Supplemental Material to Accompany:

The influence of sequence and covalent modifications on yeast tRNA dynamics

Xiaoju Zhang,[1] Ross C. Walker,[2,3] Eric M. Phizicky,[1] and David H. Mathews[1]

[1]Department of Biochemistry and Biophysics and Center for RNA Biology, University of Rochester Medical Center, Rochester, New York
[2]San Diego Supercomputer Center, University of California San Diego, 9500 Gilman Drive, La Jolla, California, 92093-0505, USA.
[3]Department of Chemistry and Biochemistry, University of California San Diego, 9500 Gilman Drive, La Jolla, California, 92093

Figure S1a. tRNA^{Asp}

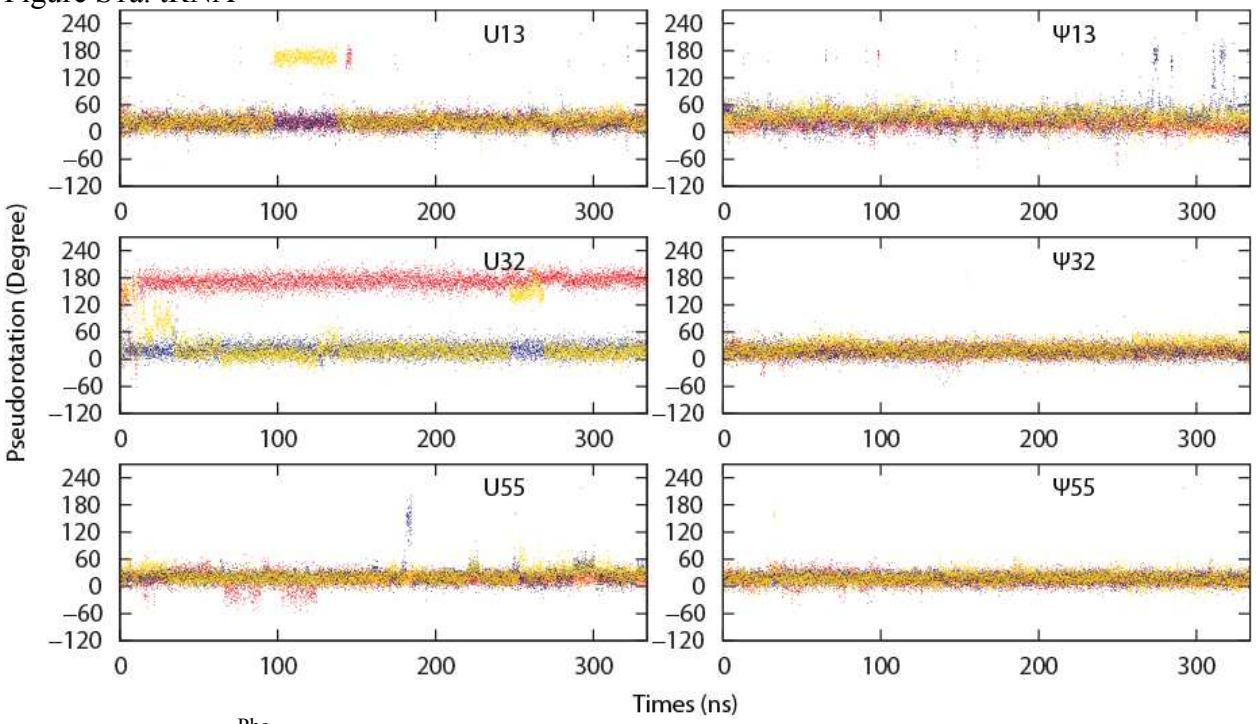

Figure S1b. tRNA^{Phe}

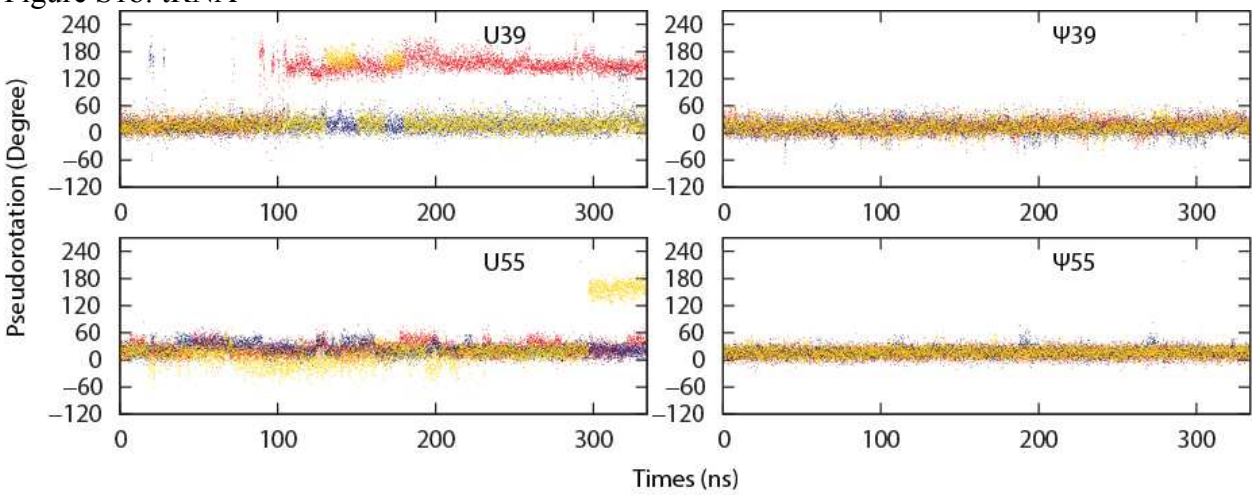

Figure S1. Sugar pucker pseudorotation values as function of time for U or Ψ base. a). The left column shows unmodified tRNA^{Asp}, and the right column shows corresponding modified tRNA^{Asp}. From top to bottom, plots for bases at position 13, 32 and 55 are listed, and each panel has three independent trajectories plotted, in red, yellow or blue. b). The left column shows unmodified tRNA^{Phe}, and the right column shows corresponding modified tRNA^{Phe}. From top to bottom, plots for bases at position 39 and 55 are listed, and each panel has three independent trajectories plotted, colored with red, yellow or blue.

