



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:09 PM BST

PDB ID : 4V6L
EMDB ID: : EMD-1850
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 : 13.20 Å (reported)
Based on PDB ID : 3FIH, 2I2U

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

A user guide is available at

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

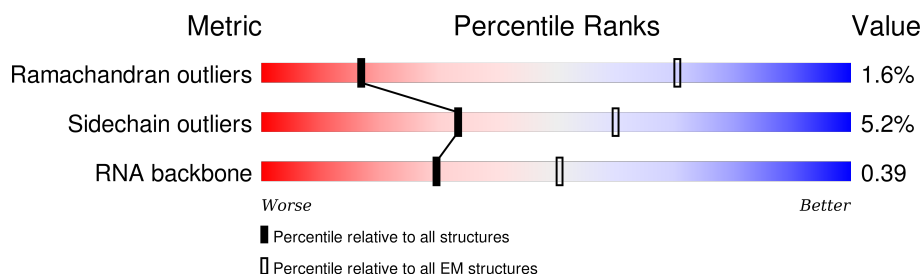
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 13.20 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.








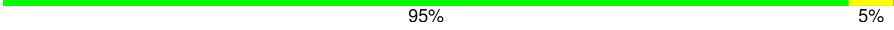

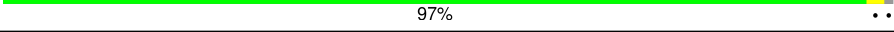


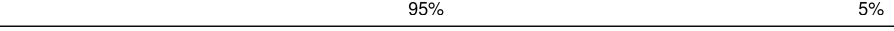
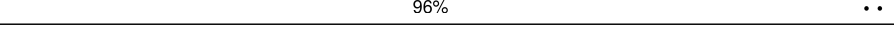

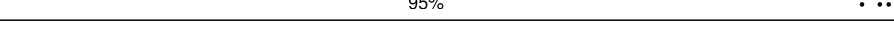
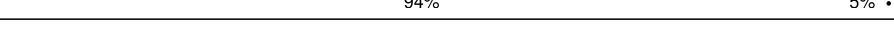



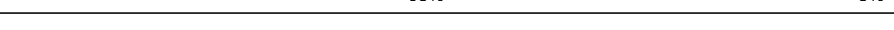
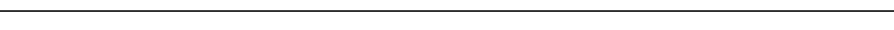

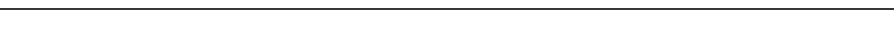
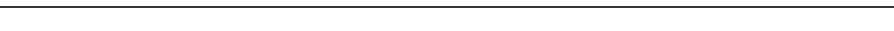


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 ≥ 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	1542	23% 49% 25% .
2	AB	76	29% 45% 25% .
2	AE	76	26% 49% 21% .
3	AC	393	95% 5%
4	AD	24	13% 50% 29% 8%
5	AF	241	94% 5%
6	AG	233	94% 5%
7	AH	206	94% 5%
8	AI	167	93% 6% .

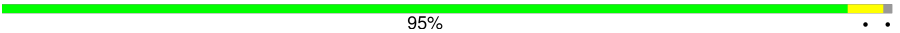
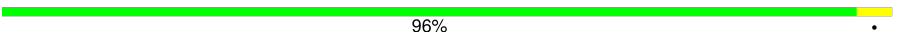








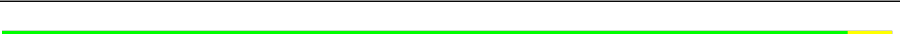


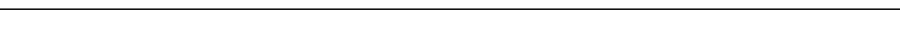
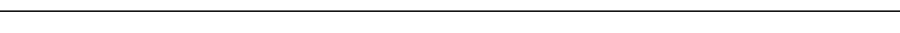
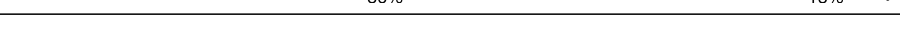

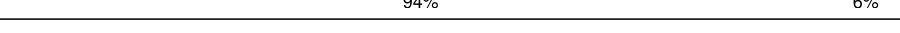
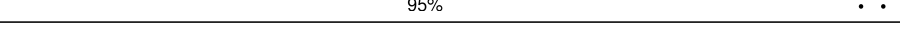
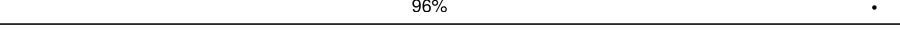

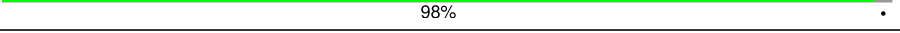
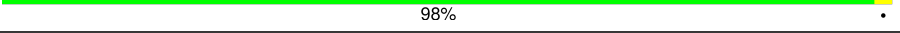

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Mol	Chain	Length	Quality of chain
9	AJ	135	 89% 10% .
10	AK	179	 92% 7% .
11	AL	130	 93% 6% .
12	AM	130	 91% 8% .
13	AN	103	 90% 9% .
14	AO	129	 95% 5% .
15	AP	124	 90% 9% .
16	AQ	118	 97% ..
17	AR	101	 85% 14% .
18	AS	89	 92% 7% .
19	AT	82	 95% 5%
20	AU	84	 96% ..
21	AV	75	 91% 8% .
22	AW	92	 95% ..
23	AX	87	 94% 5% .
24	AY	71	 87% 11% .
25	BA	120	 21% 50% 25% .
26	BB	2904	 21% 49% 26% .
27	BC	234	 95% 5%
28	BD	273	 93% 7%
29	BE	209	 91% 8%
30	BF	201	 93% 6%
31	BG	179	 92% 7% ..
32	BH	177	 91% 8% ..
33	BI	149	 93% 7% .

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Mol	Chain	Length	Quality of chain
34	BJ	142	 95% . .
35	BK	142	 96% .
36	BL	123	 93% 7% .
37	BM	144	 94% 6%
38	BN	136	 93% 7% .
39	BO	127	 94% 6%
40	BP	117	 95% 5%
41	BQ	115	 91% 8% .
42	BR	118	 96% . .
43	BS	103	 91% 8% .
44	BT	110	 95% 5%
45	BU	100	 94% 6%
46	BV	104	 95% . .
47	BW	94	 94% 6%
48	BX	85	 86% 13% .
49	BY	78	 91% 6% . .
50	BZ	63	 94% 6%
51	Ba	59	 95% . .
52	Bb	70	 96% .
53	Bc	57	 91% 7% .
54	Bd	55	 98% .
55	Be	46	 98% .
56	Bf	65	 95% . .
57	Bg	38	 87% 13%

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 16S ribosomal RNA.

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

- Molecule 2 is a RNA chain called A/T-site tRNA Phe.

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

- Molecule 3 is a protein called Elongation factor Tu 2.

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

- Molecule 4 is a RNA chain called mRNA.

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

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

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

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein S21.

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

- Molecule 25 is a RNA chain called 50S ribosomal RNA 5S.

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

- Molecule 26 is a RNA chain called 50S ribosomal RNA 23S.

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

- Molecule 27 is a protein called 50S ribosomal protein L1.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	103	Total	C	N	O		0	0
			789	498	148	143			

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L31.

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

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a protein called 50S ribosomal protein L33.

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

- Molecule 55 is a protein called 50S ribosomal protein L34.

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

- Molecule 56 is a protein called 50S ribosomal protein L35.

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

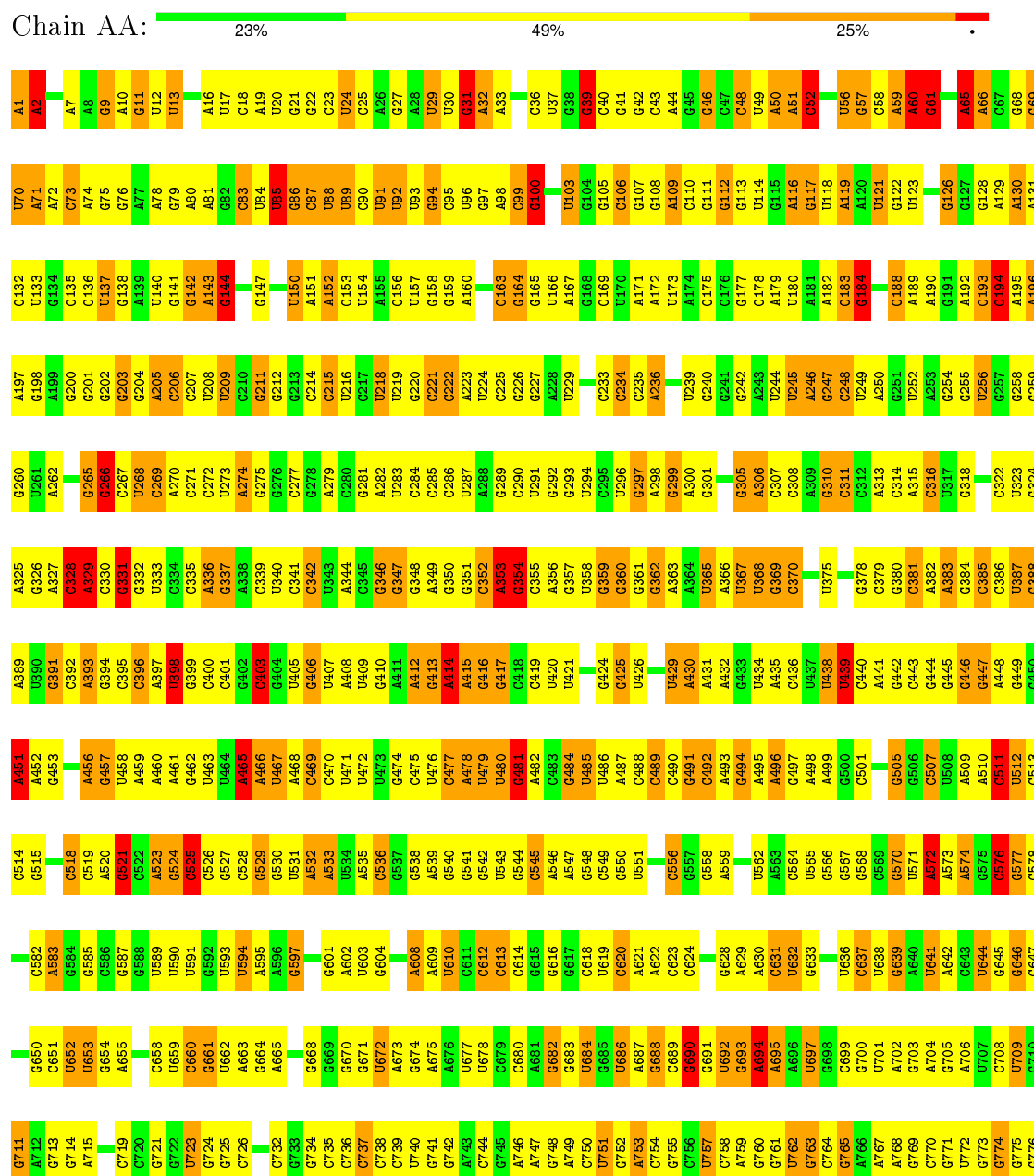
- Molecule 57 is a protein called 50S ribosomal protein L36.

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

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: 16S ribosomal RNA



A1483	G1353	A1285	G1220	A1155	A1092	U1029	G966	A900	G838	A777
C1484	U1354	A1288	G1221	G1156	A1093	U1030	C967	A901	C839	G778
U1485	G1355	A1288	G1222	A1157	G1094	G1031	A968	G902	C840	C779
G1486	G1356	A1289	C1223	G1158	U1095	G1032	A969	G903	C841	A780
G1487	U1357	U1290	U1224	U1159	C1096	G1033	C970	U904	U842	A781
G1488	U1358	U1291	A1225	G1160	C1097	G1034	G971	U905	U843	A782
G1489	C1359	G1292	C1226	C1161	C1098	A1035	G972	A906	G844	C783
U1490	U1360	C1293	C1227	C1162	G1099	C1036	G973	A907	A845	A784
A1491	G1361	U1294	C1228	A1163	C1100	C1037	A974	A908	G846	G785
A1492	A1362	A1363	C1229	G1164	A1101	C1038	A975	A909	G847	G786
G1493	U1364	U1295	C1230	U1165	A1102	G1039	G976	C910	C848	A787
G1494	G1365	U1298	U1231	A1169	C1103	U1040	A977	U911	G849	U788
G1495	C1366	G1300	U1232	A1170	G1104	G1041	A978	G912	U850	U789
G1496	U1367	U1301	G1233	C1172	A1105	A1042	G979	A913	G851	A790
G1497	C1369	U1302	U1234	C1173	C1109	U1043	C980	A914	U854	G791
U1498	G1370	U1235	U1235	A1174	A1110	A1044	U981	A915	U854	A792
A1499	G1371	U1236	C1237	G1175	A1111	C1046	A983	U916	U855	U793
A1500	G1372	G1303	G1241	A1176	C1112	U1047	C984	G917	C856	A794
C1501	U1373	G1305	G1242	G1177	G1113	G1048	C985	U920	G858	C796
A1502	G1374	A1306	G1243	G1178	C1114	U1049	U986	U921	G860	U798
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G1505	G1377	G1310	U1246	G1182	U1117	G1053	C990	G929	U863	U801
U1506	U1444	U1445	U1247	U1183	U1118	C1054	U991	A938	A864	A802
A1507	G1378	A1311	U1248	G1184	U1119	U1055	U992	C930	C866	G803
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C1509	U1380	U1313	A1250	G1186	U1121	G1057	A994	C932	G867	C806
G1510	U1381	G1314	U1251	G1187	U1122	G1058	A995	G933	C868	C807
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A1512	G1383	G1316	G1253	U1189	G1124	U1060	U997	A935	U871	G809
G1513	C1384	C1317	A1254	U1190	U1125	U1061	C998	C936	A873	C810
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G1517	C1388	C1319	G1256	U1192	G1127	G1063	A1000	G941	U875	U813
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A1531	C1400	A1333	A1269	U1202	G1138	U1073	U1010	U951	G885	C823
U1532	G1401	C1325	G1270	C1203	G1139	G1074	C1011	U952	G886	G824
G1534	U1405	U1326	U1271	A1204	C1140	U1075	A1012	U953	G887	A825
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C1536	U1407	A1339	A1273	C1208	G1142	U1077	A1014	U955	A889	U827
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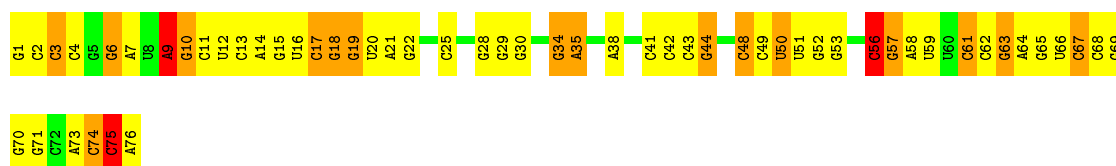
• Molecule 2: A/T-site tRNA Phe

Chain AB:  29% 45% 25%

G1	G69	G68
G2	G70	G69
G3	G71	G70
G4	G72	G71
G5	G73	G72
G6	G74	G73
G7	G75	G74
G8	G76	G75
G9	G77	G76
G10	G78	G77
G11	G79	G78
G12	G80	G79
G13	G81	G80
G14	G82	G81
G15	G83	G82
G16	G84	G83
G17	G85	G84
G18	G86	G85
G19	G87	G86
G20	G88	G87
G21	G89	G88
G22	G90	G89
G23	G91	G90
G24	G92	G91
G25	G93	G92
G26	G94	G93
G27	G95	G94
G28	G96	G95
G29	G97	G96
G30	G98	G97
G31	G99	G98
G32	G100	G99
G33	G101	G100
G34	G102	G101
G35	G103	G102
G36	G104	G103
G37	G105	G104
G38	G106	G105
G39	G107	G106
G40	G108	G107
G41	G109	G108
G42	G110	G109
G43	G111	G110
G44	G112	G111
G45	G113	G112
G46	G114	G113
G47	G115	G114
G48	G116	G115
G49	G117	G116
G50	G118	G117
G51	G119	G118
G52	G120	G119
G53	G121	G120
G54	G122	G121
G55	G123	G122
G56	G124	G123
G57	G125	G124
G58	G126	G125
G59	G127	G126
G60	G128	G127
G61	G129	G128
G62	G130	G129
G63	G131	G130
G64	G132	G131
G65	G133	G132
G66	G134	G133
G67	G135	G134

• Molecule 2: A/T-site tRNA Phe

Chain AE:  26% 49% 21%



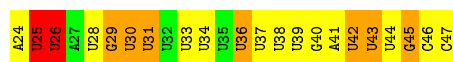
- Molecule 3: Elongation factor Tu 2

Chain AC: 95% 5%



- Molecule 4: mRNA

Chain AD: 13% 50% 29% 8%



- Molecule 5: 30S ribosomal protein S2

Chain AF: 94% 5%



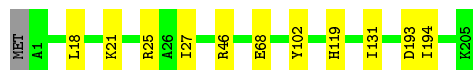
- Molecule 6: 30S ribosomal protein S3

Chain AG: 94% 5%



- Molecule 7: 30S ribosomal protein S4

Chain AH: 94% 5%



- Molecule 8: 30S ribosomal protein S5

Chain AI: 93% 6% 1%



- Molecule 9: 30S ribosomal protein S6

Chain AJ: 89% 10% 1%



- Molecule 10: 30S ribosomal protein S7

Chain AK: 92% 7%



- Molecule 11: 30S ribosomal protein S8

Chain AL: 93% 6%



- Molecule 12: 30S ribosomal protein S9

Chain AM: 91% 8%



- Molecule 13: 30S ribosomal protein S10

Chain AN: 90% 9%



- Molecule 14: 30S ribosomal protein S11

Chain AO: 95% 5%



- Molecule 15: 30S ribosomal protein S12

Chain AP: 90% 9%

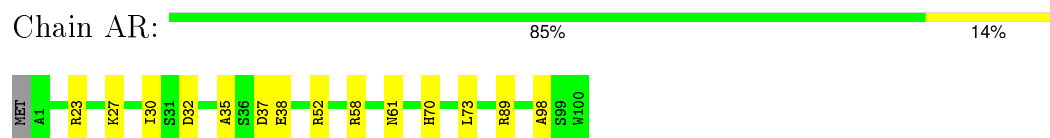


- Molecule 16: 30S ribosomal protein S13

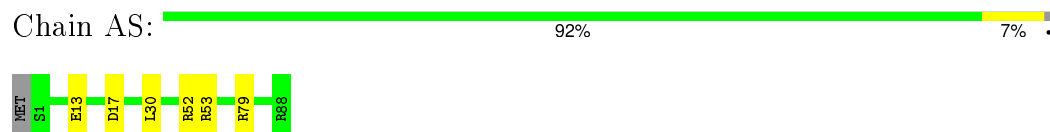
Chain AQ: 97% 2%



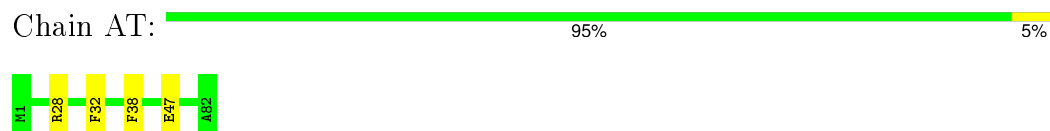
- Molecule 17: 30S ribosomal protein S14



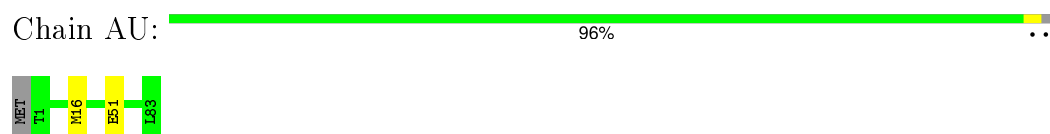
- Molecule 18: 30S ribosomal protein S15



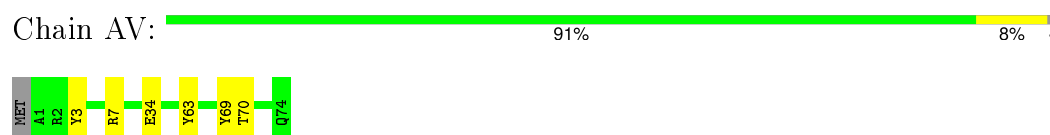
- Molecule 19: 30S ribosomal protein S16



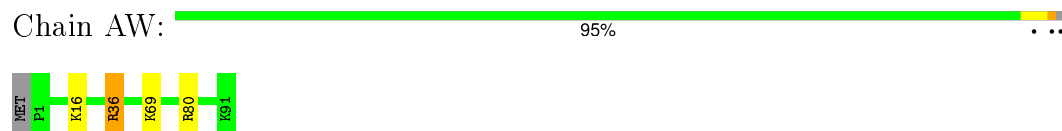
- Molecule 20: 30S ribosomal protein S17



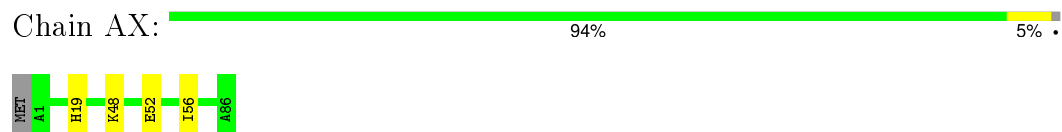
- Molecule 21: 30S ribosomal protein S18



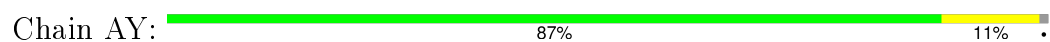
- Molecule 22: 30S ribosomal protein S19



- Molecule 23: 30S ribosomal protein S20



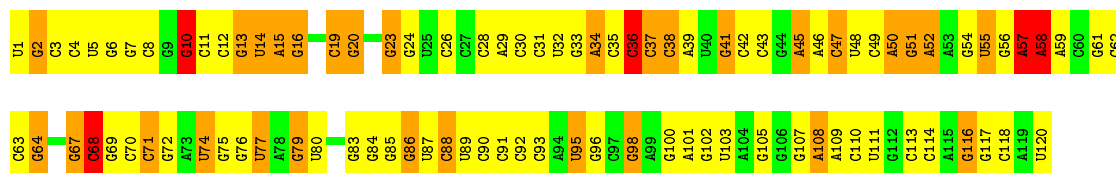
- Molecule 24: 30S ribosomal protein S21





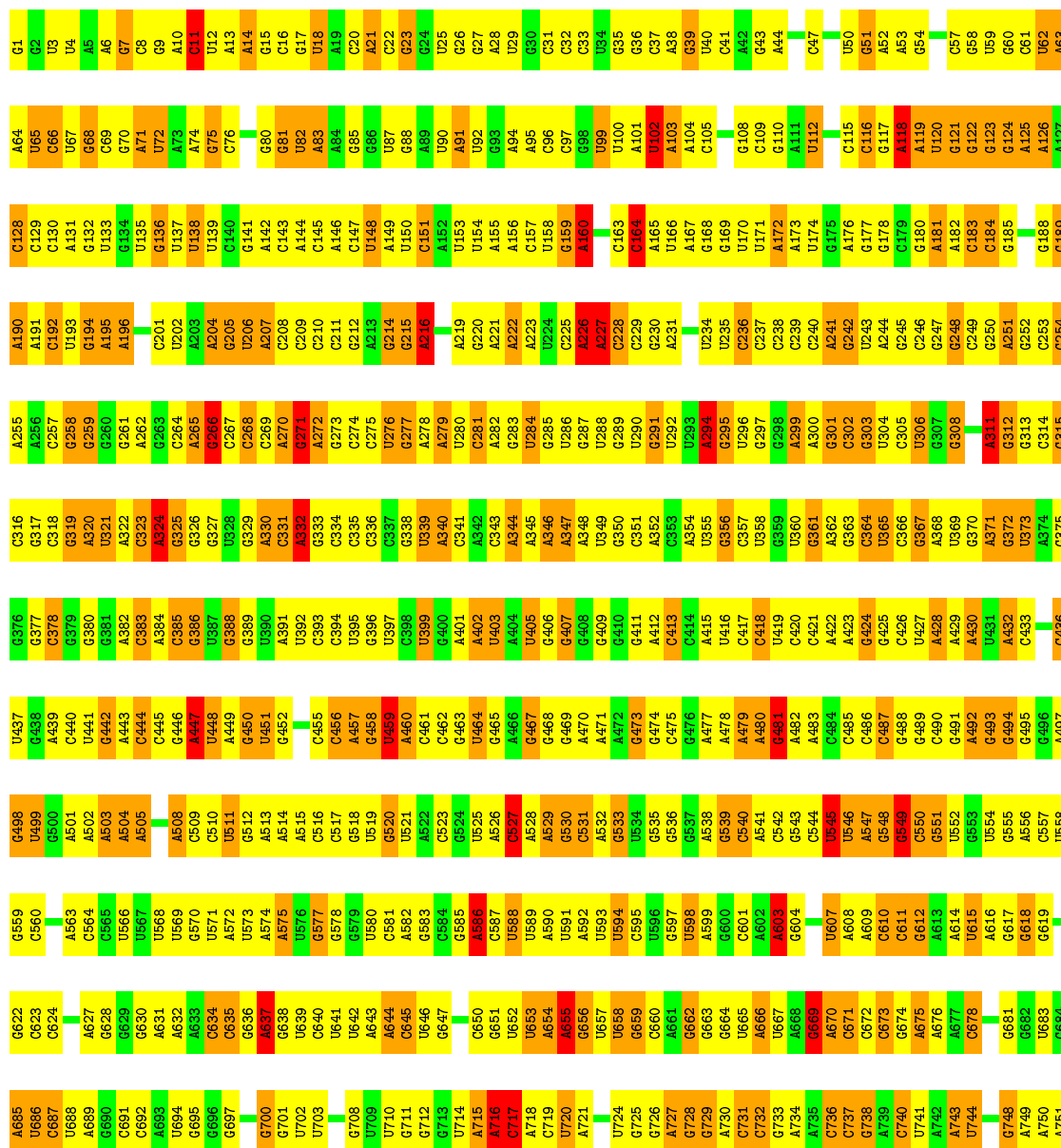
• Molecule 25: 50S ribosomal RNA 5S

Chain BA: 21% 50% 25%



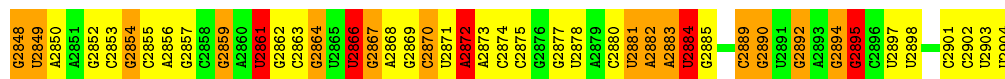
• Molecule 26: 50S ribosomal RNA 23S

Chain BB: 21% 49% 26%



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U1692	G1631	A1669	C1507	G1441	C1376	C1314	G1252	A1189	G1125	G1063	A1000	G938	G875	C814	A753
U1693	A1632	A1570	A1508	U1442	G1377	C1315	A1253	G1190	A1126	C1064	A1001	G939	C876	C815	
C1694	G1633	A1571	A1509	U1443	A1378	U1316	A1254	G1191	A1127	U1065	G1002	G940	A877	C816	A756
G1695	A1634	A1572	G1510	G1444	U1379	G1317	U1255	G1192	U1066	U1067	G1003	A941	A878	C817	G757
G1696	A1635	G1573	G1511	G1445	U1380	U1318	G1256	G1193	A1128	A1068	U1004	G942	A879	C818	C758
G1697	G1636	G1574	C1512	G1446	C1381		C1257	A1194	U1130	G1069	C1005	A943	C880	A819	G759
A1698	A1637	C1575	U1513	G1447	G1382	A1321	U1258	G1195	G1131	A1069	C1006	G944	G881	A820	G760
G1699	G1638	U1576	G1514	A1448	A1383		G1259	C1196	U1132	A1070	C1007	A945	G882	A821	A761
A1700	C1639	U1577	A1515	G1449	A1384	G1325	A1260	G1197	A1133	G1072		C946	G883	G822	G762
A1701	A1640	U1578	G1516	G1450	A1385	U1326	C1261	U1198	A1134	U1073	G1015	G951	U884	C823	G763
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G1703	G1642	A1580	G1452	G1453	A1387	A1327	U1263		G1136	G1074	U1012	G949	A886	A825	G765
C1704	G1643	G1581	U1519	A1454	G1388	A1328	A1264	G1202	G1137	C1075	C1013	G950	U887	U826	G766
A1705	G1644		G1520	G1455	U1389	U1329	G1265	U1203	G1138	A1076	A1014	C952	C888	U827	G767
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G1707	C1646	A1585	U1523		U1391	G1331	U1267	A1205	A1140	C1078	G1016	G954	C890	A829	U769
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U2724	A2660	C2594	A2531	C2467	C2332	A2267	A2205	A2142	C2078	A2013	U1951	G1884	A1819	G1753
A2725	G2661	G2595	G2532	A2468	U2333	A2268	C2206	G2143	U2079	A2014	U1952	A1885	C1822	A1754
A2726	A2662	U2533	U2334	A2469	U2401	G2269	C2207	G2144	A2080	A2015	U1953	U1886	C1822	
A2727	G2663	A2534	A2402	G2470	C2403	A2271	C2208	C2145	U2081	U2016	G1954	C1887	U1825	U1757
A2728	G2664	G2535	G2403	A2471	A2336	G2270		C2146	A2082	U2017	G1955	C1888	U1826	U1758
A2665	A2665	G2601	U2536	G2472	G2337	U2272		A2147	G2083	G2018	U1955	A1889	U1827	A1759
C2730	C2667	G2603	U2537	U2473	C2338	A2273	U2212	G2148	C2084	A2019	U1956	A1890	C1828	C1760
G2731	G2668	G2604	C2538	A2406	A2339	A2274	U2213	U2149	U2085	A2020	G1891	C1892	G1831	C1761
A2732			C2539	C2475	A2340	C2275	C2214	U2150	U2086	C2021	C1892	C1862	A1762	A1762
A2733			C2540	A2476	G2341	G2276	C2215	G2151	G2087	U2022	C1893	C1862	C1763	C1763
G2734			U2403	U2477	G2342	G2277	G2216	G2152	A2088	G2023	C1894	C1864	C1764	C1764
G2735	U2672	C2610	A2541	U2477	C2343	A2278	G2217		C2089	G2024	C1895	C1865	U1765	U1765
A2736	G2673	C2612	A2542	A2478	U2344		G2218	U2155	A2090	C2025	C1896	G1766	G1766	G1766
G2737		U2613	G2543	U2479	G2345	A2281	U2219	G2156	C2091	U2026	C1897	G1767	G1767	G1767
A2738	G2676	A2614	G2546	C2480	A2346	G2282	U2220	G2157	U2092	U2027	U1898	C1838	C1838	C1768
U2739	G2678	U2546	A2547	G2486	C2347	C2283	G2221	A2158	G2093	U2028	A1899	G1839	G1839	U1769
A2740	A2679	G2616	A2547	C2486	U2348	A2284	C2222	G2159	G2094	G2029	A1900	G1840	G1840	G1840
A2741	U2680	U2617	U2548	G2487	G2349	C2285	G2223	C2160	A2097	U2030	A1901	U1841	U1841	A1772
G2742	C2681	G2618	G2549	U2488	C2350	G2286	G2224	C2161	U2098	A2031	C1902	G1842	G1842	A1773
U2743	A2682	G2619	G2550	G2489	C2351	A2287	A2225	C2162	G1972	G2032	G1906	C1843	C1774	C1774
G2744	C2683	C2620	C2551	G2490	A2352	A2288	C2226	A2163	U2099	A2033	G1907	C1844	U1775	U1775
C2745	U2684	G2621	U2552	U2491	A2352	A2288	A2227	C2164	G1974	U2034	G1908	G1845	G1776	G1776
U2746	G2685	U2622	G2553	U2492			G2228	G2102	G1975		C1908	G1846	U1777	U1777
G2747	G2686	G2623	U2554	U2493	G2293		G2229	C2103	U1976	U2039	C1909	A1847	U1778	U1778
A2748	U2687	G2624	U2555	G2494	G2294	C2295	G2230	G2168	A1977	G2040	A1848	A1848	U1779	U1779
U2749	G2688	G2625	G2556	G2495	C2296	U2297	U2231	A2170	U1978	U2041	G1849	G1849	A1780	A1780
A2750	U2689	C2626	C2557	A2426	A2297	C2300	U2232	A2171	A2042	A2042	G1850	G1850	U1781	U1781
G2751	U2690	G2627	C2558	C2427	G2305	A2298	U2233	U2172	G1980	C2043	U1851	U1851	U1782	U1782
C2752	G2691	C2628	C2559	G2428	A2306	U2299	G2234	U2109	A2044	C2044	G1981	G1981	U1852	A1783
A2753	G2692	U2629	U2560	G2429	G2307	C2300	G2235	C2174	U1982	C2045	A1853	A1853	U1784	A1784
U2754	C2693	G2630	A2561	A2430	C2308	G2286	U2236	C2175	G1983	G2046	U1916	A1854	A1785	A1785
G2755	G2694	U2631	U2562	U2501	A2431	C2309	G2237	A2176	G1984	C2047	U1918	A1855	A1786	A1786
A2756	U2695	A2632	C2563	G2502	A2432	G2303	G2238	C2177	U2113	G2048	A1919	A1856	A1787	A1787
U2757	G2696	G2633	A2564	A2503	A2433	G2304	U2239	C2178	C1986	C1920	G1857	G1857	C1788	C1788
G2758	C2697	U2634	A2565	U2504	U2434	U2305	U2240	C2179	A1987	C2050	G1921	A1858		
U2759	U2698	A2635	A2566	G2505	G2506	C2306	A2241	U2180	G1988	A2051	G1922	U1859	A1791	A1791
C2760	C2699	C2636	G2567	U2506	G2307	G2307	G2242	U2181	G1989	G2052	U1923	A1860	G1792	G1792
A2761	U2700	U2637	U2568	C2507	A2376	G2308	U2243	U2182	C1990	G2053	C1924	G1861	C1793	C1793
G2762	U2701	G2638	G2569	G2508	A2377	A2309	U2244	A2183	U1991	A2054	C1925	G1862		
G2763	G2702	A2639	U2570	G2509	A2378	A2310	U2246	A2184	G1992	C2055	U1926	G1863	U1796	U1796
A2764	C2703	G2640	U2571	C2442	G2379	A2311	G2246	U2185	G1993	G2056	A1927	G1864	G1797	G1797
A2765	C2704	G2641	C2572	U2511	G2380	U2312		G2186	C1994	G2057	A1928	U1865	U1798	U1798
U2766	A2705	G2642	G2573	C2512	A2381	G2313	U2249	U2187	U1995	A2058	G1923	A1866	G1799	G1799
G2767	U2706	G2643	G2574	A2513	G2382	A2314	G2250	G2124	C1996	A2059	G1867	C1867	C1800	C1800
U2768	U2707	G2644		U2514	G2383		G2251	G2125	C1997	A2060	C1868	A1801	A1802	A1802
U2769	G2708	G2645	G2578	G2515	U2384	A2317	G2252	A2126	A1998	G2061	A1932	G1869	G1806	G1806
G2770	G2709	C2646	A2516	G2447	C2385	G2318	G2253	A2191	C1999	A2062	G1933	C1870	A1807	A1807
C2771	C2710	U2647	U2580	U2448	G2386	G2319	G2254	U2192	C2000	C2063	C1934	A1871	A1808	A1808
G2772	A2711	G2648	G2581	A2518	U2387	U2320	G2255	G2193	C2001	C2064	G1935	G1872	A1809	A1809
C2773		C2649	G2582	U2519	A2388	U2321	G2256	U2194	G2002	C2065	A1936	G1873	A1810	A1810
C2774	G2714	U2650	G2583	C2520	G2389	A2322	U2257	U2195	C2003	C2066	A1937	C1874	G1811	G1811
G2775	C2715	C2651	U2584	G2521	U2390	G2323	C2258	C2196	A1938	G2067	A1938	G1875	A1812	A1812
A2776	C2716	G2652	U2585	U2458	G2391	U2324	U2259	U2197	A2005	U2068	A1876	G1877	G1813	G1813
G2777	G2717	U2653	U2586	A2459	A2392	G2325	A2134	A2198	C2006	U1940	A1877	G1878	G1814	G1814
A2778	G2718	A2587	G2587	U2460	U2393	C2326	C2261	A2199	U2007	C2072	C1941	C1879	G1815	G1815
U2779	G2719	G2655	G2588	A2461	C2394	A2327	U2262	C2200	C2008	C2073	C1942	U1880	C1816	C1816
G2780	U2720	U2656	A2589	C2462	C2395	A2328	C2263	G2201	C2009	U2074	U1943	C1881		
A2781	A2721	G2657	G2396	C2462	G2397	U2329	C2264	U2202	G2010	U2075		C1882		
G2782	G2722	C2658	G2397	C2465		G2330	U2265	G2140		U2076	U2011		U1882	



- Molecule 27: 50S ribosomal protein L1

Chain BC: 95% 5%



- Molecule 28: 50S ribosomal protein L2

Chain BD: 93% 7%



- Molecule 29: 50S ribosomal protein L3

Chain BE: 91% 8%



- Molecule 30: 50S ribosomal protein L4

Chain BF: 93% 6%



- Molecule 31: 50S ribosomal protein L5

Chain BG: 92% 7% ..



- Molecule 32: 50S ribosomal protein L6

Chain BH: 91% 8% ..



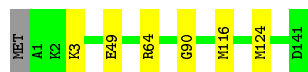
- Molecule 33: 50S ribosomal protein L9

Chain BI: 93% 7%



- Molecule 34: 50S ribosomal protein L11

Chain BJ: 95%



- Molecule 35: 50S ribosomal protein L13

Chain BK: 96%



- Molecule 36: 50S ribosomal protein L14

Chain BL: 93%



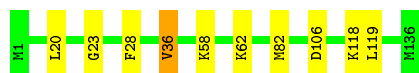
- Molecule 37: 50S ribosomal protein L15

Chain BM: 94%



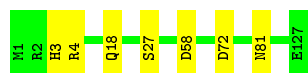
- Molecule 38: 50S ribosomal protein L16

Chain BN: 93%



- Molecule 39: 50S ribosomal protein L17

Chain BO: 94%



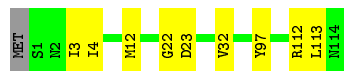
- Molecule 40: 50S ribosomal protein L18

Chain BP: 95%



- Molecule 41: 50S ribosomal protein L19

Chain BQ:  91% 8%



- Molecule 42: 50S ribosomal protein L20

Chain BR:  96%



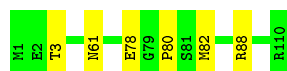
- Molecule 43: 50S ribosomal protein L21

Chain BS:  91% 8%



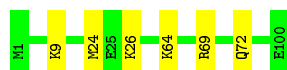
- Molecule 44: 50S ribosomal protein L22

Chain BT:  95% 5%



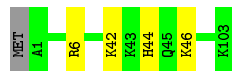
- Molecule 45: 50S ribosomal protein L23

Chain BU:  94% 6%



- Molecule 46: 50S ribosomal protein L24

Chain BV:  95%




- Molecule 47: 50S ribosomal protein L25

Chain BW:  94% 6%



- Molecule 48: 50S ribosomal protein L27

Chain BX:  86% 13%



- Molecule 49: 50S ribosomal protein L28

Chain BY:  91% 6%



- Molecule 50: 50S ribosomal protein L29

Chain BZ:  94% 6%



- Molecule 51: 50S ribosomal protein L30

Chain Ba:  95%



- Molecule 52: 50S ribosomal protein L31

Chain Bb:  96%



- Molecule 53: 50S ribosomal protein L32

Chain Bc:  91% 7%



- Molecule 54: 50S ribosomal protein L33

Chain Bd:  98%



- Molecule 55: 50S ribosomal protein L34

Chain Be:  98%



- Molecule 56: 50S ribosomal protein L35

Chain Bf: 95% . .



- Molecule 57: 50S ribosomal protein L36

Chain Bg: 87% 13%



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: 5MU, 3TD, CH, OMG, 5MC, 3AU, MA6, MIA, OMC, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 7MG, 1MG, 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	1.22	1/36769 (0.0%)	2.00	1273/57354 (2.2%)
10	AK	0.63	0/1422	1.07	1/1908 (0.1%)
11	AL	0.59	0/989	1.01	0/1326
12	AM	0.65	0/1048	1.05	1/1394 (0.1%)
13	AN	0.57	0/835	1.08	1/1127 (0.1%)
14	AO	0.61	0/982	1.04	0/1323
15	AP	0.62	0/969	1.12	0/1300
16	AQ	0.58	0/919	1.02	0/1226
17	AR	0.63	0/817	1.15	2/1088 (0.2%)
18	AS	0.59	0/724	0.96	1/966 (0.1%)
19	AT	0.63	0/659	1.08	1/884 (0.1%)
2	AB	1.25	0/1580	2.01	56/2459 (2.3%)
2	AE	1.26	0/1580	2.04	66/2459 (2.7%)
20	AU	0.58	0/681	0.97	0/913
21	AV	0.73	0/637	1.08	0/851
22	AW	0.60	0/744	1.00	1/995 (0.1%)
23	AX	0.58	0/676	0.98	0/895
24	AY	0.69	0/598	1.18	1/792 (0.1%)
25	BA	1.24	0/2869	2.16	127/4474 (2.8%)
26	BB	1.22	0/69257	2.02	2547/108040 (2.4%)
27	BC	0.55	0/1748	0.98	0/2355
28	BD	0.62	0/2131	1.09	0/2863
29	BE	0.59	0/1586	1.04	0/2134
3	AC	0.61	0/3092	0.97	1/4183 (0.0%)
30	BF	0.58	0/1571	1.01	1/2113 (0.0%)
31	BG	0.66	0/1444	1.10	0/1937
32	BH	0.59	0/1343	1.05	2/1816 (0.1%)
33	BI	0.58	0/1122	1.01	1/1515 (0.1%)
34	BJ	0.57	0/1046	0.93	0/1410
35	BK	0.64	0/1152	1.00	0/1551
36	BL	0.58	0/956	1.03	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
37	BM	0.62	0/1062	1.07	0/1413
38	BN	0.63	0/1093	1.04	0/1460
39	BO	0.62	0/1021	1.06	0/1364
4	AD	1.37	0/548	1.98	20/848 (2.4%)
40	BP	0.60	0/910	1.01	0/1219
41	BQ	0.63	0/929	1.05	0/1242
42	BR	0.67	0/960	1.03	1/1278 (0.1%)
43	BS	0.63	0/829	1.06	0/1107
44	BT	0.54	0/864	0.98	0/1156
45	BU	0.57	0/794	1.02	0/1060
46	BV	0.58	0/797	1.02	0/1062
47	BW	0.61	0/766	0.98	0/1025
48	BX	0.64	0/642	1.10	0/848
49	BY	0.64	0/635	1.10	1/848 (0.1%)
5	AF	0.60	0/1904	1.00	1/2565 (0.0%)
50	BZ	0.56	0/510	1.05	0/677
51	Ba	0.55	0/453	0.97	0/605
52	Bb	0.62	0/559	1.10	0/745
53	Bc	0.62	0/450	1.12	0/599
54	Bd	0.60	0/448	0.96	0/594
55	Be	0.64	0/380	1.04	0/498
56	Bf	0.60	0/513	1.02	0/676
57	Bg	0.55	0/303	1.09	0/397
6	AG	0.61	0/1852	1.04	0/2490
7	AH	0.64	0/1665	0.99	0/2227
8	AI	0.59	0/1239	1.07	1/1664 (0.1%)
9	AJ	0.62	0/1121	1.05	2/1509 (0.1%)
All	All	1.07	1/165193 (0.0%)	1.79	4109/246106 (1.7%)

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	502
11	AL	0	1
13	AN	0	1
14	AO	0	1
15	AP	0	1
17	AR	0	2
2	AB	0	19

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	AE	0	15
21	AV	0	1
24	AY	0	1
25	BA	0	37
26	BB	0	952
27	BC	0	3
28	BD	0	2
29	BE	0	2
3	AC	0	1
30	BF	0	2
32	BH	0	2
33	BI	0	1
4	AD	0	9
41	BQ	0	1
42	BR	0	1
43	BS	0	1
48	BX	0	1
49	BY	0	1
53	Bc	0	1
6	AG	0	1
7	AH	0	1
8	AI	0	3
9	AJ	0	1
All	All	0	1567

