wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2026 – 01:24 PM UTC

PDB ID	:	1VQ5 / pdb_00001vq5
Title	:	The structure of the transition state analogue "RAA" bound to the large ribosomal subunit of haloarcula marismortui
Authors	:	Schmeing, T.M.; Steitz, T.A.
Deposited on	:	2004-12-16
Resolution	:	2.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

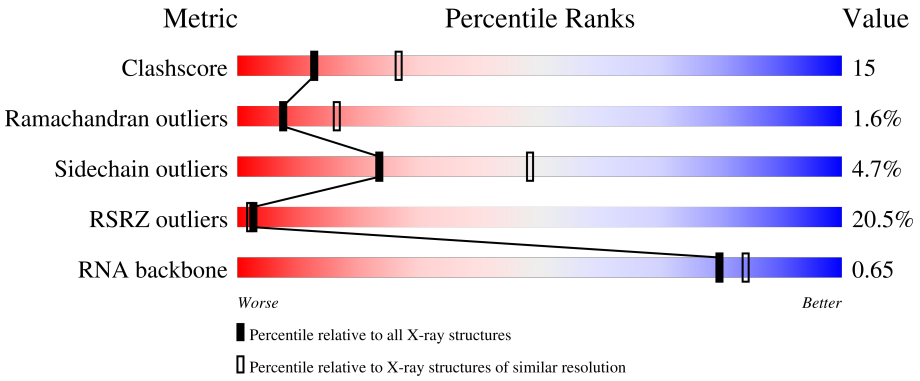
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	0	2922	15% 61% 28% 5% • 6%
2	9	122	14% 58% 32% 10%
3	4	8	38% 38% 25%
4	A	240	8% 58% 35% 5% •
5	B	338	46% 48% 45% 7%

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Mol	Chain	Length	Quality of chain
6	C	246	4% 57% 36% 6%
7	D	177	40% 29% 42% 7% 21%
8	E	178	65% 49% 44%
9	F	120	12% 52% 43%
10	G	348	6% 5% 92%
11	H	171	29% 56% 35% 6%
12	J	145	36% 60% 31% 7%
13	K	132	50% 63% 34%
14	L	165	20% 52% 32% 12%
15	M	194	% 67% 30%
16	N	187	21% 46% 42% 12%
17	O	116	14% 67% 29%
18	P	149	14% 62% 32%
19	Q	96	12% 68% 28%
20	R	155	6% 61% 34%
21	S	85	6% 65% 28% 5%
22	T	120	5% 56% 39%
23	U	66	26% 44% 36% 20%
24	V	71	24% 42% 42% 7% 8%
25	W	154	16% 50% 44% 6%
26	X	92	16% 48% 32% 10% 11%
27	Y	241	5% 38% 18% 41%
28	Z	83	16% 52% 33% 12%
29	1	57	2% 65% 30%
30	2	50	28% 50% 42% 8%

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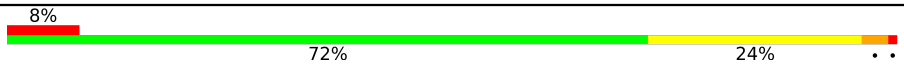
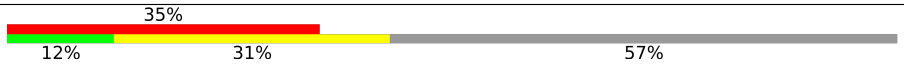
Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99060 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 ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59021	26350	10878	19048	2745	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a RNA chain called 5'-D(*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	8	126	61	23	37	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	237	1753	1072	352	324	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total 865	C 529	N 161	O 175	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total 1136	C 683	N 229	O 224	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total 735	C 450	N 141	O 144	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	150	Total 1149	C 713	N 209	O 223	S 4	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	81	Total 641	C 389	N 111	O 138	S 3	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total 950	C 568	N 180	O 202	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	53	Total 410	C 244	N 75	O 86	S 5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	106	Total	Mg	0	0
			106	106		
33	9	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	3	Total K 3 3	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	71	Total Na 71 71	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5820	Total O 5820 5820	0	0
38	9	133	Total O 133 133	0	0
38	4	8	Total O 8 8	0	0
38	A	117	Total O 117 117	0	0
38	B	150	Total O 150 150	0	0
38	C	165	Total O 165 165	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	D	49	Total O 49 49	0	0
38	E	47	Total O 47 47	0	0
38	F	21	Total O 21 21	0	0
38	G	16	Total O 16 16	0	0
38	H	66	Total O 66 66	0	0
38	J	52	Total O 52 52	0	0
38	K	54	Total O 54 54	0	0
38	L	83	Total O 83 83	0	0
38	M	118	Total O 118 118	0	0
38	N	66	Total O 66 66	0	0
38	O	39	Total O 39 39	0	0
38	P	65	Total O 65 65	0	0
38	Q	52	Total O 52 52	0	0
38	R	85	Total O 85 85	0	0
38	S	31	Total O 31 31	0	0
38	T	39	Total O 39 39	0	0
38	U	25	Total O 25 25	0	0
38	V	13	Total O 13 13	0	0
38	W	68	Total O 68 68	0	0
38	X	27	Total O 27 27	0	0
38	Y	92	Total O 92 92	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	Z	30	Total O 30 30	0	0
38	1	59	Total O 59 59	0	0
38	2	42	Total O 42 42	0	0
38	3	74	Total O 74 74	0	0
38	I	10	Total O 10 10	0	0

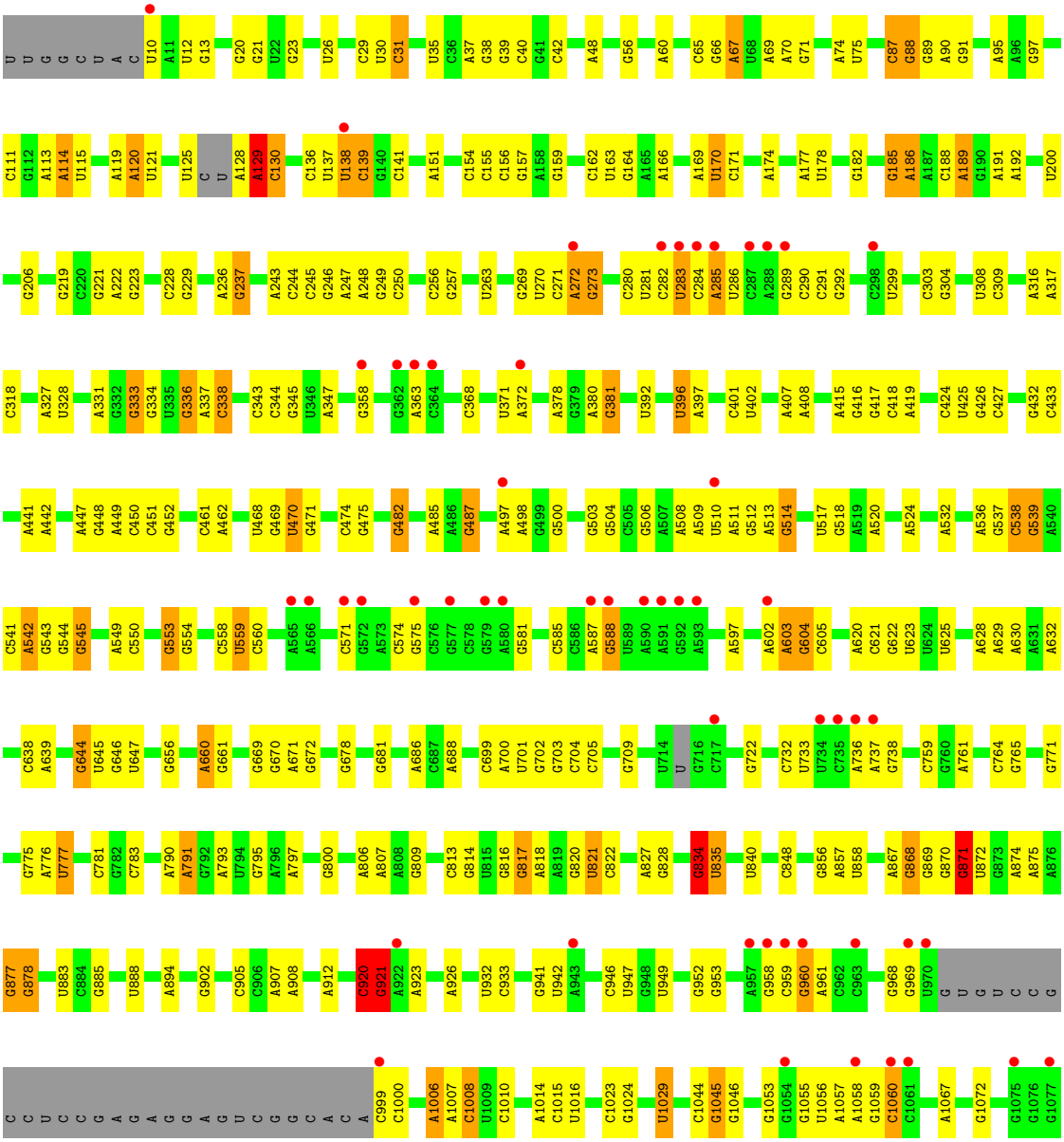
3 Residue-property plots (i)

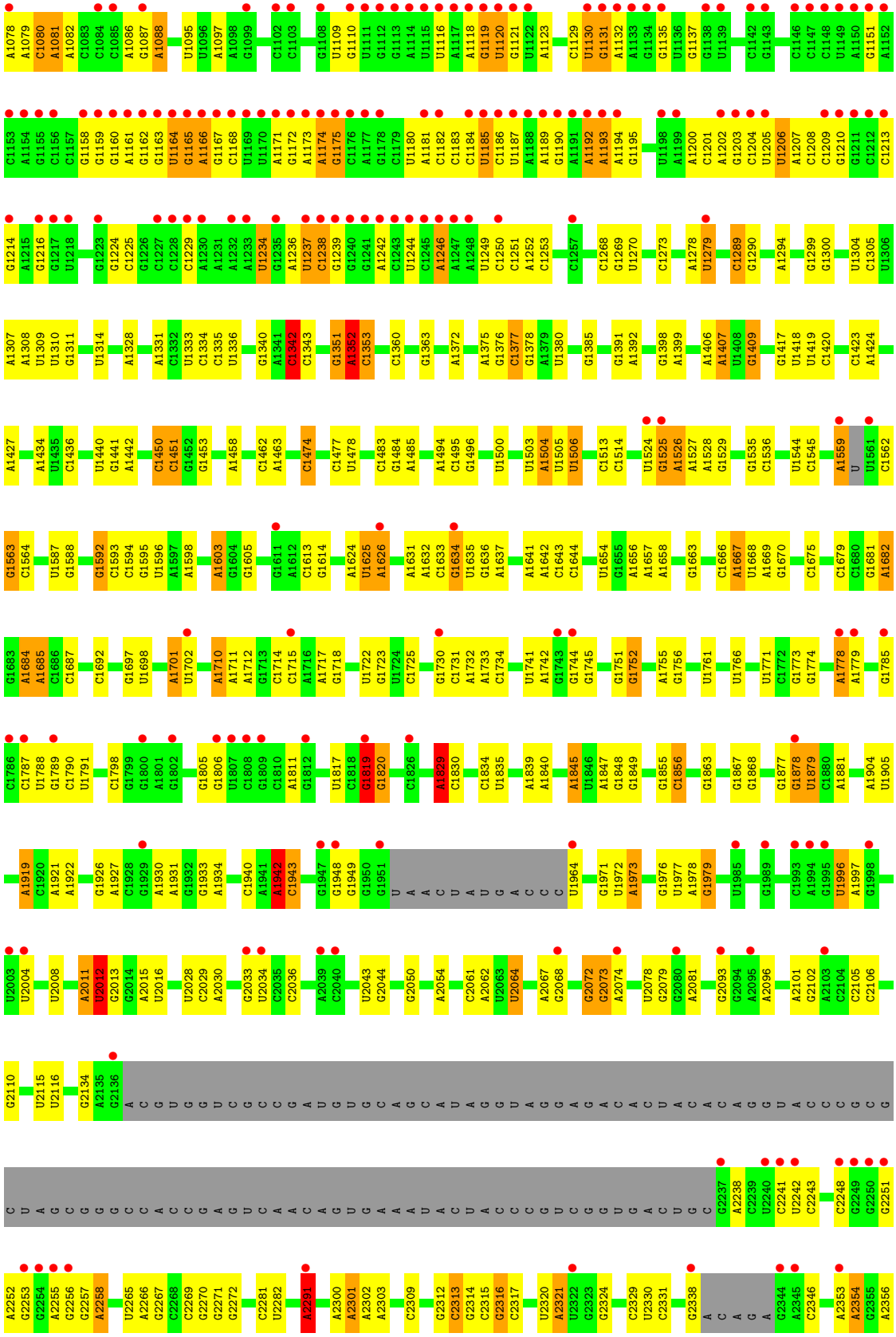
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