Figure S2a. tRNA^{Asp}

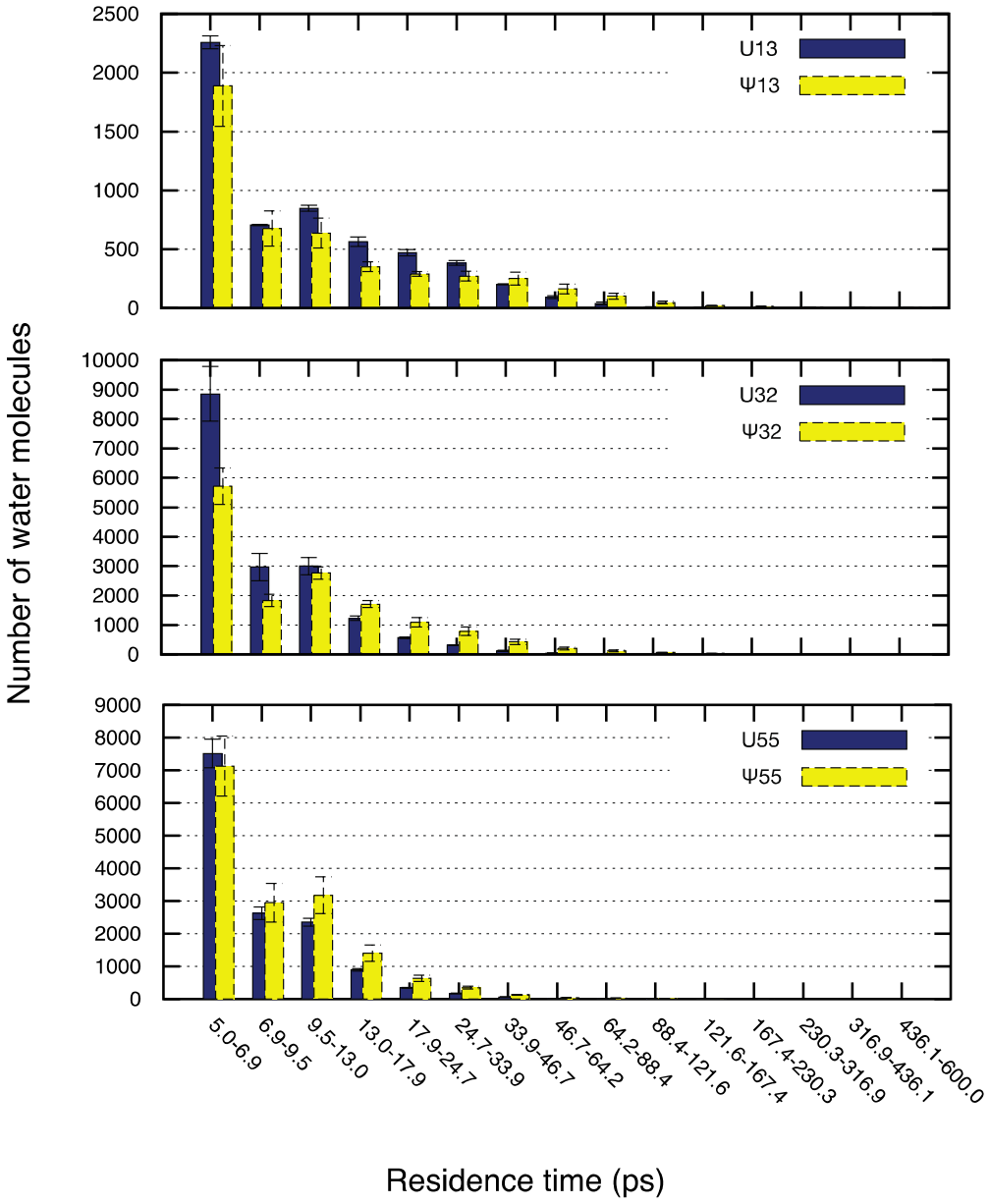

Figure S2b. tRNA^{Phe}

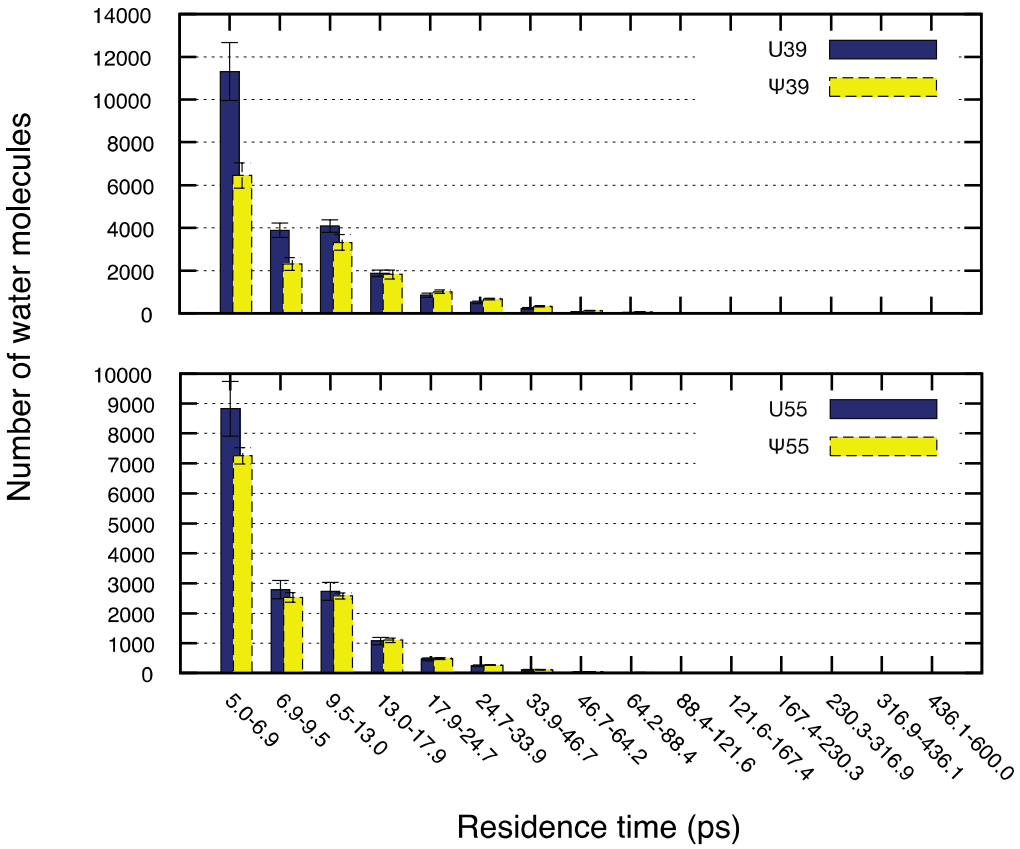

Figure S2. The averaged distribution of U or Ψ base water residence time with the full range of residence times. The frequency is averaged from three trajectories of each molecule, and the error bars represent standard error. a). From top to bottom, plots for bases at position 13, 32 and 55 of tRNA^{Asp} are provided, with unmodified tRNA^{Asp} plotted in blue and modified tRNA^{Asp} plotted in yellow. b). From top to bottom, plots for bases at position 39 and 55 tRNA^{Phe} are provided, with unmodified tRNA^{Phe} plotted in blue and modified tRNA^{Phe} plotted in yellow.

Supplemental Table 1 Missing parameter assignments

Bond Parameters

bond	k_r[a]	r_{eq}[b]	source
N* - CQ	470.3	1.35	GAFF: ca-na
N* - CA	426	1.38	GAFF: n -cd[i]
NA - CM	426	1.38	GAFF: cd-n
CA - N	372.3	1.422	GAFF: ca-n
N* - CC	390.5	1.407	GAFF: c2-n
