Full wwPDB EM Validation Report (i)

Feb 13, 2024 – 04:06 PM EST

PDB ID	:	3J9Z
EMDB ID	:	EMD-6315
Title	:	Activation of GTP Hydrolysis in mRNA-tRNA Translocation by Elongation Factor G
Authors	:	Li, W.; Liu, Z.; Koripella, R.K.; Langlois, R.; Sanyal, S.; Frank, J.
Deposited on	:	2015-03-27
Resolution	:	3.60 Å(reported)
Based on initial model	:	3J0U

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

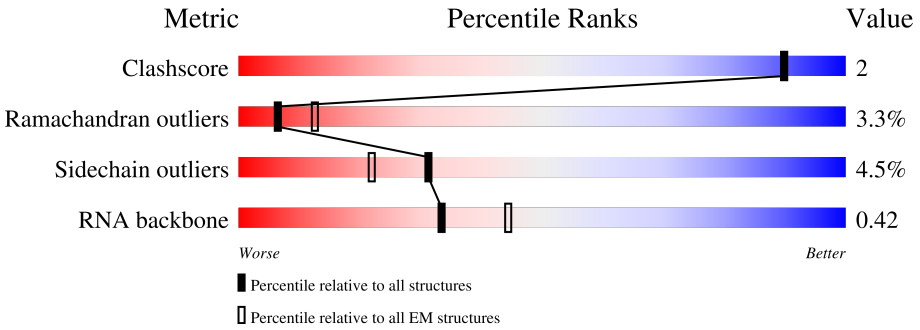
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	SA	1542	19% 44% 26% 10%
2	S6	77	19% 56% 17% 8%
3	S7	74	9% 35% 27% 28%
4	SJ	103	10% 86% 10%
5	SK	128	12% 84% 12%
6	SL	123	9% 85% 15%
7	SM	117	84% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	SN	100	89% 8%
9	SO	88	8% 89% 7% 5%
10	SP	82	6% 87% 9% 5%
11	SQ	83	11% 90% 6%
12	SR	74	16% 84% 15%
13	SS	91	11% 84% 15%
14	SB	240	18% 88% 9%
15	ST	86	10% 91% 7%
16	SU	70	29% 76% 20%
17	SC	232	14% 87% 12%
18	SD	205	86% 12%
19	SE	166	13% 90% 8%
20	SF	135	29% 89% 10%
21	SG	178	12% 89% 10%
22	SH	129	5% 88% 10%
23	SI	129	89% 9%
24	S1	702	12% 87% 12%
25	LA	2904	17% 43% 29% 11%
26	LB	120	19% 51% 24% 6%
27	LC	234	26% 85% 13%
28	LM	114	9% 82% 12% 5%
29	LN	272	11% 83% 16%
30	LO	117	80% 16%
31	LP	103	83% 14%
32	LQ	110	9% 92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	LR	100	13% 86% 14%
34	LS	103	85% 12%
35	LT	94	90% 7%
36	LU	84	10% 70% 24% 5%
37	LV	77	88% 10%
38	LD	164	41% 93% 7%
39	LW	63	21% 87% 10%
40	LX	209	7% 83% 12%
41	LY	58	91% 5%
42	L1	56	80% 18%
43	L2	54	9% 96%
44	L3	46	13% 76% 15% 7%
45	L4	64	91% 8%
46	L5	38	92% 5%
47	L6	201	5% 87% 11%
48	LE	141	13% 91% 8%
49	L7	178	75% 21%
50	L8	176	6% 88% 11%
51	L9	149	36% 87% 12%
52	LF	142	85% 13%
53	LG	123	11% 82% 16%
54	LH	144	84% 13%
55	LI	136	91% 7%
56	LJ	127	12% 80% 17%
57	LK	117	85% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	LZ	70	26% 87% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	GTP	S1	801	-	-	X	-

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 156714 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	SA	1542	33076	14754	6064	10717	1541	0	0

- Molecule 2 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	S6	77	1639	732	297	534	76	0	0

- Molecule 3 is a RNA chain called E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	S7	74	1577	704	282	518	73	0	0

- Molecule 4 is a protein called 30S ribosomal protein S10.

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

- Molecule 5 is a protein called 30S ribosomal protein S11.

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

- Molecule 6 is a protein called 30S ribosomal protein S12.

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

- Molecule 7 is a protein called 30S ribosomal protein S13.

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

- Molecule 8 is a protein called 30S ribosomal protein S14.

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

- Molecule 9 is a protein called 30S ribosomal protein S15.

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

- Molecule 10 is a protein called 30S ribosomal protein S16.

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

- Molecule 11 is a protein called 30S ribosomal protein S17.

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

- Molecule 12 is a protein called 30S ribosomal protein S18.

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

- Molecule 13 is a protein called 30S ribosomal protein S19.

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

- Molecule 14 is a protein called 30S ribosomal protein S2.

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

- Molecule 15 is a protein called 30S ribosomal protein S20.

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

- Molecule 16 is a protein called 30S ribosomal protein S21.

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

- Molecule 17 is a protein called 30S ribosomal protein S3.

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

- Molecule 18 is a protein called 30S ribosomal protein S4.

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

- Molecule 19 is a protein called 30S ribosomal protein S5.

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

- Molecule 20 is a protein called 30S ribosomal protein S6.

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

- Molecule 21 is a protein called 30S ribosomal protein S7.

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

- Molecule 22 is a protein called 30S ribosomal protein S8.

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

- Molecule 23 is a protein called 30S ribosomal protein S9.

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

- Molecule 24 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	S1	702	5431	3420	938	1048	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S1	91	ALA	HIS	engineered mutation	UNP P0A6M8

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	LA	2904	62333	27808	11464	20158	2903	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LA	1618	U	A	conflict	GB 33357927
LA	2030	C	A	conflict	GB 33357927

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

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

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

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

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

- Molecule 29 is a protein called 50S ribosomal protein L2.

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

- Molecule 30 is a protein called 50S ribosomal protein L20.

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

- Molecule 31 is a protein called 50S ribosomal protein L21.

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

- Molecule 32 is a protein called 50S ribosomal protein L22.

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

- Molecule 33 is a protein called 50S ribosomal protein L23.

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

- Molecule 34 is a protein called 50S ribosomal protein L24.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L27.

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

- Molecule 37 is a protein called 50S ribosomal protein L28.

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

- Molecule 38 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LD	164	1233	776	220	231	6	0	0

- Molecule 39 is a protein called 50S ribosomal protein L29.

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

- Molecule 40 is a protein called 50S ribosomal protein L3.

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

- Molecule 41 is a protein called 50S ribosomal protein L30.

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

- Molecule 42 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	L1	56	444	269	94	80	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	L2	54	441	284	81	76	0	0

- Molecule 44 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	L3	46	377	228	90	57	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	L4	64	504	323	105	74	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	L5	38	302	185	65	48	4	0	0

- Molecule 47 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	L6	201	1552	974	283	290	5	0	0

- Molecule 48 is a protein called 50S ribosomal protein L11.

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

- Molecule 49 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	L7	178	1420	905	251	258	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	L8	176	1323	832	243	246	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	L9	149	1111	699	197	214	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L13.

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

- Molecule 53 is a protein called 50S ribosomal protein L14.

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

- Molecule 54 is a protein called 50S ribosomal protein L15.

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

- Molecule 55 is a protein called 50S ribosomal protein L16.

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

- Molecule 56 is a protein called 50S ribosomal protein L17.

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

- Molecule 57 is a protein called 50S ribosomal protein L18.

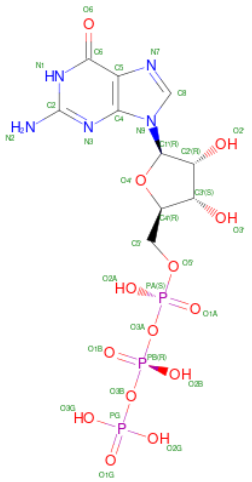
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	LK	117	900	557	179	163	1	0	0

- Molecule 58 is a protein called 50S ribosomal protein L31.

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

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

GTP



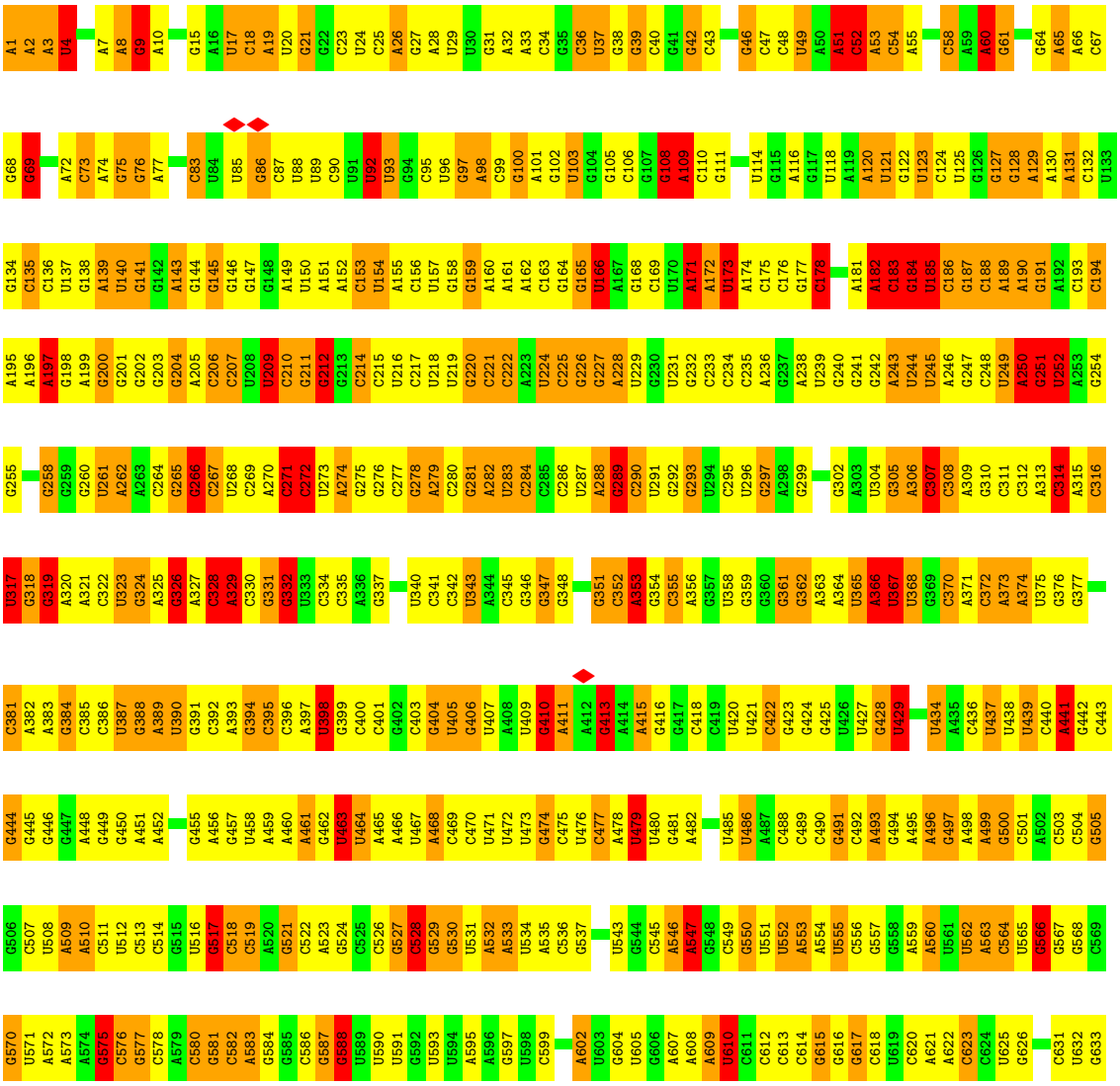
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	S1	1	32	10	5	14	3	0

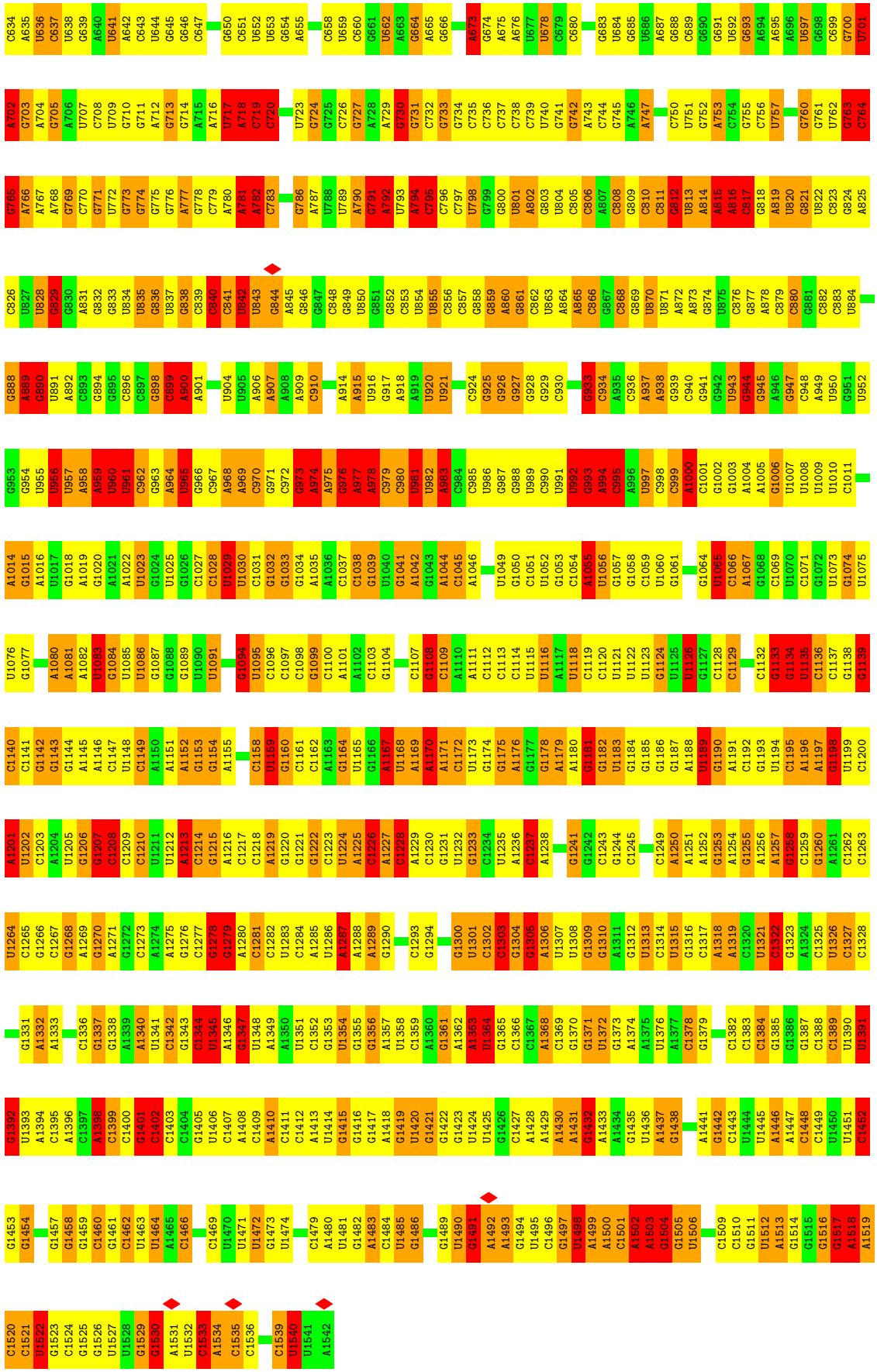
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

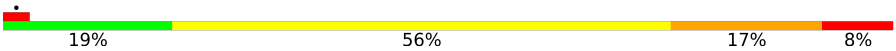
Chain SA: 19% 44% 26% 10%

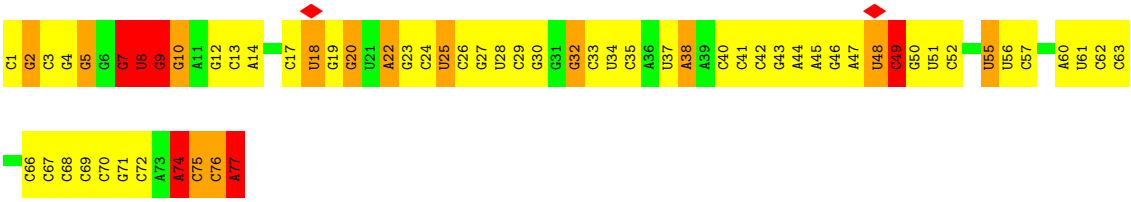



C634 A635 U636 C637 U638 G639 A640 U641 A642 C643 U644 G645 G646 C647 G650 C651 U652 U653 G654 A655 C658 U659 C660 G661 U662 A663 G664 A665 G666 A673 G674 A675 A676 U677 U678 C679 C680 G683 U684 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 G698 C699 G700 U701
A702 G703 A704 G705 A706 U707 C708 U709 G710 G711 A712 G713 G714 A715 A716 U717 A718 C719 C720 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 G733 G734 C735 G736 C737 C738 U739 U740 G741 G742 A743 C744 G745 A746 A747 C750 U751 G752 A753 C754 G755 C756 U757 G760 G761 U762 G763 C764
G765 A766 A767 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 C786 A787 U788 U789 A790 G791 A792 U793 A794 A795 C796 C797 U798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825
C826 U827 U828 G829 G830 A831 G832 G833 U834 U835 G836 U837 G838 C839 C840 C841 U842 U843 G844 A845 G846 G847 C848 G849 U850 G851 C852 C853 U854 U855 C856 C857 G858 G859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 U875 C876 G877 A878 C879 C880 G881 C882 C883 U884
G888 A889 G890 U891 A892 C893 G894 G895 C896 C897 G898 C899 A900 A901 U904 U905 A906 A907 A908 A909 C910 A914 A915 U916 G917 A918 A919 U920 U921 C924 G925 G926 G927 G928 G929 C930 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 A949 U950 G951 U952
G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 U986 G987 G988 U989 C990 U991 U992 G993 A994 C995 A996 U997 C998 C999 A1000 C1001 G1002 G1003 A1004 A1005 G1006 U1007 U1008 U1009 U1010 C1011
A1014 G1015 A1016 U1017 G1018 A1019 G1020 A1021 A1022 U1023 G1024 U1025 G1026 C1027 C1028 U1029 U1030 C1031 G1032 G1033 G1034 A1035 A1036 C1037 C1038 G1039 U1040 G1041 A1042 G1043 A1044 C1045 A1046 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 U1060 G1061 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 U1075
U1076 G1077 A1080 A1081 A1082 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 U1115 U1116 A1117 U1118 C1119 C1120 U1121 U1122 U1123 G1124 U1125 U1126 G1127 C1128 C1129 C1132 G1133 G1134 U1135 C1136 C1137 G1138 G1139
C1140 C1141 G1142 G1143 G1144 A1145 A1146 C1147 U1148 C1149 A1150 A1151 A1152 G1153 G1154 A1155 C1158 U1159 G1160 C1161 C1162 A1163 G1164 U1165 G1166 A1167 U1168 A1169 A1170 A1171 C1172 U1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 C1182 U1183 G1184 G1185 G1186 G1187 A1188 U1189 G1190 A1191 C1192 G1193 U1194 C1195 A1196 A1197 G1198 U1199 C1200
A1201 U1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 G1241 G1242 C1243 G1244 C1245 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261 C1262 C1263
U1264 C1265 G1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275 G1276 C1277 G1278 G1279 A1280 C1281 C1282 U1283 C1284 A1285 A1286 A1287 A1288 A1289 C1290 C1293 G1294 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 A1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 U1321 C1322 G1323 A1324 C1325 U1326 C1327 C1328
G1331 A1332 A1333 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 U1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 A1362 A1363 U1364 G1365 C1366 C1367 A1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 C1382 C1383 C1384 G1385 G1386 G1387 C1388 C1389 U1390 U1391
G1392 U1393 A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 A1408 C1409 A1410 C1411 C1412 A1413 U1414 G1415 G1416 G1417 A1418 G1419 U1420 G1421 G1422 G1423 U1424 U1425 G1426 C1427 A1428 A1429 A1430 A1431 G1432 A1433 A1434 G1435 U1436 A1437 G1438 A1441 G1442 C1443 U1444 U1445 A1446 A1447 C1448 C1449 U1450 U1451 C1452
G1453 G1454 G1457 G1458 G1459 C1460 G1461 C1462 U1463 U1464 A1465 C1466 C1469 U1470 U1471 U1472 G1473 U1474 C1479 A1480 U1481 G1482 A1483 C1484 U1485 G1486 G1489 U1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497 U1498 A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 C1509 C1510 G1511 U1512 A1513 G1514 G1515 G1516 G1517 A1518 A1519
C1520 C1521 U1522 G1523 C1524 G1525 G1526 U1527 U1528 G1529 G1530 A1531 U1532 C1533 A1534 C1535 C1536 C1539 U1540 U1541 A1542

- Molecule 2: P-tRNA

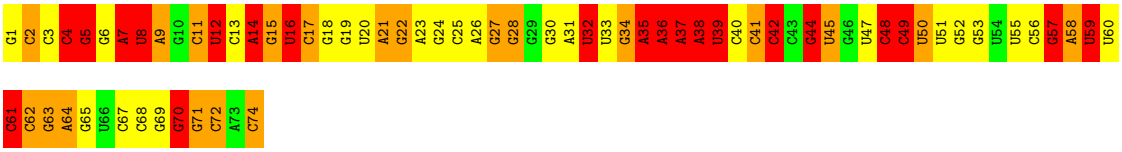
Chain S6:





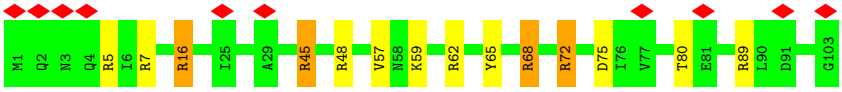
- Molecule 3: E-tRNA

Chain S7:



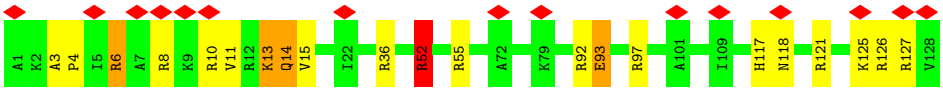
- Molecule 4: 30S ribosomal protein S10

Chain SJ:



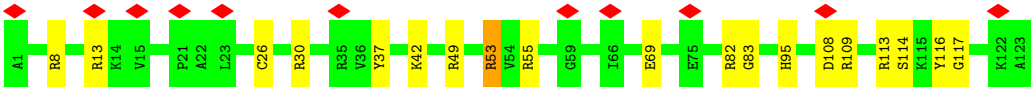
- Molecule 5: 30S ribosomal protein S11

Chain SK:



- Molecule 6: 30S ribosomal protein S12

Chain SL:

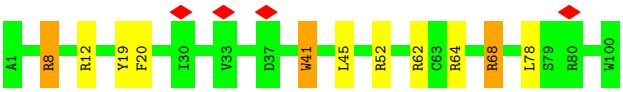


- Molecule 7: 30S ribosomal protein S13

Chain SM:

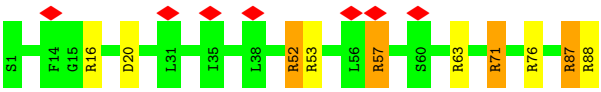
- Molecule 8: 30S ribosomal protein S14

Chain SN: 89% 8%



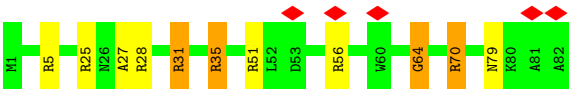
• Molecule 9: 30S ribosomal protein S15

Chain SO: 8% 89% 7% 5%



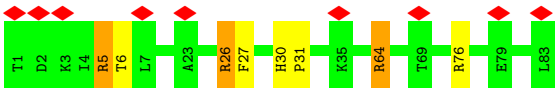
• Molecule 10: 30S ribosomal protein S16

Chain SP: 6% 87% 9% 5%



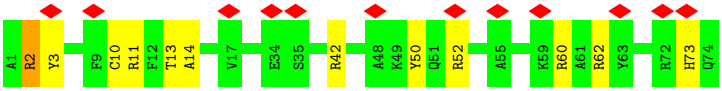
• Molecule 11: 30S ribosomal protein S17

Chain SQ: 11% 90% 6%



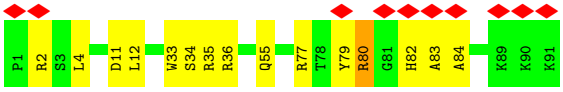
• Molecule 12: 30S ribosomal protein S18

Chain SR: 16% 84% 15%



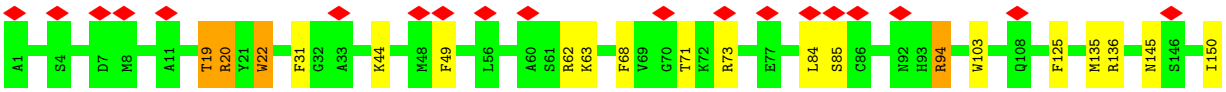
• Molecule 13: 30S ribosomal protein S19

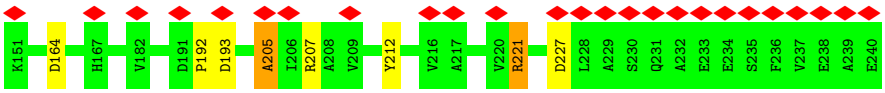
Chain SS: 11% 84% 15%



• Molecule 14: 30S ribosomal protein S2

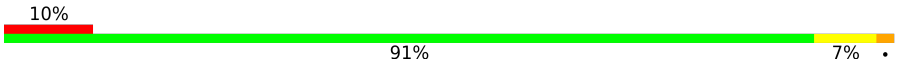
Chain SB: 18% 88% 9%

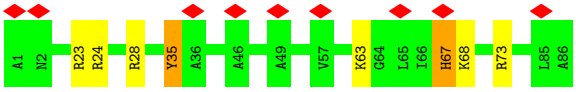




• Molecule 15: 30S ribosomal protein S20

Chain ST:



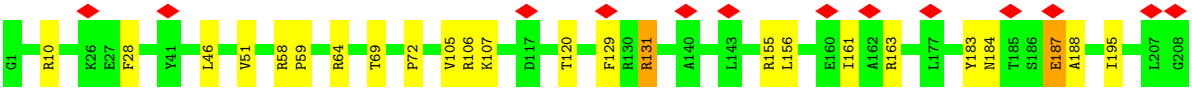


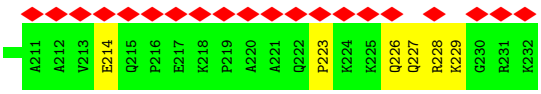
• Molecule 16: 30S ribosomal protein S21

Chain SU:

• Molecule 17: 30S ribosomal protein S3

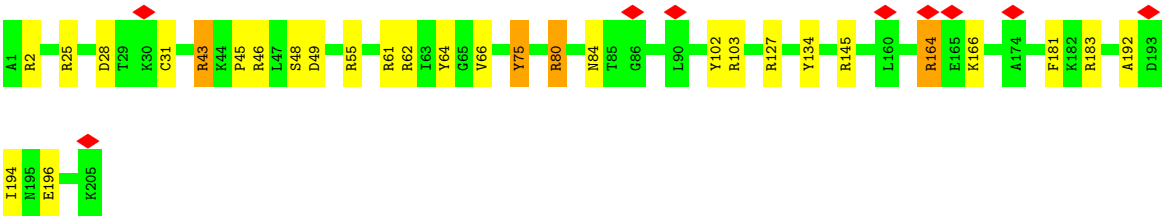
Chain SC:





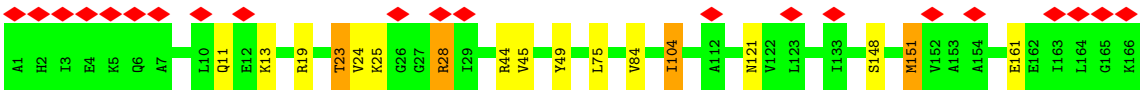
• Molecule 18: 30S ribosomal protein S4

Chain SD:



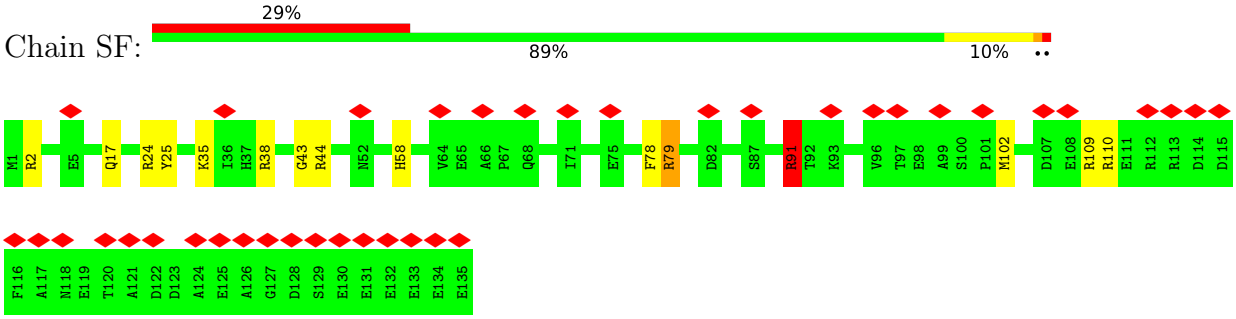
• Molecule 19: 30S ribosomal protein S5

Chain SE:



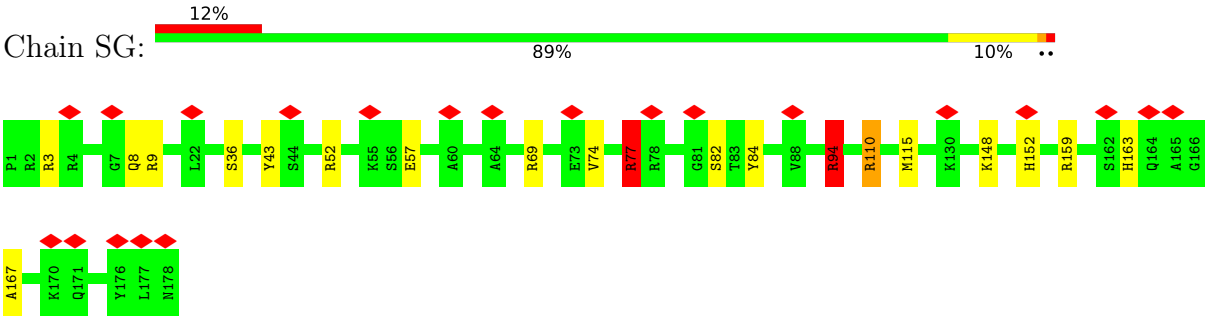
• Molecule 20: 30S ribosomal protein S6

Chain SF:



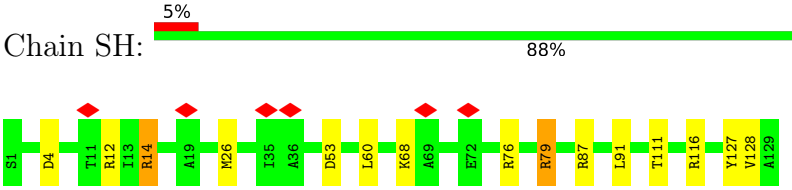
- Molecule 21: 30S ribosomal protein S7

Chain SG:



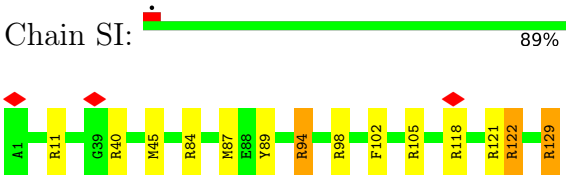
- Molecule 22: 30S ribosomal protein S8

Chain SH:



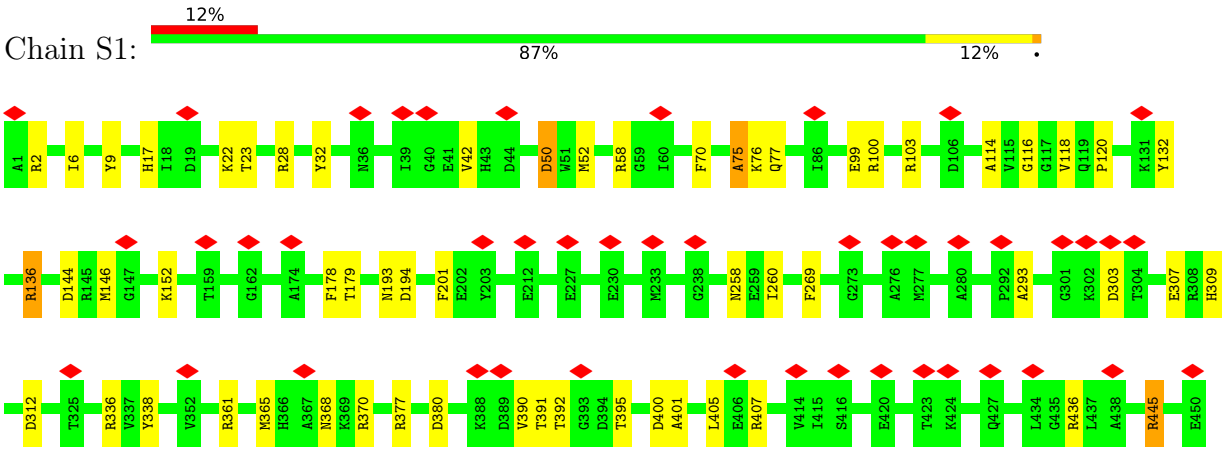
- Molecule 23: 30S ribosomal protein S9

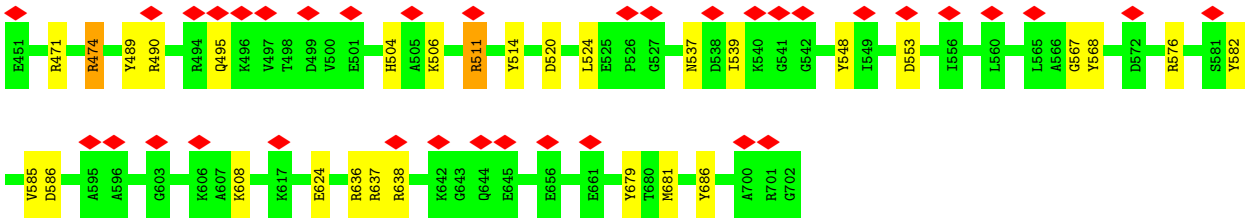
Chain SI:



- Molecule 24: Elongation factor G

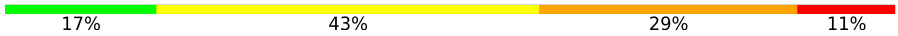
Chain S1:

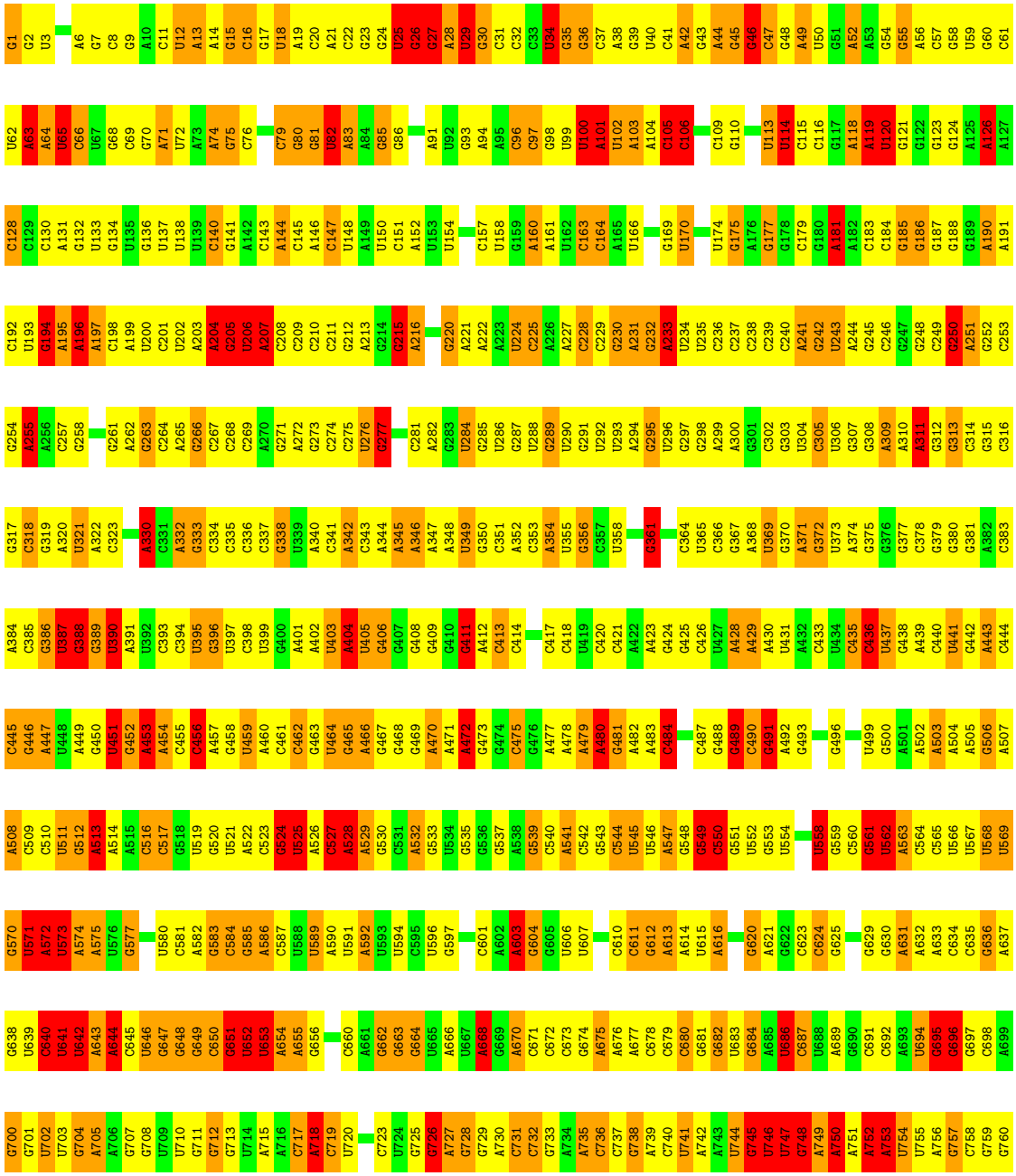


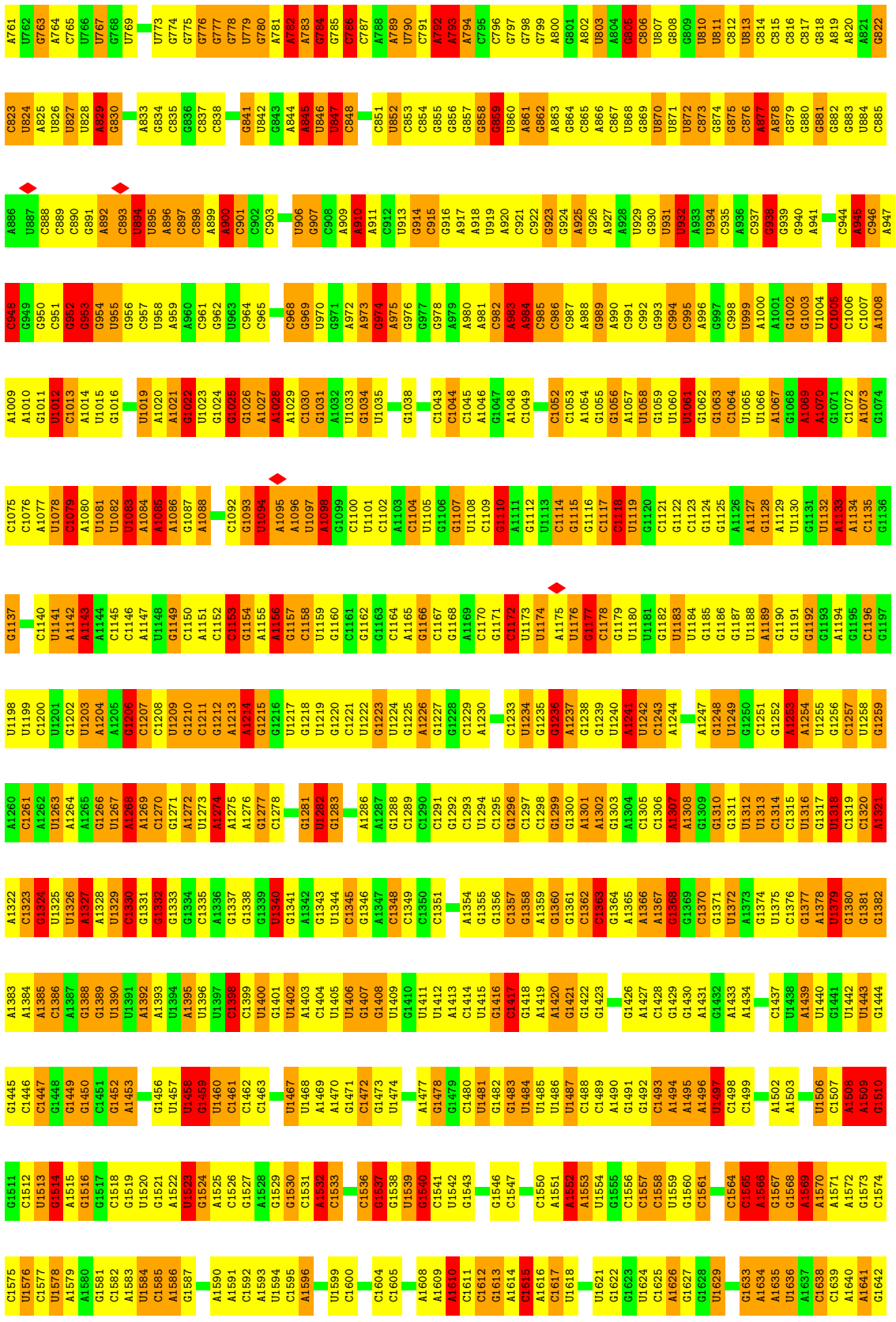


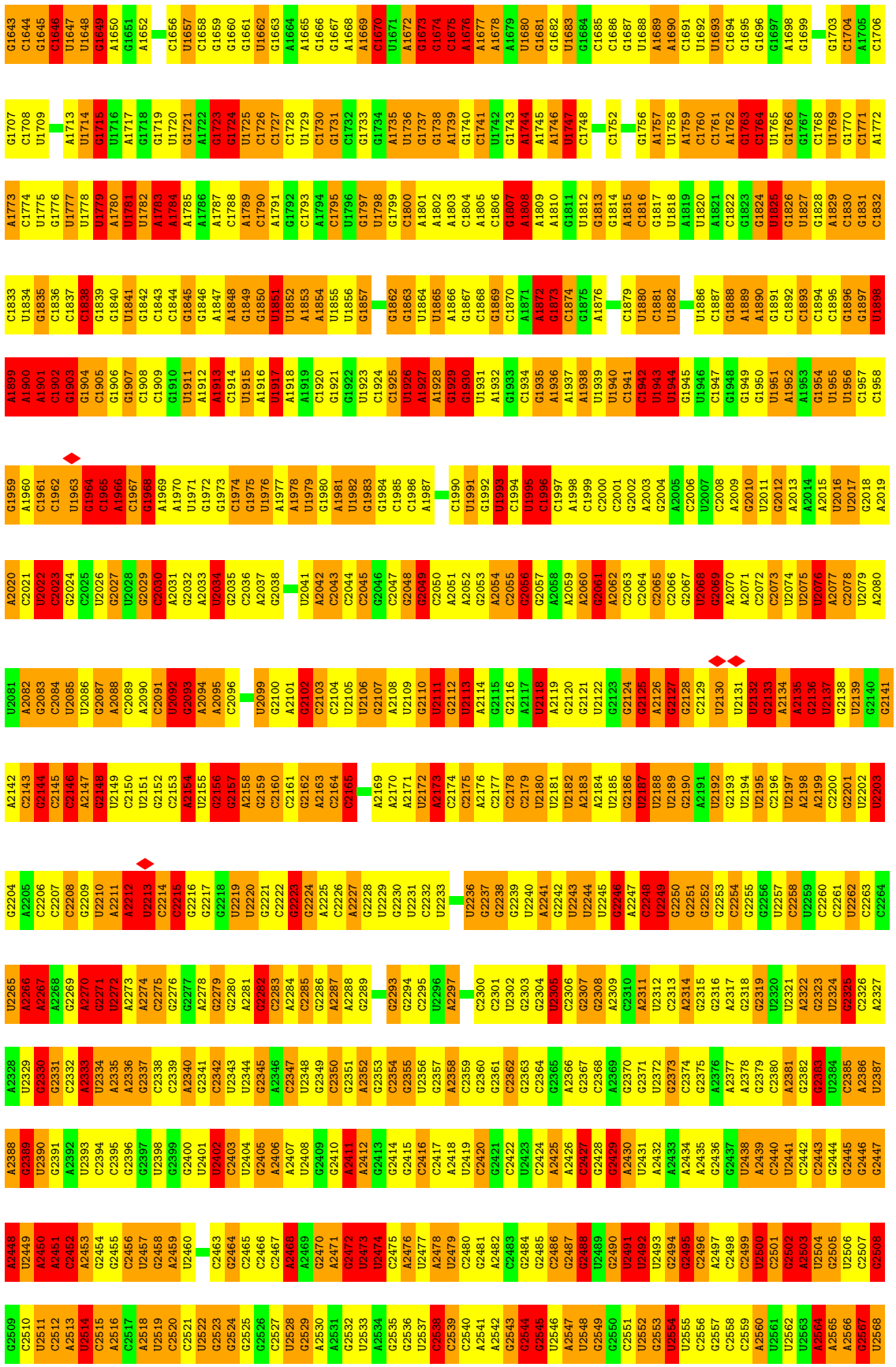
- Molecule 25: 23S ribosomal RNA

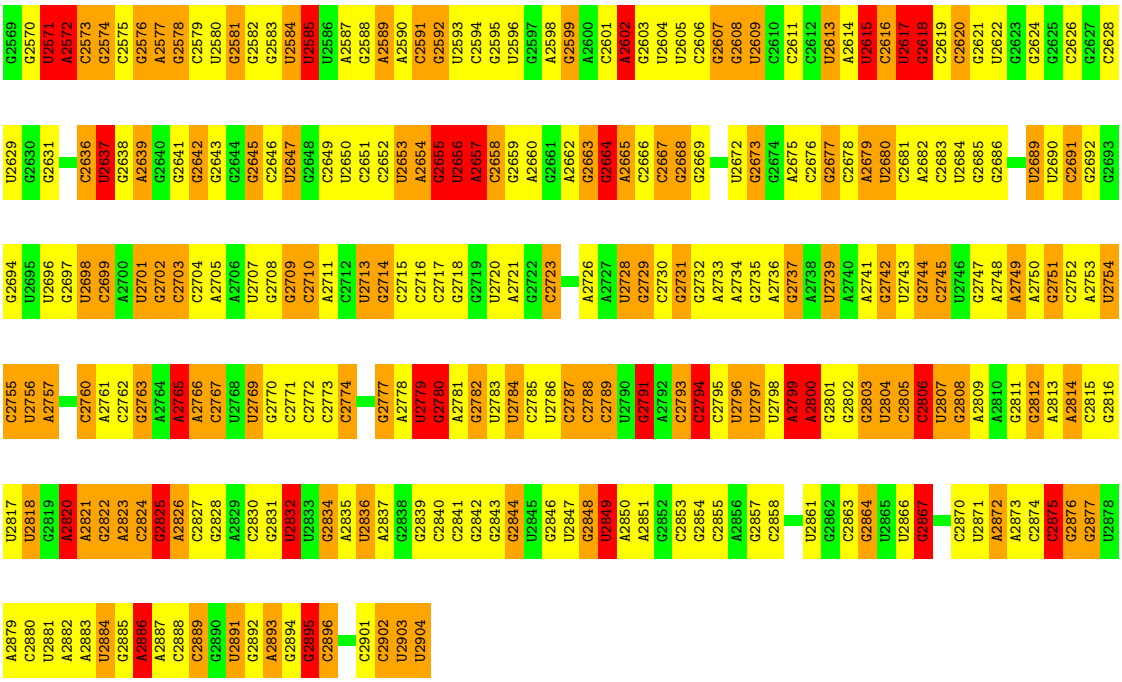
Chain LA:





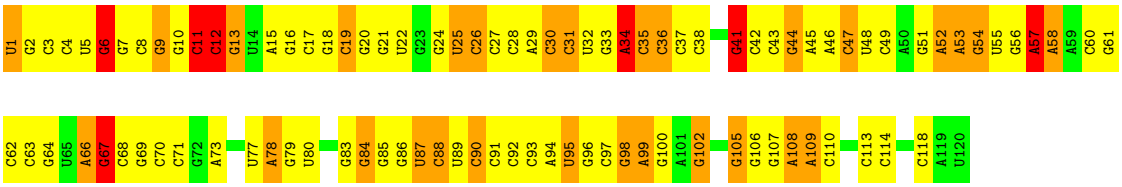

A761 U762 G763 A764 C765 U766 U767 G768 U769 U773 G774 G775 G776 G777 G778 U779 G780 A781 A782 A783 G784 G785 C786 C787 A788 A789 U790 C791 A792 A793 A794 C795 C796 G797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 G822
C823 U824 A825 U826 U827 U828 A829 G830 A833 G834 C835 G836 C837 C838 G841 U842 G843 A844 A845 U846 U847 C848 C851 U852 C853 C854 G855 G856 G857 G858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 U870 U871 U872 C873 G874 G875 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885
A886 U887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 C903 U906 G907 C908 A909 A910 A911 C912 U913 G914 C915 G916 A917 A918 U919 A920 C921 C922 G923 G924 A925 G926 A927 A928 U929 G930 U931 U932 A933 U934 C935 A936 C937 G938 G939 G940 A941 C944 A945 C946 A947
C948 G949 G950 C951 G952 G953 G954 U955 G956 C957 U958 A959 A960 C961 G962 U963 C964 C965 C968 G969 U970 G971 A972 A973 G974 A975 G976 G977 G978 A979 A980 A981 C982 A983 A984 C985 C986 C987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 U1004 C1005 C1006 C1007 A1008
A1009 A1010 G1011 U1012 C1013 A1014 U1015 G1016 U1019 A1020 A1021 G1022 U1023 G1024 G1025 G1026 A1027 A1028 A1029 C1030 G1031 A1032 U1033 G1034 U1035 G1038 C1043 C1044 C1045 A1046 G1047 A1048 C1049 C1052 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074
C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 C1114 G1115 G1116 C1117 C1118 U1119 G1120 C1121 G1122 C1123 G1124 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136
G1137 C1140 U1141 A1142 A1143 A1144 C1145 C1146 A1147 U1148 G1149 C1150 A1151 C1152 C1153 G1154 A1155 A1156 G1157 C1158 U1159 G1160 C1161 G1162 G1163 C1164 A1165 G1166 C1167 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 G1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195 C1196 G1197
U1198 U1199 C1200 U1201 G1202 U1203 A1204 A1205 G1206 C1207 C1208 U1209 G1210 C1211 C1212 A1213 A1214 G1215 G1216 U1217 C1218 U1219 G1220 C1221 U1222 G1223 U1224 G1225 A1226 G1227 G1228 C1229 A1230 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 U1242 C1243 A1244 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 U1258 G1259
A1260 C1261 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 C1278 G1281 U1282 G1283 A1286 A1287 G1288 C1289 C1290 C1291 G1292 C1293 U1294 C1295 G1296 C1297 C1298 G1299 G1300 A1301 A1302 G1303 A1304 C1305 C1306 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 G1317 U1318 C1319 C1320 A1321
A1322 C1323 G1324 U1325 U1326 A1327 A1328 U1329 C1330 G1331 G1332 G1333 G1334 C1335 A1336 G1337 G1338 G1339 U1340 G1341 A1342 G1343 U1344 U1345 G1346 A1347 C1348 C1349 C1350 C1351 A1354 G1355 G1356 C1357 G1358 A1359 G1360 G1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 G1374 U1375 C1376 G1377 A1378 U1379 G1380 G1381 G1382
A1383 A1384 A1385 C1386 A1387 G1388 G1389 U1390 U1391 A1392 A1393 U1394 A1395 U1396 U1397 C1398 C1399 U1400 G1401 U1402 A1403 C1404 U1405 U1406 G1407 G1408 U1409 G1410 U1411 U1412 A1413 C1414 U1415 G1416 C1417 G1418 A1419 A1420 G1421 G1422 G1423 G1426 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 C1437 U1438 A1439 U1440 G1441 U1442 U1443 G1444
G1445 C1446 C1447 G1448 G1449 G1450 C1451 G1452 A1453 G1456 U1457 U1458 G1459 U1460 C1461 C1462 C1463 U1467 U1468 A1469 A1470 G1471 C1472 G1473 U1474 A1477 G1478 G1479 C1480 U1481 G1482 G1483 U1484 U1485 U1486 U1487 C1488 C1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 A1502 A1503 U1506 C1507 A1508 A1509 G1510
G1511 C1512 U1513 G1514 A1515 G1516 G1517 C1518 G1519 U1520 G1521 A1522 U1523 G1524 A1525 C1526 G1527 A1528 G1529 G1530 C1531 A1532 C1533 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 G1546 C1547 C1550 A1551 A1552 A1553 U1554 G1555 C1556 C1557 C1558 U1559 G1560 C1561 C1564 C1565 A1566 G1567 G1568 A1569 A1570 A1571 A1572 G1573 C1574
C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 A1586 G1587 A1590 A1591 C1592 A1593 U1594 C1595 A1596 U1599 C1600 C1604 C1605 A1608 A1609 A1610 C1611 C1612 G1613 A1614 G1615 A1616 C1617 U1618 U1621 G1622 G1623 U1624 C1625 A1626 G1627 G1628 U1629 G1633 A1634 A1635 U1636 A1637 C1638 C1639 A1640 A1641 G1642





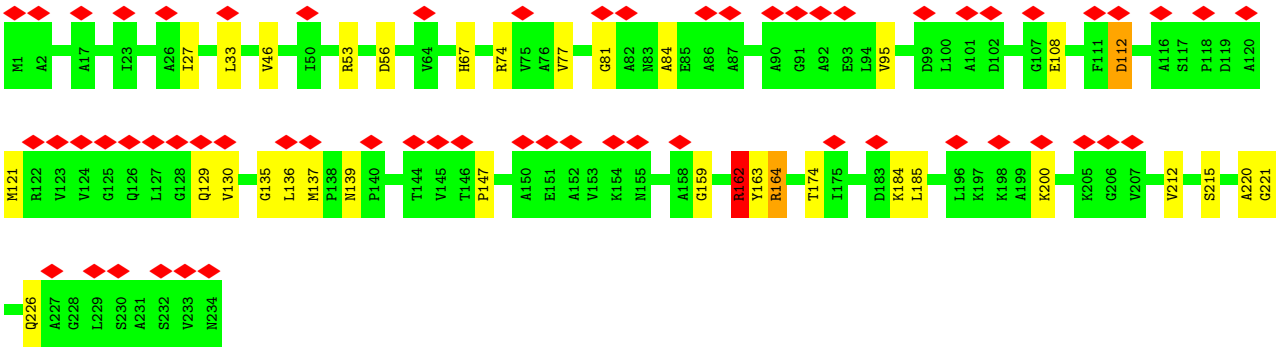
- Molecule 26: 5S ribosomal RNA

Chain LB:



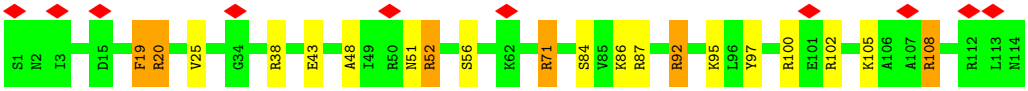
- Molecule 27: 50S ribosomal protein L1

Chain LC:



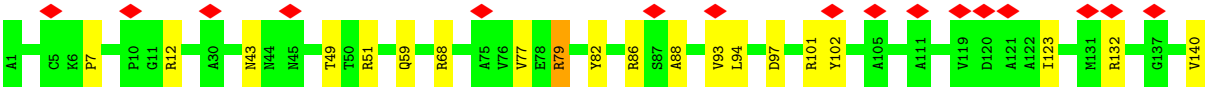
- Molecule 28: 50S ribosomal protein L19

Chain LM:



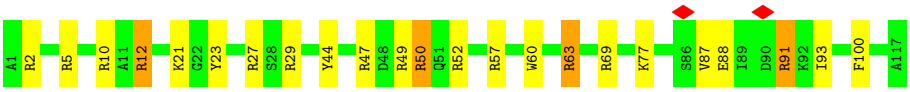
- Molecule 29: 50S ribosomal protein L2

Chain LN:



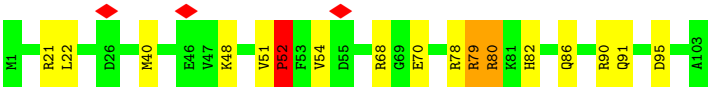
- Molecule 30: 50S ribosomal protein L20

Chain LO:



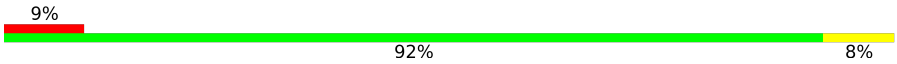
- Molecule 31: 50S ribosomal protein L21

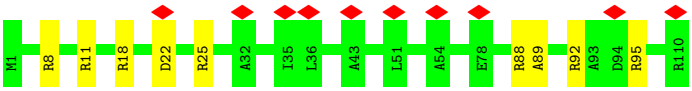
Chain LP:



- Molecule 32: 50S ribosomal protein L22

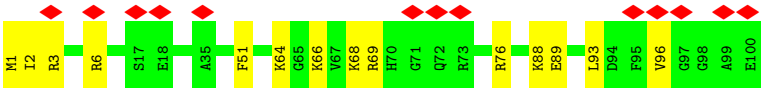
Chain LQ:





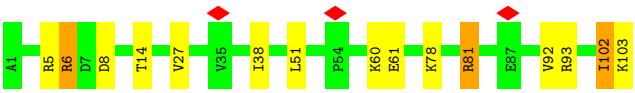
- Molecule 33: 50S ribosomal protein L23

Chain LR:



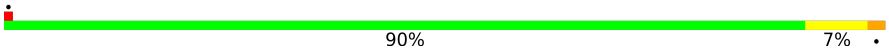
- Molecule 34: 50S ribosomal protein L24

Chain LS:



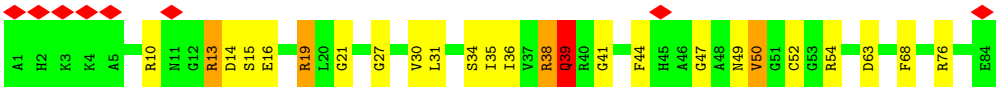
• Molecule 35: 50S ribosomal protein L25

Chain LT:



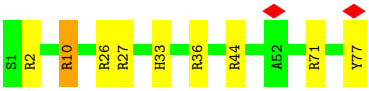
• Molecule 36: 50S ribosomal protein L27

Chain LU:



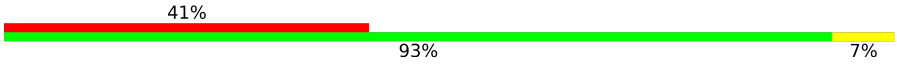
• Molecule 37: 50S ribosomal protein L28

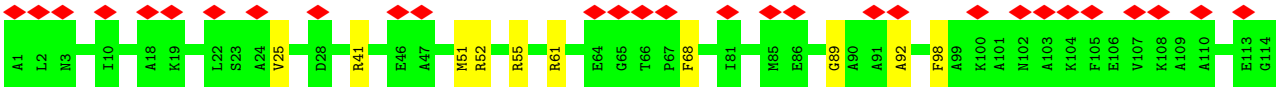
Chain LV:

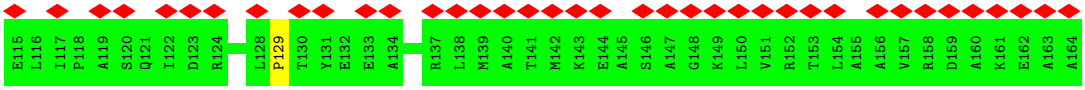


• Molecule 38: 50S ribosomal protein L10

Chain LD:

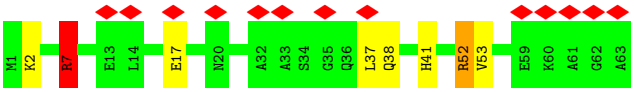






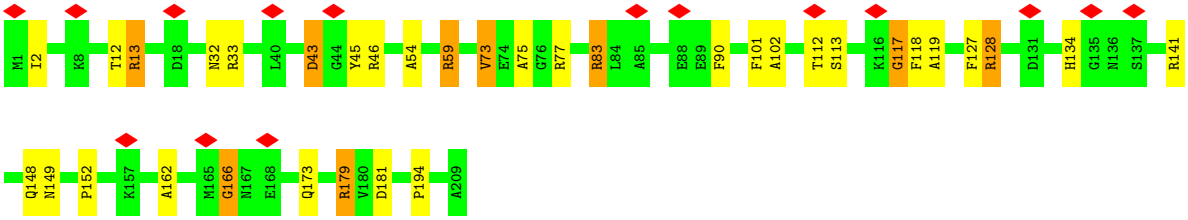
• Molecule 39: 50S ribosomal protein L29

Chain LW:



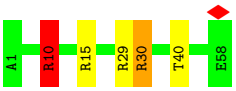
• Molecule 40: 50S ribosomal protein L3

Chain LX:



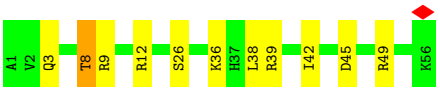
• Molecule 41: 50S ribosomal protein L30

Chain LY: 91% 5%



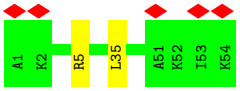
• Molecule 42: 50S ribosomal protein L32

Chain L1: 80% 18%



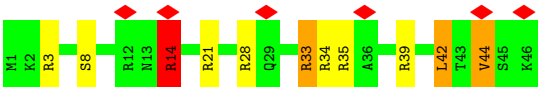
• Molecule 43: 50S ribosomal protein L33

Chain L2: 9% 96%



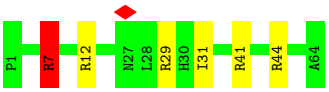
• Molecule 44: 50S ribosomal protein L34

Chain L3: 13% 76% 15% 7%



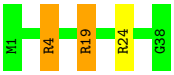
• Molecule 45: 50S ribosomal protein L35

Chain L4: 91% 8%



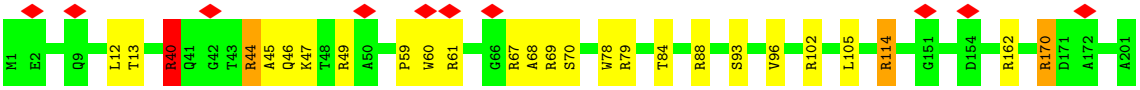
• Molecule 46: 50S ribosomal protein L36

Chain L5: 92% 5%



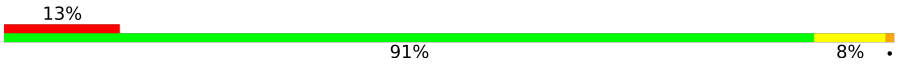
• Molecule 47: 50S ribosomal protein L4

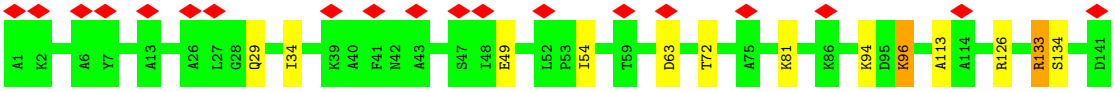
Chain L6:



• Molecule 48: 50S ribosomal protein L11

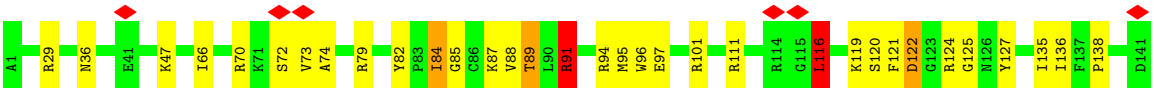
Chain LE:

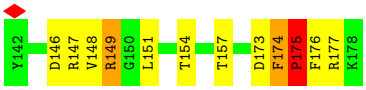




• Molecule 49: 50S ribosomal protein L5

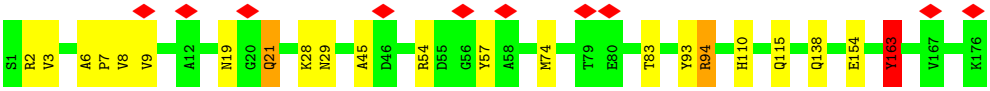
Chain L7:





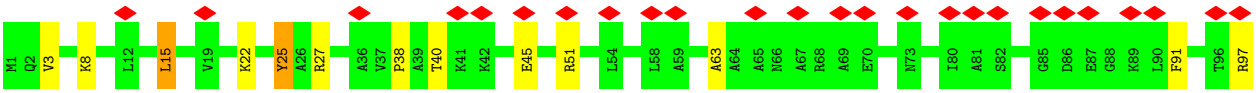
• Molecule 50: 50S ribosomal protein L6

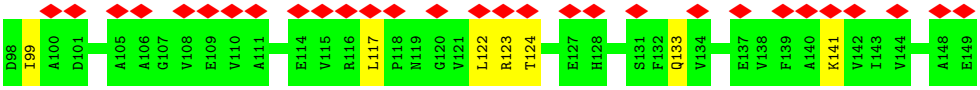
Chain L8:



• Molecule 51: 50S ribosomal protein L9

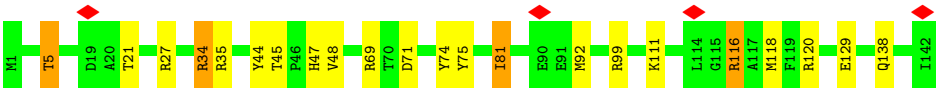
Chain L9:





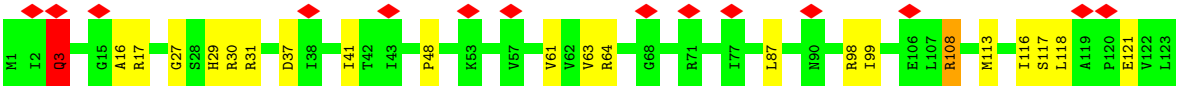
• Molecule 52: 50S ribosomal protein L13

Chain LF:



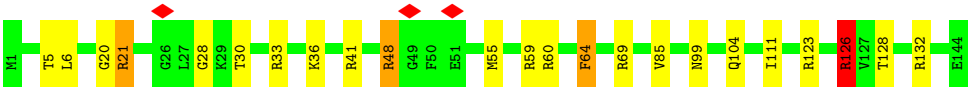
- Molecule 53: 50S ribosomal protein L14

Chain LG:



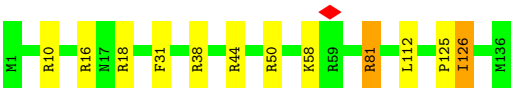
- Molecule 54: 50S ribosomal protein L15

Chain LH:



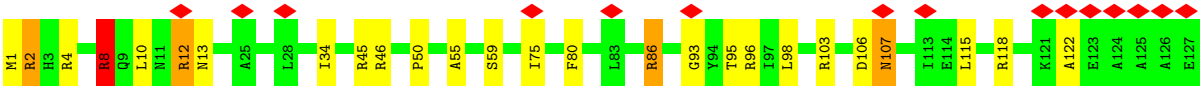
- Molecule 55: 50S ribosomal protein L16

Chain LI:



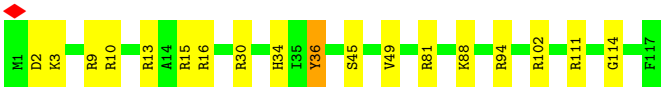
- Molecule 56: 50S ribosomal protein L17

Chain LJ:



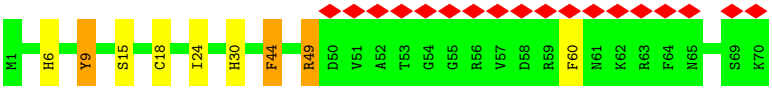
- Molecule 57: 50S ribosomal protein L18

Chain LK:



- Molecule 58: 50S ribosomal protein L31

Chain LZ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	90000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND3 and CTFIT	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	58000	Depositor
Image detector	DIRECT ELECTRON DE-12 (4k x 3k)	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	377.99997, 377.99997, 377.99997	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	SA	1.54	172/37035 (0.5%)	1.91	1570/57774 (2.7%)
2	S6	1.44	5/1831 (0.3%)	1.81	72/2853 (2.5%)
3	S7	1.36	4/1762 (0.2%)	1.97	89/2746 (3.2%)
4	SJ	0.73	0/835	1.28	10/1127 (0.9%)
5	SK	0.75	0/982	1.30	11/1323 (0.8%)
6	SL	0.75	0/969	1.37	9/1300 (0.7%)
7	SM	0.70	0/919	1.33	10/1226 (0.8%)
8	SN	0.73	0/817	1.36	8/1088 (0.7%)
9	SO	0.70	0/724	1.35	12/966 (1.2%)
10	SP	0.73	0/659	1.41	12/884 (1.4%)
11	SQ	0.74	0/681	1.24	5/913 (0.5%)
12	SR	0.76	0/637	1.37	8/851 (0.9%)
13	SS	0.70	0/744	1.28	5/995 (0.5%)
14	SB	0.71	0/1904	1.22	16/2565 (0.6%)
15	ST	0.69	0/676	1.15	3/895 (0.3%)
16	SU	0.84	0/598	1.53	8/792 (1.0%)
17	SC	0.74	0/1852	1.19	7/2490 (0.3%)
18	SD	0.70	0/1665	1.33	16/2227 (0.7%)
19	SE	0.74	0/1239	1.16	2/1664 (0.1%)
20	SF	0.75	0/1121	1.26	6/1509 (0.4%)
21	SG	0.75	0/1422	1.29	12/1908 (0.6%)
22	SH	0.71	0/989	1.22	8/1326 (0.6%)
23	SI	0.75	0/1048	1.35	17/1394 (1.2%)
24	S1	0.70	0/5532	1.21	27/7485 (0.4%)
25	LA	1.66	473/69812 (0.7%)	1.93	2989/108912 (2.7%)
26	LB	1.39	6/2869 (0.2%)	1.84	112/4474 (2.5%)
27	LC	0.70	0/1748	1.21	7/2355 (0.3%)
28	LM	0.77	0/929	1.33	12/1242 (1.0%)
29	LN	0.74	0/2131	1.38	16/2863 (0.6%)
30	LO	0.70	0/960	1.46	18/1278 (1.4%)
31	LP	0.76	0/829	1.21	6/1107 (0.5%)
32	LQ	0.74	0/864	1.28	9/1156 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	LR	0.73	0/794	1.22	6/1060 (0.6%)
34	LS	0.71	0/797	1.19	6/1062 (0.6%)
35	LT	0.71	0/766	1.18	4/1025 (0.4%)
36	LU	0.78	0/642	1.34	6/848 (0.7%)
37	LV	0.76	0/635	1.32	7/848 (0.8%)
38	LD	0.73	0/1247	1.15	3/1679 (0.2%)
39	LW	0.72	0/510	1.22	4/677 (0.6%)
40	LX	0.77	0/1586	1.35	16/2134 (0.7%)
41	LY	0.68	0/453	1.40	4/605 (0.7%)
42	L1	0.71	0/450	1.28	1/599 (0.2%)
43	L2	0.75	0/448	1.13	1/594 (0.2%)
44	L3	0.77	0/380	1.61	9/498 (1.8%)
45	L4	0.66	0/513	1.28	3/676 (0.4%)
46	L5	0.81	0/303	1.35	3/397 (0.8%)
47	L6	0.71	0/1571	1.27	11/2113 (0.5%)
48	LE	0.68	0/1046	1.19	4/1410 (0.3%)
49	L7	0.73	0/1444	1.35	18/1937 (0.9%)
50	L8	0.70	0/1343	1.20	9/1816 (0.5%)
51	L9	0.71	0/1122	1.16	8/1515 (0.5%)
52	LF	0.77	0/1152	1.30	10/1551 (0.6%)
53	LG	0.78	0/956	1.32	6/1279 (0.5%)
54	LH	0.72	0/1062	1.35	13/1413 (0.9%)
55	LI	0.75	0/1093	1.33	12/1460 (0.8%)
56	LJ	0.75	0/1021	1.36	12/1364 (0.9%)
57	LK	0.73	0/910	1.32	12/1219 (1.0%)
58	LZ	0.71	0/559	1.23	4/745 (0.5%)
All	All	1.38	660/169586 (0.4%)	1.75	5304/252212 (2.1%)

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	SA	2	423
2	S6	0	16
3	S7	0	31
4	SJ	0	7
5	SK	0	5
6	SL	0	9
7	SM	0	4
8	SN	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
9	SO	0	4
10	SP	0	4
11	SQ	0	4
12	SR	0	3
13	SS	0	2
14	SB	0	3
15	ST	0	2
16	SU	0	3
17	SC	0	7
18	SD	0	6
19	SE	0	8
20	SF	0	6
21	SG	0	4
22	SH	0	3
23	SI	0	4
24	S1	0	19
25	LA	1	941
26	LB	0	21
27	LC	0	4
28	LM	0	5
29	LN	0	9
30	LO	0	4
31	LP	0	1
32	LQ	0	2
34	LS	0	3
35	LT	0	2
36	LU	0	5
37	LV	0	3
38	LD	0	3
39	LW	0	4
40	LX	0	10
41	LY	0	1
42	L1	0	2
44	L3	0	5
45	L4	0	3
46	L5	0	1
47	L6	0	6
48	LE	0	1
49	L7	0	8
50	L8	0	3
51	L9	0	2
52	LF	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
53	LG	0	4
54	LH	0	5
55	LI	0	1
56	LJ	0	6
57	LK	0	3
58	LZ	0	4
All	All	3	1660

