



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 30, 2017 – 01:55 PM EST

PDB ID : 6AWB  
EMDB ID: : EMD-7014  
Title : Structure of 30S ribosomal subunit and RNA polymerase complex in non-rotated state  
Authors : Demo, G.; Rasouly, A.; Vasilyev, N.; Loveland, A.B.; Diaz-Avalos, R.; Grigorieff, N.; Nudler, E.; Korostelev, A.A.  
Deposited on : unknown  
Resolution : 6.70 Å(reported)

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

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

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

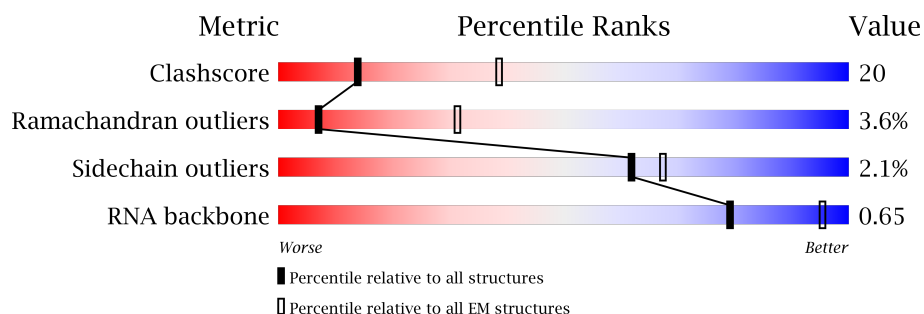
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





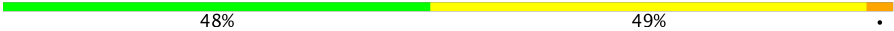








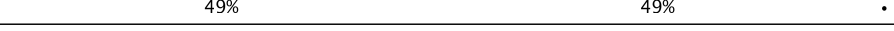







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1539	55% 35% 6%
2	01	229	47% 50% ..
2	02	229	46% 48% . ..
3	03	1340	53% 44% ..
4	04	1369	50% 46% ..
5	05	76	43% 57%
6	B	153	93% 7%
7	E	218	48% 43% 8%

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Mol	Chain	Length	Quality of chain
8	F	206	 64% 34% .
9	G	205	 43% 53% .
10	H	157	 48% 49% .
11	I	100	 51% 46% .
12	J	151	 56% 43% .
13	K	129	 64% 34% .
14	L	127	 54% 42% .
15	M	98	 63% 33% .
16	N	116	 43% 53% .
17	O	123	 59% 38% .
18	P	114	 62% 33% .
19	Q	100	 49% 49% .
20	R	88	 65% 34% .
21	S	82	 59% 38% .
22	T	80	 59% 39% .
23	U	65	 65% 32% .
24	V	79	 48% 49% .
25	W	85	 52% 44% 5%
26	X	65	 46% 45% 9%

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 75316 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1443	Total	C	N	O	P	0	0
			30955	13808	5681	10024	1442		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	01	227	Total	C	N	O	S	0	0
			1753	1091	311	345	6		
2	02	227	Total	C	N	O	S	0	0
			1757	1094	311	346	6		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	03	1327	Total	C	N	O	S	0	0
			10272	6441	1787	2001	43		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	04	1345	Total	C	N	O	S	0	0
			10372	6508	1853	1962	49		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	05	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

- Molecule 6 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	B	153	Total	C	N	O	0	0
			774	463	154	157		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

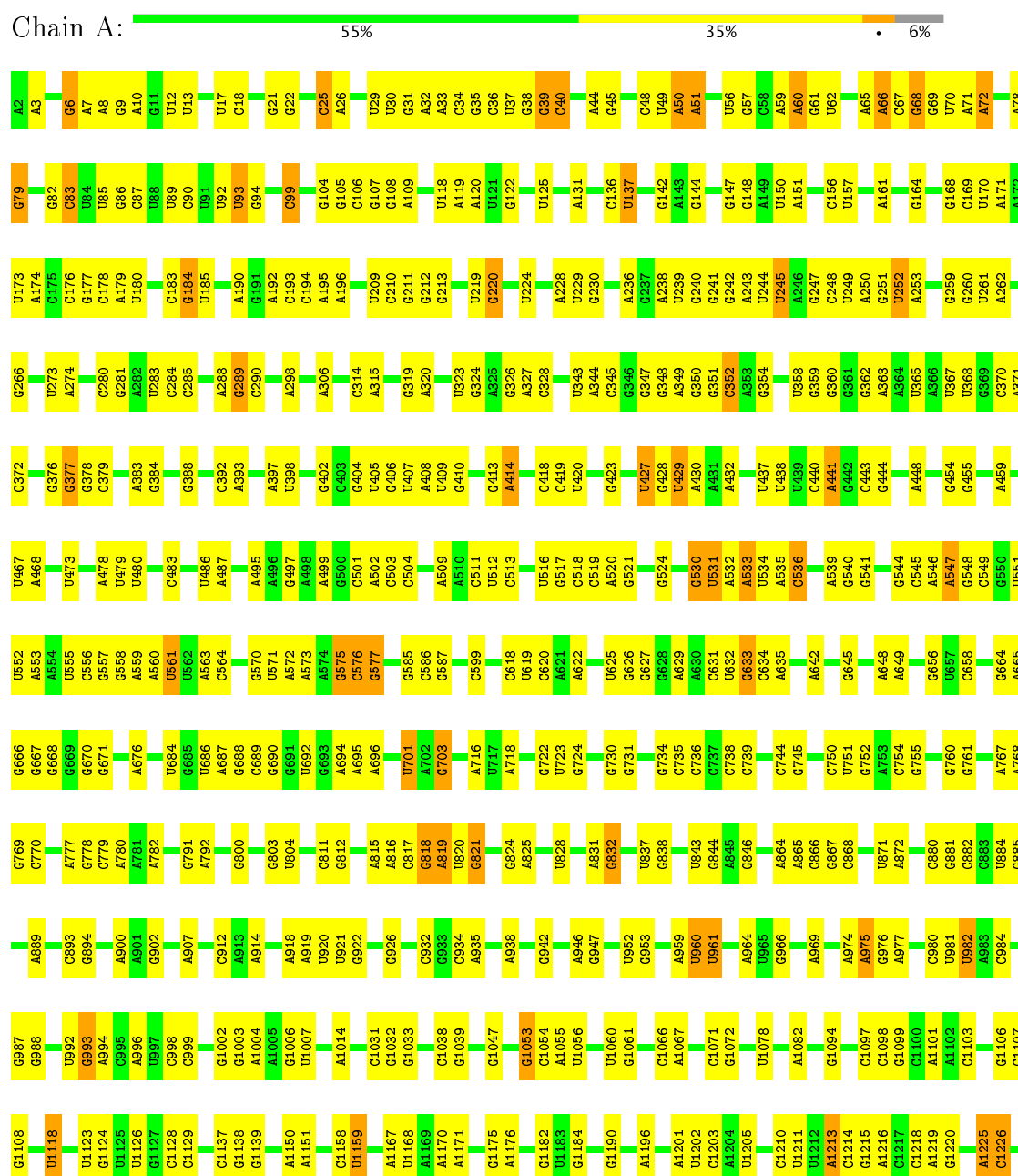
- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