CC - CC	589.7	1.324	GAFF: c2-c2
P - HO	300	2.12	See note[j]

Angle Parameters

angle	k_θ[c]	θ_{eq}[d]	source
CB - C - N*	70.2	111.86	GAFF: cd-c -na/n
CB - C - N	70.2	111.86	GAFF: cd-c -n
C - N* - CQ	65.3	125.2	GAFF: c -na-ca
N - C - N*	75.4	111.7	GAFF: n -c -na/n
N* - CQ - NC	69.7	123.86	GAFF: na/n -ca-nc
N* - CQ - H5	51.3	119.23	GAFF: h5-ca-nb and h5-ca-nc[j]
CT - N* - CQ	63.1	124.36	GAFF: c3 - na - ca
C - N* - CA	65.2	124.19	GAFF: c -n -cd
N* - CA - NC	70.9	123.86	GAFF: n -cd-nc
N* - CA - N2	72.2	117.01	GAFF: n -cd-nh
CT - N* - CA	63.3	121.17	GAFF: c3-n -cd
CT - CM - CA	64.7	115.97	GAFF: c3-cd-cd
N* - CK - N*	73.7	109.33	GAFF: na-c2-na
N* - CB - C	64.3	130.8	GAFF: c -cc-nc
CT - N* - CT	62.7	119.26	GAFF: c3-na-c3 and c3-n -c3[j]
N* - C - N	75.4	111.7	GAFF: n -c -n
C - N - C	67.4	119.63	GAFF: c -n -c
CT - N2 - CT	63.5	114.54	GAFF: c3-nh-c3
NA - CM - CM	67.9	119.89	GAFF: cd-cd-n
NA - CM - H4	50.4	117.62	GAFF: h4-cd-n
