



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 10:05 PM BST

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 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/ValidationPDFNotes.html>

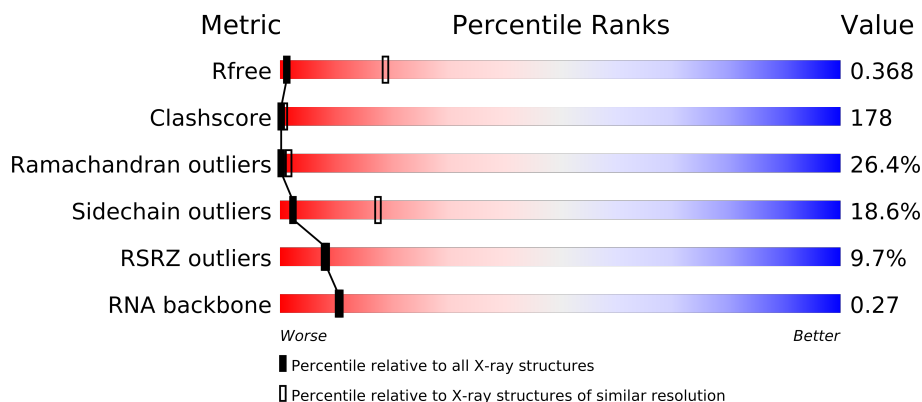
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance




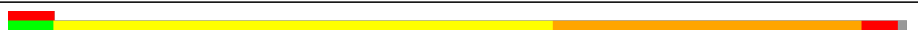

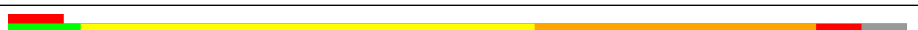
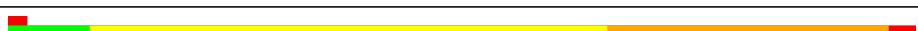
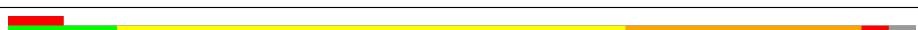




The reported resolution of this entry is 3.71 Å.

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}	66092	1103 (4.04-3.40)
Clashscore	79885	1026 (3.98-3.46)
Ramachandran outliers	78287	1082 (4.00-3.44)
Sidechain outliers	78261	1075 (4.00-3.44)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	w	2889	
2	x	121	
3	A	229	
4	B	276	
5	C	206	
6	D	205	
7	E	182	
8	F	180	
9	G	148	
10	H	163	
11	I	122	
12	J	150	

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Mol	Chain	Length	Quality of chain
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	
30	b	37	
31	y	1522	
32	z	76	
33	0	76	
34	l	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 hydrogen and 0 are deuterium.

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			

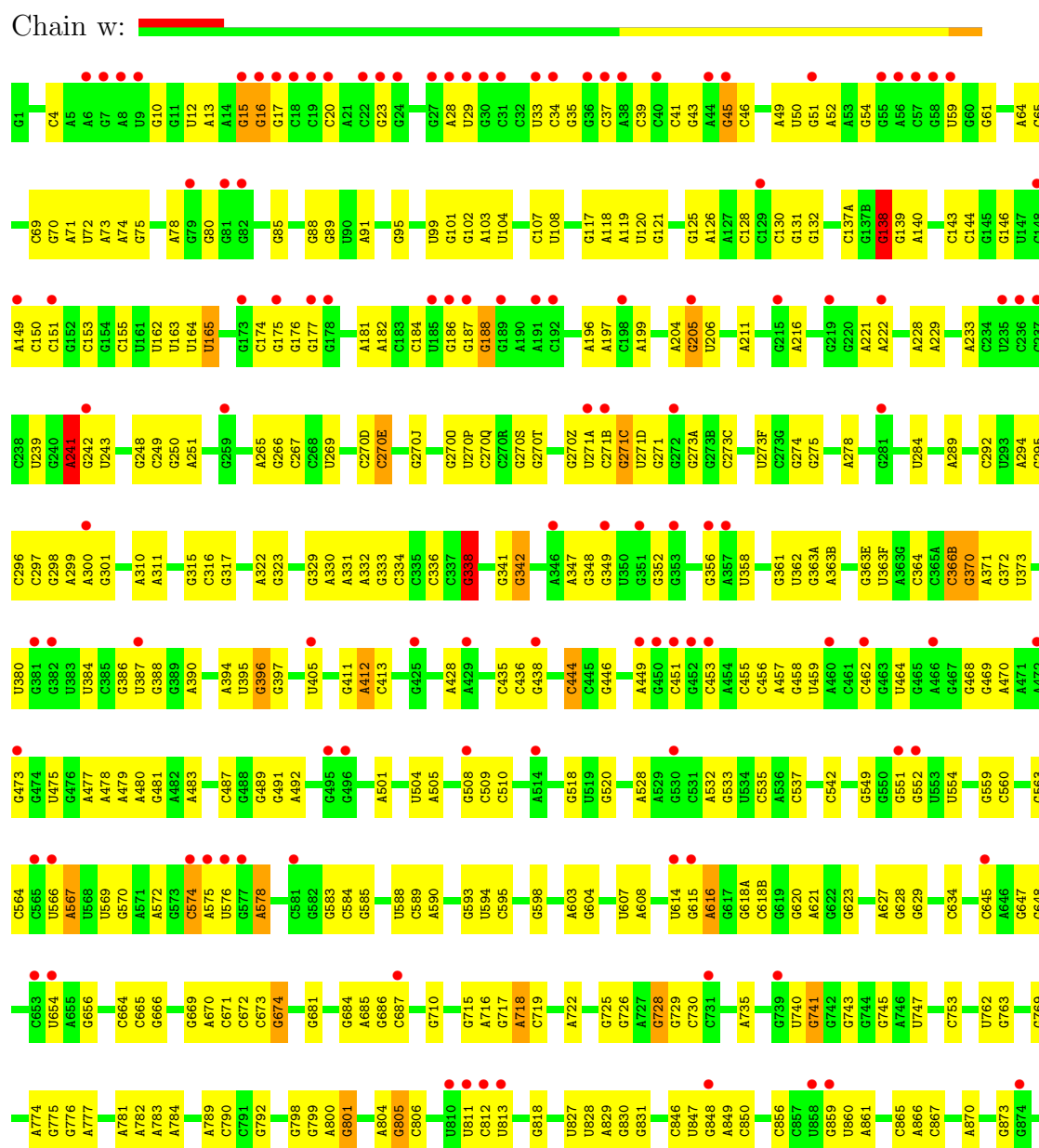
- Molecule 54 is a protein called 30S ribosomal protein Thx.

