



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:09 PM BST

PDB ID : 4V6R
EMDB ID: : EMD-5362
Title : Structural characterization of mRNA-tRNA translocation intermediates (class 6 of the six classes)
Authors : Agirrezabala, X.; Liao, H.; Schreiner, E.; Fu, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-12-08
Resolution : 11.50 Å(reported)
Based on PDB ID : 2I2U

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

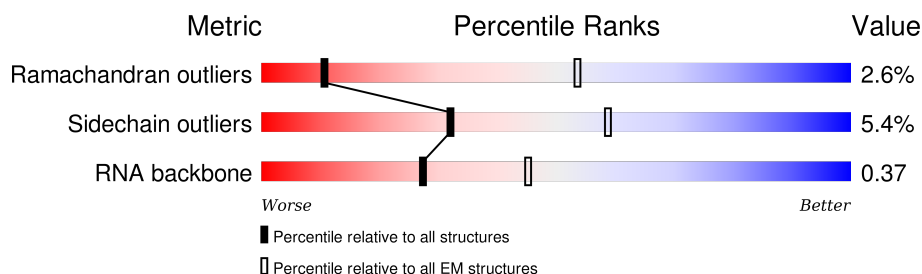
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 11.50 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.











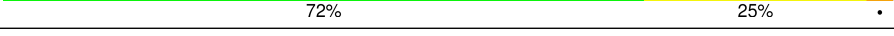

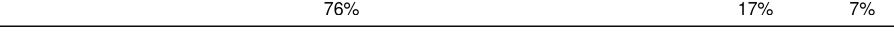
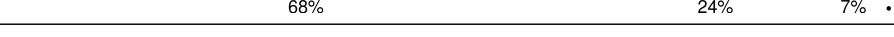

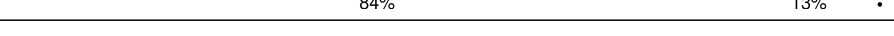


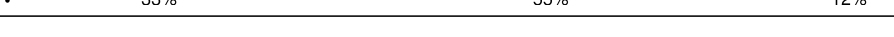

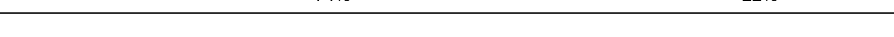






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AB	76	
3	AC	47	
4	AD	77	
5	AE	240	
6	AF	232	
7	AG	205	
8	AH	166	
9	AI	135	














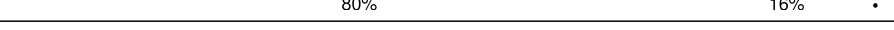







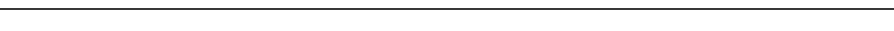


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Mol	Chain	Length	Quality of chain
10	AJ	178	
11	AK	129	
12	AL	129	
13	AM	103	
14	AN	128	
15	AO	123	
16	AP	117	
17	AQ	100	
18	AR	88	
19	AS	82	
20	AT	83	
21	AU	74	
22	AV	91	
23	AW	86	
24	AX	70	
25	BA	120	
26	BB	2904	
27	BC	234	
28	BD	272	
29	BE	209	
30	BF	201	
31	BG	178	
32	BH	176	
33	BI	149	
34	BJ	164	

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Mol	Chain	Length	Quality of chain
35	BK	141	 81% 18% .
36	BL	142	 76% 20% . .
37	BM	123	 68% 29% .
38	BN	144	 80% 18% .
39	BO	136	 74% 23% .
40	BP	127	 75% 22% .
41	BQ	117	 80% 17% .
42	BR	114	 76% 18% 5%
43	BS	117	 71% 26% . .
44	BT	103	 77% 19% .
45	BU	110	 75% 24% .
46	BV	100	 78% 19% .
47	BW	103	 79% 19% .
48	BX	94	 80% 16% .
49	BY	84	 74% 20% . .
50	BZ	77	 81% 17% .
51	B0	63	 75% 24% .
52	B1	58	 76% 21% .
53	B2	70	 73% 19% 7% .
54	B3	56	 71% 21% 7%
55	B4	54	 83% 13% .
56	B5	46	 65% 30% .
57	B6	64	 80% 19% .
58	B7	38	 71% 29%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 152351 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	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 2 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	76	Total	C	N	O	P	S	0	0
			1627	731	287	532	75	2		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	47	Total	C	N	O	P	0	0
			993	445	167	335	46		

- Molecule 4 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	77	Total	C	N	O	P	S	0	0
			1641	734	297	533	76	1		

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	240	Total	C	N	O	S	0	0
			1872	1180	332	352	8		

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	232	Total	C	N	O	S	0	0
			1822	1149	346	323	4		

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	166	Total	C	N	O	S	0	0
			1225	761	232	226	6		

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 24 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

- Molecule 27 is a protein called 50S ribosomal protein L1.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BJ	164	Total	C	N	O	S	0	0
			1233	776	220	231	6		

- Molecule 35 is a protein called 50S ribosomal protein L11.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BM	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	103	Total	C	N	O	S	0	0
			789	498	148	143			

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 50 is a protein called 50S ribosomal protein L28.

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B0	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	B4	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

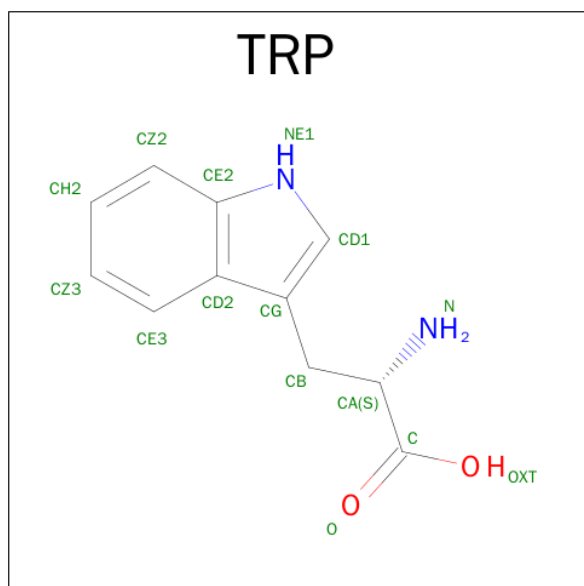
- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 58 is a protein called 50S ribosomal protein L36.

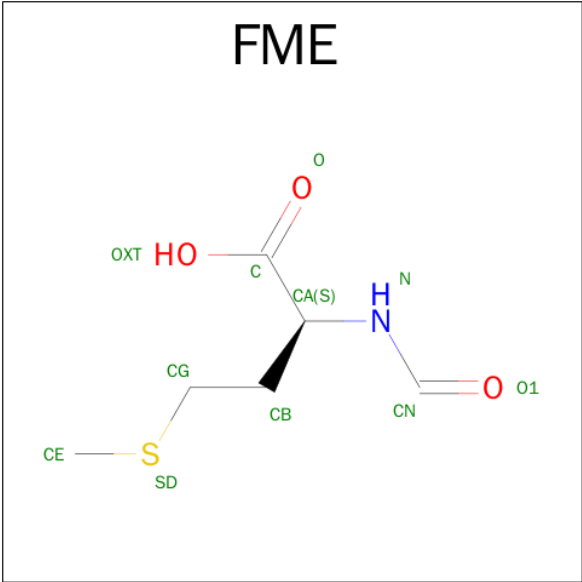
Mol	Chain	Residues	Atoms					AltConf	Trace
58	B7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
59	AB	1	Total	C	N	O	0
			14	11	2	1	

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

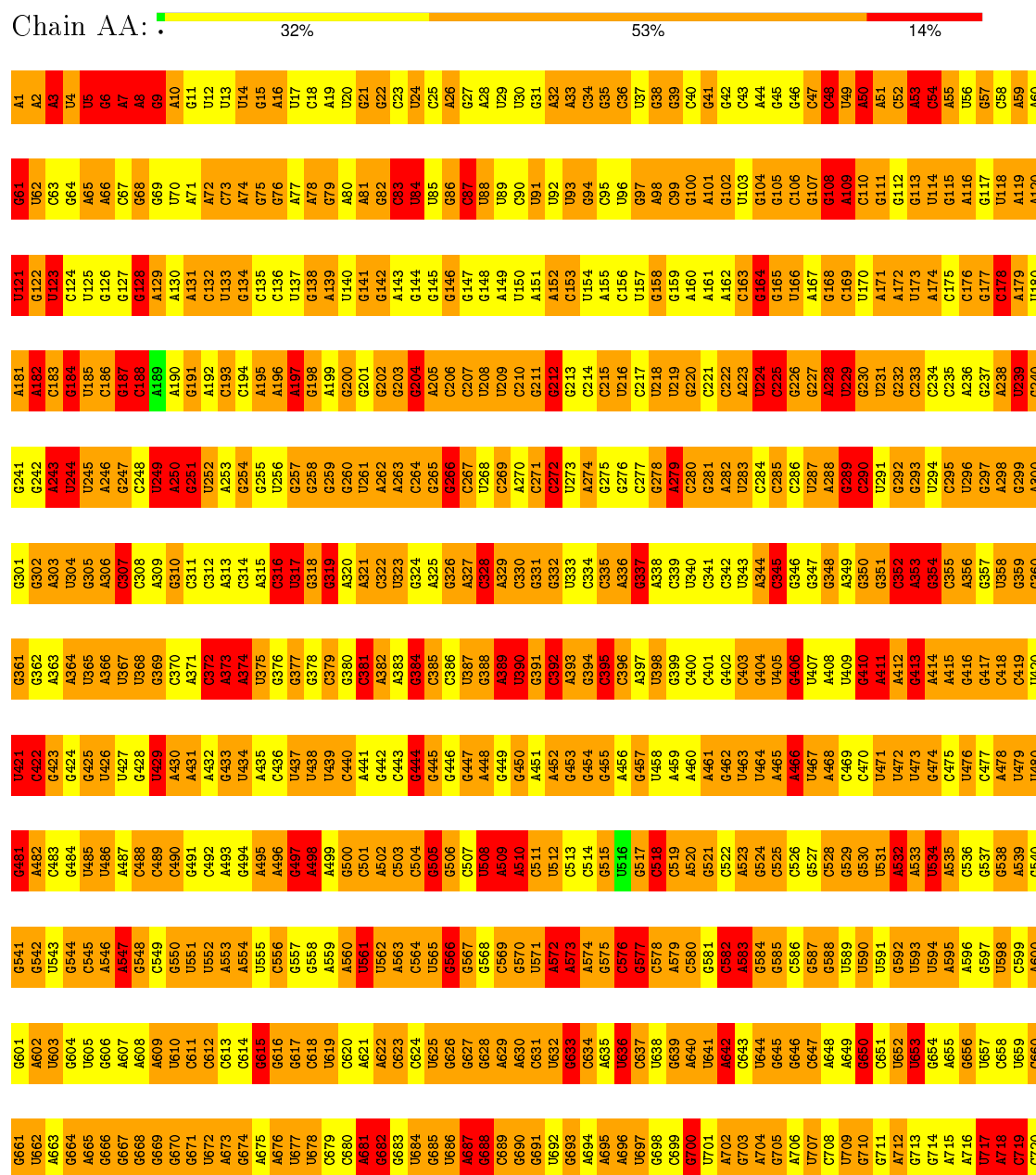


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	BB	1	10	6	1	2	1	0

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 errors 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