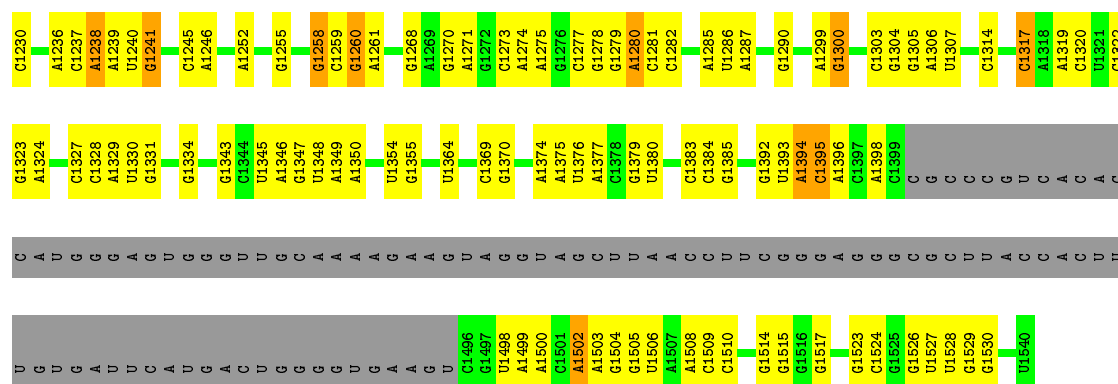
### 3 Residue-property plots

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: 16S rRNA

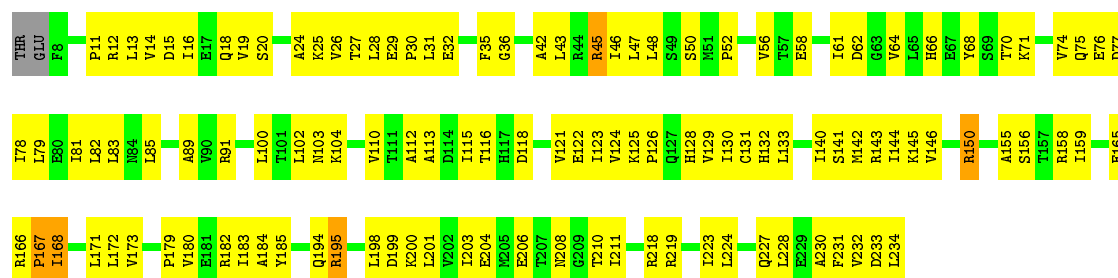






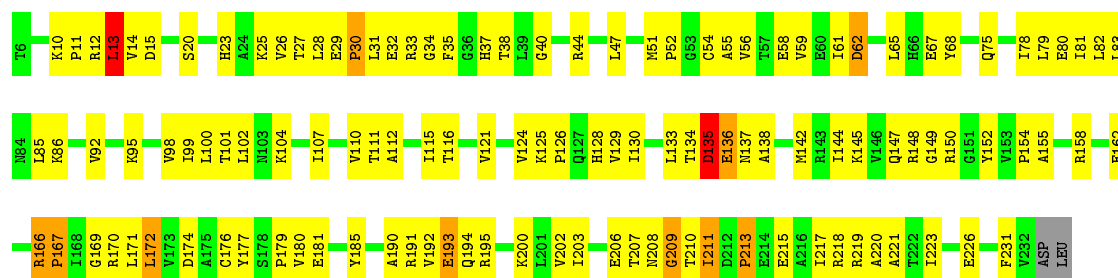
• Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain 01: 47% 50% ..



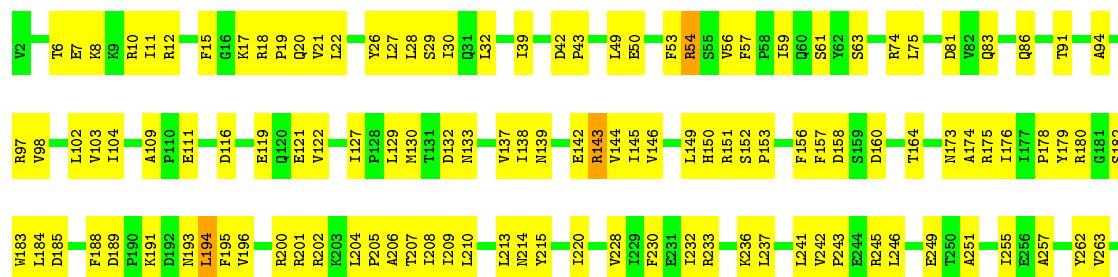
• Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain 02: 46% 48% ..

