IDEALIZED ATOMIC COORDINATES OF YEAST PHENYLALANINE TRANSFER RNA

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Abstract: The atomic coordinates are given for yeast phenylalanine transfer RNA in the orthorhombic crystal form. The structure has been refined by fitting to successively improved electron density maps at 2.7 Å resolution. The model fitting has been accomplished by using an interactive computer graphics system to minimize the errors inherent in manual model building and coordinate measurements, using an optical comparator. The atomic coordinates have then been "idealized" to make bond distances, bond angles, steric conformation and non-bonded contacts close to standard values, while constraining the model to fit the electron density maps.

The three dimensional structure of yeast phenylalanine tRNA ($tRNA^{PHE}$) in the orthorhombic crystal form has been determined by X-ray crystallographic methods. The backbone structure of the molecule was determined at 4 Å resolution by the multiple isomorphous replacement method (1), and the tertiary hydrogen bonding scheme between the bases has since been described for the yeast $tRNA^{PHE}$ in the orthorhombic (2) and the monoclinic crystal form (3), based on the electron density maps at 3 Å resolution. The refinement for the yeast $tRNA^{PHE}$ structure in the orthorhombic crystal form has been pursued along two different directions, one at M.I.T. (to be submitted to this journal), and the other at Duke University. We present the results from the latter approach here.

In fitting the models to successively improved electron density maps obtained by the "partial structure fourier method" (4), we have used initially an optical comparator (5), then an interactive computer graphics system developed in collaboration with the Department of Computer Science at the University of North Carolina at Chapel Hill. The "idealization" was achieved by the use of a program written by Hermans and McQueen (6), and modified for nucleic acid structures by Sussman (4). The idealization is accomplished by minimizing a criterion function for each atom sequentially in the structure. This function contains terms for deviations from standard bond angles, bond

