



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:03 PM BST

PDB ID : 4V6K  
EMDB ID: : EMD-1849  
Title : Structural insights into cognate vs. near-cognate discrimination during decoding.  
Authors : Agirrezabala, X.; Schreiner, E.; Trabuco, L.G.; Lei, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.  
Deposited on : 2011-01-07  
Resolution : 8.25 Å(reported)  
Based on PDB ID : 2I2V

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

---

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

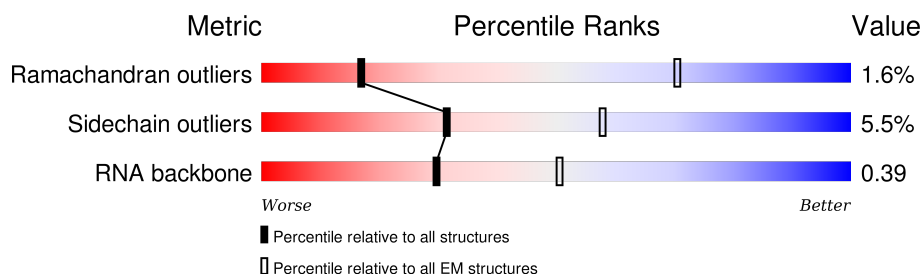
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.25 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.



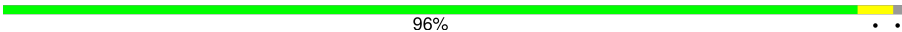
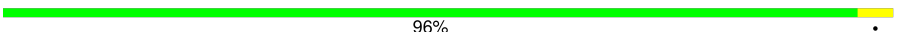










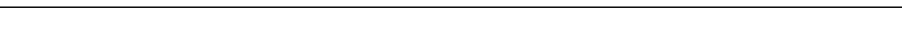

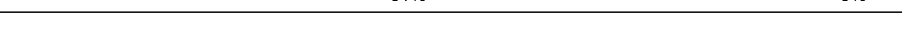

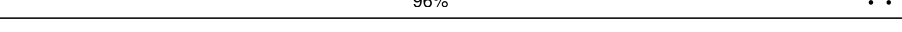







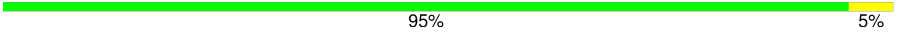
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	AA	120	33% 45% 18% .
2	AB	2904	26% 48% 23% .
3	AC	234	93% 7%
4	AD	273	92% 7%
5	AE	209	92% 8%
6	AF	201	95% 5%
7	AG	179	92% 7% ..
8	AH	177	90% 10% .
9	AI	149	90% 9% .

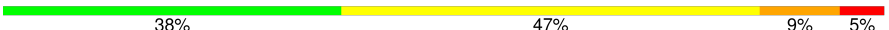

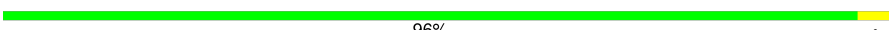
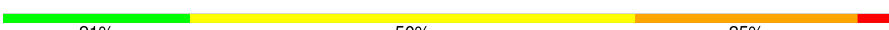








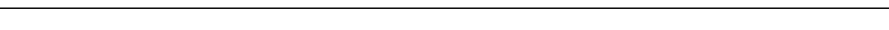
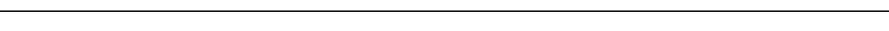
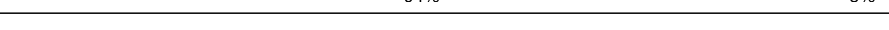
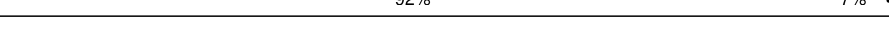
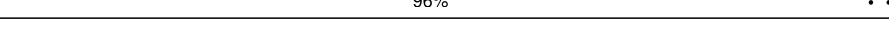

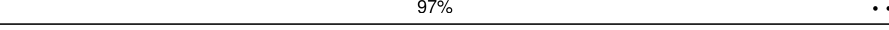
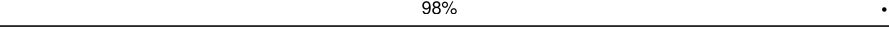
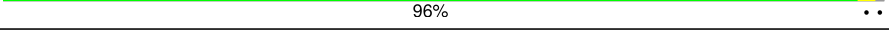


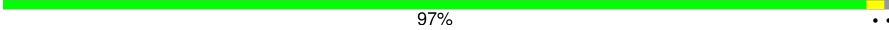
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
10	AJ	142	 96% . .
11	AK	142	 96% .
12	AL	123	 90% 10%
13	AM	144	 96% .
14	AN	136	 93% 6% .
15	AO	127	 97% .
16	AP	117	 93% 7%
17	AQ	115	 90% 8% . .
18	AR	118	 91% 8% .
19	AS	103	 90% 10%
20	AT	110	 95% 5%
21	AU	100	 93% 7%
22	AV	104	 95% . .
23	AW	94	 91% 9%
24	AX	85	 93% 6% .
25	AY	78	 96% . .
26	AZ	63	 86% 13% .
27	Aa	59	 92% 7% .
28	Ab	70	 89% 11%
29	Ac	57	 88% 11% .
30	Ad	55	 93% 5% .
31	Ae	46	 87% 13%
32	Af	65	 95% . .
33	Ag	38	 95% 5%
34	BA	1542	 25% 50% 21% .

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
35	BB	76	 38% 47% 9% 5%
35	BE	76	 34% 41% 21% .
36	BC	393	 96% .
37	BD	24	 21% 50% 25% .
38	BF	241	 94% 6%
39	BG	233	 92% 7%
40	BH	206	 94% 6%
41	BI	167	 92% 8% .
42	BJ	135	 94% 6%
43	BK	179	 93% 7% .
44	BL	130	 93% 6% .
45	BM	130	 90% 9% .
46	BN	103	 86% 14%
47	BO	129	 94% 5% .
48	BP	124	 92% 7% .
49	BQ	118	 96% . .
50	BR	101	 84% 14% . .
51	BS	89	 97% . .
52	BT	82	 98% .
53	BU	84	 96% . .
54	BV	75	 87% 9% . .
55	BW	92	 92% 5% . .
56	BX	87	 97% . .
57	BY	71	 85% 14% .

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 153634 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 ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

- Molecule 2 is a RNA chain called ribosomal RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

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

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

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

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

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

- Molecule 10 is a protein called 50S ribosomal protein L11.

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

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	103	Total	C	N	O	S	0	0
			789	498	148	143			

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ab	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	54	Total	C	N	O	S	0	0
			441	284	81	76			

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 35 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	BB	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		
35	BE	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		

- Molecule 36 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	BC	393	Total	C	N	O	S		0	0
			3036	1918	523	582	13			

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	BD	24	Total	C	N	O	P		0	0
			495	222	68	181	24			

- Molecule 38 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	BF	240	Total	C	N	O	S		0	0
			1872	1180	332	352	8			

- Molecule 39 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	BG	232	Total	C	N	O	S		0	0
			1822	1149	346	323	4			

- Molecule 40 is a protein called 30S ribosomal protein S4.

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

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	BI	166	Total	C	N	O	S		0	0
			1225	761	232	226	6			

- Molecule 42 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BJ	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BK	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 44 is a protein called 30S ribosomal protein S8.

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

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BM	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BN	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BO	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 48 is a protein called 30S ribosomal protein S12.

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

- Molecule 49 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BQ	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 50 is a protein called 30S ribosomal protein S14.

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

- Molecule 51 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BS	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 52 is a protein called 30S ribosomal protein S16.

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

- Molecule 53 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BU	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 54 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BV	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 55 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BW	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 56 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BX	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 57 is a protein called 30S ribosomal protein S21.

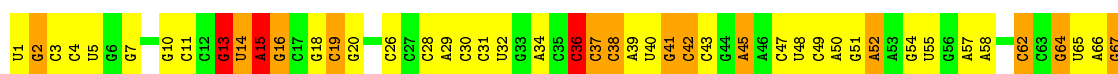
Mol	Chain	Residues	Atoms					AltConf	Trace
57	BY	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

### 3 Residue-property plots

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

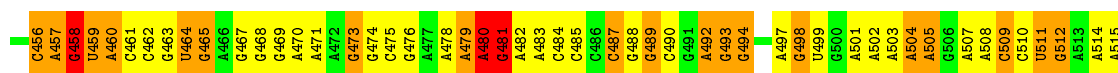
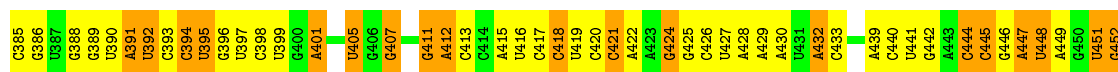
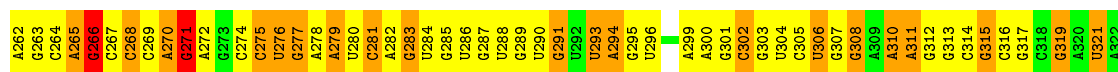
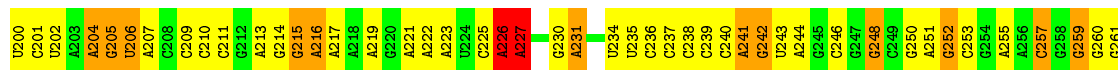
#### • Molecule 1: ribosomal RNA 5S

Chain AA: 



#### • Molecule 2: ribosomal RNA 23S

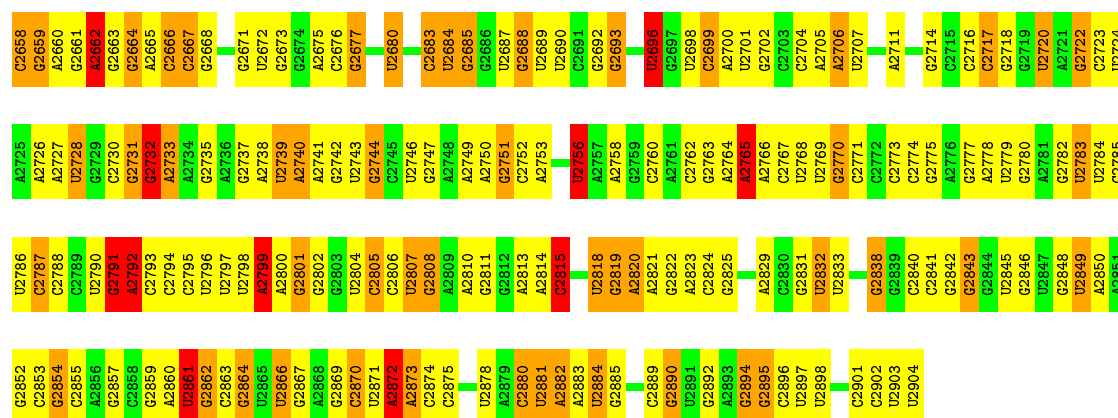
Chain AB: 



A1549	C1550	A1551	A1552	A1553	A1554	A1555	C1558	A1559	G1560	C1561	A1562	A1563	A1564	C1565	A1566	A1567	A1568	A1569	A1570	A1571	A1572	G1573	G1574	C1575	A1576	C1577	A1578	A1579	A1580	C1581	A1582	A1583	A1584	A1585	C1586	C1587	G1588	A1589	A1590	A1591	A1592	A1593	A1594	A1595	A1596	A1597	A1598	A1599	A1600	G1601	A1602	A1603	C1604	C1605	C1606	C1607	A1608	A1609		
U1486	U1487	C1488	C1489	A1490	A1491	A1492	C1493	A1494	A1495	A1496	A1497	A1498	G1499	A1500	A1501	A1502	A1503	A1504	A1505	U1506	A1507	A1508	A1509	A1510	A1511	C1512	A1513	A1514	A1515	A1516	U1520	G1521	A1522	A1523	A1524	A1525	C1526	A1527	A1528	A1529	A1530	C1531	A1532	C1533	A1534	A1535	A1536	A1537	A1538	U1539	C1540	A1541	A1542	A1543	A1544	A1545	A1546	A1547	A1548	A1549
G1416	C1417	G1418	A1419	A1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	A1433	A1434	G1435	G1436	G1437	U1440	G1441	U1442	U1443	U1444	U1445	U1446	C1447	G1448	C1451	G1452	A1453	C1454	A1455	G1389	G1390	U1457	U1458	U1459	U1460	C1461	C1462	C1463	U1467	G1471	C1472	G1473	U1474	G1475	U1476	A1477	G1478	G1479	C1480	U1481	G1482	A1483	U1484	U1485					
A1353	A1354	G1355	G1356	C1357	G1358	A1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	A1372	A1373	G1374	U1375	G1376	G1377	A1378	C1379	G1380	G1381	G1382	A1383	A1384	A1385	U1389	A1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	C1398	C1399	U1400	U1401	U1402	A1403	C1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	
A1286	A1287	G1288	G1289	C1290	G1291	C1292	C1293	U1294	C1295	G1296	C1297	C1298	G1299	G1300	A1301	A1302	G1303	A1304	C1305	C1306	A1307	A1308	G1309	G1310	U1313	U1316	G1317	G1318	A1321	G1324	U1325	U1326	A1327	C1330	G1331	G1332	G1333	G1334	C1335	G1338	G1339	G1340	U1343	U1344	G1345	G1346	A1347	C1348	C1349	C1350	C1351	C1352								
U1219	G1220	C1221	U1222	G1223	U1224	G1225	A1226	G1227	G1228	C1229	A1230	U1231	G1232	U1233	A1234	G1235	G1236	A1237	G1238	U1241	U1242	C1243	A1244	G1245	A1246	U1247	G1248	U1249	G1250	A1254	U1255	G1256	C1257	U1258	C1261	A1262	U1263	G1266	U1267	A1268	G1271	A1272	U1275	A1276	G1277	C1278	G1279	G1280	G1281	U1282	G1283	A1285								
U1159	U1160	G1161	A1096	U1097	G1163	C1164	A1165	U1166	C1167	G1170	U1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	U1184	G1185	G1186	G1187	U1188	A1189	G1190	U1191	G1192	G1193	A1194	G1195	C1196	G1197	U1198	U1199	C1200	U1201	G1202	U1203	A1204	G1206	C1207	C1208	U1209	G1210	C1211	G1212	A1213	A1214	G1215	G1216	G1217	G1218			
G1093	U1094	A1095	U1033	G1034	U1035	G1036	G1037	G1038	A1039	A1040	G1041	G1042	C1045	A1053	A1054	G1055	G1056	A1057	U1058	G1059	U1060	U1061	G1062	G1063	C1064	U1065	U1066	A1067	G1068	A1069	C1070	G1071	C1072	A1073	G1074	C1075	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	U1086	G1087	A1088	G1091	C1092	G1093	G1094							
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
A1029	U967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974	A975	G976	G977	A978	A979	A980	A981	C982	U919	A920	A983	A984	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	G938	A941	G942	A943	A945	C946	C948	G949	U1010	U1011	U1012	U1013	A1014	U1015	G1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	G1024	G1025	G1026	A1028
U0966	U0967	C968	U906	G907	U908	A972	A973	A974																																																				

U2593	G3529	C2463	U2393	A2199	C2129	G2065	A2003	U1939	G1875	G1813	U1747	C1685	A1610
C2594	A2530	G2464	C2394	C2200	U2130	C2066	G2004	U1940	A1876	C1816	C1748	C1686	C1611
G2595	C2531	C2465	C2395	G2201	U2131	G2067	A2005	C1941	A1877	G1817	A1749	G1687	C1612
U2596	G2532	A2466	G2396	U2202	U2132	U2068	C2006	G1878	C1877	U1818	U1750	U1688	G1613
G2597	U2533	C2467	G2397	G2203	G2133	C2069	C2007	U1879	U1819	U1751	C1752	U1689	A1614
A2598	C2534	C2468	U2398	G2204	A2134	A2071	A2009	U1880	U1880	A1819		A1690	C1615
G2599	G2535	A2471	G2399	A2205	A2135	C2072	G2010	C1881	C1881	U1820	A1755	A1691	A1616
A2600	U2537	U2472	G2400	C2206	A2136	C2073	G2011	U1947	U1882	A1821		U1692	G1619
G2601	U2538	U2473	U2401	C2207	U2137	U2074	G2012	U1951	A1884	C1822	G1756	U1693	G1620
A2602	C2539	U2474	U2402	C2208	U2138	U2075		A1952	A1952	U1825	A1758	U1694	U1621
	C2539	G2475	C2403	G2209	U2139	U2076		A1953	G1885	U1826		G1695	G1622
	C2540	U2476	U2404	A2212	U2140	C2077	A2015	G1954	C1886	U1827	G1761	G1696	G1623
C2606	A2541	U2477	G2405	G2213	G2140	U2078	U2016	C1887	G1887	G1828	A1762		U1624
	A2542	A2478	A2406	U2214	C2145	A2079	U2017	G1888	G1888			G1699	
C2610	G2543	U2479	U2407	C2215	A2146	A2080	G2018	A1889	A1889	G1829	C1763	A1700	G1627
C2611	C2544	U2480	U2408	C2216	A2147	U2081	A2019	U1956	U1956	A1830	C1764	U1701	G1628
U2613	A2547	G2483	A2411	G2218	C2150	G2083	C2021	A1960	G1891	G1831	C1765	U1702	A1629
A2614	U2548	G2484	G2415	U2219		G2084	U2022	C1961	C1892	G1832	G1766	G1703	A1630
U2615	G2549	G2485	G2416	U2220	G2156	U2085	C2023	C1962	G1893	C1833	G1767	G1704	A1631
C2616	G2550		C2417	U2221	U2157	U2086	G2024	U1963		G1834	C1768	A1705	G1632
			U2418	G2222	A2158	G2087	C2025	C1964	U1898	C1836	A1773	G1706	C1638
G2618	U2553	G2488	C2419	U2223	C2159	U2088	U2026	A1966	A1899	C1837	C1774	G1707	C1639
U2619	U2554	U2489	G2420	G2224	C2160	C2089	G2027	C1967	A1900	C1838	U1775	U1708	C1640
C2620	G2555	G2490	A2418	G2225	C2161	U2090	U2028	C1968	A1901	G1839	G1776	U1709	A1641
G2621	U2556	U2491	U2419	G2226	G2162	C2091	G2029	U1969	U1902	G1840	U1777	G1710	
U2622	C2557	U2492	C2420	A2227	A2163	U2092		A1970	G1903	U1841	U1778	A1711	G1642
	C2558	U2493	U2423	G2228	C2164	A2094	G2030	U1971	U1971	C1843	U1779	G1714	G1643
C2625	C2559	G2494	C2424	U2229			G2031	U1972	A1848	G1844	U1780	G1715	C1644
G2626	U2560	G2495	A2425	G2230	G2168	A2097	A2033	G1906	G1906	G1845	U1781	U1716	G1645
C2627	A2561	C2357	U2426	U2231	A2169	U2098	G2034	G1907	G1907	G1846	U1782	U1717	C1646
G2628	C2358	C2359	C2427	G2232	A2170	U2099	G2035	C1908	C1908	U1847	U1783	A1718	U1647
U2629	U2563		U2428	U2233	A2171		C2036	U1976	A1849	C1842	A1784	U1719	U1648
G2630	A2564	C2362	C2429	G2234	U2172	G2102	U2039	A1977	A1912	G1849	A1785	G1720	G1649
C2631	U2565	G2363	U2430	U2235	A2173	C2103	G2040	U1978	A1913	U1850	A1786	G1721	A1652
A2632	A2566	C2364	A2431	G2236	C2174	C2104	U2041	U1979	C1914	G1851	A1787	G1722	G1653
G2633	G2567	G2365	U2432	U2237	C2175	U2105	A2042	G1980	G1915	U1852	C1788	G1723	A1654
A2634	U2568	C2366	A2433	G2238	A2176	U2106	C2043	A1981	U1916	A1853	A1789	G1724	A1655
C2635	G2569	G2367	U2434	U2239	C2177	G2107	C2044	U1982	U1917	U1854	C1790	U1725	G1656
				U2240	U2178	U2108	C2045	G1983	A1918	U1855	A1791	C1726	U1657
C2636	U2570	G2370	U2435	G2241	C2179	U2109	G2046	G1984	A1919	U1856	G1792	C1727	C1658
G2637	G2571		A2436	U2242	U2180	G2110	C2047	C1985	C1920	G1857	U1728	U1729	U1662
U2638	A2572	C2374	U2438	U2243	U2181	G2111	U2048	A1986	G1921	A1858	U1796	C1730	G1663
C2639	G2573	G2375	A2439	U2244	U2182	G2112	G2049	A1987		U1859	G1797	C1731	A1664
G2640	U2574	A2376	U2440	U2245	U2183	U2113	C2050	U1988	C1924	G1860	U1798	G1732	A1665
C2641	C2575	A2377	U2441	U2246	U2184	A2114	A2051	G1989	C1925	G1861	U1799	C1733	G1666
	G2576	U2378	G2442	U2247	U2185	G2115	U2052	C1990	U1926	G1862	C1800	G1734	
G2642	A2577	C2379	G2443	U2248	G2186	G2116	A2053	U1991	A1927	G1863	A1801	A1735	C1670
C2643	C2578	A2380	U2444	U2249	U2187	A2117	C2054	G1992	A1928	U1864	A1802	U1736	U1671
G2644	U2579	G2381	U2445	U2250	U2188	U2118	C2055	U1993	G1929	U1865	A1803	G1737	A1672
C2645	G2580	U2382	A2446	U2251	U2189	A2119	C2056	C1994	C1930	A1866	C1804	G1738	G1673
G2646	U2581	G2383	U2447	U2252	U2190	G2120	G2057	U1995	C1926	G1867	A1805	U1739	A1674
U2647	A2582	U2384	G2448	U2253	A2191	U2121	A2058	C1996	A1932	C1868	C1806	G1740	C1675
C2648	U2583	G2385	U2449	U2254	U2192	G2122	C2059	C1997	G1933	G1869	G1807	C1741	A1676
G2649	G2584	A2386	U2450	U2255	G2193	G2123	A2060	A1998	C1934	C1870	A1808	U1742	A1677
C2650	U2585	U2387	A2451	U2256	U2194	G2124	G2061	C1999	G1935	A1871	A1809	U1743	A1678
G2651	C2586	U2388	U2452	U2257	U2195	G2125	A2062	C2000	U1936	A1872	A1810	G1744	U1679
C2652	U2587	U2389	U2453	U2258	U2196	A2126	C2063	C2001	A1937	G1873	G1811		
U2653	G2588	U2390	U2454	U2259	U2197	G2127	G2064	G2002	A1938	C1874	U1812		
A2654	C2589	A2391	U2455	U2260	U2198	G2128							
G2655	U2590	C2392	C2456	U2261	A2198								
C2656	G2591	U2393	U2457	U2262	U2199								
A2657	U2592	C2394	U2458	U2263	U2200								





- Molecule 3: 50S ribosomal protein L1

Chain AC: 93% 7%



- Molecule 4: 50S ribosomal protein L2

Chain AD: 92% 7%



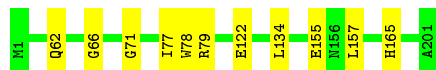
- Molecule 5: 50S ribosomal protein L3

Chain AE: 92% 8%



- Molecule 6: 50S ribosomal protein L4

Chain AF: 95% 5%



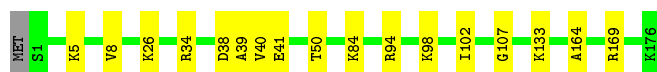
- Molecule 7: 50S ribosomal protein L5

Chain AG: 92% 7% ..



- Molecule 8: 50S ribosomal protein L6

Chain AH: 90% 10% •



- Molecule 9: 50S ribosomal protein L9

Chain AI: 90% 9%



- Molecule 10: 50S ribosomal protein L11

Chain AJ: 96%



- Molecule 11: 50S ribosomal protein L13

Chain AK: 96%



- Molecule 12: 50S ribosomal protein L14

Chain AL: 90% 10%



- Molecule 13: 50S ribosomal protein L15

Chain AM: 96%



- Molecule 14: 50S ribosomal protein L16

Chain AN: 93% 6%



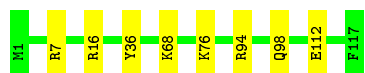
- Molecule 15: 50S ribosomal protein L17

Chain AO: 97%



- Molecule 16: 50S ribosomal protein L18

Chain AP:  93% 7%



- Molecule 17: 50S ribosomal protein L19

Chain AQ:  90% 8% ..



- Molecule 18: 50S ribosomal protein L20

Chain AR:  91% 8% .



- Molecule 19: 50S ribosomal protein L21

Chain AS:  90% 10%



- Molecule 20: 50S ribosomal protein L22

Chain AT:  95% 5%



- Molecule 21: 50S ribosomal protein L23

Chain AU:  93% 7%



- Molecule 22: 50S ribosomal protein L24

Chain AV:  95% . .



- Molecule 23: 50S ribosomal protein L25

Chain AW:  91% 9%



- Molecule 24: 50S ribosomal protein L27

Chain AX:  93% 6%




- Molecule 25: 50S ribosomal protein L28

Chain AY:  96%



- Molecule 26: 50S ribosomal protein L29

Chain AZ:  86% 13%



- Molecule 27: 50S ribosomal protein L30

Chain Aa:  92% 7%



- Molecule 28: 50S ribosomal protein L31

Chain Ab:  89% 11%



- Molecule 29: 50S ribosomal protein L32

Chain Ac:  88% 11%



- Molecule 30: 50S ribosomal protein L33

Chain Ad:  93% 5%



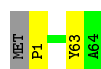
- Molecule 31: 50S ribosomal protein L34

Chain Ae: 87% 13%



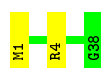
- Molecule 32: 50S ribosomal protein L35

Chain Af: 95% 5%



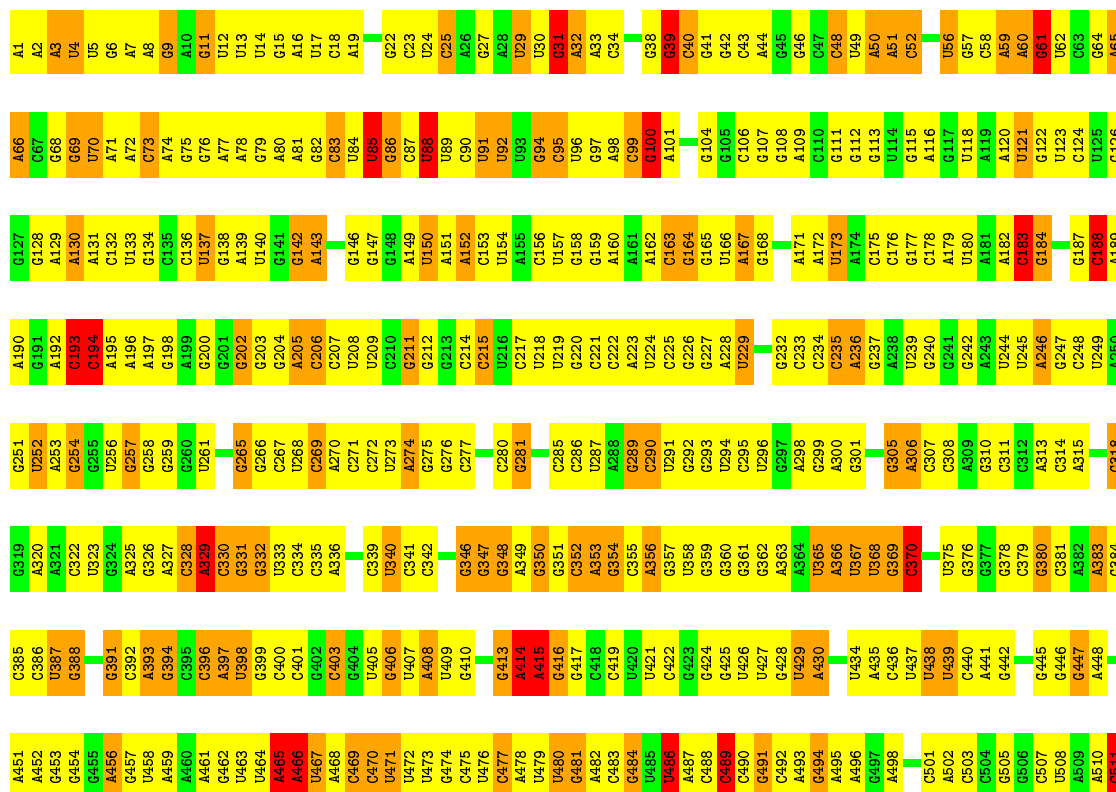
- Molecule 33: 50S ribosomal protein L36

Chain Ag: 95% 5%



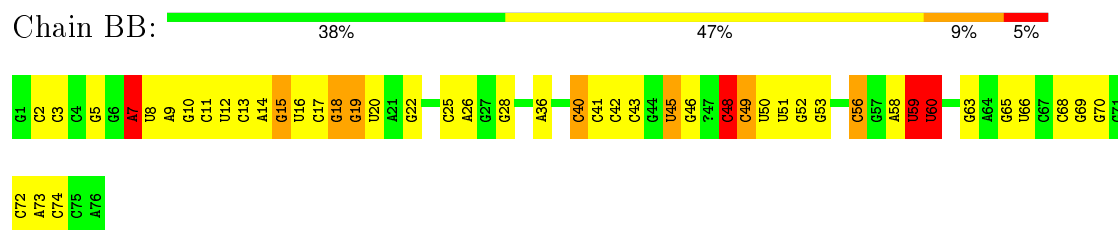
- Molecule 34: 16S ribosomal RNA

Chain BA: 25% 50% 21%

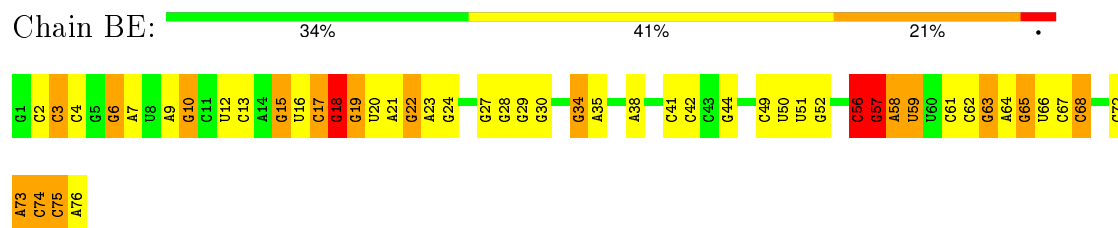


A1434	G1435	A1362	G1297	G1226	C1158	C1096	G1033	A968	U904	C841	A777	A715	G649	C582	U512
G1436	A1363	A1227	U1298	A1228	U1189	C1097	G1034	A969	U905	U842	G778	A718	G650	A583	G517
U1437	A1364	C1228	C1098	C1160	G1160	C1098	A1035	C970	A906	U843	G779	A719	G651	G584	C518
A1438	G1365	A1229	G1300	C1161	C1161	G1099	A1036	G971	A907	G844	A780	A720	U652	G585	C519
G1439	C1366	G1230	U1301	C1162	C1162	C1100	G1037	A908	A908	A845	A781	G720	G653	C586	A520
U1440	C1302	G1231	C1303	A1163	A1163	A1101	C1038	A909	A909	G846	A782	G721	G654	G587	C521
G1441	G1304	U1232	C1304	G1164	G1164	A1102	G1039	A975	C910	G847	C783	G722	G655	G588	C522
A1442	G1305	G1233	G1305	U1165	U1165	C1103	U1040	G976	U911	C848	A194	U723	G656	U589	C523
C1443	C1234	C1234	C1234	G1166	G1166	G1104	A1042	A977	C912	G849	G724	G724	G657	U590	A524
U1444	U1235	U1235	U1235	A1167	A1167	A1105	A1043	A978	A913	G850	G785	G725	G660	U591	C525
G1445	A1306	U1307	A1307	U1168	U1168	G1106	G1043	C979	A914	G851	A786	C726	G661	G592	C526
U1446	U1308	U1308	U1308	U1169	U1169	C1107	A1044	C980	A915	U854	U788	G727	U662	U593	C527
A1447	G1309	G1241	G1309	A1170	A1170	G1108	C1045	U981	U916	U855	A789	A728	U663	U594	C528
A1448	G1310	G1242	G1310	A1171	A1171	C1109	A1046	U982	G917	U856	A790	A729	G664	A595	C529
G1449	A1311	G1243	A1311	C1172	C1172	A1110	G1047	A983	A918	C857	G791	G730	G665	A596	G530
U1450	U1173	G1244	U1173	U1173	U1173	A1111	G1048	C984	A919	G858	A792	G731	G666	G597	U531
U1451	C1313	U1313	C1313	U1174	U1174	C1112	U1049	C985	U920	G859	U793	C732	U598	U532	A533
C1452	U1314	G1249	C1314	A1176	A1176	U1115	G1050	U986	U921	G860	A794	G733	G668	C599	A534
G1453	U1315	A1250	U1315	G1177	G1177	U1116	C1051	G987	G922	A860	G795	G734	G670	A600	A535
C1454	G1178	G1255	G1178	G1179	G1179	U1117	U1052	G988	A923	G861	C796	G735	G671	A601	C536
G1455	A1180	A1256	A1180	A1181	A1181	C1118	U1056	U989	G928	G862	C797	G736	G672	A602	C537
A1456	C1138	A1257	C1138	G1182	G1182	C1119	G1057	U991	C930	U863	A798	C737	A673	U603	C538
G1457	U1320	G1258	U1320	U1183	U1183	C1120	G1058	U992	C931	A865	C738	C738	A674	G604	C539
C1458	C1321	G1259	C1321	U1184	U1184	U1121	G1059	G993	C932	A866	C739	C739	A675	A607	C540
U1459	G1322	G1260	G1322	G1184	G1184	U1122	U1060	A994	C933	G867	U740	G741	U677	A608	C541
C1460	G1323	A1261	G1323	U1185	U1185	U1123	G1061	C995	G934	C868	G742	G742	U678	A609	C542
G1461	U1326	C1262	U1326	G1179	G1179	C1124	U1062	A996	C935	G869	A743	A743	G682	C612	C543
C1462	U1327	U1263	U1327	U1180	U1180	U1125	C1063	U997	A936	U870	C744	C744	G683	C613	C544
G1463	C1327	U1264	C1327	G1181	G1181	U1126	G1064	C998	C936	U871	C745	C745	G684	C614	C545
U1464	A1318	A1258	A1318	A1191	A1191	C1127	U1065	C999	A937	A872	A746	A746	U685	A546	C546
A1465	G1387	G1265	G1387	C1192	C1192	C1128	C1066	A1000	A938	A873	C810	A747	G686	C618	C547
C1466	U1398	C1266	U1398	G1193	G1193	C1129	A1067	C1001	G939	G874	C811	A748	U687	U619	C548
U1467	A1333	G1268	A1333	U1194	U1194	A1130	C1068	G1002	C940	U875	A749	A749	A688	C620	C549
C1468	C1335	U1270	C1335	G1197	G1197	C1132	G1069	G1003	G941	C876	C750	C750	G689	A621	C550
G1469	U1336	A1271	U1336	U1199	U1199	G1134	U1071	A1005	U942	A814	C751	C751	G690	A622	C551
U1470	C1337	G1272	C1337	C1200	C1200	G1135	G1072	G1006	U944	A815	G752	G752	G691	C623	C552
C1471	G1338	C1273	G1338	U1201	U1201	U1136	U1073	U1007	A945	C880	A816	A753	U692	C624	C553
A1408	A1340	G1276	A1340	U1202	U1202	C1137	U1074	U1008	A946	G881	C817	C756	G693	U625	C554
C1409	U1341	U1277	U1341	C1203	C1203	G1138	U1075	U1009	C947	C882	A818	C757	A694	G628	C555
G1410	G1342	G1278	G1342	U1204	U1204	G1139	U1076	U1010	U948	C883	A819	C758	A695	A562	C556
A1411	C1343	G1279	C1343	U1205	U1205	C1140	U1077	A949	U950	U884	U820	C759	U697	A563	C557
C1412	U1344	A1280	U1344	G1206	G1206	C1141	U1078	A951	C951	G886	U822	C760	G699	C564	C558
U1413	G1345	C1281	U1345	U1212	U1212	G1142	A1080	G952	U952	G887	C823	G761	G700	U565	C559
G1414	A1346	U1282	A1346	C1214	C1214	G1143	U1081	A1016	U955	G888	U827	U762	G701	U636	C560
C1415	U1283	G1283	U1283	G1215	G1215	G1144	U1082	U1017	U956	U889	U828	C763	A702	C637	C561
A1416	G1284	C1284	G1284	G1216	G1216	G1145	U1083	G1018	U957	U890	G829	C764	G703	U638	C562
G1417	A1285	A1285	A1285	U1217	U1217	C1147	G1084	A1019	U958	A892	G830	G765	A704	G639	C563
U1418	U1288	C1217	U1288	C1218	C1218	U1148	U1085	G1020	A958	C893	A768	G768	G705	U640	C564
C1419	A1289	A1219	A1289	A1150	A1150	C1149	U1086	A1021	A959	C896	C769	C770	A641	A572	C565
G1420	G1290	G1290	G1290	A1151	A1151	U1149	G1089	A1022	U960	C897	C771	C771	U642	A573	C566
A1421	U1291	G1291	U1291	A1152	A1152	C1150	U1090	U1025	U961	G898	U772	U772	U643	C567	C567
C1422	G1292	G1292	G1292	A1153	A1153	G1151	U091	G1026	C962	C899	G773	G773	U644	G645	C568
U1423	C1293	G1293	C1293	G1154	G1154	C1152	A1092	C1027	A964	A900	G774	G774	G646	G577	C569
G1424	U1294	G1294	U1294	A1155	A1155	U1156	A1093	G1028	U965	A901	G775	G775	G647	C578	C570
U1425	C1295	G1295	C1295	U1156	U1156	C1157	G1094	C1029	G966	G902	G776	G776	G648	A579	C571
A1426	A1296	C1296	A1296	A1157	A1157	U1157	U1095	G1032	C967	G903	C840	C840	G649	A580	C572

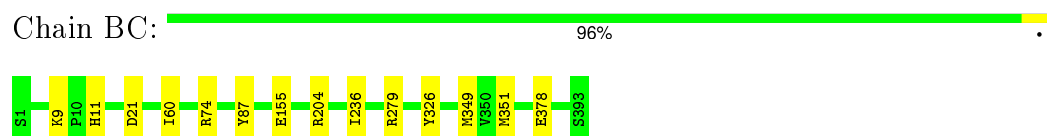
• Molecule 35: A/T-site tRNA Phe



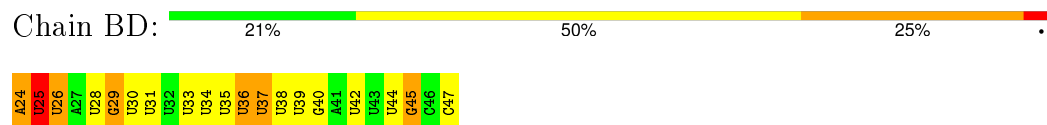
- Molecule 35: A/T-site tRNA Phe



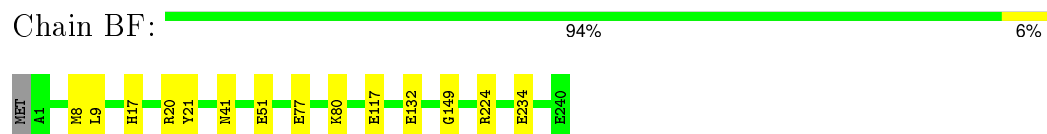
- Molecule 36: Elongation factor Tu 2



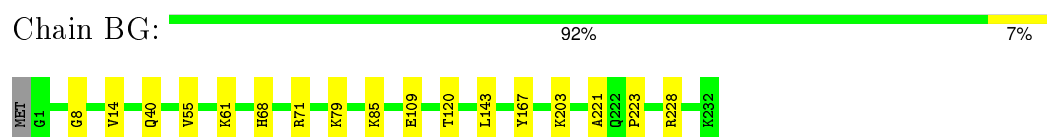
- Molecule 37: mRNA



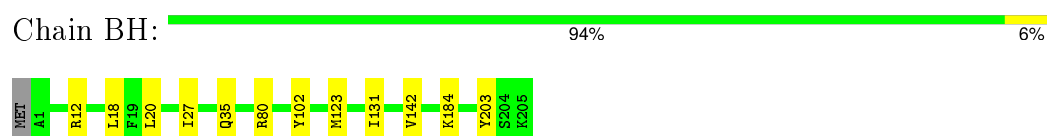
- Molecule 38: 30S ribosomal protein S2



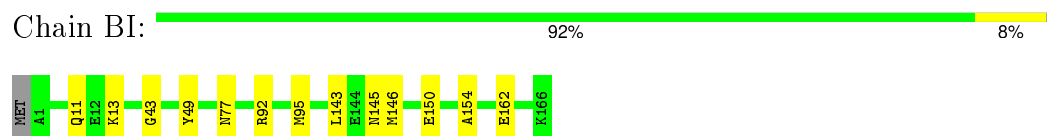
- Molecule 39: 30S ribosomal protein S3



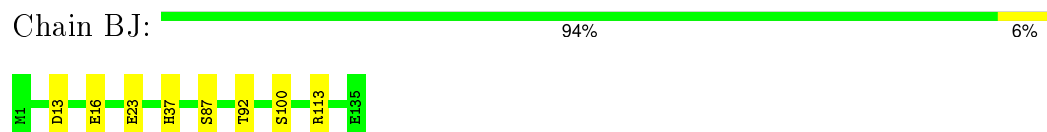
- Molecule 40: 30S ribosomal protein S4



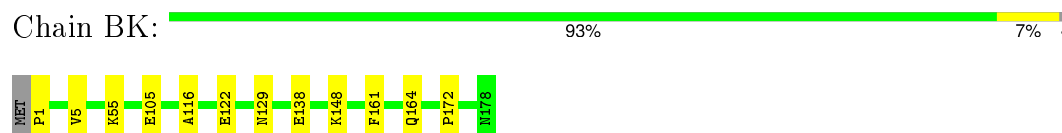
- Molecule 41: 30S ribosomal protein S5



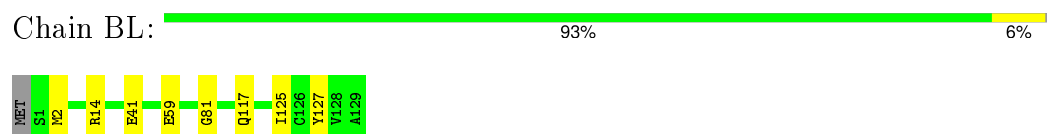
- Molecule 42: 30S ribosomal protein S6



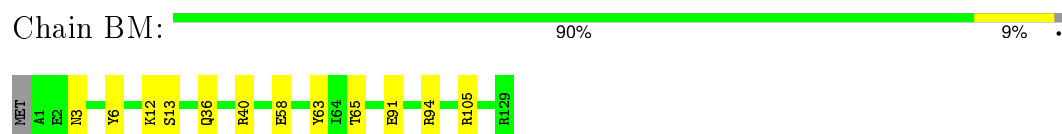
- Molecule 43: 30S ribosomal protein S7



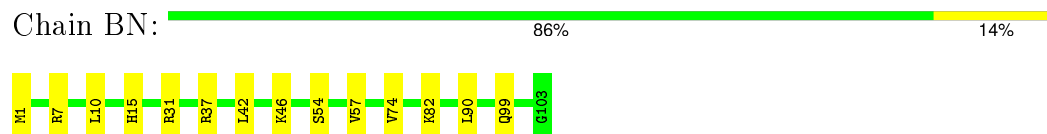
- Molecule 44: 30S ribosomal protein S8



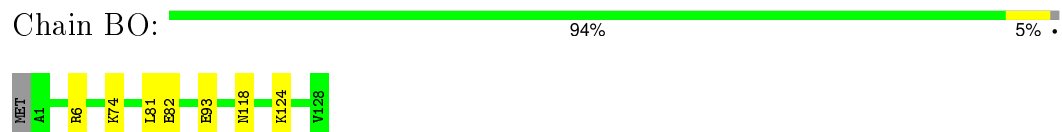
- Molecule 45: 30S ribosomal protein S9



- Molecule 46: 30S ribosomal protein S10



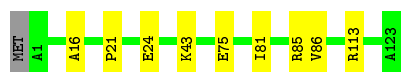
- Molecule 47: 30S ribosomal protein S11



- Molecule 48: 30S ribosomal protein S12



Chain BP:  92% 7% .




- Molecule 49: 30S ribosomal protein S13

Chain BQ:  96% ..



- Molecule 50: 30S ribosomal protein S14

Chain BR:  84% 14% ..



- Molecule 51: 30S ribosomal protein S15

Chain BS:  97% ..



- Molecule 52: 30S ribosomal protein S16

Chain BT:  98% .




- Molecule 53: 30S ribosomal protein S17

Chain BU:  96% ..



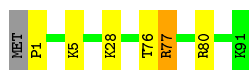
- Molecule 54: 30S ribosomal protein S18

Chain BV:  87% 9% . .



- Molecule 55: 30S ribosomal protein S19

Chain BW:  92% 5% ..



- Molecule 56: 30S ribosomal protein S20

Chain BX: 97% ..



- Molecule 57: 30S ribosomal protein S21

Chain BY: 85% 14% .



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 5MU, CH, OMG, OMU, MA6, MIA, OMC, 1MG, H2U, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, 3AU, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	AA	1.18	0/2869	2.04	104/4474 (2.3%)
10	AJ	0.57	0/1046	0.92	0/1410
11	AK	0.63	0/1152	0.99	0/1551
12	AL	0.57	0/956	1.00	0/1279
13	AM	0.60	0/1062	1.01	0/1413
14	AN	0.63	0/1093	1.05	1/1460 (0.1%)
15	AO	0.61	0/1021	1.03	0/1364
16	AP	0.60	0/910	1.00	0/1219
17	AQ	0.61	0/929	1.06	0/1242
18	AR	0.67	0/960	1.02	1/1278 (0.1%)
19	AS	0.62	0/829	1.01	0/1107
2	AB	1.17	0/69257	1.96	2261/108040 (2.1%)
20	AT	0.52	0/864	0.96	0/1156
21	AU	0.55	0/794	0.99	0/1060
22	AV	0.56	0/797	1.03	0/1062
23	AW	0.60	0/766	0.97	0/1025
24	AX	0.64	0/642	1.09	0/848
25	AY	0.64	0/635	1.06	0/848
26	AZ	0.56	0/510	1.10	1/677 (0.1%)
27	Aa	0.54	0/453	0.98	0/605
28	Ab	0.63	0/559	1.17	2/745 (0.3%)
29	Ac	0.59	0/450	1.05	0/599
3	AC	0.56	0/1748	0.96	1/2355 (0.0%)
30	Ad	0.61	0/448	1.00	0/594
31	Ae	0.63	0/380	1.11	1/498 (0.2%)
32	Af	0.58	0/513	1.01	1/676 (0.1%)
33	Ag	0.53	0/303	1.00	0/397
34	BA	1.17	1/36769 (0.0%)	1.96	1171/57354 (2.0%)
35	BB	1.23	0/1580	1.96	45/2459 (1.8%)
35	BE	1.20	0/1580	2.05	59/2459 (2.4%)
36	BC	0.61	0/3092	0.96	1/4183 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
37	BD	1.30	0/548	1.88	16/848 (1.9%)
38	BF	0.60	0/1904	1.00	0/2565
39	BG	0.60	0/1852	1.04	0/2490
4	AD	0.60	0/2131	1.07	1/2863 (0.0%)
40	BH	0.63	0/1665	1.02	0/2227
41	BI	0.56	0/1239	1.00	1/1664 (0.1%)
42	BJ	0.61	0/1121	1.05	0/1509
43	BK	0.62	0/1422	1.04	1/1908 (0.1%)
44	BL	0.58	0/989	0.97	0/1326
45	BM	0.65	0/1048	1.03	0/1394
46	BN	0.59	0/835	1.08	0/1127
47	BO	0.61	0/982	1.00	0/1323
48	BP	0.61	0/969	1.09	0/1300
49	BQ	0.57	0/919	1.01	0/1226
5	AE	0.58	0/1586	1.02	0/2134
50	BR	0.63	0/817	1.14	1/1088 (0.1%)
51	BS	0.58	0/724	1.00	1/966 (0.1%)
52	BT	0.63	0/659	1.04	0/884
53	BU	0.58	0/681	0.99	0/913
54	BV	0.71	0/637	1.06	0/851
55	BW	0.60	0/744	1.02	3/995 (0.3%)
56	BX	0.55	0/676	0.91	0/895
57	BY	0.69	0/598	1.17	1/792 (0.1%)
6	AF	0.57	0/1571	0.99	0/2113
7	AG	0.65	0/1444	1.10	4/1937 (0.2%)
8	AH	0.59	0/1343	1.02	0/1816
9	AI	0.57	0/1122	1.01	1/1515 (0.1%)
All	All	1.03	1/165193 (0.0%)	1.75	3679/246106 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	27
11	AK	0	2
15	AO	0	1
17	AQ	0	1
18	AR	0	1
2	AB	0	821
28	Ab	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AC	0	2
30	Ad	0	1
31	Ae	0	2
34	BA	0	473
35	BB	0	12
35	BE	0	15
37	BD	0	4
38	BF	0	1
39	BG	0	2
40	BH	0	2
41	BI	0	3
42	BJ	0	1
43	BK	0	2
45	BM	0	2
47	BO	0	1
48	BP	0	1
5	AE	0	3
50	BR	0	1
54	BV	0	1
55	BW	0	1
57	BY	0	3
6	AF	0	1
8	AH	0	2
9	AI	0	2
All	All	0	1392

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	1535	C	P-O5'	5.14	1.64	1.59

