



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:14 PM BST

PDB ID : 4V6S
EMDB ID: : EMD-5360
Title : Structural characterization of mRNA-tRNA translocation intermediates (class 3 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 : 2011-12-09
Resolution : 13.10 Å(reported)
Based on PDB ID : 2I2V

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>

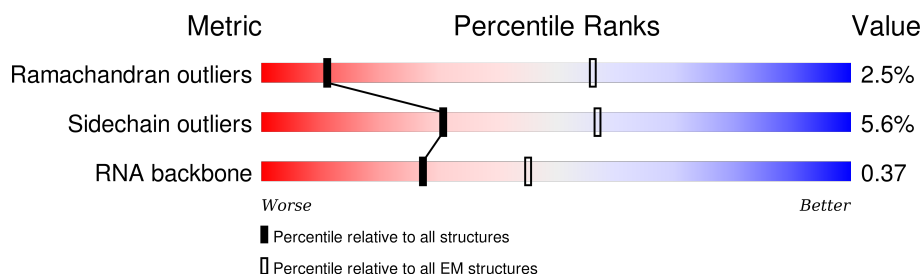
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 13.10 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	120	37% 48% 15%
2	AB	2904	34% 54% 12%
3	AC	234	85% 14% .
4	AD	272	73% 24% .
5	AE	209	78% 18% .
6	AF	201	77% 20% .
7	AG	178	72% 25% .
8	AH	176	75% 22% ..
9	AI	149	81% 16% .












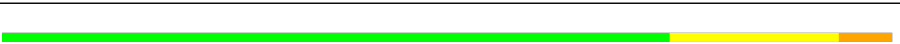




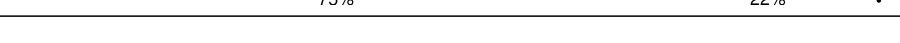
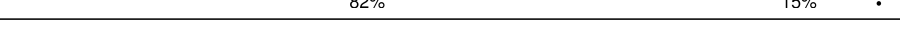

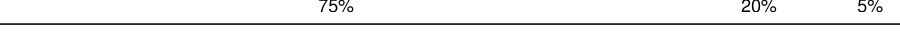

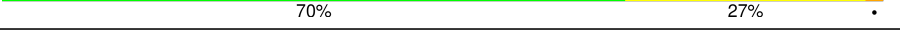

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Mol	Chain	Length	Quality of chain
10	AJ	164	 78%18%.
11	AK	141	 85%13%.
12	AL	142	 75%21%.
13	AM	123	 76%20%. .
14	AN	144	 86%11%.
15	AO	136	 79%17%.
16	AP	127	 78%19%.
17	AQ	117	 75%20%5%.
18	AR	114	 76%18%5%.
19	AS	117	 70%29%.
20	AT	103	 73%23%.
21	AU	110	 75%22%.
22	AV	100	 74%25%.
23	AW	103	 81%19%.
24	AX	94	 71%27%.
25	AY	84	 73%24%.
26	AZ	77	 60%36%.
27	A0	63	 79%14%6%.
28	A1	58	 74%19%7%.
29	A2	70	 81%16%.
30	A3	56	 77%18%.
31	A4	54	 80%17%.
32	A5	46	 61%39%.
33	A6	64	 83%13%5%.
34	A7	38	 68%29%.

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Mol	Chain	Length	Quality of chain
35	BA	1542	
36	BB	47	
37	BC	77	
38	BD	240	
39	BE	232	
40	BF	205	
41	BG	166	
42	BH	135	
43	BI	178	
44	BJ	129	
45	BK	129	
46	BL	103	
47	BM	128	
48	BN	123	
49	BO	117	
50	BP	100	
51	BQ	88	
52	BR	82	
53	BS	83	
54	BT	74	
55	BU	91	
56	BV	86	
57	BW	70	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 150700 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 5S ribosomal RNA.

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

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L1.

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

- Molecule 4 is a protein called 50S ribosomal protein L2.

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

- Molecule 5 is a protein called 50S ribosomal protein L3.

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

- Molecule 6 is a protein called 50S ribosomal protein L4.

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

- Molecule 10 is a protein called 50S ribosomal protein L10.

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

- Molecule 11 is a protein called 50S ribosomal protein L11.

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

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called 50S ribosomal protein L17.

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

- Molecule 17 is a protein called 50S ribosomal protein L18.

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

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

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

- Molecule 20 is a protein called 50S ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

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

- Molecule 23 is a protein called 50S ribosomal protein L24.

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

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L27.

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A0	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A2	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	A4	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A5	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 36 is a RNA chain called mRNA.

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

- Molecule 37 is a RNA chain called P site tRNA.

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

- Molecule 38 is a protein called 30S ribosomal protein S2.

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

- Molecule 39 is a protein called 30S ribosomal protein S3.

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

- Molecule 40 is a protein called 30S ribosomal protein S4.

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

- Molecule 41 is a protein called 30S ribosomal protein S5.

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

- Molecule 42 is a protein called 30S ribosomal protein S6.

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

- Molecule 43 is a protein called 30S ribosomal protein S7.

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

- Molecule 44 is a protein called 30S ribosomal protein S8.

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

- Molecule 45 is a protein called 30S ribosomal protein S9.

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

- Molecule 46 is a protein called 30S ribosomal protein S10.

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

- Molecule 47 is a protein called 30S ribosomal protein S11.

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

- Molecule 48 is a protein called 30S ribosomal protein S12.

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

- Molecule 49 is a protein called 30S ribosomal protein S13.

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

- Molecule 50 is a protein called 30S ribosomal protein S14.

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

- Molecule 51 is a protein called 30S ribosomal protein S15.

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

- Molecule 52 is a protein called 30S ribosomal protein S16.

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

- Molecule 53 is a protein called 30S ribosomal protein S17.

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

- Molecule 54 is a protein called 30S ribosomal protein S18.

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

- Molecule 55 is a protein called 30S ribosomal protein S19.

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

- Molecule 56 is a protein called 30S ribosomal protein S20.

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

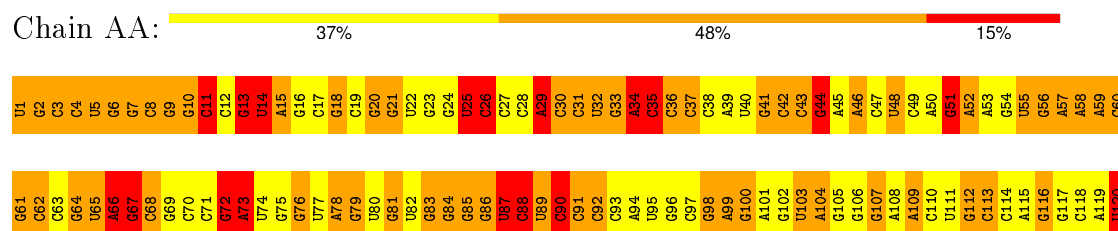
- Molecule 57 is a protein called 30S ribosomal protein S21.

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

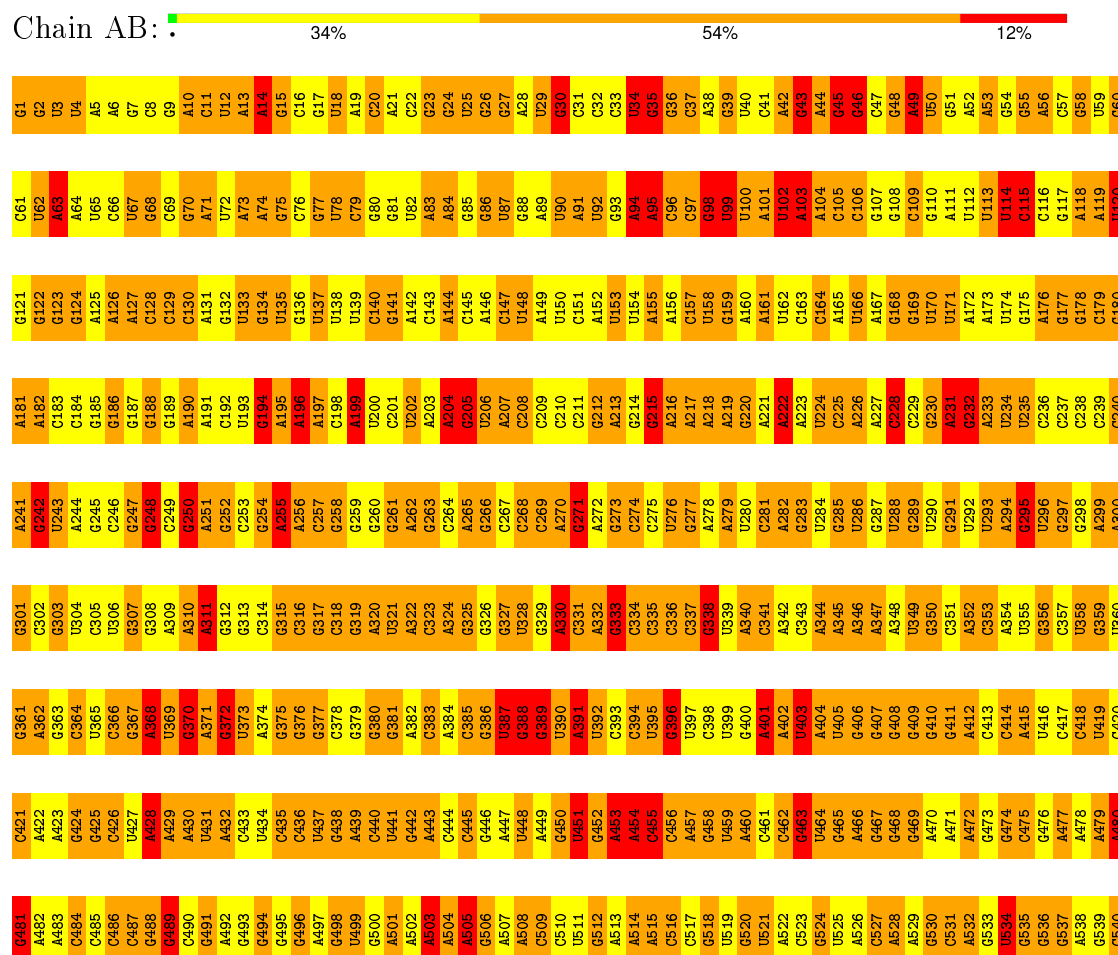
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 5S ribosomal RNA

