



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

Jul 18, 2017 – 04:43 PM EDT

PDB ID : 4V5H  
EMDB ID: : EMD-1657  
Title : E.Coli 70s Ribosome Stalled During Translation Of Tnac Leader Peptide.  
Authors : Seidelt, B.; Innis, C.A.; Wilson, D.N.; Gartmann, M.; Armache, J.; Villa, E.;  
Trabuco, L.G.; Becker, T.; Mielke, T.; Schulten, K.; Steitz, T.A.; Beckmann,  
R.  
Deposited on : unknown  
Resolution : 5.80 Å(reported)  
Based on PDB ID : 3FIH, 3FIK

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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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-20029824

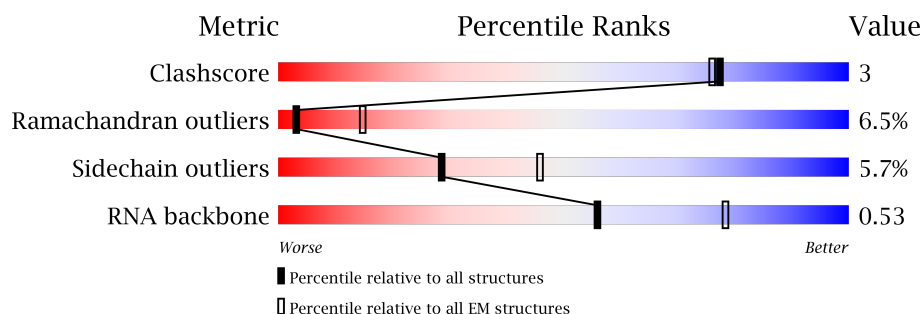
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.80 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	AA	1530	35% 47% 18%
2	AB	218	68% 28% .
3	AC	206	65% 25% 9% .
4	AD	205	67% 24% 8%
5	AE	150	65% 28% 7% .
6	AF	100	65% 28% 6% .
7	AG	150	67% 25% 7% .
8	AH	129	71% 26% .


















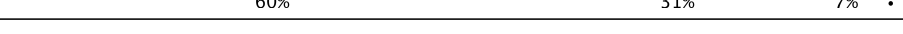





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Mol	Chain	Length	Quality of chain
9	AI	127	 59% 33% 7% .
10	AJ	98	 54% 42% .
11	AK	117	 70% 26% . .
12	AL	123	 66% 25% 8% .
13	AM	113	 60% 28% 9% .
14	AN	96	 64% 27% 9%
15	AO	88	 67% 25% 7% .
16	AP	80	 64% 33% . .
17	AQ	80	 65% 26% 8% .
18	AR	55	 64% 27% 9%
19	AS	79	 59% 30% 10%
20	AT	85	 73% 22% . .
21	AU	51	 65% 27% 8%
22	AV	77	 . 57% 29% 13%
23	AX	11	 9% 18% 27% 45%
24	AZ	20	 80% 20%
25	B0	77	 70% 25% 5%
26	B1	63	 65% 32% .
27	B2	58	 76% 24%
28	B3	56	 66% 25% 7% .
29	B4	50	 66% 30% .
30	B5	234	 77% 20% .
31	B6	46	 59% 20% 20% .
32	B7	64	 59% 39% .
33	B8	38	 76% 24%

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Mol	Chain	Length	Quality of chain
34	BA	117	 42% 43% 14% .
35	BB	2903	 38% 45% 17%
36	BC	271	 68% 25% 6% .
37	BD	209	 67% 23% 8% .
38	BE	201	 66% 27% 6%
39	BF	178	 63% 26% 10% .
40	BG	176	 72% 22% 6% .
41	BH	149	 74% 21% 5%
42	BI	141	 35% 59% 6%
43	BJ	142	 69% 21% 8% .
44	BK	121	 64% 26% 8% .
45	BL	143	 67% 29% .
46	BM	136	 68% 29% . .
47	BN	120	 67% 27% 7%
48	BO	116	 74% 22% .
49	BP	114	 68% 25% 7%
50	BQ	117	 60% 31% 7% .
51	BR	103	 59% 32% 7% .
52	BS	110	 61% 27% 12%
53	BT	93	 56% 39% 5%
54	BU	102	 62% 26% 6% . .
55	BW	94	 61% 31% 7% .
56	BY	79	 63% 27% 6% .

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 145960 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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	113	Total	C	N	O	S	0	0
			876	541	177	155	3		

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	80	Total	C	N	O	S	0	0
			638	400	126	111	1		

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called P-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0
			1649	733	297	542	77		

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AX	11	Total	C	N	O	P	0	0
			236	106	46	73	11		

- Molecule 24 is a protein called POLY-ALA NASCENT CHAIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	AZ	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B1	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L32.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	B3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B4	50	Total	C	N	O		0	0
			409	263	75	71			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B5	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	B8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 34 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	115	Total	C	N	O	P	0	0
			2464	1097	451	801	115		

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BB	2903	Total	C	N	O	P	0	0
			62321	27801	11467	20150	2903		

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BF	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BG	175	Total	C	N	O	S	0	0
			1316	827	242	245	2		

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BH	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BJ	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BK	121	Total	C	N	O	S	0	0
			930	582	179	163	6		

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BO	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BP	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BQ	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BR	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BS	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BU	99	Total	C	N	O		0	0
			755	479	140	136			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BW	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

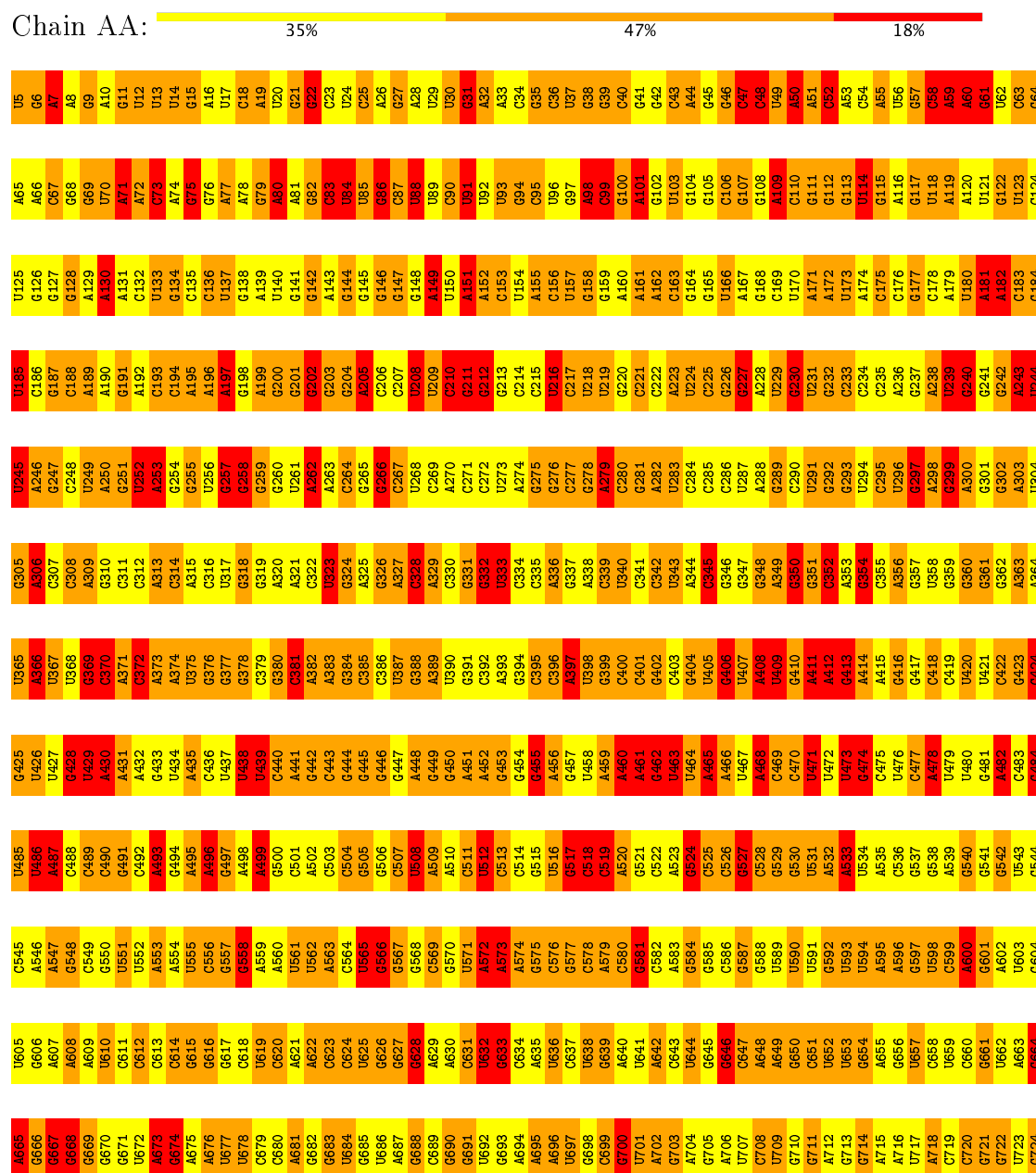
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	BY	79	596	367	120	108	1	0	0

