



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:26 PM BST

PDB ID : 5FMF  
EMDB ID: : EMD-3114  
Title : the P-lobe of RNA polymerase II pre-initiation complex  
Authors : Murakami, K.; Tsai, K.; Kalisman, N.; Bushnell, D.A.; Asturias, F.J.; Kornberg, R.D.  
Deposited on : 2015-11-03  
Resolution : 6.00 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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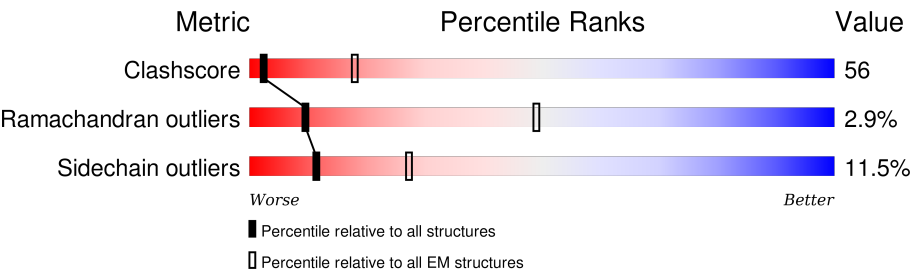
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 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 6.00 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.







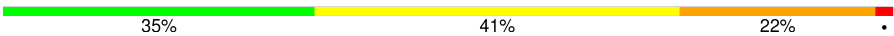

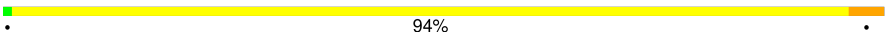

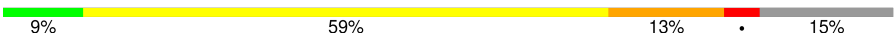

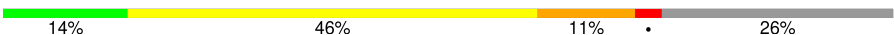
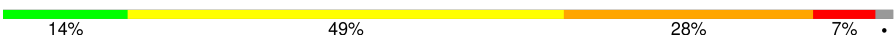
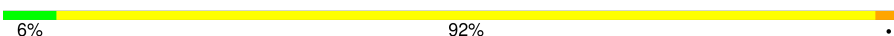




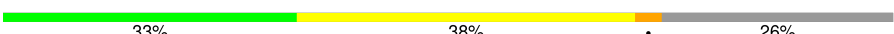
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	1	492	<div><div>35%</div><div>52%</div><div>8%</div><div>.</div><div>.</div></div>
2	2	174	<div><div>64%</div><div>28%</div><div>6%</div><div>.</div></div>
3	A	1733	<div><div>53%</div><div>24%</div><div>.</div><div>.</div><div>18%</div></div>
4	B	1224	<div><div>61%</div><div>29%</div><div>.</div><div>6%</div></div>
5	C	266	<div><div>73%</div><div>22%</div><div>5%</div></div>
6	D	178	<div><div>67%</div><div>26%</div><div>6%</div><div>.</div></div>
7	E	214	<div><div>74%</div><div>24%</div><div>.</div></div>
8	F	84	<div><div>60%</div><div>37%</div><div>.</div></div>
9	G	171	<div><div>67%</div><div>27%</div><div>5%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
10	H	146	
11	I	119	
12	J	65	
13	K	115	
14	L	46	
15	M	116	
16	N	72	
17	O	122	
18	P	345	
19	Q	180	
20	R	160	
21	S	123	
22	T	72	
23	U	150	
24	V	174	
25	W	62	
26	X	63	
27	Y	778	

## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 55363 atoms, of which 691 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 REPAIR HELICASE RAD25, SSL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	473	Total	C	N	O	S	0	0
			3797	2390	664	720	23		

- Molecule 2 is a protein called TRANSCRIPTION ELONGATION FACTOR S-II, DST1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	174	Total	C	N	O	S	0	104
			666	454	99	108	5		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1422	Total	C	N	O	S	0	0
			11174	7036	1954	2122	62		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1156	Total	C	N	O	S	0	0
			9140	5781	1606	1697	56		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 6 is a protein called RNA POLYMERASE II PRE-INITIATION COMPLEX, RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	178	Total	C	N	O	S	0	0
			1434	887	257	288	2		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1, RPB5.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2, RPB6.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3, RPB8.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5, RPB10.

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

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4, RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 15 is a protein called RNA POLYMERASE II PRE-INITIATION COMPLEX, TOA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	116	Total	C	N	O	S	0	0
			956	599	159	195	3		

- Molecule 16 is a DNA chain called NON-TEMPLATE STRAND DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	72	Total	C	N	O	P	0	0
			1500	711	300	417	72		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2, TOA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	101	Total	C	N	O	S	0	0
			792	500	132	156	4		

- Molecule 18 is a protein called TRANSCRIPTION INITIATION FACTOR IIB, SUA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	293	Total	C	N	O	S	0	0
			2269	1437	386	428	18		

- Molecule 19 is a protein called TATA-BOX-BINDING PROTEIN, TBP.

