wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:32 PM 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

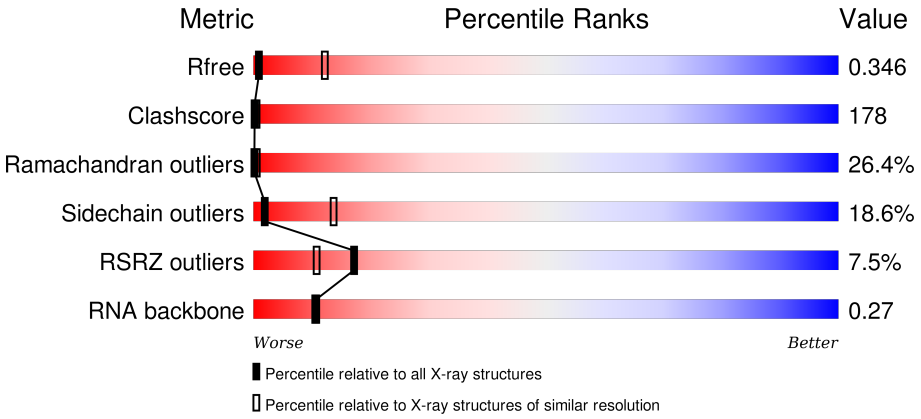
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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.



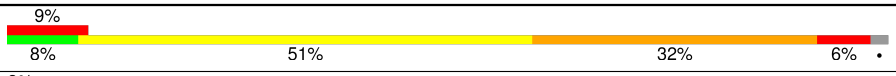
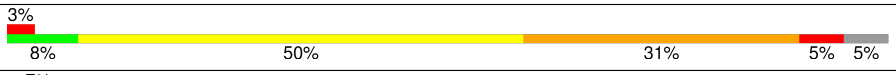
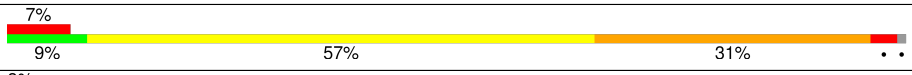
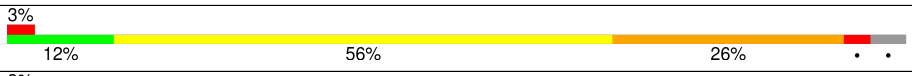
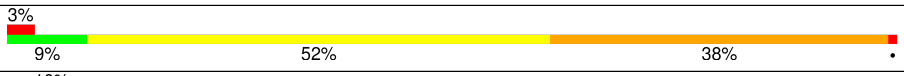
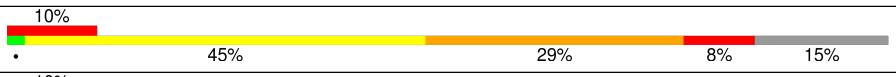
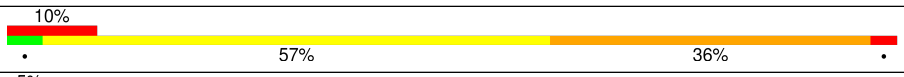
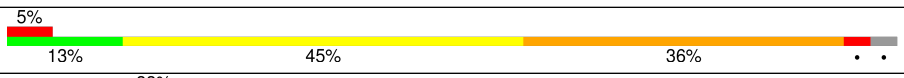
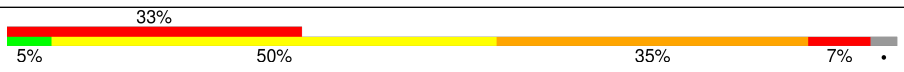
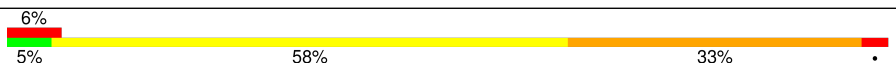
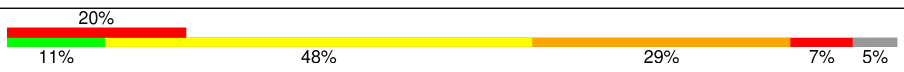
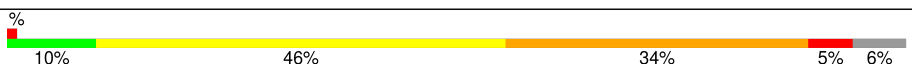
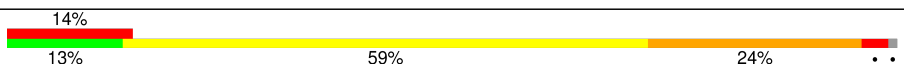
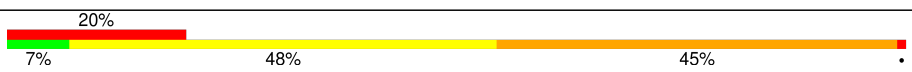
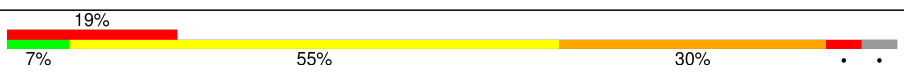
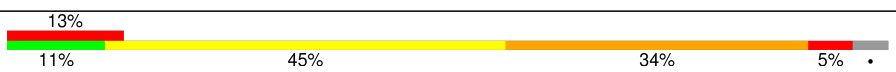
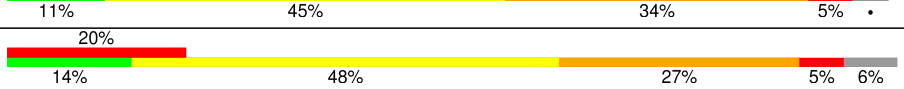
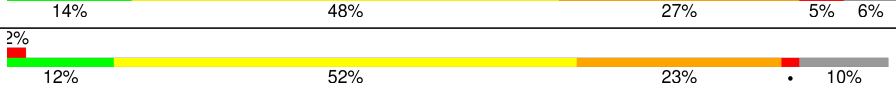
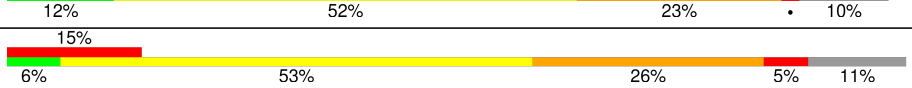
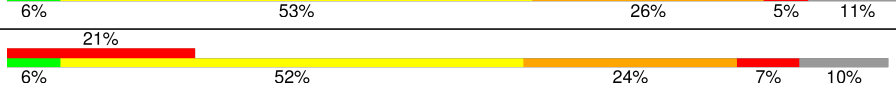
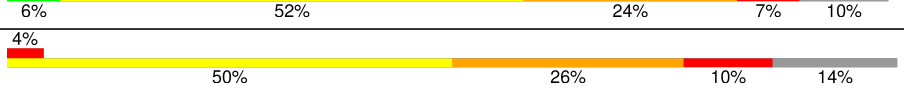
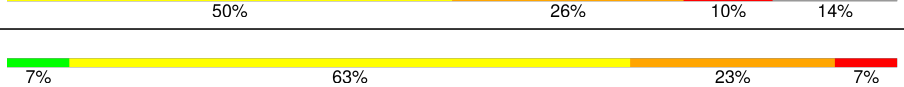
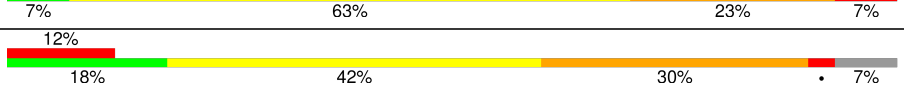
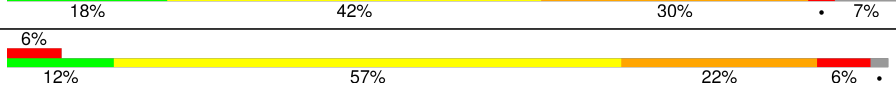
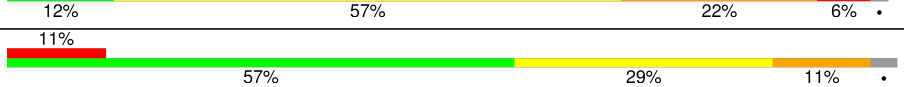
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1129 (3.94-3.50)
Clashscore	102246	1252 (3.94-3.50)
Ramachandran outliers	100387	1199 (3.94-3.50)
Sidechain outliers	100360	1197 (3.94-3.50)
RSRZ outliers	91569	1136 (3.94-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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. 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 <=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	5% 57% 39% ·
2	x	121	3% 61% 36% · ·
3	A	229	7% 6% 34% 13% · 45%
4	B	276	11% 5% 55% 34% · ·

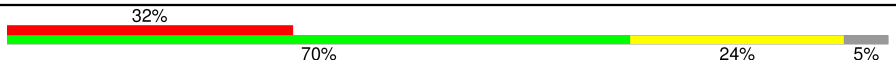
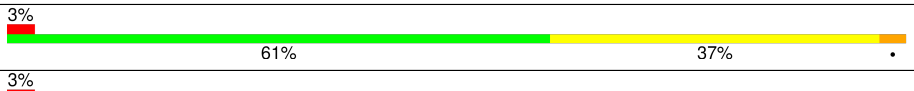
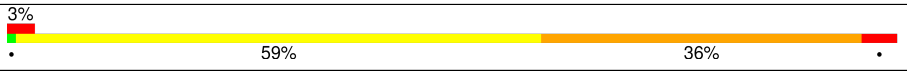
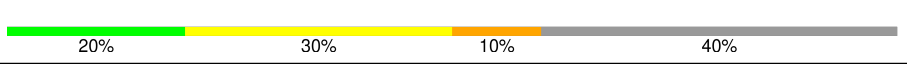
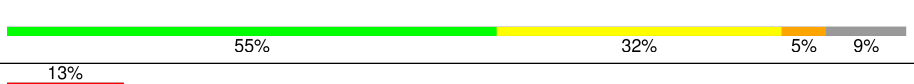
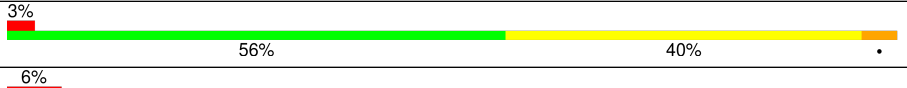
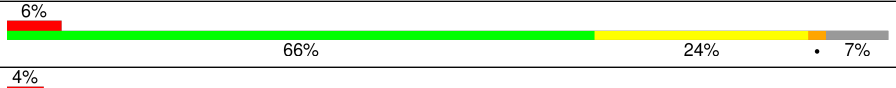
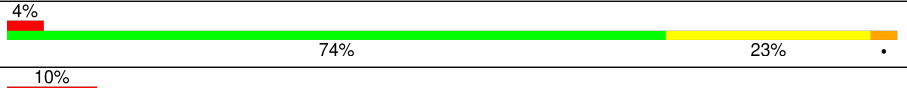
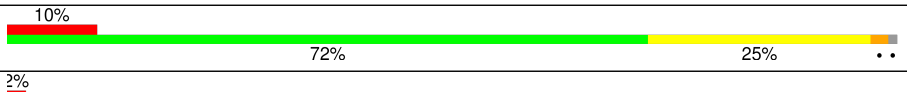
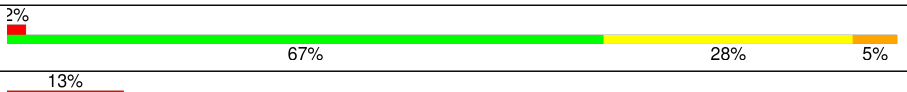
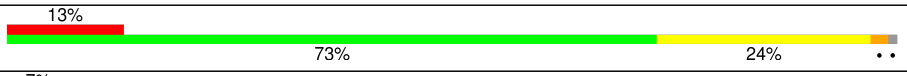
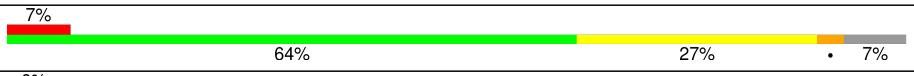
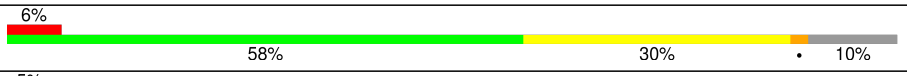
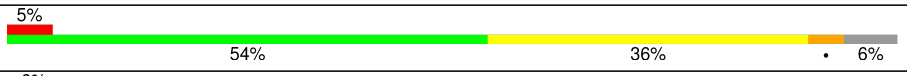
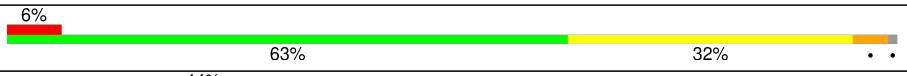
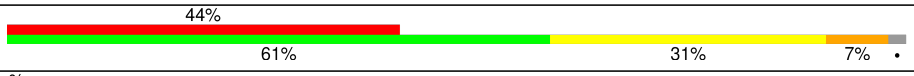
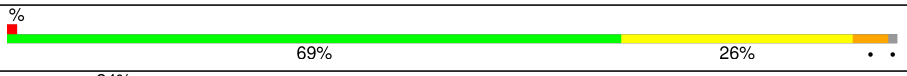
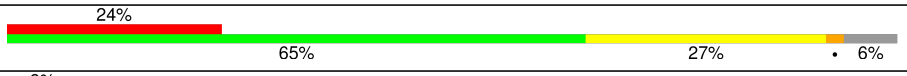
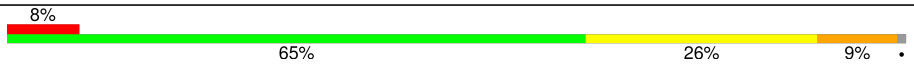
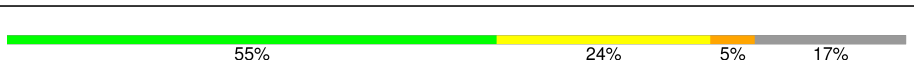
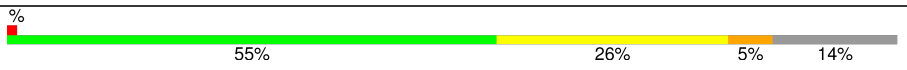
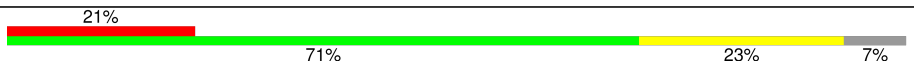
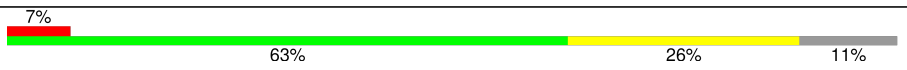
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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
			Total	C	N	O	P			
1	w	2889	62213	27690	11624	20011	2888	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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	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	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	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.