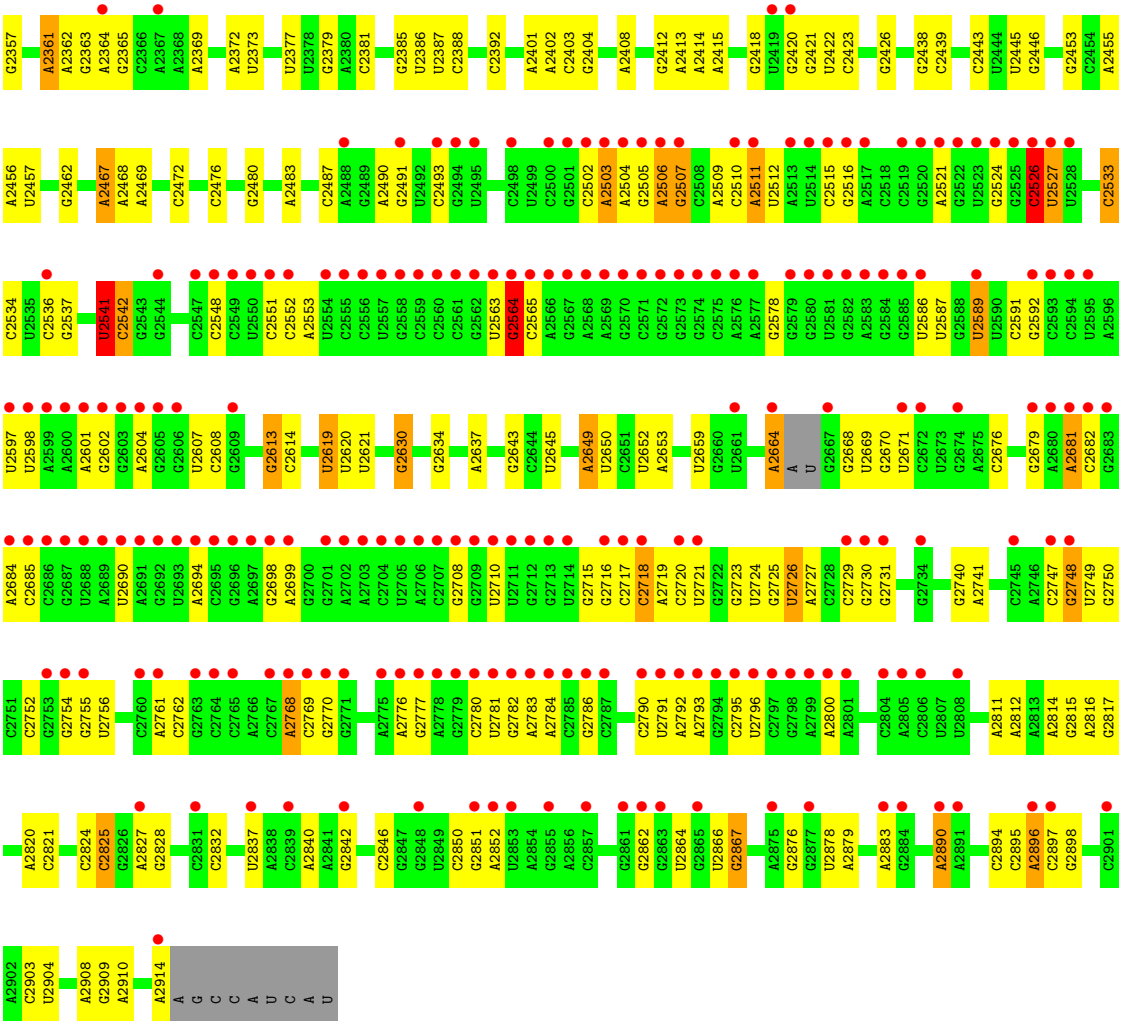
- Molecule 1: 23S ribosomal rna

Chain 0:





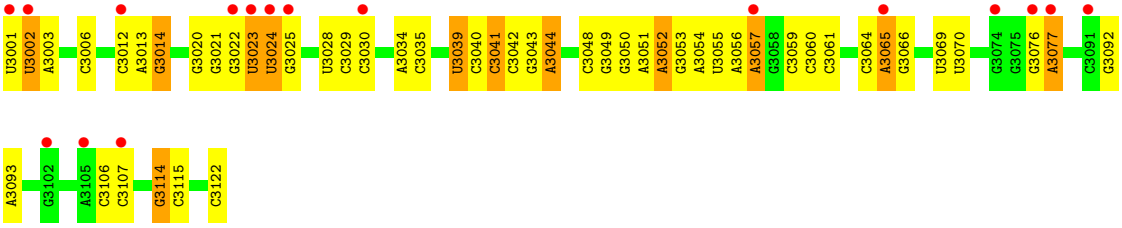

A1078 A1079 C1080 A1081 A1082 C1083 C1084 C1085 A1086 G1087 A1088 U1095 U1096 A1097 A1098 G1099 C1102 C1103 G1108 U1109 G1110 U1111 G1112 G1113 A1114 U1115 U1116 A1117 A1118 G1119 U1120 G1121 U1122 A1123 C1129 U1130 G1131 A1132 A1133 G1134 G1135 U1136 G1137 G1138 U1139 C1142 G1143 C1146 C1147 C1148 U1149 A1150 G1151 A1152
C1153 A1154 G1155 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 C1179 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213
G1214 A1215 G1216 G1217 U1218 G1223 G1224 C1225 G1226 C1227 C1228 C1229 A1230 A1231 A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 G1240 G1241 A1242 C1243 U1244 C1245 A1246 A1247 A1248 U1249 C1250 C1251 A1252 C1253 C1257 C1268 G1269 U1270 C1273 A1278 U1279 C1289 G1290 A1294 G1299 G1300 U1304 C1305 U1306
A1307 A1308 U1309 U1310 G1311 U1314 A1328 A1331 C1332 U1333 C1334 C1335 U1336 G1340 A1341 C1342 C1343 G1351 A1352 C1353 C1360 G1363 A1372 A1375 G1376 C1377 G1378 A1379 U1380 G1385 G1391 A1392 G1398 A1399 A1406 A1407 U1408 G1409 G1417 U1418 U1419 C1420 C1423 A1424
A1427 A1434 U1435 C1436 U1440 G1441 A1442 C1450 C1451 G1452 G1453 A1458 C1462 A1463 C1474 C1477 U1478 C1483 G1484 A1485 A1494 C1495 G1496 U1500 U1503 A1504 U1505 U1506 C1513 C1514 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 U1544 C1545 A1559 U U1561 C1562
G1563 C1564 U1587 G1588 G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 G1611 A1612 C1613 G1614 A1624 U1625 A1626 A1631 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 C1644 U1654 G1655 A1656 A1657 A1658 G1663 C1666 A1667 U1668 A1669 G1670 C1675 C1679 C1680 G1681 A1682
G1683 A1684 A1685 C1686 C1687 C1692 G1697 U1698 A1701 U1702 A1710 A1711 A1712 G1713 C1714 C1715 A1716 A1717 G1718 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 U1741 A1742 G1743 G1744 G1745 G1751 G1752 A1755 G1756 U1761 U1766 U1771 C1772 G1773 G1774 A1778 A1779 G1785
C1786 C1787 U1788 G1789 C1790 U1791 C1798 G1799 G1800 A1801 G1802 G1805 G1806 U1807 C1808 G1809 C1810 A1811 G1812 U1817 C1818 G1819 G1820 C1826 A1829 C1830 C1834 U1835 A1839 A1840 A1845 U1846 A1847 G1848 G1849 G1855 C1856 G1863 G1867 G1868 G1877 G1878 U1879 C1880 A1881 A1904 U1905
A1919 C1920 A1921 A1922 G1926 A1927 C1928 G1929 A1930 A1931 G1932 G1933 A1934 C1940 A1941 A1942 C1943 G1947 G1948 G1949 G1950 G1951 U C A A C U A U G C U1964 G1971 U1972 A1973 G1976 U1977 A1978 G1979 U1985 G1989 C1993 A1994 G1995 U1996 A1997 G1998
U2003 U2004 U2008 A2011 U2012 G2013 G2014 A2015 U2016 U2028 C2029 A2030 G2033 U2034 C2035 C2036 A2039 C2040 U2043 G2044 G2050 A2054 C2061 A2062 U2063 U2064 A2067 G2068 G2072 G2073 A2074 U2078 G2079 G2080 A2081 G2093 G2094 A2095 A2096 A2101 G2102 A2103 C2104 C2105 C2106
G2110 U2115 U2116 G2134 A2135 G2136 A C G U G U C G C C G G C C A C G U C A A C G U U C C C G A A C A A G U G G C C A A A U C U U C A A C U G C G2237 A2238 C2239 U2240 C2241 U2242 C2243 C2248 G2249 G2250 G2251
A2252 G2253 G2254 A2255 G2256 C2257 A2258 U2265 A2266 G2267 C2268 C2269 G2270 G2271 G2272 C2281 U2282 A2291 A2300 A2301 A2302 A2303 C2309 G2312 C2313 G2314 C2315 G2316 C2317 U2320 A2321 U2322 G2323 G2324 C2329 U2330 C2331 G2338 A C A G A G2344 A2345 C2346 A2353 A2354 G2355 A2356



• Molecule 2: 5S ribosomal RNA

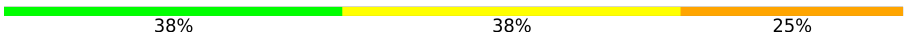
Chain 9:

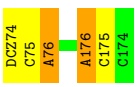




• Molecule 3: 5'-D(*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3')