C1501	A1441	U1381	U1321	A1261	A1201	C1141	A1081	A1021	U961	A901	C841	A781	G721
A1502	C1442	C1382	C1322	C1262	C1202	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	C1323	C1263	C1203	G1143	U1083	A1023	G963	G903	U843	C783	U723
G1504	U1444	C1384	A1324	U1264	A1204	G1144	G1084	G1024	A964	U904	G844	A784	G724
G1505	U1445	G1385	C1325	C1265	U1205	A1145	U1085	U1025	U965	U905	A845	G785	G725
U1506	A1446	G1386	U1326	G1266	G1206	A1146	U1086	G1026	G966	A906	G846	G786	G726
A1507	A1447	G1387	C1327	C1267	G1207	C1147	G1087	C1027	C967	A907	G847	A787	G727
A1508	C1448	C1388	C1328	G1268	C1208	U1148	A1088	C1028	A968	A908	C848	U788	A728
A1509	C1449	C1389	A1329	A1269	C1209	C1149	U1089	U1029	A969	A909	G849	U789	A729
C1510	U1450	U1390	U1330	G1270	G1210	A1150	U1090	U1030	C970	C910	U850	A790	G730
G1511	U1451	G1391	G1331	A1271	U1211	A1151	U1091	C1031	G971	U911	G851	G791	G731
C1452	G1392	A1332	A1332	C1272	U1212	A1152	A1092	G1032	C972	C912	G852	A792	C732
A1512	C1453	C1393	A1333	G1273	A1213	G1153	A1093	C1033	G973	A913	C853	U793	G733
G1514	G1454	A1394	C1334	A1274	C1214	A1154	G1094	A1034	A974	A914	A794	A794	G734
G1515	G1455	C1395	U1335	A1275	G1215	A1155	U1095	A1035	A975	A915	U855	C795	C735
G1516	A1456	A1396	G1336	G1276	A1216	G1156	C1096	A1036	G976	U916	C856	G796	G736
C1457	C1397	G1337	G1337	C1277	C1217	A1157	C1097	C1037	A977	G917	C857	C797	C737
C1458	A1398	G1338	G1338	G1278	C1218	G1158	C1098	C1038	A978	A918	C858	U798	C738
C1520	C1459	C1399	A1339	G1279	A1219	U1159	G1099	C1039	C979	A919	G859	G799	C739
C1521	C1460	C1400	A1340	A1280	C1220	G1160	C1100	U1040	C980	U920	A860	G800	U740
U1522	G1461	G1401	U1341	G1281	G1221	C1161	A1101	G1041	U981	U921	G861	U801	G741
G1523	C1462	C1402	C1342	C1282	G1222	C1162	A1102	A1042	U982	G922	C862	A802	G742
C1524	U1463	C1403	G1343	U1283	C1223	A1163	C1103	G1043	A983	A923	U863	G803	A743
G1525	U1464	C1404	C1344	G1284	U1224	G1164	G1104	A1044	C884	C924	A864	U804	C744
G1526	A1465	G1405	U1345	A1285	A1225	U1165	A1105	C1045	A985	G925	A865	C805	G745
U1527	C1466	U1406	G1346	U1286	C1226	G1166	G1106	A1046	U986	G926	C866	C806	A746
G1528	C1467	C1407	G1347	A1287	A1227	A1167	C1107	G1047	G987	G927	G867	A807	A747
A1529	A1468	A1408	U1348	A1288	C1228	U1168	G1108	U1048	G988	G928	C868	C808	G748
C1530	C1469	C1409	A1349	A1289	A1229	A1169	C1109	U1049	U989	G929	G869	G809	A749
A1531	U1470	A1410	A1350	G1290	C1230	A1170	A1110	G1050	C990	C930	U870	C810	C750
U1532	U1471	C1411	U1351	C1291	G1231	G1171	A1111	C1051	U991	C931	U871	C811	G751
C1533	U1472	C1412	C1352	G1292	U1232	C1172	A1112	U1052	U992	C932	A872	G812	G752
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G1536	G1475	G1415	G1355	U1295	U1235	G1175	U1115	A1055	C995	A935	U875	A815	G755
C1537	A1476	G1416	G1356	C1296	A1236	A1176	U1116	U1056	A996	C936	C876	A816	C756
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A1540	C1479	A1419	C1359	A1299	A1239	A1179	C1119	G1059	C999	G939	C879	A819	A759
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U1481	G1421	C1361	U1301	G1301	G1241	G1181	U1121	G1061	C1001	G941	G881	A821	G761
G1482	G1422	A1362	C1302	G1302	G1242	G1182	U1122	U1062	C882	G942	C882	U822	G762
A1483	G1423	A1363	C1303	C1303	C1243	U1183	G1123	C1063	A983	U943	C883	C823	G763
C1484	U1424	U1364	G1304	G1304	G1244	G1184	G1124	G1064	A1004	G944	U884	G824	G764
U1485	U1425	G1365	G1305	G1305	C1245	G1185	U1125	U1065	A1005	A945	A885	A825	G765
G1486	G1426	C1366	A1306	A1246	A1246	G1186	U1126	C1066	G1006	G946	G886	C826	A766
G1487	G1427	C1367	U1307	U1247	U1247	G1187	G1127	A1067	U1007	G947	G887	U827	A767
C1488	A1428	A1368	U1308	U1248	A1248	A1188	C1128	G1068	U1008	C948	C888	U828	A768
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U1490	A1430	C1370	G1310	A1250	A1250	G1190	A1130	U1070	U1010	U950	G890	G830	C770
C1491	G1431	C1371	A1311	A1311	A1251	A1191	G1131	C1071	C1011	G951	U891	A831	G771
A1492	G1432	U1372	G1312	G1312	G1252	G1192	G1132	G1072	A892	U952	G892	G832	U772
A1493	C1433	C1373	U1313	A1253	G1253	G1193	G1133	U1073	G1013	G953	C893	G833	G773
G1494	A1434	A1374	C1314	A1254	A1254	U1194	G1134	G1074	A894	G954	C894	U834	G774
U1495	U1435	G1375	U1315	U1255	G1255	C1195	U1135	U1075	G955	U955	G895	U835	G775
G1496	C1436	U1376	G1316	A1256	A1256	A1196	U1136	U1076	A896	U956	G896	G836	G776
G1497	A1437	C1377	C1317	C1317	A1257	A1197	G1137	G1077	U1017	U957	C897	U837	A777
U1498	U1438	C1378	A1318	G1258	G1258	G1198	G1138	U1078	G958	A958	G898	G838	G778
A1499	G1439	G1379	A1319	C1259	C1259	U1199	G1139	G1079	A1019	A959	C899	C839	C779
C1500	U1440	U1320	C1320	C1260	C1260	C1140	G1140	A1080	C960	A900	G840	C780	G720

• Molecule 2: A site tRNA

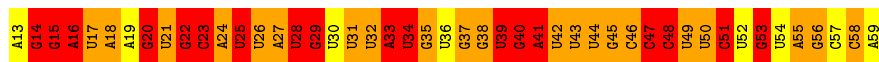
Chain AB: 7% 26% 49% 18%

A1	G2	G3	G4	G5	G6	G7	G8	A9	G10	U11	U12	C13	A14	A15	G16	G17	G18	G19	U20	A21	G22	A23	G24	G25	A26	C27	G28	G29	G30	U31	G32	U33	C34	C35	A36	A37	A38	A39	C40	C41	G42	G43	G44	G45	G46	U47	U48	G49	G50	G51	A52	G53	G54	G55	G56	G57	A58	G59	U60	G61
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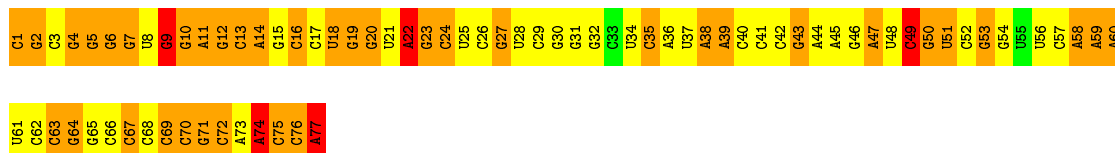
- Molecule 3: mRNA