NA - C - NA	75.4	111.7	GAFF: n -c -n
H - NA - CM	47.5	121.52	GAFF: cd-n -hn
CM - NA - C	65.2	124.19	GAFF: c -n -cd
CB - CA - N	68	119.89	GAFF: ca-ca-n
CA - N - C	64.3	123.71	GAFF: c -n -ca
CA - N - H	47.6	114.59	GAFF: ca-n -hn

N - CA - NC	71.6	123.8	GAFF: nb-ca-nb, nb-ca-nc and nb-ca-nh[j]
N - C - N	75.4	111.7	GAFF: n -c -n
OH - C - O2	77.4	122.88	GAFF: o -c -oh
N* - CB - N*	74.2	107.38	GAFF: na-c2-na and n -c2-na[j]
C - N* - CB	64.3	125.09	GAFF: c -na-c2
C - N* - CC	64.3	125.09	GAFF: c -na-c2
N* - CB - NB	71.7	123.62	GAFF: n2-c2-na
N* - CC - CC	69.8	121.38	GAFF: c2-c2-na
N* - CC - CT	65	122.54	GAFF: c3-c2-na
CB - N* - CC	67.8	110.37	GAFF: c2-na-c2
CB - N* - CB	67.8	110.37	GAFF: c2-na-c2
CB - NB - CC	70.8	118.18	GAFF: c2-n2-c2
NB - CC - CC	71.3	126.01	GAFF: c2-c2-n2
CT - CC - CC	64.3	123.42	GAFF: c2-c2-c3
N - C - OS	74.7	115.25	GAFF: n -c -os
P - HO - OH	0	0	See note[k]
O2 - P - HO	0	0	See note[k]
OS - P - HO	0	0	See note[k]
OH - P - HO	0	0	See note[k]

