Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 01:44 am BST

PDB ID	:	6Q98
EMDB ID	:	EMD-4477
Title	:	Structure of tmRNA SmpB bound in P site of E. coli 70S ribosome
Authors	:	Rae, C.D.
Deposited on	:	2018-12-17
Resolution	:	4.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

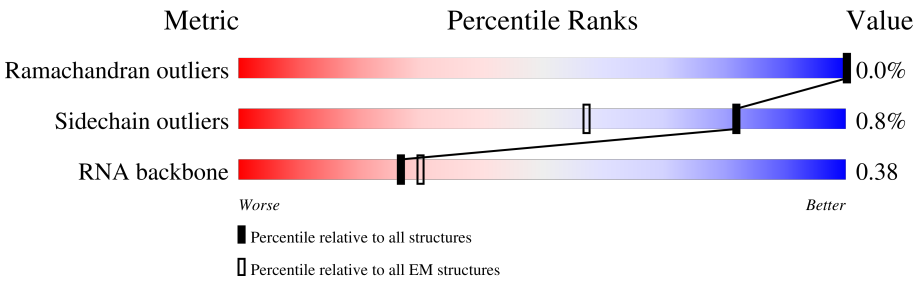
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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	1	2904	6% 58% 37% •
2	2	1535	10% 61% 34% 5%
3	3	120	7% 68% 28% •
4	5	160	59% 92% •• 6%
5	6	22	77% 100%
6	B	273	29% 99% •
7	C	209	20% 100%
8	D	201	31% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E	179	49% 98%
10	F	177	36% 98%
11	G	149	75% 100%
12	H	165	63% 78% 21%
13	I	142	80% 90% 5% 5%
14	J	142	20% 100%
15	K	123	24% 98%
16	L	144	22% 99%
17	M	136	22% 99%
18	N	127	16% 93% 6%
19	O	117	43% 98%
20	P	115	32% 97%
21	Q	118	11% 99%
22	R	103	25% 99%
23	S	110	19% 98%
24	T	100	33% 94% 6%
25	U	104	31% 97%
26	V	94	28% 100%
27	W	85	18% 88% 11%
28	X	78	19% 97%
29	Y	63	37% 97%
30	Z	59	19% 98%
31	a	70	64% 84% 16%
32	b	57	18% 93% 5%
33	c	55	40% 95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	d	46	26% 100%
35	e	65	20% 97%
36	f	38	21% 100%
37	g	241	75% 93% 7%
38	h	233	64% 89% 11%
39	i	206	61% 99%
40	j	167	30% 91% 7%
41	k	135	27% 76% 23%
42	l	179	69% 84% 16%
43	m	130	32% 98%
44	n	130	82% 96%
45	o	103	83% 94%
46	p	129	34% 90% 9%
47	q	124	35% 94%
48	r	118	82% 92% 5%
49	s	101	77% 99%
50	t	89	45% 98%
51	u	82	32% 98%
52	v	84	36% 94% 5%
53	w	75	32% 87% 12%
54	x	92	70% 89% 10%
55	y	87	44% 99%
56	z	71	56% 99%
57	4	363	79% 20% 44% 36%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	1	1618	X	-	-	-
1	PSU	1	1911	X	-	-	-
1	3TD	1	1915	X	-	-	-
1	PSU	1	1917	X	-	-	-
1	6MZ	1	2030	X	-	-	-
1	G7M	1	2069	X	-	-	-
1	OMG	1	2251	X	-	-	-
1	PSU	1	2457	X	-	-	-
1	OMC	1	2498	X	-	-	-
1	2MA	1	2503	X	-	-	-
1	PSU	1	2504	X	-	-	-
1	OMU	1	2552	X	-	-	-
1	PSU	1	2580	X	-	-	-
1	PSU	1	2605	X	-	-	-

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 153878 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	1	2903	62336	27816	11470	20147	2903	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	120	2569	1144	468	837	120	0	0

- Molecule 4 is a protein called SsrA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	150	1209	763	226	216	4	0	0

- Molecule 5 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	6	22	110	66	22	22	0	0

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	175	1313	826	241	244	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	130	980	620	174	182	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	135	984	622	171	185	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	123	946	593	181	166	6	0	0

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	144	1053	654	207	190	2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	119	951	588	195	163	5	0	0

- Molecule 19 is a protein called 50S ribosomal protein L18.

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

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	T	94	746	470	140	134	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	U	103	788	498	148	142	0	0

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	76	582	360	117	104	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	62	501	308	98	94	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	58	448	281	87	78	2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	a	59	472	293	89	84	6	0	0

- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	c	52	426	275	78	73	0	0

- Molecule 34 is a protein called 50S ribosomal protein L34.

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

- Molecule 35 is a protein called 50S ribosomal protein L35.

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

- Molecule 36 is a protein called 50S ribosomal protein L36.

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

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	225	1760	1113	316	323	8	0	0

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	208	1636	1036	307	290	3	0	0

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	156	1152	717	217	212	6	0	0

- Molecule 41 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	104	848	536	153	152	7	0	0

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

- Molecule 44 is a protein called 30S ribosomal protein S9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	99	790	495	151	143	1	0	0

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p	117	877	540	174	160	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	122	951	588	195	163	5	0	0

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	r	112	867	535	175	154	3	0	0

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s	100	805	499	164	139	3	0	0

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	w	66	544	344	102	97	1	0	0

- Molecule 54 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	x	83	663	424	126	111	2	0	0

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	y	86	669	414	138	114	3	0	0

- Molecule 56 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	z	70	589	366	125	97	1	0	0

- Molecule 57 is a RNA chain called transfer-messenger RNA (tmRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	4	363	7758	3465	1410	2520	363	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	1	283	283	283	0
58	2	126	126	126	0
58	3	8	8	8	0
58	B	2	2	2	0
58	C	1	1	1	0
58	L	2	2	2	0
58	N	1	1	1	0
58	U	1	1	1	0
58	f	1	1	1	0
58	i	1	1	1	0
58	r	2	2	2	0
58	4	1	1	1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	a	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	f	1	1	1	0

- Molecule 60 is water.

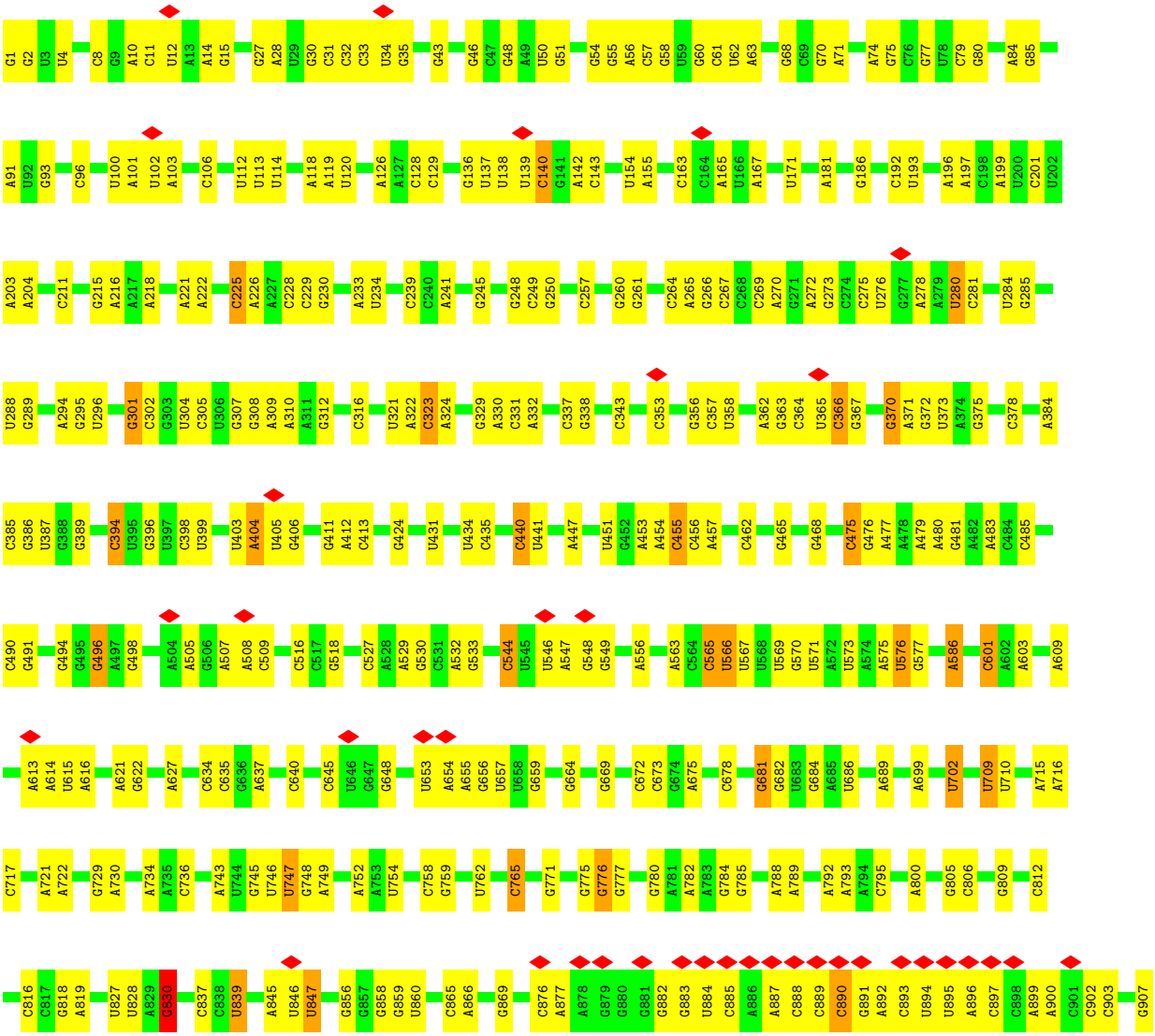
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
60	B	2	2	2	0

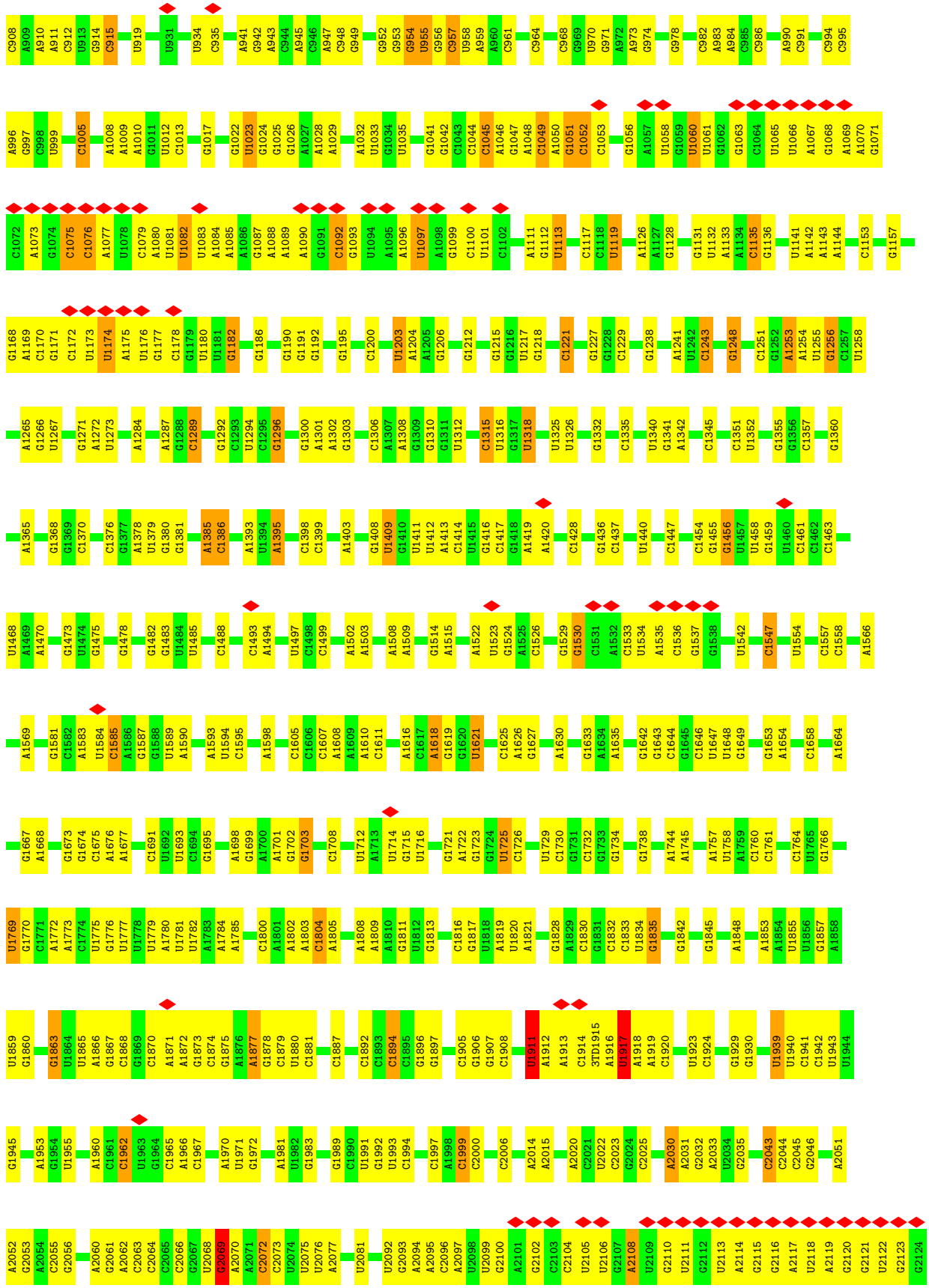
3 Residue-property plots (i)

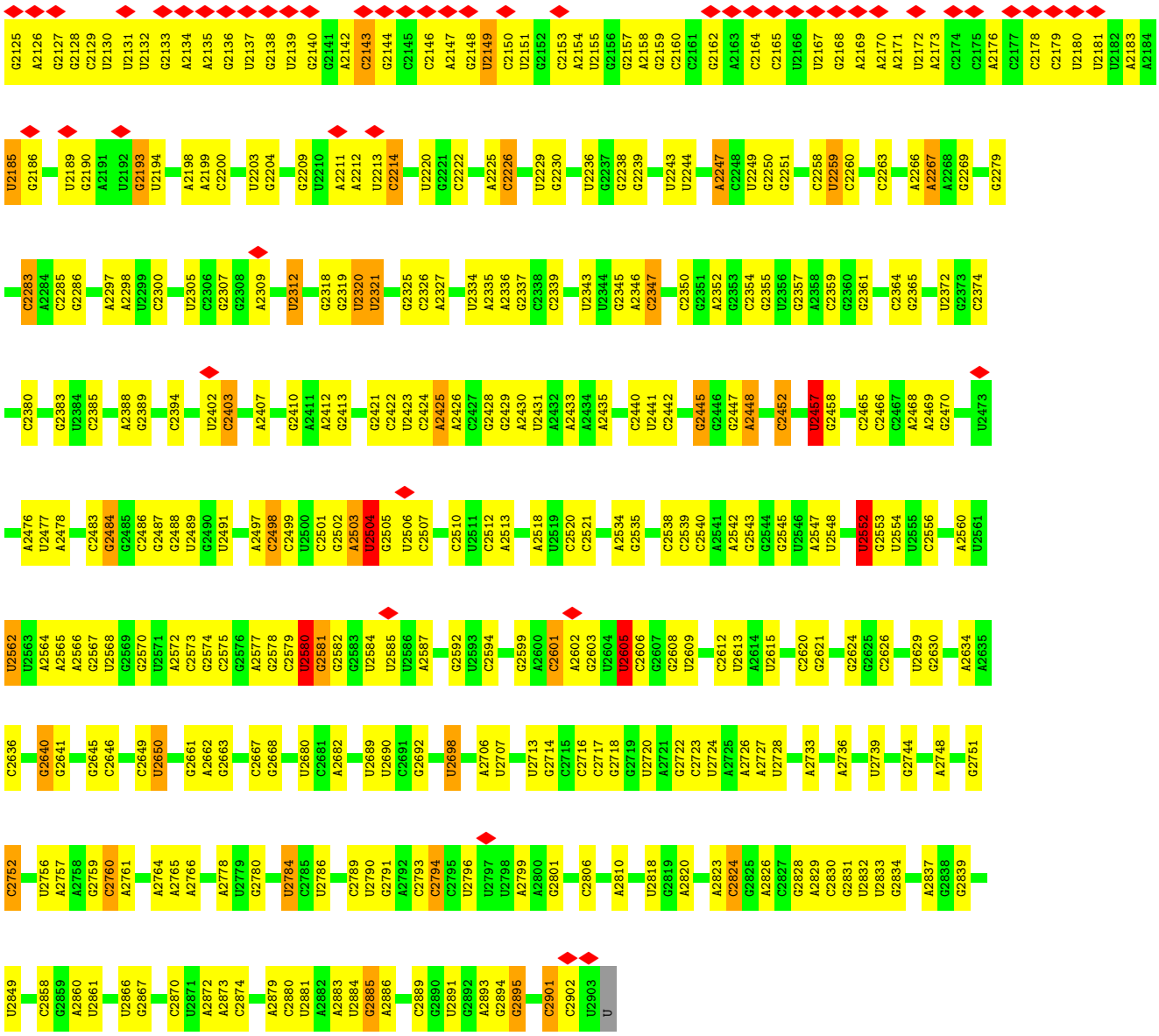
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 1:

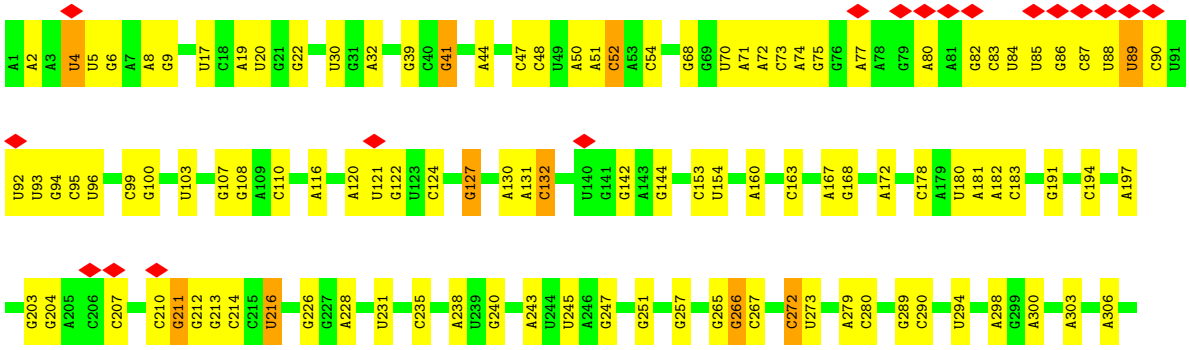


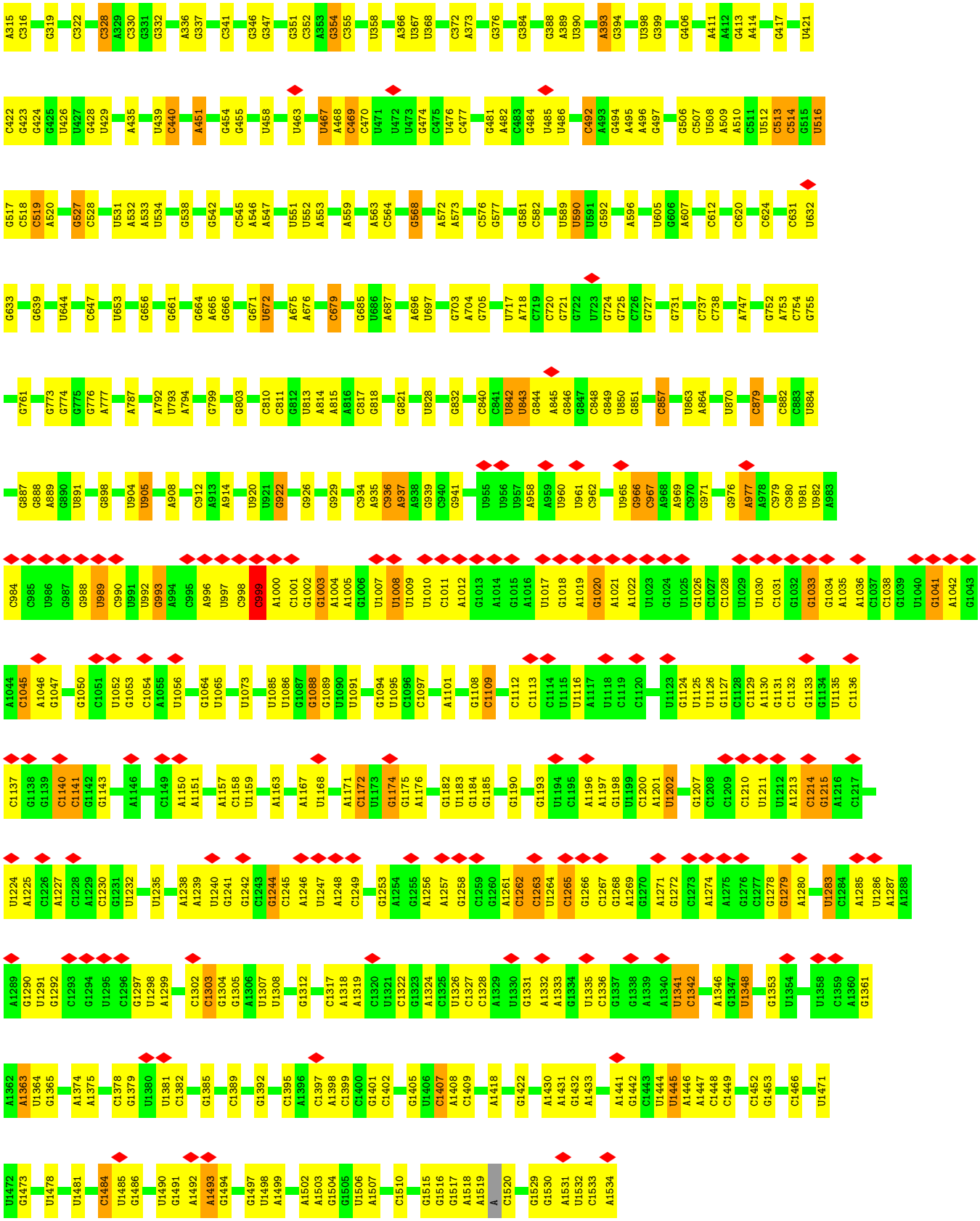

C908 A909 A910 A911 C912 U913 G914 C915 U919 U931 U934 C935 A941 G942 A943 C944 A945 C946 A947 C948 G949 G952 G953 G954 U955 G956 C957 U958 A959 A960 C961 C964 C968 G969 U970 G971 A972 A973 G974 G978 C982 A983 A984 C985 C986 A990 C991 C994 C995
A996 G997 C998 U999 C1005 A1008 A1009 A1010 G1011 U1012 C1013 G1017 G1022 U1023 G1024 G1025 G1026 A1027 A1028 A1029 A1032 U1033 G1034 U1035 G1041 G1042 C1043 C1044 C1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 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 A1111 G1112 U1113 C1117 C1118 U1119 A1126 A1127 G1128 G1131 U1132 A1133 A1134 C1135 G1136 U1141 A1142 A1143 A1144 C1153 G1157
G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 G1186 G1190 G1191 G1192 G1195 C1200 U1203 A1204 A1205 G1206 G1212 G1215 G1216 U1217 G1218 C1221 G1227 G1228 C1229 G1238 A1241 U1242 C1243 G1248 C1251 G1252 A1253 A1254 U1255 G1256 C1257 U1258
A1265 G1266 U1267 G1271 A1272 U1273 A1284 A1287 G1288 C1289 G1292 C1293 U1294 C1295 G1296 G1300 A1301 A1302 G1303 C1306 A1307 A1308 G1309 G1310 G1311 U1312 C1315 U1316 G1317 U1318 U1325 U1326 G1332 C1335 U1340 G1341 A1342 C1345 C1351 U1352 G1355 G1356 C1357 G1360
A1365 G1368 G1369 C1370 C1376 G1377 A1378 U1379 G1380 G1381 A1385 C1386 A1393 U1394 A1395 C1398 C1399 A1403 G1408 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 C1428 G1436 C1437 U1440 C1447 C1454 G1455 G1456 U1457 U1458 G1459 U1460 C1461 G1462 C1463
U1468 A1469 A1470 G1473 U1474 G1475 G1478 G1482 G1483 U1484 U1485 C1488 C1493 A1494 U1497 C1498 C1499 A1502 A1503 A1508 A1509 G1514 A1515 A1522 U1523 G1524 A1525 C1526 G1529 G1530 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1542 C1547 U1554 C1557 C1558 A1566
A1569 G1581 C1582 A1583 U1584 C1585 A1586 G1587 G1588 U1589 A1590 A1593 U1594 C1595 A1598 C1605 C1606 C1607 A1608 A1609 A1610 C1611 A1616 C1617 A1618 G1619 G1620 U1621 C1625 A1626 G1627 A1630 G1633 A1634 A1635 G1642 G1643 C1644 G1645 C1646 U1647 U1648 G1649 G1653 A1654 C1658 A1664
G1667 A1668 G1673 G1674 C1675 A1676 A1677 C1691 U1692 U1693 C1694 G1695 A1698 G1699 A1700 A1701 G1702 G1703 C1708 U1712 A1713 U1714 G1715 U1716 G1721 A1722 G1723 G1724 U1725 C1726 U1729 C1730 C1731 C1732 G1733 G1734 G1738 A1744 A1745 A1757 U1758 A1759 C1760 C1761 C1764 U1765 G1766
U1769 G1770 C1771 A1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 U1781 U1782 A1783 A1784 A1785 C1800 A1801 A1802 A1803 C1804 A1805 A1808 A1809 A1810 G1811 U1812 G1813 C1816 G1817 U1818 A1819 U1820 A1821 G1828 A1829 C1830 G1831 C1832 C1833 U1834 G1835 G1842 G1845 A1848 A1853 A1854 U1855 U1856 G1857 A1858
U1859 G1860 G1863 U1864 U1865 A1866 A1867 C1868 G1869 C1870 A1871 A1872 G1873 C1874 G1875 A1876 A1877 G1878 C1879 U1880 C1881 C1887 C1892 C1893 C1894 C1895 G1896 G1897 C1905 G1906 G1907 C1908 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 C1920 U1923 C1924 G1929 G1930 U1939 U1940 C1941 C1942 U1943 U1944
G1945 A1953 G1954 U1955 A1960 C1961 C1962 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 A1981 U1982 G1983 G1989 C1990 U1991 G1992 U1993 C1994 C1997 A1998 C1999 C2000 C2006 A2014 A2015 A2020 C2021 U2022 C2023 G2024 C2025 A2030 A2031 G2032 A2033 U2034 G2035 C2043 C2044 C2045 G2046 A2051
A2052 G2053 A2054 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 A2070 A2071 C2072 C2073 U2074 U2075 U2076 A2077 U2081 U2092 G2093 A2094 A2095 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



• Molecule 2: 16S ribosomal RNA

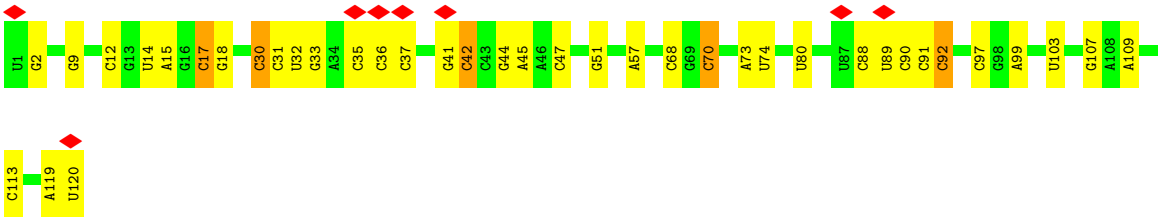
Chain 2:





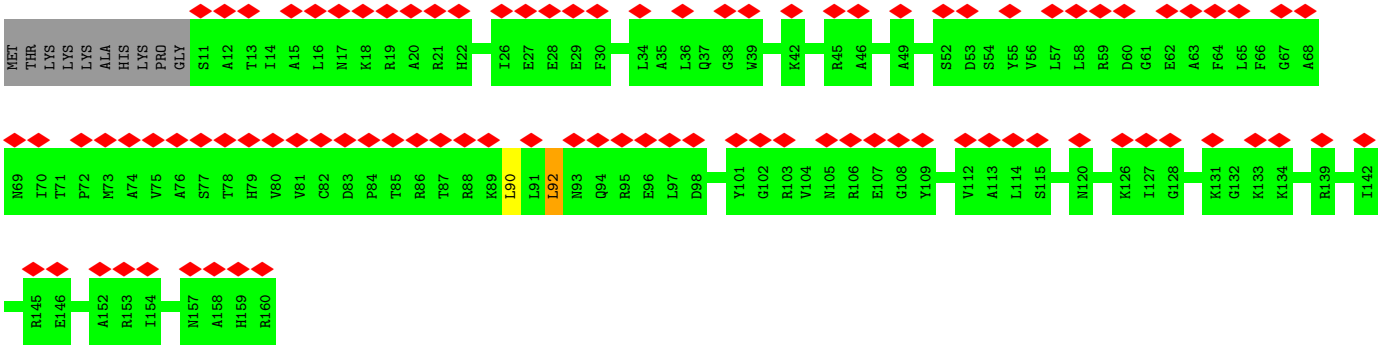
- Molecule 3: 5S ribosomal RNA

Chain 3: 7% 68% 28% •



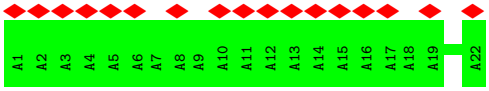
- Molecule 4: SsrA-binding protein

Chain 5: 59% 92% •• 6%



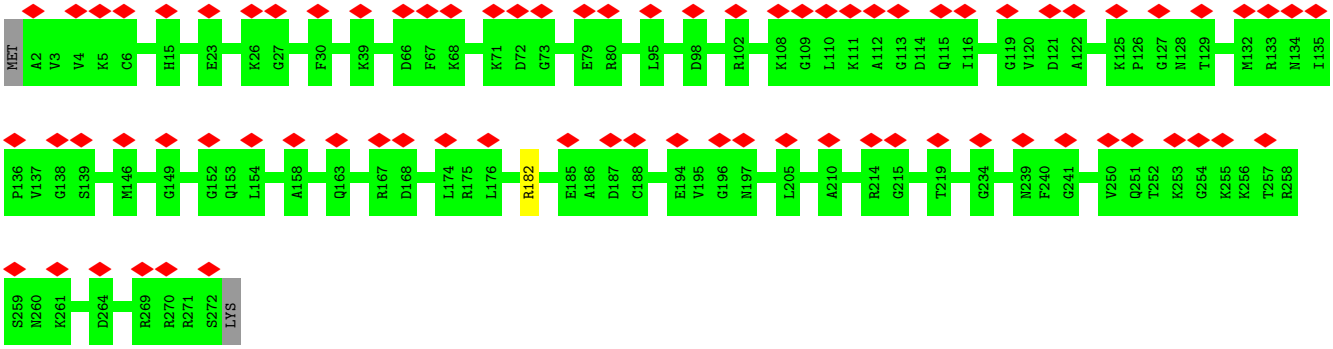
- Molecule 5: Nascent peptide

Chain 6: 77% 100%



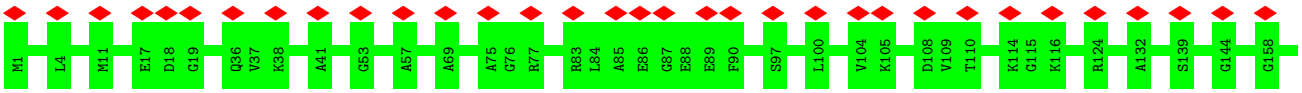
- Molecule 6: 50S ribosomal protein L2

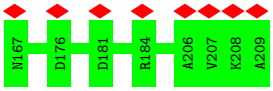
Chain B: 29% 99% •



- Molecule 7: 50S ribosomal protein L3

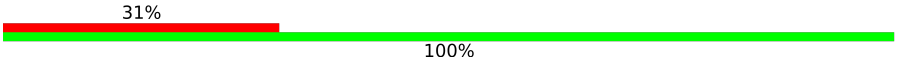
Chain C: 20% 100%

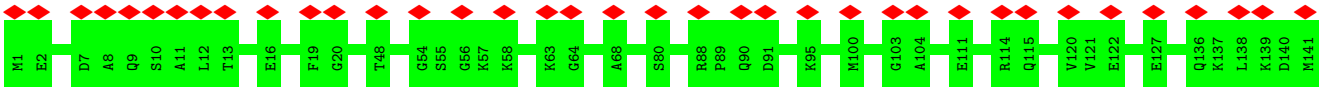


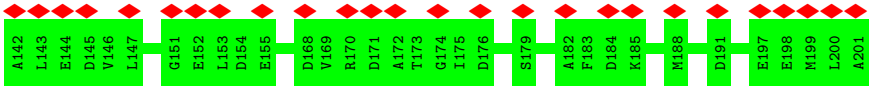


- Molecule 8: 50S ribosomal protein L4

Chain D:

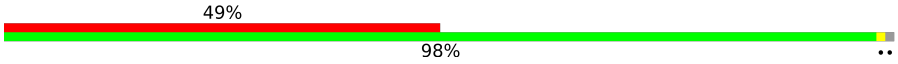


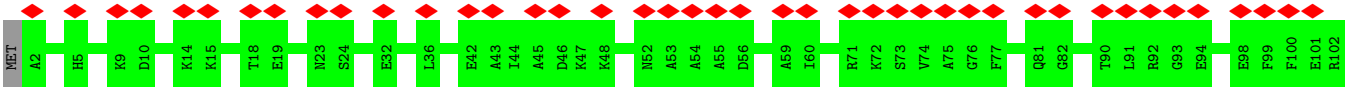


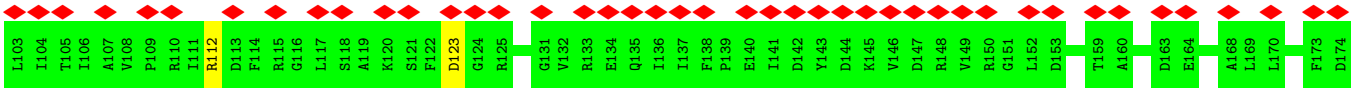


- Molecule 9: 50S ribosomal protein L5

Chain E:

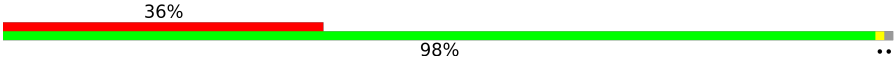


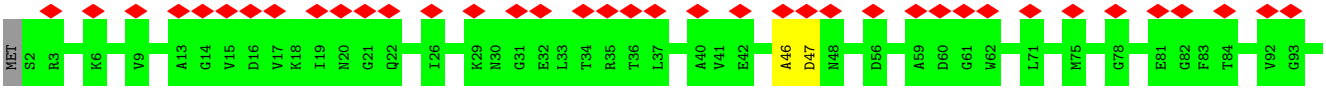


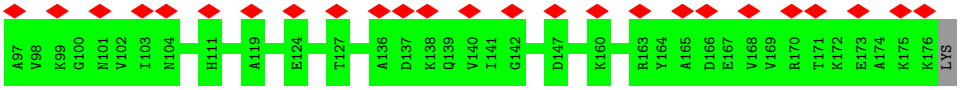


- Molecule 10: 50S ribosomal protein L6

Chain F:

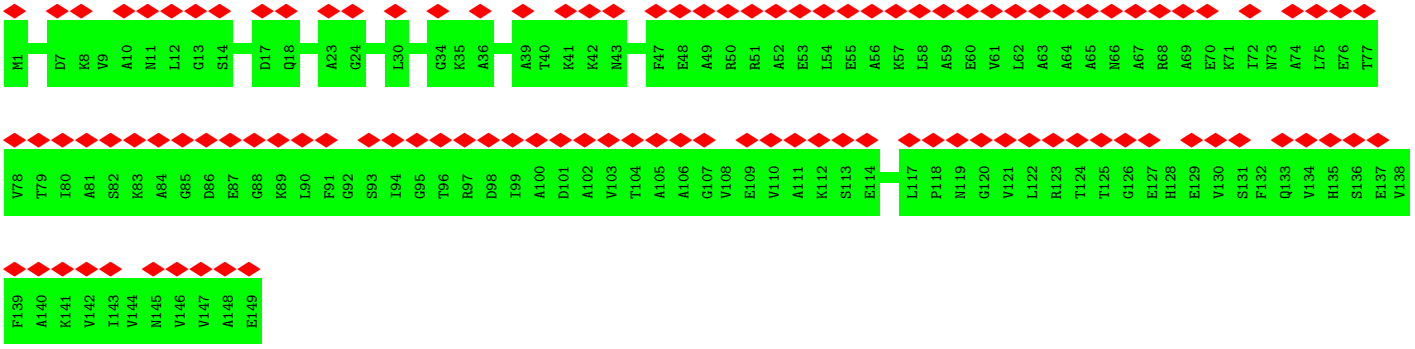






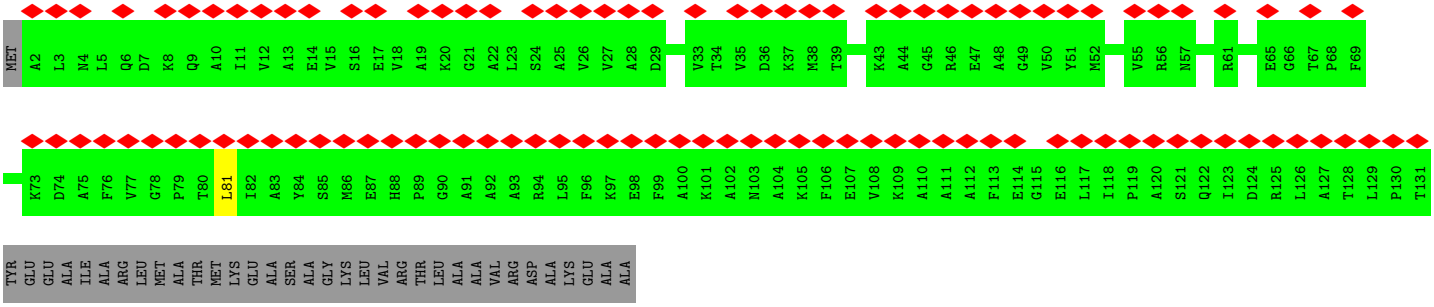
- Molecule 11: 50S ribosomal protein L9

Chain G:



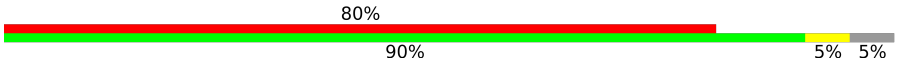
- Molecule 12: 50S ribosomal protein L10

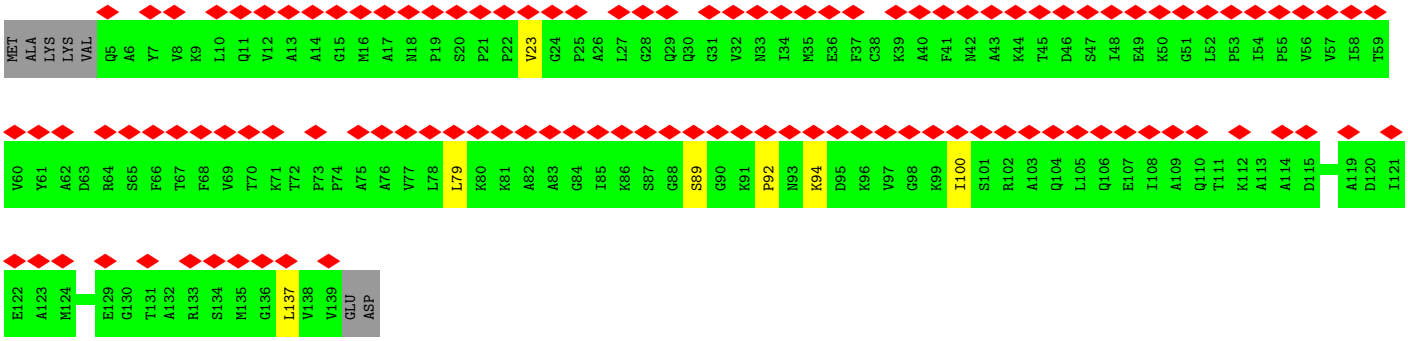
Chain H:



- Molecule 13: 50S ribosomal protein L11

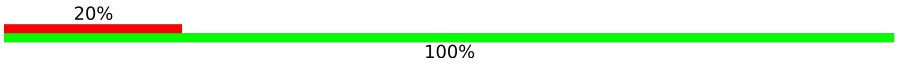
Chain I:

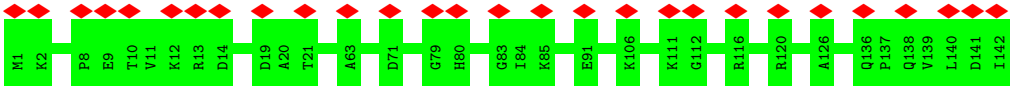




- Molecule 14: 50S ribosomal protein L13

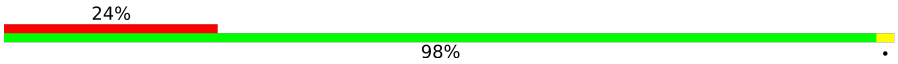
Chain J:

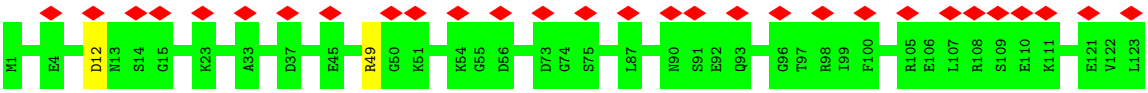




- Molecule 15: 50S ribosomal protein L14

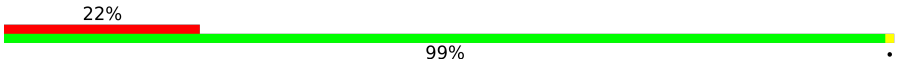
Chain K:

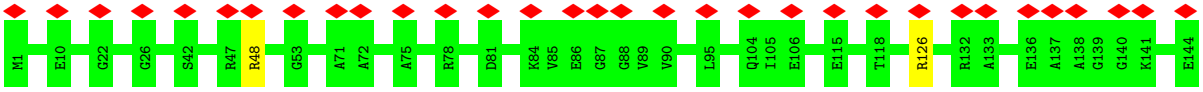




• Molecule 16: 50S ribosomal protein L15

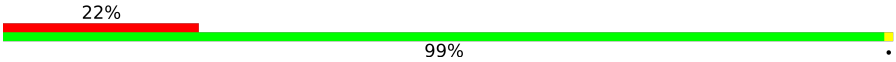
Chain L:

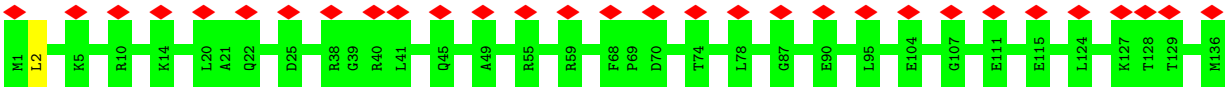




• Molecule 17: 50S ribosomal protein L16

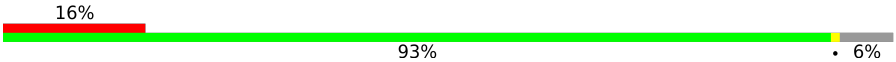
Chain M:

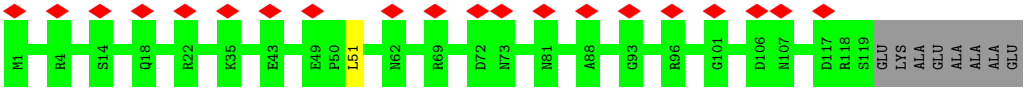




• Molecule 18: 50S ribosomal protein L17

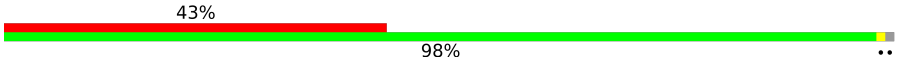
Chain N:

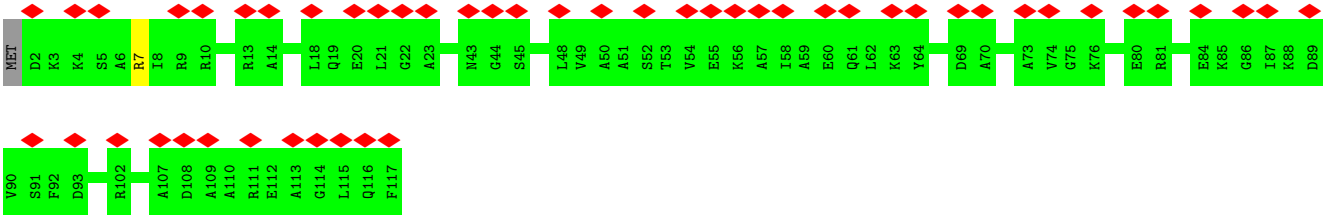




• Molecule 19: 50S ribosomal protein L18

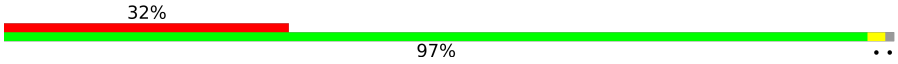
Chain O:

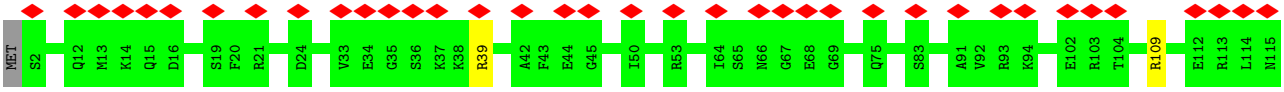




• Molecule 20: 50S ribosomal protein L19

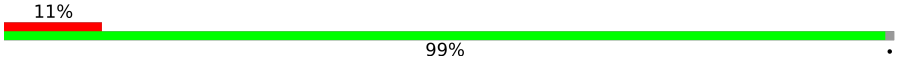
Chain P:

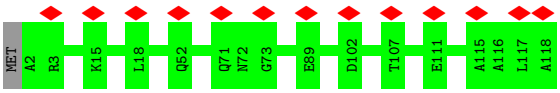




• Molecule 21: 50S ribosomal protein L20

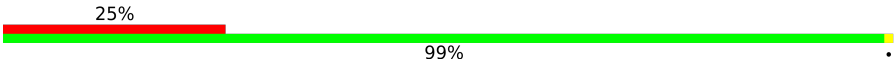
Chain Q:

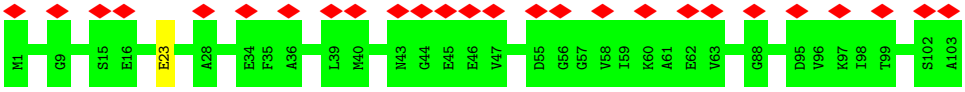




• Molecule 22: 50S ribosomal protein L21

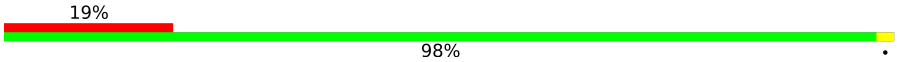
Chain R:

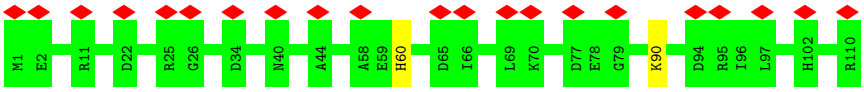




• Molecule 23: 50S ribosomal protein L22

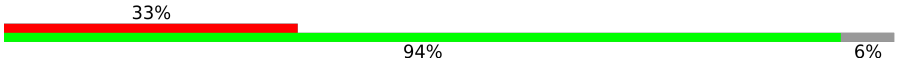
Chain S:

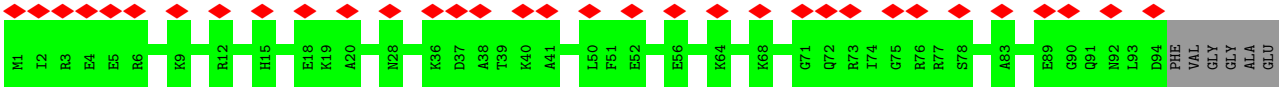




• Molecule 24: 50S ribosomal protein L23

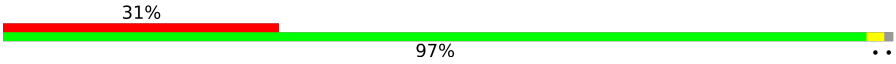
Chain T:

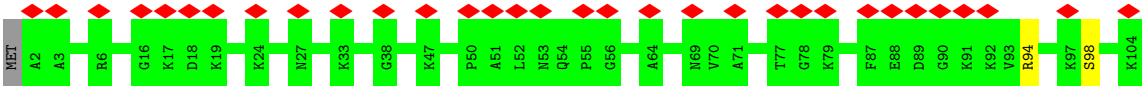




• Molecule 25: 50S ribosomal protein L24

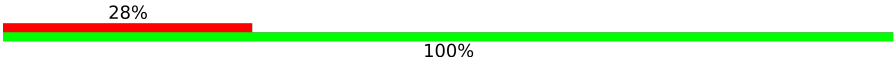
Chain U:

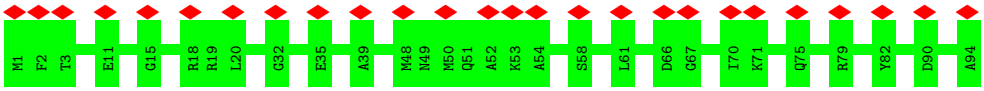




• Molecule 26: 50S ribosomal protein L25

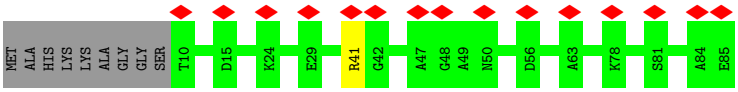
Chain V:





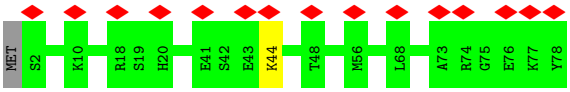
• Molecule 27: 50S ribosomal protein L27

Chain W:



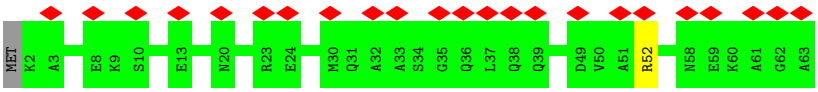
• Molecule 28: 50S ribosomal protein L28

Chain X: 19% 97%



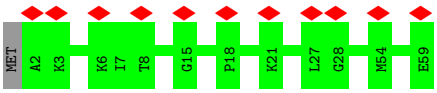
• Molecule 29: 50S ribosomal protein L29

Chain Y: 37% 97%



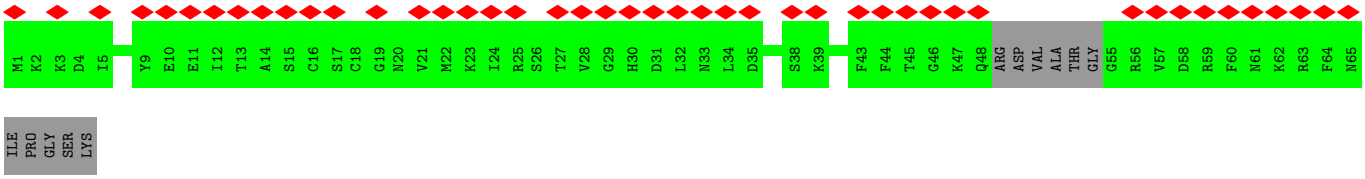
• Molecule 30: 50S ribosomal protein L30

Chain Z: 19% 98%



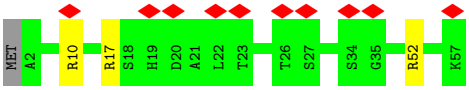
• Molecule 31: 50S ribosomal protein L31

Chain a: 64% 84% 16%



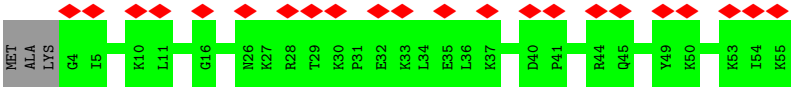
• Molecule 32: 50S ribosomal protein L32

Chain b: 18% 93% 5%



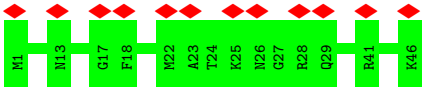
• Molecule 33: 50S ribosomal protein L33

Chain c: 40% 95% 5%



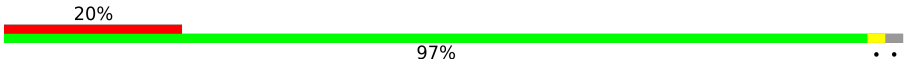
• Molecule 34: 50S ribosomal protein L34

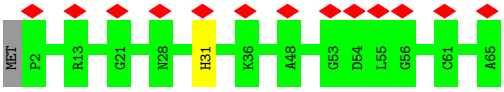
Chain d: 26% 100%



• Molecule 35: 50S ribosomal protein L35

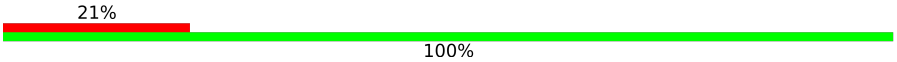
Chain e:

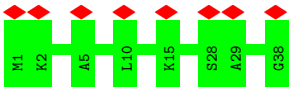




• Molecule 36: 50S ribosomal protein L36

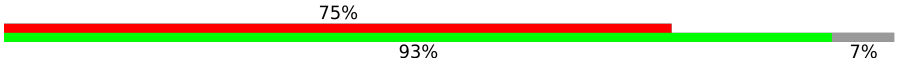
Chain f:

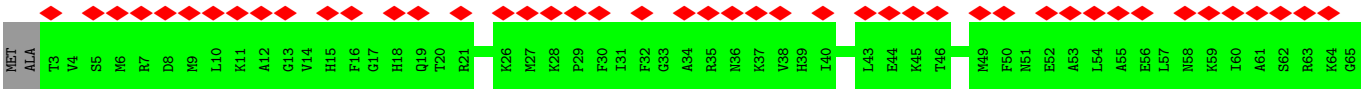


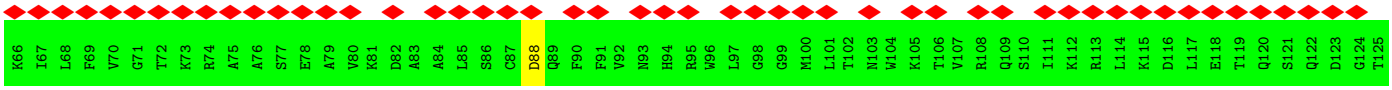


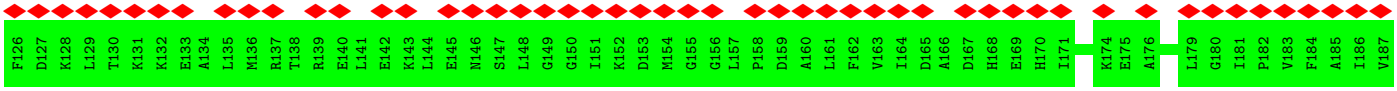
• Molecule 37: 30S ribosomal protein S2

Chain g:



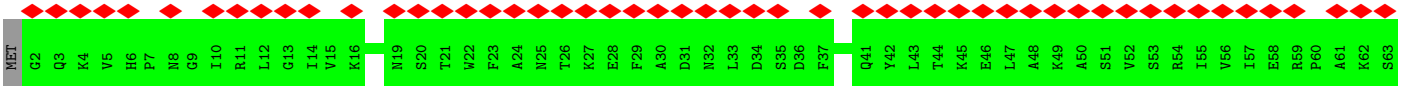


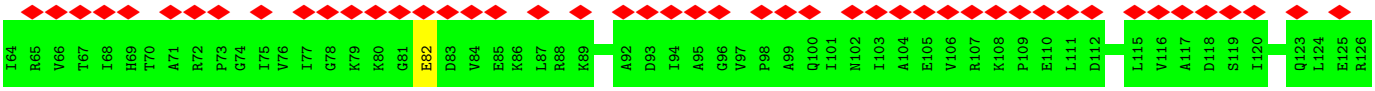


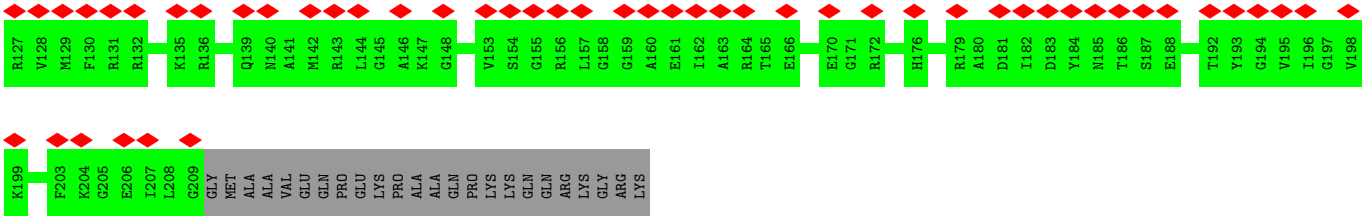


• Molecule 38: 30S ribosomal protein S3

Chain h:

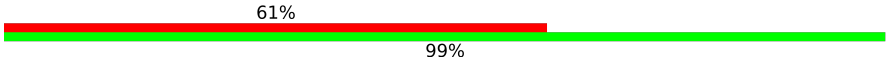


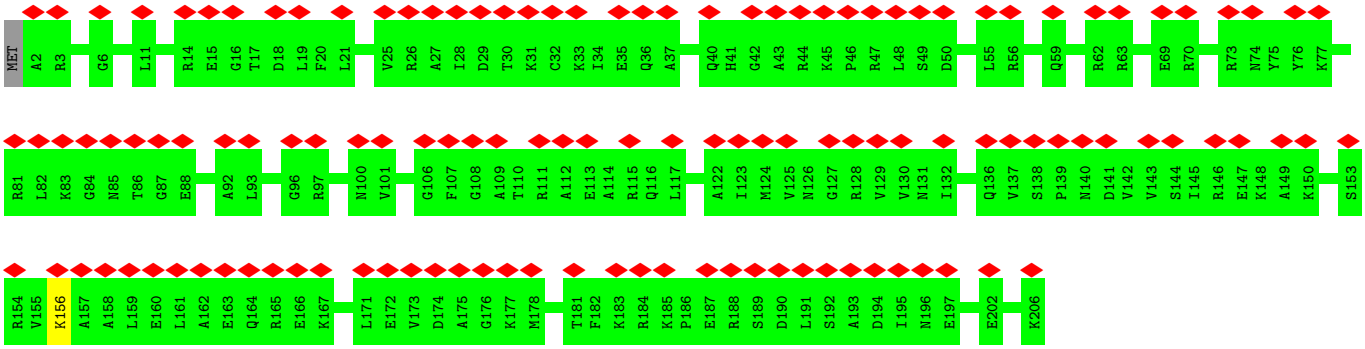




• Molecule 39: 30S ribosomal protein S4

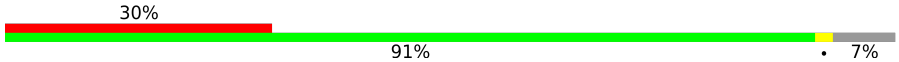
Chain i:

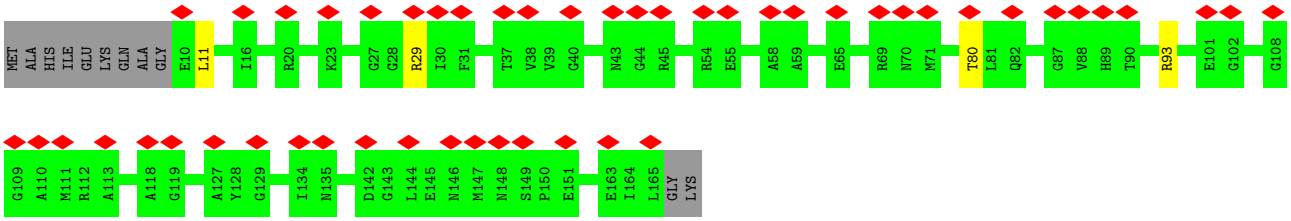




• Molecule 40: 30S ribosomal protein S5

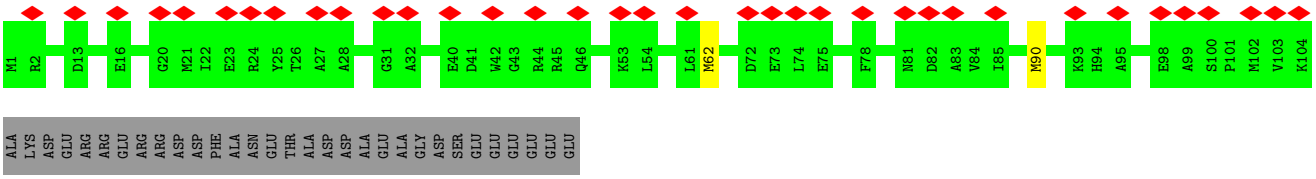
Chain j:





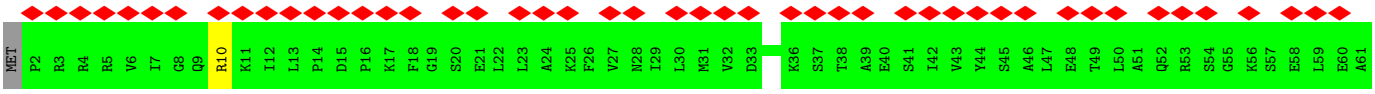
• Molecule 41: 30S ribosomal protein S6

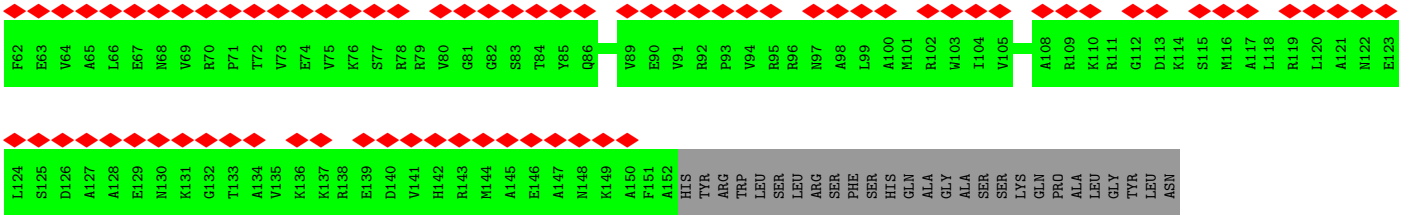
Chain k:



• Molecule 42: 30S ribosomal protein S7

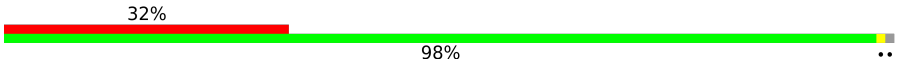
Chain l:

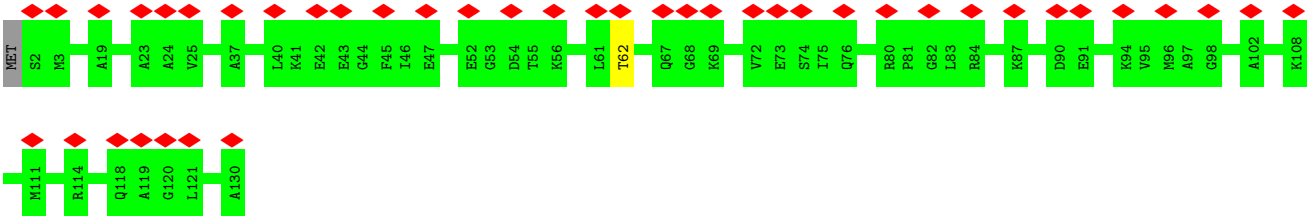




- Molecule 43: 30S ribosomal protein S8

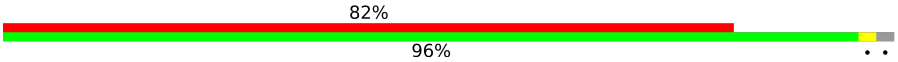
Chain m:

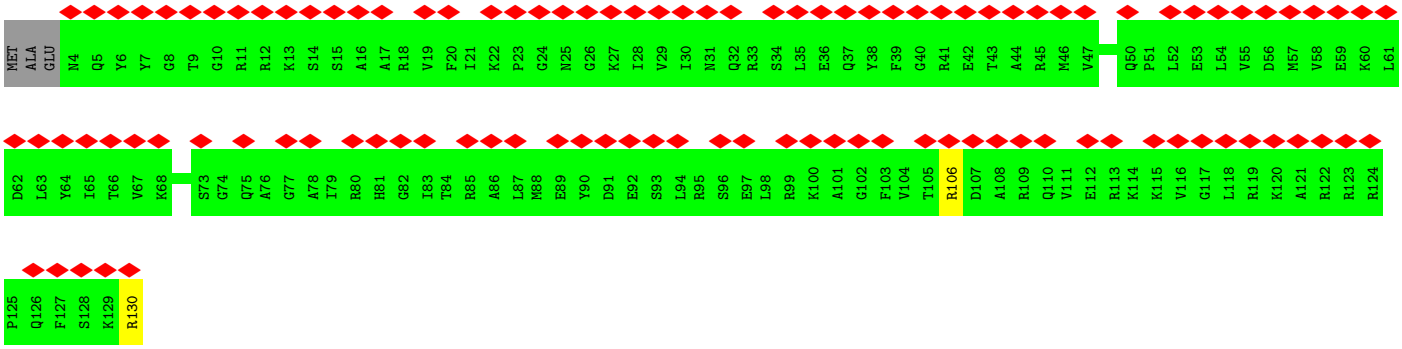




- Molecule 44: 30S ribosomal protein S9

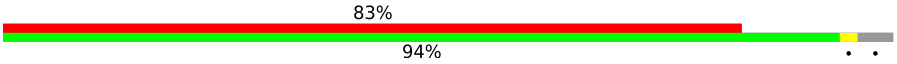
Chain n:





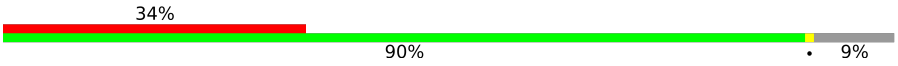
- Molecule 45: 30S ribosomal protein S10

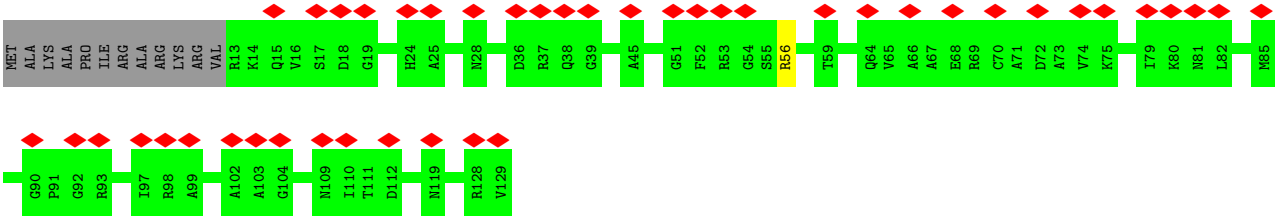
Chain o:



- Molecule 46: 30S ribosomal protein S11

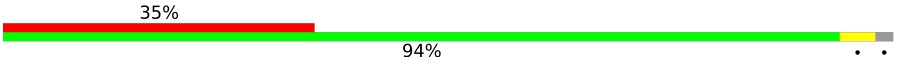
Chain p:

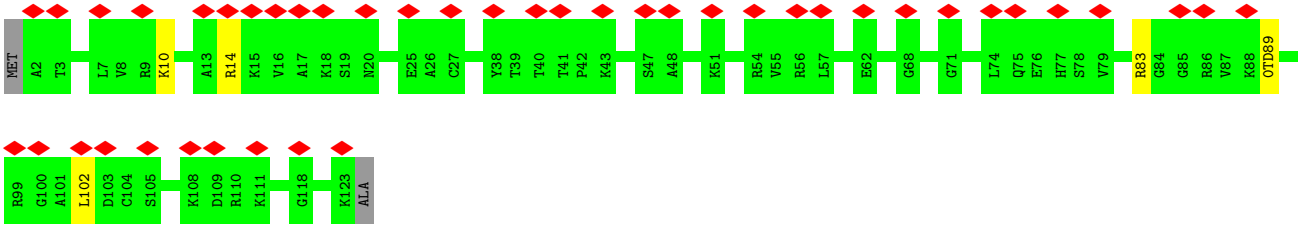




- Molecule 47: 30S ribosomal protein S12

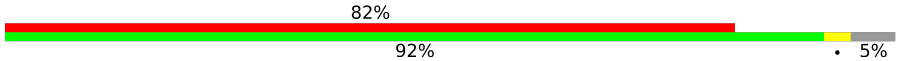
Chain q:

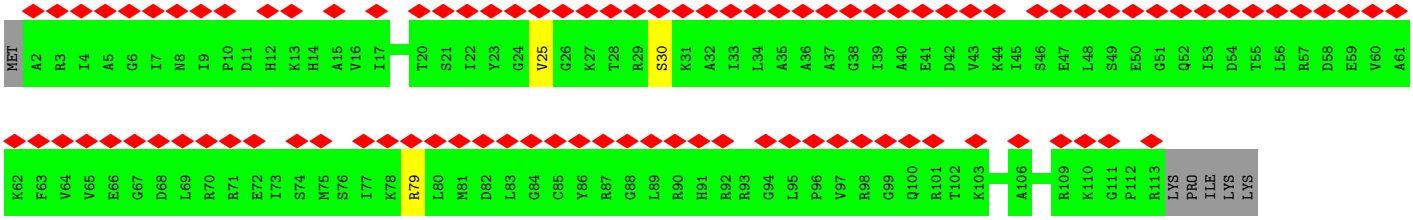




- Molecule 48: 30S ribosomal protein S13

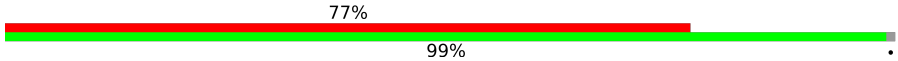
Chain r:

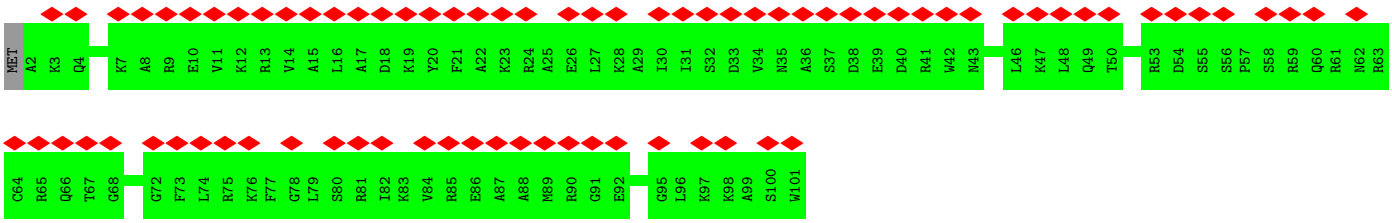




- Molecule 49: 30S ribosomal protein S14

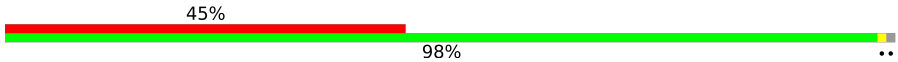
Chain s:

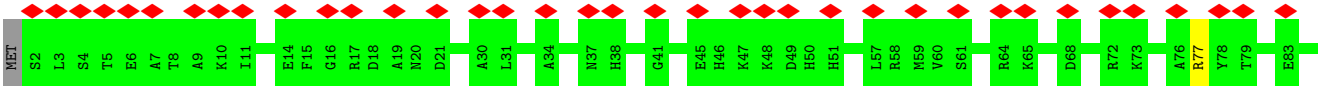




- Molecule 50: 30S ribosomal protein S15

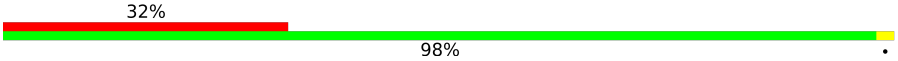
Chain t:

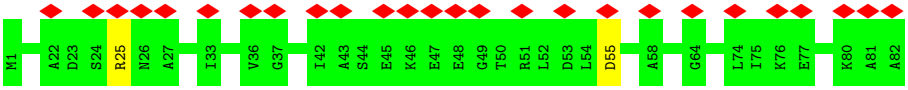




• Molecule 51: 30S ribosomal protein S16

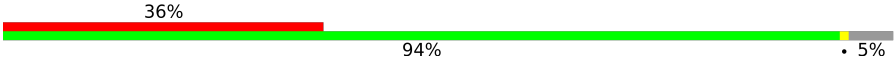
Chain u:

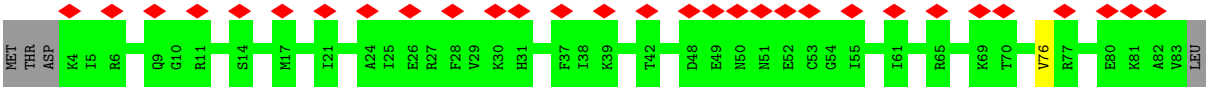




• Molecule 52: 30S ribosomal protein S17

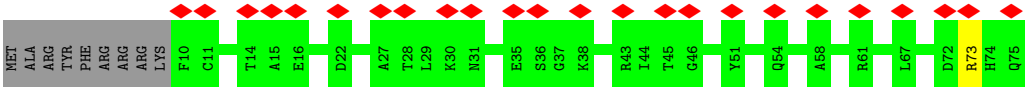
Chain v:





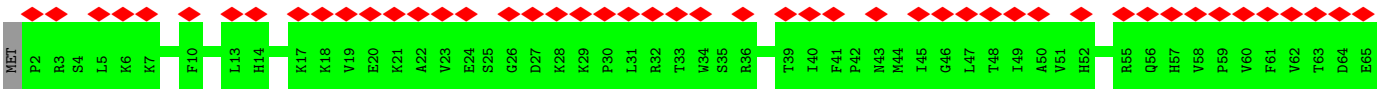
• Molecule 53: 30S ribosomal protein S18

Chain w:



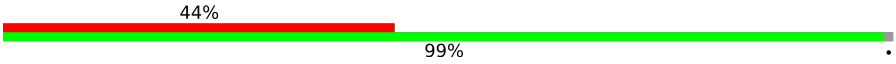
• Molecule 54: 30S ribosomal protein S19

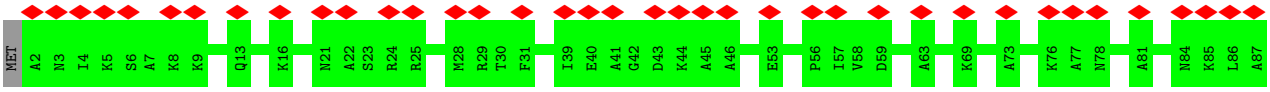
Chain x:



• Molecule 55: 30S ribosomal protein S20

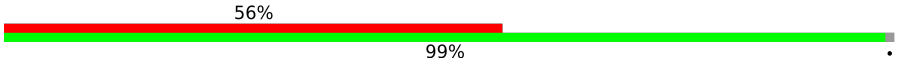
Chain y:

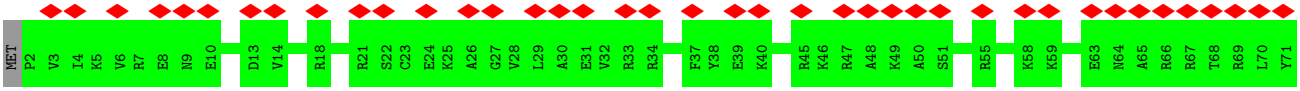




• Molecule 56: 30S ribosomal protein S21

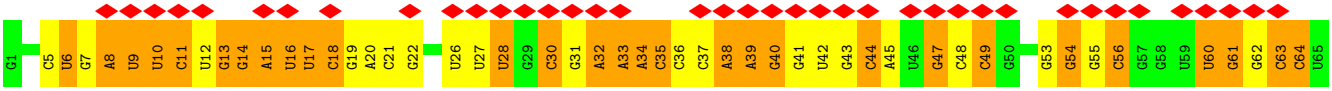
Chain z:

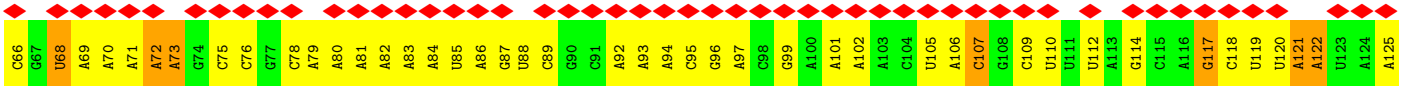


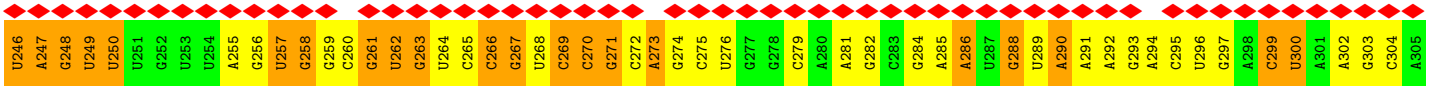


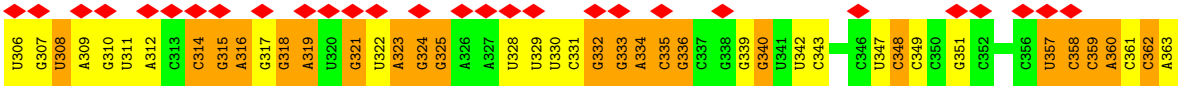
• Molecule 57: transfer-messenger RNA (tmRNA)

Chain 4:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	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	0.407	Depositor
Minimum map value	-0.269	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0934	Depositor
Map size (Å)	437.0, 437.0, 437.0	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, 5MU, G7M, MG, ZN, OMC, 6MZ, 1MG, 5MC, OMG, 0TD, 2MG, 7MG, OMU, 2MA, UR3, 3TD, PSU, MA6

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	1	0.91	8/69285 (0.0%)	1.33	664/108083 (0.6%)
2	2	0.74	0/36587	1.28	306/57062 (0.5%)
3	3	0.73	0/2872	1.22	19/4478 (0.4%)
4	5	0.42	0/1231	0.67	0/1655
5	6	0.30	0/109	0.70	0/151
6	B	0.43	0/2121	0.62	0/2852
7	C	0.42	0/1586	0.63	0/2134
8	D	0.41	0/1571	0.59	0/2113
9	E	0.37	0/1434	0.62	0/1926
10	F	0.35	0/1333	0.59	0/1805
11	G	0.32	0/1122	0.59	0/1515
12	H	0.39	0/993	0.75	1/1340 (0.1%)
13	I	0.31	0/998	0.69	3/1348 (0.2%)
14	J	0.43	0/1152	0.57	0/1551
15	K	0.42	0/955	0.62	1/1279 (0.1%)
16	L	0.38	0/1062	0.61	0/1413
17	M	0.51	1/1093 (0.1%)	0.59	0/1460
18	N	0.43	0/964	0.69	2/1289 (0.2%)
19	O	0.35	0/902	0.53	0/1209
20	P	0.42	0/929	0.59	0/1242
21	Q	0.48	0/960	0.55	0/1278
22	R	0.45	0/829	0.60	0/1107
23	S	0.42	0/864	0.61	0/1156
24	T	0.37	0/752	0.55	0/1005
25	U	0.39	0/796	0.60	1/1062 (0.1%)
26	V	0.38	0/766	0.57	0/1025
27	W	0.42	0/589	0.59	0/779
28	X	0.40	0/635	0.57	0/848
29	Y	0.33	0/502	0.52	0/667
30	Z	0.36	0/452	0.59	0/605
31	a	0.31	0/480	0.52	0/638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.42	0/450	0.66	0/599
33	c	0.38	0/433	0.61	0/576
34	d	0.39	0/380	0.62	0/498
35	e	0.42	0/513	0.67	0/676
36	f	0.44	0/303	0.62	0/397
37	g	0.33	0/1791	0.61	1/2413 (0.0%)
38	h	0.34	0/1663	0.59	0/2241
39	i	0.35	0/1665	0.53	0/2227
40	j	0.39	0/1165	0.64	0/1568
41	k	0.36	0/867	0.61	0/1171
42	l	0.31	0/1195	0.58	0/1602
43	m	0.39	0/989	0.62	0/1326
44	n	0.32	0/1034	0.60	0/1375
45	o	0.32	0/800	0.65	1/1082 (0.1%)
46	p	0.35	0/893	0.60	0/1205
47	q	0.40	0/954	0.68	0/1279
48	r	0.32	0/875	0.68	0/1170
49	s	0.31	0/817	0.52	0/1088
50	t	0.35	0/722	0.60	0/964
51	u	0.36	0/659	0.62	1/884 (0.1%)
52	v	0.38	0/657	0.62	0/881
53	w	0.36	0/553	0.50	0/743
54	x	0.32	0/680	0.56	0/915
55	y	0.30	0/675	0.50	0/895
56	z	0.35	0/597	0.53	0/792
57	4	0.80	3/8680 (0.0%)	2.16	591/13528 (4.4%)
All	All	0.74	12/165934 (0.0%)	1.23	1591/248170 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	26	1
2	2	0	1
4	5	0	1
10	F	0	1
13	I	0	2
22	R	0	1
23	S	0	1
35	e	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
38	h	0	1
43	m	0	1
47	q	0	1
53	w	0	1
All	All	26	13

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	M	2	LEU	C-N	-9.15	1.13	1.34
57	4	335	C	N1-C2	6.53	1.46	1.40
1	1	1253	A	N9-C4	-6.17	1.34	1.37
1	1	586	A	N9-C4	-6.08	1.34	1.37
57	4	237	U	N1-C2	6.07	1.44	1.38
1	1	978	G	C2-N3	-6.05	1.27	1.32
1	1	2448	A	N9-C4	-5.92	1.34	1.37
1	1	809	G	N7-C5	-5.11	1.36	1.39
57	4	32	A	N9-C4	5.11	1.41	1.37
1	1	2592	G	N7-C5	-5.10	1.36	1.39
1	1	2542	A	N9-C4	-5.10	1.34	1.37
1	1	2020	A	N9-C4	-5.08	1.34	1.37