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	X	Y	Z
1 GUANOSINE			
O	24.6	24.4	66.3
P	25.4	25.7	66.8
O1P	25.7	26.6	65.7
O2P	24.7	26.3	68.0
O5'	26.9	25.2	67.4
C5'	27.2	23.8	67.5
C4'	26.8	23.2	68.9
O1'	25.3	23.4	69.1
C1'	24.7	22.2	69.7
C3'	27.0	21.8	69.1
C2'	26.0	21.4	70.1
O2'	26.4	21.8	71.4
O3'	28.4	21.5	69.5
N9	23.6	21.6	68.8
C8	22.8	22.3	67.8
N7	22.0	21.6	67.2
C5	22.1	20.3	67.7
C6	21.4	19.2	67.3
O6	20.5	19.2	66.5
N1	21.8	18.0	67.9
C2	22.9	18.0	68.8
N2	23.1	16.8	69.3
N3	23.6	19.1	69.2
C4	23.1	20.2	68.6
2 CYTIDINE			
P	29.4	20.8	68.5
O1P	29.3	21.3	67.1
O2P	30.8	21.0	69.0
O5'	28.9	19.2	68.6
C5'	29.3	18.3	67.6
C4'	28.7	16.9	67.9
O1'	27.3	17.0	68.2
C1'	26.5	16.0	67.6
C3'	28.6	16.0	66.6
C2'	27.5	15.0	66.9
O2'	27.9	14.0	67.8
O3'	29.9	15.4	66.4
N1	25.4	16.5	66.6
C6	25.2	17.9	66.3
C5	24.3	18.3	65.5
C4	23.4	17.4	65.0
N4	22.4	17.8	64.2
N3	23.5	16.1	65.2
C2	24.4	15.6	66.1
O2	24.5	14.5	66.3
3 GUANOSINE			
P	30.4	15.1	64.9
O1P	30.0	16.2	63.9
O2P	31.9	14.8	64.9
O5'	29.6	13.8	64.4
C5'	29.8	12.5	65.1
C4'	28.7	11.4	64.7
O1'	27.5	12.0	65.2
C1'	26.4	11.7	64.3
C3'	28.5	11.2	63.3
C2'	27.1	10.7	63.3
O2'	27.0	9.4	63.8
O3'	29.4	10.3	62.7
N9	25.9	12.9	63.6
C8	26.2	14.3	63.8
N7	25.5	15.1	63.0
C5	24.6	14.3	62.4
C6	23.7	14.6	61.4
O6	23.4	15.7	61.0
N1	23.0	13.4	61.0
C2	23.3	12.2	61.4
N2	22.5	11.2	60.8
N3	24.2	11.9	62.3
C4	24.8	13.0	62.7
4 GUANOSINE			
P	30.3	10.7	61.4
O1P	30.5	12.2	61.3
O2P	31.5	9.9	61.3
O5'	29.2	10.3	60.1
C5'	29.2	8.9	59.6
C4'	27.9	8.6	58.8
O1'	26.8	9.2	59.5
C1'	25.8	9.7	58.5
C3'	27.8	9.2	57.4
C2'	26.3	9.2	57.2
O2'	25.8	8.0	56.9
O3'	28.4	8.4	56.3
N9	25.6	11.2	58.6
C8	26.4	12.2	59.4
N7	25.9	13.4	59.2
C5	24.9	13.2	58.3
C6	24.0	14.1	57.8
O6	23.9	15.3	58.0
N1	23.1	13.6	56.9
C2	23.0	12.3	56.6
N2	22.0	12.0	55.7
N3	23.8	11.4	57.1
C4	24.7	11.9	58.0
5 ADENOSINE			
P	28.9	9.1	54.9
O1P	29.6	10.3	55.T
O2P	29.6	8.1	54.1
O5'	27.5	9.5	54.2
C5'	26.7	8.6	53.3
C4'	25.5	9.3	52.6
O1'	24.8	10.1	53.6
C1'	24.4	11.3	53.0
C3'	26.0	10.4	51.6
C2'	24.8	11.3	51.5
O2'	23.7	10.8	50.8
O3'	26.3	9.8	50.3
N9	25.0	12.4	53.8
C8	26.1	12.5	54.7
N7	26.3	13.7	55.2
C5	25.3	14.4	54.6
C6	24.9	15.8	54.8
N6	25.5	16.7	55.6
N1	23.9	16.2	54.1
C2	23.3	15.3	53.3
N3	23.5	14.1	53.1
C4	24.5	13.7	53.8
6 URIDINE			
P	27.6	10.3	49.4
O1P	28.7	10.8	50.3
O2P	28.0	9.2	48.5
O5'	27.0	11.5	48.5
C5'	25.9	11.4	47.5
C4'	25.2	12.7	47.3
O1'	24.7	13.1	48.6
C1'	24.7	14.5	48.8
C3'	26.0	13.9	46.8
C2'	25.2	15.1	47.4
O2'	24.0	15.3	46.7
C3'	26.1	14.0	45.4
N1	25.6	14.9	50.0
C6	26.4	13.9	50.8
C5	27.2	14.3	51.8
C4	27.2	15.7	52.2
O4	27.9	16.2	53.1
N3	26.5	16.5	51.4
C2	25.7	16.2	50.4
O2	25.0	17.0	49.8
7 URIDINE			
P	27.3	13.5	44.5
O1P	27.8	12.2	45.0
O2P	26.9	13.4	43.1
O5'	28.4	14.6	44.8
C5'	28.6	15.8	44.0
C4'	27.5	16.9	44.4
O1'	27.3	17.0	45.8
C1'	27.6	18.3	46.3
C3'	27.9	18.3	44.0
C2'	28.5	18.9	45.2
O2'	28.6	20.3	45.2
O3'	26.8	19.1	43.5
N1	28.2	18.2	47.8
C6	28.6	17.0	48.4
C5	29.0	16.9	49.6
C4	29.2	18.0	50.5
O4	29.5	18.0	51.6
N3	28.8	19.2	49.9
C2	28.3	19.4	48.6
O2	28.1	20.5	48.3
8 URIDINE			
P	27.0	20.1	42.2
O1P	25.7	20.1	41.5
O2P	27.5	21.4	42.7
O5'	28.0	19.3	41.2
C5'	29.2	20.0	40.7
C4'	29.7	19.5	39.4
O1'	30.3	18.2	39.6
C1'	30.0	17.4	38.4
C3'	28.7	19.3	38.3
C2'	29.3	18.4	37.4
O2'	30.3	19.2	36.8
O3'	28.2	20.5	37.6
N1	29.1	16.2	38.7
C6	28.2	16.0	39.8
C5	27.4	14.9	40.0
C4	27.4	13.9	39.0
O4	26.7	12.9	39.0
N3	28.3	14.1	37.9
C2	29.1	15.2	37.7
O2	29.8	15.3	36.8
9 ADENOSINE			
P	26.7	20.9	37.8
O1P	25.8	19.7	37.4
O2P	26.5	21.4	39.1
O5'	26.7	22.0	36.7
C5'	25.6	22.2	35.7
C4'	26.2	22.8	34.5
O1'	27.0	21.8	33.8
C1'	26.6	21.7	32.5
C3'	25.3	23.4	33.5
C2'	25.2	22.3	32.5
O2'	24.8	22.8	31.2
O3'	25.7	24.7	33.0
N9	26.7	20.3	32.0
C8	26.1	19.1	32.5
N7	26.4	18.1	31.9
C5	27.4	18.5	31.0
C6	28.2	17.8	30.1
N6	28.1	16.4	29.9
N1	29.1	18.4	29.8
C2	29.2	19.8	29.6
N3	28.5	20.6	30.4
C4	27.6	19.8	31.1
10 2H-GUANOSINE			
P	25.3	26.1	33.8
O1P	25.9	26.0	35.2
O2P	25.8	27.2	32.9
O5'	23.7	26.0	33.8
C5'	22.9	26.8	34.7
C4'	21.4	26.4	34.6
O1'	21.0	26.5	33.2
C1'	20.1	25.5	32.8
C3'	21.0	25.0	35.0
C2'	19.7	24.8	34.1
O2'	18.6	25.5	34.6
O3'	20.8	24.9	36.5
N9	20.9	24.6	31.7
C8	22.0	24.9	31.0
N7	22.4	23.9	30.2
C5	21.4	23.0	30.3
C6	21.4	21.7	29.7
O6	22.2	21.2	28.9
N1	20.2	21.0	30.0
C2	19.2	21.5	30.8
N2	18.2	20.8	31.0
C2H	17.1	21.2	31.8
N3	19.3	22.7	31.5
C4	20.5	23.4	31.2
11 CYTIDINE			
P	20.3	23.5	37.3
O1P	21.3	22.4	37.0
O2P	20.2	23.8	38.7
O5'	18.9	23.2	36.5
C5'	17.6	23.0	37.2
C4'	17.1	21.6	37.0
O1'	17.2	21.3	35.5
C1'	17.5	19.9	35.3
C3'	17.9	20.5	37.6
C2'	17.5	19.3	36.8
O2'	16.2	18.9	37.0
O3'	17.5	20.4	39.0
N1	18.9	19.8	34.6
C6	19.9	20.8	34.6
C5	21.1	20.7	33.9
C4	21.2	19.6	33.0
N4	22.3	19.4	32.3
N3	20.2	18.6	33.0
C2	19.1	18.7	33.7
O2	18.2	17.9	33.8
12 URIDINE			
P	18.7	19.9	40.0
O1P	20.0	20.5	39.7
O2P	18.2	20.3	41.4
O5'	18.7	18.3	39.8
C5'	17.5	17.5	40.2
C4'	17.5	16.1	39.3
O1'	17.7	16.5	37.9
C1'	18.5	15.5	37.2
C3'	18.7	15.2	39.6
C2'	18.7	14.4	38.3
O2'	17.7	13.5	38.1
O3'	18.4	14.3	40.7
N1	19.8	16.2	36.6
C6	20.4	17.4	37.1
C5	21.5	17.9	36.6
C4	22.2	17.3	35.5
O4	23.2	17.7	35.0
N3	21.6	16.1	35.1
C2	20.5	15.5	35.6
O2	20.1	14.4	35.2
13 CYTIDINE			
P	19.6	13.5	41.5
O1P	20.5	14.5	42.0
O2P	19.0	12.7	42.5
O5'	20.2	12.6	40.3
C5'	21.6	12.2	40.4
C4'	22.0	11.5	39.0
O1'	21.8	12.6	38.0
C1'	22.9	12.4	37.0
C3'	23.4	11.1	39.0
C2'	23.7	11.1	37.5
O2'	23.1	10.0	36.9
O3'	23.7	9.8	39.6
N1	23.8	13.7	37.0
C6	23.7	14.8	37.8
C5	24.5	15.9	37.7
C4	25.5	15.9	36.7
N4	26.3	17.0	36.6
N3	25.6	14.9	35.9
C2	24.8	13.8	36.0
O2	25.0	12.9	35.2
14 ADENOSINE			
P	25.2	9.4	40.1
O1P	26.0	10.6	40.6
O2P	25.1	8.3	41.1
O5'	25.8	8.9	38.7
C5'	25.6	7.5	38.2
C4'	26.8	7.1	37.2
O1'	26.8	8.0	36.1
C1'	28.1	8.2	35.6
C3'	28.2	7.2	37.8
C2'	29.0	7.3	36.5
O2'	29.1	6.1	35.9
O3'	28.6	6.2	38.6
N9	28.6	9.7	35.7
C8	28.1	10.8	36.4
N7	28.7	11.9	36.2
C5	29.7	11.5	35.3
C6	30.7	12.2	34.7
N6	31.1	13.5	34.9
N1	31.5	11.6	33.8
C2	31.2	10.4	33.5
N3	30.3	9.6	34.0
C4	29.6	10.2	34.9
15 GUANOSINE			
P	29.6	6.5	39.9
O1P	29.0	7.4	40.8
O2P	30.0	5.1	40.5
O5'	30.9	7.2	39.2
C5'	31.7	6.4	38.3
C4'	32.7	7.2	37.5
O1'	32.0	8.3	36.8
C1'	32.9	9.4	36.8
C3'	33.8	7.8	38.2
C2'	34.3	8.9	37.3
O2'	35.1	8.4	36.3
O3'	34.9	7.0	38.6
N9	32.4	10.6	37.5
C8	31.3	10.7	38.4
N7	31.1	11.9	38.9
C5	32.1	12.7	38.3
C6	32.4	14.1	38.4
O6	31.9	14.9	39.1
N1	33.4	14.4	37.6
C2	34.1	13.6	36.7
N2	35.0	14.2	36.0
N3	33.8	12.3	36.6
C4	32.8	11.9	37.4
16 DIHYDROURIDINE			
P	35.2	6.6	40.1
O1P	35.3	7.9	40.9
O2P	34.1	5.7	40.6
O5'	36.6	5.9	39.9
C5'	37.3	5.4	41.1
C4'	37.2	3.9	41.3
O1'	35.8	3.6	41.5
C1'	35.5	2.4	40.9
C3'	37.6	3.0	40.2
C2'	36.8	1.8	40.5
O2'	37.4	1.1	41.6
O3'	38.9	2.8	40.0
N1	34.4	2.6	39.8
C6	34.7	2.9	38.3
C5	33.7	3.7	37.6
C4	32.3	3.1	37.9
O4	31.4	3.3	37.1
N3	32.2	2.5	39.1
C2	33.1	2.3	40.1
O2	32.8	1.9	41.2
17 DIHYDROURIDINE			
P	39.7	3.4	38.7
O1P	38.9	3.2	37.4
O2P	40.0	4.9	38.9
O5'	41.0	2.5	38.5
C5'	41.8	2.2	39.8
C4'	43.1	3.0	39.9
O1'	43.9	2.6	38.8
C1'	44.4	3.8	38.2
C3'	43.0	4.5	39.9
C2'	43.3	4.9	38.5
O2'	43.7	6.3	38.4
O3'	43.8	5.2	40.9
N1	44.7	3.4	36.8
C6	43.6	3.4	35.7
C5	44.0	2.4	34.6
C4	45.4	2.6	34.1
O4	45.8	2.3	33.0
N3	46.2	3.1	35.1
C2	45.9	3.4	36.4
O2	46.8	3.7	37.2
18 GUANOSINE			
P	43.2	6.3	41.9
O1P	41.7	6.1	42.1
O2P	44.0	6.4	43.1
O5'	43.5	7.7	41.0
C5'	42.4	8.5	40.4
C4'	42.9	9.8	39.8
O1'	43.5	10.6	40.8
C1'	44.6	11.4	40.2
C3'	43.9	9.7	38.6
C2'	44.7	11.1	38.7
O2'	44.0	12.1	38.1
O3'	43.1	9.5	37.4
N9	45.9	11.0	41.0
C8	46.3	9.7	41.5
N7	47.4	9.8	42.2
C5	47.8	11.1	42.1
C6	48.8	11.8	42.7
O6	49.8	11.4	43.4
N1	48.8	13.1	42.3
C2	47.9	13.7	41.6
N2	48.2	15.0	41.4
N3	46.9	13.1	41.0
C4	46.9	11.8	41.4
19 GUANOSINE			
P	43.6	9.1	36.0
O1P	44.8	8.2	36.1
O2P	42.5	8.5	35.2
O5'	44.1	10.5	35.3
C5'	43.2	11.6	35.0
C4'	44.0	12.9	34.5
O1'	45.3	12.8	34.9
C1'	46.2	12.7	33.8
C3'	44.1	13.0	32.9
C2'	45.4	12.3	32.6
O2'	45.8	12.7	31.3
O3'	44.2	14.4	32.5
N9	47.3	11.8	34.3
C8	47.3	10.4	34.6
N7	48.3	10.0	35.0
C5	49.1	11.1	35.1
C6	50.4	11.2	35.6
O6	51.1	10.3	36.0
N1	50.9	12.5	35.5
C2	50.2	13.6	35.1
N2	50.7	14.7	35.1
N3	48.9	13.5	34.6
C4	48.5	12.2	34.7
20 GUANOSINE			
P	42.9	15.2	32.1
O1P	41.9	15.2	33.2
O2P	43.4	16.6	31.8
O5'	42.2	14.4	30.9
C5'	42.8	14.8	29.6
C4'	41.7	14.2	28.5
O1'	41.0	12.9	28.8
C1'	39.6	13.1	28.6
C3'	40.6	15.2	28.5
C2'	39.4	14.5	28.0
O2'	39.5	14.3	26.6
O3'	41.0	16.4	27.8
N9	38.8	12.9	29.9
C8	39.3	12.9	31.3
N7	38.4	12.6	32.2
C5	37.2	12.4	31.4
C6	35.9	12.1	31.9
O6	35.5	11.9	33.1
N1	35.0	12.0	30.8
C2	35.3	12.1	29.5
N2	34.3	12.0	28.7
N3	36.6	12.4	29.1
C4	37.5	12.6	30.1
21 ADENOSINE			
P	41.0	17.8	28.5
O1P	41.9	17.7	29.7
O2P	41.6	18.8	27.5
O5'	39.4	18.1	28.8
C5'	38.9	18.1	30.1
C4'	37.8	17.1	30.4
O1'	37.4	17.4	31.8
C1'	36.0	17.6	31.7
C3'	36.6	17.2	29.5
C2'	35.7	18.1	30.3
O2'	34.8	18.1	30.0
O3'	36.0	16.0	29.1
N9	35.5	18.6	32.8
C8	35.9	19.8	33.2
N7	35.3	20.4	34.1
C5	34.3	19.4	34.4
C6	33.3	19.4	35.3