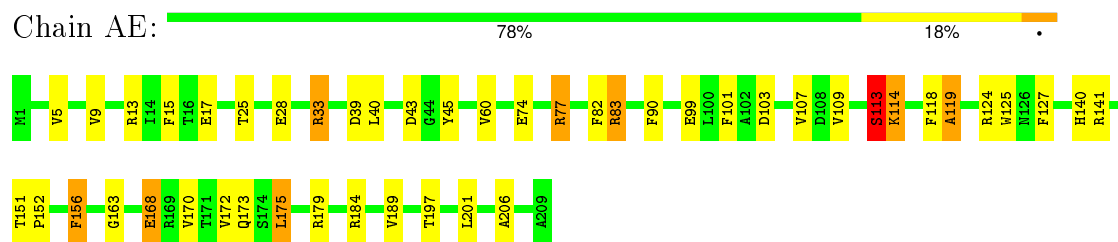


- Molecule 2: 23S ribosomal RNA

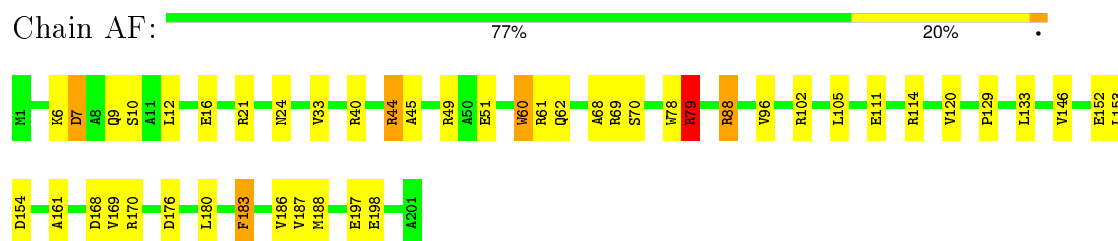


U1442	G1382	A1322	A1262	G1202	A1142	U1082	G1022	G962	C902	U842	A782	A721	G601	A541
U1443	A1383	C1323	U1263	U1203	A1143	U1083	U1023	U963	C903	G843	A783	A722	A602	C542
U1444	A1384	A1324	U1264	A1204	A1144	A1084	G1024	C964	G904	A844	G784	C723	A603	G543
U1445	A1385	U1325	A1265	A1205	C1145	A1085	G1025	C965	G905	A845	G785	U724	G604	C544
U1446	A1386	C1326	G1266	G1206	C1146	A1086	G1026	G966	U906	U846	C786	G725	U605	U545
U1447	A1387	U1327	U1267	G1207	A1147	G1087	A1027	U967	G907	U847	C787	G726	U606	U546
U1448	G1388	A1328	A1268	C1208	U1148	A1088	A1028	C968	C908	C848	A788	A727	U607	A547
U1449	G1389	U1329	A1269	U1209	G1149	A1089	C1029	G969	A909	A849	A789	G728	A608	G548
U1450	U1390	C1330	C1270	G1210	C1150	A1090	G1030	U970	A910	U850	U790	G729	A609	G549
C1451	U1391	G1331	G1271	C1211	A1151	G1091	G1031	G971	A911	U851	C791	A730	C610	C550
G1452	A1392	G1332	A1272	G1212	C1152	C1092	A1032	A972	C912	U852	A792	C731	C611	G551
A1453	C1393	G1333	U1273	A1213	G1153	U1093	U1033	A973	U913	G853	A793	G732	G612	U552
U1454	U1394	G1334	A1274	A1214	G1154	U1094	G1034	G974	G914	C854	A794	G733	A613	G553
A1455	A1395	C1335	A1275	G1215	A1155	A1095	U1035	A975	C915	G855	C795	A734	A614	U554
G1456	U1396	A1336	A1276	G1216	A1156	A1096	G1036	G976	G916	G856	C796	A735	U615	G555
U1457	G1397	G1337	G1277	U1217	G1157	U1097	G1037	G977	G917	G857	C797	C736	U616	A556
U1458	C1398	G1338	C1278	G1218	C1158	A1098	G1038	G978	A918	G858	C798	C737	G617	C557
G1459	G1399	G1339	G1279	U1219	U1159	G1099	A1039	A979	U919	G859	G799	G738	G618	U558
U1460	U1400	U1340	G1280	G1220	G1160	C1100	A1040	A980	A920	U860	A800	A739	G619	G559
C1461	G1401	G1341	G1281	C1221	C1161	U1101	G1041	A981	C921	A861	A801	C740	G620	C560
C1462	U1402	A1342	U1282	U1222	G1162	C1102	G1042	C982	C922	G862	A802	U741	A621	G561
G1463	G1343	G1343	G1283	G1223	G1163	A1103	C1043	A983	G923	A863	U803	A742	G622	U562
U1464	C1404	A1344	A1284	U1224	C1164	C1104	C1044	A984	G924	G864	A804	A743	G623	A563
G1465	A1405	G1345	A1285	G1225	A1165	U1105	C1045	C985	A925	G865	G805	U744	G624	C564
U1466	U1406	G1346	A1286	A1226	G1166	G1106	A1046	C986	G926	A866	C806	U745	G625	C565
G1467	G1407	A1347	A1287	G1227	C1167	G1107	G1047	C987	A927	C867	U807	U747	A626	U566
U1468	G1408	C1348	G1288	G1228	G1168	U1108	A1048	A988	A928	U868	G808	G748	A627	U567
A1469	U1409	C1349	G1289	C1229	A1169	C1109	C1049	G989	U929	G869	A809	A749	G628	U568
U1470	G1410	C1350	C1290	G1230	C1170	A1110	A1050	A990	G930	U870	U810	A750	G629	U569
G1471	U1411	C1351	G1291	U1231	G1171	A1111	G1051	C991	U931	U871	U811	A751	G630	G570
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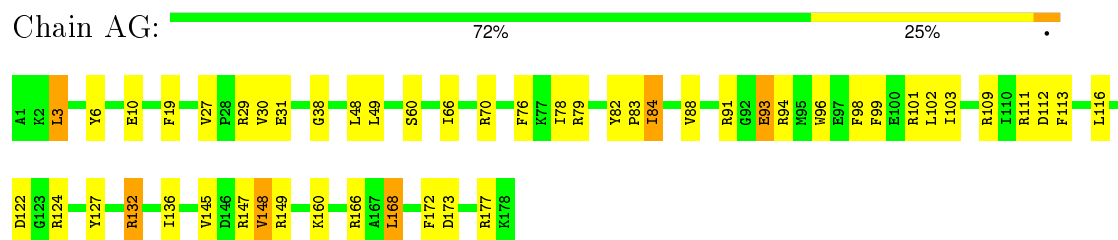
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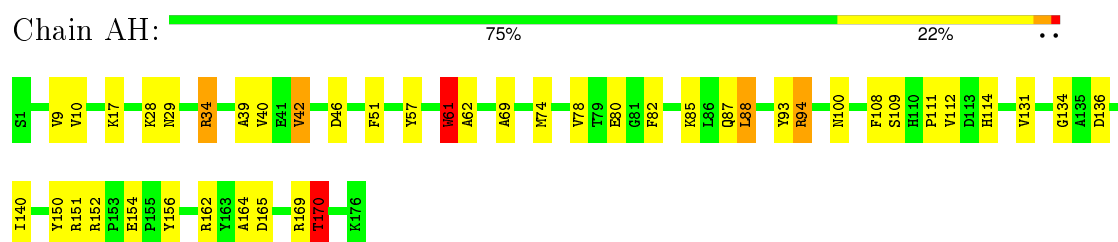
- Molecule 6: 50S ribosomal protein L4