All (1591) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	335	C	N1-C2-O2	20.18	131.01	118.90
57	4	335	C	N3-C2-O2	-19.68	108.12	121.90
57	4	335	C	C6-N1-C2	-15.59	114.06	120.30
57	4	173	C	N1-C2-O2	15.35	128.11	118.90
57	4	30	C	C6-N1-C2	-15.28	114.19	120.30
57	4	154	C	N1-C2-O2	15.28	128.07	118.90
57	4	237	U	N3-C2-O2	-14.74	111.88	122.20
57	4	154	C	N3-C2-O2	-13.87	112.19	121.90
57	4	362	C	C6-N1-C2	-13.68	114.83	120.30
57	4	335	C	C2-N1-C1'	13.48	133.63	118.80
57	4	173	C	N3-C2-O2	-13.44	112.49	121.90
57	4	258	G	O5'-P-OP1	-13.19	93.83	105.70
57	4	154	C	C2-N1-C1'	12.97	133.07	118.80
57	4	266	C	C6-N1-C2	-12.96	115.11	120.30
57	4	30	C	C5-C6-N1	12.52	127.26	121.00
57	4	154	C	C6-N1-C2	-12.50	115.30	120.30
57	4	237	U	C2-N1-C1'	12.46	132.66	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	18	C	O4'-C1'-N1	12.36	118.08	108.20
57	4	155	C	C2-N1-C1'	12.11	132.12	118.80
57	4	237	U	N1-C2-O2	12.08	131.25	122.80
57	4	34	A	O5'-P-OP1	-12.00	94.90	105.70
57	4	155	C	N1-C2-O2	11.97	126.08	118.90
57	4	35	C	O5'-P-OP1	-11.89	95.00	105.70
57	4	266	C	C5-C6-N1	11.82	126.91	121.00
57	4	75	C	C5-C6-N1	11.65	126.83	121.00
57	4	245	C	C6-N1-C2	-11.61	115.66	120.30
57	4	209	C	C6-N1-C2	-11.60	115.66	120.30
57	4	224	A	O4'-C1'-N9	11.51	117.41	108.20
57	4	299	C	N1-C2-O2	11.41	125.75	118.90
57	4	75	C	C6-N1-C2	-11.33	115.77	120.30
2	2	467	U	N3-C2-O2	-11.30	114.29	122.20
2	2	467	U	C2-N1-C1'	11.22	131.17	117.70
57	4	173	C	C2-N1-C1'	11.17	131.09	118.80
57	4	173	C	C6-N1-C2	-10.99	115.90	120.30
1	1	1621	U	N1-C2-O2	10.92	130.44	122.80
57	4	270	C	C6-N1-C2	-10.89	115.94	120.30
57	4	157	C	C6-N1-C2	-10.85	115.96	120.30
2	2	467	U	N1-C2-O2	10.82	130.37	122.80
57	4	284	G	P-O3'-C3'	10.80	132.66	119.70
1	1	544	C	C2-N1-C1'	10.78	130.66	118.80
57	4	60	U	C5-C6-N1	10.77	128.08	122.70
1	1	1621	U	N3-C2-O2	-10.76	114.67	122.20
57	4	324	G	O4'-C1'-N9	10.75	116.80	108.20
57	4	137	C	C6-N1-C2	-10.68	116.03	120.30
1	1	544	C	N1-C2-O2	10.66	125.30	118.90
57	4	161	U	P-O3'-C3'	10.60	132.42	119.70
57	4	12	U	N1-C2-O2	10.59	130.21	122.80
57	4	237	U	C6-N1-C2	-10.57	114.66	121.00
57	4	245	C	C5-C6-N1	10.53	126.27	121.00
57	4	245	C	C2-N1-C1'	10.52	130.37	118.80
57	4	299	C	C2-N1-C1'	10.41	130.25	118.80
57	4	18	C	C2-N1-C1'	10.38	130.22	118.80
57	4	262	U	N1-C2-O2	10.36	130.05	122.80
57	4	12	U	C2-N1-C1'	10.29	130.04	117.70
1	1	830	G	O4'-C1'-N9	-10.27	99.98	108.20
1	1	1621	U	C2-N1-C1'	10.21	129.96	117.70
57	4	241	C	C6-N1-C2	-10.21	116.22	120.30
57	4	210	C	C6-N1-C2	-10.21	116.22	120.30
57	4	154	C	O5'-P-OP2	-10.16	96.56	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	304	C	C6-N1-C2	-10.06	116.28	120.30
57	4	137	C	P-O3'-C3'	9.98	131.68	119.70
57	4	48	C	C6-N1-C2	-9.98	116.31	120.30
2	2	1341	U	C2-N1-C1'	9.95	129.65	117.70
2	2	1341	U	N1-C2-O2	9.85	129.69	122.80
57	4	290	A	P-O3'-C3'	9.80	131.46	119.70
57	4	214	C	C5-C6-N1	9.76	125.88	121.00
57	4	263	G	C8-N9-C4	-9.70	102.52	106.40
2	2	1303	C	C2-N1-C1'	9.65	129.41	118.80
1	1	2075	U	N3-C4-O4	9.61	126.12	119.40
57	4	214	C	C6-N1-C2	-9.54	116.48	120.30
57	4	246	U	O5'-P-OP2	-9.53	97.13	105.70
1	1	2226	C	N1-C2-O2	9.52	124.61	118.90
2	2	99	C	N1-C2-O2	9.52	124.61	118.90
57	4	261	G	OP1-P-O3'	9.49	126.07	105.20
57	4	16	U	O5'-P-OP2	-9.47	97.18	105.70
57	4	222	U	N1-C2-O2	9.45	129.42	122.80
57	4	186	A	O4'-C1'-N9	9.39	115.72	108.20
57	4	245	C	N1-C2-O2	9.39	124.54	118.90
1	1	1075	C	C2-N1-C1'	9.38	129.12	118.80
57	4	109	C	C6-N1-C2	-9.36	116.56	120.30
57	4	12	U	N3-C2-O2	-9.35	115.66	122.20
1	1	569	U	N1-C2-O2	9.31	129.32	122.80
1	1	1999	C	C6-N1-C2	-9.31	116.58	120.30
57	4	159	C	C6-N1-C2	-9.31	116.58	120.30
1	1	1092	C	C2-N1-C1'	9.27	129.00	118.80
1	1	2075	U	C5-C4-O4	-9.26	120.34	125.90
57	4	118	C	C6-N1-C2	-9.26	116.60	120.30
57	4	222	U	C2-N1-C1'	9.23	128.78	117.70
1	1	544	C	N3-C2-O2	-9.19	115.47	121.90
57	4	120	U	N3-C2-O2	-9.17	115.78	122.20
57	4	300	U	N1-C2-O2	9.14	129.20	122.80
57	4	288	G	C8-N9-C4	-9.13	102.75	106.40
2	2	514	C	N3-C2-O2	-9.11	115.52	121.90
1	1	305	C	N3-C2-O2	-9.11	115.53	121.90
1	1	1075	C	N1-C2-O2	9.10	124.36	118.90
57	4	181	G	N3-C4-C5	-9.08	124.06	128.60
1	1	2752	C	N1-C2-O2	9.06	124.34	118.90
1	1	915	C	C2-N1-C1'	9.04	128.74	118.80
1	1	2902	C	N3-C2-O2	-9.02	115.59	121.90
57	4	155	C	C6-N1-C2	-9.00	116.70	120.30
57	4	300	U	N3-C2-O2	-8.99	115.91	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	186	A	C8-N9-C4	-8.99	102.20	105.80
57	4	299	C	N3-C2-O2	-8.99	115.61	121.90
57	4	155	C	N3-C2-O2	-8.98	115.61	121.90
57	4	332	G	C5'-C4'-O4'	-8.96	98.35	109.10
1	1	378	C	N1-C2-O2	8.95	124.27	118.90
57	4	335	C	O4'-C1'-N1	8.90	115.32	108.20
1	1	1376	C	N1-C2-O2	8.89	124.23	118.90
57	4	314	C	P-O3'-C3'	8.89	130.37	119.70
2	2	999	C	C6-N1-C2	-8.87	116.75	120.30
57	4	308	U	C5-C6-N1	8.84	127.12	122.70
57	4	308	U	P-O3'-C3'	8.82	130.28	119.70
2	2	1244	G	N3-C4-N9	-8.79	120.73	126.00
2	2	1109	C	C3'-C2'-C1'	8.75	108.50	101.50
57	4	265	C	C5-C6-N1	8.74	125.37	121.00
1	1	2902	C	N1-C2-O2	8.74	124.14	118.90
57	4	362	C	C5-C6-N1	8.73	125.37	121.00
1	1	2874	C	N1-C2-O2	8.71	124.13	118.90
2	2	672	U	N1-C2-O2	8.71	128.90	122.80
2	2	514	C	C6-N1-C2	-8.69	116.82	120.30
57	4	269	C	C6-N1-C2	-8.69	116.83	120.30
57	4	299	C	C6-N1-C2	-8.66	116.84	120.30
57	4	266	C	P-O3'-C3'	8.62	130.04	119.70
57	4	222	U	N3-C2-O2	-8.61	116.17	122.20
2	2	528	C	C6-N1-C2	-8.61	116.86	120.30
57	4	151	C	C6-N1-C2	-8.61	116.86	120.30
1	1	1045	C	O4'-C1'-N1	8.60	115.08	108.20
1	1	1376	C	C2-N1-C1'	8.59	128.25	118.80
57	4	233	A	P-O3'-C3'	8.54	129.95	119.70
1	1	1082	U	O4'-C1'-N1	8.53	115.02	108.20
1	1	1081	U	N3-C2-O2	-8.51	116.24	122.20
2	2	469	C	N1-C2-O2	8.51	124.01	118.90
57	4	26	U	C5-C6-N1	8.49	126.95	122.70
57	4	316	A	C8-N9-C4	-8.48	102.41	105.80
57	4	141	C	C6-N1-C2	-8.45	116.92	120.30
1	1	2072	C	C2-N1-C1'	8.45	128.09	118.80
57	4	155	C	C5-C6-N1	8.43	125.21	121.00
1	1	729	G	C4-N9-C1'	8.42	137.44	126.50
57	4	227	C	C6-N1-C2	-8.39	116.94	120.30
57	4	241	C	C5-C6-N1	8.37	125.19	121.00
2	2	1158	C	C6-N1-C2	-8.35	116.96	120.30
57	4	335	C	C5-C6-N1	8.35	125.17	121.00
1	1	1081	U	N1-C2-O2	8.34	128.64	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	349	C	C5-C6-N1	8.33	125.17	121.00
12	H	81	LEU	CA-CB-CG	8.32	134.44	115.30
1	1	62	U	C2-N1-C1'	8.31	127.67	117.70
1	1	1594	U	C2-N1-C1'	8.31	127.67	117.70
1	1	1726	C	C6-N1-C2	-8.30	116.98	120.30
57	4	17	U	N3-C2-O2	-8.30	116.39	122.20
2	2	1158	C	C2-N1-C1'	8.29	127.91	118.80
57	4	262	U	C2-N1-C1'	8.27	127.62	117.70
57	4	349	C	C6-N1-C2	-8.27	116.99	120.30
57	4	48	C	O3'-P-O5'	8.26	119.69	104.00
57	4	13	G	P-O3'-C3'	8.25	129.60	119.70
1	1	1941	C	N1-C2-O2	8.21	123.82	118.90
2	2	1262	C	N1-C2-O2	8.19	123.81	118.90
57	4	63	C	C2-N1-C1'	8.19	127.81	118.80
1	1	839	U	C2-N1-C1'	8.16	127.49	117.70
2	2	1033	G	C4-N9-C1'	8.16	137.10	126.50
1	1	62	U	N3-C2-O2	-8.15	116.49	122.20
57	4	224	A	O5'-P-OP1	-8.15	98.37	105.70
2	2	672	U	C2-N1-C1'	8.15	127.48	117.70
57	4	18	C	N1-C2-O2	8.15	123.79	118.90
57	4	271	G	C8-N9-C4	-8.14	103.14	106.40
2	2	857	C	C2-N1-C1'	8.14	127.75	118.80
57	4	273	A	N7-C8-N9	8.13	117.87	113.80
1	1	312	G	N3-C4-N9	8.11	130.87	126.00
57	4	147	C	C6-N1-C2	-8.11	117.06	120.30
2	2	754	C	N1-C2-O2	8.10	123.76	118.90
57	4	35	C	O4'-C1'-N1	8.10	114.68	108.20
2	2	1448	C	C2-N1-C1'	8.09	127.70	118.80
1	1	2810	A	N7-C8-N9	8.08	117.84	113.80
57	4	54	G	C4-N9-C1'	8.07	137.00	126.50
57	4	63	C	C6-N1-C2	-8.07	117.07	120.30
57	4	295	C	C6-N1-C2	-8.06	117.08	120.30
57	4	76	C	C6-N1-C2	-8.05	117.08	120.30
2	2	1484	C	C6-N1-C2	-8.05	117.08	120.30
57	4	40	G	C8-N9-C4	-8.05	103.18	106.40
1	1	1221	C	N1-C2-O2	8.05	123.73	118.90
57	4	269	C	N1-C2-O2	8.03	123.72	118.90
57	4	130	C	P-O3'-C3'	8.02	129.32	119.70
57	4	155	C	C6-N1-C1'	-8.02	111.18	120.80
57	4	11	C	N1-C2-O2	8.01	123.71	118.90
57	4	154	C	C6-N1-C1'	-8.00	111.20	120.80
3	3	17	C	C2-N1-C1'	8.00	127.60	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	9	U	O5'-P-OP1	-7.97	98.52	105.70
1	1	284	U	C2-N1-C1'	7.96	127.25	117.70
57	4	181	G	N3-C4-N9	7.95	130.77	126.00
57	4	209	C	C5-C6-N1	7.94	124.97	121.00
57	4	324	G	N3-C4-C5	-7.93	124.63	128.60
1	1	2063	C	C2-N1-C1'	7.93	127.52	118.80
57	4	267	G	C2-N3-C4	7.92	115.86	111.90
57	4	137	C	C5-C6-N1	7.92	124.96	121.00
57	4	18	C	C6-N1-C1'	-7.92	111.30	120.80
57	4	262	U	N3-C2-O2	-7.91	116.66	122.20
1	1	544	C	C6-N1-C2	-7.91	117.14	120.30
57	4	7	G	C8-N9-C4	-7.91	103.23	106.40
57	4	362	C	C6-N1-C1'	7.91	130.29	120.80
57	4	315	G	C4-N9-C1'	7.91	136.78	126.50
2	2	1341	U	N3-C2-O2	-7.91	116.67	122.20
57	4	76	C	C5-C6-N1	7.91	124.95	121.00
1	1	305	C	C6-N1-C2	-7.90	117.14	120.30
2	2	1448	C	C6-N1-C2	-7.90	117.14	120.30
2	2	672	U	N3-C2-O2	-7.90	116.67	122.20
57	4	334	A	O4'-C1'-N9	-7.88	101.89	108.20
1	1	2226	C	N3-C2-O2	-7.87	116.39	121.90
1	1	569	U	N3-C2-O2	-7.86	116.70	122.20
1	1	1092	C	N1-C2-O2	7.86	123.61	118.90
2	2	1303	C	N1-C2-O2	7.85	123.61	118.90
1	1	1376	C	N3-C2-O2	-7.85	116.41	121.90
57	4	267	G	N3-C4-C5	-7.84	124.68	128.60
1	1	62	U	N1-C2-O2	7.83	128.28	122.80
57	4	154	C	C5-C6-N1	7.83	124.92	121.00
1	1	1135	C	N1-C2-O2	7.81	123.58	118.90
57	4	166	C	O4'-C1'-N1	7.81	114.45	108.20
2	2	1158	C	N3-C2-O2	-7.81	116.44	121.90
2	2	1245	C	C6-N1-C2	-7.79	117.18	120.30
1	1	2594	C	N1-C2-O2	7.79	123.58	118.90
57	4	245	C	N3-C2-O2	-7.79	116.45	121.90
57	4	120	U	N1-C2-O2	7.78	128.25	122.80
1	1	1892	C	C6-N1-C2	-7.78	117.19	120.30
57	4	142	U	C5-C6-N1	7.76	126.58	122.70
57	4	120	U	C2-N1-C1'	7.76	127.01	117.70
2	2	998	C	C2-N1-C1'	7.75	127.33	118.80
57	4	153	U	O4'-C1'-N1	7.75	114.40	108.20
1	1	2810	A	C8-N9-C4	-7.74	102.70	105.80
2	2	194	C	C6-N1-C2	-7.74	117.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2259	U	C2-N1-C1'	7.71	126.96	117.70
57	4	332	G	C8-N9-C4	-7.71	103.31	106.40
57	4	265	C	C6-N1-C2	-7.70	117.22	120.30
57	4	324	G	C2-N3-C4	7.70	115.75	111.90
57	4	187	C	N1-C2-O2	7.69	123.51	118.90
2	2	1262	C	C6-N1-C2	-7.69	117.22	120.30
57	4	200	G	O4'-C1'-N9	7.67	114.34	108.20
1	1	2200	C	C6-N1-C2	-7.66	117.23	120.30
1	1	31	C	N3-C2-O2	-7.66	116.54	121.90
1	1	2354	C	C2-N1-C1'	7.65	127.21	118.80
57	4	38	A	OP1-P-O3'	7.65	122.02	105.20
1	1	1874	C	N1-C2-O2	7.64	123.49	118.90
1	1	2226	C	C2-N1-C1'	7.64	127.20	118.80
57	4	361	C	N3-C2-O2	-7.63	116.56	121.90
1	1	1414	C	C6-N1-C2	-7.62	117.25	120.30
57	4	199	C	O4'-C1'-N1	7.61	114.29	108.20
1	1	2063	C	N1-C2-O2	7.61	123.47	118.90
57	4	256	G	O4'-C1'-N9	7.61	114.28	108.20
1	1	1594	U	N1-C2-O2	7.60	128.12	122.80
57	4	223	G	P-O3'-C3'	7.60	128.82	119.70
57	4	286	A	P-O3'-C3'	7.60	128.82	119.70
2	2	1409	C	C5-C6-N1	7.59	124.79	121.00
57	4	237	U	C5-C6-N1	7.58	126.49	122.70
57	4	266	C	O3'-P-O5'	7.58	118.41	104.00
2	2	998	C	N1-C2-O2	7.57	123.44	118.90
57	4	161	U	O3'-P-O5'	7.57	118.39	104.00
57	4	229	U	OP1-P-O3'	7.57	121.85	105.20
57	4	229	U	N3-C2-O2	-7.56	116.91	122.20
2	2	99	C	C2-N1-C1'	7.56	127.12	118.80
2	2	469	C	N3-C2-O2	-7.55	116.62	121.90
1	1	729	G	C8-N9-C1'	-7.54	117.19	127.00
1	1	1621	U	C6-N1-C1'	-7.54	110.64	121.20
2	2	1341	U	C6-N1-C1'	-7.54	110.65	121.20
2	2	1132	C	C6-N1-C2	-7.53	117.29	120.30
57	4	229	U	N1-C2-O2	7.53	128.07	122.80
1	1	1370	C	N1-C2-O2	7.52	123.41	118.90
1	1	2364	C	C6-N1-C2	-7.52	117.29	120.30
2	2	272	C	N1-C2-O2	7.51	123.40	118.90
2	2	979	C	C2-N1-C1'	7.50	127.05	118.80
1	1	2072	C	C5-C6-N1	7.50	124.75	121.00
3	3	92	C	N1-C2-O2	7.50	123.40	118.90
1	1	2752	C	N3-C2-O2	-7.49	116.65	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2870	C	C6-N1-C2	-7.48	117.31	120.30
1	1	818	G	C6-C5-N7	-7.47	125.92	130.40
1	1	2556	C	N1-C2-O2	7.47	123.38	118.90
57	4	247	A	O4'-C1'-N9	7.47	114.18	108.20
57	4	269	C	C5-C6-N1	7.46	124.73	121.00
2	2	1303	C	C6-N1-C1'	-7.46	111.85	120.80
1	1	1941	C	C2-N1-C1'	7.45	127.00	118.80
57	4	223	G	C4-N9-C1'	7.45	136.18	126.50
1	1	485	C	N3-C2-O2	-7.44	116.69	121.90
57	4	60	U	C6-N1-C2	-7.44	116.54	121.00
1	1	1318	U	N1-C2-O2	7.44	128.01	122.80
1	1	1999	C	C5-C6-N1	7.43	124.72	121.00
1	1	2193	G	C4-N9-C1'	7.42	136.14	126.50
1	1	225	C	N1-C2-O2	7.42	123.35	118.90
1	1	2636	C	C2-N1-C1'	7.41	126.95	118.80
57	4	39	A	P-O3'-C3'	7.41	128.59	119.70
1	1	1595	C	C6-N1-C2	-7.40	117.34	120.30
2	2	979	C	N1-C2-O2	7.40	123.34	118.90
1	1	2072	C	C6-N1-C2	-7.39	117.34	120.30
57	4	299	C	C5-C6-N1	7.38	124.69	121.00
1	1	986	C	N3-C2-O2	-7.38	116.74	121.90
57	4	143	C	C6-N1-C2	-7.38	117.35	120.30
57	4	18	C	C6-N1-C2	-7.37	117.35	120.30
57	4	142	U	C6-N1-C2	-7.37	116.58	121.00
1	1	373	U	N3-C2-O2	-7.36	117.05	122.20
57	4	269	C	N3-C2-O2	-7.36	116.75	121.90
3	3	17	C	C6-N1-C2	-7.36	117.36	120.30
2	2	843	U	N1-C2-O2	7.35	127.95	122.80
57	4	157	C	C5-C6-N1	7.35	124.67	121.00
57	4	214	C	O4'-C1'-N1	7.35	114.08	108.20
1	1	1113	U	C2-N1-C1'	7.35	126.52	117.70
1	1	736	C	C6-N1-C2	-7.34	117.36	120.30
1	1	2581	G	C4-N9-C1'	7.33	136.03	126.50
2	2	1132	C	C5-C6-N1	7.33	124.66	121.00
1	1	1097	U	N3-C2-O2	-7.32	117.07	122.20
2	2	1265	C	C6-N1-C2	-7.32	117.37	120.30
57	4	163	G	O3'-P-O5'	7.31	117.89	104.00
57	4	297	G	N7-C8-N9	7.30	116.75	113.10
1	1	1097	U	N1-C2-O2	7.30	127.91	122.80
1	1	765	C	C2-N1-C1'	7.29	126.83	118.80
1	1	365	U	C5-C6-N1	7.29	126.35	122.70
2	2	1448	C	N3-C2-O2	-7.29	116.80	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	818	G	N7-C8-N9	7.28	116.74	113.10
2	2	1448	C	N1-C2-O2	7.28	123.27	118.90
2	2	754	C	N3-C2-O2	-7.27	116.81	121.90
57	4	247	A	P-O3'-C3'	7.26	128.41	119.70
1	1	544	C	C6-N1-C1'	-7.25	112.10	120.80
57	4	150	G	N3-C4-C5	-7.25	124.97	128.60
1	1	1289	C	N1-C2-O2	7.25	123.25	118.90
57	4	237	U	C6-N1-C1'	-7.24	111.06	121.20
1	1	1051	G	N3-C4-N9	7.24	130.34	126.00
1	1	2874	C	N3-C2-O2	-7.22	116.84	121.90
1	1	2063	C	N3-C2-O2	-7.22	116.85	121.90
57	4	61	G	P-O3'-C3'	7.22	128.37	119.70
1	1	171	U	N1-C2-O2	7.21	127.85	122.80
1	1	2789	C	C6-N1-C2	-7.21	117.42	120.30
57	4	36	C	C6-N1-C2	-7.20	117.42	120.30
1	1	1594	U	N3-C2-O2	-7.19	117.17	122.20
1	1	2267	A	N1-C6-N6	-7.19	114.28	118.60
57	4	139	C	C6-N1-C2	-7.19	117.42	120.30
1	1	2465	C	N3-C2-O2	-7.19	116.87	121.90
1	1	2259	U	N1-C2-O2	7.19	127.83	122.80
2	2	1279	G	C4-N9-C1'	7.19	135.84	126.50
1	1	2193	G	N3-C4-N9	7.18	130.31	126.00
1	1	31	C	N1-C2-O2	7.18	123.21	118.90
1	1	305	C	N1-C2-O2	7.17	123.20	118.90
57	4	316	A	N7-C8-N9	7.17	117.38	113.80
2	2	857	C	N1-C2-O2	7.16	123.20	118.90
2	2	1263	C	C6-N1-C2	-7.16	117.44	120.30
57	4	333	G	P-O3'-C3'	7.16	128.29	119.70
1	1	2312	U	N3-C2-O2	-7.15	117.20	122.20
57	4	193	A	C5'-C4'-O4'	-7.15	100.52	109.10
57	4	269	C	P-O3'-C3'	7.15	128.28	119.70
1	1	1456	G	C4-N9-C1'	7.14	135.79	126.50
57	4	15	A	O5'-P-OP1	7.14	119.27	110.70
57	4	197	A	O5'-P-OP2	-7.14	99.27	105.70
57	4	335	C	C6-N1-C1'	-7.14	112.23	120.80
57	4	210	C	C5-C6-N1	7.14	124.57	121.00
57	4	271	G	N7-C8-N9	7.14	116.67	113.10
2	2	1172	C	N1-C2-O2	7.13	123.18	118.90
57	4	269	C	O3'-P-O5'	7.13	117.55	104.00
2	2	1389	C	N3-C2-O2	-7.13	116.91	121.90
57	4	17	U	N1-C2-O2	7.13	127.79	122.80
57	4	308	U	C2-N1-C1'	7.12	126.25	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	99	C	N3-C2-O2	-7.12	116.91	121.90
1	1	984	A	C2-N3-C4	7.12	114.16	110.60
1	1	1411	U	N1-C2-O2	7.12	127.78	122.80
1	1	1335	C	C6-N1-C2	-7.12	117.45	120.30
1	1	569	U	C2-N1-C1'	7.10	126.22	117.70
57	4	263	G	N9-C4-C5	7.10	108.24	105.40
57	4	263	G	N3-C4-N9	-7.10	121.74	126.00
1	1	1023	U	N1-C2-O2	7.10	127.77	122.80
57	4	13	G	O4'-C1'-N9	7.10	113.88	108.20
57	4	137	C	O3'-P-O5'	7.09	117.48	104.00
57	4	173	C	C5-C6-N1	7.09	124.55	121.00
1	1	316	C	C6-N1-C2	-7.08	117.47	120.30
1	1	2581	G	C8-N9-C1'	-7.08	117.79	127.00
57	4	163	G	P-O3'-C3'	7.08	128.19	119.70
57	4	130	C	O5'-P-OP1	7.07	119.19	110.70
1	1	171	U	N3-C2-O2	-7.07	117.25	122.20
57	4	165	A	P-O3'-C3'	7.06	128.18	119.70
1	1	1318	U	C2-N1-C1'	7.06	126.17	117.70
57	4	159	C	C5-C6-N1	7.06	124.53	121.00
57	4	148	U	C5-C6-N1	7.05	126.23	122.70
57	4	316	A	C5'-C4'-O4'	-7.05	100.64	109.10
1	1	1905	C	C2-N1-C1'	7.05	126.55	118.80
2	2	1158	C	N1-C2-O2	7.05	123.13	118.90
1	1	1411	U	N3-C2-O2	-7.03	117.28	122.20
1	1	758	C	C6-N1-C2	-7.03	117.49	120.30
2	2	1033	G	C8-N9-C1'	-7.03	117.86	127.00
57	4	39	A	C2-N3-C4	7.02	114.11	110.60
57	4	246	U	OP2-P-O3'	7.02	120.65	105.20
57	4	343	C	C2-N1-C1'	7.02	126.53	118.80
57	4	246	U	N3-C2-O2	-7.02	117.28	122.20
1	1	1905	C	N1-C2-O2	7.02	123.11	118.90
1	1	1769	U	N1-C2-O2	7.01	127.71	122.80
2	2	936	C	C2-N1-C1'	7.01	126.52	118.80
57	4	181	G	P-O3'-C3'	7.01	128.12	119.70
1	1	1157	G	C6-C5-N7	-7.01	126.19	130.40
57	4	325	G	N3-C4-C5	-7.01	125.09	128.60
57	4	133	A	C5'-C4'-O4'	-7.00	100.69	109.10
2	2	1262	C	N3-C2-O2	-7.00	117.00	121.90
57	4	118	C	C5-C6-N1	7.00	124.50	121.00
57	4	297	G	C6-C5-N7	-7.00	126.20	130.40
1	1	1005	C	C2-N1-C1'	6.99	126.49	118.80
1	1	1585	C	N1-C2-O2	6.99	123.09	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	978	G	C8-N9-C4	-6.99	103.61	106.40
1	1	2072	C	N1-C2-O2	6.99	123.09	118.90
57	4	157	C	O4'-C1'-N1	6.99	113.79	108.20
57	4	18	C	C5-C6-N1	6.98	124.49	121.00
57	4	54	G	N3-C4-C5	-6.96	125.12	128.60
57	4	260	C	N3-C2-O2	-6.96	117.03	121.90
1	1	2824	C	N1-C2-O2	6.95	123.07	118.90
1	1	566	U	C2-N1-C1'	6.95	126.03	117.70
2	2	1009	U	N3-C2-O2	-6.95	117.34	122.20
1	1	378	C	N3-C2-O2	-6.94	117.04	121.90
2	2	1493	A	O4'-C1'-N9	6.94	113.75	108.20
1	1	2556	C	N3-C2-O2	-6.93	117.05	121.90
2	2	440	C	N1-C2-O2	6.93	123.06	118.90
2	2	1262	C	C2-N1-C1'	6.92	126.42	118.80
1	1	2760	C	N1-C2-O2	6.92	123.05	118.90
1	1	1075	C	N3-C2-O2	-6.92	117.06	121.90
1	1	1941	C	N3-C2-O2	-6.92	117.06	121.90
57	4	311	U	O4'-C1'-N1	6.92	113.73	108.20
1	1	1	G	N3-C4-N9	6.91	130.15	126.00
57	4	187	C	C5'-C4'-C3'	-6.91	104.94	116.00
1	1	1530	G	C4-N9-C1'	6.91	135.48	126.50
2	2	1132	C	C2-N1-C1'	6.91	126.40	118.80
57	4	321	G	C8-N9-C4	-6.90	103.64	106.40
57	4	297	G	C4-C5-N7	6.90	113.56	110.80
1	1	1051	G	N3-C4-C5	-6.89	125.15	128.60
57	4	357	U	C2-N1-C1'	6.89	125.97	117.70
2	2	843	U	N3-C2-O2	-6.89	117.38	122.20
2	2	513	C	N1-C2-O2	6.88	123.03	118.90
2	2	1033	G	N3-C4-N9	6.87	130.12	126.00
1	1	839	U	N1-C2-O2	6.87	127.61	122.80
1	1	485	C	C6-N1-C2	-6.87	117.55	120.30
57	4	260	C	N1-C2-O2	6.87	123.02	118.90
57	4	5	C	C6-N1-C2	-6.87	117.55	120.30
1	1	1351	C	N1-C2-O2	6.86	123.02	118.90
1	1	1409	U	C2-N1-C1'	6.86	125.94	117.70
57	4	163	G	C8-N9-C4	-6.86	103.66	106.40
1	1	225	C	C2-N1-C1'	6.86	126.34	118.80
1	1	2149	U	C2-N1-C1'	6.85	125.92	117.70
1	1	839	U	C5-C6-N1	6.84	126.12	122.70
2	2	467	U	C6-N1-C1'	-6.84	111.62	121.20
57	4	248	G	C4-N9-C1'	-6.84	117.61	126.50
1	1	284	U	N1-C2-O2	6.84	127.58	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	681	G	C6-C5-N7	-6.84	126.30	130.40
2	2	1348	U	C2-N1-C1'	6.83	125.90	117.70
57	4	47	G	C8-N9-C4	-6.83	103.67	106.40
57	4	181	G	C4-N9-C1'	6.83	135.38	126.50
1	1	356	G	C8-N9-C4	-6.83	103.67	106.40
57	4	27	U	N3-C2-O2	-6.83	117.42	122.20
1	1	681	G	C4-C5-N7	6.82	113.53	110.80
1	1	2193	G	N3-C4-C5	-6.82	125.19	128.60
57	4	189	C	P-O3'-C3'	6.82	127.89	119.70
57	4	227	C	C5-C6-N1	6.82	124.41	121.00
2	2	998	C	N3-C2-O2	-6.82	117.13	121.90
57	4	161	U	C5-C6-N1	6.81	126.11	122.70
1	1	1081	U	C2-N1-C1'	6.81	125.87	117.70
1	1	140	C	N1-C2-O2	6.79	122.97	118.90
1	1	2579	C	N1-C2-O2	6.79	122.97	118.90
1	1	2200	C	C2-N1-C1'	6.78	126.26	118.80
1	1	1075	C	C6-N1-C1'	-6.78	112.67	120.80
57	4	54	G	N3-C4-N9	6.78	130.06	126.00
57	4	340	G	C4-N9-C1'	6.77	135.30	126.50
57	4	343	C	N1-C2-O2	6.76	122.96	118.90
1	1	114	U	C2-N1-C1'	6.76	125.81	117.70
1	1	678	C	C6-N1-C2	-6.76	117.60	120.30
1	1	672	C	C6-N1-C2	-6.75	117.60	120.30
57	4	286	A	C4-N9-C1'	-6.75	114.15	126.30
57	4	68	U	P-O3'-C3'	6.75	127.80	119.70
57	4	190	A	P-O3'-C3'	6.74	127.79	119.70
57	4	328	U	N3-C2-O2	-6.74	117.48	122.20
2	2	1328	C	N3-C2-O2	-6.73	117.19	121.90
57	4	246	U	N1-C2-O2	6.73	127.51	122.80
1	1	2312	U	C5-C6-N1	6.73	126.06	122.70
57	4	183	C	C6-N1-C1'	6.73	128.87	120.80
57	4	361	C	N1-C2-O2	6.73	122.94	118.90
1	1	2601	C	C6-N1-C2	-6.72	117.61	120.30
2	2	273	U	C2-N1-C1'	6.71	125.76	117.70
1	1	1092	C	C6-N1-C1'	-6.71	112.74	120.80
1	1	106	C	C6-N1-C2	-6.71	117.62	120.30
57	4	315	G	C8-N9-C1'	-6.71	118.28	127.00
57	4	11	C	N3-C2-O2	-6.70	117.21	121.90
1	1	8	C	C5-C6-N1	6.70	124.35	121.00
57	4	48	C	C5-C6-N1	6.69	124.35	121.00
1	1	1411	U	C5-C6-N1	6.69	126.05	122.70
2	2	1348	U	N1-C2-O2	6.68	127.48	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	54	G	C8-N9-C1'	-6.68	118.32	127.00
1	1	601	C	C2-N1-C1'	6.68	126.14	118.80
1	1	516	C	N3-C2-O2	-6.67	117.23	121.90
1	1	2752	C	C2-N1-C1'	6.67	126.14	118.80
2	2	216	U	N3-C2-O2	-6.67	117.53	122.20
57	4	270	C	C5'-C4'-O4'	-6.67	101.10	109.10
57	4	63	C	N3-C2-O2	-6.66	117.24	121.90
1	1	986	C	C6-N1-C2	-6.66	117.64	120.30
57	4	11	C	C6-N1-C2	-6.66	117.64	120.30
57	4	12	U	C6-N1-C1'	-6.65	111.89	121.20
1	1	1760	C	C6-N1-C2	-6.64	117.64	120.30
1	1	2297	A	C2-N3-C4	6.64	113.92	110.60
2	2	439	U	N3-C2-O2	-6.63	117.56	122.20
57	4	195	A	P-O3'-C3'	6.63	127.66	119.70
1	1	1052	C	C5-C6-N1	6.62	124.31	121.00
1	1	2149	U	N1-C2-O2	6.62	127.43	122.80
2	2	993	G	N3-C4-N9	6.62	129.97	126.00
1	1	1874	C	N3-C2-O2	-6.61	117.27	121.90
1	1	2786	U	N1-C2-O2	6.61	127.43	122.80
2	2	178	C	N1-C2-O2	6.61	122.87	118.90
2	2	1172	C	N3-C2-O2	-6.61	117.27	121.90
57	4	120	U	C6-N1-C2	-6.61	117.03	121.00
57	4	324	G	N3-C4-N9	6.60	129.96	126.00
1	1	8	C	C6-N1-C2	-6.59	117.67	120.30
57	4	159	C	N3-C2-O2	-6.59	117.29	121.90
1	1	2726	A	C8-N9-C4	6.58	108.43	105.80
1	1	1776	G	C4-N9-C1'	6.57	135.04	126.50
57	4	267	G	C4-N9-C1'	6.57	135.05	126.50
57	4	299	C	C6-N1-C1'	-6.57	112.91	120.80
1	1	2312	U	C6-N1-C2	-6.57	117.06	121.00
2	2	476	U	C2-N1-C1'	6.57	125.58	117.70
18	N	51	LEU	CA-CB-CG	6.57	130.41	115.30
57	4	37	C	O4'-C1'-N1	6.57	113.45	108.20
57	4	129	G	C4-N9-C1'	6.57	135.04	126.50
1	1	1170	C	C2-N1-C1'	6.56	126.02	118.80
1	1	915	C	C6-N1-C1'	-6.56	112.93	120.80
1	1	2581	G	C6-C5-N7	-6.56	126.47	130.40
2	2	632	U	C2-N1-C1'	6.56	125.57	117.70
1	1	312	G	N3-C4-C5	-6.56	125.32	128.60
57	4	6	U	C6-N1-C2	-6.55	117.07	121.00
57	4	308	U	C5'-C4'-O4'	-6.55	101.23	109.10
1	1	1023	U	N3-C2-O2	-6.55	117.61	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	78	C	C6-N1-C2	-6.55	117.68	120.30
1	1	1887	C	C6-N1-C2	-6.54	117.68	120.30
57	4	286	A	C4-C5-C6	-6.54	113.73	117.00
1	1	709	U	C2-N1-C1'	6.53	125.54	117.70
2	2	1327	C	C2-N1-C1'	6.53	125.98	118.80
57	4	44	C	P-O3'-C3'	6.53	127.53	119.70
1	1	1180	U	N1-C2-O2	6.52	127.36	122.80
1	1	2592	G	C6-C5-N7	-6.52	126.49	130.40
1	1	2581	G	N3-C4-N9	6.51	129.91	126.00
1	1	1887	C	C5-C6-N1	6.51	124.25	121.00
57	4	271	G	C5'-C4'-O4'	-6.51	101.29	109.10
57	4	273	A	C5-N7-C8	-6.51	100.65	103.90
1	1	1526	C	C6-N1-C2	-6.50	117.70	120.30
3	3	30	C	C2-N1-C1'	6.50	125.95	118.80
13	I	79	LEU	CA-CB-CG	6.50	130.24	115.30
57	4	173	C	C6-N1-C1'	-6.50	113.00	120.80
57	4	63	C	N1-C2-O2	6.49	122.80	118.90
57	4	14	G	C8-N9-C4	-6.49	103.80	106.40
57	4	257	U	C5-C6-N1	6.49	125.94	122.70
57	4	270	C	N3-C2-O2	-6.49	117.36	121.90
57	4	262	U	C6-N1-C1'	-6.48	112.12	121.20
57	4	26	U	C6-N1-C2	-6.48	117.11	121.00
57	4	56	C	P-O3'-C3'	6.48	127.48	119.70
1	1	2465	C	N1-C2-O2	6.48	122.79	118.90
2	2	590	U	N3-C2-O2	-6.48	117.67	122.20
1	1	1542	U	N1-C2-O2	6.47	127.33	122.80
57	4	66	C	O4'-C1'-N1	6.47	113.38	108.20
2	2	440	C	C2-N1-C1'	6.47	125.92	118.80
1	1	2214	C	N1-C2-O2	6.47	122.78	118.90
2	2	1342	C	N3-C2-O2	-6.46	117.38	121.90
3	3	42	C	N3-C2-O2	-6.46	117.38	121.90
57	4	34	A	O3'-P-O5'	6.45	116.26	104.00
2	2	977	A	C2-N3-C4	6.45	113.83	110.60
1	1	186	G	C4-N9-C1'	6.45	134.88	126.50
57	4	33	A	OP1-P-O3'	6.45	119.38	105.20
1	1	2562	U	N3-C2-O2	-6.44	117.69	122.20
2	2	216	U	N1-C2-O2	6.44	127.31	122.80
1	1	1117	C	N1-C2-O2	6.44	122.77	118.90
2	2	1033	G	N3-C4-C5	-6.44	125.38	128.60
1	1	1170	C	N1-C2-O2	6.44	122.76	118.90
2	2	1020	G	N3-C4-N9	6.44	129.87	126.00
57	4	332	G	N7-C8-N9	6.43	116.32	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	669	G	C4-N9-C1'	6.43	134.86	126.50
2	2	393	A	C2-N3-C4	6.43	113.81	110.60
57	4	340	G	C8-N9-C1'	-6.42	118.65	127.00
1	1	394	C	N3-C2-O2	-6.42	117.41	121.90
1	1	1386	C	C6-N1-C2	-6.42	117.73	120.30
1	1	1399	C	C6-N1-C2	-6.42	117.73	120.30
57	4	132	U	P-O3'-C3'	6.42	127.40	119.70
57	4	189	C	N1-C2-O2	6.42	122.75	118.90
1	1	2717	C	N1-C2-O2	6.41	122.75	118.90
57	4	152	C	N3-C2-O2	-6.41	117.41	121.90
1	1	971	G	C8-N9-C1'	-6.41	118.67	127.00
2	2	1395	C	C2-N1-C1'	6.41	125.85	118.80
57	4	308	U	O4'-C1'-N1	-6.41	103.08	108.20
57	4	315	G	P-O3'-C3'	6.40	127.38	119.70
1	1	1868	C	C6-N1-C2	-6.40	117.74	120.30
1	1	1157	G	C4-N9-C1'	6.39	134.81	126.50
57	4	166	C	C6-N1-C2	-6.39	117.74	120.30
1	1	1157	G	C8-N9-C1'	-6.39	118.69	127.00
57	4	334	A	C8-N9-C4	-6.39	103.24	105.80
57	4	66	C	P-O3'-C3'	6.39	127.37	119.70
1	1	1060	U	C6-N1-C2	-6.38	117.17	121.00
2	2	936	C	C6-N1-C2	-6.38	117.75	120.30
1	1	1075	C	C6-N1-C2	-6.38	117.75	120.30
57	4	217	G	C8-N9-C4	-6.38	103.85	106.40
1	1	225	C	N3-C2-O2	-6.37	117.44	121.90
1	1	1595	C	C5-C6-N1	6.37	124.18	121.00
2	2	1244	G	N3-C4-C5	6.37	131.78	128.60
2	2	697	U	N3-C2-O2	-6.37	117.74	122.20
57	4	200	G	C8-N9-C4	-6.37	103.85	106.40
57	4	361	C	C6-N1-C2	-6.36	117.76	120.30
1	1	1999	C	C2-N1-C1'	6.36	125.79	118.80
1	1	2226	C	C6-N1-C2	-6.36	117.76	120.30
1	1	2354	C	C6-N1-C2	-6.35	117.76	120.30
2	2	41	G	C6-C5-N7	-6.35	126.59	130.40
57	4	189	C	C5-C6-N1	6.35	124.17	121.00
57	4	210	C	O4'-C1'-N1	6.34	113.27	108.20
57	4	37	C	P-O3'-C3'	6.33	127.30	119.70
1	1	2200	C	C5-C6-N1	6.33	124.17	121.00
2	2	328	C	N1-C2-O2	6.33	122.70	118.90
2	2	1172	C	C2-N1-C1'	6.33	125.77	118.80
1	1	2193	G	C8-N9-C1'	-6.33	118.77	127.00
1	1	373	U	N1-C2-O2	6.33	127.23	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	952	G	C6-C5-N7	-6.32	126.61	130.40
2	2	620	C	N1-C2-O2	6.32	122.69	118.90
2	2	857	C	C6-N1-C1'	-6.32	113.22	120.80
1	1	1585	C	N3-C2-O2	-6.32	117.48	121.90
1	1	2283	C	N1-C2-O2	6.32	122.69	118.90
2	2	467	U	C6-N1-C2	-6.32	117.21	121.00
1	1	915	C	N1-C2-O2	6.32	122.69	118.90
1	1	1414	C	N3-C2-O2	-6.32	117.48	121.90
2	2	1484	C	C5-C6-N1	6.30	124.15	121.00
57	4	41	G	O4'-C1'-N9	6.30	113.24	108.20
1	1	366	C	N1-C2-O2	6.30	122.68	118.90
1	1	2247	A	N7-C8-N9	6.29	116.95	113.80
57	4	14	G	P-O3'-C3'	6.29	127.25	119.70
1	1	2312	U	N1-C2-O2	6.29	127.20	122.80
1	1	257	C	N1-C2-O2	6.28	122.67	118.90
57	4	272	C	P-O3'-C3'	6.28	127.24	119.70
1	1	1351	C	N3-C2-O2	-6.28	117.50	121.90
1	1	2720	U	N3-C2-O2	-6.28	117.81	122.20
57	4	223	G	C8-N9-C1'	-6.28	118.84	127.00
57	4	206	A	O5'-P-OP1	6.28	118.23	110.70
2	2	1326	U	N3-C2-O2	-6.27	117.81	122.20
1	1	1052	C	C6-N1-C2	-6.27	117.79	120.30
57	4	136	G	P-O3'-C3'	6.27	127.22	119.70
1	1	2601	C	C5-C6-N1	6.27	124.13	121.00
1	1	2874	C	C6-N1-C2	-6.27	117.79	120.30
1	1	1542	U	N3-C2-O2	-6.27	117.81	122.20
1	1	269	C	N1-C2-O2	6.26	122.66	118.90
1	1	2717	C	C2-N1-C1'	6.26	125.68	118.80
1	1	2466	C	C6-N1-C2	-6.25	117.80	120.30
1	1	1526	C	N3-C2-O2	-6.25	117.53	121.90
57	4	189	C	C2-N1-C1'	6.25	125.67	118.80
57	4	297	G	C5-N7-C8	-6.25	101.18	104.30
57	4	146	C	C6-N1-C2	-6.25	117.80	120.30
57	4	336	G	O4'-C1'-N9	6.25	113.20	108.20
57	4	348	C	C2-N1-C1'	6.25	125.67	118.80
1	1	2556	C	C6-N1-C2	-6.25	117.80	120.30
57	4	358	C	N3-C2-O2	-6.25	117.53	121.90
1	1	186	G	C8-N9-C1'	-6.24	118.89	127.00
57	4	176	G	C5'-C4'-O4'	-6.24	101.62	109.10
1	1	2568	U	C5-C6-N1	6.24	125.82	122.70
2	2	1088	G	N3-C4-N9	6.24	129.74	126.00
2	2	1409	C	C6-N1-C2	-6.23	117.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	272	C	C6-N1-C2	-6.23	117.81	120.30
57	4	307	G	P-O3'-C3'	-6.23	112.22	119.70
2	2	1009	U	N1-C2-O2	6.23	127.16	122.80
57	4	237	U	OP2-P-O3'	6.23	118.90	105.20
1	1	1051	G	C4-N9-C1'	6.22	134.59	126.50
57	4	215	C	C6-N1-C2	-6.22	117.81	120.30
57	4	250	U	O4'-C1'-N1	6.22	113.18	108.20
1	1	1221	C	C2-N1-C1'	6.22	125.64	118.80
1	1	2539	C	C6-N1-C2	-6.22	117.81	120.30
57	4	236	U	N3-C2-O2	-6.21	117.85	122.20
57	4	42	U	C5-C6-N1	6.21	125.81	122.70
1	1	954	G	C8-N9-C1'	-6.21	118.93	127.00
1	1	234	U	N3-C2-O2	-6.20	117.86	122.20
2	2	1471	U	N3-C2-O2	-6.20	117.86	122.20
57	4	76	C	N1-C2-O2	6.20	122.62	118.90
57	4	290	A	O4'-C1'-N9	6.20	113.16	108.20
1	1	2285	C	N3-C2-O2	-6.19	117.56	121.90
2	2	513	C	C2-N1-C1'	6.19	125.61	118.80
1	1	2570	G	C2-N3-C4	-6.19	108.80	111.90
57	4	145	C	C6-N1-C2	-6.19	117.82	120.30
57	4	152	C	N1-C2-O2	6.19	122.61	118.90
1	1	818	G	C4-N9-C1'	6.19	134.54	126.50
1	1	1082	U	C2-N1-C1'	-6.19	110.28	117.70
57	4	281	A	C5'-C4'-O4'	6.18	116.52	109.10
1	1	284	U	N3-C2-O2	-6.18	117.87	122.20
3	3	17	C	N1-C2-O2	6.18	122.61	118.90
1	1	1060	U	C2-N1-C1'	6.18	125.11	117.70
1	1	2372	U	C2-N1-C1'	6.17	125.11	117.70
1	1	1557	C	N1-C2-N3	6.17	123.52	119.20
2	2	1471	U	C2-N1-C1'	6.17	125.11	117.70
2	2	1045	C	N1-C2-O2	6.17	122.60	118.90
1	1	566	U	N1-C2-O2	6.17	127.12	122.80
1	1	1318	U	N3-C2-O2	-6.17	117.88	122.20
1	1	1411	U	C2-N1-C1'	6.17	125.10	117.70
1	1	1082	U	C6-N1-C1'	6.17	129.83	121.20
57	4	16	U	N3-C2-O2	-6.15	117.89	122.20
1	1	1605	C	C6-N1-C2	-6.15	117.84	120.30
57	4	210	C	C6-N1-C1'	6.15	128.18	120.80
57	4	53	G	P-O3'-C3'	6.15	127.08	119.70
57	4	213	G	C8-N9-C4	-6.15	103.94	106.40
57	4	221	U	C5-C6-N1	6.15	125.77	122.70
57	4	334	A	C5'-C4'-O4'	-6.14	101.73	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2230	G	N3-C4-N9	6.14	129.69	126.00
2	2	1003	G	C6-C5-N7	-6.14	126.72	130.40
57	4	33	A	P-O3'-C3'	6.14	127.07	119.70
2	2	341	C	C2-N1-C1'	6.14	125.55	118.80
57	4	159	C	O4'-C1'-N1	6.13	113.11	108.20
57	4	262	U	O5'-P-OP1	-6.13	100.18	105.70
2	2	582	C	N1-C2-O2	6.13	122.58	118.90
1	1	2380	C	N3-C2-O2	-6.13	117.61	121.90
57	4	38	A	P-O3'-C3'	6.13	127.05	119.70
1	1	1436	G	N1-C2-N3	6.12	127.58	123.90
57	4	151	C	C5-C6-N1	6.12	124.06	121.00
1	1	776	G	C4-N9-C1'	6.12	134.46	126.50
1	1	1920	C	C6-N1-C2	-6.12	117.85	120.30
1	1	601	C	N1-C2-O2	6.12	122.57	118.90
2	2	697	U	N1-C2-O2	6.12	127.08	122.80
1	1	994	C	C5-C6-N1	6.12	124.06	121.00
1	1	2053	G	C6-C5-N7	-6.11	126.73	130.40
2	2	235	C	N3-C2-O2	-6.11	117.62	121.90
2	2	1038	C	C6-N1-C2	-6.11	117.86	120.30
3	3	17	C	C5-C6-N1	6.11	124.06	121.00
2	2	1279	G	C8-N9-C1'	-6.11	119.06	127.00
57	4	314	C	OP1-P-O3'	6.11	118.64	105.20
1	1	211	C	C6-N1-C2	-6.11	117.86	120.30
2	2	1389	C	C6-N1-C2	-6.11	117.86	120.30
57	4	288	G	N3-C4-C5	-6.11	125.55	128.60
1	1	2230	G	C6-C5-N7	-6.11	126.74	130.40
2	2	679	C	N1-C2-O2	6.11	122.56	118.90
1	1	2562	U	N1-C2-O2	6.10	127.07	122.80
57	4	49	C	C6-N1-C2	-6.09	117.86	120.30
57	4	144	U	C5-C6-N1	6.09	125.75	122.70
1	1	839	U	N3-C2-O2	-6.09	117.94	122.20
2	2	492	C	N1-C2-O2	6.09	122.55	118.90
1	1	702	U	N1-C2-O2	6.08	127.06	122.80
2	2	1244	G	C8-N9-C1'	6.08	134.91	127.00
57	4	11	C	C2-N1-C1'	6.08	125.49	118.80
57	4	247	A	N9-C1'-C2'	6.08	121.91	114.00
1	1	1289	C	N3-C2-O2	-6.08	117.64	121.90
1	1	2263	C	C2-N1-C1'	6.08	125.49	118.80
1	1	1376	C	C6-N1-C2	-6.07	117.87	120.30
1	1	2874	C	C2-N1-C1'	6.07	125.48	118.80
2	2	1348	U	N3-C2-O2	-6.07	117.95	122.20
1	1	1315	C	C2-N1-C1'	6.07	125.48	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1003	G	N3-C4-N9	6.07	129.64	126.00
1	1	669	G	C8-N9-C1'	-6.06	119.12	127.00
57	4	270	C	C5-C6-N1	6.06	124.03	121.00
1	1	138	U	N3-C2-O2	-6.06	117.96	122.20
57	4	223	G	N3-C4-C5	-6.06	125.57	128.60
1	1	566	U	N3-C2-O2	-6.06	117.96	122.20
57	4	204	G	N9-C4-C5	-6.06	102.98	105.40
1	1	1256	G	C4-N9-C1'	6.04	134.36	126.50
2	2	178	C	N3-C2-O2	-6.04	117.67	121.90
2	2	476	U	N1-C2-O2	6.04	127.03	122.80
57	4	33	A	O5'-P-OP1	-6.04	100.26	105.70
1	1	2247	A	C8-N9-C4	-6.04	103.38	105.80
2	2	368	U	N3-C2-O2	-6.04	117.97	122.20
1	1	129	C	N1-C2-O2	6.04	122.52	118.90
1	1	1769	U	N3-C2-O2	-6.04	117.97	122.20
2	2	154	U	N3-C2-O2	-6.04	117.97	122.20
57	4	163	G	C5'-C4'-O4'	-6.04	101.85	109.10
1	1	1180	U	C5-C6-N1	6.03	125.72	122.70
57	4	321	G	N3-C4-N9	-6.03	122.38	126.00
1	1	1526	C	N1-C2-O2	6.03	122.52	118.90
57	4	32	A	C2-N3-C4	6.03	113.61	110.60
57	4	235	C	C6-N1-C2	-6.03	117.89	120.30
1	1	1308	A	C8-N9-C4	-6.02	103.39	105.80
57	4	36	C	C5-C6-N1	6.02	124.01	121.00
2	2	840	C	C5-C6-N1	6.02	124.01	121.00
57	4	72	A	C4-N9-C1'	6.02	137.14	126.30
1	1	2824	C	N3-C2-O2	-6.02	117.69	121.90
1	1	1994	C	N3-C2-O2	-6.02	117.69	121.90
1	1	378	C	C2-N1-C1'	6.02	125.42	118.80
1	1	1076	C	N1-C2-O2	6.01	122.51	118.90
1	1	2636	C	C6-N1-C2	-6.01	117.89	120.30
57	4	311	U	C5-C6-N1	6.01	125.71	122.70
57	4	181	G	C2-N3-C4	6.01	114.90	111.90
57	4	300	U	C5-C6-N1	6.01	125.70	122.70
57	4	221	U	P-O3'-C3'	6.01	126.91	119.70
57	4	267	G	N3-C4-N9	6.01	129.60	126.00
1	1	1170	C	N3-C2-O2	-6.00	117.70	121.90
1	1	2321	U	N3-C2-O2	-6.00	118.00	122.20
2	2	1088	G	C4-N9-C1'	6.00	134.30	126.50
1	1	1456	G	C8-N9-C1'	-5.99	119.21	127.00
57	4	18	C	N3-C2-O2	-5.99	117.71	121.90
2	2	1020	G	C4-N9-C1'	5.99	134.28	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	754	C	C2-N1-C1'	5.98	125.38	118.80
2	2	354	G	C8-N9-C1'	-5.98	119.22	127.00
57	4	236	U	N1-C2-O2	5.98	126.99	122.80
2	2	99	C	C6-N1-C1'	-5.98	113.62	120.80
2	2	843	U	C2-N1-C1'	5.98	124.88	117.70
57	4	187	C	C2-N1-C1'	5.98	125.38	118.80
57	4	286	A	C8-N9-C4	5.98	108.19	105.80
1	1	366	C	C2-N1-C1'	5.98	125.38	118.80
2	2	476	U	N3-C2-O2	-5.98	118.02	122.20
2	2	1244	G	C4-N9-C1'	-5.98	118.73	126.50
2	2	979	C	N3-C2-O2	-5.97	117.72	121.90
3	3	42	C	N1-C2-O2	5.97	122.48	118.90
57	4	183	C	C2-N1-C1'	-5.97	112.23	118.80
57	4	279	C	C5-C6-N1	5.97	123.99	121.00
1	1	2259	U	N3-C2-O2	-5.97	118.02	122.20
2	2	354	G	C4-N9-C1'	5.97	134.26	126.50
1	1	2108	A	C2-N3-C4	5.97	113.58	110.60
57	4	212	U	P-O3'-C3'	5.96	126.86	119.70
1	1	257	C	N3-C2-O2	-5.96	117.73	121.90
1	1	1060	U	C5-C6-N1	5.96	125.68	122.70
1	1	2043	C	C2-N1-C1'	5.96	125.36	118.80