Chain AC: 17% 45% 38%



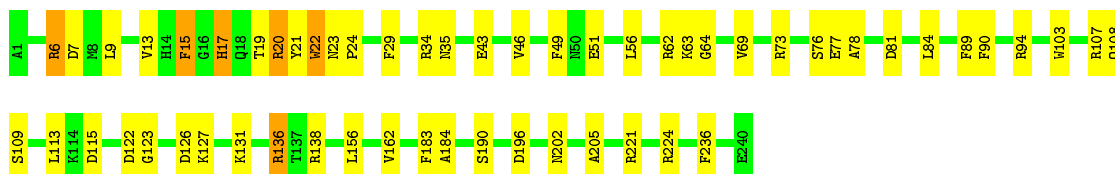
- Molecule 4: P site tRNA

Chain AD: 42% 49% 6%



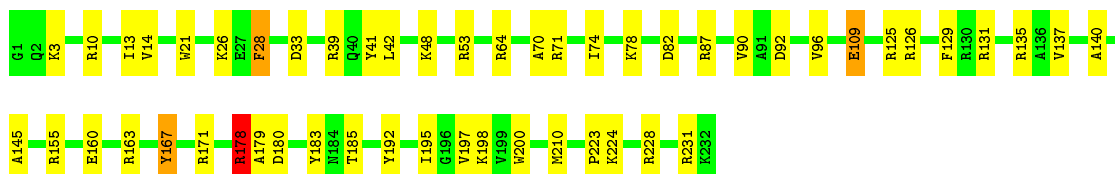
- Molecule 5: 30S ribosomal protein S2

Chain AE: 76% 21% 3%



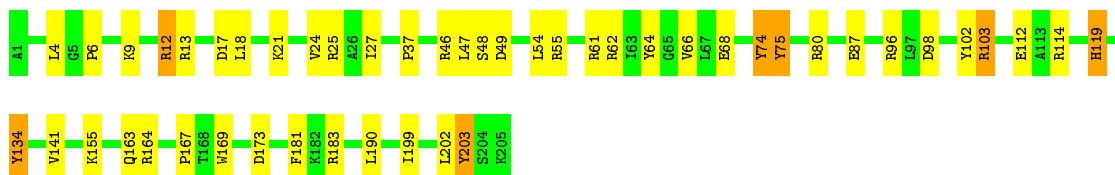
- Molecule 6: 30S ribosomal protein S3

Chain AF: 78% 21% 1%

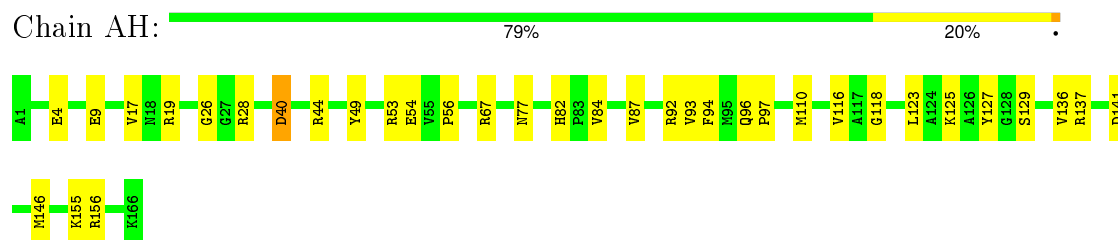


- Molecule 7: 30S ribosomal protein S4

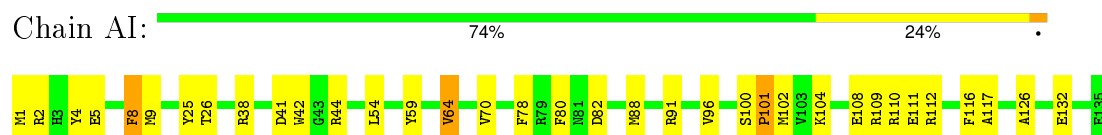
Chain AG: 77% 20% 3%



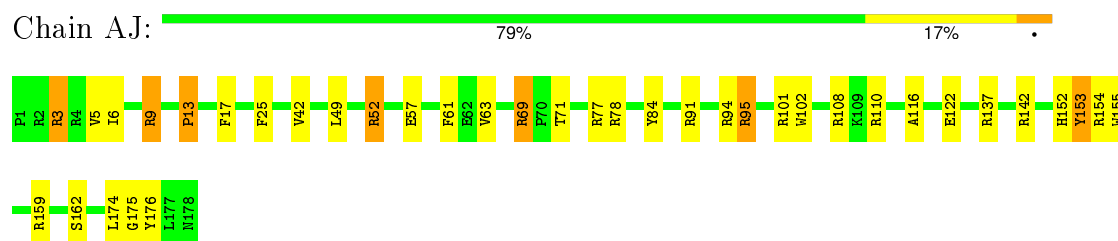
- Molecule 8: 30S ribosomal protein S5



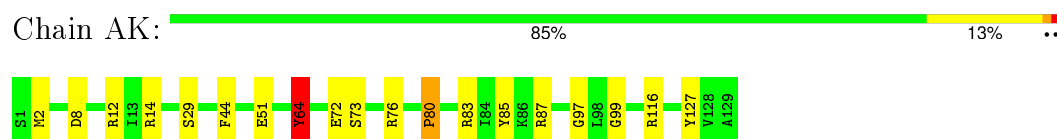
- Molecule 9: 30S ribosomal protein S6



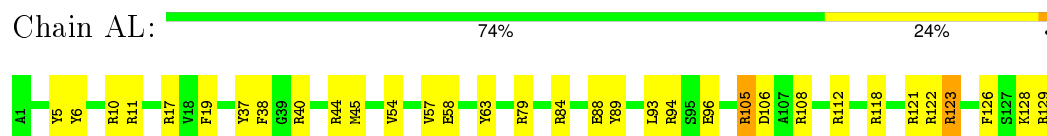
- Molecule 10: 30S ribosomal protein S7



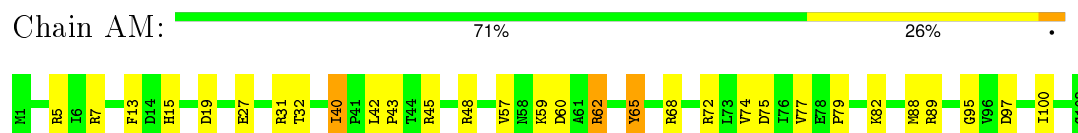
- Molecule 11: 30S ribosomal protein S8



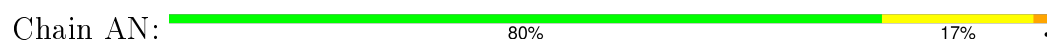
- Molecule 12: 30S ribosomal protein S9



- Molecule 13: 30S ribosomal protein S10



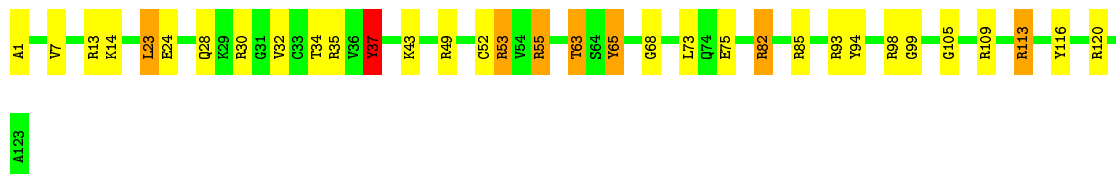
- Molecule 14: 30S ribosomal protein S11





- Molecule 15: 30S ribosomal protein S12

Chain AO: 73% 20% 6%



- Molecule 16: 30S ribosomal protein S13

Chain AP: 79% 18%



- Molecule 17: 30S ribosomal protein S14

Chain AQ: 66% 30%



- Molecule 18: 30S ribosomal protein S15

Chain AR: 72% 25%



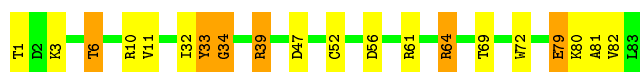
- Molecule 19: 30S ribosomal protein S16

Chain AS: 79% 16% 5%



- Molecule 20: 30S ribosomal protein S17

Chain AT: 76% 17% 7%

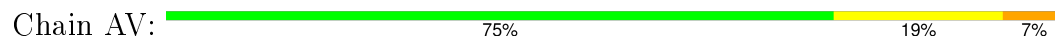


- Molecule 21: 30S ribosomal protein S18

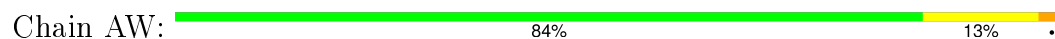
Chain AU: 68% 24% 7%



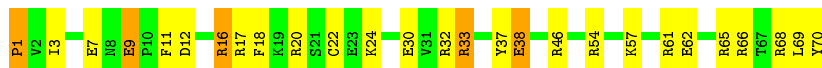
- Molecule 22: 30S ribosomal protein S19



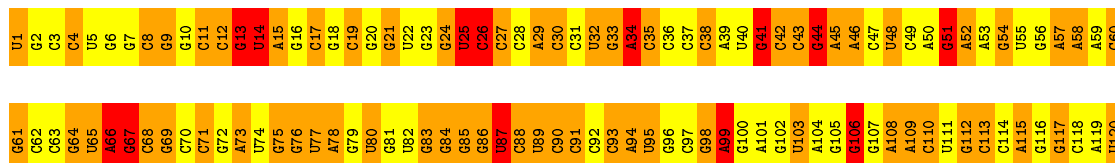
- Molecule 23: 30S ribosomal protein S20



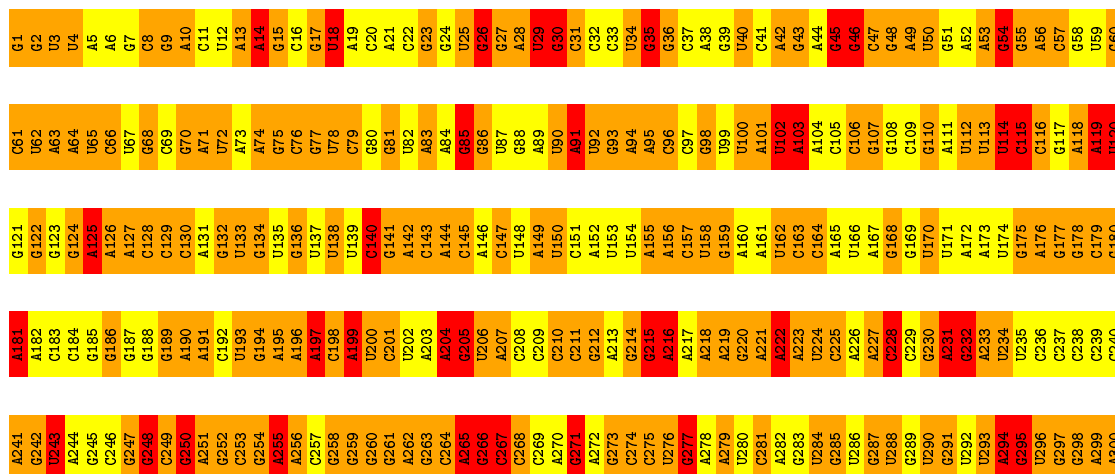
- Molecule 24: 30S ribosomal protein S21