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

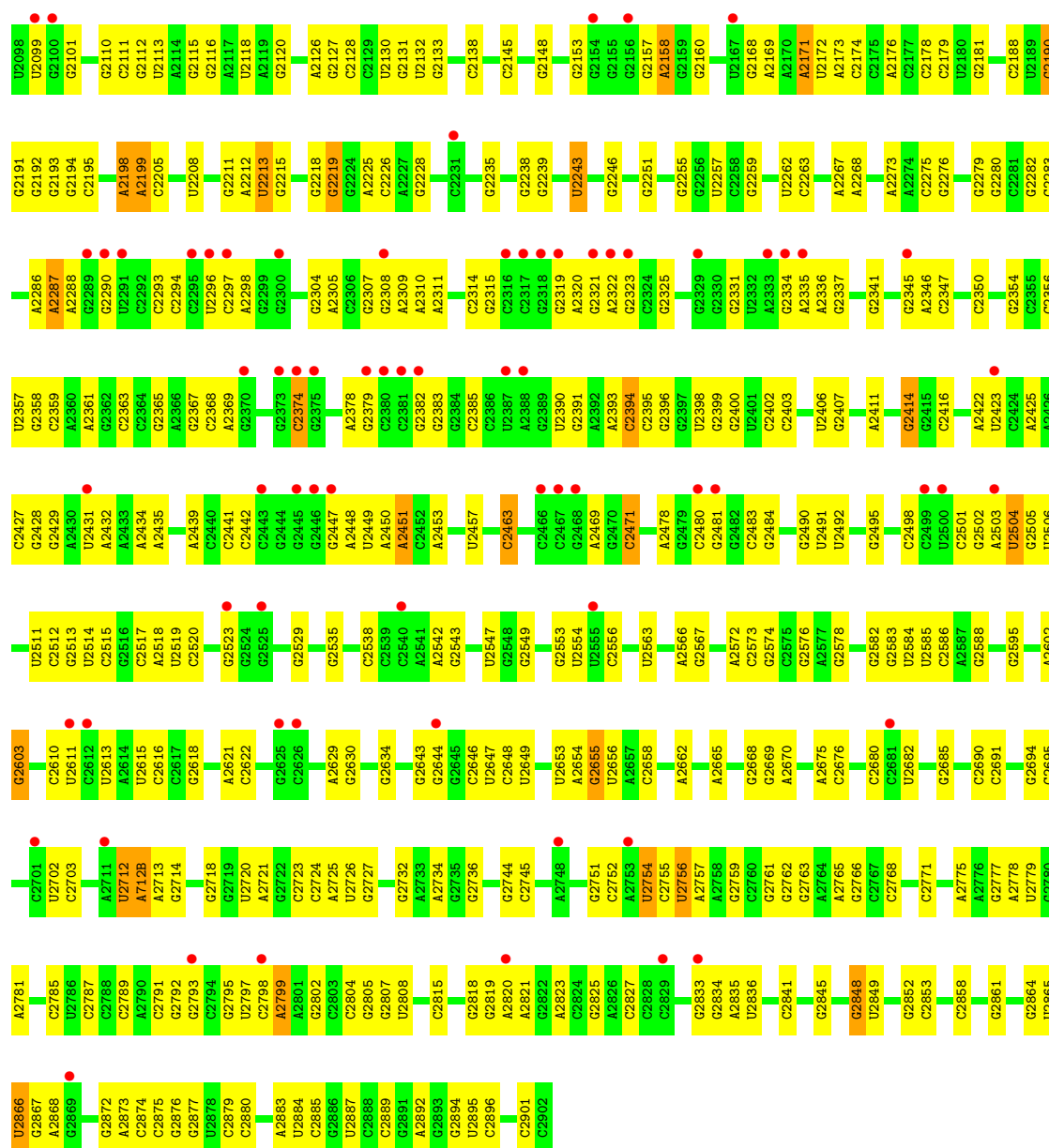
3 Residue-property plots

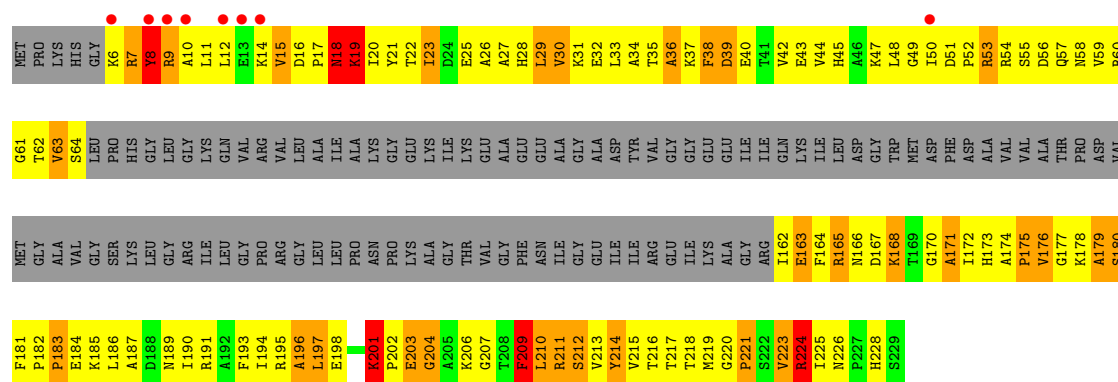
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



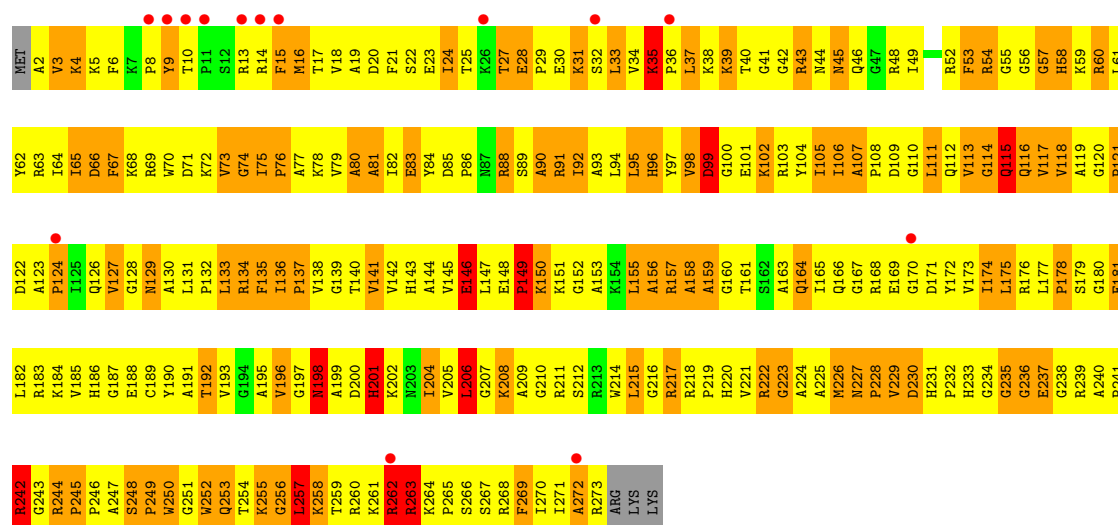
A2013	U1915	G1822	U1735	C1640	G1561	U1481	A1384	C1305	G1223	G1160	G1059	C964	A878
A2014	A1916	G1823	C1741	A1641	A1562	G1481	G1385	C1306	C1224	C1161	G1060	C965	G879
A2020	U1917	G1824	C1742	G1642	G1484	G1483	C1386	A1307	A1226	C1162	U1061	G966	G880
A2021	A1918	G1825	G1743	G1643	C1565	G1485	U1396	G1310	G1227	G1163	A1070	G972	G881
U2022	G1929	G1826	G1746	C1644	A1566	A1486	U1397	G1311	G1228	G1164	G1071	A973	G882
G2023	G1930	G1827	G1747	C1645	A1567	G1487	C1398	G1312	G1229	U1165	C1079	G974	G883
G2024	G1931	G1828	G1748	C1646	G1568	G1488	C1399	U1313	C1230	C1166	U1082	G975	C886
G2025	U1931	A1829	C1751	G1647	A1569	U1489	G1400	C1314	G1231	G1167	U1081	G976	A887
C2026	C1934	U1833	C1752	G1649	G1573	A1490	U1406	G1319	G1236	G1170	U1083	G977	C888
A2031	G1935	G1834	G1753	G1650	A1574	A1491	G1413	G1320	A1237	G1171	C1079	G978	A890
G2032	A1936	G1835	U1757	U1575	U1576	U1497	G1416	G1321	G1238	G1172	A1087	A980	U895
A2033	G1937	C1836	G1758	C1577	C1498	C1499	G1416	A1322	U1240	A1174	A1088	A981	A896
U2034	A1938	C1837	G1759	U1578	G1500	G1501	G1419	U1323	G1244	U1175	A982	A984	A897
G2035	C1838	G1839	A1759	A1579	G1502	G1503	U1420	G1324	G1245	A1177	G1093	A988	C898
C2036	U1943	G1840	G1763	C1662	G1585	C1506	G1421	G1325	G1246	C1178	U1094	A989	A899
U2041	U1944	G1841	G1764	C1663	G1586	A1509	G1422	U1326	A1247	C1179	C1098	A990	C902
G2042	G1945	G1842	G1773	A1664	A1587	A1510	G1423	G1327	G1248	C1180	G1099	A991	G906
C2043	A1953	C1843	C1774	A1665	A1588	C1508	G1424	U1328	U1249	G1181	C1100	C994	U907
U2047	U1954	G1846	U1777	A1669	A1589	A1509	G1425	G1329	G1250	A1182	C995	C996	G906
G2048	A1955	A1847	U1778	C1670	A1586	A1510	G1426	U1330	C1251	G1183	A1103	C997	C991
G2049	A1960	G1848	C1781	U1671	A1591	U1516	A1427	A1331	G1252	G1184	C1110	A996	A910
C2050	U1963	G1849	C1782	U1672	C1592	G1517	G1429	G1332	G1253	C1185	G1111	A997	A911
A2051	G1964	U1851	A1783	U1673	G1593	C1518	C1430	G1333	U1255	G1186	G1112	C1005	C912
G2052	G1965	G1852	G1784	G1682	A1596	G1519	G1436	U1334	G1256	G1187	C1113	C1006	U913
C2053	A1966	G1853	A1785	C1683	A1596	U1520	G1437	A1336	G1256	U1188	C1114	C1007	C914
A2054	G1967	G1854	U1786	G1683	G1601	G1522	U1438	G1337	C1261	A1189	C1116	C1008	G915
G2055	U1968	U1858	A1787	U1688	U1602	U1523	U1439	U1341	G1262	G1191	G1122	A1009	A917
C2056	G1969	A1859	C1791	A1603	A1604	G1526	A1448	A1342	A1264	A1194	G1125	A1010	A918
A2057	U1970	G1864	G1792	C1605	C1606	U1527	C1445	G1343	A1265	G1195	G1126	G1011	G920
G2058	A1971	U1869	C1793	G1607	G1608	A1528	G1448	G1344	G1266	C1196	A1126	U1012	G921
A2060	U1972	C1694	C1694	G1607	A1608	A1529	A1498	C1345	U1267	G1197	A1127	C1013	A926
G2061	G1973	G1695	G1795	A1609	A1610	G1530	G1449	G1346	C1270	U1198	A1128	U1014	G931
A2062	C1974	U1796	U1796	A1609	A1610	C1531	C1450	G1347	G1271	U1199	A1129	G1015	G932
G1975	C1975	G1879	C1797	A1610	A1610	U1535	A1451	G1348	A1272	U1199	U1130	G1016	G933
C2064	U1976	G1880	U1798	A1700	A1700	U1536	A1453	A1349	U1273	C1201	G1131	G1017	A933
C2065	A1977	C1885	G1800	A1701	G1613	A1536	U1454	C1350	A1274	A1204	A1132	A1020	G938
C2066	U1978	A1885	G1801	G1702	G1613	C1537	G1455	C1351	A1275	U1205	U1133	A1021	G939
G2069	A1981	C1886	G1802	G1703	A1616	G1538	G1456	G1358	A1276	G1206	G1136	G1022	G940
G2070	C1982	G1888	A1803	U1706	C1617	U1540	A1457	A1359	G1277	G1209	G1137	G1023	G943
A2071	G1987	A1889	C1806	G1707	G1619	U1541	C1459	C1362	A1278	U1211	G1138	G1024	G944
U2076	U1991	U1898	G1807	U1712	G1623	A1543	A1461	G1363	G1283	U1210	C1146	U1033	A945
A2077	G1992	G1899	U1808	U1716	C1626	C1544	G1465	G1364	A1287	G1212	U1141	U1034	G946
C2078	U1993	A1900	A1810	G1717	G1627	A1545	G1466	A1365	U1288	A1213	C1142	U1035	G954
G2087	C1994	G1903	G1811	G1725	G1628	C1546	C1467	A1367	A1289	G1216	A1148	G1043	U958
U2089	U1995	G1906	A1815	G1729	G1630	C1547	G1470	G1374	C1295	G1217	A1149	A1045	A959
G2090	C1996	C1909	G1816	U1730	C1636	U1547	A1471	G1377	G1296	C1218	G1149	A1046	A960
U2091	G1997	C1909	G1817	U1731	G1636	A1553	A1474	A1378	C1297	A1220	C1152	G1047	G962
U2092	G1998	U1818	U1818	G1731	A1634	A1558	C1474	A1379	U1300	C1221	C1155	A1054	U963
G2093	C1999	A1912	A1819	A1732	G1635	G1559	G1478	C1383	A1301	C122A			
U2096	G2000	A1913	U1820	G1733	A1634	A1560							
C2097	G2012	C1914	A1821	C1734									