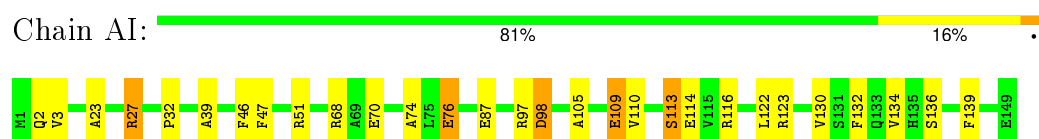
- Molecule 7: 50S ribosomal protein L5



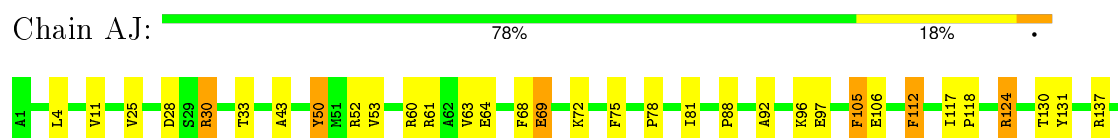
- Molecule 8: 50S ribosomal protein L6

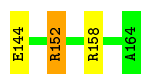


- Molecule 9: 50S ribosomal protein L9



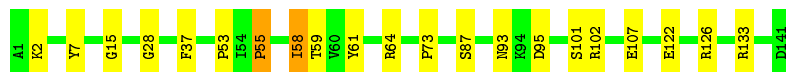
- Molecule 10: 50S ribosomal protein L10





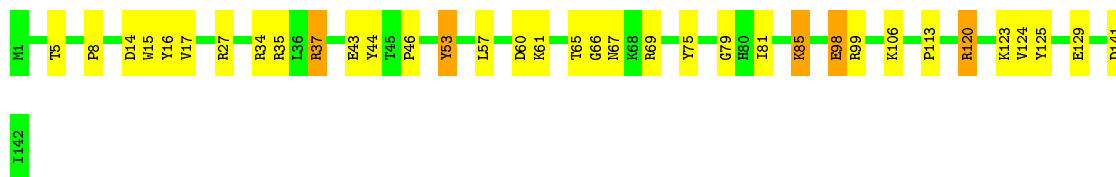
- Molecule 11: 50S ribosomal protein L11

Chain AK: 85% 13%



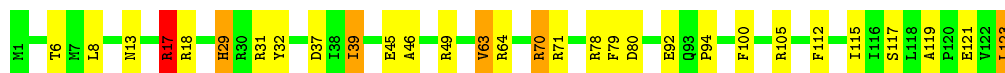
- Molecule 12: 50S ribosomal protein L13

Chain AL: 75% 21%



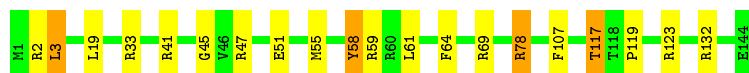
- Molecule 13: 50S ribosomal protein L14

Chain AM: 76% 20%



- Molecule 14: 50S ribosomal protein L15

Chain AN: 86% 11%



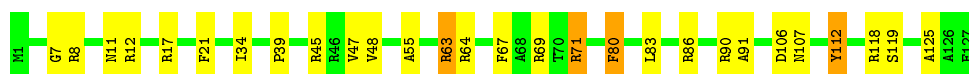
- Molecule 15: 50S ribosomal protein L16

Chain AO: 79% 17%



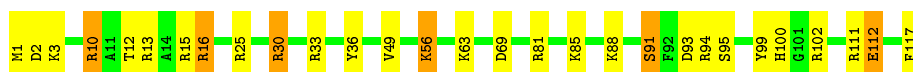
- Molecule 16: 50S ribosomal protein L17

Chain AP: 78% 19%



- Molecule 17: 50S ribosomal protein L18

Chain AQ: 75% 20% 5%



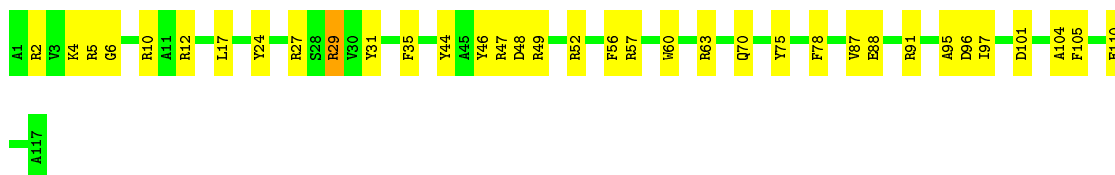
- Molecule 18: 50S ribosomal protein L19

Chain AR: 76% 18% 5%



- Molecule 19: 50S ribosomal protein L20

Chain AS: 70% 29%



- Molecule 20: 50S ribosomal protein L21

Chain AT: 73% 23%



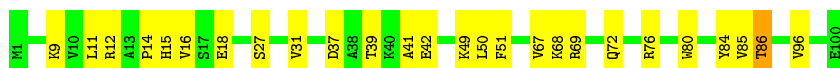
- Molecule 21: 50S ribosomal protein L22

Chain AU: 75% 22%



- Molecule 22: 50S ribosomal protein L23

Chain AV: 74% 25%



- Molecule 23: 50S ribosomal protein L24

Chain AW: 81% 19%



- Molecule 24: 50S ribosomal protein L25

Chain AX: 71% 27%



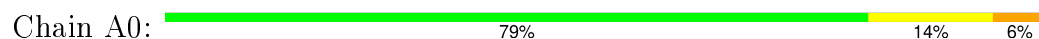
- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



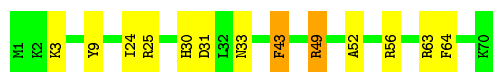
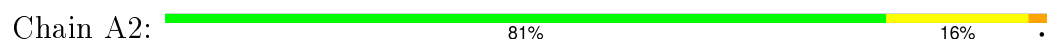
- Molecule 27: 50S ribosomal protein L29



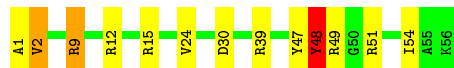
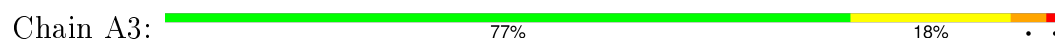
- Molecule 28: 50S ribosomal protein L30



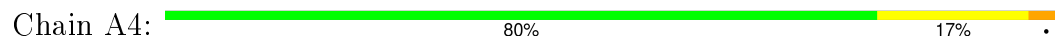
- Molecule 29: 50S ribosomal protein L31



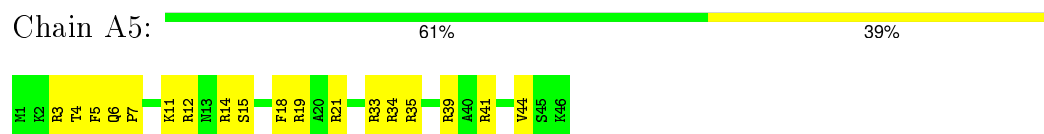
- Molecule 30: 50S ribosomal protein L32



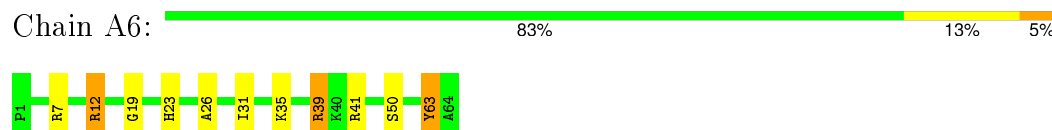
- Molecule 31: 50S ribosomal protein L33



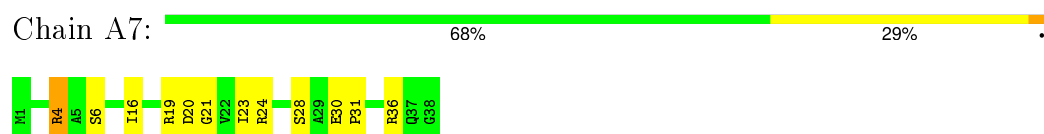
- Molecule 32: 50S ribosomal protein L34