Dihedral Parameters

dihedral	no. of paths[e]	Magnitude[f]	phase offset[g]	Periodicity[h]	source
X -N*-CQ- X	4	1.2	180	2	GAFF: X -ca-na-X
X -N*-CA- X	4	6.6	180	2	GAFF: X -n -cd-X
X -NA-CM- X	4	6.6	180	2	GAFF: X -n -cc-X
X -CA-N - X	4	1.8	180	2	GAFF: X -ca-n -X
X -N*-CC- X	4	2.6	180	2	GAFF: X -c2-n -X
X -CC-CC- X	4	26.6	180	2	GAFF: X -c2-c2-X
OS-P -HO-OH	2	0	0	2	See note[k]
O2-P -HO-OH	2	0	0	2	See note[k]

[a] Bond force constant in kcal/(mol Å^2). [b] Bond equilibrium value in Å. [c] Angle force constant in kcal/(mol radian^2). [d] Angle equilibrium value in degrees. [e] Number of bond paths that the total magnitude of torsion is divided into, which is equal to the product of the number of bonds to each of the middle two atoms. [f] Magnitude of torsion in kcal/mol. [g] Phase offset in degrees. [h] Periodicity of torsion. [i] "N*" atom type has two possible GAFF atom types: "na" and "n," however, in this particular case N* - CA only occurs in the1MG residue, and it was assigned as n -cd. [j] The parameter of GAFF assigned atom types are missing in GAFF force field, so the value is the average of all reasonable analogies. They are: N* - CQ - H5, CT - N* - CT, N - CA - NC, and N* - CB - N*. [k] Derived from Tim Meyer's and David Case's force field library for tRNA^{Phe}, which was contributed to the AMBER parameter database: http://www.pharmacy.manchester.ac.uk/bryce/amber.

Supplemental Table 2 Partial charges

5'- phosphate A		5'- phosphate G		5'- phosphate U		m^1A	
Atom	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**
H5T	0.409864	H5T	0.397689	H5T	0.427626	P	1.1662
O3P	-0.749592	O3P	-0.739785	O3P	-0.684482	O1P	-0.776
P	1.665315	P	1.686837	P	1.462946	O2P	-0.776
O1P	-0.919627	O1P	-0.916682	O1P	-0.857648	O5'	-0.4989
O2P	-0.919627	O2P	-0.916682	O2P	-0.857648	C5'	0.0558
O5'	-0.679133	O5'	-0.704177	O5'	-0.683594	H5'1	0.0679
C5'	0.0558	C5'	0.0558	C5'	0.0558	H5'2	0.0679
H5'1	0.0679	H5'1	0.0679	H5'2	0.0679	C4'	0.1065
H5'2	0.0679	H5'2	0.0679	H5'1	0.0679	H4'	0.1174
C4'	0.1065	C4'	0.1065	C4'	0.1065	O4'	-0.3548
H4'	0.1174	H4'	0.1174	H4'	0.1174	C1'	0.096366
O4'	-0.3548	O4'	-0.3548	O4'	-0.3548	H1'	0.131302
C1'	0.0394	C1'	0.0191	C1'	0.0674	N9	-0.12752
H1'	0.2007	H1'	0.2006	H1'	0.1824	C8	0.253186
C2'	0.067	C2'	0.067	C2'	0.067	H8	0.126154
H2'1	0.0972	H2'1	0.0972	H2'1	0.0972	N7	-0.596846
O2'	-0.6139	O2'	-0.6139	O2'	-0.6139	C5	0.00869
HO'2	0.4186	HO'2	0.4186	HO'2	0.4186	C6	0.550704
N9	-0.0251	N9	0.0492	N1	0.0418	N6	-0.862164
C4	0.3053	C4	0.1222	C2	0.4687	HN62	0.397056
C5	0.0515	C5	0.1744	O2	-0.5477	N1	-0.140304
C6	0.7009	C6	0.477	N3	-0.3549	CM1	-0.228134
N1	-0.7615	O6	-0.5597	H3	0.3154	HM11	0.118139
C2	0.5875	N1	-0.4787	C4	0.5952	HM12	0.118139
H2	0.0473	H1	0.3424	O4	-0.5761	HM13	0.118139
N6	-0.9019	C2	0.7657	C5	-0.3635	C2	0.239943
H61	0.4115	N2	-0.9672	H5	0.1811	H2	0.143205
H62	0.4115	H21	0.4364	C6	-0.1126	N3	-0.59396
N7	-0.6073	H22	0.4364	H6	0.2188	C4	0.363905
N3	-0.6997	N7	-0.5709	C3'	0.2022	C3'	0.2022
C8	0.2006	N3	-0.6323	H3'	0.0615	H3'	0.0615
H8	0.1553	C8	0.1374	O3'	-0.5246	C2'	0.067
C3'	0.2022	H8	0.164			H2'1	0.0972
H3'	0.0615	C3'	0.2022			O2'	-0.6139
O3'	-0.5246	H3'	0.0615			HO'2	0.4186
		O3'	-0.5246			O3'	-0.5246