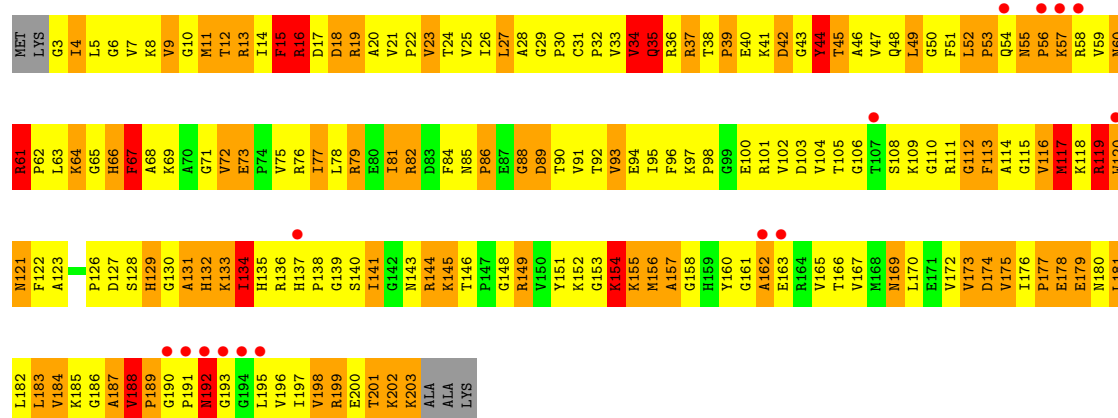
• Molecule 4: 50S ribosomal protein L2

Chain B:



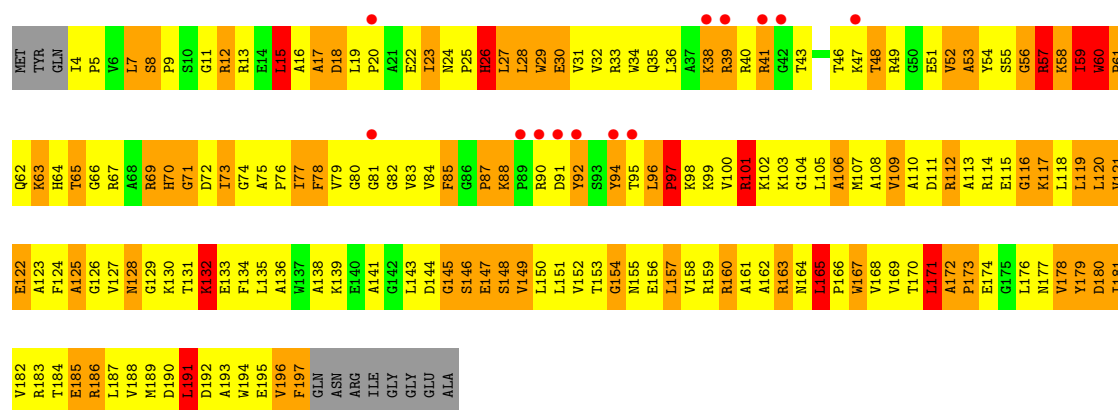
• Molecule 5: 50S ribosomal protein L3

Chain C:



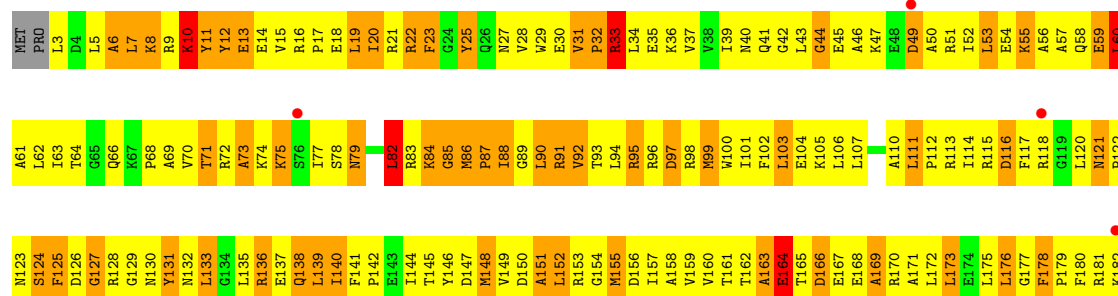
• Molecule 6: 50S ribosomal protein L4

Chain D:



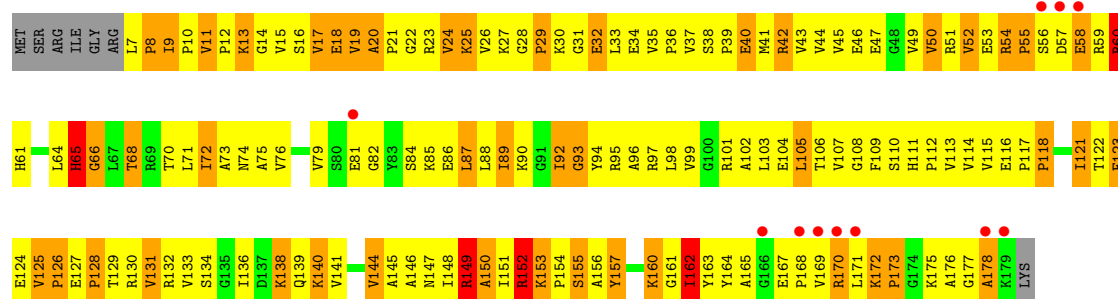
• Molecule 7: 50S ribosomal protein L5

Chain E:



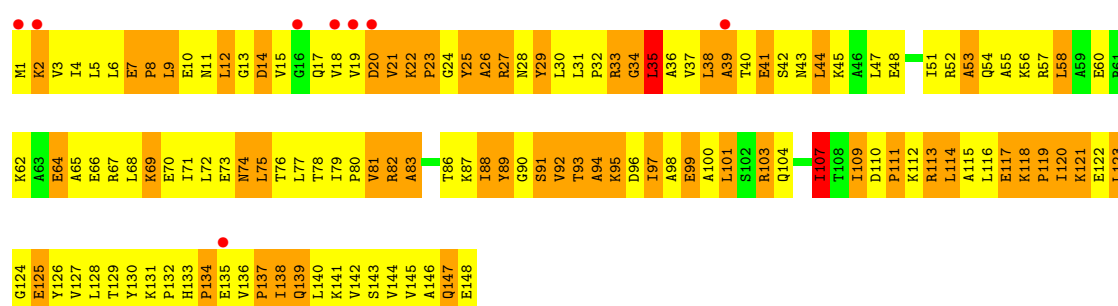
• Molecule 8: 50S ribosomal protein L6

Chain F:



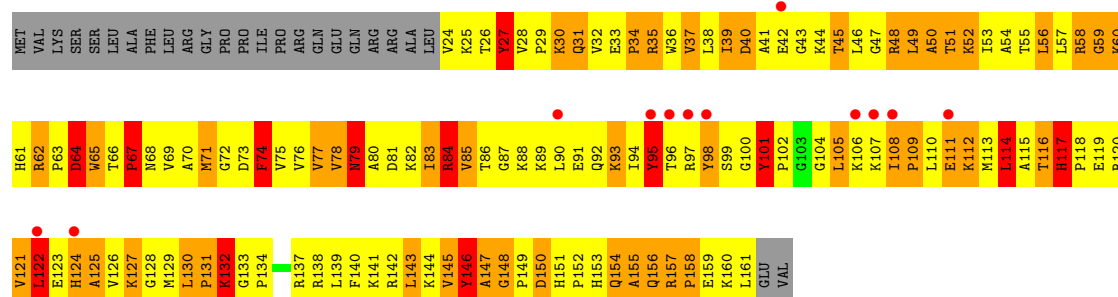
• Molecule 9: 50S ribosomal protein L9

Chain G:



- Molecule 10: 50S ribosomal protein L13

Chain H:



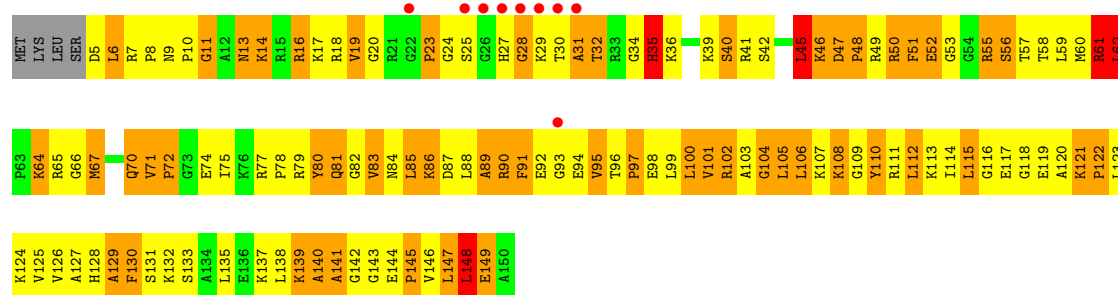
- Molecule 11: 50S ribosomal protein L14

Chain I:



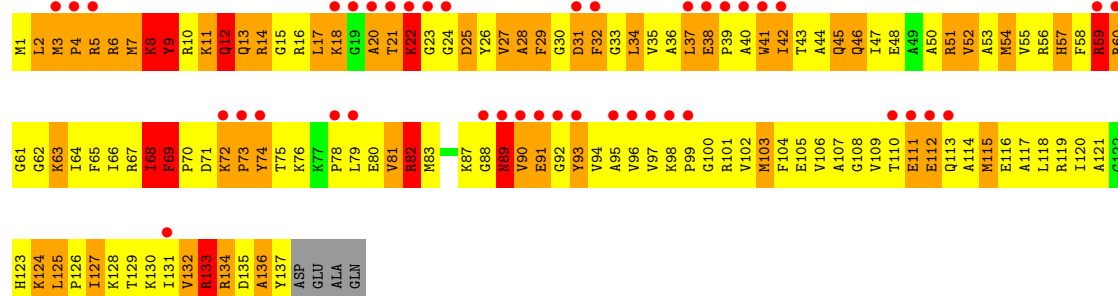
- Molecule 12: 50S ribosomal protein L15

Chain J:

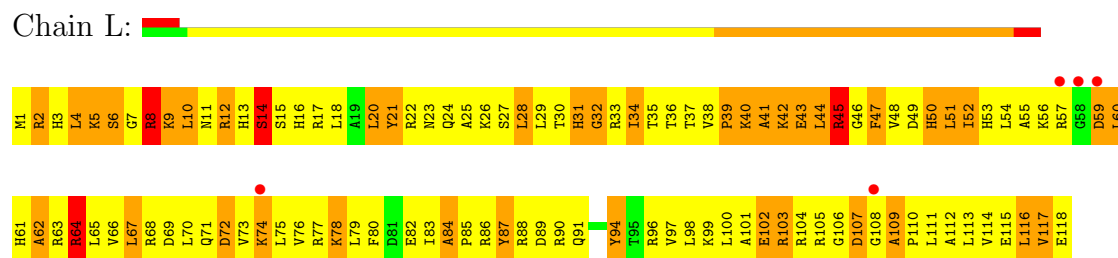


- Molecule 13: 50S ribosomal protein L16

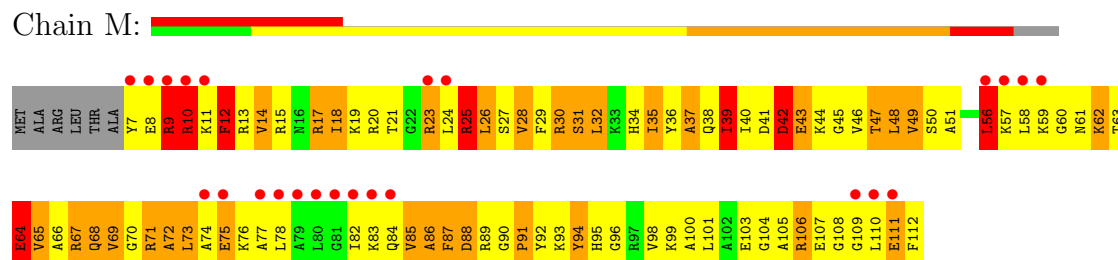
Chain K:



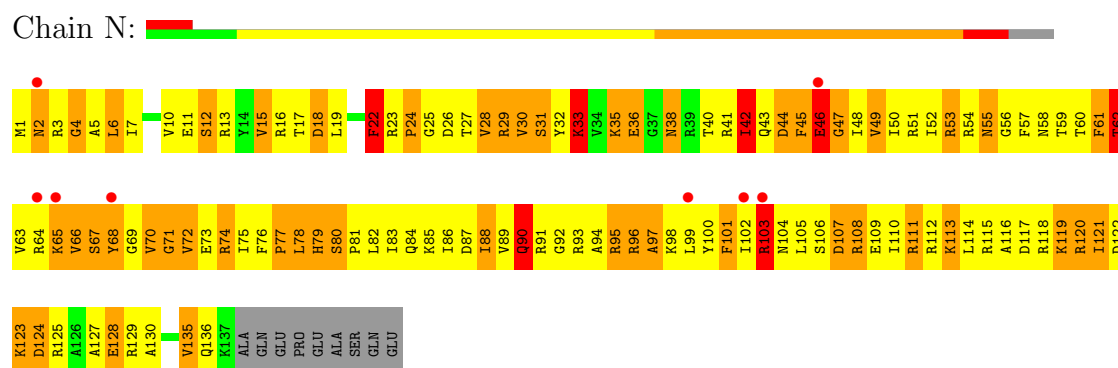
- Molecule 14: 50S ribosomal protein L17



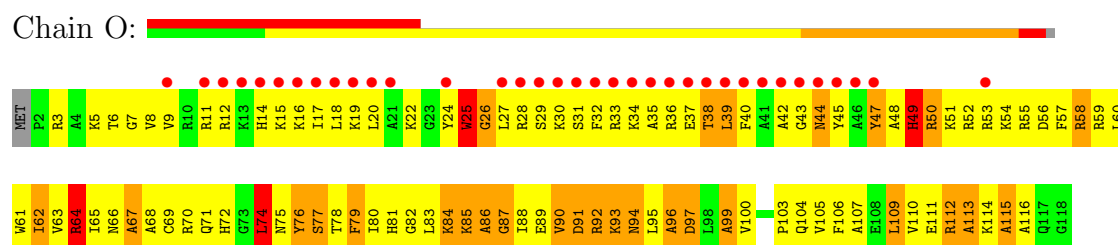
- Molecule 15: 50S ribosomal protein L18



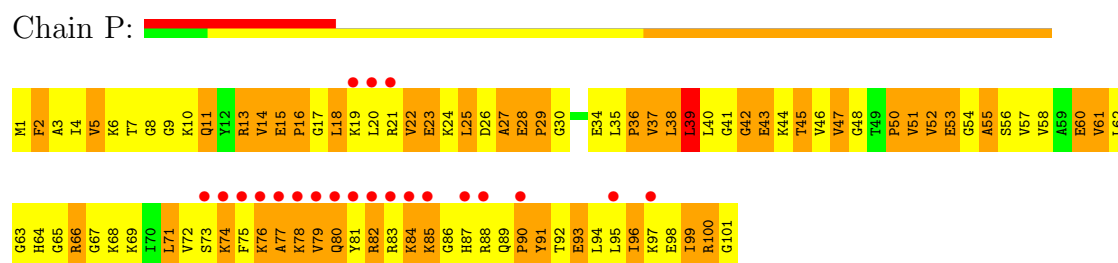
- Molecule 16: 50S ribosomal protein L19



- Molecule 17: 50S ribosomal protein L20

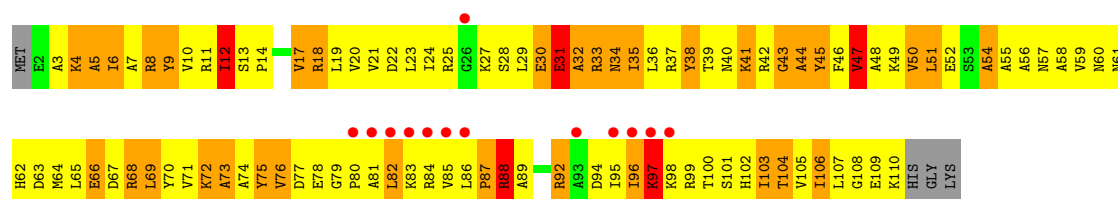


- Molecule 18: 50S ribosomal protein L21



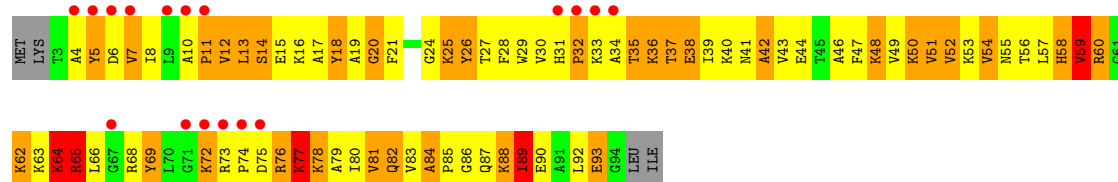
- Molecule 19: 50S ribosomal protein L22

Chain Q:



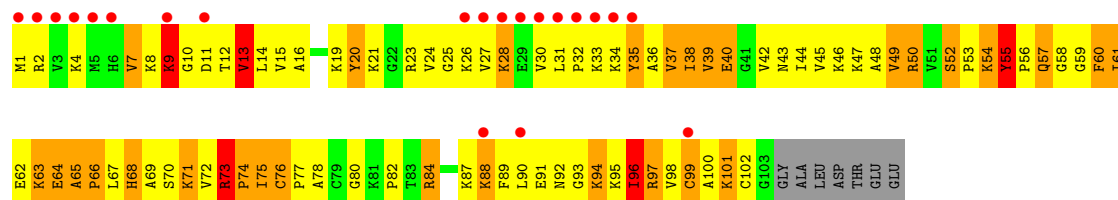
- Molecule 20: 50S ribosomal protein L23

Chain R:



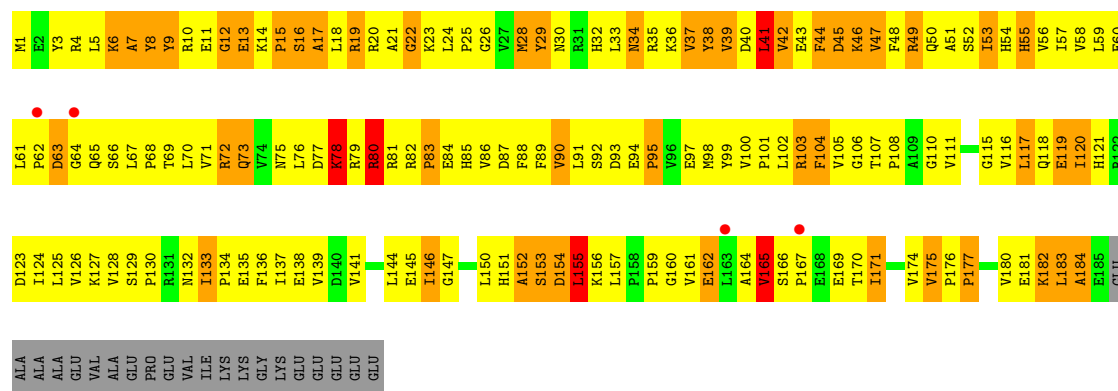
- Molecule 21: 50S ribosomal protein L24