All (3679) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	13	G	O4'-C1'-N9	15.20	120.36	108.20
2	AB	736	C	O4'-C1'-N1	14.43	119.74	108.20
34	BA	465	A	O4'-C1'-N9	13.60	119.08	108.20
2	AB	2832	U	O4'-C1'-N1	12.97	118.58	108.20
34	BA	1152	A	O4'-C1'-N9	12.96	118.57	108.20
1	AA	49	C	O4'-C1'-N1	12.84	118.47	108.20
1	AA	30	C	O4'-C1'-N1	12.65	118.32	108.20
2	AB	2092	U	O4'-C1'-N1	12.43	118.14	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1078	U	O4'-C1'-N1	12.33	118.06	108.20
2	AB	784	G	O4'-C1'-N9	12.14	117.91	108.20
2	AB	1535	A	O4'-C1'-N9	12.04	117.83	108.20
2	AB	2147	A	O4'-C1'-N9	11.81	117.64	108.20
2	AB	1730	C	O4'-C1'-N1	11.50	117.40	108.20
2	AB	1294	U	O4'-C1'-N1	11.35	117.28	108.20
2	AB	323	C	O4'-C1'-N1	11.31	117.25	108.20
2	AB	1701	A	O4'-C1'-N9	11.31	117.25	108.20
2	AB	100	U	O4'-C1'-N1	11.30	117.24	108.20
34	BA	1322	C	O4'-C1'-N1	11.10	117.08	108.20
2	AB	382	A	O4'-C1'-N9	11.09	117.07	108.20
34	BA	792	A	O4'-C1'-N9	11.03	117.02	108.20
2	AB	372	G	O4'-C1'-N9	10.99	116.99	108.20
34	BA	1212	U	O4'-C1'-N1	10.98	116.99	108.20
2	AB	1808	A	O4'-C1'-N9	10.90	116.92	108.20
34	BA	225	C	O4'-C1'-N1	10.85	116.88	108.20
2	AB	1870	C	O4'-C1'-N1	10.84	116.87	108.20
2	AB	2903	U	O4'-C1'-N1	10.77	116.81	108.20
2	AB	2742	G	O4'-C1'-N9	10.72	116.77	108.20
2	AB	2147	A	C1'-O4'-C4'	-10.71	101.33	109.90
2	AB	362	A	O4'-C1'-N9	10.70	116.76	108.20
2	AB	2667	C	O4'-C1'-N1	10.62	116.70	108.20
2	AB	740	C	O4'-C1'-N1	10.62	116.69	108.20
2	AB	2610	C	O4'-C1'-N1	10.59	116.67	108.20
2	AB	316	C	O4'-C1'-N1	10.55	116.64	108.20
2	AB	2666	C	O4'-C1'-N1	10.53	116.63	108.20
2	AB	2276	G	O4'-C1'-N9	10.52	116.62	108.20
2	AB	2637	U	O4'-C1'-N1	10.45	116.56	108.20
2	AB	346	A	O4'-C1'-N9	10.41	116.53	108.20
2	AB	277	G	C1'-O4'-C4'	-10.40	101.58	109.90
2	AB	169	G	O4'-C1'-N9	10.36	116.49	108.20
34	BA	899	C	O3'-P-O5'	-10.35	84.33	104.00
34	BA	1193	G	O4'-C1'-N9	10.34	116.47	108.20
34	BA	593	U	O4'-C1'-N1	10.29	116.43	108.20
34	BA	1435	G	O4'-C1'-N9	10.25	116.40	108.20
2	AB	302	C	O4'-C1'-N1	10.24	116.39	108.20
2	AB	1552	A	O4'-C1'-N9	10.23	116.39	108.20
2	AB	1209	U	O4'-C1'-N1	10.20	116.36	108.20
2	AB	1081	U	O4'-C1'-N1	10.19	116.35	108.20
34	BA	274	A	O4'-C1'-N9	10.17	116.33	108.20
2	AB	105	C	O4'-C1'-N1	10.13	116.31	108.20
2	AB	1195	G	O4'-C1'-N9	10.08	116.26	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	835	U	O4'-C1'-N1	10.05	116.24	108.20
34	BA	664	G	O4'-C1'-N9	10.04	116.23	108.20
2	AB	351	C	O4'-C1'-N1	10.01	116.21	108.20
2	AB	1981	A	O4'-C1'-N9	9.98	116.18	108.20
2	AB	1967	C	O4'-C1'-N1	9.96	116.17	108.20
35	BB	25	C	O4'-C1'-N1	9.95	116.16	108.20
2	AB	1016	G	O4'-C1'-N9	9.94	116.15	108.20
2	AB	2213	U	O4'-C1'-N1	9.93	116.15	108.20
2	AB	1185	G	O4'-C1'-N9	9.91	116.13	108.20
1	AA	118	C	O4'-C1'-N1	9.91	116.13	108.20
34	BA	244	U	O4'-C1'-N1	9.91	116.13	108.20
34	BA	1457	G	O4'-C1'-N9	9.91	116.13	108.20
2	AB	2518	A	O4'-C1'-N9	9.91	116.12	108.20
2	AB	550	C	O4'-C1'-N1	9.87	116.09	108.20
35	BE	17	C	O4'-C1'-N1	9.85	116.08	108.20
2	AB	1542	U	O4'-C1'-N1	9.84	116.07	108.20
2	AB	1647	U	O4'-C1'-N1	9.80	116.04	108.20
2	AB	339	U	O4'-C1'-N1	9.79	116.03	108.20
34	BA	396	C	O4'-C1'-N1	9.78	116.02	108.20
2	AB	1714	U	O4'-C1'-N1	9.75	116.00	108.20
2	AB	1901	A	O4'-C1'-N9	9.70	115.96	108.20
2	AB	1477	A	C5'-C4'-O4'	9.70	120.73	109.10
2	AB	1703	G	O4'-C1'-N9	9.69	115.95	108.20
2	AB	1026	G	O4'-C1'-N9	9.65	115.92	108.20
2	AB	206	U	O4'-C1'-N1	9.64	115.91	108.20
34	BA	277	C	O4'-C1'-N1	9.64	115.91	108.20
34	BA	811	C	O4'-C1'-N1	9.64	115.91	108.20
34	BA	488	C	O4'-C1'-N1	9.62	115.89	108.20
2	AB	744	U	O4'-C1'-N1	9.61	115.89	108.20
34	BA	834	U	O4'-C1'-N1	9.61	115.89	108.20
2	AB	876	C	O4'-C1'-N1	9.58	115.86	108.20
34	BA	936	C	O4'-C1'-N1	9.58	115.86	108.20
34	BA	532	A	O4'-C1'-N9	9.56	115.85	108.20
2	AB	512	G	O4'-C1'-N9	9.54	115.83	108.20
2	AB	614	A	O4'-C1'-N9	9.54	115.83	108.20
2	AB	1443	U	O4'-C1'-N1	9.53	115.82	108.20
34	BA	214	C	O4'-C1'-N1	9.52	115.81	108.20
34	BA	379	C	O4'-C1'-N1	9.51	115.81	108.20
34	BA	1540	U	O4'-C1'-N1	9.51	115.81	108.20
34	BA	1071	C	O4'-C1'-N1	9.49	115.79	108.20
34	BA	29	U	O4'-C1'-N1	9.49	115.79	108.20
34	BA	158	G	O4'-C1'-N9	9.46	115.77	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	52	A	O4'-C1'-N9	9.46	115.77	108.20
2	AB	1245	G	O4'-C1'-N9	9.46	115.77	108.20
34	BA	770	C	O4'-C1'-N1	9.46	115.76	108.20
34	BA	842	U	O4'-C1'-N1	9.44	115.75	108.20
34	BA	890	G	O4'-C1'-N9	9.40	115.72	108.20
1	AA	93	C	O4'-C1'-N1	9.39	115.71	108.20
2	AB	546	U	O4'-C1'-N1	9.38	115.70	108.20
2	AB	2707	U	O4'-C1'-N1	9.35	115.68	108.20
2	AB	1293	C	O4'-C1'-N1	9.33	115.67	108.20
2	AB	1520	U	O4'-C1'-N1	9.33	115.66	108.20
2	AB	2684	U	O4'-C1'-N1	9.32	115.66	108.20
2	AB	354	A	O4'-C1'-N9	9.32	115.65	108.20
34	BA	465	A	C1'-O4'-C4'	-9.31	102.45	109.90
7	AG	132	ARG	NE-CZ-NH2	9.31	124.95	120.30
34	BA	1232	U	O4'-C1'-N1	9.30	115.64	108.20
2	AB	2465	C	O4'-C1'-N1	9.26	115.61	108.20
2	AB	268	C	O4'-C1'-N1	9.26	115.61	108.20
2	AB	2098	U	O4'-C1'-N1	9.26	115.61	108.20
2	AB	1729	U	O4'-C1'-N1	9.25	115.60	108.20
2	AB	1394	U	C5'-C4'-C3'	-9.24	101.21	116.00
2	AB	39	G	O4'-C1'-N9	9.22	115.58	108.20
2	AB	1816	C	O4'-C1'-N1	9.22	115.58	108.20
34	BA	408	A	O4'-C1'-N9	9.22	115.58	108.20
2	AB	921	C	O4'-C1'-N1	9.20	115.56	108.20
2	AB	1102	C	O4'-C1'-N1	9.18	115.55	108.20
2	AB	276	U	O4'-C1'-N1	9.18	115.54	108.20
2	AB	1409	U	O4'-C1'-N1	9.18	115.54	108.20
2	AB	70	G	O4'-C1'-N9	9.16	115.53	108.20
34	BA	1449	C	O4'-C1'-N1	9.16	115.53	108.20
2	AB	321	U	O4'-C1'-N1	9.15	115.52	108.20
2	AB	2226	C	O4'-C1'-N1	9.15	115.52	108.20
34	BA	798	U	O4'-C1'-N1	9.15	115.52	108.20
1	AA	68	C	O4'-C1'-N1	9.14	115.51	108.20
2	AB	2212	A	O4'-C1'-N9	9.13	115.51	108.20
34	BA	1414	U	O4'-C1'-N1	9.13	115.50	108.20
2	AB	945	A	O4'-C1'-N9	9.12	115.50	108.20
2	AB	2864	G	C5'-C4'-C3'	-9.12	101.41	116.00
34	BA	862	C	O4'-C1'-N1	9.12	115.50	108.20
2	AB	2138	G	O4'-C1'-N9	9.11	115.49	108.20
2	AB	1639	C	O4'-C1'-N1	9.10	115.48	108.20
2	AB	306	U	O4'-C1'-N1	9.10	115.48	108.20
2	AB	2739	U	O4'-C1'-N1	9.10	115.48	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1931	U	O4'-C1'-N1	9.09	115.47	108.20
34	BA	245	U	O4'-C1'-N1	9.04	115.43	108.20
34	BA	375	U	O4'-C1'-N1	9.04	115.43	108.20
2	AB	1578	U	O4'-C1'-N1	9.03	115.42	108.20
34	BA	1541	U	O4'-C1'-N1	9.03	115.43	108.20
2	AB	1849	G	O4'-C1'-N9	9.02	115.42	108.20
2	AB	2188	U	O4'-C1'-N1	9.02	115.42	108.20
2	AB	2855	C	O4'-C1'-N1	9.02	115.42	108.20
34	BA	332	G	O4'-C1'-N9	9.01	115.41	108.20
2	AB	2652	C	O4'-C1'-N1	9.00	115.40	108.20
2	AB	1648	U	O4'-C1'-N1	8.97	115.38	108.20
2	AB	616	A	C5'-C4'-C3'	-8.96	101.66	116.00
2	AB	908	C	O4'-C1'-N1	8.96	115.37	108.20
2	AB	1304	A	O4'-C1'-N9	8.96	115.37	108.20
2	AB	1539	U	O4'-C1'-N1	8.96	115.37	108.20
2	AB	1763	G	O4'-C1'-N9	8.96	115.36	108.20
2	AB	1181	U	O4'-C1'-N1	8.94	115.35	108.20
2	AB	510	C	O4'-C1'-N1	8.92	115.33	108.20
2	AB	1774	C	O4'-C1'-N1	8.92	115.33	108.20
2	AB	365	U	O4'-C1'-N1	8.91	115.33	108.20
2	AB	1444	G	O4'-C1'-N9	8.91	115.33	108.20
34	BA	1141	C	O4'-C1'-N1	8.91	115.33	108.20
2	AB	407	G	O4'-C1'-N9	8.90	115.32	108.20
2	AB	2793	C	O4'-C1'-N1	8.89	115.31	108.20
2	AB	2559	C	O4'-C1'-N1	8.89	115.31	108.20
34	BA	1444	U	O4'-C1'-N1	8.87	115.30	108.20
2	AB	1374	G	O4'-C1'-N9	8.87	115.30	108.20
2	AB	2051	A	O4'-C1'-N9	8.86	115.29	108.20
37	BD	26	U	O4'-C1'-N1	8.85	115.28	108.20
2	AB	2264	C	O4'-C1'-N1	8.84	115.28	108.20
34	BA	90	C	O4'-C1'-N1	8.84	115.27	108.20
34	BA	353	A	O4'-C1'-N9	8.84	115.27	108.20
1	AA	11	C	O4'-C1'-N1	8.83	115.27	108.20
2	AB	279	A	O3'-P-O5'	-8.83	87.22	104.00
2	AB	116	C	O4'-C1'-N1	8.82	115.26	108.20
2	AB	2102	G	O4'-C1'-N9	8.81	115.25	108.20
2	AB	1041	G	O4'-C1'-N9	8.81	115.25	108.20
2	AB	2664	G	C8-N9-C4	-8.81	102.88	106.40
2	AB	236	C	O4'-C1'-N1	8.79	115.23	108.20
34	BA	163	C	O4'-C1'-N1	8.79	115.23	108.20
2	AB	1777	U	O4'-C1'-N1	8.78	115.22	108.20
2	AB	1941	C	O4'-C1'-N1	8.77	115.22	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1067	A	O4'-C1'-N9	8.76	115.20	108.20
2	AB	975	A	C5'-C4'-O4'	8.75	119.60	109.10
34	BA	705	G	O4'-C1'-N9	8.75	115.20	108.20
34	BA	812	G	O4'-C1'-N9	8.74	115.19	108.20
34	BA	1364	U	O4'-C1'-N1	8.74	115.20	108.20
2	AB	1434	A	O4'-C1'-N9	8.74	115.19	108.20
34	BA	69	G	O4'-C1'-N9	8.73	115.19	108.20
2	AB	125	A	C1'-O4'-C4'	-8.70	102.94	109.90
2	AB	2215	C	C5'-C4'-O4'	8.69	119.53	109.10
2	AB	718	A	O4'-C1'-N9	8.69	115.15	108.20
34	BA	1454	G	O4'-C1'-N9	8.69	115.15	108.20
34	BA	1266	G	O4'-C1'-N9	8.68	115.14	108.20
2	AB	1868	C	O4'-C1'-N1	8.68	115.14	108.20
34	BA	815	A	O4'-C1'-C2'	-8.67	97.13	105.80
2	AB	2140	G	O4'-C1'-N9	8.67	115.14	108.20
2	AB	2751	G	O4'-C1'-N9	8.66	115.13	108.20
2	AB	405	U	O4'-C1'-N1	8.66	115.13	108.20
2	AB	1318	U	O4'-C1'-N1	8.66	115.13	108.20
2	AB	870	U	O4'-C1'-N1	8.65	115.12	108.20
2	AB	2391	G	O4'-C1'-N9	8.64	115.11	108.20
34	BA	461	A	O4'-C1'-N9	8.64	115.11	108.20
2	AB	148	U	O4'-C1'-N1	8.64	115.11	108.20
34	BA	658	C	O4'-C1'-N1	8.64	115.11	108.20
2	AB	471	A	O4'-C1'-N9	8.63	115.10	108.20
2	AB	490	C	O4'-C1'-N1	8.62	115.10	108.20
2	AB	2197	U	O4'-C1'-N1	8.62	115.10	108.20
34	BA	677	U	O4'-C1'-N1	8.62	115.09	108.20
34	BA	472	U	O4'-C1'-N1	8.60	115.08	108.20
34	BA	870	U	O4'-C1'-N1	8.59	115.07	108.20
2	AB	1658	C	O4'-C1'-N1	8.58	115.06	108.20
34	BA	1105	A	O4'-C1'-N9	8.58	115.06	108.20
34	BA	1139	G	O4'-C1'-N9	8.58	115.06	108.20
2	AB	1832	C	O4'-C1'-N1	8.57	115.05	108.20
2	AB	934	U	O4'-C1'-N1	8.56	115.05	108.20
35	BE	51	U	O4'-C1'-N1	8.56	115.05	108.20
2	AB	2538	C	O4'-C1'-N1	8.56	115.05	108.20
2	AB	2773	C	O4'-C1'-N1	8.56	115.05	108.20
2	AB	2672	U	O4'-C1'-N1	8.56	115.05	108.20
34	BA	387	U	O4'-C1'-N1	8.55	115.04	108.20
2	AB	1986	C	C5'-C4'-O4'	8.54	119.34	109.10
34	BA	1425	U	O4'-C1'-N1	8.54	115.03	108.20
2	AB	92	U	O4'-C1'-N1	8.54	115.03	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1463	C	O4'-C1'-N1	8.53	115.03	108.20
2	AB	598	U	O4'-C1'-N1	8.52	115.02	108.20
34	BA	955	U	O4'-C1'-N1	8.52	115.02	108.20
2	AB	1851	U	O4'-C1'-N1	8.52	115.02	108.20
2	AB	277	G	P-O3'-C3'	8.50	129.90	119.70
2	AB	1649	G	C5'-C4'-O4'	8.50	119.30	109.10
2	AB	415	A	O4'-C1'-N9	8.49	114.99	108.20
2	AB	1933	G	O4'-C1'-N9	8.48	114.98	108.20
2	AB	2798	U	O4'-C1'-N1	8.48	114.98	108.20
1	AA	13	G	N9-C1'-C2'	-8.47	102.68	112.00
2	AB	1882	U	O4'-C1'-N1	8.47	114.97	108.20
2	AB	1784	A	O4'-C1'-N9	8.46	114.97	108.20
2	AB	1244	A	O4'-C1'-N9	8.46	114.97	108.20
2	AB	1943	U	O4'-C1'-N1	8.44	114.95	108.20
2	AB	1512	C	O4'-C1'-N1	8.43	114.94	108.20
2	AB	331	C	O4'-C1'-N1	8.42	114.93	108.20
2	AB	2175	C	O3'-P-O5'	-8.41	88.03	104.00
2	AB	2807	U	O4'-C1'-N1	8.41	114.92	108.20
2	AB	16	C	O4'-C1'-N1	8.40	114.92	108.20
2	AB	366	C	O4'-C1'-N1	8.40	114.92	108.20
2	AB	2396	G	O4'-C1'-N9	8.40	114.92	108.20
34	BA	1299	A	O4'-C1'-N9	8.40	114.92	108.20
34	BA	1377	A	C5'-C4'-O4'	8.40	119.18	109.10
34	BA	419	C	O4'-C1'-N1	8.39	114.91	108.20
34	BA	465	A	C5'-C4'-O4'	8.39	119.17	109.10
2	AB	319	G	O4'-C1'-N9	8.38	114.90	108.20
2	AB	1588	G	O3'-P-O5'	-8.38	88.08	104.00
2	AB	1720	U	O4'-C1'-N1	8.38	114.90	108.20
2	AB	2020	A	C5'-C4'-O4'	8.38	119.15	109.10
2	AB	2581	G	O4'-C1'-N9	8.38	114.90	108.20
2	AB	458	G	O4'-C1'-N9	8.37	114.90	108.20
34	BA	1315	U	C5'-C4'-O4'	8.37	119.14	109.10
2	AB	288	U	O4'-C1'-N1	8.36	114.89	108.20
2	AB	991	C	O4'-C1'-N1	8.36	114.88	108.20
34	BA	1478	U	O4'-C1'-N1	8.36	114.89	108.20
2	AB	737	C	O4'-C1'-N1	8.35	114.88	108.20
2	AB	1476	U	O4'-C1'-N1	8.35	114.88	108.20
34	BA	711	G	O4'-C1'-N9	8.34	114.87	108.20
2	AB	1372	U	O4'-C1'-N1	8.34	114.87	108.20
2	AB	2244	U	O4'-C1'-N1	8.34	114.87	108.20
34	BA	507	C	O4'-C1'-N1	8.33	114.86	108.20
34	BA	267	C	O4'-C1'-N1	8.32	114.85	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	22	G	O4'-C1'-N9	8.31	114.85	108.20
34	BA	126	G	O4'-C1'-N9	8.31	114.85	108.20
34	BA	1075	U	O4'-C1'-N1	8.31	114.85	108.20
34	BA	1372	U	O4'-C1'-N1	8.31	114.84	108.20
34	BA	567	G	O4'-C1'-N9	8.29	114.83	108.20
2	AB	2784	U	O4'-C1'-N1	8.29	114.83	108.20
34	BA	99	C	O4'-C1'-N1	8.29	114.83	108.20
34	BA	409	U	O4'-C1'-N1	8.28	114.83	108.20
2	AB	2032	G	O4'-C1'-N9	8.28	114.82	108.20
34	BA	78	A	O4'-C1'-N9	8.28	114.82	108.20
2	AB	1742	U	O4'-C1'-N1	8.27	114.81	108.20
34	BA	899	C	O4'-C1'-N1	8.26	114.81	108.20
34	BA	1255	G	O4'-C1'-N9	8.26	114.81	108.20
2	AB	1493	C	O4'-C1'-N1	8.26	114.80	108.20
2	AB	2655	G	O4'-C1'-N9	8.26	114.80	108.20
34	BA	453	G	O4'-C1'-N9	8.25	114.80	108.20
2	AB	1709	U	C5'-C4'-O4'	8.24	118.99	109.10
2	AB	2147	A	C5'-C4'-O4'	8.24	118.99	109.10
2	AB	1088	A	O4'-C1'-N9	8.24	114.79	108.20
2	AB	720	U	C5'-C4'-O4'	8.24	118.99	109.10
2	AB	1417	C	O4'-C1'-N1	8.24	114.79	108.20
2	AB	1526	C	O4'-C1'-N1	8.24	114.79	108.20
34	BA	1136	C	O4'-C1'-N1	8.24	114.79	108.20
2	AB	2473	U	O4'-C1'-N1	8.23	114.78	108.20
2	AB	2126	A	O4'-C1'-N9	8.23	114.78	108.20
34	BA	518	C	O4'-C1'-N1	8.22	114.78	108.20
2	AB	1886	U	O4'-C1'-N1	8.21	114.77	108.20
34	BA	702	A	O4'-C1'-N9	8.21	114.77	108.20
34	BA	268	U	C5'-C4'-O4'	8.21	118.95	109.10
2	AB	960	A	O4'-C1'-N9	-8.20	101.64	108.20
2	AB	865	C	O4'-C1'-N1	8.20	114.76	108.20
34	BA	25	C	O4'-C1'-N1	8.18	114.74	108.20
34	BA	384	G	O4'-C1'-N9	8.18	114.74	108.20
2	AB	63	A	O4'-C1'-N9	8.17	114.74	108.20
2	AB	2579	C	O4'-C1'-N1	8.17	114.74	108.20
34	BA	723	U	O4'-C1'-N1	8.17	114.73	108.20
2	AB	551	G	O4'-C1'-N9	8.16	114.73	108.20
35	BB	19	G	N3-C4-C5	-8.16	124.52	128.60
2	AB	1914	C	O4'-C1'-N1	8.16	114.73	108.20
2	AB	2321	U	O4'-C1'-N1	8.16	114.73	108.20
2	AB	65	U	O4'-C1'-N1	8.16	114.73	108.20
2	AB	2509	G	O4'-C1'-N9	8.15	114.72	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	59	U	O4'-C1'-N1	8.15	114.72	108.20
2	AB	517	C	O4'-C1'-N1	8.14	114.72	108.20
34	BA	1172	C	O4'-C1'-N1	8.14	114.71	108.20
34	BA	1409	C	O4'-C1'-N1	8.14	114.71	108.20
2	AB	295	G	O4'-C1'-N9	8.13	114.71	108.20
2	AB	880	G	O4'-C1'-N9	8.13	114.71	108.20
2	AB	776	G	O4'-C1'-N9	8.13	114.70	108.20
2	AB	971	G	O4'-C1'-N9	8.13	114.70	108.20
2	AB	32	C	O4'-C1'-N1	8.12	114.70	108.20
2	AB	1167	C	O4'-C1'-N1	8.12	114.70	108.20
34	BA	212	G	O4'-C1'-N9	8.12	114.69	108.20
2	AB	1798	U	O4'-C1'-N1	8.12	114.69	108.20
2	AB	345	A	C1'-O4'-C4'	-8.11	103.41	109.90
2	AB	1405	U	O4'-C1'-N1	8.11	114.69	108.20
2	AB	2843	G	O4'-C1'-N9	8.11	114.69	108.20
2	AB	1153	C	O4'-C1'-N1	8.10	114.68	108.20
2	AB	2404	U	O4'-C1'-N1	8.09	114.67	108.20
2	AB	2406	A	O4'-C1'-N9	8.09	114.67	108.20
2	AB	2438	U	O4'-C1'-N1	8.08	114.67	108.20
2	AB	1695	G	O4'-C1'-N9	8.08	114.67	108.20
2	AB	2265	U	O4'-C1'-N1	8.08	114.67	108.20
34	BA	85	U	O4'-C1'-N1	8.08	114.66	108.20
2	AB	1370	C	O4'-C1'-N1	8.07	114.66	108.20
34	BA	1281	C	O4'-C1'-N1	8.07	114.66	108.20
2	AB	2699	C	O4'-C1'-N1	8.07	114.66	108.20
2	AB	141	G	C5'-C4'-C3'	-8.07	103.09	116.00
34	BA	294	U	O4'-C1'-N1	8.07	114.65	108.20
2	AB	279	A	O4'-C1'-N9	8.06	114.65	108.20
2	AB	627	A	O4'-C1'-N9	8.06	114.65	108.20
34	BA	143	A	O4'-C1'-N9	8.06	114.65	108.20
2	AB	1549	A	O4'-C1'-N9	8.06	114.65	108.20
2	AB	1920	C	O4'-C1'-N1	8.05	114.64	108.20
2	AB	765	C	O4'-C1'-N1	8.05	114.64	108.20
34	BA	311	C	O4'-C1'-N1	8.04	114.63	108.20
34	BA	844	G	O4'-C1'-N9	8.04	114.63	108.20
2	AB	841	G	C5'-C4'-O4'	8.03	118.74	109.10
2	AB	158	U	O4'-C1'-N1	8.03	114.63	108.20
2	AB	291	G	O4'-C1'-N9	8.03	114.63	108.20
2	AB	1724	G	C8-N9-C4	-8.03	103.19	106.40
2	AB	1115	G	O4'-C1'-N9	8.02	114.62	108.20
2	AB	1767	G	O4'-C1'-N9	8.02	114.62	108.20
2	AB	2750	A	O4'-C1'-N9	8.02	114.61	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1506	U	O4'-C1'-N1	8.01	114.61	108.20
1	AA	36	C	O4'-C1'-N1	8.01	114.61	108.20
2	AB	1177	G	C5'-C4'-O4'	8.01	118.71	109.10
2	AB	1101	U	O4'-C1'-N1	8.01	114.61	108.20
2	AB	2901	C	O4'-C1'-N1	8.00	114.60	108.20
2	AB	1002	G	O4'-C1'-N9	8.00	114.60	108.20
34	BA	301	G	O4'-C1'-N9	8.00	114.60	108.20
2	AB	1887	C	O4'-C1'-N1	8.00	114.60	108.20
34	BA	1097	C	O4'-C1'-N1	7.99	114.59	108.20
34	BA	31	G	O4'-C1'-N9	7.99	114.59	108.20
2	AB	2178	C	O4'-C1'-N1	7.98	114.59	108.20
34	BA	1040	U	O4'-C1'-N1	7.98	114.59	108.20
34	BA	1258	G	O4'-C1'-N9	7.97	114.58	108.20
34	BA	465	A	C5'-C4'-C3'	-7.97	103.24	116.00
34	BA	675	A	O4'-C1'-N9	7.97	114.58	108.20
2	AB	246	C	O4'-C1'-N1	7.97	114.57	108.20
2	AB	2582	G	C8-N9-C4	-7.97	103.21	106.40
2	AB	193	U	O4'-C1'-N1	7.96	114.57	108.20
2	AB	961	C	O4'-C1'-N1	7.96	114.57	108.20
2	AB	1758	U	O4'-C1'-N1	7.96	114.57	108.20
2	AB	1484	U	O4'-C1'-N1	7.95	114.56	108.20
34	BA	150	U	O4'-C1'-N1	7.95	114.56	108.20
34	BA	860	A	O4'-C1'-N9	7.95	114.56	108.20
2	AB	856	G	C5'-C4'-O4'	7.95	118.64	109.10
34	BA	192	A	O4'-C1'-N9	7.94	114.55	108.20
2	AB	1275	A	O4'-C1'-N9	7.94	114.55	108.20
2	AB	2182	U	O4'-C1'-N1	7.94	114.55	108.20
2	AB	433	C	O4'-C1'-N1	7.93	114.55	108.20
34	BA	151	A	O4'-C1'-N9	7.93	114.55	108.20
34	BA	1315	U	C5'-C4'-C3'	-7.93	103.30	116.00
2	AB	128	C	O4'-C1'-N1	7.93	114.54	108.20
2	AB	618	G	O4'-C1'-N9	7.92	114.54	108.20
2	AB	2220	U	O4'-C1'-N1	7.91	114.52	108.20
34	BA	256	U	O4'-C1'-N1	7.91	114.53	108.20
2	AB	1118	C	O4'-C1'-N1	7.90	114.52	108.20
2	AB	2020	A	O4'-C1'-N9	7.90	114.52	108.20
2	AB	2310	C	O4'-C1'-N1	7.90	114.52	108.20
1	AA	95	U	O4'-C1'-N1	7.90	114.52	108.20
34	BA	1	A	O4'-C1'-N9	7.90	114.52	108.20
2	AB	2632	A	O4'-C1'-N9	7.89	114.52	108.20
34	BA	845	A	O4'-C1'-N9	7.89	114.52	108.20
35	BE	42	C	O4'-C1'-N1	7.89	114.52	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1196	C	O4'-C1'-N1	7.89	114.52	108.20
2	AB	266	G	C8-N9-C4	-7.89	103.24	106.40
34	BA	512	U	O4'-C1'-N1	7.89	114.51	108.20
34	BA	937	A	O4'-C1'-N9	7.89	114.51	108.20
34	BA	1480	A	O4'-C1'-N9	7.89	114.51	108.20
2	AB	1058	U	O4'-C1'-N1	7.88	114.50	108.20
35	BE	13	C	O4'-C1'-N1	7.88	114.50	108.20
2	AB	1985	C	O4'-C1'-N1	7.88	114.50	108.20
34	BA	930	C	O4'-C1'-N1	7.88	114.50	108.20
34	BA	1474	U	O4'-C1'-N1	7.88	114.50	108.20
34	BA	841	C	C6-N1-C2	-7.87	117.15	120.30
34	BA	1351	U	O4'-C1'-N1	7.87	114.49	108.20
34	BA	342	C	O4'-C1'-N1	7.86	114.49	108.20
2	AB	2110	G	O4'-C1'-N9	7.86	114.48	108.20
2	AB	891	G	O4'-C1'-N9	7.85	114.48	108.20
2	AB	1186	G	C5'-C4'-C3'	-7.85	103.44	116.00
2	AB	2882	A	C5'-C4'-O4'	7.85	118.52	109.10
2	AB	2374	C	O4'-C1'-N1	7.85	114.48	108.20
34	BA	562	U	O4'-C1'-N1	7.84	114.47	108.20
2	AB	519	U	O4'-C1'-N1	7.84	114.47	108.20
34	BA	594	U	O4'-C1'-N1	7.84	114.47	108.20
2	AB	336	C	O4'-C1'-N1	7.84	114.47	108.20
34	BA	904	U	O4'-C1'-N1	7.83	114.47	108.20
34	BA	73	C	O4'-C1'-N1	7.83	114.47	108.20
2	AB	1909	C	O4'-C1'-N1	7.83	114.46	108.20
2	AB	2769	U	O4'-C1'-N1	7.83	114.46	108.20
2	AB	1871	A	C3'-C2'-C1'	7.82	107.76	101.50
2	AB	1998	A	O4'-C1'-N9	7.82	114.46	108.20
2	AB	1148	U	O4'-C1'-N1	7.82	114.46	108.20
2	AB	1349	C	O4'-C1'-N1	7.82	114.46	108.20
2	AB	1079	C	O4'-C1'-N1	7.82	114.46	108.20
34	BA	65	A	O4'-C1'-N9	7.82	114.45	108.20
2	AB	1191	G	O4'-C1'-N9	7.81	114.45	108.20
34	BA	206	C	O4'-C1'-N1	7.81	114.45	108.20
35	BB	11	C	C5'-C4'-O4'	7.81	118.47	109.10
34	BA	359	G	O4'-C1'-N9	7.81	114.45	108.20
2	AB	651	G	O4'-C1'-N9	7.80	114.44	108.20
2	AB	1938	A	O4'-C1'-N9	7.80	114.44	108.20
2	AB	1509	A	O4'-C1'-N9	7.80	114.44	108.20
2	AB	2426	A	O4'-C1'-N9	7.80	114.44	108.20
34	BA	971	G	C5'-C4'-C3'	-7.79	103.53	116.00
2	AB	1097	U	O4'-C1'-N1	7.79	114.44	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	651	C	C5'-C4'-O4'	7.79	118.45	109.10
2	AB	803	U	O4'-C1'-N1	7.79	114.43	108.20
34	BA	898	G	O4'-C1'-N9	7.79	114.43	108.20
35	BB	49	C	O4'-C1'-N1	7.79	114.43	108.20
2	AB	1883	U	O4'-C1'-N1	7.79	114.43	108.20
2	AB	2825	G	O4'-C1'-N9	7.79	114.43	108.20
34	BA	1328	C	O4'-C1'-N1	7.78	114.43	108.20
2	AB	418	C	O4'-C1'-N1	7.78	114.42	108.20
2	AB	2470	G	O4'-C1'-N9	7.78	114.43	108.20
34	BA	211	G	N3-C4-C5	-7.78	124.71	128.60
2	AB	1282	U	O4'-C1'-N1	7.78	114.42	108.20
34	BA	1528	U	O4'-C1'-N1	7.78	114.42	108.20
2	AB	898	C	O4'-C1'-N1	7.77	114.42	108.20
2	AB	984	A	C1'-O4'-C4'	-7.77	103.69	109.90
34	BA	1202	U	O4'-C1'-N1	7.76	114.41	108.20
34	BA	972	C	O4'-C1'-N1	7.76	114.41	108.20
1	AA	70	C	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2103	C	O4'-C1'-N1	7.75	114.40	108.20
35	BE	41	C	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2001	C	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2240	U	O4'-C1'-N1	7.75	114.40	108.20
2	AB	2164	C	O4'-C1'-N1	7.74	114.39	108.20
2	AB	341	C	O4'-C1'-N1	7.74	114.39	108.20
2	AB	2743	U	O4'-C1'-N1	7.74	114.39	108.20
2	AB	2762	C	O4'-C1'-N1	7.74	114.39	108.20
34	BA	1165	U	O4'-C1'-N1	7.74	114.39	108.20
34	BA	96	U	O4'-C1'-N1	7.74	114.39	108.20
2	AB	324	A	C5'-C4'-C3'	-7.73	103.63	116.00
1	AA	120	U	O4'-C1'-N1	7.73	114.39	108.20
2	AB	1351	C	O4'-C1'-N1	7.73	114.39	108.20
2	AB	878	A	O4'-C1'-N9	7.73	114.39	108.20
2	AB	1670	C	O4'-C1'-N1	7.73	114.39	108.20
2	AB	1895	C	O4'-C1'-N1	7.73	114.39	108.20
2	AB	1300	G	O4'-C1'-N9	7.73	114.38	108.20
2	AB	2795	C	O4'-C1'-N1	7.73	114.38	108.20
34	BA	1121	U	O4'-C1'-N1	7.73	114.38	108.20
2	AB	504	A	O4'-C1'-N9	7.73	114.38	108.20
34	BA	287	U	O4'-C1'-N1	7.73	114.38	108.20
2	AB	1166	G	O4'-C1'-N9	7.72	114.38	108.20
2	AB	2181	U	O4'-C1'-N1	7.72	114.38	108.20
34	BA	1471	U	O4'-C1'-N1	7.71	114.37	108.20
2	AB	1902	C	O4'-C1'-N1	7.71	114.37	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	984	A	O4'-C1'-C2'	-7.71	98.09	105.80
34	BA	83	C	O4'-C1'-N1	7.71	114.37	108.20
34	BA	465	A	O4'-C1'-C2'	-7.71	98.09	105.80
34	BA	1066	C	O4'-C1'-N1	7.71	114.36	108.20
2	AB	1423	G	O4'-C1'-N9	7.70	114.36	108.20
2	AB	305	C	C5'-C4'-C3'	-7.70	103.69	116.00
34	BA	1017	U	O4'-C1'-N1	7.69	114.36	108.20
2	AB	2370	G	O4'-C1'-N9	7.69	114.35	108.20
2	AB	277	G	C5'-C4'-O4'	7.69	118.33	109.10
2	AB	57	C	O4'-C1'-N1	7.68	114.34	108.20
2	AB	613	A	C3'-C2'-C1'	-7.68	95.36	101.50
34	BA	490	C	O4'-C1'-N1	7.68	114.34	108.20
34	BA	1223	C	C5'-C4'-C3'	-7.68	103.71	116.00
2	AB	1605	C	O4'-C1'-N1	7.68	114.34	108.20
2	AB	1053	C	O4'-C1'-N1	7.68	114.34	108.20
2	AB	2430	A	O4'-C1'-N9	7.68	114.34	108.20
2	AB	66	C	O4'-C1'-N1	7.67	114.33	108.20
2	AB	1606	C	O4'-C1'-N1	7.67	114.33	108.20
2	AB	216	A	O4'-C1'-N9	7.66	114.33	108.20
2	AB	349	U	O4'-C1'-N1	7.66	114.33	108.20
2	AB	1227	G	O4'-C1'-N9	7.66	114.33	108.20
2	AB	2723	C	O4'-C1'-N1	7.65	114.32	108.20
2	AB	1288	G	O4'-C1'-N9	7.65	114.32	108.20
2	AB	2612	C	O4'-C1'-N1	7.65	114.32	108.20
34	BA	1294	G	O4'-C1'-N9	7.65	114.32	108.20
2	AB	797	G	O4'-C1'-N9	7.64	114.31	108.20
2	AB	972	A	O4'-C1'-N9	7.64	114.31	108.20
34	BA	258	G	O4'-C1'-N9	7.64	114.31	108.20
2	AB	1853	A	O4'-C1'-N9	7.63	114.30	108.20
2	AB	899	A	O4'-C1'-N9	7.63	114.30	108.20
2	AB	259	G	O4'-C1'-N9	7.62	114.30	108.20
2	AB	1290	C	O4'-C1'-N1	7.62	114.30	108.20
2	AB	1485	U	O4'-C1'-N1	7.62	114.30	108.20
2	AB	593	U	O4'-C1'-N1	7.62	114.30	108.20
2	AB	1144	A	O4'-C1'-N9	7.62	114.29	108.20
2	AB	1173	U	O4'-C1'-N1	7.61	114.29	108.20
2	AB	1880	U	C5'-C4'-O4'	7.61	118.23	109.10
2	AB	702	U	O4'-C1'-N1	7.61	114.29	108.20
2	AB	1736	U	O4'-C1'-N1	7.60	114.28	108.20
2	AB	1402	U	O4'-C1'-N1	7.59	114.27	108.20
2	AB	38	A	O4'-C1'-N9	7.59	114.27	108.20
2	AB	1177	G	C5'-C4'-C3'	-7.59	103.85	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	783	C	C5'-C4'-O4'	7.59	118.21	109.10
34	BA	406	G	C5'-C4'-O4'	7.59	118.21	109.10
34	BA	672	U	O4'-C1'-N1	7.59	114.27	108.20
2	AB	60	G	O4'-C1'-N9	7.59	114.27	108.20
2	AB	1425	G	O4'-C1'-N9	7.58	114.27	108.20
37	BD	33	U	O4'-C1'-N1	7.58	114.27	108.20
2	AB	1837	C	O4'-C1'-N1	7.58	114.27	108.20
34	BA	970	C	C5'-C4'-O4'	7.58	118.20	109.10
2	AB	2794	C	O4'-C1'-N1	7.58	114.26	108.20
2	AB	2507	C	O4'-C1'-N1	7.58	114.26	108.20
2	AB	1183	U	O4'-C1'-N1	7.57	114.26	108.20
2	AB	2751	G	C1'-O4'-C4'	-7.57	103.85	109.90
2	AB	1769	U	O4'-C1'-N1	7.56	114.25	108.20
2	AB	1185	G	C1'-O4'-C4'	-7.55	103.86	109.90
34	BA	1538	C	C5'-C4'-C3'	7.55	128.08	116.00
2	AB	355	U	O4'-C1'-N1	7.55	114.24	108.20
2	AB	1361	G	O4'-C1'-N9	7.54	114.23	108.20
2	AB	644	A	O4'-C1'-N9	7.54	114.23	108.20
2	AB	473	G	C5'-C4'-O4'	7.54	118.15	109.10
1	AA	86	G	O4'-C1'-N9	7.54	114.23	108.20
2	AB	1612	C	O4'-C1'-N1	7.53	114.22	108.20
1	AA	89	U	O4'-C1'-N1	7.53	114.22	108.20
2	AB	2099	U	O4'-C1'-N1	7.53	114.22	108.20
2	AB	2123	G	O4'-C1'-N9	7.53	114.22	108.20
2	AB	1182	G	O4'-C1'-N9	7.53	114.22	108.20
2	AB	2696	U	C5'-C4'-O4'	7.53	118.13	109.10
34	BA	1410	A	O4'-C1'-N9	7.52	114.22	108.20
2	AB	603	A	O4'-C1'-N9	7.52	114.22	108.20
2	AB	2687	U	O4'-C1'-N1	7.52	114.21	108.20
2	AB	185	G	O4'-C1'-N9	7.51	114.21	108.20
2	AB	2362	C	O4'-C1'-N1	7.51	114.21	108.20
34	BA	670	G	O4'-C1'-N9	7.51	114.21	108.20
34	BA	880	C	O4'-C1'-N1	7.51	114.21	108.20
2	AB	191	A	O4'-C1'-N9	7.51	114.21	108.20
34	BA	52	C	O4'-C1'-N1	7.51	114.21	108.20
34	BA	558	G	O4'-C1'-N9	7.50	114.20	108.20
2	AB	252	G	O4'-C1'-N9	7.50	114.20	108.20
34	BA	809	G	O4'-C1'-N9	7.50	114.20	108.20
2	AB	1728	C	O4'-C1'-N1	7.50	114.20	108.20
2	AB	877	A	O4'-C1'-N9	7.49	114.19	108.20
2	AB	2391	G	C1'-O4'-C4'	-7.49	103.91	109.90
2	AB	518	G	C5'-C4'-O4'	7.49	118.08	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2556	C	O4'-C1'-N1	7.49	114.19	108.20
34	BA	1323	G	C5'-C4'-O4'	7.49	118.08	109.10
34	BA	793	U	O4'-C1'-N1	7.48	114.19	108.20
34	BA	133	U	O4'-C1'-N1	7.48	114.19	108.20
34	BA	1205	U	O4'-C1'-N1	7.48	114.18	108.20
35	BE	62	C	O4'-C1'-N1	7.47	114.18	108.20
34	BA	453	G	C8-N9-C4	-7.47	103.41	106.40
2	AB	2025	C	O4'-C1'-N1	7.47	114.17	108.20
34	BA	942	G	O4'-C1'-N9	7.46	114.17	108.20
34	BA	621	A	C5'-C4'-O4'	7.46	118.05	109.10
2	AB	1242	U	O4'-C1'-N1	7.46	114.16	108.20
34	BA	273	U	O4'-C1'-N1	7.45	114.16	108.20
2	AB	683	U	O4'-C1'-N1	7.45	114.16	108.20
2	AB	2558	C	O4'-C1'-N1	7.45	114.16	108.20
34	BA	469	C	O4'-C1'-N1	7.45	114.16	108.20
34	BA	1223	C	C4'-C3'-C2'	-7.45	95.15	102.60
2	AB	1706	C	O4'-C1'-N1	7.45	114.16	108.20
34	BA	956	U	O4'-C1'-N1	7.45	114.16	108.20
34	BA	1500	A	O4'-C1'-N9	7.45	114.16	108.20
2	AB	1878	G	O4'-C1'-N9	7.44	114.15	108.20
2	AB	2293	G	O4'-C1'-N9	7.43	114.15	108.20
2	AB	343	C	O4'-C1'-N1	7.43	114.15	108.20
34	BA	620	C	C5'-C4'-O4'	7.43	118.01	109.10
2	AB	25	U	O4'-C1'-N1	7.42	114.14	108.20
2	AB	2066	C	O4'-C1'-N1	7.42	114.14	108.20
2	AB	2852	G	O4'-C1'-N9	7.42	114.14	108.20
2	AB	1841	U	O4'-C1'-N1	7.42	114.13	108.20
34	BA	682	G	O4'-C1'-N9	7.42	114.14	108.20
34	BA	1225	A	O4'-C1'-N9	-7.42	102.27	108.20
2	AB	15	G	C8-N9-C4	-7.41	103.44	106.40
34	BA	1470	U	O4'-C1'-N1	7.41	114.13	108.20
2	AB	877	A	C8-N9-C4	-7.41	102.84	105.80
2	AB	1326	U	O4'-C1'-N1	7.41	114.12	108.20
34	BA	739	C	O4'-C1'-N1	7.40	114.12	108.20
2	AB	23	G	O4'-C1'-N9	7.40	114.12	108.20
34	BA	773	G	O4'-C1'-N9	7.40	114.12	108.20
2	AB	109	C	O4'-C1'-N1	7.40	114.12	108.20
2	AB	2885	G	C5'-C4'-C3'	-7.39	104.17	116.00
2	AB	2364	C	O4'-C1'-N1	7.39	114.11	108.20
2	AB	719	C	O4'-C1'-N1	7.39	114.11	108.20
2	AB	613	A	O4'-C1'-N9	7.39	114.11	108.20
2	AB	848	C	O4'-C1'-N1	7.39	114.11	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	156	C	O4'-C1'-N1	7.39	114.11	108.20
2	AB	951	C	O4'-C1'-N1	7.38	114.11	108.20
2	AB	2688	G	O4'-C1'-N9	7.38	114.11	108.20
2	AB	1573	G	O4'-C1'-N9	7.38	114.10	108.20
34	BA	348	G	O4'-C1'-N9	7.38	114.10	108.20
34	BA	782	A	O4'-C1'-N9	7.38	114.10	108.20
34	BA	1460	C	O4'-C1'-N1	7.38	114.10	108.20
2	AB	2733	A	O4'-C1'-N9	7.38	114.10	108.20
2	AB	475	C	O4'-C1'-N1	7.37	114.09	108.20
2	AB	2073	C	O4'-C1'-N1	7.37	114.09	108.20
34	BA	1455	G	O4'-C1'-N9	7.37	114.09	108.20
2	AB	1982	U	C5'-C4'-O4'	7.36	117.94	109.10
2	AB	1487	U	O4'-C1'-N1	7.36	114.09	108.20
2	AB	1569	A	O4'-C1'-N9	7.36	114.09	108.20
2	AB	1621	U	O4'-C1'-N1	7.36	114.09	108.20
34	BA	1320	C	C5'-C4'-O4'	7.36	117.93	109.10
2	AB	906	U	O4'-C1'-N1	7.35	114.08	108.20
2	AB	1638	C	O4'-C1'-N1	7.35	114.08	108.20
34	BA	383	A	O4'-C1'-N9	7.35	114.08	108.20
2	AB	1477	A	C5'-C4'-C3'	-7.35	104.24	116.00
34	BA	361	G	O4'-C1'-N9	7.35	114.08	108.20
35	BB	19	G	C8-N9-C4	-7.35	103.46	106.40
2	AB	211	C	O4'-C1'-N1	7.34	114.07	108.20
2	AB	1384	A	O4'-C1'-N9	-7.34	102.33	108.20
2	AB	1221	C	O4'-C1'-N1	7.34	114.07	108.20
2	AB	2079	U	O4'-C1'-N1	7.34	114.07	108.20
34	BA	815	A	C1'-O4'-C4'	-7.34	104.03	109.90
34	BA	1069	C	O4'-C1'-N1	7.34	114.07	108.20
2	AB	2007	U	O4'-C1'-N1	7.34	114.07	108.20
34	BA	458	U	O4'-C1'-N1	7.34	114.07	108.20
34	BA	1443	C	O4'-C1'-N1	7.34	114.07	108.20
34	BA	1218	C	O4'-C1'-N1	7.34	114.07	108.20
34	BA	1065	U	O4'-C1'-N1	7.33	114.07	108.20
2	AB	2229	U	O4'-C1'-N1	7.33	114.07	108.20
2	AB	2805	C	O4'-C1'-N1	7.33	114.07	108.20
2	AB	1162	G	O4'-C1'-N9	7.33	114.06	108.20
2	AB	1172	C	O4'-C1'-N1	7.33	114.06	108.20
2	AB	2086	U	O4'-C1'-N1	7.33	114.07	108.20
2	AB	1347	A	O4'-C1'-N9	7.33	114.06	108.20
2	AB	664	G	O4'-C1'-N9	7.32	114.06	108.20
34	BA	290	C	C5'-C4'-O4'	7.32	117.89	109.10
2	AB	416	U	C5'-C4'-O4'	7.32	117.89	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	946	C	O4'-C1'-N1	7.32	114.05	108.20
2	AB	984	A	C4'-C3'-C2'	-7.31	95.29	102.60
2	AB	225	C	O4'-C1'-N1	7.31	114.05	108.20
2	AB	452	G	O4'-C1'-N9	7.31	114.05	108.20
2	AB	1295	C	O4'-C1'-N1	7.31	114.05	108.20
2	AB	135	U	O4'-C1'-N1	7.30	114.04	108.20
34	BA	543	U	O4'-C1'-N1	7.30	114.04	108.20
34	BA	1025	U	O4'-C1'-N1	7.30	114.04	108.20
34	BA	1132	C	O4'-C1'-N1	7.30	114.04	108.20
2	AB	700	G	N9-C1'-C2'	-7.30	103.97	112.00
2	AB	984	A	O4'-C4'-C3'	7.30	111.94	106.10
2	AB	1112	G	C5'-C4'-O4'	7.29	117.86	109.10
2	AB	1061	U	C3'-C2'-C1'	-7.29	95.67	101.50
2	AB	2841	C	O4'-C1'-N1	7.29	114.03	108.20
2	AB	2139	U	O4'-C1'-N1	7.29	114.03	108.20
34	BA	1091	U	C5'-C4'-O4'	7.28	117.84	109.10
2	AB	1573	G	C8-N9-C4	-7.28	103.49	106.40
2	AB	1686	C	O4'-C1'-N1	7.28	114.03	108.20
1	AA	111	U	O4'-C1'-N1	7.28	114.02	108.20
2	AB	919	U	O4'-C1'-N1	7.28	114.02	108.20
2	AB	1801	A	O4'-C1'-N9	7.28	114.02	108.20
2	AB	120	U	O4'-C1'-N1	7.27	114.02	108.20
2	AB	811	U	O4'-C1'-N1	7.27	114.01	108.20
2	AB	930	G	O4'-C1'-N9	7.26	114.01	108.20
2	AB	168	G	O4'-C1'-N9	7.26	114.01	108.20
2	AB	1309	G	O4'-C1'-N9	7.26	114.01	108.20
2	AB	2792	A	C5'-C4'-C3'	-7.26	104.39	116.00
34	BA	900	A	C8-N9-C4	-7.26	102.90	105.80
34	BA	585	G	C5'-C4'-O4'	7.25	117.80	109.10
2	AB	257	C	O4'-C1'-N1	7.24	114.00	108.20
34	BA	1279	G	O4'-C1'-N9	7.24	114.00	108.20
2	AB	2456	C	O4'-C1'-N1	7.24	113.99	108.20
34	BA	678	U	O4'-C1'-N1	7.24	113.99	108.20
2	AB	2582	G	N3-C4-C5	-7.23	124.98	128.60
2	AB	733	G	C5'-C4'-O4'	7.23	117.78	109.10
2	AB	748	G	C5'-C4'-O4'	7.23	117.78	109.10
2	AB	2775	G	C8-N9-C4	-7.23	103.51	106.40
34	BA	1462	C	O4'-C1'-N1	7.23	113.98	108.20
2	AB	1271	G	O4'-C1'-N9	7.23	113.98	108.20
34	BA	386	C	C5'-C4'-O4'	7.23	117.77	109.10
2	AB	834	G	C8-N9-C4	-7.22	103.51	106.40
2	AB	1045	C	O4'-C1'-N1	7.22	113.98	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1231	U	O4'-C1'-N1	7.22	113.98	108.20
2	AB	1396	U	O4'-C1'-N1	7.22	113.98	108.20
34	BA	401	C	O4'-C1'-N1	7.22	113.98	108.20
2	AB	1146	C	O4'-C1'-N1	7.22	113.98	108.20
2	AB	2466	C	O4'-C1'-N1	7.22	113.98	108.20
34	BA	202	G	O4'-C1'-N9	7.22	113.98	108.20
2	AB	1233	C	O4'-C1'-N1	7.22	113.97	108.20
34	BA	397	A	O4'-C1'-N9	7.22	113.97	108.20
34	BA	24	U	O4'-C1'-N1	7.21	113.97	108.20
2	AB	399	U	O4'-C1'-N1	7.21	113.97	108.20
34	BA	1448	C	O4'-C1'-N1	7.21	113.97	108.20
2	AB	817	C	O4'-C1'-N1	7.20	113.96	108.20
2	AB	1575	C	O4'-C1'-N1	7.20	113.96	108.20
2	AB	2586	U	O4'-C1'-N1	7.20	113.96	108.20
2	AB	160	A	O4'-C1'-N9	7.20	113.96	108.20
2	AB	772	C	O4'-C1'-N1	7.20	113.96	108.20
34	BA	1432	G	O4'-C1'-N9	7.20	113.96	108.20
2	AB	1177	G	N3-C4-C5	-7.19	125.01	128.60
2	AB	489	G	O4'-C1'-N9	7.18	113.95	108.20
34	BA	327	A	C1'-O4'-C4'	-7.18	104.16	109.90
34	BA	690	G	O4'-C1'-N9	7.18	113.94	108.20
34	BA	1216	A	O4'-C1'-N9	7.18	113.94	108.20
2	AB	2659	G	O4'-C1'-N9	7.17	113.94	108.20
2	AB	58	G	O4'-C1'-N9	7.17	113.94	108.20
34	BA	1522	U	O4'-C1'-N1	7.17	113.93	108.20
2	AB	1316	U	O4'-C1'-N1	7.17	113.93	108.20
2	AB	2633	G	O4'-C1'-N9	7.17	113.93	108.20
2	AB	970	U	O4'-C1'-N1	7.16	113.93	108.20
2	AB	1653	G	C8-N9-C4	-7.16	103.54	106.40
34	BA	415	A	O4'-C1'-N9	7.16	113.92	108.20
2	AB	1541	C	O4'-C1'-N1	7.15	113.92	108.20
1	AA	107	G	C8-N9-C4	-7.15	103.54	106.40
2	AB	853	C	O4'-C1'-N1	7.15	113.92	108.20
2	AB	889	C	O4'-C1'-N1	7.15	113.92	108.20
34	BA	614	C	O4'-C1'-N1	7.15	113.92	108.20
34	BA	818	G	O4'-C1'-C2'	-7.15	98.65	105.80
34	BA	962	C	C5'-C4'-O4'	7.15	117.68	109.10
2	AB	2200	C	O4'-C1'-N1	7.15	113.92	108.20
2	AB	913	U	O4'-C1'-N1	7.15	113.92	108.20
2	AB	2651	C	O4'-C1'-N1	7.15	113.92	108.20
34	BA	1326	U	O4'-C1'-N1	7.15	113.92	108.20
34	BA	1479	C	O4'-C1'-N1	7.15	113.92	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	208	U	O4'-C1'-N1	7.15	113.92	108.20
2	AB	1827	U	O4'-C1'-N1	7.14	113.91	108.20
2	AB	1025	G	O4'-C1'-N9	7.14	113.91	108.20
34	BA	489	C	C5'-C4'-O4'	7.14	117.67	109.10
2	AB	591	U	O4'-C1'-N1	7.14	113.91	108.20
2	AB	2693	G	O4'-C1'-N9	7.13	113.91	108.20
2	AB	2223	G	O4'-C1'-N9	7.13	113.90	108.20
2	AB	487	C	O4'-C1'-N1	7.13	113.90	108.20
2	AB	2698	U	O4'-C1'-N1	7.13	113.90	108.20
2	AB	2172	U	P-O3'-C3'	7.12	128.25	119.70
2	AB	2342	C	O4'-C1'-N1	7.12	113.90	108.20
2	AB	892	A	O4'-C1'-N9	7.12	113.89	108.20
2	AB	29	U	O4'-C1'-N1	7.11	113.89	108.20
2	AB	1052	C	O4'-C1'-N1	7.11	113.89	108.20
2	AB	2479	U	O4'-C1'-N1	7.11	113.89	108.20
2	AB	2890	G	O4'-C1'-N9	7.11	113.89	108.20
2	AB	1537	G	O4'-C1'-N9	7.10	113.88	108.20
2	AB	1080	A	O4'-C1'-N9	7.10	113.88	108.20
2	AB	1657	U	O4'-C1'-N1	7.10	113.88	108.20
2	AB	1696	G	O4'-C1'-N9	7.09	113.88	108.20
2	AB	271	G	O4'-C1'-N9	7.09	113.88	108.20
2	AB	2015	A	O4'-C1'-N9	7.09	113.87	108.20
34	BA	1061	G	O4'-C1'-N9	7.09	113.87	108.20
34	BA	952	U	O4'-C1'-N1	7.09	113.87	108.20
2	AB	1193	G	O4'-C1'-N9	7.08	113.87	108.20
2	AB	2058	A	P-O3'-C3'	7.08	128.20	119.70
34	BA	178	C	O4'-C1'-N1	7.08	113.87	108.20
34	BA	941	G	O4'-C1'-N9	7.08	113.86	108.20
34	BA	52	C	C1'-O4'-C4'	-7.08	104.24	109.90
2	AB	2112	G	C8-N9-C4	-7.08	103.57	106.40
34	BA	1467	C	O4'-C1'-N1	7.08	113.86	108.20
34	BA	992	U	O4'-C1'-N1	7.07	113.86	108.20
2	AB	2195	U	O4'-C1'-N1	7.07	113.86	108.20
34	BA	198	G	C5'-C4'-O4'	7.07	117.58	109.10
2	AB	1946	U	O4'-C1'-N1	7.07	113.86	108.20
2	AB	345	A	O4'-C1'-N9	7.07	113.85	108.20
2	AB	1299	G	O4'-C1'-N9	7.07	113.85	108.20
2	AB	2866	U	O4'-C1'-N1	7.07	113.85	108.20
34	BA	1007	U	O4'-C1'-N1	7.07	113.85	108.20
2	AB	1097	U	N1-C1'-C2'	-7.06	104.23	112.00
2	AB	1843	C	O4'-C1'-N1	7.06	113.85	108.20
34	BA	1045	C	O4'-C1'-N1	7.06	113.85	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	56	C	O4'-C1'-N1	7.06	113.85	108.20
2	AB	2054	A	C5'-C4'-C3'	-7.06	104.71	116.00
34	BA	865	A	O4'-C1'-N9	7.05	113.84	108.20
34	BA	1355	G	O4'-C1'-N9	7.05	113.84	108.20
2	AB	1577	C	C5'-C4'-O4'	7.05	117.56	109.10
2	AB	304	U	O4'-C1'-N1	7.05	113.84	108.20
2	AB	1145	C	O4'-C1'-N1	7.05	113.84	108.20
2	AB	264	C	O4'-C1'-N1	7.04	113.83	108.20
34	BA	609	A	C8-N9-C4	-7.04	102.98	105.80
34	BA	909	A	O4'-C1'-N9	7.04	113.83	108.20
2	AB	1217	U	O4'-C1'-N1	7.04	113.83	108.20
2	AB	1580	A	C5'-C4'-C3'	-7.04	104.74	116.00
35	BB	5	G	O4'-C1'-N9	7.03	113.83	108.20
34	BA	1279	G	C3'-C2'-C1'	7.03	107.13	101.50
2	AB	1482	G	O4'-C1'-N9	7.03	113.82	108.20
2	AB	2791	G	O4'-C1'-N9	7.03	113.82	108.20
34	BA	121	U	C3'-C2'-C1'	7.03	107.12	101.50
2	AB	290	U	C5'-C4'-O4'	7.03	117.53	109.10
2	AB	974	G	O4'-C1'-N9	7.02	113.82	108.20
2	AB	769	U	O4'-C1'-N1	7.02	113.82	108.20
2	AB	1761	C	O4'-C1'-N1	7.02	113.81	108.20
34	BA	137	U	O4'-C1'-N1	7.02	113.81	108.20
34	BA	886	G	O4'-C1'-N9	7.02	113.81	108.20
34	BA	1234	C	O4'-C1'-N1	7.02	113.81	108.20
35	BE	50	U	O4'-C1'-N1	7.02	113.81	108.20
2	AB	226	A	C5'-C4'-O4'	7.02	117.52	109.10
2	AB	424	G	O4'-C1'-N9	7.01	113.81	108.20
2	AB	445	C	O4'-C1'-N1	7.01	113.81	108.20
2	AB	874	G	O4'-C1'-N9	7.01	113.81	108.20
2	AB	548	G	N3-C4-C5	-7.01	125.09	128.60
2	AB	2649	C	O4'-C1'-N1	7.01	113.81	108.20
34	BA	646	G	O4'-C1'-N9	7.01	113.81	108.20
34	BA	1464	U	O4'-C1'-N1	7.01	113.81	108.20
2	AB	701	G	O4'-C1'-N9	7.01	113.81	108.20
2	AB	281	C	O4'-C1'-N1	7.01	113.81	108.20
2	AB	2358	A	O4'-C1'-N9	7.01	113.81	108.20
2	AB	2662	A	O4'-C1'-N9	7.01	113.81	108.20
34	BA	851	G	O4'-C1'-N9	7.00	113.80	108.20
2	AB	1874	C	O4'-C1'-N1	7.00	113.80	108.20
55	BW	77	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	AB	1845	G	O4'-C1'-N9	7.00	113.80	108.20
34	BA	631	C	O4'-C1'-N1	7.00	113.80	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1083	U	O4'-C1'-N1	6.99	113.80	108.20
34	BA	1094	G	O4'-C1'-N9	6.99	113.79	108.20
2	AB	502	A	O4'-C1'-N9	6.99	113.79	108.20
2	AB	552	U	O4'-C1'-N1	6.99	113.79	108.20
34	BA	270	A	O4'-C1'-N9	6.99	113.79	108.20
34	BA	778	G	O4'-C1'-N9	6.99	113.79	108.20
34	BA	1190	G	O4'-C1'-N9	6.99	113.79	108.20
2	AB	673	C	O4'-C1'-N1	6.99	113.79	108.20
2	AB	1956	U	C5'-C4'-O4'	6.99	117.48	109.10
34	BA	1169	A	O4'-C1'-N9	6.99	113.79	108.20
34	BA	1147	C	O4'-C1'-N1	6.98	113.79	108.20
2	AB	774	G	C8-N9-C4	-6.98	103.61	106.40
2	AB	913	U	O4'-C4'-C3'	6.98	111.68	106.10
34	BA	803	G	C8-N9-C4	-6.98	103.61	106.40
34	BA	1061	G	C8-N9-C4	-6.98	103.61	106.40
2	AB	357	C	O4'-C1'-N1	6.98	113.78	108.20
34	BA	1536	C	C1'-O4'-C4'	-6.98	104.32	109.90
1	AA	47	C	O4'-C1'-N1	6.97	113.78	108.20
2	AB	658	U	O4'-C1'-N1	6.97	113.78	108.20
2	AB	965	C	O4'-C1'-N1	6.97	113.78	108.20
2	AB	1188	U	O4'-C1'-N1	6.97	113.77	108.20
35	BE	29	G	C5'-C4'-O4'	6.97	117.46	109.10
2	AB	548	G	C2-N3-C4	6.96	115.38	111.90
2	AB	599	A	O4'-C1'-N9	6.96	113.77	108.20
34	BA	650	G	O4'-C1'-N9	6.96	113.77	108.20
2	AB	385	C	O4'-C1'-N1	6.96	113.77	108.20
2	AB	2416	C	O4'-C1'-N1	6.96	113.77	108.20
2	AB	1906	G	O4'-C1'-N9	6.96	113.76	108.20
2	AB	1678	A	O4'-C1'-N9	6.95	113.76	108.20
34	BA	1453	G	O4'-C1'-N9	6.95	113.76	108.20
2	AB	2489	U	O4'-C1'-N1	6.95	113.76	108.20
34	BA	142	G	C5'-C4'-O4'	6.95	117.44	109.10
35	BE	67	C	O4'-C1'-N1	6.95	113.76	108.20
2	AB	556	A	O4'-C1'-N9	6.95	113.76	108.20
2	AB	396	G	C8-N9-C4	-6.95	103.62	106.40
2	AB	2339	C	C5'-C4'-O4'	6.94	117.43	109.10
2	AB	231	A	O4'-C1'-N9	6.94	113.75	108.20
2	AB	555	G	C8-N9-C4	-6.94	103.62	106.40
37	BD	38	U	O4'-C1'-N1	6.94	113.75	108.20
34	BA	2	A	C5'-C4'-C3'	-6.94	104.90	116.00
34	BA	759	A	O4'-C1'-N9	6.94	113.75	108.20
1	AA	28	C	O4'-C1'-N1	6.94	113.75	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1414	C	O4'-C1'-N1	6.94	113.75	108.20
34	BA	1539	C	P-O3'-C3'	6.94	128.03	119.70
2	AB	1529	G	O4'-C1'-N9	6.93	113.75	108.20
34	BA	59	A	C5'-C4'-O4'	6.93	117.42	109.10
2	AB	1015	U	O4'-C1'-N1	6.93	113.75	108.20
34	BA	623	C	O4'-C1'-N1	6.93	113.75	108.20
2	AB	1629	U	O4'-C1'-N1	6.93	113.75	108.20
34	BA	1090	U	O4'-C1'-N1	6.93	113.74	108.20
35	BB	40	C	O4'-C1'-N1	6.93	113.74	108.20
2	AB	2751	G	P-O3'-C3'	6.93	128.01	119.70
37	BD	36	U	O4'-C1'-N1	6.93	113.74	108.20
34	BA	1356	G	O4'-C1'-N9	6.92	113.74	108.20
35	BE	68	C	O4'-C1'-N1	6.92	113.74	108.20
2	AB	2811	G	O4'-C1'-N9	6.92	113.74	108.20
34	BA	92	U	O4'-C1'-N1	6.92	113.74	108.20
2	AB	814	C	O4'-C1'-N1	6.92	113.73	108.20
34	BA	524	G	O4'-C1'-N9	6.92	113.73	108.20
34	BA	524	G	C3'-C2'-C1'	6.92	107.03	101.50
34	BA	619	U	C5'-C4'-C3'	-6.92	104.93	116.00
2	AB	278	A	P-O3'-C3'	6.92	128.00	119.70
34	BA	219	U	O4'-C1'-N1	6.92	113.73	108.20
34	BA	327	A	C5'-C4'-O4'	6.92	117.40	109.10
34	BA	1099	G	O4'-C1'-N9	6.92	113.73	108.20
2	AB	834	G	N3-C4-C5	-6.92	125.14	128.60
2	AB	2026	U	O4'-C1'-N1	6.92	113.73	108.20
34	BA	308	C	O4'-C1'-N1	6.91	113.73	108.20
2	AB	1572	A	C5'-C4'-O4'	6.91	117.39	109.10
2	AB	2337	G	C5'-C4'-O4'	6.91	117.39	109.10
34	BA	1307	U	O4'-C1'-N1	6.91	113.73	108.20
2	AB	2818	U	O4'-C1'-N1	6.91	113.72	108.20
2	AB	2011	U	O4'-C1'-N1	6.90	113.72	108.20
2	AB	2861	U	O4'-C1'-N1	6.90	113.72	108.20
2	AB	1499	C	O4'-C1'-N1	6.90	113.72	108.20
34	BA	1051	C	O4'-C1'-N1	6.90	113.72	108.20
2	AB	1218	G	O4'-C1'-N9	6.90	113.72	108.20
2	AB	1877	A	O4'-C1'-N9	6.90	113.72	108.20
2	AB	784	G	C1'-O4'-C4'	-6.89	104.38	109.90
2	AB	953	G	O4'-C1'-N9	6.89	113.72	108.20
2	AB	1177	G	C8-N9-C4	-6.89	103.64	106.40
34	BA	824	G	C5'-C4'-O4'	6.89	117.37	109.10
34	BA	1117	A	C5'-C4'-O4'	6.89	117.37	109.10
34	BA	1137	C	C5'-C4'-C3'	-6.89	104.97	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	112	U	O4'-C1'-N1	6.89	113.71	108.20
34	BA	837	U	O4'-C1'-N1	6.89	113.71	108.20
2	AB	280	U	O4'-C1'-N1	6.89	113.71	108.20
2	AB	2760	C	C5'-C4'-O4'	6.89	117.36	109.10
35	BE	12	U	C5'-C4'-O4'	6.89	117.36	109.10
34	BA	1361	G	O4'-C1'-N9	6.88	113.71	108.20
34	BA	1021	A	O4'-C1'-N9	6.88	113.71	108.20
34	BA	1388	C	O4'-C1'-N1	6.88	113.71	108.20
2	AB	2359	C	O4'-C1'-N1	6.88	113.70	108.20
34	BA	1499	A	C5'-C4'-O4'	6.88	117.36	109.10
2	AB	774	G	O4'-C1'-N9	6.88	113.70	108.20
2	AB	2207	C	O4'-C1'-N1	6.88	113.70	108.20
34	BA	887	G	O4'-C1'-N9	6.88	113.70	108.20
2	AB	80	G	O4'-C1'-N9	6.87	113.70	108.20
34	BA	1495	U	O4'-C1'-N1	6.87	113.70	108.20
2	AB	1887	C	C4'-C3'-C2'	6.87	109.47	102.60
1	AA	90	C	C1'-O4'-C4'	-6.87	104.41	109.90
34	BA	1225	A	C5'-C4'-O4'	6.86	117.33	109.10
34	BA	621	A	C5'-C4'-C3'	-6.86	105.02	116.00
34	BA	923	A	O4'-C1'-N9	6.86	113.69	108.20
2	AB	1584	U	O4'-C1'-N1	6.86	113.69	108.20
1	AA	41	G	O4'-C1'-N9	6.86	113.69	108.20
2	AB	1993	U	O4'-C1'-N1	6.86	113.69	108.20
2	AB	2730	C	O4'-C1'-N1	6.86	113.69	108.20
34	BA	88	U	O4'-C1'-N1	6.86	113.68	108.20
34	BA	475	C	O4'-C1'-N1	6.86	113.68	108.20
34	BA	1377	A	C1'-O4'-C4'	-6.86	104.42	109.90
2	AB	1100	C	O4'-C1'-N1	6.85	113.68	108.20
34	BA	1117	A	C5'-C4'-C3'	-6.85	105.03	116.00
35	BE	19	G	O4'-C1'-N9	6.85	113.68	108.20
2	AB	1676	A	O4'-C1'-N9	6.85	113.68	108.20
2	AB	2044	C	O4'-C1'-N1	6.85	113.68	108.20
2	AB	2215	C	C5'-C4'-C3'	-6.85	105.04	116.00
2	AB	2548	U	O4'-C1'-N1	6.85	113.68	108.20
2	AB	2125	G	O4'-C1'-N9	6.85	113.68	108.20
2	AB	2519	U	O4'-C1'-N1	6.84	113.67	108.20
34	BA	1401	G	N3-C4-C5	-6.84	125.18	128.60
2	AB	601	C	O4'-C1'-N1	6.84	113.67	108.20
2	AB	1886	U	C1'-O4'-C4'	-6.84	104.43	109.90
2	AB	1357	C	O4'-C1'-N1	6.83	113.67	108.20
2	AB	1691	C	O4'-C1'-N1	6.83	113.67	108.20
2	AB	662	G	O4'-C1'-N9	6.83	113.66	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2126	A	O3'-P-O5'	-6.83	91.03	104.00
34	BA	1028	C	O4'-C1'-N1	6.83	113.66	108.20
35	BE	66	U	O4'-C1'-N1	6.83	113.66	108.20
1	AA	95	U	C5'-C4'-O4'	6.82	117.29	109.10
34	BA	757	U	O4'-C1'-N1	6.82	113.66	108.20
35	BB	52	G	O4'-C1'-N9	6.82	113.66	108.20
2	AB	1013	C	O4'-C1'-N1	6.82	113.66	108.20
34	BA	830	G	C5'-C4'-O4'	6.82	117.28	109.10
34	BA	703	G	O4'-C1'-N9	6.82	113.65	108.20
34	BA	901	A	O4'-C1'-N9	6.82	113.66	108.20
35	BE	64	A	O4'-C1'-N9	6.81	113.65	108.20
2	AB	2496	C	O4'-C1'-N1	6.81	113.65	108.20
2	AB	1642	G	O4'-C1'-N9	6.81	113.65	108.20
34	BA	414	A	C8-N9-C4	-6.81	103.08	105.80
1	AA	69	G	O4'-C1'-N9	6.81	113.65	108.20
34	BA	582	C	O4'-C1'-N1	6.81	113.65	108.20
34	BA	1382	C	O4'-C1'-N1	6.81	113.64	108.20
2	AB	2257	U	O4'-C1'-N1	6.80	113.64	108.20
2	AB	2702	G	C5'-C4'-C3'	-6.80	105.11	116.00
2	AB	312	G	C5'-C4'-O4'	6.80	117.26	109.10
2	AB	2124	G	C5'-C4'-O4'	6.80	117.26	109.10
2	AB	700	G	O4'-C1'-N9	6.80	113.64	108.20
35	BB	13	C	O4'-C1'-N1	6.79	113.64	108.20
34	BA	1003	G	O4'-C1'-N9	6.79	113.64	108.20
34	BA	72	A	C5'-C4'-O4'	6.79	117.25	109.10
2	AB	1673	G	O4'-C1'-N9	6.79	113.63	108.20
2	AB	1747	U	O4'-C1'-N1	6.79	113.63	108.20
2	AB	2018	G	O4'-C1'-N9	6.79	113.63	108.20
34	BA	628	G	O4'-C1'-N9	6.79	113.63	108.20
34	BA	737	C	O4'-C1'-N1	6.79	113.63	108.20
2	AB	2872	A	C5'-C4'-O4'	6.78	117.24	109.10
2	AB	2129	C	N1-C2-O2	6.78	122.97	118.90
2	AB	285	G	O4'-C1'-N9	6.78	113.62	108.20
2	AB	583	G	O4'-C1'-N9	6.78	113.62	108.20
34	BA	60	A	P-O3'-C3'	6.78	127.84	119.70
34	BA	828	U	O4'-C1'-N1	6.78	113.62	108.20
34	BA	888	G	O4'-C1'-N9	6.78	113.62	108.20
2	AB	2109	U	O4'-C1'-N1	6.78	113.62	108.20
2	AB	494	G	O4'-C1'-N9	6.78	113.62	108.20
2	AB	826	U	O4'-C1'-N1	6.78	113.62	108.20
2	AB	2045	C	O4'-C1'-N1	6.78	113.62	108.20
2	AB	27	G	O4'-C1'-N9	6.77	113.62	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	559	G	C5'-C4'-O4'	6.77	117.22	109.10
2	AB	2403	C	O4'-C1'-N1	6.77	113.61	108.20
34	BA	405	U	O4'-C1'-N1	6.76	113.61	108.20
1	AA	32	U	O4'-C1'-N1	6.76	113.61	108.20
2	AB	35	G	N3-C4-C5	-6.76	125.22	128.60
34	BA	1170	A	C5'-C4'-O4'	6.76	117.21	109.10
2	AB	21	A	O4'-C1'-N9	6.76	113.61	108.20
2	AB	1710	G	C5'-C4'-O4'	6.75	117.21	109.10
2	AB	2107	G	O4'-C1'-N9	6.75	113.60	108.20
34	BA	528	C	O4'-C1'-N1	6.75	113.60	108.20
2	AB	1860	G	C8-N9-C4	-6.75	103.70	106.40
34	BA	1172	C	C5'-C4'-C3'	-6.75	105.20	116.00
2	AB	2062	A	O3'-P-O5'	-6.75	91.18	104.00
34	BA	1413	A	O4'-C1'-N9	6.75	113.60	108.20
34	BA	467	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	1986	C	O4'-C1'-N1	6.74	113.59	108.20
2	AB	296	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	2792	A	C5'-C4'-O4'	6.74	117.19	109.10
2	AB	594	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	1213	A	C5'-C4'-O4'	6.74	117.19	109.10
1	AA	85	G	O4'-C1'-N9	6.74	113.59	108.20
2	AB	244	A	O4'-C1'-N9	6.74	113.59	108.20
2	AB	538	A	O4'-C1'-N9	6.74	113.59	108.20
2	AB	1049	C	O4'-C1'-N1	6.74	113.59	108.20
2	AB	2106	U	O4'-C1'-N1	6.74	113.59	108.20
2	AB	241	A	O4'-C1'-N9	6.73	113.59	108.20
34	BA	328	C	N1-C2-O2	6.73	122.94	118.90
2	AB	869	G	O4'-C1'-N9	6.73	113.58	108.20
34	BA	235	C	O4'-C1'-N1	6.73	113.58	108.20
34	BA	803	G	N3-C4-C5	-6.73	125.23	128.60
34	BA	391	G	O4'-C1'-N9	6.73	113.58	108.20
2	AB	920	A	O4'-C1'-N9	6.73	113.58	108.20
2	AB	419	U	O4'-C1'-N1	6.72	113.58	108.20
34	BA	1221	G	O4'-C1'-N9	6.72	113.58	108.20
2	AB	1297	C	O4'-C1'-N1	6.72	113.58	108.20
34	BA	638	U	C5'-C4'-O4'	6.72	117.16	109.10
2	AB	195	A	C5'-C4'-O4'	6.72	117.16	109.10
2	AB	1833	C	O4'-C1'-N1	6.72	113.58	108.20
2	AB	1916	A	O4'-C1'-N9	6.72	113.58	108.20
2	AB	2732	G	O4'-C1'-N9	6.72	113.57	108.20
34	BA	173	U	O4'-C1'-N1	6.72	113.57	108.20
2	AB	464	U	O4'-C1'-N1	6.71	113.57	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1084	G	C8-N9-C4	-6.71	103.72	106.40
34	BA	1533	C	O3'-P-O5'	6.71	116.76	104.00
34	BA	1109	C	O4'-C1'-N1	6.71	113.57	108.20
2	AB	834	G	N7-C8-N9	6.71	116.45	113.10
2	AB	230	G	C4'-C3'-C2'	-6.71	95.89	102.60
2	AB	1069	A	O4'-C1'-N9	6.71	113.57	108.20
2	AB	2716	C	C5'-C4'-O4'	6.71	117.15	109.10
34	BA	39	G	O4'-C1'-N9	6.71	113.57	108.20
34	BA	221	C	O4'-C1'-N1	6.71	113.57	108.20
1	AA	34	A	C5'-C4'-O4'	6.71	117.15	109.10
2	AB	395	U	O4'-C1'-N1	6.71	113.56	108.20
34	BA	1015	G	O4'-C1'-N9	6.71	113.56	108.20
2	AB	1991	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	2819	G	C5'-C4'-C3'	-6.70	105.28	116.00
28	Ab	9	TYR	CB-CG-CD1	-6.70	116.98	121.00
34	BA	157	U	O4'-C1'-N1	6.70	113.56	108.20
34	BA	1283	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	827	U	P-O3'-C3'	6.70	127.74	119.70
2	AB	2838	G	C5'-C4'-O4'	6.70	117.14	109.10
34	BA	859	G	C5'-C4'-O4'	6.70	117.14	109.10
34	BA	1235	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	183	C	O4'-C1'-N1	6.70	113.56	108.20
2	AB	1261	C	O4'-C1'-N1	6.70	113.56	108.20
2	AB	2692	G	C4'-C3'-C2'	-6.70	95.90	102.60
34	BA	1131	G	C5'-C4'-O4'	6.70	117.14	109.10
2	AB	694	U	O4'-C1'-N1	6.70	113.56	108.20
2	AB	1863	G	C5'-C4'-O4'	6.70	117.14	109.10
34	BA	907	A	C5'-C4'-C3'	-6.70	105.29	116.00
1	AA	67	G	C8-N9-C4	-6.69	103.72	106.40
2	AB	2353	G	O4'-C1'-N9	6.69	113.55	108.20
2	AB	2594	C	O4'-C1'-N1	6.69	113.55	108.20
32	Af	1	PRO	CA-N-CD	-6.69	102.13	111.50
34	BA	291	U	O4'-C1'-N1	6.69	113.55	108.20
2	AB	2206	C	O4'-C1'-N1	6.69	113.55	108.20
34	BA	1271	A	C5'-C4'-C3'	-6.69	105.30	116.00
34	BA	1346	A	O4'-C1'-N9	6.69	113.55	108.20
34	BA	536	C	O4'-C1'-N1	6.68	113.55	108.20
34	BA	1312	G	C5'-C4'-O4'	6.68	117.12	109.10
2	AB	2802	G	O4'-C1'-N9	6.68	113.55	108.20
2	AB	209	C	O4'-C1'-N1	6.68	113.54	108.20
2	AB	1562	U	O4'-C1'-N1	6.68	113.54	108.20
34	BA	988	G	O4'-C1'-N9	6.68	113.54	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	51	A	O4'-C1'-N9	6.68	113.54	108.20
2	AB	2790	U	O4'-C4'-C3'	6.68	111.44	106.10
2	AB	2732	G	C5'-C4'-C3'	-6.67	105.32	116.00
34	BA	477	C	O4'-C1'-N1	6.67	113.54	108.20
34	BA	736	C	C5'-C4'-O4'	6.67	117.11	109.10
2	AB	459	U	O4'-C1'-N1	6.67	113.54	108.20
2	AB	2005	A	O4'-C1'-N9	6.67	113.54	108.20
2	AB	96	C	O4'-C1'-N1	6.67	113.54	108.20
2	AB	121	G	O4'-C1'-N9	6.67	113.54	108.20
34	BA	804	U	O4'-C1'-N1	6.67	113.54	108.20
34	BA	1225	A	N9-C1'-C2'	6.67	122.67	114.00
34	BA	659	U	O4'-C1'-N1	6.67	113.54	108.20
34	BA	848	C	O4'-C1'-N1	6.67	113.53	108.20
2	AB	2236	U	O4'-C1'-N1	6.67	113.53	108.20
34	BA	551	U	O4'-C1'-N1	6.67	113.53	108.20
35	BB	42	C	O4'-C1'-N1	6.67	113.53	108.20
2	AB	2298	A	C5'-C4'-C3'	-6.67	105.34	116.00
34	BA	1192	C	O4'-C1'-N1	6.66	113.53	108.20
34	BA	951	G	C8-N9-C4	-6.66	103.74	106.40
35	BB	56	C	O4'-C1'-N1	6.66	113.53	108.20
2	AB	832	U	O4'-C1'-N1	6.66	113.53	108.20
2	AB	967	U	O4'-C1'-N1	6.66	113.53	108.20
34	BA	612	C	O4'-C1'-N1	6.65	113.52	108.20
2	AB	1006	C	O4'-C1'-N1	6.65	113.52	108.20
2	AB	1070	A	C3'-C2'-C1'	6.65	106.82	101.50
2	AB	1159	U	O4'-C1'-N1	6.65	113.52	108.20
2	AB	360	U	O4'-C1'-N1	6.64	113.52	108.20
2	AB	806	C	O4'-C1'-N1	6.64	113.52	108.20
34	BA	414	A	O3'-P-O5'	-6.64	91.38	104.00
2	AB	1935	G	O4'-C1'-N9	6.64	113.51	108.20
34	BA	180	U	O4'-C1'-N1	6.64	113.51	108.20
2	AB	2089	C	O4'-C1'-N1	6.64	113.51	108.20
2	AB	278	A	C8-N9-C4	-6.63	103.15	105.80
2	AB	325	G	O4'-C1'-N9	6.63	113.51	108.20
2	AB	791	C	O4'-C1'-N1	6.63	113.51	108.20
2	AB	1588	G	O4'-C1'-N9	6.63	113.51	108.20
2	AB	1847	A	O4'-C4'-C3'	6.63	111.41	106.10
34	BA	52	C	C5'-C4'-O4'	6.63	117.06	109.10
34	BA	147	G	C8-N9-C4	-6.63	103.75	106.40
2	AB	1990	C	O4'-C1'-N1	6.63	113.50	108.20
2	AB	1727	C	C5'-C4'-O4'	6.63	117.05	109.10
34	BA	933	G	N3-C4-C5	-6.63	125.29	128.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1571	A	O4'-C1'-N9	6.62	113.50	108.20
34	BA	246	A	C5'-C4'-O4'	6.62	117.05	109.10
2	AB	1331	G	C8-N9-C4	-6.62	103.75	106.40
2	AB	1951	U	P-O3'-C3'	6.62	127.65	119.70
1	AA	92	C	O4'-C1'-N1	6.62	113.50	108.20
2	AB	885	C	O4'-C1'-N1	6.62	113.50	108.20
34	BA	498	A	C8-N9-C4	-6.62	103.15	105.80
2	AB	1378	A	O4'-C1'-N9	6.62	113.50	108.20
2	AB	20	C	O4'-C1'-N1	6.62	113.50	108.20
34	BA	613	C	O4'-C1'-N1	6.62	113.49	108.20
35	BB	22	G	O4'-C1'-N9	6.62	113.49	108.20
2	AB	1859	U	O4'-C1'-N1	6.61	113.49	108.20
34	BA	132	C	O4'-C1'-N1	6.61	113.49	108.20
34	BA	1530	G	O4'-C1'-N9	6.61	113.49	108.20
2	AB	1976	U	O4'-C1'-N1	6.61	113.49	108.20
2	AB	1989	G	O4'-C1'-N9	6.61	113.49	108.20
34	BA	91	U	C5'-C4'-O4'	6.61	117.03	109.10
2	AB	361	G	P-O3'-C3'	6.61	127.63	119.70
34	BA	97	G	C8-N9-C4	-6.60	103.76	106.40
2	AB	655	A	P-O3'-C3'	6.60	127.62	119.70
2	AB	350	G	O4'-C1'-N9	6.60	113.48	108.20
34	BA	694	A	O4'-C1'-N9	6.60	113.48	108.20
2	AB	672	C	O4'-C1'-N1	6.60	113.48	108.20
2	AB	1422	G	C5'-C4'-O4'	6.60	117.02	109.10
2	AB	1516	G	O4'-C1'-N9	6.60	113.48	108.20
2	AB	188	G	O4'-C1'-N9	6.60	113.48	108.20
34	BA	653	U	C3'-C2'-C1'	6.60	106.78	101.50
2	AB	1881	C	O4'-C1'-N1	6.59	113.47	108.20
2	AB	2896	C	C5'-C4'-O4'	6.59	117.01	109.10
35	BE	18	G	O4'-C1'-N9	6.59	113.48	108.20
34	BA	1430	A	O4'-C1'-N9	6.59	113.47	108.20
34	BA	118	U	O4'-C1'-N1	6.59	113.47	108.20
2	AB	137	U	O4'-C1'-N1	6.59	113.47	108.20
2	AB	788	A	O4'-C1'-N9	6.58	113.47	108.20
34	BA	160	A	O4'-C1'-N9	6.58	113.47	108.20
34	BA	861	G	C8-N9-C4	-6.58	103.77	106.40
34	BA	857	C	O4'-C1'-N1	6.58	113.46	108.20
2	AB	67	U	O4'-C1'-N1	6.58	113.46	108.20
34	BA	341	C	O4'-C1'-N1	6.58	113.46	108.20
34	BA	603	U	O4'-C1'-N1	6.58	113.46	108.20
34	BA	310	G	C8-N9-C4	-6.58	103.77	106.40
34	BA	747	A	O4'-C1'-N9	6.58	113.46	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	333	G	N3-C4-C5	-6.57	125.31	128.60
34	BA	1010	U	O4'-C1'-N1	6.57	113.46	108.20
2	AB	1460	U	O4'-C1'-N1	6.57	113.46	108.20
2	AB	2395	C	O4'-C1'-N1	6.57	113.46	108.20
34	BA	1103	C	O4'-C1'-N1	6.57	113.46	108.20
2	AB	2208	C	O4'-C1'-N1	6.57	113.45	108.20
2	AB	2067	G	O4'-C4'-C3'	6.56	111.35	106.10
34	BA	1104	G	C5'-C4'-O4'	6.56	116.98	109.10
34	BA	1409	C	C5'-C4'-C3'	-6.56	105.50	116.00
2	AB	1109	C	O4'-C1'-N1	6.56	113.45	108.20
34	BA	58	C	O4'-C1'-N1	6.56	113.45	108.20
35	BE	7	A	O4'-C1'-N9	6.56	113.44	108.20
2	AB	2523	G	C5'-C4'-O4'	6.55	116.97	109.10
1	AA	19	C	O4'-C1'-N1	6.55	113.44	108.20
2	AB	544	C	P-O3'-C3'	6.55	127.56	119.70
2	AB	2247	A	C5'-C4'-C3'	-6.55	105.52	116.00
34	BA	1006	G	O4'-C1'-N9	6.55	113.44	108.20
2	AB	424	G	N9-C1'-C2'	-6.55	104.80	112.00
2	AB	2758	A	C5'-C4'-O4'	6.55	116.96	109.10
2	AB	2804	U	O4'-C1'-N1	6.55	113.44	108.20
2	AB	234	U	O4'-C1'-N1	6.55	113.44	108.20
1	AA	42	C	O4'-C1'-N1	6.55	113.44	108.20
2	AB	831	G	O4'-C1'-N9	6.55	113.44	108.20
34	BA	379	C	C4'-C3'-C2'	-6.55	96.05	102.60
34	BA	671	G	O4'-C1'-N9	6.54	113.43	108.20
1	AA	71	C	O4'-C1'-N1	6.54	113.43	108.20
34	BA	57	G	C8-N9-C4	-6.54	103.78	106.40
34	BA	403	C	O4'-C1'-N1	6.54	113.43	108.20
34	BA	772	U	O4'-C1'-N1	6.54	113.43	108.20
34	BA	990	C	O4'-C1'-N1	6.54	113.43	108.20
2	AB	1310	G	C5'-C4'-C3'	-6.54	105.54	116.00
2	AB	1913	A	O4'-C1'-N9	6.54	113.43	108.20
2	AB	1291	C	O4'-C1'-N1	6.53	113.43	108.20
35	BB	60	U	O4'-C1'-N1	6.53	113.43	108.20
2	AB	2720	U	O4'-C1'-N1	6.53	113.42	108.20
2	AB	2819	G	C5'-C4'-O4'	6.53	116.94	109.10
34	BA	792	A	C1'-O4'-C4'	-6.53	104.67	109.90
34	BA	1304	G	O4'-C1'-N9	6.53	113.43	108.20
2	AB	394	C	O4'-C1'-N1	6.53	113.42	108.20
2	AB	166	U	O4'-C1'-N1	6.53	113.42	108.20
2	AB	2392	A	C8-N9-C4	-6.53	103.19	105.80
2	AB	999	U	O4'-C1'-N1	6.53	113.42	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1057	A	O4'-C1'-N9	6.52	113.42	108.20
35	BE	59	U	O4'-C1'-N1	6.52	113.42	108.20
34	BA	248	C	O4'-C1'-N1	6.52	113.42	108.20
2	AB	852	U	O4'-C1'-N1	6.52	113.42	108.20
2	AB	1035	U	O4'-C1'-N1	6.52	113.42	108.20
2	AB	1097	U	C5'-C4'-O4'	6.52	116.92	109.10
2	AB	2668	G	O4'-C1'-N9	6.52	113.41	108.20
2	AB	2820	A	O4'-C1'-N9	6.51	113.41	108.20
34	BA	271	C	C5'-C4'-O4'	6.51	116.92	109.10
2	AB	2043	C	O4'-C1'-N1	6.51	113.41	108.20
34	BA	1037	C	O4'-C1'-N1	6.51	113.41	108.20
34	BA	1273	C	O4'-C1'-N1	6.51	113.41	108.20
1	AA	74	U	O4'-C1'-N1	6.50	113.40	108.20
2	AB	2760	C	C5'-C4'-C3'	-6.50	105.59	116.00
35	BB	3	C	O4'-C1'-N1	6.50	113.40	108.20
2	AB	283	G	O4'-C1'-N9	6.50	113.40	108.20
2	AB	1105	U	O4'-C1'-N1	6.50	113.40	108.20
2	AB	1730	C	N1-C2-O2	6.50	122.80	118.90
2	AB	1913	A	O4'-C1'-C2'	-6.50	99.30	105.80
1	AA	91	C	O4'-C1'-N1	6.49	113.39	108.20
2	AB	352	A	O4'-C1'-N9	6.49	113.39	108.20
2	AB	954	G	C5'-C4'-O4'	6.49	116.89	109.10
2	AB	897	C	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2039	U	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2299	U	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2747	G	O4'-C1'-N9	6.49	113.39	108.20
34	BA	484	G	O4'-C1'-N9	6.49	113.39	108.20
1	AA	98	G	C5'-C4'-O4'	6.49	116.88	109.10
2	AB	1907	G	O4'-C1'-N9	6.49	113.39	108.20
2	AB	2343	U	O4'-C1'-N1	6.49	113.39	108.20
2	AB	2543	G	N3-C4-C5	-6.49	125.36	128.60
34	BA	246	A	C5'-C4'-C3'	-6.48	105.63	116.00
34	BA	850	U	O4'-C1'-N1	6.48	113.38	108.20
2	AB	2500	U	O4'-C1'-N1	6.48	113.38	108.20
2	AB	528	A	O4'-C1'-N9	6.47	113.38	108.20
2	AB	1348	C	O4'-C1'-N1	6.47	113.38	108.20
34	BA	242	G	O4'-C1'-N9	6.47	113.38	108.20
2	AB	2515	C	O4'-C1'-N1	6.47	113.38	108.20
2	AB	2097	A	O4'-C1'-N9	6.47	113.37	108.20
34	BA	194	C	C2-N3-C4	6.47	123.13	119.90
2	AB	94	A	O4'-C1'-N9	6.46	113.37	108.20
2	AB	201	C	O4'-C1'-N1	6.46	113.37	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	492	C	O4'-C1'-N1	6.46	113.37	108.20
34	BA	1110	A	O4'-C1'-N9	6.46	113.37	108.20
2	AB	26	G	O4'-C1'-N9	6.45	113.36	108.20
34	BA	1009	U	O4'-C1'-N1	6.45	113.36	108.20
34	BA	1153	G	O4'-C1'-N9	6.45	113.36	108.20
2	AB	1402	U	C5'-C4'-O4'	6.45	116.84	109.10
2	AB	2849	U	O4'-C1'-N1	6.45	113.36	108.20
34	BA	632	U	O4'-C1'-N1	6.45	113.36	108.20
34	BA	314	C	O4'-C1'-N1	6.45	113.36	108.20
34	BA	1408	A	C5'-C4'-O4'	6.44	116.83	109.10
2	AB	157	C	O4'-C1'-N1	6.44	113.35	108.20
34	BA	6	G	C5'-C4'-C3'	-6.44	105.69	116.00
34	BA	1270	G	O4'-C1'-N9	6.44	113.35	108.20
2	AB	569	U	O4'-C1'-N1	6.44	113.35	108.20
34	BA	296	U	C5'-C4'-C3'	-6.44	105.70	116.00
34	BA	360	G	O4'-C1'-N9	6.44	113.35	108.20
34	BA	741	G	O4'-C1'-N9	6.44	113.35	108.20
2	AB	441	U	O4'-C1'-N1	6.44	113.35	108.20
2	AB	1662	U	O4'-C1'-N1	6.44	113.35	108.20
2	AB	2085	U	O4'-C1'-N1	6.44	113.35	108.20
2	AB	1641	A	C5'-C4'-C3'	-6.44	105.70	116.00
2	AB	2751	G	C2'-C3'-O3'	6.44	124.00	113.70
2	AB	1844	C	O4'-C1'-N1	6.44	113.35	108.20
34	BA	123	U	O4'-C1'-N1	6.43	113.35	108.20
34	BA	1458	G	O4'-C1'-N9	6.43	113.35	108.20
2	AB	192	C	O4'-C1'-N1	6.43	113.34	108.20
2	AB	611	C	O4'-C1'-N1	6.43	113.35	108.20
2	AB	2314	A	C5'-C4'-C3'	-6.43	105.71	116.00
2	AB	200	U	O4'-C1'-N1	6.43	113.34	108.20
34	BA	220	G	N3-C4-C5	-6.43	125.39	128.60
34	BA	369	G	O4'-C1'-N9	6.43	113.34	108.20
2	AB	440	C	C5'-C4'-O4'	6.42	116.81	109.10
2	AB	872	U	O4'-C1'-N1	6.42	113.34	108.20
2	AB	1134	A	O4'-C1'-N9	6.42	113.34	108.20
2	AB	397	U	O4'-C1'-N1	6.42	113.34	108.20
2	AB	2189	U	O4'-C1'-N1	6.42	113.34	108.20
1	AA	64	G	O4'-C1'-N9	6.42	113.34	108.20
2	AB	1174	U	O4'-C1'-N1	6.42	113.34	108.20
2	AB	358	U	O4'-C1'-N1	6.42	113.33	108.20
2	AB	1703	G	C5'-C4'-C3'	-6.42	105.73	116.00
34	BA	641	U	O4'-C4'-C3'	6.42	111.23	106.10
34	BA	771	G	O4'-C1'-N9	6.42	113.33	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	70	G	O4'-C1'-N9	6.42	113.33	108.20
2	AB	916	G	C8-N9-C4	-6.41	103.83	106.40
2	AB	1114	C	C5'-C4'-O4'	6.41	116.80	109.10
2	AB	1487	U	C5'-C4'-C3'	-6.41	105.74	116.00
34	BA	929	G	O4'-C1'-N9	6.41	113.33	108.20
2	AB	701	G	C5'-C4'-C3'	-6.41	105.74	116.00
2	AB	1952	A	C3'-C2'-C1'	6.41	106.63	101.50
34	BA	1073	U	O4'-C1'-N1	6.41	113.33	108.20
2	AB	1098	A	C5'-C4'-C3'	-6.41	105.75	116.00
2	AB	2091	C	O4'-C1'-N1	6.41	113.33	108.20
2	AB	2146	C	O3'-P-O5'	-6.41	91.83	104.00
2	AB	1258	U	O4'-C1'-N1	6.41	113.33	108.20
2	AB	2683	C	O4'-C1'-N1	6.41	113.33	108.20
34	BA	770	C	C4'-C3'-C2'	-6.41	96.19	102.60
35	BB	65	G	C5'-C4'-C3'	-6.41	105.75	116.00
34	BA	358	U	O4'-C1'-N1	6.40	113.32	108.20
34	BA	933	G	C5'-C4'-O4'	6.40	116.78	109.10
2	AB	1457	U	O4'-C1'-N1	6.40	113.32	108.20
34	BA	1535	C	O5'-C5'-C4'	6.40	123.86	111.70
2	AB	1068	G	O3'-P-O5'	-6.40	91.84	104.00
34	BA	111	G	O4'-C1'-N9	6.40	113.32	108.20
34	BA	70	U	O4'-C1'-N1	6.40	113.32	108.20
34	BA	847	G	C8-N9-C4	-6.40	103.84	106.40
2	AB	1694	C	N1-C2-O2	6.39	122.74	118.90
34	BA	220	G	C8-N9-C4	-6.39	103.84	106.40
2	AB	790	U	O4'-C1'-N1	6.39	113.31	108.20
2	AB	873	C	O4'-C1'-N1	6.39	113.31	108.20
34	BA	1098	C	O4'-C1'-N1	6.39	113.31	108.20
2	AB	2779	U	O4'-C1'-N1	6.39	113.31	108.20
2	AB	286	U	O4'-C1'-N1	6.39	113.31	108.20
2	AB	2585	U	O4'-C1'-N1	6.39	113.31	108.20
34	BA	100	G	C5'-C4'-O4'	6.39	116.76	109.10
34	BA	179	A	C5'-C4'-C3'	-6.39	105.78	116.00
2	AB	1180	U	C5'-C4'-O4'	6.38	116.76	109.10
2	AB	1352	U	O4'-C1'-N1	6.38	113.31	108.20
2	AB	1599	U	O4'-C1'-N1	6.38	113.31	108.20
34	BA	218	U	O4'-C1'-N1	6.38	113.31	108.20
2	AB	2193	G	O4'-C1'-N9	6.38	113.31	108.20
35	BE	58	A	C5'-C4'-C3'	-6.38	105.79	116.00
2	AB	557	C	O4'-C1'-N1	6.38	113.30	108.20
2	AB	314	C	O4'-C1'-N1	6.38	113.30	108.20
2	AB	2854	G	C5'-C4'-O4'	6.38	116.75	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1293	C	O4'-C1'-N1	6.38	113.30	108.20
2	AB	1183	U	C5'-C4'-C3'	-6.38	105.80	116.00
2	AB	248	G	O4'-C1'-N9	6.37	113.30	108.20
2	AB	2016	U	O3'-P-O5'	-6.37	91.89	104.00
34	BA	193	C	C5'-C4'-O4'	6.37	116.74	109.10
1	AA	1	U	O4'-C1'-N1	6.36	113.29	108.20
2	AB	462	C	O4'-C1'-N1	6.36	113.29	108.20
37	BD	31	U	C5'-C4'-O4'	6.36	116.74	109.10
37	BD	34	U	O4'-C1'-N1	6.36	113.29	108.20
34	BA	265	G	C8-N9-C4	-6.36	103.86	106.40
2	AB	493	G	O4'-C1'-N9	6.36	113.29	108.20
2	AB	1054	A	O4'-C1'-N9	6.36	113.29	108.20
2	AB	1116	G	O4'-C1'-N9	6.36	113.29	108.20
2	AB	2379	G	O4'-C1'-N9	6.36	113.29	108.20
28	Ab	53	THR	C-N-CA	6.36	135.66	122.30
2	AB	722	A	C5'-C4'-C3'	-6.36	105.83	116.00
2	AB	1266	G	O4'-C1'-N9	6.36	113.29	108.20
2	AB	2408	U	O4'-C1'-N1	6.36	113.28	108.20
2	AB	2425	A	O4'-C1'-C2'	-6.36	99.44	105.80
2	AB	2718	G	C5'-C4'-O4'	6.36	116.73	109.10
2	AB	2508	G	O4'-C1'-N9	6.35	113.28	108.20
2	AB	845	A	O4'-C1'-N9	6.35	113.28	108.20
34	BA	2	A	C5'-C4'-O4'	6.35	116.72	109.10
34	BA	4	U	C5'-C4'-C3'	-6.35	105.83	116.00
34	BA	653	U	O4'-C1'-N1	6.35	113.28	108.20
2	AB	1731	G	C8-N9-C4	-6.35	103.86	106.40
2	AB	125	A	O4'-C1'-C2'	-6.35	99.45	105.80
2	AB	1872	A	C8-N9-C4	-6.35	103.26	105.80
2	AB	2131	U	O4'-C1'-N1	6.35	113.28	108.20
2	AB	310	A	C5'-C4'-C3'	-6.35	105.84	116.00
2	AB	1989	G	C5'-C4'-O4'	6.35	116.72	109.10
2	AB	2319	G	O4'-C1'-N9	6.35	113.28	108.20
34	BA	486	U	O4'-C1'-N1	6.35	113.28	108.20
2	AB	948	C	O4'-C1'-N1	6.34	113.28	108.20
2	AB	2676	C	O4'-C1'-N1	6.34	113.28	108.20
2	AB	1338	G	O4'-C1'-N9	6.34	113.27	108.20
2	AB	417	C	O4'-C1'-N1	6.34	113.27	108.20
34	BA	1453	G	N3-C4-C5	-6.34	125.43	128.60
2	AB	813	U	O4'-C1'-N1	6.34	113.27	108.20
34	BA	793	U	C1'-O4'-C4'	-6.34	104.83	109.90
34	BA	1308	U	O4'-C1'-N1	6.34	113.27	108.20
34	BA	701	U	C1'-O4'-C4'	-6.34	104.83	109.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	413	C	O4'-C1'-N1	6.33	113.27	108.20
2	AB	1702	G	O4'-C1'-N9	6.33	113.27	108.20
2	AB	798	G	O4'-C1'-N9	6.33	113.27	108.20
34	BA	228	A	C5'-C4'-C3'	-6.33	105.87	116.00
34	BA	1243	C	O4'-C1'-N1	6.33	113.26	108.20
2	AB	1123	C	C5'-C4'-O4'	6.33	116.69	109.10
2	AB	1746	A	O3'-P-O5'	-6.33	91.98	104.00
34	BA	1487	G	O4'-C1'-N9	6.33	113.26	108.20
1	AA	67	G	C5'-C4'-O4'	6.32	116.69	109.10
2	AB	2521	C	O4'-C1'-N1	6.32	113.26	108.20
34	BA	1268	G	C5'-C4'-O4'	6.32	116.69	109.10
2	AB	2554	U	O4'-C1'-N1	6.32	113.26	108.20
34	BA	812	G	O3'-P-O5'	-6.32	91.99	104.00
2	AB	267	C	O4'-C1'-N1	6.32	113.25	108.20
2	AB	2629	U	O4'-C1'-N1	6.32	113.25	108.20
2	AB	1734	G	O4'-C1'-N9	6.32	113.25	108.20
34	BA	636	U	C4'-C3'-C2'	-6.32	96.28	102.60
2	AB	1722	A	C5'-C4'-C3'	-6.31	105.90	116.00
34	BA	68	G	N9-C1'-C2'	-6.31	105.06	112.00
34	BA	939	G	O4'-C1'-N9	6.31	113.25	108.20
2	AB	2227	A	O4'-C1'-N9	6.31	113.25	108.20
34	BA	843	U	C5'-C4'-C3'	-6.31	105.90	116.00
2	AB	1504	A	O4'-C1'-N9	6.31	113.25	108.20
34	BA	259	G	O4'-C1'-N9	6.31	113.25	108.20
34	BA	884	U	O4'-C1'-N1	6.31	113.25	108.20
2	AB	1103	A	O4'-C1'-N9	6.31	113.25	108.20
2	AB	1811	G	O4'-C1'-N9	6.31	113.25	108.20
34	BA	211	G	C2-N3-C4	6.31	115.05	111.90
34	BA	1477	U	C5'-C4'-O4'	6.31	116.67	109.10
2	AB	895	U	P-O3'-C3'	6.30	127.27	119.70
35	BE	49	C	O4'-C1'-N1	6.30	113.24	108.20
35	BB	15	G	C8-N9-C4	-6.30	103.88	106.40
2	AB	1535	A	O3'-P-O5'	-6.30	92.03	104.00
2	AB	2318	G	O4'-C1'-N9	6.30	113.24	108.20
2	AB	22	C	O4'-C1'-N1	6.30	113.24	108.20
2	AB	2179	C	O4'-C1'-N1	6.30	113.24	108.20
2	AB	2040	G	C5'-C4'-C3'	-6.29	105.93	116.00
2	AB	1183	U	C3'-C2'-C1'	6.29	106.53	101.50
2	AB	1656	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	2199	A	C5'-C4'-O4'	6.29	116.65	109.10
2	AB	2675	A	O4'-C1'-N9	6.29	113.23	108.20
2	AB	1695	G	N3-C4-C5	-6.29	125.45	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2072	C	O4'-C1'-N1	6.29	113.23	108.20
1	AA	31	C	C5'-C4'-O4'	6.29	116.65	109.10
2	AB	570	G	O4'-C1'-N9	6.29	113.23	108.20
2	AB	995	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	1806	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	1763	G	C5'-C4'-C3'	-6.29	105.94	116.00
34	BA	217	C	C5'-C4'-C3'	-6.29	105.94	116.00
34	BA	233	C	O4'-C1'-N1	6.29	113.23	108.20
34	BA	286	C	O4'-C1'-N1	6.29	113.23	108.20
34	BA	620	C	O4'-C1'-N1	6.29	113.23	108.20
34	BA	779	C	O4'-C1'-N1	6.29	113.23	108.20
2	AB	1528	A	O4'-C1'-N9	6.28	113.23	108.20
2	AB	2567	G	N3-C4-C5	-6.28	125.46	128.60
2	AB	647	G	O4'-C1'-N9	6.28	113.22	108.20
2	AB	2568	U	O4'-C1'-N1	6.28	113.22	108.20
2	AB	490	C	C5'-C4'-O4'	6.28	116.64	109.10
1	AA	4	C	O4'-C1'-N1	6.28	113.22	108.20
2	AB	1180	U	O4'-C1'-N1	6.28	113.22	108.20
2	AB	2506	U	O3'-P-O5'	-6.28	92.07	104.00
34	BA	346	G	N3-C4-C5	-6.28	125.46	128.60
2	AB	586	A	O4'-C1'-N9	6.27	113.22	108.20
2	AB	989	G	O4'-C1'-N9	6.27	113.22	108.20
2	AB	47	C	O4'-C1'-N1	6.27	113.22	108.20
2	AB	2214	C	O4'-C1'-N1	6.27	113.22	108.20
34	BA	910	C	O4'-C1'-N1	6.27	113.22	108.20
2	AB	1501	G	O4'-C1'-N9	6.27	113.22	108.20
2	AB	2124	G	C5'-C4'-C3'	-6.27	105.97	116.00
34	BA	854	U	O4'-C1'-N1	6.27	113.22	108.20
34	BA	1353	G	C5'-C4'-O4'	6.27	116.62	109.10
2	AB	275	C	O4'-C1'-N1	6.27	113.21	108.20
34	BA	456	A	O4'-C1'-N9	6.27	113.21	108.20
34	BA	823	C	O4'-C1'-N1	6.27	113.21	108.20
2	AB	2599	G	O4'-C1'-N9	6.26	113.21	108.20
2	AB	1249	U	O4'-C1'-N1	6.26	113.21	108.20
2	AB	1606	C	N1-C2-O2	6.26	122.66	118.90
2	AB	2740	A	C5'-C4'-O4'	6.26	116.61	109.10
36	BC	87	TYR	CB-CG-CD1	-6.26	117.24	121.00
2	AB	2134	A	O4'-C1'-N9	6.26	113.21	108.20
34	BA	801	U	O4'-C1'-N1	6.26	113.21	108.20
2	AB	151	C	O4'-C1'-N1	6.26	113.21	108.20
2	AB	1558	C	O4'-C1'-N1	6.26	113.21	108.20
2	AB	1725	U	C5'-C4'-C3'	-6.26	105.99	116.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2194	U	O4'-C1'-N1	6.26	113.20	108.20
34	BA	462	G	O4'-C1'-N9	6.26	113.20	108.20
2	AB	364	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	215	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	896	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	1429	A	O4'-C1'-N9	6.25	113.20	108.20
2	AB	2485	G	C3'-C2'-C1'	-6.25	96.50	101.50
2	AB	687	C	O4'-C1'-N1	6.25	113.20	108.20
34	BA	154	U	C5'-C4'-O4'	6.25	116.60	109.10
34	BA	1103	C	C5'-C4'-C3'	-6.25	106.00	116.00
2	AB	184	C	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2185	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2291	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2796	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	911	A	O4'-C1'-N9	6.25	113.20	108.20
37	BD	30	U	O4'-C1'-N1	6.25	113.20	108.20
2	AB	2387	U	O4'-C1'-N1	6.24	113.19	108.20
34	BA	931	C	O4'-C1'-N1	6.24	113.19	108.20
2	AB	416	U	O4'-C1'-N1	6.24	113.19	108.20
2	AB	1303	G	C5'-C4'-C3'	-6.24	106.02	116.00
2	AB	2221	G	O4'-C1'-N9	6.24	113.19	108.20
2	AB	460	A	O4'-C1'-N9	6.24	113.19	108.20
2	AB	527	C	O4'-C1'-N1	6.24	113.19	108.20
2	AB	1142	A	P-O3'-C3'	6.24	127.19	119.70
2	AB	1688	U	C5'-C4'-O4'	6.24	116.59	109.10
34	BA	1143	G	C8-N9-C4	-6.24	103.91	106.40
2	AB	578	G	O4'-C1'-N9	6.24	113.19	108.20
2	AB	2012	G	C8-N9-C4	-6.24	103.91	106.40
2	AB	2869	G	O4'-C1'-N9	6.24	113.19	108.20
34	BA	426	U	O4'-C1'-N1	6.24	113.19	108.20
2	AB	1940	U	N1-C1'-C2'	6.23	122.10	114.00
34	BA	1052	U	O4'-C1'-N1	6.23	113.19	108.20
2	AB	131	A	O4'-C1'-N9	6.23	113.18	108.20
2	AB	2067	G	O4'-C1'-N9	6.23	113.18	108.20
34	BA	355	C	O4'-C1'-N1	6.22	113.18	108.20
34	BA	838	G	C8-N9-C4	-6.22	103.91	106.40
2	AB	425	G	O4'-C1'-N9	6.22	113.18	108.20
2	AB	1154	G	C8-N9-C4	-6.22	103.91	106.40
34	BA	406	G	N3-C4-C5	-6.22	125.49	128.60
2	AB	173	A	O4'-C1'-N9	6.22	113.17	108.20
34	BA	897	C	O4'-C1'-N1	6.22	113.17	108.20
2	AB	3	U	O4'-C1'-N1	6.22	113.17	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	172	A	O4'-C1'-N9	6.21	113.17	108.20
2	AB	2442	C	O4'-C1'-N1	6.21	113.17	108.20
2	AB	101	A	O4'-C1'-N9	6.21	113.17	108.20
2	AB	1481	U	O4'-C1'-N1	6.21	113.17	108.20
1	AA	84	G	O4'-C1'-N9	6.21	113.17	108.20
2	AB	103	A	C5'-C4'-O4'	6.21	116.55	109.10
34	BA	847	G	N3-C4-C5	-6.21	125.50	128.60
2	AB	205	G	O4'-C1'-N9	6.21	113.17	108.20
2	AB	1368	G	O4'-C1'-N9	6.21	113.17	108.20
2	AB	1600	C	O4'-C1'-N1	6.21	113.17	108.20
2	AB	2461	A	O4'-C1'-N9	6.21	113.17	108.20
2	AB	369	U	O4'-C1'-N1	6.21	113.17	108.20
2	AB	2769	U	C5'-C4'-O4'	6.21	116.55	109.10
34	BA	998	C	C5'-C4'-C3'	-6.21	106.07	116.00
2	AB	893	C	O4'-C1'-N1	6.20	113.16	108.20
34	BA	1203	C	C5'-C4'-O4'	6.20	116.54	109.10
2	AB	334	C	O4'-C1'-N1	6.20	113.16	108.20
34	BA	1434	A	O4'-C1'-N9	6.20	113.16	108.20
34	BA	1138	G	P-O3'-C3'	6.20	127.14	119.70
34	BA	269	C	O4'-C1'-N1	6.19	113.16	108.20
34	BA	1310	G	O4'-C1'-N9	6.19	113.15	108.20
2	AB	989	G	C1'-O4'-C4'	-6.19	104.95	109.90
2	AB	947	A	O4'-C1'-N9	6.19	113.15	108.20
2	AB	2513	A	C5'-C4'-O4'	6.19	116.52	109.10
34	BA	1446	A	O4'-C1'-N9	6.19	113.15	108.20
35	BB	28	G	N3-C4-C5	-6.19	125.51	128.60
2	AB	988	A	O4'-C1'-N9	6.18	113.15	108.20
2	AB	1573	G	C5'-C4'-O4'	6.18	116.52	109.10
2	AB	122	G	O4'-C1'-N9	6.18	113.15	108.20
2	AB	1467	U	O4'-C1'-N1	6.18	113.15	108.20
2	AB	2746	U	O4'-C1'-N1	6.18	113.15	108.20
35	BB	41	C	O4'-C1'-N1	6.18	113.14	108.20
2	AB	2493	U	O4'-C1'-N1	6.18	113.14	108.20
2	AB	2460	U	O4'-C1'-N1	6.18	113.14	108.20
34	BA	1173	U	O4'-C1'-N1	6.18	113.14	108.20
2	AB	2528	U	O4'-C1'-N1	6.18	113.14	108.20
34	BA	400	C	O4'-C1'-N1	6.18	113.14	108.20
34	BA	410	G	O4'-C1'-N9	6.18	113.14	108.20
2	AB	1936	A	O4'-C1'-N9	6.17	113.14	108.20
2	AB	2112	G	O4'-C1'-N9	6.17	113.14	108.20
2	AB	2753	A	C8-N9-C4	-6.17	103.33	105.80
34	BA	352	C	O4'-C1'-N1	6.17	113.14	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1790	C	O4'-C1'-N1	6.17	113.14	108.20
2	AB	2028	U	C5'-C4'-O4'	6.17	116.51	109.10
2	AB	2829	A	O4'-C1'-N9	6.17	113.14	108.20
2	AB	393	C	O4'-C1'-N1	6.17	113.14	108.20
2	AB	649	G	O4'-C1'-N9	6.17	113.13	108.20
2	AB	1214	A	O4'-C1'-N9	6.17	113.13	108.20
34	BA	644	U	O4'-C1'-N1	6.17	113.13	108.20
2	AB	10	A	C5'-C4'-C3'	-6.16	106.14	116.00
34	BA	1401	G	C8-N9-C4	-6.16	103.94	106.40
34	BA	1002	G	O4'-C1'-N9	6.16	113.13	108.20
34	BA	1089	G	O4'-C1'-N9	6.16	113.13	108.20
34	BA	1196	A	O4'-C1'-N9	6.16	113.13	108.20
2	AB	1390	U	O4'-C1'-N1	6.16	113.12	108.20
2	AB	1407	G	C5'-C4'-O4'	6.16	116.48	109.10
2	AB	650	C	O4'-C1'-N1	6.15	113.12	108.20
2	AB	1871	A	O4'-C1'-N9	6.15	113.12	108.20
2	AB	2214	C	C5'-C4'-O4'	6.15	116.48	109.10
2	AB	2366	A	O4'-C1'-N9	6.15	113.12	108.20
2	AB	2156	G	O4'-C1'-N9	6.15	113.12	108.20
2	AB	1810	A	C5'-C4'-C3'	-6.15	106.16	116.00
2	AB	1890	A	C8-N9-C4	-6.15	103.34	105.80
35	BB	12	U	O4'-C1'-N1	6.15	113.12	108.20
34	BA	934	C	C3'-C2'-C1'	6.14	106.42	101.50
2	AB	731	C	O4'-C1'-N1	6.14	113.11	108.20
2	AB	1119	U	O4'-C1'-N1	6.14	113.11	108.20
2	AB	1367	A	O4'-C1'-N9	6.14	113.11	108.20
2	AB	1082	U	O4'-C1'-N1	6.14	113.11	108.20
34	BA	730	G	C5'-C4'-C3'	-6.14	106.17	116.00
34	BA	1198	G	O4'-C1'-N9	6.14	113.11	108.20
2	AB	444	C	O4'-C1'-N1	6.14	113.11	108.20
2	AB	2567	G	C8-N9-C4	-6.14	103.94	106.40
2	AB	2880	C	N1-C2-O2	6.14	122.58	118.90
34	BA	883	C	O4'-C1'-N1	6.14	113.11	108.20
34	BA	1304	G	C5'-C4'-O4'	6.14	116.47	109.10
2	AB	1483	G	C5'-C4'-C3'	-6.14	106.18	116.00
2	AB	2253	G	O4'-C1'-N9	6.14	113.11	108.20
2	AB	1132	U	O4'-C1'-N1	6.13	113.11	108.20
2	AB	1560	G	C5'-C4'-C3'	-6.13	106.18	116.00
34	BA	1181	G	C5'-C4'-C3'	-6.13	106.18	116.00
2	AB	796	C	O4'-C1'-N1	6.13	113.11	108.20
2	AB	1199	U	O4'-C1'-N1	6.13	113.11	108.20
2	AB	2494	G	C5'-C4'-O4'	6.13	116.46	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2658	C	C5'-C4'-O4'	6.13	116.46	109.10
34	BA	1124	G	O4'-C1'-N9	6.13	113.11	108.20
2	AB	894	U	O4'-C1'-N1	6.13	113.10	108.20
34	BA	1188	A	O4'-C1'-N9	6.13	113.10	108.20
1	AA	95	U	C5'-C4'-C3'	-6.13	106.20	116.00
2	AB	2597	G	C5'-C4'-O4'	6.13	116.45	109.10
2	AB	1530	G	C8-N9-C4	-6.12	103.95	106.40
34	BA	68	G	O4'-C1'-N9	6.12	113.10	108.20
2	AB	210	C	O4'-C1'-N1	6.12	113.10	108.20
2	AB	505	A	O4'-C1'-N9	6.12	113.10	108.20
2	AB	867	C	O4'-C1'-N1	6.12	113.10	108.20
2	AB	1752	C	O4'-C1'-N1	6.12	113.10	108.20
2	AB	2635	A	O4'-C1'-N9	6.12	113.10	108.20
2	AB	2664	G	O4'-C1'-N9	6.12	113.10	108.20
34	BA	1115	U	C5'-C4'-O4'	6.12	116.44	109.10
2	AB	1792	G	C5'-C4'-O4'	6.12	116.44	109.10
2	AB	99	U	O4'-C1'-N1	6.12	113.09	108.20
2	AB	497	A	O4'-C1'-N9	6.12	113.09	108.20
2	AB	525	U	O4'-C1'-N1	6.12	113.09	108.20
34	BA	714	G	O4'-C1'-N9	6.12	113.09	108.20
2	AB	1338	G	C5'-C4'-O4'	6.12	116.44	109.10
2	AB	1446	C	O4'-C1'-N1	6.12	113.09	108.20
2	AB	2233	U	O4'-C1'-N1	6.12	113.09	108.20
2	AB	1313	U	C5'-C4'-O4'	6.11	116.44	109.10
2	AB	1925	C	O4'-C1'-N1	6.11	113.09	108.20
34	BA	249	U	O4'-C1'-N1	6.11	113.09	108.20
34	BA	108	G	N3-C4-C5	-6.11	125.54	128.60
34	BA	749	A	C5'-C4'-O4'	6.11	116.44	109.10
2	AB	289	G	O4'-C1'-N9	6.11	113.09	108.20
2	AB	1415	U	C2'-C3'-O3'	6.11	123.47	113.70
2	AB	1215	G	O4'-C1'-N9	6.11	113.09	108.20
2	AB	2860	A	C5'-C4'-C3'	-6.11	106.23	116.00
34	BA	503	C	C5'-C4'-O4'	6.11	116.43	109.10
34	BA	915	A	O4'-C1'-N9	6.11	113.09	108.20
34	BA	1276	G	C5'-C4'-O4'	6.11	116.43	109.10
2	AB	912	C	C5'-C4'-O4'	6.11	116.43	109.10
2	AB	1533	C	O4'-C1'-N1	6.10	113.08	108.20
2	AB	2059	A	O4'-C1'-N9	6.10	113.08	108.20
2	AB	2664	G	N9-C4-C5	6.10	107.84	105.40
34	BA	19	A	O4'-C1'-N9	6.10	113.08	108.20
35	BE	15	G	O4'-C1'-N9	6.10	113.08	108.20
2	AB	347	A	C5'-C4'-O4'	6.10	116.42	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1479	G	O4'-C1'-N9	6.10	113.08	108.20
34	BA	211	G	C8-N9-C4	-6.10	103.96	106.40
2	AB	607	U	O4'-C1'-N1	6.10	113.08	108.20
2	AB	1554	U	O4'-C1'-N1	6.10	113.08	108.20
2	AB	2255	G	O4'-C1'-N9	6.10	113.08	108.20
2	AB	2311	A	O4'-C1'-N9	6.10	113.08	108.20
1	AA	14	U	C5'-C4'-C3'	-6.09	106.25	116.00
2	AB	2673	G	O4'-C1'-N9	6.09	113.08	108.20
35	BE	61	C	O4'-C1'-N1	6.09	113.08	108.20
2	AB	207	A	O4'-C1'-N9	6.09	113.07	108.20
2	AB	2889	C	O4'-C1'-N1	6.09	113.07	108.20
2	AB	1525	A	O4'-C1'-N9	6.09	113.07	108.20
2	AB	2511	U	O4'-C1'-N1	6.09	113.07	108.20
2	AB	2810	A	C5'-C4'-C3'	-6.09	106.25	116.00
34	BA	254	G	O4'-C1'-N9	6.09	113.07	108.20
1	AA	79	G	C8-N9-C4	-6.09	103.96	106.40
2	AB	237	C	O4'-C1'-N1	6.09	113.07	108.20
2	AB	340	A	O4'-C1'-N9	6.09	113.07	108.20
1	AA	36	C	C5'-C4'-C3'	-6.09	106.26	116.00
2	AB	1280	G	O4'-C1'-N9	6.09	113.07	108.20
2	AB	2031	A	O4'-C4'-C3'	6.09	110.97	106.10
34	BA	57	G	N3-C4-C5	-6.09	125.56	128.60
34	BA	1264	U	C4'-C3'-C2'	-6.09	96.51	102.60
2	AB	2599	G	C4'-C3'-C2'	-6.08	96.52	102.60
2	AB	488	G	C5'-C4'-O4'	6.08	116.40	109.10
2	AB	515	A	O4'-C1'-N9	6.08	113.06	108.20
2	AB	685	A	C8-N9-C4	-6.08	103.37	105.80
2	AB	1375	U	O4'-C1'-N1	6.08	113.06	108.20
2	AB	657	U	C3'-C2'-C1'	6.08	106.36	101.50
2	AB	1445	G	C8-N9-C4	-6.08	103.97	106.40
34	BA	101	A	O4'-C1'-N9	6.08	113.06	108.20
34	BA	1135	U	O4'-C1'-N1	6.08	113.06	108.20
1	AA	77	U	C2'-C3'-O3'	6.08	123.42	113.70
2	AB	2060	A	O4'-C1'-C2'	-6.08	99.72	105.80
34	BA	652	U	O4'-C1'-N1	6.08	113.06	108.20
34	BA	124	C	O4'-C1'-N1	6.08	113.06	108.20
34	BA	251	G	C8-N9-C4	-6.08	103.97	106.40
34	BA	604	G	C3'-C2'-C1'	-6.08	96.64	101.50
34	BA	1424	U	O4'-C1'-N1	6.08	113.06	108.20
2	AB	235	U	O4'-C1'-N1	6.07	113.06	108.20
2	AB	884	U	O4'-C1'-N1	6.07	113.06	108.20
2	AB	1773	A	C5'-C4'-O4'	6.07	116.39	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	407	U	O4'-C1'-N1	6.07	113.06	108.20
2	AB	839	U	O3'-P-O5'	-6.07	92.47	104.00
34	BA	1494	G	C5'-C4'-O4'	6.07	116.39	109.10
2	AB	291	G	O3'-P-O5'	-6.07	92.47	104.00
2	AB	560	C	O4'-C1'-N1	6.07	113.05	108.20
2	AB	907	G	C5'-C4'-O4'	6.07	116.38	109.10
2	AB	1216	G	C5'-C4'-C3'	-6.07	106.29	116.00
2	AB	2118	U	O4'-C1'-N1	6.07	113.05	108.20
34	BA	871	U	O4'-C1'-N1	6.07	113.05	108.20
2	AB	966	G	O4'-C1'-N9	6.06	113.05	108.20
2	AB	461	C	O4'-C1'-N1	6.06	113.05	108.20
2	AB	531	C	C1'-O4'-C4'	-6.06	105.05	109.90
2	AB	1076	C	O4'-C1'-N1	6.06	113.05	108.20
2	AB	2238	G	C5'-C4'-O4'	-6.06	101.83	109.10
35	BB	63	G	O4'-C1'-N9	6.06	113.05	108.20
2	AB	1109	C	O4'-C4'-C3'	6.06	110.94	106.10
2	AB	2087	G	C8-N9-C4	-6.06	103.98	106.40
2	AB	789	A	C5'-C4'-C3'	-6.05	106.32	116.00
34	BA	9	G	N3-C4-C5	-6.05	125.57	128.60
34	BA	760	G	O4'-C1'-N9	6.05	113.04	108.20
34	BA	1429	A	N9-C1'-C2'	-6.05	105.34	112.00
2	AB	793	A	O4'-C1'-N9	6.05	113.04	108.20
34	BA	398	U	O4'-C1'-N1	6.05	113.04	108.20
34	BA	1383	C	O4'-C1'-N1	6.05	113.04	108.20
34	BA	882	C	O4'-C1'-N1	6.05	113.04	108.20
2	AB	688	U	O4'-C1'-N1	6.05	113.04	108.20
2	AB	878	A	C8-N9-C4	-6.05	103.38	105.80
2	AB	913	U	C5'-C4'-C3'	-6.05	106.32	116.00
2	AB	927	A	O4'-C1'-N9	6.05	113.04	108.20
2	AB	2615	U	O4'-C1'-N1	6.05	113.04	108.20
34	BA	986	U	O4'-C1'-N1	6.05	113.04	108.20
2	AB	759	G	N3-C4-C5	-6.04	125.58	128.60
2	AB	760	G	O4'-C1'-N9	6.04	113.03	108.20
1	AA	5	U	O4'-C1'-N1	6.04	113.03	108.20
2	AB	1999	C	C5'-C4'-O4'	6.04	116.35	109.10
34	BA	74	A	O4'-C1'-N9	6.04	113.03	108.20
2	AB	976	G	C8-N9-C4	-6.04	103.98	106.40
2	AB	1550	C	C3'-C2'-C1'	6.04	106.33	101.50
2	AB	2774	C	O4'-C1'-N1	6.04	113.03	108.20
2	AB	190	A	C5'-C4'-C3'	-6.04	106.34	116.00
2	AB	270	A	O4'-C1'-N9	6.04	113.03	108.20
2	AB	1404	C	C5'-C4'-O4'	6.04	116.34	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1567	G	O4'-C1'-N9	6.04	113.03	108.20
2	AB	2559	C	C1'-O4'-C4'	-6.04	105.07	109.90
7	AG	132	ARG	NE-CZ-NH1	-6.04	117.28	120.30
2	AB	2724	U	O4'-C1'-N1	6.03	113.03	108.20
34	BA	588	G	O4'-C1'-N9	6.03	113.03	108.20
2	AB	2870	C	C3'-C2'-C1'	-6.03	96.68	101.50
34	BA	899	C	C4'-C3'-C2'	6.03	108.63	102.60
1	AA	16	G	C8-N9-C4	-6.03	103.99	106.40
2	AB	1645	G	C8-N9-C4	-6.03	103.99	106.40
34	BA	1057	G	O4'-C1'-N9	6.03	113.02	108.20
2	AB	1505	A	O4'-C1'-N9	6.03	113.02	108.20
2	AB	2744	G	C5'-C4'-O4'	6.03	116.33	109.10
34	BA	81	A	O4'-C1'-N9	6.03	113.02	108.20
34	BA	436	C	O4'-C1'-N1	6.03	113.02	108.20
34	BA	971	G	O4'-C1'-N9	6.03	113.02	108.20
2	AB	667	U	O4'-C1'-N1	6.02	113.02	108.20
2	AB	1055	G	C8-N9-C4	-6.02	103.99	106.40
2	AB	2328	A	O3'-P-O5'	-6.02	92.55	104.00
34	BA	165	G	C5'-C4'-C3'	-6.02	106.36	116.00
34	BA	622	A	C8-N9-C4	-6.02	103.39	105.80
2	AB	1456	G	O4'-C1'-N9	6.02	113.02	108.20
2	AB	1604	C	C5'-C4'-O4'	6.02	116.33	109.10
2	AB	1580	A	O4'-C1'-N9	6.02	113.02	108.20
2	AB	2767	C	O4'-C1'-N1	6.02	113.01	108.20
2	AB	377	G	C5'-C4'-C3'	-6.02	106.37	116.00
34	BA	670	G	N9-C1'-C2'	-6.02	105.38	112.00
2	AB	251	A	C8-N9-C4	-6.01	103.39	105.80
2	AB	916	G	O4'-C1'-N9	6.01	113.01	108.20
34	BA	987	G	C8-N9-C4	-6.01	103.99	106.40
34	BA	1137	C	O4'-C1'-N1	6.01	113.01	108.20
2	AB	839	U	O4'-C1'-N1	6.01	113.01	108.20
2	AB	1138	G	O4'-C1'-N9	6.01	113.01	108.20
34	BA	1395	C	C5'-C4'-O4'	6.01	116.31	109.10
2	AB	2190	G	C5'-C4'-O4'	6.01	116.31	109.10
2	AB	2192	U	C5'-C4'-O4'	6.01	116.31	109.10
34	BA	261	U	C5'-C4'-O4'	6.01	116.31	109.10
34	BA	764	C	C5'-C4'-O4'	6.01	116.31	109.10
34	BA	876	C	O4'-C1'-N1	6.01	113.01	108.20
2	AB	1107	G	O4'-C1'-N9	6.00	113.00	108.20
2	AB	1954	G	O4'-C1'-N9	6.00	113.00	108.20
35	BE	10	G	C8-N9-C4	-6.00	104.00	106.40
