



wwPDB EM Map/Model Validation Report ⓘ

Aug 10, 2016 – 08:33 PM EDT

PDB ID : 5KCS
EMDB ID: : EMD-8238
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Evernimycin, mRNA, TetM and P-site tRNA at 3.9Å resolution
Authors : Arenz, S.; Juetten, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.
Deposited on : 2016-06-06
Resolution : 3.90 Å(reported)

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) : rb-20027939

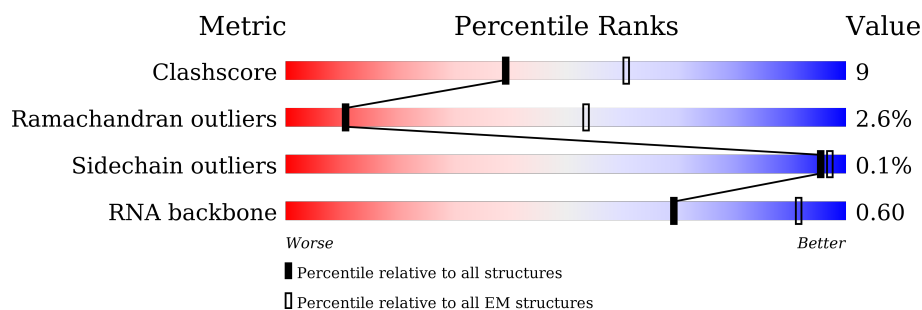
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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




























Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
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	1A	2904	54% 40% 7%
2	1B	120	63% 31% 6%
3	1D	273	64% 34% .
4	1E	209	72% 28%
5	1F	201	73% 27%
6	1G	179	71% 27% ..
7	1H	177	85% 15% .
8	1L	121	57% 43%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	1I	149	
10	1J	165	
11	1K	142	
12	1N	142	
13	1O	123	
14	1P	144	
15	1Q	136	
16	1R	127	
17	1S	117	
18	1T	115	
19	1U	118	
20	1V	103	
21	1W	110	
22	1X	100	
23	1Y	104	
24	1Z	94	
25	10	85	
26	11	78	
27	12	63	
28	13	59	
29	14	70	
30	15	57	
31	16	55	
32	17	46	
33	18	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	19	38	
35	1a	1539	
36	1b	241	
37	1c	233	
38	1d	206	
39	1e	167	
40	1f	135	
41	1g	179	
42	1h	130	
43	1i	130	
44	1j	103	
45	1k	129	
46	1l	124	
47	1m	118	
48	1n	101	
49	1o	89	
50	1p	82	
51	1q	84	
52	1r	75	
53	1s	92	
54	1t	87	
55	1u	71	
56	1v	60	
57	1w	639	
58	1x	77	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 148945 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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	2900	Total	C	N	O	P	0	0
			62276	27788	11459	20129	2900		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1D	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1E	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1F	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1L	69	Total	C	N	O	0	0
			276	138	69	69		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	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	1J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	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	1N	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	1O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1Q	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	1R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1S	116	Total	C	N	O	0	0
			892	552	178	162		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1T	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	1U	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	1V	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	1W	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	1X	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1Y	102	Total	C	N	O	S	0	0
			779	492	146	141			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Z	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	10	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	11	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	12	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	13	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	14	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	15	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	16	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	17	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	18	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	19	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	1a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	1v	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

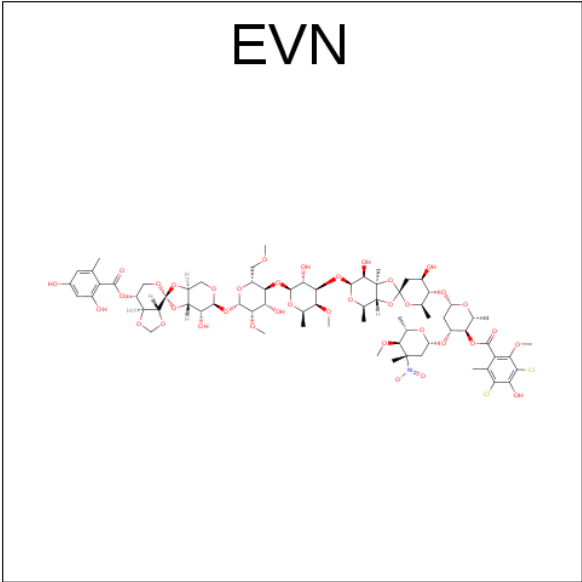
- Molecule 57 is a protein called Tetracycline resistance protein TetM from transposon Tn916.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	1w	639	Total	C	N	O	0	0
			2590	1308	640	642		

- Molecule 58 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	1x	73	Total	C	N	O	P	0	0
			1567	699	285	510	73		

- Molecule 59 is (2R,3R,4R,6S)-6-{{(2R,3aR,4R,4'R,5'S,6S,6'R,7S,7aR)-6-{{(2S,3R,4R,5S,6R)-2-{{[(2R,3S,4S,5S,6S)-6-{{(2R,3aS,3a'R,6S,7R,7'R,7aS,7a'S)-7'-[(2,4-dihydroxy-6-methylbenzoyl)oxy]-7-hydroxyoctahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}oxy)-4-hydroxy-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl}oxy}-3-hydroxy-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl}oxy}-4',7-dihydroxy-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl}oxy}-4-{{(2R,4S,5R,6S)-5-methoxy-4,6-dimethyl-4-nitrotetrahydro-2H-pyran-2-yl}oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (three-letter code: EVN) (formula: C₇₀H₉₇Cl₂NO₃₈).