### 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.

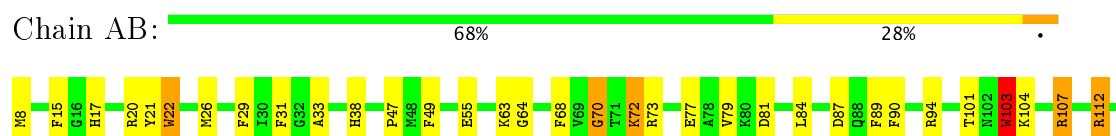
#### • Molecule 1: 16S RIBOSOMAL RNA



G1505	U1445	C1325	C1265	U1025	U965	U905	A845	G785	G725
U1506	A1446	U1326	G1266	G1026	G966	A906	A846	G786	G726
A1507	A1447	C1327	G1267	G1027	C967	A907	G847	A787	G727
A1508	C1448	C1328	G1268	C1028	A968	A908	C948	U788	A728
C1509	C1449	A1329	A1269	C1029	G1089	A909	G849	U789	A729
C1510	U1330	G1330	G1270	U1030	C970	C910	U850	U790	A730
U1511	U1331	G1331	A1271	C1031	G971	U911	G851	U791	G731
U1512	C1332	A1332	G1272	G1032	G972	C912	G852	A792	C732
A1513	A1333	G1333	G1273	G1033	C973	A913	C853	U793	G733
G1514	G1454	G1334	A1274	G1034	A974	A914	U854	A794	G734
G1515	C1335	U1335	G1275	A1035	A975	A915	U855	G795	C735
G1516	A1456	G1336	A1276	A1036	G976	U916	C856	G796	C736
U1517	C1337	G1337	G1277	C1037	A977	G917	C857	C797	C737
A1518	G1338	G1338	G1278	C1038	A978	A918	G858	U798	C738
C1519	C1339	A1339	G1279	G1039	C979	A919	G859	G799	C739
C1520	C1400	A1340	A1280	U1040	C980	U920	A860	G800	U740
G1521	G1401	U1341	C1281	G1041	U981	U921	G861	U801	G741
U1522	C1462	C1342	G1282	A1042	U982	G922	C862	A802	G742
G1523	U1463	G1343	U1283	G1043	A983	A923	U863	G803	A743
G1524	U1464	C1344	C1284	A1044	C984	G924	A864	U804	C744
G1525	A1465	U1345	A1285	A1105	C985	G925	A865	C805	G745
C1526	C1466	A1346	U1286	A1046	U986	G926	C866	C806	A746
U1527	C1467	G1347	A1287	G1047	C987	G927	G867	A807	A747
A1528	A1468	U1348	A1288	U1048	G988	G928	C868	C808	G748
G1529	C1469	A1349	A1289	G1049	U989	G929	G869	G809	A749
G1530	U1470	A1350	G1290	C1050	C990	C930	U870	C810	C750
A1531	U1471	U1351	U1291	C1051	U991	C931	U871	C811	U751
U1532	U1472	C1352	G1292	C1172	U992	C932	A872	G812	G752
C1533	G1473	G1353	C1293	C1173	G993	G933	A873	U813	A753
A1534	U1474	U1354	G1294	C1054	A994	C934	G874	A814	C754
	G1475	G1355	U1295	A1055	C995	A935	U875	A815	G755
	A1476	G1356	C1296	U1056	A996	C936	G876	A816	C756
	U1477	A1357	G1297	G1057	U997	A937	G877	C817	U757
	U1478	U1358	U1298	C1058	C998	A938	A878	G818	C758
	C1479	C1359	A1299	C1059	C999	G939	C879	A819	A759
	A1480	U1420	A1360	U1060	A1000	C940	C880	U820	G760
	U1481	G1361	U1301	G1061	G1001	G941	G881	G821	G761
	G1482	A1362	C1302	G1242	G1002	G942	C882	U822	U762
	A1483	A1363	C1303	C1243	G1003	U943	C883	C823	G763
	C1484	G1364	G1304	G1244	U804	G944	G884	G824	C764
	U1485	G1365	G1305	U1065	A1005	G945	G885	A825	G765
	G1486	C1366	A1306	C1066	G1006	A946	G886	C826	A766
	G1487	C1367	U1307	A1067	U1007	G947	G887	U827	A767
	G1488	A1368	U1308	C1068	U1008	C948	G888	U828	A768
	U1489	C1369	G1309	G1069	U1009	A949	A889	G829	G769
	U1490	G1370	U1310	U1070	U1010	U950	G890	A830	C770
	G1491	G1371	A1311	C1071	C1011	G951	U891	G831	G771
	A1492	U1372	G1312	G1252	A1012	U952	A892	G832	U772
	A1493	G1373	U1313	G1253	G1013	G953	C893	G833	G773
	G1494	A1374	C1314	G1254	A1014	G954	G894	U834	G774
	U1495	A1375	G1315	G1255	G1015	U955	G895	U835	G775
	C1496	U1376	G1316	A1256	U1016	U956	C896	G836	G776
	G1497	A1377	A1317	G1257	U1017	U957	C897	U837	A777
	U1498	C1378	A1318	G1258	G1018	A958	G898	G838	G778
	A1499	G1379	A1319	C1259	U1019	A959	C899	C839	C779
	U1500	U1380	C1320	G1260	G1020	U960	A900	C840	A780
	C1501	U1381	A1261	A1081	A1021	U961	A901	C841	A781
	A1502	C1382	C1262	A1082	A1022	C962	G902	U842	A782
	U1503	G1383	C1263	G1143	U1023	G963	G903	U843	C783
	G1504	C1384	A1324	G1144	G1024	A964	U904	G844	A784

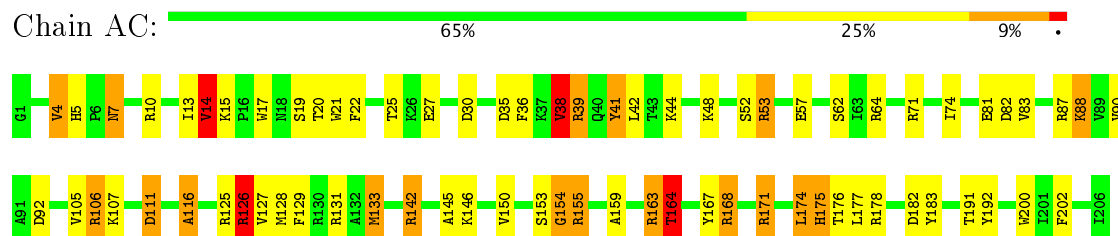
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:

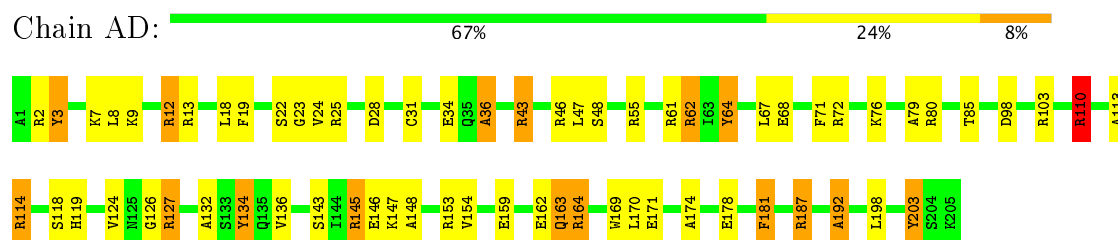




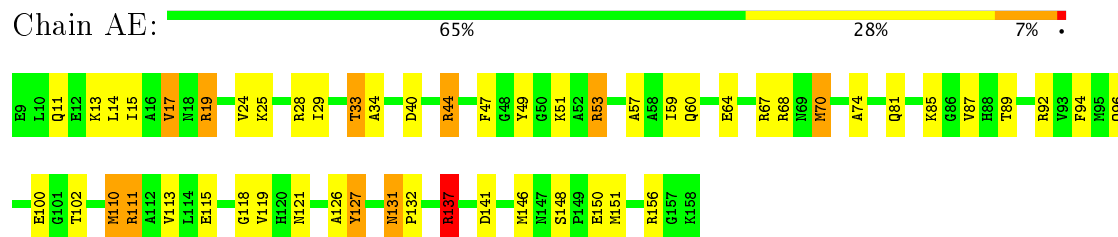
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



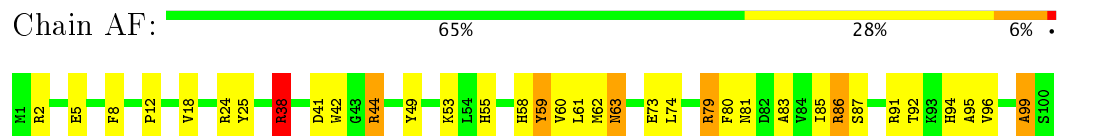
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



