



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 22, 2018 – 11:49 AM EST

PDB ID : 6F40
EMDB ID: : EMD-4180
Title : RNA Polymerase III open complex
Authors : Vorlaender, M.K.; Khatter, H.; Wetzels, R.; Hagen, W.J.H.; Mueller, C.W.
Deposited on : 2017-11-29
Resolution : 3.70 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

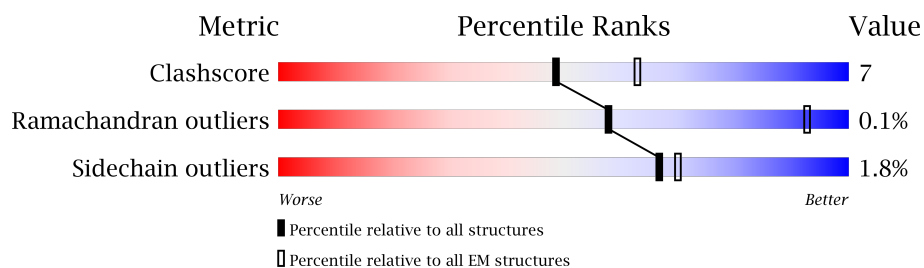
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.







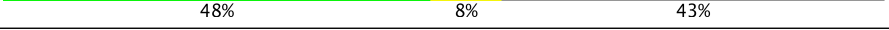

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	
2	B	1149	
3	C	335	
4	D	161	
5	E	215	
6	F	155	
7	G	212	
8	H	146	
9	I	110	

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Mol	Chain	Length	Quality of chain
10	J	70	 81% 14% .
11	K	142	 58% 13% 29%
12	L	70	 54% 10% 36%
13	M	282	 51% 14% 35%
14	N	422	 19% 5% 75%
15	O	654	 64% 17% . 18%
16	P	317	 61% 16% . 22%
17	Q	251	 12% . 86%
18	U	240	 52% 23% 25%
19	V	596	 48% 8% 43%
20	W	594	 28% 8% 63%
21	X	81	 57% 12% 31%
22	Y	81	 57% 14% 30%

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 47396 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	1398	Total	C	N	O	S	0	0
			10972	6919	1936	2059	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 RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1751	1111	309	320	11		

- 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	180	Total	C	N	O	S	0	0
			1448	950	231	261	6		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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	34	Total	C	N	O	S	0	0
			255	161	39	49	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	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 RPABC4.

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	183	Total	C	N	O	S	0	0
			1484	942	257	283	2		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	104	Total	C	N	O	S	0	0
			797	505	143	146	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	534	Total	C	N	O	S	0	0
			4293	2733	736	806	18		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	246	Total	C	N	O	S	0	0
			1990	1276	326	377	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	35	Total	C	N	O	0	0
			273	181	45	47		

- Molecule 18 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 19 is a protein called Transcription factor IIIB 70 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	337	Total	C	N	O	S	0	0
			2686	1682	486	504	14		

- Molecule 20 is a protein called Transcription factor TFIIB component B”.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	218	Total	C	N	O	S	0	0
			1798	1131	319	339	9		

- Molecule 21 is a DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	56	Total	C	N	O	P	0	0
			1137	549	186	346	56		

- Molecule 22 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	57	Total	C	N	O	P	0	0
			1179	563	226	333	57		