	X	Y	Z
N6	32.9	20.5	36.0
N1	32.6	18.3	35.4
C2	32.9	17.2	34.7
N3	33.9	17.1	33.8
C4	34.5	18.3	33.7

22 GUANOSINE

P	35.2	15.8	27.6
O1P	36.0	16.6	26.5
O2P	35.1	14.4	27.2
O5'	33.8	16.6	27.9
C5'	32.5	16.1	27.5
C4'	32.1	14.7	28.1
O1'	32.5	14.7	29.6
C1'	31.4	14.0	30.3
C3'	30.6	14.5	28.2
C2'	30.5	13.4	29.3
O2'	30.9	12.2	28.8
O3'	30.0	14.0	26.9
N9	30.8	14.9	31.4
C8	31.2	16.1	31.9
N7	30.4	16.6	32.8
C5	29.4	15.7	33.0
C6	28.4	15.9	33.9
O6	28.1	16.8	34.6
N1	27.6	14.7	33.8
C2	27.9	13.6	33.0
N2	27.1	12.6	33.1
N3	28.9	13.6	32.2
C4	29.6	14.7	32.2

23 ADENOSINE

P	28.4	13.9	26.7
O1P	27.7	15.2	27.2
O2P	28.1	13.7	25.3
O5'	28.0	12.7	27.7
C5'	27.8	11.3	27.2
C4'	26.5	10.8	27.7
O1'	26.4	11.0	29.2
C1'	25.1	11.3	29.5
C3'	25.2	11.4	27.2
C2'	24.2	11.1	28.3
O2'	23.8	9.8	28.2
O3'	24.8	10.9	25.9
N9	25.1	12.7	30.2
C8	25.9	13.8	29.9
N7	25.7	14.9	30.6
C5	24.7	14.4	31.5
C6	24.1	15.0	32.6
N6	24.5	16.2	33.0
N1	23.2	14.4	33.2
C2	22.8	13.2	32.8
N3	23.3	12.5	31.8
C4	24.3	13.2	31.2

24 GUANOSINE

P	23.9	11.8	24.9
O1P	24.3	13.2	24.9
O2P	23.8	11.1	23.6
O5'	22.4	11.7	25.7
C5'	21.6	10.5	25.7
C4'	20.5	10.6	26.8
O1'	21.2	11.0	28.1
C1'	20.4	11.9	28.8
C3'	19.4	11.6	26.6
C2'	19.0	11.9	28.1
O2'	18.2	10.9	28.6
O3'	18.4	11.0	25.8
N9	21.1	13.2	29.0
C8	22.2	13.8	28.3
N7	22.6	14.9	28.7
C5	21.7	15.2	29.8
C6	21.7	16.3	30.7
O6	22.5	17.2	30.7
N1	20.7	16.1	31.6
C2	19.8	15.1	31.6
N2	18.9	15.2	32.5
N3	19.8	14.1	30.8
C4	20.8	14.2	29.9