m^1G		m^2G		m^5C		m^5U	
Atom	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**
P	1.1662	P	1.1662	P	1.1662	P	1.1662
O1P	-0.776	O1P	-0.776	O1P	-0.776	O1P	-0.776
O2P	-0.776	O2P	-0.776	O2P	-0.776	O2P	-0.776
O5'	-0.4989	O5'	-0.4989	O5'	-0.4989	O5'	-0.4989
C5'	0.0558	C5'	0.0558	C5'	0.0558	C5'	0.0558
H5'1	0.0679	H5'1	0.0679	H5'1	0.0679	H5'1	0.0679
H5'2	0.0679	H5'2	0.0679	H5'2	0.0679	H5'2	0.0679
C4'	0.1065	C4'	0.1065	C4'	0.1065	C4'	0.1065
H4'	0.1174	H4'	0.1174	H4'	0.1174	H4'	0.1174
O4'	-0.3548	O4'	-0.3548	O4'	-0.3548	O4'	-0.3548
C1'	0.09816	C1'	0.068321	C1'	-0.002514	C1'	0.127486
H1'	0.142091	H1'	0.167336	H1'	0.223447	H1'	0.152768
N9	-0.024806	N9	-0.050463	N1	-0.159492	N1	-0.138087
C8	0.037228	C8	0.231962	C6	-0.173051	C6	-0.338213
H8	0.182333	H8	0.137729	H6	0.324799	H6	0.282658
N7	-0.496069	N7	-0.588617	C5	-0.223284	C5	-0.007369
C5	0.040707	C5	0.021564	CM5	-0.236056	CM5	-0.332308
C6	0.521633	C6	0.785635	HM51	0.079647	HM51	-0.145382
O6	-0.53576	O6	-0.599002	HM52	0.079647	HM52	0.415261
N1	-0.191741	N1	-0.847781	HM53	0.079647	HM53	0.415261
CM1	-0.077609	H1	0.398301	C4	0.874761	C4	0.415261
HM11	0.079562	C2	0.877651	N4	-1.001064	O4	-0.594517
HM12	0.079562	N2	-0.691322	H41	0.424898	N3	-0.729305
HM13	0.079562	H21	0.396574	H42	0.424898	H3	0.395007
C2	0.607242	CM2	-0.073693	N3	-0.830303	C2	0.803672
N2	-0.851637	HM21	0.087021	C2	0.85586	O2	-0.606193
H21	0.379544	HM22	0.087021	O2	-0.62584	C3'	0.2022
H22	0.379544	HM23	0.087021	C3'	0.2022	H3'	0.0615
N3	-0.593016	N3	-0.571886	H3'	0.0615	C2'	0.067
C4	0.25947	C4	0.192628	C2'	0.067	H2'1	0.0972
C3'	0.2022	C3'	0.2022	H2'1	0.0972	O2'	-0.6139
H3'	0.0615	H3'	0.0615	O2'	-0.6139	HO'2	0.4186
C2'	0.067	C2'	0.067	HO'2	0.4186	O3'	-0.5246
H2'1	0.0972	H2'1	0.0972	O3'	-0.5246		
O2'	-0.6139	O2'	-0.6139				
HO'2	0.4186	HO'2	0.4186				
O3'	-0.5246	O3'	-0.5246				

