Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:07 pm GMT

PDB ID	:	5O2R
EMDB ID	:	EMD-3730
Title	:	Cryo-EM structure of the proline-rich antimicrobial peptide Api137 bound to the terminating ribosome
Authors	:	Graf, M.; Berninghausen, O.; Beckmann, R.; Wilson, D.N.
Deposited on	:	2017-05-22
Resolution	:	3.40 Å(reported)

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

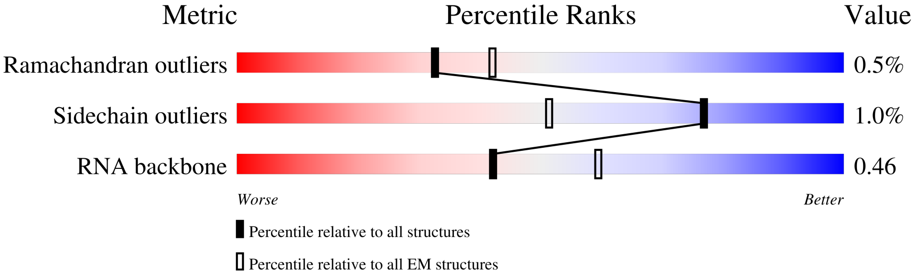
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

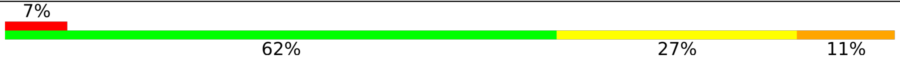
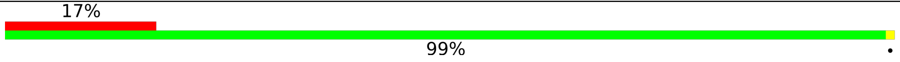
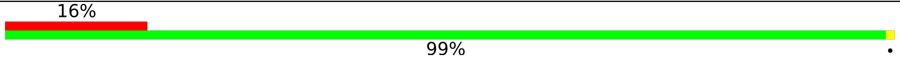
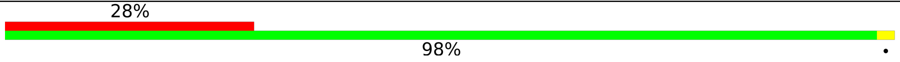
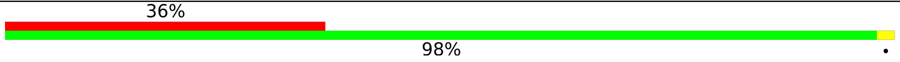
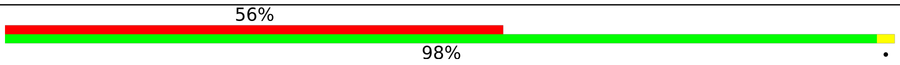
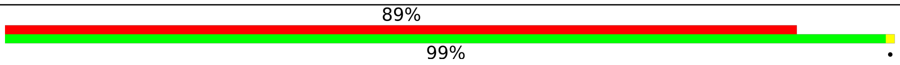
The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	H	149	

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Mol	Chain	Length	Quality of chain
9	I	141	97% 99%
10	J	142	16% 100%
11	K	122	20% 99%
12	L	143	17% 98%
13	M	136	17% 98%
14	N	120	9% 99%
15	O	116	22% 100%
16	P	114	20% 98%
17	Q	117	15% 99%
18	R	103	27% 98%
19	S	110	16% 99%
20	T	93	28% 100%
21	U	102	32% 100%
22	V	94	28% 100%
23	W	75	8% 99%
24	X	77	25% 99%
25	Y	63	41% 100%
26	Z	58	10% 100%
27	0	56	18% 100%
28	1	50	38% 100%
29	2	46	9% 100%
30	3	64	6% 98%
31	4	38	16% 100%
32	5	131	98% 98%
33	6	66	61% 100%

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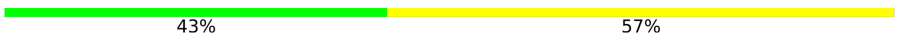
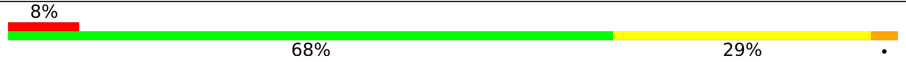
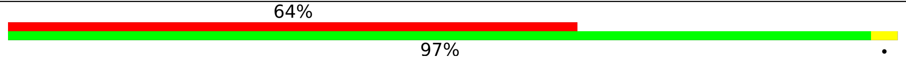
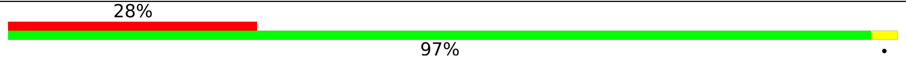
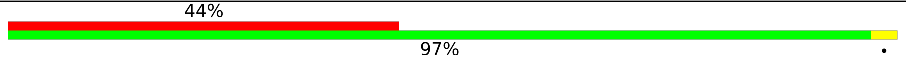
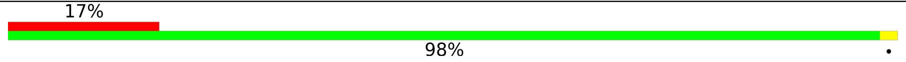
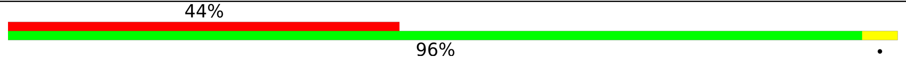
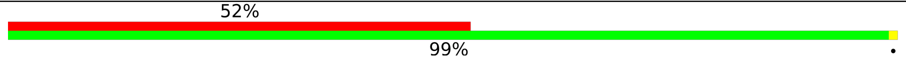
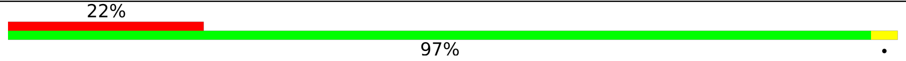
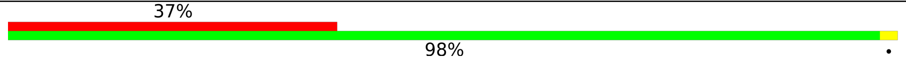
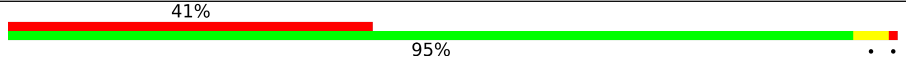
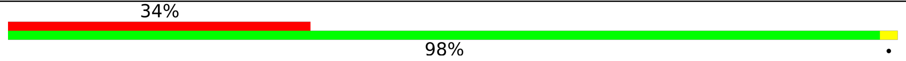
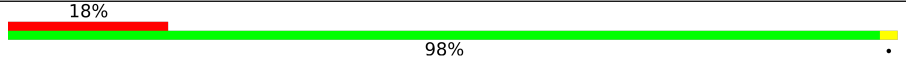
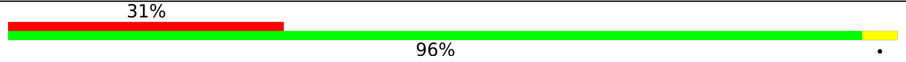
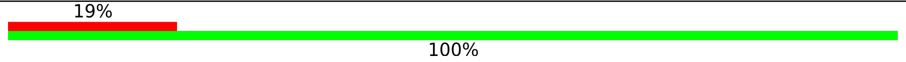
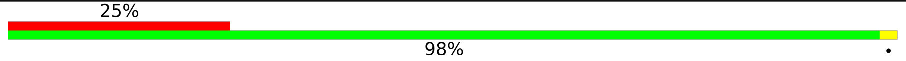
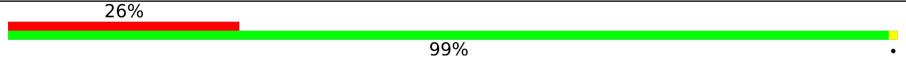
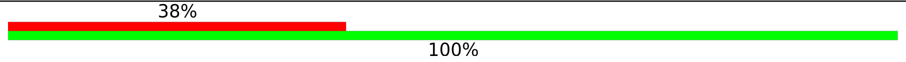
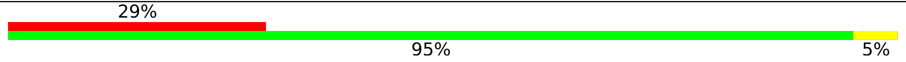
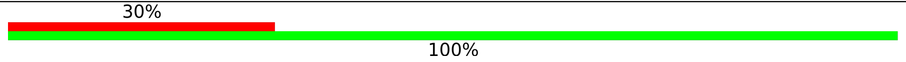
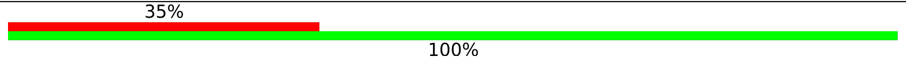
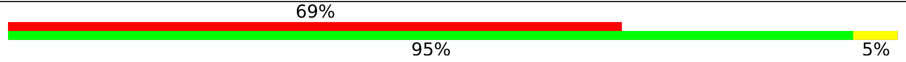
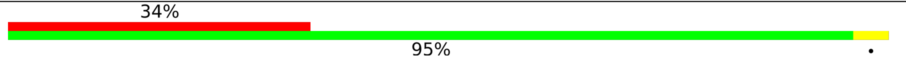
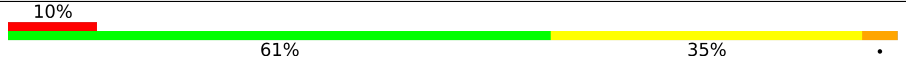
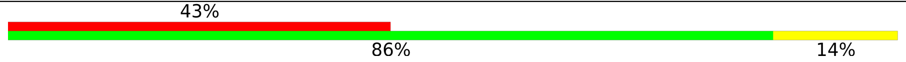
Mol	Chain	Length	Quality of chain
34	7	7	
35	a	1539	
36	b	218	
37	c	206	
38	d	205	
39	e	157	
40	f	100	
41	g	151	
42	h	129	
43	i	127	
44	j	98	
45	k	116	
46	l	123	
47	m	114	
48	n	101	
49	o	88	
50	p	82	
51	q	80	
52	r	65	
53	s	79	
54	t	85	
55	u	65	
56	v	242	
57	x	77	
58	z	14	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 147985 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2900	62262	27774	11460	20128	2900	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1150448909

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	209	1565	979	288	294	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	177	1410	899	249	256	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	176	1323	832	243	246	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	149	1111	699	197	214	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	141	1032	651	179	196	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	142	1129	714	212	199	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	122	938	587	180	165	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	143	1045	649	206	189	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	136	1074	686	205	177	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	120	960	593	196	166	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	O	116	892	552	178	162	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	114	917	574	179	163	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Q	117	947	604	192	151	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	103	816	516	153	145	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	110	857	532	166	156	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	93	738	466	139	131	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	U	102	779	492	146	141	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	94	753	479	137	134	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	75	575	356	116	102	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	77	625	388	129	106	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	63	509	313	99	95	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	58	449	281	87	79	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	0	56	444	269	94	80	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	1	50	409	263	75	71	0	0

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	2	46	377	228	90	57	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	3	64	504	323	105	74	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	4	38	302	185	65	48	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	5	131	988	625	175	183	5	0	0

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total 522	C 323	N 99	O 94	S 6	0	0

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	7	Total 149	C 67	N 27	O 48	P 7	0	0

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	1539	Total 33016	C 14725	N 6052	O 10700	P 1539	0	0

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	218	Total 1704	C 1081	N 305	O 311	S 7	0	0

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	206	Total 1624	C 1028	N 305	O 288	S 3	0	0

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	205	Total 1643	C 1026	N 315	O 298	S 4	0	0

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	157	Total 1141	C 709	N 218	O 208	S 6	0	0

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	f	100	817	515	148	148	6	0	0

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	g	151	1181	735	227	215	4	0	0

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	h	129	979	616	173	184	6	0	0

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	i	127	1022	634	206	179	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	j	98	786	493	150	142	1	0	0

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k	116	869	535	173	158	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	l	123	955	590	196	165	4	0	0

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s	79	Total 637	C 408	N 120	O 107	S 2	0	0

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	t	85	Total 665	C 411	N 137	O 114	S 3	0	0

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	65	Total 495	C 307	N 100	O 87	S 1	0	0

- Molecule 56 is a protein called Peptide chain release factor RF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	v	242	Total 1880	C 1151	N 359	O 362	S 8	0	0

- Molecule 57 is a RNA chain called P-site Ile-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	77	Total 1647	C 734	N 296	O 540	P 77	0	0

- Molecule 58 is a protein called Apidaecin.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	z	14	Total 120	C 80	N 25	O 15	0	0

There is a discrepancy between the modelled and reference sequences:

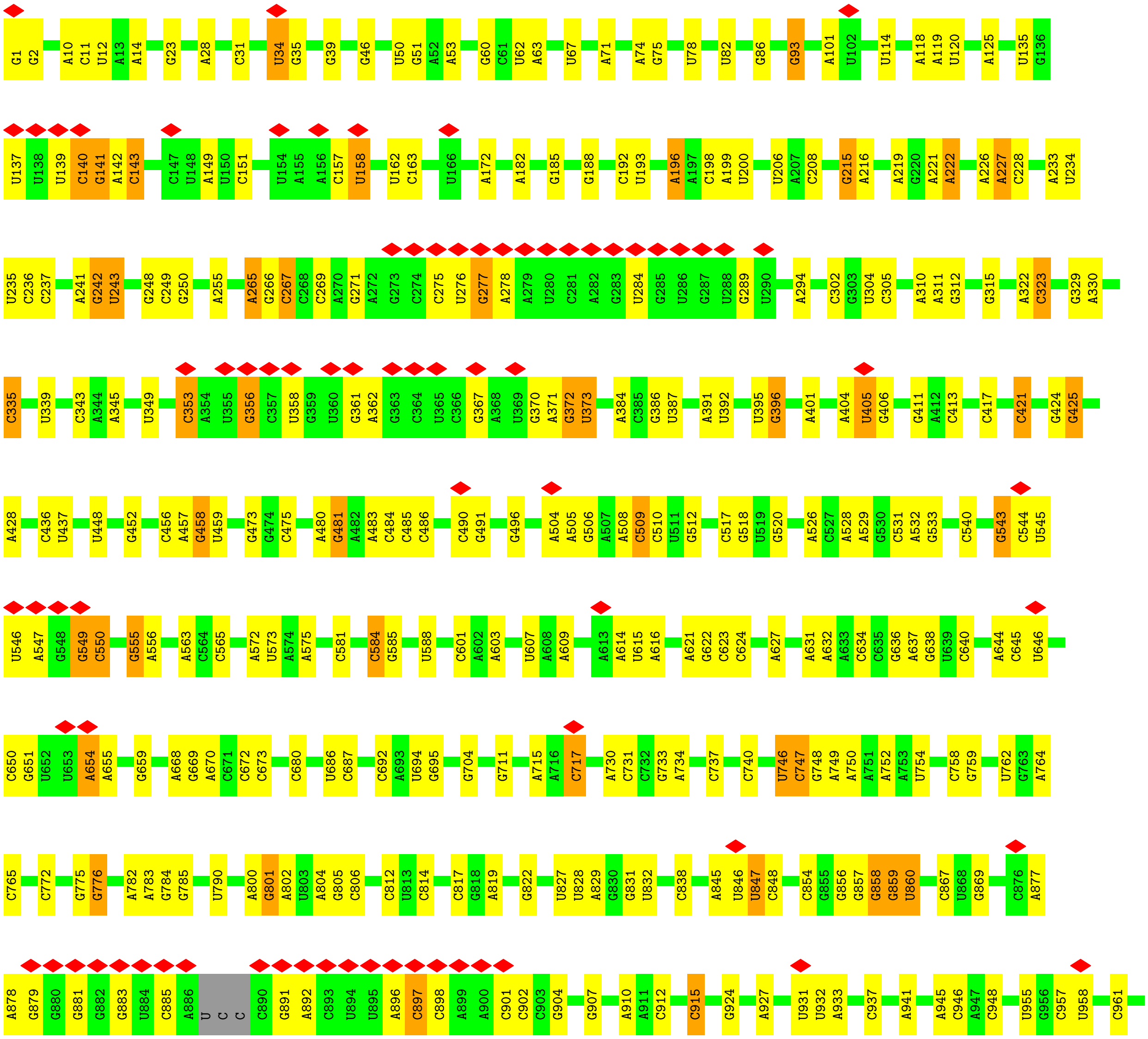
Chain	Residue	Modelled	Actual	Comment	Reference
z	10	ARG	GLN	conflict	UNP Q8WSY8

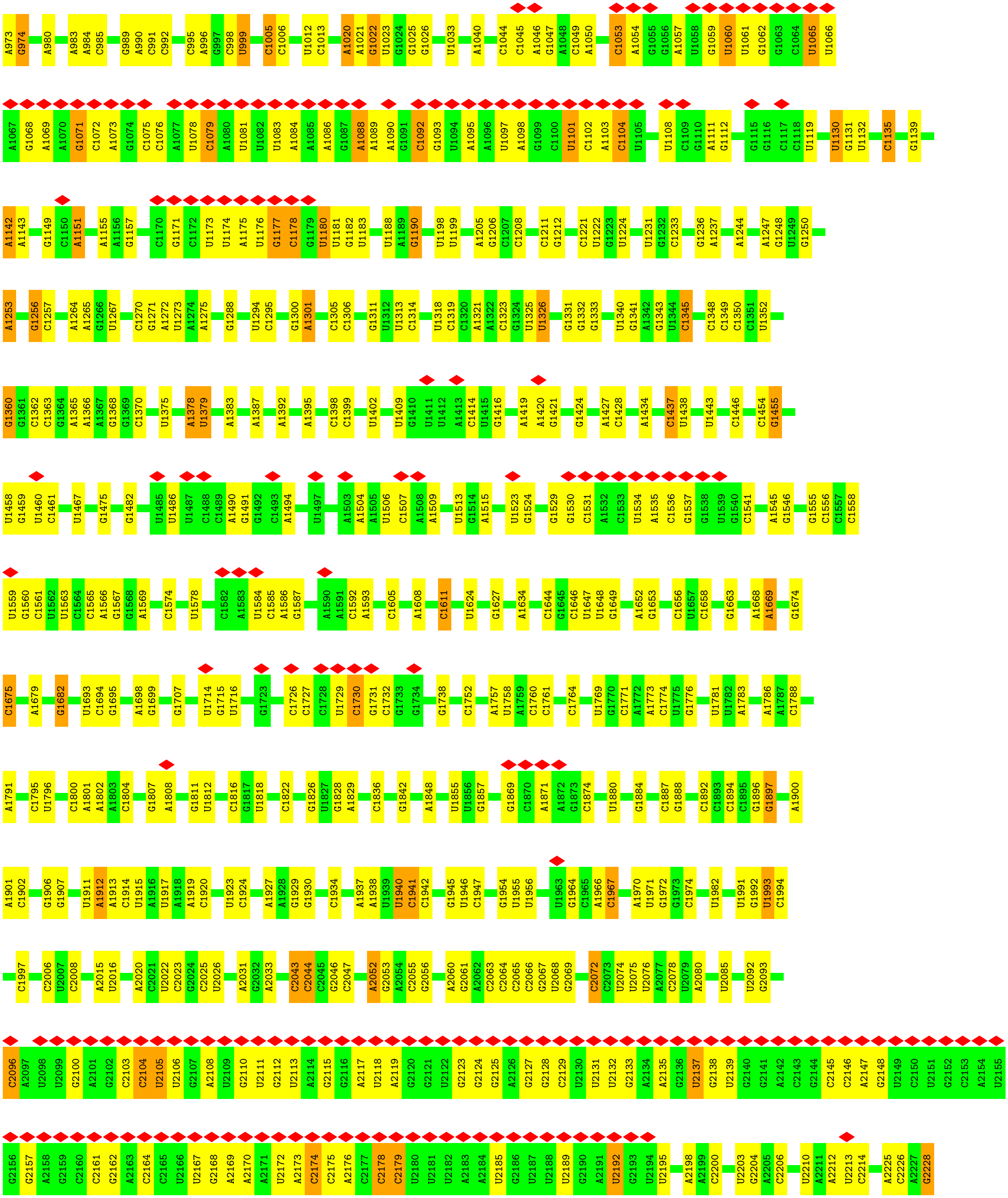
3 Residue-property plots ⓘ

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 A:

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A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 U1108 C1109 G1110 A1111 G1112 G1115 G1116 C1117 C1118 U1119 U1130 G1131 U1132 C1135 G1139
A1142 A1143 G1149 C1150 A1151 A1155 A1156 G1157 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1188 A1189 G1190 U1198 U1199 A1205 G1206 C1207 C1208 C1211 G1212 C1221 U1222 G1223 U1224 U1231 G1232 C1233 G1236 A1237 A1244 A1247 G1248 U1249 G1250
A1253 G1256 C1257 A1264 A1265 G1266 U1267 C1270 G1271 A1272 U1273 A1274 A1275 G1288 U1294 C1295 G1300 A1301 C1305 C1306 G1311 U1312 U1313 C1314 U1318 C1319 C1320 A1321 A1322 C1323 G1324 U1325 U1326 G1331 G1332 G1333 U1340 G1341 A1342 G1343 U1344 C1345 C1348 C1349 C1350 C1351 U1352
G1360 G1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 U1375 A1378 U1379 A1383 A1387 A1392 A1395 C1398 C1399 U1402 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 A1419 A1420 G1421 G1424 A1427 C1428 A1434 C1437 U1438 U1443 C1446 C1454 G1455
U1458 G1459 U1460 C1461 U1467 G1475 G1482 U1485 U1486 U1487 C1488 C1489 A1490 G1491 G1492 C1493 A1494 U1497 A1503 A1504 A1505 U1506 C1507 A1508 A1509 U1513 G1514 A1515 U1523 G1524 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 A1545 G1546 G1555 C1556 C1557 C1558
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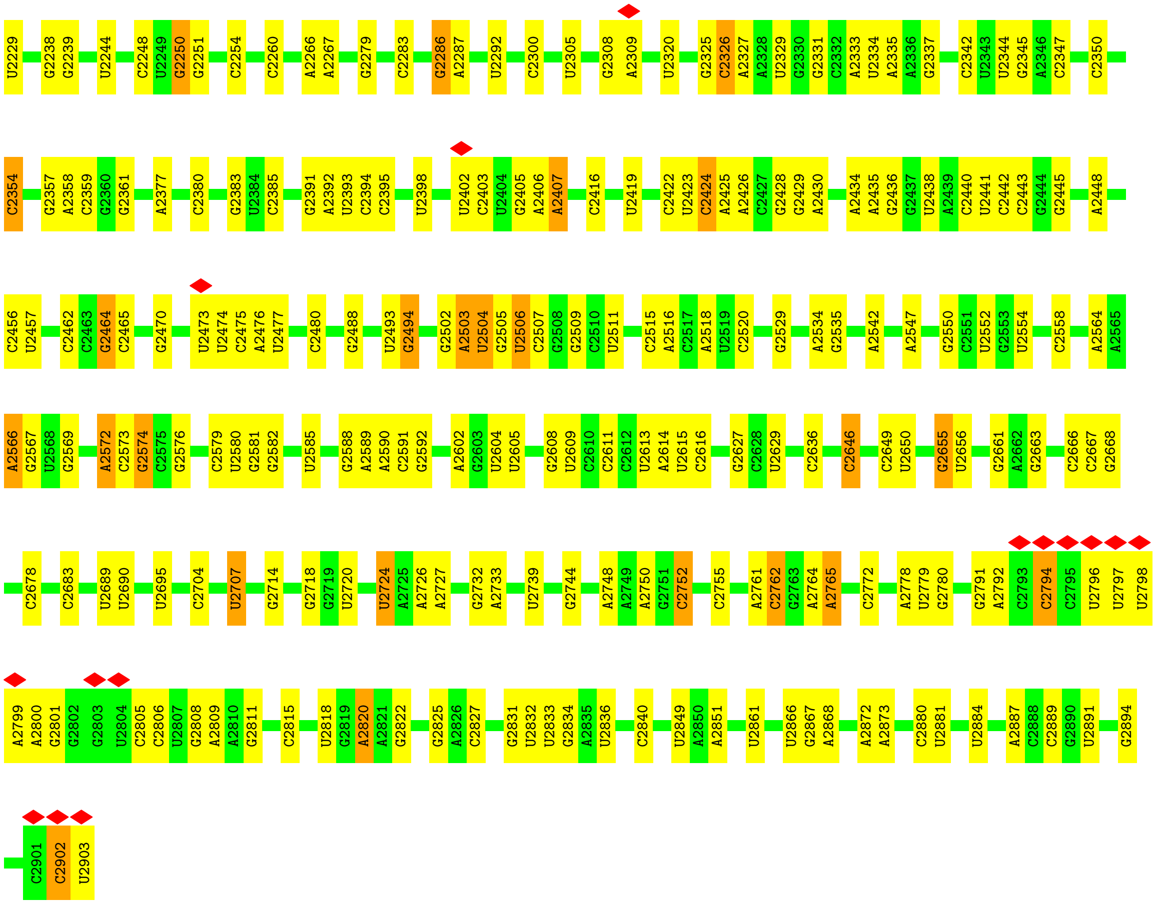
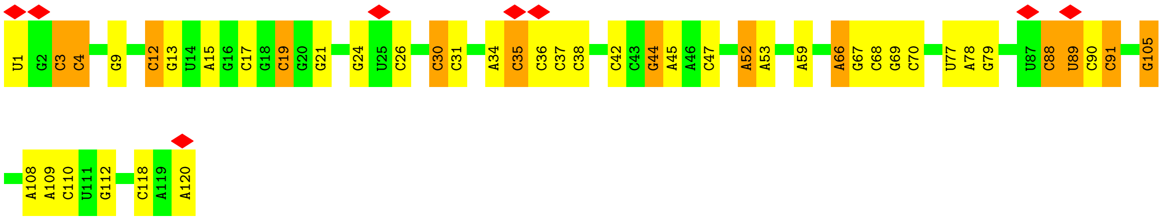
C1675 A1679 G1682 U1693 C1694 G1695 A1698 G1699 G1707 U1714 G1715 U1716 G1723 C1726 C1727 C1728 U1729 C1730 G1731 C1732 G1733 G1734 G1738 C1752 A1757 U1758 A1759 C1760 C1761 C1764 U1769 G1770 C1771 A1772 A1773 C1774 U1775 G1776 U1781 U1782 A1783 A1786 A1787 C1788
A1791 C1795 U1796 C1800 A1801 A1802 A1803 C1804 G1807 A1808 G1811 U1812 C1816 G1817 U1818 C1822 G1826 U1827 G1828 A1829 C1836 G1842 A1848 U1855 U1856 G1857 G1869 C1870 A1871 A1872 G1873 C1874 U1880 G1884 C1887 G1888 C1892 C1893 U1894 C1895 G1896 G1897 A1900
A1901 C1902 G1906 G1907 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 U1923 C1924 A1927 A1928 G1929 G1930 C1934 A1937 A1938 U1939 U1940 C1941 C1942 G1945 U1946 C1947 G1954 U1955 U1956 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1973 C1974 U1982 U1991 G1992 U1993 C1994
C1997 C2006 U2007 C2008 A2015 U2016 A2020 C2021 U2022 C2023 G2024 C2025 U2026 A2031 G2032 A2033 C2043 C2044 C2045 G2046 C2047 A2052 G2053 A2054 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 C2072 C2073 U2074 U2075 U2076 A2077 C2078 U2079 A2080 U2085 U2092 G2093
C2096 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 G2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155
G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2185 G2186 U2187 U2188 U2189 G2190 A2191 U2192 G2193 U2194 U2195 A2198 A2199 C2200 U2203 G2204 A2205 C2206 U2210 A2211 A2212 U2213 C2214 A2225 C2226 A2227 G2228



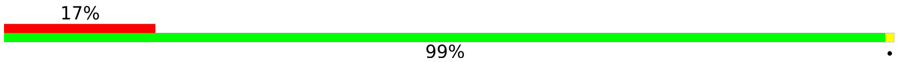
- Molecule 2: 5S ribosomal RNA

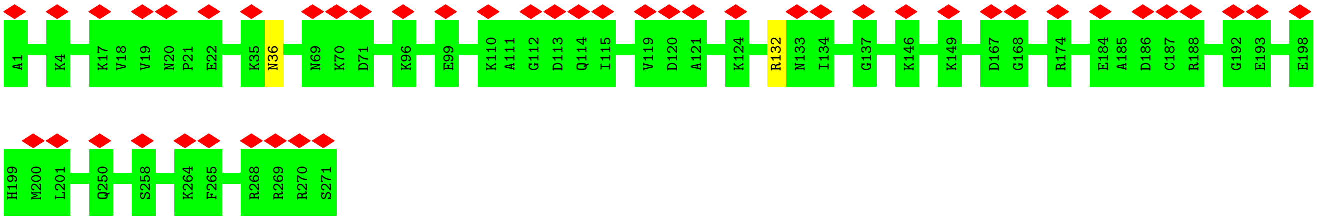
Chain B:



- Molecule 3: 50S ribosomal protein L2

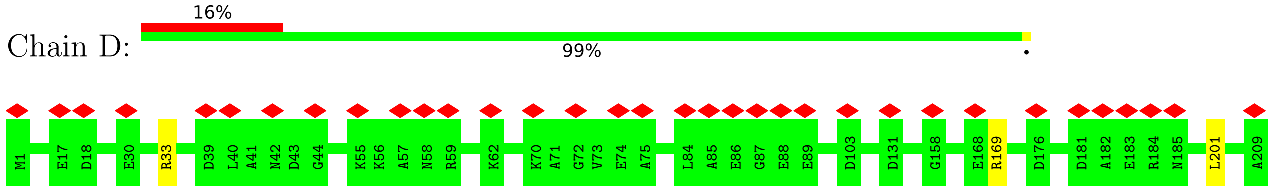
Chain C:





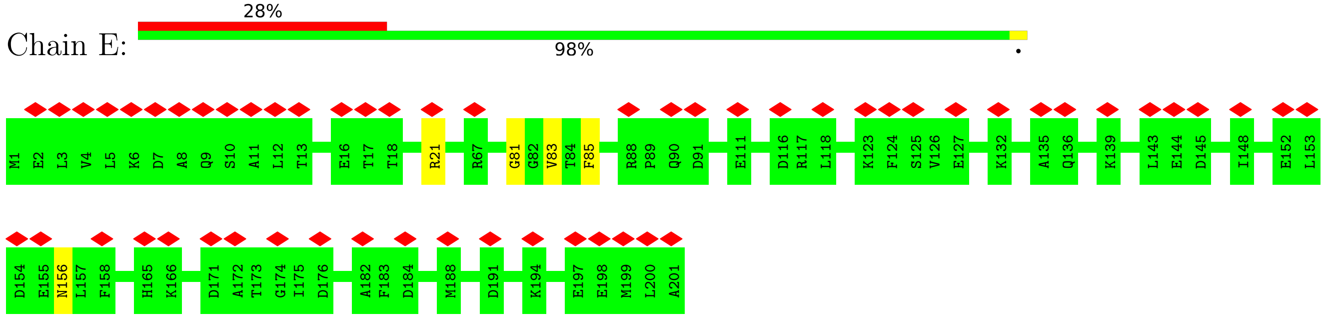
- Molecule 4: 50S ribosomal protein L3

Chain D:



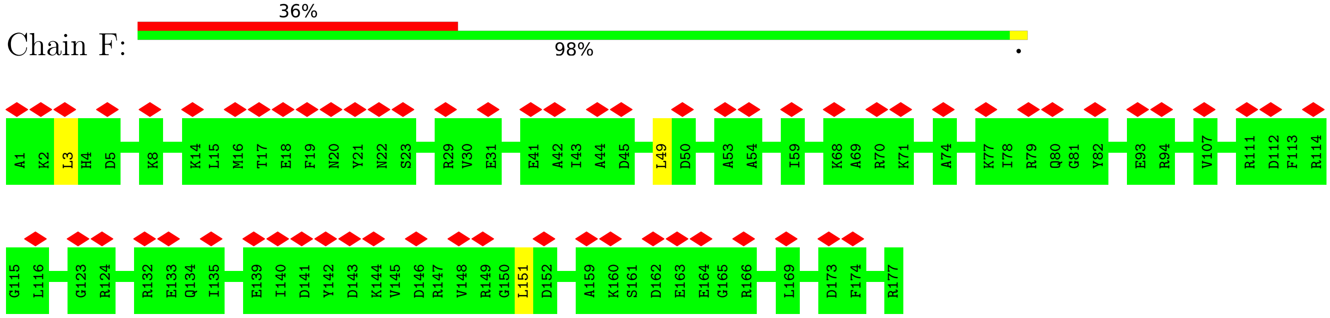
- Molecule 5: 50S ribosomal protein L4

Chain E:



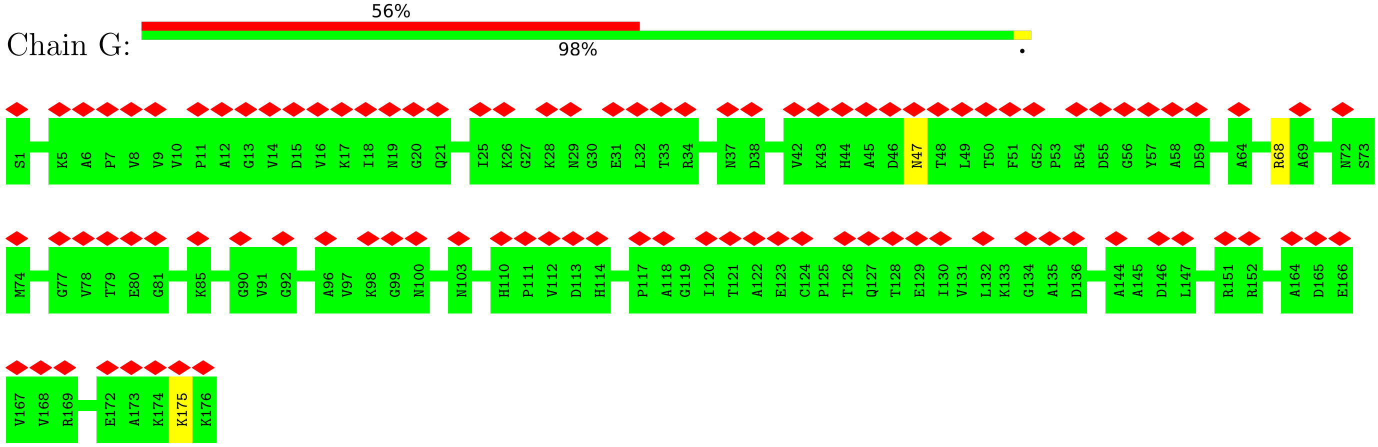
- Molecule 6: 50S ribosomal protein L5

Chain F:



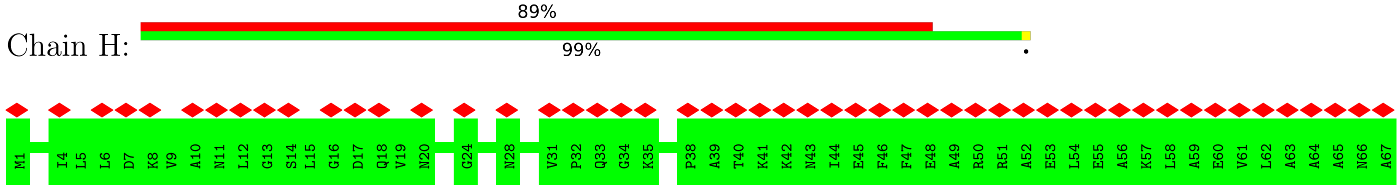
- Molecule 7: 50S ribosomal protein L6

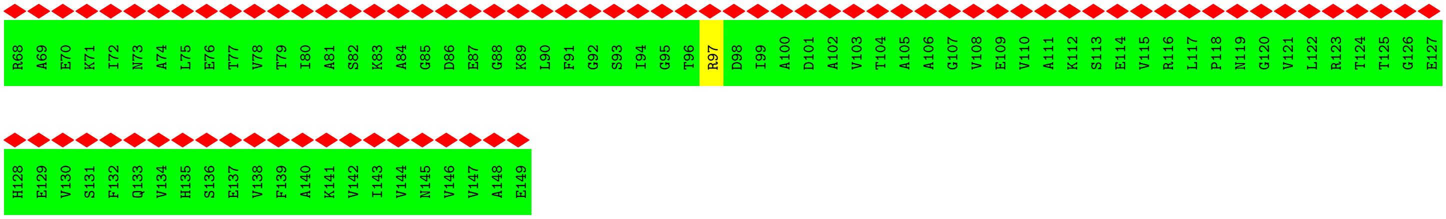
Chain G:



- Molecule 8: 50S ribosomal protein L9

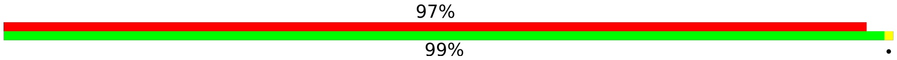
Chain H:

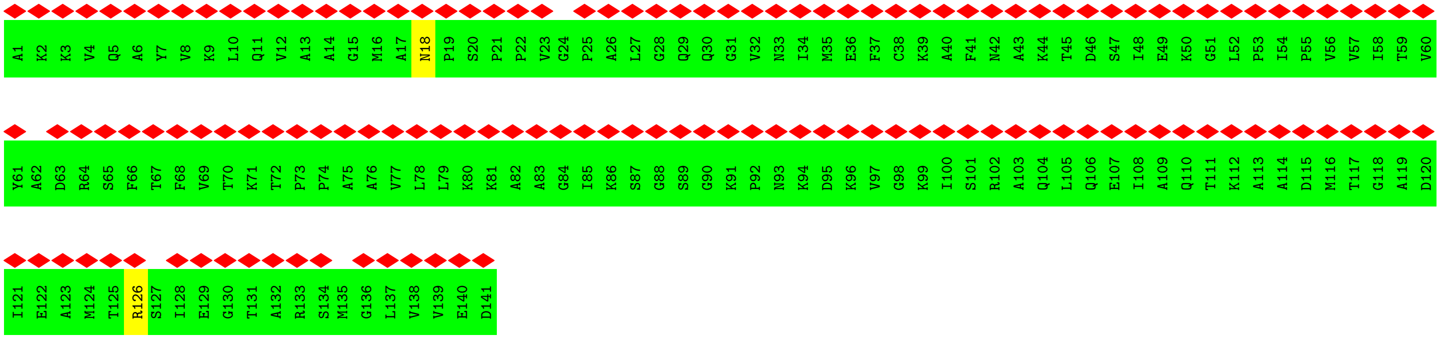




- Molecule 9: 50S ribosomal protein L11

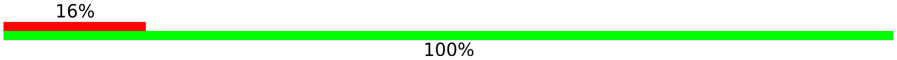
Chain I:

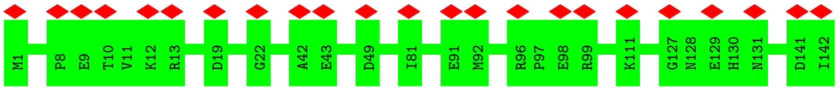




- Molecule 10: 50S ribosomal protein L13

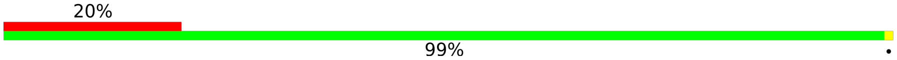
Chain J:

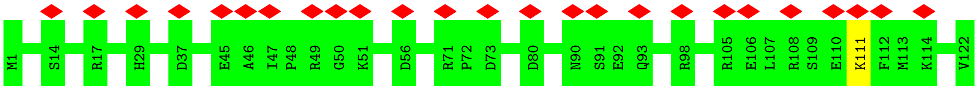




- Molecule 11: 50S ribosomal protein L14

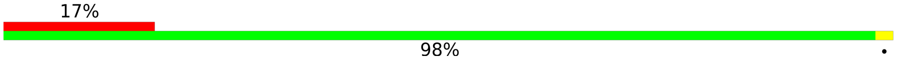
Chain K:

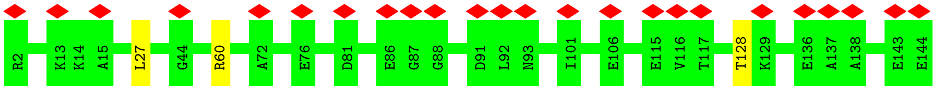




- Molecule 12: 50S ribosomal protein L15

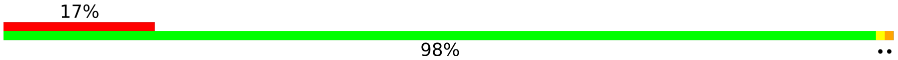
Chain L:

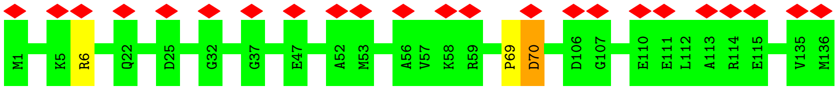




- Molecule 13: 50S ribosomal protein L16

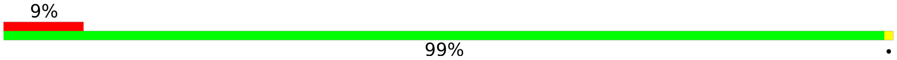
Chain M:

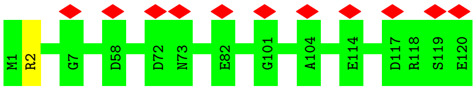




- Molecule 14: 50S ribosomal protein L17

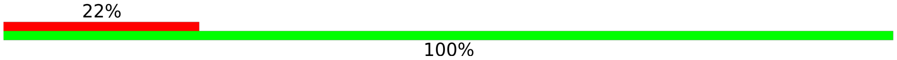
Chain N:

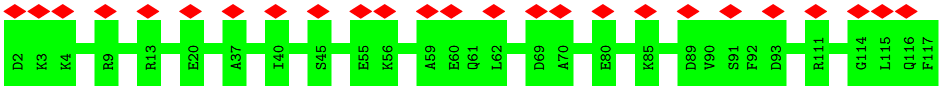




- Molecule 15: 50S ribosomal protein L18

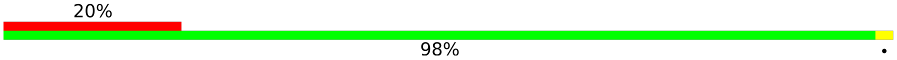
Chain O:

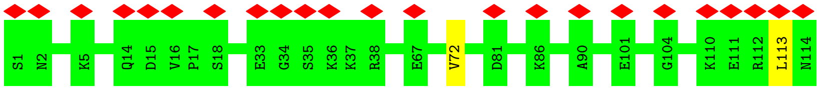




- Molecule 16: 50S ribosomal protein L19

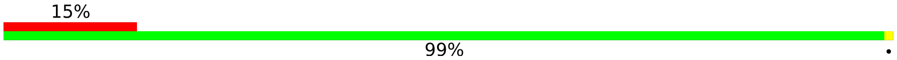
Chain P:

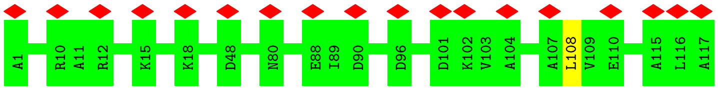




- Molecule 17: 50S ribosomal protein L20

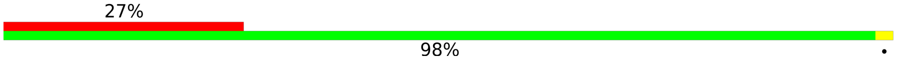
Chain Q:

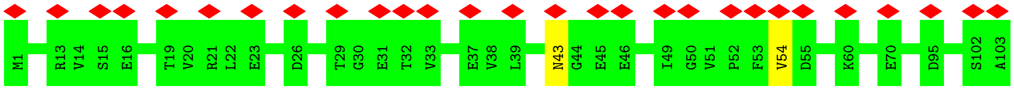




- Molecule 18: 50S ribosomal protein L21

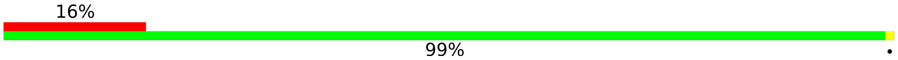
Chain R:

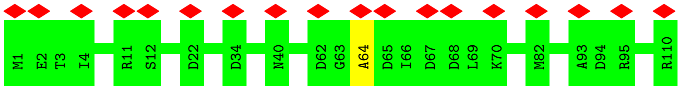




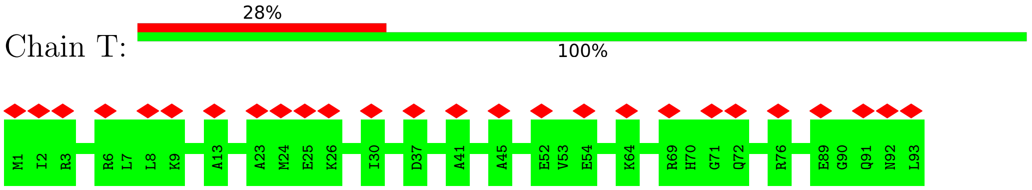
- Molecule 19: 50S ribosomal protein L22

Chain S:

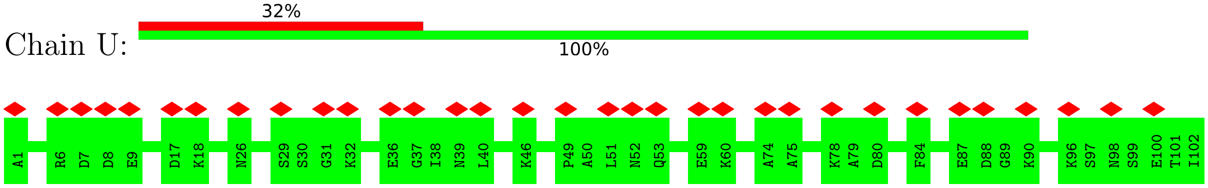




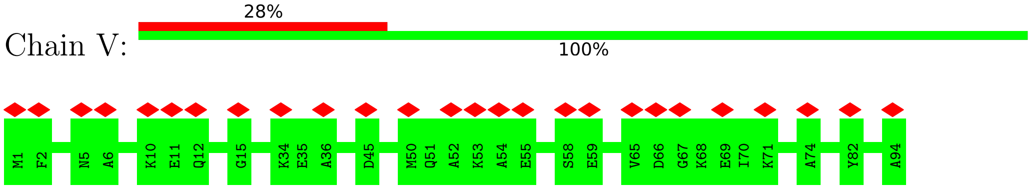
- Molecule 20: 50S ribosomal protein L23



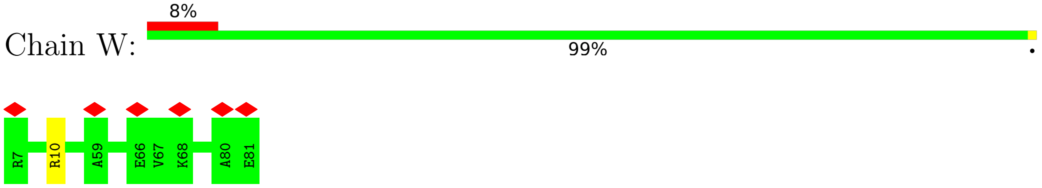
- Molecule 21: 50S ribosomal protein L24



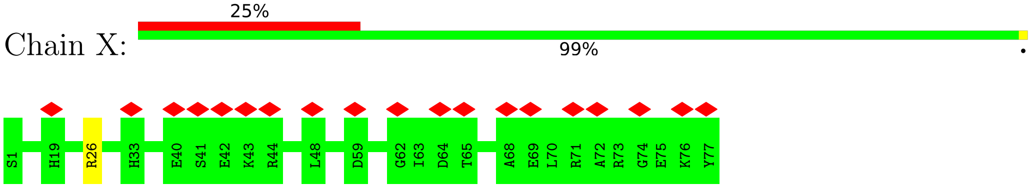
- Molecule 22: 50S ribosomal protein L25



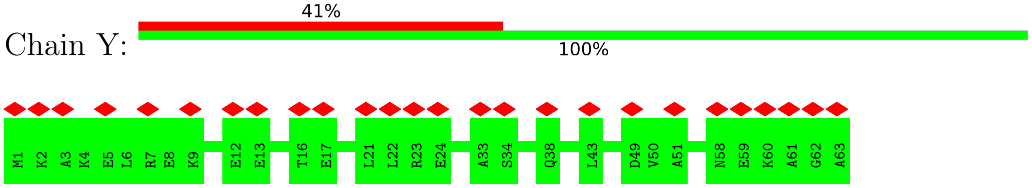
- Molecule 23: 50S ribosomal protein L27



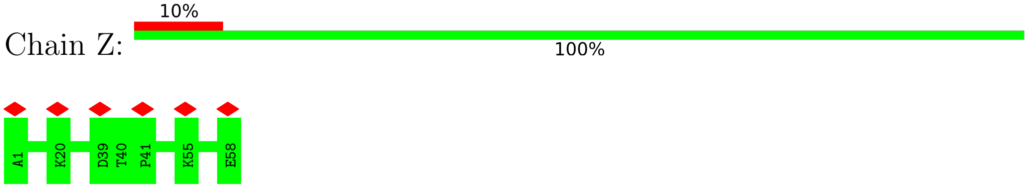
- Molecule 24: 50S ribosomal protein L28



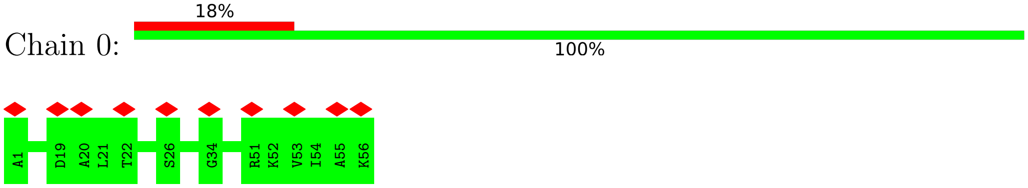
- Molecule 25: 50S ribosomal protein L29



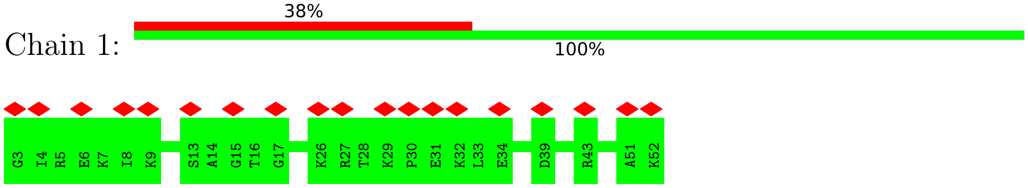
- Molecule 26: 50S ribosomal protein L30



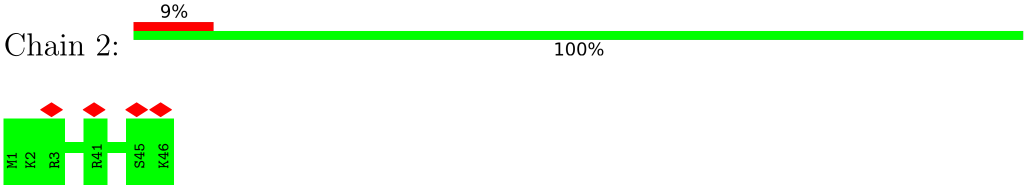
- Molecule 27: 50S ribosomal protein L32



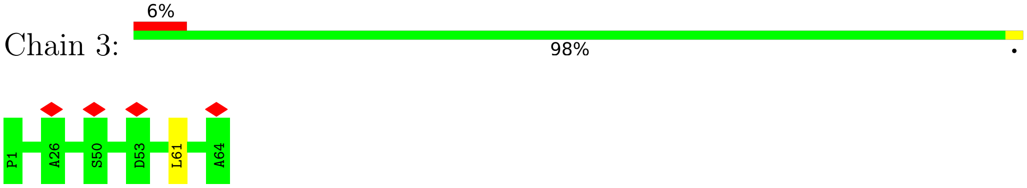
- Molecule 28: 50S ribosomal protein L33



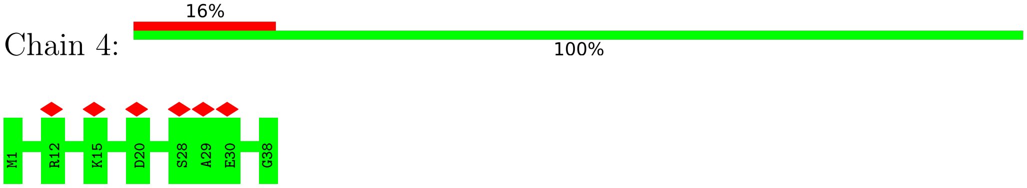
- Molecule 29: 50S ribosomal protein L34



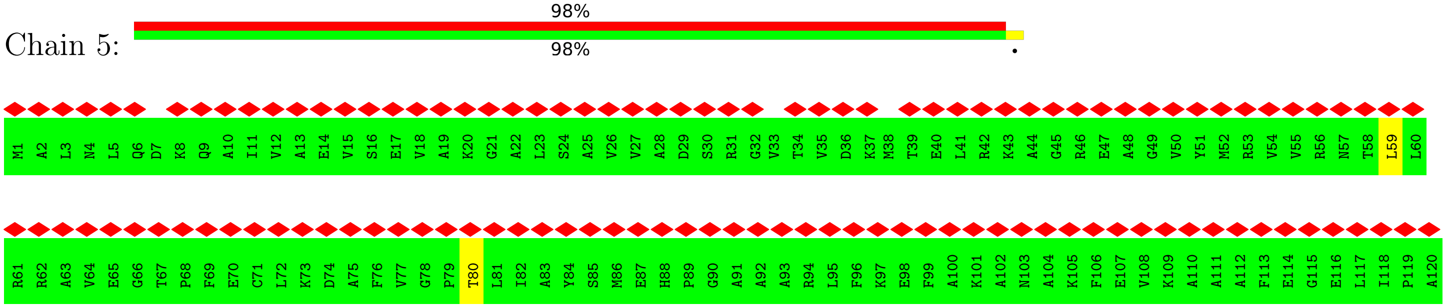
- Molecule 30: 50S ribosomal protein L35

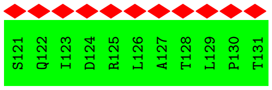


- Molecule 31: 50S ribosomal protein L36



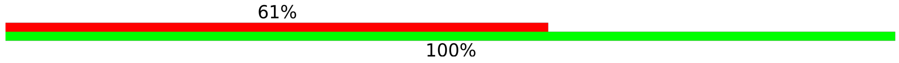
- Molecule 32: 50S ribosomal protein L10

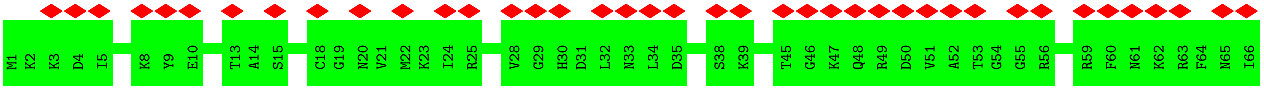




- Molecule 33: 50S ribosomal protein L31

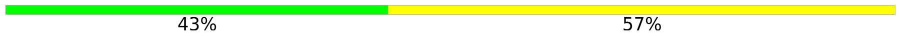
Chain 6:





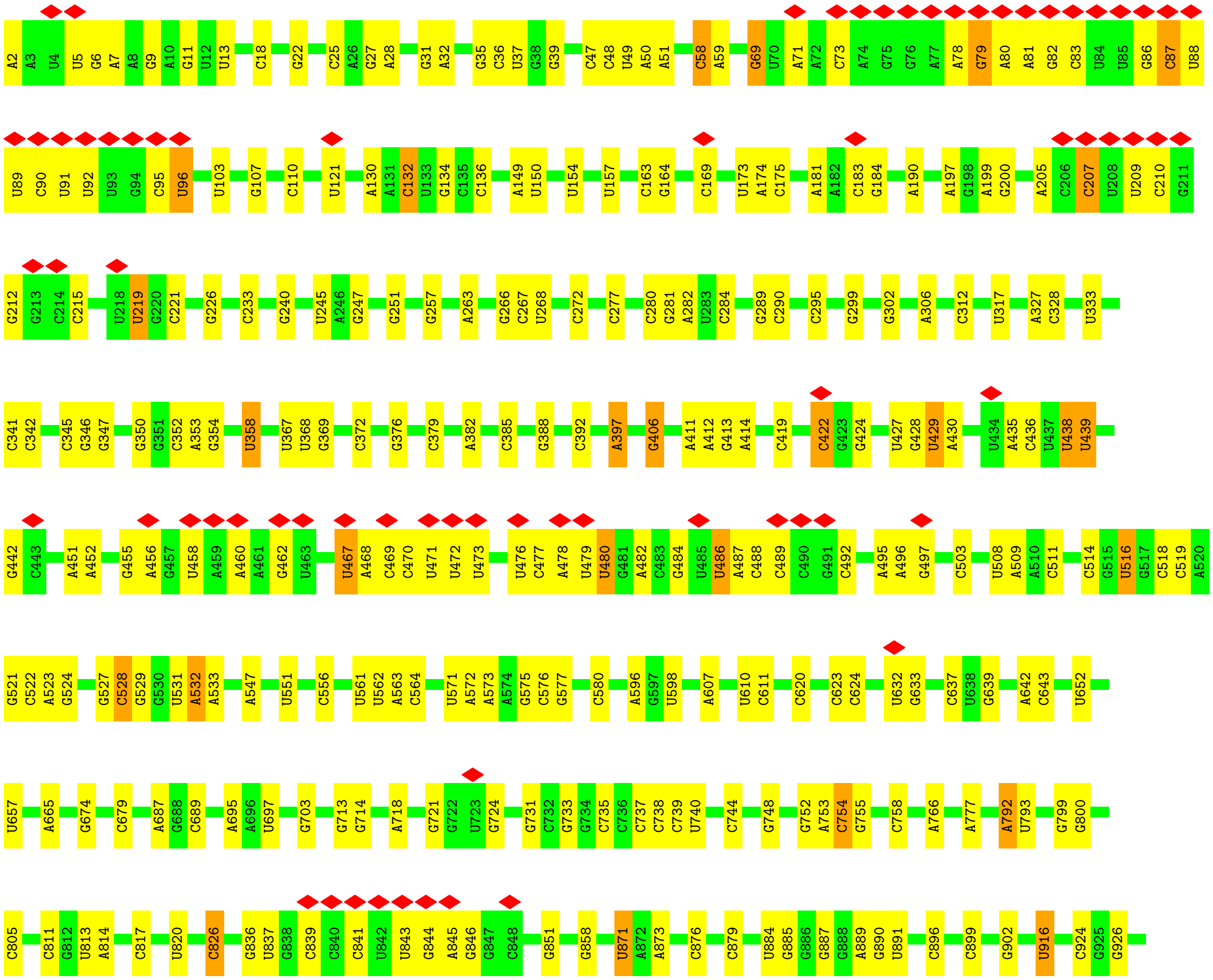
- Molecule 34: mRNA

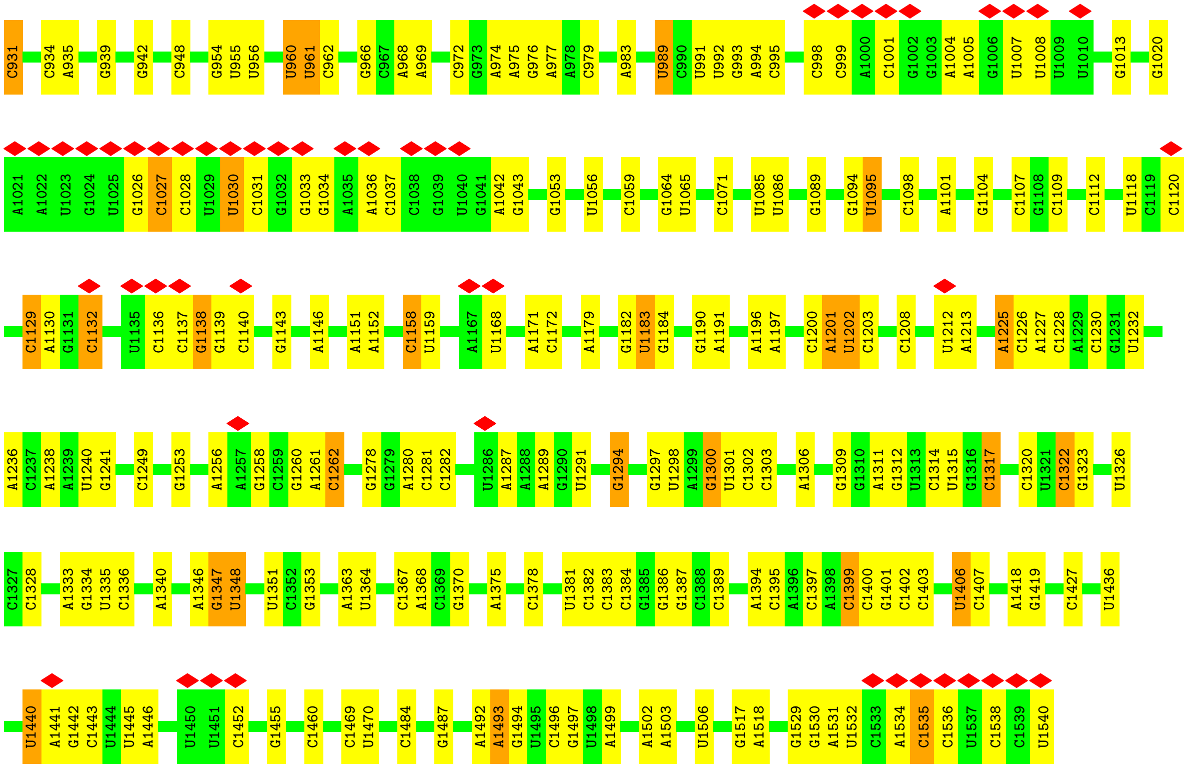
Chain 7:



- Molecule 35: 16S ribosomal RNA

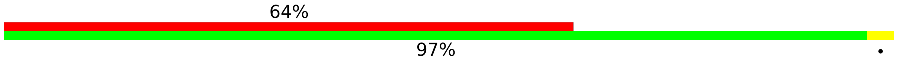
Chain a:

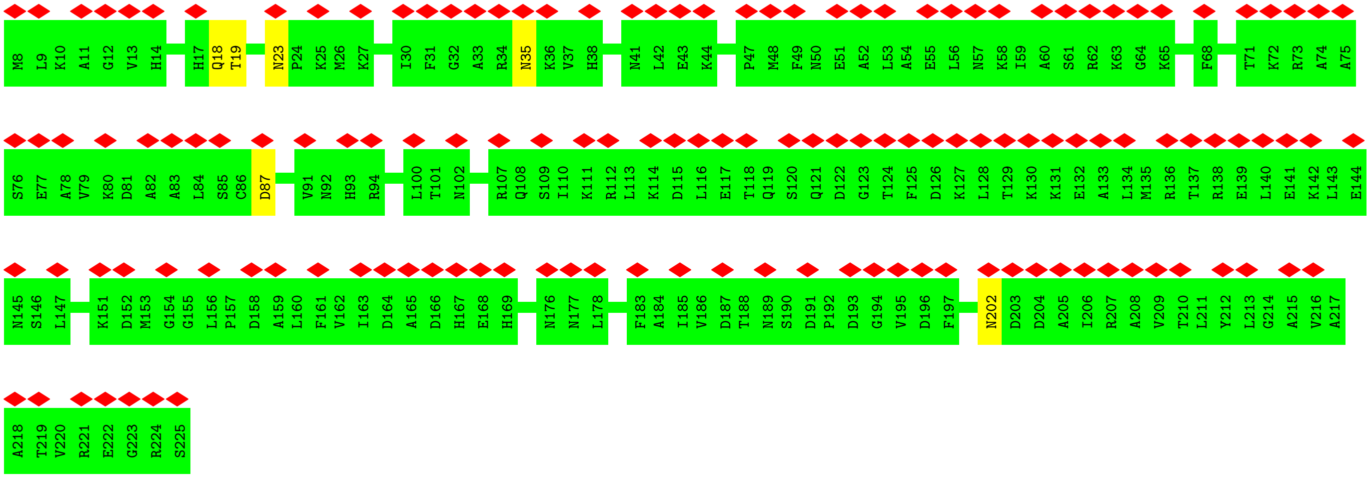




- Molecule 36: 30S ribosomal protein S2

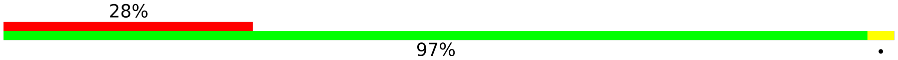
Chain b:

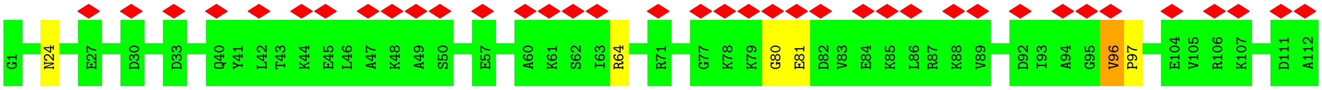


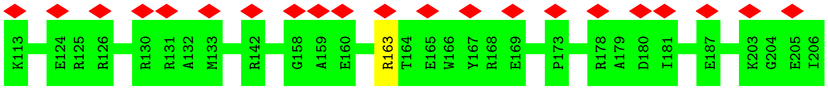


- Molecule 37: 30S ribosomal protein S3

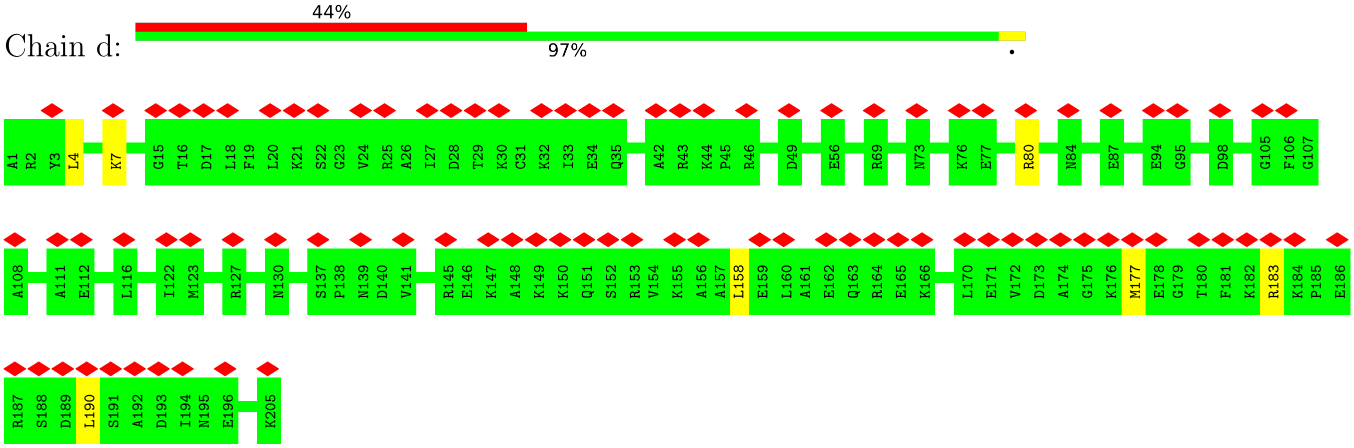
Chain c:



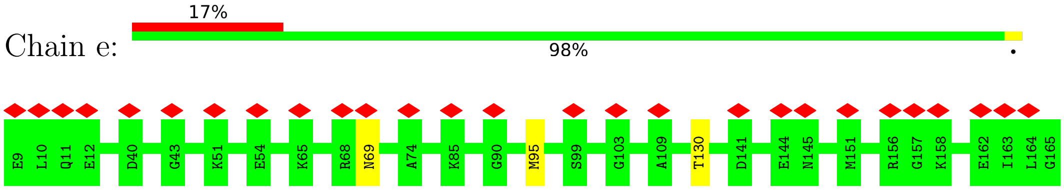




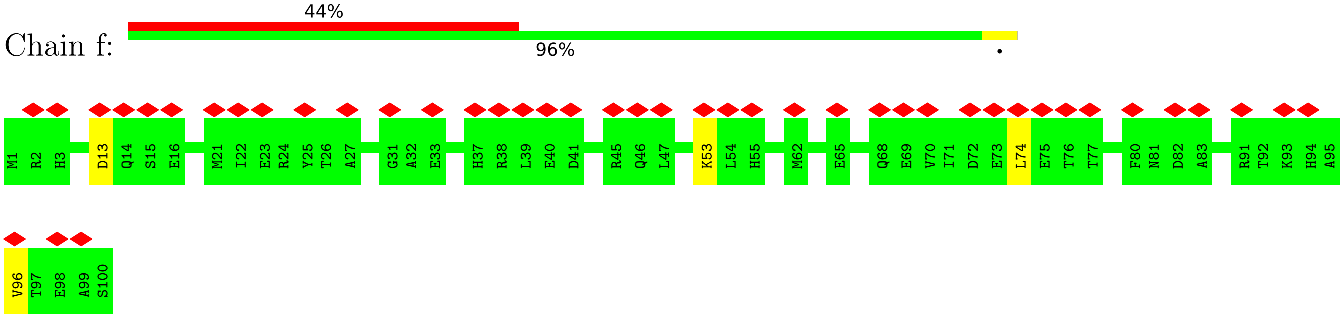
- Molecule 38: 30S ribosomal protein S4



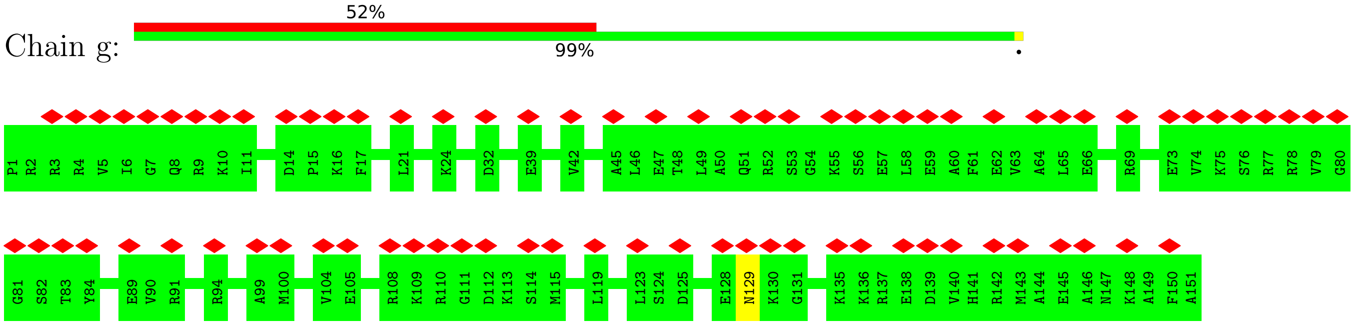
- Molecule 39: 30S ribosomal protein S5



- Molecule 40: 30S ribosomal protein S6

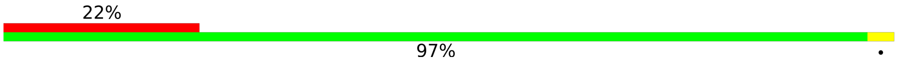


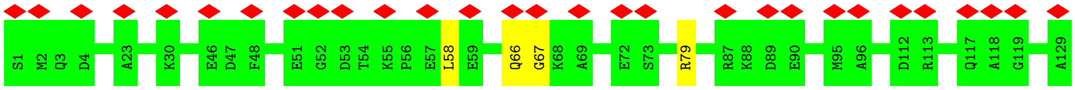
- Molecule 41: 30S ribosomal protein S7



- Molecule 42: 30S ribosomal protein S8

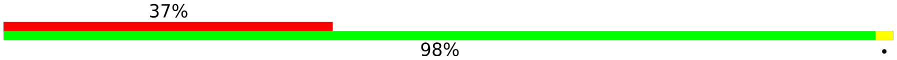
Chain h:

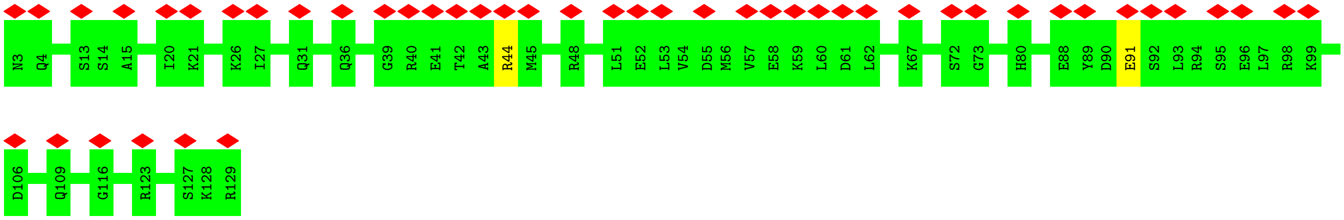




- Molecule 43: 30S ribosomal protein S9

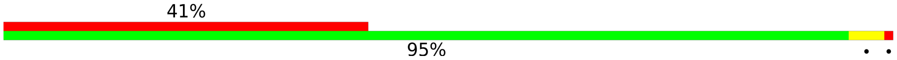
Chain i:

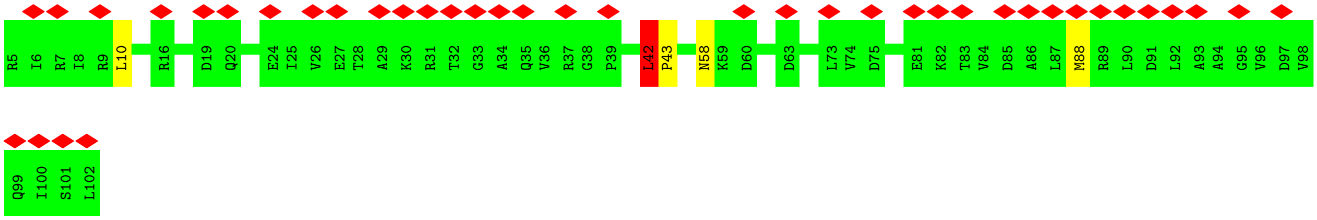




- Molecule 44: 30S ribosomal protein S10

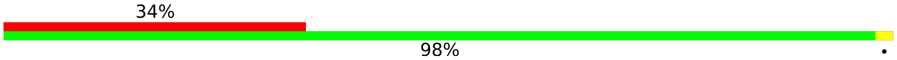
Chain j:

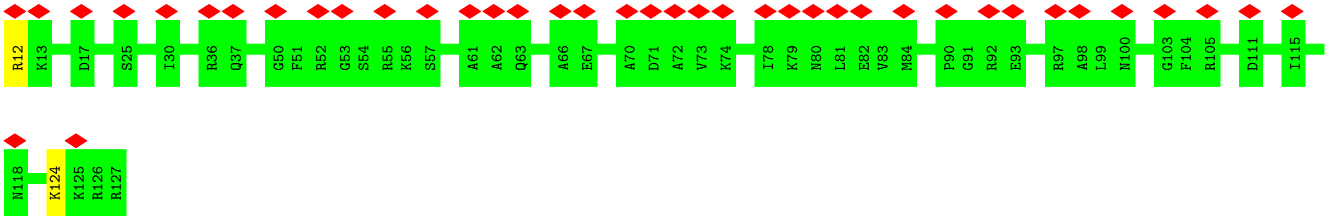




- Molecule 45: 30S ribosomal protein S11

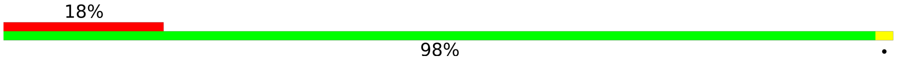
Chain k:

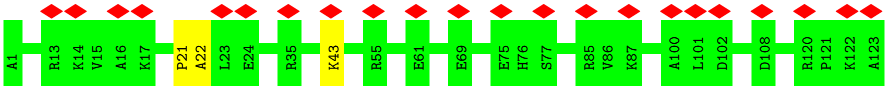




- Molecule 46: 30S ribosomal protein S12

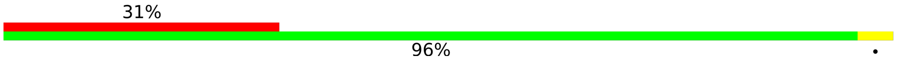
Chain l:

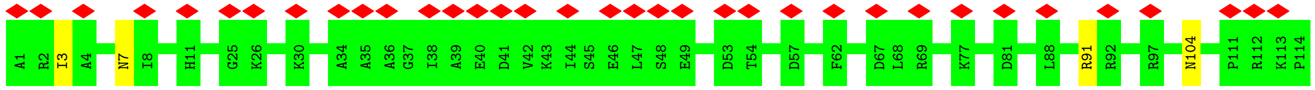




- Molecule 47: 30S ribosomal protein S13

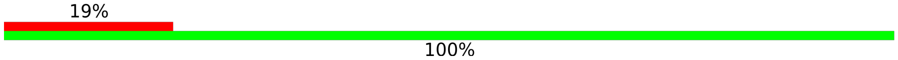
Chain m:

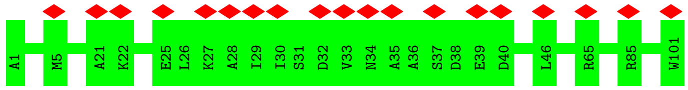




- Molecule 48: 30S ribosomal protein S14

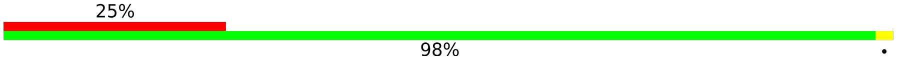
Chain n:

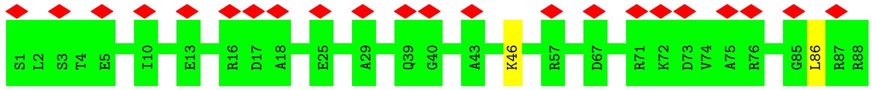




- Molecule 49: 30S ribosomal protein S15

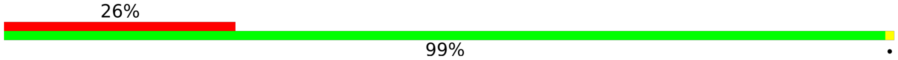
Chain o:

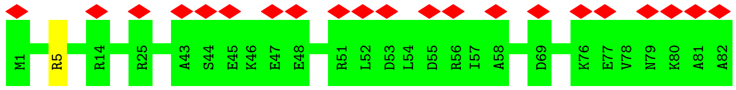




- Molecule 50: 30S ribosomal protein S16

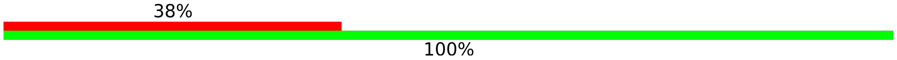
Chain p:

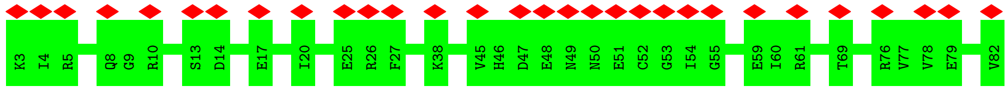




- Molecule 51: 30S ribosomal protein S17

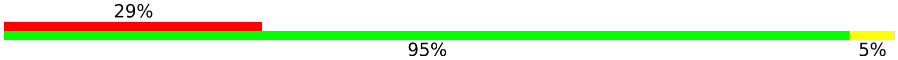
Chain q:

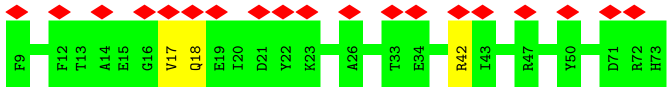




- Molecule 52: 30S ribosomal protein S18

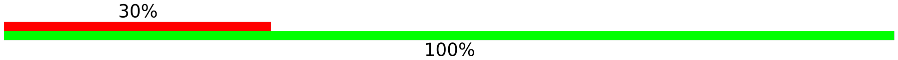
Chain r:

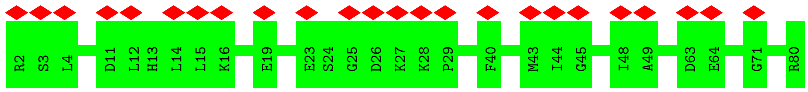




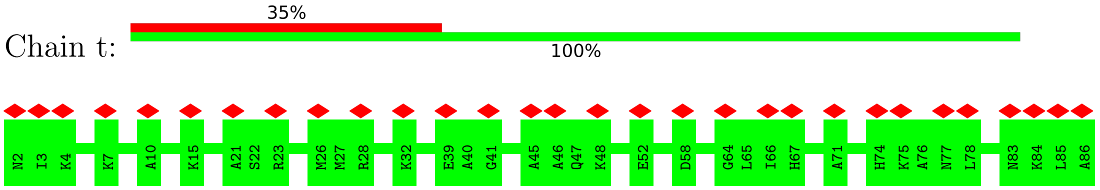
- Molecule 53: 30S ribosomal protein S19

Chain s:

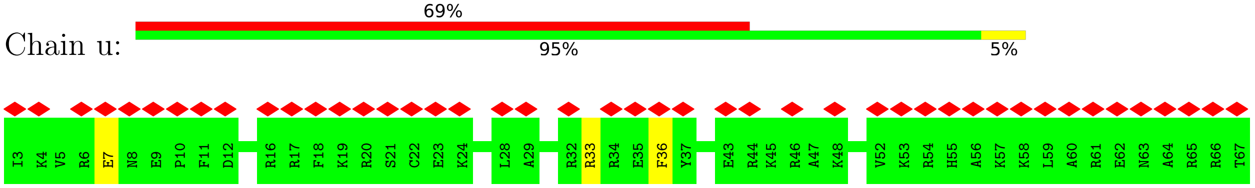




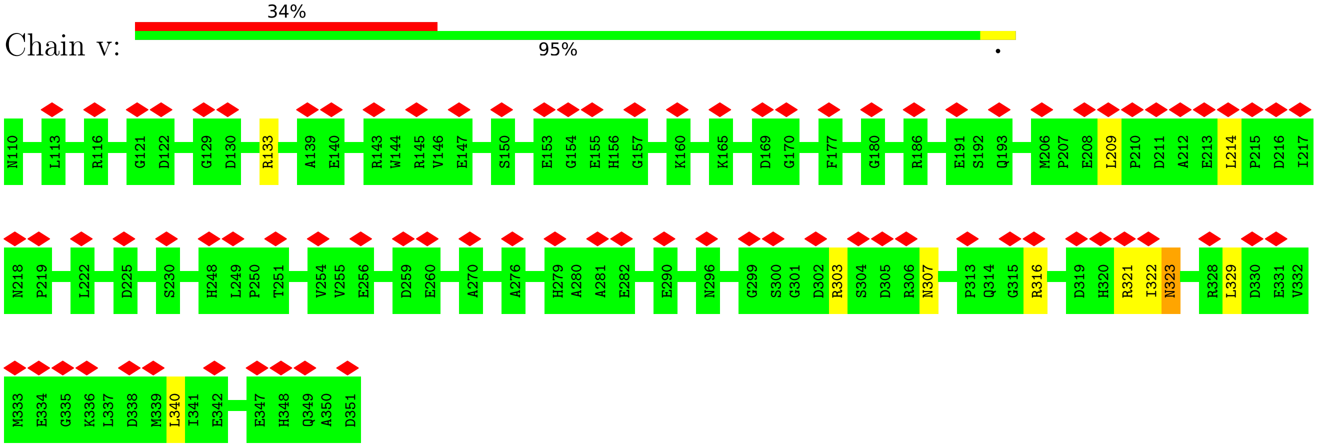
- Molecule 54: 30S ribosomal protein S20



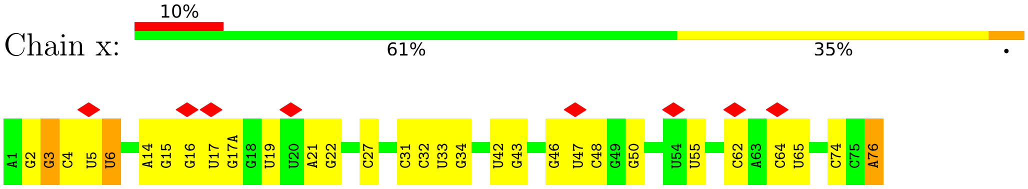
- Molecule 55: 30S ribosomal protein S21



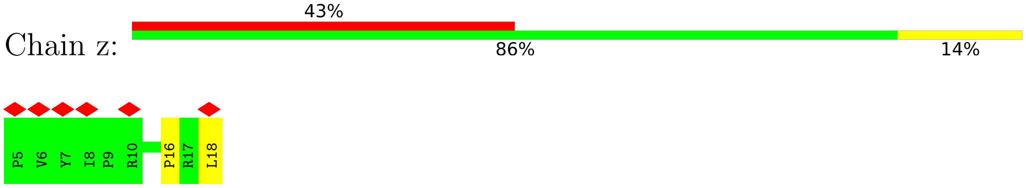
- Molecule 56: Peptide chain release factor RF1



- Molecule 57: P-site Ile-tRNA



- Molecule 58: Apidaecin



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36826	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.131	Depositor
Minimum map value	-1.467	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.407	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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	A	1.25	33/69734 (0.0%)	1.36	809/108788 (0.7%)
2	B	1.04	1/2876 (0.0%)	1.47	56/4483 (1.2%)
3	C	0.62	0/2121	0.69	0/2852
4	D	0.63	0/1586	0.69	1/2134 (0.0%)
5	E	0.61	1/1571 (0.1%)	0.68	1/2113 (0.0%)
6	F	0.51	0/1434	0.74	3/1926 (0.2%)
7	G	0.47	0/1343	0.65	0/1816
8	H	0.36	0/1122	0.60	1/1515 (0.1%)
9	I	0.35	0/1046	0.67	0/1410
10	J	0.57	0/1152	0.63	0/1551
11	K	0.59	0/947	0.76	0/1268
12	L	0.62	1/1054 (0.1%)	0.79	0/1403
13	M	0.62	0/1093	0.71	1/1460 (0.1%)
14	N	0.58	0/973	0.74	0/1301
15	O	0.56	0/902	0.67	0/1209
16	P	0.60	0/929	0.68	1/1242 (0.1%)
17	Q	0.72	0/960	0.66	0/1278
18	R	0.58	0/829	0.72	0/1107
19	S	0.58	0/864	0.70	0/1156
20	T	0.53	0/744	0.65	0/994
21	U	0.47	0/787	0.66	0/1051
22	V	0.55	0/766	0.65	0/1025
23	W	0.65	0/582	0.63	0/769
24	X	0.53	0/635	0.65	0/848
25	Y	0.41	0/510	0.66	0/677
26	Z	0.53	0/453	0.65	0/605
27	0	0.57	0/450	0.65	0/599
28	1	0.55	0/416	0.66	0/554
29	2	0.62	0/380	0.74	0/498
30	3	0.63	0/513	0.78	1/676 (0.1%)
31	4	0.65	0/303	0.59	0/397
32	5	0.39	0/1001	0.81	1/1350 (0.1%)
33	6	0.40	0/531	0.63	0/709
34	7	1.17	0/166	1.09	0/256

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	a	1.17	5/36967 (0.0%)	1.33	366/57666 (0.6%)
36	b	0.44	0/1735	0.71	0/2338
37	c	0.54	0/1651	0.79	2/2225 (0.1%)
38	d	0.51	0/1665	0.75	3/2227 (0.1%)
39	e	0.59	0/1154	0.76	1/1554 (0.1%)
40	f	0.48	0/835	0.81	2/1128 (0.2%)
41	g	0.46	0/1195	0.68	0/1602
42	h	0.54	0/989	0.78	2/1326 (0.2%)
43	i	0.53	0/1034	0.70	0/1375
44	j	0.50	0/796	0.93	3/1077 (0.3%)
45	k	0.51	0/885	0.69	0/1195
46	l	0.63	0/969	0.77	2/1300 (0.2%)
47	m	0.49	0/892	0.74	0/1193
48	n	0.52	0/811	0.63	0/1081
49	o	0.48	0/722	0.68	1/964 (0.1%)
50	p	0.54	0/659	0.71	0/884
51	q	0.57	0/657	0.73	0/881
52	r	0.53	0/511	0.69	0/689
53	s	0.52	0/652	0.69	0/877
54	t	0.48	0/671	0.66	0/888
55	u	0.43	0/500	0.82	0/668
56	v	0.53	0/1910	0.75	2/2573 (0.1%)
57	x	1.03	0/1841	1.38	26/2869 (0.9%)
58	z	0.40	0/127	0.81	0/175
All	All	1.06	41/160601 (0.0%)	1.21	1285/239775 (0.5%)

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
56	v	0	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	G	OP3-P	-11.16	1.47	1.61
35	a	2	A	OP3-P	-10.97	1.48	1.61
2	B	1	U	OP3-P	-10.32	1.48	1.61
1	A	1142	A	N9-C4	-7.34	1.33	1.37
5	E	85	PHE	CA-CB	-7.07	1.38	1.53

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	60	ARG	C-N	-6.93	1.18	1.34
1	A	783	A	N9-C4	-6.72	1.33	1.37
1	A	2604	U	N3-C4	-6.34	1.32	1.38
1	A	526	A	N9-C4	-6.33	1.34	1.37
1	A	2052	A	N7-C5	-6.31	1.35	1.39
1	A	528	A	N9-C4	-6.27	1.34	1.37
1	A	2589	A	N9-C4	-5.97	1.34	1.37
35	a	1306	A	N7-C5	-5.82	1.35	1.39
1	A	1253	A	N9-C4	-5.82	1.34	1.37
1	A	1783	A	N9-C4	-5.70	1.34	1.37
1	A	2052	A	N9-C4	-5.63	1.34	1.37
1	A	241	A	N9-C4	-5.60	1.34	1.37
1	A	1912	A	N7-C5	-5.54	1.35	1.39
1	A	1994	C	N3-C4	-5.51	1.30	1.33
35	a	28	A	N9-C4	-5.41	1.34	1.37
1	A	1264	A	N9-C4	-5.39	1.34	1.37
1	A	1605	C	N1-C6	-5.39	1.33	1.37
1	A	1791	A	N9-C4	-5.37	1.34	1.37
1	A	565	C	N1-C6	-5.35	1.33	1.37
1	A	1954	G	N9-C8	-5.33	1.34	1.37
1	A	1679	A	N9-C4	-5.32	1.34	1.37
1	A	804	A	N9-C4	-5.28	1.34	1.37
1	A	673	C	N3-C4	-5.27	1.30	1.33
1	A	2407	A	N7-C5	-5.22	1.36	1.39
1	A	2443	C	N1-C6	-5.22	1.34	1.37
1	A	198	C	C4-C5	-5.21	1.38	1.43
1	A	2542	A	N9-C4	-5.20	1.34	1.37
1	A	1791	A	N7-C5	-5.18	1.36	1.39
1	A	1086	A	N9-C4	-5.17	1.34	1.37
35	a	805	C	N1-C6	-5.17	1.34	1.37
1	A	2516	A	N7-C5	-5.15	1.36	1.39
1	A	265	A	N9-C4	-5.13	1.34	1.37
1	A	1964	G	N9-C4	-5.13	1.33	1.38
35	a	800	G	N7-C5	-5.11	1.36	1.39
1	A	2267	A	C6-N1	-5.10	1.31	1.35
1	A	2572	A	N9-C4	-5.03	1.34	1.37

