



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 01:56 pm BST

PDB ID : 5A9Z
EMDB ID : EMD-6396
Title : Complex of Thermophilus thermophilus ribosome 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 : 4.70 Å(reported)

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

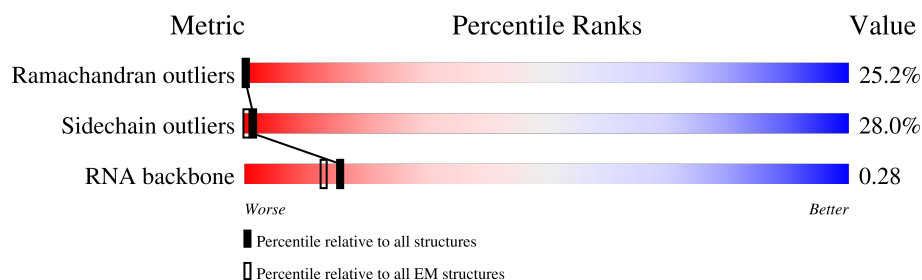
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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.





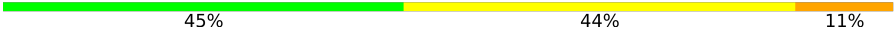








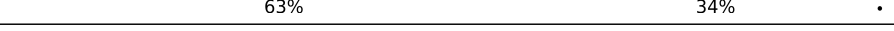







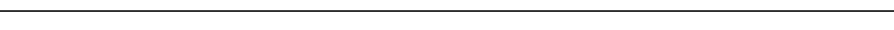

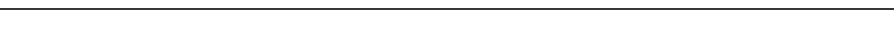
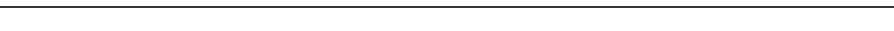


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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% 43% 10% .
2	AB	123	50% 41% 7% .
3	AC	228	75% 23% .
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	AI	153	80% 20% .










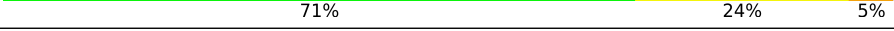



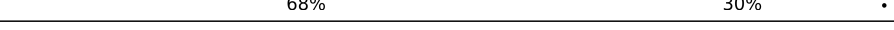







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	AJ	134	
11	AK	139	
12	AL	122	
13	AM	145	
14	AN	136	
15	AO	117	
16	AP	110	
17	AQ	117	
18	AR	117	
19	AS	101	
20	AT	110	
21	AU	94	
22	AV	110	
23	AW	180	
24	AX	85	
25	AY	67	
26	AZ	59	
27	Aa	71	
28	Ab	57	
29	Ac	49	
30	Ad	49	
31	Ae	64	
32	Af	37	
33	Ag	128	
34	BA	1515	

Continued on next page...

Continued from previous page...

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	CA	593	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 150547 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 L10.

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

- Molecule 10 is a protein called 50S ribosomal protein L11.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

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

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L31.

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

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

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

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- 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		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		

- 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		

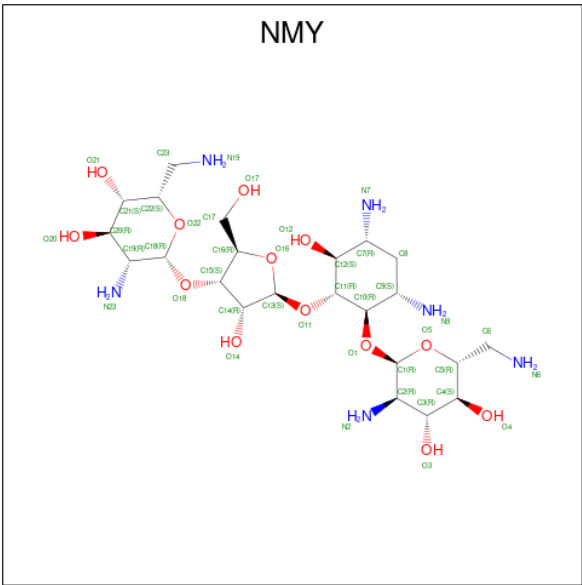
- Molecule 54 is a protein called 30S ribosomal protein Thx.

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

- Molecule 55 is a protein called BipA.

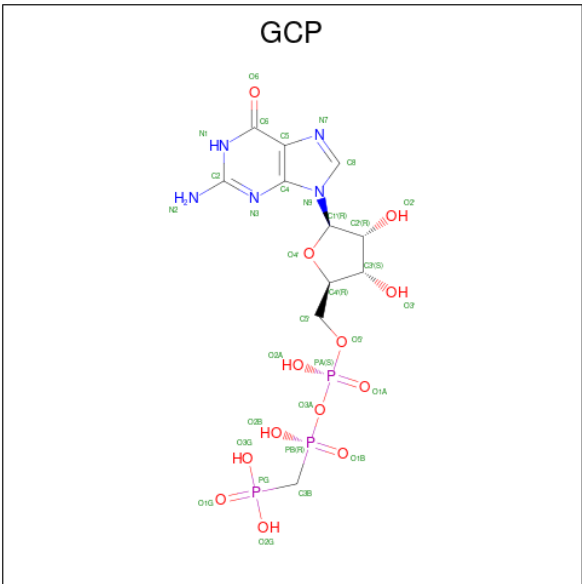
Mol	Chain	Residues	Atoms					AltConf	Trace
55	CA	593	Total	C	N	O	S	0	0
			4532	2856	791	868	17		

- Molecule 56 is NEOMYCIN (three-letter code: NMY) (formula: C₂₃H₄₆N₆O₁₃).



