



Full wwPDB EM Validation Report ⓘ

Feb 22, 2024 – 09:22 AM EST

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 initial models : 2I2U, 3FIH

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

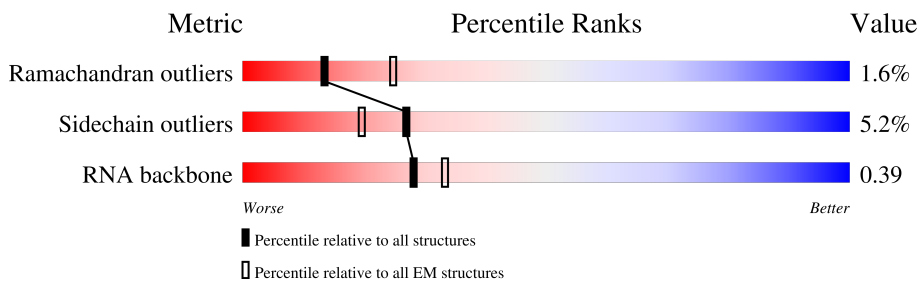
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	AA	1542	
2	AB	76	
2	AE	76	
3	AC	393	
4	AD	24	
5	AF	241	
6	AG	233	
7	AH	206	

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Mol	Chain	Length	Quality of chain
8	AI	167	9% 93% 6%
9	AJ	135	6% 89% 10%
10	AK	179	92% 7%
11	AL	130	93% 6%
12	AM	130	91% 8%
13	AN	103	5% 90% 9%
14	AO	129	12% 95% 5%
15	AP	124	6% 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	10% 87% 11%
25	BA	120	21% 50% 25%
26	BB	2904	21% 49% 26%
27	BC	234	14% 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%

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Mol	Chain	Length	Quality of chain
33	BI	149	30% 93% 7%
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	5% 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	8% 86% 13%
49	BY	78	91% 6%
50	BZ	63	94% 6%
51	Ba	59	95% ..
52	Bb	70	9% 96% .
53	Bc	57	5% 91% 7%
54	Bd	55	98% .
55	Be	46	98% .
56	Bf	65	95% ..
57	Bg	38	87% 13%

2 Entry composition [i](#)

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
			Total	C	N	O	P		
1	AA	1542	33089	14767	6064	10717	1541	0	0

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

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

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

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

- Molecule 4 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
20	AU	83	672	425	124	120	3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
34	BJ	141	1032	651	179	196	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
55	Be	46	377	228	90	57	2	0	0

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

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

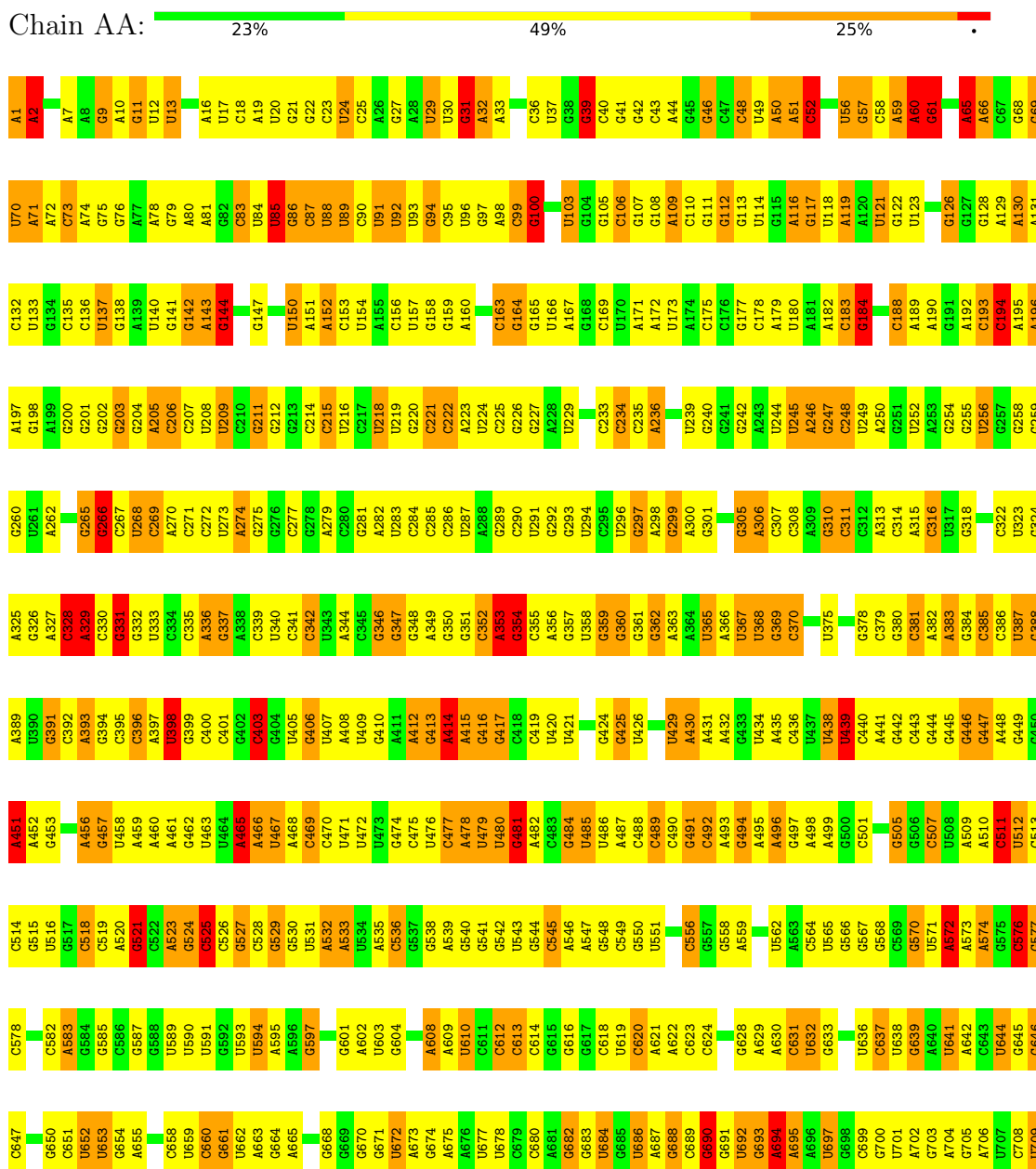
- Molecule 57 is a protein called 50S ribosomal protein L36.

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

3 Residue-property plots

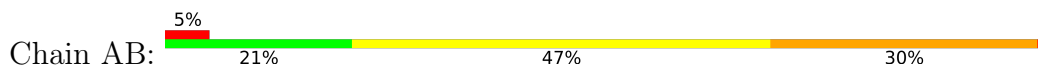
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

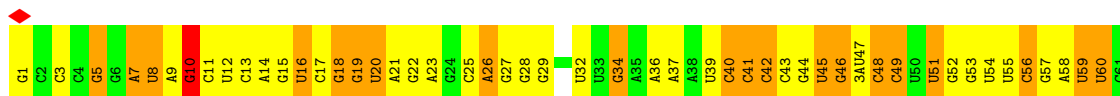
- Molecule 1: 16S ribosomal RNA



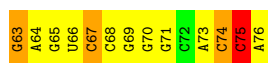
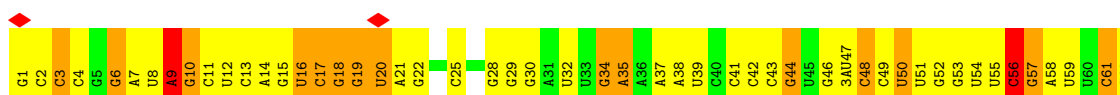
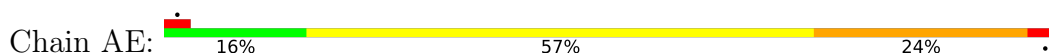
A1542	A1480	G1415	U1351	C1218	G1154	U1091	C1028	G966	C889	U837	G776	G710	
A1481	G1416	A1219	C1352	A1219	A1155	A1092	U1029	G967	A900	G838	A777	G711	
A1482	G1417	G1220	G1353	G1220	A1156	A1093	U1030	C968	A901	C839	A778	A712	
A1483	G1418	G1221	G1354	G1221	A1157	G1094	C1031	A969	G902	C840	C779	G713	
A1484	G1419	G1222	G1355	A1222	U1158	U1095	G1032	A969	G903	C841	A780	G714	
A1485	G1420	G1223	G1356	C1223	U1159	U1096	G1033	C970	G904	U842	A781	A715	
U1424	U1425	U1224	A1357	U1224	G1160	C1097	G1034	C971	U905	U843	A782	C719	
U1426	U1358	A1225	U1358	C1225	C1161	C1098	A1035	C972	A906	G844	C783	C720	
U1426	C1359	A1226	C1359	A1226	C1162	G1099	A1036	C973	A907	A845	A794	G720	
C1427	A1360	A1227	G1360	A1227	A1163	C1100	C1037	A974	A908	G846	G785	G721	
A1428	G1361	C1228	G1361	C1228	A1164	A1101	C1038	A975	A909	G847	G786	G722	
A1429	U1295	U1229	U1295	U1229	U1165	C1102	G1039	G976	C910	C848	A787	U723	
A1363	U1363	C1230	U1363	C1230	A1166	A1103	U1040	A977	U911	G849	U788	G724	
U1364	U1364	G1231	A1364	G1231	A1169	G1104	G1041	A978	G912	U850	G725	G725	
G1365	G1365	U1232	G1365	U1232	C1172	A1105	A1042	C979	A913	G851	A790	C726	
C1366	U1301	G1233	U1301	G1233	C1173	G1106	G1043	C980	G791	C732	G732	C732	
C1369	C1302	U1235	C1302	U1235	G1174	C1109	A1044	U981	A916	U855	U793	G733	
G1370	G1303	A1236	G1303	A1236	G1175	A1111	A1045	A983	U915	C856	A794	G734	
G1371	G1304	C1237	G1304	C1237	A1176	C1112	G1047	C984	G917	C857	C795	C735	
U1372	G1305	G1241	U1372	G1241	G1177	C1113	G1048	C985	U920	G858	C796	C736	
G1373	A1306	G1242	G1373	G1242	A1178	C1114	U1049	U986	U921	G859	C797	C737	
A1374	U1307	A1243	A1374	A1243	A1179	U1115	G1050	G987	A922	A860	C798	C738	
A1375	U1308	C1243	U1308	C1243	A1180	U1116	G1051	G988	A923	G861	C799	C739	
U1376	G1309	G1244	U1376	G1244	G1181	A1117	U1052	U989	G928	G862	U740	C740	
A1377	G1310	C1245	A1377	C1245	G1182	U1118	G1053	C990	G929	U863	G741	C741	
C1378	A1311	A1246	C1378	A1246	U1183	C1119	C1054	U991	G930	A864	A802	G742	
U1379	G1312	U1247	U1379	U1247	G1184	C1120	A1055	U992	C931	A865	G803	A743	
U1380	U1313	A1248	U1380	A1248	G1185	U1121	G1056	G993	C932	A866	G804	C744	
A1447	C1314	C1249	A1447	C1249	G1186	U1122	G1057	A994	C933	G867	C805	G745	
C1382	U1315	A1250	C1382	A1250	G1187	U1123	G1058	C995	G933	C868	C806	A746	
C1383	G1316	G1251	C1383	G1251	A1188	G1124	C1059	A996	C934	G869	A807	A747	
C1384	C1317	G1252	C1384	G1252	U1189	U1125	C1060	U997	A935	U870	G748	C748	
G1385	A1318	A1254	G1385	A1254	G1190	U1126	G1061	C998	C936	U871	G809	A749	
C1388	A1319	G1255	C1388	G1255	A1191	G1127	U1062	C999	A937	A872	C810	C750	
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U1392	G1323	C1259	U1392	C1259	C1195	G1131	C1066	G1003	G943	C876	A814	C754	
C1395	A1324	G1260	C1395	G1260	A1196	C1132	A1067	A1004	U943	A815	A815	G755	
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C1399	C1328	C1267	C1399	C1267	C1200	C1136	C1071	U1008	G947	U819	A819	A759	
C1400	A1329	G1268	C1400	G1268	A1201	C1137	G1072	U1009	C948	C882	U820	G760	
G1401	U1330	A1269	G1401	A1269	U1202	G1138	U1073	U1010	A949	G883	G821	G761	
C1402	A1333	G1270	C1402	G1270	A1204	C1140	G1074	C1011	U950	U884	U822	U762	
G1405	U1337	G1271	G1405	G1271	U1205	C1141	U1075	G1013	G951	G885	G823	G763	
U1406	G1338	C1272	U1406	C1272	G1206	G1142	G1077	A1014	G953	G887	G824	C764	
C1407	A1339	C1273	C1407	C1273	G1207	G1143	U1078	G1015	G954	G888	C826	A766	
A1408	A1340	A1274	A1408	A1274	C1208	G1144	U1083	A1016	A889	A889	A767	A767	
C1409	U1341	A1275	C1409	A1275	C1209	A1145	G1084	U1017	U955	G890	U828	A768	
C1410	C1342	G1276	C1410	G1276	A1146	G1146	G1085	G1018	U957	U891	G829	G769	
A1410	G1343	C1277	A1410	C1277	C1147	U1147	U1086	G1018	A958	A892	C830	C770	
C1411	U1343	G1279	C1411	G1279	U1148	U1148	U1087	A1021	A959	A895	G771	G771	
C1412	A1346	A1280	C1412	A1280	A1151	U1148	G1088	U1025	U960	C896	G833	G833	
A1414	A1347	C1281	A1414	C1281	A1152	U1152	G1089	G1026	U961	C897	U834	G773	
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												G775	G775