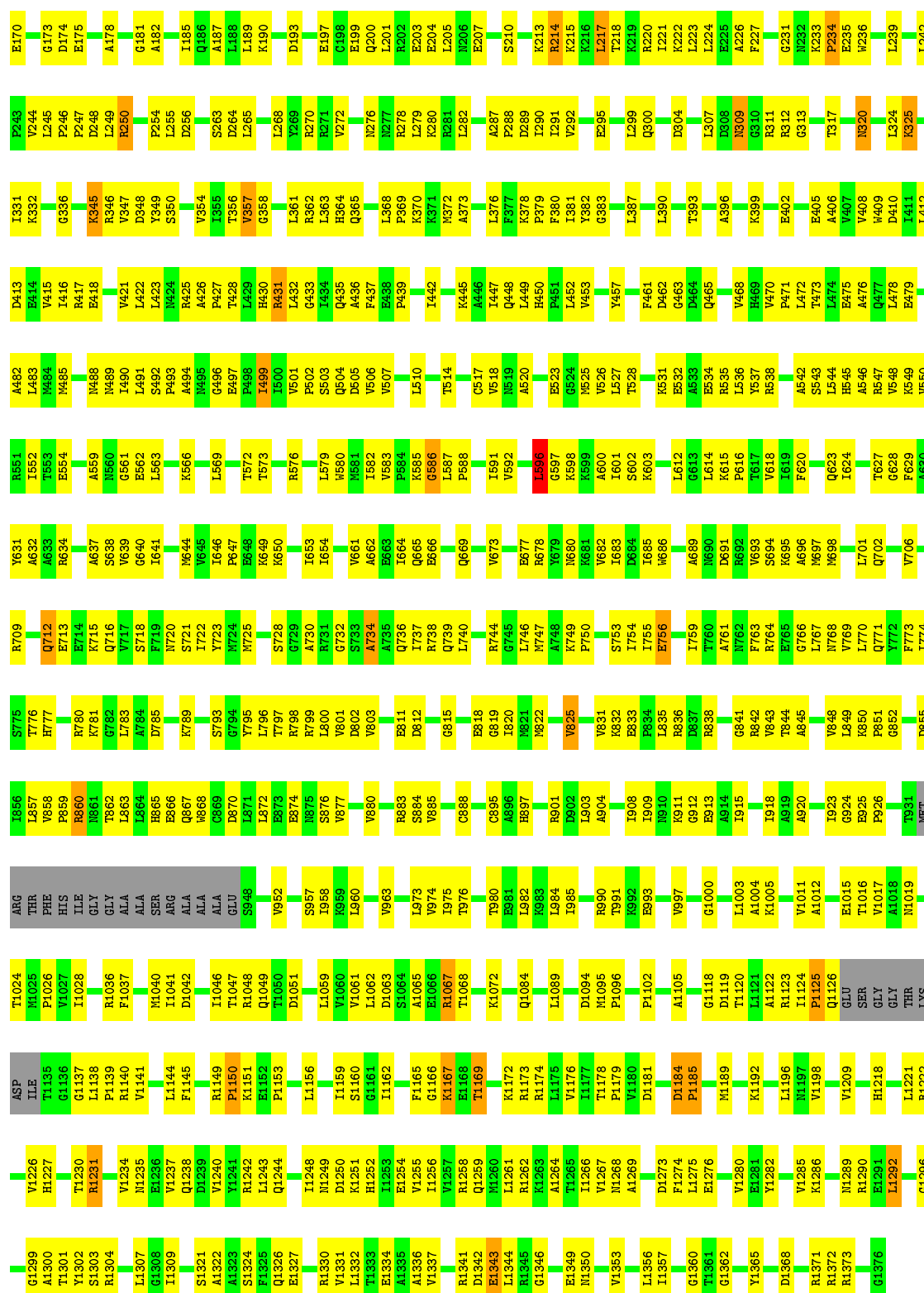


• Molecule 3: DNA-directed RNA polymerase subunit beta

Chain 03: 53% 44% ..