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

- Molecule 20 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT

ALPHA, TFA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	118	Total	C	N	O	S	0	0
			960	625	158	172	5		

- Molecule 21 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA, TFA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	121	Total	C	N	O	S	0	0
			1005	650	164	188	3		

- Molecule 22 is a DNA chain called TEMPLATE STRAND DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	72	Total	C	N	O	P	0	0
			1452	700	233	447	72		

- Molecule 23 is a protein called RNA POLYMERASE II PRE-INITIATION COMPLEX, TFG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	150	Total	C	N	O	S	0	0
			1248	793	220	232	3		

- Molecule 24 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA, TFG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	174	Total	C	N	O	S	0	0
			1455	930	250	269	6		

- Molecule 25 is a protein called RNA POLYMERASE II TRANSCRIPTION FACTOR B SUBUNIT 2, TFB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	62	Total	C	N	O	0	0
			518	334	83	101		

- Molecule 26 is a protein called RNA POLYMERASE II TRANSCRIPTION FACTOR B SUBUNIT 5, TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	63	Total	C	N	O	S	0	0
			499	316	88	93	2		

- Molecule 27 is a protein called DNA REPAIR HELICASE RAD3.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Y	578	Total	C	H	N	O	S	0	0
			5351	2975	691	790	862	33		

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	2	1	Total	Mg	0
			1	1	
28	A	1	Total	Mg	0
			1	1	

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
29	J	1	Total	Zn	0
			1	1	
29	B	1	Total	Zn	0
			1	1	
29	I	2	Total	Zn	0
			2	2	
29	C	1	Total	Zn	0
			1	1	
29	A	2	Total	Zn	0
			2	2	
29	2	1	Total	Zn	0
			1	1	
29	L	1	Total	Zn	0
			1	1	



- Molecule 1: DNA REPAIR HELICASE RAD25, SSL2



SER	TYR	THR	PRO	TYR	THR	GLN	S1392	M1284	Q1187	PHE	V958	T831	L702	P570	A457	K372	P285	P197	C77
TYR	GLY	GLY	PRO	GLY	GLY	ASP	M1393	V1291	R1193	PHE	T964	T834	H706	L571	Y465	T375	H286	E198	P78
THR	ALA	VAL	THR	THR	THR	GLY	L1194	L1295	R1194	ALA	G707	G835	M708	G574	Y465	T375	H287	L199	H80
PRO	THR	THR	THR	THR	THR	VAL	L1195	G1296	G707	GLY	I973	G836	M709	K575	F468	T375	I289	T204	P89
SER	PRO	PRO	SER	SER	PRO	ALA	L1196	E1297	E1196	SER	H974	Y836	L710	K576	L470	T381	E290	L208	V90
TYR	GLY	GLY	TYR	TYR	TYR	ALA	L1197	T1308	L1197	THR	H975	R839	R711	S579	L471	T381	E291	L208	F91
GLY	ASN	ASN	GLY	GLY	GLY	SER	M1203	D1309	M1204	K1092	T982	R840	E712	I582	L472	I385	S294	V216	H92
VAL	GLY	GLY	VAL	VAL	VAL	THR	K1205	M1312	K1205	K1093	T983	E846	F714	I582	S473	R387	Q297	F219	V93
SER	GLY	GLY	THR	THR	THR	THR	K1206	E1404	L1206	K984	T984	M849	V718	L588	T475	L388	A301	S221	I96
GLY	LEU	LEU	GLY	GLY	GLY	THR	L1207	E1405	L1207	K985	D885	M849	V718	K589	S476	L388	A301	L222	A97
LEU	VAL	VAL	LEU	LEU	LEU	THR	T1208	E1315	T1208	M1111	L993	R857	R726	K590	A480	V392	D307	F224	V106
VAL	ASN	ASN	VAL	VAL	VAL	THR	Q1218	M1316	Q1218	K1112	Q994	R857	R726	E593	D481	V392	D307	F224	V106
ALA	ALA	ALA	ALA	ALA	ALA	THR	T1113	V1317	T1113	T1113	Q994	R857	R726	E593	D481	V392	D307	F224	V106
THR	THR	THR	THR	THR	THR	THR	P1114	M1409	P1114	T1114	L998	G861	A729	G594	F482	E398	Q311	V227	D130
PRO	PRO	PRO	PRO	PRO	PRO	PRO	S1115	T1325	K1221	S1115	L998	G861	A729	G594	F482	E398	Q311	V227	D130
ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1116	H1326	M1222	L1116	M1004	R867	R731	T595	D483	R399	P312	W233	S131
VAL	VAL	VAL	VAL	VAL	VAL	VAL	T1117	I1327	D1223	T1117	M1004	R868	L732	T596	G484	P400	Q313	W233	K132
LYS	LYS	LYS	LYS	LYS	LYS	LYS	Y1118	Y1328	M1232	Y1118	M1009	R869	E734	L597	D486	G401	Q314	W234	K133
TYR	TYR	TYR	TYR	TYR	TYR	TYR	Y1119	T1329	M1232	Y1119	M1009	R870	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1120	E1426	M1232	Y1119	M1009	R870	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1121	M1336	L1236	E1121	V1015	R871	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1237	E1427	L1237	M873	T1016	R871	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1238	E1428	L1238	M874	T1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	I1341	E1429	I1341	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1340	E1430	G1340	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	I1341	E1431	I1341	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1345	E1432	R1345	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q1432	E1433	Q1432	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1433	E1434	M1433	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	I1436	E1435	I1436	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1437	E1436	G1437	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1438	E1437	T1438	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	F1441	E1438	F1441	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	D1442	E1439	D1442	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1443	E1440	V1443	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1444	E1441	M1444	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	D1445	E1442	D1445	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	D1446	E1443	D1446	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	S1362	E1444	S1362	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1363	E1445	V1363	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1365	E1446	R1365	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	F1447	E1447	F1447	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	E1448	E1448	E1448	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	S1449	E1449	S1449	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1450	E1450	L1450	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1451	E1451	V1451	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	K1452	E1452	K1452	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	D1373	E1453	D1373	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1376	E1454	T1376	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1377	E1455	T1377	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1386	E1456	R1386	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1382	E1457	T1382	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1386	E1458	L1386	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1387	E1459	R1387	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1388	E1460	G1388	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	F1389	E1461	F1389	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1390	E1462	M1390	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1282	E1463	V1282	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1391	E1464	R1391	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1283	E1465	T1283	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1285	E1466	M1285	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1261	E1467	L1261	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	K1262	E1468	K1262	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	H1263	E1469	H1263	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	E1264	E1470	E1264	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1265	E1471	M1265	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1273	E1472	L1273	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1274	E1473	R1274	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1279	E1474	T1279	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	E1280	E1475	E1280	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1281	E1476	R1281	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1282	E1477	M1282	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1282	E1478	V1282	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1283	E1479	R1283	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133
GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1283	E1480	M1283	A875	L1017	R874	E734	L597	D486	G401	Q314	W234	K133

