



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:04 am GMT

PDB ID : 4V4I
Title : Crystal Structure of a 70S Ribosome-tRNA Complex Reveals Functional Interactions and Rearrangements.
Authors : Korostelev, A.; Trakhanov, S.; Laurberg, M.; Noller, H.F.
Deposited on : 2007-02-15
Resolution : 3.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

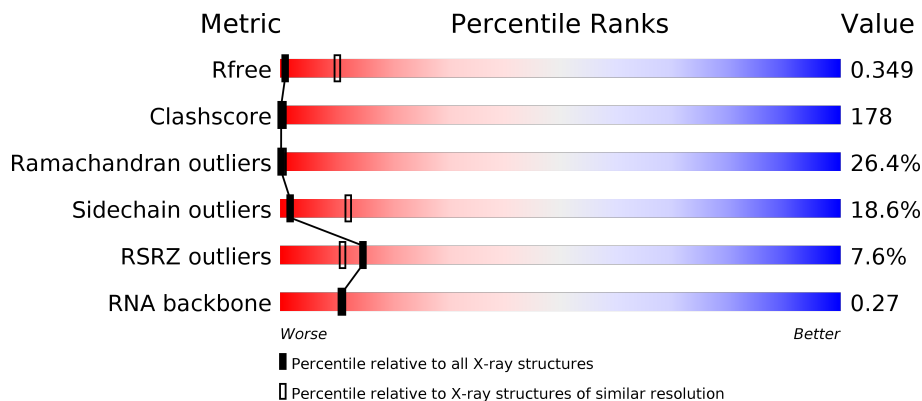
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1264 (3.94-3.50)
Clashscore	112137	1408 (3.94-3.50)
Ramachandran outliers	110173	1353 (3.94-3.50)
Sidechain outliers	110143	1350 (3.94-3.50)
RSRZ outliers	101464	1293 (3.94-3.50)
RNA backbone	2435	1012 (4.52-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	w	2889	<div> <div>5%</div> <div>57%</div> <div>39%</div> <div>.</div> </div>
2	x	121	<div> <div>3%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
3	A	229	<div> <div>7%</div> <div>6%</div> <div>34%</div> <div>13%</div> <div>.</div> <div>45%</div> </div>
4	B	276	<div> <div>10%</div> <div>5%</div> <div>55%</div> <div>34%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	206	
6	D	205	
7	E	182	
8	F	180	
9	G	148	
10	H	163	
11	I	122	
12	J	150	
13	K	141	
14	L	118	
15	M	112	
16	N	146	
17	O	118	
18	P	101	
19	Q	113	
20	R	96	
21	S	110	
22	T	206	
23	U	85	
24	V	98	
25	W	72	
26	X	60	
27	Y	60	
28	Z	49	
29	a	65	

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Mol	Chain	Length	Quality of chain
30	b	37	
31	y	1522	
32	z	76	
33	0	76	
34	1	10	
35	c	256	
36	d	239	
37	e	209	
38	f	162	
39	g	101	
40	h	156	
41	i	138	
42	j	128	
43	k	105	
44	l	129	
45	m	132	
46	n	126	
47	o	61	
48	p	89	
49	q	88	
50	r	105	
51	s	88	
52	t	93	
53	u	106	
54	v	27	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 146532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	w	2889	Total	C	N	O	P	0	0	0
			62213	27690	11624	20011	2888			

- Molecule 2 is a RNA chain called 5S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	x	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	127	Total	C	N	O	S	0	0	0
			996	627	184	184	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	201	Total	C	N	O	S	0	0	0
			1541	974	295	267	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	194	Total	C	N	O	S	0	0	0
			1517	969	283	263	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	180	Total	C	N	O	S	0	0	0
			1468	938	267	259	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	173	Total	C	N	O	S	0	0	0
			1319	839	245	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	148	Total	C	N	O	S	0	0	0
			1156	737	204	214	1			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	138	Total	C	N	O	S	0	0	0
			1103	712	206	182	3			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	137	Total	C	N	O	S	0	0	0
			1089	698	207	177	7			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	106	Total	C	N	O	S	0	0	0
			846	534	168	144				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	109	Total	C	N	O	S	0	0	0
			868	547	170	150	1			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	103	Total	C	N	O	S	0	0	0
			793	510	151	126	6			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	185	Total	C	N	O	S	0	0	0
			1475	941	262	269	3			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	88	Total	C	N	O		0	0	0
			694	435	141	118				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	62	Total	C	N	O	S	0	0	0
			520	325	102	91	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	56	Total	C	N	O	S	0	0	0
			436	275	84	72	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	a	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	b	35	Total	C	N	O	S	0	0	0
			294	181	66	44	3			

- Molecule 31 is a RNA chain called 16S SMALL SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	y	1502	Total	C	N	O	P	0	0	0
			32302	14386	5984	10431	1501			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	450	G	C	CONFLICT	GB 155076
y	516	PSU	U	MODIFIED RESIDUE	GB 155076
y	527	7MG	G	MODIFIED RESIDUE	GB 155076
y	966	M2G	G	MODIFIED RESIDUE	GB 155076
y	967	5MC	C	MODIFIED RESIDUE	GB 155076
y	1207	2MG	G	MODIFIED RESIDUE	GB 155076
y	1400	5MC	C	MODIFIED RESIDUE	GB 155076
y	1402	4OC	C	MODIFIED RESIDUE	GB 155076
y	1404	5MC	C	MODIFIED RESIDUE	GB 155076
y	1407	5MC	C	MODIFIED RESIDUE	GB 155076
y	1498	UR3	U	MODIFIED RESIDUE	GB 155076
y	1518	MA6	A	MODIFIED RESIDUE	GB 155076
y	1519	MA6	A	MODIFIED RESIDUE	GB 155076

- Molecule 32 is a RNA chain called P-site PHE-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	z	76	Total	C	N	O	P	S	0	0
			1628	731	290	530	75	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	8	4SU	U	MODIFIED RESIDUE	GB 174422
z	16	H2U	U	MODIFIED RESIDUE	GB 174422
z	20	H2U	U	MODIFIED RESIDUE	GB 174422
z	32	PSU	U	MODIFIED RESIDUE	GB 174422
z	37	MIA	A	MODIFIED RESIDUE	GB 174422
z	39	PSU	U	MODIFIED RESIDUE	GB 174422
z	46	7MG	G	MODIFIED RESIDUE	GB 174422
z	54	5MU	U	MODIFIED RESIDUE	GB 174422
z	55	PSU	U	MODIFIED RESIDUE	GB 174422

- Molecule 33 is a RNA chain called E-TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	0	76	Total	C	N	O	P	0	0	0
			1621	725	293	528	75			

- Molecule 34 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1	6	Total	C	N	O	P	0	0	0
			122	56	19	42	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	j	127	Total	C	N	O	0	0	0
			1011	639	198	174			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	l	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	n	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	s	73	Total	C	N	O	0	0	0
			598	381	118	99			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	u	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

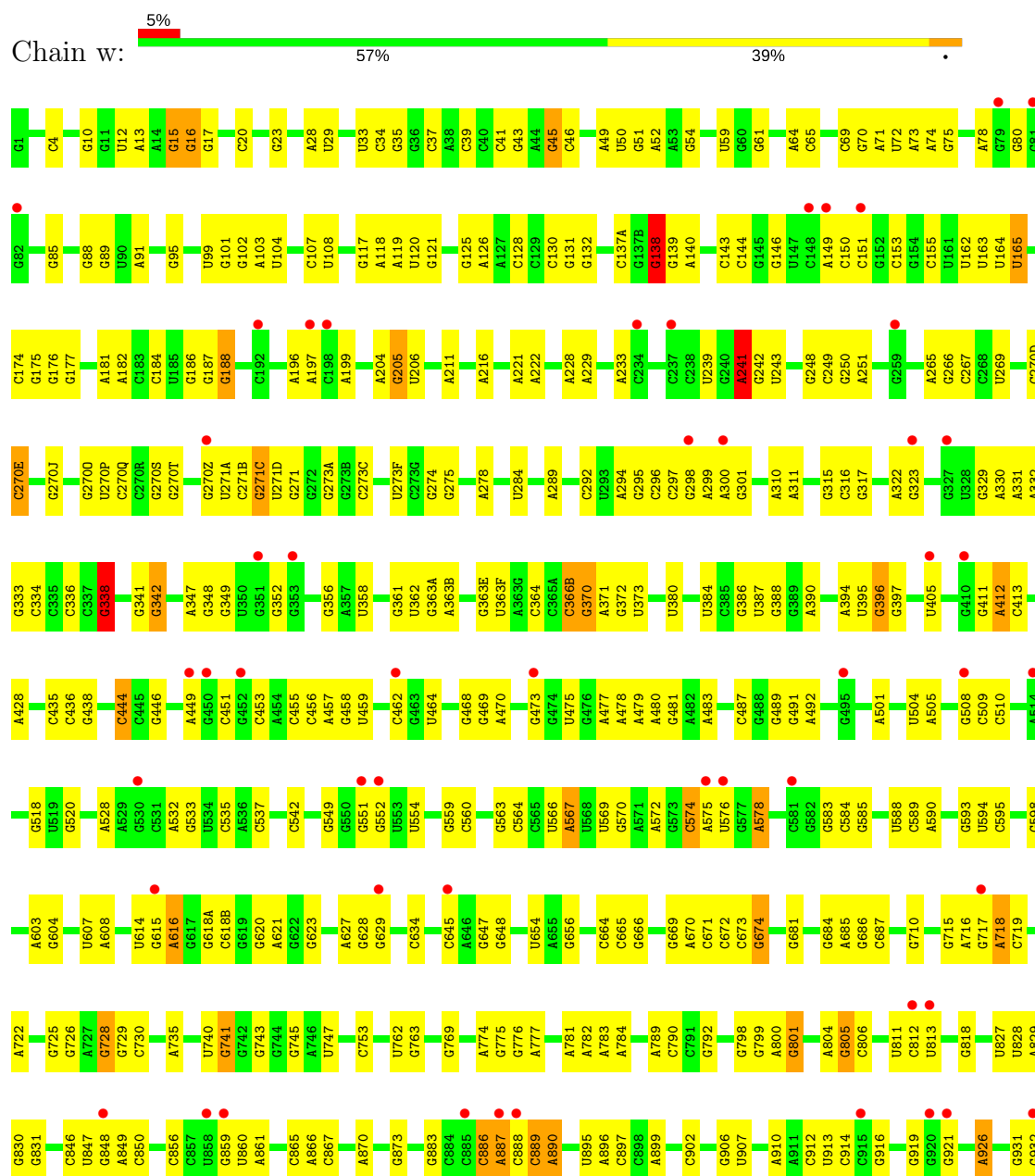
- Molecule 54 is a protein called 30S ribosomal protein Thx.