- Molecule 25: 5S ribosomal RNA



- Molecule 26: 23S ribosomal RNA

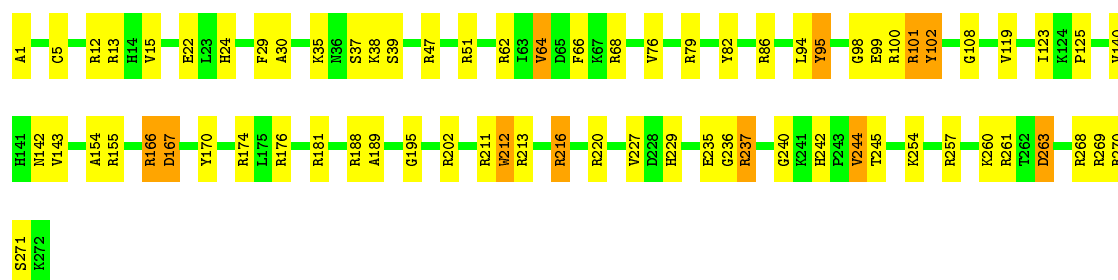


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U1263	U1203	A1143	U1083	U1023	U963	C903	G843	A783	G723	G663	A603	G543	A423	G363	G303
A1264	A1204	A1144	A1084	G1024	A844	G904	A844	G784	G724	U664	G604	C544	A424	C364	U304
A1265	G1205	C1145	A1085	G1025	C965	A905	U845	G785	G725	U665	G605	U545	G425	U365	U305
G1266	A1206	C1146	A1086	G1026	G966	A906	U846	G786	G726	U667	U607	U546	G426	C366	U306
U1267	C1207	A1147	G1087	A1027	U967	G907	U847	G787	A727	U667	A608	A547	U427	G367	G307
A1268	C1208	U1148	A1088	A1028	C968	C908	G848	A788	G728	U668	A609	G548	A428	A368	G308
U1269	U1209	G1149	A1089	A1029	G969	A909	A849	A789	G729	G669	G609	G549	A429	U369	A309
G1210	C1210	A1150	A1090	C1030	U970	A910	U850	U790	C730	A670	C610	C550	A430	G370	A310
C1211	C1211	A1151	G1091	G1031	G971	A911	C851	G791	C731	G671	G611	G551	U431	A371	A311
G1212	G1212	C1152	C1092	A1032	A972	C912	U852	A792	G732	G672	G612	U552	A432	G372	G312
A1213	A1213	C1153	G1093	U1033	G973	U913	C853	A793	G733	C673	A613	G553	C433	U373	G313
U1273	U1273	G1154	U1094	G1034	G974	G914	C854	A794	A734	G674	A614	U554	U434	A374	C314
A1274	G1215	A1155	A1095	U1035	A975	C915	G855	C795	A735	U675	U615	G555	C435	G375	G315
A1275	G1216	G1156	A1096	G1036	G976	G916	G856	C796	G736	A676	A616	A556	C436	G376	C316
G1277	U1217	G1157	U1097	G1037	G977	A917	G857	G797	G737	U677	G617	C557	U437	G377	G317
C1278	G1218	A1158	A1098	G1038	G978	A918	G858	G798	G738	G678	G618	U558	G438	C378	C318
U1279	U1219	U1159	G1099	A1039	A979	U919	G859	G799	A739	C679	G619	G559	A439	G379	G319
G1280	G1220	G1160	C1100	A1040	A980	A920	U860	A800	C740	G680	G620	C560	C440	G380	A320
U1281	C1221	A1161	U1101	G1041	C981	A921	A861	G801	U741	G681	A621	G561	U441	G381	U321
U1282	U1222	G1162	C1102	G1042	C982	C922	G862	A802	A742	U682	G622	U562	G442	A382	A322
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C1291	U1231	G1171	A1111	G1051	C991	U931	U871	U811	A751	C691	A631	U571	U451	A391	C331
G1292	G1232	C1172	G1112	C1052	C992	U932	U872	C812	A752	C692	A632	A572	G452	U392	A332
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A1302	U1242	G1182	G1122	G1062	G1002	G942	G882	G822	U762	U702	U642	A582	C462	A402	A342
G1303	C1243	U1183	C1123	G1063	G1003	A943	G883	C823	G763	U703	A643	G583	G463	U403	C343
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C1305	G1245	G1185	G1125	U1065	C1005	A945	C885	A825	C765	A705	C645	G585	G465	U405	A345
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A1307	U1247	U1187	G1127	A1067	C1007	A947	U887	U827	U767	G707	G647	C587	G467	G407	A347
A1308	G1248	U1188	G1128	G1068	C948	C948	C888	U828	G768	G708	G648	U588	G468	G408	U348
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A2225	C2165	U2105	C2045	C1985	G1925	U1865	A1805	A1745	G1685	C1625	C1565	A1505	G1445	A1385	U1325
G2226	U2166	U2106	G2046	C1986	U1926	A1866	C1806	A1746	C1686	A1626	U1566	A1506	C1446	C1386	U1326
A2227	U2167	G2107	C2047	A1987	A1927	G1867	G1807	U1747	G1687	G1627	G1567	C1507	C1447	A1387	A1327
G2228	G2168	A2108	G2048	G1988	A1928	C1868	A1808	C1748	U1688	G1628	G1568	A1508	G1448	G1388	A1328
U2229	A2169	U2109	G2049	G1989	G1929	G1869	A1809	A1749	G1689	U1629	U1569	A1509	G1449	G1389	U1329
G2230	G2170	C2050	C2050	G1990	G1930	C1870	A1810	G1750	A1690	G1630	A1570	G1510	G1450	U1390	C1330
U2231	A2171	U2111	A2051	A1991	U1931	A1871	G1811	U1751	C1691	G1631	A1571	G1511	C1451	U1391	G1331
C2232	U2172	G2112	A2052	G1992	A1932	A1872	U1812	C1752	U1692	A1632	A1572	C1512	G1452	A1392	G1332
U2233	C2173	U2113	G2053	U1993	G1933	G1873	G1813	G1753	U1693	G1633	A1573	U1513	A1453	A1393	G1333
G2234	C2174	A2114	A2054	C1994	C1934	C1874	G1814	A1754	C1694	A1634	C1574	G1514	C1454	U1394	G1334
G2235	C2175	G2115	C2055	U1995	G1935	G1875	A1815	A1755	G1695	A1635	C1575	A1515	G1455	A1395	C1335
U2236	A2176	G2116	G2056	C1996	A1936	A1876	C1816	G1756	G1696	U1636	U1576	A1516	G1456	U1396	A1336
G2237	C2177	A2117	G2057	C1997	A1937	A1877	G1817	A1757	G1697	A1637	C1577	U1517	U1457	U1397	G1337
C2238	C2178	A2118	A2058	A1998	A1938	G1878	U1818	U1758	A1698	C1638	U1578	C1518	U1458	C1398	G1338
G2239	C2179	A2119	A2059	C1999	U1939	C1879	A1819	A1759	G1699	C1639	A1579	U1519	G1459	C1399	G1339
U2240	U2180	G2120	A2060	C2000	U1940	U1880	U1820	C1760	A1700	A1640	A1580	U1520	U1460	U1400	U1340
A2241	U2181	G2121	G2061	C2001	C1941	C1881	A1821	C1761	A1701	G1641	A1581	G1521	C1461	U1401	G1341
G2242	U2182	U2122	A2062	G2002	C1942	U1882	C1822	A1762	G1702	G1642	C1582	A1522	C1462	U1402	A1342
U2243	A2183	G2123	C2063	A2003	U1943	U1883	G1823	G1763	G1703	G1643	A1583	U1523	C1463	A1403	G1343
U2244	A2184	G2124	C2064	G2004	U1944	G1884	G1824	U1764	C1704	C1644	A1584	G1524	G1464	C1404	U1344
U2245	U2185	G2125	C2065	A2005	G1945	A1885	U1825	G1765	A1705	G1645	C1585	A1525	G1465	U1405	C1345
G2246	G2186	A2126	C2066	C2006	U1946	U1886	G1826	G1766	C1706	C1646	A1586	C1526	U1466	U1406	G1346
A2247	U2187	G2127	G2067	U2007	C1947	C1887	U1827	G1767	G1707	U1647	U1587	G1527	U1467	G1407	A1347
C2248	U2188	G2128	U2068	C2008	G1948	U1888	G1828	C1768	C1708	U1648	A1588	G1528	U1468	G1408	C1348
U2249	U2189	C2129	G2069	A2009	G1949	A1889	A1830	U1769	U1709	G1649	A1589	G1529	U1469	U1409	C1349
G2250	C2190	U2130	A2070	G2010	G1950	A1890	C1830	G1770	G1710	A1650	A1590	G1530	A1470	G1410	C1350
G2251	A2191	U2131	A2071	U1951	U1951	G1891	G1831	C1771	A1711	G1651	A1591	C1531	G1471	U1411	U1351
G2252	U2192	U2132	C2072	A1952	A1952	C1892	C1832	A1772	U1712	A1652	C1592	A1532	C1472	U1412	U1352
G2253	G2193	A2133	C2073	A2013	C1953	C1893	C1833	A1773	A1713	G1653	C1593	C1533	G1473	A1413	A1353
C2254	U2194	A2134	U2074	A1954	G1954	A1894	U1834	C1774	U1714	A1654	C1594	U1534	U1474	C1414	A1354
G2255	U2195	A2135	U2075	A1955	U1955	C1895	G1835	U1775	G1715	A1655	C1595	A1535	G1475	U1415	G1355
G2256	C2196	G2136	U2076	U1956	U1956	G1896	C1836	G1776	U1716	C1656	A1596	C1536	U1476	G1416	G1356
U2257	U2197	U2137	A2077	C1957	C1957	G1897	C1837	U1777	A1717	U1657	A1597	G1537	G1477	C1357	G1357
C2258	A2198	G2138	C2078	G2018	C1958	U1898	C1838	U1778	G1718	C1658	A1598	G1538	G1478	G1418	G1358
U2259	A2199	U2139	U2079	G1959	A1959	A1899	G1839	U1779	G1719	G1659	U1599	U1539	G1479	A1419	A1359
C2260	C2200	G2140	A2080	A2020	A1960	A1900	U1840	A1780	U1720	G1660	C1600	G1540	C1480	A1420	G1360
C2261	G2201	G2141	U2081	C2021	C1961	A1901	U1841	U1781	G1721	G1661	G1601	C1541	U1481	G1421	G1361
U2262	U2202	A2142	A2082	U2022	C1962	C1902	G1842	U1782	A1722	U1662	U1602	U1542	G1482	G1422	C1362
C2263	U2203	G2143	G2083	C2023	U1963	G1903	C1843	A1783	G1723	G1663	A1603	G1543	G1483	G1423	G1363
G2264	G2204	C2144	C2084	G2024	G1964	G1904	C1844	A1784	G1724	A1664	C1604	A1544	U1484	G1424	G1364
U2265	A2205	C2145	U2085	C2025	C1965	C1905	G1845	A1785	U1725	A1665	C1605	A1545	U1485	G1425	A1365
A2266	C2206	C2146	U2086	A1966	A1966	G1906	G1846	A1786	C1726	G1666	C1606	G1546	U1486	G1426	A1366
U2267	C2207	G2147	G2087	C1967	C1967	G1907	A1847	A1787	C1727	G1667	C1607	C1547	U1487	A1427	A1367
A2268	C2208	G2148	A2088	G1968	G1968	C1908	A1848	C1788	C1728	A1668	A1608	A1548	C1488	G1428	G1368
G2269	G2209	U2149	C2089	A1969	A1969	C1909	G1849	A1789	U1729	A1669	A1609	A1549	C1489	G1429	G1369
A2270	U2210	C2150	A2090	U2030	A1970	G1910	G1850	C1790	C1730	C1670	A1610	C1550	A1490	G1430	C1370
G2271	A2211	U2151	C2091	U1971	U1911	G1911	U1851	A1791	G1731	A1671	C1611	A1551	G1491	A1431	G1371
U2272	A2212	G2152	U2092	G1972	G1972	A1912	U1852	G1792	C1732	A1672	C1612	A1552	G1492	G1432	G1372
A2273	U2213	C2153	G2093	G1973	C1973	A1913	A1853	C1793	G1733	G1673	C1613	A1553	C1493	A1433	A1373
C2274	C2214	A2154	A2094	C1974	C1974	C1914	A1854	A1794	G1734	A1674	A1614	U1554	A1494	A1434	G1374
C2275	G2215	U2155	A2095	G1975	G1975	G1915	U1855	C1795	A1735	C1675	C1615	G1555	A1495	G1435	U1375
G2276	G2216	G2156	C2096	U1976	U1976	A1916	U1856	U1796	A1736	A1676	A1616	C1556	A1496	G1436	C1376
G2277	G2217	G2157	A2097	A1977	A1977	U1917	G1857	G1797	G1737	A1677	C1617	C1557	U1497	C1437	G1377
A2278	G2218	A2158	U2098	A1978	A1978	A1918	A1858	G1798	G1738	A1678	U1618	C1558	C1498	U1438	A1378
G2279	U2219	C2159	U2099	U1979	U1979	A1919	U1859	G1799	A1739	A1679	A1619	U1559	C1499	A1439	U1379
G2280	U2220	C2160	G2100	G1980	G1980	C1920	G1860	C1800	G1740	U1680	G1620	G1560	G1500	U1440	G1380