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

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



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

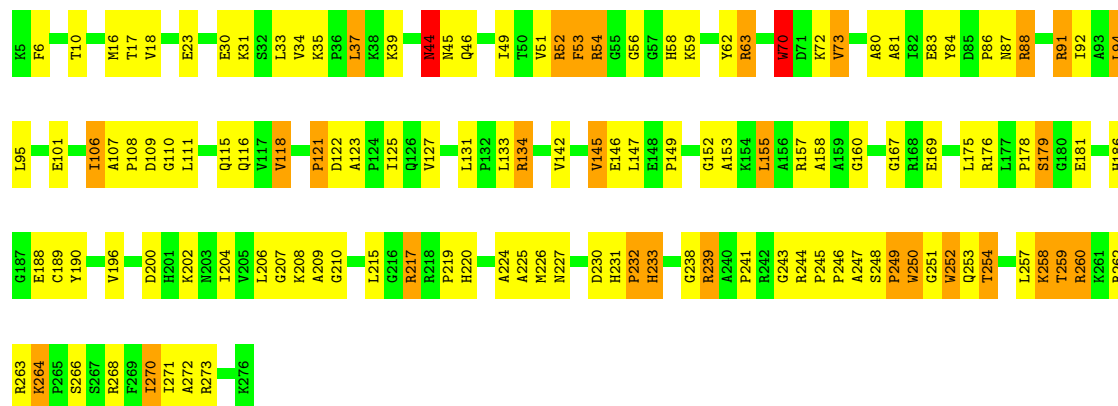
C2044	U1963	C1881	C1782	G1623	G1552	C1474	A1379	A1284	A1204	U1113	A1045	G976	G892
U2047	G1964	A1884	A1783	G1624	A1553	G1477	A1384	G1285	U1205	C1116	A1046	G971	A896
G2048	C1965	A1966	A1784	C1625	A1554	A1478	A1385	A1286	G1206	G1127	G1047	G972	A897
G2049	C1966	A1785	A1786	G1626	G1555	G1479	G1388	A1287	C1207	A1126	A1048	G973	C897
C2050	C1967	A1701	G1702	G1628	A1558	G1480	G1389	U1288	G1208	A1127	C1049	G974	C898
A2051	A1969	C1790	G1703	A1631	G1559	U1482	A1392	C1289	A1210	A1128	A1050	G975	A899
G2052	A1970	G1904	G1704	A1634	G1561	G1485	A1393	G1296	U1211	A1129	G1053	G976	A900
C2055	A1971	G1906	G1705	A1635	G1564	G1489	A1395	C1297	G1212	A1131	C1052	G977	A901
G2056	C1793	U1706	G1707	G1635	C1565	U1490	U1396	U1300	A1213	A1132	G1056	C903	C903
A2060	A1978	G1708	G1708	C1640	C1566	A1491	U1397	A1301	A1220	A1133	A1057	G978	C904
G2061	C1979	U1709	U1709	A1641	A1567	G1492	C1398	A1302	C1221	G1134	G1058	G979	U905
A2062	G1980	C1800	C1710	G1644	G1568	A1494	C1403	G1303	C1222	C1135	G1059	C982	G906
C2063	A1981	G1801	C1711	G1645	A1569	A1495	U1405	C1304	C1225	C1140	U1060	A983	C908
C2064	C1982	A1802	G1712	G1646	A1570	A1496	U1406	G1310	G1228	U1141	G1062	A984	A909
G2068	C1983	A1803	U1716	G1647	A1571	A1497	U1407	G1312	G1299	U1142	G1063	C985	A910
G2069	G1984	G1917	G1718	C1648	A1572	C1498	C1407	U1313	C1230	A1143	C1064	G987	A911
G2073	G1985	U1805	G1718	G1649	C1573	C1499	G1416	A1321	G1237	G1154	U1065	A988	U913
C2074	G1989	U1808	G1725	G1650	C1574	A1507	G1417	A1322	G1238	G1155	U1066	G989	C914
U2075	A1809	U1727	G1726	G1651	U1576	A1508	G1418	U1323	G1239	A1156	A1067	A990	C915
G2076	A1810	G1728	G1728	A1652	C1577	A1509	U1419	U1324	U1240	A1157	A1068	C995	A917
A2077	A1815	U1730	A1579	A1654	A1579	A1510	U1420	G1324	A1241	A1157	A1069	A996	A918
G2080	G1816	G1731	A1580	A1655	A1580	A1511	G1424	U1326	A1242	G1160	C1072	A997	C919
U2089	G1817	A1732	C1656	C1657	A1581	G1512	G1425	C1327	G1244	G1161	A1073	C1000	G921
G2093	A1819	G1733	C1658	C1658	C1582	U1514	G1426	U1328	G1244	G1162	G1074	U922	U922
C2095	C1930	G1735	A1659	C1659	A1585	U1515	A1427	U1329	C1330	C1005	C1075	C1005	C923
G2096	U1931	C1741	C1660	C1660	A1586	U1516	C1428	C1330	A1247	G1169	C1076	C1008	C924
U2097	G1822	G1742	G1661	G1661	A1587	U1517	G1429	U1335	G1248	G1170	A1077	A1009	U930
A2014	G1826	G1743	A1664	A1664	U1590	U1518	U1438	U1340	U1249	G1171	A1078	G931	G931
G2015	C1827	G1746	C1665	C1665	G1591	G1520	A1439	U1341	C1251	A1174	C1079	G1011	G932
U2016	G1828	G1747	G1667	G1667	A1597	G1521	G1440	A1342	G1252	U1175	C1080	U1012	A933
G2017	A1829	A1755	A1668	A1668	C1597	G1522	A1444	A1254	U1256	G1176	U1083	C1013	G939
C2018	C1830	G1756	A1669	A1669	C1600	U1523	C1445	U1255	G1257	C1178	A1085	C1018	G940
A2019	G1758	G1758	C1670	C1670	G1601	G1524	A1445	G1345	G1258	C1179	A1086	U1019	A941
C2020	A1759	A1759	U1673	U1673	U1602	G1525	C1450	G1346	C1257	C1180	G1087	A1020	G942
G2021	G1834	G1762	C1674	C1674	A1603	U1526	C1451	G1347	C1258	C1181	A1088	A1021	U943
C2022	G1839	G1763	A1675	A1675	C1604	A1528	A1453	A1348	G1259	G1182	G1089	G1022	G944
G2023	G1840	G1764	A1676	A1676	C1605	A1529	U1454	C1350	G1260	G1183	U1090	U1023	A945
C2026	C1843	G1765	A1677	A1677	G1606	U1530	G1455	C1261	C1261	G1184	G1092	G1024	G946
G2027	U1766	U1766	G1678	G1678	C1607	C1531	G1456	A1262	U1263	C1185	C1092	G1025	C946
A2030	A1847	G1767	G1681	G1681	A1608	C1532	G1456	U1357	G1264	G1186	G1093	U1026	G950
G2031	A1848	U1768	G1682	G1682	A1609	C1533	G1459	G1358	A1265	A1189	G1099	A1027	C955
A2032	C1852	C1683	C1683	C1683	A1610	G1534	A1460	A1359	G1266	G1190	C1100	G1031	G956
G2033	A1853	A1773	C1684	C1684	C1612	G1534	G1461	C1363	U1267	G1191	U1101	A1032	A957
U2034	G1953	C1774	C1685	C1685	G1613	G1539	C1462	G1364	A1268	A1194	C1102	U1033	U958
G2035	A1857	U1775	C1686	C1686	A1614	U1539	C1463	A1365	A1269	G1195	A1103	U1033	A959
G2036	G1857	G1776	C1687	C1687	C1615	G1540	C1467	A1366	C1270	C1038	A1104	C1038	A960
G2037	U1956	U1777	U1688	U1688	A1616	U1541	C1468	A1367	G1271	U1189	C1104	G1039	C961
C2040	G1878	U1778	C1691	C1691	C1617	G1542	A1468	A1368	U1272	G1200	U1108	G1041	G962
U2041	A1879	A1780	U1692	U1692	A1618	G1544	A1471	U1372	U1273	C1201	C1109	G1042	C965
G2042	C1879	U1781	U1693	U1693	G1619	C1544	A1472	A1274	A1275	C1202	G1110	G1043	U969
C2043	C1880	C1781	C1693	C1693	G1619	U1544	G1473	A1378		G1203	G1112	G1044	