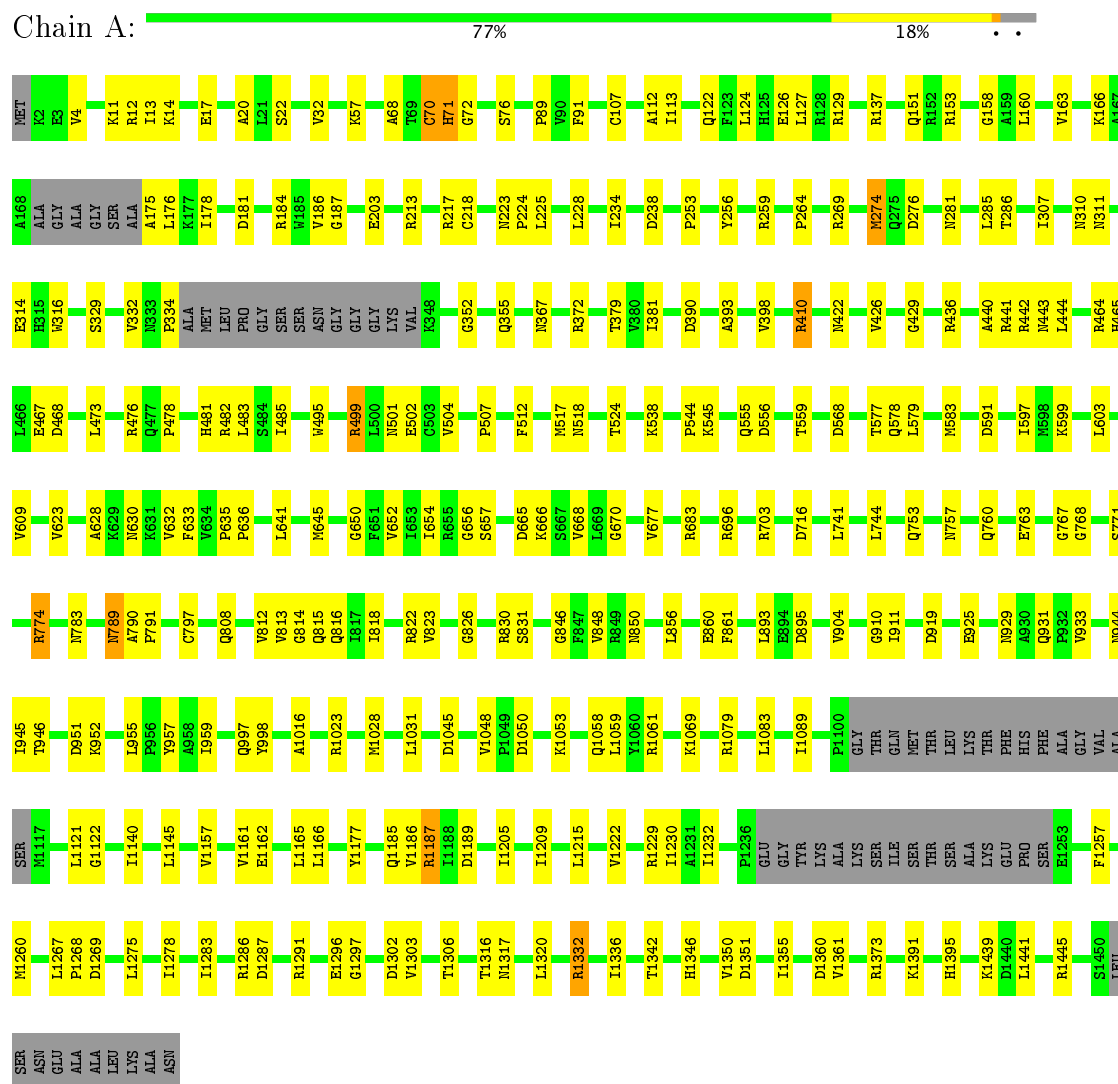
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

