



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 05:17 am BST

PDB ID : 5AA0
EMDB ID : EMD-6397
Title : Complex of Thermosus thermophilus ribosome (A-and P-site tRNA) bound to BipA-GDPCP
Authors : Kumar, V.; Chen, Y.; Ahmed, T.; Tan, J.; Ero, R.; Bhushan, S.; Gao, Y.-G.
Deposited on : 2015-07-23
Resolution : 5.00 Å(reported)
Based on initial model : 4V4Y

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

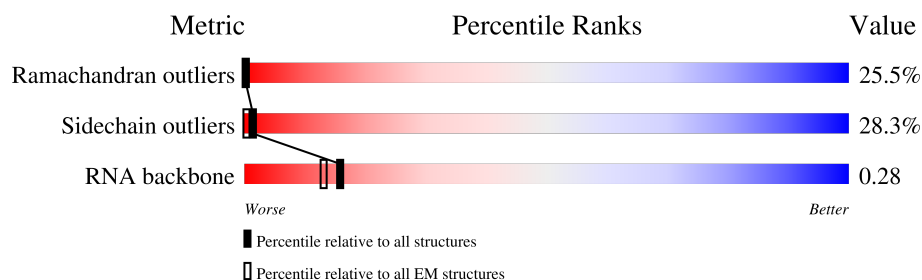
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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.



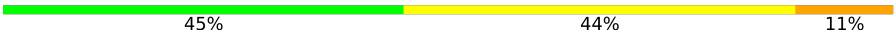
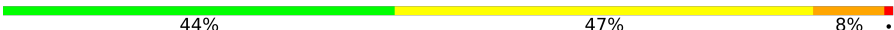
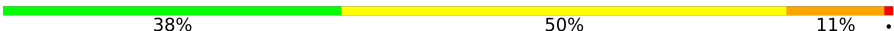


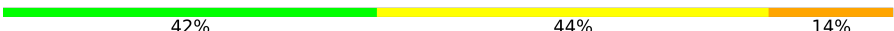









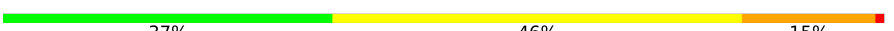
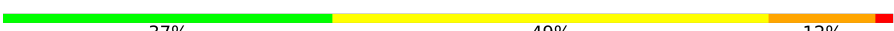
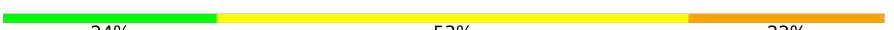







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	2889	44% 44% 9% .
2	AB	123	50% 41% 7% .
3	AC	228	76% 22% .
4	AD	272	53% 36% 11% .
5	AE	206	48% 39% 13%
6	AF	208	54% 37% 9%
7	AG	182	53% 38% 8% .
8	AH	174	59% 34% 6% .
9	AK	139	41% 50% 9%














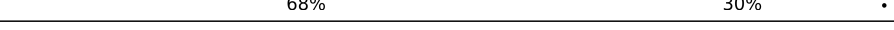







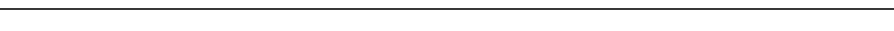


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Mol	Chain	Length	Quality of chain
10	AL	122	
11	AM	145	
12	AN	136	
13	AO	117	
14	AP	110	
15	AQ	117	
16	AR	117	
17	AS	101	
18	AT	110	
19	AU	94	
20	AV	110	
21	AW	180	
22	AX	85	
23	AY	67	
24	AZ	59	
25	Aa	71	
26	Ab	57	
27	Ac	49	
28	Ad	49	
29	Ae	64	
30	Af	37	
31	AI	153	
32	AJ	134	
33	Ag	128	
34	BA	1515	

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Mol	Chain	Length	Quality of chain
35	BF	234	
36	BG	206	
37	BH	208	
38	BI	150	
39	BJ	101	
40	BK	155	
41	BL	138	
42	BM	127	
43	BN	98	
44	BO	119	
45	BP	124	
46	BQ	114	
47	BR	60	
48	BS	88	
49	BT	83	
50	BU	104	
51	BV	73	
52	BW	80	
53	BX	99	
54	BY	24	
55	BC	76	
56	BD	75	
56	BE	75	
57	BZ	605	

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 155482 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	AA	2889	Total	C	N	O	P	0	0
			62218	27691	11629	20009	2889		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	1134	G	UNK	conflict	GB 37223181

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	123	Total	C	N	O	P	0	0
			2641	1175	488	855	123		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	228	Total	C	N	O	S	0	0
			1742	1102	318	319	3		

- 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
			2124	1339	424	358	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	206	Total	C	N	O	S	0	0
			1578	997	302	273	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	208	Total	C	N	O	S	0	0
			1625	1034	303	286	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	182	Total	C	N	O	S	0	0
			1482	947	269	261	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	174	Total	C	N	O	S	0	0
			1328	844	248	235	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AK	139	Total	C	N	O	S	0	0
			1113	717	207	186	3		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	122	Total	C	N	O	S	0	0
			932	587	171	170	4		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AM	145	Total	C	N	O	S	0	0
			1106	688	226	190	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AN	136	Total	C	N	O	S	0	0
			1080	688	204	183	5		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	AO	117	Total	C	N	O	0	0
			960	599	202	159		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AP	110	Total	C	N	O	0	0
			877	553	175	149		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AQ	117	Total	C	N	O	S	0	0
			976	614	197	164	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AR	117	Total	C	N	O	S	0	0
			964	610	202	151	1		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AS	101	Total	C	N	O	S	0	0
			779	501	142	135	1		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AT	110	Total	C	N	O	S	0	0
			876	552	171	151	2		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	AU	94	Total	C	N	O	0	0
			742	483	133	126		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AV	110	Total	C	N	O	S	0	0
			844	539	158	141	6		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AW	180	Total	C	N	O	S	0	0
			1435	916	256	260	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AX	85	Total	C	N	O	S	0	0
			670	415	141	112	2		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AY	67	Total	C	N	O	S	0	0
			567	350	116	99	2		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	AZ	59	Total	C	N	O	0	0
			469	298	90	81		

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Aa	71	Total	C	N	O	S	0	0
			581	364	108	104	5		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ab	57	Total	C	N	O	S	0	0
			445	279	87	74	5		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ac	49	Total	C	N	O	S	0	0
			426	265	87	70	4		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ad	49	Total	C	N	O	S	0	0
			430	263	108	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ae	64	Total	C	N	O	S	0	0
			515	331	102	79	3		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Af	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AI	153	Total	C	N	O		0	0
			752	446	153	153			

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AJ	134	Total	C	N	O	S	0	0
			993	632	175	181	5		

- Molecule 33 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ag	128	Total	C	N	O		0	5
			620	369	128	123			

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	1515	Total	C	N	O	P	0	0
			32554	14490	6022	10527	1515		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BF	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BG	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BH	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BI	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BJ	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BK	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BL	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BM	127	Total	C	N	O	S	0	0
			1010	639	197	174			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BN	98	Total	C	N	O	S	0	0
			794	499	156	138	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BO	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BP	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BQ	114	Total	C	N	O	S	0	0
			914	565	189	158	2		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BR	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BS	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BT	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BU	104	Total	C	N	O	S	0	0
			857	547	161	147	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	BV	73	Total	C	N	O	0	0
			597	380	118	99		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BW	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BX	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
54	BY	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 55 is a RNA chain called tRNA chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BC	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

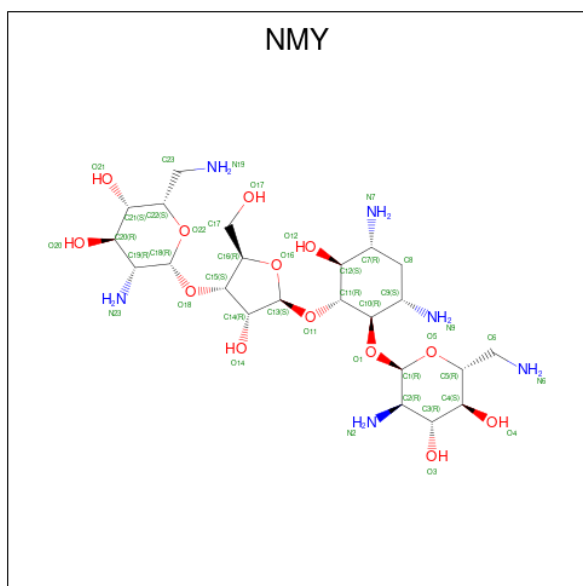
- Molecule 56 is a RNA chain called tRNA chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BD	75	Total	C	N	O	P	0	0
			1597	713	285	525	74		
56	BE	75	Total	C	N	O	P	0	0
			1597	713	285	525	74		

- Molecule 57 is a protein called GTP-binding protein.

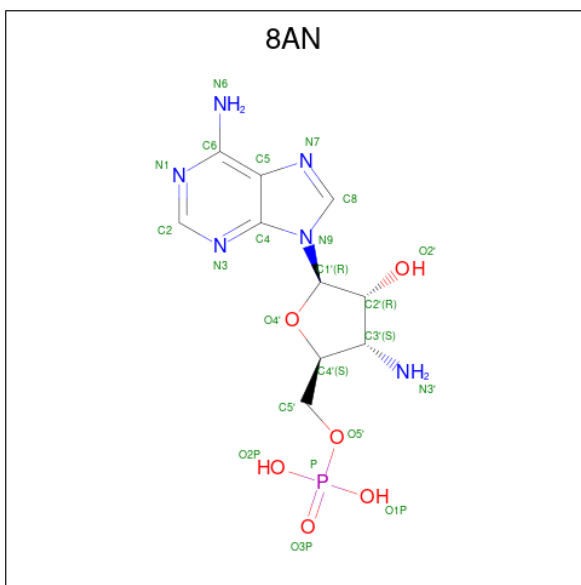
Mol	Chain	Residues	Atoms					AltConf	Trace
57	BZ	605	Total	C	N	O	S	0	0
			4610	2902	807	883	18		

- Molecule 58 is NEOMYCIN (three-letter code: NMY) (formula: $\text{C}_{23}\text{H}_{46}\text{N}_6\text{O}_{13}$).



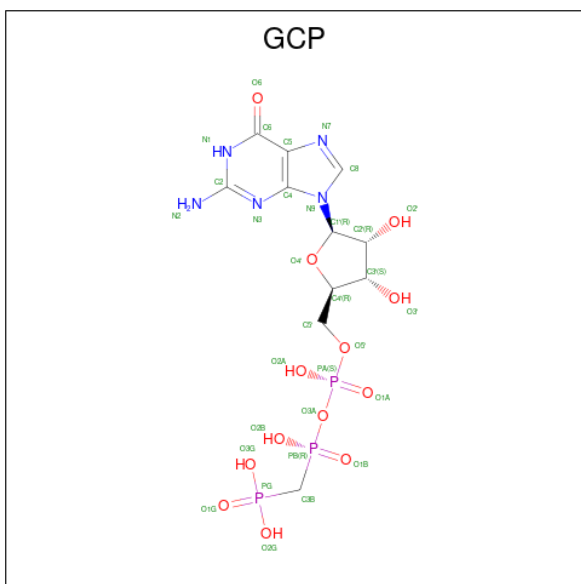
Mol	Chain	Residues	Atoms				AltConf
58	AA	1	Total 42	C 23	N 6	O 13	0
58	BA	1	Total 42	C 23	N 6	O 13	0

- Molecule 59 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_6\text{O}_6\text{P}$).