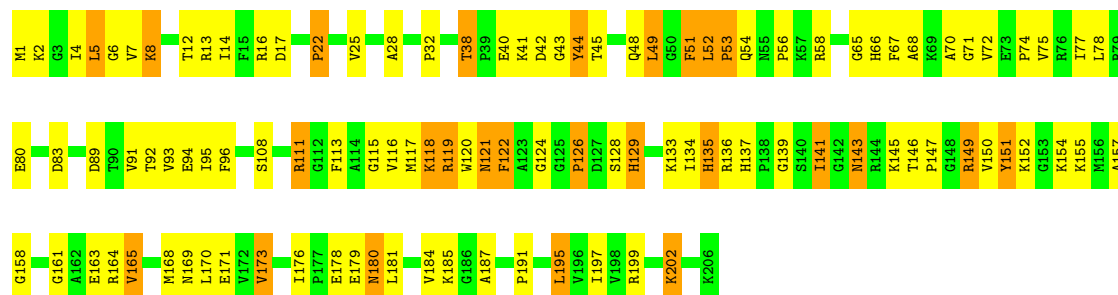
• Molecule 4: 50S ribosomal protein L2

Chain AD: 53% 36% 11% •



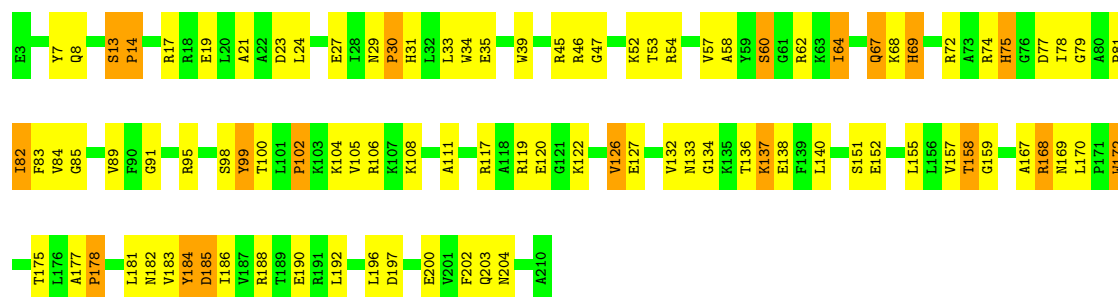
• Molecule 5: 50S ribosomal protein L3

Chain AE: 48% 39% 13%



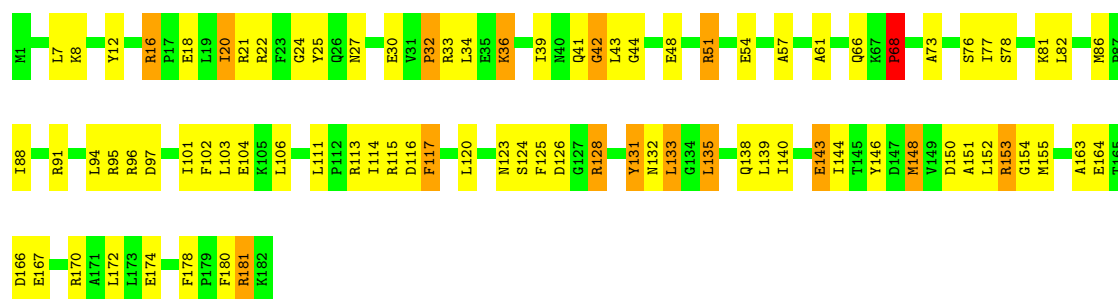
• Molecule 6: 50S ribosomal protein L4

Chain AF: 54% 37% 9%



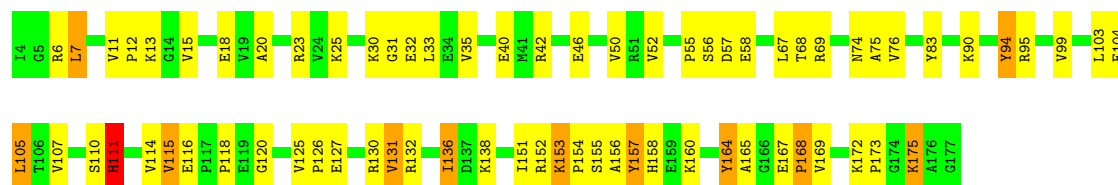
• Molecule 7: 50S ribosomal protein L5

Chain AG: 53% 38% 8% •



• Molecule 8: 50S ribosomal protein L6

Chain AH: 59% 34% 6% .



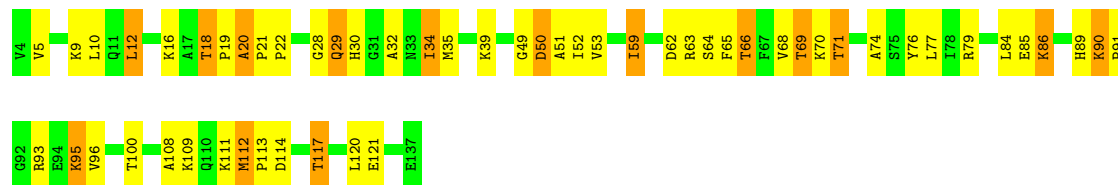
• Molecule 9: 50S ribosomal protein L10

Chain AI: 80% 20% .



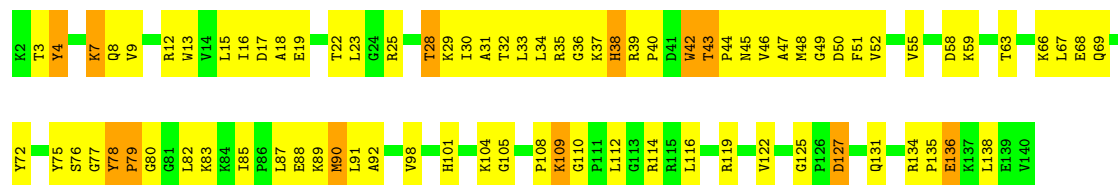
• Molecule 10: 50S ribosomal protein L11

Chain AJ: 59% 30% 11%



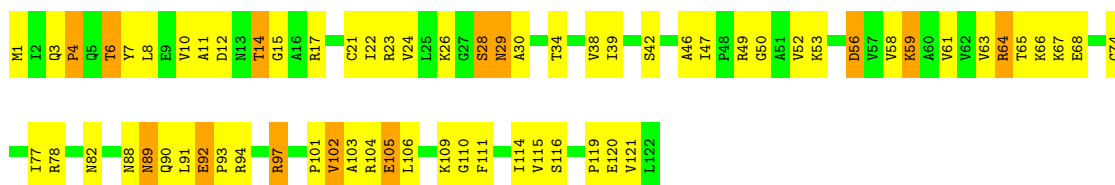
• Molecule 11: 50S ribosomal protein L13

Chain AK: 41% 50% 9%



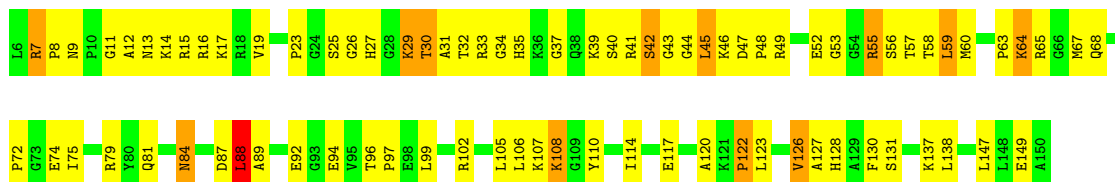
• Molecule 12: 50S ribosomal protein L14

Chain AL: 45% 44% 11%



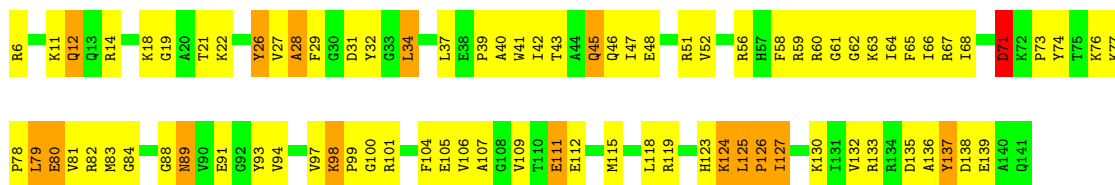
• Molecule 13: 50S ribosomal protein L15

Chain AM: 44% 47% 8% .



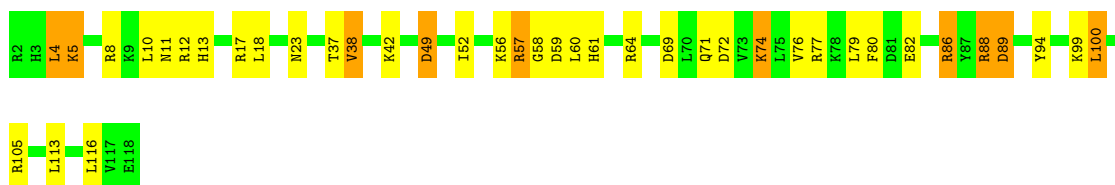
• Molecule 14: 50S ribosomal protein L16

Chain AN: 38% 50% 11% .



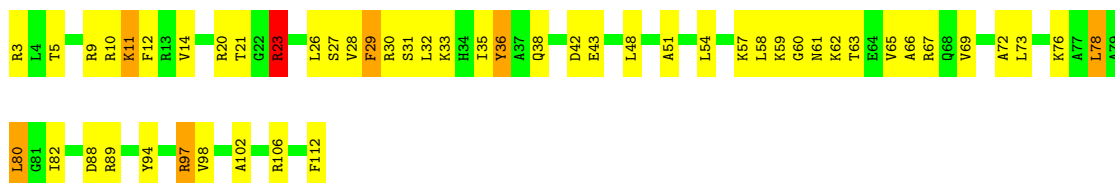
• Molecule 15: 50S ribosomal protein L17

Chain AO: 66% 26% 9% .