All (660) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	1513	A	N9-C4	-11.15	1.31	1.37
1	SA	781	A	N9-C4	-10.92	1.31	1.37
1	SA	900	A	N9-C4	-10.30	1.31	1.37
25	LA	2571	U	O3'-P	-10.16	1.49	1.61
25	LA	750	A	N9-C4	-10.00	1.31	1.37
25	LA	1977	A	N9-C4	-9.28	1.32	1.37
25	LA	2052	A	N9-C4	-9.19	1.32	1.37
25	LA	2003	A	N9-C4	-9.17	1.32	1.37
1	SA	51	A	O3'-P	-9.11	1.50	1.61
25	LA	2247	A	N9-C4	-8.96	1.32	1.37
25	LA	528	A	N9-C4	-8.67	1.32	1.37
25	LA	2009	A	N9-C4	-8.66	1.32	1.37
1	SA	1340	A	N9-C4	-8.59	1.32	1.37
25	LA	2386	A	N9-C4	-8.49	1.32	1.37
25	LA	574	A	N9-C4	-8.45	1.32	1.37
25	LA	575	A	N9-C4	-8.40	1.32	1.37
25	LA	2823	A	N9-C4	-8.25	1.32	1.37
25	LA	2445	G	C2'-C1'	-8.05	1.44	1.53
25	LA	2607	G	C2'-C1'	-8.05	1.44	1.53
25	LA	2453	A	N9-C4	-7.83	1.33	1.37
25	LA	2657	A	C2'-C1'	-7.77	1.44	1.53
1	SA	1080	A	O3'-P	-7.76	1.51	1.61
1	SA	764	C	O3'-P	-7.65	1.51	1.61
25	LA	752	A	C2'-C1'	-7.64	1.45	1.53
25	LA	1269	A	N9-C4	-7.61	1.33	1.37
25	LA	1967	C	C5'-C4'	7.58	1.60	1.51
25	LA	2064	C	C2-N3	-7.58	1.29	1.35
1	SA	768	A	N9-C4	-7.57	1.33	1.37
25	LA	2589	A	N9-C4	-7.57	1.33	1.37
25	LA	1021	A	N9-C4	-7.57	1.33	1.37
25	LA	1967	C	C2'-C1'	-7.44	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	783	A	N9-C4	-7.42	1.33	1.37
25	LA	203	A	N9-C4	-7.39	1.33	1.37
25	LA	2665	A	C2'-C1'	-7.37	1.45	1.53
25	LA	2731	G	C2'-C1'	-7.36	1.45	1.53
25	LA	2094	A	N9-C4	-7.35	1.33	1.37
25	LA	1322	A	O3'-P	-7.33	1.52	1.61
1	SA	730	G	N1-C2	-7.32	1.31	1.37
25	LA	1359	A	N9-C4	-7.30	1.33	1.37
2	S6	32	G	N9-C4	-7.28	1.32	1.38
25	LA	2766	A	N9-C4	-7.28	1.33	1.37
25	LA	811	U	P-O5'	-7.26	1.52	1.59
1	SA	1176	A	N9-C4	-7.24	1.33	1.37
25	LA	2541	A	N9-C4	-7.23	1.33	1.37
25	LA	1151	A	N9-C4	-7.22	1.33	1.37
1	SA	1416	G	C2'-C1'	-7.21	1.45	1.53
1	SA	918	A	N9-C4	-7.16	1.33	1.37
25	LA	2647	U	O3'-P	-7.14	1.52	1.61
25	LA	764	A	C2'-C1'	-7.10	1.45	1.53
25	LA	2451	A	N9-C4	-7.10	1.33	1.37
25	LA	1772	A	N9-C4	-7.07	1.33	1.37
1	SA	452	A	N9-C4	-7.06	1.33	1.37
1	SA	1419	G	C2'-C1'	-7.04	1.45	1.53
25	LA	15	G	C2'-C1'	-7.04	1.45	1.53
25	LA	2236	U	O3'-P	-7.02	1.52	1.61
25	LA	870	U	P-O5'	-6.99	1.52	1.59
25	LA	2060	A	O3'-P	-6.96	1.52	1.61
25	LA	2826	A	N9-C4	-6.96	1.33	1.37
25	LA	945	A	C2'-C1'	-6.95	1.45	1.53
25	LA	564	C	P-O5'	-6.94	1.52	1.59
1	SA	1331	G	P-O5'	-6.92	1.52	1.59
25	LA	2598	A	N9-C4	-6.92	1.33	1.37
1	SA	1402	C	C2'-C1'	-6.92	1.45	1.53
25	LA	692	C	P-O5'	-6.89	1.52	1.59
25	LA	1010	A	N9-C4	-6.85	1.33	1.37
1	SA	553	A	N9-C4	-6.84	1.33	1.37
25	LA	1434	A	N9-C4	6.82	1.42	1.37
25	LA	1787	A	N7-C5	-6.82	1.35	1.39
25	LA	684	G	C2'-C1'	-6.81	1.45	1.53
25	LA	2468	A	N9-C4	-6.80	1.33	1.37
1	SA	957	U	O3'-P	-6.80	1.52	1.61
25	LA	465	G	O3'-P	-6.73	1.53	1.61
1	SA	499	A	N9-C4	-6.72	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	2020	A	N9-C4	-6.72	1.33	1.37
1	SA	1080	A	N9-C4	-6.70	1.33	1.37
25	LA	676	A	N9-C4	-6.70	1.33	1.37
1	SA	1190	G	O3'-P	-6.69	1.53	1.61
25	LA	2665	A	C1'-N9	-6.68	1.37	1.46
1	SA	1213	A	N9-C4	-6.66	1.33	1.37
25	LA	745	G	C6-N1	6.66	1.44	1.39
25	LA	752	A	C1'-N9	-6.66	1.37	1.46
25	LA	17	G	P-O5'	-6.65	1.53	1.59
25	LA	761	A	N9-C4	-6.64	1.33	1.37
25	LA	1849	G	N9-C4	-6.63	1.32	1.38
25	LA	1808	A	P-O5'	-6.63	1.53	1.59
25	LA	2495	G	P-O5'	-6.63	1.53	1.59
25	LA	1807	G	O3'-P	-6.59	1.53	1.61
25	LA	2684	U	P-O5'	-6.59	1.53	1.59
25	LA	18	U	P-O5'	-6.59	1.53	1.59
25	LA	2698	U	C2'-C1'	-6.59	1.46	1.53
25	LA	573	U	C5'-C4'	6.58	1.59	1.51
25	LA	826	U	O3'-P	-6.57	1.53	1.61
1	SA	817	C	O3'-P	-6.57	1.53	1.61
25	LA	513	A	N9-C4	-6.57	1.33	1.37
25	LA	1302	A	N9-C4	-6.55	1.33	1.37
25	LA	2427	C	C2'-C1'	-6.55	1.46	1.53
25	LA	29	U	O3'-P	-6.55	1.53	1.61
25	LA	1543	G	O3'-P	-6.55	1.53	1.61
1	SA	652	U	O3'-P	-6.54	1.53	1.61
25	LA	2251	G	C2'-C1'	-6.54	1.46	1.53
1	SA	804	U	O3'-P	-6.53	1.53	1.61
1	SA	292	G	N9-C4	-6.52	1.32	1.38
25	LA	808	G	C2'-C1'	-6.52	1.46	1.53
25	LA	2560	A	N9-C4	-6.50	1.33	1.37
25	LA	1903	G	N9-C4	-6.49	1.32	1.38
25	LA	570	G	C1'-N9	-6.48	1.37	1.46
25	LA	458	G	C2'-C1'	-6.48	1.46	1.53
25	LA	29	U	P-O5'	-6.48	1.53	1.59
25	LA	764	A	N9-C4	-6.46	1.33	1.37
1	SA	780	A	N9-C4	-6.45	1.33	1.37
25	LA	1307	A	N9-C4	-6.43	1.33	1.37
25	LA	2566	A	C2'-C1'	-6.42	1.46	1.53
25	LA	1797	G	O3'-P	-6.42	1.53	1.61
25	LA	1427	A	N9-C4	-6.41	1.34	1.37
25	LA	1939	U	C2'-C1'	-6.41	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	983	A	N9-C4	-6.39	1.34	1.37
25	LA	2251	G	C6-N1	6.38	1.44	1.39
25	LA	668	A	N9-C4	-6.38	1.34	1.37
25	LA	195	A	C2'-C1'	-6.37	1.46	1.53
25	LA	1477	A	N9-C4	-6.37	1.34	1.37
1	SA	781	A	C1'-N9	-6.36	1.38	1.46
1	SA	1305	G	C4'-O4'	-6.35	1.37	1.45
1	SA	1255	G	N9-C4	-6.34	1.32	1.38
1	SA	552	U	C2'-C1'	-6.34	1.46	1.53
25	LA	782	A	N9-C4	-6.34	1.34	1.37
1	SA	1393	U	P-O5'	-6.33	1.53	1.59
25	LA	586	A	N9-C4	-6.33	1.34	1.37
25	LA	1568	G	P-O5'	-6.32	1.53	1.59
25	LA	2736	A	N9-C4	-6.31	1.34	1.37
25	LA	643	A	C5'-C4'	6.31	1.58	1.51
25	LA	2511	U	C2'-C1'	-6.30	1.46	1.53
25	LA	1274	A	N9-C4	-6.30	1.34	1.37
1	SA	1402	C	O3'-P	-6.28	1.53	1.61
25	LA	2444	G	C2'-C1'	-6.28	1.46	1.53
1	SA	944	G	O3'-P	-6.28	1.53	1.61
1	SA	261	U	O3'-P	-6.28	1.53	1.61
1	SA	227	G	O3'-P	-6.25	1.53	1.61
25	LA	2250	G	N9-C4	-6.24	1.32	1.38
25	LA	1966	A	N7-C5	-6.23	1.35	1.39
25	LA	2457	U	P-O5'	-6.23	1.53	1.59
1	SA	1401	G	C6-N1	-6.21	1.35	1.39
25	LA	2705	A	N9-C4	-6.21	1.34	1.37
25	LA	572	A	N9-C4	-6.20	1.34	1.37
25	LA	1686	C	P-O5'	-6.20	1.53	1.59
25	LA	2682	A	N7-C5	-6.20	1.35	1.39
25	LA	516	C	O3'-P	-6.20	1.53	1.61
25	LA	464	U	P-O5'	-6.19	1.53	1.59
25	LA	990	A	N9-C4	-6.19	1.34	1.37
25	LA	2822	G	P-O5'	-6.19	1.53	1.59
25	LA	742	A	N9-C4	-6.18	1.34	1.37
25	LA	1253	A	C2'-C1'	-6.18	1.46	1.53
25	LA	1677	A	N9-C4	-6.18	1.34	1.37
1	SA	752	G	O3'-P	-6.17	1.53	1.61
1	SA	393	A	N9-C4	-6.17	1.34	1.37
1	SA	782	A	O3'-P	-6.17	1.53	1.61
1	SA	1501	C	C2'-C1'	-6.16	1.46	1.53
25	LA	507	A	P-O5'	-6.16	1.53	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S7	64	A	N9-C4	-6.15	1.34	1.37
1	SA	1305	G	O4'-C1'	-6.15	1.33	1.41
1	SA	664	G	P-O5'	-6.14	1.53	1.59
1	SA	795	C	O3'-P	-6.14	1.53	1.61
25	LA	629	G	O3'-P	-6.14	1.53	1.61
1	SA	1124	G	O3'-P	-6.14	1.53	1.61
1	SA	1227	A	O3'-P	-6.14	1.53	1.61
1	SA	814	A	N9-C4	6.13	1.41	1.37
1	SA	1504	G	N7-C5	-6.13	1.35	1.39
1	SA	1518	A	C2'-C1'	-6.13	1.46	1.53
1	SA	1523	G	P-O5'	-6.13	1.53	1.59
25	LA	2271	G	O3'-P	-6.13	1.53	1.61
1	SA	1046	A	N9-C4	-6.12	1.34	1.37
25	LA	805	G	C6-N1	-6.12	1.35	1.39
1	SA	797	C	P-O5'	-6.12	1.53	1.59
25	LA	1901	A	N9-C4	-6.11	1.34	1.37
25	LA	2591	C	P-O5'	-6.11	1.53	1.59
25	LA	1899	A	N9-C4	-6.10	1.34	1.37
25	LA	2249	U	O3'-P	-6.09	1.53	1.61
25	LA	2664	G	O3'-P	-6.08	1.53	1.61
25	LA	2522	U	P-O5'	-6.08	1.53	1.59
25	LA	2667	C	P-O5'	-6.07	1.53	1.59
25	LA	1257	C	P-O5'	-6.07	1.53	1.59
25	LA	2498	C	C2-N3	-6.07	1.30	1.35
25	LA	787	C	C2'-C1'	-6.05	1.46	1.53
1	SA	772	U	P-O5'	-6.05	1.53	1.59
25	LA	922	C	C2'-C1'	-6.04	1.46	1.53
25	LA	2579	C	C2'-C1'	-6.03	1.46	1.53
25	LA	2589	A	C2'-C1'	-6.03	1.46	1.53
1	SA	787	A	N9-C4	-6.03	1.34	1.37
1	SA	786	G	P-O5'	-6.02	1.53	1.59
25	LA	2068	U	C2'-C1'	-6.02	1.46	1.53
25	LA	2495	G	N7-C5	-6.02	1.35	1.39
25	LA	1650	A	N9-C4	-6.02	1.34	1.37
25	LA	502	A	N9-C4	-6.01	1.34	1.37
1	SA	1074	G	P-O5'	-6.00	1.53	1.59
25	LA	1779	U	P-O5'	-6.00	1.53	1.59
25	LA	671	C	P-O5'	-6.00	1.53	1.59
25	LA	2060	A	C2'-C1'	-6.00	1.46	1.53
25	LA	751	A	O3'-P	-5.99	1.53	1.61
25	LA	752	A	C3'-C2'	-5.99	1.46	1.52
25	LA	242	G	O3'-P	-5.98	1.53	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	2730	C	P-O5'	-5.98	1.53	1.59
25	LA	611	C	O3'-P	-5.98	1.53	1.61
1	SA	1191	A	N9-C4	-5.97	1.34	1.37
25	LA	2599	G	C2'-C1'	-5.97	1.46	1.53
25	LA	948	C	P-O5'	-5.97	1.53	1.59
25	LA	119	A	C2'-C1'	-5.96	1.46	1.53
25	LA	2282	G	O3'-P	-5.96	1.53	1.61
25	LA	2572	A	C2'-C1'	-5.96	1.46	1.53
25	LA	2052	A	N7-C5	-5.96	1.35	1.39
25	LA	2595	G	P-O5'	-5.96	1.53	1.59
1	SA	609	A	N9-C4	-5.95	1.34	1.37
25	LA	1634	A	C2'-C1'	-5.94	1.46	1.53
25	LA	2266	A	N9-C4	-5.94	1.34	1.37
1	SA	1054	C	O3'-P	-5.94	1.54	1.61
1	SA	720	C	O3'-P	-5.94	1.54	1.61
25	LA	1936	A	N7-C5	-5.94	1.35	1.39
25	LA	2471	A	N9-C4	-5.93	1.34	1.37
1	SA	503	C	P-O5'	-5.93	1.53	1.59
1	SA	555	U	P-O5'	-5.92	1.53	1.59
25	LA	28	A	N7-C5	-5.92	1.35	1.39
25	LA	945	A	C1'-N9	-5.91	1.38	1.46
25	LA	826	U	C2'-C1'	-5.91	1.46	1.53
1	SA	777	A	C2'-C1'	-5.90	1.46	1.53
1	SA	527	G	N9-C4	-5.89	1.33	1.38
25	LA	947	A	P-O5'	-5.88	1.53	1.59
25	LA	1698	A	C2'-C1'	-5.88	1.46	1.53
1	SA	1523	G	O3'-P	-5.88	1.54	1.61
25	LA	2420	C	P-O5'	-5.88	1.53	1.59
25	LA	231	A	O3'-P	-5.87	1.54	1.61
25	LA	2516	A	P-O5'	-5.87	1.53	1.59
25	LA	2394	C	P-O5'	-5.86	1.53	1.59
1	SA	415	A	N9-C4	5.86	1.41	1.37
1	SA	98	A	N9-C4	-5.85	1.34	1.37
1	SA	765	G	C6-N1	-5.85	1.35	1.39
25	LA	1928	A	N9-C4	-5.84	1.34	1.37
1	SA	909	A	N7-C5	-5.84	1.35	1.39
25	LA	1165	A	C2'-C1'	-5.84	1.47	1.53
1	SA	1522	U	N1-C2	-5.84	1.33	1.38
25	LA	197	A	N9-C4	-5.84	1.34	1.37
25	LA	250	G	O3'-P	-5.84	1.54	1.61
26	LB	43	C	O3'-P	-5.84	1.54	1.61
25	LA	481	G	C2'-C1'	-5.83	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	18	C	P-O5'	-5.82	1.53	1.59
25	LA	241	A	O3'-P	-5.82	1.54	1.61
25	LA	1998	A	N9-C4	-5.82	1.34	1.37
1	SA	428	G	O3'-P	-5.81	1.54	1.61
25	LA	210	C	P-O5'	-5.81	1.53	1.59
1	SA	575	G	P-O5'	-5.81	1.53	1.59
25	LA	1019	U	C2'-C1'	-5.80	1.47	1.53
1	SA	9	G	N9-C4	-5.80	1.33	1.38
1	SA	1499	A	N7-C5	-5.79	1.35	1.39
25	LA	1978	A	N9-C4	-5.78	1.34	1.37
1	SA	9	G	C2'-C1'	-5.78	1.47	1.53
25	LA	2246	G	P-O5'	-5.78	1.53	1.59
25	LA	2496	C	P-O5'	-5.77	1.53	1.59
25	LA	1649	G	N9-C4	-5.77	1.33	1.38
25	LA	2274	A	C2'-C1'	-5.77	1.47	1.53
25	LA	1665	A	N9-C4	-5.77	1.34	1.37
25	LA	2567	G	O3'-P	-5.76	1.54	1.61
25	LA	2249	U	C2'-C1'	-5.76	1.47	1.53
25	LA	752	A	O3'-P	-5.76	1.54	1.61
1	SA	1491	G	C4'-C3'	5.75	1.59	1.53
25	LA	1960	A	C2'-C1'	-5.75	1.47	1.53
25	LA	2518	A	C2'-C1'	-5.75	1.47	1.53
1	SA	740	U	P-O5'	-5.75	1.54	1.59
25	LA	1663	G	P-O5'	-5.75	1.54	1.59
25	LA	2585	U	O3'-P	-5.75	1.54	1.61
1	SA	1368	A	N9-C4	-5.74	1.34	1.37
1	SA	1480	A	N9-C4	-5.74	1.34	1.37
25	LA	925	A	C2'-C1'	-5.74	1.47	1.53
3	S7	61	C	C5'-C4'	5.74	1.58	1.51
26	LB	91	C	P-O5'	-5.74	1.54	1.59
1	SA	1197	A	N9-C4	-5.73	1.34	1.37
25	LA	2022	U	C2'-C1'	-5.73	1.47	1.53
26	LB	78	A	P-O5'	-5.73	1.54	1.59
25	LA	630	G	O3'-P	-5.73	1.54	1.61
25	LA	1323	C	C2'-C1'	-5.73	1.47	1.53
25	LA	1831	G	P-O5'	-5.73	1.54	1.59
25	LA	2067	G	C2'-C1'	-5.72	1.47	1.53
3	S7	49	C	C5'-C4'	5.72	1.58	1.51
25	LA	2518	A	C1'-N9	-5.72	1.38	1.46
25	LA	2588	G	C1'-N9	-5.72	1.38	1.46
1	SA	777	A	N9-C4	-5.71	1.34	1.37
1	SA	1179	A	O3'-P	-5.71	1.54	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	274	A	O3'-P	-5.70	1.54	1.61
25	LA	2030	C	N1-C6	5.70	1.40	1.37
25	LA	1917	U	C2'-C1'	-5.69	1.47	1.53
1	SA	1418	A	N9-C4	-5.69	1.34	1.37
25	LA	2614	A	N9-C4	-5.69	1.34	1.37
1	SA	816	A	N9-C4	-5.69	1.34	1.37
25	LA	1600	C	P-O5'	-5.69	1.54	1.59
25	LA	1132	U	C2'-C1'	-5.68	1.47	1.53
25	LA	466	A	P-O5'	-5.68	1.54	1.59
1	SA	768	A	N3-C4	-5.68	1.31	1.34
25	LA	691	C	O3'-P	-5.68	1.54	1.61
25	LA	1826	G	C2'-C1'	-5.68	1.47	1.53
1	SA	1123	U	O3'-P	-5.67	1.54	1.61
25	LA	126	A	C2'-C1'	-5.67	1.47	1.53
25	LA	631	A	P-O5'	-5.67	1.54	1.59
25	LA	630	G	P-O5'	-5.67	1.54	1.59
25	LA	1805	A	C2'-C1'	-5.66	1.47	1.53
25	LA	2033	A	C2'-C1'	-5.66	1.47	1.53
25	LA	1788	C	P-O5'	-5.66	1.54	1.59
25	LA	2605	U	P-O5'	-5.66	1.54	1.59
25	LA	1930	G	O3'-P	-5.65	1.54	1.61
25	LA	1838	C	P-O5'	-5.65	1.54	1.59
2	S6	38	A	N9-C4	-5.65	1.34	1.37
25	LA	450	G	C2'-C1'	-5.65	1.47	1.53
2	S6	40	C	P-O5'	-5.64	1.54	1.59
25	LA	196	A	P-O5'	-5.64	1.54	1.59
25	LA	745	G	P-O5'	-5.64	1.54	1.59
25	LA	2799	A	C5'-C4'	5.64	1.58	1.51
25	LA	806	C	P-O5'	-5.64	1.54	1.59
25	LA	1269	A	C2'-C1'	-5.63	1.47	1.53
2	S6	8	U	P-O5'	-5.63	1.54	1.59
25	LA	1676	A	C2'-C1'	-5.63	1.47	1.53
1	SA	1473	G	P-O5'	-5.63	1.54	1.59
25	LA	1900	A	O3'-P	-5.63	1.54	1.61
25	LA	1825	U	C2'-C1'	-5.63	1.47	1.53
1	SA	1518	A	N9-C4	-5.62	1.34	1.37
1	SA	878	A	P-O5'	-5.62	1.54	1.59
1	SA	1499	A	C2'-C1'	-5.62	1.47	1.53
25	LA	1439	A	N7-C5	-5.61	1.35	1.39
25	LA	2607	G	P-O5'	-5.61	1.54	1.59
25	LA	1762	A	O3'-P	-5.61	1.54	1.61
26	LB	108	A	N9-C4	-5.61	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	1240	U	O3'-P	-5.61	1.54	1.61
25	LA	1649	G	C2'-C1'	-5.60	1.47	1.53
1	SA	956	U	P-O5'	-5.60	1.54	1.59
25	LA	1960	A	N9-C4	-5.60	1.34	1.37
1	SA	1207	G	C2'-C1'	-5.60	1.47	1.53
25	LA	2435	A	N7-C5	-5.60	1.35	1.39
26	LB	86	G	C3'-O3'	5.60	1.50	1.42
25	LA	2667	C	C2-N3	-5.60	1.31	1.35
25	LA	2446	G	N7-C5	-5.59	1.35	1.39
25	LA	2680	U	O3'-P	-5.59	1.54	1.61
25	LA	17	G	O3'-P	-5.59	1.54	1.61
25	LA	1430	G	P-O5'	-5.59	1.54	1.59
25	LA	1142	A	N9-C4	-5.58	1.34	1.37
25	LA	1676	A	N9-C4	-5.57	1.34	1.37
1	SA	1500	A	N9-C4	-5.57	1.34	1.37
1	SA	405	U	P-O5'	-5.57	1.54	1.59
25	LA	1470	A	N7-C5	-5.57	1.35	1.39
25	LA	1916	A	N7-C5	-5.57	1.35	1.39
25	LA	2779	U	O3'-P	-5.57	1.54	1.61
25	LA	190	A	P-O5'	-5.56	1.54	1.59
25	LA	1183	U	C2-N3	-5.56	1.33	1.37
25	LA	1904	G	N7-C5	-5.56	1.35	1.39
25	LA	1979	U	P-O5'	-5.56	1.54	1.59
1	SA	424	G	C2'-C1'	-5.56	1.47	1.53
25	LA	691	C	P-O5'	-5.56	1.54	1.59
25	LA	1324	G	C2'-C1'	-5.55	1.47	1.53
25	LA	2051	A	C2'-C1'	-5.55	1.47	1.53
25	LA	470	A	N9-C4	-5.55	1.34	1.37
1	SA	1401	G	N9-C4	-5.54	1.33	1.38
1	SA	1081	A	P-O5'	-5.53	1.54	1.59
25	LA	1277	G	C2'-C1'	-5.53	1.47	1.53
1	SA	120	A	C5'-C4'	5.53	1.57	1.51
25	LA	114	U	O3'-P	-5.53	1.54	1.61
25	LA	1648	U	N1-C2	-5.53	1.33	1.38
25	LA	2451	A	N7-C5	-5.52	1.35	1.39
25	LA	584	C	O3'-P	-5.52	1.54	1.61
2	S6	74	A	O3'-P	-5.52	1.54	1.61
25	LA	2035	G	C2-N2	-5.52	1.29	1.34
25	LA	1155	A	N9-C4	-5.51	1.34	1.37
25	LA	1813	G	C2'-C1'	-5.51	1.47	1.53
1	SA	51	A	C3'-C2'	5.50	1.58	1.52
25	LA	457	A	N9-C4	-5.50	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	726	G	C2'-C1'	-5.49	1.47	1.53
1	SA	1524	C	P-O5'	-5.49	1.54	1.59
1	SA	404	G	O3'-P	-5.49	1.54	1.61
25	LA	2352	A	N9-C4	-5.49	1.34	1.37
1	SA	1416	G	O3'-P	-5.49	1.54	1.61
25	LA	2484	G	P-O5'	-5.49	1.54	1.59
1	SA	582	C	O3'-P	-5.48	1.54	1.61
1	SA	116	A	N7-C5	-5.47	1.35	1.39
25	LA	2615	U	C2'-C1'	-5.47	1.47	1.53
25	LA	1165	A	N9-C4	-5.47	1.34	1.37
25	LA	993	G	O3'-P	-5.47	1.54	1.61
25	LA	1798	U	P-O5'	-5.46	1.54	1.59
1	SA	1067	A	N9-C4	-5.46	1.34	1.37
25	LA	2357	G	P-O5'	-5.46	1.54	1.59
25	LA	2539	C	P-O5'	-5.46	1.54	1.59
25	LA	1678	A	N3-C4	-5.46	1.31	1.34
25	LA	675	A	N3-C4	-5.45	1.31	1.34
25	LA	2678	C	C2'-C1'	-5.45	1.47	1.53
25	LA	2679	A	N9-C4	-5.45	1.34	1.37
25	LA	1829	A	N7-C5	-5.44	1.35	1.39
25	LA	1027	A	O3'-P	-5.44	1.54	1.61
1	SA	1217	C	C5'-C4'	5.43	1.57	1.51
25	LA	1889	A	N9-C4	-5.43	1.34	1.37
1	SA	1502	A	N7-C5	-5.43	1.35	1.39
25	LA	2177	C	P-O5'	-5.42	1.54	1.59
25	LA	2498	C	C2'-C1'	-5.42	1.47	1.53
25	LA	1094	U	C5'-C4'	5.42	1.57	1.51
25	LA	563	A	O3'-P	-5.41	1.54	1.61
25	LA	800	A	C2'-C1'	-5.41	1.47	1.53
25	LA	2075	U	C2-N3	-5.41	1.33	1.37
25	LA	447	A	C2'-C1'	-5.41	1.47	1.53
25	LA	818	G	N7-C5	-5.41	1.36	1.39
25	LA	807	U	P-O5'	-5.40	1.54	1.59
25	LA	2229	U	N1-C2	-5.40	1.33	1.38
25	LA	2656	U	C2'-C1'	-5.40	1.47	1.53
1	SA	1154	G	C5'-C4'	5.39	1.57	1.51
25	LA	1365	A	O3'-P	-5.39	1.54	1.61
25	LA	1806	C	C2'-C1'	-5.39	1.47	1.53
25	LA	116	C	C2'-C1'	-5.39	1.47	1.53
25	LA	1282	U	O3'-P	-5.39	1.54	1.61
25	LA	2566	A	N9-C4	-5.38	1.34	1.37
25	LA	2664	G	C2'-C1'	-5.38	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	674	G	C2'-C1'	-5.38	1.47	1.53
1	SA	781	A	N3-C4	-5.38	1.31	1.34
1	SA	1209	C	P-O5'	-5.37	1.54	1.59
1	SA	1206	G	P-O5'	-5.37	1.54	1.59
25	LA	526	A	C3'-O3'	5.37	1.49	1.42
25	LA	1010	A	O3'-P	-5.37	1.54	1.61
25	LA	2574	G	C2'-C1'	-5.37	1.47	1.53
25	LA	147	C	P-O5'	-5.36	1.54	1.59
1	SA	712	A	N9-C4	-5.36	1.34	1.37
25	LA	1226	A	P-O5'	-5.36	1.54	1.59
1	SA	1228	C	P-O5'	-5.35	1.54	1.59
25	LA	1969	A	P-O5'	-5.35	1.54	1.59
1	SA	331	G	O3'-P	-5.35	1.54	1.61
25	LA	1791	A	P-O5'	-5.34	1.54	1.59
25	LA	2564	A	N9-C4	-5.34	1.34	1.37
25	LA	570	G	O3'-P	-5.34	1.54	1.61
25	LA	1140	C	P-O5'	-5.34	1.54	1.59
25	LA	565	C	P-O5'	-5.34	1.54	1.59
25	LA	973	A	N9-C4	-5.34	1.34	1.37
25	LA	503	A	N9-C4	-5.34	1.34	1.37
25	LA	2863	C	P-O5'	-5.34	1.54	1.59
25	LA	1616	A	C1'-N9	-5.33	1.39	1.46
25	LA	2331	G	C2'-C1'	-5.33	1.47	1.53
25	LA	2332	C	C2'-C1'	-5.33	1.47	1.53
1	SA	702	A	N9-C4	-5.33	1.34	1.37
25	LA	2598	A	N7-C5	-5.33	1.36	1.39
25	LA	1825	U	O3'-P	-5.32	1.54	1.61
25	LA	2082	A	N7-C5	-5.32	1.36	1.39
25	LA	2675	A	N9-C4	-5.32	1.34	1.37
25	LA	909	A	P-O5'	-5.32	1.54	1.59
1	SA	1015	G	C2'-C1'	-5.32	1.47	1.53
25	LA	482	A	N9-C4	-5.32	1.34	1.37
25	LA	1657	U	P-O5'	-5.32	1.54	1.59
25	LA	2111	U	C5'-C4'	5.32	1.57	1.51
25	LA	2355	G	P-O5'	-5.32	1.54	1.59
25	LA	293	U	P-O5'	-5.32	1.54	1.59
25	LA	192	C	C2'-C1'	-5.31	1.47	1.53
25	LA	1237	A	N9-C4	-5.31	1.34	1.37
1	SA	804	U	N1-C2	-5.31	1.33	1.38
25	LA	428	A	C2'-C1'	-5.31	1.47	1.53
25	LA	583	G	N1-C2	-5.31	1.33	1.37
25	LA	1657	U	C2'-C1'	-5.31	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	2450	A	C2'-C1'	-5.31	1.47	1.53
1	SA	781	A	C2'-C1'	-5.30	1.47	1.53
25	LA	1525	A	N9-C4	-5.30	1.34	1.37
25	LA	1979	U	N1-C2	-5.30	1.33	1.38
25	LA	635	C	P-O5'	-5.30	1.54	1.59
1	SA	1111	A	N9-C4	-5.30	1.34	1.37
25	LA	810	U	O3'-P	-5.29	1.54	1.61
25	LA	2459	A	N9-C4	-5.29	1.34	1.37
1	SA	1207	G	N9-C4	-5.29	1.33	1.38
25	LA	2276	G	O3'-P	-5.29	1.54	1.61
25	LA	1964	G	C2'-C1'	-5.29	1.47	1.53
25	LA	2552	U	O3'-P	-5.29	1.54	1.61
1	SA	865	A	C2'-C1'	-5.29	1.47	1.53
25	LA	1251	C	P-O5'	-5.29	1.54	1.59
25	LA	439	A	N9-C4	-5.28	1.34	1.37
25	LA	969	G	N7-C5	-5.28	1.36	1.39
25	LA	2267	A	N9-C4	-5.28	1.34	1.37
25	LA	1905	C	P-O5'	-5.28	1.54	1.59
25	LA	2450	A	P-O5'	-5.28	1.54	1.59
1	SA	315	A	O3'-P	-5.28	1.54	1.61
25	LA	1928	A	O3'-P	-5.28	1.54	1.61
1	SA	675	A	N9-C4	-5.27	1.34	1.37
25	LA	805	G	N1-C2	-5.27	1.33	1.37
25	LA	1641	A	N9-C4	-5.27	1.34	1.37
25	LA	2336	A	N7-C5	-5.27	1.36	1.39
1	SA	1483	A	N7-C5	-5.27	1.36	1.39
25	LA	1249	U	O3'-P	-5.27	1.54	1.61
25	LA	481	G	O3'-P	-5.27	1.54	1.61
25	LA	753	A	N7-C5	-5.27	1.36	1.39
25	LA	1944	U	C1'-N1	5.27	1.56	1.48
25	LA	1538	G	C5'-C4'	5.26	1.57	1.51
25	LA	1649	G	O3'-P	-5.26	1.54	1.61
25	LA	1829	A	O3'-P	-5.26	1.54	1.61
25	LA	541	A	C2'-C1'	-5.25	1.47	1.53
1	SA	313	A	N9-C4	-5.25	1.34	1.37
25	LA	2077	A	N3-C4	-5.25	1.31	1.34
25	LA	692	C	C2'-C1'	-5.25	1.47	1.53
25	LA	1327	A	N9-C4	-5.25	1.34	1.37
25	LA	456	C	C2'-C1'	-5.24	1.47	1.53
25	LA	2247	A	P-O5'	-5.24	1.54	1.59
26	LB	49	C	O3'-P	-5.24	1.54	1.61
25	LA	2849	U	P-O5'	-5.24	1.54	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	1522	U	P-O5'	-5.24	1.54	1.59
25	LA	404	A	O3'-P	-5.24	1.54	1.61
25	LA	195	A	O3'-P	-5.23	1.54	1.61
25	LA	1326	U	O3'-P	-5.23	1.54	1.61
25	LA	691	C	C2'-C1'	-5.23	1.47	1.53
25	LA	2362	C	P-O5'	-5.23	1.54	1.59
1	SA	1502	A	C2'-C1'	-5.22	1.47	1.53
25	LA	507	A	O3'-P	-5.22	1.54	1.61
25	LA	1818	U	O3'-P	-5.22	1.54	1.61
25	LA	2160	C	C5'-C4'	5.22	1.57	1.51
25	LA	1688	U	P-O5'	-5.22	1.54	1.59
25	LA	456	C	O3'-P	-5.21	1.54	1.61
25	LA	2169	A	C5'-C4'	5.21	1.57	1.51
25	LA	470	A	C2'-C1'	-5.21	1.47	1.53
25	LA	2431	U	P-O5'	-5.21	1.54	1.59
1	SA	776	G	O3'-P	-5.21	1.54	1.61
1	SA	15	G	N1-C2	-5.21	1.33	1.37
1	SA	1431	A	N9-C4	-5.21	1.34	1.37
25	LA	492	A	N7-C5	-5.21	1.36	1.39
25	LA	823	C	O3'-P	-5.21	1.54	1.61
25	LA	2223	G	O3'-P	-5.21	1.54	1.61
25	LA	781	A	N9-C4	-5.21	1.34	1.37
25	LA	925	A	N9-C4	-5.21	1.34	1.37
25	LA	1784	A	N9-C4	-5.21	1.34	1.37
1	SA	1505	G	C2-N2	-5.20	1.29	1.34
25	LA	2147	A	O3'-P	-5.20	1.54	1.61
1	SA	607	A	N9-C4	-5.20	1.34	1.37
25	LA	458	G	O3'-P	-5.20	1.54	1.61
25	LA	402	A	C2'-C1'	-5.19	1.47	1.53
25	LA	1142	A	O3'-P	-5.19	1.54	1.61
25	LA	1770	G	C2'-C1'	-5.19	1.47	1.53
25	LA	774	G	C2'-C1'	-5.19	1.47	1.53
25	LA	1031	G	C2'-C1'	-5.19	1.47	1.53
1	SA	391	G	O3'-P	-5.19	1.54	1.61
25	LA	2441	U	P-O5'	-5.19	1.54	1.59
25	LA	6	A	N9-C4	-5.19	1.34	1.37
25	LA	1690	A	N9-C4	-5.19	1.34	1.37
25	LA	2566	A	C3'-C2'	-5.19	1.47	1.52
25	LA	1616	A	C2'-C1'	-5.18	1.47	1.53
25	LA	2245	U	C2'-C1'	-5.18	1.47	1.53
25	LA	208	C	C2'-C1'	-5.18	1.47	1.53
1	SA	273	U	P-O5'	-5.18	1.54	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	2821	A	C5'-C4'	5.18	1.57	1.51
25	LA	2850	A	O3'-P	-5.18	1.54	1.61
1	SA	795	C	C2'-C1'	-5.18	1.47	1.53
25	LA	2481	G	O3'-P	-5.18	1.54	1.61
1	SA	860	A	C2'-C1'	-5.17	1.47	1.53
25	LA	1453	A	C5'-C4'	5.17	1.57	1.51
25	LA	731	C	P-O5'	-5.17	1.54	1.59
25	LA	242	G	C2'-C1'	-5.17	1.47	1.53
25	LA	959	A	N9-C4	-5.17	1.34	1.37
25	LA	1380	G	N7-C5	-5.17	1.36	1.39
25	LA	2592	G	C6-N1	-5.17	1.35	1.39
1	SA	1197	A	C2'-C1'	-5.16	1.47	1.53
25	LA	2557	G	N7-C5	-5.16	1.36	1.39
25	LA	901	C	P-O5'	-5.16	1.54	1.59
25	LA	1028	A	N3-C4	-5.16	1.31	1.34
25	LA	2427	C	N1-C6	-5.16	1.34	1.37
1	SA	1495	U	P-O5'	-5.16	1.54	1.59
25	LA	2072	C	C2'-C1'	-5.16	1.47	1.53
25	LA	1810	A	C5'-C4'	5.15	1.57	1.51
1	SA	1331	G	O3'-P	-5.15	1.54	1.61
25	LA	1420	A	O3'-P	-5.15	1.54	1.61
25	LA	955	U	P-O5'	-5.15	1.54	1.59
3	S7	41	C	O3'-P	-5.15	1.54	1.61
25	LA	1567	G	N7-C5	-5.14	1.36	1.39
25	LA	2617	U	N1-C2	-5.14	1.33	1.38
25	LA	573	U	C2'-C1'	-5.14	1.47	1.53
25	LA	1826	G	P-O5'	-5.14	1.54	1.59
1	SA	535	A	N9-C4	-5.14	1.34	1.37
1	SA	1053	G	N7-C5	-5.14	1.36	1.39
25	LA	262	A	C2'-C1'	-5.14	1.47	1.53
25	LA	2088	A	N9-C4	-5.14	1.34	1.37
1	SA	139	A	N9-C4	-5.13	1.34	1.37
25	LA	683	U	P-O5'	-5.13	1.54	1.59
25	LA	528	A	C2'-C1'	-5.13	1.47	1.53
25	LA	567	U	C2'-C1'	-5.13	1.47	1.53
1	SA	815	A	N9-C8	-5.12	1.33	1.37
25	LA	1818	U	C2'-C1'	-5.12	1.47	1.53
25	LA	1981	A	O3'-P	-5.12	1.55	1.61
1	SA	808	C	P-O5'	-5.12	1.54	1.59
1	SA	832	G	N9-C4	-5.12	1.33	1.38
1	SA	1318	A	O3'-P	-5.12	1.55	1.61
25	LA	205	G	C2'-C1'	-5.11	1.47	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	LA	1634	A	N9-C4	-5.11	1.34	1.37
25	LA	1241	A	N9-C4	5.11	1.41	1.37
25	LA	1774	C	P-O5'	-5.11	1.54	1.59
25	LA	1254	A	C2'-C1'	-5.11	1.47	1.53
25	LA	2077	A	O3'-P	-5.11	1.55	1.61
1	SA	973	G	O3'-P	-5.11	1.55	1.61
25	LA	1677	A	N3-C4	-5.11	1.31	1.34
1	SA	1471	U	C2'-C1'	-5.10	1.47	1.53
25	LA	692	C	O3'-P	-5.10	1.55	1.61
25	LA	1570	A	N9-C4	-5.10	1.34	1.37
25	LA	2424	C	O3'-P	-5.10	1.55	1.61
1	SA	1431	A	O3'-P	-5.10	1.55	1.61
25	LA	194	G	C2'-C1'	-5.10	1.47	1.53
25	LA	2314	A	O3'-P	-5.10	1.55	1.61
25	LA	900	A	O3'-P	-5.10	1.55	1.61
25	LA	797	G	N7-C5	-5.09	1.36	1.39
25	LA	2086	U	P-O5'	-5.09	1.54	1.59
1	SA	61	G	C2'-C1'	-5.09	1.47	1.53
1	SA	1082	A	P-O5'	-5.09	1.54	1.59
25	LA	516	C	C2'-C1'	-5.09	1.47	1.53
25	LA	2251	G	C3'-C2'	-5.09	1.47	1.52
1	SA	1344	C	O3'-P	-5.09	1.55	1.61
1	SA	1513	A	C1'-N9	-5.09	1.39	1.46
1	SA	321	A	N9-C4	-5.08	1.34	1.37
25	LA	1837	C	P-O5'	-5.08	1.54	1.59
25	LA	2588	G	C2'-C1'	-5.08	1.47	1.53
1	SA	152	A	O3'-P	-5.08	1.55	1.61
25	LA	561	G	P-O5'	-5.08	1.54	1.59
25	LA	1854	A	N9-C4	-5.08	1.34	1.37
1	SA	933	G	C5'-C4'	5.08	1.57	1.51
25	LA	794	A	N7-C5	-5.08	1.36	1.39
25	LA	1331	G	C2'-C1'	-5.08	1.47	1.53
25	LA	1433	A	N9-C4	-5.08	1.34	1.37
25	LA	782	A	N7-C5	-5.08	1.36	1.39
25	LA	396	G	O3'-P	-5.07	1.55	1.61
25	LA	782	A	C2'-C1'	-5.07	1.47	1.53
1	SA	18	C	C2-N3	-5.07	1.31	1.35
25	LA	1975	G	N9-C4	-5.07	1.33	1.38
25	LA	972	A	O3'-P	-5.07	1.55	1.61
25	LA	1693	U	C2'-C1'	-5.07	1.47	1.53
1	SA	704	A	P-O5'	-5.07	1.54	1.59
25	LA	818	G	O3'-P	-5.06	1.55	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	SA	116	A	C2'-C1'	-5.06	1.47	1.53
25	LA	1166	G	C2'-C1'	-5.06	1.47	1.53
25	LA	739	A	N9-C4	-5.06	1.34	1.37
25	LA	2198	A	N9-C4	-5.06	1.34	1.37
25	LA	2567	G	C6-N1	-5.06	1.36	1.39
1	SA	103	U	O3'-P	-5.05	1.55	1.61
25	LA	1667	G	C2'-C1'	-5.05	1.47	1.53
1	SA	779	C	O3'-P	-5.05	1.55	1.61
25	LA	954	G	C2'-C1'	-5.05	1.47	1.53
25	LA	1935	G	C2-N2	-5.05	1.29	1.34
25	LA	2521	C	P-O5'	-5.05	1.54	1.59
1	SA	1396	A	N9-C4	-5.04	1.34	1.37
25	LA	604	G	P-O5'	-5.04	1.54	1.59
25	LA	1928	A	N7-C5	-5.04	1.36	1.39
25	LA	2073	C	N1-C6	-5.04	1.34	1.37
25	LA	1850	G	C2'-C1'	-5.04	1.47	1.53
1	SA	1181	G	C2'-C1'	-5.03	1.47	1.53
1	SA	1100	C	O3'-P	-5.03	1.55	1.61
25	LA	751	A	P-O5'	-5.03	1.54	1.59
25	LA	1264	A	P-O5'	-5.03	1.54	1.59
25	LA	1360	G	C2'-C1'	-5.03	1.47	1.53
25	LA	2391	G	C2'-C1'	-5.03	1.47	1.53
25	LA	975	A	N9-C4	-5.02	1.34	1.37
1	SA	521	G	N9-C4	-5.02	1.33	1.38
25	LA	1428	C	C5'-C4'	5.02	1.57	1.51
25	LA	1774	C	C2'-C1'	-5.02	1.47	1.53
25	LA	745	G	C2'-C1'	-5.02	1.47	1.53
25	LA	1362	C	C2'-C1'	-5.02	1.47	1.53
25	LA	562	U	O3'-P	-5.02	1.55	1.61
25	LA	2500	U	O3'-P	-5.01	1.55	1.61
1	SA	1305	G	N9-C4	-5.01	1.33	1.38
25	LA	447	A	C1'-N9	-5.01	1.39	1.46
1	SA	768	A	C2'-C1'	-5.01	1.47	1.53
25	LA	1059	G	O3'-P	-5.01	1.55	1.61
1	SA	1134	G	C2'-C1'	-5.01	1.47	1.53
25	LA	677	A	C1'-N9	-5.01	1.39	1.46
25	LA	591	U	P-O5'	-5.01	1.54	1.59
25	LA	1773	A	N7-C5	-5.00	1.36	1.39
25	LA	2250	G	N7-C5	-5.00	1.36	1.39
25	LA	2837	A	N9-C4	-5.00	1.34	1.37
1	SA	689	C	P-O5'	-5.00	1.54	1.59