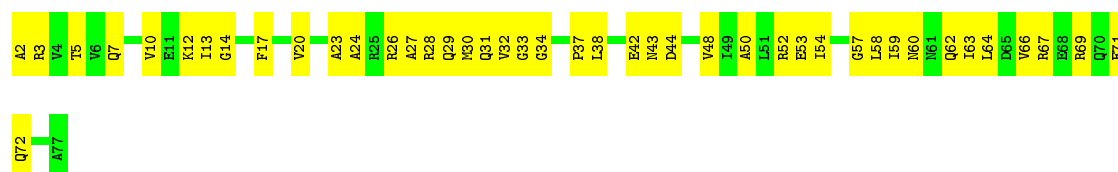


R268	R368	E458	A532	V710	G869	E962	V1046	G1123	K1200	M1290	L8
1269	M369	M459	R540	D711	1870	E963	L1047	G1123	L1204	K1294	Q11
T270	P376	N462	F545	S712	Y871	L964	K1048	M1129	L1204	L1294	T12
R273	A351	Q463	F545	A718	1872	Q965	V1052	A1130	Q1209	M1304	K13
1274	E382	F464	F545	A719	1873	1966	Y1053	A1131	11210	Y1305	R21
L277	S363	R465	V550	R720	1874	L967	Y1053	L1132	R1211	R1211	A19
V282	L384	V467	Y555	G721	1878	L971	A1055	K1133	D1214	I1308	R20
K283	N387	L468	G556	G722	1879	R974	V1056	Q1136	G1215	V1309	K21
L284	L388	V469	R557	V723	1882	1975	K1057	A1137	L1216	H1313	I22
1285	F389	R470	V558	V724	1883	1976	R1058	A1138	T1217	H1313	A23
P288	F390	V471	I561	V725	1884	A977	I1060	A1139	Q1220	M1319	L24
	S391	E472	P564	V726	1885	V978	Q1061	A1140	P1221	P1320	A25
	S391	V475	P564	V727	1886	L979	Q1062	Q1146	F1222	E1321	M29
	S391	V475	P564	V728	1887	V980	G1063	Q1146	F1223	S1322	S32
	S391	V475	P564	V729	1888	G885	G1064	Q1146	P1224	F1323	W33
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	S391	V475	P564	V731	1890	G885	K1066	Q1146	T1226	L1326	V38
	S391	V475	P564	V732	1891	V980	A1067	Q1146	Y1149	L1327	P41
	S391	V475	P564	V733	1892	G885	K1068	Q1146	D1150	K1328	E42
	S391	V475	P564	V734	1893	V980	G1069	Q1146	L1151	M1230	T43
	S391	V475	P564	V735	1894	V980	K1070	Q1146	G1152	Y1231	T44
	S391	V475	P564	V736	1895	V980	K1071	Q1146	Y1155	M1232	N45
	S391	V475	P564	V737	1896	V980	K1072	Q1146	A1156	L1233	Y46
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	S391	V475	P564	V742	1901	V980	K1077	Q1146	I1076	K1242	R53
	S391	V475	P564	V743	1902	V980	K1078	Q1146	I1076	L1243	D54
	S391	V475	P564	V744	1903	V980	K1079	Q1146	I1076	L1244	L56
	S391	V475	P564	V745	1904	V980	K1080	Q1146	I1076	D1245	F57
	S391	V475	P564	V746	1905	V980	K1081	Q1146	I1076	M1246	C58
	S391	V475	P564	V747	1906	V980	K1082	Q1146	I1076	L1253	A59
	S391	V475	P564	V748	1907	V980	K1083	Q1146	I1076	V1254	R60
	S391	V475	P564	V749	1908	V980	K1084	Q1146	I1076	Q1256	I61
	S391	V475	P564	V750	1909	V980	K1085	Q1146	I1076	Q1257	I61
	S391	V475	P564	V751	1910	V980	K1086	Q1146	I1076	P1258	P64
	S391	V475	P564	V752	1911	V980	K1087	Q1146	I1076	G1261	V65
	S391	V475	P564	V753	1912	V980	K1088	Q1146	I1076	K1262	K66
	S391	V475	P564	V754	1913	V980	K1089	Q1146	I1076	F1265	D67
	S391	V475	P564	V755	1914	V980	K1090	Q1146	I1076	F1265	Y68
	S391	V475	P564	V756	1915	V980	K1091	Q1146	I1076	F1265	E69
	S391	V475	P564	V757	1916	V980	K1092	Q1146	I1076	F1265	C70
	S391	V475	P564	V758	1917	V980	K1093	Q1146	I1076	F1265	L71
	S391	V475	P564	V759	1918	V980	K1094	Q1146	I1076	F1265	C72
	S391	V475	P564	V760	1919	V980	K1095	Q1146	I1076	F1265	K74
	S391	V475	P564	V761	1920	V980	K1096	Q1146	I1076	F1265	L78
	S391	V475	P564	V762	1921	V980	K1097	Q1146	I1076	F1265	R81
	S391	V475	P564	V763	1922	V980	K1098	Q1146	I1076	F1265	G82
	S391	V475	P564	V764	1923	V980	K1099	Q1146	I1076	F1265	V83
	S391	V475	P564	V765	1924	V980	K1100	Q1146	I1076	F1265	I84
	S391	V475	P564	V766	1925	V980	K1101	Q1146	I1076	F1265	
	S391	V475	P564	V767	1926	V980	K1102	Q1146	I1076	F1265	
	S391	V475	P564	V768	1927	V980	K1103	Q1146	I1076	F1265	
	S391	V475	P564	V769	1928	V980	K1104	Q1146	I1076	F1265	
	S391	V475	P564	V770	1929	V980	K1105	Q1146	I1076	F1265	
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	S391	V475	P564	V822	1981	V980	K1157	Q1146	I1076	F1265	
	S391	V475	P564	V823	1982	V980	K1158	Q1146	I1076	F1265	
	S391	V475	P564	V824	1983	V980	K1159	Q1146	I1076	F1265	
	S391	V475	P564	V825	1984	V980	K1160	Q1146	I1076	F1265	
	S391	V475	P564	V826	1985	V980	K1161	Q1146	I1076	F1265	
	S391	V475	P564	V827	1986	V980	K1162	Q1146	I1076	F1265	
	S391	V475	P564	V828	1987	V980	K1163	Q1146	I1076	F1265	
	S391	V475	P564	V829	1988	V980	K1164	Q1146	I1076	F1265	
	S391	V475	P564	V830	1989	V980	K1165	Q1146	I1076	F1265	
	S391	V475	P564	V831	1990	V980	K1166	Q1146	I1076	F1265	
	S391	V475	P564	V832	1991	V980	K1167	Q1146	I1076	F1265	
	S391	V475	P564	V833	1992	V980	K1168	Q1146	I1076	F1265	
	S391	V475	P564	V834	1993	V980	K1169	Q1146	I1076	F1265	
	S391	V475	P564	V835	1994	V980	K1170	Q1146	I1076	F1265	
	S391	V475	P564	V836	1995	V980					



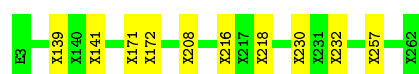
- Molecule 5: DNA-directed RNA polymerase subunit omega