THR
SER
PRO
GLY
TYR
ASN
SER
PRO
GLY
SER
PRO
ALA
TYR
ASP
GLU
GLN
LYS
HIS
ASN
GLU
ASN
GLU
ASN
SER
ARG

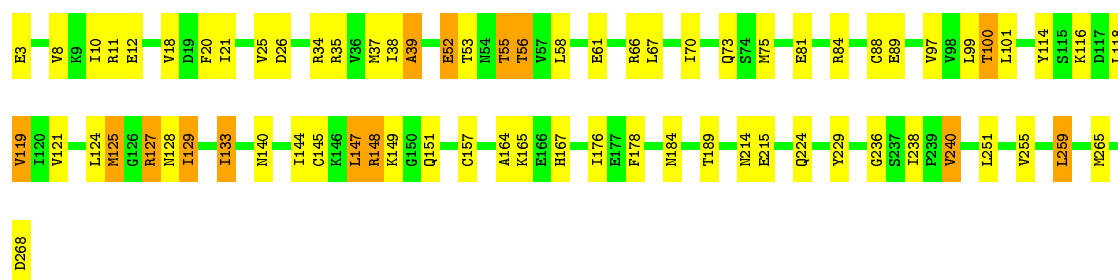
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2

Chain B: 

THR	SER	PRO	GLY	TYR	ASN	SER	PRO	GLY	SER	PRO	ALA	TYR	ASP	GLU	GLN	LYS	HIS	ASN	GLU	ASN	GLU	ASN	SER	ARG
1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240
1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265
1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290
1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315
1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340
1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365
1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390
1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415
1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440
1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465
1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490
1491	1492	1493	1494	1495	1496	1497	1498	1499	1500	1501	1502	1503	1504	1505	1506	1507	1508	1509	1510	1511	1512	1513	1514	1515
1516	1517	1518	1519	1520	1521	1522	1523	1524	1525	1526	1527	1528	1529	1530	1531	1532	1533	1534	1535	1536	1537	1538	1539	1540
1541	1542	1543	1544	1545	1546	1547	1548	1549	1550	1551	1552	1553	1554	1555	1556	1557	1558	1559	1560	1561	1562	1563	1564	1565
1566	1567	1568	1569	1570	1571	1572	1573	1574	1575	1576	1577	1578	1579	1580	1581	1582	1583	1584	1585	1586	1587	1588	1589	1590
1591	1592	1593	1594	1595	1596	1597	1598	1599	1600	1601	1602	1603	1604	1605	1606	1607	1608	1609	1610	1611	1612	1613	1614	1615
1616	1617	1618	1619	1620	1621	1622	1623	1624	1625	1626	1627	1628	1629	1630	1631	1632	1633	1634	1635	1636	1637	1638	1639	1640
1641	1642	1643	1644	1645	1646	1647	1648	1649	1650	1651	1652	1653	1654	1655	1656	1657	1658	1659	1660	1661	1662	1663	1664	1665
1666	1667	1668	1669	1670	1671	1672	1673	1674	1675	1676	1677	1678	1679	1680	1681	1682	1683	1684	1685	1686	1687	1688	1689	1690
1691	1692	1693	1694	1695	1696	1697	1698	1699	1700	1701	1702	1703	1704	1705	1706	1707	1708	1709	1710	1711	1712	1713	1714	1715
1716	1717	1718	1719	1720	1721	1722	1723	1724	1725	1726	1727	1728	1729	1730	1731	1732	1733	1734	1735	1736	1737	1738	1739	1740
1741	1742	1743	1744	1745	1746	1747	1748	1749	1750	1751	1752	1753	1754	1755	1756	1757	1758	1759	1760	1761	1762	1763	1764	1765
1766	1767	1768	1769	1770	1771	1772	1773	1774	1775	1776	1777	1778	1779	1780	1781	1782	1783	1784	1785	1786	1787	1788	1789	1790
1791	1792	1793	1794	1795	1796	1797	1798	1799	1800	1801	1802	1803	1804	1805	1806	1807	1808	1809	1810	1811	1812	1813	1814	1815
1816	1817	1818	1819	1820	1821	1822	1823	1824	1825	1826	1827	1828	1829	1830	1831	1832	1833	1834	1835	1836	1837	1838	1839	1840
1841	1842	1843	1844	1845	1846	1847	1848	1849	1850	1851	1852	1853	1854	1855	1856	1857	1858	1859	1860	1861	1862	1863	1864	1865
1866	1867	1868	1869	1870	1871	1872	1873	1874	1875	1876	1877	1878	1879	1880	1881	1882	1883	1884	1885	1886	1887	1888	1889	1890
1891	1892	1893	1894	1895	1896	1897	1898	1899	1900	1901	1902	1903	1904	1905	1906	1907	1908	1909	1910	1911	1912	1913	1914	1915
1916	1917	1918	1919	1920	1921	1922	1923	1924	1925	1926	1927	1928	1929	1930	1931	1932	1933	1934	1935	1936	1937	1938	1939	1940
1941	1942	1943	1944	1945	1946	1947	1948	1949	1950	1951	1952	1953	1954	1955	1956	1957	1958	1959	1960	1961	1962	1963	1964	1965
1966	1967	1968	1969	1970	1971	1972	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990
1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015

