



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:25 am GMT

PDB ID : 3J0K
EMDB ID: : EMD-5343
Title : Orientation of RNA polymerase II within the human VP16-Mediator-pol II-TFIIF assembly
Authors : Bernecky, C.; Grob, P.; Ebmeier, C.C.; Nogales, E.; Taatjes, D.J.
Deposited on : 2011-10-04
Resolution : 36.00 Å(reported)
Based on PDB ID : 1Y1V

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) : recalc29047

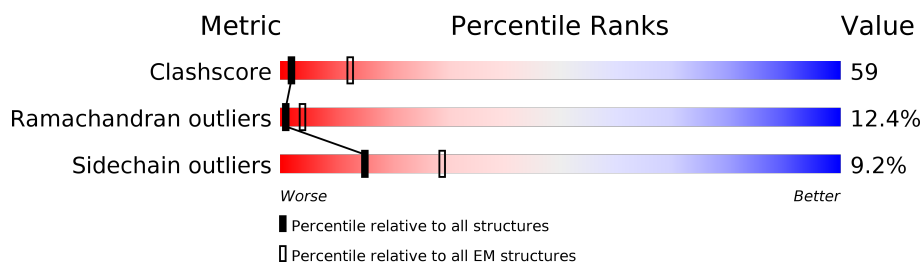
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 36.00 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	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	1455	
2	B	1224	
3	C	268	
4	D	221	
5	E	215	
6	F	84	
7	G	171	
8	H	146	
9	I	122	

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Mol	Chain	Length	Quality of chain
10	J	70	<div><div></div><div>20%54%17%7%</div></div>
11	K	120	<div><div></div><div>39%50%5%5%</div></div>
12	L	46	<div><div></div><div>9%63%26%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 31137 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 II largest subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0
			11214	7069	1959	2124	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1112	Total	C	N	O	S	0	0
			8837	5594	1548	1640	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	177	Total	C	N	O	S	0	0
			1356	840	241	273	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	114	Total	C	N	O	S	0	0
			919	590	156	171	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

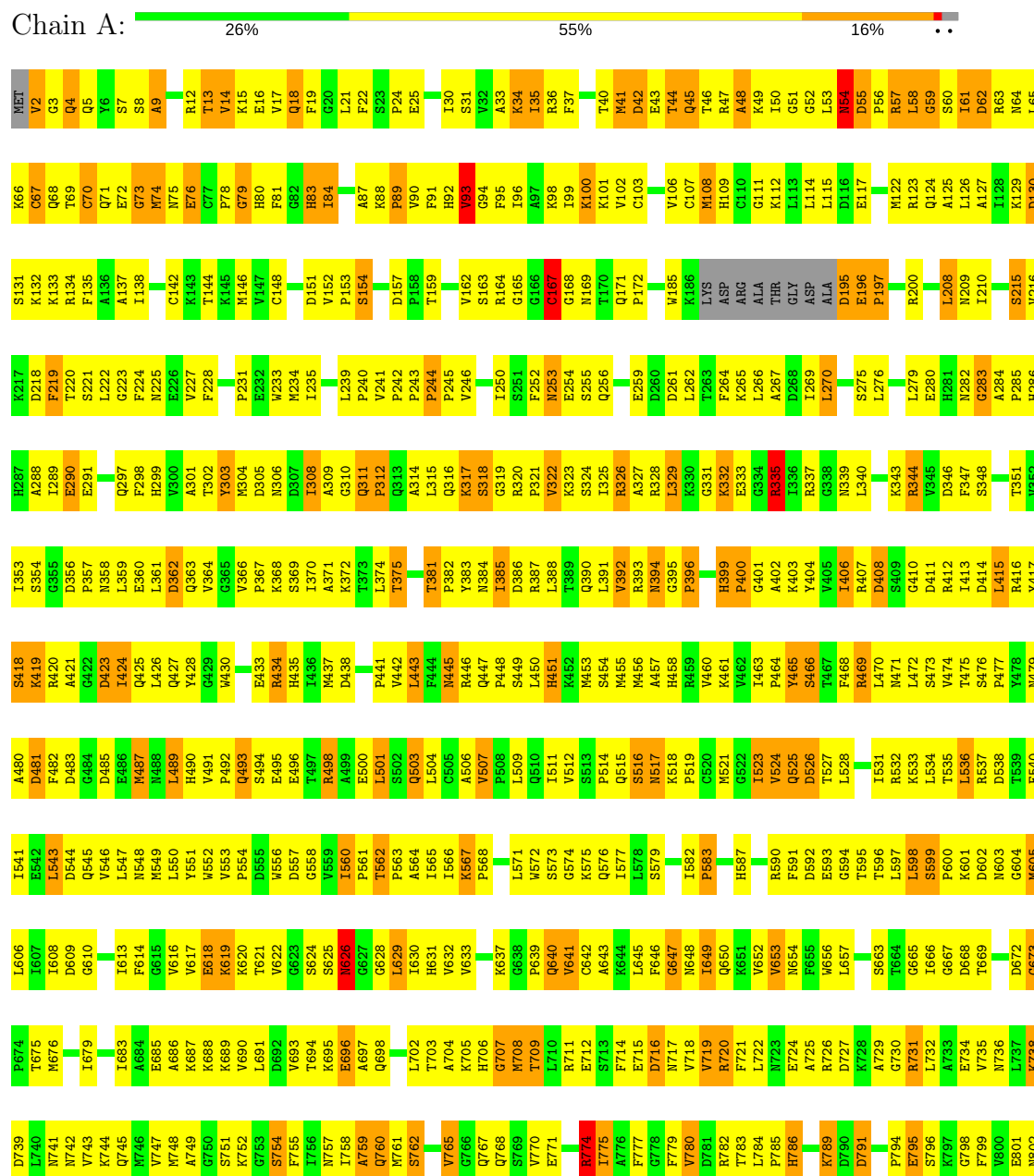
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

