



## wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 07:05 am GMT

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 Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

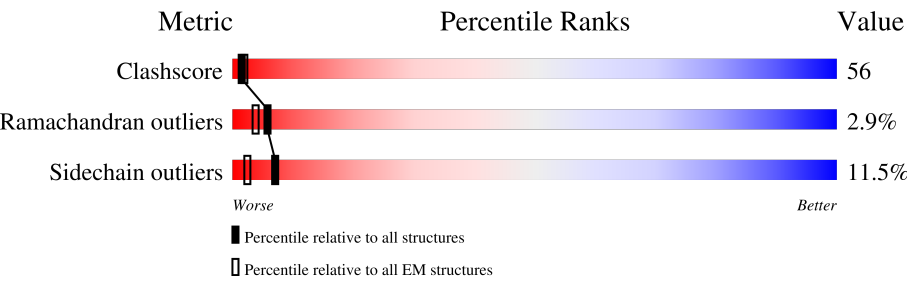
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	492	<div><div>66%</div><div><div>35%</div><div>52%</div><div>8%</div><div>.</div><div>.</div></div></div>
2	2	174	<div><div>60%</div><div><div>64%</div><div>28%</div><div>6%</div><div>.</div></div></div>
3	A	1733	<div><div>37%</div><div><div>53%</div><div>24%</div><div>.</div><div>.</div><div>18%</div></div></div>
4	B	1224	<div><div>52%</div><div><div>61%</div><div>29%</div><div>.</div><div>6%</div></div></div>
5	C	266	<div><div>34%</div><div><div>73%</div><div>22%</div><div>5%</div></div></div>
6	D	178	<div><div>57%</div><div><div>67%</div><div>26%</div><div>6%</div><div>.</div></div></div>
7	E	214	<div><div>43%</div><div><div>74%</div><div>24%</div><div>.</div></div></div>
8	F	84	<div><div>27%</div><div><div>60%</div><div>37%</div><div>.</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	G	171	
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).

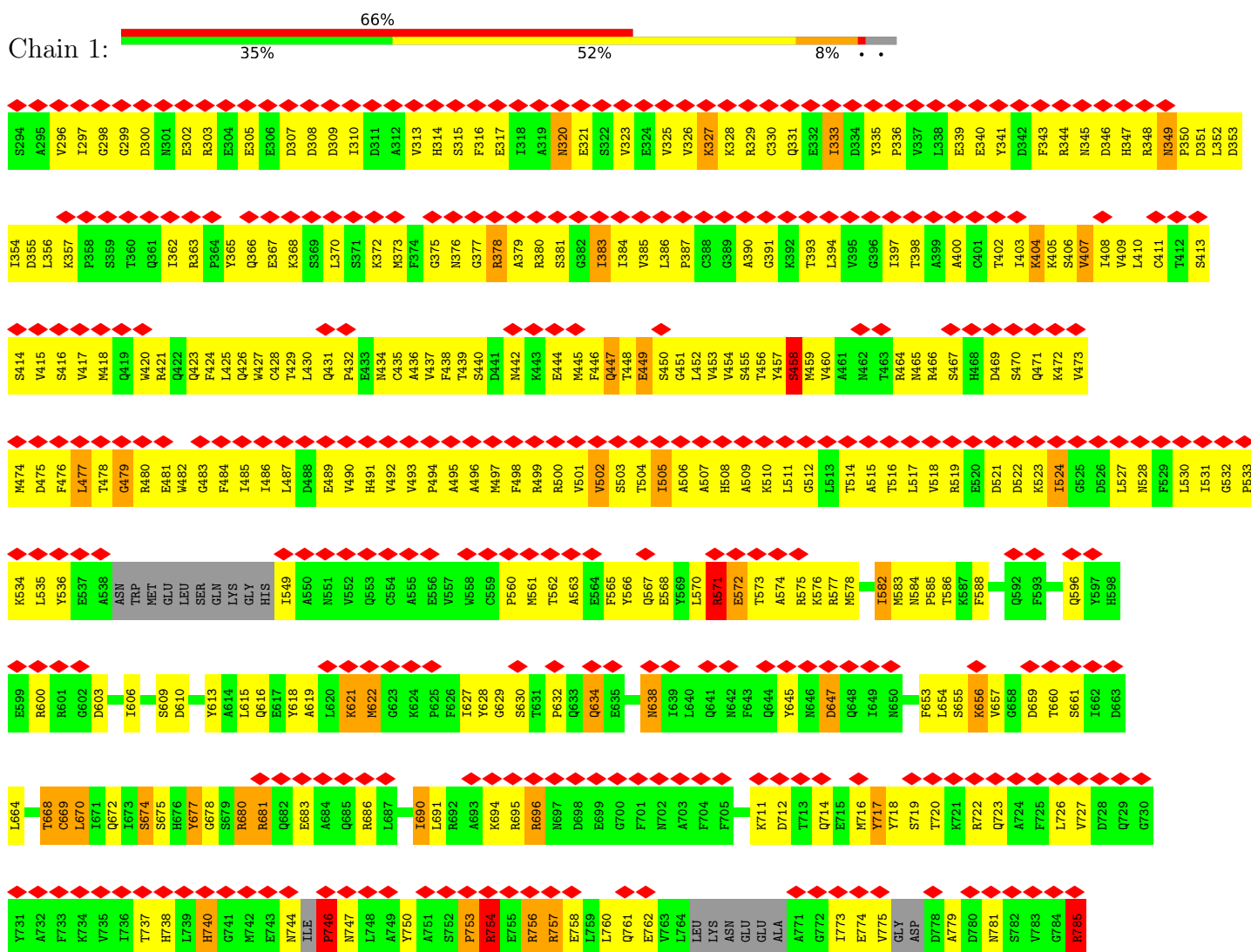
Mol	Chain	Residues	Atoms		AltConf
29	2	1	Total	Zn	0
			1	1	
29	A	2	Total	Zn	0
			2	2	
29	B	1	Total	Zn	0
			1	1	
29	C	1	Total	Zn	0
			1	1	
29	I	2	Total	Zn	0
			2	2	
29	J	1	Total	Zn	0
			1	1	
29	L	1	Total	Zn	0
			1	1	



### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 REPAIR HELICASE RAD25, SSL2



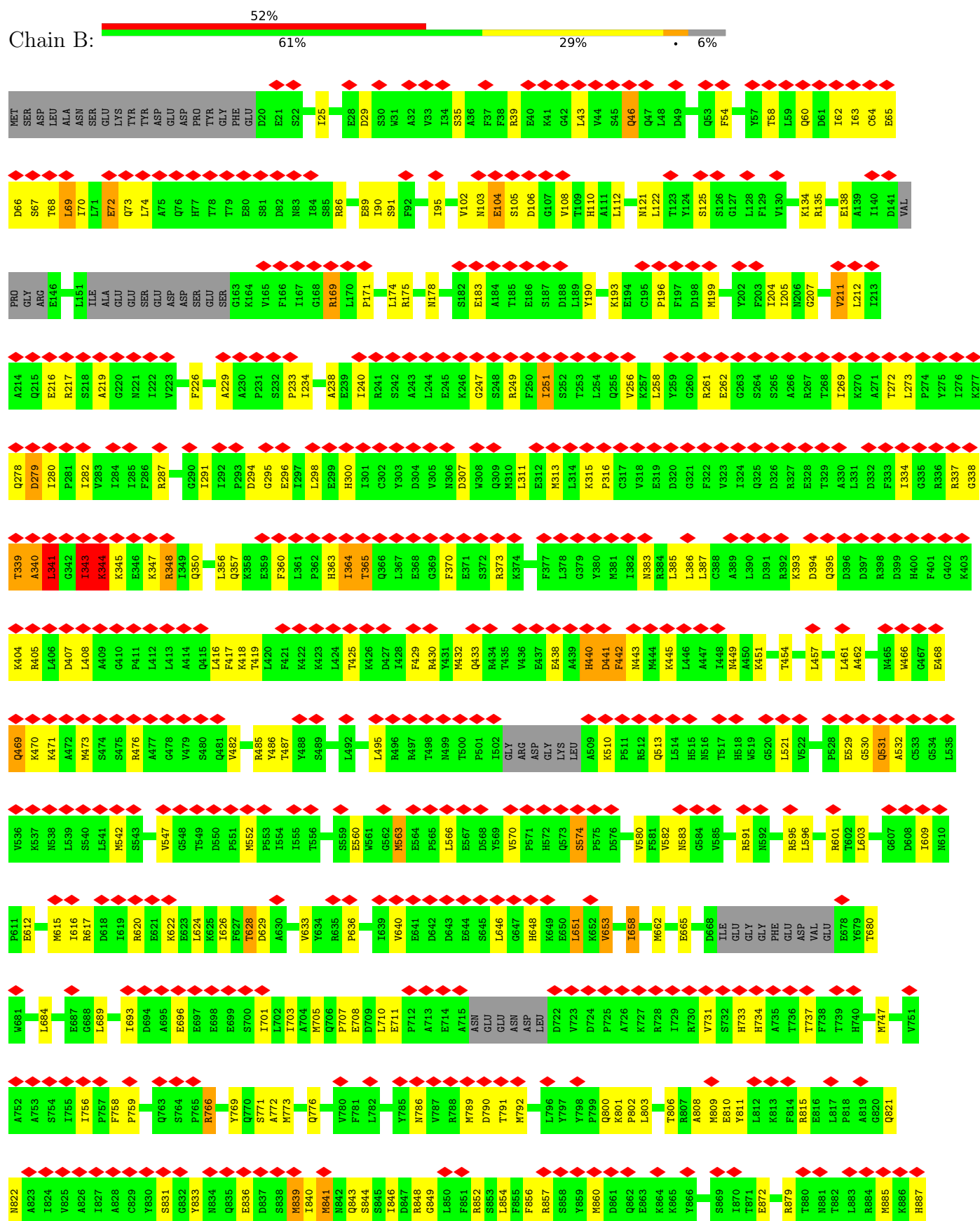
#### • Molecule 2: TRANSCRIPTION ELONGATION FACTOR S-II, DST1