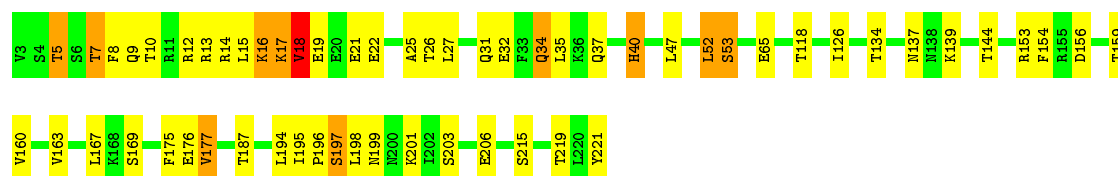
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 



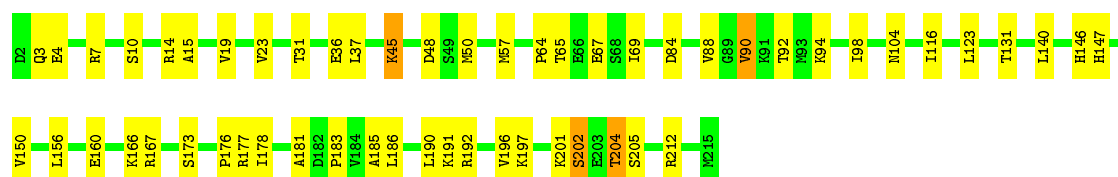
- Molecule 6: RNA POLYMERASE II PRE-INITIATION COMPLEX, RPB4

Chain D: 67% 26% 6% •



- Molecule 7: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1, RPB5

Chain E: 74% 24% •



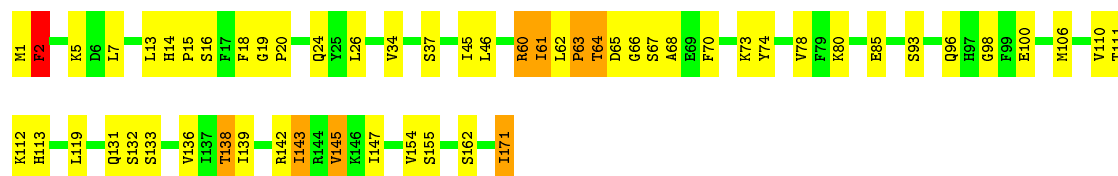
- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2, RPB6

Chain F: 60% 37% •

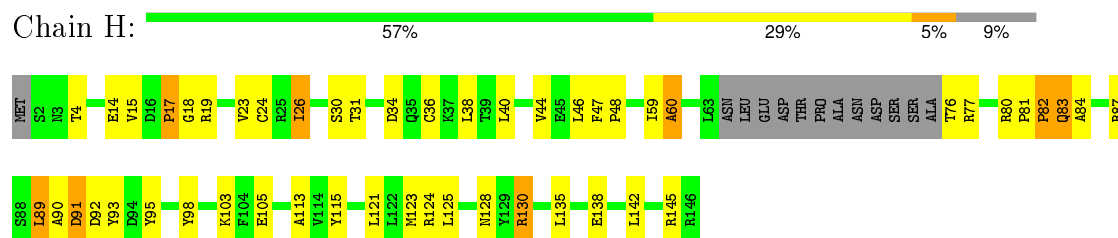


- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

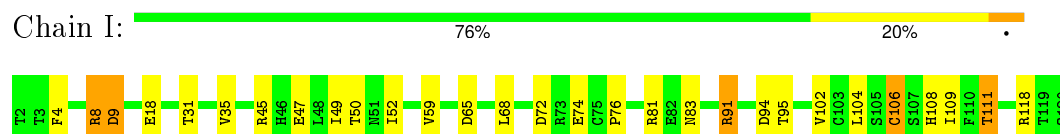
Chain G: 67% 27% 5% •



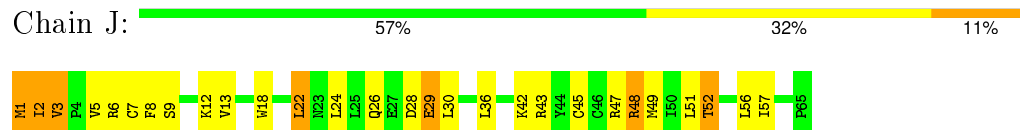
- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3, RPB8



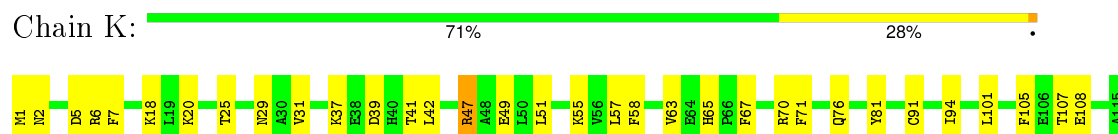
- Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



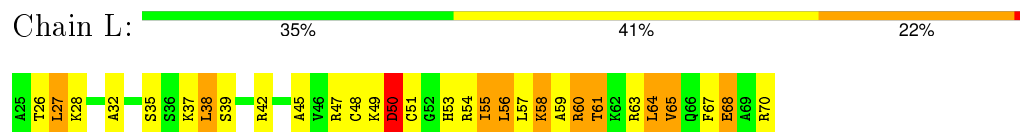
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5, RPB10



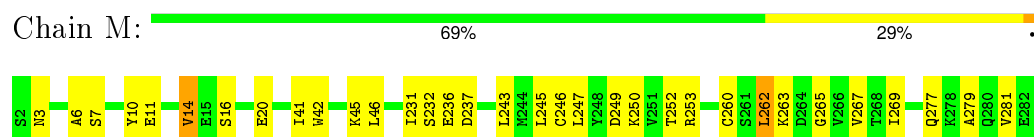
- Molecule 13: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