• Molecule 2: A/T-site tRNA Phe

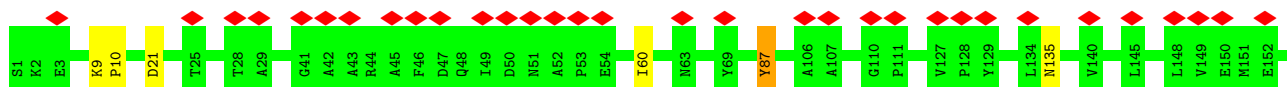




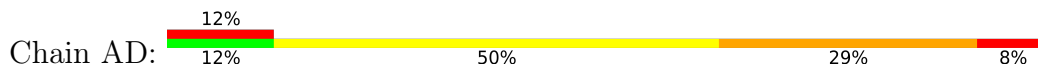
• Molecule 2: A/T-site tRNA Phe



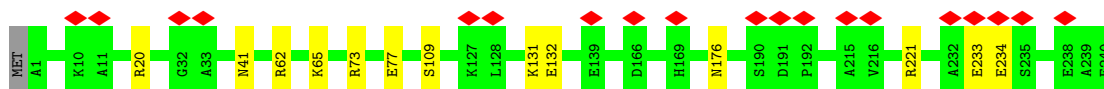
• Molecule 3: Elongation factor Tu 2



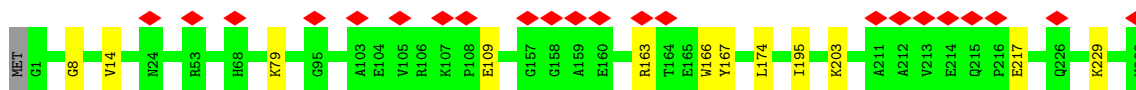
• Molecule 4: mRNA



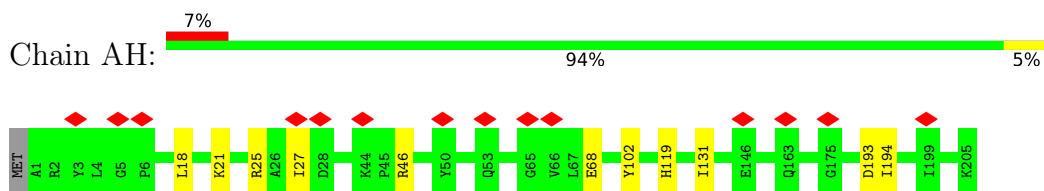
• Molecule 5: 30S ribosomal protein S2



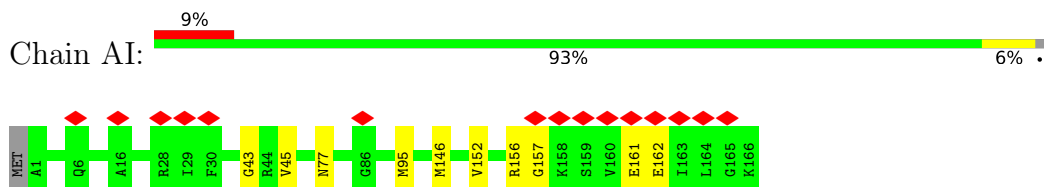
• Molecule 6: 30S ribosomal protein S3



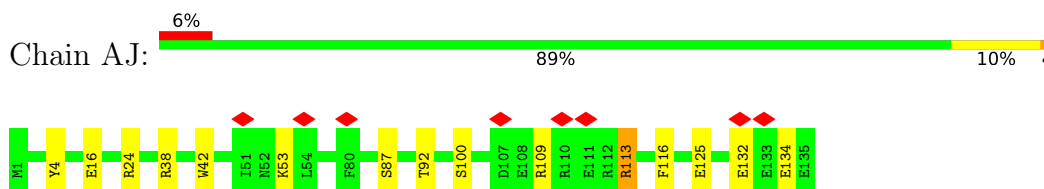
- Molecule 7: 30S ribosomal protein S4



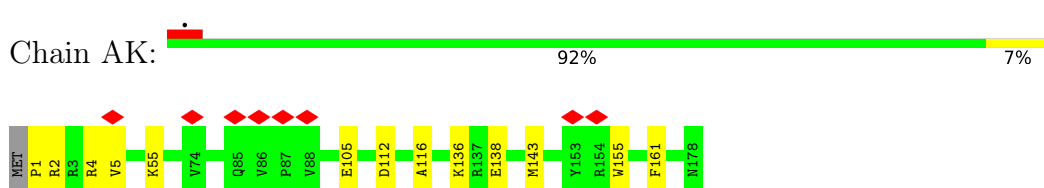
- Molecule 8: 30S ribosomal protein S5



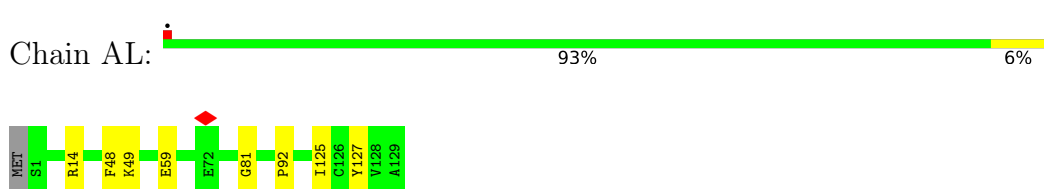
- Molecule 9: 30S ribosomal protein S6



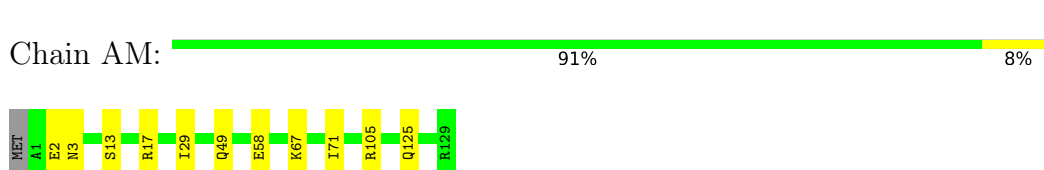
- Molecule 10: 30S ribosomal protein S7



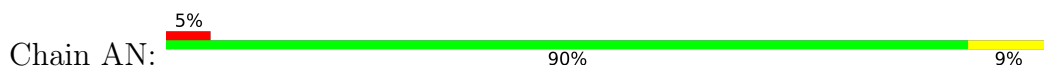
- Molecule 11: 30S ribosomal protein S8



- Molecule 12: 30S ribosomal protein S9

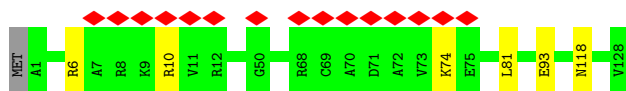


- Molecule 13: 30S ribosomal protein S10

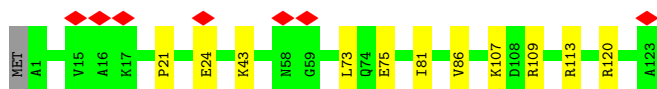
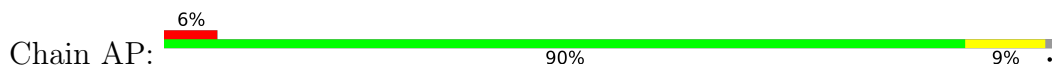




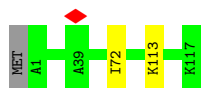
- Molecule 14: 30S ribosomal protein S11



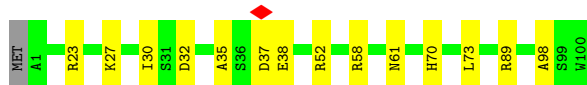
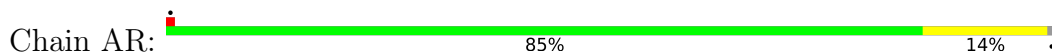
- Molecule 15: 30S ribosomal protein S12



- Molecule 16: 30S ribosomal protein S13



- Molecule 17: 30S ribosomal protein S14



- Molecule 18: 30S ribosomal protein S15



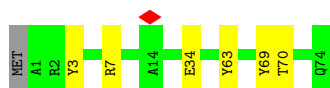
- Molecule 19: 30S ribosomal protein S16



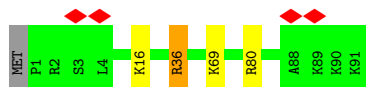
- Molecule 20: 30S ribosomal protein S17



• Molecule 21: 30S ribosomal protein S18



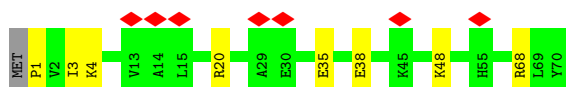
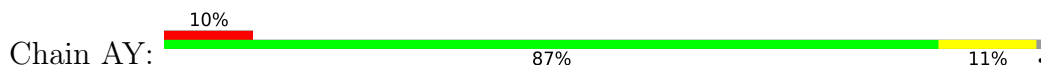
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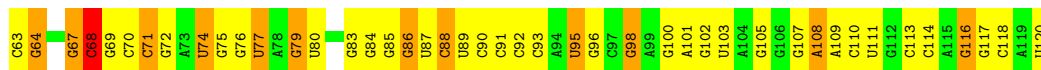
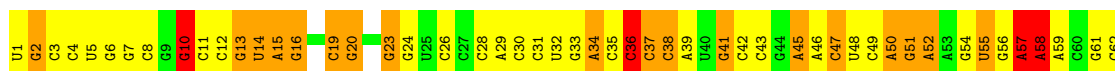
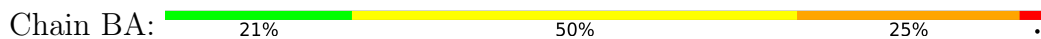
• Molecule 23: 30S ribosomal protein S20



• Molecule 24: 30S ribosomal protein S21



• Molecule 25: 50S ribosomal RNA 5S



• Molecule 26: 50S ribosomal RNA 23S



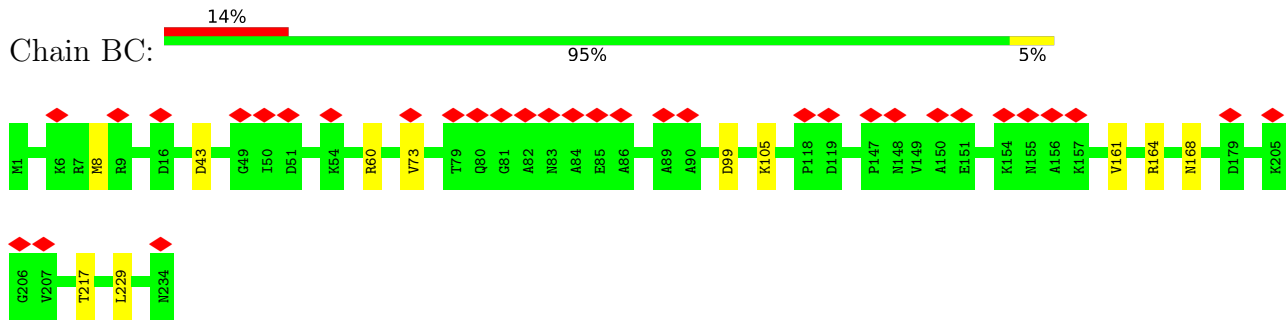
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C1881	A1819	U1751	A1690	A1439	G1374	G1313	G1250	G1187	C1123	G1061	C998
U1882	G1752	C1752	U1691	U1440	G1375	U1313	C1251	U1188	G1124	G1062	U999
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U1889	U1828	C1760	U1698	C1447	G1382	G1324	U1258	A1195	G1131	A1069	C1007
A1890	G1828	A1761	G1699	U1448	G1383	G1324	G1259	A1196	U1132	A1070	
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U1900	U1840	A1772	U1709	G1459	A1393	G1333	A1269	C1207	A1142	A1080	U1018
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	C1844	G1776		C1463	U1397	G1337	U1273	C1211	C1146	A1084	G1022
G1906	G1845	U1777			C1398	G1338	A1274	G1212	A1147	A1085	U1023
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U1909	A1847	U1779	A1685	U1467	U1340	U1340	G1276	A1214	G1149	G1087	G1025
G1910	A1848	A1780	G1686		G1341	G1341	G1277	G1215	C1150	A1088	G1026
U1911	G1849	U1781	G1687		A1342	U1342	C1278	G1216	A1151	A1089	A1027
A1912	G1850	U1782	C1688		U1403	G1343	G1279	U1217	C1152	A1090	A1028
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U1918	U1856	C1788	A1694		G1410	G1349	A1285	G1223	A1096	A1096	G1034
A1919	G1857		A1695		U1411	C1350	A1286		G1161	U1097	U1035
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C1933	A1871	G1807	U1619		A1494	G1364	G1300	U1240	G1177	A1111	C1052
C1934	A1872	A1808	G1620		A1495	A1365	A1301	A1241	C1178	G1112	C1053
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A1936	C1874	A1810	G1622		C1497	A1367	G1303	C1243	G1180	C1114	A1054
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U1939	A1877	G1813	C1625		U1500	G1370	C1306	A1246	U1183	C1117	A1057
U1940	G1878	C1814	A1626		A1502	G1371	A1307	A1247	U1184	C1118	U1058