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	439	U	C2-N3	5.10	1.41	1.37

All (4109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2092	U	O4'-C1'-N1	16.66	121.53	108.20
25	BA	49	C	O4'-C1'-N1	15.19	120.35	108.20
1	AA	465	A	O4'-C1'-N9	14.84	120.07	108.20
26	BB	736	C	O4'-C1'-N1	12.90	118.52	108.20
26	BB	1535	A	O4'-C1'-N9	12.89	118.51	108.20
26	BB	2799	A	O4'-C1'-N9	12.66	118.33	108.20
26	BB	1967	C	O4'-C1'-N1	12.66	118.33	108.20
26	BB	1195	G	O4'-C1'-N9	12.14	117.91	108.20
26	BB	354	A	O4'-C1'-N9	12.11	117.89	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1763	G	O4'-C1'-N9	12.04	117.83	108.20
1	AA	396	C	O4'-C1'-N1	12.02	117.81	108.20
26	BB	1325	U	O4'-C1'-N1	11.99	117.80	108.20
26	BB	1185	G	O4'-C1'-N9	11.97	117.78	108.20
1	AA	1227	A	O4'-C1'-N9	11.90	117.72	108.20
1	AA	1152	A	O4'-C1'-N9	11.85	117.68	108.20
1	AA	1322	C	O4'-C1'-N1	11.75	117.60	108.20
26	BB	2795	C	O4'-C1'-N1	11.71	117.57	108.20
1	AA	658	C	O4'-C1'-N1	11.70	117.56	108.20
26	BB	1730	C	O4'-C1'-N1	11.70	117.56	108.20
4	AD	30	U	O4'-C1'-N1	11.66	117.53	108.20
26	BB	2559	C	O4'-C1'-N1	11.62	117.50	108.20
26	BB	2832	U	O4'-C1'-N1	11.60	117.48	108.20
1	AA	485	U	O4'-C1'-N1	11.54	117.44	108.20
26	BB	2212	A	O4'-C1'-N9	11.54	117.43	108.20
26	BB	302	C	O4'-C1'-N1	11.51	117.41	108.20
26	BB	1493	C	O4'-C1'-N1	11.51	117.41	108.20
26	BB	169	G	O4'-C1'-N9	11.48	117.39	108.20
2	AE	17	C	O4'-C1'-N1	11.44	117.35	108.20
26	BB	2742	G	O4'-C1'-N9	11.44	117.35	108.20
26	BB	2684	U	O4'-C1'-N1	11.44	117.35	108.20
26	BB	316	C	O4'-C1'-N1	11.35	117.28	108.20
26	BB	908	C	O4'-C1'-N1	11.33	117.27	108.20
25	BA	30	C	O4'-C1'-N1	11.31	117.25	108.20
1	AA	1444	U	O4'-C1'-N1	11.25	117.20	108.20
26	BB	70	G	O4'-C1'-N9	11.25	117.20	108.20
1	AA	880	C	O4'-C1'-N1	11.24	117.19	108.20
26	BB	1275	A	O4'-C1'-N9	11.22	117.18	108.20
26	BB	546	U	O4'-C1'-N1	11.19	117.16	108.20
26	BB	1209	U	O4'-C1'-N1	11.17	117.14	108.20
26	BB	306	U	O4'-C1'-N1	11.16	117.12	108.20
26	BB	550	C	O4'-C1'-N1	11.15	117.12	108.20
26	BB	116	C	O4'-C1'-N1	11.14	117.11	108.20
26	BB	1294	U	O4'-C1'-N1	11.02	117.02	108.20
1	AA	1094	G	O4'-C1'-N9	11.02	117.01	108.20
26	BB	323	C	O4'-C1'-N1	11.00	117.00	108.20
1	AA	332	G	O4'-C1'-N9	10.91	116.93	108.20
26	BB	268	C	O4'-C1'-N1	10.90	116.92	108.20
26	BB	1901	A	O4'-C1'-N9	10.86	116.89	108.20
26	BB	1409	U	O4'-C1'-N1	10.85	116.88	108.20
26	BB	995	C	O4'-C1'-N1	10.82	116.86	108.20
1	AA	770	C	O4'-C1'-N1	10.79	116.84	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2667	C	O4'-C1'-N1	10.79	116.83	108.20
2	AB	25	C	O4'-C1'-N1	10.74	116.79	108.20
25	BA	93	C	O4'-C1'-N1	10.64	116.71	108.20
26	BB	1703	G	O4'-C1'-N9	10.63	116.70	108.20
26	BB	614	A	O4'-C1'-N9	10.62	116.69	108.20
26	BB	2903	U	O4'-C1'-N1	10.54	116.63	108.20
26	BB	2311	A	C5'-C4'-C3'	-10.49	99.21	116.00
1	AA	1212	U	O4'-C1'-N1	10.49	116.59	108.20
26	BB	382	A	O4'-C1'-N9	10.48	116.58	108.20
26	BB	1868	C	O4'-C1'-N1	10.47	116.57	108.20
26	BB	366	C	O4'-C1'-N1	10.45	116.56	108.20
1	AA	1078	U	O4'-C1'-N1	10.43	116.55	108.20
26	BB	2396	G	O4'-C1'-N9	10.40	116.52	108.20
26	BB	645	C	O4'-C1'-N1	10.38	116.51	108.20
1	AA	192	A	O4'-C1'-N9	10.37	116.50	108.20
1	AA	488	C	O4'-C1'-N1	10.36	116.49	108.20
26	BB	100	U	O4'-C1'-N1	10.36	116.49	108.20
26	BB	1081	U	O4'-C1'-N1	10.31	116.45	108.20
1	AA	90	C	O4'-C1'-N1	10.30	116.44	108.20
26	BB	2098	U	O4'-C1'-N1	10.28	116.42	108.20
26	BB	1512	C	O4'-C1'-N1	10.27	116.42	108.20
26	BB	834	G	C8-N9-C4	-10.24	102.30	106.40
26	BB	1539	U	O4'-C1'-N1	10.22	116.37	108.20
26	BB	1870	C	O4'-C1'-N1	10.21	116.37	108.20
26	BB	2864	G	C5'-C4'-C3'	-10.19	99.69	116.00
26	BB	1701	A	O4'-C1'-N9	10.19	116.35	108.20
1	AA	1061	G	O4'-C1'-N9	10.18	116.34	108.20
1	AA	1223	C	C5'-C4'-C3'	-10.11	99.82	116.00
26	BB	870	U	O4'-C1'-N1	10.10	116.28	108.20
26	BB	1025	G	O4'-C1'-N9	10.10	116.28	108.20
26	BB	2732	G	O4'-C1'-N9	10.10	116.28	108.20
26	BB	365	U	O4'-C1'-N1	10.08	116.26	108.20
26	BB	1941	C	O4'-C1'-N1	10.06	116.25	108.20
26	BB	351	C	O4'-C1'-N1	10.03	116.22	108.20
1	AA	472	U	O4'-C1'-N1	10.02	116.22	108.20
1	AA	941	G	O4'-C1'-N9	10.02	116.22	108.20
26	BB	2637	U	O4'-C1'-N1	10.02	116.22	108.20
1	AA	1534	A	O4'-C1'-N9	10.01	116.21	108.20
1	AA	1533	C	O4'-C1'-N1	9.99	116.19	108.20
1	AA	1141	C	O4'-C1'-N1	9.96	116.17	108.20
26	BB	1542	U	O4'-C1'-N1	9.96	116.17	108.20
26	BB	2076	U	C1'-O4'-C4'	-9.94	101.95	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1463	C	O4'-C1'-N1	9.92	116.13	108.20
26	BB	1549	A	O4'-C1'-N9	9.91	116.13	108.20
26	BB	1420	A	O4'-C1'-N9	9.91	116.13	108.20
1	AA	1464	U	O4'-C1'-N1	9.89	116.11	108.20
26	BB	236	C	O4'-C1'-N1	9.88	116.10	108.20
1	AA	143	A	O4'-C1'-N9	9.88	116.10	108.20
26	BB	1173	U	O4'-C1'-N1	9.86	116.09	108.20
1	AA	225	C	O4'-C1'-N1	9.83	116.06	108.20
26	BB	2076	U	O4'-C1'-N1	9.82	116.06	108.20
1	AA	1098	C	O4'-C1'-N1	9.82	116.05	108.20
26	BB	1417	C	O4'-C1'-N1	9.78	116.02	108.20
26	BB	2773	C	O4'-C1'-N1	9.77	116.02	108.20
26	BB	1658	C	O4'-C1'-N1	9.72	115.97	108.20
1	AA	1522	U	O4'-C1'-N1	9.71	115.97	108.20
26	BB	168	G	O4'-C1'-N9	9.71	115.97	108.20
1	AA	834	U	O4'-C1'-N1	9.71	115.97	108.20
26	BB	105	C	O4'-C1'-N1	9.69	115.95	108.20
1	AA	970	C	O4'-C1'-N1	9.69	115.95	108.20
1	AA	1136	C	O4'-C1'-N1	9.69	115.95	108.20
1	AA	274	A	O4'-C1'-N9	9.68	115.94	108.20
1	AA	158	G	O4'-C1'-N9	9.65	115.92	108.20
1	AA	358	U	O4'-C1'-N1	9.63	115.90	108.20
26	BB	321	U	O4'-C1'-N1	9.62	115.90	108.20
26	BB	1714	U	O4'-C1'-N1	9.61	115.89	108.20
1	AA	1382	C	O4'-C1'-N1	9.61	115.89	108.20
1	AA	1533	C	C1'-O4'-C4'	-9.61	102.21	109.90
26	BB	206	U	O4'-C1'-N1	9.58	115.86	108.20
1	AA	1351	U	O4'-C1'-N1	9.57	115.86	108.20
26	BB	1639	C	O4'-C1'-N1	9.57	115.86	108.20
26	BB	2652	C	O4'-C1'-N1	9.57	115.85	108.20
26	BB	405	U	O4'-C1'-N1	9.55	115.84	108.20
26	BB	1211	C	O4'-C1'-N1	9.55	115.84	108.20
26	BB	2750	A	O4'-C1'-N9	9.52	115.82	108.20
1	AA	1066	C	O4'-C1'-N1	9.51	115.81	108.20
1	AA	562	U	O4'-C1'-N1	9.49	115.79	108.20
25	BA	118	C	O4'-C1'-N1	9.48	115.79	108.20
26	BB	744	U	O4'-C1'-N1	9.47	115.78	108.20
26	BB	2662	A	O4'-C1'-N9	9.47	115.77	108.20
26	BB	1041	G	O4'-C1'-N9	9.46	115.77	108.20
26	BB	1588	G	O3'-P-O5'	-9.45	86.04	104.00
26	BB	991	C	O4'-C1'-N1	9.44	115.75	108.20
1	AA	1478	U	O4'-C1'-N1	9.44	115.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	458	G	O4'-C1'-N9	9.42	115.74	108.20
26	BB	1405	U	O4'-C1'-N1	9.42	115.74	108.20
1	AA	1121	U	O4'-C1'-N1	9.41	115.73	108.20
26	BB	1886	U	O4'-C1'-N1	9.41	115.72	108.20
25	BA	95	U	O4'-C1'-N1	9.39	115.71	108.20
26	BB	1016	G	O4'-C1'-N9	9.39	115.71	108.20
1	AA	1266	G	O4'-C1'-N9	9.38	115.70	108.20
26	BB	945	A	O4'-C1'-N9	9.38	115.70	108.20
26	BB	960	A	O4'-C1'-N9	-9.37	100.71	108.20
26	BB	1290	C	O4'-C1'-N1	9.37	115.69	108.20
1	AA	703	G	O4'-C1'-N9	9.36	115.69	108.20
1	AA	461	A	O4'-C1'-N9	9.35	115.68	108.20
1	AA	1457	G	O4'-C1'-N9	9.35	115.68	108.20
26	BB	1520	U	O4'-C1'-N1	9.35	115.68	108.20
26	BB	1485	U	O4'-C1'-N1	9.33	115.66	108.20
26	BB	2794	C	O4'-C1'-N1	9.30	115.64	108.20
26	BB	63	A	O4'-C1'-N9	9.28	115.62	108.20
26	BB	355	U	O4'-C1'-N1	9.27	115.61	108.20
1	AA	702	A	O4'-C1'-N9	9.27	115.61	108.20
1	AA	631	C	O4'-C1'-N1	9.26	115.61	108.20
26	BB	2110	G	O4'-C1'-N9	9.24	115.59	108.20
26	BB	1434	A	O4'-C1'-N9	9.22	115.57	108.20
1	AA	664	G	O4'-C1'-N9	9.21	115.57	108.20
26	BB	1552	A	O4'-C1'-N9	9.21	115.57	108.20
26	BB	2185	U	O4'-C1'-N1	9.20	115.56	108.20
1	AA	636	U	O4'-C1'-N1	9.19	115.55	108.20
25	BA	11	C	O4'-C1'-N1	9.18	115.54	108.20
26	BB	921	C	O4'-C1'-N1	9.17	115.54	108.20
1	AA	1443	C	O4'-C1'-N1	9.16	115.53	108.20
1	AA	614	C	O4'-C1'-N1	9.15	115.52	108.20
26	BB	1027	A	C5'-C4'-C3'	9.15	130.64	116.00
26	BB	1971	U	O4'-C1'-N1	9.15	115.52	108.20
26	BB	2786	U	O4'-C1'-N1	9.15	115.52	108.20
26	BB	1648	U	O4'-C1'-N1	9.13	115.50	108.20
1	AA	595	A	C3'-C2'-C1'	9.13	108.80	101.50
26	BB	281	C	O4'-C1'-N1	9.11	115.49	108.20
26	BB	1869	G	O4'-C1'-N9	9.10	115.48	108.20
1	AA	327	A	O4'-C1'-N9	9.10	115.48	108.20
1	AA	1528	U	O4'-C1'-N1	9.10	115.48	108.20
26	BB	2465	C	O4'-C1'-N1	9.09	115.47	108.20
26	BB	349	U	O4'-C1'-N1	9.09	115.47	108.20
26	BB	1094	U	O4'-C1'-N1	9.09	115.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2807	U	O4'-C1'-N1	9.07	115.46	108.20
26	BB	718	A	O4'-C1'-N9	9.04	115.43	108.20
2	AE	51	U	O4'-C1'-N1	9.03	115.42	108.20
26	BB	1443	U	O4'-C1'-N1	9.03	115.42	108.20
1	AA	1471	U	O4'-C1'-N1	9.02	115.42	108.20
1	AA	1283	U	O4'-C1'-N1	9.02	115.42	108.20
26	BB	1181	U	O4'-C1'-N1	9.01	115.41	108.20
1	AA	244	U	O4'-C1'-N1	9.01	115.41	108.20
26	BB	304	U	O4'-C1'-N1	9.00	115.40	108.20
26	BB	591	U	O4'-C1'-N1	8.98	115.38	108.20
26	BB	2086	U	O4'-C1'-N1	8.98	115.38	108.20
1	AA	630	A	O4'-C1'-N9	8.97	115.38	108.20
1	AA	677	U	O4'-C1'-N1	8.97	115.38	108.20
26	BB	1167	C	O4'-C1'-N1	8.96	115.37	108.20
26	BB	1976	U	O4'-C1'-N1	8.95	115.36	108.20
1	AA	818	G	O4'-C1'-N9	8.93	115.34	108.20
26	BB	1316	U	O4'-C1'-N1	8.92	115.33	108.20
1	AA	1193	G	O4'-C1'-N9	8.92	115.33	108.20
26	BB	278	A	C5'-C4'-O4'	8.92	119.80	109.10
26	BB	545	U	O4'-C1'-N1	8.92	115.33	108.20
26	BB	1798	U	O4'-C1'-N1	8.92	115.33	108.20
1	AA	353	A	O4'-C1'-N9	8.91	115.33	108.20
26	BB	2855	C	O4'-C1'-N1	8.91	115.33	108.20
26	BB	2123	G	O4'-C1'-N9	8.90	115.32	108.20
26	BB	1985	C	O4'-C1'-N1	8.89	115.31	108.20
25	BA	68	C	O4'-C1'-N1	8.89	115.31	108.20
26	BB	1887	C	O4'-C1'-N1	8.88	115.31	108.20
26	BB	2051	A	O4'-C1'-N9	8.88	115.31	108.20
26	BB	876	C	O4'-C1'-N1	8.88	115.30	108.20
26	BB	362	A	O4'-C1'-N9	8.87	115.30	108.20
26	BB	2784	U	O4'-C1'-N1	8.87	115.30	108.20
26	BB	1777	U	O4'-C1'-N1	8.87	115.30	108.20
26	BB	1902	C	O4'-C1'-N1	8.87	115.29	108.20
25	BA	100	G	C8-N9-C4	-8.87	102.85	106.40
1	AA	31	G	O4'-C1'-N9	8.86	115.29	108.20
26	BB	594	U	O4'-C1'-N1	8.86	115.28	108.20
26	BB	1182	G	O4'-C1'-N9	8.84	115.27	108.20
1	AA	593	U	O4'-C1'-N1	8.84	115.27	108.20
26	BB	1233	C	O4'-C1'-N1	8.83	115.27	108.20
1	AA	1172	C	O4'-C1'-N1	8.83	115.26	108.20
26	BB	1118	C	O4'-C1'-N1	8.82	115.25	108.20
26	BB	1444	G	O4'-C1'-N9	8.81	115.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1045	C	O4'-C1'-N1	8.80	115.24	108.20
26	BB	906	U	O4'-C1'-N1	8.80	115.24	108.20
26	BB	2276	G	O4'-C1'-N9	8.80	115.24	108.20
1	AA	379	C	O4'-C1'-N1	8.79	115.23	108.20
26	BB	1629	U	O4'-C1'-N1	8.79	115.23	108.20
1	AA	465	A	C1'-O4'-C4'	-8.78	102.88	109.90
26	BB	1115	G	O4'-C1'-N9	8.78	115.22	108.20
1	AA	29	U	O4'-C1'-N1	8.77	115.22	108.20
26	BB	1729	U	O4'-C1'-N1	8.77	115.22	108.20
26	BB	2849	U	O4'-C1'-N1	8.77	115.21	108.20
1	AA	24	U	O4'-C1'-N1	8.76	115.21	108.20
1	AA	1083	U	O4'-C1'-N1	8.75	115.20	108.20
26	BB	2841	C	O4'-C1'-N1	8.75	115.20	108.20
26	BB	700	G	O4'-C1'-N9	8.74	115.20	108.20
1	AA	1010	U	O4'-C1'-N1	8.74	115.19	108.20
26	BB	39	G	O4'-C1'-N9	8.74	115.19	108.20
26	BB	148	U	O4'-C1'-N1	8.74	115.19	108.20
26	BB	2843	G	O4'-C1'-N9	8.73	115.19	108.20
1	AA	414	A	C8-N9-C4	-8.72	102.31	105.80
1	AA	1165	U	O4'-C1'-N1	8.72	115.17	108.20
1	AA	1	A	O4'-C1'-N9	8.71	115.17	108.20
26	BB	1882	U	O4'-C1'-N1	8.71	115.17	108.20
1	AA	904	U	O4'-C1'-N1	8.71	115.17	108.20
26	BB	2793	C	O4'-C1'-N1	8.70	115.16	108.20
26	BB	2362	C	O4'-C1'-N1	8.70	115.16	108.20
26	BB	2882	A	C5'-C4'-O4'	8.70	119.53	109.10
26	BB	784	G	O4'-C1'-N9	8.69	115.15	108.20
26	BB	1166	G	O4'-C1'-N9	8.69	115.15	108.20
26	BB	2502	G	O4'-C1'-N9	8.69	115.15	108.20
26	BB	2594	C	O4'-C1'-N1	8.68	115.15	108.20
26	BB	737	C	O4'-C1'-N1	8.68	115.14	108.20
26	BB	1931	U	O4'-C1'-N1	8.68	115.14	108.20
26	BB	489	G	O4'-C1'-N9	8.68	115.14	108.20
1	AA	1232	U	O4'-C1'-N1	8.66	115.13	108.20
26	BB	1816	C	O4'-C1'-N1	8.66	115.13	108.20
26	BB	1851	U	O4'-C1'-N1	8.65	115.12	108.20
26	BB	569	U	O4'-C1'-N1	8.65	115.12	108.20
26	BB	1943	U	O4'-C1'-N1	8.65	115.12	108.20
26	BB	2391	G	O4'-C1'-N9	8.65	115.12	108.20
26	BB	2125	G	O4'-C1'-N9	8.65	115.12	108.20
26	BB	2632	A	O4'-C1'-N9	8.65	115.12	108.20
26	BB	1759	A	O4'-C1'-N9	8.64	115.11	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	277	C	O4'-C1'-N1	8.63	115.10	108.20
1	AA	212	G	O4'-C1'-N9	8.62	115.10	108.20
26	BB	593	U	O4'-C1'-N1	8.62	115.10	108.20
26	BB	1227	G	O4'-C1'-N9	8.61	115.09	108.20
26	BB	1374	G	O4'-C1'-N9	8.61	115.09	108.20
1	AA	1153	G	O4'-C1'-N9	8.61	115.09	108.20
1	AA	870	U	O4'-C1'-N1	8.60	115.08	108.20
1	AA	590	U	O4'-C1'-N1	8.60	115.08	108.20
26	BB	1245	G	O4'-C1'-N9	8.60	115.08	108.20
1	AA	256	U	O4'-C1'-N1	8.59	115.07	108.20
26	BB	1526	C	O4'-C1'-N1	8.59	115.07	108.20
1	AA	142	G	C5'-C4'-O4'	8.59	119.41	109.10
26	BB	880	G	O4'-C1'-N9	8.57	115.06	108.20
26	BB	128	C	O4'-C1'-N1	8.57	115.05	108.20
26	BB	475	C	O4'-C1'-N1	8.56	115.05	108.20
1	AA	484	G	O4'-C1'-N9	8.56	115.05	108.20
26	BB	1843	C	O4'-C1'-N1	8.56	115.05	108.20
26	BB	892	A	O4'-C1'-N9	8.55	115.04	108.20
1	AA	58	C	O4'-C1'-N1	8.55	115.04	108.20
25	BA	52	A	O4'-C1'-N9	8.55	115.04	108.20
26	BB	1107	G	O4'-C1'-N9	8.55	115.04	108.20
26	BB	1487	U	O4'-C1'-N1	8.54	115.03	108.20
26	BB	869	G	O4'-C1'-N9	8.54	115.03	108.20
1	AA	60	A	P-O3'-C3'	8.53	129.93	119.70
26	BB	1728	C	O4'-C1'-N1	8.53	115.02	108.20
1	AA	268	U	C5'-C4'-O4'	8.52	119.33	109.10
1	AA	1205	U	O4'-C1'-N1	8.52	115.02	108.20
26	BB	2666	C	O4'-C1'-N1	8.52	115.02	108.20
1	AA	453	G	O4'-C1'-N9	8.51	115.01	108.20
26	BB	16	C	O4'-C1'-N1	8.50	115.00	108.20
25	BA	50	A	C5'-C4'-C3'	-8.49	102.41	116.00
26	BB	2032	G	O4'-C1'-N9	8.49	114.99	108.20
1	AA	88	U	O4'-C1'-N1	8.49	114.99	108.20
26	BB	344	A	O4'-C1'-N9	8.49	114.99	108.20
1	AA	1381	U	P-O3'-C3'	8.48	129.88	119.70
26	BB	1076	C	O4'-C1'-N1	8.48	114.98	108.20
26	BB	2805	C	O4'-C1'-N1	8.48	114.98	108.20
26	BB	2579	C	O4'-C1'-N1	8.48	114.98	108.20
4	AD	38	U	O4'-C1'-N1	8.47	114.98	108.20
1	AA	936	C	O4'-C1'-N1	8.46	114.97	108.20
1	AA	406	G	C5'-C4'-O4'	8.46	119.25	109.10
1	AA	812	G	O4'-C1'-N9	8.46	114.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1152	A	C4'-C3'-C2'	-8.46	94.14	102.60
26	BB	2796	U	O4'-C1'-N1	8.46	114.97	108.20
26	BB	2538	C	O4'-C1'-N1	8.45	114.96	108.20
26	BB	954	G	C5'-C4'-O4'	8.45	119.24	109.10
26	BB	1244	A	O4'-C1'-N9	8.45	114.96	108.20
1	AA	214	C	O4'-C1'-N1	8.45	114.96	108.20
26	BB	1172	C	O4'-C1'-N1	8.45	114.96	108.20
26	BB	2438	U	O4'-C1'-N1	8.44	114.95	108.20
26	BB	126	A	C1'-O4'-C4'	-8.44	103.15	109.90
26	BB	137	U	O4'-C1'-N1	8.44	114.95	108.20
26	BB	343	C	O4'-C1'-N1	8.44	114.95	108.20
26	BB	519	U	O4'-C1'-N1	8.44	114.95	108.20
25	BA	92	C	O4'-C1'-N1	8.44	114.95	108.20
4	AD	26	U	O4'-C1'-N1	8.43	114.95	108.20
25	BA	57	A	O4'-C1'-N9	8.43	114.95	108.20
26	BB	2739	U	O4'-C1'-N1	8.43	114.94	108.20
1	AA	107	G	O4'-C1'-N9	8.42	114.94	108.20
25	BA	47	C	O4'-C1'-N1	8.42	114.94	108.20
1	AA	739	C	O4'-C1'-N1	8.42	114.94	108.20
26	BB	2511	U	O4'-C1'-N1	8.42	114.94	108.20
26	BB	2672	U	O4'-C1'-N1	8.40	114.92	108.20
1	AA	1425	U	O4'-C1'-N1	8.40	114.92	108.20
1	AA	69	G	O4'-C1'-N9	8.39	114.91	108.20
26	BB	1477	A	C5'-C4'-O4'	8.39	119.17	109.10
26	BB	2081	U	O4'-C1'-N1	8.39	114.91	108.20
26	BB	291	G	O4'-C1'-N9	8.38	114.91	108.20
26	BB	1678	A	O4'-C1'-N9	8.36	114.89	108.20
1	AA	1540	U	O4'-C1'-N1	8.36	114.89	108.20
1	AA	398	U	O4'-C1'-N1	8.36	114.89	108.20
26	BB	2762	C	O4'-C1'-N1	8.36	114.89	108.20
1	AA	835	U	O4'-C1'-N1	8.35	114.88	108.20
1	AA	1470	U	O4'-C1'-N1	8.35	114.88	108.20
26	BB	1509	A	O4'-C1'-N9	8.35	114.88	108.20
1	AA	471	U	O4'-C1'-N1	8.35	114.88	108.20
1	AA	929	G	O4'-C1'-N9	8.34	114.88	108.20
1	AA	871	U	O4'-C1'-N1	8.34	114.87	108.20
26	BB	1052	C	O4'-C1'-N1	8.34	114.87	108.20
26	BB	1015	U	O4'-C1'-N1	8.34	114.87	108.20
26	BB	1849	G	O4'-C1'-N9	8.34	114.87	108.20
26	BB	2707	U	O4'-C1'-N1	8.34	114.87	108.20
26	BB	2240	U	O4'-C1'-N1	8.33	114.87	108.20
1	AA	1388	C	O4'-C1'-N1	8.33	114.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	702	U	O4'-C1'-N1	8.32	114.86	108.20
1	AA	612	C	O4'-C1'-N1	8.32	114.86	108.20
1	AA	1414	U	O4'-C1'-N1	8.32	114.86	108.20
26	BB	2466	C	O4'-C1'-N1	8.32	114.86	108.20
1	AA	294	U	O4'-C1'-N1	8.31	114.85	108.20
26	BB	2178	C	O4'-C1'-N1	8.31	114.85	108.20
26	BB	1196	C	O4'-C1'-N1	8.31	114.85	108.20
26	BB	1916	A	O4'-C1'-N9	8.31	114.85	108.20
26	BB	1871	A	C3'-C2'-C1'	8.30	108.14	101.50
1	AA	206	C	O4'-C1'-N1	8.30	114.84	108.20
1	AA	194	C	C5'-C4'-O4'	8.30	119.06	109.10
26	BB	1303	G	C5'-C4'-C3'	-8.29	102.74	116.00
26	BB	510	C	O4'-C1'-N1	8.29	114.83	108.20
26	BB	165	A	C5'-C4'-C3'	-8.27	102.77	116.00
26	BB	394	C	O4'-C1'-N1	8.27	114.81	108.20
26	BB	934	U	O4'-C1'-N1	8.27	114.81	108.20
26	BB	557	C	O4'-C1'-N1	8.26	114.81	108.20
26	BB	1070	A	C8-N9-C4	-8.26	102.50	105.80
26	BB	967	U	O4'-C1'-N1	8.26	114.81	108.20
26	BB	1372	U	O4'-C1'-N1	8.26	114.81	108.20
26	BB	1612	C	O4'-C1'-N1	8.25	114.80	108.20
26	BB	651	G	O4'-C1'-N9	8.24	114.80	108.20
1	AA	122	G	C5'-C4'-O4'	8.24	118.98	109.10
26	BB	1720	U	O4'-C1'-N1	8.24	114.79	108.20
26	BB	1742	U	O4'-C1'-N1	8.23	114.79	108.20
26	BB	1191	G	O4'-C1'-N9	8.23	114.78	108.20
26	BB	2430	A	O4'-C1'-N9	8.22	114.78	108.20
1	AA	327	A	C5'-C4'-O4'	8.22	118.97	109.10
1	AA	475	C	O4'-C1'-N1	8.22	114.78	108.20
1	AA	456	A	O4'-C1'-N9	8.22	114.77	108.20
1	AA	465	A	O4'-C1'-C2'	-8.21	97.58	105.80
26	BB	58	G	O4'-C1'-N9	8.22	114.77	108.20
1	AA	1190	G	O4'-C1'-N9	8.21	114.77	108.20
1	AA	1196	A	O4'-C1'-N9	8.21	114.77	108.20
1	AA	414	A	O4'-C1'-N9	8.21	114.77	108.20
1	AA	972	C	O4'-C1'-N1	8.21	114.76	108.20
26	BB	305	C	O4'-C1'-N1	8.21	114.77	108.20
26	BB	611	C	O4'-C1'-N1	8.20	114.76	108.20
26	BB	1069	A	O4'-C1'-N9	8.20	114.76	108.20
26	BB	1736	U	O4'-C1'-N1	8.20	114.76	108.20
1	AA	1542	A	O4'-C1'-N9	8.20	114.76	108.20
25	BA	12	C	P-O3'-C3'	8.20	129.53	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AE	22	G	O4'-C1'-N9	8.19	114.75	108.20
1	AA	220	G	O4'-C1'-N9	8.18	114.75	108.20
26	BB	96	C	O4'-C1'-N1	8.18	114.74	108.20
26	BB	135	U	O4'-C1'-N1	8.17	114.74	108.20
1	AA	1479	C	O4'-C1'-N1	8.17	114.74	108.20
26	BB	173	A	O4'-C1'-N9	8.17	114.73	108.20
26	BB	1293	C	O4'-C1'-N1	8.17	114.73	108.20
1	AA	219	U	O4'-C1'-N1	8.16	114.73	108.20
26	BB	2751	G	P-O3'-C3'	8.16	129.50	119.70
26	BB	1351	C	O4'-C1'-N1	8.16	114.73	108.20
26	BB	1359	A	O4'-C1'-N9	8.16	114.73	108.20
1	AA	1086	U	C5'-C4'-C3'	-8.16	102.94	116.00
26	BB	1946	U	O4'-C1'-N1	8.16	114.73	108.20
26	BB	2558	C	O4'-C1'-N1	8.16	114.73	108.20
26	BB	288	U	O4'-C1'-N1	8.16	114.72	108.20
26	BB	331	C	O4'-C1'-N1	8.14	114.72	108.20
26	BB	1402	U	O4'-C1'-N1	8.14	114.71	108.20
26	BB	2215	C	O4'-C1'-N1	8.14	114.71	108.20
1	AA	567	G	O4'-C1'-N9	8.13	114.71	108.20
26	BB	1484	U	O4'-C1'-N1	8.14	114.71	108.20
26	BB	1425	G	O4'-C1'-N9	8.13	114.71	108.20
26	BB	2470	G	O4'-C1'-N9	8.13	114.71	108.20
26	BB	512	G	O4'-C1'-N9	8.12	114.69	108.20
26	BB	2630	G	O4'-C1'-N9	8.12	114.69	108.20
1	AA	419	C	O4'-C1'-N1	8.11	114.69	108.20
1	AA	1480	A	O4'-C1'-N9	8.11	114.69	108.20
26	BB	1185	G	C1'-O4'-C4'	-8.11	103.41	109.90
26	BB	2473	U	O4'-C1'-N1	8.11	114.69	108.20
26	BB	1933	G	O4'-C1'-N9	8.10	114.68	108.20
26	BB	57	C	O4'-C1'-N1	8.09	114.67	108.20
26	BB	1863	G	C5'-C4'-O4'	8.08	118.79	109.10
1	AA	235	C	O4'-C1'-N1	8.07	114.66	108.20
1	AA	963	G	O4'-C1'-N9	8.07	114.66	108.20
1	AA	290	C	C5'-C4'-O4'	8.07	118.78	109.10
26	BB	2054	A	C5'-C4'-C3'	-8.07	103.09	116.00
1	AA	590	U	C5'-C4'-C3'	-8.06	103.10	116.00
26	BB	1231	U	O4'-C1'-N1	8.06	114.65	108.20
26	BB	2825	G	O4'-C1'-N9	8.06	114.65	108.20
26	BB	2769	U	O4'-C1'-N1	8.06	114.65	108.20
26	BB	2724	U	O4'-C1'-N1	8.06	114.65	108.20
1	AA	971	G	C5'-C4'-C3'	-8.05	103.12	116.00
1	AA	1040	U	O4'-C1'-N1	8.05	114.64	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1279	G	O4'-C1'-N9	8.05	114.64	108.20
1	AA	52	C	O4'-C1'-N1	8.05	114.64	108.20
26	BB	1937	A	O4'-C1'-N9	8.04	114.63	108.20
26	BB	2138	G	O4'-C1'-N9	8.04	114.63	108.20
26	BB	344	A	C3'-C2'-C1'	-8.03	95.07	101.50
26	BB	971	G	O4'-C1'-N9	8.03	114.62	108.20
1	AA	701	U	O4'-C1'-N1	8.03	114.62	108.20
25	BA	13	G	C1'-O4'-C4'	-8.03	103.48	109.90
26	BB	1541	C	O4'-C1'-N1	8.03	114.62	108.20
26	BB	1695	G	O4'-C1'-N9	8.03	114.62	108.20
1	AA	613	C	O4'-C1'-N1	8.02	114.62	108.20
1	AA	1377	A	C5'-C4'-O4'	8.02	118.73	109.10
1	AA	711	G	O4'-C1'-N9	8.02	114.61	108.20
26	BB	2479	U	O4'-C1'-N1	8.02	114.61	108.20
26	BB	279	A	O4'-C1'-N9	8.02	114.61	108.20
26	BB	2500	U	O4'-C1'-N1	8.01	114.61	108.20
25	BA	19	C	O4'-C1'-N1	8.01	114.61	108.20
1	AA	726	C	O4'-C1'-N1	8.01	114.60	108.20
26	BB	1621	U	O4'-C1'-N1	8.00	114.60	108.20
26	BB	1575	C	O4'-C1'-N1	8.00	114.60	108.20
26	BB	407	G	O4'-C1'-N9	7.99	114.59	108.20
26	BB	1748	C	O4'-C1'-N1	7.99	114.59	108.20
26	BB	1506	U	O4'-C1'-N1	7.99	114.59	108.20
26	BB	2233	U	O4'-C1'-N1	7.99	114.59	108.20
26	BB	1769	U	O4'-C1'-N1	7.99	114.59	108.20
26	BB	618	G	O4'-C1'-N9	7.99	114.59	108.20
26	BB	915	C	O4'-C1'-N1	7.98	114.59	108.20
1	AA	387	U	O4'-C1'-N1	7.98	114.59	108.20
1	AA	571	U	O4'-C1'-N1	7.98	114.58	108.20
1	AA	1536	C	O4'-C1'-N1	7.98	114.58	108.20
26	BB	225	C	O4'-C1'-N1	7.97	114.58	108.20
1	AA	400	C	O4'-C1'-N1	7.97	114.57	108.20
25	BA	108	A	C1'-O4'-C4'	-7.97	103.53	109.90
2	AB	11	C	C5'-C4'-O4'	7.96	118.66	109.10
1	AA	409	U	O4'-C1'-N1	7.96	114.57	108.20
1	AA	133	U	O4'-C1'-N1	7.96	114.57	108.20
26	BB	1649	G	C5'-C4'-O4'	7.96	118.65	109.10
26	BB	2226	C	O4'-C1'-N1	7.96	114.57	108.20
1	AA	1255	G	O4'-C1'-N9	7.95	114.56	108.20
26	BB	658	U	O4'-C1'-N1	7.95	114.56	108.20
1	AA	1467	C	O4'-C1'-N1	7.95	114.56	108.20
25	BA	107	G	C5'-C4'-C3'	-7.94	103.29	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1323	G	C5'-C4'-O4'	7.94	118.63	109.10
26	BB	226	A	C5'-C4'-O4'	7.94	118.63	109.10
26	BB	1097	U	O4'-C1'-N1	7.93	114.55	108.20
26	BB	1370	C	O4'-C1'-N1	7.93	114.55	108.20
2	AE	41	C	O4'-C1'-N1	7.93	114.54	108.20
26	BB	1529	G	O4'-C1'-N9	7.93	114.54	108.20
26	BB	246	C	O4'-C1'-N1	7.93	114.54	108.20
1	AA	327	A	C1'-O4'-C4'	-7.92	103.56	109.90
26	BB	1394	U	C5'-C4'-C3'	-7.92	103.33	116.00
26	BB	210	C	O4'-C1'-N1	7.92	114.54	108.20
26	BB	1986	C	C5'-C4'-O4'	7.92	118.60	109.10
26	BB	193	U	O4'-C1'-N1	7.92	114.53	108.20
26	BB	1297	C	O4'-C1'-N1	7.92	114.53	108.20
26	BB	1479	G	O4'-C1'-N9	7.92	114.53	108.20
25	BA	105	G	O4'-C1'-N9	7.91	114.53	108.20
26	BB	1657	U	O4'-C1'-N1	7.91	114.53	108.20
26	BB	895	U	P-O3'-C3'	7.90	129.18	119.70
26	BB	415	A	O4'-C1'-N9	7.90	114.52	108.20
26	BB	158	U	O4'-C1'-N1	7.90	114.52	108.20
1	AA	1017	U	O4'-C1'-N1	7.89	114.51	108.20
1	AA	1364	U	O4'-C1'-N1	7.89	114.51	108.20
26	BB	1304	A	O4'-C1'-N9	7.89	114.51	108.20
26	BB	2374	C	O4'-C1'-N1	7.89	114.51	108.20
1	AA	163	C	O4'-C1'-N1	7.89	114.51	108.20
25	BA	86	G	O4'-C1'-N9	7.89	114.51	108.20
26	BB	1056	G	P-O3'-C3'	7.88	129.16	119.70
26	BB	863	A	C8-N9-C4	-7.88	102.65	105.80
1	AA	824	G	C5'-C4'-O4'	7.88	118.55	109.10
1	AA	1218	C	O4'-C1'-N1	7.88	114.50	108.20
25	BA	54	G	C8-N9-C4	-7.87	103.25	106.40
26	BB	1647	U	O3'-P-O5'	-7.87	89.04	104.00
26	BB	1309	G	O4'-C1'-N9	7.87	114.50	108.20
1	AA	126	G	O4'-C1'-N9	7.87	114.50	108.20
26	BB	1055	G	C8-N9-C4	-7.87	103.25	106.40
1	AA	1500	A	O4'-C1'-N9	7.87	114.49	108.20
1	AA	809	G	O4'-C1'-N9	7.87	114.49	108.20
2	AB	42	C	O4'-C1'-N1	7.87	114.49	108.20
1	AA	287	U	O4'-C1'-N1	7.86	114.49	108.20
26	BB	2404	U	O4'-C1'-N1	7.86	114.49	108.20
1	AA	151	A	O4'-C1'-N9	7.86	114.49	108.20
26	BB	2554	U	O4'-C1'-N1	7.86	114.49	108.20
1	AA	646	G	O4'-C1'-N9	7.86	114.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1435	G	O4'-C1'-N9	7.86	114.48	108.20
26	BB	1423	G	O4'-C1'-N9	7.86	114.48	108.20
1	AA	1007	U	O4'-C1'-N1	7.85	114.48	108.20
26	BB	1841	U	O4'-C1'-N1	7.84	114.48	108.20
1	AA	405	U	O4'-C1'-N1	7.84	114.47	108.20
26	BB	119	A	P-O3'-C3'	7.84	129.11	119.70
26	BB	2659	G	O4'-C1'-N9	7.83	114.46	108.20
1	AA	1413	A	O4'-C1'-N9	7.82	114.46	108.20
26	BB	1781	U	O4'-C1'-N1	7.82	114.46	108.20
26	BB	2476	A	O4'-C1'-N9	7.82	114.45	108.20
26	BB	640	C	O4'-C1'-N1	7.81	114.45	108.20
1	AA	1223	C	C4'-C3'-C2'	-7.81	94.79	102.60
26	BB	1832	C	O4'-C1'-N1	7.81	114.45	108.20
26	BB	2758	A	C5'-C4'-O4'	7.81	118.47	109.10
26	BB	1930	G	O4'-C1'-N9	7.80	114.44	108.20
26	BB	2496	C	O4'-C1'-N1	7.80	114.44	108.20
26	BB	694	U	O4'-C1'-N1	7.79	114.44	108.20
26	BB	2461	A	O4'-C1'-N9	7.79	114.43	108.20
26	BB	893	C	O4'-C1'-N1	7.79	114.43	108.20
2	AE	62	C	O4'-C1'-N1	7.78	114.43	108.20
26	BB	1153	C	O4'-C1'-N1	7.78	114.42	108.20
26	BB	1331	G	C8-N9-C4	-7.78	103.29	106.40
26	BB	1643	G	O4'-C1'-N9	7.78	114.43	108.20
1	AA	651	C	C5'-C4'-O4'	7.78	118.44	109.10
26	BB	974	G	O4'-C1'-N9	7.78	114.42	108.20
1	AA	620	C	C5'-C4'-O4'	7.77	118.43	109.10
26	BB	386	G	O4'-C1'-N9	7.77	114.42	108.20
26	BB	1146	C	O4'-C1'-N1	7.77	114.42	108.20
1	AA	401	C	O4'-C1'-N1	7.77	114.42	108.20
26	BB	32	C	O4'-C1'-N1	7.77	114.42	108.20
26	BB	2099	U	O4'-C1'-N1	7.77	114.42	108.20
1	AA	1453	G	O4'-C1'-N9	7.77	114.41	108.20
26	BB	1981	A	O4'-C1'-N9	7.76	114.41	108.20
26	BB	1833	C	O4'-C1'-N1	7.76	114.41	108.20
26	BB	2200	C	O4'-C1'-N1	7.75	114.40	108.20
25	BA	111	U	O4'-C1'-N1	7.75	114.40	108.20
26	BB	2489	U	O4'-C1'-N1	7.75	114.40	108.20
26	BB	239	C	O4'-C1'-N1	7.75	114.40	108.20
26	BB	1522	A	P-O3'-C3'	7.74	128.99	119.70
26	BB	528	A	O4'-C1'-N9	7.74	114.39	108.20
26	BB	360	U	O4'-C1'-N1	7.73	114.39	108.20
26	BB	1609	A	O4'-C1'-N9	7.73	114.39	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	372	G	O4'-C1'-N9	7.73	114.38	108.20
26	BB	2419	U	O4'-C1'-N1	7.73	114.38	108.20
26	BB	2205	A	O4'-C1'-N9	7.73	114.38	108.20
26	BB	2586	U	O4'-C1'-N1	7.72	114.38	108.20
26	BB	1033	U	C5'-C4'-C3'	-7.72	103.64	116.00
26	BB	2711	A	O4'-C1'-N9	7.72	114.38	108.20
1	AA	331	G	O4'-C1'-N9	7.72	114.38	108.20
26	BB	2109	U	O4'-C1'-N1	7.72	114.38	108.20
26	BB	1499	C	O4'-C1'-N1	7.72	114.37	108.20
26	BB	2310	C	O4'-C1'-N1	7.72	114.38	108.20
26	BB	2181	U	O4'-C1'-N1	7.72	114.37	108.20
1	AA	1097	C	O4'-C1'-N1	7.71	114.37	108.20
26	BB	975	A	C5'-C4'-O4'	7.71	118.35	109.10
26	BB	2025	C	O4'-C1'-N1	7.71	114.37	108.20
1	AA	150	U	O4'-C1'-N1	7.71	114.36	108.20
26	BB	2615	U	O4'-C1'-N1	7.71	114.36	108.20
1	AA	518	C	O4'-C1'-N1	7.70	114.36	108.20
1	AA	988	G	O4'-C1'-N9	7.70	114.36	108.20
1	AA	998	C	O4'-C1'-N1	7.70	114.36	108.20
26	BB	1676	A	O4'-C1'-N9	7.70	114.36	108.20
26	BB	2518	A	O4'-C1'-N9	7.70	114.36	108.20
1	AA	414	A	O3'-P-O5'	-7.70	89.38	104.00
26	BB	948	C	O4'-C1'-N1	7.70	114.36	108.20
1	AA	961	U	C5'-C4'-O4'	7.69	118.33	109.10
1	AA	348	G	O4'-C1'-N9	7.69	114.35	108.20
1	AA	812	G	O3'-P-O5'	-7.69	89.39	104.00
26	BB	1180	U	O4'-C1'-N1	7.69	114.35	108.20
1	AA	465	A	C5'-C4'-O4'	7.68	118.32	109.10
1	AA	890	G	O4'-C1'-N9	7.68	114.34	108.20
1	AA	930	C	O4'-C1'-N1	7.68	114.34	108.20
26	BB	1878	G	O4'-C1'-N9	7.68	114.34	108.20
26	BB	259	G	O4'-C1'-N9	7.67	114.34	108.20
26	BB	1462	C	O4'-C1'-N1	7.67	114.34	108.20
26	BB	1183	U	O4'-C1'-N1	7.67	114.33	108.20
1	AA	301	G	O4'-C1'-N9	7.66	114.33	108.20
26	BB	2044	C	O4'-C1'-N1	7.66	114.33	108.20
1	AA	299	G	C8-N9-C4	-7.66	103.34	106.40
26	BB	891	G	O4'-C1'-N9	7.66	114.33	108.20
26	BB	1696	G	O4'-C1'-N9	7.66	114.33	108.20
26	BB	2743	U	O4'-C1'-N1	7.66	114.32	108.20
26	BB	38	A	O4'-C1'-N9	7.65	114.32	108.20
26	BB	1347	A	O4'-C1'-N9	7.65	114.32	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1349	C	O4'-C1'-N1	7.65	114.32	108.20
26	BB	1920	C	O4'-C1'-N1	7.65	114.32	108.20
1	AA	99	C	O4'-C1'-N1	7.64	114.31	108.20
26	BB	424	G	O4'-C1'-N9	7.64	114.31	108.20
1	AA	1216	A	O4'-C1'-N9	7.64	114.31	108.20
1	AA	1356	G	O4'-C1'-N9	7.64	114.31	108.20
1	AA	786	G	O4'-C1'-N9	7.63	114.31	108.20
26	BB	121	G	C8-N9-C4	-7.63	103.35	106.40
26	BB	2515	C	O4'-C1'-N1	7.63	114.30	108.20
26	BB	395	U	O4'-C1'-N1	7.62	114.30	108.20
26	BB	1102	C	O4'-C1'-N1	7.62	114.30	108.20
26	BB	2218	G	O4'-C1'-N9	7.62	114.29	108.20
1	AA	9	G	C8-N9-C4	-7.62	103.35	106.40
26	BB	1271	G	C8-N9-C4	-7.62	103.35	106.40
1	AA	1124	G	O4'-C1'-N9	7.61	114.29	108.20
1	AA	477	C	O4'-C1'-N1	7.61	114.29	108.20
26	BB	2219	U	O4'-C1'-N1	7.61	114.28	108.20
25	BA	91	C	O4'-C1'-N1	7.60	114.28	108.20
26	BB	459	U	O4'-C1'-N1	7.60	114.28	108.20
1	AA	862	C	O4'-C1'-N1	7.59	114.28	108.20
26	BB	2367	G	O4'-C1'-N9	7.59	114.27	108.20
1	AA	68	G	O4'-C1'-N9	7.59	114.27	108.20
26	BB	1792	G	C5'-C4'-O4'	7.59	118.21	109.10
26	BB	2236	U	O4'-C1'-N1	7.59	114.27	108.20
26	BB	157	C	O4'-C1'-N1	7.59	114.27	108.20
1	AA	1071	C	O4'-C1'-N1	7.58	114.27	108.20
1	AA	81	A	O4'-C1'-N9	7.58	114.27	108.20
26	BB	776	G	O4'-C1'-N9	7.58	114.26	108.20
1	AA	507	C	O4'-C1'-N1	7.58	114.26	108.20
26	BB	2760	C	C5'-C4'-C3'	-7.58	103.88	116.00
26	BB	1734	G	O4'-C1'-N9	7.57	114.26	108.20
26	BB	2063	C	O4'-C1'-N1	7.57	114.25	108.20
26	BB	23	G	O4'-C1'-N9	7.57	114.25	108.20
26	BB	1767	G	O4'-C1'-N9	7.57	114.25	108.20
26	BB	583	G	O4'-C1'-N9	7.56	114.25	108.20
26	BB	1234	U	O4'-C1'-N1	7.56	114.25	108.20
25	BA	50	A	C5'-C4'-O4'	7.56	118.17	109.10
26	BB	25	U	O4'-C1'-N1	7.55	114.24	108.20
1	AA	96	U	O4'-C1'-N1	7.55	114.24	108.20
1	AA	682	G	O4'-C1'-N9	7.55	114.24	108.20
26	BB	2205	A	N9-C4-C5	7.55	108.82	105.80
1	AA	270	A	O4'-C1'-N9	7.55	114.24	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	858	G	O4'-C1'-N9	7.55	114.24	108.20
26	BB	2214	C	C5'-C4'-C3'	-7.55	103.92	116.00
26	BB	2299	U	O4'-C1'-N1	7.54	114.24	108.20
26	BB	598	U	O4'-C1'-N1	7.54	114.23	108.20
26	BB	1049	C	O4'-C1'-N1	7.54	114.23	108.20
26	BB	2901	C	O4'-C1'-N1	7.54	114.23	108.20
1	AA	684	U	O4'-C1'-N1	7.54	114.23	108.20
26	BB	1898	U	C5'-C4'-O4'	7.54	118.15	109.10
26	BB	2073	C	O4'-C1'-N1	7.54	114.23	108.20
26	BB	2212	A	N9-C1'-C2'	-7.54	103.71	112.00
26	BB	445	C	O4'-C1'-N1	7.54	114.23	108.20
2	AE	64	A	O4'-C1'-N9	7.54	114.23	108.20
1	AA	1110	A	O4'-C1'-N9	7.53	114.22	108.20
26	BB	894	U	O4'-C1'-N1	7.53	114.23	108.20
26	BB	2265	U	O4'-C1'-N1	7.53	114.22	108.20
1	AA	1380	U	O4'-C1'-N1	7.53	114.22	108.20
26	BB	538	A	O4'-C1'-N9	7.53	114.22	108.20
1	AA	458	U	O4'-C1'-N1	7.53	114.22	108.20
26	BB	1300	G	O4'-C1'-N9	7.53	114.22	108.20
26	BB	1605	C	O4'-C1'-N1	7.53	114.22	108.20
26	BB	2321	U	O4'-C1'-N1	7.52	114.22	108.20
26	BB	11	C	O4'-C1'-N1	7.52	114.22	108.20
26	BB	2406	A	O4'-C1'-N9	7.52	114.22	108.20
1	AA	386	C	C5'-C4'-O4'	7.51	118.11	109.10
1	AA	1235	U	O4'-C1'-N1	7.51	114.21	108.20
26	BB	1578	U	O4'-C1'-N1	7.51	114.21	108.20
26	BB	183	C	O4'-C1'-N1	7.51	114.21	108.20
26	BB	1002	G	O4'-C1'-N9	7.51	114.21	108.20
26	BB	2343	U	O4'-C1'-N1	7.51	114.20	108.20
26	BB	1088	A	O4'-C1'-N9	7.50	114.20	108.20
26	BB	1070	A	C3'-C2'-C1'	7.50	107.50	101.50
26	BB	2342	C	O4'-C1'-N1	7.50	114.20	108.20
1	AA	1458	G	O4'-C1'-N9	7.50	114.20	108.20
26	BB	719	C	O4'-C1'-N1	7.50	114.20	108.20
26	BB	2126	A	O3'-P-O5'	-7.50	89.75	104.00
26	BB	2687	U	O4'-C1'-N1	7.50	114.20	108.20
1	AA	265	G	C8-N9-C4	-7.50	103.40	106.40
1	AA	485	U	O4'-C1'-C2'	-7.49	98.31	105.80
1	AA	952	U	O4'-C1'-N1	7.49	114.19	108.20
26	BB	1912	A	O3'-P-O5'	-7.49	89.76	104.00
26	BB	2215	C	C5'-C4'-O4'	7.49	118.09	109.10
26	BB	2264	C	O4'-C1'-N1	7.49	114.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2853	C	O4'-C1'-N1	7.49	114.19	108.20
1	AA	384	G	O4'-C1'-N9	7.49	114.19	108.20
26	BB	1747	U	O4'-C1'-N1	7.48	114.19	108.20
26	BB	1853	A	O4'-C1'-N9	7.48	114.19	108.20
26	BB	108	G	C5'-C4'-C3'	-7.48	104.03	116.00
26	BB	2213	U	O4'-C1'-N1	7.48	114.18	108.20
1	AA	122	G	C5'-C4'-C3'	-7.47	104.04	116.00
26	BB	841	G	C5'-C4'-O4'	7.47	118.07	109.10
26	BB	1186	G	C5'-C4'-C3'	-7.47	104.05	116.00
26	BB	2015	A	O4'-C1'-N9	7.47	114.17	108.20
26	BB	464	U	O4'-C1'-N1	7.47	114.17	108.20
26	BB	185	G	O4'-C1'-N9	7.46	114.17	108.20
26	BB	2214	C	O4'-C1'-N1	7.46	114.17	108.20
26	BB	1006	C	O4'-C1'-N1	7.46	114.17	108.20
1	AA	1342	C	O4'-C1'-N1	7.46	114.17	108.20
26	BB	2633	G	O4'-C1'-N9	7.46	114.17	108.20
1	AA	1508	A	C5'-C4'-C3'	-7.46	104.07	116.00
1	AA	73	C	O4'-C1'-N1	7.45	114.16	108.20
1	AA	747	A	O4'-C1'-N9	7.45	114.16	108.20
1	AA	1462	C	O4'-C1'-N1	7.45	114.16	108.20
25	BA	33	G	O4'-C1'-N9	7.45	114.16	108.20
1	AA	827	U	O4'-C1'-N1	7.45	114.16	108.20
25	BA	71	C	O4'-C1'-N1	7.45	114.16	108.20
26	BB	2704	C	O4'-C1'-N1	7.45	114.16	108.20
26	BB	2787	C	O4'-C1'-N1	7.45	114.16	108.20
26	BB	1533	C	O4'-C1'-N1	7.45	114.16	108.20
26	BB	1573	G	C8-N9-C4	-7.44	103.42	106.40
26	BB	1907	G	O4'-C1'-N9	7.44	114.15	108.20
1	AA	1147	C	O4'-C1'-N1	7.44	114.15	108.20
26	BB	2140	G	O4'-C1'-N9	7.44	114.15	108.20
2	AE	61	C	O4'-C1'-N1	7.44	114.15	108.20
26	BB	319	G	O4'-C1'-N9	7.44	114.15	108.20
26	BB	1130	U	O4'-C1'-N1	7.44	114.15	108.20
26	BB	556	A	O4'-C1'-N9	7.43	114.15	108.20
1	AA	1058	G	C8-N9-C4	-7.43	103.43	106.40
26	BB	2139	U	O4'-C1'-N1	7.43	114.14	108.20
26	BB	965	C	O4'-C1'-N1	7.43	114.14	108.20
1	AA	254	G	O4'-C1'-N9	7.42	114.14	108.20
1	AA	375	U	O4'-C1'-N1	7.42	114.14	108.20
26	BB	1877	A	O4'-C1'-N9	7.42	114.14	108.20
1	AA	826	C	C3'-C2'-C1'	7.41	107.43	101.50
25	BA	38	C	O4'-C1'-N1	7.41	114.13	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	947	A	O4'-C1'-N9	7.41	114.13	108.20
1	AA	548	G	O4'-C1'-N9	7.41	114.13	108.20
1	AA	245	U	O4'-C1'-N1	7.41	114.12	108.20
26	BB	1691	C	O4'-C1'-N1	7.41	114.12	108.20
26	BB	1909	C	O4'-C1'-N1	7.41	114.12	108.20
26	BB	1982	U	C5'-C4'-O4'	7.40	117.98	109.10
26	BB	2391	G	C1'-O4'-C4'	-7.40	103.98	109.90
1	AA	208	U	O4'-C1'-N1	7.39	114.11	108.20
26	BB	339	U	O4'-C1'-N1	7.39	114.11	108.20
26	BB	581	C	O4'-C1'-N1	7.39	114.11	108.20
26	BB	2311	A	O4'-C1'-N9	7.39	114.12	108.20
26	BB	2684	U	N1-C2-N3	7.39	119.34	114.90
26	BB	984	A	C1'-O4'-C4'	-7.39	103.98	109.90
26	BB	2112	G	C8-N9-C4	-7.39	103.44	106.40
24	AY	1	PRO	CA-N-CD	-7.39	101.16	111.50
1	AA	1115	U	O4'-C1'-N1	7.38	114.11	108.20
26	BB	2811	G	O4'-C1'-N9	7.38	114.11	108.20
26	BB	133	U	O4'-C1'-N1	7.38	114.11	108.20
26	BB	1291	C	O4'-C1'-N1	7.38	114.11	108.20
1	AA	80	A	O4'-C1'-N9	7.38	114.10	108.20
26	BB	35	G	N3-C4-C5	-7.37	124.91	128.60
1	AA	100	G	C5'-C4'-O4'	7.37	117.94	109.10
2	AE	30	G	O4'-C1'-N9	7.37	114.09	108.20
26	BB	769	U	O4'-C1'-N1	7.37	114.09	108.20
26	BB	984	A	O4'-C1'-C2'	-7.37	98.43	105.80
26	BB	2629	U	C3'-C2'-C1'	7.37	107.39	101.50
26	BB	286	U	O4'-C1'-N1	7.37	114.09	108.20
26	BB	1580	A	O4'-C1'-N9	7.37	114.09	108.20
26	BB	1811	G	O4'-C1'-N9	7.36	114.09	108.20
26	BB	1930	G	O5'-C5'-C4'	-7.36	97.72	111.70
26	BB	2020	A	C5'-C4'-O4'	7.36	117.93	109.10
26	BB	2725	A	C8-N9-C4	-7.36	102.86	105.80
26	BB	2556	C	O4'-C1'-N1	7.36	114.09	108.20
26	BB	2610	C	O4'-C1'-N1	7.36	114.08	108.20
26	BB	2664	G	C8-N9-C4	-7.35	103.46	106.40
1	AA	117	G	O4'-C1'-N9	7.35	114.08	108.20
26	BB	559	G	C5'-C4'-O4'	7.35	117.92	109.10
26	BB	1852	U	P-O3'-C3'	7.35	128.52	119.70
1	AA	847	G	C8-N9-C4	-7.34	103.46	106.40
2	AE	42	C	O4'-C1'-N1	7.34	114.07	108.20
26	BB	47	C	O4'-C1'-N1	7.34	114.07	108.20
26	BB	2001	C	O4'-C1'-N1	7.34	114.07	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	827	U	P-O3'-C3'	7.34	128.51	119.70
26	BB	1088	A	C3'-C2'-C1'	7.34	107.37	101.50
26	BB	1112	G	C5'-C4'-O4'	7.34	117.90	109.10
26	BB	2848	G	O4'-C1'-N9	7.34	114.07	108.20
1	AA	1091	U	C5'-C4'-O4'	7.33	117.90	109.10
26	BB	2654	A	O4'-C1'-N9	7.33	114.07	108.20
26	BB	452	G	O4'-C1'-N9	7.33	114.07	108.20
1	AA	837	U	O4'-C1'-N1	7.33	114.06	108.20
1	AA	637	C	O4'-C1'-N1	7.33	114.06	108.20
26	BB	2007	U	O4'-C1'-N1	7.32	114.06	108.20
26	BB	2066	C	O4'-C1'-N1	7.32	114.06	108.20
26	BB	423	A	N1-C6-N6	-7.32	114.21	118.60
26	BB	2189	U	O4'-C1'-N1	7.32	114.06	108.20
26	BB	2804	U	O4'-C1'-N1	7.31	114.05	108.20
1	AA	165	G	C5'-C4'-C3'	-7.31	104.30	116.00
26	BB	1642	G	O4'-C1'-N9	7.31	114.05	108.20
1	AA	1203	C	C5'-C4'-O4'	7.31	117.87	109.10
1	AA	1320	C	C5'-C4'-O4'	7.31	117.87	109.10
1	AA	678	U	O4'-C1'-N1	7.31	114.05	108.20
26	BB	92	U	O4'-C1'-N1	7.31	114.05	108.20
26	BB	2064	C	O4'-C1'-N1	7.30	114.04	108.20
1	AA	78	A	O4'-C1'-N9	7.30	114.04	108.20
26	BB	1361	G	O4'-C1'-N9	7.30	114.04	108.20
26	BB	1874	C	O4'-C1'-N1	7.30	114.04	108.20
26	BB	2819	G	C5'-C4'-C3'	-7.30	104.32	116.00
1	AA	17	U	O4'-C1'-N1	7.30	114.04	108.20
26	BB	2688	G	O4'-C1'-N9	7.30	114.04	108.20
1	AA	848	C	O4'-C1'-N1	7.29	114.04	108.20
26	BB	1724	G	C8-N9-C4	-7.29	103.48	106.40
26	BB	2696	U	C5'-C4'-O4'	7.29	117.85	109.10
26	BB	2760	C	C5'-C4'-O4'	7.29	117.85	109.10
26	BB	547	A	O4'-C1'-N9	7.29	114.03	108.20
26	BB	2133	G	O4'-C1'-N9	7.29	114.03	108.20
25	BA	120	U	O4'-C1'-N1	7.29	114.03	108.20
26	BB	992	C	O4'-C1'-N1	7.28	114.03	108.20
2	AE	2	C	O4'-C1'-N1	7.28	114.02	108.20
26	BB	2716	C	O4'-C1'-N1	7.28	114.02	108.20
1	AA	180	U	O4'-C1'-N1	7.28	114.02	108.20
26	BB	444	C	O4'-C1'-N1	7.28	114.02	108.20
26	BB	1634	A	O4'-C1'-N9	7.27	114.02	108.20
26	BB	2011	U	O4'-C1'-N1	7.27	114.02	108.20
26	BB	1652	A	C5'-C4'-C3'	-7.27	104.38	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1399	C	O4'-C1'-N1	7.26	114.01	108.20
26	BB	363	G	C5'-C4'-C3'	-7.26	104.38	116.00
26	BB	2685	G	O4'-C1'-N9	7.26	114.01	108.20
1	AA	403	C	O4'-C1'-N1	7.26	114.01	108.20
26	BB	961	C	O4'-C1'-N1	7.26	114.01	108.20
1	AA	218	U	O4'-C1'-N1	7.26	114.00	108.20
26	BB	720	U	C5'-C4'-O4'	7.26	117.81	109.10
26	BB	131	A	O4'-C1'-N9	7.25	114.00	108.20
26	BB	1516	G	O4'-C1'-N9	7.25	114.00	108.20
1	AA	1151	A	O4'-C1'-N9	7.25	114.00	108.20
1	AA	737	C	O4'-C1'-N1	7.25	114.00	108.20
26	BB	242	G	O4'-C1'-N9	7.24	113.99	108.20
1	AA	1339	A	O4'-C1'-N9	7.24	113.99	108.20
26	BB	285	G	O4'-C1'-N9	7.24	113.99	108.20
26	BB	797	G	O4'-C1'-N9	7.24	113.99	108.20
26	BB	1928	A	O4'-C1'-N9	7.24	113.99	108.20
1	AA	690	G	O4'-C1'-N9	7.24	113.99	108.20
26	BB	1879	C	O4'-C1'-N1	7.24	113.99	108.20
1	AA	44	A	O4'-C1'-N9	7.23	113.99	108.20
25	BA	100	G	N7-C8-N9	7.23	116.71	113.10
26	BB	1513	U	O4'-C1'-N1	7.22	113.98	108.20
26	BB	1670	C	O4'-C1'-N1	7.22	113.98	108.20
26	BB	1073	A	C5'-C4'-O4'	7.22	117.77	109.10
26	BB	494	G	O4'-C1'-N9	7.22	113.98	108.20
26	BB	603	A	O4'-C1'-N9	7.22	113.98	108.20
26	BB	196	A	O4'-C1'-N9	7.22	113.97	108.20
1	AA	123	U	O4'-C1'-N1	7.21	113.97	108.20
26	BB	2798	U	O4'-C1'-N1	7.21	113.97	108.20
26	BB	1318	U	O4'-C1'-N1	7.21	113.97	108.20
26	BB	2147	A	O4'-C1'-N9	7.21	113.97	108.20
1	AA	1182	G	C8-N9-C4	-7.20	103.52	106.40
26	BB	2352	A	C5'-C4'-O4'	7.20	117.75	109.10
1	AA	543	U	O4'-C1'-N1	7.20	113.96	108.20
1	AA	111	G	O4'-C1'-N9	7.20	113.96	108.20
1	AA	469	C	O4'-C1'-N1	7.20	113.96	108.20
26	BB	1109	C	O4'-C1'-N1	7.20	113.96	108.20
26	BB	1392	A	O4'-C1'-N9	-7.19	102.45	108.20
26	BB	701	G	O4'-C1'-N9	7.19	113.95	108.20
1	AA	1534	A	C1'-O4'-C4'	-7.19	104.15	109.90
26	BB	817	C	O4'-C1'-N1	7.19	113.95	108.20
1	AA	1460	C	O4'-C1'-N1	7.19	113.95	108.20
26	BB	772	C	O4'-C1'-N1	7.19	113.95	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	970	C	C5'-C4'-O4'	7.18	117.72	109.10
1	AA	1410	A	O4'-C1'-N9	7.18	113.95	108.20
26	BB	683	U	O4'-C1'-N1	7.18	113.95	108.20
26	BB	2026	U	O4'-C1'-N1	7.18	113.94	108.20
1	AA	415	A	O4'-C1'-N9	7.18	113.94	108.20
25	BA	34	A	N9-C4-C5	7.18	108.67	105.80
26	BB	172	A	O4'-C1'-N9	7.18	113.94	108.20
26	BB	874	G	O4'-C1'-N9	7.18	113.94	108.20
26	BB	889	C	O4'-C1'-N1	7.18	113.94	108.20
26	BB	1854	A	O4'-C1'-N9	7.18	113.94	108.20
26	BB	21	A	O4'-C1'-N9	7.18	113.94	108.20
26	BB	341	C	O4'-C1'-N1	7.17	113.94	108.20
1	AA	883	C	O4'-C1'-N1	7.17	113.94	108.20
1	AA	1449	C	O4'-C1'-N1	7.17	113.94	108.20
1	AA	490	C	O4'-C1'-N1	7.17	113.94	108.20
1	AA	582	C	O4'-C1'-N1	7.17	113.94	108.20
26	BB	1144	A	O4'-C1'-N9	7.17	113.93	108.20
26	BB	1188	U	O4'-C1'-N1	7.17	113.93	108.20
2	AE	18	G	O4'-C1'-N9	7.17	113.93	108.20
26	BB	657	U	C3'-C2'-C1'	7.17	107.23	101.50
1	AA	369	G	O4'-C1'-N9	7.16	113.93	108.20
1	AA	1541	U	O5'-C5'-C4'	-7.16	98.09	111.70
26	BB	1159	U	O4'-C1'-N1	7.16	113.93	108.20
1	AA	269	C	O4'-C1'-N1	7.16	113.92	108.20
26	BB	266	G	C8-N9-C4	-7.15	103.54	106.40
1	AA	1086	U	C5'-C4'-O4'	7.15	117.68	109.10
26	BB	2884	U	C5'-C4'-C3'	-7.15	104.56	116.00
26	BB	1069	A	C4'-C3'-C2'	-7.15	95.45	102.60
26	BB	601	C	O4'-C1'-N1	7.14	113.92	108.20
26	BB	1162	G	O4'-C1'-N9	7.14	113.92	108.20
26	BB	560	C	O4'-C1'-N1	7.14	113.91	108.20
26	BB	1511	G	O4'-C1'-N9	7.14	113.91	108.20
26	BB	297	G	O4'-C1'-N9	7.14	113.91	108.20
2	AB	22	G	O4'-C1'-N9	7.14	113.91	108.20
1	AA	923	A	O4'-C1'-N9	7.14	113.91	108.20
1	AA	13	U	O4'-C1'-N1	7.13	113.91	108.20
1	AA	662	U	O4'-C1'-N1	7.13	113.91	108.20
26	BB	2568	U	O4'-C1'-N1	7.13	113.91	108.20
1	AA	1424	U	O4'-C1'-N1	7.13	113.91	108.20
26	BB	2617	U	O4'-C1'-N1	7.13	113.90	108.20
1	AA	956	U	O4'-C1'-N1	7.13	113.90	108.20
1	AA	1105	A	O4'-C1'-N9	7.13	113.90	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2456	C	O4'-C1'-N1	7.13	113.90	108.20
1	AA	342	C	O4'-C1'-N1	7.12	113.90	108.20
4	AD	36	U	O4'-C1'-N1	7.12	113.90	108.20
26	BB	151	C	O4'-C1'-N1	7.12	113.89	108.20
1	AA	558	G	O4'-C1'-N9	7.11	113.89	108.20
26	BB	942	G	C8-N9-C4	-7.11	103.56	106.40
1	AA	1533	C	C5'-C4'-O4'	7.11	117.63	109.10
26	BB	1600	C	O4'-C1'-N1	7.11	113.89	108.20
26	BB	1872	A	C8-N9-C4	-7.11	102.96	105.80
26	BB	1991	U	O4'-C1'-N1	7.10	113.88	108.20
1	AA	286	C	O4'-C1'-N1	7.10	113.88	108.20
2	AE	56	C	O4'-C1'-N1	7.10	113.88	108.20
26	BB	314	C	O4'-C1'-N1	7.10	113.88	108.20
26	BB	20	C	O4'-C1'-N1	7.10	113.88	108.20
26	BB	765	C	O4'-C1'-N1	7.10	113.88	108.20
26	BB	2629	U	O4'-C4'-C3'	7.10	111.78	106.10
26	BB	2890	G	O4'-C1'-N9	7.10	113.88	108.20
26	BB	1012	U	O4'-C1'-N1	7.10	113.88	108.20
1	AA	1051	C	O4'-C1'-N1	7.09	113.88	108.20
26	BB	2818	U	O4'-C1'-N1	7.09	113.88	108.20
1	AA	1355	G	O4'-C1'-N9	7.09	113.87	108.20
2	AB	44	G	C8-N9-C4	-7.09	103.56	106.40
26	BB	1584	U	O4'-C1'-N1	7.09	113.87	108.20
26	BB	2193	G	O4'-C1'-N9	7.09	113.87	108.20
26	BB	139	U	O4'-C1'-N1	7.09	113.87	108.20
26	BB	1177	G	C5'-C4'-O4'	7.09	117.60	109.10
26	BB	1752	C	O4'-C1'-N1	7.09	113.87	108.20
26	BB	1881	C	O4'-C1'-N1	7.08	113.86	108.20
26	BB	1573	G	C5'-C4'-O4'	7.08	117.59	109.10
26	BB	2401	U	O4'-C1'-N1	7.08	113.86	108.20
26	BB	2395	C	O4'-C1'-N1	7.08	113.86	108.20
1	AA	233	C	O4'-C1'-N1	7.08	113.86	108.20
26	BB	2699	C	O4'-C1'-N1	7.08	113.86	108.20
26	BB	1177	G	C8-N9-C4	-7.07	103.57	106.40
26	BB	1746	A	O3'-P-O5'	-7.07	90.56	104.00
26	BB	774	G	C8-N9-C4	-7.07	103.57	106.40
1	AA	1315	U	C5'-C4'-O4'	7.07	117.58	109.10
26	BB	174	U	O4'-C1'-N1	7.07	113.86	108.20
1	AA	811	C	O4'-C1'-N1	7.07	113.85	108.20
26	BB	1989	G	O4'-C1'-N9	7.07	113.85	108.20
26	BB	2164	C	O4'-C1'-N1	7.07	113.85	108.20
1	AA	1021	A	O4'-C1'-N9	7.06	113.85	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	4	C	O4'-C1'-N1	7.06	113.85	108.20
26	BB	393	C	O4'-C1'-N1	7.06	113.85	108.20
26	BB	109	C	O4'-C1'-N1	7.06	113.84	108.20
26	BB	2528	U	O4'-C1'-N1	7.06	113.84	108.20
1	AA	1328	C	O4'-C1'-N1	7.05	113.84	108.20
26	BB	399	U	O4'-C1'-N1	7.05	113.84	108.20
26	BB	2512	C	O4'-C1'-N1	7.05	113.84	108.20
26	BB	1104	C	C6-N1-C2	-7.05	117.48	120.30
26	BB	441	U	O4'-C1'-N1	7.05	113.84	108.20
1	AA	367	U	O4'-C4'-C3'	7.05	111.74	106.10
26	BB	627	A	O4'-C1'-N9	7.05	113.84	108.20
26	BB	1480	C	O4'-C1'-N1	7.04	113.83	108.20
26	BB	616	A	C5'-C4'-C3'	-7.04	104.74	116.00
1	AA	623	C	O4'-C1'-N1	7.04	113.83	108.20
26	BB	2405	G	O4'-C1'-N9	7.04	113.83	108.20
26	BB	2852	G	O4'-C1'-N9	7.04	113.83	108.20
2	AB	49	C	O4'-C1'-N1	7.03	113.83	108.20
26	BB	2302	U	C5'-C4'-O4'	7.03	117.54	109.10
2	AE	35	A	C5'-C4'-O4'	7.03	117.54	109.10
1	AA	694	A	O4'-C1'-N9	7.03	113.82	108.20
26	BB	147	C	O4'-C1'-N1	7.03	113.82	108.20
1	AA	650	G	O4'-C1'-N9	7.03	113.82	108.20
1	AA	1279	G	C3'-C2'-C1'	7.03	107.12	101.50
26	BB	1822	C	O4'-C1'-N1	7.03	113.82	108.20
1	AA	1380	U	N3-C2-O2	-7.02	117.28	122.20
26	BB	570	G	O4'-C1'-N9	7.02	113.82	108.20
25	BA	16	G	N3-C4-C5	-7.02	125.09	128.60
26	BB	913	U	O4'-C1'-N1	7.02	113.81	108.20
26	BB	867	C	O4'-C1'-N1	7.02	113.81	108.20
1	AA	585	G	C5'-C4'-O4'	7.02	117.52	109.10
1	AA	465	A	C5'-C4'-C3'	-7.01	104.78	116.00
26	BB	1537	G	O4'-C1'-N9	7.01	113.81	108.20
1	AA	551	U	O4'-C1'-N1	7.01	113.81	108.20
26	BB	170	U	O4'-C1'-N1	7.01	113.81	108.20
26	BB	2085	U	O4'-C1'-N1	7.01	113.81	108.20
26	BB	644	A	O4'-C1'-N9	7.01	113.81	108.20
26	BB	1242	U	O4'-C1'-N1	7.01	113.81	108.20
26	BB	1871	A	C5'-C4'-C3'	-7.01	104.78	116.00
26	BB	66	C	O4'-C1'-N1	7.00	113.80	108.20
1	AA	12	U	O4'-C1'-N1	7.00	113.80	108.20
1	AA	1117	A	C5'-C4'-C3'	-7.00	104.80	116.00
1	AA	804	U	O4'-C1'-N1	7.00	113.80	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	481	G	O4'-C1'-N9	7.00	113.80	108.20
26	BB	1551	A	O4'-C1'-N9	7.00	113.80	108.20
26	BB	1554	U	O4'-C1'-N1	7.00	113.80	108.20
26	BB	1069	A	C1'-O4'-C4'	-7.00	104.30	109.90
26	BB	2731	G	C8-N9-C4	-7.00	103.60	106.40
1	AA	845	A	O4'-C1'-N9	7.00	113.80	108.20
26	BB	803	U	O4'-C1'-N1	7.00	113.80	108.20
26	BB	2257	U	O4'-C1'-N1	6.99	113.79	108.20
26	BB	2702	G	C5'-C4'-C3'	-6.99	104.81	116.00
4	AD	31	U	C5'-C4'-O4'	6.99	117.49	109.10
1	AA	524	G	O4'-C1'-N9	6.99	113.79	108.20
1	AA	512	U	O4'-C1'-N1	6.98	113.78	108.20
26	BB	2460	U	O4'-C1'-N1	6.98	113.78	108.20
1	AA	1409	C	O4'-C1'-N1	6.97	113.78	108.20
26	BB	214	G	C8-N9-C4	-6.97	103.61	106.40
26	BB	660	C	C5'-C4'-C3'	-6.97	104.84	116.00
26	BB	789	A	C5'-C4'-C3'	-6.97	104.84	116.00
26	BB	1686	C	O4'-C1'-N1	6.97	113.78	108.20
1	AA	194	C	C5'-C4'-C3'	-6.97	104.85	116.00
1	AA	1454	G	O4'-C1'-N9	6.97	113.78	108.20
26	BB	2647	U	O4'-C1'-N1	6.97	113.77	108.20
1	AA	882	C	O4'-C1'-N1	6.96	113.77	108.20
1	AA	810	C	O4'-C1'-N1	6.96	113.77	108.20
1	AA	1148	U	O4'-C1'-N1	6.96	113.77	108.20
1	AA	1440	U	O4'-C1'-N1	6.96	113.77	108.20
1	AA	271	C	C5'-C4'-O4'	6.96	117.45	109.10
26	BB	839	U	O3'-P-O5'	-6.96	90.78	104.00
26	BB	1221	C	O4'-C1'-N1	6.96	113.77	108.20
26	BB	2718	G	C5'-C4'-O4'	6.96	117.45	109.10
26	BB	865	C	O4'-C1'-N1	6.95	113.76	108.20
26	BB	1844	C	O4'-C1'-N1	6.95	113.76	108.20
1	AA	1258	G	O4'-C1'-N9	6.95	113.76	108.20
26	BB	497	A	O4'-C1'-N9	6.95	113.76	108.20
26	BB	424	G	C5'-C4'-C3'	-6.95	104.89	116.00
2	AB	15	G	C8-N9-C4	-6.95	103.62	106.40
1	AA	89	U	O4'-C1'-N1	6.94	113.75	108.20
26	BB	529	A	C1'-O4'-C4'	-6.94	104.35	109.90
26	BB	1148	U	O4'-C1'-N1	6.94	113.75	108.20
1	AA	426	U	O4'-C1'-N1	6.94	113.75	108.20
25	BA	41	G	O4'-C1'-N9	6.94	113.75	108.20
26	BB	296	U	O4'-C1'-N1	6.94	113.75	108.20
26	BB	462	C	O4'-C1'-N1	6.94	113.75	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	3	U	O4'-C1'-N1	6.94	113.75	108.20
26	BB	1396	U	O4'-C1'-N1	6.94	113.75	108.20
1	AA	597	G	C8-N9-C4	-6.93	103.63	106.40
1	AA	1506	U	O4'-C1'-N1	6.93	113.75	108.20
26	BB	1562	U	O4'-C1'-N1	6.93	113.75	108.20
26	BB	53	A	O4'-C1'-N9	6.93	113.74	108.20