All (5304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2030	C	C6-N1-C2	-27.21	109.42	120.30
25	LA	2251	G	O4'-C1'-N9	26.55	129.44	108.20
25	LA	1900	A	P-O3'-C3'	25.97	150.87	119.70
1	SA	51	A	P-O3'-C3'	25.23	149.97	119.70
25	LA	2656	U	C2-N3-C4	-22.74	113.35	127.00
25	LA	2445	G	O4'-C1'-N9	21.16	125.13	108.20
25	LA	948	C	C6-N1-C2	-20.26	112.20	120.30
25	LA	1420	A	P-O3'-C3'	19.18	142.71	119.70
25	LA	2609	U	P-O3'-C3'	17.83	141.10	119.70
25	LA	2211	A	P-O3'-C3'	17.56	140.77	119.70
25	LA	1321	A	O4'-C1'-N9	17.49	122.19	108.20
25	LA	2308	G	P-O3'-C3'	16.73	139.78	119.70
1	SA	764	C	P-O3'-C3'	16.71	139.75	119.70
25	LA	826	U	P-O3'-C3'	16.30	139.26	119.70
1	SA	810	C	P-O5'-C5'	16.25	146.91	120.90
25	LA	1272	A	P-O3'-C3'	16.02	138.92	119.70
26	LB	34	A	P-O3'-C3'	15.69	138.53	119.70
25	LA	2118	U	P-O3'-C3'	15.65	138.48	119.70
1	SA	1140	C	C6-N1-C2	-15.57	114.07	120.30
25	LA	2701	U	P-O3'-C3'	-15.55	101.04	119.70
1	SA	752	G	P-O3'-C3'	15.30	138.06	119.70
25	LA	644	A	P-O3'-C3'	15.23	137.98	119.70
25	LA	2649	C	P-O3'-C3'	15.18	137.91	119.70
25	LA	2799	A	O4'-C1'-N9	14.54	119.84	108.20
25	LA	2448	A	P-O3'-C3'	14.49	137.09	119.70
1	SA	497	G	P-O3'-C3'	14.48	137.07	119.70
25	LA	1807	G	P-O3'-C3'	14.34	136.91	119.70
25	LA	1332	G	P-O3'-C3'	14.30	136.86	119.70
25	LA	2030	C	C2-N3-C4	-14.28	112.76	119.90
25	LA	2566	A	P-O3'-C3'	-14.12	102.76	119.70
25	LA	1409	U	P-O5'-C5'	13.98	143.26	120.90
25	LA	2146	C	P-O3'-C3'	13.91	136.39	119.70
1	SA	1159	U	P-O3'-C3'	13.73	136.18	119.70
1	SA	51	A	O4'-C1'-N9	13.57	119.05	108.20
25	LA	2568	U	P-O5'-C5'	13.43	142.40	120.90
25	LA	1460	U	P-O3'-C3'	13.35	135.72	119.70
1	SA	1502	A	O4'-C1'-N9	13.15	118.72	108.20
1	SA	1226	C	P-O3'-C3'	13.08	135.39	119.70
25	LA	1849	G	C5'-C4'-C3'	-12.99	95.22	116.00
25	LA	1142	A	P-O3'-C3'	12.97	135.26	119.70
25	LA	1274	A	P-O3'-C3'	-12.88	104.25	119.70
25	LA	2564	A	P-O3'-C3'	12.86	135.13	119.70
25	LA	2287	A	P-O3'-C3'	12.72	134.96	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2571	U	P-O3'-C3'	12.67	134.90	119.70
25	LA	900	A	P-O3'-C3'	12.60	134.82	119.70
1	SA	204	G	O4'-C1'-N9	12.59	118.27	108.20
25	LA	1902	C	C6-N1-C2	-12.57	115.27	120.30
1	SA	519	C	O4'-C1'-N1	12.52	118.22	108.20
29	LN	220	ARG	NE-CZ-NH2	-12.40	114.10	120.30
25	LA	2702	G	P-O3'-C3'	12.36	134.53	119.70
25	LA	2756	U	P-O3'-C3'	12.34	134.51	119.70
1	SA	177	G	O4'-C1'-N9	12.14	117.92	108.20
1	SA	717	U	P-O3'-C3'	12.04	134.14	119.70
25	LA	1067	A	O4'-C1'-N9	12.03	117.82	108.20
25	LA	2516	A	P-O5'-C5'	12.03	140.15	120.90
25	LA	2557	G	C4-N9-C1'	12.02	142.12	126.50
1	SA	52	C	O4'-C1'-N1	12.01	117.81	108.20
3	S7	41	C	P-O3'-C3'	11.99	134.09	119.70
25	LA	2271	G	P-O3'-C3'	11.98	134.08	119.70
25	LA	2427	C	O4'-C1'-N1	11.92	117.74	108.20
1	SA	1530	G	C1'-O4'-C4'	-11.91	100.37	109.90
25	LA	2500	U	P-O3'-C3'	11.91	133.99	119.70
25	LA	2607	G	C8-N9-C1'	11.90	142.47	127.00
25	LA	1890	A	N1-C6-N6	-11.89	111.47	118.60
25	LA	745	G	C5-C6-O6	-11.86	121.48	128.60
44	L3	14	ARG	NE-CZ-NH2	11.86	126.23	120.30
25	LA	2808	G	P-O3'-C3'	11.82	133.88	119.70
25	LA	1902	C	C2-N3-C4	-11.77	114.01	119.90
25	LA	1323	C	O4'-C1'-N1	11.72	117.58	108.20
25	LA	2667	C	P-O5'-C5'	11.69	139.61	120.90
24	S1	474	ARG	NE-CZ-NH1	11.69	126.14	120.30
25	LA	2806	C	P-O3'-C3'	11.54	133.55	119.70
54	LH	41	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	SA	1364	U	C2-N3-C4	-11.53	120.08	127.00
1	SA	1402	C	O4'-C1'-N1	11.49	117.39	108.20
25	LA	2282	G	P-O3'-C3'	11.40	133.38	119.70
1	SA	792	A	O4'-C1'-N9	11.39	117.31	108.20
26	LB	25	U	P-O3'-C3'	11.39	133.37	119.70
25	LA	1840	G	C5-C6-O6	-11.39	121.77	128.60
25	LA	2165	C	O4'-C1'-N1	11.38	117.30	108.20
1	SA	243	A	P-O3'-C3'	11.35	133.32	119.70
25	LA	229	C	O4'-C1'-N1	11.32	117.26	108.20
25	LA	1079	C	O4'-C1'-N1	11.31	117.25	108.20
25	LA	574	A	P-O3'-C3'	11.30	133.26	119.70
1	SA	974	A	O4'-C1'-N9	11.28	117.22	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	LY	10	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	SA	794	A	C5'-C4'-C3'	11.18	133.89	116.00
25	LA	2136	G	P-O5'-C5'	11.15	138.75	120.90
1	SA	844	G	P-O3'-C3'	11.15	133.08	119.70
25	LA	1899	A	P-O3'-C3'	11.14	133.07	119.70
1	SA	122	G	P-O3'-C3'	11.14	133.06	119.70
25	LA	2607	G	C4-N9-C1'	-11.13	112.03	126.50
25	LA	876	C	O4'-C1'-N1	11.11	117.09	108.20
25	LA	126	A	O4'-C1'-N9	11.11	117.08	108.20
25	LA	42	A	P-O5'-C5'	11.03	138.55	120.90
40	LX	128	ARG	NE-CZ-NH1	11.03	125.81	120.30
25	LA	2447	G	C4'-C3'-C2'	-11.01	91.59	102.60
25	LA	2572	A	O4'-C1'-N9	10.96	116.97	108.20
29	LN	257	ARG	NE-CZ-NH2	-10.95	114.82	120.30
25	LA	2030	C	O4'-C1'-C2'	-10.95	94.85	105.80
1	SA	203	G	P-O3'-C3'	10.91	132.79	119.70
26	LB	15	A	O4'-C1'-N9	10.90	116.92	108.20
29	LN	79	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	SA	693	G	O4'-C1'-N9	10.86	116.89	108.20
1	SA	307	C	P-O3'-C3'	10.85	132.72	119.70
25	LA	2336	A	O4'-C1'-N9	10.85	116.88	108.20
52	LF	35	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	SA	473	U	O4'-C1'-N1	10.78	116.82	108.20
25	LA	2156	G	O4'-C1'-N9	10.77	116.82	108.20
25	LA	670	A	P-O3'-C3'	10.74	132.59	119.70
1	SA	1518	A	O4'-C1'-N9	10.73	116.78	108.20
3	S7	33	U	P-O5'-C5'	10.71	138.04	120.90
25	LA	643	A	C5'-C4'-C3'	10.71	133.13	116.00
25	LA	1675	C	C6-N1-C2	-10.70	116.02	120.30
26	LB	86	G	P-O3'-C3'	-10.69	106.87	119.70
25	LA	2581	G	O4'-C1'-N9	10.67	116.73	108.20
25	LA	2246	G	C5'-C4'-C3'	-10.63	98.98	116.00
25	LA	1950	G	C5-C6-O6	-10.61	122.23	128.60
25	LA	1927	A	P-O3'-C3'	10.61	132.43	119.70
1	SA	451	A	P-O3'-C3'	10.61	132.43	119.70
1	SA	413	G	P-O3'-C3'	-10.60	106.98	119.70
25	LA	1888	G	O4'-C1'-N9	10.58	116.66	108.20
1	SA	890	G	O4'-C1'-N9	10.57	116.65	108.20
1	SA	1155	A	P-O5'-C5'	10.56	137.80	120.90
25	LA	547	A	C1'-O4'-C4'	-10.52	101.48	109.90
25	LA	163	C	P-O3'-C3'	10.52	132.32	119.70
1	SA	1140	C	O4'-C1'-N1	10.49	116.59	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	SU	70	TYR	CB-CG-CD2	-10.49	114.71	121.00
25	LA	2480	C	O4'-C1'-N1	10.47	116.58	108.20
25	LA	2092	U	P-O3'-C3'	10.45	132.24	119.70
25	LA	15	G	O4'-C1'-N9	10.45	116.56	108.20
1	SA	252	U	O4'-C1'-N1	10.43	116.55	108.20
35	LT	18	ARG	NE-CZ-NH1	10.38	125.49	120.30
25	LA	2412	A	P-O5'-C5'	10.36	137.48	120.90
25	LA	1211	C	P-O3'-C3'	10.35	132.12	119.70
1	SA	1301	U	P-O5'-C5'	10.33	137.43	120.90
25	LA	455	C	P-O3'-C3'	10.33	132.09	119.70
1	SA	795	C	P-O3'-C3'	10.30	132.06	119.70
25	LA	2822	G	C5'-C4'-C3'	-10.29	99.54	116.00
25	LA	311	A	O4'-C1'-N9	10.28	116.42	108.20
1	SA	1168	U	O4'-C1'-N1	10.27	116.42	108.20
25	LA	390	U	P-O3'-C3'	10.22	131.96	119.70
25	LA	2713	U	C2-N3-C4	-10.20	120.88	127.00
25	LA	1840	G	N1-C6-O6	10.16	125.99	119.90
1	SA	1277	C	O4'-C1'-N1	10.15	116.32	108.20
25	LA	1609	A	O4'-C1'-N9	10.15	116.32	108.20
25	LA	1509	A	O4'-C1'-N9	10.14	116.31	108.20
25	LA	2866	U	P-O3'-C3'	10.13	131.86	119.70
26	LB	43	C	O4'-C1'-N1	10.10	116.28	108.20
1	SA	1530	G	C5'-C4'-O4'	10.09	121.20	109.10
1	SA	676	A	P-O5'-C5'	10.06	136.99	120.90
10	SP	70	ARG	NE-CZ-NH2	-10.02	115.29	120.30
3	S7	72	C	O4'-C1'-N1	10.02	116.22	108.20
11	SQ	5	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	SA	227	G	P-O3'-C3'	10.00	131.70	119.70
25	LA	1128	G	O4'-C1'-N9	9.99	116.19	108.20
25	LA	1902	C	P-O3'-C3'	-9.99	107.72	119.70
25	LA	1012	U	C1'-O4'-C4'	-9.97	101.93	109.90
1	SA	1331	G	O4'-C1'-N9	9.96	116.17	108.20
1	SA	149	A	O4'-C1'-N9	9.96	116.17	108.20
25	LA	906	U	O4'-C1'-N1	9.96	116.17	108.20
25	LA	2656	U	O4'-C1'-N1	9.96	116.17	108.20
25	LA	1917	U	P-O3'-C3'	-9.95	107.76	119.70
25	LA	2557	G	C8-N9-C4	-9.95	102.42	106.40
25	LA	2076	U	O4'-C1'-N1	9.94	116.16	108.20
1	SA	960	U	C5'-C4'-O4'	9.94	121.02	109.10
25	LA	1837	C	C5'-C4'-C3'	-9.94	100.10	116.00
25	LA	2863	C	O4'-C1'-N1	9.93	116.14	108.20
25	LA	1110	G	O4'-C1'-N9	9.93	116.14	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2412	A	N1-C6-N6	9.93	124.56	118.60
25	LA	1324	G	O4'-C1'-N9	9.91	116.13	108.20
25	LA	2447	G	O4'-C1'-C2'	-9.91	95.89	105.80
25	LA	1386	C	O4'-C1'-N1	9.90	116.12	108.20
25	LA	1323	C	C5'-C4'-C3'	-9.89	100.17	116.00
25	LA	603	A	P-O3'-C3'	9.89	131.57	119.70
25	LA	1133	A	O4'-C1'-N9	9.87	116.10	108.20
25	LA	1453	A	O4'-C1'-N9	9.86	116.09	108.20
25	LA	2664	G	P-O3'-C3'	9.85	131.52	119.70
25	LA	1270	C	O4'-C1'-N1	9.84	116.07	108.20
1	SA	1315	U	P-O5'-C5'	9.83	136.63	120.90
25	LA	2501	C	O4'-C1'-N1	9.83	116.07	108.20
25	LA	1494	A	O4'-C1'-N9	9.82	116.06	108.20
25	LA	2574	G	P-O3'-C3'	9.82	131.49	119.70
1	SA	570	G	P-O5'-C5'	9.81	136.60	120.90
25	LA	2666	C	C5'-C4'-C3'	-9.80	100.32	116.00
25	LA	2400	G	P-O3'-C3'	9.80	131.46	119.70
25	LA	2410	G	P-O3'-C3'	9.80	131.46	119.70
56	LJ	8	ARG	NE-CZ-NH2	-9.78	115.41	120.30
25	LA	1856	U	P-O5'-C5'	9.77	136.54	120.90
25	LA	715	A	O4'-C1'-N9	9.76	116.01	108.20
25	LA	37	C	O4'-C1'-N1	9.76	116.01	108.20
25	LA	2492	U	O4'-C1'-N1	9.76	116.01	108.20
1	SA	1227	A	O4'-C1'-N9	9.75	116.00	108.20
25	LA	547	A	O4'-C1'-N9	9.74	115.99	108.20
23	SI	121	ARG	NE-CZ-NH2	-9.74	115.43	120.30
25	LA	784	G	O4'-C1'-N9	9.73	115.99	108.20
25	LA	2445	G	C4-C5-C6	-9.73	112.96	118.80
25	LA	2543	G	C5'-C4'-C3'	-9.72	100.44	116.00
25	LA	1939	U	P-O3'-C3'	-9.72	108.04	119.70
18	SD	25	ARG	NE-CZ-NH2	-9.71	115.45	120.30
25	LA	1899	A	O4'-C1'-N9	9.70	115.96	108.20
25	LA	1935	G	P-O5'-C5'	9.70	136.41	120.90
1	SA	494	G	C5-C6-O6	-9.68	122.79	128.60
25	LA	99	U	O4'-C1'-N1	9.67	115.94	108.20
1	SA	960	U	C1'-O4'-C4'	-9.67	102.17	109.90
56	LJ	118	ARG	NE-CZ-NH2	-9.66	115.47	120.30
25	LA	2657	A	O4'-C1'-N9	9.66	115.93	108.20
26	LB	31	C	O4'-C1'-N1	9.66	115.93	108.20
8	SN	19	TYR	CB-CG-CD2	-9.65	115.21	121.00
25	LA	2116	G	O4'-C1'-N9	9.65	115.92	108.20
25	LA	2821	A	C5'-C4'-C3'	-9.65	100.56	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	271	C	P-O3'-C3'	9.65	131.28	119.70
25	LA	481	G	O4'-C1'-N9	9.65	115.92	108.20
25	LA	2402	U	O4'-C1'-N1	9.64	115.92	108.20
25	LA	1592	C	O4'-C1'-N1	9.64	115.91	108.20
13	SS	77	ARG	NE-CZ-NH1	9.63	125.11	120.30
25	LA	2061	G	O4'-C1'-N9	9.62	115.89	108.20
1	SA	328	C	P-O3'-C3'	9.61	131.23	119.70
25	LA	2390	U	O4'-C1'-N1	9.61	115.89	108.20
25	LA	54	G	O4'-C1'-N9	9.60	115.88	108.20
1	SA	1383	C	O4'-C1'-N1	9.59	115.87	108.20
25	LA	1266	G	P-O3'-C3'	9.59	131.21	119.70
25	LA	2492	U	C2-N1-C1'	9.59	129.20	117.70
25	LA	2554	U	O4'-C1'-N1	9.58	115.86	108.20
25	LA	1964	G	C4-N9-C1'	-9.57	114.06	126.50
25	LA	989	G	O4'-C1'-N9	9.57	115.86	108.20
48	LE	133	ARG	NE-CZ-NH1	9.56	125.08	120.30
25	LA	2666	C	O4'-C1'-N1	9.55	115.84	108.20
25	LA	2271	G	O4'-C1'-N9	9.55	115.84	108.20
25	LA	2345	G	C5'-C4'-C3'	-9.55	100.71	116.00
26	LB	91	C	O4'-C1'-N1	9.55	115.84	108.20
1	SA	609	A	N1-C6-N6	9.55	124.33	118.60
18	SD	2	ARG	NE-CZ-NH1	9.54	125.07	120.30
25	LA	1584	U	P-O3'-C3'	9.54	131.15	119.70
25	LA	1362	C	O4'-C1'-N1	9.54	115.83	108.20
25	LA	2427	C	P-O5'-C5'	9.53	136.15	120.90
25	LA	1964	G	C8-N9-C1'	9.53	139.38	127.00
25	LA	717	C	O4'-C1'-N1	9.52	115.81	108.20
1	SA	1132	C	O4'-C1'-N1	9.51	115.81	108.20
25	LA	2238	G	P-O3'-C3'	9.51	131.11	119.70
1	SA	367	U	O3'-P-O5'	-9.49	85.96	104.00
25	LA	2106	U	P-O3'-C3'	9.49	131.09	119.70
25	LA	2055	C	C5'-C4'-C3'	9.49	131.18	116.00
25	LA	2439	A	O4'-C1'-N9	9.49	115.79	108.20
25	LA	783	A	O4'-C1'-N9	9.48	115.78	108.20
25	LA	2591	C	C6-N1-C2	-9.47	116.51	120.30
25	LA	436	C	O4'-C1'-N1	9.46	115.77	108.20
25	LA	1081	U	P-O5'-C5'	9.45	136.03	120.90
25	LA	2499	C	C6-N1-C2	-9.45	116.52	120.30
29	LN	257	ARG	NE-CZ-NH1	9.45	125.03	120.30
25	LA	1282	U	P-O3'-C3'	9.45	131.04	119.70
25	LA	157	C	O4'-C1'-N1	9.45	115.76	108.20
1	SA	1001	C	P-O5'-C5'	9.44	136.00	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	914	G	C5'-C4'-C3'	-9.44	100.90	116.00
1	SA	1141	C	O4'-C1'-N1	9.43	115.75	108.20
25	LA	1906	G	O4'-C1'-N9	9.42	115.73	108.20
1	SA	1210	C	C6-N1-C2	-9.41	116.53	120.30
18	SD	2	ARG	NE-CZ-NH2	-9.40	115.60	120.30
25	LA	1427	A	P-O3'-C3'	9.39	130.97	119.70
1	SA	899	C	P-O3'-C3'	9.39	130.97	119.70
25	LA	2445	G	N9-C4-C5	-9.38	101.65	105.40
25	LA	647	G	O4'-C1'-N9	9.38	115.70	108.20
25	LA	346	A	O4'-C1'-N9	9.36	115.69	108.20
1	SA	51	A	C1'-O4'-C4'	-9.36	102.42	109.90
30	LO	91	ARG	NE-CZ-NH1	9.36	124.98	120.30
25	LA	128	C	O4'-C1'-N1	9.35	115.68	108.20
25	LA	2656	U	C6-N1-C2	-9.35	115.39	121.00
47	L6	69	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	SA	961	U	O4'-C4'-C3'	9.34	113.57	106.10
25	LA	2252	G	O4'-C1'-N9	9.33	115.67	108.20
25	LA	2332	C	O4'-C1'-N1	9.32	115.66	108.20
25	LA	2606	C	O4'-C1'-N1	9.32	115.66	108.20
1	SA	1302	C	P-O3'-C3'	9.31	130.87	119.70
25	LA	2579	C	O4'-C1'-N1	9.30	115.64	108.20
25	LA	2451	A	C5'-C4'-C3'	-9.30	101.12	116.00
25	LA	697	G	P-O3'-C3'	9.29	130.85	119.70
25	LA	2652	C	O4'-C1'-N1	9.29	115.64	108.20
1	SA	1441	A	O4'-C1'-N9	9.29	115.63	108.20
1	SA	961	U	P-O5'-C5'	-9.28	106.05	120.90
25	LA	2755	C	C2-N1-C1'	9.27	128.99	118.80
25	LA	2385	C	O4'-C1'-N1	9.26	115.61	108.20
1	SA	863	U	P-O3'-C3'	-9.26	108.59	119.70
1	SA	889	A	P-O3'-C3'	9.26	130.81	119.70
25	LA	885	C	P-O3'-C3'	9.25	130.80	119.70
25	LA	26	G	P-O3'-C3'	9.24	130.78	119.70
1	SA	1139	G	P-O3'-C3'	-9.23	108.62	119.70
1	SA	366	A	P-O3'-C3'	9.22	130.77	119.70
25	LA	2757	A	O4'-C1'-N9	9.22	115.58	108.20
25	LA	241	A	P-O3'-C3'	9.21	130.75	119.70
1	SA	765	G	O4'-C1'-N9	9.21	115.57	108.20
36	LU	13	ARG	NE-CZ-NH2	-9.21	115.69	120.30
25	LA	105	C	O4'-C1'-N1	9.21	115.57	108.20
23	SI	122	ARG	NE-CZ-NH2	-9.21	115.70	120.30
25	LA	2222	C	O4'-C1'-N1	9.21	115.56	108.20
25	LA	464	U	O4'-C1'-N1	9.20	115.56	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	405	U	P-O3'-C3'	9.19	130.72	119.70
25	LA	1715	G	O4'-C1'-N9	9.17	115.53	108.20
1	SA	210	C	O4'-C1'-N1	9.17	115.53	108.20
25	LA	2732	G	O4'-C1'-N9	9.15	115.52	108.20
1	SA	802	A	N1-C6-N6	-9.15	113.11	118.60
1	SA	1015	G	O4'-C1'-N9	9.15	115.52	108.20
25	LA	2251	G	C5-C6-O6	-9.13	123.12	128.60
37	LV	36	ARG	NE-CZ-NH1	-9.13	115.73	120.30
25	LA	2133	G	P-O3'-C3'	9.13	130.66	119.70
1	SA	1045	C	O4'-C1'-N1	9.13	115.50	108.20
25	LA	1547	C	O4'-C1'-N1	9.13	115.50	108.20
25	LA	1962	C	P-O5'-C5'	9.13	135.50	120.90
25	LA	2901	C	O4'-C1'-N1	9.13	115.50	108.20
1	SA	781	A	P-O5'-C5'	-9.12	106.32	120.90
1	SA	1001	C	O4'-C1'-N1	9.12	115.49	108.20
1	SA	386	C	O4'-C1'-N1	9.11	115.49	108.20
1	SA	1014	A	P-O3'-C3'	9.11	130.63	119.70
25	LA	2886	A	O4'-C1'-N9	9.11	115.49	108.20
25	LA	974	G	P-O3'-C3'	9.10	130.62	119.70
25	LA	2804	U	C5'-C4'-C3'	-9.09	101.45	116.00
3	S7	49	C	P-O5'-C5'	9.08	135.43	120.90
25	LA	922	C	O4'-C1'-N1	9.08	115.47	108.20
1	SA	1447	A	O4'-C1'-N9	9.08	115.46	108.20
25	LA	1468	U	O4'-C1'-N1	9.07	115.46	108.20
41	LY	10	ARG	NE-CZ-NH1	-9.07	115.76	120.30
25	LA	1428	C	P-O5'-C5'	9.07	135.41	120.90
26	LB	90	C	C5'-C4'-C3'	-9.07	101.49	116.00
25	LA	1123	C	O4'-C1'-N1	9.05	115.44	108.20
25	LA	1416	G	P-O3'-C3'	9.05	130.56	119.70
12	SR	52	ARG	NE-CZ-NH1	9.04	124.82	120.30
25	LA	1997	C	O4'-C1'-N1	9.04	115.43	108.20
10	SP	56	ARG	NE-CZ-NH1	9.03	124.82	120.30
25	LA	2094	A	C5'-C4'-O4'	9.03	119.94	109.10
25	LA	1832	C	C6-N1-C2	-9.03	116.69	120.30
25	LA	2557	G	C8-N9-C1'	-9.03	115.26	127.00
2	S6	7	G	P-O3'-C3'	9.03	130.53	119.70
1	SA	1414	U	O3'-P-O5'	-9.02	86.86	104.00
1	SA	494	G	N1-C6-O6	9.02	125.31	119.90
25	LA	1514	G	P-O5'-C5'	9.02	135.33	120.90
25	LA	2667	C	O4'-C1'-N1	9.02	115.42	108.20
25	LA	389	G	O4'-C1'-N9	9.02	115.41	108.20
1	SA	1136	C	P-O3'-C3'	9.01	130.51	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2424	C	O3'-P-O5'	-9.01	86.88	104.00
1	SA	1462	C	O4'-C1'-N1	9.00	115.40	108.20
40	LX	77	ARG	NE-CZ-NH2	9.00	124.80	120.30
25	LA	784	G	C5-C6-O6	-9.00	123.20	128.60
25	LA	611	C	P-O3'-C3'	9.00	130.50	119.70
25	LA	745	G	O4'-C1'-N9	8.99	115.39	108.20
25	LA	2342	C	C6-N1-C2	-8.99	116.70	120.30
25	LA	1509	A	P-O3'-C3'	8.99	130.48	119.70
2	S6	1	C	O4'-C1'-N1	8.98	115.38	108.20
25	LA	292	U	O4'-C1'-N1	8.98	115.38	108.20
1	SA	909	A	C8-N9-C4	-8.97	102.21	105.80
1	SA	693	G	N1-C6-O6	8.97	125.28	119.90
25	LA	2445	G	C1'-O4'-C4'	-8.97	102.72	109.90
1	SA	224	U	P-O3'-C3'	8.97	130.46	119.70
25	LA	1564	C	P-O5'-C5'	8.97	135.25	120.90
25	LA	2307	G	P-O3'-C3'	8.97	130.46	119.70
1	SA	424	G	O4'-C1'-N9	8.96	115.37	108.20
25	LA	1253	A	P-O3'-C3'	-8.96	108.94	119.70
25	LA	1966	A	O4'-C1'-N9	8.96	115.37	108.20
25	LA	463	G	C5'-C4'-C3'	-8.95	101.67	116.00
25	LA	2297	A	C5'-C4'-C3'	-8.95	101.68	116.00
52	LF	120	ARG	NE-CZ-NH1	-8.95	115.82	120.30
25	LA	395	U	O4'-C1'-N1	8.95	115.36	108.20
25	LA	2308	G	O4'-C1'-N9	8.93	115.34	108.20
25	LA	1209	U	P-O3'-C3'	-8.92	109.00	119.70
25	LA	573	U	O4'-C1'-N1	8.91	115.33	108.20
1	SA	609	A	P-O5'-C5'	8.90	135.14	120.90
7	SM	56	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	SA	194	C	O4'-C1'-N1	8.89	115.32	108.20
52	LF	27	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	SA	1207	G	O4'-C1'-N9	8.89	115.31	108.20
1	SA	1332	A	C5'-C4'-O4'	8.89	119.76	109.10
1	SA	1160	G	C5-C6-O6	-8.88	123.27	128.60
1	SA	1332	A	C5'-C4'-C3'	-8.87	101.81	116.00
1	SA	1345	U	P-O5'-C5'	-8.87	106.71	120.90
25	LA	2566	A	O4'-C1'-N9	8.87	115.30	108.20
25	LA	2655	G	P-O5'-C5'	-8.87	106.71	120.90
25	LA	1569	A	O4'-C1'-N9	8.86	115.29	108.20
1	SA	470	C	P-O3'-C3'	8.86	130.33	119.70
12	SR	11	ARG	NE-CZ-NH2	8.86	124.73	120.30
25	LA	2322	A	O4'-C1'-N9	8.86	115.28	108.20
1	SA	86	G	P-O3'-C3'	8.85	130.32	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1008	A	O4'-C1'-N9	8.85	115.28	108.20
1	SA	693	G	C5-C6-O6	-8.84	123.29	128.60
25	LA	141	G	O4'-C1'-N9	8.84	115.27	108.20
25	LA	1582	C	O4'-C1'-N1	8.83	115.27	108.20
1	SA	1503	A	P-O3'-C3'	8.83	130.30	119.70
24	S1	9	TYR	CB-CG-CD1	-8.83	115.70	121.00
25	LA	1026	G	P-O3'-C3'	8.82	130.29	119.70
25	LA	2565	A	P-O3'-C3'	8.82	130.29	119.70
30	LO	50	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	SA	1484	C	O4'-C1'-N1	8.81	115.25	108.20
25	LA	2300	C	O4'-C1'-N1	8.81	115.25	108.20
25	LA	1595	C	O4'-C1'-N1	8.80	115.24	108.20
1	SA	1521	C	C6-N1-C2	-8.79	116.78	120.30
32	LQ	95	ARG	NE-CZ-NH1	-8.79	115.90	120.30
25	LA	428	A	O4'-C1'-N9	8.79	115.23	108.20
24	S1	637	ARG	NE-CZ-NH2	-8.78	115.91	120.30
25	LA	2677	G	O4'-C1'-N9	8.78	115.22	108.20
1	SA	428	G	C5-C6-O6	-8.77	123.34	128.60
25	LA	948	C	C5'-C4'-C3'	8.77	130.03	116.00
25	LA	1022	G	O4'-C1'-N9	8.77	115.22	108.20
25	LA	2486	C	O4'-C1'-N1	8.77	115.22	108.20
1	SA	110	C	O4'-C1'-N1	8.77	115.21	108.20
1	SA	769	G	C5-C6-O6	-8.77	123.34	128.60
25	LA	2068	U	O4'-C1'-N1	8.76	115.21	108.20
29	LN	220	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	SA	266	G	C1'-O4'-C4'	-8.76	102.89	109.90
25	LA	925	A	O4'-C1'-N9	8.76	115.21	108.20
25	LA	1772	A	P-O3'-C3'	-8.76	109.19	119.70
25	LA	2505	G	P-O3'-C3'	-8.76	109.19	119.70
1	SA	834	U	C5'-C4'-C3'	-8.74	102.02	116.00
1	SA	473	U	C2-N1-C1'	8.73	128.17	117.70
27	LC	162	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	SA	275	G	P-O5'-C5'	8.73	134.86	120.90
7	SM	56	ARG	NE-CZ-NH1	8.72	124.66	120.30
25	LA	2061	G	C5-C6-O6	-8.71	123.37	128.60
1	SA	795	C	O4'-C1'-N1	8.71	115.17	108.20
1	SA	980	C	O4'-C1'-N1	8.70	115.16	108.20
30	LO	10	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	SA	1471	U	O4'-C1'-N1	8.69	115.15	108.20
1	SA	968	A	O4'-C1'-N9	8.68	115.14	108.20
25	LA	2660	A	O4'-C1'-N9	8.68	115.14	108.20
1	SA	848	C	O4'-C1'-N1	8.67	115.14	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	LJ	96	ARG	NE-CZ-NH2	-8.67	115.97	120.30
25	LA	2445	G	C5-C6-O6	-8.67	123.40	128.60
25	LA	1967	C	O4'-C1'-N1	8.66	115.13	108.20
26	LB	109	A	O4'-C1'-N9	8.66	115.13	108.20
26	LB	42	C	O4'-C1'-N1	8.66	115.13	108.20
1	SA	335	C	O4'-C1'-N1	8.65	115.12	108.20
1	SA	87	C	O4'-C1'-N1	8.65	115.12	108.20
1	SA	971	G	O4'-C1'-N9	8.65	115.12	108.20
1	SA	504	C	O4'-C1'-N1	8.65	115.12	108.20
55	LI	81	ARG	NE-CZ-NH2	-8.64	115.98	120.30
25	LA	776	G	O4'-C1'-N9	8.64	115.11	108.20
1	SA	839	C	O4'-C1'-N1	8.64	115.11	108.20
1	SA	1158	C	C2-N1-C1'	8.63	128.29	118.80
22	SH	79	ARG	NE-CZ-NH2	-8.63	115.99	120.30
25	LA	1839	G	O4'-C1'-N9	8.62	115.10	108.20
25	LA	394	C	O4'-C1'-N1	8.62	115.10	108.20
25	LA	277	G	O4'-C1'-N9	8.62	115.10	108.20
25	LA	1808	A	P-O5'-C5'	8.62	134.69	120.90
1	SA	1501	C	O4'-C1'-N1	8.62	115.09	108.20
2	S6	8	U	C5'-C4'-C3'	-8.62	102.22	116.00
1	SA	1029	U	P-O3'-C3'	8.61	130.03	119.70
48	LE	133	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	SA	730	G	C6-N1-C2	-8.61	119.94	125.10
25	LA	1847	A	O4'-C1'-N9	8.60	115.08	108.20
50	L8	93	TYR	CB-CG-CD2	-8.60	115.84	121.00
1	SA	1100	C	O4'-C1'-N1	8.60	115.08	108.20
25	LA	948	C	P-O5'-C5'	8.59	134.65	120.90
25	LA	2045	C	C6-N1-C2	-8.58	116.87	120.30
1	SA	331	G	O4'-C1'-N9	8.58	115.06	108.20
25	LA	184	C	O4'-C1'-N1	8.58	115.06	108.20
25	LA	890	C	C2-N1-C1'	8.58	128.24	118.80
25	LA	1826	G	O4'-C1'-N9	8.57	115.06	108.20
1	SA	559	A	O4'-C1'-N9	8.57	115.06	108.20
25	LA	257	C	O4'-C1'-N1	8.57	115.06	108.20
25	LA	2403	C	O4'-C1'-N1	8.57	115.05	108.20
1	SA	480	U	O4'-C1'-N1	8.56	115.05	108.20
26	LB	86	G	O4'-C1'-N9	8.56	115.05	108.20
1	SA	1160	G	N1-C6-O6	8.56	125.04	119.90
25	LA	1681	G	O4'-C1'-N9	8.56	115.05	108.20
25	LA	1102	C	O4'-C1'-N1	8.54	115.03	108.20
25	LA	1013	C	O4'-C1'-N1	8.54	115.03	108.20
25	LA	2572	A	C1'-O4'-C4'	-8.54	103.07	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	LN	216	ARG	NE-CZ-NH1	8.54	124.57	120.30
25	LA	1392	A	O4'-C1'-N9	8.54	115.03	108.20
25	LA	2270	A	O4'-C1'-N9	8.54	115.03	108.20
25	LA	2793	C	O4'-C1'-N1	8.54	115.03	108.20
1	SA	388	G	C5-C6-O6	-8.53	123.48	128.60
7	SM	86	ARG	NE-CZ-NH2	-8.53	116.03	120.30
25	LA	2179	C	O4'-C1'-N1	8.53	115.02	108.20
25	LA	393	C	O4'-C1'-N1	8.53	115.02	108.20
22	SH	12	ARG	NE-CZ-NH2	-8.52	116.04	120.30
25	LA	2681	C	O4'-C1'-N1	8.52	115.02	108.20
1	SA	507	C	O4'-C1'-N1	8.52	115.01	108.20
1	SA	1460	C	C6-N1-C2	-8.52	116.89	120.30
1	SA	1158	C	O4'-C1'-N1	8.51	115.01	108.20
1	SA	503	C	P-O5'-C5'	8.50	134.51	120.90
25	LA	2196	C	O4'-C1'-N1	8.50	115.00	108.20
9	SO	87	ARG	NE-CZ-NH2	-8.50	116.05	120.30
25	LA	2258	C	C6-N1-C2	-8.50	116.90	120.30
25	LA	2556	C	O4'-C1'-N1	8.50	115.00	108.20
1	SA	1209	C	P-O5'-C5'	8.48	134.47	120.90
16	SU	70	TYR	CB-CG-CD1	8.48	126.09	121.00
25	LA	231	A	P-O3'-C3'	8.48	129.87	119.70
25	LA	631	A	P-O3'-C3'	8.48	129.88	119.70
25	LA	1763	G	P-O3'-C3'	8.48	129.88	119.70
25	LA	1061	U	O4'-C1'-N1	8.47	114.98	108.20
10	SP	25	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	SA	306	A	P-O3'-C3'	8.46	129.85	119.70
1	SA	765	G	N9-C1'-C2'	-8.46	102.70	112.00
25	LA	239	C	O4'-C1'-N1	8.46	114.97	108.20
25	LA	2060	A	C5'-C4'-O4'	8.46	119.25	109.10
32	LQ	95	ARG	NE-CZ-NH2	8.45	124.53	120.30
1	SA	51	A	C5'-C4'-C3'	-8.45	102.48	116.00
25	LA	2539	C	P-O5'-C5'	8.45	134.42	120.90
25	LA	2245	U	O3'-P-O5'	-8.45	87.95	104.00
1	SA	175	C	O4'-C1'-N1	8.44	114.95	108.20
25	LA	2164	C	O4'-C1'-N1	8.44	114.95	108.20
1	SA	413	G	O4'-C1'-N9	8.44	114.95	108.20
25	LA	177	G	O4'-C1'-N9	8.44	114.95	108.20
25	LA	732	C	O4'-C1'-N1	8.44	114.95	108.20
25	LA	1366	A	N1-C6-N6	-8.43	113.54	118.60
25	LA	2779	U	O4'-C1'-N1	8.43	114.94	108.20
1	SA	828	U	C5'-C4'-C3'	8.42	129.47	116.00
12	SR	11	ARG	NE-CZ-NH1	-8.42	116.09	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1493	A	O4'-C1'-N9	8.42	114.93	108.20
3	S7	39	U	O4'-C1'-N1	8.42	114.93	108.20
30	LO	57	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	SA	1206	G	C5'-C4'-C3'	-8.41	102.55	116.00
1	SA	472	U	P-O5'-C5'	8.40	134.34	120.90
3	S7	14	A	C5'-C4'-C3'	-8.40	102.55	116.00
25	LA	1923	U	P-O5'-C5'	8.40	134.34	120.90
1	SA	1148	U	P-O5'-C5'	8.40	134.34	120.90
55	LI	18	ARG	NE-CZ-NH2	8.40	124.50	120.30
1	SA	1322	C	O4'-C1'-N1	8.40	114.92	108.20
25	LA	1657	U	O4'-C1'-N1	8.40	114.92	108.20
1	SA	173	U	P-O3'-C3'	8.40	129.78	119.70
1	SA	405	U	P-O5'-C5'	8.39	134.33	120.90
1	SA	858	G	C5-C6-O6	-8.39	123.56	128.60
25	LA	798	G	C5'-C4'-C3'	-8.39	102.58	116.00
1	SA	250	A	O4'-C1'-N9	8.38	114.90	108.20
25	LA	2498	C	O4'-C1'-N1	8.38	114.90	108.20
25	LA	745	G	N1-C6-O6	8.37	124.92	119.90
25	LA	99	U	C2-N1-C1'	8.37	127.74	117.70
25	LA	1168	G	O4'-C1'-N9	8.37	114.89	108.20
1	SA	1167	A	P-O3'-C3'	8.37	129.74	119.70
6	SL	53	ARG	NE-CZ-NH2	-8.37	116.12	120.30
25	LA	540	C	O4'-C1'-N1	8.37	114.89	108.20
2	S6	74	A	O4'-C1'-N9	8.36	114.89	108.20
25	LA	1082	U	O4'-C1'-N1	8.37	114.89	108.20
1	SA	1531	A	P-O5'-C5'	-8.36	107.52	120.90
8	SN	68	ARG	NE-CZ-NH1	8.36	124.48	120.30
26	LB	114	C	O4'-C1'-N1	8.36	114.89	108.20
25	LA	147	C	O4'-C1'-N1	8.36	114.89	108.20
25	LA	1143	A	O4'-C1'-N9	8.36	114.89	108.20
25	LA	1764	C	O4'-C1'-N1	8.36	114.88	108.20
26	LB	113	C	O4'-C1'-N1	8.36	114.88	108.20
26	LB	6	G	P-O5'-C5'	8.35	134.26	120.90
13	SS	80	ARG	NE-CZ-NH1	8.35	124.47	120.30
25	LA	1204	A	O4'-C1'-N9	8.35	114.88	108.20
25	LA	1784	A	C5'-C4'-O4'	8.35	119.12	109.10
1	SA	791	G	O4'-C1'-N9	8.35	114.88	108.20
1	SA	314	C	C6-N1-C2	-8.34	116.97	120.30
25	LA	274	C	O4'-C1'-N1	8.32	114.86	108.20
27	LC	164	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	SA	65	A	O4'-C1'-N9	8.32	114.86	108.20
25	LA	2145	C	P-O3'-C3'	8.32	129.68	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	SG	52	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	SA	404	G	C5-C6-O6	-8.31	123.61	128.60
30	LO	44	TYR	CB-CG-CD1	-8.31	116.02	121.00
1	SA	916	U	O4'-C1'-N1	8.30	114.84	108.20
24	S1	636	ARG	NE-CZ-NH2	-8.30	116.15	120.30
25	LA	507	A	P-O3'-C3'	8.30	129.66	119.70
25	LA	1868	C	O4'-C1'-N1	8.30	114.84	108.20
8	SN	19	TYR	CB-CG-CD1	8.29	125.98	121.00
25	LA	1514	G	C5-C6-O6	-8.30	123.62	128.60
25	LA	387	U	C5'-C4'-O4'	8.29	119.05	109.10
25	LA	2682	A	P-O3'-C3'	-8.29	109.75	119.70
17	SC	155	ARG	NE-CZ-NH1	8.28	124.44	120.30
25	LA	719	C	O4'-C1'-N1	8.28	114.83	108.20
25	LA	2820	A	C4'-C3'-C2'	-8.28	94.32	102.60
25	LA	387	U	O4'-C1'-N1	8.28	114.82	108.20
25	LA	508	A	P-O3'-C3'	8.28	129.63	119.70
25	LA	1901	A	N1-C6-N6	-8.27	113.64	118.60
1	SA	279	A	P-O3'-C3'	8.27	129.62	119.70
1	SA	387	U	O4'-C1'-N1	8.27	114.81	108.20
25	LA	1902	C	O4'-C1'-N1	8.26	114.81	108.20
25	LA	2663	G	P-O3'-C3'	8.26	129.62	119.70
25	LA	453	A	P-O3'-C3'	8.26	129.61	119.70
32	LQ	92	ARG	NE-CZ-NH1	8.26	124.43	120.30
25	LA	2848	G	O4'-C1'-N9	8.26	114.80	108.20
26	LB	35	C	O4'-C1'-N1	8.26	114.81	108.20
25	LA	1101	U	O4'-C1'-N1	8.25	114.80	108.20
1	SA	1049	U	C5'-C4'-O4'	8.25	119.00	109.10
14	SB	212	TYR	CB-CG-CD1	-8.25	116.05	121.00
25	LA	1695	G	O4'-C1'-N9	8.25	114.80	108.20
25	LA	1531	C	O4'-C1'-N1	8.24	114.79	108.20
25	LA	2752	C	O4'-C1'-N1	8.24	114.80	108.20
52	LF	35	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	SA	964	A	P-O3'-C3'	8.24	129.59	119.70
25	LA	2458	G	N1-C6-O6	8.24	124.84	119.90
3	S7	59	U	O4'-C1'-N1	8.24	114.79	108.20
25	LA	568	U	O4'-C1'-N1	8.24	114.79	108.20
25	LA	684	G	O4'-C1'-N9	8.24	114.79	108.20
25	LA	2251	G	C1'-O4'-C4'	-8.24	103.31	109.90
25	LA	2425	A	P-O3'-C3'	8.23	129.58	119.70
1	SA	1149	C	O4'-C1'-N1	8.23	114.78	108.20
26	LB	30	C	O4'-C1'-N1	8.23	114.79	108.20
25	LA	2796	U	P-O5'-C5'	8.23	134.07	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2902	C	O4'-C1'-N1	8.23	114.78	108.20
25	LA	1542	U	O4'-C1'-N1	8.23	114.78	108.20
1	SA	1213	A	P-O3'-C3'	8.23	129.57	119.70
1	SA	1293	C	O4'-C1'-N1	8.23	114.78	108.20
1	SA	959	A	C1'-O4'-C4'	-8.22	103.32	109.90
25	LA	725	G	C5-C6-O6	-8.22	123.67	128.60
25	LA	65	U	O4'-C1'-N1	8.22	114.77	108.20
25	LA	1850	G	O4'-C1'-N9	8.22	114.77	108.20
25	LA	1913	A	O4'-C1'-N9	8.22	114.77	108.20
3	S7	31	A	P-O5'-C5'	8.22	134.04	120.90
7	SM	86	ARG	NE-CZ-NH1	8.21	124.41	120.30
25	LA	725	G	P-O3'-C3'	8.21	129.56	119.70
25	LA	1882	U	C5'-C4'-O4'	8.21	118.96	109.10
25	LA	1330	C	O4'-C1'-N1	8.21	114.77	108.20
25	LA	2538	C	O4'-C1'-N1	8.21	114.77	108.20
25	LA	2491	U	C2-N1-C1'	8.21	127.55	117.70
1	SA	637	C	O4'-C1'-N1	8.20	114.76	108.20
33	LR	69	ARG	NE-CZ-NH2	-8.20	116.20	120.30
25	LA	2504	U	P-O3'-C3'	-8.20	109.86	119.70
1	SA	1540	U	O4'-C1'-N1	8.20	114.76	108.20
1	SA	1118	U	O4'-C1'-N1	8.19	114.75	108.20
27	LC	162	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	SA	183	C	P-O3'-C3'	8.18	129.52	119.70
1	SA	1328	C	O4'-C1'-N1	8.18	114.75	108.20
1	SA	528	C	C5'-C4'-O4'	8.18	118.92	109.10
1	SA	1500	A	O4'-C1'-N9	8.18	114.74	108.20
9	SO	71	ARG	NE-CZ-NH1	8.18	124.39	120.30
25	LA	2422	C	P-O3'-C3'	8.18	129.51	119.70
25	LA	641	U	P-O3'-C3'	8.17	129.51	119.70
25	LA	787	C	O4'-C1'-N1	8.17	114.74	108.20
40	LX	77	ARG	NE-CZ-NH1	-8.17	116.21	120.30
25	LA	2073	C	O4'-C1'-N1	8.17	114.73	108.20
25	LA	1019	U	O4'-C1'-N1	8.16	114.73	108.20
40	LX	83	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	SA	73	C	O4'-C1'-N1	8.16	114.73	108.20
1	SA	1453	G	O4'-C1'-N9	8.16	114.73	108.20
1	SA	956	U	P-O5'-C5'	8.16	133.95	120.90
25	LA	267	C	P-O5'-C5'	8.16	133.95	120.90
30	LO	10	ARG	NE-CZ-NH1	8.15	124.38	120.30
25	LA	2491	U	O4'-C1'-N1	8.15	114.72	108.20
25	LA	1752	C	O4'-C1'-N1	8.14	114.72	108.20
34	LS	81	ARG	NE-CZ-NH1	8.14	124.37	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1281	C	O4'-C1'-N1	8.13	114.70	108.20
1	SA	1347	G	P-O3'-C3'	8.13	129.46	119.70
25	LA	893	C	O4'-C1'-N1	8.13	114.70	108.20
25	LA	895	U	C5'-C4'-C3'	-8.13	103.00	116.00
25	LA	2770	G	P-O3'-C3'	8.13	129.45	119.70
25	LA	2063	C	O4'-C1'-N1	8.13	114.70	108.20
25	LA	2104	C	O4'-C1'-N1	8.12	114.70	108.20
25	LA	2520	C	O4'-C1'-N1	8.12	114.70	108.20
55	LI	44	ARG	NE-CZ-NH1	-8.12	116.24	120.30
25	LA	2125	G	C5-C6-O6	-8.12	123.73	128.60
25	LA	2020	A	C5'-C4'-C3'	8.12	128.99	116.00
1	SA	83	C	O4'-C1'-N1	8.11	114.69	108.20
1	SA	1279	G	C4-N9-C1'	8.11	137.05	126.50
9	SO	76	ARG	NE-CZ-NH1	8.11	124.35	120.30
25	LA	62	U	P-O3'-C3'	8.11	129.43	119.70
25	LA	456	C	P-O5'-C5'	8.10	133.87	120.90
26	LB	68	C	O4'-C1'-N1	8.10	114.68	108.20
1	SA	3	A	P-O3'-C3'	8.10	129.41	119.70
25	LA	41	C	O4'-C1'-N1	8.10	114.68	108.20
1	SA	397	A	O4'-C1'-N9	8.09	114.67	108.20
25	LA	1104	C	O4'-C1'-N1	8.09	114.67	108.20
57	LK	102	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	SA	700	G	P-O3'-C3'	-8.08	110.00	119.70
25	LA	2665	A	O4'-C1'-N9	8.08	114.66	108.20
25	LA	1940	U	C5'-C4'-C3'	8.08	128.92	116.00
1	SA	812	G	C5'-C4'-C3'	-8.06	103.10	116.00
1	SA	1028	C	P-O5'-C5'	8.06	133.80	120.90
9	SO	71	ARG	NE-CZ-NH2	-8.06	116.27	120.30
26	LB	102	G	C5-C6-O6	-8.06	123.76	128.60
25	LA	1434	A	P-O5'-C5'	8.06	133.79	120.90
25	LA	1670	C	O4'-C1'-N1	8.06	114.65	108.20
1	SA	1530	G	O4'-C1'-N9	8.06	114.64	108.20
25	LA	740	C	O4'-C1'-N1	8.05	114.64	108.20
25	LA	1321	A	C1'-O4'-C4'	-8.05	103.46	109.90
25	LA	194	G	O4'-C1'-N9	8.05	114.64	108.20
25	LA	2666	C	C2-N1-C1'	8.05	127.65	118.80
1	SA	440	C	O4'-C1'-N1	8.04	114.64	108.20
1	SA	618	C	O4'-C1'-N1	8.04	114.64	108.20
25	LA	361	G	C5-C6-O6	-8.05	123.77	128.60
25	LA	2515	C	O4'-C1'-N1	8.05	114.64	108.20
47	L6	102	ARG	NE-CZ-NH1	-8.04	116.28	120.30
25	LA	1249	U	C5'-C4'-C3'	-8.04	103.13	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	LH	41	ARG	NE-CZ-NH1	8.04	124.32	120.30
25	LA	194	G	C4'-C3'-C2'	-8.04	94.56	102.60
25	LA	777	G	O4'-C1'-N9	8.04	114.63	108.20
25	LA	1979	U	C4'-C3'-C2'	-8.04	94.56	102.60
25	LA	774	G	O4'-C1'-N9	8.03	114.63	108.20
1	SA	328	C	O4'-C1'-N1	8.03	114.63	108.20
25	LA	876	C	P-O3'-C3'	-8.03	110.06	119.70
1	SA	1419	G	O4'-C1'-N9	8.03	114.62	108.20
1	SA	93	U	P-O3'-C3'	8.03	129.34	119.70
29	LN	101	ARG	NE-CZ-NH2	-8.03	116.29	120.30
54	LH	69	ARG	NE-CZ-NH1	8.03	124.31	120.30
25	LA	1302	A	N1-C6-N6	8.03	123.42	118.60
1	SA	1271	A	P-O3'-C3'	8.02	129.33	119.70
25	LA	1207	C	O4'-C1'-N1	8.02	114.62	108.20
25	LA	2213	U	P-O3'-C3'	8.02	129.32	119.70
25	LA	1236	G	P-O3'-C3'	-8.02	110.08	119.70
25	LA	2094	A	C5'-C4'-C3'	-8.02	103.17	116.00
25	LA	2762	C	O4'-C1'-N1	8.02	114.61	108.20
1	SA	716	A	P-O5'-C5'	-8.01	108.08	120.90
4	SJ	5	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	SA	389	A	N1-C6-N6	-8.01	113.79	118.60
25	LA	445	C	C5'-C4'-O4'	8.01	118.71	109.10
25	LA	131	A	O4'-C1'-N9	8.01	114.61	108.20
1	SA	972	C	O4'-C1'-N1	8.01	114.60	108.20
56	LJ	12	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	SA	277	C	O4'-C1'-N1	8.00	114.60	108.20
1	SA	139	A	P-O5'-C5'	8.00	133.70	120.90
25	LA	1730	C	O4'-C1'-N1	8.00	114.60	108.20
25	LA	1782	U	C2-N1-C1'	8.00	127.30	117.70
25	LA	871	U	O4'-C1'-N1	7.99	114.59	108.20
1	SA	322	C	O4'-C1'-N1	7.98	114.58	108.20
25	LA	228	C	O4'-C1'-N1	7.98	114.58	108.20
25	LA	2169	A	O4'-C1'-N9	7.98	114.58	108.20
25	LA	1585	C	O4'-C1'-N1	7.98	114.58	108.20
1	SA	941	G	O4'-C1'-N9	7.97	114.58	108.20
24	S1	336	ARG	NE-CZ-NH1	7.97	124.29	120.30
25	LA	923	G	O4'-C1'-N9	7.97	114.58	108.20
25	LA	1149	G	C5'-C4'-C3'	-7.97	103.24	116.00
25	LA	1541	C	O4'-C1'-N1	7.97	114.58	108.20
1	SA	547	A	N1-C6-N6	-7.97	113.82	118.60
25	LA	1893	C	O4'-C1'-N1	7.97	114.58	108.20
25	LA	2799	A	C1'-O4'-C4'	-7.97	103.53	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	ST	24	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	SA	1491	G	O4'-C1'-N9	7.96	114.57	108.20
25	LA	2185	U	O4'-C1'-N1	7.96	114.57	108.20
25	LA	1781	U	C1'-O4'-C4'	-7.96	103.53	109.90
25	LA	1056	G	O4'-C1'-N9	7.96	114.56	108.20
1	SA	866	C	P-O5'-C5'	7.95	133.62	120.90
25	LA	2055	C	O4'-C1'-N1	7.95	114.56	108.20
25	LA	158	U	O4'-C1'-N1	7.95	114.56	108.20
25	LA	1537	G	O4'-C1'-N9	7.95	114.56	108.20
25	LA	1926	U	C2-N1-C1'	7.95	127.23	117.70
10	SP	70	ARG	NE-CZ-NH1	7.94	124.27	120.30
25	LA	230	G	O4'-C1'-N9	7.94	114.55	108.20
25	LA	196	A	C1'-O4'-C4'	-7.94	103.55	109.90
25	LA	931	U	O4'-C1'-N1	7.94	114.55	108.20
1	SA	108	G	O4'-C1'-N9	7.94	114.55	108.20
1	SA	1034	G	O4'-C1'-N9	7.93	114.54	108.20
25	LA	2094	A	O4'-C1'-N9	7.93	114.54	108.20
25	LA	2702	G	O3'-P-O5'	-7.92	88.95	104.00
28	LM	92	ARG	NE-CZ-NH2	-7.92	116.34	120.30
47	L6	49	ARG	NE-CZ-NH2	7.92	124.26	120.30
25	LA	1361	G	C5'-C4'-C3'	-7.92	103.33	116.00
25	LA	105	C	P-O3'-C3'	7.92	129.20	119.70
1	SA	1472	U	O4'-C1'-N1	7.91	114.53	108.20
25	LA	30	G	P-O5'-C5'	-7.91	108.24	120.90
25	LA	585	G	C5-C6-O6	-7.91	123.85	128.60
25	LA	510	C	P-O3'-C3'	7.90	129.18	119.70
25	LA	403	U	O4'-C1'-N1	7.90	114.52	108.20
25	LA	1446	C	O4'-C1'-N1	7.90	114.52	108.20
40	LX	141	ARG	NE-CZ-NH2	-7.90	116.35	120.30
25	LA	1523	U	P-O3'-C3'	7.90	129.18	119.70
25	LA	450	G	O4'-C1'-N9	7.89	114.52	108.20
25	LA	1025	G	P-O3'-C3'	7.89	129.17	119.70
54	LH	69	ARG	NE-CZ-NH2	-7.89	116.35	120.30
6	SL	8	ARG	NE-CZ-NH1	7.89	124.24	120.30
25	LA	114	U	P-O3'-C3'	7.89	129.16	119.70
1	SA	522	C	O4'-C1'-N1	7.88	114.51	108.20
25	LA	2642	G	C5'-C4'-C3'	-7.88	103.39	116.00
1	SA	1327	C	C5'-C4'-C3'	-7.88	103.39	116.00
25	LA	2800	A	O4'-C1'-N9	7.88	114.50	108.20
1	SA	1421	G	O4'-C1'-N9	7.88	114.50	108.20
1	SA	346	G	C4'-C3'-C2'	-7.87	94.73	102.60
25	LA	343	C	O4'-C1'-N1	7.87	114.50	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1217	C	P-O5'-C5'	7.87	133.49	120.90
25	LA	2755	C	O4'-C1'-N1	7.87	114.49	108.20
1	SA	1398	A	O4'-C1'-N9	7.86	114.49	108.20
25	LA	1167	C	O4'-C1'-N1	7.86	114.49	108.20
1	SA	1253	G	P-O3'-C3'	7.86	129.13	119.70
25	LA	1061	U	C1'-O4'-C4'	-7.86	103.61	109.90
1	SA	1496	C	O4'-C1'-N1	7.86	114.48	108.20
25	LA	468	G	P-O3'-C3'	-7.85	110.28	119.70
1	SA	346	G	C8-N9-C1'	-7.85	116.79	127.00
9	SO	16	ARG	NE-CZ-NH2	-7.85	116.37	120.30
25	LA	2251	G	O4'-C1'-C2'	7.85	114.67	107.60
25	LA	2755	C	C6-N1-C1'	-7.85	111.38	120.80
1	SA	795	C	P-O5'-C5'	-7.85	108.34	120.90
1	SA	1089	G	O4'-C1'-N9	7.85	114.48	108.20
6	SL	55	ARG	NE-CZ-NH2	-7.85	116.38	120.30
25	LA	2054	A	N1-C6-N6	-7.84	113.89	118.60
1	SA	330	C	C5'-C4'-C3'	-7.84	103.45	116.00
25	LA	655	A	P-O3'-C3'	7.84	129.11	119.70
25	LA	1274	A	O4'-C1'-N9	7.84	114.47	108.20
25	LA	1912	A	P-O5'-C5'	7.83	133.44	120.90
25	LA	1368	G	O4'-C1'-N9	7.83	114.47	108.20
25	LA	580	U	P-O3'-C3'	7.83	129.10	119.70
25	LA	1985	C	O4'-C1'-N1	7.83	114.47	108.20
48	LE	126	ARG	NE-CZ-NH2	-7.83	116.39	120.30
25	LA	1943	U	O4'-C1'-N1	7.83	114.46	108.20
25	LA	1100	C	O4'-C1'-N1	7.82	114.46	108.20
1	SA	1120	C	O4'-C1'-N1	7.82	114.46	108.20
1	SA	1128	C	O4'-C1'-N1	7.82	114.46	108.20
25	LA	430	A	P-O3'-C3'	7.82	129.08	119.70
1	SA	1279	G	C8-N9-C1'	-7.82	116.84	127.00
25	LA	1497	U	O4'-C1'-N1	7.82	114.45	108.20
1	SA	422	C	P-O3'-C3'	7.81	129.07	119.70
1	SA	1316	G	C5-C6-O6	-7.81	123.91	128.60
25	LA	20	C	O4'-C1'-N1	7.81	114.45	108.20
25	LA	2843	G	O4'-C1'-N9	7.81	114.45	108.20
57	LK	15	ARG	NE-CZ-NH2	-7.81	116.39	120.30
25	LA	1012	U	C4'-C3'-C2'	-7.81	94.79	102.60
1	SA	120	A	P-O3'-C3'	7.81	129.07	119.70
1	SA	1201	A	C4-N9-C1'	7.81	140.35	126.30
55	LI	18	ARG	NE-CZ-NH1	-7.81	116.40	120.30
25	LA	209	C	O4'-C1'-N1	7.80	114.44	108.20
1	SA	998	C	O4'-C1'-N1	7.80	114.44	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	SD	25	ARG	NE-CZ-NH1	7.80	124.20	120.30
25	LA	456	C	O4'-C1'-N1	7.80	114.44	108.20
1	SA	202	G	C4-N9-C1'	-7.80	116.36	126.50
1	SA	882	C	O4'-C1'-N1	7.79	114.44	108.20
49	L7	121	PHE	CB-CG-CD2	7.79	126.25	120.80
26	LB	27	C	O4'-C1'-N1	7.79	114.43	108.20
1	SA	267	C	O4'-C1'-N1	7.79	114.43	108.20
1	SA	346	G	O4'-C1'-N9	7.79	114.43	108.20
25	LA	1714	U	O4'-C1'-N1	7.79	114.43	108.20
1	SA	841	C	O4'-C1'-N1	7.78	114.43	108.20
57	LK	94	ARG	NE-CZ-NH2	-7.78	116.41	120.30
25	LA	2572	A	P-O3'-C3'	7.78	129.04	119.70
1	SA	52	C	P-O5'-C5'	7.78	133.35	120.90
1	SA	750	C	O4'-C1'-N1	7.78	114.42	108.20
25	LA	650	C	O4'-C1'-N1	7.78	114.42	108.20
25	LA	315	G	O4'-C1'-N9	7.78	114.42	108.20
29	LN	79	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	SA	1259	C	O4'-C1'-N1	7.77	114.42	108.20
25	LA	1917	U	O5'-C5'-C4'	7.77	126.46	111.70
1	SA	361	G	P-O3'-C3'	7.77	129.02	119.70
25	LA	2060	A	C3'-C2'-C1'	-7.77	95.29	101.50
1	SA	1327	C	O4'-C1'-N1	7.76	114.41	108.20
25	LA	1023	U	O4'-C1'-N1	7.76	114.41	108.20
1	SA	1201	A	P-O3'-C3'	7.76	129.01	119.70
1	SA	1533	C	C6-N1-C2	-7.76	117.20	120.30
1	SA	764	C	O4'-C1'-N1	7.76	114.41	108.20
25	LA	1363	C	O4'-C1'-N1	7.76	114.41	108.20
1	SA	221	C	O4'-C1'-N1	7.75	114.40	108.20
1	SA	1392	G	C5-C6-O6	-7.75	123.95	128.60
25	LA	783	A	N1-C6-N6	-7.75	113.95	118.60
57	LK	81	ARG	NE-CZ-NH1	7.75	124.17	120.30
25	LA	2336	A	P-O3'-C3'	7.75	129.00	119.70
1	SA	979	C	O4'-C1'-N1	7.75	114.40	108.20
25	LA	242	G	P-O3'-C3'	7.74	128.99	119.70
25	LA	610	C	O4'-C1'-N1	7.74	114.39	108.20
25	LA	2021	C	O4'-C1'-N1	7.74	114.39	108.20
25	LA	1974	C	O4'-C1'-N1	7.74	114.39	108.20
1	SA	857	C	O4'-C1'-N1	7.74	114.39	108.20
25	LA	475	C	C6-N1-C2	-7.73	117.21	120.30
25	LA	611	C	O4'-C1'-N1	7.73	114.38	108.20
25	LA	1610	A	O4'-C1'-N9	7.73	114.38	108.20
25	LA	2774	C	O4'-C1'-N1	7.73	114.38	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	SI	105	ARG	NE-CZ-NH1	7.72	124.16	120.30
11	SQ	5	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	SA	166	U	O4'-C1'-N1	7.72	114.38	108.20
1	SA	169	C	O4'-C1'-N1	7.72	114.37	108.20
1	SA	1108	G	O4'-C1'-N9	7.72	114.37	108.20
25	LA	2479	U	P-O3'-C3'	7.72	128.96	119.70
1	SA	635	A	P-O3'-C3'	7.71	128.96	119.70
9	SO	87	ARG	NE-CZ-NH1	7.71	124.16	120.30
25	LA	1990	C	O4'-C1'-N1	7.71	114.37	108.20
29	LN	132	ARG	NE-CZ-NH1	7.71	124.15	120.30
25	LA	2385	C	P-O5'-C5'	7.70	133.22	120.90
23	SI	89	TYR	CB-CG-CD1	-7.70	116.38	121.00
53	LG	17	ARG	NE-CZ-NH2	-7.70	116.45	120.30
25	LA	1070	A	C5'-C4'-O4'	7.70	118.34	109.10
1	SA	38	G	P-O3'-C3'	-7.69	110.47	119.70
3	S7	23	A	C5'-C4'-C3'	-7.69	103.70	116.00
25	LA	1098	A	P-O5'-C5'	7.69	133.20	120.90
1	SA	1342	C	O4'-C1'-N1	7.68	114.35	108.20
25	LA	385	C	O4'-C1'-N1	7.68	114.35	108.20
29	LN	51	ARG	NE-CZ-NH1	7.68	124.14	120.30
25	LA	2760	C	O4'-C1'-N1	7.68	114.35	108.20
26	LB	17	C	O4'-C1'-N1	7.68	114.35	108.20
1	SA	560	A	O4'-C1'-N9	7.68	114.34	108.20
25	LA	525	U	P-O3'-C3'	7.68	128.92	119.70
1	SA	188	C	O4'-C1'-N1	7.68	114.34	108.20
25	LA	527	C	C1'-O4'-C4'	-7.68	103.76	109.90
25	LA	2504	U	C2-N1-C1'	7.68	126.92	117.70
55	LI	50	ARG	NE-CZ-NH1	-7.68	116.46	120.30
49	L7	177	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	SA	194	C	P-O3'-C3'	-7.67	110.49	119.70
1	SA	1412	C	O4'-C1'-N1	7.67	114.34	108.20
31	LP	21	ARG	NE-CZ-NH1	-7.67	116.47	120.30
25	LA	1323	C	P-O3'-C3'	7.67	128.90	119.70
25	LA	1240	U	C5'-C4'-C3'	7.67	128.27	116.00
25	LA	130	C	C5'-C4'-C3'	-7.66	103.74	116.00
1	SA	843	U	O4'-C1'-N1	7.66	114.33	108.20
25	LA	527	C	O4'-C1'-N1	7.66	114.33	108.20
25	LA	2359	C	O4'-C1'-N1	7.66	114.33	108.20
25	LA	1825	U	O4'-C1'-N1	7.66	114.32	108.20
49	L7	82	TYR	CB-CG-CD1	-7.66	116.41	121.00
1	SA	1067	A	C5'-C4'-C3'	-7.65	103.76	116.00
1	SA	1384	C	O4'-C1'-N1	7.65	114.32	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2232	C	O4'-C1'-N1	7.65	114.32	108.20
25	LA	516	C	P-O3'-C3'	7.65	128.88	119.70
25	LA	1582	C	P-O5'-C5'	7.64	133.13	120.90
25	LA	2417	C	O4'-C1'-N1	7.64	114.31	108.20
25	LA	2465	C	O4'-C1'-N1	7.64	114.31	108.20
25	LA	786	C	O4'-C1'-N1	7.64	114.31	108.20
1	SA	1265	C	O4'-C1'-N1	7.64	114.31	108.20
25	LA	517	C	O4'-C1'-N1	7.64	114.31	108.20
25	LA	2111	U	P-O3'-C3'	7.64	128.87	119.70
25	LA	2144	G	O4'-C1'-N9	7.64	114.31	108.20
1	SA	1032	G	O4'-C1'-N9	7.64	114.31	108.20
25	LA	124	G	C5-C6-O6	-7.64	124.02	128.60
25	LA	1076	C	O4'-C1'-N1	7.64	114.31	108.20
25	LA	2383	G	C5'-C4'-C3'	-7.64	103.78	116.00
47	L6	44	ARG	NE-CZ-NH1	-7.64	116.48	120.30
25	LA	1221	C	O4'-C1'-N1	7.63	114.31	108.20
25	LA	1070	A	C1'-O4'-C4'	-7.63	103.80	109.90
1	SA	1134	G	O4'-C1'-N9	7.63	114.30	108.20
1	SA	1517	G	O4'-C1'-N9	7.62	114.30	108.20
25	LA	1938	A	O4'-C1'-N9	7.62	114.30	108.20
26	LB	95	U	O4'-C1'-N1	7.62	114.30	108.20
1	SA	974	A	C4-N9-C1'	-7.62	112.59	126.30
1	SA	1203	C	O4'-C1'-N1	7.62	114.29	108.20
7	SM	22	TYR	CB-CG-CD1	-7.62	116.43	121.00
22	SH	14	ARG	NE-CZ-NH2	-7.62	116.49	120.30
25	LA	897	C	O4'-C1'-N1	7.62	114.29	108.20
1	SA	1097	C	P-O5'-C5'	7.61	133.08	120.90
47	L6	114	ARG	NE-CZ-NH1	7.61	124.11	120.30
25	LA	2545	G	P-O5'-C5'	7.61	133.08	120.90
2	S6	42	C	O4'-C1'-N1	7.61	114.29	108.20
25	LA	440	C	O4'-C1'-N1	7.61	114.29	108.20
25	LA	2093	G	C5'-C4'-C3'	7.61	128.17	116.00
25	LA	1226	A	P-O3'-C3'	7.60	128.82	119.70
25	LA	2108	A	O4'-C1'-N9	7.60	114.28	108.20
1	SA	137	U	O4'-C1'-N1	7.60	114.28	108.20
25	LA	1012	U	C5'-C4'-O4'	7.60	118.22	109.10
25	LA	2159	G	O4'-C1'-N9	7.60	114.28	108.20
26	LB	108	A	C2'-C3'-O3'	7.60	126.22	109.50
1	SA	978	A	C5'-C4'-O4'	7.60	118.22	109.10
25	LA	1210	G	C5-C6-O6	-7.60	124.04	128.60
25	LA	2492	U	C6-N1-C1'	-7.60	110.56	121.20
25	LA	272	A	O4'-C1'-N9	7.59	114.27	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	436	C	P-O5'-C5'	7.59	133.04	120.90
25	LA	1083	U	P-O3'-C3'	7.59	128.81	119.70
21	SG	159	ARG	NE-CZ-NH1	7.59	124.09	120.30
25	LA	1609	A	C1'-O4'-C4'	-7.59	103.83	109.90
1	SA	934	C	O4'-C1'-N1	7.58	114.27	108.20
1	SA	460	A	N1-C6-N6	7.58	123.15	118.60
1	SA	328	C	C5'-C4'-O4'	7.58	118.20	109.10
25	LA	366	C	O4'-C1'-N1	7.58	114.27	108.20
25	LA	2405	G	C5'-C4'-C3'	7.58	128.13	116.00
21	SG	43	TYR	CB-CG-CD2	-7.58	116.45	121.00
25	LA	351	C	O4'-C1'-N1	7.58	114.26	108.20
25	LA	126	A	C1'-O4'-C4'	-7.58	103.84	109.90
1	SA	1071	C	C6-N1-C2	-7.58	117.27	120.30
25	LA	1636	U	O4'-C1'-N1	7.58	114.26	108.20
25	LA	1849	G	O4'-C1'-N9	7.58	114.26	108.20
25	LA	654	A	O4'-C1'-N9	7.57	114.26	108.20
25	LA	2476	A	P-O3'-C3'	7.57	128.79	119.70
1	SA	841	C	C2-N1-C1'	7.57	127.13	118.80
1	SA	345	C	O4'-C1'-N1	7.57	114.26	108.20
25	LA	2789	C	O4'-C1'-N1	7.57	114.25	108.20
2	S6	69	C	O4'-C1'-N1	7.57	114.25	108.20
10	SP	5	ARG	NE-CZ-NH1	7.57	124.08	120.30
12	SR	2	ARG	NE-CZ-NH2	-7.57	116.52	120.30
25	LA	1	G	O4'-C1'-N9	7.56	114.25	108.20
25	LA	1728	C	O4'-C1'-N1	7.56	114.25	108.20
1	SA	128	G	P-O3'-C3'	7.56	128.77	119.70
25	LA	1846	G	C5'-C4'-O4'	7.56	118.17	109.10
25	LA	2067	G	P-O3'-C3'	-7.56	110.63	119.70
1	SA	1294	G	O4'-C1'-N9	7.56	114.25	108.20
1	SA	503	C	O4'-C1'-N1	7.56	114.25	108.20
1	SA	1492	A	O4'-C1'-N9	7.56	114.25	108.20
25	LA	297	G	O4'-C1'-N9	7.56	114.25	108.20
1	SA	1323	G	P-O5'-C5'	-7.55	108.82	120.90
12	SR	60	ARG	NE-CZ-NH2	-7.55	116.52	120.30
25	LA	2060	A	C1'-O4'-C4'	-7.55	103.86	109.90
25	LA	2177	C	O4'-C1'-N1	7.55	114.24	108.20
25	LA	1658	C	O4'-C1'-N1	7.55	114.24	108.20
25	LA	1743	G	N1-C6-O6	7.55	124.43	119.90
1	SA	730	G	N1-C2-N2	-7.54	109.41	116.20
25	LA	616	A	O4'-C1'-N9	7.54	114.24	108.20
30	LO	52	ARG	NE-CZ-NH2	-7.54	116.53	120.30
25	LA	2148	G	O4'-C1'-N9	7.54	114.23	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1575	C	O4'-C1'-N1	7.54	114.23	108.20
25	LA	2103	C	O4'-C1'-N1	7.54	114.23	108.20
1	SA	222	C	O4'-C1'-N1	7.54	114.23	108.20
25	LA	1994	C	O4'-C1'-N1	7.54	114.23	108.20
1	SA	990	C	O4'-C1'-N1	7.53	114.23	108.20
1	SA	1027	C	O4'-C1'-N1	7.53	114.23	108.20
25	LA	2177	C	P-O5'-C5'	7.53	132.95	120.90
1	SA	304	U	O4'-C1'-N1	7.53	114.22	108.20
25	LA	1743	G	C5-C6-O6	-7.53	124.08	128.60
1	SA	51	A	O4'-C1'-C2'	-7.53	98.27	105.80
1	SA	372	C	P-O3'-C3'	7.53	128.73	119.70
25	LA	1357	C	C6-N1-C2	-7.53	117.29	120.30
2	S6	49	C	O4'-C1'-N1	7.52	114.22	108.20
26	LB	93	C	O4'-C1'-N1	7.52	114.22	108.20
1	SA	60	A	P-O3'-C3'	7.52	128.72	119.70
2	S6	1	C	C2-N1-C1'	7.52	127.07	118.80
25	LA	1472	C	O4'-C1'-N1	7.52	114.21	108.20
25	LA	2479	U	O4'-C1'-N1	7.52	114.21	108.20
25	LA	2510	C	O4'-C1'-N1	7.51	114.21	108.20
25	LA	106	C	O4'-C1'-N1	7.51	114.21	108.20
9	SO	88	ARG	NE-CZ-NH2	-7.51	116.55	120.30
25	LA	2012	G	C5-C6-O6	-7.51	124.09	128.60
25	LA	2506	U	O4'-C1'-N1	7.51	114.21	108.20
25	LA	2651	C	O4'-C1'-N1	7.51	114.21	108.20
1	SA	362	G	O4'-C1'-N9	7.51	114.21	108.20
1	SA	815	A	C1'-O4'-C4'	-7.51	103.89	109.90
23	SI	94	ARG	NE-CZ-NH1	7.51	124.06	120.30
25	LA	692	C	O4'-C1'-N1	7.51	114.21	108.20
25	LA	2027	G	P-O3'-C3'	7.51	128.71	119.70
25	LA	1508	A	O4'-C1'-N9	7.51	114.20	108.20
25	LA	1514	G	N1-C6-O6	7.50	124.40	119.90
25	LA	890	C	O4'-C1'-N1	7.50	114.20	108.20
25	LA	952	G	O4'-C1'-N9	7.50	114.20	108.20
55	LI	44	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	SA	563	A	O4'-C1'-N9	7.50	114.20	108.20
25	LA	2110	G	P-O3'-C3'	7.50	128.70	119.70
25	LA	1590	A	C5'-C4'-C3'	-7.50	104.00	116.00
30	LO	5	ARG	NE-CZ-NH1	-7.50	116.55	120.30
25	LA	1461	C	O4'-C1'-N1	7.50	114.20	108.20
25	LA	487	C	O4'-C1'-N1	7.49	114.19	108.20
25	LA	985	C	O4'-C1'-N1	7.49	114.19	108.20
1	SA	1138	G	P-O3'-C3'	7.49	128.69	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1899	A	P-O5'-C5'	7.49	132.88	120.90
34	LS	6	ARG	NE-CZ-NH2	-7.49	116.56	120.30
25	LA	2473	U	O4'-C1'-N1	7.49	114.19	108.20
1	SA	1224	U	O4'-C1'-N1	7.48	114.19	108.20
3	S7	14	A	P-O5'-C5'	7.48	132.87	120.90
25	LA	1382	G	O4'-C1'-N9	7.48	114.18	108.20
25	LA	1178	C	O4'-C1'-N1	7.48	114.18	108.20
25	LA	1529	G	O4'-C1'-N9	7.48	114.18	108.20
1	SA	776	G	C5-C6-O6	-7.47	124.12	128.60
25	LA	1007	C	P-O3'-C3'	7.47	128.67	119.70
25	LA	1314	C	C6-N1-C2	-7.47	117.31	120.30
25	LA	1837	C	O4'-C1'-N1	7.47	114.18	108.20
1	SA	365	U	O3'-P-O5'	-7.47	89.81	104.00
1	SA	355	C	O4'-C1'-N1	7.47	114.17	108.20
1	SA	866	C	O4'-C1'-N1	7.46	114.17	108.20
25	LA	1849	G	C5'-C4'-O4'	7.46	118.06	109.10
6	SL	53	ARG	NE-CZ-NH1	7.46	124.03	120.30
25	LA	564	C	O4'-C1'-N1	7.46	114.17	108.20
25	LA	2371	G	C5-C6-O6	-7.46	124.12	128.60
25	LA	2867	G	P-O3'-C3'	7.46	128.65	119.70
2	S6	8	U	P-O3'-C3'	-7.46	110.75	119.70
38	LD	55	ARG	NE-CZ-NH1	7.46	124.03	120.30
25	LA	1150	C	O4'-C1'-N1	7.45	114.16	108.20
25	LA	2507	C	O4'-C1'-N1	7.45	114.16	108.20
25	LA	459	U	C2-N3-C4	-7.45	122.53	127.00
16	SU	20	ARG	NE-CZ-NH1	7.45	124.02	120.30
2	S6	61	U	O4'-C1'-N1	7.44	114.15	108.20
25	LA	2666	C	C6-N1-C1'	-7.44	111.87	120.80
3	S7	1	G	P-O3'-C3'	7.44	128.63	119.70
29	LN	51	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	SA	150	U	O4'-C1'-N1	7.44	114.15	108.20
25	LA	691	C	O4'-C1'-N1	7.44	114.15	108.20
54	LH	64	PHE	CB-CG-CD1	-7.44	115.59	120.80
25	LA	2275	C	O4'-C1'-N1	7.44	114.15	108.20
16	SU	44	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	SA	809	G	O4'-C1'-N9	7.43	114.15	108.20
1	SA	202	G	O4'-C1'-N9	7.43	114.14	108.20
1	SA	1539	C	O4'-C1'-N1	7.43	114.14	108.20
3	S7	49	C	O4'-C1'-N1	7.43	114.14	108.20
1	SA	75	G	O4'-C1'-N9	7.42	114.14	108.20
25	LA	2045	C	O4'-C1'-N1	7.42	114.14	108.20
25	LA	296	U	O4'-C1'-N1	7.42	114.14	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2147	A	P-O3'-C3'	7.42	128.60	119.70
25	LA	784	G	N1-C6-O6	7.42	124.35	119.90
25	LA	1046	A	O4'-C1'-N9	7.42	114.14	108.20
25	LA	2069	G	C5-C6-O6	-7.42	124.15	128.60
25	LA	2607	G	O4'-C1'-N9	7.42	114.13	108.20
25	LA	1780	A	O4'-C1'-N9	7.42	114.13	108.20
49	L7	70	ARG	NE-CZ-NH1	-7.41	116.59	120.30
2	S6	22	A	C1'-O4'-C4'	-7.41	103.97	109.90
25	LA	2503	A	O4'-C1'-N9	7.41	114.13	108.20
1	SA	252	U	P-O3'-C3'	-7.41	110.81	119.70
1	SA	1263	C	O4'-C1'-N1	7.41	114.12	108.20
25	LA	467	G	O4'-C1'-N9	7.41	114.12	108.20
25	LA	2110	G	O4'-C1'-N9	7.41	114.12	108.20
3	S7	39	U	C2-N1-C1'	7.40	126.58	117.70
25	LA	2339	C	O4'-C1'-N1	7.40	114.12	108.20
25	LA	2412	A	C5-C6-N6	-7.40	117.78	123.70
25	LA	1359	A	O4'-C1'-N9	7.39	114.12	108.20
1	SA	705	G	C5-C6-O6	-7.39	124.16	128.60
18	SD	164	ARG	NE-CZ-NH1	7.39	124.00	120.30
25	LA	516	C	O4'-C1'-N1	7.39	114.11	108.20
25	LA	1741	C	O4'-C1'-N1	7.39	114.11	108.20
25	LA	885	C	O4'-C1'-N1	7.39	114.11	108.20
25	LA	1083	U	O4'-C1'-N1	7.38	114.11	108.20
25	LA	1573	G	P-O5'-C5'	7.37	132.70	120.90
25	LA	1938	A	C1'-O4'-C4'	-7.37	104.00	109.90
55	LI	50	ARG	NE-CZ-NH2	7.37	123.99	120.30
25	LA	1625	C	O4'-C1'-N1	7.37	114.10	108.20
2	S6	70	C	O4'-C1'-N1	7.37	114.10	108.20
1	SA	929	G	C5'-C4'-C3'	-7.37	104.21	116.00
1	SA	528	C	C5'-C4'-C3'	-7.37	104.21	116.00
31	LP	68	ARG	NE-CZ-NH2	7.37	123.98	120.30
25	LA	527	C	C2-N1-C1'	7.37	126.90	118.80
25	LA	1322	A	P-O5'-C5'	7.37	132.68	120.90
36	LU	13	ARG	NE-CZ-NH1	7.37	123.98	120.30
41	LY	30	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	SA	927	G	P-O5'-C5'	7.36	132.68	120.90
5	SK	92	ARG	NE-CZ-NH1	7.36	123.98	120.30
25	LA	879	G	O4'-C1'-N9	7.36	114.09	108.20
1	SA	403	C	O4'-C1'-N1	7.36	114.09	108.20
1	SA	1196	A	O4'-C1'-N9	7.36	114.09	108.20
25	LA	2380	C	O4'-C1'-N1	7.36	114.09	108.20
25	LA	2554	U	C2-N1-C1'	7.36	126.53	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1943	U	P-O3'-C3'	7.36	128.53	119.70
25	LA	2396	G	O4'-C1'-N9	7.36	114.08	108.20
26	LB	43	C	P-O3'-C3'	7.36	128.53	119.70
1	SA	85	U	O4'-C1'-N1	7.35	114.08	108.20
25	LA	853	C	O4'-C1'-N1	7.35	114.08	108.20
25	LA	2116	G	C4-N9-C1'	7.35	136.06	126.50
25	LA	2406	A	O4'-C1'-N9	7.35	114.08	108.20
1	SA	1364	U	C6-N1-C2	-7.35	116.59	121.00
25	LA	1196	C	O4'-C1'-N1	7.35	114.08	108.20
25	LA	2853	C	O4'-C1'-N1	7.34	114.08	108.20
1	SA	388	G	O4'-C1'-N9	7.34	114.07	108.20
1	SA	781	A	C5'-C4'-C3'	7.34	127.75	116.00
3	S7	61	C	O4'-C1'-N1	7.34	114.07	108.20
25	LA	1365	A	O4'-C1'-N9	7.34	114.07	108.20
25	LA	2078	C	O4'-C1'-N1	7.34	114.07	108.20
1	SA	326	G	C4-N9-C1'	7.34	136.04	126.50
25	LA	2245	U	P-O3'-C3'	-7.34	110.89	119.70
1	SA	95	C	O4'-C1'-N1	7.33	114.07	108.20
1	SA	346	G	C4-N9-C1'	7.33	136.04	126.50
25	LA	2093	G	O4'-C1'-N9	7.33	114.07	108.20
25	LA	2047	C	O4'-C1'-N1	7.33	114.06	108.20
25	LA	2587	A	P-O3'-C3'	7.33	128.50	119.70
1	SA	971	G	P-O3'-C3'	-7.33	110.90	119.70
25	LA	1444	G	O4'-C1'-N9	7.32	114.06	108.20
1	SA	181	A	P-O5'-C5'	-7.32	109.19	120.90
25	LA	130	C	O4'-C1'-N1	7.32	114.06	108.20
45	L4	7	ARG	NE-CZ-NH1	7.32	123.96	120.30
18	SD	127	ARG	NE-CZ-NH1	7.32	123.96	120.30
25	LA	2449	U	O4'-C1'-N1	7.32	114.05	108.20
24	S1	9	TYR	CB-CG-CD2	7.31	125.39	121.00
1	SA	883	C	O4'-C1'-N1	7.31	114.05	108.20
25	LA	1901	A	O4'-C1'-N9	7.31	114.05	108.20
33	LR	3	ARG	NE-CZ-NH1	7.31	123.96	120.30
54	LH	64	PHE	CB-CG-CD2	7.31	125.92	120.80
1	SA	196	A	C5'-C4'-C3'	-7.31	104.31	116.00
25	LA	289	G	O3'-P-O5'	-7.31	90.11	104.00
25	LA	1242	U	P-O5'-C5'	7.31	132.60	120.90
25	LA	1414	C	O4'-C1'-N1	7.31	114.05	108.20
26	LB	63	C	O4'-C1'-N1	7.31	114.05	108.20
1	SA	1422	G	O4'-C1'-N9	7.31	114.05	108.20
25	LA	211	C	O4'-C1'-N1	7.31	114.05	108.20
1	SA	178	C	C5'-C4'-O4'	7.30	117.87	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	209	U	P-O3'-C3'	7.30	128.47	119.70
1	SA	973	G	C5-C6-O6	-7.30	124.22	128.60
25	LA	909	A	C5'-C4'-C3'	-7.30	104.31	116.00
25	LA	1319	C	O4'-C1'-N1	7.30	114.04	108.20
3	S7	11	C	O4'-C1'-N1	7.30	114.04	108.20
1	SA	334	C	O4'-C1'-N1	7.30	114.04	108.20
1	SA	872	A	N1-C6-N6	-7.30	114.22	118.60
25	LA	1854	A	P-O5'-C5'	-7.30	109.22	120.90
25	LA	479	A	P-O3'-C3'	7.30	128.46	119.70
1	SA	821	G	O4'-C1'-N9	7.30	114.04	108.20
2	S6	57	C	O4'-C1'-N1	7.30	114.04	108.20
1	SA	1402	C	O4'-C1'-C2'	7.29	114.17	107.60
1	SA	135	C	O4'-C1'-N1	7.29	114.03	108.20
1	SA	981	U	C6-N1-C1'	-7.29	110.99	121.20
25	LA	2769	U	C5'-C4'-C3'	-7.29	104.33	116.00
25	LA	2567	G	P-O3'-C3'	7.29	128.45	119.70
1	SA	291	U	O4'-C1'-N1	7.29	114.03	108.20
1	SA	1364	U	O4'-C1'-N1	7.29	114.03	108.20
25	LA	1648	U	P-O5'-C5'	7.28	132.55	120.90
25	LA	2823	A	C5'-C4'-C3'	-7.28	104.35	116.00
1	SA	485	U	P-O3'-C3'	-7.28	110.97	119.70
2	S6	52	C	O4'-C1'-N1	7.28	114.02	108.20
25	LA	1493	C	O4'-C1'-N1	7.28	114.02	108.20
1	SA	428	G	N1-C6-O6	7.27	124.26	119.90
1	SA	831	A	C5'-C4'-C3'	-7.27	104.37	116.00
1	SA	1134	G	C5'-C4'-C3'	7.27	127.63	116.00
1	SA	90	C	O4'-C1'-N1	7.27	114.01	108.20
25	LA	119	A	O4'-C1'-N9	7.27	114.01	108.20
30	LO	44	TYR	CB-CG-CD2	7.27	125.36	121.00
1	SA	1162	C	O4'-C1'-N1	7.26	114.01	108.20
25	LA	2372	U	O4'-C1'-N1	7.26	114.01	108.20
25	LA	164	C	O4'-C1'-N1	7.26	114.01	108.20
25	LA	1870	C	O4'-C1'-N1	7.26	114.01	108.20
49	L7	70	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	SA	221	C	C5'-C4'-C3'	-7.26	104.38	116.00
25	LA	1565	C	O4'-C1'-N1	7.26	114.01	108.20
1	SA	976	G	P-O5'-C5'	7.26	132.52	120.90
1	SA	1313	U	P-O3'-C3'	-7.26	110.99	119.70
20	SF	78	PHE	CB-CG-CD1	7.26	125.88	120.80
25	LA	568	U	C2-N1-C1'	7.26	126.41	117.70
25	LA	2505	G	O4'-C1'-N9	7.26	114.00	108.20
25	LA	414	C	O4'-C1'-N1	7.25	114.00	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2118	U	O4'-C1'-N1	7.25	114.00	108.20
25	LA	29	U	P-O3'-C3'	7.25	128.41	119.70
1	SA	1393	U	P-O5'-C5'	7.25	132.50	120.90
1	SA	810	C	O4'-C1'-N1	7.25	114.00	108.20
25	LA	234	U	O4'-C1'-N1	7.25	114.00	108.20
25	LA	2647	U	P-O5'-C5'	-7.25	109.30	120.90
1	SA	1198	G	O4'-C1'-N9	7.25	114.00	108.20
25	LA	934	U	O4'-C1'-N1	7.25	114.00	108.20
25	LA	1899	A	N1-C6-N6	-7.25	114.25	118.60
1	SA	1492	A	P-O3'-C3'	7.24	128.39	119.70
25	LA	361	G	N1-C6-O6	7.24	124.25	119.90
25	LA	2331	G	O4'-C1'-N9	7.24	114.00	108.20
25	LA	2795	C	O4'-C1'-N1	7.24	113.99	108.20
1	SA	565	U	O4'-C1'-N1	7.24	113.99	108.20
25	LA	2774	C	P-O5'-C5'	7.24	132.48	120.90
27	LC	74	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	SA	1533	C	P-O3'-C3'	7.23	128.38	119.70
25	LA	2562	U	C5'-C4'-C3'	7.23	127.57	116.00
1	SA	1279	G	P-O3'-C3'	-7.23	111.02	119.70
25	LA	1855	U	C5'-C4'-C3'	-7.23	104.43	116.00
1	SA	800	G	N1-C6-O6	7.23	124.24	119.90
25	LA	2076	U	P-O3'-C3'	7.23	128.38	119.70
25	LA	2458	G	O4'-C1'-N9	7.23	113.98	108.20
25	LA	2821	A	C5'-C4'-O4'	7.23	117.77	109.10
25	LA	890	C	C6-N1-C1'	-7.23	112.13	120.80
32	LQ	11	ARG	NE-CZ-NH1	7.23	123.91	120.30
25	LA	1685	C	O4'-C1'-N1	7.22	113.98	108.20
1	SA	800	G	C5-C6-O6	-7.22	124.27	128.60
25	LA	2676	C	O4'-C1'-N1	7.22	113.97	108.20
25	LA	1934	C	O4'-C1'-N1	7.22	113.97	108.20
25	LA	2178	C	O4'-C1'-N1	7.22	113.97	108.20
26	LB	42	C	C2-N1-C1'	7.22	126.74	118.80
1	SA	1282	C	O4'-C1'-N1	7.21	113.97	108.20
25	LA	212	G	C4'-C3'-C2'	-7.21	95.39	102.60
25	LA	2504	U	O4'-C1'-N1	7.21	113.97	108.20
25	LA	1348	C	O4'-C1'-N1	7.21	113.97	108.20
25	LA	1882	U	C5'-C4'-C3'	-7.21	104.46	116.00
1	SA	767	A	P-O5'-C5'	7.21	132.43	120.90
1	SA	808	C	O4'-C1'-N1	7.21	113.97	108.20
1	SA	999	C	O4'-C1'-N1	7.21	113.97	108.20
25	LA	1012	U	O4'-C1'-C2'	-7.21	98.59	105.80
25	LA	2801	G	C5'-C4'-C3'	-7.21	104.47	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	814	A	P-O3'-C3'	7.20	128.34	119.70
1	SA	1170	A	O4'-C1'-N9	7.20	113.96	108.20
2	S6	38	A	P-O3'-C3'	7.20	128.34	119.70
25	LA	1917	U	O4'-C1'-N1	7.20	113.96	108.20
25	LA	2094	A	C1'-O4'-C4'	-7.20	104.14	109.90
25	LA	2458	G	C5-C6-O6	-7.20	124.28	128.60
25	LA	1185	G	P-O3'-C3'	7.20	128.34	119.70
25	LA	1554	U	O4'-C1'-N1	7.20	113.96	108.20
1	SA	731	G	C5'-C4'-C3'	7.19	127.51	116.00
20	SF	24	ARG	NE-CZ-NH1	7.19	123.90	120.30
25	LA	1096	A	O4'-C1'-N9	7.19	113.95	108.20
25	LA	1662	U	O4'-C1'-N1	7.19	113.95	108.20
25	LA	2151	U	O4'-C1'-N1	7.19	113.95	108.20
1	SA	612	C	O4'-C1'-N1	7.19	113.95	108.20
1	SA	9	G	O4'-C1'-N9	7.19	113.95	108.20
1	SA	1202	U	O4'-C1'-N1	7.19	113.95	108.20
25	LA	725	G	N1-C6-O6	7.19	124.21	119.90
25	LA	737	C	O4'-C1'-N1	7.18	113.95	108.20
25	LA	1085	A	C1'-O4'-C4'	-7.18	104.15	109.90
25	LA	1306	C	O4'-C1'-N1	7.18	113.95	108.20
25	LA	2595	G	O4'-C1'-N9	7.18	113.95	108.20
25	LA	750	A	C5'-C4'-C3'	-7.18	104.51	116.00
25	LA	1561	C	O4'-C1'-N1	7.18	113.94	108.20
25	LA	1726	C	O4'-C1'-N1	7.18	113.94	108.20
26	LB	66	A	P-O3'-C3'	7.17	128.31	119.70
1	SA	441	A	C5'-C4'-C3'	-7.17	104.53	116.00
1	SA	1188	A	C5'-C4'-C3'	7.17	127.47	116.00
1	SA	743	A	C5'-C4'-C3'	-7.17	104.53	116.00
1	SA	1463	U	O4'-C1'-N1	7.17	113.94	108.20
25	LA	1317	G	P-O3'-C3'	7.17	128.30	119.70
25	LA	1604	C	C6-N1-C2	-7.17	117.43	120.30
25	LA	55	G	O4'-C1'-N9	7.16	113.93	108.20
3	S7	60	U	O4'-C1'-N1	7.16	113.93	108.20
25	LA	323	C	O4'-C1'-N1	7.16	113.93	108.20
25	LA	1053	C	O4'-C1'-N1	7.16	113.93	108.20
25	LA	1613	G	C5-C6-O6	-7.16	124.31	128.60
25	LA	2578	G	O4'-C1'-N9	7.16	113.93	108.20
3	S7	62	C	O4'-C1'-N1	7.16	113.93	108.20
3	S7	17	C	C1'-O4'-C4'	-7.16	104.17	109.90
25	LA	2163	A	O4'-C1'-N9	7.15	113.92	108.20
25	LA	100	U	O4'-C1'-N1	7.15	113.92	108.20
25	LA	1747	U	O4'-C1'-N1	7.15	113.92	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1261	C	C6-N1-C2	-7.15	117.44	120.30
1	SA	436	C	O4'-C1'-N1	7.14	113.91	108.20
25	LA	2336	A	C1'-O4'-C4'	-7.14	104.19	109.90
25	LA	81	G	C5-C6-O6	-7.14	124.31	128.60
25	LA	321	U	P-O3'-C3'	-7.14	111.13	119.70
26	LB	64	G	O4'-C1'-N9	7.14	113.91	108.20
25	LA	1565	C	C5'-C4'-O4'	7.14	117.67	109.10
25	LA	2576	G	P-O3'-C3'	-7.14	111.13	119.70
25	LA	2540	C	O4'-C1'-N1	7.14	113.91	108.20
1	SA	1317	C	P-O3'-C3'	7.13	128.26	119.70
25	LA	1775	U	O4'-C1'-N1	7.13	113.91	108.20
6	SL	30	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	SA	632	U	P-O3'-C3'	-7.13	111.14	119.70
1	SA	632	U	C2-N1-C1'	7.13	126.25	117.70
25	LA	2189	U	O4'-C1'-N1	7.13	113.90	108.20
25	LA	1012	U	O4'-C4'-C3'	7.13	111.80	106.10
1	SA	924	C	O4'-C1'-N1	7.12	113.90	108.20
25	LA	1907	G	O4'-C1'-N9	7.12	113.90	108.20
25	LA	2044	C	O4'-C1'-N1	7.12	113.90	108.20
25	LA	275	C	O4'-C1'-N1	7.12	113.89	108.20
25	LA	1895	C	O4'-C1'-N1	7.12	113.89	108.20
25	LA	1869	G	O4'-C1'-N9	7.12	113.89	108.20
1	SA	1420	U	P-O3'-C3'	7.11	128.24	119.70
25	LA	896	A	P-O3'-C3'	7.11	128.24	119.70
25	LA	1012	U	P-O5'-C5'	-7.11	109.52	120.90
25	LA	2594	C	O4'-C1'-N1	7.11	113.89	108.20
1	SA	792	A	C1'-O4'-C4'	-7.11	104.21	109.90
1	SA	792	A	P-O5'-C5'	7.11	132.28	120.90
25	LA	61	C	P-O5'-C5'	7.11	132.28	120.90
5	SK	6	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	SA	475	C	O4'-C1'-N1	7.11	113.89	108.20
1	SA	991	U	O4'-C1'-N1	7.11	113.89	108.20
1	SA	1331	G	C4-N9-C1'	-7.11	117.26	126.50
25	LA	1765	U	O4'-C1'-N1	7.11	113.89	108.20
1	SA	948	C	O4'-C1'-N1	7.11	113.89	108.20
25	LA	805	G	N3-C2-N2	7.11	124.88	119.90
25	LA	1565	C	C5'-C4'-C3'	-7.11	104.63	116.00
25	LA	2367	G	C5-C6-O6	-7.11	124.34	128.60
25	LA	2702	G	O4'-C1'-N9	7.11	113.89	108.20
25	LA	2870	C	O4'-C1'-N1	7.11	113.89	108.20
1	SA	207	C	O4'-C1'-N1	7.11	113.89	108.20
1	SA	925	G	O4'-C1'-N9	7.11	113.89	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1532	U	P-O3'-C3'	-7.11	111.17	119.70
25	LA	2145	C	O4'-C1'-N1	7.10	113.88	108.20
1	SA	40	C	O4'-C1'-N1	7.10	113.88	108.20
1	SA	387	U	P-O3'-C3'	-7.10	111.18	119.70
1	SA	609	A	C5'-C4'-O4'	7.10	117.62	109.10
1	SA	1181	G	O4'-C1'-N9	7.10	113.88	108.20
1	SA	1255	G	O4'-C1'-N9	7.10	113.88	108.20
4	SJ	72	ARG	NE-CZ-NH2	-7.10	116.75	120.30
25	LA	2279	G	C5'-C4'-C3'	7.10	127.36	116.00
1	SA	252	U	C5'-C4'-C3'	-7.10	104.64	116.00
25	LA	726	G	O4'-C1'-N9	7.10	113.88	108.20
26	LB	28	C	O4'-C1'-N1	7.10	113.88	108.20
49	L7	91	ARG	NE-CZ-NH1	-7.10	116.75	120.30
25	LA	2445	G	C5-C6-N1	7.09	115.05	111.50
25	LA	1069	A	O4'-C1'-N9	7.09	113.87	108.20
25	LA	1512	C	O4'-C1'-N1	7.09	113.87	108.20
25	LA	2618	G	P-O5'-C5'	7.09	132.25	120.90
55	LI	16	ARG	NE-CZ-NH2	-7.09	116.75	120.30
5	SK	8	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	SA	1016	A	C5'-C4'-C3'	7.09	127.34	116.00
25	LA	1941	C	O4'-C1'-N1	7.09	113.87	108.20
25	LA	2424	C	O4'-C1'-N1	7.09	113.87	108.20
1	SA	1344	C	C2'-C3'-O3'	7.09	125.09	109.50
25	LA	314	C	O4'-C1'-N1	7.09	113.87	108.20
25	LA	2283	C	O4'-C1'-N1	7.09	113.87	108.20
25	LA	2420	C	C6-N1-C2	-7.08	117.47	120.30
25	LA	776	G	P-O3'-C3'	7.08	128.20	119.70
25	LA	1495	A	O4'-C1'-N9	7.08	113.87	108.20
25	LA	490	C	O4'-C1'-N1	7.08	113.86	108.20
25	LA	2293	G	C5'-C4'-C3'	-7.08	104.67	116.00
1	SA	1065	U	O4'-C1'-C2'	-7.08	98.72	105.80
25	LA	1241	A	P-O5'-C5'	7.08	132.22	120.90
25	LA	1376	C	C6-N1-C1'	7.08	129.29	120.80
3	S7	17	C	O4'-C1'-N1	7.08	113.86	108.20
25	LA	2355	G	P-O5'-C5'	7.08	132.22	120.90
25	LA	2858	C	O4'-C1'-N1	7.08	113.86	108.20
25	LA	1167	C	C4'-C3'-C2'	-7.07	95.53	102.60
25	LA	2615	U	O4'-C1'-N1	7.07	113.86	108.20
25	LA	411	G	C4-N9-C1'	7.07	135.69	126.50
1	SA	52	C	P-O3'-C3'	-7.07	111.22	119.70
25	LA	915	C	O4'-C1'-N1	7.07	113.85	108.20
25	LA	1778	U	C3'-C2'-C1'	7.07	107.16	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1402	U	O4'-C1'-N1	7.07	113.85	108.20
1	SA	701	U	P-O3'-C3'	-7.06	111.22	119.70
1	SA	974	A	C8-N9-C1'	7.06	140.41	127.70
1	SA	1317	C	O4'-C1'-N1	7.06	113.85	108.20
8	SN	12	ARG	NE-CZ-NH1	7.06	123.83	120.30
25	LA	1375	U	O4'-C1'-N1	7.06	113.85	108.20
25	LA	1806	C	O4'-C1'-N1	7.06	113.85	108.20
25	LA	2608	G	P-O3'-C3'	-7.06	111.23	119.70
1	SA	489	C	O4'-C1'-N1	7.06	113.85	108.20
29	LN	101	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	SA	106	C	O4'-C1'-N1	7.06	113.85	108.20
1	SA	981	U	C2-N1-C1'	7.06	126.17	117.70
25	LA	2416	C	O4'-C1'-N1	7.06	113.85	108.20
1	SA	458	U	O4'-C1'-N1	7.05	113.84	108.20
25	LA	2130	U	O4'-C1'-N1	7.05	113.84	108.20
25	LA	2060	A	O4'-C1'-N9	7.05	113.84	108.20
1	SA	46	G	C4'-C3'-C2'	-7.05	95.55	102.60
25	LA	16	C	O4'-C1'-N1	7.05	113.84	108.20
1	SA	197	A	P-O5'-C5'	-7.05	109.62	120.90
20	SF	78	PHE	CB-CG-CD2	-7.05	115.87	120.80
25	LA	952	G	C4'-C3'-C2'	-7.05	95.55	102.60
25	LA	2139	U	O4'-C1'-N1	7.05	113.84	108.20
25	LA	2549	G	P-O5'-C5'	7.05	132.18	120.90
25	LA	806	C	O4'-C1'-N1	7.05	113.84	108.20
25	LA	944	C	O4'-C1'-N1	7.05	113.84	108.20
25	LA	2402	U	C1'-O4'-C4'	-7.05	104.26	109.90
2	S6	26	C	O4'-C1'-N1	7.04	113.83	108.20
2	S6	45	A	O4'-C1'-N9	7.04	113.83	108.20
25	LA	232	G	C5'-C4'-C3'	-7.04	104.73	116.00
42	L1	12	ARG	NE-CZ-NH1	7.04	123.82	120.30
25	LA	2182	U	O4'-C1'-N1	7.04	113.83	108.20
25	LA	1612	C	O4'-C1'-N1	7.04	113.83	108.20
3	S7	71	G	P-O3'-C3'	7.04	128.15	119.70
25	LA	1774	C	C6-N1-C2	-7.04	117.48	120.30
25	LA	2157	G	O4'-C1'-N9	7.04	113.83	108.20
25	LA	1278	C	O4'-C1'-N1	7.03	113.83	108.20
25	LA	1850	G	P-O3'-C3'	-7.03	111.26	119.70
1	SA	204	G	C1'-O4'-C4'	-7.03	104.27	109.90
25	LA	2076	U	C2-N1-C1'	7.03	126.14	117.70
25	LA	2794	C	O4'-C1'-N1	7.03	113.83	108.20
2	S6	76	C	O4'-C1'-N1	7.03	113.82	108.20
1	SA	328	C	C1'-O4'-C4'	-7.03	104.28	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2070	A	P-O5'-C5'	-7.03	109.66	120.90
25	LA	2787	C	O4'-C1'-N1	7.03	113.82	108.20
25	LA	523	C	O4'-C1'-N1	7.02	113.82	108.20
25	LA	1135	C	O4'-C1'-N1	7.02	113.82	108.20
25	LA	2657	A	P-O5'-C5'	7.02	132.13	120.90
25	LA	986	C	O4'-C1'-N1	7.02	113.81	108.20
25	LA	1758	U	O4'-C1'-N1	7.02	113.81	108.20
25	LA	2023	C	O4'-C1'-N1	7.02	113.81	108.20
44	L3	33	ARG	NE-CZ-NH2	7.02	123.81	120.30
25	LA	470	A	N1-C6-N6	-7.01	114.39	118.60
1	SA	316	C	O4'-C1'-N1	7.01	113.81	108.20
1	SA	962	C	C2-N1-C1'	-7.01	111.09	118.80
1	SA	1523	G	C5-C6-O6	-7.01	124.39	128.60
25	LA	784	G	C1'-O4'-C4'	-7.01	104.29	109.90
25	LA	1814	G	O4'-C1'-N9	7.01	113.81	108.20
1	SA	457	G	O4'-C1'-N9	7.01	113.81	108.20
1	SA	927	G	C5'-C4'-C3'	7.01	127.21	116.00
1	SA	1225	A	O4'-C1'-N9	7.01	113.80	108.20
25	LA	1321	A	P-O5'-C5'	-7.00	109.69	120.90
25	LA	981	A	O4'-C1'-N9	7.00	113.80	108.20
25	LA	1644	C	O4'-C1'-N1	7.00	113.80	108.20
1	SA	588	G	O4'-C1'-N9	7.00	113.80	108.20
1	SA	835	U	O4'-C1'-N1	7.00	113.80	108.20
1	SA	1033	G	O4'-C1'-N9	7.00	113.80	108.20
25	LA	1057	A	O3'-P-O5'	-7.00	90.70	104.00
25	LA	728	G	P-O3'-C3'	-7.00	111.30	119.70
25	LA	1959	G	O4'-C1'-N9	7.00	113.80	108.20
49	L7	82	TYR	CB-CG-CD2	7.00	125.20	121.00
25	LA	2295	C	O4'-C1'-N1	6.99	113.80	108.20
25	LA	145	C	O4'-C1'-N1	6.99	113.79	108.20
25	LA	882	G	O4'-C1'-N9	6.99	113.79	108.20
25	LA	1323	C	C5'-C4'-O4'	6.99	117.49	109.10
39	LW	52	ARG	NE-CZ-NH1	-6.99	116.80	120.30
7	SM	22	TYR	CB-CG-CD2	6.99	125.19	121.00
25	LA	1863	G	P-O5'-C5'	6.99	132.08	120.90
25	LA	2445	G	O4'-C1'-C2'	6.99	113.89	107.60
1	SA	1524	C	O4'-C1'-N1	6.99	113.79	108.20
25	LA	740	C	C6-N1-C2	-6.99	117.50	120.30
25	LA	1518	C	O4'-C1'-N1	6.99	113.79	108.20
25	LA	2431	U	C5'-C4'-C3'	-6.99	104.82	116.00
25	LA	2619	C	O4'-C1'-N1	6.99	113.79	108.20
25	LA	2215	C	O4'-C1'-N1	6.99	113.79	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	982	C	C2-N1-C1'	6.99	126.48	118.80
25	LA	2251	G	P-O3'-C3'	-6.99	111.32	119.70
25	LA	753	A	C5'-C4'-O4'	6.98	117.48	109.10
1	SA	1109	C	O4'-C1'-N1	6.98	113.78	108.20
1	SA	1235	U	O4'-C1'-N1	6.98	113.78	108.20
25	LA	459	U	O4'-C1'-N1	6.98	113.78	108.20
25	LA	1002	G	O4'-C1'-N9	6.98	113.78	108.20
25	LA	1227	G	C5'-C4'-C3'	6.98	127.17	116.00
25	LA	937	C	O4'-C1'-N1	6.98	113.78	108.20
25	LA	1078	U	O4'-C1'-N1	6.98	113.78	108.20
49	L7	121	PHE	CB-CG-CD1	-6.98	115.92	120.80
1	SA	139	A	O4'-C1'-N9	6.97	113.78	108.20
25	LA	7	G	O4'-C1'-N9	6.97	113.78	108.20
25	LA	2175	C	C5'-C4'-C3'	6.97	127.16	116.00
1	SA	1133	G	O4'-C1'-N9	6.97	113.78	108.20
1	SA	1176	A	O4'-C1'-N9	6.97	113.78	108.20
1	SA	1513	A	N1-C6-N6	6.97	122.78	118.60
25	LA	2197	U	C5'-C4'-C3'	-6.97	104.84	116.00
1	SA	1020	G	O4'-C1'-N9	6.97	113.78	108.20
25	LA	1379	U	O4'-C1'-N1	6.97	113.78	108.20
25	LA	1680	U	O4'-C1'-N1	6.97	113.78	108.20
50	L8	93	TYR	CB-CG-CD1	6.97	125.18	121.00
1	SA	853	C	O4'-C1'-N1	6.97	113.78	108.20
25	LA	1167	C	C5'-C4'-C3'	-6.97	104.85	116.00
26	LB	113	C	P-O3'-C3'	6.97	128.06	119.70
3	S7	25	C	O4'-C1'-N1	6.96	113.77	108.20
2	S6	29	C	O4'-C1'-N1	6.96	113.77	108.20
21	SG	9	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	SA	1147	C	O4'-C1'-N1	6.96	113.77	108.20
1	SA	182	A	O4'-C1'-N9	6.95	113.76	108.20
1	SA	977	A	O4'-C1'-N9	6.95	113.76	108.20
1	SA	981	U	O4'-C1'-N1	6.95	113.76	108.20
25	LA	305	C	O4'-C1'-N1	6.95	113.76	108.20
25	LA	464	U	C2-N1-C1'	6.95	126.05	117.70
25	LA	1489	C	C6-N1-C2	-6.95	117.52	120.30
25	LA	815	C	O4'-C1'-N1	6.95	113.76	108.20
25	LA	1928	A	P-O3'-C3'	6.95	128.04	119.70
25	LA	1481	U	O4'-C1'-N1	6.95	113.76	108.20
25	LA	2472	G	C5-C6-O6	-6.95	124.43	128.60
8	SN	12	ARG	NE-CZ-NH2	-6.95	116.83	120.30
3	S7	62	C	C6-N1-C2	-6.95	117.52	120.30
1	SA	1253	G	O4'-C1'-N9	6.94	113.75	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2186	G	O4'-C1'-N9	6.94	113.75	108.20
25	LA	2773	C	O4'-C1'-N1	6.94	113.75	108.20
1	SA	1103	C	P-O5'-C5'	6.94	132.00	120.90
25	LA	435	C	O4'-C1'-N1	6.93	113.75	108.20
25	LA	2389	G	C5-C6-O6	-6.93	124.44	128.60
1	SA	586	C	O4'-C1'-N1	6.93	113.75	108.20
25	LA	2434	A	P-O3'-C3'	-6.93	111.38	119.70
1	SA	1256	A	O4'-C1'-N9	6.93	113.74	108.20
25	LA	2187	U	O4'-C1'-N1	6.93	113.74	108.20
1	SA	55	A	O4'-C1'-N9	6.93	113.74	108.20
1	SA	1158	C	C6-N1-C1'	-6.93	112.49	120.80
25	LA	1240	U	P-O3'-C3'	6.93	128.01	119.70
58	LZ	49	ARG	NE-CZ-NH2	-6.93	116.84	120.30
25	LA	817	C	O4'-C1'-N1	6.92	113.74	108.20
25	LA	1827	U	C2-N3-C4	-6.92	122.85	127.00
25	LA	1073	A	N1-C6-N6	-6.92	114.45	118.60
1	SA	1519	A	P-O3'-C3'	6.92	128.01	119.70
25	LA	1669	A	O4'-C1'-N9	6.92	113.74	108.20
25	LA	2324	U	C2-N3-C4	-6.92	122.85	127.00
25	LA	2704	C	O4'-C1'-N1	6.92	113.74	108.20
25	LA	2657	A	P-O3'-C3'	-6.92	111.40	119.70
25	LA	811	U	C2-N1-C1'	6.92	126.00	117.70
2	S6	74	A	P-O3'-C3'	6.92	128.00	119.70
25	LA	823	C	C6-N1-C2	-6.92	117.53	120.30
25	LA	1209	U	O4'-C1'-N1	6.92	113.73	108.20
25	LA	2382	G	C5'-C4'-O4'	6.92	117.40	109.10
1	SA	1369	C	O4'-C1'-N1	6.91	113.73	108.20
25	LA	1241	A	O4'-C1'-N9	6.91	113.73	108.20
1	SA	794	A	P-O5'-C5'	-6.91	109.84	120.90
25	LA	133	U	O4'-C1'-N1	6.91	113.73	108.20
25	LA	1006	C	O4'-C1'-N1	6.91	113.73	108.20
25	LA	2254	C	O4'-C1'-N1	6.91	113.73	108.20
25	LA	1146	C	O4'-C1'-N1	6.91	113.73	108.20
25	LA	2227	A	O4'-C1'-N9	6.91	113.73	108.20
1	SA	831	A	P-O3'-C3'	-6.91	111.41	119.70
1	SA	1037	C	O4'-C1'-N1	6.91	113.72	108.20
25	LA	2305	U	O4'-C1'-N1	6.91	113.72	108.20
1	SA	54	C	O4'-C1'-N1	6.90	113.72	108.20
3	S7	59	U	C2-N1-C1'	6.90	125.98	117.70
6	SL	13	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	SA	308	C	C2-N1-C1'	6.90	126.39	118.80
18	SD	55	ARG	NE-CZ-NH1	6.90	123.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	332	A	O4'-C1'-C2'	-6.90	98.90	105.80
25	LA	1170	C	O4'-C1'-N1	6.90	113.72	108.20
25	LA	1890	A	C5-C6-N6	6.90	129.22	123.70
1	SA	521	G	C5'-C4'-C3'	6.90	127.04	116.00
24	S1	637	ARG	NE-CZ-NH1	6.90	123.75	120.30
25	LA	1072	C	O4'-C1'-N1	6.90	113.72	108.20
1	SA	173	U	O4'-C1'-N1	6.90	113.72	108.20
1	SA	1417	G	C5'-C4'-C3'	-6.90	104.96	116.00
24	S1	100	ARG	NE-CZ-NH1	6.90	123.75	120.30
25	LA	23	G	C5'-C4'-C3'	6.90	127.04	116.00
25	LA	2248	C	P-O5'-C5'	-6.90	109.87	120.90
25	LA	1966	A	C4-N9-C1'	6.89	138.71	126.30
25	LA	2250	G	N1-C6-O6	6.89	124.04	119.90
25	LA	1744	A	O4'-C1'-N9	6.89	113.71	108.20
25	LA	1943	U	C2-N1-C1'	6.89	125.97	117.70
1	SA	1312	G	O4'-C1'-N9	6.89	113.71	108.20
25	LA	163	C	O4'-C1'-N1	6.89	113.71	108.20
25	LA	2658	C	O4'-C1'-N1	6.89	113.71	108.20
1	SA	564	C	O4'-C1'-N1	6.89	113.71	108.20
25	LA	1224	U	O4'-C1'-N1	6.89	113.71	108.20
25	LA	2841	C	O4'-C1'-N1	6.89	113.71	108.20
1	SA	814	A	C4-N9-C1'	6.89	138.69	126.30
17	SC	64	ARG	NE-CZ-NH2	-6.89	116.86	120.30
25	LA	1229	C	O4'-C1'-N1	6.89	113.71	108.20
25	LA	1999	C	O4'-C1'-N1	6.89	113.71	108.20
25	LA	2326	C	O4'-C1'-N1	6.89	113.71	108.20
25	LA	2486	C	P-O5'-C5'	6.89	131.92	120.90
25	LA	1257	C	P-O5'-C5'	6.88	131.92	120.90
25	LA	2745	C	O4'-C1'-N1	6.88	113.71	108.20
25	LA	2143	C	O4'-C1'-N1	6.88	113.71	108.20
1	SA	1206	G	P-O5'-C5'	6.88	131.91	120.90
1	SA	1262	C	O4'-C1'-N1	6.88	113.70	108.20
25	LA	2106	U	O4'-C1'-N1	6.88	113.71	108.20
25	LA	1762	A	O4'-C1'-N9	6.88	113.70	108.20
25	LA	2817	U	O4'-C1'-N1	6.88	113.70	108.20
1	SA	490	C	O4'-C1'-N1	6.88	113.70	108.20
25	LA	1568	G	O4'-C1'-N9	6.88	113.70	108.20
57	LK	30	ARG	NE-CZ-NH1	6.88	123.74	120.30
25	LA	27	G	C5'-C4'-C3'	6.87	127.00	116.00
25	LA	835	C	O4'-C1'-N1	6.87	113.70	108.20
25	LA	1015	U	O4'-C1'-N1	6.87	113.70	108.20
25	LA	1881	C	O4'-C1'-N1	6.87	113.70	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	684	G	C5'-C4'-C3'	6.87	126.99	116.00
25	LA	752	A	C3'-C2'-C1'	-6.87	96.00	101.50
25	LA	1527	G	P-O5'-C5'	6.87	131.89	120.90
25	LA	1846	G	C5'-C4'-C3'	-6.87	105.01	116.00
25	LA	1191	G	O4'-C1'-N9	6.87	113.69	108.20
26	LB	1	U	C2-N1-C1'	6.87	125.94	117.70
1	SA	1	A	O4'-C1'-N9	6.86	113.69	108.20
1	SA	385	C	O4'-C1'-N1	6.86	113.69	108.20
1	SA	1158	C	C6-N1-C2	-6.86	117.55	120.30
25	LA	854	C	O4'-C1'-N1	6.86	113.69	108.20
25	LA	855	G	O4'-C1'-N9	6.86	113.69	108.20
25	LA	1092	C	O4'-C1'-N1	6.86	113.69	108.20
25	LA	2486	C	C4'-C3'-C2'	-6.86	95.74	102.60
1	SA	1284	C	O4'-C1'-N1	6.86	113.69	108.20
25	LA	568	U	C6-N1-C1'	-6.86	111.59	121.20
25	LA	2131	U	O4'-C1'-N1	6.86	113.69	108.20
1	SA	1084	G	C8-N9-C1'	6.86	135.91	127.00
1	SA	801	U	O4'-C1'-N1	6.86	113.69	108.20
1	SA	1038	C	O4'-C1'-N1	6.86	113.68	108.20
1	SA	1278	G	O4'-C1'-C2'	6.86	113.77	107.60
1	SA	388	G	N1-C6-O6	6.85	124.01	119.90
25	LA	1404	C	O4'-C1'-N1	6.85	113.68	108.20
25	LA	1649	G	O4'-C1'-N9	6.85	113.68	108.20
1	SA	375	U	O4'-C1'-N1	6.85	113.68	108.20
3	S7	7	A	P-O3'-C3'	6.85	127.92	119.70
25	LA	759	G	C5'-C4'-C3'	-6.85	105.05	116.00
1	SA	714	G	O4'-C1'-N9	6.85	113.68	108.20
25	LA	682	G	C5'-C4'-C3'	6.84	126.95	116.00
25	LA	2250	G	C5-C6-O6	-6.84	124.49	128.60
3	S7	70	G	O4'-C1'-N9	6.84	113.67	108.20
25	LA	700	G	O4'-C1'-N9	6.84	113.67	108.20
25	LA	525	U	O4'-C1'-N1	6.84	113.67	108.20
25	LA	2275	C	C6-N1-C2	-6.84	117.56	120.30
25	LA	2682	A	C4'-C3'-C2'	-6.83	95.77	102.60
25	LA	651	G	C4'-C3'-C2'	-6.83	95.77	102.60
25	LA	2219	U	O4'-C1'-N1	6.83	113.67	108.20
24	S1	548	TYR	CB-CG-CD2	-6.83	116.90	121.00
25	LA	932	U	C2-N1-C1'	6.83	125.90	117.70
25	LA	1020	A	O4'-C1'-N9	6.83	113.66	108.20
26	LB	78	A	N1-C6-N6	-6.83	114.50	118.60
1	SA	927	G	O4'-C1'-N9	6.83	113.66	108.20
25	LA	2453	A	P-O5'-C5'	-6.83	109.97	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2656	U	C5'-C4'-C3'	-6.83	105.08	116.00
1	SA	1249	C	P-O5'-C5'	6.83	131.82	120.90
1	SA	1344	C	O3'-P-O5'	6.83	116.97	104.00
1	SA	770	C	O4'-C1'-N1	6.83	113.66	108.20
12	SR	60	ARG	NE-CZ-NH1	6.83	123.71	120.30
56	LJ	8	ARG	NE-CZ-NH1	6.83	123.71	120.30
4	SJ	16	ARG	NE-CZ-NH1	6.82	123.71	120.30
25	LA	1574	C	O4'-C1'-N1	6.82	113.66	108.20
25	LA	1759	A	O4'-C1'-N9	6.82	113.66	108.20
1	SA	762	U	O4'-C1'-N1	6.82	113.66	108.20
25	LA	1909	C	O4'-C1'-N1	6.82	113.66	108.20
3	S7	61	C	C5'-C4'-C3'	-6.82	105.09	116.00
25	LA	2646	C	O4'-C1'-N1	6.82	113.65	108.20
25	LA	779	U	O4'-C1'-N1	6.82	113.65	108.20
25	LA	1322	A	P-O3'-C3'	6.82	127.88	119.70
1	SA	1399	C	O4'-C1'-N1	6.81	113.65	108.20
13	SS	35	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	SA	51	A	C8-N9-C1'	-6.81	115.44	127.70
25	LA	1879	C	O4'-C1'-N1	6.81	113.65	108.20
25	LA	2662	A	P-O5'-C5'	6.81	131.80	120.90
29	LN	269	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	SA	193	C	O4'-C1'-N1	6.81	113.65	108.20
1	SA	463	U	O4'-C1'-N1	6.81	113.65	108.20
1	SA	439	U	O4'-C1'-N1	6.81	113.65	108.20
44	L3	3	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	SA	1303	C	O4'-C1'-N1	6.81	113.64	108.20
25	LA	372	G	P-O3'-C3'	6.81	127.87	119.70
25	LA	1327	A	P-O3'-C3'	6.81	127.87	119.70
25	LA	550	C	O4'-C1'-N1	6.81	113.64	108.20
1	SA	740	U	P-O5'-C5'	6.80	131.79	120.90
25	LA	859	G	O4'-C1'-N9	6.80	113.64	108.20
25	LA	1781	U	C5'-C4'-O4'	6.80	117.27	109.10
25	LA	2379	G	O4'-C1'-N9	6.80	113.64	108.20
35	LT	79	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	SA	401	C	O4'-C1'-N1	6.80	113.64	108.20
57	LK	36	TYR	CB-CG-CD1	-6.80	116.92	121.00
25	LA	2716	C	O4'-C1'-N1	6.80	113.64	108.20
25	LA	545	U	P-O3'-C3'	6.80	127.86	119.70
30	LO	23	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	SA	705	G	N1-C6-O6	6.79	123.98	119.90
1	SA	823	C	O4'-C1'-N1	6.79	113.64	108.20
25	LA	1898	U	O4'-C1'-N1	6.79	113.63	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	967	C	O4'-C1'-N1	6.79	113.63	108.20
18	SD	62	ARG	NE-CZ-NH1	6.79	123.69	120.30
25	LA	1153	C	O4'-C1'-N1	6.79	113.63	108.20
25	LA	1407	G	O4'-C1'-N9	6.79	113.63	108.20
1	SA	730	G	N3-C2-N2	6.79	124.65	119.90
26	LB	60	C	O4'-C1'-N1	6.79	113.63	108.20
26	LB	88	C	O4'-C1'-N1	6.79	113.63	108.20
1	SA	1175	G	O4'-C1'-N9	6.79	113.63	108.20
1	SA	1419	G	C5-C6-O6	-6.79	124.53	128.60
1	SA	17	U	O4'-C1'-N1	6.79	113.63	108.20
1	SA	1182	G	P-O3'-C3'	6.79	127.84	119.70
1	SA	1352	C	O4'-C1'-N1	6.79	113.63	108.20
1	SA	605	U	O4'-C1'-N1	6.78	113.63	108.20
1	SA	1187	G	O4'-C1'-N9	6.78	113.63	108.20
25	LA	1070	A	C4'-C3'-C2'	-6.78	95.82	102.60
25	LA	1370	C	O4'-C1'-N1	6.78	113.63	108.20
25	LA	45	G	O4'-C1'-N9	6.78	113.62	108.20
25	LA	1007	C	O4'-C1'-N1	6.78	113.62	108.20
25	LA	1822	C	C6-N1-C2	-6.78	117.59	120.30
25	LA	1995	U	O4'-C1'-N1	6.78	113.62	108.20
25	LA	989	G	C5-C6-O6	-6.78	124.53	128.60
1	SA	154	U	P-O5'-C5'	6.78	131.75	120.90
10	SP	28	ARG	NE-CZ-NH1	6.78	123.69	120.30
25	LA	982	C	O4'-C1'-N1	6.78	113.62	108.20
25	LA	1149	G	O4'-C1'-N9	6.78	113.62	108.20
1	SA	880	C	O4'-C1'-N1	6.78	113.62	108.20
25	LA	1951	U	O4'-C1'-N1	6.78	113.62	108.20
25	LA	2737	G	O4'-C1'-N9	6.78	113.62	108.20
54	LH	59	ARG	NE-CZ-NH2	-6.78	116.91	120.30
25	LA	292	U	P-O3'-C3'	6.77	127.83	119.70
1	SA	1373	G	C5-C6-O6	-6.77	124.54	128.60
25	LA	52	A	P-O3'-C3'	6.77	127.82	119.70
25	LA	276	U	O4'-C1'-N1	6.77	113.62	108.20
25	LA	97	C	O4'-C1'-N1	6.77	113.61	108.20
25	LA	601	C	O4'-C1'-N1	6.77	113.61	108.20
25	LA	2427	C	O5'-C5'-C4'	6.77	124.56	111.70
3	S7	16	U	P-O3'-C3'	6.77	127.82	119.70
1	SA	286	C	O4'-C1'-N1	6.76	113.61	108.20
3	S7	38	A	O4'-C1'-N9	6.76	113.61	108.20
25	LA	2084	C	O4'-C1'-N1	6.76	113.61	108.20
1	SA	468	A	P-O5'-C5'	6.76	131.72	120.90
1	SA	1103	C	O4'-C1'-N1	6.76	113.61	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	753	A	P-O5'-C5'	-6.76	110.08	120.90
1	SA	329	A	O4'-C1'-N9	6.76	113.61	108.20
1	SA	1084	G	C4-N9-C1'	-6.76	117.71	126.50
1	SA	196	A	O4'-C1'-N9	6.76	113.61	108.20
1	SA	475	C	P-O5'-C5'	6.76	131.71	120.90
1	SA	831	A	C4'-C3'-C2'	-6.76	95.84	102.60
1	SA	1230	C	O4'-C1'-N1	6.76	113.61	108.20
25	LA	2902	C	C5'-C4'-C3'	6.76	126.81	116.00
1	SA	733	G	C1'-O4'-C4'	-6.76	104.50	109.90
25	LA	208	C	O4'-C1'-N1	6.76	113.61	108.20
25	LA	2297	A	N1-C6-N6	-6.76	114.55	118.60
25	LA	302	C	O4'-C1'-N1	6.75	113.60	108.20
25	LA	2206	C	O4'-C1'-N1	6.75	113.60	108.20
6	SL	49	ARG	NE-CZ-NH1	6.75	123.68	120.30
14	SB	212	TYR	CB-CG-CD2	6.75	125.05	121.00
1	SA	710	G	O4'-C1'-N9	6.75	113.60	108.20
1	SA	1270	G	C5-C6-O6	-6.75	124.55	128.60
2	S6	74	A	O3'-P-O5'	-6.75	91.18	104.00
25	LA	793	A	O4'-C1'-N9	6.75	113.60	108.20
25	LA	1243	C	O4'-C1'-N1	6.75	113.60	108.20
26	LB	94	A	O4'-C1'-N9	6.75	113.60	108.20
25	LA	1795	C	C6-N1-C2	-6.74	117.60	120.30
25	LA	1843	C	O4'-C1'-N1	6.74	113.59	108.20
37	LV	27	ARG	NE-CZ-NH1	6.74	123.67	120.30
25	LA	1862	G	O4'-C1'-N9	6.74	113.59	108.20
25	LA	2032	G	P-O3'-C3'	6.74	127.79	119.70
1	SA	1152	A	O4'-C1'-N9	6.74	113.59	108.20
25	LA	238	C	O4'-C1'-N1	6.74	113.59	108.20
25	LA	1044	C	P-O5'-C5'	-6.74	110.12	120.90
25	LA	2618	G	O4'-C1'-N9	6.74	113.59	108.20
1	SA	266	G	O4'-C1'-N9	6.74	113.59	108.20
1	SA	737	C	O4'-C1'-N1	6.74	113.59	108.20
31	LP	79	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	SA	123	U	P-O3'-C3'	6.74	127.78	119.70
24	S1	636	ARG	NE-CZ-NH1	6.74	123.67	120.30
25	LA	80	G	O4'-C1'-N9	6.73	113.58	108.20
25	LA	2524	G	O4'-C1'-N9	6.73	113.59	108.20
50	L8	57	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	SA	1347	G	O4'-C1'-N9	6.73	113.58	108.20
25	LA	1075	C	O4'-C1'-N1	6.73	113.58	108.20
1	SA	516	U	C6-N1-C2	-6.73	116.96	121.00
1	SA	215	C	O4'-C1'-N1	6.73	113.58	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S6	63	C	O4'-C1'-N1	6.73	113.58	108.20
1	SA	840	C	O4'-C1'-N1	6.73	113.58	108.20
3	S7	53	G	N1-C6-O6	6.73	123.94	119.90
25	LA	451	U	C1'-O4'-C4'	-6.73	104.52	109.90
25	LA	2017	U	P-O3'-C3'	6.73	127.77	119.70
1	SA	1374	A	O4'-C1'-N9	6.72	113.58	108.20
25	LA	1873	G	O4'-C1'-N9	6.72	113.58	108.20
25	LA	1385	A	O4'-C1'-N9	6.72	113.58	108.20
1	SA	776	G	N1-C6-O6	6.72	123.93	119.90
25	LA	698	C	O4'-C1'-N1	6.72	113.58	108.20
25	LA	880	G	O4'-C1'-N9	6.72	113.58	108.20
1	SA	765	G	C5'-C4'-O4'	6.72	117.16	109.10
25	LA	2682	A	O4'-C1'-N9	6.72	113.58	108.20
25	LA	205	G	O4'-C1'-N9	6.72	113.57	108.20
1	SA	1373	G	N1-C6-O6	6.72	123.93	119.90
10	SP	35	ARG	NE-CZ-NH1	6.72	123.66	120.30
25	LA	2313	C	O4'-C1'-N1	6.72	113.57	108.20
1	SA	518	C	O4'-C1'-N1	6.71	113.57	108.20
1	SA	1342	C	P-O5'-C5'	6.71	131.64	120.90
25	LA	1964	G	P-O3'-C3'	-6.71	111.64	119.70
1	SA	1201	A	C8-N9-C1'	-6.71	115.62	127.70
33	LR	3	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	SA	1055	A	N1-C6-N6	-6.71	114.57	118.60
25	LA	2086	U	P-O5'-C5'	6.71	131.64	120.90
1	SA	556	C	O4'-C1'-N1	6.71	113.57	108.20
1	SA	1419	G	C5'-C4'-C3'	6.71	126.73	116.00
1	SA	522	C	C5'-C4'-C3'	-6.71	105.27	116.00
25	LA	1828	G	O4'-C1'-N9	6.71	113.56	108.20
1	SA	307	C	O4'-C1'-N1	6.70	113.56	108.20
1	SA	437	U	O4'-C1'-N1	6.70	113.56	108.20
1	SA	1035	A	O4'-C1'-N9	6.70	113.56	108.20
25	LA	2220	U	O4'-C1'-N1	6.70	113.56	108.20
1	SA	422	C	O4'-C1'-N1	6.70	113.56	108.20
1	SA	833	G	P-O5'-C5'	-6.70	110.18	120.90
1	SA	1530	G	P-O3'-C3'	-6.70	111.66	119.70
25	LA	2226	C	O4'-C1'-N1	6.70	113.56	108.20
3	S7	47	U	P-O3'-C3'	-6.69	111.67	119.70
1	SA	356	A	O4'-C1'-N9	6.69	113.55	108.20
18	SD	183	ARG	NE-CZ-NH1	6.69	123.65	120.30
25	LA	1550	C	O4'-C1'-N1	6.69	113.55	108.20
25	LA	1643	G	O4'-C1'-N9	6.69	113.56	108.20
25	LA	2022	U	O4'-C1'-N1	6.69	113.55	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1053	G	O4'-C1'-N9	6.69	113.55	108.20
25	LA	503	A	P-O3'-C3'	6.69	127.73	119.70
25	LA	2170	A	O4'-C1'-N9	6.69	113.55	108.20
1	SA	260	G	P-O5'-C5'	6.68	131.60	120.90
25	LA	2698	U	O4'-C1'-N1	6.68	113.55	108.20
1	SA	1344	C	C6-N1-C2	-6.68	117.63	120.30
25	LA	1617	C	O4'-C1'-N1	6.68	113.55	108.20
25	LA	2657	A	N1-C6-N6	-6.68	114.59	118.60
1	SA	517	G	P-O5'-C5'	-6.68	110.21	120.90
25	LA	543	G	P-O3'-C3'	6.68	127.72	119.70
25	LA	1118	C	O4'-C1'-N1	6.68	113.54	108.20
1	SA	100	G	O4'-C1'-N9	6.68	113.54	108.20
25	LA	2006	C	O4'-C1'-N1	6.68	113.54	108.20
1	SA	870	U	P-O5'-C5'	6.68	131.58	120.90
1	SA	1046	A	O4'-C1'-N9	6.68	113.54	108.20
25	LA	1160	G	C5'-C4'-C3'	-6.68	105.32	116.00
1	SA	361	G	O4'-C1'-N9	6.67	113.54	108.20
2	S6	28	U	C5'-C4'-C3'	-6.67	105.32	116.00
1	SA	735	C	O4'-C1'-N1	6.67	113.54	108.20
1	SA	1509	C	C6-N1-C2	-6.67	117.63	120.30
25	LA	2180	U	O4'-C1'-N1	6.67	113.54	108.20
25	LA	71	A	O4'-C1'-N9	6.67	113.54	108.20
25	LA	818	G	N1-C6-O6	6.67	123.90	119.90
25	LA	2797	U	P-O3'-C3'	6.67	127.70	119.70
1	SA	862	C	O4'-C1'-N1	6.67	113.53	108.20
25	LA	16	C	C5'-C4'-C3'	-6.67	105.33	116.00
25	LA	2728	U	C5'-C4'-C3'	6.67	126.67	116.00
1	SA	1370	G	O4'-C1'-N9	6.67	113.53	108.20
25	LA	1805	A	O4'-C1'-N9	6.67	113.53	108.20
57	LK	9	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	SA	582	C	P-O3'-C3'	6.66	127.70	119.70
25	LA	1011	G	O4'-C1'-N9	6.66	113.53	108.20
25	LA	1633	G	P-O3'-C3'	6.66	127.69	119.70
25	LA	816	C	O4'-C1'-N1	6.66	113.53	108.20
25	LA	1950	G	P-O5'-C5'	6.66	131.56	120.90
1	SA	19	A	C5'-C4'-C3'	6.66	126.65	116.00
2	S6	67	C	O4'-C1'-N1	6.66	113.53	108.20
7	SM	97	ARG	NE-CZ-NH2	-6.66	116.97	120.30
25	LA	624	C	O4'-C1'-N1	6.66	113.53	108.20
25	LA	2391	G	O4'-C1'-N9	6.66	113.53	108.20
1	SA	128	G	O4'-C1'-N9	6.66	113.53	108.20
27	LC	53	ARG	NE-CZ-NH1	6.66	123.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	LX	59	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	SA	275	G	C5'-C4'-O4'	6.65	117.08	109.10
53	LG	98	ARG	NE-CZ-NH1	6.65	123.63	120.30
25	LA	1613	G	N1-C6-O6	6.65	123.89	119.90
25	LA	513	A	P-O5'-C5'	-6.65	110.26	120.90
25	LA	1098	A	N1-C6-N6	6.65	122.59	118.60
49	L7	149	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	SA	1322	C	C6-N1-C1'	-6.65	112.82	120.80
25	LA	105	C	C5'-C4'-C3'	-6.64	105.37	116.00
1	SA	638	U	O4'-C1'-N1	6.64	113.51	108.20
1	SA	992	U	P-O5'-C5'	-6.64	110.27	120.90
25	LA	2285	C	C6-N1-C2	-6.64	117.64	120.30
25	LA	873	C	O4'-C1'-N1	6.64	113.51	108.20
48	LE	126	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	SA	1448	C	O4'-C1'-N1	6.64	113.51	108.20
25	LA	591	U	O4'-C1'-N1	6.64	113.51	108.20
1	SA	46	G	C5-C6-O6	-6.64	124.62	128.60
1	SA	155	A	O4'-C1'-N9	6.64	113.51	108.20
1	SA	993	G	C4-N9-C1'	6.63	135.12	126.50
25	LA	1340	U	O4'-C1'-N1	6.63	113.51	108.20
25	LA	1911	U	C2-N3-C4	-6.63	123.02	127.00
1	SA	1325	C	O4'-C1'-N1	6.63	113.51	108.20
1	SA	1201	A	C2'-C3'-O3'	6.63	124.31	113.70
25	LA	2271	G	OP1-P-OP2	-6.63	109.65	119.60
1	SA	1118	U	C5'-C4'-C3'	-6.63	105.39	116.00
1	SA	1279	G	C5'-C4'-C3'	-6.63	105.39	116.00
25	LA	646	U	C1'-O4'-C4'	-6.63	104.60	109.90
25	LA	2029	G	C5-C6-O6	-6.63	124.62	128.60
25	LA	489	G	C5-C6-O6	-6.63	124.62	128.60
25	LA	2116	G	C8-N9-C1'	-6.63	118.39	127.00
1	SA	1449	C	O4'-C1'-N1	6.62	113.50	108.20
25	LA	1565	C	P-O5'-C5'	6.62	131.50	120.90
1	SA	28	A	O4'-C1'-N9	6.62	113.50	108.20
1	SA	1432	G	O4'-C1'-N9	6.62	113.50	108.20
25	LA	1379	U	P-O5'-C5'	6.62	131.49	120.90
25	LA	585	G	N1-C6-O6	6.62	123.87	119.90
25	LA	1489	C	C5'-C4'-C3'	-6.62	105.41	116.00
25	LA	1691	C	C5'-C4'-C3'	6.62	126.59	116.00
33	LR	69	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	SA	961	U	O5'-P-OP1	-6.62	99.75	105.70
1	SA	1358	U	O4'-C1'-N1	6.62	113.49	108.20
1	SA	1493	A	P-O3'-C3'	-6.62	111.76	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2349	G	C5-C6-O6	-6.62	124.63	128.60
25	LA	345	A	O4'-C1'-N9	6.61	113.49	108.20
25	LA	921	C	O4'-C1'-N1	6.61	113.49	108.20
25	LA	1253	A	O4'-C1'-N9	6.61	113.49	108.20
1	SA	1460	C	P-O5'-C5'	6.61	131.48	120.90
2	S6	3	C	O4'-C1'-N1	6.61	113.49	108.20
25	LA	137	U	O4'-C1'-N1	6.61	113.49	108.20
3	S7	13	C	C5'-C4'-C3'	-6.61	105.42	116.00
25	LA	2691	C	P-O3'-C3'	-6.61	111.77	119.70
25	LA	1345	C	O4'-C1'-N1	6.61	113.49	108.20
25	LA	1958	C	O4'-C1'-N1	6.61	113.49	108.20
25	LA	2617	U	O4'-C1'-N1	6.61	113.49	108.20
25	LA	2785	C	O4'-C1'-N1	6.61	113.49	108.20
25	LA	2791	G	P-O3'-C3'	-6.61	111.77	119.70
55	LI	81	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	SA	100	G	C5-C6-O6	-6.61	124.64	128.60
25	LA	1315	C	O4'-C1'-N1	6.61	113.48	108.20
25	LA	2071	A	C5'-C4'-C3'	-6.60	105.43	116.00
25	LA	2730	C	O4'-C1'-N1	6.60	113.48	108.20
2	S6	22	A	O4'-C1'-N9	6.60	113.48	108.20
25	LA	1301	A	O4'-C1'-N9	6.60	113.48	108.20
25	LA	1892	C	O4'-C1'-N1	6.60	113.48	108.20
25	LA	2609	U	C3'-C2'-C1'	-6.60	96.22	101.50
25	LA	1291	C	O4'-C1'-N1	6.60	113.48	108.20
25	LA	2362	C	C6-N1-C2	-6.60	117.66	120.30
25	LA	2874	C	O4'-C1'-N1	6.60	113.48	108.20
25	LA	820	A	O4'-C1'-N9	6.59	113.48	108.20
25	LA	976	G	C5'-C4'-C3'	-6.59	105.45	116.00
25	LA	1896	G	C5'-C4'-C3'	6.59	126.55	116.00
25	LA	2179	C	C6-N1-C2	-6.59	117.66	120.30
45	L4	44	ARG	NE-CZ-NH1	6.59	123.60	120.30
25	LA	1863	G	O4'-C1'-N9	6.59	113.47	108.20
25	LA	2521	C	C6-N1-C1'	6.59	128.71	120.80
1	SA	96	U	O4'-C1'-N1	6.59	113.47	108.20
25	LA	269	C	O4'-C1'-N1	6.59	113.47	108.20
25	LA	306	U	O4'-C1'-N1	6.59	113.47	108.20
25	LA	2096	C	O4'-C1'-N1	6.59	113.47	108.20
1	SA	888	G	C5'-C4'-C3'	-6.59	105.46	116.00
25	LA	441	U	O4'-C1'-N1	6.59	113.47	108.20
25	LA	1779	U	P-O5'-C5'	6.59	131.44	120.90
25	LA	2425	A	O4'-C1'-N9	6.59	113.47	108.20
25	LA	1515	A	O4'-C1'-N9	6.58	113.47	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1538	G	O4'-C1'-N9	6.58	113.47	108.20
25	LA	2605	U	O4'-C1'-N1	6.58	113.47	108.20
1	SA	986	U	O4'-C1'-N1	6.58	113.47	108.20
25	LA	1600	C	O4'-C1'-N1	6.58	113.47	108.20
25	LA	527	C	C6-N1-C1'	-6.58	112.90	120.80
2	S6	22	A	P-O5'-C5'	6.58	131.43	120.90
1	SA	177	G	C4-N9-C1'	6.58	135.05	126.50
1	SA	328	C	C2-N1-C1'	6.58	126.04	118.80
1	SA	1513	A	C5-C6-N6	-6.58	118.44	123.70
25	LA	229	C	C4'-C3'-C2'	-6.58	96.02	102.60
25	LA	767	U	C6-N1-C2	-6.58	117.05	121.00
25	LA	1889	A	P-O5'-C5'	6.58	131.43	120.90
25	LA	2321	U	O4'-C1'-N1	6.58	113.46	108.20
25	LA	1437	C	O4'-C1'-N1	6.58	113.46	108.20
1	SA	272	C	C5'-C4'-C3'	6.58	126.52	116.00
1	SA	1228	C	O4'-C1'-N1	6.58	113.46	108.20
1	SA	1245	C	O4'-C1'-N1	6.58	113.46	108.20
25	LA	264	C	O4'-C1'-N1	6.58	113.46	108.20
25	LA	596	U	O4'-C1'-N1	6.58	113.46	108.20
26	LB	22	U	O4'-C1'-N1	6.58	113.46	108.20
25	LA	225	C	O4'-C1'-N1	6.57	113.46	108.20
25	LA	1967	C	C2-N1-C1'	6.57	126.03	118.80
1	SA	812	G	O4'-C1'-N9	6.57	113.46	108.20
2	S6	24	C	O4'-C1'-N1	6.57	113.46	108.20
25	LA	493	G	O4'-C1'-N9	6.57	113.46	108.20
1	SA	1122	U	O4'-C1'-N1	6.57	113.45	108.20
25	LA	1539	U	O4'-C1'-N1	6.57	113.45	108.20
25	LA	2447	G	P-O3'-C3'	6.57	127.58	119.70
25	LA	354	A	O4'-C1'-N9	6.57	113.45	108.20
1	SA	693	G	C1'-O4'-C4'	-6.57	104.65	109.90
1	SA	703	G	O4'-C1'-N9	6.57	113.45	108.20
25	LA	2132	U	P-O3'-C3'	6.57	127.58	119.70
25	LA	2568	U	O4'-C1'-N1	6.57	113.45	108.20
25	LA	2723	C	O4'-C1'-N1	6.57	113.45	108.20
1	SA	25	C	C5'-C4'-O4'	6.56	116.97	109.10
1	SA	347	G	C5-C6-O6	-6.56	124.66	128.60
1	SA	472	U	O4'-C1'-N1	6.56	113.45	108.20
1	SA	965	U	O4'-C1'-N1	6.56	113.45	108.20
25	LA	154	U	P-O3'-C3'	6.56	127.57	119.70
25	LA	2473	U	C2-N1-C1'	6.56	125.57	117.70
25	LA	2551	C	O4'-C1'-N1	6.56	113.45	108.20
1	SA	609	A	C5-C6-N6	-6.56	118.45	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2032	G	O4'-C1'-N9	6.56	113.45	108.20
25	LA	2485	G	C5'-C4'-C3'	6.56	126.49	116.00
1	SA	212	G	C5-C6-O6	-6.56	124.67	128.60
25	LA	647	G	N9-C1'-C2'	-6.55	104.79	112.00
25	LA	1164	C	O4'-C1'-N1	6.55	113.44	108.20
25	LA	1358	G	C5-C6-O6	-6.55	124.67	128.60
25	LA	2538	C	C6-N1-C2	-6.55	117.68	120.30
28	LM	19	PHE	CB-CG-CD1	6.55	125.39	120.80
1	SA	177	G	C8-N9-C1'	-6.55	118.48	127.00
1	SA	233	C	O4'-C1'-N1	6.55	113.44	108.20
25	LA	1021	A	C5'-C4'-C3'	-6.55	105.52	116.00
25	LA	2213	U	O4'-C1'-N1	6.55	113.44	108.20
25	LA	2174	C	O4'-C1'-N1	6.55	113.44	108.20
25	LA	2512	C	O4'-C1'-N1	6.55	113.44	108.20
25	LA	2590	A	O4'-C1'-N9	6.55	113.44	108.20
24	S1	471	ARG	NE-CZ-NH1	6.55	123.57	120.30
25	LA	1812	U	O4'-C1'-N1	6.55	113.44	108.20
1	SA	212	G	O4'-C1'-N9	6.54	113.44	108.20
1	SA	394	G	C5-C6-O6	-6.54	124.67	128.60
18	SD	164	ARG	NE-CZ-NH2	-6.54	117.03	120.30
25	LA	2030	C	O4'-C1'-N1	6.54	113.43	108.20
25	LA	2649	C	O4'-C1'-N1	6.54	113.43	108.20
25	LA	2780	G	O4'-C1'-N9	6.54	113.44	108.20
25	LA	533	G	O4'-C1'-N9	6.54	113.43	108.20
25	LA	68	G	O4'-C1'-N9	6.54	113.43	108.20
25	LA	2111	U	C5'-C4'-O4'	6.54	116.95	109.10
1	SA	471	U	O4'-C1'-N1	6.54	113.43	108.20
22	SH	12	ARG	NE-CZ-NH1	6.54	123.57	120.30
25	LA	32	C	O4'-C1'-N1	6.54	113.43	108.20
25	LA	870	U	C5'-C4'-O4'	6.54	116.95	109.10
25	LA	2602	A	C5'-C4'-O4'	6.54	116.95	109.10
25	LA	2765	A	C5'-C4'-O4'	6.54	116.94	109.10
40	LX	59	ARG	NE-CZ-NH2	6.54	123.57	120.30
25	LA	411	G	C8-N9-C1'	-6.54	118.50	127.00
25	LA	895	U	C5'-C4'-O4'	6.54	116.94	109.10
25	LA	1611	C	O4'-C1'-N1	6.54	113.43	108.20
3	S7	3	C	O4'-C1'-N1	6.53	113.43	108.20
25	LA	1158	C	O4'-C1'-N1	6.53	113.43	108.20
25	LA	2262	U	P-O5'-C5'	-6.53	110.45	120.90
25	LA	1660	G	O4'-C1'-N9	6.53	113.42	108.20
1	SA	1114	C	O4'-C1'-N1	6.53	113.42	108.20
25	LA	945	A	C3'-C2'-C1'	-6.53	96.28	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2094	A	N1-C6-N6	6.53	122.52	118.60
1	SA	566	G	C5-C6-O6	-6.53	124.69	128.60
1	SA	989	U	O4'-C1'-N1	6.53	113.42	108.20
25	LA	458	G	C3'-C2'-C1'	-6.53	96.28	101.50
25	LA	1694	C	O4'-C1'-N1	6.53	113.42	108.20
1	SA	772	U	C5'-C4'-C3'	-6.52	105.56	116.00
1	SA	173	U	C5'-C4'-C3'	-6.52	105.56	116.00
1	SA	485	U	O4'-C1'-N1	6.52	113.42	108.20
1	SA	832	G	O4'-C1'-N9	6.52	113.42	108.20
1	SA	1378	C	O4'-C1'-N1	6.52	113.42	108.20
52	LF	120	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	SA	702	A	P-O3'-C3'	6.52	127.53	119.70
1	SA	962	C	P-O3'-C3'	-6.52	111.88	119.70
25	LA	17	G	O3'-P-O5'	-6.52	91.61	104.00
1	SA	1192	C	O4'-C1'-N1	6.52	113.41	108.20
25	LA	2742	G	C4'-C3'-C2'	-6.52	96.08	102.60
25	LA	695	G	O4'-C1'-N9	6.52	113.41	108.20
25	LA	1652	A	C5'-C4'-C3'	-6.52	105.57	116.00
25	LA	2231	U	O4'-C1'-N1	6.52	113.41	108.20
1	SA	1391	U	O4'-C1'-N1	6.51	113.41	108.20
3	S7	53	G	C5-C6-O6	-6.51	124.69	128.60
1	SA	973	G	P-O3'-C3'	6.51	127.51	119.70
1	SA	593	U	O4'-C1'-N1	6.51	113.41	108.20
25	LA	124	G	N1-C6-O6	6.51	123.81	119.90
25	LA	491	G	C5'-C4'-C3'	6.51	126.41	116.00
25	LA	1844	C	O4'-C1'-N1	6.51	113.41	108.20
1	SA	473	U	C6-N1-C1'	-6.51	112.09	121.20
1	SA	766	A	C5'-C4'-O4'	-6.51	101.29	109.10
25	LA	865	C	O4'-C1'-N1	6.51	113.41	108.20
25	LA	1532	A	O4'-C1'-N9	6.51	113.41	108.20
25	LA	1667	G	C5-C6-O6	-6.51	124.70	128.60
25	LA	2278	A	O4'-C1'-N9	6.51	113.41	108.20
25	LA	723	C	O4'-C1'-N1	6.50	113.40	108.20
26	LB	35	C	C2-N1-C1'	6.50	125.96	118.80
1	SA	1172	C	O4'-C1'-N1	6.50	113.40	108.20
25	LA	174	U	O4'-C1'-N1	6.50	113.40	108.20
25	LA	1543	G	P-O3'-C3'	6.50	127.50	119.70
1	SA	388	G	P-O3'-C3'	-6.50	111.90	119.70
1	SA	1305	G	O4'-C4'-C3'	6.50	111.30	106.10
1	SA	1498	U	O4'-C1'-N1	6.50	113.40	108.20
1	SA	527	G	N1-C6-O6	6.50	123.80	119.90
1	SA	1314	C	O4'-C1'-N1	6.50	113.40	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S6	35	C	O4'-C1'-N1	6.50	113.40	108.20
1	SA	623	C	O4'-C1'-N1	6.50	113.40	108.20
1	SA	1094	G	C5-C6-O6	-6.50	124.70	128.60
5	SK	10	ARG	NE-CZ-NH1	6.50	123.55	120.30
25	LA	1127	A	P-O3'-C3'	6.50	127.50	119.70
25	LA	1499	C	O4'-C1'-N1	6.50	113.40	108.20
25	LA	1577	C	O4'-C1'-N1	6.50	113.40	108.20
1	SA	99	C	P-O5'-C5'	6.50	131.29	120.90
25	LA	1965	C	C5'-C4'-O4'	6.50	116.89	109.10
25	LA	2330	G	O4'-C1'-N9	6.50	113.40	108.20
6	SL	13	ARG	NE-CZ-NH1	6.49	123.55	120.30
17	SC	228	ARG	NE-CZ-NH1	6.49	123.55	120.30
25	LA	417	C	O4'-C1'-N1	6.49	113.39	108.20
25	LA	1058	U	O4'-C1'-N1	6.49	113.39	108.20
25	LA	2664	G	O4'-C1'-N9	6.49	113.39	108.20
25	LA	567	U	O4'-C1'-N1	6.49	113.39	108.20
25	LA	1203	U	O4'-C1'-N1	6.49	113.39	108.20
25	LA	2638	G	C5-C6-O6	-6.49	124.71	128.60
25	LA	2086	U	O4'-C1'-N1	6.49	113.39	108.20
25	LA	470	A	P-O5'-C5'	-6.48	110.53	120.90
25	LA	318	C	O4'-C1'-N1	6.48	113.39	108.20
25	LA	2557	G	N7-C8-N9	6.48	116.34	113.10
1	SA	910	C	C4'-C3'-C2'	-6.48	96.12	102.60
25	LA	581	C	O4'-C1'-N1	6.48	113.38	108.20
1	SA	567	G	O4'-C1'-N9	6.48	113.38	108.20
25	LA	179	C	O4'-C1'-N1	6.48	113.38	108.20
25	LA	1778	U	C5'-C4'-C3'	-6.48	105.64	116.00
25	LA	2854	G	O4'-C1'-N9	6.48	113.38	108.20
1	SA	888	G	C4-N9-C1'	-6.48	118.08	126.50
25	LA	2385	C	P-O3'-C3'	-6.48	111.93	119.70
25	LA	2647	U	O4'-C1'-N1	6.48	113.38	108.20
3	S7	38	A	C5'-C4'-O4'	6.47	116.87	109.10
25	LA	915	C	P-O3'-C3'	6.47	127.47	119.70
25	LA	1389	G	O4'-C1'-N9	6.47	113.38	108.20
3	S7	59	U	C6-N1-C1'	-6.47	112.14	121.20
25	LA	34	U	C2-N1-C1'	6.47	125.47	117.70
25	LA	2498	C	P-O3'-C3'	-6.47	111.93	119.70
1	SA	1442	G	P-O5'-C5'	6.47	131.25	120.90
3	S7	5	G	P-O5'-C5'	6.47	131.25	120.90
1	SA	814	A	C5'-C4'-O4'	6.47	116.86	109.10
14	SB	31	PHE	CB-CG-CD1	-6.47	116.27	120.80
25	LA	994	C	O4'-C1'-N1	6.47	113.38	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2544	G	C4'-C3'-C2'	-6.47	96.13	102.60
25	LA	2831	G	C5-C6-O6	-6.47	124.72	128.60
1	SA	443	C	O4'-C1'-N1	6.47	113.37	108.20
1	SA	475	C	C5'-C4'-C3'	-6.47	105.65	116.00
1	SA	643	C	O4'-C1'-N1	6.47	113.37	108.20
1	SA	102	G	O4'-C1'-N9	6.46	113.37	108.20
25	LA	316	C	O4'-C1'-N1	6.46	113.37	108.20
25	LA	1966	A	C8-N9-C1'	-6.46	116.06	127.70
25	LA	803	U	O4'-C1'-N1	6.46	113.37	108.20
25	LA	298	G	P-O3'-C3'	6.46	127.45	119.70
1	SA	1002	G	O4'-C1'-N9	6.46	113.37	108.20
1	SA	1223	C	O4'-C1'-N1	6.46	113.37	108.20
25	LA	334	C	O4'-C1'-N1	6.46	113.37	108.20
25	LA	571	U	C5'-C4'-C3'	-6.46	105.67	116.00
25	LA	987	C	O4'-C1'-N1	6.46	113.37	108.20
25	LA	2022	U	P-O3'-C3'	-6.46	111.95	119.70
25	LA	2395	C	O4'-C1'-N1	6.46	113.37	108.20
26	LB	87	U	O4'-C1'-N1	6.46	113.37	108.20
1	SA	983	A	C5'-C4'-O4'	6.46	116.85	109.10
25	LA	998	C	O4'-C1'-N1	6.46	113.37	108.20
1	SA	1138	G	O4'-C1'-N9	6.46	113.36	108.20
25	LA	1012	U	N1-C1'-C2'	6.45	122.39	114.00
25	LA	1024	G	O4'-C1'-N9	6.45	113.36	108.20
25	LA	651	G	O4'-C1'-N9	6.45	113.36	108.20
25	LA	2709	G	C5'-C4'-O4'	6.45	116.84	109.10
1	SA	261	U	C2-N3-C4	-6.45	123.13	127.00
25	LA	2394	C	O4'-C1'-N1	6.45	113.36	108.20
1	SA	1416	G	O4'-C1'-N9	6.45	113.36	108.20
25	LA	44	A	P-O3'-C3'	-6.45	111.96	119.70
25	LA	2275	C	P-O3'-C3'	6.45	127.44	119.70
1	SA	530	G	C4'-C3'-C2'	6.45	109.05	102.60
1	SA	1077	G	O4'-C1'-N9	6.45	113.36	108.20
1	SA	1331	G	P-O3'-C3'	6.45	127.43	119.70
17	SC	228	ARG	NE-CZ-NH2	-6.45	117.08	120.30
25	LA	2678	C	O4'-C1'-N1	6.45	113.36	108.20
1	SA	444	G	O4'-C1'-N9	6.44	113.36	108.20
25	LA	2094	A	C8-N9-C4	6.44	108.38	105.80
30	LO	2	ARG	NE-CZ-NH2	6.44	123.52	120.30
25	LA	838	C	O4'-C1'-N1	6.44	113.35	108.20
25	LA	2297	A	C5'-C4'-O4'	6.44	116.83	109.10
25	LA	295	G	O4'-C1'-N9	6.44	113.35	108.20
25	LA	763	G	C5'-C4'-C3'	6.44	126.30	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1954	G	C5'-C4'-O4'	6.44	116.82	109.10
25	LA	1564	C	O4'-C1'-N1	6.43	113.35	108.20
26	LB	57	A	P-O3'-C3'	6.43	127.42	119.70
1	SA	578	C	O4'-C1'-N1	6.43	113.35	108.20
1	SA	610	U	P-O3'-C3'	6.43	127.42	119.70
25	LA	1277	G	O4'-C1'-N9	6.43	113.35	108.20
25	LA	2165	C	C1'-O4'-C4'	-6.43	104.75	109.90
51	L9	25	TYR	CB-CG-CD1	-6.43	117.14	121.00
1	SA	381	C	O4'-C1'-N1	6.43	113.34	108.20
25	LA	18	U	O4'-C1'-N1	6.43	113.34	108.20
25	LA	901	C	P-O3'-C3'	6.43	127.42	119.70
25	LA	1639	C	C5'-C4'-C3'	6.43	126.28	116.00
1	SA	521	G	C5-C6-O6	-6.43	124.74	128.60
1	SA	1442	G	O4'-C1'-N9	6.43	113.34	108.20
25	LA	120	U	O4'-C1'-N1	6.42	113.34	108.20
1	SA	527	G	C5-C6-O6	-6.42	124.75	128.60
25	LA	1698	A	P-O3'-C3'	6.42	127.41	119.70
25	LA	1022	G	C5-C6-O6	-6.42	124.75	128.60
25	LA	1046	A	P-O3'-C3'	6.42	127.40	119.70
1	SA	776	G	P-O3'-C3'	6.42	127.40	119.70
25	LA	574	A	O3'-P-O5'	-6.42	91.80	104.00
1	SA	202	G	C8-N9-C1'	6.42	135.34	127.00
1	SA	691	G	C5-C6-O6	-6.42	124.75	128.60
25	LA	147	C	P-O5'-C5'	6.42	131.16	120.90
25	LA	541	A	O4'-C1'-N9	6.42	113.33	108.20
25	LA	1891	G	C5-C6-O6	-6.42	124.75	128.60
25	LA	2599	G	O4'-C1'-N9	6.42	113.33	108.20
25	LA	1510	G	C4-N9-C1'	6.42	134.84	126.50
1	SA	384	G	O4'-C1'-N9	6.41	113.33	108.20
25	LA	1645	G	C5'-C4'-C3'	-6.41	105.74	116.00
28	LM	19	PHE	CB-CG-CD2	-6.41	116.31	120.80
25	LA	232	G	C5'-C4'-O4'	6.41	116.80	109.10
25	LA	2731	G	O4'-C1'-N9	6.41	113.33	108.20
26	LB	2	G	C5-C6-O6	-6.41	124.75	128.60
1	SA	673	A	C5'-C4'-C3'	-6.41	105.75	116.00
25	LA	1044	C	O4'-C1'-N1	6.41	113.33	108.20
25	LA	2429	G	O4'-C1'-N9	6.41	113.33	108.20
1	SA	114	U	C5'-C4'-C3'	6.41	126.25	116.00
1	SA	582	C	C5'-C4'-O4'	6.41	116.79	109.10
3	S7	33	U	C5'-C4'-C3'	6.41	126.25	116.00
24	S1	365	MET	CG-SD-CE	-6.41	89.95	100.20
25	LA	613	A	O4'-C1'-N9	6.41	113.32	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1686	C	O4'-C1'-N1	6.41	113.33	108.20
1	SA	469	C	O4'-C1'-N1	6.40	113.32	108.20
25	LA	881	G	O4'-C1'-N9	6.40	113.32	108.20
25	LA	25	U	C2-N3-C4	-6.40	123.16	127.00
25	LA	951	C	P-O5'-C5'	-6.40	110.66	120.90
25	LA	1355	G	O4'-C1'-N9	6.40	113.32	108.20
25	LA	2515	C	C5'-C4'-O4'	6.40	116.78	109.10
1	SA	1164	G	O4'-C1'-N9	6.40	113.32	108.20
25	LA	1064	C	O4'-C1'-N1	6.40	113.32	108.20
1	SA	768	A	C4'-C3'-C2'	-6.40	96.20	102.60
25	LA	29	U	C6-N1-C2	-6.40	117.16	121.00
25	LA	1916	A	P-O3'-C3'	-6.40	112.02	119.70
25	LA	2750	A	P-O3'-C3'	-6.40	112.02	119.70
1	SA	995	C	O4'-C1'-N1	6.40	113.32	108.20
1	SA	1243	C	O4'-C1'-N1	6.40	113.32	108.20
1	SA	1273	C	O4'-C1'-N1	6.39	113.31	108.20
1	SA	1400	C	O4'-C1'-N1	6.39	113.32	108.20
2	S6	40	C	O4'-C1'-N1	6.39	113.32	108.20
25	LA	723	C	C5'-C4'-C3'	6.39	126.23	116.00
25	LA	1080	A	O4'-C1'-N9	6.39	113.31	108.20
25	LA	1521	G	O4'-C1'-N9	6.39	113.31	108.20
1	SA	654	G	O4'-C1'-N9	6.39	113.31	108.20
1	SA	720	C	C6-N1-C2	-6.39	117.74	120.30
1	SA	937	A	P-O3'-C3'	6.39	127.36	119.70
1	SA	660	C	O4'-C1'-N1	6.39	113.31	108.20
25	LA	957	C	C6-N1-C2	-6.39	117.75	120.30
25	LA	1947	C	C4'-C3'-C2'	-6.39	96.21	102.60
25	LA	1335	C	O4'-C1'-N1	6.38	113.31	108.20
25	LA	1527	G	O4'-C1'-N9	6.38	113.31	108.20
25	LA	757	G	C5'-C4'-C3'	6.38	126.21	116.00
1	SA	1492	A	P-O5'-C5'	6.38	131.11	120.90
20	SF	91	ARG	NE-CZ-NH1	6.38	123.49	120.30
25	LA	2512	C	C6-N1-C2	-6.38	117.75	120.30
25	LA	2656	U	C1'-O4'-C4'	-6.38	104.79	109.90
25	LA	1725	U	O4'-C1'-N1	6.38	113.30	108.20
25	LA	2664	G	O3'-P-O5'	-6.38	91.88	104.00
56	LJ	46	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	SA	1443	C	O4'-C1'-N1	6.37	113.30	108.20
25	LA	2271	G	P-O5'-C5'	6.37	131.10	120.90
51	L9	51	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	SA	1510	C	O4'-C1'-N1	6.37	113.30	108.20
25	LA	194	G	P-O5'-C5'	6.37	131.09	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	837	C	O4'-C1'-N1	6.37	113.30	108.20
25	LA	2822	G	P-O3'-C3'	-6.37	112.05	119.70
54	LH	132	ARG	NE-CZ-NH1	6.37	123.48	120.30
25	LA	1121	C	O4'-C1'-N1	6.37	113.30	108.20
1	SA	1530	G	O5'-C5'-C4'	6.37	123.80	111.70
25	LA	2133	G	O4'-C1'-N9	6.37	113.30	108.20
25	LA	2192	U	O4'-C1'-N1	6.37	113.30	108.20
1	SA	239	U	P-O5'-C5'	6.37	131.09	120.90
1	SA	1436	U	O4'-C1'-N1	6.37	113.29	108.20
25	LA	1202	G	O4'-C1'-N9	6.37	113.29	108.20
25	LA	1851	U	P-O5'-C5'	-6.37	110.71	120.90
25	LA	2699	C	O4'-C1'-N1	6.37	113.29	108.20
25	LA	1480	C	O4'-C1'-N1	6.37	113.29	108.20
25	LA	663	G	O4'-C1'-N9	6.36	113.29	108.20
25	LA	2083	G	O4'-C1'-N9	6.36	113.29	108.20
26	LB	87	U	C4'-C3'-C2'	-6.36	96.24	102.60
29	LN	86	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	S7	15	G	N1-C6-O6	6.36	123.72	119.90
25	LA	1731	G	O4'-C1'-N9	6.36	113.29	108.20
25	LA	1254	A	P-O5'-C5'	-6.36	110.72	120.90
25	LA	1390	U	O4'-C1'-N1	6.36	113.29	108.20
25	LA	2207	C	C5'-C4'-O4'	6.36	116.73	109.10
26	LB	37	C	O4'-C1'-N1	6.36	113.29	108.20
57	LK	102	ARG	NE-CZ-NH1	6.36	123.48	120.30
25	LA	1986	C	O4'-C1'-N1	6.36	113.29	108.20
1	SA	29	U	O4'-C1'-N1	6.36	113.29	108.20
17	SC	131	ARG	NE-CZ-NH1	6.36	123.48	120.30
25	LA	1015	U	P-O3'-C3'	-6.36	112.07	119.70
25	LA	93	G	C4'-C3'-C2'	-6.36	96.24	102.60
25	LA	2665	A	C5'-C4'-C3'	6.36	126.17	116.00
25	LA	2673	G	C5'-C4'-C3'	6.36	126.17	116.00
1	SA	826	C	O4'-C1'-N1	6.35	113.28	108.20
25	LA	510	C	O4'-C1'-N1	6.35	113.28	108.20
25	LA	1973	G	O4'-C1'-N9	6.35	113.28	108.20
53	LG	108	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	SA	46	G	C5'-C4'-C3'	-6.35	105.84	116.00
25	LA	390	U	O4'-C1'-N1	6.35	113.28	108.20
25	LA	1382	G	P-O5'-C5'	6.35	131.06	120.90
25	LA	1406	U	O4'-C1'-N1	6.35	113.28	108.20
25	LA	1509	A	C1'-O4'-C4'	-6.35	104.82	109.90
25	LA	2717	C	C6-N1-C2	-6.35	117.76	120.30
25	LA	584	C	C2-N3-C4	-6.35	116.73	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1118	U	P-O5'-C5'	6.35	131.05	120.90
1	SA	1129	C	C6-N1-C2	-6.35	117.76	120.30
25	LA	1704	C	O4'-C1'-N1	6.34	113.28	108.20
25	LA	2500	U	O4'-C1'-N1	6.34	113.28	108.20
1	SA	351	G	P-O5'-C5'	6.34	131.05	120.90
1	SA	511	C	P-O3'-C3'	6.34	127.31	119.70
25	LA	550	C	C6-N1-C2	-6.34	117.76	120.30
25	LA	561	G	O4'-C1'-N9	6.34	113.27	108.20
25	LA	1295	C	C6-N1-C2	-6.34	117.76	120.30
25	LA	2765	A	C1'-O4'-C4'	-6.34	104.83	109.90
1	SA	176	C	O4'-C1'-N1	6.34	113.27	108.20
25	LA	2339	C	C4'-C3'-C2'	-6.34	96.26	102.60
25	LA	2888	C	O4'-C1'-N1	6.34	113.27	108.20
25	LA	2169	A	C5'-C4'-O4'	6.34	116.71	109.10
25	LA	2801	G	O4'-C1'-N9	6.34	113.27	108.20
1	SA	899	C	C6-N1-C2	-6.34	117.77	120.30
25	LA	413	C	O4'-C1'-N1	6.34	113.27	108.20
25	LA	402	A	O4'-C1'-N9	6.33	113.27	108.20
3	S7	65	G	O4'-C1'-N9	6.33	113.27	108.20
25	LA	310	A	O4'-C1'-N9	6.33	113.27	108.20
25	LA	1964	G	P-O5'-C5'	6.33	131.03	120.90
30	LO	47	ARG	NE-CZ-NH1	-6.33	117.13	120.30
53	LG	17	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	SA	1279	G	P-O5'-C5'	6.33	131.03	120.90
25	LA	287	G	O4'-C1'-N9	6.33	113.27	108.20
25	LA	2243	U	C2-N3-C4	-6.33	123.20	127.00
25	LA	2500	U	C4'-C3'-C2'	-6.33	96.27	102.60
1	SA	620	C	O4'-C1'-N1	6.33	113.26	108.20
25	LA	2012	G	N1-C6-O6	6.33	123.70	119.90
1	SA	1469	C	O4'-C1'-N1	6.33	113.26	108.20
25	LA	1152	C	O4'-C1'-N1	6.33	113.26	108.20
1	SA	189	A	O4'-C1'-N9	6.32	113.26	108.20
1	SA	1000	A	O4'-C1'-N9	6.32	113.26	108.20
25	LA	1445	G	O4'-C1'-N9	6.32	113.26	108.20
1	SA	269	C	O4'-C1'-N1	6.32	113.26	108.20
1	SA	614	C	O4'-C1'-N1	6.32	113.26	108.20
1	SA	1513	A	C5'-C4'-C3'	6.32	126.11	116.00
25	LA	220	G	C5-C6-O6	-6.32	124.81	128.60
25	LA	1748	C	O4'-C1'-N1	6.32	113.26	108.20
25	LA	2799	A	N1-C6-N6	-6.32	114.81	118.60
24	S1	58	ARG	NE-CZ-NH1	6.32	123.46	120.30
25	LA	591	U	C4'-C3'-C2'	-6.32	96.28	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1639	C	O4'-C1'-N1	6.32	113.25	108.20
25	LA	313	G	C5'-C4'-C3'	-6.32	105.89	116.00
25	LA	471	A	O4'-C1'-N9	6.32	113.25	108.20
54	LH	123	ARG	NE-CZ-NH1	6.32	123.46	120.30
25	LA	1789	A	O4'-C1'-N9	6.31	113.25	108.20
25	LA	2755	C	C6-N1-C2	-6.31	117.77	120.30
25	LA	2487	G	C5'-C4'-C3'	6.31	126.10	116.00
55	LI	16	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	SA	326	G	C8-N9-C1'	-6.31	118.80	127.00
1	SA	915	A	O4'-C1'-N9	6.31	113.25	108.20
1	SA	1486	G	O4'-C1'-N9	6.31	113.25	108.20
25	LA	285	G	C5'-C4'-C3'	6.31	126.09	116.00
25	LA	2315	G	O4'-C1'-N9	6.31	113.25	108.20
25	LA	201	C	O4'-C1'-N1	6.31	113.25	108.20
25	LA	729	G	P-O5'-C5'	-6.31	110.81	120.90
25	LA	2887	A	P-O5'-C5'	6.30	130.99	120.90
25	LA	673	C	O4'-C1'-N1	6.30	113.24	108.20
25	LA	2895	G	P-O5'-C5'	6.30	130.99	120.90
1	SA	547	A	P-O3'-C3'	6.30	127.26	119.70
2	S6	56	U	O4'-C1'-N1	6.30	113.24	108.20
25	LA	369	U	O4'-C1'-N1	6.30	113.24	108.20
25	LA	2628	C	O4'-C1'-N1	6.30	113.24	108.20
25	LA	2811	G	O4'-C1'-N9	6.30	113.24	108.20
25	LA	2338	C	O4'-C1'-N1	6.30	113.24	108.20
25	LA	468	G	O4'-C1'-N9	6.30	113.24	108.20
25	LA	1886	U	O4'-C1'-N1	6.30	113.24	108.20
25	LA	2655	G	O4'-C1'-N9	6.30	113.24	108.20
25	LA	254	G	C5-C6-O6	-6.29	124.82	128.60
1	SA	1159	U	C2'-C3'-O3'	6.29	123.77	113.70
2	S6	44	A	O4'-C1'-N9	6.29	113.23	108.20
12	SR	2	ARG	NE-CZ-NH1	6.29	123.45	120.30
25	LA	684	G	C5-C6-O6	-6.29	124.82	128.60
25	LA	2127	G	C5-C6-O6	-6.29	124.82	128.60
25	LA	2171	A	P-O3'-C3'	6.29	127.25	119.70
1	SA	295	C	O4'-C1'-N1	6.29	113.23	108.20
1	SA	452	A	O4'-C1'-N9	6.29	113.23	108.20
25	LA	330	A	C5'-C4'-C3'	-6.29	105.93	116.00
25	LA	2160	C	C5'-C4'-C3'	6.29	126.07	116.00
1	SA	1305	G	C5-C6-O6	-6.29	124.83	128.60
25	LA	2828	G	C4'-C3'-C2'	-6.29	96.31	102.60
1	SA	297	G	O4'-C1'-N9	6.29	113.23	108.20
25	LA	261	G	O4'-C1'-N9	6.29	113.23	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	731	G	O4'-C1'-N9	6.29	113.23	108.20
1	SA	1096	C	O4'-C1'-N1	6.29	113.23	108.20
1	SA	1500	A	P-O3'-C3'	-6.29	112.16	119.70
25	LA	1498	C	O4'-C1'-N1	6.29	113.23	108.20
1	SA	700	G	C5'-C4'-O4'	6.28	116.64	109.10
1	SA	896	C	O4'-C1'-N1	6.28	113.23	108.20
1	SA	1152	A	C4'-C3'-C2'	-6.28	96.32	102.60
25	LA	1124	G	O4'-C1'-N9	6.28	113.23	108.20
25	LA	2371	G	N1-C6-O6	6.28	123.67	119.90
49	L7	29	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	SA	416	G	P-O5'-C5'	6.28	130.95	120.90
25	LA	2521	C	C4'-C3'-C2'	-6.28	96.32	102.60
25	LA	1224	U	C2-N1-C1'	6.28	125.24	117.70
25	LA	47	C	O4'-C1'-N1	6.28	113.22	108.20
25	LA	1327	A	O4'-C1'-N9	6.28	113.22	108.20
25	LA	642	U	O4'-C1'-N1	6.28	113.22	108.20
34	LS	6	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	SA	510	A	P-O5'-C5'	-6.27	110.86	120.90
25	LA	1439	A	P-O5'-C5'	6.27	130.94	120.90
25	LA	2763	G	C5-C6-O6	-6.27	124.84	128.60
1	SA	410	G	C5'-C4'-C3'	-6.27	105.97	116.00
1	SA	1151	A	P-O5'-C5'	6.27	130.93	120.90
26	LB	52	A	C5'-C4'-C3'	6.27	126.03	116.00
25	LA	1298	C	P-O3'-C3'	6.27	127.22	119.70
1	SA	510	A	P-O3'-C3'	-6.27	112.18	119.70
2	S6	75	C	C5'-C4'-O4'	6.27	116.62	109.10
22	SH	14	ARG	NE-CZ-NH1	6.27	123.43	120.30
25	LA	973	A	C5'-C4'-C3'	-6.27	105.97	116.00
25	LA	2198	A	P-O3'-C3'	6.27	127.22	119.70
1	SA	816	A	P-O3'-C3'	6.26	127.22	119.70
1	SA	1087	G	P-O5'-C5'	6.26	130.92	120.90
1	SA	1168	U	C1'-O4'-C4'	-6.26	104.89	109.90
27	LC	164	ARG	NE-CZ-NH1	6.26	123.43	120.30
25	LA	1681	G	C5'-C4'-C3'	-6.26	105.98	116.00
25	LA	2808	G	O4'-C1'-N9	6.26	113.21	108.20
1	SA	930	C	O4'-C1'-N1	6.26	113.21	108.20
25	LA	236	C	O4'-C1'-N1	6.26	113.21	108.20
25	LA	1434	A	C5'-C4'-C3'	6.26	126.01	116.00
25	LA	2214	C	O4'-C1'-N1	6.26	113.21	108.20
25	LA	286	U	O4'-C1'-N1	6.26	113.20	108.20
25	LA	1449	G	O4'-C1'-N9	6.26	113.21	108.20
25	LA	1947	C	O4'-C1'-N1	6.26	113.20	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1459	G	C5-C6-O6	-6.25	124.85	128.60
7	SM	92	ARG	NE-CZ-NH1	6.25	123.43	120.30
25	LA	2091	C	O4'-C1'-N1	6.25	113.20	108.20
25	LA	2788	C	C5'-C4'-C3'	-6.25	106.00	116.00
25	LA	1127	A	C5-C6-N6	-6.25	118.70	123.70
25	LA	1240	U	O4'-C1'-N1	6.25	113.20	108.20
25	LA	2021	C	C2-N1-C1'	6.25	125.68	118.80
25	LA	2373	G	O4'-C1'-N9	6.25	113.20	108.20
28	LM	108	ARG	NE-CZ-NH2	6.25	123.43	120.30
25	LA	1046	A	C3'-C2'-C1'	-6.25	96.50	101.50
25	LA	2104	C	P-O3'-C3'	6.25	127.20	119.70
26	LB	20	G	C5'-C4'-C3'	-6.25	106.00	116.00
1	SA	501	C	O4'-C1'-N1	6.25	113.20	108.20
1	SA	655	A	O4'-C1'-N9	6.25	113.20	108.20
1	SA	1107	C	O4'-C1'-N1	6.25	113.20	108.20
21	SG	43	TYR	CB-CG-CD1	6.25	124.75	121.00
25	LA	380	G	O4'-C1'-N9	6.25	113.20	108.20
25	LA	1101	U	P-O3'-C3'	6.25	127.20	119.70
25	LA	2271	G	C5-C6-O6	-6.25	124.85	128.60
58	LZ	49	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	SA	976	G	C5-C6-O6	-6.25	124.85	128.60
1	SA	1069	C	O4'-C1'-N1	6.25	113.20	108.20
1	SA	1520	C	C6-N1-C2	-6.25	117.80	120.30
3	S7	58	A	C5'-C4'-C3'	-6.25	106.00	116.00
25	LA	906	U	P-O3'-C3'	-6.25	112.21	119.70
25	LA	634	C	O4'-C1'-N1	6.24	113.19	108.20
25	LA	984	A	O4'-C1'-C2'	-6.24	99.56	105.80
25	LA	2886	A	P-O5'-C5'	6.24	130.89	120.90
1	SA	651	C	O4'-C1'-N1	6.24	113.19	108.20
26	LB	90	C	O4'-C1'-N1	6.24	113.19	108.20
25	LA	529	A	O4'-C1'-N9	6.24	113.19	108.20
25	LA	2446	G	C5'-C4'-O4'	6.24	116.59	109.10
1	SA	815	A	N9-C1'-C2'	6.24	122.11	114.00
25	LA	39	G	O4'-C1'-N9	6.24	113.19	108.20
25	LA	1376	C	C2-N1-C1'	-6.24	111.94	118.80
25	LA	2267	A	C4-N9-C1'	-6.24	115.07	126.30
1	SA	372	C	O4'-C1'-N1	6.24	113.19	108.20
25	LA	307	G	C5-C6-O6	-6.24	124.86	128.60
25	LA	1788	C	O4'-C1'-N1	6.24	113.19	108.20
25	LA	1413	A	O4'-C1'-N9	6.23	113.19	108.20
25	LA	2095	A	P-O5'-C5'	6.23	130.87	120.90
26	LB	42	C	C6-N1-C1'	-6.23	113.32	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	L6	170	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	SA	337	G	O4'-C1'-N9	6.23	113.19	108.20
1	SA	631	C	O4'-C1'-N1	6.23	113.19	108.20
1	SA	1097	C	O4'-C1'-N1	6.23	113.19	108.20
25	LA	140	C	O4'-C1'-N1	6.23	113.19	108.20
1	SA	604	G	O4'-C1'-N9	6.23	113.18	108.20
1	SA	1071	C	C2-N1-C1'	6.23	125.65	118.80
25	LA	577	G	O4'-C1'-N9	6.23	113.19	108.20
25	LA	1061	U	P-O3'-C3'	6.23	127.18	119.70
25	LA	2609	U	O4'-C1'-N1	6.23	113.18	108.20
1	SA	956	U	O4'-C1'-N1	6.23	113.18	108.20
14	SB	68	PHE	CB-CG-CD1	-6.23	116.44	120.80
25	LA	1780	A	C1'-O4'-C4'	-6.23	104.92	109.90
25	LA	2044	C	C6-N1-C2	-6.23	117.81	120.30
1	SA	1407	C	C6-N1-C2	-6.23	117.81	120.30
25	LA	2173	A	C5'-C4'-O4'	6.23	116.57	109.10
25	LA	2214	C	P-O3'-C3'	6.23	127.17	119.70
25	LA	2367	G	N1-C6-O6	6.23	123.64	119.90
25	LA	2588	G	C8-N9-C4	-6.23	103.91	106.40
1	SA	717	U	C2'-C3'-O3'	6.22	123.66	113.70
25	LA	1208	C	O4'-C1'-N1	6.22	113.18	108.20
25	LA	2087	G	C5-C6-O6	-6.22	124.86	128.60
26	LB	85	G	C5-C6-O6	-6.22	124.86	128.60
25	LA	1386	C	C1'-O4'-C4'	-6.22	104.92	109.90
25	LA	1478	G	O4'-C1'-N9	6.22	113.18	108.20
25	LA	2844	G	O4'-C1'-N9	6.22	113.18	108.20
1	SA	817	C	C3'-C2'-C1'	-6.22	96.53	101.50
1	SA	1112	C	O4'-C1'-N1	6.22	113.18	108.20
25	LA	1645	G	O4'-C1'-N9	6.22	113.18	108.20
39	LW	7	ARG	NE-CZ-NH2	-6.22	117.19	120.30
25	LA	660	C	O4'-C1'-N1	6.22	113.17	108.20
25	LA	757	G	P-O5'-C5'	6.22	130.85	120.90
25	LA	1409	U	O4'-C1'-N1	6.22	113.17	108.20
25	LA	2251	G	C6-N1-C2	-6.22	121.37	125.10
25	LA	2313	C	P-O5'-C5'	-6.21	110.96	120.90
25	LA	2406	A	P-O3'-C3'	6.21	127.16	119.70
25	LA	2626	C	O4'-C1'-N1	6.21	113.17	108.20
25	LA	336	C	O4'-C1'-N1	6.21	113.17	108.20
25	LA	948	C	C5'-C4'-O4'	-6.21	101.65	109.10
25	LA	1154	G	P-O3'-C3'	6.21	127.15	119.70
25	LA	1795	C	O4'-C1'-N1	6.21	113.17	108.20
1	SA	960	U	OP2-P-O3'	6.21	118.86	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1105	U	O4'-C1'-N1	6.21	113.17	108.20
25	LA	1263	U	P-O3'-C3'	6.21	127.15	119.70
25	LA	2162	G	P-O3'-C3'	6.21	127.15	119.70
1	SA	346	G	P-O5'-C5'	-6.21	110.97	120.90
25	LA	562	U	C2-N3-C4	-6.21	123.28	127.00
25	LA	1361	G	O4'-C1'-N9	6.21	113.17	108.20
25	LA	1670	C	P-O5'-C5'	6.21	130.83	120.90
25	LA	2484	G	C4'-C3'-C2'	-6.21	96.39	102.60
25	LA	2626	C	C4'-C3'-C2'	-6.21	96.39	102.60
1	SA	609	A	C5'-C4'-C3'	-6.21	106.07	116.00
1	SA	713	G	C5-C6-O6	-6.21	124.88	128.60
25	LA	1519	G	O4'-C1'-N9	6.20	113.16	108.20
25	LA	2751	G	O4'-C1'-N9	6.20	113.16	108.20
1	SA	1258	G	O4'-C1'-N9	6.20	113.16	108.20
3	S7	21	A	O4'-C1'-N9	6.20	113.16	108.20
1	SA	1461	G	P-O3'-C3'	6.20	127.14	119.70
25	LA	228	C	C1'-O4'-C4'	-6.20	104.94	109.90
25	LA	532	A	O4'-C1'-N9	6.20	113.16	108.20
25	LA	1005	C	C6-N1-C2	-6.20	117.82	120.30
25	LA	2236	U	P-O3'-C3'	6.20	127.14	119.70
3	S7	37	A	P-O5'-C5'	6.20	130.82	120.90
25	LA	736	C	O4'-C1'-N1	6.20	113.16	108.20
31	LP	90	ARG	NE-CZ-NH1	6.20	123.40	120.30
10	SP	56	ARG	NE-CZ-NH2	-6.20	117.20	120.30
25	LA	2092	U	C5'-C4'-O4'	6.20	116.54	109.10
1	SA	396	C	O4'-C1'-N1	6.20	113.16	108.20
17	SC	58	ARG	NE-CZ-NH1	6.20	123.40	120.30
25	LA	470	A	C4'-C3'-C2'	-6.20	96.41	102.60
25	LA	785	G	P-O3'-C3'	6.20	127.14	119.70
2	S6	8	U	O4'-C1'-N1	6.19	113.16	108.20
25	LA	1233	C	O4'-C1'-N1	6.19	113.16	108.20
1	SA	1411	C	O4'-C1'-N1	6.19	113.15	108.20
25	LA	1305	C	O4'-C1'-N1	6.19	113.15	108.20
25	LA	93	G	O4'-C1'-N9	6.19	113.15	108.20
25	LA	1045	C	C2-N1-C1'	6.19	125.61	118.80
1	SA	609	A	P-O3'-C3'	6.19	127.13	119.70
1	SA	925	G	N1-C6-O6	-6.19	116.19	119.90
25	LA	1383	A	O4'-C1'-N9	6.19	113.15	108.20
1	SA	673	A	O4'-C1'-N9	6.19	113.15	108.20
1	SA	778	G	C5-C6-O6	-6.19	124.89	128.60
1	SA	1066	C	O4'-C1'-N1	6.19	113.15	108.20
9	SO	16	ARG	NE-CZ-NH1	6.19	123.39	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1346	G	O4'-C1'-N9	6.19	113.15	108.20
25	LA	2008	C	O4'-C1'-N1	6.19	113.15	108.20
25	LA	2101	A	O4'-C1'-N9	6.19	113.15	108.20
25	LA	752	A	P-O5'-C5'	-6.19	111.00	120.90
25	LA	1218	G	O4'-C1'-N9	6.19	113.15	108.20
25	LA	1442	U	O4'-C1'-N1	6.19	113.15	108.20
1	SA	852	G	O4'-C1'-N9	6.18	113.15	108.20
3	S7	38	A	P-O3'-C3'	-6.18	112.28	119.70
25	LA	455	C	O4'-C1'-N1	6.18	113.15	108.20
25	LA	2818	U	O4'-C1'-N1	6.18	113.15	108.20
1	SA	212	G	N1-C6-O6	6.18	123.61	119.90
1	SA	790	A	N1-C6-N6	6.18	122.31	118.60
25	LA	1416	G	O4'-C1'-N9	6.18	113.14	108.20
25	LA	2222	C	P-O3'-C3'	-6.18	112.28	119.70
1	SA	1304	G	P-O3'-C3'	6.18	127.12	119.70
1	SA	1534	A	O4'-C1'-N9	6.18	113.14	108.20
25	LA	277	G	C1'-O4'-C4'	-6.18	104.96	109.90
25	LA	752	A	O4'-C1'-N9	6.18	113.14	108.20
25	LA	2251	G	N1-C6-O6	6.18	123.61	119.90
25	LA	2896	C	O4'-C1'-N1	6.18	113.14	108.20
25	LA	729	G	C5'-C4'-C3'	-6.18	106.11	116.00
25	LA	1417	C	O4'-C1'-N1	6.18	113.14	108.20
1	SA	1437	A	O4'-C1'-N9	6.18	113.14	108.20
2	S6	23	G	O4'-C1'-N9	6.18	113.14	108.20
26	LB	47	C	O4'-C1'-N1	6.18	113.14	108.20
25	LA	1135	C	C5'-C4'-C3'	6.17	125.88	116.00
25	LA	2761	A	O4'-C1'-N9	6.17	113.14	108.20
1	SA	703	G	P-O3'-C3'	6.17	127.11	119.70
47	L6	88	ARG	NE-CZ-NH2	6.17	123.39	120.30
25	LA	183	C	C6-N1-C2	-6.17	117.83	120.30
25	LA	745	G	C4-C5-C6	-6.17	115.10	118.80
25	LA	1920	C	C6-N1-C2	-6.17	117.83	120.30
25	LA	2474	U	O4'-C1'-N1	6.17	113.14	108.20
1	SA	797	C	O4'-C1'-N1	6.17	113.14	108.20
1	SA	1267	C	C2-N1-C1'	6.17	125.58	118.80
1	SA	1305	G	N1-C6-O6	6.17	123.60	119.90
25	LA	551	G	O4'-C1'-N9	6.17	113.13	108.20
25	LA	1682	G	O4'-C1'-N9	6.17	113.14	108.20
1	SA	43	C	O4'-C1'-N1	6.17	113.13	108.20
1	SA	773	G	O4'-C1'-N9	6.17	113.13	108.20
25	LA	323	C	C2-N1-C1'	6.17	125.58	118.80
1	SA	248	C	O4'-C1'-N1	6.17	113.13	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2473	U	P-O3'-C3'	6.17	127.10	119.70
50	L8	163	TYR	CB-CG-CD1	-6.17	117.30	121.00
1	SA	802	A	C5-C6-N6	6.16	128.63	123.70
1	SA	817	C	C6-N1-C2	-6.16	117.83	120.30
1	SA	225	C	C5'-C4'-C3'	-6.16	106.14	116.00
25	LA	675	A	C4'-C3'-C2'	-6.16	96.44	102.60
25	LA	765	C	C5'-C4'-C3'	-6.16	106.14	116.00
1	SA	47	C	O4'-C1'-N1	6.16	113.13	108.20
1	SA	877	G	P-O3'-C3'	6.16	127.09	119.70
2	S6	62	C	C6-N1-C2	-6.16	117.84	120.30
3	S7	63	G	C5-C6-O6	-6.16	124.90	128.60
25	LA	1214	A	O4'-C1'-N9	6.16	113.13	108.20
1	SA	374	A	P-O5'-C5'	6.16	130.75	120.90
1	SA	568	G	C5'-C4'-C3'	6.16	125.85	116.00
25	LA	27	G	C5-C6-O6	-6.16	124.91	128.60
25	LA	1418	G	C5-C6-O6	-6.16	124.91	128.60
25	LA	2141	G	C5'-C4'-C3'	-6.16	106.15	116.00
1	SA	347	G	O4'-C1'-N9	6.16	113.13	108.20
25	LA	99	U	C6-N1-C1'	-6.16	112.58	121.20
1	SA	811	C	O4'-C1'-C2'	6.16	113.14	107.60
1	SA	1359	C	O4'-C1'-N1	6.16	113.12	108.20
25	LA	894	U	O4'-C1'-N1	6.16	113.12	108.20
25	LA	986	C	C5'-C4'-O4'	6.16	116.49	109.10
1	SA	1270	G	N1-C6-O6	6.15	123.59	119.90
25	LA	253	C	O4'-C1'-N1	6.15	113.12	108.20
25	LA	1115	G	P-O5'-C5'	6.15	130.74	120.90
1	SA	1152	A	C1'-O4'-C4'	-6.15	104.98	109.90
3	S7	27	G	O4'-C1'-N9	6.15	113.12	108.20
25	LA	341	C	O4'-C1'-N1	6.15	113.12	108.20
25	LA	1950	G	N1-C6-O6	6.15	123.59	119.90
26	LB	70	C	O4'-C1'-N1	6.15	113.12	108.20
1	SA	971	G	C5'-C4'-O4'	6.15	116.48	109.10
25	LA	233	A	C4'-C3'-C2'	-6.15	96.45	102.60
25	LA	1376	C	C5'-C4'-C3'	6.15	125.84	116.00
1	SA	248	C	P-O3'-C3'	6.15	127.08	119.70
37	LV	36	ARG	NE-CZ-NH2	6.15	123.37	120.30
26	LB	109	A	C5'-C4'-O4'	6.14	116.47	109.10
1	SA	791	G	C5'-C4'-C3'	-6.14	106.17	116.00
1	SA	1178	G	O4'-C1'-N9	6.14	113.11	108.20
25	LA	938	G	O4'-C1'-N9	6.14	113.11	108.20
25	LA	1270	C	C5'-C4'-C3'	-6.14	106.17	116.00
43	L2	5	ARG	NE-CZ-NH1	6.14	123.37	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1147	C	C5'-C4'-C3'	-6.14	106.18	116.00
1	SA	58	C	O4'-C1'-N1	6.14	113.11	108.20
1	SA	1136	C	O4'-C1'-N1	6.14	113.11	108.20
1	SA	1354	U	O4'-C1'-N1	6.14	113.11	108.20
25	LA	898	C	O4'-C1'-N1	6.14	113.11	108.20
25	LA	1302	A	C5-C6-N6	-6.14	118.79	123.70
1	SA	226	G	O4'-C1'-N9	6.13	113.11	108.20
2	S6	77	A	O4'-C1'-N9	6.13	113.11	108.20
25	LA	774	G	C5-C6-O6	-6.13	124.92	128.60
25	LA	841	G	O4'-C1'-N9	6.13	113.11	108.20
1	SA	434	U	O4'-C1'-N1	6.13	113.11	108.20
1	SA	31	G	P-O3'-C3'	-6.13	112.34	119.70
1	SA	597	G	C5'-C4'-C3'	-6.13	106.19	116.00
25	LA	756	A	C4'-C3'-C2'	-6.13	96.47	102.60
53	LG	98	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	SA	218	U	O4'-C1'-N1	6.13	113.10	108.20
25	LA	1788	C	C6-N1-C2	-6.13	117.85	120.30
25	LA	2824	C	O4'-C1'-N1	6.13	113.10	108.20
1	SA	590	U	O4'-C1'-N1	6.13	113.10	108.20
25	LA	1473	G	O4'-C1'-N9	6.13	113.10	108.20
1	SA	156	C	O4'-C1'-N1	6.12	113.10	108.20
15	ST	23	ARG	NE-CZ-NH1	6.12	123.36	120.30
25	LA	829	A	P-O3'-C3'	-6.12	112.35	119.70
25	LA	1626	A	P-O5'-C5'	6.12	130.70	120.90
1	SA	1135	U	O4'-C1'-N1	6.12	113.10	108.20
1	SA	678	U	C5'-C4'-C3'	6.12	125.79	116.00
25	LA	425	G	O4'-C1'-N9	6.12	113.10	108.20
25	LA	748	G	P-O5'-C5'	-6.12	111.11	120.90
1	SA	782	A	C4'-C3'-C2'	-6.12	96.48	102.60
25	LA	2663	G	C4'-C3'-C2'	-6.12	96.48	102.60
1	SA	318	G	O4'-C1'-N9	6.12	113.09	108.20
1	SA	683	G	P-O5'-C5'	-6.12	111.11	120.90
14	SB	221	ARG	NE-CZ-NH2	-6.12	117.24	120.30
25	LA	671	C	C6-N1-C2	-6.12	117.85	120.30
25	LA	2055	C	C4'-C3'-C2'	-6.12	96.48	102.60
25	LA	2099	U	O4'-C1'-N1	6.12	113.10	108.20
26	LB	15	A	C1'-O4'-C4'	-6.12	105.00	109.90
26	LB	33	G	O4'-C1'-N9	6.12	113.09	108.20
1	SA	441	A	C5'-C4'-O4'	6.12	116.44	109.10
25	LA	1904	G	C5-C6-O6	-6.12	124.93	128.60
1	SA	418	C	O4'-C1'-N1	6.12	113.09	108.20
1	SA	1415	G	O4'-C1'-N9	6.12	113.09	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1426	G	C5-C6-O6	-6.12	124.93	128.60
25	LA	1942	C	O4'-C1'-N1	6.12	113.09	108.20
25	LA	635	C	O4'-C1'-N1	6.11	113.09	108.20
25	LA	1950	G	O4'-C1'-N9	6.11	113.09	108.20
25	LA	2620	C	C5'-C4'-C3'	-6.11	106.22	116.00
1	SA	87	C	P-O3'-C3'	-6.11	112.37	119.70
1	SA	1197	A	O4'-C1'-N9	6.11	113.09	108.20
1	SA	1322	C	C2-N1-C1'	6.11	125.52	118.80
40	LX	101	PHE	CB-CG-CD2	6.11	125.08	120.80
40	LX	141	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	SA	261	U	C5-C4-O4	-6.11	122.23	125.90
25	LA	2562	U	O4'-C1'-N1	6.11	113.09	108.20
25	LA	1007	C	C5'-C4'-C3'	6.11	125.77	116.00
25	LA	1609	A	P-O3'-C3'	6.11	127.03	119.70
26	LB	19	C	O4'-C1'-N1	6.11	113.09	108.20
1	SA	375	U	P-O3'-C3'	-6.11	112.37	119.70
1	SA	1283	U	O4'-C1'-N1	6.11	113.08	108.20
1	SA	495	A	O4'-C1'-N9	6.10	113.08	108.20
1	SA	163	C	O4'-C1'-N1	6.10	113.08	108.20
25	LA	1344	U	C2-N3-C4	-6.10	123.34	127.00
25	LA	484	C	O4'-C1'-N1	6.10	113.08	108.20
1	SA	407	U	O4'-C1'-N1	6.10	113.08	108.20
1	SA	817	C	C5'-C4'-O4'	6.10	116.42	109.10
5	SK	10	ARG	NE-CZ-NH2	-6.10	117.25	120.30
25	LA	227	A	P-O3'-C3'	6.10	127.02	119.70
25	LA	583	G	N3-C2-N2	6.10	124.17	119.90
25	LA	1043	C	O4'-C1'-N1	6.10	113.08	108.20
25	LA	1593	A	O4'-C1'-N9	6.10	113.08	108.20
25	LA	2429	G	C4-N9-C1'	6.10	134.43	126.50
25	LA	2554	U	C6-N1-C1'	-6.10	112.66	121.20
25	LA	1447	C	O4'-C1'-N1	6.10	113.08	108.20
25	LA	1594	U	O4'-C1'-N1	6.09	113.08	108.20
26	LB	2	G	N1-C6-O6	6.09	123.56	119.90
25	LA	20	C	P-O3'-C3'	6.09	127.01	119.70
25	LA	1288	G	O4'-C1'-N9	6.09	113.07	108.20
1	SA	960	U	C2'-C3'-O3'	6.09	123.44	113.70
2	S6	27	G	O4'-C1'-N9	6.09	113.07	108.20
25	LA	791	C	O4'-C1'-N1	6.09	113.07	108.20
25	LA	1704	C	C6-N1-C2	-6.09	117.86	120.30
25	LA	1850	G	C5'-C4'-C3'	-6.09	106.26	116.00
1	SA	368	U	C5'-C4'-C3'	-6.08	106.27	116.00
25	LA	2030	C	C6-N1-C1'	-6.08	113.50	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1051	C	O4'-C1'-N1	6.08	113.07	108.20
25	LA	791	C	C5'-C4'-C3'	-6.08	106.27	116.00
25	LA	907	G	C5-C6-O6	-6.08	124.95	128.60
25	LA	1560	G	O4'-C1'-N9	6.08	113.07	108.20
25	LA	2445	G	C6-C5-N7	-6.08	126.75	130.40
1	SA	331	G	P-O5'-C5'	6.08	130.63	120.90
25	LA	1031	G	O4'-C1'-N9	6.08	113.07	108.20
25	LA	1310	G	O4'-C1'-N9	6.08	113.06	108.20
25	LA	2150	C	O4'-C1'-N1	6.08	113.06	108.20
25	LA	1990	C	P-O5'-C5'	6.08	130.63	120.90
25	LA	2893	A	P-O3'-C3'	-6.08	112.40	119.70
33	LR	6	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	SA	491	G	O4'-C1'-N9	6.08	113.06	108.20
25	LA	918	A	O4'-C1'-N9	6.08	113.06	108.20
25	LA	1266	G	C4'-C3'-C2'	-6.08	96.52	102.60
25	LA	1428	C	C4'-C3'-C2'	-6.08	96.52	102.60
25	LA	2567	G	C5'-C4'-O4'	6.08	116.39	109.10
1	SA	879	C	O4'-C1'-N1	6.08	113.06	108.20
8	SN	8	ARG	NE-CZ-NH2	-6.08	117.26	120.30
26	LB	38	C	O4'-C1'-N1	6.08	113.06	108.20
25	LA	2181	U	O4'-C1'-N1	6.07	113.06	108.20
56	LJ	118	ARG	NE-CZ-NH1	6.07	123.34	120.30
25	LA	2875	C	O4'-C1'-N1	6.07	113.06	108.20
1	SA	1275	A	O4'-C1'-N9	6.07	113.06	108.20
1	SA	1387	G	O4'-C1'-N9	6.07	113.06	108.20
25	LA	1997	C	C4'-C3'-C2'	-6.07	96.53	102.60
31	LP	78	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	SA	750	C	C5'-C4'-C3'	-6.07	106.29	116.00
1	SA	1432	G	C5'-C4'-C3'	-6.07	106.29	116.00
25	LA	2521	C	O4'-C1'-N1	6.07	113.06	108.20
1	SA	907	A	O4'-C1'-N9	6.07	113.06	108.20
23	SI	89	TYR	CB-CG-CD2	6.07	124.64	121.00
25	LA	100	U	C1'-O4'-C4'	-6.07	105.05	109.90
25	LA	1314	C	O4'-C1'-N1	6.07	113.05	108.20
25	LA	1967	C	P-O5'-C5'	6.07	130.61	120.90
25	LA	2422	C	P-O5'-C5'	6.07	130.61	120.90
1	SA	1227	A	C4'-C3'-C2'	-6.07	96.53	102.60
14	SB	221	ARG	NE-CZ-NH1	6.07	123.33	120.30
25	LA	539	G	P-O5'-C5'	-6.07	111.19	120.90
25	LA	759	G	C4'-C3'-C2'	-6.07	96.53	102.60
25	LA	818	G	C5-C6-O6	-6.07	124.96	128.60
25	LA	1908	C	O4'-C1'-N1	6.07	113.05	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1923	U	O4'-C1'-N1	6.07	113.05	108.20
25	LA	2055	C	C1'-O4'-C4'	-6.07	105.05	109.90
25	LA	1241	A	P-O3'-C3'	6.06	126.98	119.70
25	LA	799	G	N3-C2-N2	6.06	124.14	119.90
25	LA	2089	C	O4'-C1'-N1	6.06	113.05	108.20
2	S6	22	A	P-O3'-C3'	6.06	126.97	119.70
25	LA	2492	U	C5'-C4'-C3'	-6.06	106.30	116.00
1	SA	296	U	O4'-C1'-N1	6.06	113.05	108.20
1	SA	305	G	O4'-C1'-N9	6.06	113.05	108.20
1	SA	1355	G	O4'-C1'-N9	6.06	113.05	108.20
14	SB	68	PHE	CB-CG-CD2	6.06	125.04	120.80
25	LA	409	G	O4'-C1'-N9	6.06	113.05	108.20
1	SA	214	C	O4'-C1'-N1	6.06	113.05	108.20
25	LA	12	U	O4'-C1'-N1	6.06	113.05	108.20
25	LA	79	C	O4'-C1'-N1	6.06	113.05	108.20
25	LA	562	U	N1-C2-N3	6.05	118.53	114.90
25	LA	1452	G	P-O3'-C3'	-6.05	112.44	119.70
25	LA	1815	A	N1-C6-N6	-6.05	114.97	118.60
1	SA	146	G	O4'-C1'-N9	6.05	113.04	108.20
25	LA	1296	G	C5'-C4'-C3'	6.05	125.69	116.00
25	LA	1956	U	C6-N1-C2	-6.05	117.37	121.00
25	LA	2085	U	P-O3'-C3'	-6.05	112.44	119.70
1	SA	479	U	O4'-C1'-N1	6.05	113.04	108.20
1	SA	870	U	C5'-C4'-O4'	6.05	116.36	109.10
2	S6	2	G	O4'-C1'-N9	6.05	113.04	108.20
25	LA	64	A	O4'-C1'-N9	6.05	113.04	108.20
25	LA	759	G	C5-C6-O6	-6.05	124.97	128.60
25	LA	2364	C	O4'-C1'-N1	6.05	113.04	108.20
54	LH	59	ARG	NE-CZ-NH1	6.05	123.33	120.30
5	SK	126	ARG	NE-CZ-NH1	6.05	123.32	120.30
25	LA	2011	U	O4'-C1'-N1	6.05	113.04	108.20
25	LA	2147	A	P-O5'-C5'	-6.05	111.22	120.90
1	SA	452	A	N1-C6-N6	-6.05	114.97	118.60
25	LA	1088	A	N1-C6-N6	6.05	122.23	118.60
25	LA	1906	G	C5-C6-O6	-6.05	124.97	128.60
25	LA	2107	G	O4'-C1'-N9	6.05	113.04	108.20
25	LA	59	U	O4'-C1'-N1	6.04	113.03	108.20
25	LA	1327	A	C4'-C3'-C2'	-6.04	96.56	102.60
1	SA	869	G	C5-C6-O6	-6.04	124.97	128.60
25	LA	2194	U	C5'-C4'-O4'	6.04	116.35	109.10
1	SA	140	U	O4'-C1'-N1	6.04	113.03	108.20
25	LA	28	A	O3'-P-O5'	-6.04	92.52	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1488	C	O4'-C1'-N1	6.04	113.03	108.20
1	SA	89	U	O4'-C1'-N1	6.04	113.03	108.20
25	LA	623	C	O4'-C1'-N1	6.04	113.03	108.20
14	SB	136	ARG	NE-CZ-NH1	6.04	123.32	120.30
25	LA	1680	U	C4'-C3'-C2'	-6.04	96.56	102.60
25	LA	2155	U	O4'-C1'-N1	6.04	113.03	108.20
25	LA	2805	C	O4'-C1'-N1	6.04	113.03	108.20
1	SA	225	C	O4'-C1'-N1	6.03	113.03	108.20
1	SA	1466	C	O4'-C1'-N1	6.03	113.03	108.20
25	LA	687	C	O4'-C1'-N1	6.03	113.03	108.20
25	LA	2653	U	O4'-C1'-N1	6.03	113.03	108.20
1	SA	809	G	C4'-C3'-C2'	-6.03	96.57	102.60
1	SA	1099	G	C4'-C3'-C2'	-6.03	96.57	102.60
1	SA	1198	G	C4'-C3'-C2'	-6.03	96.57	102.60
25	LA	8	C	O4'-C1'-N1	6.03	113.03	108.20
25	LA	1887	C	O4'-C1'-N1	6.03	113.02	108.20
25	LA	2272	U	C5'-C4'-O4'	6.03	116.34	109.10
1	SA	947	G	C5'-C4'-C3'	-6.03	106.35	116.00
1	SA	741	G	O4'-C1'-N9	6.03	113.02	108.20
40	LX	127	PHE	CB-CG-CD1	-6.03	116.58	120.80
25	LA	2036	C	O4'-C1'-N1	6.03	113.02	108.20
1	SA	1385	G	O4'-C1'-N9	6.02	113.02	108.20
8	SN	52	ARG	NE-CZ-NH1	6.02	123.31	120.30
25	LA	648	G	P-O5'-C5'	-6.02	111.27	120.90
23	SI	40	ARG	NE-CZ-NH1	6.02	123.31	120.30
25	LA	109	C	O4'-C1'-N1	6.02	113.02	108.20
25	LA	2864	G	O4'-C1'-N9	6.02	113.02	108.20
1	SA	250	A	P-O3'-C3'	-6.02	112.48	119.70
1	SA	1259	C	C5'-C4'-C3'	-6.02	106.37	116.00
25	LA	458	G	P-O3'-C3'	6.02	126.92	119.70
25	LA	1116	G	C5'-C4'-C3'	6.02	125.63	116.00
25	LA	1793	C	O4'-C1'-N1	6.02	113.01	108.20
25	LA	1944	U	C6-N1-C1'	-6.02	112.78	121.20
1	SA	549	C	O4'-C1'-N1	6.01	113.01	108.20
1	SA	610	U	O4'-C1'-N1	6.01	113.01	108.20
3	S7	62	C	P-O5'-C5'	-6.01	111.28	120.90
25	LA	263	G	C5-C6-O6	-6.01	124.99	128.60
25	LA	712	G	O4'-C1'-N9	6.01	113.01	108.20
25	LA	1590	A	O4'-C1'-N9	6.01	113.01	108.20
25	LA	2054	A	P-O3'-C3'	6.01	126.92	119.70
1	SA	1438	G	C5'-C4'-O4'	6.01	116.31	109.10
7	SM	97	ARG	NE-CZ-NH1	6.01	123.31	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	978	G	C5-C6-O6	-6.01	124.99	128.60
25	LA	1034	G	C5-C6-O6	-6.01	124.99	128.60
28	LM	108	ARG	NE-CZ-NH1	-6.01	117.29	120.30
1	SA	1318	A	P-O3'-C3'	6.01	126.91	119.70
25	LA	822	G	O4'-C1'-N9	6.01	113.01	108.20
25	LA	1962	C	C5-C4-N4	-6.01	115.99	120.20
25	LA	2212	A	O4'-C1'-N9	6.01	113.01	108.20
21	SG	115	MET	CG-SD-CE	-6.01	90.59	100.20
25	LA	1033	U	O4'-C1'-N1	6.01	113.01	108.20
25	LA	1942	C	C5'-C4'-C3'	-6.01	106.39	116.00
25	LA	2066	C	O4'-C1'-N1	6.01	113.01	108.20
1	SA	958	A	P-O3'-C3'	6.01	126.91	119.70
3	S7	14	A	C5'-C4'-O4'	6.01	116.31	109.10
25	LA	42	A	O4'-C1'-N9	6.01	113.01	108.20
25	LA	1926	U	O4'-C1'-N1	6.01	113.00	108.20
25	LA	2741	A	P-O3'-C3'	6.01	126.91	119.70
36	LU	19	ARG	NE-CZ-NH1	6.01	123.30	120.30
25	LA	2160	C	O4'-C1'-N1	6.00	113.00	108.20
1	SA	160	A	O4'-C1'-N9	6.00	113.00	108.20
1	SA	189	A	C5'-C4'-O4'	6.00	116.31	109.10
3	S7	36	A	O4'-C1'-N9	6.00	113.00	108.20
11	SQ	76	ARG	NE-CZ-NH1	6.00	123.30	120.30
25	LA	308	G	C5-C6-O6	-6.00	125.00	128.60
25	LA	2034	U	C2-N1-C1'	-6.00	110.50	117.70
30	LO	69	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	SA	1059	C	O4'-C1'-N1	6.00	113.00	108.20
1	SA	1208	C	C6-N1-C2	-6.00	117.90	120.30
2	S6	7	G	O4'-C1'-N9	6.00	113.00	108.20
25	LA	1569	A	N1-C6-N6	-6.00	115.00	118.60
25	LA	1577	C	P-O3'-C3'	6.00	126.90	119.70
25	LA	1844	C	C6-N1-C2	-6.00	117.90	120.30
25	LA	143	C	O4'-C1'-N1	6.00	113.00	108.20
1	SA	1207	G	P-O3'-C3'	6.00	126.90	119.70
25	LA	245	G	C5'-C4'-C3'	6.00	125.60	116.00
26	LB	8	C	O4'-C1'-N1	6.00	113.00	108.20
1	SA	533	A	C5'-C4'-O4'	6.00	116.30	109.10
25	LA	2679	A	P-O3'-C3'	6.00	126.89	119.70
26	LB	20	G	O4'-C1'-N9	6.00	113.00	108.20
1	SA	271	C	O3'-P-O5'	5.99	115.39	104.00
12	SR	42	ARG	NE-CZ-NH1	5.99	123.30	120.30
25	LA	124	G	O4'-C1'-N9	5.99	112.99	108.20
25	LA	468	G	C5-C6-O6	-5.99	125.00	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1212	G	O4'-C1'-N9	5.99	112.99	108.20
25	LA	2137	U	P-O5'-C5'	5.99	130.49	120.90
1	SA	271	C	O4'-C1'-N1	5.99	112.99	108.20
1	SA	477	C	O4'-C1'-N1	5.99	112.99	108.20
25	LA	760	G	O4'-C1'-N9	5.99	112.99	108.20
25	LA	1085	A	C5'-C4'-O4'	5.99	116.29	109.10
25	LA	2311	A	C1'-O4'-C4'	-5.99	105.11	109.90
25	LA	2621	G	O4'-C1'-N9	5.99	112.99	108.20
25	LA	1192	G	P-O5'-C5'	-5.99	111.32	120.90
25	LA	1995	U	P-O3'-C3'	5.99	126.89	119.70
1	SA	127	G	C5-C6-O6	-5.99	125.01	128.60
1	SA	183	C	O4'-C1'-N1	5.99	112.99	108.20
1	SA	234	C	O4'-C1'-N1	5.99	112.99	108.20
25	LA	1293	C	C5'-C4'-O4'	5.99	116.28	109.10
32	LQ	92	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	SA	699	C	O4'-C1'-N1	5.98	112.99	108.20
1	SA	976	G	N1-C6-O6	5.98	123.49	119.90
25	LA	130	C	C4'-C3'-C2'	-5.98	96.62	102.60
25	LA	741	U	C5'-C4'-C3'	-5.98	106.43	116.00
5	SK	36	ARG	NE-CZ-NH1	5.98	123.29	120.30
25	LA	469	G	O4'-C1'-N9	5.98	112.98	108.20
25	LA	1210	G	N1-C6-O6	5.98	123.49	119.90
25	LA	2430	A	C1'-O4'-C4'	-5.98	105.12	109.90
1	SA	4	U	C2-N1-C1'	5.98	124.87	117.70
25	LA	1533	C	O4'-C1'-N1	5.98	112.98	108.20
1	SA	634	C	C5'-C4'-O4'	5.97	116.27	109.10
1	SA	740	U	C5'-C4'-O4'	5.97	116.27	109.10
1	SA	1098	C	O4'-C1'-N1	5.97	112.98	108.20
24	S1	471	ARG	NE-CZ-NH2	-5.97	117.31	120.30
25	LA	2024	G	P-O3'-C3'	5.97	126.87	119.70
25	LA	2349	G	N1-C6-O6	5.97	123.48	119.90
25	LA	2440	C	P-O3'-C3'	5.97	126.87	119.70
44	L3	35	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	SA	969	A	O4'-C1'-N9	5.97	112.98	108.20
25	LA	2575	C	O4'-C1'-N1	5.97	112.98	108.20
25	LA	974	G	P-O5'-C5'	-5.97	111.35	120.90
25	LA	2467	C	O4'-C1'-N1	5.97	112.98	108.20
1	SA	4	U	O4'-C1'-N1	5.97	112.98	108.20
1	SA	144	G	O4'-C1'-N9	5.97	112.98	108.20
25	LA	353	C	O4'-C1'-N1	5.97	112.97	108.20
25	LA	2069	G	C5'-C4'-C3'	5.97	125.55	116.00
1	SA	700	G	O4'-C1'-N9	5.97	112.97	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1049	C	O4'-C1'-N1	5.97	112.97	108.20
1	SA	162	A	O4'-C1'-N9	5.97	112.97	108.20
1	SA	814	A	C6-N1-C2	-5.97	115.02	118.60
1	SA	1215	G	O4'-C1'-N9	5.97	112.97	108.20
25	LA	992	C	O4'-C1'-N1	5.97	112.97	108.20
25	LA	1182	G	O4'-C1'-N9	5.97	112.97	108.20
25	LA	1771	C	O4'-C1'-N1	5.97	112.97	108.20
25	LA	1838	C	C5'-C4'-C3'	5.97	125.55	116.00
25	LA	2347	C	O4'-C1'-N1	5.97	112.97	108.20
25	LA	2385	C	C5'-C4'-O4'	5.97	116.26	109.10
28	LM	87	ARG	NE-CZ-NH1	5.97	123.28	120.30
40	LX	12	THR	N-CA-CB	5.97	121.64	110.30
1	SA	576	C	O4'-C1'-N1	5.96	112.97	108.20
3	S7	51	U	C5'-C4'-C3'	5.96	125.55	116.00
23	SI	102	PHE	CB-CG-CD2	-5.96	116.62	120.80
25	LA	446	G	C4-N9-C1'	5.96	134.25	126.50
25	LA	920	A	C5'-C4'-C3'	5.96	125.54	116.00
1	SA	1235	U	C4'-C3'-C2'	-5.96	96.64	102.60
25	LA	1463	C	O4'-C1'-N1	5.96	112.97	108.20
25	LA	349	U	C5'-C4'-C3'	-5.96	106.46	116.00
25	LA	808	G	O4'-C1'-N9	5.96	112.97	108.20
25	LA	1840	G	C5'-C4'-C3'	-5.96	106.46	116.00
25	LA	2472	G	N1-C6-O6	5.96	123.48	119.90
25	LA	2903	U	O4'-C1'-N1	5.96	112.97	108.20
25	LA	237	C	C6-N1-C2	-5.96	117.92	120.30
1	SA	1326	U	O4'-C1'-N1	5.96	112.97	108.20
25	LA	332	A	C1'-O4'-C4'	-5.96	105.13	109.90
25	LA	625	G	O4'-C1'-N9	5.96	112.97	108.20
25	LA	694	U	O4'-C1'-N1	5.96	112.97	108.20
25	LA	2165	C	C5'-C4'-O4'	5.96	116.25	109.10
25	LA	2172	U	P-O3'-C3'	-5.96	112.55	119.70
1	SA	108	G	C8-N9-C1'	-5.96	119.26	127.00
1	SA	438	U	O4'-C1'-N1	5.96	112.97	108.20
2	S6	68	C	O4'-C1'-N1	5.96	112.97	108.20
20	SF	2	ARG	NE-CZ-NH1	5.96	123.28	120.30
22	SH	127	TYR	CB-CG-CD2	-5.96	117.43	121.00
25	LA	404	A	N1-C6-N6	-5.96	115.03	118.60
25	LA	404	A	O4'-C1'-N9	5.96	112.97	108.20
26	LB	56	G	C5-C6-O6	-5.96	125.03	128.60
26	LB	110	C	C6-N1-C2	-5.96	117.92	120.30
1	SA	138	G	O4'-C1'-N9	5.96	112.96	108.20
25	LA	2342	C	O3'-P-O5'	5.96	115.31	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	LB	97	C	O4'-C1'-N1	5.96	112.96	108.20
25	LA	2425	A	C1'-O4'-C4'	-5.95	105.14	109.90
25	LA	2767	C	O4'-C1'-N1	5.95	112.96	108.20
1	SA	697	U	O4'-C1'-N1	5.95	112.96	108.20
25	LA	2211	A	C2'-C3'-O3'	5.95	123.22	113.70
25	LA	2686	G	O4'-C1'-N9	5.95	112.96	108.20
32	LQ	95	ARG	CD-NE-CZ	5.95	131.93	123.60
1	SA	186	C	O4'-C1'-N1	5.95	112.96	108.20
3	S7	42	C	O4'-C1'-N1	5.95	112.96	108.20
25	LA	2574	G	C5'-C4'-C3'	5.95	125.52	116.00
25	LA	377	G	C4'-C3'-C2'	-5.95	96.65	102.60
25	LA	1896	G	P-O5'-C5'	5.95	130.42	120.90
25	LA	2128	G	C5-C6-O6	-5.95	125.03	128.60
25	LA	2195	U	C4'-C3'-C2'	-5.95	96.65	102.60
1	SA	308	C	C6-N1-C1'	-5.95	113.66	120.80
1	SA	814	A	C8-N9-C1'	-5.95	117.00	127.70
1	SA	404	G	N1-C6-O6	5.95	123.47	119.90
1	SA	841	C	C6-N1-C1'	-5.95	113.67	120.80
25	LA	2263	C	P-O5'-C5'	-5.95	111.39	120.90
25	LA	2344	U	P-O5'-C5'	5.94	130.41	120.90
1	SA	99	C	O4'-C1'-N1	5.94	112.95	108.20
1	SA	1365	G	C5-C6-O6	-5.94	125.03	128.60
23	SI	40	ARG	NE-CZ-NH2	-5.94	117.33	120.30
25	LA	458	G	O4'-C1'-N9	5.94	112.95	108.20
1	SA	772	U	C5'-C4'-O4'	5.94	116.23	109.10
1	SA	1142	G	N1-C6-O6	5.94	123.47	119.90
1	SA	1497	G	O4'-C1'-N9	5.94	112.95	108.20
1	SA	1524	C	P-O3'-C3'	5.94	126.83	119.70
2	S6	37	U	O4'-C1'-N1	5.94	112.95	108.20
25	LA	1295	C	O4'-C1'-N1	5.94	112.95	108.20
25	LA	2336	A	C5'-C4'-O4'	5.94	116.23	109.10
26	LB	5	U	O4'-C1'-N1	5.94	112.95	108.20
25	LA	2260	C	O4'-C1'-N1	5.94	112.95	108.20
1	SA	1011	C	O4'-C1'-N1	5.94	112.95	108.20
25	LA	438	G	O4'-C1'-N9	5.94	112.95	108.20
25	LA	1965	C	C5'-C4'-C3'	-5.94	106.50	116.00
25	LA	2208	C	C6-N1-C2	-5.94	117.92	120.30
1	SA	597	G	O4'-C1'-N9	5.94	112.95	108.20
23	SI	102	PHE	CB-CG-CD1	5.94	124.95	120.80
25	LA	151	C	O4'-C1'-N1	5.94	112.95	108.20
25	LA	284	U	O4'-C1'-N1	5.94	112.95	108.20
1	SA	292	G	N3-C2-N2	5.93	124.05	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	348	G	O4'-C1'-N9	5.93	112.95	108.20
25	LA	1762	A	C1'-O4'-C4'	-5.93	105.15	109.90
25	LA	1894	C	O4'-C1'-N1	5.93	112.95	108.20
25	LA	2498	C	O4'-C1'-C2'	5.93	112.94	107.60
1	SA	909	A	N7-C8-N9	5.93	116.77	113.80
3	S7	21	A	C1'-O4'-C4'	-5.93	105.15	109.90
25	LA	1526	C	O4'-C1'-N1	5.93	112.94	108.20
25	LA	289	G	C5'-C4'-C3'	5.93	125.49	116.00
1	SA	678	U	P-O5'-C5'	-5.93	111.41	120.90
1	SA	1210	C	O4'-C1'-N1	5.93	112.94	108.20
1	SA	1344	C	O4'-C1'-N1	5.93	112.94	108.20
25	LA	891	G	P-O5'-C5'	5.93	130.39	120.90
25	LA	2521	C	C2-N1-C1'	-5.93	112.28	118.80
25	LA	2753	A	O4'-C1'-N9	5.93	112.94	108.20
1	SA	136	C	O4'-C1'-N1	5.93	112.94	108.20
1	SA	757	U	O4'-C1'-N1	5.93	112.94	108.20
10	SP	31	ARG	NE-CZ-NH1	5.93	123.26	120.30
25	LA	420	C	O4'-C1'-N1	5.93	112.94	108.20
9	SO	88	ARG	NE-CZ-NH1	5.93	123.26	120.30
25	LA	1872	A	O4'-C1'-N9	5.93	112.94	108.20
25	LA	2128	G	N1-C6-O6	5.93	123.46	119.90
25	LA	288	U	O4'-C1'-N1	5.92	112.94	108.20
25	LA	982	C	C6-N1-C1'	-5.92	113.69	120.80
1	SA	341	C	O4'-C1'-N1	5.92	112.94	108.20
1	SA	812	G	C4'-C3'-C2'	-5.92	96.68	102.60
3	S7	15	G	C5-C6-O6	-5.92	125.05	128.60
25	LA	1503	A	O4'-C1'-N9	5.92	112.94	108.20
25	LA	1694	C	C2-N1-C1'	5.92	125.31	118.80
1	SA	332	G	C5-C6-O6	-5.92	125.05	128.60
1	SA	771	G	O4'-C1'-N9	5.92	112.93	108.20
1	SA	1057	G	C5-C6-O6	-5.92	125.05	128.60
25	LA	896	A	O4'-C1'-N9	5.92	112.94	108.20
26	LB	110	C	O4'-C1'-N1	5.92	112.93	108.20
25	LA	1418	G	N3-C2-N2	5.92	124.04	119.90
1	SA	1316	G	N1-C6-O6	5.92	123.45	119.90
19	SE	28	ARG	NE-CZ-NH1	5.91	123.26	120.30
25	LA	63	A	P-O5'-C5'	-5.91	111.44	120.90
25	LA	348	A	O4'-C1'-N9	5.91	112.93	108.20
25	LA	907	G	O4'-C1'-N9	5.91	112.93	108.20
25	LA	1721	G	N1-C6-O6	5.91	123.45	119.90
1	SA	1408	A	C5'-C4'-O4'	5.91	116.19	109.10
1	SA	1410	A	O4'-C1'-N9	5.91	112.93	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	695	G	C4'-C3'-C2'	-5.91	96.69	102.60
25	LA	1757	A	P-O3'-C3'	5.91	126.79	119.70
25	LA	2079	U	O4'-C1'-N1	5.91	112.93	108.20
25	LA	2333	A	O4'-C1'-N9	5.91	112.93	108.20
25	LA	2620	C	O4'-C1'-N1	5.91	112.93	108.20
25	LA	2783	U	O4'-C1'-N1	5.91	112.93	108.20
51	L9	91	PHE	CB-CG-CD1	5.91	124.94	120.80
1	SA	726	C	C6-N1-C2	-5.91	117.94	120.30
1	SA	925	G	P-O5'-C5'	5.91	130.35	120.90
25	LA	953	G	C5-C6-O6	-5.91	125.06	128.60
1	SA	769	G	C4-N9-C1'	-5.91	118.82	126.50
1	SA	985	C	O4'-C1'-N1	5.91	112.92	108.20
25	LA	679	C	O4'-C1'-N1	5.91	112.92	108.20
25	LA	1814	G	P-O3'-C3'	5.91	126.79	119.70
25	LA	2043	C	P-O3'-C3'	5.91	126.79	119.70
26	LB	48	U	O4'-C1'-N1	5.90	112.92	108.20
1	SA	954	G	C5'-C4'-C3'	5.90	125.44	116.00
1	SA	1454	G	C5-C6-O6	-5.90	125.06	128.60
1	SA	1499	A	O4'-C1'-N9	5.90	112.92	108.20
25	LA	790	U	C2-N1-C1'	5.90	124.78	117.70
25	LA	1022	G	C1'-O4'-C4'	-5.90	105.18	109.90
25	LA	1022	G	N1-C6-O6	5.90	123.44	119.90
25	LA	1069	A	C1'-O4'-C4'	-5.90	105.18	109.90
1	SA	1400	C	C2-N1-C1'	5.90	125.29	118.80
1	SA	1419	G	N1-C6-O6	5.90	123.44	119.90
25	LA	567	U	C4'-C3'-C2'	-5.90	96.70	102.60
1	SA	1524	C	C6-N1-C2	-5.90	117.94	120.30
25	LA	1782	U	O4'-C1'-N1	5.90	112.92	108.20
4	SJ	68	ARG	NE-CZ-NH2	-5.90	117.35	120.30
25	LA	1635	A	C6-N1-C2	-5.90	115.06	118.60
25	LA	1640	A	P-O5'-C5'	5.90	130.34	120.90
1	SA	143	A	P-O5'-C5'	5.90	130.33	120.90
25	LA	741	U	C4'-C3'-C2'	-5.90	96.70	102.60
1	SA	1060	U	O4'-C1'-N1	5.89	112.92	108.20
2	S6	72	C	O4'-C1'-N1	5.89	112.92	108.20
25	LA	308	G	O4'-C1'-N9	5.89	112.92	108.20
25	LA	976	G	C5'-C4'-O4'	5.89	116.17	109.10
25	LA	1714	U	C2-N1-C1'	5.89	124.77	117.70
25	LA	2451	A	O4'-C1'-N9	5.89	112.92	108.20
1	SA	1073	U	C4'-C3'-C2'	-5.89	96.71	102.60
3	S7	4	C	C6-N1-C2	-5.89	117.94	120.30
22	SH	116	ARG	NE-CZ-NH1	5.89	123.25	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	93	G	C5'-C4'-C3'	-5.89	106.57	116.00
25	LA	1957	C	O4'-C1'-N1	5.89	112.91	108.20
25	LA	2175	C	O4'-C1'-N1	5.89	112.91	108.20
25	LA	2583	G	C5'-C4'-C3'	-5.89	106.57	116.00
24	S1	28	ARG	NE-CZ-NH1	5.89	123.25	120.30
25	LA	962	G	O4'-C1'-N9	5.89	112.91	108.20
1	SA	388	G	C5'-C4'-C3'	-5.89	106.58	116.00
1	SA	1379	G	O4'-C1'-N9	5.89	112.91	108.20
25	LA	81	G	O4'-C1'-N9	5.89	112.91	108.20
25	LA	1495	A	P-O5'-C5'	5.89	130.32	120.90
26	LB	102	G	N1-C6-O6	5.89	123.43	119.90
44	L3	39	ARG	NE-CZ-NH1	5.89	123.25	120.30
57	LK	94	ARG	NE-CZ-NH1	5.89	123.25	120.30
25	LA	143	C	P-O5'-C5'	5.89	130.32	120.90
25	LA	973	A	P-O3'-C3'	-5.89	112.63	119.70
56	LJ	2	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	SA	26	A	N1-C6-N6	-5.89	115.07	118.60
1	SA	195	A	O4'-C1'-N9	5.89	112.91	108.20
24	S1	576	ARG	NE-CZ-NH1	5.89	123.24	120.30
25	LA	96	C	O4'-C1'-N1	5.89	112.91	108.20
25	LA	1516	G	O4'-C1'-N9	5.89	112.91	108.20
25	LA	2549	G	O4'-C1'-N9	5.89	112.91	108.20
26	LB	36	C	O4'-C1'-N1	5.89	112.91	108.20
1	SA	1052	U	O4'-C1'-N1	5.88	112.91	108.20
1	SA	1194	U	P-O5'-C5'	5.88	130.31	120.90
25	LA	1646	C	C5'-C4'-C3'	5.88	125.41	116.00
25	LA	984	A	N1-C6-N6	-5.88	115.07	118.60
32	LQ	11	ARG	NE-CZ-NH2	-5.88	117.36	120.30
25	LA	1557	C	O4'-C1'-N1	5.88	112.90	108.20
1	SA	251	G	P-O3'-C3'	5.88	126.75	119.70
1	SA	270	A	C4'-C3'-C2'	-5.88	96.72	102.60
1	SA	708	C	O4'-C1'-N1	5.88	112.90	108.20
1	SA	765	G	N1-C6-O6	-5.88	116.38	119.90
25	LA	1070	A	P-O3'-C3'	-5.88	112.65	119.70
25	LA	2265	U	C2-N3-C4	-5.88	123.47	127.00
25	LA	2435	A	C4'-C3'-C2'	-5.88	96.72	102.60
9	SO	76	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	SA	1390	U	O4'-C1'-N1	5.87	112.90	108.20
25	LA	575	A	O4'-C1'-N9	5.87	112.90	108.20
25	LA	2602	A	O4'-C1'-N9	5.87	112.90	108.20
1	SA	888	G	C8-N9-C1'	5.87	134.63	127.00
1	SA	783	C	O4'-C1'-N1	5.87	112.90	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1053	G	C1'-O4'-C4'	-5.87	105.20	109.90
25	LA	2043	C	C5'-C4'-C3'	5.87	125.39	116.00
1	SA	993	G	C8-N9-C1'	-5.87	119.37	127.00
1	SA	1214	C	P-O3'-C3'	5.87	126.74	119.70
1	SA	1401	G	O4'-C1'-N9	5.87	112.89	108.20
25	LA	224	U	C5'-C4'-O4'	5.87	116.14	109.10
25	LA	1155	A	O3'-P-O5'	-5.87	92.86	104.00
25	LA	1452	G	C5-C6-O6	-5.87	125.08	128.60
1	SA	1213	A	C2'-C3'-O3'	5.86	123.08	113.70
1	SA	1531	A	C5'-C4'-C3'	5.86	125.38	116.00
25	LA	2095	A	O4'-C1'-N9	5.86	112.89	108.20
1	SA	1321	U	O4'-C1'-N1	5.86	112.89	108.20
1	SA	398	U	O4'-C1'-N1	5.86	112.89	108.20
1	SA	1173	U	O4'-C1'-N1	5.86	112.89	108.20
1	SA	1251	A	O4'-C1'-N9	5.86	112.89	108.20
25	LA	1234	U	O4'-C1'-N1	5.86	112.89	108.20
25	LA	2831	G	P-O3'-C3'	5.86	126.73	119.70
10	SP	28	ARG	NE-CZ-NH2	-5.86	117.37	120.30
25	LA	2120	G	O4'-C1'-N9	5.86	112.89	108.20
25	LA	2508	G	C5-C6-O6	-5.86	125.08	128.60
1	SA	455	G	O4'-C1'-N9	5.86	112.89	108.20
5	SK	52	ARG	NE-CZ-NH1	5.86	123.23	120.30
25	LA	718	A	O4'-C1'-N9	5.86	112.89	108.20
25	LA	1128	G	C5-C6-O6	-5.86	125.09	128.60
25	LA	2158	A	O4'-C1'-N9	5.86	112.89	108.20
1	SA	58	C	C6-N1-C2	-5.86	117.96	120.30
1	SA	1220	G	O4'-C1'-N9	5.86	112.89	108.20
25	LA	606	U	P-O3'-C3'	5.86	126.73	119.70
25	LA	1449	G	P-O5'-C5'	5.86	130.27	120.90
25	LA	297	G	C5'-C4'-C3'	-5.85	106.63	116.00
1	SA	1003	G	C5'-C4'-C3'	5.85	125.36	116.00
25	LA	3	U	C5'-C4'-C3'	-5.85	106.64	116.00
25	LA	1408	G	O4'-C1'-N9	5.85	112.88	108.20
58	LZ	44	PHE	CB-CG-CD1	-5.85	116.70	120.80
25	LA	463	G	C2'-C3'-O3'	5.85	123.06	113.70
25	LA	2691	C	O4'-C1'-N1	5.85	112.88	108.20
1	SA	778	G	O4'-C1'-N9	5.85	112.88	108.20
1	SA	1364	U	C5'-C4'-O4'	5.85	116.12	109.10
25	LA	965	C	O4'-C1'-N1	5.85	112.88	108.20
25	LA	1351	C	O4'-C1'-N1	5.85	112.88	108.20
25	LA	1514	G	P-O3'-C3'	-5.85	112.68	119.70
25	LA	1536	C	O4'-C1'-N1	5.85	112.88	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	381	C	C2-N1-C1'	5.85	125.23	118.80
3	S7	6	G	C5'-C4'-C3'	5.85	125.36	116.00
25	LA	1543	G	C5'-C4'-C3'	-5.85	106.64	116.00
25	LA	1119	U	P-O3'-C3'	-5.84	112.69	119.70
25	LA	1647	U	O4'-C1'-N1	5.84	112.88	108.20
25	LA	1880	U	O4'-C1'-N1	5.84	112.88	108.20
1	SA	933	G	O4'-C1'-N9	5.84	112.88	108.20
25	LA	2535	G	O4'-C1'-N9	5.84	112.87	108.20
1	SA	1192	C	P-O5'-C5'	-5.84	111.55	120.90
1	SA	1532	U	O4'-C1'-N1	5.84	112.87	108.20
3	S7	48	C	P-O3'-C3'	5.84	126.71	119.70
25	LA	181	A	P-O5'-C5'	-5.84	111.55	120.90
25	LA	246	C	O4'-C1'-N1	5.84	112.87	108.20
25	LA	676	A	O4'-C1'-N9	5.84	112.87	108.20
25	LA	1132	U	O4'-C1'-N1	5.84	112.87	108.20
25	LA	2125	G	N1-C6-O6	5.84	123.41	119.90
25	LA	2197	U	O4'-C1'-N1	5.84	112.87	108.20
1	SA	49	U	O4'-C1'-N1	5.84	112.87	108.20
1	SA	838	G	O4'-C1'-N9	5.84	112.87	108.20
25	LA	1986	C	C6-N1-C2	-5.84	117.96	120.30
1	SA	659	U	P-O3'-C3'	5.84	126.70	119.70
25	LA	388	G	C6-N1-C2	-5.84	121.60	125.10
37	LV	2	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	SA	1176	A	C5'-C4'-C3'	-5.84	106.66	116.00
1	SA	1323	G	C5-C6-O6	-5.84	125.10	128.60
23	SI	11	ARG	NE-CZ-NH2	-5.84	117.38	120.30
25	LA	452	G	C3'-C2'-C1'	5.84	106.17	101.50
25	LA	2002	G	C4'-C3'-C2'	-5.84	96.76	102.60
26	LB	109	A	C1'-O4'-C4'	-5.84	105.23	109.90
25	LA	1552	A	C8-N9-C1'	-5.83	117.20	127.70
1	SA	320	A	C5'-C4'-C3'	-5.83	106.67	116.00
1	SA	639	G	O4'-C1'-N9	5.83	112.87	108.20
25	LA	9	G	C5-C6-O6	-5.83	125.10	128.60
25	LA	58	G	O4'-C1'-N9	5.83	112.87	108.20
25	LA	413	C	P-O5'-C5'	5.83	130.23	120.90
25	LA	1236	G	C5-C6-O6	-5.83	125.10	128.60
25	LA	2159	G	P-O3'-C3'	-5.83	112.70	119.70
40	LX	101	PHE	CB-CG-CD1	-5.83	116.72	120.80
25	LA	35	G	O4'-C1'-N9	5.83	112.87	108.20
25	LA	188	G	O4'-C1'-N9	5.83	112.86	108.20
25	LA	1867	G	P-O5'-C5'	-5.83	111.57	120.90
25	LA	2107	G	C1'-O4'-C4'	-5.83	105.23	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2319	G	O4'-C1'-N9	5.83	112.86	108.20
1	SA	769	G	C8-N9-C1'	5.83	134.58	127.00
25	LA	2076	U	C6-N1-C1'	-5.83	113.04	121.20
25	LA	2272	U	C2'-C3'-O3'	5.83	123.03	113.70
1	SA	8	A	O4'-C1'-N9	5.83	112.86	108.20
1	SA	1454	G	N1-C6-O6	5.83	123.40	119.90
7	SM	78	ARG	NE-CZ-NH1	5.83	123.21	120.30
25	LA	2245	U	O4'-C1'-N1	5.83	112.86	108.20
23	SI	84	ARG	NE-CZ-NH1	5.83	123.21	120.30
23	SI	122	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	SA	1119	C	O4'-C1'-N1	5.82	112.86	108.20
25	LA	1401	G	O4'-C1'-N9	5.82	112.86	108.20
26	LB	67	G	O4'-C1'-N9	5.82	112.86	108.20
28	LM	71	ARG	NE-CZ-NH1	5.82	123.21	120.30
25	LA	1145	C	O4'-C1'-N1	5.82	112.86	108.20
1	SA	556	C	C6-N1-C2	-5.82	117.97	120.30
1	SA	1313	U	C5'-C4'-O4'	5.82	116.08	109.10
25	LA	811	U	N3-C2-O2	-5.82	118.12	122.20
25	LA	1804	C	O4'-C1'-N1	5.82	112.86	108.20
1	SA	550	G	O4'-C1'-N9	5.82	112.86	108.20
1	SA	924	C	C4'-C3'-C2'	-5.82	96.78	102.60
1	SA	988	G	O4'-C1'-N9	5.82	112.86	108.20
25	LA	1316	U	O4'-C1'-N1	5.82	112.86	108.20
25	LA	1647	U	C2-N3-C4	-5.82	123.51	127.00
25	LA	2354	C	C4'-C3'-C2'	-5.82	96.78	102.60
25	LA	2770	G	C5-C6-O6	-5.82	125.11	128.60
25	LA	1703	G	O4'-C1'-N9	5.82	112.85	108.20
25	LA	2000	C	O4'-C1'-N1	5.82	112.85	108.20
36	LU	38	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	SA	1485	U	O4'-C1'-N1	5.81	112.85	108.20
25	LA	938	G	P-O5'-C5'	5.81	130.20	120.90
25	LA	268	C	O4'-C1'-N1	5.81	112.85	108.20
25	LA	1159	U	C5'-C4'-C3'	-5.81	106.70	116.00
25	LA	1217	U	C4'-C3'-C2'	-5.81	96.79	102.60
25	LA	2024	G	C5'-C4'-O4'	5.81	116.08	109.10
1	SA	1490	U	P-O5'-C5'	5.81	130.20	120.90
25	LA	731	C	C6-N1-C2	-5.81	117.98	120.30
25	LA	827	U	P-O3'-C3'	-5.81	112.73	119.70
25	LA	1156	A	P-O3'-C3'	-5.81	112.73	119.70
25	LA	1831	G	C5-C6-O6	-5.81	125.11	128.60
1	SA	1460	C	O4'-C1'-N1	5.81	112.85	108.20
25	LA	1325	U	O4'-C1'-N1	5.81	112.85	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2049	G	C5-C6-O6	-5.81	125.11	128.60
25	LA	2779	U	C3'-C2'-C1'	-5.81	96.85	101.50
1	SA	1280	A	P-O5'-C5'	5.81	130.19	120.90
1	SA	1517	G	C5-C6-O6	-5.81	125.11	128.60
2	S6	4	G	O4'-C1'-N9	5.81	112.85	108.20
25	LA	829	A	P-O5'-C5'	5.81	130.19	120.90
25	LA	1248	G	C5-C6-O6	-5.81	125.12	128.60
25	LA	1398	C	O4'-C1'-N1	5.81	112.85	108.20
25	LA	2244	U	O4'-C1'-N1	5.81	112.85	108.20
1	SA	786	G	O4'-C1'-N9	5.81	112.84	108.20
2	S6	5	G	O4'-C1'-N9	5.81	112.84	108.20
3	S7	42	C	P-O3'-C3'	-5.81	112.73	119.70
25	LA	2236	U	O4'-C1'-N1	5.81	112.84	108.20
1	SA	368	U	C1'-O4'-C4'	-5.80	105.26	109.90
2	S6	51	U	O4'-C1'-N1	5.80	112.84	108.20
25	LA	741	U	O4'-C1'-N1	5.80	112.84	108.20
25	LA	884	U	O4'-C1'-N1	5.80	112.84	108.20
3	S7	40	C	O4'-C1'-N1	5.80	112.84	108.20
35	LT	1	MET	CG-SD-CE	-5.80	90.92	100.20
25	LA	480	A	O4'-C1'-N9	5.80	112.84	108.20
25	LA	1880	U	P-O3'-C3'	-5.80	112.74	119.70
25	LA	2073	C	C6-N1-C2	-5.80	117.98	120.30
25	LA	2840	C	O4'-C1'-N1	5.80	112.84	108.20
1	SA	700	G	C4'-C3'-C2'	-5.80	96.80	102.60
1	SA	764	C	C3'-C2'-C1'	-5.80	96.86	101.50
1	SA	952	U	O4'-C1'-N1	5.80	112.84	108.20
1	SA	1314	C	O3'-P-O5'	-5.80	92.98	104.00
25	LA	1967	C	C6-N1-C1'	-5.80	113.84	120.80
25	LA	2448	A	O5'-P-OP1	-5.80	100.48	105.70
25	LA	2496	C	O4'-C1'-N1	5.80	112.84	108.20
25	LA	2578	G	P-O3'-C3'	5.80	126.66	119.70
36	LU	54	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	SA	124	C	O4'-C1'-N1	5.79	112.84	108.20
1	SA	1392	G	N1-C6-O6	5.79	123.38	119.90
3	S7	67	C	O4'-C1'-N1	5.79	112.84	108.20
25	LA	1386	C	C5'-C4'-O4'	5.79	116.05	109.10
1	SA	736	C	O4'-C1'-N1	5.79	112.83	108.20
25	LA	1179	G	O4'-C1'-N9	5.79	112.83	108.20
25	LA	2880	C	O4'-C1'-N1	5.79	112.83	108.20
25	LA	1831	G	P-O5'-C5'	5.79	130.16	120.90
25	LA	2551	C	P-O3'-C3'	-5.79	112.75	119.70
24	S1	489	TYR	CB-CG-CD2	-5.79	117.53	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1201	A	C5'-C4'-O4'	5.79	116.05	109.10
25	LA	148	U	O4'-C1'-N1	5.79	112.83	108.20
25	LA	973	A	O4'-C1'-N9	5.79	112.83	108.20
25	LA	1035	U	O4'-C1'-N1	5.79	112.83	108.20
25	LA	1673	G	P-O3'-C3'	5.79	126.65	119.70
25	LA	1774	C	O4'-C1'-N1	5.79	112.83	108.20
25	LA	134	G	O4'-C1'-N9	5.79	112.83	108.20
25	LA	1523	U	O4'-C1'-N1	5.79	112.83	108.20
25	LA	2799	A	C5'-C4'-O4'	5.79	116.04	109.10
25	LA	746	U	O4'-C1'-N1	5.78	112.83	108.20
25	LA	796	C	C5'-C4'-C3'	-5.78	106.75	116.00
25	LA	2178	C	P-O3'-C3'	-5.78	112.76	119.70
25	LA	2488	G	C5-C6-O6	-5.78	125.13	128.60
25	LA	2705	A	O4'-C1'-N9	5.78	112.83	108.20
1	SA	774	G	C5'-C4'-C3'	5.78	125.25	116.00
1	SA	872	A	O4'-C1'-N9	5.78	112.82	108.20
1	SA	1123	U	O4'-C1'-N1	5.78	112.82	108.20
1	SA	1331	G	C8-N9-C1'	5.78	134.51	127.00
25	LA	31	C	O4'-C1'-N1	5.78	112.83	108.20
25	LA	70	G	P-O3'-C3'	5.78	126.64	119.70
25	LA	197	A	P-O3'-C3'	5.78	126.64	119.70
25	LA	512	G	O4'-C1'-N9	5.78	112.83	108.20
25	LA	1222	U	O4'-C1'-N1	5.78	112.83	108.20
25	LA	1857	G	O4'-C1'-N9	5.78	112.82	108.20
25	LA	2528	U	O4'-C1'-N1	5.78	112.83	108.20
25	LA	1961	C	O4'-C1'-N1	5.78	112.82	108.20
25	LA	2276	G	P-O5'-C5'	5.78	130.15	120.90
1	SA	410	G	C5-C6-O6	-5.78	125.13	128.60
25	LA	2338	C	P-O3'-C3'	-5.78	112.77	119.70
25	LA	2520	C	C2-N3-C4	-5.78	117.01	119.90
55	LI	38	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	SA	97	G	P-O3'-C3'	5.78	126.63	119.70
1	SA	363	A	P-O5'-C5'	-5.78	111.66	120.90
1	SA	513	C	O4'-C1'-N1	5.78	112.82	108.20
1	SA	813	U	C5'-C4'-C3'	5.78	125.24	116.00
2	S6	14	A	O4'-C1'-N9	5.77	112.82	108.20
25	LA	1024	G	P-O3'-C3'	5.77	126.63	119.70
1	SA	768	A	O4'-C1'-N9	5.77	112.82	108.20
1	SA	1414	U	O4'-C1'-N1	5.77	112.82	108.20
25	LA	612	G	O4'-C1'-N9	5.77	112.82	108.20
1	SA	647	C	O4'-C1'-N1	5.77	112.82	108.20
1	SA	1237	C	C6-N1-C2	-5.77	117.99	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1479	C	O4'-C1'-N1	5.77	112.82	108.20
2	S6	17	C	O4'-C1'-N1	5.77	112.82	108.20
25	LA	765	C	O4'-C1'-N1	5.77	112.82	108.20
25	LA	1591	A	O4'-C1'-N9	5.77	112.81	108.20
4	SJ	89	ARG	NE-CZ-NH1	5.77	123.18	120.30
25	LA	1252	G	C5-C6-O6	-5.77	125.14	128.60
25	LA	1841	U	O4'-C1'-N1	5.77	112.81	108.20
25	LA	2083	G	C4'-C3'-C2'	-5.77	96.83	102.60
25	LA	2094	A	C4'-C3'-C2'	-5.77	96.83	102.60
1	SA	158	G	C5'-C4'-O4'	5.76	116.02	109.10
25	LA	932	U	P-O3'-C3'	5.76	126.62	119.70
25	LA	1513	U	P-O5'-C5'	5.76	130.12	120.90
25	LA	2691	C	C4'-C3'-C2'	-5.76	96.83	102.60
32	LQ	18	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	S6	66	C	O4'-C1'-N1	5.76	112.81	108.20
25	LA	735	A	P-O3'-C3'	5.76	126.62	119.70
25	LA	1640	A	O4'-C1'-N9	5.76	112.81	108.20
1	SA	51	A	P-O5'-C5'	-5.76	111.68	120.90
1	SA	724	G	P-O5'-C5'	5.76	130.12	120.90
2	S6	41	C	O4'-C1'-N1	5.76	112.81	108.20
19	SE	151	MET	CG-SD-CE	-5.76	90.98	100.20
25	LA	38	A	P-O5'-C5'	5.76	130.12	120.90
25	LA	1957	C	C6-N1-C2	-5.76	118.00	120.30
1	SA	552	U	O4'-C1'-C2'	5.76	112.78	107.60
1	SA	933	G	C5-C6-O6	-5.76	125.14	128.60
1	SA	1139	G	O5'-C5'-C4'	5.76	122.64	111.70
2	S6	33	C	C2-N3-C4	-5.76	117.02	119.90
25	LA	1917	U	C3'-C2'-C1'	5.76	106.11	101.50
50	L8	94	ARG	NE-CZ-NH1	5.76	123.18	120.30
25	LA	2422	C	C4'-C3'-C2'	5.76	108.36	102.60
1	SA	806	C	O4'-C1'-N1	5.76	112.81	108.20
25	LA	1140	C	O4'-C1'-N1	5.76	112.81	108.20
1	SA	468	A	C4-N9-C1'	5.75	136.66	126.30
1	SA	529	G	O4'-C1'-N9	5.75	112.80	108.20
25	LA	830	G	O4'-C1'-N9	5.75	112.80	108.20
1	SA	566	G	N1-C6-O6	5.75	123.35	119.90
1	SA	995	C	C5'-C4'-C3'	-5.75	106.80	116.00
25	LA	544	C	O4'-C1'-N1	5.75	112.80	108.20
25	LA	953	G	C5'-C4'-C3'	5.75	125.20	116.00
25	LA	2495	G	C5'-C4'-O4'	5.75	116.00	109.10
46	L5	24	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	SA	395	C	C5'-C4'-O4'	5.75	116.00	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1091	U	C5'-C4'-O4'	5.75	116.00	109.10
1	SA	1154	G	O5'-C5'-C4'	5.75	122.63	111.70
25	LA	1906	G	C4'-C3'-C2'	-5.75	96.85	102.60
25	LA	2068	U	P-O3'-C3'	5.75	126.60	119.70
25	LA	2368	C	O4'-C1'-N1	5.75	112.80	108.20
25	LA	2549	G	C5'-C4'-C3'	5.75	125.20	116.00
25	LA	1605	C	O4'-C1'-N1	5.75	112.80	108.20
1	SA	413	G	C5-C6-O6	-5.75	125.15	128.60
25	LA	561	G	C4'-C3'-C2'	-5.75	96.85	102.60
25	LA	2043	C	O4'-C1'-N1	5.75	112.80	108.20
25	LA	2133	G	C1'-O4'-C4'	-5.75	105.30	109.90
25	LA	2707	U	O4'-C1'-N1	5.75	112.80	108.20
39	LW	52	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	SA	132	C	O4'-C1'-N1	5.75	112.80	108.20
1	SA	1014	A	C2'-C3'-O3'	5.75	122.89	113.70
1	SA	1280	A	C4'-C3'-C2'	-5.74	96.86	102.60
24	S1	548	TYR	CB-CG-CD1	5.74	124.45	121.00
25	LA	853	C	C5'-C4'-C3'	-5.74	106.81	116.00
25	LA	1187	G	N1-C6-O6	5.74	123.35	119.90
25	LA	2255	G	C5'-C4'-O4'	5.74	115.99	109.10
25	LA	2891	U	O4'-C1'-N1	5.74	112.80	108.20
47	L6	79	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	SA	825	A	O4'-C1'-N9	5.74	112.79	108.20
1	SA	1104	G	O4'-C1'-N9	5.74	112.79	108.20
25	LA	2321	U	C3'-C2'-C1'	5.74	106.09	101.50
25	LA	38	A	C5'-C4'-O4'	5.74	115.99	109.10
25	LA	930	G	O4'-C1'-N9	5.74	112.79	108.20
25	LA	2237	G	C5'-C4'-C3'	-5.74	106.81	116.00
1	SA	970	C	O4'-C1'-N1	5.74	112.79	108.20
3	S7	5	G	O4'-C1'-N9	5.74	112.79	108.20
25	LA	2523	G	C5-C6-O6	-5.74	125.16	128.60
25	LA	2566	A	P-O5'-C5'	-5.74	111.72	120.90
26	LB	49	C	O4'-C1'-N1	5.74	112.79	108.20
25	LA	1209	U	C4'-C3'-C2'	-5.74	96.86	102.60
25	LA	1903	G	O4'-C1'-N9	5.74	112.79	108.20
1	SA	1441	A	C4'-C3'-C2'	-5.74	96.86	102.60
25	LA	216	A	O4'-C1'-N9	5.74	112.79	108.20
25	LA	720	U	O4'-C1'-N1	5.74	112.79	108.20
25	LA	1003	G	C5'-C4'-C3'	5.74	125.18	116.00
25	LA	2613	U	O4'-C1'-N1	5.74	112.79	108.20
25	LA	2804	U	O4'-C1'-N1	5.74	112.79	108.20
26	LB	78	A	C5'-C4'-C3'	-5.74	106.82	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	982	U	P-O5'-C5'	-5.73	111.73	120.90
25	LA	386	G	C5-C6-O6	-5.73	125.16	128.60
1	SA	317	U	O4'-C1'-N1	5.73	112.79	108.20
1	SA	467	U	O4'-C1'-N1	5.73	112.79	108.20
5	SK	6	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	SA	255	G	C5'-C4'-C3'	-5.73	106.83	116.00
1	SA	429	U	C4'-C3'-C2'	-5.73	96.87	102.60
3	S7	63	G	N1-C6-O6	5.73	123.34	119.90
25	LA	2607	G	P-O5'-C5'	5.73	130.07	120.90
26	LB	86	G	C4-N9-C1'	-5.73	119.05	126.50
26	LB	87	U	C5'-C4'-O4'	5.73	115.98	109.10
25	LA	2435	A	N1-C6-N6	-5.73	115.16	118.60
1	SA	1423	G	O4'-C1'-N9	5.73	112.78	108.20
25	LA	946	C	P-O3'-C3'	-5.73	112.83	119.70
25	LA	2336	A	P-O5'-C5'	5.73	130.06	120.90
25	LA	2345	G	C5'-C4'-O4'	5.73	115.97	109.10
25	LA	662	G	P-O3'-C3'	-5.73	112.83	119.70
25	LA	923	G	C5'-C4'-O4'	5.73	115.97	109.10
26	LB	3	C	O4'-C1'-N1	5.73	112.78	108.20
1	SA	514	C	O4'-C1'-N1	5.72	112.78	108.20
1	SA	590	U	C5'-C4'-C3'	-5.72	106.84	116.00
25	LA	2571	U	P-O5'-C5'	5.72	130.06	120.90
25	LA	2710	C	O4'-C1'-N1	5.72	112.78	108.20
25	LA	2715	C	O4'-C1'-N1	5.72	112.78	108.20
26	LB	54	G	P-O5'-C5'	5.72	130.06	120.90
1	SA	822	U	O4'-C1'-N1	5.72	112.78	108.20
25	LA	14	A	C5'-C4'-C3'	-5.72	106.84	116.00
23	SI	45	MET	CG-SD-CE	-5.72	91.05	100.20
25	LA	475	C	P-O5'-C5'	5.72	130.05	120.90
25	LA	2537	U	P-O5'-C5'	-5.72	111.75	120.90
1	SA	51	A	C4-N9-C1'	5.72	136.59	126.30
25	LA	1443	U	O4'-C1'-N1	5.72	112.77	108.20
25	LA	1581	G	C5-C6-O6	-5.72	125.17	128.60
25	LA	2065	C	C6-N1-C2	-5.72	118.01	120.30
1	SA	626	G	C5-C6-O6	-5.71	125.17	128.60
25	LA	1968	G	C5'-C4'-C3'	-5.71	106.86	116.00
25	LA	2654	A	C5'-C4'-O4'	5.71	115.96	109.10
47	L6	102	ARG	NE-CZ-NH2	5.71	123.16	120.30
52	LF	92	MET	CG-SD-CE	-5.71	91.06	100.20
1	SA	173	U	O3'-P-O5'	-5.71	93.14	104.00
1	SA	632	U	C6-N1-C1'	-5.71	113.20	121.20
25	LA	499	U	O4'-C1'-N1	5.71	112.77	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	862	G	P-O3'-C3'	5.71	126.56	119.70
25	LA	2052	A	C4'-C3'-C2'	-5.71	96.89	102.60
25	LA	2387	U	P-O3'-C3'	5.71	126.55	119.70
25	LA	2557	G	C5'-C4'-O4'	5.71	115.95	109.10
25	LA	2827	C	O4'-C1'-N1	5.71	112.77	108.20
3	S7	1	G	C5-C6-O6	-5.71	125.17	128.60
25	LA	2680	U	O4'-C1'-N1	5.71	112.77	108.20
25	LA	175	G	O4'-C1'-N9	5.71	112.77	108.20
25	LA	1573	G	O4'-C1'-N9	5.71	112.77	108.20
26	LB	62	C	O4'-C1'-N1	5.71	112.77	108.20
1	SA	766	A	O3'-P-O5'	-5.71	93.16	104.00
1	SA	1437	A	C5'-C4'-O4'	5.71	115.95	109.10
14	SB	135	MET	CG-SD-CE	-5.71	91.07	100.20
25	LA	953	G	O4'-C1'-N9	5.71	112.77	108.20
26	LB	3	C	C6-N1-C2	-5.71	118.02	120.30
25	LA	463	G	C5'-C4'-O4'	5.71	115.95	109.10
1	SA	370	C	P-O5'-C5'	5.70	130.03	120.90
1	SA	581	G	C5-C6-O6	-5.70	125.18	128.60
1	SA	1533	C	C2-N1-C1'	5.70	125.07	118.80
25	LA	57	C	C5'-C4'-C3'	5.70	125.13	116.00
25	LA	1497	U	C2-N1-C1'	5.70	124.54	117.70
25	LA	1557	C	C6-N1-C2	-5.70	118.02	120.30
52	LF	99	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	SA	415	A	C5'-C4'-O4'	5.70	115.94	109.10
25	LA	304	U	O4'-C1'-N1	5.70	112.76	108.20
25	LA	1715	G	C5-C6-O6	-5.70	125.18	128.60
1	SA	979	C	C6-N1-C2	-5.70	118.02	120.30
3	S7	9	A	O4'-C1'-N9	5.70	112.76	108.20
14	SB	73	ARG	NE-CZ-NH1	5.70	123.15	120.30
25	LA	386	G	C4'-C3'-C2'	-5.70	96.90	102.60
25	LA	1515	A	C4'-C3'-C2'	-5.70	96.90	102.60
25	LA	1813	G	O4'-C1'-N9	5.70	112.76	108.20
25	LA	1911	U	N1-C2-N3	5.70	118.32	114.90
1	SA	599	C	O4'-C1'-N1	5.70	112.76	108.20
25	LA	2316	G	O4'-C1'-N9	5.70	112.76	108.20
1	SA	726	C	O4'-C1'-N1	5.70	112.76	108.20
1	SA	1222	G	O4'-C1'-N9	5.70	112.76	108.20
1	SA	1260	G	O4'-C1'-N9	5.70	112.76	108.20
25	LA	1313	U	N3-C2-O2	-5.70	118.21	122.20
26	LB	4	C	O4'-C1'-N1	5.70	112.76	108.20
1	SA	278	G	P-O3'-C3'	-5.70	112.87	119.70
1	SA	1374	A	C4'-C3'-C2'	-5.70	96.91	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	130	C	C5'-C4'-O4'	5.70	115.93	109.10
25	LA	511	U	C2-N1-C1'	-5.70	110.87	117.70
25	LA	700	G	C4'-C3'-C2'	-5.70	96.91	102.60
25	LA	1802	A	P-O3'-C3'	5.70	126.53	119.70
25	LA	1827	U	O4'-C1'-N1	5.70	112.76	108.20
25	LA	2060	A	P-O3'-C3'	5.70	126.54	119.70
25	LA	2356	U	O4'-C1'-N1	5.70	112.76	108.20
1	SA	1276	G	O4'-C1'-N9	5.69	112.75	108.20
25	LA	20	C	C5'-C4'-C3'	5.69	125.11	116.00
25	LA	290	U	O4'-C1'-N1	5.69	112.75	108.20
25	LA	1399	C	O4'-C1'-N1	5.69	112.75	108.20
30	LO	23	TYR	CB-CG-CD2	5.69	124.42	121.00
25	LA	1925	C	C6-N1-C2	-5.69	118.02	120.30
1	SA	157	U	O4'-C1'-N1	5.69	112.75	108.20
1	SA	701	U	OP2-P-O3'	5.69	117.71	105.20
1	SA	894	G	O4'-C1'-N9	5.69	112.75	108.20
25	LA	704	G	C5'-C4'-C3'	5.69	125.10	116.00
25	LA	1147	A	C5'-C4'-C3'	5.69	125.10	116.00
25	LA	1200	C	C6-N1-C2	-5.69	118.03	120.30
21	SG	3	ARG	NE-CZ-NH1	5.69	123.14	120.30
25	LA	116	C	O4'-C1'-N1	5.69	112.75	108.20
25	LA	867	C	P-O3'-C3'	5.69	126.52	119.70
25	LA	1483	G	P-O5'-C5'	5.69	130.00	120.90
1	SA	370	C	O4'-C1'-N1	5.68	112.75	108.20
1	SA	693	G	C8-N9-C1'	-5.68	119.61	127.00
25	LA	132	G	O4'-C1'-N9	5.68	112.75	108.20
25	LA	2410	G	O4'-C1'-N9	5.68	112.75	108.20
25	LA	2651	C	P-O5'-C5'	5.68	130.00	120.90
1	SA	147	G	O4'-C1'-N9	5.68	112.75	108.20
1	SA	319	G	O4'-C1'-N9	5.68	112.75	108.20
1	SA	1121	U	C5'-C4'-O4'	5.68	115.92	109.10
25	LA	1012	U	P-O3'-C3'	5.68	126.52	119.70
25	LA	1816	C	O4'-C1'-N1	5.68	112.75	108.20
25	LA	2539	C	P-O3'-C3'	-5.68	112.88	119.70
1	SA	713	G	N1-C6-O6	5.68	123.31	119.90
25	LA	1964	G	O3'-P-O5'	5.68	114.80	104.00
1	SA	273	U	P-O5'-C5'	5.68	129.99	120.90
1	SA	960	U	O3'-P-O5'	5.68	114.79	104.00
1	SA	1183	U	P-O3'-C3'	5.68	126.52	119.70
14	SB	49	PHE	CB-CG-CD2	5.68	124.78	120.80
25	LA	472	A	C5'-C4'-O4'	5.68	115.92	109.10
25	LA	807	U	O4'-C1'-N1	5.68	112.74	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1434	A	O4'-C1'-N9	5.68	112.74	108.20
25	LA	1560	G	C5'-C4'-C3'	-5.68	106.91	116.00
25	LA	2544	G	C6-N1-C2	-5.68	121.69	125.10
25	LA	2580	U	O4'-C1'-N1	5.68	112.74	108.20
25	LA	1337	G	C5-C6-O6	-5.68	125.19	128.60
25	LA	2279	G	O4'-C1'-N9	5.68	112.74	108.20
1	SA	273	U	C4'-C3'-C2'	-5.67	96.92	102.60
1	SA	857	C	C5'-C4'-C3'	5.67	125.08	116.00
3	S7	8	U	P-O5'-C5'	5.67	129.98	120.90
25	LA	878	A	C5'-C4'-C3'	-5.67	106.92	116.00
1	SA	790	A	C5-C6-N6	-5.67	119.16	123.70
1	SA	1165	U	O4'-C1'-N1	5.67	112.74	108.20
25	LA	220	G	N1-C6-O6	5.67	123.30	119.90
25	LA	1358	G	N1-C6-O6	5.67	123.30	119.90
49	L7	91	ARG	N-CA-CB	5.67	120.81	110.60
50	L8	74	MET	CG-SD-CE	-5.67	91.13	100.20
51	L9	25	TYR	CB-CG-CD2	5.67	124.40	121.00
3	S7	24	G	O4'-C1'-N9	5.67	112.74	108.20
3	S7	67	C	C6-N1-C2	-5.67	118.03	120.30
25	LA	371	A	C5'-C4'-C3'	5.67	125.07	116.00
25	LA	2030	C	C5-C6-N1	5.67	123.83	121.00
25	LA	2355	G	C5'-C4'-C3'	5.67	125.07	116.00
25	LA	2579	C	C3'-C2'-C1'	-5.67	96.97	101.50
25	LA	2889	C	O4'-C1'-N1	5.67	112.73	108.20
1	SA	217	C	C6-N1-C2	-5.67	118.03	120.30
1	SA	1181	G	C5'-C4'-C3'	-5.67	106.93	116.00
25	LA	1213	A	C5'-C4'-C3'	-5.67	106.93	116.00
25	LA	1638	C	C6-N1-C2	-5.67	118.03	120.30
25	LA	2831	G	N1-C6-O6	5.67	123.30	119.90
25	LA	584	C	O4'-C1'-N1	5.67	112.73	108.20
25	LA	644	A	P-O5'-C5'	-5.67	111.84	120.90
1	SA	1300	G	C5-C6-O6	-5.66	125.20	128.60
25	LA	94	A	P-O5'-C5'	5.66	129.96	120.90
25	LA	295	G	C5'-C4'-O4'	5.66	115.90	109.10
1	SA	752	G	O3'-P-O5'	-5.66	93.24	104.00
25	LA	11	C	O4'-C1'-N1	5.66	112.73	108.20
1	SA	767	A	O4'-C1'-N9	5.66	112.73	108.20
3	S7	57	G	P-O5'-C5'	-5.66	111.84	120.90
25	LA	1282	U	C2'-C3'-O3'	5.66	122.76	113.70
25	LA	1675	C	C2-N3-C4	-5.66	117.07	119.90
25	LA	1683	U	O4'-C1'-N1	5.66	112.73	108.20
25	LA	1143	A	C4-N9-C1'	-5.66	116.12	126.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2252	G	P-O5'-C5'	5.66	129.95	120.90
1	SA	938	A	P-O5'-C5'	-5.66	111.85	120.90
25	LA	545	U	O4'-C1'-N1	5.66	112.73	108.20
25	LA	635	C	C5'-C4'-O4'	5.66	115.89	109.10
25	LA	663	G	P-O3'-C3'	-5.66	112.91	119.70
25	LA	1220	G	O4'-C1'-N9	5.66	112.73	108.20
25	LA	1721	G	C5-C6-O6	-5.66	125.21	128.60
25	LA	1836	C	O4'-C1'-N1	5.66	112.73	108.20
1	SA	1028	C	O4'-C1'-N1	5.66	112.72	108.20
21	SG	69	ARG	NE-CZ-NH1	5.66	123.13	120.30
25	LA	1355	G	P-O3'-C3'	5.66	126.49	119.70
56	LJ	1	MET	CG-SD-CE	-5.66	91.15	100.20
25	LA	765	C	C4'-C3'-C2'	-5.65	96.95	102.60
1	SA	1345	U	C5'-C4'-C3'	-5.65	106.95	116.00
2	S6	23	G	C5-C6-O6	-5.65	125.21	128.60
25	LA	785	G	O4'-C1'-N9	5.65	112.72	108.20
25	LA	1371	G	C5-C6-O6	-5.65	125.21	128.60
32	LQ	25	ARG	NE-CZ-NH1	5.65	123.13	120.30
25	LA	1093	G	O4'-C1'-N9	5.65	112.72	108.20
1	SA	546	A	P-O5'-C5'	-5.65	111.86	120.90
25	LA	335	C	O4'-C1'-N1	5.65	112.72	108.20
25	LA	1644	C	C5'-C4'-C3'	-5.65	106.97	116.00
25	LA	1840	G	O4'-C1'-N9	5.65	112.72	108.20
25	LA	2822	G	C5-C6-O6	-5.65	125.21	128.60
1	SA	129	A	P-O3'-C3'	5.65	126.48	119.70
25	LA	138	U	C5'-C4'-O4'	5.65	115.88	109.10
25	LA	2708	G	O4'-C1'-N9	5.65	112.72	108.20
26	LB	118	C	O4'-C1'-N1	5.65	112.72	108.20
1	SA	428	G	P-O3'-C3'	5.64	126.47	119.70
25	LA	29	U	C6-N1-C1'	5.64	129.10	121.20
25	LA	1045	C	C6-N1-C1'	-5.64	114.03	120.80
25	LA	2544	G	O4'-C1'-N9	5.64	112.72	108.20
1	SA	1251	A	N1-C6-N6	-5.64	115.21	118.60
25	LA	727	A	P-O3'-C3'	5.64	126.47	119.70
25	LA	1842	G	O4'-C1'-N9	5.64	112.71	108.20
25	LA	2135	A	C5'-C4'-C3'	5.64	125.03	116.00
1	SA	343	U	C5'-C4'-C3'	-5.64	106.98	116.00
1	SA	858	G	N1-C6-O6	5.64	123.28	119.90
25	LA	516	C	C2-N3-C4	-5.64	117.08	119.90
25	LA	1052	C	O4'-C1'-N1	5.64	112.71	108.20
26	LB	21	G	O4'-C1'-N9	5.64	112.71	108.20
25	LA	2032	G	C5-C6-O6	-5.64	125.22	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2494	G	C5-C6-O6	-5.64	125.22	128.60
25	LA	2616	C	O4'-C1'-N1	5.64	112.71	108.20
25	LA	2665	A	N9-C1'-C2'	-5.64	105.80	112.00
25	LA	69	C	O4'-C1'-N1	5.64	112.71	108.20
25	LA	675	A	O4'-C1'-N9	5.64	112.71	108.20
25	LA	1366	A	C5-C6-N6	5.64	128.21	123.70
25	LA	1867	G	O4'-C1'-N9	5.64	112.71	108.20
25	LA	2714	G	P-O5'-C5'	5.64	129.92	120.90
1	SA	24	U	O4'-C1'-N1	5.63	112.71	108.20
1	SA	476	U	O4'-C1'-N1	5.63	112.71	108.20
1	SA	1207	G	N1-C6-O6	5.63	123.28	119.90
25	LA	1477	A	O4'-C1'-N9	5.63	112.71	108.20
25	LA	1793	C	C2-N1-C1'	-5.63	112.60	118.80
25	LA	2548	U	C4'-C3'-C2'	-5.63	96.97	102.60
1	SA	604	G	C5-C6-O6	-5.63	125.22	128.60
1	SA	287	U	O4'-C1'-N1	5.63	112.70	108.20
1	SA	1394	A	P-O3'-C3'	5.63	126.46	119.70
25	LA	2114	A	N1-C6-N6	-5.63	115.22	118.60
25	LA	2495	G	C5'-C4'-C3'	-5.63	106.99	116.00
1	SA	944	G	P-O3'-C3'	5.63	126.45	119.70
1	SA	1193	G	C4-N9-C1'	-5.63	119.18	126.50
25	LA	1158	C	P-O5'-C5'	-5.63	111.90	120.90
25	LA	1901	A	C5-C6-N6	5.63	128.20	123.70
25	LA	2348	U	O4'-C1'-N1	5.63	112.70	108.20
25	LA	2694	G	O4'-C1'-N9	5.63	112.70	108.20
1	SA	1525	G	O4'-C1'-N9	5.63	112.70	108.20
25	LA	285	G	O4'-C1'-N9	5.63	112.70	108.20
25	LA	254	G	O4'-C1'-N9	5.62	112.70	108.20
1	SA	266	G	N1-C6-O6	5.62	123.28	119.90
1	SA	1217	C	O4'-C1'-N1	5.62	112.70	108.20
25	LA	2267	A	C8-N9-C1'	5.62	137.82	127.70
39	LW	7	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	SA	323	U	P-O5'-C5'	5.62	129.89	120.90
1	SA	474	G	O4'-C1'-N9	5.62	112.70	108.20
25	LA	1312	U	P-O3'-C3'	-5.62	112.95	119.70
1	SA	1235	U	C5'-C4'-C3'	-5.62	107.01	116.00
25	LA	1715	G	N1-C6-O6	5.62	123.27	119.90
25	LA	1403	A	O4'-C1'-N9	5.62	112.69	108.20
25	LA	1838	C	P-O3'-C3'	-5.62	112.96	119.70
25	LA	2424	C	C5'-C4'-C3'	-5.62	107.01	116.00
25	LA	2505	G	C1'-O4'-C4'	-5.62	105.41	109.90
1	SA	324	G	C5-C6-O6	-5.62	125.23	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1777	U	P-O5'-C5'	-5.62	111.92	120.90
1	SA	34	C	O4'-C1'-N1	5.61	112.69	108.20
25	LA	1400	U	O4'-C1'-N1	5.61	112.69	108.20
25	LA	1405	U	O4'-C1'-N1	5.61	112.69	108.20
25	LA	2441	U	P-O5'-C5'	5.61	129.88	120.90
25	LA	1135	C	P-O3'-C3'	5.61	126.43	119.70
1	SA	1083	U	O4'-C1'-N1	5.61	112.69	108.20
25	LA	1086	A	O3'-P-O5'	-5.61	93.34	104.00
25	LA	2668	G	O4'-C1'-N9	5.61	112.69	108.20
25	LA	166	U	O4'-C1'-N1	5.61	112.69	108.20
25	LA	1532	A	C5'-C4'-O4'	5.61	115.83	109.10
25	LA	2452	C	C1'-O4'-C4'	-5.61	105.41	109.90
1	SA	1207	G	C1'-O4'-C4'	-5.61	105.42	109.90
3	S7	40	C	C6-N1-C2	-5.61	118.06	120.30
14	SB	62	ARG	NE-CZ-NH1	5.61	123.10	120.30
24	S1	686	TYR	CB-CG-CD1	-5.61	117.64	121.00
25	LA	262	A	O4'-C1'-N9	5.61	112.68	108.20
25	LA	1282	U	O4'-C1'-N1	5.61	112.68	108.20
25	LA	1343	G	P-O3'-C3'	5.61	126.43	119.70
25	LA	1457	U	P-O3'-C3'	5.61	126.43	119.70
1	SA	1071	C	C5-C6-N1	5.60	123.80	121.00
24	S1	2	ARG	NE-CZ-NH1	5.60	123.10	120.30
25	LA	36	G	C5-C6-O6	-5.60	125.24	128.60
25	LA	311	A	C1'-O4'-C4'	-5.60	105.42	109.90
25	LA	1241	A	C6-N1-C2	-5.60	115.24	118.60
25	LA	1926	U	C4'-C3'-C2'	-5.60	97.00	102.60
25	LA	2448	A	O4'-C4'-C3'	-5.60	98.40	104.00
26	LB	60	C	P-O5'-C5'	5.60	129.86	120.90
25	LA	782	A	C5'-C4'-C3'	-5.60	107.04	116.00
25	LA	2440	C	O4'-C1'-N1	5.60	112.68	108.20
1	SA	396	C	P-O5'-C5'	5.60	129.86	120.90
1	SA	1019	A	O4'-C1'-N9	5.60	112.68	108.20
25	LA	872	U	C5'-C4'-O4'	5.60	115.82	109.10
25	LA	1241	A	C5'-C4'-C3'	-5.60	107.04	116.00
25	LA	1530	G	C5'-C4'-O4'	5.60	115.82	109.10
25	LA	2730	C	C4'-C3'-C2'	-5.60	97.00	102.60
34	LS	93	ARG	NE-CZ-NH1	5.60	123.10	120.30
11	SQ	76	ARG	NE-CZ-NH2	-5.60	117.50	120.30
25	LA	1320	C	C3'-C2'-C1'	-5.60	97.02	101.50
25	LA	1991	U	C5'-C4'-C3'	5.60	124.96	116.00
25	LA	2325	G	C1'-O4'-C4'	-5.60	105.42	109.90
51	L9	51	ARG	NE-CZ-NH2	-5.60	117.50	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	405	U	O4'-C1'-N1	5.60	112.68	108.20
1	SA	449	G	O4'-C1'-N9	5.60	112.68	108.20
1	SA	1153	G	O4'-C1'-N9	5.60	112.68	108.20
25	LA	336	C	C5'-C4'-O4'	5.60	115.81	109.10
1	SA	877	G	O4'-C1'-N9	5.59	112.67	108.20
1	SA	1087	G	O4'-C1'-N9	5.59	112.68	108.20
25	LA	868	U	C5'-C4'-C3'	-5.59	107.05	116.00
25	LA	1926	U	C6-N1-C1'	-5.59	113.37	121.20
25	LA	1492	G	O4'-C1'-N9	5.59	112.67	108.20
26	LB	57	A	N1-C6-N6	5.59	121.96	118.60
1	SA	111	G	O4'-C1'-N9	5.59	112.67	108.20
25	LA	144	A	C5'-C4'-C3'	-5.59	107.05	116.00
25	LA	671	C	O4'-C1'-N1	5.59	112.67	108.20
25	LA	826	U	O4'-C1'-N1	5.59	112.67	108.20
25	LA	1164	C	C5'-C4'-C3'	-5.59	107.05	116.00
25	LA	1782	U	N3-C2-O2	-5.59	118.29	122.20
25	LA	811	U	N1-C2-O2	5.59	126.71	122.80
25	LA	1695	G	C5-C6-O6	-5.59	125.25	128.60
25	LA	2124	G	O4'-C1'-N9	5.59	112.67	108.20
25	LA	2443	C	C6-N1-C2	-5.59	118.06	120.30
25	LA	2431	U	C5'-C4'-O4'	5.59	115.81	109.10
1	SA	1244	G	O4'-C1'-N9	5.59	112.67	108.20
1	SA	1309	G	O4'-C1'-N9	5.59	112.67	108.20
25	LA	379	G	C4'-C3'-C2'	-5.59	97.01	102.60
25	LA	1761	C	O4'-C1'-N1	5.59	112.67	108.20
25	LA	2527	C	O4'-C1'-N1	5.59	112.67	108.20
1	SA	1183	U	O4'-C1'-N1	5.58	112.67	108.20
1	SA	1337	G	P-O3'-C3'	5.58	126.40	119.70
2	S6	12	G	O4'-C1'-N9	5.58	112.67	108.20
25	LA	1709	U	O4'-C1'-N1	5.58	112.67	108.20
1	SA	445	G	O4'-C1'-N9	5.58	112.67	108.20
1	SA	861	G	O4'-C1'-N9	5.58	112.67	108.20
1	SA	1480	A	O4'-C1'-N9	5.58	112.67	108.20
25	LA	421	C	O4'-C1'-N1	5.58	112.67	108.20
25	LA	2317	A	O4'-C1'-N9	5.58	112.67	108.20
25	LA	2385	C	C1'-O4'-C4'	-5.58	105.44	109.90
1	SA	878	A	O4'-C1'-N9	5.58	112.66	108.20
1	SA	891	U	C5'-C4'-O4'	5.58	115.80	109.10
25	LA	377	G	C5'-C4'-C3'	-5.58	107.07	116.00
1	SA	1208	C	C4'-C3'-C2'	-5.58	97.02	102.60
25	LA	14	A	O4'-C1'-N9	5.58	112.66	108.20
25	LA	1567	G	O4'-C1'-N9	5.58	112.66	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1729	U	O4'-C1'-N1	5.58	112.66	108.20
25	LA	2200	C	C6-N1-C2	-5.58	118.07	120.30
1	SA	890	G	C1'-O4'-C4'	-5.58	105.44	109.90
25	LA	333	G	P-O5'-C5'	-5.58	111.98	120.90
25	LA	1223	G	N1-C6-O6	5.58	123.25	119.90
57	LK	15	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	SA	470	C	O4'-C1'-N1	5.58	112.66	108.20
25	LA	1283	G	O4'-C1'-N9	5.57	112.66	108.20
1	SA	791	G	C5-C6-O6	-5.57	125.26	128.60
1	SA	1133	G	O3'-P-O5'	-5.57	93.42	104.00
18	SD	75	TYR	CB-CG-CD2	-5.57	117.66	121.00
25	LA	744	U	C4'-C3'-C2'	-5.57	97.03	102.60
25	LA	1165	A	O4'-C1'-N9	5.57	112.66	108.20
25	LA	1363	C	C6-N1-C2	-5.57	118.07	120.30
25	LA	2017	U	C5'-C4'-O4'	5.57	115.79	109.10
28	LM	102	ARG	NE-CZ-NH1	5.57	123.09	120.30
25	LA	185	G	O4'-C1'-N9	5.57	112.66	108.20
25	LA	737	C	C4'-C3'-C2'	-5.57	97.03	102.60
25	LA	889	C	O4'-C1'-N1	5.57	112.66	108.20
1	SA	824	G	O4'-C1'-N9	5.57	112.65	108.20
1	SA	1099	G	O4'-C1'-N9	5.57	112.65	108.20
1	SA	1171	A	O4'-C1'-N9	5.57	112.66	108.20
25	LA	1077	A	O4'-C1'-N9	5.57	112.65	108.20
25	LA	1194	A	O4'-C1'-N9	5.57	112.65	108.20
25	LA	1736	U	O4'-C1'-N1	5.57	112.65	108.20
25	LA	1743	G	C5'-C4'-C3'	-5.57	107.09	116.00
1	SA	742	G	O4'-C1'-N9	5.57	112.65	108.20
25	LA	2335	A	P-O3'-C3'	5.57	126.38	119.70
1	SA	617	G	C5'-C4'-C3'	-5.56	107.10	116.00
2	S6	10	G	O4'-C1'-N9	5.56	112.65	108.20
25	LA	2734	A	O4'-C1'-N9	5.56	112.65	108.20
25	LA	2779	U	C1'-O4'-C4'	-5.56	105.45	109.90
1	SA	815	A	P-O3'-C3'	-5.56	113.03	119.70
25	LA	195	A	O4'-C1'-N9	5.56	112.65	108.20
25	LA	1385	A	C5'-C4'-C3'	-5.56	107.10	116.00
25	LA	2016	U	O4'-C1'-N1	5.56	112.65	108.20
30	LO	52	ARG	NE-CZ-NH1	5.56	123.08	120.30
34	LS	5	ARG	NE-CZ-NH2	-5.56	117.52	120.30
25	LA	1456	G	O4'-C1'-N9	5.56	112.65	108.20
25	LA	2720	U	O4'-C1'-N1	5.56	112.65	108.20
1	SA	781	A	C1'-O4'-C4'	-5.56	105.45	109.90
1	SA	1395	C	C6-N1-C2	-5.56	118.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	475	C	O4'-C1'-N1	5.56	112.65	108.20
25	LA	929	U	O4'-C1'-N1	5.56	112.65	108.20
25	LA	1609	A	O4'-C1'-C2'	-5.56	100.24	105.80
25	LA	1656	C	C5'-C4'-O4'	5.56	115.77	109.10
25	LA	1757	A	C2'-C3'-O3'	5.56	122.59	113.70
25	LA	2161	C	O4'-C1'-N1	5.56	112.65	108.20
30	LO	29	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	SA	1305	G	C2'-C3'-O3'	5.56	122.59	113.70
1	SA	1458	G	O4'-C1'-N9	5.56	112.64	108.20
25	LA	45	G	P-O3'-C3'	5.56	126.37	119.70
25	LA	732	C	P-O5'-C5'	5.56	129.79	120.90
25	LA	2486	C	C5'-C4'-O4'	5.56	115.77	109.10
25	LA	2583	G	O4'-C1'-N9	5.56	112.65	108.20
1	SA	1399	C	P-O5'-C5'	-5.56	112.01	120.90
25	LA	937	C	C4'-C3'-C2'	-5.56	97.04	102.60
1	SA	171	A	O4'-C1'-N9	5.55	112.64	108.20
25	LA	652	U	O4'-C1'-N1	5.55	112.64	108.20
25	LA	1172	C	O4'-C1'-N1	5.55	112.64	108.20
25	LA	1553	A	O4'-C1'-N9	5.55	112.64	108.20
25	LA	1994	C	O3'-P-O5'	5.55	114.55	104.00
26	LB	92	C	O4'-C1'-N1	5.55	112.64	108.20
25	LA	1141	U	C5'-C4'-C3'	-5.55	107.11	116.00
1	SA	206	C	C5'-C4'-O4'	5.55	115.76	109.10
1	SA	235	C	C5'-C4'-O4'	5.55	115.76	109.10
1	SA	940	C	O4'-C1'-N1	5.55	112.64	108.20
1	SA	1459	G	O4'-C1'-N9	5.55	112.64	108.20
3	S7	61	C	C5'-C4'-O4'	5.55	115.76	109.10
1	SA	450	G	P-O3'-C3'	-5.55	113.04	119.70
25	LA	597	G	O4'-C1'-N9	5.55	112.64	108.20
25	LA	1763	G	C4'-C3'-C2'	-5.55	97.05	102.60
1	SA	738	C	O4'-C1'-N1	5.55	112.64	108.20
25	LA	2743	U	O4'-C1'-N1	5.55	112.64	108.20
25	LA	2763	G	P-O3'-C3'	5.55	126.36	119.70
25	LA	697	G	C5-C6-O6	-5.55	125.27	128.60
1	SA	83	C	C1'-O4'-C4'	-5.54	105.46	109.90
1	SA	1170	A	P-O3'-C3'	-5.54	113.05	119.70
2	S6	27	G	P-O3'-C3'	-5.54	113.05	119.70
1	SA	39	G	C5'-C4'-C3'	5.54	124.87	116.00
1	SA	578	C	C5'-C4'-O4'	5.54	115.75	109.10
1	SA	662	U	P-O5'-C5'	-5.54	112.03	120.90
1	SA	1168	U	C2-N1-C1'	5.54	124.35	117.70
1	SA	563	A	C1'-O4'-C4'	-5.54	105.47	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S7	30	G	O4'-C1'-N9	5.54	112.63	108.20
25	LA	674	G	C4'-C3'-C2'	-5.54	97.06	102.60
25	LA	842	U	O4'-C1'-N1	5.54	112.63	108.20
25	LA	1510	G	C8-N9-C1'	-5.54	119.80	127.00
1	SA	92	U	O4'-C1'-N1	5.54	112.63	108.20
1	SA	1095	U	O4'-C1'-N1	5.54	112.63	108.20
1	SA	127	G	O4'-C1'-N9	5.54	112.63	108.20
1	SA	131	A	O4'-C1'-N9	5.54	112.63	108.20
25	LA	991	C	O4'-C1'-N1	5.54	112.63	108.20
25	LA	1484	U	O4'-C1'-N1	5.54	112.63	108.20
25	LA	1843	C	C5'-C4'-C3'	-5.54	107.14	116.00
25	LA	1904	G	C5'-C4'-C3'	-5.54	107.14	116.00
25	LA	2222	C	C4'-C3'-C2'	-5.54	97.06	102.60
25	LA	1070	A	C3'-C2'-C1'	-5.54	97.07	101.50
9	SO	57	ARG	NE-CZ-NH1	5.54	123.07	120.30
25	LA	939	G	P-O5'-C5'	-5.54	112.04	120.90
25	LA	2322	A	C5'-C4'-C3'	5.54	124.86	116.00
25	LA	2650	U	P-O3'-C3'	-5.54	113.06	119.70
50	L8	54	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	SA	178	C	O4'-C1'-N1	5.53	112.63	108.20
25	LA	1297	C	C5'-C4'-C3'	5.53	124.85	116.00
25	LA	2851	A	O4'-C1'-N9	5.53	112.63	108.20
25	LA	2873	A	O4'-C1'-N9	5.53	112.63	108.20
26	LB	35	C	C6-N1-C1'	-5.53	114.16	120.80
1	SA	774	G	O4'-C1'-N9	5.53	112.62	108.20
1	SA	1409	C	O4'-C1'-N1	5.53	112.62	108.20
25	LA	22	C	C4'-C3'-C2'	-5.53	97.07	102.60
25	LA	488	G	P-O5'-C5'	5.53	129.75	120.90
25	LA	1530	G	C5'-C4'-C3'	-5.53	107.15	116.00
25	LA	1659	G	O4'-C1'-N9	5.53	112.62	108.20
18	SD	103	ARG	NE-CZ-NH1	5.53	123.06	120.30
25	LA	1374	G	C5-C6-O6	-5.53	125.28	128.60
25	LA	2464	G	O4'-C1'-N9	5.53	112.62	108.20
1	SA	1083	U	P-O3'-C3'	5.53	126.33	119.70
1	SA	1436	U	C5'-C4'-C3'	-5.53	107.16	116.00
25	LA	246	C	C5'-C4'-O4'	5.53	115.73	109.10
25	LA	1359	A	C1'-O4'-C4'	-5.53	105.48	109.90
25	LA	1965	C	O4'-C4'-C3'	5.53	110.52	106.10
25	LA	2418	A	O4'-C1'-N9	5.53	112.62	108.20
1	SA	191	G	O4'-C1'-N9	5.53	112.62	108.20
25	LA	964	C	C4'-C3'-C2'	-5.53	97.07	102.60
25	LA	2638	G	N1-C6-O6	5.53	123.22	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2717	C	O4'-C1'-N1	5.53	112.62	108.20
1	SA	1142	G	C5-C6-O6	-5.52	125.29	128.60
25	LA	263	G	O4'-C1'-N9	5.52	112.62	108.20
1	SA	925	G	C5-C6-O6	5.52	131.91	128.60
25	LA	542	C	O4'-C1'-N1	5.52	112.62	108.20
25	LA	2143	C	C5'-C4'-C3'	-5.52	107.16	116.00
25	LA	2445	G	OP1-P-OP2	-5.52	111.31	119.60
1	SA	202	G	P-O5'-C5'	5.52	129.73	120.90
1	SA	944	G	C2'-C3'-O3'	5.52	122.53	113.70
1	SA	971	G	C5'-C4'-C3'	-5.52	107.17	116.00
1	SA	1168	U	C3'-C2'-C1'	-5.52	97.08	101.50
25	LA	1127	A	N1-C6-N6	5.52	121.91	118.60
25	LA	2349	G	O4'-C1'-N9	5.52	112.61	108.20
25	LA	2573	C	O4'-C1'-N1	5.52	112.61	108.20
25	LA	2646	C	C6-N1-C2	-5.52	118.09	120.30
1	SA	602	A	O4'-C1'-N9	5.52	112.61	108.20
1	SA	1058	G	O3'-P-O5'	-5.52	93.52	104.00
25	LA	66	C	O4'-C1'-N1	5.52	112.61	108.20
25	LA	2684	U	C5'-C4'-C3'	-5.52	107.17	116.00
38	LD	41	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	SA	406	G	P-O5'-C5'	-5.51	112.08	120.90
1	SA	1086	U	O4'-C1'-N1	5.51	112.61	108.20
25	LA	449	A	O4'-C1'-N9	5.51	112.61	108.20
25	LA	2001	C	O4'-C1'-N1	5.51	112.61	108.20
25	LA	2030	C	P-O3'-C3'	-5.51	113.08	119.70
25	LA	2438	U	O4'-C1'-N1	5.51	112.61	108.20
25	LA	2744	G	O4'-C1'-N9	5.51	112.61	108.20
1	SA	1186	G	O4'-C1'-N9	5.51	112.61	108.20
1	SA	1388	C	O4'-C1'-N1	5.51	112.61	108.20
25	LA	2806	C	O4'-C1'-N1	5.51	112.61	108.20
1	SA	1133	G	C5'-C4'-O4'	5.51	115.71	109.10
18	SD	181	PHE	CB-CG-CD1	5.51	124.66	120.80
25	LA	529	A	P-O3'-C3'	-5.51	113.09	119.70
25	LA	689	A	C4'-C3'-C2'	-5.51	97.09	102.60
25	LA	1807	G	C5-C6-O6	-5.51	125.29	128.60
1	SA	1364	U	O4'-C1'-C2'	5.51	112.56	107.60
25	LA	1458	U	O4'-C1'-N1	5.51	112.61	108.20
25	LA	1945	G	P-O5'-C5'	5.51	129.72	120.90
25	LA	2613	U	P-O3'-C3'	5.51	126.31	119.70
25	LA	2814	A	O4'-C1'-N9	5.51	112.61	108.20
1	SA	343	U	C5'-C4'-O4'	5.51	115.71	109.10
25	LA	660	C	C6-N1-C2	-5.51	118.10	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1241	G	O4'-C1'-N9	5.51	112.61	108.20
25	LA	40	U	O4'-C1'-N1	5.51	112.60	108.20
25	LA	1520	U	O4'-C1'-N1	5.51	112.61	108.20
25	LA	2786	U	O4'-C1'-N1	5.51	112.61	108.20
1	SA	1452	C	O4'-C1'-N1	5.50	112.60	108.20
2	S6	25	U	O4'-C1'-N1	5.50	112.60	108.20
3	S7	41	C	O4'-C1'-N1	5.50	112.60	108.20
25	LA	46	G	C4'-C3'-C2'	-5.50	97.10	102.60
25	LA	1340	U	P-O3'-C3'	5.50	126.31	119.70
25	LA	2111	U	O4'-C1'-N1	5.50	112.60	108.20
25	LA	2391	G	C5'-C4'-C3'	-5.50	107.20	116.00
25	LA	264	C	P-O3'-C3'	-5.50	113.10	119.70
25	LA	1891	G	N1-C6-O6	5.50	123.20	119.90
25	LA	2763	G	O4'-C1'-N9	5.50	112.60	108.20
25	LA	1865	U	O4'-C1'-N1	5.50	112.60	108.20
25	LA	2045	C	C4'-C3'-C2'	-5.50	97.10	102.60
1	SA	297	G	C4-N9-C1'	-5.50	119.35	126.50
1	SA	580	C	C6-N1-C2	-5.50	118.10	120.30
1	SA	675	A	C4'-C3'-C2'	-5.50	97.10	102.60
3	S7	2	C	P-O3'-C3'	5.50	126.30	119.70
25	LA	1187	G	C5-C6-O6	-5.50	125.30	128.60
25	LA	2718	G	O4'-C1'-N9	5.50	112.60	108.20
1	SA	856	C	O4'-C1'-N1	5.50	112.60	108.20
2	S6	74	A	P-O5'-C5'	-5.50	112.11	120.90
25	LA	464	U	N3-C2-O2	-5.50	118.35	122.20
25	LA	1559	U	P-O5'-C5'	5.50	129.69	120.90
25	LA	1746	A	O4'-C1'-N9	5.50	112.60	108.20
25	LA	2061	G	O4'-C1'-C2'	-5.50	100.30	105.80
25	LA	2464	G	C5-C6-O6	-5.50	125.30	128.60
25	LA	2491	U	P-O3'-C3'	5.50	126.30	119.70
25	LA	752	A	C1'-O4'-C4'	-5.50	105.50	109.90
25	LA	2128	G	C5'-C4'-C3'	-5.50	107.21	116.00
25	LA	2429	G	C8-N9-C1'	-5.50	119.86	127.00
23	SI	105	ARG	NE-CZ-NH2	-5.49	117.55	120.30
25	LA	747	U	C2'-C3'-O3'	5.49	122.49	113.70
25	LA	1426	G	N1-C6-O6	5.49	123.20	119.90
25	LA	1496	A	O4'-C1'-N9	5.49	112.59	108.20
1	SA	1361	G	O4'-C1'-N9	5.49	112.59	108.20
25	LA	951	C	O4'-C1'-N1	5.49	112.59	108.20
2	S6	71	G	O4'-C1'-N9	5.49	112.59	108.20
25	LA	2703	C	C5'-C4'-C3'	5.49	124.78	116.00
1	SA	976	G	O4'-C1'-N9	5.49	112.59	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1424	U	O4'-C1'-N1	5.49	112.59	108.20
1	SA	936	C	O4'-C1'-N1	5.49	112.59	108.20
1	SA	1516	G	C5-C6-O6	-5.49	125.31	128.60
25	LA	213	A	O4'-C1'-N9	5.49	112.59	108.20
25	LA	1242	U	O4'-C1'-N1	5.49	112.59	108.20
25	LA	1848	A	O4'-C1'-N9	5.49	112.59	108.20
25	LA	1982	U	O4'-C1'-N1	5.49	112.59	108.20
25	LA	2137	U	O4'-C1'-N1	5.49	112.59	108.20
25	LA	2301	C	O4'-C1'-N1	5.49	112.59	108.20
25	LA	3	U	O4'-C1'-N1	5.48	112.59	108.20
25	LA	558	U	C5'-C4'-C3'	-5.48	107.23	116.00
25	LA	2723	C	C6-N1-C2	-5.48	118.11	120.30
44	L3	21	ARG	NE-CZ-NH2	5.48	123.04	120.30
25	LA	634	C	C5'-C4'-O4'	5.48	115.68	109.10
25	LA	968	C	O4'-C1'-N1	5.48	112.59	108.20
25	LA	1766	G	O4'-C1'-N9	5.48	112.59	108.20
26	LB	29	A	C5'-C4'-C3'	-5.48	107.23	116.00
1	SA	1368	A	C5'-C4'-O4'	5.48	115.68	109.10
25	LA	956	G	P-O5'-C5'	-5.48	112.13	120.90
25	LA	1308	A	C4'-C3'-C2'	-5.48	97.12	102.60
1	SA	100	G	N1-C6-O6	5.48	123.19	119.90
1	SA	1287	A	O4'-C1'-N9	5.48	112.58	108.20
25	LA	1738	G	O4'-C1'-N9	5.48	112.58	108.20
1	SA	769	G	O4'-C1'-N9	5.48	112.58	108.20
1	SA	1207	G	C5-C6-O6	-5.48	125.31	128.60
1	SA	744	C	O4'-C1'-N1	5.48	112.58	108.20
25	LA	2730	C	P-O5'-C5'	5.48	129.66	120.90
1	SA	910	C	C5'-C4'-C3'	-5.47	107.24	116.00
25	LA	554	U	O4'-C1'-N1	5.47	112.58	108.20
25	LA	847	U	O4'-C1'-N1	5.47	112.58	108.20
26	LB	78	A	C5'-C4'-O4'	5.47	115.67	109.10
1	SA	47	C	O4'-C1'-C2'	-5.47	100.33	105.80
1	SA	987	G	O4'-C1'-N9	5.47	112.58	108.20
3	S7	4	C	P-O5'-C5'	-5.47	112.14	120.90
3	S7	67	C	C5'-C4'-C3'	5.47	124.75	116.00
25	LA	2319	G	C5-C6-O6	-5.47	125.32	128.60
25	LA	110	G	C5-C6-O6	-5.47	125.32	128.60
25	LA	1046	A	C1'-O4'-C4'	-5.47	105.53	109.90
25	LA	1895	C	C5'-C4'-C3'	-5.47	107.25	116.00
1	SA	187	G	P-O3'-C3'	5.47	126.26	119.70
1	SA	1178	G	C5-C6-O6	-5.47	125.32	128.60
1	SA	1472	U	C4'-C3'-C2'	-5.47	97.13	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1665	A	C4'-C3'-C2'	-5.47	97.13	102.60
25	LA	2558	C	O4'-C1'-N1	5.47	112.58	108.20
1	SA	777	A	O4'-C1'-N9	5.47	112.57	108.20
1	SA	877	G	C5'-C4'-C3'	5.47	124.75	116.00
25	LA	774	G	C5'-C4'-C3'	-5.47	107.25	116.00
25	LA	1367	A	O4'-C1'-N9	5.47	112.57	108.20
25	LA	1670	C	C2-N3-C4	-5.47	117.17	119.90
25	LA	1775	U	C4'-C3'-C2'	-5.47	97.13	102.60
25	LA	2702	G	P-O5'-C5'	-5.47	112.16	120.90
1	SA	1007	U	C5'-C4'-O4'	5.46	115.66	109.10
1	SA	1116	U	O4'-C1'-N1	5.46	112.57	108.20
25	LA	856	G	O4'-C1'-N9	5.46	112.57	108.20
25	LA	1571	A	O4'-C1'-N9	5.46	112.57	108.20
1	SA	1203	C	C5'-C4'-C3'	-5.46	107.26	116.00
1	SA	1267	C	O4'-C1'-N1	5.46	112.57	108.20
25	LA	704	G	P-O3'-C3'	5.46	126.25	119.70
25	LA	194	G	C1'-O4'-C4'	-5.46	105.53	109.90
25	LA	931	U	C5'-C4'-C3'	5.46	124.74	116.00
49	L7	175	PRO	N-CA-C	5.46	126.30	112.10
25	LA	680	C	O4'-C1'-N1	5.46	112.57	108.20
25	LA	1292	G	O4'-C1'-N9	5.46	112.57	108.20
25	LA	2340	A	P-O5'-C5'	5.46	129.64	120.90
1	SA	302	G	O4'-C1'-N9	5.46	112.57	108.20
1	SA	756	C	C4'-C3'-C2'	-5.46	97.14	102.60
25	LA	686	U	O4'-C1'-N1	5.46	112.57	108.20
25	LA	2030	C	C1'-O4'-C4'	-5.46	105.54	109.90
1	SA	376	G	O4'-C1'-N9	5.45	112.56	108.20
1	SA	763	G	O4'-C1'-N9	5.45	112.56	108.20
1	SA	962	C	C4'-C3'-C2'	-5.45	97.15	102.60
25	LA	453	A	O4'-C1'-N9	5.45	112.56	108.20
25	LA	2021	C	C6-N1-C1'	-5.45	114.25	120.80
25	LA	2047	C	C6-N1-C2	-5.45	118.12	120.30
25	LA	2485	G	P-O3'-C3'	5.45	126.25	119.70
25	LA	2802	G	O3'-P-O5'	-5.45	93.64	104.00
25	LA	2803	G	O4'-C1'-N9	5.45	112.56	108.20
3	S7	52	G	C5-C6-O6	-5.45	125.33	128.60
25	LA	106	C	P-O3'-C3'	-5.45	113.16	119.70
49	L7	111	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	SA	1432	G	P-O5'-C5'	-5.45	112.18	120.90
25	LA	150	U	O4'-C1'-N1	5.45	112.56	108.20
25	LA	378	C	O4'-C1'-N1	5.45	112.56	108.20
25	LA	877	A	C5'-C4'-C3'	5.45	124.72	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1270	C	P-O3'-C3'	-5.45	113.16	119.70
25	LA	2847	U	O4'-C1'-N1	5.45	112.56	108.20
1	SA	460	A	C5-C6-N6	-5.45	119.34	123.70
1	SA	1029	U	O4'-C1'-N1	5.45	112.56	108.20
25	LA	215	G	O4'-C1'-N9	5.45	112.56	108.20
25	LA	790	U	C6-N1-C1'	-5.45	113.57	121.20
25	LA	1963	U	C5'-C4'-C3'	5.45	124.72	116.00
1	SA	125	U	O4'-C1'-N1	5.45	112.56	108.20
1	SA	340	U	O4'-C1'-N1	5.45	112.56	108.20
1	SA	545	C	O4'-C1'-N1	5.45	112.56	108.20
25	LA	1122	G	O4'-C1'-N9	5.45	112.56	108.20
25	LA	2514	U	O4'-C1'-N1	5.45	112.56	108.20
1	SA	243	A	C2'-C3'-O3'	5.45	122.41	113.70
25	LA	1326	U	O4'-C1'-N1	5.45	112.56	108.20
25	LA	1418	G	N1-C6-O6	5.45	123.17	119.90
25	LA	2490	G	C5-C6-O6	-5.45	125.33	128.60
1	SA	383	A	O4'-C1'-N9	5.44	112.56	108.20
25	LA	364	C	O4'-C1'-N1	5.44	112.56	108.20
21	SG	110	ARG	NE-CZ-NH2	-5.44	117.58	120.30
25	LA	2143	C	C5'-C4'-O4'	5.44	115.63	109.10
25	LA	2491	U	C6-N1-C1'	-5.44	113.58	121.20
1	SA	1318	A	N1-C6-N6	5.44	121.86	118.60
3	S7	44	G	N1-C6-O6	5.44	123.16	119.90
25	LA	1890	A	C5'-C4'-C3'	5.44	124.70	116.00
25	LA	506	G	O4'-C1'-N9	5.44	112.55	108.20
25	LA	2362	C	P-O5'-C5'	5.44	129.60	120.90
1	SA	410	G	N1-C6-O6	5.44	123.16	119.90
1	SA	961	U	C6-N1-C2	-5.44	117.74	121.00
1	SA	1438	G	C5'-C4'-C3'	-5.44	107.30	116.00
25	LA	295	G	C1'-O4'-C4'	-5.44	105.55	109.90
25	LA	1266	G	C5-C6-O6	-5.44	125.34	128.60
25	LA	1667	G	N1-C6-O6	5.44	123.16	119.90
25	LA	2444	G	O4'-C1'-N9	5.44	112.55	108.20
25	LA	2789	C	C6-N1-C2	-5.44	118.12	120.30
1	SA	1159	U	C2-N1-C1'	5.44	124.22	117.70
25	LA	462	C	O4'-C1'-N1	5.44	112.55	108.20
25	LA	2341	G	C5'-C4'-C3'	-5.44	107.30	116.00
1	SA	145	G	O4'-C1'-N9	5.43	112.55	108.20
3	S7	12	U	O4'-C1'-N1	5.43	112.55	108.20
25	LA	57	C	O4'-C1'-N1	5.43	112.55	108.20
25	LA	1743	G	C5'-C4'-O4'	5.43	115.62	109.10
25	LA	1944	U	C3'-C2'-C1'	5.43	105.85	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	143	A	O3'-P-O5'	-5.43	93.68	104.00
25	LA	1551	A	P-O5'-C5'	5.43	129.59	120.90
25	LA	2069	G	O5'-P-OP2	-5.43	100.81	105.70
25	LA	2286	G	C5-C6-O6	-5.43	125.34	128.60
25	LA	2718	G	C4'-C3'-C2'	-5.43	97.17	102.60
25	LA	2609	U	C6-N1-C2	-5.43	117.74	121.00
1	SA	270	A	O4'-C1'-N9	5.43	112.54	108.20
1	SA	1018	G	C5'-C4'-O4'	5.43	115.61	109.10
25	LA	195	A	C5'-C4'-C3'	5.43	124.69	116.00
25	LA	366	C	C4'-C3'-C2'	-5.43	97.17	102.60
25	LA	745	G	P-O5'-C5'	5.43	129.59	120.90
25	LA	1543	G	C5'-C4'-O4'	5.43	115.62	109.10
25	LA	2069	G	N1-C6-O6	5.43	123.16	119.90
54	LH	48	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	SA	40	C	C4'-C3'-C2'	-5.43	97.17	102.60
1	SA	328	C	C6-N1-C1'	-5.43	114.29	120.80
1	SA	468	A	C8-N9-C1'	-5.43	117.93	127.70
1	SA	559	A	C1'-O4'-C4'	-5.43	105.56	109.90
1	SA	1023	U	O4'-C1'-N1	5.43	112.54	108.20
25	LA	231	A	C5'-C4'-O4'	5.43	115.61	109.10
25	LA	398	C	O4'-C1'-N1	5.43	112.54	108.20
25	LA	678	C	C6-N1-C2	-5.43	118.13	120.30
25	LA	1764	C	C4'-C3'-C2'	-5.43	97.17	102.60
25	LA	2393	U	O4'-C1'-N1	5.43	112.54	108.20
25	LA	97	C	C5'-C4'-C3'	5.42	124.68	116.00
25	LA	1289	C	O4'-C1'-N1	5.42	112.54	108.20
25	LA	1459	G	C5-C6-O6	-5.42	125.34	128.60
25	LA	1864	U	O4'-C1'-N1	5.42	112.54	108.20
25	LA	2504	U	C6-N1-C1'	-5.42	113.61	121.20
1	SA	635	A	O4'-C1'-N9	5.42	112.54	108.20
11	SQ	26	ARG	NE-CZ-NH1	5.42	123.01	120.30
25	LA	457	A	C8-N9-C4	5.42	107.97	105.80
25	LA	811	U	O4'-C1'-N1	5.42	112.54	108.20
1	SA	644	U	O4'-C1'-N1	5.42	112.54	108.20
25	LA	1656	C	C5'-C4'-C3'	-5.42	107.33	116.00
25	LA	2094	A	C5-C6-N6	-5.42	119.36	123.70
1	SA	275	G	C5'-C4'-C3'	-5.42	107.33	116.00
25	LA	231	A	C2'-C3'-O3'	5.42	122.37	113.70
25	LA	503	A	O4'-C1'-N9	5.42	112.53	108.20
25	LA	956	G	C4'-C3'-C2'	-5.42	97.18	102.60
25	LA	974	G	C5-C6-O6	-5.42	125.35	128.60
25	LA	2460	U	O4'-C1'-N1	5.42	112.53	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1430	A	P-O5'-C5'	-5.42	112.23	120.90
1	SA	1464	U	O4'-C1'-N1	5.42	112.53	108.20
25	LA	356	G	C5-C6-O6	-5.42	125.35	128.60
25	LA	487	C	C5'-C4'-C3'	-5.42	107.33	116.00
25	LA	2249	U	O3'-P-O5'	-5.42	93.71	104.00
58	LZ	44	PHE	CB-CG-CD2	5.42	124.59	120.80
25	LA	553	G	C5'-C4'-C3'	-5.42	107.34	116.00
49	L7	111	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	SA	18	C	O4'-C1'-N1	5.41	112.53	108.20
1	SA	1535	C	O4'-C1'-N1	5.41	112.53	108.20
25	LA	1618	U	O4'-C1'-N1	5.41	112.53	108.20
25	LA	2241	A	N1-C6-N6	-5.41	115.35	118.60
1	SA	879	C	C4'-C3'-C2'	-5.41	97.19	102.60
2	S6	55	U	C5'-C4'-C3'	-5.41	107.34	116.00
1	SA	42	G	C5-C6-O6	-5.41	125.35	128.60
1	SA	1443	C	P-O3'-C3'	-5.41	113.21	119.70
21	SG	110	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	SA	240	G	C4'-C3'-C2'	-5.41	97.19	102.60
1	SA	311	C	O4'-C1'-N1	5.41	112.53	108.20
1	SA	850	U	C5'-C4'-C3'	-5.41	107.35	116.00
1	SA	166	U	P-O5'-C5'	5.41	129.55	120.90
26	LB	96	G	C8-N9-C4	-5.41	104.24	106.40
1	SA	523	A	P-O3'-C3'	5.41	126.19	119.70
25	LA	296	U	C5'-C4'-C3'	-5.41	107.35	116.00
25	LA	512	G	C5'-C4'-C3'	5.41	124.65	116.00
25	LA	1599	U	O4'-C1'-N1	5.41	112.53	108.20
52	LF	99	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	SA	1152	A	C5'-C4'-O4'	5.40	115.58	109.10
13	SS	80	ARG	NE-CZ-NH2	-5.40	117.60	120.30
24	S1	136	ARG	NE-CZ-NH1	5.40	123.00	120.30
25	LA	1556	C	O4'-C1'-N1	5.40	112.52	108.20
1	SA	492	C	O4'-C1'-N1	5.40	112.52	108.20
1	SA	1498	U	C1'-O4'-C4'	-5.40	105.58	109.90
25	LA	1388	G	O4'-C1'-N9	5.40	112.52	108.20
1	SA	103	U	P-O5'-C5'	-5.40	112.26	120.90
1	SA	1061	G	O4'-C1'-N9	5.40	112.52	108.20
3	S7	44	G	C5-C6-O6	-5.40	125.36	128.60
25	LA	1752	C	C6-N1-C2	-5.40	118.14	120.30
25	LA	1983	G	C4'-C3'-C2'	-5.40	97.20	102.60
25	LA	2271	G	N1-C6-O6	5.40	123.14	119.90
25	LA	2363	G	P-O5'-C5'	-5.40	112.26	120.90
25	LA	566	U	O4'-C1'-N1	5.40	112.52	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	749	A	O4'-C1'-N9	5.40	112.52	108.20
26	LB	41	G	P-O3'-C3'	5.40	126.18	119.70
26	LB	71	C	O4'-C1'-N1	5.40	112.52	108.20
1	SA	613	C	O4'-C1'-N1	5.40	112.52	108.20
1	SA	680	C	O4'-C1'-N1	5.40	112.52	108.20
1	SA	1270	G	O4'-C1'-N9	5.40	112.52	108.20
24	S1	436	ARG	NE-CZ-NH2	-5.40	117.60	120.30
25	LA	642	U	P-O5'-C5'	5.40	129.54	120.90
25	LA	892	A	N1-C6-N6	-5.40	115.36	118.60
25	LA	924	G	C5'-C4'-O4'	5.40	115.58	109.10
25	LA	1376	C	C5'-C4'-O4'	-5.40	102.62	109.10
25	LA	2042	A	P-O3'-C3'	5.40	126.18	119.70
25	LA	2275	C	C5'-C4'-O4'	-5.40	102.62	109.10
25	LA	2431	U	C4'-C3'-C2'	-5.40	97.20	102.60
50	L8	57	TYR	CB-CG-CD1	5.40	124.24	121.00
57	LK	10	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	SA	1179	A	O4'-C1'-N9	5.40	112.52	108.20
25	LA	1423	G	O4'-C1'-N9	5.40	112.52	108.20
1	SA	184	G	C5'-C4'-O4'	5.39	115.57	109.10
25	LA	830	G	C5'-C4'-O4'	5.39	115.57	109.10
25	LA	940	G	O4'-C1'-N9	5.39	112.52	108.20
25	LA	1929	G	C5-C6-O6	-5.39	125.36	128.60
26	LB	11	C	O4'-C1'-N1	5.39	112.52	108.20
44	L3	39	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	SA	868	C	C6-N1-C2	-5.39	118.14	120.30
25	LA	2638	G	O4'-C1'-N9	5.39	112.51	108.20
1	SA	1310	G	P-O5'-C5'	-5.39	112.28	120.90
8	SN	52	ARG	NE-CZ-NH2	-5.39	117.60	120.30
25	LA	1388	G	O3'-P-O5'	-5.39	93.76	104.00
28	LM	20	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	SA	921	U	O4'-C1'-N1	5.39	112.51	108.20
1	SA	990	C	C6-N1-C2	-5.39	118.14	120.30
1	SA	1140	C	C2-N3-C4	-5.39	117.20	119.90
25	LA	848	C	O4'-C1'-N1	5.39	112.51	108.20
25	LA	1269	A	P-O5'-C5'	5.39	129.52	120.90
25	LA	1299	G	C5-C6-O6	-5.39	125.37	128.60
25	LA	1924	C	P-O5'-C5'	-5.39	112.28	120.90
25	LA	2056	G	O4'-C1'-N9	5.39	112.51	108.20
25	LA	2857	G	O4'-C1'-N9	5.39	112.51	108.20
1	SA	1194	U	C6-N1-C2	-5.39	117.77	121.00
25	LA	1757	A	P-O5'-C5'	5.39	129.52	120.90
25	LA	2609	U	C2-N1-C1'	-5.39	111.23	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	L6	170	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	SA	1517	G	C1'-O4'-C4'	-5.38	105.59	109.90
25	LA	1056	G	O3'-P-O5'	5.38	114.23	104.00
25	LA	2575	C	C2-N3-C4	-5.38	117.21	119.90
1	SA	838	G	C5-C6-O6	-5.38	125.37	128.60
1	SA	1161	C	O4'-C1'-N1	5.38	112.51	108.20
25	LA	1771	C	C6-N1-C2	-5.38	118.15	120.30
25	LA	2150	C	C5'-C4'-O4'	5.38	115.56	109.10
1	SA	23	C	O4'-C1'-N1	5.38	112.51	108.20
1	SA	346	G	N1-C6-O6	5.38	123.13	119.90
1	SA	499	A	P-O5'-C5'	-5.38	112.29	120.90
1	SA	1042	A	C5'-C4'-C3'	5.38	124.61	116.00
1	SA	1124	G	O4'-C1'-N9	5.38	112.50	108.20
25	LA	570	G	C5'-C4'-C3'	-5.38	107.39	116.00
25	LA	2271	G	C4-N9-C1'	5.38	133.50	126.50
25	LA	2665	A	P-O5'-C5'	-5.38	112.29	120.90
1	SA	1407	C	P-O3'-C3'	-5.38	113.24	119.70
25	LA	805	G	N1-C2-N2	-5.38	111.36	116.20
25	LA	2034	U	O4'-C1'-N1	5.38	112.50	108.20
1	SA	950	U	O4'-C1'-N1	5.38	112.50	108.20
25	LA	437	U	O4'-C1'-N1	5.38	112.50	108.20
25	LA	2142	A	O4'-C1'-N9	5.38	112.50	108.20
26	LB	84	G	O4'-C1'-N9	5.38	112.50	108.20
1	SA	274	A	O4'-C1'-N9	5.38	112.50	108.20
1	SA	1492	A	C1'-O4'-C4'	-5.38	105.60	109.90
14	SB	49	PHE	CB-CG-CD1	-5.38	117.04	120.80
25	LA	385	C	C2-N1-C1'	-5.38	112.89	118.80
25	LA	2065	C	C1'-O4'-C4'	5.38	114.20	109.90
25	LA	2323	G	P-O5'-C5'	-5.38	112.30	120.90
25	LA	2636	C	O4'-C1'-N1	5.38	112.50	108.20
25	LA	2756	U	C2'-C3'-O3'	5.38	122.30	113.70
25	LA	1211	C	C2-N1-C1'	5.38	124.71	118.80
1	SA	1278	G	O4'-C1'-N9	5.37	112.50	108.20
25	LA	754	U	O4'-C1'-N1	5.37	112.50	108.20
25	LA	2637	U	P-O5'-C5'	5.37	129.50	120.90
1	SA	318	G	C4'-C3'-C2'	-5.37	97.23	102.60
1	SA	556	C	C4'-C3'-C2'	-5.37	97.23	102.60
1	SA	1006	G	O4'-C1'-N9	5.37	112.50	108.20
1	SA	1237	C	O4'-C1'-N1	5.37	112.50	108.20
25	LA	9	G	N1-C6-O6	5.37	123.12	119.90
25	LA	373	U	C5'-C4'-O4'	5.37	115.55	109.10
25	LA	1853	A	O4'-C1'-N9	5.37	112.50	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2448	A	C5'-C4'-C3'	5.37	124.60	116.00
1	SA	342	C	O4'-C1'-N1	5.37	112.50	108.20
1	SA	1388	C	C5'-C4'-C3'	-5.37	107.41	116.00
25	LA	2463	C	C6-N1-C2	-5.37	118.15	120.30
1	SA	352	C	O4'-C1'-N1	5.37	112.50	108.20
1	SA	757	U	P-O5'-C5'	5.37	129.49	120.90
1	SA	817	C	O4'-C1'-N1	5.37	112.49	108.20
25	LA	1258	U	O4'-C1'-N1	5.37	112.49	108.20
1	SA	924	C	C2-N3-C4	-5.37	117.22	119.90
1	SA	1016	A	P-O5'-C5'	5.37	129.48	120.90
25	LA	207	A	P-O5'-C5'	5.37	129.49	120.90
25	LA	212	G	O4'-C1'-N9	5.37	112.49	108.20
25	LA	383	C	O4'-C1'-N1	5.37	112.49	108.20
25	LA	1249	U	C5'-C4'-O4'	5.37	115.54	109.10
25	LA	2692	G	O4'-C1'-N9	5.37	112.49	108.20
1	SA	718	A	P-O5'-C5'	-5.36	112.32	120.90
1	SA	1308	U	O4'-C1'-N1	5.36	112.49	108.20
25	LA	2023	C	P-O3'-C3'	-5.36	113.27	119.70
25	LA	2146	C	O4'-C1'-N1	5.36	112.49	108.20
56	LJ	86	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	S7	17	C	P-O3'-C3'	5.36	126.13	119.70
16	SU	33	ARG	NE-CZ-NH1	5.36	122.98	120.30
25	LA	195	A	P-O5'-C5'	5.36	129.48	120.90
1	SA	1195	C	C6-N1-C2	-5.36	118.16	120.30
25	LA	1223	G	C5-C6-O6	-5.36	125.38	128.60
25	LA	2100	G	O4'-C1'-N9	5.36	112.49	108.20
25	LA	2287	A	N1-C6-N6	-5.36	115.38	118.60
25	LA	2805	C	C6-N1-C2	-5.36	118.16	120.30
1	SA	401	C	C5'-C4'-C3'	-5.36	107.43	116.00
25	LA	401	A	O4'-C1'-N9	5.36	112.48	108.20
25	LA	1252	G	P-O3'-C3'	-5.36	113.27	119.70
25	LA	2564	A	N1-C6-N6	-5.36	115.39	118.60
1	SA	1133	G	C5'-C4'-C3'	-5.36	107.43	116.00
25	LA	1782	U	P-O3'-C3'	-5.36	113.27	119.70
25	LA	1920	C	O4'-C1'-N1	5.36	112.48	108.20
25	LA	2391	G	C5'-C4'-O4'	5.36	115.53	109.10
1	SA	797	C	C6-N1-C2	-5.35	118.16	120.30
37	LV	10	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	SA	1113	C	O4'-C1'-N1	5.35	112.48	108.20
25	LA	356	G	N1-C6-O6	5.35	123.11	119.90
30	LO	12	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	SA	1030	U	O4'-C1'-N1	5.35	112.48	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1438	G	C4'-C3'-C2'	-5.35	97.25	102.60
1	SA	391	G	P-O3'-C3'	5.35	126.12	119.70
1	SA	689	C	O4'-C1'-N1	5.35	112.48	108.20
1	SA	1235	U	C5'-C4'-O4'	5.35	115.52	109.10
25	LA	792	A	C3'-C2'-C1'	5.35	105.78	101.50
1	SA	314	C	O4'-C1'-N1	5.35	112.48	108.20
1	SA	1395	C	O4'-C1'-N1	5.35	112.48	108.20
9	SO	52	ARG	NE-CZ-NH1	5.35	122.97	120.30
25	LA	903	C	P-O3'-C3'	5.35	126.12	119.70
25	LA	1376	C	O4'-C1'-N1	5.35	112.48	108.20
25	LA	1874	C	O4'-C1'-N1	5.35	112.48	108.20
25	LA	1950	G	C5-C6-N1	5.35	114.17	111.50
25	LA	2458	G	C4-N9-C1'	5.35	133.45	126.50
25	LA	696	G	O4'-C1'-N9	5.35	112.48	108.20
25	LA	2578	G	C6-N1-C2	-5.34	121.89	125.10
25	LA	2784	U	O4'-C1'-N1	5.34	112.47	108.20
25	LA	2803	G	C5'-C4'-C3'	-5.34	107.45	116.00
1	SA	868	C	O4'-C1'-N1	5.34	112.47	108.20
25	LA	1450	G	C5-C6-O6	-5.34	125.39	128.60
25	LA	2019	A	P-O3'-C3'	5.34	126.11	119.70
1	SA	109	A	O4'-C1'-C2'	-5.34	100.46	105.80
1	SA	636	U	O4'-C1'-N1	5.34	112.47	108.20
1	SA	1144	G	O4'-C1'-N9	5.34	112.47	108.20
25	LA	140	C	C2-N1-C1'	5.34	124.67	118.80
25	LA	1219	U	C5'-C4'-O4'	5.34	115.51	109.10
25	LA	1483	G	O4'-C1'-N9	5.34	112.47	108.20
25	LA	1687	G	N1-C6-O6	5.34	123.11	119.90
1	SA	394	G	C6-N1-C2	-5.34	121.90	125.10
1	SA	1323	G	C4'-C3'-C2'	-5.34	97.26	102.60
2	S6	9	G	O4'-C1'-N9	5.34	112.47	108.20
25	LA	945	A	P-O5'-C5'	5.34	129.44	120.90
25	LA	968	C	C6-N1-C2	-5.34	118.16	120.30
25	LA	1790	C	O4'-C1'-N1	5.34	112.47	108.20
44	L3	33	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	SA	60	A	O4'-C1'-N9	5.34	112.47	108.20
1	SA	96	U	P-O5'-C5'	-5.34	112.36	120.90
25	LA	568	U	C2-N3-C4	5.34	130.20	127.00
1	SA	254	G	C5-C6-O6	-5.34	125.40	128.60
25	LA	242	G	C5'-C4'-C3'	-5.34	107.46	116.00
25	LA	251	A	O4'-C1'-N9	5.34	112.47	108.20
25	LA	1768	C	O4'-C1'-N1	5.34	112.47	108.20
25	LA	1888	G	P-O3'-C3'	-5.34	113.30	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2042	A	C4'-C3'-C2'	-5.34	97.26	102.60
25	LA	2656	U	C5'-C4'-O4'	5.34	115.50	109.10
25	LA	105	C	P-O5'-C5'	5.33	129.44	120.90
29	LN	68	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	SA	536	C	O4'-C1'-N1	5.33	112.47	108.20
1	SA	751	U	O4'-C1'-N1	5.33	112.47	108.20
1	SA	1008	U	O4'-C1'-N1	5.33	112.47	108.20
25	LA	281	C	O4'-C1'-N1	5.33	112.47	108.20
25	LA	1332	G	N1-C6-O6	5.33	123.10	119.90
25	LA	1898	U	P-O5'-C5'	5.33	129.43	120.90
1	SA	1353	G	C5'-C4'-C3'	5.33	124.53	116.00
3	S7	45	U	O4'-C1'-N1	5.33	112.47	108.20
25	LA	350	G	O4'-C1'-N9	5.33	112.47	108.20
25	LA	926	G	O4'-C1'-N9	5.33	112.47	108.20
25	LA	1585	C	C5'-C4'-O4'	5.33	115.50	109.10
25	LA	2836	U	O4'-C1'-N1	5.33	112.47	108.20
1	SA	108	G	C1'-O4'-C4'	-5.33	105.64	109.90
25	LA	815	C	C5'-C4'-C3'	-5.33	107.47	116.00
25	LA	1981	A	C5'-C4'-C3'	-5.33	107.47	116.00
1	SA	1509	C	O4'-C1'-N1	5.33	112.46	108.20
21	SG	94	ARG	NE-CZ-NH1	5.33	122.96	120.30
25	LA	420	C	C6-N1-C2	-5.33	118.17	120.30
25	LA	564	C	C4'-C3'-C2'	-5.33	97.27	102.60
25	LA	858	G	O4'-C1'-N9	5.33	112.46	108.20
25	LA	872	U	O4'-C1'-N1	5.33	112.46	108.20
25	LA	2281	A	P-O3'-C3'	-5.33	113.31	119.70
25	LA	2855	C	O4'-C1'-N1	5.33	112.46	108.20
28	LM	102	ARG	NE-CZ-NH2	-5.33	117.64	120.30
2	S6	43	G	O4'-C1'-N9	5.33	112.46	108.20
16	SU	17	ARG	NE-CZ-NH1	5.33	122.96	120.30
25	LA	1627	G	C5-C6-O6	-5.33	125.40	128.60
25	LA	2073	C	C2-N3-C4	-5.33	117.24	119.90
1	SA	831	A	O4'-C1'-N9	5.33	112.46	108.20
25	LA	1318	U	O4'-C1'-N1	5.33	112.46	108.20
1	SA	842	U	P-O5'-C5'	-5.32	112.38	120.90
1	SA	921	U	C4'-C3'-C2'	-5.32	97.28	102.60
1	SA	1052	U	C5'-C4'-C3'	-5.32	107.48	116.00
14	SB	20	ARG	NE-CZ-NH1	5.32	122.96	120.30
25	LA	1366	A	O4'-C1'-N9	5.32	112.46	108.20
25	LA	2042	A	O4'-C1'-N9	5.32	112.46	108.20
25	LA	2763	G	N3-C2-N2	5.32	123.63	119.90
25	LA	2822	G	N1-C6-O6	5.32	123.09	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	192	C	O4'-C1'-N1	5.32	112.46	108.20
25	LA	1993	U	N1-C2-N3	5.32	118.09	114.90
25	LA	307	G	P-O3'-C3'	5.32	126.08	119.70
25	LA	465	G	P-O3'-C3'	5.32	126.08	119.70
25	LA	1162	G	C4'-C3'-C2'	-5.32	97.28	102.60
25	LA	1211	C	C6-N1-C1'	-5.32	114.42	120.80
25	LA	2650	U	O4'-C1'-N1	5.32	112.46	108.20
1	SA	29	U	P-O5'-C5'	-5.32	112.39	120.90
1	SA	617	G	O4'-C1'-N9	5.32	112.45	108.20
1	SA	898	G	C4'-C3'-C2'	-5.32	97.28	102.60
25	LA	1085	A	C2'-C3'-O3'	5.32	122.21	113.70
25	LA	1676	A	C5'-C4'-C3'	5.32	124.50	116.00
25	LA	1800	C	O4'-C1'-N1	5.32	112.45	108.20
26	LB	18	G	O4'-C1'-N9	5.32	112.45	108.20
1	SA	444	G	C5'-C4'-O4'	5.31	115.48	109.10
25	LA	426	C	O4'-C1'-N1	5.31	112.45	108.20
25	LA	570	G	C5-C6-O6	-5.31	125.41	128.60
1	SA	329	A	N1-C6-N6	-5.31	115.41	118.60
1	SA	1264	U	O4'-C1'-N1	5.31	112.45	108.20
25	LA	147	C	C5'-C4'-C3'	-5.31	107.50	116.00
25	LA	2502	G	C8-N9-C4	-5.31	104.28	106.40
25	LA	2832	U	O4'-C1'-N1	5.31	112.45	108.20
26	LB	41	G	C4-N9-C1'	5.31	133.41	126.50
1	SA	1174	G	O4'-C1'-N9	5.31	112.45	108.20
4	SJ	48	ARG	NE-CZ-NH1	5.31	122.95	120.30
25	LA	1114	C	O4'-C1'-N1	5.31	112.45	108.20
25	LA	2067	G	C5'-C4'-O4'	5.31	115.47	109.10
25	LA	2512	C	C2-N3-C4	-5.31	117.25	119.90
1	SA	1206	G	C5'-C4'-O4'	5.31	115.47	109.10
1	SA	1233	G	O4'-C1'-N9	5.31	112.45	108.20
25	LA	1408	G	C4'-C3'-C2'	-5.31	97.29	102.60
25	LA	1467	U	O4'-C1'-N1	5.31	112.45	108.20
2	S6	26	C	C5'-C4'-C3'	-5.31	107.51	116.00
25	LA	481	G	C1'-O4'-C4'	-5.31	105.66	109.90
25	LA	1332	G	C5-C6-O6	-5.31	125.42	128.60
25	LA	713	G	C5-C6-O6	-5.30	125.42	128.60
25	LA	862	G	O4'-C1'-N9	5.30	112.44	108.20
25	LA	2088	A	N1-C6-N6	5.30	121.78	118.60
25	LA	2559	C	C5'-C4'-O4'	5.30	115.47	109.10
26	LB	85	G	N1-C6-O6	5.30	123.08	119.90
33	LR	51	PHE	CB-CG-CD1	-5.30	117.09	120.80
52	LF	116	ARG	NE-CZ-NH2	5.30	122.95	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	521	G	N1-C6-O6	5.30	123.08	119.90
1	SA	1447	A	C3'-C2'-C1'	-5.30	97.26	101.50
14	SB	125	PHE	CB-CG-CD2	5.30	124.51	120.80
25	LA	2246	G	C5'-C4'-O4'	5.30	115.46	109.10
1	SA	673	A	P-O5'-C5'	5.30	129.38	120.90
1	SA	849	G	O4'-C1'-N9	5.30	112.44	108.20
25	LA	2703	C	C6-N1-C2	-5.30	118.18	120.30
18	SD	181	PHE	CB-CG-CD2	-5.30	117.09	120.80
25	LA	350	G	C5'-C4'-C3'	-5.30	107.52	116.00
25	LA	553	G	O4'-C1'-N9	5.30	112.44	108.20
25	LA	1723	G	C4'-C3'-C2'	-5.30	97.30	102.60
25	LA	1900	A	O3'-P-O5'	5.30	114.07	104.00
1	SA	944	G	C5-C6-O6	-5.30	125.42	128.60
5	SK	55	ARG	NE-CZ-NH1	5.30	122.95	120.30
25	LA	293	U	O4'-C1'-N1	5.30	112.44	108.20
25	LA	2436	G	C4'-C3'-C2'	-5.30	97.30	102.60
25	LA	2441	U	C2-N1-C1'	5.30	124.06	117.70
25	LA	2466	C	O4'-C1'-N1	5.30	112.44	108.20
25	LA	429	A	O4'-C1'-N9	5.30	112.44	108.20
25	LA	1259	G	O4'-C1'-N9	5.30	112.44	108.20
25	LA	2607	G	C1'-O4'-C4'	-5.30	105.66	109.90
37	LV	26	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	SA	374	A	O4'-C1'-N9	5.29	112.44	108.20
1	SA	1382	C	O4'-C1'-N1	5.29	112.44	108.20
25	LA	85	G	C5-C6-O6	-5.29	125.42	128.60
25	LA	1000	A	O4'-C1'-N9	5.29	112.44	108.20
25	LA	1954	G	C5-C6-O6	-5.29	125.42	128.60
25	LA	2754	U	O4'-C1'-N1	5.29	112.44	108.20
27	LC	137	MET	CG-SD-CE	-5.29	91.73	100.20
1	SA	224	U	O4'-C1'-N1	5.29	112.43	108.20
1	SA	224	U	P-O5'-C5'	-5.29	112.43	120.90
25	LA	183	C	O4'-C1'-N1	5.29	112.43	108.20
25	LA	1673	G	O4'-C1'-N9	5.29	112.43	108.20
25	LA	1782	U	C6-N1-C1'	-5.29	113.79	121.20
25	LA	2594	C	C5'-C4'-C3'	-5.29	107.53	116.00
25	LA	2834	G	P-O3'-C3'	5.29	126.05	119.70
1	SA	739	C	O4'-C1'-N1	5.29	112.43	108.20
25	LA	369	U	P-O3'-C3'	-5.29	113.35	119.70
25	LA	813	U	O4'-C1'-N1	5.29	112.43	108.20
25	LA	1645	G	C5-C6-O6	-5.29	125.42	128.60
25	LA	2456	C	O4'-C1'-N1	5.29	112.43	108.20
40	LX	90	PHE	CB-CG-CD2	5.29	124.50	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	83	C	C5'-C4'-O4'	5.29	115.45	109.10
1	SA	194	C	C5'-C4'-C3'	-5.29	107.54	116.00
1	SA	641	U	O4'-C1'-N1	5.29	112.43	108.20
25	LA	1005	C	P-O3'-C3'	5.29	126.05	119.70
1	SA	351	G	O4'-C1'-N9	5.29	112.43	108.20
1	SA	1403	C	O4'-C1'-N1	5.29	112.43	108.20
22	SH	79	ARG	NE-CZ-NH1	5.29	122.94	120.30
25	LA	2436	G	O4'-C1'-N9	5.29	112.43	108.20
25	LA	2683	C	O4'-C1'-N1	5.29	112.43	108.20
1	SA	1205	U	C2-N1-C1'	-5.29	111.36	117.70
25	LA	811	U	C6-N1-C1'	-5.29	113.80	121.20
25	LA	1581	G	N1-C6-O6	5.29	123.07	119.90
25	LA	1633	G	N3-C2-N2	5.29	123.60	119.90
1	SA	1305	G	O4'-C1'-N9	-5.28	103.97	108.20
25	LA	2002	G	O4'-C1'-N9	5.28	112.43	108.20
25	LA	2154	A	O4'-C1'-N9	5.28	112.43	108.20
25	LA	2622	U	O4'-C1'-N1	5.28	112.43	108.20
26	LB	88	C	C2-N1-C1'	5.28	124.61	118.80
1	SA	220	G	C5'-C4'-O4'	5.28	115.44	109.10
25	LA	552	U	O4'-C1'-N1	5.28	112.42	108.20
25	LA	1491	G	O4'-C1'-N9	5.28	112.42	108.20
25	LA	1587	G	O4'-C1'-N9	5.28	112.42	108.20
25	LA	2609	U	N1-C1'-C2'	5.28	120.86	114.00
26	LB	11	C	C4'-C3'-C2'	-5.28	97.32	102.60
1	SA	330	C	C5'-C4'-O4'	5.28	115.43	109.10
1	SA	783	C	C6-N1-C2	-5.28	118.19	120.30
25	LA	2261	C	O4'-C1'-N1	5.28	112.42	108.20
25	LA	681	G	C5-C6-O6	-5.28	125.43	128.60
25	LA	1906	G	P-O3'-C3'	-5.28	113.37	119.70
25	LA	2414	G	O4'-C1'-N9	5.28	112.42	108.20
25	LA	2784	U	P-O3'-C3'	-5.28	113.37	119.70
25	LA	375	G	O4'-C1'-N9	5.28	112.42	108.20
25	LA	1157	G	C5-C6-O6	-5.28	125.44	128.60
25	LA	1582	C	C6-N1-C2	-5.28	118.19	120.30
25	LA	2048	G	P-O5'-C5'	5.28	129.34	120.90
25	LA	2877	G	C5-C6-O6	-5.28	125.43	128.60
52	LF	118	MET	CG-SD-CE	-5.28	91.76	100.20
1	SA	36	C	O4'-C1'-N1	5.27	112.42	108.20
1	SA	840	C	C5'-C4'-O4'	5.27	115.43	109.10
1	SA	1389	C	O4'-C1'-N1	5.27	112.42	108.20
25	LA	851	C	O4'-C1'-N1	5.27	112.42	108.20
25	LA	2325	G	C5'-C4'-O4'	5.27	115.43	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	760	G	C5-C6-O6	-5.27	125.44	128.60
25	LA	852	U	O4'-C1'-N1	5.27	112.42	108.20
25	LA	1067	A	C1'-O4'-C4'	-5.27	105.68	109.90
25	LA	1182	G	P-O5'-C5'	5.27	129.34	120.90
25	LA	2024	G	C4'-C3'-C2'	-5.27	97.33	102.60
25	LA	2490	G	N1-C6-O6	5.27	123.06	119.90
25	LA	845	A	N1-C6-N6	5.27	121.76	118.60
25	LA	1698	A	O4'-C1'-N9	5.27	112.42	108.20
1	SA	1445	U	O4'-C1'-N1	5.27	112.42	108.20
25	LA	1299	G	N1-C6-O6	5.27	123.06	119.90
1	SA	101	A	N1-C6-N6	-5.27	115.44	118.60
1	SA	1387	G	C5-C6-O6	-5.27	125.44	128.60
25	LA	1117	C	O4'-C1'-N1	5.27	112.41	108.20
25	LA	1866	A	O4'-C1'-N9	5.27	112.42	108.20
25	LA	2249	U	C4'-C3'-C2'	5.27	107.87	102.60
25	LA	2645	G	C5-C6-O6	-5.27	125.44	128.60
1	SA	1189	U	O4'-C1'-N1	5.27	112.41	108.20
2	S6	1	C	C6-N1-C1'	-5.27	114.48	120.80
10	SP	31	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	SA	1517	G	N1-C6-O6	5.26	123.06	119.90
4	SJ	45	ARG	NE-CZ-NH1	5.26	122.93	120.30
25	LA	41	C	O3'-P-O5'	-5.26	94.00	104.00
25	LA	560	C	O4'-C1'-N1	5.26	112.41	108.20
25	LA	2229	U	O4'-C1'-N1	5.26	112.41	108.20
1	SA	892	A	O4'-C1'-N9	5.26	112.41	108.20
1	SA	591	U	O4'-C1'-N1	5.26	112.41	108.20
1	SA	526	C	O4'-C1'-N1	5.26	112.41	108.20
1	SA	769	G	C4'-C3'-C2'	-5.26	97.34	102.60
1	SA	1002	G	C5'-C4'-C3'	5.26	124.41	116.00
1	SA	1364	U	C6-N1-C1'	-5.26	113.84	121.20
25	LA	767	U	C5'-C4'-C3'	-5.26	107.58	116.00
25	LA	1054	A	O4'-C1'-N9	5.26	112.41	108.20
25	LA	2148	G	C5-C6-O6	-5.26	125.44	128.60
25	LA	2499	C	C5'-C4'-C3'	-5.26	107.59	116.00
25	LA	2717	C	C4'-C3'-C2'	-5.26	97.34	102.60
25	LA	418	C	O4'-C1'-N1	5.26	112.41	108.20
1	SA	210	C	C6-N1-C1'	-5.26	114.49	120.80
1	SA	769	G	N1-C6-O6	5.26	123.05	119.90
1	SA	1153	G	C5'-C4'-C3'	5.26	124.41	116.00
25	LA	186	G	C5-C6-O6	-5.26	125.45	128.60
25	LA	559	G	C5-C6-O6	-5.26	125.45	128.60
25	LA	670	A	OP1-P-O3'	5.26	116.77	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1362	C	C5'-C4'-O4'	5.26	115.41	109.10
25	LA	2018	G	O4'-C1'-N9	5.26	112.41	108.20
40	LX	179	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	SA	578	C	C5'-C4'-C3'	-5.25	107.59	116.00
1	SA	1435	G	O4'-C1'-N9	5.25	112.40	108.20
2	S6	37	U	P-O5'-C5'	-5.25	112.49	120.90
3	S7	35	A	P-O3'-C3'	5.25	126.01	119.70
1	SA	1051	C	P-O5'-C5'	5.25	129.31	120.90
25	LA	668	A	O4'-C1'-N9	5.25	112.40	108.20
25	LA	1471	G	O4'-C1'-N9	5.25	112.40	108.20
1	SA	216	U	O4'-C1'-N1	5.25	112.40	108.20
1	SA	261	U	C5'-C4'-C3'	5.25	124.40	116.00
1	SA	747	A	O4'-C1'-N9	5.25	112.40	108.20
1	SA	1209	C	O4'-C1'-N1	5.25	112.40	108.20
25	LA	22	C	O4'-C1'-N1	5.25	112.40	108.20
25	LA	1133	A	N1-C6-N6	-5.25	115.45	118.60
25	LA	2061	G	C5-C6-N1	5.25	114.12	111.50
25	LA	2251	G	C3'-C2'-C1'	-5.25	97.30	101.50
1	SA	732	C	O4'-C1'-N1	5.25	112.40	108.20
25	LA	549	G	O4'-C1'-N9	5.25	112.40	108.20
25	LA	1415	U	O4'-C1'-N1	5.25	112.40	108.20
25	LA	2442	C	O4'-C1'-N1	5.25	112.40	108.20
1	SA	68	G	C5-C6-O6	-5.25	125.45	128.60
1	SA	1221	G	O4'-C1'-N9	5.25	112.40	108.20
1	SA	1441	A	P-O5'-C5'	5.25	129.30	120.90
25	LA	228	C	C3'-C2'-C1'	-5.25	97.30	101.50
25	LA	1696	G	O4'-C1'-N9	5.25	112.40	108.20
1	SA	1058	G	O4'-C1'-N9	5.25	112.40	108.20
1	SA	1140	C	C6-N1-C1'	-5.25	114.50	120.80
25	LA	1381	G	O4'-C1'-N9	5.25	112.40	108.20
25	LA	1967	C	O5'-C5'-C4'	5.25	121.67	111.70
25	LA	2280	G	C5'-C4'-C3'	5.25	124.39	116.00
1	SA	587	G	O4'-C1'-N9	5.25	112.40	108.20
25	LA	344	A	C5'-C4'-O4'	5.25	115.39	109.10
25	LA	604	G	C5-C6-O6	-5.25	125.45	128.60
25	LA	2334	U	O4'-C1'-N1	5.25	112.40	108.20
25	LA	2536	G	P-O3'-C3'	5.25	125.99	119.70
26	LB	107	G	C5-C6-O6	-5.25	125.45	128.60
1	SA	406	G	P-O3'-C3'	5.24	125.99	119.70
25	LA	1566	A	O4'-C1'-N9	5.24	112.39	108.20
25	LA	1636	U	P-O5'-C5'	-5.24	112.51	120.90
25	LA	2412	A	C5'-C4'-O4'	5.24	115.39	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1277	C	C5'-C4'-C3'	5.24	124.39	116.00
25	LA	573	U	P-O3'-C3'	5.24	125.99	119.70
25	LA	1641	A	P-O3'-C3'	5.24	125.99	119.70
25	LA	2113	U	O4'-C1'-N1	5.24	112.39	108.20
1	SA	168	G	C4'-C3'-C2'	-5.24	97.36	102.60
1	SA	920	U	P-O5'-C5'	5.24	129.28	120.90
1	SA	960	U	O4'-C1'-N1	5.24	112.39	108.20
25	LA	445	C	O4'-C1'-N1	5.24	112.39	108.20
25	LA	464	U	C6-N1-C1'	-5.24	113.86	121.20
25	LA	1905	C	C5'-C4'-O4'	5.24	115.39	109.10
25	LA	2278	A	C4'-C3'-C2'	-5.24	97.36	102.60
36	LU	76	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	SA	219	U	C4'-C3'-C2'	-5.24	97.36	102.60
1	SA	658	C	O4'-C1'-N1	5.24	112.39	108.20
25	LA	18	U	P-O5'-C5'	5.24	129.28	120.90
25	LA	1489	C	C5'-C4'-O4'	5.24	115.39	109.10
25	LA	1656	C	O4'-C1'-N1	5.24	112.39	108.20
25	LA	2876	G	O4'-C1'-N9	5.24	112.39	108.20
1	SA	111	G	P-O3'-C3'	-5.24	113.42	119.70
1	SA	1279	G	C5'-C4'-O4'	5.24	115.38	109.10
25	LA	647	G	C4'-C3'-C2'	-5.24	97.36	102.60
25	LA	1462	C	O4'-C1'-N1	5.24	112.39	108.20
1	SA	890	G	C5'-C4'-O4'	5.23	115.38	109.10
1	SA	1067	A	P-O5'-C5'	-5.23	112.53	120.90
25	LA	702	U	P-O3'-C3'	5.23	125.98	119.70
1	SA	521	G	O4'-C1'-N9	5.23	112.39	108.20
1	SA	962	C	C6-N1-C1'	5.23	127.08	120.80
25	LA	38	A	P-O3'-C3'	-5.23	113.42	119.70
25	LA	457	A	P-O5'-C5'	5.23	129.27	120.90
44	L3	35	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	SA	158	G	O4'-C1'-N9	5.23	112.39	108.20
1	SA	944	G	C5'-C4'-O4'	5.23	115.38	109.10
1	SA	970	C	P-O3'-C3'	-5.23	113.42	119.70
25	LA	1895	C	C4'-C3'-C2'	-5.23	97.37	102.60
25	LA	2301	C	C5'-C4'-O4'	5.23	115.38	109.10
53	LG	3	GLN	N-CA-C	-5.23	96.88	111.00
25	LA	1021	A	C4-N9-C1'	-5.23	116.89	126.30
25	LA	2471	A	O4'-C1'-N9	5.23	112.38	108.20
25	LA	2709	G	C2'-C3'-O3'	5.23	122.07	113.70
54	LH	126	ARG	NE-CZ-NH1	5.23	122.92	120.30
25	LA	204	A	P-O3'-C3'	5.23	125.97	119.70
25	LA	1739	A	C5'-C4'-C3'	-5.23	107.64	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1824	G	N9-C1'-C2'	-5.23	106.25	112.00
25	LA	2393	U	C4'-C3'-C2'	-5.23	97.37	102.60
25	LA	2885	G	C5-C6-O6	-5.23	125.46	128.60
25	LA	2730	C	C6-N1-C2	-5.23	118.21	120.30
1	SA	446	G	O4'-C1'-N9	5.22	112.38	108.20
1	SA	1126	U	O4'-C1'-N1	5.22	112.38	108.20
1	SA	1345	U	O5'-C5'-C4'	5.22	121.63	111.70
25	LA	2056	G	O5'-C5'-C4'	5.22	121.63	111.70
25	LA	2110	G	O3'-P-O5'	5.22	113.93	104.00
25	LA	2669	G	O4'-C1'-N9	5.22	112.38	108.20
1	SA	410	G	O4'-C1'-N9	5.22	112.38	108.20
25	LA	451	U	O4'-C1'-N1	5.22	112.38	108.20
25	LA	516	C	C6-N1-C2	-5.22	118.21	120.30
25	LA	846	U	P-O3'-C3'	5.22	125.97	119.70
25	LA	1010	A	P-O3'-C3'	5.22	125.97	119.70
25	LA	1021	A	C5'-C4'-O4'	5.22	115.37	109.10
25	LA	198	C	O4'-C1'-N1	5.22	112.38	108.20
25	LA	611	C	C5'-C4'-O4'	5.22	115.37	109.10
25	LA	2585	U	O4'-C1'-N1	5.22	112.38	108.20
1	SA	796	C	O4'-C1'-N1	5.22	112.38	108.20
1	SA	904	U	O4'-C1'-N1	5.22	112.38	108.20
1	SA	1082	A	O4'-C1'-N9	5.22	112.38	108.20
1	SA	1327	C	C5'-C4'-O4'	5.22	115.36	109.10
41	LY	29	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	SA	993	G	C5'-C4'-O4'	5.22	115.36	109.10
4	SJ	68	ARG	NE-CZ-NH1	5.22	122.91	120.30
25	LA	570	G	N1-C6-O6	5.22	123.03	119.90
25	LA	2871	U	O3'-P-O5'	-5.22	94.09	104.00
26	LB	16	G	P-O3'-C3'	-5.22	113.44	119.70
1	SA	241	G	O4'-C1'-N9	5.21	112.37	108.20
1	SA	1124	G	C1'-O4'-C4'	-5.21	105.73	109.90
25	LA	193	U	C5'-C4'-C3'	-5.21	107.66	116.00
25	LA	664	G	C8-N9-C1'	5.21	133.78	127.00
25	LA	1159	U	O4'-C1'-N1	5.21	112.37	108.20
25	LA	1244	A	O4'-C1'-N9	5.21	112.37	108.20
25	LA	1695	G	C5'-C4'-C3'	5.21	124.34	116.00
25	LA	2330	G	C5'-C4'-C3'	5.21	124.34	116.00
25	LA	2478	A	O4'-C1'-N9	5.21	112.37	108.20
25	LA	2867	G	O4'-C1'-N9	5.21	112.37	108.20
1	SA	219	U	O4'-C1'-N1	5.21	112.37	108.20
25	LA	1841	U	C2-N3-C4	-5.21	123.87	127.00
25	LA	1952	A	P-O5'-C5'	-5.21	112.56	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2434	A	O4'-C1'-N9	5.21	112.37	108.20
1	SA	181	A	P-O3'-C3'	-5.21	113.44	119.70
1	SA	278	G	O4'-C1'-N9	5.21	112.37	108.20
1	SA	456	A	O4'-C1'-N9	5.21	112.37	108.20
1	SA	933	G	P-O5'-C5'	5.21	129.24	120.90
16	SU	20	ARG	NE-CZ-NH2	-5.21	117.69	120.30
20	SF	25	TYR	CB-CG-CD2	-5.21	117.87	121.00
25	LA	261	G	P-O5'-C5'	5.21	129.24	120.90
18	SD	43	ARG	NE-CZ-NH1	5.21	122.91	120.30
25	LA	2193	G	O4'-C1'-N9	5.21	112.37	108.20
25	LA	2269	G	P-O3'-C3'	5.21	125.95	119.70
1	SA	77	A	O4'-C1'-N9	5.21	112.37	108.20
25	LA	82	U	O4'-C1'-N1	5.21	112.37	108.20
25	LA	2246	G	C2'-C3'-O3'	5.21	122.03	113.70
1	SA	21	G	O4'-C1'-N9	5.21	112.36	108.20
1	SA	869	G	N1-C6-O6	5.21	123.02	119.90
1	SA	1081	A	C4'-C3'-C2'	-5.21	97.39	102.60
25	LA	1402	U	N1-C2-N3	5.21	118.02	114.90
25	LA	2136	G	O4'-C1'-N9	5.21	112.36	108.20
25	LA	2708	G	C4'-C3'-C2'	-5.21	97.39	102.60
1	SA	278	G	C4-N9-C1'	-5.21	119.73	126.50
3	S7	48	C	C5'-C4'-O4'	5.21	115.35	109.10
25	LA	2208	C	O4'-C1'-N1	5.21	112.36	108.20
1	SA	283	U	O4'-C1'-N1	5.20	112.36	108.20
4	SJ	89	ARG	NE-CZ-NH2	-5.20	117.70	120.30
25	LA	398	C	O3'-P-O5'	5.20	113.89	104.00
25	LA	1489	C	O4'-C1'-N1	5.20	112.36	108.20
25	LA	2129	C	O4'-C1'-N1	5.20	112.36	108.20
25	LA	2802	G	C5'-C4'-O4'	5.20	115.34	109.10
26	LB	26	C	C2-N1-C1'	5.20	124.53	118.80
16	SU	46	ARG	NE-CZ-NH1	5.20	122.90	120.30
25	LA	2248	C	O4'-C1'-N1	5.20	112.36	108.20
1	SA	74	A	O4'-C1'-N9	5.20	112.36	108.20
1	SA	232	G	C5-C6-O6	-5.20	125.48	128.60
1	SA	943	U	O4'-C1'-N1	5.20	112.36	108.20
1	SA	1427	C	C6-N1-C2	-5.20	118.22	120.30
25	LA	1708	C	C6-N1-C2	-5.20	118.22	120.30
25	LA	2361	G	C5'-C4'-C3'	5.20	124.32	116.00
25	LA	2826	A	P-O5'-C5'	5.20	129.22	120.90
1	SA	368	U	C5'-C4'-O4'	5.20	115.34	109.10
1	SA	1366	C	O4'-C1'-N1	5.20	112.36	108.20
25	LA	69	C	C6-N1-C2	-5.20	118.22	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	205	G	C3'-C2'-C1'	-5.20	97.34	101.50
25	LA	1236	G	N1-C6-O6	5.20	123.02	119.90
1	SA	46	G	O4'-C1'-N9	5.20	112.36	108.20
1	SA	516	U	C5'-C4'-C3'	5.20	124.31	116.00
1	SA	1198	G	P-O3'-C3'	-5.20	113.47	119.70
25	LA	473	G	O4'-C1'-N9	5.20	112.36	108.20
30	LO	57	ARG	NE-CZ-NH2	-5.20	117.70	120.30
46	L5	19	ARG	NE-CZ-NH1	5.20	122.90	120.30
25	LA	1634	A	P-O3'-C3'	-5.19	113.47	119.70
26	LB	52	A	O4'-C1'-N9	5.19	112.36	108.20
1	SA	345	C	C1'-O4'-C4'	-5.19	105.75	109.90
1	SA	356	A	N1-C6-N6	-5.19	115.48	118.60
25	LA	220	G	P-O5'-C5'	5.19	129.21	120.90
25	LA	1943	U	C6-N1-C1'	-5.19	113.93	121.20
34	LS	8	ASP	CB-CG-OD2	5.19	122.97	118.30
1	SA	1039	G	O4'-C1'-N9	5.19	112.35	108.20
1	SA	1180	A	O4'-C1'-N9	5.19	112.35	108.20
1	SA	1447	A	C1'-O4'-C4'	-5.19	105.75	109.90
25	LA	753	A	C1'-O4'-C4'	-5.19	105.75	109.90
25	LA	895	U	O4'-C1'-N1	5.19	112.35	108.20
25	LA	921	C	P-O3'-C3'	5.19	125.93	119.70
25	LA	2631	G	C5'-C4'-O4'	5.19	115.33	109.10
25	LA	2873	A	O4'-C1'-C2'	-5.19	100.61	105.80
1	SA	309	A	P-O5'-C5'	5.19	129.20	120.90
1	SA	1356	G	O4'-C1'-N9	5.19	112.35	108.20
1	SA	1512	U	C2'-C3'-O3'	5.19	122.00	113.70
2	S6	13	C	O4'-C1'-N1	5.19	112.35	108.20
25	LA	405	U	O4'-C1'-N1	5.19	112.35	108.20
25	LA	1372	U	O4'-C1'-N1	5.19	112.35	108.20
25	LA	1968	G	O4'-C1'-N9	5.19	112.35	108.20
1	SA	332	G	N1-C6-O6	5.19	123.01	119.90
1	SA	997	U	O4'-C1'-N1	5.19	112.35	108.20
25	LA	1005	C	O4'-C1'-N1	5.19	112.35	108.20
25	LA	1331	G	C4-N9-C1'	5.19	133.24	126.50
25	LA	1411	U	O4'-C1'-N1	5.19	112.35	108.20
25	LA	1675	C	P-O5'-C5'	-5.19	112.60	120.90
1	SA	1005	A	O4'-C1'-N9	5.19	112.35	108.20
3	S7	70	G	C5'-C4'-O4'	-5.19	102.88	109.10
25	LA	177	G	C5-C6-O6	-5.19	125.49	128.60
25	LA	397	U	P-O5'-C5'	-5.19	112.60	120.90
25	LA	40	U	C5'-C4'-C3'	-5.18	107.70	116.00
25	LA	526	A	O3'-P-O5'	5.18	113.85	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	906	U	O4'-C4'-C3'	-5.18	98.81	104.00
25	LA	1239	G	C4'-C3'-C2'	-5.18	97.42	102.60
25	LA	2406	A	O3'-P-O5'	-5.18	94.15	104.00
1	SA	859	G	O4'-C1'-N9	5.18	112.34	108.20
1	SA	1539	C	C1'-O4'-C4'	-5.18	105.75	109.90
25	LA	282	A	O4'-C1'-N9	5.18	112.35	108.20
25	LA	1149	G	C5'-C4'-O4'	5.18	115.32	109.10
25	LA	2086	U	C4'-C3'-C2'	-5.18	97.42	102.60
25	LA	2341	G	C5'-C4'-O4'	5.18	115.32	109.10
25	LA	2772	C	C6-N1-C2	-5.18	118.23	120.30
51	L9	123	ARG	NE-CZ-NH1	5.18	122.89	120.30
3	S7	56	C	P-O3'-C3'	5.18	125.91	119.70
25	LA	672	C	C4'-C3'-C2'	-5.18	97.42	102.60
25	LA	672	C	O4'-C1'-N1	5.18	112.34	108.20
25	LA	1031	G	C5'-C4'-O4'	5.18	115.32	109.10
25	LA	1268	A	C4'-C3'-C2'	-5.18	97.42	102.60
1	SA	283	U	P-O3'-C3'	5.18	125.91	119.70
25	LA	34	U	P-O5'-C5'	5.18	129.18	120.90
25	LA	1162	G	O4'-C1'-N9	5.18	112.34	108.20
25	LA	1778	U	O4'-C1'-N1	5.18	112.34	108.20
25	LA	2091	C	C6-N1-C2	-5.18	118.23	120.30
25	LA	2343	U	P-O3'-C3'	5.18	125.91	119.70
1	SA	240	G	O4'-C1'-N9	5.17	112.34	108.20
1	SA	1345	U	O4'-C1'-N1	5.17	112.34	108.20
1	SA	1504	G	N1-C6-O6	5.17	123.00	119.90
25	LA	1727	C	O4'-C1'-N1	5.17	112.34	108.20
25	LA	2511	U	C2-N3-C4	-5.17	123.90	127.00
25	LA	2895	G	C5-C6-O6	-5.17	125.50	128.60
1	SA	67	C	O4'-C1'-N1	5.17	112.34	108.20
5	SK	126	ARG	NE-CZ-NH2	-5.17	117.71	120.30
25	LA	101	A	O4'-C1'-N9	5.17	112.34	108.20
25	LA	1107	G	O4'-C1'-N9	5.17	112.34	108.20
25	LA	1417	C	P-O3'-C3'	5.17	125.91	119.70
25	LA	1715	G	P-O3'-C3'	5.17	125.91	119.70
25	LA	2190	G	O4'-C1'-N9	5.17	112.34	108.20
25	LA	2293	G	C5'-C4'-O4'	5.17	115.31	109.10
25	LA	2319	G	N1-C6-O6	5.17	123.00	119.90
25	LA	2445	G	C8-N9-C4	5.17	108.47	106.40
25	LA	2577	A	P-O3'-C3'	-5.17	113.49	119.70
25	LA	134	G	C5'-C4'-C3'	-5.17	107.73	116.00
25	LA	338	G	C5-C6-O6	-5.17	125.50	128.60
25	LA	381	G	O4'-C1'-N9	5.17	112.34	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1059	G	C5-C6-O6	-5.17	125.50	128.60
25	LA	1596	A	P-O3'-C3'	-5.17	113.50	119.70
25	LA	2721	A	C4'-C3'-C2'	-5.17	97.43	102.60
25	LA	2737	G	P-O5'-C5'	5.17	129.18	120.90
10	SP	5	ARG	NE-CZ-NH2	-5.17	117.72	120.30
25	LA	1540	G	O4'-C1'-N9	5.17	112.34	108.20
25	LA	592	A	P-O3'-C3'	5.17	125.90	119.70
25	LA	914	G	C4'-C3'-C2'	-5.17	97.43	102.60
25	LA	2471	A	C5'-C4'-O4'	5.17	115.30	109.10
26	LB	13	G	C5-C6-O6	-5.17	125.50	128.60
38	LD	98	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	SA	399	G	O4'-C1'-N9	5.17	112.33	108.20
2	S6	55	U	O4'-C1'-N1	5.17	112.33	108.20
25	LA	2521	C	C2-N3-C4	-5.17	117.32	119.90
26	LB	98	G	O4'-C1'-N9	5.17	112.33	108.20
1	SA	683	G	C5-C6-O6	-5.17	125.50	128.60
25	LA	1072	C	P-O3'-C3'	-5.17	113.50	119.70
25	LA	1487	U	O4'-C1'-N1	5.17	112.33	108.20
25	LA	2828	G	O4'-C1'-N9	5.17	112.33	108.20
54	LH	123	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	SA	1169	A	O4'-C1'-N9	5.16	112.33	108.20
2	S6	70	C	C4'-C3'-C2'	-5.16	97.44	102.60
15	ST	28	ARG	NE-CZ-NH1	5.16	122.88	120.30
25	LA	507	A	C2'-C3'-O3'	5.16	121.96	113.70
25	LA	1257	C	C6-N1-C2	-5.16	118.23	120.30
25	LA	2718	G	C5'-C4'-C3'	5.16	124.26	116.00
25	LA	1706	C	O4'-C1'-N1	5.16	112.33	108.20
25	LA	1820	U	O4'-C1'-N1	5.16	112.33	108.20
25	LA	2252	G	C5'-C4'-O4'	5.16	115.29	109.10
1	SA	159	G	O4'-C1'-N9	5.16	112.33	108.20
1	SA	507	C	P-O5'-C5'	5.16	129.16	120.90
1	SA	1278	G	C4'-C3'-C2'	5.16	107.76	102.60
1	SA	1517	G	C5'-C4'-O4'	5.16	115.29	109.10
3	S7	39	U	C6-N1-C1'	-5.16	113.98	121.20
25	LA	352	A	O4'-C1'-N9	5.16	112.33	108.20
25	LA	935	C	O4'-C1'-N1	5.16	112.33	108.20
25	LA	1911	U	O4'-C1'-C2'	5.16	112.24	107.60
25	LA	2120	G	P-O5'-C5'	-5.16	112.64	120.90
25	LA	2523	G	P-O5'-C5'	-5.16	112.64	120.90
25	LA	2802	G	C2'-C3'-O3'	5.16	121.95	113.70
49	L7	154	THR	N-CA-CB	5.16	120.11	110.30
1	SA	123	U	O4'-C1'-N1	5.16	112.33	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	137	U	C5'-C4'-C3'	-5.16	107.75	116.00
1	SA	1099	G	N9-C1'-C2'	-5.16	106.33	112.00
1	SA	1180	A	N1-C6-N6	5.16	121.69	118.60
1	SA	1400	C	C6-N1-C1'	-5.16	114.61	120.80
1	SA	1499	A	P-O3'-C3'	-5.16	113.51	119.70
25	LA	1247	A	C5'-C4'-O4'	5.16	115.29	109.10
25	LA	2389	G	C5'-C4'-O4'	5.16	115.29	109.10
26	LB	88	C	C6-N1-C1'	-5.16	114.61	120.80
1	SA	297	G	C8-N9-C1'	5.16	133.70	127.00
1	SA	486	U	O4'-C1'-N1	5.16	112.32	108.20
25	LA	589	U	O4'-C1'-N1	5.16	112.32	108.20
25	LA	668	A	P-O3'-C3'	5.16	125.89	119.70
25	LA	1987	A	C5'-C4'-O4'	5.16	115.29	109.10
25	LA	2556	C	P-O3'-C3'	-5.16	113.51	119.70
1	SA	420	U	P-O3'-C3'	5.15	125.89	119.70
1	SA	1104	G	C5'-C4'-C3'	5.15	124.25	116.00
1	SA	1416	G	C5-C6-O6	-5.15	125.51	128.60
25	LA	2184	A	O4'-C1'-N9	5.15	112.32	108.20
1	SA	305	G	C5-C6-O6	-5.15	125.51	128.60
1	SA	582	C	O4'-C1'-N1	5.15	112.32	108.20
1	SA	1511	G	P-O3'-C3'	5.15	125.88	119.70
25	LA	1003	G	C5-C6-O6	-5.15	125.51	128.60
25	LA	1094	U	O4'-C1'-N1	5.15	112.32	108.20
25	LA	2846	G	P-O3'-C3'	-5.15	113.52	119.70
25	LA	2903	U	C5'-C4'-O4'	5.15	115.28	109.10
56	LJ	46	ARG	NE-CZ-NH1	5.15	122.88	120.30
57	LK	36	TYR	CB-CG-CD2	5.15	124.09	121.00
1	SA	709	U	O4'-C1'-N1	5.15	112.32	108.20
1	SA	1094	G	N1-C6-O6	5.15	122.99	119.90
21	SG	77	ARG	NE-CZ-NH2	-5.15	117.72	120.30
25	LA	1016	G	C4'-C3'-C2'	-5.15	97.45	102.60
25	LA	1251	C	C5'-C4'-O4'	5.15	115.28	109.10
25	LA	1917	U	C1'-O4'-C4'	5.15	114.02	109.90
25	LA	2581	G	C5'-C4'-C3'	-5.15	107.76	116.00
25	LA	2825	G	O4'-C1'-N9	5.15	112.32	108.20
25	LA	2830	C	C5'-C4'-O4'	5.15	115.28	109.10
51	L9	15	LEU	N-CA-CB	5.15	120.70	110.40
1	SA	204	G	C5'-C4'-O4'	5.15	115.28	109.10
1	SA	394	G	N1-C6-O6	5.15	122.99	119.90
1	SA	854	U	O4'-C1'-N1	5.15	112.32	108.20
25	LA	408	G	O4'-C1'-N9	5.15	112.32	108.20
25	LA	1081	U	O4'-C1'-N1	5.15	112.32	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1721	G	O4'-C1'-N9	5.15	112.32	108.20
25	LA	1976	U	C2-N3-C4	-5.15	123.91	127.00
25	LA	2199	A	O4'-C1'-N9	5.15	112.32	108.20
25	LA	2624	G	O4'-C1'-N9	5.15	112.32	108.20
25	LA	2850	A	P-O5'-C5'	-5.15	112.67	120.90
25	LA	1133	A	C1'-O4'-C4'	-5.15	105.78	109.90
25	LA	2403	C	C5'-C4'-C3'	5.15	124.23	116.00
40	LX	113	SER	N-CA-CB	5.15	118.22	110.50
25	LA	640	C	C6-N1-C2	-5.14	118.24	120.30
25	LA	1879	C	C6-N1-C2	-5.14	118.24	120.30
25	LA	2322	A	O4'-C4'-C3'	-5.14	98.86	104.00
1	SA	840	C	C1'-O4'-C4'	-5.14	105.79	109.90
1	SA	1481	U	C5'-C4'-O4'	5.14	115.27	109.10
25	LA	423	A	N1-C6-N6	-5.14	115.52	118.60
25	LA	946	C	C6-N1-C2	-5.14	118.24	120.30
25	LA	1223	G	C4'-C3'-C2'	-5.14	97.46	102.60
25	LA	1507	C	O4'-C1'-N1	5.14	112.31	108.20
25	LA	1941	C	P-O5'-C5'	-5.14	112.67	120.90
25	LA	2350	C	O4'-C1'-N1	5.14	112.31	108.20
25	LA	899	A	O4'-C1'-N9	5.14	112.31	108.20
1	SA	1073	U	C5'-C4'-C3'	-5.14	107.78	116.00
25	LA	1192	G	O4'-C1'-N9	5.14	112.31	108.20
25	LA	1502	A	O4'-C1'-N9	5.14	112.31	108.20
25	LA	2236	U	C2'-C3'-O3'	5.14	121.92	113.70
26	LB	107	G	N1-C6-O6	5.14	122.98	119.90
25	LA	2495	G	O4'-C1'-N9	5.14	112.31	108.20
1	SA	206	C	O4'-C1'-N1	5.14	112.31	108.20
1	SA	761	G	O4'-C1'-N9	5.14	112.31	108.20
24	S1	146	MET	CG-SD-CE	-5.14	91.98	100.20
25	LA	231	A	O4'-C1'-N9	5.14	112.31	108.20
25	LA	1030	C	C5'-C4'-C3'	5.14	124.22	116.00
25	LA	1611	C	P-O3'-C3'	5.14	125.86	119.70
25	LA	1999	C	C4'-C3'-C2'	-5.14	97.46	102.60
25	LA	2206	C	P-O5'-C5'	5.14	129.12	120.90
1	SA	266	G	C5-C6-O6	-5.13	125.52	128.60
1	SA	693	G	C4-N9-C1'	5.13	133.17	126.50
25	LA	1118	C	C6-N1-C2	-5.13	118.25	120.30
25	LA	2071	A	C5'-C4'-O4'	5.13	115.26	109.10
25	LA	2358	A	O4'-C1'-N9	5.13	112.31	108.20
25	LA	2559	C	O4'-C1'-N1	5.13	112.31	108.20
25	LA	2430	A	O3'-P-O5'	5.13	113.75	104.00
1	SA	37	U	C5'-C4'-O4'	5.13	115.26	109.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S7	32	U	O4'-C1'-N1	5.13	112.31	108.20
25	LA	874	G	O4'-C1'-N9	5.13	112.30	108.20
25	LA	1227	G	O4'-C1'-N9	5.13	112.31	108.20
25	LA	2697	G	C5'-C4'-O4'	5.13	115.26	109.10
25	LA	2747	G	C5-C6-O6	-5.13	125.52	128.60
1	SA	979	C	P-O5'-C5'	5.13	129.11	120.90
25	LA	344	A	O4'-C1'-N9	5.13	112.30	108.20
25	LA	365	U	O4'-C1'-N1	5.13	112.30	108.20
1	SA	898	G	C4-N9-C1'	-5.13	119.83	126.50
25	LA	76	C	O4'-C1'-N1	5.13	112.30	108.20
25	LA	300	A	P-O3'-C3'	-5.13	113.55	119.70
25	LA	491	G	O4'-C1'-N9	5.13	112.30	108.20
25	LA	818	G	N3-C2-N2	5.13	123.49	119.90
25	LA	931	U	C2-N1-C1'	5.13	123.85	117.70
25	LA	1615	C	C6-N1-C2	-5.13	118.25	120.30
25	LA	1927	A	C2'-C3'-O3'	5.13	121.91	113.70
25	LA	2472	G	C8-N9-C1'	-5.13	120.33	127.00
25	LA	2643	G	C5-C6-O6	-5.13	125.52	128.60
1	SA	105	G	O4'-C1'-N9	5.13	112.30	108.20
1	SA	1413	A	O4'-C1'-N9	5.13	112.30	108.20
25	LA	437	U	C5'-C4'-O4'	5.13	115.25	109.10
25	LA	1921	G	C5-C6-O6	-5.13	125.52	128.60
25	LA	2442	C	C2-N3-C4	-5.13	117.34	119.90
25	LA	2621	G	C5'-C4'-C3'	5.13	124.20	116.00
25	LA	2815	C	P-O5'-C5'	-5.13	112.70	120.90
26	LB	5	U	P-O3'-C3'	-5.13	113.55	119.70
1	SA	151	A	O4'-C1'-N9	5.12	112.30	108.20
1	SA	290	C	O4'-C1'-N1	5.12	112.30	108.20
1	SA	334	C	P-O5'-C5'	5.12	129.10	120.90
1	SA	578	C	P-O3'-C3'	-5.12	113.55	119.70
1	SA	1395	C	P-O5'-C5'	5.12	129.10	120.90
17	SC	106	ARG	NE-CZ-NH2	-5.12	117.74	120.30
25	LA	1924	C	O4'-C1'-N1	5.12	112.30	108.20
40	LX	33	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	SA	143	A	O4'-C1'-N9	5.12	112.30	108.20
1	SA	185	U	P-O5'-C5'	5.12	129.10	120.90
1	SA	924	C	C5-C4-N4	-5.12	116.61	120.20
25	LA	307	G	C4-N9-C1'	-5.12	119.84	126.50
25	LA	309	A	O4'-C1'-N9	5.12	112.30	108.20
25	LA	1846	G	N3-C2-N2	5.12	123.49	119.90
1	SA	779	C	O4'-C1'-N1	5.12	112.30	108.20
1	SA	836	G	O4'-C1'-N9	5.12	112.30	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1472	C	C6-N1-C2	-5.12	118.25	120.30
25	LA	1537	G	C5-C6-O6	-5.12	125.53	128.60
25	LA	1841	U	N1-C2-N3	5.12	117.97	114.90
1	SA	479	U	C4'-C3'-C2'	-5.12	97.48	102.60
1	SA	1162	C	C5'-C4'-O4'	5.12	115.24	109.10
1	SA	165	G	O4'-C1'-N9	5.12	112.29	108.20
1	SA	798	U	C5'-C4'-O4'	5.12	115.24	109.10
25	LA	1212	G	C5-C6-O6	-5.12	125.53	128.60
25	LA	2435	A	O4'-C1'-N9	5.12	112.30	108.20
56	LJ	2	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	SA	254	G	P-O5'-C5'	-5.12	112.71	120.90
25	LA	484	C	C6-N1-C2	-5.12	118.25	120.30
25	LA	1733	G	P-O3'-C3'	5.12	125.84	119.70
25	LA	1267	U	O4'-C1'-N1	5.12	112.29	108.20
25	LA	1360	G	O4'-C1'-N9	5.12	112.29	108.20
25	LA	1857	G	C5-C6-O6	-5.12	125.53	128.60
1	SA	185	U	O4'-C1'-N1	5.11	112.29	108.20
25	LA	777	G	C4'-C3'-C2'	-5.11	97.49	102.60
1	SA	1420	U	O4'-C1'-N1	5.11	112.29	108.20
25	LA	1277	G	P-O3'-C3'	5.11	125.83	119.70
25	LA	2224	G	N3-C2-N2	5.11	123.48	119.90
1	SA	719	C	C2'-C3'-O3'	5.11	121.88	113.70
1	SA	1035	A	P-O5'-C5'	5.11	129.08	120.90
1	SA	1313	U	C5'-C4'-C3'	-5.11	107.82	116.00
1	SA	1379	G	C5'-C4'-C3'	5.11	124.18	116.00
25	LA	1215	G	O4'-C1'-N9	5.11	112.29	108.20
25	LA	1421	G	O4'-C1'-N9	5.11	112.29	108.20
25	LA	2458	G	C8-N9-C1'	-5.11	120.36	127.00
1	SA	839	C	C5'-C4'-C3'	5.11	124.17	116.00
25	LA	2572	A	N1-C6-N6	-5.11	115.53	118.60
28	LM	52	ARG	NE-CZ-NH2	-5.11	117.75	120.30
50	L8	163	TYR	CB-CG-CD2	5.11	124.07	121.00
1	SA	307	C	C2'-C3'-O3'	5.11	121.87	113.70
1	SA	1009	U	O4'-C1'-N1	5.11	112.29	108.20
23	SI	121	ARG	NE-CZ-NH1	5.11	122.85	120.30
25	LA	31	C	C5'-C4'-O4'	5.11	115.23	109.10
25	LA	206	U	C2-N3-C4	-5.11	123.94	127.00
25	LA	747	U	P-O5'-C5'	-5.11	112.73	120.90
25	LA	755	U	O4'-C1'-N1	5.11	112.29	108.20
25	LA	1070	A	C5'-C4'-C3'	-5.11	107.83	116.00
1	SA	69	G	O4'-C1'-N9	5.11	112.28	108.20
1	SA	268	U	O4'-C1'-N1	5.11	112.28	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	461	C	O4'-C1'-N1	5.11	112.28	108.20
25	LA	797	G	C5-C6-O6	-5.11	125.54	128.60
25	LA	2092	U	C1'-O4'-C4'	-5.11	105.82	109.90
25	LA	367	G	O4'-C1'-N9	5.10	112.28	108.20
25	LA	1689	A	O4'-C1'-N9	5.10	112.28	108.20
1	SA	258	G	O4'-C1'-N9	5.10	112.28	108.20
1	SA	500	G	C5-C6-O6	-5.10	125.54	128.60
1	SA	855	U	C2-N3-C4	-5.10	123.94	127.00
2	S6	62	C	O4'-C1'-N1	5.10	112.28	108.20
25	LA	79	C	P-O3'-C3'	-5.10	113.58	119.70
25	LA	491	G	C5-C6-O6	-5.10	125.54	128.60
25	LA	573	U	P-O5'-C5'	5.10	129.06	120.90
25	LA	646	U	C2-N3-C4	-5.10	123.94	127.00
25	LA	814	C	O4'-C1'-N1	5.10	112.28	108.20
25	LA	861	A	C4'-C3'-C2'	-5.10	97.50	102.60
25	LA	932	U	P-O5'-C5'	-5.10	112.73	120.90
25	LA	1206	G	C1'-O4'-C4'	-5.10	105.82	109.90
25	LA	1550	C	C5'-C4'-O4'	5.10	115.22	109.10
25	LA	1667	G	O4'-C1'-N9	5.10	112.28	108.20
25	LA	2370	G	O4'-C1'-N9	5.10	112.28	108.20
25	LA	2541	A	C5'-C4'-C3'	-5.10	107.83	116.00
1	SA	320	A	C5'-C4'-O4'	5.10	115.22	109.10
25	LA	2572	A	P-O5'-C5'	-5.10	112.74	120.90
26	LB	91	C	P-O5'-C5'	5.10	129.06	120.90
1	SA	537	G	O4'-C1'-N9	5.10	112.28	108.20
25	LA	266	G	C5'-C4'-C3'	5.10	124.16	116.00
25	LA	1604	C	O4'-C1'-N1	5.10	112.28	108.20
25	LA	1930	G	C4'-C3'-C2'	-5.10	97.50	102.60
25	LA	1947	C	C6-N1-C2	-5.10	118.26	120.30
24	S1	75	ALA	N-CA-CB	5.10	117.24	110.10
25	LA	769	U	O4'-C1'-N1	5.10	112.28	108.20
25	LA	1012	U	O4'-C1'-N1	5.10	112.28	108.20
25	LA	1157	G	O4'-C1'-N9	5.10	112.28	108.20
25	LA	1745	A	O4'-C1'-N9	5.10	112.28	108.20
25	LA	1021	A	P-O3'-C3'	-5.10	113.58	119.70
25	LA	1239	G	C5-C6-O6	-5.10	125.54	128.60
25	LA	1905	C	C6-N1-C2	-5.10	118.26	120.30
25	LA	2669	G	C5'-C4'-C3'	5.10	124.15	116.00
1	SA	829	G	C5'-C4'-O4'	5.09	115.21	109.10
24	S1	436	ARG	NE-CZ-NH1	5.09	122.85	120.30
25	LA	444	C	O4'-C1'-N1	5.09	112.28	108.20
25	LA	589	U	P-O3'-C3'	5.09	125.81	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1067	A	C4-N9-C1'	5.09	135.47	126.30
25	LA	549	G	C5-C6-O6	-5.09	125.54	128.60
1	SA	156	C	P-O5'-C5'	-5.09	112.75	120.90
1	SA	290	C	C6-N1-C2	-5.09	118.26	120.30
1	SA	634	C	O4'-C1'-N1	5.09	112.27	108.20
1	SA	1501	C	O3'-P-O5'	-5.09	94.33	104.00
25	LA	1845	G	O4'-C1'-N9	5.09	112.27	108.20
25	LA	1996	C	P-O3'-C3'	5.09	125.81	119.70
25	LA	2357	G	C5-C6-O6	-5.09	125.55	128.60
25	LA	2645	G	N1-C6-O6	5.09	122.95	119.90
25	LA	2840	C	C5'-C4'-C3'	-5.09	107.85	116.00
37	LV	2	ARG	NE-CZ-NH2	5.09	122.85	120.30
46	L5	4	ARG	NE-CZ-NH2	-5.09	117.75	120.30
25	LA	347	A	C5'-C4'-O4'	5.09	115.21	109.10
25	LA	869	G	O4'-C1'-N9	5.09	112.27	108.20
25	LA	1376	C	N3-C2-O2	-5.09	118.34	121.90
26	LB	106	G	O4'-C1'-N9	5.09	112.27	108.20
25	LA	2495	G	N3-C2-N2	5.09	123.46	119.90
1	SA	961	U	C3'-C2'-C1'	5.09	105.57	101.50
1	SA	1056	U	O4'-C1'-N1	5.09	112.27	108.20
1	SA	1389	C	P-O5'-C5'	5.09	129.04	120.90
4	SJ	16	ARG	NE-CZ-NH2	-5.09	117.76	120.30
25	LA	569	U	P-O5'-C5'	-5.09	112.76	120.90
25	LA	1164	C	P-O3'-C3'	-5.09	113.59	119.70
25	LA	2757	A	C1'-O4'-C4'	-5.09	105.83	109.90
1	SA	882	C	C5'-C4'-C3'	-5.08	107.86	116.00
1	SA	1085	U	P-O3'-C3'	5.08	125.80	119.70
25	LA	332	A	P-O5'-C5'	-5.08	112.77	120.90
47	L6	40	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	SA	320	A	C4'-C3'-C2'	-5.08	97.52	102.60
1	SA	583	A	P-O5'-C5'	-5.08	112.77	120.90
25	LA	433	C	O4'-C1'-N1	5.08	112.27	108.20
25	LA	1281	G	O4'-C1'-N9	5.08	112.27	108.20
25	LA	1381	G	N3-C2-N2	5.08	123.46	119.90
1	SA	25	C	O4'-C1'-N1	5.08	112.27	108.20
1	SA	371	A	O4'-C1'-N9	5.08	112.27	108.20
25	LA	411	G	O4'-C1'-C2'	-5.08	100.72	105.80
25	LA	873	C	C6-N1-C2	-5.08	118.27	120.30
25	LA	1168	G	O3'-P-O5'	-5.08	94.35	104.00
25	LA	2047	C	C5'-C4'-C3'	-5.08	107.87	116.00
25	LA	2683	C	P-O5'-C5'	-5.08	112.77	120.90
25	LA	2872	A	C4'-C3'-C2'	-5.08	97.52	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	353	A	O4'-C1'-N9	5.08	112.26	108.20
25	LA	1235	G	N1-C6-O6	5.08	122.95	119.90
51	L9	27	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	SA	1267	C	C6-N1-C1'	-5.08	114.70	120.80
25	LA	1649	G	P-O3'-C3'	5.08	125.80	119.70
25	LA	1945	G	C5-C6-O6	-5.08	125.55	128.60
25	LA	2891	U	C5'-C4'-O4'	5.08	115.19	109.10
1	SA	604	G	C4'-C3'-C2'	-5.08	97.52	102.60
25	LA	204	A	O4'-C1'-N9	5.08	112.26	108.20
25	LA	1638	C	O4'-C1'-N1	5.08	112.26	108.20
1	SA	308	C	O4'-C1'-N1	5.08	112.26	108.20
1	SA	1304	G	C4'-C3'-C2'	-5.08	97.52	102.60
25	LA	1202	G	O3'-P-O5'	-5.08	94.36	104.00
25	LA	2470	G	O4'-C1'-N9	5.08	112.26	108.20
28	LM	100	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	SA	810	C	C6-N1-C1'	-5.07	114.71	120.80
1	SA	906	A	O4'-C1'-N9	5.07	112.26	108.20
1	SA	1167	A	O4'-C1'-N9	5.07	112.26	108.20
1	SA	1415	G	C5'-C4'-C3'	5.07	124.12	116.00
24	S1	638	ARG	NE-CZ-NH1	5.07	122.84	120.30
25	LA	1585	C	C5'-C4'-C3'	-5.07	107.88	116.00
25	LA	1675	C	O4'-C1'-N1	5.07	112.26	108.20
25	LA	1994	C	C6-N1-C2	-5.07	118.27	120.30
25	LA	2332	C	P-O3'-C3'	-5.07	113.61	119.70
25	LA	2450	A	C3'-C2'-C1'	-5.07	97.44	101.50
25	LA	623	C	P-O3'-C3'	5.07	125.79	119.70
25	LA	1785	A	P-O3'-C3'	5.07	125.79	119.70
25	LA	1799	G	P-O3'-C3'	5.07	125.79	119.70
1	SA	564	C	O4'-C1'-C2'	5.07	112.16	107.60
1	SA	961	U	C2'-C3'-O3'	5.07	121.81	113.70
3	S7	28	G	O4'-C1'-N9	5.07	112.26	108.20
25	LA	403	U	C5'-C4'-O4'	5.07	115.19	109.10
25	LA	524	G	C5-C6-O6	-5.07	125.56	128.60
25	LA	649	G	O4'-C1'-N9	5.07	112.26	108.20
25	LA	1735	A	O4'-C1'-N9	5.07	112.25	108.20
25	LA	2663	G	O4'-C1'-N9	5.07	112.25	108.20
1	SA	1513	A	P-O3'-C3'	-5.07	113.62	119.70
25	LA	907	G	N1-C6-O6	5.07	122.94	119.90
25	LA	1252	G	C5'-C4'-O4'	5.07	115.18	109.10
25	LA	2448	A	C5-C6-N6	-5.07	119.65	123.70
25	LA	2887	A	C5'-C4'-O4'	5.07	115.18	109.10
26	LB	6	G	C5-C6-O6	-5.07	125.56	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	1519	A	O4'-C1'-N9	5.07	112.25	108.20
25	LA	1985	C	C4'-C3'-C2'	-5.07	97.53	102.60
25	LA	2566	A	C4'-C3'-C2'	5.07	107.67	102.60
1	SA	1148	U	C5'-C4'-O4'	5.06	115.18	109.10
1	SA	1288	A	P-O3'-C3'	-5.06	113.62	119.70
25	LA	1579	A	O4'-C1'-N9	5.06	112.25	108.20
25	LA	1993	U	C6-N1-C2	-5.06	117.96	121.00
1	SA	252	U	C2-N3-C4	-5.06	123.96	127.00
25	LA	2224	G	C5-C6-O6	-5.06	125.56	128.60
1	SA	265	G	P-O5'-C5'	5.06	129.00	120.90
25	LA	664	G	C4-N9-C1'	-5.06	119.92	126.50
25	LA	2087	G	O4'-C1'-N9	5.06	112.25	108.20
25	LA	2105	U	O4'-C1'-N1	5.06	112.25	108.20
25	LA	2749	A	O4'-C1'-N9	5.06	112.25	108.20
26	LB	86	G	C8-N9-C1'	5.06	133.58	127.00
3	S7	34	G	C5-C6-O6	-5.06	125.57	128.60
25	LA	573	U	O4'-C4'-C3'	-5.06	98.94	104.00
25	LA	1063	G	O4'-C1'-N9	5.06	112.25	108.20
25	LA	920	A	O4'-C1'-N9	5.06	112.25	108.20
25	LA	1223	G	C5'-C4'-C3'	-5.06	107.91	116.00
1	SA	183	C	C6-N1-C2	-5.05	118.28	120.30
1	SA	1260	G	C5-C6-O6	-5.05	125.57	128.60
25	LA	532	A	P-O3'-C3'	5.05	125.77	119.70
25	LA	1012	U	C6-N1-C1'	-5.05	114.12	121.20
25	LA	1837	C	C5'-C4'-O4'	5.05	115.16	109.10
25	LA	2223	G	P-O3'-C3'	5.05	125.77	119.70
25	LA	2408	U	O4'-C1'-N1	5.05	112.24	108.20
1	SA	332	G	C5'-C4'-O4'	5.05	115.16	109.10
1	SA	665	A	O4'-C1'-N9	5.05	112.24	108.20
6	SL	55	ARG	NE-CZ-NH1	5.05	122.83	120.30
25	LA	2102	G	O4'-C1'-N9	5.05	112.24	108.20
25	LA	2506	U	O3'-P-O5'	5.05	113.60	104.00
1	SA	289	G	C4'-C3'-C2'	-5.05	97.55	102.60
1	SA	488	C	O4'-C1'-N1	5.05	112.24	108.20
1	SA	849	G	N1-C6-O6	5.05	122.93	119.90
25	LA	999	U	O4'-C1'-N1	5.05	112.24	108.20
25	LA	1576	U	O4'-C1'-N1	5.05	112.24	108.20
25	LA	2463	C	O4'-C1'-N1	5.05	112.24	108.20
25	LA	2799	A	C8-N9-C4	-5.05	103.78	105.80
26	LB	105	G	O4'-C1'-N9	5.05	112.24	108.20
1	SA	235	C	P-O5'-C5'	-5.05	112.82	120.90
1	SA	249	U	O4'-C1'-N1	5.05	112.24	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	SA	991	U	C5'-C4'-O4'	5.05	115.16	109.10
25	LA	1781	U	P-O3'-C3'	-5.05	113.64	119.70
25	LA	1832	C	C5'-C4'-O4'	5.05	115.16	109.10
25	LA	2157	G	C5-C6-O6	-5.05	125.57	128.60
1	SA	229	U	C4'-C3'-C2'	-5.05	97.55	102.60
1	SA	292	G	P-O3'-C3'	5.05	125.76	119.70
1	SA	1522	U	C3'-C2'-C1'	5.05	105.54	101.50
23	SI	129	ARG	NE-CZ-NH1	5.05	122.82	120.30
25	LA	1362	C	C4'-C3'-C2'	-5.05	97.55	102.60
25	LA	1836	C	C5'-C4'-C3'	5.05	124.07	116.00
25	LA	1920	C	C2-N3-C4	-5.05	117.38	119.90
25	LA	2830	C	C5'-C4'-C3'	-5.05	107.92	116.00
26	LB	53	A	O4'-C1'-N9	5.05	112.24	108.20
1	SA	221	C	C5'-C4'-O4'	5.04	115.15	109.10
1	SA	241	G	C4'-C3'-C2'	-5.04	97.56	102.60
1	SA	496	A	C1'-O4'-C4'	-5.04	105.86	109.90
1	SA	505	G	O4'-C1'-N9	5.04	112.24	108.20
25	LA	778	G	C5'-C4'-C3'	-5.04	107.93	116.00
25	LA	1180	U	O4'-C1'-N1	5.04	112.24	108.20
25	LA	2401	U	O4'-C1'-N1	5.04	112.24	108.20
1	SA	1148	U	O4'-C1'-N1	5.04	112.24	108.20
25	LA	470	A	O4'-C1'-N9	5.04	112.23	108.20
25	LA	510	C	O3'-P-O5'	-5.04	94.42	104.00
25	LA	1801	A	O4'-C1'-N9	5.04	112.23	108.20
25	LA	2280	G	C4'-C3'-C2'	-5.04	97.56	102.60
25	LA	2387	U	C4'-C3'-C2'	-5.04	97.56	102.60
49	L7	157	THR	N-CA-CB	5.04	119.88	110.30
1	SA	794	A	O5'-C5'-C4'	5.04	121.28	111.70
13	SS	36	ARG	NE-CZ-NH1	5.04	122.82	120.30
25	LA	2083	G	P-O3'-C3'	5.04	125.75	119.70
25	LA	2147	A	O3'-P-O5'	-5.04	94.42	104.00
25	LA	2272	U	N1-C1'-C2'	5.04	120.55	114.00
25	LA	2836	U	C2-N3-C4	-5.04	123.97	127.00
1	SA	365	U	P-O5'-C5'	5.04	128.97	120.90
1	SA	1154	G	C5-C6-O6	-5.04	125.58	128.60
25	LA	2881	U	C5'-C4'-O4'	5.04	115.15	109.10
1	SA	27	G	O4'-C1'-N9	5.04	112.23	108.20
1	SA	1119	C	C1'-O4'-C4'	-5.04	105.87	109.90
1	SA	1485	U	C2-N1-C1'	-5.04	111.65	117.70
25	LA	481	G	C3'-C2'-C1'	-5.04	97.47	101.50
25	LA	507	A	C5'-C4'-C3'	-5.04	107.94	116.00
25	LA	1016	G	O4'-C1'-N9	5.04	112.23	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	1422	G	O4'-C1'-N9	5.04	112.23	108.20
25	LA	1615	C	P-O3'-C3'	-5.04	113.65	119.70
25	LA	1956	U	P-O5'-C5'	-5.04	112.84	120.90
49	L7	95	MET	CG-SD-CE	-5.04	92.14	100.20
1	SA	727	G	C5'-C4'-C3'	5.04	124.06	116.00
25	LA	710	U	O4'-C1'-N1	5.04	112.23	108.20
25	LA	2452	C	C6-N1-C2	-5.04	118.28	120.30
25	LA	2681	C	P-O3'-C3'	-5.04	113.66	119.70
1	SA	1121	U	P-O3'-C3'	5.04	125.74	119.70
25	LA	379	G	O4'-C1'-N9	5.04	112.23	108.20
25	LA	940	G	C4'-C3'-C2'	-5.04	97.56	102.60
25	LA	1831	G	O4'-C1'-N9	5.04	112.23	108.20
25	LA	2138	G	C5'-C4'-O4'	5.04	115.14	109.10
1	SA	10	A	C5'-C4'-C3'	-5.03	107.95	116.00
1	SA	465	A	N1-C6-N6	5.03	121.62	118.60
1	SA	1022	A	C4'-C3'-C2'	-5.03	97.57	102.60
14	SB	205	ALA	N-CA-CB	5.03	117.15	110.10
25	LA	389	G	C4-N9-C1'	5.03	133.04	126.50
25	LA	901	C	C2'-C3'-O3'	5.03	121.75	113.70
25	LA	2281	A	O4'-C1'-N9	5.03	112.23	108.20
25	LA	2579	C	C1'-O4'-C4'	-5.03	105.87	109.90
29	LN	268	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	SA	312	C	O4'-C1'-N1	5.03	112.23	108.20
25	LA	1513	U	O4'-C1'-N1	5.03	112.23	108.20
25	LA	1849	G	N1-C6-O6	5.03	122.92	119.90
1	SA	199	A	C5'-C4'-O4'	5.03	115.14	109.10
1	SA	1305	G	P-O5'-C5'	-5.03	112.85	120.90
25	LA	1022	G	P-O5'-C5'	5.03	128.95	120.90
25	LA	1557	C	C5'-C4'-C3'	5.03	124.05	116.00
25	LA	2122	U	O4'-C1'-N1	5.03	112.22	108.20
1	SA	1503	A	O4'-C1'-N9	5.03	112.22	108.20
25	LA	704	G	O4'-C1'-N9	5.03	112.22	108.20
25	LA	1452	G	N1-C6-O6	5.03	122.92	119.90
25	LA	203	A	P-O3'-C3'	5.03	125.73	119.70
25	LA	299	A	P-O3'-C3'	5.03	125.73	119.70
25	LA	587	C	C2-N1-C1'	5.03	124.33	118.80
25	LA	1629	U	O4'-C1'-N1	5.03	112.22	108.20
25	LA	1769	U	O4'-C1'-N1	5.03	112.22	108.20
25	LA	1784	A	P-O5'-C5'	-5.03	112.86	120.90
25	LA	2036	C	O3'-P-O5'	-5.03	94.45	104.00
25	LA	2080	A	C4'-C3'-C2'	-5.03	97.57	102.60
25	LA	2141	G	O4'-C1'-N9	5.03	112.22	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2252	G	N9-C1'-C2'	-5.03	106.47	112.00
25	LA	2497	A	C5'-C4'-C3'	-5.03	107.95	116.00
1	SA	400	C	O4'-C1'-N1	5.03	112.22	108.20
1	SA	675	A	O4'-C1'-N9	5.03	112.22	108.20
1	SA	1305	G	C4-N9-C1'	-5.03	119.97	126.50
2	S6	38	A	P-O5'-C5'	-5.03	112.86	120.90
25	LA	715	A	C1'-O4'-C4'	-5.03	105.88	109.90
25	LA	947	A	C5'-C4'-C3'	-5.03	107.96	116.00
25	LA	1898	U	P-O3'-C3'	5.03	125.73	119.70
1	SA	415	A	O4'-C1'-N9	5.02	112.22	108.20
25	LA	705	A	P-O3'-C3'	5.02	125.73	119.70
26	LB	67	G	C5-C6-O6	-5.02	125.59	128.60
1	SA	222	C	C6-N1-C2	-5.02	118.29	120.30
1	SA	532	A	P-O3'-C3'	5.02	125.73	119.70
25	LA	186	G	N1-C6-O6	5.02	122.91	119.90
25	LA	238	C	C5'-C4'-C3'	5.02	124.03	116.00
25	LA	1022	G	C5'-C4'-O4'	5.02	115.13	109.10
25	LA	1951	U	C2-N1-C1'	5.02	123.73	117.70
25	LA	2352	A	N1-C6-N6	5.02	121.61	118.60
1	SA	1112	C	P-O5'-C5'	5.02	128.93	120.90
1	SA	1514	G	O4'-C1'-N9	5.02	112.22	108.20
25	LA	1377	G	O4'-C1'-N9	5.02	112.22	108.20
25	LA	1956	U	N1-C2-N3	5.02	117.91	114.90
49	L7	91	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	SA	141	G	C4'-C3'-C2'	-5.02	97.58	102.60
1	SA	260	G	C2'-C3'-O3'	5.02	121.73	113.70
1	SA	1044	A	O4'-C1'-N9	5.02	112.22	108.20
1	SA	1425	U	O3'-P-O5'	-5.02	94.46	104.00
1	SA	1429	A	O4'-C1'-N9	5.02	112.22	108.20
25	LA	269	C	P-O5'-C5'	5.02	128.93	120.90
25	LA	824	U	C5'-C4'-O4'	5.02	115.12	109.10
25	LA	2226	C	C4'-C3'-C2'	-5.02	97.58	102.60
25	LA	2757	A	C5'-C4'-O4'	5.02	115.12	109.10
1	SA	852	G	P-O3'-C3'	5.02	125.72	119.70
25	LA	224	U	O4'-C1'-N1	5.02	112.21	108.20
25	LA	1694	C	C6-N1-C1'	-5.02	114.78	120.80
25	LA	2318	G	P-O3'-C3'	5.02	125.72	119.70
25	LA	1182	G	N1-C6-O6	5.02	122.91	119.90
1	SA	545	C	C6-N1-C2	-5.01	118.30	120.30
2	S6	72	C	C6-N1-C2	-5.01	118.29	120.30
3	S7	42	C	C6-N1-C2	-5.01	118.29	120.30
24	S1	445	ARG	NE-CZ-NH1	5.01	122.81	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	738	G	C4'-C3'-C2'	-5.01	97.58	102.60
25	LA	1521	G	C5-C6-O6	-5.01	125.59	128.60
25	LA	2061	G	N9-C1'-C2'	-5.01	106.48	112.00
25	LA	2242	G	C4'-C3'-C2'	-5.01	97.59	102.60
1	SA	621	A	O4'-C1'-N9	5.01	112.21	108.20
1	SA	355	C	C5'-C4'-O4'	5.01	115.11	109.10
1	SA	1182	G	O4'-C1'-N9	5.01	112.21	108.20
2	S6	34	U	O4'-C1'-N1	5.01	112.21	108.20
25	LA	235	U	O4'-C1'-N1	5.01	112.21	108.20
25	LA	1506	U	O4'-C1'-N1	5.01	112.21	108.20
25	LA	2680	U	P-O3'-C3'	5.01	125.71	119.70
35	LT	21	ARG	NE-CZ-NH2	-5.01	117.79	120.30
55	LI	10	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	SA	1402	C	P-O3'-C3'	5.01	125.71	119.70
25	LA	170	U	O4'-C1'-N1	5.01	112.21	108.20
25	LA	756	A	C5'-C4'-C3'	-5.01	107.99	116.00
25	LA	1167	C	C5'-C4'-O4'	5.01	115.11	109.10
25	LA	1835	G	P-O5'-C5'	-5.01	112.89	120.90
45	L4	44	ARG	NE-CZ-NH2	-5.01	117.80	120.30
25	LA	342	A	P-O3'-C3'	-5.01	113.69	119.70
25	LA	1984	G	C4'-C3'-C2'	-5.01	97.59	102.60
1	SA	284	C	O4'-C1'-N1	5.01	112.20	108.20
1	SA	563	A	C5'-C4'-O4'	5.01	115.11	109.10
1	SA	1289	A	O4'-C1'-N9	5.01	112.20	108.20
25	LA	1402	U	C2-N3-C4	-5.01	124.00	127.00
25	LA	1921	G	O4'-C1'-N9	5.01	112.20	108.20
25	LA	2010	G	C1'-O4'-C4'	-5.01	105.89	109.90
25	LA	2203	U	C2-N1-C1'	5.01	123.71	117.70
25	LA	2639	A	N1-C6-N6	-5.01	115.60	118.60
1	SA	1038	C	C4'-C3'-C2'	-5.00	97.59	102.60
25	LA	649	G	C5-C6-O6	-5.00	125.60	128.60
25	LA	2405	G	O4'-C1'-N9	5.00	112.20	108.20
1	SA	580	C	O4'-C1'-N1	5.00	112.20	108.20
1	SA	580	C	P-O5'-C5'	-5.00	112.89	120.90
1	SA	813	U	P-O5'-C5'	-5.00	112.90	120.90
1	SA	814	A	O4'-C1'-N9	5.00	112.20	108.20
1	SA	1457	G	C5-C6-O6	-5.00	125.60	128.60
1	SA	1531	A	O3'-P-O5'	-5.00	94.49	104.00
3	S7	55	U	C2-N1-C1'	5.00	123.70	117.70
18	SD	62	ARG	CG-CD-NE	-5.00	101.29	111.80
25	LA	374	A	N1-C6-N6	5.00	121.60	118.60
25	LA	2448	A	N1-C6-N6	5.00	121.60	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LA	2479	U	C2-N3-C4	-5.00	124.00	127.00
26	LB	12	C	N3-C4-N4	5.00	121.50	118.00
26	LB	87	U	C1'-O4'-C4'	-5.00	105.90	109.90
1	SA	645	G	O4'-C1'-N9	5.00	112.20	108.20
25	LA	439	A	O4'-C1'-N9	5.00	112.20	108.20
25	LA	446	G	C8-N9-C1'	-5.00	120.50	127.00
25	LA	875	G	C1'-O4'-C4'	-5.00	105.90	109.90
25	LA	947	A	P-O5'-C5'	5.00	128.90	120.90
25	LA	1459	G	N1-C6-O6	5.00	122.90	119.90
25	LA	1616	A	C3'-C2'-C1'	-5.00	97.50	101.50
31	LP	80	ARG	NE-CZ-NH2	-5.00	117.80	120.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	SA	1498	U	C3',C4'
25	LA	2251	G	C1'