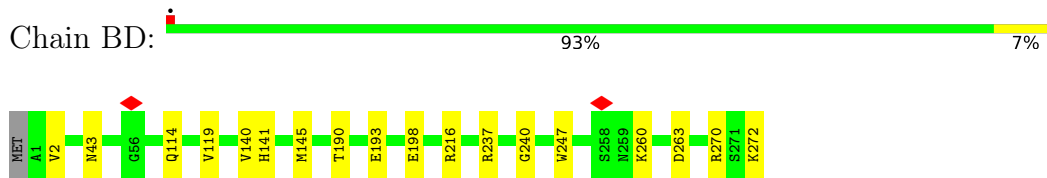
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A2134	A2135	G2138	G2139	G2140	G2141	A2142	A2143	A2144	G2145	G2146	G2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	G2157	G2158	G2159	G2160	C2161	A2162	A2163	C2164	G2168	A2169	A2170	A2171	U2172	U2173	G2174	G2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2185	U2186	U2187	U2188	U2189	G2190	A2191	U2192	G2193	U2194	U2195	C2196	U2197	A2198	A2199	G2200	G2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	G2230	U2231	U2232	U2233	U2234	G2235	U2236	G2237	U2238	G2239	U2240	A2241	G2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	U2257	U2258	U2259	U2260	U2261	U2262	U2263	U2264	U2265	U2266	U2267	U2268	U2269	U2270	U2271	U2272	A2273	A2274	A2275	A2276	A2277	A2278	A2281	G2282	C2283	A2284	C2285	G2286	A2287	A2288	G2293	G2294	C2295	U2296	A2297	A2298	U2299	G2300	C2301	U2302	G2303	G2304	U2305	G2306	G2307	G2308	A2309	A2310	A2311	U2312	G2313	A2314	A2317	G2318	G2319	G2320	G2321	G2322	U2323	U2324	G2325	G2326	U2327	U2328	U2329	U2330	U2331	U2332	U2333	U2334	U2335	U2336	U2337	U2338	U2339	U2340	U2341	U2342	U2343	U2344	U2345	U2346	U2347	U2348	U2349	U2350	U2351	U2352	U2353	U2354	U2355	U2356	U2357	U2358	U2359	U2360	U2361	U2362	U2363	U2364	U2365	U2366	U2367	U2368	U2369	U2370	U2371	U2372	U2373	U2374	U2375	U2376	U2377	U2378	U2379	U2380	U2381	U2382	U2383	U2384	U2385	U2386	U2387	U2388	U2389	U2390	U2391	U2392	U2393	U2394	U2395	U2396	U2397	U2398	U2399	U2400	U2401	U2402	U2403	U2404	U2405	U2406	U2407	U2408	U2409	U2410	U2411	U2412	U2413	U2414	U2415	U2416	U2417	U2418	U2419	U2420	U2421	U2422	U2423	U2424	U2425	U2426	U2427	U2428	U2429	U2430	U2431	U2432	U2433	U2434	U2435	U2436	U2437	U2438	U2439	U2440	U2441	U2442	U2443	U2444	U2445	U2446	U2447	U2448	U2449	U2450	U2451	U2452	U2453	U2454	U2455	U2456	U2457	U2458	U2459	U2460	U2461	U2462	U2463	U2464	U2465	U2466	U2467	U2468	U2469	U2470	U2471	U2472	U2473	U2474	U2475	U2476	U2477	U2478	U2479	U2480	U2481	U2482	U2483	U2484	U2485	U2486	U2487	U2488	U2489	U2490	U2491	U2492	U2493	U2494	U2495	U2496	U2497	U2498	U2499	U2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	A2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550	C2551	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625	C2626	C2627	C2628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	C2712	C2713	C2714	C2715	C2716	C2717	C2718	C2719	C2720	C2721	C2722	C2723	C2724	C2725	C2726	C2727	C2728	C2729	C2730	C2731	C2732	C2733	C2734	C2735	C2736	C2737	C2738	C2739	C2740	C2741	C2742	C2743	C2744	C2745	C2746	C2747	C2748	C2749	C2750	C2751	C2752	C2753	C2754	C2755	C2756	C2757	C2758	C2759	C2760	C2761	C2762	C2763	C2764	C2765	C2766	C2767	C2768	C2769	C2770	C2771	C2772	C2773	C2774	C2775	C2776	C2777	C2778	C2779	C2780	C2781	C2782	C2783	C2784	C2785	C2786	C2787	C2788	C2789	C2790	C2791	C2792	C2793	C2794	C2795	C2796	C2797	C2798	C2799	C2800	C2801	C2802	C2803	C2804	C2805	C2806	C2807	C2808	C2809	C2810	C2811	C2812	C2813	C2814	C2815	C2816	C2817	C2818	C2819	C2820	C2821	C2822	C2823	C2824	C2825	C2826	C2827	C2828	C2829	C2830	C2831	C2832	C2833	C2834	C2835	C2836	C2837	C2838	C2839	C2840	C2841	C2842	C2843	C2844	C2845	C2846	C2847	C2848	C2849	C2850	C2851	C2852	C2853	C2854	C2855	C2856	C2857	C2858	C2859	C2860	C2861	C2862	C2863	C2864	C2865	C2866	C2867	C2868	C2869	C2870	C2871	C2872	C2873	C2874	C2875	C2876	C2877	C2878	C2879	C2880	C2881	C2882	C2883	C2884	C2885	C2886	C2887	C2888	C2889	C2890	C2891	C2892	C2893	C2894	C2895	C2896	C2897	C2898	C2899	C2900	C2901	C2902

U2903
U2904

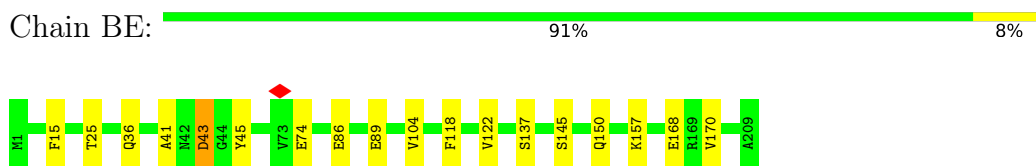
- Molecule 27: 50S ribosomal protein L1



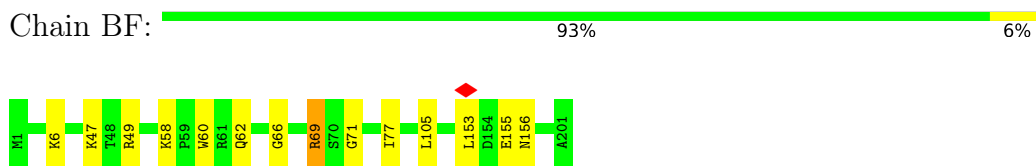
- Molecule 28: 50S ribosomal protein L2



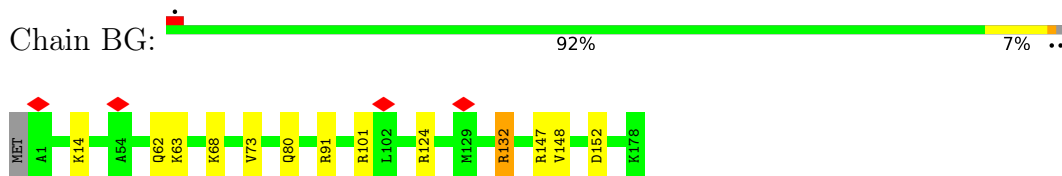
- Molecule 29: 50S ribosomal protein L3



- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5

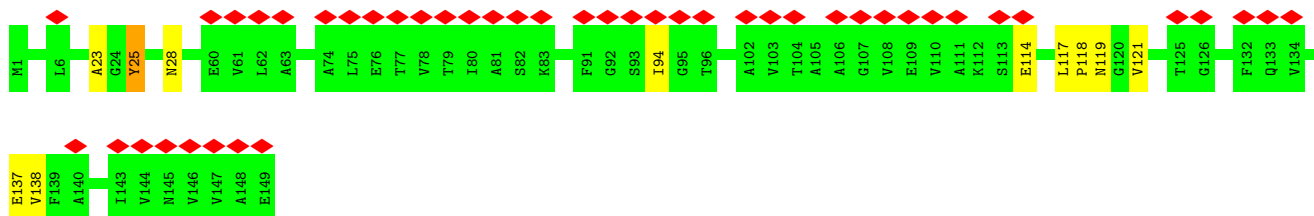


- Molecule 32: 50S ribosomal protein L6

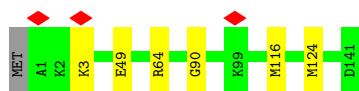




- Molecule 33: 50S ribosomal protein L9



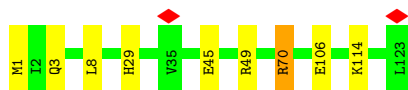
- Molecule 34: 50S ribosomal protein L11



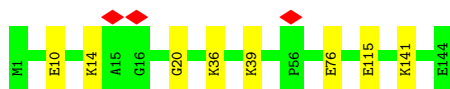
- Molecule 35: 50S ribosomal protein L13



- Molecule 36: 50S ribosomal protein L14



- Molecule 37: 50S ribosomal protein L15

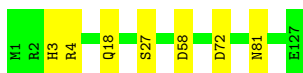


- Molecule 38: 50S ribosomal protein L16





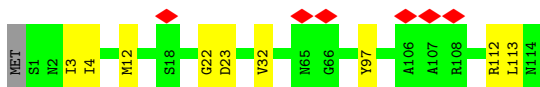
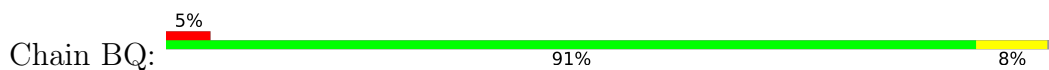
- Molecule 39: 50S ribosomal protein L17



- Molecule 40: 50S ribosomal protein L18



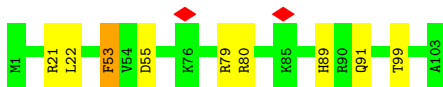
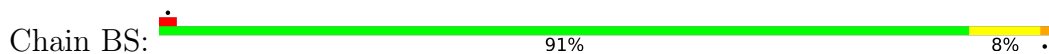
- Molecule 41: 50S ribosomal protein L19



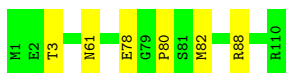
- Molecule 42: 50S ribosomal protein L20



- Molecule 43: 50S ribosomal protein L21

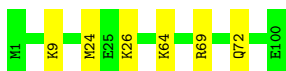


- Molecule 44: 50S ribosomal protein L22

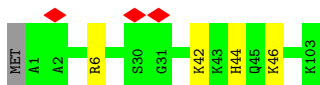


- Molecule 45: 50S ribosomal protein L23





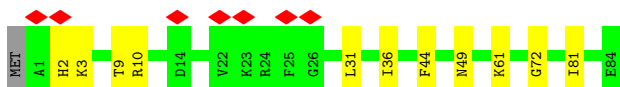
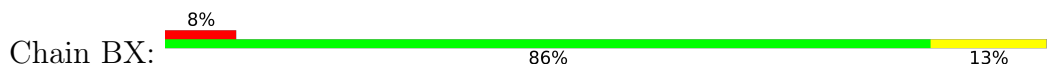
- Molecule 46: 50S ribosomal protein L24