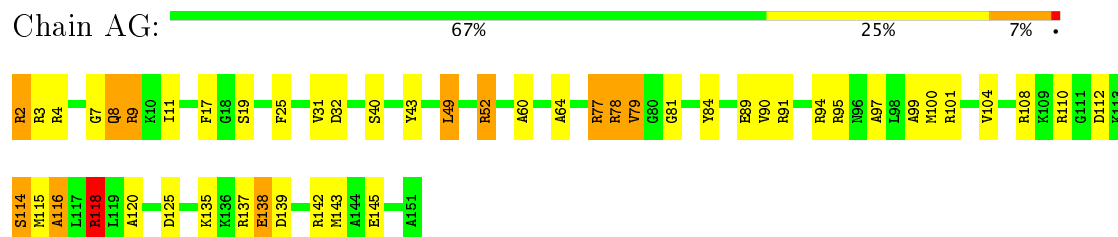
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

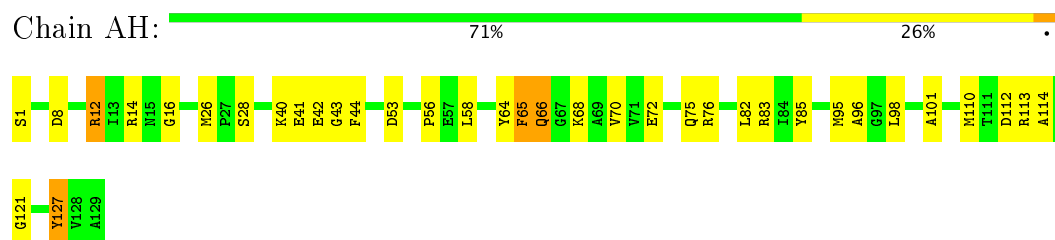


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

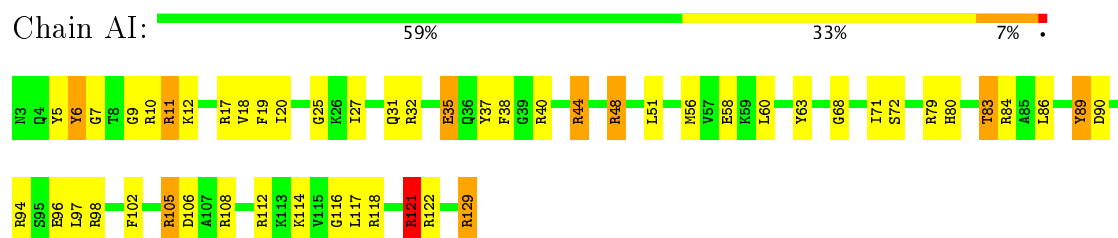




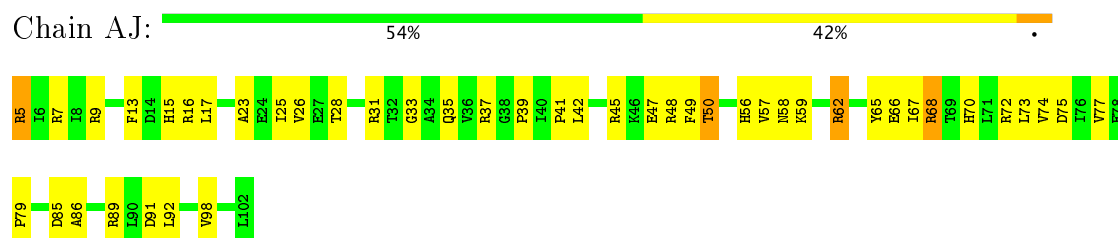
- Molecule 8: 30S RIBOSOMAL PROTEIN S8



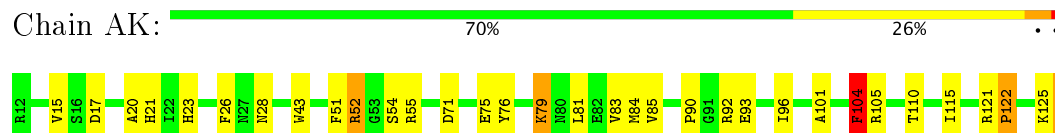
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



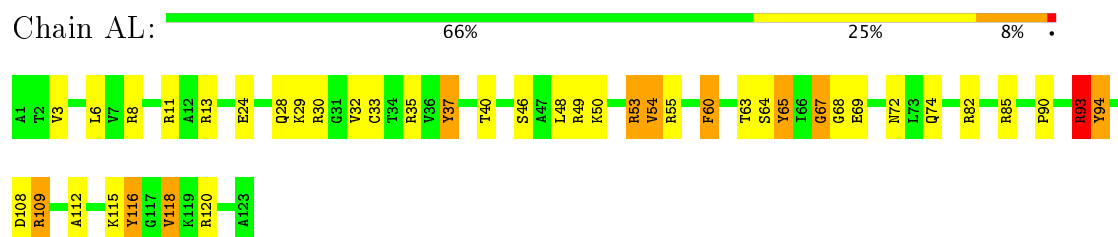
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



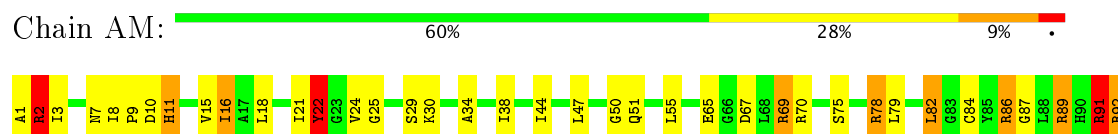
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



- Molecule 12: 30S RIBOSOMAL PROTEIN S12



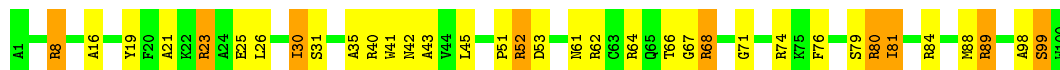
- Molecule 13: 30S RIBOSOMAL PROTEIN S13





- Molecule 14: 30S RIBOSOMAL PROTEIN S14

Chain AN: 



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 



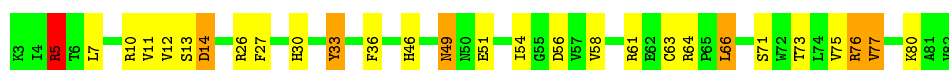
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:  64% 33% .



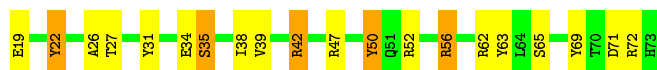
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 



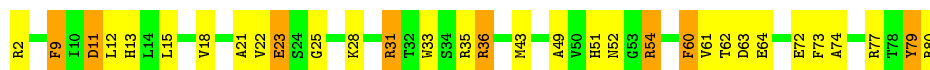
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 

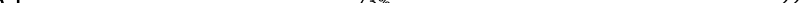


- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 



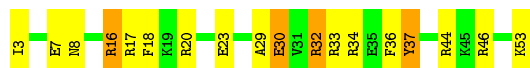
- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:  73% 22% 5%



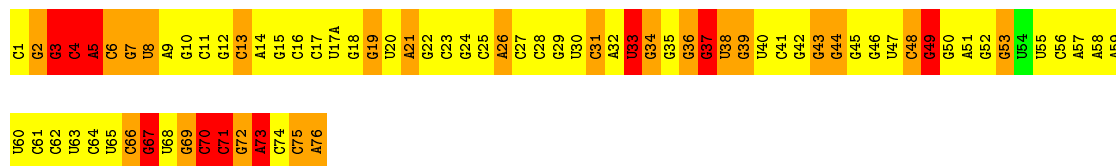
- Molecule 21: 30S RIBOSOMAL PROTEIN S21

Chain AU:  65% 27% 8%




- Molecule 22: P-SITE TRNA

Chain AV:  57% 29% 13%




- Molecule 23: MRNA

Chain AX:  9% 18% 27% 45%



- Molecule 24: POLY-ALA NASCENT CHAIN

Chain AZ:  80% 20%



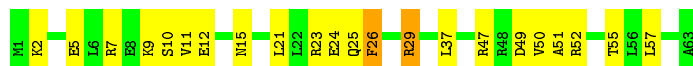
- Molecule 25: 50S RIBOSOMAL PROTEIN L28

Chain B0:  70% 25% 5%




- Molecule 26: 50S RIBOSOMAL PROTEIN L29

Chain B1:  65% 32% 3%



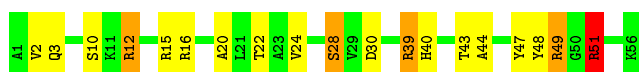
- Molecule 27: 50S RIBOSOMAL PROTEIN L30

Chain B2:  76% 24%



- Molecule 28: 50S RIBOSOMAL PROTEIN L32

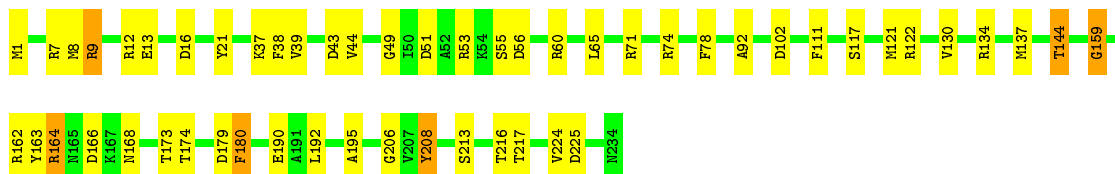
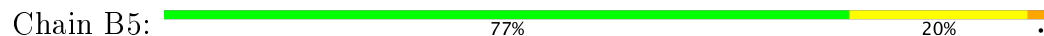
Chain B3:  66% 25% 7% 2%