Mol	Chain	Residues	Atoms					AltConf
59	AA	1	Total	C	N	O	P	0
			22	10	6	5	1	
59	AA	1	Total	C	N	O	P	0
			22	10	6	5	1	

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

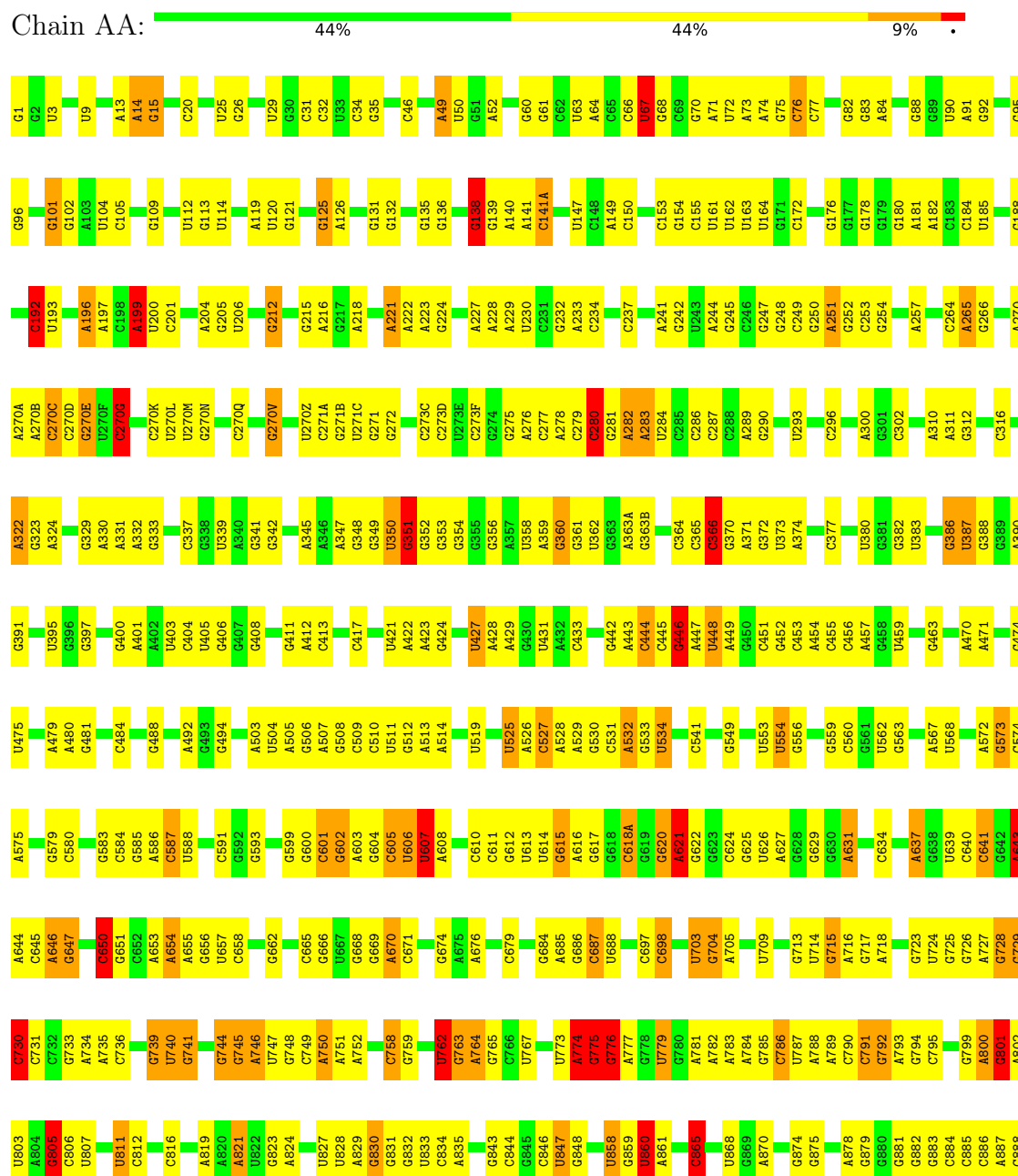


Mol	Chain	Residues	Atoms					AltConf
60	BZ	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

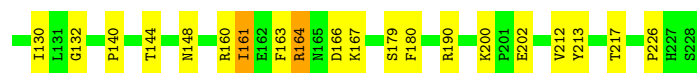
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S ribosomal RNA



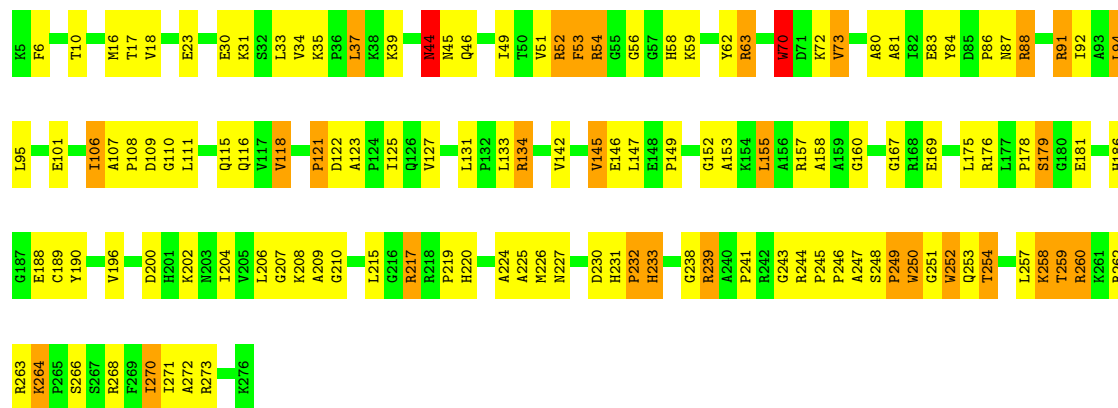
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U2041	C1958	C1879	U1779	A1618	A1943	A1472	A1378	A1274	C1201	G1110	G1042	C966	A890
A2042	C1959	C1880	C1781	G1619	C1544	A1473	A1379	A1275	G1202	A1111	C1043	C967	C892
C2043	C1960	C1881	C1782	G1620	G1552	C1474	A1384	A1284	G1203	U1113	A1045	C968	C893
C2044	C1961	C1882	A1783	G1621	A1553	A1475	A1385	A1285	U1205	C1116	A1046	C969	C894
U2047	C1962	A1884	A1784	G1622	A1554	A1476	A1386	A1286	G1206	C1117	A1047	C970	U895
G2048	C1963	A1901	A1785	G1623	A1555	A1477	A1387	A1287	G1207	C1118	A1048	C971	U896
G2049	C1964	C1902	A1786	G1624	A1556	A1478	A1388	A1288	C1208	A1126	C1049	C972	A896
C2050	C1965	C1903	A1787	G1625	A1557	A1479	A1389	C1289	U1209	A1127	A1050	C973	C897
G2051	C1966	G1904	C1790	G1626	A1558	A1480	A1390	C1290	A1210	A1128	G1051	C974	C898
G2052	C1967	G1905	C1791	G1627	G1559	A1481	A1391	C1291	U1211	A1129	C1052	C975	A900
C2053	C1968	G1906	A1792	A1631	G1560	A1482	A1392	C1292	U1212	U1130	C1053	C976	A901
G2054	C1969	G1907	C1793	A1632	G1561	A1483	A1393	C1293	A1213	G1131	C1054	C977	C902
C2055	C1970	C1908	C1794	A1633	C1562	A1484	A1394	C1294	C1225	C1140	U1061	C978	C903
G2056	C1971	G1909	A1794	G1635	C1563	A1485	A1395	U1300	C1226	U1141	G1062	C979	C904
A2060	C1972	C1910	C1795	G1636	C1564	U1489	U1396	U1301	A1220	U1142	A1057	C980	U905
G2061	C1973	U1911	U1798	G1637	C1565	A1490	U1397	A1302	G1228	A1143	G1058	C981	A906
A2062	C1974	A1912	C1799	A1640	C1566	A1491	C1398	A1303	U1229	U1144	G1059	C982	U907
C2063	C1975	A1913	C1800	A1641	A1567	A1492	C1399	C1304	C1230	U1145	U1060	C983	C908
C2064	C1976	C1914	G1801	C1644	G1568	A1493	C1403	C1305	G1231	U1146	U1061	C984	A909
C2065	C1977	C1915	A1802	G1645	A1569	A1494	C1404	C1306	U1232	U1147	U1062	C985	A910
G2066	C1978	U1916	A1803	G1646	A1570	A1495	U1405	G1310	G1228	U1148	U1063	C986	A911
C2067	C1979	G1917	C1804	G1647	A1571	A1496	U1406	G1311	U1229	A1149	C1064	C987	C912
G2068	C1980	U1918	C1805	G1648	A1572	A1497	C1407	U1312	C1230	U1150	U1065	C988	U913
C2069	C1981	A1919	U1806	G1649	G1573	C1498	G1416	U1313	C1231	U1151	U1066	C989	C914
G2070	C1982	C1920	U1807	G1650	G1574	C1499	C1417	A1321	A1237	U1152	U1067	C990	C915
U2071	C1983	G1921	C1808	G1651	G1575	A1507	C1418	A1322	G1238	U1153	U1068	C991	C916
C2072	C1984	U1922	A1809	A1652	C1576	A1508	C1419	U1323	U1239	U1154	U1069	C992	A917
U2073	C1985	C1923	C1810	A1653	C1577	C1509	U1420	G1324	A1156	U1155	A1070	C993	A918
G2074	C1986	U1924	A1811	G1654	U1578	A1510	C1421	U1240	G1157	U1156	G1071	C994	A919
C2075	C1987	C1925	A1812	G1655	A1579	A1511	C1422	U1326	U1160	U1157	U1072	C995	G920
U2076	C1988	G1926	C1813	G1656	G1580	A1512	C1423	U1327	C1161	U1158	A1073	C996	G921
C2077	C1989	A1927	U1814	C1657	C1581	C1513	C1424	G1328	U1162	U1159	G1074	C997	G922
G2080	C1990	C1928	U1815	G1658	C1582	C1514	C1425	U1329	U1163	U1160	C1075	C1005	U922
U2081	C1991	G1929	A1816	C1659	C1583	C1515	C1426	U1330	A1247	U1161	A1076	C1006	C924
C2082	C1992	C1930	U1817	G1660	C1584	C1516	C1427	C1330	U1248	U1162	A1077	C1007	U923
U2083	C1993	U1931	C1821	C1661	A1586	C1517	C1428	U1335	U1249	U1163	U1078	A1009	A930
G2084	C1994	A1932	G1822	G1662	A1587	C1518	C1429	U1336	G1248	U1164	C1079	A1010	G931
C2085	C1995	C1933	U1823	A1664	U1590	C1519	U1438	U1340	C1251	U1165	C1080	G1011	G932
G2086	C1996	G1934	C1824	G1665	G1591	C1520	A1439	U1341	C1252	U1166	U1083	G1012	A933
C2087	C1997	A1935	U1825	G1666	G1592	C1521	G1440	U1342	C1253	U1167	A1084	C1013	G939
U2088	C1998	C1936	C1826	C1667	A1597	C1522	A1441	A1253	A1254	U1168	A1085	U1019	G940
C2089	C1999	A1937	G1827	A1668	C1598	C1523	C1442	G1343	U1255	U1169	A1086	U1020	A941
U2090	C2000	U1938	C1830	C1669	C1600	C1524	C1443	G1344	G1256	U1170	A1087	A1021	G942
G2091	C2001	C1939	G1831	C1670	G1601	G1525	C1444	C1345	C1257	U1171	U1088	U1022	U943
C2092	C2002	U1940	U1832	U1673	U1602	C1526	C1445	G1346	C1258	U1172	A1089	G1023	A944
U2093	C2003	C1941	C1833	G1674	A1603	C1527	C1446	G1347	G1259	U1173	U1090	U1024	G945
G2094	C2004	A1942	G1834	C1675	C1604	A1528	C1447	A1348	C1260	U1174	G1091	G1025	G946
C2095	C2005	C1943	U1835	A1676	G1605	C1529	C1448	C1349	C1261	U1175	C1092	U1026	G950
U2096	C2006	G1944	C1836	A1677	G1606	C1530	C1449	A1350	U1262	U1176	G1093	U1027	C955
C2097	C2007	U1945	U1837	G1678	C1607	C1531	C1450	U1357	U1263	U1177	A1099	G1031	G956
G2098	C2008	C1946	A1838	G1679	C1608	C1532	C1451	G1358	C1264	U1178	A1085	A1032	A957
C2103	C2009	U1947	C1839	G1680	A1609	C1533	C1452	A1359	A1265	U1179	A1086	U1033	U958
G2110	C2010	G1950	U1840	C1681	C1610	C1534	C1453	C1363	U1267	U1180	A1087	C1034	A959
C2111	C2011	U1951	A1841	G1682	A1611	G1535	C1454	C1364	A1268	U1181	U1088	U1103	A960
U2112	C2012	C1952	C1842	C1683	C1612	C1536	C1455	A1269	C1270	U1182	A1089	C1104	C961
G2113	C2013	A1953	U1843	C1684	G1613	C1537	C1456	C1365	U1271	U1183	G1092	U1108	G962
C2114	C2014	C1954	A1844	C1685	C1614	C1538	C1457	C1366	A1272	U1184	C1093		
G2115	C2015	U1955	C1845	C1686	A1615	G1539	C1458	A1367		U1185	A1099		
U2116	C2016	G1956	U1846	C1687	C1616	C1540	C1459	U1368		U1186	A1085		
C2117	C2017	A1957	A1847	G1688	C1617	C1541	C1460	A1369		U1187	A1086		
G2118	C2018	C1958	C1848	C1689	C1618	C1542	C1461	A1266		U1188	A1087		
U2119	C2019	U1959	U1849	C1690	C1619	C1543	C1462	U1267		U1189	A1088		
C2120	C2020	A1960	A1850	C1691	C1620	C1544	C1463	A1268		U1190	A1089		
G2121	C2021	C1961	C1851	C1692	C1621	C1545	C1464	C1269		U1191	A1090		
U2122	C2022	U1962	U1852	C1693	C1622	C1546	C1465	A1270		U1192	A1091		
C2123	C2023	A1963	A1853	C1694	C1623	C1547	C1466	C1271		U1193	A1092		
G2124	C2024	G1964	C1854	C1695	C1624	C1548	C1467	U1272		U1194	A1093		
U2125	C2025	U1965	U1855	C1696	C1625	C1549	C1468	U1273		U1195	A1094		
C2126	C2026	C1966	G1856	C1697	C1626	C1550	C1469	C1368		U1196	A1095		
G2127	C2027	A1967	C1857	C1698	C1627	C1551	C1470	U1369		U1197	A1096		