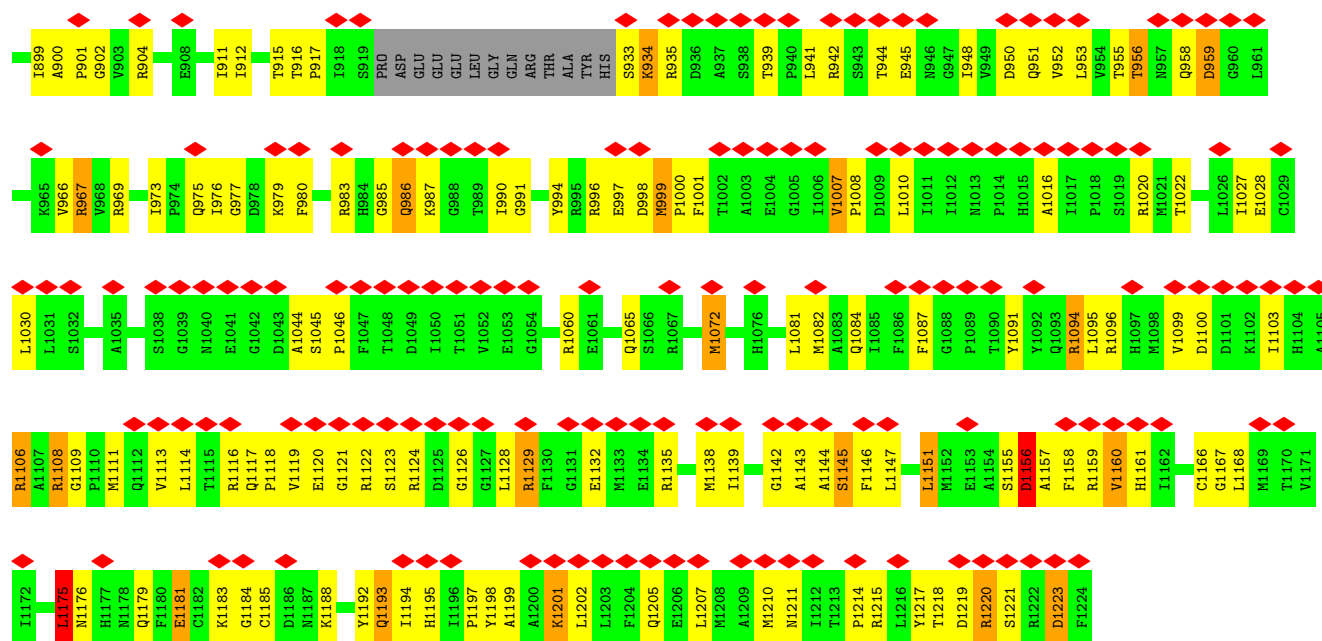




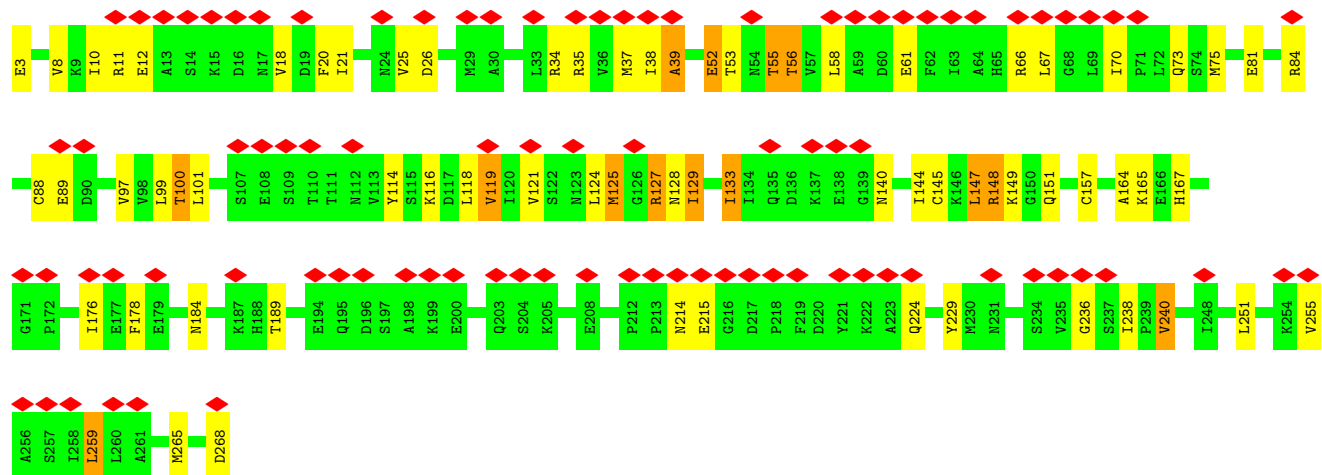
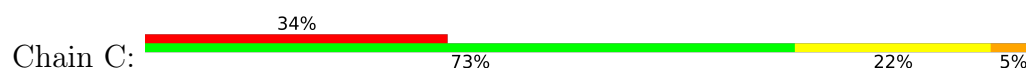
THR	GLN	SER	THR	SER	THR	PRO	THR	LEU	V1424	M1364	R1281	D1206	L1133	M1063	D980	L883	T809	E712
LYS	LYS	PRO	SER	VAL	ASP	THR	THR	ASP	S1425	Y1365	V1282	L1207	I1134	L1067	L981	D884	P810	S713
ASN	ASN	PRO	SER	LYS	VAL	THR	THR	LYS	E1426	R1366	V1283	T1208	R1135	A1068	T982	T885	P811	F714
ASN	GLU	THR	THR	ASP	GLU	THR	THR	GLU	N1427	M1367	M1284	M1209	T1142	A1069	T983	I386	Q811	V718
ASN	GLU	PRO	SER	GLU	LEU	THR	THR	LEU	V1428	M1368	V1291	G1210	K1144	A1069	T984	I387	F813	R726
ASN	THR	PRO	SER	MET	THR	THR	THR	MET	I1429	A1369	P1294	Q1211	S1145	I1072	H816	G888	F813	
THR	THR	THR	THR	PHE	THR	THR	THR	PHE	L1430	L1371	T1296	E1214		G1073	A817	G887	H816	A729
THR	THR	THR	THR	THR	THR	THR	THR	THR	Q1431	V1372	T1296	R1215	I1148	E1074	A817	A891	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	Q1432	D1373	E1297	R1216	A1149	P1075	M818	A892	M818	G730
THR	THR	THR	THR	THR	THR	THR	THR	THR	M1433	V1374	E1297	I1216	A1149	P1075	G819	A892	G819	L732
THR	THR	THR	THR	THR	THR	THR	THR	THR	A1434	M1375	K1300	K1217	S1150	A1076	K991	R896	G820	L732
THR	THR	THR	THR	THR	THR	THR	THR	THR	M1435	T1376	K1300	Q1218	E1151	T1077	D992	G887	G820	E734
THR	THR	THR	THR	THR	THR	THR	THR	THR	I1436	T1377	D1308	Q1219	Y1154	Q1078	L901	G887	H816	
THR	THR	THR	THR	THR	THR	THR	THR	THR	G1437	Q1378	D1309	F1220		Q1078	L902	A891	A817	A729
THR	THR	THR	THR	THR	THR	THR	THR	THR	T1438	Q1379	D1309	F1220		Q1078	L903	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	A1440	G1380	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	F1441	G1381	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	D1442	T1382	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	V1443	T1383	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	M1444	T1383	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	I1445	T1383	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	D1446	R1386	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	E1447	G1387	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	E1448	G1388	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	S1449	F1389	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	L1450	N1390	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	V1451	R1391	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	K1452	S1392	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	M1454	S1392	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	P1455	T1394	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	GLU	G1395	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	GLN	G1396	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	A1396	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L1397	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	M1398	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	R1399	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	C1400	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	S1401	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F1402	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	E1403	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L1404	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	T1405	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	V1406	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	E1407	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	I1408	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L1409	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	F1410	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	E1411	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	A1412	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	G1413	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L1414	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	S1415	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	A1416	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	E1417	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L1418	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	D1419	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	D1420	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	R1421	N1312	N1222		Q1078	L904	A892	A817	
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	G1423	N1312	N1222		Q1078	L904	A892	A817	