26	BB	253	C	C5'-C4'-O4'	6.93	117.41	109.10
1	AA	1372	U	O4'-C1'-N1	6.93	113.74	108.20
1	AA	1092	A	C8-N9-C4	-6.92	103.03	105.80
26	BB	358	U	O4'-C1'-N1	6.92	113.74	108.20
26	BB	1078	U	O4'-C1'-N1	6.92	113.74	108.20
26	BB	2197	U	O4'-C1'-N1	6.92	113.74	108.20
26	BB	2244	U	O4'-C1'-N1	6.92	113.74	108.20
26	BB	280	U	O4'-C1'-N1	6.92	113.74	108.20
26	BB	347	A	C8-N9-C4	-6.92	103.03	105.80
1	AA	655	A	O4'-C1'-N9	6.92	113.74	108.20
1	AA	1117	A	C5'-C4'-O4'	6.92	117.40	109.10
26	BB	416	U	C5'-C4'-O4'	6.92	117.40	109.10
26	BB	1283	G	C8-N9-C4	-6.92	103.63	106.40
26	BB	2188	U	O4'-C1'-N1	6.92	113.73	108.20
1	AA	48	C	O4'-C1'-N1	6.92	113.73	108.20
26	BB	2622	U	C5'-C4'-O4'	6.92	117.40	109.10
1	AA	215	C	C5'-C4'-C3'	-6.91	104.94	116.00
1	AA	782	A	O4'-C1'-N9	6.91	113.73	108.20
2	AB	19	G	N3-C4-C5	-6.91	125.14	128.60
26	BB	238	C	C5'-C4'-O4'	6.91	117.39	109.10
26	BB	1080	A	O4'-C1'-N9	6.91	113.73	108.20
26	BB	184	C	O4'-C1'-N1	6.91	113.73	108.20
25	BA	32	U	O4'-C1'-N1	6.90	113.72	108.20
26	BB	2419	U	C5'-C4'-O4'	6.90	117.38	109.10
26	BB	2500	U	P-O3'-C3'	6.90	127.98	119.70
26	BB	2651	C	O4'-C1'-N1	6.90	113.72	108.20
26	BB	2174	C	O4'-C1'-N1	6.90	113.72	108.20
26	BB	2549	G	O4'-C1'-N9	6.89	113.72	108.20
26	BB	2079	U	O4'-C1'-N1	6.89	113.71	108.20
26	BB	423	A	N9-C4-C5	6.89	108.56	105.80
2	AE	67	C	O4'-C1'-N1	6.89	113.71	108.20
26	BB	650	C	O4'-C1'-N1	6.89	113.71	108.20
1	AA	1389	C	O4'-C1'-N1	6.89	113.71	108.20
26	BB	276	U	O4'-C1'-N1	6.89	113.71	108.20
26	BB	2207	C	O4'-C1'-N1	6.89	113.71	108.20
26	BB	1348	C	O4'-C1'-N1	6.89	113.71	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1411	U	O4'-C1'-N1	6.89	113.71	108.20
26	BB	1067	A	O4'-C1'-N9	6.88	113.71	108.20
26	BB	1209	U	N1-C1'-C2'	-6.88	104.43	112.00
1	AA	659	U	O4'-C1'-N1	6.88	113.70	108.20
1	AA	884	U	O4'-C1'-N1	6.88	113.70	108.20
26	BB	1560	G	C8-N9-C4	-6.88	103.65	106.40
26	BB	2753	A	C8-N9-C4	-6.88	103.05	105.80
26	BB	417	C	O4'-C1'-N1	6.88	113.70	108.20
26	BB	2293	G	O4'-C1'-N9	6.88	113.70	108.20
1	AA	361	G	O4'-C1'-N9	6.88	113.70	108.20
1	AA	273	U	O4'-C1'-N1	6.87	113.70	108.20
1	AA	1137	C	C5'-C4'-C3'	-6.87	105.00	116.00
26	BB	622	G	O4'-C1'-N9	6.87	113.69	108.20
26	BB	790	U	O4'-C1'-N1	6.87	113.69	108.20
26	BB	1523	U	C4'-C3'-C2'	-6.87	95.73	102.60
26	BB	2869	G	O4'-C1'-N9	6.87	113.69	108.20
1	AA	211	G	N3-C4-C5	-6.86	125.17	128.60
26	BB	1727	C	C5'-C4'-O4'	6.86	117.33	109.10
1	AA	266	G	O4'-C1'-N9	6.86	113.69	108.20
1	AA	92	U	O4'-C1'-N1	6.86	113.69	108.20
26	BB	1199	U	O4'-C1'-N1	6.86	113.69	108.20
1	AA	991	U	C5'-C4'-O4'	6.85	117.32	109.10
26	BB	1722	A	C5'-C4'-C3'	-6.85	105.04	116.00
26	BB	2411	A	C5'-C4'-O4'	6.85	117.32	109.10
1	AA	1162	C	O4'-C1'-N1	6.85	113.68	108.20
26	BB	555	G	C8-N9-C4	-6.85	103.66	106.40
1	AA	1103	C	O4'-C1'-N1	6.84	113.67	108.20
26	BB	490	C	O4'-C4'-C3'	6.84	111.57	106.10
26	BB	672	C	O4'-C1'-N1	6.84	113.67	108.20
26	BB	2097	A	O4'-C1'-N9	6.84	113.67	108.20
26	BB	1895	C	O4'-C1'-N1	6.84	113.67	108.20
26	BB	2751	G	C1'-O4'-C4'	-6.84	104.43	109.90
1	AA	909	A	C8-N9-C4	-6.84	103.06	105.80
25	BA	5	U	O4'-C1'-N1	6.84	113.67	108.20
26	BB	1827	U	O4'-C1'-N1	6.84	113.67	108.20
26	BB	1340	U	O4'-C1'-N1	6.84	113.67	108.20
26	BB	1384	A	O4'-C1'-N9	-6.84	102.73	108.20
26	BB	1525	A	O4'-C1'-N9	6.84	113.67	108.20
26	BB	160	A	C5'-C4'-C3'	-6.83	105.06	116.00
26	BB	291	G	O3'-P-O5'	-6.83	91.01	104.00
26	BB	811	U	O4'-C1'-N1	6.83	113.67	108.20
26	BB	1331	G	N3-C4-C5	-6.83	125.18	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1588	G	O4'-C1'-N9	6.83	113.67	108.20
26	BB	1856	U	O4'-C1'-N1	6.83	113.67	108.20
26	BB	2780	G	C8-N9-C4	-6.83	103.67	106.40
26	BB	1524	G	C8-N9-C4	-6.83	103.67	106.40
1	AA	1374	A	O4'-C1'-N9	6.83	113.66	108.20
26	BB	481	G	C8-N9-C4	-6.83	103.67	106.40
1	AA	884	U	C1'-O4'-C4'	-6.82	104.44	109.90
26	BB	493	G	O4'-C1'-N9	6.82	113.66	108.20
26	BB	1706	C	O4'-C1'-N1	6.82	113.66	108.20
26	BB	813	U	O4'-C1'-N1	6.82	113.66	108.20
26	BB	2091	C	O4'-C1'-N1	6.82	113.66	108.20
1	AA	1520	C	O4'-C1'-N1	6.82	113.65	108.20
26	BB	357	C	O4'-C1'-N1	6.82	113.65	108.20
26	BB	848	C	O4'-C1'-N1	6.82	113.65	108.20
1	AA	686	U	O4'-C1'-N1	6.81	113.65	108.20
1	AA	570	G	O4'-C1'-N9	6.81	113.65	108.20
26	BB	433	C	O4'-C1'-N1	6.81	113.65	108.20
1	AA	296	U	C5'-C4'-C3'	-6.81	105.11	116.00
26	BB	919	U	O4'-C1'-N1	6.81	113.65	108.20
26	BB	1634	A	O3'-P-O5'	-6.81	91.06	104.00
1	AA	406	G	N3-C4-C5	-6.81	125.20	128.60
1	AA	525	C	C5'-C4'-O4'	6.81	117.27	109.10
26	BB	607	U	O4'-C1'-N1	6.81	113.65	108.20
26	BB	779	U	O4'-C1'-N1	6.81	113.65	108.20
26	BB	815	C	C3'-C2'-C1'	6.81	106.95	101.50
26	BB	1058	U	O4'-C1'-N1	6.81	113.64	108.20
1	AA	1073	U	O4'-C1'-N1	6.81	113.64	108.20
1	AA	1319	A	C5'-C4'-C3'	-6.80	105.11	116.00
26	BB	884	U	O4'-C1'-N1	6.80	113.64	108.20
26	BB	1332	G	O4'-C1'-N9	6.80	113.64	108.20
1	AA	1448	C	O4'-C1'-N1	6.80	113.64	108.20
26	BB	595	C	O4'-C1'-N1	6.80	113.64	108.20
26	BB	2442	C	O4'-C1'-N1	6.80	113.64	108.20
26	BB	1453	A	O4'-C1'-N9	6.80	113.64	108.20
1	AA	538	G	O4'-C1'-N9	6.80	113.64	108.20
1	AA	147	G	C8-N9-C4	-6.79	103.68	106.40
1	AA	838	G	C8-N9-C4	-6.79	103.68	106.40
1	AA	823	C	O4'-C1'-N1	6.79	113.63	108.20
26	BB	403	U	O4'-C1'-N1	6.79	113.63	108.20
1	AA	907	A	C5'-C4'-C3'	-6.79	105.14	116.00
26	BB	2751	G	C2'-C3'-O3'	6.79	124.56	113.70
1	AA	25	C	O4'-C1'-N1	6.78	113.63	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1492	G	O4'-C1'-N9	6.78	113.63	108.20
26	BB	2799	A	C3'-C2'-C1'	-6.78	96.07	101.50
1	AA	1006	G	O4'-C1'-N9	6.78	113.62	108.20
26	BB	2043	C	C5'-C4'-C3'	-6.78	105.15	116.00
1	AA	259	G	O4'-C1'-N9	6.78	113.62	108.20
1	AA	1244	G	O4'-C1'-N9	6.78	113.62	108.20
26	BB	970	U	O4'-C1'-N1	6.78	113.62	108.20
1	AA	844	G	O4'-C1'-N9	6.78	113.62	108.20
26	BB	1073	A	C5'-C4'-C3'	-6.78	105.16	116.00
2	AB	3	C	O4'-C1'-N1	6.78	113.62	108.20
26	BB	1145	C	C5'-C4'-O4'	6.78	117.23	109.10
1	AA	574	A	O4'-C1'-N9	6.77	113.62	108.20
26	BB	1709	U	C5'-C4'-O4'	6.77	117.23	109.10
26	BB	2698	U	O4'-C1'-N1	6.77	113.62	108.20
2	AB	5	G	O4'-C1'-N9	6.77	113.62	108.20
26	BB	333	G	N3-C4-C5	-6.77	125.22	128.60
1	AA	1059	C	O4'-C1'-N1	6.77	113.61	108.20
26	BB	418	C	O4'-C1'-N1	6.77	113.61	108.20
26	BB	1482	G	O4'-C1'-N9	6.77	113.62	108.20
26	BB	1652	A	C5'-C4'-O4'	6.77	117.22	109.10
26	BB	1662	U	O4'-C1'-N1	6.77	113.62	108.20
1	AA	328	C	N1-C2-O2	6.77	122.96	118.90
26	BB	1119	U	O4'-C1'-N1	6.77	113.61	108.20
1	AA	327	A	C5'-C4'-C3'	-6.76	105.18	116.00
1	AA	46	G	O4'-C1'-N9	6.76	113.61	108.20
26	BB	416	U	O4'-C1'-N1	6.76	113.61	108.20
26	BB	153	U	O4'-C1'-N1	6.76	113.61	108.20
26	BB	834	G	N3-C4-C5	-6.76	125.22	128.60
1	AA	85	U	O4'-C1'-N1	6.75	113.60	108.20
26	BB	231	A	O4'-C1'-N9	6.75	113.60	108.20
26	BB	1339	G	O3'-P-O5'	6.75	116.83	104.00
26	BB	1796	U	O4'-C1'-N1	6.75	113.60	108.20
1	AA	60	A	C2'-C3'-O3'	6.75	124.50	113.70
1	AA	1415	G	O4'-C1'-N9	6.75	113.60	108.20
26	BB	1786	A	C5'-C4'-O4'	6.75	117.20	109.10
26	BB	2723	C	O4'-C1'-N1	6.75	113.60	108.20
26	BB	1573	G	O4'-C1'-N9	6.75	113.60	108.20
26	BB	2819	G	C5'-C4'-O4'	6.75	117.20	109.10
26	BB	1403	A	O4'-C1'-N9	6.75	113.60	108.20
26	BB	1594	U	O4'-C1'-N1	6.74	113.59	108.20
1	AA	1213	A	P-O3'-C3'	6.74	127.79	119.70
26	BB	2370	G	O4'-C1'-N9	6.74	113.59	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	171	U	O4'-C1'-N1	6.74	113.59	108.20
26	BB	1501	G	N9-C4-C5	6.74	108.09	105.40
26	BB	2788	C	O4'-C1'-N1	6.74	113.59	108.20
26	BB	1523	U	P-O3'-C3'	6.74	127.78	119.70
1	AA	1138	G	O4'-C1'-N9	6.74	113.59	108.20
2	AE	29	G	C5'-C4'-O4'	6.74	117.18	109.10
26	BB	335	C	O4'-C1'-N1	6.74	113.59	108.20
26	BB	2089	C	O4'-C1'-N1	6.74	113.59	108.20
26	BB	2692	G	C4'-C3'-C2'	-6.74	95.86	102.60
1	AA	1002	G	O4'-C1'-N9	6.73	113.59	108.20
1	AA	1385	G	C5'-C4'-O4'	6.73	117.18	109.10
1	AA	1075	U	O4'-C1'-N1	6.73	113.58	108.20
1	AA	1292	G	O4'-C1'-N9	6.73	113.58	108.20
1	AA	621	A	C5'-C4'-O4'	6.73	117.17	109.10
2	AE	68	C	O4'-C1'-N1	6.73	113.58	108.20
26	BB	1930	G	C3'-C2'-C1'	6.73	106.88	101.50
1	AA	291	U	O4'-C1'-N1	6.73	113.58	108.20
1	AA	1303	C	O4'-C1'-N1	6.73	113.58	108.20
1	AA	850	U	O4'-C1'-N1	6.72	113.58	108.20
25	BA	85	G	O4'-C1'-N9	6.72	113.58	108.20
1	AA	421	U	O4'-C1'-N1	6.72	113.58	108.20
26	BB	1784	A	O4'-C1'-N9	6.72	113.58	108.20
26	BB	277	G	C5'-C4'-O4'	6.72	117.17	109.10
1	AA	11	G	C5'-C4'-O4'	6.72	117.16	109.10
1	AA	97	G	C8-N9-C4	-6.72	103.71	106.40
25	BA	70	C	O4'-C1'-N1	6.72	113.58	108.20
26	BB	872	U	O4'-C1'-N1	6.72	113.58	108.20
26	BB	1758	U	O4'-C1'-N1	6.72	113.58	108.20
26	BB	2770	G	O4'-C1'-N9	6.72	113.57	108.20
1	AA	1281	C	O4'-C1'-N1	6.72	113.57	108.20
26	BB	895	U	C4'-C3'-O3'	-6.72	95.30	109.40
26	BB	2488	G	C8-N9-C4	-6.72	103.71	106.40
1	AA	868	C	O4'-C1'-N1	6.71	113.57	108.20
26	BB	2799	A	C5'-C4'-O4'	6.71	117.16	109.10
1	AA	154	U	O4'-C1'-N1	6.71	113.57	108.20
2	AE	10	G	N3-C4-C5	-6.71	125.25	128.60
26	BB	2838	G	C5'-C4'-O4'	6.71	117.15	109.10
1	AA	1173	U	C5'-C4'-C3'	-6.71	105.27	116.00
26	BB	896	A	O3'-P-O5'	-6.71	91.26	104.00
26	BB	1303	G	C5'-C4'-O4'	6.71	117.15	109.10
26	BB	2329	U	O4'-C1'-N1	6.71	113.56	108.20
1	AA	987	G	C8-N9-C4	-6.70	103.72	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1266	G	C3'-C2'-C1'	-6.70	96.14	101.50
1	AA	1502	A	C5'-C4'-C3'	-6.70	105.28	116.00
26	BB	764	A	O4'-C1'-C2'	-6.70	99.10	105.80
26	BB	853	C	O4'-C1'-N1	6.70	113.56	108.20
26	BB	2182	U	O4'-C1'-N1	6.70	113.56	108.20
26	BB	548	G	C2-N3-C4	6.70	115.25	111.90
26	BB	1193	G	O4'-C1'-N9	6.70	113.56	108.20
26	BB	946	C	O4'-C1'-N1	6.70	113.56	108.20
1	AA	688	G	C8-N9-C4	-6.69	103.72	106.40
26	BB	1433	A	O4'-C1'-N9	6.69	113.55	108.20
26	BB	2010	G	C5'-C4'-O4'	6.69	117.13	109.10
1	AA	791	G	C8-N9-C4	-6.69	103.72	106.40
26	BB	1740	G	C8-N9-C4	-6.69	103.72	106.40
1	AA	970	C	N1-C1'-C2'	-6.69	104.64	112.00
4	AD	33	U	O4'-C1'-N1	6.69	113.55	108.20
26	BB	647	G	O4'-C1'-N9	6.69	113.55	108.20
26	BB	1210	G	P-O3'-C3'	6.69	127.72	119.70
1	AA	1408	A	C5'-C4'-O4'	6.69	117.12	109.10
1	AA	356	A	O4'-C1'-N9	6.68	113.55	108.20
1	AA	1482	G	O4'-C1'-N9	6.68	113.55	108.20
26	BB	1681	G	O4'-C1'-N9	6.68	113.55	108.20
1	AA	108	G	O4'-C1'-N9	6.68	113.54	108.20
1	AA	121	U	P-O3'-C3'	6.68	127.71	119.70
26	BB	65	U	O4'-C1'-N1	6.68	113.54	108.20
26	BB	667	U	O4'-C1'-N1	6.68	113.54	108.20
26	BB	2634	A	O4'-C1'-N9	6.68	113.54	108.20
26	BB	1914	C	O4'-C1'-N1	6.68	113.54	108.20
26	BB	2471	A	O4'-C1'-N9	6.68	113.54	108.20
26	BB	2582	G	C8-N9-C4	-6.67	103.73	106.40
2	AB	40	C	O4'-C1'-N1	6.67	113.53	108.20
1	AA	1401	G	C8-N9-C4	-6.67	103.73	106.40
26	BB	1258	U	O4'-C1'-N1	6.66	113.53	108.20
1	AA	167	A	O4'-C1'-N9	6.66	113.53	108.20
26	BB	999	U	O4'-C1'-N1	6.66	113.53	108.20
26	BB	2649	C	O4'-C1'-N1	6.66	113.53	108.20
2	AB	7	A	O4'-C1'-N9	6.66	113.53	108.20
26	BB	520	G	O4'-C1'-N9	6.66	113.53	108.20
26	BB	1271	G	N9-C4-C5	6.66	108.06	105.40
26	BB	2889	C	O4'-C1'-N1	6.66	113.53	108.20
1	AA	715	A	O4'-C1'-N9	6.66	113.52	108.20
1	AA	1028	C	O4'-C1'-N1	6.66	113.52	108.20
1	AA	1156	G	O4'-C1'-N9	6.66	113.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	498	A	C8-N9-C4	-6.65	103.14	105.80
1	AA	196	A	O4'-C1'-N9	6.65	113.52	108.20
26	BB	1414	C	O4'-C1'-N1	6.65	113.52	108.20
26	BB	160	A	C5'-C4'-O4'	6.65	117.08	109.10
26	BB	1154	G	C8-N9-C4	-6.65	103.74	106.40
26	BB	2509	G	O4'-C1'-N9	6.65	113.52	108.20
26	BB	2797	U	O4'-C1'-N1	6.65	113.52	108.20
26	BB	97	C	O4'-C1'-N1	6.64	113.51	108.20
26	BB	1501	G	O4'-C1'-N9	6.64	113.51	108.20
1	AA	193	C	C5'-C4'-O4'	6.64	117.06	109.10
26	BB	873	C	O4'-C1'-N1	6.64	113.51	108.20
26	BB	1437	C	O4'-C1'-N1	6.64	113.51	108.20
26	BB	1938	A	O4'-C1'-N9	6.64	113.51	108.20
26	BB	2493	U	O4'-C1'-N1	6.64	113.51	108.20
26	BB	352	A	O4'-C1'-N9	6.63	113.51	108.20
26	BB	2658	C	O4'-C1'-N1	6.63	113.51	108.20
1	AA	166	U	O4'-C1'-N1	6.63	113.51	108.20
19	AT	28	ARG	NE-CZ-NH2	-6.63	116.98	120.30
26	BB	487	C	O4'-C1'-N1	6.63	113.51	108.20
26	BB	740	C	O4'-C1'-N1	6.63	113.51	108.20
1	AA	1352	C	O4'-C1'-N1	6.63	113.50	108.20
26	BB	2546	U	O4'-C1'-N1	6.63	113.50	108.20
26	BB	1151	A	O4'-C1'-N9	6.63	113.50	108.20
1	AA	383	A	O4'-C1'-N9	6.63	113.50	108.20
26	BB	451	U	O4'-C1'-N1	6.63	113.50	108.20
26	BB	1788	C	C5'-C4'-O4'	6.63	117.06	109.10
26	BB	1045	C	O4'-C1'-N1	6.62	113.50	108.20
1	AA	436	C	O4'-C1'-N1	6.62	113.50	108.20
1	AA	797	C	C2'-C3'-O3'	6.62	124.29	113.70
1	AA	1315	U	C5'-C4'-C3'	-6.62	105.41	116.00
26	BB	1952	A	C3'-C2'-C1'	6.62	106.80	101.50
26	BB	326	G	O4'-C1'-N9	6.62	113.49	108.20
26	BB	1116	G	O4'-C1'-N9	6.62	113.49	108.20
26	BB	1490	A	C8-N9-C4	-6.62	103.15	105.80
1	AA	778	G	C5'-C4'-C3'	-6.62	105.42	116.00
26	BB	839	U	O4'-C1'-N1	6.62	113.49	108.20
26	BB	527	C	N1-C2-O2	6.61	122.87	118.90
26	BB	2068	U	O4'-C1'-N1	6.61	113.49	108.20
26	BB	2238	G	C8-N9-C4	-6.61	103.75	106.40
26	BB	2779	U	O4'-C1'-N1	6.61	113.49	108.20
26	BB	2050	C	O4'-C1'-N1	6.61	113.49	108.20
26	BB	257	C	O4'-C1'-N1	6.61	113.49	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1053	C	O4'-C1'-N1	6.61	113.49	108.20
26	BB	2223	G	O4'-C1'-N9	6.61	113.49	108.20
26	BB	2368	C	O4'-C1'-N1	6.61	113.49	108.20
26	BB	1100	C	O4'-C1'-N1	6.61	113.49	108.20
26	BB	1865	U	P-O3'-C3'	6.61	127.63	119.70
1	AA	542	G	O4'-C1'-N9	6.61	113.49	108.20
26	BB	214	G	N3-C4-C5	-6.61	125.30	128.60
26	BB	834	G	O4'-C1'-N9	6.61	113.49	108.20
26	BB	2254	C	C5'-C4'-O4'	6.61	117.03	109.10
1	AA	777	A	C5'-C4'-C3'	-6.61	105.43	116.00
26	BB	1738	G	N9-C4-C5	6.61	108.04	105.40
1	AA	1060	U	O4'-C1'-N1	6.60	113.48	108.20
1	AA	818	G	C8-N9-C4	-6.60	103.76	106.40
1	AA	886	G	O4'-C1'-N9	6.60	113.48	108.20
1	AA	1379	G	C5'-C4'-C3'	-6.60	105.44	116.00
4	AD	31	U	C1'-O4'-C4'	-6.60	104.62	109.90
26	BB	586	A	C8-N9-C4	-6.60	103.16	105.80
26	BB	1282	U	O4'-C1'-N1	6.60	113.48	108.20
26	BB	2417	C	O4'-C1'-N1	6.60	113.48	108.20
2	AB	13	C	O4'-C1'-N1	6.60	113.48	108.20
2	AB	28	G	C8-N9-C4	-6.60	103.76	106.40
26	BB	336	C	O4'-C1'-N1	6.60	113.48	108.20
26	BB	1070	A	C5'-C4'-C3'	-6.60	105.44	116.00
26	BB	1441	G	O4'-C1'-N9	6.60	113.48	108.20
26	BB	671	C	O4'-C1'-N1	6.60	113.48	108.20
26	BB	2317	A	O4'-C1'-N9	6.60	113.48	108.20
26	BB	189	G	C5'-C4'-O4'	6.59	117.01	109.10
26	BB	1906	G	O4'-C1'-N9	6.59	113.48	108.20
26	BB	2537	U	O4'-C1'-N1	6.59	113.48	108.20
1	AA	1299	A	O4'-C1'-N9	6.59	113.47	108.20
26	BB	237	C	O4'-C1'-N1	6.59	113.47	108.20
1	AA	738	C	O4'-C1'-N1	6.59	113.47	108.20
26	BB	1079	C	O4'-C1'-N1	6.59	113.47	108.20
26	BB	2629	U	O4'-C1'-N1	6.59	113.47	108.20
26	BB	188	G	O4'-C1'-N9	6.59	113.47	108.20
26	BB	854	C	O4'-C1'-N1	6.59	113.47	108.20
1	AA	589	U	O4'-C1'-N1	6.59	113.47	108.20
26	BB	252	G	O4'-C1'-N9	6.59	113.47	108.20
26	BB	277	G	O4'-C1'-N9	6.59	113.47	108.20
26	BB	356	G	O4'-C1'-N9	6.59	113.47	108.20
26	BB	1645	G	C8-N9-C4	-6.59	103.77	106.40
26	BB	1778	U	O4'-C1'-N1	6.59	113.47	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1105	U	O4'-C1'-N1	6.58	113.47	108.20
26	BB	2582	G	N3-C4-C5	-6.58	125.31	128.60
1	AA	129	A	O4'-C1'-N9	6.58	113.47	108.20
26	BB	2635	A	O4'-C1'-N9	6.58	113.47	108.20
1	AA	849	G	C8-N9-C4	-6.58	103.77	106.40
26	BB	1973	G	C5'-C4'-O4'	6.58	117.00	109.10
26	BB	1114	C	C5'-C4'-O4'	6.58	116.99	109.10
1	AA	1477	U	C5'-C4'-O4'	6.58	116.99	109.10
26	BB	518	G	C5'-C4'-O4'	6.58	116.99	109.10
1	AA	61	G	C8-N9-C4	-6.57	103.77	106.40
26	BB	920	A	O4'-C1'-N9	6.57	113.46	108.20
26	BB	1063	G	C8-N9-C4	-6.57	103.77	106.40
26	BB	1504	A	O4'-C1'-N9	6.57	113.46	108.20
2	AB	28	G	N3-C4-C5	-6.57	125.31	128.60
26	BB	748	G	C5'-C4'-O4'	6.57	116.99	109.10
1	AA	1390	U	O4'-C1'-N1	6.57	113.46	108.20
26	BB	333	G	C8-N9-C4	-6.57	103.77	106.40
26	BB	2045	C	O4'-C1'-N1	6.57	113.46	108.20
25	BA	36	C	C5'-C4'-C3'	-6.57	105.50	116.00
26	BB	1993	U	O4'-C1'-N1	6.56	113.45	108.20
26	BB	592	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	793	U	O3'-P-O5'	-6.56	91.54	104.00
26	BB	10	A	C5'-C4'-C3'	-6.56	105.50	116.00
26	BB	195	A	C5'-C4'-O4'	6.56	116.97	109.10
26	BB	1897	G	O4'-C1'-N9	6.56	113.45	108.20
26	BB	2238	G	N9-C4-C5	6.56	108.02	105.40
26	BB	2393	U	O4'-C1'-N1	6.56	113.45	108.20
1	AA	759	A	O4'-C1'-N9	6.56	113.45	108.20
1	AA	798	U	O4'-C1'-N1	6.56	113.44	108.20
1	AA	1230	C	O4'-C1'-N1	6.56	113.44	108.20
26	BB	566	U	C5'-C4'-O4'	6.55	116.97	109.10
26	BB	2060	A	O4'-C1'-C2'	-6.55	99.25	105.80
26	BB	1751	U	O4'-C1'-N1	6.55	113.44	108.20
26	BB	2744	G	C5'-C4'-O4'	6.55	116.96	109.10
26	BB	599	A	O4'-C1'-N9	6.55	113.44	108.20
26	BB	796	C	O4'-C1'-N1	6.55	113.44	108.20
1	AA	224	U	O4'-C1'-N1	6.55	113.44	108.20
26	BB	2260	C	O4'-C1'-N1	6.55	113.44	108.20
26	BB	2738	A	O4'-C1'-N9	6.55	113.44	108.20
26	BB	122	G	O4'-C1'-N9	6.54	113.44	108.20
1	AA	156	C	O4'-C1'-N1	6.54	113.44	108.20
1	AA	787	A	O4'-C1'-N9	6.54	113.44	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1318	A	C5'-C4'-C3'	-6.54	105.53	116.00
26	BB	548	G	O4'-C1'-N9	6.54	113.44	108.20
26	BB	1261	C	O4'-C1'-N1	6.54	113.43	108.20
1	AA	2	A	C3'-C2'-C1'	-6.54	96.27	101.50
1	AA	70	U	O4'-C1'-N1	6.54	113.43	108.20
26	BB	15	G	C8-N9-C4	-6.54	103.78	106.40
26	BB	558	U	O4'-C1'-N1	6.54	113.43	108.20
26	BB	2219	U	C2-N3-C4	-6.54	123.08	127.00
26	BB	2131	U	O4'-C1'-N1	6.54	113.43	108.20
26	BB	124	G	O4'-C1'-N9	6.54	113.43	108.20
26	BB	205	G	O4'-C1'-N9	6.54	113.43	108.20
26	BB	2693	G	O4'-C1'-N9	6.53	113.43	108.20
1	AA	1380	U	N1-C2-N3	6.53	118.82	114.90
1	AA	360	G	O4'-C1'-N9	6.53	113.42	108.20
26	BB	2890	G	C8-N9-C4	-6.52	103.79	106.40
4	AD	39	U	O4'-C1'-N1	6.52	113.42	108.20
26	BB	2319	G	O4'-C1'-N9	6.52	113.42	108.20
26	BB	160	A	O4'-C1'-N9	6.52	113.42	108.20
26	BB	691	C	O4'-C1'-N1	6.52	113.42	108.20
1	AA	267	C	O4'-C1'-N1	6.52	113.41	108.20
1	AA	595	A	O4'-C4'-C3'	6.52	111.31	106.10
26	BB	1606	C	N1-C2-O2	6.52	122.81	118.90
26	BB	1127	A	O4'-C1'-N9	-6.52	102.99	108.20
26	BB	2739	U	C4'-C3'-C2'	-6.52	96.08	102.60
26	BB	2008	C	O4'-C1'-N1	6.51	113.41	108.20
26	BB	2134	A	O4'-C1'-N9	6.51	113.41	108.20
1	AA	1455	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	628	G	O4'-C1'-N9	6.51	113.41	108.20
1	AA	865	A	C3'-C2'-C1'	6.51	106.71	101.50
1	AA	1452	C	O4'-C1'-N1	6.51	113.41	108.20
26	BB	2338	C	O4'-C1'-N1	6.51	113.41	108.20
1	AA	1374	A	C5'-C4'-C3'	-6.51	105.59	116.00
26	BB	2000	C	O4'-C1'-N1	6.51	113.41	108.20
26	BB	2800	A	O4'-C1'-N9	6.51	113.41	108.20
26	BB	2847	U	O4'-C1'-N1	6.51	113.41	108.20
26	BB	1883	U	O4'-C1'-N1	6.50	113.40	108.20
1	AA	628	G	C8-N9-C4	-6.50	103.80	106.40
26	BB	525	U	O4'-C1'-N1	6.50	113.40	108.20
26	BB	2007	U	C5'-C4'-C3'	-6.50	105.59	116.00
1	AA	352	C	C5'-C4'-O4'	6.50	116.90	109.10
26	BB	664	G	O4'-C1'-N9	6.50	113.40	108.20
1	AA	732	C	O4'-C1'-N1	6.50	113.40	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1481	U	O4'-C1'-N1	6.50	113.40	108.20
1	AA	955	U	O4'-C1'-N1	6.50	113.40	108.20
1	AA	1474	U	O4'-C1'-N1	6.50	113.40	108.20
26	BB	368	A	C8-N9-C4	-6.50	103.20	105.80
26	BB	568	U	O4'-C1'-N1	6.50	113.40	108.20
26	BB	2379	G	O4'-C1'-N9	6.50	113.40	108.20
26	BB	612	G	C8-N9-C4	-6.50	103.80	106.40
2	AE	19	G	O4'-C1'-N9	6.49	113.39	108.20
26	BB	1828	G	O4'-C1'-N9	6.49	113.39	108.20
26	BB	1837	C	O4'-C1'-N1	6.49	113.39	108.20
26	BB	1986	C	O4'-C1'-N1	6.49	113.39	108.20
26	BB	2705	A	C4'-C3'-C2'	-6.49	96.11	102.60
26	BB	540	C	O4'-C1'-N1	6.49	113.39	108.20
1	AA	1291	U	O4'-C1'-N1	6.49	113.39	108.20
26	BB	502	A	O4'-C1'-N9	6.49	113.39	108.20
26	BB	862	G	C8-N9-C4	-6.49	103.81	106.40
26	BB	2053	G	O4'-C1'-N9	6.49	113.39	108.20
1	AA	911	U	O4'-C1'-N1	6.48	113.39	108.20
25	BA	59	A	C8-N9-C4	-6.48	103.21	105.80
26	BB	1847	A	O4'-C1'-N9	6.48	113.39	108.20
1	AA	644	U	O4'-C1'-N1	6.48	113.38	108.20
26	BB	144	A	O4'-C1'-N9	6.48	113.38	108.20
1	AA	359	G	O4'-C1'-N9	6.48	113.38	108.20
25	BA	62	C	O4'-C1'-N1	6.48	113.38	108.20
26	BB	99	U	O4'-C1'-N1	6.48	113.38	108.20
1	AA	398	U	C5'-C4'-C3'	-6.47	105.64	116.00
26	BB	216	A	O4'-C1'-N9	6.47	113.38	108.20
26	BB	455	C	C3'-C2'-C1'	6.47	106.68	101.50
26	BB	1707	G	C8-N9-C4	-6.47	103.81	106.40
1	AA	909	A	O4'-C1'-N9	6.47	113.38	108.20
26	BB	231	A	C5'-C4'-C3'	-6.47	105.65	116.00
26	BB	2339	C	C5'-C4'-O4'	6.47	116.86	109.10
26	BB	94	A	O4'-C1'-N9	6.47	113.38	108.20
26	BB	1812	U	O4'-C1'-N1	6.47	113.38	108.20
26	BB	2149	U	O4'-C1'-N1	6.47	113.38	108.20
26	BB	1901	A	C1'-O4'-C4'	-6.47	104.73	109.90
26	BB	2507	C	O4'-C1'-N1	6.47	113.38	108.20
1	AA	896	C	O4'-C1'-N1	6.47	113.37	108.20
26	BB	1717	A	O4'-C1'-N9	6.47	113.37	108.20
2	AE	66	U	O4'-C1'-N1	6.46	113.37	108.20
1	AA	178	C	O4'-C1'-N1	6.46	113.37	108.20
26	BB	1606	C	O4'-C1'-N1	6.46	113.37	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2728	U	O4'-C1'-N1	6.46	113.37	108.20
2	AB	41	C	O4'-C1'-N1	6.46	113.37	108.20
26	BB	843	G	C8-N9-C4	-6.46	103.82	106.40
26	BB	1070	A	C1'-O4'-C4'	-6.46	104.73	109.90
26	BB	2560	A	O3'-P-O5'	-6.46	91.72	104.00
1	AA	1432	G	O4'-C1'-N9	6.46	113.37	108.20
26	BB	1974	C	O4'-C1'-N1	6.46	113.37	108.20
26	BB	1402	U	C5'-C4'-O4'	6.46	116.85	109.10
26	BB	1279	G	O4'-C1'-N9	6.45	113.36	108.20
26	BB	2428	G	C8-N9-C4	-6.45	103.82	106.40
1	AA	1100	C	O4'-C1'-N1	6.45	113.36	108.20
3	AC	87	TYR	CB-CG-CD1	-6.45	117.13	121.00
2	AB	44	G	N3-C4-C5	-6.45	125.38	128.60
26	BB	1933	G	C5'-C4'-C3'	-6.45	105.68	116.00
26	BB	1765	U	O4'-C1'-N1	6.45	113.36	108.20
26	BB	2191	A	O4'-C1'-N9	6.45	113.36	108.20
26	BB	2783	U	O4'-C1'-N1	6.45	113.36	108.20
1	AA	1184	G	C8-N9-C4	-6.45	103.82	106.40
1	AA	1225	A	O4'-C1'-N9	-6.45	103.04	108.20
1	AA	118	U	O4'-C1'-N1	6.44	113.36	108.20
26	BB	2172	U	P-O3'-C3'	6.44	127.43	119.70
26	BB	461	C	O4'-C1'-N1	6.44	113.35	108.20
1	AA	532	A	O4'-C1'-N9	6.44	113.35	108.20
26	BB	1656	C	O4'-C1'-N1	6.44	113.35	108.20
26	BB	1727	C	O4'-C1'-N1	6.44	113.35	108.20
1	AA	891	U	O4'-C1'-N1	6.44	113.35	108.20
26	BB	191	A	O4'-C1'-N9	6.44	113.35	108.20
26	BB	1999	C	C5'-C4'-O4'	6.44	116.83	109.10
26	BB	2665	A	C5'-C4'-C3'	-6.44	105.70	116.00
26	BB	1637	A	C5'-C4'-C3'	-6.43	105.70	116.00
25	BA	113	C	O4'-C1'-N1	6.43	113.34	108.20
26	BB	759	G	N3-C4-C5	-6.43	125.38	128.60
25	BA	37	C	C6-N1-C2	-6.43	117.73	120.30
26	BB	2162	G	C8-N9-C4	-6.43	103.83	106.40
26	BB	1845	G	O4'-C1'-N9	6.43	113.34	108.20
25	BA	79	G	C8-N9-C4	-6.42	103.83	106.40
2	AE	70	G	O4'-C1'-N9	6.42	113.34	108.20
26	BB	332	A	C5'-C4'-O4'	6.42	116.80	109.10
26	BB	1103	A	O4'-C1'-N9	6.42	113.34	108.20
26	BB	597	G	O4'-C1'-N9	6.42	113.33	108.20
1	AA	108	G	N3-C4-C5	-6.42	125.39	128.60
1	AA	639	G	C8-N9-C4	-6.42	103.83	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	836	G	C8-N9-C4	-6.42	103.83	106.40
1	AA	1300	G	P-O3'-C3'	6.42	127.40	119.70
26	BB	2875	C	O4'-C1'-N1	6.42	113.33	108.20
1	AA	414	A	C1'-O4'-C4'	6.41	115.03	109.90
26	BB	1773	A	C5'-C4'-O4'	6.41	116.80	109.10
25	BA	20	G	O4'-C1'-N9	6.41	113.33	108.20
1	AA	1273	C	O4'-C1'-N1	6.41	113.33	108.20
26	BB	2344	U	O4'-C1'-N1	6.41	113.33	108.20
26	BB	954	G	C5'-C4'-C3'	-6.41	105.75	116.00
26	BB	966	G	O4'-C1'-N9	6.41	113.33	108.20
25	BA	77	U	C3'-C2'-C1'	-6.40	96.38	101.50
25	BA	16	G	C8-N9-C4	-6.40	103.84	106.40
26	BB	970	U	C4'-C3'-C2'	6.40	109.00	102.60
26	BB	1060	U	P-O3'-C3'	6.40	127.38	119.70
26	BB	2350	C	O4'-C1'-N1	6.40	113.32	108.20
1	AA	847	G	N3-C4-C5	-6.40	125.40	128.60
26	BB	1410	G	O4'-C1'-N9	6.40	113.32	108.20
26	BB	1792	G	C5'-C4'-C3'	-6.40	105.77	116.00
26	BB	350	G	O4'-C1'-N9	6.39	113.32	108.20
26	BB	1694	C	N1-C2-O2	6.39	122.74	118.90
26	BB	1869	G	N9-C4-C5	6.39	107.96	105.40
26	BB	2308	G	C8-N9-C4	-6.39	103.84	106.40
26	BB	2006	C	C5'-C4'-O4'	6.39	116.77	109.10
1	AA	876	C	O4'-C1'-N1	6.39	113.31	108.20
26	BB	1026	G	O4'-C1'-N9	6.39	113.31	108.20
26	BB	397	U	O4'-C1'-N1	6.39	113.31	108.20
26	BB	688	U	O4'-C1'-N1	6.39	113.31	108.20
1	AA	594	U	O4'-C1'-N1	6.39	113.31	108.20
26	BB	1610	A	O4'-C1'-N9	6.39	113.31	108.20
26	BB	1177	G	C5'-C4'-C3'	-6.39	105.78	116.00
26	BB	2574	G	C8-N9-C4	-6.38	103.85	106.40
26	BB	2767	C	O4'-C1'-N1	6.38	113.31	108.20
1	AA	1288	A	C8-N9-C4	-6.38	103.25	105.80
26	BB	935	C	O4'-C1'-N1	6.38	113.30	108.20
26	BB	1064	C	C3'-C2'-C1'	-6.38	96.40	101.50
1	AA	1013	G	O4'-C1'-N9	6.38	113.30	108.20
2	AB	12	U	O4'-C1'-N1	6.38	113.30	108.20
26	BB	419	U	O4'-C1'-N1	6.38	113.30	108.20
26	BB	29	U	O4'-C1'-N1	6.38	113.30	108.20
26	BB	1489	C	O4'-C1'-N1	6.38	113.30	108.20
1	AA	1009	U	O4'-C1'-N1	6.37	113.30	108.20
1	AA	1015	G	O4'-C1'-N9	6.37	113.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1103	C	C5'-C4'-C3'	-6.37	105.80	116.00
26	BB	1408	G	C3'-C2'-C1'	-6.37	96.40	101.50
26	BB	2771	C	O4'-C1'-N1	6.37	113.30	108.20
1	AA	160	A	O4'-C1'-N9	6.37	113.30	108.20
25	BA	43	C	O4'-C1'-N1	6.37	113.30	108.20
26	BB	378	C	C5'-C4'-O4'	6.37	116.75	109.10
26	BB	2301	C	O4'-C1'-N1	6.37	113.30	108.20
26	BB	1177	G	N3-C4-C5	-6.37	125.42	128.60
26	BB	1990	C	O4'-C1'-N1	6.37	113.30	108.20
1	AA	619	U	C5'-C4'-C3'	-6.36	105.82	116.00
26	BB	1313	U	C5'-C4'-O4'	6.36	116.73	109.10
1	AA	200	G	C5'-C4'-C3'	-6.36	105.82	116.00
1	AA	268	U	C5'-C4'-C3'	-6.36	105.82	116.00
1	AA	705	G	O4'-C1'-N9	6.36	113.29	108.20
2	AE	4	C	O4'-C1'-N1	6.36	113.29	108.20
1	AA	72	A	C5'-C4'-O4'	6.36	116.73	109.10
1	AA	860	A	O4'-C1'-N9	6.36	113.29	108.20
1	AA	962	C	C5'-C4'-O4'	6.36	116.73	109.10
26	BB	1889	A	C8-N9-C4	-6.36	103.26	105.80
26	BB	2018	G	O4'-C1'-N9	6.36	113.29	108.20
26	BB	2852	G	C8-N9-C4	-6.36	103.86	106.40
1	AA	1158	C	C3'-C2'-C1'	6.35	106.58	101.50
26	BB	2565	A	C8-N9-C4	-6.35	103.26	105.80
26	BB	810	U	O4'-C1'-N1	6.35	113.28	108.20
1	AA	818	G	O4'-C1'-C2'	-6.35	99.45	105.80
26	BB	1746	A	O4'-C1'-N9	6.35	113.28	108.20
1	AA	222	C	O4'-C1'-N1	6.35	113.28	108.20
1	AA	603	U	O4'-C1'-N1	6.35	113.28	108.20
2	AB	76	A	O4'-C1'-N9	6.35	113.28	108.20
26	BB	1592	C	O4'-C1'-N1	6.35	113.28	108.20
26	BB	1998	A	O4'-C1'-N9	6.35	113.28	108.20
26	BB	2192	U	C5'-C4'-O4'	6.35	116.72	109.10
26	BB	2822	G	C5'-C4'-C3'	-6.35	105.84	116.00
1	AA	1089	G	C8-N9-C4	-6.34	103.86	106.40
26	BB	1560	G	C5'-C4'-C3'	-6.34	105.85	116.00
1	AA	65	A	O4'-C1'-N9	6.34	113.27	108.20
26	BB	1476	U	O4'-C1'-N1	6.34	113.27	108.20
26	BB	2548	U	O4'-C1'-N1	6.34	113.27	108.20
26	BB	1218	G	O4'-C1'-N9	6.34	113.27	108.20
26	BB	2741	A	C4'-C3'-C2'	-6.34	96.26	102.60
1	AA	1046	A	C5'-C4'-O4'	6.34	116.70	109.10
2	AE	44	G	O4'-C1'-N9	6.34	113.27	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	59	U	P-O3'-C3'	6.34	127.31	119.70
26	BB	856	G	C5'-C4'-O4'	6.34	116.70	109.10
26	BB	2206	C	O4'-C1'-N1	6.33	113.27	108.20
26	BB	2398	U	C5'-C4'-O4'	6.33	116.70	109.10
1	AA	1128	C	C5'-C4'-O4'	6.33	116.70	109.10
1	AA	1401	G	N3-C4-C5	-6.33	125.44	128.60
26	BB	126	A	C5'-C4'-O4'	6.33	116.70	109.10
26	BB	364	C	O4'-C1'-N1	6.33	113.26	108.20
1	AA	826	C	O4'-C4'-C3'	6.33	111.16	106.10
26	BB	469	G	C8-N9-C4	-6.33	103.87	106.40
1	AA	632	U	O4'-C1'-N1	6.33	113.26	108.20
26	BB	2810	A	C8-N9-C4	-6.33	103.27	105.80
26	BB	60	G	O4'-C1'-N9	6.33	113.26	108.20
26	BB	402	A	C8-N9-C4	-6.33	103.27	105.80
26	BB	2541	A	C5'-C4'-O4'	6.32	116.69	109.10
1	AA	843	U	C3'-C2'-C1'	6.32	106.56	101.50
26	BB	575	A	O4'-C1'-N9	6.32	113.26	108.20
26	BB	989	G	C1'-O4'-C4'	-6.32	104.84	109.90
1	AA	793	U	O4'-C1'-N1	6.32	113.26	108.20
26	BB	834	G	N7-C8-N9	6.32	116.26	113.10
26	BB	2255	G	C8-N9-C4	-6.32	103.87	106.40
26	BB	2393	U	N1-C1'-C2'	-6.32	105.05	112.00
1	AA	79	G	O4'-C1'-N9	6.32	113.25	108.20
26	BB	548	G	N3-C4-C5	-6.32	125.44	128.60
1	AA	91	U	C5'-C4'-O4'	6.32	116.68	109.10
26	BB	1637	A	C5'-C4'-O4'	6.32	116.68	109.10
2	AB	70	G	O4'-C1'-N9	6.31	113.25	108.20
26	BB	389	G	N3-C4-C5	-6.31	125.44	128.60
26	BB	988	A	O4'-C1'-N9	6.31	113.25	108.20
26	BB	1154	G	N7-C8-N9	6.31	116.26	113.10
26	BB	724	U	O4'-C1'-N1	6.31	113.25	108.20
26	BB	230	G	C4'-C3'-C2'	-6.31	96.29	102.60
1	AA	915	A	O4'-C1'-N9	6.31	113.25	108.20
26	BB	2643	G	O4'-C1'-N9	6.31	113.25	108.20
1	AA	246	A	C5'-C4'-O4'	6.30	116.67	109.10
1	AA	760	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	1025	U	O4'-C1'-N1	6.30	113.24	108.20
26	BB	236	C	N1-C1'-C2'	-6.30	105.07	112.00
26	BB	798	G	O4'-C1'-N9	6.30	113.24	108.20
1	AA	285	C	O4'-C1'-N1	6.30	113.24	108.20
1	AA	843	U	O4'-C4'-C3'	6.30	111.14	106.10
1	AA	1143	G	C8-N9-C4	-6.30	103.88	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	103	A	C8-N9-C4	-6.30	103.28	105.80
26	BB	2733	A	O4'-C1'-N9	6.30	113.24	108.20
9	AJ	113	ARG	NE-CZ-NH1	6.30	123.45	120.30
26	BB	925	A	O4'-C1'-N9	6.30	113.24	108.20
26	BB	1564	C	O4'-C1'-N1	6.30	113.24	108.20
26	BB	1561	C	O4'-C1'-N1	6.30	113.24	108.20
1	AA	858	G	C8-N9-C4	-6.29	103.88	106.40
26	BB	1535	A	O3'-P-O5'	-6.29	92.04	104.00
26	BB	1730	C	N1-C2-O2	6.29	122.68	118.90
1	AA	1227	A	O3'-P-O5'	-6.29	92.05	104.00
1	AA	861	G	N3-C4-C5	-6.29	125.45	128.60
1	AA	699	C	O4'-C1'-N1	6.29	113.23	108.20
1	AA	951	G	C8-N9-C4	-6.29	103.89	106.40
26	BB	1511	G	C5'-C4'-O4'	6.29	116.64	109.10
1	AA	122	G	N3-C4-C5	-6.29	125.46	128.60
1	AA	1037	C	O4'-C1'-N1	6.29	113.23	108.20
26	BB	473	G	C5'-C4'-O4'	6.28	116.64	109.10
1	AA	1052	U	O4'-C1'-N1	6.28	113.23	108.20
25	BA	34	A	C5'-C4'-O4'	6.28	116.64	109.10
26	BB	244	A	O4'-C1'-N9	6.28	113.23	108.20
26	BB	1337	G	C8-N9-C4	-6.28	103.89	106.40
26	BB	1867	G	O4'-C1'-N9	6.28	113.23	108.20
26	BB	2386	A	C3'-C2'-C1'	-6.28	96.47	101.50
26	BB	2429	G	P-O3'-C3'	6.28	127.24	119.70
25	BA	100	G	N3-C4-C5	-6.28	125.46	128.60
26	BB	14	A	C5'-C4'-O4'	6.28	116.64	109.10
26	BB	1455	G	C5'-C4'-O4'	6.28	116.64	109.10
26	BB	2094	A	O4'-C1'-N9	6.28	113.22	108.20
26	BB	2306	C	P-O3'-C3'	6.28	127.23	119.70
25	BA	64	G	O4'-C1'-N9	6.28	113.22	108.20
26	BB	324	A	C5'-C4'-C3'	-6.28	105.95	116.00
26	BB	1918	A	O4'-C1'-N9	6.28	113.22	108.20
26	BB	22	C	O4'-C1'-N1	6.28	113.22	108.20
26	BB	1175	A	C5'-C4'-C3'	-6.28	105.96	116.00
26	BB	190	A	C5'-C4'-C3'	-6.27	105.97	116.00
26	BB	1793	C	O4'-C1'-N1	6.27	113.22	108.20
26	BB	1343	G	N3-C4-C5	-6.27	125.47	128.60
26	BB	1543	G	C5'-C4'-O4'	6.27	116.62	109.10
26	BB	1761	C	P-O3'-C3'	6.27	127.22	119.70
26	BB	1138	G	C8-N9-C4	-6.27	103.89	106.40
1	AA	157	U	O4'-C1'-N1	6.26	113.21	108.20
1	AA	1164	G	O4'-C1'-N9	6.26	113.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1203	U	N3-C2-O2	-6.26	117.82	122.20
26	BB	1460	U	O4'-C1'-N1	6.26	113.21	108.20
26	BB	479	A	P-O3'-C3'	6.26	127.21	119.70
26	BB	1242	U	N1-C2-N3	6.26	118.66	114.90
26	BB	1887	C	C4'-C3'-C2'	6.26	108.86	102.60
1	AA	351	G	O4'-C1'-N9	6.26	113.21	108.20
2	AB	43	C	O4'-C1'-N1	6.26	113.21	108.20
25	BA	34	A	P-O3'-C3'	6.26	127.21	119.70
26	BB	209	C	O4'-C1'-N1	6.26	113.21	108.20
26	BB	1101	U	O4'-C1'-N1	6.26	113.21	108.20
26	BB	1574	C	O4'-C1'-N1	6.26	113.21	108.20
26	BB	1964	G	C8-N9-C1'	6.26	135.14	127.00
26	BB	820	A	C5'-C4'-O4'	6.25	116.61	109.10
26	BB	1036	G	O4'-C1'-N9	6.25	113.20	108.20
1	AA	803	G	N3-C4-C5	-6.25	125.47	128.60
1	AA	249	U	O4'-C1'-N1	6.25	113.20	108.20
1	AA	779	C	O4'-C1'-N1	6.25	113.20	108.20
26	BB	2780	G	O4'-C1'-N9	6.25	113.20	108.20
26	BB	2806	C	O4'-C1'-N1	6.25	113.20	108.20
1	AA	652	U	O4'-C1'-N1	6.24	113.19	108.20
1	AA	986	U	O4'-C1'-N1	6.24	113.20	108.20
26	BB	827	U	O4'-C1'-N1	6.24	113.19	108.20
1	AA	709	U	O4'-C1'-N1	6.24	113.19	108.20
26	BB	733	G	C5'-C4'-O4'	6.24	116.59	109.10
1	AA	1312	G	C5'-C4'-O4'	6.24	116.59	109.10
26	BB	1726	C	O4'-C1'-N1	6.24	113.19	108.20
1	AA	59	A	C5'-C4'-O4'	6.24	116.58	109.10
2	AE	65	G	O4'-C1'-N9	6.24	113.19	108.20
26	BB	1786	A	C5'-C4'-C3'	-6.24	106.02	116.00
1	AA	901	A	O4'-C1'-N9	6.23	113.19	108.20
26	BB	241	A	O4'-C1'-N9	6.23	113.18	108.20
26	BB	2192	U	O4'-C1'-N1	6.23	113.19	108.20
1	AA	207	C	O4'-C1'-N1	6.23	113.18	108.20
26	BB	2810	A	C5'-C4'-C3'	-6.23	106.03	116.00
26	BB	26	G	O4'-C1'-N9	6.23	113.18	108.20
26	BB	997	G	O4'-C1'-N9	6.23	113.18	108.20
1	AA	1085	U	C3'-C2'-C1'	-6.23	96.52	101.50
1	AA	661	G	C8-N9-C4	-6.22	103.91	106.40
1	AA	266	G	C5'-C4'-O4'	-6.22	101.63	109.10
1	AA	854	U	C5'-C4'-O4'	6.22	116.57	109.10
26	BB	998	C	O4'-C1'-N1	6.22	113.18	108.20
26	BB	1963	U	P-O3'-C3'	6.22	127.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1060	U	P-O3'-C3'	6.22	127.17	119.70
1	AA	1512	U	O4'-C1'-N1	6.22	113.18	108.20
26	BB	54	G	C8-N9-C4	-6.22	103.91	106.40
26	BB	969	G	O4'-C1'-N9	6.22	113.18	108.20
26	BB	1240	U	O4'-C1'-N1	6.22	113.17	108.20
26	BB	2114	A	O4'-C1'-N9	6.22	113.17	108.20
26	BB	2740	A	C5'-C4'-O4'	6.22	116.56	109.10
26	BB	2881	U	C2-N3-C4	-6.22	123.27	127.00
1	AA	675	A	O4'-C1'-N9	6.22	113.17	108.20
1	AA	1326	U	O4'-C1'-N1	6.22	113.17	108.20
26	BB	1355	G	O4'-C1'-N9	6.22	113.17	108.20
26	BB	2241	A	O4'-C1'-N9	6.22	113.17	108.20
26	BB	2807	U	C4'-C3'-C2'	-6.22	96.38	102.60
1	AA	1358	U	N1-C2-N3	6.21	118.63	114.90
26	BB	536	G	O4'-C1'-N9	6.21	113.17	108.20
26	BB	2497	A	O4'-C1'-N9	6.21	113.17	108.20
1	AA	741	G	C8-N9-C4	-6.21	103.92	106.40
26	BB	743	A	C5'-C4'-O4'	6.21	116.55	109.10
26	BB	1217	U	O4'-C1'-N1	6.21	113.17	108.20
1	AA	776	G	C8-N9-C4	-6.21	103.92	106.40
1	AA	817	C	O4'-C1'-N1	6.21	113.16	108.20
1	AA	937	A	O4'-C1'-N9	6.21	113.17	108.20
26	BB	662	G	O4'-C1'-N9	6.21	113.17	108.20
1	AA	57	G	O4'-C1'-N9	6.21	113.16	108.20
26	BB	413	C	O4'-C1'-N1	6.20	113.16	108.20
26	BB	1786	A	C1'-O4'-C4'	-6.20	104.94	109.90
1	AA	1485	U	O4'-C1'-N1	6.20	113.16	108.20
1	AA	672	U	O4'-C1'-N1	6.20	113.16	108.20
25	BA	10	G	O4'-C1'-N9	6.20	113.16	108.20
26	BB	40	U	O4'-C1'-N1	6.20	113.16	108.20
26	BB	825	A	C5'-C4'-O4'	6.20	116.54	109.10
26	BB	2176	A	O4'-C1'-N9	6.20	113.16	108.20
1	AA	1099	G	O4'-C1'-N9	6.20	113.16	108.20
1	AA	997	U	O4'-C1'-N1	6.19	113.15	108.20
26	BB	356	G	C8-N9-C4	-6.19	103.92	106.40
1	AA	631	C	P-O3'-C3'	6.19	127.13	119.70
1	AA	1430	A	O4'-C1'-N9	6.19	113.15	108.20
26	BB	1531	C	O4'-C1'-N1	6.19	113.15	108.20
26	BB	2458	G	O4'-C1'-N9	6.19	113.15	108.20
26	BB	1572	A	C5'-C4'-O4'	6.19	116.53	109.10
26	BB	1680	U	C5'-C4'-O4'	6.19	116.53	109.10
1	AA	515	G	C8-N9-C4	-6.19	103.92	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	523	A	O4'-C1'-N9	6.19	113.15	108.20
1	AA	1316	G	C4'-C3'-C2'	-6.19	96.41	102.60
2	AE	75	C	O4'-C1'-N1	6.19	113.15	108.20
26	BB	897	C	O4'-C1'-N1	6.19	113.15	108.20
26	BB	1454	C	O4'-C1'-N1	6.19	113.15	108.20
26	BB	609	A	C8-N9-C4	-6.18	103.33	105.80
26	BB	121	G	O4'-C1'-N9	6.18	113.14	108.20
26	BB	1850	G	O4'-C1'-N9	6.18	113.15	108.20
26	BB	1963	U	O3'-P-O5'	-6.18	92.25	104.00
26	BB	2559	C	C1'-O4'-C4'	-6.18	104.95	109.90
26	BB	2601	C	C2-N3-C4	6.18	122.99	119.90
1	AA	1131	G	C5'-C4'-O4'	6.18	116.52	109.10
26	BB	2268	A	N9-C1'-C2'	-6.18	105.20	112.00
1	AA	74	A	O4'-C1'-N9	6.18	113.14	108.20
1	AA	742	G	N9-C4-C5	6.18	107.87	105.40
1	AA	1109	C	O4'-C1'-N1	6.18	113.14	108.20
26	BB	1929	G	O4'-C1'-N9	6.18	113.14	108.20
26	BB	2732	G	N9-C1'-C2'	-6.18	105.20	112.00
26	BB	2882	A	C5'-C4'-C3'	-6.18	106.11	116.00
1	AA	1385	G	C5'-C4'-C3'	-6.18	106.11	116.00
1	AA	226	G	C5'-C4'-O4'	6.18	116.51	109.10
26	BB	1138	G	N3-C4-C5	-6.18	125.51	128.60
26	BB	2161	C	N1-C2-O2	6.18	122.61	118.90
26	BB	2585	U	O4'-C1'-N1	6.17	113.14	108.20
26	BB	2892	G	C5'-C4'-C3'	-6.17	106.12	116.00
26	BB	2043	C	O4'-C1'-N1	6.17	113.14	108.20
1	AA	462	G	O4'-C1'-N9	6.17	113.14	108.20
1	AA	865	A	O4'-C1'-N9	6.17	113.13	108.20
26	BB	272	A	O4'-C1'-N9	6.17	113.13	108.20
26	BB	1393	A	O4'-C1'-N9	-6.17	103.27	108.20
26	BB	2523	G	C5'-C4'-O4'	6.17	116.50	109.10
26	BB	2802	G	O4'-C1'-N9	6.17	113.13	108.20
1	AA	1192	C	O4'-C1'-N1	6.16	113.13	108.20
1	AA	1245	C	O4'-C1'-N1	6.16	113.13	108.20
26	BB	2829	A	O4'-C1'-N9	6.16	113.13	108.20
1	AA	742	G	C8-N9-C4	-6.16	103.94	106.40
26	BB	1333	G	C5'-C4'-O4'	6.16	116.49	109.10
26	BB	910	A	O4'-C1'-N9	6.16	113.13	108.20
26	BB	2255	G	O4'-C1'-N9	6.16	113.13	108.20
26	BB	2784	U	C5'-C4'-C3'	-6.16	106.15	116.00
1	AA	1153	G	C8-N9-C4	-6.16	103.94	106.40
26	BB	2039	U	O4'-C1'-N1	6.16	113.12	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	830	G	C5'-C4'-O4'	6.15	116.48	109.10
2	AE	52	G	O4'-C1'-N9	6.15	113.12	108.20
26	BB	1864	U	O4'-C1'-N1	6.15	113.12	108.20
26	BB	2243	U	C5'-C4'-O4'	6.15	116.48	109.10
1	AA	1337	G	O3'-P-O5'	-6.15	92.32	104.00
26	BB	2502	G	C8-N9-C4	-6.15	103.94	106.40
26	BB	880	G	C8-N9-C4	-6.15	103.94	106.40
1	AA	670	G	O4'-C1'-N9	6.14	113.11	108.20
25	BA	34	A	C8-N9-C4	-6.14	103.34	105.80
26	BB	624	C	O4'-C1'-N1	6.14	113.12	108.20
26	BB	2048	G	C8-N9-C4	-6.14	103.94	106.40
1	AA	98	A	O4'-C1'-N9	6.14	113.11	108.20
26	BB	2012	G	C8-N9-C4	-6.14	103.94	106.40
26	BB	1304	A	C5'-C4'-C3'	-6.14	106.17	116.00
26	BB	1440	U	O4'-C1'-N1	6.14	113.11	108.20
1	AA	367	U	C1'-O4'-C4'	-6.14	104.99	109.90
1	AA	541	G	O4'-C1'-N9	6.14	113.11	108.20
26	BB	424	G	C3'-C2'-C1'	-6.14	96.59	101.50
26	BB	812	C	O4'-C1'-N1	6.14	113.11	108.20
26	BB	1500	G	O4'-C1'-N9	6.14	113.11	108.20
26	BB	1299	G	O4'-C1'-N9	6.14	113.11	108.20
26	BB	2060	A	O3'-P-O5'	-6.14	92.34	104.00
26	BB	2229	U	O4'-C1'-N1	6.14	113.11	108.20
26	BB	2318	G	O4'-C1'-N9	6.14	113.11	108.20
1	AA	61	G	C5'-C4'-C3'	6.13	125.82	116.00
1	AA	1304	G	O4'-C1'-N9	6.13	113.11	108.20
1	AA	202	G	O4'-C1'-N9	6.13	113.11	108.20
26	BB	373	U	O4'-C1'-N1	6.13	113.11	108.20
26	BB	1308	A	C5'-C4'-C3'	-6.13	106.19	116.00
26	BB	251	A	C8-N9-C4	-6.13	103.35	105.80
1	AA	653	U	C3'-C2'-C1'	6.13	106.40	101.50
26	BB	354	A	C8-N9-C4	-6.13	103.35	105.80
26	BB	2663	G	N3-C4-C5	-6.13	125.54	128.60
26	BB	2842	G	O4'-C1'-N9	6.13	113.10	108.20
1	AA	873	A	C5'-C4'-O4'	6.13	116.45	109.10
1	AA	916	U	O4'-C1'-N1	6.13	113.10	108.20
1	AA	1223	C	O4'-C4'-C3'	6.13	111.00	106.10
26	BB	112	U	O4'-C1'-N1	6.13	113.10	108.20
1	AA	859	G	C5'-C4'-O4'	6.12	116.45	109.10
2	AE	69	G	O4'-C1'-N9	6.12	113.10	108.20
25	BA	45	A	C5-C6-N6	-6.12	118.80	123.70
26	BB	2775	G	C8-N9-C4	-6.12	103.95	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1323	G	N3-C4-C5	-6.12	125.54	128.60
26	BB	290	U	C5'-C4'-O4'	6.12	116.45	109.10
26	BB	440	C	O4'-C1'-N1	6.12	113.10	108.20
26	BB	635	C	O4'-C1'-N1	6.12	113.10	108.20
26	BB	2398	U	C5'-C4'-C3'	-6.12	106.20	116.00
26	BB	2872	A	C5'-C4'-O4'	6.12	116.45	109.10
26	BB	235	U	O4'-C1'-N1	6.12	113.10	108.20
1	AA	1256	A	O4'-C1'-N9	6.12	113.09	108.20
26	BB	308	G	O4'-C1'-N9	6.12	113.09	108.20
2	AE	10	G	C5'-C4'-O4'	6.12	116.44	109.10
2	AE	10	G	C8-N9-C4	-6.12	103.95	106.40
25	BA	79	G	N3-C4-C5	-6.12	125.54	128.60
26	BB	1378	A	O4'-C1'-N9	6.12	113.09	108.20
26	BB	2193	G	C5'-C4'-C3'	-6.12	106.21	116.00
1	AA	1353	G	C5'-C4'-O4'	6.11	116.44	109.10
1	AA	346	G	C3'-C2'-C1'	6.11	106.39	101.50
1	AA	601	G	O4'-C1'-N9	6.11	113.09	108.20
26	BB	1488	C	O4'-C1'-N1	6.11	113.09	108.20
26	BB	1731	G	C8-N9-C4	-6.11	103.96	106.40
26	BB	2242	G	O4'-C1'-N9	6.11	113.09	108.20
26	BB	2387	U	O4'-C1'-N1	6.11	113.09	108.20
2	AB	45	U	C3'-C2'-C1'	6.11	106.39	101.50
26	BB	784	G	C1'-O4'-C4'	-6.11	105.01	109.90
26	BB	2199	A	C5'-C4'-O4'	6.11	116.43	109.10
26	BB	118	A	O4'-C4'-C3'	6.11	110.98	106.10
26	BB	824	U	C5'-C4'-O4'	6.11	116.43	109.10
26	BB	1230	A	O4'-C1'-N9	6.11	113.08	108.20
26	BB	764	A	O4'-C1'-N9	6.10	113.08	108.20
26	BB	1338	G	O4'-C1'-N9	6.10	113.08	108.20
1	AA	1209	C	O4'-C1'-N1	6.10	113.08	108.20
26	BB	1695	G	N3-C4-C5	-6.10	125.55	128.60
26	BB	2256	G	C8-N9-C4	-6.10	103.96	106.40
26	BB	2898	U	O4'-C1'-N1	6.10	113.08	108.20
1	AA	132	C	O4'-C1'-N1	6.10	113.08	108.20
26	BB	481	G	N3-C4-C5	-6.10	125.55	128.60
26	BB	806	C	O4'-C1'-N1	6.10	113.08	108.20
26	BB	132	G	O4'-C1'-N9	6.09	113.08	108.20
26	BB	1142	A	O4'-C1'-N9	6.09	113.08	108.20
26	BB	1923	U	C5'-C4'-C3'	-6.09	106.25	116.00
26	BB	2631	G	C5'-C4'-O4'	6.09	116.41	109.10
2	AE	63	G	O4'-C1'-N9	6.09	113.08	108.20
25	BA	51	G	O4'-C1'-N9	6.09	113.07	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	617	G	O4'-C1'-N9	6.09	113.07	108.20
26	BB	899	A	O4'-C1'-N9	6.09	113.07	108.20
26	BB	2513	A	C5'-C4'-O4'	6.09	116.41	109.10
1	AA	314	C	C4'-C3'-C2'	-6.09	96.51	102.60
1	AA	944	G	O4'-C1'-N9	6.09	113.07	108.20
1	AA	1295	U	O4'-C1'-N1	6.09	113.07	108.20
26	BB	973	A	O4'-C1'-N9	6.09	113.07	108.20
26	BB	2683	C	O4'-C1'-N1	6.09	113.07	108.20
1	AA	137	U	O4'-C1'-N1	6.09	113.07	108.20
26	BB	903	C	C5'-C4'-O4'	6.09	116.40	109.10
26	BB	976	G	C8-N9-C4	-6.09	103.97	106.40
1	AA	877	G	O4'-C1'-N9	6.08	113.07	108.20
1	AA	109	A	O4'-C1'-N9	6.08	113.06	108.20
26	BB	1599	U	O4'-C1'-N1	6.08	113.06	108.20
26	BB	1951	U	P-O3'-C3'	6.08	127.00	119.70
26	BB	2252	G	C4'-C3'-C2'	-6.08	96.52	102.60
1	AA	764	C	O4'-C1'-N1	6.08	113.06	108.20
2	AB	29	G	C8-N9-C4	-6.08	103.97	106.40
26	BB	1375	U	O4'-C1'-N1	6.08	113.06	108.20
42	BR	23	TYR	CB-CG-CD1	-6.08	117.35	121.00
2	AE	3	C	C5'-C4'-O4'	6.08	116.39	109.10
26	BB	1703	G	C5'-C4'-C3'	-6.08	106.28	116.00
26	BB	2074	U	O4'-C1'-N1	6.08	113.06	108.20
26	BB	1451	C	C2'-C3'-O3'	6.07	123.42	113.70
26	BB	729	G	O3'-P-O5'	-6.07	92.47	104.00
26	BB	1337	G	N3-C4-C5	-6.07	125.56	128.60
1	AA	1489	G	N3-C4-C5	-6.07	125.57	128.60
26	BB	119	A	C1'-O4'-C4'	-6.07	105.05	109.90
26	BB	1308	A	C8-N9-C4	-6.07	103.37	105.80
26	BB	1446	C	O4'-C1'-N1	6.07	113.06	108.20
26	BB	2485	G	C3'-C2'-C1'	-6.07	96.65	101.50
26	BB	2488	G	N3-C4-C5	-6.07	125.57	128.60
26	BB	2655	G	O4'-C1'-N9	6.07	113.05	108.20
1	AA	792	A	O4'-C1'-N9	6.07	113.05	108.20
1	AA	540	G	O4'-C1'-N9	6.06	113.05	108.20
26	BB	770	G	O4'-C1'-N9	6.06	113.05	108.20
26	BB	1886	U	P-O3'-C3'	6.06	126.97	119.70
26	BB	2269	G	C5'-C4'-C3'	-6.06	106.30	116.00
26	BB	2601	C	C3'-C2'-C1'	6.06	106.35	101.50
1	AA	863	U	C1'-O4'-C4'	-6.06	105.05	109.90
26	BB	1416	G	N9-C4-C5	6.06	107.83	105.40
1	AA	175	C	C5'-C4'-O4'	6.06	116.37	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	408	A	C8-N9-C4	-6.06	103.38	105.80
1	AA	847	G	O4'-C1'-N9	6.06	113.05	108.20
26	BB	2627	G	C8-N9-C4	-6.06	103.98	106.40
26	BB	2863	C	C5'-C4'-O4'	6.06	116.37	109.10
1	AA	1329	A	O4'-C1'-N9	6.06	113.05	108.20
25	BA	76	G	O4'-C1'-N9	6.06	113.05	108.20
26	BB	1550	C	C3'-C2'-C1'	6.06	106.34	101.50
26	BB	1921	G	O4'-C1'-N9	6.06	113.05	108.20
26	BB	1183	U	C3'-C2'-C1'	6.05	106.34	101.50
26	BB	1206	G	C5'-C4'-C3'	-6.05	106.31	116.00
26	BB	2667	C	C5'-C4'-C3'	-6.05	106.31	116.00
1	AA	1323	G	C8-N9-C4	-6.05	103.98	106.40
26	BB	2425	A	O4'-C1'-C2'	-6.05	99.75	105.80
26	BB	2023	C	O4'-C1'-N1	6.05	113.04	108.20
26	BB	2047	C	O4'-C1'-N1	6.05	113.04	108.20
1	AA	59	A	C3'-C2'-C1'	-6.05	96.66	101.50
1	AA	726	C	C5'-C4'-O4'	6.05	116.36	109.10
1	AA	1085	U	O4'-C1'-N1	6.05	113.04	108.20
1	AA	1497	G	O4'-C1'-N9	6.05	113.04	108.20
26	BB	471	A	O4'-C1'-N9	6.05	113.04	108.20
26	BB	809	G	N3-C4-C5	-6.05	125.58	128.60
26	BB	2622	U	O4'-C1'-N1	6.05	113.04	108.20
26	BB	521	U	C5'-C4'-O4'	6.04	116.35	109.10
26	BB	2219	U	N1-C2-N3	6.04	118.53	114.90
1	AA	694	A	C3'-C2'-C1'	6.04	106.33	101.50
26	BB	2730	C	O4'-C1'-N1	6.04	113.03	108.20
2	AB	63	G	O4'-C1'-N9	6.04	113.03	108.20
26	BB	1033	U	O4'-C4'-C3'	6.04	110.93	106.10
26	BB	447	A	C8-N9-C4	-6.04	103.39	105.80
26	BB	673	C	O4'-C1'-N1	6.04	113.03	108.20
26	BB	1952	A	O4'-C4'-C3'	6.04	110.93	106.10
26	BB	2364	C	O4'-C1'-N1	6.04	113.03	108.20
2	AE	2	C	C5'-C4'-O4'	6.04	116.34	109.10
26	BB	442	G	O4'-C1'-N9	6.04	113.03	108.20
26	BB	1138	G	O4'-C1'-N9	6.04	113.03	108.20
26	BB	2078	C	C5'-C4'-O4'	6.04	116.34	109.10
26	BB	2747	G	O4'-C1'-N9	6.04	113.03	108.20
1	AA	154	U	C5'-C4'-O4'	6.04	116.34	109.10
26	BB	689	A	C5'-C4'-O4'	6.04	116.34	109.10
26	BB	1560	G	N3-C4-C5	-6.03	125.58	128.60
2	AE	12	U	O4'-C1'-N1	6.03	113.03	108.20
26	BB	960	A	C2'-C3'-O3'	6.03	123.35	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1136	G	N3-C4-C5	-6.03	125.58	128.60
26	BB	1109	C	C3'-C2'-C1'	6.03	106.32	101.50
26	BB	1507	C	O4'-C1'-N1	6.03	113.02	108.20
26	BB	2551	C	C5'-C4'-C3'	-6.03	106.35	116.00
1	AA	740	U	O4'-C1'-N1	6.03	113.02	108.20
26	BB	7	G	C5'-C4'-C3'	-6.03	106.35	116.00
26	BB	167	A	C5'-C4'-O4'	6.03	116.33	109.10
26	BB	1972	G	N3-C2-N2	-6.03	115.68	119.90
26	BB	1975	G	O4'-C1'-N9	6.03	113.02	108.20
26	BB	421	C	O4'-C1'-N1	6.03	113.02	108.20
26	BB	731	C	O4'-C1'-N1	6.03	113.02	108.20
26	BB	1940	U	N1-C1'-C2'	6.03	121.83	114.00
1	AA	757	U	O3'-P-O5'	-6.02	92.55	104.00
26	BB	675	A	C5'-C4'-O4'	6.02	116.33	109.10
1	AA	922	G	O4'-C1'-N9	6.02	113.02	108.20
26	BB	809	G	C8-N9-C4	-6.02	103.99	106.40
26	BB	1352	U	O4'-C1'-N1	6.02	113.02	108.20
26	BB	2384	U	O4'-C1'-N1	6.02	113.02	108.20
1	AA	1006	G	C8-N9-C4	-6.02	103.99	106.40
1	AA	1010	U	N1-C2-N3	6.02	118.51	114.90
26	BB	2423	U	O4'-C1'-N1	6.02	113.02	108.20
2	AB	14	A	O4'-C1'-N9	6.02	113.01	108.20
26	BB	515	A	O4'-C1'-N9	6.02	113.01	108.20
26	BB	1208	C	O4'-C1'-N1	6.02	113.01	108.20
26	BB	1997	C	O4'-C1'-N1	6.02	113.01	108.20
49	BY	36	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	AA	1490	U	O4'-C1'-N1	6.02	113.01	108.20
26	BB	1361	G	N3-C4-C5	-6.02	125.59	128.60
26	BB	1619	G	C5'-C4'-O4'	6.02	116.32	109.10
1	AA	1319	A	C5'-C4'-O4'	6.01	116.32	109.10
26	BB	1570	A	O4'-C1'-N9	6.01	113.01	108.20
26	BB	2129	C	N1-C2-O2	6.01	122.51	118.90
26	BB	150	U	O4'-C1'-N1	6.01	113.01	108.20
26	BB	211	C	O4'-C1'-N1	6.01	113.01	108.20
1	AA	1276	G	C5'-C4'-O4'	6.01	116.31	109.10
26	BB	294	A	C8-N9-C4	-6.01	103.39	105.80
26	BB	1054	A	O4'-C1'-N9	6.01	113.01	108.20
26	BB	1688	U	C5'-C4'-O4'	6.01	116.31	109.10
26	BB	2403	C	O4'-C1'-N1	6.01	113.01	108.20
26	BB	1088	A	P-O3'-C3'	6.01	126.91	119.70
26	BB	1324	G	C5'-C4'-C3'	-6.01	106.39	116.00
26	BB	1913	A	O4'-C1'-C2'	-6.01	99.79	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2668	G	C8-N9-C4	-6.01	104.00	106.40
26	BB	2864	G	C5'-C4'-O4'	6.01	116.31	109.10
26	BB	141	G	C4'-C3'-C2'	-6.00	96.59	102.60
26	BB	871	U	O4'-C1'-N1	6.00	113.00	108.20
26	BB	2854	G	C5'-C4'-O4'	6.00	116.31	109.10
25	BA	4	C	O3'-P-O5'	6.00	115.41	104.00
26	BB	1954	G	O4'-C1'-N9	6.00	113.00	108.20
26	BB	50	U	O4'-C1'-N1	6.00	113.00	108.20
26	BB	485	C	O4'-C1'-N1	6.00	113.00	108.20
26	BB	1084	A	O4'-C1'-N9	6.00	113.00	108.20
26	BB	2041	U	O4'-C1'-N1	6.00	113.00	108.20
26	BB	2769	U	C5'-C4'-O4'	6.00	116.30	109.10
1	AA	183	C	C5'-C4'-C3'	-6.00	106.40	116.00
26	BB	1532	A	C8-N9-C4	-6.00	103.40	105.80
26	BB	2408	U	O4'-C1'-N1	6.00	113.00	108.20
26	BB	2508	G	C3'-C2'-C1'	-6.00	96.70	101.50
26	BB	951	C	O4'-C1'-N1	6.00	113.00	108.20
26	BB	1525	A	C5'-C4'-O4'	6.00	116.30	109.10
1	AA	858	G	C5'-C4'-O4'	5.99	116.29	109.10
1	AA	1036	A	C5'-C4'-C3'	-5.99	106.41	116.00
26	BB	486	C	O4'-C1'-N1	5.99	112.99	108.20
26	BB	2309	A	O4'-C1'-N9	5.99	113.00	108.20
1	AA	898	G	O4'-C1'-N9	5.99	112.99	108.20
1	AA	1018	G	O4'-C1'-N9	5.99	112.99	108.20
26	BB	736	C	C3'-C2'-C1'	5.99	106.29	101.50