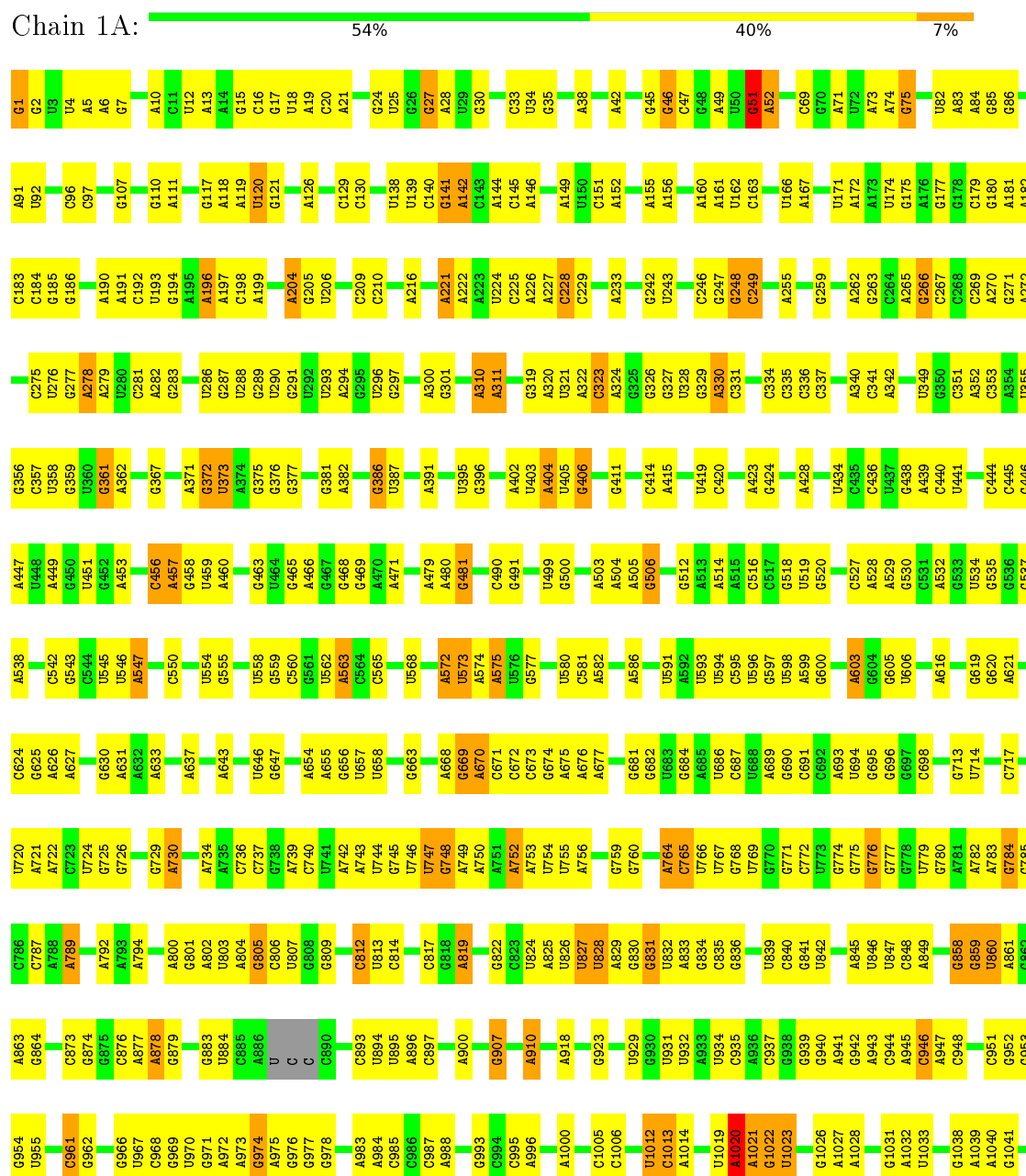


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
59	1A	1	111	70	2	1	38	0

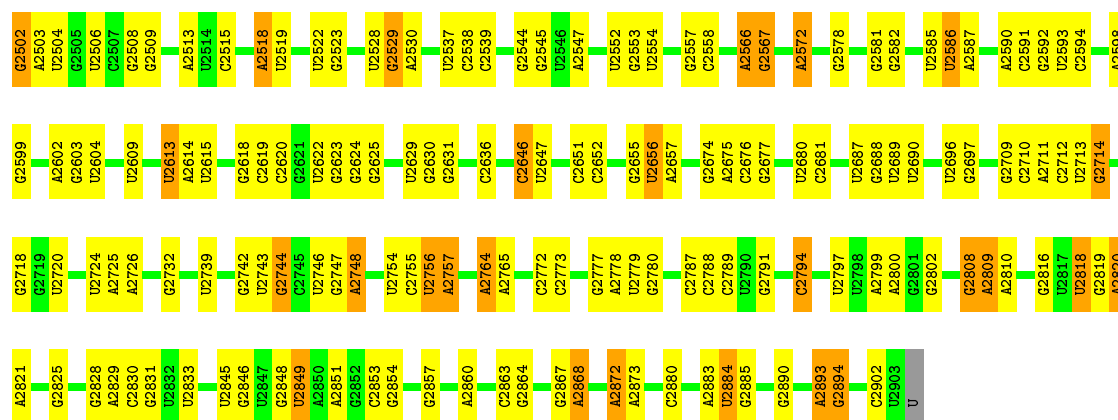
3 Residue-property plots

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: 23S Ribosomal RNA

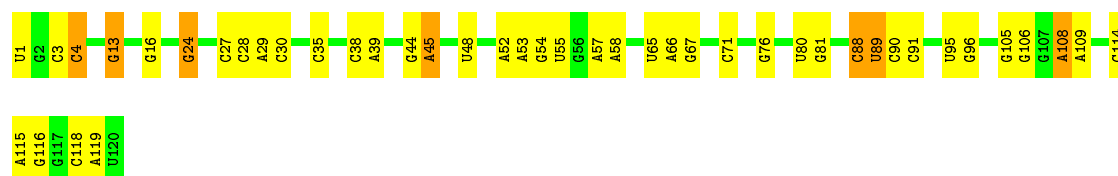


G2421	A2346	U2259	C2146	A2062	G1972	G1897	A1808	G1516	C1417	U1326	A1247	G1131	A1046
C2422	C2347	C2260	A2147	C2063	G1972	U1896	A1809	G1517	G1418	A1327	G1248	U1132	G1047
C2423	U2348	C2261	G2162	U2068	A1981	A1899	A1810	G1517	A1419	A1328	U1249	A1133	A1048
C2424	C2349	C2262	C2163	G2069	U1991	A1900	G1813	G1524	A1420	U1329	U1250	A1134	
A2425	C2350	A2267	C2164	A2070	U1992	A1901	G1814	A1528	G1421	G1330	G1251	C1135	C1053
C2427	G2353	A2268	A2170	C2072	U1993	C1906	A1815	A1529	G1422	G1331	G1252	A1054	A1054
G2428	C2354	G2269	A2171	C2073	U1994	G1906	G1816	G1530	G1423	G1332	A1253	G1055	G1055
G2429	C2355	A2270	U2172	U2074	C1996	C1909	G1817	C1533	C1428	A1336	G1256	U1141	G1056
A2430	U2356	G2271	U2173	A1998	C1997	G1910	G1818	U1534	A1429	G1337	C1261	A1142	U1058
U2431	G2357	G2272	A2173	U2075	A1998	G1910	A1819	A1535	A1430	U1340	C1261	A1143	G1059
A2432	A2358	G2273	U2189	A2080	G2002	A1913	U1820	G1536	A1431	G1341	A1264	A1147	U1060
A2433	C2359	G2274	G2190	U2081	A2003	C1914	A1821	G1537	G1432	A1342	A1265		U1061
A2434	G2360	A2278	A2191	A2082	G2004	U1915	A1822	U1538	A1433	G1343	A1266	G1154	G1062
A2435	G2361	G2279	U2192	G2083	A2005	A1916	G1823	G1538	A1434	U1344	U1267	A1155	C1063
G2436	C2362	A2281	G2193	A2095	A2006	U1917	G1824	U1539	G1435	G1345	A1268	U1158	U1065
G2437	G2364	G2282	U2194	U2086	C2008	A1918	G1825	C1541	U1442	G1346	A1269	U1166	U1066
	G2365	U2087	U2195	G2087	A2009	A1919	U1827	U1542	U1443	A1347	C1270	A1165	A1067
C2440	A2369	A2088		A2088	G2010		G1828	G1543			G1271	G1166	G1068
U2441	C2285	C2285	A2198	G2093	U2011	C1924	A1829	A1549	G1448	C1351	A1272	C1167	A1069
C2442	G2286	C2286	A2199	C2012	G2012	C1925	U1830	A1549	G1449	U1352	U1273	U1174	U1070
C2443	A2287	A2287	C2200	A2094	A2013	U1926	G1831	U1647	G1450	A1353	A1274	A1175	G1071
G2445	G2374	A2095	G2201	A2095	A2013	A1927	U1834	U1648	C1451	G1354		U1176	C1072
G2446	C2375	U2291	U2202	C2096	A2020	G1928	G1835	G1651	G1452	G1355	C1278	G1177	C1075
G2447	A2376	U2292	U2203	A2097	C2021	G1929	U1836	C1557	G1453	G1356	G1279		C1076
A2448	A2377	U2098	G2204	U2098	U2022	G1930	A1837	C1558	C1454				
	A2378				C2023	U1931	G1838	C1559	A1454				
A2453	A2297	A2298	A2211	A2101	G2027	G1935	U1843	C1560	C1461	G1361	G1283		C1079
G2454	A2298	A2298	A2212	G2102	U2028	A1936	G1844	U1562		G1362	A1286	U1180	A1080
	U2305	U2305	U2213	C2103	G2029	U1937	G1845	U1563		G1363	A1287	U1182	A1084
A2461	A2309	A2309	C2215	C2104	U2030	A1938		C1564	A1469	A1365	G1288	U1183	
C2462	C2313	C2313	G2221	G2110	A2031	U1938	G1849	C1565	A1470	A1366	G1289	U1184	
C2463	G2314	A2314	C2222	G2111	G2032	A1939	G1850	C1566	G1475	A1367	C1290	A1088	A1089
C2465	G2315	G2315	G2223	U2112	A2033	U1940	G1851	G1567		G1368	C1291	U1187	A1089
C2466	A2391	G2315	G2223	U2113	U2034	C1941	G1852	U1568	U1481	A1378	G1292	U1188	G1092
	A2392		G2224	U2113	G2035			A1569	G1482	U1379	G1296	A1189	G1093
G2470	U2393	G2319	G2225	G2116	C2036	U1944	G1863	A1570				G1190	U1094
A2471	C2394	U2320	A2226	A2117	G1945	G1945	U1864	A1571	U1485	G1382	G1300	G1191	A1095
G2472			C2226	U2118	U2039	G1949	U1865	A1572	U1486	A1383	A1301	U1199	A1096
G2475	G2399	G2325	U2233	A2119	G2040	G1949	U1866	G1573				A1205	U1097
A2476	C2326	C2326	G2234	G2120	U2041	G1954	G1869	A1579	A1490	U1394	A1307	A1206	A1098
U2477	A2327	A2327	G2235	G2121	A2042	U1955	C1870	A1580	A1491	U1397	A1308	G1210	G1099
U2478	U2402	A2328	U2236	G2127	C2043	U1956	A1871	G1581	G1492	C1398	G1310	G1211	C1100
	U2404	G2330	G2237	G2127	G2048	C1957	G1872	C1585	A1493	U1400		G1212	A1103
G2484	C2403	G2331	G2238	G2127	C2048	C1958	G1873	A1586	G1501	G1401	C1313	A1213	U1105
G2485	U2404	U2131	A2241	G2133	A2051	G1959	G1874	G1587				A1214	
A2407	A2408	U2132	G2242	G2133	A2052	A1960	G1875	G1588	A1504	U1405	U1316	G1218	G1110
G2408	G2409	U2137	U2245	G2138	C2053	C1962	G1878	G1589	A1505	U1406	G1317	G1218	A1111
G2487	G2488	G2138	G2246	U1963	A2054	U1963	G1879	U1589	U1506	G1407	U1318	G1112	G1112
U2489	A2411	U2139	G2246	G1964	C2055	G1964	U1882	A1591	C1507	G1408	C1319	G1225	
		G2140	G2250	G1964	G2056	U1798	U1883	G1592	A1508	U1409	C1320	U1119	
G2496	G2415	G2141	G2251	G2057	A2058	C1967	G1884	U1593	A1509	G1410	A1321	G1236	G1125
A2497	C2416	A2142	G2252	A2059	A2058	G1968		U1594	G1510	U1411	A1322	A1237	
C2498	C2417	C2143	G2253	A2059	A2059	A1969	A1890	C1595	G1514	U1415	G1323	G1238	
C2499	A2418	G2144	U2257	A2060	A2060	A1970	G1891	C1694	G1514	A1515	G1324	G1239	
U2500	U2344	G2345	U2258	C2145	G2061	U1971	G1896	A1597					U1130