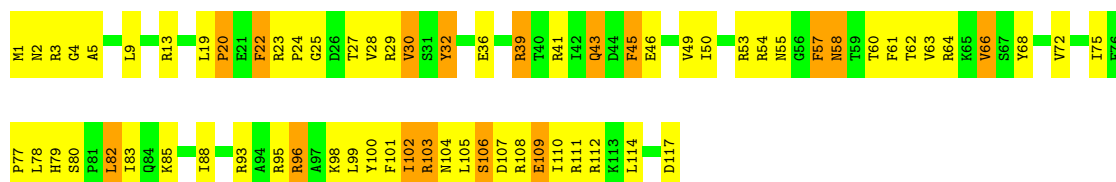
• Molecule 16: 50S ribosomal protein L18

Chain AP: 54% 40% 5% .



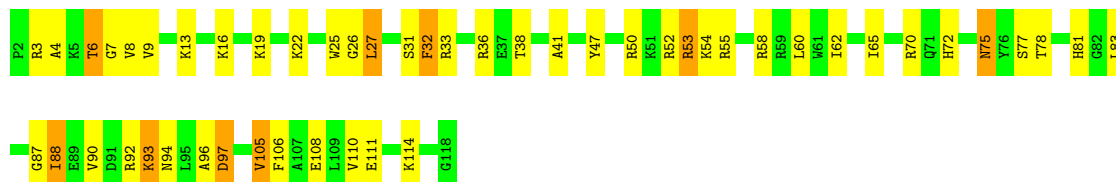
• Molecule 17: 50S ribosomal protein L19

Chain AQ: 42% 44% 14% .



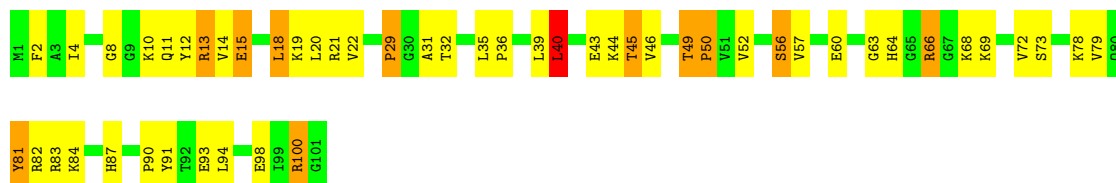
• Molecule 18: 50S ribosomal protein L20

Chain AR: 57% 35% 8%



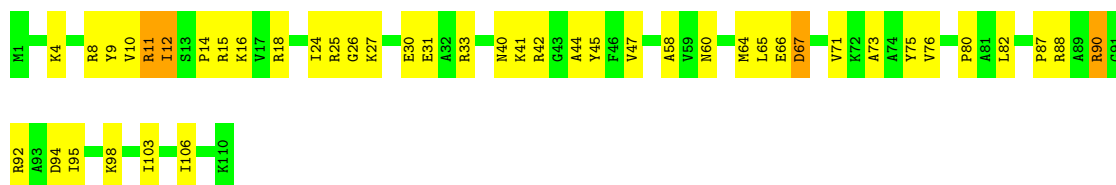
• Molecule 19: 50S ribosomal protein L21

Chain AS: 50% 39% 11%



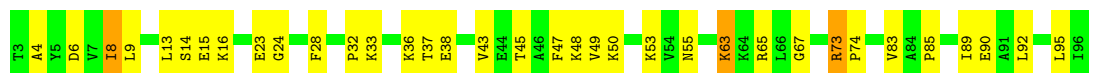
• Molecule 20: 50S ribosomal protein L22

Chain AT: 60% 36% 4%



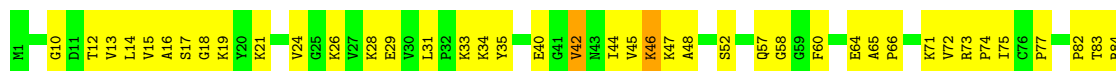
• Molecule 21: 50S ribosomal protein L23

Chain AU: 63% 34% 3%



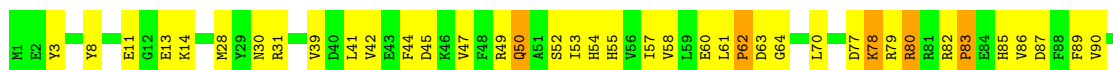
• Molecule 22: 50S ribosomal protein L24

Chain AV: 53% 45% 2%





- Molecule 23: 50S ribosomal protein L25



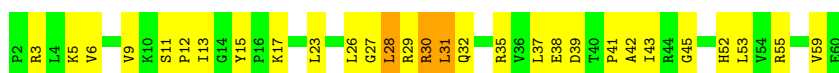
- Molecule 24: 50S ribosomal protein L27



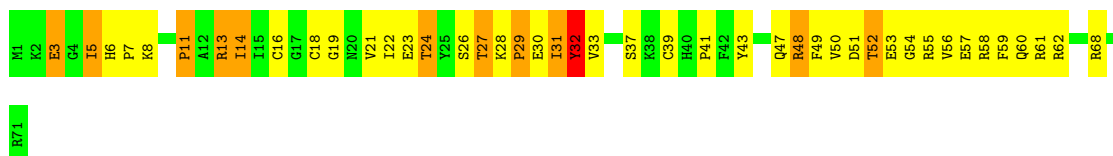
- Molecule 25: 50S ribosomal protein L29



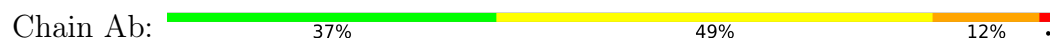
- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L31



- Molecule 28: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L33

Chain Ac:  27% 51% 22%



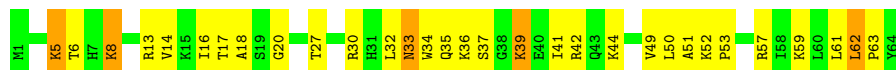
- Molecule 30: 50S ribosomal protein L34

Chain Ad:  53% 37% 10%



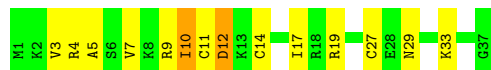
- Molecule 31: 50S ribosomal protein L35

Chain Ae:  52% 41% 8%



- Molecule 32: 50S ribosomal protein L36

Chain Af:  62% 32% 5%



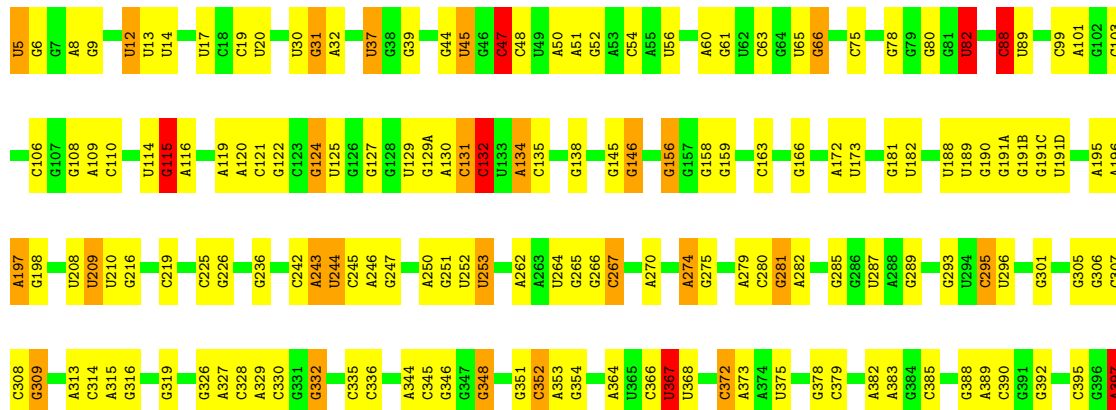
- Molecule 33: Unknown peptide

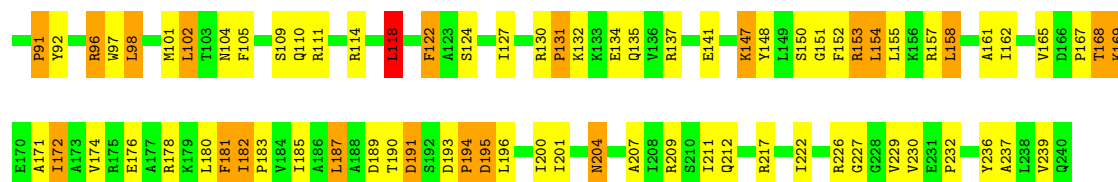
Chain Ag:  100%

There are no outlier residues recorded for this chain.