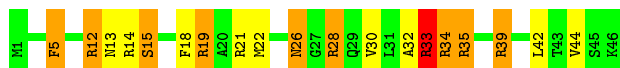
- Molecule 29: 50S RIBOSOMAL PROTEIN L33



- Molecule 30: 50S RIBOSOMAL PROTEIN L1



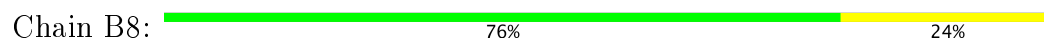
- Molecule 31: 50S RIBOSOMAL PROTEIN L34



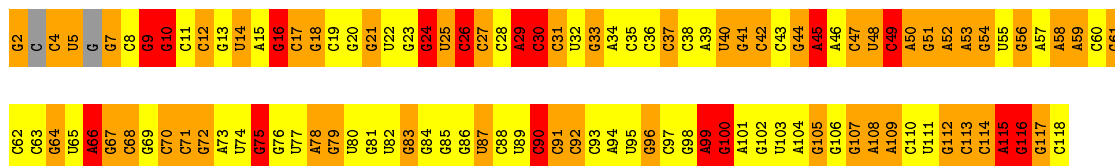
- Molecule 32: 50S RIBOSOMAL PROTEIN L35



- Molecule 33: 50S RIBOSOMAL PROTEIN L36



- Molecule 34: 5S RIBOSOMAL RNA



- Molecule 35: 23S RIBOSOMAL RNA

Chain BB:

38%

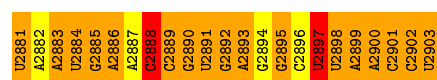
45%

17%

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G2	U62	G122	A182	G242	G302	A362	A422	A482	C542	A602	G662	A722	A782	G842	C902
G3	A63	G123	C183	U243	G303	G363	A423	A483	G543	A603	G663	C723	A783	G843	C903
U4	U64	G124	C184	A244	U304	G364	G424	C484	C544	G604	G664	U724	A784	A844	G904
A5	U65	A125	G185	G245	C305	U365	G425	C485	U545	G605	U665	G725	A785	A845	A905
A6	C66	A126	G186	C246	U306	C366	C426	C486	U546	G606	A666	G726	A786	U846	U906
G7	U67	A127	G187	G247	G307	G367	U427	C487	A547	G607	U667	A727	A787	U847	G907
C8	G68	C128	G188	U248	G308	A368	A428	C488	G548	A608	A668	G728	A788	C848	C908
G9	C69	C129	G189	C249	A309	U369	A429	C489	G549	A609	G669	G729	A789	C849	A909
A10	G70	C130	A190	G250	A310	G370	A430	C490	C550	G610	A670	A730	A790	U850	A910
C11	A71	A131	A191	A251	A311	A371	U431	C491	G551	C611	C671	C731	A791	C851	A911
U12	U72	G132	C192	G252	G312	G372	A432	C492	U552	G612	G672	G732	A792	U852	C912
A13	A73	U133	U193	C263	G313	U373	C433	C493	G553	A613	C673	G733	A793	C853	U913
A14	A74	G134	G194	G264	C314	A374	U434	C494	U554	A614	G674	A734	A794	C854	G914
G15	G75	U135	A195	A265	G315	G375	C435	C495	G555	U615	A675	A735	A795	G855	G915
C16	C76	G136	A196	A266	C316	A376	U436	C496	U556	A616	A676	A736	A796	G856	A916
G17	U77	U137	A197	G267	G317	G377	U437	C497	G557	G617	A677	G737	A797	G857	A917
U18	U78	U138	C198	G268	C318	C378	U438	C498	U558	G618	C678	G738	A798	G858	A918
A19	C79	U139	A199	G269	G319	G379	A439	C499	G559	G619	C679	A739	A799	G859	U919
C20	G80	C140	U200	G270	A320	G380	C440	C500	G560	G620	C680	C740	A800	U860	A920
A21	G81	G141	C201	G271	U321	G381	U441	C501	G561	A621	G681	C741	A801	U861	C921
G22	U82	C142	U202	G272	A322	C382	A442	C502	U562	G622	G682	A742	A802	G862	C922
C23	A83	C143	A203	G273	C323	C383	A443	C503	A563	C623	U683	A743	A803	G863	G923
G24	A84	A144	A204	C264	A324	A384	C444	C504	C564	G624	G684	U744	A804	G864	G924
U25	G85	C145	G205	A265	G325	C385	C445	C505	U565	G625	A685	G745	A805	C865	A925
G26	G86	A146	U206	G266	G326	G386	U446	C506	U566	A626	U686	U746	A806	A866	G926
G27	U87	C147	A207	C267	G327	U387	A447	C507	U567	A627	C687	U747	A807	C867	A927
U29	A89	U149	C209	G268	U328	G388	U448	C508	U568	G628	U688	G748	A808	U868	A928
G30	U90	U150	C210	G269	G329	C389	A449	C509	U569	G629	A689	A749	A809	G869	U929
C31	A91	C151	C211	G271	C331	U391	U451	C511	U571	A631	C691	A751	A811	U871	U931
C32	U92	A152	G212	A272	A332	U392	A452	C512	A572	A632	C692	A752	A812	U872	U932
C33	G93	U153	A213	G273	G333	C393	A453	C513	U573	A633	C693	A753	A813	U873	A933
U34	A94	A154	G214	C274	C334	C394	A454	C514	A574	A634	U694	U754	A814	G874	U934
G35	A95	A155	G215	C275	C335	U395	C455	C515	A575	A635	U695	U755	A815	C875	C935
G36	C96	A156	A216	U276	C336	G396	C456	C516	U576	A636	G696	A756	A816	C876	A936
C37	U97	C157	A217	G277	C337	U397	A457	C517	G577	A637	C697	A757	A817	C877	C937
A38	G98	U158	A218	G278	G338	C398	U458	C518	G578	A638	C698	A758	A818	U878	C938
G39	U99	A159	A219	G279	U339	U399	U459	C519	U579	A639	C699	A759	A819	G879	G939
U40	A100	A160	G220	U280	A340	G400	A460	C520	U580	A640	U700	A760	A820	U880	G940
C41	A101	C161	A221	C281	C341	A401	C461	C521	C581	U641	G701	A761	A821	U881	A941
A42	U102	A162	A222	A282	A342	A402	C462	C522	A582	U642	U702	A762	A822	G882	G942
G43	A103	C163	A223	G283	C343	U403	C463	C523	G583	A643	G703	A763	A823	G883	A943
A44	A104	C164	U224	U284	C344	A404	U464	C524	G584	A644	U704	A764	A824	U884	C944
G45	C105	A165	C225	G285	A345	U405	C465	C525	G585	A645	U705	A765	A825	C885	A945
G46	C106	U166	A226	U286	A346	A406	A466	C526	A586	U646	G706	A766	A826	U886	C946
C47	G107	A167	A227	G287	A347	G407	C467	C527	C587	U647	G707	A767	A827	U887	A947
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U50	G110	U170	G230	U290	G350	C410	A470	C530	A590	A650	U710	A770	A830	C890	G950
G51	A111	U171	A231	G291	C351	G411	A471	C531	U591	A651	G711	A771	A831	C891	C951
A52	U112	A172	G232	U292	A352	A412	A472	C532	A592	U652	G712	A772	A832	U892	G952
G53	U113	A173	A233	U293	C353	C413	G473	C533	U593	A653	G713	A773	A833	C893	G953
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G55	C115	G175	U235	G295	G355	A415	C475	C535	C595	A655	A715	A775	A835	U895	U955
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G58	A118	G178	C238	G298	U358	C418	A478	C538	U598	A658	A718	A778	A838	U898	U958
U59	C119	C179	C239	A299	G359	U419	A479	C539	A599	U659	C719	A779	A839	C899	G959
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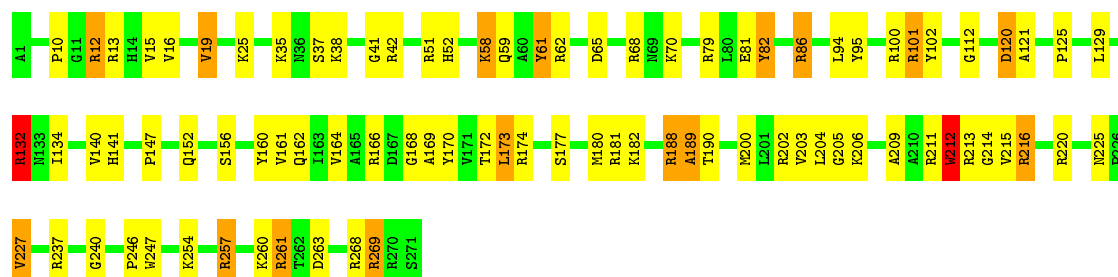
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G1863	A1803	G1743	G1683	G1623	U1563	A1503	U1443	G1383	C1323	A1263	U1203	A1143	U1083	G1023	U963
G1864	C1804	A1744	G1684	U1624	C1564	A1504	G1444	A1384	G1324	A1264	A1204	A1144	A1084	G1024	C964
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G1867	G1807	U1747	G1687	G1627	G1567	C1507	C1447	A1387	A1327	U1267	G1207	A1147	G1087	A1027	U967
C1868	A1808	C1748	U1688	G1628	G1568	A1508	G1448	G1388	A1328	A1268	C1208	U1148	A1088	A1028	C968
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C1881	A1821	C1760	A1701	A1641	G1581	G1521	C1461	G1401	G1341	G1281	C1221	C1161	U1101	G1041	A981
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A1884	G1824	C1764	C1704	G1644	U1584	G1524	G1464	A1404	U1344	A1284	U1224	C1164	C1104	C1044	A984
A1885	U1825	U1765	A1705	G1645	C1585	A1525	G1465	U1405	C1345	A1285	G1225	A1165	U1105	C1045	C985
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G1888	G1828	C1768	C1708	U1648	G1588	A1528	U1468	A1408	G1348	G1288	G1228	C1168	U1108	A1048	A988
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A1899	G1839	U1779	G1719	G1659	U1599	U1539	G1479	A1419	A1359	G1299	G1239	G1179	U1119	G1059	U999
A1900	G1840	A1780	U1720	G1660	C1600	G1540	C1480	A1420	G1360	G1300	U1240	U1180	G1120	U1060	A1000
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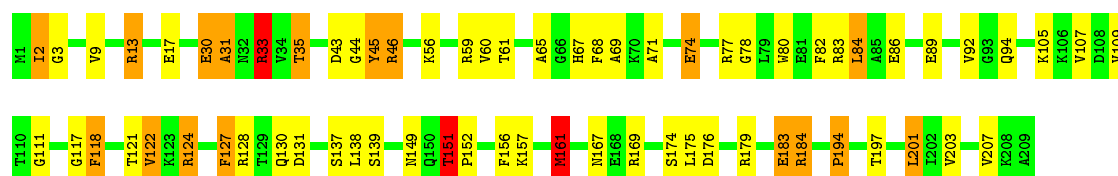
• Molecule 36: 50S RIBOSOMAL PROTEIN L2