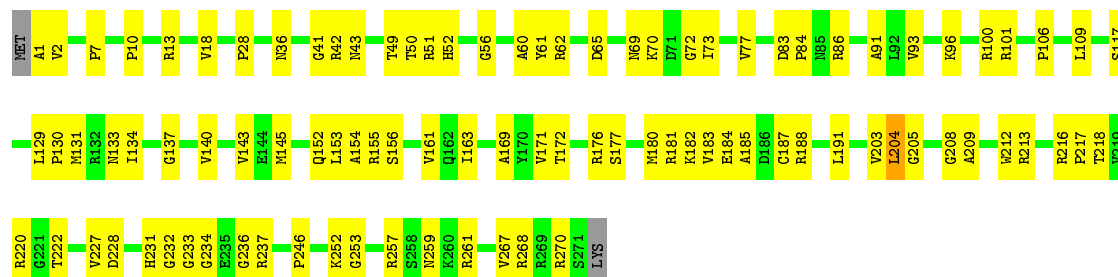
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 63% 31% 6%



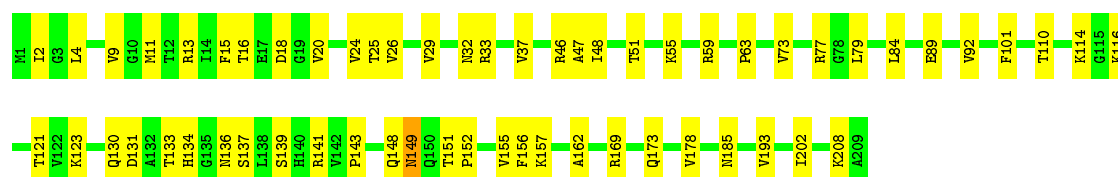
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 64% 34% 2%



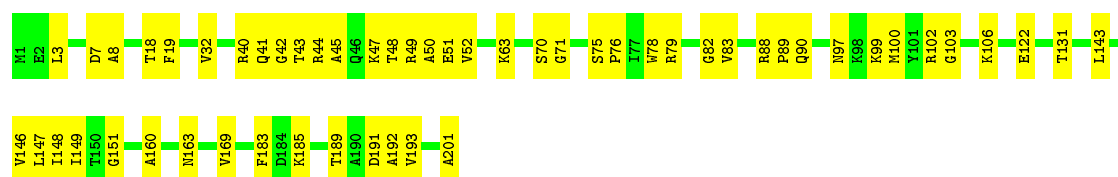
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 72% 28% 0%