Chain 05:  43% 57%



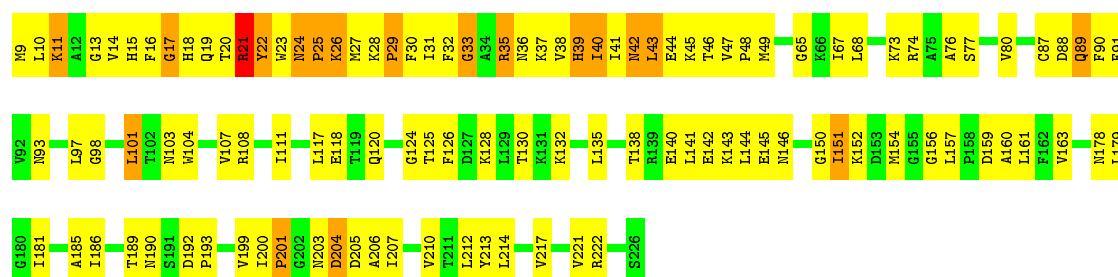
• Molecule 6: 30S ribosomal protein S1

Chain B: 93% 7%



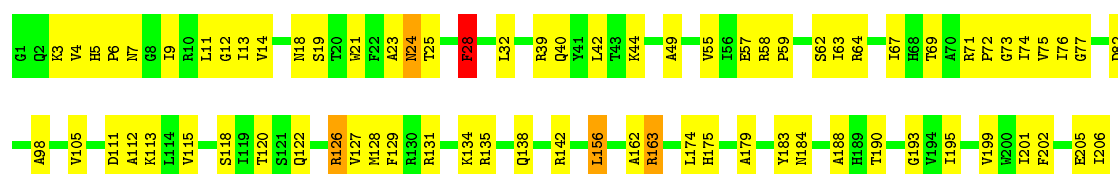
• Molecule 7: 30S ribosomal protein S2

Chain E: 48% 43% 8%



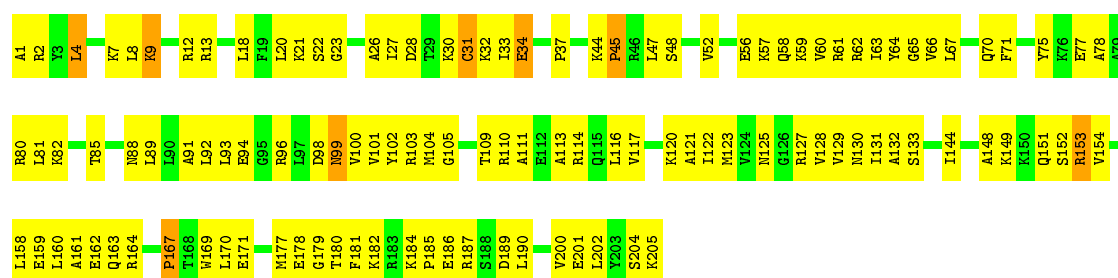
• Molecule 8: 30S ribosomal protein S3

Chain F: 64% 34% 2%

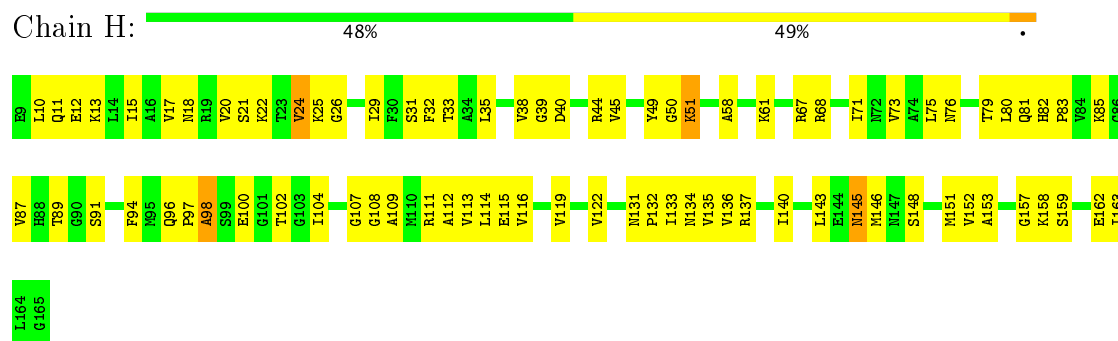


• Molecule 9: 30S ribosomal protein S4

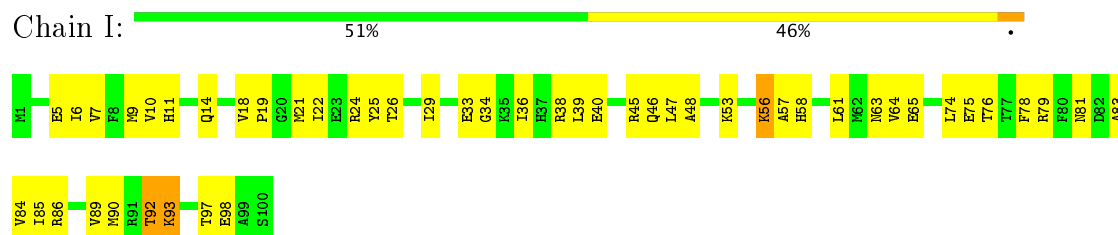
Chain G: 43% 53% 4%



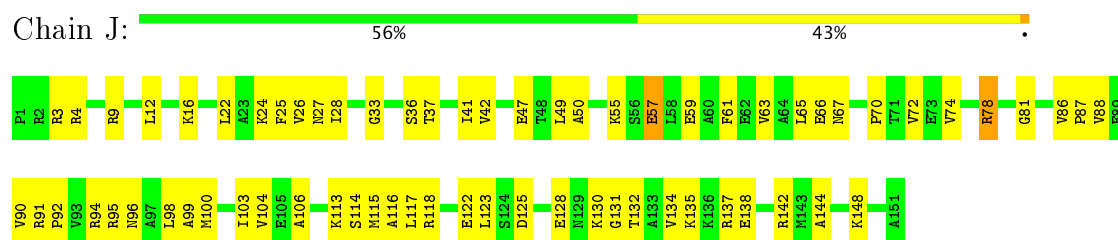
• Molecule 10: 30S ribosomal protein S5



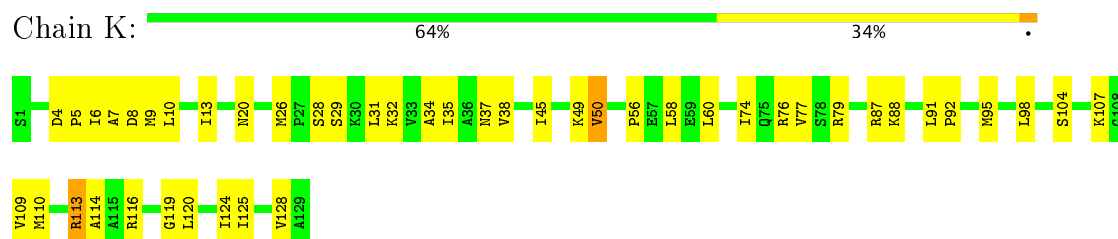
- Molecule 11: 30S ribosomal protein S6