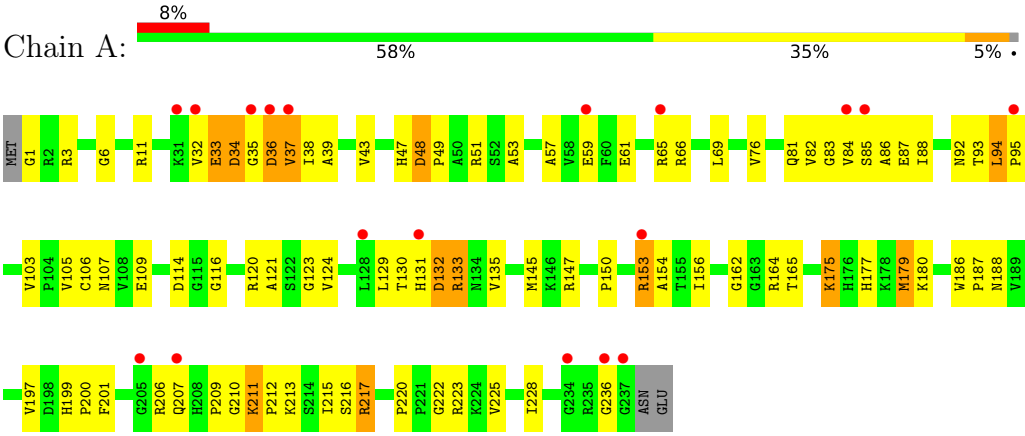
Chain 4:





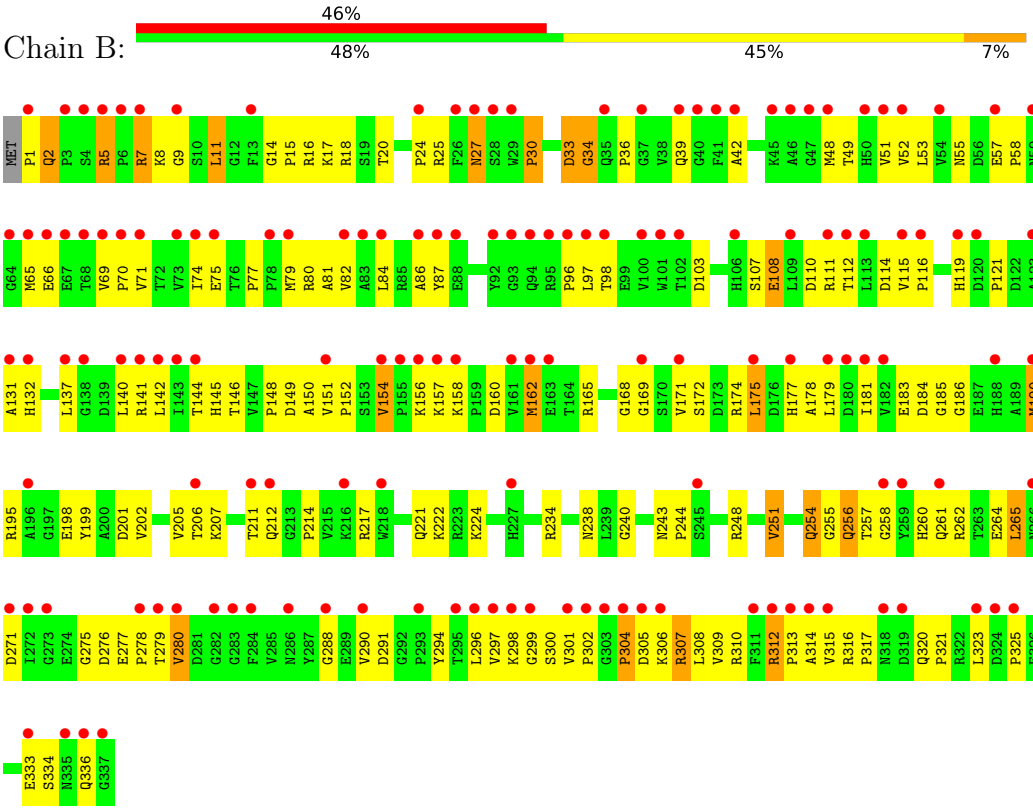
• Molecule 4: 50S ribosomal protein L2P

Chain A:



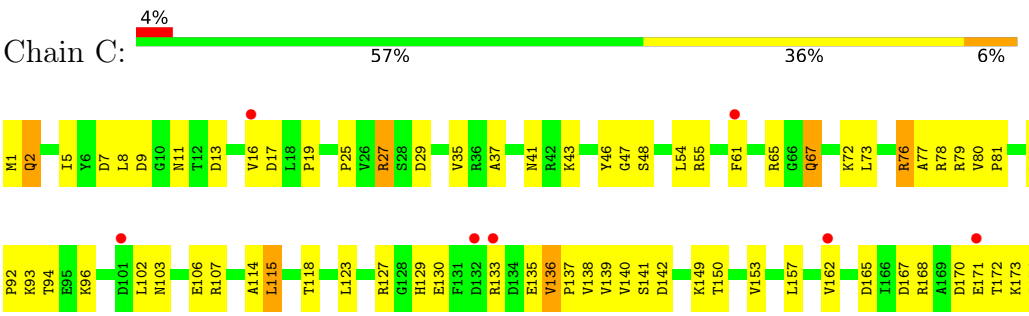
• Molecule 5: 50S ribosomal protein L3P

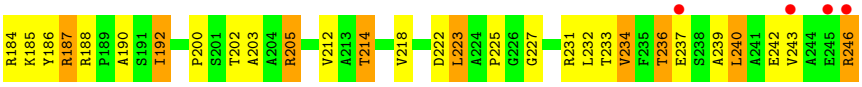
Chain B:



• Molecule 6: 50S ribosomal protein L4E

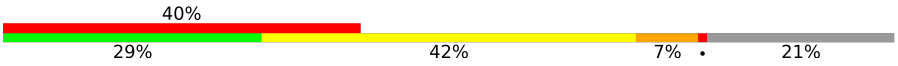
Chain C:

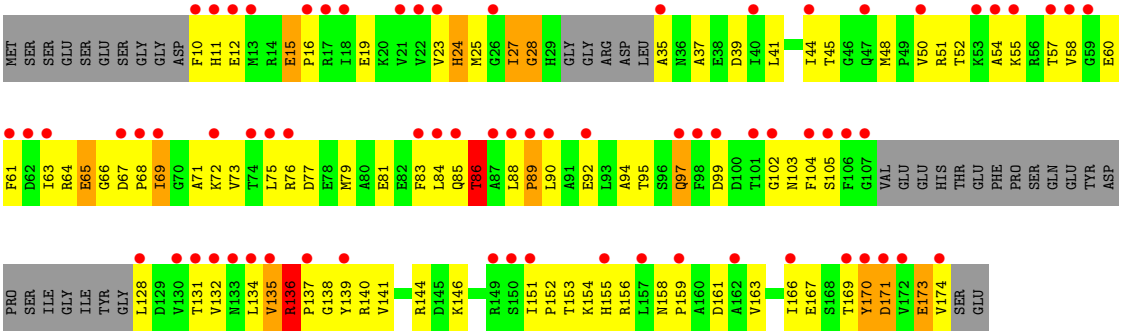




• Molecule 7: 50S ribosomal protein L5P

Chain D:

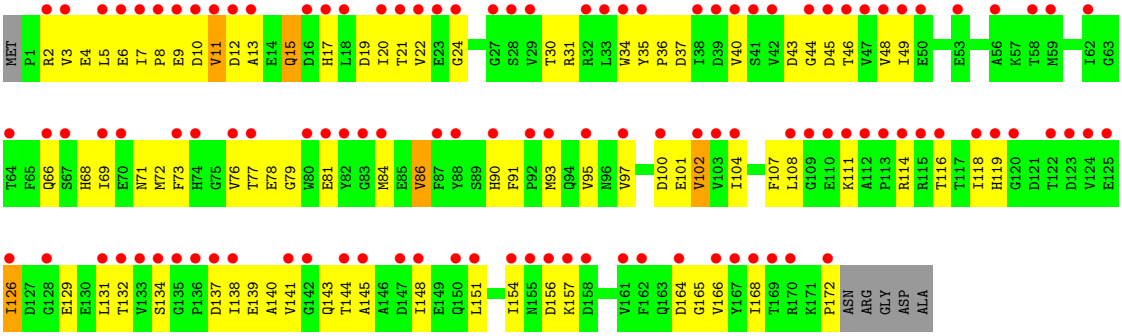




• Molecule 8: 50S ribosomal protein L6P

Chain E:

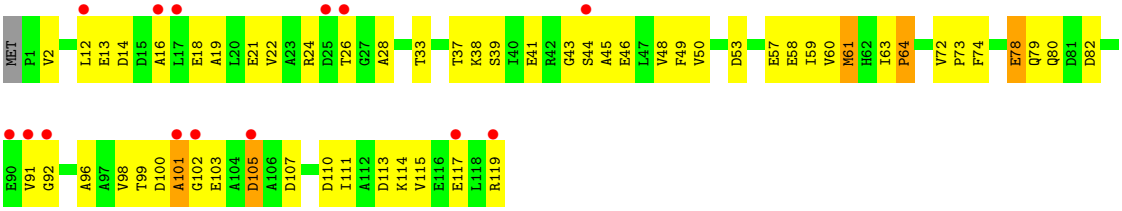




• Molecule 9: 50S ribosomal protein L7AE

Chain F:

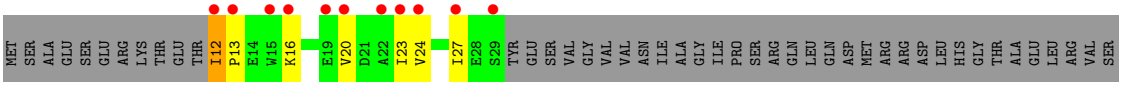


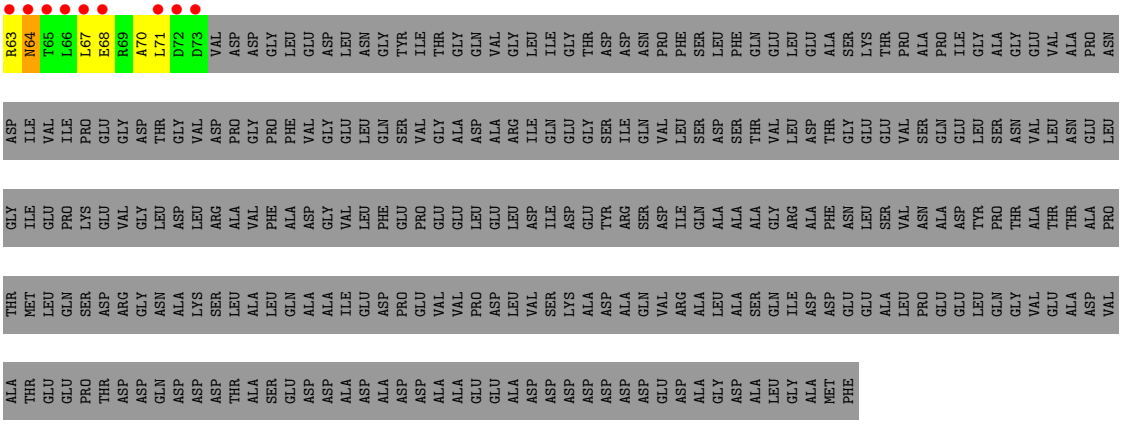


• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



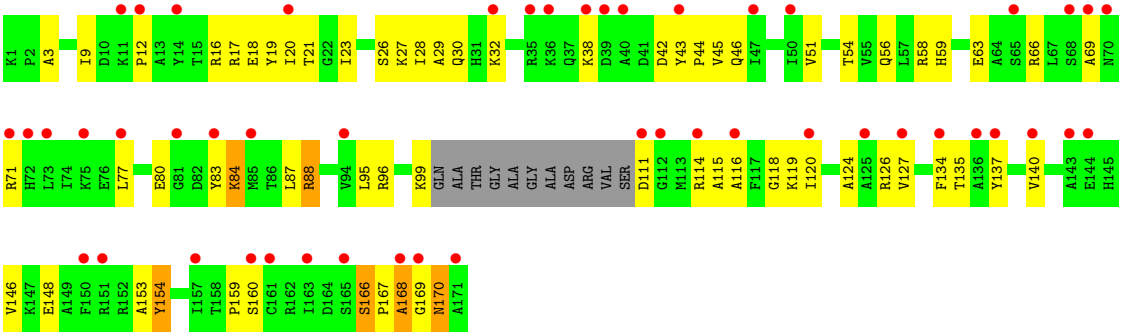




• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:

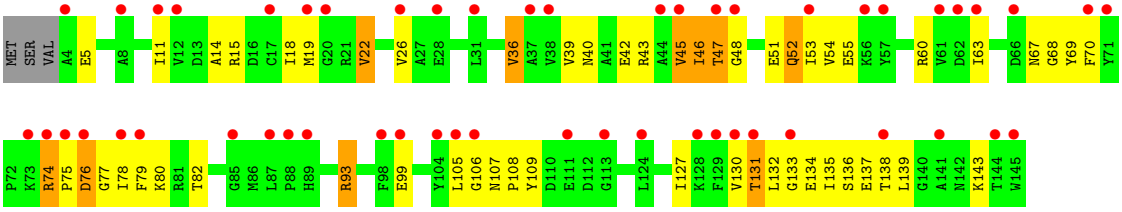




• Molecule 12: 50S ribosomal protein L13P

Chain J:

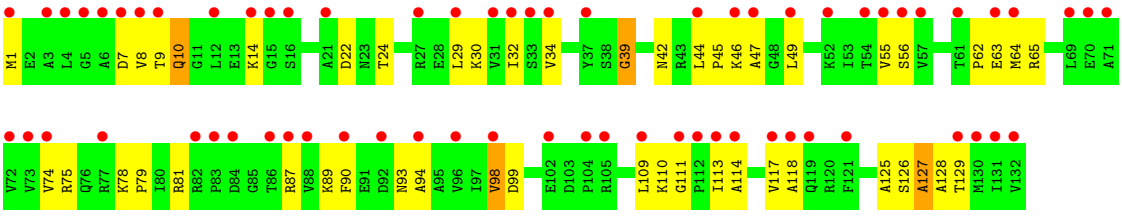




• Molecule 13: 50S ribosomal protein L14P

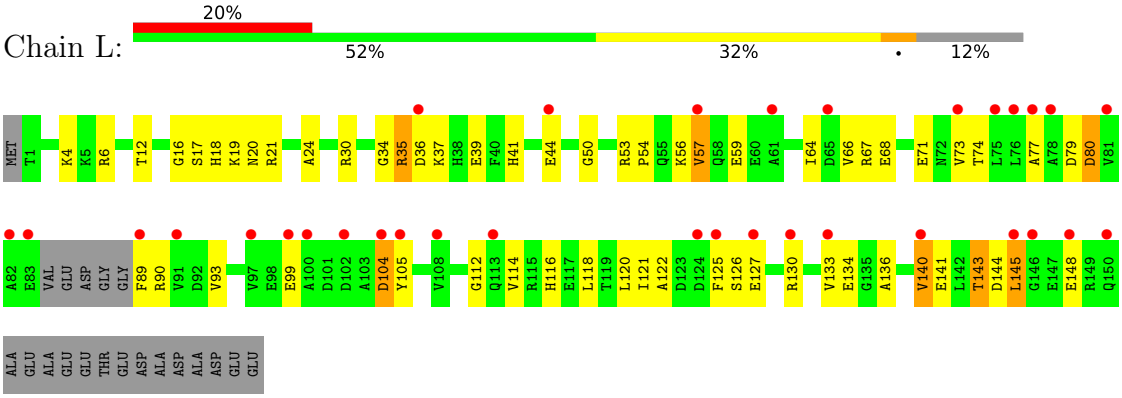
Chain K:





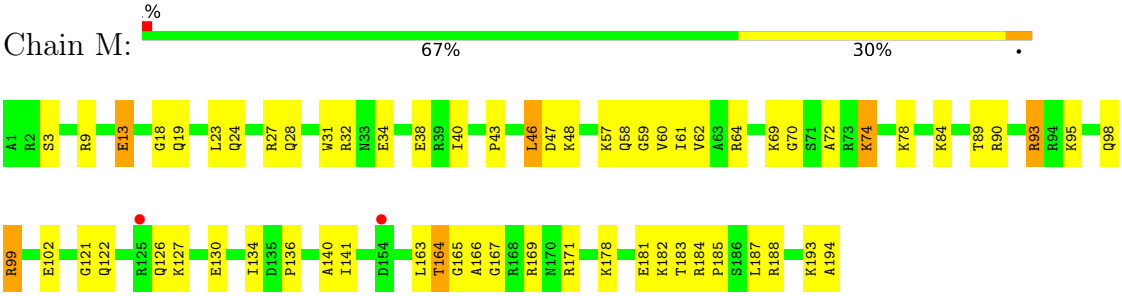
• Molecule 14: 50S ribosomal protein L15P

Chain L:



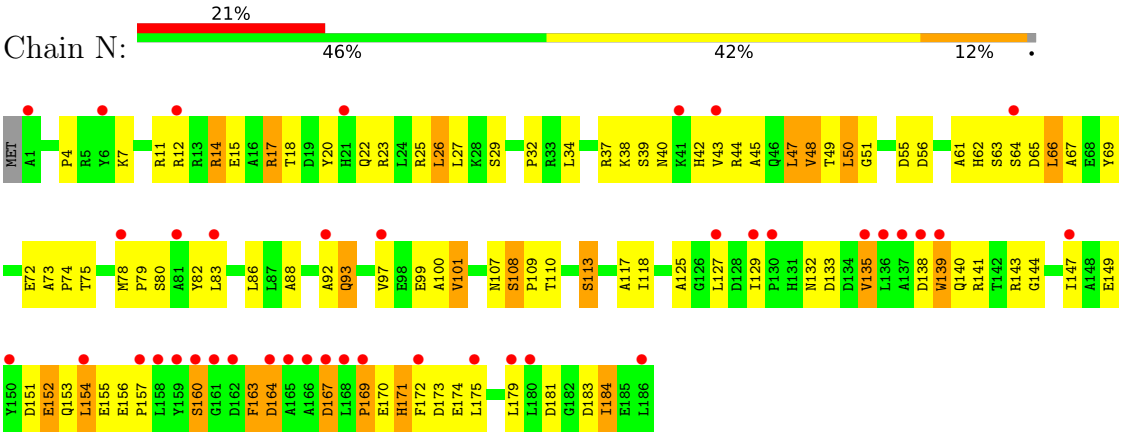
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



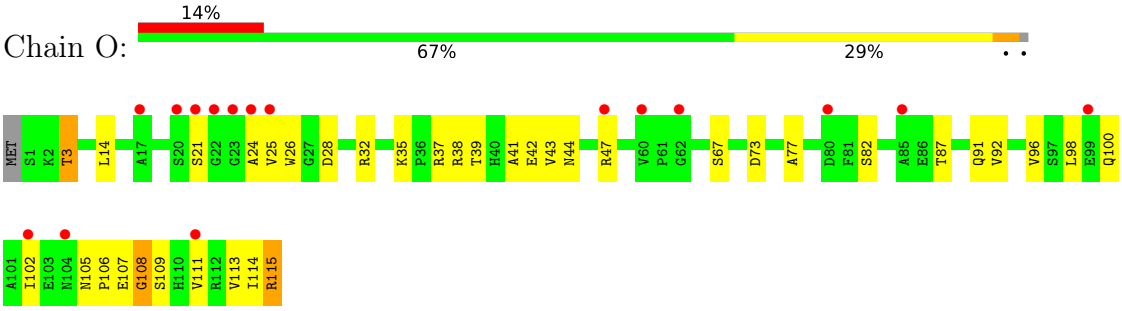
• Molecule 16: 50S ribosomal protein L18P

Chain N:

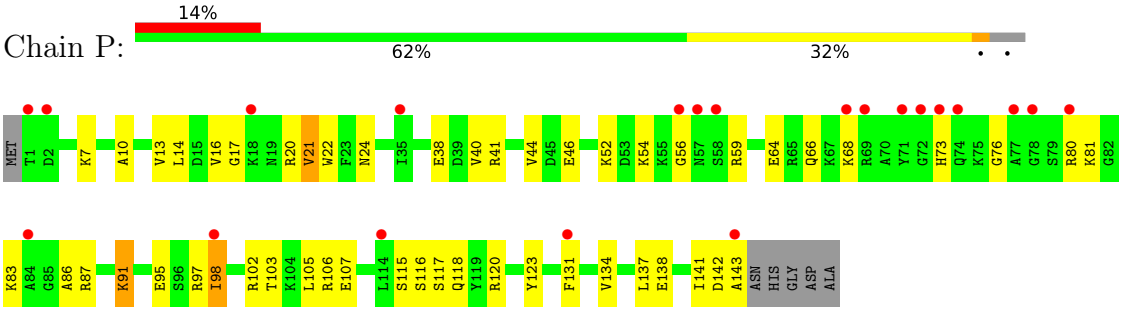


• Molecule 17: 50S ribosomal protein L18e

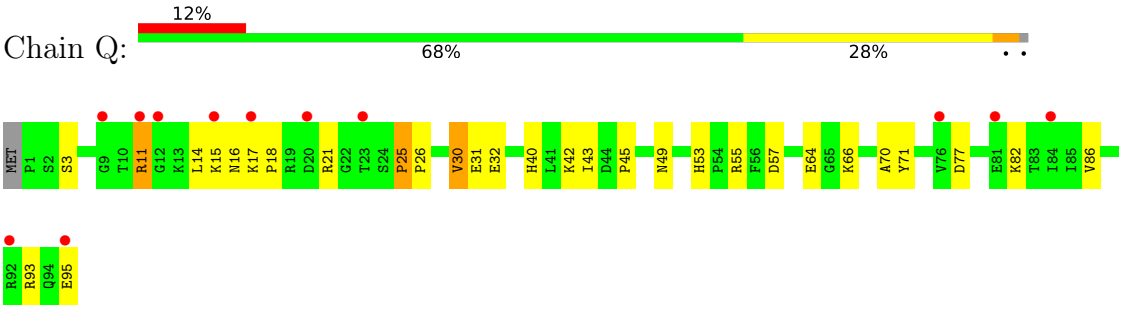
Chain O:



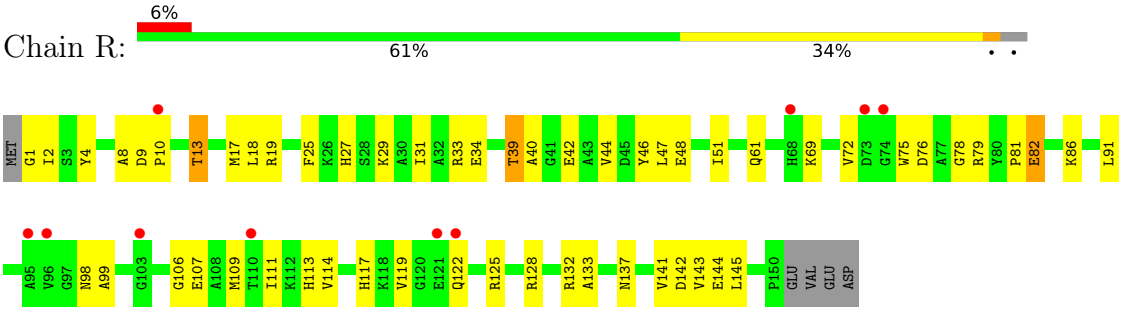
• Molecule 18: 50S ribosomal protein L19E