All (1285) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	j	42	LEU	C-N-CD	-15.77	85.92	120.60
37	c	96	VAL	C-N-CD	-15.69	86.08	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	516	U	N3-C2-O2	-13.84	112.52	122.20
1	A	1917	U	N3-C2-O2	-13.13	113.01	122.20
1	A	2072	C	C6-N1-C2	-13.04	115.08	120.30
1	A	2072	C	C5-C6-N1	12.75	127.38	121.00
2	B	36	C	C6-N1-C2	-11.58	115.67	120.30
1	A	2506	U	N1-C2-O2	11.15	130.60	122.80
1	A	1101	U	N3-C2-O2	-10.91	114.56	122.20
1	A	2590	A	C6-N1-C2	-10.87	112.08	118.60
1	A	2506	U	N3-C2-O2	-10.79	114.65	122.20
35	a	1306	A	C8-N9-C4	-10.77	101.49	105.80
1	A	998	C	C5-C6-N1	10.63	126.31	121.00
1	A	998	C	C6-N1-C2	-10.55	116.08	120.30
1	A	2580	U	N3-C2-O2	-10.26	115.02	122.20
1	A	1092	C	N1-C2-O2	10.23	125.04	118.90
2	B	26	C	N1-C2-O2	10.21	125.03	118.90
1	A	550	C	C2-N1-C1'	10.19	130.01	118.80
35	a	516	U	N1-C2-O2	10.12	129.89	122.80
1	A	1349	C	C6-N1-C2	-10.11	116.26	120.30
1	A	2504	U	N3-C2-O2	-10.09	115.14	122.20
1	A	2342	C	C6-N1-C2	-10.04	116.28	120.30
1	A	2506	U	C2-N1-C1'	10.04	129.75	117.70
1	A	1104	C	C6-N1-C2	-9.98	116.31	120.30
1	A	2457	U	N3-C2-O2	-9.86	115.30	122.20
35	a	58	C	C6-N1-C2	-9.86	116.36	120.30
35	a	1306	A	N7-C8-N9	9.84	118.72	113.80
1	A	234	U	N3-C2-O2	-9.79	115.34	122.20
1	A	1804	C	C6-N1-C2	-9.77	116.39	120.30
1	A	1314	C	C2-N1-C1'	9.75	129.53	118.80
1	A	1914	C	N1-C2-O2	9.72	124.73	118.90
2	B	30	C	N1-C2-O2	9.70	124.72	118.90
1	A	1313	U	N3-C2-O2	-9.69	115.42	122.20
1	A	405	U	C2-N1-C1'	9.68	129.31	117.70
1	A	1914	C	C2-N1-C1'	9.66	129.42	118.80
1	A	405	U	N1-C2-O2	9.62	129.53	122.80
1	A	2326	C	C6-N1-C2	-9.62	116.45	120.30
1	A	2646	C	C5-C6-N1	9.61	125.81	121.00
1	A	2604	U	C5-C4-O4	9.60	131.66	125.90
1	A	1104	C	N1-C2-O2	9.54	124.63	118.90
1	A	898	C	C5-C6-N1	9.52	125.76	121.00
1	A	1313	U	C2-N1-C1'	9.52	129.12	117.70
2	B	4	C	C5-C6-N1	9.50	125.75	121.00
35	a	891	U	N3-C2-O2	-9.31	115.68	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	36	C	N1-C2-O2	9.29	124.48	118.90
1	A	2504	U	C2-N1-C1'	9.25	128.80	117.70
35	a	972	C	C6-N1-C2	-9.24	116.60	120.30
1	A	1362	C	C6-N1-C2	-9.23	116.61	120.30
1	A	1079	C	C6-N1-C2	-9.22	116.61	120.30
1	A	1917	U	N1-C2-O2	9.21	129.25	122.80
1	A	2474	U	N1-C2-O2	9.20	129.24	122.80
35	a	1037	C	N1-C2-O2	9.11	124.36	118.90
2	B	36	C	C5-C6-N1	9.08	125.54	121.00
1	A	1104	C	N3-C2-O2	-9.03	115.58	121.90
35	a	58	C	N1-C2-O2	9.03	124.31	118.90
1	A	2605	U	N3-C2-O2	-8.99	115.91	122.20
2	B	12	C	C2-N1-C1'	8.99	128.69	118.80
1	A	2072	C	C2-N1-C1'	8.95	128.65	118.80
57	x	32	C	N1-C2-O2	8.95	124.27	118.90
1	A	1101	U	N1-C2-O2	8.93	129.05	122.80
1	A	1313	U	N1-C2-O2	8.91	129.04	122.80
1	A	2063	C	C2-N1-C1'	8.88	128.57	118.80
35	a	422	C	O5'-P-OP2	-8.87	97.71	105.70
1	A	854	C	N3-C2-O2	-8.84	115.71	121.90
1	A	1914	C	N3-C2-O2	-8.82	115.72	121.90
35	a	1109	C	C6-N1-C2	-8.82	116.77	120.30
1	A	2456	C	C5-C6-N1	8.81	125.41	121.00
1	A	1092	C	N3-C2-O2	-8.80	115.74	121.90
1	A	758	C	C6-N1-C2	-8.80	116.78	120.30
1	A	2605	U	C2-N1-C1'	8.79	128.25	117.70
35	a	83	C	C6-N1-C2	-8.79	116.79	120.30
35	a	528	C	C6-N1-C2	-8.72	116.81	120.30
35	a	1098	C	C6-N1-C2	-8.71	116.82	120.30
2	B	30	C	N3-C2-O2	-8.68	115.83	121.90
35	a	58	C	C2-N1-C1'	8.68	128.35	118.80
1	A	1362	C	C5-C6-N1	8.65	125.32	121.00
1	A	550	C	C5-C6-N1	8.65	125.32	121.00
1	A	1911	U	N3-C2-O2	-8.64	116.15	122.20
1	A	1531	C	N1-C2-O2	8.63	124.08	118.90
1	A	1348	C	N1-C2-O2	8.63	124.08	118.90
1	A	2504	U	N1-C2-O2	8.62	128.84	122.80
1	A	2473	U	C2-N1-C1'	8.61	128.03	117.70
1	A	413	C	C5-C6-N1	8.59	125.30	121.00
1	A	1437	C	C5-C6-N1	8.59	125.29	121.00
1	A	2354	C	C6-N1-C2	-8.58	116.87	120.30
57	x	6	U	C2-N1-C1'	8.54	127.95	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	955	U	N3-C2-O2	-8.53	116.23	122.20
1	A	2354	C	C5-C6-N1	8.53	125.27	121.00
35	a	528	C	C5-C6-N1	8.50	125.25	121.00
1	A	1092	C	C2-N1-C1’	8.49	128.14	118.80
35	a	826	C	C6-N1-C2	-8.45	116.92	120.30
35	a	470	C	C6-N1-C2	-8.44	116.92	120.30
35	a	1120	C	N1-C2-O2	8.42	123.95	118.90
35	a	35	G	N3-C4-N9	8.42	131.05	126.00
2	B	26	C	N3-C2-O2	-8.37	116.04	121.90
35	a	826	C	C5-C6-N1	8.37	125.18	121.00
35	a	35	G	N3-C4-C5	-8.36	124.42	128.60
1	A	1611	C	C6-N1-C2	-8.36	116.96	120.30
1	A	2656	U	N3-C2-O2	-8.32	116.37	122.20
1	A	405	U	N3-C2-O2	-8.32	116.38	122.20
1	A	2590	A	C5-C6-N1	8.30	121.85	117.70
35	a	1203	C	C6-N1-C2	-8.30	116.98	120.30
35	a	679	C	C5-C6-N1	8.28	125.14	121.00
1	A	1104	C	C5-C6-N1	8.23	125.11	121.00
1	A	2605	U	N1-C2-O2	8.21	128.55	122.80
57	x	32	C	N3-C2-O2	-8.20	116.16	121.90
1	A	2063	C	N1-C2-O2	8.19	123.81	118.90
35	a	891	U	N1-C2-O2	8.19	128.53	122.80
35	a	439	U	N3-C2-O2	-8.16	116.48	122.20
1	A	2326	C	C5-C6-N1	8.16	125.08	121.00
1	A	2616	C	C6-N1-C2	-8.15	117.04	120.30
35	a	528	C	N1-C2-O2	8.15	123.79	118.90
1	A	1656	C	C5-C6-N1	8.14	125.07	121.00
1	A	1941	C	N1-C2-O2	8.14	123.78	118.90
1	A	847	U	N3-C2-O2	-8.13	116.51	122.20
1	A	901	C	N1-C2-O2	8.13	123.78	118.90
1	A	924	G	N3-C4-N9	-8.13	121.12	126.00
1	A	2720	U	N3-C2-O2	-8.11	116.52	122.20
2	B	4	C	C6-N1-C2	-8.10	117.06	120.30
2	B	36	C	N3-C2-O2	-8.10	116.23	121.90
1	A	1956	U	N1-C2-O2	8.09	128.46	122.80
1	A	2473	U	N3-C2-O2	-8.08	116.54	122.20
1	A	2192	U	C2-N1-C1’	8.06	127.38	117.70
1	A	2604	U	C2-N1-C1’	8.06	127.38	117.70
1	A	1314	C	C5-C6-N1	8.04	125.02	121.00
1	A	912	C	C6-N1-C2	-8.03	117.09	120.30
2	B	4	C	C2-N1-C1’	8.02	127.62	118.80
1	A	135	U	N1-C2-O2	8.01	128.41	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	358	U	C5-C6-N1	8.00	126.70	122.70
1	A	2580	U	N1-C2-O2	8.00	128.40	122.80
1	A	1917	U	C2-N1-C1'	7.99	127.29	117.70
1	A	955	U	C2-N1-C1'	7.94	127.23	117.70
1	A	1531	C	N3-C2-O2	-7.92	116.36	121.90
35	a	58	C	N3-C2-O2	-7.88	116.38	121.90
1	A	1092	C	C6-N1-C2	-7.88	117.15	120.30
2	B	35	C	N1-C2-O2	7.88	123.62	118.90
2	B	37	C	N1-C2-O2	7.86	123.62	118.90
1	A	1578	U	N3-C2-O2	-7.85	116.70	122.20
1	A	1314	C	C6-N1-C2	-7.83	117.17	120.30
1	A	2456	C	C6-N1-C2	-7.82	117.17	120.30
1	A	1804	C	C5-C6-N1	7.81	124.91	121.00
1	A	2473	U	N1-C2-O2	7.81	128.26	122.80
1	A	2161	C	N1-C2-O2	7.79	123.57	118.90
35	a	83	C	C5-C6-N1	7.78	124.89	121.00
1	A	2395	C	C6-N1-C2	-7.77	117.19	120.30
1	A	284	U	N3-C2-O2	-7.77	116.76	122.20
1	A	373	U	C2-N1-C1'	7.76	127.01	117.70
2	B	26	C	C2-N1-C1'	7.76	127.33	118.80
35	a	439	U	N1-C2-O2	7.76	128.23	122.80
1	A	1044	C	N1-C2-O2	7.74	123.54	118.90
35	a	488	C	C6-N1-C2	-7.71	117.22	120.30
1	A	783	A	C5-N7-C8	-7.68	100.06	103.90
1	A	343	C	C6-N1-C2	-7.67	117.23	120.30
1	A	284	U	N1-C2-O2	7.66	128.16	122.80
1	A	2474	U	C5-C6-N1	7.66	126.53	122.70
1	A	1180	U	N3-C2-O2	-7.65	116.85	122.20
1	A	2474	U	C2-N1-C1'	7.65	126.88	117.70
1	A	2656	U	N1-C2-O2	7.64	128.15	122.80
1	A	2666	C	C6-N1-C2	-7.61	117.26	120.30
1	A	284	U	C2-N1-C1'	7.60	126.82	117.70
1	A	2646	C	C6-N1-C2	-7.58	117.27	120.30
56	v	209	LEU	CA-CB-CG	7.58	132.74	115.30
35	a	35	G	C4-N9-C1'	7.58	136.35	126.50
42	h	58	LEU	CA-CB-CG	7.58	132.73	115.30
1	A	2666	C	N1-C2-O2	7.57	123.44	118.90
35	a	528	C	C2-N1-C1'	7.57	127.12	118.80
1	A	459	U	N3-C2-O2	-7.56	116.91	122.20
1	A	2329	U	C5-C6-N1	7.56	126.48	122.70
35	a	1027	C	C5-C6-N1	7.56	124.78	121.00
35	a	1086	U	N1-C2-O2	7.55	128.08	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2192	U	N3-C4-O4	7.54	124.67	119.40
1	A	235	U	N3-C2-O2	-7.51	116.95	122.20
1	A	601	C	C6-N1-C2	-7.50	117.30	120.30
35	a	110	C	N1-C2-O2	7.50	123.40	118.90
35	a	1037	C	N3-C2-O2	-7.48	116.67	121.90
35	a	58	C	C5-C6-N1	7.47	124.74	121.00
37	c	81	GLU	N-CA-C	7.45	131.11	111.00
1	A	143	C	C2-N1-C1’	7.44	126.98	118.80
1	A	475	C	C5-C6-N1	7.44	124.72	121.00
1	A	2457	U	C2-N1-C1’	7.43	126.62	117.70
35	a	529	G	C5-C6-O6	-7.43	124.14	128.60
1	A	2342	C	C5-C6-N1	7.43	124.72	121.00
1	A	2666	C	C2-N1-C1’	7.43	126.98	118.80
1	A	2064	C	C6-N1-C2	-7.42	117.33	120.30
39	e	95	MET	C-N-CA	7.42	140.25	121.70
1	A	2043	C	C2-N1-C1’	7.40	126.94	118.80
1	A	158	U	N3-C2-O2	-7.38	117.03	122.20
35	a	36	C	C5-C6-N1	7.38	124.69	121.00
2	B	3	C	P-O3’-C3’	7.38	128.55	119.70
1	A	2580	U	C2-N1-C1’	7.37	126.54	117.70
1	A	2457	U	N1-C2-O2	7.36	127.95	122.80
2	B	36	C	C2-N1-C1’	7.35	126.88	118.80
35	a	469	C	N1-C2-O2	7.33	123.30	118.90
1	A	2889	C	C6-N1-C2	-7.32	117.37	120.30
1	A	1180	U	N1-C2-O2	7.31	127.92	122.80
1	A	413	C	C6-N1-C2	-7.30	117.38	120.30
1	A	2063	C	N3-C2-O2	-7.30	116.79	121.90
35	a	1071	C	C6-N1-C2	-7.29	117.39	120.30
1	A	1956	U	N3-C2-O2	-7.29	117.10	122.20
1	A	2507	C	C5-C6-N1	7.28	124.64	121.00
1	A	2025	C	C5-C6-N1	7.27	124.64	121.00
1	A	2794	C	N3-C2-O2	-7.27	116.81	121.90
1	A	2248	C	C2-N1-C1’	7.26	126.79	118.80
1	A	2616	C	C5-C6-N1	7.25	124.62	121.00
1	A	1437	C	C2-N1-C1’	7.25	126.77	118.80
38	d	158	LEU	CA-CB-CG	7.22	131.91	115.30
1	A	373	U	N3-C2-O2	-7.22	117.14	122.20
1	A	924	G	N9-C4-C5	7.21	108.28	105.40
35	a	611	C	N1-C2-O2	7.21	123.22	118.90
1	A	2611	C	C6-N1-C2	-7.21	117.42	120.30
57	x	31	C	C2-N1-C1’	7.21	126.72	118.80
35	a	221	C	C2-N1-C1’	7.20	126.72	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	x	3	G	P-O3'-C3'	7.19	128.33	119.70
30	3	61	LEU	CA-CB-CG	7.17	131.80	115.30
1	A	623	C	C5-C6-N1	7.16	124.58	121.00
35	a	1203	C	N3-C2-O2	-7.16	116.89	121.90
1	A	1071	G	C4-N9-C1'	-7.15	117.20	126.50
2	B	12	C	O4'-C1'-N1	7.15	113.92	108.20
1	A	859	G	P-O3'-C3'	7.15	128.28	119.70
1	A	2636	C	N1-C2-O2	7.12	123.17	118.90
1	A	1348	C	N3-C2-O2	-7.12	116.92	121.90
1	A	1578	U	N1-C2-O2	7.11	127.78	122.80
1	A	783	A	C4-C5-N7	7.11	114.25	110.70
35	a	1120	C	N3-C2-O2	-7.10	116.93	121.90
1	A	425	G	C4-C5-N7	7.10	113.64	110.80
1	A	624	C	C6-N1-C2	-7.09	117.46	120.30
1	A	1658	C	C5-C6-N1	7.09	124.55	121.00
1	A	2442	C	C6-N1-C2	-7.09	117.47	120.30
1	A	510	C	C2-N1-C1'	7.08	126.59	118.80
35	a	341	C	C5-C6-N1	7.08	124.54	121.00
1	A	2260	C	C6-N1-C2	-7.07	117.47	120.30
1	A	1716	U	C5-C6-N1	7.07	126.24	122.70
35	a	979	C	N1-C2-O2	7.07	123.14	118.90
35	a	1314	C	C5-C6-N1	7.07	124.53	121.00
1	A	640	C	C6-N1-C2	-7.05	117.48	120.30
1	A	2006	C	C6-N1-C2	-7.05	117.48	120.30
1	A	82	U	N1-C2-O2	7.05	127.73	122.80
1	A	1178	C	C2-N1-C1'	7.04	126.55	118.80
35	a	674	G	N7-C8-N9	7.04	116.62	113.10
1	A	2214	C	N1-C2-O2	7.04	123.12	118.90
35	a	516	U	C5-C4-O4	7.04	130.12	125.90
2	B	35	C	N3-C2-O2	-7.03	116.98	121.90
1	A	1081	U	C2-N1-C1'	7.03	126.14	117.70
1	A	550	C	C6-N1-C2	-7.03	117.49	120.30
1	A	854	C	C6-N1-C2	-7.03	117.49	120.30
35	a	1406	U	N1-C2-O2	7.02	127.72	122.80
1	A	550	C	C6-N1-C1'	-7.01	112.39	120.80
1	A	1044	C	N3-C2-O2	-7.01	116.99	121.90
1	A	1771	C	C5-C6-N1	7.01	124.50	121.00
1	A	1924	C	C6-N1-C2	-7.01	117.50	120.30
1	A	1760	C	C5-C6-N1	7.01	124.50	121.00
35	a	35	G	C8-N9-C1'	-7.01	117.89	127.00
1	A	339	U	C5-C6-N1	7.00	126.20	122.70
1	A	2178	C	C6-N1-C2	-7.00	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	1535	C	C6-N1-C2	-7.00	117.50	120.30
1	A	1343	G	C8-N9-C1'	-6.99	117.92	127.00
1	A	1006	C	C6-N1-C2	-6.98	117.51	120.30
1	A	2474	U	N3-C2-O2	-6.98	117.31	122.20
1	A	1267	U	N1-C2-O2	6.98	127.69	122.80
35	a	737	C	C5-C6-N1	6.98	124.49	121.00
57	x	2	G	P-O3'-C3'	6.96	128.06	119.70
1	A	867	C	N1-C2-O2	6.96	123.07	118.90
1	A	158	U	N1-C2-O2	6.95	127.67	122.80
1	A	1437	C	C6-N1-C2	-6.95	117.52	120.30
1	A	991	C	C6-N1-C2	-6.95	117.52	120.30
1	A	623	C	C6-N1-C2	-6.95	117.52	120.30
1	A	1349	C	C2-N1-C1'	6.95	126.44	118.80
1	A	2192	U	N1-C2-O2	6.95	127.66	122.80
35	a	503	C	C6-N1-C2	-6.95	117.52	120.30
1	A	2515	C	C5-C6-N1	6.94	124.47	121.00
2	B	12	C	C6-N1-C1'	-6.94	112.47	120.80
1	A	2063	C	C6-N1-C2	-6.94	117.52	120.30
2	B	12	C	N1-C2-O2	6.94	123.06	118.90
1	A	1917	U	C5-C4-O4	6.94	130.06	125.90
35	a	436	C	N1-C2-O2	6.92	123.06	118.90
35	a	1518	A	N7-C8-N9	6.92	117.26	113.80
1	A	1005	C	C6-N1-C2	-6.92	117.53	120.30
1	A	1233	C	C6-N1-C2	-6.92	117.53	120.30
2	B	26	C	C6-N1-C2	-6.91	117.53	120.30
1	A	82	U	N3-C2-O2	-6.91	117.36	122.20
1	A	747	C	N1-C2-O2	6.90	123.04	118.90
57	x	32	C	C6-N1-C2	-6.90	117.54	120.30
1	A	2075	U	N3-C4-O4	6.89	124.22	119.40
35	a	679	C	C6-N1-C2	-6.89	117.54	120.30
1	A	1022	G	P-O3'-C3'	6.89	127.96	119.70
35	a	207	C	C2-N1-C1'	6.88	126.36	118.80
1	A	2683	C	N1-C2-O2	6.86	123.02	118.90
35	a	1460	C	C6-N1-C2	-6.86	117.56	120.30
1	A	2424	C	N1-C2-O2	6.85	123.01	118.90
35	a	826	C	C2-N1-C1'	6.85	126.34	118.80
35	a	436	C	N3-C2-O2	-6.85	117.10	121.90
1	A	2192	U	N3-C2-O2	-6.85	117.40	122.20
1	A	373	U	N1-C2-O2	6.84	127.59	122.80
1	A	1130	U	P-O3'-C3'	6.84	127.91	119.70
1	A	372	G	P-O3'-C3'	6.84	127.90	119.70
1	A	1071	G	N3-C4-N9	-6.84	121.90	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	1158	C	C2-N1-C1'	6.84	126.32	118.80
1	A	234	U	N1-C2-O2	6.83	127.58	122.80
1	A	343	C	C5-C6-N1	6.83	124.41	121.00
1	A	1343	G	C4-N9-C1'	6.83	135.37	126.50
35	a	472	U	N3-C2-O2	-6.82	117.43	122.20
1	A	948	C	C6-N1-C2	-6.82	117.57	120.30
35	a	516	U	C2-N1-C1'	6.81	125.88	117.70
13	M	70	ASP	CB-CG-OD1	6.80	124.42	118.30
35	a	1001	C	C5-C6-N1	6.79	124.40	121.00
1	A	2840	C	C6-N1-C2	-6.79	117.58	120.30
35	a	1086	U	N3-C2-O2	-6.79	117.45	122.20
1	A	858	G	P-O3'-C3'	6.79	127.85	119.70
35	a	1382	C	C6-N1-C2	-6.78	117.59	120.30
1	A	2254	C	N1-C2-O2	6.78	122.97	118.90
35	a	979	C	N3-C2-O2	-6.78	117.16	121.90
1	A	640	C	C5-C6-N1	6.77	124.39	121.00
1	A	2066	C	C6-N1-C2	-6.77	117.59	120.30
2	B	37	C	N3-C2-O2	-6.77	117.16	121.90
1	A	2815	C	C6-N1-C2	-6.76	117.59	120.30
35	a	1300	G	P-O3'-C3'	6.76	127.81	119.70
1	A	1443	U	C5-C6-N1	6.76	126.08	122.70
1	A	1020	A	P-O3'-C3'	6.75	127.80	119.70
1	A	1761	C	C5-C6-N1	6.75	124.37	121.00
35	a	470	C	C5-C6-N1	6.74	124.37	121.00
1	A	1053	C	C6-N1-C2	-6.74	117.61	120.30
1	A	2592	G	N3-C4-N9	6.74	130.04	126.00
35	a	1202	U	N3-C2-O2	-6.74	117.48	122.20
1	A	237	C	C6-N1-C2	-6.72	117.61	120.30
1	A	193	U	N3-C2-O2	-6.71	117.50	122.20
35	a	551	U	C5-C6-N1	6.71	126.05	122.70
1	A	2515	C	C6-N1-C2	-6.71	117.62	120.30
1	A	528	A	C2-N3-C4	-6.69	107.26	110.60
1	A	1104	C	C2-N1-C1'	6.69	126.15	118.80
1	A	2504	U	C6-N1-C1'	-6.69	111.84	121.20
35	a	1406	U	N3-C2-O2	-6.68	117.52	122.20
2	B	70	C	C6-N1-C2	-6.68	117.63	120.30
35	a	317	U	C5-C6-N1	6.67	126.04	122.70
35	a	467	U	N1-C2-O2	6.67	127.47	122.80
1	A	1294	U	N1-C2-O2	6.67	127.47	122.80
35	a	972	C	C5-C6-N1	6.67	124.33	121.00
1	A	2192	U	C5-C4-O4	-6.67	121.90	125.90
16	P	113	LEU	CA-CB-CG	6.67	130.63	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	341	C	C6-N1-C2	-6.67	117.63	120.30
1	A	2511	U	C5-C6-N1	6.66	126.03	122.70
1	A	1771	C	C6-N1-C2	-6.66	117.64	120.30
1	A	2794	C	N1-C2-O2	6.64	122.89	118.90
1	A	2889	C	C5-C6-N1	6.64	124.32	121.00
1	A	1130	U	N3-C4-O4	6.63	124.04	119.40
35	a	1518	A	C8-N9-C4	-6.63	103.15	105.80
1	A	1914	C	C6-N1-C2	-6.63	117.65	120.30
1	A	2443	C	N1-C2-O2	6.63	122.88	118.90
1	A	2806	C	C5-C6-N1	6.62	124.31	121.00
35	a	132	C	C6-N1-C2	-6.62	117.65	120.30
35	a	1001	C	C6-N1-C2	-6.62	117.65	120.30
1	A	2473	U	C5-C6-N1	6.62	126.01	122.70
1	A	157	C	C5-C6-N1	6.61	124.31	121.00
35	a	272	C	C6-N1-C2	-6.61	117.66	120.30
1	A	1914	C	C6-N1-C1'	-6.60	112.88	120.80
1	A	1941	C	N3-C2-O2	-6.60	117.28	121.90
1	A	1964	G	N3-C4-N9	-6.60	122.04	126.00
35	a	1030	U	N1-C2-O2	6.59	127.42	122.80
1	A	585	G	N3-C4-C5	-6.59	125.30	128.60
1	A	1940	U	P-O3'-C3'	6.59	127.61	119.70
35	a	960	U	P-O3'-C3'	6.59	127.61	119.70
1	A	1993	U	N3-C2-O2	-6.58	117.59	122.20
1	A	2872	A	C8-N9-C4	-6.58	103.17	105.80
35	a	471	U	C5-C6-N1	6.58	125.99	122.70
35	a	623	C	C6-N1-C2	-6.58	117.67	120.30
1	A	243	U	N1-C2-O2	6.57	127.40	122.80
35	a	1172	C	C5-C6-N1	6.57	124.28	121.00
1	A	2161	C	C2-N1-C1'	6.57	126.03	118.80
1	A	2805	C	C6-N1-C2	-6.57	117.67	120.30
35	a	132	C	C2-N1-C1'	6.57	126.02	118.80
35	a	1158	C	N1-C2-O2	6.57	122.84	118.90
35	a	1203	C	C2-N1-C1'	6.56	126.02	118.80
35	a	219	U	N1-C2-O2	6.56	127.39	122.80
35	a	103	U	N3-C2-O2	-6.55	117.61	122.20
1	A	2666	C	N3-C2-O2	-6.55	117.31	121.90
1	A	373	U	C5-C6-N1	6.55	125.97	122.70
1	A	1313	U	C6-N1-C1'	-6.55	112.03	121.20
1	A	1378	A	P-O3'-C3'	6.55	127.56	119.70
1	A	1446	C	C6-N1-C2	-6.54	117.68	120.30
35	a	1027	C	C6-N1-C2	-6.54	117.68	120.30
35	a	556	C	C5-C6-N1	6.54	124.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2076	U	N1-C2-O2	6.53	127.37	122.80
35	a	1008	U	N3-C2-O2	-6.53	117.63	122.20
1	A	1611	C	C5-C6-N1	6.53	124.27	121.00
1	A	2822	G	C4-C5-N7	6.53	113.41	110.80
1	A	2724	U	N3-C2-O2	-6.53	117.63	122.20
35	a	1059	C	C6-N1-C2	-6.53	117.69	120.30
1	A	898	C	C6-N1-C2	-6.52	117.69	120.30
35	a	1427	C	C6-N1-C2	-6.52	117.69	120.30
35	a	792	A	O4'-C1'-N9	6.52	113.42	108.20
1	A	1541	C	C6-N1-C2	-6.52	117.69	120.30
1	A	2720	U	N1-C2-O2	6.52	127.36	122.80
1	A	1345	C	C6-N1-C2	-6.51	117.69	120.30
35	a	643	C	C6-N1-C2	-6.51	117.70	120.30
35	a	737	C	C6-N1-C2	-6.51	117.69	120.30
35	a	469	C	N3-C2-O2	-6.51	117.34	121.90
1	A	2752	C	N1-C2-O2	6.50	122.80	118.90
35	a	1098	C	C5-C6-N1	6.50	124.25	121.00
1	A	67	U	C5-C4-O4	-6.50	122.00	125.90
1	A	11	C	N1-C2-O2	6.50	122.80	118.90
1	A	992	C	C6-N1-C2	-6.50	117.70	120.30
1	A	1340	U	N3-C2-O2	-6.50	117.65	122.20
1	A	2103	C	C5-C6-N1	6.50	124.25	121.00
35	a	744	C	C6-N1-C2	-6.50	117.70	120.30
35	a	1297	G	P-O3'-C3'	6.49	127.49	119.70
1	A	2192	U	C5-C6-N1	6.49	125.94	122.70
1	A	1135	C	N1-C2-O2	6.49	122.79	118.90
1	A	2129	C	C5-C6-N1	6.48	124.24	121.00
35	a	1317	C	N3-C2-O2	-6.48	117.37	121.90
1	A	1005	C	C2-N1-C1'	6.46	125.91	118.80
1	A	198	C	C5-C6-N1	6.46	124.23	121.00
1	A	1379	U	N3-C2-O2	-6.46	117.68	122.20
35	a	1403	C	C6-N1-C2	-6.46	117.72	120.30
1	A	2424	C	C6-N1-C2	-6.45	117.72	120.30
35	a	1109	C	C2-N1-C1'	6.45	125.90	118.80
1	A	1752	C	C5-C6-N1	6.45	124.22	121.00
57	x	64	C	C6-N1-C2	-6.44	117.72	120.30
1	A	544	C	N3-C2-O2	-6.44	117.39	121.90
35	a	739	C	C6-N1-C2	-6.44	117.72	120.30
35	a	529	G	N1-C6-O6	6.43	123.76	119.90
1	A	2137	U	N1-C2-O2	6.43	127.30	122.80
1	A	305	C	C6-N1-C2	-6.43	117.73	120.30
1	A	82	U	C2-N1-C1'	6.42	125.41	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	C	OP1-P-O3'	6.42	119.33	105.20
1	A	1340	U	C2-N1-C1'	6.42	125.41	117.70
1	A	158	U	C2-N1-C1'	6.41	125.39	117.70
35	a	931	C	C2-N1-C1'	6.41	125.85	118.80
1	A	1836	C	C5-C6-N1	6.41	124.20	121.00
57	x	27	C	C6-N1-C2	-6.41	117.74	120.30
35	a	456	A	N1-C6-N6	6.41	122.44	118.60
1	A	157	C	C6-N1-C2	-6.40	117.74	120.30
35	a	1314	C	C6-N1-C2	-6.40	117.74	120.30
1	A	135	U	C2-N1-C1'	6.40	125.38	117.70
35	a	1201	A	P-O3'-C3'	6.39	127.37	119.70
35	a	931	C	C5-C6-N1	6.39	124.20	121.00
1	A	1370	C	C6-N1-C2	-6.39	117.74	120.30
1	A	746	U	N1-C2-O2	6.39	127.27	122.80
35	a	1375	A	C8-N9-C4	-6.39	103.25	105.80
1	A	1314	C	N1-C2-O2	6.39	122.73	118.90
1	A	2292	U	C5-C6-N1	6.38	125.89	122.70
1	A	669	G	C4-N9-C1'	6.38	134.79	126.50
1	A	2137	U	N3-C2-O2	-6.38	117.74	122.20
38	d	4	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	510	C	N1-C2-O2	6.37	122.72	118.90
1	A	1911	U	C2-N1-C1'	6.37	125.35	117.70
35	a	472	U	N1-C2-O2	6.37	127.26	122.80
35	a	110	C	N3-C2-O2	-6.36	117.45	121.90
1	A	2834	G	C8-N9-C4	-6.36	103.86	106.40
1	A	1319	C	C6-N1-C2	-6.36	117.76	120.30
1	A	2065	C	C5-C6-N1	6.36	124.18	121.00
35	a	25	C	C5-C6-N1	6.35	124.18	121.00
1	A	901	C	N3-C2-O2	-6.35	117.45	121.90
2	B	77	U	N1-C2-O2	6.35	127.24	122.80
35	a	1158	C	N3-C2-O2	-6.35	117.46	121.90
1	A	2161	C	C5-C6-N1	6.34	124.17	121.00
1	A	1092	C	C5-C6-N1	6.34	124.17	121.00
35	a	439	U	C5-C6-N1	6.34	125.87	122.70
1	A	2043	C	N1-C2-O2	6.34	122.70	118.90
1	A	1716	U	C2-N1-C1'	6.34	125.31	117.70
35	a	1190	G	P-O3'-C3'	6.33	127.30	119.70
35	a	476	U	N3-C4-O4	-6.33	114.97	119.40
1	A	1314	C	C6-N1-C1'	-6.33	113.21	120.80
1	A	867	C	N3-C2-O2	-6.33	117.47	121.90
35	a	455	G	N1-C6-O6	-6.33	116.10	119.90
35	a	486	U	N3-C2-O2	-6.32	117.77	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1920	C	C6-N1-C2	-6.32	117.77	120.30
1	A	405	U	C6-N1-C1'	-6.32	112.35	121.20
1	A	854	C	N1-C2-N3	6.32	123.62	119.20
1	A	2649	C	N1-C2-O2	6.32	122.69	118.90
1	A	1081	U	N1-C2-O2	6.31	127.22	122.80
1	A	1379	U	O5'-P-OP2	-6.31	100.02	105.70
1	A	2104	C	C6-N1-C2	-6.31	117.78	120.30
1	A	737	C	C6-N1-C2	-6.31	117.78	120.30
1	A	2075	U	C5-C4-O4	-6.30	122.12	125.90
1	A	974	G	C4-N9-C1'	6.30	134.69	126.50
2	B	89	U	OP1-P-OP2	-6.30	110.14	119.60
1	A	353	C	N1-C2-O2	6.30	122.68	118.90
1	A	859	G	OP2-P-O3'	6.30	119.06	105.20
2	B	77	U	N3-C2-O2	-6.30	117.79	122.20
35	a	529	G	C6-C5-N7	-6.30	126.62	130.40
1	A	2342	C	N3-C2-O2	-6.30	117.49	121.90
35	a	1043	G	N3-C2-N2	-6.30	115.49	119.90
35	a	1182	G	P-O3'-C3'	6.30	127.26	119.70
35	a	1132	C	C6-N1-C2	-6.29	117.78	120.30
1	A	1071	G	N3-C4-C5	6.28	131.74	128.60
1	A	2394	C	N1-C2-O2	6.28	122.67	118.90
35	a	1249	C	C6-N1-C2	-6.28	117.79	120.30
1	A	2044	C	C6-N1-C2	-6.27	117.79	120.30
1	A	2124	G	C4-N9-C1'	6.27	134.65	126.50
1	A	2137	U	C2-N1-C1'	6.27	125.22	117.70
35	a	467	U	N3-C2-O2	-6.27	117.81	122.20
35	a	754	C	C2-N1-C1'	6.27	125.69	118.80
1	A	405	U	C5-C6-N1	6.27	125.83	122.70
1	A	208	C	C5-C6-N1	6.26	124.13	121.00
1	A	1360	G	N3-C4-N9	6.25	129.75	126.00
35	a	735	C	C6-N1-C2	-6.25	117.80	120.30
1	A	1855	U	C5-C6-N1	6.25	125.82	122.70
35	a	219	U	N3-C2-O2	-6.24	117.83	122.20
1	A	974	G	C6-C5-N7	-6.24	126.66	130.40
35	a	1118	U	N3-C2-O2	-6.24	117.83	122.20
1	A	632	A	N7-C8-N9	6.24	116.92	113.80
1	A	1294	U	N3-C2-O2	-6.23	117.84	122.20
1	A	2008	C	C6-N1-C2	-6.22	117.81	120.30
1	A	2043	C	C6-N1-C2	-6.22	117.81	120.30
35	a	1317	C	N1-C2-O2	6.22	122.63	118.90
1	A	1005	C	C5-C6-N1	6.21	124.11	121.00
1	A	1142	A	N3-C4-C5	6.21	131.15	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1656	C	C6-N1-C2	-6.21	117.82	120.30
35	a	169	C	N1-C2-O2	6.21	122.63	118.90
35	a	379	C	C5-C6-N1	6.21	124.10	121.00
1	A	1414	C	C2-N1-C1'	6.20	125.62	118.80
35	a	1347	G	P-O3'-C3'	6.20	127.14	119.70
35	a	478	A	C8-N9-C4	-6.19	103.32	105.80
35	a	1436	U	C5-C6-N1	6.18	125.79	122.70
1	A	2552	U	C2-N1-C1'	6.18	125.12	117.70
35	a	1132	C	C5-C6-N1	6.18	124.09	121.00
1	A	1349	C	N3-C4-C5	-6.18	119.43	121.90
35	a	514	C	C5-C6-N1	6.18	124.09	121.00
1	A	2605	U	C6-N1-C1'	-6.17	112.56	121.20
1	A	242	G	P-O3'-C3'	6.17	127.10	119.70
35	a	37	U	N3-C2-O2	-6.16	117.89	122.20
35	a	1109	C	N1-C2-O2	6.16	122.59	118.90
35	a	472	U	C2-N1-C1'	6.16	125.09	117.70
1	A	746	U	N3-C2-O2	-6.16	117.89	122.20
35	a	438	U	P-O3'-C3'	6.16	127.09	119.70
1	A	2047	C	C5-C6-N1	6.15	124.08	121.00
1	A	2666	C	C5-C6-N1	6.15	124.08	121.00
2	B	3	C	C6-N1-C2	-6.15	117.84	120.30
35	a	1030	U	N3-C2-O2	-6.15	117.90	122.20
1	A	1071	G	C8-N9-C1'	6.15	134.99	127.00
1	A	1060	U	N1-C2-O2	6.14	127.10	122.80
1	A	1323	C	N1-C2-O2	6.14	122.58	118.90
35	a	528	C	N3-C2-O2	-6.14	117.60	121.90
1	A	2822	G	C6-C5-N7	-6.14	126.72	130.40
1	A	1658	C	C6-N1-C2	-6.14	117.85	120.30
1	A	2678	C	C5-C6-N1	6.13	124.07	121.00
2	B	110	C	C6-N1-C2	-6.13	117.85	120.30
35	a	899	C	C6-N1-C2	-6.13	117.85	120.30
35	a	924	C	C6-N1-C2	-6.13	117.85	120.30
1	A	948	C	C5-C6-N1	6.13	124.06	121.00
1	A	2552	U	N3-C2-O2	-6.12	117.92	122.20
35	a	1348	U	N1-C2-O2	6.12	127.09	122.80
35	a	358	U	C6-N1-C2	-6.12	117.33	121.00
2	B	52	A	P-O3'-C3'	6.11	127.03	119.70
1	A	607	U	N3-C2-O2	-6.11	117.92	122.20
1	A	955	U	N1-C2-O2	6.11	127.08	122.80
1	A	2591	C	C6-N1-C2	-6.11	117.86	120.30
1	A	2558	C	C6-N1-C2	-6.11	117.86	120.30
35	a	157	U	N3-C2-O2	-6.11	117.93	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	f	74	LEU	CB-CG-CD1	-6.10	100.63	111.00
1	A	2493	U	C5-C4-O4	-6.09	122.25	125.90
1	A	2506	U	C6-N1-C1’	-6.09	112.67	121.20
1	A	2678	C	C6-N1-C2	-6.09	117.86	120.30
35	a	280	C	P-O3’-C3’	6.09	127.01	119.70
1	A	1398	C	C2-N1-C1’	6.09	125.49	118.80
35	a	87	C	C2-N1-C1’	6.09	125.50	118.80
35	a	436	C	C6-N1-C2	-6.08	117.87	120.30
1	A	2254	C	N3-C2-O2	-6.08	117.64	121.90
1	A	2026	U	C5-C6-N1	6.08	125.74	122.70
1	A	2103	C	C6-N1-C2	-6.08	117.87	120.30
1	A	2506	U	C5-C6-N1	6.08	125.74	122.70
1	A	459	U	N1-C2-O2	6.07	127.05	122.80
35	a	611	C	C6-N1-C2	-6.07	117.87	120.30
1	A	2566	A	P-O3’-C3’	6.07	126.98	119.70
35	a	826	C	N1-C2-O2	6.07	122.54	118.90
1	A	2464	G	N3-C4-N9	6.07	129.64	126.00
40	f	13	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	838	C	C2-N1-C1’	6.06	125.47	118.80
1	A	1180	U	C2-N1-C1’	6.06	124.97	117.70
1	A	1760	C	C6-N1-C2	-6.06	117.88	120.30
1	A	1795	C	C5-C6-N1	6.06	124.03	121.00
1	A	1911	U	N1-C2-O2	6.06	127.04	122.80
35	a	674	G	C8-N9-C4	-6.06	103.98	106.40
35	a	955	U	N3-C2-O2	-6.06	117.96	122.20
1	A	2267	A	N1-C6-N6	-6.05	114.97	118.60
1	A	243	U	C2-N1-C1’	6.05	124.96	117.70
1	A	2185	U	C6-N1-C2	-6.04	117.38	121.00
35	a	207	C	N1-C2-O2	6.04	122.52	118.90
35	a	1138	G	C4-N9-C1’	6.04	134.35	126.50
1	A	1993	U	C5-C6-N1	6.03	125.72	122.70
57	x	31	C	C5-C6-N1	6.03	124.02	121.00
57	x	31	C	C6-N1-C2	-6.03	117.89	120.30
35	a	800	G	C6-C5-N7	-6.03	126.78	130.40
35	a	931	C	C6-N1-C2	-6.03	117.89	120.30
1	A	1208	C	C2-N1-C1’	6.03	125.43	118.80
35	a	87	C	N1-C2-O2	6.03	122.52	118.90
35	a	858	G	C4-N9-C1’	6.03	134.33	126.50
1	A	1345	C	N3-C2-O2	-6.02	117.68	121.90
1	A	550	C	N3-C4-N4	6.02	122.22	118.00
35	a	611	C	C5-C6-N1	6.02	124.01	121.00
35	a	107	G	N1-C6-O6	-6.02	116.29	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	1172	C	C6-N1-C2	-6.02	117.89	120.30
1	A	1752	C	C6-N1-C2	-6.01	117.89	120.30
35	a	738	C	C6-N1-C2	-6.01	117.89	120.30
35	a	1086	U	C2-N1-C1'	6.01	124.91	117.70
35	a	284	C	C5-C6-N1	6.00	124.00	121.00
35	a	624	C	C6-N1-C2	-5.99	117.91	120.30
1	A	2044	C	C5-C6-N1	5.99	123.99	121.00
2	B	47	C	C6-N1-C2	-5.99	117.91	120.30
35	a	1460	C	C5-C6-N1	5.99	123.99	121.00
1	A	192	C	N1-C2-O2	5.98	122.49	118.90
35	a	841	C	N1-C2-O2	5.98	122.49	118.90
35	a	406	G	C5-C6-O6	-5.98	125.01	128.60
1	A	151	C	C5-C6-N1	5.98	123.99	121.00
35	a	358	U	C2-N1-C1'	5.98	124.88	117.70
1	A	776	G	C4-N9-C1'	5.97	134.26	126.50
1	A	806	C	C6-N1-C2	-5.97	117.91	120.30
1	A	1142	A	C2-N3-C4	-5.97	107.61	110.60
1	A	2752	C	C5-C6-N1	5.97	123.99	121.00
1	A	1221	C	C2-N1-C1'	5.97	125.36	118.80
1	A	717	C	N1-C2-O2	5.96	122.48	118.90
1	A	1414	C	N1-C2-O2	5.96	122.48	118.90
1	A	2354	C	C2-N1-C1'	5.96	125.36	118.80
35	a	735	C	C5-C6-N1	5.96	123.98	121.00
1	A	2473	U	C6-N1-C2	-5.96	117.43	121.00
35	a	948	C	C5-C6-N1	5.96	123.98	121.00
35	a	1348	U	C2-N1-C1'	5.95	124.84	117.70
35	a	674	G	N3-C4-C5	-5.95	125.62	128.60
1	A	1574	C	C5-C6-N1	5.95	123.97	121.00
1	A	236	C	C6-N1-C2	-5.95	117.92	120.30
35	a	516	U	N3-C4-O4	-5.94	115.24	119.40
35	a	961	U	C5-C6-N1	5.94	125.67	122.70
1	A	2832	U	N3-C2-O2	-5.94	118.04	122.20
35	a	295	C	C5-C6-N1	5.94	123.97	121.00
1	A	543	G	C5-C6-O6	-5.94	125.04	128.60
1	A	624	C	C5-C6-N1	5.94	123.97	121.00
1	A	2078	C	C5-C6-N1	5.94	123.97	121.00
35	a	948	C	C6-N1-C2	-5.94	117.92	120.30
35	a	1333	A	C2-N3-C4	5.94	113.57	110.60
35	a	1538	C	C6-N1-C2	-5.94	117.92	120.30
1	A	1437	C	N1-C2-O2	5.93	122.46	118.90
35	a	674	G	C4-N9-C1'	5.93	134.22	126.50
35	a	896	C	C5-C6-N1	5.93	123.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1414	C	C5-C6-N1	5.93	123.97	121.00
1	A	2636	C	N3-C2-O2	-5.93	117.75	121.90
35	a	1109	C	N3-C2-O2	-5.93	117.75	121.90
35	a	1440	U	C2-N1-C1'	5.93	124.82	117.70
46	l	22	ALA	N-CA-C	-5.93	94.98	111.00
35	a	333	U	C5-C4-O4	-5.92	122.34	125.90
1	A	2393	U	N3-C2-O2	-5.92	118.05	122.20
1	A	353	C	C6-N1-C2	-5.92	117.93	120.30
1	A	1198	U	N3-C2-O2	-5.92	118.06	122.20
35	a	69	G	C4-N9-C1'	5.92	134.19	126.50
1	A	1902	C	C5-C6-N1	5.92	123.96	121.00
35	a	1518	A	O4'-C1'-N9	5.92	112.93	108.20
1	A	955	U	O4'-C1'-N1	5.91	112.93	108.20
2	B	4	C	N1-C2-O2	5.91	122.45	118.90
1	A	517	C	C6-N1-C2	-5.91	117.94	120.30
1	A	475	C	C6-N1-C2	-5.91	117.94	120.30
1	A	1409	U	N3-C2-O2	-5.90	118.07	122.20
1	A	1887	C	C5-C6-N1	5.90	123.95	121.00
1	A	1319	C	C5-C6-N1	5.89	123.95	121.00
35	a	379	C	C6-N1-C2	-5.89	117.94	120.30
35	a	1306	A	C5-N7-C8	-5.89	100.95	103.90
1	A	2072	C	N1-C2-O2	5.89	122.43	118.90
1	A	2872	A	N7-C8-N9	5.88	116.74	113.80
35	a	1496	C	C6-N1-C2	-5.88	117.95	120.30
35	a	1225	A	C4-N9-C1'	5.88	136.88	126.30
35	a	611	C	N3-C2-O2	-5.88	117.79	121.90
57	x	55	U	C2-N1-C1'	5.87	124.75	117.70
1	A	1714	U	C5-C6-N1	5.87	125.64	122.70
1	A	2244	U	N3-C4-O4	5.87	123.51	119.40
57	x	3	G	C4-C5-N7	5.87	113.15	110.80
1	A	1675	C	N1-C2-O2	5.87	122.42	118.90
1	A	817	C	C6-N1-C2	-5.87	117.95	120.30
1	A	1178	C	N1-C2-O2	5.87	122.42	118.90
1	A	2576	G	C2-N3-C4	5.86	114.83	111.90
1	A	2646	C	C4-C5-C6	-5.86	114.47	117.40
2	B	17	C	C6-N1-C2	-5.86	117.96	120.30
1	A	458	G	P-O3'-C3'	5.86	126.73	119.70
1	A	2832	U	N1-C2-O2	5.86	126.90	122.80
35	a	1294	G	N3-C4-N9	5.86	129.51	126.00
1	A	2477	U	C5-C6-N1	5.85	125.63	122.70
1	A	392	U	N3-C2-O2	-5.85	118.10	122.20
1	A	549	G	C8-N9-C4	-5.85	104.06	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	a	1493	A	O4'-C1'-N9	5.85	112.88	108.20
35	a	486	U	N1-C2-O2	5.85	126.89	122.80
46	l	43	LYS	N-CA-C	5.85	126.79	111.00
35	a	916	U	C5-C6-N1	5.85	125.62	122.70
1	A	1103	A	OP1-P-O3'	5.84	118.06	105.20
1	A	898	C	C2-N3-C4	5.84	122.82	119.90
1	A	222	A	O4'-C1'-N9	-5.84	103.53	108.20
1	A	2655	G	OP2-P-O3'	5.84	118.05	105.20
1	A	1326	U	N1-C2-O2	5.84	126.89	122.80
35	a	290	C	C5-C6-N1	5.84	123.92	121.00
1	A	1894	C	N1-C2-O2	5.84	122.40	118.90
35	a	989	U	N3-C2-O2	-5.84	118.11	122.20
1	A	227	A	P-O3'-C3'	5.83	126.70	119.70
35	a	991	U	C2-N1-C1'	5.83	124.70	117.70
35	a	1183	U	OP1-P-O3'	5.83	118.03	105.20
35	a	563	A	C4-N9-C1'	5.83	136.79	126.30
1	A	1267	U	C5-C6-N1	5.82	125.61	122.70
1	A	2588	G	C4-C5-N7	5.82	113.13	110.80
1	A	459	U	C2-N1-C1'	5.82	124.68	117.70
1	A	1130	U	C5-C4-O4	-5.82	122.41	125.90
1	A	654	A	C4-N9-C1'	5.81	136.76	126.30
1	A	2063	C	C6-N1-C1'	-5.81	113.83	120.80
1	A	358	U	C5-C6-N1	5.81	125.60	122.70
2	B	88	C	OP1-P-O3'	5.81	117.97	105.20
1	A	1208	C	C6-N1-C2	-5.80	117.98	120.30
1	A	2805	C	N1-C2-O2	5.80	122.38	118.90
1	A	235	U	N1-C2-O2	5.80	126.86	122.80
1	A	999	U	N3-C2-O2	-5.80	118.14	122.20
1	A	550	C	C5-C4-N4	-5.79	116.15	120.20
1	A	34	U	N1-C2-O2	5.79	126.85	122.80
1	A	1049	C	N1-C2-O2	5.79	122.37	118.90
1	A	198	C	C2-N1-C1'	5.79	125.17	118.80
1	A	860	U	C5-C6-N1	5.79	125.59	122.70
1	A	2105	U	C2-N1-C1'	5.79	124.64	117.70
35	a	284	C	C6-N1-C2	-5.78	117.99	120.30
35	a	1383	C	N1-C2-O2	5.78	122.37	118.90
1	A	1053	C	C5-C6-N1	5.77	123.89	121.00
1	A	2822	G	C5-C6-O6	-5.77	125.14	128.60
57	x	55	U	N3-C2-O2	-5.77	118.16	122.20
32	5	59	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	2063	C	C5-C6-N1	5.76	123.88	121.00
1	A	2494	G	C5-C6-O6	-5.76	125.14	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2395	C	C5-C6-N1	5.76	123.88	121.00
35	a	931	C	N1-C2-O2	5.76	122.36	118.90
1	A	898	C	N1-C2-O2	5.75	122.35	118.90
35	a	11	G	N3-C4-N9	5.75	129.45	126.00
35	a	439	U	C2-N1-C1’	5.75	124.61	117.70
1	A	1788	C	C5-C6-N1	5.75	123.88	121.00
2	B	31	C	C6-N1-C2	-5.75	118.00	120.30
1	A	731	C	C6-N1-C2	-5.75	118.00	120.30
1	A	39	G	C4-N9-C1’	5.74	133.96	126.50
1	A	1326	U	N3-C2-O2	-5.74	118.18	122.20
1	A	2762	C	C6-N1-C2	-5.74	118.00	120.30
1	A	2827	C	C5-C6-N1	5.74	123.87	121.00
1	A	267	C	C5-C6-N1	5.74	123.87	121.00
1	A	2424	C	C5-C6-N1	5.73	123.86	121.00
1	A	135	U	N3-C2-O2	-5.73	118.19	122.20
35	a	470	C	C2-N1-C1’	5.72	125.09	118.80
1	A	1177	G	C6-C5-N7	-5.72	126.97	130.40
1	A	2161	C	C6-N1-C2	-5.72	118.01	120.30
35	a	1427	C	C5-C6-N1	5.72	123.86	121.00
1	A	114	U	C2-N1-C1’	5.71	124.55	117.70
1	A	2506	U	C6-N1-C2	-5.71	117.57	121.00
35	a	69	G	C8-N9-C1’	-5.71	119.58	127.00
35	a	1253	G	N3-C4-N9	5.70	129.42	126.00
1	A	898	C	C2-N1-C1’	5.70	125.07	118.80
1	A	2464	G	C4-N9-C1’	5.70	133.91	126.50
35	a	1120	C	C6-N1-C2	-5.69	118.02	120.30
2	B	35	C	C6-N1-C2	-5.69	118.02	120.30
35	a	132	C	N1-C2-O2	5.69	122.31	118.90
35	a	1208	C	C6-N1-C2	-5.69	118.03	120.30
1	A	486	C	C6-N1-C2	-5.68	118.03	120.30
1	A	912	C	C2-N1-C1’	5.68	125.05	118.80
35	a	317	U	C6-N1-C2	-5.68	117.59	121.00
1	A	2616	C	N1-C2-O2	5.68	122.31	118.90
35	a	1469	C	N1-C2-O2	5.67	122.31	118.90
1	A	2105	U	N3-C2-O2	-5.67	118.23	122.20
1	A	2228	G	C6-C5-N7	-5.67	127.00	130.40
5	E	81	GLY	N-CA-C	-5.66	98.94	113.10
35	a	1382	C	C2-N1-C1’	5.66	125.03	118.80
1	A	2772	C	C5-C6-N1	5.66	123.83	121.00
44	j	10	LEU	CA-CB-CG	5.66	128.32	115.30
1	A	1352	U	N3-C2-O2	-5.66	118.24	122.20
1	A	1993	U	N1-C2-O2	5.66	126.76	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	985	C	N1-C2-O2	5.65	122.29	118.90
35	a	954	G	N3-C4-C5	-5.65	125.77	128.60
1	A	867	C	C6-N1-C2	-5.65	118.04	120.30
1	A	550	C	N1-C2-O2	5.65	122.29	118.90
1	A	2667	C	C6-N1-C2	-5.64	118.04	120.30
1	A	2135	A	C2-N3-C4	5.64	113.42	110.60
1	A	1994	C	C6-N1-C2	-5.63	118.05	120.30
35	a	11	G	C4-N9-C1'	5.63	133.82	126.50
1	A	141	G	N3-C4-C5	-5.63	125.78	128.60
1	A	67	U	N3-C4-O4	5.63	123.34	119.40
57	x	6	U	N1-C2-O2	5.63	126.74	122.80
1	A	1561	C	N1-C2-O2	5.63	122.28	118.90
1	A	2650	U	C5-C6-N1	5.63	125.51	122.70
35	a	90	C	C6-N1-C2	-5.63	118.05	120.30
57	x	32	C	C2-N1-C1'	5.63	124.99	118.80
1	A	1331	G	N1-C6-O6	-5.62	116.53	119.90
35	a	610	U	N3-C2-O2	-5.62	118.27	122.20
1	A	1923	U	C5-C6-N1	5.62	125.51	122.70
35	a	1203	C	N1-C2-O2	5.62	122.27	118.90
1	A	34	U	N3-C2-O2	-5.61	118.27	122.20
1	A	271	G	O4'-C1'-N9	5.61	112.69	108.20
57	x	55	U	N1-C2-O2	5.61	126.73	122.80
1	A	1964	G	N3-C4-C5	5.61	131.40	128.60
35	a	960	U	N3-C2-O2	-5.61	118.27	122.20
1	A	206	U	C2-N1-C1'	5.61	124.43	117.70
1	A	2464	G	C8-N9-C1'	-5.61	119.71	127.00
35	a	643	C	C5-C6-N1	5.61	123.80	121.00
35	a	1348	U	N3-C2-O2	-5.61	118.28	122.20
1	A	1982	U	C5-C6-N1	5.60	125.50	122.70
2	B	47	C	C5-C6-N1	5.60	123.80	121.00
35	a	175	C	N1-C2-O2	5.60	122.26	118.90
35	a	529	G	C4-C5-N7	5.60	113.04	110.80
35	a	758	C	C6-N1-C2	-5.60	118.06	120.30
1	A	998	C	N3-C4-N4	5.60	121.92	118.00
1	A	2615	U	C2-N1-C1'	5.60	124.42	117.70
2	B	91	C	C6-N1-C2	-5.60	118.06	120.30
1	A	2074	U	O5'-P-OP2	-5.59	100.67	105.70
1	A	1934	C	C5-C6-N1	5.59	123.80	121.00
1	A	193	U	N1-C2-O2	5.59	126.72	122.80
1	A	2185	U	N3-C2-O2	-5.59	118.29	122.20
1	A	1716	U	C6-N1-C2	-5.59	117.65	121.00
1	A	11	C	N3-C2-O2	-5.58	117.99	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2076	U	N3-C2-O2	-5.58	118.29	122.20
1	A	2185	U	C5-C6-N1	5.58	125.49	122.70
1	A	1669	A	C2-N3-C4	5.58	113.39	110.60
1	A	31	C	C5-C6-N1	5.58	123.79	121.00
2	B	26	C	C5-C6-N1	5.57	123.79	121.00
35	a	277	C	C6-N1-C2	-5.57	118.07	120.30
1	A	2825	G	C4-N9-C1’	5.57	133.74	126.50
35	a	611	C	C2-N1-C1’	5.57	124.93	118.80
1	A	143	C	N1-C2-O2	5.57	122.24	118.90
35	a	598	U	N3-C2-O2	-5.57	118.30	122.20
1	A	93	G	C6-C5-N7	-5.57	127.06	130.40
1	A	278	A	C4-N9-C1’	5.57	136.32	126.30
1	A	991	C	C5-C6-N1	5.57	123.78	121.00
1	A	2178	C	N3-C2-O2	-5.57	118.00	121.90
1	A	62	U	C2-N1-C1’	5.56	124.38	117.70
1	A	484	C	N1-C2-O2	5.56	122.23	118.90
1	A	1343	G	N3-C4-N9	5.56	129.33	126.00
1	A	277	G	N3-C4-C5	-5.55	125.82	128.60
1	A	1065	U	N3-C2-O2	-5.55	118.31	122.20
1	A	1911	U	C6-N1-C2	-5.55	117.67	121.00
1	A	1333	G	N3-C4-N9	5.55	129.33	126.00
1	A	2480	C	C6-N1-C2	-5.55	118.08	120.30
35	a	1109	C	C5-C6-N1	5.55	123.77	121.00
1	A	11	C	C6-N1-C2	-5.54	118.08	120.30
1	A	93	G	C4-N9-C1’	5.54	133.70	126.50
57	x	6	U	C6-N1-C1’	-5.54	113.45	121.20
35	a	458	U	N3-C2-O2	-5.53	118.33	122.20
1	A	510	C	C5-C6-N1	5.53	123.77	121.00
1	A	581	C	C5-C6-N1	5.53	123.77	121.00
1	A	912	C	N3-C4-C5	-5.53	119.69	121.90
1	A	1880	U	N1-C2-O2	5.53	126.67	122.80
1	A	759	G	N9-C4-C5	-5.53	103.19	105.40
1	A	2161	C	N3-C2-O2	-5.53	118.03	121.90
1	A	2739	U	N1-C2-O2	5.53	126.67	122.80
1	A	208	C	C6-N1-C2	-5.52	118.09	120.30
1	A	2047	C	C6-N1-C2	-5.52	118.09	120.30
35	a	272	C	C5-C6-N1	5.52	123.76	121.00
1	A	417	C	C2-N1-C1’	5.52	124.87	118.80
1	A	801	G	C4-N9-C1’	-5.52	119.33	126.50
1	A	1081	U	C5-C6-N1	5.52	125.46	122.70
2	B	12	C	C5-C6-N1	5.52	123.76	121.00
35	a	169	C	N3-C2-O2	-5.52	118.04	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	532	A	C5-C6-N6	-5.52	119.29	123.70
35	a	858	G	C8-N9-C1'	-5.51	119.83	127.00
35	a	995	C	N3-C2-O2	-5.51	118.04	121.90
2	B	79	G	C4-N9-C1'	5.51	133.67	126.50
1	A	1663	G	OP2-P-O3'	5.51	117.33	105.20
35	a	1126	U	N3-C2-O2	-5.51	118.34	122.20
1	A	669	G	C8-N9-C1'	-5.51	119.84	127.00
4	D	201	LEU	CB-CG-CD1	-5.50	101.64	111.00
1	A	1101	U	C6-N1-C2	-5.50	117.70	121.00
35	a	1202	U	N1-C2-O2	5.50	126.65	122.80
1	A	237	C	C5-C6-N1	5.49	123.75	121.00
1	A	847	U	N1-C2-O2	5.49	126.64	122.80
35	a	738	C	C5-C6-N1	5.49	123.75	121.00
1	A	1946	U	C5-C6-N1	5.48	125.44	122.70
1	A	2424	C	N3-C2-O2	-5.48	118.06	121.90
1	A	2805	C	C5-C6-N1	5.48	123.74	121.00
35	a	1158	C	C6-N1-C1'	-5.48	114.22	120.80
1	A	1135	C	C2-N1-C1'	5.48	124.83	118.80
1	A	2752	C	C6-N1-C2	-5.48	118.11	120.30
1	A	2076	U	C2-N1-C1'	5.48	124.28	117.70
1	A	2006	C	C2-N1-C1'	5.48	124.83	118.80
1	A	373	U	C6-N1-C2	-5.47	117.72	121.00
1	A	1190	G	C4-C5-N7	5.47	112.99	110.80
35	a	899	C	N1-C2-O2	5.47	122.18	118.90
1	A	39	G	C8-N9-C1'	-5.47	119.89	127.00
57	x	43	G	N3-C2-N2	-5.47	116.07	119.90
1	A	2611	C	C5-C6-N1	5.47	123.73	121.00
1	A	2465	C	C6-N1-C2	-5.47	118.11	120.30
2	B	37	C	C6-N1-C2	-5.47	118.11	120.30
35	a	342	C	C6-N1-C2	-5.47	118.11	120.30
35	a	1230	C	C6-N1-C2	-5.47	118.11	120.30
1	A	509	C	C6-N1-C2	-5.46	118.11	120.30
1	A	915	C	C2-N1-C1'	5.46	124.81	118.80
1	A	2755	C	C2-N1-C1'	5.46	124.81	118.80
35	a	439	U	C6-N1-C2	-5.46	117.72	121.00
1	A	759	G	N3-C4-N9	5.46	129.28	126.00
1	A	1917	U	C6-N1-C2	-5.46	117.72	121.00
1	A	897	C	N1-C2-O2	5.46	122.18	118.90
35	a	233	C	C6-N1-C2	-5.46	118.12	120.30
35	a	1460	C	N1-C2-O2	5.46	122.18	118.90
57	x	76	A	C4-C5-C6	-5.46	114.27	117.00
1	A	912	C	C5-C6-N1	5.46	123.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1379	U	N1-C2-O2	5.45	126.62	122.80
1	A	1993	U	C2-N1-C1'	5.45	124.24	117.70
1	A	985	C	C6-N1-C2	-5.45	118.12	120.30
1	A	2016	U	C6-N1-C2	-5.45	117.73	121.00
1	A	2064	C	C2-N1-C1'	5.45	124.79	118.80
1	A	1350	C	C6-N1-C2	-5.45	118.12	120.30
1	A	1967	C	N1-C2-O2	5.45	122.17	118.90
1	A	2300	C	C2-N1-C1'	5.45	124.79	118.80
1	A	1222	U	N3-C2-O2	-5.44	118.39	122.20
1	A	1896	G	N3-C2-N2	-5.44	116.09	119.90
1	A	200	U	N1-C2-O2	5.44	126.61	122.80
1	A	2200	C	C6-N1-C2	-5.44	118.12	120.30
1	A	1956	U	C2-N1-C1'	5.44	124.22	117.70
1	A	2902	C	N1-C2-O2	5.44	122.16	118.90
1	A	1267	U	C2-N1-C1'	5.43	124.22	117.70
1	A	2755	C	C6-N1-C2	-5.43	118.13	120.30
35	a	687	A	C8-N9-C4	-5.43	103.63	105.80
35	a	1375	A	N7-C8-N9	5.43	116.52	113.80
35	a	1470	U	N1-C2-O2	5.43	126.60	122.80
1	A	848	C	C2-N1-C1'	5.43	124.77	118.80
1	A	2178	C	N1-C2-O2	5.43	122.16	118.90
35	a	1008	U	N1-C2-O2	5.43	126.60	122.80
44	j	88	MET	C-N-CA	5.43	135.27	121.70
2	B	105	G	N9-C4-C5	-5.43	103.23	105.40
1	A	392	U	N1-C2-O2	5.42	126.60	122.80
35	a	697	U	N3-C2-O2	-5.42	118.40	122.20
1	A	2068	U	C5-C6-N1	5.42	125.41	122.70
1	A	860	U	N1-C2-O2	5.42	126.59	122.80
1	A	2822	G	N1-C6-O6	5.42	123.15	119.90
1	A	421	C	N1-C2-O2	5.42	122.15	118.90
1	A	2195	U	N3-C2-O2	-5.42	118.41	122.20
1	A	2840	C	C5-C6-N1	5.42	123.71	121.00
38	d	158	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	A	585	G	N3-C4-N9	5.41	129.25	126.00
1	A	2616	C	C2-N1-C1'	5.41	124.75	118.80
35	a	429	U	OP1-P-O3'	5.41	117.11	105.20
1	A	974	G	C4-C5-N7	5.41	112.96	110.80
35	a	839	C	N3-C2-O2	-5.41	118.11	121.90
42	h	66	GLN	C-N-CA	5.41	133.66	122.30
1	A	1340	U	N1-C2-O2	5.41	126.59	122.80
35	a	397	A	C2-N3-C4	5.41	113.30	110.60
35	a	571	U	C5-C6-N1	5.41	125.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1892	C	C5-C6-N1	5.40	123.70	121.00
1	A	343	C	C2-N1-C1'	5.40	124.74	118.80
1	A	206	U	N3-C2-O2	-5.40	118.42	122.20
1	A	1314	C	C2-N3-C4	5.40	122.60	119.90
1	A	2511	U	C6-N1-C2	-5.40	117.76	121.00
35	a	150	U	N3-C2-O2	-5.40	118.42	122.20
1	A	2025	C	C6-N1-C2	-5.40	118.14	120.30
1	A	1459	G	N3-C4-N9	-5.40	122.76	126.00
1	A	2558	C	C5-C6-N1	5.40	123.70	121.00
35	a	839	C	N1-C2-O2	5.39	122.14	118.90
57	x	3	G	C6-C5-N7	-5.39	127.16	130.40
35	a	1118	U	O5'-P-OP1	-5.39	100.85	105.70
1	A	2124	G	N3-C4-C5	-5.39	125.91	128.60
1	A	2192	U	C6-N1-C2	-5.39	117.77	121.00
35	a	1382	C	C5-C6-N1	5.39	123.69	121.00
35	a	754	C	N1-C2-O2	5.39	122.13	118.90
35	a	1294	G	N3-C4-C5	-5.39	125.91	128.60
1	A	437	U	N3-C2-O2	-5.39	118.43	122.20
1	A	1730	C	C6-N1-C2	-5.39	118.14	120.30
35	a	1086	U	C5-C6-N1	5.38	125.39	122.70
1	A	1088	A	N7-C8-N9	5.38	116.49	113.80
1	A	1378	A	OP1-P-O3'	5.38	117.03	105.20
1	A	2286	G	N3-C4-C5	5.38	131.29	128.60
1	A	2592	G	N3-C4-C5	-5.38	125.91	128.60
35	a	879	C	C5-C6-N1	5.38	123.69	121.00
35	a	1407	C	C6-N1-C2	-5.38	118.15	120.30
57	x	6	U	C5-C6-N1	5.38	125.39	122.70
35	a	556	C	C6-N1-C2	-5.37	118.15	120.30
35	a	1367	C	C6-N1-C2	-5.37	118.15	120.30
2	B	66	A	P-O3'-C3'	5.37	126.14	119.70
1	A	1982	U	C6-N1-C2	-5.37	117.78	121.00
1	A	1624	U	N3-C2-O2	-5.37	118.44	122.20
1	A	356	G	N3-C4-N9	5.36	129.22	126.00
1	A	93	G	C4-C5-N7	5.36	112.94	110.80
1	A	2072	C	C2-N3-C4	5.36	122.58	119.90
35	a	998	C	N3-C2-O2	-5.36	118.15	121.90
1	A	34	U	C2-N1-C1'	5.36	124.13	117.70
35	a	1326	U	N1-C2-O2	5.36	126.55	122.80
1	A	2507	C	C6-N1-C2	-5.36	118.16	120.30
2	B	4	C	C2-N3-C4	5.36	122.58	119.90
35	a	563	A	C8-N9-C1'	-5.35	118.06	127.70
1	A	692	C	C6-N1-C2	-5.35	118.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2380	C	C6-N1-C2	-5.35	118.16	120.30
1	A	2043	C	N3-C2-O2	-5.34	118.16	121.90
1	A	2806	C	C6-N1-C2	-5.34	118.16	120.30
1	A	206	U	N1-C2-O2	5.34	126.54	122.80
2	B	105	G	C4-C5-N7	5.34	112.94	110.80
56	v	214	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	243	U	N3-C2-O2	-5.34	118.46	122.20
1	A	1199	U	C5-C6-N1	5.33	125.37	122.70
1	A	1915	U	N3-C2-O2	-5.33	118.47	122.20
35	a	91	U	C2-N1-C1’	5.33	124.10	117.70
35	a	175	C	N3-C2-O2	-5.33	118.17	121.90
1	A	1924	C	C5-C6-N1	5.33	123.67	121.00
2	B	38	C	N3-C2-O2	-5.33	118.17	121.90
35	a	1322	C	C6-N1-C2	5.33	122.43	120.30
1	A	1044	C	C6-N1-C2	-5.32	118.17	120.30
35	a	529	G	N3-C4-N9	5.32	129.19	126.00
1	A	860	U	C2-N1-C1’	5.32	124.09	117.70
35	a	1460	C	C2-N1-C1’	5.32	124.65	118.80
1	A	2006	C	C5-C6-N1	5.32	123.66	121.00
1	A	2096	C	C6-N1-C2	-5.32	118.17	120.30
1	A	2457	U	C6-N1-C2	-5.32	117.81	121.00
35	a	623	C	C5-C6-N1	5.32	123.66	121.00
1	A	1049	C	N3-C4-C5	-5.32	119.77	121.90
1	A	2248	C	C6-N1-C1’	-5.32	114.42	120.80
1	A	2393	U	N1-C2-O2	5.32	126.52	122.80
35	a	1037	C	C2-N1-C1’	5.32	124.65	118.80
1	A	485	C	N1-C2-O2	5.32	122.09	118.90
1	A	1760	C	N1-C2-O2	5.32	122.09	118.90
1	A	2124	G	N3-C4-N9	5.32	129.19	126.00
35	a	1399	C	P-O3’-C3’	5.32	126.08	119.70
1	A	1205	A	C8-N9-C4	5.31	107.93	105.80
1	A	1438	U	N1-C2-O2	5.31	126.52	122.80
1	A	2755	C	N1-C2-O2	5.31	122.09	118.90
1	A	1915	U	N1-C2-O2	5.31	126.52	122.80
1	A	2604	U	O4’-C1’-N1	5.31	112.45	108.20
1	A	140	C	N1-C2-O2	5.31	122.08	118.90
1	A	484	C	C2-N1-C1’	5.31	124.64	118.80
1	A	1157	G	C4-C5-N7	5.31	112.92	110.80
1	A	2300	C	C5-C6-N1	5.31	123.65	121.00
35	a	998	C	N1-C2-O2	5.31	122.08	118.90
35	a	1440	U	N1-C2-O2	5.31	126.52	122.80
1	A	192	C	N3-C2-O2	-5.31	118.19	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	C	O4'-C1'-N1	5.31	112.44	108.20
1	A	832	U	C6-N1-C2	-5.30	117.82	121.00
1	A	985	C	C5-C6-N1	5.30	123.65	121.00
1	A	2695	U	C5-C6-N1	5.30	125.35	122.70
1	A	2214	C	N3-C2-O2	-5.30	118.19	121.90
35	a	207	C	C5-C6-N1	5.30	123.65	121.00
35	a	740	U	N3-C2-O2	-5.30	118.49	122.20
1	A	2416	C	C6-N1-C2	-5.30	118.18	120.30
1	A	196	A	O4'-C1'-N9	5.29	112.43	108.20
1	A	198	C	C6-N1-C2	-5.29	118.18	120.30
1	A	1270	C	C6-N1-C2	-5.29	118.19	120.30
1	A	2881	U	C5-C6-N1	5.29	125.34	122.70
35	a	1007	U	C2-N1-C1'	5.29	124.04	117.70
35	a	800	G	C8-N9-C4	-5.28	104.29	106.40
1	A	1005	C	N1-C2-O2	5.28	122.07	118.90
1	A	1486	U	N3-C2-O2	-5.28	118.51	122.20
1	A	2214	C	C5-C6-N1	5.28	123.64	121.00
1	A	1783	A	N3-C4-N9	-5.28	123.18	127.40
35	a	995	C	C6-N1-C2	-5.28	118.19	120.30
1	A	267	C	C2-N1-C1'	5.27	124.60	118.80
35	a	13	U	C5-C4-O4	-5.27	122.73	125.90
1	A	1941	C	C2-N1-C1'	5.27	124.60	118.80
1	A	801	G	C8-N9-C1'	5.27	133.85	127.00
1	A	1414	C	C6-N1-C2	-5.27	118.19	120.30
1	A	2579	C	C6-N1-C2	-5.27	118.19	120.30
35	a	358	U	N1-C2-O2	5.26	126.48	122.80
1	A	937	C	C6-N1-C2	-5.26	118.20	120.30
1	A	999	U	N1-C2-O2	5.26	126.48	122.80
35	a	811	C	C6-N1-C2	-5.26	118.20	120.30
35	a	1071	C	C5-C6-N1	5.26	123.63	121.00
1	A	2248	C	N1-C2-O2	5.26	122.05	118.90
35	a	1126	U	N1-C2-O2	5.25	126.47	122.80
1	A	638	G	C4-N9-C1'	5.25	133.32	126.50
1	A	1079	C	C5-C6-N1	5.25	123.62	121.00
1	A	1574	C	C6-N1-C2	-5.25	118.20	120.30
1	A	1796	U	N3-C2-O2	-5.25	118.53	122.20
1	A	2398	U	N3-C2-O2	-5.25	118.53	122.20
35	a	1112	C	C5-C6-N1	5.25	123.62	121.00
1	A	1151	A	N9-C4-C5	-5.25	103.70	105.80
2	B	78	A	O5'-P-OP1	-5.25	100.98	105.70
35	a	580	C	N1-C2-O2	5.25	122.05	118.90
57	x	74	C	C5-C6-N1	5.25	123.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	G	N3-C4-N9	5.24	129.14	126.00
1	A	1177	G	N7-C8-N9	5.24	115.72	113.10
1	A	1675	C	N3-C2-O2	-5.24	118.23	121.90
1	A	1726	C	N1-C2-O2	5.24	122.05	118.90
1	A	1288	G	C4-N9-C1'	5.24	133.31	126.50
1	A	1343	G	C6-C5-N7	-5.24	127.26	130.40
1	A	1894	C	N3-C2-O2	-5.24	118.23	121.90
1	A	2655	G	P-O3'-C3'	5.24	125.98	119.70
1	A	512	G	O4'-C1'-N9	5.24	112.39	108.20
1	A	1349	C	N3-C2-O2	-5.23	118.24	121.90
1	A	540	C	C6-N1-C2	-5.23	118.21	120.30
1	A	520	G	C8-N9-C4	-5.23	104.31	106.40
1	A	1318	U	C5-C6-N1	5.23	125.31	122.70
1	A	2752	C	C2-N1-C1'	5.23	124.55	118.80
35	a	1138	G	N3-C4-C5	-5.22	125.99	128.60
1	A	151	C	C6-N1-C2	-5.22	118.21	120.30
1	A	1333	G	C8-N9-C1'	-5.22	120.22	127.00
1	A	1668	A	C2-N3-C4	5.22	113.21	110.60
1	A	1081	U	N3-C2-O2	-5.21	118.55	122.20
1	A	1446	C	C5-C6-N1	5.21	123.61	121.00
35	a	657	U	N3-C2-O2	-5.21	118.55	122.20
1	A	2078	C	C6-N1-C2	-5.21	118.22	120.30
1	A	1301	A	C4-N9-C1'	5.21	135.67	126.30
1	A	1363	C	C6-N1-C2	-5.21	118.22	120.30
35	a	813	U	N3-C2-O2	-5.21	118.56	122.20
1	A	1065	U	N1-C2-O2	5.21	126.44	122.80
35	a	998	C	C6-N1-C2	-5.21	118.22	120.30
1	A	747	C	N3-C2-O2	-5.20	118.26	121.90
35	a	871	U	P-O3'-C3'	5.20	125.94	119.70
35	a	962	C	C6-N1-C2	-5.20	118.22	120.30
35	a	1129	C	C2-N1-C1'	5.20	124.52	118.80
35	a	302	G	N3-C4-C5	-5.20	126.00	128.60
1	A	1669	A	C4-N9-C1'	5.20	135.66	126.30
1	A	2329	U	N3-C4-O4	5.20	123.04	119.40
1	A	2704	C	N1-C2-O2	5.20	122.02	118.90
6	F	49	LEU	CA-CB-CG	5.19	127.24	115.30
35	a	960	U	N1-C2-O2	5.19	126.43	122.80
35	a	1518	A	C5-N7-C8	-5.19	101.31	103.90
1	A	1188	U	N3-C2-O2	-5.19	118.57	122.20
49	o	86	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	1370	C	C5-C6-N1	5.18	123.59	121.00
1	A	733	G	N1-C6-O6	-5.17	116.80	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1343	G	N9-C4-C5	-5.17	103.33	105.40
1	A	1402	U	C5-C6-N1	5.17	125.29	122.70
2	B	88	C	P-O3'-C3'	5.17	125.91	119.70
35	a	480	U	O4'-C1'-N1	5.17	112.34	108.20
1	A	2591	C	C5-C6-N1	5.17	123.59	121.00
35	a	35	G	C2-N3-C4	5.17	114.49	111.90
8	H	97	ARG	N-CA-C	5.17	124.96	111.00
57	x	33	U	N3-C2-O2	-5.17	118.58	122.20
1	A	2104	C	C5-C6-N1	5.17	123.58	121.00
1	A	1653	G	N1-C6-O6	5.17	123.00	119.90
1	A	2683	C	N3-C2-O2	-5.17	118.28	121.90
35	a	79	G	C4-N9-C1'	5.17	133.22	126.50
1	A	2436	G	C6-N1-C2	-5.17	122.00	125.10
35	a	190	A	N7-C8-N9	5.17	116.38	113.80
1	A	62	U	O4'-C1'-N1	5.16	112.33	108.20
35	a	799	G	N3-C4-C5	-5.16	126.02	128.60
1	A	790	U	C5-C6-N1	-5.16	120.12	122.70
1	A	143	C	C6-N1-C1'	-5.16	114.61	120.80
35	a	11	G	C6-C5-N7	-5.16	127.30	130.40
35	a	1095	U	N3-C2-O2	-5.16	118.59	122.20
35	a	1532	U	C5-C6-N1	5.16	125.28	122.70
2	B	36	C	C2-N3-C4	5.16	122.48	119.90
1	A	234	U	C2-N1-C1'	5.15	123.88	117.70
1	A	510	C	C6-N1-C1'	-5.15	114.62	120.80
1	A	717	C	C6-N1-C2	-5.15	118.24	120.30
1	A	1513	U	N3-C2-O2	-5.15	118.59	122.20
1	A	1716	U	N3-C2-O2	-5.15	118.59	122.20
35	a	837	U	N3-C2-O2	-5.15	118.59	122.20
1	A	425	G	C6-C5-N7	-5.15	127.31	130.40
1	A	2329	U	C6-N1-C2	-5.15	117.91	121.00
1	A	2615	U	N1-C2-O2	5.15	126.40	122.80
1	A	694	U	C5-C6-N1	5.15	125.27	122.70
35	a	956	U	N3-C2-O2	-5.15	118.60	122.20
1	A	1157	G	N9-C4-C5	-5.14	103.34	105.40
1	A	2248	C	C5-C6-N1	5.14	123.57	121.00
35	a	1138	G	N3-C4-N9	5.14	129.09	126.00
35	a	1232	U	C5-C6-N1	5.14	125.27	122.70
35	a	1314	C	C2-N1-C1'	5.14	124.46	118.80
35	a	1382	C	N1-C2-O2	5.14	121.99	118.90
1	A	315	G	N3-C4-N9	5.14	129.09	126.00
1	A	1188	U	N1-C2-O2	5.14	126.40	122.80
1	A	2380	C	C5-C6-N1	5.14	123.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	299	G	C8-N9-C4	-5.14	104.34	106.40
1	A	1818	U	C2-N1-C1'	5.14	123.87	117.70
1	A	2065	C	C6-N1-C2	-5.14	118.24	120.30
1	A	484	C	C5-C6-N1	5.14	123.57	121.00
35	a	18	C	C5-C6-N1	5.14	123.57	121.00
35	a	522	C	N3-C4-C5	5.14	123.95	121.90
35	a	805	C	N1-C2-O2	5.14	121.98	118.90
1	A	680	C	C5-C6-N1	5.13	123.57	121.00
1	A	1531	C	C6-N1-C2	-5.13	118.25	120.30
1	A	269	C	C6-N1-C2	-5.13	118.25	120.30
1	A	2627	G	N9-C4-C5	5.13	107.45	105.40
1	A	1092	C	C6-N1-C1'	-5.13	114.64	120.80
1	A	2250	G	C4-C5-N7	5.13	112.85	110.80
35	a	961	U	N1-C2-O2	5.13	126.39	122.80
1	A	2179	C	N1-C2-O2	5.12	121.97	118.90
1	A	1822	C	C6-N1-C2	-5.12	118.25	120.30
35	a	221	C	C5-C6-N1	5.12	123.56	121.00
35	a	312	C	N3-C2-O2	-5.12	118.31	121.90
1	A	584	C	C5-C6-N1	5.12	123.56	121.00
1	A	2592	G	C8-N9-C1'	-5.12	120.34	127.00
1	A	2067	G	N9-C4-C5	-5.12	103.35	105.40
1	A	2105	U	N1-C2-O2	5.12	126.38	122.80
2	B	19	C	C5-C6-N1	5.12	123.56	121.00
1	A	93	G	C8-N9-C1'	-5.12	120.35	127.00
1	A	2206	C	C6-N1-C2	-5.12	118.25	120.30
1	A	1295	C	C6-N1-C2	-5.12	118.25	120.30
1	A	215	G	OP1-P-O3'	5.11	116.44	105.20
1	A	1974	C	C5-C6-N1	5.11	123.56	121.00
1	A	2124	G	C8-N9-C1'	-5.11	120.36	127.00
35	a	620	C	N1-C2-O2	5.11	121.97	118.90
35	a	1230	C	C5-C6-N1	5.11	123.56	121.00
1	A	672	C	C5-C6-N1	5.11	123.55	121.00
35	a	961	U	C2-N1-C1'	5.11	123.83	117.70
1	A	137	U	N3-C2-O2	-5.10	118.63	122.20
35	a	1328	C	C6-N1-C2	-5.10	118.26	120.30
1	A	2695	U	C6-N1-C2	-5.10	117.94	121.00
2	B	37	C	C2-N1-C1'	5.10	124.41	118.80
57	x	3	G	N7-C8-N9	5.10	115.65	113.10
1	A	1256	G	C4-C5-N7	5.10	112.84	110.80
1	A	2174	C	C6-N1-C2	-5.10	118.26	120.30
1	A	2592	G	C4-N9-C1'	5.10	133.13	126.50
1	A	1459	G	C8-N9-C1'	5.10	133.63	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1644	C	C6-N1-C2	-5.10	118.26	120.30
1	A	1682	G	N3-C4-N9	5.10	129.06	126.00
35	a	752	G	C4-N9-C1'	5.10	133.13	126.50
35	a	1303	C	C2-N1-C1'	5.10	124.41	118.80
1	A	692	C	C5-C6-N1	5.10	123.55	121.00
1	A	801	G	N3-C4-N9	-5.10	122.94	126.00
1	A	1130	U	C2-N1-C1'	5.09	123.81	117.70
1	A	1348	C	C2-N1-C1'	5.09	124.41	118.80
1	A	2337	G	C6-N1-C2	-5.09	122.04	125.10
1	A	496	G	N9-C4-C5	-5.09	103.36	105.40
1	A	632	A	C8-N9-C4	-5.09	103.76	105.80
35	a	514	C	N1-C2-O2	5.09	121.95	118.90
1	A	353	C	N3-C2-O2	-5.09	118.34	121.90
1	A	1142	A	N3-C4-N9	-5.09	123.33	127.40
1	A	1848	A	N7-C8-N9	5.09	116.34	113.80
35	a	488	C	C2-N1-C1'	5.09	124.40	118.80
1	A	356	G	N3-C4-C5	-5.09	126.06	128.60
1	A	158	U	C5-C6-N1	5.09	125.24	122.70
1	A	395	U	N1-C2-O2	5.09	126.36	122.80
1	A	654	A	C8-N9-C1'	-5.09	118.54	127.70
1	A	584	C	N1-C2-O2	5.08	121.95	118.90
6	F	151	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	157	C	C2-N1-C1'	5.08	124.39	118.80
35	a	689	C	C5-C6-N1	5.08	123.54	121.00
1	A	1947	C	C5-C6-N1	5.08	123.54	121.00
1	A	1956	U	C5-C6-N1	5.08	125.24	122.70
35	a	899	C	N3-C2-O2	-5.08	118.34	121.90
35	a	1389	C	C5-C6-N1	5.08	123.54	121.00
1	A	2438	U	C5-C6-N1	5.08	125.24	122.70
35	a	11	G	C8-N9-C1'	-5.08	120.40	127.00
35	a	637	C	C5-C6-N1	5.08	123.54	121.00
1	A	1108	U	C5-C6-N1	5.07	125.24	122.70
1	A	2043	C	C5-C6-N1	5.07	123.54	121.00
1	A	2550	G	C6-C5-N7	-5.07	127.36	130.40
1	A	2825	G	C8-N9-C1'	-5.07	120.41	127.00
35	a	1262	C	N3-C2-O2	-5.07	118.35	121.90
35	a	1262	C	N1-C2-O2	5.07	121.94	118.90
35	a	1348	U	C5-C6-N1	5.07	125.23	122.70
1	A	867	C	C2-N1-C1'	5.07	124.38	118.80
2	B	17	C	C5-C6-N1	5.07	123.53	121.00
35	a	136	C	C2-N1-C1'	5.07	124.37	118.80
35	a	516	U	C6-N1-C2	-5.07	117.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	481	G	C8-N9-C4	5.07	108.43	106.40
1	A	974	G	C8-N9-C1’	-5.07	120.41	127.00
1	A	2581	G	C2-N3-C4	5.07	114.43	111.90
1	A	1178	C	N3-C2-O2	-5.06	118.36	121.90
1	A	2214	C	C6-N1-C2	-5.06	118.28	120.30
1	A	2509	G	C4-C5-N7	5.06	112.82	110.80
35	a	1107	C	C6-N1-C2	-5.06	118.28	120.30
1	A	242	G	OP2-P-O3’	5.06	116.32	105.20
6	F	3	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	1333	G	C6-C5-N7	-5.05	127.37	130.40
1	A	2462	C	C5-C6-N1	5.05	123.53	121.00
1	A	2329	U	C2-N1-C1’	5.05	123.76	117.70
1	A	740	C	C5-C6-N1	5.05	123.53	121.00
1	A	2085	U	N3-C2-O2	-5.05	118.66	122.20
35	a	752	G	N3-C4-N9	5.05	129.03	126.00
1	A	417	C	N1-C2-O2	5.05	121.93	118.90
35	a	1253	G	N3-C4-C5	-5.05	126.08	128.60
1	A	304	U	C2-N1-C1’	5.04	123.75	117.70
1	A	370	G	N3-C2-N2	-5.04	116.37	119.90
1	A	2707	U	C5-C6-N1	5.04	125.22	122.70
35	a	333	U	C2-N1-C1’	5.04	123.75	117.70
1	A	1333	G	C4-N9-C1’	5.04	133.05	126.50
1	A	1774	C	N3-C2-O2	-5.04	118.37	121.90
1	A	2762	C	C2-N1-C1’	5.04	124.35	118.80
35	a	96	U	N1-C2-O2	5.04	126.33	122.80
57	x	3	G	C5-N7-C8	-5.04	101.78	104.30
1	A	2254	C	C6-N1-C2	-5.04	118.28	120.30
1	A	335	C	C6-N1-C2	-5.04	118.29	120.30
1	A	2724	U	C5-C4-O4	5.04	128.92	125.90
1	A	2820	A	OP1-P-O3’	5.04	116.28	105.20
35	a	1179	A	N7-C8-N9	5.04	116.32	113.80
1	A	1060	U	N3-C2-O2	-5.03	118.68	122.20
1	A	1897	G	C6-C5-N7	-5.03	127.38	130.40
1	A	2831	G	N1-C6-O6	-5.03	116.88	119.90
35	a	752	G	N3-C4-C5	-5.03	126.08	128.60
1	A	1157	G	N3-C4-N9	5.03	129.02	126.00
1	A	1912	A	N9-C4-C5	5.03	107.81	105.80
1	A	2656	U	C6-N1-C2	-5.03	117.98	121.00
1	A	814	C	C6-N1-C2	-5.03	118.29	120.30
1	A	1233	C	C5-C6-N1	5.03	123.51	121.00
1	A	1874	C	C5-C6-N1	5.03	123.51	121.00
35	a	221	C	C6-N1-C2	-5.03	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1360	G	N3-C4-C5	-5.02	126.09	128.60
1	A	2503	A	C2-N3-C4	5.02	113.11	110.60
1	A	555	G	P-O3'-C3'	5.02	125.72	119.70
35	a	1294	G	C4-N9-C1'	5.02	133.03	126.50
35	a	1351	U	C5-C6-N1	5.02	125.21	122.70
1	A	496	G	N3-C4-N9	5.02	129.01	126.00
1	A	1231	U	N3-C2-O2	-5.01	118.69	122.20
2	B	44	G	C4-C5-N7	-5.01	108.79	110.80
1	A	1563	U	C5-C6-N1	5.01	125.21	122.70
1	A	1343	G	C4-C5-N7	5.01	112.81	110.80
1	A	2574	G	C6-C5-N7	-5.01	127.39	130.40
2	B	30	C	C6-N1-C2	-5.01	118.30	120.30
35	a	11	G	N3-C4-C5	-5.01	126.10	128.60
35	a	419	C	C5-C6-N1	5.01	123.50	121.00
35	a	523	A	N1-C6-N6	5.01	121.61	118.60
1	A	650	C	C6-N1-C2	-5.01	118.30	120.30
35	a	219	U	C2-N1-C1'	5.01	123.71	117.70
35	a	610	U	N1-C2-O2	5.01	126.31	122.80
1	A	1455	G	C8-N9-C1'	-5.00	120.49	127.00
1	A	2765	A	C2-N3-C4	5.00	113.10	110.60
1	A	528	A	N3-C4-N9	-5.00	123.40	127.40
1	A	1198	U	C6-N1-C2	-5.00	118.00	121.00
35	a	532	A	N1-C6-N6	5.00	121.60	118.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	v	303	ARG	Sidechain