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

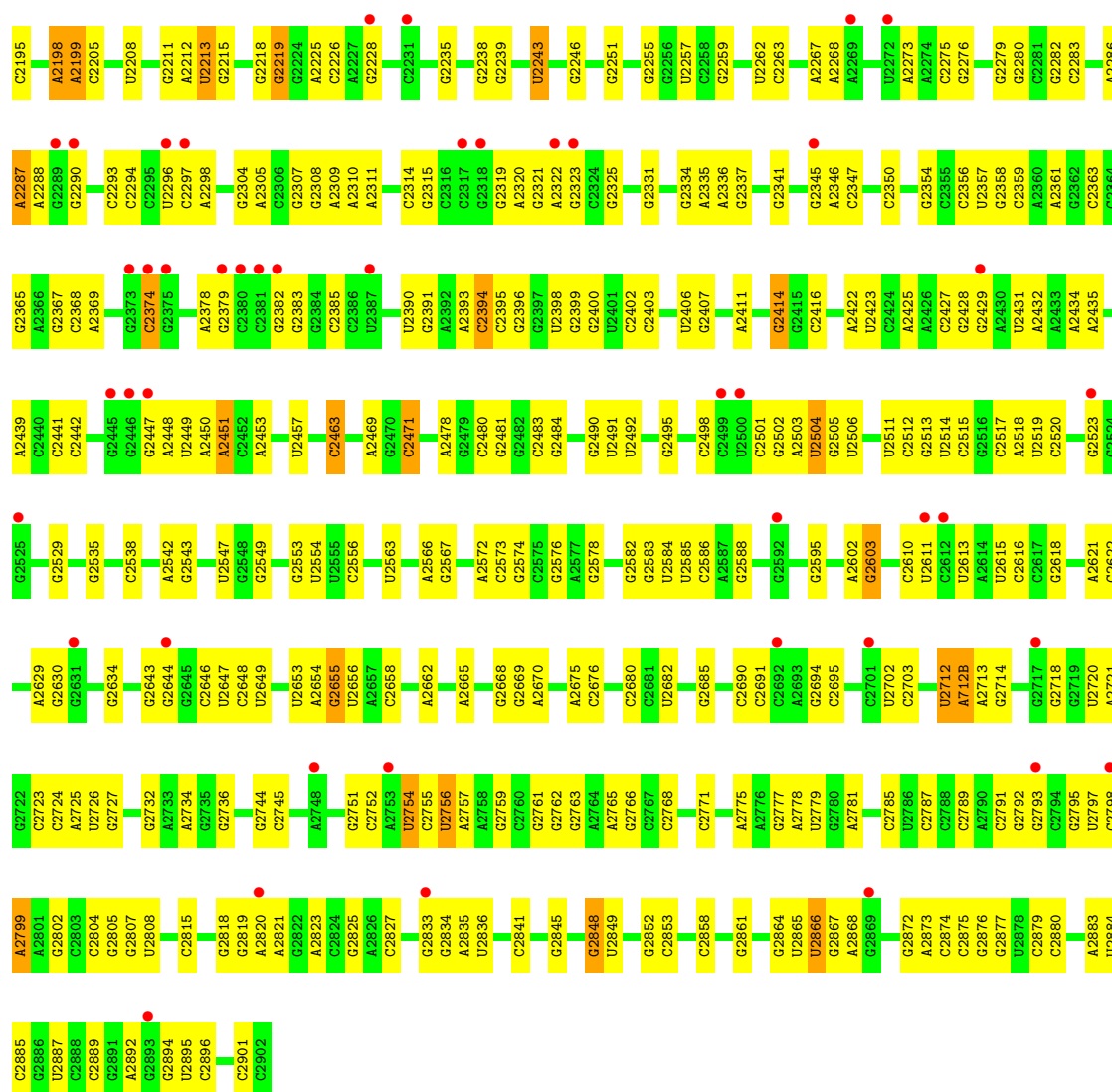
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

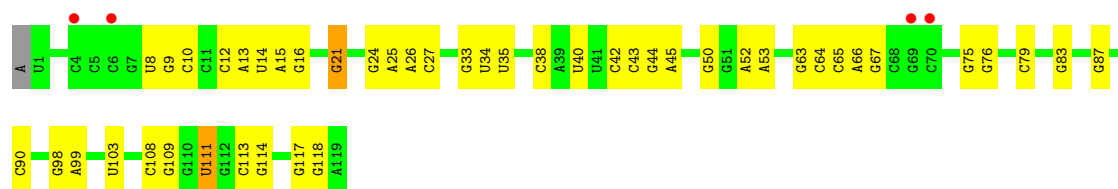
• Molecule 1: 23S LARGE SUBUNIT RIBOSOMAL RNA



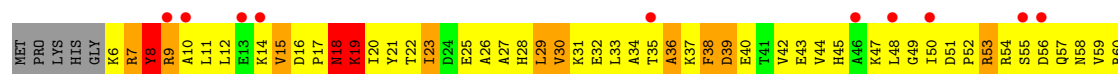
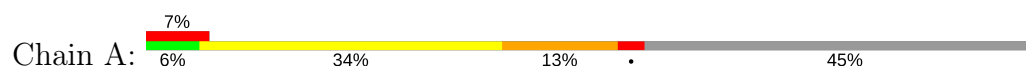
G2101	A2020	U1917	U1818	A1732	G1830	G1542	A1460	A1359	U1273	C1201	A1129	G1015	A933
G2110	C2021	A1918	A1819	G1733	G183B	A1543	G1461	C1362	A1274	A1204	U1130	G1016	G938
G2111	U2022	G1929	U1820	C1734	A1634	A1544	G1465	C1363	A1275	U1205	A1131	G1017	G939
G2112	G2023	U1930	A1821	G1735	G1635	A1545	G1466	G1364	A1276	G1206	U1205		
U2113	G2024	U1931	G1822	C1741	G1636	A1546	G1467	A1365	A1277		A1020		U943
A2114	C2025	G1934	G1824	G1743	C1840	C1547	G1470	A1366	G1283	G1209	G1022		G944
G2115	C2026	G1935	A1825	G1746	C1644	A1553	A1471	A1367	U1288	A1210	G1023		G945
G2116	A2031	A1936	G1826	G1747	G1747	A1558	C1474	G1374	G1287	U1211	G1024		G946
A2117	G2032	G1937	G1827	G1748	C1646	A1560	G1478	G1377	U1289	A1213	G1025		G954
G2118	A2033	A1938	G1828	C1751	G1647	A1561	G1481	A1378	C1295	G1216	U1033		U958
A2119	U2034	U1939	A1829	G1752	C1648	G1562	G1481	A1379	G1296	G1217	G1034		A959
G2120	G2035	A1943	C1836	G1753	G1849	G1563	U1481		G1297	G1218	C1043		A960
A2126	C2036	U1944	C1837	U1757	G1650	A1564	G1483	A1384	C1298	G1219	G1044		C961
G2127	U2041	G1945	G1838	G1758	G1651	C1565	G1484	G1385	G1299	A1148	G1045		G962
C2128	A2042	A1953	G1839	A1759	A1652	A1566	G1485	G1386	U1300	A1220	A1046		U963
U2130	C2043	G1954	G1840	G1763	A1655	A1567	A1486	C1398	A1301	C1221	G1047		C964
G2131	U2047	U1955	U1841	G1764	C1662	G1568	G1487	C1399	A1302	G1222			C965
G2132	G2048	G1956	G1842	G1765	C1663	A1569	U1488	G1400	C1305	G1223	A1054		G966
G2133	G2049	A1960	G1846	G1769	A1665	G1573	U1489	U1406	G1310	G1224			G972
C2138	A2050	U1963	A1847	A1773	A1669	C1574	U1490	G1413	G1311	G1225			U973
G2139	G2051	G1964	A1848	C1774	U1670	C1575	U1491	G1414	U1312	A1226			C974A
C2145	G2052	C1965	G1849	G1777	G1671	U1576	U1492	G1415	U1313	G1227			C974B
A2054	A2053	A1966	G1850	U1777	U1672	C1577	U1493	G1416	U1314	G1228			G975
G2148	G2055	G1967	G1858	U1778	G1673	A1578	U1500	G1417	G1319	G1229			C976
G2153	C2056	G1968	U1673	C1781	U1674	A1579	C1501	A1419	G1320	U1231			G977
G2154	A2057	U1969	G1874	G1782	G1675	A1580	C1502	U1420	U1321	G1236			G978
A2157	A2060	A1970	G1864	A1783	G1676	C1582	C1506	G1421	A1322	U1237			G979
G2158	C2061	G1971	U1869	A1784	G1682	A1583	U1516	A1422	U1323	G1238			A980
A2159	A2062	A1972	G1878	A1785	C1683	A1584	U1517	G1423	U1324	U1081			A983
G2160	C2063	G1973	G1879	A1786	U1688	A1586	U1518	G1424	G1325	G1239			A984
	C2064	U1974	C1880	A1787	U1689	A1596	U1519	G1425	U1326	U1240			
	C2065	U1975	A1885	A1791	U1690	A1597	U1520	G1426	G1327	G1244			A988
	C2066	A1976	C1886	G1792	C1694	U1601	U1521	G1427	C1328	G1245			G989
G2168	G2069	A1977	A1887	C1793	G1695	U1602	U1522	A1428	U1329	A1246			A990
A2170	G2070	A1978	C1888	U1794	A1698	A1603	U1523	G1429	C1330	A1247			C991
A2171	A2071	A1981	G1889	C1795	G1699	C1604	G1524	G1430	U1331	U1249			C992
A2172		C1982	A1889	U1796	A1700	A1608	U1525	G1436	G1332	G1250			C993
A2173		G1987	U1898	G1797	A1701	A1609	U1526	U1437	U1333	C1251			C994
C2174	U2076	U1991	G1899	G1799	G1702	A1610	G1527	U1438	G1334	G1252			C995
	C2077	G1992	A1900	C1800	G1703	G1613	U1528	A1448	U1335	A1253			A996
C2175	C2078	U1993	G1903	G1801	G1704	A1614	G1529	G1449	G1337	U1255			G997
C2176		C1994	G1906	A1802	U1706	A1615	U1530	G1450	U1341	G1256			
C2177		U1995	G1907	C1806	G1707	C1616	G1531	A1498	A1342	C1261			G1002
C2178	G2087	C1996	C1909	U1716	C1712	A1617	U1532	G1451	G1343				G1003
C2179		G1997	A1912	G1717	U1716	G1619	U1533	C1452	C1344	C1116			G1004
U2180	G2090	U1998	G1913	G1718	G1718	G1623	U1534	U1453	C1345	G1122			C1005
G2181	U2091	G2000	A1914	G1725	G1725	G1628	G1535	U1454	G1346	G1190			C1006
	C2096	G2001	A1915	G1811	G1726	G1629	G1536	U1455	G1347	G1191			C1007
C2188	U2097	G2002	A1916	A1815	U1729	G1629	G1537	U1456	C1351	G1267			C1008
G2189	U2098	A2013	U1915	G1816	U1730	G1629	G1538	G1457	C1351	G1270			A1009
G2190	G2100	A2014	A1916	G1817	G1731	U1629	U1541	G1459	G1358	A1272			A1010
G2191													G1011
G2192													G1012
G2193													C1013
G2194													U1014