26	BB	738	G	C8-N9-C4	-5.99	104.00	106.40
26	BB	1025	G	C8-N9-C4	-5.99	104.00	106.40
1	AA	706	A	C5'-C4'-C3'	-5.99	106.42	116.00
2	AE	59	U	O4'-C1'-N1	5.99	112.99	108.20
26	BB	494	G	N9-C1'-C2'	-5.99	105.41	112.00
26	BB	1198	U	O4'-C1'-N1	5.99	112.99	108.20
26	BB	2640	G	C5'-C4'-O4'	5.99	116.29	109.10
1	AA	341	C	O4'-C1'-N1	5.99	112.99	108.20
26	BB	301	G	P-O3'-C3'	5.99	126.88	119.70
26	BB	1511	G	C5'-C4'-C3'	-5.99	106.42	116.00
1	AA	221	C	O4'-C1'-N1	5.98	112.99	108.20
1	AA	240	G	N3-C4-C5	-5.98	125.61	128.60
25	BA	84	G	O4'-C1'-N9	5.98	112.99	108.20
26	BB	160	A	N9-C1'-C2'	-5.98	105.42	112.00
26	BB	1734	G	N3-C4-C5	-5.98	125.61	128.60
26	BB	2262	U	C5'-C4'-C3'	-5.98	106.43	116.00
1	AA	339	C	O4'-C1'-N1	5.98	112.98	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2650	U	O4'-C1'-N1	5.98	112.98	108.20
1	AA	1495	U	O4'-C1'-N1	5.98	112.98	108.20
1	AA	196	A	C4'-C3'-C2'	-5.98	96.62	102.60
1	AA	1541	U	O4'-C1'-N1	5.98	112.98	108.20
1	AA	52	C	C1'-O4'-C4'	-5.97	105.12	109.90
1	AA	783	C	C5'-C4'-O4'	5.97	116.27	109.10
1	AA	863	U	O4'-C1'-N1	5.97	112.98	108.20
1	AA	1395	C	C5'-C4'-O4'	5.97	116.27	109.10
26	BB	1301	A	N9-C1'-C2'	5.97	121.77	114.00
1	AA	772	U	O4'-C1'-N1	5.97	112.98	108.20
1	AA	1216	A	C3'-C2'-C1'	5.97	106.28	101.50
26	BB	1740	G	O4'-C1'-N9	5.97	112.98	108.20
26	BB	1810	A	C4'-C3'-C2'	-5.97	96.63	102.60
26	BB	2187	U	C5'-C4'-O4'	5.97	116.27	109.10
26	BB	580	U	O4'-C1'-N1	5.97	112.98	108.20
2	AE	50	U	O4'-C1'-N1	5.97	112.97	108.20
26	BB	845	A	O4'-C1'-N9	5.97	112.98	108.20
26	BB	2543	G	C8-N9-C4	-5.97	104.01	106.40
26	BB	2685	G	C5'-C4'-O4'	5.97	116.26	109.10
26	BB	1068	G	O3'-P-O5'	-5.97	92.66	104.00
26	BB	1074	G	O4'-C1'-N9	5.97	112.97	108.20
1	AA	406	G	C8-N9-C4	-5.96	104.01	106.40
1	AA	1043	G	C8-N9-C4	-5.96	104.01	106.40
1	AA	1221	G	O4'-C1'-N9	5.96	112.97	108.20
26	BB	303	G	C8-N9-C4	-5.96	104.01	106.40
26	BB	301	G	N9-C4-C5	5.96	107.78	105.40
26	BB	2676	C	O4'-C1'-N1	5.96	112.97	108.20
26	BB	315	G	O4'-C1'-N9	5.96	112.97	108.20
26	BB	2516	A	O4'-C1'-N9	5.96	112.97	108.20
25	BA	87	U	O4'-C1'-N1	5.96	112.97	108.20
1	AA	326	G	C8-N9-C4	-5.96	104.02	106.40
26	BB	826	U	O4'-C1'-N1	5.96	112.97	108.20
1	AA	513	C	O4'-C1'-N1	5.96	112.97	108.20
26	BB	578	G	O4'-C1'-N9	5.96	112.97	108.20
26	BB	2519	U	O4'-C1'-N1	5.96	112.97	108.20
1	AA	258	G	O4'-C1'-N9	5.96	112.96	108.20
1	AA	1192	C	N1-C2-O2	5.96	122.47	118.90
26	BB	1035	U	O4'-C1'-N1	5.96	112.96	108.20
26	BB	1326	U	O4'-C1'-N1	5.96	112.96	108.20
26	BB	2625	G	N3-C4-C5	-5.95	125.62	128.60
1	AA	453	G	C8-N9-C4	-5.95	104.02	106.40
2	AE	17	C	N1-C2-O2	5.95	122.47	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	610	C	O4'-C1'-N1	5.95	112.96	108.20
26	BB	1033	U	C3'-C2'-C1'	5.95	106.26	101.50
1	AA	255	G	C5'-C4'-C3'	-5.95	106.48	116.00
26	BB	700	G	N9-C1'-C2'	-5.95	105.46	112.00
26	BB	989	G	O4'-C1'-N9	5.95	112.96	108.20
26	BB	2385	C	C5'-C4'-O4'	5.95	116.24	109.10
1	AA	463	U	O4'-C1'-N1	5.95	112.96	108.20
26	BB	59	U	O4'-C1'-N1	5.94	112.95	108.20
26	BB	1528	A	O4'-C1'-N9	5.94	112.95	108.20
26	BB	2272	U	O4'-C1'-N1	5.94	112.95	108.20
1	AA	1378	C	C5'-C4'-C3'	-5.94	106.49	116.00
1	AA	1514	G	O4'-C1'-N9	5.94	112.95	108.20
25	BA	95	U	C5'-C4'-O4'	5.94	116.23	109.10
26	BB	311	A	O4'-C1'-N9	5.94	112.95	108.20
26	BB	1070	A	N9-C4-C5	5.94	108.18	105.80
26	BB	1593	A	O4'-C1'-N9	5.94	112.95	108.20
26	BB	1634	A	C3'-C2'-C1'	-5.94	96.75	101.50
1	AA	9	G	N3-C4-C5	-5.94	125.63	128.60
26	BB	637	A	O4'-C1'-N9	5.94	112.95	108.20
26	BB	983	A	O4'-C4'-C3'	5.94	110.85	106.10
26	BB	1664	A	C5'-C4'-C3'	-5.94	106.50	116.00
26	BB	407	G	C8-N9-C4	-5.94	104.02	106.40
26	BB	1732	C	O4'-C4'-C3'	5.94	110.85	106.10
26	BB	1615	C	O4'-C1'-N1	5.94	112.95	108.20
1	AA	622	A	C8-N9-C4	-5.94	103.43	105.80
26	BB	1638	C	O4'-C1'-N1	5.94	112.95	108.20
1	AA	869	G	C8-N9-C4	-5.93	104.03	106.40
26	BB	1760	C	O4'-C1'-N1	5.93	112.95	108.20
26	BB	2062	A	O4'-C1'-N9	5.93	112.94	108.20
26	BB	340	A	O4'-C1'-N9	5.93	112.94	108.20
26	BB	1108	U	O4'-C1'-N1	5.93	112.94	108.20
26	BB	2763	G	C8-N9-C4	-5.93	104.03	106.40
1	AA	491	G	C5'-C4'-C3'	-5.93	106.52	116.00
1	AA	1417	G	C5'-C4'-O4'	5.93	116.21	109.10
26	BB	1388	G	O4'-C1'-N9	5.93	112.94	108.20
26	BB	1490	A	O4'-C1'-N9	-5.93	103.46	108.20
1	AA	1160	G	N3-C4-C5	-5.92	125.64	128.60
26	BB	192	C	O4'-C1'-N1	5.92	112.94	108.20
26	BB	1540	G	N3-C4-C5	-5.92	125.64	128.60
26	BB	312	G	C8-N9-C4	-5.92	104.03	106.40
26	BB	1956	U	C5'-C4'-O4'	5.92	116.21	109.10
1	AA	107	G	N9-C1'-C2'	-5.92	105.49	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1860	G	C8-N9-C4	-5.92	104.03	106.40
1	AA	1429	A	O4'-C1'-N9	5.92	112.93	108.20
1	AA	1065	U	O4'-C4'-C3'	5.91	110.83	106.10
26	BB	389	G	C8-N9-C4	-5.91	104.03	106.40
1	AA	1088	G	O3'-P-O5'	-5.91	92.77	104.00
26	BB	69	C	O4'-C1'-N1	5.91	112.93	108.20
26	BB	1091	G	O4'-C1'-N9	5.91	112.93	108.20
26	BB	1908	C	O4'-C1'-N1	5.91	112.93	108.20
26	BB	62	U	O4'-C1'-N1	5.91	112.93	108.20
1	AA	989	U	O4'-C1'-N1	5.91	112.93	108.20
1	AA	1161	C	O4'-C1'-N1	5.91	112.93	108.20
1	AA	1509	C	O4'-C1'-N1	5.91	112.93	108.20
2	AB	21	A	O4'-C1'-N9	5.91	112.93	108.20
26	BB	2318	G	C8-N9-C4	-5.91	104.04	106.40
1	AA	1223	C	C3'-C2'-C1'	5.90	106.22	101.50
25	BA	55	U	C5'-C4'-C3'	-5.90	106.56	116.00
26	BB	852	U	N1-C2-N3	5.90	118.44	114.90
1	AA	861	G	C8-N9-C4	-5.90	104.04	106.40
1	AA	1153	G	N3-C4-C5	-5.90	125.65	128.60
25	BA	108	A	O4'-C1'-N9	5.90	112.92	108.20
26	BB	1926	U	C5'-C4'-C3'	-5.90	106.56	116.00
26	BB	710	U	O3'-P-O5'	-5.90	92.79	104.00
1	AA	220	G	N3-C4-C5	-5.90	125.65	128.60
2	AE	9	A	C3'-C2'-C1'	5.90	106.22	101.50
26	BB	1075	C	O4'-C1'-N1	5.89	112.92	108.20
26	BB	2295	C	O4'-C1'-N1	5.89	112.92	108.20
26	BB	2514	U	O4'-C1'-N1	5.89	112.92	108.20
1	AA	171	A	C5'-C4'-C3'	-5.89	106.57	116.00
26	BB	283	G	O4'-C1'-N9	5.89	112.91	108.20
1	AA	1312	G	N3-C4-C5	-5.89	125.65	128.60
26	BB	2112	G	N3-C4-C5	-5.89	125.65	128.60
26	BB	976	G	C5'-C4'-O4'	5.89	116.17	109.10
26	BB	1523	U	N1-C1'-C2'	5.89	121.66	114.00
26	BB	1577	C	C5'-C4'-O4'	5.89	116.17	109.10
1	AA	616	G	O4'-C1'-N9	5.89	112.91	108.20
1	AA	1072	G	C8-N9-C4	-5.89	104.05	106.40
1	AA	1489	G	C8-N9-C4	-5.89	104.05	106.40
2	AB	69	G	O4'-C1'-N9	5.89	112.91	108.20
26	BB	508	A	O4'-C1'-N9	5.88	112.91	108.20
26	BB	832	U	O4'-C1'-N1	5.88	112.91	108.20
26	BB	511	U	C5'-C4'-O4'	5.88	116.16	109.10
25	BA	67	G	O4'-C1'-N9	5.88	112.91	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1573	G	C5'-C4'-C3'	-5.88	106.59	116.00
26	BB	2491	U	O4'-C1'-N1	5.88	112.90	108.20
1	AA	528	C	O4'-C1'-N1	5.88	112.90	108.20
26	BB	412	A	C5'-C4'-C3'	-5.88	106.59	116.00
26	BB	2380	C	C4'-C3'-C2'	-5.88	96.72	102.60
26	BB	1551	A	C3'-C2'-C1'	-5.88	96.80	101.50
26	BB	1801	A	O4'-C1'-N9	5.88	112.90	108.20
26	BB	636	G	C3'-C2'-C1'	5.88	106.20	101.50
26	BB	499	U	O4'-C1'-N1	5.87	112.90	108.20
26	BB	968	C	O4'-C1'-N1	5.87	112.90	108.20
1	AA	347	G	O4'-C1'-N9	5.87	112.90	108.20
25	BA	10	G	N3-C4-C5	-5.87	125.66	128.60
26	BB	1069	A	O4'-C4'-C3'	5.87	110.80	106.10
26	BB	503	A	O4'-C1'-N9	5.87	112.90	108.20
26	BB	2205	A	C8-N9-C4	-5.87	103.45	105.80
26	BB	279	A	O3'-P-O5'	-5.87	92.85	104.00
26	BB	2017	U	C3'-C2'-C1'	5.87	106.19	101.50
26	BB	2751	G	N9-C1'-C2'	5.87	121.63	114.00
26	BB	2863	C	O4'-C1'-N1	5.87	112.89	108.20
1	AA	198	G	C5'-C4'-O4'	5.87	116.14	109.10
1	AA	240	G	C8-N9-C4	-5.87	104.05	106.40
26	BB	1390	U	O4'-C1'-N1	5.87	112.89	108.20
26	BB	1532	A	O4'-C1'-N9	5.87	112.89	108.20
1	AA	1496	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	439	A	O4'-C1'-N9	5.86	112.89	108.20
26	BB	76	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	802	A	C5'-C4'-C3'	-5.86	106.62	116.00
26	BB	1855	U	C5'-C4'-O4'	5.86	116.13	109.10
26	BB	1937	A	C8-N9-C4	-5.86	103.46	105.80
1	AA	545	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	2072	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	2462	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	33	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	2195	U	O4'-C1'-N1	5.86	112.89	108.20
26	BB	2862	G	O4'-C1'-N9	5.86	112.89	108.20
1	AA	1234	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	564	C	O4'-C1'-N1	5.86	112.89	108.20
26	BB	2087	G	N3-C4-C5	-5.85	125.67	128.60
1	AA	536	C	O4'-C1'-N1	5.85	112.88	108.20
2	AB	34	G	C8-N9-C4	-5.85	104.06	106.40
26	BB	9	G	C5'-C4'-C3'	-5.85	106.64	116.00
26	BB	1145	C	O4'-C1'-N1	5.85	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1236	G	O4'-C1'-N9	5.85	112.88	108.20
26	BB	961	C	C6-N1-C2	-5.85	117.96	120.30
26	BB	1379	U	O4'-C1'-N1	5.85	112.88	108.20
26	BB	1710	G	C5'-C4'-O4'	5.85	116.12	109.10
26	BB	2179	C	O4'-C1'-N1	5.85	112.88	108.20
26	BB	2373	G	N9-C1'-C2'	-5.85	105.57	112.00
26	BB	2494	G	C5'-C4'-O4'	5.85	116.11	109.10
26	BB	2581	G	O4'-C1'-N9	5.85	112.88	108.20
1	AA	177	G	C8-N9-C4	-5.84	104.06	106.40
1	AA	300	A	C8-N9-C4	-5.84	103.46	105.80
1	AA	1186	G	N3-C4-C5	-5.84	125.68	128.60
2	AE	1	G	N3-C4-C5	-5.84	125.68	128.60
26	BB	1303	G	N3-C4-C5	-5.84	125.68	128.60
1	AA	1529	G	O4'-C1'-N9	5.84	112.87	108.20
1	AA	195	A	C5'-C4'-C3'	-5.84	106.66	116.00
1	AA	887	G	O4'-C1'-N9	5.84	112.87	108.20
26	BB	2352	A	C5'-C4'-C3'	-5.84	106.66	116.00
26	BB	1195	G	N9-C1'-C2'	-5.84	105.58	112.00
26	BB	1270	C	O4'-C1'-N1	5.83	112.87	108.20
1	AA	51	A	O4'-C1'-N9	5.83	112.87	108.20
1	AA	236	A	O4'-C1'-N9	5.83	112.87	108.20
1	AA	917	G	N3-C4-C5	-5.83	125.68	128.60
26	BB	1940	U	O4'-C4'-C3'	5.83	110.77	106.10
26	BB	1986	C	C5'-C4'-C3'	-5.83	106.67	116.00
26	BB	9	G	P-O3'-C3'	5.83	126.70	119.70
26	BB	964	C	O4'-C1'-N1	5.83	112.86	108.20
26	BB	2848	G	C2-N3-C4	5.83	114.81	111.90
25	BA	69	G	O4'-C1'-N9	5.83	112.86	108.20
26	BB	669	G	N3-C4-C5	-5.83	125.69	128.60
26	BB	734	A	C5'-C4'-O4'	5.83	116.09	109.10
26	BB	2418	A	O4'-C1'-N9	5.83	112.86	108.20
1	AA	1521	C	O4'-C1'-N1	5.83	112.86	108.20
26	BB	2716	C	C5'-C4'-O4'	5.83	116.09	109.10
26	BB	2751	G	O4'-C1'-N9	5.83	112.86	108.20
26	BB	81	G	O4'-C1'-N9	5.82	112.86	108.20
1	AA	172	A	C8-N9-C4	-5.82	103.47	105.80
1	AA	457	G	C8-N9-C4	-5.82	104.07	106.40
26	BB	820	A	C5'-C4'-C3'	-5.82	106.69	116.00
26	BB	821	A	O4'-C1'-N9	5.82	112.86	108.20
26	BB	243	U	O4'-C1'-N1	5.82	112.86	108.20
26	BB	1140	C	O4'-C1'-N1	5.82	112.86	108.20
26	BB	1280	G	O4'-C1'-N9	5.82	112.86	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1617	C	O4'-C1'-N1	5.82	112.86	108.20
26	BB	2656	U	O4'-C1'-N1	5.82	112.86	108.20
26	BB	907	G	C5'-C4'-O4'	5.82	116.08	109.10
26	BB	1736	U	N1-C2-N3	5.82	118.39	114.90
26	BB	345	A	P-O3'-C3'	5.82	126.68	119.70
26	BB	1325	U	O4'-C1'-C2'	-5.82	99.98	105.80
26	BB	1622	G	N3-C4-C5	-5.82	125.69	128.60
26	BB	2790	U	O4'-C4'-C3'	5.82	110.75	106.10
1	AA	1120	C	O3'-P-O5'	-5.82	92.95	104.00
26	BB	226	A	C5'-C4'-C3'	-5.82	106.69	116.00
1	AA	1151	A	O3'-P-O5'	-5.81	92.96	104.00
26	BB	1972	G	N9-C4-C5	5.81	107.72	105.40
26	BB	2440	C	O4'-C1'-N1	5.81	112.85	108.20
26	BB	2480	C	O4'-C1'-N1	5.81	112.85	108.20
1	AA	367	U	C5'-C4'-C3'	-5.81	106.70	116.00
1	AA	533	A	P-O3'-C3'	5.81	126.67	119.70
1	AA	697	U	C5'-C4'-O4'	5.81	116.07	109.10
1	AA	773	G	O4'-C1'-N9	5.81	112.85	108.20
1	AA	1304	G	C5'-C4'-O4'	5.81	116.07	109.10
25	BA	14	U	C5'-C4'-C3'	-5.81	106.70	116.00
26	BB	1597	A	O4'-C1'-N9	5.81	112.85	108.20
26	BB	793	A	O4'-C1'-N9	5.81	112.84	108.20
26	BB	1232	G	O4'-C1'-N9	5.81	112.84	108.20
26	BB	1473	G	C3'-C2'-C1'	-5.81	96.86	101.50
1	AA	367	U	C3'-C2'-C1'	5.80	106.14	101.50
1	AA	1505	G	N9-C4-C5	5.80	107.72	105.40
26	BB	284	U	O4'-C1'-N1	5.80	112.84	108.20
26	BB	2620	C	O4'-C1'-N1	5.80	112.84	108.20
26	BB	230	G	O4'-C1'-N9	5.80	112.84	108.20
26	BB	2567	G	C8-N9-C4	-5.80	104.08	106.40
1	AA	1358	U	O4'-C1'-C2'	-5.80	100.00	105.80
25	BA	11	C	O3'-P-O5'	-5.80	92.98	104.00
26	BB	687	C	O4'-C1'-N1	5.80	112.84	108.20
26	BB	1072	C	O4'-C1'-N1	5.80	112.84	108.20
26	BB	1406	U	O4'-C1'-N1	5.80	112.84	108.20
26	BB	1566	A	C3'-C2'-C1'	5.80	106.14	101.50
26	BB	902	C	C5'-C4'-O4'	5.80	116.06	109.10
26	BB	831	G	O4'-C1'-N9	5.79	112.84	108.20
26	BB	1284	A	O4'-C1'-N9	5.79	112.84	108.20
1	AA	357	G	C5'-C4'-O4'	5.79	116.05	109.10
1	AA	539	A	C5'-C4'-O4'	5.79	116.05	109.10
1	AA	876	C	C5'-C4'-O4'	5.79	116.05	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	892	A	C5'-C4'-C3'	-5.79	106.73	116.00
1	AA	1099	G	C5'-C4'-C3'	-5.79	106.73	116.00
26	BB	368	A	C5'-C4'-C3'	-5.79	106.73	116.00
26	BB	555	G	N3-C4-C5	-5.79	125.70	128.60
26	BB	922	C	O4'-C1'-N1	5.79	112.84	108.20
26	BB	1024	G	O4'-C1'-N9	5.79	112.83	108.20
26	BB	2664	G	C5'-C4'-O4'	5.79	116.05	109.10
26	BB	2777	G	N3-C4-C5	-5.79	125.70	128.60
1	AA	623	C	C5'-C4'-O4'	5.79	116.05	109.10
26	BB	1128	G	O4'-C1'-N9	5.79	112.83	108.20
26	BB	385	C	O4'-C1'-N1	5.79	112.83	108.20
1	AA	512	U	C4'-C3'-C2'	-5.79	96.81	102.60
1	AA	653	U	O4'-C1'-N1	5.79	112.83	108.20
26	BB	1653	G	O4'-C1'-N9	5.79	112.83	108.20
26	BB	1930	G	C8-N9-C4	-5.79	104.08	106.40
26	BB	2485	G	N3-C4-C5	-5.79	125.71	128.60
1	AA	1392	G	N9-C1'-C2'	-5.79	105.63	112.00
26	BB	960	A	P-O3'-C3'	5.79	126.64	119.70
1	AA	525	C	C5'-C4'-C3'	-5.79	106.74	116.00
1	AA	1463	U	O4'-C1'-N1	5.79	112.83	108.20
26	BB	361	G	O4'-C1'-N9	5.79	112.83	108.20
26	BB	1171	G	C8-N9-C4	-5.79	104.09	106.40
26	BB	1661	G	O4'-C1'-N9	5.79	112.83	108.20
26	BB	1467	U	O4'-C1'-N1	5.78	112.83	108.20
26	BB	1855	U	O4'-C1'-N1	5.78	112.83	108.20
26	BB	1109	C	O4'-C4'-C3'	5.78	110.72	106.10
2	AB	56	C	O4'-C1'-N1	5.78	112.82	108.20
26	BB	1197	G	C5'-C4'-O4'	5.78	116.03	109.10
1	AA	813	U	C4'-C3'-C2'	-5.77	96.83	102.60
26	BB	437	U	O4'-C1'-N1	5.77	112.82	108.20
26	BB	673	C	C5'-C4'-O4'	5.77	116.03	109.10
26	BB	930	G	N3-C4-C5	-5.77	125.71	128.60
26	BB	808	G	C8-N9-C4	-5.77	104.09	106.40
26	BB	2820	A	C4'-C3'-C2'	-5.77	96.83	102.60
1	AA	1119	C	O4'-C1'-N1	5.77	112.81	108.20
1	AA	1188	A	O4'-C1'-N9	5.77	112.81	108.20
26	BB	2720	U	C5'-C4'-O4'	5.77	116.02	109.10
26	BB	2765	A	O4'-C1'-N9	5.77	112.81	108.20
1	AA	491	G	N3-C4-C5	-5.77	125.72	128.60
1	AA	639	G	N3-C4-C5	-5.77	125.72	128.60
1	AA	931	C	O4'-C1'-N1	5.77	112.81	108.20
4	AD	42	U	O4'-C1'-N1	5.77	112.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1135	C	C5'-C4'-O4'	5.77	116.02	109.10
26	BB	1890	A	C8-N9-C4	-5.77	103.49	105.80
1	AA	943	U	O4'-C1'-N1	5.77	112.81	108.20
1	AA	1377	A	C5'-C4'-C3'	-5.76	106.78	116.00
26	BB	2283	C	O4'-C1'-N1	5.76	112.81	108.20
26	BB	305	C	C5'-C4'-C3'	-5.76	106.78	116.00
26	BB	1029	A	C8-N9-C4	-5.76	103.50	105.80
26	BB	2102	G	O4'-C1'-N9	5.76	112.81	108.20
1	AA	597	G	N3-C4-C5	-5.76	125.72	128.60
26	BB	623	C	O4'-C1'-N1	5.76	112.81	108.20
26	BB	1385	A	C1'-O4'-C4'	-5.76	105.29	109.90
26	BB	2543	G	N3-C4-C5	-5.76	125.72	128.60
26	BB	2589	A	C5'-C4'-C3'	-5.76	106.79	116.00
2	AB	59	U	O4'-C1'-N1	5.76	112.81	108.20
1	AA	1294	G	O4'-C1'-N9	5.76	112.80	108.20
26	BB	628	G	O4'-C1'-N9	5.76	112.81	108.20
26	BB	1294	U	C2-N1-C1'	5.76	124.61	117.70
26	BB	2567	G	N3-C4-C5	-5.76	125.72	128.60
1	AA	1275	A	C5'-C4'-C3'	-5.75	106.79	116.00
2	AE	28	G	C8-N9-C4	-5.75	104.10	106.40
26	BB	612	G	N3-C4-C5	-5.75	125.72	128.60
26	BB	2312	U	C5'-C4'-C3'	-5.75	106.80	116.00
1	AA	114	U	O4'-C1'-N1	5.75	112.80	108.20
25	BA	29	A	O4'-C1'-N9	5.75	112.80	108.20
26	BB	1074	G	N3-C4-C5	-5.75	125.72	128.60
26	BB	2266	A	O4'-C1'-N9	5.75	112.80	108.20
26	BB	312	G	N3-C4-C5	-5.75	125.72	128.60
26	BB	1183	U	C5'-C4'-C3'	-5.75	106.80	116.00
1	AA	721	G	O4'-C1'-N9	5.75	112.80	108.20
1	AA	863	U	C5'-C4'-O4'	5.75	116.00	109.10
26	BB	164	C	O4'-C1'-N1	5.75	112.80	108.20
26	BB	315	G	N9-C4-C5	5.75	107.70	105.40
26	BB	1106	G	C8-N9-C4	-5.75	104.10	106.40
1	AA	897	C	O4'-C1'-N1	5.75	112.80	108.20
25	BA	89	U	O4'-C1'-N1	5.75	112.80	108.20
1	AA	929	G	N9-C1'-C2'	-5.74	105.68	112.00
1	AA	1066	C	N1-C2-O2	5.74	122.35	118.90
26	BB	2554	U	O3'-P-O5'	-5.74	93.09	104.00
26	BB	554	U	C5'-C4'-O4'	5.74	115.99	109.10
1	AA	460	A	O4'-C1'-N9	5.74	112.79	108.20
1	AA	491	G	C8-N9-C4	-5.74	104.10	106.40
1	AA	246	A	C5'-C4'-C3'	-5.74	106.82	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	857	C	O4'-C1'-N1	5.74	112.79	108.20
25	BA	72	G	C8-N9-C4	-5.74	104.11	106.40
26	BB	1534	U	O4'-C1'-N1	5.74	112.79	108.20
26	BB	1888	G	N3-C4-C5	-5.74	125.73	128.60
26	BB	2029	G	C5'-C4'-O4'	5.74	115.99	109.10
26	BB	2127	G	C5'-C4'-O4'	5.74	115.99	109.10
1	AA	873	A	C5'-C4'-C3'	-5.74	106.82	116.00
1	AA	451	A	O4'-C1'-N9	5.74	112.79	108.20
26	BB	551	G	O4'-C1'-N9	5.73	112.79	108.20
26	BB	953	G	C5'-C4'-C3'	-5.73	106.83	116.00
1	AA	1225	A	N9-C1'-C2'	5.73	121.45	114.00
26	BB	913	U	O4'-C4'-C3'	5.73	110.68	106.10
1	AA	171	A	C5'-C4'-O4'	5.73	115.97	109.10
26	BB	1230	A	C5'-C4'-C3'	-5.73	106.83	116.00
26	BB	2494	G	O4'-C1'-N9	5.73	112.78	108.20
26	BB	1003	G	O4'-C1'-N9	5.72	112.78	108.20
26	BB	2506	U	O4'-C1'-N1	5.72	112.78	108.20
1	AA	688	G	N3-C4-C5	-5.72	125.74	128.60
26	BB	589	U	O4'-C1'-N1	5.72	112.78	108.20
26	BB	949	G	O4'-C1'-N9	5.72	112.78	108.20
1	AA	1325	C	C5'-C4'-O4'	5.72	115.97	109.10
26	BB	790	U	P-O3'-C3'	5.72	126.56	119.70
26	BB	2878	U	O4'-C1'-N1	5.72	112.78	108.20
1	AA	119	A	O4'-C1'-N9	5.72	112.78	108.20
25	BA	8	C	O4'-C1'-N1	5.72	112.78	108.20
26	BB	2744	G	C1'-O4'-C4'	-5.72	105.32	109.90
1	AA	583	A	O4'-C1'-N9	5.72	112.77	108.20
26	BB	1175	A	O4'-C1'-N9	5.72	112.78	108.20
26	BB	1359	A	C5'-C4'-C3'	-5.72	106.85	116.00
26	BB	2190	G	C5'-C4'-O4'	5.72	115.96	109.10
1	AA	204	G	C8-N9-C4	-5.72	104.11	106.40
1	AA	314	C	O4'-C1'-N1	5.72	112.77	108.20
26	BB	2663	G	C8-N9-C4	-5.72	104.11	106.40
1	AA	177	G	N3-C4-C5	-5.71	125.74	128.60
1	AA	874	G	N3-C4-C5	-5.71	125.74	128.60
26	BB	91	A	C4'-C3'-C2'	-5.71	96.89	102.60
26	BB	1738	G	C4-N9-C1'	-5.71	119.07	126.50
26	BB	1859	U	O4'-C1'-N1	5.71	112.77	108.20
26	BB	1571	A	O4'-C1'-N9	5.71	112.77	108.20
1	AA	83	C	O4'-C1'-N1	5.71	112.77	108.20
1	AA	1123	U	O4'-C1'-N1	5.71	112.77	108.20
1	AA	1132	C	O4'-C1'-N1	5.71	112.77	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2678	C	O4'-C1'-N1	5.71	112.77	108.20
1	AA	1223	C	C5'-C4'-O4'	5.71	115.95	109.10
26	BB	2588	G	N3-C4-C5	-5.71	125.75	128.60
25	BA	107	G	C3'-C2'-C1'	5.71	106.07	101.50
26	BB	1586	A	C4'-C3'-C2'	-5.71	96.89	102.60
26	BB	2252	G	O4'-C1'-N9	5.71	112.77	108.20
26	BB	2648	G	C8-N9-C4	-5.71	104.12	106.40
26	BB	657	U	O4'-C1'-N1	5.71	112.77	108.20
26	BB	2521	C	O4'-C1'-N1	5.71	112.77	108.20
26	BB	480	A	C5'-C4'-O4'	5.71	115.95	109.10
26	BB	2825	G	N3-C4-C5	-5.70	125.75	128.60
26	BB	2877	G	C4'-C3'-C2'	-5.70	96.90	102.60
26	BB	194	G	C5'-C4'-O4'	5.70	115.94	109.10
26	BB	274	C	C5'-C4'-O4'	5.70	115.94	109.10
26	BB	2028	U	O4'-C1'-N1	5.70	112.76	108.20
26	BB	2508	G	O4'-C1'-N9	5.70	112.76	108.20
1	AA	501	C	C4'-C3'-C2'	-5.70	96.90	102.60
26	BB	1442	U	O4'-C1'-N1	5.70	112.76	108.20
26	BB	1779	U	O4'-C1'-N1	5.70	112.76	108.20
1	AA	780	A	O3'-P-O5'	-5.70	93.18	104.00
26	BB	1069	A	O4'-C1'-C2'	-5.70	100.10	105.80
26	BB	2720	U	O4'-C1'-N1	5.70	112.76	108.20
1	AA	442	G	C5'-C4'-C3'	-5.70	106.89	116.00
26	BB	1124	G	N3-C4-C5	-5.70	125.75	128.60
26	BB	80	G	O4'-C1'-N9	5.69	112.75	108.20
26	BB	271	G	N9-C1'-C2'	5.69	121.40	114.00
26	BB	555	G	O4'-C1'-N9	5.69	112.75	108.20
26	BB	1241	A	O4'-C1'-N9	5.69	112.75	108.20
1	AA	795	C	O4'-C1'-N1	5.69	112.75	108.20
1	AA	1453	G	N3-C4-C5	-5.69	125.75	128.60
26	BB	1385	A	C4'-C3'-C2'	-5.69	96.91	102.60
1	AA	169	C	N1-C2-O2	5.69	122.31	118.90
1	AA	1017	U	C5'-C4'-O4'	5.69	115.93	109.10
26	BB	2135	A	C3'-C2'-C1'	5.69	106.05	101.50
26	BB	2143	C	O4'-C1'-N1	5.69	112.75	108.20
26	BB	1346	G	N3-C4-C5	-5.69	125.75	128.60
26	BB	1822	C	N1-C2-O2	5.69	122.31	118.90
1	AA	1104	G	C5'-C4'-O4'	5.69	115.92	109.10
1	AA	1118	U	O4'-C1'-N1	5.69	112.75	108.20
26	BB	896	A	C4'-C3'-C2'	5.69	108.29	102.60
26	BB	2380	C	C5'-C4'-O4'	5.69	115.92	109.10
26	BB	2792	A	C8-N9-C4	-5.69	103.53	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2262	U	O4'-C1'-N1	5.69	112.75	108.20
26	BB	2571	U	O4'-C1'-N1	5.69	112.75	108.20
1	AA	337	G	C5'-C4'-C3'	-5.68	106.90	116.00
1	AA	32	A	O4'-C1'-N9	5.68	112.75	108.20
1	AA	1058	G	N3-C4-C5	-5.68	125.76	128.60
26	BB	866	A	C5'-C4'-O4'	5.68	115.92	109.10
26	BB	1266	G	C3'-C2'-C1'	-5.68	96.95	101.50
26	BB	1694	C	O4'-C1'-N1	5.68	112.75	108.20
26	BB	2222	C	O4'-C1'-N1	5.68	112.75	108.20
26	BB	2277	G	N3-C4-C5	-5.68	125.76	128.60
26	BB	2424	C	O4'-C1'-N1	5.68	112.75	108.20
1	AA	435	A	O4'-C1'-N9	5.68	112.75	108.20
1	AA	1057	G	N3-C4-C5	-5.68	125.76	128.60
1	AA	1173	U	O4'-C1'-N1	5.68	112.75	108.20
26	BB	514	A	C5'-C4'-O4'	5.68	115.92	109.10
1	AA	140	U	C5'-C4'-O4'	5.68	115.92	109.10
1	AA	1313	U	O4'-C1'-N1	5.68	112.74	108.20
26	BB	868	U	O4'-C1'-N1	5.68	112.74	108.20
26	BB	2214	C	C5'-C4'-O4'	5.68	115.92	109.10
1	AA	597	G	N9-C4-C5	5.68	107.67	105.40
2	AE	44	G	C8-N9-C4	-5.68	104.13	106.40
26	BB	505	A	O4'-C1'-N9	5.68	112.74	108.20
26	BB	2184	A	C5'-C4'-O4'	5.68	115.91	109.10
26	BB	290	U	O4'-C1'-N1	5.68	112.74	108.20
26	BB	2801	G	C5'-C4'-C3'	-5.68	106.92	116.00
1	AA	496	A	C8-N9-C4	-5.67	103.53	105.80
1	AA	636	U	C5'-C4'-O4'	5.67	115.91	109.10
1	AA	1143	G	N7-C8-N9	5.67	115.94	113.10
26	BB	646	U	O4'-C1'-N1	5.67	112.74	108.20
26	BB	1104	C	C5'-C4'-O4'	5.67	115.91	109.10
26	BB	1215	G	C8-N9-C4	-5.67	104.13	106.40
26	BB	1733	G	N3-C4-C5	-5.67	125.76	128.60
26	BB	2220	U	O4'-C1'-N1	5.67	112.74	108.20
26	BB	2231	U	O4'-C1'-N1	5.67	112.74	108.20
26	BB	814	C	C6-N1-C2	-5.67	118.03	120.30
26	BB	2855	C	C5'-C4'-C3'	-5.67	106.92	116.00
1	AA	937	A	C8-N9-C4	-5.67	103.53	105.80
1	AA	996	A	C5'-C4'-O4'	5.67	115.91	109.10
26	BB	1203	U	C2-N3-C4	-5.67	123.60	127.00
26	BB	2059	A	C8-N9-C4	-5.67	103.53	105.80
25	BA	91	C	C5'-C4'-C3'	-5.67	106.93	116.00
26	BB	554	U	C5'-C4'-C3'	-5.67	106.93	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	813	U	C5'-C4'-O4'	5.67	115.90	109.10
1	AA	683	G	C8-N9-C4	-5.67	104.13	106.40
2	AE	34	G	O4'-C1'-N9	5.67	112.73	108.20
26	BB	481	G	C2-N3-C4	5.67	114.73	111.90
26	BB	1007	C	C5'-C4'-O4'	5.67	115.90	109.10
26	BB	1209	U	C2-N1-C1'	5.67	124.50	117.70
26	BB	2065	C	C5'-C4'-O4'	5.67	115.90	109.10
26	BB	2328	A	C5'-C4'-O4'	5.67	115.90	109.10
1	AA	247	G	N3-C4-C5	-5.67	125.77	128.60
1	AA	1142	G	O4'-C1'-N9	5.67	112.73	108.20
26	BB	1187	G	O4'-C4'-C3'	5.67	110.63	106.10
26	BB	1452	G	N3-C4-C5	-5.67	125.77	128.60
26	BB	1929	G	N9-C4-C5	5.67	107.67	105.40
26	BB	1996	C	O4'-C1'-N1	5.67	112.73	108.20
26	BB	2398	U	O4'-C1'-N1	5.67	112.73	108.20
1	AA	800	G	C8-N9-C4	-5.67	104.13	106.40
2	AB	26	A	C8-N9-C4	-5.67	103.53	105.80
26	BB	1875	G	O4'-C1'-N9	5.67	112.73	108.20
1	AA	216	U	O4'-C1'-N1	5.66	112.73	108.20
26	BB	549	G	C5'-C4'-C3'	-5.66	106.94	116.00
26	BB	1128	G	C1'-O4'-C4'	-5.66	105.37	109.90
26	BB	1847	A	C1'-O4'-C4'	-5.66	105.37	109.90
2	AB	29	G	N3-C4-C5	-5.66	125.77	128.60
26	BB	665	U	O4'-C1'-N1	5.66	112.72	108.20
26	BB	2431	U	C2'-C3'-O3'	5.66	122.75	113.70
26	BB	712	G	O4'-C1'-N9	5.66	112.72	108.20
26	BB	817	C	C5'-C4'-O4'	5.66	115.89	109.10
26	BB	166	U	C4'-C3'-C2'	-5.65	96.95	102.60
26	BB	2750	A	C5'-C4'-C3'	-5.65	106.95	116.00
1	AA	446	G	O4'-C1'-N9	5.65	112.72	108.20
1	AA	1222	G	O4'-C1'-N9	5.65	112.72	108.20
26	BB	733	G	O4'-C1'-N9	5.65	112.72	108.20
26	BB	1569	A	O4'-C1'-N9	5.65	112.72	108.20
26	BB	1591	A	C8-N9-C4	-5.65	103.54	105.80
26	BB	2216	G	C5'-C4'-C3'	-5.65	106.96	116.00
2	AB	52	G	C8-N9-C4	-5.65	104.14	106.40
26	BB	4	U	O4'-C1'-N1	5.65	112.72	108.20
26	BB	146	A	O4'-C1'-N9	5.65	112.72	108.20
26	BB	703	U	O4'-C1'-N1	5.65	112.72	108.20
26	BB	843	G	N3-C4-C5	-5.65	125.78	128.60
26	BB	1308	A	C5'-C4'-O4'	5.65	115.88	109.10
26	BB	2312	U	C5'-C4'-O4'	5.65	115.88	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1090	U	O4'-C1'-N1	5.65	112.72	108.20
26	BB	758	C	O4'-C1'-N1	5.65	112.72	108.20
26	BB	2040	G	N3-C4-C5	-5.65	125.78	128.60
26	BB	2732	G	C5'-C4'-C3'	-5.65	106.96	116.00
1	AA	854	U	O4'-C1'-N1	5.64	112.72	108.20
1	AA	1293	C	O4'-C1'-N1	5.64	112.72	108.20
1	AA	1324	A	O4'-C1'-N9	5.64	112.72	108.20
2	AE	28	G	N3-C4-C5	-5.64	125.78	128.60
25	BA	20	G	C8-N9-C4	-5.64	104.14	106.40
26	BB	703	U	C5'-C4'-C3'	-5.64	106.97	116.00
1	AA	1035	A	O4'-C1'-N9	5.64	112.71	108.20
26	BB	1869	G	C8-N9-C4	-5.64	104.14	106.40
1	AA	705	G	C8-N9-C4	-5.64	104.14	106.40
1	AA	1058	G	N7-C8-N9	5.64	115.92	113.10
1	AA	1212	U	C5'-C4'-O4'	-5.64	102.33	109.10
26	BB	2486	C	O4'-C1'-N1	5.64	112.71	108.20
1	AA	406	G	C5'-C4'-C3'	-5.64	106.98	116.00
26	BB	1603	A	C5'-C4'-O4'	5.64	115.86	109.10
26	BB	2468	A	O4'-C1'-N9	5.64	112.71	108.20
25	BA	46	A	N1-C6-N6	-5.64	115.22	118.60
1	AA	378	G	O4'-C1'-N9	5.63	112.71	108.20
26	BB	1357	C	O4'-C1'-N1	5.63	112.71	108.20
26	BB	1446	C	C5'-C4'-O4'	5.63	115.86	109.10
26	BB	2261	C	O4'-C1'-N1	5.63	112.71	108.20
26	BB	1056	G	C2'-C3'-O3'	5.63	122.71	113.70
26	BB	2506	U	C4'-C3'-C2'	-5.63	96.97	102.60
33	BI	25	TYR	CB-CG-CD1	-5.63	117.62	121.00
25	BA	1	U	O4'-C1'-N1	5.63	112.70	108.20
26	BB	2366	A	O4'-C1'-N9	5.63	112.70	108.20
1	AA	311	C	O4'-C1'-N1	5.63	112.70	108.20
1	AA	1182	G	C3'-C2'-C1'	5.63	106.00	101.50
26	BB	436	C	O4'-C1'-N1	5.63	112.70	108.20
26	BB	1278	C	O4'-C1'-N1	5.63	112.70	108.20
26	BB	498	G	O4'-C1'-N9	5.63	112.70	108.20
26	BB	655	A	P-O3'-C3'	5.62	126.45	119.70
26	BB	738	G	N9-C4-C5	5.62	107.65	105.40
26	BB	247	G	C5'-C4'-O4'	5.62	115.85	109.10
26	BB	732	C	O4'-C1'-N1	5.62	112.70	108.20
26	BB	880	G	N3-C4-C5	-5.62	125.79	128.60
26	BB	1376	C	O4'-C1'-N1	5.62	112.70	108.20
25	BA	31	C	C5'-C4'-O4'	5.62	115.85	109.10
26	BB	824	U	C5'-C4'-C3'	-5.62	107.01	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2258	C	P-O3'-C3'	5.62	126.45	119.70
26	BB	68	G	C8-N9-C4	-5.62	104.15	106.40
26	BB	245	G	C8-N9-C4	-5.62	104.15	106.40
26	BB	2697	G	O4'-C1'-N9	5.62	112.70	108.20
1	AA	512	U	C1'-O4'-C4'	-5.62	105.41	109.90
1	AA	742	G	C2-N3-C4	5.62	114.71	111.90
2	AE	59	U	C3'-C2'-C1'	5.62	105.99	101.50
26	BB	802	A	C5'-C4'-O4'	5.62	115.84	109.10
26	BB	890	C	C5'-C4'-O4'	5.62	115.84	109.10
26	BB	1507	C	C4'-C3'-C2'	-5.62	96.98	102.60
26	BB	270	A	C3'-C2'-C1'	-5.62	97.01	101.50
26	BB	344	A	C1'-O4'-C4'	-5.62	105.41	109.90
26	BB	656	G	N3-C4-C5	-5.62	125.79	128.60
26	BB	2885	G	C8-N9-C4	-5.62	104.15	106.40
1	AA	1426	G	O4'-C1'-N9	5.61	112.69	108.20
26	BB	685	A	C8-N9-C4	-5.61	103.56	105.80
26	BB	1995	U	O4'-C1'-N1	5.61	112.69	108.20
26	BB	2639	A	C5'-C4'-C3'	-5.61	107.02	116.00
26	BB	2082	A	C8-N9-C4	-5.61	103.56	105.80
1	AA	1242	G	C8-N9-C4	-5.61	104.16	106.40
26	BB	1448	G	C5'-C4'-O4'	5.61	115.83	109.10
1	AA	818	G	C3'-C2'-C1'	5.61	105.99	101.50
1	AA	885	G	C8-N9-C4	-5.61	104.16	106.40
26	BB	123	G	O4'-C1'-N9	5.61	112.69	108.20
26	BB	938	G	N3-C4-C5	-5.61	125.80	128.60
1	AA	226	G	C3'-C2'-C1'	-5.61	97.02	101.50
1	AA	893	C	O4'-C1'-N1	5.61	112.68	108.20
26	BB	2337	G	C5'-C4'-O4'	5.61	115.83	109.10
26	BB	108	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	184	G	O4'-C1'-N9	5.60	112.68	108.20
1	AA	440	C	O4'-C1'-N1	5.60	112.68	108.20
1	AA	1443	C	P-O3'-C3'	5.60	126.42	119.70
25	BA	101	A	C5'-C4'-O4'	5.60	115.82	109.10
26	BB	2781	A	C3'-C2'-C1'	-5.60	97.02	101.50
5	AF	221	ARG	NE-CZ-NH1	5.60	123.10	120.30
26	BB	1759	A	N9-C1'-C2'	-5.60	105.84	112.00
1	AA	1163	A	O4'-C1'-N9	5.60	112.68	108.20
1	AA	1200	C	P-O3'-C3'	5.60	126.42	119.70
26	BB	1645	G	C3'-C2'-C1'	5.60	105.98	101.50
1	AA	212	G	N3-C4-C5	-5.60	125.80	128.60
26	BB	1538	G	N3-C4-C5	-5.60	125.80	128.60
26	BB	2268	A	C5'-C4'-O4'	5.60	115.82	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2741	A	C5'-C4'-C3'	-5.60	107.04	116.00
4	AD	44	U	O4'-C1'-N1	5.60	112.68	108.20
26	BB	2704	C	C5'-C4'-O4'	5.60	115.81	109.10
26	BB	163	C	O4'-C1'-N1	5.59	112.68	108.20
26	BB	242	G	C5'-C4'-C3'	-5.59	107.05	116.00
26	BB	367	G	O4'-C1'-N9	5.59	112.68	108.20
26	BB	1569	A	C5'-C4'-O4'	5.59	115.81	109.10
26	BB	653	U	P-O3'-C3'	5.59	126.41	119.70
1	AA	441	A	C5'-C4'-C3'	-5.59	107.05	116.00
26	BB	1292	G	C8-N9-C4	-5.59	104.16	106.40
26	BB	1775	U	O4'-C1'-N1	5.59	112.67	108.20
26	BB	2119	A	O4'-C1'-N9	5.59	112.67	108.20
1	AA	836	G	O3'-P-O5'	-5.59	93.38	104.00
1	AA	1038	C	O4'-C1'-N1	5.59	112.67	108.20
2	AE	7	A	O4'-C1'-N9	5.59	112.67	108.20
25	BA	39	A	O4'-C1'-N9	5.59	112.67	108.20
26	BB	895	U	O3'-P-O5'	-5.59	93.38	104.00
26	BB	2156	G	C8-N9-C4	-5.59	104.17	106.40
26	BB	2870	C	C5'-C4'-O4'	5.59	115.81	109.10
1	AA	844	G	C8-N9-C4	-5.59	104.17	106.40
1	AA	1032	G	N3-C4-C5	-5.59	125.81	128.60
26	BB	716	A	O4'-C1'-N9	5.59	112.67	108.20
26	BB	1086	A	C8-N9-C4	-5.59	103.56	105.80
26	BB	1491	G	C8-N9-C4	-5.59	104.17	106.40
1	AA	164	G	C5'-C4'-O4'	5.59	115.80	109.10
26	BB	855	G	N9-C4-C5	5.59	107.63	105.40
26	BB	1724	G	O4'-C1'-N9	5.59	112.67	108.20
26	BB	2348	U	O4'-C1'-N1	5.59	112.67	108.20
1	AA	1003	G	O4'-C1'-N9	5.58	112.67	108.20
26	BB	1514	G	C8-N9-C4	-5.58	104.17	106.40
1	AA	443	C	O4'-C1'-N1	5.58	112.67	108.20
1	AA	995	C	O4'-C1'-N1	5.58	112.67	108.20
1	AA	1027	C	C5'-C4'-O4'	5.58	115.80	109.10
25	BA	33	G	N9-C1'-C2'	-5.58	105.86	112.00
26	BB	531	C	O4'-C4'-C3'	5.58	110.56	106.10
26	BB	552	U	O4'-C1'-N1	5.58	112.66	108.20
26	BB	1834	U	O4'-C1'-N1	5.58	112.66	108.20
26	BB	2190	G	O4'-C1'-N9	5.58	112.66	108.20
26	BB	2760	C	O4'-C1'-N1	5.58	112.66	108.20
1	AA	741	G	O4'-C1'-N9	5.58	112.66	108.20
1	AA	1310	G	O4'-C1'-N9	5.58	112.66	108.20
26	BB	540	C	C5'-C4'-O4'	5.58	115.80	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	308	C	O4'-C1'-N1	5.58	112.66	108.20
26	BB	229	C	O4'-C1'-N1	5.58	112.66	108.20
1	AA	1350	A	C5'-C4'-C3'	-5.58	107.08	116.00
26	BB	1135	C	C5'-C4'-C3'	-5.58	107.08	116.00
26	BB	1650	A	O4'-C1'-N9	5.58	112.66	108.20
25	BA	86	G	C8-N9-C4	-5.57	104.17	106.40
26	BB	923	G	C8-N9-C4	-5.57	104.17	106.40
26	BB	1187	G	C8-N9-C4	-5.57	104.17	106.40
1	AA	111	G	N3-C4-C5	-5.57	125.81	128.60
1	AA	136	C	O4'-C1'-N1	5.57	112.66	108.20
1	AA	529	G	O4'-C1'-N9	5.57	112.66	108.20
26	BB	283	G	C5'-C4'-C3'	-5.57	107.09	116.00
26	BB	1187	G	C5'-C4'-O4'	5.57	115.78	109.10
26	BB	1395	A	O4'-C4'-C3'	5.57	110.56	106.10
1	AA	654	G	C8-N9-C4	-5.57	104.17	106.40
1	AA	1074	G	C5'-C4'-O4'	5.57	115.78	109.10
26	BB	103	A	C5'-C4'-O4'	5.57	115.78	109.10
1	AA	861	G	C5'-C4'-O4'	5.57	115.78	109.10
25	BA	98	G	C5'-C4'-O4'	5.57	115.78	109.10
26	BB	1587	G	C8-N9-C4	-5.57	104.17	106.40
1	AA	211	G	C8-N9-C4	-5.56	104.17	106.40
26	BB	1604	C	C5'-C4'-O4'	5.56	115.78	109.10
26	BB	2636	C	O4'-C1'-N1	5.56	112.65	108.20
1	AA	1010	U	N3-C2-O2	-5.56	118.31	122.20
1	AA	1380	U	C1'-O4'-C4'	-5.56	105.45	109.90
1	AA	1258	G	N3-C4-C5	-5.56	125.82	128.60
1	AA	858	G	C5'-C4'-C3'	-5.56	107.10	116.00
26	BB	442	G	C8-N9-C4	-5.56	104.18	106.40
26	BB	879	G	C8-N9-C4	-5.56	104.18	106.40
1	AA	332	G	C1'-O4'-C4'	-5.56	105.45	109.90
1	AA	492	C	O4'-C1'-N1	5.56	112.65	108.20
26	BB	1233	C	C5'-C4'-O4'	-5.56	102.43	109.10
25	BA	54	G	N3-C4-C5	-5.56	125.82	128.60
26	BB	987	C	O4'-C1'-N1	5.56	112.64	108.20
1	AA	633	G	C8-N9-C4	-5.55	104.18	106.40
1	AA	993	G	N3-C4-C5	-5.55	125.82	128.60
26	BB	1929	G	C8-N9-C4	-5.55	104.18	106.40
1	AA	867	G	N3-C4-C5	-5.55	125.82	128.60
1	AA	944	G	C8-N9-C4	-5.55	104.18	106.40
1	AA	1084	G	C8-N9-C4	-5.55	104.18	106.40
26	BB	1044	C	O4'-C1'-N1	5.55	112.64	108.20
26	BB	2731	G	N3-C4-C5	-5.55	125.82	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	544	G	O4'-C1'-N9	5.55	112.64	108.20
1	AA	1257	A	O4'-C1'-N9	5.55	112.64	108.20
1	AA	1357	A	O4'-C1'-N9	5.55	112.64	108.20
26	BB	1256	G	N3-C4-C5	-5.55	125.83	128.60
26	BB	2814	A	O4'-C1'-N9	5.55	112.64	108.20
1	AA	362	G	C5'-C4'-C3'	-5.55	107.12	116.00
1	AA	893	C	C5'-C4'-O4'	5.55	115.76	109.10
26	BB	972	A	O4'-C1'-N9	5.55	112.64	108.20
26	BB	1408	G	C8-N9-C4	-5.55	104.18	106.40
26	BB	1538	G	O4'-C1'-N9	5.55	112.64	108.20
26	BB	2028	U	C5'-C4'-O4'	5.55	115.76	109.10
26	BB	2268	A	O3'-P-O5'	-5.55	93.45	104.00
26	BB	2040	G	C8-N9-C4	-5.55	104.18	106.40
1	AA	1381	U	O4'-C1'-N1	5.55	112.64	108.20
2	AE	13	C	O4'-C1'-N1	5.55	112.64	108.20
2	AE	18	G	C8-N9-C4	-5.55	104.18	106.40
26	BB	1757	A	P-O3'-C3'	5.55	126.36	119.70
26	BB	2399	G	O4'-C1'-N9	5.54	112.64	108.20
26	BB	2644	G	C8-N9-C4	-5.54	104.18	106.40
26	BB	571	U	O4'-C1'-N1	5.54	112.64	108.20
1	AA	1031	C	O4'-C1'-N1	5.54	112.63	108.20
26	BB	1538	G	C8-N9-C4	-5.54	104.18	106.40
26	BB	2345	G	N3-C4-C5	-5.54	125.83	128.60
26	BB	1509	A	P-O3'-C3'	5.54	126.35	119.70
1	AA	346	G	N3-C4-C5	-5.54	125.83	128.60
26	BB	323	C	N1-C2-O2	5.54	122.22	118.90
26	BB	424	G	N9-C1'-C2'	-5.54	105.91	112.00
26	BB	2126	A	O4'-C1'-N9	5.54	112.63	108.20
1	AA	780	A	O4'-C1'-N9	5.54	112.63	108.20
25	BA	103	U	O4'-C1'-N1	5.54	112.63	108.20
26	BB	765	C	C5'-C4'-O4'	5.54	115.74	109.10
26	BB	869	G	N9-C1'-C2'	-5.54	105.91	112.00
26	BB	1062	G	C8-N9-C4	-5.54	104.19	106.40
26	BB	1338	G	C8-N9-C4	-5.54	104.19	106.40
26	BB	2232	C	O4'-C1'-N1	5.54	112.63	108.20
26	BB	2653	U	O4'-C1'-N1	5.54	112.63	108.20
1	AA	392	C	O4'-C1'-N1	5.53	112.63	108.20
26	BB	90	U	C5'-C4'-C3'	-5.53	107.15	116.00
26	BB	201	C	C2-N3-C4	5.53	122.67	119.90
26	BB	808	G	O4'-C1'-N9	5.53	112.63	108.20
26	BB	1722	A	C8-N9-C4	-5.53	103.59	105.80
26	BB	2834	G	C8-N9-C4	-5.53	104.19	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1114	C	C3'-C2'-C1'	5.53	105.93	101.50
26	BB	1368	G	O4'-C1'-N9	5.53	112.62	108.20
1	AA	23	C	O4'-C1'-N1	5.53	112.62	108.20
1	AA	765	G	C8-N9-C4	-5.53	104.19	106.40
26	BB	997	G	C8-N9-C4	-5.53	104.19	106.40
26	BB	1731	G	N3-C4-C5	-5.53	125.83	128.60
26	BB	2271	G	C5'-C4'-C3'	-5.53	107.15	116.00
1	AA	1184	G	N3-C4-C5	-5.53	125.83	128.60
26	BB	942	G	O4'-C1'-N9	5.53	112.62	108.20
26	BB	740	C	C5'-C4'-O4'	5.53	115.73	109.10
26	BB	759	G	C8-N9-C4	-5.53	104.19	106.40
26	BB	1018	U	O4'-C1'-N1	5.53	112.62	108.20
26	BB	1042	G	C5'-C4'-O4'	5.53	115.73	109.10
26	BB	1206	G	C5'-C4'-O4'	5.53	115.73	109.10
26	BB	2640	G	N3-C4-C5	-5.53	125.84	128.60
1	AA	652	U	C5'-C4'-C3'	-5.53	107.16	116.00
2	AB	36	A	C5'-C4'-O4'	5.53	115.73	109.10
26	BB	2824	C	O4'-C1'-N1	5.53	112.62	108.20
1	AA	248	C	O4'-C1'-N1	5.52	112.62	108.20
1	AA	736	C	C5'-C4'-O4'	5.52	115.73	109.10
26	BB	354	A	N9-C4-C5	5.52	108.01	105.80
26	BB	938	G	C8-N9-C4	-5.52	104.19	106.40
26	BB	1537	G	C8-N9-C4	-5.52	104.19	106.40
1	AA	1191	A	O4'-C1'-N9	5.52	112.62	108.20
26	BB	2751	G	N3-C4-C5	-5.52	125.84	128.60
26	BB	190	A	O4'-C1'-N9	5.52	112.62	108.20
26	BB	334	C	O4'-C1'-N1	5.52	112.62	108.20
1	AA	838	G	N3-C4-C5	-5.52	125.84	128.60
1	AA	874	G	C8-N9-C4	-5.52	104.19	106.40
1	AA	1178	G	C8-N9-C4	-5.52	104.19	106.40
1	AA	671	G	O4'-C1'-N9	5.52	112.61	108.20
1	AA	892	A	C5'-C4'-O4'	5.52	115.72	109.10
1	AA	1310	G	C5'-C4'-O4'	5.52	115.72	109.10
26	BB	1611	C	C5'-C4'-O4'	5.52	115.72	109.10
26	BB	2186	G	C8-N9-C4	-5.51	104.19	106.40
1	AA	998	C	C5'-C4'-C3'	-5.51	107.18	116.00
25	BA	77	U	C2'-C3'-O3'	5.51	122.52	113.70
26	BB	1227	G	O3'-P-O5'	-5.51	93.53	104.00
26	BB	1523	U	O4'-C4'-C3'	5.51	110.51	106.10
26	BB	1989	G	C5'-C4'-O4'	5.51	115.71	109.10
1	AA	524	G	C3'-C2'-C1'	5.51	105.91	101.50
1	AA	641	U	O4'-C4'-C3'	5.51	110.51	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1138	G	N3-C4-C5	-5.51	125.84	128.60
26	BB	240	C	N1-C2-O2	5.51	122.20	118.90
26	BB	1479	G	N9-C4-C5	5.51	107.60	105.40
26	BB	2796	U	C2-N3-C4	-5.51	123.69	127.00
26	BB	18	U	O4'-C1'-N1	5.51	112.61	108.20
26	BB	409	G	C5'-C4'-O4'	5.51	115.71	109.10
26	BB	822	G	O4'-C1'-N9	5.51	112.61	108.20
4	AD	31	U	O4'-C1'-N1	5.51	112.61	108.20
26	BB	2845	U	O4'-C1'-N1	5.51	112.61	108.20
1	AA	391	G	O4'-C1'-N9	5.50	112.60	108.20
1	AA	803	G	C8-N9-C4	-5.50	104.20	106.40
26	BB	1278	C	C4'-C3'-C2'	-5.50	97.09	102.60
1	AA	818	G	N3-C4-C5	-5.50	125.85	128.60
26	BB	119	A	O4'-C1'-N9	5.50	112.60	108.20
26	BB	905	A	O4'-C1'-N9	5.50	112.60	108.20
26	BB	2386	A	C5'-C4'-O4'	5.50	115.70	109.10
32	BH	162	ARG	NE-CZ-NH2	5.50	123.05	120.30
26	BB	2648	G	C5'-C4'-O4'	5.50	115.70	109.10
1	AA	1541	U	C3'-C2'-C1'	5.50	105.90	101.50
26	BB	1800	C	O4'-C4'-C3'	5.50	110.50	106.10
26	BB	2040	G	C5'-C4'-C3'	-5.50	107.20	116.00
26	BB	2866	U	O4'-C1'-N1	5.50	112.60	108.20
1	AA	1072	G	N3-C4-C5	-5.50	125.85	128.60
26	BB	913	U	N1-C2-N3	5.50	118.20	114.90
26	BB	1013	C	O4'-C1'-N1	5.50	112.60	108.20
26	BB	1495	A	O4'-C1'-N9	5.50	112.60	108.20
26	BB	2083	G	O4'-C1'-N9	5.50	112.60	108.20
1	AA	899	C	O3'-P-O5'	-5.50	93.56	104.00
4	AD	31	U	C3'-C2'-C1'	5.50	105.90	101.50
26	BB	242	G	C3'-C2'-C1'	-5.50	97.10	101.50
1	AA	1467	C	N1-C2-O2	5.50	122.20	118.90
26	BB	1973	G	C5'-C4'-C3'	-5.50	107.21	116.00
26	BB	2751	G	C4'-C3'-O3'	-5.50	97.86	109.40
1	AA	1346	A	O4'-C1'-N9	5.49	112.59	108.20
26	BB	517	C	O4'-C1'-N1	5.49	112.59	108.20
26	BB	1540	G	O4'-C1'-N9	5.49	112.59	108.20
1	AA	93	U	O4'-C1'-N1	5.49	112.59	108.20
1	AA	112	G	C1'-O4'-C4'	-5.49	105.51	109.90
26	BB	189	G	C8-N9-C4	-5.49	104.20	106.40
26	BB	545	U	C5'-C4'-C3'	-5.49	107.22	116.00
26	BB	835	C	O4'-C1'-N1	5.49	112.59	108.20
26	BB	1047	G	O3'-P-O5'	-5.49	93.57	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2328	A	C5'-C4'-C3'	-5.49	107.22	116.00
1	AA	1001	C	O4'-C1'-N1	5.49	112.59	108.20
26	BB	1695	G	C8-N9-C4	-5.49	104.20	106.40
1	AA	211	G	C2-N3-C4	5.49	114.64	111.90
1	AA	1246	A	O4'-C1'-N9	5.49	112.59	108.20
26	BB	880	G	N9-C4-C5	5.49	107.59	105.40
1	AA	227	G	O4'-C1'-N9	5.48	112.59	108.20
26	BB	2874	C	O4'-C1'-N1	5.48	112.59	108.20
1	AA	234	C	O4'-C1'-N1	5.48	112.59	108.20
1	AA	1530	G	O4'-C1'-N9	5.48	112.59	108.20
26	BB	148	U	P-O3'-C3'	5.48	126.28	119.70
26	BB	728	G	N3-C4-C5	-5.48	125.86	128.60
26	BB	2145	C	C3'-C2'-C1'	-5.48	97.11	101.50
1	AA	624	C	O4'-C1'-N1	5.48	112.58	108.20
1	AA	906	A	O4'-C1'-N9	5.48	112.58	108.20
1	AA	1395	C	C5'-C4'-C3'	-5.48	107.23	116.00
25	BA	54	G	N9-C4-C5	5.48	107.59	105.40
26	BB	1180	U	C5'-C4'-O4'	5.48	115.68	109.10
26	BB	1869	G	C8-N9-C1'	5.48	134.12	127.00
1	AA	511	C	O3'-P-O5'	-5.48	93.59	104.00
1	AA	774	G	C5'-C4'-O4'	5.48	115.67	109.10
2	AE	74	C	O3'-P-O5'	-5.48	93.59	104.00
26	BB	990	A	O3'-P-O5'	-5.48	93.59	104.00
26	BB	1059	G	C8-N9-C4	-5.48	104.21	106.40
26	BB	1687	G	C8-N9-C4	-5.48	104.21	106.40
26	BB	1859	U	C5'-C4'-O4'	5.48	115.67	109.10
26	BB	2416	C	O4'-C1'-N1	5.48	112.58	108.20
26	BB	2537	U	C5'-C4'-O4'	5.48	115.67	109.10
26	BB	2756	U	P-O3'-C3'	5.48	126.27	119.70
1	AA	856	C	O4'-C1'-N1	5.48	112.58	108.20
4	AD	43	U	N1-C1'-C2'	5.48	121.12	114.00
26	BB	1361	G	C8-N9-C4	-5.48	104.21	106.40
1	AA	46	G	C8-N9-C4	-5.47	104.21	106.40
26	BB	1510	G	O4'-C1'-N9	5.47	112.58	108.20
26	BB	2357	G	C5'-C4'-O4'	5.47	115.67	109.10
1	AA	112	G	C8-N9-C4	-5.47	104.21	106.40
26	BB	467	G	C8-N9-C4	-5.47	104.21	106.40
26	BB	871	U	C5'-C4'-O4'	5.47	115.67	109.10
26	BB	1324	G	O4'-C1'-N9	5.47	112.58	108.20
26	BB	1360	G	O4'-C1'-N9	5.47	112.58	108.20
26	BB	1623	G	O4'-C1'-N9	5.47	112.58	108.20
26	BB	2087	G	C8-N9-C4	-5.47	104.21	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2588	G	O4'-C1'-N9	5.47	112.58	108.20
1	AA	1200	C	N1-C2-O2	5.47	122.18	118.90
1	AA	1225	A	C5'-C4'-O4'	5.47	115.67	109.10
26	BB	207	A	O4'-C1'-N9	5.47	112.58	108.20
26	BB	1934	C	O4'-C1'-N1	5.47	112.58	108.20
1	AA	520	A	C8-N9-C4	-5.47	103.61	105.80
1	AA	1198	G	O4'-C1'-N9	5.47	112.58	108.20
26	BB	412	A	O4'-C1'-N9	5.47	112.58	108.20
26	BB	1145	C	C5'-C4'-C3'	-5.47	107.25	116.00
26	BB	2164	C	N1-C2-O2	5.47	122.18	118.90
1	AA	447	G	C8-N9-C4	-5.47	104.21	106.40
1	AA	725	G	O4'-C1'-N9	5.47	112.57	108.20
26	BB	301	G	C8-N9-C4	-5.47	104.21	106.40
1	AA	1159	U	O4'-C1'-N1	5.46	112.57	108.20
1	AA	1499	A	C5'-C4'-O4'	5.46	115.66	109.10
25	BA	108	A	C5'-C4'-O4'	5.46	115.66	109.10
26	BB	695	G	O4'-C1'-N9	5.46	112.57	108.20
1	AA	75	G	O4'-C1'-N9	5.46	112.57	108.20
26	BB	2780	G	N3-C4-C5	-5.46	125.87	128.60
1	AA	324	G	C8-N9-C4	-5.46	104.22	106.40
1	AA	668	G	C5'-C4'-O4'	5.46	115.65	109.10
1	AA	768	A	C5'-C4'-O4'	5.46	115.65	109.10
26	BB	2578	G	C5'-C4'-O4'	5.46	115.66	109.10
2	AE	71	G	O4'-C1'-N9	5.46	112.57	108.20
26	BB	2408	U	C5'-C4'-O4'	5.46	115.65	109.10
26	BB	164	C	C5'-C4'-O4'	5.46	115.65	109.10
26	BB	942	G	N3-C4-C5	-5.46	125.87	128.60
26	BB	2557	G	O4'-C1'-N9	5.46	112.57	108.20
26	BB	2625	G	C5'-C4'-O4'	5.46	115.65	109.10
2	AB	18	G	O4'-C1'-N9	5.46	112.56	108.20
26	BB	912	C	O4'-C1'-N1	5.46	112.57	108.20
26	BB	2447	G	P-O3'-C3'	5.46	126.25	119.70
1	AA	310	G	C8-N9-C4	-5.45	104.22	106.40
26	BB	253	C	O4'-C1'-N1	5.45	112.56	108.20
26	BB	885	C	O4'-C1'-N1	5.45	112.56	108.20
26	BB	2619	C	C5'-C4'-O4'	5.45	115.64	109.10
26	BB	2744	G	C8-N9-C4	-5.45	104.22	106.40
1	AA	50	A	O4'-C1'-N9	5.45	112.56	108.20
1	AA	1049	U	O3'-P-O5'	-5.45	93.64	104.00
26	BB	870	U	N1-C2-N3	5.45	118.17	114.90
1	AA	1461	G	C5'-C4'-O4'	5.45	115.64	109.10
26	BB	15	G	N7-C8-N9	5.45	115.83	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	806	C	C5'-C4'-C3'	-5.45	107.28	116.00
26	BB	2706	A	O4'-C1'-N9	5.45	112.56	108.20
1	AA	1208	C	O4'-C1'-N1	5.45	112.56	108.20
2	AE	49	C	O4'-C1'-N1	5.45	112.56	108.20
12	AM	17	ARG	NE-CZ-NH1	5.45	123.02	120.30
26	BB	1150	C	O4'-C1'-N1	5.45	112.56	108.20
26	BB	1478	G	C5'-C4'-O4'	5.45	115.64	109.10
26	BB	1605	C	C5'-C4'-C3'	-5.45	107.28	116.00
26	BB	1338	G	C5'-C4'-O4'	5.45	115.64	109.10
26	BB	2416	C	C5'-C4'-C3'	-5.45	107.28	116.00
26	BB	370	G	C8-N9-C4	-5.45	104.22	106.40
26	BB	1219	U	O4'-C1'-N1	5.45	112.56	108.20
26	BB	109	C	C5'-C4'-C3'	-5.44	107.29	116.00
26	BB	1063	G	C3'-C2'-C1'	-5.44	97.14	101.50
26	BB	1298	C	O4'-C1'-N1	5.44	112.56	108.20
1	AA	329	A	O4'-C1'-N9	5.44	112.55	108.20
1	AA	1377	A	C1'-O4'-C4'	-5.44	105.55	109.90
26	BB	1826	G	N3-C4-C5	-5.44	125.88	128.60
1	AA	910	C	C5'-C4'-C3'	-5.44	107.30	116.00
1	AA	1279	G	N3-C4-C5	-5.44	125.88	128.60
26	BB	654	A	P-O3'-C3'	5.44	126.23	119.70
1	AA	394	G	N9-C4-C5	5.44	107.58	105.40
26	BB	1204	A	O4'-C1'-N9	5.44	112.55	108.20
26	BB	1263	U	O4'-C1'-N1	5.44	112.55	108.20
26	BB	2791	G	C1'-O4'-C4'	-5.44	105.55	109.90
1	AA	1203	C	C5'-C4'-C3'	-5.44	107.30	116.00
26	BB	1446	C	C5'-C4'-C3'	-5.44	107.30	116.00
26	BB	1871	A	C5'-C4'-O4'	5.44	115.63	109.10
26	BB	2549	G	N9-C4-C5	5.44	107.58	105.40
1	AA	763	G	O4'-C1'-N9	5.44	112.55	108.20
26	BB	36	G	C4'-C3'-C2'	-5.44	97.16	102.60
26	BB	456	C	O4'-C1'-N1	5.44	112.55	108.20
25	BA	3	C	O4'-C1'-N1	5.43	112.55	108.20
26	BB	554	U	O4'-C1'-N1	5.43	112.55	108.20
26	BB	1089	A	O3'-P-O5'	-5.43	93.67	104.00
26	BB	1341	G	O4'-C1'-N9	5.43	112.55	108.20
1	AA	403	C	C5'-C4'-O4'	5.43	115.62	109.10
1	AA	439	U	O4'-C1'-N1	5.43	112.55	108.20
2	AE	30	G	C8-N9-C4	-5.43	104.23	106.40
26	BB	1850	G	C8-N9-C4	-5.43	104.23	106.40
26	BB	2129	C	O4'-C1'-N1	5.43	112.55	108.20
1	AA	103	U	O4'-C1'-N1	5.43	112.54	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	169	C	C2-N3-C4	5.43	122.61	119.90
26	BB	35	G	C8-N9-C4	-5.43	104.23	106.40
26	BB	566	U	C5'-C4'-C3'	-5.43	107.31	116.00
26	BB	1968	G	C3'-C2'-C1'	-5.43	97.16	101.50
26	BB	2135	A	C4'-C3'-C2'	-5.43	97.17	102.60
26	BB	2870	C	O4'-C1'-N1	5.43	112.54	108.20
1	AA	299	G	N7-C8-N9	5.43	115.81	113.10
1	AA	1436	U	C4'-C3'-C2'	-5.43	97.17	102.60
26	BB	185	G	N9-C1'-C2'	-5.43	106.03	112.00
26	BB	280	U	C5'-C4'-C3'	-5.43	107.31	116.00
26	BB	1096	A	C5'-C4'-O4'	5.43	115.61	109.10
26	BB	1563	U	O4'-C1'-N1	5.43	112.54	108.20
26	BB	1786	A	O4'-C1'-C2'	-5.43	100.37	105.80
26	BB	322	A	C5'-C4'-C3'	-5.43	107.32	116.00
26	BB	396	G	C8-N9-C4	-5.43	104.23	106.40
26	BB	504	A	O4'-C1'-N9	5.43	112.54	108.20
26	BB	686	U	C3'-C2'-C1'	5.43	105.84	101.50
26	BB	864	G	C8-N9-C4	-5.43	104.23	106.40
26	BB	1314	C	N1-C2-O2	5.43	122.16	118.90
26	BB	2602	A	O4'-C1'-N9	5.43	112.54	108.20
1	AA	663	A	C8-N9-C4	-5.42	103.63	105.80
26	BB	273	G	N3-C4-C5	-5.42	125.89	128.60
2	AB	28	G	O4'-C1'-N9	5.42	112.54	108.20
25	BA	48	U	C4'-C3'-C2'	-5.42	97.18	102.60
26	BB	943	A	C5'-C4'-O4'	5.42	115.61	109.10
26	BB	2208	C	C4'-C3'-C2'	-5.42	97.18	102.60
26	BB	2797	U	O4'-C1'-C2'	-5.42	100.38	105.80
1	AA	1409	C	C5'-C4'-C3'	-5.42	107.32	116.00
26	BB	2407	A	C4'-C3'-C2'	-5.42	97.18	102.60
1	AA	768	A	C2'-C3'-O3'	5.42	122.37	113.70
26	BB	687	C	N1-C2-O2	5.42	122.15	118.90
26	BB	1885	A	C5'-C4'-O4'	5.42	115.61	109.10
1	AA	39	G	N3-C4-C5	-5.42	125.89	128.60
26	BB	143	C	O4'-C1'-N1	5.42	112.53	108.20
26	BB	317	G	O4'-C1'-N9	5.42	112.53	108.20
26	BB	1788	C	C5'-C4'-C3'	-5.42	107.33	116.00
1	AA	762	U	O4'-C1'-N1	5.42	112.53	108.20
1	AA	1033	G	N3-C4-C5	-5.42	125.89	128.60
1	AA	1091	U	C5'-C4'-C3'	-5.42	107.33	116.00
26	BB	1587	G	C4'-C3'-C2'	-5.42	97.18	102.60
26	BB	2344	U	P-O3'-C3'	5.42	126.20	119.70
26	BB	815	C	C4'-C3'-C2'	-5.42	97.19	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	175	C	O4'-C1'-N1	5.41	112.53	108.20
1	AA	1011	C	O4'-C1'-N1	5.41	112.53	108.20
26	BB	388	G	P-O3'-C3'	5.41	126.19	119.70
26	BB	545	U	O3'-P-O5'	-5.41	93.72	104.00
26	BB	651	G	C8-N9-C4	-5.41	104.23	106.40
26	BB	1964	G	N9-C4-C5	5.41	107.56	105.40
26	BB	2426	A	O4'-C1'-N9	5.41	112.53	108.20
1	AA	689	C	O4'-C1'-N1	5.41	112.53	108.20
26	BB	165	A	C5'-C4'-O4'	5.41	115.59	109.10
26	BB	2278	A	O4'-C1'-N9	5.41	112.53	108.20
1	AA	130	A	O4'-C1'-N9	5.41	112.53	108.20
26	BB	757	G	O4'-C1'-N9	5.41	112.53	108.20
1	AA	336	A	C5'-C4'-O4'	5.41	115.59	109.10
1	AA	356	A	N9-C1'-C2'	-5.41	106.05	112.00
1	AA	921	U	O4'-C1'-N1	5.41	112.53	108.20
26	BB	292	U	O4'-C1'-N1	5.41	112.53	108.20
26	BB	332	A	C1'-O4'-C4'	-5.41	105.57	109.90
26	BB	716	A	P-O3'-C3'	5.41	126.19	119.70
26	BB	997	G	N3-C4-C5	-5.41	125.90	128.60
26	BB	1404	C	O4'-C1'-N1	5.41	112.53	108.20
26	BB	2051	A	C5'-C4'-C3'	-5.41	107.34	116.00
32	BH	108	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	AA	694	A	C8-N9-C4	-5.41	103.64	105.80
1	AA	849	G	C5'-C4'-O4'	5.41	115.59	109.10
26	BB	2611	C	O4'-C1'-N1	5.41	112.53	108.20
1	AA	165	G	O4'-C1'-N9	5.41	112.52	108.20
1	AA	467	U	O4'-C1'-N1	5.41	112.53	108.20
2	AE	75	C	C3'-C2'-C1'	5.41	105.83	101.50
26	BB	1865	U	O4'-C1'-N1	5.41	112.53	108.20
26	BB	2768	U	O4'-C1'-N1	5.40	112.52	108.20
1	AA	410	G	O4'-C1'-N9	5.40	112.52	108.20
1	AA	1418	A	O4'-C1'-N9	5.40	112.52	108.20
25	BA	111	U	C5'-C4'-C3'	-5.40	107.36	116.00
26	BB	1581	G	C8-N9-C4	-5.40	104.24	106.40
1	AA	18	C	O4'-C1'-N1	5.40	112.52	108.20
1	AA	521	G	N3-C4-C5	-5.40	125.90	128.60
2	AB	26	A	O4'-C1'-N9	5.40	112.52	108.20
2	AE	43	C	O4'-C1'-N1	5.40	112.52	108.20
26	BB	949	G	C8-N9-C4	-5.40	104.24	106.40
1	AA	608	A	C5'-C4'-O4'	5.40	115.58	109.10
1	AA	1047	G	N3-C4-C5	-5.40	125.90	128.60
1	AA	1361	G	O4'-C1'-N9	5.40	112.52	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	159	G	P-O3'-C3'	5.40	126.18	119.70