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	242 (90%)	27 (10%)	0	100	100
4	D	207/209 (99%)	182 (88%)	25 (12%)	0	100	100
5	E	199/201 (99%)	182 (92%)	16 (8%)	1 (0%)	29	61
6	F	175/177 (99%)	159 (91%)	16 (9%)	0	100	100
7	G	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	25	57
8	H	147/149 (99%)	127 (86%)	20 (14%)	0	100	100
9	I	139/141 (99%)	114 (82%)	25 (18%)	0	100	100
10	J	140/142 (99%)	129 (92%)	11 (8%)	0	100	100
11	K	120/122 (98%)	103 (86%)	16 (13%)	1 (1%)	19	51
12	L	141/143 (99%)	117 (83%)	23 (16%)	1 (1%)	22	55
13	M	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10	36
14	N	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
15	O	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
16	P	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	87 (86%)	13 (13%)	1 (1%)	15	46
19	S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	49
20	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
21	U	100/102 (98%)	84 (84%)	16 (16%)	0	100	100
22	V	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
23	W	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
24	X	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
25	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
26	Z	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
27	0	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	1	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
29	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	54 (87%)	8 (13%)	0	100	100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	101 (78%)	27 (21%)	1 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	6	64/66 (97%)	53 (83%)	11 (17%)	0	100	100
36	b	216/218 (99%)	177 (82%)	37 (17%)	2 (1%)	17	49
37	c	204/206 (99%)	183 (90%)	18 (9%)	3 (2%)	10	36
38	d	203/205 (99%)	180 (89%)	23 (11%)	0	100	100
39	e	155/157 (99%)	136 (88%)	19 (12%)	0	100	100
40	f	98/100 (98%)	82 (84%)	15 (15%)	1 (1%)	15	46
41	g	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	22	55
42	h	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	51
43	i	125/127 (98%)	105 (84%)	19 (15%)	1 (1%)	19	51
44	j	96/98 (98%)	79 (82%)	15 (16%)	2 (2%)	7	30
45	k	114/116 (98%)	91 (80%)	23 (20%)	0	100	100
46	l	121/123 (98%)	94 (78%)	26 (22%)	1 (1%)	19	51
47	m	112/114 (98%)	98 (88%)	13 (12%)	1 (1%)	17	49
48	n	99/101 (98%)	88 (89%)	11 (11%)	0	100	100
49	o	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	41
50	p	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
51	q	78/80 (98%)	62 (80%)	16 (20%)	0	100	100
52	r	63/65 (97%)	50 (79%)	11 (18%)	2 (3%)	4	22
53	s	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
54	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
55	u	63/65 (97%)	43 (68%)	17 (27%)	3 (5%)	2	15
56	v	240/242 (99%)	213 (89%)	24 (10%)	3 (1%)	12	39
58	z	12/14 (86%)	10 (83%)	1 (8%)	1 (8%)	1	5
All	All	6099/6205 (98%)	5361 (88%)	706 (12%)	32 (0%)	32	61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	175	LYS
18	R	54	VAL
32	5	80	THR
36	b	19	THR
37	c	96	VAL
37	c	97	PRO