34	BA	941	G	C5'-C4'-C3'	-6.00	106.40	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1441	G	O4'-C1'-N9	6.00	113.00	108.20
2	AB	1451	C	C2'-C3'-O3'	6.00	123.30	113.70
2	AB	2338	C	O4'-C1'-N1	6.00	113.00	108.20
2	AB	1448	G	C5'-C4'-O4'	6.00	116.30	109.10
2	AB	2398	U	C5'-C4'-O4'	6.00	116.30	109.10
2	AB	2704	C	C5'-C4'-O4'	6.00	116.30	109.10
34	BA	13	U	O4'-C1'-N1	6.00	113.00	108.20
34	BA	846	G	C2-N3-C4	6.00	114.90	111.90
34	BA	1128	C	C5'-C4'-O4'	6.00	116.30	109.10
34	BA	1322	C	N1-C2-O2	6.00	122.50	118.90
34	BA	48	C	O4'-C1'-N1	6.00	113.00	108.20
2	AB	344	A	C3'-C2'-C1'	-5.99	96.70	101.50
2	AB	490	C	C1'-O4'-C4'	-5.99	105.11	109.90
2	AB	1343	G	N3-C4-C5	-5.99	125.60	128.60
2	AB	2008	C	O4'-C1'-N1	5.99	113.00	108.20
2	AB	2411	A	C5'-C4'-O4'	5.99	116.29	109.10
34	BA	1288	A	C8-N9-C4	-5.99	103.40	105.80
34	BA	352	C	N1-C2-O2	5.99	122.50	118.90
34	BA	1490	U	O4'-C1'-N1	5.99	112.99	108.20
2	AB	181	A	C5'-C4'-O4'	5.99	116.29	109.10
2	AB	1033	U	C5'-C4'-O4'	5.99	116.29	109.10
34	BA	415	A	C5'-C4'-O4'	5.99	116.29	109.10
34	BA	438	U	O4'-C1'-N1	5.99	112.99	108.20
34	BA	1156	G	O4'-C1'-N9	5.99	112.99	108.20
34	BA	44	A	O4'-C1'-N9	5.99	112.99	108.20
2	AB	1359	A	O4'-C1'-N9	5.98	112.99	108.20
34	BA	1227	A	O4'-C1'-N9	5.98	112.98	108.20
35	BE	38	A	C5'-C4'-O4'	5.98	116.28	109.10
2	AB	1072	C	O4'-C1'-N1	5.98	112.98	108.20
2	AB	2110	G	O4'-C4'-C3'	5.98	110.88	106.10
2	AB	558	U	O4'-C1'-N1	5.98	112.98	108.20
2	AB	1278	C	O4'-C1'-N1	5.98	112.98	108.20
2	AB	2302	U	C5'-C4'-O4'	5.98	116.27	109.10
34	BA	758	C	N1-C2-O2	5.98	122.49	118.90
34	BA	1482	G	O4'-C1'-N9	5.98	112.98	108.20
35	BE	18	G	C4'-C3'-C2'	-5.98	96.62	102.60
55	BW	77	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	AB	532	A	C1'-O4'-C4'	-5.98	105.12	109.90
2	AB	2150	C	O4'-C1'-N1	5.98	112.98	108.20
2	AB	412	A	C5'-C4'-C3'	-5.97	106.44	116.00
2	AB	1029	A	O4'-C1'-N9	5.97	112.98	108.20
2	AB	2787	C	O4'-C1'-N1	5.97	112.98	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	17	C	N1-C2-O2	5.97	122.48	118.90
2	AB	1840	G	C8-N9-C4	-5.97	104.01	106.40
34	BA	1380	U	O4'-C1'-N1	5.97	112.98	108.20
2	AB	238	C	C5'-C4'-O4'	5.97	116.27	109.10
2	AB	407	G	C8-N9-C4	-5.97	104.01	106.40
2	AB	949	G	C8-N9-C4	-5.97	104.01	106.40
34	BA	1027	C	C5'-C4'-O4'	5.97	116.27	109.10
34	BA	538	G	O4'-C1'-N9	5.97	112.98	108.20
34	BA	948	C	O4'-C1'-N1	5.97	112.97	108.20
2	AB	542	C	C5'-C4'-O4'	5.97	116.26	109.10
2	AB	239	C	O4'-C1'-N1	5.97	112.97	108.20
2	AB	673	C	C5'-C4'-O4'	5.97	116.26	109.10
2	AB	1609	A	O4'-C1'-N9	5.97	112.97	108.20
34	BA	9	G	C8-N9-C4	-5.97	104.01	106.40
34	BA	601	G	C5'-C4'-O4'	5.97	116.26	109.10
2	AB	1475	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	1748	C	O4'-C1'-N1	5.96	112.97	108.20
34	BA	437	U	O4'-C1'-N1	5.96	112.97	108.20
34	BA	725	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	767	U	C5'-C4'-O4'	5.96	116.26	109.10
2	AB	2252	G	O4'-C1'-N9	5.96	112.97	108.20
34	BA	108	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	748	G	C1'-O4'-C4'	-5.96	105.13	109.90
2	AB	326	G	O4'-C1'-N9	5.96	112.97	108.20
2	AB	2059	A	C8-N9-C4	-5.96	103.42	105.80
2	AB	2497	A	O4'-C1'-N9	5.96	112.97	108.20
2	AB	943	A	C5'-C4'-O4'	5.95	116.25	109.10
2	AB	1933	G	C5'-C4'-C3'	-5.95	106.47	116.00
34	BA	1106	G	C8-N9-C4	-5.95	104.02	106.40
34	BA	1120	C	C5'-C4'-O4'	5.95	116.24	109.10
2	AB	1855	U	O4'-C1'-N1	5.95	112.96	108.20
34	BA	639	G	O4'-C1'-N9	5.95	112.96	108.20
2	AB	1363	C	O4'-C1'-N1	5.95	112.96	108.20
2	AB	1996	C	O4'-C1'-N1	5.95	112.96	108.20
34	BA	204	G	C8-N9-C4	-5.95	104.02	106.40
2	AB	121	G	C8-N9-C4	-5.95	104.02	106.40
35	BE	65	G	O4'-C1'-N9	5.95	112.96	108.20
2	AB	1822	C	O4'-C1'-N1	5.95	112.96	108.20
34	BA	1359	C	C5'-C4'-C3'	-5.95	106.49	116.00
35	BE	30	G	O4'-C1'-N9	5.95	112.96	108.20
34	BA	1417	G	C5'-C4'-O4'	5.94	116.23	109.10
2	AB	854	C	O4'-C1'-N1	5.94	112.95	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	270	A	C1'-O4'-C4'	-5.94	105.15	109.90
34	BA	398	U	C5'-C4'-C3'	-5.94	106.50	116.00
34	BA	346	G	C3'-C2'-C1'	5.94	106.25	101.50
34	BA	780	A	O4'-C1'-N9	5.94	112.95	108.20
2	AB	2247	A	C5'-C4'-O4'	5.93	116.22	109.10
34	BA	164	G	C5'-C4'-O4'	5.93	116.22	109.10
34	BA	207	C	O4'-C1'-N1	5.93	112.95	108.20
1	AA	34	A	P-O3'-C3'	5.93	126.82	119.70
2	AB	1727	C	O4'-C1'-N1	5.93	112.94	108.20
2	AB	2874	C	O4'-C1'-N1	5.93	112.94	108.20
2	AB	2784	U	C5'-C4'-C3'	-5.93	106.52	116.00
2	AB	2807	U	C4'-C3'-C2'	-5.93	96.67	102.60
34	BA	272	C	O4'-C1'-N1	5.93	112.94	108.20
2	AB	2716	C	O4'-C1'-N1	5.92	112.94	108.20
34	BA	154	U	O4'-C1'-N1	5.92	112.94	108.20
2	AB	2537	U	C5'-C4'-O4'	5.92	116.21	109.10
2	AB	2377	A	O4'-C1'-N9	5.92	112.94	108.20
2	AB	2514	U	O4'-C1'-N1	5.92	112.94	108.20
35	BB	7	A	O4'-C1'-N9	5.92	112.94	108.20
2	AB	1788	C	C5'-C4'-O4'	5.92	116.20	109.10
34	BA	1213	A	P-O3'-C3'	5.92	126.80	119.70
2	AB	890	C	C5'-C4'-O4'	5.92	116.20	109.10
2	AB	2274	A	C5'-C4'-C3'	-5.92	106.53	116.00
2	AB	2625	G	C5'-C4'-O4'	5.92	116.20	109.10
2	AB	165	A	O4'-C1'-N9	5.92	112.93	108.20
2	AB	997	G	N3-C4-C5	-5.92	125.64	128.60
2	AB	2050	C	O4'-C1'-N1	5.92	112.93	108.20
2	AB	2254	C	C5'-C4'-O4'	5.92	116.20	109.10
2	AB	2500	U	P-O3'-C3'	5.92	126.80	119.70
2	AB	2601	C	C3'-C2'-C1'	5.92	106.23	101.50
2	AB	97	C	O4'-C1'-N1	5.91	112.93	108.20
2	AB	998	C	O4'-C1'-N1	5.91	112.93	108.20
34	BA	501	C	C4'-C3'-C2'	-5.91	96.69	102.60
34	BA	945	G	C5'-C4'-O4'	5.91	116.19	109.10
34	BA	1341	U	O4'-C1'-N1	5.91	112.93	108.20
2	AB	759	G	C8-N9-C4	-5.91	104.04	106.40
2	AB	1078	U	O4'-C1'-N1	5.91	112.93	108.20
2	AB	1623	G	O4'-C1'-N9	5.91	112.93	108.20
2	AB	743	A	C5'-C4'-O4'	5.91	116.19	109.10
2	AB	2074	U	O4'-C1'-N1	5.91	112.92	108.20
2	AB	2222	C	O4'-C1'-N1	5.91	112.92	108.20
34	BA	856	C	O4'-C1'-N1	5.91	112.92	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	656	G	N3-C4-C5	-5.90	125.65	128.60
34	BA	718	A	C5'-C4'-O4'	5.90	116.19	109.10
2	AB	549	G	C2-N3-C4	5.90	114.85	111.90
2	AB	779	U	O4'-C1'-N1	5.90	112.92	108.20
2	AB	1994	C	O4'-C1'-N1	5.90	112.92	108.20
2	AB	2262	U	C5'-C4'-C3'	-5.90	106.56	116.00
2	AB	2318	G	C8-N9-C4	-5.90	104.04	106.40
34	BA	732	C	O4'-C1'-N1	5.90	112.92	108.20
2	AB	1416	G	N9-C4-C5	5.90	107.76	105.40
2	AB	1492	G	O4'-C1'-N9	5.90	112.92	108.20
2	AB	1511	G	C5'-C4'-C3'	-5.90	106.56	116.00
2	AB	274	C	C5'-C4'-O4'	5.90	116.18	109.10
2	AB	1564	C	O4'-C1'-N1	5.90	112.92	108.20
34	BA	177	G	O4'-C1'-N9	5.90	112.92	108.20
35	BE	72	C	O4'-C1'-N1	5.90	112.92	108.20
2	AB	896	A	O3'-P-O5'	-5.90	92.80	104.00
2	AB	1648	U	C5'-C4'-O4'	5.89	116.17	109.10
2	AB	1610	A	O4'-C1'-N9	5.89	112.91	108.20
2	AB	1869	G	O4'-C1'-N9	5.89	112.91	108.20
34	BA	583	A	O4'-C1'-N9	5.89	112.91	108.20
34	BA	1150	A	C5'-C4'-O4'	5.89	116.17	109.10
2	AB	2622	U	C5'-C4'-O4'	5.89	116.17	109.10
34	BA	608	A	C5'-C4'-O4'	5.89	116.17	109.10
2	AB	243	U	O4'-C1'-N1	5.89	112.91	108.20
2	AB	540	C	O4'-C1'-N1	5.89	112.91	108.20
2	AB	1331	G	N3-C4-C5	-5.89	125.66	128.60
2	AB	1331	G	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	1865	U	P-O3'-C3'	5.89	126.77	119.70
34	BA	327	A	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	549	G	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	1036	G	O4'-C1'-N9	5.89	112.91	108.20
2	AB	2550	G	C5'-C4'-C3'	-5.89	106.58	116.00
2	AB	2788	C	C5'-C4'-O4'	5.89	116.16	109.10
2	AB	1690	A	O4'-C1'-N9	5.88	112.91	108.20
2	AB	2768	U	O4'-C1'-N1	5.88	112.91	108.20
34	BA	380	G	O4'-C1'-N9	5.88	112.91	108.20
2	AB	1462	C	O4'-C1'-N1	5.88	112.90	108.20
2	AB	714	U	O4'-C1'-N1	5.88	112.90	108.20
2	AB	1717	A	O4'-C1'-N9	5.88	112.90	108.20
2	AB	2814	A	O4'-C1'-N9	5.88	112.90	108.20
2	AB	2405	G	O4'-C1'-N9	5.88	112.90	108.20
34	BA	1489	G	O4'-C1'-N9	5.88	112.90	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	253	C	O4'-C1'-N1	5.87	112.90	108.20
34	BA	893	C	O4'-C1'-N1	5.87	112.90	108.20
2	AB	810	U	O4'-C1'-N1	5.87	112.90	108.20
1	AA	50	A	C5'-C4'-C3'	-5.87	106.61	116.00
2	AB	2417	C	O4'-C1'-N1	5.87	112.90	108.20
2	AB	481	G	C8-N9-C4	-5.87	104.05	106.40
34	BA	847	G	O4'-C1'-N9	5.87	112.89	108.20
34	BA	858	G	C8-N9-C4	-5.87	104.05	106.40
2	AB	1643	G	O4'-C1'-N9	5.87	112.89	108.20
2	AB	2639	A	O4'-C1'-N9	5.87	112.89	108.20
34	BA	891	U	O4'-C1'-N1	5.87	112.89	108.20
34	BA	1262	C	O4'-C1'-N1	5.87	112.89	108.20
34	BA	865	A	C3'-C2'-C1'	5.86	106.19	101.50
34	BA	1376	U	O4'-C1'-N1	5.86	112.89	108.20
35	BE	34	G	O4'-C1'-N9	5.86	112.89	108.20
2	AB	2199	A	C5'-C4'-C3'	-5.86	106.62	116.00
2	AB	2328	A	C5'-C4'-C3'	-5.86	106.62	116.00
34	BA	366	A	C4'-C3'-C2'	-5.86	96.74	102.60
34	BA	1366	C	O4'-C1'-N1	5.86	112.89	108.20
2	AB	136	G	C3'-C2'-C1'	-5.86	96.81	101.50
2	AB	1136	G	N3-C4-C5	-5.86	125.67	128.60
34	BA	23	C	O4'-C1'-N1	5.86	112.89	108.20
34	BA	874	G	N3-C4-C5	-5.86	125.67	128.60
2	AB	2862	G	O4'-C1'-N9	5.86	112.89	108.20
34	BA	760	G	N1-C6-O6	-5.86	116.39	119.90
2	AB	1447	C	O4'-C1'-N1	5.85	112.88	108.20
34	BA	1158	C	C3'-C2'-C1'	5.85	106.18	101.50
34	BA	1362	A	C8-N9-C4	-5.85	103.46	105.80
2	AB	1091	G	O4'-C1'-N9	5.85	112.88	108.20
2	AB	2578	G	C5'-C4'-O4'	5.85	116.12	109.10
34	BA	1206	G	C8-N9-C4	-5.85	104.06	106.40
34	BA	1291	U	C5'-C4'-O4'	5.85	116.12	109.10
2	AB	833	A	O4'-C1'-N9	5.85	112.88	108.20
2	AB	2380	C	C5'-C4'-O4'	5.85	116.12	109.10
2	AB	2458	G	O4'-C1'-N9	5.85	112.88	108.20
2	AB	2653	U	O4'-C1'-N1	5.85	112.88	108.20
2	AB	1266	G	C3'-C2'-C1'	-5.84	96.83	101.50
2	AB	1472	C	O4'-C1'-N1	5.84	112.87	108.20
2	AB	1166	G	C5'-C4'-C3'	-5.84	106.66	116.00
2	AB	581	C	O4'-C1'-N1	5.84	112.87	108.20
2	AB	2295	C	O4'-C1'-N1	5.84	112.87	108.20
2	AB	2741	A	C4'-C3'-C2'	-5.84	96.76	102.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	623	C	C5'-C4'-O4'	5.84	116.11	109.10
34	BA	688	G	C8-N9-C4	-5.84	104.06	106.40
34	BA	1111	A	C5'-C4'-C3'	-5.84	106.66	116.00
2	AB	622	G	O4'-C1'-N9	5.83	112.87	108.20
2	AB	818	G	C8-N9-C4	-5.83	104.07	106.40
2	AB	1930	G	O4'-C4'-C3'	5.83	110.77	106.10
2	AB	2298	A	C5'-C4'-O4'	5.83	116.10	109.10
34	BA	544	G	O4'-C1'-N9	5.83	112.87	108.20
2	AB	90	U	C5'-C4'-C3'	-5.83	106.67	116.00
2	AB	490	C	C5'-C4'-C3'	-5.83	106.67	116.00
34	BA	993	G	N3-C4-C5	-5.83	125.68	128.60
2	AB	1902	C	C5'-C4'-C3'	-5.83	106.67	116.00
34	BA	3	A	P-O3'-C3'	5.83	126.70	119.70
34	BA	466	A	C5'-C4'-C3'	-5.83	106.67	116.00
34	BA	869	G	C8-N9-C4	-5.83	104.07	106.40
2	AB	1404	C	O4'-C1'-N1	5.83	112.86	108.20
2	AB	942	G	O4'-C1'-N9	5.83	112.86	108.20
34	BA	347	G	O4'-C1'-N9	5.83	112.86	108.20
2	AB	396	G	N3-C4-C5	-5.83	125.69	128.60
2	AB	2611	C	C3'-C2'-C1'	5.83	106.16	101.50
34	BA	457	G	O4'-C1'-N9	5.83	112.86	108.20
2	AB	1271	G	N9-C1'-C2'	-5.82	105.59	112.00
2	AB	1411	U	O4'-C1'-N1	5.82	112.86	108.20
34	BA	1049	U	O4'-C1'-N1	5.82	112.86	108.20
2	AB	2563	U	C5'-C4'-O4'	5.82	116.09	109.10
34	BA	1313	U	O4'-C1'-N1	5.82	112.86	108.20
34	BA	205	A	C8-N9-C4	-5.82	103.47	105.80
34	BA	624	C	O4'-C1'-N1	5.82	112.86	108.20
34	BA	1300	G	P-O3'-C3'	5.82	126.68	119.70
34	BA	768	A	O4'-C1'-N9	5.82	112.86	108.20
2	AB	1242	U	N1-C2-N3	5.82	118.39	114.90
2	AB	701	G	N9-C1'-C2'	-5.82	105.60	112.00
2	AB	820	A	C5'-C4'-O4'	5.82	116.08	109.10
2	AB	821	A	O4'-C1'-N9	5.82	112.85	108.20
34	BA	98	A	O4'-C1'-N9	5.82	112.85	108.20
34	BA	474	G	O4'-C1'-N9	5.82	112.85	108.20
34	BA	660	C	O4'-C1'-N1	5.82	112.85	108.20
34	BA	709	U	O4'-C1'-N1	5.82	112.85	108.20
34	BA	1329	A	O4'-C1'-N9	5.82	112.85	108.20
2	AB	1161	C	O4'-C1'-N1	5.81	112.85	108.20
2	AB	2537	U	O4'-C1'-N1	5.81	112.85	108.20
34	BA	1178	G	C8-N9-C4	-5.81	104.08	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	229	U	O4'-C1'-N1	5.81	112.85	108.20
2	AB	33	C	O4'-C1'-N1	5.81	112.85	108.20
2	AB	1149	G	O4'-C1'-N9	5.81	112.84	108.20
2	AB	283	G	C5'-C4'-C3'	-5.81	106.71	116.00
2	AB	2783	U	O4'-C1'-N1	5.81	112.84	108.20
35	BE	4	C	O4'-C1'-N1	5.81	112.84	108.20
2	AB	718	A	C5'-C4'-O4'	5.80	116.06	109.10
2	AB	1866	A	C8-N9-C4	-5.80	103.48	105.80
2	AB	1879	C	O4'-C1'-N1	5.80	112.84	108.20
2	AB	2540	C	O4'-C1'-N1	5.80	112.84	108.20
2	AB	758	C	O4'-C1'-N1	5.80	112.84	108.20
9	AI	25	TYR	CB-CG-CD2	-5.80	117.52	121.00
34	BA	447	G	C8-N9-C4	-5.80	104.08	106.40
2	AB	37	C	C5'-C4'-O4'	5.80	116.06	109.10
2	AB	119	A	C1'-O4'-C4'	-5.80	105.26	109.90
2	AB	1741	C	C5'-C4'-O4'	5.80	116.06	109.10
37	BD	45	G	O4'-C1'-N9	5.80	112.84	108.20
2	AB	864	G	C5'-C4'-C3'	-5.80	106.72	116.00
2	AB	2203	U	O4'-C1'-N1	5.80	112.84	108.20
2	AB	1513	U	O4'-C1'-N1	5.80	112.84	108.20
34	BA	357	G	C5'-C4'-O4'	5.80	116.06	109.10
34	BA	757	U	O3'-P-O5'	-5.80	92.99	104.00
2	AB	726	G	C8-N9-C1'	5.79	134.53	127.00
34	BA	1035	A	C4'-C3'-C2'	-5.79	96.81	102.60
34	BA	1224	U	O3'-P-O5'	-5.79	92.99	104.00
2	AB	91	A	C4'-C3'-C2'	-5.79	96.81	102.60
2	AB	2494	G	O4'-C1'-N9	5.79	112.83	108.20
2	AB	2553	G	C5'-C4'-C3'	-5.79	106.73	116.00
34	BA	868	C	O4'-C1'-N1	5.79	112.83	108.20
34	BA	1116	U	O4'-C1'-N1	5.79	112.83	108.20
35	BE	28	G	O4'-C1'-N9	5.79	112.83	108.20
2	AB	863	A	C8-N9-C4	-5.79	103.48	105.80
2	AB	1964	G	C8-N9-C1'	5.79	134.53	127.00
2	AB	2704	C	C5'-C4'-C3'	-5.79	106.74	116.00
34	BA	1461	G	C5'-C4'-O4'	5.79	116.05	109.10
2	AB	857	G	N9-C4-C5	5.79	107.72	105.40
2	AB	1974	C	O4'-C1'-N1	5.79	112.83	108.20
2	AB	2783	U	C5'-C4'-C3'	-5.79	106.74	116.00
34	BA	590	U	O4'-C1'-N1	5.79	112.83	108.20
34	BA	744	C	O4'-C1'-N1	5.79	112.83	108.20
34	BA	1342	C	O4'-C1'-N1	5.79	112.83	108.20
2	AB	1185	G	N3-C4-C5	-5.79	125.71	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1044	A	C5'-C4'-C3'	-5.79	106.74	116.00
2	AB	2875	C	O4'-C1'-N1	5.78	112.83	108.20
34	BA	762	U	O4'-C1'-N1	5.78	112.83	108.20
2	AB	2480	C	O4'-C1'-N1	5.78	112.83	108.20
2	AB	293	U	O4'-C1'-N1	5.78	112.83	108.20
2	AB	465	G	C5'-C4'-O4'	5.78	116.04	109.10
34	BA	1144	G	C8-N9-C4	-5.78	104.09	106.40
2	AB	10	A	O4'-C1'-N9	5.78	112.82	108.20
2	AB	657	U	O4'-C1'-N1	5.78	112.82	108.20
2	AB	2796	U	C5'-C4'-O4'	5.78	116.03	109.10
34	BA	920	U	O4'-C1'-N1	5.78	112.82	108.20
2	AB	340	A	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	1033	U	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	1175	A	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	1707	G	C8-N9-C4	-5.78	104.09	106.40
2	AB	2855	C	C5'-C4'-C3'	-5.78	106.76	116.00
2	AB	310	A	C5'-C4'-O4'	5.77	116.03	109.10
2	AB	770	G	O4'-C1'-N9	5.77	112.82	108.20
2	AB	1758	U	P-O3'-C3'	5.77	126.63	119.70
2	AB	2118	U	C3'-C2'-C1'	5.77	106.12	101.50
2	AB	2186	G	N3-C4-C5	-5.77	125.71	128.60
2	AB	2863	C	C5'-C4'-O4'	5.77	116.03	109.10
34	BA	950	U	O4'-C1'-N1	5.77	112.82	108.20
34	BA	1447	A	O4'-C1'-N9	5.77	112.82	108.20
2	AB	858	G	O4'-C1'-N9	5.77	112.82	108.20
2	AB	2352	A	C5'-C4'-O4'	5.77	116.03	109.10
34	BA	129	A	O4'-C1'-N9	5.77	112.82	108.20
2	AB	174	U	O4'-C1'-N1	5.77	112.81	108.20
2	AB	1208	C	O4'-C1'-N1	5.77	112.82	108.20
2	AB	1451	C	P-O3'-C3'	5.77	126.62	119.70
1	AA	29	A	O4'-C1'-N9	5.77	112.81	108.20
2	AB	2260	C	O4'-C1'-N1	5.77	112.81	108.20
2	AB	2462	C	O4'-C1'-N1	5.77	112.81	108.20
2	AB	1041	G	C5'-C4'-C3'	-5.77	106.78	116.00
2	AB	1885	A	C5'-C4'-O4'	5.77	116.02	109.10
34	BA	576	C	N1-C2-O2	5.77	122.36	118.90
1	AA	32	U	C3'-C2'-C1'	-5.76	96.89	101.50
2	AB	1648	U	C1'-O4'-C4'	-5.76	105.29	109.90
34	BA	18	C	O4'-C1'-N1	5.76	112.81	108.20
1	AA	54	G	C8-N9-C4	-5.76	104.10	106.40
2	AB	21	A	C5'-C4'-O4'	5.76	116.01	109.10
2	AB	1019	U	C5'-C4'-C3'	-5.76	106.79	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1861	G	C4'-C3'-C2'	-5.76	96.84	102.60
34	BA	271	C	O4'-C1'-N1	5.76	112.81	108.20
34	BA	392	C	O4'-C1'-N1	5.76	112.81	108.20
2	AB	1088	A	C1'-O4'-C4'	-5.76	105.29	109.90
34	BA	1514	G	O4'-C1'-N9	5.76	112.81	108.20
35	BB	18	G	C8-N9-C4	-5.76	104.10	106.40
1	AA	16	G	N3-C4-C5	-5.75	125.72	128.60
2	AB	2112	G	N3-C4-C5	-5.75	125.72	128.60
34	BA	935	A	O4'-C1'-N9	5.75	112.80	108.20
2	AB	937	C	O4'-C1'-N1	5.75	112.80	108.20
2	AB	1928	A	C8-N9-C4	-5.75	103.50	105.80
2	AB	2543	G	C8-N9-C4	-5.75	104.10	106.40
2	AB	2667	C	C5'-C4'-C3'	-5.75	106.80	116.00
2	AB	2801	G	C5'-C4'-C3'	-5.75	106.80	116.00
34	BA	484	G	C3'-C2'-C1'	-5.75	96.90	101.50
34	BA	911	U	O4'-C1'-N1	5.75	112.80	108.20
34	BA	1018	G	O4'-C1'-N9	5.75	112.80	108.20
2	AB	712	G	O4'-C1'-N9	5.75	112.80	108.20
2	AB	1395	A	O4'-C4'-C3'	5.75	110.70	106.10
2	AB	2348	U	O4'-C1'-N1	5.75	112.80	108.20
34	BA	1162	C	O4'-C1'-N1	5.75	112.80	108.20
2	AB	1652	A	C5'-C4'-C3'	-5.75	106.81	116.00
2	AB	2625	G	N3-C4-C5	-5.75	125.73	128.60
34	BA	322	C	O4'-C1'-N1	5.75	112.80	108.20
34	BA	429	U	C5'-C4'-C3'	-5.75	106.80	116.00
34	BA	814	A	C5'-C4'-C3'	-5.75	106.80	116.00
2	AB	1511	G	C5'-C4'-O4'	5.75	115.99	109.10
2	AB	1765	U	O4'-C1'-N1	5.75	112.80	108.20
34	BA	1534	A	C3'-C2'-C1'	5.75	106.10	101.50
2	AB	1033	U	C1'-O4'-C4'	-5.74	105.31	109.90
2	AB	545	U	O4'-C4'-C3'	5.74	110.69	106.10
2	AB	1210	G	P-O3'-C3'	5.74	126.59	119.70
35	BE	63	G	O4'-C1'-N9	5.74	112.79	108.20
2	AB	2452	C	O4'-C1'-N1	5.74	112.79	108.20
2	AB	2692	G	C5'-C4'-O4'	5.74	115.99	109.10
34	BA	505	G	N3-C4-C5	-5.74	125.73	128.60
34	BA	1034	G	C5'-C4'-O4'	5.74	115.99	109.10
2	AB	2399	G	O4'-C1'-N9	5.74	112.79	108.20
2	AB	1627	G	C5'-C4'-O4'	5.74	115.98	109.10
34	BA	236	A	O4'-C1'-N9	5.74	112.79	108.20
34	BA	921	U	O4'-C1'-N1	5.74	112.79	108.20
2	AB	2053	G	O4'-C1'-N9	5.73	112.79	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2491	U	O4'-C1'-N1	5.73	112.79	108.20
34	BA	678	U	C5'-C4'-O4'	5.73	115.98	109.10
35	BB	17	C	P-O3'-C3'	5.73	126.58	119.70
2	AB	2588	G	N3-C4-C5	-5.73	125.73	128.60
34	BA	329	A	C5'-C4'-C3'	-5.73	106.83	116.00
34	BA	1303	C	O4'-C1'-N1	5.73	112.78	108.20
2	AB	1507	C	O4'-C1'-N1	5.73	112.78	108.20
34	BA	1046	A	C5'-C4'-O4'	5.73	115.98	109.10
1	AA	39	A	O4'-C1'-N9	5.73	112.78	108.20
2	AB	1757	A	P-O3'-C3'	5.73	126.58	119.70
2	AB	2440	C	O4'-C1'-N1	5.73	112.78	108.20
2	AB	1024	G	O4'-C1'-N9	5.73	112.78	108.20
34	BA	156	C	C5'-C4'-C3'	-5.73	106.84	116.00
34	BA	684	U	O4'-C1'-N1	5.73	112.78	108.20
2	AB	368	A	C5'-C4'-C3'	-5.73	106.84	116.00
34	BA	46	G	O4'-C1'-N9	5.73	112.78	108.20
2	AB	1104	C	O4'-C1'-N1	5.72	112.78	108.20
2	AB	1909	C	C4'-C3'-C2'	-5.72	96.88	102.60
34	BA	367	U	C3'-C2'-C1'	5.72	106.08	101.50
1	AA	100	G	C8-N9-C4	-5.72	104.11	106.40
2	AB	1160	G	O4'-C1'-N9	5.72	112.78	108.20
2	AB	1581	G	N9-C4-C5	5.72	107.69	105.40
34	BA	668	G	C5'-C4'-O4'	5.72	115.96	109.10
34	BA	1155	A	C5'-C4'-C3'	-5.72	106.85	116.00
2	AB	820	A	O4'-C1'-N9	5.72	112.78	108.20
2	AB	2196	C	C5'-C4'-O4'	5.72	115.96	109.10
2	AB	52	A	C5'-C4'-C3'	-5.72	106.85	116.00
2	AB	277	G	C2'-C3'-O3'	5.72	122.85	113.70
2	AB	1187	G	C5'-C4'-O4'	5.72	115.96	109.10
2	AB	1510	G	O4'-C1'-N9	5.72	112.77	108.20
2	AB	1645	G	C5'-C4'-C3'	-5.72	106.86	116.00
2	AB	2104	C	O4'-C1'-N1	5.72	112.77	108.20
2	AB	2610	C	C3'-C2'-C1'	-5.71	96.93	101.50
34	BA	281	G	C5'-C4'-O4'	5.71	115.96	109.10
34	BA	751	U	O4'-C1'-N1	5.71	112.77	108.20
34	BA	1535	C	C5'-C4'-C3'	5.71	125.14	116.00
2	AB	295	G	N9-C1'-C2'	-5.71	105.72	112.00
34	BA	410	G	C5'-C4'-C3'	-5.71	106.86	116.00
2	AB	922	C	O4'-C1'-N1	5.71	112.77	108.20
2	AB	2739	U	C4'-C3'-C2'	-5.71	96.89	102.60
2	AB	811	U	C5'-C4'-C3'	-5.71	106.87	116.00
2	AB	1781	U	O4'-C1'-N1	5.71	112.77	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	30	U	C3'-C2'-C1'	5.71	106.07	101.50
34	BA	140	U	O4'-C1'-N1	5.71	112.76	108.20
2	AB	1408	G	O3'-P-O5'	-5.70	93.17	104.00
2	AB	1454	C	N1-C2-O2	5.70	122.32	118.90
35	BB	43	C	O4'-C1'-N1	5.70	112.76	108.20
2	AB	147	C	O4'-C1'-N1	5.70	112.76	108.20
2	AB	1309	G	C8-N9-C4	-5.70	104.12	106.40
2	AB	1501	G	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	2191	A	O4'-C1'-N9	5.70	112.76	108.20
2	AB	2365	G	C5'-C4'-O4'	5.70	115.94	109.10
34	BA	261	U	C5'-C4'-C3'	-5.70	106.88	116.00
34	BA	494	G	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	480	A	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	1840	G	N7-C8-N9	5.70	115.95	113.10
2	AB	2078	C	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	2303	G	C5'-C4'-C3'	-5.70	106.88	116.00
34	BA	111	G	C8-N9-C4	-5.70	104.12	106.40
35	BE	35	A	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	59	U	O4'-C1'-N1	5.70	112.76	108.20
2	AB	566	U	C5'-C4'-O4'	5.70	115.94	109.10
2	AB	1592	C	O4'-C1'-N1	5.70	112.76	108.20
34	BA	787	A	O4'-C1'-N9	5.70	112.76	108.20
2	AB	1560	G	C8-N9-C4	-5.70	104.12	106.40
2	AB	1751	U	O4'-C1'-N1	5.70	112.76	108.20
2	AB	1994	C	C4'-C3'-C2'	-5.70	96.90	102.60
2	AB	2023	C	O4'-C1'-N1	5.69	112.75	108.20
2	AB	141	G	O4'-C1'-N9	5.69	112.75	108.20
2	AB	170	U	O4'-C1'-N1	5.69	112.75	108.20
2	AB	1007	C	C5'-C4'-O4'	5.69	115.93	109.10
2	AB	1543	G	C5'-C4'-O4'	5.69	115.93	109.10
34	BA	1390	U	O4'-C1'-N1	5.69	112.75	108.20
2	AB	1283	G	C8-N9-C4	-5.69	104.12	106.40
34	BA	1201	A	C5'-C4'-O4'	5.69	115.93	109.10
2	AB	317	G	O4'-C1'-N9	5.69	112.75	108.20
2	AB	1420	A	O4'-C1'-N9	5.69	112.75	108.20
2	AB	1325	U	O4'-C1'-N1	5.69	112.75	108.20
34	BA	1035	A	O4'-C1'-N9	5.69	112.75	108.20
2	AB	871	U	C5'-C4'-O4'	5.68	115.92	109.10
2	AB	1416	G	C8-N9-C1'	5.68	134.39	127.00
34	BA	289	G	O4'-C1'-N9	5.68	112.75	108.20
2	AB	549	G	C8-N9-C4	-5.68	104.13	106.40
2	AB	1535	A	N9-C1'-C2'	-5.68	105.75	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1603	A	C5'-C4'-O4'	5.68	115.92	109.10
2	AB	1978	A	O4'-C1'-N9	5.68	112.75	108.20
2	AB	2205	A	O4'-C1'-N9	5.68	112.75	108.20
34	BA	394	G	N9-C4-C5	5.68	107.67	105.40
2	AB	311	A	C3'-C2'-C1'	5.68	106.04	101.50
2	AB	510	C	C5'-C4'-C3'	-5.68	106.91	116.00
2	AB	1203	U	N3-C2-O2	-5.68	118.23	122.20
34	BA	1333	A	C8-N9-C4	-5.68	103.53	105.80
2	AB	1154	G	N7-C8-N9	5.67	115.94	113.10
2	AB	2485	G	N3-C4-C5	-5.67	125.76	128.60
2	AB	2744	G	C1'-O4'-C4'	-5.67	105.36	109.90
34	BA	512	U	C1'-O4'-C4'	-5.67	105.36	109.90
2	AB	783	A	O4'-C1'-N9	5.67	112.74	108.20
2	AB	2076	U	O4'-C1'-N1	5.67	112.74	108.20
2	AB	2705	A	C5'-C4'-C3'	-5.67	106.93	116.00
34	BA	523	A	O4'-C1'-N9	5.67	112.74	108.20
34	BA	822	U	C5'-C4'-O4'	5.67	115.91	109.10
2	AB	738	G	O4'-C1'-N9	5.67	112.74	108.20
2	AB	964	C	O4'-C1'-N1	5.67	112.74	108.20
34	BA	618	C	O4'-C1'-N1	5.67	112.74	108.20
2	AB	863	A	O4'-C1'-N9	5.67	112.73	108.20
2	AB	871	U	C5'-C4'-C3'	-5.67	106.93	116.00
2	AB	1865	U	O4'-C1'-N1	5.67	112.73	108.20
2	AB	1934	C	O4'-C1'-N1	5.67	112.73	108.20
34	BA	352	C	C5'-C4'-O4'	5.67	115.90	109.10
34	BA	1489	G	C8-N9-C4	-5.67	104.13	106.40
34	BA	846	G	N3-C4-C5	-5.67	125.77	128.60
34	BA	1292	G	O4'-C1'-N9	5.67	112.73	108.20
2	AB	2057	G	C4'-C3'-C2'	-5.66	96.94	102.60
2	AB	2650	U	O4'-C1'-N1	5.66	112.73	108.20
34	BA	636	U	C5'-C4'-C3'	-5.66	106.94	116.00
34	BA	1374	A	O4'-C1'-N9	5.66	112.73	108.20
35	BE	57	G	P-O3'-C3'	5.66	126.50	119.70
2	AB	440	C	O4'-C1'-N1	5.66	112.73	108.20
2	AB	1238	G	N3-C4-C5	-5.66	125.77	128.60
2	AB	1695	G	C2-N3-C4	5.66	114.73	111.90
34	BA	1505	G	N9-C4-C5	5.66	107.66	105.40
2	AB	116	C	C5'-C4'-C3'	-5.66	106.95	116.00
34	BA	463	U	O4'-C1'-N1	5.66	112.73	108.20
34	BA	763	G	O4'-C1'-N9	5.66	112.73	108.20
34	BA	1347	G	O4'-C1'-N9	5.66	112.73	108.20
2	AB	2814	A	C5'-C4'-C3'	-5.66	106.95	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	106	C	O4'-C1'-N1	5.66	112.73	108.20
34	BA	719	C	O4'-C1'-N1	5.66	112.72	108.20
2	AB	1695	G	C8-N9-C4	-5.65	104.14	106.40
2	AB	2329	U	O4'-C1'-N1	5.65	112.72	108.20
2	AB	1206	G	C5'-C4'-O4'	5.65	115.88	109.10
34	BA	152	A	O4'-C1'-N9	5.65	112.72	108.20
2	AB	1813	G	C8-N9-C4	-5.65	104.14	106.40
2	AB	2771	C	O4'-C1'-N1	5.65	112.72	108.20
34	BA	40	C	O4'-C1'-N1	5.65	112.72	108.20
34	BA	943	U	O4'-C1'-N1	5.65	112.72	108.20
34	BA	1289	A	C8-N9-C4	-5.65	103.54	105.80
34	BA	1408	A	C5'-C4'-C3'	-5.65	106.96	116.00
2	AB	580	U	O4'-C1'-N1	5.65	112.72	108.20
2	AB	451	U	O4'-C1'-N1	5.65	112.72	108.20
2	AB	1973	G	C5'-C4'-O4'	5.65	115.88	109.10
2	AB	2897	U	C5'-C4'-O4'	5.65	115.88	109.10
2	AB	457	A	P-O3'-C3'	5.65	126.47	119.70
34	BA	686	U	O4'-C4'-C3'	5.65	110.62	106.10
2	AB	133	U	O4'-C1'-N1	5.64	112.72	108.20
2	AB	669	G	N3-C4-C5	-5.64	125.78	128.60
2	AB	1597	A	O4'-C1'-N9	5.64	112.72	108.20
2	AB	2845	U	O4'-C1'-N1	5.64	112.72	108.20
2	AB	368	A	C5'-C4'-O4'	5.64	115.87	109.10
2	AB	1094	U	O4'-C1'-N1	5.64	112.71	108.20
2	AB	2123	G	C8-N9-C4	-5.64	104.14	106.40
2	AB	2214	C	C5'-C4'-C3'	-5.64	106.97	116.00
34	BA	999	C	O4'-C1'-N1	5.64	112.71	108.20
37	BD	28	U	O3'-P-O5'	-5.64	93.28	104.00
2	AB	695	G	O4'-C1'-N9	5.64	112.71	108.20
2	AB	2717	C	C5'-C4'-O4'	5.64	115.87	109.10
2	AB	284	U	O4'-C1'-N1	5.64	112.71	108.20
2	AB	763	G	N3-C4-C5	-5.64	125.78	128.60
2	AB	266	G	N3-C4-C5	-5.64	125.78	128.60
2	AB	1885	A	C5'-C4'-C3'	-5.64	106.98	116.00
2	AB	1346	G	O4'-C1'-N9	5.64	112.71	108.20
2	AB	2350	C	O4'-C1'-N1	5.64	112.71	108.20
2	AB	2821	A	C5'-C4'-C3'	-5.64	106.98	116.00
34	BA	708	C	O4'-C1'-N1	5.64	112.71	108.20
34	BA	1309	G	O4'-C1'-N9	5.64	112.71	108.20
1	AA	50	A	C8-N9-C4	-5.63	103.55	105.80
2	AB	2656	U	O4'-C1'-N1	5.63	112.71	108.20
2	AB	278	A	O3'-P-O5'	-5.63	93.30	104.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1551	A	O4'-C1'-N9	5.63	112.70	108.20
2	AB	541	A	O4'-C1'-N9	5.63	112.70	108.20
2	AB	1627	G	N3-C4-C5	-5.63	125.79	128.60
2	AB	2337	G	C5'-C4'-C3'	-5.63	106.99	116.00
34	BA	821	G	C5'-C4'-O4'	5.63	115.86	109.10
2	AB	356	G	O4'-C1'-N9	5.63	112.70	108.20
2	AB	392	U	C5'-C4'-O4'	5.63	115.85	109.10
2	AB	1590	A	C5'-C4'-C3'	-5.63	107.00	116.00
2	AB	2731	G	C5'-C4'-O4'	5.63	115.85	109.10
34	BA	607	A	O4'-C1'-N9	5.63	112.70	108.20
35	BE	6	G	O3'-P-O5'	-5.63	93.31	104.00
2	AB	242	G	C3'-C2'-C1'	-5.62	97.00	101.50
2	AB	545	U	C4'-C3'-O3'	5.62	124.25	113.00
34	BA	1100	C	C5'-C4'-O4'	5.62	115.85	109.10
34	BA	1385	G	C5'-C4'-O4'	5.62	115.85	109.10
2	AB	2262	U	C5'-C4'-O4'	5.62	115.85	109.10
34	BA	892	A	C5'-C4'-C3'	-5.62	107.00	116.00
2	AB	1988	G	C5'-C4'-O4'	5.62	115.84	109.10
2	AB	2554	U	O3'-P-O5'	-5.62	93.32	104.00
34	BA	183	C	C5'-C4'-C3'	-5.62	107.00	116.00
34	BA	699	C	O4'-C1'-N1	5.62	112.70	108.20
34	BA	774	G	C5'-C4'-O4'	5.62	115.84	109.10
2	AB	2043	C	C5'-C4'-C3'	-5.62	107.01	116.00
2	AB	2431	U	C2'-C3'-O3'	5.62	122.69	113.70
2	AB	2791	G	C5'-C4'-C3'	-5.62	107.01	116.00
34	BA	1178	G	N9-C4-C5	5.62	107.65	105.40
35	BE	13	C	O3'-P-O5'	5.62	114.68	104.00
2	AB	378	C	C5'-C4'-O4'	5.62	115.84	109.10
2	AB	492	A	C8-N9-C4	-5.62	103.55	105.80
34	BA	416	G	O4'-C1'-N9	5.62	112.69	108.20
2	AB	2885	G	C8-N9-C4	-5.62	104.15	106.40
34	BA	166	U	O4'-C1'-N1	5.62	112.69	108.20
2	AB	424	G	C5'-C4'-C3'	-5.61	107.02	116.00
2	AB	2666	C	N1-C1'-C2'	-5.61	105.83	112.00
34	BA	4	U	C5'-C4'-O4'	5.61	115.84	109.10
34	BA	41	G	O4'-C1'-N9	5.61	112.69	108.20
34	BA	226	G	C5'-C4'-O4'	5.61	115.84	109.10
2	AB	2506	U	C4'-C3'-C2'	-5.61	96.99	102.60
34	BA	130	A	O4'-C1'-N9	5.61	112.69	108.20
2	AB	2560	A	O3'-P-O5'	-5.61	93.34	104.00
34	BA	900	A	C3'-C2'-C1'	5.61	105.99	101.50
1	AA	32	U	N1-C2-N3	5.61	118.27	114.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	428	A	O4'-C1'-N9	5.61	112.69	108.20
2	AB	2256	G	C8-N9-C4	-5.61	104.16	106.40
2	AB	2853	C	O4'-C1'-N1	5.61	112.69	108.20
34	BA	421	U	O4'-C1'-N1	5.61	112.69	108.20
2	AB	498	G	O4'-C1'-N9	5.61	112.69	108.20
2	AB	674	G	O4'-C1'-N9	5.61	112.68	108.20
2	AB	2648	G	C8-N9-C4	-5.61	104.16	106.40
34	BA	347	G	N3-C4-C5	-5.61	125.80	128.60
34	BA	453	G	N7-C8-N9	5.61	115.90	113.10
34	BA	471	U	O4'-C1'-N1	5.61	112.69	108.20
34	BA	955	U	N1-C1'-C2'	-5.61	105.83	112.00
34	BA	1148	U	O4'-C1'-N1	5.61	112.68	108.20
2	AB	2788	C	O4'-C1'-N1	5.60	112.68	108.20
2	AB	976	G	C5'-C4'-O4'	5.60	115.82	109.10
2	AB	1454	C	O4'-C1'-N1	5.60	112.68	108.20
34	BA	347	G	N9-C1'-C2'	-5.60	105.84	112.00
34	BA	394	G	C5'-C4'-O4'	5.60	115.82	109.10
2	AB	714	U	C5'-C4'-C3'	-5.60	107.04	116.00
2	AB	921	C	C5'-C4'-C3'	-5.60	107.04	116.00
2	AB	1256	G	N3-C4-C5	-5.60	125.80	128.60
2	AB	1511	G	O4'-C1'-N9	5.60	112.68	108.20
2	AB	2040	G	N3-C4-C5	-5.60	125.80	128.60
34	BA	810	C	O4'-C1'-N1	5.60	112.68	108.20
2	AB	439	A	O4'-C1'-N9	5.60	112.68	108.20
34	BA	991	U	O4'-C4'-C3'	5.60	110.58	106.10
2	AB	564	C	O4'-C1'-N1	5.59	112.68	108.20
2	AB	1243	C	O4'-C1'-N1	5.59	112.68	108.20
2	AB	2626	C	O4'-C1'-N1	5.59	112.68	108.20
34	BA	769	G	C5'-C4'-O4'	5.59	115.81	109.10
2	AB	1195	G	N9-C1'-C2'	-5.59	105.85	112.00
2	AB	2272	U	O4'-C1'-N1	5.59	112.67	108.20
34	BA	1201	A	C3'-C2'-C1'	5.59	105.97	101.50
34	BA	585	G	N3-C4-C5	-5.59	125.81	128.60
34	BA	1415	G	O4'-C1'-N9	5.59	112.67	108.20
34	BA	1418	A	O4'-C1'-N9	5.59	112.67	108.20
2	AB	18	U	O4'-C1'-N1	5.59	112.67	108.20
2	AB	141	G	C5'-C4'-O4'	5.59	115.81	109.10
2	AB	969	G	O4'-C1'-N9	5.59	112.67	108.20
2	AB	2317	A	O4'-C1'-N9	5.59	112.67	108.20
2	AB	966	G	C8-N9-C4	-5.59	104.17	106.40
34	BA	1152	A	C3'-C2'-C1'	5.59	105.97	101.50
34	BA	1223	C	O4'-C4'-C3'	5.59	110.57	106.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	332	A	O4'-C1'-C2'	-5.58	100.22	105.80
2	AB	1986	C	C5'-C4'-C3'	-5.58	107.07	116.00
34	BA	280	C	O4'-C1'-N1	5.58	112.67	108.20
35	BB	28	G	C8-N9-C4	-5.58	104.17	106.40
2	AB	1483	G	C8-N9-C4	-5.58	104.17	106.40
2	AB	1645	G	C3'-C2'-C1'	5.58	105.97	101.50
2	AB	2283	C	O4'-C1'-N1	5.58	112.67	108.20
34	BA	1017	U	C5'-C4'-O4'	5.58	115.80	109.10
34	BA	1200	C	N1-C2-O2	5.58	122.25	118.90
2	AB	11	C	O4'-C1'-C2'	-5.58	100.22	105.80
2	AB	1119	U	C5'-C4'-O4'	5.58	115.80	109.10
2	AB	1624	U	O4'-C1'-N1	5.58	112.66	108.20
34	BA	1440	U	O4'-C1'-N1	5.58	112.66	108.20
2	AB	895	U	O3'-P-O5'	-5.58	93.40	104.00
2	AB	2871	U	O4'-C1'-N1	5.58	112.66	108.20
34	BA	855	U	C5'-C4'-O4'	5.58	115.80	109.10
34	BA	1223	C	C3'-C2'-C1'	5.58	105.96	101.50
34	BA	1277	C	O4'-C1'-N1	5.58	112.66	108.20
2	AB	1069	A	O4'-C4'-C3'	5.58	110.56	106.10
2	AB	2073	C	C5'-C4'-O4'	5.58	115.79	109.10
2	AB	2175	C	C4'-C3'-C2'	5.58	108.17	102.60
2	AB	2756	U	P-O3'-C3'	5.58	126.39	119.70
34	BA	147	G	N3-C4-C5	-5.58	125.81	128.60
1	AA	103	U	O4'-C1'-N1	5.57	112.66	108.20
2	AB	964	C	C5'-C4'-O4'	5.57	115.79	109.10
2	AB	997	G	O4'-C1'-N9	5.57	112.66	108.20
2	AB	1725	U	C5'-C4'-O4'	5.57	115.79	109.10
34	BA	980	C	N1-C2-O2	5.57	122.25	118.90
35	BB	36	A	C5'-C4'-O4'	5.57	115.79	109.10
34	BA	1435	G	C8-N9-C4	-5.57	104.17	106.40
2	AB	1038	G	N3-C4-C5	-5.57	125.81	128.60
2	AB	2477	U	O4'-C4'-C3'	5.57	110.56	106.10
34	BA	56	U	O4'-C1'-N1	5.57	112.66	108.20
34	BA	327	A	O4'-C1'-N9	5.57	112.66	108.20
34	BA	1109	C	C5'-C4'-C3'	-5.57	107.09	116.00
2	AB	325	G	N9-C1'-C2'	-5.57	105.87	112.00
2	AB	2738	A	O4'-C1'-N9	5.57	112.66	108.20
34	BA	651	C	C1'-O4'-C4'	-5.57	105.44	109.90
2	AB	481	G	N3-C4-C5	-5.57	125.82	128.60
2	AB	1652	A	C5'-C4'-O4'	5.57	115.78	109.10
2	AB	2268	A	N9-C1'-C2'	-5.57	105.88	112.00
34	BA	1161	C	O4'-C1'-N1	5.57	112.65	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1145	C	C5'-C4'-O4'	5.57	115.78	109.10
2	AB	2276	G	C5'-C4'-O4'	5.57	115.78	109.10
34	BA	1337	G	P-O3'-C3'	5.57	126.38	119.70
2	AB	617	G	O4'-C1'-N9	5.56	112.65	108.20
2	AB	1640	A	O4'-C1'-N9	5.56	112.65	108.20
34	BA	1264	U	O4'-C1'-N1	5.56	112.65	108.20
2	AB	681	G	C5'-C4'-O4'	5.56	115.78	109.10
2	AB	1699	G	C5'-C4'-C3'	-5.56	107.10	116.00
2	AB	2133	G	C8-N9-C4	-5.56	104.17	106.40
2	AB	2815	C	C5'-C4'-O4'	5.56	115.78	109.10
34	BA	70	U	N3-C2-O2	-5.56	118.31	122.20
2	AB	767	U	C5'-C4'-C3'	-5.56	107.10	116.00
2	AB	1685	C	O4'-C1'-N1	5.56	112.65	108.20
2	AB	2187	U	C5'-C4'-O4'	5.56	115.77	109.10
2	AB	725	G	P-O3'-C3'	5.56	126.37	119.70
2	AB	862	G	C8-N9-C4	-5.56	104.18	106.40
34	BA	1485	U	O4'-C1'-N1	5.56	112.65	108.20
2	AB	521	U	C5'-C4'-O4'	5.56	115.77	109.10
2	AB	2170	A	O4'-C1'-N9	5.56	112.65	108.20
34	BA	531	U	O4'-C1'-C2'	-5.56	100.24	105.80
2	AB	2161	C	N1-C2-O2	5.55	122.23	118.90
2	AB	182	A	O4'-C1'-N9	5.55	112.64	108.20
2	AB	718	A	C5'-C4'-C3'	-5.55	107.12	116.00
2	AB	1726	C	C5'-C4'-C3'	-5.55	107.12	116.00
2	AB	1933	G	C4'-C3'-C2'	-5.55	97.05	102.60
34	BA	970	C	O4'-C1'-N1	5.55	112.64	108.20
2	AB	427	U	C5'-C4'-O4'	5.55	115.76	109.10
2	AB	2192	U	O4'-C1'-N1	5.55	112.64	108.20
2	AB	2862	G	C5'-C4'-O4'	5.55	115.76	109.10
34	BA	1102	A	C5'-C4'-O4'	5.55	115.76	109.10
34	BA	1118	U	O4'-C1'-N1	5.55	112.64	108.20
1	AA	2	G	N3-C4-C5	-5.55	125.83	128.60
2	AB	817	C	C5'-C4'-O4'	5.55	115.76	109.10
2	AB	1437	C	O4'-C1'-N1	5.55	112.64	108.20
2	AB	2534	A	C5'-C4'-O4'	5.55	115.76	109.10
34	BA	123	U	C5'-C4'-C3'	-5.55	107.13	116.00
2	AB	282	A	O4'-C1'-N9	5.54	112.64	108.20
2	AB	1555	G	C8-N9-C4	-5.54	104.18	106.40
2	AB	1921	G	O4'-C1'-N9	5.54	112.64	108.20
2	AB	2492	U	O4'-C1'-N1	5.54	112.63	108.20
34	BA	61	G	C8-N9-C4	-5.54	104.18	106.40
34	BA	194	C	C5'-C4'-O4'	5.54	115.75	109.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1108	G	O4'-C1'-N9	5.54	112.64	108.20
2	AB	1454	C	N3-C2-O2	-5.54	118.02	121.90
2	AB	2278	A	O4'-C1'-N9	5.54	112.63	108.20
2	AB	2673	G	C3'-C2'-C1'	-5.54	97.07	101.50
34	BA	1144	G	C5'-C4'-O4'	5.54	115.75	109.10
34	BA	1333	A	C5'-C4'-O4'	5.54	115.75	109.10
2	AB	900	A	C8-N9-C4	-5.54	103.58	105.80
2	AB	1566	A	C5'-C4'-O4'	5.54	115.75	109.10
34	BA	906	A	O4'-C1'-N9	5.54	112.63	108.20
34	BA	1021	A	N9-C1'-C2'	-5.54	105.91	112.00
34	BA	1456	A	O3'-P-O5'	-5.54	93.48	104.00
2	AB	1573	G	C5'-C4'-C3'	-5.54	107.14	116.00
2	AB	1947	C	O4'-C1'-N1	5.54	112.63	108.20
34	BA	637	C	O4'-C1'-N1	5.54	112.63	108.20
1	AA	114	C	O4'-C1'-N1	5.54	112.63	108.20
2	AB	1201	U	O4'-C1'-N1	5.54	112.63	108.20
34	BA	1267	C	O4'-C1'-N1	5.54	112.63	108.20
2	AB	274	C	O4'-C1'-N1	5.53	112.63	108.20
2	AB	1746	A	O4'-C1'-N9	5.53	112.63	108.20
2	AB	2249	U	O4'-C4'-C3'	5.53	110.53	106.10
2	AB	2365	G	C8-N9-C4	-5.53	104.19	106.40
34	BA	480	U	C5'-C4'-C3'	-5.53	107.15	116.00
34	BA	1199	U	O4'-C1'-N1	5.53	112.63	108.20
2	AB	1140	C	O4'-C1'-N1	5.53	112.63	108.20
2	AB	2864	G	C5'-C4'-O4'	5.53	115.74	109.10
34	BA	339	C	O4'-C1'-N1	5.53	112.63	108.20
34	BA	556	C	O4'-C1'-N1	5.53	112.62	108.20
34	BA	601	G	N9-C1'-C2'	-5.53	105.92	112.00
34	BA	844	G	C8-N9-C4	-5.53	104.19	106.40
1	AA	107	G	O4'-C1'-N9	5.53	112.62	108.20
2	AB	1997	C	O4'-C1'-N1	5.53	112.62	108.20
34	BA	200	G	C5'-C4'-C3'	-5.53	107.15	116.00
34	BA	1297	G	O4'-C1'-N9	5.53	112.62	108.20
34	BA	1510	C	C5'-C4'-O4'	5.53	115.74	109.10
37	BD	39	U	O4'-C1'-N1	5.53	112.62	108.20
2	AB	1433	A	O4'-C1'-N9	5.53	112.62	108.20
2	AB	660	C	C5'-C4'-C3'	-5.53	107.16	116.00
2	AB	1685	C	C5'-C4'-O4'	5.53	115.73	109.10
2	AB	2047	C	O4'-C1'-N1	5.53	112.62	108.20
34	BA	1096	C	N1-C2-O2	5.53	122.22	118.90
2	AB	1645	G	O4'-C4'-C3'	5.53	110.52	106.10
2	AB	1740	G	C8-N9-C4	-5.53	104.19	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	14	A	O4'-C1'-N9	5.53	112.62	108.20
34	BA	473	U	O4'-C1'-N1	5.52	112.62	108.20
34	BA	1115	U	O4'-C1'-N1	5.52	112.62	108.20
57	BY	1	PRO	CA-N-CD	-5.52	103.77	111.50
2	AB	1222	U	O4'-C1'-N1	5.52	112.62	108.20
2	AB	2114	A	O4'-C1'-N9	5.52	112.62	108.20
34	BA	521	G	N3-C4-C5	-5.52	125.84	128.60
34	BA	529	G	O4'-C1'-N9	5.52	112.62	108.20
34	BA	1150	A	C5'-C4'-C3'	-5.52	107.16	116.00
2	AB	2786	U	O4'-C1'-N1	5.52	112.62	108.20
2	AB	1804	C	O4'-C1'-N1	5.52	112.62	108.20
1	AA	20	G	C8-N9-C4	-5.52	104.19	106.40
2	AB	469	G	C8-N9-C4	-5.52	104.19	106.40
2	AB	1022	G	O4'-C1'-N9	5.52	112.61	108.20
2	AB	2506	U	O4'-C1'-N1	5.52	112.61	108.20
34	BA	414	A	O4'-C1'-N9	5.52	112.61	108.20
34	BA	643	C	O4'-C1'-N1	5.52	112.61	108.20
34	BA	1502	A	C5'-C4'-C3'	-5.52	107.17	116.00
2	AB	2664	G	N7-C8-N9	5.51	115.86	113.10
34	BA	1284	C	O4'-C1'-N1	5.51	112.61	108.20
2	AB	1092	C	O4'-C1'-N1	5.51	112.61	108.20
2	AB	1890	A	O4'-C1'-N9	5.51	112.61	108.20
2	AB	1796	U	O4'-C1'-N1	5.51	112.61	108.20
2	AB	2627	G	C8-N9-C4	-5.51	104.19	106.40
2	AB	2557	G	O4'-C1'-N9	5.51	112.61	108.20
34	BA	1040	U	C5'-C4'-O4'	5.51	115.71	109.10
34	BA	1074	G	C5'-C4'-O4'	5.51	115.71	109.10
1	AA	105	G	O4'-C1'-N9	5.51	112.61	108.20
2	AB	335	C	O4'-C1'-N1	5.51	112.61	108.20
2	AB	665	U	O4'-C1'-N1	5.51	112.61	108.20
2	AB	1114	C	C5'-C4'-C3'	-5.51	107.19	116.00
2	AB	2087	G	N3-C4-C5	-5.51	125.85	128.60
2	AB	829	A	O4'-C1'-N9	5.51	112.61	108.20
34	BA	357	G	O4'-C1'-N9	5.51	112.61	108.20
34	BA	1289	A	O4'-C1'-N9	5.51	112.61	108.20
34	BA	1386	G	O4'-C1'-N9	5.51	112.61	108.20
2	AB	371	A	O4'-C1'-N9	5.50	112.60	108.20
2	AB	2282	G	O4'-C1'-N9	5.50	112.60	108.20
2	AB	2419	U	O4'-C1'-N1	5.50	112.60	108.20
2	AB	2896	C	C1'-O4'-C4'	-5.50	105.50	109.90
34	BA	1047	G	C8-N9-C4	-5.50	104.20	106.40
1	AA	50	A	C5'-C4'-O4'	5.50	115.70	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	924	G	C3'-C2'-C1'	-5.50	97.10	101.50
2	AB	2299	U	C5'-C4'-C3'	-5.50	107.20	116.00
34	BA	728	A	C5'-C4'-O4'	5.50	115.70	109.10
2	AB	308	G	C3'-C2'-C1'	5.50	105.90	101.50
34	BA	80	A	O4'-C1'-N9	5.50	112.60	108.20
34	BA	139	A	C5'-C4'-C3'	-5.50	107.20	116.00
34	BA	806	C	C5'-C4'-O4'	5.50	115.70	109.10
34	BA	1469	C	C5'-C4'-O4'	5.50	115.70	109.10
2	AB	270	A	C3'-C2'-C1'	-5.50	97.10	101.50
2	AB	356	G	C8-N9-C4	-5.50	104.20	106.40
2	AB	2049	G	O4'-C1'-N9	5.50	112.60	108.20
34	BA	995	C	O4'-C1'-N1	5.50	112.60	108.20
34	BA	1340	A	O4'-C1'-N9	5.50	112.60	108.20
2	AB	740	C	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	2068	U	O4'-C1'-N1	5.49	112.59	108.20
2	AB	1211	C	O4'-C1'-N1	5.49	112.59	108.20
34	BA	164	G	C5'-C4'-C3'	-5.49	107.21	116.00
34	BA	972	C	N1-C1'-C2'	-5.49	105.96	112.00
2	AB	2611	C	C5'-C4'-C3'	-5.49	107.21	116.00
37	BD	35	U	O4'-C1'-N1	5.49	112.59	108.20
1	AA	84	G	N9-C1'-C2'	-5.49	105.96	112.00
2	AB	305	C	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	843	G	N3-C4-C5	-5.49	125.86	128.60
2	AB	2459	A	C8-N9-C4	-5.49	103.60	105.80
2	AB	2647	U	O4'-C1'-N1	5.49	112.59	108.20
34	BA	215	C	C5'-C4'-C3'	-5.49	107.22	116.00
2	AB	278	A	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	1035	U	C5'-C4'-O4'	5.49	115.69	109.10
2	AB	2802	G	N9-C1'-C2'	-5.49	105.96	112.00
2	AB	903	C	C5'-C4'-O4'	5.49	115.68	109.10
2	AB	1084	A	C1'-O4'-C4'	-5.49	105.51	109.90
2	AB	1740	G	O4'-C1'-N9	5.48	112.59	108.20
2	AB	1984	G	O4'-C1'-N9	5.48	112.59	108.20
34	BA	355	C	N3-C2-O2	-5.48	118.06	121.90
2	AB	2408	U	C5'-C4'-O4'	5.48	115.68	109.10
34	BA	740	U	O4'-C1'-N1	5.48	112.58	108.20
34	BA	1022	A	O4'-C1'-N9	5.48	112.58	108.20
2	AB	1574	C	O4'-C1'-N1	5.48	112.58	108.20
2	AB	2472	G	C8-N9-C4	-5.48	104.21	106.40
2	AB	1822	C	C2-N3-C4	5.48	122.64	119.90
2	AB	2588	G	C8-N9-C4	-5.48	104.21	106.40
34	BA	326	G	C8-N9-C4	-5.48	104.21	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1377	A	C4'-C3'-C2'	-5.48	97.12	102.60
2	AB	2878	U	O4'-C1'-N1	5.48	112.58	108.20
2	AB	974	G	N3-C4-C5	-5.47	125.86	128.60
2	AB	1184	U	C5'-C4'-C3'	-5.47	107.24	116.00
2	AB	2606	C	O4'-C1'-N1	5.47	112.58	108.20
1	AA	75	G	C8-N9-C4	-5.47	104.21	106.40
2	AB	635	C	O4'-C1'-N1	5.47	112.58	108.20
2	AB	1852	U	P-O3'-C3'	5.47	126.27	119.70
2	AB	2447	G	P-O3'-C3'	5.47	126.27	119.70
34	BA	1244	G	O4'-C1'-N9	5.47	112.58	108.20
2	AB	1483	G	C5'-C4'-O4'	5.47	115.66	109.10
34	BA	587	G	C5'-C4'-C3'	-5.47	107.25	116.00
34	BA	1228	C	O4'-C4'-C3'	5.47	110.47	106.10
34	BA	1021	A	C4'-C3'-C2'	-5.47	97.13	102.60
2	AB	374	A	C5'-C4'-O4'	5.46	115.66	109.10
2	AB	2400	G	O4'-C1'-N9	5.46	112.57	108.20
34	BA	32	A	O4'-C1'-N9	5.46	112.57	108.20
34	BA	346	G	C2-N3-C4	5.46	114.63	111.90
2	AB	2685	G	O4'-C1'-N9	5.46	112.57	108.20
34	BA	545	C	O4'-C1'-N1	5.46	112.57	108.20
2	AB	1724	G	N3-C4-C5	-5.46	125.87	128.60
2	AB	2308	G	C8-N9-C4	-5.46	104.22	106.40
2	AB	119	A	C5'-C4'-C3'	-5.46	107.26	116.00
2	AB	1355	G	O4'-C1'-N9	5.46	112.57	108.20
34	BA	12	U	O4'-C1'-N1	5.46	112.57	108.20
2	AB	398	C	O4'-C1'-N1	5.46	112.57	108.20
2	AB	671	C	C4'-C3'-C2'	-5.46	97.14	102.60
2	AB	984	A	N9-C1'-C2'	5.46	121.09	114.00
18	AR	23	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	AB	2354	C	O4'-C1'-N1	5.46	112.57	108.20
2	AB	479	A	P-O3'-C3'	5.46	126.25	119.70
2	AB	554	U	C5'-C4'-C3'	-5.46	107.27	116.00
2	AB	2451	A	O4'-C1'-N9	5.45	112.56	108.20
2	AB	2846	G	C8-N9-C4	-5.45	104.22	106.40
34	BA	964	A	O4'-C1'-N9	5.45	112.56	108.20
1	AA	38	C	O4'-C1'-N1	5.45	112.56	108.20
34	BA	731	G	C5'-C4'-O4'	5.45	115.64	109.10
2	AB	623	C	O4'-C1'-N1	5.45	112.56	108.20
2	AB	656	G	C8-N9-C4	-5.45	104.22	106.40
2	AB	925	A	O4'-C1'-N9	5.45	112.56	108.20
2	AB	1561	C	O4'-C1'-N1	5.45	112.56	108.20
34	BA	107	G	C5'-C4'-O4'	5.45	115.64	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	527	C	N1-C2-O2	5.45	122.17	118.90
2	AB	1002	G	C8-N9-C4	-5.45	104.22	106.40
35	BB	53	G	O4'-C1'-N9	5.45	112.56	108.20
1	AA	32	U	N3-C2-O2	-5.45	118.39	122.20
2	AB	345	A	P-O3'-C3'	5.44	126.23	119.70
2	AB	2640	G	C5'-C4'-O4'	5.44	115.63	109.10
2	AB	1723	G	C8-N9-C4	-5.44	104.22	106.40
3	AC	228	GLY	C-N-CA	5.44	135.31	121.70
34	BA	790	A	C5'-C4'-O4'	5.44	115.63	109.10
34	BA	1272	G	O4'-C1'-N9	5.44	112.55	108.20
2	AB	40	U	O4'-C1'-N1	5.44	112.55	108.20
2	AB	549	G	N3-C4-C5	-5.44	125.88	128.60
2	AB	1360	G	N9-C4-C5	5.44	107.58	105.40
34	BA	292	G	C4'-C3'-C2'	-5.44	97.16	102.60
2	AB	6	A	C5'-C4'-O4'	5.44	115.63	109.10
2	AB	2439	A	C5'-C4'-C3'	-5.44	107.30	116.00
2	AB	832	U	C5'-C4'-C3'	-5.44	107.30	116.00
2	AB	917	A	O4'-C1'-N9	5.44	112.55	108.20
2	AB	1410	G	N3-C4-C5	-5.44	125.88	128.60
2	AB	2401	U	O4'-C1'-N1	5.44	112.55	108.20
37	BD	37	U	O4'-C1'-N1	5.44	112.55	108.20
1	AA	14	U	C1'-O4'-C4'	-5.44	105.55	109.90
2	AB	545	U	O4'-C1'-N1	5.43	112.55	108.20
2	AB	690	G	C8-N9-C4	-5.43	104.23	106.40
2	AB	768	G	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	1507	C	C4'-C3'-C2'	-5.43	97.17	102.60
2	AB	1847	A	C1'-O4'-C4'	-5.43	105.55	109.90
2	AB	2488	G	N3-C4-C5	-5.43	125.88	128.60
34	BA	347	G	C8-N9-C4	-5.43	104.23	106.40
34	BA	636	U	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	2363	G	C8-N9-C4	-5.43	104.23	106.40
34	BA	9	G	O4'-C1'-N9	5.43	112.55	108.20
34	BA	1086	U	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	217	A	C5'-C4'-C3'	-5.43	107.31	116.00
1	AA	43	C	O4'-C1'-N1	5.43	112.54	108.20
2	AB	15	G	N7-C8-N9	5.43	115.81	113.10
2	AB	421	C	O4'-C1'-N1	5.43	112.54	108.20
2	AB	547	A	O4'-C1'-N9	5.43	112.54	108.20
2	AB	1893	C	O4'-C1'-N1	5.43	112.54	108.20
2	AB	2136	G	C5'-C4'-O4'	5.43	115.62	109.10
2	AB	2711	A	O4'-C1'-N9	5.43	112.54	108.20
34	BA	1184	G	C5'-C4'-O4'	5.43	115.62	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2162	G	C5'-C4'-C3'	-5.43	107.31	116.00
34	BA	139	A	C4'-C3'-C2'	-5.43	97.17	102.60
34	BA	1319	A	O4'-C1'-N9	5.43	112.54	108.20
2	AB	242	G	C5'-C4'-C3'	-5.43	107.32	116.00
2	AB	2705	A	C4'-C3'-C2'	-5.43	97.17	102.60
34	BA	1061	G	N7-C8-N9	5.43	115.81	113.10
34	BA	1213	A	C2'-C3'-O3'	5.43	122.38	113.70
2	AB	623	C	C5'-C4'-C3'	-5.42	107.32	116.00
2	AB	2020	A	C1'-O4'-C4'	-5.42	105.56	109.90
2	AB	2571	U	P-O3'-C3'	5.42	126.21	119.70
34	BA	168	G	C5'-C4'-O4'	5.42	115.61	109.10
2	AB	240	C	O4'-C1'-N1	5.42	112.54	108.20
2	AB	253	C	C5'-C4'-O4'	5.42	115.61	109.10
2	AB	764	A	O4'-C1'-N9	5.42	112.54	108.20
2	AB	767	U	O4'-C1'-N1	5.42	112.54	108.20
34	BA	403	C	C5'-C4'-O4'	5.42	115.61	109.10
34	BA	1280	A	C5'-C4'-C3'	-5.42	107.33	116.00
2	AB	119	A	O4'-C1'-N9	5.42	112.54	108.20
2	AB	1410	G	C8-N9-C4	-5.42	104.23	106.40
2	AB	2562	U	O4'-C1'-N1	5.42	112.54	108.20
34	BA	85	U	C1'-O4'-C4'	-5.42	105.56	109.90
2	AB	1603	A	C5'-C4'-C3'	-5.42	107.33	116.00
34	BA	439	U	N1-C2-N3	5.42	118.15	114.90
34	BA	909	A	O3'-P-O5'	5.42	114.29	104.00
1	AA	75	G	O4'-C1'-N9	5.42	112.53	108.20
2	AB	531	C	O4'-C4'-C3'	5.42	110.43	106.10
2	AB	987	C	O4'-C1'-N1	5.42	112.53	108.20
2	AB	2263	C	O4'-C1'-N1	5.42	112.53	108.20
34	BA	234	C	O4'-C1'-N1	5.42	112.53	108.20
34	BA	1230	C	O4'-C1'-N1	5.42	112.53	108.20
2	AB	769	U	C5'-C4'-O4'	5.42	115.60	109.10
2	AB	1952	A	O4'-C4'-C3'	5.41	110.43	106.10
2	AB	2186	G	O4'-C1'-N9	5.41	112.53	108.20
2	AB	2806	C	O4'-C1'-N1	5.41	112.53	108.20
34	BA	715	A	O4'-C1'-N9	5.41	112.53	108.20
2	AB	536	G	O4'-C1'-N9	5.41	112.53	108.20
2	AB	763	G	C8-N9-C4	-5.41	104.23	106.40
34	BA	336	A	O4'-C1'-N9	5.41	112.53	108.20
1	AA	107	G	N7-C8-N9	5.41	115.81	113.10
2	AB	735	A	O4'-C1'-N9	5.41	112.53	108.20
2	AB	824	U	C5'-C4'-O4'	5.41	115.59	109.10
2	AB	1495	A	O4'-C1'-N9	5.41	112.53	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	491	G	C8-N9-C4	-5.41	104.24	106.40
2	AB	554	U	C5'-C4'-O4'	5.41	115.59	109.10
2	AB	787	C	O4'-C1'-N1	5.41	112.53	108.20
2	AB	1139	G	O4'-C1'-N9	5.41	112.53	108.20
2	AB	2174	C	O4'-C1'-N1	5.41	112.53	108.20
34	BA	136	C	O4'-C1'-N1	5.41	112.53	108.20
34	BA	861	G	N3-C4-C5	-5.41	125.90	128.60
34	BA	1008	U	C5'-C4'-O4'	5.41	115.59	109.10
34	BA	1256	A	O4'-C1'-N9	5.41	112.53	108.20
34	BA	277	C	N1-C1'-C2'	-5.41	106.05	112.00
2	AB	842	U	C5'-C4'-C3'	-5.41	107.35	116.00
2	AB	1566	A	C5'-C4'-C3'	-5.41	107.35	116.00
2	AB	742	A	O4'-C1'-N9	5.40	112.52	108.20
2	AB	2735	G	C5'-C4'-O4'	5.40	115.58	109.10
34	BA	175	C	C5'-C4'-O4'	5.40	115.58	109.10
34	BA	1242	G	C8-N9-C4	-5.40	104.24	106.40
2	AB	545	U	O3'-P-O5'	-5.40	93.74	104.00
2	AB	1332	G	N3-C4-C5	-5.40	125.90	128.60
2	AB	2398	U	C5'-C4'-C3'	-5.40	107.36	116.00
34	BA	356	A	O4'-C1'-N9	5.40	112.52	108.20
34	BA	793	U	O3'-P-O5'	-5.40	93.74	104.00
34	BA	1090	U	N1-C1'-C2'	-5.40	106.06	112.00
2	AB	383	C	N1-C2-O2	5.40	122.14	118.90
2	AB	996	A	C5'-C4'-O4'	5.40	115.58	109.10
2	AB	2309	A	O4'-C1'-N9	5.40	112.52	108.20
34	BA	705	G	C8-N9-C4	-5.40	104.24	106.40
34	BA	913	A	P-O3'-C3'	5.40	126.18	119.70
2	AB	1292	G	O3'-P-O5'	-5.40	93.74	104.00
34	BA	1138	G	N3-C4-C5	-5.40	125.90	128.60
1	AA	13	G	C4'-C3'-O3'	5.40	123.80	113.00
2	AB	1164	C	O4'-C1'-N1	5.40	112.52	108.20
2	AB	389	G	C8-N9-C4	-5.40	104.24	106.40
2	AB	1118	C	C5'-C4'-C3'	-5.40	107.37	116.00
2	AB	2234	G	C8-N9-C4	-5.40	104.24	106.40
2	AB	2299	U	C5'-C4'-O4'	5.40	115.58	109.10
34	BA	253	A	O3'-P-O5'	-5.40	93.75	104.00
2	AB	1710	G	C5'-C4'-C3'	-5.39	107.37	116.00
2	AB	2677	G	O4'-C1'-N9	5.39	112.52	108.20
2	AB	2902	C	O4'-C1'-N1	5.39	112.52	108.20
34	BA	310	G	N3-C4-C5	-5.39	125.90	128.60
2	AB	1799	G	O4'-C1'-N9	5.39	112.52	108.20
2	AB	1822	C	N1-C2-O2	5.39	122.14	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2471	A	O4'-C1'-N9	5.39	112.51	108.20
34	BA	1061	G	N3-C4-C5	-5.39	125.90	128.60
2	AB	72	U	O4'-C4'-C3'	5.39	110.41	106.10
2	AB	121	G	N3-C4-C5	-5.39	125.91	128.60
2	AB	123	G	C5'-C4'-O4'	5.39	115.57	109.10
2	AB	654	A	P-O3'-C3'	5.39	126.17	119.70
2	AB	2006	C	C5'-C4'-O4'	5.39	115.56	109.10
34	BA	843	U	C3'-C2'-C1'	5.39	105.81	101.50
1	AA	51	G	C8-N9-C4	-5.39	104.25	106.40
2	AB	589	U	O4'-C1'-N1	5.39	112.51	108.20
2	AB	942	G	C8-N9-C4	-5.39	104.25	106.40
34	BA	415	A	N9-C1'-C2'	-5.39	106.08	112.00
2	AB	216	A	N9-C1'-C2'	-5.38	106.08	112.00
2	AB	2842	G	O4'-C1'-N9	5.38	112.51	108.20
34	BA	917	G	N3-C4-C5	-5.38	125.91	128.60
34	BA	1395	C	C5'-C4'-C3'	-5.38	107.38	116.00
2	AB	1403	A	O4'-C1'-N9	5.38	112.51	108.20
34	BA	188	C	O3'-P-O5'	-5.38	93.77	104.00
34	BA	240	G	O4'-C1'-N9	5.38	112.51	108.20
34	BA	378	G	O4'-C1'-N9	5.38	112.51	108.20
2	AB	1444	G	C8-N9-C4	-5.38	104.25	106.40
2	AB	1666	G	O4'-C1'-N9	5.38	112.51	108.20
2	AB	2614	A	O4'-C1'-N9	5.38	112.50	108.20
34	BA	542	G	O4'-C1'-N9	5.38	112.51	108.20
35	BB	72	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	426	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	2328	A	C5'-C4'-O4'	5.38	115.55	109.10
2	AB	2890	G	C8-N9-C4	-5.38	104.25	106.40
37	BD	26	U	N3-C2-O2	-5.38	118.44	122.20
34	BA	688	G	N3-C4-C5	-5.38	125.91	128.60
2	AB	337	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	1214	A	C5'-C4'-C3'	-5.38	107.40	116.00
2	AB	1566	A	C3'-C2'-C1'	5.38	105.80	101.50
2	AB	1812	U	O4'-C1'-N1	5.38	112.50	108.20
34	BA	1001	C	C5'-C4'-C3'	-5.38	107.40	116.00
34	BA	1107	C	O4'-C1'-N1	5.38	112.50	108.20
2	AB	54	G	C8-N9-C4	-5.37	104.25	106.40
2	AB	2083	G	C8-N9-C4	-5.37	104.25	106.40
2	AB	2619	C	C5'-C4'-O4'	5.37	115.55	109.10
34	BA	75	G	O4'-C1'-N9	5.37	112.50	108.20
34	BA	470	C	O4'-C1'-N1	5.37	112.50	108.20
34	BA	1512	U	O4'-C1'-N1	5.37	112.50	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1171	G	O4'-C1'-N9	5.37	112.50	108.20
2	AB	1767	G	N3-C4-C5	-5.37	125.92	128.60
2	AB	2202	U	C5'-C4'-O4'	5.37	115.55	109.10
34	BA	422	C	O4'-C1'-N1	5.37	112.50	108.20
34	BA	1076	U	C2'-C3'-O3'	5.37	122.29	113.70
34	BA	235	C	C5'-C4'-O4'	5.37	115.54	109.10
2	AB	98	G	C8-N9-C4	-5.37	104.25	106.40
34	BA	749	A	C3'-C2'-C1'	-5.37	97.20	101.50
34	BA	777	A	C5'-C4'-C3'	-5.37	107.41	116.00
34	BA	743	A	C5'-C4'-O4'	5.37	115.54	109.10
2	AB	79	C	O4'-C1'-N1	5.37	112.49	108.20
2	AB	329	G	C8-N9-C4	-5.37	104.25	106.40
2	AB	687	C	N1-C2-O2	5.37	122.12	118.90
2	AB	1868	C	C5'-C4'-C3'	-5.37	107.42	116.00
2	AB	2123	G	N9-C4-C5	5.37	107.55	105.40
2	AB	494	G	N9-C1'-C2'	-5.36	106.10	112.00
2	AB	686	U	C5'-C4'-O4'	5.36	115.54	109.10
2	AB	1454	C	C6-N1-C2	-5.36	118.16	120.30
2	AB	2135	A	C3'-C2'-C1'	5.36	105.79	101.50
2	AB	2792	A	P-O5'-C5'	5.36	129.48	120.90
34	BA	72	A	C5'-C4'-C3'	-5.36	107.42	116.00
34	BA	318	G	C3'-C2'-C1'	-5.36	97.21	101.50
2	AB	1718	G	C5'-C4'-O4'	5.36	115.53	109.10
2	AB	401	A	C5'-C4'-C3'	-5.36	107.42	116.00
2	AB	807	U	C4'-C3'-C2'	-5.36	97.24	102.60
2	AB	866	A	C5'-C4'-O4'	5.36	115.53	109.10
2	AB	1138	G	N3-C4-C5	-5.36	125.92	128.60
2	AB	2631	G	C5'-C4'-O4'	5.36	115.53	109.10
34	BA	1038	C	O4'-C1'-N1	5.36	112.49	108.20
35	BE	52	G	O4'-C1'-N9	5.36	112.49	108.20
2	AB	181	A	C3'-C2'-C1'	-5.36	97.21	101.50
2	AB	2800	A	C5'-C4'-C3'	-5.36	107.43	116.00
2	AB	857	G	C8-N9-C1'	5.36	133.96	127.00
2	AB	981	A	C5'-C4'-O4'	5.36	115.53	109.10
2	AB	1474	U	O4'-C1'-N1	5.36	112.48	108.20
2	AB	2186	G	C8-N9-C4	-5.36	104.26	106.40
2	AB	2258	C	P-O3'-C3'	5.35	126.12	119.70
35	BB	69	G	O4'-C1'-N9	5.35	112.48	108.20
2	AB	843	G	C8-N9-C4	-5.35	104.26	106.40
34	BA	1255	G	N9-C4-C5	5.35	107.54	105.40
34	BA	1533	C	O4'-C1'-N1	5.35	112.48	108.20
2	AB	712	G	C8-N9-C4	-5.35	104.26	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1540	G	N3-C4-C5	-5.35	125.93	128.60
2	AB	1737	G	C5'-C4'-C3'	-5.35	107.44	116.00
34	BA	633	G	O4'-C1'-N9	5.35	112.48	108.20
2	AB	841	G	C1'-O4'-C4'	-5.35	105.62	109.90
2	AB	1538	G	O4'-C1'-N9	5.35	112.48	108.20
34	BA	251	G	O4'-C1'-N9	5.35	112.48	108.20
34	BA	1344	C	O4'-C1'-N1	5.35	112.48	108.20
2	AB	545	U	C3'-C2'-C1'	5.35	105.78	101.50
2	AB	2039	U	C5'-C4'-C3'	-5.34	107.45	116.00
2	AB	2345	G	N3-C4-C5	-5.34	125.93	128.60
34	BA	435	A	O4'-C1'-N9	5.34	112.48	108.20
35	BE	6	G	P-O3'-C3'	5.34	126.11	119.70
2	AB	2219	U	O4'-C1'-N1	5.34	112.47	108.20
2	AB	2344	U	O4'-C1'-N1	5.34	112.47	108.20
2	AB	757	G	O4'-C1'-N9	5.34	112.47	108.20
2	AB	1186	G	C8-N9-C4	-5.34	104.26	106.40
34	BA	756	C	O4'-C1'-N1	5.34	112.47	108.20
34	BA	996	A	C5'-C4'-O4'	5.34	115.51	109.10
2	AB	2036	C	N1-C2-O2	5.34	122.10	118.90
2	AB	2639	A	C5'-C4'-C3'	-5.34	107.46	116.00
35	BE	12	U	O4'-C1'-N1	5.34	112.47	108.20
35	BE	19	G	N3-C4-C5	-5.34	125.93	128.60
34	BA	115	G	O4'-C1'-N9	5.33	112.47	108.20
34	BA	1013	G	O4'-C1'-N9	5.33	112.47	108.20
2	AB	1446	C	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	2680	U	O4'-C1'-N1	5.33	112.47	108.20
34	BA	79	G	O4'-C1'-N9	5.33	112.47	108.20
35	BB	66	U	C5'-C4'-O4'	5.33	115.50	109.10
35	BE	61	C	C5'-C4'-C3'	-5.33	107.47	116.00
2	AB	323	C	C5'-C4'-C3'	-5.33	107.47	116.00
2	AB	2666	C	N1-C2-O2	5.33	122.10	118.90
34	BA	909	A	C8-N9-C4	-5.33	103.67	105.80
35	BE	18	G	P-O3'-C3'	5.33	126.10	119.70
2	AB	2550	G	C5'-C4'-O4'	5.33	115.50	109.10
34	BA	1373	G	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	1117	C	O4'-C1'-N1	5.33	112.46	108.20
2	AB	1451	C	C5'-C4'-O4'	5.33	115.49	109.10
2	AB	1680	U	C5'-C4'-O4'	5.33	115.49	109.10
2	AB	1776	G	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	2357	G	C5'-C4'-O4'	5.33	115.50	109.10
2	AB	2399	G	C8-N9-C4	-5.33	104.27	106.40
34	BA	981	U	C5'-C4'-C3'	-5.33	107.47	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BD	44	U	O4'-C1'-N1	5.33	112.46	108.20
1	AA	13	G	N3-C4-C5	-5.33	125.94	128.60
2	AB	1451	C	N1-C2-O2	5.33	122.10	118.90
2	AB	1732	C	O4'-C4'-C3'	5.33	110.36	106.10
2	AB	171	U	O4'-C1'-N1	5.33	112.46	108.20
2	AB	227	A	O4'-C1'-N9	5.33	112.46	108.20
2	AB	968	C	O4'-C1'-N1	5.33	112.46	108.20
2	AB	1455	G	C5'-C4'-O4'	5.33	115.49	109.10
2	AB	1873	G	N3-C4-C5	-5.33	125.94	128.60
2	AB	1159	U	C5'-C4'-O4'	5.32	115.49	109.10
2	AB	2587	A	O4'-C1'-N9	5.32	112.46	108.20
34	BA	602	A	O4'-C1'-N9	5.32	112.46	108.20
35	BE	75	C	O4'-C1'-N1	5.32	112.46	108.20
2	AB	1385	A	C4'-C3'-C2'	-5.32	97.28	102.60
34	BA	1386	G	C8-N9-C4	-5.32	104.27	106.40
2	AB	1236	G	O4'-C1'-N9	5.32	112.46	108.20
2	AB	2261	C	O4'-C1'-N1	5.32	112.46	108.20
2	AB	424	G	N3-C4-C5	-5.32	125.94	128.60
2	AB	514	A	C5'-C4'-O4'	5.32	115.48	109.10
2	AB	2019	A	O4'-C1'-N9	5.32	112.45	108.20
2	AB	875	G	N3-C4-C5	-5.32	125.94	128.60
34	BA	351	G	O4'-C1'-N9	5.32	112.45	108.20
1	AA	3	C	C5'-C4'-O4'	5.32	115.48	109.10
2	AB	1107	G	N3-C4-C5	-5.32	125.94	128.60
34	BA	1310	G	C5'-C4'-O4'	5.32	115.48	109.10
2	AB	1241	A	O4'-C1'-N9	5.31	112.45	108.20
2	AB	2731	G	C8-N9-C4	-5.31	104.27	106.40
34	BA	520	A	C8-N9-C4	-5.31	103.67	105.80
2	AB	1718	G	C8-N9-C4	-5.31	104.28	106.40
2	AB	2301	C	O4'-C1'-N1	5.31	112.45	108.20
35	BE	28	G	N3-C4-C5	-5.31	125.94	128.60
2	AB	1490	A	C8-N9-C4	-5.31	103.68	105.80
2	AB	1552	A	C1'-O4'-C4'	-5.31	105.65	109.90
2	AB	468	G	C8-N9-C4	-5.31	104.28	106.40
34	BA	1058	G	O4'-C1'-N9	5.31	112.45	108.20
2	AB	15	G	N3-C4-C5	-5.31	125.95	128.60
2	AB	2488	G	C8-N9-C4	-5.31	104.28	106.40
34	BA	86	G	C3'-C2'-C1'	5.31	105.75	101.50
34	BA	765	G	C8-N9-C4	-5.31	104.28	106.40
34	BA	933	G	C5'-C4'-C3'	-5.31	107.51	116.00
34	BA	1053	G	P-O3'-C3'	5.31	126.07	119.70
34	BA	1279	G	O5'-C5'-C4'	-5.31	101.61	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	618	G	C8-N9-C4	-5.31	104.28	106.40
2	AB	1817	G	C8-N9-C4	-5.31	104.28	106.40
2	AB	53	A	O4'-C1'-N9	5.30	112.44	108.20
2	AB	678	C	O4'-C1'-N1	5.30	112.44	108.20
2	AB	1588	G	C3'-C2'-C1'	-5.30	97.26	101.50
2	AB	1850	G	O4'-C1'-N9	5.30	112.44	108.20
2	AB	1995	U	O4'-C1'-N1	5.30	112.44	108.20
34	BA	257	G	C5'-C4'-O4'	5.30	115.47	109.10
34	BA	789	U	C5'-C4'-O4'	5.30	115.47	109.10
2	AB	17	G	C8-N9-C4	-5.30	104.28	106.40
2	AB	1726	C	O4'-C1'-N1	5.30	112.44	108.20
2	AB	2190	G	C5'-C4'-C3'	-5.30	107.52	116.00
34	BA	331	G	O4'-C1'-N9	5.30	112.44	108.20
2	AB	1263	U	O4'-C1'-N1	5.30	112.44	108.20
34	BA	376	G	O4'-C1'-N9	5.30	112.44	108.20
34	BA	815	A	C4'-C3'-C2'	-5.30	97.30	102.60
2	AB	1165	A	C5'-C4'-O4'	5.30	115.46	109.10
2	AB	2238	G	N3-C4-C5	-5.30	125.95	128.60
2	AB	2692	G	N3-C4-C5	-5.30	125.95	128.60
2	AB	532	A	O4'-C4'-C3'	5.30	110.34	106.10
2	AB	301	G	N9-C4-C5	5.30	107.52	105.40
2	AB	347	A	C8-N9-C4	-5.30	103.68	105.80
34	BA	938	A	C5'-C4'-O4'	5.30	115.46	109.10
34	BA	1033	G	N3-C4-C5	-5.30	125.95	128.60
2	AB	2248	C	O4'-C1'-N1	5.29	112.44	108.20
34	BA	1257	A	O4'-C4'-C3'	5.29	110.34	106.10
2	AB	1869	G	N9-C4-C5	5.29	107.52	105.40
2	AB	1972	G	O4'-C1'-N9	5.29	112.44	108.20
35	BE	73	A	O4'-C1'-N9	5.29	112.44	108.20
2	AB	1502	A	O4'-C1'-N9	5.29	112.43	108.20
2	AB	1569	A	C5'-C4'-O4'	5.29	115.45	109.10
2	AB	2448	A	C1'-O4'-C4'	-5.29	105.67	109.90
2	AB	2483	C	O4'-C1'-N1	5.29	112.43	108.20
2	AB	2881	U	C2-N3-C4	-5.29	123.83	127.00
34	BA	367	U	O4'-C4'-C3'	5.29	110.33	106.10
34	BA	426	U	O3'-P-O5'	-5.29	93.94	104.00
2	AB	2296	U	O4'-C4'-C3'	5.29	110.33	106.10
34	BA	1520	C	O4'-C1'-N1	5.29	112.43	108.20
35	BB	26	A	O4'-C1'-N9	5.29	112.43	108.20
2	AB	2049	G	C4'-C3'-C2'	-5.29	97.31	102.60
2	AB	2429	G	P-O3'-C3'	5.29	126.05	119.70
34	BA	112	G	C1'-O4'-C4'	-5.29	105.67	109.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1144	G	N3-C4-C5	-5.29	125.96	128.60
34	BA	227	G	O4'-C1'-N9	5.29	112.43	108.20
1	AA	15	A	O3'-P-O5'	-5.28	93.96	104.00
1	AA	72	G	C8-N9-C4	-5.28	104.29	106.40
2	AB	21	A	C5'-C4'-C3'	-5.28	107.55	116.00
2	AB	1165	A	N9-C1'-C2'	-5.28	106.19	112.00
2	AB	1975	G	N9-C1'-C2'	-5.28	106.19	112.00
2	AB	2394	C	C4'-C3'-C2'	-5.28	97.32	102.60
2	AB	2553	G	C4'-C3'-C2'	-5.28	97.32	102.60
34	BA	1279	G	C1'-O4'-C4'	-5.28	105.67	109.90
2	AB	729	G	N3-C4-C5	-5.28	125.96	128.60
2	AB	1559	U	O4'-C1'-N1	5.28	112.42	108.20
34	BA	38	G	C8-N9-C4	-5.28	104.29	106.40
34	BA	276	G	C5'-C4'-O4'	5.28	115.44	109.10
35	BE	34	G	C5'-C4'-C3'	-5.28	107.55	116.00
2	AB	447	A	C8-N9-C4	-5.28	103.69	105.80
34	BA	214	C	N3-C2-O2	-5.28	118.20	121.90
34	BA	439	U	O4'-C1'-N1	5.28	112.42	108.20
34	BA	689	C	O4'-C1'-N1	5.28	112.42	108.20
34	BA	793	U	C5'-C4'-O4'	5.28	115.43	109.10
2	AB	458	G	C3'-C2'-C1'	-5.28	97.28	101.50
2	AB	533	G	N3-C4-C5	-5.28	125.96	128.60
2	AB	671	C	O4'-C1'-N1	5.28	112.42	108.20
2	AB	1786	A	C1'-O4'-C4'	-5.28	105.68	109.90
2	AB	2302	U	O4'-C1'-N1	5.28	112.42	108.20
35	BE	66	U	N1-C2-N3	5.28	118.06	114.90
2	AB	910	A	O4'-C1'-N9	5.27	112.42	108.20
34	BA	1225	A	O5'-C5'-C4'	-5.27	101.68	111.70
2	AB	690	G	N3-C4-C5	-5.27	125.96	128.60
2	AB	1042	G	C5'-C4'-O4'	5.27	115.43	109.10
2	AB	1138	G	C8-N9-C4	-5.27	104.29	106.40
2	AB	1538	G	N3-C4-C5	-5.27	125.96	128.60
2	AB	2625	G	C8-N9-C4	-5.27	104.29	106.40
34	BA	39	G	C4'-C3'-C2'	-5.27	97.33	102.60
34	BA	42	G	C5'-C4'-C3'	-5.27	107.56	116.00
34	BA	100	G	O4'-C1'-N9	5.27	112.42	108.20
2	AB	1838	C	N1-C2-O2	5.27	122.06	118.90
2	AB	2665	A	O4'-C1'-N9	5.27	112.42	108.20
2	AB	333	G	C8-N9-C4	-5.27	104.29	106.40
2	AB	485	C	C5'-C4'-C3'	-5.27	107.57	116.00
2	AB	1024	G	C8-N9-C4	-5.27	104.29	106.40
2	AB	1291	C	C5'-C4'-C3'	-5.27	107.57	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1900	A	O4'-C1'-N9	5.27	112.42	108.20
2	AB	1992	G	O4'-C1'-N9	5.27	112.42	108.20
34	BA	408	A	C8-N9-C4	-5.27	103.69	105.80
34	BA	686	U	C4'-C3'-C2'	-5.27	97.33	102.60
34	BA	1042	A	O4'-C1'-N9	5.27	112.42	108.20
2	AB	1895	C	C5'-C4'-O4'	5.27	115.42	109.10
34	BA	651	C	C5'-C4'-C3'	-5.27	107.57	116.00
34	BA	842	U	C5'-C4'-C3'	-5.27	107.57	116.00
34	BA	1072	G	C8-N9-C4	-5.27	104.29	106.40
34	BA	1397	C	C5'-C4'-C3'	-5.27	107.57	116.00
2	AB	346	A	C5'-C4'-O4'	5.26	115.42	109.10
34	BA	300	A	O4'-C1'-N9	5.26	112.41	108.20
34	BA	511	C	O3'-P-O5'	-5.26	94.00	104.00
2	AB	2706	A	O4'-C1'-N9	5.26	112.41	108.20
34	BA	738	C	O4'-C1'-N1	5.26	112.41	108.20
34	BA	1312	G	N3-C4-C5	-5.26	125.97	128.60
2	AB	1345	C	C5'-C4'-C3'	-5.26	107.58	116.00
2	AB	1989	G	C5'-C4'-C3'	-5.26	107.58	116.00
2	AB	2241	A	O4'-C1'-N9	5.26	112.41	108.20
34	BA	193	C	O4'-C1'-N1	5.26	112.41	108.20
34	BA	1041	G	C5'-C4'-O4'	5.26	115.41	109.10
34	BA	1233	G	C5'-C4'-O4'	5.26	115.41	109.10
2	AB	1042	G	C5'-C4'-C3'	-5.26	107.58	116.00
2	AB	1307	A	O4'-C1'-N9	5.26	112.41	108.20
2	AB	2212	A	N9-C1'-C2'	-5.26	106.22	112.00
2	AB	2285	C	C5'-C4'-O4'	5.26	115.41	109.10
34	BA	525	C	C5'-C4'-O4'	5.26	115.41	109.10
34	BA	579	A	O4'-C1'-N9	5.26	112.41	108.20
35	BE	28	G	C8-N9-C4	-5.26	104.30	106.40
2	AB	4	U	C5'-C4'-O4'	5.26	115.41	109.10
2	AB	916	G	N3-C4-C5	-5.26	125.97	128.60
34	BA	14	U	O4'-C1'-N1	5.26	112.41	108.20
34	BA	1040	U	C5'-C4'-C3'	-5.26	107.59	116.00
2	AB	187	G	N3-C4-C5	-5.25	125.97	128.60
2	AB	1186	G	C5'-C4'-O4'	5.25	115.41	109.10
2	AB	474	G	O4'-C1'-N9	5.25	112.40	108.20
2	AB	1738	G	N9-C4-C5	5.25	107.50	105.40
34	BA	70	U	N1-C2-N3	5.25	118.05	114.90
34	BA	268	U	C5'-C4'-C3'	-5.25	107.60	116.00
34	BA	1043	G	C8-N9-C4	-5.25	104.30	106.40
34	BA	1426	G	C8-N9-C4	-5.25	104.30	106.40
35	BB	18	G	N3-C4-C5	-5.25	125.97	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1201	U	C5'-C4'-O4'	5.25	115.40	109.10
2	AB	2637	U	N1-C2-N3	5.25	118.05	114.90
34	BA	162	A	C8-N9-C4	-5.25	103.70	105.80
34	BA	794	A	C5'-C4'-O4'	5.25	115.40	109.10
2	AB	550	C	P-O5'-C5'	5.25	129.30	120.90
2	AB	1508	A	C3'-C2'-C1'	5.25	105.70	101.50
2	AB	2380	C	C4'-C3'-C2'	-5.25	97.35	102.60
2	AB	2462	C	N3-C2-O2	-5.25	118.23	121.90
2	AB	2648	G	C5'-C4'-O4'	5.25	115.40	109.10
34	BA	660	C	C4'-C3'-C2'	-5.25	97.35	102.60
34	BA	1016	A	C5'-C4'-O4'	5.25	115.40	109.10
34	BA	1138	G	O4'-C1'-N9	5.25	112.40	108.20
35	BB	18	G	C3'-C2'-C1'	5.25	105.70	101.50
35	BB	22	G	N3-C4-C5	-5.25	125.98	128.60
2	AB	305	C	O4'-C1'-N1	5.25	112.40	108.20
2	AB	1040	A	O4'-C1'-N9	5.25	112.40	108.20
2	AB	2728	U	O4'-C1'-N1	5.25	112.40	108.20
2	AB	2808	G	P-O3'-C3'	5.25	126.00	119.70
34	BA	172	A	C8-N9-C4	-5.25	103.70	105.80
2	AB	2028	U	C3'-C2'-C1'	-5.25	97.30	101.50
2	AB	2822	G	C5'-C4'-O4'	5.25	115.39	109.10
2	AB	616	A	C5'-C4'-O4'	5.24	115.39	109.10
2	AB	1241	A	C8-N9-C4	-5.24	103.70	105.80
2	AB	2485	G	C8-N9-C4	-5.24	104.30	106.40
2	AB	2512	C	O4'-C1'-N1	5.24	112.39	108.20
2	AB	2777	G	N3-C4-C5	-5.24	125.98	128.60
2	AB	1243	C	C5'-C4'-C3'	-5.24	107.61	116.00
2	AB	2029	G	C5'-C4'-O4'	5.24	115.39	109.10
1	AA	18	G	C5'-C4'-O4'	5.24	115.39	109.10
34	BA	310	G	N7-C8-N9	5.24	115.72	113.10
2	AB	523	C	C5'-C4'-O4'	5.24	115.39	109.10
2	AB	712	G	N3-C4-C5	-5.24	125.98	128.60
2	AB	722	A	O4'-C1'-N9	5.24	112.39	108.20
2	AB	1330	C	C5'-C4'-O4'	5.24	115.39	109.10
2	AB	1530	G	C5'-C4'-O4'	5.24	115.39	109.10
34	BA	858	G	C5'-C4'-O4'	5.24	115.39	109.10
34	BA	1203	C	O4'-C1'-N1	5.24	112.39	108.20
2	AB	852	U	N1-C2-N3	5.24	118.04	114.90
1	AA	51	G	O4'-C1'-N9	5.23	112.39	108.20
2	AB	2133	G	O4'-C1'-C2'	-5.23	100.57	105.80
34	BA	1233	G	N3-C4-C5	-5.23	125.98	128.60
1	AA	75	G	O5'-C5'-C4'	-5.23	101.76	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	76	G	O4'-C1'-N9	5.23	112.38	108.20
2	AB	2119	A	C3'-C2'-C1'	5.23	105.69	101.50
34	BA	77	A	O4'-C1'-N9	5.23	112.39	108.20
34	BA	1501	C	C3'-C2'-C1'	5.23	105.68	101.50
2	AB	2685	G	C5'-C4'-O4'	5.23	115.38	109.10
2	AB	756	A	C3'-C2'-C1'	-5.23	97.32	101.50
2	AB	1941	C	C3'-C2'-C1'	5.23	105.68	101.50
2	AB	2051	A	C5'-C4'-C3'	-5.23	107.64	116.00
2	AB	2104	C	C5'-C4'-C3'	-5.23	107.64	116.00
2	AB	2749	A	O4'-C1'-N9	5.23	112.38	108.20
1	AA	11	C	N1-C2-O2	5.23	122.04	118.90
2	AB	167	A	C8-N9-C4	-5.23	103.71	105.80
2	AB	344	A	O4'-C1'-N9	5.23	112.38	108.20
2	AB	69	C	C5'-C4'-O4'	5.22	115.37	109.10
2	AB	724	U	O4'-C1'-N1	5.22	112.38	108.20
2	AB	1104	C	C2-N3-C4	5.22	122.51	119.90
34	BA	1347	G	C3'-C2'-C1'	-5.22	97.32	101.50
2	AB	1017	G	O4'-C1'-N9	5.22	112.38	108.20
2	AB	1395	A	C5'-C4'-C3'	-5.22	107.64	116.00
2	AB	1782	U	O4'-C1'-N1	5.22	112.38	108.20
34	BA	122	G	N3-C4-C5	-5.22	125.99	128.60
34	BA	625	U	O4'-C1'-N1	5.22	112.38	108.20
34	BA	749	A	C5'-C4'-C3'	-5.22	107.64	116.00
35	BB	19	G	O4'-C1'-N9	5.22	112.38	108.20
34	BA	295	C	O4'-C1'-N1	5.22	112.38	108.20
34	BA	1032	G	N3-C4-C5	-5.22	125.99	128.60
2	AB	1816	C	C1'-O4'-C4'	-5.22	105.72	109.90
2	AB	2791	G	C1'-O4'-C4'	-5.22	105.72	109.90
34	BA	817	C	O4'-C4'-C3'	5.22	110.28	106.10
2	AB	1498	C	O4'-C1'-N1	5.22	112.37	108.20
34	BA	1176	A	C8-N9-C4	-5.22	103.71	105.80
2	AB	555	G	N3-C4-C5	-5.22	125.99	128.60
2	AB	1850	G	C8-N9-C4	-5.22	104.31	106.40
2	AB	2190	G	O4'-C1'-N9	5.22	112.37	108.20
34	BA	729	A	O4'-C1'-N9	5.22	112.37	108.20
34	BA	989	U	O4'-C1'-N1	5.22	112.37	108.20
1	AA	110	C	O4'-C1'-N1	5.21	112.37	108.20
2	AB	205	G	C8-N9-C4	-5.21	104.31	106.40
2	AB	1048	A	C8-N9-C4	-5.21	103.71	105.80
34	BA	911	U	C5'-C4'-C3'	-5.21	107.66	116.00
1	AA	107	G	N3-C4-C5	-5.21	125.99	128.60
2	AB	979	A	C5'-C4'-C3'	-5.21	107.66	116.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	378	C	C5'-C4'-C3'	-5.21	107.66	116.00
2	AB	533	G	O4'-C4'-C3'	5.21	110.27	106.10
2	AB	711	G	C8-N9-C4	-5.21	104.32	106.40
2	AB	766	U	C5'-C4'-O4'	5.21	115.35	109.10
2	AB	1537	G	N3-C4-C5	-5.21	126.00	128.60
2	AB	1875	G	O3'-P-O5'	-5.21	94.10	104.00
34	BA	477	C	O4'-C4'-C3'	5.21	110.27	106.10
34	BA	851	G	C3'-C2'-C1'	-5.21	97.33	101.50
34	BA	1295	U	O4'-C1'-N1	5.21	112.37	108.20
1	AA	72	G	C5'-C4'-O4'	5.21	115.35	109.10
2	AB	509	C	O4'-C4'-C3'	5.21	110.27	106.10
2	AB	1411	U	C5'-C4'-C3'	-5.21	107.66	116.00
2	AB	1491	G	N3-C4-C5	-5.21	126.00	128.60
2	AB	2401	U	C5'-C4'-C3'	-5.21	107.66	116.00
34	BA	1047	G	C5'-C4'-O4'	5.21	115.35	109.10
2	AB	407	G	N3-C4-C5	-5.21	126.00	128.60
2	AB	483	A	O4'-C1'-N9	5.21	112.37	108.20
2	AB	509	C	O4'-C1'-N1	5.21	112.37	108.20
2	AB	1358	G	C8-N9-C4	-5.21	104.32	106.40
2	AB	2094	A	O4'-C1'-N9	5.21	112.37	108.20
2	AB	2618	G	C5'-C4'-O4'	5.21	115.35	109.10
34	BA	781	A	C5'-C4'-O4'	5.21	115.35	109.10
34	BA	1006	G	C8-N9-C4	-5.21	104.32	106.40
35	BE	2	C	C5'-C4'-O4'	5.21	115.35	109.10
34	BA	1446	A	C5'-C4'-C3'	-5.21	107.67	116.00
2	AB	646	U	C4'-C3'-C2'	-5.21	97.39	102.60
2	AB	824	U	C5'-C4'-C3'	-5.20	107.67	116.00
2	AB	844	A	O4'-C1'-N9	5.20	112.36	108.20
2	AB	983	A	O4'-C4'-C3'	5.20	110.26	106.10
2	AB	1197	G	C5'-C4'-O4'	5.20	115.34	109.10
2	AB	1594	U	O4'-C1'-N1	5.20	112.36	108.20
2	AB	2256	G	O4'-C1'-N9	5.20	112.36	108.20
34	BA	232	G	C5'-C4'-O4'	5.20	115.34	109.10
34	BA	1091	U	C5'-C4'-C3'	-5.20	107.67	116.00
34	BA	1314	C	N1-C2-O2	5.20	122.02	118.90
2	AB	1385	A	C1'-O4'-C4'	-5.20	105.74	109.90
2	AB	604	G	N9-C1'-C2'	-5.20	106.28	112.00
2	AB	1538	G	C8-N9-C4	-5.20	104.32	106.40
2	AB	1569	A	C5'-C4'-C3'	-5.20	107.68	116.00
2	AB	1757	A	O4'-C4'-C3'	5.20	110.26	106.10
2	AB	2168	G	C8-N9-C4	-5.20	104.32	106.40
34	BA	987	G	N3-C4-C5	-5.20	126.00	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1641	A	C5'-C4'-O4'	5.20	115.34	109.10
2	AB	2407	A	C4'-C3'-C2'	-5.20	97.40	102.60
2	AB	240	C	N1-C2-O2	5.20	122.02	118.90
34	BA	447	G	N3-C4-C5	-5.20	126.00	128.60
2	AB	316	C	N1-C1'-C2'	-5.20	106.28	112.00
2	AB	651	G	C5'-C4'-C3'	5.20	124.31	116.00
34	BA	1481	U	C5'-C4'-O4'	5.20	115.33	109.10
2	AB	305	C	C4'-C3'-C2'	-5.19	97.41	102.60
34	BA	252	U	O4'-C1'-N1	5.19	112.36	108.20
2	AB	684	G	O4'-C1'-N9	5.19	112.35	108.20
2	AB	811	U	O4'-C1'-C2'	-5.19	100.61	105.80
2	AB	1360	G	O4'-C1'-N9	5.19	112.35	108.20
2	AB	705	A	C8-N9-C4	-5.19	103.72	105.80
2	AB	1579	A	C5'-C4'-O4'	5.19	115.33	109.10
34	BA	140	U	C5'-C4'-O4'	5.19	115.33	109.10
2	AB	1848	A	C5'-C4'-O4'	5.19	115.33	109.10
34	BA	563	A	C1'-O4'-C4'	-5.19	105.75	109.90
2	AB	555	G	C2-N3-C4	5.19	114.49	111.90
2	AB	1537	G	C8-N9-C4	-5.19	104.33	106.40
2	AB	1855	U	C5'-C4'-O4'	5.19	115.32	109.10
2	AB	2344	U	P-O3'-C3'	5.19	125.92	119.70
34	BA	1399	C	O4'-C1'-N1	5.19	112.35	108.20
2	AB	2300	C	C5'-C4'-O4'	5.19	115.32	109.10
1	AA	62	C	O4'-C1'-N1	5.18	112.35	108.20
2	AB	978	G	C3'-C2'-C1'	-5.18	97.35	101.50
2	AB	2653	U	C5'-C4'-O4'	5.18	115.32	109.10
2	AB	2799	A	O4'-C1'-C2'	-5.18	100.62	105.80
2	AB	992	C	O4'-C1'-N1	5.18	112.35	108.20
34	BA	668	G	C5'-C4'-C3'	-5.18	107.71	116.00
2	AB	1209	U	C2-N1-C1'	5.18	123.92	117.70
2	AB	1396	U	C5'-C4'-C3'	-5.18	107.71	116.00
2	AB	1583	A	C4'-C3'-O3'	5.18	123.36	113.00
2	AB	1731	G	N9-C4-C5	5.18	107.47	105.40
2	AB	2801	G	C5'-C4'-O4'	5.18	115.31	109.10
34	BA	601	G	C5'-C4'-C3'	-5.18	107.71	116.00
34	BA	1149	C	C5'-C4'-O4'	5.18	115.31	109.10
2	AB	2158	A	P-O3'-C3'	5.18	125.91	119.70
2	AB	14	A	C5'-C4'-O4'	5.18	115.31	109.10
2	AB	957	C	O3'-P-O5'	-5.18	94.17	104.00
2	AB	1082	U	C5'-C4'-O4'	5.18	115.31	109.10
2	AB	1845	G	C8-N9-C4	-5.18	104.33	106.40
2	AB	2276	G	N9-C1'-C2'	-5.18	106.31	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	177	G	O4'-C1'-N9	5.17	112.34	108.20
2	AB	1331	G	C5'-C4'-O4'	5.17	115.31	109.10
2	AB	1902	C	C5'-C4'-O4'	5.17	115.31	109.10
2	AB	2228	G	C8-N9-C4	-5.17	104.33	106.40
34	BA	1279	G	N3-C4-C5	-5.17	126.01	128.60
1	AA	38	C	N1-C1'-C2'	-5.17	106.31	112.00
2	AB	2055	C	O4'-C1'-N1	5.17	112.34	108.20
34	BA	340	U	C5'-C4'-O4'	5.17	115.31	109.10
34	BA	662	U	O4'-C1'-N1	5.17	112.34	108.20
1	AA	45	A	C5'-C4'-C3'	-5.17	107.72	116.00
2	AB	855	G	C5'-C4'-C3'	-5.17	107.73	116.00
2	AB	1927	A	O4'-C1'-N9	5.17	112.34	108.20
34	BA	370	C	O4'-C1'-N1	5.17	112.34	108.20
34	BA	597	G	N3-C4-C5	-5.17	126.01	128.60
34	BA	726	C	O4'-C1'-N1	5.17	112.34	108.20
35	BE	3	C	C5'-C4'-O4'	5.17	115.31	109.10
2	AB	592	A	O4'-C1'-N9	5.17	112.34	108.20
2	AB	793	A	C8-N9-C4	-5.17	103.73	105.80
34	BA	1315	U	O4'-C1'-N1	5.17	112.34	108.20
2	AB	573	U	C5'-C4'-C3'	-5.17	107.73	116.00
2	AB	979	A	O4'-C1'-N9	5.17	112.33	108.20
2	AB	1521	G	O4'-C1'-N9	5.17	112.33	108.20
2	AB	2164	C	N1-C2-O2	5.17	122.00	118.90
2	AB	2533	U	N1-C1'-C2'	-5.17	106.31	112.00
2	AB	732	C	O4'-C1'-N1	5.17	112.33	108.20
2	AB	1372	U	C5'-C4'-O4'	5.17	115.30	109.10
34	BA	335	C	C5'-C4'-O4'	5.17	115.30	109.10
34	BA	1120	C	O3'-P-O5'	-5.17	94.18	104.00
37	BD	29	G	O4'-C4'-C3'	5.17	110.23	106.10
34	BA	1360	A	O4'-C1'-N9	5.17	112.33	108.20
2	AB	2393	U	O4'-C1'-N1	5.16	112.33	108.20
34	BA	1204	A	C5'-C4'-O4'	5.16	115.30	109.10
35	BB	45	U	O4'-C1'-N1	5.16	112.33	108.20
2	AB	179	C	C5'-C4'-O4'	5.16	115.30	109.10
2	AB	277	G	N9-C1'-C2'	5.16	120.71	114.00
2	AB	489	G	N9-C1'-C2'	-5.16	106.32	112.00
2	AB	597	G	O4'-C1'-N9	5.16	112.33	108.20
2	AB	2111	U	P-O3'-C3'	5.16	125.89	119.70
2	AB	1525	A	C5'-C4'-O4'	5.16	115.29	109.10
34	BA	245	U	C1'-O4'-C4'	-5.16	105.77	109.90
34	BA	441	A	O4'-C1'-N9	5.16	112.33	108.20
2	AB	716	A	C1'-O4'-C4'	-5.16	105.77	109.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1219	U	O4'-C1'-N1	5.16	112.33	108.20
2	AB	1408	G	C3'-C2'-C1'	-5.16	97.37	101.50
2	AB	1461	C	C1'-O4'-C4'	-5.16	105.77	109.90
2	AB	1591	A	C5'-C4'-C3'	-5.16	107.75	116.00
2	AB	1722	A	C8-N9-C4	-5.16	103.74	105.80
2	AB	2234	G	N7-C8-N9	5.16	115.68	113.10
2	AB	2324	U	O4'-C4'-C3'	5.16	110.23	106.10
34	BA	932	C	O4'-C1'-N1	5.16	112.33	108.20
1	AA	77	U	C3'-C2'-C1'	-5.16	97.38	101.50
2	AB	1646	C	O4'-C1'-N1	5.16	112.33	108.20
2	AB	1800	C	C6-N1-C2	-5.16	118.24	120.30
34	BA	1057	G	N3-C4-C5	-5.16	126.02	128.60
2	AB	573	U	C4'-C3'-C2'	-5.15	97.45	102.60
2	AB	1888	G	C8-N9-C4	-5.15	104.34	106.40
34	BA	916	U	O4'-C1'-N1	5.15	112.32	108.20
34	BA	1094	G	C8-N9-C4	-5.15	104.34	106.40
2	AB	367	G	C5'-C4'-C3'	-5.15	107.76	116.00
2	AB	1786	A	C5'-C4'-C3'	-5.15	107.76	116.00
2	AB	2517	C	N1-C2-O2	5.15	121.99	118.90
2	AB	2870	C	C5'-C4'-O4'	5.15	115.28	109.10
34	BA	434	U	C5'-C4'-O4'	5.15	115.28	109.10
34	BA	688	G	O4'-C1'-N9	5.15	112.32	108.20
34	BA	812	G	N3-C4-C5	-5.15	126.02	128.60
34	BA	1217	C	O4'-C1'-N1	5.15	112.32	108.20
2	AB	214	G	C8-N9-C4	-5.15	104.34	106.40
2	AB	302	C	C4'-C3'-C2'	-5.15	97.45	102.60
2	AB	2476	A	C2'-C3'-O3'	5.15	121.94	113.70
34	BA	50	A	O4'-C1'-N9	5.15	112.32	108.20
34	BA	430	A	C5'-C4'-O4'	5.15	115.28	109.10
2	AB	1324	G	O4'-C1'-N9	5.15	112.32	108.20
34	BA	212	G	N3-C4-C5	-5.15	126.03	128.60
34	BA	886	G	N9-C1'-C2'	-5.15	106.34	112.00
34	BA	998	C	O4'-C1'-N1	5.15	112.32	108.20
34	BA	1291	U	O4'-C1'-N1	5.15	112.32	108.20
2	AB	890	C	O4'-C1'-N1	5.15	112.32	108.20
34	BA	1081	A	O4'-C1'-N9	5.15	112.32	108.20
35	BE	27	G	O4'-C1'-N9	5.15	112.32	108.20
2	AB	345	A	C5'-C4'-O4'	5.15	115.28	109.10
2	AB	363	G	C5'-C4'-C3'	-5.15	107.77	116.00
2	AB	2378	A	C5'-C4'-O4'	5.15	115.28	109.10
34	BA	394	G	C8-N9-C4	-5.15	104.34	106.40
2	AB	1011	G	N9-C4-C5	5.14	107.46	105.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2638	G	C5'-C4'-C3'	-5.14	107.77	116.00
34	BA	183	C	O4'-C1'-N1	5.14	112.31	108.20
2	AB	81	G	O4'-C1'-N9	5.14	112.31	108.20
2	AB	1308	A	C5'-C4'-C3'	-5.14	107.77	116.00
2	AB	726	G	C4-N9-C1'	-5.14	119.82	126.50
2	AB	1478	G	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	1776	G	N3-C4-C5	-5.14	126.03	128.60
34	BA	146	G	O4'-C1'-N9	5.14	112.31	108.20
34	BA	332	G	C1'-O4'-C4'	-5.14	105.79	109.90
34	BA	764	C	O4'-C1'-N1	5.14	112.31	108.20
34	BA	1051	C	P-O3'-C3'	5.14	125.87	119.70
43	BK	1	PRO	CA-N-CD	-5.14	104.31	111.50
2	AB	380	G	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	669	G	C2-N3-C4	5.14	114.47	111.90
2	AB	2840	C	O4'-C1'-N1	5.14	112.31	108.20
34	BA	1020	G	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	1379	U	O4'-C1'-N1	5.14	112.31	108.20
2	AB	1830	C	C5'-C4'-O4'	5.14	115.26	109.10
2	AB	1898	U	C5'-C4'-O4'	5.14	115.27	109.10
2	AB	2041	U	O4'-C1'-N1	5.14	112.31	108.20
2	AB	2801	G	N9-C1'-C2'	-5.14	106.35	112.00
34	BA	406	G	C8-N9-C4	-5.14	104.35	106.40
34	BA	885	G	N3-C4-C5	-5.14	126.03	128.60
34	BA	1119	C	O4'-C1'-N1	5.14	112.31	108.20
34	BA	1162	C	C5'-C4'-C3'	-5.14	107.78	116.00
35	BB	2	C	O4'-C1'-N1	5.14	112.31	108.20
2	AB	190	A	O5'-C5'-C4'	5.13	121.45	111.70
2	AB	898	C	C1'-O4'-C4'	-5.13	105.79	109.90
1	AA	49	C	N1-C1'-C2'	-5.13	106.35	112.00
2	AB	2177	C	N1-C2-O2	5.13	121.98	118.90
2	AB	2885	G	C4'-C3'-O3'	5.13	123.27	113.00
1	AA	77	U	C5'-C4'-O4'	5.13	115.26	109.10
2	AB	1034	G	O4'-C1'-N9	5.13	112.31	108.20
2	AB	2477	U	C4'-C3'-C2'	-5.13	97.47	102.60
26	AZ	7	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	AB	1422	G	C3'-C2'-C1'	-5.13	97.40	101.50
2	AB	2543	G	C5'-C4'-O4'	5.13	115.26	109.10
2	AB	167	A	C5'-C4'-O4'	5.13	115.25	109.10
2	AB	389	G	N3-C4-C5	-5.13	126.04	128.60
2	AB	1360	G	C8-N9-C4	-5.13	104.35	106.40
2	AB	2230	G	N3-C4-C5	-5.13	126.04	128.60
2	AB	2540	C	C1'-O4'-C4'	-5.13	105.80	109.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1361	G	C8-N9-C4	-5.13	104.35	106.40
34	BA	1380	U	C1'-O4'-C4'	-5.13	105.80	109.90
2	AB	1154	G	N3-C4-C5	-5.13	126.04	128.60
2	AB	1203	U	C2-N3-C4	-5.13	123.92	127.00
2	AB	1743	G	C4'-C3'-C2'	-5.13	97.47	102.60
34	BA	540	G	O4'-C1'-N9	5.13	112.30	108.20
34	BA	1084	G	C2'-C3'-O3'	5.13	121.90	113.70
31	Ae	19	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	AA	88	C	O4'-C1'-N1	5.12	112.30	108.20
2	AB	841	G	O4'-C1'-C2'	5.12	112.21	107.60
2	AB	1555	G	N9-C4-C5	5.12	107.45	105.40
2	AB	1560	G	N3-C4-C5	-5.12	126.04	128.60
2	AB	2666	C	C4'-C3'-C2'	-5.12	97.48	102.60
2	AB	2765	A	O4'-C1'-N9	5.12	112.30	108.20
2	AB	1799	G	C8-N9-C4	-5.12	104.35	106.40
2	AB	1989	G	C8-N9-C4	-5.12	104.35	106.40
2	AB	2588	G	O4'-C1'-N9	5.12	112.30	108.20
34	BA	94	G	N3-C4-C5	-5.12	126.04	128.60
2	AB	381	G	O4'-C1'-N9	5.12	112.30	108.20
34	BA	393	A	O4'-C1'-N9	5.12	112.30	108.20
35	BB	18	G	O4'-C1'-N9	5.12	112.30	108.20
2	AB	202	U	O4'-C1'-N1	5.12	112.30	108.20
2	AB	242	G	O4'-C1'-N9	5.12	112.30	108.20
2	AB	1645	G	N3-C4-C5	-5.12	126.04	128.60
2	AB	1776	G	C5'-C4'-C3'	-5.12	107.81	116.00
2	AB	2731	G	C5'-C4'-C3'	-5.12	107.81	116.00
34	BA	502	A	O4'-C1'-N9	5.12	112.30	108.20
34	BA	1159	U	O4'-C1'-N1	5.12	112.30	108.20
2	AB	277	G	O4'-C1'-N9	5.12	112.29	108.20
2	AB	2060	A	O4'-C1'-N9	5.12	112.29	108.20
34	BA	176	C	O4'-C1'-N1	5.12	112.29	108.20
34	BA	884	U	C1'-O4'-C4'	-5.12	105.81	109.90
2	AB	150	U	O4'-C1'-N1	5.12	112.29	108.20
2	AB	483	A	C5'-C4'-O4'	5.12	115.24	109.10
2	AB	1881	C	C5'-C4'-C3'	-5.12	107.81	116.00
2	AB	1938	A	C5'-C4'-O4'	5.12	115.24	109.10
34	BA	549	C	C5'-C4'-O4'	5.12	115.24	109.10
34	BA	1227	A	C8-N9-C4	-5.12	103.75	105.80
2	AB	168	G	C3'-C2'-C1'	-5.11	97.41	101.50
2	AB	663	G	C8-N9-C4	-5.11	104.36	106.40
2	AB	1332	G	O3'-P-O5'	-5.11	94.28	104.00
2	AB	2292	U	O4'-C1'-N1	5.11	112.29	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	522	C	O4'-C1'-N1	5.11	112.29	108.20
34	BA	901	A	C4'-C3'-C2'	-5.11	97.49	102.60
34	BA	1426	G	O4'-C1'-N9	5.11	112.29	108.20
2	AB	231	A	C5'-C4'-C3'	-5.11	107.82	116.00
2	AB	326	G	C8-N9-C4	-5.11	104.36	106.40
2	AB	2898	U	O4'-C1'-N1	5.11	112.29	108.20
2	AB	1230	A	C5'-C4'-C3'	-5.11	107.82	116.00
34	BA	305	G	P-O3'-C3'	5.11	125.83	119.70
34	BA	991	U	O4'-C1'-N1	5.11	112.29	108.20
2	AB	287	G	N3-C4-C5	-5.11	126.05	128.60
2	AB	473	G	C5'-C4'-C3'	-5.11	107.83	116.00
2	AB	511	U	C5'-C4'-C3'	-5.11	107.83	116.00
2	AB	2872	A	C1'-O4'-C4'	-5.11	105.81	109.90
34	BA	1452	C	O4'-C1'-N1	5.11	112.29	108.20
1	AA	43	C	C3'-C2'-C1'	5.11	105.59	101.50
2	AB	1705	A	O4'-C1'-N9	5.11	112.29	108.20
2	AB	2831	G	O3'-P-O5'	-5.11	94.30	104.00
34	BA	758	C	N3-C2-O2	-5.11	118.33	121.90
51	BS	88	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	AA	111	U	C5'-C4'-C3'	-5.11	107.83	116.00
2	AB	663	G	O4'-C1'-N9	5.11	112.28	108.20
2	AB	725	G	C2'-C3'-O3'	5.11	121.87	113.70
2	AB	2530	A	C5'-C4'-O4'	5.11	115.23	109.10
2	AB	2642	G	N3-C4-C5	-5.11	126.05	128.60
34	BA	11	G	C5'-C4'-O4'	5.11	115.23	109.10
34	BA	1256	A	O3'-P-O5'	-5.11	94.30	104.00
35	BB	60	U	O4'-C1'-C2'	-5.11	100.69	105.80
2	AB	90	U	P-O3'-C3'	5.10	125.82	119.70
2	AB	136	G	N9-C1'-C2'	-5.10	106.39	112.00
2	AB	1491	G	C8-N9-C4	-5.10	104.36	106.40
2	AB	2031	A	C3'-C2'-C1'	5.10	105.58	101.50
2	AB	178	G	O4'-C1'-N9	5.10	112.28	108.20
2	AB	1530	G	N3-C4-C5	-5.10	126.05	128.60
2	AB	2162	G	N9-C4-C5	5.10	107.44	105.40
2	AB	2537	U	C5'-C4'-C3'	-5.10	107.83	116.00
2	AB	2825	G	N3-C4-C5	-5.10	126.05	128.60
34	BA	1047	G	N3-C4-C5	-5.10	126.05	128.60
1	AA	34	A	C8-N9-C4	-5.10	103.76	105.80
2	AB	532	A	O4'-C1'-C2'	-5.10	100.70	105.80
2	AB	1345	C	O4'-C1'-N1	5.10	112.28	108.20
34	BA	933	G	C8-N9-C4	-5.10	104.36	106.40
34	BA	194	C	N1-C2-O2	5.10	121.96	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1333	A	O4'-C1'-N9	5.10	112.28	108.20
2	AB	915	C	O4'-C1'-N1	5.10	112.28	108.20
2	AB	1446	C	C5'-C4'-C3'	-5.10	107.84	116.00
2	AB	2749	A	C3'-C2'-C1'	-5.10	97.42	101.50
34	BA	330	C	C5'-C4'-C3'	-5.10	107.84	116.00
34	BA	591	U	C5'-C4'-O4'	5.10	115.22	109.10
34	BA	936	C	C5'-C4'-C3'	-5.10	107.84	116.00
34	BA	874	G	C8-N9-C4	-5.10	104.36	106.40
2	AB	1785	A	C4'-C3'-C2'	-5.09	97.50	102.60
2	AB	1826	G	N3-C4-C5	-5.09	126.05	128.60
2	AB	111	A	O4'-C1'-N9	5.09	112.27	108.20
2	AB	388	G	P-O3'-C3'	5.09	125.81	119.70
2	AB	1586	A	C4'-C3'-C2'	-5.09	97.51	102.60
2	AB	1892	C	O4'-C1'-N1	5.09	112.28	108.20
34	BA	217	C	C5'-C4'-O4'	5.09	115.21	109.10
2	AB	141	G	C1'-O4'-C4'	-5.09	105.83	109.90
2	AB	739	A	O4'-C1'-N9	-5.09	104.13	108.20
2	AB	1854	A	C5'-C4'-C3'	-5.09	107.85	116.00
2	AB	2211	A	O4'-C1'-N9	5.09	112.27	108.20
2	AB	2782	G	C5'-C4'-O4'	5.09	115.21	109.10
2	AB	1848	A	C8-N9-C4	-5.09	103.77	105.80
2	AB	2464	G	N9-C4-C5	5.09	107.44	105.40
34	BA	335	C	O4'-C1'-N1	5.09	112.27	108.20
34	BA	596	A	C5'-C4'-C3'	-5.09	107.86	116.00
2	AB	1559	U	N1-C1'-C2'	5.09	120.61	114.00
2	AB	2490	G	C8-N9-C4	-5.09	104.36	106.40
35	BB	48	C	C5'-C4'-O4'	5.09	115.21	109.10
2	AB	255	A	C5'-C4'-C3'	-5.09	107.86	116.00
2	AB	710	U	O3'-P-O5'	-5.09	94.33	104.00
2	AB	1800	C	C3'-C2'-C1'	5.09	105.57	101.50
4	AD	132	ARG	NE-CZ-NH1	5.09	122.84	120.30
34	BA	318	G	C5'-C4'-O4'	5.09	115.20	109.10
35	BE	23	A	O4'-C1'-N9	5.09	112.27	108.20
1	AA	37	C	C6-N1-C2	-5.08	118.27	120.30
34	BA	1143	G	N3-C4-C5	-5.08	126.06	128.60
2	AB	570	G	C5'-C4'-O4'	5.08	115.20	109.10
2	AB	1234	U	O4'-C1'-N1	5.08	112.27	108.20
2	AB	1313	U	C5'-C4'-C3'	-5.08	107.86	116.00
2	AB	1500	G	C5'-C4'-O4'	5.08	115.20	109.10
34	BA	120	A	C5'-C4'-C3'	-5.08	107.87	116.00
34	BA	929	G	N9-C1'-C2'	-5.08	106.41	112.00
2	AB	425	G	N9-C1'-C2'	-5.08	106.41	112.00