1	AA	645	G	C8-N9-C4	-5.40	104.24	106.40
26	BB	1848	A	C8-N9-C4	-5.40	103.64	105.80
1	AA	202	G	N9-C4-C5	5.39	107.56	105.40
26	BB	904	G	N9-C1'-C2'	-5.39	106.06	112.00
26	BB	1425	G	C8-N9-C4	-5.39	104.24	106.40
26	BB	2455	G	N3-C4-C5	-5.39	125.90	128.60
1	AA	445	G	O4'-C1'-N9	5.39	112.51	108.20
1	AA	595	A	C5'-C4'-C3'	-5.39	107.37	116.00
26	BB	2233	U	N1-C1'-C2'	-5.39	106.07	112.00
26	BB	2705	A	C5'-C4'-C3'	-5.39	107.37	116.00
25	BA	105	G	N3-C4-C5	-5.39	125.91	128.60
26	BB	1269	A	C5'-C4'-C3'	-5.39	107.37	116.00
26	BB	2843	G	C3'-C2'-C1'	-5.39	97.19	101.50
1	AA	1270	G	O4'-C1'-N9	5.39	112.51	108.20
26	BB	984	A	N9-C1'-C2'	5.39	121.01	114.00
26	BB	1519	G	C8-N9-C4	-5.39	104.25	106.40
26	BB	2540	C	O4'-C1'-N1	5.39	112.51	108.20
1	AA	1160	G	C5'-C4'-O4'	5.39	115.56	109.10
1	AA	1213	A	C5'-C4'-O4'	5.39	115.56	109.10
26	BB	541	A	O4'-C1'-N9	5.39	112.51	108.20
26	BB	646	U	C4'-C3'-C2'	-5.39	97.21	102.60
26	BB	1587	G	O5'-C5'-C4'	-5.39	101.47	111.70
26	BB	1685	C	O4'-C1'-N1	5.39	112.51	108.20
26	BB	1738	G	C8-N9-C4	-5.39	104.25	106.40
26	BB	2124	G	C5'-C4'-O4'	5.39	115.56	109.10
1	AA	851	G	O4'-C1'-N9	5.38	112.51	108.20
1	AA	1501	C	C3'-C2'-C1'	5.38	105.81	101.50
26	BB	1892	C	O4'-C1'-N1	5.38	112.51	108.20
26	BB	2488	G	O4'-C1'-N9	5.38	112.51	108.20
26	BB	177	G	N3-C4-C5	-5.38	125.91	128.60
26	BB	492	A	C8-N9-C4	-5.38	103.65	105.80
26	BB	930	G	O4'-C1'-N9	5.38	112.51	108.20
26	BB	2563	U	C5'-C4'-O4'	5.38	115.56	109.10
1	AA	209	U	O4'-C1'-N1	5.38	112.50	108.20
26	BB	495	G	N9-C4-C5	5.38	107.55	105.40
26	BB	1334	G	C8-N9-C4	-5.38	104.25	106.40
26	BB	2883	A	O4'-C1'-N9	5.38	112.51	108.20
2	AE	30	G	N9-C4-C5	5.38	107.55	105.40
26	BB	11	C	O4'-C1'-C2'	-5.38	100.42	105.80
26	BB	1063	G	N3-C4-C5	-5.38	125.91	128.60
1	AA	214	C	C3'-C2'-C1'	-5.38	97.20	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	432	A	C5'-C4'-C3'	-5.38	107.40	116.00
26	BB	829	A	O4'-C4'-C3'	5.38	110.40	106.10
26	BB	1104	C	C5-C6-N1	5.38	123.69	121.00
26	BB	1776	G	N3-C4-C5	-5.38	125.91	128.60
1	AA	768	A	C8-N9-C4	-5.38	103.65	105.80
1	AA	1083	U	C3'-C2'-C1'	5.38	105.80	101.50
9	AJ	113	ARG	NE-CZ-NH2	-5.38	117.61	120.30
26	BB	136	G	C3'-C2'-C1'	-5.38	97.20	101.50
26	BB	1627	G	C5'-C4'-O4'	5.38	115.55	109.10
26	BB	2564	A	C5'-C4'-O4'	5.38	115.55	109.10
26	BB	2766	A	C5'-C4'-O4'	5.38	115.55	109.10
1	AA	909	A	O3'-P-O5'	5.38	114.21	104.00
26	BB	1474	U	O4'-C1'-N1	5.38	112.50	108.20
26	BB	460	A	O4'-C1'-N9	5.37	112.50	108.20
26	BB	808	G	N3-C4-C5	-5.37	125.91	128.60
26	BB	2302	U	C5'-C4'-C3'	-5.37	107.40	116.00
1	AA	385	C	C2'-C3'-O3'	5.37	122.30	113.70
1	AA	1138	G	P-O3'-C3'	5.37	126.14	119.70
10	AK	1	PRO	CA-N-CD	-5.37	103.98	111.50
26	BB	1501	G	C8-N9-C4	-5.37	104.25	106.40
26	BB	2612	C	C3'-C2'-C1'	5.37	105.80	101.50
26	BB	1171	G	O4'-C1'-N9	5.37	112.50	108.20
1	AA	1264	U	O4'-C1'-N1	5.37	112.49	108.20
26	BB	787	C	O3'-P-O5'	-5.37	93.80	104.00
26	BB	864	G	O4'-C1'-N9	5.37	112.50	108.20
26	BB	1065	U	C3'-C2'-C1'	5.37	105.80	101.50
26	BB	1535	A	N9-C1'-C2'	-5.37	106.09	112.00
26	BB	2111	U	P-O3'-C3'	5.37	126.14	119.70
26	BB	1277	G	O4'-C1'-N9	5.37	112.49	108.20
26	BB	2133	G	O4'-C1'-C2'	-5.37	100.43	105.80
1	AA	576	C	N1-C2-O2	5.37	122.12	118.90
26	BB	205	G	C8-N9-C4	-5.37	104.25	106.40
1	AA	1096	C	N1-C2-O2	5.36	122.12	118.90
26	BB	362	A	C5'-C4'-C3'	-5.36	107.42	116.00
26	BB	2673	G	O4'-C1'-N9	5.36	112.49	108.20
1	AA	1508	A	O4'-C1'-N9	5.36	112.49	108.20
1	AA	1530	G	O5'-C5'-C4'	-5.36	101.51	111.70
1	AA	758	C	N1-C2-O2	5.36	122.12	118.90
2	AB	53	G	O4'-C1'-N9	5.36	112.49	108.20
26	BB	2459	A	C8-N9-C4	-5.36	103.66	105.80
26	BB	450	G	O4'-C1'-N9	5.36	112.49	108.20
26	BB	663	G	C8-N9-C4	-5.36	104.26	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2378	A	C5'-C4'-O4'	5.36	115.53	109.10
25	BA	28	C	C5'-C4'-O4'	5.36	115.53	109.10
26	BB	1640	A	O4'-C1'-N9	5.36	112.49	108.20
1	AA	801	U	O4'-C1'-N1	5.36	112.48	108.20
1	AA	950	U	O4'-C1'-N1	5.36	112.48	108.20
1	AA	1450	U	C3'-C2'-C1'	5.36	105.78	101.50
26	BB	6	A	O4'-C1'-N9	5.36	112.48	108.20
26	BB	2861	U	O4'-C1'-N1	5.36	112.48	108.20
1	AA	395	C	O4'-C1'-N1	5.35	112.48	108.20
26	BB	246	C	C5'-C4'-C3'	-5.35	107.43	116.00
1	AA	629	A	O4'-C1'-N9	5.35	112.48	108.20
26	BB	37	C	C5'-C4'-O4'	5.35	115.52	109.10
26	BB	543	G	C1'-O4'-C4'	-5.35	105.62	109.90
26	BB	2005	A	O4'-C1'-N9	5.35	112.48	108.20
2	AB	52	G	N3-C4-C5	-5.35	125.92	128.60
26	BB	481	G	O4'-C1'-C2'	-5.35	100.45	105.80
26	BB	1512	C	N1-C1'-C2'	-5.35	106.12	112.00
26	BB	2180	U	O4'-C1'-N1	5.35	112.48	108.20
26	BB	2770	G	C8-N9-C4	-5.35	104.26	106.40
1	AA	792	A	O4'-C4'-C3'	5.35	110.38	106.10
26	BB	314	C	C2-N3-C4	5.35	122.57	119.90
26	BB	1445	G	C8-N9-C4	-5.35	104.26	106.40
1	AA	42	G	C8-N9-C4	-5.35	104.26	106.40
1	AA	708	C	O4'-C1'-N1	5.35	112.48	108.20
26	BB	555	G	C2-N3-C4	5.35	114.57	111.90
26	BB	2378	A	O4'-C1'-N9	5.35	112.48	108.20
1	AA	116	A	N9-C1'-C2'	-5.34	106.12	112.00
1	AA	484	G	C3'-C2'-C1'	-5.34	97.22	101.50
25	BA	23	G	C8-N9-C4	-5.34	104.26	106.40
26	BB	2054	A	O3'-P-O5'	-5.34	93.85	104.00
1	AA	56	U	O4'-C1'-N1	5.34	112.47	108.20
1	AA	214	C	N3-C2-O2	-5.34	118.16	121.90
26	BB	862	G	N3-C4-C5	-5.34	125.93	128.60
1	AA	1289	A	C8-N9-C4	-5.34	103.66	105.80
1	AA	1522	U	N1-C2-N3	5.34	118.10	114.90
26	BB	1757	A	O4'-C4'-C3'	5.34	110.37	106.10
26	BB	2895	G	C8-N9-C4	-5.34	104.26	106.40
1	AA	87	C	O4'-C1'-N1	5.34	112.47	108.20
26	BB	289	G	O4'-C1'-N9	5.34	112.47	108.20
26	BB	639	U	O4'-C1'-N1	5.34	112.47	108.20
26	BB	1330	C	C5'-C4'-O4'	5.34	115.51	109.10
26	BB	1826	G	C4'-C3'-C2'	-5.34	97.26	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2666	C	N1-C2-O2	5.34	122.10	118.90
1	AA	1144	G	C5'-C4'-O4'	5.34	115.50	109.10
26	BB	660	C	C5'-C4'-O4'	5.34	115.50	109.10
26	BB	2785	C	O4'-C1'-N1	5.34	112.47	108.20
1	AA	68	G	N3-C4-C5	-5.33	125.93	128.60
1	AA	203	G	C8-N9-C4	-5.33	104.27	106.40
26	BB	659	G	C8-N9-C4	-5.33	104.27	106.40
26	BB	2234	G	N7-C8-N9	5.33	115.77	113.10
1	AA	322	C	O4'-C1'-N1	5.33	112.47	108.20
1	AA	480	U	O4'-C1'-N1	5.33	112.47	108.20
4	AD	37	U	O4'-C1'-N1	5.33	112.47	108.20
26	BB	526	A	O4'-C1'-N9	-5.33	103.93	108.20
26	BB	1928	A	C8-N9-C4	-5.33	103.67	105.80
1	AA	410	G	C5'-C4'-C3'	-5.33	107.47	116.00
1	AA	1152	A	C3'-C2'-C1'	5.33	105.77	101.50
26	BB	514	A	O4'-C1'-N9	5.33	112.47	108.20
1	AA	489	C	C5'-C4'-O4'	5.33	115.50	109.10
1	AA	1135	U	O4'-C1'-N1	5.33	112.46	108.20
2	AB	48	C	C5'-C4'-O4'	5.33	115.49	109.10
26	BB	1505	A	O4'-C1'-N9	5.33	112.46	108.20
26	BB	1888	G	C8-N9-C4	-5.33	104.27	106.40
1	AA	354	G	C8-N9-C4	-5.33	104.27	106.40
1	AA	843	U	O4'-C1'-N1	5.33	112.46	108.20
26	BB	1645	G	O4'-C4'-C3'	5.33	110.36	106.10
1	AA	489	C	O4'-C1'-N1	5.33	112.46	108.20
26	BB	2150	C	O4'-C1'-N1	5.33	112.46	108.20
26	BB	2303	G	C8-N9-C4	-5.33	104.27	106.40
1	AA	1314	C	C5'-C4'-C3'	-5.32	107.48	116.00
1	AA	1436	U	C3'-C2'-C1'	5.32	105.76	101.50
26	BB	1092	C	C5'-C4'-O4'	5.32	115.49	109.10
26	BB	1580	A	C5'-C4'-C3'	-5.32	107.48	116.00
26	BB	1855	U	C5'-C4'-C3'	-5.32	107.48	116.00
30	BF	69	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	AA	407	U	O4'-C1'-N1	5.32	112.46	108.20
26	BB	491	G	N3-C4-C5	-5.32	125.94	128.60
26	BB	2243	U	O4'-C1'-N1	5.32	112.46	108.20
26	BB	764	A	C8-N9-C4	-5.32	103.67	105.80
26	BB	1540	G	C8-N9-C4	-5.32	104.27	106.40
26	BB	1555	G	P-O3'-C3'	5.32	126.08	119.70
1	AA	19	A	O4'-C1'-N9	5.32	112.45	108.20
1	AA	572	A	C1'-O4'-C4'	-5.32	105.64	109.90
1	AA	849	G	N9-C4-C5	5.32	107.53	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1505	G	C8-N9-C4	-5.32	104.27	106.40
1	AA	94	G	N3-C4-C5	-5.32	125.94	128.60
1	AA	1337	G	P-O3'-C3'	5.32	126.08	119.70
26	BB	145	C	O4'-C1'-N1	5.32	112.45	108.20
26	BB	1967	C	N1-C2-O2	5.32	122.09	118.90
26	BB	2115	G	C8-N9-C4	-5.32	104.27	106.40
26	BB	2297	A	C8-N9-C4	-5.32	103.67	105.80
1	AA	907	A	C5'-C4'-O4'	5.32	115.48	109.10
1	AA	1087	G	C4'-C3'-C2'	-5.32	97.28	102.60
26	BB	267	C	O4'-C1'-N1	5.32	112.45	108.20
26	BB	2885	G	O4'-C1'-N9	5.32	112.45	108.20
25	BA	85	G	C8-N9-C4	-5.31	104.27	106.40
26	BB	21	A	C5'-C4'-O4'	5.31	115.48	109.10
26	BB	655	A	O4'-C1'-N9	5.31	112.45	108.20
1	AA	272	C	O4'-C1'-N1	5.31	112.45	108.20
1	AA	1208	C	C5'-C4'-O4'	5.31	115.47	109.10
1	AA	1366	C	O4'-C1'-N1	5.31	112.45	108.20
25	BA	76	G	C8-N9-C4	-5.31	104.28	106.40
26	BB	666	A	O4'-C1'-N9	5.31	112.45	108.20
26	BB	1367	A	O4'-C1'-N9	5.31	112.45	108.20
26	BB	1016	G	N9-C4-C5	5.31	107.52	105.40
1	AA	212	G	C8-N9-C4	-5.31	104.28	106.40
1	AA	1061	G	C8-N9-C4	-5.31	104.28	106.40
26	BB	235	U	C5'-C4'-C3'	-5.31	107.50	116.00
26	BB	1947	C	O4'-C1'-N1	5.31	112.45	108.20
1	AA	1373	G	C5'-C4'-O4'	5.31	115.47	109.10
26	BB	302	C	C4'-C3'-C2'	-5.31	97.29	102.60
26	BB	348	A	O4'-C1'-N9	5.31	112.45	108.20
26	BB	2808	G	P-O3'-C3'	5.31	126.07	119.70
26	BB	2872	A	C1'-O4'-C4'	-5.31	105.65	109.90
1	AA	481	G	C2'-C3'-O3'	5.31	122.19	113.70
1	AA	1089	G	O4'-C1'-N9	5.31	112.44	108.20
26	BB	1850	G	N9-C4-C5	5.31	107.52	105.40
1	AA	1384	C	C5'-C4'-C3'	-5.30	107.51	116.00
26	BB	468	G	C8-N9-C4	-5.30	104.28	106.40
1	AA	987	G	O4'-C1'-N9	5.30	112.44	108.20
1	AA	1114	C	N3-C2-O2	-5.30	118.19	121.90
26	BB	1416	G	C8-N9-C1'	5.30	133.89	127.00
1	AA	1176	A	C8-N9-C4	-5.30	103.68	105.80
26	BB	426	C	O4'-C1'-N1	5.30	112.44	108.20
26	BB	1124	G	C8-N9-C4	-5.30	104.28	106.40
1	AA	1507	A	C5'-C4'-O4'	5.30	115.46	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1683	U	O4'-C1'-N1	5.30	112.44	108.20
26	BB	1786	A	O4'-C1'-N9	5.30	112.44	108.20
26	BB	2403	C	N1-C2-O2	5.30	122.08	118.90
26	BB	15	G	N3-C4-C5	-5.30	125.95	128.60
26	BB	363	G	C5'-C4'-O4'	5.30	115.46	109.10
1	AA	610	U	O4'-C1'-N1	5.30	112.44	108.20
26	BB	67	U	O4'-C1'-N1	5.30	112.44	108.20
26	BB	1025	G	N3-C4-C5	-5.30	125.95	128.60
26	BB	2208	C	O4'-C1'-N1	5.30	112.44	108.20
26	BB	2488	G	N9-C4-C5	5.30	107.52	105.40
1	AA	866	C	P-O3'-C3'	5.29	126.06	119.70
4	AD	46	C	O4'-C1'-N1	5.29	112.44	108.20
25	BA	55	U	C5'-C4'-O4'	5.29	115.45	109.10
26	BB	634	C	O4'-C1'-N1	5.29	112.44	108.20
26	BB	612	G	N7-C8-N9	5.29	115.75	113.10
26	BB	718	A	C5'-C4'-O4'	5.29	115.45	109.10
26	BB	2664	G	N9-C4-C5	5.29	107.52	105.40
26	BB	274	C	O4'-C1'-N1	5.29	112.43	108.20
26	BB	749	A	O4'-C1'-N9	5.29	112.43	108.20
26	BB	1325	U	C3'-C2'-C1'	-5.29	97.27	101.50
26	BB	1698	A	C8-N9-C4	-5.29	103.68	105.80
13	AN	7	ARG	NE-CZ-NH2	-5.29	117.66	120.30
26	BB	181	A	C5'-C4'-O4'	5.29	115.45	109.10
1	AA	1528	U	O3'-P-O5'	-5.29	93.95	104.00
25	BA	38	C	N1-C1'-C2'	-5.29	106.18	112.00
26	BB	2028	U	C3'-C2'-C1'	-5.29	97.27	101.50
26	BB	2432	A	O4'-C1'-N9	5.29	112.43	108.20
26	BB	320	A	O4'-C1'-N9	5.29	112.43	108.20
26	BB	852	U	O4'-C1'-N1	5.29	112.43	108.20
26	BB	1092	C	O4'-C1'-N1	5.29	112.43	108.20
26	BB	1732	C	C3'-C2'-C1'	5.29	105.73	101.50
26	BB	818	G	C8-N9-C4	-5.28	104.29	106.40
26	BB	1724	G	N9-C4-C5	5.28	107.51	105.40
26	BB	2277	G	C5'-C4'-C3'	-5.28	107.55	116.00
26	BB	2281	A	C5'-C4'-C3'	-5.28	107.55	116.00
26	BB	717	C	O4'-C1'-N1	5.28	112.43	108.20
26	BB	838	C	C5'-C4'-O4'	5.28	115.44	109.10
1	AA	36	C	O4'-C1'-N1	5.28	112.42	108.20
1	AA	41	G	C8-N9-C4	-5.28	104.29	106.40
1	AA	969	A	O4'-C1'-N9	5.28	112.42	108.20
26	BB	533	G	O4'-C1'-N9	5.28	112.42	108.20
26	BB	2298	A	C5'-C4'-O4'	5.28	115.44	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1076	U	C2'-C3'-O3'	5.28	122.15	113.70
1	AA	999	C	O4'-C1'-N1	5.28	112.42	108.20
26	BB	1808	A	O4'-C1'-N9	5.28	112.42	108.20
26	BB	2347	C	O4'-C1'-N1	5.28	112.42	108.20
26	BB	2874	C	O3'-P-O5'	-5.28	93.97	104.00
1	AA	591	U	O4'-C1'-N1	5.28	112.42	108.20
1	AA	1098	C	N1-C1'-C2'	-5.28	106.20	112.00
17	AR	58	ARG	NE-CZ-NH1	5.28	122.94	120.30
25	BA	107	G	O4'-C4'-C3'	5.28	110.32	106.10
26	BB	1840	G	C8-N9-C4	-5.28	104.29	106.40
26	BB	2006	C	C5'-C4'-C3'	-5.28	107.56	116.00
1	AA	1487	G	O4'-C1'-N9	5.27	112.42	108.20
26	BB	102	U	C1'-O4'-C4'	-5.27	105.68	109.90
26	BB	323	C	N3-C2-O2	-5.27	118.21	121.90
26	BB	1919	A	C4'-C3'-O3'	5.27	123.55	113.00
26	BB	2216	G	C5'-C4'-O4'	5.27	115.43	109.10
26	BB	2234	G	C8-N9-C4	-5.27	104.29	106.40
1	AA	57	G	C8-N9-C4	-5.27	104.29	106.40
1	AA	163	C	C4'-C3'-C2'	-5.27	97.33	102.60
1	AA	1178	G	O4'-C1'-N9	5.27	112.42	108.20
1	AA	1491	G	N3-C4-C5	-5.27	125.96	128.60
4	AD	41	A	O4'-C1'-N9	5.27	112.42	108.20
26	BB	774	G	O4'-C1'-N9	5.27	112.42	108.20
26	BB	1345	C	O4'-C1'-N1	5.27	112.42	108.20
1	AA	549	C	C5'-C4'-O4'	5.27	115.42	109.10
26	BB	1880	U	O4'-C1'-N1	5.27	112.42	108.20
26	BB	2379	G	C8-N9-C4	-5.27	104.29	106.40
1	AA	71	A	C8-N9-C4	-5.27	103.69	105.80
1	AA	1435	G	C8-N9-C4	-5.27	104.29	106.40
26	BB	1416	G	C4-C5-N7	-5.27	108.69	110.80
26	BB	2488	G	C2-N3-C4	5.27	114.53	111.90
26	BB	756	A	C3'-C2'-C1'	-5.27	97.29	101.50
1	AA	126	G	N9-C4-C5	5.26	107.51	105.40
1	AA	1162	C	C5'-C4'-C3'	-5.26	107.58	116.00
26	BB	1292	G	N3-C4-C5	-5.26	125.97	128.60
1	AA	1363	A	C1'-O4'-C4'	-5.26	105.69	109.90
1	AA	340	U	O4'-C1'-N1	5.26	112.41	108.20
1	AA	736	C	O4'-C1'-N1	5.26	112.41	108.20
1	AA	833	G	C5'-C4'-O4'	5.26	115.41	109.10
26	BB	917	A	O4'-C1'-N9	5.26	112.41	108.20
26	BB	1806	C	O4'-C1'-N1	5.26	112.41	108.20
1	AA	242	G	O4'-C1'-N9	5.26	112.41	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	751	U	O4'-C1'-N1	5.26	112.41	108.20
26	BB	2043	C	C5'-C4'-O4'	5.26	115.41	109.10
26	BB	2057	G	O4'-C1'-N9	5.26	112.41	108.20
26	BB	2449	H2U	P-O3'-C3'	5.26	126.01	119.70
26	BB	2049	G	C4'-C3'-C2'	-5.26	97.34	102.60
26	BB	2486	C	C5'-C4'-C3'	-5.26	107.59	116.00
26	BB	2581	G	C8-N9-C4	-5.26	104.30	106.40
1	AA	412	A	O4'-C1'-N9	5.26	112.41	108.20
26	BB	87	U	C3'-C2'-C1'	5.26	105.70	101.50
1	AA	497	G	C8-N9-C4	-5.25	104.30	106.40
26	BB	285	G	C8-N9-C4	-5.25	104.30	106.40
26	BB	2646	C	O4'-C1'-N1	5.25	112.40	108.20
1	AA	595	A	O4'-C1'-N9	5.25	112.40	108.20
1	AA	947	G	C8-N9-C4	-5.25	104.30	106.40
1	AA	1418	A	C8-N9-C4	-5.25	103.70	105.80
26	BB	156	A	O4'-C1'-N9	5.25	112.40	108.20
26	BB	488	G	C5'-C4'-O4'	5.25	115.40	109.10
26	BB	511	U	O4'-C1'-N1	5.25	112.40	108.20
26	BB	2902	C	O4'-C1'-N1	5.25	112.40	108.20
26	BB	264	C	O4'-C1'-N1	5.25	112.40	108.20
26	BB	702	U	C5'-C4'-O4'	5.25	115.40	109.10
26	BB	2642	G	C8-N9-C4	-5.25	104.30	106.40
1	AA	37	U	O4'-C1'-N1	5.25	112.40	108.20
1	AA	509	A	C5'-C4'-C3'	-5.25	107.60	116.00
1	AA	638	U	O4'-C1'-N1	5.25	112.40	108.20
1	AA	1440	U	N1-C1'-C2'	-5.25	106.23	112.00
26	BB	170	U	C4'-C3'-C2'	-5.25	97.35	102.60
26	BB	1510	G	N3-C4-C5	-5.25	125.97	128.60
26	BB	2640	G	C8-N9-C4	-5.25	104.30	106.40
1	AA	316	C	O4'-C1'-N1	5.25	112.40	108.20
26	BB	959	A	O4'-C1'-N9	5.25	112.40	108.20
1	AA	1217	C	O4'-C1'-N1	5.25	112.40	108.20
1	AA	1247	U	O4'-C1'-N1	5.25	112.40	108.20
26	BB	295	G	C5'-C4'-C3'	-5.25	107.61	116.00
26	BB	2171	A	O4'-C1'-N9	5.25	112.40	108.20
1	AA	791	G	N3-C4-C5	-5.24	125.98	128.60
1	AA	808	C	O4'-C1'-N1	5.24	112.39	108.20
26	BB	58	G	C4'-C3'-C2'	-5.24	97.36	102.60
26	BB	993	G	N3-C4-C5	-5.24	125.98	128.60
1	AA	714	G	O4'-C1'-N9	5.24	112.39	108.20
26	BB	555	G	C5'-C4'-O4'	5.24	115.39	109.10
26	BB	1544	A	C5'-C4'-O4'	5.24	115.39	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	147	G	N3-C4-C5	-5.24	125.98	128.60
1	AA	556	C	O4'-C1'-N1	5.24	112.39	108.20
1	AA	621	A	C4'-C3'-C2'	-5.24	97.36	102.60
1	AA	742	G	N3-C4-C5	-5.24	125.98	128.60
1	AA	1454	G	C8-N9-C4	-5.24	104.30	106.40
26	BB	1416	G	N3-C4-C5	-5.24	125.98	128.60
1	AA	106	C	O4'-C1'-N1	5.24	112.39	108.20
26	BB	311	A	O3'-P-O5'	-5.24	94.05	104.00
26	BB	368	A	C5'-C4'-O4'	5.24	115.39	109.10
1	AA	628	G	N9-C4-C5	5.24	107.50	105.40
1	AA	203	G	N3-C4-C5	-5.24	125.98	128.60
1	AA	1062	U	O4'-C1'-N1	5.24	112.39	108.20
1	AA	1068	G	C5'-C4'-C3'	-5.24	107.62	116.00
26	BB	315	G	C8-N9-C4	-5.24	104.31	106.40
26	BB	923	G	N9-C4-C5	5.24	107.49	105.40
26	BB	966	G	C8-N9-C4	-5.24	104.31	106.40
26	BB	1198	U	C5'-C4'-C3'	-5.24	107.62	116.00
26	BB	1774	C	O4'-C1'-N1	5.24	112.39	108.20
1	AA	122	G	O4'-C4'-C3'	5.23	110.29	106.10
1	AA	744	C	C5'-C4'-C3'	-5.23	107.63	116.00
25	BA	96	G	O4'-C1'-N9	5.23	112.39	108.20
26	BB	428	A	O4'-C1'-N9	5.23	112.39	108.20
26	BB	1601	G	O4'-C1'-N9	5.23	112.39	108.20
1	AA	1258	G	C8-N9-C4	-5.23	104.31	106.40
25	BA	55	U	C4'-C3'-C2'	-5.23	97.37	102.60
25	BA	83	G	C8-N9-C4	-5.23	104.31	106.40
26	BB	2032	G	C8-N9-C4	-5.23	104.31	106.40
1	AA	604	G	C8-N9-C4	-5.23	104.31	106.40
26	BB	869	G	N9-C4-C5	5.23	107.49	105.40
26	BB	1749	A	O4'-C1'-N9	5.23	112.39	108.20
26	BB	2162	G	N9-C4-C5	5.23	107.49	105.40
1	AA	205	A	C8-N9-C4	-5.23	103.71	105.80
25	BA	56	G	O4'-C1'-N9	5.23	112.38	108.20
1	AA	457	G	O4'-C1'-N9	5.23	112.38	108.20
1	AA	1233	G	N3-C4-C5	-5.23	125.99	128.60
4	AD	25	U	C3'-C2'-C1'	5.23	105.68	101.50
25	BA	77	U	C5'-C4'-O4'	5.23	115.37	109.10
26	BB	1346	G	O4'-C1'-N9	5.23	112.38	108.20
26	BB	1407	G	C5'-C4'-O4'	5.23	115.37	109.10
1	AA	591	U	C5'-C4'-O4'	5.23	115.37	109.10
1	AA	863	U	C5'-C4'-C3'	-5.23	107.64	116.00
1	AA	1457	G	C4'-C3'-C2'	-5.23	97.37	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AE	3	C	O4'-C1'-N1	5.23	112.38	108.20
26	BB	1745	A	O4'-C1'-N9	5.23	112.38	108.20
1	AA	200	G	C4'-C3'-C2'	-5.22	97.38	102.60
1	AA	416	G	C8-N9-C4	-5.22	104.31	106.40
1	AA	1193	G	N9-C1'-C2'	-5.22	106.25	112.00
25	BA	74	U	O4'-C1'-N1	5.22	112.38	108.20
26	BB	957	C	O4'-C1'-N1	5.22	112.38	108.20
26	BB	2839	G	C8-N9-C4	-5.22	104.31	106.40
1	AA	975	A	C2'-C3'-O3'	5.22	122.06	113.70
1	AA	1069	C	O4'-C1'-N1	5.22	112.38	108.20
4	AD	30	U	C5'-C4'-O4'	5.22	115.37	109.10
2	AE	38	A	C5'-C4'-O4'	5.22	115.37	109.10
26	BB	1396	U	C3'-C2'-C1'	-5.22	97.32	101.50
26	BB	1537	G	N3-C4-C5	-5.22	125.99	128.60
1	AA	558	G	C8-N9-C4	-5.22	104.31	106.40
1	AA	631	C	C4'-C3'-C2'	-5.22	97.38	102.60
26	BB	2485	G	C8-N9-C4	-5.22	104.31	106.40
1	AA	674	G	C4'-C3'-C2'	-5.22	97.38	102.60
26	BB	8	C	O4'-C1'-N1	5.22	112.38	108.20
26	BB	1936	A	O4'-C1'-N9	5.22	112.38	108.20
26	BB	2194	U	O4'-C1'-N1	5.22	112.38	108.20
26	BB	2833	U	O4'-C1'-N1	5.22	112.38	108.20
26	BB	1161	C	O4'-C1'-N1	5.22	112.38	108.20
26	BB	2148	G	N3-C4-C5	-5.22	125.99	128.60
1	AA	1065	U	C1'-O4'-C4'	-5.22	105.73	109.90
26	BB	803	U	C4'-C3'-C2'	-5.22	97.38	102.60
26	BB	852	U	C2-N3-C4	-5.22	123.87	127.00
26	BB	1074	G	N9-C4-C5	5.22	107.49	105.40
26	BB	1158	C	O4'-C1'-N1	5.22	112.37	108.20
26	BB	1171	G	C1'-O4'-C4'	-5.22	105.73	109.90
26	BB	1559	U	O4'-C1'-N1	5.22	112.37	108.20
26	BB	2065	C	C5'-C4'-C3'	-5.22	107.65	116.00
26	BB	2147	A	C1'-O4'-C4'	-5.22	105.73	109.90
26	BB	2581	G	N3-C4-C5	-5.22	125.99	128.60
26	BB	2645	G	P-O3'-C3'	5.22	125.96	119.70
25	BA	107	G	O3'-P-O5'	5.21	113.91	104.00
26	BB	318	C	O4'-C1'-N1	5.21	112.37	108.20
26	BB	1222	U	O4'-C1'-N1	5.21	112.37	108.20
26	BB	1525	A	C5'-C4'-C3'	-5.21	107.66	116.00
26	BB	1758	U	P-O3'-C3'	5.21	125.96	119.70
26	BB	2792	A	C5'-C4'-O4'	5.21	115.36	109.10
26	BB	255	A	C5'-C4'-C3'	-5.21	107.66	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1984	G	O4'-C1'-N9	5.21	112.37	108.20
26	BB	2412	A	C5'-C4'-C3'	-5.21	107.66	116.00
2	AE	12	U	C5'-C4'-O4'	5.21	115.35	109.10
26	BB	389	G	N7-C8-N9	5.21	115.71	113.10
26	BB	727	A	O4'-C1'-N9	5.21	112.37	108.20
26	BB	855	G	O4'-C1'-N9	5.21	112.37	108.20
26	BB	2501	C	O4'-C1'-N1	-5.21	104.03	108.20
1	AA	693	G	C8-N9-C4	-5.21	104.32	106.40
26	BB	945	A	P-O3'-C3'	5.21	125.95	119.70
26	BB	2883	A	N9-C1'-C2'	-5.21	106.27	112.00
1	AA	1048	G	C8-N9-C4	-5.21	104.32	106.40
26	BB	1645	G	N3-C4-C5	-5.21	126.00	128.60
26	BB	2611	C	C3'-C2'-C1'	5.21	105.67	101.50
26	BB	2688	G	C8-N9-C4	-5.21	104.32	106.40
26	BB	2760	C	C4'-C3'-C2'	-5.21	97.39	102.60
1	AA	1517	G	N3-C4-C5	-5.21	126.00	128.60
26	BB	810	U	C3'-C2'-C1'	5.21	105.66	101.50
26	BB	1491	G	N9-C4-C5	5.21	107.48	105.40
1	AA	165	G	N3-C4-C5	-5.20	126.00	128.60
1	AA	702	A	C3'-C2'-C1'	5.20	105.66	101.50
1	AA	1453	G	C8-N9-C4	-5.20	104.32	106.40
26	BB	1845	G	C8-N9-C4	-5.20	104.32	106.40
26	BB	2307	G	N3-C4-C5	-5.20	126.00	128.60
26	BB	2777	G	C8-N9-C4	-5.20	104.32	106.40
1	AA	1320	C	C3'-C2'-C1'	-5.20	97.34	101.50
26	BB	1238	G	N3-C4-C5	-5.20	126.00	128.60
1	AA	1046	A	C2'-C3'-O3'	5.20	122.02	113.70
26	BB	141	G	C3'-C2'-C1'	5.20	105.66	101.50
26	BB	212	G	N3-C4-C5	-5.20	126.00	128.60
26	BB	659	G	C5'-C4'-O4'	5.20	115.34	109.10
26	BB	953	G	N9-C4-C5	5.20	107.48	105.40
22	AW	36	ARG	NE-CZ-NH1	5.20	122.90	120.30
26	BB	465	G	C5'-C4'-O4'	5.20	115.34	109.10
26	BB	1074	G	C8-N9-C4	-5.20	104.32	106.40
26	BB	2365	G	C8-N9-C4	-5.20	104.32	106.40
1	AA	494	G	C5'-C4'-O4'	5.20	115.34	109.10
1	AA	1384	C	P-O5'-C5'	5.20	129.21	120.90
26	BB	297	G	C8-N9-C4	-5.20	104.32	106.40
26	BB	681	G	O4'-C1'-N9	5.20	112.36	108.20
26	BB	860	U	O4'-C1'-N1	5.20	112.36	108.20
26	BB	1408	G	O3'-P-O5'	-5.20	94.13	104.00
26	BB	1853	A	P-O3'-C3'	5.20	125.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	141	G	O4'-C1'-N9	5.19	112.36	108.20
2	AB	15	G	N9-C4-C5	5.19	107.48	105.40
26	BB	371	A	O4'-C1'-N9	5.19	112.36	108.20
26	BB	1332	G	N3-C4-C5	-5.19	126.00	128.60
26	BB	2048	G	C5'-C4'-O4'	5.19	115.33	109.10
2	AE	15	G	O4'-C1'-N9	5.19	112.35	108.20
26	BB	442	G	N9-C4-C5	5.19	107.48	105.40
26	BB	530	G	C8-N9-C4	-5.19	104.32	106.40
26	BB	1591	A	O4'-C1'-N9	5.19	112.35	108.20
26	BB	1627	G	N3-C4-C5	-5.19	126.00	128.60
26	BB	1998	A	N9-C1'-C2'	-5.19	106.29	112.00
1	AA	723	U	O4'-C1'-N1	5.19	112.35	108.20
26	BB	54	G	N3-C4-C5	-5.19	126.01	128.60
26	BB	240	C	O4'-C1'-N1	5.19	112.35	108.20
26	BB	2117	A	O3'-P-O5'	5.19	113.86	104.00
26	BB	2159	G	C8-N9-C4	-5.19	104.33	106.40
26	BB	2211	A	C3'-C2'-C1'	5.19	105.65	101.50
26	BB	2363	G	C8-N9-C4	-5.19	104.33	106.40
1	AA	379	C	C4'-C3'-C2'	-5.19	97.41	102.60
25	BA	116	G	N9-C4-C5	5.19	107.47	105.40
26	BB	1724	G	N3-C4-C5	-5.19	126.01	128.60
1	AA	1307	U	O4'-C1'-N1	5.18	112.35	108.20
26	BB	276	U	P-O3'-C3'	5.18	125.92	119.70
26	BB	1078	U	O3'-P-O5'	-5.18	94.15	104.00
26	BB	1567	G	O4'-C1'-N9	5.18	112.35	108.20
26	BB	1994	C	O4'-C1'-N1	5.18	112.35	108.20
26	BB	2218	G	C5'-C4'-C3'	-5.18	107.70	116.00
1	AA	355	C	O4'-C1'-N1	5.18	112.35	108.20
26	BB	117	G	C2-N3-C4	5.18	114.49	111.90
26	BB	906	U	N3-C2-O2	-5.18	118.57	122.20
26	BB	1548	A	C8-N9-C4	-5.18	103.73	105.80
26	BB	1695	G	C2-N3-C4	5.18	114.49	111.90
26	BB	2399	G	C8-N9-C4	-5.18	104.33	106.40
26	BB	2731	G	C5'-C4'-O4'	5.18	115.32	109.10
26	BB	2735	G	C5'-C4'-O4'	5.18	115.32	109.10
26	BB	2780	G	N7-C8-N9	5.18	115.69	113.10
1	AA	126	G	N9-C1'-C2'	-5.18	106.30	112.00
1	AA	1154	G	C5'-C4'-O4'	5.18	115.32	109.10
1	AA	1484	C	O4'-C1'-N1	5.18	112.34	108.20
26	BB	430	A	C5'-C4'-O4'	5.18	115.32	109.10
26	BB	1174	U	O4'-C1'-N1	5.18	112.34	108.20
26	BB	1380	G	C8-N9-C4	-5.18	104.33	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	878	A	O4'-C1'-N9	5.18	112.34	108.20
1	AA	1461	G	C8-N9-C4	-5.18	104.33	106.40
26	BB	274	C	C5'-C4'-C3'	-5.18	107.71	116.00
26	BB	1622	G	C8-N9-C4	-5.18	104.33	106.40
26	BB	2369	A	O4'-C1'-N9	5.18	112.34	108.20
2	AB	71	G	C5'-C4'-O4'	5.18	115.31	109.10
26	BB	287	G	C8-N9-C4	-5.18	104.33	106.40
26	BB	681	G	C5'-C4'-O4'	5.18	115.31	109.10
26	BB	1763	G	O4'-C1'-C2'	-5.18	100.62	105.80
1	AA	1088	G	N3-C4-C5	-5.18	126.01	128.60
1	AA	1189	U	P-O3'-C3'	5.18	125.91	119.70
2	AB	22	G	N3-C4-C5	-5.18	126.01	128.60
26	BB	1392	A	C3'-C2'-C1'	5.18	105.64	101.50
26	BB	1913	A	C5'-C4'-C3'	-5.18	107.72	116.00
26	BB	2666	C	C4'-C3'-C2'	-5.18	97.42	102.60
1	AA	621	A	C5'-C4'-C3'	-5.17	107.72	116.00
1	AA	806	C	C5'-C4'-O4'	5.17	115.31	109.10
1	AA	1446	A	C5'-C4'-C3'	-5.17	107.72	116.00
25	BA	51	G	N1-C6-O6	-5.17	116.80	119.90
26	BB	305	C	C4'-C3'-C2'	-5.17	97.42	102.60
1	AA	1220	G	O4'-C1'-N9	5.17	112.34	108.20
25	BA	83	G	N3-C4-C5	-5.17	126.01	128.60
26	BB	2684	U	C3'-C2'-C1'	-5.17	97.36	101.50
1	AA	41	G	N3-C4-C5	-5.17	126.01	128.60
1	AA	628	G	N9-C1'-C2'	-5.17	106.31	112.00
1	AA	1053	G	P-O3'-C3'	5.17	125.91	119.70
1	AA	1268	G	C5'-C4'-O4'	5.17	115.31	109.10
26	BB	1651	G	N3-C4-C5	-5.17	126.01	128.60
26	BB	2145	C	O4'-C1'-N1	5.17	112.34	108.20
1	AA	247	G	C8-N9-C4	-5.17	104.33	106.40
1	AA	1438	G	O4'-C1'-N9	5.17	112.34	108.20
8	AI	156	ARG	NE-CZ-NH1	5.17	122.89	120.30
26	BB	670	A	C5'-C4'-C3'	-5.17	107.73	116.00
1	AA	282	A	C8-N9-C4	-5.17	103.73	105.80
1	AA	602	A	O4'-C1'-N9	5.17	112.33	108.20
1	AA	769	G	C5'-C4'-O4'	5.17	115.30	109.10
1	AA	1102	A	C5'-C4'-O4'	5.17	115.30	109.10
2	AB	10	G	N3-C4-C5	-5.17	126.02	128.60
26	BB	136	G	C5'-C4'-O4'	5.17	115.30	109.10
26	BB	343	C	P-O3'-C3'	5.17	125.90	119.70
26	BB	1782	U	O4'-C1'-N1	5.17	112.33	108.20
26	BB	1800	C	N1-C2-O2	5.17	122.00	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1838	C	N1-C2-O2	5.17	122.00	118.90
26	BB	2527	C	O4'-C1'-N1	5.17	112.33	108.20
1	AA	420	U	O4'-C1'-N1	5.17	112.33	108.20
1	AA	735	C	C5'-C4'-O4'	5.17	115.30	109.10
26	BB	650	C	C4'-C3'-C2'	-5.17	97.43	102.60
26	BB	1233	C	P-O3'-C3'	5.17	125.90	119.70
26	BB	1546	G	O3'-P-O5'	-5.17	94.19	104.00
1	AA	434	U	O4'-C1'-N1	5.17	112.33	108.20
2	AB	56	C	C3'-C2'-C1'	5.17	105.63	101.50
1	AA	888	G	O4'-C1'-N9	5.16	112.33	108.20
2	AB	62	C	O4'-C1'-N1	5.16	112.33	108.20
4	AD	30	U	C1'-O4'-C4'	-5.16	105.77	109.90
2	AE	74	C	O4'-C1'-C2'	-5.16	100.64	105.80
26	BB	82	U	O4'-C1'-N1	5.16	112.33	108.20
26	BB	1385	A	O4'-C4'-C3'	5.16	110.23	106.10
26	BB	1925	C	N1-C2-O2	5.16	122.00	118.90
1	AA	1195	C	N1-C2-O2	5.16	122.00	118.90
26	BB	282	A	O4'-C1'-N9	5.16	112.33	108.20
26	BB	425	G	O4'-C1'-N9	5.16	112.33	108.20
26	BB	1389	G	O4'-C1'-N9	5.16	112.33	108.20
26	BB	1493	C	O3'-P-O5'	-5.16	94.19	104.00
26	BB	1726	C	C5'-C4'-C3'	-5.16	107.74	116.00
26	BB	711	G	C8-N9-C4	-5.16	104.34	106.40
26	BB	1004	U	O4'-C1'-N1	5.16	112.33	108.20
26	BB	1502	A	O4'-C1'-N9	5.16	112.33	108.20
26	BB	1690	A	O4'-C1'-N9	5.16	112.33	108.20
1	AA	514	C	C4'-C3'-C2'	-5.16	97.44	102.60
1	AA	1310	G	C5'-C4'-C3'	-5.16	107.75	116.00
1	AA	1419	G	O4'-C1'-N9	5.16	112.33	108.20
1	AA	1508	A	C5'-C4'-O4'	5.16	115.29	109.10
26	BB	70	G	C5'-C4'-C3'	-5.16	107.75	116.00
26	BB	641	U	C5'-C4'-O4'	5.16	115.29	109.10
26	BB	1937	A	P-O3'-C3'	5.16	125.89	119.70
26	BB	2400	G	O4'-C1'-N9	5.16	112.33	108.20
26	BB	2722	G	C5'-C4'-O4'	5.16	115.29	109.10
25	BA	69	G	C5'-C4'-C3'	-5.16	107.75	116.00
25	BA	75	G	C8-N9-C4	-5.16	104.34	106.40
26	BB	1649	G	C8-N9-C4	-5.16	104.34	106.40
1	AA	682	G	C8-N9-C4	-5.16	104.34	106.40
26	BB	248	G	O4'-C1'-N9	5.16	112.32	108.20
1	AA	30	U	C3'-C2'-C1'	5.15	105.62	101.50
26	BB	2802	G	N9-C1'-C2'	-5.15	106.33	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	980	C	N1-C2-O2	5.15	121.99	118.90
25	BA	63	C	O4'-C1'-N1	5.15	112.32	108.20
26	BB	83	A	C8-N9-C4	-5.15	103.74	105.80
26	BB	130	C	O4'-C1'-N1	5.15	112.32	108.20
26	BB	1444	G	C8-N9-C4	-5.15	104.34	106.40
1	AA	1267	C	O4'-C1'-N1	5.15	112.32	108.20
1	AA	1333	A	C5'-C4'-O4'	5.15	115.28	109.10
26	BB	641	U	O4'-C1'-N1	5.15	112.32	108.20
26	BB	842	U	C5'-C4'-C3'	-5.15	107.76	116.00
26	BB	1501	G	C2-N3-C4	5.15	114.47	111.90
26	BB	1601	G	C5'-C4'-C3'	-5.15	107.76	116.00
26	BB	2175	C	O3'-P-O5'	-5.15	94.22	104.00
26	BB	2578	G	N3-C4-C5	-5.15	126.03	128.60
26	BB	2823	A	C8-N9-C4	-5.15	103.74	105.80
1	AA	568	G	C8-N9-C4	-5.15	104.34	106.40
26	BB	325	G	C8-N9-C4	-5.15	104.34	106.40
26	BB	615	U	O3'-P-O5'	-5.15	94.22	104.00
26	BB	1741	C	C5'-C4'-O4'	5.15	115.28	109.10
26	BB	1872	A	O4'-C1'-C2'	-5.15	100.65	105.80
26	BB	2790	U	C5'-C4'-C3'	-5.15	107.76	116.00
1	AA	1504	G	N3-C4-C5	-5.15	126.03	128.60
26	BB	16	C	C5'-C4'-C3'	-5.15	107.77	116.00
26	BB	2156	G	O4'-C1'-N9	5.15	112.32	108.20
26	BB	2337	G	N3-C4-C5	-5.15	126.03	128.60
26	BB	2103	C	O4'-C1'-N1	5.15	112.32	108.20
1	AA	505	G	N3-C4-C5	-5.14	126.03	128.60
1	AA	622	A	O4'-C1'-N9	5.14	112.32	108.20
1	AA	633	G	O4'-C1'-N9	5.14	112.32	108.20
1	AA	941	G	N3-C4-C5	-5.14	126.03	128.60
1	AA	1333	A	C8-N9-C4	-5.14	103.74	105.80
1	AA	1360	A	O4'-C1'-N9	5.14	112.31	108.20
2	AB	51	U	O4'-C1'-N1	5.14	112.32	108.20
26	BB	728	G	C8-N9-C4	-5.14	104.34	106.40
26	BB	1154	G	N3-C4-C5	-5.14	126.03	128.60
26	BB	1859	U	C5'-C4'-C3'	-5.14	107.77	116.00
26	BB	1916	A	C8-N9-C4	-5.14	103.74	105.80
26	BB	2506	U	O4'-C1'-C2'	-5.14	100.66	105.80
26	BB	2569	G	O4'-C1'-N9	5.14	112.31	108.20
2	AB	66	U	C5'-C4'-O4'	5.14	115.27	109.10
26	BB	121	G	N3-C4-C5	-5.14	126.03	128.60
26	BB	716	A	O4'-C1'-C2'	-5.14	100.66	105.80
26	BB	891	G	C8-N9-C4	-5.14	104.34	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1461	C	C1'-O4'-C4'	-5.14	105.79	109.90
26	BB	1647	U	P-O3'-C3'	5.14	125.87	119.70
26	BB	2823	A	C3'-C2'-C1'	5.14	105.61	101.50
26	BB	2892	G	O4'-C1'-N9	5.14	112.31	108.20
26	BB	275	C	O4'-C1'-N1	5.14	112.31	108.20
26	BB	1139	G	C8-N9-C4	-5.14	104.34	106.40
26	BB	2133	G	C8-N9-C4	-5.14	104.34	106.40
1	AA	479	U	O4'-C1'-N1	5.14	112.31	108.20
1	AA	774	G	O4'-C1'-N9	5.14	112.31	108.20
25	BA	80	U	O4'-C1'-N1	5.14	112.31	108.20
26	BB	1189	A	C5'-C4'-O4'	5.14	115.27	109.10
26	BB	2392	A	C8-N9-C4	-5.14	103.74	105.80
26	BB	1445	G	N3-C4-C5	-5.14	126.03	128.60
1	AA	435	A	C5'-C4'-O4'	5.14	115.26	109.10
1	AA	922	G	C8-N9-C4	-5.14	104.34	106.40
25	BA	102	G	C8-N9-C4	-5.14	104.34	106.40
26	BB	325	G	O4'-C1'-N9	5.14	112.31	108.20
26	BB	542	C	C5'-C4'-O4'	5.14	115.27	109.10
26	BB	652	U	C5'-C4'-C3'	-5.14	107.78	116.00
26	BB	1073	A	C5-C6-N6	-5.14	119.59	123.70
1	AA	194	C	C2'-C3'-O3'	5.13	121.92	113.70
1	AA	595	A	C8-N9-C4	-5.13	103.75	105.80
1	AA	678	U	C5'-C4'-O4'	5.13	115.26	109.10
1	AA	985	C	O4'-C1'-N1	5.13	112.31	108.20
1	AA	1140	C	O4'-C1'-N1	5.13	112.31	108.20
2	AB	72	C	O4'-C1'-N1	5.13	112.31	108.20
26	BB	1014	A	O4'-C1'-N9	5.13	112.31	108.20
26	BB	1371	G	C3'-C2'-C1'	5.13	105.61	101.50
26	BB	1386	C	O4'-C1'-N1	5.13	112.31	108.20
26	BB	2692	G	N3-C4-C5	-5.13	126.03	128.60
26	BB	2702	G	C5'-C4'-O4'	5.13	115.26	109.10
1	AA	954	G	C8-N9-C4	-5.13	104.35	106.40
1	AA	1077	G	C8-N9-C4	-5.13	104.35	106.40
1	AA	485	U	C1'-O4'-C4'	-5.13	105.80	109.90
1	AA	604	G	C3'-C2'-C1'	-5.13	97.39	101.50
1	AA	920	U	O4'-C1'-N1	5.13	112.31	108.20
1	AA	1142	G	C8-N9-C4	-5.13	104.35	106.40
26	BB	2382	G	N3-C4-C5	-5.13	126.03	128.60
26	BB	2544	G	C8-N9-C4	-5.13	104.35	106.40
26	BB	2668	G	O4'-C1'-N9	5.13	112.31	108.20
26	BB	878	A	O4'-C1'-N9	5.13	112.30	108.20
26	BB	1095	A	C4'-C3'-O3'	5.13	123.26	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2682	A	O4'-C1'-N9	5.13	112.30	108.20
1	AA	750	C	C5'-C4'-C3'	-5.13	107.79	116.00
26	BB	958	U	P-O3'-C3'	5.13	125.85	119.70
26	BB	980	A	C5'-C4'-C3'	-5.13	107.80	116.00
26	BB	1259	G	C8-N9-C4	-5.13	104.35	106.40
26	BB	2499	C	O4'-C1'-N1	5.13	112.30	108.20
1	AA	1342	C	P-O3'-C3'	5.13	125.85	119.70
1	AA	1451	U	O3'-P-O5'	-5.13	94.26	104.00
25	BA	43	C	C3'-C2'-C1'	5.13	105.60	101.50
26	BB	798	G	N9-C1'-C2'	-5.13	106.36	112.00
26	BB	2062	A	P-O3'-C3'	5.13	125.85	119.70
1	AA	183	C	N1-C2-O2	5.12	121.97	118.90
1	AA	1439	G	C8-N9-C4	-5.12	104.35	106.40
26	BB	544	C	O4'-C4'-C3'	5.12	110.20	106.10
26	BB	2031	A	O4'-C4'-C3'	5.12	110.20	106.10
26	BB	2883	A	C5'-C4'-O4'	5.12	115.25	109.10
1	AA	20	U	O4'-C1'-N1	5.12	112.30	108.20
26	BB	752	A	O4'-C1'-N9	5.12	112.30	108.20
26	BB	1625	C	C2'-C3'-O3'	5.12	121.89	113.70
1	AA	1173	U	C5'-C4'-O4'	5.12	115.24	109.10
26	BB	530	G	N3-C4-C5	-5.12	126.04	128.60
26	BB	712	G	N3-C4-C5	-5.12	126.04	128.60
26	BB	1936	A	O3'-P-O5'	5.12	113.73	104.00
1	AA	284	C	O4'-C1'-N1	5.12	112.30	108.20
1	AA	753	A	O4'-C1'-N9	5.12	112.30	108.20
1	AA	1255	G	N9-C4-C5	5.12	107.45	105.40
26	BB	278	A	O4'-C1'-N9	-5.12	104.11	108.20
26	BB	383	C	N1-C2-O2	5.12	121.97	118.90
26	BB	2676	C	C5'-C4'-O4'	5.12	115.24	109.10
1	AA	1265	C	C5'-C4'-O4'	5.12	115.24	109.10
26	BB	1223	G	C8-N9-C4	-5.12	104.35	106.40
26	BB	2067	G	O4'-C1'-N9	5.12	112.29	108.20
26	BB	2875	C	O3'-P-O5'	-5.12	94.28	104.00
1	AA	188	C	O3'-P-O5'	-5.12	94.28	104.00
26	BB	102	U	C3'-C2'-C1'	5.12	105.59	101.50
26	BB	1585	C	N1-C2-O2	5.12	121.97	118.90
26	BB	2027	G	C8-N9-C4	-5.12	104.35	106.40
26	BB	2462	C	N3-C2-O2	-5.12	118.32	121.90
1	AA	826	C	N3-C2-O2	-5.11	118.32	121.90
1	AA	1537	U	N3-C2-O2	-5.11	118.62	122.20
25	BA	72	G	C5'-C4'-O4'	5.11	115.24	109.10
26	BB	2256	G	N3-C4-C5	-5.11	126.04	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	65	A	O4'-C1'-C2'	-5.11	100.69	105.80
1	AA	690	G	C5'-C4'-C3'	-5.11	107.82	116.00
26	BB	1241	A	C8-N9-C4	-5.11	103.75	105.80
26	BB	1422	G	C5'-C4'-O4'	5.11	115.23	109.10
26	BB	1483	G	C5'-C4'-O4'	5.11	115.23	109.10
26	BB	1636	U	O4'-C1'-N1	5.11	112.29	108.20
1	AA	583	A	N1-C6-N6	-5.11	115.53	118.60
26	BB	1064	C	C2-N3-C4	-5.11	117.35	119.90
26	BB	2090	A	C4'-C3'-C2'	-5.11	97.49	102.60
26	BB	2106	U	O4'-C1'-N1	5.11	112.29	108.20
1	AA	827	U	C1'-O4'-C4'	-5.11	105.81	109.90
26	BB	277	G	C5'-C4'-C3'	-5.11	107.83	116.00
26	BB	2127	G	O4'-C4'-C3'	5.11	110.19	106.10
26	BB	2550	G	C5'-C4'-C3'	-5.11	107.83	116.00
1	AA	425	G	C8-N9-C4	-5.11	104.36	106.40
26	BB	363	G	N3-C4-C5	-5.11	126.05	128.60
1	AA	1358	U	C1'-O4'-C4'	-5.10	105.82	109.90
1	AA	144	G	N3-C4-C5	-5.10	126.05	128.60
1	AA	842	U	C5'-C4'-O4'	5.10	115.22	109.10
1	AA	1152	A	C1'-O4'-C4'	-5.10	105.82	109.90
1	AA	1428	A	N9-C1'-C2'	-5.10	106.39	112.00
26	BB	178	G	C8-N9-C4	-5.10	104.36	106.40
26	BB	1718	G	C8-N9-C4	-5.10	104.36	106.40
26	BB	1866	A	C8-N9-C4	-5.10	103.76	105.80
1	AA	1383	C	C5'-C4'-O4'	5.10	115.22	109.10
1	AA	811	C	C5'-C4'-C3'	-5.10	107.84	116.00
1	AA	1308	U	O4'-C1'-N1	5.10	112.28	108.20
26	BB	550	C	C2-N1-C1'	-5.10	113.19	118.80
26	BB	1105	U	C5'-C4'-O4'	5.10	115.22	109.10
26	BB	1648	U	N3-C2-O2	-5.10	118.63	122.20
26	BB	2073	C	C5'-C4'-O4'	5.10	115.22	109.10
26	BB	2444	G	C8-N9-C4	-5.10	104.36	106.40
1	AA	430	A	C5'-C4'-O4'	5.10	115.22	109.10
26	BB	440	C	C5'-C4'-O4'	5.10	115.22	109.10
26	BB	2061	G	P-O3'-C3'	5.10	125.82	119.70
1	AA	439	U	C2-N3-C4	-5.10	123.94	127.00
25	BA	58	A	P-O3'-C3'	5.10	125.81	119.70
26	BB	278	A	O3'-P-O5'	-5.10	94.32	104.00
26	BB	1569	A	C5'-C4'-C3'	-5.10	107.85	116.00
26	BB	1635	A	C5'-C4'-C3'	-5.10	107.85	116.00
1	AA	417	G	C8-N9-C4	-5.09	104.36	106.40
1	AA	628	G	N3-C4-C5	-5.09	126.05	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AR	58	ARG	NE-CZ-NH2	-5.09	117.75	120.30
26	BB	182	A	O4'-C1'-N9	5.09	112.28	108.20
26	BB	1962	5MC	P-O3'-C3'	5.09	125.81	119.70
1	AA	39	G	O4'-C1'-N9	5.09	112.28	108.20
26	BB	1112	G	C4'-C3'-C2'	-5.09	97.51	102.60
26	BB	1432	G	C8-N9-C4	-5.09	104.36	106.40
26	BB	2110	G	O4'-C4'-C3'	5.09	110.17	106.10
1	AA	357	G	C5'-C4'-C3'	-5.09	107.86	116.00
1	AA	644	U	C2-N3-C4	-5.09	123.94	127.00
1	AA	1219	A	O4'-C1'-N9	5.09	112.27	108.20
1	AA	1456	A	C8-N9-C4	-5.09	103.76	105.80
26	BB	871	U	C5'-C4'-C3'	-5.09	107.85	116.00
26	BB	1242	U	C6-N1-C2	-5.09	117.94	121.00
26	BB	2054	A	C3'-C2'-C1'	5.09	105.57	101.50
1	AA	41	G	O4'-C1'-N9	5.09	112.27	108.20
2	AE	19	G	N3-C4-C5	-5.09	126.06	128.60
26	BB	228	C	O4'-C1'-N1	5.09	112.27	108.20
26	BB	375	G	C8-N9-C4	-5.09	104.36	106.40
26	BB	1380	G	N3-C4-C5	-5.09	126.06	128.60
26	BB	1616	A	C1'-O4'-C4'	-5.09	105.83	109.90
26	BB	2885	G	O3'-P-O5'	-5.09	94.33	104.00
1	AA	577	G	N3-C4-C5	-5.09	126.06	128.60
1	AA	992	U	O4'-C1'-N1	5.09	112.27	108.20
18	AS	53	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	AA	1008	U	O4'-C1'-N1	5.09	112.27	108.20
25	BA	11	C	N1-C2-O2	5.09	121.95	118.90
26	BB	227	A	O3'-P-O5'	-5.09	94.34	104.00
26	BB	539	G	O4'-C1'-N9	5.09	112.27	108.20
26	BB	2365	G	C5'-C4'-O4'	5.09	115.20	109.10
26	BB	2502	G	N9-C4-C5	5.09	107.44	105.40
1	AA	945	G	N3-C4-C5	-5.08	126.06	128.60
26	BB	1585	C	C6-N1-C2	-5.08	118.27	120.30
26	BB	1988	G	C5'-C4'-O4'	5.08	115.20	109.10
26	BB	2238	G	C2-N3-C4	5.08	114.44	111.90
1	AA	449	G	C8-N9-C4	-5.08	104.37	106.40
1	AA	790	A	C5'-C4'-O4'	5.08	115.20	109.10
26	BB	2745	C	O4'-C1'-N1	5.08	112.27	108.20
1	AA	913	A	P-O3'-C3'	5.08	125.80	119.70
26	BB	41	C	O4'-C1'-N1	5.08	112.27	108.20
26	BB	258	G	C5'-C4'-O4'	5.08	115.20	109.10
26	BB	2093	G	N3-C4-C5	-5.08	126.06	128.60
25	BA	2	G	N3-C4-C5	-5.08	126.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	864	G	C8-N9-C1'	5.08	133.60	127.00
26	BB	1177	G	N7-C8-N9	5.08	115.64	113.10
1	AA	1225	A	O4'-C4'-C3'	5.08	110.16	106.10
2	AB	48	C	C3'-C2'-C1'	-5.08	97.44	101.50
26	BB	349	U	P-O3'-C3'	5.08	125.79	119.70
26	BB	1346	G	C8-N9-C4	-5.08	104.37	106.40
26	BB	1514	G	P-O3'-C3'	5.08	125.80	119.70
26	BB	1987	A	C5'-C4'-O4'	5.08	115.19	109.10
26	BB	489	G	N9-C1'-C2'	-5.08	106.42	112.00
26	BB	1416	G	C6-N1-C2	-5.08	122.05	125.10
26	BB	2253	G	O4'-C1'-N9	5.08	112.26	108.20
1	AA	734	G	C5'-C4'-O4'	5.08	115.19	109.10
1	AA	1065	U	O4'-C1'-N1	5.08	112.26	108.20
1	AA	1439	G	N3-C4-C5	-5.08	126.06	128.60
1	AA	1529	G	C8-N9-C4	-5.08	104.37	106.40
26	BB	370	G	N3-C4-C5	-5.08	126.06	128.60
26	BB	617	G	C8-N9-C4	-5.08	104.37	106.40
1	AA	981	U	C5'-C4'-O4'	5.07	115.19	109.10
1	AA	1029	U	P-O3'-C3'	5.07	125.79	119.70
26	BB	275	C	N1-C2-O2	5.07	121.94	118.90
26	BB	1551	A	C8-N9-C4	-5.07	103.77	105.80
2	AE	15	G	C8-N9-C4	-5.07	104.37	106.40
26	BB	377	G	C5'-C4'-C3'	-5.07	107.89	116.00
26	BB	2010	G	C5'-C4'-C3'	-5.07	107.89	116.00
1	AA	1070	U	C5'-C4'-C3'	-5.07	107.89	116.00
26	BB	807	U	C4'-C3'-C2'	-5.07	97.53	102.60
26	BB	1069	A	O3'-P-O5'	5.07	113.63	104.00
26	BB	2791	G	C5'-C4'-C3'	-5.07	107.89	116.00
1	AA	855	U	O4'-C1'-N1	5.07	112.25	108.20
26	BB	2225	A	O3'-P-O5'	5.07	113.63	104.00
1	AA	135	C	O4'-C1'-N1	5.07	112.25	108.20
1	AA	220	G	C2-N3-C4	5.07	114.43	111.90
2	AB	19	G	C8-N9-C4	-5.07	104.37	106.40
26	BB	155	A	N9-C1'-C2'	-5.07	106.43	112.00
26	BB	1439	A	C8-N9-C4	-5.07	103.77	105.80
26	BB	1479	G	N9-C1'-C2'	-5.07	106.42	112.00
26	BB	1725	U	C5'-C4'-C3'	-5.07	107.89	116.00
26	BB	1776	G	C8-N9-C4	-5.07	104.37	106.40
26	BB	2057	G	C5'-C4'-C3'	-5.07	107.89	116.00
1	AA	292	G	C4'-C3'-C2'	-5.07	97.53	102.60
1	AA	352	C	N1-C2-O2	5.07	121.94	118.90
1	AA	438	U	O4'-C1'-N1	5.07	112.25	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1036	A	C5'-C4'-O4'	5.07	115.18	109.10
1	AA	1461	G	N3-C4-C5	-5.07	126.07	128.60
26	BB	829	A	C4'-C3'-C2'	-5.07	97.53	102.60
26	BB	1142	A	P-O3'-C3'	5.07	125.78	119.70
26	BB	1451	C	P-O3'-C3'	5.07	125.78	119.70
1	AA	16	A	O4'-C1'-N9	5.06	112.25	108.20
1	AA	389	A	N9-C1'-C2'	-5.06	106.43	112.00
1	AA	550	G	N3-C4-C5	-5.06	126.07	128.60
1	AA	1174	G	N3-C4-C5	-5.06	126.07	128.60
26	BB	11	C	C1'-O4'-C4'	-5.06	105.85	109.90
26	BB	1483	G	C5'-C4'-C3'	-5.06	107.90	116.00
1	AA	352	C	O4'-C1'-N1	5.06	112.25	108.20
1	AA	942	G	P-O3'-C3'	5.06	125.77	119.70
1	AA	1467	C	N3-C2-O2	-5.06	118.36	121.90
26	BB	1016	G	N3-C2-N2	-5.06	116.36	119.90
2	AB	34	G	O4'-C1'-N9	5.06	112.25	108.20
26	BB	1140	C	C5'-C4'-O4'	5.06	115.17	109.10
25	BA	14	U	O4'-C4'-C3'	5.06	110.15	106.10
26	BB	503	A	P-O3'-C3'	5.06	125.77	119.70
26	BB	1973	G	N3-C4-C5	-5.06	126.07	128.60
26	BB	2201	G	N3-C4-C5	-5.06	126.07	128.60
26	BB	2366	A	C5'-C4'-C3'	-5.06	107.91	116.00
26	BB	2433	A	P-O3'-C3'	5.06	125.77	119.70
26	BB	577	G	O4'-C1'-N9	5.06	112.25	108.20
26	BB	2446	G	P-O3'-C3'	5.06	125.77	119.70
26	BB	2641	G	N3-C4-C5	-5.06	126.07	128.60
26	BB	2897	U	O4'-C1'-N1	5.06	112.24	108.20
1	AA	305	G	P-O3'-C3'	5.05	125.77	119.70
26	BB	780	G	C8-N9-C4	-5.05	104.38	106.40
26	BB	940	G	C5'-C4'-C3'	-5.05	107.91	116.00
26	BB	678	C	O4'-C1'-N1	5.05	112.24	108.20
1	AA	1078	U	C4-C5-C6	5.05	122.73	119.70
1	AA	1353	G	C5'-C4'-C3'	-5.05	107.92	116.00
26	BB	902	C	P-O5'-C5'	5.05	128.98	120.90
26	BB	1416	G	C8-N9-C4	-5.05	104.38	106.40
26	BB	2184	A	O4'-C1'-N9	5.05	112.24	108.20
1	AA	65	A	C8-N9-C4	-5.05	103.78	105.80
1	AA	333	U	O4'-C1'-N1	5.05	112.24	108.20
1	AA	470	C	C5'-C4'-O4'	5.05	115.16	109.10
1	AA	558	G	N3-C4-C5	-5.05	126.08	128.60
1	AA	1354	U	C5'-C4'-O4'	5.05	115.16	109.10
26	BB	458	G	C3'-C2'-C1'	-5.05	97.46	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1165	A	O4'-C1'-N9	5.05	112.24	108.20
26	BB	1987	A	O4'-C1'-N9	5.05	112.24	108.20
26	BB	2228	G	C8-N9-C4	-5.05	104.38	106.40
26	BB	2269	G	O4'-C1'-N9	5.05	112.24	108.20
26	BB	2394	C	C4'-C3'-C2'	-5.05	97.55	102.60
1	AA	1535	C	O4'-C1'-N1	5.05	112.24	108.20
2	AE	48	C	N1-C2-O2	5.05	121.93	118.90
26	BB	1252	G	C3'-C2'-C1'	5.05	105.54	101.50
26	BB	2534	A	O4'-C1'-N9	5.05	112.24	108.20
1	AA	2	A	O4'-C1'-N9	5.05	112.24	108.20
26	BB	1884	G	C8-N9-C4	-5.05	104.38	106.40
26	BB	1975	G	N9-C1'-C2'	-5.05	106.45	112.00
1	AA	990	C	C5'-C4'-O4'	5.04	115.15	109.10
25	BA	54	G	N7-C8-N9	5.04	115.62	113.10
26	BB	424	G	N3-C4-C5	-5.04	126.08	128.60
26	BB	791	C	P-O3'-C3'	5.04	125.75	119.70
26	BB	2490	G	C8-N9-C4	-5.04	104.38	106.40
1	AA	439	U	N1-C2-N3	5.04	117.93	114.90
26	BB	832	U	C5'-C4'-O4'	5.04	115.15	109.10
26	BB	1087	G	C8-N9-C4	-5.04	104.38	106.40
26	BB	1334	G	C5'-C4'-C3'	-5.04	107.93	116.00
26	BB	1929	G	C2-N3-C4	5.04	114.42	111.90
26	BB	1933	G	C4'-C3'-C2'	-5.04	97.56	102.60
1	AA	394	G	C5'-C4'-O4'	5.04	115.15	109.10
1	AA	830	G	O4'-C1'-N9	5.04	112.23	108.20
26	BB	1636	U	C5'-C4'-O4'	5.04	115.15	109.10
26	BB	2523	G	N3-C4-C5	-5.04	126.08	128.60
26	BB	2579	C	C3'-C2'-C1'	5.04	105.53	101.50
1	AA	660	C	O4'-C1'-N1	5.04	112.23	108.20
2	AB	57	G	N3-C4-C5	-5.04	126.08	128.60
26	BB	863	A	N7-C8-N9	5.04	116.32	113.80
26	BB	2169	A	C8-N9-C4	-5.04	103.78	105.80
1	AA	152	A	O4'-C1'-N9	5.04	112.23	108.20
1	AA	570	G	C8-N9-C4	-5.04	104.38	106.40
1	AA	1124	G	C8-N9-C4	-5.04	104.39	106.40
1	AA	1208	C	C5'-C4'-C3'	-5.04	107.94	116.00
2	AE	53	G	N3-C4-C5	-5.04	126.08	128.60
25	BA	32	U	C3'-C2'-C1'	-5.04	97.47	101.50
26	BB	266	G	N3-C4-C5	-5.04	126.08	128.60
26	BB	271	G	P-O3'-C3'	5.04	125.75	119.70
26	BB	1049	C	C2'-C3'-O3'	5.04	121.76	113.70
26	BB	1267	U	C5'-C4'-O4'	5.04	115.15	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2061	G	C4'-C3'-C2'	-5.04	97.56	102.60
4	AD	47	C	N1-C2-O2	5.04	121.92	118.90
26	BB	121	G	C5'-C4'-C3'	-5.04	107.94	116.00
26	BB	1339	G	C8-N9-C4	-5.04	104.39	106.40
26	BB	1576	U	O4'-C1'-N1	5.04	112.23	108.20
26	BB	2429	G	N3-C4-C5	-5.04	126.08	128.60
26	BB	2871	U	O4'-C1'-N1	5.04	112.23	108.20
1	AA	429	U	C5'-C4'-C3'	-5.03	107.94	116.00
1	AA	515	G	N3-C4-C5	-5.03	126.08	128.60
1	AA	973	G	C5'-C4'-O4'	5.03	115.14	109.10
1	AA	1087	G	N3-C4-C5	-5.03	126.08	128.60
26	BB	996	A	C5'-C4'-C3'	-5.03	107.95	116.00
1	AA	744	C	O4'-C1'-N1	5.03	112.22	108.20
1	AA	1253	G	O4'-C1'-N9	5.03	112.22	108.20
2	AB	5	G	N3-C4-C5	-5.03	126.08	128.60
25	BA	14	U	P-O3'-C3'	-5.03	113.66	119.70
26	BB	254	G	C2-N3-C4	5.03	114.42	111.90
26	BB	369	U	O4'-C1'-N1	5.03	112.22	108.20
26	BB	1498	C	C5'-C4'-O4'	5.03	115.14	109.10
26	BB	2017	U	P-O3'-C3'	5.03	125.74	119.70
26	BB	2709	G	C5'-C4'-C3'	-5.03	107.95	116.00
26	BB	2831	G	O3'-P-O5'	-5.03	94.44	104.00
26	BB	2867	G	O4'-C1'-N9	5.03	112.22	108.20
1	AA	384	G	N3-C4-C5	-5.03	126.09	128.60
26	BB	364	C	C4'-C3'-C2'	-5.03	97.57	102.60
26	BB	2083	G	C8-N9-C4	-5.03	104.39	106.40
1	AA	1473	G	N3-C4-C5	-5.03	126.09	128.60
2	AE	28	G	O4'-C1'-N9	5.03	112.22	108.20
26	BB	763	G	C8-N9-C4	-5.03	104.39	106.40
26	BB	1869	G	O5'-C5'-C4'	-5.03	102.15	111.70
26	BB	2227	A	O4'-C1'-N9	5.03	112.22	108.20
1	AA	1006	G	N3-C4-C5	-5.03	126.09	128.60
26	BB	1	G	N3-C4-C5	-5.03	126.09	128.60
26	BB	1452	G	C3'-C2'-C1'	5.03	105.52	101.50
26	BB	1558	C	O4'-C1'-N1	5.03	112.22	108.20
26	BB	1725	U	C5'-C4'-O4'	5.03	115.13	109.10
26	BB	1837	C	P-O3'-C3'	5.03	125.73	119.70
26	BB	2694	G	O4'-C1'-N9	5.03	112.22	108.20
1	AA	297	G	O4'-C1'-N9	5.02	112.22	108.20
1	AA	781	A	C5'-C4'-O4'	5.02	115.13	109.10
1	AA	1405	G	N3-C4-C5	-5.02	126.09	128.60
26	BB	814	C	O4'-C1'-N1	5.02	112.22	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1171	G	N3-C4-C5	-5.02	126.09	128.60
1	AA	969	A	C4'-C3'-C2'	-5.02	97.58	102.60
2	AE	11	C	C5'-C4'-O4'	5.02	115.13	109.10
26	BB	890	C	O4'-C1'-N1	5.02	112.22	108.20
26	BB	1619	G	C5'-C4'-C3'	-5.02	107.97	116.00
26	BB	2749	A	O3'-P-O5'	-5.02	94.46	104.00
25	BA	75	G	O4'-C1'-N9	5.02	112.22	108.20
26	BB	14	A	C5'-C4'-C3'	-5.02	107.97	116.00
26	BB	1907	G	N9-C1'-C2'	-5.02	106.48	112.00
1	AA	1224	U	O3'-P-O5'	-5.02	94.46	104.00
1	AA	1383	C	C2-N3-C4	5.02	122.41	119.90
2	AB	1	G	N3-C4-C5	-5.02	126.09	128.60
2	AE	57	G	C8-N9-C4	-5.02	104.39	106.40
25	BA	32	U	N1-C2-N3	5.02	117.91	114.90
26	BB	521	U	O4'-C1'-N1	5.02	112.22	108.20
26	BB	708	G	C8-N9-C4	-5.02	104.39	106.40
26	BB	1377	G	C8-N9-C4	-5.02	104.39	106.40
1	AA	1010	U	C2-N3-C4	-5.02	123.99	127.00
26	BB	725	G	C2'-C3'-O3'	5.02	121.73	113.70
26	BB	1266	G	N9-C4-C5	5.02	107.41	105.40
26	BB	1345	C	C5'-C4'-C3'	-5.02	107.97	116.00
26	BB	898	C	O4'-C1'-N1	5.02	112.21	108.20
26	BB	1058	U	N1-C2-N3	5.02	117.91	114.90
26	BB	1064	C	C5-C4-N4	-5.02	116.69	120.20
26	BB	1123	C	C5'-C4'-O4'	5.02	115.12	109.10
26	BB	1314	C	C5'-C4'-O4'	5.02	115.12	109.10
1	AA	410	G	C8-N9-C4	-5.01	104.39	106.40
1	AA	692	U	N3-C2-O2	-5.01	118.69	122.20
1	AA	846	G	N3-C4-C5	-5.01	126.09	128.60
1	AA	1264	U	C4'-C3'-C2'	-5.01	97.58	102.60
2	AE	38	A	O4'-C1'-N9	5.01	112.21	108.20
25	BA	49	C	N1-C2-O2	5.01	121.91	118.90
26	BB	363	G	C8-N9-C4	-5.01	104.39	106.40
26	BB	474	G	O4'-C1'-N9	5.01	112.21	108.20
26	BB	2148	G	C8-N9-C4	-5.01	104.39	106.40
26	BB	2296	U	O4'-C4'-C3'	5.01	110.11	106.10
26	BB	2604	U	O4'-C1'-N1	5.01	112.21	108.20
26	BB	2625	G	C8-N9-C4	-5.01	104.39	106.40
26	BB	1139	G	N3-C4-C5	-5.01	126.09	128.60
26	BB	2802	G	C5'-C4'-C3'	-5.01	107.98	116.00
1	AA	930	C	C5'-C4'-O4'	5.01	115.11	109.10
1	AA	1199	U	O4'-C1'-N1	5.01	112.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	1274	A	P-O3'-C3'	5.01	125.71	119.70
26	BB	1936	A	P-O3'-C3'	5.01	125.71	119.70
26	BB	2177	C	N1-C2-O2	5.01	121.91	118.90
26	BB	2859	G	P-O3'-C3'	5.01	125.71	119.70
1	AA	761	G	O4'-C1'-N9	5.01	112.21	108.20
1	AA	1047	G	C8-N9-C4	-5.01	104.40	106.40
1	AA	1229	A	O4'-C1'-N9	5.01	112.21	108.20
25	BA	67	G	C8-N9-C4	-5.01	104.40	106.40
26	BB	1864	U	C3'-C2'-C1'	5.01	105.51	101.50
26	BB	2517	C	N1-C2-O2	5.01	121.91	118.90
26	BB	2642	G	N3-C4-C5	-5.01	126.10	128.60
2	AB	11	C	O4'-C1'-N1	5.01	112.21	108.20
26	BB	1420	A	C8-N9-C4	-5.01	103.80	105.80
1	AA	734	G	N3-C4-C5	-5.01	126.10	128.60
2	AE	6	G	C5'-C4'-O4'	5.01	115.11	109.10
26	BB	2328	A	O3'-P-O5'	-5.01	94.49	104.00
1	AA	1354	U	O4'-C1'-N1	5.00	112.20	108.20
26	BB	1191	G	N3-C4-C5	-5.00	126.10	128.60
1	AA	142	G	C5'-C4'-C3'	-5.00	108.00	116.00
1	AA	344	A	C5'-C4'-O4'	5.00	115.10	109.10
26	BB	51	G	O4'-C1'-N9	5.00	112.20	108.20
26	BB	1503	A	O4'-C1'-N9	5.00	112.20	108.20
26	BB	1988	G	O4'-C1'-N9	5.00	112.20	108.20
1	AA	164	G	N3-C4-C5	-5.00	126.10	128.60
26	BB	172	A	N9-C1'-C2'	-5.00	106.50	112.00
26	BB	1420	A	O3'-P-O5'	-5.00	94.50	104.00