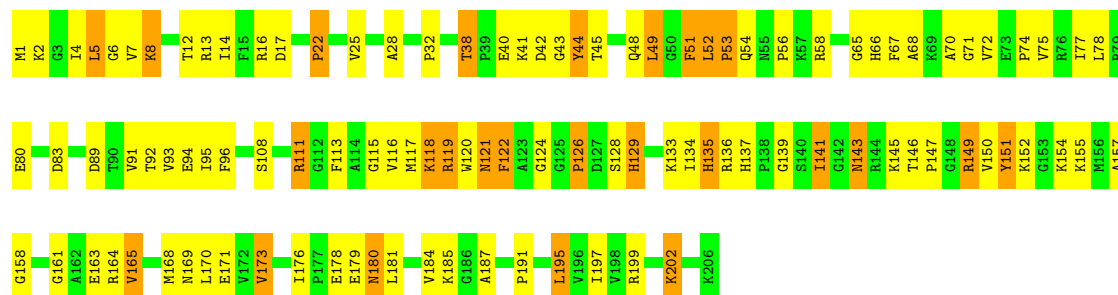
• Molecule 4: 50S ribosomal protein L2

Chain AD: 53% 36% 11% •



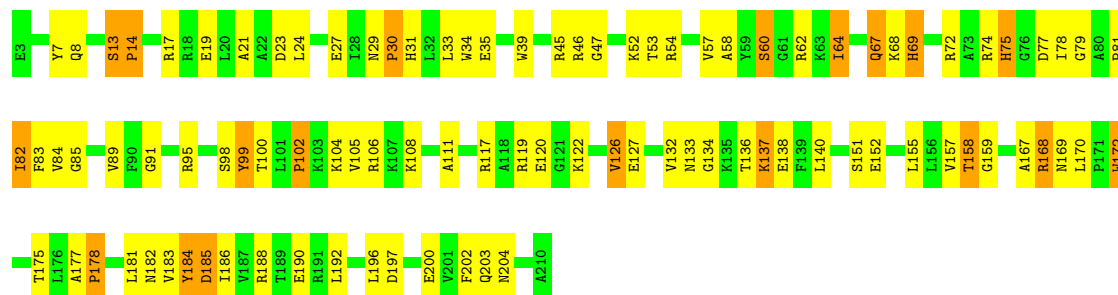
• Molecule 5: 50S ribosomal protein L3

Chain AE: 48% 39% 13%



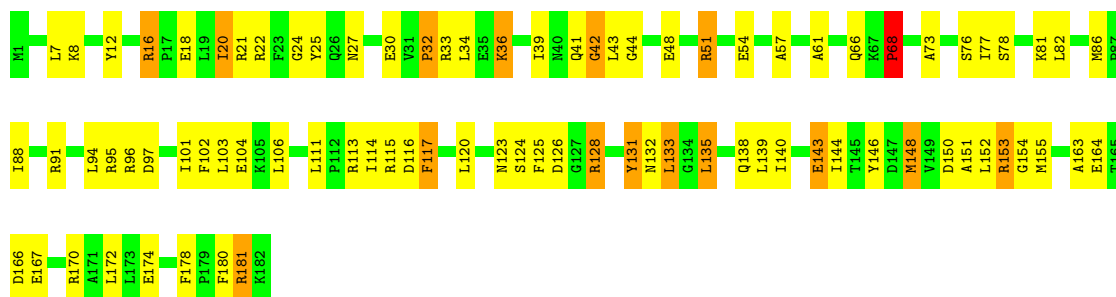
• Molecule 6: 50S ribosomal protein L4

Chain AF: 54% 37% 9%



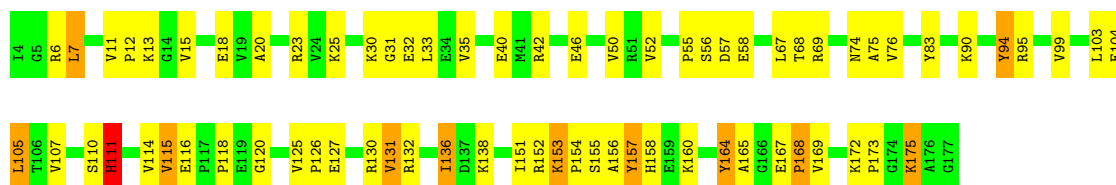
• Molecule 7: 50S ribosomal protein L5

Chain AG: 53% 38% 8% •



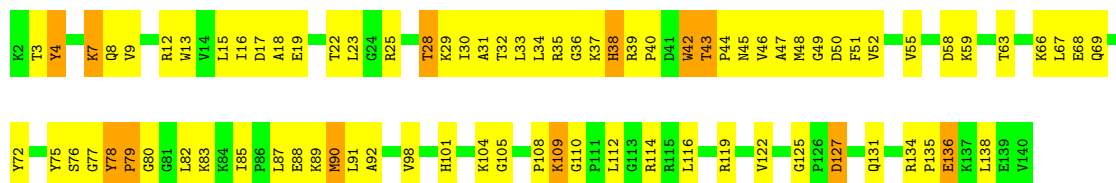
• Molecule 8: 50S ribosomal protein L6

Chain AH: 59% 34% 6% .



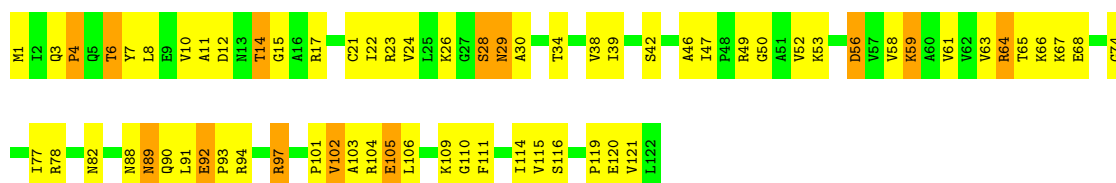
• Molecule 9: 50S ribosomal protein L13

Chain AK: 41% 50% 9%



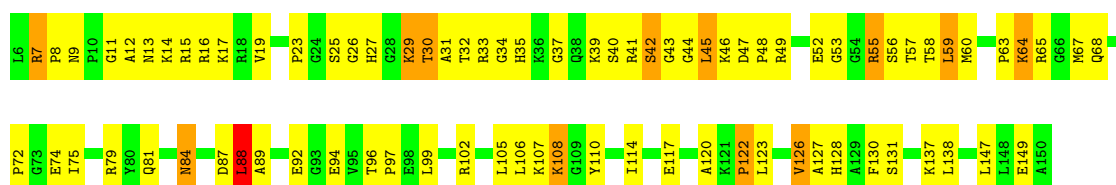
• Molecule 10: 50S ribosomal protein L14

Chain AL: 45% 44% 11%



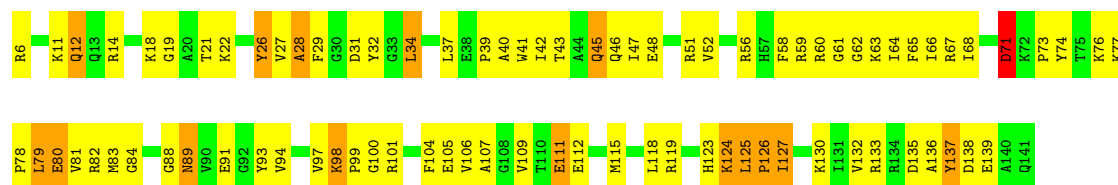
• Molecule 11: 50S ribosomal protein L15

Chain AM: 44% 47% 8% .



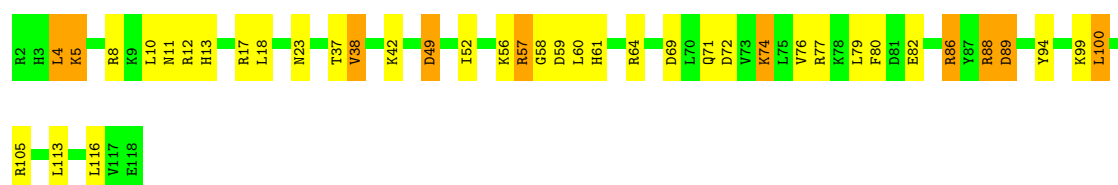
- Molecule 12: 50S ribosomal protein L16

Chain AN:  38% 50% 11%



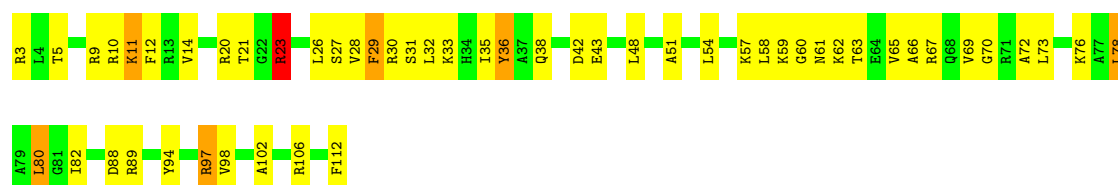
- Molecule 13: 50S ribosomal protein L17

Chain AO:  66% 26% 9%



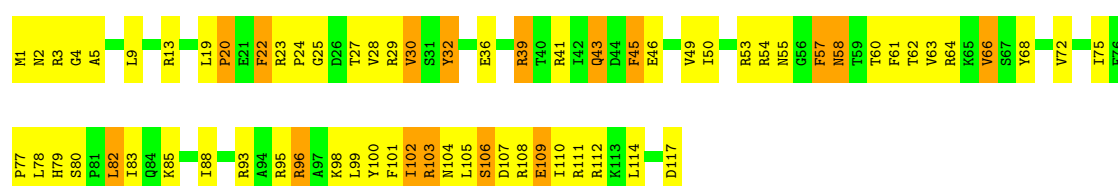
- Molecule 14: 50S ribosomal protein L18