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2081	U	O4'-C1'-N1	5.08	112.27	108.20
34	BA	111	G	N3-C4-C5	-5.08	126.06	128.60
34	BA	440	C	O4'-C1'-N1	5.08	112.27	108.20
2	AB	624	C	O4'-C1'-N1	5.08	112.26	108.20
2	AB	1489	C	O4'-C1'-N1	5.08	112.26	108.20
34	BA	760	G	N9-C1'-C2'	-5.08	106.41	112.00
1	AA	20	G	N3-C4-C5	-5.08	126.06	128.60
2	AB	315	G	N9-C4-C5	5.08	107.43	105.40
2	AB	516	C	O4'-C1'-N1	5.08	112.26	108.20
2	AB	530	G	C5'-C4'-C3'	-5.08	107.87	116.00
7	AG	132	ARG	CD-NE-CZ	5.08	130.71	123.60
34	BA	167	A	O4'-C1'-N9	5.08	112.26	108.20
34	BA	340	U	O4'-C1'-N1	5.08	112.26	108.20
34	BA	1270	G	N9-C4-C5	5.08	107.43	105.40
34	BA	1378	C	C4'-C3'-C2'	-5.08	97.52	102.60
2	AB	914	G	C2-N3-C4	5.08	114.44	111.90
2	AB	949	G	N3-C4-C5	-5.08	126.06	128.60
2	AB	1151	A	O4'-C1'-N9	5.08	112.26	108.20
2	AB	619	G	C8-N9-C4	-5.08	104.37	106.40
2	AB	1162	G	N9-C1'-C2'	-5.08	106.42	112.00
2	AB	1345	C	C5'-C4'-O4'	5.08	115.19	109.10
34	BA	42	G	O4'-C1'-N9	5.08	112.26	108.20
34	BA	481	G	C2'-C3'-O3'	5.08	121.82	113.70
34	BA	1001	C	O4'-C1'-N1	5.08	112.26	108.20
34	BA	1164	G	O4'-C1'-N9	5.08	112.26	108.20
34	BA	1359	C	O4'-C4'-C3'	5.08	110.16	106.10
41	BI	145	ASN	C-N-CA	5.08	134.39	121.70
2	AB	21	A	N9-C1'-C2'	-5.07	106.42	112.00
2	AB	407	G	C3'-C2'-C1'	-5.07	97.44	101.50
2	AB	1761	C	C2'-C3'-O3'	5.07	121.82	113.70
2	AB	1882	U	C5'-C4'-C3'	-5.07	107.88	116.00
2	AB	2811	G	N9-C1'-C2'	-5.07	106.42	112.00
34	BA	543	U	C5'-C4'-O4'	5.07	115.19	109.10
2	AB	514	A	O4'-C1'-N9	5.07	112.26	108.20
2	AB	2823	A	C3'-C2'-C1'	5.07	105.56	101.50
14	AN	38	ARG	NE-CZ-NH1	5.07	122.84	120.30
34	BA	599	C	O4'-C1'-N1	5.07	112.26	108.20
34	BA	648	A	C5'-C4'-C3'	-5.07	107.89	116.00
2	AB	1509	A	P-O3'-C3'	5.07	125.78	119.70
34	BA	292	G	C8-N9-C4	-5.07	104.37	106.40
2	AB	2565	A	C8-N9-C4	-5.07	103.77	105.80
2	AB	2692	G	C5'-C4'-C3'	-5.07	107.89	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	454	G	C8-N9-C4	-5.07	104.37	106.40
34	BA	1047	G	C1'-O4'-C4'	-5.07	105.84	109.90
34	BA	1078	U	N3-C2-O2	-5.07	118.65	122.20
34	BA	1228	C	C5'-C4'-O4'	5.07	115.18	109.10
1	AA	54	G	N9-C4-C5	5.07	107.43	105.40
2	AB	1193	G	C5'-C4'-C3'	-5.07	107.89	116.00
2	AB	2093	G	O5'-C5'-C4'	-5.07	102.07	111.70
2	AB	2664	G	N3-C4-C5	-5.07	126.07	128.60
34	BA	441	A	C8-N9-C4	-5.07	103.77	105.80
34	BA	682	G	N9-C1'-C2'	-5.07	106.42	112.00
34	BA	1381	U	O4'-C1'-N1	5.07	112.25	108.20
2	AB	1340	U	O4'-C1'-N1	5.07	112.25	108.20
2	AB	2332	C	O4'-C1'-N1	5.06	112.25	108.20
34	BA	163	C	C4'-C3'-C2'	-5.06	97.54	102.60
34	BA	727	G	C5'-C4'-O4'	5.06	115.18	109.10
2	AB	529	A	C1'-O4'-C4'	-5.06	105.85	109.90
34	BA	1022	A	C8-N9-C4	-5.06	103.78	105.80
34	BA	1056	U	C5'-C4'-O4'	5.06	115.17	109.10
34	BA	1450	U	C3'-C2'-C1'	5.06	105.55	101.50
50	BR	58	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	AA	77	U	O4'-C1'-N1	5.06	112.25	108.20
2	AB	7	G	C5'-C4'-C3'	-5.06	107.90	116.00
2	AB	380	G	N9-C1'-C2'	-5.06	106.43	112.00
34	BA	887	G	N9-C1'-C2'	-5.06	106.43	112.00
55	BW	1	PRO	CA-N-CD	-5.06	104.42	111.50
2	AB	1694	C	O4'-C1'-N1	5.06	112.25	108.20
2	AB	2584	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	17	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	30	U	O4'-C4'-C3'	5.06	110.15	106.10
34	BA	620	C	C1'-O4'-C4'	-5.06	105.85	109.90
34	BA	1000	A	C5'-C4'-O4'	5.06	115.17	109.10
2	AB	1189	A	C5'-C4'-O4'	5.06	115.17	109.10
2	AB	2195	U	C5'-C4'-C3'	-5.06	107.91	116.00
2	AB	2423	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	1436	U	C4'-C3'-C2'	-5.06	97.54	102.60
2	AB	1206	G	C5'-C4'-C3'	-5.06	107.91	116.00
2	AB	1619	G	C8-N9-C4	-5.06	104.38	106.40
2	AB	1971	U	O4'-C1'-N1	5.06	112.25	108.20
34	BA	503	C	N1-C2-O2	5.06	121.93	118.90
1	AA	55	U	O4'-C1'-N1	5.05	112.24	108.20
2	AB	62	U	O4'-C1'-N1	5.05	112.24	108.20
2	AB	69	C	O4'-C1'-N1	5.05	112.24	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	481	G	C2-N3-C4	5.05	114.43	111.90
2	AB	520	G	C5'-C4'-C3'	-5.05	107.91	116.00
2	AB	533	G	C8-N9-C4	-5.05	104.38	106.40
2	AB	877	A	O3'-P-O5'	-5.05	94.40	104.00
2	AB	2478	A	C3'-C2'-C1'	-5.05	97.46	101.50
2	AB	1778	U	P-O3'-C3'	5.05	125.76	119.70
34	BA	893	C	C5'-C4'-O4'	5.05	115.16	109.10
35	BE	74	C	O4'-C1'-N1	5.05	112.24	108.20
2	AB	1938	A	C5'-C4'-C3'	-5.05	107.92	116.00
2	AB	2035	G	O4'-C1'-N9	5.05	112.24	108.20
2	AB	2617	U	O4'-C1'-N1	5.05	112.24	108.20
34	BA	663	A	C8-N9-C4	-5.05	103.78	105.80
34	BA	846	G	C8-N9-C4	-5.05	104.38	106.40
2	AB	1064	C	O3'-P-O5'	-5.05	94.41	104.00
2	AB	1390	U	C5'-C4'-C3'	-5.05	107.92	116.00
2	AB	1980	G	P-O3'-C3'	5.05	125.76	119.70
2	AB	2516	A	O4'-C1'-N9	5.05	112.24	108.20
34	BA	164	G	N3-C4-C5	-5.05	126.08	128.60
2	AB	103	A	C8-N9-C4	-5.05	103.78	105.80
2	AB	468	G	N3-C4-C5	-5.05	126.08	128.60
2	AB	1099	G	C4'-C3'-C2'	-5.05	97.55	102.60
2	AB	1416	G	C4-C5-N7	-5.05	108.78	110.80
2	AB	1418	G	C5'-C4'-O4'	5.05	115.16	109.10
2	AB	1888	G	N3-C4-C5	-5.05	126.08	128.60
34	BA	907	A	C5'-C4'-O4'	5.05	115.16	109.10
35	BB	73	A	O4'-C1'-N9	5.05	112.24	108.20
2	AB	1187	G	C8-N9-C4	-5.04	104.38	106.40
2	AB	2854	G	C5'-C4'-C3'	-5.04	107.93	116.00
7	AG	19	PHE	CB-CG-CD1	-5.04	117.27	120.80
34	BA	1231	G	C3'-C2'-C1'	-5.04	97.46	101.50
34	BA	1266	G	C3'-C2'-C1'	-5.04	97.46	101.50
2	AB	900	A	O4'-C1'-N9	5.04	112.23	108.20
2	AB	1603	A	C3'-C2'-C1'	-5.04	97.47	101.50
2	AB	1649	G	C1'-O4'-C4'	-5.04	105.86	109.90
2	AB	2186	G	N9-C1'-C2'	-5.04	106.45	112.00
2	AB	2347	C	P-O3'-C3'	5.04	125.75	119.70
34	BA	1527	U	O4'-C1'-N1	5.04	112.23	108.20
35	BE	10	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	1046	A	C4'-C3'-C2'	-5.04	97.56	102.60
2	AB	1289	C	C5'-C4'-O4'	5.04	115.15	109.10
34	BA	445	G	O4'-C1'-N9	5.04	112.23	108.20
34	BA	521	G	C5'-C4'-O4'	5.04	115.15	109.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1517	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	219	A	O4'-C1'-N9	5.04	112.23	108.20
2	AB	1191	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	1711	A	O4'-C1'-N9	5.04	112.23	108.20
2	AB	776	G	C8-N9-C4	-5.04	104.38	106.40
2	AB	1587	G	C4'-C3'-C2'	-5.04	97.56	102.60
34	BA	481	G	C8-N9-C4	-5.04	104.38	106.40
34	BA	1041	G	O4'-C1'-N9	5.04	112.23	108.20
34	BA	1353	G	C5'-C4'-C3'	-5.04	107.94	116.00
34	BA	95	C	O4'-C1'-N1	5.04	112.23	108.20
2	AB	133	U	C5'-C4'-O4'	5.04	115.14	109.10
2	AB	1731	G	N3-C4-C5	-5.04	126.08	128.60
2	AB	2280	G	O4'-C1'-N9	5.04	112.23	108.20
2	AB	2699	C	C5'-C4'-C3'	-5.04	107.94	116.00
34	BA	171	A	C5'-C4'-O4'	5.04	115.14	109.10
34	BA	1002	G	C5'-C4'-O4'	5.04	115.14	109.10
34	BA	1021	A	C5'-C4'-C3'	-5.04	107.94	116.00
34	BA	1200	C	P-O3'-C3'	5.04	125.74	119.70
2	AB	1619	G	N3-C4-C5	-5.03	126.08	128.60
2	AB	2145	C	N1-C2-O2	5.03	121.92	118.90
2	AB	416	U	C5'-C4'-C3'	-5.03	107.95	116.00
34	BA	407	U	C4'-C3'-C2'	-5.03	97.57	102.60
2	AB	1606	C	N3-C2-O2	-5.03	118.38	121.90
2	AB	2051	A	O4'-C4'-C3'	5.03	110.12	106.10
2	AB	2194	U	C5'-C4'-C3'	-5.03	107.95	116.00
2	AB	2367	G	C3'-C2'-C1'	-5.03	97.48	101.50
37	BD	25	U	O4'-C1'-N1	5.03	112.22	108.20
2	AB	1504	A	C5'-C4'-C3'	-5.03	107.95	116.00
34	BA	1329	A	C4'-C3'-C2'	-5.03	97.57	102.60
2	AB	301	G	P-O3'-C3'	5.03	125.73	119.70
2	AB	390	U	C5'-C4'-O4'	5.03	115.13	109.10
2	AB	1736	U	N1-C2-N3	5.03	117.92	114.90
34	BA	1528	U	C4'-C3'-C2'	-5.03	97.57	102.60
1	AA	32	U	C2-N3-C4	-5.02	123.98	127.00
2	AB	1480	C	O4'-C1'-N1	5.02	112.22	108.20
2	AB	1583	A	P-O3'-C3'	5.02	125.73	119.70
34	BA	214	C	C3'-C2'-C1'	-5.02	97.48	101.50
2	AB	214	G	N3-C4-C5	-5.02	126.09	128.60
2	AB	301	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	1333	G	C5'-C4'-O4'	5.02	115.13	109.10
2	AB	1348	C	C5'-C4'-O4'	5.02	115.13	109.10
34	BA	1511	G	C5'-C4'-C3'	-5.02	107.96	116.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BB	69	G	C5'-C4'-C3'	-5.02	107.96	116.00
2	AB	23	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	35	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	1066	U	C5'-C4'-C3'	-5.02	107.97	116.00
2	AB	2000	C	O4'-C1'-N1	5.02	112.22	108.20
2	AB	938	G	O4'-C1'-N9	5.02	112.22	108.20
2	AB	942	G	N3-C4-C5	-5.02	126.09	128.60
2	AB	1191	G	C4'-C3'-C2'	-5.02	97.58	102.60
2	AB	2378	A	C5'-C4'-C3'	-5.02	107.97	116.00
34	BA	1026	G	C8-N9-C4	-5.02	104.39	106.40
2	AB	2117	A	P-O3'-C3'	5.02	125.72	119.70
2	AB	1171	G	C4'-C3'-C2'	-5.02	97.58	102.60
2	AB	1954	G	C3'-C2'-C1'	-5.02	97.49	101.50
34	BA	847	G	C2-N3-C4	5.02	114.41	111.90
34	BA	1403	C	C5'-C4'-C3'	-5.02	107.97	116.00
1	AA	79	G	N3-C4-C5	-5.01	126.09	128.60
2	AB	1734	G	N3-C4-C5	-5.01	126.09	128.60
34	BA	911	U	C1'-O4'-C4'	-5.01	105.89	109.90
34	BA	1219	A	O4'-C1'-N9	5.01	112.21	108.20
35	BE	10	G	C5'-C4'-O4'	5.01	115.12	109.10
2	AB	1799	G	N9-C4-C5	5.01	107.41	105.40
2	AB	2010	G	C5'-C4'-O4'	5.01	115.12	109.10
2	AB	2288	A	O4'-C1'-N9	5.01	112.21	108.20
34	BA	989	U	C5'-C4'-O4'	5.01	115.12	109.10
34	BA	1532	U	O4'-C1'-N1	5.01	112.21	108.20
35	BE	49	C	C5'-C4'-O4'	5.01	115.11	109.10
2	AB	323	C	N1-C2-O2	5.01	121.91	118.90
2	AB	2741	A	C5'-C4'-C3'	-5.01	107.98	116.00
2	AB	860	U	O4'-C1'-N1	5.01	112.21	108.20
2	AB	912	C	O4'-C1'-N1	5.01	112.21	108.20
2	AB	948	C	N1-C2-O2	5.01	121.91	118.90
2	AB	1245	G	C4'-C3'-C2'	-5.01	97.59	102.60
2	AB	1533	C	N1-C2-O2	5.01	121.91	118.90
2	AB	1763	G	O3'-P-O5'	-5.01	94.48	104.00
2	AB	1937	A	O4'-C1'-N9	5.01	112.21	108.20
2	AB	2722	G	C8-N9-C4	-5.01	104.40	106.40
2	AB	1171	G	C8-N9-C4	-5.01	104.40	106.40
2	AB	2297	A	C5'-C4'-O4'	5.01	115.11	109.10
2	AB	420	C	N3-C2-O2	-5.01	118.40	121.90
2	AB	1228	G	O4'-C1'-N9	5.01	112.20	108.20
2	AB	1359	A	N9-C1'-C2'	-5.01	106.49	112.00
2	AB	1501	G	C2-N3-C4	5.01	114.40	111.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2278	A	C4'-C3'-C2'	-5.01	97.59	102.60
2	AB	2395	C	C5'-C4'-C3'	-5.01	107.99	116.00
2	AB	2770	G	O4'-C1'-N9	5.01	112.20	108.20
34	BA	590	U	C5'-C4'-C3'	-5.01	107.99	116.00
34	BA	1153	G	N9-C1'-C2'	-5.01	106.49	112.00
34	BA	1259	C	C5'-C4'-O4'	5.01	115.11	109.10
2	AB	720	U	C5'-C4'-C3'	-5.00	107.99	116.00
2	AB	1054	A	P-O3'-C3'	5.00	125.71	119.70
2	AB	1266	G	N9-C4-C5	5.00	107.40	105.40
34	BA	350	G	P-O3'-C3'	5.00	125.71	119.70
1	AA	43	C	N1-C2-O2	5.00	121.90	118.90
2	AB	840	C	O4'-C1'-N1	5.00	112.20	108.20
2	AB	2870	C	O4'-C1'-N1	5.00	112.20	108.20
34	BA	761	G	O4'-C1'-N9	5.00	112.20	108.20
34	BA	1475	G	C8-N9-C4	-5.00	104.40	106.40
2	AB	8	C	O4'-C1'-N1	5.00	112.20	108.20
35	BE	2	C	O4'-C1'-N1	5.00	112.20	108.20