- Molecule 34: 16S ribosomal RNA

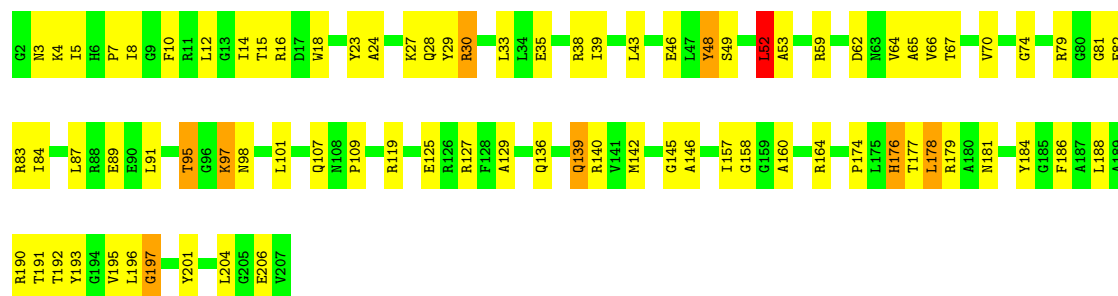
Chain BA:  56% 37% 6%





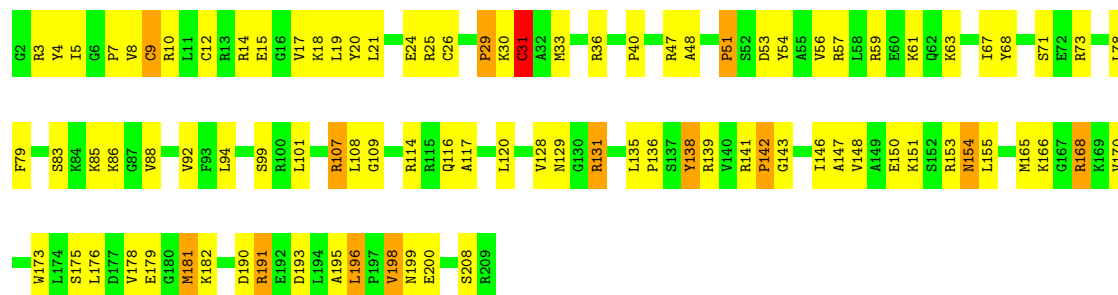
- Molecule 36: 30S ribosomal protein S3

Chain BG: 60% 35%



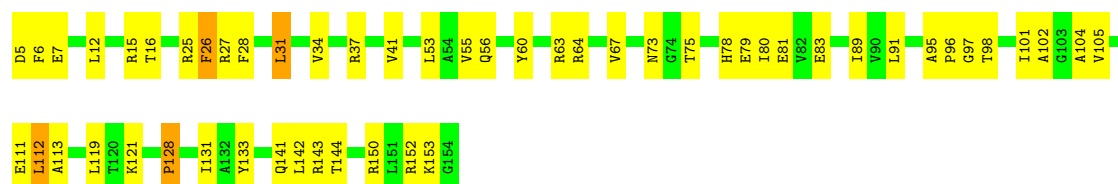
- Molecule 37: 30S ribosomal protein S4

Chain BH: 55% 38% 6%



- Molecule 38: 30S ribosomal protein S5

Chain BI: 65% 33%



- Molecule 39: 30S ribosomal protein S6

Chain BJ: 55% 38% 7%





- Molecule 40: 30S ribosomal protein S7

Chain BK: 63% 29% 8%



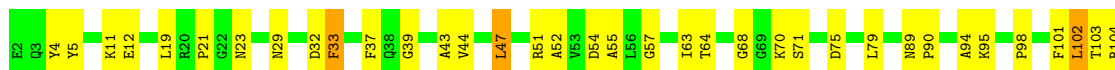
- Molecule 41: 30S ribosomal protein S8

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

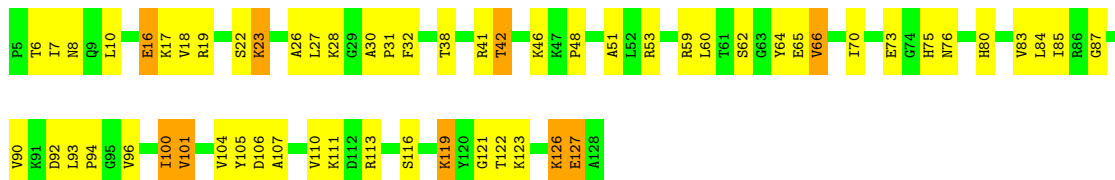
Chain BO: 71% 24% 5%





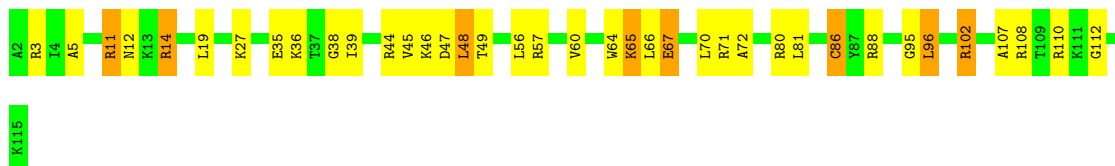
- Molecule 45: 30S ribosomal protein S12

Chain BP: 52% 40% 7%



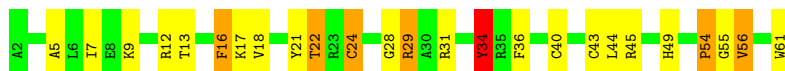
- Molecule 46: 30S ribosomal protein S13

Chain BQ: 67% 26% 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%



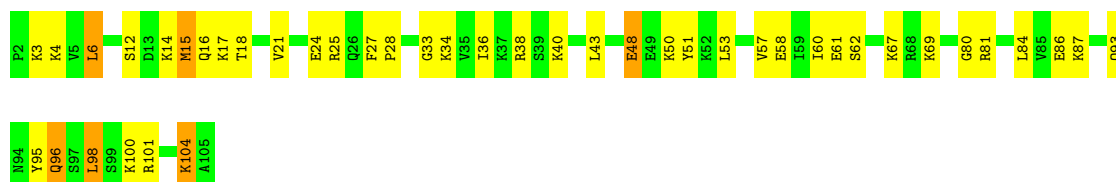
- Molecule 49: 30S ribosomal protein S16

Chain BT: 58% 36% 6%



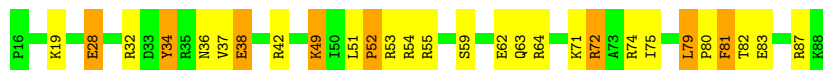
- Molecule 50: 30S ribosomal protein S17

Chain BU: 59% 36% 6%



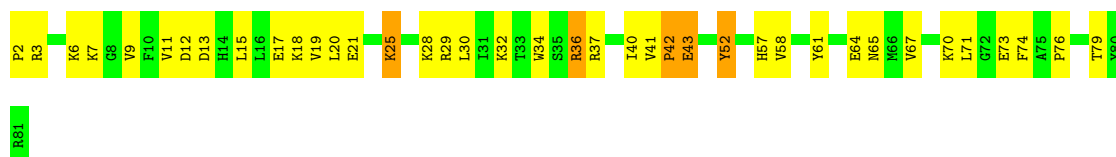
- Molecule 51: 30S ribosomal protein S18

Chain BV: 62% 27% 11%



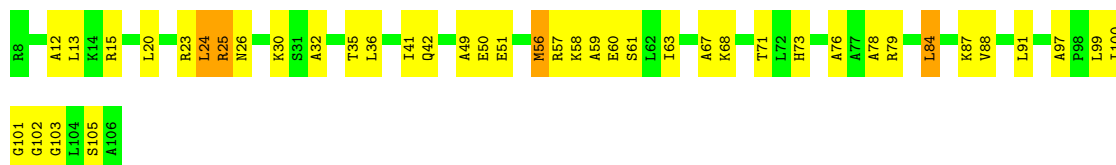
- Molecule 52: 30S ribosomal protein S19

Chain BW: 51% 42% 6%



- Molecule 53: 30S ribosomal protein S20

Chain BX: 58% 38% .