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

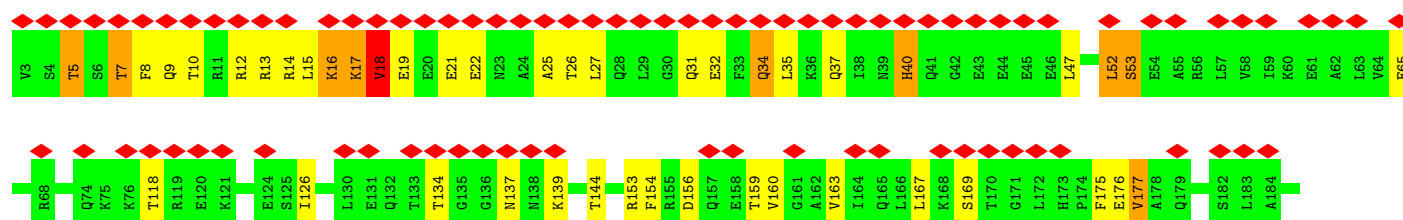




• Molecule 5: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

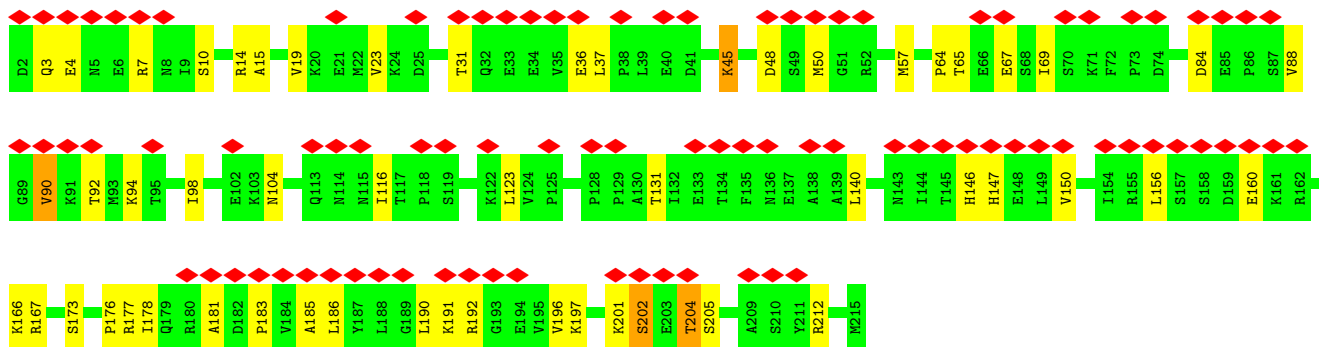
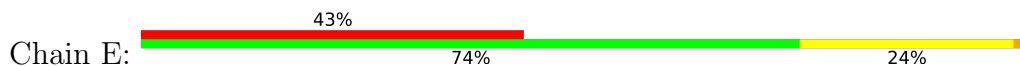


• Molecule 6: RNA POLYMERASE II PRE-INITIATION COMPLEX, RPB4

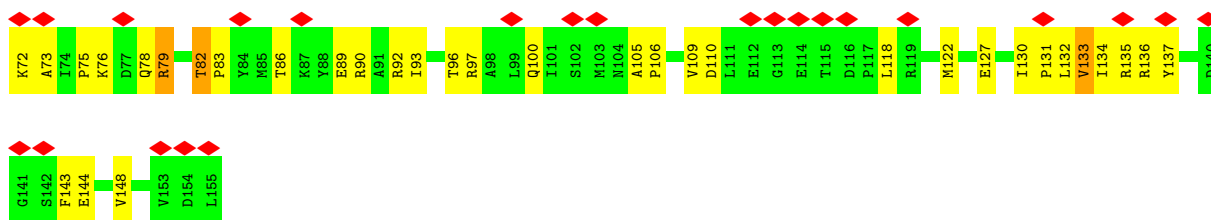




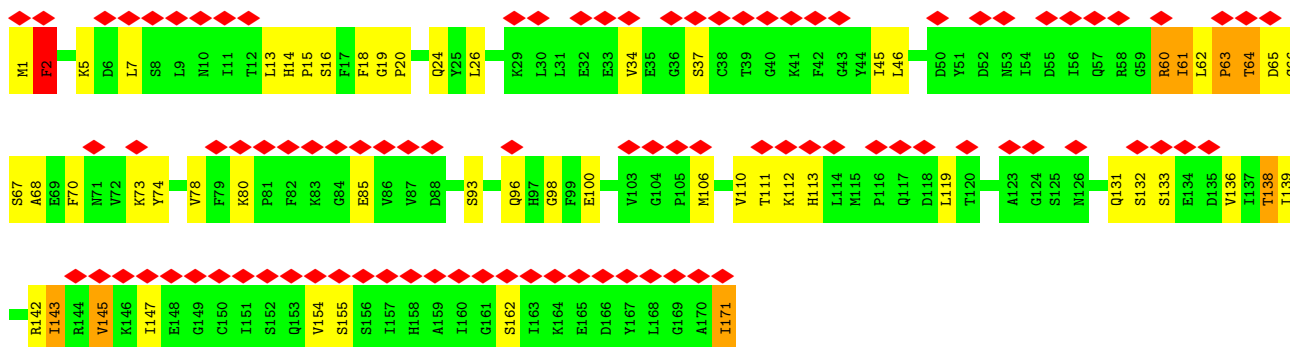
- Molecule 7: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1, RPB5



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

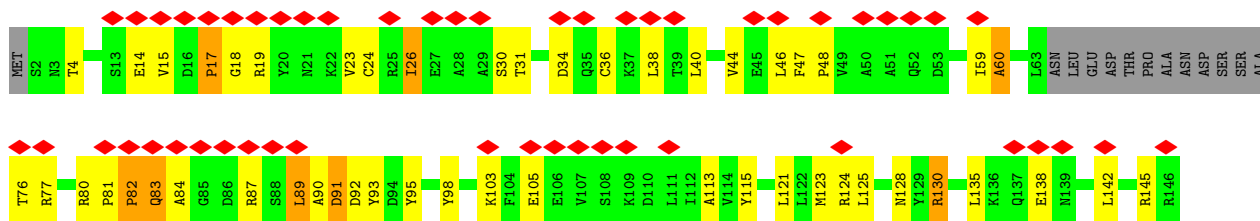


- Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

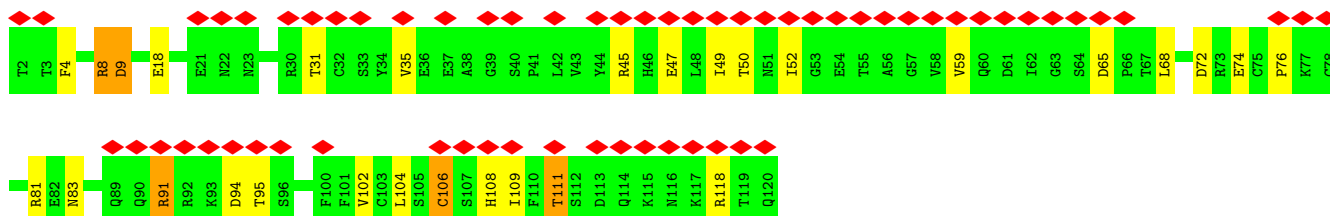


- Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3, RPB8

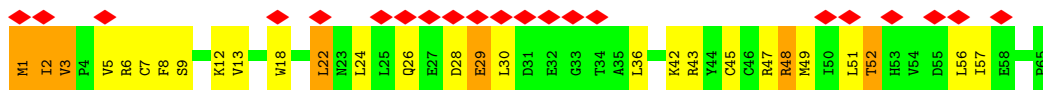




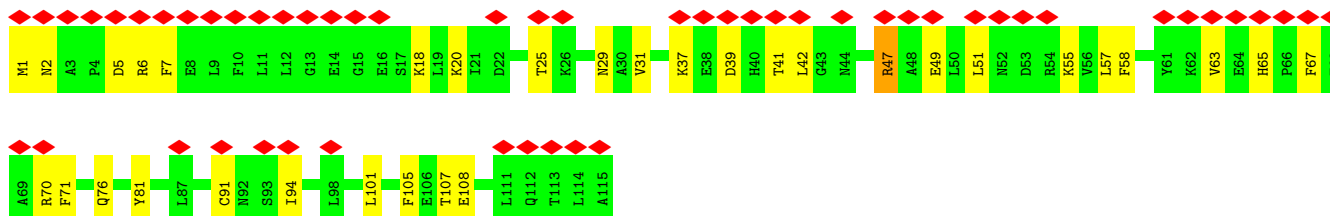
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