All (1660) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	L1	49	ARG	Sidechain
42	L1	9	ARG	Sidechain
44	L3	14	ARG	Sidechain
44	L3	28	ARG	Sidechain
44	L3	33	ARG	Sidechain
44	L3	34	ARG	Sidechain
44	L3	44	VAL	Peptide
45	L4	12	ARG	Sidechain
45	L4	41	ARG	Sidechain
45	L4	7	ARG	Sidechain
46	L5	4	ARG	Sidechain
47	L6	114	ARG	Sidechain
47	L6	162	ARG	Sidechain
47	L6	170	ARG	Sidechain
47	L6	40	ARG	Sidechain
47	L6	61	ARG	Sidechain
47	L6	67	ARG	Sidechain
49	L7	101	ARG	Peptide
49	L7	116	LEU	Peptide
49	L7	124	ARG	Sidechain
49	L7	127	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
49	L7	174	PHE	Peptide
49	L7	72	SER	Peptide
49	L7	91	ARG	Sidechain
49	L7	94	ARG	Sidechain
50	L8	154	GLU	Peptide
50	L8	163	TYR	Sidechain
50	L8	6	ALA	Peptide
51	L9	22	LYS	Peptide
51	L9	63	ALA	Peptide
25	LA	1	G	Sidechain
25	LA	1004	U	Sidechain
25	LA	1005	C	Sidechain
25	LA	1012	U	Sidechain
25	LA	1019	U	Sidechain
25	LA	102	U	Sidechain
25	LA	1021	A	Sidechain
25	LA	1022	G	Sidechain
25	LA	1025	G	Sidechain
25	LA	1026	G	Sidechain
25	LA	1028	A	Sidechain
25	LA	1029	A	Sidechain
25	LA	1030	C	Sidechain
25	LA	1031	G	Sidechain
25	LA	1034	G	Sidechain
25	LA	1038	G	Sidechain
25	LA	105	C	Sidechain
25	LA	1055	G	Sidechain
25	LA	1056	G	Sidechain
25	LA	1058	U	Sidechain
25	LA	106	C	Sidechain
25	LA	1061	U	Sidechain
25	LA	1063	G	Sidechain
25	LA	1069	A	Sidechain
25	LA	1079	C	Sidechain
25	LA	1083	U	Sidechain
25	LA	1084	A	Sidechain
25	LA	1085	A	Sidechain
25	LA	1086	A	Sidechain
25	LA	1088	A	Sidechain
25	LA	1093	G	Sidechain
25	LA	1094	U	Sidechain
25	LA	1095	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1097	U	Sidechain
25	LA	1098	A	Sidechain
25	LA	1110	G	Sidechain
25	LA	1118	C	Sidechain
25	LA	1125	G	Sidechain
25	LA	113	U	Sidechain
25	LA	1130	U	Sidechain
25	LA	1133	A	Sidechain
25	LA	1134	A	Sidechain
25	LA	1137	G	Sidechain
25	LA	114	U	Sidechain
25	LA	1143	A	Sidechain
25	LA	1153	C	Sidechain
25	LA	1156	A	Sidechain
25	LA	1166	G	Sidechain
25	LA	1172	C	Sidechain
25	LA	1174	U	Sidechain
25	LA	1176	U	Sidechain
25	LA	1177	G	Sidechain
25	LA	1183	U	Sidechain
25	LA	1186	G	Sidechain
25	LA	1188	U	Sidechain
25	LA	1189	A	Sidechain
25	LA	1190	G	Sidechain
25	LA	1192	G	Sidechain
25	LA	1196	C	Sidechain
25	LA	1198	U	Sidechain
25	LA	1199	U	Sidechain
25	LA	12	U	Sidechain
25	LA	120	U	Sidechain
25	LA	1203	U	Sidechain
25	LA	1204	A	Sidechain
25	LA	1206	G	Sidechain
25	LA	1209	U	Sidechain
25	LA	121	G	Sidechain
25	LA	1214	A	Sidechain
25	LA	1215	G	Sidechain
25	LA	1223	G	Sidechain
25	LA	1225	G	Sidechain
25	LA	1226	A	Sidechain
25	LA	123	G	Sidechain
25	LA	1230	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1234	U	Sidechain
25	LA	1236	G	Sidechain
25	LA	1248	G	Sidechain
25	LA	1249	U	Sidechain
25	LA	1253	A	Sidechain
25	LA	1257	C	Sidechain
25	LA	1259	G	Sidechain
25	LA	126	A	Sidechain
25	LA	1261	C	Sidechain
25	LA	1263	U	Sidechain
25	LA	1267	U	Sidechain
25	LA	1268	A	Sidechain
25	LA	1269	A	Sidechain
25	LA	1270	C	Sidechain
25	LA	1271	G	Sidechain
25	LA	1275	A	Sidechain
25	LA	1294	U	Sidechain
25	LA	1296	G	Sidechain
25	LA	1299	G	Sidechain
25	LA	1307	A	Sidechain
25	LA	1310	G	Sidechain
25	LA	1311	G	Sidechain
25	LA	1312	U	Sidechain
25	LA	1313	U	Sidechain
25	LA	1314	C	Sidechain
25	LA	1316	U	Sidechain
25	LA	1318	U	Sidechain
25	LA	1321	A	Sidechain
25	LA	1324	G	Sidechain
25	LA	1326	U	Sidechain
25	LA	1327	A	Sidechain
25	LA	1330	C	Sidechain
25	LA	1332	G	Sidechain
25	LA	1338	G	Sidechain
25	LA	1340	U	Sidechain
25	LA	1345	C	Sidechain
25	LA	1354	A	Sidechain
25	LA	1356	G	Sidechain
25	LA	1357	C	Sidechain
25	LA	1358	G	Sidechain
25	LA	136	G	Sidechain
25	LA	1360	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1363	C	Sidechain
25	LA	1364	G	Sidechain
25	LA	1370	C	Sidechain
25	LA	1372	U	Sidechain
25	LA	1377	G	Sidechain
25	LA	1378	A	Sidechain
25	LA	1379	U	Sidechain
25	LA	1381	G	Sidechain
25	LA	1382	G	Sidechain
25	LA	1388	G	Sidechain
25	LA	1389	G	Sidechain
25	LA	1390	U	Sidechain
25	LA	1393	A	Sidechain
25	LA	1396	U	Sidechain
25	LA	1398	C	Sidechain
25	LA	1400	U	Sidechain
25	LA	1406	U	Sidechain
25	LA	1407	G	Sidechain
25	LA	1408	G	Sidechain
25	LA	1412	U	Sidechain
25	LA	1417	C	Sidechain
25	LA	1419	A	Sidechain
25	LA	1431	A	Sidechain
25	LA	144	A	Sidechain
25	LA	1440	U	Sidechain
25	LA	1443	U	Sidechain
25	LA	1447	C	Sidechain
25	LA	1449	G	Sidechain
25	LA	1450	G	Sidechain
25	LA	1458	U	Sidechain
25	LA	1459	G	Sidechain
25	LA	146	A	Sidechain
25	LA	1469	A	Sidechain
25	LA	147	C	Sidechain
25	LA	1472	C	Sidechain
25	LA	1474	U	Sidechain
25	LA	1478	G	Sidechain
25	LA	1481	U	Sidechain
25	LA	1485	U	Sidechain
25	LA	1496	A	Sidechain
25	LA	1497	U	Sidechain
25	LA	15	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1506	U	Sidechain
25	LA	1508	A	Sidechain
25	LA	1510	G	Sidechain
25	LA	1513	U	Sidechain
25	LA	1514	G	Sidechain
25	LA	1516	G	Sidechain
25	LA	152	A	Sidechain
25	LA	1523	U	Sidechain
25	LA	1524	G	Sidechain
25	LA	1530	G	Sidechain
25	LA	1532	A	Sidechain
25	LA	1533	C	Sidechain
25	LA	1537	G	Sidechain
25	LA	1539	U	Sidechain
25	LA	1540	G	Sidechain
25	LA	1552	A	Sidechain
25	LA	1561	C	Sidechain
25	LA	1564	C	Sidechain
25	LA	1565	C	Sidechain
25	LA	1566	A	Sidechain
25	LA	1567	G	Sidechain
25	LA	1568	G	Sidechain
25	LA	1569	A	Sidechain
25	LA	1570	A	Sidechain
25	LA	1572	A	Sidechain
25	LA	1576	U	Sidechain
25	LA	1578	U	Sidechain
25	LA	1583	A	Sidechain
25	LA	1584	U	Sidechain
25	LA	1586	A	Sidechain
25	LA	1596	A	Sidechain
25	LA	16	C	Sidechain
25	LA	160	A	Sidechain
25	LA	1610	A	Sidechain
25	LA	1613	G	Sidechain
25	LA	1614	A	Sidechain
25	LA	1615	C	Sidechain
25	LA	1621	U	Sidechain
25	LA	1622	G	Sidechain
25	LA	1624	U	Sidechain
25	LA	1629	U	Sidechain
25	LA	1633	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1636	U	Sidechain
25	LA	1638	C	Sidechain
25	LA	1641	A	Sidechain
25	LA	1642	G	Sidechain
25	LA	1643	G	Sidechain
25	LA	1644	C	Sidechain
25	LA	1646	C	Sidechain
25	LA	1647	U	Sidechain
25	LA	1649	G	Sidechain
25	LA	1657	U	Sidechain
25	LA	1666	G	Sidechain
25	LA	1668	A	Sidechain
25	LA	1672	A	Sidechain
25	LA	1674	G	Sidechain
25	LA	1675	C	Sidechain
25	LA	1676	A	Sidechain
25	LA	1677	A	Sidechain
25	LA	1678	A	Sidechain
25	LA	1680	U	Sidechain
25	LA	1681	G	Sidechain
25	LA	1683	U	Sidechain
25	LA	1689	A	Sidechain
25	LA	169	G	Sidechain
25	LA	1690	A	Sidechain
25	LA	1692	U	Sidechain
25	LA	1693	U	Sidechain
25	LA	1699	G	Sidechain
25	LA	170	U	Sidechain
25	LA	1704	C	Sidechain
25	LA	1707	G	Sidechain
25	LA	1715	G	Sidechain
25	LA	1719	G	Sidechain
25	LA	1720	U	Sidechain
25	LA	1721	G	Sidechain
25	LA	1723	G	Sidechain
25	LA	1724	G	Sidechain
25	LA	1727	C	Sidechain
25	LA	1731	G	Sidechain
25	LA	1736	U	Sidechain
25	LA	1737	G	Sidechain
25	LA	1738	G	Sidechain
25	LA	1741	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1744	A	Sidechain
25	LA	1747	U	Sidechain
25	LA	175	G	Sidechain
25	LA	1756	G	Sidechain
25	LA	1760	C	Sidechain
25	LA	1766	G	Sidechain
25	LA	1769	U	Sidechain
25	LA	177	G	Sidechain
25	LA	1771	C	Sidechain
25	LA	1777	U	Sidechain
25	LA	1779	U	Sidechain
25	LA	1781	U	Sidechain
25	LA	1782	U	Sidechain
25	LA	1783	A	Sidechain
25	LA	1784	A	Sidechain
25	LA	1795	C	Sidechain
25	LA	1803	A	Sidechain
25	LA	1807	G	Sidechain
25	LA	1808	A	Sidechain
25	LA	1813	G	Sidechain
25	LA	1824	G	Sidechain
25	LA	1825	U	Sidechain
25	LA	1826	G	Sidechain
25	LA	1827	U	Sidechain
25	LA	1829	A	Sidechain
25	LA	1830	C	Sidechain
25	LA	1832	C	Sidechain
25	LA	1834	U	Sidechain
25	LA	1835	G	Sidechain
25	LA	1838	C	Sidechain
25	LA	1841	U	Sidechain
25	LA	1845	G	Sidechain
25	LA	1848	A	Sidechain
25	LA	1849	G	Sidechain
25	LA	185	G	Sidechain
25	LA	1850	G	Sidechain
25	LA	1851	U	Sidechain
25	LA	1852	U	Sidechain
25	LA	1857	G	Sidechain
25	LA	186	G	Sidechain
25	LA	1862	G	Sidechain
25	LA	1863	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1865	U	Sidechain
25	LA	1869	G	Sidechain
25	LA	187	G	Sidechain
25	LA	1872	A	Sidechain
25	LA	1876	A	Sidechain
25	LA	1880	U	Sidechain
25	LA	1890	A	Sidechain
25	LA	1893	C	Sidechain
25	LA	1896	G	Sidechain
25	LA	1897	G	Sidechain
25	LA	1898	U	Sidechain
25	LA	1899	A	Sidechain
25	LA	1900	A	Sidechain
25	LA	1901	A	Sidechain
25	LA	1902	C	Sidechain
25	LA	1903	G	Sidechain
25	LA	1904	G	Sidechain
25	LA	1905	C	Sidechain
25	LA	1907	G	Sidechain
25	LA	191	A	Sidechain
25	LA	1911	U	Sidechain
25	LA	1913	A	Sidechain
25	LA	1915	U	Sidechain
25	LA	1917	U	Sidechain
25	LA	1925	C	Sidechain
25	LA	1926	U	Sidechain
25	LA	1927	A	Sidechain
25	LA	1929	G	Sidechain
25	LA	1930	G	Sidechain
25	LA	1931	U	Sidechain
25	LA	1932	A	Sidechain
25	LA	1935	G	Sidechain
25	LA	1936	A	Sidechain
25	LA	194	G	Sidechain
25	LA	1942	C	Sidechain
25	LA	1943	U	Sidechain
25	LA	1944	U	Sidechain
25	LA	1949	G	Sidechain
25	LA	1951	U	Sidechain
25	LA	1952	A	Sidechain
25	LA	1955	U	Sidechain
25	LA	1956	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	1959	G	Sidechain
25	LA	196	A	Sidechain
25	LA	1961	C	Sidechain
25	LA	1962	C	Sidechain
25	LA	1964	G	Sidechain
25	LA	1968	G	Sidechain
25	LA	1974	C	Sidechain
25	LA	1975	G	Sidechain
25	LA	1976	U	Sidechain
25	LA	1978	A	Sidechain
25	LA	1979	U	Sidechain
25	LA	1983	G	Sidechain
25	LA	199	A	Sidechain
25	LA	1991	U	Sidechain
25	LA	1992	G	Sidechain
25	LA	1993	U	Sidechain
25	LA	1995	U	Sidechain
25	LA	1996	C	Sidechain
25	LA	2	G	Sidechain
25	LA	200	U	Sidechain
25	LA	2010	G	Sidechain
25	LA	2015	A	Sidechain
25	LA	2016	U	Sidechain
25	LA	2017	U	Sidechain
25	LA	202	U	Sidechain
25	LA	2022	U	Sidechain
25	LA	2023	C	Sidechain
25	LA	2026	U	Sidechain
25	LA	2027	G	Sidechain
25	LA	2029	G	Sidechain
25	LA	2030	C	Sidechain
25	LA	2034	U	Sidechain
25	LA	2037	A	Sidechain
25	LA	2038	G	Sidechain
25	LA	2041	U	Sidechain
25	LA	2045	C	Sidechain
25	LA	2049	G	Sidechain
25	LA	205	G	Sidechain
25	LA	2050	C	Sidechain
25	LA	2053	G	Sidechain
25	LA	2054	A	Sidechain
25	LA	2056	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2057	G	Sidechain
25	LA	206	U	Sidechain
25	LA	2060	A	Sidechain
25	LA	2061	G	Sidechain
25	LA	2062	A	Sidechain
25	LA	2065	C	Sidechain
25	LA	2068	U	Sidechain
25	LA	2069	G	Sidechain
25	LA	207	A	Sidechain
25	LA	2073	C	Sidechain
25	LA	2074	U	Sidechain
25	LA	2075	U	Sidechain
25	LA	2076	U	Sidechain
25	LA	2078	C	Sidechain
25	LA	2082	A	Sidechain
25	LA	2083	G	Sidechain
25	LA	2087	G	Sidechain
25	LA	2088	A	Sidechain
25	LA	2090	A	Sidechain
25	LA	2091	C	Sidechain
25	LA	2092	U	Sidechain
25	LA	2093	G	Sidechain
25	LA	2094	A	Sidechain
25	LA	2099	U	Sidechain
25	LA	2102	G	Sidechain
25	LA	2109	U	Sidechain
25	LA	2110	G	Sidechain
25	LA	2111	U	Sidechain
25	LA	2112	G	Sidechain
25	LA	2113	U	Sidechain
25	LA	2118	U	Sidechain
25	LA	2121	G	Sidechain
25	LA	2124	G	Sidechain
25	LA	2125	G	Sidechain
25	LA	2126	A	Sidechain
25	LA	2127	G	Sidechain
25	LA	2132	U	Sidechain
25	LA	2133	G	Sidechain
25	LA	2134	A	Sidechain
25	LA	2135	A	Sidechain
25	LA	2136	G	Sidechain
25	LA	2137	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2139	U	Sidechain
25	LA	2141	G	Sidechain
25	LA	2144	G	Sidechain
25	LA	2148	G	Sidechain
25	LA	2149	U	Sidechain
25	LA	215	G	Sidechain
25	LA	2154	A	Sidechain
25	LA	2156	G	Sidechain
25	LA	2157	G	Sidechain
25	LA	2160	C	Sidechain
25	LA	2165	C	Sidechain
25	LA	2172	U	Sidechain
25	LA	2173	A	Sidechain
25	LA	2175	C	Sidechain
25	LA	2176	A	Sidechain
25	LA	2179	C	Sidechain
25	LA	2180	U	Sidechain
25	LA	2183	A	Sidechain
25	LA	2186	G	Sidechain
25	LA	2187	U	Sidechain
25	LA	2188	U	Sidechain
25	LA	2190	G	Sidechain
25	LA	2192	U	Sidechain
25	LA	2195	U	Sidechain
25	LA	2197	U	Sidechain
25	LA	2201	G	Sidechain
25	LA	2203	U	Sidechain
25	LA	2208	C	Sidechain
25	LA	221	A	Sidechain
25	LA	2210	U	Sidechain
25	LA	2213	U	Sidechain
25	LA	2215	C	Sidechain
25	LA	2216	G	Sidechain
25	LA	2217	G	Sidechain
25	LA	2219	U	Sidechain
25	LA	2220	U	Sidechain
25	LA	2221	G	Sidechain
25	LA	2223	G	Sidechain
25	LA	2227	A	Sidechain
25	LA	2228	G	Sidechain
25	LA	2230	G	Sidechain
25	LA	2233	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2240	U	Sidechain
25	LA	2241	A	Sidechain
25	LA	2243	U	Sidechain
25	LA	2244	U	Sidechain
25	LA	2246	G	Sidechain
25	LA	2248	C	Sidechain
25	LA	2249	U	Sidechain
25	LA	2251	G	Sidechain
25	LA	2252	G	Sidechain
25	LA	2254	C	Sidechain
25	LA	2257	U	Sidechain
25	LA	2258	C	Sidechain
25	LA	2262	U	Sidechain
25	LA	2265	U	Sidechain
25	LA	2266	A	Sidechain
25	LA	2267	A	Sidechain
25	LA	2270	A	Sidechain
25	LA	2272	U	Sidechain
25	LA	2273	A	Sidechain
25	LA	2274	A	Sidechain
25	LA	2275	C	Sidechain
25	LA	2279	G	Sidechain
25	LA	228	C	Sidechain
25	LA	2282	G	Sidechain
25	LA	2284	A	Sidechain
25	LA	2285	C	Sidechain
25	LA	2289	G	Sidechain
25	LA	2293	G	Sidechain
25	LA	2294	G	Sidechain
25	LA	2297	A	Sidechain
25	LA	230	G	Sidechain
25	LA	2302	U	Sidechain
25	LA	2303	G	Sidechain
25	LA	2304	G	Sidechain
25	LA	2305	U	Sidechain
25	LA	2314	A	Sidechain
25	LA	2319	G	Sidechain
25	LA	2323	G	Sidechain
25	LA	2324	U	Sidechain
25	LA	2325	G	Sidechain
25	LA	2327	A	Sidechain
25	LA	2329	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	233	A	Sidechain
25	LA	2330	G	Sidechain
25	LA	2331	G	Sidechain
25	LA	2333	A	Sidechain
25	LA	2337	G	Sidechain
25	LA	2342	C	Sidechain
25	LA	2351	G	Sidechain
25	LA	2352	A	Sidechain
25	LA	2353	G	Sidechain
25	LA	2355	G	Sidechain
25	LA	2360	G	Sidechain
25	LA	2362	C	Sidechain
25	LA	2366	A	Sidechain
25	LA	2375	G	Sidechain
25	LA	2383	G	Sidechain
25	LA	2387	U	Sidechain
25	LA	2388	A	Sidechain
25	LA	2398	U	Sidechain
25	LA	24	G	Sidechain
25	LA	240	C	Sidechain
25	LA	2402	U	Sidechain
25	LA	2403	C	Sidechain
25	LA	2404	U	Sidechain
25	LA	2405	G	Sidechain
25	LA	2411	A	Sidechain
25	LA	2419	U	Sidechain
25	LA	2420	C	Sidechain
25	LA	2429	G	Sidechain
25	LA	243	U	Sidechain
25	LA	2438	U	Sidechain
25	LA	2443	C	Sidechain
25	LA	2445	G	Sidechain
25	LA	2446	G	Sidechain
25	LA	2448	A	Sidechain
25	LA	2451	A	Sidechain
25	LA	2452	C	Sidechain
25	LA	2454	G	Sidechain
25	LA	2455	G	Sidechain
25	LA	2458	G	Sidechain
25	LA	2459	A	Sidechain
25	LA	2464	G	Sidechain
25	LA	2468	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2471	A	Sidechain
25	LA	2472	G	Sidechain
25	LA	2473	U	Sidechain
25	LA	2474	U	Sidechain
25	LA	2475	C	Sidechain
25	LA	2477	U	Sidechain
25	LA	2479	U	Sidechain
25	LA	2482	A	Sidechain
25	LA	2488	G	Sidechain
25	LA	249	C	Sidechain
25	LA	2490	G	Sidechain
25	LA	2491	U	Sidechain
25	LA	2492	U	Sidechain
25	LA	2495	G	Sidechain
25	LA	2499	C	Sidechain
25	LA	25	U	Sidechain
25	LA	250	G	Sidechain
25	LA	2500	U	Sidechain
25	LA	2501	C	Sidechain
25	LA	2504	U	Sidechain
25	LA	2505	G	Sidechain
25	LA	2508	G	Sidechain
25	LA	251	A	Sidechain
25	LA	2511	U	Sidechain
25	LA	2512	C	Sidechain
25	LA	2513	A	Sidechain
25	LA	2514	U	Sidechain
25	LA	252	G	Sidechain
25	LA	2520	C	Sidechain
25	LA	2522	U	Sidechain
25	LA	2523	G	Sidechain
25	LA	2524	G	Sidechain
25	LA	2525	G	Sidechain
25	LA	2528	U	Sidechain
25	LA	2529	G	Sidechain
25	LA	2532	G	Sidechain
25	LA	2533	U	Sidechain
25	LA	2538	C	Sidechain
25	LA	2544	G	Sidechain
25	LA	2545	G	Sidechain
25	LA	2546	U	Sidechain
25	LA	2547	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2548	U	Sidechain
25	LA	2549	G	Sidechain
25	LA	255	A	Sidechain
25	LA	2552	U	Sidechain
25	LA	2553	G	Sidechain
25	LA	2554	U	Sidechain
25	LA	2555	U	Sidechain
25	LA	2560	A	Sidechain
25	LA	2564	A	Sidechain
25	LA	2567	G	Sidechain
25	LA	2568	U	Sidechain
25	LA	2570	G	Sidechain
25	LA	2571	U	Sidechain
25	LA	2572	A	Sidechain
25	LA	2576	G	Sidechain
25	LA	2577	A	Sidechain
25	LA	2578	G	Sidechain
25	LA	258	G	Sidechain
25	LA	2582	G	Sidechain
25	LA	2584	U	Sidechain
25	LA	2585	U	Sidechain
25	LA	2589	A	Sidechain
25	LA	2591	C	Sidechain
25	LA	2592	G	Sidechain
25	LA	2596	U	Sidechain
25	LA	26	G	Sidechain
25	LA	2601	C	Sidechain
25	LA	2602	A	Sidechain
25	LA	2603	G	Sidechain
25	LA	2604	U	Sidechain
25	LA	2607	G	Sidechain
25	LA	2608	G	Sidechain
25	LA	2609	U	Sidechain
25	LA	2611	C	Sidechain
25	LA	2615	U	Sidechain
25	LA	2617	U	Sidechain
25	LA	2618	G	Sidechain
25	LA	2620	C	Sidechain
25	LA	263	G	Sidechain
25	LA	2637	U	Sidechain
25	LA	2641	G	Sidechain
25	LA	2642	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2645	G	Sidechain
25	LA	2647	U	Sidechain
25	LA	2653	U	Sidechain
25	LA	2655	G	Sidechain
25	LA	2656	U	Sidechain
25	LA	2657	A	Sidechain
25	LA	2659	G	Sidechain
25	LA	2664	G	Sidechain
25	LA	2667	C	Sidechain
25	LA	2668	G	Sidechain
25	LA	2672	U	Sidechain
25	LA	2673	G	Sidechain
25	LA	2677	G	Sidechain
25	LA	2680	U	Sidechain
25	LA	2689	U	Sidechain
25	LA	2691	C	Sidechain
25	LA	2696	U	Sidechain
25	LA	2698	U	Sidechain
25	LA	2699	C	Sidechain
25	LA	27	G	Sidechain
25	LA	2701	U	Sidechain
25	LA	2702	G	Sidechain
25	LA	2703	C	Sidechain
25	LA	2713	U	Sidechain
25	LA	2723	C	Sidechain
25	LA	2728	U	Sidechain
25	LA	2729	G	Sidechain
25	LA	273	G	Sidechain
25	LA	2731	G	Sidechain
25	LA	2733	A	Sidechain
25	LA	2735	G	Sidechain
25	LA	2739	U	Sidechain
25	LA	2745	C	Sidechain
25	LA	2751	G	Sidechain
25	LA	2754	U	Sidechain
25	LA	2755	C	Sidechain
25	LA	276	U	Sidechain
25	LA	2760	C	Sidechain
25	LA	2763	G	Sidechain
25	LA	2767	C	Sidechain
25	LA	2777	G	Sidechain
25	LA	2779	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2780	G	Sidechain
25	LA	2782	G	Sidechain
25	LA	2784	U	Sidechain
25	LA	2787	C	Sidechain
25	LA	2791	G	Sidechain
25	LA	2794	C	Sidechain
25	LA	2796	U	Sidechain
25	LA	2799	A	Sidechain
25	LA	2803	G	Sidechain
25	LA	2806	C	Sidechain
25	LA	2807	U	Sidechain
25	LA	2812	G	Sidechain
25	LA	2814	A	Sidechain
25	LA	2816	G	Sidechain
25	LA	2820	A	Sidechain
25	LA	2822	G	Sidechain
25	LA	2823	A	Sidechain
25	LA	2824	C	Sidechain
25	LA	2825	G	Sidechain
25	LA	2826	A	Sidechain
25	LA	2832	U	Sidechain
25	LA	2834	G	Sidechain
25	LA	2836	U	Sidechain
25	LA	2839	G	Sidechain
25	LA	284	U	Sidechain
25	LA	2844	G	Sidechain
25	LA	2848	G	Sidechain
25	LA	2849	U	Sidechain
25	LA	2867	G	Sidechain
25	LA	2875	C	Sidechain
25	LA	2877	G	Sidechain
25	LA	2879	A	Sidechain
25	LA	2882	A	Sidechain
25	LA	2884	U	Sidechain
25	LA	289	G	Sidechain
25	LA	2891	U	Sidechain
25	LA	2892	G	Sidechain
25	LA	2894	G	Sidechain
25	LA	2895	G	Sidechain
25	LA	2896	C	Sidechain
25	LA	29	U	Sidechain
25	LA	2902	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	2904	U	Sidechain
25	LA	291	G	Sidechain
25	LA	294	A	Sidechain
25	LA	303	G	Sidechain
25	LA	305	C	Sidechain
25	LA	311	A	Sidechain
25	LA	312	G	Sidechain
25	LA	313	G	Sidechain
25	LA	319	G	Sidechain
25	LA	320	A	Sidechain
25	LA	330	A	Sidechain
25	LA	337	C	Sidechain
25	LA	34	U	Sidechain
25	LA	342	A	Sidechain
25	LA	345	A	Sidechain
25	LA	349	U	Sidechain
25	LA	354	A	Sidechain
25	LA	358	U	Sidechain
25	LA	36	G	Sidechain
25	LA	361	G	Sidechain
25	LA	370	G	Sidechain
25	LA	384	A	Sidechain
25	LA	387	U	Sidechain
25	LA	388	G	Sidechain
25	LA	390	U	Sidechain
25	LA	395	U	Sidechain
25	LA	399	U	Sidechain
25	LA	403	U	Sidechain
25	LA	404	A	Sidechain
25	LA	406	G	Sidechain
25	LA	411	G	Sidechain
25	LA	412	A	Sidechain
25	LA	413	C	Sidechain
25	LA	43	G	Sidechain
25	LA	436	C	Sidechain
25	LA	437	U	Sidechain
25	LA	441	U	Sidechain
25	LA	442	G	Sidechain
25	LA	445	C	Sidechain
25	LA	446	G	Sidechain
25	LA	451	U	Sidechain
25	LA	454	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	456	C	Sidechain
25	LA	459	U	Sidechain
25	LA	462	C	Sidechain
25	LA	464	U	Sidechain
25	LA	465	G	Sidechain
25	LA	466	A	Sidechain
25	LA	47	C	Sidechain
25	LA	472	A	Sidechain
25	LA	477	A	Sidechain
25	LA	48	G	Sidechain
25	LA	489	G	Sidechain
25	LA	49	A	Sidechain
25	LA	491	G	Sidechain
25	LA	496	G	Sidechain
25	LA	50	U	Sidechain
25	LA	500	G	Sidechain
25	LA	503	A	Sidechain
25	LA	506	G	Sidechain
25	LA	511	U	Sidechain
25	LA	512	G	Sidechain
25	LA	514	A	Sidechain
25	LA	516	C	Sidechain
25	LA	517	C	Sidechain
25	LA	519	U	Sidechain
25	LA	52	A	Sidechain
25	LA	521	U	Sidechain
25	LA	524	G	Sidechain
25	LA	525	U	Sidechain
25	LA	528	A	Sidechain
25	LA	535	G	Sidechain
25	LA	537	G	Sidechain
25	LA	539	G	Sidechain
25	LA	541	A	Sidechain
25	LA	549	G	Sidechain
25	LA	550	C	Sidechain
25	LA	558	U	Sidechain
25	LA	561	G	Sidechain
25	LA	562	U	Sidechain
25	LA	569	U	Sidechain
25	LA	570	G	Sidechain
25	LA	571	U	Sidechain
25	LA	572	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	577	G	Sidechain
25	LA	582	A	Sidechain
25	LA	583	G	Sidechain
25	LA	584	C	Sidechain
25	LA	585	G	Sidechain
25	LA	589	U	Sidechain
25	LA	592	A	Sidechain
25	LA	594	U	Sidechain
25	LA	60	G	Sidechain
25	LA	603	A	Sidechain
25	LA	607	U	Sidechain
25	LA	616	A	Sidechain
25	LA	620	G	Sidechain
25	LA	624	C	Sidechain
25	LA	633	A	Sidechain
25	LA	636	G	Sidechain
25	LA	640	C	Sidechain
25	LA	641	U	Sidechain
25	LA	642	U	Sidechain
25	LA	644	A	Sidechain
25	LA	646	U	Sidechain
25	LA	65	U	Sidechain
25	LA	651	G	Sidechain
25	LA	652	U	Sidechain
25	LA	653	U	Sidechain
25	LA	654	A	Sidechain
25	LA	662	G	Sidechain
25	LA	663	G	Sidechain
25	LA	664	G	Sidechain
25	LA	666	A	Sidechain
25	LA	668	A	Sidechain
25	LA	670	A	Sidechain
25	LA	680	C	Sidechain
25	LA	682	G	Sidechain
25	LA	686	U	Sidechain
25	LA	687	C	Sidechain
25	LA	694	U	Sidechain
25	LA	695	G	Sidechain
25	LA	696	G	Sidechain
25	LA	700	G	Sidechain
25	LA	701	G	Sidechain
25	LA	703	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	704	G	Sidechain
25	LA	707	G	Sidechain
25	LA	708	G	Sidechain
25	LA	711	G	Sidechain
25	LA	712	G	Sidechain
25	LA	718	A	Sidechain
25	LA	72	U	Sidechain
25	LA	726	G	Sidechain
25	LA	731	C	Sidechain
25	LA	733	G	Sidechain
25	LA	738	G	Sidechain
25	LA	74	A	Sidechain
25	LA	741	U	Sidechain
25	LA	744	U	Sidechain
25	LA	745	G	Sidechain
25	LA	746	U	Sidechain
25	LA	747	U	Sidechain
25	LA	748	G	Sidechain
25	LA	749	A	Sidechain
25	LA	75	G	Sidechain
25	LA	750	A	Sidechain
25	LA	752	A	Sidechain
25	LA	753	A	Sidechain
25	LA	754	U	Sidechain
25	LA	757	G	Sidechain
25	LA	767	U	Sidechain
25	LA	773	U	Sidechain
25	LA	777	G	Sidechain
25	LA	778	G	Sidechain
25	LA	779	U	Sidechain
25	LA	780	G	Sidechain
25	LA	783	A	Sidechain
25	LA	786	C	Sidechain
25	LA	789	A	Sidechain
25	LA	79	C	Sidechain
25	LA	790	U	Sidechain
25	LA	793	A	Sidechain
25	LA	803	U	Sidechain
25	LA	805	G	Sidechain
25	LA	806	C	Sidechain
25	LA	810	U	Sidechain
25	LA	811	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	813	U	Sidechain
25	LA	82	U	Sidechain
25	LA	822	G	Sidechain
25	LA	823	C	Sidechain
25	LA	824	U	Sidechain
25	LA	827	U	Sidechain
25	LA	828	U	Sidechain
25	LA	829	A	Sidechain
25	LA	83	A	Sidechain
25	LA	830	G	Sidechain
25	LA	834	G	Sidechain
25	LA	841	G	Sidechain
25	LA	844	A	Sidechain
25	LA	845	A	Sidechain
25	LA	852	U	Sidechain
25	LA	857	G	Sidechain
25	LA	858	G	Sidechain
25	LA	859	G	Sidechain
25	LA	86	G	Sidechain
25	LA	860	U	Sidechain
25	LA	862	G	Sidechain
25	LA	863	A	Sidechain
25	LA	872	U	Sidechain
25	LA	873	C	Sidechain
25	LA	875	G	Sidechain
25	LA	876	C	Sidechain
25	LA	877	A	Sidechain
25	LA	881	G	Sidechain
25	LA	883	G	Sidechain
25	LA	888	C	Sidechain
25	LA	892	A	Sidechain
25	LA	894	U	Sidechain
25	LA	895	U	Sidechain
25	LA	898	C	Sidechain
25	LA	900	A	Sidechain
25	LA	906	U	Sidechain
25	LA	907	G	Sidechain
25	LA	910	A	Sidechain
25	LA	913	U	Sidechain
25	LA	914	G	Sidechain
25	LA	916	G	Sidechain
25	LA	919	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
25	LA	923	G	Sidechain
25	LA	927	A	Sidechain
25	LA	931	U	Sidechain
25	LA	932	U	Sidechain
25	LA	934	U	Sidechain
25	LA	938	G	Sidechain
25	LA	945	A	Sidechain
25	LA	948	C	Sidechain
25	LA	950	G	Sidechain
25	LA	952	G	Sidechain
25	LA	953	G	Sidechain
25	LA	954	G	Sidechain
25	LA	955	U	Sidechain
25	LA	958	U	Sidechain
25	LA	968	C	Sidechain
25	LA	969	G	Sidechain
25	LA	97	C	Sidechain
25	LA	970	U	Sidechain
25	LA	974	G	Sidechain
25	LA	980	A	Sidechain
25	LA	983	A	Sidechain
25	LA	984	A	Sidechain
25	LA	989	G	Sidechain
25	LA	994	C	Sidechain
25	LA	995	C	Sidechain
25	LA	999	U	Sidechain
26	LB	1	U	Sidechain
26	LB	100	G	Sidechain
26	LB	102	G	Sidechain
26	LB	105	G	Sidechain
26	LB	19	C	Sidechain
26	LB	24	G	Sidechain
26	LB	32	U	Sidechain
26	LB	34	A	Sidechain
26	LB	41	G	Sidechain
26	LB	6	G	Sidechain
26	LB	61	G	Sidechain
26	LB	67	G	Sidechain
26	LB	69	G	Sidechain
26	LB	7	G	Sidechain
26	LB	77	U	Sidechain
26	LB	79	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
26	LB	80	U	Sidechain
26	LB	83	G	Sidechain
26	LB	84	G	Sidechain
26	LB	95	U	Sidechain
26	LB	98	G	Sidechain
27	LC	163	TYR	Sidechain
27	LC	164	ARG	Sidechain
27	LC	56	ASP	Peptide
27	LC	84	ALA	Peptide
38	LD	52	ARG	Sidechain
38	LD	61	ARG	Sidechain
38	LD	89	GLY	Peptide
48	LE	133	ARG	Sidechain
52	LF	116	ARG	Sidechain
52	LF	34	ARG	Sidechain
52	LF	5	THR	Peptide
52	LF	69	ARG	Sidechain
52	LF	74	TYR	Sidechain
52	LF	75	TYR	Sidechain
53	LG	117	SER	Peptide
53	LG	30	ARG	Sidechain
53	LG	31	ARG	Sidechain
53	LG	64	ARG	Sidechain
54	LH	126	ARG	Sidechain
54	LH	21	ARG	Sidechain
54	LH	28	GLY	Peptide
54	LH	33	ARG	Sidechain
54	LH	60	ARG	Sidechain
55	LI	81	ARG	Sidechain
56	LJ	103	ARG	Sidechain
56	LJ	2	ARG	Sidechain
56	LJ	4	ARG	Sidechain
56	LJ	45	ARG	Sidechain
56	LJ	8	ARG	Sidechain
56	LJ	86	ARG	Sidechain
57	LK	111	ARG	Sidechain
57	LK	13	ARG	Sidechain
57	LK	16	ARG	Sidechain
28	LM	20	ARG	Sidechain
28	LM	38	ARG	Sidechain
28	LM	48	ALA	Peptide
28	LM	92	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
28	LM	97	TYR	Sidechain
29	LN	102	TYR	Sidechain
29	LN	12	ARG	Sidechain
29	LN	170	TYR	Sidechain
29	LN	176	ARG	Sidechain
29	LN	194	VAL	Peptide
29	LN	211	ARG	Sidechain
29	LN	225	ASN	Peptide
29	LN	79	ARG	Sidechain
29	LN	82	TYR	Sidechain
30	LO	12	ARG	Sidechain
30	LO	27	ARG	Sidechain
30	LO	49	ARG	Sidechain
30	LO	63	ARG	Sidechain
31	LP	52	PRO	Peptide
32	LQ	8	ARG	Sidechain
32	LQ	88	ARG	Sidechain
34	LS	14	THR	Peptide
34	LS	6	ARG	Sidechain
34	LS	81	ARG	Sidechain
35	LT	82	TYR	Sidechain
35	LT	93	ARG	Sidechain
36	LU	10	ARG	Peptide
36	LU	14	ASP	Peptide
36	LU	16	GLU	Peptide
36	LU	38	ARG	Sidechain
36	LU	39	GLN	Peptide
37	LV	10	ARG	Sidechain
37	LV	44	ARG	Sidechain
37	LV	71	ARG	Sidechain
39	LW	37	LEU	Peptide
39	LW	38	GLN	Peptide
39	LW	52	ARG	Sidechain
39	LW	7	ARG	Sidechain
40	LX	117	GLY	Peptide
40	LX	128	ARG	Sidechain
40	LX	13	ARG	Sidechain
40	LX	166	GLY	Peptide
40	LX	179	ARG	Sidechain
40	LX	43	ASP	Peptide
40	LX	45	TYR	Sidechain
40	LX	46	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
40	LX	59	ARG	Sidechain
40	LX	83	ARG	Sidechain
41	LY	15	ARG	Sidechain
58	LZ	15	SER	Peptide
58	LZ	49	ARG	Sidechain
58	LZ	6	HIS	Peptide
58	LZ	9	TYR	Sidechain
24	S1	103	ARG	Sidechain
24	S1	132	TYR	Sidechain
24	S1	179	THR	Peptide
24	S1	193	ASN	Peptide
24	S1	303	ASP	Peptide
24	S1	338	TYR	Sidechain
24	S1	361	ARG	Sidechain
24	S1	400	ASP	Peptide
24	S1	401	ALA	Peptide
24	S1	407	ARG	Sidechain
24	S1	445	ARG	Sidechain
24	S1	474	ARG	Sidechain
24	S1	490	ARG	Sidechain
24	S1	506	LYS	Peptide
24	S1	511	ARG	Peptide,Sidechain
24	S1	568	TYR	Sidechain
24	S1	585	VAL	Peptide
24	S1	586	ASP	Peptide
2	S6	18	U	Sidechain
2	S6	2	G	Sidechain
2	S6	20	G	Sidechain
2	S6	25	U	Sidechain
2	S6	30	G	Sidechain
2	S6	32	G	Sidechain
2	S6	46	G	Sidechain
2	S6	47	A	Sidechain
2	S6	5	G	Sidechain
2	S6	55	U	Sidechain
2	S6	60	A	Sidechain
2	S6	7	G	Sidechain
2	S6	74	A	Sidechain
2	S6	77	A	Sidechain
2	S6	8	U	Sidechain
2	S6	9	G	Sidechain
3	S7	12	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	S7	14	A	Sidechain
3	S7	15	G	Sidechain
3	S7	16	U	Sidechain
3	S7	19	G	Sidechain
3	S7	2	C	Sidechain
3	S7	22	G	Sidechain
3	S7	27	G	Sidechain
3	S7	28	G	Sidechain
3	S7	32	U	Sidechain
3	S7	34	G	Sidechain
3	S7	37	A	Sidechain
3	S7	39	U	Sidechain
3	S7	4	C	Sidechain
3	S7	42	C	Sidechain
3	S7	44	G	Sidechain
3	S7	48	C	Sidechain
3	S7	49	C	Sidechain
3	S7	5	G	Sidechain
3	S7	50	U	Sidechain
3	S7	57	G	Sidechain
3	S7	59	U	Sidechain
3	S7	61	C	Sidechain
3	S7	64	A	Sidechain
3	S7	69	G	Sidechain
3	S7	7	A	Sidechain
3	S7	70	G	Sidechain
3	S7	71	G	Sidechain
3	S7	72	C	Sidechain
3	S7	74	C	Sidechain
3	S7	8	U	Sidechain
1	SA	100	G	Sidechain
1	SA	1000	A	Sidechain
1	SA	1010	U	Sidechain
1	SA	1023	U	Sidechain
1	SA	1025	U	Sidechain
1	SA	1029	U	Sidechain
1	SA	103	U	Sidechain
1	SA	1032	G	Sidechain
1	SA	1033	G	Sidechain
1	SA	1038	C	Sidechain
1	SA	1039	G	Sidechain
1	SA	1041	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	1044	A	Sidechain
1	SA	1055	A	Sidechain
1	SA	1056	U	Sidechain
1	SA	1065	U	Sidechain
1	SA	1066	C	Sidechain
1	SA	1067	A	Sidechain
1	SA	1076	U	Sidechain
1	SA	108	G	Sidechain
1	SA	1080	A	Sidechain
1	SA	1083	U	Sidechain
1	SA	1086	U	Sidechain
1	SA	109	A	Sidechain
1	SA	1091	U	Sidechain
1	SA	1094	G	Sidechain
1	SA	1099	G	Sidechain
1	SA	1108	G	Sidechain
1	SA	1115	U	Sidechain
1	SA	1116	U	Sidechain
1	SA	1124	G	Sidechain
1	SA	1126	U	Sidechain
1	SA	1129	C	Sidechain
1	SA	1133	G	Sidechain
1	SA	1134	G	Sidechain
1	SA	1135	U	Sidechain
1	SA	1139	G	Sidechain
1	SA	1140	C	Sidechain
1	SA	1143	G	Sidechain
1	SA	1145	A	Sidechain
1	SA	1153	G	Sidechain
1	SA	1164	G	Sidechain
1	SA	1167	A	Sidechain
1	SA	1170	A	Sidechain
1	SA	1175	G	Sidechain
1	SA	1176	A	Sidechain
1	SA	1178	G	Sidechain
1	SA	1179	A	Sidechain
1	SA	1181	G	Sidechain
1	SA	1182	G	Sidechain
1	SA	1184	G	Sidechain
1	SA	1185	G	Sidechain
1	SA	1189	U	Sidechain
1	SA	1195	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	1198	G	Sidechain
1	SA	1199	U	Sidechain
1	SA	1201	A	Sidechain
1	SA	1206	G	Sidechain
1	SA	1207	G	Sidechain
1	SA	1208	C	Sidechain
1	SA	121	U	Sidechain
1	SA	1210	C	Sidechain
1	SA	1213	A	Sidechain
1	SA	1219	A	Sidechain
1	SA	1222	G	Sidechain
1	SA	1225	A	Sidechain
1	SA	1226	C	Sidechain
1	SA	1237	C	Sidechain
1	SA	1252	A	Sidechain
1	SA	1257	A	Sidechain
1	SA	1258	G	Sidechain
1	SA	1260	G	Sidechain
1	SA	1266	G	Sidechain
1	SA	1268	G	Sidechain
1	SA	1269	A	Sidechain
1	SA	127	G	Sidechain
1	SA	1278	G	Sidechain
1	SA	1279	G	Sidechain
1	SA	1285	A	Sidechain
1	SA	130	A	Sidechain
1	SA	1303	C	Sidechain
1	SA	1304	G	Sidechain
1	SA	1306	A	Sidechain
1	SA	1307	U	Sidechain
1	SA	1313	U	Sidechain
1	SA	1318	A	Sidechain
1	SA	1321	U	Sidechain
1	SA	1322	C	Sidechain
1	SA	1326	U	Sidechain
1	SA	1327	C	Sidechain
1	SA	1337	G	Sidechain
1	SA	1338	G	Sidechain
1	SA	1341	U	Sidechain
1	SA	1344	C	Sidechain
1	SA	1345	U	Sidechain
1	SA	1347	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	1349	A	Sidechain
1	SA	1351	U	Sidechain
1	SA	1354	U	Sidechain
1	SA	1356	G	Sidechain
1	SA	1357	A	Sidechain
1	SA	1361	G	Sidechain
1	SA	1363	A	Sidechain
1	SA	1364	U	Sidechain
1	SA	1371	G	Sidechain
1	SA	1372	U	Sidechain
1	SA	1376	U	Sidechain
1	SA	1384	C	Sidechain
1	SA	1389	C	Sidechain
1	SA	139	A	Sidechain
1	SA	1391	U	Sidechain
1	SA	1392	G	Sidechain
1	SA	1398	A	Sidechain
1	SA	1399	C	Sidechain
1	SA	140	U	Sidechain
1	SA	1401	G	Sidechain
1	SA	1402	C	Sidechain
1	SA	1405	G	Sidechain
1	SA	1406	U	Sidechain
1	SA	141	G	Sidechain
1	SA	1415	G	Sidechain
1	SA	1420	U	Sidechain
1	SA	1421	G	Sidechain
1	SA	1428	A	Sidechain
1	SA	143	A	Sidechain
1	SA	1432	G	Sidechain
1	SA	1433	A	Sidechain
1	SA	1438	G	Sidechain
1	SA	1442	G	Sidechain
1	SA	1446	A	Sidechain
1	SA	145	G	Sidechain
1	SA	1458	G	Sidechain
1	SA	1460	C	Sidechain
1	SA	1464	U	Sidechain
1	SA	1472	U	Sidechain
1	SA	1474	U	Sidechain
1	SA	1482	G	Sidechain
1	SA	1483	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	1485	U	Sidechain
1	SA	1486	G	Sidechain
1	SA	1489	G	Sidechain
1	SA	1491	G	Sidechain
1	SA	1497	G	Sidechain
1	SA	1500	A	Sidechain
1	SA	1504	G	Sidechain
1	SA	1506	U	Sidechain
1	SA	1512	U	Sidechain
1	SA	1513	A	Sidechain
1	SA	1516	G	Sidechain
1	SA	1517	G	Sidechain
1	SA	1518	A	Sidechain
1	SA	1519	A	Sidechain
1	SA	1521	C	Sidechain
1	SA	1522	U	Sidechain
1	SA	1526	G	Sidechain
1	SA	1527	U	Sidechain
1	SA	1529	G	Sidechain
1	SA	153	C	Sidechain
1	SA	1530	G	Sidechain
1	SA	1533	C	Sidechain
1	SA	154	U	Sidechain
1	SA	1540	U	Sidechain
1	SA	159	G	Sidechain
1	SA	161	A	Sidechain
1	SA	165	G	Sidechain
1	SA	166	U	Sidechain
1	SA	171	A	Sidechain
1	SA	172	A	Sidechain
1	SA	173	U	Sidechain
1	SA	178	C	Sidechain
1	SA	182	A	Sidechain
1	SA	183	C	Sidechain
1	SA	184	G	Sidechain
1	SA	185	U	Sidechain
1	SA	190	A	Sidechain
1	SA	194	C	Sidechain
1	SA	197	A	Sidechain
1	SA	20	U	Sidechain
1	SA	200	G	Sidechain
1	SA	201	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	209	U	Sidechain
1	SA	21	G	Sidechain
1	SA	210	C	Sidechain
1	SA	211	G	Sidechain
1	SA	212	G	Sidechain
1	SA	214	C	Sidechain
1	SA	220	G	Sidechain
1	SA	228	A	Sidechain
1	SA	231	U	Sidechain
1	SA	236	A	Sidechain
1	SA	238	A	Sidechain
1	SA	242	G	Sidechain
1	SA	244	U	Sidechain
1	SA	245	U	Sidechain
1	SA	246	A	Sidechain
1	SA	249	U	Sidechain
1	SA	250	A	Sidechain
1	SA	251	G	Sidechain
1	SA	252	U	Sidechain
1	SA	258	G	Sidechain
1	SA	261	U	Sidechain
1	SA	262	A	Sidechain
1	SA	264	C	Sidechain
1	SA	265	G	Sidechain
1	SA	266	G	Sidechain
1	SA	271	C	Sidechain
1	SA	274	A	Sidechain
1	SA	276	G	Sidechain
1	SA	278	G	Sidechain
1	SA	281	G	Sidechain
1	SA	288	A	Sidechain
1	SA	297	G	Sidechain
1	SA	299	G	Sidechain
1	SA	305	G	Sidechain
1	SA	310	G	Sidechain
1	SA	314	C	Sidechain
1	SA	317	U	Sidechain
1	SA	318	G	Sidechain
1	SA	319	G	Sidechain
1	SA	33	A	Sidechain
1	SA	331	G	Sidechain
1	SA	332	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	343	U	Sidechain
1	SA	347	G	Sidechain
1	SA	351	G	Sidechain
1	SA	353	A	Sidechain
1	SA	355	C	Sidechain
1	SA	358	U	Sidechain
1	SA	361	G	Sidechain
1	SA	362	G	Sidechain
1	SA	365	U	Sidechain
1	SA	366	A	Sidechain
1	SA	367	U	Sidechain
1	SA	368	U	Sidechain
1	SA	37	U	Sidechain
1	SA	370	C	Sidechain
1	SA	377	G	Sidechain
1	SA	387	U	Sidechain
1	SA	388	G	Sidechain
1	SA	390	U	Sidechain
1	SA	394	G	Sidechain
1	SA	398	U	Sidechain
1	SA	4	U	Sidechain
1	SA	405	U	Sidechain
1	SA	410	G	Sidechain
1	SA	411	A	Sidechain
1	SA	413	G	Sidechain
1	SA	42	G	Sidechain
1	SA	423	G	Sidechain
1	SA	425	G	Sidechain
1	SA	427	U	Sidechain
1	SA	429	U	Sidechain
1	SA	434	U	Sidechain
1	SA	437	U	Sidechain
1	SA	439	U	Sidechain
1	SA	441	A	Sidechain
1	SA	442	G	Sidechain
1	SA	448	A	Sidechain
1	SA	459	A	Sidechain
1	SA	46	G	Sidechain
1	SA	461	A	Sidechain
1	SA	463	U	Sidechain
1	SA	464	U	Sidechain
1	SA	466	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	474	G	Sidechain
1	SA	479	U	Sidechain
1	SA	481	G	Sidechain
1	SA	486	U	Sidechain
1	SA	491	G	Sidechain
1	SA	493	A	Sidechain
1	SA	509	A	Sidechain
1	SA	51	A	Sidechain
1	SA	512	U	Sidechain
1	SA	517	G	Sidechain
1	SA	52	C	Sidechain
1	SA	521	G	Sidechain
1	SA	524	G	Sidechain
1	SA	528	C	Sidechain
1	SA	529	G	Sidechain
1	SA	530	G	Sidechain
1	SA	534	U	Sidechain
1	SA	543	U	Sidechain
1	SA	554	A	Sidechain
1	SA	555	U	Sidechain
1	SA	557	G	Sidechain
1	SA	562	U	Sidechain
1	SA	564	C	Sidechain
1	SA	570	G	Sidechain
1	SA	571	U	Sidechain
1	SA	575	G	Sidechain
1	SA	577	G	Sidechain
1	SA	58	C	Sidechain
1	SA	580	C	Sidechain
1	SA	581	G	Sidechain
1	SA	584	G	Sidechain
1	SA	587	G	Sidechain
1	SA	588	G	Sidechain
1	SA	595	A	Sidechain
1	SA	60	A	Sidechain
1	SA	602	A	Sidechain
1	SA	610	U	Sidechain
1	SA	615	G	Sidechain
1	SA	616	G	Sidechain
1	SA	617	G	Sidechain
1	SA	622	A	Sidechain
1	SA	623	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	625	U	Sidechain
1	SA	637	C	Sidechain
1	SA	64	G	Sidechain
1	SA	641	U	Sidechain
1	SA	646	G	Sidechain
1	SA	65	A	Sidechain
1	SA	66	A	Sidechain
1	SA	662	U	Sidechain
1	SA	664	G	Sidechain
1	SA	666	G	Sidechain
1	SA	673	A	Sidechain
1	SA	678	U	Sidechain
1	SA	684	U	Sidechain
1	SA	685	G	Sidechain
1	SA	69	G	Sidechain
1	SA	692	U	Sidechain
1	SA	693	G	Sidechain
1	SA	695	A	Sidechain
1	SA	697	U	Sidechain
1	SA	701	U	Sidechain
1	SA	703	G	Sidechain
1	SA	705	G	Sidechain
1	SA	707	U	Sidechain
1	SA	711	G	Sidechain
1	SA	713	G	Sidechain
1	SA	717	U	Sidechain
1	SA	719	C	Sidechain
1	SA	72	A	Sidechain
1	SA	720	C	Sidechain
1	SA	727	G	Sidechain
1	SA	730	G	Sidechain
1	SA	742	G	Sidechain
1	SA	745	G	Sidechain
1	SA	747	A	Sidechain
1	SA	753	A	Sidechain
1	SA	757	U	Sidechain
1	SA	76	G	Sidechain
1	SA	763	G	Sidechain
1	SA	764	C	Sidechain
1	SA	765	G	Sidechain
1	SA	769	G	Sidechain
1	SA	771	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	773	G	Sidechain
1	SA	774	G	Sidechain
1	SA	775	G	Sidechain
1	SA	782	A	Sidechain
1	SA	786	G	Sidechain
1	SA	789	U	Sidechain
1	SA	791	G	Sidechain
1	SA	792	A	Sidechain
1	SA	795	C	Sidechain
1	SA	798	U	Sidechain
1	SA	801	U	Sidechain
1	SA	802	A	Sidechain
1	SA	803	G	Sidechain
1	SA	806	C	Sidechain
1	SA	808	C	Sidechain
1	SA	812	G	Sidechain
1	SA	813	U	Sidechain
1	SA	815	A	Sidechain
1	SA	816	A	Sidechain
1	SA	817	C	Sidechain
1	SA	819	A	Sidechain
1	SA	820	U	Sidechain
1	SA	829	G	Sidechain
1	SA	835	U	Sidechain
1	SA	838	G	Sidechain
1	SA	842	U	Sidechain
1	SA	855	U	Sidechain
1	SA	859	G	Sidechain
1	SA	86	G	Sidechain
1	SA	860	A	Sidechain
1	SA	861	G	Sidechain
1	SA	866	C	Sidechain
1	SA	868	C	Sidechain
1	SA	871	U	Sidechain
1	SA	88	U	Sidechain
1	SA	880	C	Sidechain
1	SA	884	U	Sidechain
1	SA	888	G	Sidechain
1	SA	890	G	Sidechain
1	SA	899	C	Sidechain
1	SA	9	G	Sidechain
1	SA	900	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	SA	907	A	Sidechain
1	SA	915	A	Sidechain
1	SA	92	U	Sidechain
1	SA	920	U	Sidechain
1	SA	921	U	Sidechain
1	SA	925	G	Sidechain
1	SA	926	G	Sidechain
1	SA	928	G	Sidechain
1	SA	933	G	Sidechain
1	SA	943	U	Sidechain
1	SA	944	G	Sidechain
1	SA	945	G	Sidechain
1	SA	947	G	Sidechain
1	SA	956	U	Sidechain
1	SA	957	U	Sidechain
1	SA	958	A	Sidechain
1	SA	959	A	Sidechain
1	SA	961	U	Sidechain
1	SA	963	G	Sidechain
1	SA	965	U	Sidechain
1	SA	973	G	Sidechain
1	SA	975	A	Sidechain
1	SA	976	G	Sidechain
1	SA	977	A	Sidechain
1	SA	978	A	Sidechain
1	SA	979	C	Sidechain
1	SA	980	C	Sidechain
1	SA	981	U	Sidechain
1	SA	983	A	Sidechain
1	SA	992	U	Sidechain
1	SA	993	G	Sidechain
1	SA	994	A	Sidechain
1	SA	997	U	Sidechain
14	SB	150	ILE	Peptide
14	SB	164	ASP	Peptide
14	SB	94	ARG	Sidechain
17	SC	10	ARG	Sidechain
17	SC	105	VAL	Peptide
17	SC	131	ARG	Peptide,Sidechain
17	SC	163	ARG	Sidechain
17	SC	183	TYR	Sidechain
17	SC	187	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
18	SD	102	TYR	Sidechain
18	SD	61	ARG	Sidechain
18	SD	64	TYR	Sidechain
18	SD	75	TYR	Sidechain
18	SD	80	ARG	Sidechain
18	SD	84	ASN	Peptide
19	SE	104	ILE	Peptide
19	SE	11	GLN	Peptide
19	SE	121	ASN	Peptide
19	SE	19	ARG	Sidechain
19	SE	25	LYS	Peptide
19	SE	28	ARG	Sidechain
19	SE	44	ARG	Sidechain
19	SE	49	TYR	Sidechain
20	SF	109	ARG	Sidechain
20	SF	110	ARG	Sidechain
20	SF	17	GLN	Peptide
20	SF	38	ARG	Sidechain
20	SF	44	ARG	Sidechain
20	SF	79	ARG	Sidechain
21	SG	110	ARG	Sidechain
21	SG	148	LYS	Peptide
21	SG	77	ARG	Sidechain
21	SG	94	ARG	Sidechain
22	SH	14	ARG	Sidechain
22	SH	79	ARG	Sidechain
22	SH	87	ARG	Sidechain
23	SI	118	ARG	Sidechain
23	SI	122	ARG	Sidechain
23	SI	129	ARG	Sidechain
23	SI	98	ARG	Sidechain
4	SJ	16	ARG	Sidechain
4	SJ	45	ARG	Sidechain
4	SJ	62	ARG	Sidechain
4	SJ	65	TYR	Sidechain
4	SJ	68	ARG	Sidechain
4	SJ	72	ARG	Sidechain
4	SJ	80	THR	Peptide
5	SK	121	ARG	Sidechain
5	SK	127	ARG	Sidechain
5	SK	3	ALA	Peptide
5	SK	52	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
5	SK	97	ARG	Sidechain
6	SL	108	ASP	Peptide
6	SL	109	ARG	Sidechain
6	SL	113	ARG	Sidechain
6	SL	114	SER	Peptide
6	SL	26	CYS	Peptide
6	SL	37	TYR	Peptide
6	SL	42	LYS	Peptide
6	SL	53	ARG	Sidechain
6	SL	82	ARG	Sidechain
7	SM	108	ARG	Sidechain
7	SM	69	ARG	Sidechain
7	SM	70	ARG	Sidechain
7	SM	97	ARG	Sidechain
8	SN	41	TRP	Peptide
8	SN	62	ARG	Sidechain
8	SN	64	ARG	Sidechain
8	SN	68	ARG	Sidechain
8	SN	8	ARG	Sidechain
9	SO	52	ARG	Sidechain
9	SO	53	ARG	Sidechain
9	SO	63	ARG	Sidechain
9	SO	71	ARG	Sidechain
10	SP	35	ARG	Sidechain
10	SP	51	ARG	Sidechain
10	SP	64	GLY	Peptide
10	SP	70	ARG	Sidechain
11	SQ	26	ARG	Sidechain
11	SQ	30	HIS	Peptide
11	SQ	5	ARG	Sidechain
11	SQ	6	THR	Peptide
12	SR	3	TYR	Sidechain
12	SR	50	TYR	Sidechain
12	SR	62	ARG	Sidechain
13	SS	11	ASP	Peptide
13	SS	2	ARG	Sidechain
15	ST	35	TYR	Sidechain
15	ST	73	ARG	Sidechain
16	SU	36	PHE	Peptide
16	SU	38	GLU	Peptide
16	SU	70	TYR	Sidechain