D		Cm		Gm		Ψ	
Atom	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**
P	1.1662	P	1.1662	P	1.1662	P	1.1662
O1P	-0.776	O1P	-0.776	O1P	-0.776	O1P	-0.776
O2P	-0.776	O2P	-0.776	O2P	-0.776	O2P	-0.776
O5'	-0.4989	O5'	-0.4989	O5'	-0.4989	O5'	-0.4989
C5'	0.0558	C5'	0.057167	C5'	0.007835	C5'	0.0558
H5'1	0.0679	H5'1	0.069407	H5'1	0.103793	H5'1	0.0679
H5'2	0.0679	H5'2	0.069407	H5'2	0.103793	H5'2	0.0679
C4'	0.1065	C4'	0.237211	C4'	0.049736	C4'	0.1065
H4'	0.1174	H4'	0.016263	H4'	0.094709	H4'	0.1174
O4'	-0.3548	O4'	-0.34379	O4'	-0.441272	O4'	-0.3548
C1'	0.025251	C1'	-0.052069	C1'	0.326094	C1'	-0.042993
H1'	0.206415	H1'	0.199764	H1'	0.05097	H1'	0.179765
N1	-0.325289	N1	-0.0484	N9	0.0492	N1	-0.479198
C6	0.35287	C6	0.0053	C8	0.1374	H1	0.35505
H61	-0.018653	H6	0.1958	H8	0.164	C6	0.03412
H62	-0.018653	C5	-0.5215	N7	-0.5709	H6	0.145461
C5	-0.406811	H5	0.1928	C5	0.1744	C5	-0.178682
H51	0.137176	C4	0.8185	C6	0.477	C4	0.745914
H52	0.137176	N4	-0.953	O6	-0.5597	O4	-0.550401
C4	0.780503	HN41	0.4234	N1	-0.4787	N3	-0.645585
O4	-0.596282	HN42	0.4234	H1	0.3424	H3	0.369073
N3	-0.730344	N3	-0.7584	C2	0.7657	C2	0.799618
HN3	0.389263	C2	0.7538	N2	-0.9672	O2	-0.616142
C2	0.786488	O2	-0.6252	HN21	0.4364	C3'	0.2022
O2	-0.60311	C3'	0.15863	HN22	0.4364	H3'	0.0615
C3'	0.2022	H3'	0.098689	N3	-0.6323	C2'	0.067
H3'	0.0615	C2'	-0.050237	C4	0.1222	H2'1	0.0972
C2'	0.067	H2'1	0.158115	C3'	0.327771	O2'	-0.6139
H2'1	0.0972	O2'	-0.31312	H3'	0.015523	HO'2	0.4186
O2'	-0.6139	CM2	-0.054982	C2'	-0.012428	O3'	-0.5246
HO'2	0.4186	HM21	0.084115	H2'1	0.058128		
O3'	-0.5246	HM22	0.084115	O2'	-0.365119		
		HM23	0.084115	CM2	-0.049974		
		O3'	-0.5246	HM21	0.081147		
				HM22	0.081147		
				HM23	0.081147		
				O3'	-0.5246		