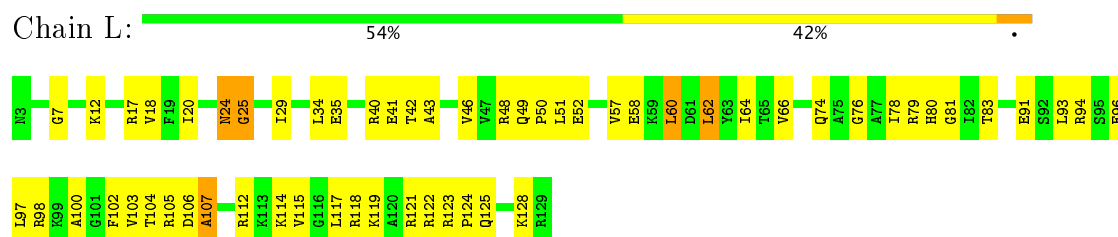
- Molecule 12: 30S ribosomal protein S7



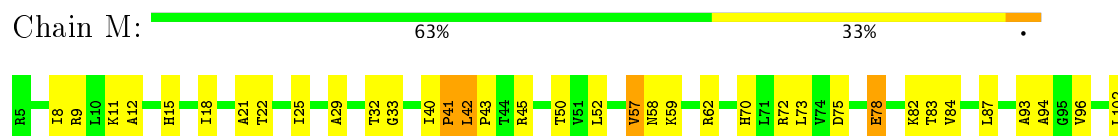
- Molecule 13: 30S ribosomal protein S8



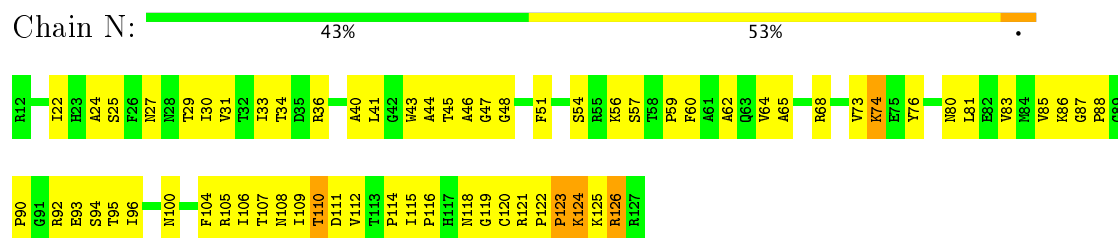
- Molecule 14: 30S ribosomal protein S9



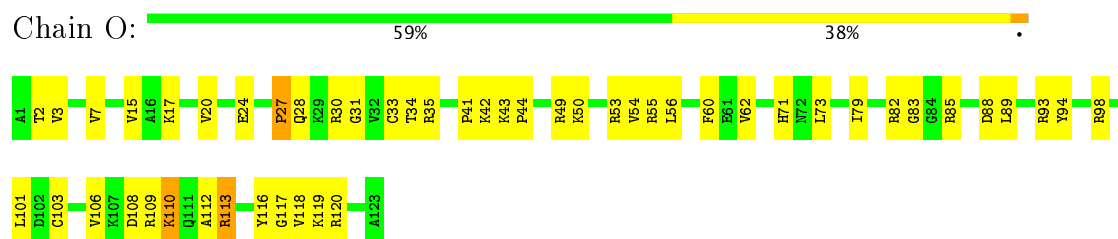
- Molecule 15: 30S ribosomal protein S10



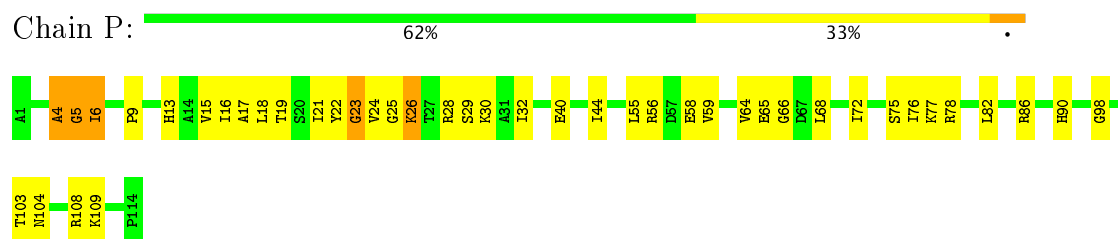
- Molecule 16: 30S ribosomal protein S11



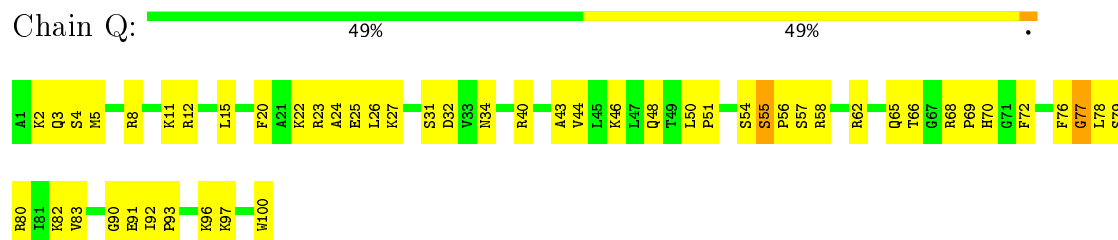
- Molecule 17: 30S ribosomal protein S12



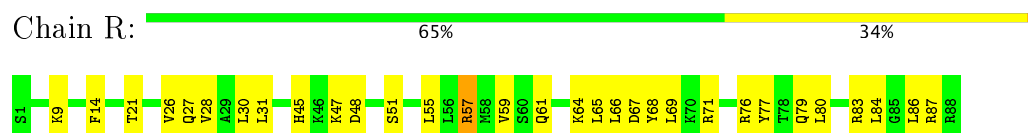
- Molecule 18: 30S ribosomal protein S13



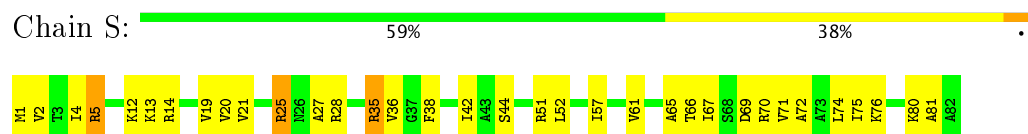
- Molecule 19: 30S ribosomal protein S14