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	SA	33076	0	16648	111	0
2	S6	1639	0	837	1	0
3	S7	1577	0	800	5	0
4	SJ	825	0	865	0	0
5	SK	965	0	997	3	0
6	SL	955	0	1019	1	0
7	SM	910	0	981	2	0
8	SN	805	0	847	1	0
9	SO	716	0	742	0	0
10	SP	649	0	666	0	0
11	SQ	672	0	716	0	0
12	SR	626	0	651	0	0
13	SS	727	0	769	2	0
14	SB	1872	0	1885	1	0
15	ST	670	0	722	3	0
16	SU	590	0	631	0	0
17	SC	1822	0	1913	2	0
18	SD	1643	0	1710	1	0
19	SE	1225	0	1273	1	0
20	SF	1101	0	1050	1	0
21	SG	1400	0	1449	2	0
22	SH	979	0	1034	1	0
23	SI	1036	0	1084	0	0
24	S1	5431	0	5403	16	0
25	LA	62333	0	31349	251	0
26	LB	2566	0	1302	10	0
27	LC	1733	0	1824	6	0
28	LM	917	0	965	1	0
29	LN	2092	0	2170	6	0
30	LO	947	0	1022	1	0
31	LP	816	0	839	2	0
32	LQ	857	0	922	0	0
33	LR	787	0	846	0	0
34	LS	789	0	847	1	0
35	LT	753	0	780	0	0
36	LU	634	0	656	3	0
37	LV	625	0	655	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LD	1233	0	1283	1	0
39	LW	509	0	543	2	0
40	LX	1565	0	1616	1	0
41	LY	449	0	491	1	0
42	L1	444	0	461	5	0
43	L2	441	0	485	0	0
44	L3	377	0	418	0	0
45	L4	504	0	574	0	0
46	L5	302	0	343	0	0
47	L6	1552	0	1619	3	0
48	LE	1032	0	1088	0	0
49	L7	1420	0	1460	4	0
50	L8	1323	0	1374	1	0
51	L9	1111	0	1148	0	0
52	LF	1129	0	1162	6	0
53	LG	947	0	1023	5	0
54	LH	1053	0	1129	2	0
55	LI	1074	0	1157	1	0
56	LJ	1008	0	1045	4	0
57	LK	900	0	935	0	0
58	LZ	549	0	552	1	0
59	S1	32	0	12	15	0
All	All	156714	0	108787	450	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (450) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S1:22:LYS:CE	59:S1:801:GTP:O3G	2.13	0.97
24:S1:23:THR:N	59:S1:801:GTP:O2B	2.08	0.86
24:S1:22:LYS:HE3	59:S1:801:GTP:O3G	1.76	0.85
21:SG:77:ARG:HE	21:SG:152:HIS:CD2	2.05	0.74
24:S1:144:ASP:CG	59:S1:801:GTP:HN1	1.89	0.74
25:LA:2799:A:H3'	25:LA:2800:A:H5'	1.73	0.71
25:LA:2849:U:H3	25:LA:2867:G:H1'	1.57	0.70
24:S1:144:ASP:OD2	59:S1:801:GTP:N1	2.27	0.68
24:S1:269:PHE:HB2	59:S1:801:GTP:C5	2.29	0.67
25:LA:45:G:H4'	25:LA:46:G:H5'	1.76	0.67
25:LA:1241:A:C2	25:LA:1242:U:C4	2.87	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:701:U:H4'	1:SA:702:A:OP2	1.98	0.61
17:SC:120:THR:HG23	17:SC:188:ALA:HB1	1.83	0.60
25:LA:1127:A:H61	25:LA:2488:G:H21	1.48	0.59
25:LA:1367:A:H2'	25:LA:1368:G:H5'	1.85	0.59
20:SF:43:GLY:HA2	20:SF:58:HIS:CE1	2.37	0.59
8:SN:45:LEU:H	8:SN:45:LEU:HD22	1.68	0.59
24:S1:22:LYS:HE2	59:S1:801:GTP:O3G	2.02	0.58
25:LA:877:A:H62	25:LA:900:A:H61	1.53	0.57
25:LA:82:U:H2'	25:LA:83:A:C8	2.40	0.57
25:LA:63:A:H2'	25:LA:64:A:C8	2.41	0.56
3:S7:5:G:H1	3:S7:68:C:H42	1.54	0.55
24:S1:269:PHE:CB	59:S1:801:GTP:C5	2.89	0.55
25:LA:948:C:H1'	25:LA:984:A:C8	2.42	0.55
25:LA:1615:C:C5	25:LA:1617:C:C4	2.95	0.54
1:SA:92:U:H2'	1:SA:93:U:C6	2.42	0.54
25:LA:2210:U:C6	25:LA:2212:A:C2	2.95	0.54
25:LA:1763:G:H3'	25:LA:1764:C:H5"	1.89	0.54
25:LA:2657:A:C2	25:LA:2665:A:C4	2.95	0.54
25:LA:1783:A:H3'	25:LA:1783:A:C8	2.43	0.54
25:LA:780:G:C2	25:LA:782:A:C2	2.96	0.54
25:LA:2125:G:H21	25:LA:2173:A:H62	1.56	0.54
1:SA:794:A:C5	1:SA:795:C:C5	2.94	0.54
25:LA:452:G:H2'	25:LA:453:A:C8	2.42	0.54
1:SA:1401:G:C6	1:SA:1402:C:N3	2.76	0.53
25:LA:2427:C:H5'	25:LA:2429:G:H5'	1.90	0.53
25:LA:322:A:H5'	25:LA:340:A:H1'	1.89	0.53
25:LA:745:G:C2	25:LA:750:A:C6	2.97	0.53
13:SS:12:LEU:HD12	13:SS:12:LEU:H	1.73	0.53
1:SA:171:A:H2'	1:SA:172:A:C8	2.44	0.52
1:SA:994:A:C5	1:SA:995:C:C5	2.97	0.52
25:LA:1899:A:C2	25:LA:1902:C:N4	2.78	0.52
1:SA:190:A:C6	1:SA:191:G:H1'	2.44	0.52
25:LA:784:G:C5	29:LN:227:VAL:HG11	2.44	0.52
24:S1:23:THR:CB	59:S1:801:GTP:O2B	2.58	0.52
25:LA:1899:A:C2	25:LA:1903:G:C2	2.98	0.51
42:L1:38:LEU:HD22	42:L1:38:LEU:H	1.75	0.51
25:LA:489:G:H22	25:LA:1320:C:H3'	1.74	0.51
25:LA:590:A:C2	25:LA:668:A:C2	2.98	0.51
25:LA:2330:G:C2	25:LA:2386:A:C2	2.98	0.51
1:SA:1391:U:H2'	1:SA:1392:G:C8	2.46	0.51
25:LA:2125:G:N2	25:LA:2173:A:H62	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:1942:C:C5	25:LA:1943:U:C5	2.99	0.51
25:LA:2799:A:H3'	25:LA:2800:A:C5'	2.39	0.51
25:LA:96:C:H5'	39:LW:41:HIS:CD2	2.46	0.51
1:SA:1501:C:C5	1:SA:1504:G:C5	2.99	0.51
1:SA:560:A:C2	1:SA:566:G:C5	2.99	0.50
25:LA:2657:A:C2	25:LA:2665:A:C5	2.99	0.50
1:SA:609:A:C6	1:SA:610:U:C4	2.99	0.50
1:SA:1236:A:H5'	1:SA:1305:G:OP1	2.11	0.50
25:LA:1670:C:H42	25:LA:1674:G:H5'	1.77	0.50
52:LF:47:HIS:CE1	52:LF:48:VAL:HG23	2.46	0.50
1:SA:118:U:C5	1:SA:288:A:C6	2.99	0.50
1:SA:293:G:H4'	1:SA:610:U:C4	2.46	0.50
5:SK:93:GLU:H	5:SK:93:GLU:CD	2.15	0.50
25:LA:451:U:C5	25:LA:453:A:H3'	2.46	0.50
26:LB:30:C:H2'	26:LB:31:C:H5'	1.94	0.50
25:LA:745:G:N2	25:LA:750:A:C6	2.80	0.50
25:LA:573:U:C6	25:LA:2030:C:H2'	2.46	0.50
25:LA:1366:A:H62	25:LA:1808:A:N6	2.10	0.50
1:SA:283:U:C4	1:SA:284:C:C4	3.00	0.50
25:LA:2519:U:C4	25:LA:2542:A:C5	3.00	0.49
1:SA:889:A:H4'	1:SA:890:G:H5'	1.95	0.49
25:LA:25:U:C5	25:LA:26:G:C6	3.01	0.49
25:LA:1174:U:H3'	25:LA:1175:A:H5"	1.94	0.49
25:LA:2061:G:H5'	25:LA:2502:G:H4'	1.94	0.49
56:LJ:95:THR:HG22	56:LJ:115:LEU:HD23	1.93	0.49
56:LJ:106:ASP:CG	56:LJ:107:ASN:H	2.15	0.49
25:LA:1274:A:C2	25:LA:1646:C:C2	3.01	0.49
25:LA:1851:U:C5	25:LA:1852:U:C4	3.01	0.49
1:SA:609:A:N1	1:SA:610:U:C4	2.81	0.49
25:LA:244:A:C2	25:LA:255:A:C4	3.01	0.49
25:LA:1439:A:C2	25:LA:1553:A:C6	3.01	0.49
25:LA:2710:C:H2'	25:LA:2711:A:C8	2.48	0.49
1:SA:49:U:C4	1:SA:364:A:C6	3.00	0.49
1:SA:1158:C:H2'	1:SA:1159:U:H4'	1.95	0.49
25:LA:443:A:H3'	47:L6:40:ARG:HH12	1.78	0.49
1:SA:1342:C:H2'	1:SA:1343:G:C8	2.48	0.49
25:LA:55:G:H2'	25:LA:56:A:C8	2.47	0.49
25:LA:877:A:H62	25:LA:900:A:N6	2.10	0.49
25:LA:861:A:C2	25:LA:917:A:C4	3.01	0.49
25:LA:2451:A:N7	25:LA:2452:C:C5	2.81	0.49
25:LA:1028:A:H1'	25:LA:2487:G:H5'	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:204:G:H2'	1:SA:205:A:C8	2.48	0.48
25:LA:1082:U:C5	25:LA:1083:U:C5	3.01	0.48
25:LA:2748:A:C2	25:LA:2749:A:C4	3.02	0.48
50:L8:110:HIS:CD2	50:L8:110:HIS:O	2.67	0.48
52:LF:81:ILE:HD13	52:LF:81:ILE:H	1.78	0.48
25:LA:983:A:C8	25:LA:983:A:H3'	2.49	0.48
27:LC:112:ASP:CG	27:LC:162:ARG:HH21	2.17	0.48
38:LD:25:VAL:HG21	38:LD:92:ALA:HA	1.94	0.48
52:LF:5:THR:HA	52:LF:44:TYR:CE1	2.48	0.48
1:SA:978:A:C4	1:SA:1319:A:C2	3.02	0.48
25:LA:1127:A:H61	25:LA:2488:G:N2	2.12	0.48
25:LA:1268:A:C2	25:LA:2013:A:C4	3.01	0.48
36:LU:47:GLY:O	36:LU:50:VAL:HG23	2.13	0.48
1:SA:461:A:C6	1:SA:462:G:C6	3.02	0.48
25:LA:1242:U:C4	25:LA:1243:C:C4	3.02	0.48
27:LC:77:VAL:HB	27:LC:95:VAL:HG22	1.95	0.48
25:LA:2812:G:C6	25:LA:2813:A:C6	3.01	0.48
53:LG:61:VAL:HG13	53:LG:87:LEU:HD11	1.95	0.48
1:SA:811:C:H5'	1:SA:898:G:H4'	1.95	0.47
34:LS:102:ILE:HG23	34:LS:103:LYS:H	1.79	0.47
25:LA:1789:A:C5	25:LA:1790:C:C4	3.02	0.47
25:LA:45:G:C4'	25:LA:46:G:H5'	2.42	0.47
1:SA:325:A:C6	1:SA:326:G:C2	3.02	0.47
1:SA:500:G:C6	1:SA:546:A:C2	3.02	0.47
1:SA:864:A:H2'	1:SA:865:A:C8	2.49	0.47
1:SA:934:C:C5	1:SA:1345:U:C6	3.01	0.47
24:S1:269:PHE:HB2	59:S1:801:GTP:C4	2.50	0.47
25:LA:489:G:C6	25:LA:491:G:C2	3.02	0.47
27:LC:215:SER:HA	27:LC:221:GLY:HA2	1.97	0.47
29:LN:229:HIS:CD2	29:LN:231:HIS:H	2.33	0.47
25:LA:2584:U:C5	25:LA:2585:U:C4	3.03	0.47
1:SA:794:A:C4	1:SA:795:C:C5	3.03	0.47
25:LA:478:A:C6	25:LA:480:A:C5	3.03	0.47
1:SA:109:A:C4	1:SA:327:A:C2	3.02	0.47
1:SA:293:G:H4'	1:SA:610:U:C5	2.50	0.47
25:LA:643:A:H62	25:LA:644:A:N6	2.13	0.47
1:SA:1502:A:H3'	1:SA:1503:A:H5'	1.96	0.47
1:SA:53:A:C2	1:SA:359:G:C2	3.03	0.47
1:SA:306:A:H2'	1:SA:307:C:H5'	1.97	0.47
25:LA:640:C:C4	25:LA:641:U:C4	3.03	0.47
52:LF:45:THR:OG1	52:LF:47:HIS:CD2	2.68	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:673:A:C2	1:SA:734:G:C2	3.03	0.46
1:SA:477:C:H2'	1:SA:478:A:C8	2.50	0.46
25:LA:388:G:C8	25:LA:390:U:C6	3.03	0.46
25:LA:1242:U:C5	25:LA:1243:C:C4	3.04	0.46
26:LB:11:C:C5	26:LB:12:C:C4	3.03	0.46
25:LA:819:A:C4	25:LA:1189:A:C2	3.04	0.46
25:LA:864:G:H21	25:LA:866:A:N6	2.13	0.46
25:LA:1760:C:C5	25:LA:1761:C:C4	3.03	0.46
25:LA:2447:G:C5	25:LA:2500:U:C5	3.03	0.46
1:SA:1074:G:C6	1:SA:1075:U:C4	3.04	0.46
25:LA:13:A:H61	25:LA:525:U:H3'	1.81	0.46
25:LA:1467:U:C4	25:LA:1546:G:C2	3.04	0.46
1:SA:1134:G:H2'	1:SA:1135:U:H5'	1.98	0.46
36:LU:30:VAL:HG12	36:LU:30:VAL:O	2.16	0.46
1:SA:840:C:C4	1:SA:842:U:H1'	2.50	0.46
1:SA:1332:A:C2	1:SA:1333:A:C4	3.04	0.46
3:S7:35:A:H5"	3:S7:36:A:C8	2.50	0.46
25:LA:27:G:H1'	25:LA:513:A:H62	1.81	0.46
25:LA:983:A:C5	25:LA:984:A:C6	3.03	0.46
25:LA:1838:C:C5	25:LA:1899:A:N7	2.84	0.46
1:SA:282:A:C6	1:SA:283:U:C2	3.03	0.46
1:SA:864:A:C6	1:SA:865:A:C6	3.04	0.46
1:SA:994:A:C5	1:SA:1216:A:H4'	2.51	0.46
25:LA:44:A:C6	25:LA:45:G:C5	3.04	0.46
25:LA:277:G:H1'	25:LA:361:G:H1	1.81	0.46
25:LA:2584:U:C5	25:LA:2585:U:C5	3.04	0.46
25:LA:717:C:H3'	25:LA:718:A:H5"	1.98	0.45
53:LG:113:MET:HA	53:LG:116:ILE:HG22	1.98	0.45
25:LA:1853:A:C6	25:LA:1854:A:C2	3.05	0.45
25:LA:2061:G:O6	25:LA:2503:A:C5	2.70	0.45
25:LA:2373:G:C2	25:LA:2381:A:C2	3.04	0.45
25:LA:586:A:H5"	47:L6:84:THR:HG21	1.99	0.45
25:LA:2657:A:C8	25:LA:2658:C:C6	3.05	0.45
25:LA:1329:U:OP2	25:LA:1330:C:C5	2.69	0.45
25:LA:65:U:H2'	25:LA:66:C:C6	2.51	0.45
25:LA:2636:C:H2'	25:LA:2637:U:C6	2.51	0.45
18:SD:196:GLU:CD	18:SD:196:GLU:H	2.19	0.45
25:LA:1797:G:C6	25:LA:1798:U:C4	3.05	0.45
30:LO:60:TRP:CZ2	30:LO:93:ILE:HD13	2.51	0.45
42:L1:42:ILE:HD11	56:LJ:98:LEU:HB3	1.98	0.45
1:SA:185:U:H2'	1:SA:186:C:C6	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:221:C:H2'	1:SA:222:C:C6	2.52	0.45
1:SA:1171:A:H2'	1:SA:1172:C:C6	2.52	0.45
3:S7:37:A:C5	3:S7:38:A:H1'	2.52	0.45
25:LA:983:A:C8	25:LA:983:A:C3'	3.00	0.45
25:LA:1171:G:H2'	25:LA:1172:C:C6	2.52	0.45
25:LA:2061:G:O6	25:LA:2503:A:C6	2.70	0.45
25:LA:2788:C:H2'	25:LA:2789:C:C6	2.51	0.45
1:SA:499:A:C6	1:SA:547:A:C8	3.05	0.45
25:LA:2584:U:C6	25:LA:2585:U:C5	3.05	0.45
27:LC:67:HIS:CE1	27:LC:184:LYS:HA	2.51	0.45
39:LW:17:GLU:HA	39:LW:53:VAL:HG21	1.98	0.45
2:S6:48:U:H4'	2:S6:49:C:OP2	2.17	0.45
25:LA:2377:A:H2'	25:LA:2378:A:C8	2.51	0.45
1:SA:441:A:H61	1:SA:493:A:N6	2.14	0.45
25:LA:524:G:C5	25:LA:525:U:C5	3.05	0.45
25:LA:1276:A:C2	25:LA:1277:G:C5	3.05	0.45
25:LA:2875:C:H2'	25:LA:2876:G:C8	2.53	0.44
1:SA:960:U:H4'	1:SA:961:U:OP2	2.18	0.44
25:LA:1872:A:C6	25:LA:1873:G:H1'	2.53	0.44
25:LA:2188:U:C4	25:LA:2189:U:C4	3.04	0.44
1:SA:2:A:C8	1:SA:4:U:O4	2.70	0.44
1:SA:976:G:C6	1:SA:1363:A:C2	3.05	0.44
1:SA:1236:A:H2'	1:SA:1237:C:C6	2.53	0.44
24:S1:22:LYS:NZ	59:S1:801:GTP:O3G	2.49	0.44
24:S1:23:THR:OG1	59:S1:801:GTP:O2B	2.28	0.44
25:LA:652:U:H4'	25:LA:653:U:C4	2.52	0.44
1:SA:323:U:C4	1:SA:324:G:C5	3.05	0.44
1:SA:949:A:C2	1:SA:1233:G:C2	3.05	0.44
15:ST:67:HIS:CG	15:ST:68:LYS:H	2.35	0.44
25:LA:28:A:C4	25:LA:513:A:C8	3.06	0.44
25:LA:85:G:C5	25:LA:98:G:C2	3.05	0.44
25:LA:1064:C:C4	25:LA:1065:U:C4	3.06	0.44
25:LA:1490:A:C8	29:LN:97:ASP:HB3	2.52	0.44
1:SA:271:C:H3'	1:SA:272:C:H5"	2.00	0.44
1:SA:1517:G:N1	1:SA:1518:A:C2	2.86	0.44
25:LA:19:A:C2	25:LA:522:A:C2	3.06	0.44
25:LA:845:A:C5	25:LA:847:U:O2	2.71	0.44
1:SA:588:G:C5	1:SA:753:A:C5	3.06	0.44
25:LA:638:G:C5	25:LA:639:U:C4	3.06	0.44
25:LA:705:A:H1'	25:LA:727:A:C2	2.53	0.44
25:LA:782:A:N7	29:LN:219:VAL:HG11	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:845:A:C2	25:LA:847:U:H1'	2.53	0.44
25:LA:1917:U:H2'	25:LA:1918:A:C8	2.52	0.44
25:LA:1966:A:C8	25:LA:2593:U:H5'	2.52	0.44
25:LA:983:A:C5	25:LA:984:A:C5	3.06	0.44
25:LA:1213:A:C2	25:LA:1214:A:C4	3.05	0.44
1:SA:999:C:H2'	1:SA:1000:A:C8	2.53	0.44
25:LA:181:A:C2	25:LA:435:C:C5	3.06	0.44
25:LA:780:G:H1	29:LN:228:ASP:CG	2.21	0.44
25:LA:1153:C:C4	25:LA:1154:G:C6	3.05	0.44
25:LA:1717:A:C2	25:LA:1744:A:C4	3.05	0.44
25:LA:2209:G:C4	25:LA:2210:U:C5	3.06	0.44
1:SA:1432:G:H5'	28:LM:105:LYS:HB2	2.00	0.44
25:LA:2187:U:H2'	25:LA:2188:U:C6	2.53	0.44
25:LA:2451:A:H2'	25:LA:2452:C:H5'	1.99	0.44
1:SA:1041:G:C2	1:SA:1042:A:C5	3.06	0.43
1:SA:1142:G:C2	1:SA:1143:G:H1'	2.53	0.43
25:LA:782:A:C2	29:LN:224:MET:HG2	2.53	0.43
25:LA:792:A:O3'	25:LA:793:A:C2	2.70	0.43
25:LA:1675:C:C5	25:LA:1676:A:C4	3.05	0.43
41:LY:10:ARG:HE	41:LY:10:ARG:HA	1.82	0.43
1:SA:373:A:C2	1:SA:482:A:C6	3.06	0.43
1:SA:1231:G:C6	1:SA:1232:U:C4	3.06	0.43
1:SA:1401:G:C6	1:SA:1402:C:C2	3.05	0.43
25:LA:705:A:H62	25:LA:726:G:H1'	1.83	0.43
25:LA:983:A:C6	25:LA:984:A:C6	3.06	0.43
25:LA:2373:G:C6	25:LA:2374:C:C4	3.06	0.43
56:LJ:55:ALA:HA	56:LJ:80:PHE:CE1	2.53	0.43
1:SA:1501:C:C5	1:SA:1504:G:C4	3.07	0.43
14:SB:19:THR:HG23	14:SB:20:ARG:H	1.83	0.43
25:LA:81:G:C6	25:LA:82:U:C2	3.06	0.43
25:LA:2030:C:HO2'	25:LA:2030:C:H6	1.63	0.43
25:LA:2799:A:C3'	25:LA:2800:A:H5'	2.43	0.43
26:LB:52:A:C6	26:LB:53:A:C5	3.07	0.43
26:LB:54:G:C6	26:LB:55:U:C4	3.06	0.43
54:LH:126:ARG:HH22	54:LH:128:THR:HG22	1.82	0.43
1:SA:1065:U:C5	1:SA:1189:U:N3	2.87	0.43
25:LA:1486:U:H2'	25:LA:1487:U:C6	2.52	0.43
25:LA:2411:A:H2'	25:LA:2412:A:C8	2.53	0.43
25:LA:2447:G:C4	25:LA:2500:U:C5	3.06	0.43
25:LA:2495:G:C6	25:LA:2496:C:C4	3.07	0.43
1:SA:1451:U:H3'	1:SA:1452:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:1502:A:H2'	1:SA:1504:G:C8	2.53	0.43
25:LA:893:C:C5	25:LA:894:U:C2	3.07	0.43
25:LA:1242:U:C5	25:LA:1243:C:C5	3.06	0.43
25:LA:103:A:C6	25:LA:104:A:C4	3.06	0.43
25:LA:103:A:C2	25:LA:104:A:H1'	2.53	0.43
25:LA:204:A:C5	25:LA:206:U:O4	2.72	0.43
25:LA:652:U:H4'	25:LA:653:U:C5	2.53	0.43
25:LA:1022:G:C6	25:LA:1141:U:C5	3.07	0.43
25:LA:1206:G:C6	25:LA:1207:C:C4	3.06	0.43
26:LB:78:A:C2	26:LB:99:A:C4	3.06	0.43
49:L7:84:ILE:HG23	49:L7:85:GLY:H	1.83	0.43
3:S7:48:C:C4	3:S7:59:U:C5	3.07	0.43
25:LA:558:U:H5"	52:LF:111:LYS:HD3	2.01	0.43
25:LA:568:U:H5"	25:LA:945:A:N6	2.34	0.43
25:LA:748:G:C4	25:LA:750:A:C6	3.06	0.43
25:LA:1557:C:H2'	25:LA:1558:C:C5	2.53	0.43
25:LA:1779:U:C4	25:LA:1783:A:C8	3.06	0.43
1:SA:1517:G:C6	1:SA:1518:A:C6	3.06	0.43
19:SE:23:THR:HG22	19:SE:24:VAL:HG13	2.00	0.43
25:LA:194:G:C6	25:LA:195:A:C5	3.06	0.43
25:LA:1645:G:H5"	25:LA:1646:C:H5'	1.99	0.43
25:LA:2709:G:C6	25:LA:2710:C:C4	3.06	0.43
31:LP:82:HIS:O	31:LP:82:HIS:CG	2.72	0.43
53:LG:99:ILE:HG22	53:LG:118:LEU:HB2	2.00	0.43
1:SA:17:U:H2'	1:SA:18:C:C6	2.53	0.43
1:SA:328:C:C5'	1:SA:329:A:H5'	2.49	0.43
24:S1:269:PHE:HB2	59:S1:801:GTP:N7	2.33	0.43
25:LA:1118:C:C5	25:LA:1119:U:C5	3.07	0.43
25:LA:2886:A:H62	42:L1:39:ARG:CZ	2.32	0.43
25:LA:2886:A:H62	42:L1:39:ARG:NE	2.17	0.43
1:SA:206:C:H2'	1:SA:207:C:C6	2.53	0.43
1:SA:608:A:C6	1:SA:609:A:N6	2.87	0.43
1:SA:729:A:H2'	1:SA:730:G:C8	2.54	0.43
1:SA:900:A:H2'	1:SA:901:A:C8	2.53	0.43
25:LA:21:A:C2	25:LA:520:G:C2	3.06	0.43
25:LA:1965:C:C6	25:LA:1966:A:H2'	2.54	0.43
25:LA:2389:G:H5"	25:LA:2390:U:H5'	2.00	0.43
25:LA:2615:U:C2	42:L1:3:GLN:HA	2.53	0.43
1:SA:75:G:H2'	1:SA:76:G:C8	2.54	0.42
5:SK:4:PRO:HA	25:LA:2146:C:H2'	2.00	0.42
13:SS:4:LEU:HD23	13:SS:4:LEU:H	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:1508:A:H1'	25:LA:1509:A:H3'	2.00	0.42
25:LA:1873:G:H2'	25:LA:1874:C:C6	2.54	0.42
49:L7:135:ILE:HG13	49:L7:136:ILE:H	1.84	0.42
25:LA:2136:G:H2'	25:LA:2137:U:C6	2.54	0.42
25:LA:684:G:C2	25:LA:794:A:C2	3.07	0.42
25:LA:1395:A:C6	25:LA:1398:C:C2	3.07	0.42
25:LA:2048:G:C6	25:LA:2049:G:C5	3.07	0.42
25:LA:2135:A:N6	25:LA:2156:G:H1'	2.34	0.42
25:LA:2201:G:C5	25:LA:2202:U:C4	3.08	0.42
25:LA:2513:A:C2	25:LA:2514:U:C2	3.06	0.42
25:LA:317:G:C6	25:LA:318:C:C4	3.07	0.42
1:SA:409:U:C4	1:SA:410:G:C5	3.07	0.42
25:LA:80:G:H5'	25:LA:346:A:H1'	2.01	0.42
25:LA:309:A:C6	25:LA:330:A:C6	3.08	0.42
25:LA:1114:C:H2'	25:LA:1115:G:C8	2.54	0.42
25:LA:1726:C:C2	25:LA:1735:A:C2	3.08	0.42
25:LA:2492:U:O2'	25:LA:2493:U:C6	2.72	0.42
25:LA:2617:U:O4	25:LA:2618:G:C6	2.72	0.42
36:LU:36:ILE:HG22	36:LU:39:GLN:HG2	2.01	0.42
25:LA:1536:C:H4'	25:LA:1537:G:H5"	2.01	0.42
25:LA:2084:C:C4	25:LA:2085:U:C4	3.08	0.42
1:SA:1218:C:H2'	1:SA:1219:A:C8	2.55	0.42
25:LA:636:G:C5	54:LH:111:ILE:HD12	2.55	0.42
25:LA:952:G:C6	25:LA:953:G:C5	3.07	0.42
26:LB:44:G:H4'	26:LB:46:A:H62	1.84	0.42
26:LB:57:A:H2'	26:LB:58:A:C8	2.55	0.42
52:LF:5:THR:HA	52:LF:44:TYR:CD1	2.54	0.42
1:SA:1133:G:C6	1:SA:1134:G:C5	3.08	0.42
1:SA:1410:A:C2	1:SA:1491:G:C2	3.08	0.42
25:LA:695:G:H5'	25:LA:1380:G:H4'	2.01	0.42
25:LA:1724:G:C6	25:LA:1725:U:C4	3.07	0.42
25:LA:1779:U:H2'	25:LA:1783:A:C6	2.55	0.42
25:LA:2513:A:C6	25:LA:2574:G:C6	3.08	0.42
25:LA:2567:G:H4'	25:LA:2567:G:OP1	2.20	0.42
1:SA:9:G:C2	1:SA:26:A:C2	3.08	0.42
1:SA:718:A:C4	5:SK:117:HIS:CD2	3.08	0.42
1:SA:955:U:C4	1:SA:956:U:C4	3.08	0.42
1:SA:961:U:H3	1:SA:974:A:H61	1.68	0.42
1:SA:1108:G:C5	1:SA:1109:C:C5	3.07	0.42
3:S7:11:C:H2'	3:S7:12:U:C6	2.55	0.42
7:SM:108:ARG:HB2	7:SM:108:ARG:CZ	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:1014:A:C2	25:LA:1149:G:C2	3.08	0.42
25:LA:1135:C:C6	25:LA:1137:G:OP2	2.73	0.42
25:LA:1281:G:H2'	25:LA:1282:U:C6	2.55	0.42
25:LA:1926:U:C5	25:LA:1929:G:C2	3.07	0.42
25:LA:2456:C:C5	25:LA:2457:U:C5	3.08	0.42
49:L7:88:VAL:HG12	49:L7:89:THR:H	1.83	0.42
1:SA:1000:A:C2	1:SA:1041:G:C2	3.08	0.42
1:SA:1083:U:C5	1:SA:1084:G:C6	3.08	0.42
7:SM:26:LYS:HD2	7:SM:27:THR:H	1.84	0.42
24:S1:144:ASP:OD1	59:S1:801:GTP:N1	2.52	0.42
25:LA:572:A:C5	25:LA:573:U:H1'	2.55	0.42
25:LA:2182:U:H2'	25:LA:2183:A:C8	2.55	0.42
1:SA:226:G:C6	1:SA:227:G:C5	3.07	0.41
25:LA:745:G:C2	25:LA:753:A:C2	3.08	0.41
26:LB:30:C:H1'	26:LB:57:A:H61	1.85	0.41
25:LA:649:G:C5	25:LA:650:C:C4	3.08	0.41
1:SA:109:A:C6	1:SA:325:A:N1	2.88	0.41
1:SA:1074:G:C5	1:SA:1075:U:C5	3.08	0.41
31:LP:51:VAL:H	31:LP:54:VAL:HG22	1.85	0.41
1:SA:19:A:C2	1:SA:917:G:C6	3.09	0.41
1:SA:1309:G:C6	1:SA:1310:G:C5	3.09	0.41
15:ST:67:HIS:CD2	15:ST:68:LYS:H	2.38	0.41
25:LA:28:A:C2	25:LA:513:A:H1'	2.56	0.41
25:LA:190:A:C4	25:LA:207:A:C2	3.09	0.41
25:LA:355:U:H2'	25:LA:356:G:C8	2.56	0.41
25:LA:586:A:C5'	47:L6:84:THR:HG21	2.50	0.41
25:LA:1980:G:H3'	25:LA:1981:A:H5"	2.03	0.41
55:LI:126:ILE:HD13	55:LI:126:ILE:H	1.84	0.41
25:LA:571:U:H3	25:LA:2030:C:N4	2.14	0.41
25:LA:1061:U:H1'	25:LA:1070:A:H4'	2.03	0.41
25:LA:2543:G:C2	25:LA:2765:A:C8	3.08	0.41
1:SA:1255:G:C5	1:SA:1279:G:C6	3.08	0.41
25:LA:528:A:C8	25:LA:528:A:H3'	2.56	0.41
25:LA:647:G:C6	25:LA:648:G:C5	3.08	0.41
25:LA:1897:G:C6	25:LA:1898:U:C4	3.09	0.41
25:LA:2584:U:C6	25:LA:2585:U:C6	3.09	0.41
25:LA:2804:U:H2'	25:LA:2805:C:C6	2.56	0.41
1:SA:550:G:C5	1:SA:551:U:C5	3.08	0.41
1:SA:836:G:C6	1:SA:837:U:C2	3.08	0.41
25:LA:745:G:N2	25:LA:753:A:C4	2.89	0.41
25:LA:910:A:C6	25:LA:911:A:C6	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:1065:U:C5	25:LA:1066:U:C5	3.09	0.41
25:LA:2102:G:C5	25:LA:2103:C:C4	3.09	0.41
25:LA:2502:G:H3'	25:LA:2503:A:H5'	2.02	0.41
26:LB:46:A:C5	26:LB:47:C:C4	3.08	0.41
27:LC:27:ILE:HG21	27:LC:185:LEU:HB2	2.03	0.41
1:SA:289:G:C5	1:SA:290:C:C5	3.09	0.41
1:SA:1306:A:C2	1:SA:1332:A:C8	3.09	0.41
1:SA:1401:G:C5	1:SA:1402:C:N3	2.89	0.41
22:SH:4:ASP:CG	22:SH:76:ARG:HH12	2.23	0.41
27:LC:46:VAL:HG13	27:LC:212:VAL:HG22	2.03	0.41
15:ST:63:LYS:HA	15:ST:63:LYS:HD3	1.98	0.41
25:LA:105:C:H2'	25:LA:106:C:C6	2.56	0.41
25:LA:118:A:C8	25:LA:119:A:C8	3.09	0.41
25:LA:483:A:C8	25:LA:484:C:C5	3.09	0.41
25:LA:878:A:C2	25:LA:900:A:N6	2.89	0.41
25:LA:1117:C:H2'	25:LA:1118:C:C6	2.56	0.41
25:LA:1174:U:C4	25:LA:1177:G:C6	3.09	0.41
25:LA:1661:G:C5	25:LA:1662:U:C5	3.09	0.41
25:LA:2270:A:H3'	25:LA:2271:G:H5'	2.03	0.41
25:LA:2450:A:H2'	25:LA:2451:A:C8	2.56	0.41
25:LA:2544:G:C6	25:LA:2545:G:C5	3.09	0.41
1:SA:51:A:H61	1:SA:314:C:H1'	1.86	0.41
1:SA:325:A:C2	1:SA:326:G:H2'	2.56	0.41
1:SA:1503:A:H4'	1:SA:1504:G:OP2	2.21	0.41
24:S1:269:PHE:HB2	59:S1:801:GTP:C8	2.56	0.41
25:LA:524:G:C6	25:LA:525:U:C4	3.09	0.41
25:LA:825:A:C2	25:LA:833:A:C2	3.09	0.41
25:LA:948:C:H3'	25:LA:948:C:C6	2.55	0.41
25:LA:1012:U:N3	25:LA:1143:A:N7	2.69	0.41
25:LA:1107:G:C6	25:LA:1108:U:C4	3.09	0.41
25:LA:1881:C:C5	25:LA:1882:U:C5	3.09	0.41
25:LA:2538:C:H2'	25:LA:2539:C:C6	2.56	0.41
1:SA:811:C:H1'	1:SA:901:A:H61	1.86	0.40
25:LA:527:C:C6	25:LA:2779:U:C5	3.09	0.40
25:LA:2793:C:H2'	25:LA:2794:C:C6	2.55	0.40
49:L7:176:PHE:CG	58:LZ:30:HIS:HB3	2.56	0.40
53:LG:108:ARG:HH22	53:LG:121:GLU:CD	2.24	0.40
1:SA:730:G:C6	1:SA:731:G:H1'	2.56	0.40
1:SA:763:G:H2'	1:SA:764:C:C6	2.56	0.40
1:SA:781:A:H4'	1:SA:1522:U:O2'	2.22	0.40
1:SA:1228:C:H2'	1:SA:1229:A:C8	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LA:194:G:C6	25:LA:195:A:C6	3.09	0.40
25:LA:194:G:O6	25:LA:195:A:C6	2.74	0.40
25:LA:644:A:H2'	25:LA:647:G:C5	2.56	0.40
25:LA:1483:G:C6	25:LA:1484:U:C4	3.09	0.40
25:LA:1532:A:C2	25:LA:1540:G:C2	3.09	0.40
1:SA:32:A:C2	1:SA:553:A:C2	3.09	0.40
1:SA:552:U:H4'	6:SL:83:GLY:O	2.22	0.40
1:SA:1371:G:C5	1:SA:1372:U:C5	3.09	0.40
17:SC:51:VAL:HA	17:SC:69:THR:HA	2.04	0.40
21:SG:57:GLU:H	21:SG:57:GLU:CD	2.25	0.40
24:S1:395:THR:HG21	24:S1:405:LEU:H	1.86	0.40
25:LA:847:U:O4	25:LA:932:U:C6	2.75	0.40
25:LA:1673:G:H2'	25:LA:1674:G:H5"	2.03	0.40
25:LA:1739:A:C6	25:LA:1740:G:C6	3.10	0.40
25:LA:1746:A:C2	25:LA:1747:U:C2	3.10	0.40
25:LA:1897:G:C5	25:LA:1898:U:C4	3.09	0.40
1:SA:1083:U:H3'	1:SA:1084:G:C8	2.56	0.40
1:SA:1250:A:C2	1:SA:1287:A:C6	3.09	0.40
25:LA:460:A:C2	25:LA:470:A:C4	3.10	0.40
25:LA:1995:U:H1'	53:LG:3:GLN:HG2	2.03	0.40
25:LA:2248:C:C5	25:LA:2249:U:C4	3.10	0.40
25:LA:2415:G:C6	25:LA:2416:C:C4	3.10	0.40
25:LA:2574:G:N2	40:LX:148:GLN:HE21	2.20	0.40
25:LA:100:U:O2'	25:LA:101:A:C5	2.75	0.40
25:LA:160:A:C6	25:LA:161:A:C6	3.10	0.40
25:LA:1783:A:C8	25:LA:1783:A:C3'	2.99	0.40
25:LA:2210:U:C5	25:LA:2212:A:C2	3.09	0.40
25:LA:2679:A:C2	25:LA:2729:G:C2	3.10	0.40
26:LB:9:G:C6	26:LB:10:G:C5	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SJ	101/103 (98%)	98 (97%)	0	3 (3%)	4	33
5	SK	126/128 (98%)	104 (82%)	17 (14%)	5 (4%)	3	26
6	SL	121/123 (98%)	109 (90%)	10 (8%)	2 (2%)	9	45
7	SM	115/117 (98%)	101 (88%)	9 (8%)	5 (4%)	2	24
8	SN	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	55
9	SO	86/88 (98%)	83 (96%)	1 (1%)	2 (2%)	6	38
10	SP	80/82 (98%)	72 (90%)	4 (5%)	4 (5%)	2	21
11	SQ	81/83 (98%)	71 (88%)	8 (10%)	2 (2%)	5	36
12	SR	72/74 (97%)	58 (81%)	11 (15%)	3 (4%)	3	25
13	SS	89/91 (98%)	74 (83%)	10 (11%)	5 (6%)	2	19
14	SB	238/240 (99%)	217 (91%)	13 (6%)	8 (3%)	3	31
15	ST	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	13	51
16	SU	68/70 (97%)	52 (76%)	11 (16%)	5 (7%)	1	13
17	SC	230/232 (99%)	212 (92%)	13 (6%)	5 (2%)	6	39
18	SD	203/205 (99%)	177 (87%)	18 (9%)	8 (4%)	3	27
19	SE	164/166 (99%)	149 (91%)	13 (8%)	2 (1%)	13	51
20	SF	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	19	59
21	SG	176/178 (99%)	158 (90%)	15 (8%)	3 (2%)	9	45
22	SH	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	9	46
23	SI	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
24	S1	700/702 (100%)	632 (90%)	45 (6%)	23 (3%)	4	31
27	LC	232/234 (99%)	206 (89%)	19 (8%)	7 (3%)	4	33
28	LM	112/114 (98%)	99 (88%)	10 (9%)	3 (3%)	5	35
29	LN	270/272 (99%)	244 (90%)	16 (6%)	10 (4%)	3	28
30	LO	115/117 (98%)	108 (94%)	4 (4%)	3 (3%)	5	35
31	LP	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	7	41
32	LQ	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17	57
33	LR	98/100 (98%)	84 (86%)	9 (9%)	5 (5%)	2	20
34	LS	101/103 (98%)	89 (88%)	8 (8%)	4 (4%)	3	26
35	LT	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	14	53
36	LU	82/84 (98%)	56 (68%)	15 (18%)	11 (13%)	0	4
37	LV	75/77 (97%)	71 (95%)	4 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	LD	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
39	LW	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
40	LX	207/209 (99%)	168 (81%)	25 (12%)	14 (7%)	1	15
41	LY	56/58 (97%)	52 (93%)	3 (5%)	1 (2%)	8	43
42	L1	54/56 (96%)	47 (87%)	5 (9%)	2 (4%)	3	28
43	L2	52/54 (96%)	44 (85%)	7 (14%)	1 (2%)	8	42
44	L3	44/46 (96%)	39 (89%)	2 (4%)	3 (7%)	1	15
45	L4	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	9	46
46	L5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
47	L6	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	2	23
48	LE	139/141 (99%)	123 (88%)	12 (9%)	4 (3%)	4	33
49	L7	176/178 (99%)	137 (78%)	21 (12%)	18 (10%)	0	7
50	L8	174/176 (99%)	156 (90%)	9 (5%)	9 (5%)	2	20
51	L9	147/149 (99%)	132 (90%)	9 (6%)	6 (4%)	3	26
52	LF	140/142 (99%)	122 (87%)	16 (11%)	2 (1%)	11	48
53	LG	121/123 (98%)	107 (88%)	12 (10%)	2 (2%)	9	45
54	LH	142/144 (99%)	129 (91%)	5 (4%)	8 (6%)	2	19
55	LI	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	47
56	LJ	125/127 (98%)	110 (88%)	9 (7%)	6 (5%)	2	22
57	LK	115/117 (98%)	107 (93%)	5 (4%)	3 (3%)	5	35
58	LZ	68/70 (97%)	56 (82%)	10 (15%)	2 (3%)	4	33
All	All	7019/7125 (98%)	6254 (89%)	534 (8%)	231 (3%)	6	31