Chain AP:  53% 41% 5%



- Molecule 15: 50S ribosomal protein L19

Chain AQ:  42% 44% 14%

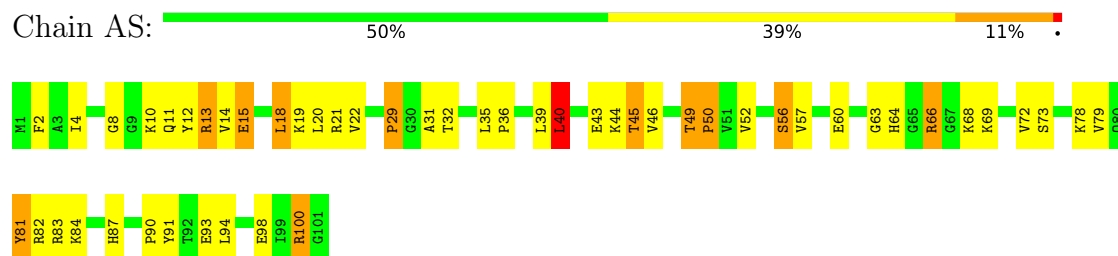


- Molecule 16: 50S ribosomal protein L20

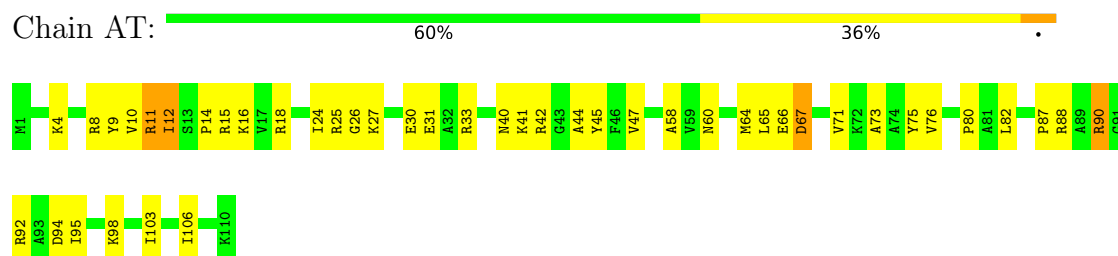
Chain AR:  57% 35% 8%



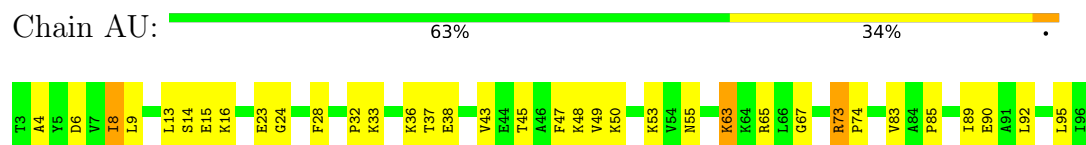
- Molecule 17: 50S ribosomal protein L21



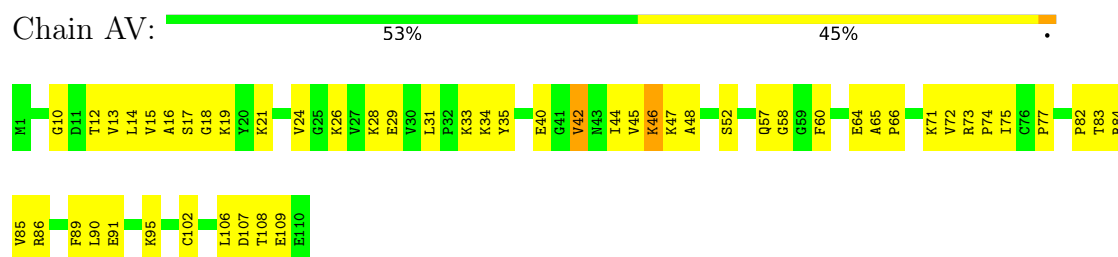
- Molecule 18: 50S ribosomal protein L22



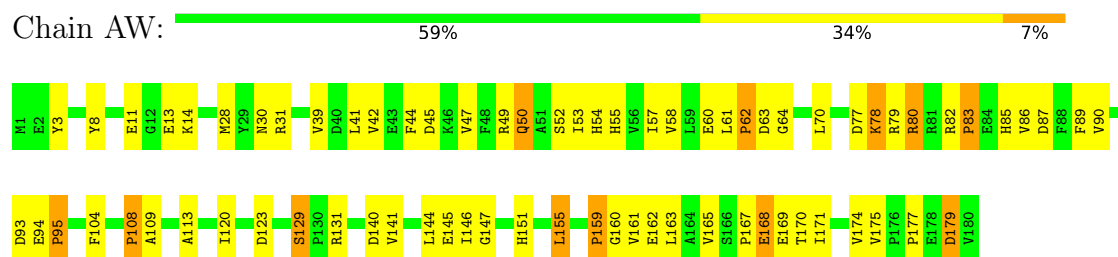
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



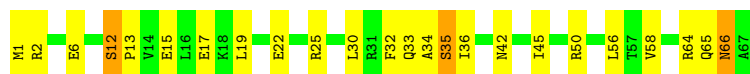
- Molecule 22: 50S ribosomal protein L27

Chain AX:  71% 27% .



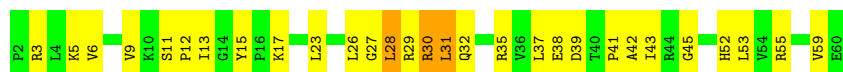
- Molecule 23: 50S ribosomal protein L29

Chain AY:  64% 31% .




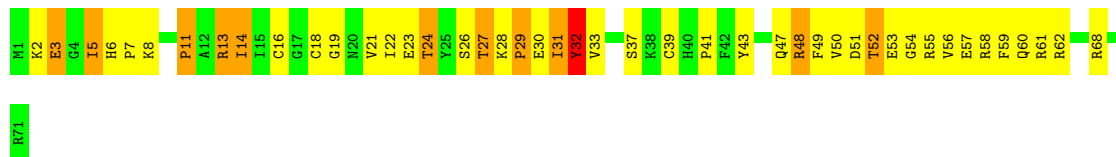
- Molecule 24: 50S ribosomal protein L30

Chain AZ:  51% 44% 5% .



- Molecule 25: 50S ribosomal protein L31

Chain Aa:  37% 46% 15% .



- Molecule 26: 50S ribosomal protein L32

Chain Ab:  37% 49% 12% .



- Molecule 27: 50S ribosomal protein L33

Chain Ac:  24% 53% 22% .



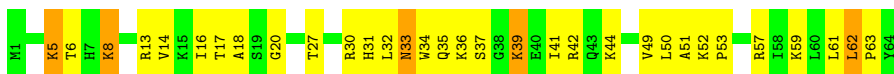
- Molecule 28: 50S ribosomal protein L34

Chain Ad:  53% 37% 10% .



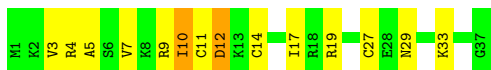
- Molecule 29: 50S ribosomal protein L35

Chain Ae:  50% 42% 8%




- Molecule 30: 50S ribosomal protein L36

Chain Af:  62% 32% 5%



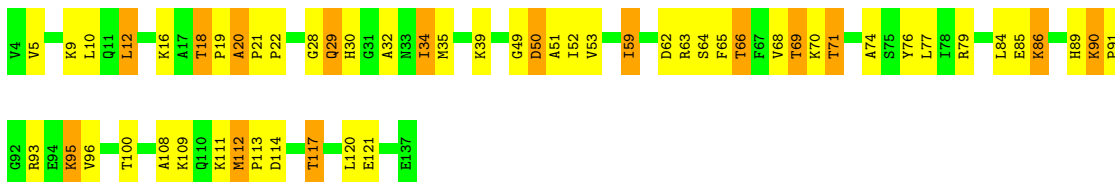
- Molecule 31: 50S ribosomal protein L10

Chain Ai:  80% 20% 0%



- Molecule 32: 50S ribosomal protein L11

Chain Aj:  59% 30% 11%



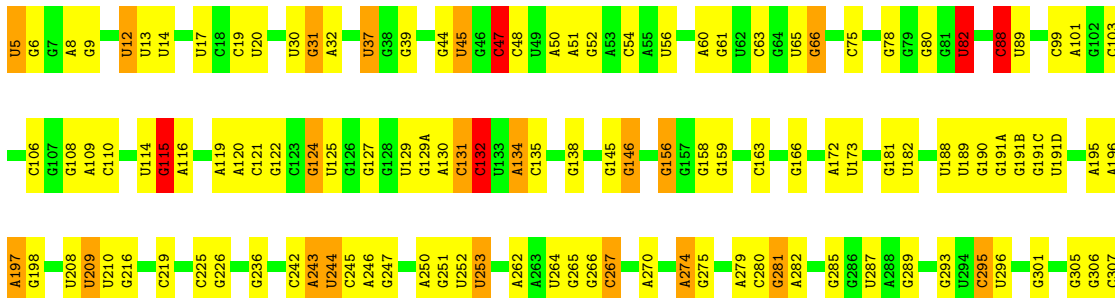
- Molecule 33: Unknown peptide

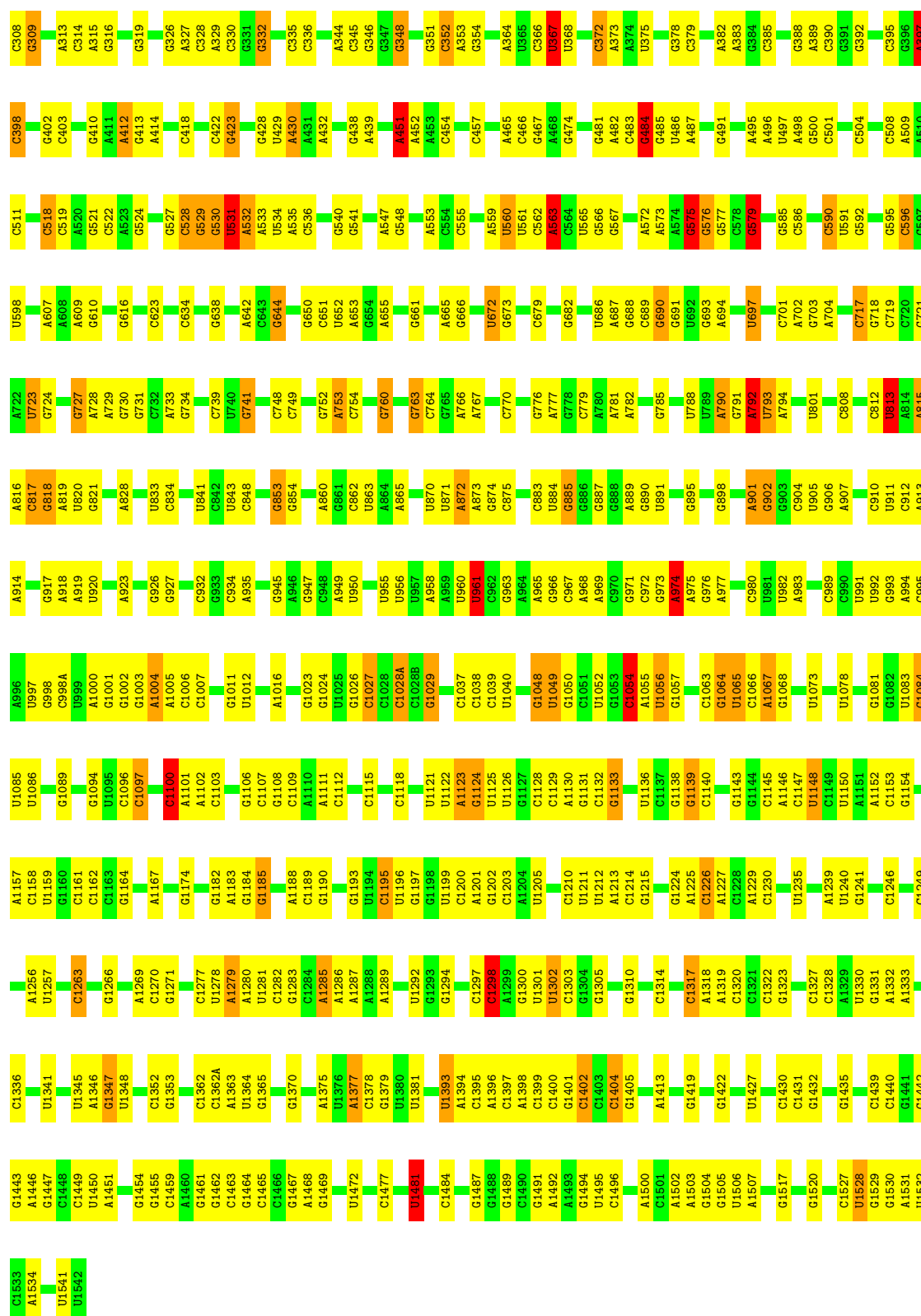
Chain Ag:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 16S ribosomal RNA