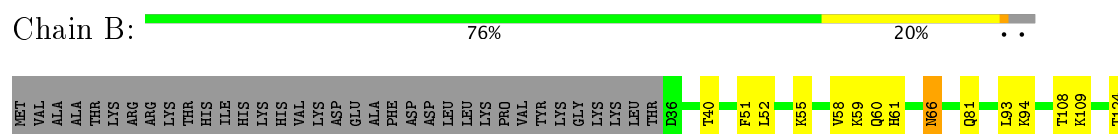
3 Residue-property plots

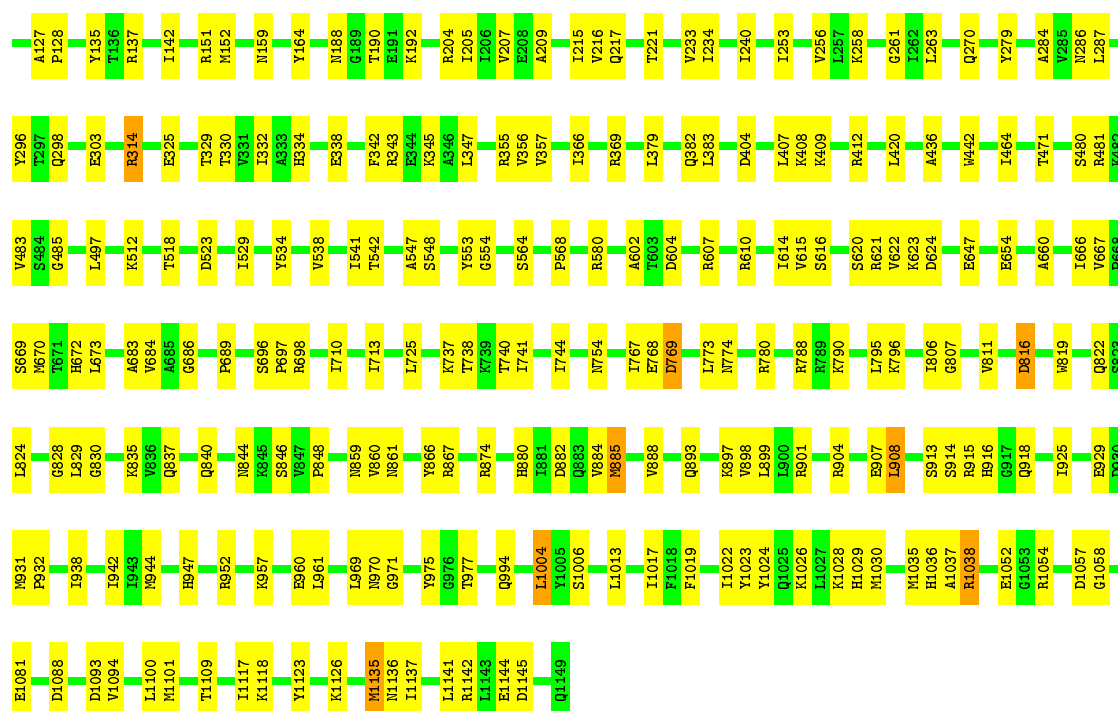
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



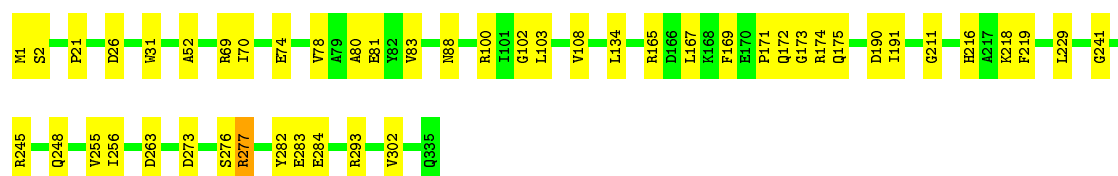
- Molecule 2: DNA-directed RNA polymerase III subunit RPC2





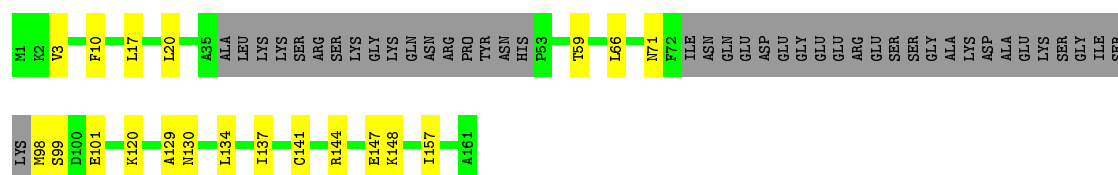
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 86% 14%