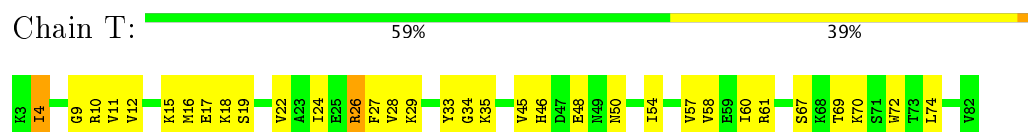
- Molecule 20: 30S ribosomal protein S15



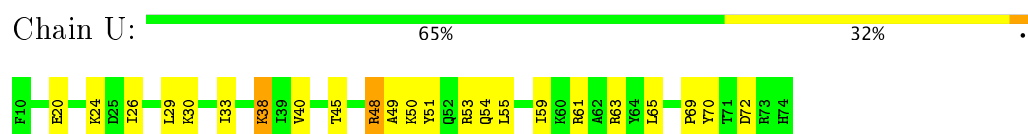
- Molecule 21: 30S ribosomal protein S16



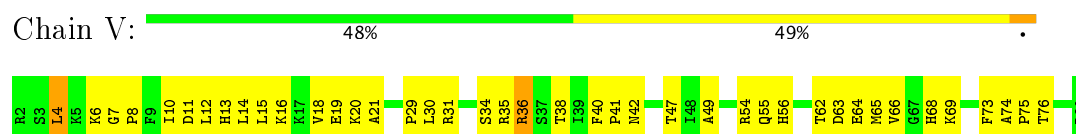
- Molecule 22: 30S ribosomal protein S17



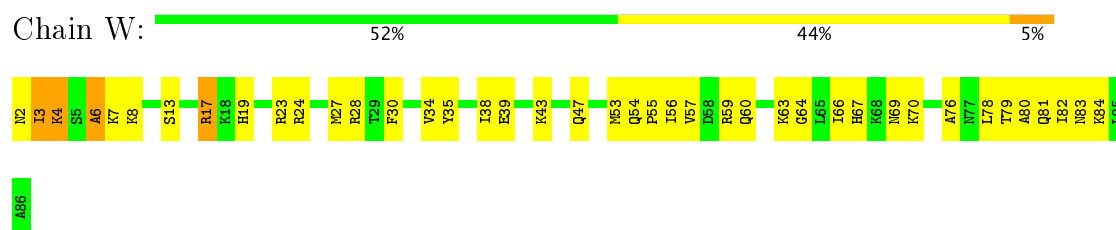
- Molecule 23: 30S ribosomal protein S18



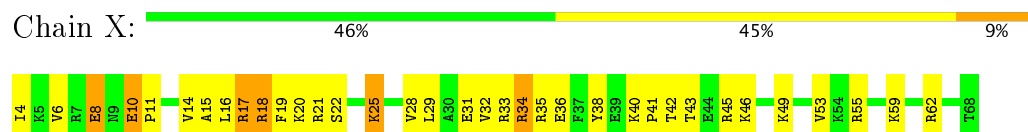
- Molecule 24: 30S ribosomal protein S19



- Molecule 25: 30S ribosomal protein S20



- Molecule 26: 30S ribosomal protein S21



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.32	0/34660	0.67	0/54067
10	H	0.30	0/1170	0.63	0/1573
11	I	0.30	0/836	0.56	0/1128
12	J	0.28	0/1196	0.63	0/1602
13	K	0.31	0/989	0.65	0/1326
14	L	0.30	0/1034	0.60	0/1375
15	M	0.32	0/797	0.60	0/1077
16	N	0.33	0/886	0.64	0/1195
17	O	0.30	0/969	0.65	0/1300
18	P	0.28	0/893	0.60	0/1193
19	Q	0.33	0/817	0.63	1/1088 (0.1%)
2	01	0.25	0/1774	0.61	0/2405
2	02	0.28	0/1779	0.66	2/2411 (0.1%)
20	R	0.30	0/722	0.62	0/964
21	S	0.31	0/659	0.55	0/884
22	T	0.31	0/658	0.60	0/881
23	U	0.35	0/545	0.72	0/731
24	V	0.34	0/653	0.60	0/877
25	W	0.31	0/671	0.59	0/888
26	X	0.39	0/551	0.70	0/728
3	03	0.30	0/10433	0.66	3/14101 (0.0%)
4	04	0.29	0/10528	0.67	4/14224 (0.0%)
5	05	0.28	0/607	0.60	0/817
6	B	0.64	0/65	0.56	0/86
7	E	0.36	0/1736	0.73	2/2338 (0.1%)
8	F	0.30	0/1652	0.59	1/2225 (0.0%)
9	G	0.30	0/1665	0.61	1/2227 (0.0%)
All	All	0.31	0/78945	0.66	14/113711 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	04	1296	GLY	N-CA-C	-6.35	97.22	113.10
2	02	135	ASP	N-CA-C	6.33	128.10	111.00
3	03	843	THR	N-CA-C	-6.31	93.96	111.00
3	03	891	GLY	N-CA-C	6.30	128.84	113.10
4	04	1184	ASP	N-CA-C	6.16	127.63	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	C	Sidechain
1	A	872	A	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	30955	0	15586	433	0
2	01	1753	0	1780	113	0
2	02	1757	0	1778	110	0
3	03	10272	0	10138	556	0
4	04	10372	0	10512	598	0
5	05	605	0	612	41	0
6	B	774	0	200	5	0
7	E	1705	0	1732	157	0
8	F	1625	0	1699	60	0
9	G	1643	0	1710	100	0
10	H	1157	0	1199	66	0
11	I	818	0	808	43	0
12	J	1182	0	1240	59	0
13	K	979	0	1034	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L	1022	0	1070	64	0
15	M	787	0	828	43	0
16	N	870	0	878	60	0
17	O	955	0	1019	38	0
18	P	884	0	944	41	0
19	Q	805	0	847	47	0
20	R	714	0	737	30	0
21	S	649	0	666	25	0
22	T	649	0	691	30	0
23	U	536	0	552	21	0
24	V	638	0	665	50	0
25	W	665	0	714	54	0
26	X	545	0	579	37	0
All	All	75316	0	60218	2681	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 20.