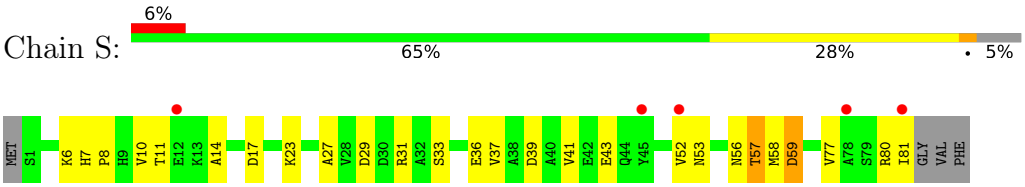
• Molecule 19: 50S ribosomal protein L21e



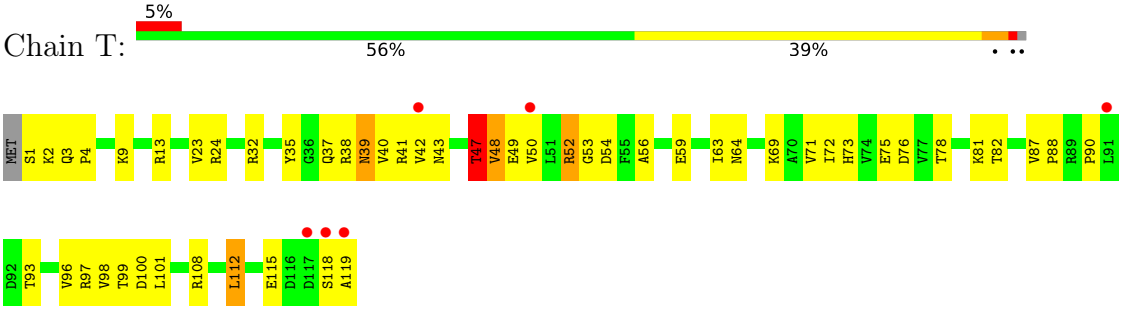
• Molecule 20: 50S ribosomal protein L22P



• Molecule 21: 50S ribosomal protein L23P

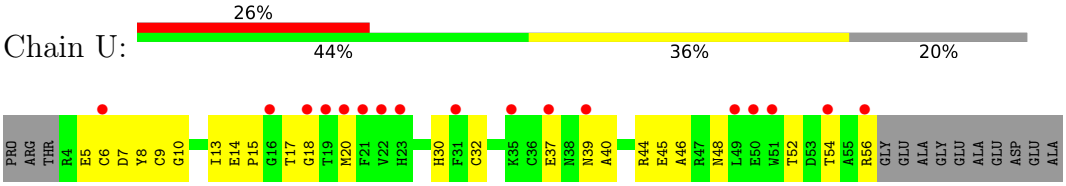


• Molecule 22: 50S ribosomal protein L24P



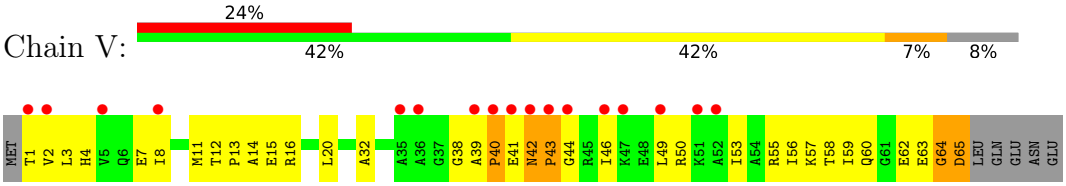
• Molecule 23: 50S ribosomal protein L24E

Chain U:



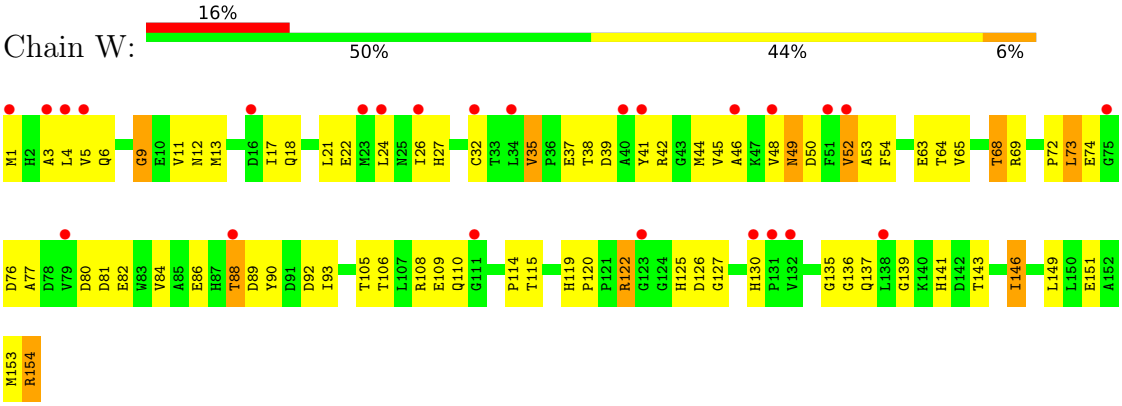
• Molecule 24: 50S ribosomal protein L29P

Chain V:



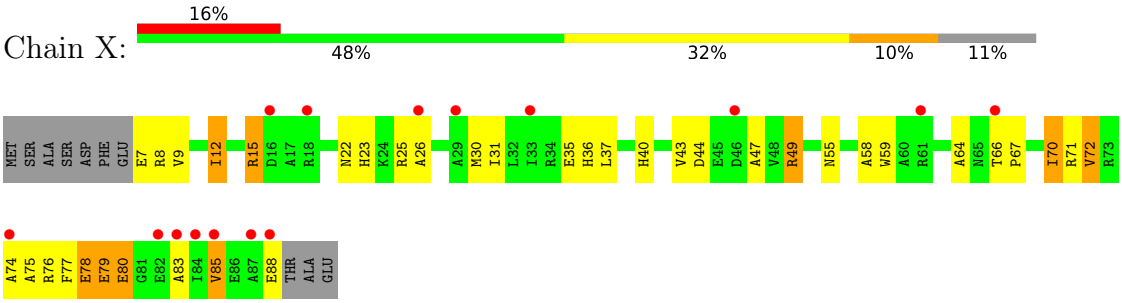
• Molecule 25: 50S ribosomal protein L30P

Chain W:



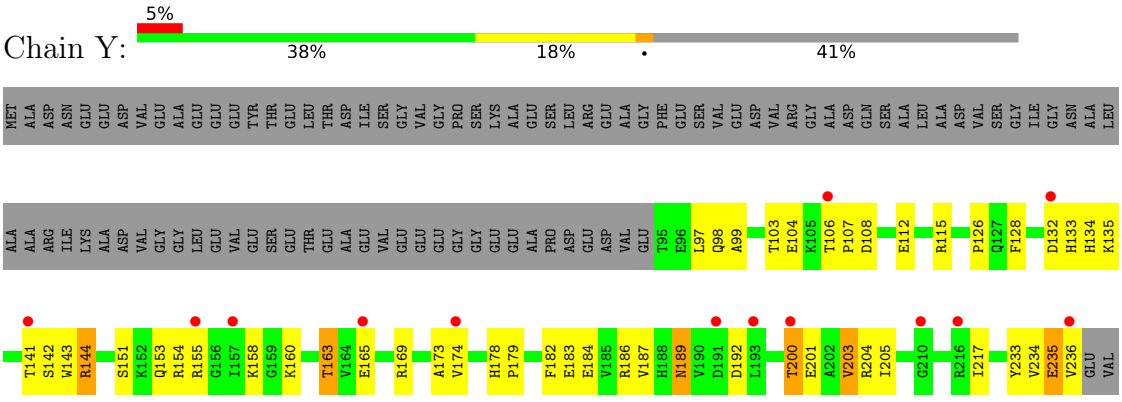
• Molecule 26: 50S ribosomal protein L31e

Chain X:



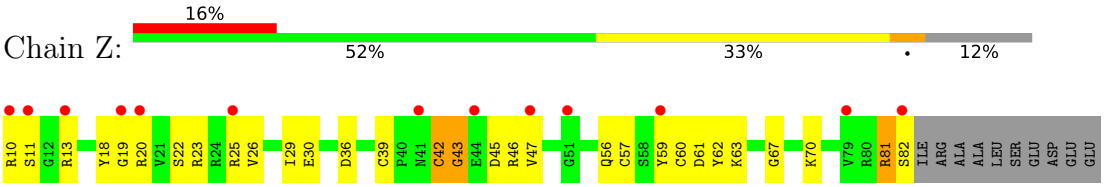
• Molecule 27: 50S ribosomal protein L32E

Chain Y:

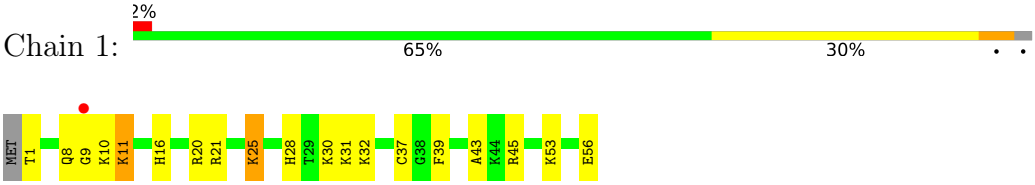




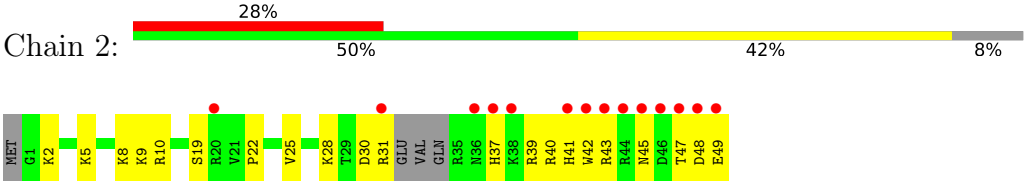
• Molecule 28: 50S ribosomal protein L37Ae



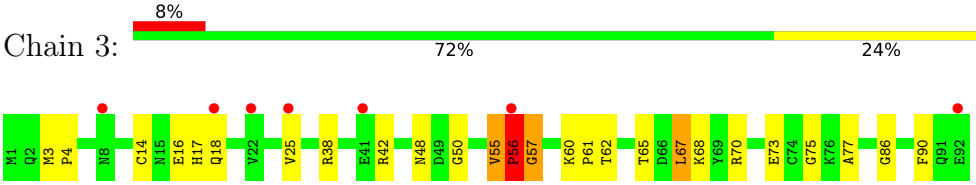
• Molecule 29: 50S ribosomal protein L37e