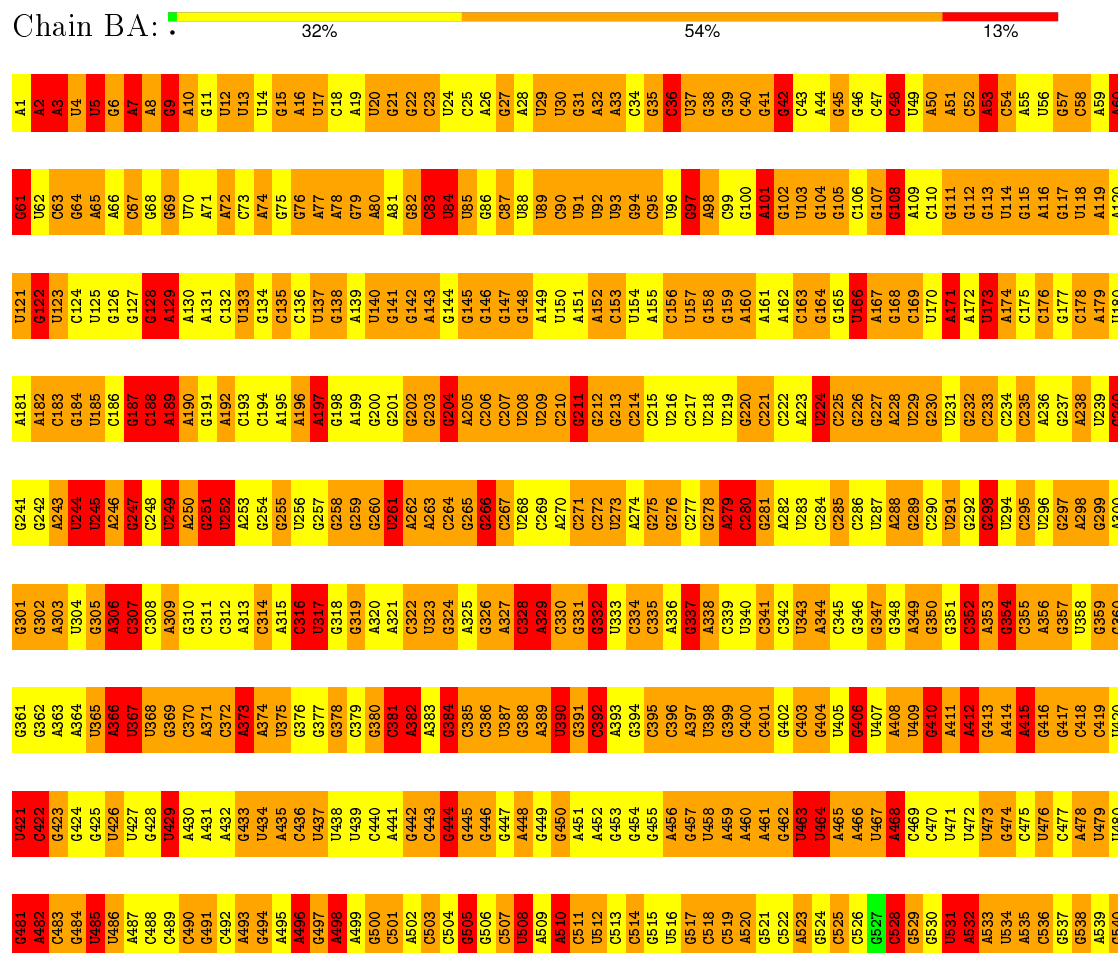
- Molecule 33: 50S ribosomal protein L35



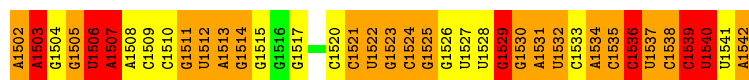
- Molecule 34: 50S ribosomal protein L36



- Molecule 35: 16S ribosomal RNA



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C1460	A1400	G1280	A1280	G1160	C1100	U1040	C980	A919	G859	G799	C739	C679	U619	A559
G1461	G1401	C1341	C1281	C1161	A1101	G1041	U981	U920	A860	G800	U740	C680	C620	A560
A1462	C1402	C1342	C1282	C1162	A1102	A1042	U982	U921	G861	U801	G741	A681	A621	U561
U1463	C1403	G1283	C1223	A1163	C1103	G1043	A983	G922	C862	A802	G742	G682	A622	U562
U1464	C1404	C1284	U1224	G1164	G1104	A1044	C984	A923	U863	G803	A743	G683	C623	A563
A1465	G1405	U1345	A1285	U1165	A1105	A1045	C985	C924	A864	U804	C744	U684	C624	C564
A1466	U1406	U1346	C1226	G1166	G1106	A1046	U986	G925	A865	C805	G745	G685	U625	U565
C1467	C1407	A1287	A1227	A1167	C1107	G1047	G987	G926	C866	C806	A746	U686	G626	G566
A1468	A1408	U1348	A1288	U1168	G1108	U1048	G988	G927	G867	A807	A747	A687	G627	G567
C1469	C1409	A1289	A1229	A1169	C1109	U1049	U989	G928	C868	C808	G748	G688	G628	G568
U1470	A1410	A1350	G1290	A1170	A1110	G1050	C990	G929	A869	A789	A749	C689	A629	C569
A1471	C1411	U1351	G1291	A1171	A1111	G1051	U991	C930	U870	C810	C750	G690	A630	G570
A1472	G1412	C1352	G1292	C1172	C1112	U1052	U992	C931	U871	C811	U751	G691	C631	U571
G1473	A1413	C1353	C1293	U1173	C1113	G1053	G993	C932	A872	G812	G752	U692	U632	A572
U1474	U1414	U1354	G1294	G1174	C1114	C1054	A994	G933	A873	U813	G753	G693	G633	A573
G1475	G1415	G1355	U1295	A1175	U1115	A1055	C995	C934	G874	A814	C754	A694	C634	A574
A1476	G1416	G1356	A1236	A1176	U1116	U1056	A996	A935	U875	A815	G755	A695	A635	G575
G1477	G1417	A1357	G1237	G1177	G1117	G1057	U997	C936	C876	A816	G756	A696	U636	C576
A1478	U1418	U1358	U1238	G1178	U1118	G1058	C998	A937	G877	C817	U757	U697	C637	G577
C1479	G1419	A1239	A1239	A1179	C1119	C1059	C999	A938	A878	G818	C758	G698	U638	C578
A1480	U1420	A1360	U1240	A1180	C1120	U1060	A1000	G939	C879	A819	A759	C699	G639	A579
U1481	G1421	G1361	G1241	G1181	U1121	G1061	C1001	C940	C880	U820	G760	G700	A640	C580
G1482	G1422	A1362	C1242	G1182	U1122	U1062	G1002	G941	G881	G821	G761	U701	U641	G581
A1483	C1423	C1363	C1243	U1183	U1123	C1063	G1003	G942	C882	U822	U762	A702	A642	C582
C1484	U1424	G1364	G1244	G1184	G1124	G1064	A1004	U943	C883	C923	G763	G703	C643	A583
U1485	U1425	G1365	C1245	G1185	U1125	U1065	A1005	G944	U884	G824	G764	A704	U644	G584
G1486	G1426	C1366	A1246	G1186	U1126	C1066	A1006	G945	G885	A825	G765	G705	G645	G585
G1487	C1427	C1367	U1247	G1187	G1127	A1067	U1007	A946	G886	C826	A766	A706	C646	C586
G1488	A1428	U1368	A1248	A1188	C1128	G1068	U1008	G947	G887	U827	G767	U707	G647	G587
C1489	C1369	G1309	C1249	U1189	C1129	C1069	U1009	C948	G888	U828	A768	C708	A648	G588
U1490	A1430	G1370	G1310	G1190	A1130	U1070	U1010	A949	A889	G829	G769	U709	A649	U589
G1491	A1431	U1371	A1311	A1191	G1131	C1071	C1011	U950	G890	G830	C770	G710	G650	U590
A1492	G1432	U1372	A1251	C1191	G1132	G1072	A1012	G951	U891	A831	G771	G711	C651	U591
A1493	A1433	G1373	G1253	G1193	C1133	U1073	G1013	U952	A892	A772	G772	A712	U652	G592
G1494	C1434	C1314	A1254	U1194	G1134	G1074	A1014	G953	C893	G833	G773	G713	U653	U593
U1495	G1435	U1375	G1255	U1195	U1135	U1075	G894	G954	G894	G774	G774	G714	G654	U594
C1496	A1436	G1316	A1256	A1196	C1136	U1076	A1016	U955	G895	U835	G775	A715	A655	A595
G1497	U1437	U1377	C1257	A1197	C1137	G1077	U1017	U956	C896	G836	G776	A716	G656	A596
U1498	G1438	C1378	G1258	G1198	G1138	U1078	G1018	U957	C897	U837	A777	U717	U657	G597
A1499	G1439	C1379	C1259	U1199	G1139	U1079	A1019	A958	G898	G838	G778	A718	C658	U598
U1500	U1440	C1380	C1260	C1200	A1080	G1079	G1020	A959	C899	C779	G779	C719	U659	C599
C1501	A1441	U1381	A1261	A1201	C1141	A1081	A1021	U960	A900	C940	A780	C720	C660	A600



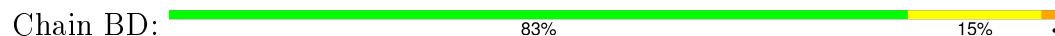
- Molecule 36: mRNA



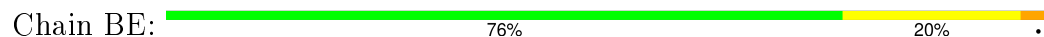
- Molecule 37: P site tRNA



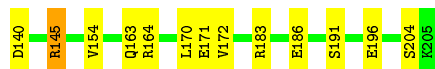
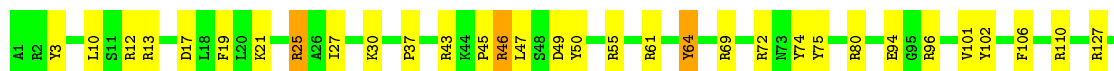
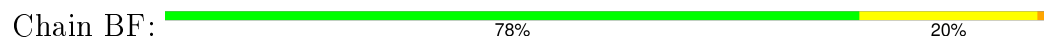
- Molecule 38: 30S ribosomal protein S2