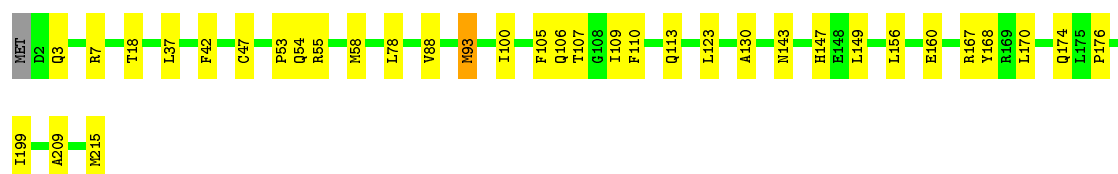
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

Chain D: 61% 12% 26%



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

Chain E: 83% 16%

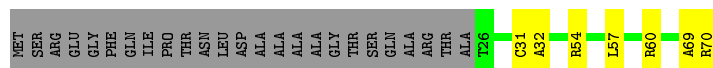


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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | THR | GLU | ASP | ILE | GLU | GLN | LYS | THR | THR | ALA | THR | VAL | GLU | GLN | PRO | GLN | GLU | GLU | GLU | GLU | GLN | ASP | VAL | ASP | MET | THR | THR | GLY | ASP | GLU | GLU | GLN | GLU | GLU | GLU | GLU | GLU | P42 | S65 | E56 | D57 | G58 | S62 | T71 | N74 | R77 | K82 | F88 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



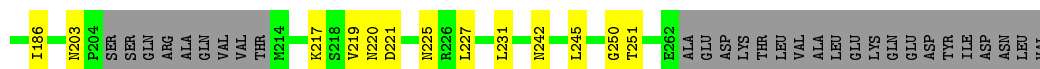
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 54% 10% 36%



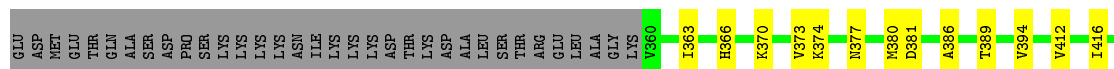
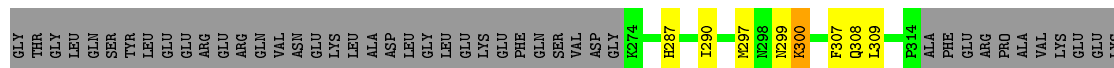
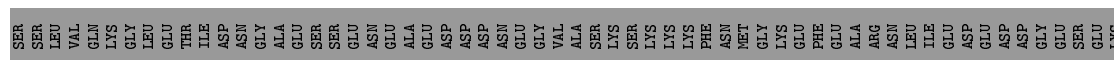
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5

Chain M: 51% 14% 35%



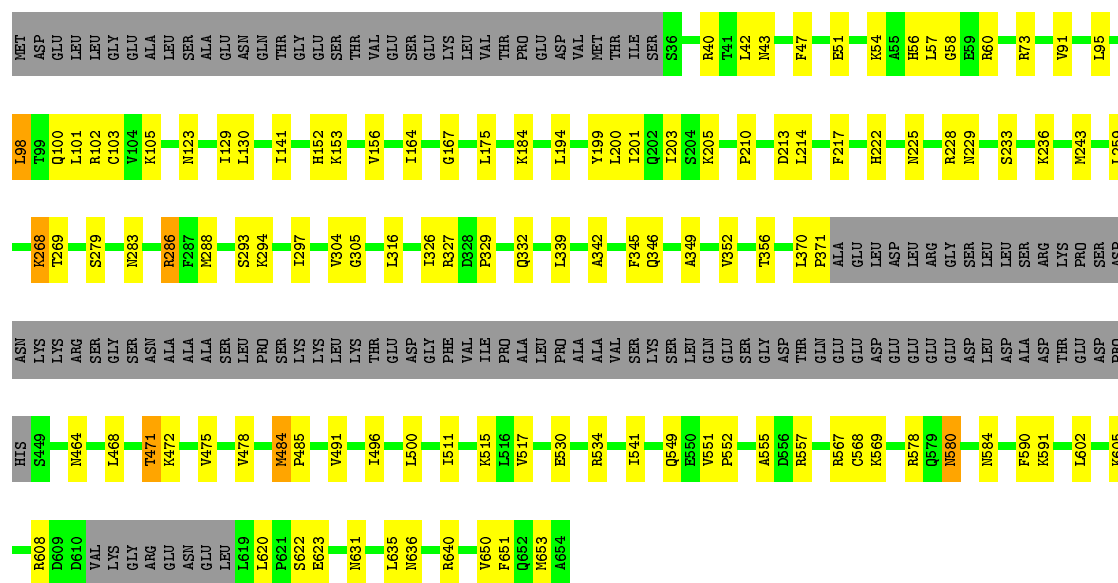
- Molecule 14: DNA-directed RNA polymerase III subunit RPC4