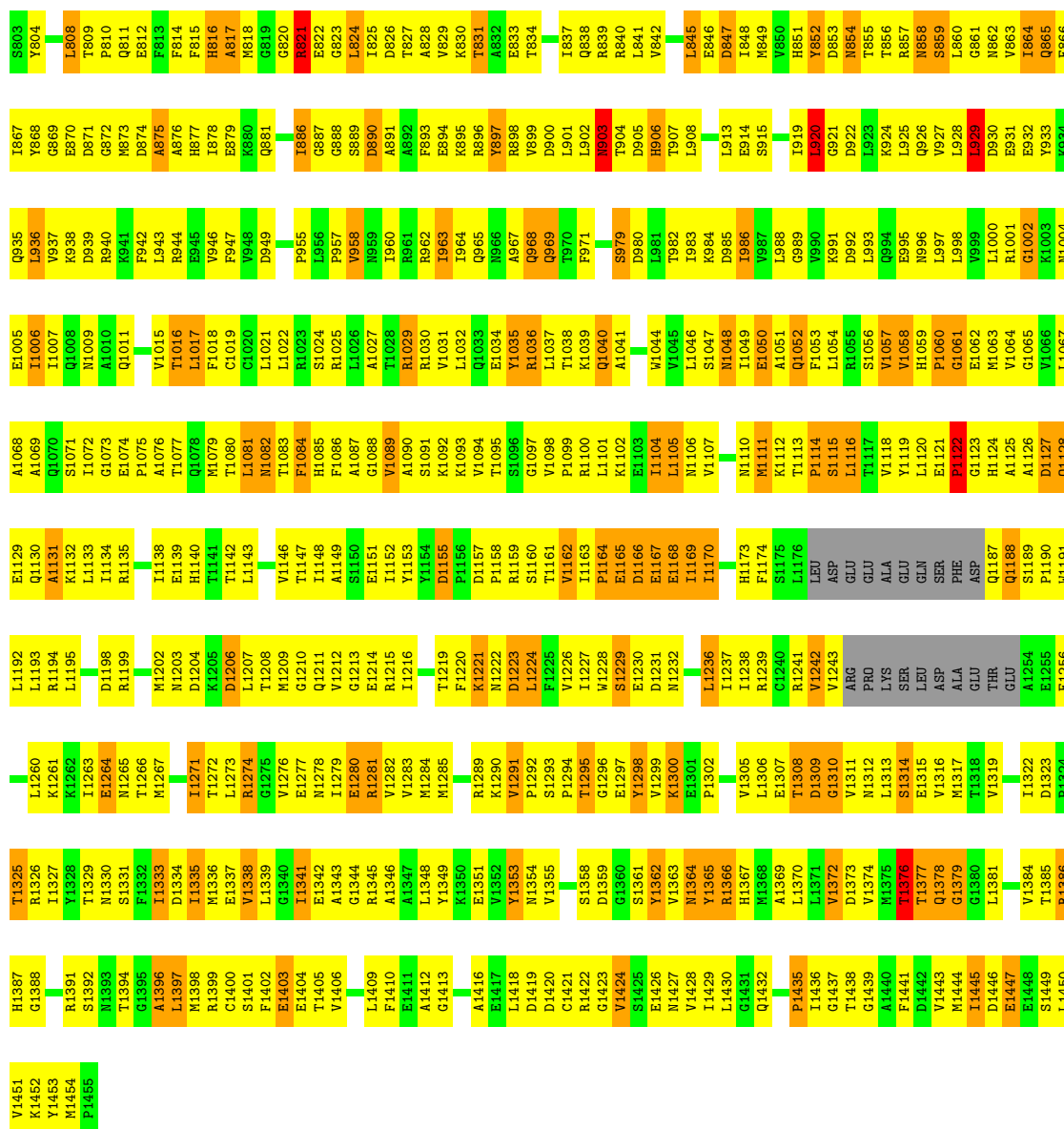
Mol	Chain	Residues	Atoms		AltConf
14	J	1	Total	Zn	0
			1	1	
14	B	1	Total	Zn	0
			1	1	
14	I	2	Total	Zn	0
			2	2	
14	C	1	Total	Zn	0
			1	1	
14	A	3	Total	Zn	0
			3	3	
14	L	1	Total	Zn	0
			1	1	