Chain BC: 68% 25% 6% .



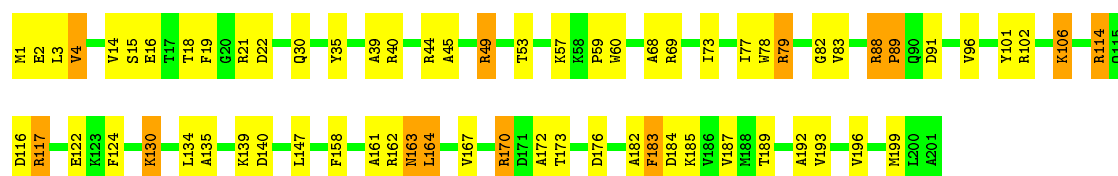
• Molecule 37: 50S RIBOSOMAL PROTEIN L3

Chain BD: 67% 23% 8% .



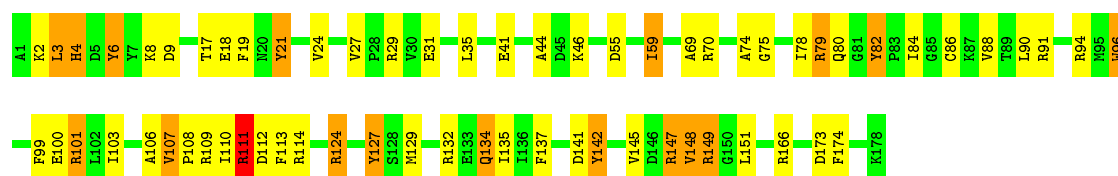
• Molecule 38: 50S RIBOSOMAL PROTEIN L4

Chain BE: 66% 27% 6% .



• Molecule 39: 50S RIBOSOMAL PROTEIN L5

Chain BF: 63% 26% 10% .

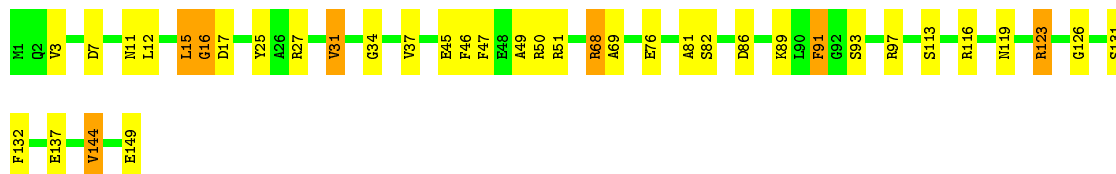






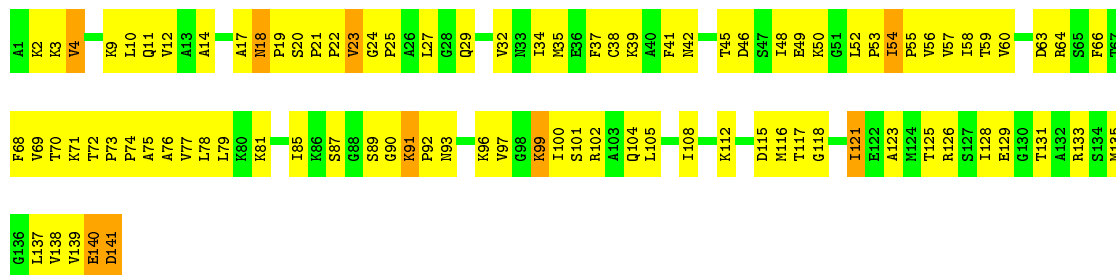
• Molecule 41: 50S RIBOSOMAL PROTEIN L9

Chain BH: 74% 21% 5%



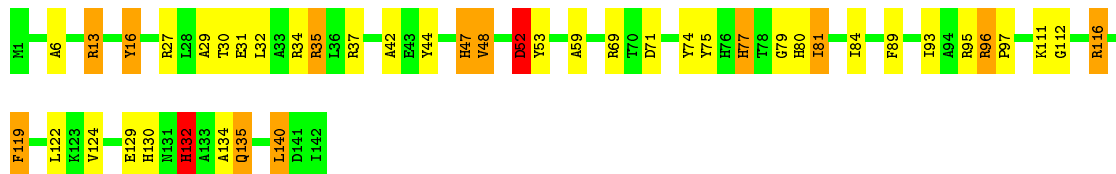
• Molecule 42: 50S RIBOSOMAL PROTEIN L11

Chain BI: 35% 59% 6%



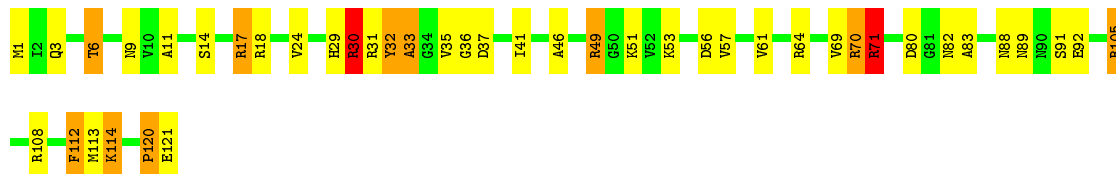
• Molecule 43: 50S RIBOSOMAL PROTEIN L13

Chain BJ: 69% 21% 8%



• Molecule 44: 50S RIBOSOMAL PROTEIN L14

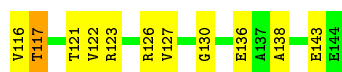
Chain BK: 64% 26% 8%



• Molecule 45: 50S RIBOSOMAL PROTEIN L15

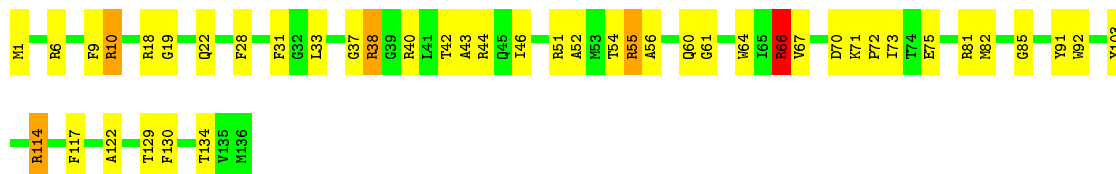
Chain BL: 67% 29%





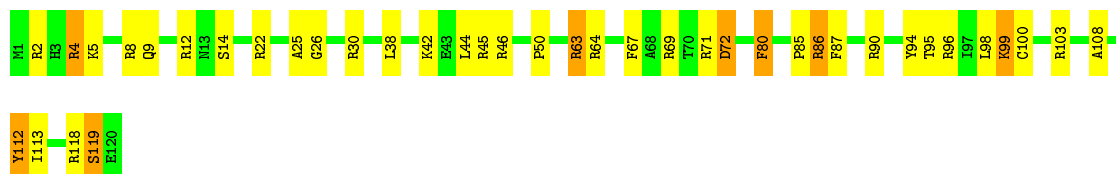
- Molecule 46: 50S RIBOSOMAL PROTEIN L16