Chain N: 19% 5% 75%



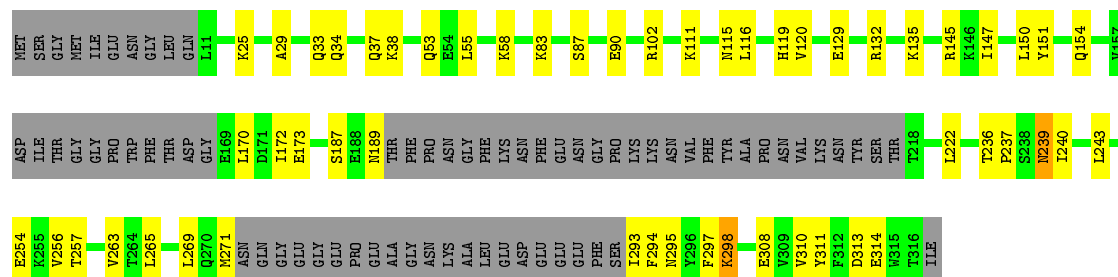
- Molecule 15: DNA-directed RNA polymerase III subunit RPC3

Chain O: 64% 17% 18%



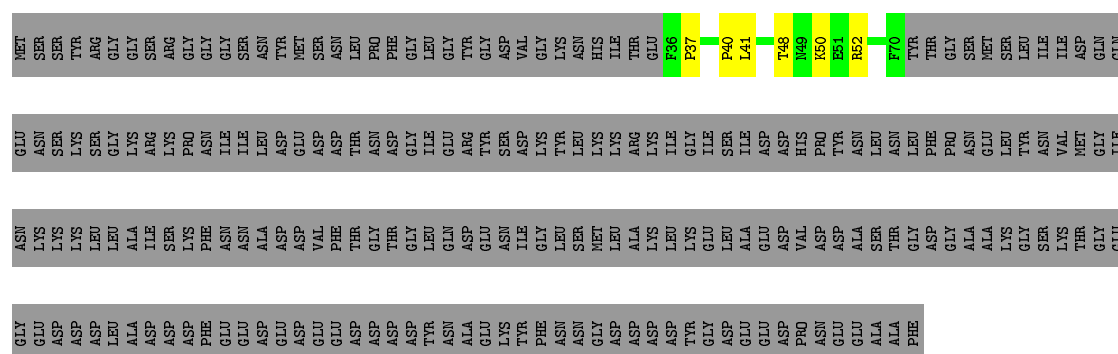
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6

Chain P: 61% 16% 22%



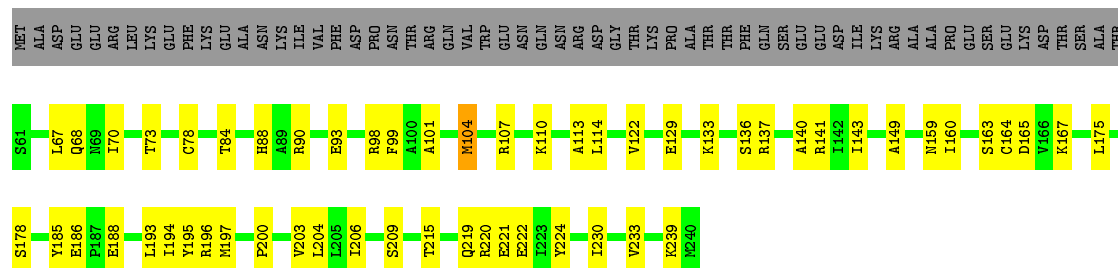
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