There are no chirality outliers.

All (1392) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	103	U	Sidechain
1	AA	107	G	Sidechain
1	AA	108	A	Sidechain
1	AA	109	A	Sidechain
1	AA	13	G	Sidechain
1	AA	14	U	Sidechain
1	AA	15	A	Sidechain
1	AA	19	C	Sidechain
1	AA	2	G	Sidechain
1	AA	26	C	Sidechain
1	AA	36	C	Sidechain
1	AA	37	C	Sidechain
1	AA	40	U	Sidechain
1	AA	41	G	Sidechain
1	AA	48	U	Sidechain
1	AA	52	A	Sidechain
1	AA	62	C	Sidechain
1	AA	64	G	Sidechain
1	AA	65	U	Sidechain
1	AA	66	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	AA	67	G	Sidechain
1	AA	7	G	Sidechain
1	AA	72	G	Sidechain
1	AA	87	U	Sidechain
1	AA	88	C	Sidechain
1	AA	95	U	Sidechain
1	AA	99	A	Sidechain
2	AB	1000	A	Sidechain
2	AB	1003	G	Sidechain
2	AB	1004	U	Sidechain
2	AB	1005	C	Sidechain
2	AB	1006	C	Sidechain
2	AB	1010	A	Sidechain
2	AB	1011	G	Sidechain
2	AB	1012	U	Sidechain
2	AB	1014	A	Sidechain
2	AB	1017	G	Sidechain
2	AB	1022	G	Sidechain
2	AB	1025	G	Sidechain
2	AB	1026	G	Sidechain
2	AB	1027	A	Sidechain
2	AB	1028	A	Sidechain
2	AB	1029	A	Sidechain
2	AB	103	A	Sidechain
2	AB	104	A	Sidechain
2	AB	1042	G	Sidechain
2	AB	1048	A	Sidechain
2	AB	105	C	Sidechain
2	AB	1052	C	Sidechain
2	AB	1053	C	Sidechain
2	AB	1054	A	Sidechain
2	AB	1057	A	Sidechain
2	AB	1059	G	Sidechain
2	AB	1061	U	Sidechain
2	AB	1063	G	Sidechain
2	AB	1064	C	Sidechain
2	AB	1067	A	Sidechain
2	AB	1069	A	Sidechain
2	AB	1073	A	Sidechain
2	AB	1074	G	Sidechain
2	AB	1075	C	Sidechain
2	AB	1076	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	1084	A	Sidechain
2	AB	1087	G	Sidechain
2	AB	1094	U	Sidechain
2	AB	1096	A	Sidechain
2	AB	1097	U	Sidechain
2	AB	1098	A	Sidechain
2	AB	1099	G	Sidechain
2	AB	1111	A	Sidechain
2	AB	1116	G	Sidechain
2	AB	1117	C	Sidechain
2	AB	1118	C	Sidechain
2	AB	112	U	Sidechain
2	AB	1120	G	Sidechain
2	AB	1121	C	Sidechain
2	AB	1123	C	Sidechain
2	AB	1124	G	Sidechain
2	AB	1130	U	Sidechain
2	AB	1131	G	Sidechain
2	AB	1132	U	Sidechain
2	AB	1133	A	Sidechain
2	AB	1135	C	Sidechain
2	AB	1138	G	Sidechain
2	AB	1141	U	Sidechain
2	AB	1143	A	Sidechain
2	AB	1144	A	Sidechain
2	AB	1145	C	Sidechain
2	AB	115	C	Sidechain
2	AB	1153	C	Sidechain
2	AB	1154	G	Sidechain
2	AB	116	C	Sidechain
2	AB	1161	C	Sidechain
2	AB	1174	U	Sidechain
2	AB	1179	G	Sidechain
2	AB	118	A	Sidechain
2	AB	1182	G	Sidechain
2	AB	119	A	Sidechain
2	AB	1198	U	Sidechain
2	AB	1199	U	Sidechain
2	AB	1203	U	Sidechain
2	AB	1204	A	Sidechain
2	AB	1212	G	Sidechain
2	AB	1224	U	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	1226	A	Sidechain
2	AB	1227	G	Sidechain
2	AB	1230	A	Sidechain
2	AB	1234	U	Sidechain
2	AB	1236	G	Sidechain
2	AB	1242	U	Sidechain
2	AB	1246	A	Sidechain
2	AB	1256	G	Sidechain
2	AB	1262	A	Sidechain
2	AB	1263	U	Sidechain
2	AB	1266	G	Sidechain
2	AB	1268	A	Sidechain
2	AB	127	A	Sidechain
2	AB	1271	G	Sidechain
2	AB	1276	A	Sidechain
2	AB	1281	G	Sidechain
2	AB	1282	U	Sidechain
2	AB	1283	G	Sidechain
2	AB	1284	A	Sidechain
2	AB	1287	A	Sidechain
2	AB	1288	G	Sidechain
2	AB	1289	C	Sidechain
2	AB	129	C	Sidechain
2	AB	1293	C	Sidechain
2	AB	1295	C	Sidechain
2	AB	1296	G	Sidechain
2	AB	1299	G	Sidechain
2	AB	1309	G	Sidechain
2	AB	1317	G	Sidechain
2	AB	132	G	Sidechain
2	AB	1321	A	Sidechain
2	AB	1324	G	Sidechain
2	AB	1327	A	Sidechain
2	AB	133	U	Sidechain
2	AB	1330	C	Sidechain
2	AB	1334	G	Sidechain
2	AB	1335	C	Sidechain
2	AB	1345	C	Sidechain
2	AB	1353	A	Sidechain
2	AB	1356	G	Sidechain
2	AB	1359	A	Sidechain
2	AB	1368	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	137	U	Sidechain
2	AB	1371	G	Sidechain
2	AB	1376	C	Sidechain
2	AB	1377	G	Sidechain
2	AB	1379	U	Sidechain
2	AB	138	U	Sidechain
2	AB	1381	G	Sidechain
2	AB	1389	G	Sidechain
2	AB	1390	U	Sidechain
2	AB	1392	A	Sidechain
2	AB	1393	A	Sidechain
2	AB	1394	U	Sidechain
2	AB	1396	U	Sidechain
2	AB	1398	C	Sidechain
2	AB	1399	C	Sidechain
2	AB	140	C	Sidechain
2	AB	1400	U	Sidechain
2	AB	141	G	Sidechain
2	AB	1410	G	Sidechain
2	AB	1416	G	Sidechain
2	AB	1417	C	Sidechain
2	AB	1418	G	Sidechain
2	AB	1419	A	Sidechain
2	AB	1424	G	Sidechain
2	AB	1426	G	Sidechain
2	AB	1427	A	Sidechain
2	AB	143	C	Sidechain
2	AB	1436	G	Sidechain
2	AB	1440	U	Sidechain
2	AB	1442	U	Sidechain
2	AB	145	C	Sidechain
2	AB	1453	A	Sidechain
2	AB	1454	C	Sidechain
2	AB	1456	G	Sidechain
2	AB	1458	U	Sidechain
2	AB	1459	G	Sidechain
2	AB	146	A	Sidechain
2	AB	1471	G	Sidechain
2	AB	1473	G	Sidechain
2	AB	1481	U	Sidechain
2	AB	149	A	Sidechain
2	AB	1495	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	1501	G	Sidechain
2	AB	1514	G	Sidechain
2	AB	1521	G	Sidechain
2	AB	1527	G	Sidechain
2	AB	1532	A	Sidechain
2	AB	1535	A	Sidechain
2	AB	1537	G	Sidechain
2	AB	1544	A	Sidechain
2	AB	1546	G	Sidechain
2	AB	1548	A	Sidechain
2	AB	1549	A	Sidechain
2	AB	1552	A	Sidechain
2	AB	1553	A	Sidechain
2	AB	1554	U	Sidechain
2	AB	1555	G	Sidechain
2	AB	1564	C	Sidechain
2	AB	1566	A	Sidechain
2	AB	1568	G	Sidechain
2	AB	1577	C	Sidechain
2	AB	1578	U	Sidechain
2	AB	1581	G	Sidechain
2	AB	1588	G	Sidechain
2	AB	1592	C	Sidechain
2	AB	1596	A	Sidechain
2	AB	1603	A	Sidechain
2	AB	1605	C	Sidechain
2	AB	1606	C	Sidechain
2	AB	1607	C	Sidechain
2	AB	1608	A	Sidechain
2	AB	1609	A	Sidechain
2	AB	161	A	Sidechain
2	AB	1620	G	Sidechain
2	AB	1622	G	Sidechain
2	AB	163	C	Sidechain
2	AB	1631	G	Sidechain
2	AB	1632	A	Sidechain
2	AB	164	C	Sidechain
2	AB	1641	A	Sidechain
2	AB	1644	C	Sidechain
2	AB	1646	C	Sidechain
2	AB	1652	A	Sidechain
2	AB	1656	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	166	U	Sidechain
2	AB	1664	A	Sidechain
2	AB	1671	U	Sidechain
2	AB	1672	A	Sidechain
2	AB	1675	C	Sidechain
2	AB	1680	U	Sidechain
2	AB	1687	G	Sidechain
2	AB	1689	A	Sidechain
2	AB	169	G	Sidechain
2	AB	1690	A	Sidechain
2	AB	1693	U	Sidechain
2	AB	1695	G	Sidechain
2	AB	17	G	Sidechain
2	AB	1701	A	Sidechain
2	AB	1706	C	Sidechain
2	AB	1710	G	Sidechain
2	AB	1711	A	Sidechain
2	AB	1721	G	Sidechain
2	AB	1722	A	Sidechain
2	AB	1723	G	Sidechain
2	AB	1726	C	Sidechain
2	AB	1733	G	Sidechain
2	AB	1734	G	Sidechain
2	AB	1736	U	Sidechain
2	AB	1738	G	Sidechain
2	AB	1739	A	Sidechain
2	AB	174	U	Sidechain
2	AB	1740	G	Sidechain
2	AB	1742	U	Sidechain
2	AB	1750	G	Sidechain
2	AB	1752	C	Sidechain
2	AB	1755	A	Sidechain
2	AB	1757	A	Sidechain
2	AB	177	G	Sidechain
2	AB	1777	U	Sidechain
2	AB	1780	A	Sidechain
2	AB	1788	C	Sidechain
2	AB	1791	A	Sidechain
2	AB	1797	G	Sidechain
2	AB	1799	G	Sidechain
2	AB	180	G	Sidechain
2	AB	1800	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	1801	A	Sidechain
2	AB	1802	A	Sidechain
2	AB	1805	A	Sidechain
2	AB	1806	C	Sidechain
2	AB	1809	A	Sidechain
2	AB	1810	A	Sidechain
2	AB	1818	U	Sidechain
2	AB	1819	A	Sidechain
2	AB	1820	U	Sidechain
2	AB	1822	C	Sidechain
2	AB	1825	U	Sidechain
2	AB	1828	G	Sidechain
2	AB	1831	G	Sidechain
2	AB	1834	U	Sidechain
2	AB	1836	C	Sidechain
2	AB	1837	C	Sidechain
2	AB	1839	G	Sidechain
2	AB	1841	U	Sidechain
2	AB	1846	G	Sidechain
2	AB	1847	A	Sidechain
2	AB	1848	A	Sidechain
2	AB	1850	G	Sidechain
2	AB	1852	U	Sidechain
2	AB	1854	A	Sidechain
2	AB	1857	G	Sidechain
2	AB	1865	U	Sidechain
2	AB	1869	G	Sidechain
2	AB	1870	C	Sidechain
2	AB	1871	A	Sidechain
2	AB	1872	A	Sidechain
2	AB	1878	G	Sidechain
2	AB	188	G	Sidechain
2	AB	1886	U	Sidechain
2	AB	1887	C	Sidechain
2	AB	1888	G	Sidechain
2	AB	189	G	Sidechain
2	AB	1898	U	Sidechain
2	AB	190	A	Sidechain
2	AB	1903	G	Sidechain
2	AB	1906	G	Sidechain
2	AB	1909	C	Sidechain
2	AB	1912	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	1918	A	Sidechain
2	AB	192	C	Sidechain
2	AB	1920	C	Sidechain
2	AB	1924	C	Sidechain
2	AB	1925	C	Sidechain
2	AB	1926	U	Sidechain
2	AB	1927	A	Sidechain
2	AB	1928	A	Sidechain
2	AB	1929	G	Sidechain
2	AB	1932	A	Sidechain
2	AB	1938	A	Sidechain
2	AB	194	G	Sidechain
2	AB	1942	C	Sidechain
2	AB	195	A	Sidechain
2	AB	1959	G	Sidechain
2	AB	1961	C	Sidechain
2	AB	1968	G	Sidechain
2	AB	1969	A	Sidechain
2	AB	1970	A	Sidechain
2	AB	1973	G	Sidechain
2	AB	1975	G	Sidechain
2	AB	1976	U	Sidechain
2	AB	1995	U	Sidechain
2	AB	1996	C	Sidechain
2	AB	1997	C	Sidechain
2	AB	20	C	Sidechain
2	AB	2002	G	Sidechain
2	AB	2005	A	Sidechain
2	AB	2017	U	Sidechain
2	AB	2020	A	Sidechain
2	AB	2021	C	Sidechain
2	AB	2025	C	Sidechain
2	AB	2029	G	Sidechain
2	AB	2031	A	Sidechain
2	AB	2032	G	Sidechain
2	AB	2033	A	Sidechain
2	AB	2034	U	Sidechain
2	AB	204	A	Sidechain
2	AB	2040	G	Sidechain
2	AB	2042	A	Sidechain
2	AB	2046	G	Sidechain
2	AB	2048	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	2051	A	Sidechain
2	AB	2053	G	Sidechain
2	AB	2055	C	Sidechain
2	AB	2058	A	Sidechain
2	AB	2059	A	Sidechain
2	AB	206	U	Sidechain
2	AB	2064	C	Sidechain
2	AB	2068	U	Sidechain
2	AB	2071	A	Sidechain
2	AB	2072	C	Sidechain
2	AB	2073	C	Sidechain
2	AB	2074	U	Sidechain
2	AB	2075	U	Sidechain
2	AB	2077	A	Sidechain
2	AB	2079	U	Sidechain
2	AB	2092	U	Sidechain
2	AB	2094	A	Sidechain
2	AB	2097	A	Sidechain
2	AB	2107	G	Sidechain
2	AB	2112	G	Sidechain
2	AB	2113	U	Sidechain
2	AB	2115	G	Sidechain
2	AB	2117	A	Sidechain
2	AB	2126	A	Sidechain
2	AB	2127	G	Sidechain
2	AB	2128	G	Sidechain
2	AB	213	A	Sidechain
2	AB	2133	G	Sidechain
2	AB	2134	A	Sidechain
2	AB	215	G	Sidechain
2	AB	2159	G	Sidechain
2	AB	2160	C	Sidechain
2	AB	2168	G	Sidechain
2	AB	2179	C	Sidechain
2	AB	2183	A	Sidechain
2	AB	2185	U	Sidechain
2	AB	2188	U	Sidechain
2	AB	2190	G	Sidechain
2	AB	2193	G	Sidechain
2	AB	2198	A	Sidechain
2	AB	22	C	Sidechain
2	AB	2202	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	2204	G	Sidechain
2	AB	2218	G	Sidechain
2	AB	2223	G	Sidechain
2	AB	2226	C	Sidechain
2	AB	2233	U	Sidechain
2	AB	2234	G	Sidechain
2	AB	2238	G	Sidechain
2	AB	2250	G	Sidechain
2	AB	2259	U	Sidechain
2	AB	226	A	Sidechain
2	AB	2261	C	Sidechain
2	AB	2262	U	Sidechain
2	AB	2263	C	Sidechain
2	AB	2268	A	Sidechain
2	AB	2269	G	Sidechain
2	AB	227	A	Sidechain
2	AB	2271	G	Sidechain
2	AB	2273	A	Sidechain
2	AB	2274	A	Sidechain
2	AB	2275	C	Sidechain
2	AB	2277	G	Sidechain
2	AB	2282	G	Sidechain
2	AB	2285	C	Sidechain
2	AB	2287	A	Sidechain
2	AB	2289	G	Sidechain
2	AB	2299	U	Sidechain
2	AB	23	G	Sidechain
2	AB	2301	C	Sidechain
2	AB	2304	G	Sidechain
2	AB	2306	C	Sidechain
2	AB	2307	G	Sidechain
2	AB	2308	G	Sidechain
2	AB	231	A	Sidechain
2	AB	2310	C	Sidechain
2	AB	2317	A	Sidechain
2	AB	2318	G	Sidechain
2	AB	2321	U	Sidechain
2	AB	2323	G	Sidechain
2	AB	2324	U	Sidechain
2	AB	2325	G	Sidechain
2	AB	2328	A	Sidechain
2	AB	2330	G	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	2331	G	Sidechain
2	AB	2333	A	Sidechain
2	AB	2335	A	Sidechain
2	AB	2338	C	Sidechain
2	AB	2342	C	Sidechain
2	AB	2344	U	Sidechain
2	AB	2348	U	Sidechain
2	AB	2357	G	Sidechain
2	AB	2359	C	Sidechain
2	AB	2362	C	Sidechain
2	AB	2365	G	Sidechain
2	AB	2375	G	Sidechain
2	AB	2376	A	Sidechain
2	AB	2380	C	Sidechain
2	AB	2383	G	Sidechain
2	AB	2387	U	Sidechain
2	AB	2389	G	Sidechain
2	AB	2391	G	Sidechain
2	AB	24	G	Sidechain
2	AB	2402	U	Sidechain
2	AB	2407	A	Sidechain
2	AB	241	A	Sidechain
2	AB	2411	A	Sidechain
2	AB	2414	G	Sidechain
2	AB	2416	C	Sidechain
2	AB	2419	U	Sidechain
2	AB	242	G	Sidechain
2	AB	2420	C	Sidechain
2	AB	2424	C	Sidechain
2	AB	2427	C	Sidechain
2	AB	2430	A	Sidechain
2	AB	2434	A	Sidechain
2	AB	2450	A	Sidechain
2	AB	2458	G	Sidechain
2	AB	2460	U	Sidechain
2	AB	2464	G	Sidechain
2	AB	2466	C	Sidechain
2	AB	2471	A	Sidechain
2	AB	2480	C	Sidechain
2	AB	2490	G	Sidechain
2	AB	2492	U	Sidechain
2	AB	2496	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	2497	A	Sidechain
2	AB	250	G	Sidechain
2	AB	2500	U	Sidechain
2	AB	2505	G	Sidechain
2	AB	2507	C	Sidechain
2	AB	2510	C	Sidechain
2	AB	2515	C	Sidechain
2	AB	2516	A	Sidechain
2	AB	2519	U	Sidechain
2	AB	252	G	Sidechain
2	AB	2521	C	Sidechain
2	AB	2526	G	Sidechain
2	AB	2529	G	Sidechain
2	AB	2531	A	Sidechain
2	AB	2533	U	Sidechain
2	AB	2536	G	Sidechain
2	AB	2538	C	Sidechain
2	AB	2539	C	Sidechain
2	AB	2547	A	Sidechain
2	AB	2550	G	Sidechain
2	AB	2554	U	Sidechain
2	AB	2563	U	Sidechain
2	AB	2565	A	Sidechain
2	AB	2569	G	Sidechain
2	AB	257	C	Sidechain
2	AB	2573	C	Sidechain
2	AB	2574	G	Sidechain
2	AB	2576	G	Sidechain
2	AB	2579	C	Sidechain
2	AB	2581	G	Sidechain
2	AB	2583	G	Sidechain
2	AB	2587	A	Sidechain
2	AB	2588	G	Sidechain
2	AB	2589	A	Sidechain
2	AB	259	G	Sidechain
2	AB	2592	G	Sidechain
2	AB	2595	G	Sidechain
2	AB	2599	G	Sidechain
2	AB	260	G	Sidechain
2	AB	261	G	Sidechain
2	AB	2611	C	Sidechain
2	AB	2612	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	2616	C	Sidechain
2	AB	262	A	Sidechain
2	AB	2621	G	Sidechain
2	AB	2625	G	Sidechain
2	AB	2627	G	Sidechain
2	AB	263	G	Sidechain
2	AB	2637	U	Sidechain
2	AB	2643	G	Sidechain
2	AB	2644	G	Sidechain
2	AB	2645	G	Sidechain
2	AB	265	A	Sidechain
2	AB	2658	C	Sidechain
2	AB	2659	G	Sidechain
2	AB	266	G	Sidechain
2	AB	2660	A	Sidechain
2	AB	2661	G	Sidechain
2	AB	2662	A	Sidechain
2	AB	2663	G	Sidechain
2	AB	2664	G	Sidechain
2	AB	2666	C	Sidechain
2	AB	2671	G	Sidechain
2	AB	2677	G	Sidechain
2	AB	268	C	Sidechain
2	AB	2680	U	Sidechain
2	AB	2683	C	Sidechain
2	AB	2684	U	Sidechain
2	AB	2688	G	Sidechain
2	AB	2693	G	Sidechain
2	AB	2696	U	Sidechain
2	AB	2701	U	Sidechain
2	AB	2706	A	Sidechain
2	AB	271	G	Sidechain
2	AB	2720	U	Sidechain
2	AB	2722	G	Sidechain
2	AB	2727	A	Sidechain
2	AB	2728	U	Sidechain
2	AB	2731	G	Sidechain
2	AB	2732	G	Sidechain
2	AB	2737	G	Sidechain
2	AB	2739	U	Sidechain
2	AB	2740	A	Sidechain
2	AB	275	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	2756	U	Sidechain
2	AB	276	U	Sidechain
2	AB	2763	G	Sidechain
2	AB	2764	A	Sidechain
2	AB	2765	A	Sidechain
2	AB	2770	G	Sidechain
2	AB	2783	U	Sidechain
2	AB	2785	C	Sidechain
2	AB	2787	C	Sidechain
2	AB	2791	G	Sidechain
2	AB	2792	A	Sidechain
2	AB	2797	U	Sidechain
2	AB	2799	A	Sidechain
2	AB	2801	G	Sidechain
2	AB	2805	C	Sidechain
2	AB	2807	U	Sidechain
2	AB	2808	G	Sidechain
2	AB	281	C	Sidechain
2	AB	2813	A	Sidechain
2	AB	2815	C	Sidechain
2	AB	2818	U	Sidechain
2	AB	2819	G	Sidechain
2	AB	2824	C	Sidechain
2	AB	283	G	Sidechain
2	AB	2832	U	Sidechain
2	AB	2843	G	Sidechain
2	AB	2849	U	Sidechain
2	AB	2854	G	Sidechain
2	AB	2857	G	Sidechain
2	AB	2859	G	Sidechain
2	AB	2861	U	Sidechain
2	AB	2862	G	Sidechain
2	AB	2864	G	Sidechain
2	AB	2872	A	Sidechain
2	AB	2873	A	Sidechain
2	AB	2881	U	Sidechain
2	AB	2882	A	Sidechain
2	AB	2884	U	Sidechain
2	AB	2890	G	Sidechain
2	AB	2892	G	Sidechain
2	AB	2894	G	Sidechain
2	AB	2895	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	29	U	Sidechain
2	AB	291	G	Sidechain
2	AB	293	U	Sidechain
2	AB	294	A	Sidechain
2	AB	299	A	Sidechain
2	AB	300	A	Sidechain
2	AB	303	G	Sidechain
2	AB	306	U	Sidechain
2	AB	307	G	Sidechain
2	AB	308	G	Sidechain
2	AB	310	A	Sidechain
2	AB	311	A	Sidechain
2	AB	313	G	Sidechain
2	AB	315	G	Sidechain
2	AB	319	G	Sidechain
2	AB	32	C	Sidechain
2	AB	321	U	Sidechain
2	AB	329	G	Sidechain
2	AB	33	C	Sidechain
2	AB	339	U	Sidechain
2	AB	34	U	Sidechain
2	AB	340	A	Sidechain
2	AB	341	C	Sidechain
2	AB	342	A	Sidechain
2	AB	345	A	Sidechain
2	AB	346	A	Sidechain
2	AB	347	A	Sidechain
2	AB	356	G	Sidechain
2	AB	360	U	Sidechain
2	AB	362	A	Sidechain
2	AB	363	G	Sidechain
2	AB	364	C	Sidechain
2	AB	365	U	Sidechain
2	AB	367	G	Sidechain
2	AB	368	A	Sidechain
2	AB	369	U	Sidechain
2	AB	378	C	Sidechain
2	AB	382	A	Sidechain
2	AB	391	A	Sidechain
2	AB	392	U	Sidechain
2	AB	394	C	Sidechain
2	AB	395	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	401	A	Sidechain
2	AB	405	U	Sidechain
2	AB	407	G	Sidechain
2	AB	411	G	Sidechain
2	AB	412	A	Sidechain
2	AB	421	C	Sidechain
2	AB	422	A	Sidechain
2	AB	424	G	Sidechain
2	AB	429	A	Sidechain
2	AB	430	A	Sidechain
2	AB	432	A	Sidechain
2	AB	442	G	Sidechain
2	AB	445	C	Sidechain
2	AB	446	G	Sidechain
2	AB	448	U	Sidechain
2	AB	449	A	Sidechain
2	AB	45	G	Sidechain
2	AB	452	G	Sidechain
2	AB	456	C	Sidechain
2	AB	458	G	Sidechain
2	AB	460	A	Sidechain
2	AB	463	G	Sidechain
2	AB	464	U	Sidechain
2	AB	465	G	Sidechain
2	AB	467	G	Sidechain
2	AB	47	C	Sidechain
2	AB	470	A	Sidechain
2	AB	473	G	Sidechain
2	AB	476	G	Sidechain
2	AB	478	A	Sidechain
2	AB	480	A	Sidechain
2	AB	481	G	Sidechain
2	AB	484	C	Sidechain
2	AB	487	C	Sidechain
2	AB	489	G	Sidechain
2	AB	492	A	Sidechain
2	AB	493	G	Sidechain
2	AB	494	G	Sidechain
2	AB	498	G	Sidechain
2	AB	499	U	Sidechain
2	AB	501	A	Sidechain
2	AB	507	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	511	U	Sidechain
2	AB	512	G	Sidechain
2	AB	517	C	Sidechain
2	AB	518	G	Sidechain
2	AB	520	G	Sidechain
2	AB	522	A	Sidechain
2	AB	526	A	Sidechain
2	AB	527	C	Sidechain
2	AB	535	G	Sidechain
2	AB	536	G	Sidechain
2	AB	539	G	Sidechain
2	AB	546	U	Sidechain
2	AB	547	A	Sidechain
2	AB	551	G	Sidechain
2	AB	553	G	Sidechain
2	AB	554	U	Sidechain
2	AB	555	G	Sidechain
2	AB	572	A	Sidechain
2	AB	582	A	Sidechain
2	AB	585	G	Sidechain
2	AB	586	A	Sidechain
2	AB	588	U	Sidechain
2	AB	590	A	Sidechain
2	AB	591	U	Sidechain
2	AB	594	U	Sidechain
2	AB	595	C	Sidechain
2	AB	60	G	Sidechain
2	AB	604	G	Sidechain
2	AB	608	A	Sidechain
2	AB	611	C	Sidechain
2	AB	612	G	Sidechain
2	AB	613	A	Sidechain
2	AB	614	A	Sidechain
2	AB	62	U	Sidechain
2	AB	630	G	Sidechain
2	AB	631	A	Sidechain
2	AB	632	A	Sidechain
2	AB	635	C	Sidechain
2	AB	642	U	Sidechain
2	AB	644	A	Sidechain
2	AB	647	G	Sidechain
2	AB	65	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	655	A	Sidechain
2	AB	666	A	Sidechain
2	AB	674	G	Sidechain
2	AB	676	A	Sidechain
2	AB	678	C	Sidechain
2	AB	68	G	Sidechain
2	AB	692	C	Sidechain
2	AB	693	A	Sidechain
2	AB	696	G	Sidechain
2	AB	697	G	Sidechain
2	AB	7	G	Sidechain
2	AB	700	G	Sidechain
2	AB	701	G	Sidechain
2	AB	704	G	Sidechain
2	AB	71	A	Sidechain
2	AB	714	U	Sidechain
2	AB	716	A	Sidechain
2	AB	717	C	Sidechain
2	AB	72	U	Sidechain
2	AB	721	A	Sidechain
2	AB	726	G	Sidechain
2	AB	727	A	Sidechain
2	AB	730	A	Sidechain
2	AB	738	G	Sidechain
2	AB	739	A	Sidechain
2	AB	74	A	Sidechain
2	AB	744	U	Sidechain
2	AB	750	A	Sidechain
2	AB	751	A	Sidechain
2	AB	753	A	Sidechain
2	AB	757	G	Sidechain
2	AB	758	C	Sidechain
2	AB	765	C	Sidechain
2	AB	766	U	Sidechain
2	AB	767	U	Sidechain
2	AB	77	G	Sidechain
2	AB	775	G	Sidechain
2	AB	778	G	Sidechain
2	AB	780	G	Sidechain
2	AB	788	A	Sidechain
2	AB	789	A	Sidechain
2	AB	791	C	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	794	A	Sidechain
2	AB	798	G	Sidechain
2	AB	801	G	Sidechain
2	AB	809	G	Sidechain
2	AB	81	G	Sidechain
2	AB	810	U	Sidechain
2	AB	814	C	Sidechain
2	AB	816	C	Sidechain
2	AB	818	G	Sidechain
2	AB	83	A	Sidechain
2	AB	834	G	Sidechain
2	AB	836	G	Sidechain
2	AB	839	U	Sidechain
2	AB	841	G	Sidechain
2	AB	843	G	Sidechain
2	AB	844	A	Sidechain
2	AB	845	A	Sidechain
2	AB	847	U	Sidechain
2	AB	848	C	Sidechain
2	AB	852	U	Sidechain
2	AB	856	G	Sidechain
2	AB	857	G	Sidechain
2	AB	858	G	Sidechain
2	AB	859	G	Sidechain
2	AB	864	G	Sidechain
2	AB	866	A	Sidechain
2	AB	867	C	Sidechain
2	AB	868	U	Sidechain
2	AB	870	U	Sidechain
2	AB	871	U	Sidechain
2	AB	872	U	Sidechain
2	AB	88	G	Sidechain
2	AB	882	G	Sidechain
2	AB	886	A	Sidechain
2	AB	887	U	Sidechain
2	AB	888	C	Sidechain
2	AB	892	A	Sidechain
2	AB	894	U	Sidechain
2	AB	895	U	Sidechain
2	AB	896	A	Sidechain
2	AB	898	C	Sidechain
2	AB	901	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	AB	910	A	Sidechain
2	AB	911	A	Sidechain
2	AB	912	C	Sidechain
2	AB	913	U	Sidechain
2	AB	918	A	Sidechain
2	AB	92	U	Sidechain
2	AB	924	G	Sidechain
2	AB	925	A	Sidechain
2	AB	930	G	Sidechain
2	AB	932	U	Sidechain
2	AB	933	A	Sidechain
2	AB	936	A	Sidechain
2	AB	945	A	Sidechain
2	AB	947	A	Sidechain
2	AB	949	G	Sidechain
2	AB	95	A	Sidechain
2	AB	960	A	Sidechain
2	AB	961	C	Sidechain
2	AB	962	G	Sidechain
2	AB	965	C	Sidechain
2	AB	966	G	Sidechain
2	AB	976	G	Sidechain
2	AB	978	G	Sidechain
2	AB	979	A	Sidechain
2	AB	98	G	Sidechain
2	AB	980	A	Sidechain
2	AB	983	A	Sidechain
2	AB	99	U	Sidechain
2	AB	990	A	Sidechain
2	AB	993	G	Sidechain
3	AC	43	ASP	Peptide
3	AC	44	VAL	Peptide
5	AE	24	VAL	Mainchain
5	AE	47	ALA	Mainchain,Peptide
6	AF	77	ILE	Peptide
8	AH	107	GLY	Peptide
8	AH	39	ALA	Peptide
9	AI	117	LEU	Peptide
9	AI	31	VAL	Mainchain
11	AK	51	GLY	Peptide
11	AK	75	TYR	Sidechain
15	AO	16	HIS	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
17	AQ	98	TYR	Sidechain
18	AR	4	LYS	Peptide
28	Ab	54	GLY	Mainchain
30	Ad	48	TYR	Sidechain
31	Ae	45	SER	Peptide
31	Ae	6	GLN	Peptide
34	BA	100	G	Sidechain
34	BA	1003	G	Sidechain
34	BA	1008	U	Sidechain
34	BA	1009	U	Sidechain
34	BA	1010	U	Sidechain
34	BA	1013	G	Sidechain
34	BA	1014	A	Sidechain
34	BA	1016	A	Sidechain
34	BA	1026	G	Sidechain
34	BA	1027	C	Sidechain
34	BA	1032	G	Sidechain
34	BA	104	G	Sidechain
34	BA	1048	G	Sidechain
34	BA	1058	G	Sidechain
34	BA	1061	G	Sidechain
34	BA	1062	U	Sidechain
34	BA	1065	U	Sidechain
34	BA	1068	G	Sidechain
34	BA	1071	C	Sidechain
34	BA	1072	G	Sidechain
34	BA	1074	G	Sidechain
34	BA	1077	G	Sidechain
34	BA	1078	U	Sidechain
34	BA	1079	G	Sidechain
34	BA	1086	U	Sidechain
34	BA	1091	U	Sidechain
34	BA	1092	A	Sidechain
34	BA	1093	A	Sidechain
34	BA	1094	G	Sidechain
34	BA	1095	U	Sidechain
34	BA	1097	C	Sidechain
34	BA	11	G	Sidechain
34	BA	1100	C	Sidechain
34	BA	1101	A	Sidechain
34	BA	1106	G	Sidechain
34	BA	1119	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	1120	C	Sidechain
34	BA	1121	U	Sidechain
34	BA	1122	U	Sidechain
34	BA	1123	U	Sidechain
34	BA	1124	G	Sidechain
34	BA	1126	U	Sidechain
34	BA	1127	G	Sidechain
34	BA	113	G	Sidechain
34	BA	1130	A	Sidechain
34	BA	1132	C	Sidechain
34	BA	1134	G	Sidechain
34	BA	1135	U	Sidechain
34	BA	1136	C	Sidechain
34	BA	1140	C	Sidechain
34	BA	1141	C	Sidechain
34	BA	1144	G	Sidechain
34	BA	1148	U	Sidechain
34	BA	1149	C	Sidechain
34	BA	1151	A	Sidechain
34	BA	1153	G	Sidechain
34	BA	1155	A	Sidechain
34	BA	1158	C	Sidechain
34	BA	1159	U	Sidechain
34	BA	116	A	Sidechain
34	BA	1160	G	Sidechain
34	BA	1167	A	Sidechain
34	BA	1169	A	Sidechain
34	BA	1176	A	Sidechain
34	BA	1177	G	Sidechain
34	BA	1179	A	Sidechain
34	BA	1181	G	Sidechain
34	BA	1182	G	Sidechain
34	BA	1183	U	Sidechain
34	BA	1197	A	Sidechain
34	BA	1201	A	Sidechain
34	BA	1202	U	Sidechain
34	BA	1206	G	Sidechain
34	BA	1212	U	Sidechain
34	BA	1213	A	Sidechain
34	BA	1214	C	Sidechain
34	BA	1216	A	Sidechain
34	BA	1222	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	1225	A	Sidechain
34	BA	1227	A	Sidechain
34	BA	1232	U	Sidechain
34	BA	1233	G	Sidechain
34	BA	1234	C	Sidechain
34	BA	1235	U	Sidechain
34	BA	1240	U	Sidechain
34	BA	1242	G	Sidechain
34	BA	1249	C	Sidechain
34	BA	1250	A	Sidechain
34	BA	1256	A	Sidechain
34	BA	1258	G	Sidechain
34	BA	1260	G	Sidechain
34	BA	1266	G	Sidechain
34	BA	1267	C	Sidechain
34	BA	1269	A	Sidechain
34	BA	1277	C	Sidechain
34	BA	128	G	Sidechain
34	BA	1285	A	Sidechain
34	BA	1288	A	Sidechain
34	BA	1289	A	Sidechain
34	BA	1298	U	Sidechain
34	BA	1301	U	Sidechain
34	BA	1303	C	Sidechain
34	BA	1305	G	Sidechain
34	BA	1307	U	Sidechain
34	BA	1319	A	Sidechain
34	BA	1322	C	Sidechain
34	BA	1323	G	Sidechain
34	BA	1326	U	Sidechain
34	BA	1333	A	Sidechain
34	BA	1335	U	Sidechain
34	BA	1337	G	Sidechain
34	BA	134	G	Sidechain
34	BA	1340	A	Sidechain
34	BA	1341	U	Sidechain
34	BA	1343	G	Sidechain
34	BA	1345	U	Sidechain
34	BA	1346	A	Sidechain
34	BA	1347	G	Sidechain
34	BA	1354	U	Sidechain
34	BA	1356	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	1357	A	Sidechain
34	BA	1358	U	Sidechain
34	BA	1364	U	Sidechain
34	BA	137	U	Sidechain
34	BA	1371	G	Sidechain
34	BA	1373	G	Sidechain
34	BA	1376	U	Sidechain
34	BA	1377	A	Sidechain
34	BA	1378	C	Sidechain
34	BA	1379	G	Sidechain
34	BA	138	G	Sidechain
34	BA	1382	C	Sidechain
34	BA	1383	C	Sidechain
34	BA	1390	U	Sidechain
34	BA	1391	U	Sidechain
34	BA	1392	G	Sidechain
34	BA	1398	A	Sidechain
34	BA	1403	C	Sidechain
34	BA	1411	C	Sidechain
34	BA	1412	C	Sidechain
34	BA	1414	U	Sidechain
34	BA	1416	G	Sidechain
34	BA	1417	G	Sidechain
34	BA	142	G	Sidechain
34	BA	1424	U	Sidechain
34	BA	1425	U	Sidechain
34	BA	1429	A	Sidechain
34	BA	143	A	Sidechain
34	BA	1432	G	Sidechain
34	BA	1433	A	Sidechain
34	BA	1438	G	Sidechain
34	BA	1441	A	Sidechain
34	BA	1444	U	Sidechain
34	BA	1446	A	Sidechain
34	BA	1447	A	Sidechain
34	BA	1450	U	Sidechain
34	BA	1456	A	Sidechain
34	BA	1459	G	Sidechain
34	BA	1464	U	Sidechain
34	BA	1465	A	Sidechain
34	BA	1467	C	Sidechain
34	BA	1469	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	1470	U	Sidechain
34	BA	1477	U	Sidechain
34	BA	1478	U	Sidechain
34	BA	1479	C	Sidechain
34	BA	1482	G	Sidechain
34	BA	1483	A	Sidechain
34	BA	149	A	Sidechain
34	BA	1491	G	Sidechain
34	BA	1492	A	Sidechain
34	BA	1499	A	Sidechain
34	BA	15	G	Sidechain
34	BA	150	U	Sidechain
34	BA	1501	C	Sidechain
34	BA	1502	A	Sidechain
34	BA	1503	A	Sidechain
34	BA	1505	G	Sidechain
34	BA	1509	C	Sidechain
34	BA	1512	U	Sidechain
34	BA	1517	G	Sidechain
34	BA	152	A	Sidechain
34	BA	1520	C	Sidechain
34	BA	1521	C	Sidechain
34	BA	1522	U	Sidechain
34	BA	1528	U	Sidechain
34	BA	1529	G	Sidechain
34	BA	153	C	Sidechain
34	BA	1530	G	Sidechain
34	BA	1531	A	Sidechain
34	BA	1536	C	Sidechain
34	BA	1540	U	Sidechain
34	BA	1541	U	Sidechain
34	BA	1542	A	Sidechain
34	BA	159	G	Sidechain
34	BA	16	A	Sidechain
34	BA	163	C	Sidechain
34	BA	167	A	Sidechain
34	BA	173	U	Sidechain
34	BA	182	A	Sidechain
34	BA	183	C	Sidechain
34	BA	184	G	Sidechain
34	BA	187	G	Sidechain
34	BA	188	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	189	A	Sidechain
34	BA	190	A	Sidechain
34	BA	193	C	Sidechain
34	BA	194	C	Sidechain
34	BA	195	A	Sidechain
34	BA	196	A	Sidechain
34	BA	197	A	Sidechain
34	BA	202	G	Sidechain
34	BA	203	G	Sidechain
34	BA	205	A	Sidechain
34	BA	206	C	Sidechain
34	BA	211	G	Sidechain
34	BA	215	C	Sidechain
34	BA	22	G	Sidechain
34	BA	222	C	Sidechain
34	BA	223	A	Sidechain
34	BA	224	U	Sidechain
34	BA	229	U	Sidechain
34	BA	235	C	Sidechain
34	BA	236	A	Sidechain
34	BA	237	G	Sidechain
34	BA	239	U	Sidechain
34	BA	246	A	Sidechain
34	BA	25	C	Sidechain
34	BA	252	U	Sidechain
34	BA	254	G	Sidechain
34	BA	257	G	Sidechain
34	BA	265	G	Sidechain
34	BA	269	C	Sidechain
34	BA	27	G	Sidechain
34	BA	274	A	Sidechain
34	BA	285	C	Sidechain
34	BA	29	U	Sidechain
34	BA	290	C	Sidechain
34	BA	298	A	Sidechain
34	BA	299	G	Sidechain
34	BA	3	A	Sidechain
34	BA	305	G	Sidechain
34	BA	306	A	Sidechain
34	BA	307	C	Sidechain
34	BA	31	G	Sidechain
34	BA	313	A	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	315	A	Sidechain
34	BA	320	A	Sidechain
34	BA	323	U	Sidechain
34	BA	325	A	Sidechain
34	BA	329	A	Sidechain
34	BA	33	A	Sidechain
34	BA	330	C	Sidechain
34	BA	332	G	Sidechain
34	BA	333	U	Sidechain
34	BA	334	C	Sidechain
34	BA	34	C	Sidechain
34	BA	340	U	Sidechain
34	BA	346	G	Sidechain
34	BA	347	G	Sidechain
34	BA	348	G	Sidechain
34	BA	349	A	Sidechain
34	BA	350	G	Sidechain
34	BA	354	G	Sidechain
34	BA	356	A	Sidechain
34	BA	362	G	Sidechain
34	BA	363	A	Sidechain
34	BA	365	U	Sidechain
34	BA	368	U	Sidechain
34	BA	370	C	Sidechain
34	BA	380	G	Sidechain
34	BA	383	A	Sidechain
34	BA	387	U	Sidechain
34	BA	388	G	Sidechain
34	BA	39	G	Sidechain
34	BA	391	G	Sidechain
34	BA	394	G	Sidechain
34	BA	396	C	Sidechain
34	BA	399	G	Sidechain
34	BA	4	U	Sidechain
34	BA	408	A	Sidechain
34	BA	413	G	Sidechain
34	BA	414	A	Sidechain
34	BA	415	A	Sidechain
34	BA	417	G	Sidechain
34	BA	427	U	Sidechain
34	BA	428	G	Sidechain
34	BA	43	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	430	A	Sidechain
34	BA	442	G	Sidechain
34	BA	446	G	Sidechain
34	BA	447	G	Sidechain
34	BA	448	A	Sidechain
34	BA	452	A	Sidechain
34	BA	456	A	Sidechain
34	BA	459	A	Sidechain
34	BA	464	U	Sidechain
34	BA	465	A	Sidechain
34	BA	466	A	Sidechain
34	BA	467	U	Sidechain
34	BA	469	C	Sidechain
34	BA	470	C	Sidechain
34	BA	471	U	Sidechain
34	BA	476	U	Sidechain
34	BA	477	C	Sidechain
34	BA	479	U	Sidechain
34	BA	480	U	Sidechain
34	BA	481	G	Sidechain
34	BA	483	C	Sidechain
34	BA	486	U	Sidechain
34	BA	487	A	Sidechain
34	BA	489	C	Sidechain
34	BA	491	G	Sidechain
34	BA	493	A	Sidechain
34	BA	496	A	Sidechain
34	BA	5	U	Sidechain
34	BA	50	A	Sidechain
34	BA	508	U	Sidechain
34	BA	510	A	Sidechain
34	BA	511	C	Sidechain
34	BA	517	G	Sidechain
34	BA	519	C	Sidechain
34	BA	520	A	Sidechain
34	BA	523	A	Sidechain
34	BA	525	C	Sidechain
34	BA	532	A	Sidechain
34	BA	533	A	Sidechain
34	BA	542	G	Sidechain
34	BA	546	A	Sidechain
34	BA	556	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	565	U	Sidechain
34	BA	568	G	Sidechain
34	BA	576	C	Sidechain
34	BA	577	G	Sidechain
34	BA	589	U	Sidechain
34	BA	594	U	Sidechain
34	BA	596	A	Sidechain
34	BA	597	G	Sidechain
34	BA	608	A	Sidechain
34	BA	609	A	Sidechain
34	BA	61	G	Sidechain
34	BA	613	C	Sidechain
34	BA	614	C	Sidechain
34	BA	618	C	Sidechain
34	BA	62	U	Sidechain
34	BA	636	U	Sidechain
34	BA	64	G	Sidechain
34	BA	641	U	Sidechain
34	BA	642	A	Sidechain
34	BA	646	G	Sidechain
34	BA	654	G	Sidechain
34	BA	66	A	Sidechain
34	BA	660	C	Sidechain
34	BA	661	G	Sidechain
34	BA	670	G	Sidechain
34	BA	671	G	Sidechain
34	BA	673	A	Sidechain
34	BA	682	G	Sidechain
34	BA	686	U	Sidechain
34	BA	687	A	Sidechain
34	BA	688	G	Sidechain
34	BA	69	G	Sidechain
34	BA	692	U	Sidechain
34	BA	693	G	Sidechain
34	BA	694	A	Sidechain
34	BA	697	U	Sidechain
34	BA	7	A	Sidechain
34	BA	701	U	Sidechain
34	BA	702	A	Sidechain
34	BA	704	A	Sidechain
34	BA	705	G	Sidechain
34	BA	71	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	713	G	Sidechain
34	BA	714	G	Sidechain
34	BA	719	C	Sidechain
34	BA	721	G	Sidechain
34	BA	723	U	Sidechain
34	BA	728	A	Sidechain
34	BA	73	C	Sidechain
34	BA	737	C	Sidechain
34	BA	738	C	Sidechain
34	BA	739	C	Sidechain
34	BA	745	G	Sidechain
34	BA	748	G	Sidechain
34	BA	749	A	Sidechain
34	BA	751	U	Sidechain
34	BA	752	G	Sidechain
34	BA	754	C	Sidechain
34	BA	757	U	Sidechain
34	BA	758	C	Sidechain
34	BA	76	G	Sidechain
34	BA	762	U	Sidechain
34	BA	765	G	Sidechain
34	BA	771	G	Sidechain
34	BA	773	G	Sidechain
34	BA	775	G	Sidechain
34	BA	776	G	Sidechain
34	BA	786	G	Sidechain
34	BA	789	U	Sidechain
34	BA	790	A	Sidechain
34	BA	792	A	Sidechain
34	BA	794	A	Sidechain
34	BA	797	C	Sidechain
34	BA	8	A	Sidechain
34	BA	804	U	Sidechain
34	BA	817	C	Sidechain
34	BA	82	G	Sidechain
34	BA	820	U	Sidechain
34	BA	823	C	Sidechain
34	BA	828	U	Sidechain
34	BA	833	G	Sidechain
34	BA	838	G	Sidechain
34	BA	84	U	Sidechain
34	BA	840	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	841	C	Sidechain
34	BA	842	U	Sidechain
34	BA	843	U	Sidechain
34	BA	847	G	Sidechain
34	BA	849	G	Sidechain
34	BA	85	U	Sidechain
34	BA	851	G	Sidechain
34	BA	854	U	Sidechain
34	BA	861	G	Sidechain
34	BA	864	A	Sidechain
34	BA	866	C	Sidechain
34	BA	869	G	Sidechain
34	BA	870	U	Sidechain
34	BA	873	A	Sidechain
34	BA	874	G	Sidechain
34	BA	876	C	Sidechain
34	BA	877	G	Sidechain
34	BA	88	U	Sidechain
34	BA	880	C	Sidechain
34	BA	884	U	Sidechain
34	BA	888	G	Sidechain
34	BA	89	U	Sidechain
34	BA	899	C	Sidechain
34	BA	900	A	Sidechain
34	BA	901	A	Sidechain
34	BA	902	G	Sidechain
34	BA	908	A	Sidechain
34	BA	91	U	Sidechain
34	BA	919	A	Sidechain
34	BA	92	U	Sidechain
34	BA	920	U	Sidechain
34	BA	923	A	Sidechain
34	BA	928	G	Sidechain
34	BA	933	G	Sidechain
34	BA	934	C	Sidechain
34	BA	935	A	Sidechain
34	BA	937	A	Sidechain
34	BA	938	A	Sidechain
34	BA	94	G	Sidechain
34	BA	940	C	Sidechain
34	BA	946	A	Sidechain
34	BA	948	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
34	BA	951	G	Sidechain
34	BA	955	U	Sidechain
34	BA	958	A	Sidechain
34	BA	959	A	Sidechain
34	BA	960	U	Sidechain
34	BA	972	C	Sidechain
34	BA	975	A	Sidechain
34	BA	977	A	Sidechain
34	BA	978	A	Sidechain
34	BA	980	C	Sidechain
34	BA	983	A	Sidechain
34	BA	984	C	Sidechain
34	BA	99	C	Sidechain
34	BA	991	U	Sidechain
34	BA	992	U	Sidechain
34	BA	994	A	Sidechain
34	BA	995	C	Sidechain
35	BB	15	G	Sidechain
35	BB	40	C	Sidechain
35	BB	48	C	Sidechain
35	BB	50	U	Sidechain
35	BB	51	U	Sidechain
35	BB	56	C	Sidechain
35	BB	58	A	Sidechain
35	BB	59	U	Sidechain
35	BB	60	U	Sidechain
35	BB	68	C	Sidechain
35	BB	7	A	Sidechain
35	BB	74	C	Sidechain
37	BD	24	A	Sidechain
37	BD	25	U	Sidechain
37	BD	37	U	Sidechain
37	BD	47	C	Sidechain
35	BE	15	G	Sidechain
35	BE	18	G	Sidechain
35	BE	19	G	Sidechain
35	BE	21	A	Sidechain
35	BE	22	G	Sidechain
35	BE	24	G	Sidechain
35	BE	34	G	Sidechain
35	BE	44	G	Sidechain
35	BE	56	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
35	BE	57	G	Sidechain
35	BE	59	U	Sidechain
35	BE	6	G	Sidechain
35	BE	63	G	Sidechain
35	BE	65	G	Sidechain
35	BE	68	C	Sidechain
38	BF	21	TYR	Sidechain
39	BG	221	ALA	Peptide
39	BG	223	PRO	Mainchain
40	BH	102	TYR	Sidechain
40	BH	203	TYR	Sidechain
41	BI	146	MET	Mainchain,Peptide
41	BI	154	ALA	Peptide
42	BJ	87	SER	Peptide
43	BK	172	PRO	Mainchain
43	BK	5	VAL	Peptide
45	BM	6	TYR	Sidechain
45	BM	63	TYR	Sidechain
47	BO	81	LEU	Peptide
48	BP	16	ALA	Mainchain
50	BR	60	ARG	Mainchain
54	BV	3	TYR	Sidechain
55	BW	77	ARG	Sidechain
57	BY	17	ARG	Sidechain
57	BY	37	TYR	Sidechain
57	BY	4	LYS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2566	0	1302	0	0
2	AB	62351	0	31387	0	0
3	AC	1733	0	1824	0	0
4	AD	2092	0	2170	0	0
5	AE	1565	0	1616	0	0
6	AF	1552	0	1619	0	0
7	AG	1420	0	1460	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	1323	0	1374	0	0
9	AI	1111	0	1148	0	0
10	AJ	1032	0	1088	0	0
11	AK	1129	0	1162	0	0
12	AL	947	0	1023	0	0
13	AM	1053	0	1129	0	0
14	AN	1074	0	1157	0	0
15	AO	1008	0	1045	0	0
16	AP	900	0	935	0	0
17	AQ	917	0	965	0	0
18	AR	947	0	1022	0	0
19	AS	816	0	839	0	0
20	AT	857	0	922	0	0
21	AU	787	0	846	0	0
22	AV	789	0	847	0	0
23	AW	753	0	780	0	0
24	AX	634	0	656	0	0
25	AY	625	0	655	0	0
26	AZ	509	0	543	0	0
27	Aa	449	0	491	0	0
28	Ab	549	0	552	0	0
29	Ac	444	0	461	0	0
30	Ad	441	0	485	0	0
31	Ae	377	0	418	0	0
32	Af	504	0	574	0	0
33	Ag	302	0	343	0	0
34	BA	33089	0	16678	0	0
35	BB	1635	0	849	0	0
35	BE	1635	0	849	0	0
36	BC	3036	0	3052	0	0
37	BD	495	0	249	0	0
38	BF	1872	0	1885	0	0
39	BG	1822	0	1913	0	0
40	BH	1643	0	1710	0	0
41	BI	1225	0	1273	0	0
42	BJ	1101	0	1050	0	0
43	BK	1400	0	1449	0	0
44	BL	979	0	1034	0	0
45	BM	1036	0	1084	0	0
46	BN	825	0	865	0	0
47	BO	965	0	997	0	0
48	BP	955	0	1019	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	BQ	910	0	981	0	0
50	BR	805	0	847	0	0
51	BS	716	0	742	0	0
52	BT	649	0	666	0	0
53	BU	672	0	716	0	0
54	BV	626	0	651	0	0
55	BW	727	0	769	0	0
56	BX	670	0	722	0	0
57	BY	590	0	631	0	0
All	All	153634	0	105519	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	15	60
4	AD	270/273 (99%)	239 (88%)	23 (8%)	8 (3%)	5	42
5	AE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	6	43
6	AF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	13	57
7	AG	176/179 (98%)	147 (84%)	27 (15%)	2 (1%)	17	63
8	AH	174/177 (98%)	163 (94%)	8 (5%)	3 (2%)	11	55
9	AI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	5	40
10	AJ	139/142 (98%)	123 (88%)	15 (11%)	1 (1%)	26	71
11	AK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
12	AL	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	11	55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	AM	142/144 (99%)	125 (88%)	15 (11%)	2 (1%)	14	58
14	AN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	8	49
15	AO	125/127 (98%)	117 (94%)	7 (6%)	1 (1%)	24	69
16	AP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	21	67
17	AQ	112/115 (97%)	100 (89%)	10 (9%)	2 (2%)	11	53
18	AR	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	21	67
19	AS	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	4	35
20	AT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	21	67
21	AU	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	9	51
22	AV	101/104 (97%)	89 (88%)	11 (11%)	1 (1%)	19	65
23	AW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	8	49
24	AX	82/85 (96%)	67 (82%)	12 (15%)	3 (4%)	4	38
25	AY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	6	45
26	AZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	3	31
27	Aa	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	11	53
28	Ab	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	13	57
29	Ac	54/57 (95%)	47 (87%)	5 (9%)	2 (4%)	4	38
30	Ad	52/55 (94%)	45 (86%)	7 (14%)	0	100	100
31	Ae	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
32	Af	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	Ag	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	44
36	BC	391/393 (100%)	368 (94%)	20 (5%)	3 (1%)	24	69
38	BF	238/241 (99%)	215 (90%)	20 (8%)	3 (1%)	15	60
39	BG	230/233 (99%)	211 (92%)	17 (7%)	2 (1%)	21	67
40	BH	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	19	65
41	BI	164/167 (98%)	144 (88%)	17 (10%)	3 (2%)	11	53
42	BJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	13	57
43	BK	176/179 (98%)	160 (91%)	14 (8%)	2 (1%)	17	63
44	BL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	12	56
45	BM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	12	56
46	BN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	4	35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	12	56
48	BP	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	3	35
49	BQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
50	BR	98/101 (97%)	83 (85%)	8 (8%)	7 (7%)	1	22
51	BS	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
52	BT	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
53	BU	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
54	BV	72/75 (96%)	65 (90%)	5 (7%)	2 (3%)	6	44
55	BW	89/92 (97%)	80 (90%)	9 (10%)	0	100	100
56	BX	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
57	BY	68/71 (96%)	60 (88%)	7 (10%)	1 (2%)	13	57
All	All	6548/6682 (98%)	5904 (90%)	536 (8%)	108 (2%)	17	56