2	2	620	C	N3-C2-O2	-5.96	117.73	121.90
2	2	1045	C	C6-N1-C2	-5.95	117.92	120.30
57	4	146	C	O4'-C1'-N1	5.95	112.96	108.20
2	2	922	G	C4-N9-C1'	5.95	134.24	126.50
1	1	2320	U	N1-C2-O2	-5.95	118.64	122.80
1	1	2312	U	C2-N1-C1'	5.95	124.84	117.70
2	2	1008	U	C2-N1-C1'	5.95	124.84	117.70
57	4	325	G	C8-N9-C4	-5.95	104.02	106.40
1	1	2594	C	N3-C2-O2	-5.94	117.74	121.90
57	4	306	U	C5-C6-N1	5.94	125.67	122.70
1	1	912	C	N3-C2-O2	-5.94	117.74	121.90
1	1	1192	G	N1-C6-O6	-5.94	116.34	119.90
1	1	1908	C	C6-N1-C2	-5.93	117.93	120.30
1	1	2717	C	N3-C2-O2	-5.93	117.75	121.90
57	4	241	C	N3-C2-O2	-5.93	117.75	121.90
57	4	189	C	C6-N1-C2	-5.93	117.93	120.30
1	1	1221	C	N3-C2-O2	-5.92	117.75	121.90
3	3	74	U	C5-C6-N1	5.92	125.66	122.70
1	1	1775	U	N3-C2-O2	-5.92	118.06	122.20
2	2	679	C	C2-N1-C1'	5.92	125.31	118.80
57	4	117	G	N7-C8-N9	5.92	116.06	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	462	C	N3-C2-O2	-5.92	117.76	121.90
1	1	971	G	C6-C5-N7	-5.92	126.85	130.40
57	4	349	C	C2-N1-C1'	5.92	125.31	118.80
57	4	245	C	C6-N1-C1'	-5.92	113.70	120.80
1	1	1045	C	C6-N1-C2	-5.91	117.94	120.30
57	4	10	U	O5'-P-OP1	5.91	117.80	110.70
1	1	673	C	N3-C2-O2	-5.91	117.76	121.90
2	2	937	A	N1-C6-N6	5.91	122.14	118.60
57	4	73	A	C4-N9-C1'	5.91	136.94	126.30
1	1	1776	G	C8-N9-C4	-5.91	104.04	106.40
1	1	816	C	N1-C2-O2	5.90	122.44	118.90
1	1	818	G	C8-N9-C4	-5.90	104.04	106.40
2	2	936	C	N1-C2-O2	5.90	122.44	118.90
57	4	30	C	N3-C4-N4	5.90	122.13	118.00
2	2	1172	C	C6-N1-C2	-5.90	117.94	120.30
57	4	281	A	O4'-C1'-N9	5.90	112.92	108.20
1	1	2452	C	C2-N1-C1'	5.89	125.28	118.80
1	1	1135	C	C2-N1-C1'	5.89	125.28	118.80
1	1	2636	C	C5-C6-N1	5.89	123.94	121.00
1	1	2786	U	N3-C2-O2	-5.89	118.08	122.20
1	1	954	G	C4-N9-C1'	5.88	134.15	126.50
2	2	328	C	N3-C2-O2	-5.88	117.78	121.90
57	4	144	U	O4'-C1'-N1	5.88	112.91	108.20
1	1	1157	G	N3-C4-N9	5.88	129.53	126.00
57	4	232	A	C8-N9-C4	-5.88	103.45	105.80
1	1	1370	C	N3-C2-O2	-5.88	117.78	121.90
57	4	209	C	N3-C2-O2	-5.88	117.78	121.90
2	2	4	U	C2-N1-C1'	5.88	124.75	117.70
57	4	223	G	N3-C4-N9	5.88	129.53	126.00
57	4	132	U	C5-C6-N1	5.88	125.64	122.70
3	3	92	C	C2-N1-C1'	5.87	125.26	118.80
2	2	341	C	N1-C2-O2	5.87	122.42	118.90
1	1	2615	U	C2-N1-C1'	5.87	124.74	117.70
2	2	492	C	C2-N1-C1'	5.87	125.26	118.80
2	2	879	C	N1-C2-O2	5.87	122.42	118.90
1	1	2209	G	C6-C5-N7	-5.87	126.88	130.40
2	2	4	U	N1-C2-O2	5.86	126.90	122.80
57	4	273	A	C8-N9-C4	-5.86	103.45	105.80
1	1	1859	U	N3-C2-O2	-5.86	118.10	122.20
2	2	1174	G	N3-C4-N9	5.86	129.51	126.00
57	4	200	G	N7-C8-N9	5.86	116.03	113.10
57	4	214	C	C4-C5-C6	-5.86	114.47	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	229	U	C2-N1-C1'	5.86	124.73	117.70
57	4	229	U	C5-C6-N1	5.86	125.63	122.70
57	4	340	G	C6-C5-N7	-5.86	126.89	130.40
2	2	1510	C	C6-N1-C2	-5.85	117.96	120.30
1	1	1376	C	C6-N1-C1'	-5.85	113.78	120.80
2	2	1008	U	N1-C2-O2	5.85	126.89	122.80
1	1	1804	C	C6-N1-C2	-5.85	117.96	120.30
57	4	167	G	P-O3'-C3'	5.85	126.72	119.70
57	4	304	C	C5-C6-N1	5.84	123.92	121.00
57	4	304	C	O4'-C1'-N1	5.84	112.88	108.20
57	4	159	C	N1-C2-O2	5.84	122.41	118.90
1	1	1725	U	C2-N1-C1'	5.83	124.70	117.70
57	4	5	C	O4'-C1'-N1	5.83	112.86	108.20
2	2	1327	C	C6-N1-C2	-5.83	117.97	120.30
2	2	1003	G	C4-N9-C1'	5.83	134.08	126.50
57	4	117	G	C8-N9-C4	-5.83	104.07	106.40
57	4	204	G	C4-C5-N7	5.83	113.13	110.80
2	2	467	U	C5-C6-N1	5.83	125.61	122.70
1	1	2789	C	C5-C6-N1	5.82	123.91	121.00
1	1	709	U	N3-C2-O2	-5.82	118.12	122.20
1	1	2025	C	C2-N1-C1'	5.82	125.20	118.80
2	2	737	C	C5-C6-N1	5.82	123.91	121.00
57	4	129	G	C8-N9-C1'	-5.82	119.44	127.00
1	1	1920	C	C5-C6-N1	5.82	123.91	121.00
1	1	565	C	C6-N1-C2	-5.81	117.97	120.30
57	4	297	G	N1-C6-O6	5.81	123.39	119.90
57	4	27	U	C5-C6-N1	5.81	125.61	122.70
57	4	163	G	N7-C8-N9	5.81	116.01	113.10
1	1	2594	C	C5-C6-N1	5.81	123.91	121.00
57	4	263	G	N3-C2-N2	-5.81	115.83	119.90
57	4	232	A	N7-C8-N9	5.81	116.70	113.80
1	1	269	C	C6-N1-C2	-5.81	117.98	120.30
1	1	729	G	N3-C4-C5	-5.80	125.70	128.60
57	4	31	G	O4'-C1'-N9	5.80	112.84	108.20
57	4	223	G	OP1-P-O3'	5.80	117.96	105.20
1	1	143	C	N3-C2-O2	-5.80	117.84	121.90
1	1	729	G	N3-C4-N9	5.80	129.48	126.00
57	4	199	C	C6-N1-C2	-5.80	117.98	120.30
57	4	122	A	C5-C6-N1	5.79	120.60	117.70
57	4	319	A	P-O3'-C3'	5.79	126.65	119.70
1	1	2425	A	P-O3'-C3'	5.79	126.64	119.70
1	1	2006	C	C6-N1-C2	-5.79	117.98	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	263	G	P-O3'-C3'	5.79	126.64	119.70
2	2	882	C	C6-N1-C2	-5.78	117.99	120.30
1	1	1873	G	N7-C8-N9	5.78	115.99	113.10
57	4	48	C	P-O3'-C3'	5.78	126.64	119.70
1	1	2149	U	N3-C2-O2	-5.78	118.16	122.20
1	1	2185	U	C5-C6-N1	5.78	125.59	122.70
1	1	1894	C	N3-C2-O2	-5.77	117.86	121.90
1	1	2548	U	N3-C2-O2	-5.77	118.16	122.20
1	1	971	G	C4-N9-C1'	5.77	134.00	126.50
57	4	56	C	O5'-P-OP2	-5.77	100.51	105.70
1	1	1357	C	N3-C2-O2	-5.77	117.86	121.90
57	4	27	U	N1-C2-O2	5.77	126.84	122.80
57	4	289	U	C6-N1-C2	-5.77	117.54	121.00
1	1	2889	C	C2-N1-C1'	5.76	125.14	118.80
2	2	272	C	N3-C2-O2	-5.76	117.87	121.90
1	1	818	G	N1-C2-N2	-5.76	111.02	116.20
1	1	860	U	N3-C2-O2	-5.76	118.17	122.20
1	1	1945	G	N3-C4-N9	5.76	129.45	126.00
57	4	204	G	C5-C6-O6	-5.76	125.15	128.60
1	1	860	U	N1-C2-O2	5.75	126.83	122.80
1	1	648	G	C4-N9-C1'	5.75	133.98	126.50
1	1	765	C	C5-C6-N1	5.75	123.87	121.00
1	1	1153	C	C6-N1-C2	-5.75	118.00	120.30
57	4	311	U	C6-N1-C2	-5.75	117.55	121.00
2	2	937	A	C5-N7-C8	-5.75	101.03	103.90
1	1	2649	C	C2-N1-C1'	5.75	125.12	118.80
57	4	6	U	C5'-C4'-O4'	-5.75	102.21	109.10
57	4	40	G	N7-C8-N9	5.75	115.97	113.10
57	4	267	G	C8-N9-C4	-5.74	104.10	106.40
1	1	2200	C	N1-C2-O2	5.74	122.34	118.90
1	1	404	A	P-O3'-C3'	5.73	126.58	119.70
1	1	1170	C	C6-N1-C2	-5.73	118.01	120.30
1	1	1859	U	C2-N1-C1'	5.73	124.58	117.70
1	1	138	U	C2-N1-C1'	5.73	124.58	117.70
57	4	175	A	O3'-P-O5'	5.73	114.89	104.00
1	1	2000	C	C5-C6-N1	5.73	123.86	121.00
57	4	229	U	P-O3'-C3'	5.73	126.57	119.70
1	1	171	U	C2-N1-C1'	5.73	124.57	117.70
57	4	222	U	C6-N1-C1'	-5.73	113.18	121.20
1	1	2885	G	N3-C4-N9	5.72	129.44	126.00
1	1	2901	C	C5-C6-N1	5.72	123.86	121.00
1	1	2902	C	C6-N1-C2	-5.72	118.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	30	C	N1-C2-O2	5.72	122.33	118.90
57	4	275	C	O4'-C1'-N1	5.72	112.78	108.20
2	2	519	C	N1-C2-O2	5.72	122.33	118.90
1	1	1557	C	C2-N3-C4	-5.72	117.04	119.90
57	4	263	G	C5'-C4'-C3'	5.72	125.15	116.00
1	1	280	U	N3-C2-O2	-5.72	118.20	122.20
1	1	860	U	C2-N1-C1'	5.72	124.56	117.70
1	1	2650	U	N1-C2-O2	5.72	126.80	122.80
57	4	73	A	N7-C8-N9	5.72	116.66	113.80
57	4	200	G	N3-C4-C5	-5.72	125.74	128.60
57	4	222	U	C5-C6-N1	5.72	125.56	122.70
57	4	73	A	C8-N9-C4	-5.71	103.52	105.80
2	2	492	C	C6-N1-C2	-5.71	118.02	120.30
57	4	144	U	OP2-P-O3'	5.71	117.76	105.20
57	4	248	G	C8-N9-C1'	5.71	134.43	127.00
1	1	2229	U	C6-N1-C2	-5.71	117.58	121.00
2	2	989	U	N1-C2-O2	5.71	126.80	122.80
1	1	2540	C	N3-C2-O2	-5.70	117.91	121.90
2	2	469	C	C6-N1-C2	-5.70	118.02	120.30
2	2	1020	G	N3-C4-C5	-5.70	125.75	128.60
1	1	544	C	C5-C6-N1	5.69	123.85	121.00
1	1	1092	C	C6-N1-C2	-5.69	118.02	120.30
57	4	17	U	P-O3'-C3'	5.69	126.53	119.70
2	2	738	C	C6-N1-C2	-5.69	118.02	120.30
57	4	122	A	N1-C6-N6	-5.69	115.19	118.60
1	1	2786	U	C2-N1-C1'	5.69	124.52	117.70
2	2	528	C	C5-C6-N1	5.68	123.84	121.00
57	4	257	U	OP1-P-O3'	5.68	117.70	105.20
1	1	269	C	N3-C2-O2	-5.68	117.92	121.90
1	1	1243	C	N1-C2-O2	5.68	122.31	118.90
1	1	2760	C	N3-C2-O2	-5.68	117.92	121.90
57	4	336	G	P-O5'-C5'	-5.68	111.81	120.90
2	2	612	C	C6-N1-C2	-5.68	118.03	120.30
1	1	876	C	C5-C6-N1	5.67	123.84	121.00
1	1	2680	U	C2-N1-C1'	5.67	124.51	117.70
57	4	199	C	N3-C2-O2	-5.67	117.93	121.90
57	4	211	C	P-O3'-C3'	5.67	126.51	119.70
1	1	2063	C	C6-N1-C2	-5.67	118.03	120.30
57	4	329	U	C5-C6-N1	5.67	125.54	122.70
1	1	2488	G	C4-N9-C1'	5.67	133.87	126.50
2	2	341	C	C5-C6-N1	5.67	123.83	121.00
1	1	1804	C	C5-C6-N1	5.67	123.83	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2064	C	C6-N1-C2	-5.67	118.03	120.30
3	3	92	C	N3-C2-O2	-5.67	117.93	121.90
57	4	144	U	C6-N1-C2	-5.67	117.60	121.00
1	1	2452	C	N1-C2-O2	5.67	122.30	118.90
2	2	439	U	N1-C2-O2	5.67	126.77	122.80
1	1	31	C	C6-N1-C2	-5.66	118.03	120.30
57	4	141	C	C5-C6-N1	5.66	123.83	121.00
2	2	1303	C	N3-C2-O2	-5.66	117.94	121.90
2	2	1533	C	C6-N1-C2	-5.66	118.04	120.30
1	1	635	C	C6-N1-C2	-5.66	118.04	120.30
1	1	942	G	N1-C2-N2	-5.66	111.11	116.20
1	1	323	C	C2-N1-C1'	5.65	125.02	118.80
1	1	1097	U	C2-N1-C1'	5.65	124.48	117.70
1	1	462	C	C6-N1-C2	-5.65	118.04	120.30
1	1	816	C	N3-C2-O2	-5.65	117.95	121.90
57	4	132	U	O5'-P-OP2	-5.65	100.62	105.70
57	4	335	C	C5-C4-N4	5.65	124.15	120.20
1	1	1075	C	C5-C6-N1	5.64	123.82	121.00
1	1	1594	U	C6-N1-C1'	-5.64	113.30	121.20
1	1	2624	G	C8-N9-C4	-5.64	104.14	106.40
57	4	53	G	OP2-P-O3'	-5.64	92.79	105.20
1	1	1	G	N3-C4-C5	-5.64	125.78	128.60
1	1	968	C	C6-N1-C2	-5.64	118.05	120.30
1	1	2885	G	C4-N9-C1'	5.64	133.83	126.50
2	2	1008	U	N3-C2-O2	-5.64	118.25	122.20
2	2	1073	U	N3-C2-O2	-5.63	118.26	122.20
57	4	241	C	N1-C2-O2	5.63	122.28	118.90
1	1	2214	C	N3-C2-O2	-5.63	117.96	121.90
57	4	335	C	P-O3'-C3'	5.63	126.46	119.70
2	2	1116	U	N1-C2-O2	5.63	126.74	122.80
57	4	229	U	C6-N1-C2	-5.63	117.62	121.00
57	4	12	U	C5-C6-N1	5.62	125.51	122.70
57	4	187	C	N3-C2-O2	-5.62	117.96	121.90
1	1	1357	C	N1-C2-O2	5.62	122.27	118.90
1	1	2403	C	C2-N1-C1'	5.62	124.98	118.80
1	1	1905	C	N3-C2-O2	-5.62	117.97	121.90
57	4	321	G	N9-C4-C5	5.62	107.65	105.40
1	1	709	U	N1-C2-O2	5.61	126.73	122.80
2	2	993	G	C4-N9-C1'	5.61	133.80	126.50
1	1	957	C	N1-C2-O2	5.61	122.27	118.90
1	1	1117	C	N3-C2-O2	-5.61	117.97	121.90
1	1	1547	C	N3-C2-O2	-5.61	117.97	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1859	U	N1-C2-O2	5.61	126.73	122.80
1	1	2484	G	C8-N9-C1'	-5.61	119.71	127.00
2	2	582	C	N3-C2-O2	-5.61	117.98	121.90
1	1	1157	G	C4-C5-N7	5.60	113.04	110.80
2	2	1009	U	C2-N1-C1'	5.60	124.42	117.70
1	1	2488	G	N3-C4-N9	5.60	129.36	126.00
2	2	727	G	C6-C5-N7	-5.60	127.04	130.40
2	2	979	C	C6-N1-C2	-5.60	118.06	120.30
2	2	1245	C	C5-C6-N1	5.60	123.80	121.00
57	4	134	G	C8-N9-C4	-5.60	104.16	106.40
1	1	1725	U	N3-C2-O2	-5.60	118.28	122.20
1	1	2283	C	N3-C2-O2	-5.60	117.98	121.90
1	1	2507	C	C6-N1-C2	-5.60	118.06	120.30
57	4	304	C	N3-C2-O2	-5.59	117.98	121.90
18	N	51	LEU	CB-CG-CD1	-5.59	101.50	111.00
1	1	648	G	C6-C5-N7	-5.59	127.05	130.40
1	1	1725	U	N1-C2-O2	5.59	126.71	122.80
1	1	1351	C	C2-N1-C1'	5.59	124.94	118.80
57	4	13	G	OP1-P-O3'	5.58	117.49	105.20
57	4	16	U	N1-C2-O2	5.58	126.71	122.80
57	4	330	U	C5-C6-N1	5.58	125.49	122.70
57	4	333	G	C4-N9-C1'	5.58	133.75	126.50
57	4	248	G	O4'-C1'-N9	5.58	112.66	108.20
1	1	2347	C	N1-C2-O2	5.57	122.24	118.90
1	1	1385	A	O4'-C1'-N9	5.57	112.66	108.20
1	1	2667	C	N1-C2-O2	5.57	122.24	118.90
2	2	937	A	C4-C5-N7	5.57	113.49	110.70
57	4	358	C	N1-C2-O2	5.57	122.24	118.90
1	1	876	C	C6-N1-C2	-5.56	118.08	120.30
1	1	2889	C	C6-N1-C2	-5.56	118.08	120.30
1	1	1447	C	C6-N1-C2	-5.56	118.08	120.30
57	4	343	C	N3-C2-O2	-5.56	118.01	121.90
57	4	146	C	C5-C6-N1	5.56	123.78	121.00
2	2	1215	G	C4-N9-C1'	5.55	133.72	126.50
57	4	49	C	P-O5'-C5'	5.55	129.79	120.90
1	1	2510	C	N3-C2-O2	-5.55	118.01	121.90
1	1	2562	U	C2-N1-C1'	5.55	124.36	117.70
1	1	2594	C	C2-N1-C1'	5.55	124.90	118.80
2	2	470	C	N3-C2-O2	-5.55	118.02	121.90
2	2	1471	U	N1-C2-O2	5.55	126.68	122.80
1	1	2552	OMU	P-O3'-C3'	5.55	126.36	119.70
2	2	1262	C	C5-C6-N1	5.55	123.77	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	492	C	C5-C6-N1	5.54	123.77	121.00
2	2	563	A	C4-N9-C1'	5.54	136.27	126.30
2	2	451	A	C4-N9-C1'	5.54	136.27	126.30
1	1	2620	C	C6-N1-C2	-5.54	118.08	120.30
57	4	323	A	C8-N9-C4	-5.54	103.58	105.80
1	1	2720	U	N1-C2-O2	5.54	126.67	122.80
2	2	1041	G	C5-C6-O6	5.53	131.92	128.60
1	1	281	C	C6-N1-C2	-5.53	118.09	120.30
1	1	2698	U	C5-C6-N1	5.53	125.47	122.70
1	1	295	G	N3-C4-N9	5.53	129.32	126.00
1	1	2339	C	C2-N1-C1'	5.53	124.88	118.80
2	2	989	U	C5-C6-N1	5.53	125.46	122.70
57	4	152	C	O4'-C1'-N1	5.53	112.62	108.20
57	4	300	U	C6-N1-C2	-5.53	117.68	121.00
1	1	307	G	C8-N9-C4	-5.53	104.19	106.40
57	4	137	C	N1-C2-O2	5.53	122.22	118.90
2	2	1003	G	C4-C5-N7	5.52	113.01	110.80
1	1	269	C	C2-N1-C1'	5.52	124.88	118.80
1	1	2300	C	C6-N1-C2	-5.52	118.09	120.30
2	2	1244	G	N3-C2-N2	-5.52	116.03	119.90
57	4	66	C	C6-N1-C2	-5.52	118.09	120.30
1	1	77	G	C4-N9-C1'	5.52	133.68	126.50
1	1	1153	C	C2-N1-C1'	5.52	124.87	118.80
1	1	1182	G	C6-C5-N7	-5.52	127.09	130.40
1	1	1119	U	N3-C2-O2	-5.51	118.34	122.20
1	1	1785	A	C8-N9-C4	-5.51	103.59	105.80
1	1	1892	C	C5-C6-N1	5.51	123.76	121.00
3	3	68	C	N1-C2-O2	5.51	122.21	118.90
57	4	36	C	O4'-C1'-N1	5.51	112.61	108.20
1	1	1894	C	N1-C2-O2	5.51	122.20	118.90
1	1	1200	C	C6-N1-C2	-5.51	118.10	120.30
2	2	1097	C	C6-N1-C2	-5.51	118.10	120.30
1	1	669	G	N3-C4-N9	5.50	129.30	126.00
57	4	132	U	C6-N1-C2	-5.50	117.70	121.00
1	1	155	A	N9-C4-C5	-5.50	103.60	105.80
1	1	2457	PSU	P-O3'-C3'	5.50	126.30	119.70
1	1	2698	U	C2-N1-C1'	5.50	124.30	117.70
57	4	286	A	C8-N9-C1'	5.50	137.59	127.70
1	1	455	C	C6-N1-C2	-5.49	118.10	120.30
2	2	1445	U	N1-C2-O2	5.49	126.64	122.80
57	4	249	U	P-O3'-C3'	5.49	126.29	119.70
25	U	98	SER	C-N-CA	5.49	135.43	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	333	G	C6-C5-N7	-5.49	127.11	130.40
1	1	681	G	N9-C4-C5	-5.49	103.20	105.40
37	g	88	ASP	CB-CG-OD1	5.49	123.24	118.30
57	4	127	C	C6-N1-C2	-5.49	118.11	120.30
57	4	148	U	C6-N1-C2	-5.49	117.71	121.00
57	4	273	A	C6-C5-N7	-5.49	128.46	132.30
2	2	1132	C	N1-C2-O2	5.49	122.19	118.90
1	1	1611	C	N1-C2-O2	5.48	122.19	118.90
2	2	266	G	C4-C5-N7	5.48	112.99	110.80
2	2	842	U	N1-C2-O2	5.48	126.64	122.80
57	4	144	U	P-O3'-C3'	5.48	126.28	119.70
1	1	1399	C	C5-C6-N1	5.48	123.74	121.00
1	1	2321	U	N1-C2-O2	5.48	126.63	122.80
2	2	54	C	N3-C2-O2	-5.48	118.07	121.90
1	1	1135	C	N3-C2-O2	-5.48	118.07	121.90
57	4	172	U	O4'-C1'-N1	5.47	112.58	108.20
2	2	211	G	C4-N9-C1'	5.47	133.62	126.50
2	2	936	C	N3-C2-O2	-5.47	118.07	121.90
57	4	150	G	N3-C4-N9	5.47	129.28	126.00
2	2	4	U	N3-C2-O2	-5.47	118.37	122.20
1	1	780	G	C6-C5-N7	-5.46	127.12	130.40
1	1	1023	U	C2-N1-C1'	5.46	124.26	117.70
1	1	1267	U	N1-C2-O2	5.46	126.63	122.80
1	1	2512	C	C5-C6-N1	5.46	123.73	121.00
2	2	842	U	N3-C2-O2	-5.46	118.38	122.20
2	2	1264	U	C5-C6-N1	5.46	125.43	122.70
57	4	186	A	N7-C8-N9	5.46	116.53	113.80
57	4	246	U	C2-N1-C1'	5.46	124.26	117.70
1	1	1296	G	C6-C5-N7	-5.46	127.12	130.40
57	4	120	U	C5-C6-N1	5.46	125.43	122.70
1	1	702	U	C2-N1-C1'	5.46	124.25	117.70
1	1	2901	C	C6-N1-C2	-5.46	118.12	120.30
1	1	312	G	C4-N9-C1'	5.46	133.59	126.50
2	2	1445	U	N3-C2-O2	-5.46	118.38	122.20
1	1	301	G	O4'-C1'-N9	5.46	112.56	108.20
1	1	721	A	C4-C5-N7	5.46	113.43	110.70
1	1	1557	C	N3-C2-O2	-5.45	118.08	121.90
2	2	1020	G	C8-N9-C1'	-5.45	119.91	127.00
1	1	1092	C	N3-C2-O2	-5.45	118.08	121.90
2	2	632	U	N3-C2-O2	-5.45	118.39	122.20
1	1	1664	A	C4-N9-C1'	5.45	136.11	126.30
2	2	110	C	C2-N1-C1'	5.45	124.79	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	153	U	OP2-P-O3'	5.45	117.19	105.20
1	1	1675	C	C6-N1-C2	-5.45	118.12	120.30
1	1	952	G	N7-C8-N9	5.45	115.82	113.10
1	1	2761	A	O4'-C1'-N9	5.45	112.56	108.20
57	4	38	A	O4'-C1'-N9	5.45	112.56	108.20
57	4	48	C	N3-C2-O2	-5.44	118.09	121.90
57	4	193	A	O4'-C1'-N9	5.44	112.56	108.20
1	1	1157	G	N9-C4-C5	-5.44	103.22	105.40
2	2	590	U	N1-C2-O2	5.44	126.61	122.80
2	2	738	C	C5-C6-N1	5.44	123.72	121.00
3	3	30	C	C5-C6-N1	5.44	123.72	121.00
1	1	129	C	N3-C2-O2	-5.44	118.09	121.90
57	4	36	C	P-O3'-C3'	5.44	126.22	119.70
2	2	647	C	C6-N1-C2	-5.43	118.13	120.30
57	4	359	C	C6-N1-C2	-5.43	118.13	120.30
1	1	485	C	N1-C2-O2	5.43	122.16	118.90
1	1	991	C	C2-N1-C1'	5.43	124.77	118.80
2	2	1088	G	C8-N9-C1'	-5.43	119.94	127.00
2	2	358	U	N3-C2-O2	-5.43	118.40	122.20
57	4	286	A	N7-C8-N9	-5.43	111.09	113.80
57	4	121	A	P-O3'-C3'	5.43	126.21	119.70
1	1	1267	U	N3-C2-O2	-5.42	118.40	122.20
1	1	1916	A	N7-C8-N9	5.42	116.51	113.80
1	1	2488	G	N3-C4-C5	-5.42	125.89	128.60
1	1	2592	G	C4-C5-N7	5.42	112.97	110.80
1	1	1605	C	N1-C2-O2	5.42	122.15	118.90
57	4	76	C	C2-N1-C1'	5.42	124.76	118.80
1	1	373	U	C2-N1-C1'	5.42	124.20	117.70
2	2	1346	A	OP1-P-O3'	5.41	117.11	105.20
2	2	1174	G	N9-C4-C5	-5.41	103.24	105.40
1	1	1547	C	C6-N1-C2	-5.41	118.14	120.30
1	1	2624	G	C6-N1-C2	-5.41	121.86	125.10
57	4	48	C	O4'-C1'-N1	5.41	112.53	108.20
2	2	294	U	C2-N1-C1'	5.41	124.19	117.70
57	4	240	U	O4'-C1'-N1	5.41	112.52	108.20
1	1	1174	U	N1-C2-O2	5.40	126.58	122.80
1	1	1605	C	N3-C2-O2	-5.40	118.12	121.90
1	1	2594	C	C6-N1-C2	-5.40	118.14	120.30
2	2	993	G	C8-N9-C1'	-5.40	119.98	127.00
2	2	1533	C	N1-C2-O2	5.40	122.14	118.90
57	4	290	A	O3'-P-O5'	5.40	114.26	104.00
1	1	1785	A	N7-C8-N9	5.40	116.50	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2063	C	C6-N1-C1'	-5.40	114.32	120.80
1	1	2794	C	C2-N1-C1'	5.40	124.74	118.80
1	1	2222	C	C6-N1-C2	-5.40	118.14	120.30
57	4	289	U	N3-C2-O2	-5.40	118.42	122.20
57	4	147	C	C5-C6-N1	5.40	123.70	121.00
1	1	2259	U	C6-N1-C1'	-5.39	113.65	121.20
1	1	2285	C	N1-C2-O2	5.39	122.14	118.90
1	1	1456	G	C6-C5-N7	-5.39	127.17	130.40
57	4	141	C	O4'-C1'-N1	5.39	112.51	108.20
1	1	143	C	N1-C2-O2	5.39	122.13	118.90
1	1	2380	C	N1-C2-O2	5.39	122.13	118.90
2	2	1113	C	C6-N1-C2	-5.39	118.14	120.30
57	4	121	A	O4'-C1'-N9	-5.39	103.89	108.20
2	2	20	U	N3-C2-O2	-5.38	118.43	122.20
57	4	27	U	C6-N1-C2	-5.38	117.77	121.00
57	4	214	C	C6-N1-C1'	5.38	127.26	120.80
1	1	284	U	C5-C6-N1	5.38	125.39	122.70
57	4	16	U	C6-N1-C2	-5.38	117.77	121.00
1	1	702	U	N3-C2-O2	-5.38	118.43	122.20
1	1	1941	C	C6-N1-C1'	-5.38	114.34	120.80
1	1	1530	G	N3-C4-N9	5.38	129.23	126.00
1	1	1190	G	C8-N9-C4	-5.38	104.25	106.40
1	1	2601	C	C2-N1-C1'	5.38	124.72	118.80
1	1	1881	C	N3-C2-O2	-5.38	118.14	121.90
57	4	132	U	O3'-P-O5'	5.38	114.21	104.00
2	2	879	C	N3-C2-O2	-5.37	118.14	121.90
2	2	1163	A	N9-C4-C5	-5.37	103.65	105.80
57	4	284	G	P-O5'-C5'	5.37	129.50	120.90
57	4	288	G	N7-C8-N9	5.37	115.79	113.10
1	1	1456	G	N3-C4-N9	5.37	129.22	126.00
2	2	1392	G	C6-C5-N7	-5.37	127.18	130.40
2	2	1038	C	C5-C6-N1	5.37	123.68	121.00
57	4	360	A	O5'-C5'-C4'	5.37	121.90	111.70
1	1	284	U	C6-N1-C1'	-5.37	113.69	121.20
1	1	847	U	C2-N1-C1'	5.37	124.14	117.70
1	1	2512	C	C6-N1-C2	-5.37	118.15	120.30
1	1	2874	C	C5-C6-N1	5.37	123.68	121.00
2	2	1088	G	N3-C4-C5	-5.37	125.92	128.60
2	2	1163	A	C4-C5-N7	5.37	113.38	110.70
57	4	189	C	O3'-P-O5'	5.37	114.19	104.00
1	1	1547	C	C2-N1-C1'	5.36	124.70	118.80
1	1	1658	C	C5-C6-N1	5.36	123.68	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1945	G	C4-N9-C1'	5.36	133.47	126.50
1	1	1873	G	C6-C5-N7	-5.36	127.19	130.40
2	2	476	U	C5-C6-N1	5.36	125.38	122.70
57	4	273	A	C4-C5-N7	5.36	113.38	110.70
1	1	358	U	C6-N1-C2	-5.35	117.79	121.00
1	1	2236	U	N3-C2-O2	-5.35	118.45	122.20
1	1	2902	C	C2-N1-C1'	5.35	124.69	118.80
2	2	1283	U	N3-C2-O2	-5.35	118.45	122.20
57	4	137	C	C2-N1-C1'	5.35	124.69	118.80
57	4	328	U	C6-N1-C2	-5.35	117.79	121.00
1	1	1999	C	N3-C2-O2	-5.35	118.16	121.90
1	1	2556	C	C2-N1-C1'	5.35	124.68	118.80
1	1	1530	G	N7-C8-N9	5.34	115.77	113.10
2	2	1382	C	C6-N1-C2	-5.34	118.16	120.30
1	1	475	C	N1-C2-O2	5.34	122.10	118.90
2	2	455	G	N3-C4-N9	5.34	129.20	126.00
2	2	1531	A	C8-N9-C4	-5.34	103.66	105.80
57	4	237	U	C5'-C4'-O4'	-5.34	102.69	109.10
57	4	191	A	O3'-P-O5'	5.34	114.14	104.00
57	4	213	G	N7-C8-N9	5.33	115.77	113.10
1	1	1776	G	N3-C4-C5	-5.33	125.93	128.60
1	1	2760	C	C2-N1-C1'	5.33	124.67	118.80
2	2	52	C	N3-C2-O2	-5.33	118.17	121.90
2	2	273	U	N3-C2-O2	-5.33	118.47	122.20
1	1	2752	C	C6-N1-C2	-5.33	118.17	120.30
2	2	568	G	C4-N9-C1'	5.33	133.42	126.50
2	2	998	C	C6-N1-C1'	-5.33	114.41	120.80
1	1	1113	U	N1-C2-O2	5.32	126.53	122.80
57	4	35	C	P-O3'-C3'	5.32	126.09	119.70
57	4	259	G	C8-N9-C4	-5.32	104.27	106.40
57	4	224	A	C5'-C4'-O4'	5.32	115.49	109.10
1	1	1306	C	N3-C2-O2	-5.32	118.18	121.90
57	4	193	A	O5'-C5'-C4'	5.32	121.81	111.70
2	2	672	U	C6-N1-C1'	-5.32	113.75	121.20
2	2	1141	C	O4'-C1'-N1	5.32	112.45	108.20
57	4	142	U	C5'-C4'-O4'	-5.32	102.72	109.10
1	1	999	U	N3-C2-O2	-5.31	118.48	122.20
1	1	1092	C	C5-C6-N1	5.31	123.66	121.00
57	4	131	U	P-O5'-C5'	5.31	129.40	120.90
13	I	137	LEU	CA-CB-CG	5.31	127.52	115.30
57	4	16	U	C5-C6-N1	5.31	125.36	122.70
1	1	62	U	C6-N1-C2	-5.31	117.81	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1547	C	N1-C2-O2	5.31	122.09	118.90
1	1	1916	A	C8-N9-C4	-5.31	103.68	105.80
2	2	272	C	C6-N1-C2	-5.31	118.18	120.30
57	4	60	U	C5'-C4'-O4'	-5.31	102.73	109.10
57	4	117	G	C6-C5-N7	-5.31	127.21	130.40
2	2	17	U	N3-C2-O2	-5.31	118.48	122.20
2	2	1008	U	C5-C6-N1	5.31	125.35	122.70
1	1	370	G	N1-C2-N2	-5.30	111.43	116.20
1	1	994	C	C6-N1-C2	-5.30	118.18	120.30
1	1	1877	A	N1-C6-N6	-5.30	115.42	118.60
57	4	47	G	N7-C8-N9	5.30	115.75	113.10
1	1	1463	C	C5-C6-N1	5.30	123.65	121.00
57	4	155	C	C2-N3-C4	5.30	122.55	119.90
1	1	681	G	C8-N9-C1'	-5.30	120.11	127.00
1	1	1605	C	C5-C6-N1	5.30	123.65	121.00
1	1	2539	C	C5-C6-N1	5.30	123.65	121.00
57	4	75	C	C2-N3-C4	5.30	122.55	119.90
1	1	2723	C	N3-C2-O2	-5.29	118.19	121.90
57	4	176	G	C8-N9-C4	-5.29	104.28	106.40
57	4	328	U	N1-C2-O2	5.29	126.50	122.80
1	1	2108	A	N3-C4-N9	5.29	131.63	127.40
57	4	246	U	P-O3'-C3'	-5.29	113.35	119.70
1	1	1530	G	C8-N9-C1'	-5.29	120.13	127.00
57	4	184	A	O5'-P-OP1	-5.29	100.94	105.70
57	4	297	G	C5-C6-O6	-5.29	125.43	128.60
57	4	56	C	O4'-C1'-N1	5.29	112.43	108.20
1	1	915	C	C6-N1-C2	-5.28	118.19	120.30
1	1	1530	G	C6-C5-N7	-5.28	127.23	130.40
1	1	765	C	C6-N1-C2	-5.28	118.19	120.30
1	1	1192	G	C5-C6-O6	5.28	131.77	128.60
1	1	576	U	N1-C2-O2	5.28	126.50	122.80
1	1	1294	U	C2-N1-C1'	5.28	124.04	117.70
1	1	1436	G	C6-N1-C2	-5.28	121.93	125.10
1	1	565	C	C2-N1-C1'	5.28	124.60	118.80
1	1	1051	G	C8-N9-C1'	-5.27	120.15	127.00
57	4	78	C	N1-C2-O2	5.27	122.06	118.90
1	1	440	C	C6-N1-C2	-5.27	118.19	120.30
1	1	2072	C	C6-N1-C1'	-5.27	114.48	120.80
1	1	2072	C	N3-C2-O2	-5.27	118.21	121.90
2	2	1003	G	C8-N9-C1'	-5.27	120.15	127.00
2	2	336	A	N7-C8-N9	5.27	116.43	113.80
57	4	191	A	P-O3'-C3'	5.27	126.02	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1499	C	C2-N1-C1'	5.26	124.59	118.80
1	1	1664	A	C8-N9-C1'	-5.26	118.22	127.70
1	1	455	C	N1-C2-O2	5.26	122.06	118.90
1	1	681	G	C4-N9-C1'	5.26	133.34	126.50
1	1	678	C	C2-N1-C1'	5.26	124.59	118.80
2	2	89	U	N3-C2-O2	-5.26	118.52	122.20
57	4	129	G	C8-N9-C4	-5.26	104.30	106.40
1	1	890	C	C6-N1-C2	-5.26	118.20	120.30
57	4	329	U	N3-C2-O2	-5.26	118.52	122.20
1	1	837	C	N3-C2-O2	-5.26	118.22	121.90
1	1	2698	U	N3-C2-O2	-5.25	118.52	122.20
57	4	330	U	N3-C2-O2	-5.25	118.52	122.20
1	1	1409	U	N1-C2-O2	5.25	126.48	122.80
2	2	1232	U	N3-C2-O2	-5.25	118.52	122.20
57	4	315	G	N3-C4-N9	5.25	129.15	126.00
1	1	978	G	N9-C4-C5	5.25	107.50	105.40
57	4	78	C	C5-C6-N1	5.25	123.62	121.00
57	4	249	U	C2-N1-C1'	-5.25	111.40	117.70
1	1	356	G	N7-C8-N9	5.25	115.72	113.10
1	1	1180	U	N3-C2-O2	-5.25	118.53	122.20
2	2	273	U	N1-C2-O2	5.25	126.47	122.80
57	4	255	A	N7-C8-N9	5.25	116.42	113.80
1	1	1878	G	C8-N9-C4	-5.25	104.30	106.40
2	2	1210	C	N1-C2-O2	5.25	122.05	118.90
1	1	154	U	C5-C6-N1	5.24	125.32	122.70
1	1	496	G	N1-C6-O6	-5.24	116.75	119.90
1	1	912	C	C6-N1-C2	-5.24	118.20	120.30
2	2	1116	U	C2-N1-C1'	5.24	123.99	117.70
57	4	171	A	C8-N9-C4	-5.24	103.70	105.80
57	4	185	A	P-O3'-C3'	5.24	125.99	119.70
1	1	971	G	N9-C4-C5	-5.24	103.31	105.40
2	2	864	A	N7-C8-N9	5.24	116.42	113.80
2	2	538	G	N1-C2-N3	5.24	127.04	123.90
57	4	324	G	C5'-C4'-O4'	5.24	115.38	109.10
57	4	191	A	C8-N9-C4	-5.23	103.71	105.80
1	1	758	C	N3-C2-O2	-5.23	118.24	121.90
1	1	2143	C	N1-C2-O2	5.23	122.04	118.90
2	2	1214	C	P-O3'-C3'	5.23	125.98	119.70
1	1	1294	U	N3-C2-O2	-5.23	118.54	122.20
1	1	2484	G	C4-N9-C1'	5.23	133.30	126.50
2	2	1283	U	N1-C2-O2	5.23	126.46	122.80
1	1	1296	G	C4-C5-N7	5.23	112.89	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	127	G	C8-N9-C4	-5.22	104.31	106.40
1	1	1113	U	C6-N1-C1'	-5.22	113.89	121.20
51	u	55	ASP	CB-CG-OD1	5.22	123.00	118.30
1	1	943	A	N7-C8-N9	5.22	116.41	113.80
1	1	1817	G	O5'-P-OP2	-5.22	101.00	105.70
57	4	318	G	N3-C4-C5	-5.22	125.99	128.60
2	2	962	C	C2-N1-C1'	5.22	124.54	118.80
1	1	1053	C	N1-C2-O2	5.22	122.03	118.90
1	1	2784	U	C2-N1-C1'	5.22	123.96	117.70
2	2	1244	G	N9-C4-C5	5.22	107.49	105.40
3	3	47	C	N1-C2-O2	5.22	122.03	118.90
57	4	181	G	C8-N9-C1'	-5.22	120.22	127.00
1	1	302	C	N1-C2-O2	5.21	122.03	118.90
57	4	294	A	N1-C6-N6	-5.21	115.47	118.60
1	1	2442	C	N3-C2-O2	-5.21	118.25	121.90
2	2	272	C	C2-N1-C1'	5.21	124.53	118.80
1	1	1708	C	C2-N1-C1'	5.21	124.53	118.80
1	1	1805	A	C5-C6-N1	5.21	120.30	117.70
2	2	1116	U	N3-C2-O2	-5.21	118.56	122.20
57	4	28	U	P-O3'-C3'	5.21	125.95	119.70
57	4	261	G	P-O5'-C5'	5.21	129.23	120.90
57	4	41	G	C8-N9-C4	-5.20	104.32	106.40
1	1	1248	G	C6-C5-N7	-5.20	127.28	130.40
57	4	138	C	C6-N1-C2	-5.20	118.22	120.30
1	1	1308	A	N7-C8-N9	5.20	116.40	113.80
1	1	2326	C	C2-N1-C1'	5.20	124.52	118.80
1	1	2582	G	N3-C4-N9	5.20	129.12	126.00
57	4	109	C	N3-C2-O2	-5.20	118.26	121.90
57	4	145	C	O4'-C1'-N1	5.20	112.36	108.20
1	1	2260	C	C6-N1-C2	-5.20	118.22	120.30
1	1	2626	C	C6-N1-C2	-5.20	118.22	120.30
57	4	357	U	C6-N1-C1'	-5.20	113.93	121.20
2	2	999	C	N3-C2-O2	-5.19	118.26	121.90
1	1	1	G	C4-N9-C1'	5.19	133.25	126.50
2	2	132	C	C6-N1-C2	-5.19	118.22	120.30
2	2	1230	C	C6-N1-C2	-5.19	118.22	120.30
2	2	368	U	N1-C2-O2	5.19	126.43	122.80
57	4	331	C	O4'-C1'-N1	5.19	112.35	108.20
3	3	97	C	C6-N1-C2	-5.19	118.22	120.30
1	1	999	U	C2-N1-C1'	5.19	123.93	117.70
1	1	968	C	C5-C6-N1	5.19	123.59	121.00
1	1	8	C	C2-N1-C1'	5.18	124.50	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1760	C	N3-C2-O2	-5.18	118.27	121.90
1	1	2465	C	C6-N1-C2	-5.18	118.23	120.30
57	4	75	C	C2-N1-C1'	5.18	124.50	118.80
1	1	912	C	N1-C2-O2	5.18	122.01	118.90
1	1	2560	A	N7-C8-N9	5.18	116.39	113.80
1	1	1703	G	N3-C4-N9	5.18	129.11	126.00
57	4	343	C	C6-N1-C2	-5.18	118.23	120.30
57	4	130	C	C6-N1-C2	-5.17	118.23	120.30
57	4	232	A	C5-C6-N1	5.17	120.29	117.70
1	1	640	C	C6-N1-C2	-5.17	118.23	120.30
57	4	133	A	P-O3'-C3'	5.17	125.91	119.70
57	4	157	C	C6-N1-C1'	5.17	127.01	120.80
57	4	204	G	C8-N9-C1'	-5.17	120.28	127.00
1	1	2483	C	C6-N1-C2	-5.17	118.23	120.30
1	1	2650	U	N3-C2-O2	-5.17	118.58	122.20
1	1	1370	C	C2-N1-C1'	5.17	124.48	118.80
1	1	496	G	C5-C6-O6	5.16	131.70	128.60
1	1	2466	C	N3-C2-O2	-5.16	118.29	121.90
57	4	72	A	C8-N9-C1'	-5.16	118.41	127.70
57	4	306	U	C6-N1-C2	-5.16	117.90	121.00
2	2	180	U	C2-N1-C1'	5.16	123.89	117.70
2	2	1363	A	O4'-C1'-N9	5.16	112.33	108.20
57	4	240	U	C5'-C4'-O4'	5.16	115.30	109.10
2	2	440	C	C5-C6-N1	5.16	123.58	121.00
57	4	53	G	OP1-P-O3'	5.16	116.55	105.20
57	4	266	C	N3-C4-N4	5.15	121.61	118.00
1	1	1437	C	C6-N1-C2	-5.15	118.24	120.30
57	4	133	A	C8-N9-C4	-5.15	103.74	105.80
1	1	1832	C	C6-N1-C2	-5.15	118.24	120.30
1	1	2000	C	C6-N1-C2	-5.15	118.24	120.30
1	1	795	C	C6-N1-C2	-5.15	118.24	120.30
57	4	6	U	C5-C6-N1	5.15	125.27	122.70
57	4	22	G	N7-C8-N9	5.15	115.67	113.10
2	2	761	G	C4-N9-C1'	5.15	133.19	126.50
1	1	2108	A	C4-N9-C1'	5.14	135.56	126.30
1	1	2347	C	C6-N1-C2	-5.14	118.24	120.30
1	1	2579	C	N3-C2-O2	-5.14	118.30	121.90
1	1	2230	G	N3-C4-C5	-5.14	126.03	128.60
57	4	110	U	N1-C2-O2	5.14	126.40	122.80
1	1	140	C	N3-C2-O2	-5.14	118.31	121.90
2	2	52	C	N1-C2-O2	5.14	121.98	118.90
45	o	42	LEU	CA-CB-CG	5.14	127.11	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	4	9	U	OP1-P-O3'	5.13	116.50	105.20
1	1	305	C	C5-C6-N1	5.13	123.57	121.00
1	1	1530	G	N3-C4-C5	-5.13	126.03	128.60
2	2	1244	G	C6-C5-N7	5.13	133.48	130.40
1	1	635	C	C5-C6-N1	5.13	123.56	121.00
57	4	37	C	C6-N1-C2	-5.13	118.25	120.30
57	4	263	G	N1-C2-N2	5.13	120.82	116.20
1	1	77	G	C8-N9-C1'	-5.13	120.33	127.00
2	2	103	U	N3-C2-O2	-5.13	118.61	122.20
57	4	64	C	P-O5'-C5'	5.13	129.10	120.90
1	1	1180	U	C2-N1-C1'	5.12	123.85	117.70
2	2	1140	C	O4'-C1'-N1	5.12	112.30	108.20
1	1	2540	C	C6-N1-C2	-5.12	118.25	120.30
1	1	2723	C	C6-N1-C2	-5.12	118.25	120.30
57	4	192	A	O4'-C1'-N9	5.12	112.30	108.20
1	1	2605	PSU	OP2-P-O3'	5.12	116.47	105.20
57	4	318	G	O4'-C1'-N9	5.12	112.30	108.20
1	1	1296	G	C4-N9-C1'	5.12	133.16	126.50
1	1	1488	C	C2-N1-C1'	5.12	124.43	118.80
57	4	212	U	C6-N1-C2	-5.12	117.93	121.00
2	2	1333	A	N7-C8-N9	5.12	116.36	113.80
57	4	288	G	C2-N3-C4	5.12	114.46	111.90
1	1	754	U	C5-C6-N1	5.12	125.26	122.70
1	1	1395	A	O4'-C1'-N9	5.12	112.29	108.20
2	2	1009	U	C6-N1-C2	-5.12	117.93	121.00
57	4	342	U	C5-C6-N1	5.12	125.26	122.70
2	2	1327	C	N3-C2-O2	-5.11	118.32	121.90
57	4	263	G	C2-N3-C4	5.11	114.46	111.90
2	2	589	U	N3-C2-O2	-5.11	118.62	122.20
2	2	632	U	N1-C2-O2	5.11	126.38	122.80
2	2	563	A	C8-N9-C1'	-5.11	118.51	127.70
2	2	1448	C	C5-C6-N1	5.11	123.55	121.00
57	4	6	U	O4'-C1'-N1	5.11	112.29	108.20
1	1	2698	U	C6-N1-C2	-5.11	117.94	121.00
57	4	332	G	P-O3'-C3'	5.11	125.83	119.70
57	4	216	U	P-O3'-C3'	5.10	125.83	119.70
1	1	672	C	N3-C2-O2	-5.10	118.33	121.90
1	1	2640	G	C4-C5-N7	5.10	112.84	110.80
2	2	624	C	C6-N1-C2	-5.10	118.26	120.30
2	2	891	U	N3-C2-O2	-5.10	118.63	122.20
2	2	1515	G	N3-C4-C5	-5.10	126.05	128.60
1	1	358	U	N3-C2-O2	-5.10	118.63	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2885	G	N3-C4-C5	-5.10	126.05	128.60
1	1	2073	C	C6-N1-C2	-5.09	118.26	120.30
1	1	2895	G	C6-C5-N7	-5.09	127.34	130.40
57	4	184	A	O4'-C1'-N9	5.09	112.28	108.20
57	4	315	G	N3-C4-C5	-5.09	126.05	128.60
2	2	990	C	N1-C2-O2	5.09	121.95	118.90
2	2	998	C	C6-N1-C2	-5.09	118.26	120.30
57	4	142	U	O4'-C1'-N1	5.09	112.27	108.20
1	1	288	U	C5-C6-N1	5.09	125.25	122.70
2	2	929	G	N3-C4-N9	-5.09	122.95	126.00
2	2	1327	C	N1-C2-O2	5.09	121.95	118.90
57	4	324	G	N1-C6-O6	-5.09	116.85	119.90
1	1	2507	C	C2-N1-C1'	5.09	124.40	118.80
2	2	20	U	N1-C2-O2	5.09	126.36	122.80
2	2	980	C	C2-N1-C1'	5.09	124.40	118.80
2	2	1002	G	N7-C8-N9	5.09	115.64	113.10
57	4	14	G	N7-C8-N9	5.09	115.64	113.10
1	1	2521	C	N1-C2-O2	5.08	121.95	118.90
1	1	1611	C	C2-N1-C1'	5.08	124.39	118.80
1	1	2053	G	C4-N9-C1'	5.08	133.11	126.50
57	4	154	C	C2-N3-C4	5.08	122.44	119.90
1	1	1256	G	C8-N9-C1'	-5.08	120.40	127.00
2	2	54	C	N1-C2-O2	5.08	121.95	118.90
2	2	1202	U	N1-C2-O2	5.08	126.35	122.80
1	1	468	G	C5-C6-O6	5.08	131.65	128.60
1	1	565	C	N1-C2-O2	5.08	121.94	118.90
1	1	1296	G	N7-C8-N9	5.07	115.64	113.10
15	K	12	ASP	CB-CG-OD1	5.07	122.87	118.30
2	2	1322	C	N1-C2-O2	5.07	121.94	118.90
2	2	1174	G	C4-C5-N7	5.07	112.83	110.80
2	2	341	C	C6-N1-C2	-5.07	118.27	120.30
57	4	126	C	C5-C4-N4	-5.07	116.65	120.20
1	1	743	A	N7-C8-N9	5.07	116.33	113.80
2	2	458	U	C2-N1-C1'	5.07	123.78	117.70
57	4	276	U	O4'-C1'-N1	5.07	112.25	108.20
2	2	904	U	N3-C2-O2	-5.06	118.66	122.20
2	2	1449	C	N1-C2-O2	5.06	121.94	118.90
2	2	905	U	N1-C2-O2	5.06	126.34	122.80
57	4	323	A	C2-N3-C4	5.06	113.13	110.60
57	4	32	A	P-O3'-C3'	5.05	125.77	119.70
1	1	62	U	C5-C6-N1	5.05	125.23	122.70
1	1	280	U	N1-C2-O2	5.05	126.34	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	439	U	C2-N1-C1'	5.05	123.76	117.70
13	I	100	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	1	2457	PSU	OP2-P-O3'	5.05	116.31	105.20
1	1	2895	G	C4-N9-C1'	5.05	133.07	126.50
2	2	605	U	N3-C2-O2	-5.05	118.66	122.20
57	4	330	U	C6-N1-C2	-5.05	117.97	121.00
1	1	1409	U	C5-C6-N1	5.05	125.22	122.70
2	2	110	C	N1-C2-O2	5.05	121.93	118.90
3	3	92	C	C5-C6-N1	5.05	123.52	121.00
57	4	331	C	P-O3'-C3'	5.05	125.76	119.70
1	1	2510	C	N1-C2-O2	5.04	121.93	118.90
1	1	1119	U	N1-C2-O2	5.04	126.33	122.80
1	1	2230	G	C4-N9-C1'	5.04	133.06	126.50
2	2	458	U	C5-C6-N1	5.04	125.22	122.70
1	1	809	G	N1-C6-O6	-5.04	116.88	119.90
1	1	1049	C	N3-C2-O2	-5.04	118.37	121.90
1	1	776	G	C8-N9-C1'	-5.04	120.45	127.00
1	1	1203	U	N3-C2-O2	-5.04	118.68	122.20
1	1	1243	C	N3-C2-O2	-5.04	118.38	121.90
1	1	1412	U	N3-C2-O2	-5.03	118.68	122.20
57	4	110	U	N3-C2-O2	-5.03	118.68	122.20
57	4	181	G	C8-N9-C4	-5.03	104.39	106.40
1	1	952	G	C4-C5-N7	5.03	112.81	110.80
2	2	514	C	N1-C2-O2	5.03	121.92	118.90
1	1	1488	C	C6-N1-C2	-5.03	118.29	120.30
57	4	107	C	OP2-P-O3'	5.03	116.26	105.20
2	2	937	A	C5-C6-N6	-5.02	119.68	123.70
57	4	325	G	C4-N9-C1'	5.02	133.03	126.50
1	1	1658	C	C6-N1-C2	-5.02	118.29	120.30
1	1	1999	C	N1-C2-O2	5.02	121.91	118.90
3	3	70	C	C6-N1-C2	-5.02	118.29	120.30
57	4	160	U	N3-C2-O2	-5.02	118.69	122.20
57	4	335	C	C4'-C3'-O3'	5.02	123.05	113.00
1	1	1530	G	C8-N9-C4	-5.02	104.39	106.40
1	1	2045	C	C6-N1-C2	-5.02	118.29	120.30
1	1	2806	C	C2-N1-C1'	5.02	124.32	118.80
1	1	570	G	C6-C5-N7	-5.02	127.39	130.40
1	1	2442	C	N1-C2-O2	5.02	121.91	118.90
2	2	153	C	C6-N1-C2	-5.02	118.29	120.30
2	2	1515	G	C6-C5-N7	-5.02	127.39	130.40
1	1	1459	G	C8-N9-C4	-5.02	104.39	106.40
1	1	1905	C	C6-N1-C1'	-5.02	114.78	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	300	A	C8-N9-C4	-5.02	103.79	105.80
57	4	112	U	N3-C2-O2	-5.02	118.69	122.20
1	1	1863	G	N3-C4-C5	5.02	131.11	128.60
57	4	180	G	N3-C4-C5	-5.02	126.09	128.60
1	1	2108	A	N3-C4-C5	-5.01	123.29	126.80
2	2	882	C	N3-C2-O2	-5.01	118.39	121.90
57	4	9	U	P-O3'-C3'	5.01	125.72	119.70
57	4	266	C	C5'-C4'-O4'	-5.01	103.08	109.10
1	1	1303	G	N1-C6-O6	-5.01	116.89	119.90
2	2	857	C	C5-C6-N1	5.01	123.51	121.00
57	4	348	C	N3-C4-N4	5.01	121.51	118.00
2	2	41	G	C4-C5-N7	5.01	112.81	110.80
57	4	137	C	N3-C2-O2	-5.01	118.39	121.90
57	4	266	C	C5-C4-N4	-5.01	116.69	120.20
1	1	2831	G	N3-C4-N9	-5.01	122.99	126.00
1	1	312	G	C8-N9-C1'	-5.01	120.49	127.00
3	3	30	C	C6-N1-C2	-5.01	118.30	120.30
57	4	73	A	O4'-C1'-N9	-5.00	104.20	108.20
1	1	1398	C	C2-N1-C1'	5.00	124.30	118.80
57	4	8	A	O4'-C1'-N9	5.00	112.20	108.20