Chain BM: 68% 29%



- Molecule 47: 50S RIBOSOMAL PROTEIN L17

Chain BN: 67% 27% 7%



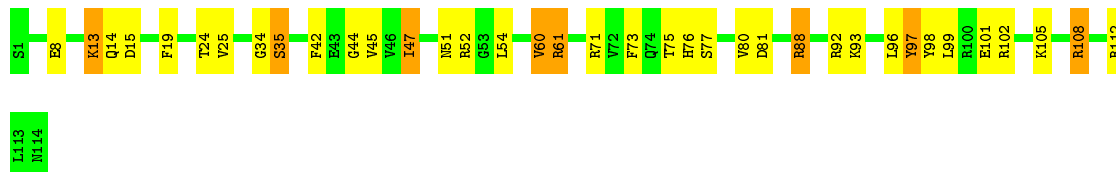
- Molecule 48: 50S RIBOSOMAL PROTEIN L18

Chain BO: 74% 22%



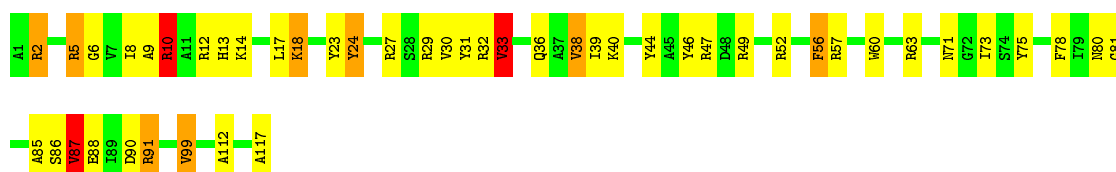
- Molecule 49: 50S RIBOSOMAL PROTEIN L19

Chain BP: 68% 25% 7%

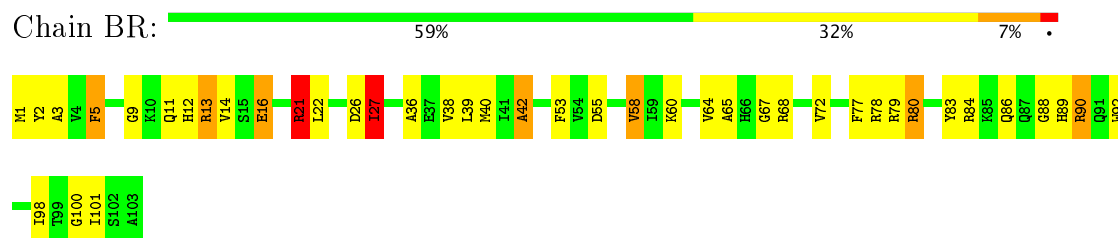


- Molecule 50: 50S RIBOSOMAL PROTEIN L20

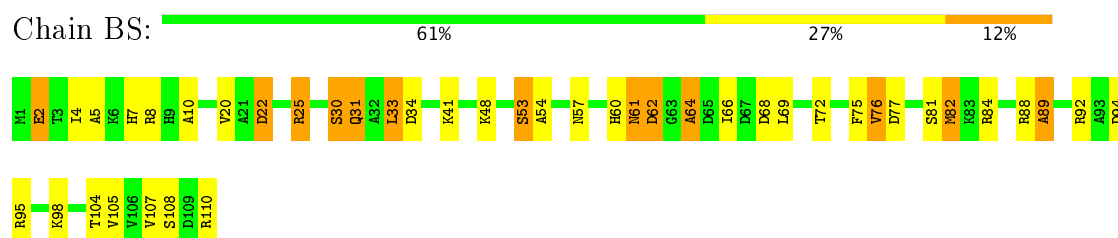
Chain BQ: 60% 31% 7%



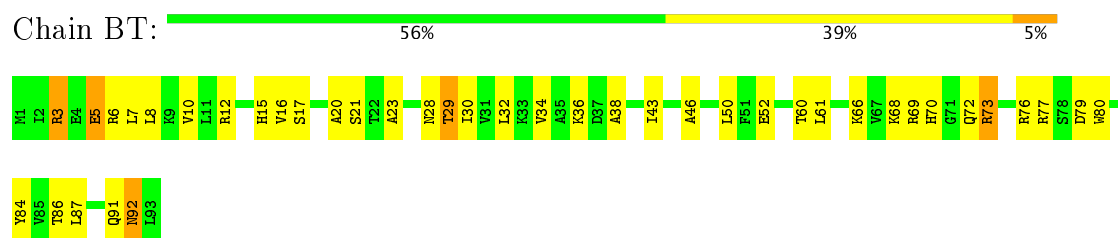
- Molecule 51: 50S RIBOSOMAL PROTEIN L21



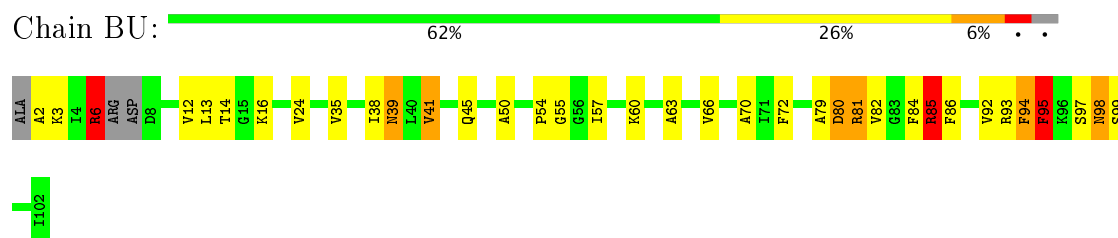
• Molecule 52: 50S RIBOSOMAL PROTEIN L22



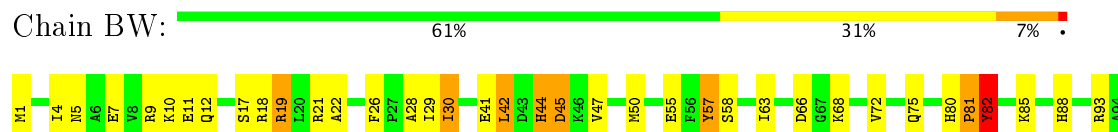
• Molecule 53: 50S RIBOSOMAL PROTEIN L23



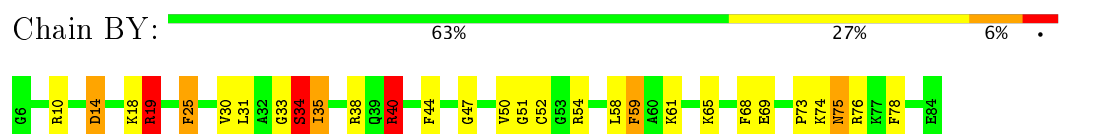
• Molecule 54: 50S RIBOSOMAL PROTEIN L24



• Molecule 55: 50S RIBOSOMAL PROTEIN L25



• Molecule 56: 50S RIBOSOMAL PROTEIN L27



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	263000	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	38900	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU

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	AA	3.37	4837/36762 (13.2%)	3.72	8282/57350 (14.4%)
10	AJ	1.78	11/796 (1.4%)	1.89	15/1077 (1.4%)
11	AK	1.75	7/893 (0.8%)	1.96	18/1205 (1.5%)
12	AL	1.85	13/969 (1.3%)	1.98	28/1300 (2.2%)
13	AM	1.73	12/884 (1.4%)	2.02	28/1181 (2.4%)
14	AN	1.80	6/785 (0.8%)	1.92	19/1043 (1.8%)
15	AO	1.77	11/724 (1.5%)	1.90	24/966 (2.5%)
16	AP	1.84	9/648 (1.4%)	2.16	26/870 (3.0%)
17	AQ	1.73	4/657 (0.6%)	1.93	18/881 (2.0%)
18	AR	1.74	6/462 (1.3%)	2.28	16/621 (2.6%)
19	AS	1.78	8/652 (1.2%)	2.15	26/877 (3.0%)
2	AB	1.71	14/1735 (0.8%)	2.05	53/2338 (2.3%)
20	AT	1.66	4/671 (0.6%)	1.93	17/888 (1.9%)
21	AU	1.82	6/430 (1.4%)	2.16	13/570 (2.3%)
22	AV	2.38	76/1820 (4.2%)	2.84	256/2836 (9.0%)
23	AX	1.81	4/264 (1.5%)	2.14	19/407 (4.7%)
24	AZ	1.97	1/99 (1.0%)	1.94	5/137 (3.6%)
25	B0	1.75	7/635 (1.1%)	2.27	19/848 (2.2%)
26	B1	1.72	5/510 (1.0%)	1.94	14/677 (2.1%)
27	B2	1.75	4/453 (0.9%)	1.86	10/605 (1.7%)
28	B3	1.82	6/450 (1.3%)	2.19	16/599 (2.7%)
29	B4	1.63	4/416 (1.0%)	2.02	13/554 (2.3%)
3	AC	1.73	20/1651 (1.2%)	2.05	55/2225 (2.5%)
30	B5	1.56	11/1748 (0.6%)	1.95	40/2355 (1.7%)
31	B6	1.85	4/380 (1.1%)	2.31	17/498 (3.4%)
32	B7	1.68	4/513 (0.8%)	2.03	12/676 (1.8%)
33	B8	1.83	4/303 (1.3%)	2.01	7/397 (1.8%)
34	BA	3.34	356/2753 (12.9%)	3.78	615/4288 (14.3%)
35	BB	3.39	9308/69800 (13.3%)	3.73	15832/108892 (14.5%)
36	BC	1.81	24/2121 (1.1%)	2.05	60/2852 (2.1%)
37	BD	1.77	16/1586 (1.0%)	2.01	31/2134 (1.5%)
38	BE	1.69	8/1571 (0.5%)	1.97	41/2113 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BF	1.73	14/1444 (1.0%)	2.17	40/1937 (2.1%)
4	AD	1.80	24/1665 (1.4%)	2.05	48/2227 (2.2%)
40	BG	1.76	13/1335 (1.0%)	2.04	28/1803 (1.6%)
41	BH	1.74	11/1122 (1.0%)	2.05	35/1515 (2.3%)
42	BI	0.62	2/1046 (0.2%)	0.56	1/1410 (0.1%)
43	BJ	1.77	12/1152 (1.0%)	2.04	30/1551 (1.9%)
44	BK	1.76	13/939 (1.4%)	1.99	23/1257 (1.8%)
45	BL	1.78	10/1054 (0.9%)	1.94	28/1403 (2.0%)
46	BM	1.83	9/1093 (0.8%)	2.07	30/1460 (2.1%)
47	BN	1.76	12/973 (1.2%)	2.22	32/1301 (2.5%)
48	BO	1.79	15/902 (1.7%)	2.02	24/1209 (2.0%)
49	BP	1.68	5/929 (0.5%)	2.03	20/1242 (1.6%)
5	AE	1.73	17/1118 (1.5%)	1.97	27/1504 (1.8%)
50	BQ	1.89	15/960 (1.6%)	2.11	29/1278 (2.3%)
51	BR	1.80	11/829 (1.3%)	2.03	23/1107 (2.1%)
52	BS	1.71	7/864 (0.8%)	2.16	34/1156 (2.9%)
53	BT	1.69	5/744 (0.7%)	1.99	18/994 (1.8%)
54	BU	1.73	3/761 (0.4%)	2.02	25/1013 (2.5%)
55	BW	1.79	13/766 (1.7%)	2.05	18/1025 (1.8%)
56	BY	1.73	3/603 (0.5%)	2.11	23/797 (2.9%)
6	AF	1.77	7/835 (0.8%)	1.96	17/1128 (1.5%)
7	AG	1.82	18/1187 (1.5%)	2.01	40/1591 (2.5%)
8	AH	1.79	10/989 (1.0%)	2.07	29/1326 (2.2%)
9	AI	1.97	21/1034 (2.0%)	2.09	33/1375 (2.4%)
All	All	2.98	15080/158485 (9.5%)	3.34	26300/236869 (11.1%)

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	AA	0	740
10	AJ	0	6
11	AK	0	3
12	AL	0	5
13	AM	0	9
14	AN	0	3
15	AO	0	6
16	AP	0	4
17	AQ	0	1
18	AR	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	AS	0	4
2	AB	0	5
20	AT	0	3
22	AV	0	13
23	AX	0	4
25	B0	0	4
26	B1	0	1
28	B3	0	2
29	B4	0	3
3	AC	0	7
30	B5	0	6
31	B6	0	3
32	B7	0	1
34	BA	0	50
35	BB	0	1343
36	BC	0	8
37	BD	0	6
38	BE	0	5
39	BF	0	10
4	AD	0	11
40	BG	0	3
41	BH	0	1
43	BJ	0	4
44	BK	0	5
45	BL	0	1
46	BM	0	3
47	BN	0	5
48	BO	0	2
49	BP	0	5
5	AE	0	5
50	BQ	0	5
51	BR	0	3
52	BS	0	1
53	BT	0	1
54	BU	0	2
55	BW	0	4
56	BY	0	5
6	AF	0	3
7	AG	0	3
8	AH	0	3
9	AI	0	7
All	All	0	2342

The worst 5 of 15080 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	1403	A	N9-C4	21.34	1.50	1.37
35	BB	1301	A	N7-C5	-20.38	1.27	1.39
1	AA	930	C	N1-C6	19.80	1.49	1.37
1	AA	816	A	N7-C5	-19.29	1.27	1.39
35	BB	1821	A	N9-C4	19.18	1.49	1.37

The worst 5 of 26300 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	753	A	N1-C6-N6	30.52	136.91	118.60
35	BB	666	A	N1-C6-N6	26.10	134.26	118.60
35	BB	533	G	N1-C6-O6	25.90	135.44	119.90
1	AA	242	G	C5-C6-O6	-25.60	113.24	128.60
35	BB	1014	A	N1-C6-N6	25.57	133.94	118.60

There are no chirality outliers.

5 of 2342 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	11	G	Sidechain
1	AA	12	U	Sidechain
1	AA	5	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	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	AA	32831	0	16502	183	0
2	AB	1704	0	1732	3	0
3	AC	1624	0	1699	12	0
4	AD	1643	0	1710	5	0
5	AE	1105	0	1148	6	0
6	AF	817	0	808	7	0
7	AG	1174	0	1230	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	979	0	1034	1	0
9	AI	1022	0	1070	9	0
10	AJ	786	0	828	3	0
11	AK	877	0	887	9	0
12	AL	955	0	1019	2	0
13	AM	876	0	937	7	0
14	AN	774	0	827	2	0
15	AO	716	0	742	3	0
16	AP	638	0	656	0	0
17	AQ	648	0	691	4	0
18	AR	455	0	478	1	0
19	AS	637	0	665	5	0
20	AT	665	0	714	4	0
21	AU	425	0	449	2	0
22	AV	1649	0	832	21	0
23	AX	236	0	121	10	0
24	AZ	100	0	99	0	0
25	B0	625	0	655	1	0
26	B1	509	0	543	1	0
27	B2	449	0	491	1	0
28	B3	444	0	461	3	0
29	B4	409	0	440	0	0
30	B5	1733	0	1824	4	0
31	B6	377	0	418	3	0
32	B7	504	0	574	5	0
33	B8	302	0	343	0	0
34	BA	2464	0	1246	8	0
35	BB	62321	0	31294	336	0
36	BC	2082	0	2157	14	0
37	BD	1565	0	1616	8	0
38	BE	1552	0	1619	9	0
39	BF	1420	0	1460	9	0
40	BG	1316	0	1364	4	0
41	BH	1111	0	1148	1	0
42	BI	1032	0	1088	118	0
43	BJ	1129	0	1162	8	0
44	BK	930	0	1003	6	0
45	BL	1045	0	1117	6	0
46	BM	1074	0	1157	4	0
47	BN	960	0	1000	2	0
48	BO	892	0	923	2	0
49	BP	917	0	965	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BQ	947	0	1022	8	0
51	BR	816	0	839	8	0
52	BS	857	0	922	3	0
53	BT	738	0	807	5	0
54	BU	755	0	807	10	0
55	BW	753	0	780	5	0
56	BY	596	0	610	1	0
All	All	145960	0	98733	840	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 3.

The worst 5 of 840 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:AV:35:G:N2	23:AX:18:C:C2	2.08	1.22
42:BI:11:GLN:HG2	42:BI:55:PRO:HB3	1.51	0.91
42:BI:140:GLU:O	42:BI:141:ASP:OXT	1.91	0.89
42:BI:27:LEU:H	42:BI:27:LEU:HD23	1.43	0.82
42:BI:121:ILE:HD13	42:BI:121:ILE:H	1.44	0.82