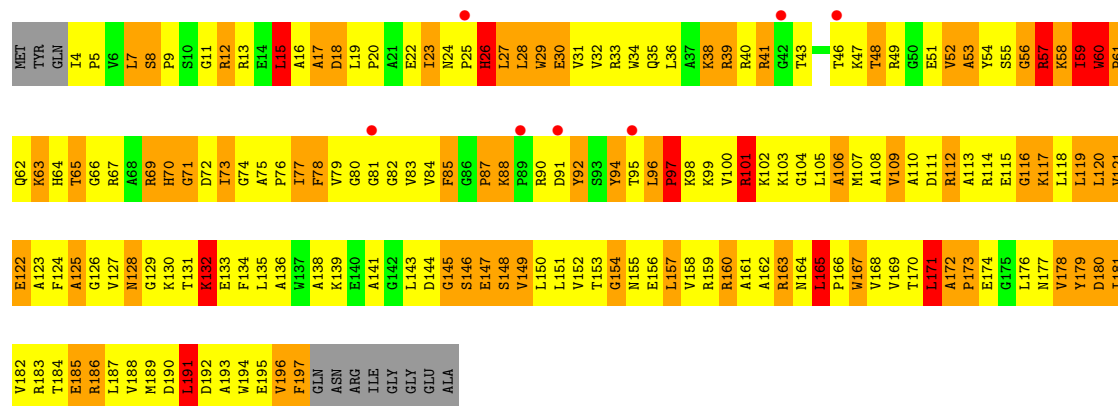


• Molecule 2: 5S LARGE SUBUNIT RIBOSOMAL RNA

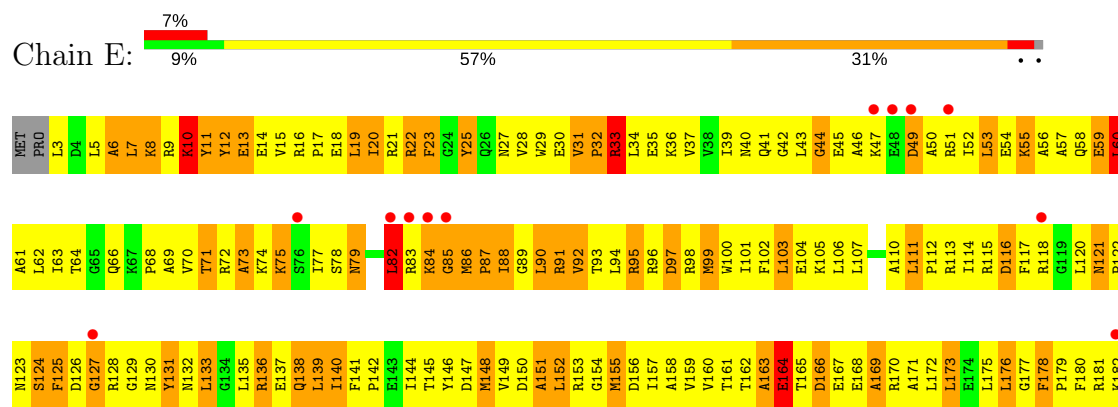


• Molecule 3: 50S ribosomal protein L1

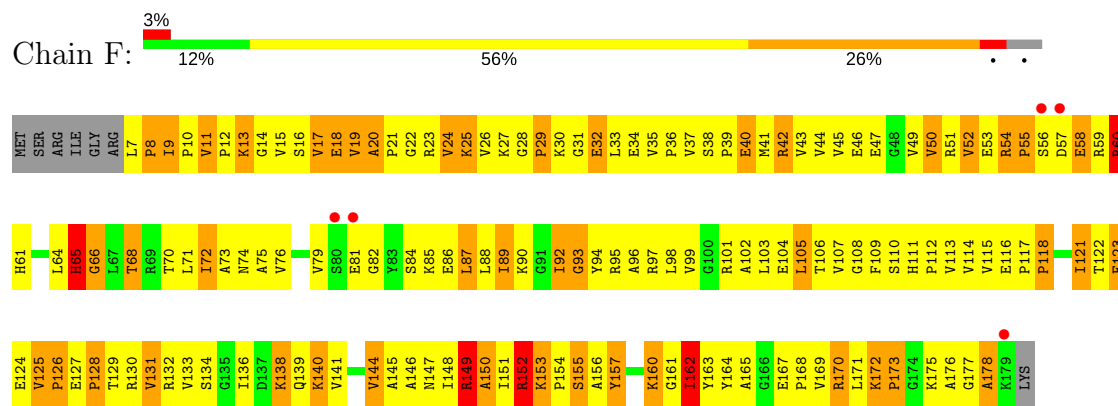




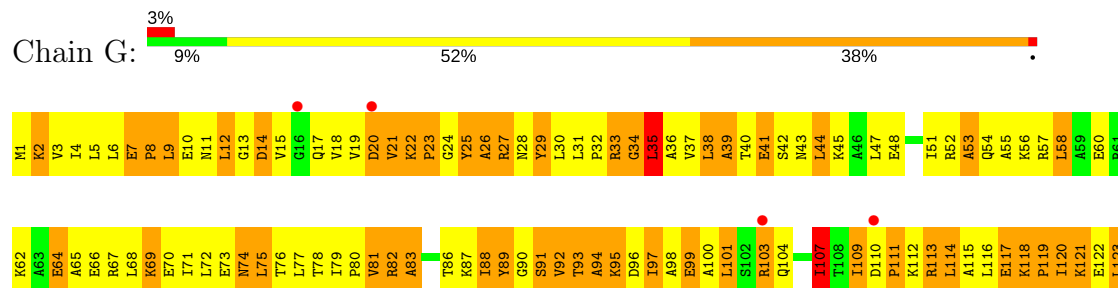
• Molecule 7: 50S ribosomal protein L5



• Molecule 8: 50S ribosomal protein L6

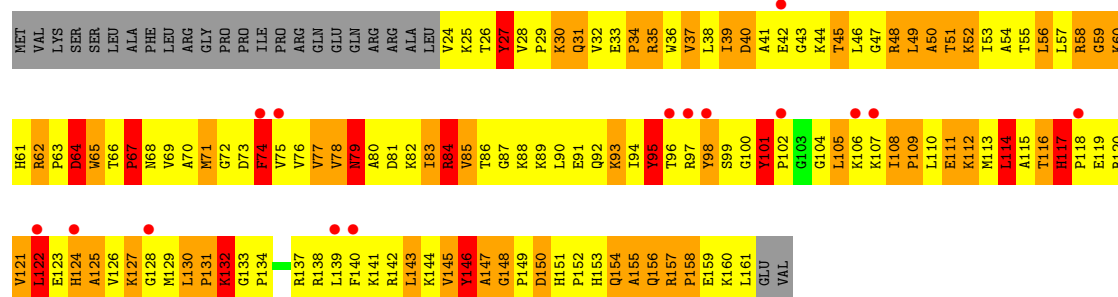


• Molecule 9: 50S ribosomal protein L9

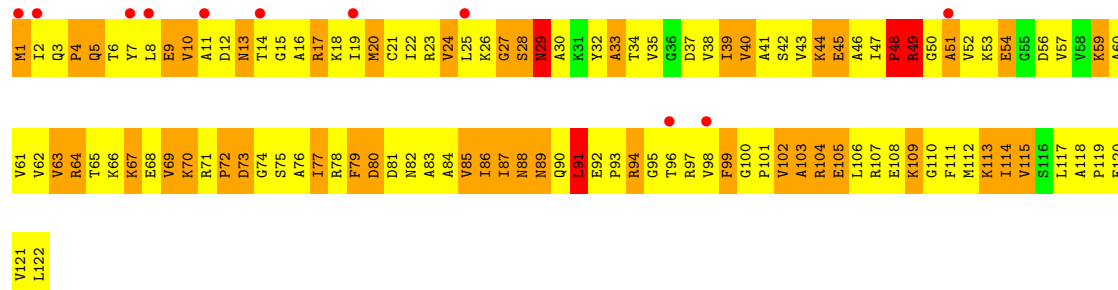




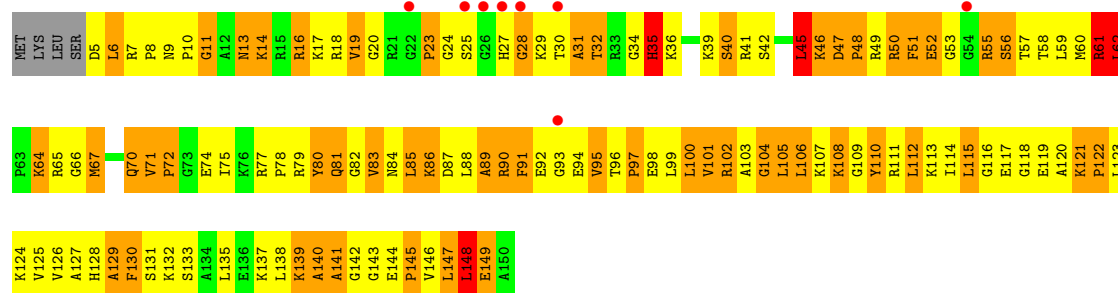
• Molecule 10: 50S ribosomal protein L13



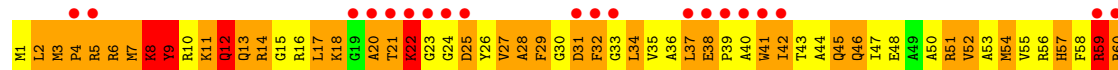
• Molecule 11: 50S ribosomal protein L14

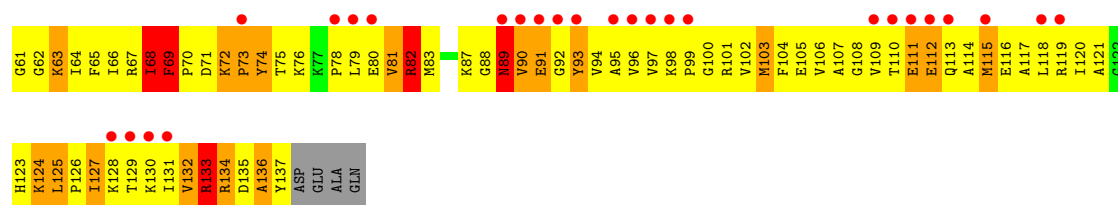


• Molecule 12: 50S ribosomal protein L15

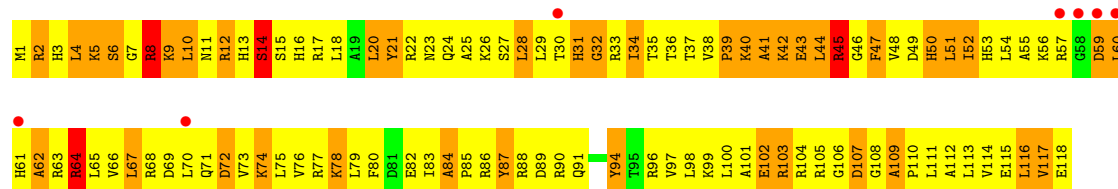


• Molecule 13: 50S ribosomal protein L16

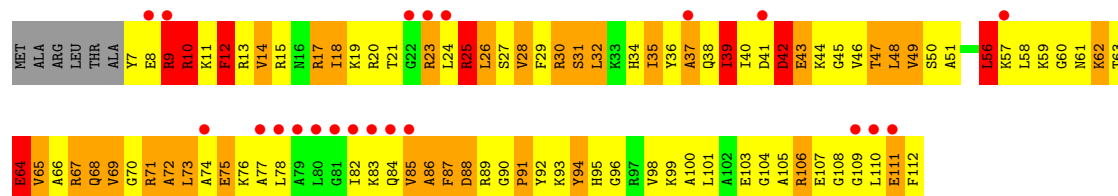




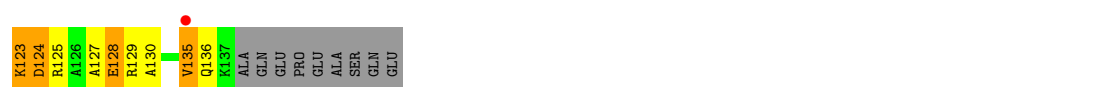
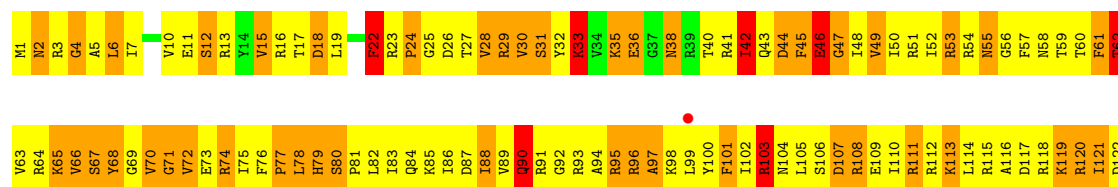
• Molecule 14: 50S ribosomal protein L17