There are no chirality outliers.

All (1567) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	10	A	Sidechain
1	AA	100	G	Sidechain
1	AA	1008	U	Sidechain
1	AA	1009	U	Sidechain
1	AA	1010	U	Sidechain
1	AA	1013	G	Sidechain
1	AA	1014	A	Sidechain
1	AA	1016	A	Sidechain
1	AA	1026	G	Sidechain
1	AA	1027	C	Sidechain
1	AA	103	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1035	A	Sidechain
1	AA	1037	C	Sidechain
1	AA	1039	G	Sidechain
1	AA	1046	A	Sidechain
1	AA	1049	U	Sidechain
1	AA	105	G	Sidechain
1	AA	1054	C	Sidechain
1	AA	1055	A	Sidechain
1	AA	1058	G	Sidechain
1	AA	106	C	Sidechain
1	AA	1061	G	Sidechain
1	AA	1062	U	Sidechain
1	AA	1072	G	Sidechain
1	AA	1073	U	Sidechain
1	AA	1074	G	Sidechain
1	AA	1075	U	Sidechain
1	AA	1077	G	Sidechain
1	AA	1093	A	Sidechain
1	AA	1094	G	Sidechain
1	AA	1096	C	Sidechain
1	AA	1097	C	Sidechain
1	AA	11	G	Sidechain
1	AA	110	C	Sidechain
1	AA	1100	C	Sidechain
1	AA	1101	A	Sidechain
1	AA	1109	C	Sidechain
1	AA	1110	A	Sidechain
1	AA	1114	C	Sidechain
1	AA	1115	U	Sidechain
1	AA	1117	A	Sidechain
1	AA	1119	C	Sidechain
1	AA	112	G	Sidechain
1	AA	1121	U	Sidechain
1	AA	1124	G	Sidechain
1	AA	1125	U	Sidechain
1	AA	1126	U	Sidechain
1	AA	1127	G	Sidechain
1	AA	113	G	Sidechain
1	AA	1130	A	Sidechain
1	AA	1132	C	Sidechain
1	AA	1134	G	Sidechain
1	AA	1135	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1138	G	Sidechain
1	AA	1139	G	Sidechain
1	AA	1140	C	Sidechain
1	AA	1142	G	Sidechain
1	AA	1143	G	Sidechain
1	AA	1145	A	Sidechain
1	AA	1148	U	Sidechain
1	AA	1151	A	Sidechain
1	AA	1153	G	Sidechain
1	AA	1155	A	Sidechain
1	AA	1158	C	Sidechain
1	AA	116	A	Sidechain
1	AA	1160	G	Sidechain
1	AA	1162	C	Sidechain
1	AA	1169	A	Sidechain
1	AA	117	G	Sidechain
1	AA	1174	G	Sidechain
1	AA	1175	G	Sidechain
1	AA	1176	A	Sidechain
1	AA	1178	G	Sidechain
1	AA	1179	A	Sidechain
1	AA	1181	G	Sidechain
1	AA	1184	G	Sidechain
1	AA	119	A	Sidechain
1	AA	1196	A	Sidechain
1	AA	1197	A	Sidechain
1	AA	1201	A	Sidechain
1	AA	1202	U	Sidechain
1	AA	1212	U	Sidechain
1	AA	1213	A	Sidechain
1	AA	1214	C	Sidechain
1	AA	1215	G	Sidechain
1	AA	1216	A	Sidechain
1	AA	1219	A	Sidechain
1	AA	1222	G	Sidechain
1	AA	1226	C	Sidechain
1	AA	1228	C	Sidechain
1	AA	1230	C	Sidechain
1	AA	1233	G	Sidechain
1	AA	1234	C	Sidechain
1	AA	1237	C	Sidechain
1	AA	1249	C	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1250	A	Sidechain
1	AA	1258	G	Sidechain
1	AA	1259	C	Sidechain
1	AA	126	G	Sidechain
1	AA	1260	G	Sidechain
1	AA	1266	G	Sidechain
1	AA	1267	C	Sidechain
1	AA	1268	G	Sidechain
1	AA	1269	A	Sidechain
1	AA	1270	G	Sidechain
1	AA	1272	G	Sidechain
1	AA	1274	A	Sidechain
1	AA	1276	G	Sidechain
1	AA	128	G	Sidechain
1	AA	1284	C	Sidechain
1	AA	1289	A	Sidechain
1	AA	1294	G	Sidechain
1	AA	1298	U	Sidechain
1	AA	13	U	Sidechain
1	AA	1301	U	Sidechain
1	AA	1305	G	Sidechain
1	AA	1307	U	Sidechain
1	AA	1313	U	Sidechain
1	AA	1314	C	Sidechain
1	AA	1317	C	Sidechain
1	AA	1318	A	Sidechain
1	AA	1319	A	Sidechain
1	AA	1322	C	Sidechain
1	AA	1323	G	Sidechain
1	AA	1325	C	Sidechain
1	AA	1328	C	Sidechain
1	AA	1330	U	Sidechain
1	AA	1333	A	Sidechain
1	AA	1337	G	Sidechain
1	AA	1339	A	Sidechain
1	AA	1343	G	Sidechain
1	AA	1346	A	Sidechain
1	AA	1351	U	Sidechain
1	AA	1357	A	Sidechain
1	AA	1358	U	Sidechain
1	AA	1361	G	Sidechain
1	AA	1363	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1364	U	Sidechain
1	AA	1369	C	Sidechain
1	AA	137	U	Sidechain
1	AA	1370	G	Sidechain
1	AA	1371	G	Sidechain
1	AA	1373	G	Sidechain
1	AA	1376	U	Sidechain
1	AA	1377	A	Sidechain
1	AA	1378	C	Sidechain
1	AA	138	G	Sidechain
1	AA	1380	U	Sidechain
1	AA	1390	U	Sidechain
1	AA	1391	U	Sidechain
1	AA	1392	G	Sidechain
1	AA	1400	C	Sidechain
1	AA	1405	G	Sidechain
1	AA	1406	U	Sidechain
1	AA	1412	C	Sidechain
1	AA	1416	G	Sidechain
1	AA	1417	G	Sidechain
1	AA	142	G	Sidechain
1	AA	1424	U	Sidechain
1	AA	1429	A	Sidechain
1	AA	143	A	Sidechain
1	AA	1432	G	Sidechain
1	AA	1433	A	Sidechain
1	AA	1435	G	Sidechain
1	AA	144	G	Sidechain
1	AA	1440	U	Sidechain
1	AA	1444	U	Sidechain
1	AA	1447	A	Sidechain
1	AA	1450	U	Sidechain
1	AA	1455	G	Sidechain
1	AA	1456	A	Sidechain
1	AA	1457	G	Sidechain
1	AA	1459	G	Sidechain
1	AA	1464	U	Sidechain
1	AA	1465	A	Sidechain
1	AA	1470	U	Sidechain
1	AA	1477	U	Sidechain
1	AA	1479	C	Sidechain
1	AA	1482	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1483	A	Sidechain
1	AA	1491	G	Sidechain
1	AA	1493	A	Sidechain
1	AA	150	U	Sidechain
1	AA	1500	A	Sidechain
1	AA	1501	C	Sidechain
1	AA	1502	A	Sidechain
1	AA	1506	U	Sidechain
1	AA	1517	G	Sidechain
1	AA	152	A	Sidechain
1	AA	1521	C	Sidechain
1	AA	1523	G	Sidechain
1	AA	1526	G	Sidechain
1	AA	153	C	Sidechain
1	AA	1530	G	Sidechain
1	AA	1531	A	Sidechain
1	AA	1534	A	Sidechain
1	AA	1535	C	Sidechain
1	AA	1536	C	Sidechain
1	AA	1537	U	Sidechain
1	AA	1539	C	Sidechain
1	AA	1540	U	Sidechain
1	AA	159	G	Sidechain
1	AA	163	C	Sidechain
1	AA	173	U	Sidechain
1	AA	179	A	Sidechain
1	AA	182	A	Sidechain
1	AA	184	G	Sidechain
1	AA	189	A	Sidechain
1	AA	190	A	Sidechain
1	AA	194	C	Sidechain
1	AA	196	A	Sidechain
1	AA	197	A	Sidechain
1	AA	2	A	Sidechain
1	AA	201	G	Sidechain
1	AA	203	G	Sidechain
1	AA	205	A	Sidechain
1	AA	206	C	Sidechain
1	AA	21	G	Sidechain
1	AA	211	G	Sidechain
1	AA	215	C	Sidechain
1	AA	218	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	22	G	Sidechain
1	AA	221	C	Sidechain
1	AA	222	C	Sidechain
1	AA	223	A	Sidechain
1	AA	229	U	Sidechain
1	AA	234	C	Sidechain
1	AA	236	A	Sidechain
1	AA	239	U	Sidechain
1	AA	24	U	Sidechain
1	AA	245	U	Sidechain
1	AA	246	A	Sidechain
1	AA	248	C	Sidechain
1	AA	250	A	Sidechain
1	AA	252	U	Sidechain
1	AA	256	U	Sidechain
1	AA	260	G	Sidechain
1	AA	262	A	Sidechain
1	AA	265	G	Sidechain
1	AA	266	G	Sidechain
1	AA	268	U	Sidechain
1	AA	269	C	Sidechain
1	AA	27	G	Sidechain
1	AA	274	A	Sidechain
1	AA	279	A	Sidechain
1	AA	283	U	Sidechain
1	AA	29	U	Sidechain
1	AA	297	G	Sidechain
1	AA	298	A	Sidechain
1	AA	299	G	Sidechain
1	AA	305	G	Sidechain
1	AA	306	A	Sidechain
1	AA	307	C	Sidechain
1	AA	31	G	Sidechain
1	AA	310	G	Sidechain
1	AA	311	C	Sidechain
1	AA	313	A	Sidechain
1	AA	315	A	Sidechain
1	AA	316	C	Sidechain
1	AA	323	U	Sidechain
1	AA	325	A	Sidechain
1	AA	328	C	Sidechain
1	AA	329	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	33	A	Sidechain
1	AA	330	C	Sidechain
1	AA	331	G	Sidechain
1	AA	335	C	Sidechain
1	AA	336	A	Sidechain
1	AA	337	G	Sidechain
1	AA	342	C	Sidechain
1	AA	346	G	Sidechain
1	AA	347	G	Sidechain
1	AA	349	A	Sidechain
1	AA	350	G	Sidechain
1	AA	353	A	Sidechain
1	AA	354	G	Sidechain
1	AA	359	G	Sidechain
1	AA	360	G	Sidechain
1	AA	362	G	Sidechain
1	AA	363	A	Sidechain
1	AA	365	U	Sidechain
1	AA	368	U	Sidechain
1	AA	370	C	Sidechain
1	AA	380	G	Sidechain
1	AA	381	C	Sidechain
1	AA	382	A	Sidechain
1	AA	383	A	Sidechain
1	AA	387	U	Sidechain
1	AA	388	G	Sidechain
1	AA	39	G	Sidechain
1	AA	391	G	Sidechain
1	AA	393	A	Sidechain
1	AA	396	C	Sidechain
1	AA	398	U	Sidechain
1	AA	399	G	Sidechain
1	AA	403	C	Sidechain
1	AA	412	A	Sidechain
1	AA	413	G	Sidechain
1	AA	414	A	Sidechain
1	AA	417	G	Sidechain
1	AA	425	G	Sidechain
1	AA	43	C	Sidechain
1	AA	430	A	Sidechain
1	AA	431	A	Sidechain
1	AA	439	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	444	G	Sidechain
1	AA	446	G	Sidechain
1	AA	447	G	Sidechain
1	AA	448	A	Sidechain
1	AA	451	A	Sidechain
1	AA	452	A	Sidechain
1	AA	456	A	Sidechain
1	AA	457	G	Sidechain
1	AA	459	A	Sidechain
1	AA	46	G	Sidechain
1	AA	465	A	Sidechain
1	AA	466	A	Sidechain
1	AA	467	U	Sidechain
1	AA	469	C	Sidechain
1	AA	474	G	Sidechain
1	AA	476	U	Sidechain
1	AA	477	C	Sidechain
1	AA	478	A	Sidechain
1	AA	479	U	Sidechain
1	AA	480	U	Sidechain
1	AA	481	G	Sidechain
1	AA	485	U	Sidechain
1	AA	487	A	Sidechain
1	AA	491	G	Sidechain
1	AA	492	C	Sidechain
1	AA	493	A	Sidechain
1	AA	496	A	Sidechain
1	AA	499	A	Sidechain
1	AA	50	A	Sidechain
1	AA	505	G	Sidechain
1	AA	507	C	Sidechain
1	AA	510	A	Sidechain
1	AA	511	C	Sidechain
1	AA	519	C	Sidechain
1	AA	52	C	Sidechain
1	AA	521	G	Sidechain
1	AA	523	A	Sidechain
1	AA	525	C	Sidechain
1	AA	526	C	Sidechain
1	AA	529	G	Sidechain
1	AA	530	G	Sidechain
1	AA	533	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	535	A	Sidechain
1	AA	536	C	Sidechain
1	AA	545	C	Sidechain
1	AA	546	A	Sidechain
1	AA	556	C	Sidechain
1	AA	565	U	Sidechain
1	AA	57	G	Sidechain
1	AA	572	A	Sidechain
1	AA	574	A	Sidechain
1	AA	576	C	Sidechain
1	AA	577	G	Sidechain
1	AA	578	C	Sidechain
1	AA	583	A	Sidechain
1	AA	587	G	Sidechain
1	AA	594	U	Sidechain
1	AA	597	G	Sidechain
1	AA	60	A	Sidechain
1	AA	608	A	Sidechain
1	AA	609	A	Sidechain
1	AA	61	G	Sidechain
1	AA	610	U	Sidechain
1	AA	612	C	Sidechain
1	AA	613	C	Sidechain
1	AA	618	C	Sidechain
1	AA	631	C	Sidechain
1	AA	637	C	Sidechain
1	AA	639	G	Sidechain
1	AA	641	U	Sidechain
1	AA	642	A	Sidechain
1	AA	644	U	Sidechain
1	AA	646	G	Sidechain
1	AA	647	C	Sidechain
1	AA	65	A	Sidechain
1	AA	652	U	Sidechain
1	AA	66	A	Sidechain
1	AA	660	C	Sidechain
1	AA	661	G	Sidechain
1	AA	672	U	Sidechain
1	AA	673	A	Sidechain
1	AA	680	C	Sidechain
1	AA	682	G	Sidechain
1	AA	684	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	686	U	Sidechain
1	AA	688	G	Sidechain
1	AA	69	G	Sidechain
1	AA	690	G	Sidechain
1	AA	692	U	Sidechain
1	AA	693	G	Sidechain
1	AA	694	A	Sidechain
1	AA	695	A	Sidechain
1	AA	697	U	Sidechain
1	AA	7	A	Sidechain
1	AA	704	A	Sidechain
1	AA	709	U	Sidechain
1	AA	71	A	Sidechain
1	AA	711	G	Sidechain
1	AA	713	G	Sidechain
1	AA	719	C	Sidechain
1	AA	723	U	Sidechain
1	AA	73	C	Sidechain
1	AA	737	C	Sidechain
1	AA	748	G	Sidechain
1	AA	751	U	Sidechain
1	AA	752	G	Sidechain
1	AA	754	C	Sidechain
1	AA	757	U	Sidechain
1	AA	76	G	Sidechain
1	AA	762	U	Sidechain
1	AA	763	G	Sidechain
1	AA	765	G	Sidechain
1	AA	767	A	Sidechain
1	AA	771	G	Sidechain
1	AA	774	G	Sidechain
1	AA	775	G	Sidechain
1	AA	779	C	Sidechain
1	AA	786	G	Sidechain
1	AA	787	A	Sidechain
1	AA	789	U	Sidechain
1	AA	790	A	Sidechain
1	AA	793	U	Sidechain
1	AA	800	G	Sidechain
1	AA	801	U	Sidechain
1	AA	802	A	Sidechain
1	AA	804	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	808	C	Sidechain
1	AA	817	C	Sidechain
1	AA	820	U	Sidechain
1	AA	826	C	Sidechain
1	AA	827	U	Sidechain
1	AA	836	G	Sidechain
1	AA	838	G	Sidechain
1	AA	84	U	Sidechain
1	AA	840	C	Sidechain
1	AA	841	C	Sidechain
1	AA	846	G	Sidechain
1	AA	847	G	Sidechain
1	AA	849	G	Sidechain
1	AA	85	U	Sidechain
1	AA	851	G	Sidechain
1	AA	855	U	Sidechain
1	AA	858	G	Sidechain
1	AA	86	G	Sidechain
1	AA	864	A	Sidechain
1	AA	866	C	Sidechain
1	AA	870	U	Sidechain
1	AA	873	A	Sidechain
1	AA	874	G	Sidechain
1	AA	876	C	Sidechain
1	AA	879	C	Sidechain
1	AA	880	C	Sidechain
1	AA	884	U	Sidechain
1	AA	888	G	Sidechain
1	AA	89	U	Sidechain
1	AA	900	A	Sidechain
1	AA	901	A	Sidechain
1	AA	902	G	Sidechain
1	AA	905	U	Sidechain
1	AA	908	A	Sidechain
1	AA	91	U	Sidechain
1	AA	916	U	Sidechain
1	AA	92	U	Sidechain
1	AA	920	U	Sidechain
1	AA	922	G	Sidechain
1	AA	923	A	Sidechain
1	AA	928	G	Sidechain
1	AA	932	C	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	933	G	Sidechain
1	AA	934	C	Sidechain
1	AA	936	C	Sidechain
1	AA	937	A	Sidechain
1	AA	938	A	Sidechain
1	AA	94	G	Sidechain
1	AA	944	G	Sidechain
1	AA	946	A	Sidechain
1	AA	948	C	Sidechain
1	AA	949	A	Sidechain
1	AA	951	G	Sidechain
1	AA	952	U	Sidechain
1	AA	953	G	Sidechain
1	AA	954	G	Sidechain
1	AA	958	A	Sidechain
1	AA	959	A	Sidechain
1	AA	970	C	Sidechain
1	AA	972	C	Sidechain
1	AA	973	G	Sidechain
1	AA	977	A	Sidechain
1	AA	978	A	Sidechain
1	AA	980	C	Sidechain
1	AA	983	A	Sidechain
1	AA	984	C	Sidechain
1	AA	99	C	Sidechain
1	AA	991	U	Sidechain
1	AA	992	U	Sidechain
1	AA	993	G	Sidechain
1	AA	995	C	Sidechain
2	AB	10	G	Sidechain
2	AB	17	C	Sidechain
2	AB	23	A	Sidechain
2	AB	26	A	Sidechain
2	AB	27	G	Sidechain
2	AB	34	G	Sidechain
2	AB	40	C	Sidechain
2	AB	41	C	Sidechain
2	AB	42	C	Sidechain
2	AB	5	G	Sidechain
2	AB	51	U	Sidechain
2	AB	56	C	Sidechain
2	AB	58	A	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	60	U	Sidechain
2	AB	66	U	Sidechain
2	AB	68	C	Sidechain
2	AB	70	G	Sidechain
2	AB	71	G	Sidechain
2	AB	75	C	Sidechain
3	AC	10	PRO	Mainchain
4	AD	25	U	Sidechain
4	AD	26	U	Sidechain
4	AD	28	U	Sidechain
4	AD	29	G	Sidechain
4	AD	30	U	Sidechain
4	AD	31	U	Sidechain
4	AD	34	U	Sidechain
4	AD	43	U	Sidechain
4	AD	45	G	Sidechain
2	AE	14	A	Sidechain
2	AE	19	G	Sidechain
2	AE	21	A	Sidechain
2	AE	25	C	Sidechain
2	AE	34	G	Sidechain
2	AE	35	A	Sidechain
2	AE	44	G	Sidechain
2	AE	48	C	Sidechain
2	AE	50	U	Sidechain
2	AE	56	C	Sidechain
2	AE	6	G	Sidechain
2	AE	63	G	Sidechain
2	AE	67	C	Sidechain
2	AE	75	C	Sidechain
2	AE	9	A	Sidechain
6	AG	229	LYS	Mainchain
7	AH	102	TYR	Sidechain
8	AI	146	MET	Mainchain
8	AI	157	GLY	Peptide
8	AI	161	GLU	Mainchain
9	AJ	87	SER	Peptide
11	AL	92	PRO	Peptide
13	AN	40	ILE	Mainchain
14	AO	81	LEU	Peptide
15	AP	120	ARG	Peptide
17	AR	38	GLU	Mainchain