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	260	LYS
5	AE	122	VAL
5	AE	150	GLN
5	AE	170	VAL
9	AI	23	ALA
14	AN	36	VAL
16	AP	68	LYS
19	AS	91	GLN
22	AV	6	ARG
26	AZ	46	VAL
29	Ac	26	SER
40	BH	18	LEU
45	BM	3	ASN
46	BN	74	VAL
47	BO	118	ASN
48	BP	86	VAL
50	BR	37	ASP
50	BR	70	HIS
57	BY	3	ILE
3	AC	217	THR
3	AC	229	LEU
4	AD	119	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	AD	237	ARG
5	AE	43	ASP
7	AG	148	VAL
13	AM	36	LYS
18	AR	104	ALA
24	AX	9	THR
24	AX	72	GLY
25	AY	27	ARG
25	AY	62	GLY
26	AZ	23	ARG
27	Aa	9	THR
29	Ac	39	ARG
36	BC	21	ASP
36	BC	60	ILE
38	BF	41	ASN
41	BI	77	ASN
43	BK	55	LYS
54	BV	11	ARG
4	AD	193	GLU
4	AD	240	GLY
5	AE	41	ALA
5	AE	137	SER
6	AF	62	GLN
8	AH	50	THR
8	AH	164	ALA
12	AL	70	ARG
33	Ag	4	ARG
41	BI	43	GLY
41	BI	162	GLU
43	BK	116	ALA
46	BN	90	LEU
47	BO	74	LYS
48	BP	75	GLU
50	BR	61	ASN
50	BR	73	LEU
4	AD	140	VAL
4	AD	190	THR
12	AL	3	GLN
19	AS	53	PHE
19	AS	80	ARG
21	AU	69	ARG
23	AW	85	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	BF	132	GLU
42	BJ	92	THR
45	BM	13	SER
48	BP	24	GLU
50	BR	32	ASP
50	BR	35	ALA
54	BV	3	TYR
6	AF	66	GLY
8	AH	8	VAL
14	AN	106	ASP
15	AO	81	ASN
36	BC	9	LYS
39	BG	14	VAL
42	BJ	100	SER
46	BN	42	LEU
48	BP	21	PRO
48	BP	43	LYS
3	AC	73	VAL
4	AD	141	HIS
6	AF	71	GLY
7	AG	73	VAL
9	AI	28	ASN
10	AJ	90	GLY
21	AU	23	ALA
26	AZ	17	GLU
38	BF	149	GLY
13	AM	20	GLY
14	AN	23	GLY
39	BG	8	GLY
46	BN	57	VAL
9	AI	118	PRO
9	AI	121	VAL
17	AQ	22	GLY
23	AW	65	VAL
40	BH	27	ILE
28	Ab	36	VAL
44	BL	81	GLY
44	BL	125	ILE
50	BR	30	ILE
9	AI	94	ILE
17	AQ	32	VAL
19	AS	101	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	AT	80	PRO
24	AX	36	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	181/181 (100%)	171 (94%)	10 (6%)	27	63
4	AD	217/218 (100%)	204 (94%)	13 (6%)	24	60
5	AE	164/164 (100%)	154 (94%)	10 (6%)	23	60
6	AF	165/165 (100%)	158 (96%)	7 (4%)	36	70
7	AG	149/150 (99%)	138 (93%)	11 (7%)	17	54
8	AH	137/138 (99%)	125 (91%)	12 (9%)	12	45
9	AI	114/114 (100%)	106 (93%)	8 (7%)	19	56
10	AJ	109/110 (99%)	105 (96%)	4 (4%)	41	73
11	AK	116/116 (100%)	113 (97%)	3 (3%)	54	80
12	AL	104/104 (100%)	94 (90%)	10 (10%)	10	40
13	AM	103/103 (100%)	99 (96%)	4 (4%)	39	72
14	AN	109/109 (100%)	103 (94%)	6 (6%)	27	63
15	AO	103/103 (100%)	101 (98%)	2 (2%)	65	86
16	AP	87/87 (100%)	80 (92%)	7 (8%)	15	50
17	AQ	99/100 (99%)	91 (92%)	8 (8%)	15	50
18	AR	89/90 (99%)	82 (92%)	7 (8%)	15	51
19	AS	84/84 (100%)	78 (93%)	6 (7%)	18	55
20	AT	93/93 (100%)	89 (96%)	4 (4%)	35	70
21	AU	84/84 (100%)	79 (94%)	5 (6%)	24	60
22	AV	84/85 (99%)	81 (96%)	3 (4%)	42	74
23	AW	78/78 (100%)	72 (92%)	6 (8%)	16	52
24	AX	62/63 (98%)	60 (97%)	2 (3%)	46	76