• 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

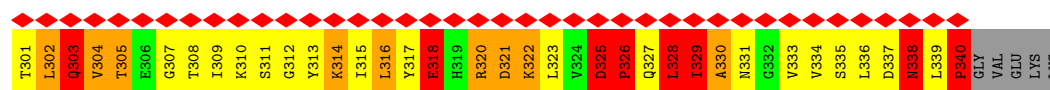


• Molecule 15: RNA POLYMERASE II PRE-INITIATION COMPLEX, TOA1

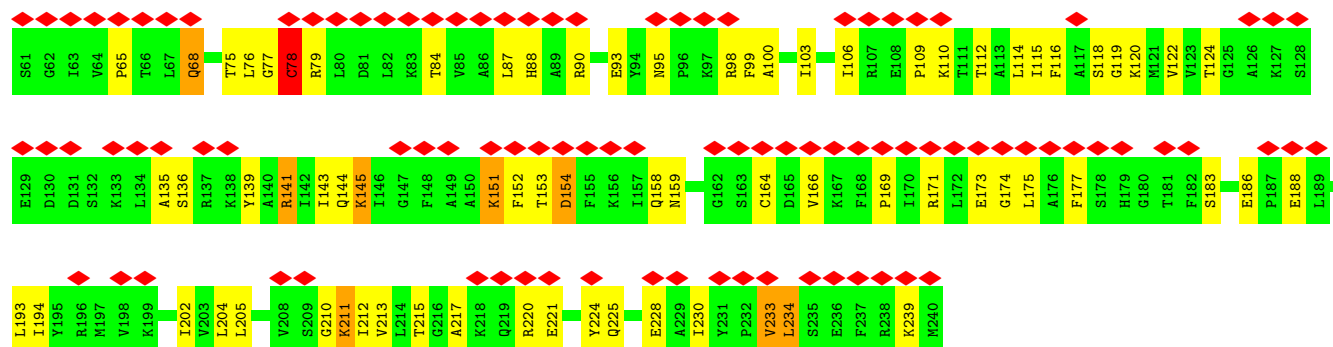




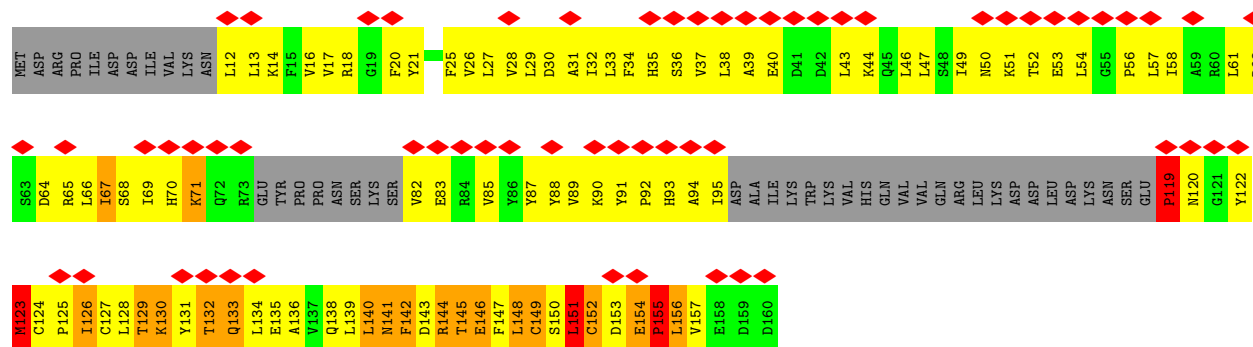
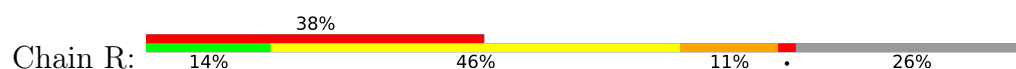




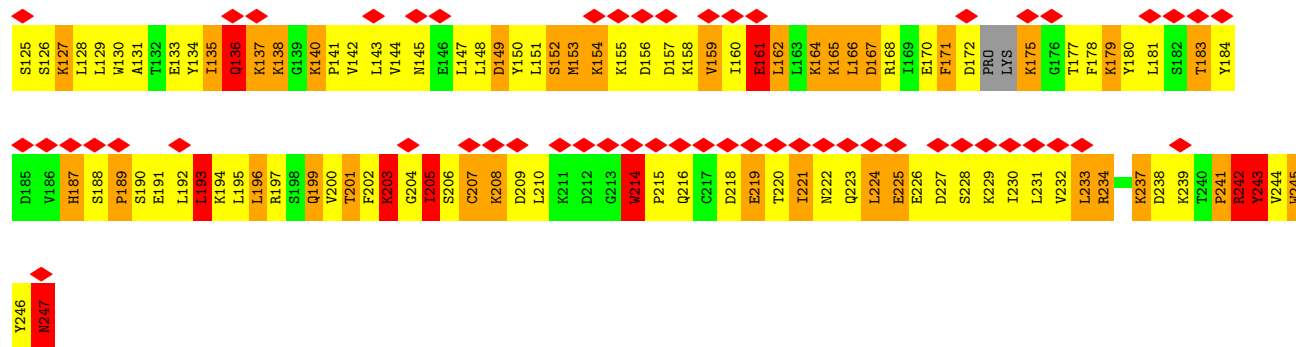
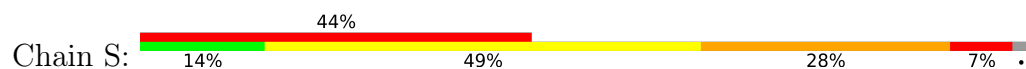
• Molecule 19: TATA-BOX-BINDING PROTEIN, TBP



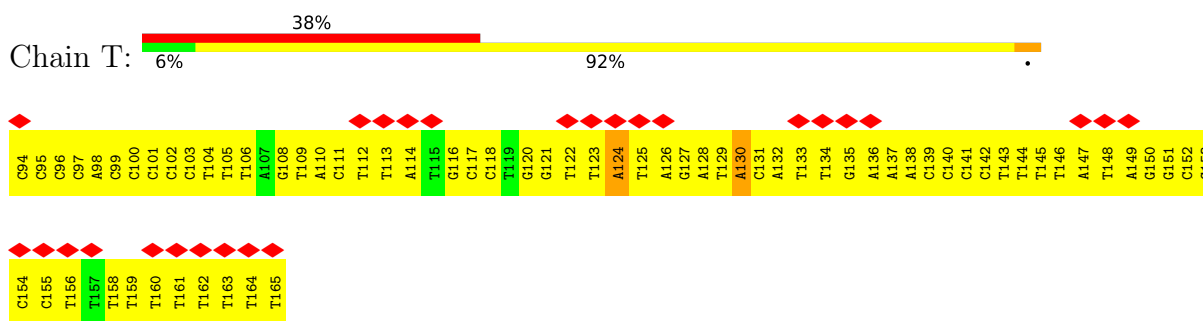
• Molecule 20: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA, TFA1



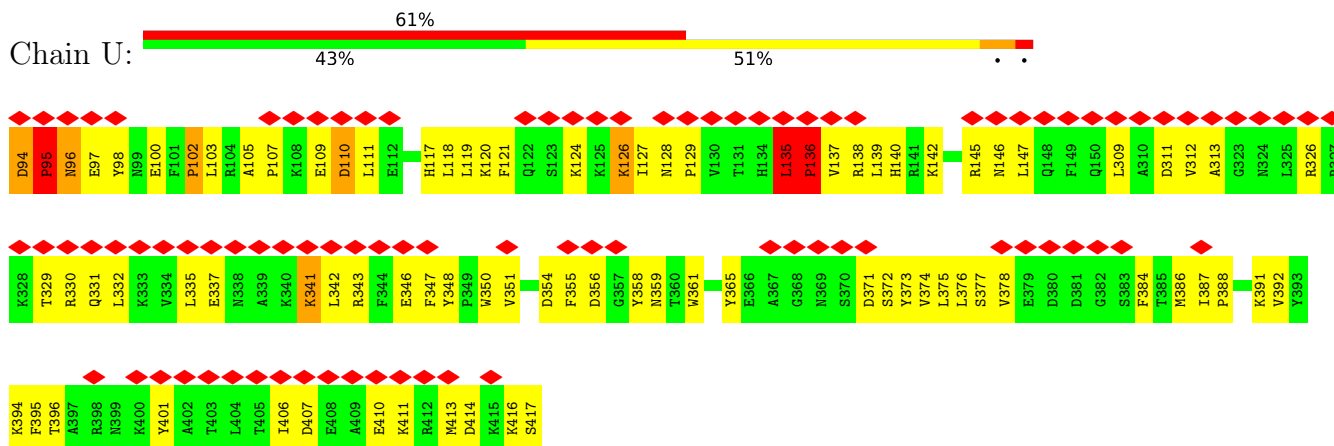
• Molecule 21: TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA, TFA2



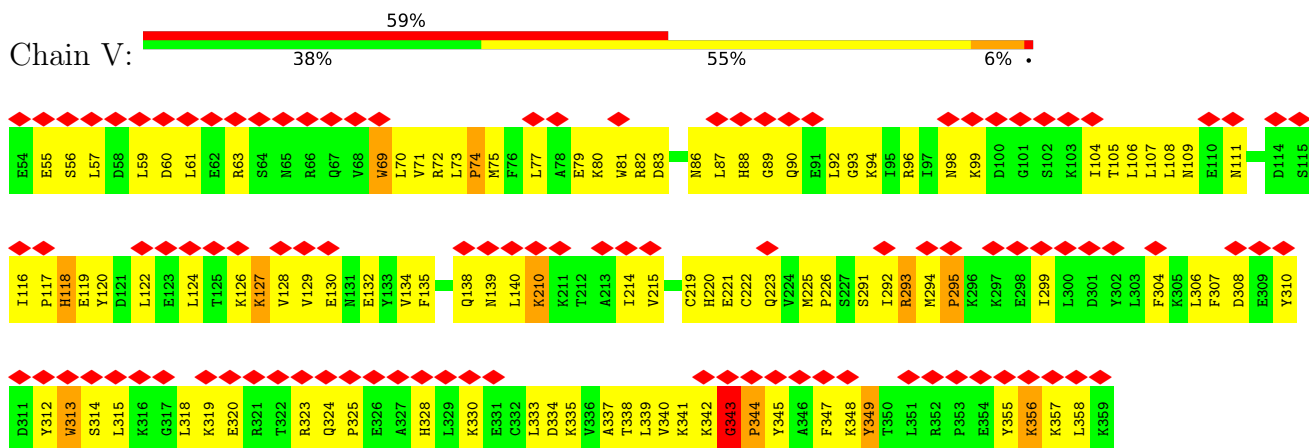
• Molecule 22: TEMPLATE STRAND DNA



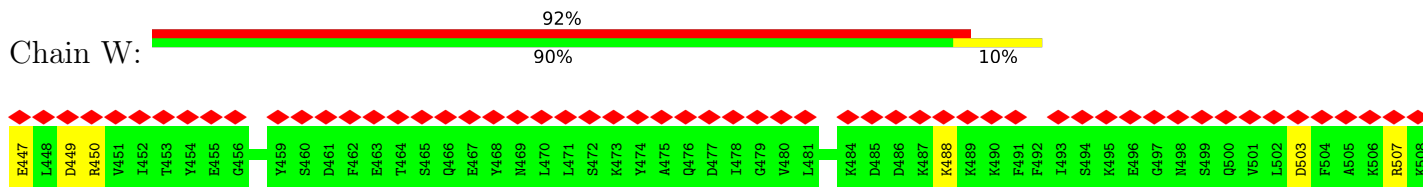
• Molecule 23: RNA POLYMERASE II PRE-INITIATION COMPLEX, TFG1