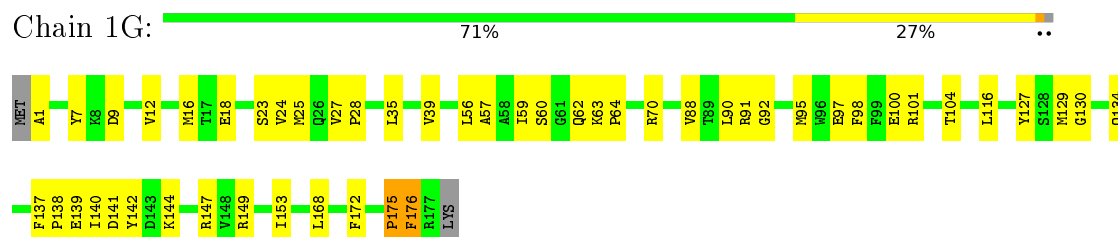


• Molecule 5: 50S ribosomal protein L4

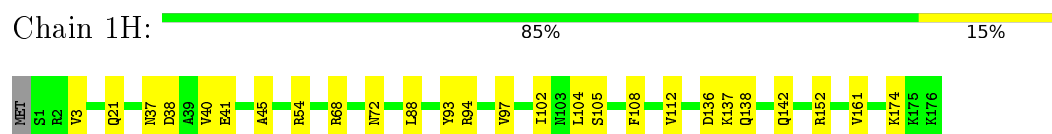
Chain 1F: 73% 27% 0%



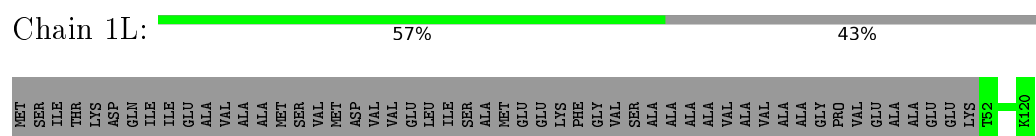
- Molecule 6: 50S ribosomal protein L5



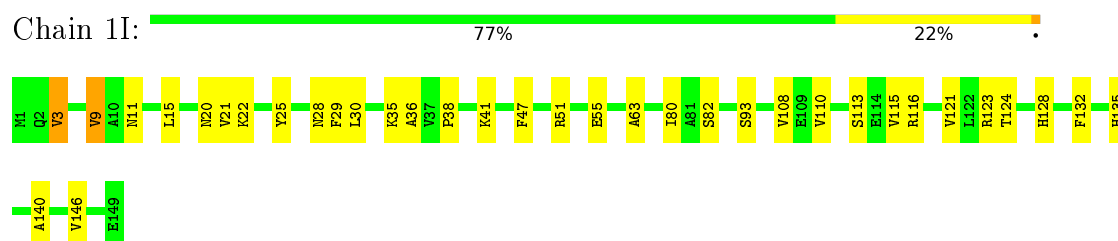
- Molecule 7: 50S ribosomal protein L6



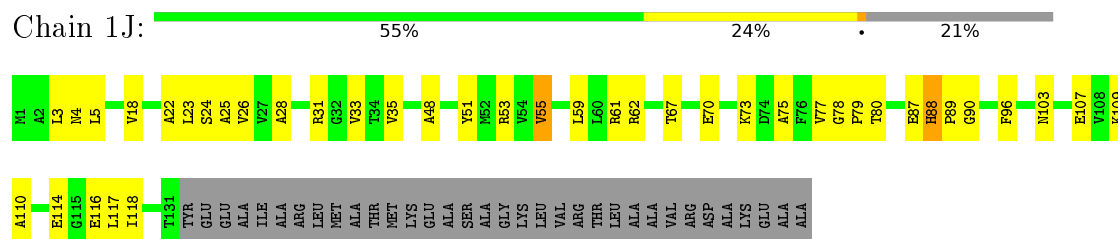
- Molecule 8: 50S ribosomal protein L7/L12



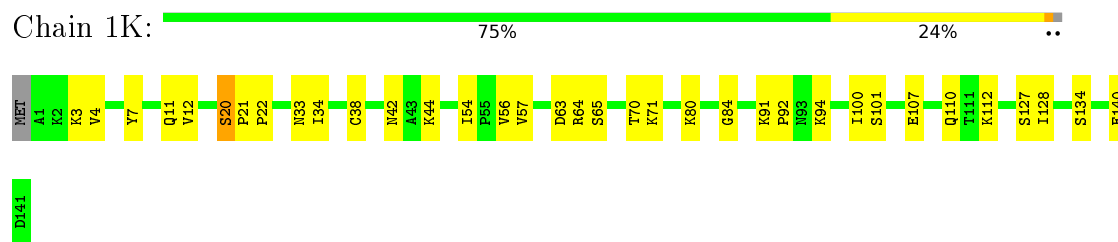
- Molecule 9: 50S ribosomal protein L9



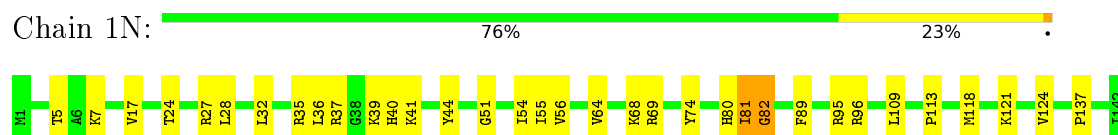
- Molecule 10: 50S ribosomal protein L10



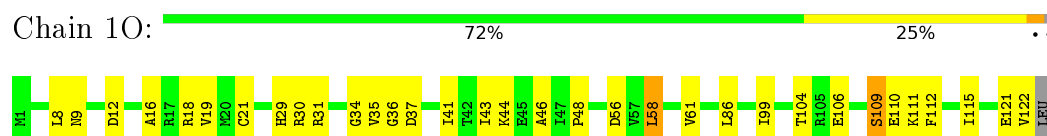
- Molecule 11: 50S ribosomal protein L11



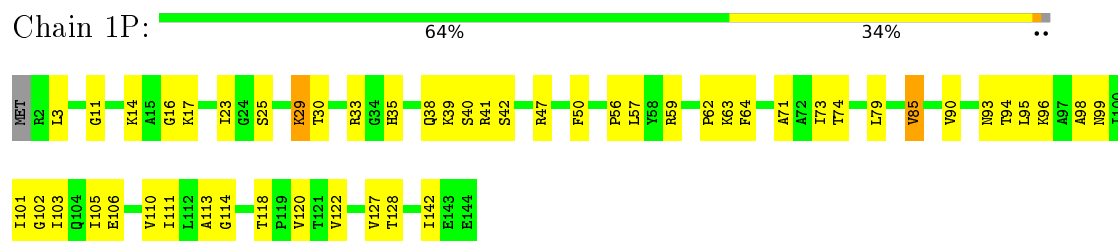
- Molecule 12: 50S ribosomal protein L13



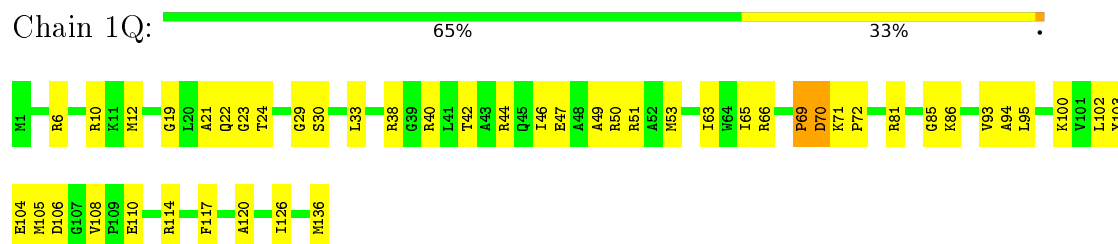
- Molecule 13: 50S ribosomal protein L14



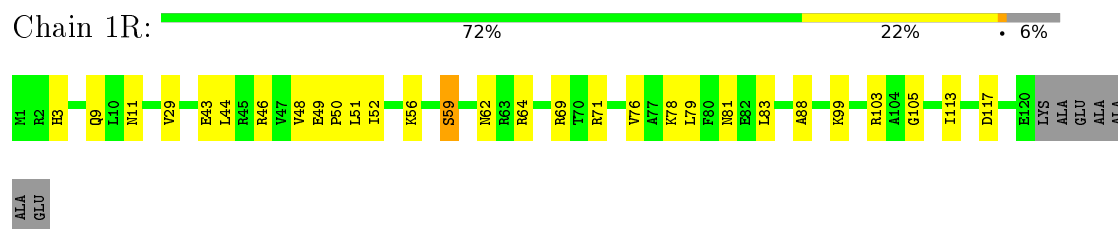
- Molecule 14: 50S ribosomal protein L15



- Molecule 15: 50S ribosomal protein L16



- Molecule 16: 50S ribosomal protein L17



- Molecule 17: 50S ribosomal protein L18

Chain 1S:  86% 13%




- Molecule 18: 50S ribosomal protein L19

Chain 1T:  86% 13%




- Molecule 19: 50S ribosomal protein L20

Chain 1U:  79% 20%




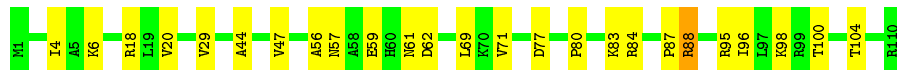
- Molecule 20: 50S ribosomal protein L21

Chain 1V:  76% 24%




- Molecule 21: 50S ribosomal protein L22

Chain 1W:  77% 22%



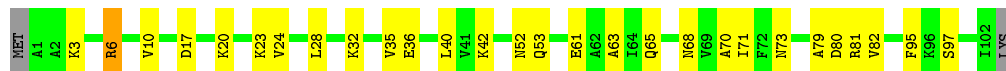
- Molecule 22: 50S ribosomal protein L23

Chain 1X:  73% 19% 7%



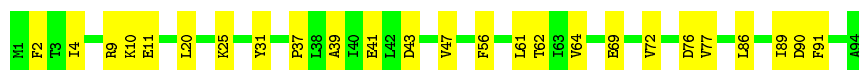
- Molecule 23: 50S ribosomal protein L24

Chain 1Y:  71% 26%



- Molecule 24: 50S ribosomal protein L25

Chain 1Z:  73% 27%




- Molecule 25: 50S ribosomal protein L27

Chain 10:  62% 26% 12%




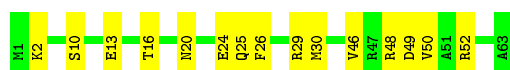
- Molecule 26: 50S ribosomal protein L28

Chain 11:  77% 22% .