Chain Q: 12% 86%



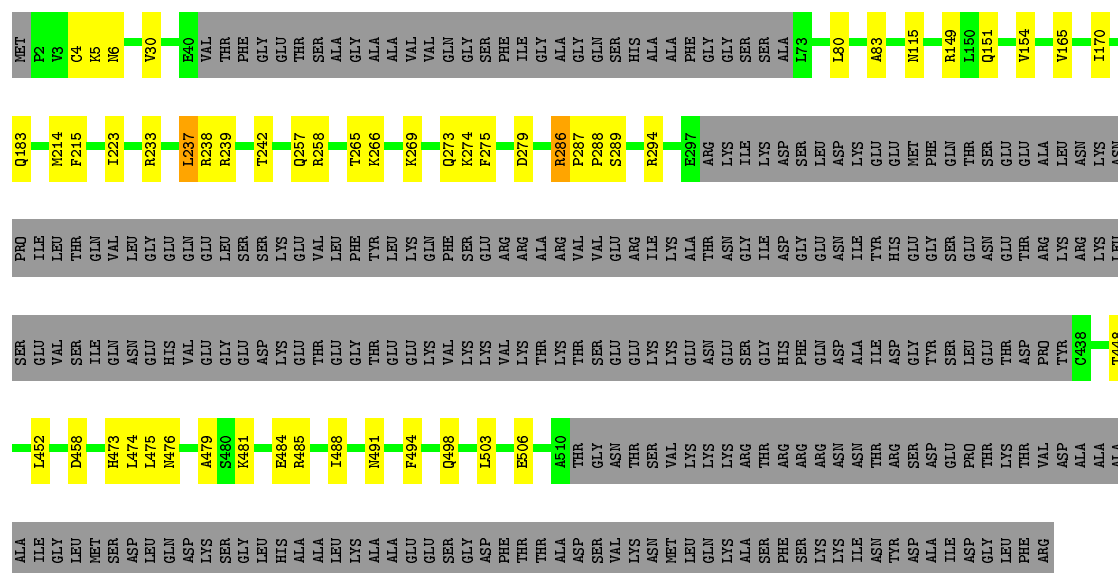
• Molecule 18: TATA-box-binding protein

Chain U: 52% 23% 25%



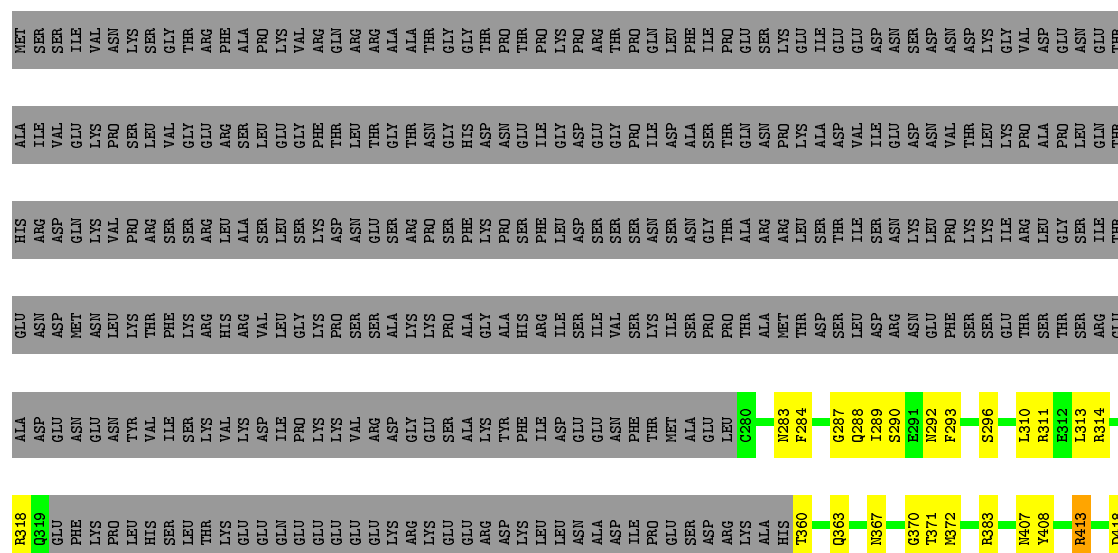
• Molecule 19: Transcription factor IIIB 70 kDa subunit