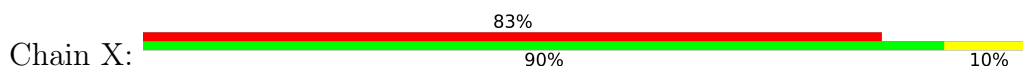
• Molecule 24: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA, TFG2



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

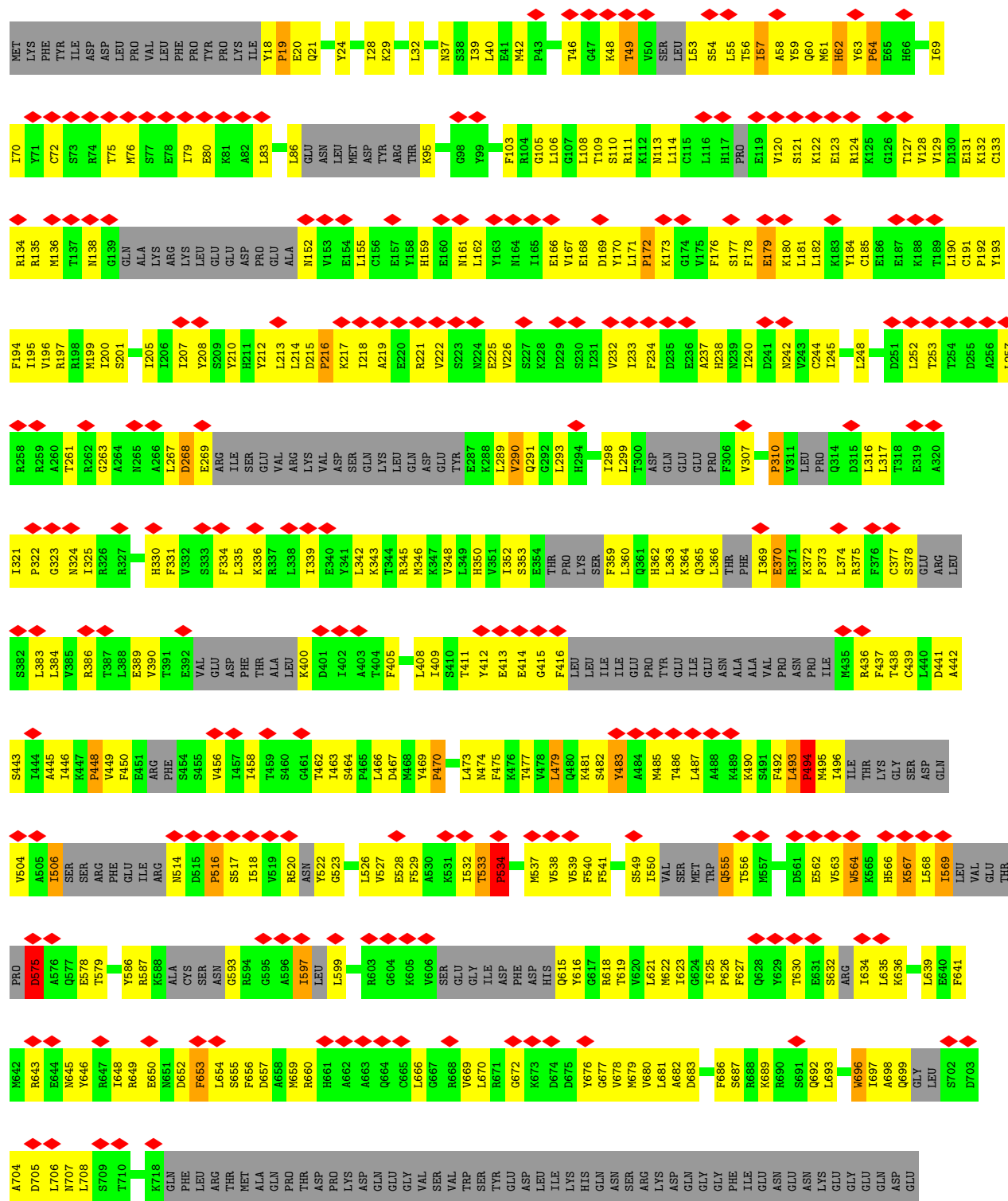


• Molecule 26: RNA POLYMERASE II TRANSCRIPTION FACTOR B SUBUNIT 5, TFB5





## • Molecule 27: DNA REPAIR HELICASE RAD3



ASP  
GLU  
ASP  
GLU  
ASP  
ASP  
ILE  
GLU  
MET  
GLN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7578	Depositor
Resolution determination method	Not provided	
CTF correction method	SPARX	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	9.151	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.142	Depositor
Map value standard deviation	0.652	Depositor
Recommended contour level	3.99	Depositor
Map size ( $\text{\AA}$ )	399.76, 399.76, 399.76	wwPDB
Map dimensions	152, 152, 152	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.63, 2.63, 2.63	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	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	4.34	6/3867 (0.2%)	2.05	41/5221 (0.8%)
2	2	1.31	4/571 (0.7%)	1.64	7/765 (0.9%)
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
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
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%)
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
2	2	0	2
3	A	0	2
4	B	0	1
18	P	2	0
20	R	1	0
21	S	0	1
27	Y	0	2
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	2	269	PHE	Peptide,Sidechain
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

*Continued on next page...*



*Continued from previous page...*

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
18:P:137:CYS:SG	18:P:142:LEU:HB3	1.34	1.64
27:Y:132:LYS:HD3	27:Y:155:LEU:CD1	1.24	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%)	12 47
2	2	68/174 (39%)	51 (75%)	10 (15%)	7 (10%)	0 6
3	A	1414/1733 (82%)	1250 (88%)	113 (8%)	51 (4%)	3 20
4	B	1140/1224 (93%)	1018 (89%)	86 (8%)	36 (3%)	3 21

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	264/266 (99%)	242 (92%)	20 (8%)	2 (1%)	16	55
6	D	174/178 (98%)	148 (85%)	18 (10%)	8 (5%)	2	17
7	E	212/214 (99%)	195 (92%)	13 (6%)	4 (2%)	6	32
8	F	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
9	G	169/171 (99%)	158 (94%)	8 (5%)	3 (2%)	7	34
10	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1	11
11	I	117/119 (98%)	98 (84%)	16 (14%)	3 (3%)	4	25
12	J	63/65 (97%)	51 (81%)	9 (14%)	3 (5%)	2	16
13	K	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
14	L	44/46 (96%)	27 (61%)	9 (20%)	8 (18%)	0	2
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	12
19	Q	178/180 (99%)	170 (96%)	5 (3%)	3 (2%)	7	36
20	R	112/160 (70%)	100 (89%)	10 (9%)	2 (2%)	7	34
21	S	105/123 (85%)	94 (90%)	7 (7%)	4 (4%)	2	19
23	U	142/150 (95%)	131 (92%)	6 (4%)	5 (4%)	3	20
24	V	166/174 (95%)	145 (87%)	16 (10%)	5 (3%)	3	22
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%)	9	40
All	All	6332/7300 (87%)	5668 (90%)	479 (8%)	185 (3%)	6	23

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%)	5	19
2	2	62/151 (41%)	55 (89%)	7 (11%)	4	17
3	A	1240/1520 (82%)	1066 (86%)	174 (14%)	3	12
4	B	985/1061 (93%)	868 (88%)	117 (12%)	4	16
5	C	234/234 (100%)	206 (88%)	28 (12%)	4	16
6	D	160/160 (100%)	129 (81%)	31 (19%)	1	7
7	E	196/196 (100%)	175 (89%)	21 (11%)	5	19
8	F	74/74 (100%)	67 (90%)	7 (10%)	7	22
9	G	152/152 (100%)	135 (89%)	17 (11%)	5	17
10	H	117/128 (91%)	103 (88%)	14 (12%)	4	16
11	I	113/113 (100%)	106 (94%)	7 (6%)	15	36
12	J	60/60 (100%)	49 (82%)	11 (18%)	1	8
13	K	99/99 (100%)	87 (88%)	12 (12%)	4	16
14	L	40/40 (100%)	27 (68%)	13 (32%)	0	2
15	M	107/107 (100%)	104 (97%)	3 (3%)	38	57
17	O	91/108 (84%)	83 (91%)	8 (9%)	8	25
18	P	256/299 (86%)	215 (84%)	41 (16%)	2	10
19	Q	152/152 (100%)	143 (94%)	9 (6%)	16	38
20	R	108/149 (72%)	88 (82%)	20 (18%)	1	8
21	S	116/118 (98%)	69 (60%)	47 (40%)	0	0
23	U	136/136 (100%)	133 (98%)	3 (2%)	47	65
24	V	163/163 (100%)	158 (97%)	5 (3%)	35	54
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%)	33	52
All	All	5711/6472 (88%)	5054 (88%)	657 (12%)	7	16

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

Mol	Chain	Res	Type
11	I	35	VAL
20	R	133	GLN
12	J	42	LYS
11	I	31	THR
18	P	255	SER

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

Mol	Chain	Res	Type
10	H	35	GLN
18	P	84	ASN
27	Y	60	GLN
11	I	83	ASN
15	M	59	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	S	7
27	Y	7
24	V	3
23	U	3
15	M	2
3	A	2
6	D	1
1	1	1
4	B	1
2	2	1

The worst 5 of 28 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	227:SER	C	291:SER	N	84.31
1	M	61:ASN	C	228:ASP	N	43.11
1	D	76:LYS	C	118:THR	N	35.68
1	S	184:TYR	C	185:ASP	N	14.79
1	U	313:ALA	C	323:GLY	N	13.13

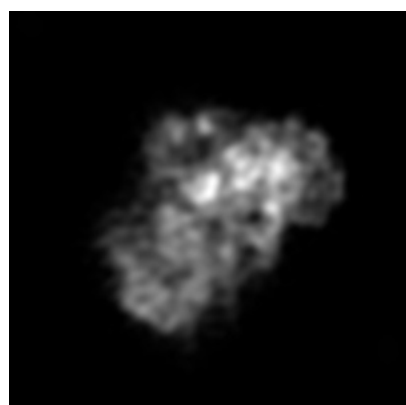
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3114. These allow visual inspection of the internal detail of the map and identification of artifacts.