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AY	67/68 (98%)	67 (100%)	0	100	100
26	AZ	55/55 (100%)	49 (89%)	6 (11%)	8	35
27	Aa	48/49 (98%)	45 (94%)	3 (6%)	22	59
28	Ab	62/62 (100%)	58 (94%)	4 (6%)	21	58
29	Ac	47/48 (98%)	43 (92%)	4 (8%)	13	48
30	Ad	48/49 (98%)	46 (96%)	2 (4%)	36	70
31	Ae	38/38 (100%)	35 (92%)	3 (8%)	15	51
32	Af	51/52 (98%)	50 (98%)	1 (2%)	63	85
33	Ag	34/34 (100%)	33 (97%)	1 (3%)	50	78
36	BC	326/326 (100%)	316 (97%)	10 (3%)	47	77
38	BF	198/199 (100%)	188 (95%)	10 (5%)	29	66
39	BG	189/190 (100%)	176 (93%)	13 (7%)	19	56
40	BH	172/173 (99%)	164 (95%)	8 (5%)	32	68
41	BI	125/126 (99%)	118 (94%)	7 (6%)	26	62
42	BJ	116/116 (100%)	111 (96%)	5 (4%)	35	70
43	BK	146/147 (99%)	139 (95%)	7 (5%)	31	67
44	BL	104/105 (99%)	98 (94%)	6 (6%)	25	61
45	BM	106/107 (99%)	98 (92%)	8 (8%)	17	53
46	BN	90/90 (100%)	80 (89%)	10 (11%)	8	34
47	BO	98/99 (99%)	94 (96%)	4 (4%)	37	71
48	BP	103/104 (99%)	100 (97%)	3 (3%)	50	78
49	BQ	95/96 (99%)	91 (96%)	4 (4%)	36	70
50	BR	83/84 (99%)	76 (92%)	7 (8%)	14	48
51	BS	76/77 (99%)	75 (99%)	1 (1%)	76	89
52	BT	65/65 (100%)	63 (97%)	2 (3%)	47	77
53	BU	77/78 (99%)	75 (97%)	2 (3%)	54	80
54	BV	64/65 (98%)	56 (88%)	8 (12%)	6	30
55	BW	78/79 (99%)	74 (95%)	4 (5%)	29	66
56	BX	65/66 (98%)	63 (97%)	2 (3%)	47	77
57	BY	60/61 (98%)	55 (92%)	5 (8%)	14	49
All	All	5417/5447 (99%)	5119 (94%)	298 (6%)	31	63