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.

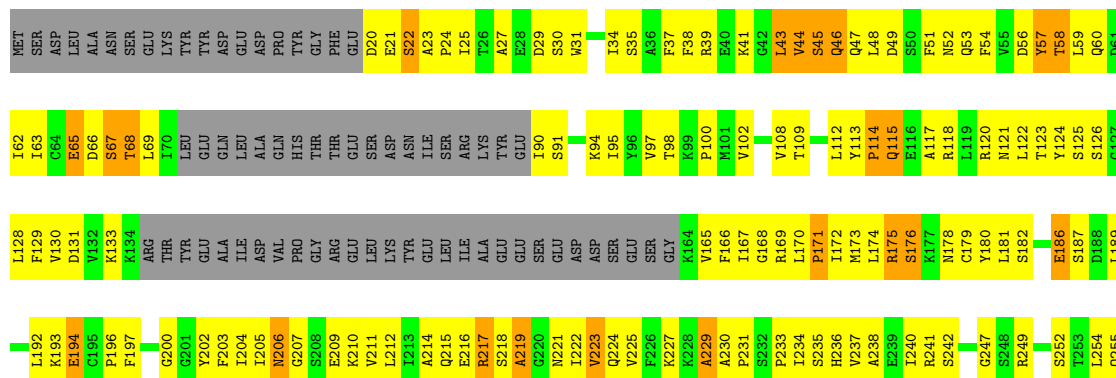
- Molecule 1: DNA-directed RNA polymerase II largest subunit