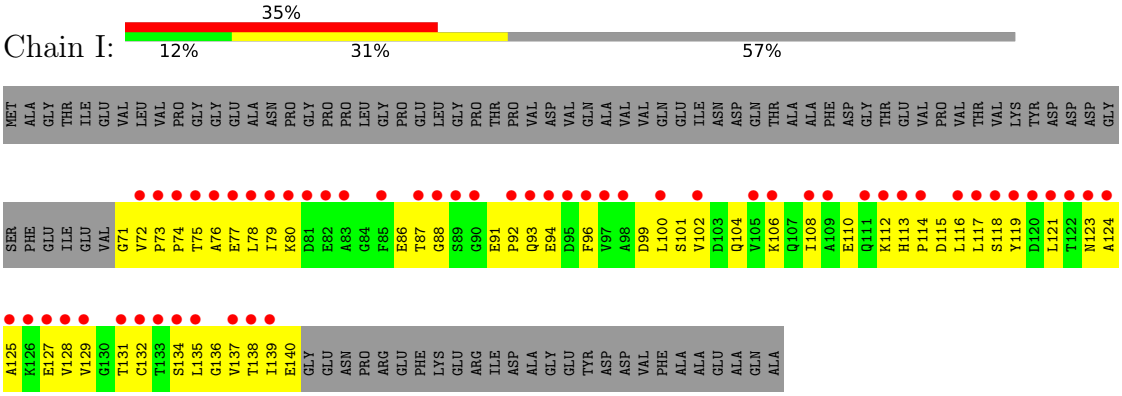
• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.79Å 300.61Å 573.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 94.1 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.83 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.237 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	53.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMU, PO2, CD, CL, UR3, NA, 5AA, PSU, K, 2OP, OMG, 1MA, DCZ

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	0	0.39	0/65959	0.61	29/102870 (0.0%)
2	9	0.38	0/2905	0.60	2/4528 (0.0%)
3	4	0.44	0/83	0.99	1/119 (0.8%)
4	A	0.43	0/1786	1.00	7/2408 (0.3%)
5	B	0.41	0/2690	0.99	9/3652 (0.2%)
6	C	0.48	0/1884	1.01	7/2551 (0.3%)
7	D	0.33	0/1111	0.87	5/1498 (0.3%)
8	E	0.38	0/1382	0.89	3/1880 (0.2%)
9	F	0.37	0/901	0.87	0/1224
10	G	0.36	0/241	0.72	0/324
11	H	0.39	0/1287	0.95	4/1725 (0.2%)
12	J	0.42	0/1136	0.94	5/1530 (0.3%)
13	K	0.44	0/1001	1.03	3/1347 (0.2%)
14	L	0.38	0/1130	0.96	4/1509 (0.3%)
15	M	0.42	0/1584	0.90	5/2119 (0.2%)
16	N	0.37	0/1474	1.05	15/1999 (0.8%)
17	O	0.43	0/874	0.93	1/1181 (0.1%)
18	P	0.40	0/1147	0.89	3/1528 (0.2%)
19	Q	0.44	0/749	1.03	5/1005 (0.5%)
20	R	0.45	0/1172	0.94	3/1578 (0.2%)
21	S	0.37	0/648	0.88	3/875 (0.3%)
22	T	0.39	0/958	0.97	3/1289 (0.2%)
23	U	0.39	0/417	0.86	0/562
24	V	0.36	0/502	0.94	3/675 (0.4%)
25	W	0.45	0/1219	0.99	4/1655 (0.2%)
26	X	0.44	0/664	1.00	3/895 (0.3%)
27	Y	0.45	0/1146	0.99	3/1536 (0.2%)
28	Z	0.42	0/589	0.94	1/787 (0.1%)
29	1	0.47	0/438	0.94	2/578 (0.3%)
30	2	0.40	0/401	0.76	0/529
31	3	0.42	0/771	0.89	3/1024 (0.3%)
32	I	0.35	0/526	0.91	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.39	0/98775	0.72	136/147696 (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	0	1	52
25	W	0	1
All	All	1	53

There are no bond length outliers.

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	13.94	130.40	109.50
4	A	222	GLY	N-CA-C	-9.56	103.11	114.48
16	N	163	PHE	N-CA-C	-9.01	102.42	113.41
1	0	1563	G	C4'-C3'-O3'	8.84	122.66	109.40
19	Q	17	LYS	N-CA-C	-8.54	97.77	110.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 53 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	189	A	Sidechain
1	0	26	U	Sidechain
1	0	333	G	Sidechain
1	0	48	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	0	59021	0	29813	781	1
2	9	2600	0	1326	52	1
3	4	126	0	75	5	0
4	A	1753	0	1766	109	0
5	B	2625	0	2533	165	1
6	C	1859	0	1816	114	0
7	D	1094	0	1085	99	0
8	E	1357	0	1266	79	0
9	F	890	0	843	55	0
10	G	240	0	231	11	0
11	H	1266	0	1268	60	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	52	1
14	L	1118	0	1076	59	0
15	M	1560	0	1568	65	0
16	N	1445	0	1401	114	0
17	O	865	0	873	31	0
18	P	1136	0	1123	53	0
19	Q	735	0	729	24	0
20	R	1149	0	1122	55	0
21	S	641	0	605	19	0
22	T	950	0	923	51	0
23	U	410	0	364	23	0
24	V	499	0	511	37	0
25	W	1196	0	1137	98	0
26	X	654	0	653	45	0
27	Y	1130	0	1133	54	0
28	Z	578	0	539	23	0
29	1	431	0	426	28	0
30	2	396	0	413	29	0
31	3	755	0	728	19	0
32	I	519	0	500	59	0
33	0	106	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	3	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5820	0	0	111	0
38	1	59	0	0	2	0
38	2	42	0	0	2	0
38	3	74	0	0	4	0
38	4	8	0	0	0	0
38	9	133	0	0	3	0
38	A	117	0	0	10	0
38	B	150	0	0	16	0
38	C	165	0	0	15	0
38	D	49	0	0	11	0
38	E	47	0	0	7	0
38	F	21	0	0	3	0
38	G	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	66	0	0	6	0
38	I	10	0	0	2	0
38	J	52	0	0	1	0
38	K	54	0	0	3	0
38	L	83	0	0	10	0
38	M	118	0	0	3	0
38	N	66	0	0	8	0
38	O	39	0	0	4	0
38	P	65	0	0	3	0
38	Q	52	0	0	5	0
38	R	85	0	0	5	0
38	S	31	0	0	3	0
38	T	39	0	0	1	0
38	U	25	0	0	0	0
38	V	13	0	0	2	0
38	W	68	0	0	6	0
38	X	27	0	0	2	0
38	Y	92	0	0	5	0
38	Z	30	0	0	2	0
All	All	99060	0	59975	2299	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 15.

The worst 5 of 2299 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
5:B:62:ARG:HA	5:B:65:MET:HE3	1.31	1.10
15:M:164:THR:HG22	15:M:167:GLY:H	1.13	1.09
1:0:156:C:H5"	15:M:171:ARG:HD3	1.35	1.08
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.30	1.08

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)
2:9:3020:G:OP1	5:B:195:ARG:NH2[7_545]	1.98	0.22
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	2.13	0.07
13:K:63:GLU:CB	13:K:63:GLU:CB[3_655]	2.13	0.07

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
4	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	5 11
5	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	6 14
6	C	244/246 (99%)	217 (89%)	26 (11%)	1 (0%)	30 51
7	D	134/177 (76%)	97 (72%)	25 (19%)	12 (9%)	0 0
8	E	170/178 (96%)	156 (92%)	13 (8%)	1 (1%)	21 42
9	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	3 4
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
11	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	6 13
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	9 19
13	K	130/132 (98%)	119 (92%)	8 (6%)	3 (2%)	5 9
14	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	9 19
15	M	192/194 (99%)	178 (93%)	14 (7%)	0	100 100
16	N	184/187 (98%)	167 (91%)	11 (6%)	6 (3%)	3 5
17	O	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	14 30
18	P	141/149 (95%)	135 (96%)	6 (4%)	0	100 100
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100 100
20	R	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	9 19
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100 100
22	T	117/120 (98%)	107 (92%)	10 (8%)	0	100 100
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	6 12
24	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	3 5
25	W	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	18 38
26	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	4 8
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100 100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
31	3	90/92 (98%)	88 (98%)	0	2 (2%)	5 10
32	I	68/162 (42%)	51 (75%)	17 (25%)	0	100 100
All	All	3705/4430 (84%)	3350 (90%)	295 (8%)	60 (2%)	7 16

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	ASP
4	A	132	ASP
9	F	101	ALA
11	H	168	ALA
12	J	5	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
4	A	179/182 (98%)	169 (94%)	10 (6%)	19 40
5	B	282/283 (100%)	263 (93%)	19 (7%)	15 33
6	C	193/193 (100%)	176 (91%)	17 (9%)	9 21
7	D	117/148 (79%)	114 (97%)	3 (3%)	40 68
8	E	152/156 (97%)	148 (97%)	4 (3%)	40 68
9	F	93/94 (99%)	91 (98%)	2 (2%)	45 72
10	G	27/283 (10%)	25 (93%)	2 (7%)	13 29
11	H	132/138 (96%)	124 (94%)	8 (6%)	17 37
12	J	118/121 (98%)	111 (94%)	7 (6%)	18 38
13	K	106/106 (100%)	101 (95%)	5 (5%)	23 48
14	L	113/127 (89%)	108 (96%)	5 (4%)	25 50
15	M	158/158 (100%)	151 (96%)	7 (4%)	25 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	N	149/150 (99%)	141 (95%)	8 (5%)	20 42
17	O	93/94 (99%)	89 (96%)	4 (4%)	26 51
18	P	113/117 (97%)	109 (96%)	4 (4%)	32 59
19	Q	79/80 (99%)	75 (95%)	4 (5%)	21 45
20	R	117/122 (96%)	114 (97%)	3 (3%)	40 68
21	S	71/74 (96%)	70 (99%)	1 (1%)	59 81
22	T	105/106 (99%)	99 (94%)	6 (6%)	18 40
23	U	44/52 (85%)	44 (100%)	0	100 100
24	V	51/57 (90%)	49 (96%)	2 (4%)	28 55
25	W	130/130 (100%)	122 (94%)	8 (6%)	16 36
26	X	66/74 (89%)	61 (92%)	5 (8%)	12 27
27	Y	120/196 (61%)	112 (93%)	8 (7%)	15 33
28	Z	60/68 (88%)	60 (100%)	0	100 100
29	1	46/47 (98%)	45 (98%)	1 (2%)	45 72
30	2	42/46 (91%)	42 (100%)	0	100 100
31	3	79/79 (100%)	77 (98%)	2 (2%)	42 69
32	I	58/130 (45%)	57 (98%)	1 (2%)	53 78
All	All	3093/3611 (86%)	2947 (95%)	146 (5%)	23 48

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	T	48	VAL
31	3	42	ARG
24	V	43	PRO
26	X	49	ARG
7	D	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
18	P	118	GLN
21	S	55	GLN
31	3	2	GLN
19	Q	40	HIS

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Mol	Chain	Res	Type
20	R	113	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	260 (9%)	33 (1%)

5 of 260 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2649	A
1	0	2718	C
2	9	3065	A
1	0	1246	A
1	0	1237	U

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

7 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	$\#\|Z\|>2$
3	DCZ	4	74	3	17,17,17	0.30	0	24,24,24	0.28	0
1	PSU	0	2621	1	18,21,22	1.59	2 (11%)	21,30,33	1.39	3 (14%)
1	1MA	0	628	1	21,25,26	0.77	1 (4%)	30,37,40	0.81	1 (3%)
1	OMU	0	2587	1,35	19,22,23	0.22	0	25,31,34	0.37	0
1	UR3	0	2619	1	19,22,23	0.33	0	26,32,35	0.67	1 (3%)
1	OMG	0	2588	1,3	23,26,27	0.33	0	32,38,41	0.33	0
3	5AA	4	76	1,3	23,26,27	0.27	0	29,38,41	0.79	1 (3%)