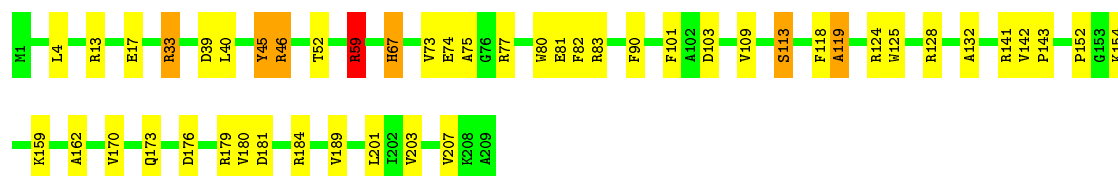
WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM



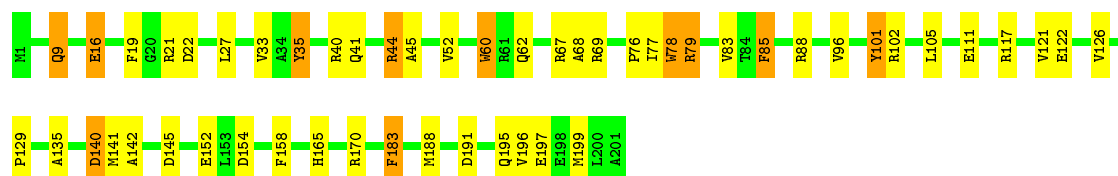
- Molecule 29: 50S ribosomal protein L3

Chain BE: 77% 20% .



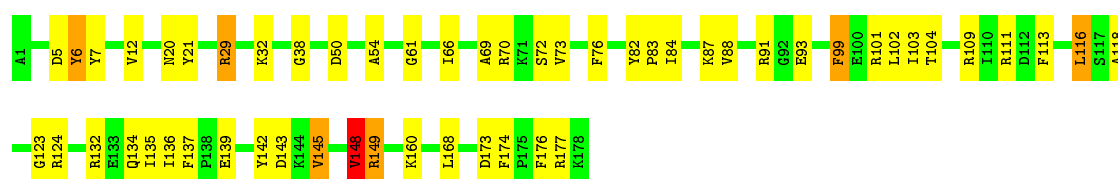
- Molecule 30: 50S ribosomal protein L4

Chain BF: 74% 20% 5%



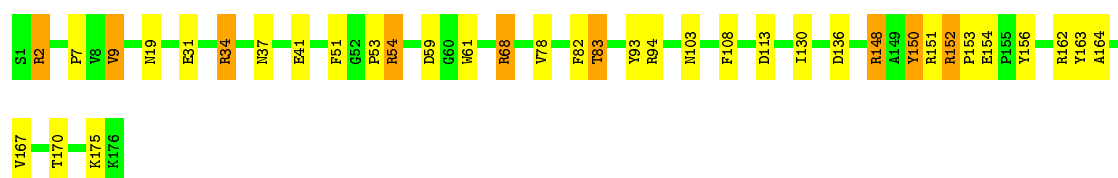
- Molecule 31: 50S ribosomal protein L5

Chain BG: 70% 26% . .

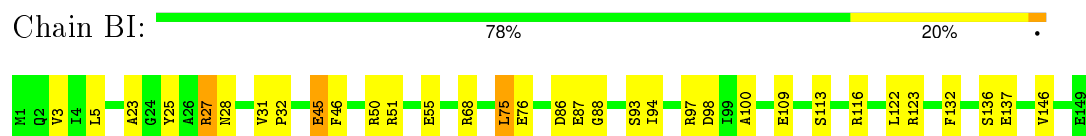


- Molecule 32: 50S ribosomal protein L6

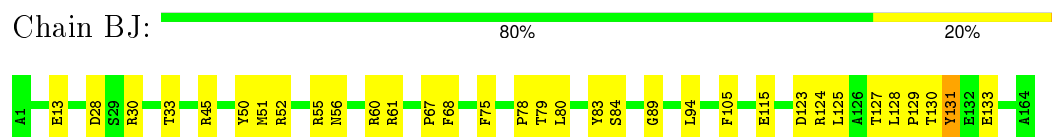
Chain BH: 79% 16% 5%



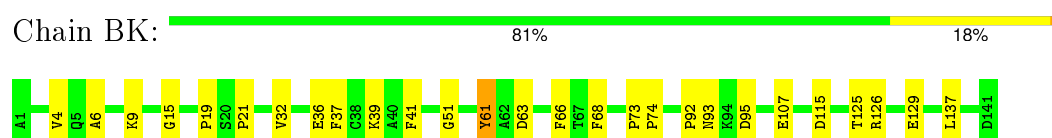
- Molecule 33: 50S ribosomal protein L9



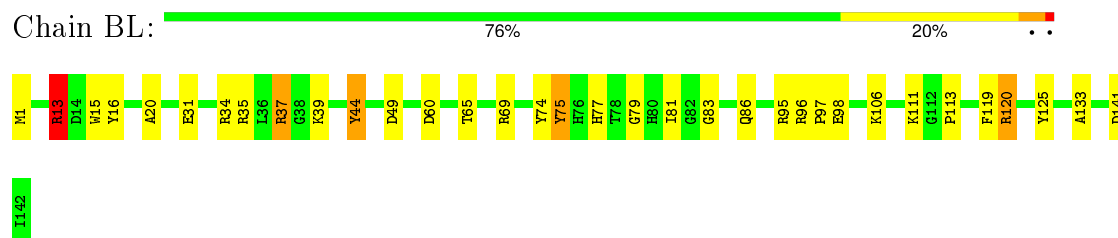
- Molecule 34: 50S ribosomal protein L10



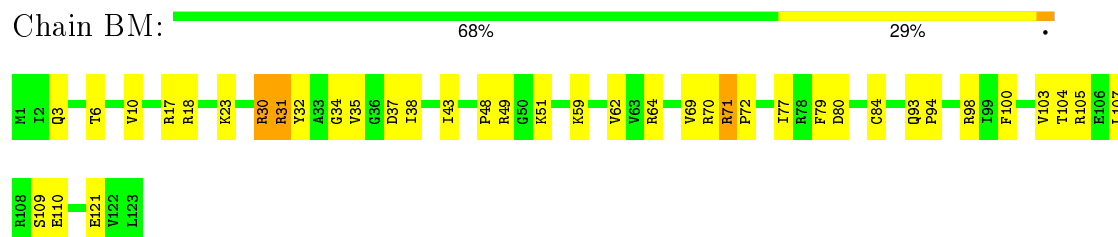
- Molecule 35: 50S ribosomal protein L11



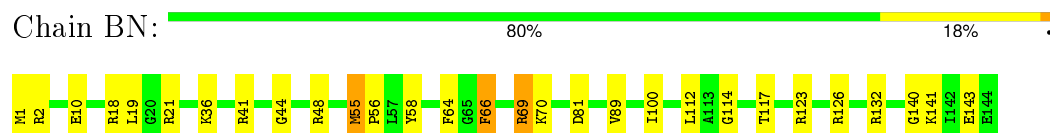
- Molecule 36: 50S ribosomal protein L13



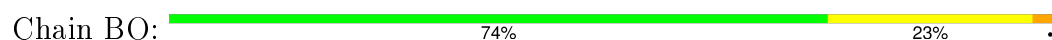
- Molecule 37: 50S ribosomal protein L14

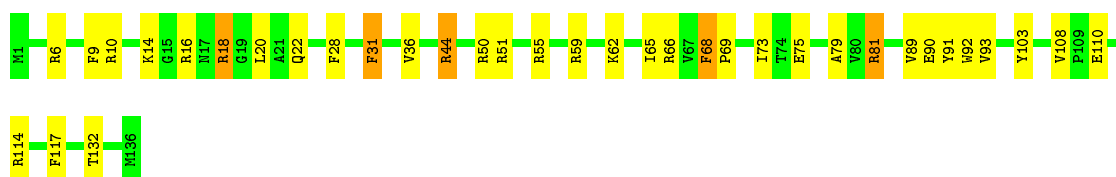


- Molecule 38: 50S ribosomal protein L15



- Molecule 39: 50S ribosomal protein L16





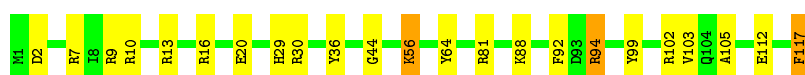
- Molecule 40: 50S ribosomal protein L17

Chain BP: 75% 22%



- Molecule 41: 50S ribosomal protein L18

Chain BQ: 80% 17%



- Molecule 42: 50S ribosomal protein L19

Chain BR: 76% 18% 5%



- Molecule 43: 50S ribosomal protein L20

Chain BS: 71% 26%



- Molecule 44: 50S ribosomal protein L21

Chain BT: 77% 19%

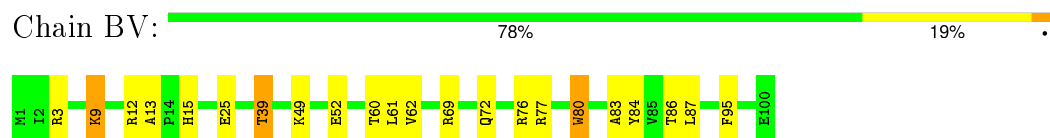


- Molecule 45: 50S ribosomal protein L22

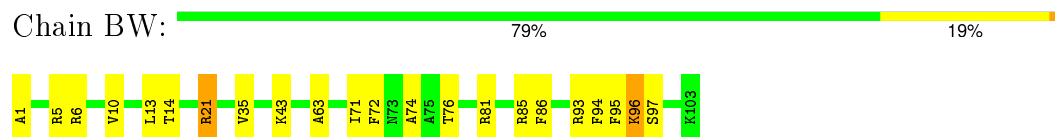
Chain BU: 75% 24%



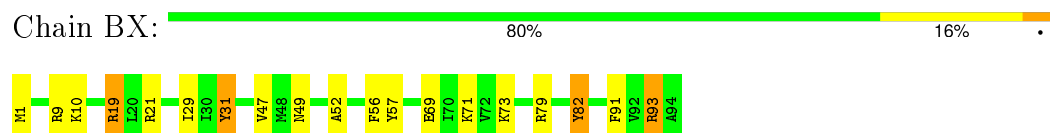
- Molecule 46: 50S ribosomal protein L23