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Mol	Chain	Res	Type
49	o	46	LYS
55	u	36	PHE
56	v	323	ASN
12	L	128	THR
36	b	18	GLN
40	f	96	VAL
44	j	42	LEU
58	z	16	PRO
11	K	111	LYS
52	r	17	VAL
52	r	18	GLN
55	u	33	ARG
56	v	329	LEU
42	h	67	GLY
44	j	43	PRO
56	v	307	ASN
13	M	70	ASP
19	S	64	ALA
41	g	129	ASN
47	m	104	ASN
43	i	91	GLU
55	u	7	GLU
37	c	80	GLY
5	E	83	VAL
13	M	69	PRO
46	l	21	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	214 (99%)	2 (1%)	78	90
4	D	164/164 (100%)	162 (99%)	2 (1%)	71	85
5	E	165/165 (100%)	163 (99%)	2 (1%)	71	85
6	F	148/148 (100%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	137/137 (100%)	135 (98%)	2 (2%)	65	82
8	H	114/114 (100%)	114 (100%)	0	100	100
9	I	109/109 (100%)	107 (98%)	2 (2%)	59	79
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/103 (100%)	103 (100%)	0	100	100
12	L	102/102 (100%)	101 (99%)	1 (1%)	76	88
13	M	109/109 (100%)	108 (99%)	1 (1%)	78	90
14	N	100/100 (100%)	99 (99%)	1 (1%)	76	88
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	98 (99%)	1 (1%)	76	88
17	Q	89/89 (100%)	88 (99%)	1 (1%)	73	86
18	R	84/84 (100%)	83 (99%)	1 (1%)	71	85
19	S	93/93 (100%)	93 (100%)	0	100	100
20	T	80/80 (100%)	80 (100%)	0	100	100
21	U	83/83 (100%)	83 (100%)	0	100	100
22	V	78/78 (100%)	78 (100%)	0	100	100
23	W	57/57 (100%)	56 (98%)	1 (2%)	59	79
24	X	67/67 (100%)	66 (98%)	1 (2%)	65	82
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/48 (100%)	48 (100%)	0	100	100
27	0	47/47 (100%)	47 (100%)	0	100	100
28	1	45/45 (100%)	45 (100%)	0	100	100
29	2	38/38 (100%)	38 (100%)	0	100	100
30	3	51/51 (100%)	51 (100%)	0	100	100
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	100 (100%)	0	100	100
33	6	59/59 (100%)	59 (100%)	0	100	100
36	b	180/180 (100%)	176 (98%)	4 (2%)	52	75
37	c	170/170 (100%)	167 (98%)	3 (2%)	59	79
38	d	172/172 (100%)	167 (97%)	5 (3%)	42	69
39	e	114/119 (96%)	112 (98%)	2 (2%)	59	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	f	87/87 (100%)	86 (99%)	1 (1%)	73	86
41	g	124/124 (100%)	124 (100%)	0	100	100
42	h	104/104 (100%)	103 (99%)	1 (1%)	76	88
43	i	105/105 (100%)	104 (99%)	1 (1%)	76	88
44	j	86/86 (100%)	84 (98%)	2 (2%)	50	74
45	k	89/89 (100%)	87 (98%)	2 (2%)	52	75
46	l	103/103 (100%)	103 (100%)	0	100	100
47	m	92/92 (100%)	89 (97%)	3 (3%)	38	66
48	n	79/83 (95%)	79 (100%)	0	100	100
49	o	76/76 (100%)	76 (100%)	0	100	100
50	p	65/65 (100%)	64 (98%)	1 (2%)	65	82
51	q	74/74 (100%)	74 (100%)	0	100	100
52	r	48/56 (86%)	47 (98%)	1 (2%)	53	76
53	s	70/70 (100%)	70 (100%)	0	100	100
54	t	65/65 (100%)	65 (100%)	0	100	100
55	u	44/55 (80%)	44 (100%)	0	100	100
56	v	195/195 (100%)	189 (97%)	6 (3%)	40	68
58	z	14/14 (100%)	13 (93%)	1 (7%)	14	44
All	All	5032/5060 (99%)	4981 (99%)	51 (1%)	77	88