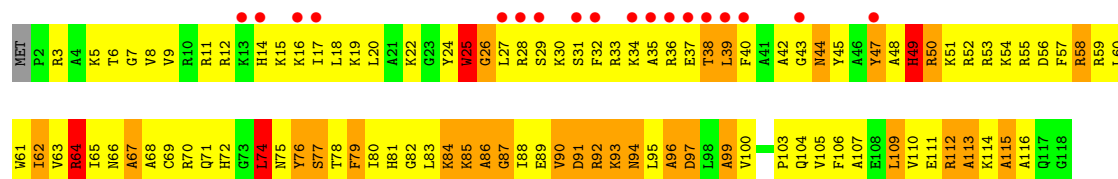
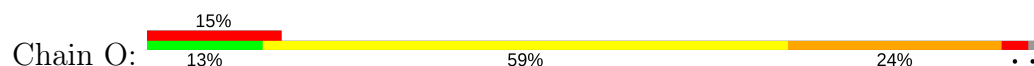
• Molecule 15: 50S ribosomal protein L18



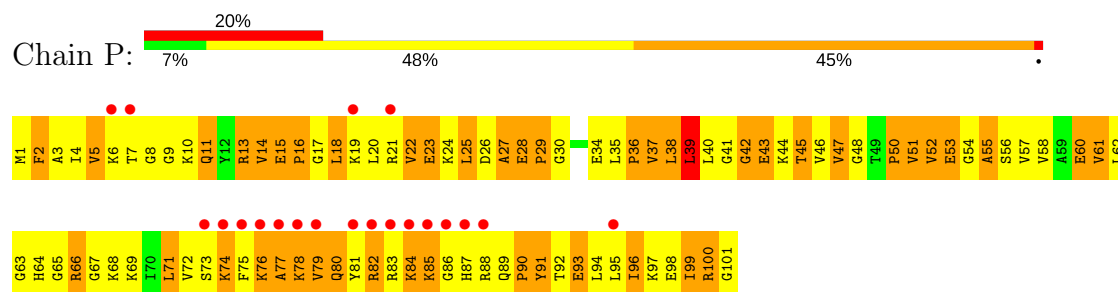
• Molecule 16: 50S ribosomal protein L19



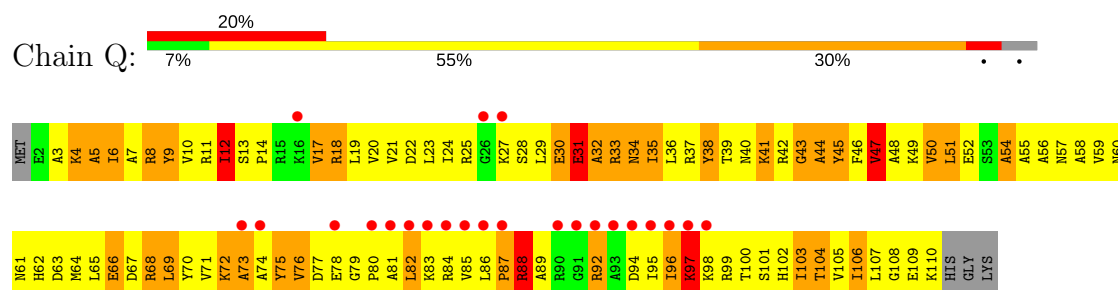
• Molecule 17: 50S ribosomal protein L20



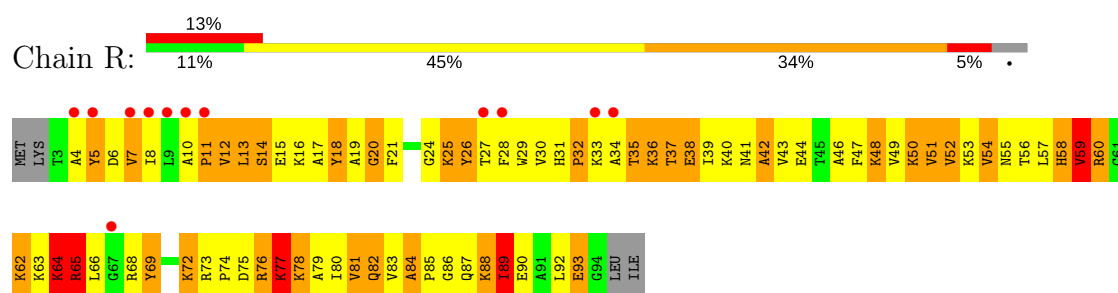
- Molecule 18: 50S ribosomal protein L21



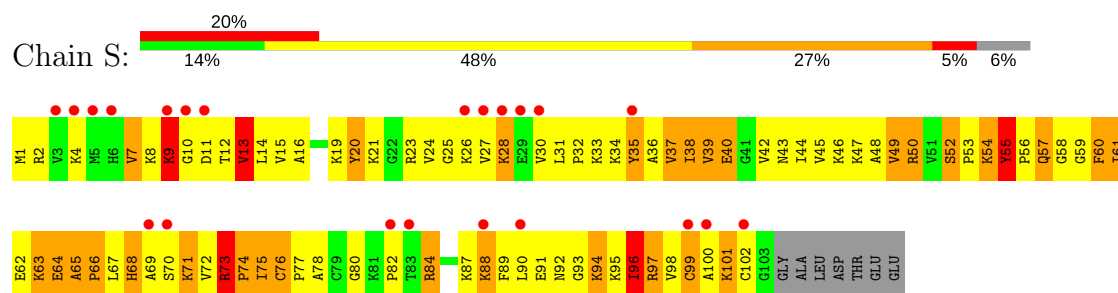
- Molecule 19: 50S ribosomal protein L22



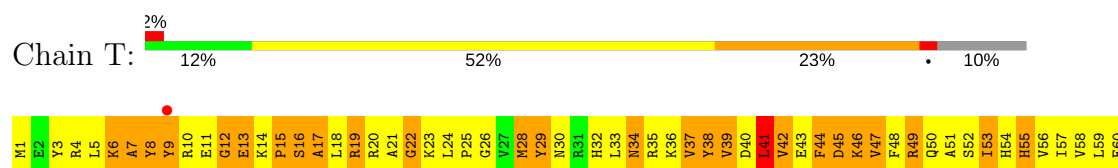
- Molecule 20: 50S ribosomal protein L23

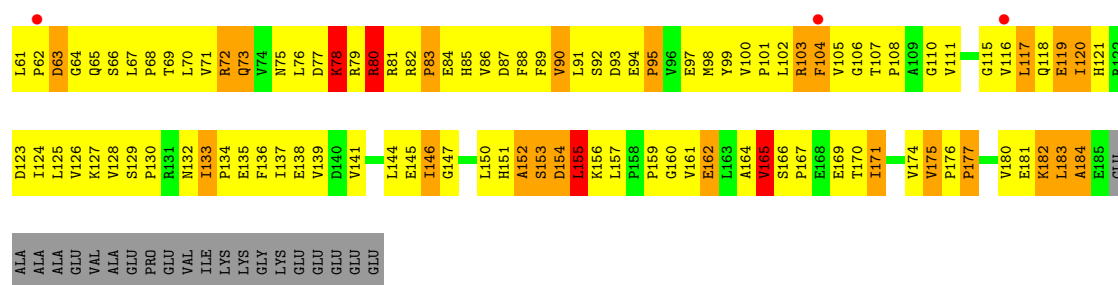


- Molecule 21: 50S ribosomal protein L24

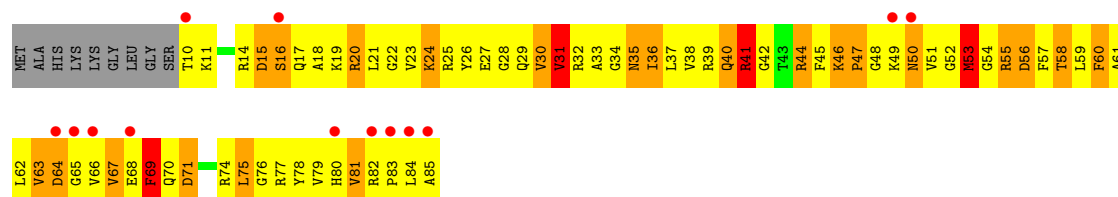


- Molecule 22: 50S ribosomal protein L25

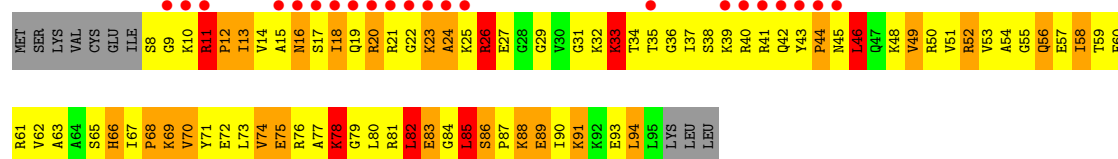




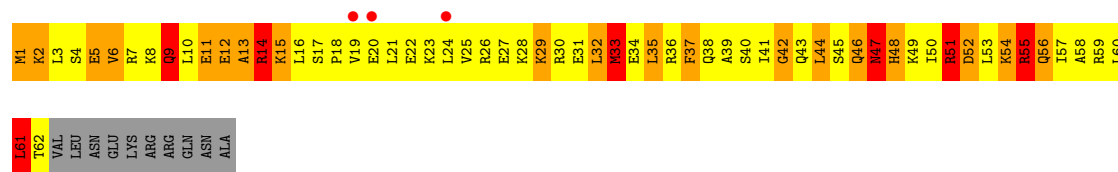
• Molecule 23: 50S ribosomal protein L27



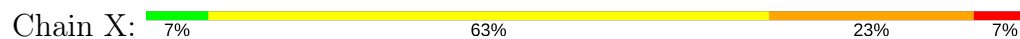
• Molecule 24: 50S ribosomal protein L28



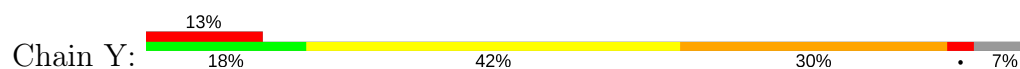
• Molecule 25: 50S ribosomal protein L29