25 CYTIDINE

P	17.0	11.8	25.4
O1P	16.4	11.1	24.3
O2P	16.1	11.8	26.7
O5'	17.5	13.2	25.0
C5'	16.6	14.4	25.0
C4'	16.2	14.9	26.4
O1'	17.3	14.8	27.3
C1'	17.4	15.9	28.2
C3'	15.9	16.4	26.4
C2'	16.1	16.7	27.9
O2'	15.0	16.3	28.7
O3'	14.5	16.6	26.0
N1	18.7	16.7	28.1
C6	19.8	16.3	27.1
C5	20.9	17.0	27.0
C4	21.1	18.1	27.8
N4	22.2	18.8	27.8
N3	20.1	18.5	28.7
C2	19.0	17.8	28.8
O2	18.1	18.2	29.7

26 2,2DIM-GUANOSINE

P	14.2	17.8	24.9
O1P	15.0	17.5	23.7
O2P	12.7	17.8	24.6
O5'	14.7	19.1	25.6
C5'	14.0	19.7	26.7
C8'	14.7	21.0	27.3
O1'	16.0	20.6	27.8
C1'	16.9	21.6	27.5
C3'	15.1	22.0	26.2
C2'	16.2	22.7	26.8
O2'	15.8	23.6	27.8
O3'	14.0	22.8	25.9
N9	18.1	21.0	26.7
C8	18.2	19.8	26.0
N7	19.4	19.6	25.5
C5	20.1	20.7	25.8
C6	21.5	21.1	25.5
C6	22.3	20.4	24.9
N1	21.8	22.3	26.0
C2	20.8	23.1	26.7
N2	21.1	24.3	27.1
C2N1	20.1	25.2	27.7
C2N2	22.5	24.9	27.0
N3	19.6	22.8	26.9
C4	19.3	21.6	26.5

27 CYTIDINE

P	13.6	23.1	24.3
O1P	13.8	21.8	23.5
O2P	12.2	23.6	24.2
O5'	14.7	24.2	23.9
C5'	14.6	25.6	24.5
C4'	16.0	26.3	24.3
O1'	17.0	25.5	25.0
C1'	18.2	25.5	24.3
C3'	16.5	26.4	22.9
C2'	18.0	26.6	23.1
O2'	18.3	27.8	23.6
O3'	15.9	27.5	22.2
N1	18.7	24.1	23.7
C6	17.9	23.0	23.8
C5	18.3	21.8	23.3
C4	19.5	21.8	22.7
N4	20.0	20.7	22.3
N3	20.3	22.9	22.6
O2	19.9	24.0	23.1
	20.7	25.0	23.0

28 CYTIDINE

P	15.8	27.5	20.6
O1P	15.2	26.2	20.1
O2P	15.0	28.6	20.0
O5'	17.4	27.5	20.1
C5'	18.1	28.8	20.0
C4'	19.3	28.6	19.0
O1'	20.3	27.7	19.7
C1'	20.9	26.9	18.7
C3'	19.0	27.8	17.7
C2'	20.4	27.4	17.4
O2'	21.2	28.5	16.9
O3'	18.4	28.6	16.7
N1	20.6	25.4	18.9
C6	19.6	24.9	19.7
C5	19.3	23.6	19.9
C4	20.2	22.7	19.3
N4	20.0	21.5	19.4
N3	21.2	23.1	18.5
C2	21.4	24.4	18.3
O2	22.3	24.8	17.6

29 ADENOSINE

P	16.8	28.2	16.3
O1P	16.1	27.4	17.4
O2P	16.1	29.5	16.1
O5'	16.9	27.3	15.0
C5'	17.6	27.8	13.8
C4'	19.0	27.1	13.5
O1'	19.5	26.5	14.8
C1'	20.2	25.3	14.6
C3'	19.0	25.9	12.6
C2'	20.2	25.1	13.1
O2'	21.4	25.7	12.6
O3'	19.1	26.2	11.2
N9	19.5	24.2	15.3
C8	18.3	24.2	16.1
N7	18.0	23.0	16.6
C5	18.9	22.2	16.1
C6	19.2	20.8	16.2
N6	18.4	19.9	16.8
N1	20.2	20.3	15.6
C2	21.0	21.1	15.0
N3	20.9	22.4	14.8
C4	19.9	22.8	15.4

30 GUANOSINE

P	18.7	25.2	10.0
O1P	17.3	24.6	10.2
O2P	18.8	25.9	8.7
O5'	19.7	23.9	10.2
C5'	21.1	24.0	9.7
C4'	21.7	22.6	9.5
O1'	21.8	22.0	10.8
C1'	21.5	20.6	10.6
C3'	20.9	21.6	8.6
C2'	21.4	20.3	9.1
O2'	22.7	20.0	8.6
O3'	21.1	21.8	7.2
N9	20.3	20.2	11.5
C8	19.3	21.0	12.1
N7	18.5	20.3	12.8
C5	18.9	19.0	12.7
C6	18.4	17.9	13.4
O6	17.5	17.8	14.2
N1	19.0	16.7	12.9
C2	20.0	16.7	12.0
N2	20.5	15.5	11.7
N3	20.5	17.8	11.4
C4	19.9	18.9	11.9

31 ADENOSINE

P	19.9	22.4	6.4
O1P	19.1	23.4	7.1
O2P	20.4	23.0	5.1
O5'	18.9	21.1	6.1
C5'	19.3	20.2	5.1
C4'	19.3	18.7	5.5
O1'	19.6	18.6	7.0
C1'	18.9	17.5	7.6
C3'	17.9	18.0	5.4
C2'	18.1	16.9	6.4
O2'	18.9	15.8	5.9
O3'	17.7	17.5	4.0
N9	17.9	18.0	8.7
C8	17.6	19.3	9.1
N7	16.8	19.3	10.1
C5	16.6	17.9	10.4
C6	15.8	17.3	11.4
N6	15.0	17.9	12.2
N1	15.8	16.0	11.4
C2	16.6	15.3	10.5
N3	17.3	15.8	9.6
C4	17.3	17.2	9.6

32 2'OM-CYTIDINE

P	16.3	16.8	3.5
O1P	15.1	17.6	3.9
O2P	16.3	16.6	2.1
O5'	16.3	15.4	4.4
C5'	15.6	14.3	4.0
C4'	14.3	14.0	4.8
O1'	14.7	14.2	6.3
C1'	13.5	14.7	6.9
C3'	13.1	14.8	4.6
C2'	12.3	14.6	5.9
O2'	11.6	13.3	5.8
C2'M	11.6	12.2	7.0
O3'	12.4	14.5	3.5
N1	13.7	16.1	7.5
C6	14.3	17.2	6.9
C5	14.3	18.4	7.4
C4	13.7	18.5	8.7
N4	13.6	19.7	9.3
N3	13.1	17.5	9.3
C2	13.1	16.3	8.8
O2	12.7	15.3	9.4

33 URIDINE

P	12.1	15.6	2.4
O1P	12.6	17.0	2.7
O2P	12.6	15.1	1.1
O5'	10.5	15.7	2.3
C5'	9.7	14.5	2.3
C4'	8.5	14.5	3.3
O1'	9.1	14.8	4.6
C1'	8.2	15.7	5.3
C3'	7.5	15.6	3.1
C2'	6.9	15.7	4.5
O2'	6.1	14.6	4.8
O3'	6.5	15.4	2.1
N1	8.0	17.1	5.7
C6	9.9	17.7	5.0
C5	10.3	18.9	5.4
C4	9.6	19.7	6.5
O4	9.9	20.8	6.9
N3	8.6	19.0	7.0
C2	8.1	17.8	6.7
O2	7.2	17.3	7.2