- Molecule 47: 50S ribosomal protein L25



- Molecule 48: 50S ribosomal protein L27



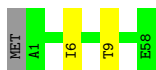
- Molecule 49: 50S ribosomal protein L28



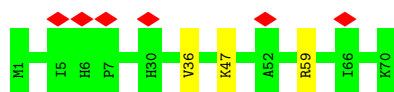
- Molecule 50: 50S ribosomal protein L29



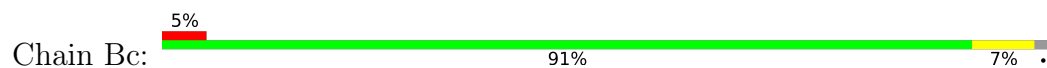
- Molecule 51: 50S ribosomal protein L30



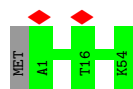
- Molecule 52: 50S ribosomal protein L31



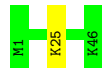
- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L33



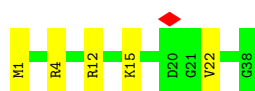
- Molecule 55: 50S ribosomal protein L34



- Molecule 56: 50S ribosomal protein L35



- Molecule 57: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26873	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	267.364	Depositor
Minimum map value	-80.270	Depositor
Average map value	5.966	Depositor
Map value standard deviation	25.669	Depositor
Recommended contour level	32.5	Depositor
Map size (\AA)	375, 375, 375	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	1.5, 1.5, 1.5	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	1.22	1/36769 (0.0%)	2.00	1273/57354 (2.2%)
2	AB	1.25	0/1580	2.01	56/2459 (2.3%)
2	AE	1.26	0/1580	2.04	66/2459 (2.7%)
3	AC	0.61	0/3092	0.97	1/4183 (0.0%)
4	AD	1.37	0/548	1.98	20/848 (2.4%)
5	AF	0.60	0/1904	1.00	1/2565 (0.0%)
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%)
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%)
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
30	BF	0.58	0/1571	1.01	1/2113 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
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
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
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%)
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
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
2	AB	0	19
2	AE	0	15
3	AC	0	1
4	AD	0	9
6	AG	0	1
7	AH	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	AI	0	3
9	AJ	0	1
11	AL	0	1
13	AN	0	1
14	AO	0	1
15	AP	0	1
17	AR	0	2
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
30	BF	0	2
32	BH	0	2
33	BI	0	1
41	BQ	0	1
42	BR	0	1
43	BS	0	1
48	BX	0	1
49	BY	0	1
53	Bc	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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%)	19	60
5	AF	238/241 (99%)	215 (90%)	21 (9%)	2 (1%)	19	60
6	AG	230/233 (99%)	210 (91%)	18 (8%)	2 (1%)	17	57
7	AH	203/206 (98%)	189 (93%)	12 (6%)	2 (1%)	15	55
8	AI	164/167 (98%)	143 (87%)	18 (11%)	3 (2%)	8	40
9	AJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	10	46
10	AK	176/179 (98%)	159 (90%)	15 (8%)	2 (1%)	14	52
11	AL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	9	44
12	AM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	9	44
13	AN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	3	23
14	AO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	9	44
15	AP	121/124 (98%)	103 (85%)	13 (11%)	5 (4%)	3	23
16	AQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
17	AR	98/101 (97%)	82 (84%)	9 (9%)	7 (7%)	1	14
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%)	11	46
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%)	10	46
27	BC	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	12	48
28	BD	270/273 (99%)	239 (88%)	22 (8%)	9 (3%)	4	26
29	BE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	4	29
30	BF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	10	46
31	BG	176/179 (98%)	148 (84%)	25 (14%)	3 (2%)	9	42
32	BH	174/177 (98%)	162 (93%)	9 (5%)	3 (2%)	9	42
33	BI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	3	26
34	BJ	139/142 (98%)	121 (87%)	17 (12%)	1 (1%)	22	63
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%)	9	42
37	BM	142/144 (99%)	124 (87%)	16 (11%)	2 (1%)	11	46
38	BN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	6	35
39	BO	125/127 (98%)	116 (93%)	8 (6%)	1 (1%)	19	60
40	BP	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17	57
41	BQ	112/115 (97%)	99 (88%)	11 (10%)	2 (2%)	8	40
42	BR	115/118 (98%)	109 (95%)	5 (4%)	1 (1%)	17	57
43	BS	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	4	28
44	BT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	17	57
45	BU	98/100 (98%)	86 (88%)	11 (11%)	1 (1%)	15	55
46	BV	101/104 (97%)	90 (89%)	10 (10%)	1 (1%)	15	55
47	BW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	6	35
48	BX	82/85 (96%)	68 (83%)	11 (13%)	3 (4%)	3	24
49	BY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	5	31
50	BZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	2	20
51	Ba	56/59 (95%)	53 (95%)	2 (4%)	1 (2%)	8	40
52	Bb	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	46
53	Bc	54/57 (95%)	46 (85%)	6 (11%)	2 (4%)	3	24
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%)	5	30
All	All	6548/6682 (98%)	5895 (90%)	547 (8%)	106 (2%)	13	44

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	326/326 (100%)	311 (95%)	15 (5%)	27	52
5	AF	198/199 (100%)	188 (95%)	10 (5%)	24	48
6	AG	189/190 (100%)	180 (95%)	9 (5%)	25	51
7	AH	172/173 (99%)	164 (95%)	8 (5%)	26	51
8	AI	125/126 (99%)	122 (98%)	3 (2%)	49	69
9	AJ	116/116 (100%)	104 (90%)	12 (10%)	7	25
10	AK	146/147 (99%)	136 (93%)	10 (7%)	16	41
11	AL	104/105 (99%)	99 (95%)	5 (5%)	25	51
12	AM	106/107 (99%)	98 (92%)	8 (8%)	13	38
13	AN	90/90 (100%)	85 (94%)	5 (6%)	21	46
14	AO	98/99 (99%)	95 (97%)	3 (3%)	40	62
15	AP	103/104 (99%)	98 (95%)	5 (5%)	25	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AQ	95/96 (99%)	93 (98%)	2 (2%)	53	72
17	AR	83/84 (99%)	79 (95%)	4 (5%)	25	51
18	AS	76/77 (99%)	71 (93%)	5 (7%)	16	41
19	AT	65/65 (100%)	62 (95%)	3 (5%)	27	52
20	AU	77/78 (99%)	75 (97%)	2 (3%)	46	66
21	AV	64/65 (98%)	60 (94%)	4 (6%)	18	43
22	AW	78/79 (99%)	74 (95%)	4 (5%)	24	48
23	AX	65/66 (98%)	61 (94%)	4 (6%)	18	43
24	AY	60/61 (98%)	55 (92%)	5 (8%)	11	34
27	BC	181/181 (100%)	176 (97%)	5 (3%)	43	65
28	BD	217/218 (100%)	210 (97%)	7 (3%)	39	61
29	BE	164/164 (100%)	153 (93%)	11 (7%)	16	41
30	BF	165/165 (100%)	156 (94%)	9 (6%)	21	47
31	BG	149/150 (99%)	138 (93%)	11 (7%)	13	38
32	BH	137/138 (99%)	128 (93%)	9 (7%)	16	41
33	BI	114/114 (100%)	109 (96%)	5 (4%)	28	53
34	BJ	109/110 (99%)	104 (95%)	5 (5%)	27	52
35	BK	116/116 (100%)	110 (95%)	6 (5%)	23	48
36	BL	104/104 (100%)	96 (92%)	8 (8%)	13	37
37	BM	103/103 (100%)	97 (94%)	6 (6%)	20	45
38	BN	109/109 (100%)	101 (93%)	8 (7%)	14	39
39	BO	103/103 (100%)	97 (94%)	6 (6%)	20	45
40	BP	87/87 (100%)	82 (94%)	5 (6%)	20	45
41	BQ	99/100 (99%)	93 (94%)	6 (6%)	18	44
42	BR	89/90 (99%)	88 (99%)	1 (1%)	73	84
43	BS	84/84 (100%)	78 (93%)	6 (7%)	14	39
44	BT	93/93 (100%)	88 (95%)	5 (5%)	22	47
45	BU	84/84 (100%)	79 (94%)	5 (6%)	19	44
46	BV	84/85 (99%)	81 (96%)	3 (4%)	35	59
47	BW	78/78 (100%)	74 (95%)	4 (5%)	24	48
48	BX	62/63 (98%)	55 (89%)	7 (11%)	6	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BY	67/68 (98%)	64 (96%)	3 (4%)	27	52
50	BZ	55/55 (100%)	54 (98%)	1 (2%)	59	77
51	Ba	48/49 (98%)	47 (98%)	1 (2%)	53	72
52	Bb	62/62 (100%)	60 (97%)	2 (3%)	39	61
53	Bc	47/48 (98%)	46 (98%)	1 (2%)	53	72
54	Bd	48/49 (98%)	48 (100%)	0	100	100
55	Be	38/38 (100%)	37 (97%)	1 (3%)	46	66
56	Bf	51/52 (98%)	49 (96%)	2 (4%)	32	56
57	Bg	34/34 (100%)	30 (88%)	4 (12%)	5	20
All	All	5417/5447 (99%)	5138 (95%)	279 (5%)	27	48