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	1618	6MZ	C2',C3'
1	1	1911	PSU	C4',C3'
1	1	1915	3TD	C3'
1	1	1917	PSU	C4',C3'
1	1	2030	6MZ	C2',C3'
1	1	2069	G7M	C4',C2',C3'
1	1	2251	OMG	C2'
1	1	2457	PSU	C4',C3'
1	1	2498	OMC	C4'
1	1	2503	2MA	C2',C3'
1	1	2504	PSU	C4',C3'
1	1	2552	OMU	C2',C3'
1	1	2580	PSU	C4',C3'
1	1	2605	PSU	C4',C3'

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	830	G	Sidechain
2	2	999	C	Sidechain
4	5	90	LEU	Mainchain
10	F	46	ALA	Peptide
13	I	89	SER	Peptide
13	I	94	LYS	Peptide
22	R	23	GLU	Peptide
23	S	60	HIS	Peptide
35	e	31	HIS	Peptide
38	h	82	GLU	Peptide
43	m	62	THR	Peptide
47	q	102	LEU	Peptide
53	w	73	ARG	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	5	148/160 (92%)	127 (86%)	20 (14%)	1 (1%)	22	62
5	6	20/22 (91%)	12 (60%)	8 (40%)	0	100	100
6	B	269/273 (98%)	236 (88%)	33 (12%)	0	100	100
7	C	207/209 (99%)	183 (88%)	24 (12%)	0	100	100
8	D	199/201 (99%)	177 (89%)	22 (11%)	0	100	100
9	E	175/179 (98%)	152 (87%)	23 (13%)	0	100	100
10	F	173/177 (98%)	154 (89%)	18 (10%)	1 (1%)	25	65
11	G	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
12	H	128/165 (78%)	94 (73%)	34 (27%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	I	133/142 (94%)	104 (78%)	28 (21%)	1 (1%)	19	60
14	J	140/142 (99%)	125 (89%)	15 (11%)	0	100	100
15	K	121/123 (98%)	109 (90%)	12 (10%)	0	100	100
16	L	142/144 (99%)	122 (86%)	20 (14%)	0	100	100
17	M	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
18	N	117/127 (92%)	106 (91%)	11 (9%)	0	100	100
19	O	114/117 (97%)	98 (86%)	16 (14%)	0	100	100
20	P	112/115 (97%)	103 (92%)	9 (8%)	0	100	100
21	Q	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
22	R	101/103 (98%)	86 (85%)	15 (15%)	0	100	100
23	S	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
24	T	92/100 (92%)	84 (91%)	8 (9%)	0	100	100
25	U	101/104 (97%)	90 (89%)	11 (11%)	0	100	100
26	V	92/94 (98%)	83 (90%)	9 (10%)	0	100	100
27	W	74/85 (87%)	63 (85%)	11 (15%)	0	100	100
28	X	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
29	Y	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
30	Z	56/59 (95%)	50 (89%)	6 (11%)	0	100	100
31	a	55/70 (79%)	47 (86%)	8 (14%)	0	100	100
32	b	54/57 (95%)	45 (83%)	9 (17%)	0	100	100
33	c	50/55 (91%)	44 (88%)	6 (12%)	0	100	100
34	d	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
35	e	62/65 (95%)	52 (84%)	10 (16%)	0	100	100
36	f	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
37	g	223/241 (92%)	195 (87%)	28 (13%)	0	100	100
38	h	206/233 (88%)	179 (87%)	27 (13%)	0	100	100
39	i	203/206 (98%)	185 (91%)	18 (9%)	0	100	100
40	j	154/167 (92%)	135 (88%)	19 (12%)	0	100	100
41	k	102/135 (76%)	97 (95%)	5 (5%)	0	100	100
42	l	149/179 (83%)	135 (91%)	14 (9%)	0	100	100
43	m	127/130 (98%)	113 (89%)	14 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	n	125/130 (96%)	110 (88%)	15 (12%)	0	100	100
45	o	97/103 (94%)	88 (91%)	9 (9%)	0	100	100
46	p	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
47	q	119/124 (96%)	99 (83%)	20 (17%)	0	100	100
48	r	110/118 (93%)	89 (81%)	21 (19%)	0	100	100
49	s	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
50	t	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
51	u	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
52	v	78/84 (93%)	67 (86%)	11 (14%)	0	100	100
53	w	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
54	x	81/92 (88%)	66 (82%)	15 (18%)	0	100	100
55	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
56	z	68/71 (96%)	60 (88%)	8 (12%)	0	100	100
All	All	6023/6402 (94%)	5297 (88%)	723 (12%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	47	ASP
4	5	92	LEU
13	I	92	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
4	5	125/133 (94%)	124 (99%)	1 (1%)	81	89
6	B	216/218 (99%)	215 (100%)	1 (0%)	88	93
7	C	164/164 (100%)	164 (100%)	0	100	100
8	D	165/165 (100%)	165 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	E	148/150 (99%)	146 (99%)	2 (1%)	67	81
10	F	136/138 (99%)	136 (100%)	0	100	100
11	G	114/114 (100%)	114 (100%)	0	100	100
12	H	99/123 (80%)	99 (100%)	0	100	100
13	I	104/110 (94%)	103 (99%)	1 (1%)	76	86
14	J	116/116 (100%)	116 (100%)	0	100	100
15	K	104/104 (100%)	103 (99%)	1 (1%)	76	86
16	L	103/103 (100%)	101 (98%)	2 (2%)	57	75
17	M	109/109 (100%)	109 (100%)	0	100	100
18	N	99/103 (96%)	99 (100%)	0	100	100
19	O	86/87 (99%)	85 (99%)	1 (1%)	71	84
20	P	99/100 (99%)	97 (98%)	2 (2%)	55	73
21	Q	89/90 (99%)	89 (100%)	0	100	100
22	R	84/84 (100%)	84 (100%)	0	100	100
23	S	93/93 (100%)	92 (99%)	1 (1%)	73	85
24	T	81/84 (96%)	81 (100%)	0	100	100
25	U	84/85 (99%)	83 (99%)	1 (1%)	71	84
26	V	78/78 (100%)	78 (100%)	0	100	100
27	W	58/63 (92%)	57 (98%)	1 (2%)	60	78
28	X	67/68 (98%)	66 (98%)	1 (2%)	65	80
29	Y	54/55 (98%)	53 (98%)	1 (2%)	57	75
30	Z	48/49 (98%)	48 (100%)	0	100	100
31	a	54/62 (87%)	54 (100%)	0	100	100
32	b	47/48 (98%)	44 (94%)	3 (6%)	17	44
33	c	47/49 (96%)	47 (100%)	0	100	100
34	d	38/38 (100%)	38 (100%)	0	100	100
35	e	51/52 (98%)	51 (100%)	0	100	100
36	f	34/34 (100%)	34 (100%)	0	100	100
37	g	187/199 (94%)	187 (100%)	0	100	100
38	h	171/190 (90%)	171 (100%)	0	100	100
39	i	172/173 (99%)	171 (99%)	1 (1%)	86	92

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	j	119/126 (94%)	115 (97%)	4 (3%)	37	61
41	k	91/116 (78%)	89 (98%)	2 (2%)	52	71
42	l	124/147 (84%)	123 (99%)	1 (1%)	81	89
43	m	104/105 (99%)	104 (100%)	0	100	100
44	n	105/107 (98%)	103 (98%)	2 (2%)	57	75
45	o	86/90 (96%)	85 (99%)	1 (1%)	71	84
46	p	90/99 (91%)	89 (99%)	1 (1%)	73	85
47	q	102/103 (99%)	99 (97%)	3 (3%)	42	64
48	r	90/96 (94%)	87 (97%)	3 (3%)	38	62
49	s	83/84 (99%)	83 (100%)	0	100	100
50	t	76/77 (99%)	75 (99%)	1 (1%)	69	82
51	u	65/65 (100%)	64 (98%)	1 (2%)	65	80
52	v	74/78 (95%)	73 (99%)	1 (1%)	67	81
53	w	57/65 (88%)	57 (100%)	0	100	100
54	x	72/79 (91%)	71 (99%)	1 (1%)	67	81
55	y	65/66 (98%)	65 (100%)	0	100	100
56	z	60/61 (98%)	60 (100%)	0	100	100
All	All	4987/5195 (96%)	4946 (99%)	41 (1%)	82	89

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	92	LEU
6	B	182	ARG
9	E	112	ARG
9	E	123	ASP
13	I	23	VAL
15	K	49	ARG
16	L	48	ARG
16	L	126	ARG
19	O	7	ARG
20	P	39	ARG
20	P	109	ARG
23	S	90	LYS
25	U	94	ARG
27	W	41	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	X	44	LYS
29	Y	52	ARG
32	b	10	ARG
32	b	17	ARG
32	b	52	ARG
39	i	156	LYS
40	j	11	LEU
40	j	29	ARG
40	j	80	THR
40	j	93	ARG
41	k	62	MET
41	k	90	MET
42	l	10	ARG
44	n	106	ARG
44	n	130	ARG
45	o	5	ARG
46	p	56	ARG
47	q	10	LYS
47	q	14	ARG
47	q	83	ARG
48	r	25	VAL
48	r	30	SER
48	r	79	ARG
50	t	77	ARG
51	u	25	ARG
52	v	76	VAL
54	x	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
4	5	93	ASN
4	5	148	GLN
6	B	70	ASN
6	B	134	ASN
7	C	150	GLN
7	C	173	GLN
8	D	97	ASN
8	D	115	GLN
8	D	163	ASN
10	F	22	GLN
10	F	73	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	G	11	ASN
11	G	28	ASN
15	K	93	GLN
17	M	45	GLN
17	M	60	GLN
19	O	61	GLN
20	P	12	GLN
20	P	15	GLN
23	S	40	ASN
23	S	57	ASN
23	S	60	HIS
23	S	61	ASN
23	S	102	HIS
24	T	15	HIS
24	T	59	ASN
27	W	76	ASN
29	Y	15	ASN
31	a	41	HIS
31	a	61	ASN
31	a	65	ASN
32	b	19	HIS
34	d	29	GLN
35	e	26	HIS
37	g	42	ASN
37	g	109	GLN
38	h	32	ASN
38	h	123	GLN
38	h	185	ASN
39	i	71	GLN
39	i	152	GLN
40	j	70	ASN
41	k	46	GLN
42	l	68	ASN
43	m	16	ASN
44	n	31	ASN
45	o	15	HIS
48	r	14	HIS
49	s	66	GLN
49	s	71	HIS
54	x	83	HIS
55	y	3	ASN
55	y	52	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	y	55	GLN
55	y	68	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2897/2904 (99%)	989 (34%)	22 (0%)
2	2	1526/1535 (99%)	495 (32%)	7 (0%)
3	3	119/120 (99%)	35 (29%)	0
57	4	361/363 (99%)	211 (58%)	31 (8%)
All	All	4903/4922 (99%)	1730 (35%)	60 (1%)

All (1730) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	G
1	1	4	U
1	1	10	A
1	1	11	C
1	1	12	U
1	1	14	A
1	1	15	G
1	1	27	G
1	1	28	A
1	1	30	G
1	1	32	C
1	1	33	C
1	1	34	U
1	1	35	G
1	1	43	G
1	1	46	G
1	1	48	G
1	1	50	U
1	1	51	G
1	1	54	G
1	1	55	G
1	1	57	C
1	1	58	G
1	1	60	G
1	1	61	C
1	1	63	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	68	G
1	1	71	A
1	1	74	A
1	1	75	G
1	1	79	C
1	1	80	G
1	1	84	A
1	1	85	G
1	1	91	A
1	1	93	G
1	1	96	C
1	1	100	U
1	1	101	A
1	1	102	U
1	1	103	A
1	1	112	U
1	1	113	U
1	1	118	A
1	1	119	A
1	1	120	U
1	1	126	A
1	1	128	C
1	1	136	G
1	1	137	U
1	1	139	U
1	1	140	C
1	1	142	A
1	1	163	C
1	1	165	A
1	1	167	A
1	1	181	A
1	1	192	C
1	1	193	U
1	1	196	A
1	1	197	A
1	1	199	A
1	1	201	C
1	1	203	A
1	1	204	A
1	1	215	G
1	1	216	A
1	1	218	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	221	A
1	1	222	A
1	1	225	C
1	1	226	A
1	1	228	C
1	1	229	C
1	1	230	G
1	1	233	A
1	1	239	C
1	1	241	A
1	1	245	G
1	1	248	G
1	1	249	C
1	1	250	G
1	1	260	G
1	1	261	G
1	1	264	C
1	1	265	A
1	1	266	G
1	1	267	C
1	1	270	A
1	1	272	A
1	1	273	G
1	1	275	C
1	1	276	U
1	1	278	A
1	1	280	U
1	1	285	G
1	1	289	G
1	1	294	A
1	1	296	U
1	1	301	G
1	1	304	U
1	1	308	G
1	1	309	A
1	1	310	A
1	1	321	U
1	1	322	A
1	1	323	C
1	1	324	A
1	1	329	G
1	1	330	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	331	C
1	1	332	A
1	1	337	C
1	1	338	G
1	1	343	C
1	1	353	C
1	1	357	C
1	1	362	A
1	1	363	G
1	1	364	C
1	1	366	C
1	1	367	G
1	1	370	G
1	1	371	A
1	1	372	G
1	1	375	G
1	1	384	A
1	1	385	C
1	1	386	G
1	1	387	U
1	1	389	G
1	1	394	C
1	1	396	G
1	1	398	C
1	1	399	U
1	1	403	U
1	1	404	A
1	1	405	U
1	1	406	G
1	1	411	G
1	1	412	A
1	1	413	C
1	1	424	G
1	1	431	U
1	1	434	U
1	1	435	C
1	1	440	C
1	1	441	U
1	1	447	A
1	1	451	U
1	1	453	A
1	1	454	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	455	C
1	1	456	C
1	1	457	A
1	1	465	G
1	1	475	C
1	1	476	G
1	1	477	A
1	1	479	A
1	1	480	A
1	1	481	G
1	1	483	A
1	1	490	C
1	1	491	G
1	1	494	G
1	1	496	G
1	1	498	G
1	1	505	A
1	1	507	A
1	1	508	A
1	1	509	C
1	1	518	G
1	1	527	C
1	1	529	A
1	1	530	G
1	1	532	A
1	1	533	G
1	1	544	C
1	1	546	U
1	1	547	A
1	1	548	G
1	1	549	G
1	1	556	A
1	1	563	A
1	1	565	C
1	1	566	U
1	1	567	U
1	1	571	U
1	1	573	U
1	1	575	A
1	1	576	U
1	1	577	G
1	1	586	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	601	C
1	1	603	A
1	1	609	A
1	1	613	A
1	1	614	A
1	1	615	U
1	1	616	A
1	1	621	A
1	1	622	G
1	1	627	A
1	1	634	C
1	1	637	A
1	1	645	C
1	1	653	U
1	1	654	A
1	1	655	A
1	1	656	G
1	1	657	U
1	1	659	G
1	1	664	G
1	1	675	A
1	1	681	G
1	1	682	G
1	1	684	G
1	1	686	U
1	1	689	A
1	1	699	A
1	1	702	U
1	1	709	U
1	1	710	U
1	1	715	A
1	1	716	A
1	1	717	C
1	1	722	A
1	1	730	A
1	1	734	A
1	1	747	5MU
1	1	748	G
1	1	749	A
1	1	752	A
1	1	759	G
1	1	762	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	765	C
1	1	771	G
1	1	775	G
1	1	776	G
1	1	777	G
1	1	782	A
1	1	784	G
1	1	785	G
1	1	788	A
1	1	789	A
1	1	792	A
1	1	793	A
1	1	800	A
1	1	805	G
1	1	806	C
1	1	812	C
1	1	819	A
1	1	827	U
1	1	828	U
1	1	830	G
1	1	839	U
1	1	845	A
1	1	846	U
1	1	847	U
1	1	856	G
1	1	858	G
1	1	859	G
1	1	865	C
1	1	866	A
1	1	869	G
1	1	877	A
1	1	882	G
1	1	884	U
1	1	885	C
1	1	887	A
1	1	888	C
1	1	889	C
1	1	890	C
1	1	891	G
1	1	892	A
1	1	893	C
1	1	895	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	896	A
1	1	897	C
1	1	899	A
1	1	900	A
1	1	902	C
1	1	903	C
1	1	907	G
1	1	908	C
1	1	910	A
1	1	911	A
1	1	914	G
1	1	915	C
1	1	919	U
1	1	934	U
1	1	935	C
1	1	941	A
1	1	945	A
1	1	947	A
1	1	948	C
1	1	949	G
1	1	953	G
1	1	954	G
1	1	955	PSU
1	1	956	G
1	1	957	C
1	1	958	U
1	1	959	A
1	1	961	C
1	1	964	C
1	1	970	U
1	1	973	A
1	1	974	G
1	1	982	C
1	1	983	A
1	1	990	A
1	1	995	C
1	1	996	A
1	1	997	G
1	1	1005	C
1	1	1008	A
1	1	1009	A
1	1	1010	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1012	U
1	1	1013	C
1	1	1017	G
1	1	1022	G
1	1	1023	U
1	1	1024	G
1	1	1025	G
1	1	1026	G
1	1	1028	A
1	1	1029	A
1	1	1032	A
1	1	1033	U
1	1	1035	U
1	1	1041	G
1	1	1042	G
1	1	1044	C
1	1	1045	C
1	1	1046	A
1	1	1047	G
1	1	1048	A
1	1	1049	C
1	1	1050	A
1	1	1051	G
1	1	1052	C
1	1	1056	G
1	1	1058	U
1	1	1060	U
1	1	1061	U
1	1	1063	G
1	1	1065	U
1	1	1066	U
1	1	1067	A
1	1	1068	G
1	1	1069	A
1	1	1070	A
1	1	1071	G
1	1	1073	A
1	1	1075	C
1	1	1076	C
1	1	1077	A
1	1	1079	C
1	1	1080	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1082	U
1	1	1083	U
1	1	1084	A
1	1	1085	A
1	1	1087	G
1	1	1088	A
1	1	1089	A
1	1	1090	A
1	1	1092	C
1	1	1093	G
1	1	1096	A
1	1	1097	U
1	1	1099	G
1	1	1100	C
1	1	1101	U
1	1	1111	A
1	1	1112	G
1	1	1113	U
1	1	1119	U
1	1	1126	A
1	1	1128	G
1	1	1131	G
1	1	1132	U
1	1	1133	A
1	1	1135	C
1	1	1136	G
1	1	1141	U
1	1	1142	A
1	1	1143	A
1	1	1144	A
1	1	1168	G
1	1	1169	A
1	1	1171	G
1	1	1172	C
1	1	1173	U
1	1	1174	U
1	1	1175	A
1	1	1176	U
1	1	1177	G
1	1	1178	C
1	1	1182	G
1	1	1186	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1191	G
1	1	1195	G
1	1	1203	U
1	1	1204	A
1	1	1206	G
1	1	1212	G
1	1	1215	G
1	1	1217	U
1	1	1218	G
1	1	1221	C
1	1	1227	G
1	1	1229	C
1	1	1238	G
1	1	1241	A
1	1	1243	C
1	1	1248	G
1	1	1251	C
1	1	1253	A
1	1	1254	A
1	1	1255	U
1	1	1256	G
1	1	1258	U
1	1	1265	A
1	1	1266	G
1	1	1271	G
1	1	1272	A
1	1	1273	U
1	1	1284	A
1	1	1287	A
1	1	1289	C
1	1	1292	G
1	1	1296	G
1	1	1300	G
1	1	1301	A
1	1	1302	A
1	1	1310	G
1	1	1312	U
1	1	1315	C
1	1	1316	U
1	1	1318	U
1	1	1325	U
1	1	1326	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1332	G
1	1	1340	U
1	1	1341	G
1	1	1342	A
1	1	1345	C
1	1	1352	U
1	1	1355	G
1	1	1360	G
1	1	1365	A
1	1	1368	G
1	1	1378	A
1	1	1379	U
1	1	1380	G
1	1	1381	G
1	1	1385	A
1	1	1386	C
1	1	1393	A
1	1	1395	A
1	1	1403	A
1	1	1408	G
1	1	1409	U
1	1	1413	A
1	1	1416	G
1	1	1417	C
1	1	1419	A
1	1	1420	A
1	1	1428	C
1	1	1440	U
1	1	1454	C
1	1	1455	G
1	1	1456	G
1	1	1458	U
1	1	1461	C
1	1	1468	U
1	1	1470	A
1	1	1473	G
1	1	1475	G
1	1	1478	G
1	1	1482	G
1	1	1483	G
1	1	1485	U
1	1	1493	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1494	A
1	1	1497	U
1	1	1502	A
1	1	1503	A
1	1	1508	A
1	1	1509	A
1	1	1514	G
1	1	1515	A
1	1	1522	A
1	1	1523	U
1	1	1524	G
1	1	1529	G
1	1	1530	G
1	1	1533	C
1	1	1534	U
1	1	1535	A
1	1	1536	C
1	1	1537	G
1	1	1547	C
1	1	1554	U
1	1	1558	C
1	1	1566	A
1	1	1569	A
1	1	1581	G
1	1	1583	A
1	1	1584	U
1	1	1585	C
1	1	1587	G
1	1	1589	U
1	1	1590	A
1	1	1593	A
1	1	1598	A
1	1	1607	C
1	1	1608	A
1	1	1610	A
1	1	1616	A
1	1	1619	G
1	1	1621	U
1	1	1625	C
1	1	1626	A
1	1	1627	G
1	1	1630	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1633	G
1	1	1635	A
1	1	1642	G
1	1	1643	G
1	1	1644	C
1	1	1646	C
1	1	1647	U
1	1	1648	U
1	1	1649	G
1	1	1653	G
1	1	1654	A
1	1	1667	G
1	1	1668	A
1	1	1673	G
1	1	1674	G
1	1	1676	A
1	1	1677	A
1	1	1691	C
1	1	1693	U
1	1	1695	G
1	1	1698	A
1	1	1699	G
1	1	1701	A
1	1	1702	G
1	1	1703	G
1	1	1712	U
1	1	1714	U
1	1	1715	G
1	1	1716	U
1	1	1721	G
1	1	1722	A
1	1	1723	G
1	1	1725	U
1	1	1729	U
1	1	1730	C
1	1	1732	C
1	1	1734	G
1	1	1738	G
1	1	1744	A
1	1	1745	A
1	1	1757	A
1	1	1758	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1761	C
1	1	1764	C
1	1	1766	G
1	1	1769	U
1	1	1770	G
1	1	1772	A
1	1	1773	A
1	1	1777	U
1	1	1779	U
1	1	1780	A
1	1	1781	U
1	1	1782	U
1	1	1784	A
1	1	1800	C
1	1	1802	A
1	1	1803	A
1	1	1804	C
1	1	1808	A
1	1	1809	A
1	1	1811	G
1	1	1813	G
1	1	1816	C
1	1	1819	A
1	1	1820	U
1	1	1821	A
1	1	1828	G
1	1	1830	C
1	1	1833	C
1	1	1834	U
1	1	1835	2MG
1	1	1842	G
1	1	1845	G
1	1	1848	A
1	1	1853	A
1	1	1855	U
1	1	1857	G
1	1	1860	G
1	1	1863	G
1	1	1865	U
1	1	1866	A
1	1	1867	G
1	1	1870	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1871	A
1	1	1872	A
1	1	1875	G
1	1	1877	A
1	1	1879	C
1	1	1880	U
1	1	1894	C
1	1	1896	G
1	1	1897	G
1	1	1906	G
1	1	1907	G
1	1	1911	PSU
1	1	1912	A
1	1	1913	A
1	1	1914	C
1	1	1917	PSU
1	1	1918	A
1	1	1919	A
1	1	1923	U
1	1	1924	C
1	1	1929	G
1	1	1930	G
1	1	1939	5MU
1	1	1940	U
1	1	1942	C
1	1	1943	U
1	1	1953	A
1	1	1955	U
1	1	1960	A
1	1	1962	5MC
1	1	1965	C
1	1	1966	A
1	1	1967	C
1	1	1970	A
1	1	1971	U
1	1	1972	G
1	1	1981	A
1	1	1983	G
1	1	1989	G
1	1	1991	U
1	1	1992	G
1	1	1993	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1997	C
1	1	1999	C
1	1	2014	A
1	1	2015	A
1	1	2022	U
1	1	2023	C
1	1	2031	A
1	1	2032	G
1	1	2033	A
1	1	2035	G
1	1	2043	C
1	1	2044	C
1	1	2046	G
1	1	2051	A
1	1	2052	A
1	1	2055	C
1	1	2056	G
1	1	2060	A
1	1	2061	G
1	1	2062	A
1	1	2066	C
1	1	2068	U
1	1	2069	G7M
1	1	2070	A
1	1	2072	C
1	1	2076	U
1	1	2077	A
1	1	2081	U
1	1	2092	U
1	1	2093	G
1	1	2094	A
1	1	2095	A
1	1	2096	C
1	1	2097	A
1	1	2099	U
1	1	2100	G
1	1	2102	G
1	1	2104	C
1	1	2105	U
1	1	2106	U
1	1	2108	A
1	1	2110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2111	U
1	1	2113	U
1	1	2114	A
1	1	2115	G
1	1	2116	G
1	1	2117	A
1	1	2118	U
1	1	2119	A
1	1	2120	G
1	1	2121	G
1	1	2122	U
1	1	2123	G
1	1	2125	G
1	1	2126	A
1	1	2127	G
1	1	2128	G
1	1	2129	C
1	1	2130	U
1	1	2131	U
1	1	2132	U
1	1	2133	G
1	1	2134	A
1	1	2135	A
1	1	2136	G
1	1	2137	U
1	1	2138	G
1	1	2139	U
1	1	2140	G
1	1	2142	A
1	1	2143	C
1	1	2144	G
1	1	2146	C
1	1	2147	A
1	1	2148	G
1	1	2149	U
1	1	2150	C
1	1	2151	U
1	1	2153	C
1	1	2154	A
1	1	2155	U
1	1	2157	G
1	1	2158	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2159	G
1	1	2160	C
1	1	2162	G
1	1	2164	C
1	1	2165	C
1	1	2167	U
1	1	2168	G
1	1	2169	A
1	1	2170	A
1	1	2171	A
1	1	2172	U
1	1	2173	A
1	1	2176	A
1	1	2178	C
1	1	2179	C
1	1	2180	U
1	1	2181	U
1	1	2183	A
1	1	2185	U
1	1	2186	G
1	1	2189	U
1	1	2190	G
1	1	2193	G
1	1	2194	U
1	1	2198	A
1	1	2199	A
1	1	2203	U
1	1	2204	G
1	1	2211	A
1	1	2212	A
1	1	2213	U
1	1	2214	C
1	1	2220	U
1	1	2225	A
1	1	2226	C
1	1	2238	G
1	1	2239	G
1	1	2243	U
1	1	2244	U
1	1	2247	A
1	1	2249	U
1	1	2250	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2258	C
1	1	2259	U
1	1	2266	A
1	1	2267	A
1	1	2269	G
1	1	2279	G
1	1	2283	C
1	1	2286	G
1	1	2298	A
1	1	2305	U
1	1	2307	G
1	1	2309	A
1	1	2312	U
1	1	2318	G
1	1	2319	G
1	1	2320	U
1	1	2321	U
1	1	2325	G
1	1	2327	A
1	1	2334	U
1	1	2335	A
1	1	2336	A
1	1	2337	G
1	1	2343	U
1	1	2345	G
1	1	2346	A
1	1	2347	C
1	1	2350	C
1	1	2352	A
1	1	2355	G
1	1	2357	G
1	1	2359	C
1	1	2361	G
1	1	2365	G
1	1	2374	C
1	1	2383	G
1	1	2385	C
1	1	2388	A
1	1	2389	G
1	1	2394	C
1	1	2402	U
1	1	2403	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2407	A
1	1	2410	G
1	1	2412	A
1	1	2413	G
1	1	2421	G
1	1	2422	C
1	1	2423	U
1	1	2424	C
1	1	2425	A
1	1	2426	A
1	1	2428	G
1	1	2429	G
1	1	2430	A
1	1	2431	U
1	1	2433	A
1	1	2435	A
1	1	2440	C
1	1	2441	U
1	1	2445	2MG
1	1	2447	G
1	1	2448	A
1	1	2452	C
1	1	2457	PSU
1	1	2458	G
1	1	2468	A
1	1	2469	A
1	1	2470	G
1	1	2476	A
1	1	2477	U
1	1	2478	A
1	1	2484	G
1	1	2486	C
1	1	2487	G
1	1	2489	U
1	1	2491	U
1	1	2497	A
1	1	2498	OMC
1	1	2499	C
1	1	2501	C
1	1	2502	G
1	1	2504	PSU
1	1	2505	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2506	U
1	1	2513	A
1	1	2518	A
1	1	2520	C
1	1	2534	A
1	1	2535	G
1	1	2538	C
1	1	2543	G
1	1	2545	G
1	1	2547	A
1	1	2552	OMU
1	1	2553	G
1	1	2554	U
1	1	2562	U
1	1	2564	A
1	1	2565	A
1	1	2566	A
1	1	2567	G
1	1	2572	A
1	1	2573	C
1	1	2574	G
1	1	2575	C
1	1	2577	A
1	1	2578	G
1	1	2580	PSU
1	1	2581	G
1	1	2584	U
1	1	2585	U
1	1	2587	A
1	1	2599	G
1	1	2601	C
1	1	2602	A
1	1	2603	G
1	1	2605	PSU
1	1	2606	C
1	1	2608	G
1	1	2609	U
1	1	2612	C
1	1	2613	U
1	1	2621	G
1	1	2629	U
1	1	2630	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2634	A
1	1	2640	G
1	1	2641	G
1	1	2645	G
1	1	2646	C
1	1	2650	U
1	1	2661	G
1	1	2662	A
1	1	2663	G
1	1	2668	G
1	1	2682	A
1	1	2689	U
1	1	2690	U
1	1	2692	G
1	1	2698	U
1	1	2706	A
1	1	2707	U
1	1	2713	U
1	1	2714	G
1	1	2716	C
1	1	2718	G
1	1	2722	G
1	1	2724	U
1	1	2727	A
1	1	2728	U
1	1	2733	A
1	1	2736	A
1	1	2739	U
1	1	2744	G
1	1	2748	A
1	1	2751	G
1	1	2752	C
1	1	2757	A
1	1	2759	G
1	1	2760	C
1	1	2764	A
1	1	2765	A
1	1	2766	A
1	1	2778	A
1	1	2780	G
1	1	2784	U
1	1	2790	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2791	G
1	1	2793	C
1	1	2794	C
1	1	2796	U
1	1	2799	A
1	1	2801	G
1	1	2818	U
1	1	2820	A
1	1	2823	A
1	1	2824	C
1	1	2826	A
1	1	2828	G
1	1	2829	A
1	1	2830	C
1	1	2832	U
1	1	2833	U
1	1	2834	G
1	1	2837	A
1	1	2839	G
1	1	2849	U
1	1	2858	C
1	1	2860	A
1	1	2861	U
1	1	2866	U
1	1	2867	G
1	1	2872	A
1	1	2873	A
1	1	2879	A
1	1	2880	C
1	1	2881	U
1	1	2883	A
1	1	2884	U
1	1	2885	G
1	1	2886	A
1	1	2891	U
1	1	2893	A
1	1	2894	G
1	1	2895	G
1	1	2901	C
2	2	2	A
2	2	4	U
2	2	5	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	6	G
2	2	9	G
2	2	19	A
2	2	22	G
2	2	30	U
2	2	32	A
2	2	39	G
2	2	41	G
2	2	44	A
2	2	47	C
2	2	48	C
2	2	50	A
2	2	51	A
2	2	52	C
2	2	68	G
2	2	70	U
2	2	71	A
2	2	72	A
2	2	73	C
2	2	74	A
2	2	75	G
2	2	77	A
2	2	80	A
2	2	82	G
2	2	83	C
2	2	84	U
2	2	85	U
2	2	86	G
2	2	87	C
2	2	88	U
2	2	89	U
2	2	90	C
2	2	92	U
2	2	93	U
2	2	94	G
2	2	95	C
2	2	96	U
2	2	100	G
2	2	107	G
2	2	108	G
2	2	116	A
2	2	120	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	121	U
2	2	122	G
2	2	124	C
2	2	127	G
2	2	130	A
2	2	131	A
2	2	132	C
2	2	142	G
2	2	144	G
2	2	160	A
2	2	163	C
2	2	167	A
2	2	168	G
2	2	172	A
2	2	181	A
2	2	182	A
2	2	183	C
2	2	191	G
2	2	197	A
2	2	203	G
2	2	204	G
2	2	207	C
2	2	210	C
2	2	211	G
2	2	212	G
2	2	213	G
2	2	214	C
2	2	216	U
2	2	226	G
2	2	228	A
2	2	231	U
2	2	238	A
2	2	240	G
2	2	243	A
2	2	245	U
2	2	247	G
2	2	251	G
2	2	257	G
2	2	265	G
2	2	266	G
2	2	267	C
2	2	272	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	279	A
2	2	280	C
2	2	289	G
2	2	290	C
2	2	298	A
2	2	303	A
2	2	306	A
2	2	315	A
2	2	316	C
2	2	319	G
2	2	322	C
2	2	328	C
2	2	330	C
2	2	332	G
2	2	337	G
2	2	346	G
2	2	347	G
2	2	351	G
2	2	352	C
2	2	354	G
2	2	355	C
2	2	366	A
2	2	367	U
2	2	372	C
2	2	373	A
2	2	376	G
2	2	384	G
2	2	388	G
2	2	389	A
2	2	390	U
2	2	393	A
2	2	394	G
2	2	398	U
2	2	399	G
2	2	406	G
2	2	411	A
2	2	413	G
2	2	414	A
2	2	417	G
2	2	421	U
2	2	422	C
2	2	423	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	424	G
2	2	426	U
2	2	428	G
2	2	429	U
2	2	435	A
2	2	440	C
2	2	451	A
2	2	454	G
2	2	463	U
2	2	467	U
2	2	468	A
2	2	469	C
2	2	474	G
2	2	477	C
2	2	481	G
2	2	482	A
2	2	484	G
2	2	485	U
2	2	486	U
2	2	492	C
2	2	494	G
2	2	495	A
2	2	496	A
2	2	497	G
2	2	506	G
2	2	507	C
2	2	508	U
2	2	509	A
2	2	510	A
2	2	513	C
2	2	514	C
2	2	516	PSU
2	2	517	G
2	2	518	C
2	2	519	C
2	2	520	A
2	2	527	7MG
2	2	531	U
2	2	532	A
2	2	533	A
2	2	534	U
2	2	542	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	545	C
2	2	546	A
2	2	547	A
2	2	551	U
2	2	552	U
2	2	553	A
2	2	559	A
2	2	564	C
2	2	568	G
2	2	572	A
2	2	573	A
2	2	576	C
2	2	577	G
2	2	581	G
2	2	590	U
2	2	592	G
2	2	596	A
2	2	607	A
2	2	631	C
2	2	633	G
2	2	639	G
2	2	644	U
2	2	653	U
2	2	656	G
2	2	661	G
2	2	664	G
2	2	665	A
2	2	666	G
2	2	671	G
2	2	672	U
2	2	675	A
2	2	676	A
2	2	679	C
2	2	685	G
2	2	687	A
2	2	696	A
2	2	703	G
2	2	704	A
2	2	705	G
2	2	717	U
2	2	718	A
2	2	720	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	721	G
2	2	724	G
2	2	725	G
2	2	731	G
2	2	747	A
2	2	752	G
2	2	753	A
2	2	755	G
2	2	773	G
2	2	774	G
2	2	776	G
2	2	777	A
2	2	787	A
2	2	792	A
2	2	793	U
2	2	794	A
2	2	799	G
2	2	803	G
2	2	810	C
2	2	811	C
2	2	813	U
2	2	814	A
2	2	815	A
2	2	817	C
2	2	818	G
2	2	821	G
2	2	828	U
2	2	832	G
2	2	842	U
2	2	843	U
2	2	844	G
2	2	845	A
2	2	846	G
2	2	848	C
2	2	849	G
2	2	850	U
2	2	851	G
2	2	857	C
2	2	863	U
2	2	870	U
2	2	879	C
2	2	887	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	888	G
2	2	889	A
2	2	898	G
2	2	905	U
2	2	908	A
2	2	912	C
2	2	914	A
2	2	920	U
2	2	922	G
2	2	926	G
2	2	934	C
2	2	935	A
2	2	936	C
2	2	937	A
2	2	939	G
2	2	941	G
2	2	958	A
2	2	960	U
2	2	961	U
2	2	965	U
2	2	966	2MG
2	2	967	5MC
2	2	969	A
2	2	971	G
2	2	976	G
2	2	977	A
2	2	981	U
2	2	982	U
2	2	984	C
2	2	988	G
2	2	989	U
2	2	992	U
2	2	993	G
2	2	996	A
2	2	997	U
2	2	999	C
2	2	1000	A
2	2	1001	C
2	2	1003	G
2	2	1004	A
2	2	1005	A
2	2	1007	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1008	U
2	2	1010	U
2	2	1011	C
2	2	1012	A
2	2	1017	U
2	2	1018	G
2	2	1019	A
2	2	1020	G
2	2	1021	A
2	2	1022	A
2	2	1026	G
2	2	1028	C
2	2	1030	U
2	2	1031	C
2	2	1033	G
2	2	1034	G
2	2	1035	A
2	2	1036	A
2	2	1041	G
2	2	1042	A
2	2	1045	C
2	2	1046	A
2	2	1047	G
2	2	1050	G
2	2	1052	U
2	2	1053	G
2	2	1054	C
2	2	1056	U
2	2	1064	G
2	2	1065	U
2	2	1085	U
2	2	1086	U
2	2	1088	G
2	2	1089	G
2	2	1091	U
2	2	1094	G
2	2	1095	U
2	2	1101	A
2	2	1108	G
2	2	1112	C
2	2	1124	G
2	2	1125	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1126	U
2	2	1127	G
2	2	1129	C
2	2	1130	A
2	2	1131	G
2	2	1133	G
2	2	1135	U
2	2	1136	C
2	2	1137	C
2	2	1140	C
2	2	1141	C
2	2	1143	G
2	2	1150	A
2	2	1151	A
2	2	1157	A
2	2	1159	U
2	2	1167	A
2	2	1168	U
2	2	1171	A
2	2	1172	C
2	2	1174	G
2	2	1175	G
2	2	1176	A
2	2	1182	G
2	2	1183	U
2	2	1184	G
2	2	1185	G
2	2	1190	G
2	2	1193	G
2	2	1196	A
2	2	1197	A
2	2	1198	G
2	2	1200	C
2	2	1201	A
2	2	1202	U
2	2	1211	U
2	2	1213	A
2	2	1214	C
2	2	1215	G
2	2	1224	U
2	2	1225	A
2	2	1227	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1235	U
2	2	1238	A
2	2	1239	A
2	2	1240	U
2	2	1241	G
2	2	1242	G
2	2	1244	G
2	2	1246	A
2	2	1247	U
2	2	1248	A
2	2	1249	C
2	2	1253	G
2	2	1256	A
2	2	1257	A
2	2	1258	G
2	2	1261	A
2	2	1262	C
2	2	1263	C
2	2	1265	C
2	2	1266	G
2	2	1267	C
2	2	1268	G
2	2	1269	A
2	2	1271	A
2	2	1272	G
2	2	1274	A
2	2	1278	G
2	2	1279	G
2	2	1280	A
2	2	1283	U
2	2	1285	A
2	2	1286	U
2	2	1287	A
2	2	1290	G
2	2	1291	U
2	2	1292	G
2	2	1297	G
2	2	1298	U
2	2	1299	A
2	2	1302	C
2	2	1303	C
2	2	1304	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1305	G
2	2	1307	U
2	2	1308	U
2	2	1312	G
2	2	1317	C
2	2	1318	A
2	2	1319	A
2	2	1324	A
2	2	1331	G
2	2	1332	A
2	2	1335	U
2	2	1336	C
2	2	1341	U
2	2	1342	C
2	2	1348	U
2	2	1353	G
2	2	1361	G
2	2	1363	A
2	2	1364	U
2	2	1365	G
2	2	1374	A
2	2	1375	A
2	2	1378	C
2	2	1379	G
2	2	1381	U
2	2	1385	G
2	2	1397	C
2	2	1398	A
2	2	1399	C
2	2	1401	G
2	2	1405	G
2	2	1407	5MC
2	2	1408	A
2	2	1418	A
2	2	1422	G
2	2	1430	A
2	2	1431	A
2	2	1432	G
2	2	1433	A
2	2	1441	A
2	2	1442	G
2	2	1444	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	1445	U
2	2	1446	A
2	2	1447	A
2	2	1452	C
2	2	1453	G
2	2	1466	C
2	2	1473	G
2	2	1478	U
2	2	1481	U
2	2	1484	C
2	2	1485	U
2	2	1486	G
2	2	1490	U
2	2	1491	G
2	2	1492	A
2	2	1493	A
2	2	1494	G
2	2	1497	G
2	2	1499	A
2	2	1502	A
2	2	1503	A
2	2	1504	G
2	2	1506	U
2	2	1507	A
2	2	1517	G
2	2	1520	C
2	2	1529	G
2	2	1530	G
2	2	1532	U
2	2	1534	A
3	3	2	G
3	3	9	G
3	3	12	C
3	3	14	U
3	3	15	A
3	3	17	C
3	3	18	G
3	3	30	C
3	3	31	C
3	3	32	U
3	3	33	G
3	3	35	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	36	C
3	3	37	C
3	3	41	G
3	3	42	C
3	3	44	G
3	3	45	A
3	3	51	G
3	3	57	A
3	3	70	C
3	3	73	A
3	3	80	U
3	3	88	C
3	3	89	U
3	3	90	C
3	3	91	C
3	3	92	C
3	3	99	A
3	3	103	U
3	3	107	G
3	3	109	A
3	3	113	C
3	3	119	A
3	3	120	U
57	4	6	U
57	4	8	A
57	4	9	U
57	4	10	U
57	4	11	C
57	4	13	G
57	4	14	G
57	4	15	A
57	4	16	U
57	4	17	U
57	4	18	C
57	4	19	G
57	4	20	A
57	4	21	C
57	4	28	U
57	4	30	C
57	4	32	A
57	4	33	A
57	4	34	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	4	35	C
57	4	38	A
57	4	39	A
57	4	40	G
57	4	43	G
57	4	44	C
57	4	45	A
57	4	47	G
57	4	49	C
57	4	54	G
57	4	55	G
57	4	56	C
57	4	60	U
57	4	61	G
57	4	62	G
57	4	63	C
57	4	64	C
57	4	68	U
57	4	69	A
57	4	70	A
57	4	71	A
57	4	72	A
57	4	73	A
57	4	79	A
57	4	80	A
57	4	81	A
57	4	82	A
57	4	83	A
57	4	84	A
57	4	85	U
57	4	86	A
57	4	87	G
57	4	88	U
57	4	89	C
57	4	92	A
57	4	93	A
57	4	94	A
57	4	95	C
57	4	96	G
57	4	97	A
57	4	99	G
57	4	101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	4	102	A
57	4	105	U
57	4	106	A
57	4	107	C
57	4	114	G
57	4	117	G
57	4	119	U
57	4	121	A
57	4	122	A
57	4	125	A
57	4	127	C
57	4	129	G
57	4	130	C
57	4	131	U
57	4	132	U
57	4	133	A
57	4	138	C
57	4	143	C
57	4	145	C
57	4	149	A
57	4	150	G
57	4	151	C
57	4	154	C
57	4	155	C
57	4	156	G
57	4	158	U
57	4	162	A
57	4	164	G
57	4	165	A
57	4	166	C
57	4	168	G
57	4	169	G
57	4	170	G
57	4	172	U
57	4	173	C
57	4	174	A
57	4	175	A
57	4	176	G
57	4	180	G
57	4	181	G
57	4	182	U
57	4	183	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	4	184	A
57	4	185	A
57	4	186	A
57	4	188	C
57	4	189	C
57	4	190	A
57	4	191	A
57	4	192	A
57	4	193	A
57	4	194	G
57	4	195	A
57	4	197	A
57	4	198	U
57	4	199	C
57	4	200	G
57	4	203	U
57	4	204	G
57	4	205	G
57	4	206	A
57	4	207	A
57	4	210	C
57	4	211	C
57	4	213	G
57	4	216	U
57	4	218	G
57	4	219	G
57	4	222	U
57	4	223	G
57	4	224	A
57	4	225	A
57	4	226	G
57	4	227	C
57	4	228	G
57	4	229	U
57	4	230	U
57	4	231	A
57	4	233	A
57	4	234	A
57	4	235	C
57	4	236	U
57	4	237	U
57	4	238	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	4	239	A
57	4	241	C
57	4	242	A
57	4	244	G
57	4	245	C
57	4	246	U
57	4	247	A
57	4	248	G
57	4	249	U
57	4	250	U
57	4	257	U
57	4	258	G
57	4	261	G
57	4	262	U
57	4	263	G
57	4	264	U
57	4	266	C
57	4	267	G
57	4	268	U
57	4	269	C
57	4	270	C
57	4	271	G
57	4	273	A
57	4	274	G
57	4	282	G
57	4	285	A
57	4	286	A
57	4	288	G
57	4	291	A
57	4	292	A
57	4	293	G
57	4	296	U
57	4	299	C
57	4	300	U
57	4	302	A
57	4	303	G
57	4	308	U
57	4	309	A
57	4	310	G
57	4	312	A
57	4	315	G
57	4	316	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	4	317	G
57	4	318	G
57	4	319	A
57	4	321	G
57	4	322	U
57	4	323	A
57	4	324	G
57	4	325	G
57	4	332	G
57	4	333	G
57	4	334	A
57	4	335	C
57	4	336	G
57	4	339	G
57	4	340	G
57	4	347	U
57	4	348	C
57	4	351	G
57	4	357	U
57	4	358	C
57	4	359	C
57	4	360	A
57	4	362	C
57	4	363	A