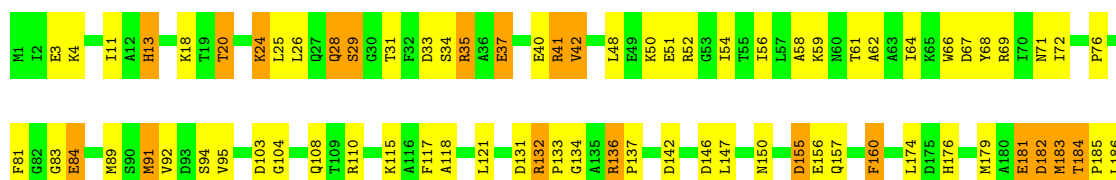
- Molecule 54: 30S ribosomal protein Thx

Chain BY: 71% 21% 8%



- Molecule 55: BipA

Chain CA: 63% 31% 5%



I489	S490	N491	G492	Q493	D506	R507	G508	K509	L512	A516	E517	V518	I526	R527	S528	V535	N536	G537	L538	T539	K542	A554	P559	D574	T583	R588	K589	L592	T593	R597	R598	R599	R602	A603	F604	K605													
T404	V407	E408	E409	Q410	H411	Q417	A418	L419	G424	K427	N428	N429	N430	K434	G435	R436	V437	V442	I443	P444	S445	L448	I449	G450	S460	G461	T462	G463	L464	L465	Y466	S467	T468	F469	S470	H471	Y472	D473	D474	V475	R476	P477	V480	G481	Q482	R483	Q484	N485	G486
C289	D290	T291	V294	E295	A296	L297	E304	P305	T306	V307	S308	S316	G320	K321	K324	F325	V326	R329	L332	D333	L339	N342	R346	R357	V358	S359	G360	R361	L364	L380	A381	V382	S383	R384	P385	K386	V387	R390	E391	I392	D393	G394	R395	E398					
V194	P195	A196	P197	D198	W199	L200	L201	D202	G203	M207	Q208	I209	L212	S216	Y217	V218	G222	I223	G224	R225	K230	N234	D241	S242	E243	G244	K245	K250	V251	G252	K253	L258	G259	L260	E261	R262	T265	D266	L267	A268	E269	D272	I273	N283	I284				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61165	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)	2700	Depositor
Magnification	53000	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: 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	106/69677 (0.2%)	1.08	349/108754 (0.3%)
2	AB	0.83	4/2954 (0.1%)	0.99	7/4606 (0.2%)
3	AC	0.54	0/1775	0.86	0/2393
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	AI	0.50	1/751 (0.1%)	0.82	4/1042 (0.4%)
10	AJ	0.52	0/1012	0.64	8/1373 (0.6%)
11	AK	0.78	1/1140 (0.1%)	1.16	8/1537 (0.5%)
12	AL	0.92	1/942 (0.1%)	1.31	10/1268 (0.8%)
13	AM	0.71	0/1123	1.12	5/1493 (0.3%)
14	AN	0.72	0/1100	1.19	8/1470 (0.5%)
15	AO	0.70	0/974	1.06	2/1302 (0.2%)
16	AP	0.72	0/887	1.06	4/1180 (0.3%)
17	AQ	0.85	0/990	1.31	9/1325 (0.7%)
18	AR	0.76	0/982	1.08	0/1306
19	AS	0.87	1/790 (0.1%)	1.28	9/1057 (0.9%)
20	AT	0.66	0/886	1.04	1/1189 (0.1%)
21	AU	0.57	0/756	0.93	0/1015
22	AV	0.54	0/857	1.04	2/1142 (0.2%)
23	AW	0.66	0/1467	1.11	7/1992 (0.4%)
24	AX	0.65	0/679	1.04	1/902 (0.1%)
25	AY	0.59	0/569	0.88	0/751
26	AZ	0.59	0/474	1.09	2/635 (0.3%)
27	Aa	0.84	1/594 (0.2%)	1.31	8/795 (1.0%)
28	Ab	0.72	0/459	1.16	3/621 (0.5%)
29	Ac	0.85	1/433 (0.2%)	1.36	5/576 (0.9%)
30	Ad	0.73	0/438	1.01	0/575
31	Ae	0.60	0/523	1.14	5/690 (0.7%)
32	Af	0.59	0/310	1.08	1/407 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BA	0.92	25/36437 (0.1%)	1.09	139/56865 (0.2%)
35	BF	0.64	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	0.63	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	2/963 (0.2%)
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	CA	0.36	0/4598	0.49	15/6200 (0.2%)
All	All	0.87	146/162336 (0.1%)	1.06	689/241736 (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	430
2	AB	0	17
3	AC	0	1
5	AE	0	1
6	AF	0	1
9	AI	0	2
11	AK	0	1
14	AN	0	1
17	AQ	0	1
19	AS	0	1
27	Aa	0	1
28	Ab	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
34	BA	0	170
37	BH	0	1
39	BJ	0	1
44	BO	0	1
47	BR	0	1
55	CA	0	1
All	All	0	633

The worst 5 of 146 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	-70.09	0.77	1.61
1	AA	1203	G	O3'-P	-34.69	1.19	1.61
34	BA	1167	A	O3'-P	20.86	1.86	1.61
1	AA	2500	U	C4-O4	18.53	1.38	1.23

The worst 5 of 689 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	57.69	160.28	119.90
34	BA	1317	C	P-O3'-C3'	-48.76	61.18	119.70
34	BA	1317	C	O3'-P-O5'	30.59	162.12	104.00
1	AA	1060	U	O3'-P-O5'	28.66	158.46	104.00

There are no chirality outliers.

5 of 633 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

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	226/228 (99%)	155 (69%)	41 (18%)	30 (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	AI	151/153 (99%)	89 (59%)	33 (22%)	29 (19%)	0	2
10	AJ	132/134 (98%)	56 (42%)	44 (33%)	32 (24%)	0	1
11	AK	137/139 (99%)	64 (47%)	28 (20%)	45 (33%)	0	0
12	AL	120/122 (98%)	59 (49%)	23 (19%)	38 (32%)	0	0
13	AM	143/145 (99%)	57 (40%)	36 (25%)	50 (35%)	0	0
14	AN	134/136 (98%)	49 (37%)	33 (25%)	52 (39%)	0	0
15	AO	115/117 (98%)	57 (50%)	39 (34%)	19 (16%)	0	3
16	AP	108/110 (98%)	48 (44%)	29 (27%)	31 (29%)	0	0
17	AQ	115/117 (98%)	52 (45%)	26 (23%)	37 (32%)	0	0
18	AR	115/117 (98%)	35 (30%)	50 (44%)	30 (26%)	0	1
19	AS	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	0
20	AT	108/110 (98%)	63 (58%)	24 (22%)	21 (19%)	0	2
21	AU	92/94 (98%)	57 (62%)	16 (17%)	19 (21%)	0	2
22	AV	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	0
23	AW	178/180 (99%)	96 (54%)	43 (24%)	39 (22%)	0	1
24	AX	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	5
25	AY	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	4
26	AZ	57/59 (97%)	34 (60%)	8 (14%)	15 (26%)	0	1
27	Aa	69/71 (97%)	23 (33%)	16 (23%)	30 (44%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Ab	55/57 (96%)	14 (26%)	19 (34%)	22 (40%)	0	0
29	Ac	47/49 (96%)	14 (30%)	7 (15%)	26 (55%)	0	0
30	Ad	47/49 (96%)	20 (43%)	12 (26%)	15 (32%)	0	0
31	Ae	62/64 (97%)	23 (37%)	18 (29%)	21 (34%)	0	0
32	Af	35/37 (95%)	20 (57%)	5 (14%)	10 (29%)	0	0
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%)	57 (28%)	54 (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%)	29 (26%)	19 (17%)	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
55	CA	587/593 (99%)	313 (53%)	170 (29%)	104 (18%)	0	2
All	All	6565/6671 (98%)	3259 (50%)	1650 (25%)	1656 (25%)	0	1