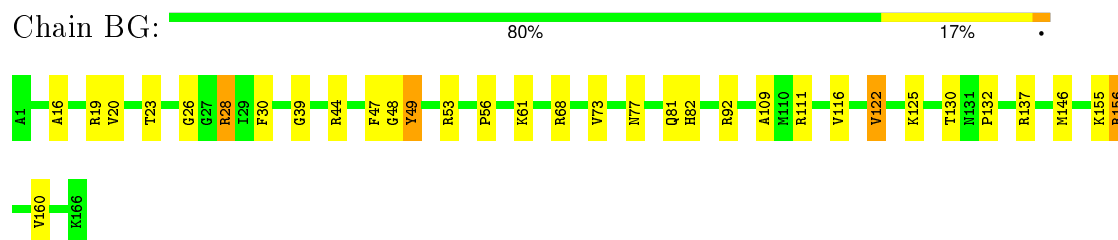
- Molecule 39: 30S ribosomal protein S3



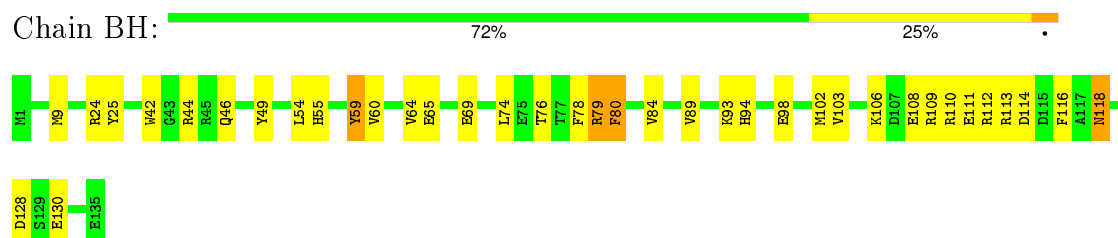
- Molecule 40: 30S ribosomal protein S4



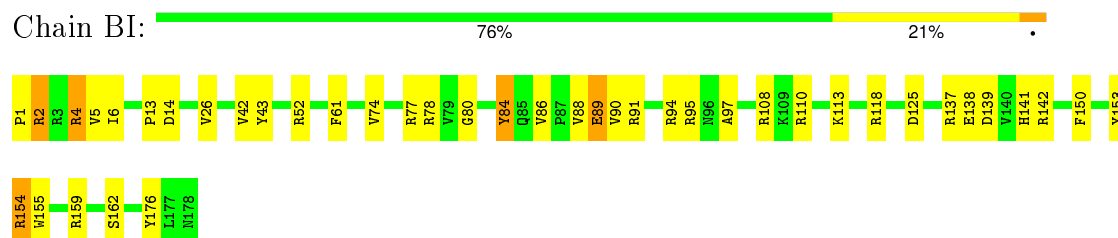
- Molecule 41: 30S ribosomal protein S5



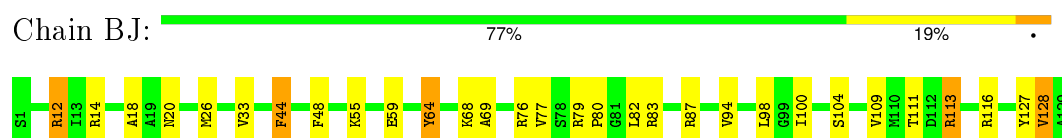
- Molecule 42: 30S ribosomal protein S6



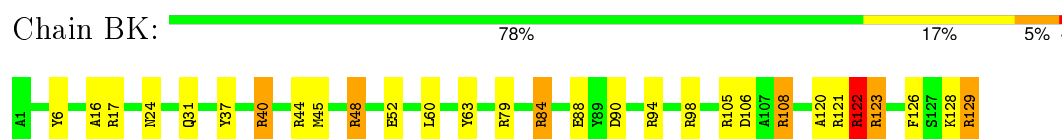
- Molecule 43: 30S ribosomal protein S7



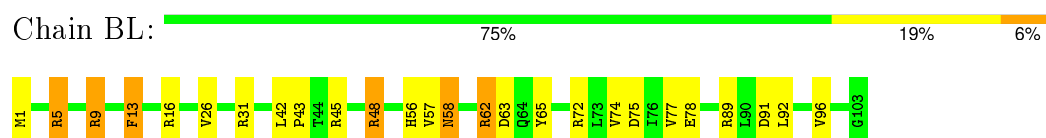
- Molecule 44: 30S ribosomal protein S8



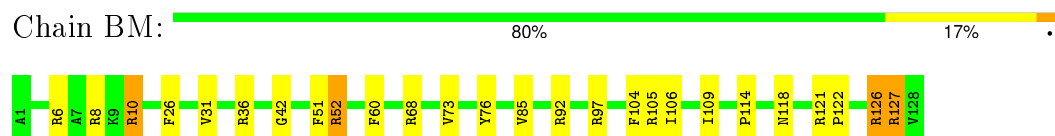
- Molecule 45: 30S ribosomal protein S9



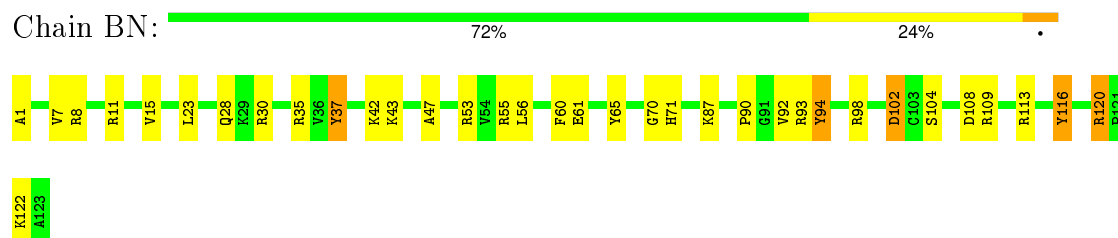
- Molecule 46: 30S ribosomal protein S10



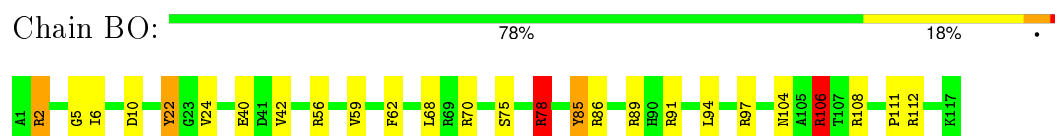
- Molecule 47: 30S ribosomal protein S11



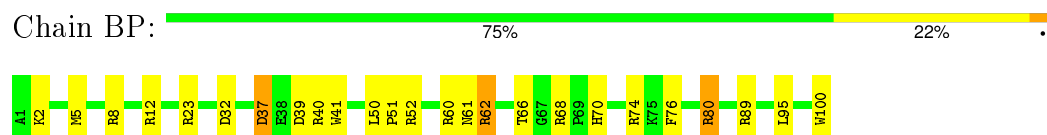
- Molecule 48: 30S ribosomal protein S12



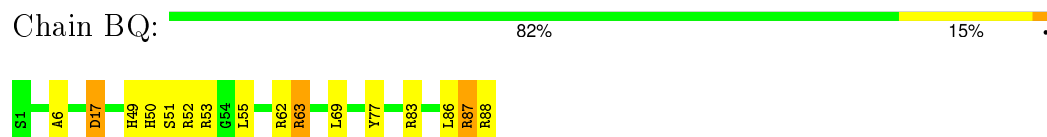
- Molecule 49: 30S ribosomal protein S13



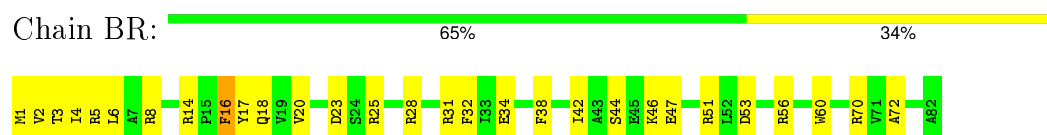
- Molecule 50: 30S ribosomal protein S14



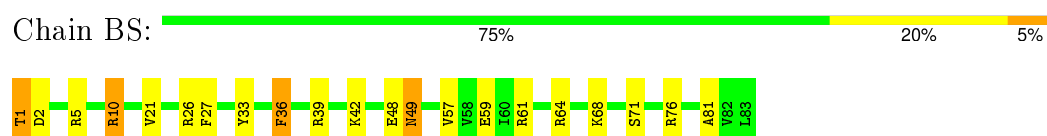
- Molecule 51: 30S ribosomal protein S15