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Mol	Chain	Res	Type	Group
17	AR	98	ALA	Mainchain
21	AV	63	TYR	Sidechain
24	AY	48	LYS	Mainchain
25	BA	10	G	Sidechain
25	BA	110	C	Sidechain
25	BA	114	C	Sidechain
25	BA	116	G	Sidechain
25	BA	117	G	Sidechain
25	BA	14	U	Sidechain
25	BA	15	A	Sidechain
25	BA	19	C	Sidechain
25	BA	2	G	Sidechain
25	BA	20	G	Sidechain
25	BA	23	G	Sidechain
25	BA	24	G	Sidechain
25	BA	26	C	Sidechain
25	BA	34	A	Sidechain
25	BA	35	C	Sidechain
25	BA	36	C	Sidechain
25	BA	37	C	Sidechain
25	BA	41	G	Sidechain
25	BA	47	C	Sidechain
25	BA	50	A	Sidechain
25	BA	51	G	Sidechain
25	BA	52	A	Sidechain
25	BA	55	U	Sidechain
25	BA	57	A	Sidechain
25	BA	58	A	Sidechain
25	BA	6	G	Sidechain
25	BA	61	G	Sidechain
25	BA	64	G	Sidechain
25	BA	67	G	Sidechain
25	BA	68	C	Sidechain
25	BA	7	G	Sidechain
25	BA	74	U	Sidechain
25	BA	79	G	Sidechain
25	BA	86	G	Sidechain
25	BA	88	C	Sidechain
25	BA	95	U	Sidechain
25	BA	98	G	Sidechain
26	BB	1000	A	Sidechain
26	BB	1005	C	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1006	C	Sidechain
26	BB	1010	A	Sidechain
26	BB	1011	G	Sidechain
26	BB	1014	A	Sidechain
26	BB	1017	G	Sidechain
26	BB	102	U	Sidechain
26	BB	1020	A	Sidechain
26	BB	1022	G	Sidechain
26	BB	1026	G	Sidechain
26	BB	1027	A	Sidechain
26	BB	1028	A	Sidechain
26	BB	103	A	Sidechain
26	BB	1030	C	Sidechain
26	BB	1038	G	Sidechain
26	BB	104	A	Sidechain
26	BB	1042	G	Sidechain
26	BB	1048	A	Sidechain
26	BB	1053	C	Sidechain
26	BB	1054	A	Sidechain
26	BB	1055	G	Sidechain
26	BB	1056	G	Sidechain
26	BB	1057	A	Sidechain
26	BB	1060	U	Sidechain
26	BB	1061	U	Sidechain
26	BB	1062	G	Sidechain
26	BB	1063	G	Sidechain
26	BB	1064	C	Sidechain
26	BB	1069	A	Sidechain
26	BB	1070	A	Sidechain
26	BB	1073	A	Sidechain
26	BB	1076	C	Sidechain
26	BB	1077	A	Sidechain
26	BB	1082	U	Sidechain
26	BB	1083	U	Sidechain
26	BB	1085	A	Sidechain
26	BB	1095	A	Sidechain
26	BB	1097	U	Sidechain
26	BB	1099	G	Sidechain
26	BB	11	C	Sidechain
26	BB	1101	U	Sidechain
26	BB	1102	C	Sidechain
26	BB	1106	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1107	G	Sidechain
26	BB	1114	C	Sidechain
26	BB	112	U	Sidechain
26	BB	1126	A	Sidechain
26	BB	1130	U	Sidechain
26	BB	1131	G	Sidechain
26	BB	1132	U	Sidechain
26	BB	1135	C	Sidechain
26	BB	1138	G	Sidechain
26	BB	1141	U	Sidechain
26	BB	1142	A	Sidechain
26	BB	1144	A	Sidechain
26	BB	1145	C	Sidechain
26	BB	1147	A	Sidechain
26	BB	115	C	Sidechain
26	BB	1153	C	Sidechain
26	BB	1154	G	Sidechain
26	BB	116	C	Sidechain
26	BB	1161	C	Sidechain
26	BB	1167	C	Sidechain
26	BB	1174	U	Sidechain
26	BB	1177	G	Sidechain
26	BB	1179	G	Sidechain
26	BB	118	A	Sidechain
26	BB	1182	G	Sidechain
26	BB	1187	G	Sidechain
26	BB	1198	U	Sidechain
26	BB	12	U	Sidechain
26	BB	120	U	Sidechain
26	BB	1202	G	Sidechain
26	BB	1204	A	Sidechain
26	BB	1207	C	Sidechain
26	BB	121	G	Sidechain
26	BB	1211	C	Sidechain
26	BB	1216	G	Sidechain
26	BB	122	G	Sidechain
26	BB	1226	A	Sidechain
26	BB	1227	G	Sidechain
26	BB	123	G	Sidechain
26	BB	1230	A	Sidechain
26	BB	1234	U	Sidechain
26	BB	1236	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1237	A	Sidechain
26	BB	1238	G	Sidechain
26	BB	124	G	Sidechain
26	BB	1240	U	Sidechain
26	BB	1242	U	Sidechain
26	BB	1246	A	Sidechain
26	BB	125	A	Sidechain
26	BB	1250	G	Sidechain
26	BB	1265	A	Sidechain
26	BB	1266	G	Sidechain
26	BB	1268	A	Sidechain
26	BB	1271	G	Sidechain
26	BB	1275	A	Sidechain
26	BB	1278	C	Sidechain
26	BB	1281	G	Sidechain
26	BB	1282	U	Sidechain
26	BB	1283	G	Sidechain
26	BB	1284	A	Sidechain
26	BB	1285	A	Sidechain
26	BB	1287	A	Sidechain
26	BB	1289	C	Sidechain
26	BB	129	C	Sidechain
26	BB	1293	C	Sidechain
26	BB	1295	C	Sidechain
26	BB	1296	G	Sidechain
26	BB	1299	G	Sidechain
26	BB	1303	G	Sidechain
26	BB	1306	C	Sidechain
26	BB	1309	G	Sidechain
26	BB	1317	G	Sidechain
26	BB	1318	U	Sidechain
26	BB	1321	A	Sidechain
26	BB	1324	G	Sidechain
26	BB	1325	U	Sidechain
26	BB	1327	A	Sidechain
26	BB	1328	A	Sidechain
26	BB	1335	C	Sidechain
26	BB	1340	U	Sidechain
26	BB	1353	A	Sidechain
26	BB	1356	G	Sidechain
26	BB	1358	G	Sidechain
26	BB	136	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1360	G	Sidechain
26	BB	1363	C	Sidechain
26	BB	1368	G	Sidechain
26	BB	1376	C	Sidechain
26	BB	138	U	Sidechain
26	BB	1382	G	Sidechain
26	BB	1384	A	Sidechain
26	BB	1389	G	Sidechain
26	BB	1390	U	Sidechain
26	BB	1392	A	Sidechain
26	BB	1393	A	Sidechain
26	BB	1394	U	Sidechain
26	BB	1396	U	Sidechain
26	BB	1397	U	Sidechain
26	BB	1398	C	Sidechain
26	BB	1399	C	Sidechain
26	BB	1408	G	Sidechain
26	BB	1410	G	Sidechain
26	BB	1416	G	Sidechain
26	BB	1417	C	Sidechain
26	BB	1418	G	Sidechain
26	BB	1419	A	Sidechain
26	BB	1420	A	Sidechain
26	BB	1424	G	Sidechain
26	BB	1426	G	Sidechain
26	BB	1427	A	Sidechain
26	BB	1431	A	Sidechain
26	BB	1432	G	Sidechain
26	BB	1433	A	Sidechain
26	BB	1439	A	Sidechain
26	BB	1440	U	Sidechain
26	BB	1441	G	Sidechain
26	BB	1445	G	Sidechain
26	BB	1449	G	Sidechain
26	BB	1450	G	Sidechain
26	BB	1453	A	Sidechain
26	BB	1454	C	Sidechain
26	BB	1459	G	Sidechain
26	BB	1466	U	Sidechain
26	BB	1472	C	Sidechain
26	BB	1473	G	Sidechain
26	BB	148	U	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1490	A	Sidechain
26	BB	1492	G	Sidechain
26	BB	1493	C	Sidechain
26	BB	1495	A	Sidechain
26	BB	1501	G	Sidechain
26	BB	1502	A	Sidechain
26	BB	151	C	Sidechain
26	BB	1511	G	Sidechain
26	BB	1514	G	Sidechain
26	BB	1515	A	Sidechain
26	BB	1519	G	Sidechain
26	BB	1521	G	Sidechain
26	BB	1523	U	Sidechain
26	BB	1532	A	Sidechain
26	BB	1535	A	Sidechain
26	BB	1537	G	Sidechain
26	BB	1542	U	Sidechain
26	BB	1544	A	Sidechain
26	BB	1548	A	Sidechain
26	BB	1549	A	Sidechain
26	BB	1550	C	Sidechain
26	BB	1551	A	Sidechain
26	BB	1553	A	Sidechain
26	BB	1554	U	Sidechain
26	BB	1555	G	Sidechain
26	BB	1561	C	Sidechain
26	BB	1564	C	Sidechain
26	BB	1565	C	Sidechain
26	BB	1567	G	Sidechain
26	BB	1568	G	Sidechain
26	BB	1574	C	Sidechain
26	BB	1577	C	Sidechain
26	BB	1581	G	Sidechain
26	BB	1585	C	Sidechain
26	BB	1587	G	Sidechain
26	BB	1588	G	Sidechain
26	BB	159	G	Sidechain
26	BB	1592	C	Sidechain
26	BB	1593	A	Sidechain
26	BB	1594	U	Sidechain
26	BB	1596	A	Sidechain
26	BB	160	A	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1601	G	Sidechain
26	BB	1603	A	Sidechain
26	BB	1605	C	Sidechain
26	BB	1607	C	Sidechain
26	BB	1608	A	Sidechain
26	BB	1609	A	Sidechain
26	BB	1616	A	Sidechain
26	BB	1619	G	Sidechain
26	BB	1620	G	Sidechain
26	BB	1626	A	Sidechain
26	BB	1631	G	Sidechain
26	BB	1632	A	Sidechain
26	BB	1633	G	Sidechain
26	BB	164	C	Sidechain
26	BB	1641	A	Sidechain
26	BB	1644	C	Sidechain
26	BB	1645	G	Sidechain
26	BB	1646	C	Sidechain
26	BB	1652	A	Sidechain
26	BB	1653	G	Sidechain
26	BB	1658	C	Sidechain
26	BB	1660	G	Sidechain
26	BB	1664	A	Sidechain
26	BB	1665	A	Sidechain
26	BB	1667	G	Sidechain
26	BB	1671	U	Sidechain
26	BB	1673	G	Sidechain
26	BB	1680	U	Sidechain
26	BB	1681	G	Sidechain
26	BB	1687	G	Sidechain
26	BB	1689	A	Sidechain
26	BB	1690	A	Sidechain
26	BB	1693	U	Sidechain
26	BB	1695	G	Sidechain
26	BB	17	G	Sidechain
26	BB	1701	A	Sidechain
26	BB	1702	G	Sidechain
26	BB	1706	C	Sidechain
26	BB	1710	G	Sidechain
26	BB	1711	A	Sidechain
26	BB	1715	G	Sidechain
26	BB	172	A	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1720	U	Sidechain
26	BB	1721	G	Sidechain
26	BB	1722	A	Sidechain
26	BB	1723	G	Sidechain
26	BB	1724	G	Sidechain
26	BB	1726	C	Sidechain
26	BB	1731	G	Sidechain
26	BB	1733	G	Sidechain
26	BB	1734	G	Sidechain
26	BB	1736	U	Sidechain
26	BB	1738	G	Sidechain
26	BB	1739	A	Sidechain
26	BB	1740	G	Sidechain
26	BB	1741	C	Sidechain
26	BB	1742	U	Sidechain
26	BB	1744	A	Sidechain
26	BB	1745	A	Sidechain
26	BB	1750	G	Sidechain
26	BB	1752	C	Sidechain
26	BB	1754	A	Sidechain
26	BB	1757	A	Sidechain
26	BB	1759	A	Sidechain
26	BB	176	A	Sidechain
26	BB	1762	A	Sidechain
26	BB	1772	A	Sidechain
26	BB	1773	A	Sidechain
26	BB	1777	U	Sidechain
26	BB	1779	U	Sidechain
26	BB	1780	A	Sidechain
26	BB	1784	A	Sidechain
26	BB	1788	C	Sidechain
26	BB	1791	A	Sidechain
26	BB	1792	G	Sidechain
26	BB	1798	U	Sidechain
26	BB	18	U	Sidechain
26	BB	180	G	Sidechain
26	BB	1802	A	Sidechain
26	BB	1809	A	Sidechain
26	BB	181	A	Sidechain
26	BB	1811	G	Sidechain
26	BB	1812	U	Sidechain
26	BB	1814	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1819	A	Sidechain
26	BB	1822	C	Sidechain
26	BB	1825	U	Sidechain
26	BB	183	C	Sidechain
26	BB	1831	G	Sidechain
26	BB	1834	U	Sidechain
26	BB	1837	C	Sidechain
26	BB	1839	G	Sidechain
26	BB	184	C	Sidechain
26	BB	1841	U	Sidechain
26	BB	1846	G	Sidechain
26	BB	1847	A	Sidechain
26	BB	1848	A	Sidechain
26	BB	1850	G	Sidechain
26	BB	1852	U	Sidechain
26	BB	1854	A	Sidechain
26	BB	1855	U	Sidechain
26	BB	1856	U	Sidechain
26	BB	1857	G	Sidechain
26	BB	1858	A	Sidechain
26	BB	1862	G	Sidechain
26	BB	1863	G	Sidechain
26	BB	1865	U	Sidechain
26	BB	1869	G	Sidechain
26	BB	1870	C	Sidechain
26	BB	1871	A	Sidechain
26	BB	1875	G	Sidechain
26	BB	1878	G	Sidechain
26	BB	1885	A	Sidechain
26	BB	1886	U	Sidechain
26	BB	1887	C	Sidechain
26	BB	1888	G	Sidechain
26	BB	189	G	Sidechain
26	BB	1893	C	Sidechain
26	BB	1898	U	Sidechain
26	BB	190	A	Sidechain
26	BB	1901	A	Sidechain
26	BB	1906	G	Sidechain
26	BB	1907	G	Sidechain
26	BB	1909	C	Sidechain
26	BB	1919	A	Sidechain
26	BB	192	C	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	1920	C	Sidechain
26	BB	1924	C	Sidechain
26	BB	1925	C	Sidechain
26	BB	1926	U	Sidechain
26	BB	1927	A	Sidechain
26	BB	1928	A	Sidechain
26	BB	1929	G	Sidechain
26	BB	1930	G	Sidechain
26	BB	1938	A	Sidechain
26	BB	194	G	Sidechain
26	BB	1940	U	Sidechain
26	BB	195	A	Sidechain
26	BB	1961	C	Sidechain
26	BB	1965	C	Sidechain
26	BB	1966	A	Sidechain
26	BB	1968	G	Sidechain
26	BB	1969	A	Sidechain
26	BB	1970	A	Sidechain
26	BB	1973	G	Sidechain
26	BB	1976	U	Sidechain
26	BB	1977	A	Sidechain
26	BB	1978	A	Sidechain
26	BB	1979	U	Sidechain
26	BB	1995	U	Sidechain
26	BB	1997	C	Sidechain
26	BB	1998	A	Sidechain
26	BB	2001	C	Sidechain
26	BB	2004	G	Sidechain
26	BB	2008	C	Sidechain
26	BB	2012	G	Sidechain
26	BB	2013	A	Sidechain
26	BB	202	U	Sidechain
26	BB	2020	A	Sidechain
26	BB	2021	C	Sidechain
26	BB	2022	U	Sidechain
26	BB	2029	G	Sidechain
26	BB	2031	A	Sidechain
26	BB	2032	G	Sidechain
26	BB	2033	A	Sidechain
26	BB	2034	U	Sidechain
26	BB	204	A	Sidechain
26	BB	2040	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	2046	G	Sidechain
26	BB	2048	G	Sidechain
26	BB	2050	C	Sidechain
26	BB	2053	G	Sidechain
26	BB	2054	A	Sidechain
26	BB	2055	C	Sidechain
26	BB	2058	A	Sidechain
26	BB	2059	A	Sidechain
26	BB	206	U	Sidechain
26	BB	2060	A	Sidechain
26	BB	2061	G	Sidechain
26	BB	2062	A	Sidechain
26	BB	2068	U	Sidechain
26	BB	207	A	Sidechain
26	BB	2077	A	Sidechain
26	BB	2079	U	Sidechain
26	BB	208	C	Sidechain
26	BB	2081	U	Sidechain
26	BB	2092	U	Sidechain
26	BB	21	A	Sidechain
26	BB	2107	G	Sidechain
26	BB	2109	U	Sidechain
26	BB	2112	G	Sidechain
26	BB	2113	U	Sidechain
26	BB	2115	G	Sidechain
26	BB	2117	A	Sidechain
26	BB	2118	U	Sidechain
26	BB	2121	G	Sidechain
26	BB	2123	G	Sidechain
26	BB	2126	A	Sidechain
26	BB	2127	G	Sidechain
26	BB	214	G	Sidechain
26	BB	2141	G	Sidechain
26	BB	2143	C	Sidechain
26	BB	2145	C	Sidechain
26	BB	2147	A	Sidechain
26	BB	2148	G	Sidechain
26	BB	2149	U	Sidechain
26	BB	215	G	Sidechain
26	BB	2152	G	Sidechain
26	BB	2155	U	Sidechain
26	BB	2158	A	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	216	A	Sidechain
26	BB	2160	C	Sidechain
26	BB	2161	C	Sidechain
26	BB	2162	G	Sidechain
26	BB	2168	G	Sidechain
26	BB	2170	A	Sidechain
26	BB	2178	C	Sidechain
26	BB	2179	C	Sidechain
26	BB	2180	U	Sidechain
26	BB	2183	A	Sidechain
26	BB	2185	U	Sidechain
26	BB	2187	U	Sidechain
26	BB	219	A	Sidechain
26	BB	2193	G	Sidechain
26	BB	2196	C	Sidechain
26	BB	2198	A	Sidechain
26	BB	220	G	Sidechain
26	BB	2205	A	Sidechain
26	BB	2206	C	Sidechain
26	BB	2208	C	Sidechain
26	BB	2216	G	Sidechain
26	BB	2218	G	Sidechain
26	BB	222	A	Sidechain
26	BB	2220	U	Sidechain
26	BB	2221	G	Sidechain
26	BB	2224	G	Sidechain
26	BB	2228	G	Sidechain
26	BB	2233	U	Sidechain
26	BB	2234	G	Sidechain
26	BB	2238	G	Sidechain
26	BB	2239	G	Sidechain
26	BB	2246	G	Sidechain
26	BB	2249	U	Sidechain
26	BB	2250	G	Sidechain
26	BB	2254	C	Sidechain
26	BB	2258	C	Sidechain
26	BB	2259	U	Sidechain
26	BB	226	A	Sidechain
26	BB	2262	U	Sidechain
26	BB	2268	A	Sidechain
26	BB	2269	G	Sidechain
26	BB	227	A	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	2273	A	Sidechain
26	BB	2274	A	Sidechain
26	BB	2275	C	Sidechain
26	BB	2276	G	Sidechain
26	BB	2277	G	Sidechain
26	BB	228	C	Sidechain
26	BB	2282	G	Sidechain
26	BB	2284	A	Sidechain
26	BB	2285	C	Sidechain
26	BB	2287	A	Sidechain
26	BB	2288	A	Sidechain
26	BB	23	G	Sidechain
26	BB	2305	U	Sidechain
26	BB	2306	C	Sidechain
26	BB	2307	G	Sidechain
26	BB	2308	G	Sidechain
26	BB	2310	C	Sidechain
26	BB	2311	A	Sidechain
26	BB	2312	U	Sidechain
26	BB	2314	A	Sidechain
26	BB	2317	A	Sidechain
26	BB	2318	G	Sidechain
26	BB	2323	G	Sidechain
26	BB	2324	U	Sidechain
26	BB	2325	G	Sidechain
26	BB	2326	C	Sidechain
26	BB	2328	A	Sidechain
26	BB	2330	G	Sidechain
26	BB	2331	G	Sidechain
26	BB	2333	A	Sidechain
26	BB	2335	A	Sidechain
26	BB	234	U	Sidechain
26	BB	2340	A	Sidechain
26	BB	2344	U	Sidechain
26	BB	2345	G	Sidechain
26	BB	2348	U	Sidechain
26	BB	2357	G	Sidechain
26	BB	236	C	Sidechain
26	BB	2362	C	Sidechain
26	BB	2365	G	Sidechain
26	BB	2369	A	Sidechain
26	BB	2375	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	2376	A	Sidechain
26	BB	2380	C	Sidechain
26	BB	2383	G	Sidechain
26	BB	2384	U	Sidechain
26	BB	2386	A	Sidechain
26	BB	2388	A	Sidechain
26	BB	2389	G	Sidechain
26	BB	2391	G	Sidechain
26	BB	2392	A	Sidechain
26	BB	2394	C	Sidechain
26	BB	2401	U	Sidechain
26	BB	2402	U	Sidechain
26	BB	2403	C	Sidechain
26	BB	2405	G	Sidechain
26	BB	2407	A	Sidechain
26	BB	2408	U	Sidechain
26	BB	241	A	Sidechain
26	BB	2411	A	Sidechain
26	BB	2414	G	Sidechain
26	BB	2416	C	Sidechain
26	BB	2418	A	Sidechain
26	BB	242	G	Sidechain
26	BB	2420	C	Sidechain
26	BB	2421	G	Sidechain
26	BB	2424	C	Sidechain
26	BB	2427	C	Sidechain
26	BB	2429	G	Sidechain
26	BB	2430	A	Sidechain
26	BB	2434	A	Sidechain
26	BB	2438	U	Sidechain
26	BB	2442	C	Sidechain
26	BB	2458	G	Sidechain
26	BB	2459	A	Sidechain
26	BB	2460	U	Sidechain
26	BB	2465	C	Sidechain
26	BB	2468	A	Sidechain
26	BB	2469	A	Sidechain
26	BB	2471	A	Sidechain
26	BB	2472	G	Sidechain
26	BB	2476	A	Sidechain
26	BB	2480	C	Sidechain
26	BB	2488	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	2489	U	Sidechain
26	BB	249	C	Sidechain
26	BB	2491	U	Sidechain
26	BB	2492	U	Sidechain
26	BB	2496	C	Sidechain
26	BB	250	G	Sidechain
26	BB	2500	U	Sidechain
26	BB	2502	G	Sidechain
26	BB	2509	G	Sidechain
26	BB	251	A	Sidechain
26	BB	2510	C	Sidechain
26	BB	2515	C	Sidechain
26	BB	2517	C	Sidechain
26	BB	2518	A	Sidechain
26	BB	2519	U	Sidechain
26	BB	2520	C	Sidechain
26	BB	2521	C	Sidechain
26	BB	2522	U	Sidechain
26	BB	2526	G	Sidechain
26	BB	2529	G	Sidechain
26	BB	2531	A	Sidechain
26	BB	2533	U	Sidechain
26	BB	2534	A	Sidechain
26	BB	2536	G	Sidechain
26	BB	2538	C	Sidechain
26	BB	2539	C	Sidechain
26	BB	254	G	Sidechain
26	BB	2547	A	Sidechain
26	BB	2550	G	Sidechain
26	BB	2553	G	Sidechain
26	BB	2554	U	Sidechain
26	BB	2557	G	Sidechain
26	BB	2561	U	Sidechain
26	BB	2565	A	Sidechain
26	BB	2569	G	Sidechain
26	BB	2570	G	Sidechain
26	BB	2574	G	Sidechain
26	BB	258	G	Sidechain
26	BB	2582	G	Sidechain
26	BB	2588	G	Sidechain
26	BB	2589	A	Sidechain
26	BB	259	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	2592	G	Sidechain
26	BB	2595	G	Sidechain
26	BB	2599	G	Sidechain
26	BB	2602	A	Sidechain
26	BB	261	G	Sidechain
26	BB	2610	C	Sidechain
26	BB	2611	C	Sidechain
26	BB	262	A	Sidechain
26	BB	2621	G	Sidechain
26	BB	2624	G	Sidechain
26	BB	2625	G	Sidechain
26	BB	2627	G	Sidechain
26	BB	2633	G	Sidechain
26	BB	2637	U	Sidechain
26	BB	2638	G	Sidechain
26	BB	2640	G	Sidechain
26	BB	2643	G	Sidechain
26	BB	2644	G	Sidechain
26	BB	2645	G	Sidechain
26	BB	265	A	Sidechain
26	BB	2655	G	Sidechain
26	BB	2656	U	Sidechain
26	BB	2658	C	Sidechain
26	BB	2659	G	Sidechain
26	BB	266	G	Sidechain
26	BB	2661	G	Sidechain
26	BB	2662	A	Sidechain
26	BB	2663	G	Sidechain
26	BB	2664	G	Sidechain
26	BB	268	C	Sidechain
26	BB	2680	U	Sidechain
26	BB	2681	C	Sidechain
26	BB	2684	U	Sidechain
26	BB	2685	G	Sidechain
26	BB	2686	G	Sidechain
26	BB	2688	G	Sidechain
26	BB	2694	G	Sidechain
26	BB	2696	U	Sidechain
26	BB	27	G	Sidechain
26	BB	2701	U	Sidechain
26	BB	2706	A	Sidechain
26	BB	271	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	2711	A	Sidechain
26	BB	2720	U	Sidechain
26	BB	2722	G	Sidechain
26	BB	2725	A	Sidechain
26	BB	2727	A	Sidechain
26	BB	2731	G	Sidechain
26	BB	2732	G	Sidechain
26	BB	2737	G	Sidechain
26	BB	2739	U	Sidechain
26	BB	2740	A	Sidechain
26	BB	2743	U	Sidechain
26	BB	2744	G	Sidechain
26	BB	2751	G	Sidechain
26	BB	2753	A	Sidechain
26	BB	2755	C	Sidechain
26	BB	2759	G	Sidechain
26	BB	276	U	Sidechain
26	BB	2763	G	Sidechain
26	BB	2764	A	Sidechain
26	BB	2765	A	Sidechain
26	BB	2774	C	Sidechain
26	BB	2783	U	Sidechain
26	BB	2787	C	Sidechain
26	BB	2791	G	Sidechain
26	BB	2792	A	Sidechain
26	BB	2796	U	Sidechain
26	BB	2797	U	Sidechain
26	BB	2799	A	Sidechain
26	BB	2807	U	Sidechain
26	BB	2808	G	Sidechain
26	BB	2809	A	Sidechain
26	BB	281	C	Sidechain
26	BB	2810	A	Sidechain
26	BB	2813	A	Sidechain
26	BB	2815	C	Sidechain
26	BB	2819	G	Sidechain
26	BB	2822	G	Sidechain
26	BB	2833	U	Sidechain
26	BB	2838	G	Sidechain
26	BB	284	U	Sidechain
26	BB	2843	G	Sidechain
26	BB	2849	U	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	2854	G	Sidechain
26	BB	2856	A	Sidechain
26	BB	2857	G	Sidechain
26	BB	2859	G	Sidechain
26	BB	2861	U	Sidechain
26	BB	2864	G	Sidechain
26	BB	2866	U	Sidechain
26	BB	2868	A	Sidechain
26	BB	2872	A	Sidechain
26	BB	2881	U	Sidechain
26	BB	2882	A	Sidechain
26	BB	2884	U	Sidechain
26	BB	2889	C	Sidechain
26	BB	2890	G	Sidechain
26	BB	2892	G	Sidechain
26	BB	2894	G	Sidechain
26	BB	2895	G	Sidechain
26	BB	291	G	Sidechain
26	BB	294	A	Sidechain
26	BB	295	G	Sidechain
26	BB	299	A	Sidechain
26	BB	300	A	Sidechain
26	BB	301	G	Sidechain
26	BB	303	G	Sidechain
26	BB	306	U	Sidechain
26	BB	308	G	Sidechain
26	BB	31	C	Sidechain
26	BB	311	A	Sidechain
26	BB	312	G	Sidechain
26	BB	313	G	Sidechain
26	BB	315	G	Sidechain
26	BB	319	G	Sidechain
26	BB	320	A	Sidechain
26	BB	321	U	Sidechain
26	BB	324	A	Sidechain
26	BB	325	G	Sidechain
26	BB	327	G	Sidechain
26	BB	329	G	Sidechain
26	BB	330	A	Sidechain
26	BB	332	A	Sidechain
26	BB	339	U	Sidechain
26	BB	340	A	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	344	A	Sidechain
26	BB	346	A	Sidechain
26	BB	347	A	Sidechain
26	BB	356	G	Sidechain
26	BB	361	G	Sidechain
26	BB	364	C	Sidechain
26	BB	365	U	Sidechain
26	BB	367	G	Sidechain
26	BB	371	A	Sidechain
26	BB	378	C	Sidechain
26	BB	384	A	Sidechain
26	BB	385	C	Sidechain
26	BB	388	G	Sidechain
26	BB	39	G	Sidechain
26	BB	392	U	Sidechain
26	BB	399	U	Sidechain
26	BB	401	A	Sidechain
26	BB	402	A	Sidechain
26	BB	403	U	Sidechain
26	BB	405	U	Sidechain
26	BB	406	G	Sidechain
26	BB	407	G	Sidechain
26	BB	413	C	Sidechain
26	BB	420	C	Sidechain
26	BB	422	A	Sidechain
26	BB	424	G	Sidechain
26	BB	427	U	Sidechain
26	BB	428	A	Sidechain
26	BB	429	A	Sidechain
26	BB	43	G	Sidechain
26	BB	430	A	Sidechain
26	BB	432	A	Sidechain
26	BB	436	C	Sidechain
26	BB	44	A	Sidechain
26	BB	442	G	Sidechain
26	BB	443	A	Sidechain
26	BB	446	G	Sidechain
26	BB	447	A	Sidechain
26	BB	448	U	Sidechain
26	BB	449	A	Sidechain
26	BB	450	G	Sidechain
26	BB	457	A	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	459	U	Sidechain
26	BB	460	A	Sidechain
26	BB	463	G	Sidechain
26	BB	464	U	Sidechain
26	BB	467	G	Sidechain
26	BB	470	A	Sidechain
26	BB	473	G	Sidechain
26	BB	477	A	Sidechain
26	BB	478	A	Sidechain
26	BB	481	G	Sidechain
26	BB	483	A	Sidechain
26	BB	487	C	Sidechain
26	BB	492	A	Sidechain
26	BB	493	G	Sidechain
26	BB	494	G	Sidechain
26	BB	498	G	Sidechain
26	BB	499	U	Sidechain
26	BB	501	A	Sidechain
26	BB	51	G	Sidechain
26	BB	511	U	Sidechain
26	BB	513	A	Sidechain
26	BB	516	C	Sidechain
26	BB	520	G	Sidechain
26	BB	523	C	Sidechain
26	BB	527	C	Sidechain
26	BB	535	G	Sidechain
26	BB	539	G	Sidechain
26	BB	540	C	Sidechain
26	BB	545	U	Sidechain
26	BB	549	G	Sidechain
26	BB	550	C	Sidechain
26	BB	551	G	Sidechain
26	BB	572	A	Sidechain
26	BB	577	G	Sidechain
26	BB	582	A	Sidechain
26	BB	585	G	Sidechain
26	BB	586	A	Sidechain
26	BB	587	C	Sidechain
26	BB	588	U	Sidechain
26	BB	590	A	Sidechain
26	BB	594	U	Sidechain
26	BB	598	U	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	603	A	Sidechain
26	BB	604	G	Sidechain
26	BB	608	A	Sidechain
26	BB	610	C	Sidechain
26	BB	611	C	Sidechain
26	BB	612	G	Sidechain
26	BB	618	G	Sidechain
26	BB	619	G	Sidechain
26	BB	62	U	Sidechain
26	BB	63	A	Sidechain
26	BB	630	G	Sidechain
26	BB	631	A	Sidechain
26	BB	632	A	Sidechain
26	BB	634	C	Sidechain
26	BB	635	C	Sidechain
26	BB	637	A	Sidechain
26	BB	638	G	Sidechain
26	BB	642	U	Sidechain
26	BB	643	A	Sidechain
26	BB	644	A	Sidechain
26	BB	653	U	Sidechain
26	BB	655	A	Sidechain
26	BB	658	U	Sidechain
26	BB	659	G	Sidechain
26	BB	66	C	Sidechain
26	BB	662	G	Sidechain
26	BB	666	A	Sidechain
26	BB	669	G	Sidechain
26	BB	674	G	Sidechain
26	BB	675	A	Sidechain
26	BB	676	A	Sidechain
26	BB	678	C	Sidechain
26	BB	68	G	Sidechain
26	BB	685	A	Sidechain
26	BB	687	C	Sidechain
26	BB	692	C	Sidechain
26	BB	697	G	Sidechain
26	BB	7	G	Sidechain
26	BB	700	G	Sidechain
26	BB	71	A	Sidechain
26	BB	714	U	Sidechain
26	BB	715	A	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	716	A	Sidechain
26	BB	717	C	Sidechain
26	BB	72	U	Sidechain
26	BB	721	A	Sidechain
26	BB	726	G	Sidechain
26	BB	727	A	Sidechain
26	BB	731	C	Sidechain
26	BB	732	C	Sidechain
26	BB	738	G	Sidechain
26	BB	74	A	Sidechain
26	BB	741	U	Sidechain
26	BB	744	U	Sidechain
26	BB	75	G	Sidechain
26	BB	750	A	Sidechain
26	BB	751	A	Sidechain
26	BB	753	A	Sidechain
26	BB	757	G	Sidechain
26	BB	758	C	Sidechain
26	BB	761	A	Sidechain
26	BB	764	A	Sidechain
26	BB	765	C	Sidechain
26	BB	767	U	Sidechain
26	BB	775	G	Sidechain
26	BB	778	G	Sidechain
26	BB	780	G	Sidechain
26	BB	782	A	Sidechain
26	BB	783	A	Sidechain
26	BB	789	A	Sidechain
26	BB	794	A	Sidechain
26	BB	800	A	Sidechain
26	BB	801	G	Sidechain
26	BB	802	A	Sidechain
26	BB	803	U	Sidechain
26	BB	807	U	Sidechain
26	BB	81	G	Sidechain
26	BB	810	U	Sidechain
26	BB	811	U	Sidechain
26	BB	813	U	Sidechain
26	BB	814	C	Sidechain
26	BB	816	C	Sidechain
26	BB	817	C	Sidechain
26	BB	82	U	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	820	A	Sidechain
26	BB	822	G	Sidechain
26	BB	83	A	Sidechain
26	BB	834	G	Sidechain
26	BB	836	G	Sidechain
26	BB	837	C	Sidechain
26	BB	841	G	Sidechain
26	BB	843	G	Sidechain
26	BB	844	A	Sidechain
26	BB	845	A	Sidechain
26	BB	848	C	Sidechain
26	BB	85	G	Sidechain
26	BB	850	U	Sidechain
26	BB	855	G	Sidechain
26	BB	856	G	Sidechain
26	BB	857	G	Sidechain
26	BB	858	G	Sidechain
26	BB	863	A	Sidechain
26	BB	864	G	Sidechain
26	BB	866	A	Sidechain
26	BB	867	C	Sidechain
26	BB	868	U	Sidechain
26	BB	870	U	Sidechain
26	BB	871	U	Sidechain
26	BB	872	U	Sidechain
26	BB	88	G	Sidechain
26	BB	881	G	Sidechain
26	BB	882	G	Sidechain
26	BB	887	U	Sidechain
26	BB	888	C	Sidechain
26	BB	897	C	Sidechain
26	BB	899	A	Sidechain
26	BB	903	C	Sidechain
26	BB	904	G	Sidechain
26	BB	910	A	Sidechain
26	BB	911	A	Sidechain
26	BB	912	C	Sidechain
26	BB	913	U	Sidechain
26	BB	914	G	Sidechain
26	BB	918	A	Sidechain
26	BB	921	C	Sidechain
26	BB	924	G	Sidechain

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Mol	Chain	Res	Type	Group
26	BB	925	A	Sidechain
26	BB	926	G	Sidechain
26	BB	930	G	Sidechain
26	BB	933	A	Sidechain
26	BB	936	A	Sidechain
26	BB	941	A	Sidechain
26	BB	945	A	Sidechain
26	BB	947	A	Sidechain
26	BB	949	G	Sidechain
26	BB	95	A	Sidechain
26	BB	950	G	Sidechain
26	BB	954	G	Sidechain
26	BB	959	A	Sidechain
26	BB	960	A	Sidechain
26	BB	961	C	Sidechain
26	BB	962	G	Sidechain
26	BB	966	G	Sidechain
26	BB	974	G	Sidechain
26	BB	976	G	Sidechain
26	BB	978	G	Sidechain
26	BB	979	A	Sidechain
26	BB	980	A	Sidechain
26	BB	982	C	Sidechain
26	BB	983	A	Sidechain
26	BB	99	U	Sidechain
26	BB	993	G	Sidechain
27	BC	161	VAL	Mainchain
27	BC	43	ASP	Peptide
27	BC	99	ASP	Mainchain
28	BD	216	ARG	Sidechain
28	BD	270	ARG	Sidechain
29	BE	118	PHE	Sidechain
29	BE	45	TYR	Sidechain
30	BF	69	ARG	Peptide
30	BF	77	ILE	Peptide
32	BH	114	HIS	Peptide
32	BH	61	TRP	Mainchain
33	BI	117	LEU	Peptide
41	BQ	4	ILE	Peptide
42	BR	4	LYS	Peptide
43	BS	99	THR	Mainchain
48	BX	3	LYS	Peptide

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Mol	Chain	Res	Type	Group
49	BY	77	TYR	Sidechain
53	Bc	36	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	33089	0	16678	0	0
2	AB	1635	0	849	0	0
2	AE	1635	0	849	0	0
3	AC	3036	0	3052	0	0
4	AD	495	0	249	0	0
5	AF	1872	0	1885	0	0
6	AG	1822	0	1913	0	0
7	AH	1643	0	1710	0	0
8	AI	1225	0	1273	0	0
9	AJ	1101	0	1050	0	0
10	AK	1400	0	1449	0	0
11	AL	979	0	1034	0	0
12	AM	1036	0	1084	0	0
13	AN	825	0	865	0	0
14	AO	965	0	997	0	0
15	AP	955	0	1019	0	0
16	AQ	910	0	981	0	0
17	AR	805	0	847	0	0
18	AS	716	0	742	0	0
19	AT	649	0	666	0	0
20	AU	672	0	716	0	0
21	AV	626	0	651	0	0
22	AW	727	0	769	0	0
23	AX	670	0	722	0	0
24	AY	590	0	631	0	0
25	BA	2566	0	1302	0	0
26	BB	62351	0	31387	0	0
27	BC	1733	0	1824	0	0
28	BD	2092	0	2170	0	0
29	BE	1565	0	1616	0	0
30	BF	1552	0	1619	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BG	1420	0	1460	0	0
32	BH	1323	0	1374	0	0
33	BI	1111	0	1148	0	0
34	BJ	1032	0	1088	0	0
35	BK	1129	0	1162	0	0
36	BL	947	0	1023	0	0
37	BM	1053	0	1129	0	0
38	BN	1074	0	1157	0	0
39	BO	1008	0	1045	0	0
40	BP	900	0	935	0	0
41	BQ	917	0	965	0	0
42	BR	947	0	1022	0	0
43	BS	816	0	839	0	0
44	BT	857	0	922	0	0
45	BU	787	0	846	0	0
46	BV	789	0	847	0	0
47	BW	753	0	780	0	0
48	BX	634	0	656	0	0
49	BY	625	0	655	0	0
50	BZ	509	0	543	0	0
51	Ba	449	0	491	0	0
52	Bb	549	0	552	0	0
53	Bc	444	0	461	0	0
54	Bd	441	0	485	0	0
55	Be	377	0	418	0	0
56	Bf	504	0	574	0	0
57	Bg	302	0	343	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	391/393 (100%)	367 (94%)	21 (5%)	3 (1%)	24	69
5	AF	238/241 (99%)	215 (90%)	21 (9%)	2 (1%)	24	69
6	AG	230/233 (99%)	210 (91%)	18 (8%)	2 (1%)	21	67
7	AH	203/206 (98%)	189 (93%)	12 (6%)	2 (1%)	19	65
8	AI	164/167 (98%)	143 (87%)	18 (11%)	3 (2%)	11	53
9	AJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	13	57
10	AK	176/179 (98%)	159 (90%)	15 (8%)	2 (1%)	17	63
11	AL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	12	56
12	AM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	12	56
13	AN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	4	35
14	AO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	12	56
15	AP	121/124 (98%)	103 (85%)	13 (11%)	5 (4%)	3	35
16	AQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
17	AR	98/101 (97%)	82 (84%)	9 (9%)	7 (7%)	1	22
18	AS	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
19	AT	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
20	AU	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
21	AV	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	14	58
22	AW	89/92 (97%)	81 (91%)	8 (9%)	0	100	100
23	AX	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
24	AY	68/71 (96%)	62 (91%)	5 (7%)	1 (2%)	13	57
27	BC	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	15	60
28	BD	270/273 (99%)	239 (88%)	22 (8%)	9 (3%)	5	40
29	BE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	6	43
30	BF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	13	57
31	BG	176/179 (98%)	148 (84%)	25 (14%)	3 (2%)	11	55
32	BH	174/177 (98%)	162 (93%)	9 (5%)	3 (2%)	11	55
33	BI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	5	40
34	BJ	139/142 (98%)	121 (87%)	17 (12%)	1 (1%)	26	71
35	BK	140/142 (99%)	131 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	BL	121/123 (98%)	107 (88%)	12 (10%)	2 (2%)	11	55
37	BM	142/144 (99%)	124 (87%)	16 (11%)	2 (1%)	14	58
38	BN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	8	49
39	BO	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	24	69
40	BP	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	21	67
41	BQ	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	11	53
42	BR	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	21	67
43	BS	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	5	42
44	BT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	21	67
45	BU	98/100 (98%)	86 (88%)	11 (11%)	1 (1%)	19	65
46	BV	101/104 (97%)	90 (89%)	10 (10%)	1 (1%)	19	65
47	BW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	8	49
48	BX	82/85 (96%)	68 (83%)	11 (13%)	3 (4%)	4	38
49	BY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	6	45
50	BZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	3	31
51	Ba	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	11	53
52	Bb	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	13	57
53	Bc	54/57 (95%)	46 (85%)	6 (11%)	2 (4%)	4	38
54	Bd	52/55 (94%)	45 (86%)	7 (14%)	0	100	100
55	Be	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
56	Bf	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
57	Bg	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	44
All	All	6548/6682 (98%)	5895 (90%)	547 (8%)	106 (2%)	17	56

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	AH	18	LEU
12	AM	3	ASN
13	AN	74	VAL
14	AO	118	ASN
15	AP	86	VAL
17	AR	70	HIS
24	AY	3	ILE

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Mol	Chain	Res	Type
28	BD	260	LYS
29	BE	43	ASP
29	BE	122	VAL
29	BE	150	GLN
29	BE	170	VAL
38	BN	36	VAL
40	BP	68	LYS
43	BS	91	GLN
46	BV	6	ARG
48	BX	9	THR
53	Bc	26	SER
3	AC	21	ASP
3	AC	60	ILE
5	AF	41	ASN
8	AI	77	ASN
10	AK	55	LYS
13	AN	90	LEU
14	AO	74	LYS
17	AR	37	ASP
27	BC	217	THR
27	BC	229	LEU
28	BD	119	VAL
28	BD	237	ARG
33	BI	23	ALA
37	BM	36	LYS
42	BR	104	ALA
48	BX	72	GLY
49	BY	27	ARG
49	BY	62	GLY
50	BZ	46	VAL
51	Ba	9	THR
53	Bc	39	ARG
5	AF	132	GLU
8	AI	43	GLY
8	AI	162	GLU
10	AK	116	ALA
15	AP	24	GLU
15	AP	75	GLU
17	AR	73	LEU
28	BD	193	GLU
28	BD	240	GLY
29	BE	137	SER

