	0/532
2	B	0.22	0/8943	0.45	0/12068
20	T	0.13	0/218	0.69	0/338
3	C	0.23	0/2711	0.46	1/3676 (0.0%)
4	D	0.23	0/991	0.51	0/1328
5	E	0.23	0/1795	0.45	0/2416
6	F	0.21	0/683	0.42	0/923
7	G	0.23	0/1583	0.49	0/2146
8	H	0.21	0/1138	0.45	0/1540
9	I	0.30	0/328	0.48	0/445
All	All	0.23	0/39898	0.49	2/54074 (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
11	K	0	1
14	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	120	LEU	CA-CB-CG	5.32	127.52	115.30
15	O	516	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	ASP	Peptide
1	A	599	LYS	Peptide
1	A	601	TYR	Peptide
2	B	319	ILE	Peptide
2	B	839	GLY	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	A	11130	0	11258	310	0
2	B	8788	0	8902	246	0
3	C	2655	0	2628	73	0
4	D	977	0	983	35	0
5	E	1759	0	1788	53	0
6	F	671	0	692	12	0
7	G	1544	0	1540	66	0
8	H	1120	0	1089	24	0
9	I	321	0	304	11	0
10	J	549	0	560	13	0
11	K	792	0	790	22	0
12	L	358	0	381	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1338	0	1307	41	0
14	N	845	0	891	36	0
15	O	4329	0	4497	168	0
16	P	738	0	719	41	0
17	Q	390	0	269	5	0
18	R	470	0	260	12	0
19	S	309	0	171	6	0
20	T	195	0	100	2	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
All	All	39284	0	39129	1053	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 1053 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:1163:LYS:HZ1	1:A:1280:ARG:HA	1.36	0.91
1:A:829:ASP:OD2	1:A:838:ASN:ND2	2.03	0.91
1:A:615:LYS:NZ	1:A:620:SER:O	2.05	0.88
4:D:126:GLN:HG3	4:D:127:LEU:HG	1.56	0.88
3:C:16:THR:O	3:C:295:ARG:NH1	2.07	0.87

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	1414/1460 (97%)	1166 (82%)	234 (16%)	14 (1%)	19	64
2	B	1112/1149 (97%)	943 (85%)	160 (14%)	9 (1%)	24	68
3	C	333/335 (99%)	284 (85%)	44 (13%)	5 (2%)	13	57
4	D	113/161 (70%)	83 (74%)	30 (26%)	0	100	100
5	E	213/215 (99%)	172 (81%)	39 (18%)	2 (1%)	21	65
6	F	81/155 (52%)	73 (90%)	8 (10%)	0	100	100
7	G	185/212 (87%)	155 (84%)	24 (13%)	6 (3%)	5	43
8	H	136/146 (93%)	115 (85%)	21 (15%)	0	100	100
9	I	40/110 (36%)	33 (82%)	6 (15%)	1 (2%)	7	48
10	J	65/70 (93%)	53 (82%)	11 (17%)	1 (2%)	13	57
11	K	99/142 (70%)	84 (85%)	15 (15%)	0	100	100
12	L	43/70 (61%)	34 (79%)	9 (21%)	0	100	100
13	M	160/282 (57%)	138 (86%)	20 (12%)	2 (1%)	15	59
14	N	106/422 (25%)	82 (77%)	23 (22%)	1 (1%)	21	65
15	O	533/654 (82%)	437 (82%)	89 (17%)	7 (1%)	15	59
16	P	83/317 (26%)	54 (65%)	24 (29%)	5 (6%)	2	27
17	Q	26/104 (25%)	23 (88%)	2 (8%)	1 (4%)	4	38
All	All	4742/6004 (79%)	3929 (83%)	759 (16%)	54 (1%)	23	63

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ILE
1	A	1371	ILE
13	M	97	VAL
13	M	107	ILE
15	O	88	VAL

### 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	1231/1257 (98%)	1213 (98%)	18 (2%)	72	89
2	B	975/1006 (97%)	960 (98%)	15 (2%)	72	89
3	C	296/296 (100%)	289 (98%)	7 (2%)	57	82
4	D	110/145 (76%)	107 (97%)	3 (3%)	52	80
5	E	197/197 (100%)	192 (98%)	5 (2%)	55	82
6	F	73/137 (53%)	70 (96%)	3 (4%)	37	73
7	G	170/190 (90%)	167 (98%)	3 (2%)	66	87
8	H	123/128 (96%)	121 (98%)	2 (2%)	70	88
9	I	38/98 (39%)	37 (97%)	1 (3%)	54	81
10	J	62/65 (95%)	60 (97%)	2 (3%)	46	78
11	K	91/130 (70%)	91 (100%)	0	100	100
12	L	40/57 (70%)	38 (95%)	2 (5%)	30	68
13	M	142/249 (57%)	136 (96%)	6 (4%)	36	72
14	N	92/360 (26%)	88 (96%)	4 (4%)	35	72
15	O	495/593 (84%)	477 (96%)	18 (4%)	42	76
16	P	86/285 (30%)	85 (99%)	1 (1%)	78	90
17	Q	24/56 (43%)	24 (100%)	0	100	100
All	All	4245/5249 (81%)	4155 (98%)	90 (2%)	64	85

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	29	TRP
6	F	133	VAL
15	O	468	LEU
4	D	127	LEU
5	E	78	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	299	GLN
2	B	552	ASN
15	O	580	ASN
2	B	60	GLN
13	M	190	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	T	9/9 (100%)	2 (22%)	1 (11%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	T	8	G
20	T	10	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	T	7	A

## 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.