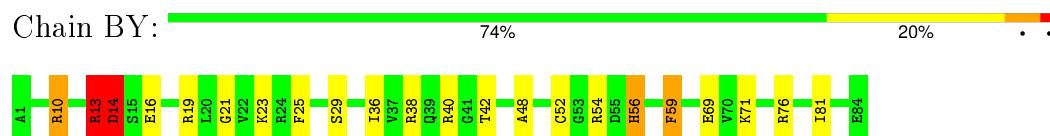
- Molecule 47: 50S ribosomal protein L24



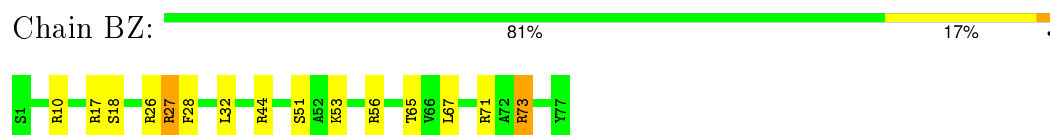
- Molecule 48: 50S ribosomal protein L25



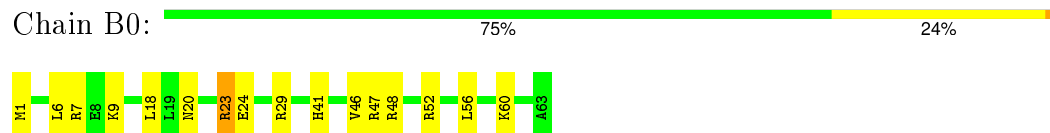
- Molecule 49: 50S ribosomal protein L27



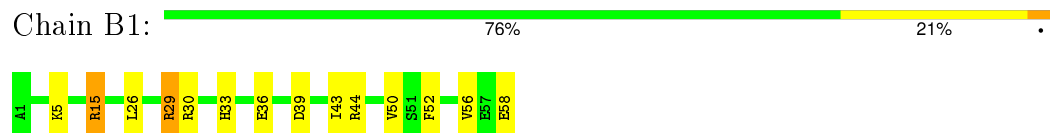
- Molecule 50: 50S ribosomal protein L28



- Molecule 51: 50S ribosomal protein L29

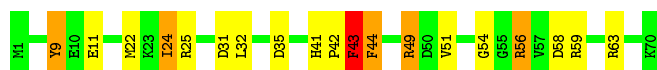


- Molecule 52: 50S ribosomal protein L30



- Molecule 53: 50S ribosomal protein L31

Chain B2:  73% 19% 7% •




- Molecule 54: 50S ribosomal protein L32

Chain B3:  71% 21% 7%



- Molecule 55: 50S ribosomal protein L33

Chain B4:  83% 13% •




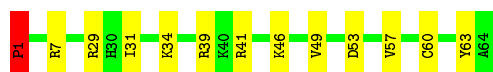
- Molecule 56: 50S ribosomal protein L34

Chain B5:  65% 30% •



- Molecule 57: 50S ribosomal protein L35

Chain B6:  80% 19% •



- Molecule 58: 50S ribosomal protein L36

Chain B7:  71% 29%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	37000	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Volumes were CTF-corrected in defocus groups	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	TVIPS TemCam-F415 (CCD)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 3TD, CH, OMG, 5MC, MA6, MIA, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, FME, 4SU, 7MG, 5MU, 1MG, PSU

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	3.08	3895/36769 (10.6%)	3.56	8470/57354 (14.8%)
10	AJ	1.47	2/1422 (0.1%)	2.07	39/1908 (2.0%)
11	AK	1.53	8/989 (0.8%)	1.89	16/1326 (1.2%)
12	AL	1.52	4/1048 (0.4%)	2.03	33/1394 (2.4%)
13	AM	1.50	5/835 (0.6%)	2.00	23/1127 (2.0%)
14	AN	1.54	6/982 (0.6%)	1.99	24/1323 (1.8%)
15	AO	1.52	4/969 (0.4%)	2.06	33/1300 (2.5%)
16	AP	1.57	5/919 (0.5%)	2.09	26/1226 (2.1%)
17	AQ	1.60	8/817 (1.0%)	1.99	27/1088 (2.5%)
18	AR	1.44	0/724	2.09	30/966 (3.1%)
19	AS	1.53	4/659 (0.6%)	1.92	13/884 (1.5%)
2	AB	3.15	171/1600 (10.7%)	3.56	384/2492 (15.4%)
20	AT	1.56	2/681 (0.3%)	1.83	18/913 (2.0%)
21	AU	1.59	7/637 (1.1%)	2.19	20/851 (2.4%)
22	AV	1.48	2/744 (0.3%)	1.98	20/995 (2.0%)
23	AW	1.46	1/676 (0.1%)	1.88	14/895 (1.6%)
24	AX	1.61	4/598 (0.7%)	2.21	25/792 (3.2%)
25	BA	3.02	293/2869 (10.2%)	3.44	610/4474 (13.6%)
26	BB	3.09	7348/69257 (10.6%)	3.54	15639/108040 (14.5%)
27	BC	1.46	3/1748 (0.2%)	1.85	33/2355 (1.4%)
28	BD	1.51	10/2131 (0.5%)	2.03	68/2863 (2.4%)
29	BE	1.54	3/1586 (0.2%)	2.03	41/2134 (1.9%)
3	AC	3.09	117/1108 (10.6%)	3.61	256/1724 (14.8%)
30	BF	1.53	6/1571 (0.4%)	1.97	51/2113 (2.4%)
31	BG	1.58	11/1444 (0.8%)	1.94	33/1937 (1.7%)
32	BH	1.50	7/1343 (0.5%)	1.89	33/1816 (1.8%)
33	BI	1.50	8/1122 (0.7%)	1.93	22/1515 (1.5%)
34	BJ	1.52	4/1247 (0.3%)	1.95	29/1679 (1.7%)
35	BK	1.45	4/1046 (0.4%)	1.81	17/1410 (1.2%)
36	BL	1.53	5/1152 (0.4%)	1.98	24/1551 (1.5%)
37	BM	1.53	3/956 (0.3%)	1.99	28/1279 (2.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	BN	1.53	4/1062 (0.4%)	1.93	21/1413 (1.5%)
39	BO	1.53	6/1093 (0.5%)	1.96	31/1460 (2.1%)
4	AD	3.09	193/1721 (11.2%)	3.54	391/2683 (14.6%)
40	BP	1.53	3/1021 (0.3%)	2.11	37/1364 (2.7%)
41	BQ	1.60	4/910 (0.4%)	1.96	26/1219 (2.1%)
42	BR	1.53	1/929 (0.1%)	2.18	29/1242 (2.3%)
43	BS	1.57	5/960 (0.5%)	2.38	37/1278 (2.9%)
44	BT	1.58	2/829 (0.2%)	2.03	21/1107 (1.9%)
45	BU	1.43	4/864 (0.5%)	2.00	28/1156 (2.4%)
46	BV	1.52	3/794 (0.4%)	1.92	14/1060 (1.3%)
47	BW	1.46	1/797 (0.1%)	2.06	20/1062 (1.9%)
48	BX	1.48	1/766 (0.1%)	1.93	16/1025 (1.6%)
49	BY	1.49	4/642 (0.6%)	2.00	16/848 (1.9%)
5	AE	1.51	6/1904 (0.3%)	1.92	45/2565 (1.8%)
50	BZ	1.50	0/635	1.84	17/848 (2.0%)
51	B0	1.43	1/510 (0.2%)	2.02	13/677 (1.9%)
52	B1	1.54	1/453 (0.2%)	1.96	12/605 (2.0%)
53	B2	1.58	4/559 (0.7%)	1.92	13/745 (1.7%)
54	B3	1.55	2/450 (0.4%)	2.05	10/599 (1.7%)
55	B4	1.41	0/448	1.83	6/594 (1.0%)
56	B5	1.50	1/380 (0.3%)	2.36	22/498 (4.4%)
57	B6	1.43	0/513	1.79	11/676 (1.6%)
58	B7	1.44	1/303 (0.3%)	2.17	7/397 (1.8%)
6	AF	1.52	7/1852 (0.4%)	1.92	47/2490 (1.9%)
7	AG	1.49	7/1665 (0.4%)	2.08	46/2227 (2.1%)
8	AH	1.51	6/1239 (0.5%)	1.87	24/1664 (1.4%)
9	AI	1.55	6/1121 (0.5%)	1.91	29/1509 (1.9%)
All	All	2.70	12223/164069 (7.4%)	3.19	27088/244735 (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	910
10	AJ	0	6
11	AK	0	2
12	AL	0	3
13	AM	0	2
14	AN	0	4
15	AO	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	AP	0	4
17	AQ	0	1
18	AR	0	3
19	AS	0	3
2	AB	0	43
20	AT	0	2
21	AU	0	5
22	AV	0	3
23	AW	0	2
24	AX	0	4
25	BA	0	65
26	BB	0	1685
27	BC	0	1
28	BD	0	10
29	BE	0	8
3	AC	0	30
30	BF	0	6
31	BG	0	7
32	BH	0	6
33	BI	0	3
34	BJ	0	4
35	BK	0	5
36	BL	0	8
37	BM	0	4
38	BN	0	2
39	BO	0	4
4	AD	0	37
40	BP	0	2
41	BQ	0	2
42	BR	0	5
43	BS	0	6
44	BT	0	3
45	BU	0	1
46	BV	0	2
47	BW	0	1
48	BX	0	5
49	BY	0	4
5	AE	0	1
50	BZ	0	1
51	B0	0	1
53	B2	0	5
54	B3	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	B4	0	3
56	B5	0	2
57	B6	0	1
6	AF	0	3
7	AG	0	9
8	AH	0	2
9	AI	0	5
All	All	0	2959

The worst 5 of 12223 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	2448	A	N3-C4	21.86	1.48	1.34
1	AA	451	A	N3-C4	17.17	1.45	1.34
26	BB	492	A	N7-C5	-16.23	1.29	1.39
26	BB	2241	A	N3-C4	15.98	1.44	1.34
26	BB	833	A	N7-C5	-15.82	1.29	1.39

The worst 5 of 27088 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AG	164	ARG	NE-CZ-NH2	-25.71	107.44	120.30
7	AG	164	ARG	NE-CZ-NH1	23.24	131.92	120.30
7	AG	114	ARG	NE-CZ-NH2	-22.43	109.08	120.30
26	BB	1929	G	C2-N3-C4	22.14	122.97	111.90
26	BB	2512	C	N3-C4-C5	-21.97	113.11	121.90

There are no chirality outliers.