- Molecule 27: 50S ribosomal protein L29

Chain 12:  76% 24%




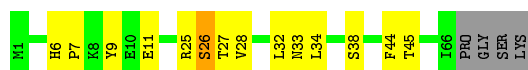
- Molecule 28: 50S ribosomal protein L30

Chain 13:  73% 25% .



- Molecule 29: 50S ribosomal protein L31

Chain 14:  74% 19% . 6%



- Molecule 30: 50S ribosomal protein L32

Chain 15:  70% 26% . .



- Molecule 31: 50S ribosomal protein L33

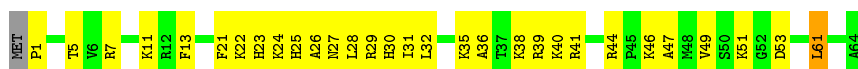
Chain 16:  69% 22% 9%



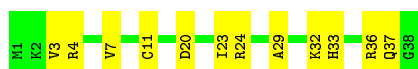
- Molecule 32: 50S ribosomal protein L34



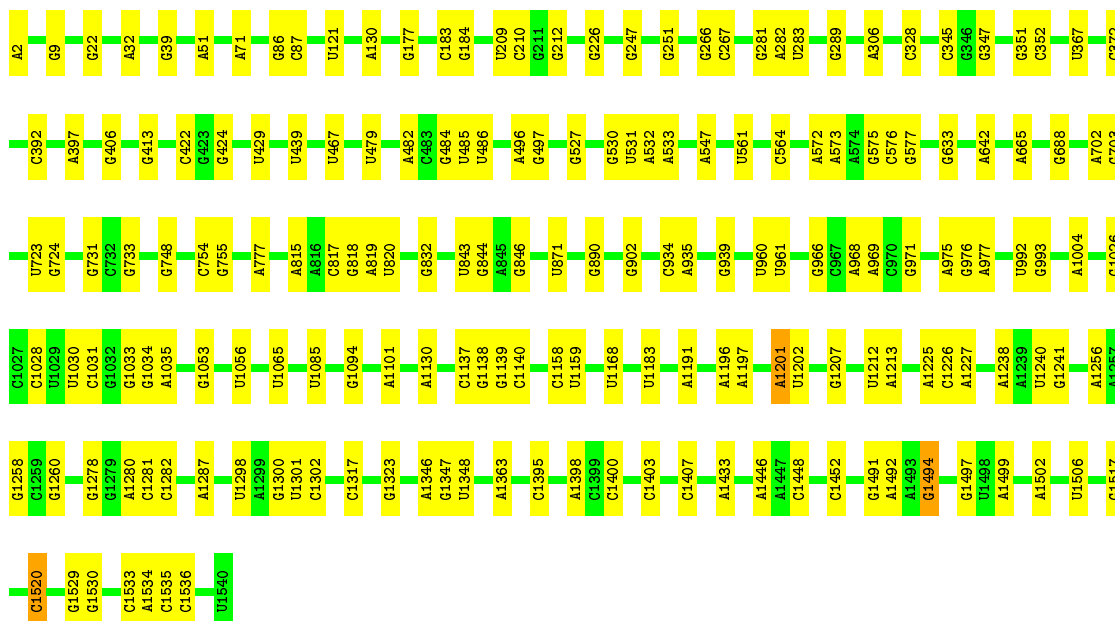
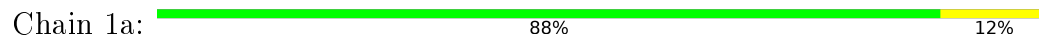
- Molecule 33: 50S ribosomal protein L35



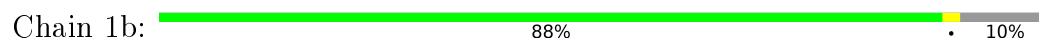
- Molecule 34: 50S ribosomal protein L36



- Molecule 35: 16S Ribosomal RNA



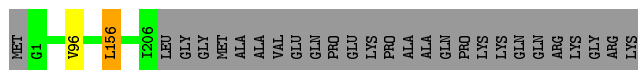
- Molecule 36: 30S ribosomal protein S2





- Molecule 37: 30S ribosomal protein S3

Chain 1c: 88% 12%



- Molecule 38: 30S ribosomal protein S4

Chain 1d: 98%



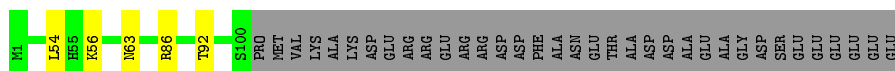
- Molecule 39: 30S ribosomal protein S5

Chain 1e: 89% 5% 6%



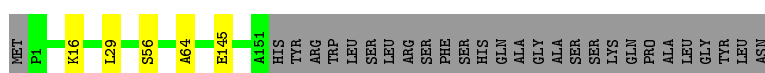
- Molecule 40: 30S ribosomal protein S6

Chain 1f: 70% 26%



- Molecule 41: 30S ribosomal protein S7

Chain 1g: 82% 16%



- Molecule 42: 30S ribosomal protein S8

Chain 1h: 98%




- Molecule 43: 30S ribosomal protein S9

Chain 1i: 93% 5%




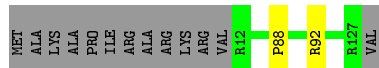
- Molecule 44: 30S ribosomal protein S10

Chain 1j:  89% 6% 5%



- Molecule 45: 30S ribosomal protein S11

Chain 1k:  88% 10%



- Molecule 46: 30S ribosomal protein S12

Chain 1l:  94% 6%



- Molecule 47: 30S ribosomal protein S13

Chain 1m:  94%



- Molecule 48: 30S ribosomal protein S14

Chain 1n:  92% 7%



- Molecule 49: 30S ribosomal protein S15

Chain 1o:  94%



- Molecule 50: 30S ribosomal protein S16

Chain 1p:  99%




- Molecule 51: 30S ribosomal protein S17

Chain 1q:  92% • 5%




- Molecule 52: 30S ribosomal protein S18

Chain 1r:  83% • 13%



- Molecule 53: 30S ribosomal protein S19

Chain 1s:  85% • 14%




- Molecule 54: 30S ribosomal protein S20

Chain 1t:  98% •



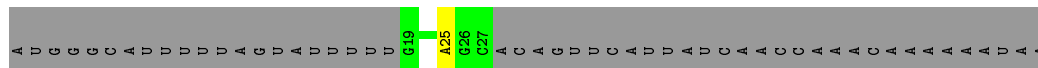
- Molecule 55: 30S ribosomal protein S21