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
3	DCZ	4	74	3	-	0/6/18/18	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3
1	OMU	0	2587	1,35	-	0/9/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1,3	-	0/9/27/28	0/3/3/3
3	5AA	4	76	1,3	-	0/11/29/30	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.20	1.43	1.36
1	0	2621	PSU	C6-C5	3.27	1.38	1.35
1	0	628	1MA	C6-N6	2.73	1.34	1.28

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.49	120.53	118.17
1	0	2621	PSU	C6-N1-C2	-3.39	119.54	122.69
1	0	628	1MA	N1-C2-N3	2.88	129.42	126.00
3	4	76	5AA	C2-N1-C6	2.87	118.83	111.83
1	0	2621	PSU	O2-C2-N1	2.72	125.59	122.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	74	DCZ	3	0
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0
3	4	76	5AA	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 234 ligands modelled in this entry, 234 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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	0	2749/2922 (94%)	1.01	449 (16%) 4 3	24, 51, 98, 161	0
2	9	122/122 (100%)	1.45	17 (13%) 6 5	46, 68, 96, 153	0
3	4	4/8 (50%)	0.76	0 100 100	42, 42, 46, 46	0
4	A	237/240 (98%)	0.86	18 (7%) 20 16	31, 55, 94, 120	0
5	B	337/338 (99%)	2.02	157 (46%) 0 0	33, 65, 94, 103	0
6	C	246/246 (100%)	0.69	11 (4%) 38 32	26, 51, 75, 86	0
7	D	140/177 (79%)	2.27	71 (50%) 0 0	64, 110, 134, 141	0
8	E	172/178 (96%)	2.56	116 (67%) 0 0	50, 81, 105, 115	0
9	F	119/120 (99%)	1.12	14 (11%) 9 7	57, 81, 107, 122	0
10	G	29/348 (8%)	2.57	20 (68%) 0 0	74, 95, 105, 107	0
11	H	160/171 (93%)	1.69	49 (30%) 1 1	42, 63, 94, 101	0
12	J	142/145 (97%)	1.85	52 (36%) 1 0	42, 59, 82, 97	0
13	K	132/132 (100%)	2.09	66 (50%) 0 0	37, 62, 86, 90	0
14	L	145/165 (87%)	1.22	33 (22%) 2 2	28, 74, 118, 131	0
15	M	194/194 (100%)	0.39	2 (1%) 79 76	33, 48, 64, 72	0
16	N	186/187 (99%)	1.43	40 (21%) 2 2	43, 69, 118, 124	0
17	O	115/116 (99%)	1.05	16 (13%) 6 5	43, 61, 79, 89	0
18	P	143/149 (95%)	1.25	21 (14%) 6 4	46, 62, 75, 81	0
19	Q	95/96 (98%)	1.07	12 (12%) 8 6	40, 50, 66, 77	0
20	R	150/155 (96%)	0.91	10 (6%) 24 19	36, 51, 72, 82	0
21	S	81/85 (95%)	0.85	5 (6%) 26 21	48, 65, 85, 94	0
22	T	119/120 (99%)	0.80	6 (5%) 34 28	44, 61, 90, 111	0
23	U	53/66 (80%)	1.76	17 (32%) 1 1	48, 63, 80, 88	0
24	V	65/71 (91%)	1.45	17 (26%) 1 1	59, 83, 117, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	1.32	25 (16%) 4 3	41, 57, 78, 88	0
26	X	82/92 (89%)	1.43	15 (18%) 3 3	49, 66, 89, 106	0
27	Y	142/241 (58%)	1.02	13 (9%) 14 11	32, 51, 74, 95	0
28	Z	73/83 (87%)	1.32	13 (17%) 4 3	45, 64, 78, 96	0
29	1	56/57 (98%)	0.30	1 (1%) 67 63	31, 38, 46, 61	0
30	2	46/50 (92%)	1.73	14 (30%) 1 1	40, 70, 123, 128	0
31	3	92/92 (100%)	0.84	7 (7%) 20 16	37, 60, 74, 89	0
32	I	70/162 (43%)	3.14	56 (80%) 0 0	108, 129, 152, 155	0
All	All	6650/7482 (88%)	1.22	1363 (20%) 2 2	24, 58, 109, 161	0

The worst 5 of 1363 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	133	THR	8.6
24	V	1	THR	6.4
7	D	10	PHE	6.3
16	N	168	LEU	6.2
32	I	132	CYS	5.9