- Molecule 52: 30S ribosomal protein S16



- Molecule 53: 30S ribosomal protein S17



- Molecule 54: 30S ribosomal protein S18

Chain BT:  74% 20% 5%




- Molecule 55: 30S ribosomal protein S19

Chain BU:  70% 27% 3%



- Molecule 56: 30S ribosomal protein S20

Chain BV:  86% 13% 1%



- Molecule 57: 30S ribosomal protein S21

Chain BW:  66% 27% 6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	21000	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: 3TD, 5MU, CH, OMG, OMU, MA6, H2U, OMC, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, 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	3.07	298/2869 (10.4%)	3.56	669/4474 (15.0%)
10	AJ	1.52	5/1247 (0.4%)	1.94	27/1679 (1.6%)
11	AK	1.44	5/1046 (0.5%)	1.86	18/1410 (1.3%)
12	AL	1.50	6/1152 (0.5%)	2.08	30/1551 (1.9%)
13	AM	1.53	5/956 (0.5%)	1.95	25/1279 (2.0%)
14	AN	1.52	5/1062 (0.5%)	1.89	20/1413 (1.4%)
15	AO	1.49	3/1093 (0.3%)	2.07	38/1460 (2.6%)
16	AP	1.48	5/1021 (0.5%)	2.09	28/1364 (2.1%)
17	AQ	1.57	4/910 (0.4%)	1.90	27/1219 (2.2%)
18	AR	1.54	2/929 (0.2%)	1.95	26/1242 (2.1%)
19	AS	1.52	6/960 (0.6%)	2.20	39/1278 (3.1%)
2	AB	3.08	7422/69257 (10.7%)	3.52	15483/108040 (14.3%)
20	AT	1.60	5/829 (0.6%)	1.89	18/1107 (1.6%)
21	AU	1.49	1/864 (0.1%)	1.96	21/1156 (1.8%)
22	AV	1.54	3/794 (0.4%)	1.90	17/1060 (1.6%)
23	AW	1.44	2/797 (0.3%)	1.90	13/1062 (1.2%)
24	AX	1.49	5/766 (0.7%)	1.79	15/1025 (1.5%)
25	AY	1.48	2/642 (0.3%)	1.92	14/848 (1.7%)
26	AZ	1.50	3/635 (0.5%)	2.21	25/848 (2.9%)
27	A0	1.37	1/510 (0.2%)	1.90	12/677 (1.8%)
28	A1	1.52	2/453 (0.4%)	2.11	13/605 (2.1%)
29	A2	1.55	3/559 (0.5%)	1.96	12/745 (1.6%)
3	AC	1.42	3/1748 (0.2%)	1.86	30/2355 (1.3%)
30	A3	1.49	1/450 (0.2%)	2.05	15/599 (2.5%)
31	A4	1.46	1/448 (0.2%)	1.82	7/594 (1.2%)
32	A5	1.53	1/380 (0.3%)	2.15	14/498 (2.8%)
33	A6	1.55	4/513 (0.8%)	1.80	7/676 (1.0%)
34	A7	1.57	2/303 (0.7%)	1.98	6/397 (1.5%)
35	BA	3.07	3871/36769 (10.5%)	3.53	8462/57354 (14.8%)
36	BB	3.23	131/1108 (11.8%)	3.61	262/1724 (15.2%)
37	BC	3.09	176/1721 (10.2%)	3.61	392/2683 (14.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	BD	1.43	2/1904 (0.1%)	1.86	32/2565 (1.2%)
39	BE	1.55	11/1852 (0.6%)	1.94	38/2490 (1.5%)
4	AD	1.56	11/2131 (0.5%)	2.03	60/2863 (2.1%)
40	BF	1.51	8/1665 (0.5%)	1.96	51/2227 (2.3%)
41	BG	1.54	5/1239 (0.4%)	2.01	27/1664 (1.6%)
42	BH	1.50	3/1121 (0.3%)	1.92	27/1509 (1.8%)
43	BI	1.54	5/1422 (0.4%)	2.05	48/1908 (2.5%)
44	BJ	1.49	3/989 (0.3%)	2.00	23/1326 (1.7%)
45	BK	1.55	5/1048 (0.5%)	2.08	34/1394 (2.4%)
46	BL	1.47	1/835 (0.1%)	2.19	25/1127 (2.2%)
47	BM	1.52	7/982 (0.7%)	2.02	28/1323 (2.1%)
48	BN	1.52	4/969 (0.4%)	2.10	39/1300 (3.0%)
49	BO	1.51	8/919 (0.9%)	1.98	30/1226 (2.4%)
5	AE	1.49	5/1586 (0.3%)	1.92	39/2134 (1.8%)
50	BP	1.53	1/817 (0.1%)	2.02	23/1088 (2.1%)
51	BQ	1.43	1/724 (0.1%)	1.93	16/966 (1.7%)
52	BR	1.53	2/659 (0.3%)	2.14	25/884 (2.8%)
53	BS	1.55	6/681 (0.9%)	1.99	18/913 (2.0%)
54	BT	1.60	6/637 (0.9%)	2.07	18/851 (2.1%)
55	BU	1.53	3/744 (0.4%)	1.84	16/995 (1.6%)
56	BV	1.39	1/676 (0.1%)	1.86	14/895 (1.6%)
57	BW	1.46	5/598 (0.8%)	2.19	23/792 (2.9%)
6	AF	1.52	7/1571 (0.4%)	1.92	42/2113 (2.0%)
7	AG	1.53	3/1444 (0.2%)	2.02	45/1937 (2.3%)
8	AH	1.53	6/1343 (0.4%)	1.96	35/1816 (1.9%)
9	AI	1.45	3/1122 (0.3%)	1.94	25/1515 (1.7%)
All	All	2.69	12105/162469 (7.5%)	3.17	26586/242243 (11.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	69
10	AJ	0	8
11	AK	0	1
12	AL	0	3
13	AM	0	3
14	AN	0	2
15	AO	0	3
16	AP	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	AQ	0	4
18	AR	0	6
19	AS	0	3
2	AB	0	1654
20	AT	0	5
21	AU	0	5
22	AV	0	1
24	AX	0	5
25	AY	0	4
26	AZ	0	2
27	A0	0	4
28	A1	0	4
29	A2	0	3
3	AC	0	3
30	A3	0	1
31	A4	0	2
32	A5	0	2
33	A6	0	2
34	A7	0	2
35	BA	0	882
36	BB	0	30
37	BC	0	41
38	BD	0	4
39	BE	0	9
4	AD	0	11
40	BF	0	3
41	BG	0	3
42	BH	0	9
43	BI	0	3
44	BJ	0	7
45	BK	0	5
46	BL	0	2
47	BM	0	1
48	BN	0	6
49	BO	0	4
5	AE	0	7
50	BP	0	1
51	BQ	0	2
52	BR	0	2
53	BS	0	1
54	BT	0	2
55	BU	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
57	BW	0	4
6	AF	0	2
7	AG	0	1
8	AH	0	2
9	AI	0	3
All	All	0	2857

The worst 5 of 12105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	504	A	N3-C4	18.22	1.45	1.34
2	AB	2682	A	N3-C4	18.21	1.45	1.34
2	AB	744	U	C2-N3	17.97	1.50	1.37
35	BA	1484	C	N1-C6	16.21	1.46	1.37
2	AB	2829	A	P-O5'	15.96	1.75	1.59

The worst 5 of 26586 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AL	120	ARG	NE-CZ-NH2	24.50	132.55	120.30
2	AB	1193	G	C8-N9-C4	-23.95	96.82	106.40
35	BA	581	G	N9-C4-C5	22.36	114.35	105.40
46	BL	45	ARG	NE-CZ-NH1	21.76	131.18	120.30
44	BJ	116	ARG	NE-CZ-NH2	-21.74	109.43	120.30

There are no chirality outliers.