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

Sometimes 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 [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	AE	32	2	18,21,22	0.95	1 (5%)	22,30,33	1.14	2 (9%)
26	3TD	BB	1915	26	18,22,23	0.86	0	22,32,35	1.18	2 (9%)
2	MIA	AB	37	2	24,31,32	1.04	3 (12%)	26,44,47	1.61	4 (15%)
2	PSU	AB	32	2	18,21,22	0.93	1 (5%)	22,30,33	1.10	1 (4%)
2	H2U	AB	20	2	18,21,22	0.85	0	21,30,33	1.05	1 (4%)
2	4SU	AE	8	2	18,21,22	1.38	2 (11%)	26,30,33	1.45	3 (11%)
26	PSU	BB	1917	26	18,21,22	0.92	0	22,30,33	0.99	2 (9%)
2	H2U	AE	16	2	18,21,22	0.79	0	21,30,33	1.01	1 (4%)
26	PSU	BB	2605	26	18,21,22	0.91	1 (5%)	22,30,33	0.93	1 (4%)
2	5MU	AE	54	2	19,22,23	0.64	0	28,32,35	0.98	2 (7%)
26	CH	BB	2575	26	16,21,22	1.02	1 (6%)	20,30,33	1.06	1 (5%)
2	3AU	AB	47	-	24,28,29	0.83	1 (4%)	33,40,43	0.80	1 (3%)
2	3AU	AE	47	-	24,28,29	0.85	1 (4%)	33,40,43	1.19	2 (6%)
26	OMU	BB	2552	26	19,22,23	0.75	0	26,31,34	0.99	1 (3%)
1	MA6	AA	1518	1	19,26,27	1.01	1 (5%)	18,38,41	1.03	0
2	PSU	AB	55	2	18,21,22	0.95	1 (5%)	22,30,33	0.93	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	H2U	AE	20	2	18,21,22	0.81	0	21,30,33	1.00	1 (4%)
26	5MC	BB	1962	26	18,22,23	0.56	0	26,32,35	1.22	2 (7%)
26	PSU	BB	2457	26	18,21,22	0.97	1 (5%)	22,30,33	1.31	3 (13%)
1	UR3	AA	1498	1	19,22,23	0.70	0	26,32,35	1.17	3 (11%)
26	PSU	BB	746	26	18,21,22	0.97	1 (5%)	22,30,33	1.10	2 (9%)
2	PSU	AE	39	2	18,21,22	0.89	1 (5%)	22,30,33	1.20	1 (4%)
26	5MU	BB	747	26	19,22,23	0.73	0	28,32,35	1.39	3 (10%)
2	7MG	AE	46	2	22,26,27	4.46	2 (9%)	29,39,42	1.50	3 (10%)
1	5MC	AA	967	1	18,22,23	0.67	0	26,32,35	0.85	1 (3%)
2	H2U	AB	16	2	18,21,22	0.86	0	21,30,33	1.32	2 (9%)
26	2MA	BB	2503	26	17,25,26	1.19	3 (17%)	17,37,40	1.43	3 (17%)
2	4SU	AB	8	2	18,21,22	1.42	1 (5%)	26,30,33	1.01	2 (7%)
26	OMC	BB	2498	26	19,22,23	0.61	0	26,31,34	0.87	0
1	2MG	AA	966	1	18,26,27	1.18	1 (5%)	16,38,41	1.34	2 (12%)
26	5MU	BB	1939	26	19,22,23	0.82	0	28,32,35	1.37	3 (10%)
2	5MU	AB	54	2	19,22,23	0.66	0	28,32,35	1.21	4 (14%)
26	6MZ	BB	2030	26	18,25,26	1.01	1 (5%)	16,36,39	1.45	3 (18%)
1	4OC	AA	1402	1	20,23,24	0.72	0	26,32,35	1.11	1 (3%)
2	MIA	AE	37	2	24,31,32	1.08	3 (12%)	26,44,47	1.55	3 (11%)
26	PSU	BB	2580	26	18,21,22	0.95	0	22,30,33	0.94	0
2	PSU	AB	39	2	18,21,22	0.91	0	22,30,33	0.92	1 (4%)
26	2MG	BB	1835	26	18,26,27	1.22	3 (16%)	16,38,41	0.73	0
1	MA6	AA	1519	1	19,26,27	1.01	1 (5%)	18,38,41	1.20	1 (5%)
26	2MG	BB	2445	26	18,26,27	1.24	3 (16%)	16,38,41	0.60	0
1	5MC	AA	1407	1	18,22,23	0.62	0	26,32,35	0.81	1 (3%)
26	1MG	BB	745	26	18,26,27	1.13	1 (5%)	19,39,42	1.26	1 (5%)
26	PSU	BB	2504	26	18,21,22	0.95	0	22,30,33	1.20	2 (9%)
1	7MG	AA	527	1	22,26,27	4.57	2 (9%)	29,39,42	1.35	1 (3%)
26	6MZ	BB	1618	26	18,25,26	0.95	1 (5%)	16,36,39	1.35	2 (12%)
26	OMG	BB	2251	26	18,26,27	1.11	2 (11%)	19,38,41	1.02	1 (5%)
26	PSU	BB	955	26	18,21,22	0.96	1 (5%)	22,30,33	1.08	1 (4%)
1	2MG	AA	1207	1	18,26,27	1.22	2 (11%)	16,38,41	0.95	0
2	7MG	AB	46	2	22,26,27	4.64	2 (9%)	29,39,42	1.32	1 (3%)
26	7MG	BB	2069	26	22,26,27	4.58	1 (4%)	29,39,42	1.39	2 (6%)
26	H2U	BB	2449	26	18,21,22	0.81	0	21,30,33	1.12	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	AA	1516	1	18,26,27	1.20	2 (11%)	16,38,41	0.79	0
2	PSU	AE	55	2	18,21,22	0.98	1 (5%)	22,30,33	1.08	1 (4%)
1	PSU	AA	516	1	18,21,22	0.85	0	22,30,33	1.31	2 (9%)
26	PSU	BB	1911	26	18,21,22	0.84	0	22,30,33	1.02	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	AE	32	2	-	0/7/25/26	0/2/2/2
26	3TD	BB	1915	26	-	0/7/25/26	0/2/2/2
2	MIA	AB	37	2	-	0/11/33/34	0/3/3/3
2	PSU	AB	32	2	-	0/7/25/26	0/2/2/2
2	H2U	AB	20	2	-	1/7/38/39	0/2/2/2
2	4SU	AE	8	2	-	0/7/25/26	0/2/2/2
26	PSU	BB	1917	26	-	0/7/25/26	0/2/2/2
2	H2U	AE	16	2	-	0/7/38/39	0/2/2/2
26	PSU	BB	2605	26	-	0/7/25/26	0/2/2/2
2	5MU	AE	54	2	-	0/7/25/26	0/2/2/2
26	CH	BB	2575	26	-	1/5/25/26	0/2/2/2
2	3AU	AB	47	-	-	2/16/34/35	0/2/2/2
2	3AU	AE	47	-	-	5/16/34/35	0/2/2/2
26	OMU	BB	2552	26	-	0/9/27/28	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
2	PSU	AB	55	2	-	1/7/25/26	0/2/2/2
2	H2U	AE	20	2	-	0/7/38/39	0/2/2/2
26	5MC	BB	1962	26	-	5/7/25/26	0/2/2/2
26	PSU	BB	2457	26	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
26	PSU	BB	746	26	-	4/7/25/26	0/2/2/2
2	PSU	AE	39	2	-	0/7/25/26	0/2/2/2
26	5MU	BB	747	26	-	4/7/25/26	0/2/2/2
2	7MG	AE	46	2	-	0/7/37/38	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
2	H2U	AB	16	2	-	1/7/38/39	0/2/2/2
26	2MA	BB	2503	26	-	0/3/25/26	0/3/3/3
2	4SU	AB	8	2	-	0/7/25/26	0/2/2/2
26	OMC	BB	2498	26	-	1/9/27/28	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	5MU	BB	1939	26	-	0/7/25/26	0/2/2/2
2	5MU	AB	54	2	-	0/7/25/26	0/2/2/2
26	6MZ	BB	2030	26	-	1/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
2	MIA	AE	37	2	-	0/11/33/34	0/3/3/3
26	PSU	BB	2580	26	-	2/7/25/26	0/2/2/2
2	PSU	AB	39	2	-	0/7/25/26	0/2/2/2
26	2MG	BB	1835	26	-	0/5/27/28	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
26	2MG	BB	2445	26	-	0/5/27/28	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
26	1MG	BB	745	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	2504	26	-	1/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	1/7/37/38	0/3/3/3
26	6MZ	BB	1618	26	-	0/5/27/28	0/3/3/3
26	OMG	BB	2251	26	-	0/5/27/28	0/3/3/3
26	PSU	BB	955	26	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
2	7MG	AB	46	2	-	1/7/37/38	0/3/3/3
26	7MG	BB	2069	26	-	0/7/37/38	0/3/3/3
26	H2U	BB	2449	26	-	0/7/38/39	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
2	PSU	AE	55	2	-	1/7/25/26	0/2/2/2
1	PSU	AA	516	1	-	0/7/25/26	0/2/2/2
26	PSU	BB	1911	26	-	1/7/25/26	0/2/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	46	7MG	C8-N9	-21.46	1.34	1.46
26	BB	2069	7MG	C8-N9	-21.24	1.34	1.46
1	AA	527	7MG	C8-N9	-21.18	1.34	1.46
2	AE	46	7MG	C8-N9	-20.62	1.34	1.46
2	AB	8	4SU	C5-C4	-5.15	1.35	1.42
2	AE	8	4SU	C5-C4	-4.78	1.36	1.42
26	BB	2575	CH	C5-C4	3.16	1.44	1.39
26	BB	745	1MG	C8-N7	-2.87	1.30	1.35
26	BB	2445	2MG	C8-N7	-2.68	1.30	1.35
1	AA	1516	2MG	C8-N7	-2.64	1.30	1.35
1	AA	1207	2MG	C8-N7	-2.55	1.30	1.35
26	BB	2503	2MA	C8-N7	-2.52	1.30	1.35
26	BB	2030	6MZ	C8-N7	-2.51	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	966	2MG	C8-N7	-2.48	1.30	1.35
26	BB	1835	2MG	C8-N7	-2.43	1.30	1.35
2	AE	37	MIA	C2-S10	2.42	1.77	1.75
1	AA	1519	MA6	C8-N7	-2.42	1.30	1.34
26	BB	2251	OMG	C8-N7	-2.38	1.31	1.35
2	AB	37	MIA	C2-S10	2.35	1.77	1.75
1	AA	1518	MA6	C8-N7	-2.33	1.30	1.34
2	AB	37	MIA	C8-N7	-2.30	1.30	1.34
2	AE	37	MIA	C6-N1	2.30	1.36	1.32
26	BB	955	PSU	C2-N1	2.29	1.39	1.36
26	BB	1618	6MZ	C8-N7	-2.28	1.30	1.34
26	BB	746	PSU	C2-N1	2.25	1.39	1.36
2	AE	37	MIA	C8-N7	-2.24	1.30	1.34
26	BB	2457	PSU	C2-N1	2.22	1.39	1.36
2	AB	32	PSU	C2-N1	2.22	1.39	1.36
2	AB	55	PSU	C2-N1	2.21	1.39	1.36
2	AE	39	PSU	C2-N1	2.20	1.39	1.36
2	AE	47	3AU	O31-C13	-2.20	1.23	1.30
2	AB	47	3AU	O31-C13	-2.16	1.23	1.30
26	BB	2503	2MA	O4'-C4'	-2.14	1.40	1.45
2	AE	32	PSU	C2-N1	2.13	1.39	1.36
26	BB	2503	2MA	C5-C4	-2.10	1.37	1.43
26	BB	2605	PSU	C2-N1	2.10	1.39	1.36
26	BB	1835	2MG	C5-C4	-2.10	1.37	1.43
2	AB	46	7MG	C5-N7	2.09	1.38	1.35
26	BB	2445	2MG	C5-C6	-2.09	1.43	1.47
1	AA	527	7MG	C5-N7	2.09	1.38	1.35
2	AB	37	MIA	C6-N1	2.09	1.35	1.32
2	AE	8	4SU	C4-S4	-2.06	1.64	1.68
26	BB	2445	2MG	C5-C4	-2.06	1.37	1.43
26	BB	1835	2MG	C5-C6	-2.04	1.43	1.47
26	BB	2251	OMG	C5-C4	-2.03	1.37	1.43
1	AA	1516	2MG	C5-C6	-2.03	1.43	1.47
2	AE	55	PSU	C2-N1	2.02	1.39	1.36
2	AE	46	7MG	C5-N7	2.01	1.38	1.35
1	AA	1207	2MG	C5-C4	-2.01	1.38	1.43