m^2_2G		m^7G		Ar(p)			
Atom	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**
P	1.1662	P	1.1662	P	1.1662	N1	-0.7615
O1P	-0.776	O1P	-0.776	O1P	-0.776	C2	0.5875
O2P	-0.776	O2P	-0.776	O2P	-0.776	H2	0.0473
O5'	-0.4989	O5'	-0.4989	O5A	-0.4989	N6	-0.9019
C5'	0.0558	C5'	0.0558	C5A	-0.015008	HN61	0.4115
H5'1	0.0679	H5'1	0.0679	H5A1	0.081781	HN62	0.4115
H5'2	0.0679	H5'2	0.0679	H5A2	0.081781	N7	-0.6073
C4'	0.1065	C4'	0.1065	C4A	0.011975	N3	-0.6997
H4'	0.1174	H4'	0.1174	O4'	-0.183639	C8	0.2006
O4'	-0.3548	O4'	-0.3548	C1A	-0.373664	H8	0.1553
C1'	0.091595	C1'	0.483035	H1A	0.386804	H4A	0.23049
H1'	0.150813	H1'	0.075941	C2A	-0.215723	C3A	0.232812
N9	-0.075868	N9	-0.351153	H2A	0.245994	H3A	0.170251
C8	0.07491	C8	0.0375	O2A	-0.427945	O3A	-0.5246
H8	0.180271	H81	0.197097	C1'	0.415152		
N7	-0.531587	N7	0.233874	H1'	0.083186		
C5	0.067484	CM7	-0.368449	C2'	0.420531		
C6	0.65836	HM71	0.180051	H2'	-0.032329		
O6	-0.580309	HM72	0.180051	C3'	0.193051		
N1	-0.658799	HM73	0.180051	H3'	0.028531		
H1	0.378871	C5	-0.452906	C4'	0.172609		
C2	0.597736	C6	0.8095	H4'	0.073578		
N2	-0.145837	O6	-0.558777	C5'	0.327854		
CM1	-0.278445	N1	-0.768094	H5'1	-0.026178		
HM11	0.125637	HN1	0.423999	H5'2	-0.026178		
HM12	0.125637	C2	1.038857	O5'	-0.61577		
HM13	0.125637	N2	-1.07866	P'	1.503572		
CM2	-0.278444	HN21	0.487941	O2X	-0.87719		
HM21	0.125637	HN22	0.487941	O3X	-0.87719		
HM22	0.125637	N3	-0.785196	HO1X	0.438961		
HM23	0.125637	C4	0.663397	O1X	-0.763731		
N3	-0.575923	C3'	0.2022	O3'	-0.80961		
C4	0.28735	H3'	0.0615	HO3'	0.534074		
C3'	0.2022	C2'	0.067	O2'	-0.788001		
H3'	0.0615	H2'1	0.0972	HO'2	0.487615		
C2'	0.067	O2'	-0.6139	O1'	-0.555045		
H2'1	0.0972	HO2'	0.4186	N9	-0.025101		
O2'	-0.6139	O3'	-0.5246	C4	0.3053		
HO2'	0.4186			C5	0.0515		
O3'	-0.5246			C6	0.7009		

t^6A				yW			
Atom	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**	**Atom**	**Charge**
P	1.1662	H152	0.061593	P	1.1662	C15	0.416213
O1P	-0.776	H153	0.061593	O1P	-0.776	H15	-0.041559
O2P	-0.776	C3'	0.2022	O2P	-0.776	C16	0.6149
O5'	-0.4989	H3'	0.0615	O5'	-0.4989	O17	-0.53739
C5'	0.0558	C2'	0.067	C5'	0.0558	O18	-0.424994
H5'2	0.0679	H2'	0.0972	H5'1	0.0679	C19	0.159256
H5'1	0.0679	O2'	-0.6139	H5'2	0.0679	H191	0.026232
C4'	0.1065	HO'2	0.4186	C4'	0.1065	H192	0.026232
H4'	0.1174	O3'	-0.5246	H4'	0.1174	H193	0.026232
O4'	-0.3548			O4'	-0.3548	N20	-0.932881
C1'	-0.085723			C1'	0.191167	H20	0.420465
H1'	0.189544			H1'	0.100834	C21	0.998769
N9	0.016959			N9	-0.067783	O22	-0.650244
C8	0.202397			C8	0.215094	O23	-0.297564
H8	0.133014			H8	0.153545	C24	-0.186421
N7	-0.593702			N7	-0.55884	H241	0.118318
C5	0.045686			C5	0.077045	H242	0.118318
C6	0.55803			C6	0.617249	H243	0.118318
N6	-0.591393			O6	-0.52166	C3'	0.2022
HN6	0.349977			N1	-0.149504	H3'	0.0615
N1	-0.589285			C2	0.337632	C2'	0.067
C2	0.48629			N2	-0.562283	H2'	0.0972
H2	0.076868			N3	-0.092322	O2'	-0.6139
N3	-0.645618			H31	0.056374	HO'2	0.4186
C4	0.354039			H32	0.056374	O3'	-0.5246
C10	0.762945			H33	0.056374		
O10	-0.658434			C3	0.034583		
N11	-0.370628			C4	-0.008591		
HN11	0.262234			C10	-0.573403		
C12	-0.198945			H101	0.159192		
H12	0.088908			H102	0.159192		
C13	0.863589			H103	0.159192		
ODA	-0.761017			C11	0.41044		
ODB	-0.808249			C12	-0.229091		
C14	0.478546			C13	0.07747		
H14	0.019433			H131	0.031895		
O14	-0.783782			H132	0.031895		
HO14	0.460398			C14	-0.12428		
C15	-0.33086			H141	0.053005		
H151	0.061593			H142	0.053005		