Chain 1u:  82% 8% • 8%



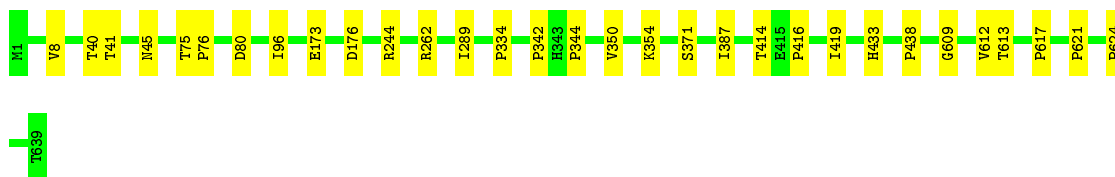
- Molecule 56: mRNA

Chain 1v:  13% • 85%



- Molecule 57: Tetracycline resistance protein TetM from transposon Tn916

Chain 1w:  95% 5%



- Molecule 58: P-site tRNA

87% 8% 5%



4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	78186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, OMG, OMU, EVN, MA6, G7M, H2U, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 3TD, 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	1A	0.19	1/69174 (0.0%)	0.69	11/107910 (0.0%)
10	1J	0.29	0/1001	0.47	0/1350
11	1K	0.27	0/1046	0.44	0/1410
12	1N	0.25	0/1152	0.42	0/1551
13	1O	0.26	0/947	0.45	0/1268
14	1P	0.27	0/1054	0.45	0/1403
15	1Q	0.30	0/1093	0.49	0/1460
16	1R	0.25	0/973	0.41	0/1301
17	1S	0.26	0/902	0.39	0/1209
18	1T	0.26	0/929	0.46	0/1242
19	1U	0.25	0/960	0.35	0/1278
2	1B	0.26	1/2873 (0.0%)	0.68	0/4478
20	1V	0.27	0/829	0.45	0/1107
21	1W	0.26	0/864	0.44	0/1156
22	1X	0.26	0/744	0.42	0/994
23	1Y	0.27	0/787	0.45	0/1051
24	1Z	0.28	0/766	0.42	0/1025
25	10	0.27	0/582	0.42	0/769
26	11	0.25	0/635	0.41	0/848
27	12	0.24	0/510	0.40	0/677
28	13	0.24	0/453	0.45	0/605
29	14	0.28	0/531	0.43	0/709
3	1D	0.28	0/2121	0.47	0/2852
30	15	0.24	0/450	0.43	0/599
31	16	0.26	0/416	0.43	0/554
32	17	0.25	0/380	0.43	0/498
33	18	0.26	0/513	0.44	0/676
34	19	0.25	0/303	0.40	0/397
35	1a	0.19	1/36701 (0.0%)	0.70	13/57246 (0.0%)
36	1b	0.26	0/1735	0.41	0/2338
37	1c	0.26	0/1651	0.44	0/2225

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	1d	0.26	0/1665	0.42	0/2227
39	1e	0.26	0/1154	0.44	0/1554
4	1E	0.27	0/1586	0.46	0/2134
40	1f	0.25	0/835	0.43	0/1128
41	1g	0.26	0/1195	0.42	0/1602
42	1h	0.26	0/989	0.46	0/1326
43	1i	0.26	0/1034	0.45	0/1375
44	1j	0.25	0/796	0.47	0/1077
45	1k	0.26	0/885	0.43	0/1195
46	1l	0.26	0/969	0.46	0/1300
47	1m	0.25	0/892	0.43	0/1193
48	1n	0.26	0/806	0.43	0/1074
49	1o	0.24	0/722	0.38	0/964
5	1F	0.25	0/1571	0.41	0/2113
50	1p	0.26	0/659	0.42	0/884
51	1q	0.28	0/657	0.46	0/881
52	1r	0.26	0/511	0.42	0/689
53	1s	0.25	0/652	0.40	0/877
54	1t	0.26	0/671	0.37	0/888
55	1u	0.38	1/500 (0.2%)	0.40	0/668
56	1v	0.53	0/214	1.10	3/331 (0.9%)
57	1w	0.26	0/2594	0.47	0/3251
58	1x	0.36	1/1656 (0.1%)	0.72	0/2575
6	1G	0.27	0/1434	0.42	0/1926
7	1H	0.26	0/1343	0.44	0/1816
8	1L	0.25	0/275	0.43	0/342
9	1I	0.27	0/1122	0.43	0/1515
All	All	0.22	5/160462 (0.0%)	0.63	27/239091 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1x	1	A	OP3-P	-10.60	1.48	1.61
35	1a	2	A	OP3-P	-10.55	1.48	1.61
2	1B	1	U	OP3-P	-10.46	1.48	1.61
1	1A	1	G	OP3-P	-10.44	1.48	1.61
55	1u	9	GLU	C-N	5.99	1.45	1.34

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	754	C	C2-N1-C1'	8.93	128.63	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	754	C	N1-C2-O2	8.83	124.20	118.90
35	1a	1158	C	C2-N1-C1'	8.63	128.30	118.80
35	1a	1158	C	N1-C2-O2	8.58	124.05	118.90
1	1A	2884	U	C2-N1-C1'	7.77	127.02	117.70

There are no chirality outliers.

There are no planarity outliers.

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	1A	62276	0	31344	905	0
2	1B	2570	0	1301	26	0
3	1D	2082	0	2157	78	0
4	1E	1565	0	1616	47	0
5	1F	1552	0	1619	38	0
6	1G	1410	0	1447	37	0
7	1H	1323	0	1374	17	0
8	1L	276	0	79	0	0
9	1I	1111	0	1148	22	0
10	1J	988	0	1025	24	0
11	1K	1032	0	1088	17	0
12	1N	1129	0	1162	26	0
13	1O	938	0	1012	22	0
14	1P	1045	0	1117	40	0
15	1Q	1074	0	1157	33	0
16	1R	960	0	1000	21	0
17	1S	892	0	923	9	0
18	1T	917	0	965	13	0
19	1U	947	0	1022	19	0
20	1V	816	0	839	17	0
21	1W	857	0	922	21	0
22	1X	738	0	807	12	0
23	1Y	779	0	834	19	0
24	1Z	753	0	780	16	0
25	10	575	0	592	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	11	625	0	655	15	0
27	12	509	0	543	10	0
28	13	449	0	491	9	0
29	14	522	0	522	12	0
30	15	444	0	461	12	0
31	16	409	0	440	9	0
32	17	377	0	418	22	0
33	18	504	0	574	25	0
34	19	302	0	343	9	0
35	1a	33029	0	16644	0	0
36	1b	1704	0	1732	0	0
37	1c	1624	0	1699	0	0
38	1d	1643	0	1710	0	0
39	1e	1141	0	1170	0	0
40	1f	817	0	808	0	0
41	1g	1181	0	1240	0	0
42	1h	979	0	1034	0	0
43	1i	1022	0	1070	0	0
44	1j	786	0	828	0	0
45	1k	869	0	878	0	0
46	1l	955	0	1019	0	0
47	1m	883	0	944	0	0
48	1n	794	0	833	0	0
49	1o	714	0	737	0	0
50	1p	649	0	666	0	0
51	1q	648	0	691	0	0
52	1r	504	0	502	0	0
53	1s	637	0	665	0	0
54	1t	665	0	714	0	0
55	1u	495	0	486	0	0
56	1v	192	0	98	0	0
57	1w	2590	0	731	0	0
58	1x	1567	0	798	0	0
59	1A	111	0	0	0	0
All	All	148945	0	99474	1397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1397 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:827:U:H2'	1:1A:2068:U:O2	1.20	1.28
1:1A:827:U:C2'	1:1A:2068:U:O2	1.98	1.12
1:1A:827:U:H2'	1:1A:2068:U:C2	1.97	1.00
1:1A:776:G:H22	1:1A:2072:C:H5'	1.35	0.89
6:1G:140:ILE:HG22	6:1G:142:TYR:H	1.43	0.84