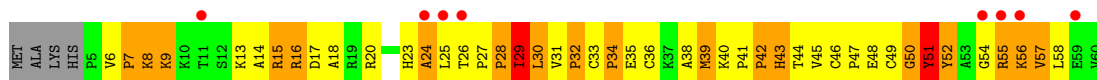


• Molecule 26: 50S ribosomal protein L30

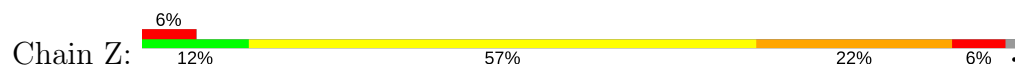


• Molecule 27: 50S ribosomal protein L32

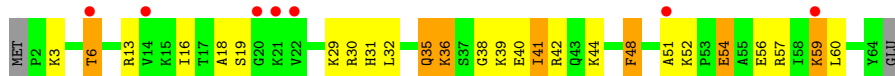




- Molecule 28: 50S ribosomal protein L34



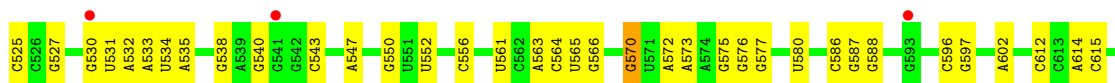
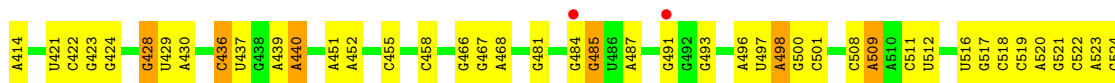
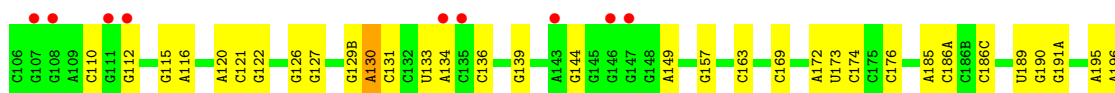
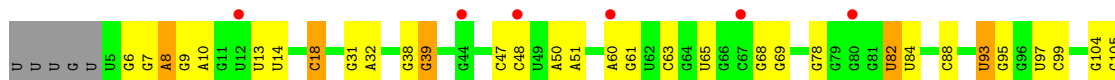
- Molecule 29: 50S ribosomal protein L35