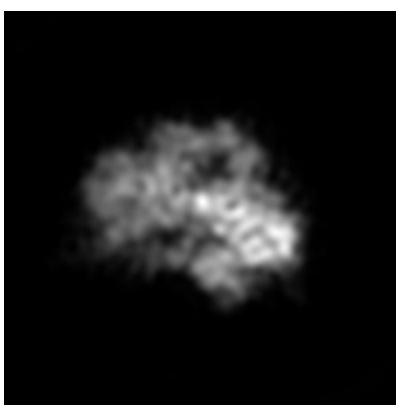
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

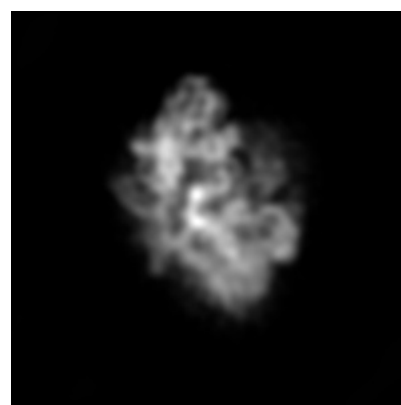
#### 6.1.1 Primary map



X



Y

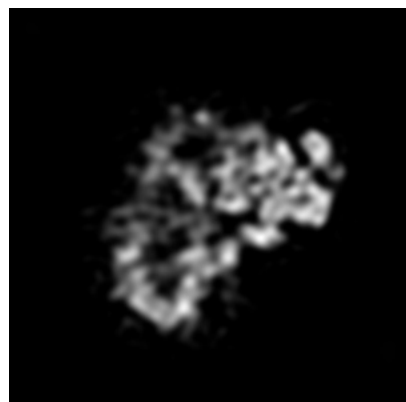


Z

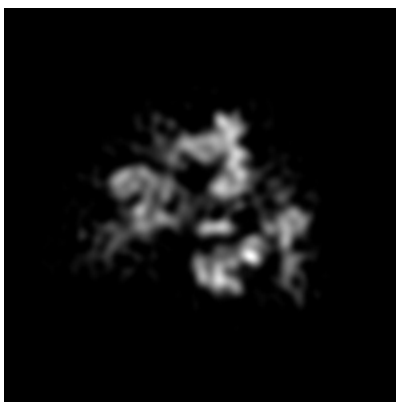
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

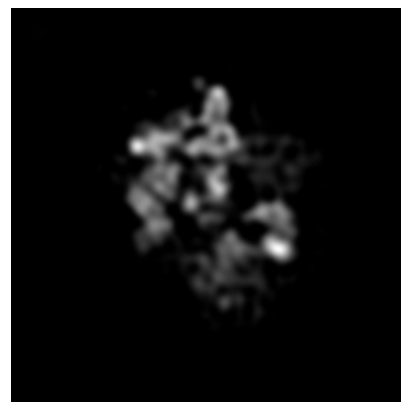
#### 6.2.1 Primary map



X Index: 76



Y Index: 76



Z Index: 76

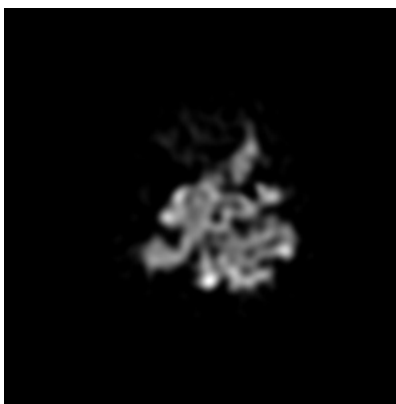
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 69



Y Index: 99

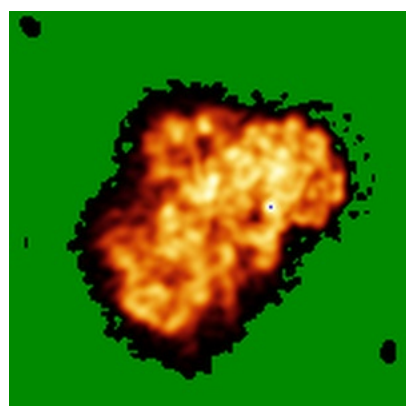


Z Index: 88

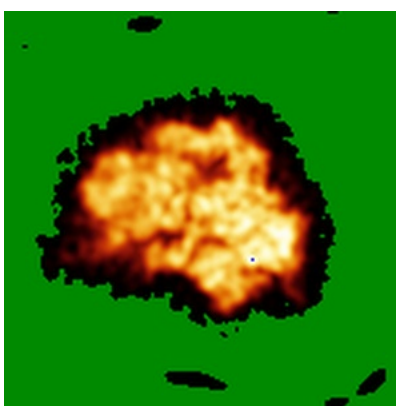
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

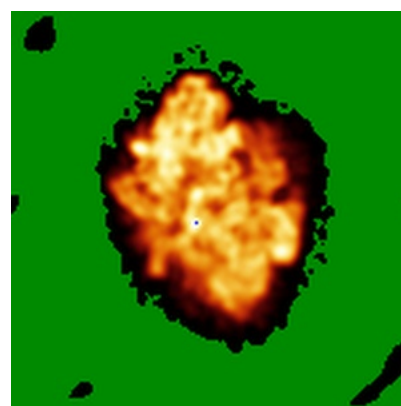
### 6.4.1 Primary map



X



Y

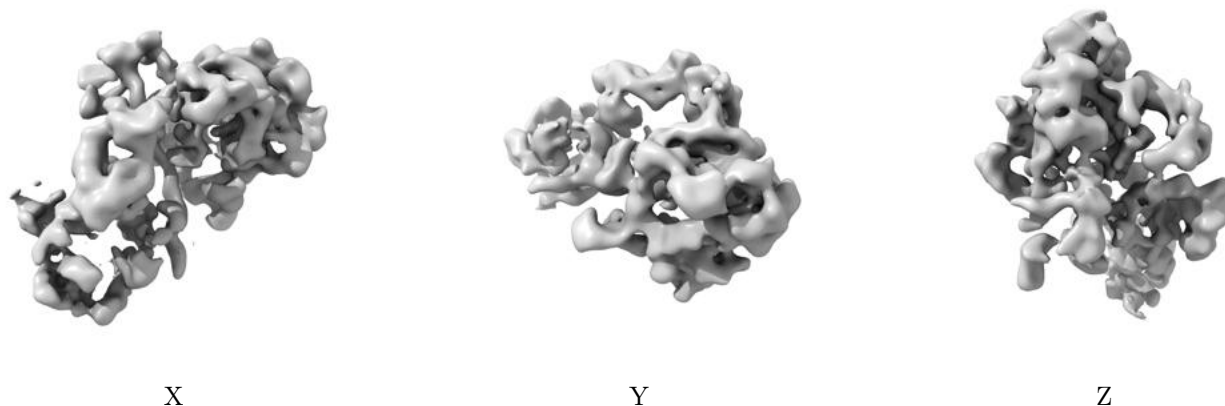


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.99. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

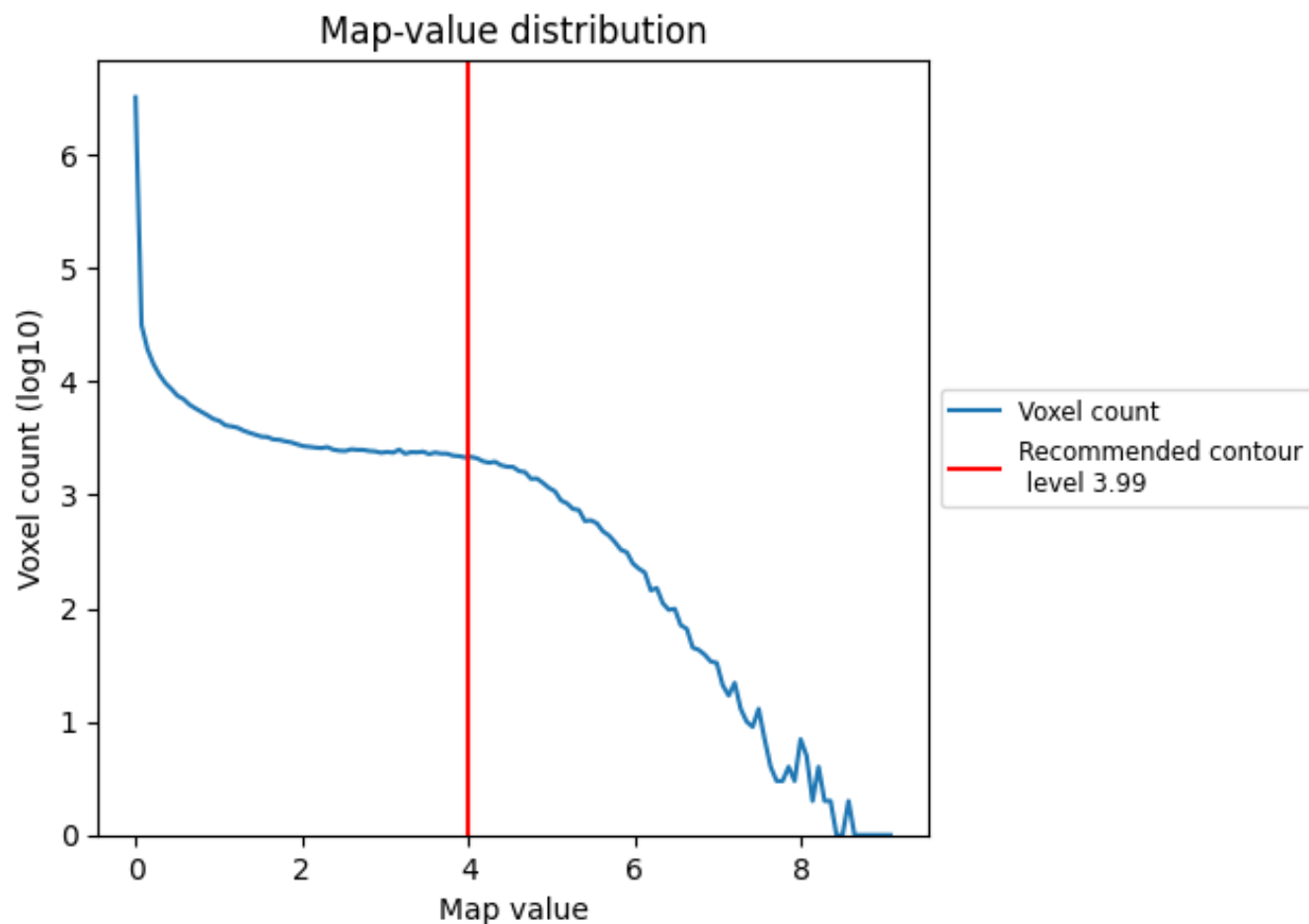
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