34 2'OM-GUANOSINE

P	6.6	16.3	0.8
O1P	7.9	16.1	0.0
O2P	5.4	16.2	0.0
O5'	6.7	17.8	1.5
C5'	6.6	19.0	0.6
C4'	5.4	19.9	1.1
O1'	4.2	19.1	0.8
C1'	3.2	19.4	1.8
C3'	5.3	20.3	2.5
C2'	3.8	20.5	2.7
O2'	3.4	21.8	2.1
C2'M	2.5	22.6	2.7
O3'	6.2	21.4	2.8
N9	2.9	18.0	2.5
C8	3.3	16.7	2.3
N7	2.8	15.8	3.1
C5	2.0	16.5	3.9
C6	1.1	16.1	5.0
O6	1.0	15.0	5.4
N1	0.5	17.2	5.6
C2	0.6	18.5	5.3
N2	0.0	19.4	6.0
N3	1.4	18.9	4.3
C4	2.0	17.9	3.6

35 ADENOSINE

P	6.5	22.0	4.4
O1P	7.0	20.9	5.3
O2P	7.5	23.1	4.3
O5'	5.0	22.5	4.8
C5'	4.8	23.7	5.6
C4'	4.1	23.3	7.0
O1'	3.1	22.3	6.7
C1'	3.1	21.4	7.8
C3'	5.0	22.6	8.0
C2'	4.0	22.0	8.8
O2'	3.3	22.9	9.6
O3'	5.9	23.4	8.7
N9	3.5	20.0	7.3
C8	4.4	19.6	6.3
N7	4.5	18.4	6.2
C5	3.7	17.8	7.1
C6	3.4	16.6	7.3
N6	4.0	15.7	6.6
N1	2.5	16.3	8.3
C2	1.9	17.3	8.9
N3	2.1	18.6	8.8
C4	3.0	18.8	7.8

36 ADENOSINE

P	7.5	23.2	8.5
O1P	7.9	23.5	7.1
O2P	8.3	23.9	9.5
O5'	7.8	21.5	8.6
C5'	7.9	20.8	9.9
C4'	6.6	20.8	10.6
O1'	5.8	19.8	9.8
C1'	4.9	19.1	10.7
C3'	6.5	20.2	12.0
C2'	5.1	19.8	12.1
O2'	4.2	20.9	12.2
O3'	6.9	21.2	13.0
N9	5.1	17.6	10.6
C8	6.0	16.9	9.8
N7	5.9	15.6	9.9
C5	4.9	15.4	10.8
C6	4.3	14.2	11.3
N6	4.7	13.0	10.9
N1	3.3	14.4	12.1
C2	3.0	15.6	12.5
N3	3.5	16.8	12.1
C4	4.4	16.6	11.2

37 Y

P	7.8	20.7	14.3
O1P	9.2	20.5	13.9
O2P	7.6	21.7	15.3
O5'	7.1	19.3	14.7
C5'	5.9	19.2	15.5
C4'	5.6	17.7	16.0
O1'	5.2	17.0	14.8
C1'	5.7	15.6	15.0
C3'	6.8	17.0	16.5
C2'	6.4	15.6	16.3
O2'	5.5	15.2	17.3
O3'	7.2	17.2	17.8
N9	6.7	15.3	13.8
C8	7.5	16.1	13.0
N7	8.2	15.5	12.1
C5	7.8	14.2	12.3
C6	8.2	13.0	11.7
O6	8.9	12.9	10.8
N1	7.6	11.9	12.2
C10	7.9	10.7	11.6
C13	8.8	10.7	10.3
C14	8.0	10.4	8.9
C15	7.2	11.7	8.5
C16	8.0	12.8	7.6
O17	8.4	12.5	6.5
O18	8.1	14.1	8.1
C19M	9.4	14.8	8.4
N20	6.0	11.3	7.8
C21	4.7	12.3	7.7
O22	4.9	13.5	8.0
O23	3.5	11.8	7.5
C24M	2.5	11.6	8.6
C11	7.2	9.8	12.4
C11M	7.3	8.3	12.1
N12	6.6	10.5	13.4
C2	6.8	11.9	13.2
N3	6.4	12.9	13.9
C3M	5.5	12.6	15.0
C4	6.9	14.0	13.4

38 ADENOSINE

P	8.8	17.3	18.1
O1P	9.7	17.1	16.8
O2P	9.1	18.6	18.7
O5'	9.0	16.1	19.2
C5'	10.1	15.2	19.1
C4'	9.6	13.8	18.8
O1'	8.8	13.8	17.5
C1'	9.1	12.6	16.8
C3'	10.7	12.8	18.6
C2'	9.9	11.7	17.8
O2'	9.1	11.0	18.6
O3'	11.3	12.3	19.8
N9	9.8	12.8	15.5
C8	10.2	14.0	14.9
N7	10.8	13.9	13.7
C5	10.8	12.5	13.5
C6	11.3	11.7	12.5
N6	12.0	12.3	11.4
N1	11.2	10.4	12.6
C2	10.5	9.9	13.7
N3	10.0	10.5	14.7
C4	10.2	11.9	14.5

39 PSEUDOURIDINE

P	12.4	11.0	19.9
O1P	13.6	11.4	20.7
O2P	11.6	9.8	20.4
O5'	12.9	10.8	18.3
C5'	12.8	9.5	17.6
C4'	13.6	9.4	16.3
O1'	13.1	10.3	15.3
C1'	14.1	10.8	14.5
C3'	15.1	9.9	16.4
C2'	15.4	10.2	15.0
O2'	15.6	9.0	14.2
O3'	15.9	9.0	16.9
C5	14.0	12.4	14.6
C6	13.4	13.2	15.6
N1	13.3	14.5	15.6
C2	13.9	15.2	14.5
O2	13.9	16.4	14.3
N3	14.6	14.4	13.5
C4	14.7	13.1	13.6
O4	15.3	12.5	12.7

40 5M-CYTIDINE

P	16.6	9.3	18.4
O1P	16.1	10.5	19.1
O2P	16.5	8.0	19.2
O5'	18.2	9.6	17.9
C5'	19.0	8.5	17.3
C4'	19.6	8.9	15.9
O1'	18.5	9.6	15.1
C1'	19.0	10.7	14.3
C3'	20.7	10.0	15.9
C2'	20.5	10.6	14.6
O2'	21.1	9.8	13.6
O3'	22.0	9.5	16.2
N1	18.4	12.1	14.7
C6	17.5	12.2	15.8
C5	17.0	13.4	16.1
C4	17.3	14.5	15.4
N4	16.9	15.7	15.7
N3	18.2	14.4	14.3
C2	18.7	13.2	14.0
O2	19.5	13.1	13.0
C5M	16.0	13.5	17.3

41 URIDINE

P	23.1	10.5	16.9
O1P	22.7	11.0	18.2
O2P	24.4	9.8	17.0
O5'	23.2	11.8	15.9
C5'	23.9	11.6	14.5
C4'	24.2	13.0	13.9
O1'	22.9	13.6	13.5
C1'	23.0	15.1	13.8
C3'	24.8	14.0	14.8
C2'	24.5	15.3	14.1
O2'	25.2	15.5	12.9
O3'	26.2	13.8	14.9
N1	22.0	15.6	14.8
C6	21.3	14.8	15.7
C5	20.4	15.3	16.6