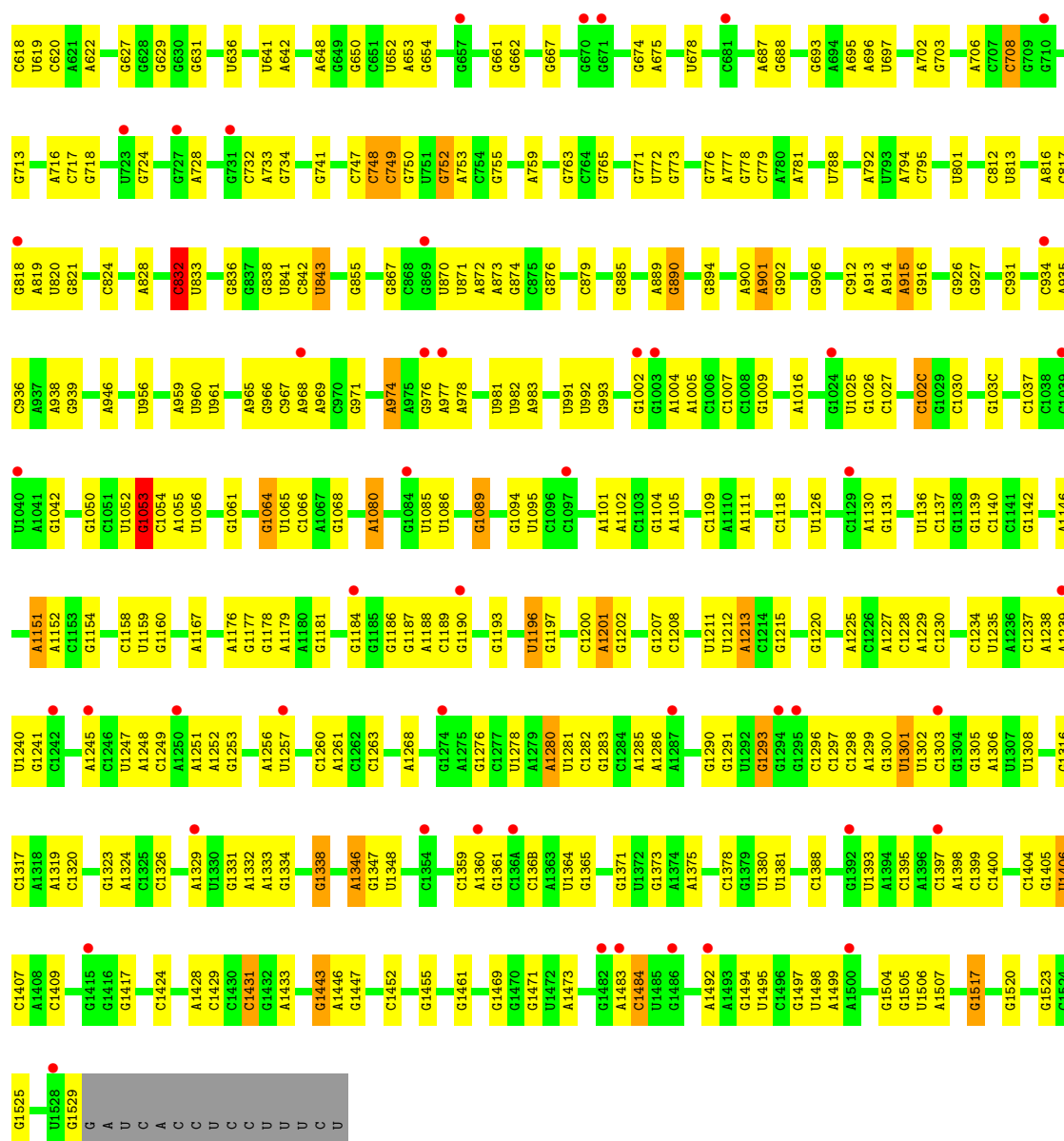


- Molecule 30: 50S ribosomal protein L36

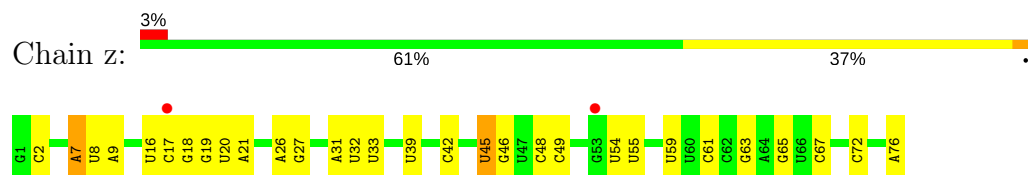


- Molecule 31: 16S SMALL SUBUNIT RIBOSOMAL RNA

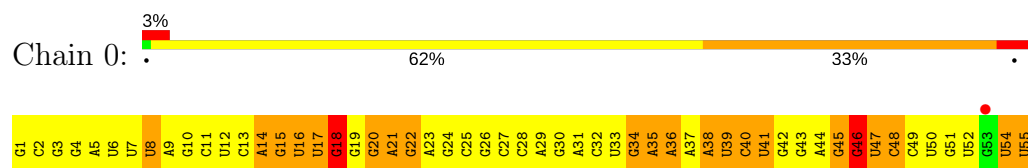


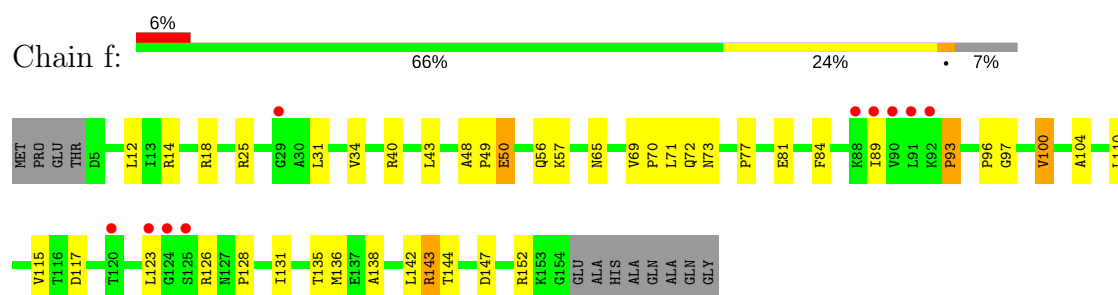


• Molecule 32: P-site PHE-tRNA

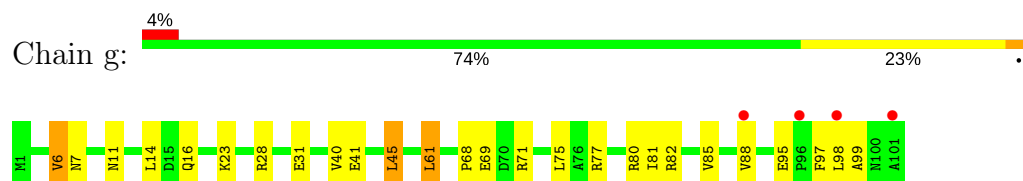


• Molecule 33: E-TRNA

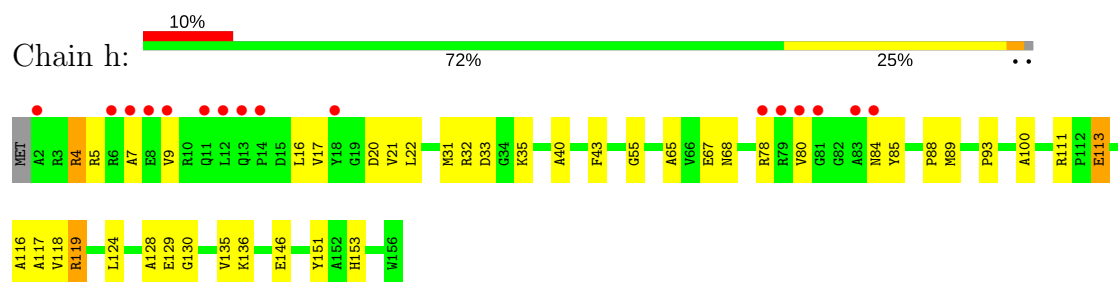




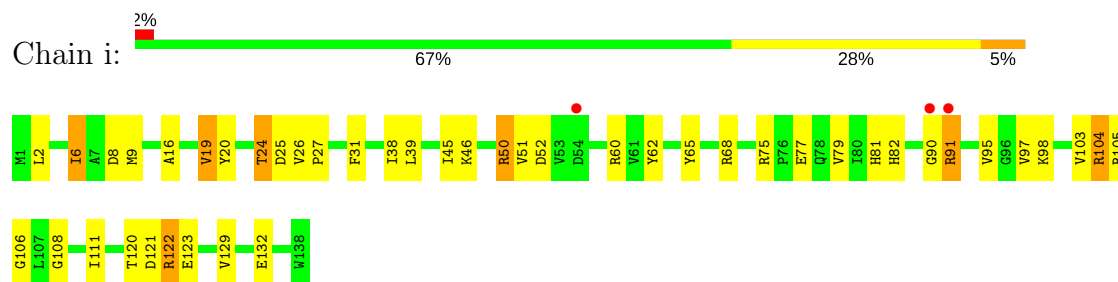
• Molecule 39: 30S ribosomal protein S6



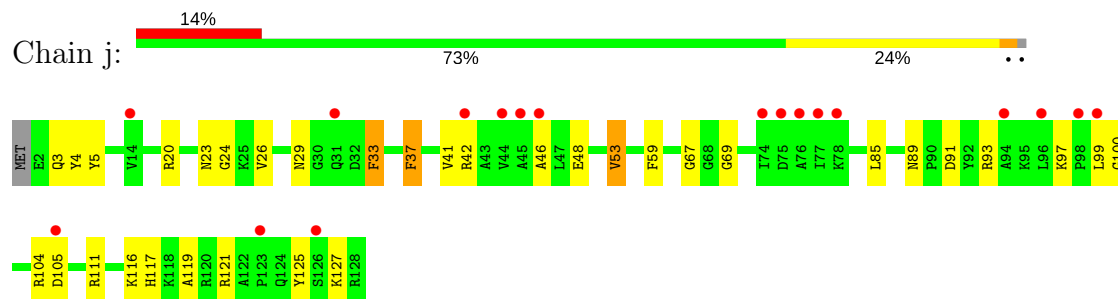
• Molecule 40: 30S ribosomal protein S7



• Molecule 41: 30S ribosomal protein S8

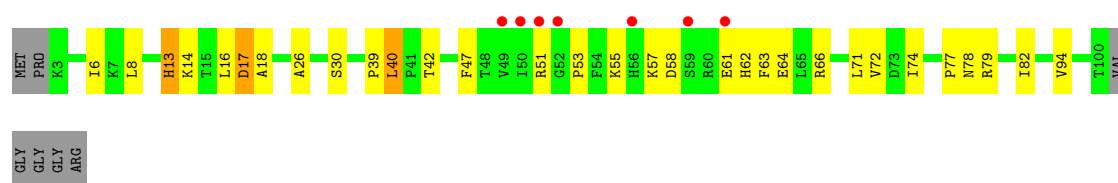


• Molecule 42: 30S ribosomal protein S9

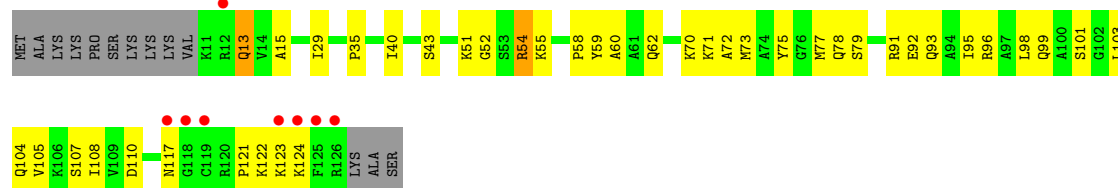


• Molecule 43: 30S ribosomal protein S10





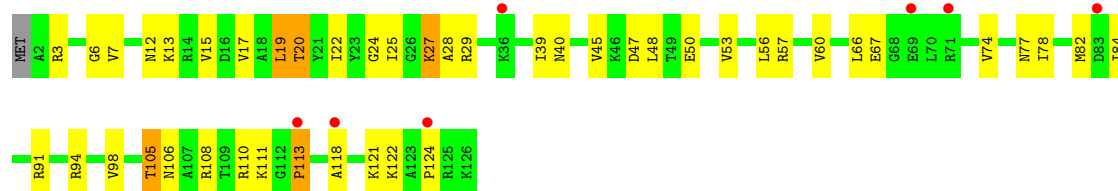
• Molecule 44: 30S ribosomal protein S11



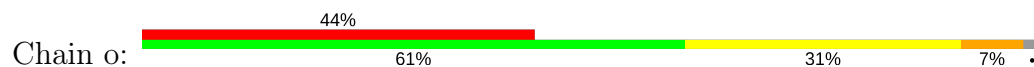
• Molecule 45: 30S ribosomal protein S12



• Molecule 46: 30S ribosomal protein S13



• Molecule 47: 30S ribosomal protein S14

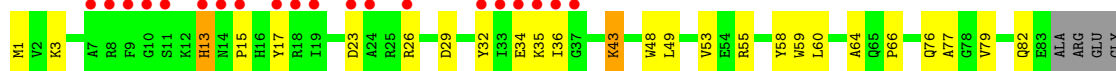


• Molecule 48: 30S ribosomal protein S15



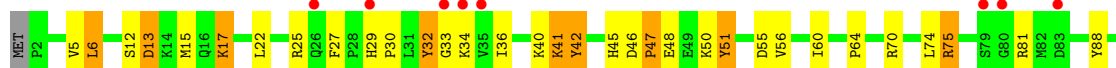


- Molecule 49: 30S ribosomal protein S16



ALA

- Molecule 50: 30S ribosomal protein S17

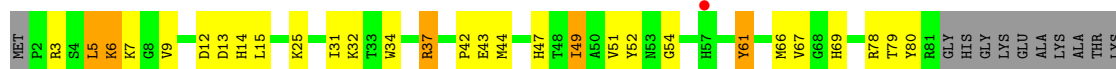


Y95
Q96
K100
A105

- Molecule 51: 30S ribosomal protein S18

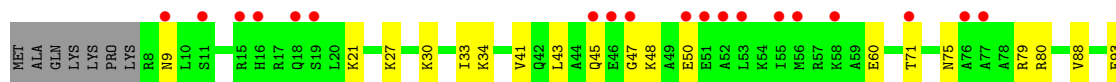


- Molecule 52: 30S ribosomal protein S19



LYS
LYS

- Molecule 53: 30S ribosomal protein S20



A97
P98
L99
I100
G101
G102
G103
L104
S105
A106

- Molecule 54: 30S ribosomal protein Thx

Chain v: 7% 63% 26% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	507.81Å 507.81Å 689.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.71 72.78 – 3.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.71) 97.9 (72.78-3.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.348 , 0.353 0.346 , 0.349	Depositor DCC
R_{free} test set	11369 reflections (2.55%)	DCC
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.70 , 508.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.228 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.219 for -1/2*h-1/2*k+1/2*l, -1/2*h-1/2*k-1/2*l, h-k	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	146532	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, M2G, MA6, MIA, H2U, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	w	1.06	48/69679 (0.1%)	1.11	232/108779 (0.2%)
2	x	0.89	0/2878	1.03	11/4490 (0.2%)
3	A	0.50	0/1015	0.57	0/1369
4	B	0.49	0/2165	0.63	0/2919
5	C	0.57	0/1574	0.68	0/2125
6	D	0.57	0/1551	0.66	0/2101
7	E	0.55	0/1492	0.65	0/2006
8	F	0.55	0/1345	0.66	1/1819 (0.1%)
9	G	0.53	0/1171	0.65	0/1583
10	H	0.47	0/1130	0.59	0/1525
11	I	0.54	0/942	0.66	0/1268
12	J	0.50	0/1131	0.64	0/1504
13	K	0.62	0/1110	0.71	1/1483 (0.1%)
14	L	0.51	0/982	0.65	0/1312
15	M	0.54	0/856	0.63	0/1138
16	N	0.49	0/1157	0.62	0/1544
17	O	0.54	0/982	0.67	0/1306
18	P	0.51	0/790	0.62	0/1057
19	Q	0.56	0/878	0.66	0/1179
20	R	0.59	0/739	0.69	0/993
21	S	0.58	0/806	0.64	0/1074
22	T	0.54	0/1507	0.64	0/2045
23	U	0.57	0/613	0.65	0/816
24	V	0.49	0/701	0.60	0/932
25	W	0.52	0/522	0.65	0/690
26	X	0.56	0/482	0.73	0/646
27	Y	0.45	0/449	0.55	0/606
28	Z	0.80	0/426	0.73	0/561
29	a	0.58	0/515	0.69	0/679
30	b	0.55	0/297	0.61	0/392
31	y	0.97	13/35859 (0.0%)	1.07	96/55966 (0.2%)
32	z	0.98	1/1603 (0.1%)	1.05	3/2497 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	0	0.89	1/1791 (0.1%)	0.97	2/2791 (0.1%)
34	1	0.94	0/135	1.02	0/208
35	c	0.55	0/1935	0.60	0/2609
36	d	0.51	0/1636	0.62	0/2205
37	e	0.53	0/1733	0.62	1/2318 (0.0%)
38	f	0.51	0/1162	0.60	0/1564
39	g	0.56	0/856	0.63	0/1154
40	h	0.53	0/1276	0.57	0/1709
41	i	0.51	0/1136	0.62	0/1527
42	j	0.47	0/1029	0.53	0/1378
43	k	0.52	0/807	0.59	0/1085
44	l	0.49	0/879	0.59	0/1187
45	m	0.57	0/986	0.72	0/1320
46	n	0.52	0/1008	0.61	0/1347
47	o	0.53	0/501	0.57	0/664
48	p	0.49	0/745	0.58	0/992
49	q	0.49	0/716	0.63	0/963
50	r	0.55	0/870	0.63	0/1159
51	s	0.51	0/604	0.63	0/801
52	t	0.54	0/661	0.64	0/890
53	u	0.21	0/764	0.44	0/1006
54	v	0.57	0/212	0.52	0/277
All	All	0.91	63/158789 (0.0%)	0.99	347/237558 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	w	0	24
2	x	2	0
31	y	0	8
All	All	2	32

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	926	A	O3'-P	30.08	1.97	1.61
1	w	1506	C	O3'-P	29.80	1.97	1.61
1	w	1171	G	O3'-P	28.10	1.94	1.61
1	w	890	A	O3'-P	28.02	1.94	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	1481	U	O3'-P	24.13	1.90	1.61

The worst 5 of 347 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	1822	G	N9-C1'-C2'	-18.71	89.67	114.00
1	w	1577	C	N1-C1'-C2'	-15.42	93.96	114.00
1	w	712(B)	A	P-O3'-C3'	-14.26	102.58	119.70
31	y	93	U	N1-C1'-C2'	-14.11	95.66	114.00
31	y	832	C	N1-C1'-C2'	-13.21	96.82	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	x	14	U	C3'
2	x	24	G	C3'

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	w	138	G	Sidechain
1	w	241	A	Sidechain
1	w	338	G	Sidechain
1	w	566	U	Sidechain
1	w	74	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	w	62213	0	31360	0	1
2	x	2573	0	1306	0	0
3	A	996	0	1013	324	0
4	B	2115	0	2195	865	0
5	C	1541	0	1599	658	0
6	D	1517	0	1565	619	0
7	E	1468	0	1529	570	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	1319	0	1399	472	0
9	G	1156	0	1239	549	2
10	H	1103	0	1177	595	0
11	I	932	0	994	481	0
12	J	1114	0	1187	402	0
13	K	1089	0	1156	504	0
14	L	968	0	1033	432	0
15	M	846	0	902	322	0
16	N	1143	0	1211	519	0
17	O	964	0	1022	345	0
18	P	779	0	852	345	0
19	Q	868	0	929	344	0
20	R	725	0	778	264	0
21	S	793	0	890	240	0
22	T	1475	0	1504	524	0
23	U	605	0	628	287	0
24	V	694	0	764	335	0
25	W	520	0	575	182	0
26	X	477	0	529	208	0
27	Y	436	0	460	135	0
28	Z	418	0	467	83	0
29	a	507	0	576	0	0
30	b	294	0	323	0	0
31	y	32302	0	16327	0	2
32	z	1628	0	844	0	0
33	0	1621	0	821	271	0
34	1	122	0	65	2	0
35	c	1900	0	1951	0	0
36	d	1612	0	1677	0	0
37	e	1703	0	1767	0	0
38	f	1146	0	1207	0	0
39	g	843	0	857	0	0
40	h	1257	0	1296	0	0
41	i	1116	0	1177	0	0
42	j	1011	0	1043	0	0
43	k	794	0	840	0	0
44	l	864	0	881	0	0
45	m	970	0	1057	0	0
46	n	997	0	1072	0	0
47	o	492	0	533	0	0
48	p	734	0	771	0	0
49	q	700	0	720	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	r	857	0	930	0	0
51	s	598	0	670	0	0
52	t	647	0	673	0	0
53	u	762	0	859	0	0
54	v	208	0	221	0	0
All	All	146532	0	99421	10655	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 178.