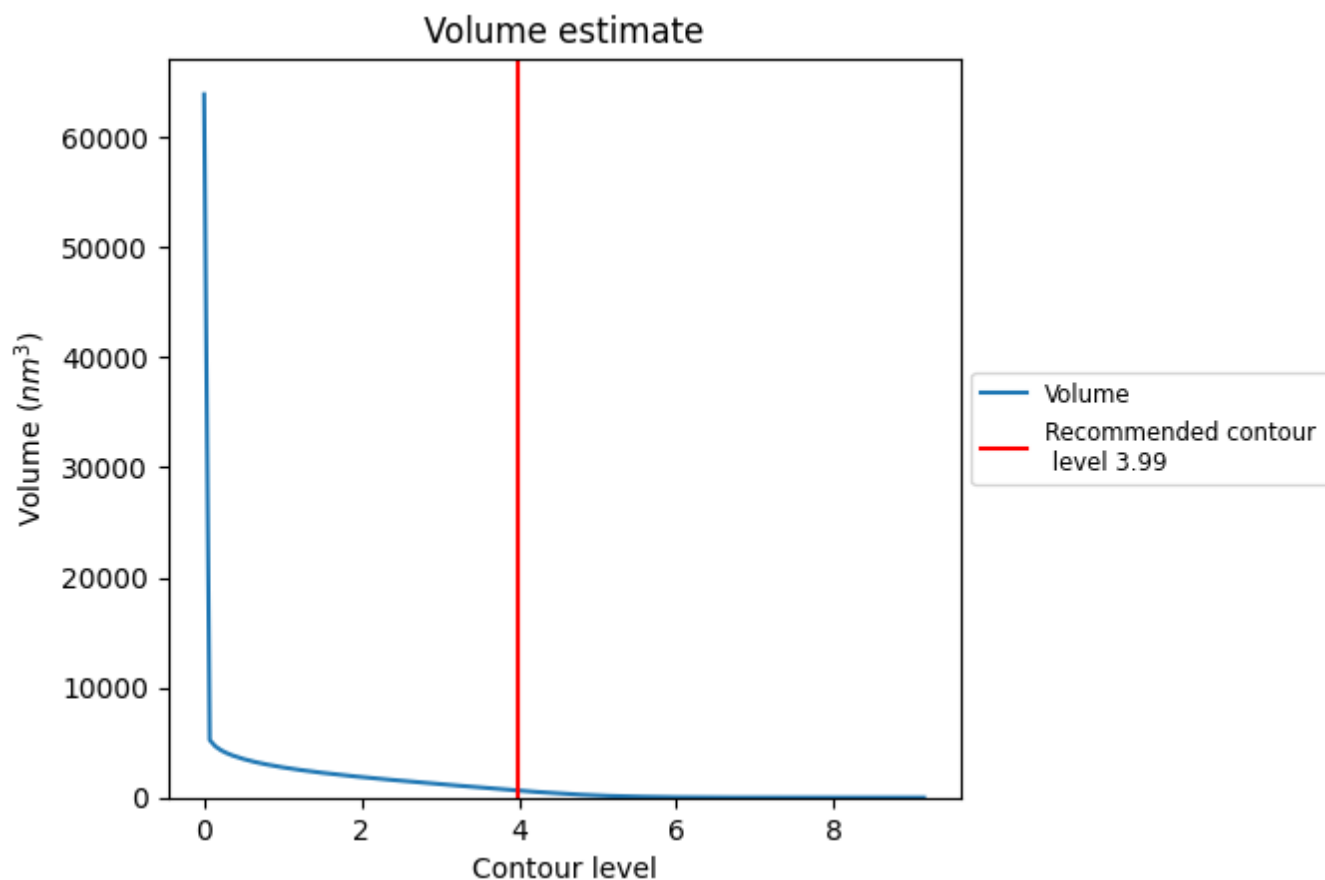
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

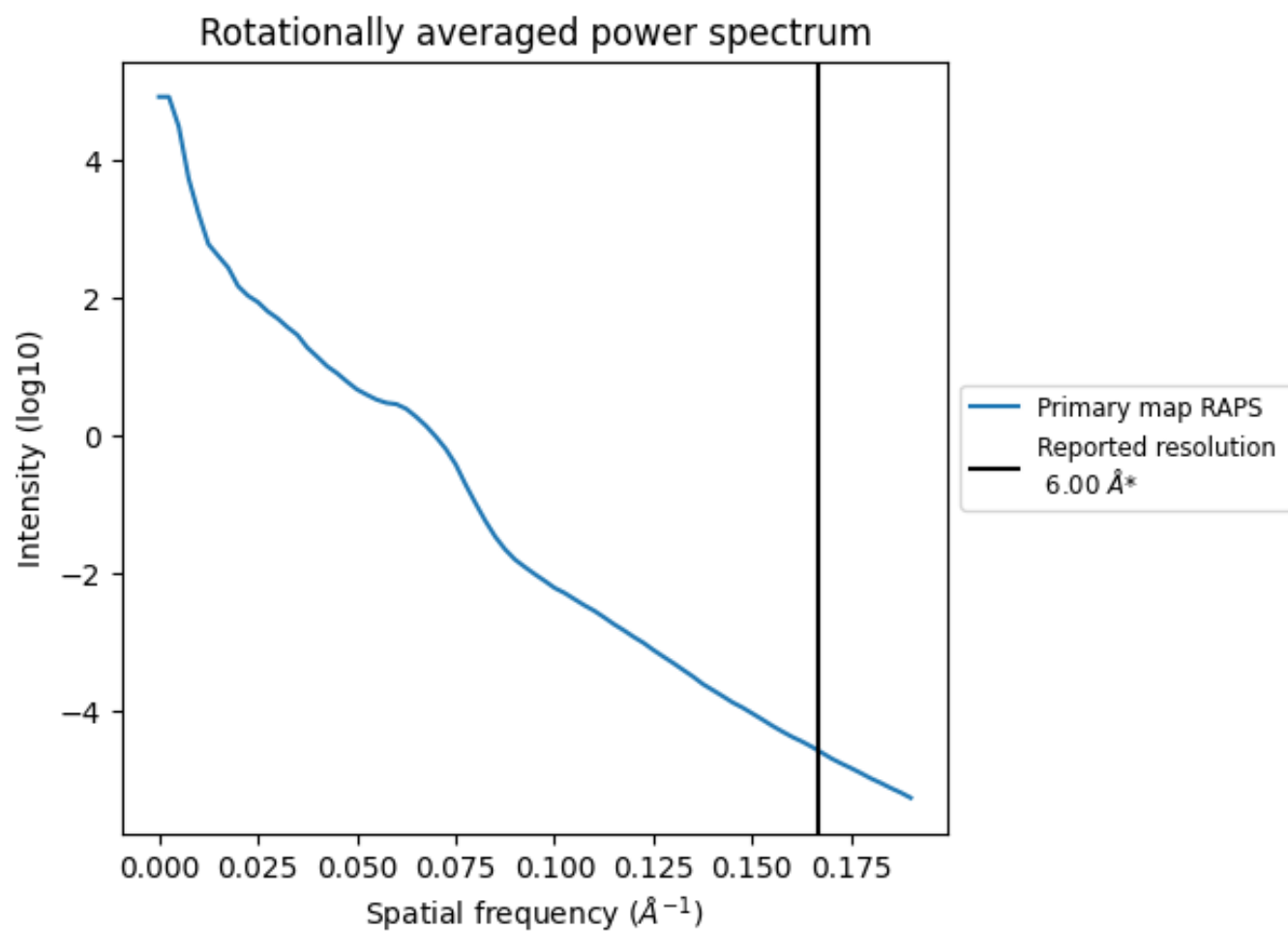
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 637 nm<sup>3</sup>; this corresponds to an approximate mass of 575 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

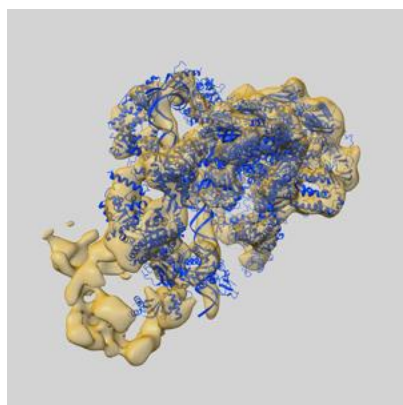
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

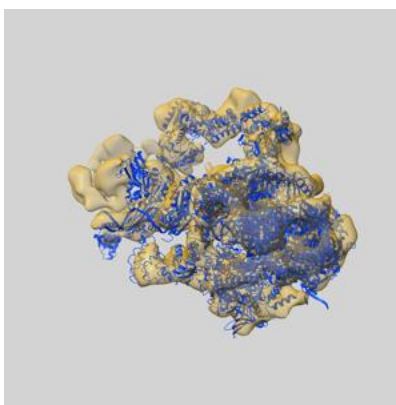
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3114 and PDB model 5FMF. Per-residue inclusion information can be found in section [3](#) on page [9](#).