5 of 2959 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1	A	Sidechain
1	AA	2	A	Sidechain
1	AA	3	A	Sidechain
1	AA	5	U	Sidechain
1	AA	6	G	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	33089	0	16599	0	0
2	AB	1627	0	841	0	0
3	AC	993	0	498	0	0
4	AD	1641	0	839	0	0
5	AE	1872	0	1885	0	0
6	AF	1822	0	1913	0	0
7	AG	1643	0	1710	0	0
8	AH	1225	0	1273	0	0
9	AI	1101	0	1050	0	0
10	AJ	1400	0	1449	0	0
11	AK	979	0	1034	0	0
12	AL	1036	0	1084	0	0
13	AM	825	0	865	0	0
14	AN	965	0	997	0	0
15	AO	955	0	1019	0	0
16	AP	910	0	981	0	0
17	AQ	805	0	847	0	0
18	AR	716	0	742	0	0
19	AS	649	0	666	0	0
20	AT	672	0	716	0	0
21	AU	626	0	651	0	0
22	AV	727	0	769	0	0
23	AW	670	0	722	0	0
24	AX	590	0	631	0	0
25	BA	2566	0	1294	0	0
26	BB	62351	0	31277	0	0
27	BC	1733	0	1824	0	0
28	BD	2092	0	2170	0	0
29	BE	1565	0	1616	0	0
30	BF	1552	0	1619	0	0
31	BG	1420	0	1460	0	0
32	BH	1323	0	1374	0	0
33	BI	1111	0	1148	0	0
34	BJ	1233	0	1283	0	0
35	BK	1032	0	1088	0	0
36	BL	1129	0	1162	0	0
37	BM	947	0	1023	0	0
38	BN	1053	0	1129	0	0
39	BO	1074	0	1157	0	0
40	BP	1008	0	1045	0	0
41	BQ	900	0	935	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BR	917	0	965	0	0
43	BS	947	0	1022	0	0
44	BT	816	0	839	0	0
45	BU	857	0	922	0	0
46	BV	787	0	846	0	0
47	BW	789	0	847	0	0
48	BX	753	0	780	0	0
49	BY	634	0	656	0	0
50	BZ	625	0	655	0	0
51	B0	509	0	543	0	0
52	B1	449	0	491	0	0
53	B2	549	0	552	0	0
54	B3	444	0	461	0	0
55	B4	441	0	485	0	0
56	B5	377	0	418	0	0
57	B6	504	0	574	0	0
58	B7	302	0	343	0	0
59	AB	14	0	9	0	0
60	BB	10	0	10	0	0
All	All	152351	0	103803	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	
5	AE	238/240 (99%)	219 (92%)	10 (4%)	9 (4%)	4	37
6	AF	230/232 (99%)	215 (94%)	10 (4%)	5 (2%)	8	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	AG	203/205 (99%)	187 (92%)	13 (6%)	3 (2%)	13	57
8	AH	164/166 (99%)	151 (92%)	11 (7%)	2 (1%)	16	61
9	AI	133/135 (98%)	122 (92%)	10 (8%)	1 (1%)	24	69
10	AJ	176/178 (99%)	164 (93%)	10 (6%)	2 (1%)	17	63
11	AK	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	24	69
12	AL	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	7	47
13	AM	101/103 (98%)	92 (91%)	4 (4%)	5 (5%)	3	31
14	AN	126/128 (98%)	111 (88%)	13 (10%)	2 (2%)	12	56
15	AO	121/123 (98%)	105 (87%)	13 (11%)	3 (2%)	7	46
16	AP	115/117 (98%)	109 (95%)	4 (4%)	2 (2%)	11	55
17	AQ	98/100 (98%)	85 (87%)	6 (6%)	7 (7%)	1	22
18	AR	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	16	61
19	AS	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
20	AT	81/83 (98%)	72 (89%)	7 (9%)	2 (2%)	7	46
21	AU	72/74 (97%)	61 (85%)	7 (10%)	4 (6%)	2	28
22	AV	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	17	63
23	AW	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	16	61
24	AX	68/70 (97%)	61 (90%)	4 (6%)	3 (4%)	3	33
27	BC	232/234 (99%)	215 (93%)	13 (6%)	4 (2%)	11	55
28	BD	270/272 (99%)	238 (88%)	23 (8%)	9 (3%)	5	40
29	BE	207/209 (99%)	173 (84%)	27 (13%)	7 (3%)	5	40
30	BF	199/201 (99%)	173 (87%)	17 (8%)	9 (4%)	3	33
31	BG	176/178 (99%)	152 (86%)	13 (7%)	11 (6%)	2	25
32	BH	174/176 (99%)	158 (91%)	13 (8%)	3 (2%)	11	55
33	BI	147/149 (99%)	131 (89%)	11 (8%)	5 (3%)	5	40
34	BJ	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	30	74
35	BK	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	26	71
36	BL	140/142 (99%)	119 (85%)	14 (10%)	7 (5%)	3	31
37	BM	121/123 (98%)	109 (90%)	9 (7%)	3 (2%)	7	46
38	BN	142/144 (99%)	126 (89%)	13 (9%)	3 (2%)	9	50
39	BO	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	13	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BP	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	24	69
41	BQ	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
42	BR	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	6	45
43	BS	115/117 (98%)	107 (93%)	5 (4%)	3 (3%)	7	45
44	BT	101/103 (98%)	89 (88%)	7 (7%)	5 (5%)	3	31
45	BU	108/110 (98%)	99 (92%)	6 (6%)	3 (3%)	6	44
46	BV	98/100 (98%)	75 (76%)	19 (19%)	4 (4%)	3	35
47	BW	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	9	51
48	BX	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	17	63
49	BY	82/84 (98%)	65 (79%)	12 (15%)	5 (6%)	2	26
50	BZ	75/77 (97%)	67 (89%)	5 (7%)	3 (4%)	4	35
51	B0	61/63 (97%)	56 (92%)	3 (5%)	2 (3%)	5	40
52	B1	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
53	B2	68/70 (97%)	63 (93%)	4 (6%)	1 (2%)	13	57
54	B3	54/56 (96%)	48 (89%)	3 (6%)	3 (6%)	2	28
55	B4	52/54 (96%)	49 (94%)	1 (2%)	2 (4%)	4	37
56	B5	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	3	33
57	B6	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	12	56
58	B7	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	28
All	All	6319/6423 (98%)	5707 (90%)	447 (7%)	165 (3%)	11	45

5 of 165 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	AH	77	ASN
13	AM	57	VAL
17	AQ	2	LYS
17	AQ	61	ASN
17	AQ	70	HIS

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	
5	AE	198/198 (100%)	186 (94%)	12 (6%)	23	60
6	AF	189/189 (100%)	180 (95%)	9 (5%)	31	67
7	AG	172/172 (100%)	166 (96%)	6 (4%)	43	74
8	AH	125/125 (100%)	116 (93%)	9 (7%)	18	55
9	AI	116/116 (100%)	109 (94%)	7 (6%)	24	60
10	AJ	146/146 (100%)	138 (94%)	8 (6%)	27	63
11	AK	104/104 (100%)	100 (96%)	4 (4%)	40	73
12	AL	106/106 (100%)	102 (96%)	4 (4%)	40	73
13	AM	90/90 (100%)	84 (93%)	6 (7%)	20	57
14	AN	98/98 (100%)	95 (97%)	3 (3%)	47	77
15	AO	103/103 (100%)	98 (95%)	5 (5%)	31	67
16	AP	95/95 (100%)	94 (99%)	1 (1%)	80	91
17	AQ	83/83 (100%)	79 (95%)	4 (5%)	31	67
18	AR	76/76 (100%)	74 (97%)	2 (3%)	54	80
19	AS	65/65 (100%)	60 (92%)	5 (8%)	16	52
20	AT	77/77 (100%)	71 (92%)	6 (8%)	16	51
21	AU	64/64 (100%)	60 (94%)	4 (6%)	22	59
22	AV	78/78 (100%)	70 (90%)	8 (10%)	9	37
23	AW	65/65 (100%)	62 (95%)	3 (5%)	33	68
24	AX	60/60 (100%)	57 (95%)	3 (5%)	30	66
27	BC	181/181 (100%)	173 (96%)	8 (4%)	35	69
28	BD	217/217 (100%)	210 (97%)	7 (3%)	46	76
29	BE	164/164 (100%)	153 (93%)	11 (7%)	20	57
30	BF	165/165 (100%)	157 (95%)	8 (5%)	31	67
31	BG	149/149 (100%)	141 (95%)	8 (5%)	27	64
32	BH	137/137 (100%)	129 (94%)	8 (6%)	25	61
33	BI	114/114 (100%)	107 (94%)	7 (6%)	23	60
34	BJ	122/122 (100%)	115 (94%)	7 (6%)	25	62
35	BK	109/109 (100%)	106 (97%)	3 (3%)	51	78
36	BL	116/116 (100%)	111 (96%)	5 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BM	104/104 (100%)	96 (92%)	8 (8%)	16	52
38	BN	103/103 (100%)	96 (93%)	7 (7%)	20	57
39	BO	109/109 (100%)	102 (94%)	7 (6%)	22	58
40	BP	103/103 (100%)	98 (95%)	5 (5%)	31	67
41	BQ	87/87 (100%)	84 (97%)	3 (3%)	44	75
42	BR	99/99 (100%)	94 (95%)	5 (5%)	29	66
43	BS	89/89 (100%)	88 (99%)	1 (1%)	80	91
44	BT	84/84 (100%)	79 (94%)	5 (6%)	24	60
45	BU	93/93 (100%)	90 (97%)	3 (3%)	46	76
46	BV	84/84 (100%)	77 (92%)	7 (8%)	14	49
47	BW	84/84 (100%)	79 (94%)	5 (6%)	24	60
48	BX	78/78 (100%)	73 (94%)	5 (6%)	22	58
49	BY	62/62 (100%)	57 (92%)	5 (8%)	15	50
50	BZ	67/67 (100%)	66 (98%)	1 (2%)	72	88
51	B0	55/55 (100%)	50 (91%)	5 (9%)	12	43
52	B1	48/48 (100%)	43 (90%)	5 (10%)	9	36
53	B2	62/62 (100%)	55 (89%)	7 (11%)	7	33
54	B3	47/47 (100%)	44 (94%)	3 (6%)	22	58
55	B4	48/48 (100%)	47 (98%)	1 (2%)	61	84
56	B5	38/38 (100%)	35 (92%)	3 (8%)	15	51
57	B6	51/51 (100%)	46 (90%)	5 (10%)	10	39
58	B7	34/34 (100%)	32 (94%)	2 (6%)	24	61
All	All	5213/5213 (100%)	4934 (95%)	279 (5%)	32	64