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	AB	216/218 (99%)	159 (74%)	41 (19%)	16 (7%)	1	18
3	AC	204/206 (99%)	158 (78%)	31 (15%)	15 (7%)	1	18
4	AD	203/205 (99%)	160 (79%)	34 (17%)	9 (4%)	3	29
5	AE	148/150 (99%)	110 (74%)	27 (18%)	11 (7%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	98/100 (98%)	73 (74%)	18 (18%)	7 (7%)	1	19
7	AG	148/150 (99%)	109 (74%)	33 (22%)	6 (4%)	3	30
8	AH	127/129 (98%)	94 (74%)	27 (21%)	6 (5%)	3	28
9	AI	125/127 (98%)	99 (79%)	21 (17%)	5 (4%)	3	31
10	AJ	96/98 (98%)	71 (74%)	14 (15%)	11 (12%)	0	8
11	AK	115/117 (98%)	96 (84%)	14 (12%)	5 (4%)	3	30
12	AL	121/123 (98%)	100 (83%)	12 (10%)	9 (7%)	1	18
13	AM	111/113 (98%)	80 (72%)	19 (17%)	12 (11%)	0	10
14	AN	92/96 (96%)	57 (62%)	22 (24%)	13 (14%)	0	5
15	AO	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	7	43
16	AP	78/80 (98%)	62 (80%)	10 (13%)	6 (8%)	1	17
17	AQ	78/80 (98%)	65 (83%)	7 (9%)	6 (8%)	1	17
18	AR	53/55 (96%)	42 (79%)	8 (15%)	3 (6%)	2	24
19	AS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	3	31
20	AT	83/85 (98%)	68 (82%)	13 (16%)	2 (2%)	7	42
21	AU	49/51 (96%)	41 (84%)	5 (10%)	3 (6%)	2	22
24	AZ	18/20 (90%)	16 (89%)	1 (6%)	1 (6%)	2	24
25	B0	75/77 (97%)	52 (69%)	20 (27%)	3 (4%)	3	31
26	B1	61/63 (97%)	45 (74%)	14 (23%)	2 (3%)	4	36
27	B2	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
28	B3	54/56 (96%)	42 (78%)	9 (17%)	3 (6%)	2	24
29	B4	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	30
30	B5	232/234 (99%)	190 (82%)	37 (16%)	5 (2%)	8	44
31	B6	44/46 (96%)	29 (66%)	11 (25%)	4 (9%)	1	14
32	B7	62/64 (97%)	52 (84%)	5 (8%)	5 (8%)	1	16
33	B8	36/38 (95%)	30 (83%)	4 (11%)	2 (6%)	2	24
36	BC	269/271 (99%)	209 (78%)	47 (18%)	13 (5%)	2	27
37	BD	207/209 (99%)	149 (72%)	37 (18%)	21 (10%)	1	12
38	BE	199/201 (99%)	161 (81%)	23 (12%)	15 (8%)	1	18
39	BF	176/178 (99%)	131 (74%)	26 (15%)	19 (11%)	0	10
40	BG	171/176 (97%)	134 (78%)	28 (16%)	9 (5%)	2	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BH	147/149 (99%)	111 (76%)	31 (21%)	5 (3%)	4	35
42	BI	139/141 (99%)	113 (81%)	21 (15%)	5 (4%)	4	34
43	BJ	140/142 (99%)	106 (76%)	24 (17%)	10 (7%)	1	19
44	BK	119/121 (98%)	95 (80%)	14 (12%)	10 (8%)	1	15
45	BL	141/143 (99%)	115 (82%)	16 (11%)	10 (7%)	1	19
46	BM	134/136 (98%)	105 (78%)	21 (16%)	8 (6%)	2	22
47	BN	118/120 (98%)	96 (81%)	16 (14%)	6 (5%)	2	26
48	BO	114/116 (98%)	98 (86%)	14 (12%)	2 (2%)	10	49
49	BP	112/114 (98%)	85 (76%)	19 (17%)	8 (7%)	1	19
50	BQ	115/117 (98%)	84 (73%)	21 (18%)	10 (9%)	1	15
51	BR	101/103 (98%)	80 (79%)	13 (13%)	8 (8%)	1	17
52	BS	108/110 (98%)	76 (70%)	21 (19%)	11 (10%)	1	11
53	BT	91/93 (98%)	60 (66%)	25 (28%)	6 (7%)	1	21
54	BU	94/102 (92%)	71 (76%)	16 (17%)	7 (7%)	1	18
55	BW	92/94 (98%)	76 (83%)	10 (11%)	6 (6%)	1	21
56	BY	77/79 (98%)	46 (60%)	18 (23%)	13 (17%)	0	4
All	All	5858/5971 (98%)	4523 (77%)	956 (16%)	379 (6%)	3	21

5 of 379 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	TRP
3	AC	116	ALA
5	AE	11	GLN
5	AE	17	VAL
9	AI	58	GLU

### 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	AB	180/180 (100%)	171 (95%)	9 (5%)	28	60
3	AC	170/170 (100%)	158 (93%)	12 (7%)	17	50
4	AD	172/172 (100%)	165 (96%)	7 (4%)	35	65
5	AE	113/113 (100%)	103 (91%)	10 (9%)	12	40
6	AF	87/87 (100%)	85 (98%)	2 (2%)	56	78
7	AG	123/123 (100%)	120 (98%)	3 (2%)	54	77
8	AH	104/104 (100%)	99 (95%)	5 (5%)	30	62
9	AI	105/105 (100%)	100 (95%)	5 (5%)	30	62
10	AJ	86/86 (100%)	81 (94%)	5 (6%)	23	56
11	AK	90/90 (100%)	86 (96%)	4 (4%)	33	63
12	AL	103/103 (100%)	98 (95%)	5 (5%)	29	61
13	AM	91/91 (100%)	89 (98%)	2 (2%)	57	79
14	AN	79/79 (100%)	76 (96%)	3 (4%)	38	67
15	AO	76/76 (100%)	69 (91%)	7 (9%)	11	38
16	AP	65/65 (100%)	62 (95%)	3 (5%)	31	63
17	AQ	74/74 (100%)	68 (92%)	6 (8%)	14	44
18	AR	48/48 (100%)	44 (92%)	4 (8%)	13	44
19	AS	70/70 (100%)	64 (91%)	6 (9%)	12	42
20	AT	65/65 (100%)	64 (98%)	1 (2%)	70	85
21	AU	44/44 (100%)	38 (86%)	6 (14%)	4	23
25	B0	67/67 (100%)	65 (97%)	2 (3%)	46	72
26	B1	55/55 (100%)	50 (91%)	5 (9%)	11	38
27	B2	48/48 (100%)	47 (98%)	1 (2%)	59	80
28	B3	47/47 (100%)	46 (98%)	1 (2%)	59	80
29	B4	45/45 (100%)	42 (93%)	3 (7%)	19	51
30	B5	181/181 (100%)	175 (97%)	6 (3%)	43	70
31	B6	38/38 (100%)	33 (87%)	5 (13%)	5	24
32	B7	51/51 (100%)	48 (94%)	3 (6%)	23	56
33	B8	34/34 (100%)	34 (100%)	0	100	100
36	BC	216/216 (100%)	204 (94%)	12 (6%)	25	57
37	BD	164/164 (100%)	146 (89%)	18 (11%)	7	30
38	BE	165/165 (100%)	157 (95%)	8 (5%)	30	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BF	149/149 (100%)	143 (96%)	6 (4%)	36	65
40	BG	136/137 (99%)	125 (92%)	11 (8%)	14	44
41	BH	114/114 (100%)	110 (96%)	4 (4%)	41	69
42	BI	109/109 (100%)	104 (95%)	5 (5%)	31	63
43	BJ	116/116 (100%)	112 (97%)	4 (3%)	42	70
44	BK	102/102 (100%)	92 (90%)	10 (10%)	9	34
45	BL	102/102 (100%)	98 (96%)	4 (4%)	37	66
46	BM	109/109 (100%)	104 (95%)	5 (5%)	31	63
47	BN	100/100 (100%)	96 (96%)	4 (4%)	36	65
48	BO	86/86 (100%)	84 (98%)	2 (2%)	56	78
49	BP	99/99 (100%)	96 (97%)	3 (3%)	46	72
50	BQ	89/89 (100%)	83 (93%)	6 (7%)	19	51
51	BR	84/84 (100%)	76 (90%)	8 (10%)	10	36
52	BS	93/93 (100%)	87 (94%)	6 (6%)	20	53
53	BT	80/80 (100%)	68 (85%)	12 (15%)	3	20
54	BU	81/83 (98%)	76 (94%)	5 (6%)	21	54
55	BW	78/78 (100%)	73 (94%)	5 (6%)	20	53
56	BY	59/59 (100%)	54 (92%)	5 (8%)	12	43
All	All	4842/4845 (100%)	4568 (94%)	274 (6%)	28	57

5 of 274 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	B6	5	PHE
37	BD	105	LYS
53	BT	34	VAL
31	B6	34	ARG
36	BC	164	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
27	B2	33	HIS
32	B7	42	HIS
52	BS	102	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
28	B3	41	HIS
30	B5	103	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1530 (99%)	269 (17%)	34 (2%)
22	AV	76/77 (98%)	15 (19%)	0
23	AX	10/11 (90%)	8 (80%)	0
34	BA	112/117 (95%)	16 (14%)	2 (1%)
35	BB	2902/2903 (99%)	471 (16%)	56 (1%)
All	All	4629/4638 (99%)	779 (16%)	92 (1%)

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	15	G
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BB	670	A
35	BB	973	A
35	BB	2406	A
35	BB	827	U
35	BB	880	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is

the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	5MU	AV	54	22	14,21,23	1.48	2 (14%)	15,30,35	4.17	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	AV	54	22	-	0/3/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	54	5MU	C6-N1	2.18	1.38	1.35
22	AV	54	5MU	C4-N3	4.29	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	54	5MU	C5-C4-N3	-3.99	113.59	123.12
22	AV	54	5MU	O4'-C1'-N1	2.91	113.90	108.08
22	AV	54	5MU	C4-N3-C2	15.26	127.24	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
54	BU	1
14	AN	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BU	4:ILE	C	6:ARG	N	4.65
1	AN	35:ALA	C	40:ARG	N	4.56