Chain BA:  56% 37% 6%

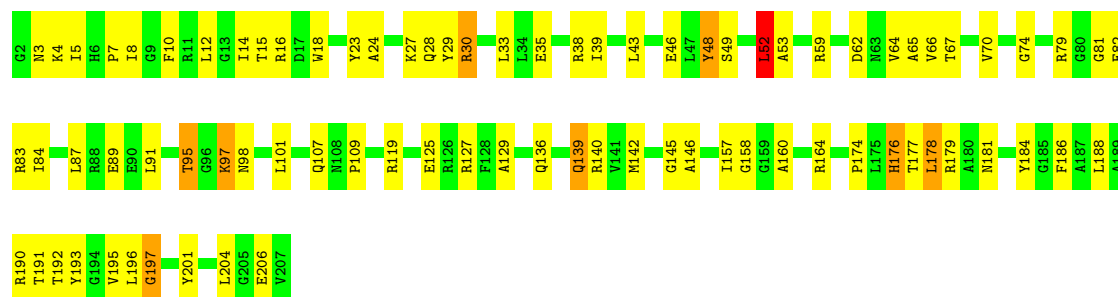




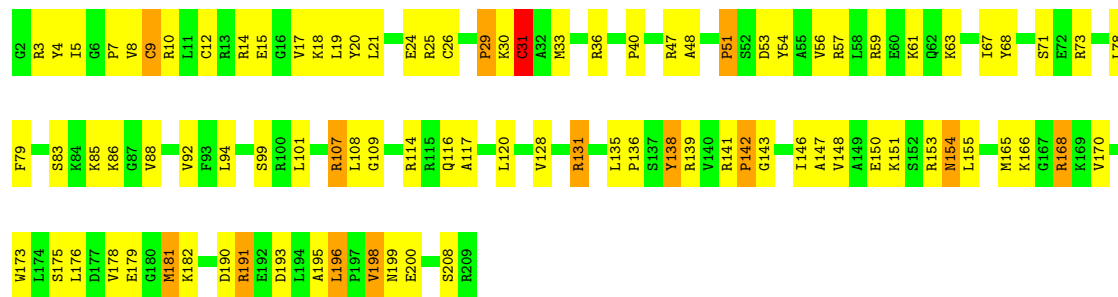
• Molecule 35: 30S ribosomal protein S2

Chain BF: 51% 37% 12%

- Molecule 36: 30S ribosomal protein S3



- Molecule 37: 30S ribosomal protein S4



- Molecule 38: 30S ribosomal protein S5



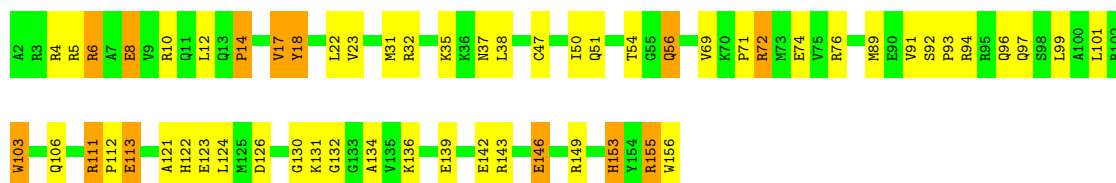
- Molecule 39: 30S ribosomal protein S6





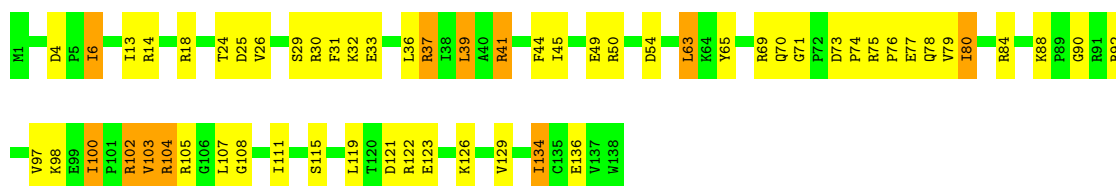
- Molecule 40: 30S ribosomal protein S7

Chain BK: 63% 29% 8%



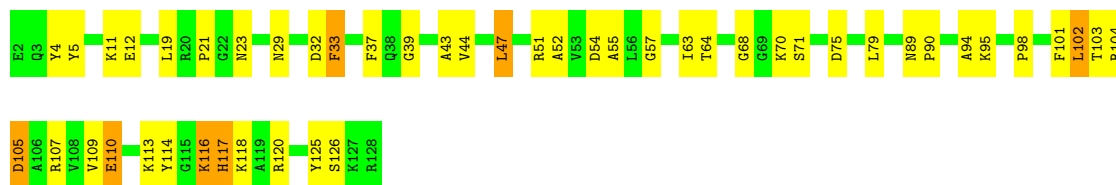
- Molecule 41: 30S ribosomal protein S8

Chain BL: 58% 34% 8%



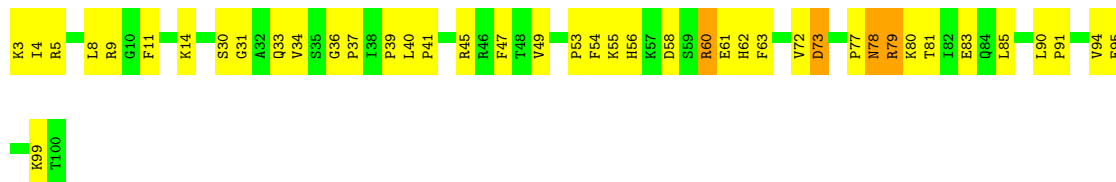
- Molecule 42: 30S ribosomal protein S9

Chain BM: 62% 32% 6%



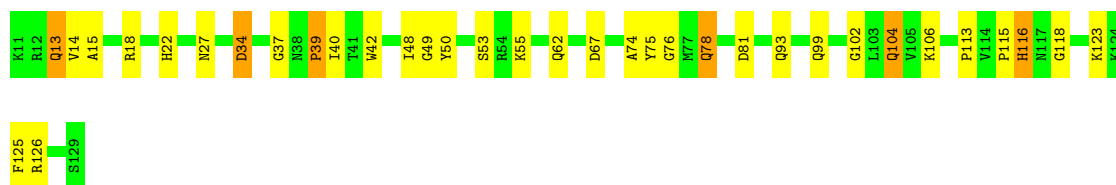
- Molecule 43: 30S ribosomal protein S10

Chain BN: 57% 39% 4%



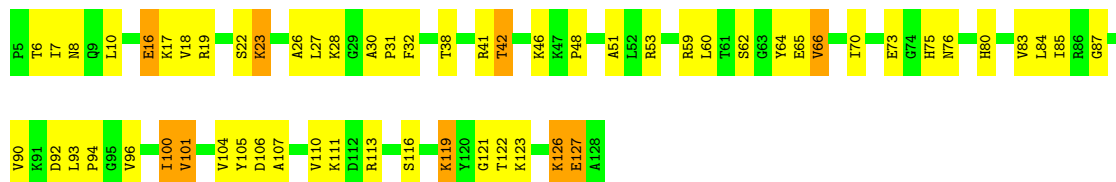
- Molecule 44: 30S ribosomal protein S11

Chain BO: 71% 24% 5%



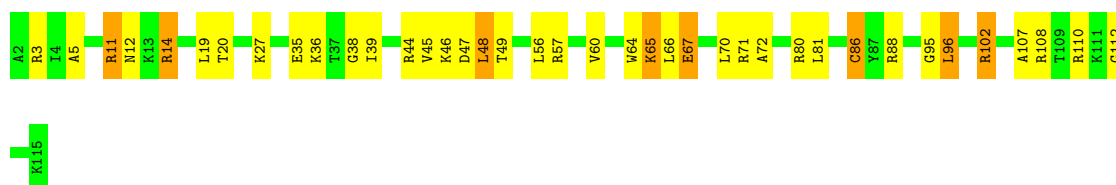
- Molecule 45: 30S ribosomal protein S12

Chain BP: 52% 40% 7%



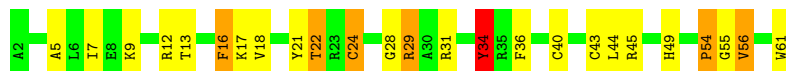
- Molecule 46: 30S ribosomal protein S13

Chain BQ: 66% 27% 7%



- Molecule 47: 30S ribosomal protein S14 type Z

Chain BR: 58% 30% 10%



- Molecule 48: 30S ribosomal protein S15

Chain BS: 68% 30% 2%



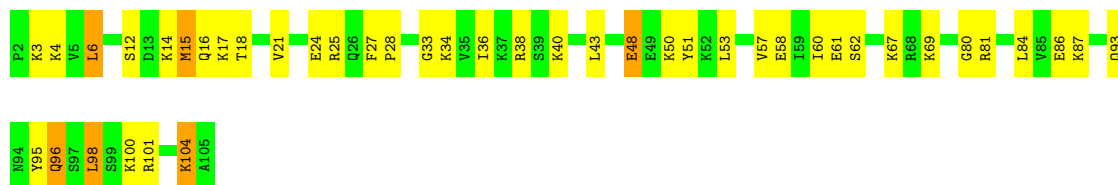
- Molecule 49: 30S ribosomal protein S16

Chain BT: 59% 35% 6%



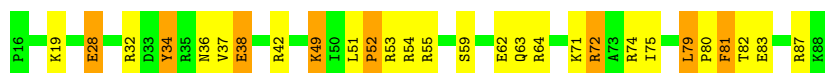
- Molecule 50: 30S ribosomal protein S17

Chain BU:  59% 36% 6%



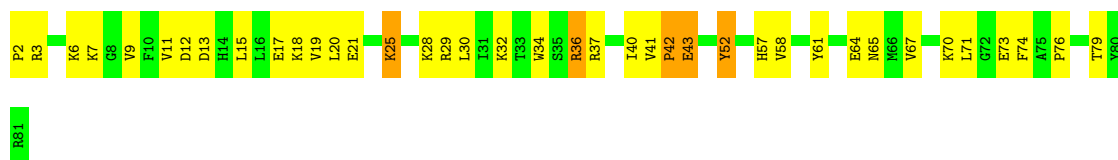
- Molecule 51: 30S ribosomal protein S18

Chain BV:  62% 27% 11%



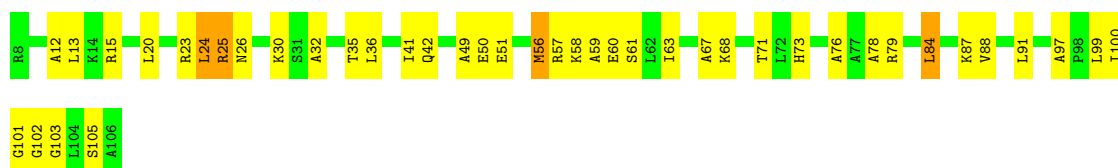
- Molecule 52: 30S ribosomal protein S19

Chain BW:  51% 42% 6%



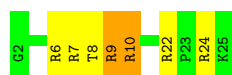
- Molecule 53: 30S ribosomal protein S20