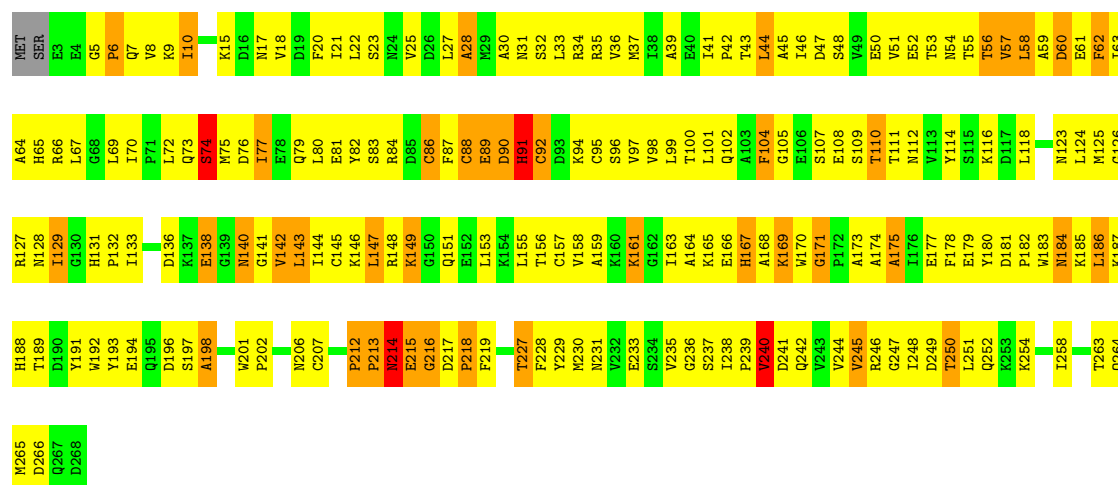


• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

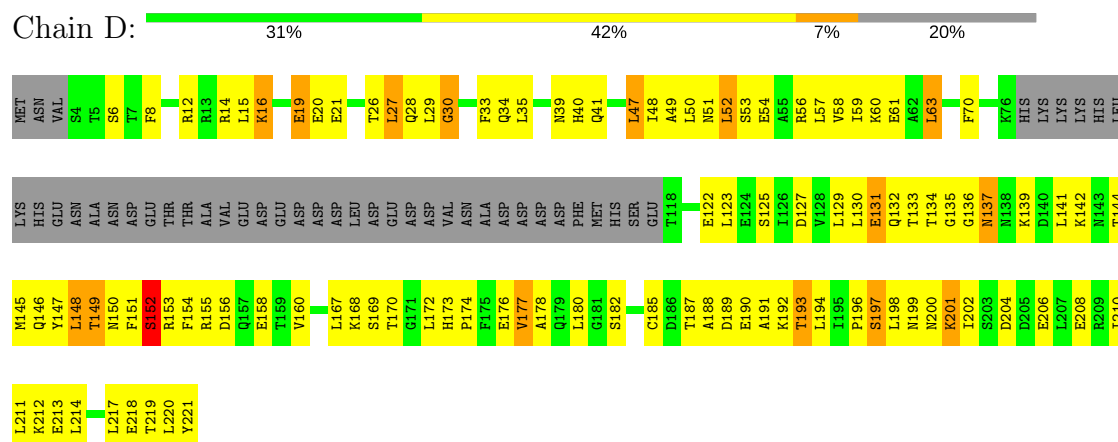
Chain B: 25% 52% 13% 9%



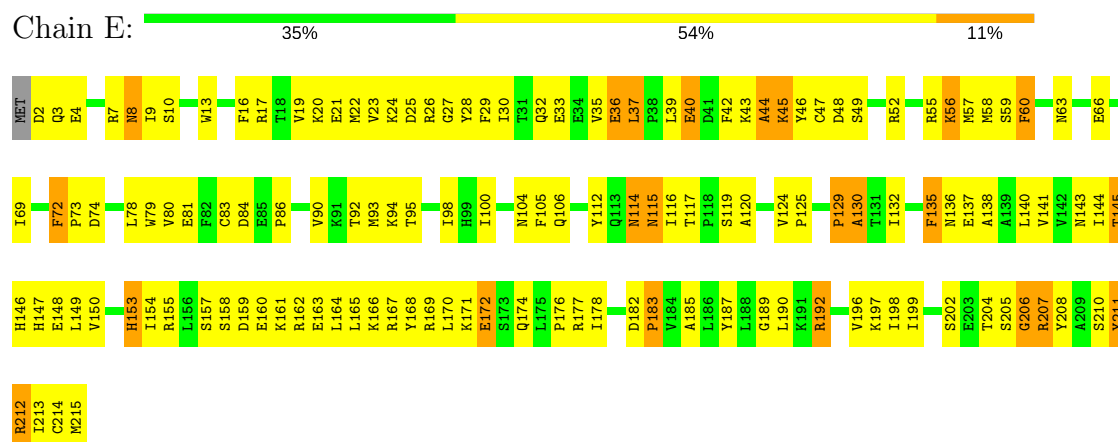




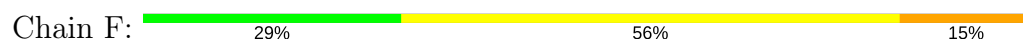
- Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide