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DCZ	4	74	16/16	0.81	0.17	48,52,56,60	0
1	OMG	0	2588	24/25	0.88	0.15	30,33,38,40	0
1	1MA	0	628	23/24	0.90	0.14	28,34,37,38	0
1	OMU	0	2587	21/22	0.90	0.15	31,35,40,41	0
3	5AA	4	76	24/25	0.91	0.14	40,44,46,47	0
1	UR3	0	2619	21/22	0.91	0.14	33,38,39,42	0
1	PSU	0	2621	20/21	0.94	0.09	31,34,40,41	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9124	1/1	0.52	0.33	66,66,66,66	0
35	NA	0	9182	1/1	0.53	0.32	81,81,81,81	0
35	NA	0	9164	1/1	0.62	0.24	53,53,53,53	0
35	NA	0	9110	1/1	0.62	0.21	43,43,43,43	0
35	NA	0	9129	1/1	0.64	0.16	57,57,57,57	0
35	NA	0	9102	1/1	0.65	0.17	45,45,45,45	0
35	NA	R	9186	1/1	0.68	0.26	78,78,78,78	0
35	NA	0	9157	1/1	0.69	0.18	73,73,73,73	0
35	NA	0	9170	1/1	0.69	0.18	49,49,49,49	0
35	NA	9	9151	1/1	0.70	0.23	64,64,64,64	0
33	MG	0	8117	1/1	0.71	0.13	37,37,37,37	0
35	NA	0	9121	1/1	0.71	0.36	55,55,55,55	0
33	MG	0	8053	1/1	0.72	0.17	57,57,57,57	0
35	NA	0	9176	1/1	0.73	0.20	49,49,49,49	0
35	NA	0	9156	1/1	0.74	0.24	49,49,49,49	0
35	NA	S	9112	1/1	0.74	0.15	73,73,73,73	0
35	NA	0	9181	1/1	0.75	0.14	56,56,56,56	0
33	MG	0	8050	1/1	0.76	0.14	69,69,69,69	0
35	NA	0	9155	1/1	0.77	0.24	79,79,79,79	0
33	MG	0	8101	1/1	0.77	0.20	72,72,72,72	0
35	NA	0	9184	1/1	0.77	0.17	83,83,83,83	0
33	MG	9	8095	1/1	0.78	0.17	77,77,77,77	0
35	NA	0	9139	1/1	0.78	0.12	31,31,31,31	0
35	NA	0	9166	1/1	0.79	0.16	69,69,69,69	0
36	CL	N	9307	1/1	0.79	0.24	72,72,72,72	0
35	NA	H	9109	1/1	0.80	0.11	34,34,34,34	0
33	MG	0	8063	1/1	0.80	0.13	71,71,71,71	0
33	MG	0	8023	1/1	0.80	0.15	52,52,52,52	0
33	MG	0	8047	1/1	0.80	0.17	86,86,86,86	0
35	NA	0	9105	1/1	0.81	0.16	44,44,44,44	0
35	NA	0	9133	1/1	0.81	0.15	34,34,34,34	0
36	CL	J	9321	1/1	0.81	0.18	55,55,55,55	0
35	NA	0	9113	1/1	0.81	0.17	67,67,67,67	0
33	MG	0	8049	1/1	0.82	0.16	81,81,81,81	0
36	CL	0	9315	1/1	0.83	0.24	80,80,80,80	0
33	MG	0	8087	1/1	0.83	0.18	59,59,59,59	0
35	NA	0	9141	1/1	0.83	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9144	1/1	0.84	0.10	33,33,33,33	0
35	NA	0	9150	1/1	0.84	0.13	42,42,42,42	0
35	NA	0	9175	1/1	0.84	0.28	52,52,52,52	0
33	MG	0	8113	1/1	0.84	0.10	52,52,52,52	0
33	MG	0	8041	1/1	0.84	0.12	79,79,79,79	0
36	CL	J	9301	1/1	0.84	0.19	78,78,78,78	0
33	MG	0	8072	1/1	0.84	0.15	60,60,60,60	0
35	NA	0	9125	1/1	0.84	0.15	59,59,59,59	0
36	CL	0	9312	1/1	0.85	0.16	59,59,59,59	0
35	NA	0	9123	1/1	0.85	0.33	44,44,44,44	0
33	MG	0	8092	1/1	0.85	0.23	90,90,90,90	0
33	MG	0	8082	1/1	0.85	0.19	76,76,76,76	0
35	NA	0	9162	1/1	0.85	0.25	64,64,64,64	0
36	CL	0	9311	1/1	0.86	0.14	53,53,53,53	0
35	NA	0	9163	1/1	0.86	0.18	65,65,65,65	0
35	NA	0	9108	1/1	0.86	0.12	49,49,49,49	0
36	CL	0	9316	1/1	0.86	0.18	66,66,66,66	0
35	NA	0	9177	1/1	0.86	0.23	68,68,68,68	0
36	CL	J	9302	1/1	0.86	0.19	79,79,79,79	0
33	MG	0	8100	1/1	0.86	0.18	70,70,70,70	0
35	NA	0	9131	1/1	0.86	0.13	41,41,41,41	0
36	CL	3	9304	1/1	0.86	0.14	61,61,61,61	0
35	NA	0	9135	1/1	0.87	0.15	52,52,52,52	0
35	NA	0	9159	1/1	0.87	0.21	50,50,50,50	0
33	MG	0	8099	1/1	0.87	0.12	53,53,53,53	0
33	MG	0	8057	1/1	0.87	0.12	42,42,42,42	0
35	NA	0	9117	1/1	0.87	0.11	61,61,61,61	0
35	NA	0	9106	1/1	0.87	0.27	38,38,38,38	0
35	NA	B	9158	1/1	0.87	0.38	70,70,70,70	0
33	MG	0	8064	1/1	0.87	0.09	30,30,30,30	0
35	NA	R	9137	1/1	0.87	0.10	44,44,44,44	0
35	NA	0	9134	1/1	0.87	0.13	41,41,41,41	0
35	NA	Q	9148	1/1	0.88	0.11	38,38,38,38	0
35	NA	0	9120	1/1	0.88	0.17	52,52,52,52	0
35	NA	0	9171	1/1	0.88	0.15	52,52,52,52	0
33	MG	0	8045	1/1	0.88	0.17	73,73,73,73	0
35	NA	0	9111	1/1	0.88	0.17	61,61,61,61	0
35	NA	0	9101	1/1	0.88	0.12	40,40,40,40	0
35	NA	0	9136	1/1	0.88	0.14	55,55,55,55	0
35	NA	0	9115	1/1	0.88	0.12	37,37,37,37	0
35	NA	0	9126	1/1	0.88	0.15	41,41,41,41	0
33	MG	0	8103	1/1	0.88	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	9	9183	1/1	0.88	0.11	60,60,60,60	0
35	NA	0	9165	1/1	0.88	0.16	47,47,47,47	0
35	NA	0	9149	1/1	0.88	0.10	38,38,38,38	0
37	CD	U	9201	1/1	0.88	0.09	74,74,74,74	0
33	MG	0	8090	1/1	0.89	0.18	65,65,65,65	0
33	MG	0	8115	1/1	0.89	0.09	57,57,57,57	0
35	NA	0	9185	1/1	0.89	0.17	51,51,51,51	0
33	MG	0	8116	1/1	0.89	0.10	62,62,62,62	0
33	MG	0	8059	1/1	0.89	0.12	51,51,51,51	0
33	MG	0	8046	1/1	0.89	0.10	59,59,59,59	0
33	MG	Y	8109	1/1	0.89	0.09	44,44,44,44	0
36	CL	0	9322	1/1	0.90	0.27	77,77,77,77	0
36	CL	A	9309	1/1	0.90	0.18	61,61,61,61	0
36	CL	B	9319	1/1	0.90	0.22	55,55,55,55	0
33	MG	0	8119	1/1	0.90	0.11	62,62,62,62	0
35	NA	A	9145	1/1	0.90	0.10	48,48,48,48	0
34	K	0	9002	1/1	0.90	0.10	48,48,48,48	0
35	NA	0	9143	1/1	0.90	0.10	33,33,33,33	0
33	MG	0	8068	1/1	0.90	0.09	60,60,60,60	0
35	NA	0	9178	1/1	0.90	0.24	57,57,57,57	0
33	MG	0	8081	1/1	0.91	0.07	52,52,52,52	0
33	MG	0	8111	1/1	0.91	0.08	52,52,52,52	0
35	NA	C	9104	1/1	0.91	0.07	40,40,40,40	0
35	NA	0	9114	1/1	0.91	0.22	64,64,64,64	0
35	NA	H	9122	1/1	0.91	0.17	72,72,72,72	0
35	NA	0	9152	1/1	0.91	0.29	61,61,61,61	0
33	MG	3	8078	1/1	0.91	0.08	43,43,43,43	0
35	NA	0	9169	1/1	0.91	0.15	60,60,60,60	0
33	MG	0	8102	1/1	0.91	0.07	58,58,58,58	0
35	NA	0	9119	1/1	0.91	0.07	44,44,44,44	0
33	MG	0	8114	1/1	0.91	0.07	56,56,56,56	0
33	MG	T	8073	1/1	0.92	0.07	59,59,59,59	0
33	MG	0	8088	1/1	0.92	0.09	38,38,38,38	0
36	CL	0	9313	1/1	0.92	0.12	60,60,60,60	0
33	MG	0	8075	1/1	0.92	0.07	57,57,57,57	0
33	MG	0	8084	1/1	0.92	0.09	38,38,38,38	0
36	CL	0	9317	1/1	0.92	0.09	61,61,61,61	0
35	NA	0	9173	1/1	0.92	0.08	62,62,62,62	0
33	MG	9	8052	1/1	0.92	0.08	54,54,54,54	0
33	MG	0	8044	1/1	0.92	0.08	55,55,55,55	0
35	NA	0	9161	1/1	0.92	0.14	56,56,56,56	0
35	NA	0	9142	1/1	0.92	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9103	1/1	0.92	0.11	43,43,43,43	0
36	CL	L	9310	1/1	0.92	0.19	63,63,63,63	0
33	MG	B	8055	1/1	0.92	0.12	62,62,62,62	0
36	CL	Y	9320	1/1	0.92	0.13	52,52,52,52	0
35	NA	0	9118	1/1	0.92	0.17	62,62,62,62	0
36	CL	0	9303	1/1	0.92	0.14	53,53,53,53	0
33	MG	0	8037	1/1	0.93	0.07	45,45,45,45	0
35	NA	0	9168	1/1	0.93	0.11	49,49,49,49	0
33	MG	0	8106	1/1	0.93	0.07	54,54,54,54	0
33	MG	0	8021	1/1	0.93	0.08	32,32,32,32	0
33	MG	B	8056	1/1	0.93	0.11	47,47,47,47	0
35	NA	0	9172	1/1	0.93	0.18	62,62,62,62	0
33	MG	0	8093	1/1	0.93	0.08	66,66,66,66	0
35	NA	0	9174	1/1	0.93	0.15	62,62,62,62	0
35	NA	0	9140	1/1	0.93	0.09	47,47,47,47	0
35	NA	L	9180	1/1	0.93	0.19	51,51,51,51	0
33	MG	0	8094	1/1	0.93	0.10	73,73,73,73	0
33	MG	0	8085	1/1	0.93	0.13	72,72,72,72	0
33	MG	0	8086	1/1	0.93	0.07	50,50,50,50	0
36	CL	O	9308	1/1	0.93	0.20	79,79,79,79	0
35	NA	0	9179	1/1	0.93	0.15	70,70,70,70	0
33	MG	0	8051	1/1	0.93	0.10	72,72,72,72	0
33	MG	0	8025	1/1	0.93	0.07	46,46,46,46	0
34	K	0	9003	1/1	0.94	0.17	64,64,64,64	0
33	MG	0	8009	1/1	0.94	0.06	30,30,30,30	0
33	MG	0	8070	1/1	0.94	0.10	57,57,57,57	0
33	MG	0	8058	1/1	0.94	0.07	56,56,56,56	0
35	NA	R	9138	1/1	0.94	0.08	63,63,63,63	0
33	MG	0	8108	1/1	0.94	0.10	58,58,58,58	0
33	MG	0	8110	1/1	0.94	0.07	32,32,32,32	0
33	MG	0	8096	1/1	0.94	0.06	53,53,53,53	0
35	NA	0	9160	1/1	0.94	0.16	46,46,46,46	0
33	MG	0	8097	1/1	0.94	0.08	40,40,40,40	0
33	MG	0	8039	1/1	0.94	0.06	52,52,52,52	0
33	MG	0	8026	1/1	0.94	0.07	24,24,24,24	0
37	CD	O	9205	1/1	0.94	0.15	143,143,143,143	0
33	MG	0	8043	1/1	0.94	0.06	47,47,47,47	0
33	MG	0	8098	1/1	0.95	0.07	47,47,47,47	0
35	NA	0	9167	1/1	0.95	0.08	52,52,52,52	0
35	NA	0	9107	1/1	0.95	0.07	46,46,46,46	0
33	MG	0	8077	1/1	0.95	0.05	28,28,28,28	0
33	MG	0	8015	1/1	0.95	0.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	9127	1/1	0.95	0.08	42,42,42,42	0
35	NA	0	9153	1/1	0.95	0.14	21,21,21,21	0
33	MG	0	8091	1/1	0.95	0.06	79,79,79,79	0
33	MG	0	8032	1/1	0.95	0.07	41,41,41,41	0
34	K	0	9001	1/1	0.95	0.19	71,71,71,71	0
33	MG	0	8042	1/1	0.95	0.06	44,44,44,44	0
35	NA	0	9116	1/1	0.95	0.08	42,42,42,42	0
33	MG	0	8034	1/1	0.95	0.07	38,38,38,38	0
33	MG	0	8006	1/1	0.95	0.06	37,37,37,37	0
33	MG	0	8060	1/1	0.95	0.10	46,46,46,46	0
33	MG	4	8118	1/1	0.95	0.05	41,41,41,41	0
33	MG	A	8065	1/1	0.95	0.07	45,45,45,45	0
33	MG	A	8066	1/1	0.96	0.06	66,66,66,66	0
33	MG	0	8007	1/1	0.96	0.06	27,27,27,27	0
33	MG	0	8020	1/1	0.96	0.05	31,31,31,31	0
35	NA	0	9128	1/1	0.96	0.09	43,43,43,43	0
33	MG	0	8112	1/1	0.96	0.08	39,39,39,39	0
33	MG	0	8004	1/1	0.96	0.05	34,34,34,34	0
33	MG	2	8076	1/1	0.96	0.07	55,55,55,55	0
35	NA	J	9146	1/1	0.96	0.04	42,42,42,42	0
33	MG	0	8036	1/1	0.96	0.06	35,35,35,35	0
33	MG	0	8071	1/1	0.96	0.10	66,66,66,66	0
33	MG	0	8010	1/1	0.96	0.05	28,28,28,28	0
33	MG	0	8089	1/1	0.96	0.06	56,56,56,56	0
33	MG	0	8024	1/1	0.96	0.07	39,39,39,39	0
36	CL	R	9306	1/1	0.96	0.08	57,57,57,57	0
33	MG	0	8012	1/1	0.96	0.04	32,32,32,32	0
33	MG	0	8104	1/1	0.96	0.07	55,55,55,55	0
33	MG	0	8080	1/1	0.96	0.07	41,41,41,41	0
33	MG	0	8061	1/1	0.96	0.05	37,37,37,37	0
37	CD	Z	9203	1/1	0.96	0.05	67,67,67,67	0
37	CD	1	9202	1/1	0.96	0.06	62,62,62,62	0
33	MG	0	8048	1/1	0.97	0.05	56,56,56,56	0
33	MG	0	8038	1/1	0.97	0.04	32,32,32,32	0
33	MG	0	8067	1/1	0.97	0.08	49,49,49,49	0
33	MG	K	8069	1/1	0.97	0.04	52,52,52,52	0
33	MG	0	8003	1/1	0.97	0.04	31,31,31,31	0
35	NA	M	9147	1/1	0.97	0.03	25,25,25,25	0
33	MG	0	8027	1/1	0.97	0.04	37,37,37,37	0
33	MG	0	8030	1/1	0.97	0.07	35,35,35,35	0
33	MG	0	8022	1/1	0.97	0.05	35,35,35,35	0
36	CL	M	9318	1/1	0.97	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	8001	1/1	0.97	0.05	35,35,35,35	0
33	MG	0	8035	1/1	0.97	0.06	49,49,49,49	0
35	NA	0	9130	1/1	0.97	0.08	45,45,45,45	0
36	CL	0	9305	1/1	0.97	0.07	55,55,55,55	0
33	MG	0	8079	1/1	0.97	0.05	29,29,29,29	0
35	NA	0	9154	1/1	0.97	0.06	33,33,33,33	0
33	MG	0	8018	1/1	0.97	0.06	42,42,42,42	0
36	CL	0	9314	1/1	0.97	0.10	49,49,49,49	0
33	MG	0	8002	1/1	0.97	0.05	39,39,39,39	0
33	MG	0	8033	1/1	0.98	0.05	38,38,38,38	0
33	MG	0	8005	1/1	0.98	0.07	36,36,36,36	0
33	MG	0	8107	1/1	0.98	0.07	53,53,53,53	0
33	MG	0	8014	1/1	0.98	0.08	43,43,43,43	0
33	MG	0	8008	1/1	0.98	0.04	37,37,37,37	0
33	MG	0	8028	1/1	0.98	0.05	41,41,41,41	0
33	MG	0	8016	1/1	0.98	0.14	50,50,50,50	0
33	MG	0	8031	1/1	0.98	0.06	30,30,30,30	0
33	MG	0	8062	1/1	0.98	0.04	51,51,51,51	0
33	MG	0	8040	1/1	0.98	0.05	56,56,56,56	0
33	MG	0	8011	1/1	0.98	0.09	20,20,20,20	0
35	NA	0	9132	1/1	0.98	0.03	34,34,34,34	0
33	MG	0	8074	1/1	0.99	0.03	37,37,37,37	0
33	MG	0	8083	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	8019	1/1	0.99	0.08	35,35,35,35	0
33	MG	0	8054	1/1	0.99	0.03	29,29,29,29	0
33	MG	0	8029	1/1	0.99	0.03	36,36,36,36	0
33	MG	0	8017	1/1	0.99	0.08	29,29,29,29	0
33	MG	0	8013	1/1	0.99	0.03	33,33,33,33	0
37	CD	3	9204	1/1	0.99	0.03	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.