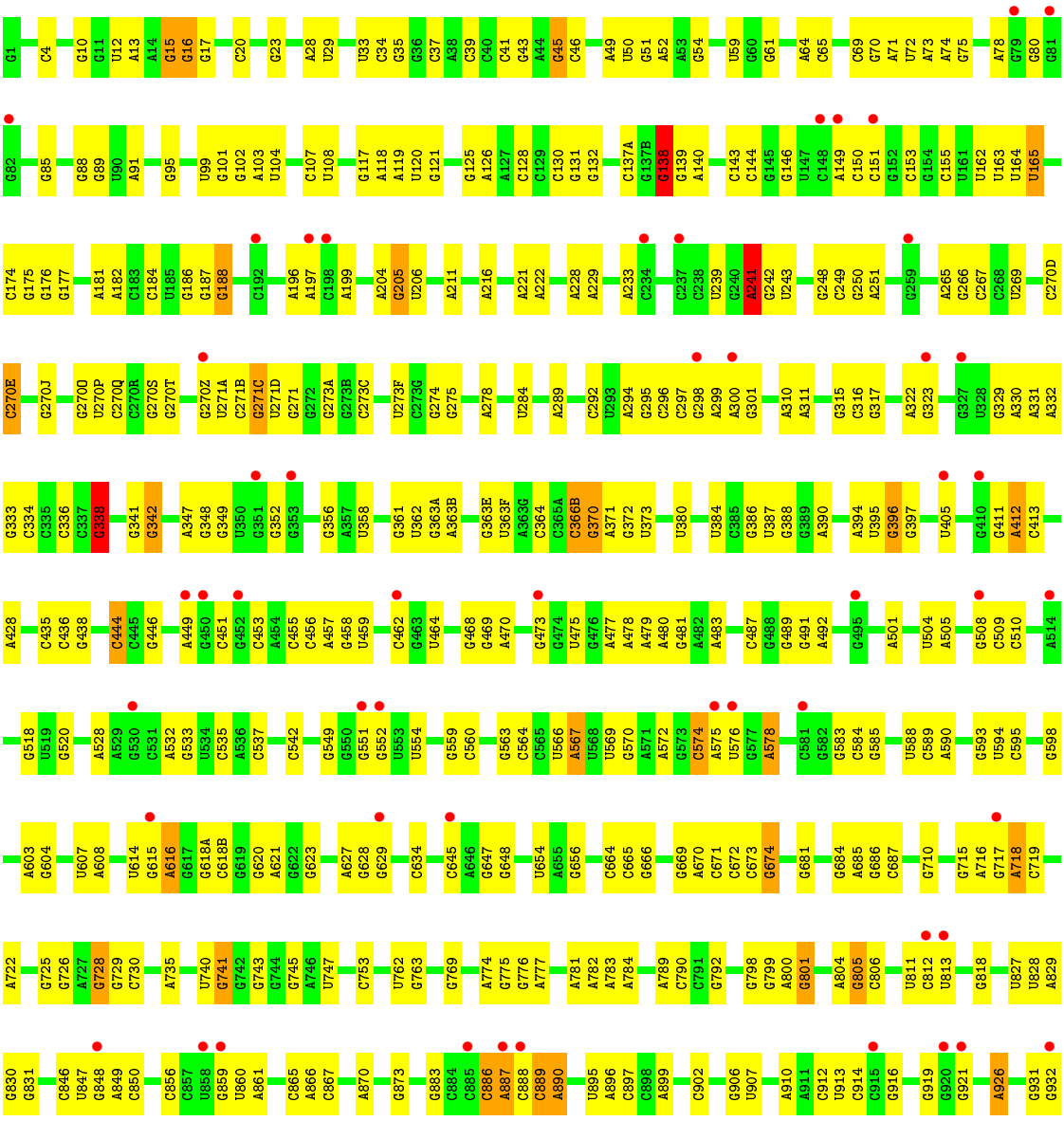
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	v	24	Total	C	N	O	0	0	0
			208	128	50	30			

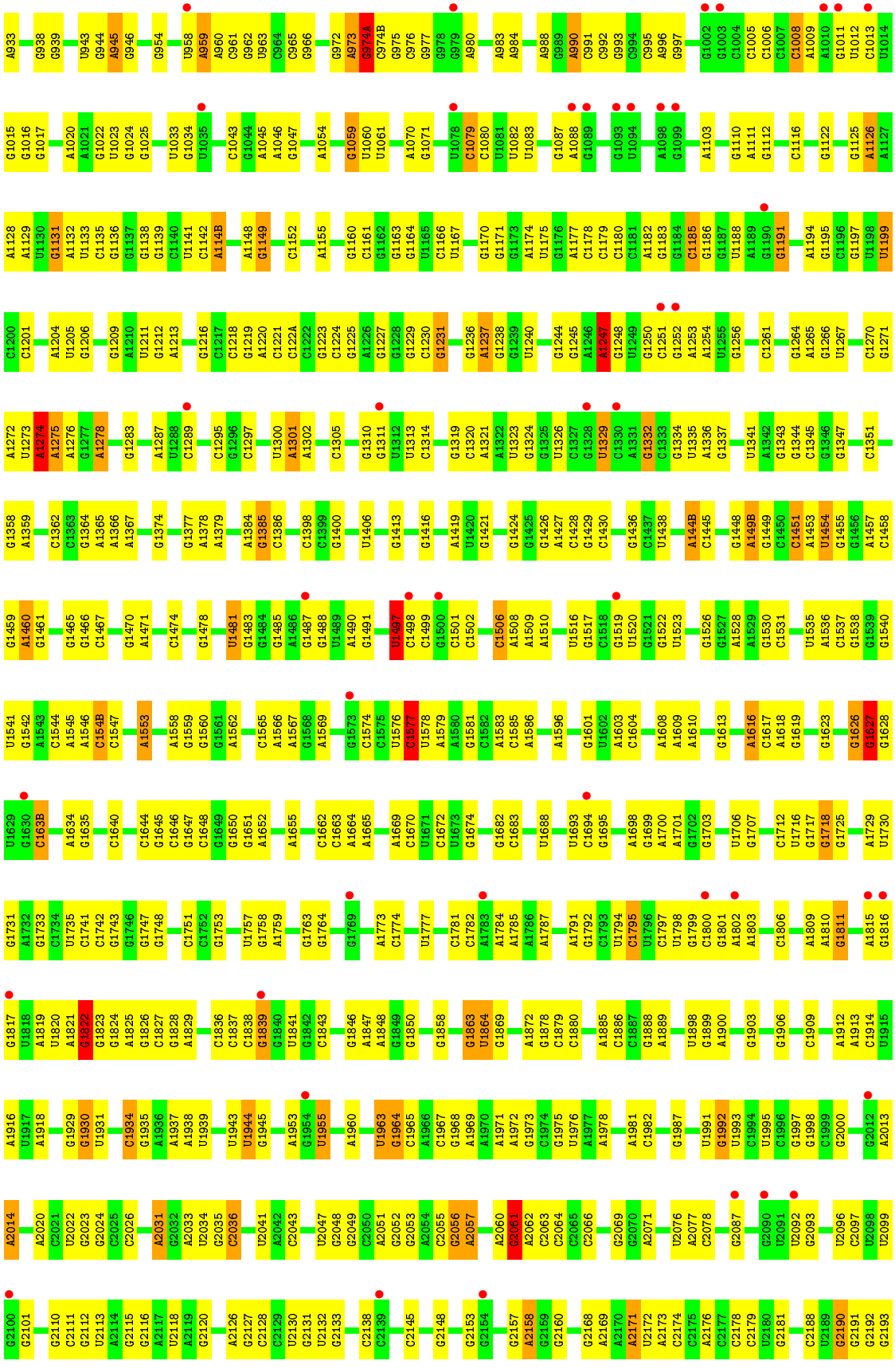
3 Residue-property plots (i)

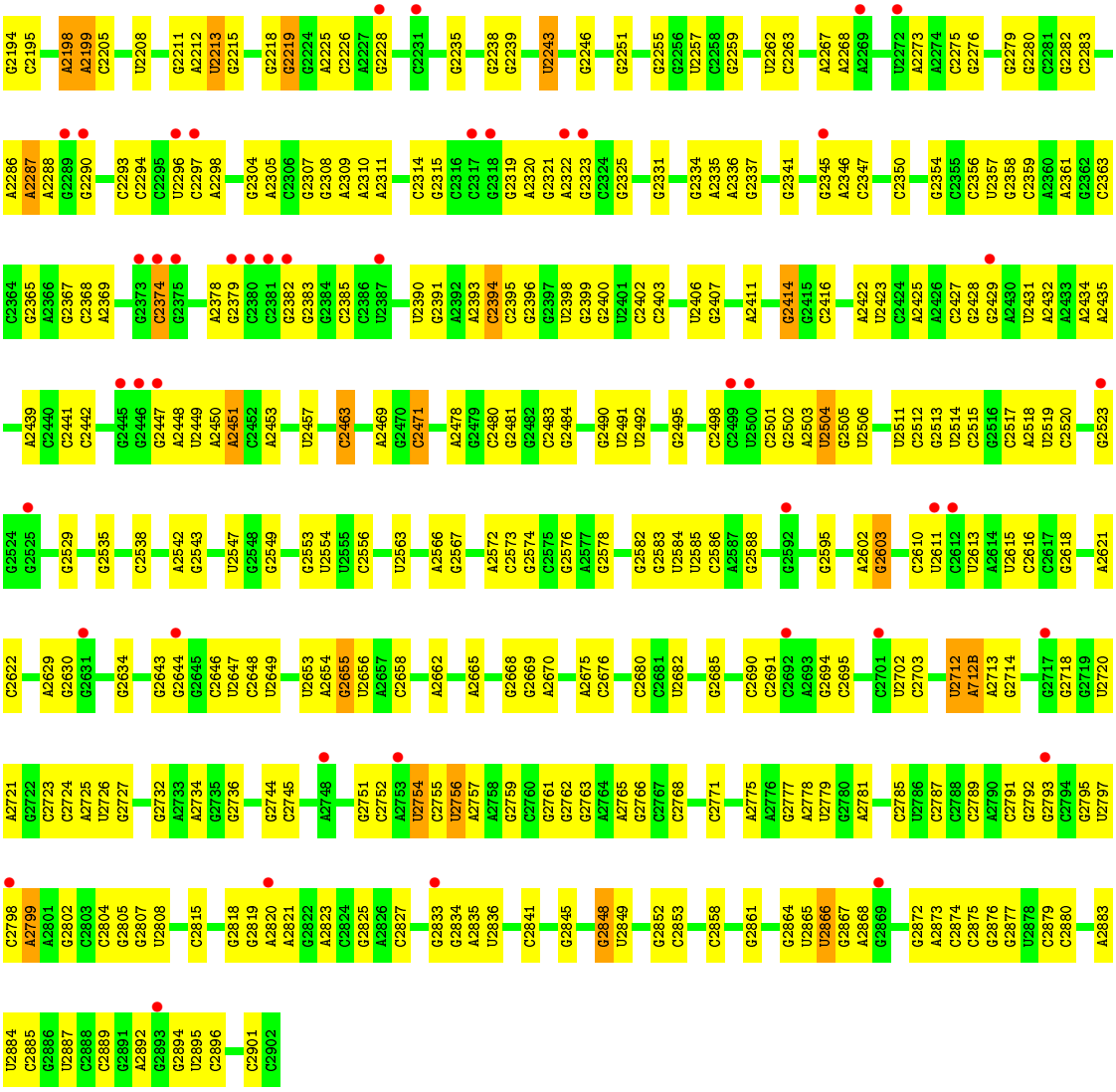
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Chain w:

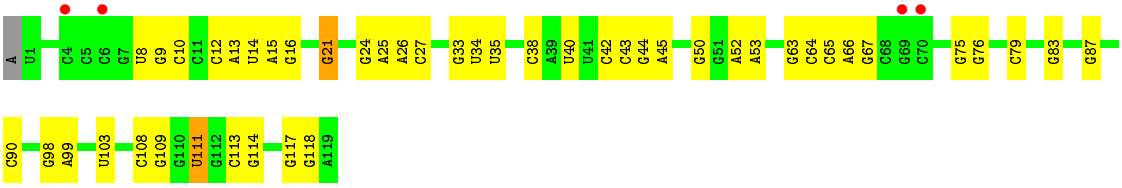



A933 G938 G939 U943 G944 A945 G946 G954 U958 A959 A960 C961 G962 U963 C964 C965 G966 G972 A973 G974A C974B G975 C976 G977 G978 G979 A980 A983 A984 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014
G1015 G1016 G1017 A1020 A1021 G1022 U1023 G1024 G1025 U1033 G1034 U1035 C1043 G1044 A1045 A1046 G1047 A1054 G1059 U1060 U1061 A1070 G1071 U1078 C1079 C1080 U1081 U1082 U1083 G1087 A1088 G1089 G1093 U1094 A1098 G1099 A1103 G1110 A1111 G1112 C1116 G1122 G1125 A1126 A1127
A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 C1142 A1114B A1148 G1149 C1152 A1155 G1160 C1161 G1162 G1163 G1164 U1165 C1166 U1167 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186 G1187 U1188 A1189 G1190 G1191 A1194 G1195 C1196 G1197 U1198 U1199
C1200 C1201 A1204 U1205 G1206 G1209 A1210 U1211 U1212 A1213 G1216 C1217 C1218 G1219 A1220 C1221 C122A C1222 G1223 C1224 G1225 A1226 G1227 G1228 G1229 C1230 G1231 G1236 A1237 G1238 G1239 U1240 G1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1261 G1264 A1265 G1266 U1267 C1270 G1271
A1272 U1273 A1274 A1275 A1276 G1277 A1278 G1283 A1287 U1288 C1289 C1295 G1296 C1297 U1300 A1301 A1302 C1305 G1310 G1311 U1312 U1313 C1314 G1319 C1320 A1321 A1322 U1323 G1324 G1325 U1326 C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 U1341 A1342 G1343 G1344 C1345 G1346 G1347 C1351
G1358 A1359 C1362 C1363 G1364 A1365 A1366 A1367 G1374 G1377 A1378 A1379 A1384 G1385 C1386 C1398 C1399 G1400 U1406 G1413 G1416 A1419 U1420 G1421 G1424 G1425 G1426 A1427 C1428 G1429 C1430 G1436 C1437 U1438 A1444B C1445 G1448 A149B G1449 C1450 C1451 A1453 U1454 G1455 G1456 A1457 C1458
G1459 A1460 G1461 G1465 G1466 C1467 G1470 A1471 C1474 G1478 U1481 G1483 G1484 G1485 A1486 G1487 G1488 U1489 A1490 G1491 U1497 C1498 C1499 G1500 C1501 C1502 C1506 A1508 A1509 A1510 U1516 G1517 C1518 G1519 U1520 G1521 G1522 U1523 G1526 G1527 A1528 A1529 G1530 C1531 U1535 A1536 C1537 G1538 G1539 G1540
U1541 G1542 A1543 C1544 A1545 A1546 C154B C1547 A1553 A1558 G1559 G1560 G1561 A1562 C1565 A1566 A1567 G1568 A1569 G1573 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1596 G1601 U1602 A1603 C1604 A1608 A1609 A1610 G1613 A1616 C1617 A1618 G1619 G1623 G1626 G1627 G1628
U1629 G1630 C163B A1634 G1635 C1640 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652 A1655 C1662 C1663 A1664 A1665 A1669 C1670 U1671 C1672 U1673 G1674 G1682 C1683 U1688 U1693 C1694 G1695 A1698 G1699 A1700 A1701 G1702 G1703 U1706 G1707 C1712 U1716 G1717 G1718 G1725 A1729 U1730
G1731 A1732 G1733 C1734 U1735 C1741 C1742 G1743 G1746 G1747 G1748 C1751 C1752 G1753 U1757 G1758 A1759 G1763 G1764 G1769 A1773 C1774 U1777 C1781 C1782 A1783 A1784 A1785 A1786 A1787 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1806 A1809 A1810 G1811 A1815 G1816
G1817 U1818 A1819 U1820 A1821 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1836 C1837 C1838 G1839 G1840 U1841 G1842 C1843 G1846 A1847 A1848 G1849 G1850 G1858 G1863 U1864 G1869 A1872 G1878 C1879 C1880 A1885 C1886 G1887 G1888 A1889 U1898 G1899 A1900 G1903 G1906 C1909 A1912 A1913 C1914 U1915
A1916 U1917 A1918 G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 U1939 U1943 U1944 G1945 A1953 G1954 U1955 A1960 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 U1976 A1977 A1978 A1981 C1982 G1987 U1991 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2000 G2012 A2013
A2014 A2020 C2021 U2022 G2023 G2024 C2025 C2026 A2031 G2032 A2033 U2034 G2035 C2036 U2041 A2042 C2043 U2047 G2048 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2057 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 G2070 A2071 U2076 A2077 C2078 G2087 G2090 U2091 U2092 G2093 U2096 C2097 U2098 U2099
G2100 G2101 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 C2138 C2139 C2145 G2149 G2153 G2154 G2157 A2158 G2159 G2160 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 G2180 G2181 C2188 U2189 G2190 G2191 G2192 G2193



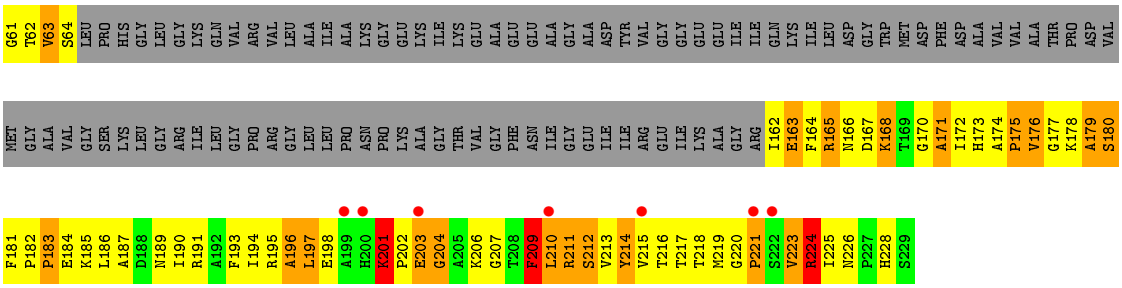
- Molecule 2: 5S LARGE SUBUNIT RIBOSOMAL RNA

Chain x:



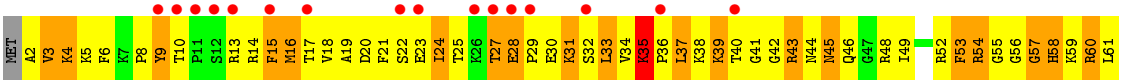
- Molecule 3: 50S ribosomal protein L1

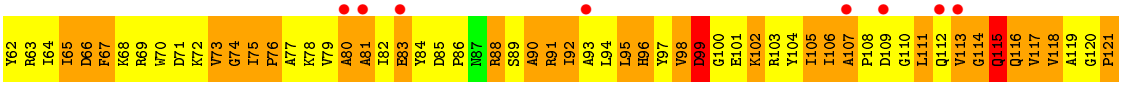
Chain A:

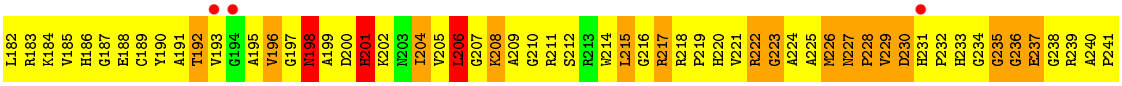


• Molecule 4: 50S ribosomal protein L2

Chain B:

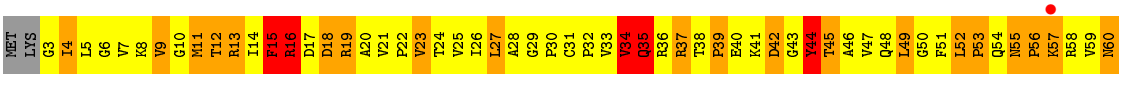






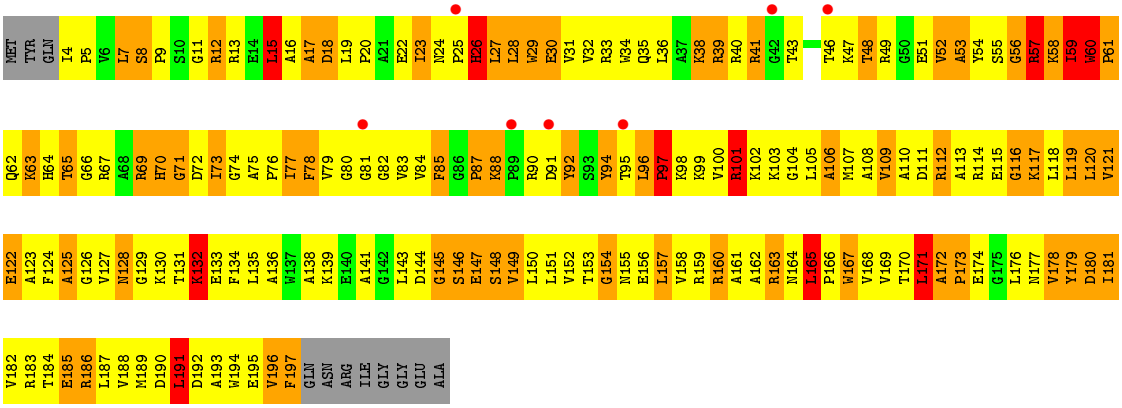
• Molecule 5: 50S ribosomal protein L3

Chain C:

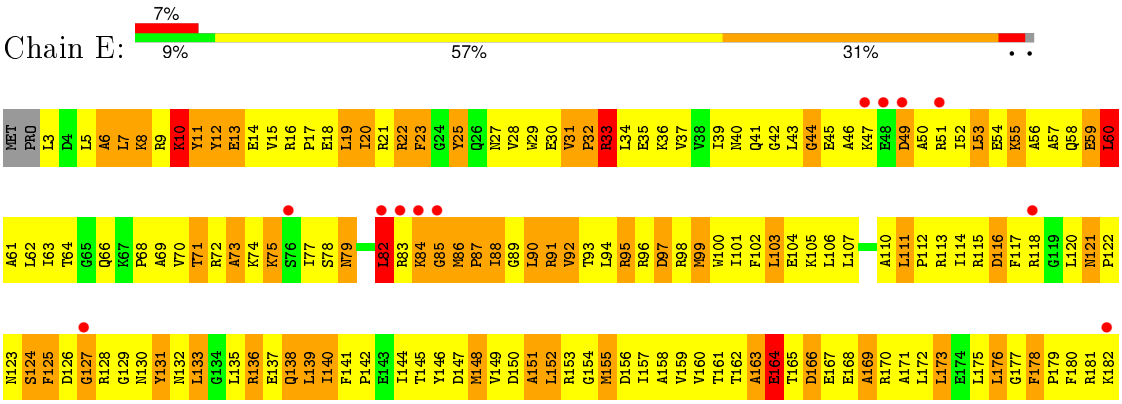


• Molecule 6: 50S ribosomal protein L4

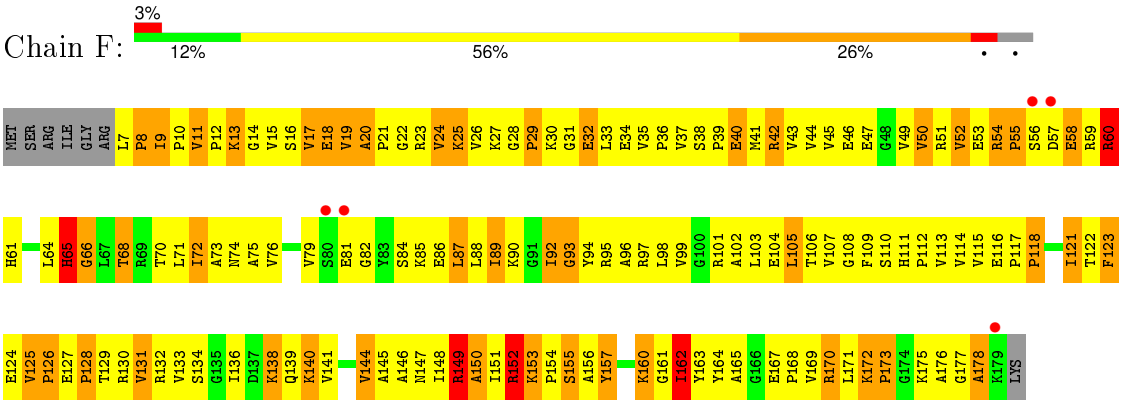
Chain D:



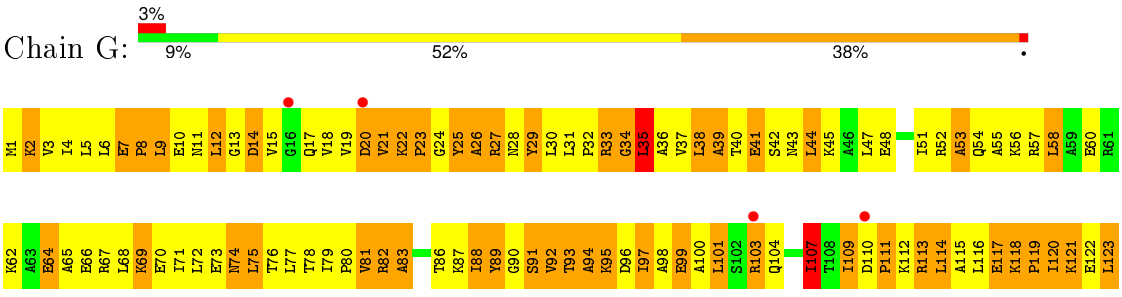
• Molecule 7: 50S ribosomal protein L5

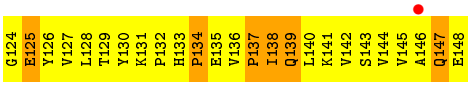


• Molecule 8: 50S ribosomal protein L6



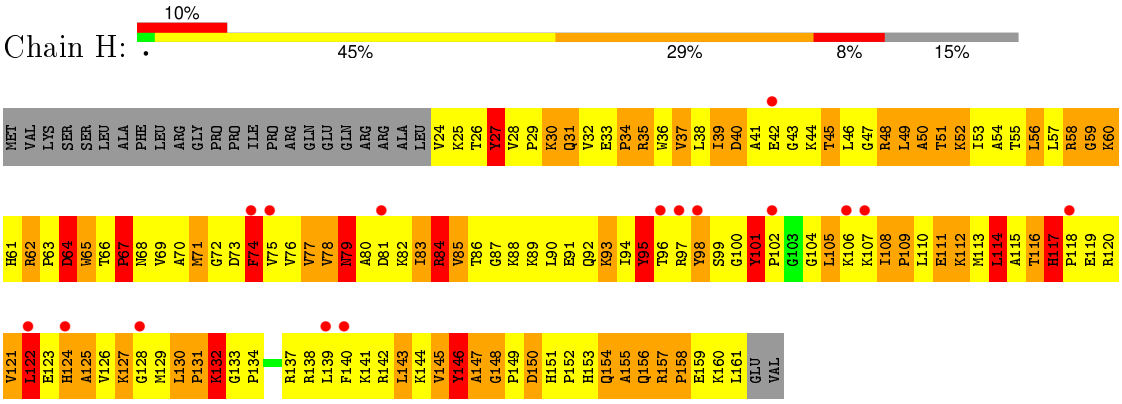
• Molecule 9: 50S ribosomal protein L9





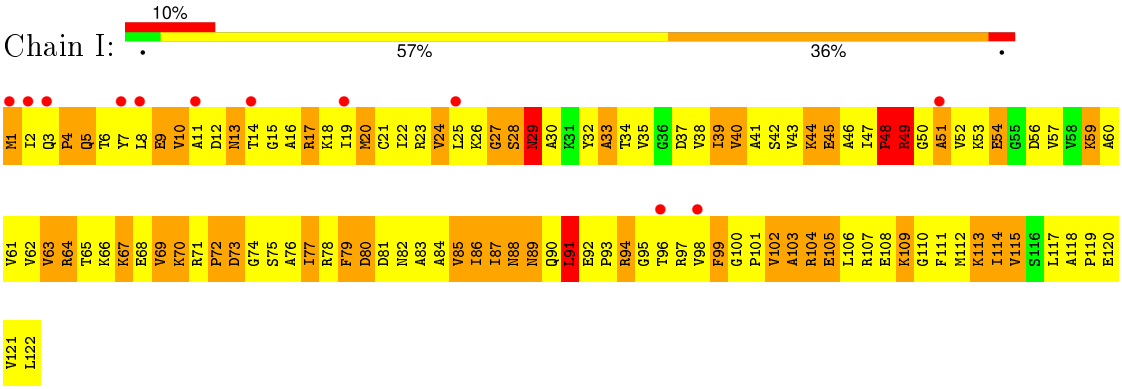
- Molecule 10: 50S ribosomal protein L13

Chain H:



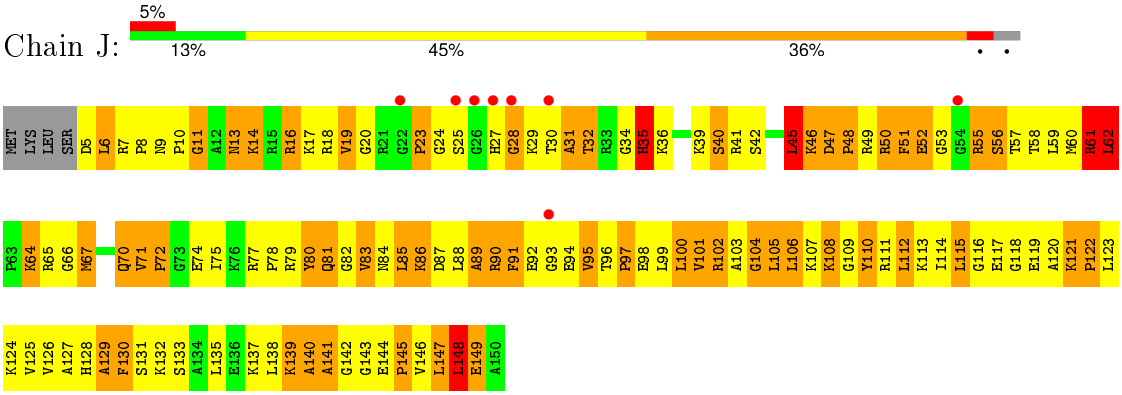
- Molecule 11: 50S ribosomal protein L14

Chain I:



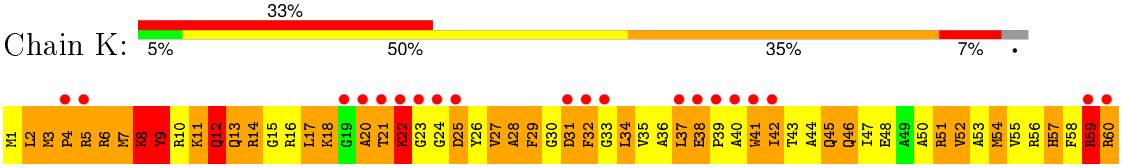
- Molecule 12: 50S ribosomal protein L15

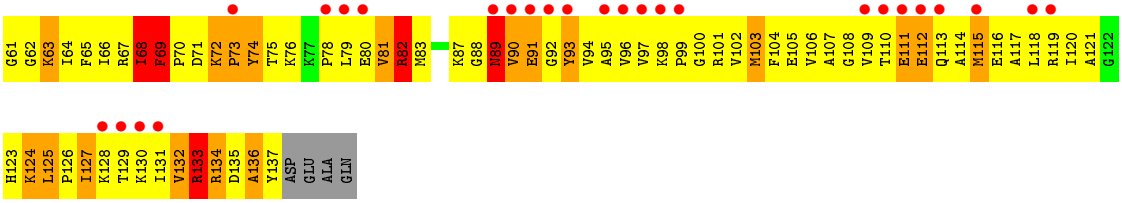
Chain J:



- Molecule 13: 50S ribosomal protein L16

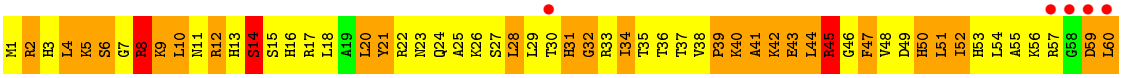
Chain K:

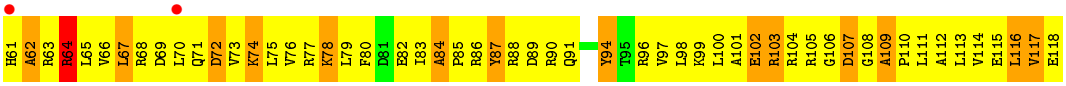




- Molecule 14: 50S ribosomal protein L17

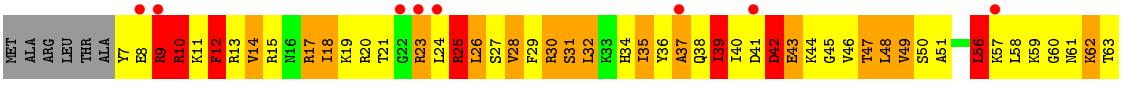
Chain L:

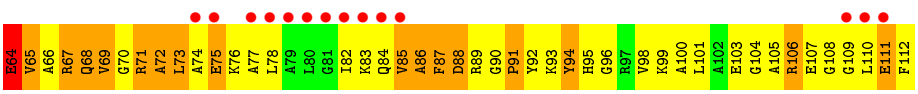




- Molecule 15: 50S ribosomal protein L18

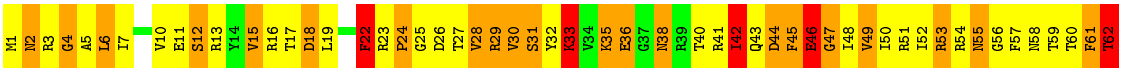
Chain M:

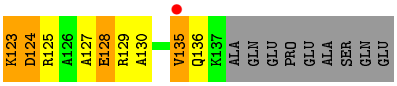




- Molecule 16: 50S ribosomal protein L19

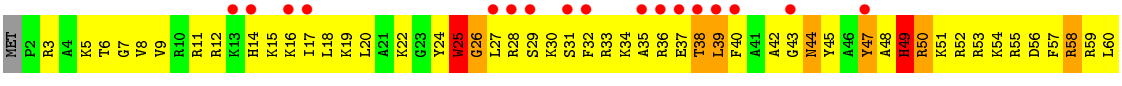
Chain N:

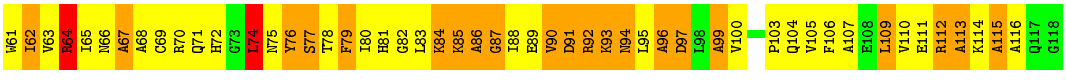




- Molecule 17: 50S ribosomal protein L20

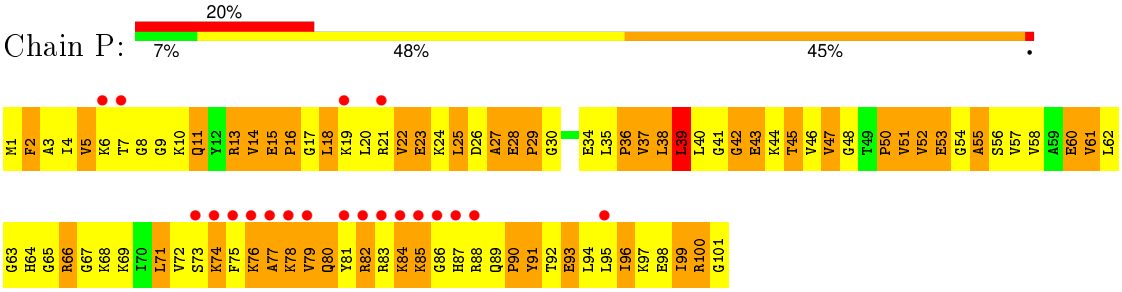
Chain O:





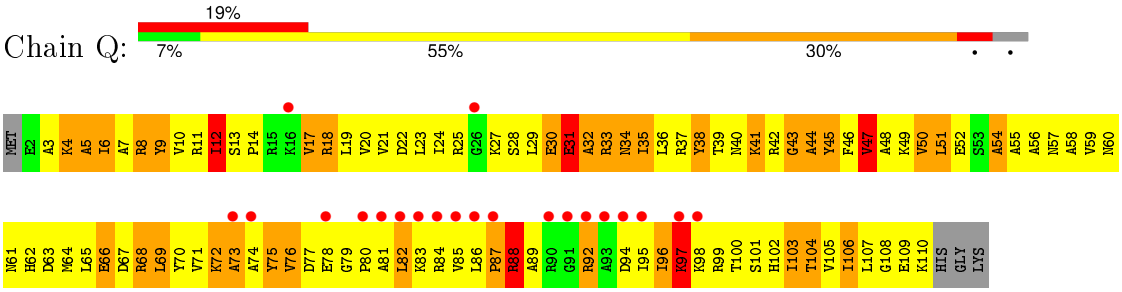
- Molecule 18: 50S ribosomal protein L21

Chain P:



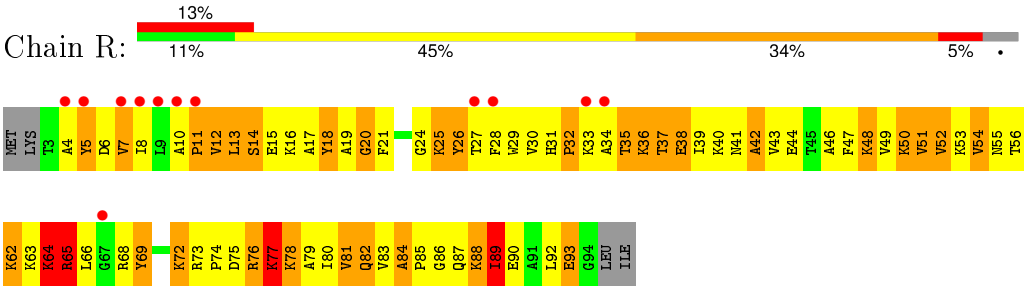
- Molecule 19: 50S ribosomal protein L22

Chain Q:



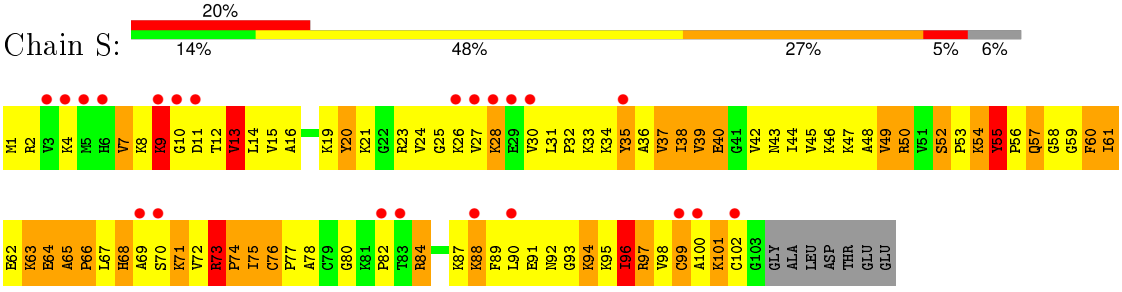
- Molecule 20: 50S ribosomal protein L23

Chain R:



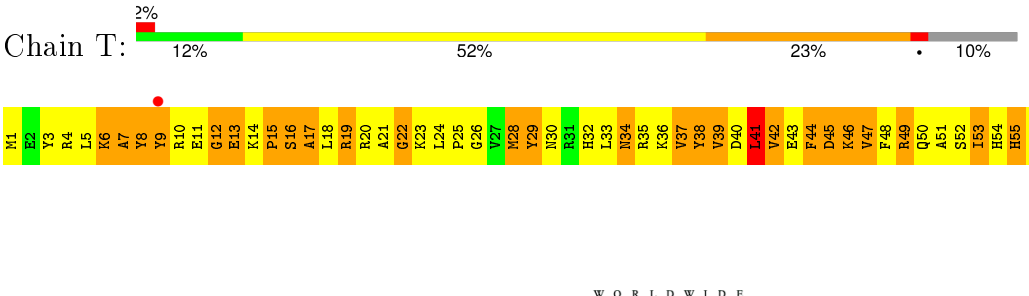
- Molecule 21: 50S ribosomal protein L24

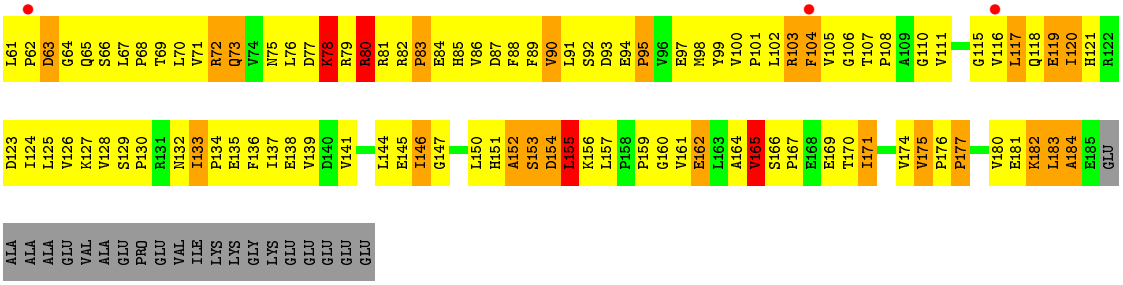
Chain S:



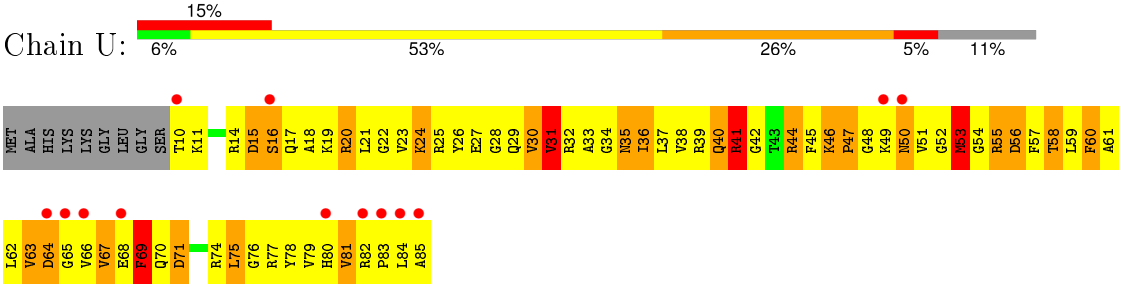
- Molecule 22: 50S ribosomal protein L25

Chain T:

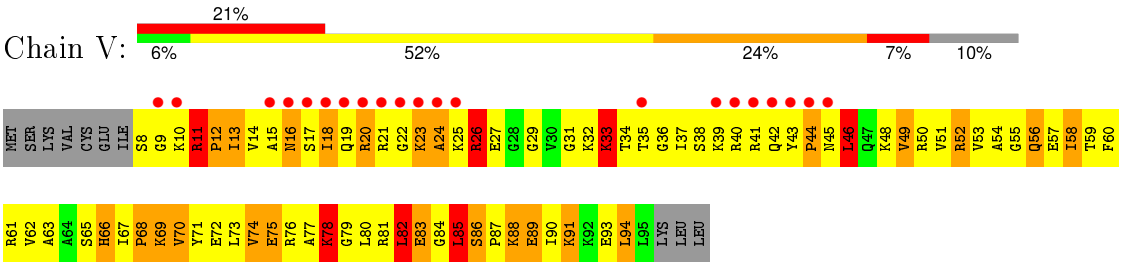




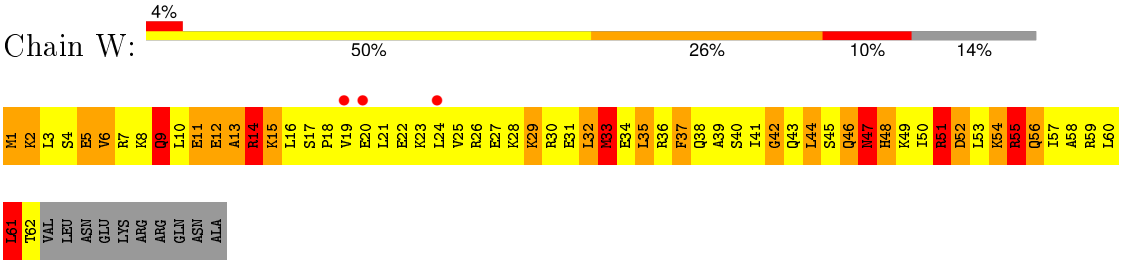
- Molecule 23: 50S ribosomal protein L27



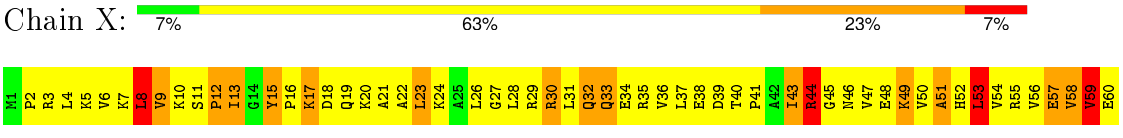
- Molecule 24: 50S ribosomal protein L28



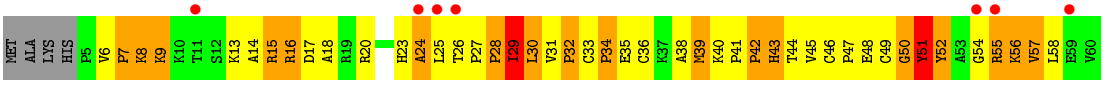
- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L32

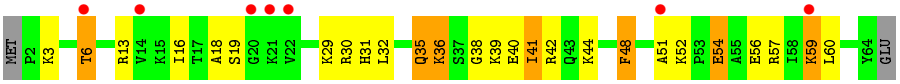


- Molecule 28: 50S ribosomal protein L34

Chain Z:

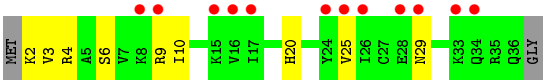
- Molecule 29: 50S ribosomal protein L35

Chain a:



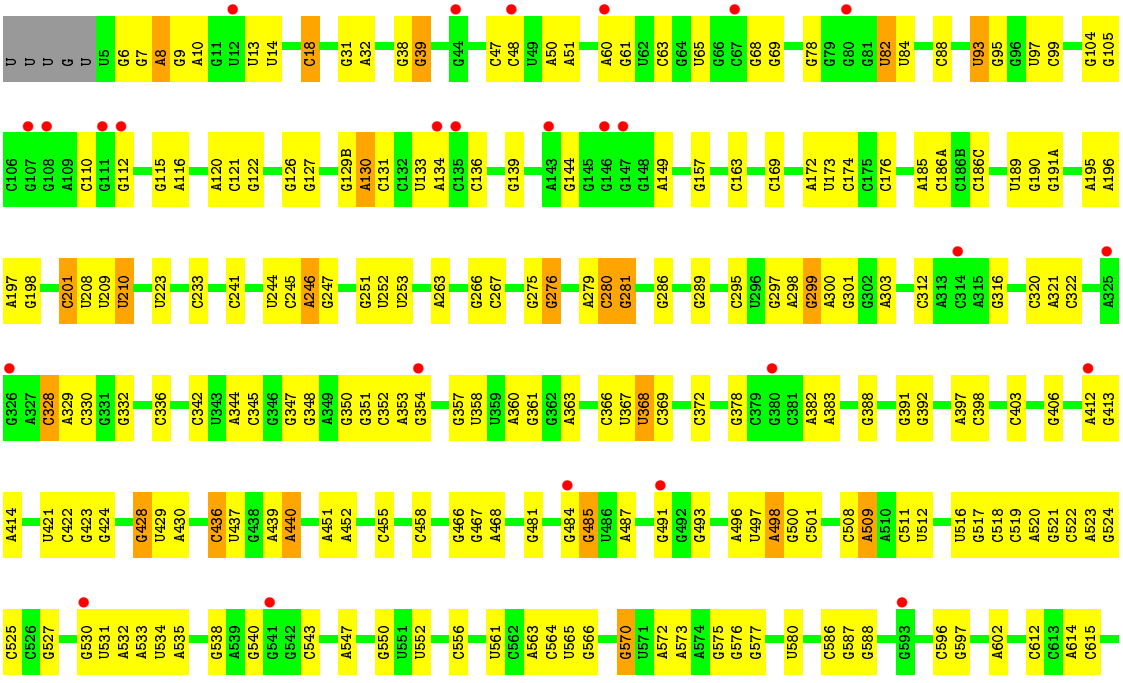
- Molecule 30: 50S ribosomal protein L36

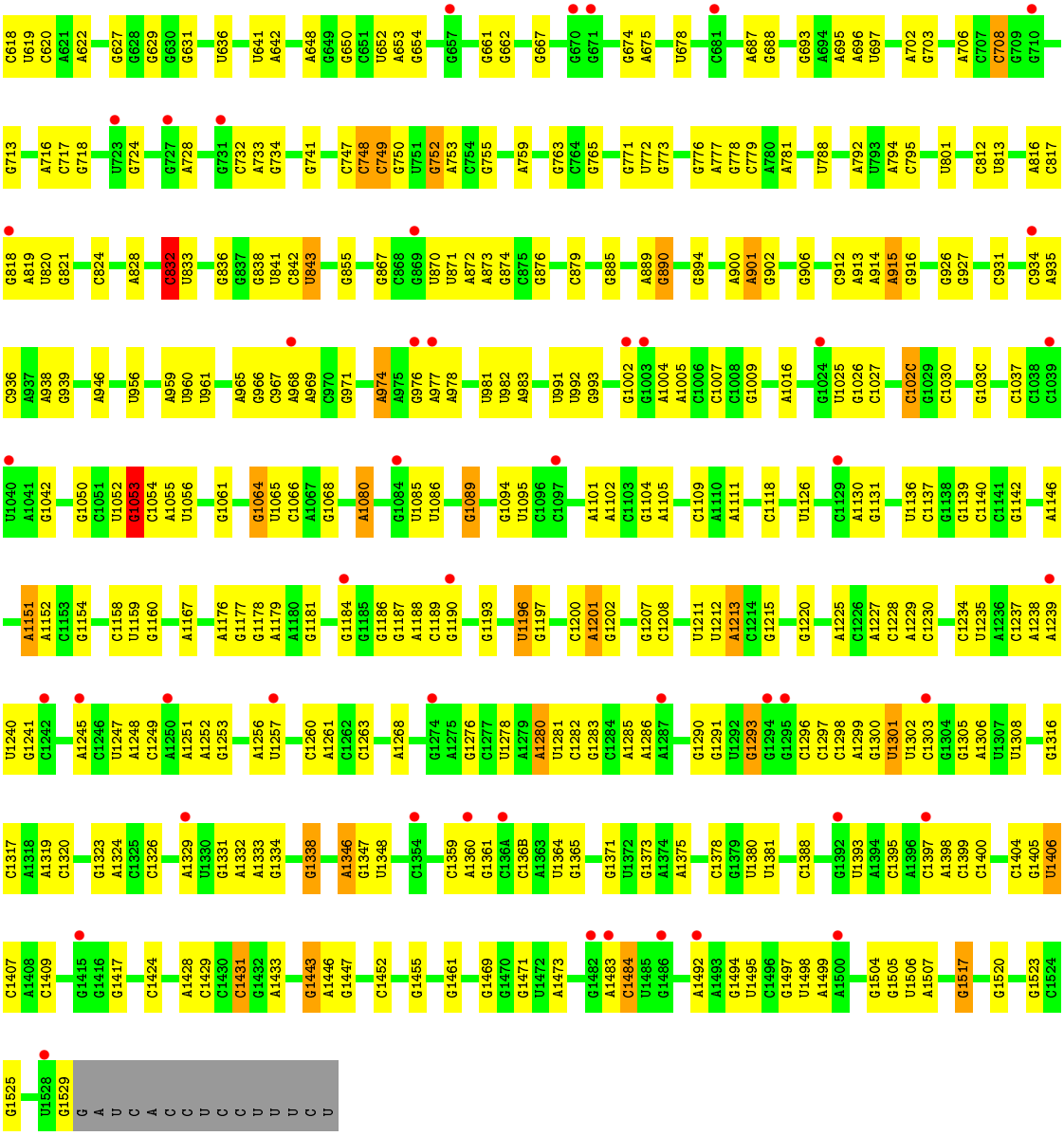
Chain b:



- Molecule 31: 16S SMALL SUBUNIT RIBOSOMAL RNA

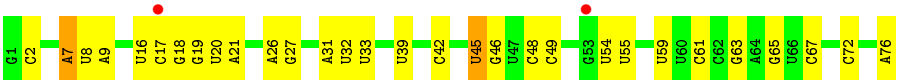
Chain y:





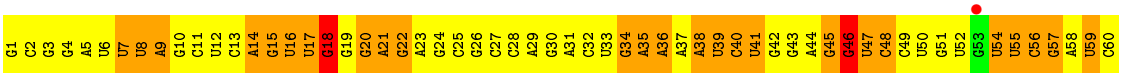
• Molecule 32: P-site PHE-tRNA

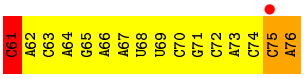
Chain z:



• Molecule 33: E-TRNA

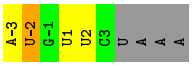
Chain 0:





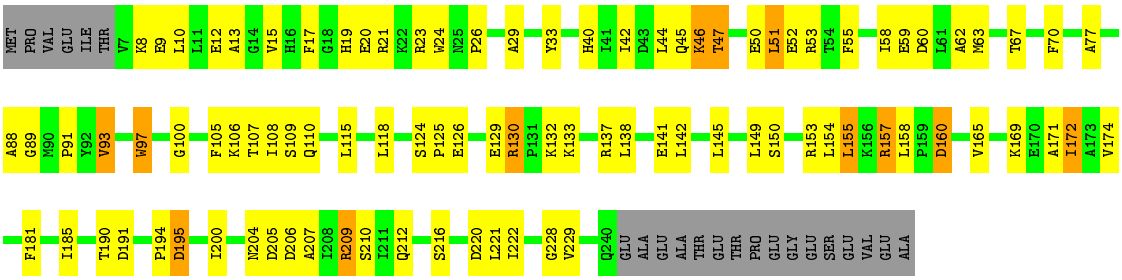
- Molecule 34: MRNA

Chain 1:



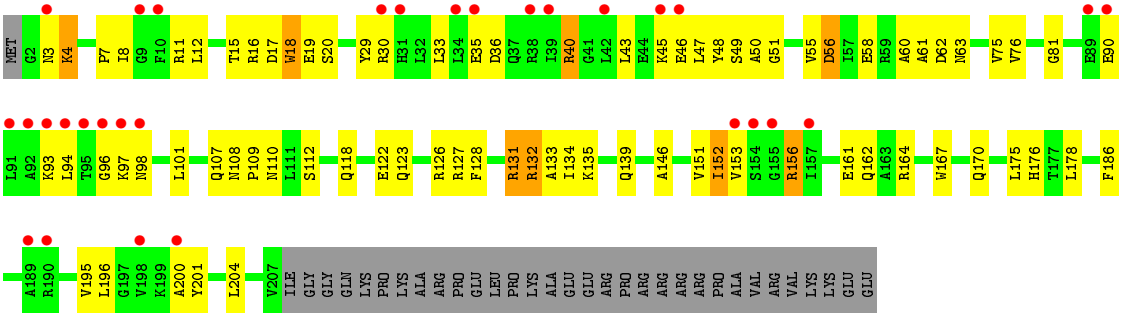
- Molecule 35: 30S ribosomal protein S2

Chain c:



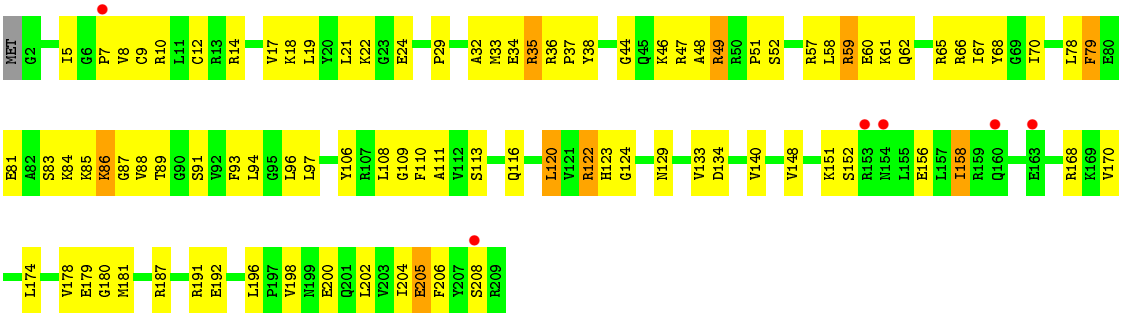
- Molecule 36: 30S ribosomal protein S3

Chain d:



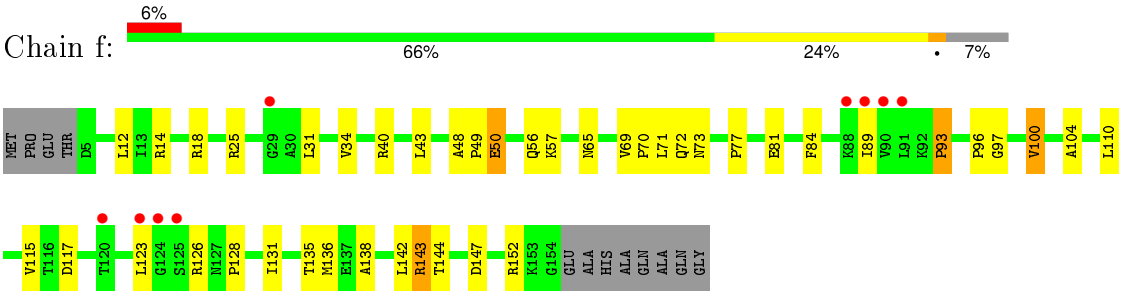
- Molecule 37: 30S ribosomal protein S4

Chain e:



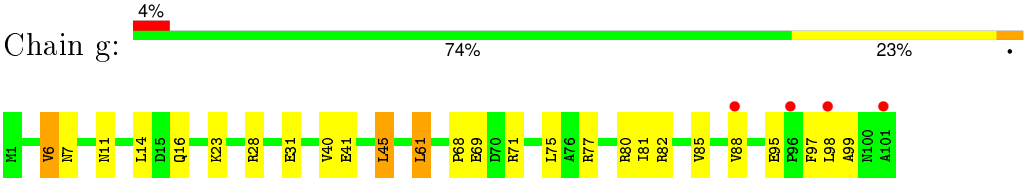
- Molecule 38: 30S ribosomal protein S5

Chain f:



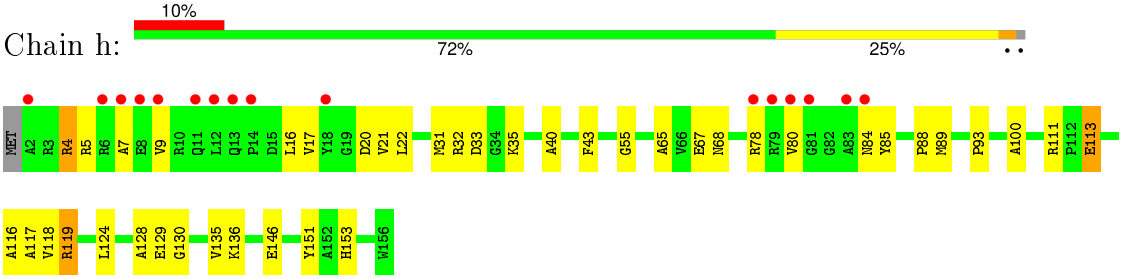
• Molecule 39: 30S ribosomal protein S6

Chain g:



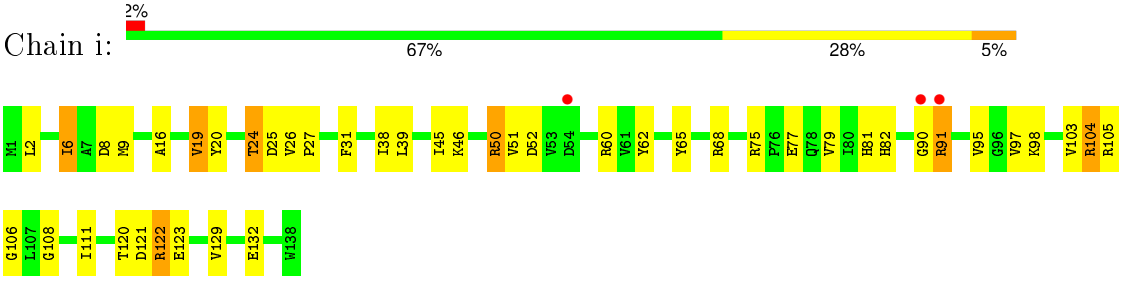
• Molecule 40: 30S ribosomal protein S7

Chain h:



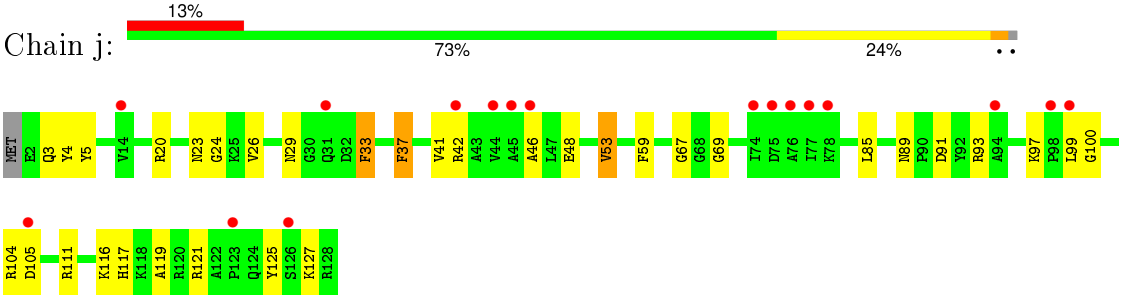
• Molecule 41: 30S ribosomal protein S8

Chain i:



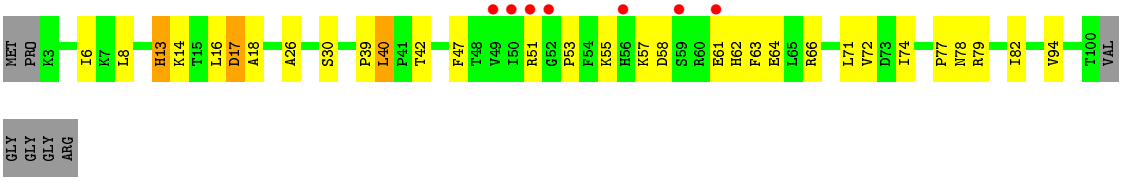
• Molecule 42: 30S ribosomal protein S9

Chain j:



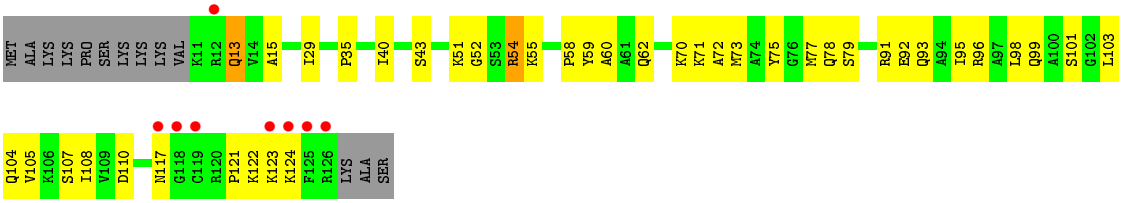
• Molecule 43: 30S ribosomal protein S10

Chain k:



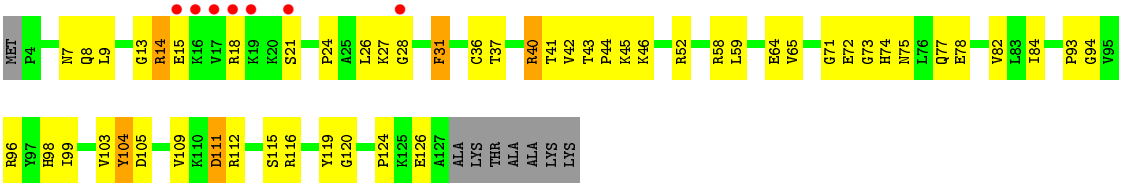
• Molecule 44: 30S ribosomal protein S11

Chain l:



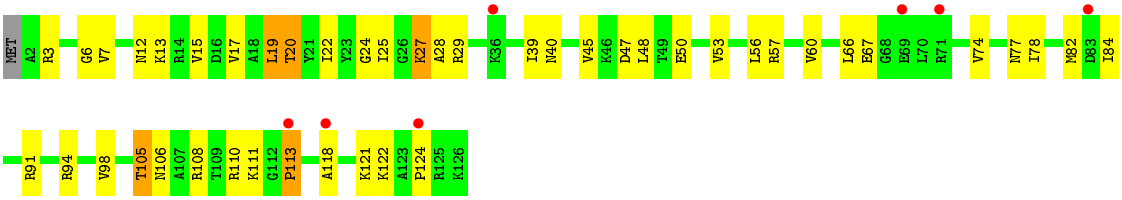
• Molecule 45: 30S ribosomal protein S12

Chain m:



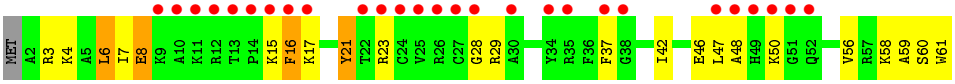
• Molecule 46: 30S ribosomal protein S13

Chain n:



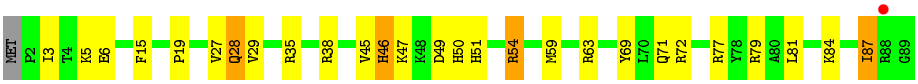
• Molecule 47: 30S ribosomal protein S14

Chain o:



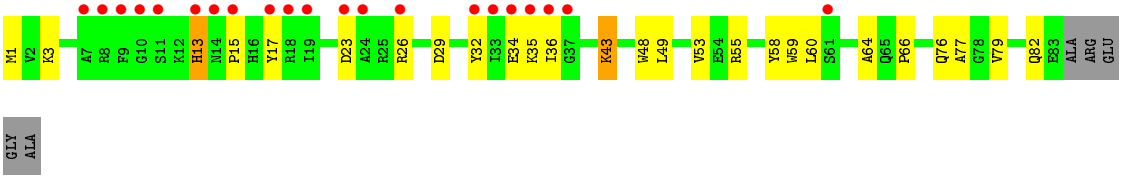
• Molecule 48: 30S ribosomal protein S15

Chain p:



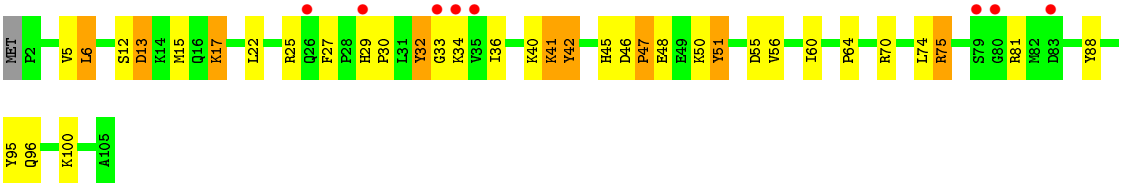
- Molecule 49: 30S ribosomal protein S16

Chain q:



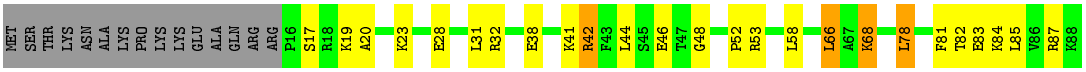
- Molecule 50: 30S ribosomal protein S17

Chain r:



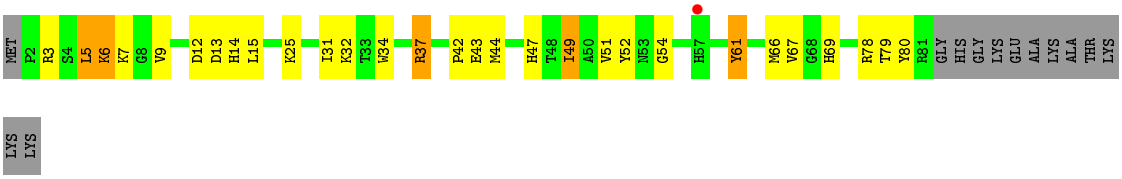
- Molecule 51: 30S ribosomal protein S18

Chain s:



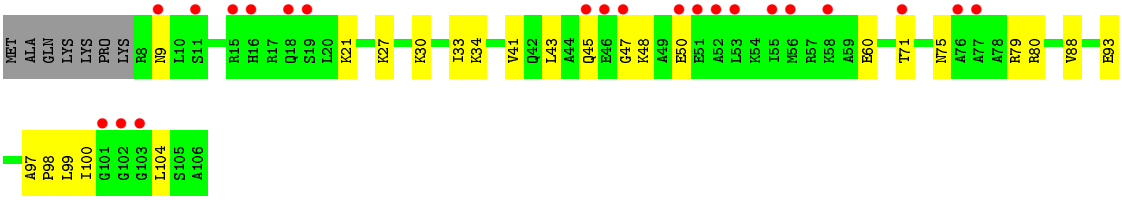
- Molecule 52: 30S ribosomal protein S19

Chain t:



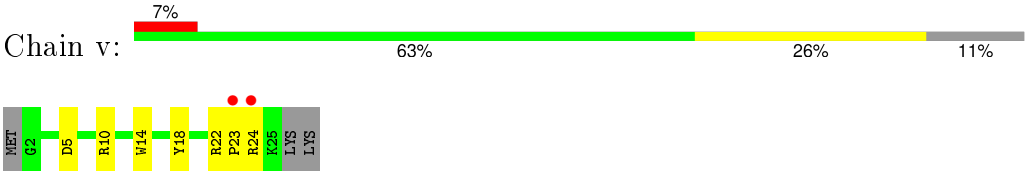
- Molecule 53: 30S ribosomal protein S20

Chain u:



• Molecule 54: 30S ribosomal protein Thx

Chain v:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.68 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.348 , 0.353 0.342 , 0.346	Depositor DCC
R_{free} test set	11349 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)	-0.71 , 506.5	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[2]	$< \|L\| > = 0.26$, $< L^2 > = 0.11$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

Continued on next page...

Continued from previous page...