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	11	ILE
3	AC	60	ARG
3	AC	85	GLU
3	AC	98	GLU
3	AC	164	ARG
3	AC	165	ASN
3	AC	167	LYS
3	AC	174	THR
3	AC	203	GLN
3	AC	218	MET
4	AD	6	LYS
4	AD	17	LYS
4	AD	43	ASN
4	AD	59	GLN
4	AD	62	ARG
4	AD	90	ILE
4	AD	129	LEU
4	AD	132	ARG
4	AD	145	MET
4	AD	200	MET
4	AD	222	THR
4	AD	231	HIS
4	AD	270	ARG
5	AE	36	GLN
5	AE	40	LEU
5	AE	74	GLU
5	AE	86	GLU
5	AE	89	GLU
5	AE	122	VAL
5	AE	148	GLN
5	AE	159	LYS
5	AE	168	GLU
5	AE	183	GLU
6	AF	78	TRP
6	AF	79	ARG
6	AF	122	GLU
6	AF	134	LEU
6	AF	155	GLU
6	AF	157	LEU
6	AF	165	HIS
7	AG	21	TYR
7	AG	22	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
7	AG	25	MET
7	AG	41	GLU
7	AG	46	LYS
7	AG	79	ARG
7	AG	91	ARG
7	AG	109	ARG
7	AG	129	MET
7	AG	132	ARG
7	AG	149	ARG
8	AH	5	LYS
8	AH	26	LYS
8	AH	34	ARG
8	AH	38	ASP
8	AH	40	VAL
8	AH	41	GLU
8	AH	84	LYS
8	AH	94	ARG
8	AH	98	LYS
8	AH	102	ILE
8	AH	133	LYS
8	AH	169	ARG
9	AI	8	LYS
9	AI	17	ASP
9	AI	25	TYR
9	AI	53	GLU
9	AI	75	LEU
9	AI	87	GLU
9	AI	109	GLU
9	AI	116	ARG
10	AJ	9	LYS
10	AJ	39	LYS
10	AJ	49	GLU
10	AJ	106	GLN
11	AK	120	ARG
11	AK	129	GLU
11	AK	136	GLN
12	AL	17	ARG
12	AL	20	MET
12	AL	45	GLU
12	AL	73	ASP
12	AL	78	ARG
12	AL	106	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	AL	110	GLU
12	AL	112	PHE
12	AL	113	MET
12	AL	114	LYS
13	AM	2	ARG
13	AM	10	GLU
13	AM	30	THR
13	AM	103	ILE
14	AN	6	ARG
14	AN	28	PHE
14	AN	36	VAL
14	AN	47	GLU
14	AN	59	ARG
14	AN	100	LYS
15	AO	114	GLU
15	AO	127	GLU
16	AP	7	ARG
16	AP	16	ARG
16	AP	36	TYR
16	AP	76	LYS
16	AP	94	ARG
16	AP	98	GLN
16	AP	112	GLU
17	AQ	31	VAL
17	AQ	33	GLU
17	AQ	39	LEU
17	AQ	54	LEU
17	AQ	98	TYR
17	AQ	100	ARG
17	AQ	109	ILE
17	AQ	114	ASN
18	AR	5	ARG
18	AR	43	GLN
18	AR	70	GLN
18	AR	77	LYS
18	AR	91	ARG
18	AR	102	LYS
18	AR	110	GLU
19	AS	6	GLN
19	AS	10	LYS
19	AS	16	GLU
19	AS	22	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	AS	37	GLU
19	AS	70	GLU
20	AT	28	LYS
20	AT	59	GLU
20	AT	66	ILE
20	AT	86	MET
21	AU	6	ARG
21	AU	9	LYS
21	AU	24	MET
21	AU	26	LYS
21	AU	73	ARG
22	AV	46	LYS
22	AV	85	ARG
22	AV	91	LYS
23	AW	11	GLU
23	AW	34	LYS
23	AW	51	GLN
23	AW	55	GLU
23	AW	79	ARG
23	AW	90	ASP
24	AX	31	LEU
24	AX	69	GLU
26	AZ	5	GLU
26	AZ	7	ARG
26	AZ	24	GLU
26	AZ	30	MET
26	AZ	31	GLN
26	AZ	60	LYS
27	Aa	5	LYS
27	Aa	38	GLU
27	Aa	58	GLU
28	Ab	56	ARG
28	Ab	59	ARG
28	Ab	62	LYS
28	Ab	65	ASN
29	Ac	3	GLN
29	Ac	9	ARG
29	Ac	12	ARG
29	Ac	47	TYR
30	Ad	29	LYS
30	Ad	34	GLU
31	Ae	3	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
31	Ae	34	ARG
31	Ae	41	ARG
32	Af	63	TYR
33	Ag	1	MET
36	BC	11	HIS
36	BC	74	ARG
36	BC	155	GLU
36	BC	204	ARG
36	BC	236	ILE
36	BC	279	ARG
36	BC	326	TYR
36	BC	349	MET
36	BC	351	MET
36	BC	378	GLU
38	BF	8	MET
38	BF	9	LEU
38	BF	17	HIS
38	BF	20	ARG
38	BF	51	GLU
38	BF	77	GLU
38	BF	80	LYS
38	BF	117	GLU
38	BF	224	ARG
38	BF	234	GLU
39	BG	40	GLN
39	BG	55	VAL
39	BG	61	LYS
39	BG	68	HIS
39	BG	71	ARG
39	BG	79	LYS
39	BG	85	LYS
39	BG	109	GLU
39	BG	120	THR
39	BG	143	LEU
39	BG	167	TYR
39	BG	203	LYS
39	BG	228	ARG
40	BH	12	ARG
40	BH	20	LEU
40	BH	35	GLN
40	BH	80	ARG
40	BH	123	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
40	BH	131	ILE
40	BH	142	VAL
40	BH	184	LYS
41	BI	11	GLN
41	BI	13	LYS
41	BI	49	TYR
41	BI	92	ARG
41	BI	95	MET
41	BI	143	LEU
41	BI	150	GLU
42	BJ	13	ASP
42	BJ	16	GLU
42	BJ	23	GLU
42	BJ	37	HIS
42	BJ	113	ARG
43	BK	105	GLU
43	BK	122	GLU
43	BK	129	ASN
43	BK	138	GLU
43	BK	148	LYS
43	BK	161	PHE
43	BK	164	GLN
44	BL	2	MET
44	BL	14	ARG
44	BL	41	GLU
44	BL	59	GLU
44	BL	117	GLN
44	BL	127	TYR
45	BM	12	LYS
45	BM	36	GLN
45	BM	40	ARG
45	BM	58	GLU
45	BM	65	THR
45	BM	91	GLU
45	BM	94	ARG
45	BM	105	ARG
46	BN	1	MET
46	BN	7	ARG
46	BN	10	LEU
46	BN	15	HIS
46	BN	31	ARG
46	BN	37	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
46	BN	46	LYS
46	BN	54	SER
46	BN	82	LYS
46	BN	99	GLN
47	BO	6	ARG
47	BO	82	GLU
47	BO	93	GLU
47	BO	124	LYS
48	BP	81	ILE
48	BP	85	ARG
48	BP	113	ARG
49	BQ	16	ILE
49	BQ	26	LYS
49	BQ	61	LYS
49	BQ	85	TYR
50	BR	20	PHE
50	BR	29	ILE
50	BR	33	VAL
50	BR	41	TRP
50	BR	66	THR
50	BR	70	HIS
50	BR	84	ARG
51	BS	13	GLU
52	BT	5	ARG
52	BT	67	ILE
53	BU	17	GLU
53	BU	54	ILE
54	BV	5	ARG
54	BV	6	ARG
54	BV	8	LYS
54	BV	11	ARG
54	BV	34	GLU
54	BV	42	ARG
54	BV	47	ARG
54	BV	69	TYR
55	BW	5	LYS
55	BW	28	LYS
55	BW	76	THR
55	BW	80	ARG
56	BX	57	VAL
56	BX	73	ARG
57	BY	15	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
57	BY	36	PHE
57	BY	38	GLU
57	BY	39	LYS
57	BY	62	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	119/120 (99%)	15 (12%)	3 (2%)
2	AB	2898/2904 (99%)	396 (13%)	130 (4%)
34	BA	1538/1542 (99%)	192 (12%)	77 (5%)
35	BB	73/76 (96%)	12 (16%)	2 (2%)
35	BE	73/76 (96%)	12 (16%)	6 (8%)
37	BD	24/24 (100%)	4 (16%)	5 (20%)
All	All	4725/4742 (99%)	631 (13%)	223 (4%)

All (631) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	13	G
1	AA	15	A
1	AA	16	G
1	AA	36	C
1	AA	38	C
1	AA	42	C
1	AA	45	A
1	AA	57	A
1	AA	58	A
1	AA	68	C
1	AA	71	C
1	AA	88	C
1	AA	90	C
1	AA	109	A
2	AB	11	C
2	AB	13	A
2	AB	14	A
2	AB	28	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	52	A
2	AB	61	C
2	AB	64	A
2	AB	65	U
2	AB	71	A
2	AB	72	U
2	AB	75	G
2	AB	91	A
2	AB	101	A
2	AB	102	U
2	AB	118	A
2	AB	119	A
2	AB	120	U
2	AB	125	A
2	AB	126	A
2	AB	128	C
2	AB	138	U
2	AB	142	A
2	AB	149	A
2	AB	154	U
2	AB	165	A
2	AB	196	A
2	AB	204	A
2	AB	205	G
2	AB	215	G
2	AB	216	A
2	AB	221	A
2	AB	222	A
2	AB	223	A
2	AB	226	A
2	AB	248	G
2	AB	265	A
2	AB	266	G
2	AB	269	C
2	AB	270	A
2	AB	271	G
2	AB	272	A
2	AB	277	G
2	AB	279	A
2	AB	294	A
2	AB	302	C
2	AB	323	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	324	A
2	AB	330	A
2	AB	331	C
2	AB	338	G
2	AB	346	A
2	AB	373	U
2	AB	383	C
2	AB	386	G
2	AB	391	A
2	AB	411	G
2	AB	418	C
2	AB	432	A
2	AB	444	C
2	AB	447	A
2	AB	448	U
2	AB	451	U
2	AB	456	C
2	AB	457	A
2	AB	458	G
2	AB	459	U
2	AB	479	A
2	AB	480	A
2	AB	481	G
2	AB	482	A
2	AB	504	A
2	AB	505	A
2	AB	508	A
2	AB	509	C
2	AB	527	C
2	AB	529	A
2	AB	530	G
2	AB	531	C
2	AB	532	A
2	AB	533	G
2	AB	546	U
2	AB	547	A
2	AB	548	G
2	AB	549	G
2	AB	563	A
2	AB	573	U
2	AB	574	A
2	AB	575	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	586	A
2	AB	588	U
2	AB	603	A
2	AB	607	U
2	AB	637	A
2	AB	645	C
2	AB	654	A
2	AB	655	A
2	AB	656	G
2	AB	669	G
2	AB	670	A
2	AB	686	U
2	AB	715	A
2	AB	717	C
2	AB	728	G
2	AB	730	A
2	AB	736	C
2	AB	737	C
2	AB	740	C
2	AB	747	5MU
2	AB	748	G
2	AB	753	A
2	AB	764	A
2	AB	775	G
2	AB	776	G
2	AB	782	A
2	AB	784	G
2	AB	786	C
2	AB	790	U
2	AB	791	C
2	AB	792	A
2	AB	793	A
2	AB	805	G
2	AB	812	C
2	AB	828	U
2	AB	910	A
2	AB	914	G
2	AB	931	U
2	AB	941	A
2	AB	945	A
2	AB	946	C
2	AB	959	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	962	G
2	AB	974	G
2	AB	980	A
2	AB	984	A
2	AB	995	C
2	AB	996	A
2	AB	1012	U
2	AB	1013	C
2	AB	1016	G
2	AB	1022	G
2	AB	1025	G
2	AB	1026	G
2	AB	1033	U
2	AB	1034	G
2	AB	1047	G
2	AB	1048	A
2	AB	1056	G
2	AB	1067	A
2	AB	1069	A
2	AB	1070	A
2	AB	1079	C
2	AB	1086	A
2	AB	1088	A
2	AB	1095	A
2	AB	1110	G
2	AB	1112	G
2	AB	1128	G
2	AB	1129	A
2	AB	1130	U
2	AB	1132	U
2	AB	1133	A
2	AB	1134	A
2	AB	1135	C
2	AB	1136	G
2	AB	1143	A
2	AB	1170	C
2	AB	1175	A
2	AB	1177	G
2	AB	1184	U
2	AB	1185	G
2	AB	1186	G
2	AB	1206	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	1211	C
2	AB	1212	G
2	AB	1213	A
2	AB	1249	U
2	AB	1250	G
2	AB	1255	U
2	AB	1256	G
2	AB	1266	G
2	AB	1271	G
2	AB	1272	A
2	AB	1286	A
2	AB	1287	A
2	AB	1296	G
2	AB	1300	G
2	AB	1301	A
2	AB	1365	A
2	AB	1378	A
2	AB	1379	U
2	AB	1391	U
2	AB	1416	G
2	AB	1417	C
2	AB	1427	A
2	AB	1440	U
2	AB	1452	G
2	AB	1453	A
2	AB	1455	G
2	AB	1458	U
2	AB	1459	G
2	AB	1460	U
2	AB	1462	C
2	AB	1482	G
2	AB	1493	C
2	AB	1509	A
2	AB	1510	G
2	AB	1523	U
2	AB	1558	C
2	AB	1566	A
2	AB	1569	A
2	AB	1584	U
2	AB	1585	C
2	AB	1596	A
2	AB	1607	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	1608	A
2	AB	1616	A
2	AB	1646	C
2	AB	1647	U
2	AB	1648	U
2	AB	1654	A
2	AB	1700	A
2	AB	1705	A
2	AB	1715	G
2	AB	1732	C
2	AB	1733	G
2	AB	1757	A
2	AB	1762	A
2	AB	1773	A
2	AB	1781	U
2	AB	1782	U
2	AB	1791	A
2	AB	1800	C
2	AB	1802	A
2	AB	1808	A
2	AB	1809	A
2	AB	1839	G
2	AB	1840	G
2	AB	1871	A
2	AB	1873	G
2	AB	1900	A
2	AB	1901	A
2	AB	1906	G
2	AB	1907	G
2	AB	1929	G
2	AB	1930	G
2	AB	1931	U
2	AB	1937	A
2	AB	1938	A
2	AB	1943	U
2	AB	1952	A
2	AB	1954	G
2	AB	1955	U
2	AB	1956	U
2	AB	1962	5MC
2	AB	1964	G
2	AB	1965	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	1966	A
2	AB	1970	A
2	AB	1971	U
2	AB	1972	G
2	AB	1981	A
2	AB	1992	G
2	AB	1993	U
2	AB	1997	C
2	AB	2003	A
2	AB	2021	C
2	AB	2023	C
2	AB	2032	G
2	AB	2042	A
2	AB	2043	C
2	AB	2056	G
2	AB	2059	A
2	AB	2061	G
2	AB	2068	U
2	AB	2076	U
2	AB	2092	U
2	AB	2112	G
2	AB	2119	A
2	AB	2120	G
2	AB	2127	G
2	AB	2129	C
2	AB	2131	U
2	AB	2132	U
2	AB	2133	G
2	AB	2135	A
2	AB	2140	G
2	AB	2147	A
2	AB	2158	A
2	AB	2159	G
2	AB	2172	U
2	AB	2173	A
2	AB	2174	C
2	AB	2179	C
2	AB	2199	A
2	AB	2203	U
2	AB	2212	A
2	AB	2213	U
2	AB	2214	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	2225	A
2	AB	2238	G
2	AB	2239	G
2	AB	2250	G
2	AB	2266	A
2	AB	2273	A
2	AB	2283	C
2	AB	2287	A
2	AB	2288	A
2	AB	2305	U
2	AB	2308	G
2	AB	2309	A
2	AB	2310	C
2	AB	2321	U
2	AB	2322	A
2	AB	2325	G
2	AB	2333	A
2	AB	2335	A
2	AB	2350	C
2	AB	2357	G
2	AB	2363	G
2	AB	2382	G
2	AB	2383	G
2	AB	2385	C
2	AB	2390	U
2	AB	2391	G
2	AB	2399	G
2	AB	2406	A
2	AB	2407	A
2	AB	2408	U
2	AB	2425	A
2	AB	2429	G
2	AB	2432	A
2	AB	2439	A
2	AB	2440	C
2	AB	2441	U
2	AB	2448	A
2	AB	2449	H2U
2	AB	2466	C
2	AB	2472	G
2	AB	2475	C
2	AB	2476	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	2478	A
2	AB	2491	U
2	AB	2501	C
2	AB	2502	G
2	AB	2504	PSU
2	AB	2506	U
2	AB	2507	C
2	AB	2530	A
2	AB	2543	G
2	AB	2566	A
2	AB	2567	G
2	AB	2573	C
2	AB	2574	G
2	AB	2578	G
2	AB	2586	U
2	AB	2599	G
2	AB	2610	C
2	AB	2613	U
2	AB	2615	U
2	AB	2629	U
2	AB	2630	G
2	AB	2639	A
2	AB	2655	G
2	AB	2685	G
2	AB	2689	U
2	AB	2690	U
2	AB	2699	C
2	AB	2700	A
2	AB	2714	G
2	AB	2726	A
2	AB	2732	G
2	AB	2733	A
2	AB	2751	G
2	AB	2752	C
2	AB	2756	U
2	AB	2765	A
2	AB	2766	A
2	AB	2778	A
2	AB	2780	G
2	AB	2791	G
2	AB	2792	A
2	AB	2799	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	2815	C
2	AB	2820	A
2	AB	2833	U
2	AB	2848	G
2	AB	2850	A
2	AB	2861	U
2	AB	2867	G
2	AB	2873	A
2	AB	2880	C
2	AB	2883	A
2	AB	2884	U
2	AB	2894	G
2	AB	2895	G
2	AB	2904	U
34	BA	9	G
34	BA	31	G
34	BA	32	A
34	BA	39	G
34	BA	40	C
34	BA	48	C
34	BA	49	U
34	BA	51	A
34	BA	60	A
34	BA	61	G
34	BA	66	A
34	BA	83	C
34	BA	86	G
34	BA	87	C
34	BA	88	U
34	BA	95	C
34	BA	109	A
34	BA	121	U
34	BA	130	A
34	BA	131	A
34	BA	164	G
34	BA	183	C
34	BA	184	G
34	BA	188	C
34	BA	247	G
34	BA	266	G
34	BA	275	G
34	BA	281	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	BA	289	G
34	BA	293	G
34	BA	306	A
34	BA	328	C
34	BA	329	A
34	BA	331	G
34	BA	352	C
34	BA	353	A
34	BA	354	G
34	BA	366	A
34	BA	367	U
34	BA	368	U
34	BA	369	G
34	BA	370	C
34	BA	381	C
34	BA	388	G
34	BA	393	A
34	BA	397	A
34	BA	398	U
34	BA	406	G
34	BA	413	G
34	BA	414	A
34	BA	416	G
34	BA	424	G
34	BA	429	U
34	BA	439	U
34	BA	465	A
34	BA	466	A
34	BA	468	A
34	BA	478	A
34	BA	482	A
34	BA	484	G
34	BA	486	U
34	BA	495	A
34	BA	511	C
34	BA	512	U
34	BA	518	C
34	BA	521	G
34	BA	524	G
34	BA	525	C
34	BA	527	7MG
34	BA	531	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	BA	532	A
34	BA	547	A
34	BA	559	A
34	BA	564	C
34	BA	566	G
34	BA	570	G
34	BA	572	A
34	BA	573	A
34	BA	576	C
34	BA	632	U
34	BA	653	U
34	BA	665	A
34	BA	687	A
34	BA	690	G
34	BA	691	G
34	BA	694	A
34	BA	695	A
34	BA	700	G
34	BA	724	G
34	BA	734	G
34	BA	746	A
34	BA	749	A
34	BA	755	G
34	BA	793	U
34	BA	794	A
34	BA	796	C
34	BA	811	C
34	BA	815	A
34	BA	817	C
34	BA	818	G
34	BA	819	A
34	BA	820	U
34	BA	821	G
34	BA	827	U
34	BA	828	U
34	BA	841	C
34	BA	843	U
34	BA	846	G
34	BA	864	A
34	BA	867	G
34	BA	872	A
34	BA	884	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	BA	885	G
34	BA	889	A
34	BA	890	G
34	BA	899	C
34	BA	922	G
34	BA	934	C
34	BA	935	A
34	BA	941	G
34	BA	949	A
34	BA	960	U
34	BA	961	U
34	BA	966	2MG
34	BA	968	A
34	BA	969	A
34	BA	975	A
34	BA	993	G
34	BA	1004	A
34	BA	1041	G
34	BA	1064	G
34	BA	1065	U
34	BA	1066	C
34	BA	1085	U
34	BA	1094	G
34	BA	1101	A
34	BA	1129	C
34	BA	1130	A
34	BA	1138	G
34	BA	1139	G
34	BA	1152	A
34	BA	1159	U
34	BA	1189	U
34	BA	1190	G
34	BA	1196	A
34	BA	1202	U
34	BA	1212	U
34	BA	1213	A
34	BA	1214	C
34	BA	1225	A
34	BA	1226	C
34	BA	1227	A
34	BA	1241	G
34	BA	1250	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	BA	1256	A
34	BA	1278	G
34	BA	1279	G
34	BA	1280	A
34	BA	1285	A
34	BA	1298	U
34	BA	1299	A
34	BA	1300	G
34	BA	1301	U
34	BA	1303	C
34	BA	1317	C
34	BA	1320	C
34	BA	1322	C
34	BA	1338	G
34	BA	1340	A
34	BA	1341	U
34	BA	1343	G
34	BA	1346	A
34	BA	1359	C
34	BA	1360	A
34	BA	1379	G
34	BA	1381	U
34	BA	1382	C
34	BA	1397	C
34	BA	1399	C
34	BA	1432	G
34	BA	1447	A
34	BA	1494	G
34	BA	1505	G
34	BA	1506	U
34	BA	1517	G
34	BA	1529	G
34	BA	1530	G
34	BA	1534	A
34	BA	1535	C
34	BA	1537	U
34	BA	1539	C
34	BA	1542	A
35	BB	7	A
35	BB	8	4SU
35	BB	10	G
35	BB	16	H2U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	BB	18	G
35	BB	19	G
35	BB	20	H2U
35	BB	46	7MG
35	BB	48	C
35	BB	49	C
35	BB	59	U
35	BB	60	U
37	BD	25	U
37	BD	26	U
37	BD	36	U
37	BD	40	G
35	BE	10	G
35	BE	16	H2U
35	BE	17	C
35	BE	18	G
35	BE	20	H2U
35	BE	56	C
35	BE	57	G
35	BE	58	A
35	BE	73	A
35	BE	74	C
35	BE	75	C
35	BE	76	A

All (223) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	15	A
1	AA	77	U
1	AA	109	A
2	AB	13	A
2	AB	72	U
2	AB	75	G
2	AB	125	A
2	AB	164	C
2	AB	194	G
2	AB	196	A
2	AB	221	A
2	AB	222	A
2	AB	227	A
2	AB	277	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	331	C
2	AB	332	A
2	AB	345	A
2	AB	372	G
2	AB	380	G
2	AB	448	U
2	AB	479	A
2	AB	503	A
2	AB	504	A
2	AB	529	A
2	AB	532	A
2	AB	545	U
2	AB	586	A
2	AB	615	U
2	AB	669	G
2	AB	671	C
2	AB	673	C
2	AB	720	U
2	AB	729	G
2	AB	736	C
2	AB	743	A
2	AB	786	C
2	AB	790	U
2	AB	791	C
2	AB	805	G
2	AB	810	U
2	AB	827	U
2	AB	979	A
2	AB	995	C
2	AB	1032	A
2	AB	1033	U
2	AB	1045	C
2	AB	1046	A
2	AB	1068	G
2	AB	1069	A
2	AB	1084	A
2	AB	1087	G
2	AB	1109	C
2	AB	1112	G
2	AB	1128	G
2	AB	1132	U
2	AB	1133	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	1134	A
2	AB	1142	A
2	AB	1185	G
2	AB	1210	G
2	AB	1241	A
2	AB	1248	G
2	AB	1254	A
2	AB	1262	A
2	AB	1286	A
2	AB	1288	G
2	AB	1305	C
2	AB	1365	A
2	AB	1383	A
2	AB	1390	U
2	AB	1407	G
2	AB	1420	A
2	AB	1451	C
2	AB	1458	U
2	AB	1508	A
2	AB	1552	A
2	AB	1602	U
2	AB	1608	A
2	AB	1614	A
2	AB	1616	A
2	AB	1646	C
2	AB	1647	U
2	AB	1649	G
2	AB	1674	G
2	AB	1714	U
2	AB	1732	C
2	AB	1761	C
2	AB	1816	C
2	AB	1839	G
2	AB	1847	A
2	AB	1870	C
2	AB	1887	C
2	AB	1900	A
2	AB	1930	G
2	AB	1952	A
2	AB	1955	U
2	AB	1969	A
2	AB	2020	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	AB	2021	C
2	AB	2119	A
2	AB	2130	U
2	AB	2172	U
2	AB	2309	A
2	AB	2339	C
2	AB	2357	G
2	AB	2380	C
2	AB	2389	G
2	AB	2390	U
2	AB	2391	G
2	AB	2448	A
2	AB	2465	C
2	AB	2500	U
2	AB	2542	A
2	AB	2581	G
2	AB	2584	U
2	AB	2602	A
2	AB	2619	C
2	AB	2654	A
2	AB	2655	G
2	AB	2662	A
2	AB	2667	C
2	AB	2696	U
2	AB	2717	C
2	AB	2726	A
2	AB	2732	G
2	AB	2744	G
2	AB	2751	G
2	AB	2791	G
2	AB	2838	G
2	AB	2866	U
2	AB	2870	C
2	AB	2872	A
2	AB	2894	G
34	BA	31	G
34	BA	52	C
34	BA	56	U
34	BA	59	A
34	BA	60	A
34	BA	65	A
34	BA	70	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	BA	85	U
34	BA	86	G
34	BA	100	G
34	BA	193	C
34	BA	194	C
34	BA	209	U
34	BA	318	G
34	BA	365	U
34	BA	367	U
34	BA	368	U
34	BA	369	G
34	BA	385	C
34	BA	403	C
34	BA	415	A
34	BA	425	G
34	BA	438	U
34	BA	451	A
34	BA	465	A
34	BA	484	G
34	BA	489	C
34	BA	494	G
34	BA	524	G
34	BA	531	U
34	BA	570	G
34	BA	620	C
34	BA	641	U
34	BA	674	G
34	BA	690	G
34	BA	694	A
34	BA	753	A
34	BA	785	G
34	BA	793	U
34	BA	794	A
34	BA	815	A
34	BA	817	C
34	BA	824	G
34	BA	843	U
34	BA	884	U
34	BA	889	A
34	BA	899	C
34	BA	934	C
34	BA	968	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	BA	975	A
34	BA	1065	U
34	BA	1104	G
34	BA	1112	C
34	BA	1124	G
34	BA	1129	C
34	BA	1131	G
34	BA	1212	U
34	BA	1213	A
34	BA	1227	A
34	BA	1257	A
34	BA	1278	G
34	BA	1279	G
34	BA	1280	A
34	BA	1298	U
34	BA	1299	A
34	BA	1300	G
34	BA	1302	C
34	BA	1312	G
34	BA	1323	G
34	BA	1340	A
34	BA	1347	G
34	BA	1377	A
34	BA	1399	C
34	BA	1441	A
34	BA	1529	G
34	BA	1534	A
34	BA	1536	C
35	BB	9	A
35	BB	45	U
37	BD	24	A
37	BD	25	U
37	BD	29	G
37	BD	42	U
37	BD	45	G
35	BE	3	C
35	BE	9	A
35	BE	18	G
35	BE	20	H2U
35	BE	56	C
35	BE	73	A

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

55 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
2	6MZ	AB	1618	2	17,25,26	0.92	1 (5%)	15,36,39	1.44	2 (13%)
2	2MG	AB	1835	2	18,26,27	1.32	1 (5%)	21,38,41	2.47	5 (23%)
2	PSU	AB	1911	2	15,21,22	1.32	1 (6%)	16,30,33	3.53	2 (12%)
2	3TD	AB	1915	2	15,22,23	0.97	0	17,32,35	1.42	3 (17%)
2	PSU	AB	1917	2	15,21,22	1.35	1 (6%)	16,30,33	3.57	3 (18%)
2	5MU	AB	1939	2	13,22,23	1.22	1 (7%)	16,32,35	4.86	4 (25%)
2	5MC	AB	1962	2	14,22,23	0.97	1 (7%)	17,32,35	1.17	3 (17%)
2	6MZ	AB	2030	2	17,25,26	0.91	1 (5%)	15,36,39	1.65	5 (33%)
2	7MG	AB	2069	2	20,26,27	2.22	3 (15%)	23,39,42	2.23	2 (8%)
2	OMG	AB	2251	2	18,26,27	1.25	2 (11%)	21,38,41	2.69	4 (19%)
2	2MG	AB	2445	2	18,26,27	1.29	2 (11%)	21,38,41	2.48	6 (28%)
2	H2U	AB	2449	2	17,21,22	0.84	1 (5%)	23,30,33	0.93	1 (4%)
2	PSU	AB	2457	2	15,21,22	1.32	1 (6%)	16,30,33	3.69	6 (37%)
2	OMC	AB	2498	2	15,22,23	0.83	0	20,31,34	1.06	2 (10%)
2	2MA	AB	2503	2	17,25,26	1.02	2 (11%)	18,37,40	1.80	1 (5%)
2	PSU	AB	2504	2	15,21,22	1.44	3 (20%)	16,30,33	3.57	5 (31%)
2	OMU	AB	2552	2	14,22,23	1.23	1 (7%)	19,31,34	2.84	4 (21%)
2	CH	AB	2575	2	14,21,22	0.97	1 (7%)	18,30,33	1.12	2 (11%)
2	PSU	AB	2580	2	15,21,22	1.34	1 (6%)	16,30,33	3.50	3 (18%)
2	PSU	AB	2605	2	15,21,22	1.29	1 (6%)	16,30,33	3.66	4 (25%)
2	1MG	AB	745	2	17,26,27	0.97	1 (5%)	19,39,42	1.85	4 (21%)
2	PSU	AB	746	2	15,21,22	1.36	2 (13%)	16,30,33	3.63	5 (31%)
2	5MU	AB	747	2	13,22,23	1.20	1 (7%)	16,32,35	4.79	5 (31%)
2	PSU	AB	955	2	15,21,22	1.25	1 (6%)	16,30,33	3.63	4 (25%)
34	2MG	BA	1207	34	18,26,27	1.29	2 (11%)	21,38,41	2.59	3 (14%)
34	4OC	BA	1402	34	15,23,24	1.01	1 (6%)	21,32,35	1.60	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	5MC	BA	1407	34	14,22,23	0.96	1 (7%)	17,32,35	1.00	1 (5%)
34	UR3	BA	1498	34	13,22,23	0.93	0	18,32,35	1.21	2 (11%)
34	2MG	BA	1516	34	18,26,27	1.22	2 (11%)	21,38,41	2.77	5 (23%)
34	MA6	BA	1518	34	18,26,27	0.94	1 (5%)	15,38,41	1.32	1 (6%)
34	MA6	BA	1519	34	18,26,27	0.87	1 (5%)	15,38,41	1.92	5 (33%)
34	PSU	BA	516	34	15,21,22	1.28	1 (6%)	16,30,33	3.49	5 (31%)
34	7MG	BA	527	34	20,26,27	2.22	3 (15%)	23,39,42	2.42	3 (13%)
34	2MG	BA	966	34	18,26,27	1.26	2 (11%)	21,38,41	3.00	9 (42%)
34	5MC	BA	967	34	14,22,23	0.94	1 (7%)	17,32,35	0.79	0
35	H2U	BB	16	35	17,21,22	0.78	0	23,30,33	1.21	2 (8%)
35	H2U	BB	20	35	17,21,22	0.79	0	23,30,33	1.12	1 (4%)
35	PSU	BB	32	35	15,21,22	1.30	1 (6%)	16,30,33	3.53	4 (25%)
35	MIA	BB	37	35	22,31,32	1.08	4 (18%)	26,44,47	1.80	5 (19%)
35	PSU	BB	39	35	15,21,22	1.23	1 (6%)	16,30,33	3.64	5 (31%)
35	7MG	BB	46	35	20,26,27	2.23	3 (15%)	23,39,42	2.51	3 (13%)
35	3AU	BB	47	-	16,28,29	0.87	0	16,40,43	1.00	1 (6%)
35	5MU	BB	54	35	13,22,23	1.20	1 (7%)	16,32,35	4.68	3 (18%)
35	PSU	BB	55	35	15,21,22	1.28	2 (13%)	16,30,33	3.51	4 (25%)
35	4SU	BB	8	35	12,21,22	1.01	1 (8%)	15,30,33	1.71	1 (6%)
35	H2U	BE	16	35	17,21,22	0.79	0	23,30,33	1.03	2 (8%)
35	H2U	BE	20	35	17,21,22	0.77	0	23,30,33	1.36	4 (17%)
35	PSU	BE	32	35	15,21,22	1.29	1 (6%)	16,30,33	3.49	3 (18%)
35	MIA	BE	37	35	22,31,32	1.08	4 (18%)	26,44,47	1.68	6 (23%)
35	PSU	BE	39	35	15,21,22	1.30	1 (6%)	16,30,33	3.54	3 (18%)
35	7MG	BE	46	35	20,26,27	2.24	3 (15%)	23,39,42	2.30	2 (8%)
35	3AU	BE	47	-	16,28,29	0.90	0	16,40,43	2.06	4 (25%)
35	5MU	BE	54	35	13,22,23	1.24	1 (7%)	16,32,35	4.82	3 (18%)
35	PSU	BE	55	35	15,21,22	1.35	1 (6%)	16,30,33	3.44	3 (18%)
35	4SU	BE	8	35	12,21,22	0.94	0	15,30,33	2.20	5 (33%)

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
2	6MZ	AB	1618	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	1835	2	-	0/5/27/28	0/3/3/3
2	PSU	AB	1911	2	-	0/7/25/26	0/2/2/2
2	3TD	AB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	1917	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	1939	2	-	0/3/25/26	0/2/2/2
2	5MC	AB	1962	2	-	0/3/25/26	0/2/2/2
2	6MZ	AB	2030	2	-	0/5/27/28	0/3/3/3
2	7MG	AB	2069	2	-	0/7/37/38	0/3/3/3
2	OMG	AB	2251	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	2445	2	-	0/5/27/28	0/3/3/3
2	H2U	AB	2449	2	-	0/7/38/39	0/2/2/2
2	PSU	AB	2457	2	-	0/7/25/26	0/2/2/2
2	OMC	AB	2498	2	-	0/5/27/28	0/2/2/2
2	2MA	AB	2503	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2504	2	-	0/7/25/26	0/2/2/2
2	OMU	AB	2552	2	-	0/5/27/28	0/2/2/2
2	CH	AB	2575	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	2580	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	2605	2	-	0/7/25/26	0/2/2/2
2	1MG	AB	745	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	746	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	747	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	955	2	-	0/7/25/26	0/2/2/2
34	2MG	BA	1207	34	-	0/5/27/28	0/3/3/3
34	4OC	BA	1402	34	-	0/7/29/30	0/2/2/2
34	5MC	BA	1407	34	-	0/3/25/26	0/2/2/2
34	UR3	BA	1498	34	-	0/3/25/26	0/2/2/2
34	2MG	BA	1516	34	-	0/5/27/28	0/3/3/3
34	MA6	BA	1518	34	-	0/7/29/30	0/3/3/3
34	MA6	BA	1519	34	-	0/7/29/30	0/3/3/3
34	PSU	BA	516	34	-	0/7/25/26	0/2/2/2
34	7MG	BA	527	34	-	0/7/37/38	0/3/3/3
34	2MG	BA	966	34	-	0/5/27/28	0/3/3/3
34	5MC	BA	967	34	-	0/3/25/26	0/2/2/2
35	H2U	BB	16	35	-	0/7/38/39	0/2/2/2
35	H2U	BB	20	35	-	0/7/38/39	0/2/2/2
35	PSU	BB	32	35	-	0/7/25/26	0/2/2/2
35	MIA	BB	37	35	-	0/11/33/34	0/3/3/3
35	PSU	BB	39	35	-	0/7/25/26	0/2/2/2
35	7MG	BB	46	35	-	0/7/37/38	0/3/3/3
35	3AU	BB	47	-	-	0/8/34/35	0/2/2/2
35	5MU	BB	54	35	-	0/3/25/26	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	BB	55	35	-	0/7/25/26	0/2/2/2
35	4SU	BB	8	35	-	0/3/25/26	0/2/2/2
35	H2U	BE	16	35	-	0/7/38/39	0/2/2/2
35	H2U	BE	20	35	-	0/7/38/39	0/2/2/2
35	PSU	BE	32	35	-	0/7/25/26	0/2/2/2
35	MIA	BE	37	35	-	0/11/33/34	0/3/3/3
35	PSU	BE	39	35	-	0/7/25/26	0/2/2/2
35	7MG	BE	46	35	-	0/7/37/38	0/3/3/3
35	3AU	BE	47	-	-	0/8/34/35	0/2/2/2
35	5MU	BE	54	35	-	0/3/25/26	0/2/2/2
35	PSU	BE	55	35	-	0/7/25/26	0/2/2/2
35	4SU	BE	8	35	-	0/3/25/26	0/2/2/2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	46	7MG	C8-N9	-7.95	1.33	1.45
2	AB	2069	7MG	C8-N9	-7.91	1.34	1.45
35	BE	46	7MG	C8-N9	-7.89	1.34	1.45
34	BA	527	7MG	C8-N9	-7.84	1.34	1.45
2	AB	2069	7MG	C8-N7	-2.79	1.30	1.43
35	BB	46	7MG	C8-N7	-2.74	1.30	1.43
34	BA	527	7MG	C8-N7	-2.72	1.31	1.43
35	BE	46	7MG	C8-N7	-2.65	1.31	1.43
2	AB	2504	PSU	O4'-C1'	-2.44	1.40	1.44
34	BA	1518	MA6	C8-N7	-2.35	1.30	1.34
2	AB	2030	6MZ	C8-N7	-2.33	1.30	1.34
2	AB	745	1MG	C8-N7	-2.22	1.30	1.34
34	BA	1519	MA6	C8-N7	-2.14	1.30	1.34
34	BA	1207	2MG	C8-N7	-2.13	1.30	1.34
2	AB	1618	6MZ	C8-N7	-2.12	1.30	1.34
2	AB	2445	2MG	C8-N7	-2.12	1.30	1.34
34	BA	1516	2MG	C8-N7	-2.10	1.30	1.34
35	BB	37	MIA	C8-N7	-2.08	1.30	1.34
35	BE	37	MIA	C8-N7	-2.07	1.30	1.34
34	BA	966	2MG	C8-N7	-2.05	1.30	1.34
2	AB	2251	OMG	C8-N7	-2.05	1.30	1.34
35	BE	37	MIA	C13-C14	-2.05	1.36	1.51
2	AB	2503	2MA	C8-N7	-2.03	1.30	1.34
35	BB	37	MIA	C13-C14	-2.03	1.36	1.51
2	AB	2449	H2U	C4-N3	-2.02	1.34	1.37
2	AB	2504	PSU	C6-N1	2.01	1.38	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	37	MIA	C6-N1	2.01	1.35	1.33
2	AB	746	PSU	C6-N1	2.02	1.38	1.34
35	BB	55	PSU	C6-N1	2.05	1.38	1.34
35	BE	37	MIA	C6-N1	2.09	1.35	1.33
34	BA	1407	5MC	C5-C4	2.12	1.44	1.41
2	AB	2575	CH	C6-N1	2.15	1.38	1.35
34	BA	967	5MC	C5-C4	2.17	1.44	1.41
35	BB	8	4SU	C6-N1	2.21	1.38	1.35
34	BA	1402	4OC	C5-C4	2.25	1.44	1.39
2	AB	1962	5MC	C5-C4	2.39	1.45	1.41
35	BB	37	MIA	C2-S10	2.43	1.77	1.75
35	BE	37	MIA	C2-S10	2.58	1.77	1.75
2	AB	2503	2MA	C6-N6	2.63	1.33	1.29
2	AB	747	5MU	C4-N3	3.28	1.38	1.33
2	AB	1939	5MU	C4-N3	3.42	1.39	1.33
2	AB	2552	OMU	C4-N3	3.49	1.39	1.33
35	BE	54	5MU	C4-N3	3.49	1.39	1.33
34	BA	516	PSU	C4-N3	3.51	1.39	1.33
35	BB	39	PSU	C4-N3	3.51	1.39	1.33
35	BB	54	5MU	C4-N3	3.54	1.39	1.33
2	AB	2457	PSU	C4-N3	3.54	1.39	1.33
35	BB	55	PSU	C4-N3	3.58	1.39	1.33
2	AB	746	PSU	C4-N3	3.60	1.39	1.33
2	AB	955	PSU	C4-N3	3.61	1.39	1.33
2	AB	2580	PSU	C4-N3	3.64	1.39	1.33
2	AB	1911	PSU	C4-N3	3.67	1.39	1.33
2	AB	2605	PSU	C4-N3	3.69	1.39	1.33
35	BE	55	PSU	C4-N3	3.69	1.39	1.33
35	BE	39	PSU	C4-N3	3.70	1.39	1.33
35	BB	46	7MG	C6-N1	3.71	1.39	1.33
35	BE	32	PSU	C4-N3	3.72	1.39	1.33
34	BA	1516	2MG	C6-N1	3.73	1.39	1.33
2	AB	2069	7MG	C6-N1	3.75	1.39	1.33
2	AB	1917	PSU	C4-N3	3.75	1.39	1.33
2	AB	2504	PSU	C4-N3	3.77	1.39	1.33
34	BA	527	7MG	C6-N1	3.78	1.39	1.33
34	BA	966	2MG	C6-N1	3.79	1.39	1.33
35	BB	32	PSU	C4-N3	3.81	1.39	1.33
2	AB	2251	OMG	C6-N1	3.82	1.39	1.33
34	BA	1207	2MG	C6-N1	3.87	1.40	1.33
35	BE	46	7MG	C6-N1	3.89	1.40	1.33
2	AB	2445	2MG	C6-N1	4.03	1.40	1.33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	1835	2MG	C6-N1	4.19	1.40	1.33

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	54	5MU	C5-C4-N3	-13.38	114.12	125.35
2	AB	1939	5MU	C5-C4-N3	-13.30	114.19	125.35
2	AB	747	5MU	C5-C4-N3	-13.28	114.20	125.35
35	BB	54	5MU	C5-C4-N3	-13.25	114.23	125.35
34	BA	1516	2MG	C5-C6-N1	-8.68	112.17	123.52
2	AB	2251	OMG	C5-C6-N1	-8.47	112.45	123.52
34	BA	966	2MG	C5-C6-N1	-8.45	112.47	123.52
34	BA	1207	2MG	C5-C6-N1	-8.20	112.80	123.52
2	AB	2445	2MG	C5-C6-N1	-7.97	113.10	123.52
2	AB	1835	2MG	C5-C6-N1	-7.93	113.16	123.52
35	BB	46	7MG	C5-C6-N1	-7.73	111.88	123.39
34	BA	527	7MG	C5-C6-N1	-7.48	112.26	123.39
35	BE	46	7MG	C5-C6-N1	-7.41	112.36	123.39
2	AB	2069	7MG	C5-C6-N1	-7.25	112.60	123.39
2	AB	2503	2MA	C2-N3-C4	-6.23	112.28	115.29
35	BE	8	4SU	C5-C4-N3	-6.07	117.13	123.56
35	BE	47	3AU	C4'-O4'-C1'	-5.86	103.44	109.64
35	BB	8	4SU	C5-C4-N3	-5.65	117.57	123.56
2	AB	745	1MG	C5-C6-N1	-4.85	112.00	118.35
2	AB	2605	PSU	C5-C1'-C2'	-3.94	108.74	115.44
2	AB	955	PSU	C5-C1'-C2'	-3.79	109.01	115.44
34	BA	966	2MG	C4'-O4'-C1'	-3.61	105.82	109.64
2	AB	2552	OMU	C5-C4-N3	-3.61	114.43	123.28
2	AB	2457	PSU	C5-C1'-C2'	-3.58	109.35	115.44
34	BA	1519	MA6	C4'-O4'-C1'	-3.45	105.98	109.64
2	AB	2457	PSU	C5-C6-N1	-3.43	119.60	124.38
2	AB	2580	PSU	C5-C6-N1	-3.33	119.73	124.38
2	AB	746	PSU	C5-C6-N1	-3.32	119.75	124.38
34	BA	516	PSU	C5-C6-N1	-3.32	119.75	124.38
35	BB	55	PSU	C5-C6-N1	-3.18	119.94	124.38
2	AB	955	PSU	C5-C6-N1	-3.14	120.00	124.38
35	BB	32	PSU	C5-C6-N1	-3.13	120.01	124.38
35	BE	32	PSU	C5-C6-N1	-3.12	120.03	124.38
34	BA	1516	2MG	C1'-N9-C4	-3.11	123.33	126.81
2	AB	2251	OMG	N3-C2-N1	-3.11	123.33	127.56
34	BA	1519	MA6	C1'-N9-C4	-3.10	123.34	126.81
2	AB	2504	PSU	C5-C6-N1	-3.09	120.08	124.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1915	3TD	C5-C1'-C2'	-3.03	110.28	115.44
2	AB	1915	3TD	C5-C4-N3	-3.01	116.20	118.65
35	BE	55	PSU	C5-C6-N1	-3.01	120.19	124.38
35	BE	39	PSU	C5-C6-N1	-2.98	120.22	124.38
35	BE	37	MIA	C1'-N9-C4	-2.86	123.61	126.81
2	AB	1915	3TD	C5-C6-N1	-2.85	120.40	124.38
35	BB	39	PSU	C5-C6-N1	-2.83	120.43	124.38
35	BB	32	PSU	C5-C1'-C2'	-2.80	110.68	115.44
35	BE	20	H2U	C6-N1-C2	-2.68	118.02	122.16
2	AB	2030	6MZ	C2'-C3'-C4'	-2.68	97.16	102.64
2	AB	2575	CH	C4'-O4'-C1'	-2.63	106.85	109.64
2	AB	2605	PSU	C5-C6-N1	-2.57	120.80	124.38
2	AB	745	1MG	C1'-N9-C4	-2.51	124.00	126.81
2	AB	1835	2MG	C1'-N9-C4	-2.51	124.00	126.81
35	BB	16	H2U	O3'-C3'-C4'	-2.51	103.52	111.01
2	AB	1911	PSU	C5-C6-N1	-2.49	120.90	124.38
34	BA	966	2MG	C2'-C3'-C4'	-2.49	97.53	102.64
34	BA	1519	MA6	C2'-C1'-N9	-2.48	106.82	113.47
34	BA	1516	2MG	N3-C2-N1	-2.46	122.51	126.19
35	BB	37	MIA	C5-C6-N1	-2.42	118.13	120.58
35	BE	54	5MU	C5'-C4'-C3'	-2.41	105.87	115.20
2	AB	1917	PSU	C5-C6-N1	-2.40	121.04	124.38
35	BE	37	MIA	C5-C6-N1	-2.37	118.18	120.58
2	AB	2030	6MZ	O3'-C3'-C4'	-2.32	104.08	111.01
35	BB	55	PSU	C5-C1'-C2'	-2.31	111.50	115.44
35	BE	37	MIA	C2'-C1'-N9	-2.31	107.27	113.47
35	BB	39	PSU	C4-C5-C1'	-2.29	117.37	121.22
35	BB	39	PSU	C5-C1'-C2'	-2.27	111.59	115.44
2	AB	746	PSU	O2'-C2'-C1'	-2.23	107.08	111.93
35	BE	8	4SU	C6-N1-C2	-2.23	117.70	121.33
2	AB	1917	PSU	C4-C5-C1'	-2.22	117.48	121.22
35	BE	16	H2U	C5-C6-N1	-2.21	108.34	110.76
2	AB	2457	PSU	C4-C5-C1'	-2.20	117.51	121.22
34	BA	516	PSU	C5-C1'-C2'	-2.20	111.70	115.44
2	AB	745	1MG	O3'-C3'-C2'	-2.18	104.79	111.86
2	AB	2504	PSU	O2'-C2'-C1'	-2.17	107.20	111.93
35	BE	20	H2U	C5-C6-N1	-2.16	108.40	110.76
2	AB	747	5MU	O4'-C1'-N1	-2.14	104.03	108.10
34	BA	966	2MG	N3-C2-N1	-2.10	123.04	126.19
2	AB	2251	OMG	C1'-N9-C4	-2.09	124.47	126.81
2	AB	1962	5MC	O3'-C3'-C2'	-2.08	105.14	111.86
35	BB	37	MIA	C1'-N9-C4	-2.06	124.51	126.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2030	6MZ	C4'-O4'-C1'	-2.06	107.46	109.64
2	AB	1939	5MU	C4'-O4'-C1'	-2.05	107.47	109.64
35	BB	46	7MG	C2'-C3'-C4'	-2.04	98.45	102.64
2	AB	955	PSU	C4-C5-C1'	-2.04	117.78	121.22
35	BB	16	H2U	C5-C6-N1	-2.04	108.53	110.76
2	AB	2552	OMU	C4'-O4'-C1'	-2.03	107.49	109.64
35	BB	39	PSU	O2'-C2'-C1'	-2.02	107.53	111.93
2	AB	2445	2MG	N3-C2-N1	-2.02	123.17	126.19
34	BA	516	PSU	C4-C5-C1'	-2.02	117.82	121.22
2	AB	2552	OMU	C6-C5-C4	2.02	121.03	117.30
2	AB	2605	PSU	O4'-C1'-C2'	2.02	106.88	104.69
34	BA	1407	5MC	O4'-C1'-N1	2.04	111.99	108.10
2	AB	2449	H2U	C4-N3-C2	2.07	127.64	125.77
2	AB	2498	OMC	C4'-O4'-C1'	2.07	111.84	109.64
35	BE	47	3AU	C6-C5-C4	2.09	121.17	117.30
34	BA	1498	UR3	C6-C5-C4	2.09	121.17	117.30
35	BE	55	PSU	O4'-C1'-C2'	2.09	106.95	104.69
2	AB	2575	CH	O4'-C1'-N1	2.10	112.09	108.10
35	BE	20	H2U	O4'-C4'-C3'	2.12	109.47	105.16
2	AB	2445	2MG	O4'-C1'-N9	2.14	112.16	108.11
35	BE	8	4SU	O4'-C1'-N1	2.14	112.18	108.10
35	BE	20	H2U	C1'-N1-C2	2.16	121.22	118.19
2	AB	747	5MU	O3'-C3'-C2'	2.17	118.86	111.86
35	BE	47	3AU	O4'-C4'-C3'	2.17	109.56	105.16
34	BA	966	2MG	O3'-C3'-C4'	2.17	117.50	111.01
35	BB	54	5MU	O3'-C3'-C2'	2.18	118.92	111.86
35	BB	37	MIA	C2-N1-C6	2.22	119.22	113.13
2	AB	746	PSU	O3'-C3'-C2'	2.23	119.06	111.86
35	BE	37	MIA	C2-N1-C6	2.27	119.37	113.13
35	BE	16	H2U	C1'-N1-C2	2.28	121.39	118.19
35	BB	55	PSU	O4'-C1'-C2'	2.29	107.16	104.69
2	AB	747	5MU	O4'-C4'-C5'	2.29	117.48	109.29
35	BB	37	MIA	C12-N6-C6	2.31	126.13	123.46
2	AB	2504	PSU	O4'-C1'-C2'	2.33	107.21	104.69
35	BB	47	3AU	C6-C5-C4	2.33	121.62	117.30
2	AB	2498	OMC	O4'-C1'-N1	2.35	112.56	108.10
34	BA	966	2MG	O4'-C1'-N9	2.40	112.64	108.11
2	AB	1835	2MG	O3'-C3'-C2'	2.42	119.69	111.86
34	BA	527	7MG	O5'-C5'-C4'	2.42	117.78	109.09
2	AB	1962	5MC	O4'-C1'-N1	2.44	112.73	108.10
2	AB	2457	PSU	C3'-C2'-C1'	2.45	104.62	101.71
2	AB	2030	6MZ	O4'-C1'-N9	2.46	112.75	108.11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	516	PSU	O4'-C1'-C2'	2.46	107.35	104.69
2	AB	2445	2MG	CM2-N2-C2	2.49	125.83	123.03
35	BE	37	MIA	O4'-C1'-N9	2.52	112.87	108.11
2	AB	1618	6MZ	O4'-C1'-N9	2.66	113.13	108.11
35	BB	20	H2U	C1'-N1-C2	2.66	121.92	118.19
35	BE	8	4SU	O3'-C3'-C4'	2.68	119.00	111.01
34	BA	966	2MG	CM2-N2-C2	2.70	126.08	123.03
2	AB	2504	PSU	C3'-C2'-C1'	2.74	104.96	101.71
34	BA	1402	4OC	O4'-C1'-N1	2.75	113.33	108.10
2	AB	1962	5MC	CM5-C5-C4	2.76	124.38	121.47
34	BA	1516	2MG	N2-C2-N3	2.81	120.20	116.94
2	AB	746	PSU	O4'-C1'-C2'	2.84	107.76	104.69
35	BE	39	PSU	O4'-C1'-C2'	2.97	107.90	104.69
35	BE	8	4SU	C5'-C4'-C3'	2.97	126.70	115.20
34	BA	1519	MA6	O3'-C3'-C2'	2.98	121.47	111.86
35	BE	32	PSU	O4'-C1'-C2'	3.11	108.05	104.69
35	BB	32	PSU	O4'-C1'-C2'	3.14	108.08	104.69
2	AB	1835	2MG	N2-C2-N3	3.17	120.62	116.94
34	BA	1498	UR3	O4'-C1'-N1	3.17	114.13	108.10
34	BA	1402	4OC	CM4-N4-C4	3.18	125.55	122.87
2	AB	2030	6MZ	C2-N1-C6	3.39	118.91	116.47
2	AB	2445	2MG	N2-C2-N3	3.39	120.88	116.94
2	AB	1939	5MU	O4'-C1'-N1	3.41	114.58	108.10
2	AB	2457	PSU	O4'-C1'-C2'	3.49	108.46	104.69
34	BA	1518	MA6	C2-N1-C6	3.56	120.04	111.64
34	BA	1519	MA6	C2-N1-C6	3.67	120.31	111.64
34	BA	1207	2MG	N2-C2-N3	3.70	121.24	116.94
2	AB	1618	6MZ	C2-N1-C6	3.71	119.14	116.47
2	AB	745	1MG	O4'-C1'-N9	3.90	115.48	108.11
2	AB	2580	PSU	O4'-C1'-C2'	4.13	109.16	104.69
35	BE	47	3AU	O4'-C1'-N1	4.21	116.10	108.10
34	BA	966	2MG	N2-C2-N3	4.59	122.27	116.94
34	BA	1402	4OC	C2-N3-C4	4.98	121.76	115.43
35	BE	37	MIA	C11-S10-C2	5.01	105.84	102.31
2	AB	1835	2MG	C6-N1-C2	5.56	123.20	115.24
2	AB	2445	2MG	C6-N1-C2	5.58	123.23	115.24
34	BA	1207	2MG	C6-N1-C2	5.82	123.58	115.24
35	BB	37	MIA	C11-S10-C2	6.27	106.73	102.31
34	BA	966	2MG	C6-N1-C2	6.36	124.35	115.24
2	AB	2069	7MG	C6-N1-C2	6.60	123.62	115.88
34	BA	1516	2MG	C6-N1-C2	6.68	124.81	115.24
35	BE	46	7MG	C6-N1-C2	6.75	123.79	115.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2251	OMG	C6-N1-C2	7.14	124.24	115.88
34	BA	527	7MG	C6-N1-C2	7.18	124.29	115.88
35	BB	46	7MG	C6-N1-C2	7.70	124.90	115.88
2	AB	2552	OMU	C4-N3-C2	10.77	125.56	114.21
2	AB	2580	PSU	C4-N3-C2	12.40	125.50	115.16
35	BB	54	5MU	C4-N3-C2	12.65	125.71	115.16
2	AB	2457	PSU	C4-N3-C2	12.73	125.78	115.16
34	BA	516	PSU	C4-N3-C2	12.74	125.79	115.16
35	BB	32	PSU	C4-N3-C2	12.82	125.86	115.16
35	BE	32	PSU	C4-N3-C2	12.84	125.88	115.16
35	BE	55	PSU	C4-N3-C2	12.90	125.92	115.16
35	BB	55	PSU	C4-N3-C2	12.90	125.92	115.16
2	AB	747	5MU	C4-N3-C2	12.93	125.94	115.16
2	AB	2504	PSU	C4-N3-C2	12.99	126.00	115.16
2	AB	746	PSU	C4-N3-C2	12.99	126.00	115.16
2	AB	955	PSU	C4-N3-C2	13.05	126.05	115.16
35	BE	39	PSU	C4-N3-C2	13.09	126.08	115.16
2	AB	2605	PSU	C4-N3-C2	13.31	126.26	115.16
2	AB	1939	5MU	C4-N3-C2	13.32	126.27	115.16
35	BE	54	5MU	C4-N3-C2	13.37	126.31	115.16
2	AB	1911	PSU	C4-N3-C2	13.49	126.41	115.16
2	AB	1917	PSU	C4-N3-C2	13.52	126.44	115.16
35	BB	39	PSU	C4-N3-C2	13.57	126.48	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.