Chain BX:  58% 38% 4%



- Molecule 54: 30S ribosomal protein Thx

Chain BY:  71% 21% 8%



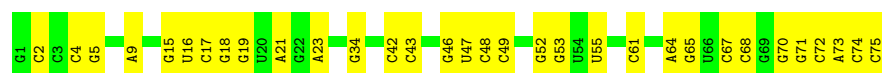
- Molecule 55: tRNA chain 1

Chain BC:  66% 34% 0%



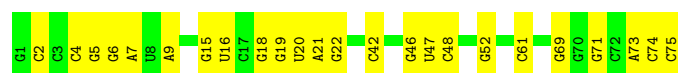
- Molecule 56: tRNA chain 2

Chain BD:  57% 43%



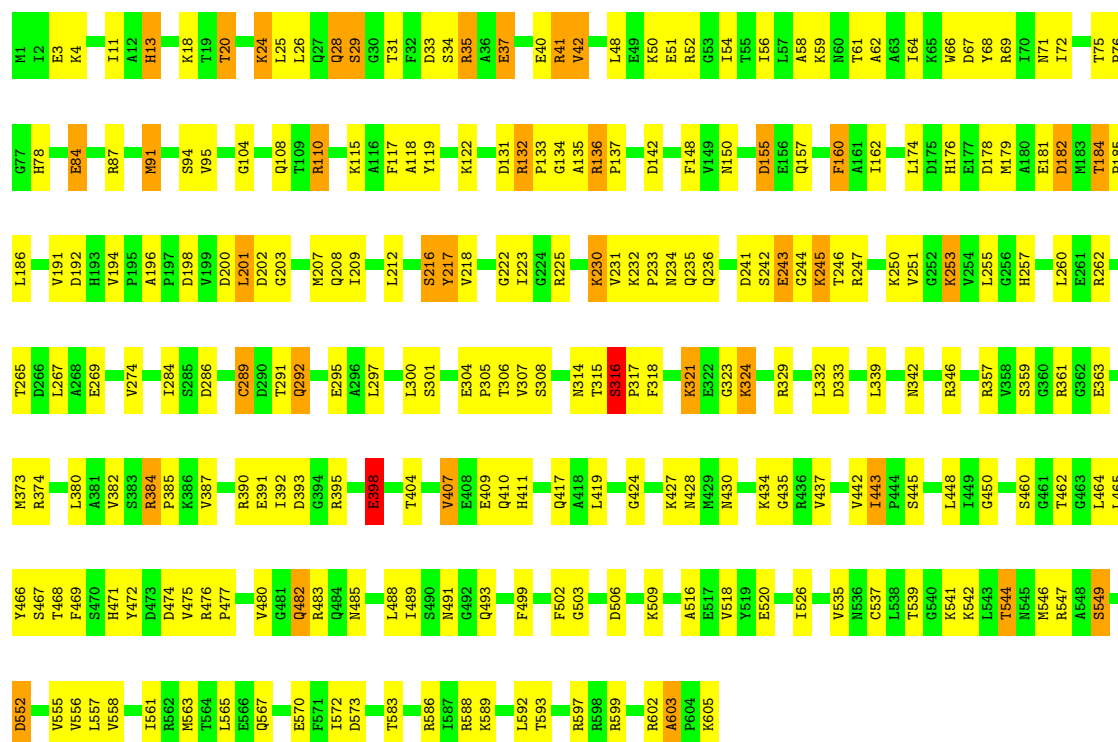
• Molecule 56: tRNA chain 2

Chain BE:  68% 32%



• Molecule 57: GTP-binding protein

Chain BZ:  59% 34% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77127	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	73684	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, NMY, GCP

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	1.00	107/69678 (0.2%)	1.08	348/108758 (0.3%)
2	AB	0.83	4/2954 (0.1%)	0.99	7/4606 (0.2%)
3	AC	0.54	0/1772	0.87	0/2383
4	AD	0.72	2/2174 (0.1%)	1.19	13/2927 (0.4%)
5	AE	0.75	0/1611	1.16	13/2171 (0.6%)
6	AF	0.64	0/1660	1.03	4/2247 (0.2%)
7	AG	0.62	0/1507	1.06	4/2027 (0.2%)
8	AH	0.59	0/1354	0.98	4/1831 (0.2%)
9	AK	0.78	1/1140 (0.1%)	1.16	8/1537 (0.5%)
10	AL	0.92	1/942 (0.1%)	1.31	10/1268 (0.8%)
11	AM	0.71	0/1123	1.12	5/1493 (0.3%)
12	AN	0.72	0/1100	1.19	8/1470 (0.5%)
13	AO	0.70	0/974	1.06	2/1302 (0.2%)
14	AP	0.72	0/887	1.06	4/1180 (0.3%)
15	AQ	0.85	0/990	1.31	9/1325 (0.7%)
16	AR	0.76	0/982	1.08	0/1306
17	AS	0.87	1/790 (0.1%)	1.28	9/1057 (0.9%)
18	AT	0.66	0/886	1.04	1/1189 (0.1%)
19	AU	0.57	0/756	0.93	0/1015
20	AV	0.54	0/857	1.05	2/1142 (0.2%)
21	AW	0.66	0/1467	1.11	7/1992 (0.4%)
22	AX	0.65	0/679	1.04	1/902 (0.1%)
23	AY	0.59	0/569	0.88	0/751
24	AZ	0.59	0/474	1.10	2/635 (0.3%)
25	Aa	0.84	1/594 (0.2%)	1.31	8/795 (1.0%)
26	Ab	0.72	0/459	1.16	3/621 (0.5%)
27	Ac	0.85	1/433 (0.2%)	1.36	5/576 (0.9%)
28	Ad	0.73	0/438	1.01	0/575
29	Ae	0.59	0/523	1.14	5/690 (0.7%)
30	Af	0.59	0/310	1.08	1/407 (0.2%)
31	AI	0.50	1/751 (0.1%)	0.82	4/1042 (0.4%)
32	AJ	0.52	0/1012	0.64	8/1373 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BA	0.92	26/36437 (0.1%)	1.10	139/56865 (0.2%)
35	BF	0.65	0/1935	1.00	4/2609 (0.2%)
36	BG	0.55	0/1636	0.92	4/2205 (0.2%)
37	BH	0.64	1/1733 (0.1%)	0.98	3/2318 (0.1%)
38	BI	0.63	0/1162	1.01	3/1564 (0.2%)
39	BJ	0.60	0/856	0.95	0/1154
40	BK	0.57	0/1276	0.90	3/1709 (0.2%)
41	BL	0.62	0/1136	1.01	3/1527 (0.2%)
42	BM	0.54	0/1029	0.83	0/1379
43	BN	0.48	0/807	0.89	1/1085 (0.1%)
44	BO	0.62	0/900	0.98	0/1213
45	BP	0.60	0/986	1.00	3/1320 (0.2%)
46	BQ	0.33	0/924	0.45	2/1238 (0.2%)
47	BR	0.55	0/501	0.97	1/664 (0.2%)
48	BS	0.62	0/745	0.95	0/992
49	BT	0.62	0/716	0.95	1/963 (0.1%)
50	BU	0.68	1/870 (0.1%)	0.99	2/1159 (0.2%)
51	BV	0.59	0/603	1.01	1/799 (0.1%)
52	BW	0.53	1/661 (0.2%)	1.34	5/890 (0.6%)
53	BX	0.65	0/765	1.00	2/1007 (0.2%)
54	BY	0.45	0/212	0.80	0/277
55	BC	0.36	0/1809	0.67	0/2819
56	BD	0.37	0/1784	0.68	0/2780
56	BE	0.35	0/1784	0.70	0/2780
57	BZ	0.37	0/4678	0.50	16/6310 (0.3%)
All	All	0.86	148/167791 (0.1%)	1.05	688/250219 (0.3%)

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	432
2	AB	0	17
3	AC	0	1
5	AE	0	1
6	AF	0	1
9	AK	0	1
12	AN	0	1
15	AQ	0	1
17	AS	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	Aa	0	1
26	Ab	0	1
31	AI	0	2
34	BA	0	170
37	BH	0	1
39	BJ	0	1
44	BO	0	1
47	BR	0	1
All	All	0	634

The worst 5 of 148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1060	U	O3'-P	-80.27	0.64	1.61
34	BA	1317	C	O3'-P	-70.10	0.77	1.61
1	AA	1203	G	O3'-P	-34.75	1.19	1.61
34	BA	1167	A	O3'-P	20.86	1.86	1.61
1	AA	2500	U	C4-O4	18.56	1.38	1.23

The worst 5 of 688 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1064	G	N1-C2-N2	-71.66	51.71	116.20
34	BA	1064	G	N3-C2-N2	57.63	160.24	119.90
34	BA	1317	C	P-O3'-C3'	-48.78	61.17	119.70
34	BA	1317	C	O3'-P-O5'	30.58	162.11	104.00
1	AA	1060	U	O3'-P-O5'	28.68	158.49	104.00

There are no chirality outliers.

5 of 634 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	14	A	Sidechain
1	AA	25	U	Sidechain
1	AA	3	U	Sidechain
1	AA	31	C	Sidechain
1	AA	9	U	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	220/228 (96%)	153 (70%)	39 (18%)	28 (13%)	0	4
4	AD	270/272 (99%)	125 (46%)	59 (22%)	86 (32%)	0	0
5	AE	204/206 (99%)	117 (57%)	31 (15%)	56 (28%)	0	0
6	AF	206/208 (99%)	109 (53%)	46 (22%)	51 (25%)	0	1
7	AG	180/182 (99%)	79 (44%)	47 (26%)	54 (30%)	0	0
8	AH	172/174 (99%)	80 (46%)	46 (27%)	46 (27%)	0	0
9	AK	137/139 (99%)	64 (47%)	28 (20%)	45 (33%)	0	0
10	AL	120/122 (98%)	59 (49%)	23 (19%)	38 (32%)	0	0
11	AM	143/145 (99%)	57 (40%)	36 (25%)	50 (35%)	0	0
12	AN	134/136 (98%)	49 (37%)	33 (25%)	52 (39%)	0	0
13	AO	115/117 (98%)	57 (50%)	39 (34%)	19 (16%)	0	3
14	AP	108/110 (98%)	48 (44%)	28 (26%)	32 (30%)	0	0
15	AQ	115/117 (98%)	52 (45%)	26 (23%)	37 (32%)	0	0
16	AR	115/117 (98%)	35 (30%)	50 (44%)	30 (26%)	0	1
17	AS	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	0
18	AT	108/110 (98%)	63 (58%)	24 (22%)	21 (19%)	0	2
19	AU	92/94 (98%)	57 (62%)	16 (17%)	19 (21%)	0	2
20	AV	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	0
21	AW	178/180 (99%)	96 (54%)	43 (24%)	39 (22%)	0	1
22	AX	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	5
23	AY	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	4
24	AZ	57/59 (97%)	34 (60%)	8 (14%)	15 (26%)	0	1
25	Aa	69/71 (97%)	23 (33%)	15 (22%)	31 (45%)	0	0
26	Ab	55/57 (96%)	14 (26%)	19 (34%)	22 (40%)	0	0
27	Ac	47/49 (96%)	14 (30%)	7 (15%)	26 (55%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Ad	47/49 (96%)	20 (43%)	12 (26%)	15 (32%)	0	0
29	Ae	62/64 (97%)	23 (37%)	17 (27%)	22 (36%)	0	0
30	Af	35/37 (95%)	20 (57%)	5 (14%)	10 (29%)	0	0
31	AI	151/153 (99%)	89 (59%)	33 (22%)	29 (19%)	0	2
32	AJ	132/134 (98%)	56 (42%)	44 (33%)	32 (24%)	0	1
35	BF	232/234 (99%)	114 (49%)	41 (18%)	77 (33%)	0	0
36	BG	204/206 (99%)	107 (52%)	46 (22%)	51 (25%)	0	1
37	BH	206/208 (99%)	95 (46%)	58 (28%)	53 (26%)	0	1
38	BI	148/150 (99%)	93 (63%)	38 (26%)	17 (12%)	0	5
39	BJ	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
40	BK	153/155 (99%)	73 (48%)	45 (29%)	35 (23%)	0	1
41	BL	136/138 (99%)	68 (50%)	35 (26%)	33 (24%)	0	1
42	BM	125/127 (98%)	62 (50%)	33 (26%)	30 (24%)	0	1
43	BN	96/98 (98%)	52 (54%)	20 (21%)	24 (25%)	0	1
44	BO	117/119 (98%)	65 (56%)	29 (25%)	23 (20%)	0	2
45	BP	122/124 (98%)	50 (41%)	30 (25%)	42 (34%)	0	0
46	BQ	112/114 (98%)	64 (57%)	28 (25%)	20 (18%)	0	2
47	BR	58/60 (97%)	24 (41%)	16 (28%)	18 (31%)	0	0
48	BS	86/88 (98%)	36 (42%)	35 (41%)	15 (17%)	0	2
49	BT	81/83 (98%)	42 (52%)	24 (30%)	15 (18%)	0	2
50	BU	102/104 (98%)	62 (61%)	23 (22%)	17 (17%)	0	3
51	BV	71/73 (97%)	26 (37%)	26 (37%)	19 (27%)	0	0
52	BW	78/80 (98%)	30 (38%)	25 (32%)	23 (30%)	0	0
53	BX	97/99 (98%)	38 (39%)	32 (33%)	27 (28%)	0	0
54	BY	22/24 (92%)	9 (41%)	6 (27%)	7 (32%)	0	0
57	BZ	603/605 (100%)	280 (46%)	200 (33%)	123 (20%)	0	2
All	All	6575/6683 (98%)	3224 (49%)	1675 (26%)	1676 (26%)	0	1

5 of 1676 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	35	ALA
3	AC	39	GLU