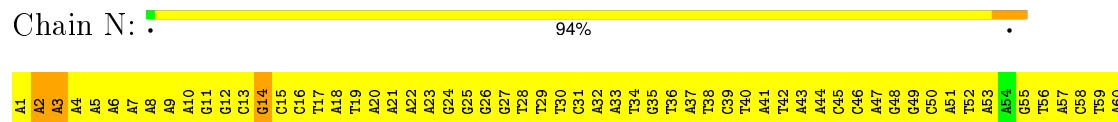
- Molecule 14: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4, RPB12



- Molecule 15: RNA POLYMERASE II PRE-INITIATION COMPLEX, TOA1



- Molecule 16: NON-TEMPLATE STRAND DNA




A61  
A62  
G63  
G64  
G65  
G66  
G67  
T68  
G69  
G70  
G71  
G72

- Molecule 17: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2, TOA2

Chain O: 

MET ALA VAL P4 G5 Y6 I15 L19 V20 D21 A22 L23 T25 D29 M38 R39 V40 L41 E42 T43 F44 D45 K46 V47 V48 A49 E50 T51 L52 T56 L60 G64 N65 L66 F71 D74 C83 Q84 V85 T86 V87 E88 ASP SER HIS ARG ASP ALA SER  
GLN ASN GLY SER GLY ASP SER LYS V105 I106 L111 N117 S118 K119 K120 SER GLU

- Molecule 18: TRANSCRIPTION INITIATION FACTOR IIB, SUA7

Chain P: 

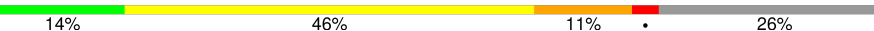
MET MET THR GLU SER ILE ASP LYS ARG ALA GLY ARG GLY PRO N17 L18 N19 I20 V21 L22 T23 T24 C24 P25 E26 C27 K28 V29 N30 P31 P32 R33 K34 I35 V35 E36 K37 F38 S39 E40 G41 D42 V43 V44 C45 A46 L47 L48 C49 G49 L50 L51 V51 L52 S53 D54 K55 K56 V57 D58 T59 R60  
S61 S62 W63 F66 SER ASN ASP ASP HIS ASN GLY ASP PRO SER ARG VAL GLY E61 A62 S63 S64 P65 Q66 Q67 Q68 Q69 Q70 Q71 Q72 Q73 Q74 Q75 Q76 Q77 Q78 Q79 Q80 Q81 Q82 Q83 Q84 Q85 Q86 Q87 Q88 Q89 Q90 Q91 Q92 Q93 Q94 Q95 Q96 Q97 Q98 Q99  
K122 D123 N124 E125 Q126 Q127 A128 A129 F130 K131 K132 I133 T134 M135 L136 C137 D138 A139 A140 A141 E142 P143 P144 N145 I146 L147 D148 D149 N150 N151 K152 L153 Y154 K155 R156 C157 K158 H159 D160 E161 T162 T163 D164 K165 R166 K167 M168 M169 E170 S171 L172 M173 A174 Q175 G176 I177 L178 I179 G180 K181  
R182 A183 T184 V185 E186 R187 T188 F189 R190 E191 I192 Q193 Q194 L195 I196 H197 V198 R199 T200 K201 E202 F203 G204 K205 K206 L207 N208 N209 K210 K211 N212 I213 L214 L215 L216 L217 L218 L219 L220 L221 L222 L223 L224 L225 L226 L227 L228 L229 L230 L231 L232 L233 L234 L235 L236 L237 L238 L239 L240 L241 L242 L243 L244 L245 L246 L247 L248 L249 L250 L251 L252 L253 L254 L255 L256 L257 L258 L259 L260 L261 L262 L263 L264 L265 L266 L267 L268 L269 L270 L271 L272 L273 L274 L275 L276 L277 L278 L279 L280 L281 L282 L283 L284 L285 L286 L287 L288 L289 L290 L291 L292 L293 L294 L295 L296 L297 L298 L299 L300 L301 L302 L303  
V304 T305 E306 G307 T308 T309 K310 K311 S312 G313 V314 K315 L316 L317 F318 F319 R320 A321 K322 L323 L324 D325 P326 Q327 L328 L329 A330 N331 G332 G333 V334 S335 S336 L337 D338 L339 P340 GLY VAL GLU LYS

- Molecule 19: TATA-BOX-BINDING PROTEIN, TBP

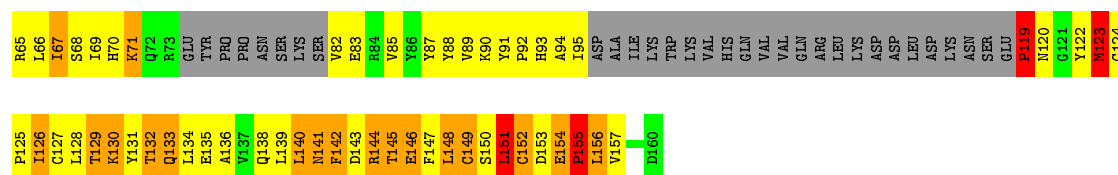
Chain Q: 

S61 P65 Q68 T75 L76 G77 C78 R79 T84 L87 H88 A89 R90 E93 Y94 N95 R98 F99 A100 I103 I106 P109 K110 T111 T112 A113 L114 I115 F116 A117 S118 G119 K120 M121 V122 T123 T124 A135 S136 Y139 A140 R141 I142 I143 Q144 K145 K151  
F152 T153 D154 Q158 N159 C164 D165 V166 P169 I170 R171 L172 E173 G174 L175 A176 F177 S183 E186 P187 E188 L193 I194 I196 T202 V203 L204 L205 T210 K211 T212 V213 T215 G216 A217 R220 E221 Y224 Q225 E228 A229 T230 V233 L234 K239 L240 K151