The worst 5 of 10655 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:71:VAL:HG13	12:J:72:PRO:CD	1.47	1.43
9:G:124:GLY:CA	9:G:144:VAL:H	1.33	1.38
11:I:17:ARG:NE	11:I:47:ILE:HB	1.39	1.37
33:O:9:A:N6	33:O:23:A:N7	1.74	1.36
16:N:100:TYR:HA	16:N:103:ARG:NH2	1.36	1.36

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:w:1457:A:OP1	1:w:1457:A:OP1[6_555]	1.38	0.82
9:G:89:TYR:O	31:y:357:G:O2'[4_555]	2.01	0.19
9:G:91:SER:O	31:y:368:U:OP1[4_555]	2.19	0.01

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	123/229 (54%)	54 (44%)	39 (32%)	30 (24%)	0	0
4	B	270/276 (98%)	103 (38%)	84 (31%)	83 (31%)	0	0
5	C	199/206 (97%)	89 (45%)	48 (24%)	62 (31%)	0	0
6	D	192/205 (94%)	76 (40%)	54 (28%)	62 (32%)	0	0
7	E	178/182 (98%)	84 (47%)	53 (30%)	41 (23%)	0	1
8	F	171/180 (95%)	76 (44%)	53 (31%)	42 (25%)	0	0
9	G	146/148 (99%)	75 (51%)	30 (20%)	41 (28%)	0	0
10	H	136/163 (83%)	48 (35%)	40 (29%)	48 (35%)	0	0
11	I	120/122 (98%)	50 (42%)	37 (31%)	33 (28%)	0	0
12	J	144/150 (96%)	59 (41%)	39 (27%)	46 (32%)	0	0
13	K	135/141 (96%)	52 (38%)	44 (33%)	39 (29%)	0	0
14	L	116/118 (98%)	60 (52%)	28 (24%)	28 (24%)	0	1
15	M	104/112 (93%)	40 (38%)	31 (30%)	33 (32%)	0	0
16	N	135/146 (92%)	59 (44%)	36 (27%)	40 (30%)	0	0
17	O	115/118 (98%)	64 (56%)	27 (24%)	24 (21%)	0	2
18	P	99/101 (98%)	30 (30%)	32 (32%)	37 (37%)	0	0
19	Q	107/113 (95%)	49 (46%)	30 (28%)	28 (26%)	0	0
20	R	90/96 (94%)	28 (31%)	29 (32%)	33 (37%)	0	0
21	S	101/110 (92%)	36 (36%)	34 (34%)	31 (31%)	0	0
22	T	183/206 (89%)	104 (57%)	41 (22%)	38 (21%)	0	2
23	U	74/85 (87%)	35 (47%)	23 (31%)	16 (22%)	0	1
24	V	86/98 (88%)	30 (35%)	31 (36%)	25 (29%)	0	0
25	W	60/72 (83%)	28 (47%)	12 (20%)	20 (33%)	0	0
26	X	58/60 (97%)	32 (55%)	15 (26%)	11 (19%)	0	2
27	Y	54/60 (90%)	22 (41%)	12 (22%)	20 (37%)	0	0
28	Z	46/49 (94%)	25 (54%)	9 (20%)	12 (26%)	0	0
29	a	61/65 (94%)	20 (33%)	22 (36%)	19 (31%)	0	0
30	b	33/37 (89%)	22 (67%)	5 (15%)	6 (18%)	0	2
35	c	232/256 (91%)	109 (47%)	66 (28%)	57 (25%)	0	0
36	d	204/239 (85%)	98 (48%)	49 (24%)	57 (28%)	0	0
37	e	206/209 (99%)	99 (48%)	44 (21%)	63 (31%)	0	0
38	f	148/162 (91%)	89 (60%)	33 (22%)	26 (18%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	g	99/101 (98%)	61 (62%)	24 (24%)	14 (14%)	0	5
40	h	153/156 (98%)	84 (55%)	40 (26%)	29 (19%)	0	2
41	i	136/138 (99%)	71 (52%)	35 (26%)	30 (22%)	0	1
42	j	125/128 (98%)	73 (58%)	31 (25%)	21 (17%)	0	4
43	k	96/105 (91%)	50 (52%)	24 (25%)	22 (23%)	0	1
44	l	114/129 (88%)	59 (52%)	28 (25%)	27 (24%)	0	1
45	m	122/132 (92%)	51 (42%)	32 (26%)	39 (32%)	0	0
46	n	123/126 (98%)	53 (43%)	35 (28%)	35 (28%)	0	0
47	o	58/61 (95%)	22 (38%)	19 (33%)	17 (29%)	0	0
48	p	86/89 (97%)	46 (54%)	23 (27%)	17 (20%)	0	2
49	q	81/88 (92%)	37 (46%)	28 (35%)	16 (20%)	0	2
50	r	102/105 (97%)	46 (45%)	31 (30%)	25 (24%)	0	0
51	s	71/88 (81%)	42 (59%)	12 (17%)	17 (24%)	0	1
52	t	78/93 (84%)	26 (33%)	31 (40%)	21 (27%)	0	0
53	u	97/106 (92%)	42 (43%)	37 (38%)	18 (19%)	0	2
54	v	22/27 (82%)	11 (50%)	7 (32%)	4 (18%)	0	2
All	All	5689/6186 (92%)	2619 (46%)	1567 (28%)	1503 (26%)	0	0

5 of 1503 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	63	VAL
3	A	179	ALA
3	A	180	SER
3	A	201	LYS
3	A	203	GLU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	106/181 (59%)	91 (86%)	15 (14%)	4	26
4	B	214/218 (98%)	169 (79%)	45 (21%)	1	8
5	C	163/166 (98%)	126 (77%)	37 (23%)	1	7
6	D	154/162 (95%)	123 (80%)	31 (20%)	1	10
7	E	154/156 (99%)	127 (82%)	27 (18%)	2	15
8	F	142/148 (96%)	124 (87%)	18 (13%)	5	30
9	G	124/124 (100%)	103 (83%)	21 (17%)	2	17
10	H	117/139 (84%)	90 (77%)	27 (23%)	1	7
11	I	100/100 (100%)	79 (79%)	21 (21%)	1	8
12	J	112/116 (97%)	89 (80%)	23 (20%)	1	9
13	K	108/111 (97%)	77 (71%)	31 (29%)	0	3
14	L	101/101 (100%)	79 (78%)	22 (22%)	1	8
15	M	84/88 (96%)	66 (79%)	18 (21%)	1	8
16	N	121/128 (94%)	97 (80%)	24 (20%)	1	10
17	O	93/94 (99%)	79 (85%)	14 (15%)	3	23
18	P	82/82 (100%)	70 (85%)	12 (15%)	3	24
19	Q	89/92 (97%)	72 (81%)	17 (19%)	2	11
20	R	74/78 (95%)	62 (84%)	12 (16%)	3	19
21	S	86/91 (94%)	75 (87%)	11 (13%)	5	29
22	T	163/179 (91%)	140 (86%)	23 (14%)	4	26
23	U	61/67 (91%)	47 (77%)	14 (23%)	1	7
24	V	73/83 (88%)	60 (82%)	13 (18%)	2	14
25	W	58/67 (87%)	42 (72%)	16 (28%)	0	4
26	X	52/52 (100%)	41 (79%)	11 (21%)	1	8
27	Y	49/52 (94%)	44 (90%)	5 (10%)	8	39
28	Z	41/42 (98%)	32 (78%)	9 (22%)	1	7
29	a	53/55 (96%)	39 (74%)	14 (26%)	0	4
30	b	33/34 (97%)	30 (91%)	3 (9%)	11	45
35	c	202/220 (92%)	154 (76%)	48 (24%)	1	6
36	d	160/188 (85%)	130 (81%)	30 (19%)	2	12
37	e	180/181 (99%)	143 (79%)	37 (21%)	1	9
38	f	115/123 (94%)	94 (82%)	21 (18%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	g	90/90 (100%)	75 (83%)	15 (17%)	2	18
40	h	126/127 (99%)	110 (87%)	16 (13%)	5	30
41	i	119/119 (100%)	97 (82%)	22 (18%)	2	12
42	j	98/99 (99%)	82 (84%)	16 (16%)	3	19
43	k	88/92 (96%)	76 (86%)	12 (14%)	4	28
44	l	88/99 (89%)	72 (82%)	16 (18%)	2	13
45	m	104/109 (95%)	85 (82%)	19 (18%)	2	13
46	n	100/101 (99%)	85 (85%)	15 (15%)	3	23
47	o	49/50 (98%)	39 (80%)	10 (20%)	1	9
48	p	79/80 (99%)	65 (82%)	14 (18%)	2	15
49	q	72/74 (97%)	60 (83%)	12 (17%)	2	18
50	r	96/97 (99%)	76 (79%)	20 (21%)	1	9
51	s	64/77 (83%)	52 (81%)	12 (19%)	2	12
52	t	71/80 (89%)	58 (82%)	13 (18%)	2	13
53	u	76/82 (93%)	70 (92%)	6 (8%)	14	51
54	v	19/22 (86%)	16 (84%)	3 (16%)	3	21
All	All	4803/5116 (94%)	3912 (81%)	891 (19%)	2	12

5 of 891 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	R	26	TYR
26	X	43	ILE
48	p	84	LYS
20	R	89	ILE
23	U	36	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
23	U	35	ASN
35	c	113	HIS
48	p	71	GLN
23	U	50	ASN
28	Z	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	w	2888/2889 (99%)	1138 (39%)	0
2	x	119/121 (98%)	42 (35%)	0
31	y	1498/1522 (98%)	502 (33%)	0
32	z	74/76 (97%)	28 (37%)	0
33	0	75/76 (98%)	30 (40%)	0
34	1	5/10 (50%)	2 (40%)	0
All	All	4659/4694 (99%)	1742 (37%)	0

5 of 1742 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	w	10	G
1	w	12	U
1	w	13	A
1	w	15	G
1	w	16	G

There are no RNA pucker outliers to report.