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Mol	Chain	Res	Type
3	AC	54	SER
3	AC	61	THR
3	AC	72	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	180/180 (100%)	151 (84%)	29 (16%)	2	11
4	AD	215/215 (100%)	153 (71%)	62 (29%)	0	2
5	AE	166/166 (100%)	102 (61%)	64 (39%)	0	0
6	AF	164/164 (100%)	105 (64%)	59 (36%)	0	1
7	AG	156/156 (100%)	112 (72%)	44 (28%)	0	2
8	AH	143/143 (100%)	108 (76%)	35 (24%)	0	3
9	AK	118/118 (100%)	79 (67%)	39 (33%)	0	2
10	AL	100/100 (100%)	69 (69%)	31 (31%)	0	2
11	AM	111/111 (100%)	71 (64%)	40 (36%)	0	1
12	AN	106/106 (100%)	65 (61%)	41 (39%)	0	0
13	AO	100/100 (100%)	71 (71%)	29 (29%)	0	2
14	AP	87/87 (100%)	63 (72%)	24 (28%)	0	3
15	AQ	105/105 (100%)	68 (65%)	37 (35%)	0	1
16	AR	93/93 (100%)	64 (69%)	29 (31%)	0	2
17	AS	82/82 (100%)	57 (70%)	25 (30%)	0	2
18	AT	90/90 (100%)	64 (71%)	26 (29%)	0	2
19	AU	76/76 (100%)	57 (75%)	19 (25%)	0	3
20	AV	91/91 (100%)	72 (79%)	19 (21%)	1	5
21	AW	159/159 (100%)	120 (76%)	39 (24%)	0	3
22	AX	67/67 (100%)	51 (76%)	16 (24%)	0	4
23	AY	62/62 (100%)	44 (71%)	18 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AZ	51/51 (100%)	36 (71%)	15 (29%)	0	2
25	Aa	63/63 (100%)	45 (71%)	18 (29%)	0	2
26	Ab	50/50 (100%)	31 (62%)	19 (38%)	0	0
27	Ac	48/48 (100%)	32 (67%)	16 (33%)	0	2
28	Ad	42/42 (100%)	29 (69%)	13 (31%)	0	2
29	Ae	54/54 (100%)	44 (82%)	10 (18%)	1	8
30	Af	34/34 (100%)	29 (85%)	5 (15%)	2	12
32	AJ	101/101 (100%)	71 (70%)	30 (30%)	0	2
35	BF	202/202 (100%)	138 (68%)	64 (32%)	0	2
36	BG	160/160 (100%)	123 (77%)	37 (23%)	0	4
37	BH	180/180 (100%)	131 (73%)	49 (27%)	0	3
38	BI	115/115 (100%)	78 (68%)	37 (32%)	0	2
39	BJ	90/90 (100%)	61 (68%)	29 (32%)	0	2
40	BK	126/126 (100%)	93 (74%)	33 (26%)	0	3
41	BL	119/119 (100%)	86 (72%)	33 (28%)	0	3
42	BM	98/98 (100%)	73 (74%)	25 (26%)	0	3
43	BN	88/88 (100%)	67 (76%)	21 (24%)	0	4
44	BO	90/90 (100%)	73 (81%)	17 (19%)	1	7
45	BP	104/104 (100%)	81 (78%)	23 (22%)	1	5
46	BQ	92/92 (100%)	67 (73%)	25 (27%)	0	3
47	BR	49/49 (100%)	36 (74%)	13 (26%)	0	3
48	BS	79/79 (100%)	64 (81%)	15 (19%)	1	7
49	BT	72/72 (100%)	49 (68%)	23 (32%)	0	2
50	BU	96/96 (100%)	67 (70%)	29 (30%)	0	2
51	BV	64/64 (100%)	48 (75%)	16 (25%)	0	3
52	BW	71/71 (100%)	52 (73%)	19 (27%)	0	3
53	BX	76/76 (100%)	59 (78%)	17 (22%)	1	5
54	BY	19/19 (100%)	17 (90%)	2 (10%)	5	20
57	BZ	486/514 (95%)	338 (70%)	148 (30%)	0	2
All	All	5390/5418 (100%)	3864 (72%)	1526 (28%)	1	2

5 of 1526 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	BG	48	TYR
42	BM	63	ILE
37	BH	8	VAL
36	BG	46	GLU
39	BJ	5	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
38	BI	56	GLN
43	BN	56	HIS
39	BJ	13	ASN
40	BK	106	GLN
44	BO	38	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2881/2889 (99%)	1265 (43%)	253 (8%)
2	AB	122/123 (99%)	46 (37%)	3 (2%)
34	BA	1514/1515 (99%)	484 (31%)	140 (9%)
55	BC	75/76 (98%)	26 (34%)	0
56	BD	74/75 (98%)	31 (41%)	2 (2%)
56	BE	74/75 (98%)	23 (31%)	1 (1%)
All	All	4740/4753 (99%)	1875 (39%)	399 (8%)

5 of 1875 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	13	A
1	AA	14	A
1	AA	15	G
1	AA	20	C
1	AA	26	G

5 of 399 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	2610	C
34	BA	327	A
1	AA	2690	C

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Mol	Chain	Res	Type
34	BA	47	C
34	BA	495	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	8AN	AA	3002	-	19,24,25	1.10	1 (5%)	13,35,38	1.70	4 (30%)
59	8AN	AA	3003	56	19,24,25	1.09	1 (5%)	13,35,38	1.70	4 (30%)
60	GCP	BZ	701	-	27,34,34	1.84	7 (25%)	34,54,54	1.99	8 (23%)
58	NMY	BA	1601	-	45,45,45	0.51	0	63,67,67	1.06	6 (9%)
58	NMY	AA	3001	-	45,45,45	0.51	0	63,67,67	1.19	7 (11%)

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	8AN	AA	3002	-	-	2/3/25/26	0/3/3/3
59	8AN	AA	3003	56	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	GCP	BZ	701	-	-	5/15/38/38	0/3/3/3
58	NMY	BA	1601	-	-	5/18/94/94	0/4/4/4
58	NMY	AA	3001	-	-	4/18/94/94	1/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BZ	701	GCP	PG-O1G	5.39	1.61	1.50
60	BZ	701	GCP	C5-C6	4.19	1.48	1.41
60	BZ	701	GCP	PG-O2G	-2.85	1.48	1.54
60	BZ	701	GCP	PG-O3G	2.85	1.61	1.54
60	BZ	701	GCP	PB-O3A	2.72	1.61	1.58

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BZ	701	GCP	C2-N3-C4	5.02	121.09	115.36
60	BZ	701	GCP	C2-N1-C6	3.99	122.27	115.93
60	BZ	701	GCP	C5-C6-N1	-3.93	118.06	123.43
60	BZ	701	GCP	PB-O3A-PA	-3.80	120.51	132.56
60	BZ	701	GCP	C4-C5-C6	-3.75	117.22	120.80

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	3001	NMY	C19-C18-O18-C15
58	BA	1601	NMY	O5-C5-C6-N6
58	BA	1601	NMY	C14-C13-O11-C11
59	AA	3003	8AN	C4'-C5'-O5'-P
59	AA	3003	8AN	O4'-C4'-C5'-O5'

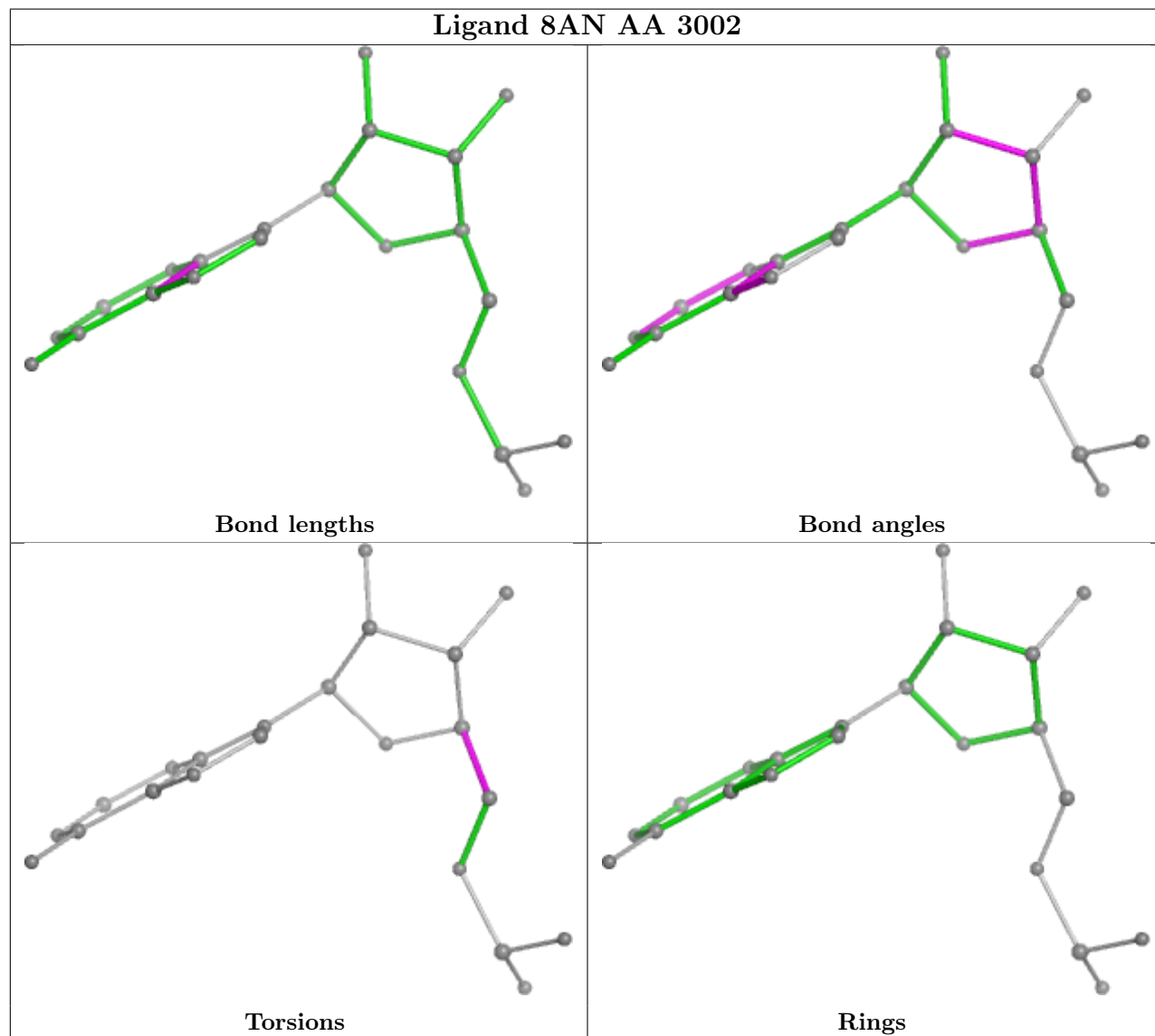
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	3001	NMY	C10-C11-C12-C7-C8-C9