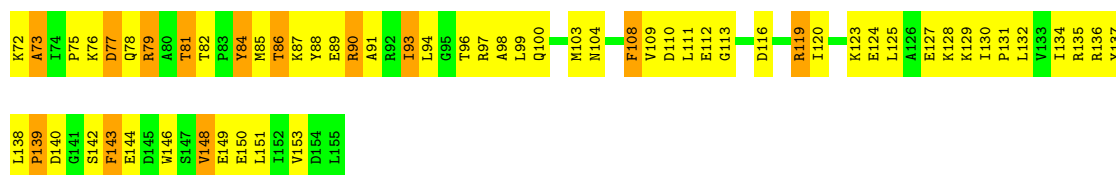


- Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



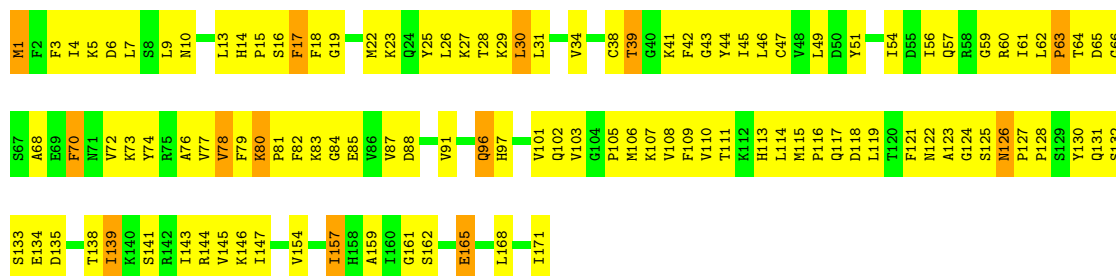
- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide





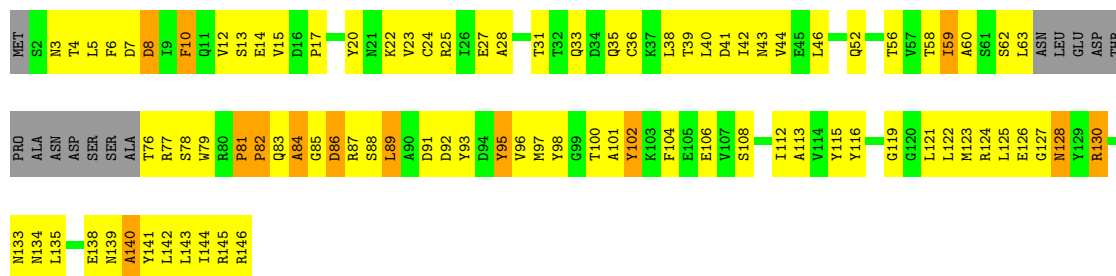
• Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

Chain G: 33% 59% 8%



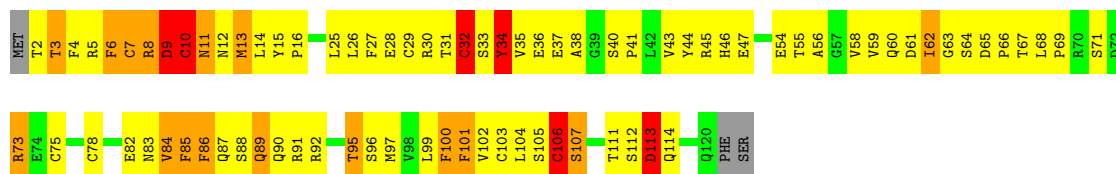
• Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H: 29% 53% 9% 9%