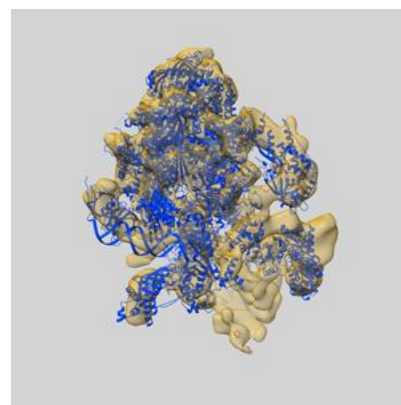
### 9.1 Map-model overlay [i](#)



X



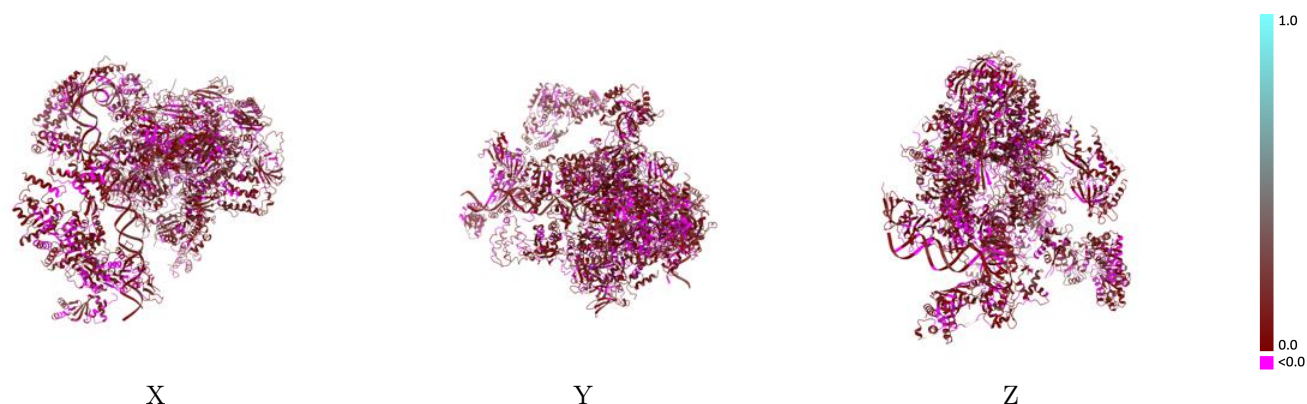
Y



Z

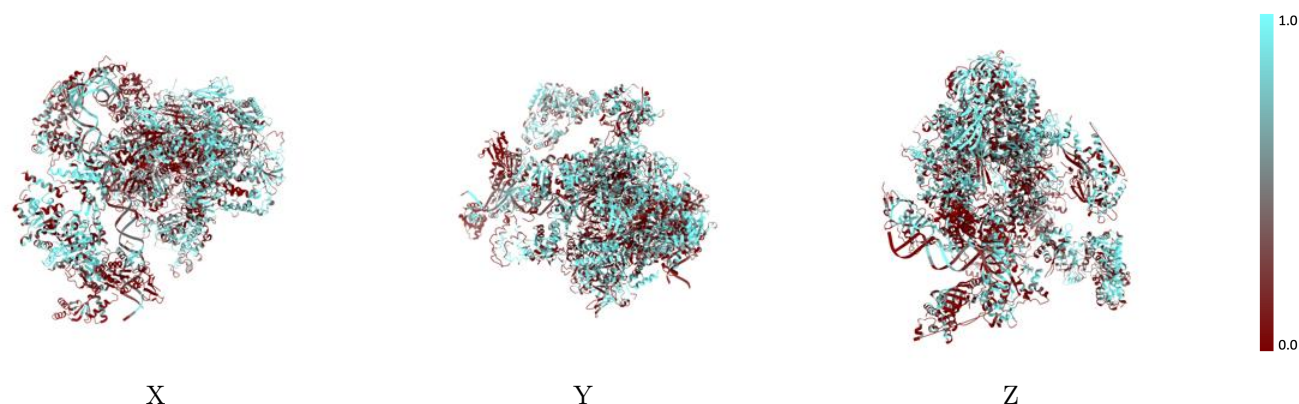
The images above show the 3D surface view of the map at the recommended contour level 3.99 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



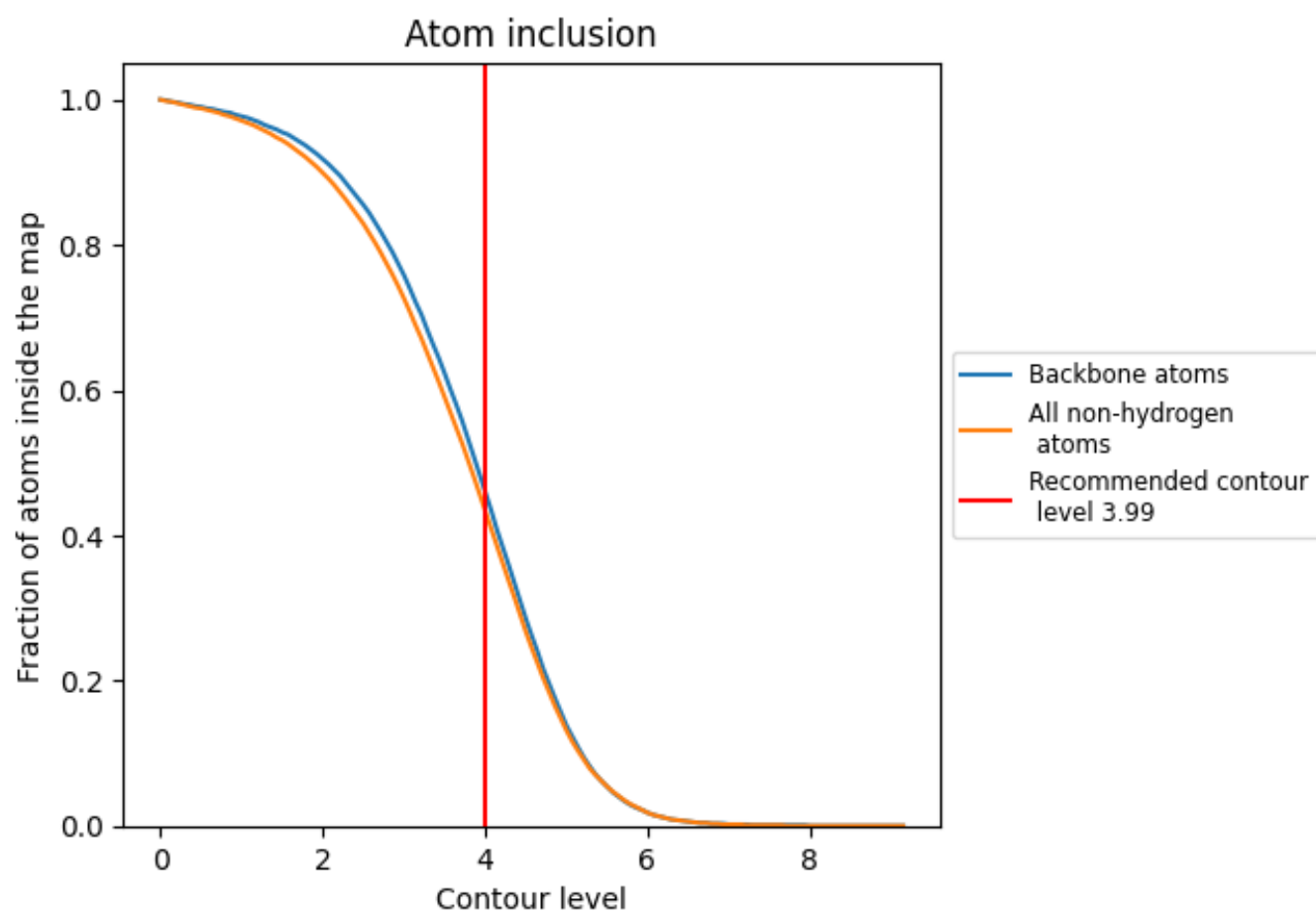
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.99).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.99) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4370	 0.0620
1	 0.2960	 0.0410
2	 0.2870	 0.0410
A	 0.5000	 0.0770
B	 0.4000	 0.0490
C	 0.6130	 0.0640
D	 0.3740	 0.0700
E	 0.5310	 0.0900
F	 0.6780	 0.0690
G	 0.4180	 0.0690
H	 0.5760	 0.0720
I	 0.4410	 0.0600
J	 0.5840	 0.0660
K	 0.5140	 0.0540
L	 0.6550	 0.0600
M	 0.3350	 0.0730
N	 0.3930	 0.0730
O	 0.2420	 0.0580
P	 0.1210	 0.0240
Q	 0.4330	 0.0640
R	 0.4710	 0.0730
S	 0.5090	 0.1020
T	 0.5020	 0.1110
U	 0.3740	 0.0320
V	 0.3860	 0.0590
W	 0.0920	 0.0590
X	 0.1870	 0.0240
Y	 0.5870	 0.0570