	X	Y	Z
C4	20.2	16.7	16.6
O4	19.4	17.3	17.3
N3	20.9	17.5	15.7
C2	21.8	17.0	14.8
O2	22.4	17.8	14.1

42 GUANOSINE

P	26.8	13.3	16.3
O1P	25.8	12.8	17.3
O2P	27.8	12.2	16.1
O5'	27.5	14.7	16.8
C5'	28.7	15.3	16.1
C4'	28.5	16.7	15.6
O1'	27.1	16.8	15.1
C1'	26.6	18.1	15.3
C3'	28.6	17.8	16.6
C2'	27.8	18.9	15.9
O2'	28.4	19.5	14.9
O3'	29.9	18.2	16.8
N9	25.4	18.1	16.3
C8	24.7	17.1	17.0
N7	23.7	17.5	17.7
C5	23.6	18.8	17.4
C6	22.7	19.7	17.9
O6	21.8	19.5	18.7
N1	23.0	21.0	17.5
C2	24.0	21.4	16.6
N2	24.0	22.6	16.3
N3	24.8	20.5	16.1
C4	24.6	19.2	16.6

43 GUANOSINE

P	30.4	19.0	18.2
O1P	29.9	18.2	19.4
O2P	31.8	19.3	18.2
O5'	29.5	20.4	18.2
C5'	29.9	21.4	17.2
C4'	29.0	22.7	17.4
O1'	27.6	22.3	17.2
C1'	26.7	23.0	18.2
C3'	28.9	23.3	18.8
C2'	27.7	24.0	18.8
O2'	27.7	25.2	18.1
O3'	30.0	24.1	19.1
N9	26.0	22.1	19.1
C8	26.1	20.7	19.4
N7	25.3	20.3	20.2
C5	24.5	21.3	20.6
C6	23.4	21.4	21.4
O6	22.7	20.5	22.0
N1	22.9	22.7	21.5
C2	23.4	23.8	20.9
N2	22.8	24.9	21.3
N3	24.5	23.8	20.1
C4	24.9	22.5	20.0

44 ADENOSINE

P	31.2	23.6	20.1
O1P	31.1	22.2	20.5
O2P	32.5	23.8	19.4
O5'	31.1	24.6	21.3
C5'	31.1	26.1	21.2
C4'	29.7	26.7	21.6
O1'	28.6	25.9	21.1
C1'	27.5	25.8	22.0
C3'	29.5	26.7	23.1
C2'	27.9	26.8	23.1
O2'	27.5	28.1	22.8
O3'	30.1	27.8	23.8
N9	27.2	24.4	22.4
C8	27.9	23.2	22.1
N7	27.4	22.1	22.6
C5	26.3	22.6	23.3
C6	25.3	22.0	24.1
N6	25.2	20.6	24.2
N1	24.3	22.7	24.6
C2	24.4	24.0	24.4
N3	25.3	24.7	23.8
C4	26.2	23.9	23.2

45 GUANOSINE

P	30.1	27.9	25.5
O1P	31.2	27.0	26.0
O2P	30.3	29.4	25.8
O5'	28.7	27.4	25.9
C5'	27.8	28.0	26.8
C4'	27.2	27.0	27.8
O1'	26.6	25.9	27.0
C1'	26.9	24.6	27.6
C3'	28.2	26.3	28.7
C2'	27.5	25.0	29.0
O2'	26.4	25.1	30.0
O3'	28.5	27.1	29.9
N9	27.8	23.8	26.7
C8	28.8	24.2	25.8
N7	29.4	23.2	25.2
C5	28.7	22.1	25.7
C6	28.9	20.7	25.4
C6	29.7	20.2	24.6
N1	28.0	19.9	26.1
C2	27.0	20.4	27.0
N2	26.3	19.5	27.6
N3	26.9	21.7	27.3
C4	27.7	22.4	26.6

46 7M-GUANOSINE

P	29.9	28.0	29.9
C1P	30.2	28.7	28.6
O2P	29.7	29.0	31.0
O5'	31.1	26.9	30.1
C5'	31.9	26.9	31.3
C4'	31.1	26.4	32.5
O1'	30.9	25.0	32.2
C1'	31.4	24.3	33.3
C3'	31.8	26.6	33.8
C2'	32.4	25.3	34.0
O2'	32.6	25.1	35.4
O3'	30.8	26.9	34.8
N9	31.9	23.0	32.8
C8	33.0	22.8	31.9
N7	33.1	21.6	31.5
C5	32.0	21.0	32.2
C6	31.6	19.7	32.1
O6	32.1	18.9	31.4
N1	30.5	19.5	32.9
C2	29.9	20.3	33.7
N2	28.9	19.7	34.3
N3	30.2	21.6	33.8
C4	31.3	21.8	33.0
C7M	34.1	21.3	30.6

47 URIDINE

P	31.0	28.3	35.7
O1P	31.2	29.5	34.7
O2P	29.9	28.4	36.6
O5'	32.4	27.9	36.4
C5'	33.0	28.9	37.3
C4'	34.3	28.3	38.0
O1'	34.7	29.3	39.0
C1'	35.1	28.6	40.2
C3'	34.1	27.0	38.8
C2'	35.2	27.1	39.8
O2'	36.5	26.9	39.3
O3'	34.1	25.8	37.8
N1	34.2	29.1	41.4
C6	32.8	29.3	41.2
C5	32.0	29.7	42.2
C4	32.6	30.0	43.5
O4	32.0	30.4	44.5
N3	34.0	29.8	43.6
C2	34.8	29.3	42.6
O2	36.0	29.2	42.8

48 CYTIDINE

P	34.8	24.3	38.1
C1P	34.1	23.4	37.2
O2P	36.3	24.4	37.9
O5'	34.5	24.1	39.7
C5'	34.8	22.9	40.4
C4'	33.7	21.9	40.2
O1'	34.0	21.1	39.0
C1'	34.0	19.7	39.2
C3'	33.6	20.8	41.3
C2'	34.3	19.7	40.7
O2'	34.0	18.5	41.4
O3'	32.3	20.5	41.7
N1	35.0	19.0	38.3
C6	36.1	19.6	37.7
O6	36.9	18.8	36.8
C4	36.5	17.5	36.5
N4	37.2	16.8	35.7
N3	35.4	17.0	37.1
C2	34.6	17.7	37.9
O2	33.6	17.2	38.5

49 5M-CYTIDINE

P	31.8	20.6	43.3
C1P	31.3	19.3	43.7
C2P	32.9	21.2	44.2
O5'	30.6	21.7	43.2
C5'	30.7	23.0	42.6
C4'	30.9	24.2	43.7
O1'	30.1	23.9	44.9
C1'	30.8	24.3	46.1
C3'	32.3	24.4	44.2
C2'	32.0	25.1	45.5
O2'	31.6	26.5	45.3
C3'	33.2	25.2	43.4
N1	31.2	23.2	47.1
C2	31.1	21.8	46.8
O2	31.5	20.9	47.6
C4	31.9	21.3	48.9
N4	32.1	20.3	49.8
N3	32.0	22.6	49.2
C2	31.7	23.5	48.4
O2	31.8	24.7	48.7
C5M	31.4	19.4	47.2

50 URIDINE

P	34.8	25.2	43.7
O1P	35.4	23.8	43.7
O2P	35.5	26.2	42.8
O5'	35.0	25.8	45.2
C5'	34.6	27.2	45.6
C4'	35.0	27.6	47.0
O1'	34.3	26.8	48.0
C1'	35.3	26.6	49.2
C3'	36.4	27.5	47.3
C2'	36.5	27.5	48.8
O2'	36.3	28.7	49.3
O3'	37.1	28.5	46.7
N1	35.6	25.1	49.4
C6	35.2	24.0	48.6
C5	35.5	22.8	48.8
C4	36.1	22.4	50.0
O4	36.3	21.3	50.3
N3	36.4	23.4	50.9
C2	36.2	24.7	50.7
O2	36.6	25.5	51.5