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(^{o})	Ideal(^{o})
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 (i)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
33:0:9:A:N6	33:0:23: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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1
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	1
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	1
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	3
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	1
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	3
35	c	232/256 (91%)	109 (47%)	66 (28%)	57 (25%)	0	1
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	g	99/101 (98%)	61 (62%)	24 (24%)	14 (14%)	0	6
40	h	153/156 (98%)	84 (55%)	40 (26%)	29 (19%)	0	3
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	1
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	3
54	v	22/27 (82%)	11 (50%)	7 (32%)	4 (18%)	0	3
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 (i)

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 29
4	B	214/218 (98%)	169 (79%)	45 (21%)	1 10
5	C	163/166 (98%)	126 (77%)	37 (23%)	1 8
6	D	154/162 (95%)	123 (80%)	31 (20%)	1 11
7	E	154/156 (99%)	127 (82%)	27 (18%)	2 17
8	F	142/148 (96%)	124 (87%)	18 (13%)	5 32
9	G	124/124 (100%)	103 (83%)	21 (17%)	2 19
10	H	117/139 (84%)	90 (77%)	27 (23%)	1 8
11	I	100/100 (100%)	79 (79%)	21 (21%)	1 10
12	J	112/116 (97%)	89 (80%)	23 (20%)	1 11
13	K	108/111 (97%)	77 (71%)	31 (29%)	0 4
14	L	101/101 (100%)	79 (78%)	22 (22%)	1 9
15	M	84/88 (96%)	66 (79%)	18 (21%)	1 9
16	N	121/128 (94%)	97 (80%)	24 (20%)	1 12
17	O	93/94 (99%)	79 (85%)	14 (15%)	3 25
18	P	82/82 (100%)	70 (85%)	12 (15%)	4 27
19	Q	89/92 (97%)	72 (81%)	17 (19%)	2 13
20	R	74/78 (95%)	62 (84%)	12 (16%)	3 21
21	S	86/91 (94%)	75 (87%)	11 (13%)	5 32
22	T	163/179 (91%)	140 (86%)	23 (14%)	4 29
23	U	61/67 (91%)	47 (77%)	14 (23%)	1 8
24	V	73/83 (88%)	60 (82%)	13 (18%)	2 16
25	W	58/67 (87%)	42 (72%)	16 (28%)	0 4
26	X	52/52 (100%)	41 (79%)	11 (21%)	1 9
27	Y	49/52 (94%)	44 (90%)	5 (10%)	9 43
28	Z	41/42 (98%)	32 (78%)	9 (22%)	1 8
29	a	53/55 (96%)	39 (74%)	14 (26%)	0 5
30	b	33/34 (97%)	30 (91%)	3 (9%)	12 49
35	c	202/220 (92%)	154 (76%)	48 (24%)	1 7
36	d	160/188 (85%)	130 (81%)	30 (19%)	2 13
37	e	180/181 (99%)	143 (79%)	37 (21%)	1 10
38	f	115/123 (94%)	94 (82%)	21 (18%)	2 14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	g	90/90 (100%)	75 (83%)	15 (17%)	3 19
40	h	126/127 (99%)	110 (87%)	16 (13%)	5 32
41	i	119/119 (100%)	97 (82%)	22 (18%)	2 14
42	j	98/99 (99%)	82 (84%)	16 (16%)	3 21
43	k	88/92 (96%)	76 (86%)	12 (14%)	5 30
44	l	88/99 (89%)	72 (82%)	16 (18%)	2 15
45	m	104/109 (95%)	85 (82%)	19 (18%)	2 14
46	n	100/101 (99%)	85 (85%)	15 (15%)	3 26
47	o	49/50 (98%)	39 (80%)	10 (20%)	1 11
48	p	79/80 (99%)	65 (82%)	14 (18%)	2 16
49	q	72/74 (97%)	60 (83%)	12 (17%)	3 19
50	r	96/97 (99%)	76 (79%)	20 (21%)	1 10
51	s	64/77 (83%)	52 (81%)	12 (19%)	2 13
52	t	71/80 (89%)	58 (82%)	13 (18%)	2 14
53	u	76/82 (93%)	70 (92%)	6 (8%)	15 55
54	v	19/22 (86%)	16 (84%)	3 (16%)	3 23
All	All	4803/5116 (94%)	3912 (81%)	891 (19%)	2 14

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	13,21,22	2.11	2 (15%)	18,30,33	4.81	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	2MG	y	1207	31	17,26,27	1.95	3 (17%)	21,38,41	3.85	8 (38%)
31	5MC	y	1400	31	13,22,23	1.32	2 (15%)	15,32,35	1.15	0
31	4OC	y	1402	31	13,23,24	1.64	3 (23%)	18,32,35	1.56	3 (16%)
31	5MC	y	1404	31	13,22,23	1.69	2 (15%)	15,32,35	1.99	2 (13%)
31	5MC	y	1407	31	13,22,23	1.59	3 (23%)	15,32,35	1.00	1 (6%)
31	UR3	y	1498	31	12,22,23	1.76	2 (16%)	16,32,35	1.29	3 (18%)
31	MA6	y	1518	31	16,26,27	1.84	1 (6%)	18,38,41	2.82	7 (38%)
31	MA6	y	1519	31	16,26,27	2.35	2 (12%)	18,38,41	3.25	6 (33%)
31	PSU	y	516	31	13,21,22	1.28	2 (15%)	18,30,33	4.19	7 (38%)
31	7MG	y	527	31	19,26,27	2.43	5 (26%)	24,39,42	2.21	4 (16%)
31	M2G	y	966	31	17,27,28	2.97	5 (29%)	22,40,43	2.77	7 (31%)
31	5MC	y	967	31	13,22,23	1.19	1 (7%)	15,32,35	0.96	0
32	H2U	z	16	32	17,21,22	1.01	1 (5%)	23,30,33	0.97	2 (8%)
32	H2U	z	20	32	17,21,22	0.83	0	23,30,33	0.95	1 (4%)
32	PSU	z	32	32	13,21,22	1.13	2 (15%)	18,30,33	4.17	8 (44%)
32	MIA	z	37	32	21,31,32	1.68	5 (23%)	26,44,47	2.45	6 (23%)
32	PSU	z	39	32	13,21,22	1.87	4 (30%)	18,30,33	4.16	7 (38%)
32	7MG	z	46	32	19,26,27	2.45	5 (26%)	24,39,42	2.12	5 (20%)
32	5MU	z	54	32	12,22,23	2.01	4 (33%)	14,32,35	3.50	3 (21%)
32	PSU	z	55	32	13,21,22	2.20	1 (7%)	18,30,33	4.27	7 (38%)
32	4SU	z	8	32	11,21,22	1.95	3 (27%)	13,30,33	2.11	3 (23%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	z	55	PSU	C5-C1'	-7.17	1.46	1.52
31	y	527	7MG	C8-N9	-6.02	1.36	1.45
33	0	55	PSU	C5-C1'	-5.93	1.47	1.52
32	z	46	7MG	C8-N9	-5.62	1.37	1.45
32	z	39	PSU	C5-C1'	-4.62	1.48	1.52

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	0	55	PSU	N1-C2-N3	-14.33	119.19	128.33
32	z	32	PSU	N1-C2-N3	-14.27	119.23	128.33
32	z	39	PSU	N1-C2-N3	-14.03	119.38	128.33
31	y	516	PSU	N1-C2-N3	-13.68	119.61	128.33
32	z	55	PSU	N1-C2-N3	-13.17	119.93	128.33

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

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, 95^{th} 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%)	0.97	141 (4%) 33 22	5, 5, 117, 159	0
2	x	120/121 (99%)	1.04	4 (3%) 50 36	5, 13, 95, 127	0
3	A	127/229 (55%)	0.44	17 (13%) 4 4	5, 50, 148, 151	0
4	B	272/276 (98%)	0.59	29 (10%) 8 5	5, 60, 148, 155	0
5	C	201/206 (97%)	0.43	19 (9%) 10 7	5, 49, 148, 159	0
6	D	194/205 (94%)	0.06	7 (3%) 46 33	5, 55, 148, 165	0
7	E	180/182 (98%)	-0.02	12 (6%) 21 12	5, 58, 148, 156	0
8	F	173/180 (96%)	-0.27	5 (2%) 55 40	5, 67, 148, 160	0
9	G	148/148 (100%)	-0.19	5 (3%) 49 35	5, 43, 148, 151	0
10	H	138/163 (84%)	0.68	16 (11%) 6 5	5, 52, 147, 152	0
11	I	122/122 (100%)	0.67	12 (9%) 10 6	5, 35, 142, 148	0
12	J	146/150 (97%)	0.20	8 (5%) 29 19	5, 90, 150, 160	0
13	K	137/141 (97%)	1.51	46 (33%) 0 1	5, 24, 148, 152	0
14	L	118/118 (100%)	0.23	7 (5%) 26 16	5, 44, 148, 148	0
15	M	106/112 (94%)	0.97	22 (20%) 1 1	5, 48, 148, 160	0
16	N	137/146 (93%)	0.04	2 (1%) 76 63	5, 74, 150, 167	0
17	O	117/118 (99%)	0.48	17 (14%) 3 3	5, 35, 114, 148	0
18	P	101/101 (100%)	0.56	20 (19%) 1 1	5, 79, 148, 159	0
19	Q	109/113 (96%)	0.63	21 (19%) 2 1	5, 33, 137, 149	0
20	R	92/96 (95%)	0.43	12 (13%) 5 4	5, 73, 148, 161	0
21	S	103/110 (93%)	0.67	22 (21%) 1 1	5, 86, 160, 163	0
22	T	185/206 (89%)	-0.22	4 (2%) 65 51	5, 50, 148, 161	0
23	U	76/85 (89%)	0.76	13 (17%) 2 2	5, 57, 151, 166	0
24	V	88/98 (89%)	0.93	21 (23%) 1 1	5, 91, 148, 154	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	62/72 (86%)	0.09	3 (4%) 34 23	5, 88, 149, 155	0
26	X	60/60 (100%)	-0.45	0 100 100	5, 36, 148, 150	0
27	Y	56/60 (93%)	0.28	7 (12%) 5 5	7, 77, 164, 168	0
28	Z	48/49 (97%)	0.43	3 (6%) 23 14	5, 5, 42, 126	0
29	a	63/65 (96%)	0.56	7 (11%) 7 5	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%)	0.97	73 (4%) 33 22	5, 9, 113, 163	0
32	z	67/76 (88%)	0.81	2 (2%) 54 38	5, 6, 82, 117	0
33	0	75/76 (98%)	0.71	2 (2%) 58 43	5, 37, 129, 148	0
34	1	6/10 (60%)	0.76	0 100 100	5, 5, 54, 67	0
35	c	234/256 (91%)	-0.34	0 100 100	5, 50, 151, 165	0
36	d	206/239 (86%)	0.37	30 (14%) 3 3	5, 57, 148, 151	0
37	e	208/209 (99%)	-0.00	6 (2%) 55 40	5, 50, 148, 157	0
38	f	150/162 (92%)	0.12	9 (6%) 25 15	5, 62, 148, 154	0
39	g	101/101 (100%)	-0.06	4 (3%) 42 29	5, 72, 148, 156	0
40	h	155/156 (99%)	0.20	16 (10%) 9 6	5, 73, 155, 163	0
41	i	138/138 (100%)	0.01	3 (2%) 65 51	5, 43, 148, 149	0
42	j	127/128 (99%)	0.58	17 (13%) 4 4	5, 85, 150, 154	0
43	k	98/105 (93%)	-0.00	7 (7%) 19 11	5, 83, 151, 164	0
44	l	116/129 (89%)	-0.03	8 (6%) 20 12	5, 71, 150, 162	0
45	m	124/132 (93%)	0.13	7 (5%) 28 18	5, 30, 148, 152	0
46	n	125/126 (99%)	0.01	7 (5%) 28 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%)	-0.28	1 (1%) 82 70	5, 57, 148, 163	0
49	q	83/88 (94%)	0.90	21 (25%) 1 1	5, 50, 148, 148	0
50	r	104/105 (99%)	0.43	8 (7%) 16 10	5, 52, 148, 158	0
51	s	73/88 (82%)	-0.49	0 100 100	5, 69, 149, 157	0
52	t	80/93 (86%)	-0.37	1 (1%) 79 66	5, 52, 148, 159	0
53	u	99/106 (93%)	1.08	22 (22%) 1 1	10, 66, 199, 199	0
54	v	24/27 (88%)	0.43	2 (8%) 14 9	5, 47, 139, 142	0
All	All	10434/10880 (95%)	0.59	787 (7%) 17 11	5, 32, 148, 199	0

The worst 5 of 787 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	49	ASP	10.3
15	M	81	GLY	9.3
14	L	58	GLY	8.9
47	o	13	THR	8.2
15	M	82	ILE	8.1

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, 95^{th} 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	0.76	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.