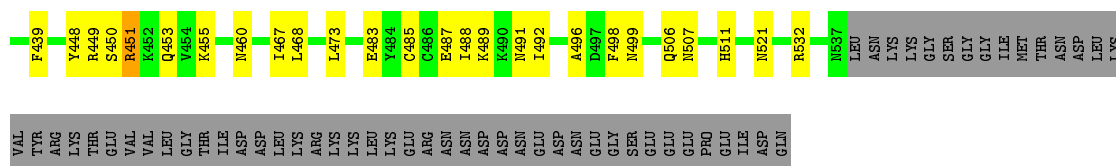
Chain V: 48% 8% 43%



• Molecule 20: Transcription factor TFIIB component B"

Chain W: 28% 8% 63%

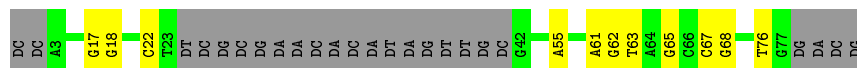




- Molecule 21: Non-Template DNA



- Molecule 22: Template DNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.9	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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	0.24	0/11168	0.47	0/15086
10	J	0.23	0/558	0.43	0/750
11	K	0.23	0/803	0.44	0/1083
12	L	0.22	0/360	0.47	0/478
13	M	0.24	0/1518	0.47	0/2054
14	N	0.23	0/805	0.48	0/1081
15	O	0.23	0/4358	0.45	1/5879 (0.0%)
16	P	0.23	0/2020	0.47	0/2718
17	Q	0.26	0/281	0.45	0/381
18	U	0.25	0/1443	0.47	0/1942
19	V	0.23	0/2728	0.44	0/3676
2	B	0.24	0/8943	0.47	0/12068
20	W	0.23	0/1831	0.42	0/2454
21	X	0.55	0/1268	1.06	0/1951
22	Y	0.56	0/1326	0.96	0/2043
3	C	0.25	0/2711	0.47	0/3676
4	D	0.23	0/991	0.42	0/1328
5	E	0.24	0/1787	0.45	0/2406
6	F	0.23	0/683	0.44	0/923
7	G	0.24	0/1486	0.45	0/2017
8	H	0.24	0/1138	0.52	0/1540
9	I	0.25	0/261	0.57	0/354
All	All	0.26	0/48467	0.51	1/65888 (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	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	471	THR	C-N-CA	6.69	138.43	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	CYS	Peptide
2	B	1057	ASP	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10972	0	11096	177	0
2	B	8788	0	8901	160	0
3	C	2655	0	2628	32	0
4	D	977	0	983	9	0
5	E	1751	0	1776	23	0
6	F	671	0	692	6	0
7	G	1448	0	1446	23	0
8	H	1120	0	1089	19	0
9	I	255	0	243	8	0
10	J	549	0	559	7	0
11	K	792	0	790	12	0
12	L	358	0	384	6	0
13	M	1484	0	1448	25	0
14	N	797	0	846	13	0
15	O	4293	0	4456	70	0
16	P	1990	0	2030	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	273	0	285	6	0
18	U	1416	0	1493	37	0
19	V	2686	0	2704	42	0
20	W	1798	0	1789	39	0
21	X	1137	0	642	8	0
22	Y	1179	0	644	9	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	V	1	0	0	0	0
All	All	47396	0	46924	659	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 7.