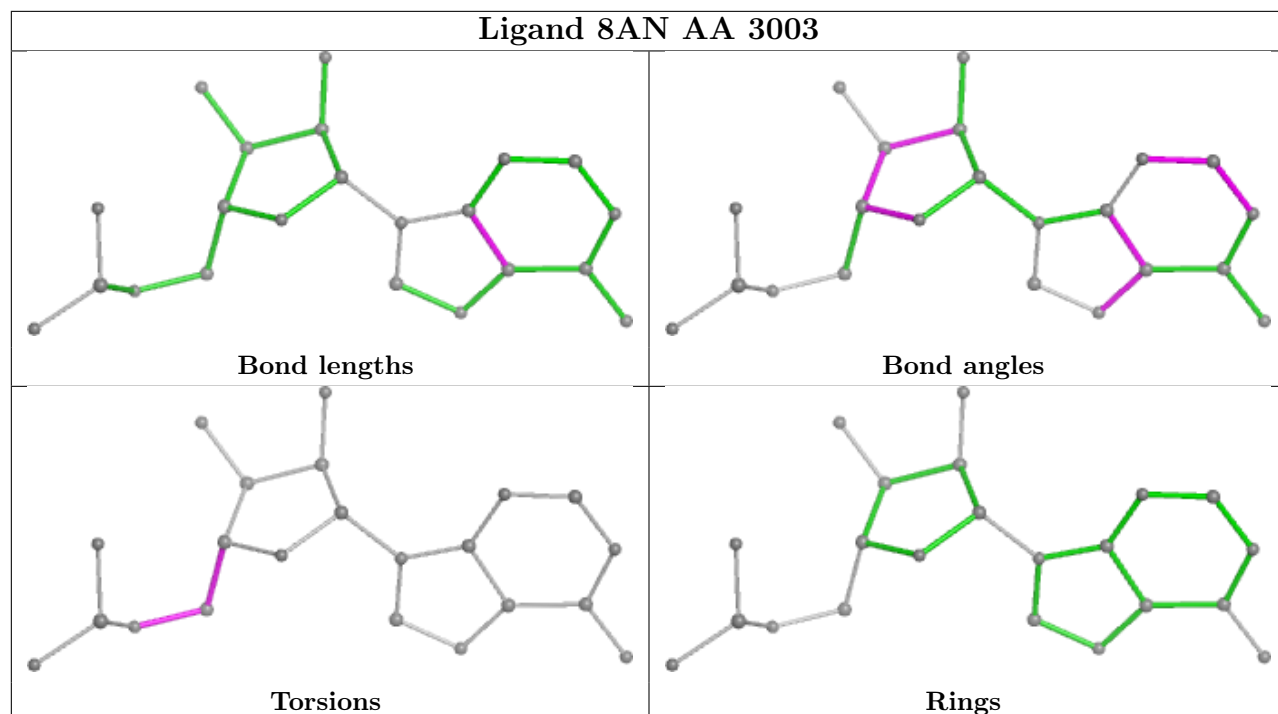
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

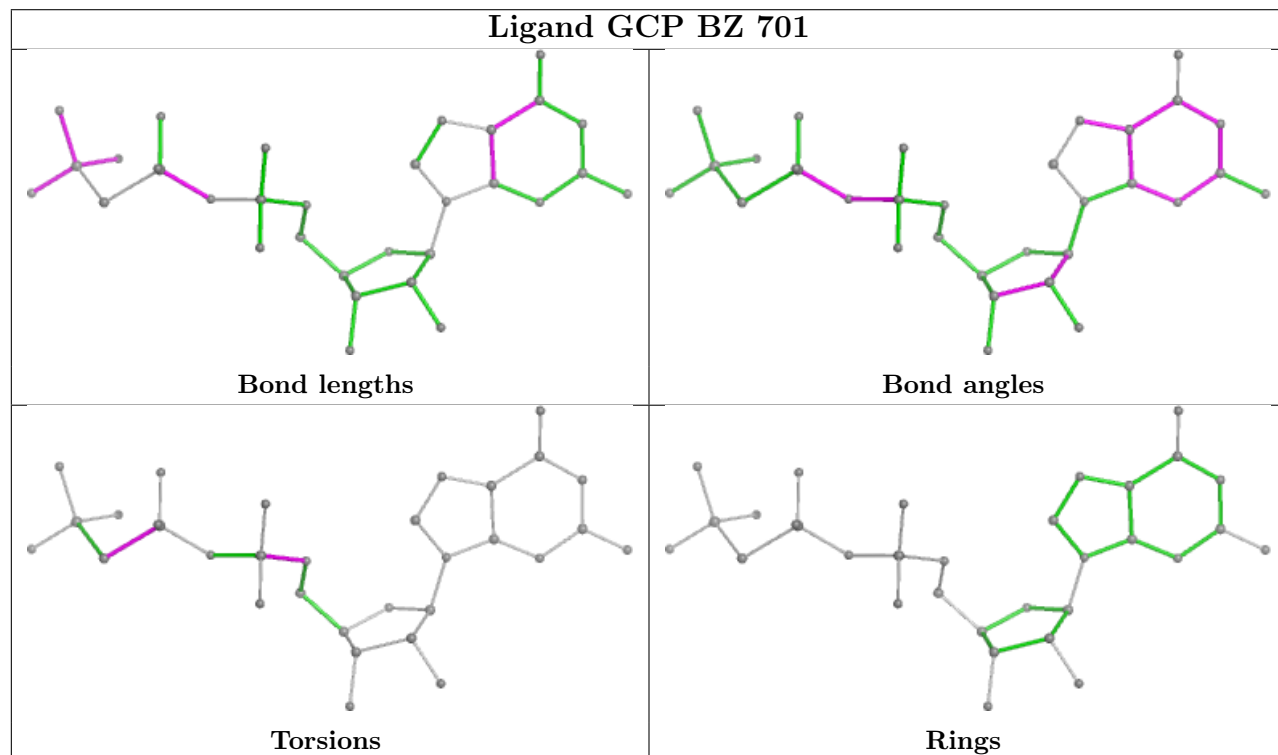
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



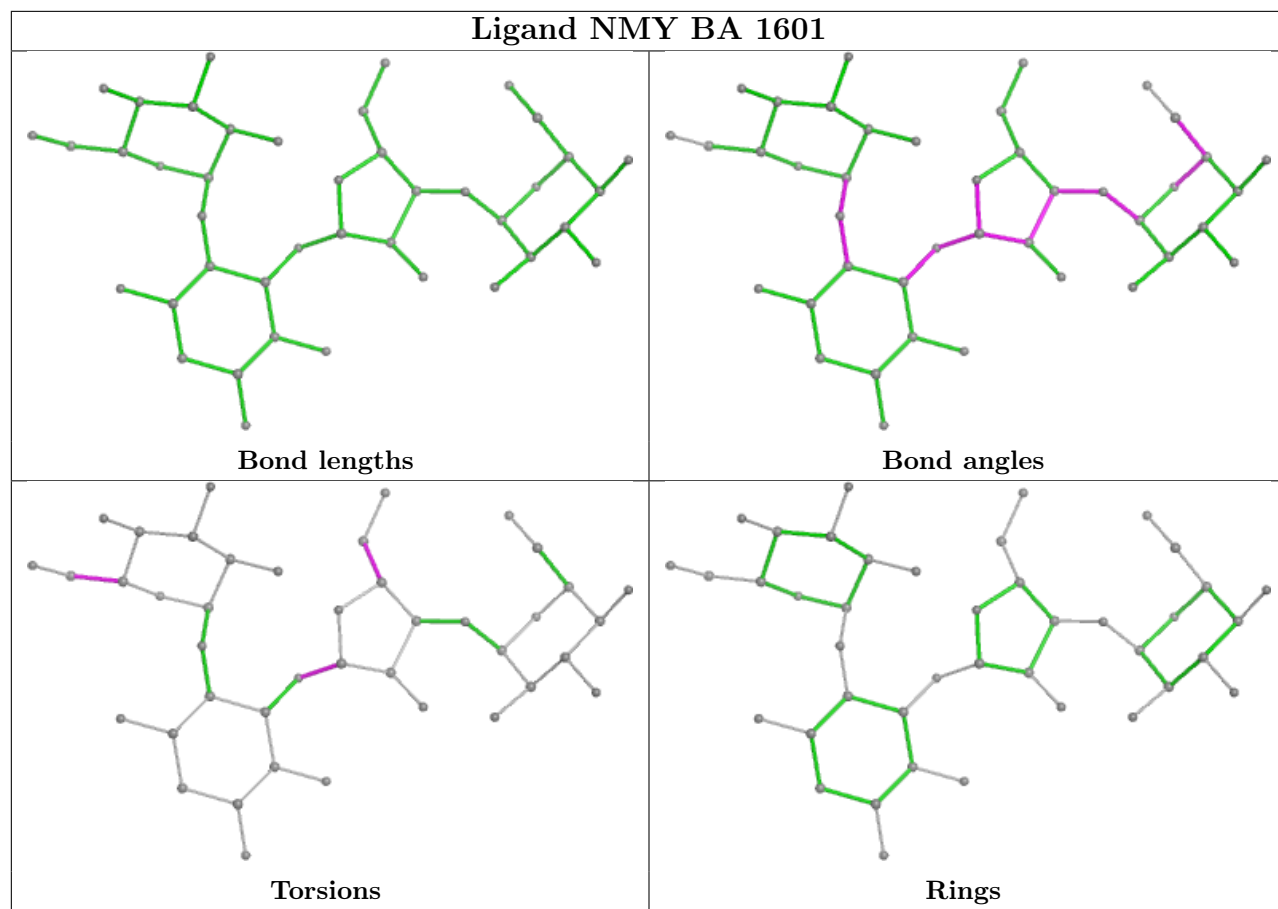
Ligand 8AN AA 3003



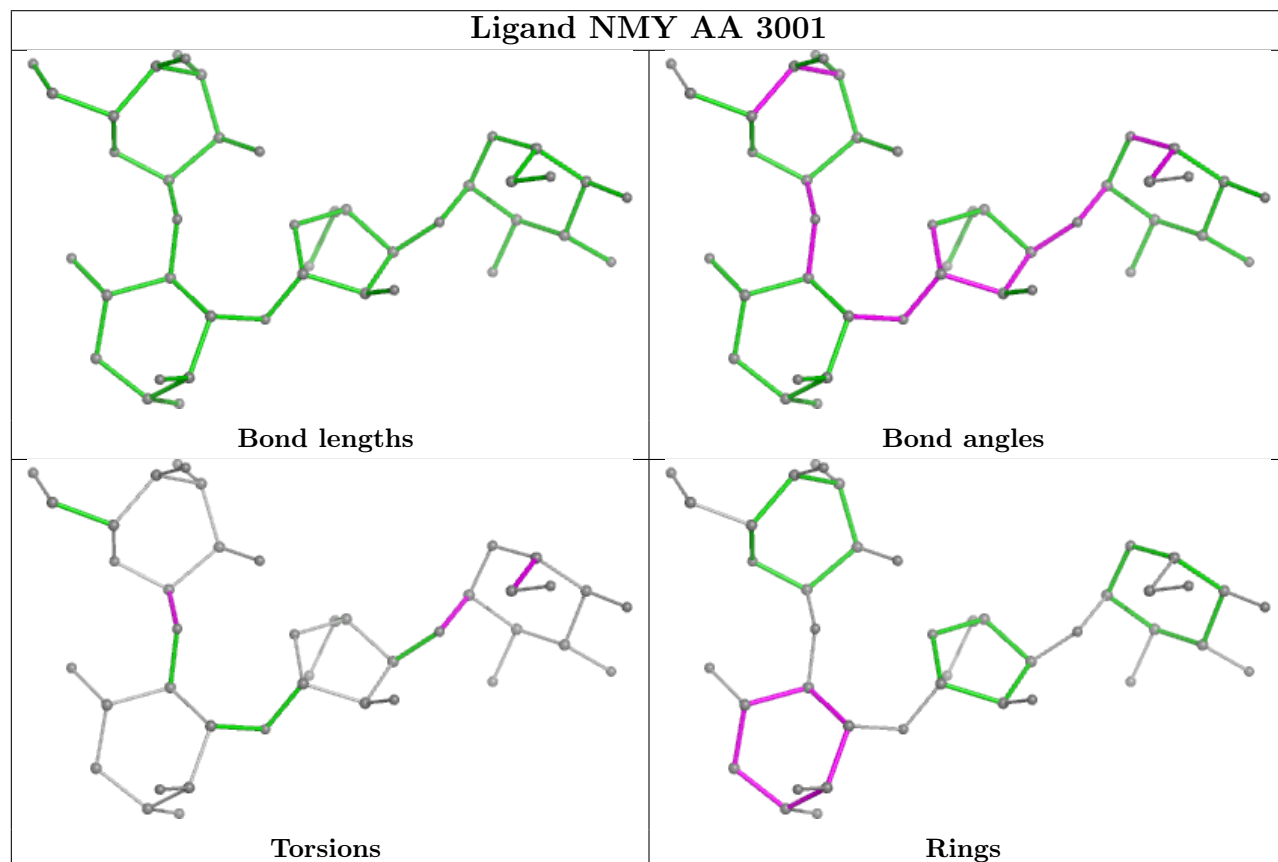
Ligand GCP BZ 701



Ligand NMY BA 1601



Ligand NMY AA 3001



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	10
3	AC	3
34	BA	3
33	Ag	2
31	AI	1

The worst 5 of 19 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ag	30:UNK	C	123:UNK	N	31.39
1	AA	164:U	O3'	171:G	P	7.68
1	AA	2893:G	O3'	2894:G	P	5.34
1	AA	2107:C	O3'	2108:C	P	4.97
1	AC	180:PHE	C	181:PRO	N	4.62

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6397. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.