All (231) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	SK	125	LYS
7	SM	62	PHE
16	SU	7	GLU
18	SD	48	SER
18	SD	134	TYR
18	SD	192	ALA
24	S1	539	ILE
27	LC	147	PRO
27	LC	220	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	LM	25	VAL
29	LN	140	VAL
33	LR	88	LYS
36	LU	15	SER
36	LU	34	SER
40	LX	43	ASP
40	LX	102	ALA
40	LX	112	THR
40	LX	119	ALA
40	LX	162	ALA
42	L1	8	THR
45	L4	31	ILE
47	L6	13	THR
48	LE	96	LYS
49	L7	122	ASP
49	L7	138	PRO
51	L9	3	VAL
51	L9	15	LEU
51	L9	124	THR
4	SJ	57	VAL
4	SJ	75	ASP
7	SM	3	ILE
7	SM	104	ASN
12	SR	14	ALA
13	SS	84	ALA
14	SB	22	TRP
14	SB	71	THR
14	SB	84	LEU
15	ST	67	HIS
16	SU	3	ILE
16	SU	22	CYS
16	SU	23	GLU
17	SC	156	LEU
18	SD	45	PRO
18	SD	66	VAL
19	SE	23	THR
21	SG	8	GLN
24	S1	75	ALA
24	S1	116	GLY
24	S1	258	ASN
24	S1	390	VAL
24	S1	392	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	S1	495	GLN
24	S1	511	ARG
27	LC	135	GLY
27	LC	200	LYS
29	LN	94	LEU
30	LO	88	GLU
33	LR	2	ILE
33	LR	93	LEU
33	LR	96	VAL
36	LU	52	CYS
40	LX	73	VAL
40	LX	117	GLY
40	LX	166	GLY
42	L1	26	SER
47	L6	45	ALA
47	L6	68	ALA
47	L6	70	SER
47	L6	93	SER
48	LE	113	ALA
49	L7	36	ASN
49	L7	73	VAL
49	L7	79	ARG
49	L7	116	LEU
49	L7	119	LYS
50	L8	7	PRO
51	L9	40	THR
52	LF	21	THR
52	LF	129	GLU
54	LH	21	ARG
54	LH	30	THR
55	LI	58	LYS
56	LJ	10	LEU
56	LJ	13	ASN
57	LK	2	ASP
58	LZ	24	ILE
5	SK	11	VAL
5	SK	13	LYS
5	SK	52	ARG
7	SM	22	TYR
7	SM	111	PRO
9	SO	20	ASP
9	SO	87	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	SP	27	ALA
10	SP	31	ARG
14	SB	19	THR
14	SB	192	PRO
17	SC	59	PRO
17	SC	72	PRO
17	SC	223	PRO
17	SC	229	LYS
18	SD	31	CYS
21	SG	84	TYR
22	SH	91	LEU
24	S1	17	HIS
24	S1	50	ASP
24	S1	52	MET
24	S1	114	ALA
24	S1	293	ALA
24	S1	391	THR
24	S1	524	LEU
27	LC	81	GLY
28	LM	86	LYS
29	LN	43	ASN
29	LN	240	GLY
29	LN	253	GLY
31	LP	91	GLN
35	LT	84	PRO
36	LU	27	GLY
36	LU	41	GLY
40	LX	54	ALA
40	LX	75	ALA
40	LX	149	ASN
44	L3	8	SER
47	L6	44	ARG
48	LE	49	GLU
49	L7	87	LYS
49	L7	175	PRO
50	L8	21	GLN
50	L8	45	ALA
51	L9	38	PRO
53	LG	16	ALA
54	LH	5	THR
54	LH	99	ASN
56	LJ	59	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	LJ	107	ASN
58	LZ	18	CYS
6	SL	116	TYR
6	SL	117	GLY
10	SP	64	GLY
10	SP	79	ASN
11	SQ	31	PRO
12	SR	2	ARG
12	SR	10	CYS
13	SS	34	SER
14	SB	63	LYS
14	SB	205	ALA
18	SD	164	ARG
19	SE	148	SER
24	S1	76	LYS
24	S1	567	GLY
24	S1	608	LYS
27	LC	159	GLY
29	LN	59	GLN
29	LN	88	ALA
31	LP	52	PRO
34	LS	51	LEU
36	LU	68	PHE
38	LD	129	PRO
40	LX	134	HIS
44	L3	42	LEU
49	L7	74	ALA
49	L7	146	ASP
49	L7	148	VAL
50	L8	2	ARG
50	L8	8	VAL
50	L8	29	ASN
54	LH	36	LYS
55	LI	125	PRO
57	LK	45	SER
57	LK	114	GLY
4	SJ	7	ARG
5	SK	14	GLN
13	SS	79	TYR
14	SB	85	SER
16	SU	24	LYS
20	SF	91	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	SG	167	ALA
24	S1	42	VAL
24	S1	178	PHE
28	LM	56	SER
29	LN	7	PRO
32	LQ	89	ALA
33	LR	89	GLU
34	LS	92	VAL
36	LU	13	ARG
36	LU	39	GLN
40	LX	118	PHE
40	LX	173	GLN
41	LY	40	THR
47	L6	59	PRO
48	LE	72	THR
49	L7	66	ILE
49	L7	149	ARG
49	L7	173	ASP
51	L9	122	LEU
54	LH	20	GLY
56	LJ	122	ALA
8	SN	41	TRP
13	SS	33	TRP
13	SS	83	ALA
18	SD	145	ARG
22	SH	53	ASP
24	S1	6	ILE
24	S1	194	ASP
30	LO	100	PHE
36	LU	21	GLY
43	L2	35	LEU
47	L6	46	GLN
49	L7	84	ILE
49	L7	89	THR
49	L7	125	GLY
50	L8	83	THR
54	LH	6	LEU
56	LJ	93	GLY
24	S1	118	VAL
29	LN	77	VAL
30	LO	87	VAL
34	LS	38	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	L6	96	VAL
50	L8	3	VAL
27	LC	130	VAL
53	LG	27	GLY
29	LN	123	ILE
34	LS	102	ILE
36	LU	35	ILE
36	LU	50	VAL
44	L3	44	VAL
11	SQ	64	ARG
50	L8	9	VAL
54	LH	85	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	SJ	90/90 (100%)	89 (99%)	1 (1%)	73	88
5	SK	98/98 (100%)	92 (94%)	6 (6%)	18	53
6	SL	103/103 (100%)	101 (98%)	2 (2%)	57	80
7	SM	95/95 (100%)	89 (94%)	6 (6%)	18	53
8	SN	83/83 (100%)	81 (98%)	2 (2%)	49	75
9	SO	76/76 (100%)	75 (99%)	1 (1%)	69	86
10	SP	65/65 (100%)	65 (100%)	0	100	100
11	SQ	77/77 (100%)	75 (97%)	2 (3%)	46	74
12	SR	64/64 (100%)	62 (97%)	2 (3%)	40	71
13	SS	78/78 (100%)	75 (96%)	3 (4%)	33	66
14	SB	198/198 (100%)	189 (96%)	9 (4%)	27	62
15	ST	65/65 (100%)	64 (98%)	1 (2%)	65	84
16	SU	60/60 (100%)	54 (90%)	6 (10%)	7	35
17	SC	189/189 (100%)	178 (94%)	11 (6%)	20	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	SD	172/172 (100%)	165 (96%)	7 (4%)	30	64
19	SE	125/125 (100%)	118 (94%)	7 (6%)	21	56
20	SF	116/116 (100%)	112 (97%)	4 (3%)	37	69
21	SG	146/146 (100%)	141 (97%)	5 (3%)	37	69
22	SH	104/104 (100%)	99 (95%)	5 (5%)	25	60
23	SI	106/106 (100%)	104 (98%)	2 (2%)	57	80
24	S1	575/575 (100%)	549 (96%)	26 (4%)	27	62
27	LC	181/181 (100%)	171 (94%)	10 (6%)	21	57
28	LM	99/99 (100%)	91 (92%)	8 (8%)	11	43
29	LN	217/217 (100%)	207 (95%)	10 (5%)	27	61
30	LO	89/89 (100%)	84 (94%)	5 (6%)	21	56
31	LP	84/84 (100%)	75 (89%)	9 (11%)	6	32
32	LQ	93/93 (100%)	92 (99%)	1 (1%)	73	88
33	LR	84/84 (100%)	79 (94%)	5 (6%)	19	54
34	LS	84/84 (100%)	80 (95%)	4 (5%)	25	60
35	LT	78/78 (100%)	74 (95%)	4 (5%)	24	58
36	LU	62/62 (100%)	57 (92%)	5 (8%)	11	43
37	LV	67/67 (100%)	65 (97%)	2 (3%)	41	71
38	LD	122/122 (100%)	120 (98%)	2 (2%)	62	83
39	LW	55/55 (100%)	53 (96%)	2 (4%)	35	67
40	LX	164/164 (100%)	157 (96%)	7 (4%)	29	63
41	LY	48/48 (100%)	46 (96%)	2 (4%)	30	63
42	L1	47/47 (100%)	44 (94%)	3 (6%)	17	52
43	L2	48/48 (100%)	48 (100%)	0	100	100
44	L3	38/38 (100%)	36 (95%)	2 (5%)	22	58
45	L4	51/51 (100%)	49 (96%)	2 (4%)	32	65
46	L5	34/34 (100%)	33 (97%)	1 (3%)	42	72
47	L6	165/165 (100%)	160 (97%)	5 (3%)	41	71
48	LE	109/109 (100%)	101 (93%)	8 (7%)	14	46
49	L7	149/149 (100%)	138 (93%)	11 (7%)	13	46
50	L8	137/137 (100%)	130 (95%)	7 (5%)	24	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	L9	114/114 (100%)	106 (93%)	8 (7%)	15	48
52	LF	116/116 (100%)	112 (97%)	4 (3%)	37	69
53	LG	104/104 (100%)	98 (94%)	6 (6%)	20	55
54	LH	103/103 (100%)	98 (95%)	5 (5%)	25	59
55	LI	109/109 (100%)	106 (97%)	3 (3%)	43	72
56	LJ	103/103 (100%)	98 (95%)	5 (5%)	25	59
57	LK	87/87 (100%)	82 (94%)	5 (6%)	20	55
58	LZ	62/62 (100%)	59 (95%)	3 (5%)	25	60
All	All	5788/5788 (100%)	5526 (96%)	262 (4%)	31	62