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	132	ARG
4	D	33	ARG
4	D	169	ARG
5	E	21	ARG
5	E	156	ASN
7	G	47	ASN
7	G	68	ARG
9	I	18	ASN
9	I	126	ARG
12	L	27	LEU
13	M	6	ARG
14	N	2	ARG

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Mol	Chain	Res	Type
16	P	72	VAL
17	Q	108	LEU
18	R	43	ASN
23	W	10	ARG
24	X	26	ARG
36	b	23	ASN
36	b	35	ASN
36	b	87	ASP
36	b	202	ASN
37	c	24	ASN
37	c	64	ARG
37	c	163	ARG
38	d	7	LYS
38	d	80	ARG
38	d	177	MET
38	d	183	ARG
38	d	190	LEU
39	e	69	ASN
39	e	130	THR
40	f	53	LYS
42	h	79	ARG
43	i	44	ARG
44	j	42	LEU
44	j	58	ASN
45	k	12	ARG
45	k	124	LYS
47	m	3	ILE
47	m	7	ASN
47	m	91	ARG
50	p	5	ARG
52	r	42	ARG
56	v	133	ARG
56	v	316	ARG
56	v	321	ARG
56	v	322	ILE
56	v	323	ASN
56	v	340	LEU
58	z	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	36	ASN
3	C	114	GLN
4	D	164	GLN
5	E	156	ASN
7	G	47	ASN
7	G	63	GLN
7	G	110	HIS
7	G	138	GLN
8	H	66	ASN
10	J	47	HIS
10	J	135	GLN
10	J	136	GLN
13	M	13	HIS
15	O	38	GLN
18	R	6	GLN
18	R	18	GLN
18	R	43	ASN
18	R	89	HIS
18	R	91	GLN
19	S	7	HIS
19	S	57	ASN
20	T	15	HIS
21	U	68	ASN
23	W	8	ASN
25	Y	27	ASN
25	Y	58	ASN
26	Z	19	HIS
27	0	41	HIS
30	3	42	HIS
31	4	35	GLN
33	6	41	HIS
36	b	18	GLN
36	b	23	ASN
36	b	35	ASN
36	b	119	GLN
36	b	121	GLN
36	b	202	ASN
37	c	24	ASN
37	c	189	HIS
38	d	151	GLN
39	e	69	ASN
39	e	82	HIS
39	e	131	ASN

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Mol	Chain	Res	Type
40	f	11	HIS
40	f	55	HIS
41	g	67	ASN
41	g	121	ASN
41	g	147	ASN
42	h	3	GLN
42	h	66	GLN
43	i	4	GLN
43	i	125	GLN
44	j	56	HIS
46	l	58	ASN
47	m	7	ASN
47	m	99	GLN
48	n	43	ASN
50	p	63	GLN
51	q	30	HIS
52	r	51	GLN
53	s	68	HIS
56	v	258	GLN
56	v	323	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2898/2903 (99%)	681 (23%)	27 (0%)
2	B	119/120 (99%)	30 (25%)	5 (4%)
34	7	6/7 (85%)	4 (66%)	0
35	a	1538/1539 (99%)	345 (22%)	0
57	x	76/77 (98%)	21 (27%)	0
All	All	4637/4646 (99%)	1081 (23%)	32 (0%)

All (1081) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	10	A
1	A	12	U
1	A	14	A
1	A	23	G
1	A	28	A
1	A	34	U

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Mol	Chain	Res	Type
1	A	35	G
1	A	46	G
1	A	50	U
1	A	51	G
1	A	53	A
1	A	60	G
1	A	63	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	78	U
1	A	86	G
1	A	93	G
1	A	101	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	143	C
1	A	149	A
1	A	158	U
1	A	162	U
1	A	163	C
1	A	172	A
1	A	182	A
1	A	185	G
1	A	188	G
1	A	196	A
1	A	199	A
1	A	215	G
1	A	216	A
1	A	219	A
1	A	221	A
1	A	222	A
1	A	226	A
1	A	227	A
1	A	228	C
1	A	233	A

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Mol	Chain	Res	Type
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	250	G
1	A	255	A
1	A	265	A
1	A	266	G
1	A	267	C
1	A	275	C
1	A	276	U
1	A	277	G
1	A	289	G
1	A	294	A
1	A	302	C
1	A	310	A
1	A	311	A
1	A	312	G
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	335	C
1	A	345	A
1	A	349	U
1	A	353	C
1	A	356	G
1	A	361	G
1	A	362	A
1	A	367	G
1	A	371	A
1	A	372	G
1	A	373	U
1	A	384	A
1	A	386	G
1	A	387	U
1	A	391	A
1	A	396	G
1	A	401	A
1	A	404	A
1	A	405	U
1	A	406	G

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Mol	Chain	Res	Type
1	A	411	G
1	A	421	C
1	A	424	G
1	A	425	G
1	A	428	A
1	A	436	C
1	A	448	U
1	A	452	G
1	A	456	C
1	A	457	A
1	A	458	G
1	A	473	G
1	A	480	A
1	A	481	G
1	A	483	A
1	A	490	C
1	A	491	G
1	A	504	A
1	A	505	A
1	A	506	G
1	A	508	A
1	A	509	C
1	A	518	G
1	A	529	A
1	A	531	C
1	A	532	A
1	A	533	G
1	A	543	G
1	A	545	U
1	A	546	U
1	A	547	A
1	A	550	C
1	A	556	A
1	A	563	A
1	A	572	A
1	A	573	U
1	A	575	A
1	A	584	C
1	A	588	U
1	A	603	A
1	A	609	A
1	A	614	A

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Mol	Chain	Res	Type
1	A	615	U
1	A	616	A
1	A	621	A
1	A	622	G
1	A	627	A
1	A	631	A
1	A	634	C
1	A	636	G
1	A	637	A
1	A	644	A
1	A	645	C
1	A	646	U
1	A	651	G
1	A	654	A
1	A	655	A
1	A	659	G
1	A	668	A
1	A	670	A
1	A	686	U
1	A	687	C
1	A	695	G
1	A	704	G
1	A	711	G
1	A	715	A
1	A	717	C
1	A	730	A
1	A	734	A
1	A	746	U
1	A	747	C
1	A	748	G
1	A	749	A
1	A	750	A
1	A	752	A
1	A	754	U
1	A	762	U
1	A	764	A
1	A	765	C
1	A	772	C
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G

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Mol	Chain	Res	Type
1	A	785	G
1	A	800	A
1	A	801	G
1	A	802	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	822	G
1	A	827	U
1	A	828	U
1	A	829	A
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	856	G
1	A	857	G
1	A	858	G
1	A	859	G
1	A	860	U
1	A	869	G
1	A	877	A
1	A	878	A
1	A	879	G
1	A	881	G
1	A	883	G
1	A	885	C
1	A	891	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	902	C
1	A	904	G
1	A	907	G
1	A	910	A
1	A	915	C
1	A	927	A
1	A	931	U
1	A	932	U
1	A	933	A
1	A	941	A
1	A	945	A

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Mol	Chain	Res	Type
1	A	946	C
1	A	957	C
1	A	958	U
1	A	961	C
1	A	973	A
1	A	974	G
1	A	980	A
1	A	983	A
1	A	984	A
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	999	U
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1040	A
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1050	A
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1071	G
1	A	1072	C
1	A	1073	A

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Mol	Chain	Res	Type
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	C
1	A	1083	U
1	A	1084	A
1	A	1088	A
1	A	1089	A
1	A	1090	A
1	A	1092	C
1	A	1093	G
1	A	1095	A
1	A	1097	U
1	A	1098	A
1	A	1101	U
1	A	1102	C
1	A	1104	C
1	A	1111	A
1	A	1112	G
1	A	1119	U
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1135	C
1	A	1139	G
1	A	1142	A
1	A	1143	A
1	A	1149	G
1	A	1151	A
1	A	1155	A
1	A	1171	G
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1181	U
1	A	1183	U
1	A	1206	G
1	A	1211	C

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Mol	Chain	Res	Type
1	A	1212	G
1	A	1224	U
1	A	1236	G
1	A	1237	A
1	A	1244	A
1	A	1247	A
1	A	1248	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1257	C
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1275	A
1	A	1300	G
1	A	1301	A
1	A	1305	C
1	A	1306	C
1	A	1311	G
1	A	1321	A
1	A	1325	U
1	A	1326	U
1	A	1332	G
1	A	1341	G
1	A	1345	C
1	A	1360	G
1	A	1365	A
1	A	1366	A
1	A	1368	G
1	A	1375	U
1	A	1378	A
1	A	1379	U
1	A	1383	A
1	A	1387	A
1	A	1392	A
1	A	1395	A
1	A	1416	G
1	A	1419	A
1	A	1420	A
1	A	1421	G

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Mol	Chain	Res	Type
1	A	1424	G
1	A	1427	A
1	A	1428	C
1	A	1434	A
1	A	1437	C
1	A	1454	C
1	A	1455	G
1	A	1458	U
1	A	1460	U
1	A	1461	C
1	A	1467	U
1	A	1475	G
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1494	A
1	A	1504	A
1	A	1506	U
1	A	1507	C
1	A	1509	A
1	A	1515	A
1	A	1523	U
1	A	1524	G
1	A	1529	G
1	A	1530	G
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1545	A
1	A	1546	G
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1559	U
1	A	1560	G
1	A	1565	C
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1584	U
1	A	1585	C

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Mol	Chain	Res	Type
1	A	1586	A
1	A	1587	G
1	A	1592	C
1	A	1593	A
1	A	1608	A
1	A	1611	C
1	A	1627	G
1	A	1634	A
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1652	A
1	A	1669	A
1	A	1674	G
1	A	1675	C
1	A	1682	G
1	A	1693	U
1	A	1694	C
1	A	1695	G
1	A	1698	A
1	A	1699	G
1	A	1707	G
1	A	1715	G
1	A	1727	C
1	A	1729	U
1	A	1730	C
1	A	1731	G
1	A	1732	C
1	A	1738	G
1	A	1757	A
1	A	1758	U
1	A	1764	C
1	A	1769	U
1	A	1773	A
1	A	1776	G
1	A	1781	U
1	A	1786	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1807	G

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Mol	Chain	Res	Type
1	A	1808	A
1	A	1811	G
1	A	1812	U
1	A	1816	C
1	A	1826	G
1	A	1828	G
1	A	1829	A
1	A	1842	G
1	A	1857	G
1	A	1869	G
1	A	1871	A
1	A	1884	G
1	A	1888	G
1	A	1897	G
1	A	1900	A
1	A	1901	A
1	A	1906	G
1	A	1907	G
1	A	1912	A
1	A	1919	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1940	U
1	A	1941	C
1	A	1942	C
1	A	1945	G
1	A	1955	U
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	C
1	A	2015	A
1	A	2020	A
1	A	2022	U

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Mol	Chain	Res	Type
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2044	C
1	A	2046	G
1	A	2052	A
1	A	2053	G
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2069	G
1	A	2072	C
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2096	C
1	A	2100	G
1	A	2104	C
1	A	2105	U
1	A	2106	U
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2123	G
1	A	2125	G
1	A	2127	G
1	A	2128	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2137	U
1	A	2138	G
1	A	2139	U
1	A	2145	C

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Mol	Chain	Res	Type
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2167	U
1	A	2168	G
1	A	2169	A
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2175	C
1	A	2176	A
1	A	2178	C
1	A	2179	C
1	A	2189	U
1	A	2192	U
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2210	U
1	A	2212	A
1	A	2213	U
1	A	2225	A
1	A	2226	C
1	A	2228	G
1	A	2229	U
1	A	2238	G
1	A	2239	G
1	A	2250	G
1	A	2251	G
1	A	2266	A
1	A	2279	G
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2305	U
1	A	2308	G
1	A	2309	A
1	A	2320	U

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Mol	Chain	Res	Type
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2334	U
1	A	2335	A
1	A	2344	U
1	A	2345	G
1	A	2350	C
1	A	2354	C
1	A	2357	G
1	A	2358	A
1	A	2359	C
1	A	2361	G
1	A	2377	A
1	A	2383	G
1	A	2385	C
1	A	2391	G
1	A	2392	A
1	A	2402	U
1	A	2403	C
1	A	2405	G
1	A	2406	A
1	A	2407	A
1	A	2419	U
1	A	2422	C
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2426	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2434	A
1	A	2435	A
1	A	2440	C
1	A	2441	U
1	A	2445	G
1	A	2448	A
1	A	2464	G
1	A	2470	G

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Mol	Chain	Res	Type
1	A	2475	C
1	A	2476	A
1	A	2488	G
1	A	2494	G
1	A	2502	G
1	A	2503	A
1	A	2504	U
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2520	C
1	A	2529	G
1	A	2534	A
1	A	2535	G
1	A	2547	A
1	A	2554	U
1	A	2564	A
1	A	2567	G
1	A	2569	G
1	A	2572	A
1	A	2573	C
1	A	2574	G
1	A	2582	G
1	A	2585	U
1	A	2602	A
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2629	U
1	A	2646	C
1	A	2655	G
1	A	2661	G
1	A	2663	G
1	A	2668	G
1	A	2689	U
1	A	2690	U
1	A	2707	U
1	A	2714	G
1	A	2718	G
1	A	2724	U
1	A	2726	A

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Mol	Chain	Res	Type
1	A	2727	A
1	A	2732	G
1	A	2733	A
1	A	2744	G
1	A	2748	A
1	A	2750	A
1	A	2752	C
1	A	2761	A
1	A	2762	C
1	A	2764	A
1	A	2765	A
1	A	2778	A
1	A	2779	U
1	A	2780	G
1	A	2791	G
1	A	2792	A
1	A	2794	C
1	A	2796	U
1	A	2797	U
1	A	2798	U
1	A	2799	A
1	A	2800	A
1	A	2801	G
1	A	2808	G
1	A	2809	A
1	A	2811	G
1	A	2818	U
1	A	2820	A
1	A	2833	U
1	A	2836	U
1	A	2849	U
1	A	2851	A
1	A	2861	U
1	A	2866	U
1	A	2867	G
1	A	2868	A
1	A	2873	A
1	A	2880	C
1	A	2884	U
1	A	2887	A
1	A	2891	U
1	A	2894	G

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Mol	Chain	Res	Type
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	9	G
2	B	12	C
2	B	13	G
2	B	15	A
2	B	19	C
2	B	21	G
2	B	24	G
2	B	30	C
2	B	34	A
2	B	35	C
2	B	42	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	59	A
2	B	66	A
2	B	67	G
2	B	68	C
2	B	69	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	105	G
2	B	108	A
2	B	109	A
2	B	112	G
2	B	118	C
2	B	120	A
34	7	27	C
34	7	29	A
34	7	30	G
34	7	31	A
35	a	5	U
35	a	6	G
35	a	7	A
35	a	9	G
35	a	22	G
35	a	27	G

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Mol	Chain	Res	Type
35	a	31	G
35	a	32	A
35	a	39	G
35	a	47	C
35	a	48	C
35	a	49	U
35	a	50	A
35	a	51	A
35	a	58	C
35	a	59	A
35	a	69	G
35	a	71	A
35	a	73	C
35	a	78	A
35	a	79	G
35	a	80	A
35	a	81	A
35	a	82	G
35	a	86	G
35	a	87	C
35	a	88	U
35	a	89	U
35	a	92	U
35	a	95	C
35	a	96	U
35	a	121	U
35	a	130	A
35	a	132	C
35	a	134	G
35	a	149	A
35	a	154	U
35	a	163	C
35	a	164	G
35	a	173	U
35	a	174	A
35	a	181	A
35	a	183	C
35	a	184	G
35	a	197	A
35	a	199	A
35	a	200	G
35	a	205	A

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Mol	Chain	Res	Type
35	a	207	C
35	a	209	U
35	a	210	C
35	a	212	G
35	a	215	C
35	a	219	U
35	a	226	G
35	a	240	G
35	a	245	U
35	a	247	G
35	a	251	G
35	a	257	G
35	a	263	A
35	a	266	G
35	a	267	C
35	a	268	U
35	a	281	G
35	a	282	A
35	a	289	G
35	a	306	A
35	a	327	A
35	a	328	C
35	a	345	C
35	a	346	G
35	a	347	G
35	a	350	G
35	a	352	C
35	a	353	A
35	a	354	G
35	a	358	U
35	a	367	U
35	a	368	U
35	a	369	G
35	a	372	C
35	a	376	G
35	a	382	A
35	a	385	C
35	a	388	G
35	a	392	C
35	a	397	A
35	a	406	G
35	a	411	A

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Mol	Chain	Res	Type
35	a	412	A
35	a	413	G
35	a	414	A
35	a	422	C
35	a	424	G
35	a	427	U
35	a	428	G
35	a	429	U
35	a	430	A
35	a	435	A
35	a	438	U
35	a	439	U
35	a	442	G
35	a	451	A
35	a	452	A
35	a	460	A
35	a	462	G
35	a	467	U
35	a	468	A
35	a	473	U
35	a	477	C
35	a	479	U
35	a	480	U
35	a	482	A
35	a	484	G
35	a	486	U
35	a	487	A
35	a	489	C
35	a	492	C
35	a	495	A
35	a	496	A
35	a	497	G
35	a	508	U
35	a	509	A
35	a	511	C
35	a	516	U
35	a	518	C
35	a	519	C
35	a	521	G
35	a	524	G
35	a	527	G
35	a	528	C

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Mol	Chain	Res	Type
35	a	531	U
35	a	532	A
35	a	533	A
35	a	547	A
35	a	561	U
35	a	562	U
35	a	564	C
35	a	572	A
35	a	573	A
35	a	575	G
35	a	576	C
35	a	577	G
35	a	596	A
35	a	607	A
35	a	632	U
35	a	633	G
35	a	639	G
35	a	642	A
35	a	652	U
35	a	665	A
35	a	695	A
35	a	703	G
35	a	713	G
35	a	714	G
35	a	718	A
35	a	721	G
35	a	724	G
35	a	731	G
35	a	733	G
35	a	748	G
35	a	753	A
35	a	754	C
35	a	755	G
35	a	766	A
35	a	777	A
35	a	792	A
35	a	793	U
35	a	814	A
35	a	817	C
35	a	820	U
35	a	826	C
35	a	836	G

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Mol	Chain	Res	Type
35	a	843	U
35	a	844	G
35	a	845	A
35	a	846	G
35	a	851	G
35	a	871	U
35	a	873	A
35	a	876	C
35	a	884	U
35	a	885	G
35	a	887	G
35	a	889	A
35	a	890	G
35	a	902	G
35	a	916	U
35	a	926	G
35	a	931	C
35	a	934	C
35	a	935	A
35	a	939	G
35	a	942	G
35	a	960	U
35	a	961	U
35	a	966	G
35	a	968	A
35	a	969	A
35	a	974	A
35	a	975	A
35	a	976	G
35	a	977	A
35	a	983	A
35	a	989	U
35	a	992	U
35	a	993	G
35	a	994	A
35	a	999	C
35	a	1004	A
35	a	1005	A
35	a	1013	G
35	a	1020	G
35	a	1026	G
35	a	1027	C

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Mol	Chain	Res	Type
35	a	1028	C
35	a	1030	U
35	a	1031	C
35	a	1033	G
35	a	1034	G
35	a	1036	A
35	a	1042	A
35	a	1053	G
35	a	1056	U
35	a	1064	G
35	a	1065	U
35	a	1085	U
35	a	1089	G
35	a	1094	G
35	a	1095	U
35	a	1101	A
35	a	1104	G
35	a	1129	C
35	a	1130	A
35	a	1132	C
35	a	1136	C
35	a	1137	C
35	a	1138	G
35	a	1139	G
35	a	1140	C
35	a	1143	G
35	a	1146	A
35	a	1151	A
35	a	1152	A
35	a	1158	C
35	a	1159	U
35	a	1168	U
35	a	1171	A
35	a	1183	U
35	a	1184	G
35	a	1191	A
35	a	1196	A
35	a	1197	A
35	a	1200	C
35	a	1201	A
35	a	1202	U
35	a	1212	U

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Mol	Chain	Res	Type
35	a	1213	A
35	a	1225	A
35	a	1226	C
35	a	1227	A
35	a	1228	C
35	a	1236	A
35	a	1238	A
35	a	1240	U
35	a	1241	G
35	a	1256	A
35	a	1258	G
35	a	1260	G
35	a	1261	A
35	a	1262	C
35	a	1278	G
35	a	1280	A
35	a	1281	C
35	a	1282	C
35	a	1287	A
35	a	1289	A
35	a	1291	U
35	a	1294	G
35	a	1298	U
35	a	1300	G
35	a	1301	U
35	a	1302	C
35	a	1309	G
35	a	1311	A
35	a	1312	G
35	a	1315	U
35	a	1317	C
35	a	1320	C
35	a	1322	C
35	a	1323	G
35	a	1334	G
35	a	1335	U
35	a	1336	C
35	a	1340	A
35	a	1346	A
35	a	1347	G
35	a	1348	U
35	a	1353	G

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Mol	Chain	Res	Type
35	a	1363	A
35	a	1364	U
35	a	1368	A
35	a	1370	G
35	a	1378	C
35	a	1381	U
35	a	1384	C
35	a	1386	G
35	a	1387	G
35	a	1394	A
35	a	1395	C
35	a	1397	C
35	a	1399	C
35	a	1400	C
35	a	1401	G
35	a	1402	C
35	a	1406	U
35	a	1418	A
35	a	1419	G
35	a	1440	U
35	a	1441	A
35	a	1442	G
35	a	1443	C
35	a	1445	U
35	a	1446	A
35	a	1452	C
35	a	1455	G
35	a	1484	C
35	a	1487	G
35	a	1492	A
35	a	1493	A
35	a	1494	G
35	a	1497	G
35	a	1499	A
35	a	1502	A
35	a	1503	A
35	a	1506	U
35	a	1517	G
35	a	1529	G
35	a	1530	G
35	a	1531	A
35	a	1534	A