The worst 5 of 2681 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)
7:E:26:LYS:O	7:E:29:PRO:HD2	1.44	1.14
1:A:664:G:H5"	23:U:53:ARG:HH12	1.05	1.10
7:E:47:VAL:HB	7:E:48:PRO:HD3	1.37	1.05
7:E:19:GLN:H	7:E:40:ILE:HA	1.14	1.04
4:04:246:PRO:HD2	4:04:249:LEU:HD12	1.38	1.03

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	
2	01	225/229 (98%)	183 (81%)	38 (17%)	4 (2%)	10	49
2	02	225/229 (98%)	177 (79%)	37 (16%)	11 (5%)	2	27
3	03	1323/1340 (99%)	1053 (80%)	221 (17%)	49 (4%)	4	33
4	04	1339/1369 (98%)	1091 (82%)	205 (15%)	43 (3%)	5	36
5	05	74/76 (97%)	60 (81%)	13 (18%)	1 (1%)	13	54
6	B	6/153 (4%)	6 (100%)	0	0	100	100
7	E	216/218 (99%)	161 (74%)	40 (18%)	15 (7%)	1	20
8	F	204/206 (99%)	178 (87%)	24 (12%)	2 (1%)	18	61
9	G	203/205 (99%)	158 (78%)	38 (19%)	7 (3%)	4	35
10	H	155/157 (99%)	119 (77%)	33 (21%)	3 (2%)	9	47
11	I	98/100 (98%)	78 (80%)	15 (15%)	5 (5%)	2	26
12	J	149/151 (99%)	126 (85%)	20 (13%)	3 (2%)	9	46
13	K	127/129 (98%)	110 (87%)	14 (11%)	3 (2%)	7	42
14	L	125/127 (98%)	94 (75%)	28 (22%)	3 (2%)	7	42
15	M	96/98 (98%)	79 (82%)	11 (12%)	6 (6%)	1	22
16	N	114/116 (98%)	96 (84%)	14 (12%)	4 (4%)	4	34
17	O	121/123 (98%)	87 (72%)	25 (21%)	9 (7%)	1	18
18	P	112/114 (98%)	93 (83%)	12 (11%)	7 (6%)	1	22
19	Q	98/100 (98%)	66 (67%)	28 (29%)	4 (4%)	3	30
20	R	86/88 (98%)	74 (86%)	12 (14%)	0	100	100
21	S	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	2	27
22	T	78/80 (98%)	61 (78%)	13 (17%)	4 (5%)	2	26
23	U	63/65 (97%)	48 (76%)	11 (18%)	4 (6%)	1	22
24	V	77/79 (98%)	59 (77%)	17 (22%)	1 (1%)	14	56
25	W	83/85 (98%)	68 (82%)	10 (12%)	5 (6%)	2	23
26	X	63/65 (97%)	49 (78%)	9 (14%)	5 (8%)	1	17
All	All	5540/5784 (96%)	4435 (80%)	903 (16%)	202 (4%)	7	33

5 of 202 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	02	13	LEU
2	02	62	ASP
2	02	135	ASP

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Mol	Chain	Res	Type
2	02	193	GLU
3	03	288	PRO

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	01	194/197 (98%)	191 (98%)	3 (2%)	70	86
2	02	194/197 (98%)	188 (97%)	6 (3%)	45	71
3	03	1098/1155 (95%)	1079 (98%)	19 (2%)	66	84
4	04	1103/1141 (97%)	1087 (98%)	16 (2%)	70	86
5	05	65/65 (100%)	65 (100%)	0	100	100
6	B	6/7 (86%)	6 (100%)	0	100	100
7	E	180/180 (100%)	173 (96%)	7 (4%)	37	66
8	F	170/170 (100%)	165 (97%)	5 (3%)	48	73
9	G	172/172 (100%)	167 (97%)	5 (3%)	48	73
10	H	119/119 (100%)	116 (98%)	3 (2%)	53	77
11	I	87/87 (100%)	86 (99%)	1 (1%)	78	89
12	J	124/124 (100%)	123 (99%)	1 (1%)	85	92
13	K	104/104 (100%)	100 (96%)	4 (4%)	38	67
14	L	105/105 (100%)	102 (97%)	3 (3%)	48	73
15	M	86/86 (100%)	86 (100%)	0	100	100
16	N	89/89 (100%)	85 (96%)	4 (4%)	32	63
17	O	103/103 (100%)	99 (96%)	4 (4%)	37	66
18	P	92/92 (100%)	92 (100%)	0	100	100
19	Q	83/83 (100%)	83 (100%)	0	100	100
20	R	76/76 (100%)	75 (99%)	1 (1%)	73	87
21	S	65/65 (100%)	62 (95%)	3 (5%)	31	62
22	T	74/74 (100%)	73 (99%)	1 (1%)	71	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	56/56 (100%)	54 (96%)	2 (4%)	40	68
24	V	70/70 (100%)	68 (97%)	2 (3%)	48	73
25	W	65/65 (100%)	62 (95%)	3 (5%)	31	62
26	X	55/55 (100%)	52 (94%)	3 (6%)	25	58
All	All	4635/4737 (98%)	4539 (98%)	96 (2%)	62	80

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	04	1332	LEU
8	F	126	ARG
24	V	4	LEU
7	E	11	LYS
7	E	89	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
4	04	1235	ASN
7	E	178	ASN
20	R	39	GLN
4	04	1279	GLN
5	05	43	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1441/1539 (93%)	170 (11%)	2 (0%)

5 of 170 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	A
1	A	31	G
1	A	32	A
1	A	39	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	69	G
1	A	343	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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
6	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	10:GLU	C	107:UNK	N	56.44
1	B	179:UNK	C	191:UNK	N	18.18