51 GUANOSINE

P	38.3	28.3	45.6
O1P	38.0	27.0	44.8
O2P	38.4	29.4	44.8
O5'	39.6	28.0	46.7
C5'	40.0	29.2	47.5
C4'	40.4	28.8	48.9
O1'	39.4	27.9	49.6
C1'	40.1	27.0	50.4
C3'	41.7	28.0	49.1
C2'	41.6	27.3	50.4
O2'	41.8	28.2	51.5
O3'	42.8	28.9	49.0
N9	39.8	25.5	50.1
C8	39.2	24.9	48.9
N7	39.1	23.6	48.9
C5	39.7	23.3	50.2
C6	39.8	22.0	50.8
O6	39.5	20.9	50.4
N1	40.5	22.1	52.0
C2	40.9	23.2	52.6
N2	41.5	23.1	53.8
N3	40.7	24.4	52.1
C4	40.1	24.4	50.9

52 URIDINE

P	44.3	28.4	48.7
O1P	44.3	27.5	47.5
O2P	45.2	29.6	48.5
O5'	44.7	27.6	50.0
C5'	45.2	28.2	51.2
C4'	45.8	27.1	52.1
O1'	44.7	26.3	52.6
C1'	45.2	24.9	52.7
C3'	46.8	26.2	51.5
C2'	46.7	25.0	52.4
O2'	47.4	25.3	53.6
O3'	48.0	26.7	51.3
N1	44.5	23.9	51.7
C6	43.9	24.3	50.5
C5	43.3	23.4	49.7
C4	43.2	22.1	50.0
O4	42.7	21.2	49.4
N3	43.8	21.7	51.2
C2	44.5	22.5	52.1
O2	45.0	22.1	53.1

53 GUANOSINE

P	48.9	26.2	50.0
O1P	48.0	26.2	48.7
O2P	50.1	27.1	49.8
O5'	49.3	24.7	50.4
C5'	50.1	24.4	51.6
C4'	50.0	23.0	52.1
O1'	48.5	22.6	52.2
C1'	48.4	21.2	51.9
C3'	50.6	22.0	51.3
C2'	49.8	20.7	51.7
O2'	50.3	20.2	52.9
O3'	52.0	21.9	51.5
N9	47.5	21.0	50.7
C8	47.0	21.8	49.7
N7	46.3	21.3	48.8
C5	46.3	19.9	49.2
C6	45.6	18.8	48.6
O6	44.9	18.8	47.6
N1	45.9	17.6	49.2
C2	46.7	17.5	50.3
N2	46.8	16.3	50.8
N3	47.3	18.5	50.9
C4	47.0	19.7	50.3

54 RIBOSYLTHYMINE

P	53.0	21.4	50.2
O1P	52.6	22.1	49.0
O2P	54.4	21.6	50.7
O5'	52.6	19.9	50.0
C5'	52.8	18.9	51.1
C4'	52.2	17.6	50.9
O1'	50.7	17.8	50.7
C1'	50.2	16.9	49.7
C3'	52.5	16.9	49.6
C2'	51.4	16.0	49.3
O2'	51.5	14.9	50.2
O3'	53.8	16.2	49.6
N1	49.5	17.6	48.5
C6	49.8	18.9	48.1
C5	49.2	19.5	47.0
C4	48.3	18.7	46.2
O4	47.7	19.1	45.2
N3	48.1	17.4	46.6
C2	48.7	16.9	47.7
O2	48.4	15.7	48.0
C5M	49.5	20.9	46.7

55 PSEUDOURIDINE

P	55.0	16.8	48.7
O1P	55.0	18.3	48.5
O2P	56.3	16.4	49.4
O5'	54.8	16.1	47.3
C5'	55.2	14.7	47.1
C4'	54.6	14.1	45.8
O1'	53.2	14.3	45.8
C1'	52.8	14.6	44.4
C3'	55.1	14.8	44.5
C2'	54.0	14.4	43.5
O2'	54.0	13.1	43.1
O3'	56.4	14.2	44.0
C5	52.1	15.9	44.3
C6	52.7	17.1	44.8
N1	52.1	18.3	44.6
C2	50.8	18.4	43.9
O2	50.2	19.4	43.8
N3	50.3	17.2	43.5
C4	50.9	15.9	43.6
O4	50.5	15.0	43.2

56 CYTIDINE

P	57.6	15.2	43.6
O1P	57.3	16.6	44.2
O2P	58.9	14.6	43.9
O5'	57.4	15.4	42.0
C5'	56.1	15.9	41.5
C4'	56.3	16.3	40.1
O1'	56.6	15.2	39.3
C1'	56.0	15.1	38.0
C3'	55.0	16.8	39.4
C2'	55.3	16.5	37.9
O2'	56.2	17.5	37.4
O3'	54.7	18.2	39.7
N1	55.1	13.9	38.0
C6	55.5	12.8	38.7
C5	54.8	11.6	38.8
C4	53.5	11.6	38.1
N4	52.8	10.6	38.1
N3	53.1	12.7	37.4
C2	53.9	13.8	37.3
O2	53.5	14.8	36.7

57 GUANOSINE

P	54.1	18.6	41.1
O1P	53.4	17.4	41.7
O2P	55.1	19.2	42.0
O5'	53.0	19.6	40.7
C5'	51.6	19.2	40.7
C4'	51.2	18.9	39.3
O1'	51.9	17.7	38.8
C1'	51.1	16.9	38.0
C3'	49.7	18.6	39.0
C2'	49.8	17.7	37.8
O2'	50.0	18.5	36.6
O3'	49.0	19.8	38.9
N9	51.0	15.5	38.7
C8	51.8	14.8	39.5
N7	51.5	13.6	39.9
C5	50.3	13.4	39.2
C6	49.5	12.2	39.2
O6	49.7	11.1	39.7
N1	48.3	12.4	38.4
C2	48.0	13.6	37.8
N2	46.8	13.6	37.2
N3	48.8	14.7	37.8
C4	49.9	14.5	38.5

58 1M-ADENOSINE

P	47.8	20.2	39.9
O1P	48.3	19.9	41.3
O2P	47.4	21.5	39.7
O5'	46.7	19.1	39.6
C5'	45.6	18.9	40.4
C4'	44.9	17.6	40.1
O1'	45.8	16.6	40.6
C1'	45.0	15.5	41.1
C3'	43.5	17.4	40.7
C2'	43.5	15.8	40.7
O2'	43.4	15.3	39.4
O3'	42.6	18.0	39.8
N9	45.4	15.4	42.6
C8	45.9	16.4	43.4
N7	46.3	16.0	44.6
C5	46.0	14.7	44.6
C6	46.2	13.6	45.5
N6	46.9	13.8	46.7
N1	45.7	12.4	45.2
C2	45.1	12.2	44.1
N3	44.8	13.1	43.1
C4	45.4	14.3	43.4
C1M	46.0	11.2	46.2

59 URIDINE

P	41.0	17.5	39.7
O1P	40.6	17.6	38.3
O2P	40.8	16.2	40.3
O5'	40.3	18.6	40.6
C5'	39.0	19.1	40.2
C4'	37.9	18.4	41.0
O1'	36.9	17.8	40.1
C1'	36.4	16.6	40.7
C3'	38.3	17.3	41.9
C2'	37.0	16.5	42.1
O2'	36.1	17.2	43.0
O3'	38.8	17.7	43.2
N1	36.8	15.4	39.8
C6	37.9	15.3	38.9
C5	38.1	14.2	38.2
C4	37.3	13.1	38.2
O4	37.5	12.0	37.6
N3	36.2	13.2	39.1
C2	35.9	14.3	39.8
O2	34.9	14.4	40.5