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AE	46	7MG	N9-C8-N7	6.12	112.13	103.38
26	BB	2069	7MG	N9-C8-N7	6.09	112.09	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	527	7MG	N9-C8-N7	6.04	112.02	103.38
2	AB	46	7MG	N9-C8-N7	5.67	111.49	103.38
1	AA	516	PSU	C6-C5-C4	4.37	121.26	118.20
2	AE	8	4SU	C4-N3-C2	-4.18	123.28	127.34
2	AE	37	MIA	C11-S10-C2	4.13	105.35	102.27
2	AB	37	MIA	C11-S10-C2	4.05	105.29	102.27
26	BB	2457	PSU	C6-C5-C4	3.99	120.99	118.20
26	BB	745	1MG	C2-N1-C6	3.95	124.16	120.95
2	AE	39	PSU	C6-C5-C4	3.89	120.92	118.20
2	AE	8	4SU	C5-C4-N3	3.85	118.26	114.69
26	BB	1939	5MU	C6-C5-C4	3.79	121.20	118.03
2	AE	37	MIA	C5-C6-N1	-3.69	117.75	120.81
2	AE	32	PSU	C6-C5-C4	3.69	120.78	118.20
26	BB	955	PSU	C6-C5-C4	3.65	120.75	118.20
26	BB	746	PSU	C6-C5-C4	3.64	120.75	118.20
2	AE	55	PSU	C6-C5-C4	3.60	120.71	118.20
2	AB	37	MIA	C5-C6-N1	-3.55	117.86	120.81
26	BB	1915	3TD	C6-C5-C4	3.53	120.66	118.22
26	BB	747	5MU	C6-C5-C4	3.49	120.95	118.03
2	AB	32	PSU	C6-C5-C4	3.45	120.61	118.20
2	AB	37	MIA	C12-N6-C6	3.40	127.58	122.55
26	BB	2504	PSU	C3'-C2'-C1'	3.28	105.45	101.64
2	AE	47	3AU	O4'-C4'-C3'	3.26	111.56	105.11
26	BB	1911	PSU	C6-C5-C4	3.14	120.40	118.20
26	BB	747	5MU	O3'-C3'-C2'	3.12	121.93	111.82
26	BB	1618	6MZ	C2-N1-C6	3.07	119.22	116.59
2	AE	16	H2U	O4'-C1'-N1	3.06	113.47	109.30
2	AB	54	5MU	C6-C5-C4	3.02	120.55	118.03
26	BB	747	5MU	C5M-C5-C6	-3.00	118.85	122.85
2	AB	8	4SU	C5-C4-N3	2.95	117.43	114.69
26	BB	2605	PSU	C6-C5-C4	2.95	120.26	118.20
26	BB	2504	PSU	C6-C5-C4	2.94	120.25	118.20
1	AA	1519	MA6	O3'-C3'-C2'	2.89	121.19	111.82
2	AE	54	5MU	C6-C5-C4	2.89	120.44	118.03
26	BB	1618	6MZ	C9-N6-C6	2.88	125.36	122.87
26	BB	1962	5MC	C3'-C2'-C1'	-2.88	95.96	101.43
26	BB	2030	6MZ	C9-N6-C6	2.86	125.34	122.87
2	AB	37	MIA	C2-N3-C4	-2.85	111.40	115.32
1	AA	966	2MG	C2'-C3'-C4'	-2.78	97.24	102.64
26	BB	2503	2MA	N1-C2-N3	2.75	127.62	123.06
26	BB	2575	CH	C5-C4-N3	2.75	119.61	118.04
26	BB	2030	6MZ	C2-N1-C6	2.73	118.93	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	16	H2U	O4'-C1'-C2'	-2.68	100.79	106.64
26	BB	2457	PSU	C3'-C2'-C1'	2.68	104.76	101.64
26	BB	1917	PSU	C3'-C2'-C1'	2.68	104.76	101.64
2	AE	37	MIA	C2-N3-C4	-2.66	111.66	115.32
26	BB	1915	3TD	C2'-C3'-C4'	-2.65	97.49	102.64
2	AB	55	PSU	C6-C5-C4	2.65	120.05	118.20
26	BB	2503	2MA	C5-C6-N1	2.63	118.56	114.02
2	AB	54	5MU	C5M-C5-C6	-2.63	119.33	122.85
2	AB	39	PSU	C6-C5-C4	2.61	120.03	118.20
2	AE	20	H2U	O4'-C1'-N1	2.59	112.83	109.30
26	BB	1939	5MU	C5M-C5-C6	-2.52	119.48	122.85
1	AA	1498	UR3	O5'-C5'-C4'	2.52	117.56	108.99
2	AE	46	7MG	O3'-C3'-C4'	2.50	118.28	111.05
1	AA	1498	UR3	O4'-C1'-N1	2.46	113.99	108.36
2	AB	8	4SU	C4-N3-C2	-2.39	125.02	127.34
26	BB	2503	2MA	O3'-C3'-C2'	2.38	119.51	111.82
1	AA	1402	4OC	O4'-C1'-N1	2.37	113.79	108.36
26	BB	2449	H2U	O3'-C3'-C4'	-2.37	104.20	111.05
2	AE	32	PSU	O4'-C1'-C2'	2.34	108.44	105.14
26	BB	1939	5MU	C5-C6-N1	-2.32	120.95	123.34
1	AA	967	5MC	CM5-C5-C6	-2.32	119.75	122.85
2	AB	54	5MU	O3'-C3'-C2'	2.29	119.24	111.82
26	BB	746	PSU	O3'-C3'-C4'	-2.27	104.48	111.05
2	AE	8	4SU	O3'-C3'-C4'	2.26	117.60	111.05
26	BB	1917	PSU	C6-C5-C4	2.23	119.76	118.20
26	BB	2251	OMG	O5'-C5'-C4'	2.18	116.40	108.99
1	AA	966	2MG	O3'-C3'-C4'	2.15	117.26	111.05
2	AE	54	5MU	C5M-C5-C6	-2.11	120.02	122.85
26	BB	1962	5MC	C5-C6-N1	-2.09	121.18	123.34
1	AA	1498	UR3	O3'-C3'-C2'	-2.08	105.09	111.82
2	AB	54	5MU	O4'-C4'-C5'	2.07	116.20	109.37
1	AA	1407	5MC	CM5-C5-C6	-2.07	120.08	122.85
26	BB	2030	6MZ	C2'-C3'-C4'	-2.07	98.62	102.64
2	AB	47	3AU	O4-C4-N3	2.06	121.63	119.16
26	BB	2457	PSU	O4'-C1'-C2'	2.04	108.01	105.14
26	BB	2552	OMU	C2'-C3'-C4'	-2.03	97.58	101.99
26	BB	2069	7MG	O5'-C5'-C4'	2.03	115.91	108.99
2	AE	47	3AU	O3'-C3'-C4'	-2.03	105.18	111.05
2	AB	20	H2U	O4'-C1'-N1	2.03	112.06	109.30
2	AB	16	H2U	O4'-C1'-N1	2.01	112.04	109.30
2	AE	46	7MG	O4'-C1'-N9	2.01	112.04	109.30
1	AA	516	PSU	O4'-C1'-C2'	2.01	107.97	105.14

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	7MG	C4'-C5'-O5'-P
2	AB	46	7MG	C4'-C5'-O5'-P
26	BB	746	PSU	C2'-C1'-C5-C4
26	BB	746	PSU	C2'-C1'-C5-C6
26	BB	747	5MU	C2'-C1'-N1-C2
26	BB	747	5MU	C2'-C1'-N1-C6
26	BB	2580	PSU	C2'-C1'-C5-C4
26	BB	2580	PSU	C2'-C1'-C5-C6
2	AE	47	3AU	N40-C12-C13-O31
26	BB	1962	5MC	C2'-C1'-N1-C6
2	AB	47	3AU	O4'-C4'-C5'-O5'
2	AB	47	3AU	C3'-C4'-C5'-O5'
2	AE	47	3AU	N40-C12-C13-O30
26	BB	1962	5MC	O4'-C1'-N1-C6
2	AE	47	3AU	O4'-C1'-N1-C2
26	BB	1962	5MC	O4'-C1'-N1-C2
2	AE	47	3AU	O4'-C1'-N1-C6
26	BB	747	5MU	O4'-C1'-N1-C6
2	AB	16	H2U	O4'-C4'-C5'-O5'
2	AE	47	3AU	O4'-C4'-C5'-O5'
2	AB	55	PSU	O4'-C1'-C5-C4
26	BB	746	PSU	O4'-C1'-C5-C4
26	BB	1911	PSU	O4'-C1'-C5-C4
26	BB	1962	5MC	C2'-C1'-N1-C2
26	BB	2504	PSU	O4'-C4'-C5'-O5'
2	AE	55	PSU	O4'-C1'-C5-C6
26	BB	746	PSU	O4'-C1'-C5-C6
26	BB	2575	CH	O4'-C1'-N1-C2
26	BB	747	5MU	O4'-C1'-N1-C2
26	BB	2030	6MZ	O4'-C4'-C5'-O5'
26	BB	1962	5MC	C4'-C5'-O5'-P
2	AB	20	H2U	O4'-C4'-C5'-O5'
26	BB	2498	OMC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

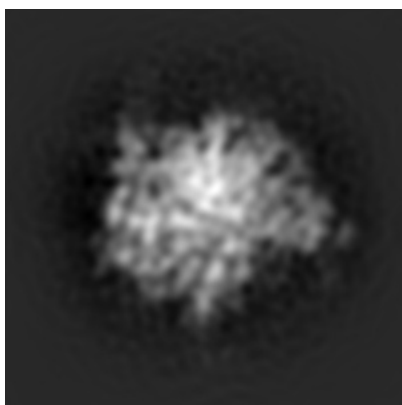
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1850. These allow visual inspection of the internal detail of the map and identification of artifacts.

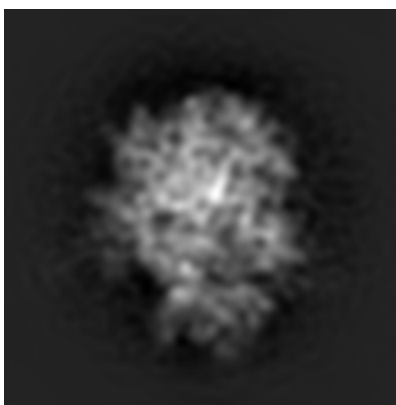
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

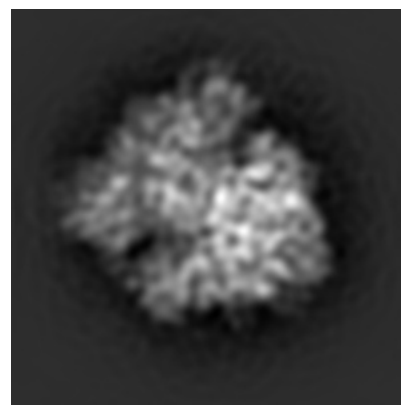
6.1.1 Primary map



X



Y

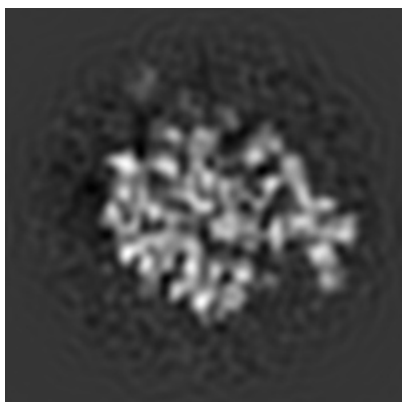


Z

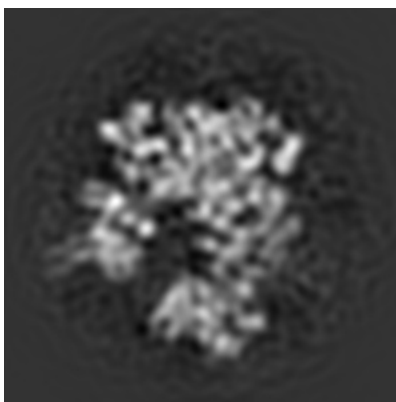
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

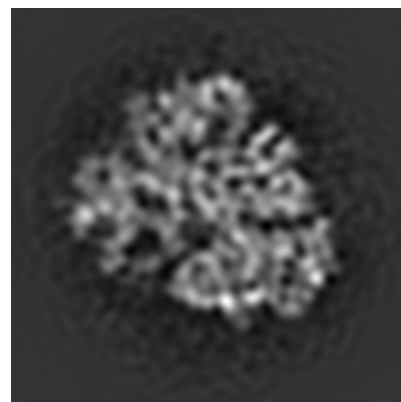
6.2.1 Primary map



X Index: 125



Y Index: 125

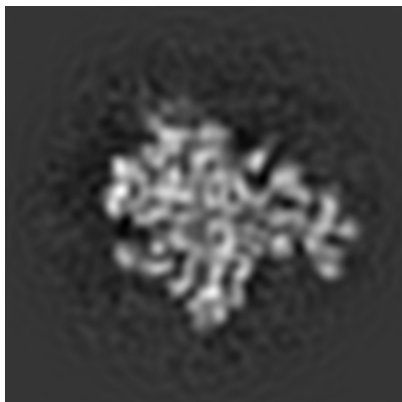


Z Index: 125

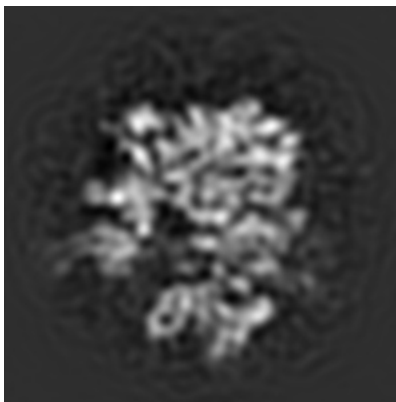
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

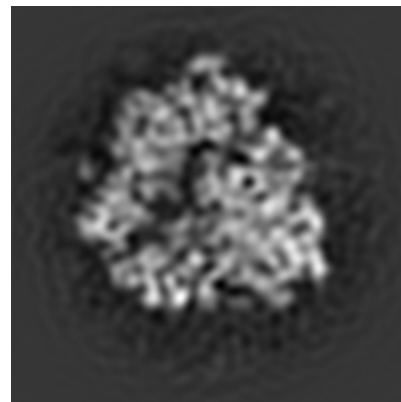
6.3.1 Primary map



X Index: 131



Y Index: 130

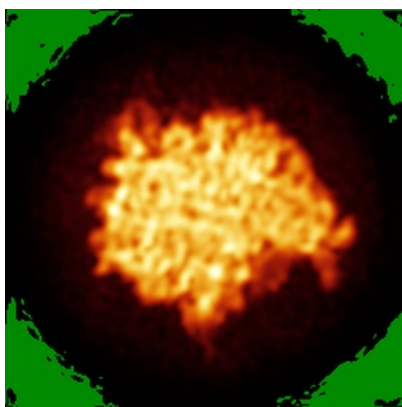


Z Index: 115

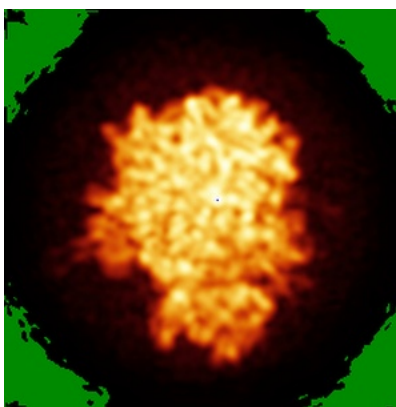
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