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BE	40	LEU
32	BH	156	TYR
52	B1	43	ILE
29	BE	74	GLU
30	BF	154	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1538/1542 (99%)	300 (19%)	101 (6%)
2	AB	74/76 (97%)	24 (32%)	7 (9%)
25	BA	119/120 (99%)	17 (14%)	10 (8%)
26	BB	2898/2904 (99%)	525 (18%)	177 (6%)
3	AC	46/47 (97%)	23 (50%)	12 (26%)
4	AD	76/77 (98%)	10 (13%)	5 (6%)
All	All	4751/4766 (99%)	899 (18%)	312 (6%)

5 of 899 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	3	A
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	7	A

5 of 312 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BB	54	G
26	BB	575	A
26	BB	2447	G
26	BB	94	A
26	BB	253	C

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

49 non-standard protein/DNA/RNA residues are 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
1	2MG	AA	1207	1	18,26,27	2.01	6 (33%)	21,38,41	3.30	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	AA	1402	1	15,23,24	2.05	5 (33%)	21,32,35	2.84	8 (38%)
1	5MC	AA	1407	1	14,22,23	1.45	3 (21%)	17,32,35	1.97	4 (23%)
1	UR3	AA	1498	1	13,22,23	1.05	0	18,32,35	1.38	3 (16%)
1	2MG	AA	1516	1	18,26,27	1.62	4 (22%)	21,38,41	3.51	9 (42%)
1	MA6	AA	1518	1	18,26,27	1.73	4 (22%)	15,38,41	1.81	3 (20%)
1	MA6	AA	1519	1	18,26,27	2.07	8 (44%)	15,38,41	2.05	5 (33%)
1	PSU	AA	516	1	15,21,22	2.25	5 (33%)	16,30,33	4.06	4 (25%)
1	7MG	AA	527	1	20,26,27	3.01	6 (30%)	23,39,42	3.05	6 (26%)
1	2MG	AA	966	1	18,26,27	1.73	6 (33%)	21,38,41	3.82	10 (47%)
1	5MC	AA	967	1	14,22,23	1.71	4 (28%)	17,32,35	2.36	6 (35%)
2	H2U	AB	16	2	17,21,22	1.47	3 (17%)	23,30,33	1.23	2 (8%)
2	H2U	AB	17	2	17,21,22	1.44	1 (5%)	23,30,33	1.94	4 (17%)
2	H2U	AB	20	2	17,21,22	1.28	2 (11%)	23,30,33	1.70	4 (17%)
2	OMC	AB	32	2	15,22,23	1.11	2 (13%)	20,31,34	2.27	4 (20%)
2	MIA	AB	37	2	22,31,32	1.90	4 (18%)	26,44,47	3.07	6 (23%)
2	7MG	AB	46	2	20,26,27	3.11	8 (40%)	23,39,42	2.75	5 (21%)
2	5MU	AB	54	2	13,22,23	2.08	7 (53%)	16,32,35	3.04	2 (12%)
2	PSU	AB	55	2	15,21,22	2.21	3 (20%)	16,30,33	4.85	6 (37%)
2	4SU	AB	8	2	12,21,22	2.23	5 (41%)	15,30,33	2.18	4 (26%)
4	H2U	AD	21	4	17,21,22	1.82	4 (23%)	23,30,33	1.96	7 (30%)
4	OMC	AD	33	4	15,22,23	1.49	3 (20%)	20,31,34	3.24	5 (25%)
4	5MU	AD	55	4	13,22,23	2.12	3 (23%)	16,32,35	4.19	4 (25%)
4	PSU	AD	56	4	15,21,22	1.69	6 (40%)	16,30,33	3.84	6 (37%)
4	4SU	AD	8	4	12,21,22	1.83	3 (25%)	15,30,33	1.99	4 (26%)
26	6MZ	BB	1618	26	17,25,26	2.03	6 (35%)	15,36,39	2.05	4 (26%)
26	2MG	BB	1835	26	18,26,27	2.07	5 (27%)	21,38,41	2.37	6 (28%)
26	PSU	BB	1911	26	15,21,22	2.15	4 (26%)	16,30,33	2.79	6 (37%)
26	3TD	BB	1915	26	15,22,23	1.74	4 (26%)	17,32,35	1.74	3 (17%)
26	PSU	BB	1917	26	15,21,22	3.07	7 (46%)	16,30,33	3.89	9 (56%)
26	5MU	BB	1939	26	13,22,23	1.73	1 (7%)	16,32,35	6.08	2 (12%)
26	5MC	BB	1962	26	14,22,23	1.43	3 (21%)	17,32,35	1.29	1 (5%)
26	6MZ	BB	2030	26	17,25,26	1.61	3 (17%)	15,36,39	2.43	4 (26%)
26	7MG	BB	2069	26	20,26,27	2.16	4 (20%)	23,39,42	2.62	6 (26%)
26	OMG	BB	2251	26	18,26,27	1.66	5 (27%)	21,38,41	2.19	9 (42%)
26	2MG	BB	2445	26	18,26,27	1.43	3 (16%)	21,38,41	3.06	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	H2U	BB	2449	26	17,21,22	1.50	3 (17%)	23,30,33	1.72	4 (17%)
26	PSU	BB	2457	26	15,21,22	1.92	5 (33%)	16,30,33	5.07	7 (43%)
26	OMC	BB	2498	26	15,22,23	1.41	3 (20%)	20,31,34	1.19	2 (10%)
26	2MA	BB	2503	26	17,25,26	1.74	3 (17%)	18,37,40	2.24	5 (27%)
26	PSU	BB	2504	26	15,21,22	2.47	6 (40%)	16,30,33	4.51	9 (56%)
26	OMU	BB	2552	26	14,22,23	1.55	2 (14%)	19,31,34	2.93	6 (31%)
26	CH	BB	2575	26	14,21,22	2.16	4 (28%)	18,30,33	2.63	6 (33%)
26	PSU	BB	2580	26	15,21,22	2.03	4 (26%)	16,30,33	3.69	7 (43%)
26	PSU	BB	2605	26	15,21,22	2.64	5 (33%)	16,30,33	3.48	5 (31%)
26	1MG	BB	745	26	17,26,27	1.88	5 (29%)	19,39,42	2.45	7 (36%)
26	PSU	BB	746	26	15,21,22	3.03	5 (33%)	16,30,33	3.41	5 (31%)
26	5MU	BB	747	26	13,22,23	1.75	4 (30%)	16,32,35	4.52	7 (43%)
26	PSU	BB	955	26	15,21,22	2.12	3 (20%)	16,30,33	5.29	6 (37%)

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
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1	-	0/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	0/7/37/38	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
2	H2U	AB	16	2	-	0/7/38/39	0/2/2/2
2	H2U	AB	17	2	-	0/7/38/39	0/2/2/2
2	H2U	AB	20	2	-	0/7/38/39	0/2/2/2
2	OMC	AB	32	2	-	0/5/27/28	0/2/2/2
2	MIA	AB	37	2	-	0/11/33/34	0/3/3/3
2	7MG	AB	46	2	-	0/7/37/38	0/3/3/3
2	5MU	AB	54	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	55	2	-	0/7/25/26	0/2/2/2
2	4SU	AB	8	2	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H2U	AD	21	4	-	0/7/38/39	0/2/2/2
4	OMC	AD	33	4	-	0/5/27/28	0/2/2/2
4	5MU	AD	55	4	-	0/3/25/26	0/2/2/2
4	PSU	AD	56	4	-	0/7/25/26	0/2/2/2
4	4SU	AD	8	4	-	0/3/25/26	0/2/2/2
26	6MZ	BB	1618	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	BB	1911	26	-	0/7/25/26	0/2/2/2
26	3TD	BB	1915	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	1939	26	-	0/3/25/26	0/2/2/2
26	5MC	BB	1962	26	-	0/3/25/26	0/2/2/2
26	6MZ	BB	2030	26	-	0/5/27/28	0/3/3/3
26	7MG	BB	2069	26	-	0/7/37/38	0/3/3/3
26	OMG	BB	2251	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	2445	26	-	0/5/27/28	0/3/3/3
26	H2U	BB	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	BB	2457	26	-	0/7/25/26	0/2/2/2
26	OMC	BB	2498	26	-	0/5/27/28	0/2/2/2
26	2MA	BB	2503	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	2504	26	-	0/7/25/26	0/2/2/2
26	OMU	BB	2552	26	-	0/5/27/28	0/2/2/2
26	CH	BB	2575	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	2580	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	BB	745	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	746	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	747	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	955	26	-	0/7/25/26	0/2/2/2

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	7MG	C8-N9	-10.96	1.29	1.45
2	AB	46	7MG	C8-N9	-9.33	1.31	1.45
26	BB	2069	7MG	C8-N9	-6.81	1.35	1.45
26	BB	2504	PSU	C2'-C1'	-5.67	1.48	1.53
26	BB	746	PSU	C6-C5	-4.75	1.31	1.38

The worst 5 of 263 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1939	5MU	C5-C4-N3	-17.64	110.54	125.35
26	BB	747	5MU	C5-C4-N3	-11.62	115.60	125.35
4	AD	55	5MU	C5-C4-N3	-11.33	115.84	125.35
1	AA	966	2MG	C4'-O4'-C1'	-9.56	99.51	109.64
1	AA	1207	2MG	C5-C6-N1	-9.52	111.08	123.52

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are 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
59	TRP	AB	101	60,2	14,15,16	1.64	3 (21%)	8,20,22	1.60	2 (25%)
60	FME	BB	3001	59	8,9,10	0.97	0	5,9,11	2.34	3 (60%)

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
59	TRP	AB	101	60,2	-	0/5/6/8	0/2/2/2
60	FME	BB	3001	59	-	1/6/9/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AB	101	TRP	OXT-C	-4.61	1.22	1.42
59	AB	101	TRP	CE3-CD2	-2.21	1.37	1.42
59	AB	101	TRP	CH2-CZ2	2.22	1.41	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BB	3001	FME	O1-CN-N	-3.74	119.08	124.80
59	AB	101	TRP	CZ3-CH2-CZ2	-2.31	117.12	120.45
60	BB	3001	FME	O-C-CA	-2.22	119.61	125.69
60	BB	3001	FME	CG-CB-CA	-2.06	106.89	113.07
59	AB	101	TRP	OXT-C-CA	3.22	120.29	111.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	BB	3001	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.