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	1D	269/273 (98%)	242 (90%)	23 (9%)	4 (2%)	13	57
4	1E	207/209 (99%)	187 (90%)	19 (9%)	1 (0%)	34	76
5	1F	199/201 (99%)	185 (93%)	11 (6%)	3 (2%)	13	57
6	1G	175/179 (98%)	153 (87%)	19 (11%)	3 (2%)	11	55
7	1H	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	17	63
8	1L	67/121 (55%)	64 (96%)	3 (4%)	0	100	100
9	1I	147/149 (99%)	130 (88%)	13 (9%)	4 (3%)	6	46
10	1J	129/165 (78%)	101 (78%)	23 (18%)	5 (4%)	4	37
11	1K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	3	31
12	1N	140/142 (99%)	132 (94%)	6 (4%)	2 (1%)	14	58
13	1O	120/123 (98%)	106 (88%)	11 (9%)	3 (2%)	7	48
14	1P	141/144 (98%)	120 (85%)	16 (11%)	5 (4%)	4	41
15	1Q	134/136 (98%)	120 (90%)	9 (7%)	5 (4%)	4	39
16	1R	118/127 (93%)	103 (87%)	13 (11%)	2 (2%)	11	55
17	1S	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	11	54
18	1T	112/115 (97%)	105 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1U	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
20	1V	101/103 (98%)	89 (88%)	8 (8%)	4 (4%)	4	37
21	1W	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
22	1X	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	8	50
23	1Y	100/104 (96%)	86 (86%)	12 (12%)	2 (2%)	9	52
24	1Z	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
25	10	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
26	11	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
27	12	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
28	13	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
29	14	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	12	56
30	15	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	10	53
31	16	48/55 (87%)	42 (88%)	5 (10%)	1 (2%)	9	51
32	17	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
33	18	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
34	19	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	6	46
36	1b	216/241 (90%)	187 (87%)	24 (11%)	5 (2%)	8	50
37	1c	204/233 (88%)	190 (93%)	12 (6%)	2 (1%)	19	64
38	1d	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	9	52
39	1e	155/167 (93%)	136 (88%)	11 (7%)	8 (5%)	2	31
40	1f	98/135 (73%)	87 (89%)	6 (6%)	5 (5%)	2	31
41	1g	149/179 (83%)	129 (87%)	15 (10%)	5 (3%)	5	42
42	1h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	24	68
43	1i	125/130 (96%)	107 (86%)	12 (10%)	6 (5%)	3	32
44	1j	96/103 (93%)	80 (83%)	10 (10%)	6 (6%)	2	26
45	1k	114/129 (88%)	98 (86%)	14 (12%)	2 (2%)	11	54
46	1l	121/124 (98%)	100 (83%)	14 (12%)	7 (6%)	2	28
47	1m	112/118 (95%)	102 (91%)	7 (6%)	3 (3%)	6	46
48	1n	98/101 (97%)	83 (85%)	9 (9%)	6 (6%)	2	27
49	1o	86/89 (97%)	76 (88%)	6 (7%)	4 (5%)	3	33
50	1p	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	15	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1q	78/84 (93%)	65 (83%)	10 (13%)	3 (4%)	4	38
52	1r	63/75 (84%)	57 (90%)	3 (5%)	3 (5%)	3	32
53	1s	77/92 (84%)	70 (91%)	6 (8%)	1 (1%)	15	59
54	1t	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
55	1u	63/71 (89%)	45 (71%)	11 (18%)	7 (11%)	0	10
57	1w	637/639 (100%)	548 (86%)	58 (9%)	31 (5%)	3	32
All	All	6550/6980 (94%)	5803 (89%)	577 (9%)	170 (3%)	11	47

5 of 170 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	18	GLU
7	1H	108	PHE
11	1K	22	PRO
11	1K	92	PRO
12	1N	81	ILE

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	1D	216/218 (99%)	216 (100%)	0	100	100
4	1E	164/164 (100%)	164 (100%)	0	100	100
5	1F	165/165 (100%)	165 (100%)	0	100	100
6	1G	148/150 (99%)	148 (100%)	0	100	100
7	1H	137/138 (99%)	137 (100%)	0	100	100
9	1I	114/114 (100%)	114 (100%)	0	100	100
10	1J	100/123 (81%)	100 (100%)	0	100	100
11	1K	109/110 (99%)	109 (100%)	0	100	100
12	1N	116/116 (100%)	116 (100%)	0	100	100
13	1O	103/104 (99%)	102 (99%)	1 (1%)	82	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1P	102/103 (99%)	102 (100%)	0	100	100
15	1Q	109/109 (100%)	108 (99%)	1 (1%)	84	92
16	1R	100/103 (97%)	100 (100%)	0	100	100
17	1S	86/87 (99%)	86 (100%)	0	100	100
18	1T	99/100 (99%)	99 (100%)	0	100	100
19	1U	89/90 (99%)	89 (100%)	0	100	100
20	1V	84/84 (100%)	84 (100%)	0	100	100
21	1W	93/93 (100%)	92 (99%)	1 (1%)	80	90
22	1X	80/84 (95%)	80 (100%)	0	100	100
23	1Y	83/85 (98%)	83 (100%)	0	100	100
24	1Z	78/78 (100%)	78 (100%)	0	100	100
25	10	57/63 (90%)	57 (100%)	0	100	100
26	11	67/68 (98%)	67 (100%)	0	100	100
27	12	55/55 (100%)	55 (100%)	0	100	100
28	13	48/49 (98%)	48 (100%)	0	100	100
29	14	59/62 (95%)	59 (100%)	0	100	100
30	15	47/48 (98%)	47 (100%)	0	100	100
31	16	45/49 (92%)	45 (100%)	0	100	100
32	17	38/38 (100%)	38 (100%)	0	100	100
33	18	51/52 (98%)	50 (98%)	1 (2%)	63	86
34	19	34/34 (100%)	34 (100%)	0	100	100
36	1b	180/199 (90%)	180 (100%)	0	100	100
37	1c	170/190 (90%)	169 (99%)	1 (1%)	90	95
38	1d	172/173 (99%)	172 (100%)	0	100	100
39	1e	114/126 (90%)	114 (100%)	0	100	100
40	1f	87/116 (75%)	87 (100%)	0	100	100
41	1g	124/147 (84%)	124 (100%)	0	100	100
42	1h	104/105 (99%)	104 (100%)	0	100	100
43	1i	105/107 (98%)	105 (100%)	0	100	100
44	1j	86/90 (96%)	86 (100%)	0	100	100
45	1k	89/99 (90%)	89 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	1l	103/104 (99%)	103 (100%)	0	100	100
47	1m	92/96 (96%)	92 (100%)	0	100	100
48	1n	79/84 (94%)	78 (99%)	1 (1%)	76	89
49	1o	76/77 (99%)	76 (100%)	0	100	100
50	1p	65/65 (100%)	65 (100%)	0	100	100
51	1q	74/78 (95%)	74 (100%)	0	100	100
52	1r	48/65 (74%)	48 (100%)	0	100	100
53	1s	70/79 (89%)	70 (100%)	0	100	100
54	1t	65/66 (98%)	65 (100%)	0	100	100
55	1u	44/61 (72%)	44 (100%)	0	100	100
57	1w	6/576 (1%)	6 (100%)	0	100	100
All	All	4829/5639 (86%)	4823 (100%)	6 (0%)	95	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	1W	88	ARG
48	1n	34	VAL
33	18	61	LEU
15	1Q	136	MET
37	1c	156	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
21	1W	40	ASN
26	11	16	ASN
53	1s	55	GLN
22	1X	15	HIS
27	12	25	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2894/2904 (99%)	424 (14%)	33 (1%)
2	1B	119/120 (99%)	14 (11%)	2 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	1a	1535/1539 (99%)	179 (11%)	0
56	1v	8/60 (13%)	0	0
58	1x	70/77 (90%)	5 (7%)	0
All	All	4626/4700 (98%)	622 (13%)	35 (0%)

5 of 622 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	27	G
1	1A	34	U
1	1A	35	G

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	1111	A
1	1A	1300	G
1	1A	2808	G
1	1A	1130	U
1	1A	1182	G