5 of 1656 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	AC	54	SER
3	AC	61	THR
3	AC	66	HIS

5.3.2 Protein sidechains [i](#)

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
10	AJ	101/101 (100%)	71 (70%)	30 (30%)	0	2
11	AK	118/118 (100%)	79 (67%)	39 (33%)	0	2
12	AL	100/100 (100%)	69 (69%)	31 (31%)	0	2
13	AM	111/111 (100%)	71 (64%)	40 (36%)	0	1
14	AN	106/106 (100%)	65 (61%)	41 (39%)	0	0
15	AO	100/100 (100%)	71 (71%)	29 (29%)	0	2
16	AP	87/87 (100%)	63 (72%)	24 (28%)	0	3
17	AQ	105/105 (100%)	68 (65%)	37 (35%)	0	1
18	AR	93/93 (100%)	64 (69%)	29 (31%)	0	2
19	AS	82/82 (100%)	57 (70%)	25 (30%)	0	2
20	AT	90/90 (100%)	64 (71%)	26 (29%)	0	2
21	AU	76/76 (100%)	57 (75%)	19 (25%)	0	3
22	AV	91/91 (100%)	72 (79%)	19 (21%)	1	6
23	AW	159/159 (100%)	120 (76%)	39 (24%)	0	3
24	AX	67/67 (100%)	51 (76%)	16 (24%)	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AY	62/62 (100%)	44 (71%)	18 (29%)	0	2
26	AZ	51/51 (100%)	36 (71%)	15 (29%)	0	2
27	Aa	63/63 (100%)	45 (71%)	18 (29%)	0	2
28	Ab	50/50 (100%)	31 (62%)	19 (38%)	0	0
29	Ac	48/48 (100%)	33 (69%)	15 (31%)	0	2
30	Ad	42/42 (100%)	29 (69%)	13 (31%)	0	2
31	Ae	54/54 (100%)	44 (82%)	10 (18%)	1	8
32	Af	34/34 (100%)	29 (85%)	5 (15%)	2	13
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	8
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
55	CA	479/507 (94%)	349 (73%)	130 (27%)	0	3
All	All	5383/5411 (100%)	3876 (72%)	1507 (28%)	1	3

5 of 1507 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	BG	52	LEU
42	BM	64	THR
37	BH	9	CYS
36	BG	48	TYR
39	BJ	6	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
38	BI	72	GLN
43	BN	68	HIS
39	BJ	18	GLN
40	BK	110	GLN
44	BO	117	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2880/2889 (99%)	1261 (43%)	253 (8%)
2	AB	122/123 (99%)	46 (37%)	3 (2%)
34	BA	1514/1515 (99%)	484 (31%)	140 (9%)
All	All	4516/4527 (99%)	1791 (39%)	396 (8%)

5 of 1791 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 396 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	2610	C
34	BA	327	A
1	AA	2690	C
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](#)

3 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$
57	GCP	CA	701	-	27,34,34	1.53	6 (22%)	34,54,54	1.98	8 (23%)
56	NMY	BA	1601	-	45,45,45	0.51	0	63,67,67	1.07	6 (9%)
56	NMY	AA	3001	-	45,45,45	0.52	0	63,67,67	1.19	6 (9%)

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
57	GCP	CA	701	-	-	6/15/38/38	0/3/3/3
56	NMY	BA	1601	-	-	5/18/94/94	0/4/4/4
56	NMY	AA	3001	-	-	4/18/94/94	1/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CA	701	GCP	C5-C6	4.22	1.48	1.41
57	CA	701	GCP	PG-O2G	2.85	1.61	1.54
57	CA	701	GCP	PG-O3G	2.84	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	CA	701	GCP	PB-O3A	2.75	1.61	1.58
57	CA	701	GCP	C5-C4	2.50	1.47	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CA	701	GCP	C2-N3-C4	4.97	121.03	115.36
57	CA	701	GCP	C2-N1-C6	4.00	122.29	115.93
57	CA	701	GCP	C5-C6-N1	-3.95	118.03	123.43
57	CA	701	GCP	PB-O3A-PA	-3.80	120.51	132.56
57	CA	701	GCP	C4-C5-C6	-3.74	117.22	120.80

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	AA	3001	NMY	C19-C18-O18-C15
56	BA	1601	NMY	O5-C5-C6-N6
56	BA	1601	NMY	C14-C13-O11-C11
57	CA	701	GCP	PG-C3B-PB-O1B
57	CA	701	GCP	PG-C3B-PB-O2B

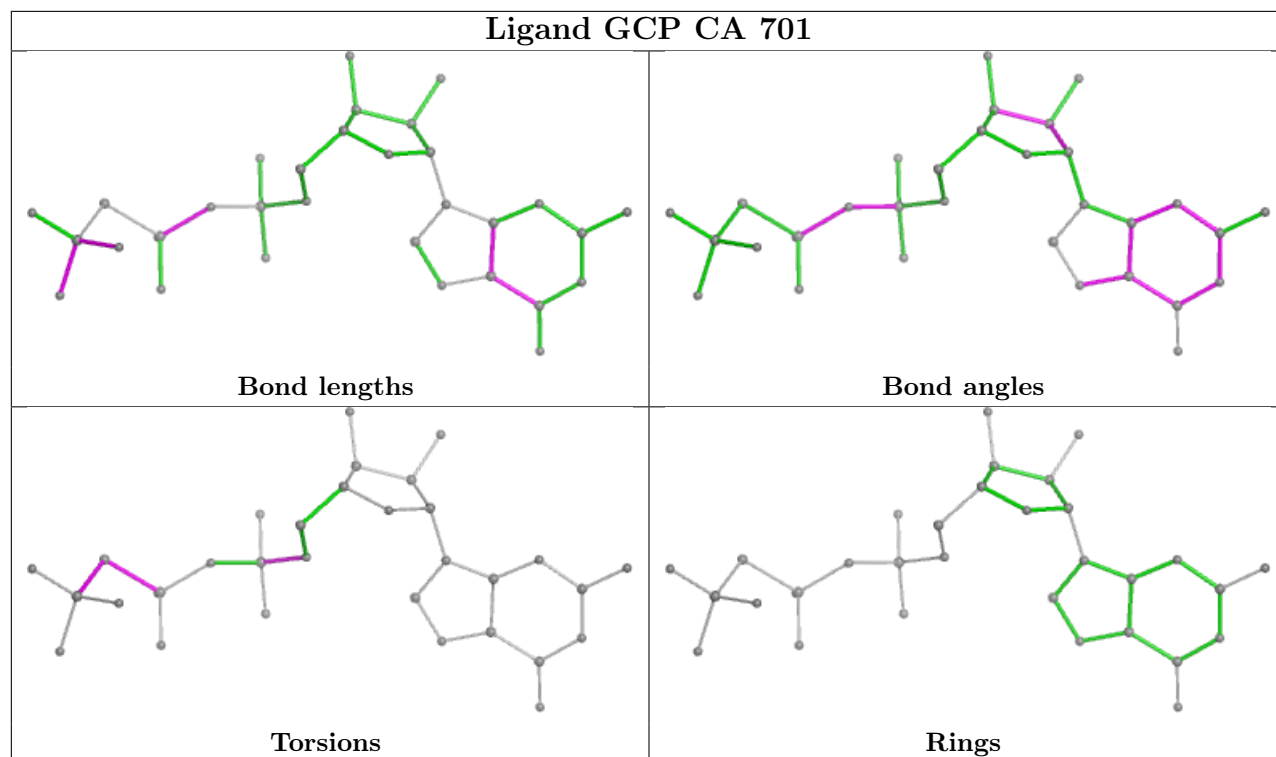
All (1) ring outliers are listed below:

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

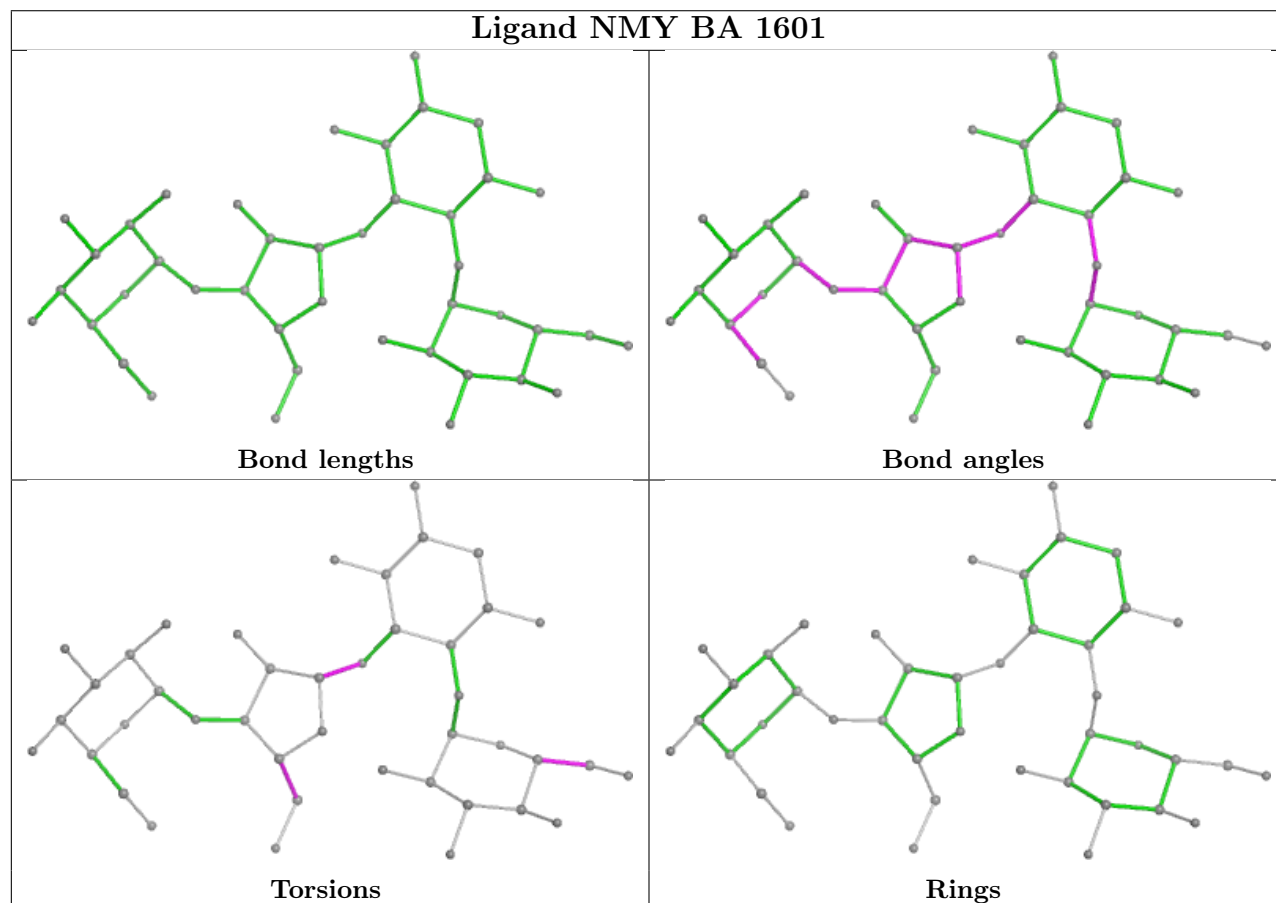
No monomer is involved in short contacts.

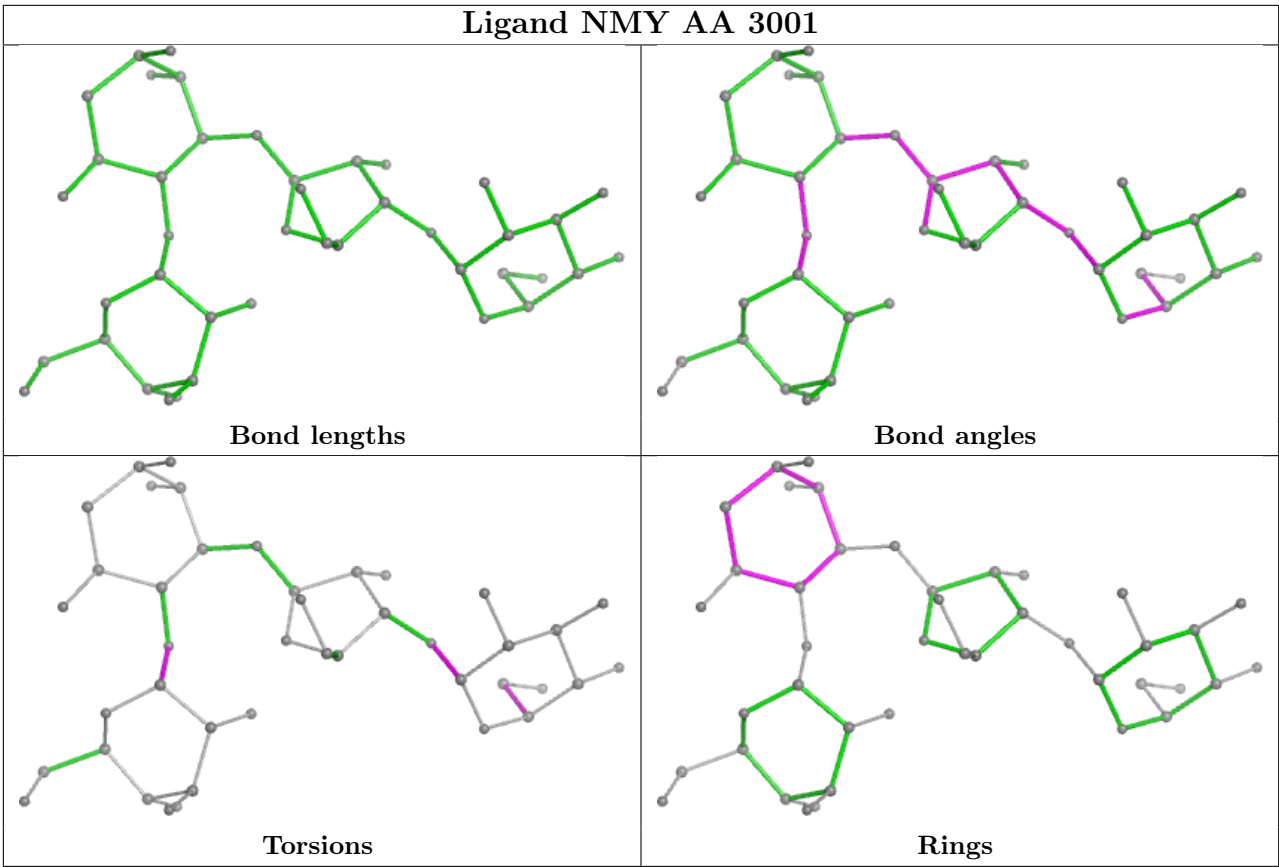
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GCP CA 701



Ligand NMY BA 1601





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	11
33	Ag	3
34	BA	3
55	CA	2
9	AI	1

The worst 5 of 20 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	CA	542:LYS	C	552:ASP	N	16.28
1	AA	164:U	O3'	171:G	P	7.69

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	2893:G	O3'	2894:G	P	5.34
1	CA	277:THR	C	281:GLU	N	5.08

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6396. 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.