All (60) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	56	A
1	1	70	G
1	1	404	A
1	1	613	A
1	1	784	G
1	1	882	G
1	1	883	G
1	1	894	U
1	1	955	PSU
1	1	1379	U
1	1	1911	PSU
1	1	1917	PSU
1	1	2132	U
1	1	2146	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	2425	A
1	1	2457	PSU
1	1	2498	OMC
1	1	2504	PSU
1	1	2580	PSU
1	1	2605	PSU
1	1	2706	A
1	1	2756	U
2	2	8	A
2	2	83	C
2	2	512	U
2	2	516	PSU
2	2	884	U
2	2	1109	C
2	2	1214	C
57	4	9	U
57	4	10	U
57	4	13	G
57	4	14	G
57	4	15	A
57	4	17	U
57	4	19	G
57	4	20	A
57	4	32	A
57	4	33	A
57	4	38	A
57	4	61	G
57	4	68	U
57	4	130	C
57	4	153	U
57	4	183	C
57	4	212	U
57	4	223	G
57	4	229	U
57	4	233	A
57	4	237	U
57	4	245	C
57	4	247	A
57	4	249	U
57	4	257	U
57	4	261	G
57	4	290	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	4	308	U
57	4	314	C
57	4	332	G
57	4	333	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	1	955	1	18,21,22	1.43	3 (16%)	22,30,33	2.08	5 (22%)
1	PSU	1	2504	1	18,21,22	2.05	6 (33%)	22,30,33	2.15	5 (22%)
1	5MU	1	1939	58,1	19,22,23	1.41	4 (21%)	28,32,35	2.35	7 (25%)
1	3TD	1	1915	1	18,22,23	2.71	7 (38%)	22,32,35	1.45	1 (4%)
1	5MU	1	747	1	19,22,23	1.41	5 (26%)	28,32,35	2.17	7 (25%)
1	5MC	1	1962	1	18,22,23	2.08	3 (16%)	26,32,35	1.59	2 (7%)
1	PSU	1	2457	1	18,21,22	1.96	5 (27%)	22,30,33	2.30	5 (22%)
2	5MC	2	1407	2	18,22,23	2.13	3 (16%)	26,32,35	1.40	3 (11%)
2	2MG	2	1207	2	18,26,27	2.95	5 (27%)	16,38,41	1.29	4 (25%)
1	2MG	1	2445	1	18,26,27	2.98	6 (33%)	16,38,41	1.53	3 (18%)
1	PSU	1	1911	1	18,21,22	1.96	5 (27%)	22,30,33	2.14	4 (18%)
1	PSU	1	746	1	18,21,22	1.40	2 (11%)	22,30,33	2.23	6 (27%)
1	OMU	1	2552	1	19,22,23	2.60	7 (36%)	26,31,34	2.09	7 (26%)
2	MA6	2	1518	2	18,26,27	0.85	0	19,38,41	1.59	4 (21%)
2	MA6	2	1519	2	18,26,27	0.90	0	19,38,41	1.44	2 (10%)
2	4OC	2	1402	2	20,23,24	0.83	1 (5%)	26,32,35	1.33	4 (15%)
47	0TD	q	89	47	7,9,10	1.40	1 (14%)	6,11,13	2.63	3 (50%)
1	OMG	1	2251	1,57	18,26,27	3.02	7 (38%)	19,38,41	1.50	4 (21%)
1	1MG	1	745	1	18,26,27	0.99	0	19,39,42	1.28	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2MG	2	1516	2	18,26,27	2.93	5 (27%)	16,38,41	1.33	3 (18%)
1	OMC	1	2498	58,1	19,22,23	1.86	6 (31%)	26,31,34	2.16	6 (23%)
2	5MC	2	967	2	18,22,23	2.07	3 (16%)	26,32,35	1.43	4 (15%)
2	UR3	2	1498	58,2	19,22,23	2.76	6 (31%)	26,32,35	1.23	2 (7%)
2	PSU	2	516	58,2	18,21,22	1.44	3 (16%)	22,30,33	2.14	5 (22%)
1	PSU	1	2580	1	18,21,22	2.07	5 (27%)	22,30,33	2.35	6 (27%)
1	6MZ	1	1618	1	18,25,26	1.92	1 (5%)	16,36,39	2.53	4 (25%)
1	PSU	1	1917	58,1	18,21,22	2.00	5 (27%)	22,30,33	1.95	5 (22%)
1	6MZ	1	2030	1	18,25,26	1.92	2 (11%)	16,36,39	3.37	5 (31%)
2	7MG	2	527	2	22,26,27	1.37	4 (18%)	29,39,42	2.59	8 (27%)
1	G7M	1	2069	1	20,26,27	1.19	2 (10%)	17,39,42	0.94	1 (5%)
1	PSU	1	2605	1	18,21,22	1.93	5 (27%)	22,30,33	2.09	3 (13%)
1	2MA	1	2503	58,1	17,25,26	1.63	3 (17%)	17,37,40	1.38	2 (11%)
1	2MG	1	1835	1	18,26,27	2.88	6 (33%)	16,38,41	1.60	4 (25%)
2	2MG	2	966	2	18,26,27	2.87	5 (27%)	16,38,41	1.42	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1	955	1	-	3/7/25/26	0/2/2/2
1	PSU	1	2504	1	2/2/5/5	4/7/25/26	0/2/2/2
1	5MU	1	1939	58,1	-	0/7/25/26	0/2/2/2
1	3TD	1	1915	1	1/1/5/5	4/7/25/26	0/2/2/2
1	5MU	1	747	1	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	1	2457	1	2/2/5/5	0/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	2/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	2/5/27/28	0/3/3/3
1	2MG	1	2445	1	-	4/5/27/28	0/3/3/3
1	PSU	1	1911	1	2/2/5/5	3/7/25/26	0/2/2/2
1	OMU	1	2552	1	2/2/5/5	3/9/27/28	0/2/2/2
1	PSU	1	746	1	-	2/7/25/26	0/2/2/2
2	MA6	2	1518	2	-	3/7/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA6	2	1519	2	-	3/7/29/30	0/3/3/3
2	4OC	2	1402	2	-	3/9/29/30	0/2/2/2
47	0TD	q	89	47	-	2/7/12/14	-
1	OMG	1	2251	1,57	1/1/5/5	2/5/27/28	0/3/3/3
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
2	2MG	2	1516	2	-	1/5/27/28	0/3/3/3
1	OMC	1	2498	58,1	1/1/5/5	5/9/27/28	0/2/2/2
2	5MC	2	967	2	-	3/7/25/26	0/2/2/2
2	UR3	2	1498	58,2	-	6/7/25/26	0/2/2/2
2	PSU	2	516	58,2	-	3/7/25/26	0/2/2/2
1	PSU	1	2580	1	2/2/5/5	2/7/25/26	0/2/2/2
1	6MZ	1	1618	1	2/2/5/6	5/5/27/28	0/3/3/3
1	PSU	1	1917	58,1	2/2/5/5	1/7/25/26	0/2/2/2
1	6MZ	1	2030	1	2/2/5/6	4/5/27/28	0/3/3/3
2	7MG	2	527	2	-	2/7/37/38	0/3/3/3
1	G7M	1	2069	1	3/3/5/5	2/3/25/26	0/3/3/3
1	PSU	1	2605	1	2/2/5/5	3/7/25/26	0/2/2/2
1	2MA	1	2503	58,1	2/2/5/5	3/3/25/26	0/3/3/3
1	2MG	1	1835	1	-	3/5/27/28	0/3/3/3
2	2MG	2	966	2	-	0/5/27/28	0/3/3/3

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	966	2MG	O6-C6	8.97	1.41	1.23
2	2	1207	2MG	O6-C6	8.83	1.41	1.23
1	1	2251	OMG	O6-C6	8.78	1.41	1.23
2	2	1516	2MG	O6-C6	8.70	1.41	1.23
1	1	2445	2MG	O6-C6	8.54	1.40	1.23
2	2	1498	UR3	O4-C4	8.46	1.41	1.23
1	1	1835	2MG	O6-C6	8.30	1.40	1.23
1	1	1915	3TD	O4-C4	8.18	1.40	1.23
1	1	2552	OMU	O4-C4	7.95	1.39	1.24
1	1	1618	6MZ	C6-N6	7.18	1.46	1.35
1	1	2030	6MZ	C6-N6	6.56	1.45	1.35
2	2	967	5MC	C4-N4	6.43	1.50	1.34
1	1	1962	5MC	C4-N4	6.21	1.50	1.34
2	2	1407	5MC	C4-N4	6.15	1.50	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	966	2MG	C2-N2	6.08	1.46	1.33
2	2	1516	2MG	C2-N2	5.81	1.46	1.33
2	2	1207	2MG	C2-N2	5.75	1.46	1.33
1	1	1835	2MG	C2-N2	5.41	1.45	1.33
2	2	1407	5MC	C2-N1	-5.12	1.28	1.40
1	1	2445	2MG	C2-N2	4.99	1.44	1.33
1	1	1962	5MC	C2-N1	-4.89	1.29	1.40
1	1	2251	OMG	C2-N2	4.88	1.45	1.34
1	1	2504	PSU	C4-N3	-4.87	1.29	1.38
1	1	2445	2MG	C6-N1	-4.79	1.30	1.37
2	2	967	5MC	C2-N1	-4.71	1.29	1.40
1	1	2498	OMC	C4-N4	4.71	1.45	1.33
1	1	2457	PSU	C4-N3	-4.61	1.30	1.38
1	1	2605	PSU	C4-N3	-4.58	1.30	1.38
1	1	2580	PSU	C2-N1	-4.45	1.30	1.36
1	1	2251	OMG	C6-N1	-4.44	1.31	1.37
1	1	1917	PSU	C6-C5	4.42	1.40	1.35
1	1	1911	PSU	C4-N3	-4.41	1.30	1.38
1	1	2580	PSU	C4-N3	-4.34	1.30	1.38
1	1	1917	PSU	C4-N3	-4.33	1.30	1.38
1	1	1915	3TD	C2-N1	-4.21	1.31	1.37
2	2	1498	UR3	C4-N3	-4.12	1.31	1.40
2	2	1498	UR3	C2-N1	-4.11	1.32	1.38
1	1	1835	2MG	C6-N1	-4.09	1.31	1.37
1	1	2552	OMU	C4-N3	-3.91	1.31	1.38
1	1	2503	2MA	C6-N6	3.89	1.44	1.28
2	2	1207	2MG	C6-N1	-3.87	1.32	1.37
1	1	2580	PSU	C6-N1	-3.81	1.29	1.36
1	1	2445	2MG	C2-N1	-3.79	1.30	1.36
1	1	2605	PSU	C6-C5	3.78	1.39	1.35
2	2	1516	2MG	C6-N1	-3.77	1.32	1.37
1	1	2580	PSU	C6-C5	3.75	1.39	1.35
1	1	2457	PSU	C6-C5	3.73	1.39	1.35
2	2	1516	2MG	C5-C6	-3.67	1.39	1.47
1	1	2504	PSU	C2-N1	-3.61	1.31	1.36
1	1	1911	PSU	C6-C5	3.61	1.39	1.35
1	1	1911	PSU	C2-N1	-3.60	1.31	1.36
1	1	2504	PSU	C6-C5	3.53	1.39	1.35
1	1	2251	OMG	C5-C6	-3.50	1.40	1.47
2	2	527	7MG	C4-N9	-3.49	1.33	1.37
1	1	2445	2MG	C5-C6	-3.49	1.40	1.47
1	1	2552	OMU	C2-N3	-3.46	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1917	PSU	C2-N1	-3.45	1.32	1.36
1	1	2457	PSU	C6-N1	-3.43	1.30	1.36
1	1	1835	2MG	C5-C6	-3.42	1.40	1.47
2	2	1207	2MG	C5-C6	-3.41	1.40	1.47
1	1	2552	OMU	C2-N1	-3.33	1.33	1.38
1	1	2457	PSU	C2-N1	-3.31	1.32	1.36
1	1	1911	PSU	C6-N1	-3.30	1.30	1.36
1	1	1915	3TD	C4-N3	-3.29	1.33	1.40
1	1	1835	2MG	C2-N1	-3.27	1.31	1.36
1	1	2504	PSU	C6-N1	-3.22	1.30	1.36
1	1	2605	PSU	C6-N1	-3.21	1.30	1.36
2	2	1498	UR3	C2-N3	-3.21	1.32	1.39
1	1	746	PSU	C6-C5	3.19	1.39	1.35
1	1	1917	PSU	C6-N1	-3.19	1.30	1.36
1	1	1915	3TD	C6-C5	3.12	1.39	1.35
1	1	2498	OMC	O2-C2	-3.09	1.18	1.23
2	2	1498	UR3	O2-C2	-3.08	1.16	1.22
1	1	2605	PSU	C2-N1	-3.06	1.32	1.36
2	2	516	PSU	C6-C5	3.03	1.38	1.35
1	1	955	PSU	C4-N3	-3.02	1.33	1.38
2	2	516	PSU	C4-N3	-2.99	1.33	1.38
1	1	2069	G7M	C5-C4	2.96	1.45	1.39
2	2	966	2MG	C6-N1	-2.95	1.33	1.37
1	1	1939	5MU	C4-N3	-2.94	1.33	1.38
1	1	1915	3TD	C2-N3	-2.89	1.32	1.38
1	1	2503	2MA	C6-N1	-2.89	1.31	1.38
1	1	2069	G7M	C6-N1	-2.89	1.33	1.37
1	1	747	5MU	C6-C5	2.82	1.39	1.34
2	2	1207	2MG	C2-N1	-2.82	1.32	1.36
2	2	966	2MG	C5-C6	-2.82	1.41	1.47
1	1	2251	OMG	C5-C4	-2.79	1.36	1.43
1	1	746	PSU	C4-N3	-2.79	1.33	1.38
1	1	955	PSU	C6-C5	2.78	1.38	1.35
1	1	747	5MU	C4-N3	-2.77	1.33	1.38
2	2	527	7MG	C5-C4	2.76	1.47	1.38
2	2	1498	UR3	C6-N1	-2.68	1.31	1.38
2	2	1407	5MC	C2-N3	-2.66	1.30	1.36
1	1	2251	OMG	C2-N1	-2.62	1.31	1.37
1	1	2251	OMG	O2'-CM2	-2.62	1.33	1.42
1	1	1939	5MU	C6-N1	-2.61	1.33	1.38
1	1	2503	2MA	C5-C4	-2.61	1.36	1.43
1	1	2498	OMC	C2-N1	-2.55	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2498	OMC	C5-C4	-2.52	1.37	1.42
1	1	2498	OMC	C2-N3	-2.48	1.31	1.36
1	1	1915	3TD	C6-N1	-2.46	1.32	1.36
1	1	2552	OMU	C6-N1	-2.46	1.32	1.38
1	1	1962	5MC	C2-N3	-2.44	1.31	1.36
2	2	527	7MG	C6-N1	-2.43	1.34	1.38
1	1	1939	5MU	C2-N3	-2.41	1.33	1.38
1	1	1939	5MU	C6-C5	2.41	1.38	1.34
2	2	1516	2MG	C2-N1	-2.38	1.32	1.36
1	1	2504	PSU	C2-N3	-2.36	1.33	1.37
1	1	2552	OMU	O2-C2	-2.36	1.18	1.23
1	1	2580	PSU	C2-N3	-2.32	1.33	1.37
1	1	747	5MU	C4-C5	2.31	1.48	1.44
1	1	1911	PSU	C2-N3	-2.30	1.33	1.37
1	1	2498	OMC	C4-N3	-2.29	1.30	1.34
1	1	2605	PSU	C2-N3	-2.29	1.33	1.37
1	1	1835	2MG	C5-C4	-2.26	1.37	1.43
2	2	516	PSU	C2-N3	-2.24	1.33	1.37
1	1	747	5MU	C6-N1	-2.22	1.34	1.38
2	2	527	7MG	C5-N7	-2.20	1.33	1.35
2	2	967	5MC	C2-N3	-2.20	1.31	1.36
1	1	2552	OMU	C5-C4	-2.19	1.38	1.43
1	1	955	PSU	C2-N3	-2.19	1.33	1.37
1	1	1915	3TD	O2-C2	-2.18	1.19	1.23
1	1	2504	PSU	O4'-C1'	-2.16	1.40	1.43
2	2	966	2MG	C2-N1	-2.14	1.33	1.36
1	1	1917	PSU	O4'-C1'	-2.11	1.40	1.43
1	1	747	5MU	C2-N3	-2.07	1.34	1.38
1	1	2457	PSU	C2-N3	-2.03	1.34	1.37
2	2	1402	4OC	C6-N1	-2.03	1.33	1.38
1	1	2030	6MZ	C2'-C1'	-2.02	1.50	1.53
1	1	2445	2MG	C5-C4	-2.01	1.37	1.43
47	q	89	0TD	CSB-SB	-2.00	1.75	1.79