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

22 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	PSU	0	55	33	16,21,22	2.09	4 (25%)	20,30,33	4.59	9 (45%)
31	2MG	y	1207	31	19,26,27	1.97	4 (21%)	20,38,41	3.92	9 (45%)
31	5MC	y	1400	31	15,22,23	1.17	1 (6%)	17,32,35	1.33	2 (11%)
31	4OC	y	1402	31	16,23,24	1.66	4 (25%)	19,32,35	1.59	4 (21%)
31	5MC	y	1404	31	15,22,23	1.49	2 (13%)	17,32,35	1.92	2 (11%)
31	5MC	y	1407	31	15,22,23	1.53	3 (20%)	17,32,35	1.01	1 (5%)
31	UR3	y	1498	31	14,22,23	1.86	3 (21%)	16,32,35	1.29	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	MA6	y	1518	31	16,26,27	1.11	0	18,38,41	2.57	7 (38%)
31	MA6	y	1519	31	16,26,27	1.76	1 (6%)	18,38,41	2.28	5 (27%)
31	PSU	y	516	31	16,21,22	1.16	2 (12%)	20,30,33	3.88	8 (40%)
31	7MG	y	527	31	20,26,27	2.74	6 (30%)	22,39,42	2.19	4 (18%)
31	M2G	y	966	31	20,27,28	2.95	6 (30%)	21,40,43	2.70	6 (28%)
31	5MC	y	967	31	15,22,23	1.11	1 (6%)	17,32,35	0.91	0
32	H2U	z	16	32	17,21,22	0.93	0	21,30,33	0.91	1 (4%)
32	H2U	z	20	32	17,21,22	0.79	0	21,30,33	0.90	1 (4%)
32	PSU	z	32	32	16,21,22	1.38	2 (12%)	20,30,33	3.94	9 (45%)
32	MIA	z	37	32	23,31,32	1.63	5 (21%)	25,44,47	2.09	4 (16%)
32	PSU	z	39	32	16,21,22	1.81	4 (25%)	20,30,33	4.12	9 (45%)
32	7MG	z	46	32	20,26,27	2.88	7 (35%)	22,39,42	2.13	4 (18%)
32	5MU	z	54	32	14,22,23	2.02	4 (28%)	16,32,35	3.32	4 (25%)
32	PSU	z	55	32	16,21,22	2.08	1 (6%)	20,30,33	4.19	9 (45%)
32	4SU	z	8	32	14,21,22	1.94	4 (28%)	15,30,33	2.19	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PSU	0	55	33	-	0/7/25/26	0/2/2/2
31	2MG	y	1207	31	-	0/5/27/28	0/3/3/3
31	5MC	y	1400	31	-	0/3/25/26	0/2/2/2
31	4OC	y	1402	31	-	0/7/29/30	0/2/2/2
31	5MC	y	1404	31	-	0/3/25/26	0/2/2/2
31	5MC	y	1407	31	-	0/3/25/26	0/2/2/2
31	UR3	y	1498	31	-	0/3/25/26	0/2/2/2
31	MA6	y	1518	31	-	0/7/29/30	0/3/3/3
31	MA6	y	1519	31	-	0/7/29/30	0/3/3/3
31	PSU	y	516	31	-	0/7/25/26	0/2/2/2
31	7MG	y	527	31	-	0/7/37/38	0/3/3/3
31	M2G	y	966	31	-	0/7/29/30	0/3/3/3
31	5MC	y	967	31	-	0/3/25/26	0/2/2/2
32	H2U	z	16	32	-	0/7/38/39	0/2/2/2
32	H2U	z	20	32	-	0/7/38/39	0/2/2/2
32	PSU	z	32	32	-	0/7/25/26	0/2/2/2
32	MIA	z	37	32	-	0/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	z	39	32	-	0/7/25/26	0/2/2/2
32	7MG	z	46	32	-	0/7/37/38	0/3/3/3
32	5MU	z	54	32	-	0/3/25/26	0/2/2/2
32	PSU	z	55	32	-	0/7/25/26	0/2/2/2
32	4SU	z	8	32	-	0/3/25/26	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	z	55	PSU	C5-C1'	-7.21	1.46	1.52
31	y	527	7MG	C8-N9	-6.02	1.36	1.45
33	0	55	PSU	C5-C1'	-5.96	1.47	1.52
32	z	46	7MG	C8-N9	-5.62	1.37	1.45
32	z	39	PSU	C5-C1'	-4.65	1.48	1.52

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	55	PSU	N1-C2-N3	-12.81	119.19	128.40
32	z	32	PSU	N1-C2-N3	-12.75	119.23	128.40
32	z	39	PSU	N1-C2-N3	-12.54	119.38	128.40
31	y	516	PSU	N1-C2-N3	-12.22	119.61	128.40
31	y	1207	2MG	C4'-O4'-C1'	-12.16	96.83	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	55	PSU	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	w	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	926:A	O3'	928:G	P	1.97
1	w	1506:C	O3'	1508:A	P	1.96
1	w	890:A	O3'	892:G	P	1.94
1	w	1171:G	O3'	1173:G	P	1.94

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	w	2889/2889 (100%)	0.95	142 (4%) 30 23	5, 5, 117, 159	0
2	x	120/121 (99%)	1.02	4 (3%) 47 36	5, 13, 95, 127	0
3	A	127/229 (55%)	0.42	17 (13%) 4 4	5, 50, 148, 151	0
4	B	272/276 (98%)	0.57	27 (9%) 8 7	5, 60, 148, 155	0
5	C	201/206 (97%)	0.41	19 (9%) 9 7	5, 49, 148, 159	0
6	D	194/205 (94%)	0.04	7 (3%) 43 33	5, 55, 148, 165	0
7	E	180/182 (98%)	-0.05	12 (6%) 19 13	5, 58, 148, 156	0
8	F	173/180 (96%)	-0.31	5 (2%) 52 40	5, 67, 148, 160	0
9	G	148/148 (100%)	-0.21	5 (3%) 46 35	5, 43, 148, 151	0
10	H	138/163 (84%)	0.66	15 (10%) 6 6	5, 52, 147, 152	0
11	I	122/122 (100%)	0.64	11 (9%) 10 8	5, 35, 142, 148	0
12	J	146/150 (97%)	0.18	8 (5%) 26 19	5, 90, 150, 160	0
13	K	137/141 (97%)	1.50	46 (33%) 0 1	5, 24, 148, 152	0
14	L	118/118 (100%)	0.21	7 (5%) 23 16	5, 44, 148, 148	0
15	M	106/112 (94%)	0.95	21 (19%) 1 1	5, 48, 148, 160	0
16	N	137/146 (93%)	0.01	2 (1%) 74 62	5, 74, 150, 167	0
17	O	117/118 (99%)	0.46	18 (15%) 2 2	5, 35, 114, 148	0
18	P	101/101 (100%)	0.55	20 (19%) 1 1	5, 79, 148, 159	0
19	Q	109/113 (96%)	0.61	23 (21%) 1 1	5, 33, 137, 149	0
20	R	92/96 (95%)	0.41	12 (13%) 4 4	5, 73, 148, 161	0
21	S	103/110 (93%)	0.65	22 (21%) 1 1	5, 86, 160, 163	0
22	T	185/206 (89%)	-0.25	4 (2%) 62 50	5, 50, 148, 161	0
23	U	76/85 (89%)	0.75	13 (17%) 2 2	5, 57, 151, 166	0
24	V	88/98 (89%)	0.91	22 (25%) 1 1	5, 91, 148, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	62/72 (86%)	0.07	3 (4%) 31 23	5, 88, 149, 155	0
26	X	60/60 (100%)	-0.49	0 100 100	5, 36, 148, 150	0
27	Y	56/60 (93%)	0.26	8 (14%) 3 3	7, 77, 164, 168	0
28	Z	48/49 (97%)	0.41	3 (6%) 21 14	5, 5, 42, 126	0
29	a	63/65 (96%)	0.54	7 (11%) 6 6	5, 50, 151, 157	0
30	b	35/37 (94%)	1.91	12 (34%) 0 1	5, 102, 149, 153	0
31	y	1490/1522 (97%)	0.94	73 (4%) 30 23	5, 9, 113, 163	0
32	z	67/76 (88%)	0.79	2 (2%) 51 38	5, 6, 82, 117	0
33	0	75/76 (98%)	0.68	2 (2%) 55 43	5, 37, 129, 148	0
34	1	6/10 (60%)	0.73	0 100 100	5, 5, 54, 67	0
35	c	234/256 (91%)	-0.38	0 100 100	5, 50, 151, 165	0
36	d	206/239 (86%)	0.35	30 (14%) 3 3	5, 57, 148, 151	0
37	e	208/209 (99%)	-0.03	6 (2%) 52 40	5, 50, 148, 157	0
38	f	150/162 (92%)	0.09	10 (6%) 19 13	5, 62, 148, 154	0
39	g	101/101 (100%)	-0.09	4 (3%) 39 29	5, 72, 148, 156	0
40	h	155/156 (99%)	0.18	16 (10%) 7 6	5, 73, 155, 163	0
41	i	138/138 (100%)	-0.02	3 (2%) 62 50	5, 43, 148, 149	0
42	j	127/128 (99%)	0.56	18 (14%) 3 3	5, 85, 150, 154	0
43	k	98/105 (93%)	-0.03	7 (7%) 17 12	5, 83, 151, 164	0
44	l	116/129 (89%)	-0.06	8 (6%) 18 13	5, 71, 150, 162	0
45	m	124/132 (93%)	0.10	7 (5%) 25 18	5, 30, 148, 152	0
46	n	125/126 (99%)	-0.02	7 (5%) 25 18	5, 74, 148, 162	0
47	o	60/61 (98%)	2.19	27 (45%) 0 1	5, 66, 151, 161	0
48	p	88/89 (98%)	-0.31	1 (1%) 80 70	5, 57, 148, 163	0
49	q	83/88 (94%)	0.89	20 (24%) 1 1	5, 50, 148, 148	0
50	r	104/105 (99%)	0.41	8 (7%) 14 11	5, 52, 148, 158	0
51	s	73/88 (82%)	-0.53	0 100 100	5, 69, 149, 157	0
52	t	80/93 (86%)	-0.41	1 (1%) 77 66	5, 52, 148, 159	0
53	u	99/106 (93%)	1.07	22 (22%) 1 1	10, 66, 199, 199	0
54	v	24/27 (88%)	0.41	2 (8%) 12 10	5, 47, 139, 142	0
All	All	10434/10880 (95%)	0.57	789 (7%) 15 11	5, 32, 148, 199	0

The worst 5 of 789 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	49	ASP	10.2
15	M	81	GLY	9.5
14	L	58	GLY	9.1
47	o	13	THR	8.2
15	M	82	ILE	8.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	2MG	y	1207	24/25	0.87	0.28	-	21,22,26,26	0
32	7MG	z	46	24/25	0.82	0.24	-	5,5,12,12	0
31	PSU	y	516	20/21	0.78	0.27	-	137,138,148,148	0
32	H2U	z	20	20/21	0.77	0.41	-	124,124,133,133	0
33	PSU	0	55	20/21	0.70	0.25	-	36,36,36,36	0
32	MIA	z	37	29/30	0.77	0.33	-	20,26,32,32	0
31	M2G	y	966	25/26	0.83	0.30	-	15,16,20,31	0
31	4OC	y	1402	22/23	0.79	0.30	-	10,13,16,16	0
31	5MC	y	1404	21/22	0.87	0.33	-	5,6,8,9	0
31	UR3	y	1498	21/22	0.93	0.27	-	5,5,5,5	0
32	PSU	z	55	20/21	0.60	0.36	-	40,50,52,53	0
31	5MC	y	1407	21/22	0.94	0.22	-	25,28,30,30	0
32	PSU	z	39	20/21	0.89	0.26	-	5,5,5,5	0
32	H2U	z	16	20/21	0.78	0.48	-	80,92,93,95	0
32	4SU	z	8	20/21	0.84	0.28	-	5,5,5,5	0
31	7MG	y	527	24/25	0.89	0.25	-	7,10,24,26	0
32	5MU	z	54	21/22	0.88	0.28	-	5,5,5,5	0
31	MA6	y	1519	24/25	0.80	0.30	-	5,5,6,8	0
31	5MC	y	1400	21/22	0.90	0.26	-	5,5,5,5	0
31	MA6	y	1518	24/25	0.79	0.29	-	31,39,52,53	0
31	5MC	y	967	21/22	0.79	0.38	-	124,124,133,133	0
32	PSU	z	32	20/21	0.88	0.32	-	42,52,58,59	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.