5 of 2857 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1	U	Sidechain
1	AA	2	G	Sidechain
1	AA	3	C	Sidechain
1	AA	4	C	Sidechain
1	AA	5	U	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	2566	0	1299	0	0
2	AB	62351	0	31248	0	0
3	AC	1733	0	1824	0	0
4	AD	2092	0	2170	0	0
5	AE	1565	0	1616	0	0
6	AF	1552	0	1619	0	0
7	AG	1420	0	1460	0	0
8	AH	1323	0	1374	0	0
9	AI	1111	0	1148	0	0
10	AJ	1233	0	1283	0	0
11	AK	1032	0	1088	0	0
12	AL	1129	0	1162	0	0
13	AM	947	0	1023	0	0
14	AN	1053	0	1129	0	0
15	AO	1074	0	1157	0	0
16	AP	1008	0	1045	0	0
17	AQ	900	0	935	0	0
18	AR	917	0	965	0	0
19	AS	947	0	1022	0	0
20	AT	816	0	839	0	0
21	AU	857	0	922	0	0
22	AV	787	0	846	0	0
23	AW	789	0	847	0	0
24	AX	753	0	780	0	0
25	AY	634	0	656	0	0
26	AZ	625	0	655	0	0
27	A0	509	0	543	0	0
28	A1	449	0	491	0	0
29	A2	549	0	552	0	0
30	A3	444	0	461	0	0
31	A4	441	0	485	0	0
32	A5	377	0	418	0	0
33	A6	504	0	574	0	0
34	A7	302	0	343	0	0
35	BA	33089	0	16599	0	0
36	BB	993	0	501	0	0
37	BC	1641	0	841	0	0
38	BD	1872	0	1885	0	0
39	BE	1822	0	1913	0	0
40	BF	1643	0	1710	0	0
41	BG	1225	0	1273	0	0
42	BH	1101	0	1050	0	0
43	BI	1400	0	1449	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BJ	979	0	1034	0	0
45	BK	1036	0	1084	0	0
46	BL	825	0	865	0	0
47	BM	965	0	997	0	0
48	BN	955	0	1019	0	0
49	BO	910	0	981	0	0
50	BP	805	0	847	0	0
51	BQ	716	0	742	0	0
52	BR	649	0	666	0	0
53	BS	672	0	716	0	0
54	BT	626	0	651	0	0
55	BU	727	0	769	0	0
56	BV	670	0	722	0	0
57	BW	590	0	631	0	0
All	All	150700	0	102924	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	
3	AC	232/234 (99%)	215 (93%)	12 (5%)	5 (2%)	8	49
4	AD	270/272 (99%)	237 (88%)	24 (9%)	9 (3%)	5	40
5	AE	207/209 (99%)	175 (84%)	24 (12%)	8 (4%)	4	36
6	AF	199/201 (99%)	173 (87%)	16 (8%)	10 (5%)	3	31
7	AG	176/178 (99%)	151 (86%)	15 (8%)	10 (6%)	2	28
8	AH	174/176 (99%)	159 (91%)	11 (6%)	4 (2%)	8	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	147/149 (99%)	131 (89%)	12 (8%)	4 (3%)	6	45
10	AJ	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	30	74
11	AK	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	26	71
12	AL	140/142 (99%)	120 (86%)	15 (11%)	5 (4%)	4	38
13	AM	121/123 (98%)	105 (87%)	12 (10%)	4 (3%)	5	40
14	AN	142/144 (99%)	125 (88%)	14 (10%)	3 (2%)	9	50
15	AO	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	13	57
16	AP	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	24	69
17	AQ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
18	AR	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	11	53
19	AS	115/117 (98%)	108 (94%)	3 (3%)	4 (4%)	4	39
20	AT	101/103 (98%)	89 (88%)	9 (9%)	3 (3%)	5	42
21	AU	108/110 (98%)	99 (92%)	5 (5%)	4 (4%)	4	38
22	AV	98/100 (98%)	77 (79%)	18 (18%)	3 (3%)	5	42
23	AW	101/103 (98%)	89 (88%)	9 (9%)	3 (3%)	5	42
24	AX	92/94 (98%)	84 (91%)	7 (8%)	1 (1%)	17	63
25	AY	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	3	31
26	AZ	75/77 (97%)	68 (91%)	4 (5%)	3 (4%)	4	35
27	A0	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	12	56
28	A1	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
29	A2	68/70 (97%)	64 (94%)	3 (4%)	1 (2%)	13	57
30	A3	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	4	38
31	A4	52/54 (96%)	49 (94%)	1 (2%)	2 (4%)	4	37
32	A5	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	3	33
33	A6	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	12	56
34	A7	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	18
38	BD	238/240 (99%)	218 (92%)	14 (6%)	6 (2%)	7	46
39	BE	230/232 (99%)	217 (94%)	9 (4%)	4 (2%)	11	55
40	BF	203/205 (99%)	186 (92%)	13 (6%)	4 (2%)	9	51
41	BG	164/166 (99%)	150 (92%)	12 (7%)	2 (1%)	16	61
42	BH	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BI	176/178 (99%)	168 (96%)	5 (3%)	3 (2%)	11	55
44	BJ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	24	69
45	BK	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	7	47
46	BL	101/103 (98%)	91 (90%)	4 (4%)	6 (6%)	2	27
47	BM	126/128 (98%)	109 (86%)	15 (12%)	2 (2%)	12	56
48	BN	121/123 (98%)	103 (85%)	16 (13%)	2 (2%)	11	55
49	BO	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	21	67
50	BP	98/100 (98%)	85 (87%)	6 (6%)	7 (7%)	1	22
51	BQ	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	16	61
52	BR	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
53	BS	81/83 (98%)	73 (90%)	7 (9%)	1 (1%)	16	61
54	BT	72/74 (97%)	62 (86%)	7 (10%)	3 (4%)	3	34
55	BU	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	17	63
56	BV	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	16	61
57	BW	68/70 (97%)	61 (90%)	4 (6%)	3 (4%)	3	33
All	All	6319/6423 (98%)	5708 (90%)	453 (7%)	158 (2%)	11	46

5 of 158 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	94	LEU
6	AF	62	GLN
6	AF	188	MET
7	AG	136	ILE
9	AI	3	VAL

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	
3	AC	181/181 (100%)	176 (97%)	5 (3%)	51	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	217/217 (100%)	205 (94%)	12 (6%)	27	63
5	AE	164/164 (100%)	152 (93%)	12 (7%)	17	54
6	AF	165/165 (100%)	160 (97%)	5 (3%)	48	77
7	AG	149/149 (100%)	140 (94%)	9 (6%)	24	60
8	AH	137/137 (100%)	123 (90%)	14 (10%)	9	37
9	AI	114/114 (100%)	109 (96%)	5 (4%)	35	69
10	AJ	122/122 (100%)	115 (94%)	7 (6%)	25	62
11	AK	109/109 (100%)	104 (95%)	5 (5%)	33	68
12	AL	116/116 (100%)	107 (92%)	9 (8%)	16	51
13	AM	104/104 (100%)	98 (94%)	6 (6%)	25	61
14	AN	103/103 (100%)	102 (99%)	1 (1%)	82	92
15	AO	109/109 (100%)	101 (93%)	8 (7%)	17	54
16	AP	103/103 (100%)	99 (96%)	4 (4%)	39	72
17	AQ	87/87 (100%)	79 (91%)	8 (9%)	11	43
18	AR	99/99 (100%)	94 (95%)	5 (5%)	29	66
19	AS	89/89 (100%)	86 (97%)	3 (3%)	44	75
20	AT	84/84 (100%)	78 (93%)	6 (7%)	18	55
21	AU	93/93 (100%)	88 (95%)	5 (5%)	27	64
22	AV	84/84 (100%)	78 (93%)	6 (7%)	18	55
23	AW	84/84 (100%)	80 (95%)	4 (5%)	31	67
24	AX	78/78 (100%)	73 (94%)	5 (6%)	22	58
25	AY	62/62 (100%)	57 (92%)	5 (8%)	15	50
26	AZ	67/67 (100%)	60 (90%)	7 (10%)	9	36
27	A0	55/55 (100%)	52 (94%)	3 (6%)	27	63
28	A1	48/48 (100%)	42 (88%)	6 (12%)	6	30
29	A2	62/62 (100%)	61 (98%)	1 (2%)	70	88
30	A3	47/47 (100%)	45 (96%)	2 (4%)	35	70
31	A4	48/48 (100%)	44 (92%)	4 (8%)	14	49
32	A5	38/38 (100%)	35 (92%)	3 (8%)	15	51
33	A6	51/51 (100%)	50 (98%)	1 (2%)	63	85
34	A7	34/34 (100%)	33 (97%)	1 (3%)	50	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BD	198/198 (100%)	188 (95%)	10 (5%)	29	66
39	BE	189/189 (100%)	174 (92%)	15 (8%)	15	51
40	BF	172/172 (100%)	168 (98%)	4 (2%)	58	83
41	BG	125/125 (100%)	118 (94%)	7 (6%)	26	62
42	BH	116/116 (100%)	107 (92%)	9 (8%)	16	51
43	BI	146/146 (100%)	139 (95%)	7 (5%)	31	67
44	BJ	104/104 (100%)	99 (95%)	5 (5%)	31	67
45	BK	106/106 (100%)	100 (94%)	6 (6%)	25	62
46	BL	90/90 (100%)	83 (92%)	7 (8%)	16	51
47	BM	98/98 (100%)	96 (98%)	2 (2%)	63	85
48	BN	103/103 (100%)	99 (96%)	4 (4%)	39	72
49	BO	95/95 (100%)	89 (94%)	6 (6%)	22	59
50	BP	83/83 (100%)	79 (95%)	4 (5%)	31	67
51	BQ	76/76 (100%)	75 (99%)	1 (1%)	76	89
52	BR	65/65 (100%)	57 (88%)	8 (12%)	6	30
53	BS	77/77 (100%)	72 (94%)	5 (6%)	21	58
54	BT	64/64 (100%)	61 (95%)	3 (5%)	32	68
55	BU	78/78 (100%)	69 (88%)	9 (12%)	7	32
56	BV	65/65 (100%)	65 (100%)	0	100	100
57	BW	60/60 (100%)	55 (92%)	5 (8%)	14	49
All	All	5213/5213 (100%)	4919 (94%)	294 (6%)	31	62