Chain S:



- Molecule 22: 50S ribosomal protein L25

Chain T:



- Molecule 23: 50S ribosomal protein L27

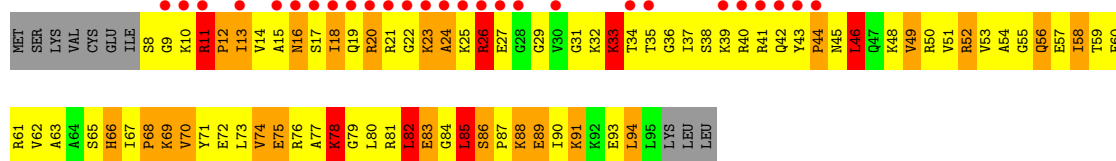
Chain U:





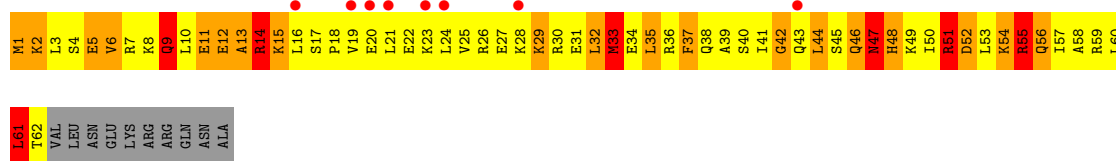
- Molecule 24: 50S ribosomal protein L28

Chain V:



- Molecule 25: 50S ribosomal protein L29

Chain W:



- Molecule 26: 50S ribosomal protein L30

Chain X:



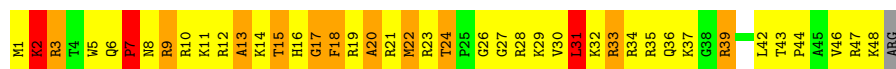
- Molecule 27: 50S ribosomal protein L32

Chain Y:



- Molecule 28: 50S ribosomal protein L34

Chain Z:



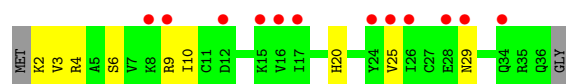
- Molecule 29: 50S ribosomal protein L35

Chain a:



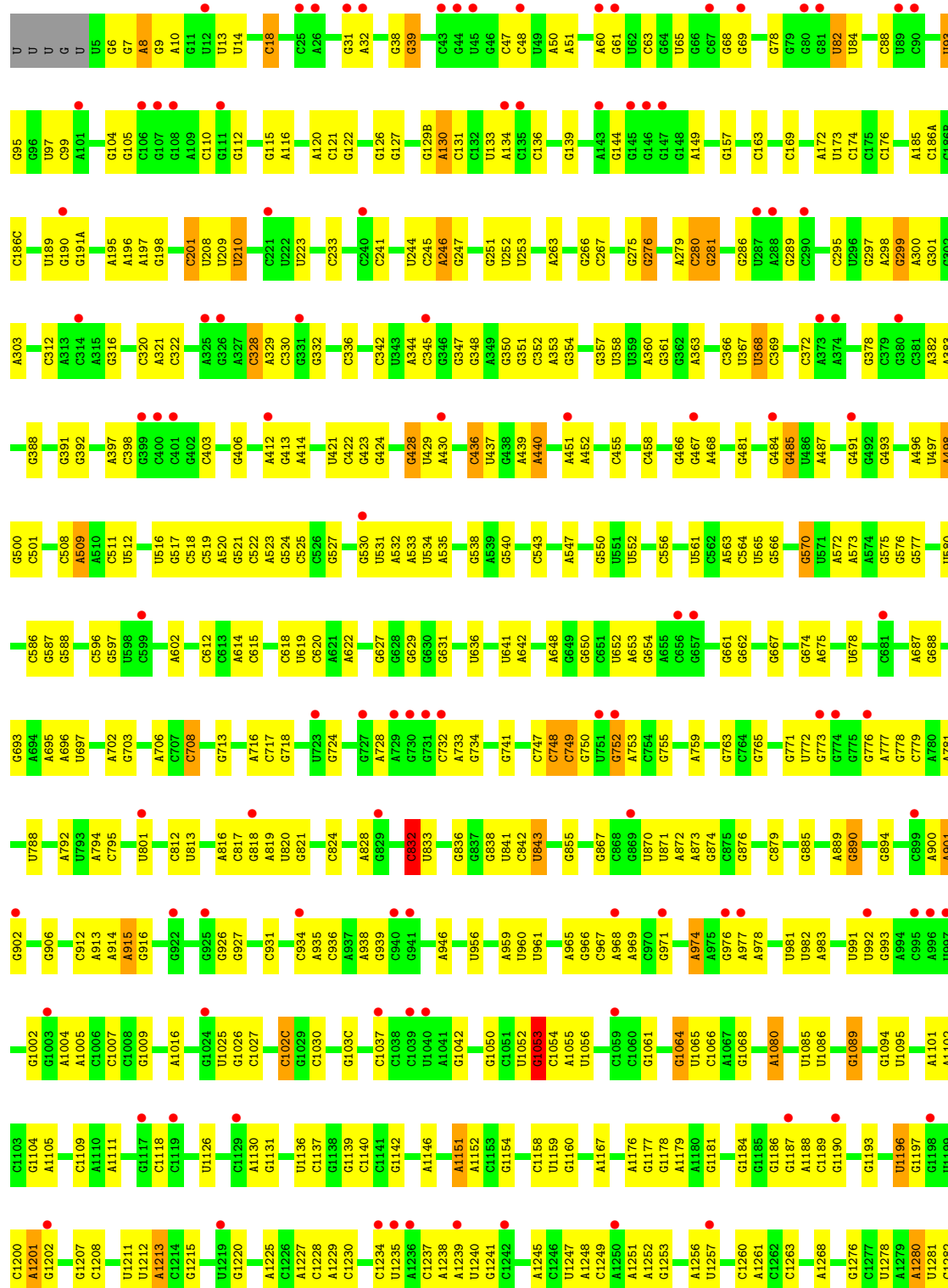
- Molecule 30: 50S ribosomal protein L36

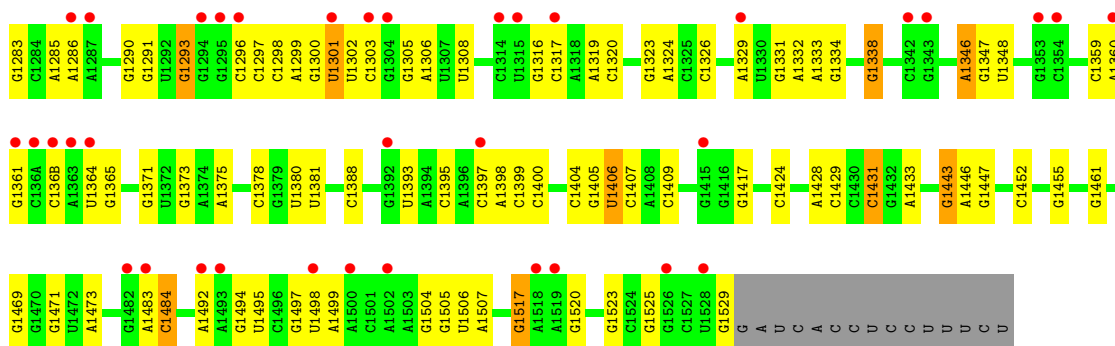
Chain b:



• Molecule 31: 16S SMALL SUBUNIT RIBOSOMAL RNA

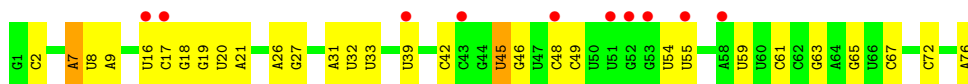
Chain y:





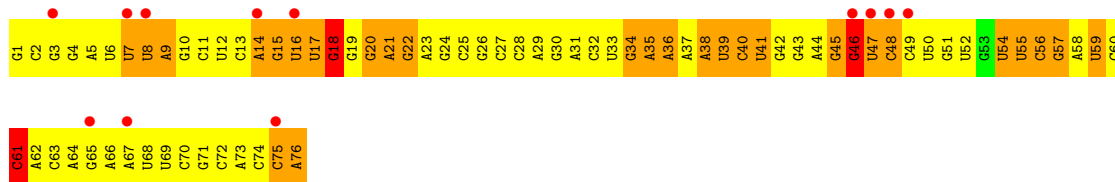
• Molecule 32: P-site PHE-tRNA

Chain z:



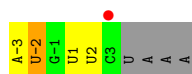
• Molecule 33: E-TRNA

Chain 0:



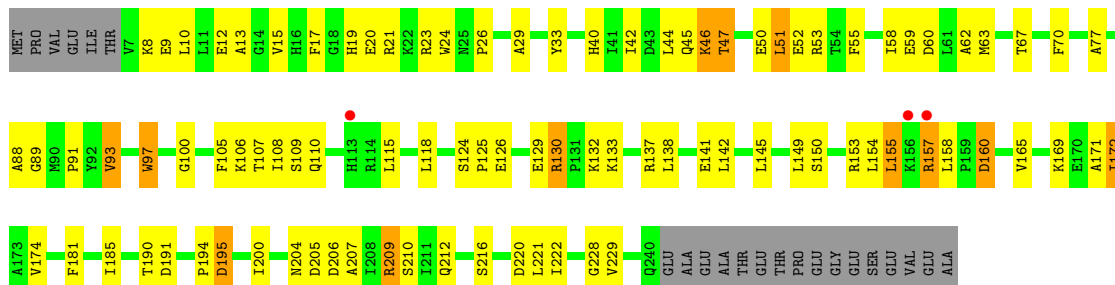
• Molecule 34: MRNA

Chain 1:



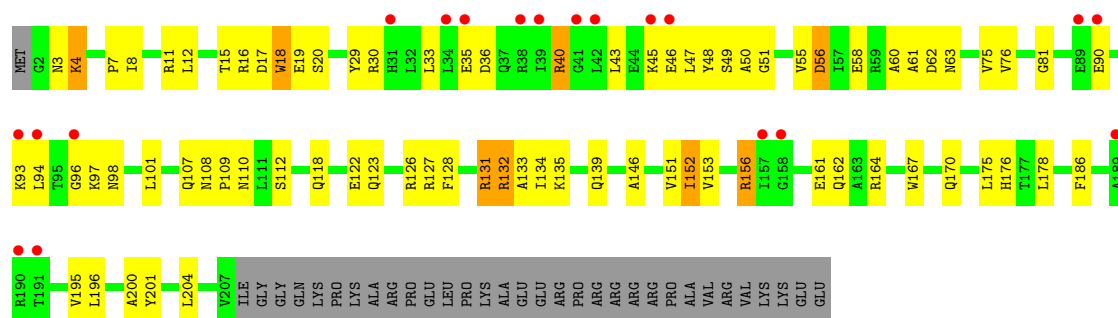
• Molecule 35: 30S ribosomal protein S2

Chain c:



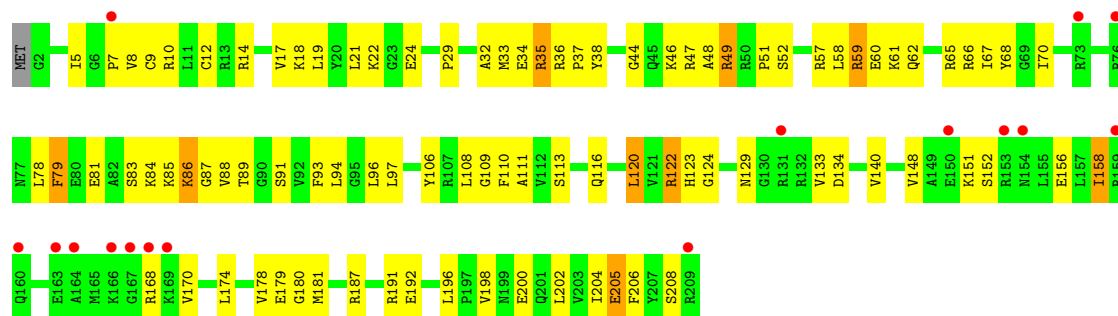
• Molecule 36: 30S ribosomal protein S3

Chain d:



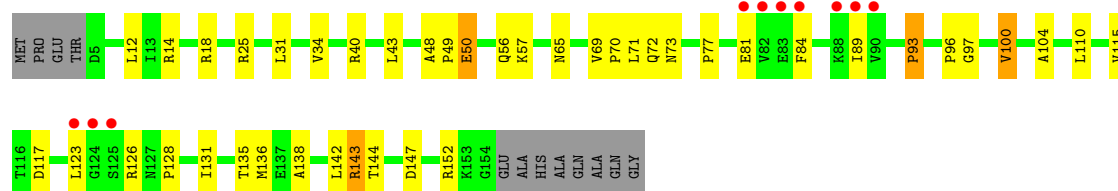
• Molecule 37: 30S ribosomal protein S4

Chain e:



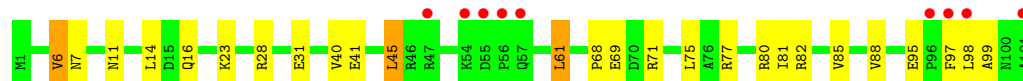
• Molecule 38: 30S ribosomal protein S5

Chain f:



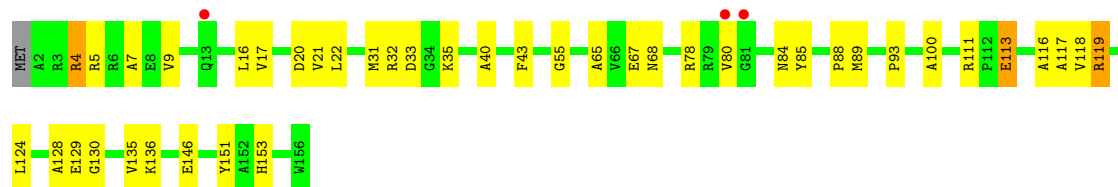
• Molecule 39: 30S ribosomal protein S6

Chain g:



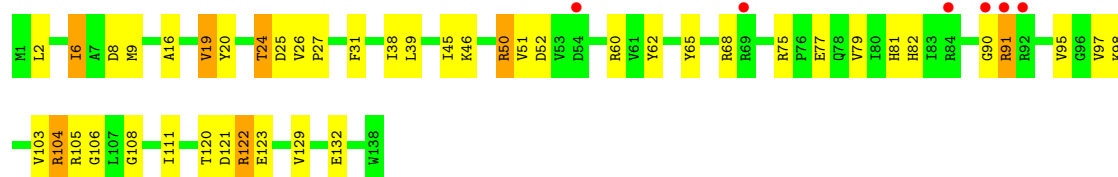
• Molecule 40: 30S ribosomal protein S7

Chain h:



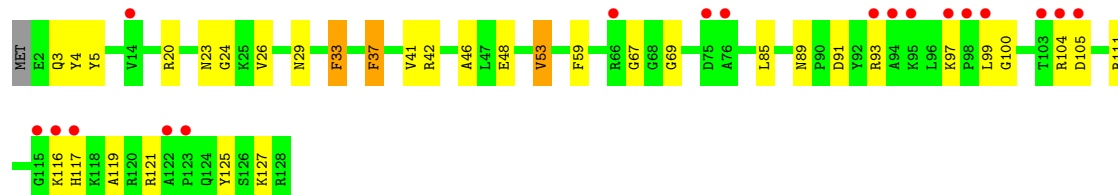
• Molecule 41: 30S ribosomal protein S8

Chain i:



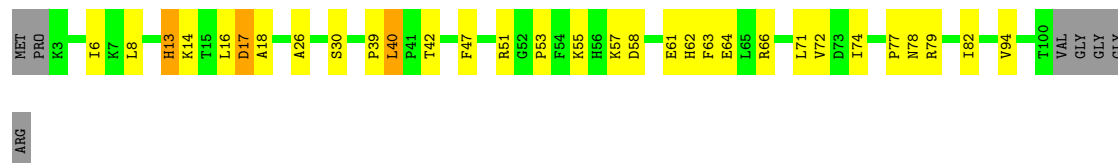
- Molecule 42: 30S ribosomal protein S9

Chain j:



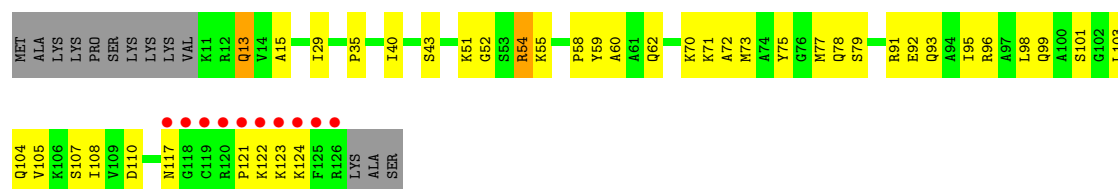
- Molecule 43: 30S ribosomal protein S10

Chain k:



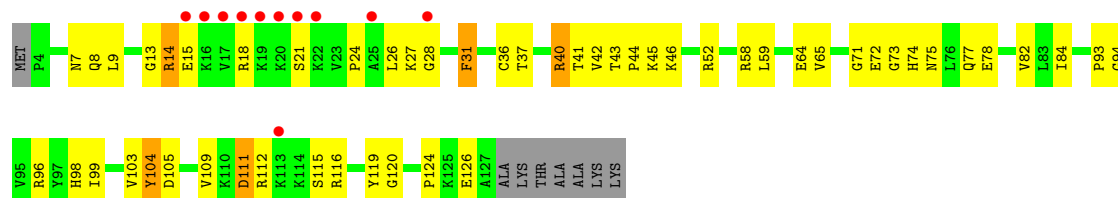
- Molecule 44: 30S ribosomal protein S11

Chain l:



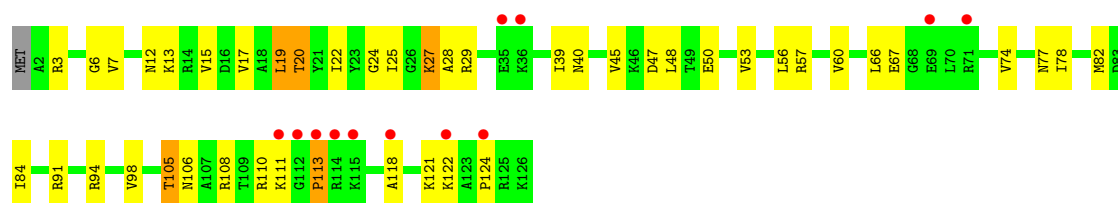
- Molecule 45: 30S ribosomal protein S12

Chain m:



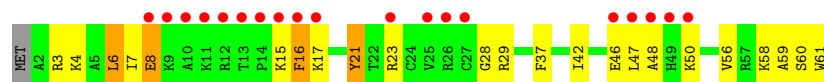
- Molecule 46: 30S ribosomal protein S13

Chain n:



- Molecule 47: 30S ribosomal protein S14

Chain o:



- Molecule 48: 30S ribosomal protein S15

Chain p:



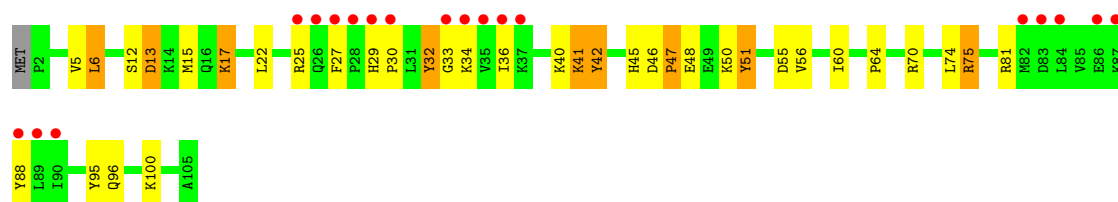
- Molecule 49: 30S ribosomal protein S16

Chain q:



- Molecule 50: 30S ribosomal protein S17

Chain r:



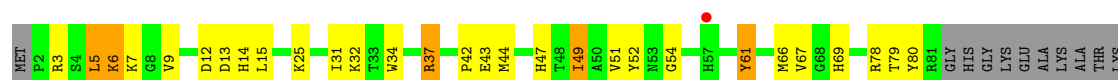
- Molecule 51: 30S ribosomal protein S18

Chain s:



- Molecule 52: 30S ribosomal protein S19

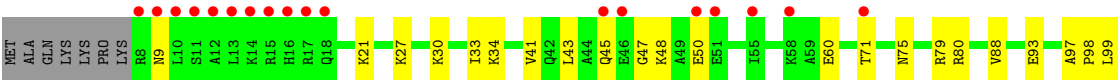
Chain t:



LYS
LYS

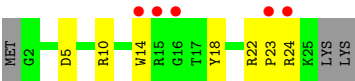
• Molecule 53: 30S ribosomal protein S20

Chain u:



• Molecule 54: 30S ribosomal protein Thx

Chain v:



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 0.363 , 0.368	Depositor DCC
R_{free} test set	11428 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 , 446.3	EDS
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
L-test for twinning	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	4 of 459965 reflections (0.001%)	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1517	0	1565	619	0
7	E	1468	0	1529	570	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	p	734	0	771	0	0
49	q	700	0	720	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 178.

The worst 5 of 10655 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	270/276 (98%)	103 (38%)	84 (31%)	83 (31%)	0	1
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	2
8	F	171/180 (95%)	76 (44%)	53 (31%)	42 (25%)	0	2
9	G	146/148 (99%)	75 (51%)	30 (20%)	41 (28%)	0	1
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	1
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	1
14	L	116/118 (98%)	60 (52%)	28 (24%)	28 (24%)	0	2
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	1
17	O	115/118 (98%)	64 (56%)	27 (24%)	24 (21%)	0	3
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	2
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	1
22	T	183/206 (89%)	104 (57%)	41 (22%)	38 (21%)	0	3
23	U	74/85 (87%)	35 (47%)	23 (31%)	16 (22%)	0	3
24	V	86/98 (88%)	30 (35%)	31 (36%)	25 (29%)	0	1
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	5
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	2
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	5
35	c	232/256 (91%)	109 (47%)	66 (28%)	57 (25%)	0	2
36	d	204/239 (85%)	98 (48%)	49 (24%)	57 (28%)	0	1
37	e	206/209 (99%)	99 (48%)	44 (21%)	63 (31%)	0	1
38	f	148/162 (91%)	89 (60%)	33 (22%)	26 (18%)	0	6

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

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%)	5	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	B	214/218 (98%)	169 (79%)	45 (21%)	1	12
5	C	163/166 (98%)	126 (77%)	37 (23%)	1	10
6	D	154/162 (95%)	123 (80%)	31 (20%)	2	14
7	E	154/156 (99%)	127 (82%)	27 (18%)	3	21
8	F	142/148 (96%)	124 (87%)	18 (13%)	6	39
9	G	124/124 (100%)	103 (83%)	21 (17%)	3	24
10	H	117/139 (84%)	90 (77%)	27 (23%)	1	9
11	I	100/100 (100%)	79 (79%)	21 (21%)	1	12
12	J	112/116 (97%)	89 (80%)	23 (20%)	2	13
13	K	108/111 (97%)	77 (71%)	31 (29%)	0	5
14	L	101/101 (100%)	79 (78%)	22 (22%)	1	11
15	M	84/88 (96%)	66 (79%)	18 (21%)	1	12
16	N	121/128 (94%)	97 (80%)	24 (20%)	2	15
17	O	93/94 (99%)	79 (85%)	14 (15%)	4	30
18	P	82/82 (100%)	70 (85%)	12 (15%)	5	31
19	Q	89/92 (97%)	72 (81%)	17 (19%)	2	16
20	R	74/78 (95%)	62 (84%)	12 (16%)	3	26
21	S	86/91 (94%)	75 (87%)	11 (13%)	6	39
22	T	163/179 (91%)	140 (86%)	23 (14%)	5	34
23	U	61/67 (91%)	47 (77%)	14 (23%)	1	9
24	V	73/83 (88%)	60 (82%)	13 (18%)	2	20
25	W	58/67 (87%)	42 (72%)	16 (28%)	0	6
26	X	52/52 (100%)	41 (79%)	11 (21%)	1	12
27	Y	49/52 (94%)	44 (90%)	5 (10%)	11	51
28	Z	41/42 (98%)	32 (78%)	9 (22%)	1	11
29	a	53/55 (96%)	39 (74%)	14 (26%)	1	7
30	b	33/34 (97%)	30 (91%)	3 (9%)	14	58
35	c	202/220 (92%)	154 (76%)	48 (24%)	1	8
36	d	160/188 (85%)	130 (81%)	30 (19%)	2	17
37	e	180/181 (99%)	143 (79%)	37 (21%)	2	13
38	f	115/123 (94%)	94 (82%)	21 (18%)	2	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	g	90/90 (100%)	75 (83%)	15 (17%)	3	24
40	h	126/127 (99%)	110 (87%)	16 (13%)	6	39
41	i	119/119 (100%)	97 (82%)	22 (18%)	2	18
42	j	98/99 (99%)	82 (84%)	16 (16%)	3	26
43	k	88/92 (96%)	76 (86%)	12 (14%)	5	36
44	l	88/99 (89%)	72 (82%)	16 (18%)	2	19
45	m	104/109 (95%)	85 (82%)	19 (18%)	2	18
46	n	100/101 (99%)	85 (85%)	15 (15%)	4	30
47	o	49/50 (98%)	39 (80%)	10 (20%)	2	13
48	p	79/80 (99%)	65 (82%)	14 (18%)	3	20
49	q	72/74 (97%)	60 (83%)	12 (17%)	3	24
50	r	96/97 (99%)	76 (79%)	20 (21%)	2	12
51	s	64/77 (83%)	52 (81%)	12 (19%)	2	17
52	t	71/80 (89%)	58 (82%)	13 (18%)	2	18
53	u	76/82 (93%)	70 (92%)	6 (8%)	18	65
54	v	19/22 (86%)	16 (84%)	3 (16%)	4	28
All	All	4803/5116 (94%)	3912 (81%)	891 (19%)	2	17

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%)	5 (6%)
34	1	5/10 (50%)	2 (40%)	0
All	All	4659/4694 (99%)	1742 (37%)	5 (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

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	0	7	U
33	0	9	A
33	0	46	G
33	0	48	C
33	0	56	C

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	19,21,22	5.15	4 (21%)	23,30,33	2.93	7 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	2MG	y	1207	31	24,26,27	1.72	3 (12%)	33,38,41	5.36	8 (24%)
31	5MC	y	1400	31	20,22,23	1.38	3 (15%)	26,32,35	1.87	6 (23%)
31	4OC	y	1402	31	21,23,24	1.59	4 (19%)	26,32,35	1.91	7 (26%)
31	5MC	y	1404	31	20,22,23	1.79	4 (20%)	26,32,35	2.12	5 (19%)
31	5MC	y	1407	31	20,22,23	1.53	4 (20%)	26,32,35	1.78	6 (23%)
31	UR3	y	1498	31	20,22,23	2.02	6 (30%)	23,32,35	1.66	6 (26%)
31	MA6	y	1518	31	26,26,27	1.74	5 (19%)	37,38,41	2.50	12 (32%)
31	MA6	y	1519	31	26,26,27	2.14	5 (19%)	37,38,41	2.35	12 (32%)
31	PSU	y	516	31	19,21,22	2.68	3 (15%)	23,30,33	1.84	6 (26%)
31	7MG	y	527	31	24,26,27	3.34	8 (33%)	34,39,42	1.88	5 (14%)
31	M2G	y	966	31	25,27,28	2.51	6 (24%)	35,40,43	4.24	8 (22%)
31	5MC	y	967	31	20,22,23	1.16	1 (5%)	26,32,35	1.60	3 (11%)
32	H2U	z	16	32	19,21,22	1.36	2 (10%)	27,30,33	1.08	3 (11%)
32	H2U	z	20	32	19,21,22	1.25	1 (5%)	27,30,33	1.04	2 (7%)
32	PSU	z	32	32	19,21,22	2.85	4 (21%)	23,30,33	1.81	5 (21%)
32	MIA	z	37	32	29,31,32	1.79	7 (24%)	41,44,47	1.77	5 (12%)
32	PSU	z	39	32	19,21,22	3.28	4 (21%)	23,30,33	1.88	7 (30%)
32	7MG	z	46	32	24,26,27	3.36	9 (37%)	34,39,42	1.97	8 (23%)
32	5MU	z	54	32	20,22,23	2.04	5 (25%)	25,32,35	2.27	6 (24%)
32	PSU	z	55	32	19,21,22	3.13	3 (15%)	23,30,33	2.37	7 (30%)
32	4SU	z	8	32	19,21,22	2.74	8 (42%)	23,30,33	4.36	7 (30%)