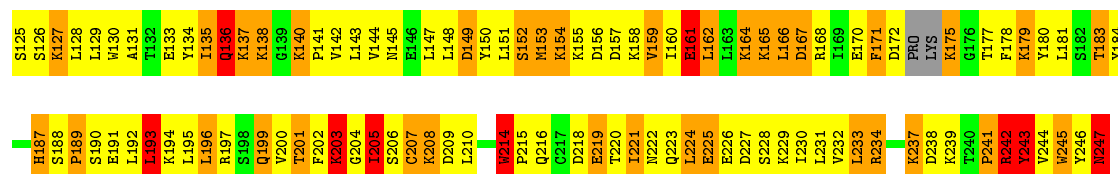
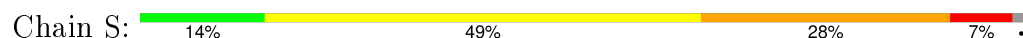
- Molecule 20: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA, TFA1

Chain R: 

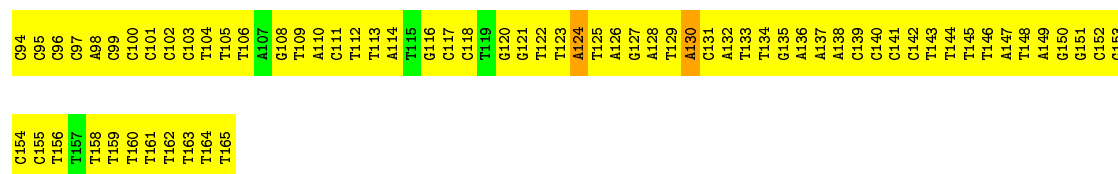
MET ASP ARG PRO ILE ASP ILE VAL LYS ASN L12 L13 L14 F15 V16 V17 R18 R19 G19 F20 Y21 F25 V26 L27 V28 L29 D30 A31 I32 I33 L34 F35 S36 V37 V38 L39 A39 E40 L43 K44 Q45 L46 L47 S48 L49 N50 K51 T52 E53 L54 G55 P56 L57 L58 L61 R62 S63 D64



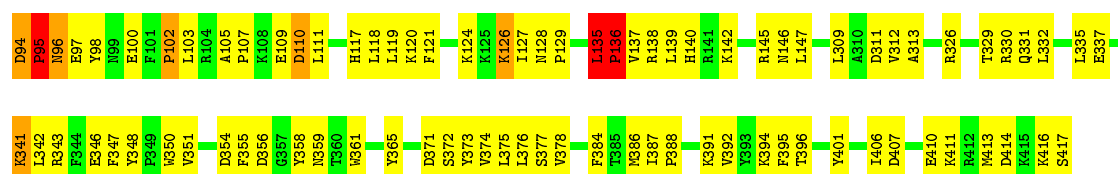
• Molecule 21: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA, TFA2



• Molecule 22: TEMPLATE STRAND DNA



• Molecule 23: RNA POLYMERASE II PRE-INITIATION COMPLEX, TFG1



• Molecule 24: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA, TFG2



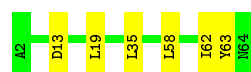
• Molecule 25: RNA POLYMERASE II TRANSCRIPTION FACTOR B SUBUNIT 2, TFB2

Chain W:



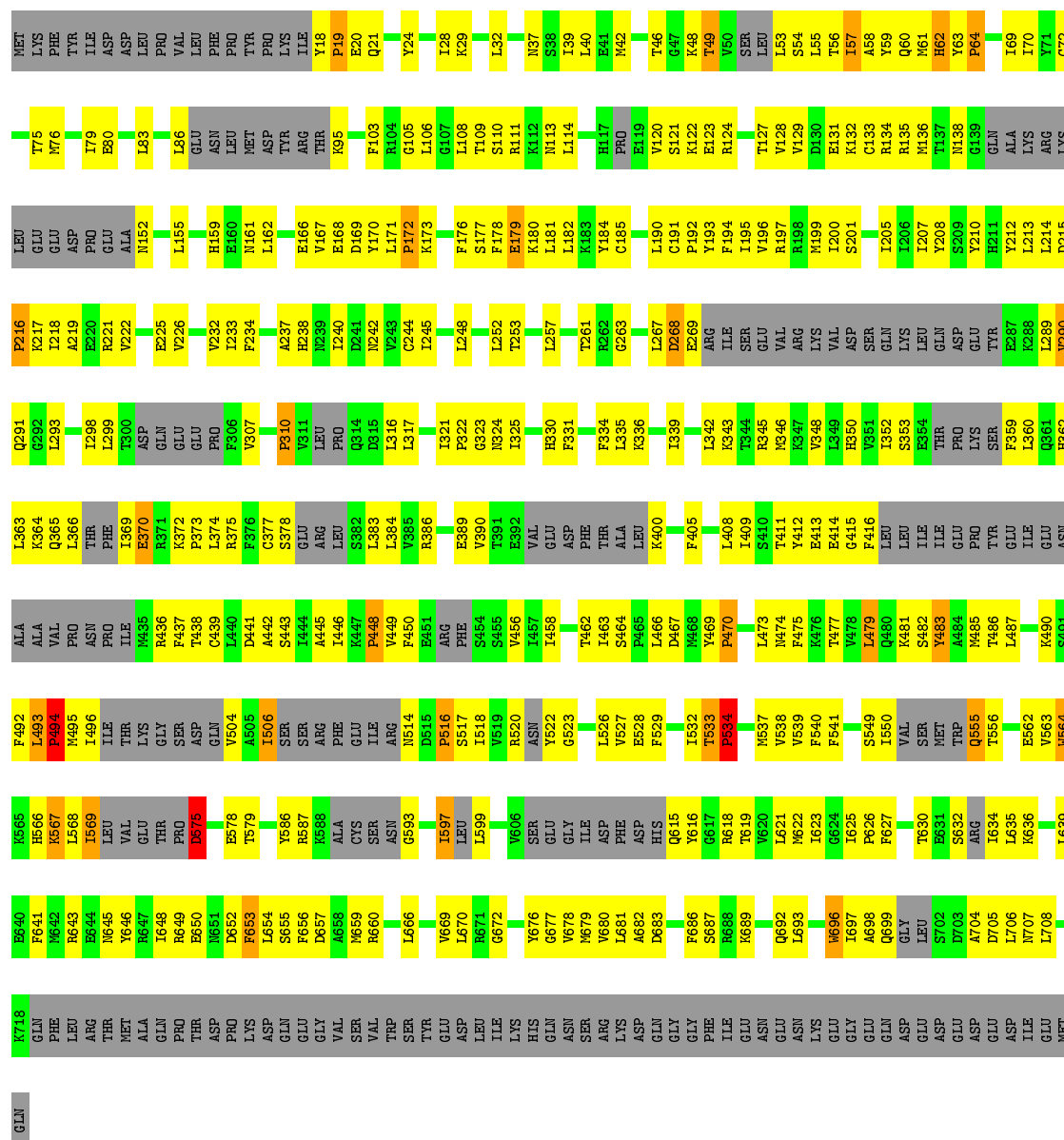
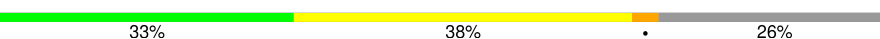
- Molecule 26: RNA POLYMERASE II TRANSCRIPTION FACTOR B SUBUNIT 5, TFB5