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

39 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	6MZ	1A	1618	1	17,25,26	0.94	1 (5%)	15,36,39	2.40	3 (20%)
1	2MG	1A	1835	1	18,26,27	1.13	2 (11%)	21,38,41	2.17	5 (23%)
1	PSU	1A	1911	1	15,21,22	1.42	1 (6%)	16,30,33	2.10	4 (25%)
1	3TD	1A	1915	1	15,22,23	1.52	3 (20%)	17,32,35	1.87	4 (23%)
1	PSU	1A	1917	1	15,21,22	1.33	1 (6%)	16,30,33	1.99	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1939	1	13,22,23	0.62	0	16,32,35	2.41	2 (12%)
1	5MC	1A	1962	1	14,22,23	1.33	1 (7%)	17,32,35	0.89	1 (5%)
1	6MZ	1A	2030	1	17,25,26	0.99	1 (5%)	15,36,39	2.42	2 (13%)
1	G7M	1A	2069	1	18,26,27	1.07	1 (5%)	21,39,42	2.02	4 (19%)
1	OMG	1A	2251	1,58	18,26,27	1.13	2 (11%)	21,38,41	2.17	4 (19%)
1	2MG	1A	2445	1	18,26,27	1.12	2 (11%)	21,38,41	2.21	6 (28%)
1	H2U	1A	2449	1	17,21,22	1.15	2 (11%)	23,30,33	1.81	5 (21%)
1	PSU	1A	2457	1	15,21,22	1.29	1 (6%)	16,30,33	1.95	3 (18%)
1	OMC	1A	2498	1	15,22,23	0.62	0	20,31,34	1.55	2 (10%)
1	2MA	1A	2503	1	17,25,26	1.62	3 (17%)	18,37,40	3.15	1 (5%)
1	PSU	1A	2504	1	15,21,22	1.41	1 (6%)	16,30,33	2.09	4 (25%)
1	OMU	1A	2552	1	14,22,23	0.73	0	19,31,34	1.64	1 (5%)
1	PSU	1A	2580	1	15,21,22	1.34	1 (6%)	16,30,33	2.02	4 (25%)
1	PSU	1A	2604	1	15,21,22	1.38	1 (6%)	16,30,33	2.07	4 (25%)
1	PSU	1A	2605	1	15,21,22	1.24	1 (6%)	16,30,33	2.00	3 (18%)
1	1MG	1A	745	1	17,26,27	1.47	3 (17%)	19,39,42	0.87	1 (5%)
1	PSU	1A	746	1	15,21,22	1.48	2 (13%)	16,30,33	2.39	3 (18%)
1	5MU	1A	747	1	13,22,23	0.65	0	16,32,35	2.52	3 (18%)
1	PSU	1A	955	1	15,21,22	1.36	1 (6%)	16,30,33	2.08	4 (25%)
35	2MG	1a	1207	35	18,26,27	1.11	2 (11%)	21,38,41	2.19	5 (23%)
35	4OC	1a	1402	35	15,23,24	0.68	0	21,32,35	1.85	4 (19%)
35	5MC	1a	1407	35	14,22,23	1.31	1 (7%)	17,32,35	0.85	1 (5%)
35	UR3	1a	1498	35	13,22,23	0.66	0	18,32,35	0.86	0
35	2MG	1a	1516	35	18,26,27	1.33	2 (11%)	21,38,41	2.39	6 (28%)
35	MA6	1a	1518	35	18,26,27	1.00	1 (5%)	15,38,41	2.46	4 (26%)
35	MA6	1a	1519	35	18,26,27	0.97	1 (5%)	15,38,41	2.28	3 (20%)
35	PSU	1a	516	35	15,21,22	1.35	1 (6%)	16,30,33	2.03	4 (25%)
35	7MG	1a	527	35	20,26,27	1.53	2 (10%)	23,39,42	2.97	5 (21%)
35	2MG	1a	966	35	18,26,27	1.14	2 (11%)	21,38,41	2.25	7 (33%)
35	5MC	1a	967	35	14,22,23	1.42	1 (7%)	17,32,35	0.97	1 (5%)
58	7MG	1x	46	58	20,26,27	1.54	3 (15%)	23,39,42	3.49	6 (26%)
58	5MU	1x	54	58	13,22,23	0.56	0	16,32,35	2.50	2 (12%)
58	PSU	1x	55	58	15,21,22	1.20	1 (6%)	16,30,33	2.07	3 (18%)
58	PSU	1x	65	58	15,21,22	1.53	2 (13%)	16,30,33	2.27	4 (25%)

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	6MZ	1A	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	1A	1835	1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	3TD	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/3/25/26	0/2/2/2
1	6MZ	1A	2030	1	-	0/5/27/28	0/3/3/3
1	G7M	1A	2069	1	-	0/3/25/26	0/3/3/3
1	OMG	1A	2251	1,58	-	0/5/27/28	0/3/3/3
1	2MG	1A	2445	1	-	0/5/27/28	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	1A	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	2498	1	-	0/5/27/28	0/2/2/2
1	2MA	1A	2503	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	2504	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/5/27/28	0/2/2/2
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	1MG	1A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	746	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	747	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
35	2MG	1a	1207	35	-	0/5/27/28	0/3/3/3
35	4OC	1a	1402	35	-	0/7/29/30	0/2/2/2
35	5MC	1a	1407	35	-	0/3/25/26	0/2/2/2
35	UR3	1a	1498	35	-	0/3/25/26	0/2/2/2
35	2MG	1a	1516	35	-	0/5/27/28	0/3/3/3
35	MA6	1a	1518	35	-	0/7/29/30	0/3/3/3
35	MA6	1a	1519	35	-	0/7/29/30	0/3/3/3
35	PSU	1a	516	35	-	0/7/25/26	0/2/2/2
35	7MG	1a	527	35	-	0/7/37/38	0/3/3/3
35	2MG	1a	966	35	-	0/5/27/28	0/3/3/3
35	5MC	1a	967	35	-	0/3/25/26	0/2/2/2
58	7MG	1x	46	58	-	0/7/37/38	0/3/3/3
58	5MU	1x	54	58	-	0/3/25/26	0/2/2/2
58	PSU	1x	55	58	-	0/7/25/26	0/2/2/2
58	PSU	1x	65	58	-	0/7/25/26	0/2/2/2

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1x	65	PSU	C5-C1'	-4.67	1.48	1.52
1	1A	2504	PSU	C5-C1'	-4.64	1.48	1.52
1	1A	1911	PSU	C5-C1'	-4.59	1.48	1.52
1	1A	2604	PSU	C5-C1'	-4.49	1.48	1.52
35	1a	516	PSU	C5-C1'	-4.34	1.48	1.52

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1x	46	7MG	C5-C4-N3	-9.35	117.21	126.74
35	1a	527	7MG	C5-C4-N3	-8.07	118.52	126.74
1	1A	747	5MU	C5-C4-N3	-7.22	119.29	125.35
58	1x	54	5MU	C5-C4-N3	-7.19	119.32	125.35
1	1A	1939	5MU	C5-C4-N3	-7.15	119.35	125.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1618	6MZ	1	0
1	1A	1835	2MG	1	0
1	1A	1915	3TD	1	0
1	1A	1917	PSU	1	0
1	1A	1939	5MU	1	0
1	1A	1962	5MC	1	0
1	1A	2030	6MZ	2	0
1	1A	2069	G7M	2	0
1	1A	2251	OMG	2	0
1	1A	2445	2MG	2	0
1	1A	2498	OMC	1	0
1	1A	2503	2MA	4	0
1	1A	2604	PSU	1	0
1	1A	745	1MG	2	0
1	1A	747	5MU	2	0
1	1A	955	PSU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	EVN	1A	3001	1	114,123,123	1.57	15 (13%)	150,191,191	1.67	33 (22%)

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	EVN	1A	3001	1	-	0/50/234/234	1/13/13/13

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3001	EVN	CDN-CAC	-6.61	1.38	1.51
59	1A	3001	EVN	CEG-CDI	-5.75	1.39	1.51
59	1A	3001	EVN	CDD-CDB	-4.32	1.39	1.50
59	1A	3001	EVN	CAD-CAJ	-4.09	1.40	1.50
59	1A	3001	EVN	CCT-CCS	-2.83	1.48	1.53

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	3001	EVN	OCR-CCL-CCK	-5.21	94.64	103.48
59	1A	3001	EVN	CAP-OAQ-CAR	-4.22	104.28	114.31
59	1A	3001	EVN	OCP-CCK-CCL	-3.61	98.90	103.51
59	1A	3001	EVN	CBD-CBC-CBB	-2.83	107.48	112.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	3001	EVN	CAA-CAB-CAC	-2.80	120.09	122.56

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	3001	EVN	CAU-CAW-CAX-CAY-CAZ-OAV

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.