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Mol	Chain	Res	Type
35	a	1535	C
35	a	1536	C
35	a	1540	U
57	x	3	G
57	x	4	C
57	x	5	U
57	x	6	U
57	x	14	A
57	x	15	G
57	x	16	G
57	x	17	U
57	x	17(A)	G
57	x	19	U
57	x	21	A
57	x	22	G
57	x	34	G
57	x	42	U
57	x	46	G
57	x	47	U
57	x	48	C
57	x	50	G
57	x	62	C
57	x	65	U
57	x	76	A

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	86	G
1	A	227	A
1	A	242	G
1	A	372	G
1	A	490	C
1	A	549	G
1	A	555	G
1	A	846	U
1	A	858	G
1	A	859	G
1	A	931	U
1	A	1020	A
1	A	1022	G
1	A	1130	U

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1190	G
1	A	1300	G
1	A	1378	A
1	A	1399	C
1	A	1565	C
1	A	1566	A
1	A	1913	A
1	A	1940	U
1	A	2326	C
1	A	2347	C
1	A	2566	A
1	A	2808	G
2	B	3	C
2	B	12	C
2	B	52	A
2	B	66	A
2	B	88	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides 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
12	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	60:ARG	C	61:LEU	N	1.18

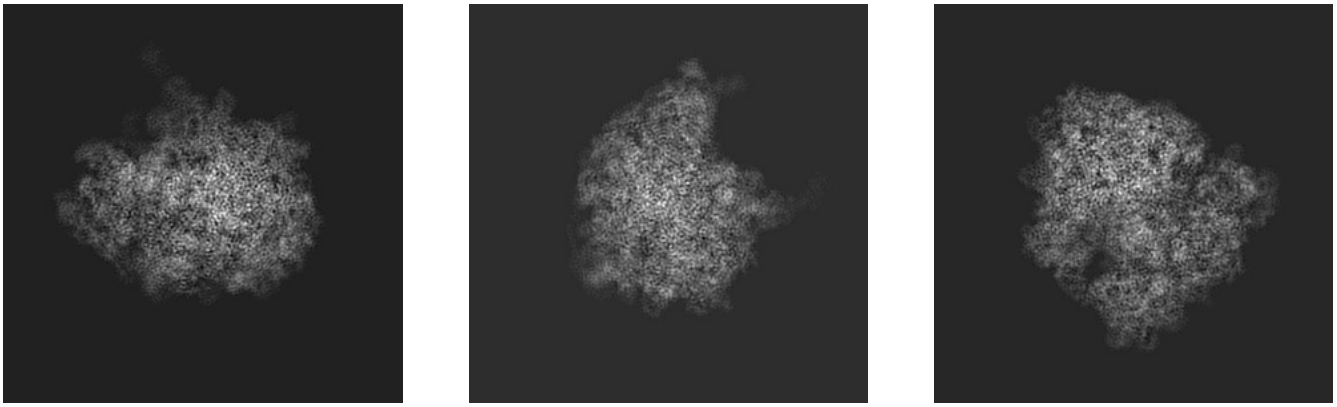
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3730. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

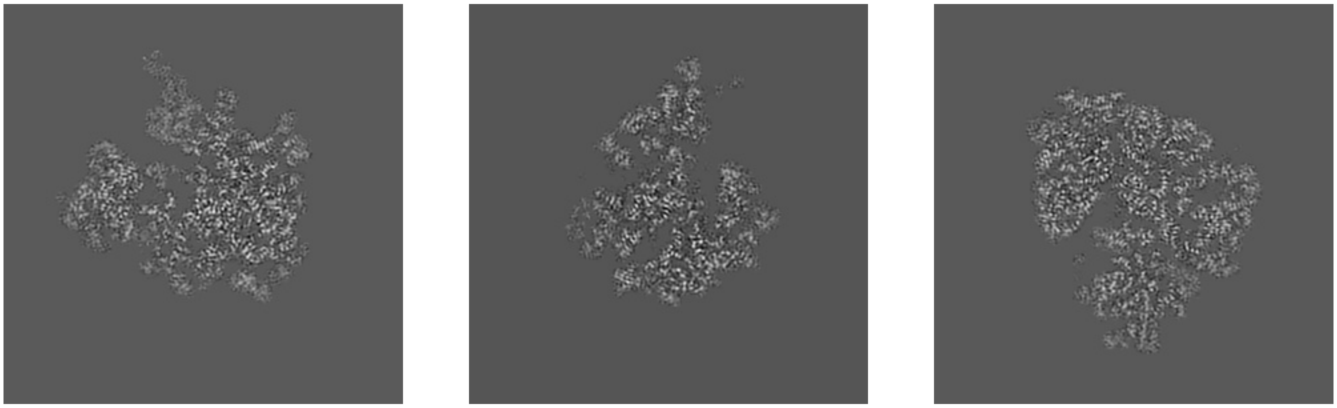


X Y Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

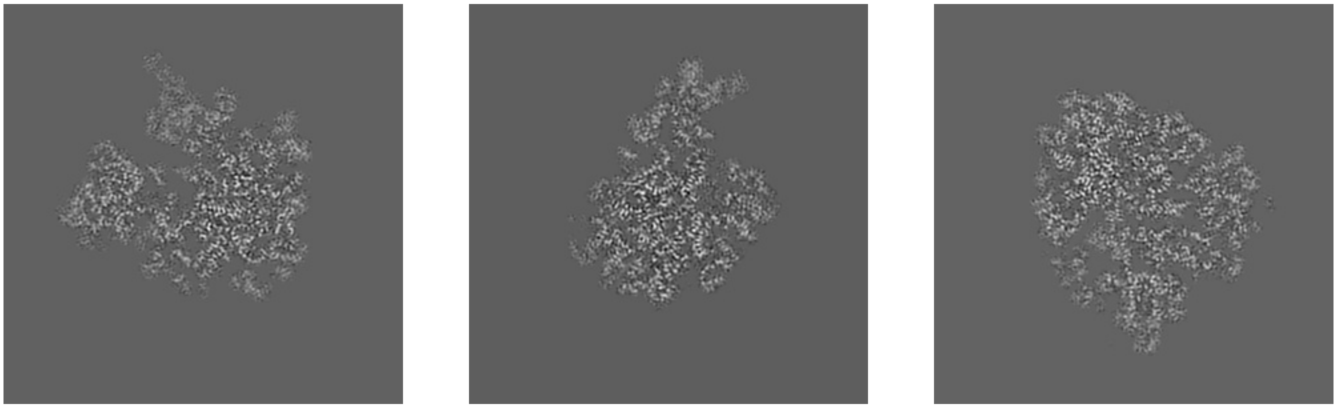


X Index: 180 Y Index: 180 Z Index: 180

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map

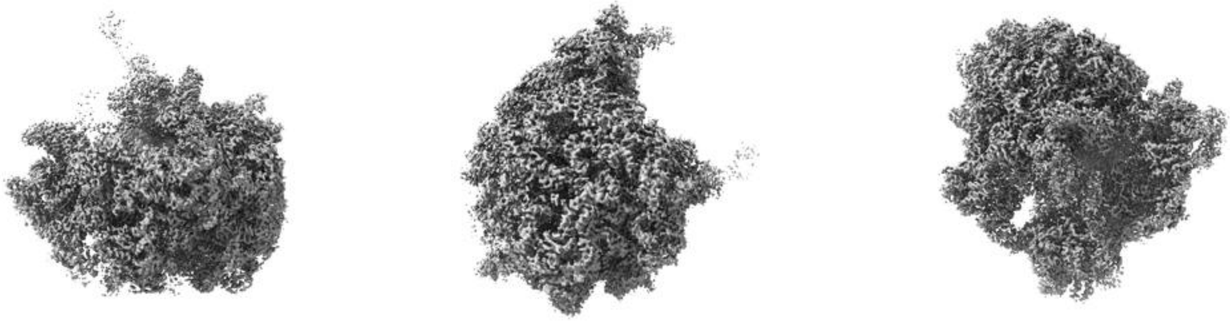


X Index: 178 Y Index: 190 Z Index: 186

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.407. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

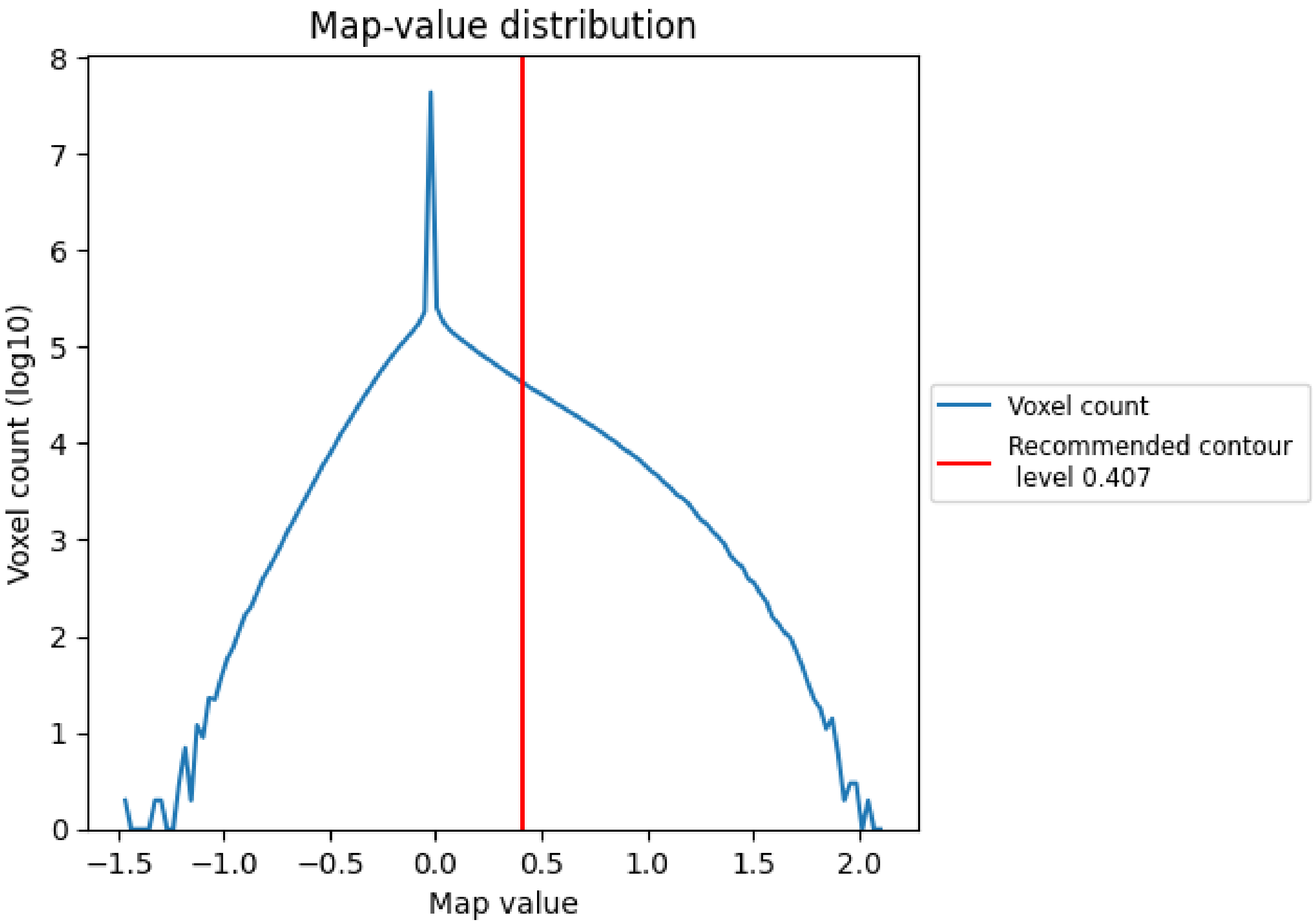
6.5 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

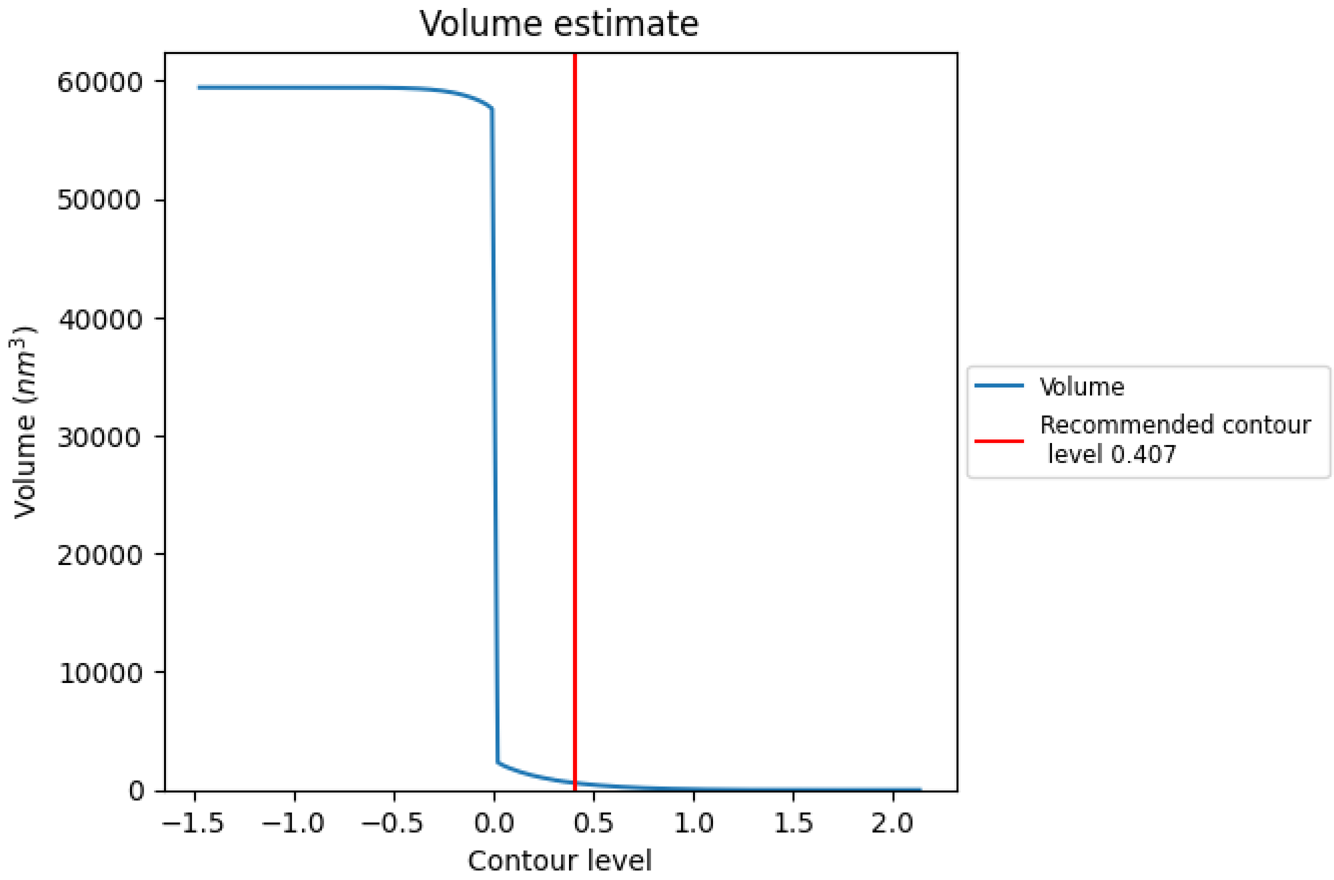
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

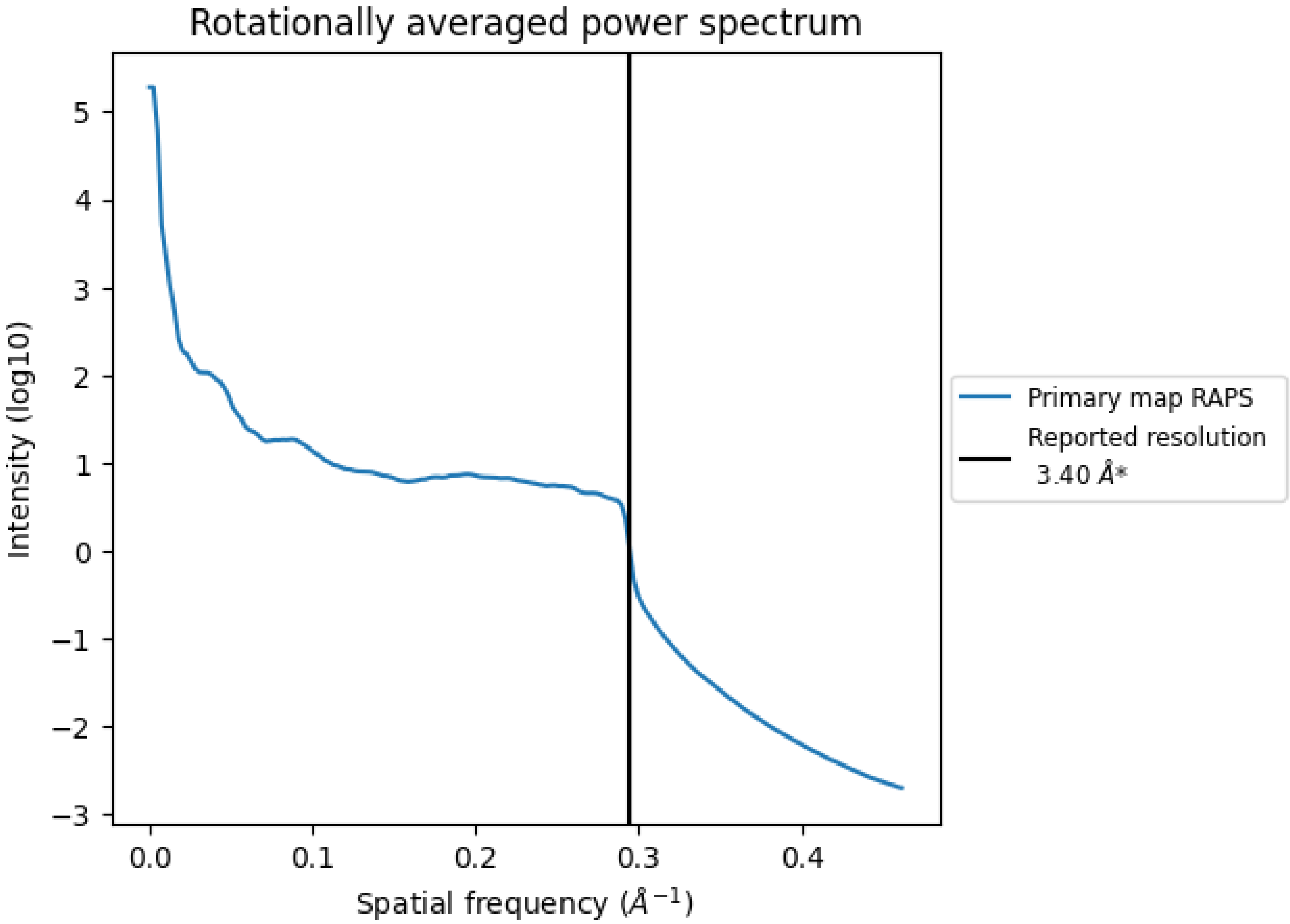
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 595 nm^3; this corresponds to an approximate mass of 537 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

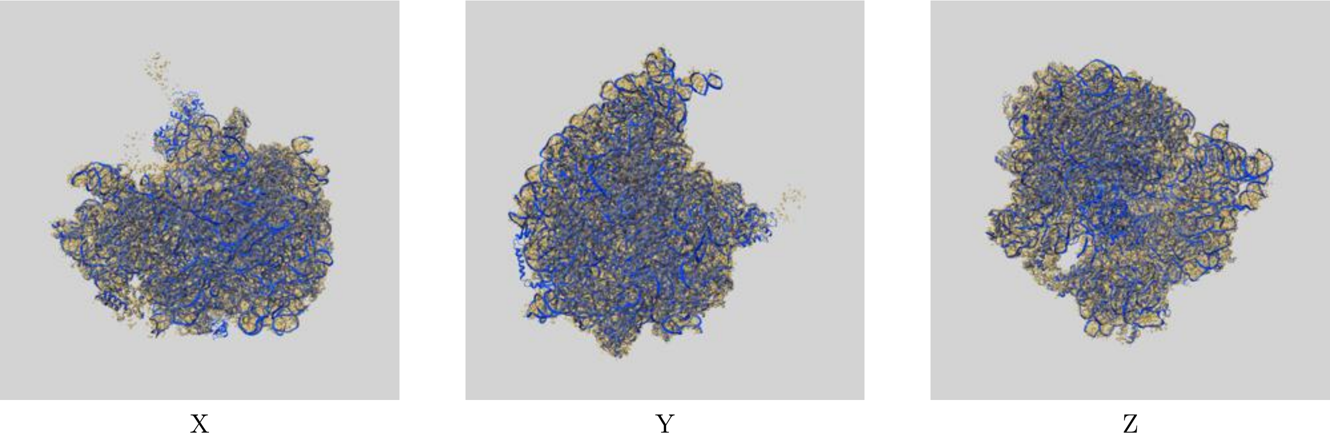
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

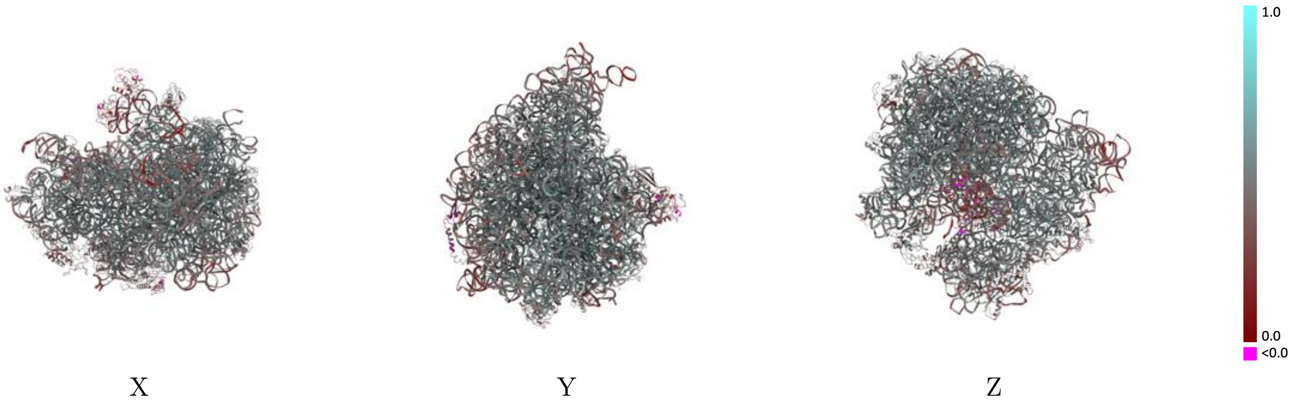
This section contains information regarding the fit between EMDB map EMD-3730 and PDB model 5O2R. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay ⓘ



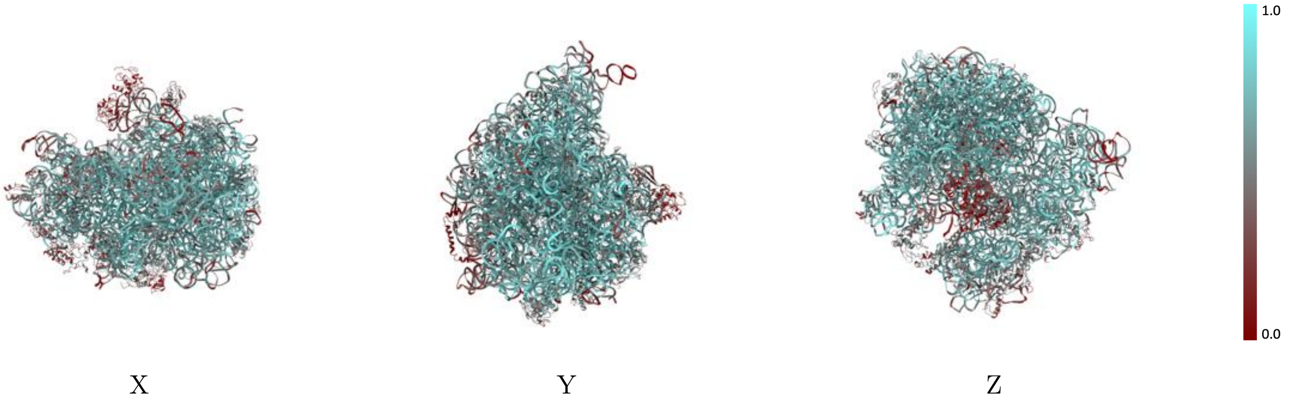
The images above show the 3D surface view of the map at the recommended contour level 0.407 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



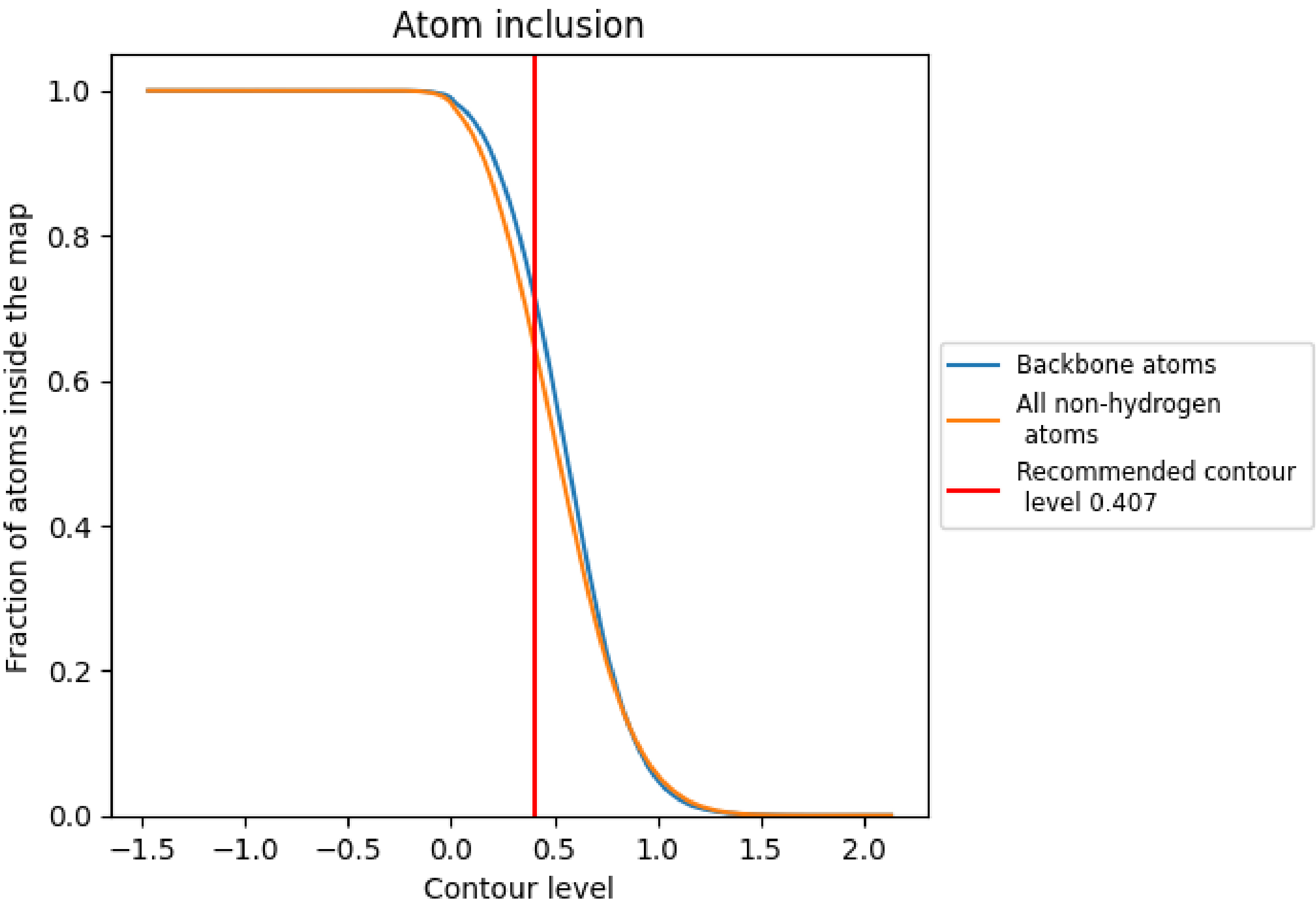
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.407).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.407) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.4760
0	0.6098	0.5100
1	0.5012	0.4880
2	0.6789	0.5170
3	0.6721	0.5400
4	0.5753	0.5170
5	0.0682	0.2130
6	0.3523	0.3920
7	0.8121	0.5450
A	0.7198	0.4880
B	0.7076	0.4730
C	0.6042	0.5210
D	0.5982	0.5120
E	0.5526	0.4840
F	0.4836	0.4530
G	0.3763	0.4170
H	0.1122	0.2790
I	0.0616	0.2140
J	0.5973	0.5110
K	0.5816	0.5030
L	0.5837	0.5060
M	0.5969	0.5180
N	0.6410	0.5220
O	0.5423	0.4760
P	0.5833	0.5040
Q	0.6564	0.5180
R	0.5521	0.4840
S	0.6005	0.5050
T	0.5277	0.4810
U	0.4889	0.4640
V	0.5461	0.4820
W	0.6440	0.5380
X	0.5474	0.4820
Y	0.4447	0.4330
Z	0.6133	0.5050

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Chain	Atom inclusion	Q-score
a	0.7026	0.4770
b	0.3552	0.3970
c	0.5209	0.4600
d	0.4428	0.4240
e	0.5862	0.4980
f	0.4334	0.4270
g	0.3934	0.4250
h	0.5385	0.4820
i	0.4709	0.4450
j	0.4389	0.4410
k	0.4959	0.4620
l	0.5787	0.4960
m	0.4853	0.4370
n	0.5664	0.4680
o	0.5435	0.4700
p	0.5295	0.4710
q	0.4699	0.4610
r	0.5381	0.4760
s	0.5040	0.4620
t	0.5031	0.4530
u	0.3130	0.3610
v	0.5063	0.4820
x	0.6132	0.4550
z	0.4779	0.4720