Chain X:



- Molecule 27: DNA REPAIR HELICASE RAD3

Chain Y:



## 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	SPARX, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (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, 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	1	4.34	6/3867 (0.2%)	2.05	41/5221 (0.8%)
10	H	0.51	0/1086	0.80	0/1470
11	I	0.47	0/989	0.78	0/1331
12	J	0.54	0/541	0.88	1/727 (0.1%)
13	K	0.47	0/938	0.71	0/1267
14	L	0.54	0/365	0.95	0/485
15	M	0.40	0/970	0.57	0/1310
16	N	1.27	20/1692 (1.2%)	1.41	34/2613 (1.3%)
17	O	0.42	0/800	0.63	0/1080
18	P	4.21	7/2297 (0.3%)	2.23	41/3090 (1.3%)
19	Q	0.41	0/1443	0.62	0/1942
2	2	1.31	4/571 (0.7%)	1.64	7/765 (0.9%)
20	R	9.51	2/978 (0.2%)	3.28	11/1321 (0.8%)
21	S	5.35	7/1017 (0.7%)	3.30	36/1356 (2.7%)
22	T	1.38	45/1618 (2.8%)	1.50	49/2491 (2.0%)
23	U	0.93	4/1273 (0.3%)	0.92	9/1710 (0.5%)
24	V	1.09	3/1481 (0.2%)	0.88	10/1988 (0.5%)
25	W	0.67	0/527	0.68	0/704
26	X	0.60	0/504	0.69	0/679
27	Y	0.88	11/4735 (0.2%)	0.84	19/6369 (0.3%)
3	A	0.57	4/11374 (0.0%)	0.81	11/15384 (0.1%)
4	B	0.49	1/9316 (0.0%)	0.74	4/12564 (0.0%)
5	C	0.49	0/2133	0.78	2/2891 (0.1%)
6	D	0.51	0/1444	0.83	2/1935 (0.1%)
7	E	0.48	0/1788	0.72	0/2406
8	F	0.62	0/691	0.81	0/933
9	G	0.52	0/1368	0.81	0/1844
All	All	2.13	114/55806 (0.2%)	1.23	277/75876 (0.4%)

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	1	1	1
18	P	2	0
2	2	0	2
20	R	1	0
21	S	0	1
27	Y	0	2
3	A	0	2
4	B	0	1
All	All	4	9

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	R	155	PRO	N-CD	213.23	4.46	1.47
20	R	119	PRO	N-CD	204.92	4.34	1.47
1	1	753	PRO	N-CD	203.03	4.32	1.47
18	P	292	PRO	N-CD	198.01	4.25	1.47
1	1	746	PRO	N-CD	168.34	3.83	1.47

The worst 5 of 277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	155	PRO	CA-N-CD	-66.71	18.11	111.50
20	R	119	PRO	N-CD-CG	-58.68	15.18	103.20
21	S	189	PRO	CA-N-CD	-53.80	36.18	111.50
1	1	753	PRO	N-CD-CG	-48.67	30.19	103.20
18	P	292	PRO	N-CD-CG	-48.02	31.17	103.20

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	690	ILE	CB
18	P	269	ILE	CB
18	P	277	ILE	CB
20	R	126	ILE	CB

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	661	SER	Peptide

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Mol	Chain	Res	Type	Group
2	2	269	PHE	Sidechain,Peptide
3	A	234	MET	Mainchain
3	A	95	PHE	Mainchain
4	B	43	LEU	Mainchain

## 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	1	3797	0	3727	916	0
2	2	666	0	546	251	0
3	A	11174	0	11217	712	0
4	B	9140	0	9107	421	0
5	C	2095	0	2051	43	0
6	D	1434	0	1460	69	0
7	E	1752	0	1776	30	0
8	F	679	0	699	94	0
9	G	1340	0	1353	174	0
10	H	1068	0	1040	21	0
11	I	971	0	927	16	0
12	J	532	0	542	14	0
13	K	920	0	929	19	0
14	L	363	0	386	24	0
15	M	956	0	916	32	0
16	N	1500	0	805	235	0
17	O	792	0	806	49	0
18	P	2269	0	2346	1242	0
19	Q	1416	0	1491	154	0
20	R	960	0	969	345	0
21	S	1005	0	1024	580	0
22	T	1452	0	822	273	0
23	U	1248	0	1229	236	0
24	V	1455	0	1465	465	0
25	W	518	0	514	27	0
26	X	499	0	525	12	0
27	Y	4660	691	4743	807	0
28	2	1	0	0	0	0
28	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	2	1	0	0	0	0
29	A	2	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	I	2	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
All	All	54672	691	53415	6017	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 56.