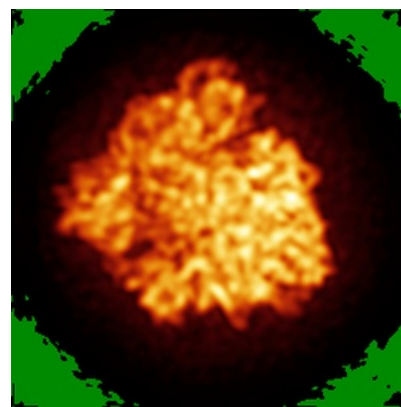
6.4.1 Primary map



X



Y

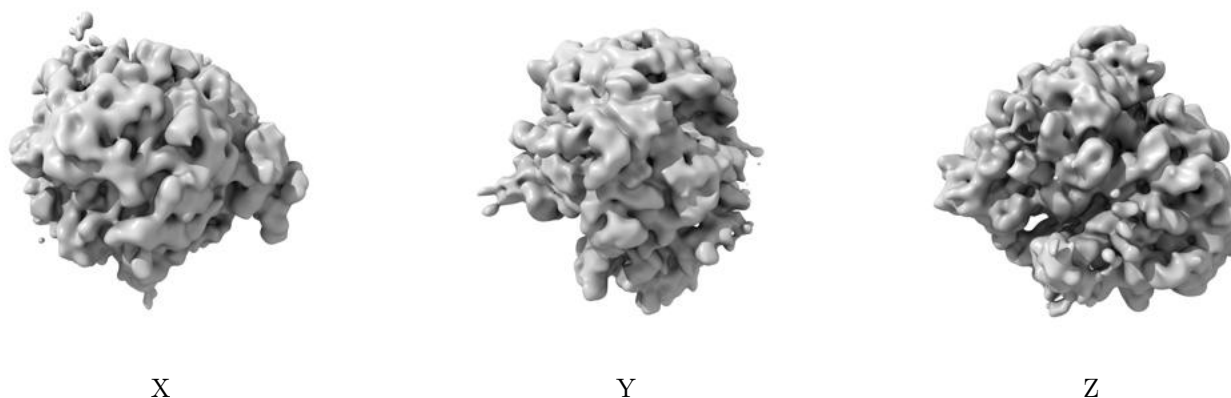


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 32.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

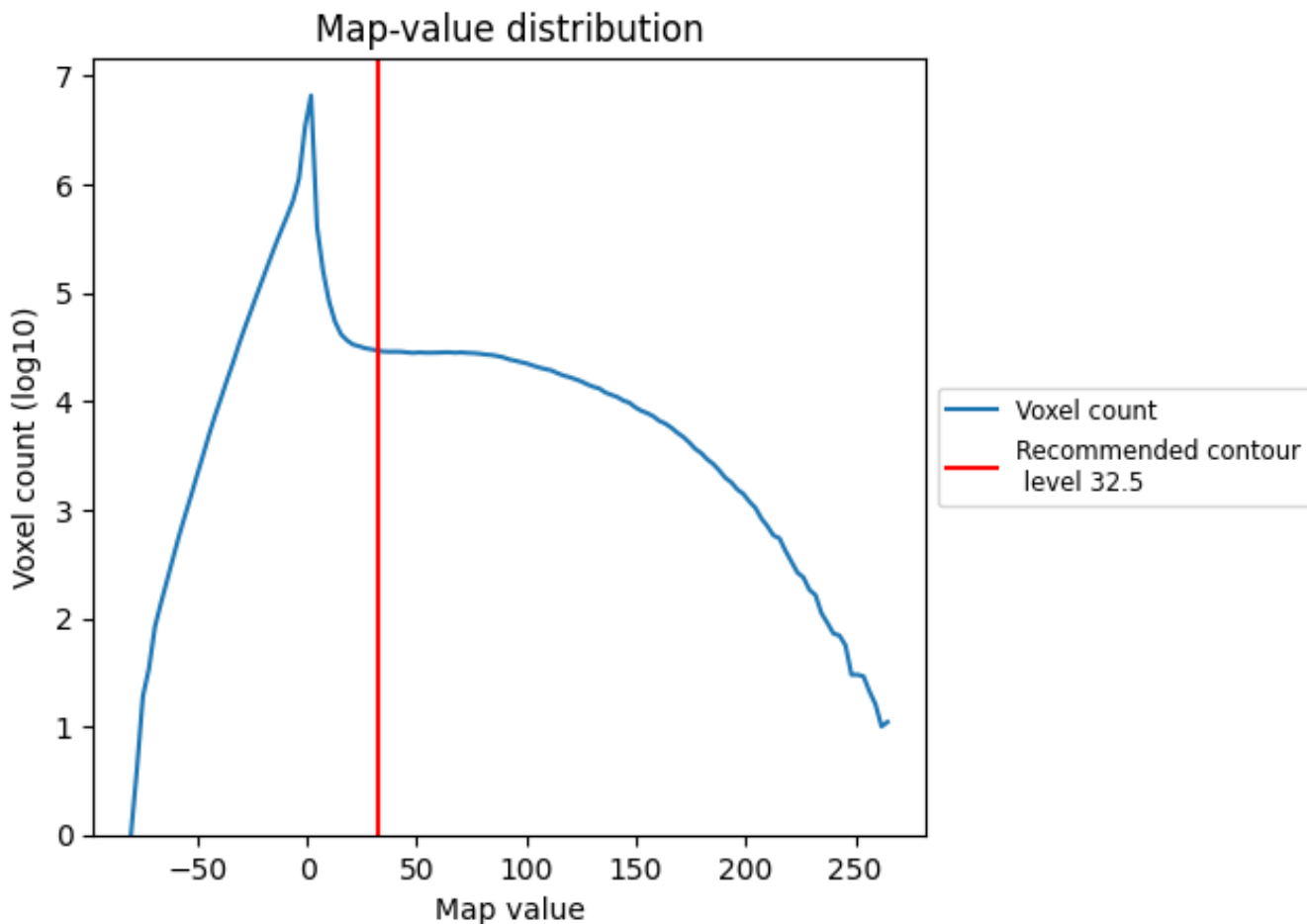
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

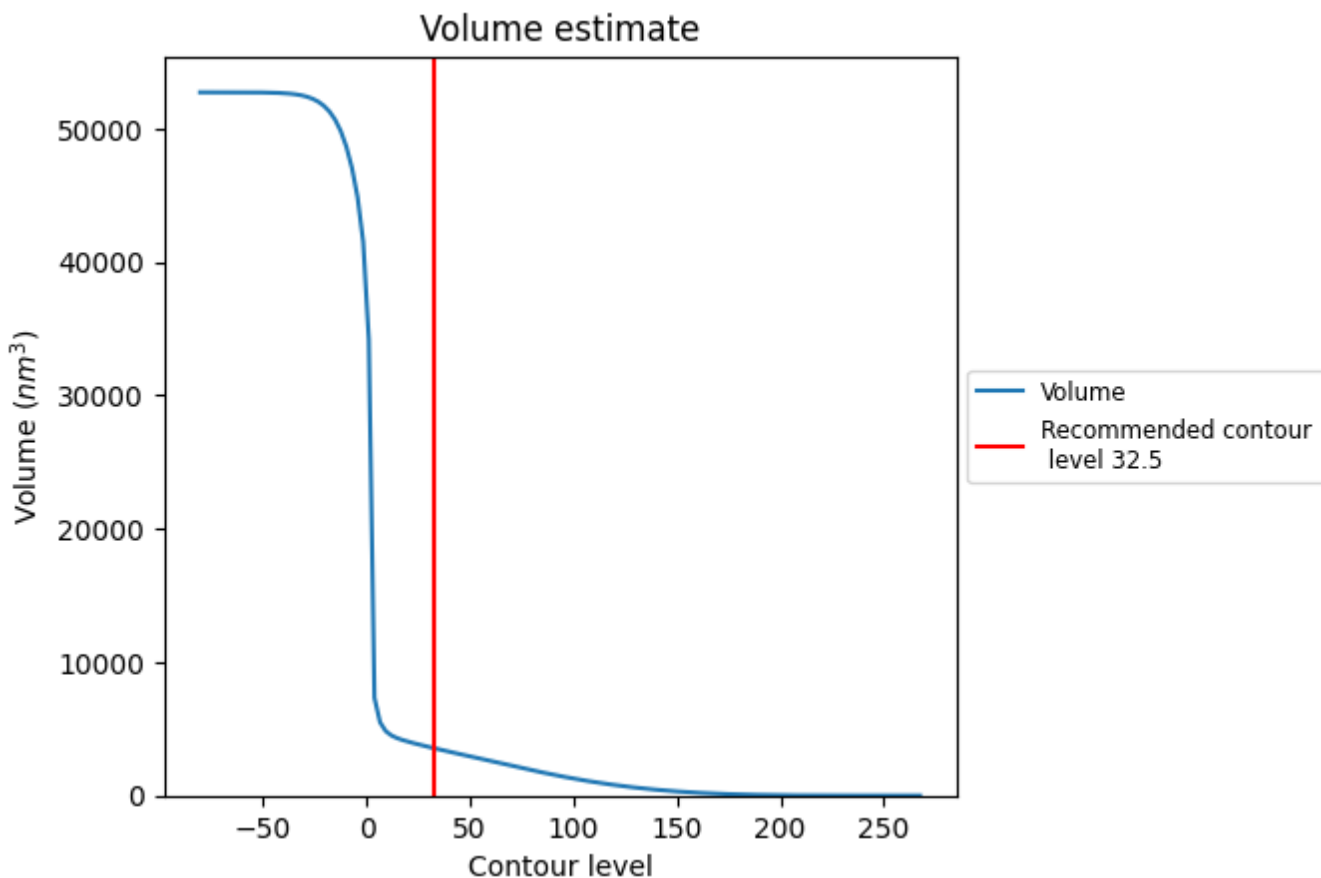
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

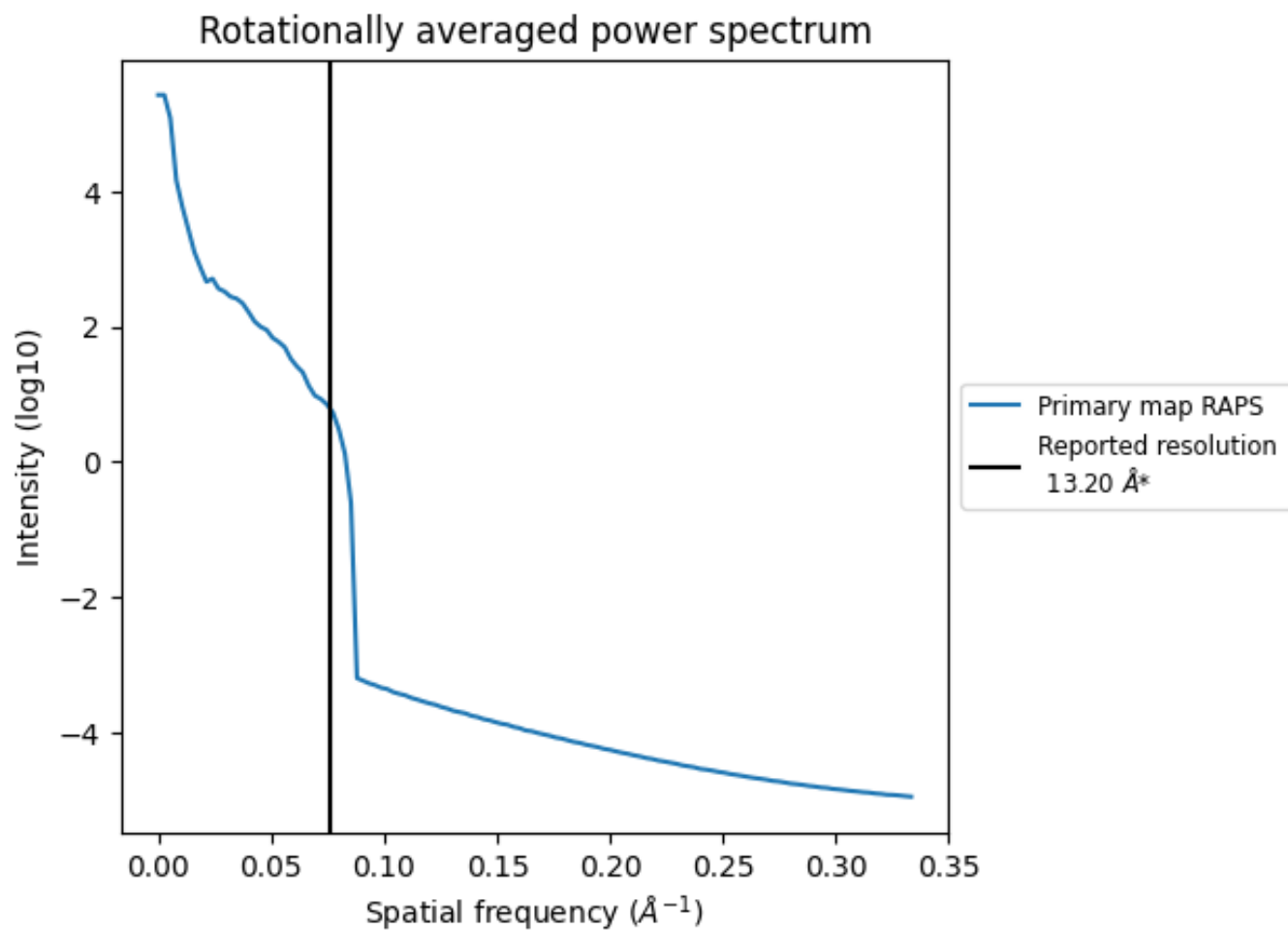
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3559 nm³; this corresponds to an approximate mass of 3215 kDa.