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SJ	59	LYS
5	SK	6	ARG
5	SK	13	LYS
5	SK	14	GLN
5	SK	15	VAL
5	SK	93	GLU
5	SK	118	ASN
6	SL	69	GLU
6	SL	95	HIS
7	SM	6	ILE
7	SM	26	LYS
7	SM	90	HIS
7	SM	91	ARG
7	SM	108	ARG
7	SM	112	ARG
8	SN	20	PHE
8	SN	78	LEU
9	SO	57	ARG
11	SQ	27	PHE
11	SQ	64	ARG
12	SR	13	THR
12	SR	73	HIS
13	SS	55	GLN
13	SS	80	ARG
13	SS	82	HIS
14	SB	22	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	SB	44	LYS
14	SB	94	ARG
14	SB	103	TRP
14	SB	145	ASN
14	SB	193	ASP
14	SB	207	ARG
14	SB	221	ARG
14	SB	227	ASP
15	ST	35	TYR
16	SU	2	VAL
16	SU	16	ARG
16	SU	23	GLU
16	SU	24	LYS
16	SU	40	PRO
16	SU	55	HIS
17	SC	28	PHE
17	SC	46	LEU
17	SC	107	LYS
17	SC	129	PHE
17	SC	161	ILE
17	SC	184	ASN
17	SC	187	GLU
17	SC	195	ILE
17	SC	214	GLU
17	SC	226	GLN
17	SC	227	GLN
18	SD	28	ASP
18	SD	43	ARG
18	SD	46	ARG
18	SD	49	ASP
18	SD	80	ARG
18	SD	166	LYS
18	SD	194	ILE
19	SE	13	LYS
19	SE	45	VAL
19	SE	75	LEU
19	SE	84	VAL
19	SE	104	ILE
19	SE	151	MET
19	SE	161	GLU
20	SF	35	LYS
20	SF	79	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	SF	91	ARG
20	SF	102	MET
21	SG	36	SER
21	SG	74	VAL
21	SG	82	SER
21	SG	94	ARG
21	SG	163	HIS
22	SH	26	MET
22	SH	60	LEU
22	SH	68	LYS
22	SH	111	THR
22	SH	128	VAL
23	SI	87	MET
23	SI	94	ARG
24	S1	32	TYR
24	S1	50	ASP
24	S1	70	PHE
24	S1	77	GLN
24	S1	99	GLU
24	S1	120	PRO
24	S1	136	ARG
24	S1	152	LYS
24	S1	201	PHE
24	S1	260	ILE
24	S1	307	GLU
24	S1	309	HIS
24	S1	312	ASP
24	S1	368	ASN
24	S1	370	ARG
24	S1	377	ARG
24	S1	380	ASP
24	S1	504	HIS
24	S1	514	TYR
24	S1	520	ASP
24	S1	537	ASN
24	S1	553	ASP
24	S1	582	TYR
24	S1	624	GLU
24	S1	679	TYR
24	S1	681	MET
27	LC	33	LEU
27	LC	108	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	LC	112	ASP
27	LC	121	MET
27	LC	129	GLN
27	LC	136	LEU
27	LC	139	ASN
27	LC	162	ARG
27	LC	174	THR
27	LC	226	GLN
28	LM	19	PHE
28	LM	43	GLU
28	LM	51	ASN
28	LM	52	ARG
28	LM	71	ARG
28	LM	84	SER
28	LM	95	LYS
28	LM	108	ARG
29	LN	49	THR
29	LN	93	VAL
29	LN	145	MET
29	LN	179	GLU
29	LN	200	MET
29	LN	212	TRP
29	LN	217	PRO
29	LN	250	GLN
29	LN	257	ARG
29	LN	263	ASP
30	LO	21	LYS
30	LO	50	ARG
30	LO	63	ARG
30	LO	77	LYS
30	LO	91	ARG
31	LP	22	LEU
31	LP	40	MET
31	LP	48	LYS
31	LP	52	PRO
31	LP	70	GLU
31	LP	79	ARG
31	LP	80	ARG
31	LP	86	GLN
31	LP	95	ASP
32	LQ	22	ASP
33	LR	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	LR	64	LYS
33	LR	66	LYS
33	LR	68	LYS
33	LR	76	ARG
34	LS	27	VAL
34	LS	60	LYS
34	LS	61	GLU
34	LS	78	LYS
35	LT	1	MET
35	LT	53	LYS
35	LT	69	GLU
35	LT	82	TYR
36	LU	19	ARG
36	LU	31	LEU
36	LU	44	PHE
36	LU	49	ASN
36	LU	63	ASP
37	LV	33	HIS
37	LV	77	TYR
38	LD	51	MET
38	LD	68	PHE
39	LW	2	LYS
39	LW	7	ARG
40	LX	2	ILE
40	LX	13	ARG
40	LX	32	ASN
40	LX	73	VAL
40	LX	152	PRO
40	LX	181	ASP
40	LX	194	PRO
41	LY	10	ARG
41	LY	30	ARG
42	L1	8	THR
42	L1	36	LYS
42	L1	45	ASP
44	L3	14	ARG
44	L3	42	LEU
45	L4	7	ARG
45	L4	29	ARG
46	L5	19	ARG
47	L6	12	LEU
47	L6	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	L6	60	TRP
47	L6	78	TRP
47	L6	105	LEU
48	LE	29	GLN
48	LE	34	ILE
48	LE	54	ILE
48	LE	63	ASP
48	LE	81	LYS
48	LE	94	LYS
48	LE	96	LYS
48	LE	134	SER
49	L7	47	LYS
49	L7	91	ARG
49	L7	96	TRP
49	L7	97	GLU
49	L7	116	LEU
49	L7	120	SER
49	L7	122	ASP
49	L7	147	ARG
49	L7	151	LEU
49	L7	174	PHE
49	L7	175	PRO
50	L8	19	ASN
50	L8	21	GLN
50	L8	28	LYS
50	L8	94	ARG
50	L8	115	GLN
50	L8	138	GLN
50	L8	163	TYR
51	L9	8	LYS
51	L9	25	TYR
51	L9	45	GLU
51	L9	97	ARG
51	L9	99	ILE
51	L9	117	LEU
51	L9	133	GLN
51	L9	141	LYS
52	LF	34	ARG
52	LF	71	ASP
52	LF	81	ILE
52	LF	138	GLN
53	LG	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	LG	29	HIS
53	LG	37	ASP
53	LG	41	ILE
53	LG	48	PRO
53	LG	63	VAL
54	LH	48	ARG
54	LH	55	MET
54	LH	64	PHE
54	LH	104	GLN
54	LH	126	ARG
55	LI	31	PHE
55	LI	112	LEU
55	LI	126	ILE
56	LJ	8	ARG
56	LJ	12	ARG
56	LJ	34	ILE
56	LJ	50	PRO
56	LJ	75	ILE
57	LK	3	LYS
57	LK	34	HIS
57	LK	36	TYR
57	LK	49	VAL
57	LK	88	LYS
58	LZ	9	TYR
58	LZ	44	PHE
58	LZ	60	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
5	SK	63	GLN
7	SM	90	HIS
10	SP	9	HIS
10	SP	18	GLN
10	SP	63	GLN
11	SQ	30	HIS
12	SR	73	HIS
12	SR	74	GLN
19	SE	147	ASN
21	SG	152	HIS
24	S1	119	GLN
29	LN	14	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	LN	152	GLN
29	LN	229	HIS
30	LO	43	GLN
33	LR	15	HIS
36	LU	45	HIS
36	LU	56	HIS
38	LD	56	ASN
40	LX	148	GLN
44	L3	16	HIS
45	L4	27	ASN
45	L4	30	HIS
49	L7	62	GLN
50	L8	115	GLN
50	L8	142	GLN
51	L9	135	HIS
52	LF	47	HIS
52	LF	77	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	SA	1542/1542 (100%)	308 (19%)	87 (5%)
2	S6	76/77 (98%)	13 (17%)	4 (5%)
25	LA	2903/2904 (99%)	557 (19%)	141 (4%)
26	LB	119/120 (99%)	20 (16%)	11 (9%)
3	S7	73/74 (98%)	29 (39%)	7 (9%)
All	All	4713/4717 (99%)	927 (19%)	250 (5%)