The worst 5 of 6017 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)
22:T:134:DT:C6	24:V:323:ARG:HD2	1.24	1.69
18:P:279:VAL:HG23	18:P:302:LEU:CG	1.19	1.66
20:R:34:PHE:CE2	20:R:134:LEU:HD11	1.25	1.65
27:Y:132:LYS:HD3	27:Y:155:LEU:CD1	1.24	1.64
18:P:137:CYS:SG	18:P:142:LEU:HB3	1.34	1.64

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	1	467/492 (95%)	436 (93%)	26 (6%)	5 (1%)	17 63
2	2	68/174 (39%)	51 (75%)	10 (15%)	7 (10%)	1 12
3	A	1414/1733 (82%)	1250 (88%)	113 (8%)	51 (4%)	4 38
4	B	1140/1224 (93%)	1018 (89%)	86 (8%)	36 (3%)	5 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	264/266 (99%)	242 (92%)	20 (8%)	2 (1%)	24	69
6	D	174/178 (98%)	148 (85%)	18 (10%)	8 (5%)	3	32
7	E	212/214 (99%)	195 (92%)	13 (6%)	4 (2%)	10	52
8	F	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
9	G	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	11	53
10	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1	22
11	I	117/119 (98%)	98 (84%)	16 (14%)	3 (3%)	7	45
12	J	63/65 (97%)	51 (81%)	9 (14%)	3 (5%)	3	31
13	K	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
14	L	44/46 (96%)	27 (61%)	9 (20%)	8 (18%)	0	4
15	M	110/116 (95%)	103 (94%)	7 (6%)	0	100	100
17	O	97/122 (80%)	93 (96%)	4 (4%)	0	100	100
18	P	287/345 (83%)	235 (82%)	33 (12%)	19 (7%)	1	24
19	Q	178/180 (99%)	170 (96%)	5 (3%)	3 (2%)	11	55
20	R	112/160 (70%)	100 (89%)	10 (9%)	2 (2%)	11	53
21	S	105/123 (85%)	94 (90%)	7 (7%)	4 (4%)	4	37
23	U	142/150 (95%)	131 (92%)	6 (4%)	5 (4%)	4	39
24	V	166/174 (95%)	145 (87%)	16 (10%)	5 (3%)	5	42
25	W	60/62 (97%)	60 (100%)	0	0	100	100
26	X	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
27	Y	558/778 (72%)	515 (92%)	35 (6%)	8 (1%)	14	58
All	All	6332/7300 (87%)	5668 (90%)	479 (8%)	185 (3%)	9	43

5 of 185 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	447	GLN
1	1	458	SER
2	2	275	LYS
2	2	292	PRO
3	A	74	MET

### 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	1	415/431 (96%)	370 (89%)	45 (11%)	8	36
2	2	62/151 (41%)	55 (89%)	7 (11%)	7	33
3	A	1240/1520 (82%)	1066 (86%)	174 (14%)	4	26
4	B	985/1061 (93%)	868 (88%)	117 (12%)	6	31
5	C	234/234 (100%)	206 (88%)	28 (12%)	6	31
6	D	160/160 (100%)	129 (81%)	31 (19%)	2	13
7	E	196/196 (100%)	175 (89%)	21 (11%)	8	36
8	F	74/74 (100%)	67 (90%)	7 (10%)	11	41
9	G	152/152 (100%)	135 (89%)	17 (11%)	7	34
10	H	117/128 (91%)	103 (88%)	14 (12%)	6	31
11	I	113/113 (100%)	106 (94%)	7 (6%)	23	60
12	J	60/60 (100%)	49 (82%)	11 (18%)	2	15
13	K	99/99 (100%)	87 (88%)	12 (12%)	6	31
14	L	40/40 (100%)	27 (68%)	13 (32%)	0	2
15	M	107/107 (100%)	104 (97%)	3 (3%)	51	78
17	O	91/108 (84%)	83 (91%)	8 (9%)	12	45
18	P	256/299 (86%)	215 (84%)	41 (16%)	3	21
19	Q	152/152 (100%)	143 (94%)	9 (6%)	24	61
20	R	108/149 (72%)	88 (82%)	20 (18%)	2	14
21	S	116/118 (98%)	69 (60%)	47 (40%)	0	0
23	U	136/136 (100%)	133 (98%)	3 (2%)	60	83
24	V	163/163 (100%)	158 (97%)	5 (3%)	47	77
25	W	57/57 (100%)	57 (100%)	0	100	100
26	X	57/57 (100%)	57 (100%)	0	100	100
27	Y	521/707 (74%)	504 (97%)	17 (3%)	45	76
All	All	5711/6472 (88%)	5054 (88%)	657 (12%)	11	32

5 of 657 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	801	LYS
5	C	240	VAL
21	S	189	PRO
4	B	939	THR
4	B	1175	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	1193	GLN
11	I	108	HIS
27	Y	100	GLN
4	B	1195	HIS
9	G	71	ASN

### 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 11 ligands modelled in this entry, 11 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.