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	AV	50	LEU
28	A1	56	VAL
52	BR	47	GLU
23	AW	46	LYS
26	AZ	7	THR

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	119/120 (99%)	18 (15%)	13 (10%)
2	AB	2898/2904 (99%)	527 (18%)	180 (6%)
35	BA	1538/1542 (99%)	294 (19%)	112 (7%)
36	BB	46/47 (97%)	15 (32%)	6 (13%)
37	BC	76/77 (98%)	14 (18%)	1 (1%)
All	All	4677/4690 (99%)	868 (18%)	312 (6%)

5 of 868 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	13	G
1	AA	14	U
1	AA	25	U
1	AA	26	C

5 of 312 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AB	2068	U
2	AB	2610	C
35	BA	1313	U
2	AB	2118	U
2	AB	2353	G

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

40 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	$\# Z > 2$
2	6MZ	AB	1618	2	17,25,26	1.66	6 (35%)	15,36,39	2.20	4 (26%)
2	2MG	AB	1835	2	18,26,27	1.81	4 (22%)	21,38,41	3.41	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	AB	1911	2	15,21,22	3.39	6 (40%)	16,30,33	2.67	4 (25%)
2	3TD	AB	1915	2	15,22,23	1.95	2 (13%)	17,32,35	2.36	5 (29%)
2	PSU	AB	1917	2	15,21,22	1.77	3 (20%)	16,30,33	3.70	5 (31%)
2	5MU	AB	1939	2	13,22,23	1.75	3 (23%)	16,32,35	3.64	7 (43%)
2	5MC	AB	1962	2	14,22,23	1.32	2 (14%)	17,32,35	1.38	3 (17%)
2	6MZ	AB	2030	2	17,25,26	1.76	3 (17%)	15,36,39	1.57	3 (20%)
2	7MG	AB	2069	2	20,26,27	2.46	5 (25%)	23,39,42	2.40	8 (34%)
2	OMG	AB	2251	2	18,26,27	1.70	5 (27%)	21,38,41	3.77	7 (33%)
2	2MG	AB	2445	2	18,26,27	2.05	4 (22%)	21,38,41	3.56	6 (28%)
2	H2U	AB	2449	2	17,21,22	1.25	2 (11%)	23,30,33	2.61	9 (39%)
2	PSU	AB	2457	2	15,21,22	1.70	2 (13%)	16,30,33	3.11	5 (31%)
2	OMC	AB	2498	2	15,22,23	1.61	5 (33%)	20,31,34	1.97	4 (20%)
2	2MA	AB	2503	2	17,25,26	1.30	3 (17%)	18,37,40	2.12	7 (38%)
2	PSU	AB	2504	2	15,21,22	1.90	3 (20%)	16,30,33	3.68	5 (31%)
2	OMU	AB	2552	2	14,22,23	1.82	2 (14%)	19,31,34	2.43	4 (21%)
2	CH	AB	2575	2	14,21,22	1.86	4 (28%)	18,30,33	1.60	5 (27%)
2	PSU	AB	2580	2	15,21,22	1.58	4 (26%)	16,30,33	3.86	8 (50%)
2	PSU	AB	2605	2	15,21,22	1.56	6 (40%)	16,30,33	3.93	8 (50%)
2	1MG	AB	745	2	17,26,27	1.88	8 (47%)	19,39,42	2.31	7 (36%)
2	PSU	AB	746	2	15,21,22	2.23	7 (46%)	16,30,33	3.28	7 (43%)
2	5MU	AB	747	2	13,22,23	1.70	3 (23%)	16,32,35	2.90	7 (43%)
2	PSU	AB	955	2	15,21,22	2.93	4 (26%)	16,30,33	3.96	3 (18%)
35	2MG	BA	1207	35	18,26,27	1.70	4 (22%)	21,38,41	3.22	11 (52%)
35	4OC	BA	1402	35	15,23,24	1.44	4 (26%)	21,32,35	4.16	8 (38%)
35	5MC	BA	1407	35	14,22,23	1.48	3 (21%)	17,32,35	1.38	4 (23%)
35	UR3	BA	1498	35	13,22,23	2.10	4 (30%)	18,32,35	2.18	4 (22%)
35	2MG	BA	1516	35	18,26,27	1.71	5 (27%)	21,38,41	2.63	8 (38%)
35	MA6	BA	1518	35	18,26,27	1.46	2 (11%)	15,38,41	1.35	1 (6%)
35	MA6	BA	1519	35	18,26,27	1.40	4 (22%)	15,38,41	2.21	4 (26%)
35	PSU	BA	516	35	15,21,22	1.43	3 (20%)	16,30,33	3.77	6 (37%)
35	7MG	BA	527	35	20,26,27	2.39	10 (50%)	23,39,42	2.02	4 (17%)
35	2MG	BA	966	35	18,26,27	1.84	4 (22%)	21,38,41	2.11	5 (23%)
35	5MC	BA	967	35	14,22,23	1.47	2 (14%)	17,32,35	1.21	2 (11%)
37	H2U	BC	21	37	17,21,22	1.67	6 (35%)	23,30,33	2.11	9 (39%)
37	OMC	BC	33	37	15,22,23	1.41	3 (20%)	20,31,34	2.26	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	5MU	BC	55	37	13,22,23	1.52	4 (30%)	16,32,35	4.96	4 (25%)
37	PSU	BC	56	37	15,21,22	3.60	5 (33%)	16,30,33	4.11	4 (25%)
37	4SU	BC	8	37	12,21,22	1.34	2 (16%)	15,30,33	2.99	4 (26%)

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
2	6MZ	AB	1618	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	1835	2	-	0/5/27/28	0/3/3/3
2	PSU	AB	1911	2	-	0/7/25/26	0/2/2/2
2	3TD	AB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	1917	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	1939	2	-	0/3/25/26	0/2/2/2
2	5MC	AB	1962	2	-	0/3/25/26	0/2/2/2
2	6MZ	AB	2030	2	-	0/5/27/28	0/3/3/3
2	7MG	AB	2069	2	-	0/7/37/38	0/3/3/3
2	OMG	AB	2251	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	2445	2	-	0/5/27/28	0/3/3/3
2	H2U	AB	2449	2	-	0/7/38/39	0/2/2/2
2	PSU	AB	2457	2	-	0/7/25/26	0/2/2/2
2	OMC	AB	2498	2	-	0/5/27/28	0/2/2/2
2	2MA	AB	2503	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2504	2	-	0/7/25/26	0/2/2/2
2	OMU	AB	2552	2	-	0/5/27/28	0/2/2/2
2	CH	AB	2575	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	2580	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	2605	2	-	0/7/25/26	0/2/2/2
2	1MG	AB	745	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	746	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	747	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	955	2	-	0/7/25/26	0/2/2/2
35	2MG	BA	1207	35	-	0/5/27/28	0/3/3/3
35	4OC	BA	1402	35	-	0/7/29/30	0/2/2/2
35	5MC	BA	1407	35	-	0/3/25/26	0/2/2/2
35	UR3	BA	1498	35	-	0/3/25/26	0/2/2/2
35	2MG	BA	1516	35	-	0/5/27/28	0/3/3/3
35	MA6	BA	1518	35	-	0/7/29/30	0/3/3/3
35	MA6	BA	1519	35	-	0/7/29/30	0/3/3/3
35	PSU	BA	516	35	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	7MG	BA	527	35	-	0/7/37/38	0/3/3/3
35	2MG	BA	966	35	-	0/5/27/28	0/3/3/3
35	5MC	BA	967	35	-	0/3/25/26	0/2/2/2
37	H2U	BC	21	37	-	0/7/38/39	0/2/2/2
37	OMC	BC	33	37	-	0/5/27/28	0/2/2/2
37	5MU	BC	55	37	-	0/3/25/26	0/2/2/2
37	PSU	BC	56	37	-	0/7/25/26	0/2/2/2
37	4SU	BC	8	37	-	0/3/25/26	0/2/2/2

The worst 5 of 161 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	2069	7MG	C8-N9	-7.60	1.34	1.45
2	AB	1911	PSU	C2'-C1'	-7.49	1.46	1.53
2	AB	955	PSU	C2'-C1'	-7.36	1.46	1.53
2	AB	955	PSU	C5-C1'	-6.63	1.46	1.52
2	AB	1915	3TD	C5-C1'	-5.76	1.47	1.52

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	1402	4OC	C6-C5-C4	-15.65	111.26	117.42
37	BC	55	5MU	C5-C4-N3	-11.94	115.33	125.35
2	AB	2445	2MG	C5-C6-N1	-11.45	108.55	123.52
2	AB	1835	2MG	C5-C6-N1	-10.71	109.52	123.52
37	BC	8	4SU	C5-C4-N3	-9.45	113.54	123.56

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](#)

There are no chain breaks in this entry.