• Molecule 9: DNA-directed RNA polymerase II subunit 9

Chain I: 30% 49% 13% 5%

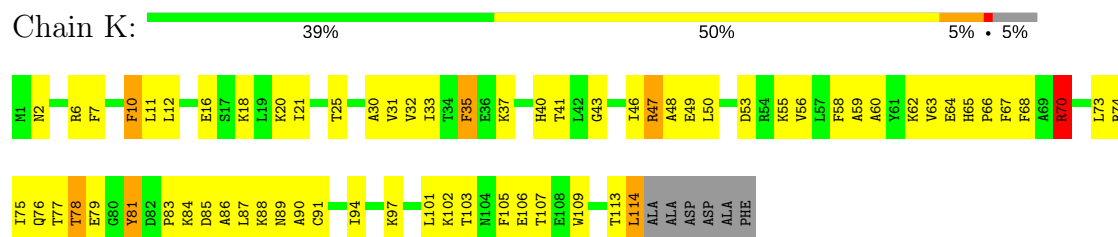


• Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10

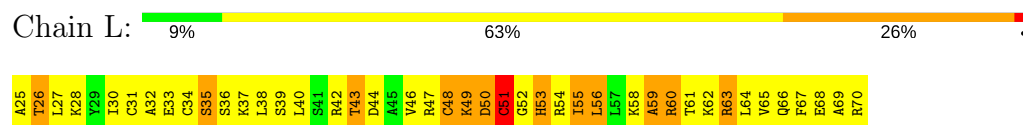
Chain J: 20% 54% 17% 7%



- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	3146	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	29000	Depositor
Image detector	Kodak SO-163 film	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, 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 > 2$	RMSZ	# $ Z > 2$
1	A	0.50	2/11417 (0.0%)	0.78	4/15442 (0.0%)
10	J	0.48	0/541	0.75	0/727
11	K	0.45	0/937	0.67	0/1265
12	L	0.54	0/366	0.79	0/485
2	B	0.52	4/9009 (0.0%)	0.76	8/12146 (0.1%)
3	C	0.48	0/2133	0.77	1/2891 (0.0%)
4	D	0.41	0/1365	0.64	0/1837
5	E	0.43	0/1788	0.66	0/2406
6	F	0.52	0/691	0.77	0/933
7	G	0.49	0/1368	0.72	0/1844
8	H	0.38	0/1086	0.65	1/1470 (0.1%)
9	I	0.46	0/989	0.77	1/1331 (0.1%)
All	All	0.49	6/31690 (0.0%)	0.75	15/42777 (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
2	B	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	467	GLY	C-O	-11.91	1.04	1.23
2	B	468	GLU	CB-CG	8.45	1.68	1.52
2	B	510	LYS	CB-CG	5.58	1.67	1.52
1	A	195	ASP	N-CA	5.49	1.57	1.46
2	B	468	GLU	CG-CD	5.21	1.59	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASP	N-CA-C	9.36	136.28	111.00
2	B	510	LYS	CB-CA-C	-7.65	95.10	110.40
2	B	510	LYS	C-N-CD	-7.45	104.21	120.60
3	C	92	CYS	CA-CB-SG	-6.78	101.80	114.00
1	A	1310	GLY	N-CA-C	-6.49	96.88	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	833	TYR	Sidechain

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	A	11214	0	11281	1475	0
2	B	8837	0	8871	1203	0
3	C	2095	0	2052	263	0
4	D	1356	0	1319	106	0
5	E	1752	0	1776	189	0
6	F	679	0	701	84	0
7	G	1340	0	1357	161	0
8	H	1068	0	1040	120	0
9	I	971	0	929	113	0
10	J	532	0	542	110	0
11	K	919	0	929	97	0
12	L	364	0	387	68	0
13	A	1	0	0	0	0
14	A	3	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31137	0	31184	3684	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 59.

The worst 5 of 3684 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)
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.28	1.13
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.10	1.12
7:G:138:THR:HG22	7:G:139:ILE:H	1.11	1.11
1:A:913:LEU:HD12	1:A:914:GLU:H	1.15	1.11
6:F:82:THR:HG22	6:F:84:TYR:H	1.15	1.11

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	1418/1455 (98%)	914 (64%)	316 (22%)	188 (13%)	0	6
2	B	1096/1224 (90%)	725 (66%)	223 (20%)	148 (14%)	0	6
3	C	264/268 (98%)	169 (64%)	62 (24%)	33 (12%)	0	7
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	1	13
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	1	12
6	F	82/84 (98%)	60 (73%)	15 (18%)	7 (8%)	1	15
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1	19
8	H	129/146 (88%)	93 (72%)	25 (19%)	11 (8%)	1	15
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	2
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	3	29
12	L	44/46 (96%)	18 (41%)	14 (32%)	12 (27%)	0	0
All	All	3879/4142 (94%)	2570 (66%)	827 (21%)	482 (12%)	1	7

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP

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	1246/1270 (98%)	1133 (91%)	113 (9%)	11	38
2	B	964/1061 (91%)	880 (91%)	84 (9%)	12	40
3	C	234/236 (99%)	205 (88%)	29 (12%)	5	26
4	D	140/200 (70%)	126 (90%)	14 (10%)	9	33
5	E	196/197 (100%)	184 (94%)	12 (6%)	22	55
6	F	74/74 (100%)	63 (85%)	11 (15%)	3	20
7	G	152/152 (100%)	143 (94%)	9 (6%)	23	55
8	H	117/128 (91%)	110 (94%)	7 (6%)	22	55
9	I	113/116 (97%)	97 (86%)	16 (14%)	4	22
10	J	60/65 (92%)	55 (92%)	5 (8%)	13	43
11	K	99/102 (97%)	91 (92%)	8 (8%)	14	44
12	L	40/40 (100%)	33 (82%)	7 (18%)	2	14
All	All	3435/3641 (94%)	3120 (91%)	315 (9%)	15	37

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	582	VAL
2	B	1002	THR
9	I	100	PHE
2	B	635	ARG
2	B	830	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
2	B	835	GLN
9	I	12	ASN
2	B	366	GLN
2	B	518	HIS

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 10 ligands modelled in this entry, 10 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.