All (927) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	SA	2	A
1	SA	3	A
1	SA	4	U
1	SA	7	A
1	SA	8	A
1	SA	9	G
1	SA	36	C
1	SA	48	C
1	SA	51	A
1	SA	52	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	53	A
1	SA	54	C
1	SA	60	A
1	SA	61	G
1	SA	69	G
1	SA	73	C
1	SA	83	C
1	SA	98	A
1	SA	108	G
1	SA	120	A
1	SA	121	U
1	SA	123	U
1	SA	129	A
1	SA	131	A
1	SA	135	C
1	SA	153	C
1	SA	164	G
1	SA	166	U
1	SA	171	A
1	SA	174	A
1	SA	182	A
1	SA	183	C
1	SA	184	G
1	SA	188	C
1	SA	189	A
1	SA	197	A
1	SA	198	G
1	SA	200	G
1	SA	209	U
1	SA	211	G
1	SA	212	G
1	SA	225	C
1	SA	228	A
1	SA	244	U
1	SA	245	U
1	SA	247	G
1	SA	250	A
1	SA	251	G
1	SA	252	U
1	SA	262	A
1	SA	266	G
1	SA	267	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	272	C
1	SA	280	C
1	SA	282	A
1	SA	289	G
1	SA	293	G
1	SA	307	C
1	SA	308	C
1	SA	316	C
1	SA	317	U
1	SA	319	G
1	SA	328	C
1	SA	329	A
1	SA	332	G
1	SA	352	C
1	SA	353	A
1	SA	354	G
1	SA	367	U
1	SA	372	C
1	SA	373	A
1	SA	374	A
1	SA	381	C
1	SA	382	A
1	SA	384	G
1	SA	389	A
1	SA	390	U
1	SA	392	C
1	SA	395	C
1	SA	398	U
1	SA	404	G
1	SA	406	G
1	SA	411	A
1	SA	413	G
1	SA	415	A
1	SA	422	C
1	SA	428	G
1	SA	429	U
1	SA	444	G
1	SA	463	U
1	SA	464	U
1	SA	468	A
1	SA	479	U
1	SA	496	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	497	G
1	SA	498	A
1	SA	505	G
1	SA	508	U
1	SA	509	A
1	SA	510	A
1	SA	517	G
1	SA	518	C
1	SA	519	C
1	SA	527	G
1	SA	528	C
1	SA	531	U
1	SA	532	A
1	SA	533	A
1	SA	547	A
1	SA	562	U
1	SA	563	A
1	SA	566	G
1	SA	572	A
1	SA	573	A
1	SA	575	G
1	SA	576	C
1	SA	577	G
1	SA	583	A
1	SA	615	G
1	SA	633	G
1	SA	636	U
1	SA	642	A
1	SA	650	G
1	SA	653	U
1	SA	687	A
1	SA	688	G
1	SA	702	A
1	SA	718	A
1	SA	720	C
1	SA	723	U
1	SA	724	G
1	SA	755	G
1	SA	760	G
1	SA	765	G
1	SA	766	A
1	SA	777	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	783	C
1	SA	790	A
1	SA	791	G
1	SA	792	A
1	SA	793	U
1	SA	794	A
1	SA	805	C
1	SA	810	C
1	SA	812	G
1	SA	815	A
1	SA	816	A
1	SA	817	C
1	SA	818	G
1	SA	819	A
1	SA	820	U
1	SA	821	G
1	SA	828	U
1	SA	829	G
1	SA	841	C
1	SA	842	U
1	SA	843	U
1	SA	845	A
1	SA	846	G
1	SA	870	U
1	SA	873	A
1	SA	874	G
1	SA	876	C
1	SA	889	A
1	SA	890	G
1	SA	900	A
1	SA	910	C
1	SA	914	A
1	SA	926	G
1	SA	927	G
1	SA	933	G
1	SA	938	A
1	SA	939	G
1	SA	945	G
1	SA	959	A
1	SA	960	U
1	SA	961	U
1	SA	962	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	965	U
1	SA	966	G
1	SA	968	A
1	SA	969	A
1	SA	970	C
1	SA	973	G
1	SA	974	A
1	SA	975	A
1	SA	977	A
1	SA	978	A
1	SA	981	U
1	SA	982	U
1	SA	983	A
1	SA	992	U
1	SA	993	G
1	SA	994	A
1	SA	995	C
1	SA	1004	A
1	SA	1006	G
1	SA	1014	A
1	SA	1015	G
1	SA	1028	C
1	SA	1030	U
1	SA	1031	C
1	SA	1045	C
1	SA	1050	G
1	SA	1055	A
1	SA	1064	G
1	SA	1065	U
1	SA	1081	A
1	SA	1094	G
1	SA	1095	U
1	SA	1101	A
1	SA	1118	U
1	SA	1126	U
1	SA	1136	C
1	SA	1137	C
1	SA	1139	G
1	SA	1146	A
1	SA	1149	C
1	SA	1152	A
1	SA	1154	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	1159	U
1	SA	1160	G
1	SA	1168	U
1	SA	1169	A
1	SA	1170	A
1	SA	1181	G
1	SA	1183	U
1	SA	1190	G
1	SA	1196	A
1	SA	1197	A
1	SA	1198	G
1	SA	1200	C
1	SA	1201	A
1	SA	1202	U
1	SA	1208	C
1	SA	1212	U
1	SA	1214	C
1	SA	1215	G
1	SA	1224	U
1	SA	1226	C
1	SA	1227	A
1	SA	1228	C
1	SA	1238	A
1	SA	1241	G
1	SA	1250	A
1	SA	1254	A
1	SA	1257	A
1	SA	1258	G
1	SA	1264	U
1	SA	1268	G
1	SA	1270	G
1	SA	1278	G
1	SA	1279	G
1	SA	1281	C
1	SA	1286	U
1	SA	1287	A
1	SA	1290	G
1	SA	1300	G
1	SA	1301	U
1	SA	1302	C
1	SA	1303	C
1	SA	1305	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	1315	U
1	SA	1319	A
1	SA	1322	C
1	SA	1336	C
1	SA	1340	A
1	SA	1345	U
1	SA	1346	A
1	SA	1347	G
1	SA	1348	U
1	SA	1362	A
1	SA	1363	A
1	SA	1364	U
1	SA	1368	A
1	SA	1378	C
1	SA	1398	A
1	SA	1401	G
1	SA	1419	G
1	SA	1431	A
1	SA	1432	G
1	SA	1437	A
1	SA	1446	A
1	SA	1448	C
1	SA	1452	C
1	SA	1454	G
1	SA	1462	C
1	SA	1466	C
1	SA	1490	U
1	SA	1492	A
1	SA	1493	A
1	SA	1494	G
1	SA	1498	U
1	SA	1499	A
1	SA	1502	A
1	SA	1503	A
1	SA	1504	G
1	SA	1505	G
1	SA	1506	U
1	SA	1520	C
1	SA	1529	G
1	SA	1530	G
1	SA	1533	C
1	SA	1534	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	1535	C
1	SA	1536	C
1	SA	1539	C
1	SA	1540	U
2	S6	8	U
2	S6	10	G
2	S6	18	U
2	S6	19	G
2	S6	20	G
2	S6	22	A
2	S6	38	A
2	S6	48	U
2	S6	49	C
2	S6	50	G
2	S6	75	C
2	S6	76	C
2	S6	77	A
3	S7	4	C
3	S7	8	U
3	S7	9	A
3	S7	14	A
3	S7	16	U
3	S7	17	C
3	S7	18	G
3	S7	20	U
3	S7	21	A
3	S7	22	G
3	S7	26	A
3	S7	32	U
3	S7	35	A
3	S7	36	A
3	S7	37	A
3	S7	38	A
3	S7	39	U
3	S7	42	C
3	S7	44	G
3	S7	45	U
3	S7	49	C
3	S7	50	U
3	S7	57	G
3	S7	58	A
3	S7	61	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S7	62	C
3	S7	63	G
3	S7	70	G
3	S7	74	C
25	LA	18	U
25	LA	30	G
25	LA	34	U
25	LA	35	G
25	LA	42	A
25	LA	46	G
25	LA	49	A
25	LA	63	A
25	LA	71	A
25	LA	74	A
25	LA	75	G
25	LA	91	A
25	LA	100	U
25	LA	101	A
25	LA	102	U
25	LA	103	A
25	LA	113	U
25	LA	115	C
25	LA	119	A
25	LA	120	U
25	LA	126	A
25	LA	128	C
25	LA	140	C
25	LA	163	C
25	LA	164	C
25	LA	181	A
25	LA	194	G
25	LA	196	A
25	LA	197	A
25	LA	204	A
25	LA	205	G
25	LA	215	G
25	LA	216	A
25	LA	220	G
25	LA	222	A
25	LA	224	U
25	LA	225	C
25	LA	232	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	233	A
25	LA	242	G
25	LA	243	U
25	LA	248	G
25	LA	250	G
25	LA	255	A
25	LA	265	A
25	LA	266	G
25	LA	271	G
25	LA	277	G
25	LA	295	G
25	LA	311	A
25	LA	321	U
25	LA	330	A
25	LA	333	G
25	LA	338	G
25	LA	369	U
25	LA	371	A
25	LA	372	G
25	LA	386	G
25	LA	387	U
25	LA	388	G
25	LA	389	G
25	LA	390	U
25	LA	391	A
25	LA	396	G
25	LA	404	A
25	LA	405	U
25	LA	406	G
25	LA	411	G
25	LA	424	G
25	LA	428	A
25	LA	429	A
25	LA	431	U
25	LA	436	C
25	LA	443	A
25	LA	447	A
25	LA	453	A
25	LA	454	A
25	LA	456	C
25	LA	472	A
25	LA	475	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	480	A
25	LA	481	G
25	LA	484	C
25	LA	490	C
25	LA	504	A
25	LA	505	A
25	LA	508	A
25	LA	509	C
25	LA	513	A
25	LA	527	C
25	LA	530	G
25	LA	532	A
25	LA	544	C
25	LA	546	U
25	LA	547	A
25	LA	549	G
25	LA	550	C
25	LA	562	U
25	LA	563	A
25	LA	573	U
25	LA	574	A
25	LA	575	A
25	LA	603	A
25	LA	604	G
25	LA	612	G
25	LA	613	A
25	LA	614	A
25	LA	615	U
25	LA	620	G
25	LA	621	A
25	LA	632	A
25	LA	637	A
25	LA	642	U
25	LA	645	C
25	LA	652	U
25	LA	653	U
25	LA	655	A
25	LA	656	G
25	LA	675	A
25	LA	686	U
25	LA	696	G
25	LA	702	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	718	A
25	LA	719	C
25	LA	728	G
25	LA	730	A
25	LA	732	C
25	LA	736	C
25	LA	746	U
25	LA	747	U
25	LA	748	G
25	LA	752	A
25	LA	758	C
25	LA	763	G
25	LA	775	G
25	LA	776	G
25	LA	782	A
25	LA	784	G
25	LA	786	C
25	LA	789	A
25	LA	792	A
25	LA	802	A
25	LA	805	G
25	LA	812	C
25	LA	829	A
25	LA	846	U
25	LA	847	U
25	LA	848	C
25	LA	859	G
25	LA	870	U
25	LA	894	U
25	LA	896	A
25	LA	897	C
25	LA	901	C
25	LA	910	A
25	LA	915	C
25	LA	925	A
25	LA	932	U
25	LA	938	G
25	LA	941	A
25	LA	945	A
25	LA	946	C
25	LA	961	C
25	LA	973	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	974	G
25	LA	975	A
25	LA	985	C
25	LA	986	C
25	LA	988	A
25	LA	995	C
25	LA	996	A
25	LA	1002	G
25	LA	1003	G
25	LA	1005	C
25	LA	1008	A
25	LA	1009	A
25	LA	1012	U
25	LA	1013	C
25	LA	1022	G
25	LA	1025	G
25	LA	1027	A
25	LA	1044	C
25	LA	1048	A
25	LA	1052	C
25	LA	1060	U
25	LA	1061	U
25	LA	1062	G
25	LA	1067	A
25	LA	1069	A
25	LA	1070	A
25	LA	1073	A
25	LA	1078	U
25	LA	1079	C
25	LA	1081	U
25	LA	1084	A
25	LA	1087	G
25	LA	1094	U
25	LA	1095	A
25	LA	1096	A
25	LA	1097	U
25	LA	1098	A
25	LA	1104	C
25	LA	1109	C
25	LA	1110	G
25	LA	1112	G
25	LA	1128	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	1129	A
25	LA	1132	U
25	LA	1133	A
25	LA	1134	A
25	LA	1143	A
25	LA	1156	A
25	LA	1158	C
25	LA	1173	U
25	LA	1176	U
25	LA	1177	G
25	LA	1178	C
25	LA	1184	U
25	LA	1211	C
25	LA	1212	G
25	LA	1236	G
25	LA	1237	A
25	LA	1238	G
25	LA	1241	A
25	LA	1253	A
25	LA	1254	A
25	LA	1255	U
25	LA	1256	G
25	LA	1266	G
25	LA	1272	A
25	LA	1273	U
25	LA	1274	A
25	LA	1283	G
25	LA	1300	G
25	LA	1301	A
25	LA	1302	A
25	LA	1303	G
25	LA	1307	A
25	LA	1308	A
25	LA	1318	U
25	LA	1321	A
25	LA	1323	C
25	LA	1324	G
25	LA	1327	A
25	LA	1328	A
25	LA	1329	U
25	LA	1332	G
25	LA	1333	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	1341	G
25	LA	1349	C
25	LA	1362	C
25	LA	1363	C
25	LA	1368	G
25	LA	1378	A
25	LA	1379	U
25	LA	1384	A
25	LA	1385	A
25	LA	1386	C
25	LA	1392	A
25	LA	1416	G
25	LA	1417	C
25	LA	1420	A
25	LA	1421	G
25	LA	1429	G
25	LA	1452	G
25	LA	1453	A
25	LA	1458	U
25	LA	1459	G
25	LA	1460	U
25	LA	1461	C
25	LA	1482	G
25	LA	1493	C
25	LA	1494	A
25	LA	1495	A
25	LA	1497	U
25	LA	1508	A
25	LA	1509	A
25	LA	1510	G
25	LA	1514	G
25	LA	1522	A
25	LA	1523	U
25	LA	1524	G
25	LA	1552	A
25	LA	1558	C
25	LA	1565	C
25	LA	1566	A
25	LA	1569	A
25	LA	1578	U
25	LA	1585	C
25	LA	1586	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	1608	A
25	LA	1610	A
25	LA	1612	C
25	LA	1615	C
25	LA	1626	A
25	LA	1634	A
25	LA	1635	A
25	LA	1646	C
25	LA	1648	U
25	LA	1649	G
25	LA	1669	A
25	LA	1670	C
25	LA	1672	A
25	LA	1673	G
25	LA	1674	G
25	LA	1713	A
25	LA	1714	U
25	LA	1715	G
25	LA	1724	G
25	LA	1730	C
25	LA	1737	G
25	LA	1757	A
25	LA	1759	A
25	LA	1762	A
25	LA	1763	G
25	LA	1764	C
25	LA	1773	A
25	LA	1776	G
25	LA	1780	A
25	LA	1781	U
25	LA	1783	A
25	LA	1800	C
25	LA	1808	A
25	LA	1809	A
25	LA	1815	A
25	LA	1816	C
25	LA	1817	G
25	LA	1825	U
25	LA	1830	C
25	LA	1831	G
25	LA	1833	C
25	LA	1851	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	1873	G
25	LA	1889	A
25	LA	1900	A
25	LA	1901	A
25	LA	1913	A
25	LA	1914	C
25	LA	1915	U
25	LA	1917	U
25	LA	1928	A
25	LA	1930	G
25	LA	1937	A
25	LA	1938	A
25	LA	1941	C
25	LA	1943	U
25	LA	1955	U
25	LA	1963	U
25	LA	1964	G
25	LA	1965	C
25	LA	1966	A
25	LA	1967	C
25	LA	1968	G
25	LA	1970	A
25	LA	1971	U
25	LA	1972	G
25	LA	1982	U
25	LA	1993	U
25	LA	1996	C
25	LA	2004	G
25	LA	2012	G
25	LA	2020	A
25	LA	2023	C
25	LA	2030	C
25	LA	2031	A
25	LA	2034	U
25	LA	2043	C
25	LA	2055	C
25	LA	2056	G
25	LA	2059	A
25	LA	2061	G
25	LA	2062	A
25	LA	2069	G
25	LA	2077	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	2092	U
25	LA	2093	G
25	LA	2095	A
25	LA	2107	G
25	LA	2111	U
25	LA	2112	G
25	LA	2113	U
25	LA	2118	U
25	LA	2119	A
25	LA	2126	A
25	LA	2127	G
25	LA	2128	G
25	LA	2130	U
25	LA	2132	U
25	LA	2133	G
25	LA	2134	A
25	LA	2137	U
25	LA	2143	C
25	LA	2144	G
25	LA	2145	C
25	LA	2146	C
25	LA	2147	A
25	LA	2148	G
25	LA	2152	G
25	LA	2153	C
25	LA	2154	A
25	LA	2157	G
25	LA	2158	A
25	LA	2159	G
25	LA	2163	A
25	LA	2164	C
25	LA	2165	C
25	LA	2178	C
25	LA	2198	A
25	LA	2199	A
25	LA	2203	U
25	LA	2204	G
25	LA	2211	A
25	LA	2212	A
25	LA	2214	C
25	LA	2215	C
25	LA	2224	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	2225	A
25	LA	2237	G
25	LA	2238	G
25	LA	2239	G
25	LA	2246	G
25	LA	2249	U
25	LA	2250	G
25	LA	2253	G
25	LA	2266	A
25	LA	2267	A
25	LA	2270	A
25	LA	2271	G
25	LA	2272	U
25	LA	2282	G
25	LA	2283	C
25	LA	2287	A
25	LA	2288	A
25	LA	2305	U
25	LA	2306	C
25	LA	2307	G
25	LA	2308	G
25	LA	2309	A
25	LA	2311	A
25	LA	2312	U
25	LA	2322	A
25	LA	2325	G
25	LA	2333	A
25	LA	2334	U
25	LA	2335	A
25	LA	2336	A
25	LA	2337	G
25	LA	2340	A
25	LA	2345	G
25	LA	2347	C
25	LA	2350	C
25	LA	2354	C
25	LA	2358	A
25	LA	2381	A
25	LA	2383	G
25	LA	2385	C
25	LA	2388	A
25	LA	2389	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	2402	U
25	LA	2406	A
25	LA	2407	A
25	LA	2411	A
25	LA	2426	A
25	LA	2427	C
25	LA	2428	G
25	LA	2429	G
25	LA	2432	A
25	LA	2439	A
25	LA	2441	U
25	LA	2448	A
25	LA	2449	U
25	LA	2450	A
25	LA	2452	C
25	LA	2453	A
25	LA	2470	G
25	LA	2472	G
25	LA	2474	U
25	LA	2476	A
25	LA	2478	A
25	LA	2486	C
25	LA	2491	U
25	LA	2494	G
25	LA	2502	G
25	LA	2503	A
25	LA	2508	G
25	LA	2515	C
25	LA	2516	A
25	LA	2518	A
25	LA	2519	U
25	LA	2529	G
25	LA	2530	A
25	LA	2547	A
25	LA	2553	G
25	LA	2554	U
25	LA	2564	A
25	LA	2565	A
25	LA	2566	A
25	LA	2567	G
25	LA	2572	A
25	LA	2573	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	2581	G
25	LA	2585	U
25	LA	2599	G
25	LA	2602	A
25	LA	2613	U
25	LA	2616	C
25	LA	2629	U
25	LA	2639	A
25	LA	2654	A
25	LA	2655	G
25	LA	2656	U
25	LA	2664	G
25	LA	2685	G
25	LA	2689	U
25	LA	2690	U
25	LA	2714	G
25	LA	2726	A
25	LA	2737	G
25	LA	2739	U
25	LA	2742	G
25	LA	2744	G
25	LA	2757	A
25	LA	2765	A
25	LA	2766	A
25	LA	2769	U
25	LA	2771	C
25	LA	2774	C
25	LA	2777	G
25	LA	2778	A
25	LA	2779	U
25	LA	2780	G
25	LA	2781	A
25	LA	2782	G
25	LA	2791	G
25	LA	2798	U
25	LA	2800	A
25	LA	2807	U
25	LA	2808	G
25	LA	2809	A
25	LA	2820	A
25	LA	2821	A
25	LA	2825	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	2832	U
25	LA	2842	G
25	LA	2849	U
25	LA	2861	U
25	LA	2864	G
25	LA	2867	G
25	LA	2872	A
25	LA	2883	A
25	LA	2884	U
25	LA	2886	A
25	LA	2889	C
25	LA	2893	A
25	LA	2895	G
25	LA	2903	U
25	LA	2904	U
26	LB	6	G
26	LB	9	G
26	LB	12	C
26	LB	13	G
26	LB	25	U
26	LB	26	C
26	LB	35	C
26	LB	41	G
26	LB	44	G
26	LB	45	A
26	LB	51	G
26	LB	57	A
26	LB	58	A
26	LB	66	A
26	LB	67	G
26	LB	73	A
26	LB	88	C
26	LB	89	U
26	LB	90	C
26	LB	99	A

All (250) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	SA	1	A
1	SA	7	A
1	SA	39	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	51	A
1	SA	97	G
1	SA	128	G
1	SA	134	G
1	SA	173	U
1	SA	178	C
1	SA	187	G
1	SA	224	U
1	SA	243	A
1	SA	244	U
1	SA	250	A
1	SA	251	G
1	SA	279	A
1	SA	281	G
1	SA	307	C
1	SA	326	G
1	SA	328	C
1	SA	366	A
1	SA	372	C
1	SA	421	U
1	SA	497	G
1	SA	533	A
1	SA	562	U
1	SA	582	C
1	SA	700	G
1	SA	701	U
1	SA	717	U
1	SA	719	C
1	SA	733	G
1	SA	764	C
1	SA	765	G
1	SA	781	A
1	SA	782	A
1	SA	793	U
1	SA	814	A
1	SA	815	A
1	SA	816	A
1	SA	840	C
1	SA	844	G
1	SA	870	U
1	SA	899	C
1	SA	937	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	SA	944	G
1	SA	960	U
1	SA	964	A
1	SA	965	U
1	SA	968	A
1	SA	976	G
1	SA	992	U
1	SA	993	G
1	SA	1014	A
1	SA	1029	U
1	SA	1159	U
1	SA	1167	A
1	SA	1168	U
1	SA	1190	G
1	SA	1196	A
1	SA	1201	A
1	SA	1207	G
1	SA	1213	A
1	SA	1214	C
1	SA	1226	C
1	SA	1227	A
1	SA	1253	G
1	SA	1278	G
1	SA	1286	U
1	SA	1289	A
1	SA	1302	C
1	SA	1344	C
1	SA	1346	A
1	SA	1347	G
1	SA	1362	A
1	SA	1364	U
1	SA	1430	A
1	SA	1491	G
1	SA	1492	A
1	SA	1498	U
1	SA	1502	A
1	SA	1503	A
1	SA	1529	G
1	SA	1530	G
1	SA	1533	C
1	SA	1534	A
1	SA	1539	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S6	7	G
2	S6	9	G
2	S6	22	A
2	S6	74	A
3	S7	7	A
3	S7	16	U
3	S7	17	C
3	S7	21	A
3	S7	38	A
3	S7	41	C
3	S7	57	G
25	LA	13	A
25	LA	29	U
25	LA	49	A
25	LA	71	A
25	LA	114	U
25	LA	118	A
25	LA	126	A
25	LA	163	C
25	LA	196	A
25	LA	231	A
25	LA	241	A
25	LA	242	G
25	LA	265	A
25	LA	332	A
25	LA	368	A
25	LA	386	G
25	LA	387	U
25	LA	428	A
25	LA	453	A
25	LA	479	A
25	LA	527	C
25	LA	529	A
25	LA	545	U
25	LA	547	A
25	LA	548	G
25	LA	561	G
25	LA	603	A
25	LA	611	C
25	LA	620	G
25	LA	631	A
25	LA	644	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	651	G
25	LA	652	U
25	LA	735	A
25	LA	805	G
25	LA	846	U
25	LA	847	U
25	LA	900	A
25	LA	974	G
25	LA	982	C
25	LA	1012	U
25	LA	1061	U
25	LA	1069	A
25	LA	1085	A
25	LA	1133	A
25	LA	1142	A
25	LA	1157	G
25	LA	1176	U
25	LA	1210	G
25	LA	1211	C
25	LA	1254	A
25	LA	1282	U
25	LA	1286	A
25	LA	1327	A
25	LA	1328	A
25	LA	1329	U
25	LA	1332	G
25	LA	1340	U
25	LA	1348	C
25	LA	1386	C
25	LA	1395	A
25	LA	1402	U
25	LA	1416	G
25	LA	1460	U
25	LA	1508	A
25	LA	1509	A
25	LA	1510	G
25	LA	1523	U
25	LA	1608	A
25	LA	1634	A
25	LA	1723	G
25	LA	1762	A
25	LA	1764	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	1781	U
25	LA	1784	A
25	LA	1807	G
25	LA	1888	G
25	LA	1900	A
25	LA	1914	C
25	LA	1927	A
25	LA	1938	A
25	LA	1940	U
25	LA	1944	U
25	LA	1954	G
25	LA	1955	U
25	LA	2022	U
25	LA	2030	C
25	LA	2042	A
25	LA	2055	C
25	LA	2068	U
25	LA	2076	U
25	LA	2092	U
25	LA	2106	U
25	LA	2118	U
25	LA	2133	G
25	LA	2145	C
25	LA	2146	C
25	LA	2162	G
25	LA	2198	A
25	LA	2211	A
25	LA	2213	U
25	LA	2223	G
25	LA	2225	A
25	LA	2236	U
25	LA	2238	G
25	LA	2249	U
25	LA	2271	G
25	LA	2282	G
25	LA	2287	A
25	LA	2305	U
25	LA	2307	G
25	LA	2308	G
25	LA	2311	A
25	LA	2336	A
25	LA	2385	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	LA	2402	U
25	LA	2425	A
25	LA	2430	A
25	LA	2439	A
25	LA	2440	C
25	LA	2448	A
25	LA	2452	C
25	LA	2468	A
25	LA	2473	U
25	LA	2515	C
25	LA	2564	A
25	LA	2571	U
25	LA	2585	U
25	LA	2602	A
25	LA	2655	G
25	LA	2663	G
25	LA	2756	U
25	LA	2765	A
25	LA	2797	U
25	LA	2806	C
25	LA	2808	G
25	LA	2818	U
25	LA	2832	U
25	LA	2835	A
25	LA	2849	U
25	LA	2861	U
26	LB	11	C
26	LB	12	C
26	LB	25	U
26	LB	34	A
26	LB	36	C
26	LB	44	G
26	LB	57	A
26	LB	66	A
26	LB	87	U
26	LB	108	A
26	LB	109	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
59	GTP	S1	801	-	26,34,34	1.81	3 (11%)	32,54,54	2.02	8 (25%)

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
59	GTP	S1	801	-	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	S1	801	GTP	C5-C6	-6.84	1.33	1.47
59	S1	801	GTP	C5-C4	-3.59	1.33	1.43
59	S1	801	GTP	O4'-C1'	2.02	1.43	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	S1	801	GTP	PB-O3B-PG	-6.78	109.56	132.83
59	S1	801	GTP	PA-O3A-PB	-3.75	119.94	132.83
59	S1	801	GTP	C2-N1-C6	-3.73	118.24	125.10
59	S1	801	GTP	C5-C6-N1	3.17	119.55	113.95
59	S1	801	GTP	C8-N7-C5	2.69	108.12	102.99
59	S1	801	GTP	O3G-PG-O2G	2.30	116.41	107.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	S1	801	GTP	C3'-C2'-C1'	2.08	104.10	100.98
59	S1	801	GTP	N1-C2-N3	-2.07	119.46	123.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

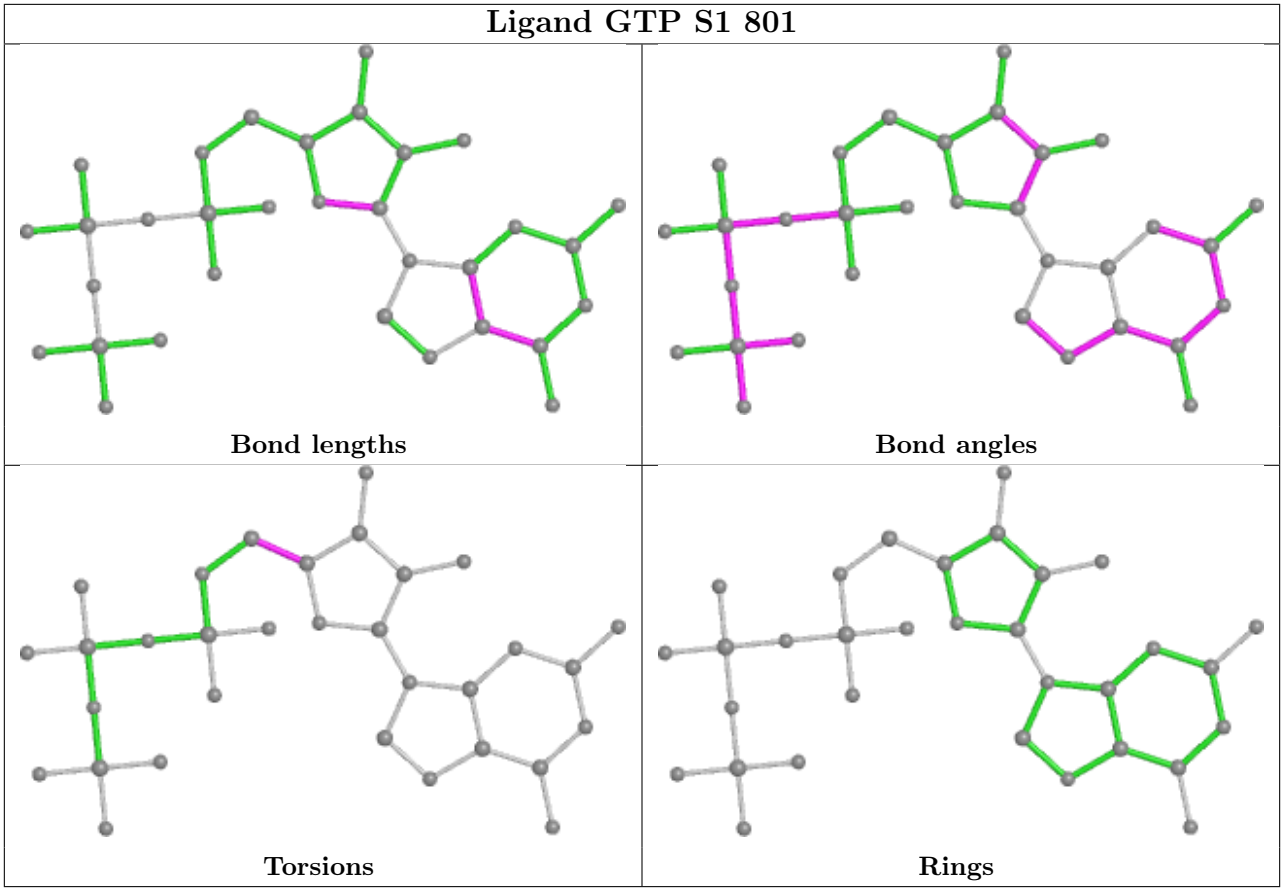
Mol	Chain	Res	Type	Atoms
59	S1	801	GTP	O4'-C4'-C5'-O5'
59	S1	801	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	S1	801	GTP	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

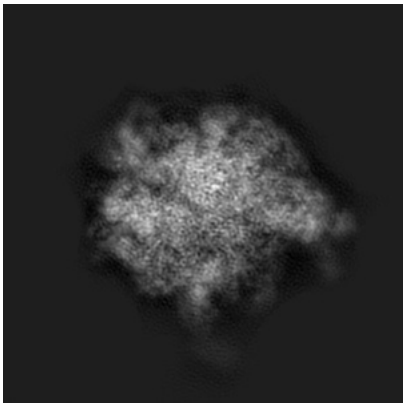
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6315. These allow visual inspection of the internal detail of the map and identification of artifacts.

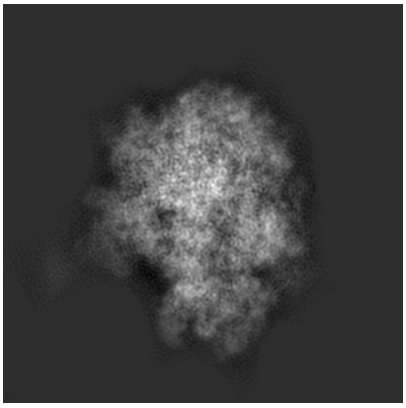
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

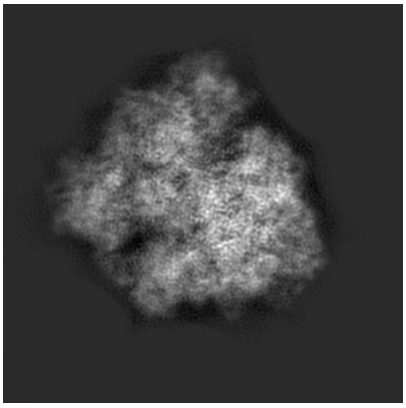
6.1.1 Primary map



X



Y

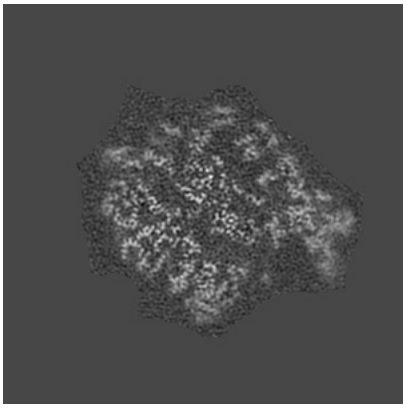


Z

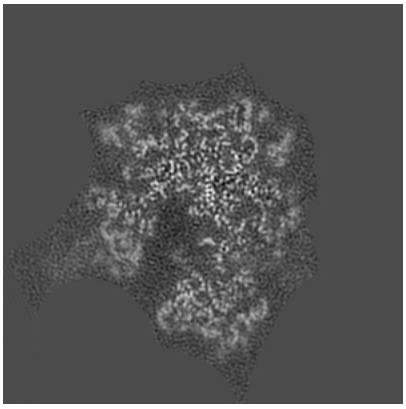
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

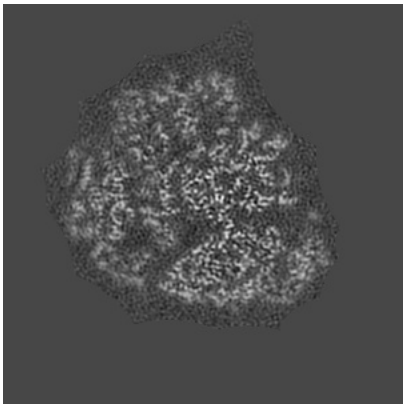
6.2.1 Primary map



X Index: 180



Y Index: 180

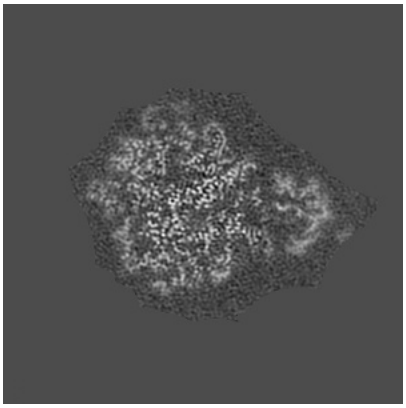


Z Index: 180

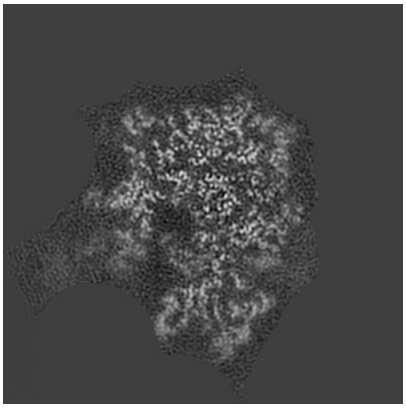
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

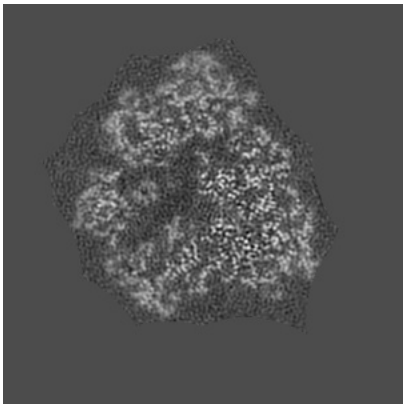
6.3.1 Primary map



X Index: 201



Y Index: 187

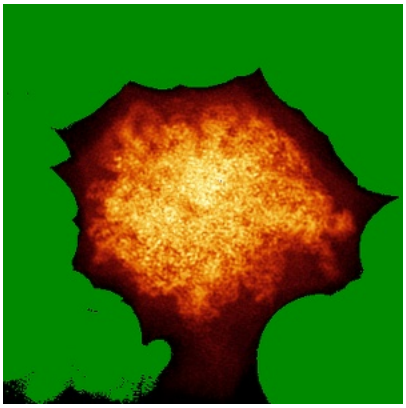


Z Index: 164

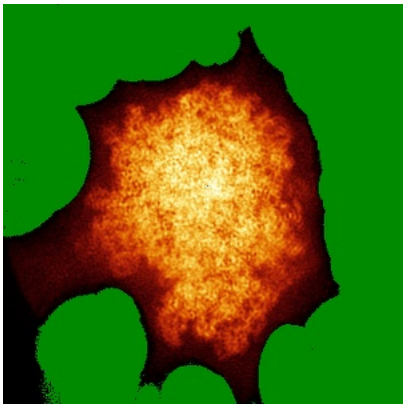
The images above show the largest variance slices of the map in three orthogonal directions.

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

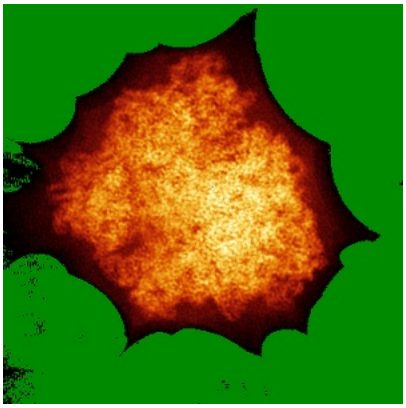
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

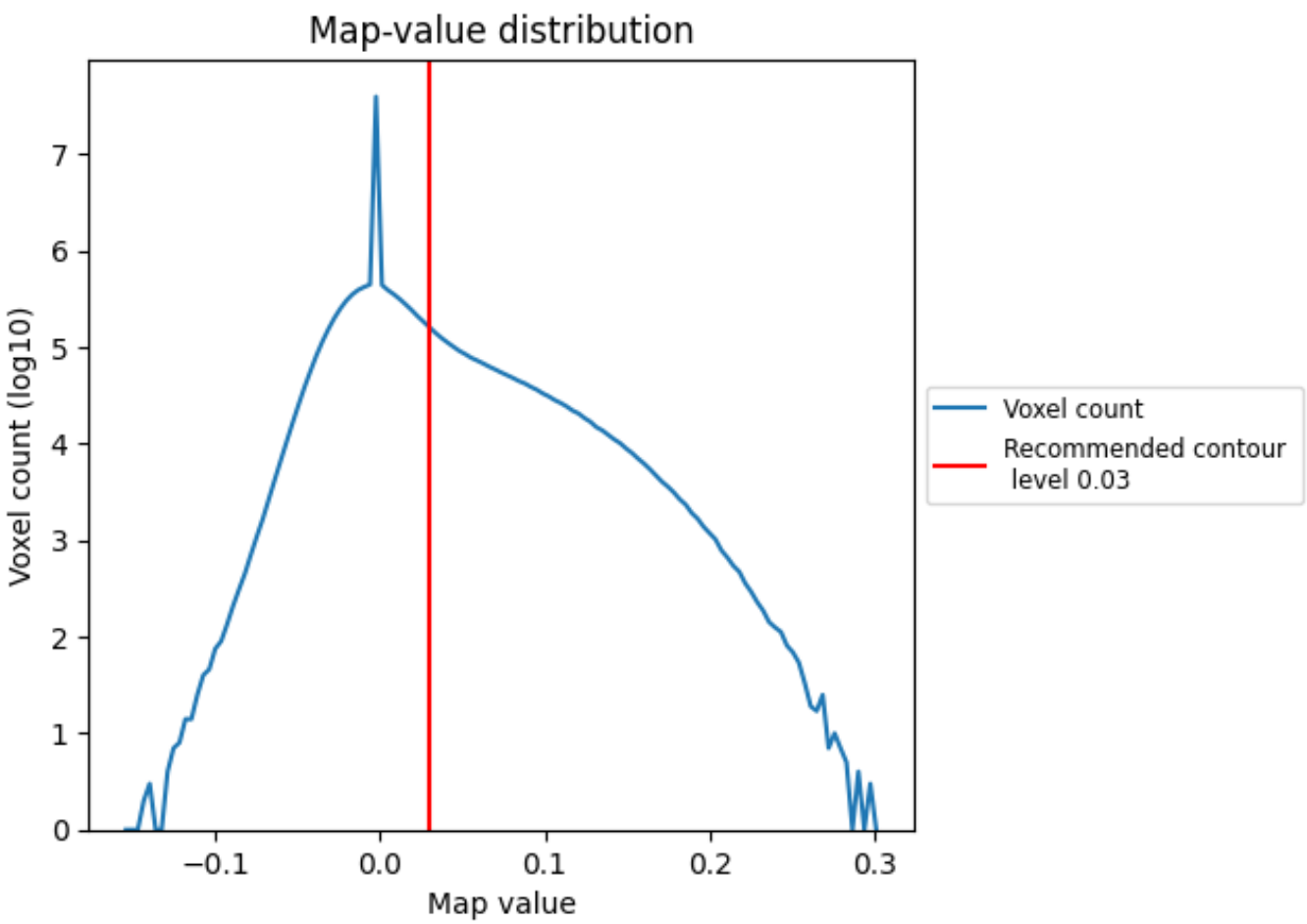
6.6 Mask visualisation (i)

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

7 Map analysis (i)

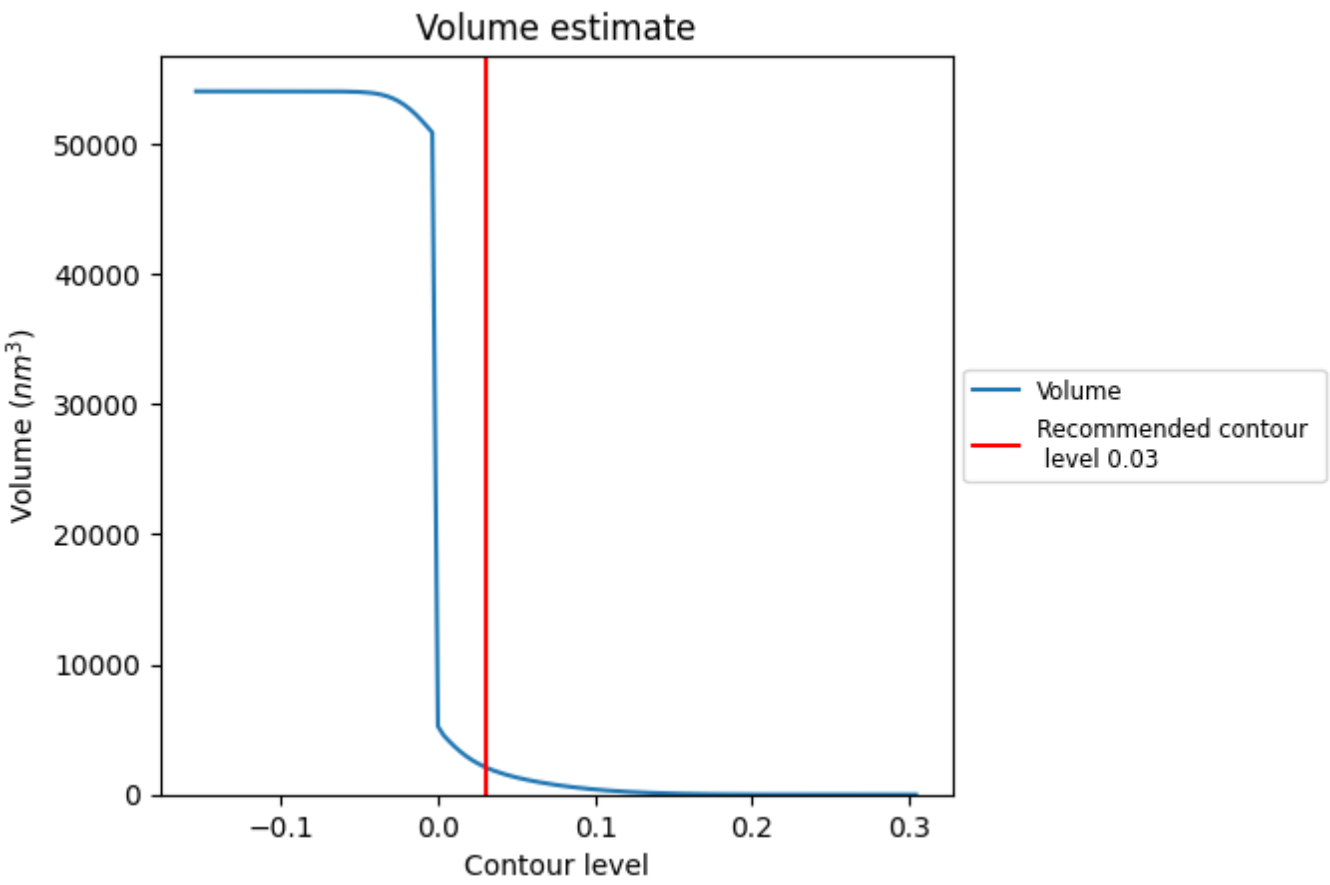
This section contains the results of statistical analysis of the map.

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.

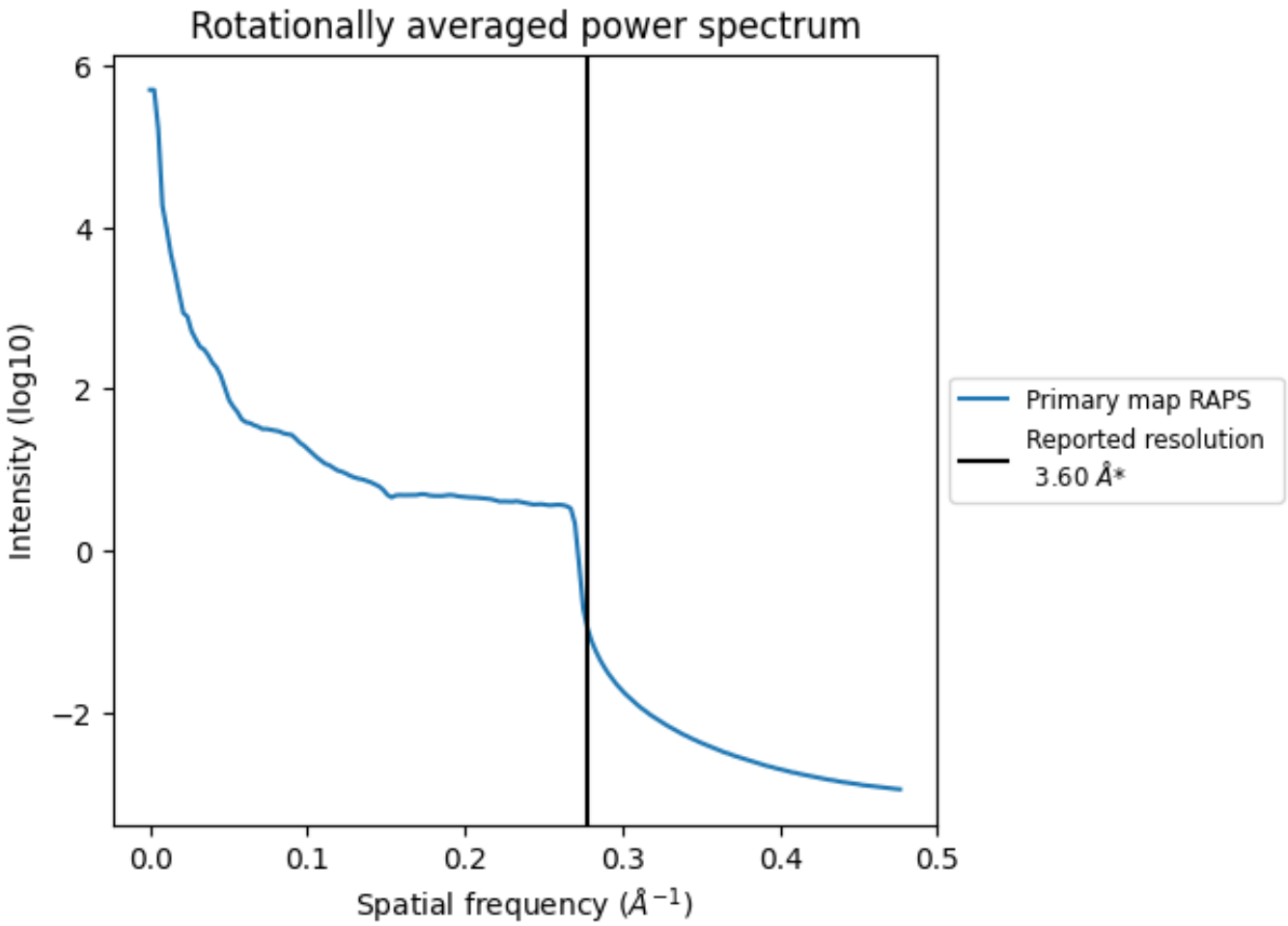
7.2 Volume estimate (i)



The volume at the recommended contour level is 2119 nm^3; this corresponds to an approximate mass of 1915 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 0.278 Å^{-1}

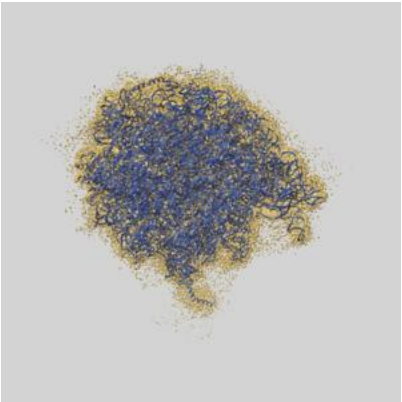
8 Fourier-Shell correlation (i)

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

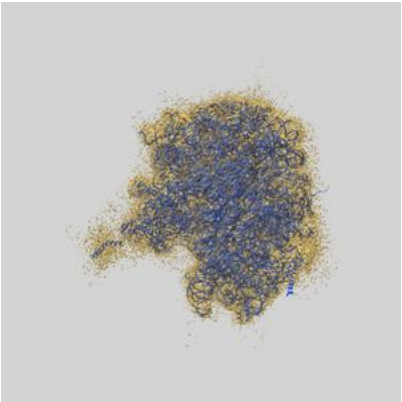
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6315 and PDB model 3J9Z. Per-residue inclusion information can be found in section 3 on page 16.

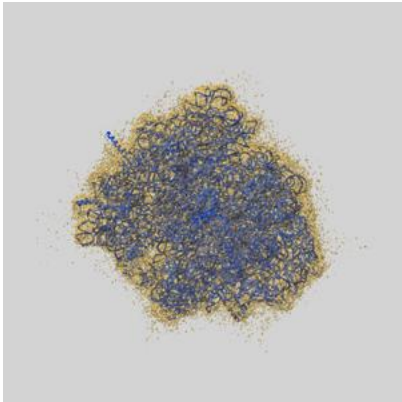
9.1 Map-model overlay (i)



X



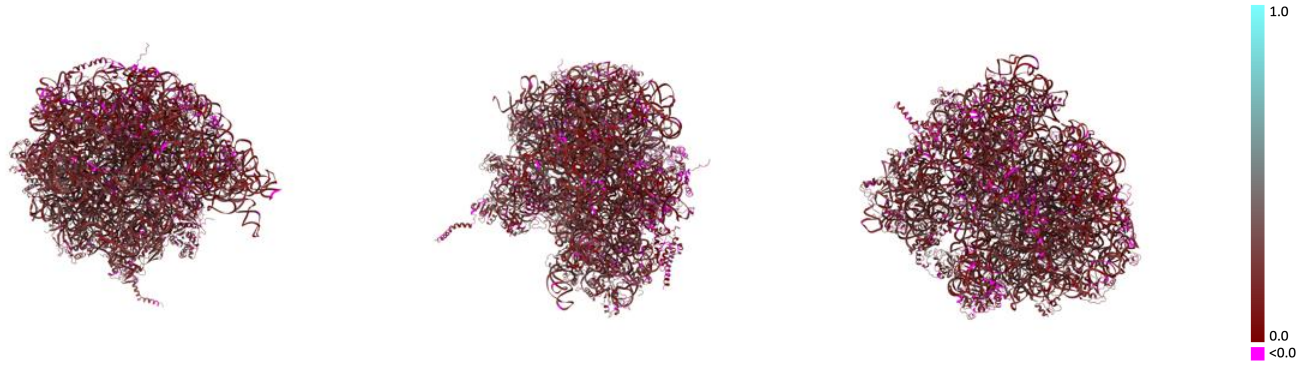
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

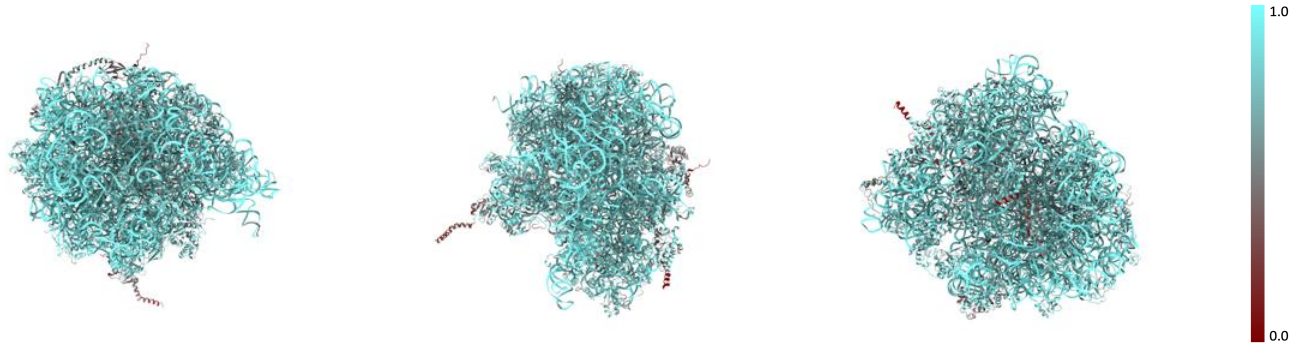
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

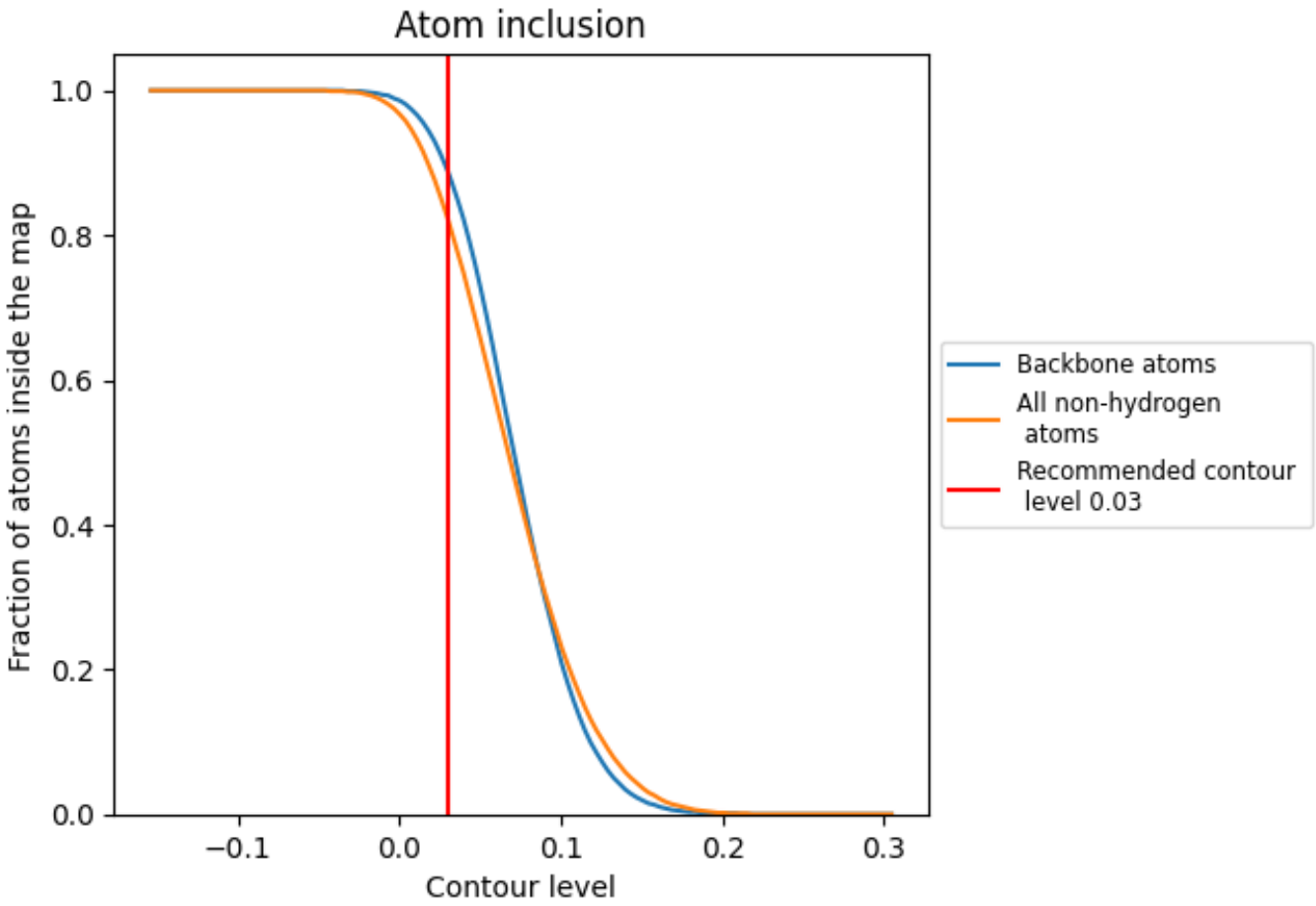
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.1940
L1	0.7380	0.1660
L2	0.7570	0.2300
L3	0.6760	0.1490
L4	0.7720	0.2340
L5	0.7880	0.2560
L6	0.7570	0.1840
L7	0.8160	0.2540
L8	0.8020	0.2460
L9	0.5100	0.1070
LA	0.8750	0.2050
LB	0.9630	0.2750
LC	0.6100	0.1060
LD	0.4940	0.1870
LE	0.7120	0.1980
LF	0.7910	0.2260
LG	0.6440	0.1730
LH	0.7810	0.2110
LI	0.8080	0.2900
LJ	0.6830	0.1270
LK	0.8530	0.2540
LM	0.6860	0.1430
LN	0.6740	0.1470
LO	0.7950	0.2170
LP	0.7880	0.2220
LQ	0.7140	0.1760
LR	0.6780	0.1130
LS	0.7900	0.1340
LT	0.8500	0.3110
LU	0.7280	0.2380
LV	0.7350	0.1800
LW	0.6800	0.0770
LX	0.7220	0.1850
LY	0.7990	0.2660
LZ	0.6410	0.1850

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	0.7010	0.1850
S6	0.8650	0.2260
S7	0.8100	0.1550
SA	0.8840	0.1920
SB	0.6410	0.1240
SC	0.6850	0.1890
SD	0.7720	0.1700
SE	0.6680	0.1570
SF	0.5730	0.0870
SG	0.7070	0.1740
SH	0.7160	0.1140
SI	0.7600	0.1720
SJ	0.7000	0.1970
SK	0.6910	0.1670
SL	0.7130	0.1850
SM	0.7940	0.2500
SN	0.8000	0.2190
SO	0.6800	0.0970
SP	0.7580	0.1140
SQ	0.6980	0.1110
SR	0.6760	0.1380
SS	0.7610	0.2490
ST	0.7270	0.1220
SU	0.5980	0.1600