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

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.076 Å⁻¹

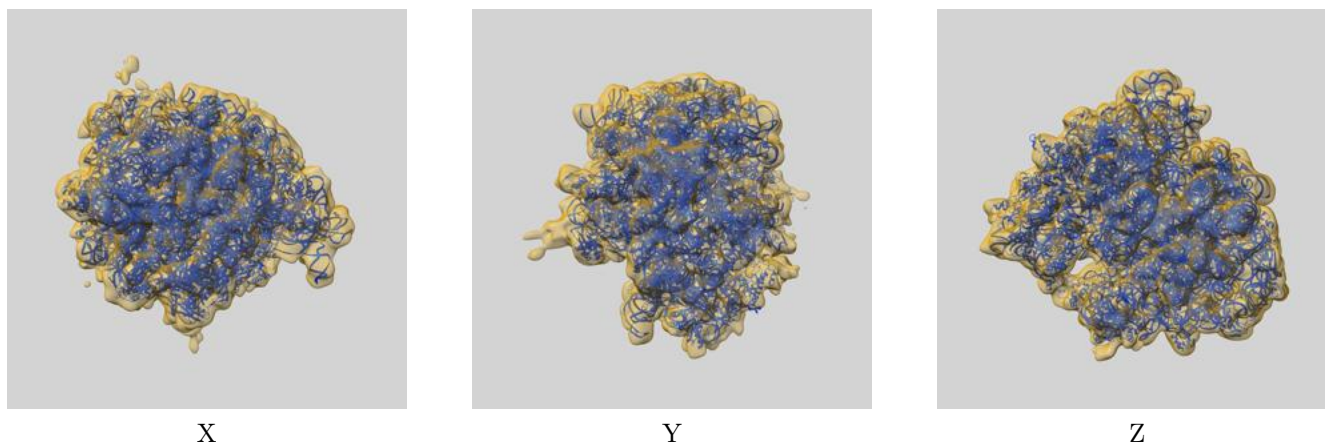
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

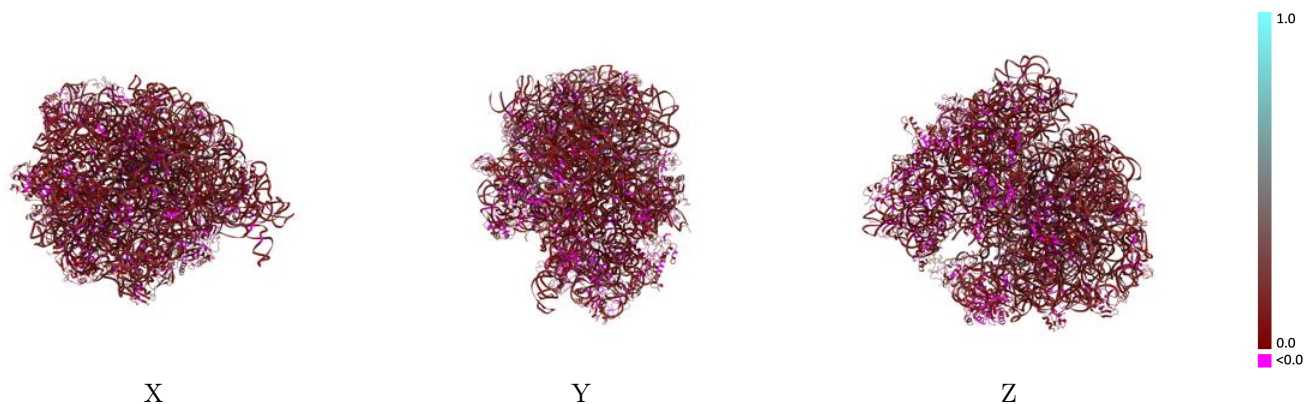
This section contains information regarding the fit between EMDB map EMD-1850 and PDB model 4V6L. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



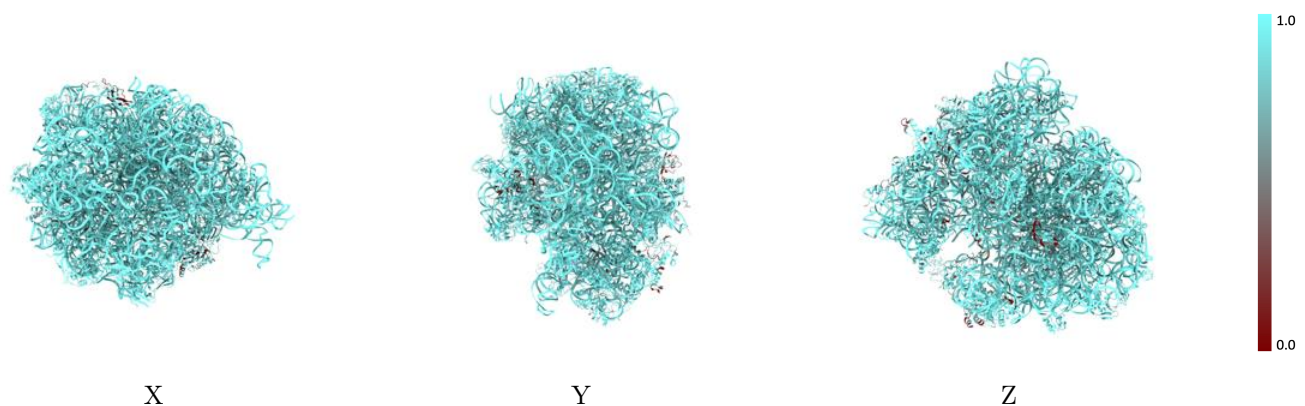
The images above show the 3D surface view of the map at the recommended contour level 32.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



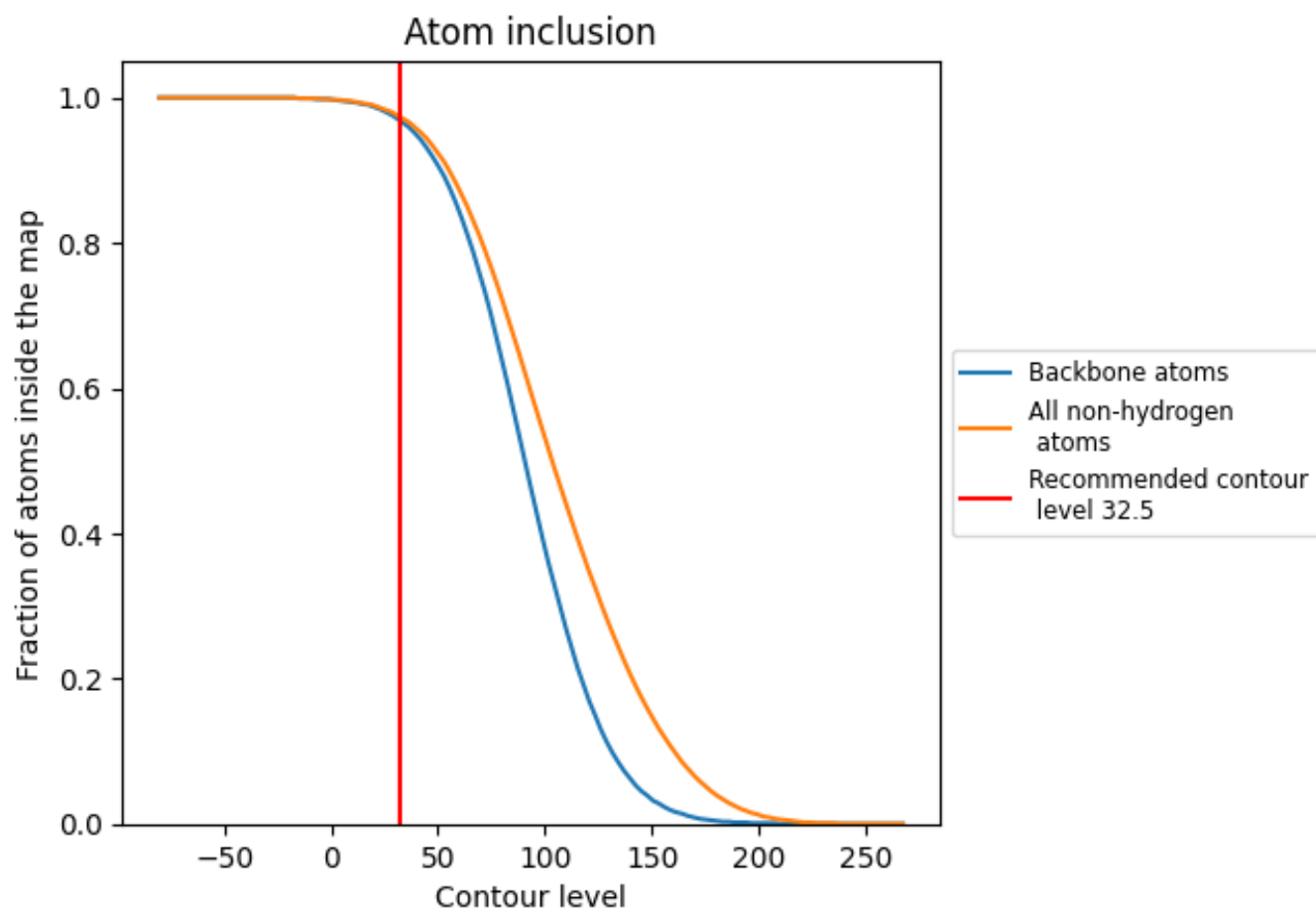
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (32.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

















































The table lists the average atom inclusion at the recommended contour level (32.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9730	0.0980
AA	0.9910	0.1100
AB	0.8780	0.0990
AC	0.8430	0.0640
AD	0.8790	0.0820
AE	0.9550	0.1100
AF	0.9030	0.0860
AG	0.9010	0.0700
AH	0.9080	0.0520
AI	0.8840	0.0690
AJ	0.8840	0.0670
AK	0.9320	0.0820
AL	0.9760	0.0640
AM	0.9880	0.0900
AN	0.9310	0.0220
AO	0.8600	0.0650
AP	0.9350	0.0400
AQ	0.9820	0.0790
AR	0.9870	0.0490
AS	0.9990	0.0720
AT	0.9870	0.0420
AU	0.9860	0.0910
AV	0.9730	0.0630
AW	0.9560	0.0560
AX	0.9570	0.0440
AY	0.8980	0.0720
BA	0.9970	0.1240
BB	0.9950	0.1180
BC	0.8210	0.0410
BD	0.9890	0.0490
BE	0.9830	0.0520
BF	0.9810	0.0670
BG	0.9740	0.0790
BH	0.9890	0.0910
BI	0.6640	0.0550



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Chain	Atom inclusion	Q-score
BJ	 0.9630	 0.0800
BK	 0.9630	 0.0660
BL	 0.9730	 0.0580
BM	 0.9760	 0.0380
BN	 0.9520	 0.0600
BO	 0.9970	 0.0630
BP	 0.9890	 0.0680
BQ	 0.9450	 0.0880
BR	 0.9870	 0.0620
BS	 0.9670	 0.0750
BT	 0.9960	 0.0720
BU	 0.9900	 0.0730
BV	 0.9650	 0.0830
BW	 0.9840	 0.0860
BX	 0.8830	 0.0410
BY	 0.9780	 0.0720
BZ	 0.9780	 0.0990
Ba	 0.9840	 0.0660
Bb	 0.9030	 0.0860
Bc	 0.9490	 0.0380
Bd	 0.9540	 0.0570
Be	 0.9970	 0.0200
Bf	 0.9590	 0.0230
Bg	 0.9800	 0.0240