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Mol	Chain	Res	Type
30	BF	62	GLN
31	BG	148	VAL
32	BH	50	THR
32	BH	164	ALA
36	BL	70	ARG
43	BS	53	PHE
43	BS	80	ARG
47	BW	85	LYS
50	BZ	23	ARG
57	Bg	4	ARG
9	AJ	92	THR
12	AM	13	SER
17	AR	32	ASP
17	AR	35	ALA
17	AR	61	ASN
28	BD	140	VAL
28	BD	190	THR
28	BD	263	ASP
29	BE	41	ALA
30	BF	66	GLY
36	BL	3	GLN
39	BO	81	ASN
45	BU	69	ARG
3	AC	9	LYS
6	AG	14	VAL
9	AJ	100	SER
13	AN	42	LEU
15	AP	21	PRO
15	AP	43	LYS
31	BG	132	ARG
32	BH	8	VAL
38	BN	106	ASP
50	BZ	17	GLU
6	AG	8	GLY
21	AV	3	TYR
28	BD	141	HIS
30	BF	71	GLY
33	BI	28	ASN
37	BM	20	GLY
38	BN	23	GLY
13	AN	57	VAL
27	BC	73	VAL

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Mol	Chain	Res	Type
31	BG	73	VAL
47	BW	65	VAL
11	AL	125	ILE
17	AR	30	ILE
33	BI	121	VAL
34	BJ	90	GLY
41	BQ	22	GLY
52	Bb	36	VAL
7	AH	27	ILE
11	AL	81	GLY
33	BI	118	PRO
41	BQ	32	VAL
44	BT	80	PRO
33	BI	94	ILE
48	BX	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	326/326 (100%)	311 (95%)	15 (5%)	33	68
5	AF	198/199 (100%)	188 (95%)	10 (5%)	29	66
6	AG	189/190 (100%)	180 (95%)	9 (5%)	31	67
7	AH	172/173 (99%)	164 (95%)	8 (5%)	32	68
8	AI	125/126 (99%)	122 (98%)	3 (2%)	57	82
9	AJ	116/116 (100%)	104 (90%)	12 (10%)	9	37
10	AK	146/147 (99%)	136 (93%)	10 (7%)	20	57
11	AL	104/105 (99%)	99 (95%)	5 (5%)	31	67
12	AM	106/107 (99%)	98 (92%)	8 (8%)	17	53
13	AN	90/90 (100%)	85 (94%)	5 (6%)	26	62
14	AO	98/99 (99%)	95 (97%)	3 (3%)	47	77
15	AP	103/104 (99%)	98 (95%)	5 (5%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AQ	95/96 (99%)	93 (98%)	2 (2%)	61	84
17	AR	83/84 (99%)	79 (95%)	4 (5%)	31	67
18	AS	76/77 (99%)	71 (93%)	5 (7%)	21	57
19	AT	65/65 (100%)	62 (95%)	3 (5%)	33	68
20	AU	77/78 (99%)	75 (97%)	2 (3%)	54	80
21	AV	64/65 (98%)	60 (94%)	4 (6%)	22	59
22	AW	78/79 (99%)	74 (95%)	4 (5%)	29	66
23	AX	65/66 (98%)	61 (94%)	4 (6%)	23	60
24	AY	60/61 (98%)	55 (92%)	5 (8%)	14	49
27	BC	181/181 (100%)	176 (97%)	5 (3%)	51	78
28	BD	217/218 (100%)	210 (97%)	7 (3%)	46	76
29	BE	164/164 (100%)	153 (93%)	11 (7%)	20	57
30	BF	165/165 (100%)	156 (94%)	9 (6%)	27	63
31	BG	149/150 (99%)	138 (93%)	11 (7%)	17	54
32	BH	137/138 (99%)	128 (93%)	9 (7%)	21	57
33	BI	114/114 (100%)	109 (96%)	5 (4%)	35	69
34	BJ	109/110 (99%)	104 (95%)	5 (5%)	33	68
35	BK	116/116 (100%)	110 (95%)	6 (5%)	29	65
36	BL	104/104 (100%)	96 (92%)	8 (8%)	16	52
37	BM	103/103 (100%)	97 (94%)	6 (6%)	25	61
38	BN	109/109 (100%)	101 (93%)	8 (7%)	17	54
39	BO	103/103 (100%)	97 (94%)	6 (6%)	25	61
40	BP	87/87 (100%)	82 (94%)	5 (6%)	25	62
41	BQ	99/100 (99%)	93 (94%)	6 (6%)	23	60
42	BR	89/90 (99%)	88 (99%)	1 (1%)	80	91
43	BS	84/84 (100%)	78 (93%)	6 (7%)	18	55
44	BT	93/93 (100%)	88 (95%)	5 (5%)	27	64
45	BU	84/84 (100%)	79 (94%)	5 (6%)	24	60
46	BV	84/85 (99%)	81 (96%)	3 (4%)	42	74
47	BW	78/78 (100%)	74 (95%)	4 (5%)	29	66
48	BX	62/63 (98%)	55 (89%)	7 (11%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BY	67/68 (98%)	64 (96%)	3 (4%)	34	69
50	BZ	55/55 (100%)	54 (98%)	1 (2%)	66	87
51	Ba	48/49 (98%)	47 (98%)	1 (2%)	61	84
52	Bb	62/62 (100%)	60 (97%)	2 (3%)	46	76
53	Bc	47/48 (98%)	46 (98%)	1 (2%)	61	84
54	Bd	48/49 (98%)	48 (100%)	0	100	100
55	Be	38/38 (100%)	37 (97%)	1 (3%)	54	80
56	Bf	51/52 (98%)	49 (96%)	2 (4%)	39	72
57	Bg	34/34 (100%)	30 (88%)	4 (12%)	6	32
All	All	5417/5447 (99%)	5138 (95%)	279 (5%)	33	65

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	87	TYR
3	AC	135	ASN
3	AC	189	LEU
3	AC	223	ARG
3	AC	236	ILE
3	AC	244	ILE
3	AC	249	GLU
3	AC	251	GLN
3	AC	252	LYS
3	AC	262	ARG
3	AC	323	PHE
3	AC	333	ARG
3	AC	345	GLU
3	AC	363	ILE
3	AC	378	GLU
5	AF	20	ARG
5	AF	62	ARG
5	AF	65	LYS
5	AF	73	ARG
5	AF	77	GLU
5	AF	109	SER
5	AF	131	LYS
5	AF	176	ASN
5	AF	233	GLU
5	AF	234	GLU

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Mol	Chain	Res	Type
6	AG	79	LYS
6	AG	109	GLU
6	AG	163	ARG
6	AG	166	TRP
6	AG	167	TYR
6	AG	174	LEU
6	AG	195	ILE
6	AG	203	LYS
6	AG	217	GLU
7	AH	21	LYS
7	AH	25	ARG
7	AH	46	ARG
7	AH	68	GLU
7	AH	119	HIS
7	AH	131	ILE
7	AH	193	ASP
7	AH	194	ILE
8	AI	45	VAL
8	AI	95	MET
8	AI	152	VAL
9	AJ	4	TYR
9	AJ	16	GLU
9	AJ	24	ARG
9	AJ	38	ARG
9	AJ	42	TRP
9	AJ	53	LYS
9	AJ	109	ARG
9	AJ	113	ARG
9	AJ	116	PHE
9	AJ	125	GLU
9	AJ	132	GLU
9	AJ	134	GLU
10	AK	2	ARG
10	AK	4	ARG
10	AK	5	VAL
10	AK	105	GLU
10	AK	112	ASP
10	AK	136	LYS
10	AK	138	GLU
10	AK	143	MET
10	AK	155	TRP
10	AK	161	PHE

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Mol	Chain	Res	Type
11	AL	14	ARG
11	AL	48	PHE
11	AL	49	LYS
11	AL	59	GLU
11	AL	127	TYR
12	AM	2	GLU
12	AM	29	ILE
12	AM	49	GLN
12	AM	58	GLU
12	AM	67	LYS
12	AM	71	ILE
12	AM	105	ARG
12	AM	125	GLN
13	AN	1	MET
13	AN	7	ARG
13	AN	32	THR
13	AN	48	ARG
13	AN	59	LYS
14	AO	6	ARG
14	AO	10	ARG
14	AO	93	GLU
15	AP	73	LEU
15	AP	81	ILE
15	AP	107	LYS
15	AP	109	ARG
15	AP	113	ARG
16	AQ	72	ILE
16	AQ	113	LYS
17	AR	23	ARG
17	AR	27	LYS
17	AR	52	ARG
17	AR	89	ARG
18	AS	13	GLU
18	AS	17	ASP
18	AS	30	LEU
18	AS	52	ARG
18	AS	79	ARG
19	AT	32	PHE
19	AT	38	PHE
19	AT	47	GLU
20	AU	16	MET
20	AU	51	GLU

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Mol	Chain	Res	Type
21	AV	7	ARG
21	AV	34	GLU
21	AV	69	TYR
21	AV	70	THR
22	AW	16	LYS
22	AW	36	ARG
22	AW	69	LYS
22	AW	80	ARG
23	AX	19	HIS
23	AX	48	LYS
23	AX	52	GLU
23	AX	56	ILE
24	AY	4	LYS
24	AY	20	ARG
24	AY	35	GLU
24	AY	38	GLU
24	AY	68	ARG
27	BC	8	MET
27	BC	60	ARG
27	BC	105	LYS
27	BC	164	ARG
27	BC	168	ASN
28	BD	2	VAL
28	BD	43	ASN
28	BD	114	GLN
28	BD	145	MET
28	BD	198	GLU
28	BD	247	TRP
28	BD	272	LYS
29	BE	15	PHE
29	BE	25	THR
29	BE	36	GLN
29	BE	43	ASP
29	BE	74	GLU
29	BE	86	GLU
29	BE	89	GLU
29	BE	104	VAL
29	BE	145	SER
29	BE	157	LYS
29	BE	168	GLU
30	BF	6	LYS
30	BF	47	LYS

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Mol	Chain	Res	Type
30	BF	49	ARG
30	BF	58	LYS
30	BF	60	TRP
30	BF	105	LEU
30	BF	153	LEU
30	BF	155	GLU
30	BF	156	ASN
31	BG	14	LYS
31	BG	62	GLN
31	BG	63	LYS
31	BG	68	LYS
31	BG	80	GLN
31	BG	91	ARG
31	BG	101	ARG
31	BG	124	ARG
31	BG	132	ARG
31	BG	147	ARG
31	BG	152	ASP
32	BH	18	ILE
32	BH	40	VAL
32	BH	84	LYS
32	BH	94	ARG
32	BH	98	LYS
32	BH	102	ILE
32	BH	108	PHE
32	BH	110	HIS
32	BH	169	ARG
33	BI	25	TYR
33	BI	114	GLU
33	BI	119	ASN
33	BI	137	GLU
33	BI	138	VAL
34	BJ	3	LYS
34	BJ	49	GLU
34	BJ	64	ARG
34	BJ	116	MET
34	BJ	124	MET
35	BK	12	LYS
35	BK	37	ARG
35	BK	71	ASP
35	BK	72	LYS
35	BK	84	ILE

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Mol	Chain	Res	Type
35	BK	96	ARG
36	BL	1	MET
36	BL	8	LEU
36	BL	29	HIS
36	BL	45	GLU
36	BL	49	ARG
36	BL	70	ARG
36	BL	106	GLU
36	BL	114	LYS
37	BM	10	GLU
37	BM	14	LYS
37	BM	39	LYS
37	BM	76	GLU
37	BM	115	GLU
37	BM	141	LYS
38	BN	20	LEU
38	BN	28	PHE
38	BN	36	VAL
38	BN	58	LYS
38	BN	62	LYS
38	BN	82	MET
38	BN	118	LYS
38	BN	119	LEU
39	BO	3	HIS
39	BO	4	ARG
39	BO	18	GLN
39	BO	27	SER
39	BO	58	ASP
39	BO	72	ASP
40	BP	7	ARG
40	BP	27	VAL
40	BP	35	ILE
40	BP	61	GLN
40	BP	94	ARG
41	BQ	3	ILE
41	BQ	12	MET
41	BQ	23	ASP
41	BQ	97	TYR
41	BQ	112	ARG
41	BQ	113	LEU
42	BR	101	ASP
43	BS	21	ARG

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Mol	Chain	Res	Type
43	BS	22	LEU
43	BS	53	PHE
43	BS	55	ASP
43	BS	79	ARG
43	BS	89	HIS
44	BT	3	THR
44	BT	61	ASN
44	BT	78	GLU
44	BT	82	MET
44	BT	88	ARG
45	BU	9	LYS
45	BU	24	MET
45	BU	26	LYS
45	BU	64	LYS
45	BU	72	GLN
46	BV	42	LYS
46	BV	44	HIS
46	BV	46	LYS
47	BW	11	GLU
47	BW	34	LYS
47	BW	55	GLU
47	BW	61	LEU
48	BX	2	HIS
48	BX	10	ARG
48	BX	31	LEU
48	BX	44	PHE
48	BX	49	ASN
48	BX	61	LYS
48	BX	81	ILE
49	BY	36	ARG
49	BY	40	GLU
49	BY	64	ASP
50	BZ	5	GLU
51	Ba	6	ILE
52	Bb	47	LYS
52	Bb	59	ARG
53	Bc	40	HIS
55	Be	25	LYS
56	Bf	1	PRO
56	Bf	49	VAL
57	Bg	1	MET
57	Bg	12	ARG

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Mol	Chain	Res	Type
57	Bg	15	LYS
57	Bg	22	VAL

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	1539/1542 (99%)	193 (12%)	73 (4%)
2	AB	73/76 (96%)	12 (16%)	2 (2%)
2	AE	73/76 (96%)	13 (17%)	6 (8%)
25	BA	119/120 (99%)	15 (12%)	4 (3%)
26	BB	2898/2904 (99%)	401 (13%)	137 (4%)
4	AD	24/24 (100%)	4 (16%)	5 (20%)
All	All	4726/4742 (99%)	638 (13%)	227 (4%)

All (638) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	40	C
1	AA	48	C
1	AA	49	U
1	AA	51	A
1	AA	60	A
1	AA	61	G
1	AA	65	A
1	AA	66	A
1	AA	83	C
1	AA	86	G
1	AA	87	C
1	AA	88	U
1	AA	95	C
1	AA	109	A
1	AA	121	U
1	AA	130	A

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Mol	Chain	Res	Type
1	AA	131	A
1	AA	144	G
1	AA	164	G
1	AA	183	C
1	AA	184	G
1	AA	188	C
1	AA	247	G
1	AA	266	G
1	AA	275	G
1	AA	281	G
1	AA	289	G
1	AA	293	G
1	AA	306	A
1	AA	328	C
1	AA	329	A
1	AA	331	G
1	AA	352	C
1	AA	353	A
1	AA	354	G
1	AA	366	A
1	AA	367	U
1	AA	368	U
1	AA	369	G
1	AA	370	C
1	AA	381	C
1	AA	388	G
1	AA	393	A
1	AA	397	A
1	AA	398	U
1	AA	406	G
1	AA	413	G
1	AA	414	A
1	AA	416	G
1	AA	424	G
1	AA	429	U
1	AA	439	U
1	AA	465	A
1	AA	466	A
1	AA	468	A
1	AA	478	A
1	AA	482	A
1	AA	484	G

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Mol	Chain	Res	Type
1	AA	486	U
1	AA	495	A
1	AA	511	C
1	AA	512	U
1	AA	518	C
1	AA	521	G
1	AA	525	C
1	AA	527	7MG
1	AA	531	U
1	AA	532	A
1	AA	547	A
1	AA	559	A
1	AA	564	C
1	AA	566	G
1	AA	570	G
1	AA	572	A
1	AA	573	A
1	AA	576	C
1	AA	632	U
1	AA	653	U
1	AA	665	A
1	AA	687	A
1	AA	690	G
1	AA	691	G
1	AA	694	A
1	AA	695	A
1	AA	700	G
1	AA	724	G
1	AA	746	A
1	AA	749	A
1	AA	755	G
1	AA	792	A
1	AA	793	U
1	AA	794	A
1	AA	796	C
1	AA	811	C
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	819	A
1	AA	820	U
1	AA	821	G

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Mol	Chain	Res	Type
1	AA	827	U
1	AA	828	U
1	AA	841	C
1	AA	846	G
1	AA	864	A
1	AA	867	G
1	AA	871	U
1	AA	872	A
1	AA	884	U
1	AA	885	G
1	AA	889	A
1	AA	890	G
1	AA	899	C
1	AA	922	G
1	AA	934	C
1	AA	935	A
1	AA	941	G
1	AA	949	A
1	AA	960	U
1	AA	961	U
1	AA	966	2MG
1	AA	968	A
1	AA	969	A
1	AA	975	A
1	AA	993	G
1	AA	1004	A
1	AA	1041	G
1	AA	1064	G
1	AA	1065	U
1	AA	1066	C
1	AA	1085	U
1	AA	1094	G
1	AA	1101	A
1	AA	1129	C
1	AA	1130	A
1	AA	1138	G
1	AA	1139	G
1	AA	1152	A
1	AA	1159	U
1	AA	1189	U
1	AA	1190	G
1	AA	1196	A

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Mol	Chain	Res	Type
1	AA	1202	U
1	AA	1212	U
1	AA	1213	A
1	AA	1214	C
1	AA	1225	A
1	AA	1226	C
1	AA	1227	A
1	AA	1241	G
1	AA	1250	A
1	AA	1256	A
1	AA	1278	G
1	AA	1279	G
1	AA	1280	A
1	AA	1285	A
1	AA	1298	U
1	AA	1299	A
1	AA	1300	G
1	AA	1301	U
1	AA	1303	C
1	AA	1317	C
1	AA	1320	C
1	AA	1322	C
1	AA	1338	G
1	AA	1340	A
1	AA	1341	U
1	AA	1343	G
1	AA	1346	A
1	AA	1359	C
1	AA	1379	G
1	AA	1381	U
1	AA	1382	C
1	AA	1397	C
1	AA	1399	C
1	AA	1432	G
1	AA	1447	A
1	AA	1494	G
1	AA	1505	G
1	AA	1506	U
1	AA	1517	G
1	AA	1529	G
1	AA	1530	G
1	AA	1534	A

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Mol	Chain	Res	Type
1	AA	1535	C
1	AA	1537	U
1	AA	1539	C
1	AA	1542	A
2	AB	7	A
2	AB	8	4SU
2	AB	10	G
2	AB	16	H2U
2	AB	18	G
2	AB	19	G
2	AB	20	H2U
2	AB	46	7MG
2	AB	48	C
2	AB	49	C
2	AB	59	U
2	AB	60	U
4	AD	25	U
4	AD	26	U
4	AD	36	U
4	AD	40	G
2	AE	10	G
2	AE	16	H2U
2	AE	17	C
2	AE	18	G
2	AE	20	H2U
2	AE	56	C
2	AE	57	G
2	AE	58	A
2	AE	61	C
2	AE	73	A
2	AE	74	C
2	AE	75	C
2	AE	76	A
25	BA	10	G
25	BA	13	G
25	BA	15	A
25	BA	16	G
25	BA	36	C
25	BA	38	C
25	BA	42	C
25	BA	45	A
25	BA	57	A

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Mol	Chain	Res	Type
25	BA	58	A
25	BA	68	C
25	BA	71	C
25	BA	88	C
25	BA	90	C
25	BA	109	A
26	BB	11	C
26	BB	13	A
26	BB	14	A
26	BB	28	A
26	BB	52	A
26	BB	61	C
26	BB	64	A
26	BB	65	U
26	BB	71	A
26	BB	72	U
26	BB	75	G
26	BB	91	A
26	BB	101	A
26	BB	102	U
26	BB	118	A
26	BB	119	A
26	BB	120	U
26	BB	125	A
26	BB	126	A
26	BB	128	C
26	BB	138	U
26	BB	142	A
26	BB	149	A
26	BB	154	U
26	BB	196	A
26	BB	204	A
26	BB	205	G
26	BB	215	G
26	BB	216	A
26	BB	221	A
26	BB	222	A
26	BB	223	A
26	BB	226	A
26	BB	248	G
26	BB	265	A
26	BB	266	G

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Mol	Chain	Res	Type
26	BB	269	C
26	BB	270	A
26	BB	271	G
26	BB	272	A
26	BB	277	G
26	BB	279	A
26	BB	294	A
26	BB	299	A
26	BB	302	C
26	BB	323	C
26	BB	324	A
26	BB	330	A
26	BB	331	C
26	BB	338	G
26	BB	346	A
26	BB	373	U
26	BB	383	C
26	BB	386	G
26	BB	391	A
26	BB	411	G
26	BB	418	C
26	BB	432	A
26	BB	444	C
26	BB	447	A
26	BB	448	U
26	BB	451	U
26	BB	456	C
26	BB	457	A
26	BB	458	G
26	BB	459	U
26	BB	479	A
26	BB	480	A
26	BB	481	G
26	BB	482	A
26	BB	504	A
26	BB	505	A
26	BB	508	A
26	BB	509	C
26	BB	527	C
26	BB	529	A
26	BB	530	G
26	BB	531	C

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Mol	Chain	Res	Type
26	BB	532	A
26	BB	533	G
26	BB	546	U
26	BB	547	A
26	BB	548	G
26	BB	549	G
26	BB	563	A
26	BB	573	U
26	BB	574	A
26	BB	575	A
26	BB	586	A
26	BB	588	U
26	BB	603	A
26	BB	607	U
26	BB	637	A
26	BB	645	C
26	BB	654	A
26	BB	655	A
26	BB	656	G
26	BB	669	G
26	BB	670	A
26	BB	686	U
26	BB	715	A
26	BB	717	C
26	BB	728	G
26	BB	730	A
26	BB	736	C
26	BB	737	C
26	BB	740	C
26	BB	748	G
26	BB	753	A
26	BB	764	A
26	BB	775	G
26	BB	776	G
26	BB	782	A
26	BB	784	G
26	BB	786	C
26	BB	790	U
26	BB	791	C
26	BB	792	A
26	BB	793	A
26	BB	805	G

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Mol	Chain	Res	Type
26	BB	812	C
26	BB	828	U
26	BB	910	A
26	BB	914	G
26	BB	931	U
26	BB	941	A
26	BB	945	A
26	BB	946	C
26	BB	948	C
26	BB	959	A
26	BB	962	G
26	BB	974	G
26	BB	980	A
26	BB	984	A
26	BB	995	C
26	BB	996	A
26	BB	1012	U
26	BB	1013	C
26	BB	1016	G
26	BB	1022	G
26	BB	1025	G
26	BB	1026	G
26	BB	1033	U
26	BB	1034	G
26	BB	1047	G
26	BB	1048	A
26	BB	1056	G
26	BB	1067	A
26	BB	1069	A
26	BB	1070	A
26	BB	1079	C
26	BB	1086	A
26	BB	1088	A
26	BB	1095	A
26	BB	1096	A
26	BB	1110	G
26	BB	1112	G
26	BB	1128	G
26	BB	1129	A
26	BB	1130	U
26	BB	1132	U
26	BB	1133	A

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Mol	Chain	Res	Type
26	BB	1134	A
26	BB	1135	C
26	BB	1136	G
26	BB	1143	A
26	BB	1170	C
26	BB	1175	A
26	BB	1177	G
26	BB	1184	U
26	BB	1185	G
26	BB	1186	G
26	BB	1206	G
26	BB	1211	C
26	BB	1212	G
26	BB	1213	A
26	BB	1249	U
26	BB	1250	G
26	BB	1256	G
26	BB	1266	G
26	BB	1271	G
26	BB	1272	A
26	BB	1286	A
26	BB	1287	A
26	BB	1296	G
26	BB	1300	G
26	BB	1301	A
26	BB	1365	A
26	BB	1378	A
26	BB	1379	U
26	BB	1391	U
26	BB	1416	G
26	BB	1417	C
26	BB	1427	A
26	BB	1440	U
26	BB	1452	G
26	BB	1453	A
26	BB	1455	G
26	BB	1458	U
26	BB	1459	G
26	BB	1460	U
26	BB	1462	C
26	BB	1482	G
26	BB	1493	C

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Mol	Chain	Res	Type
26	BB	1509	A
26	BB	1510	G
26	BB	1523	U
26	BB	1558	C
26	BB	1566	A
26	BB	1569	A
26	BB	1584	U
26	BB	1585	C
26	BB	1596	A
26	BB	1607	C
26	BB	1608	A
26	BB	1616	A
26	BB	1617	C
26	BB	1646	C
26	BB	1647	U
26	BB	1648	U
26	BB	1654	A
26	BB	1700	A
26	BB	1705	A
26	BB	1715	G
26	BB	1732	C
26	BB	1733	G
26	BB	1762	A
26	BB	1773	A
26	BB	1781	U
26	BB	1782	U
26	BB	1791	A
26	BB	1800	C
26	BB	1802	A
26	BB	1808	A
26	BB	1809	A
26	BB	1839	G
26	BB	1840	G
26	BB	1871	A
26	BB	1873	G
26	BB	1900	A
26	BB	1901	A
26	BB	1906	G
26	BB	1907	G
26	BB	1918	A
26	BB	1929	G
26	BB	1930	G

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Mol	Chain	Res	Type
26	BB	1931	U
26	BB	1937	A
26	BB	1938	A
26	BB	1939	5MU
26	BB	1943	U
26	BB	1952	A
26	BB	1954	G
26	BB	1955	U
26	BB	1956	U
26	BB	1962	5MC
26	BB	1964	G
26	BB	1965	C
26	BB	1966	A
26	BB	1970	A
26	BB	1971	U
26	BB	1972	G
26	BB	1981	A
26	BB	1992	G
26	BB	1993	U
26	BB	1997	C
26	BB	2003	A
26	BB	2021	C
26	BB	2023	C
26	BB	2032	G
26	BB	2042	A
26	BB	2043	C
26	BB	2056	G
26	BB	2059	A
26	BB	2061	G
26	BB	2062	A
26	BB	2068	U
26	BB	2076	U
26	BB	2092	U
26	BB	2112	G
26	BB	2119	A
26	BB	2120	G
26	BB	2127	G
26	BB	2129	C
26	BB	2131	U
26	BB	2132	U
26	BB	2133	G
26	BB	2135	A

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Mol	Chain	Res	Type
26	BB	2140	G
26	BB	2147	A
26	BB	2158	A
26	BB	2159	G
26	BB	2172	U
26	BB	2173	A
26	BB	2174	C
26	BB	2179	C
26	BB	2199	A
26	BB	2203	U
26	BB	2212	A
26	BB	2213	U
26	BB	2214	C
26	BB	2225	A
26	BB	2238	G
26	BB	2239	G
26	BB	2250	G
26	BB	2266	A
26	BB	2273	A
26	BB	2283	C
26	BB	2287	A
26	BB	2288	A
26	BB	2296	U
26	BB	2305	U
26	BB	2308	G
26	BB	2309	A
26	BB	2310	C
26	BB	2321	U
26	BB	2322	A
26	BB	2325	G
26	BB	2333	A
26	BB	2335	A
26	BB	2350	C
26	BB	2357	G
26	BB	2363	G
26	BB	2382	G
26	BB	2383	G
26	BB	2385	C
26	BB	2390	U
26	BB	2391	G
26	BB	2399	G
26	BB	2406	A

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Mol	Chain	Res	Type
26	BB	2407	A
26	BB	2408	U
26	BB	2425	A
26	BB	2428	G
26	BB	2429	G
26	BB	2432	A
26	BB	2439	A
26	BB	2440	C
26	BB	2441	U
26	BB	2448	A
26	BB	2449	H2U
26	BB	2465	C
26	BB	2466	C
26	BB	2472	G
26	BB	2475	C
26	BB	2476	A
26	BB	2478	A
26	BB	2491	U
26	BB	2501	C
26	BB	2502	G
26	BB	2504	PSU
26	BB	2506	U
26	BB	2507	C
26	BB	2530	A
26	BB	2543	G
26	BB	2566	A
26	BB	2567	G
26	BB	2573	C
26	BB	2574	G
26	BB	2578	G
26	BB	2586	U
26	BB	2599	G
26	BB	2610	C
26	BB	2613	U
26	BB	2615	U
26	BB	2629	U
26	BB	2630	G
26	BB	2639	A
26	BB	2655	G
26	BB	2689	U
26	BB	2690	U
26	BB	2699	C

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Mol	Chain	Res	Type
26	BB	2700	A
26	BB	2714	G
26	BB	2726	A
26	BB	2732	G
26	BB	2733	A
26	BB	2751	G
26	BB	2752	C
26	BB	2756	U
26	BB	2765	A
26	BB	2766	A
26	BB	2778	A
26	BB	2780	G
26	BB	2791	G
26	BB	2792	A
26	BB	2799	A
26	BB	2815	C
26	BB	2820	A
26	BB	2833	U
26	BB	2848	G
26	BB	2850	A
26	BB	2861	U
26	BB	2867	G
26	BB	2873	A
26	BB	2880	C
26	BB	2883	A
26	BB	2884	U
26	BB	2894	G
26	BB	2895	G
26	BB	2904	U

All (227) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	1	A
1	AA	31	G
1	AA	52	C
1	AA	56	U
1	AA	59	A
1	AA	60	A
1	AA	65	A
1	AA	70	U
1	AA	85	U

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Mol	Chain	Res	Type
1	AA	100	G
1	AA	193	C
1	AA	194	C
1	AA	209	U
1	AA	318	G
1	AA	365	U
1	AA	367	U
1	AA	368	U
1	AA	369	G
1	AA	385	C
1	AA	403	C
1	AA	415	A
1	AA	438	U
1	AA	451	A
1	AA	465	A
1	AA	481	G
1	AA	484	G
1	AA	489	C
1	AA	494	G
1	AA	524	G
1	AA	531	U
1	AA	572	A
1	AA	620	C
1	AA	690	G
1	AA	694	A
1	AA	753	A
1	AA	785	G
1	AA	793	U
1	AA	794	A
1	AA	797	C
1	AA	815	A
1	AA	817	C
1	AA	818	G
1	AA	824	G
1	AA	884	U
1	AA	889	A
1	AA	934	C
1	AA	968	A
1	AA	975	A
1	AA	1065	U
1	AA	1104	G
1	AA	1112	C

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Mol	Chain	Res	Type
1	AA	1124	G
1	AA	1129	C
1	AA	1131	G
1	AA	1212	U
1	AA	1213	A
1	AA	1227	A
1	AA	1257	A
1	AA	1278	G
1	AA	1279	G
1	AA	1280	A
1	AA	1298	U
1	AA	1299	A
1	AA	1300	G
1	AA	1302	C
1	AA	1312	G
1	AA	1320	C
1	AA	1323	G
1	AA	1340	A
1	AA	1399	C
1	AA	1441	A
1	AA	1529	G
1	AA	1534	A
2	AB	9	A
2	AB	45	U
4	AD	24	A
4	AD	25	U
4	AD	29	G
4	AD	42	U
4	AD	45	G
2	AE	3	C
2	AE	9	A
2	AE	18	G
2	AE	20	H2U
2	AE	56	C
2	AE	73	A
25	BA	15	A
25	BA	77	U
25	BA	108	A
25	BA	109	A
26	BB	13	A
26	BB	72	U
26	BB	75	G

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Mol	Chain	Res	Type
26	BB	102	U
26	BB	110	G
26	BB	125	A
26	BB	126	A
26	BB	160	A
26	BB	164	C
26	BB	196	A
26	BB	221	A
26	BB	222	A
26	BB	227	A
26	BB	311	A
26	BB	331	C
26	BB	332	A
26	BB	372	G
26	BB	380	G
26	BB	448	U
26	BB	479	A
26	BB	503	A
26	BB	504	A
26	BB	529	A
26	BB	532	A
26	BB	545	U
26	BB	574	A
26	BB	586	A
26	BB	615	U
26	BB	669	G
26	BB	671	C
26	BB	673	C
26	BB	716	A
26	BB	720	U
26	BB	729	G
26	BB	736	C
26	BB	743	A
26	BB	752	A
26	BB	786	C
26	BB	790	U
26	BB	791	C
26	BB	805	G
26	BB	827	U
26	BB	896	A
26	BB	898	C
26	BB	912	C

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Mol	Chain	Res	Type
26	BB	979	A
26	BB	995	C
26	BB	1032	A
26	BB	1033	U
26	BB	1045	C
26	BB	1046	A
26	BB	1068	G
26	BB	1069	A
26	BB	1085	A
26	BB	1087	G
26	BB	1109	C
26	BB	1112	G
26	BB	1128	G
26	BB	1132	U
26	BB	1133	A
26	BB	1185	G
26	BB	1210	G
26	BB	1241	A
26	BB	1248	G
26	BB	1254	A
26	BB	1262	A
26	BB	1286	A
26	BB	1305	C
26	BB	1365	A
26	BB	1383	A
26	BB	1390	U
26	BB	1407	G
26	BB	1420	A
26	BB	1451	C
26	BB	1458	U
26	BB	1508	A
26	BB	1552	A
26	BB	1602	U
26	BB	1608	A
26	BB	1614	A
26	BB	1616	A
26	BB	1646	C
26	BB	1647	U
26	BB	1649	G
26	BB	1674	G
26	BB	1714	U
26	BB	1732	C

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Mol	Chain	Res	Type
26	BB	1761	C
26	BB	1773	A
26	BB	1816	C
26	BB	1839	G
26	BB	1870	C
26	BB	1887	C
26	BB	1900	A
26	BB	1918	A
26	BB	1930	G
26	BB	1952	A
26	BB	1955	U
26	BB	1968	G
26	BB	1969	A
26	BB	1980	G
26	BB	2020	A
26	BB	2021	C
26	BB	2119	A
26	BB	2130	U
26	BB	2172	U
26	BB	2309	A
26	BB	2339	C
26	BB	2357	G
26	BB	2380	C
26	BB	2390	U
26	BB	2391	G
26	BB	2439	A
26	BB	2448	A
26	BB	2465	C
26	BB	2500	U
26	BB	2542	A
26	BB	2581	G
26	BB	2584	U
26	BB	2602	A
26	BB	2619	C
26	BB	2655	G
26	BB	2662	A
26	BB	2667	C
26	BB	2696	U
26	BB	2717	C
26	BB	2726	A
26	BB	2732	G
26	BB	2744	G

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Mol	Chain	Res	Type
26	BB	2751	G
26	BB	2758	A
26	BB	2791	G
26	BB	2838	G
26	BB	2866	U
26	BB	2870	C
26	BB	2872	A
26	BB	2894	G

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
1	2MG	AA	1207	1	18,26,27	1.29	2 (11%)	21,38,41	2.60	3 (14%)
1	4OC	AA	1402	1	15,23,24	1.04	2 (13%)	21,32,35	1.78	3 (14%)
1	5MC	AA	1407	1	14,22,23	0.90	1 (7%)	17,32,35	0.87	0
1	UR3	AA	1498	1	13,22,23	0.84	0	18,32,35	1.44	4 (22%)
1	2MG	AA	1516	1	18,26,27	1.23	2 (11%)	21,38,41	2.73	6 (28%)
1	MA6	AA	1518	1	18,26,27	0.91	1 (5%)	15,38,41	1.78	4 (26%)
1	MA6	AA	1519	1	18,26,27	0.84	1 (5%)	15,38,41	1.86	5 (33%)
1	PSU	AA	516	1	15,21,22	1.32	1 (6%)	16,30,33	3.60	5 (31%)
1	7MG	AA	527	1	20,26,27	2.22	4 (20%)	23,39,42	2.39	2 (8%)
1	2MG	AA	966	1	18,26,27	1.28	2 (11%)	21,38,41	2.97	8 (38%)
1	5MC	AA	967	1	14,22,23	0.95	1 (7%)	17,32,35	0.80	1 (5%)
2	H2U	AB	16	2	17,21,22	0.83	0	23,30,33	1.39	2 (8%)
2	H2U	AB	20	2	17,21,22	0.80	0	23,30,33	1.13	1 (4%)
2	PSU	AB	32	2	15,21,22	1.29	2 (13%)	16,30,33	3.58	4 (25%)
2	MIA	AB	37	2	22,31,32	1.04	3 (13%)	26,44,47	1.70	6 (23%)
2	PSU	AB	39	2	15,21,22	1.27	1 (6%)	16,30,33	3.61	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7MG	AB	46	2	20,26,27	2.21	3 (15%)	23,39,42	2.54	2 (8%)
2	3AU	AB	47	-	15,28,29	0.89	0	17,40,43	0.88	1 (5%)
2	5MU	AB	54	2	13,22,23	1.25	1 (7%)	16,32,35	4.85	3 (18%)
2	PSU	AB	55	2	15,21,22	1.31	2 (13%)	16,30,33	3.45	3 (18%)
2	4SU	AB	8	2	12,21,22	1.01	1 (8%)	15,30,33	1.68	1 (6%)
2	H2U	AE	16	2	17,21,22	0.80	0	23,30,33	1.00	1 (4%)
2	H2U	AE	20	2	17,21,22	0.81	0	23,30,33	1.06	1 (4%)
2	PSU	AE	32	2	15,21,22	1.32	1 (6%)	16,30,33	3.47	4 (25%)
2	MIA	AE	37	2	22,31,32	1.05	4 (18%)	26,44,47	1.68	5 (19%)
2	PSU	AE	39	2	15,21,22	1.23	1 (6%)	16,30,33	3.57	4 (25%)
2	7MG	AE	46	2	20,26,27	2.18	3 (15%)	23,39,42	2.43	4 (17%)
2	3AU	AE	47	-	15,28,29	0.83	0	17,40,43	1.31	1 (5%)
2	5MU	AE	54	2	13,22,23	1.23	1 (7%)	16,32,35	4.89	2 (12%)
2	PSU	AE	55	2	15,21,22	1.33	1 (6%)	16,30,33	3.52	3 (18%)
2	4SU	AE	8	2	12,21,22	0.95	0	15,30,33	1.64	2 (13%)
26	6MZ	BB	1618	26	17,25,26	0.88	1 (5%)	15,36,39	1.33	1 (6%)
26	2MG	BB	1835	26	18,26,27	1.32	1 (5%)	21,38,41	2.43	5 (23%)
26	PSU	BB	1911	26	15,21,22	1.32	1 (6%)	16,30,33	3.35	2 (12%)
26	3TD	BB	1915	26	15,22,23	0.98	0	17,32,35	1.66	4 (23%)
26	PSU	BB	1917	26	15,21,22	1.36	1 (6%)	16,30,33	3.61	4 (25%)
26	5MU	BB	1939	26	13,22,23	1.24	1 (7%)	16,32,35	4.44	2 (12%)
26	5MC	BB	1962	26	14,22,23	0.97	1 (7%)	17,32,35	1.00	1 (5%)
26	6MZ	BB	2030	26	17,25,26	0.93	1 (5%)	15,36,39	1.57	3 (20%)
26	7MG	BB	2069	26	20,26,27	2.21	3 (15%)	23,39,42	2.31	3 (13%)
26	OMG	BB	2251	26	18,26,27	1.29	1 (5%)	21,38,41	2.65	5 (23%)
26	2MG	BB	2445	26	18,26,27	1.28	2 (11%)	21,38,41	2.47	5 (23%)
26	H2U	BB	2449	26	17,21,22	0.79	0	23,30,33	1.23	2 (8%)
26	PSU	BB	2457	26	15,21,22	1.32	1 (6%)	16,30,33	3.67	6 (37%)
26	OMC	BB	2498	26	15,22,23	0.87	0	20,31,34	1.18	1 (5%)
26	2MA	BB	2503	26	17,25,26	1.10	3 (17%)	18,37,40	1.85	2 (11%)
26	PSU	BB	2504	26	15,21,22	1.33	1 (6%)	16,30,33	3.62	5 (31%)
26	OMU	BB	2552	26	14,22,23	1.26	2 (14%)	19,31,34	2.84	4 (21%)
26	CH	BB	2575	26	14,21,22	0.99	1 (7%)	18,30,33	0.96	1 (5%)
26	PSU	BB	2580	26	15,21,22	1.39	1 (6%)	16,30,33	3.48	3 (18%)
26	PSU	BB	2605	26	15,21,22	1.27	1 (6%)	16,30,33	3.62	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	1MG	BB	745	26	17,26,27	0.95	1 (5%)	19,39,42	1.61	2 (10%)
26	PSU	BB	746	26	15,21,22	1.35	1 (6%)	16,30,33	3.46	4 (25%)
26	5MU	BB	747	26	13,22,23	1.19	1 (7%)	16,32,35	4.70	3 (18%)
26	PSU	BB	955	26	15,21,22	1.28	1 (6%)	16,30,33	3.56	3 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1	-	0/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	0/7/37/38	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
2	H2U	AB	16	2	-	0/7/38/39	0/2/2/2
2	H2U	AB	20	2	-	0/7/38/39	0/2/2/2
2	PSU	AB	32	2	-	0/7/25/26	0/2/2/2
2	MIA	AB	37	2	-	0/11/33/34	0/3/3/3
2	PSU	AB	39	2	-	0/7/25/26	0/2/2/2
2	7MG	AB	46	2	-	0/7/37/38	0/3/3/3
2	3AU	AB	47	-	-	0/8/34/35	0/2/2/2
2	5MU	AB	54	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	55	2	-	0/7/25/26	0/2/2/2
2	4SU	AB	8	2	-	0/3/25/26	0/2/2/2
2	H2U	AE	16	2	-	0/7/38/39	0/2/2/2
2	H2U	AE	20	2	-	0/7/38/39	0/2/2/2
2	PSU	AE	32	2	-	0/7/25/26	0/2/2/2
2	MIA	AE	37	2	-	0/11/33/34	0/3/3/3
2	PSU	AE	39	2	-	0/7/25/26	0/2/2/2
2	7MG	AE	46	2	-	0/7/37/38	0/3/3/3
2	3AU	AE	47	-	-	0/8/34/35	0/2/2/2
2	5MU	AE	54	2	-	0/3/25/26	0/2/2/2
2	PSU	AE	55	2	-	0/7/25/26	0/2/2/2
2	4SU	AE	8	2	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	6MZ	BB	1618	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	BB	1911	26	-	0/7/25/26	0/2/2/2
26	3TD	BB	1915	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	1939	26	-	0/3/25/26	0/2/2/2
26	5MC	BB	1962	26	-	0/3/25/26	0/2/2/2
26	6MZ	BB	2030	26	-	0/5/27/28	0/3/3/3
26	7MG	BB	2069	26	-	0/7/37/38	0/3/3/3
26	OMG	BB	2251	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	2445	26	-	0/5/27/28	0/3/3/3
26	H2U	BB	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	BB	2457	26	-	0/7/25/26	0/2/2/2
26	OMC	BB	2498	26	-	0/5/27/28	0/2/2/2
26	2MA	BB	2503	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	2504	26	-	0/7/25/26	0/2/2/2
26	OMU	BB	2552	26	-	0/5/27/28	0/2/2/2
26	CH	BB	2575	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	2580	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	BB	745	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	746	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	747	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	955	26	-	0/7/25/26	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	46	7MG	C8-N9	-7.90	1.34	1.45
26	BB	2069	7MG	C8-N9	-7.81	1.34	1.45
1	AA	527	7MG	C8-N9	-7.79	1.34	1.45
2	AE	46	7MG	C8-N9	-7.57	1.34	1.45
26	BB	2069	7MG	C8-N7	-2.79	1.30	1.43
1	AA	527	7MG	C8-N7	-2.75	1.30	1.43
2	AB	46	7MG	C8-N7	-2.69	1.31	1.43
2	AE	46	7MG	C8-N7	-2.68	1.31	1.43
26	BB	745	1MG	C8-N7	-2.36	1.30	1.34
26	BB	2030	6MZ	C8-N7	-2.31	1.30	1.34
1	AA	1519	MA6	C8-N7	-2.22	1.30	1.34
26	BB	2445	2MG	C8-N7	-2.19	1.30	1.34
1	AA	1516	2MG	C8-N7	-2.15	1.30	1.34
1	AA	1518	MA6	C8-N7	-2.14	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	37	MIA	C8-N7	-2.12	1.30	1.34
26	BB	2503	2MA	O4'-C4'	-2.10	1.40	1.45
2	AB	37	MIA	C13-C14	-2.10	1.36	1.51
26	BB	1618	6MZ	C8-N7	-2.09	1.30	1.34
1	AA	1207	2MG	C8-N7	-2.07	1.30	1.34
2	AE	37	MIA	C8-N7	-2.05	1.30	1.34
26	BB	2503	2MA	C8-N7	-2.05	1.30	1.34
2	AE	37	MIA	C13-C14	-2.04	1.36	1.51
1	AA	966	2MG	C8-N7	-2.01	1.30	1.34
26	BB	2552	OMU	C6-N1	2.03	1.38	1.35
2	AB	55	PSU	C6-N1	2.03	1.38	1.34
1	AA	1407	5MC	C5-C4	2.08	1.44	1.41
2	AB	32	PSU	C6-N1	2.09	1.38	1.34
1	AA	527	7MG	C4-N3	2.11	1.37	1.34
2	AE	37	MIA	C6-N1	2.18	1.36	1.33
26	BB	1962	5MC	C5-C4	2.21	1.44	1.41
1	AA	1402	4OC	C6-N1	2.22	1.38	1.35
2	AB	8	4SU	C6-N1	2.22	1.38	1.35
1	AA	967	5MC	C5-C4	2.26	1.44	1.41
1	AA	1402	4OC	C5-C4	2.26	1.44	1.39
2	AB	37	MIA	C2-S10	2.32	1.77	1.75
26	BB	2575	CH	C6-N1	2.34	1.38	1.35
2	AE	37	MIA	C2-S10	2.39	1.77	1.75
26	BB	2503	2MA	C6-N6	2.83	1.34	1.29
26	BB	747	5MU	C4-N3	3.35	1.39	1.33
2	AE	54	5MU	C4-N3	3.54	1.39	1.33
26	BB	2069	7MG	C6-N1	3.57	1.39	1.33
26	BB	2457	PSU	C4-N3	3.57	1.39	1.33
2	AE	39	PSU	C4-N3	3.58	1.39	1.33
2	AB	54	5MU	C4-N3	3.59	1.39	1.33
2	AB	46	7MG	C6-N1	3.59	1.39	1.33
26	BB	2552	OMU	C4-N3	3.60	1.39	1.33
26	BB	1939	5MU	C4-N3	3.60	1.39	1.33
2	AB	55	PSU	C4-N3	3.62	1.39	1.33
1	AA	516	PSU	C4-N3	3.62	1.39	1.33
2	AE	55	PSU	C4-N3	3.63	1.39	1.33
26	BB	2605	PSU	C4-N3	3.63	1.39	1.33
2	AB	39	PSU	C4-N3	3.66	1.39	1.33
2	AB	32	PSU	C4-N3	3.68	1.39	1.33
1	AA	1516	2MG	C6-N1	3.69	1.39	1.33
2	AE	32	PSU	C4-N3	3.71	1.39	1.33
2	AE	46	7MG	C6-N1	3.73	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BB	2504	PSU	C4-N3	3.73	1.39	1.33
26	BB	955	PSU	C4-N3	3.74	1.39	1.33
26	BB	2580	PSU	C4-N3	3.75	1.39	1.33
26	BB	746	PSU	C4-N3	3.80	1.39	1.33
1	AA	527	7MG	C6-N1	3.81	1.39	1.33
26	BB	1917	PSU	C4-N3	3.86	1.40	1.33
26	BB	2251	OMG	C6-N1	3.89	1.40	1.33
26	BB	1911	PSU	C4-N3	3.92	1.40	1.33
1	AA	966	2MG	C6-N1	3.94	1.40	1.33
1	AA	1207	2MG	C6-N1	3.94	1.40	1.33
26	BB	2445	2MG	C6-N1	4.00	1.40	1.33
26	BB	1835	2MG	C6-N1	4.14	1.40	1.33

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AE	54	5MU	C5-C4-N3	-13.67	113.88	125.35
2	AB	54	5MU	C5-C4-N3	-13.43	114.08	125.35
26	BB	747	5MU	C5-C4-N3	-13.18	114.28	125.35
26	BB	1939	5MU	C5-C4-N3	-12.79	114.62	125.35
1	AA	1516	2MG	C5-C6-N1	-8.60	112.27	123.52
1	AA	966	2MG	C5-C6-N1	-8.35	112.60	123.52
1	AA	1207	2MG	C5-C6-N1	-8.31	112.66	123.52
26	BB	2251	OMG	C5-C6-N1	-8.27	112.71	123.52
26	BB	2445	2MG	C5-C6-N1	-8.11	112.91	123.52
26	BB	1835	2MG	C5-C6-N1	-7.93	113.15	123.52
2	AB	46	7MG	C5-C6-N1	-7.92	111.61	123.39
1	AA	527	7MG	C5-C6-N1	-7.54	112.16	123.39
2	AE	46	7MG	C5-C6-N1	-7.51	112.21	123.39
26	BB	2069	7MG	C5-C6-N1	-7.49	112.25	123.39
26	BB	2503	2MA	C2-N3-C4	-6.31	112.25	115.29
2	AB	8	4SU	C5-C4-N3	-5.78	117.43	123.56
2	AE	8	4SU	C5-C4-N3	-5.00	118.26	123.56
1	AA	516	PSU	C5-C1'-C2'	-4.99	106.97	115.44
26	BB	745	1MG	C5-C6-N1	-4.86	111.99	118.35
1	AA	966	2MG	C4'-O4'-C1'	-4.74	104.61	109.64
2	AE	39	PSU	C5-C1'-C2'	-4.06	108.54	115.44
26	BB	955	PSU	C5-C1'-C2'	-3.82	108.95	115.44
26	BB	2605	PSU	C5-C1'-C2'	-3.75	109.07	115.44
26	BB	2552	OMU	C5-C4-N3	-3.73	114.12	123.28
1	AA	516	PSU	C5-C6-N1	-3.62	119.33	124.38
2	AE	39	PSU	C5-C6-N1	-3.58	119.39	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	32	PSU	C5-C1'-C2'	-3.41	109.65	115.44
26	BB	2457	PSU	C5-C6-N1	-3.39	119.65	124.38
2	AB	32	PSU	C5-C6-N1	-3.38	119.67	124.38
26	BB	2457	PSU	C5-C1'-C2'	-3.34	109.76	115.44
2	AE	32	PSU	C5-C6-N1	-3.24	119.86	124.38
26	BB	1915	3TD	C5-C6-N1	-3.21	119.91	124.38
26	BB	955	PSU	C5-C6-N1	-3.18	119.94	124.38
26	BB	746	PSU	C5-C6-N1	-3.18	119.95	124.38
1	AA	1519	MA6	C4'-O4'-C1'	-3.13	106.33	109.64
26	BB	1915	3TD	C5-C1'-C2'	-3.11	110.15	115.44
26	BB	1915	3TD	C5-C4-N3	-3.09	116.13	118.65
2	AE	55	PSU	C5-C6-N1	-3.08	120.08	124.38
26	BB	2251	OMG	N3-C2-N1	-3.05	123.40	127.56
26	BB	2605	PSU	C5-C6-N1	-2.97	120.24	124.38
2	AB	55	PSU	C5-C6-N1	-2.96	120.25	124.38
1	AA	1518	MA6	C1'-N9-C4	-2.91	123.56	126.81
1	AA	516	PSU	C4-C5-C1'	-2.88	116.37	121.22
26	BB	2030	6MZ	C4'-O4'-C1'	-2.80	106.67	109.64
2	AE	37	MIA	C5-C6-N1	-2.79	117.75	120.58
2	AB	37	MIA	C13-C12-N6	-2.79	107.04	112.25
26	BB	2504	PSU	C5-C6-N1	-2.78	120.51	124.38
2	AB	39	PSU	C5-C6-N1	-2.77	120.52	124.38
2	AB	16	H2U	C5-C6-N1	-2.77	107.73	110.76
2	AB	37	MIA	C5-C6-N1	-2.68	117.86	120.58
26	BB	1911	PSU	C5-C6-N1	-2.67	120.65	124.38
1	AA	966	2MG	C2'-C3'-C4'	-2.64	97.24	102.64
26	BB	2580	PSU	C5-C6-N1	-2.59	120.76	124.38
2	AB	16	H2U	O4'-C1'-C2'	-2.57	100.79	106.61
26	BB	1917	PSU	C5-C6-N1	-2.53	120.85	124.38
26	BB	1915	3TD	C2'-C3'-C4'	-2.52	97.49	102.64
1	AA	1519	MA6	C2'-C1'-N9	-2.51	106.73	113.47
2	AE	37	MIA	C1'-N9-C4	-2.49	124.03	126.81
1	AA	1519	MA6	C1'-N9-C4	-2.35	124.18	126.81
26	BB	746	PSU	C5-C1'-C2'	-2.33	111.48	115.44
26	BB	2449	H2U	O3'-C3'-C4'	-2.28	104.20	111.01
1	AA	1516	2MG	C1'-N9-C4	-2.27	124.27	126.81
2	AB	39	PSU	O2'-C2'-C1'	-2.21	107.12	111.93
26	BB	746	PSU	O3'-C3'-C4'	-2.18	104.48	111.01
26	BB	2030	6MZ	C1'-N9-C4	-2.16	124.39	126.81
26	BB	1835	2MG	C1'-N9-C4	-2.16	124.39	126.81
26	BB	1835	2MG	N3-C2-N1	-2.15	122.97	126.19
1	AA	966	2MG	N3-C2-N1	-2.15	122.97	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AE	32	PSU	C5-C1'-C2'	-2.14	111.80	115.44
1	AA	1518	MA6	O2'-C2'-C1'	-2.14	104.93	111.61
26	BB	2457	PSU	C4-C5-C1'	-2.11	117.67	121.22
1	AA	1498	UR3	O3'-C3'-C2'	-2.09	105.09	111.86
26	BB	2251	OMG	C1'-N9-C4	-2.09	124.47	126.81
26	BB	2504	PSU	O2'-C2'-C1'	-2.08	107.39	111.93
26	BB	2445	2MG	N3-C2-N1	-2.06	123.10	126.19
1	AA	1516	2MG	N3-C2-N1	-2.05	123.13	126.19
2	AB	55	PSU	O4'-C1'-C2'	2.00	106.86	104.69
1	AA	967	5MC	CM5-C5-C4	2.00	123.59	121.47
26	BB	2552	OMU	O4'-C1'-N1	2.01	111.93	108.10
26	BB	2069	7MG	N2-C2-N3	2.02	120.54	117.20
26	BB	2251	OMG	O5'-C5'-C4'	2.04	116.40	109.09
26	BB	2575	CH	O4'-C1'-N1	2.09	112.07	108.10
1	AA	966	2MG	O3'-C3'-C4'	2.09	117.26	111.01
2	AE	39	PSU	O4'-C1'-C2'	2.09	106.95	104.69
2	AB	37	MIA	C2-N1-C6	2.15	119.04	113.13
26	BB	1962	5MC	O4'-C1'-N1	2.17	112.23	108.10
26	BB	2552	OMU	C6-C5-C4	2.18	121.34	117.30
26	BB	2504	PSU	O4'-C1'-C2'	2.19	107.05	104.69
26	BB	2605	PSU	O4'-C1'-C2'	2.19	107.06	104.69
2	AE	8	4SU	O3'-C3'-C4'	2.21	117.60	111.01
2	AB	39	PSU	C4'-O4'-C1'	2.22	111.83	109.54
1	AA	1516	2MG	O4'-C1'-N9	2.23	112.32	108.11
1	AA	1498	UR3	C6-C5-C4	2.24	121.45	117.30
2	AB	32	PSU	O4'-C1'-C2'	2.25	107.13	104.69
2	AB	54	5MU	O3'-C3'-C2'	2.29	119.24	111.86
1	AA	966	2MG	O4'-C1'-N9	2.29	112.42	108.11
2	AB	47	3AU	C6-C5-C4	2.29	121.55	117.30
2	AE	37	MIA	C2-N1-C6	2.33	119.53	113.13
26	BB	2449	H2U	C1'-N1-C2	2.35	121.48	118.19
1	AA	1498	UR3	O5'-C5'-C4'	2.36	117.56	109.09
26	BB	2503	2MA	O3'-C3'-C2'	2.37	119.51	111.86
2	AB	20	H2U	C1'-N1-C2	2.38	121.52	118.19
2	AE	16	H2U	C1'-N1-C2	2.41	121.57	118.19
2	AB	37	MIA	N6-C6-N1	2.42	121.43	118.55
2	AE	46	7MG	O3'-C3'-C4'	2.43	118.28	111.01
2	AE	46	7MG	C8-N9-C1'	2.48	129.86	122.43
2	AE	20	H2U	C1'-N1-C2	2.51	121.70	118.19
26	BB	1917	PSU	C3'-C2'-C1'	2.57	104.76	101.71
26	BB	2457	PSU	C3'-C2'-C1'	2.57	104.76	101.71
26	BB	2580	PSU	O4'-C1'-C2'	2.72	107.64	104.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	2445	2MG	N2-C2-N3	2.72	120.10	116.94
1	AA	1518	MA6	O4'-C1'-N9	2.75	113.31	108.11
26	BB	1917	PSU	C4'-O4'-C1'	2.81	112.44	109.54
2	AE	55	PSU	O4'-C1'-C2'	2.81	107.73	104.69
26	BB	2445	2MG	O4'-C1'-N9	2.82	113.42	108.11
1	AA	1519	MA6	O3'-C3'-C2'	2.89	121.19	111.86
2	AE	37	MIA	O4'-C1'-N9	2.89	113.56	108.11
26	BB	1835	2MG	N2-C2-N3	2.93	120.34	116.94
1	AA	1402	4OC	O4'-C1'-N1	2.99	113.79	108.10
1	AA	516	PSU	O4'-C1'-C2'	3.04	107.97	104.69
26	BB	2457	PSU	O4'-C1'-C2'	3.07	108.01	104.69
1	AA	1498	UR3	O4'-C1'-N1	3.10	113.99	108.10
26	BB	745	1MG	O4'-C1'-N9	3.11	113.98	108.11
26	BB	747	5MU	O3'-C3'-C2'	3.12	121.93	111.86
26	BB	2504	PSU	C3'-C2'-C1'	3.16	105.45	101.71
2	AE	47	3AU	O4'-C4'-C3'	3.16	111.56	105.16
26	BB	2498	OMC	C4'-O4'-C1'	3.20	113.03	109.64
1	AA	1207	2MG	N2-C2-N3	3.32	120.79	116.94
1	AA	1402	4OC	CM4-N4-C4	3.36	125.70	122.87
26	BB	2030	6MZ	C2-N1-C6	3.42	118.93	116.47
1	AA	1516	2MG	N2-C2-N3	3.43	120.93	116.94
2	AE	32	PSU	O4'-C1'-C2'	3.46	108.44	104.69
2	AB	37	MIA	C12-N6-C6	3.56	127.58	123.46
26	BB	1618	6MZ	C2-N1-C6	3.83	119.22	116.47
1	AA	1519	MA6	C2-N1-C6	3.89	120.82	111.64
1	AA	966	2MG	N2-C2-N3	3.91	121.48	116.94
1	AA	1518	MA6	C2-N1-C6	4.02	121.11	111.64
2	AB	37	MIA	C11-S10-C2	4.23	105.29	102.31
2	AE	37	MIA	C11-S10-C2	4.31	105.35	102.31
1	AA	1402	4OC	C2-N3-C4	5.62	122.58	115.43
26	BB	1835	2MG	C6-N1-C2	5.72	123.43	115.24
26	BB	2445	2MG	C6-N1-C2	5.74	123.46	115.24
1	AA	1207	2MG	C6-N1-C2	5.95	123.76	115.24
1	AA	966	2MG	C6-N1-C2	6.29	124.24	115.24
1	AA	1516	2MG	C6-N1-C2	6.44	124.47	115.24
26	BB	2251	OMG	C6-N1-C2	6.77	123.81	115.88
26	BB	2069	7MG	C6-N1-C2	6.84	123.90	115.88
2	AE	46	7MG	C6-N1-C2	7.01	124.10	115.88
1	AA	527	7MG	C6-N1-C2	7.31	124.45	115.88
2	AB	46	7MG	C6-N1-C2	7.82	125.05	115.88
26	BB	2552	OMU	C4-N3-C2	10.78	125.57	114.21
26	BB	1939	5MU	C4-N3-C2	11.69	124.92	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	516	PSU	C4-N3-C2	11.88	125.07	115.16
2	AE	39	PSU	C4-N3-C2	12.43	125.53	115.16
2	AE	32	PSU	C4-N3-C2	12.60	125.67	115.16
26	BB	1911	PSU	C4-N3-C2	12.63	125.69	115.16
26	BB	747	5MU	C4-N3-C2	12.73	125.78	115.16
26	BB	955	PSU	C4-N3-C2	12.77	125.81	115.16
2	AB	32	PSU	C4-N3-C2	12.88	125.90	115.16
2	AB	55	PSU	C4-N3-C2	12.89	125.91	115.16
26	BB	746	PSU	C4-N3-C2	12.90	125.92	115.16
26	BB	2457	PSU	C4-N3-C2	12.91	125.93	115.16
26	BB	2580	PSU	C4-N3-C2	13.03	126.03	115.16
26	BB	2605	PSU	C4-N3-C2	13.14	126.12	115.16
2	AE	55	PSU	C4-N3-C2	13.15	126.13	115.16
26	BB	1917	PSU	C4-N3-C2	13.32	126.27	115.16
26	BB	2504	PSU	C4-N3-C2	13.33	126.28	115.16
2	AB	54	5MU	C4-N3-C2	13.33	126.28	115.16
2	AB	39	PSU	C4-N3-C2	13.49	126.42	115.16
2	AE	54	5MU	C4-N3-C2	13.75	126.63	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.