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	-	0/8/25/26	0/2/2/2
31	2MG	y	1207	31	-	0/10/27/28	0/3/3/3
31	5MC	y	1400	31	-	0/6/25/26	0/2/2/2
31	4OC	y	1402	31	-	0/10/29/30	0/2/2/2
31	5MC	y	1404	31	-	0/6/25/26	0/2/2/2
31	5MC	y	1407	31	-	0/6/25/26	0/2/2/2
31	UR3	y	1498	31	-	0/6/25/26	0/2/2/2
31	MA6	y	1518	31	-	0/13/29/30	0/3/3/3
31	MA6	y	1519	31	-	0/13/29/30	0/3/3/3
31	PSU	y	516	31	-	0/8/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	7MG	y	527	31	-	0/8/37/38	0/3/3/3
31	M2G	y	966	31	-	0/12/29/30	0/3/3/3
31	5MC	y	967	31	-	0/6/25/26	0/2/2/2
32	H2U	z	16	32	-	0/8/38/39	0/2/2/2
32	H2U	z	20	32	-	0/8/38/39	0/2/2/2
32	PSU	z	32	32	-	0/8/25/26	0/2/2/2
32	MIA	z	37	32	-	1/16/33/34	0/3/3/3
32	PSU	z	39	32	-	0/8/25/26	0/2/2/2
32	7MG	z	46	32	-	0/8/37/38	0/3/3/3
32	5MU	z	54	32	-	0/6/25/26	0/2/2/2
32	PSU	z	55	32	-	0/8/25/26	0/2/2/2
32	4SU	z	8	32	-	0/6/25/26	0/2/2/2

The worst 5 of 99 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	0	55	PSU	O2-C2	20.88	1.48	1.21
32	z	39	PSU	O2-C2	12.54	1.38	1.21
31	y	527	7MG	C8-N9	-12.22	1.36	1.46
32	z	46	7MG	C8-N9	-11.45	1.37	1.46
32	z	32	PSU	O2-C2	11.19	1.36	1.21

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	1207	2MG	C6-C5-N7	-26.85	130.53	134.14
31	y	966	M2G	C6-C5-N7	-22.38	131.13	134.14
32	z	8	4SU	C4-N3-C2	19.06	122.42	121.60
31	y	1207	2MG	C4'-O4'-C1'	-11.73	96.83	109.72
33	0	55	PSU	C5-C1'-C2'	-9.22	98.62	115.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	z	37	MIA	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	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%)	1.27	282 (9%) 8 8	5, 5, 117, 159	0
2	x	120/121 (99%)	1.36	24 (20%) 2 2	5, 13, 95, 127	0
3	A	127/229 (55%)	0.28	8 (6%) 19 13	5, 50, 148, 151	0
4	B	272/276 (98%)	0.52	14 (5%) 27 17	5, 60, 148, 155	0
5	C	201/206 (97%)	0.53	15 (7%) 14 11	5, 49, 148, 159	0
6	D	194/205 (94%)	0.32	13 (6%) 17 13	5, 55, 148, 165	0
7	E	180/182 (98%)	0.20	4 (2%) 59 37	5, 58, 148, 156	0
8	F	173/180 (96%)	0.18	11 (6%) 19 13	5, 67, 148, 160	0
9	G	148/148 (100%)	0.07	8 (5%) 25 16	5, 43, 148, 151	0
10	H	138/163 (84%)	0.75	12 (8%) 10 9	5, 52, 147, 152	0
11	I	122/122 (100%)	0.27	4 (3%) 44 28	5, 35, 142, 148	0
12	J	146/150 (97%)	0.56	9 (6%) 20 14	5, 90, 150, 160	0
13	K	137/141 (97%)	1.48	41 (29%) 1 2	5, 24, 148, 152	0
14	L	118/118 (100%)	0.34	5 (4%) 35 22	5, 44, 148, 148	0
15	M	106/112 (94%)	1.14	24 (22%) 1 2	5, 48, 148, 160	0
16	N	137/146 (93%)	0.44	8 (5%) 22 15	5, 74, 150, 167	0
17	O	117/118 (99%)	1.07	35 (29%) 1 2	5, 35, 114, 148	0
18	P	101/101 (100%)	0.89	21 (20%) 1 2	5, 79, 148, 159	0
19	Q	109/113 (96%)	0.56	13 (11%) 5 6	5, 33, 137, 149	0
20	R	92/96 (95%)	0.81	17 (18%) 2 3	5, 73, 148, 161	0
21	S	103/110 (93%)	1.14	21 (20%) 1 2	5, 86, 160, 163	0
22	T	185/206 (89%)	0.02	4 (2%) 59 37	5, 50, 148, 161	0
23	U	76/85 (89%)	1.16	9 (11%) 5 6	5, 57, 151, 166	0
24	V	88/98 (89%)	1.13	27 (30%) 1 2	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%)	0.60	8 (12%) 4 5	5, 88, 149, 155	0
26	X	60/60 (100%)	0.15	0 100 100	5, 36, 148, 150	0
27	Y	56/60 (93%)	0.44	5 (8%) 10 9	7, 77, 164, 168	0
28	Z	48/49 (97%)	0.61	0 100 100	5, 5, 42, 126	0
29	a	63/65 (96%)	1.05	10 (15%) 3 3	5, 50, 151, 157	0
30	b	35/37 (94%)	1.71	12 (34%) 1 1	5, 102, 149, 153	0
31	y	1501/1522 (98%)	1.27	143 (9%) 8 8	5, 9, 114, 163	0
32	z	75/76 (98%)	1.28	10 (13%) 4 4	5, 7, 90, 128	0
33	0	76/76 (100%)	1.27	12 (15%) 3 4	5, 37, 129, 148	0
34	1	6/10 (60%)	1.15	1 (16%) 2 3	5, 5, 54, 67	0
35	c	234/256 (91%)	0.16	3 (1%) 74 50	5, 50, 151, 165	0
36	d	206/239 (86%)	0.51	19 (9%) 9 8	5, 57, 148, 151	0
37	e	208/209 (99%)	0.51	16 (7%) 13 10	5, 50, 148, 157	0
38	f	150/162 (92%)	0.47	10 (6%) 17 13	5, 62, 148, 154	0
39	g	101/101 (100%)	0.18	9 (8%) 10 9	5, 72, 148, 156	0
40	h	155/156 (99%)	0.28	3 (1%) 64 41	5, 73, 155, 163	0
41	i	138/138 (100%)	0.32	6 (4%) 34 22	5, 43, 148, 149	0
42	j	127/128 (99%)	0.67	18 (14%) 3 4	5, 85, 150, 154	0
43	k	98/105 (93%)	0.14	0 100 100	5, 83, 151, 164	0
44	l	116/129 (89%)	0.62	10 (8%) 11 9	5, 71, 150, 162	0
45	m	124/132 (93%)	0.38	11 (8%) 10 9	5, 30, 148, 152	0
46	n	125/126 (99%)	0.55	12 (9%) 8 8	5, 74, 148, 162	0
47	o	60/61 (98%)	1.73	19 (31%) 1 2	5, 66, 151, 161	0
48	p	88/89 (98%)	0.27	1 (1%) 77 54	5, 57, 148, 163	0
49	q	83/88 (94%)	0.65	9 (10%) 6 7	5, 50, 148, 148	0
50	r	104/105 (99%)	0.84	19 (18%) 2 3	5, 52, 148, 158	0
51	s	73/88 (82%)	-0.02	0 100 100	5, 69, 149, 157	0
52	t	80/93 (86%)	-0.07	1 (1%) 74 50	5, 52, 148, 159	0
53	u	99/106 (93%)	1.06	18 (18%) 2 3	10, 66, 199, 199	0
54	v	24/27 (88%)	1.23	5 (20%) 1 2	5, 47, 139, 142	0
All	All	10454/10880 (96%)	0.86	1019 (9%) 8 8	5, 32, 148, 199	0

The worst 5 of 1019 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	y	1498	UR3	11.8
1	w	508	G	7.9
13	K	92	GLY	7.5
15	M	82	ILE	7.5
15	M	81	GLY	7.5

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	2MG	y	1207	24/25	0.30	-	21,22,26,26	0
32	7MG	z	46	24/25	0.30	-	5,5,12,12	0
31	PSU	y	516	20/21	0.32	-	137,138,148,148	0
32	H2U	z	20	20/21	0.35	-	124,124,133,133	0
33	PSU	0	55	20/21	0.26	-	36,36,36,36	0
32	MIA	z	37	29/30	0.36	-	20,26,32,32	0
31	M2G	y	966	25/26	0.36	-	15,16,20,31	0
31	4OC	y	1402	22/23	0.36	-	10,13,16,16	0
31	5MC	y	1404	21/22	0.36	-	5,6,8,9	0
31	UR3	y	1498	21/22	0.31	-	5,5,5,5	0
32	PSU	z	55	20/21	0.38	-	40,50,52,53	0
31	5MC	y	1407	21/22	0.28	-	25,28,30,30	0
32	PSU	z	39	20/21	0.37	-	5,5,5,5	0
32	H2U	z	16	20/21	0.58	-	80,92,93,95	0
32	4SU	z	8	20/21	0.34	-	5,5,5,5	0
31	7MG	y	527	24/25	0.29	-	7,10,24,26	0
32	5MU	z	54	21/22	0.29	-	5,5,5,5	0
31	MA6	y	1519	24/25	0.30	-	5,5,6,8	0
31	5MC	y	1400	21/22	0.35	-	5,5,5,5	0
31	MA6	y	1518	24/25	0.28	-	31,39,52,53	0
31	5MC	y	967	21/22	0.38	-	124,124,133,133	0
32	PSU	z	32	20/21	0.32	-	42,52,58,59	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.