The worst 5 of 659 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)
20:W:371:THR:HG22	20:W:372:MET:HG3	1.68	0.76
2:B:667:VAL:HG12	2:B:669:SER:H	1.51	0.74
13:M:164:LYS:HB3	13:M:167:GLN:HB2	1.70	0.74
1:A:181:ASP:OD2	1:A:184:ARG:NH2	2.21	0.73
5:E:170:LEU:HB2	5:E:174:GLN:HE21	1.51	0.73

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	1388/1460 (95%)	1211 (87%)	176 (13%)	1 (0%)	55	88
2	B	1112/1149 (97%)	980 (88%)	131 (12%)	1 (0%)	55	88
3	C	333/335 (99%)	296 (89%)	37 (11%)	0	100	100
4	D	113/161 (70%)	100 (88%)	13 (12%)	0	100	100
5	E	212/215 (99%)	191 (90%)	21 (10%)	0	100	100
6	F	81/155 (52%)	72 (89%)	9 (11%)	0	100	100
7	G	174/212 (82%)	152 (87%)	21 (12%)	1 (1%)	28	70
8	H	136/146 (93%)	118 (87%)	18 (13%)	0	100	100
9	I	32/110 (29%)	25 (78%)	7 (22%)	0	100	100
10	J	65/70 (93%)	60 (92%)	5 (8%)	0	100	100
11	K	99/142 (70%)	94 (95%)	5 (5%)	0	100	100
12	L	43/70 (61%)	36 (84%)	7 (16%)	0	100	100
13	M	179/282 (64%)	161 (90%)	18 (10%)	0	100	100
14	N	100/422 (24%)	84 (84%)	16 (16%)	0	100	100
15	O	528/654 (81%)	493 (93%)	35 (7%)	0	100	100
16	P	238/317 (75%)	214 (90%)	24 (10%)	0	100	100
17	Q	33/251 (13%)	29 (88%)	4 (12%)	0	100	100
18	U	178/240 (74%)	163 (92%)	15 (8%)	0	100	100
19	V	331/596 (56%)	302 (91%)	29 (9%)	0	100	100
20	W	214/594 (36%)	194 (91%)	20 (9%)	0	100	100
All	All	5589/7581 (74%)	4975 (89%)	611 (11%)	3 (0%)	58	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	769	ASP
1	A	71	HIS
7	G	79	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1214/1257 (97%)	1194 (98%)	20 (2%)	68	88
2	B	975/1006 (97%)	958 (98%)	17 (2%)	66	87
3	C	296/296 (100%)	294 (99%)	2 (1%)	87	94
4	D	110/145 (76%)	106 (96%)	4 (4%)	40	74
5	E	196/197 (100%)	193 (98%)	3 (2%)	70	88
6	F	73/137 (53%)	72 (99%)	1 (1%)	71	89
7	G	160/190 (84%)	158 (99%)	2 (1%)	73	89
8	H	123/128 (96%)	122 (99%)	1 (1%)	85	93
9	I	31/98 (32%)	31 (100%)	0	100	100
10	J	62/65 (95%)	62 (100%)	0	100	100
11	K	91/130 (70%)	90 (99%)	1 (1%)	78	90
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	160/249 (64%)	154 (96%)	6 (4%)	38	73
14	N	88/360 (24%)	86 (98%)	2 (2%)	56	82
15	O	490/593 (83%)	479 (98%)	11 (2%)	57	83
16	P	227/285 (80%)	222 (98%)	5 (2%)	57	83
17	Q	31/212 (15%)	31 (100%)	0	100	100
18	U	152/205 (74%)	147 (97%)	5 (3%)	43	76
19	V	295/513 (58%)	289 (98%)	6 (2%)	60	84
20	W	194/534 (36%)	189 (97%)	5 (3%)	51	80
All	All	5008/6657 (75%)	4917 (98%)	91 (2%)	67	86

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	120	LYS
11	K	74	ASN
19	V	286	ARG
4	D	130	ASN
6	F	90	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	71	ASN
12	L	53	HIS
19	V	140	HIS
4	D	130	ASN
7	G	113	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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.