

Supplementary Material

ATOM	1	O5*	A	A	1	-2.782	7.087	1.372	1.00	0.00
ATOM	2	O3*	A	A	1	-0.635	8.754	-1.756	1.00	0.00
ATOM	3	C1*	A	A	1	0.552	6.337	-1.486	1.00	0.00
ATOM	4	C2*	A	A	1	-0.984	6.307	-1.734	1.00	0.00
ATOM	5	C3*	A	A	1	-1.249	7.682	-1.095	1.00	0.00
ATOM	6	C4*	A	A	1	-0.616	7.377	0.267	1.00	0.00
ATOM	7	C5*	A	A	1	-1.473	6.524	1.192	1.00	0.00
ATOM	8	O4*	A	A	1	0.604	6.639	-0.086	1.00	0.00
ATOM	9	O2*	A	A	1	-1.195	6.272	-3.114	1.00	0.00
ATOM	10	N6	A	A	1	4.768	2.223	-2.774	1.00	0.00
ATOM	11	C6	A	A	1	4.300	3.307	-2.129	1.00	0.00
ATOM	12	C5	A	A	1	2.985	3.781	-2.282	1.00	0.00
ATOM	13	N7	A	A	1	1.907	3.304	-3.004	1.00	0.00
ATOM	14	C8	A	A	1	0.969	4.149	-2.749	1.00	0.00
ATOM	15	N9	A	A	1	1.335	5.182	-1.917	1.00	0.00
ATOM	16	C4	A	A	1	2.644	4.905	-1.584	1.00	0.00
ATOM	17	N3	A	A	1	3.424	5.606	-0.747	1.00	0.00
ATOM	18	C2	A	A	1	4.626	5.060	-0.669	1.00	0.00
ATOM	19	N1	A	A	1	5.108	3.984	-1.301	1.00	0.00
ATOM	20	H1*	A	A	1	0.957	7.233	-1.987	1.00	0.00
ATOM	21	H2*	A	A	1	-1.458	5.511	-1.161	1.00	0.00
ATOM	22	H3*	A	A	1	-2.312	7.880	-1.001	1.00	0.00
ATOM	23	H4*	A	A	1	-0.432	8.332	0.739	1.00	0.00
ATOM	24	H5*	A	A	1	-0.975	6.413	2.157	1.00	0.00
ATOM	25	1H	A	A	1	-1.602	5.524	0.760	1.00	0.00
ATOM	26	1H6	A	A	1	5.743	1.919	-2.645	1.00	0.00
ATOM	27	2H6	A	A	1	4.151	1.704	-3.417	1.00	0.00
ATOM	28	H8	A	A	1	-0.041	4.062	-3.151	1.00	0.00
ATOM	29	H2	A	A	1	5.323	5.546	0.012	1.00	0.00
ATOM	30	P	U	A	2	-1.198	10.187	-2.065	1.00	0.00
ATOM	31	O1P	U	A	2	-2.311	10.543	-1.132	1.00	0.00
ATOM	32	O2P	U	A	2	-0.082	11.180	-2.059	1.00	0.00
ATOM	33	O5*	U	A	2	-1.782	10.110	-3.544	1.00	0.00
ATOM	34	C5*	U	A	2	-2.066	8.922	-4.289	1.00	0.00
ATOM	35	C4*	U	A	2	-3.527	8.525	-4.121	1.00	0.00
ATOM	36	O4*	U	A	2	-3.767	7.273	-4.856	1.00	0.00
ATOM	37	C3*	U	A	2	-3.999	8.264	-2.700	1.00	0.00
ATOM	38	O3*	U	A	2	-5.143	9.021	-2.354	1.00	0.00
ATOM	39	C2*	U	A	2	-4.220	6.756	-2.666	1.00	0.00
ATOM	40	O2*	U	A	2	-5.228	6.369	-1.768	1.00	0.00
ATOM	41	C1*	U	A	2	-4.804	6.630	-4.104	1.00	0.00
ATOM	42	N1	U	A	2	-5.176	5.278	-4.483	1.00	0.00
ATOM	43	C2	U	A	2	-4.279	4.479	-5.149	1.00	0.00
ATOM	44	O2	U	A	2	-3.146	4.843	-5.427	1.00	0.00
ATOM	45	N3	U	A	2	-4.710	3.213	-5.481	1.00	0.00
ATOM	46	C4	U	A	2	-5.953	2.661	-5.210	1.00	0.00
ATOM	47	O4	U	A	2	-6.234	1.515	-5.561	1.00	0.00
ATOM	48	C5	U	A	2	-6.835	3.558	-4.502	1.00	0.00
ATOM	49	C6	U	A	2	-6.438	4.793	-4.172	1.00	0.00
ATOM	50	H5*	U	A	2	-1.855	9.085	-5.349	1.00	0.00
ATOM	51	1H	U	A	2	-1.431	8.099	-3.947	1.00	0.00
ATOM	52	H4*	U	A	2	-4.137	9.344	-4.498	1.00	0.00
ATOM	53	H3T	U	A	2	-3.224	8.561	-1.984	1.00	0.00
ATOM	54	H2*	U	A	2	-3.277	6.218	-2.571	1.00	0.00
ATOM	55	H1*	U	A	2	-5.643	7.342	-4.193	1.00	0.00

[illegible]