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2030	6MZ	C9-N6-C6	-9.62	114.59	122.87
2	2	527	7MG	N9-C4-N3	8.69	138.46	125.47
1	1	2498	OMC	O2-C2-N3	-6.85	111.18	122.33
1	1	2457	PSU	N1-C2-N3	6.77	122.80	115.13
2	2	516	PSU	N1-C2-N3	6.77	122.80	115.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1962	5MC	C5-C6-N1	-6.46	116.69	123.34
1	1	2580	PSU	N1-C2-N3	6.41	122.39	115.13
1	1	746	PSU	N1-C2-N3	6.39	122.37	115.13
1	1	2605	PSU	N1-C2-N3	6.36	122.33	115.13
1	1	955	PSU	N1-C2-N3	6.35	122.32	115.13
1	1	1911	PSU	N1-C2-N3	6.25	122.21	115.13
1	1	1618	6MZ	C9-N6-C6	-6.15	117.58	122.87
1	1	2504	PSU	N1-C2-N3	6.14	122.09	115.13
1	1	2030	6MZ	C2-N1-C6	5.94	121.69	116.59
1	1	2030	6MZ	N3-C2-N1	-5.75	119.69	128.68
1	1	1939	5MU	C4-N3-C2	-5.66	120.02	127.35
1	1	1917	PSU	N1-C2-N3	5.65	121.53	115.13
2	2	527	7MG	N9-C8-N7	-5.61	95.35	103.38
1	1	1915	3TD	N1-C2-N3	5.41	120.41	116.14
2	2	527	7MG	C5-C4-N3	-5.34	117.96	128.13
1	1	747	5MU	N3-C2-N1	5.28	121.89	114.89
1	1	2580	PSU	O2-C2-N1	-5.25	117.01	122.79
2	2	967	5MC	C5-C6-N1	-5.22	117.97	123.34
1	1	747	5MU	C4-N3-C2	-5.17	120.66	127.35
1	1	1618	6MZ	C2-N1-C6	5.14	121.00	116.59
2	2	1407	5MC	C5-C6-N1	-5.06	118.13	123.34
1	1	1939	5MU	C5-C4-N3	5.03	119.61	115.31
1	1	2552	OMU	N3-C2-N1	5.01	121.54	114.89
1	1	1939	5MU	N3-C2-N1	4.97	121.48	114.89
2	2	1519	MA6	N3-C2-N1	-4.82	121.14	128.68
1	1	2552	OMU	C4-N3-C2	-4.81	120.24	126.58
1	1	2457	PSU	O2-C2-N1	-4.64	117.68	122.79
1	1	2457	PSU	C4-N3-C2	-4.59	119.73	126.34
1	1	1939	5MU	C5-C6-N1	-4.56	118.65	123.34
2	2	1518	MA6	N3-C2-N1	-4.52	121.61	128.68
1	1	1618	6MZ	N3-C2-N1	-4.49	121.66	128.68
1	1	2605	PSU	C4-N3-C2	-4.49	119.87	126.34
1	1	955	PSU	C4-N3-C2	-4.38	120.03	126.34
1	1	2498	OMC	C1'-N1-C2	4.36	128.14	118.42
1	1	1939	5MU	O4-C4-C5	-4.34	119.87	124.90
1	1	2504	PSU	C4-N3-C2	-4.29	120.16	126.34
1	1	1911	PSU	O2-C2-N1	-4.17	118.20	122.79
2	2	516	PSU	C4-N3-C2	-4.13	120.39	126.34
1	1	747	5MU	C5-C4-N3	4.12	118.83	115.31
1	1	746	PSU	C4-N3-C2	-4.11	120.41	126.34
47	q	89	0TD	OD2-CG-CB	4.10	122.01	113.15
2	2	527	7MG	C2-N3-C4	4.09	119.59	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1911	PSU	C4-N3-C2	-4.06	120.49	126.34
1	1	2503	2MA	C5-C6-N1	4.05	121.02	114.02
1	1	2498	OMC	O2-C2-N1	3.99	127.12	118.89
1	1	2445	2MG	CM2-N2-C2	-3.86	115.33	123.86
1	1	1835	2MG	C5-C6-N1	3.84	120.73	113.95
1	1	2580	PSU	C4-N3-C2	-3.79	120.89	126.34
2	2	1498	UR3	C4-N3-C2	-3.78	121.01	124.56
1	1	2504	PSU	O2-C2-N1	-3.76	118.65	122.79
1	1	747	5MU	C5-C6-N1	-3.73	119.50	123.34
1	1	1917	PSU	O2-C2-N1	-3.73	118.69	122.79
1	1	747	5MU	O4-C4-C5	-3.71	120.60	124.90
1	1	2580	PSU	C6-C5-C4	-3.68	115.63	118.20
1	1	2552	OMU	C5-C4-N3	3.61	120.25	114.84
1	1	1917	PSU	C4-N3-C2	-3.57	121.20	126.34
2	2	516	PSU	O2-C2-N1	-3.55	118.88	122.79
1	1	955	PSU	O2-C2-N1	-3.49	118.95	122.79
1	1	1618	6MZ	C4-C5-N7	-3.48	105.78	109.40
1	1	746	PSU	O2'-C2'-C1'	-3.46	102.98	111.23
2	2	1402	4OC	C2'-C1'-N1	-3.46	107.51	114.22
1	1	1939	5MU	O2-C2-N1	-3.41	118.25	122.79
1	1	746	PSU	O2-C2-N1	-3.40	119.04	122.79
2	2	966	2MG	C5-C6-N1	3.36	119.88	113.95
1	1	2251	OMG	C5-C6-N1	3.35	119.87	113.95
47	q	89	0TD	CSB-SB-CB	3.30	108.41	102.44
1	1	747	5MU	O2-C2-N1	-3.29	118.41	122.79
1	1	2605	PSU	O2-C2-N1	-3.24	119.22	122.79
1	1	2445	2MG	C5-C6-N1	3.20	119.59	113.95
1	1	2552	OMU	CM2-O2'-C2'	-3.18	106.19	114.52
1	1	2498	OMC	C6-N1-C2	-3.15	115.02	120.49
1	1	1835	2MG	CM2-N2-C2	-3.10	117.02	123.86
47	q	89	0TD	OD1-CG-CB	-3.06	116.03	122.44
1	1	2251	OMG	C2-N1-C6	-3.05	119.49	125.10
2	2	1516	2MG	C5-C6-N1	2.97	119.20	113.95
1	1	2552	OMU	O4-C4-C5	-2.88	120.09	125.16
1	1	2580	PSU	C6-N1-C2	-2.86	119.76	122.68
2	2	1407	5MC	O2-C2-N3	-2.86	117.69	122.33
2	2	1207	2MG	C5-C6-N1	2.85	118.99	113.95
1	1	2069	G7M	C3'-C2'-C1'	2.83	105.23	100.98
1	1	2030	6MZ	C1'-N9-C4	-2.82	121.69	126.64
2	2	516	PSU	O3'-C3'-C2'	2.81	120.93	111.82
2	2	1518	MA6	C4-C5-N7	-2.78	106.50	109.40
1	1	2030	6MZ	C4-C5-N7	-2.77	106.51	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	745	1MG	C8-N7-C5	2.76	108.25	102.99
1	1	1835	2MG	C8-N7-C5	2.75	108.24	102.99
2	2	1516	2MG	O6-C6-C5	-2.72	119.07	124.37
1	1	2503	2MA	C8-N7-C5	2.71	108.15	102.99
2	2	966	2MG	C8-N7-C5	2.69	108.11	102.99
2	2	1402	4OC	O4'-C1'-N1	2.67	114.46	108.36
1	1	2552	OMU	O3'-C3'-C4'	2.66	118.74	111.05
2	2	527	7MG	O3'-C3'-C4'	2.65	118.72	111.05
1	1	2251	OMG	O6-C6-C5	-2.64	119.22	124.37
2	2	967	5MC	O2-C2-N3	-2.63	118.06	122.33
1	1	747	5MU	C2'-C1'-N1	-2.63	105.78	113.22
1	1	1939	5MU	O3'-C3'-C4'	-2.62	103.47	111.05
1	1	2251	OMG	CM2-O2'-C2'	-2.62	107.66	114.52
2	2	527	7MG	C5-C6-N1	2.61	115.59	110.99
2	2	1519	MA6	C4-C5-N7	-2.61	106.68	109.40
2	2	1518	MA6	C1'-N9-C4	2.57	131.16	126.64
1	1	1962	5MC	O2-C2-N3	-2.55	118.18	122.33
1	1	1911	PSU	C6-N1-C2	-2.54	120.08	122.68
1	1	955	PSU	C2'-C3'-C4'	2.53	107.56	102.64
2	2	1207	2MG	CM2-N2-C2	-2.48	118.38	123.86
1	1	745	1MG	C5-C6-N1	2.47	117.61	113.90
1	1	746	PSU	O3'-C3'-C2'	2.43	119.69	111.82
1	1	746	PSU	C5-C6-N1	-2.41	118.50	122.11
2	2	1518	MA6	C9-N6-C6	2.40	126.78	119.51
1	1	2445	2MG	C8-N7-C5	2.40	107.55	102.99
2	2	1207	2MG	C8-N7-C5	2.37	107.50	102.99
2	2	1498	UR3	C3U-N3-C2	2.31	121.36	117.31
2	2	1516	2MG	CM2-N2-C2	-2.30	118.79	123.86
1	1	2498	OMC	CM2-O2'-C2'	-2.29	108.53	114.52
2	2	1402	4OC	C6-C5-C4	2.28	119.75	116.96
2	2	966	2MG	O6-C6-C5	-2.27	119.94	124.37
2	2	967	5MC	C5-C4-N3	-2.24	119.25	121.67
2	2	527	7MG	O6-C6-C5	-2.23	122.06	127.54
2	2	967	5MC	N1-C2-N3	2.22	122.86	118.81
1	1	1835	2MG	O6-C6-C5	-2.22	120.03	124.37
1	1	2504	PSU	C6-N1-C2	-2.22	120.41	122.68
1	1	2457	PSU	O3'-C3'-C4'	2.20	117.40	111.05
1	1	1917	PSU	C6-N1-C2	-2.17	120.47	122.68
1	1	2457	PSU	C6-N1-C2	-2.15	120.48	122.68
2	2	516	PSU	O2'-C2'-C1'	-2.14	106.12	111.23
1	1	2552	OMU	O2-C2-N3	-2.14	117.51	121.50
2	2	527	7MG	C5-C4-N9	-2.14	103.57	106.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1917	PSU	C6-C5-C4	-2.12	116.72	118.20
2	2	1207	2MG	O6-C6-C5	-2.08	120.30	124.37
1	1	2580	PSU	C3'-C2'-C1'	-2.07	99.22	101.64
1	1	955	PSU	C5-C6-N1	-2.07	119.00	122.11
2	2	1407	5MC	N1-C2-N3	2.06	122.56	118.81
1	1	2504	PSU	O4-C4-C5	-2.02	118.77	124.05
1	1	2498	OMC	C4-N3-C2	2.01	123.51	120.25
2	2	1402	4OC	CM4-N4-C4	-2.01	118.53	122.45

All (26) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	1618	6MZ	C2'
1	1	1618	6MZ	C3'
1	1	1911	PSU	C4'
1	1	1911	PSU	C3'
1	1	1915	3TD	C3'
1	1	1917	PSU	C4'
1	1	1917	PSU	C3'
1	1	2030	6MZ	C2'
1	1	2030	6MZ	C3'
1	1	2069	G7M	C4'
1	1	2069	G7M	C2'
1	1	2069	G7M	C3'
1	1	2251	OMG	C2'
1	1	2457	PSU	C4'
1	1	2457	PSU	C3'
1	1	2498	OMC	C4'
1	1	2503	2MA	C2'
1	1	2503	2MA	C3'
1	1	2504	PSU	C4'
1	1	2504	PSU	C3'
1	1	2552	OMU	C2'
1	1	2552	OMU	C3'
1	1	2580	PSU	C4'
1	1	2580	PSU	C3'
1	1	2605	PSU	C4'
1	1	2605	PSU	C3'

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	955	PSU	C2'-C1'-C5-C4
1	1	955	PSU	C4'-C5'-O5'-P
1	1	1618	6MZ	C5-C6-N6-C9
1	1	1618	6MZ	N1-C6-N6-C9
1	1	1618	6MZ	O4'-C4'-C5'-O5'
1	1	1618	6MZ	C3'-C4'-C5'-O5'
1	1	1835	2MG	N1-C2-N2-CM2
1	1	1835	2MG	N3-C2-N2-CM2
1	1	1911	PSU	C4'-C5'-O5'-P
1	1	1915	3TD	O4'-C1'-C5-C4
1	1	1915	3TD	O4'-C1'-C5-C6
1	1	1962	5MC	O4'-C4'-C5'-O5'
1	1	1962	5MC	C3'-C4'-C5'-O5'
1	1	2030	6MZ	N1-C6-N6-C9
1	1	2030	6MZ	O4'-C4'-C5'-O5'
1	1	2030	6MZ	C3'-C4'-C5'-O5'
1	1	2069	G7M	C3'-C4'-C5'-O5'
1	1	2445	2MG	C3'-C4'-C5'-O5'
1	1	2445	2MG	N1-C2-N2-CM2
1	1	2445	2MG	N3-C2-N2-CM2
1	1	2498	OMC	C3'-C4'-C5'-O5'
1	1	2498	OMC	C4'-C5'-O5'-P
1	1	2504	PSU	C2'-C1'-C5-C6
1	1	2552	OMU	O4'-C4'-C5'-O5'
1	1	2580	PSU	C2'-C1'-C5-C4
1	1	2580	PSU	C2'-C1'-C5-C6
1	1	2605	PSU	C3'-C4'-C5'-O5'
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	516	PSU	C4'-C5'-O5'-P
2	2	527	7MG	C3'-C4'-C5'-O5'
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1207	2MG	N1-C2-N2-CM2
2	2	1207	2MG	N3-C2-N2-CM2
2	2	1402	4OC	C1'-C2'-O2'-CM2
2	2	1407	5MC	O4'-C4'-C5'-O5'
2	2	1516	2MG	N3-C2-N2-CM2
2	2	1518	MA6	O4'-C4'-C5'-O5'
2	2	1518	MA6	C3'-C4'-C5'-O5'
2	2	1519	MA6	C5-C6-N6-C10
1	1	2504	PSU	C4'-C5'-O5'-P
1	1	1915	3TD	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1	2503	2MA	O4'-C4'-C5'-O5'
1	1	2503	2MA	C3'-C4'-C5'-O5'
1	1	2504	PSU	C3'-C4'-C5'-O5'
1	1	2552	OMU	C3'-C4'-C5'-O5'
2	2	1407	5MC	C3'-C4'-C5'-O5'
1	1	2445	2MG	O4'-C4'-C5'-O5'
1	1	2504	PSU	O4'-C4'-C5'-O5'
1	1	2605	PSU	O4'-C4'-C5'-O5'
2	2	527	7MG	O4'-C4'-C5'-O5'
2	2	1519	MA6	N1-C6-N6-C10
1	1	1911	PSU	C3'-C4'-C5'-O5'
1	1	1915	3TD	C3'-C4'-C5'-O5'
1	1	2069	G7M	O4'-C4'-C5'-O5'
1	1	2251	OMG	O4'-C4'-C5'-O5'
1	1	1917	PSU	C4'-C5'-O5'-P
1	1	2498	OMC	O4'-C4'-C5'-O5'
1	1	2605	PSU	C4'-C5'-O5'-P
2	2	1402	4OC	C4'-C5'-O5'-P
1	1	2030	6MZ	C5-C6-N6-C9
1	1	1911	PSU	O4'-C4'-C5'-O5'
1	1	2498	OMC	C2'-C1'-N1-C6
1	1	1618	6MZ	C4'-C5'-O5'-P
1	1	2552	OMU	C4'-C5'-O5'-P
47	q	89	0TD	SB-CB-CG-OD1
2	2	1402	4OC	C3'-C2'-O2'-CM2
2	2	1498	UR3	C2'-C1'-N1-C6
1	1	2498	OMC	C2'-C1'-N1-C2
2	2	1519	MA6	C5-C6-N6-C9
2	2	967	5MC	C4'-C5'-O5'-P
1	1	2503	2MA	C4'-C5'-O5'-P
1	1	746	PSU	O4'-C1'-C5-C4
1	1	955	PSU	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C1'-N1-C6
47	q	89	0TD	CA-CB-SB-CSB
1	1	1835	2MG	O4'-C4'-C5'-O5'
1	1	2251	OMG	C3'-C4'-C5'-O5'
2	2	1498	UR3	O4'-C4'-C5'-O5'
2	2	1518	MA6	C4'-C5'-O5'-P
1	1	746	PSU	O4'-C1'-C5-C6
2	2	1498	UR3	C2'-C1'-N1-C2
2	2	1498	UR3	O4'-C1'-N1-C2
2	2	1498	UR3	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 431 ligands modelled in this entry, 431 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	3
57	4	1
1	1	1
17	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	342:U	O3'	343:C	P	3.61
1	2	1276:G	O3'	1277:C	P	3.26
1	1	2314:A	O3'	2315:G	P	3.25
1	2	147:G	O3'	148:G	P	3.25

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1383:C	O3'	1384:C	P	3.17
1	M	2:LEU	C	3:GLN	N	1.13

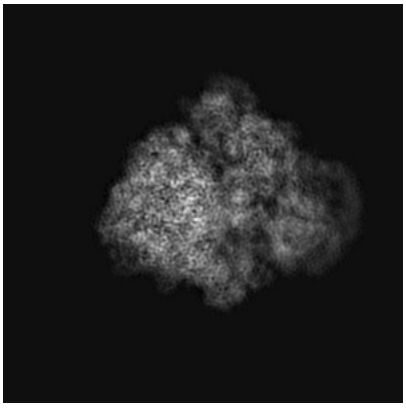
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4477. These allow visual inspection of the internal detail of the map and identification of artifacts.

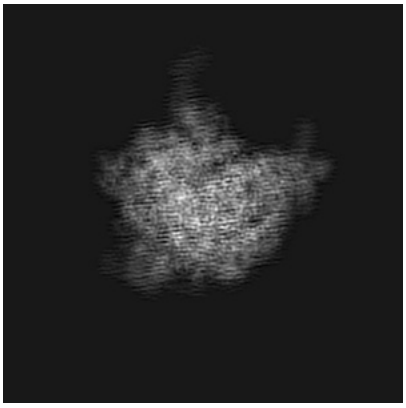
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

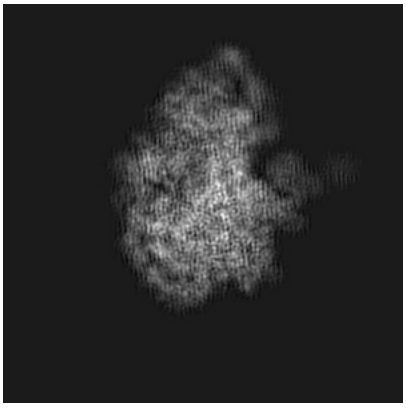
6.1.1 Primary map



X



Y

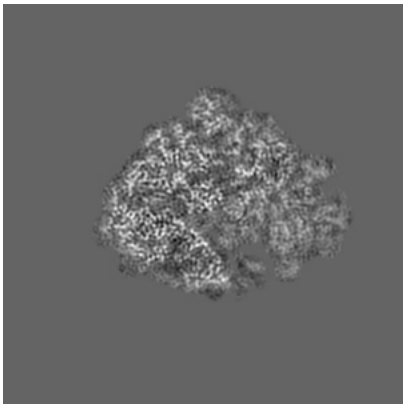


Z

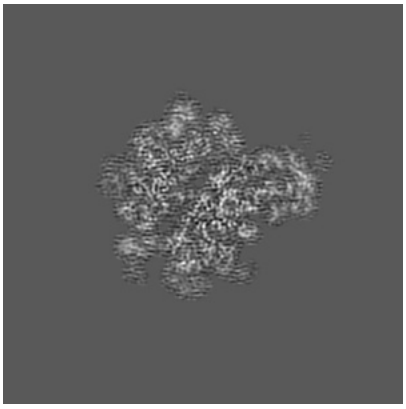
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

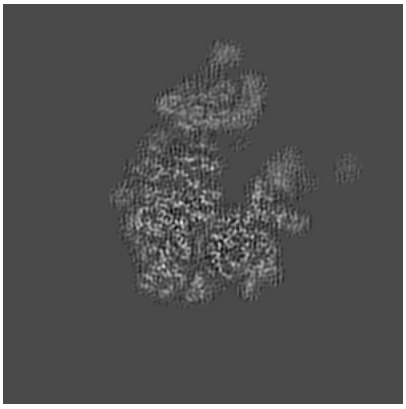
6.2.1 Primary map



X Index: 190



Y Index: 190

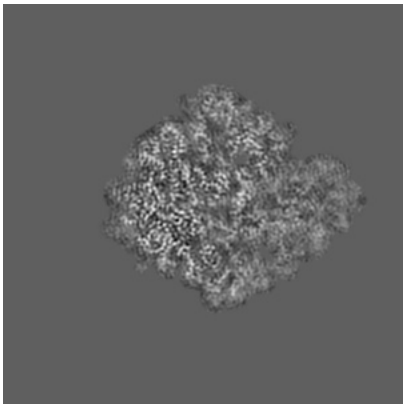


Z Index: 190

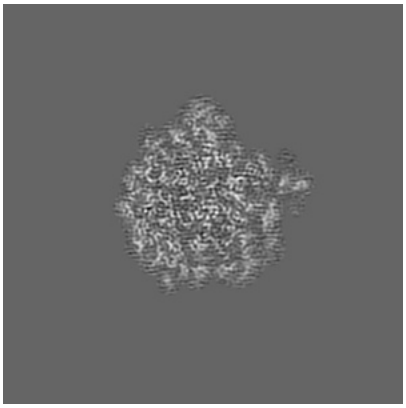
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

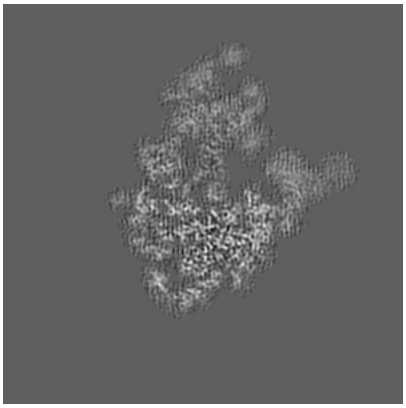
6.3.1 Primary map



X Index: 199



Y Index: 176

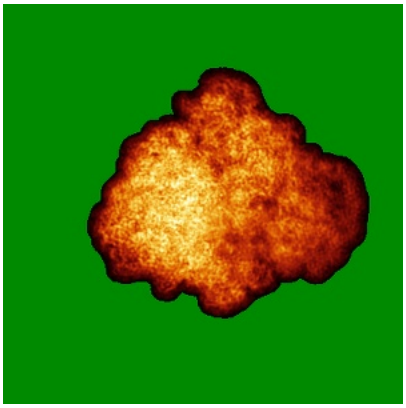


Z Index: 174

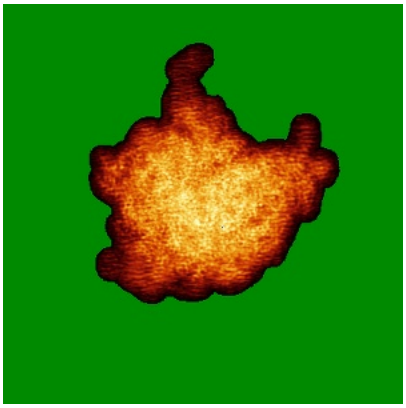
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

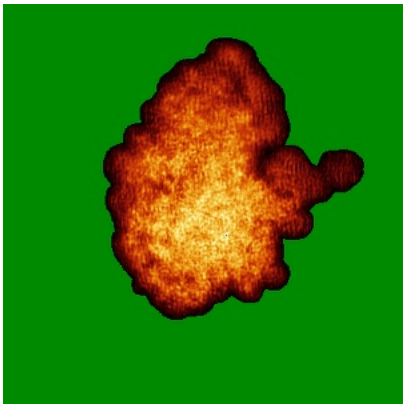
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0934. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

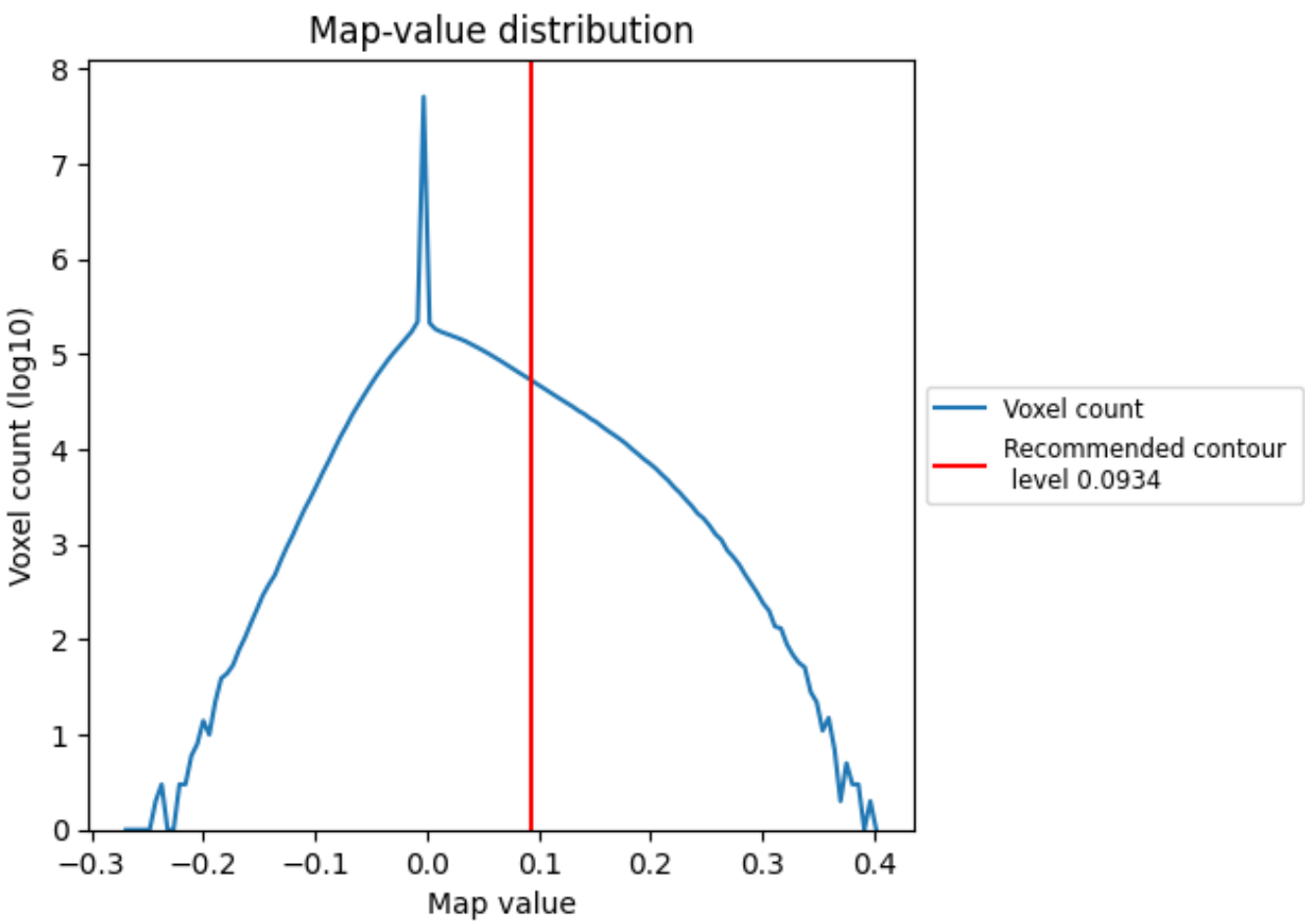
6.6 Mask visualisation (i)

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

7 Map analysis (i)

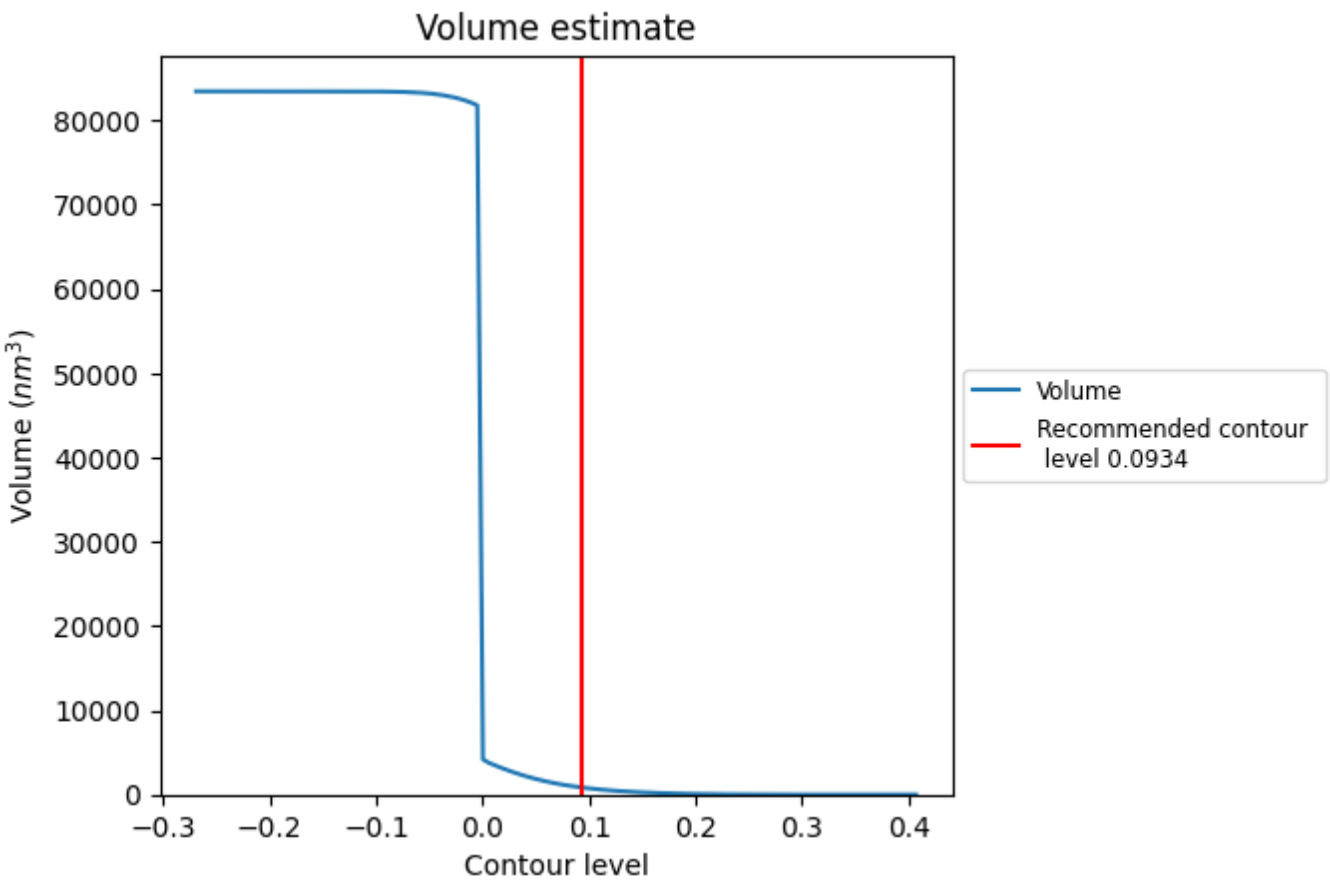
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

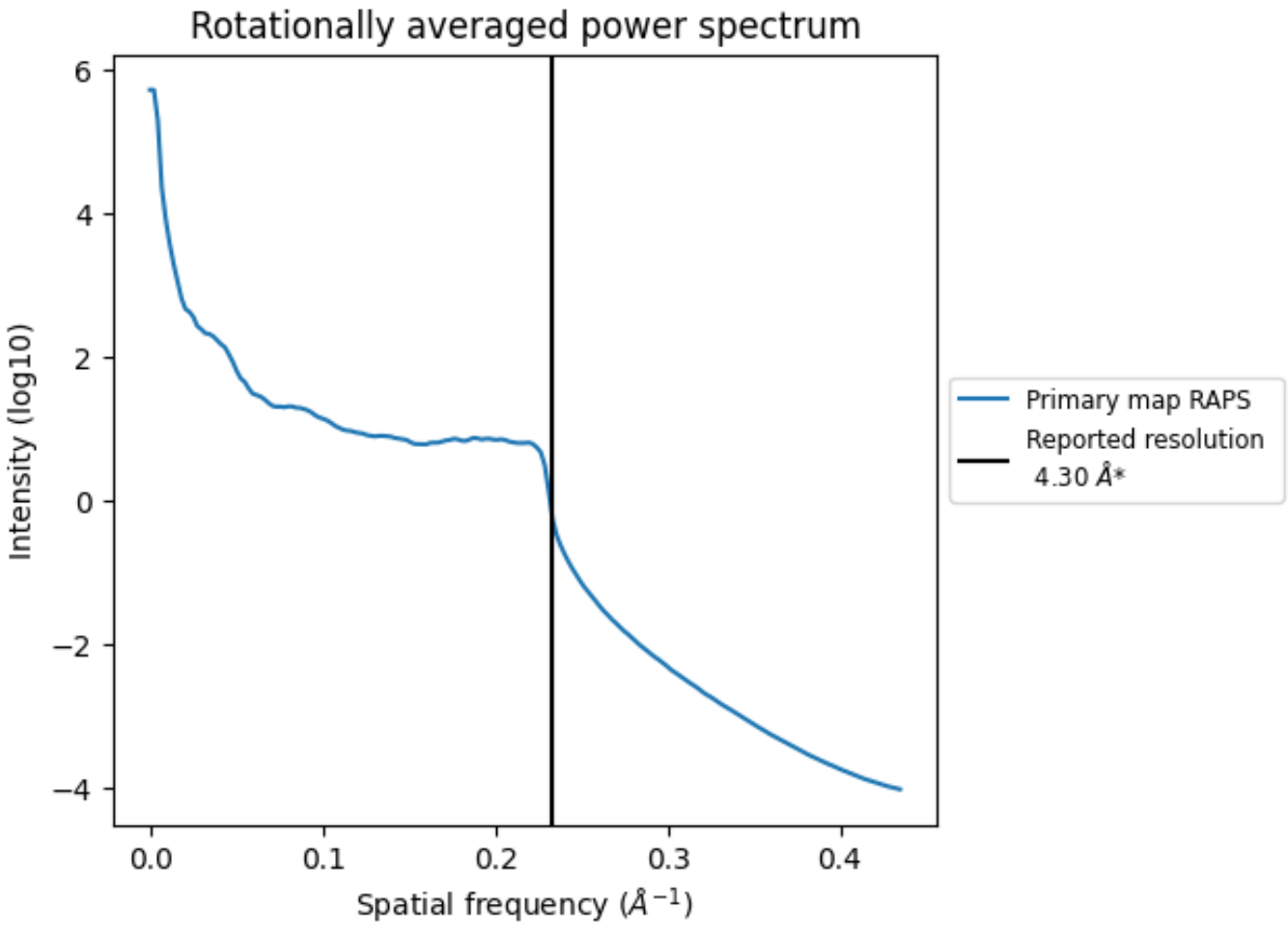
7.2 Volume estimate (i)



The volume at the recommended contour level is 836 nm^3; this corresponds to an approximate mass of 755 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 (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

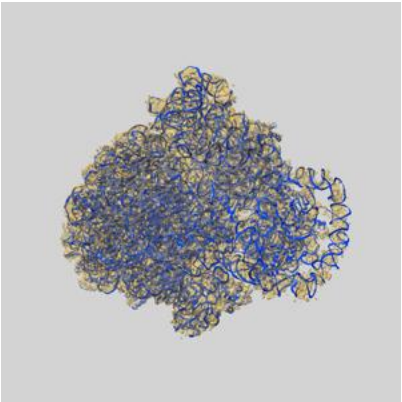
8 Fourier-Shell correlation (i)

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

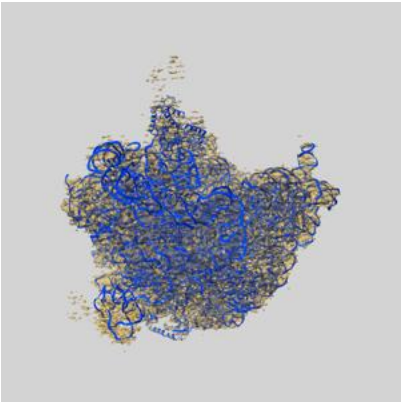
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4477 and PDB model 6Q98. Per-residue inclusion information can be found in section 3 on page 16.

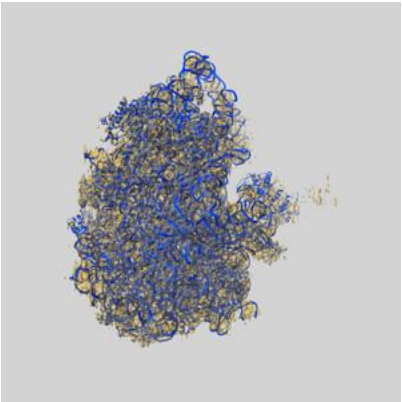
9.1 Map-model overlay (i)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0934 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.

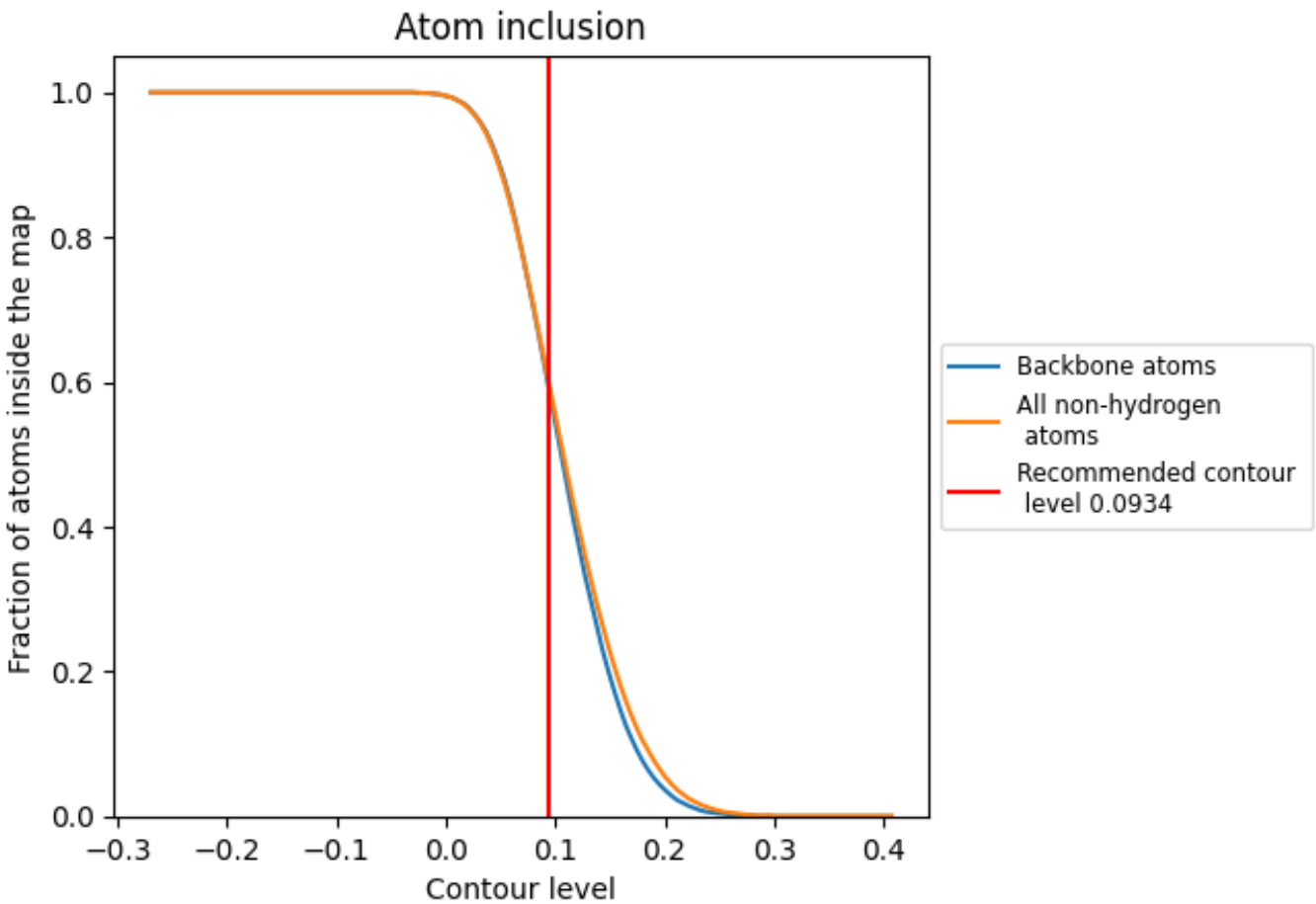
9.2 Q-score mapped to coordinate model (i)

This section was not generated.

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0934) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.6050
1	0.7470
2	0.6730
3	0.7410
4	0.2510
5	0.3400
6	0.1910
B	0.5360
C	0.5700
D	0.5280
E	0.3970
F	0.4770
G	0.2300
H	0.1950
I	0.1690
J	0.5620
K	0.5360
L	0.5580
M	0.5440
N	0.5940
O	0.4770
P	0.4830
Q	0.6410
R	0.5480
S	0.5730
T	0.5000
U	0.5020
V	0.5470
W	0.5620
X	0.5440
Y	0.4930
Z	0.5620
a	0.2390
b	0.5940
c	0.4330

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
d	0.5630
e	0.5930
f	0.5750
g	0.2340
h	0.2910
i	0.3530
j	0.4890
k	0.4870
l	0.2300
m	0.4980
n	0.2160
o	0.1920
p	0.4850
q	0.4700
r	0.1890
s	0.2520
t	0.4940
u	0.4880
v	0.4710
w	0.4910
x	0.2100
y	0.4680
z	0.3790