60 CYTIDINE

P	40.2	16.9	43.7
O1P	41.3	17.1	42.9
O2P	40.5	17.3	45.2
O5'	39.8	15.3	43.7
C5'	38.8	14.7	44.5
C4'	38.6	13.2	44.4
O1'	38.6	12.9	42.9
C1'	39.6	11.9	42.7
C3'	39.7	12.4	45.0
C2'	40.6	12.1	43.8
O2'	41.5	11.0	44.1
O3'	39.3	11.2	45.6
N1	40.0	12.0	41.3
C6	40.8	13.1	40.7
C5	41.2	13.1	39.4
C4	40.7	12.0	38.6
N4	41.0	12.0	37.4
N3	40.0	11.0	39.1
C2	39.6	11.0	40.4
O2	39.0	10.1	40.9

61 CYTIDINE

P	39.3	11.0	47.3
O1P	40.0	12.2	47.9
O2P	38.0	10.8	47.8
O5'	40.2	9.7	47.5
C5'	41.6	9.6	47.1
C4'	42.7	9.9	48.2
O1'	43.7	10.7	47.6
C1'	44.2	11.7	48.5
C3'	42.2	10.7	49.4
C2'	43.5	11.4	49.9
O2'	44.3	10.5	50.6
O3'	41.6	10.0	50.4
N1	43.9	13.1	48.0
C6	42.9	13.4	47.0
C5	42.7	14.7	46.5
C4	43.5	15.7	47.1
N4	43.3	16.9	46.6
N3	44.4	15.5	48.0
C2	44.6	14.2	48.5
O2	45.4	14.0	49.4

62 ADENOSINE

P	40.5	10.7	51.4
O1P	39.6	11.7	50.7
O2P	39.8	9.7	52.2
O5'	41.5	11.5	52.4
C5'	42.5	10.8	53.3
C4'	43.5	11.8	54.0
O1'	44.2	12.5	52.9
C1'	44.4	13.9	53.3
C3'	42.8	12.9	54.8
C2'	43.9	14.0	54.8
O2'	45.0	13.7	55.6
O3'	42.6	12.5	56.1
N9	43.7	14.9	52.3
C8	42.7	14.6	51.3

	X	Y	Z
N7	42.4	15.7	50.7
C5	43.0	16.7	51.3
C6	43.1	18.0	51.0
N6	42.4	18.5	50.0
N1	43.8	18.8	51.8
C2	44.5	18.3	52.8
N3	44.6	17.0	53.2
C4	43.8	16.3	52.3
63 CYTIDINE			
P	41.3	13.0	56.9
O1P	40.0	13.0	56.1
O2P	41.1	12.3	58.2
O5'	41.6	14.6	57.2
C5'	42.8	15.0	58.0
C4'	43.0	16.5	58.0
O1'	43.4	16.8	56.6
C1'	42.9	18.2	56.3
C3'	41.9	17.4	58.2
C2'	42.2	18.7	57.6
O2'	43.2	19.4	58.3
O3'	41.6	17.5	59.6
N1	41.9	18.2	55.1
C6	41.1	17.1	54.6
C5	40.3	17.2	53.6
C4	40.2	18.4	52.9
N4	39.4	18.6	51.9
N3	40.9	19.5	53.3
C2	41.7	19.4	54.4
O2	42.4	20.4	54.8
64 ADENOSINE			
P	40.2	17.1	60.2
O1P	39.5	16.0	59.4
O2P	40.3	16.6	61.6
O5'	39.3	18.5	60.1
C5'	39.7	19.6	61.0
C4'	39.9	21.0	60.3
O1'	40.5	20.8	59.0
C1'	40.0	21.8	58.1
C3'	38.7	21.8	60.1
C2'	39.2	22.7	58.9
O2'	40.0	23.7	59.4
O3'	38.3	22.6	61.2
N9	39.3	21.1	56.9
C8	39.0	19.8	56.6
N7	38.4	19.6	55.5
C5	38.2	20.9	54.9
C6	37.6	21.3	53.8
N6	37.1	20.5	52.9
N1	37.5	22.6	53.5
C2	38.0	23.5	54.4
N3	38.6	23.2	55.6
C4	38.7	21.8	55.8
65 GUANOSINE			
P	36.8	23.0	61.4
O1P	35.9	21.8	61.4
O2P	36.7	23.8	62.7
O5'	36.5	24.0	60.1
C5'	35.2	24.2	59.6
C4'	35.1	25.2	58.6
O1'	35.8	24.8	57.4
C1'	35.1	25.1	56.2
C3'	33.7	25.3	58.1
C2'	33.8	25.9	56.7
O2'	34.1	27.3	56.7
O3'	32.9	26.2	58.9
N9	34.7	23.9	55.4
C8	34.8	22.5	55.7
N7	34.4	21.7	54.7
C5	34.0	22.6	53.7
C6	33.6	22.2	52.5
O6	33.5	21.1	52.0
N1	33.2	23.3	51.7
C2	33.3	24.6	52.2
N2	32.9	25.6	51.4
N3	33.8	25.0	53.4
C4	34.1	23.9	54.1
66 ADENOSINE			
P	31.4	25.7	59.4
O1P	31.3	24.3	59.7
O2P	30.9	26.6	60.4
O5'	30.6	25.9	58.0
C5'	30.4	27.3	57.4
C4'	30.2	27.3	55.9
C1'	31.1	26.5	55.2
C1'	30.5	25.8	54.1
C3'	28.8	26.8	55.5
C2'	29.1	26.4	54.0
C2'	29.1	27.5	53.2
O3'	27.8	27.7	55.6
N9	30.5	24.3	54.2
C8	30.9	23.5	55.3
N7	30.9	22.2	55.1
C5	30.4	22.2	53.7
C6	30.2	21.1	52.9
N6	30.6	19.9	53.3
N1	29.7	21.4	51.6
C2	29.5	22.7	51.3
N3	29.7	23.7	52.0
C4	30.2	23.4	53.2
67 ADENOSINE			
P	26.3	27.3	56.1
O1P	26.4	26.4	57.2
O2P	25.5	28.5	56.4
O5'	25.8	26.5	54.8
C5'	25.3	27.2	53.6
C4'	24.9	26.3	52.4
C1'	26.0	25.4	52.1
C1'	25.5	24.1	51.8
C3'	23.8	25.3	52.8
C2'	24.0	24.2	51.9
O2'	23.5	24.5	50.6
O3'	22.5	25.9	52.7
N9	26.1	23.1	52.7
C8	26.7	23.1	54.0
N7	27.1	22.0	54.4
C5	26.8	21.1	53.8
C6	26.9	19.7	53.2
N6	27.5	18.9	54.0
N1	26.5	19.3	52.0
C2	25.9	20.1	51.2
N3	25.7	21.3	51.2
C4	26.2	21.8	52.4
68 URIDINE			
P	21.3	25.6	53.7
O1P	21.7	25.4	55.1
O2P	20.2	26.7	53.5
O5'	20.8	24.2	53.1
C5'	19.9	24.1	51.8
C4'	19.8	22.6	51.4
O1'	21.2	22.2	51.1
C1'	21.3	20.8	51.5
C3'	19.3	21.6	52.4
C2'	19.8	20.3	51.9
O2'	19.2	19.8	50.8
O3'	17.8	21.6	52.5
N1	22.2	20.5	52.7
C6	22.9	21.5	53.5
C5	23.6	21.2	54.5
C4	23.9	19.9	54.8
O4	24.6	19.4	55.7
N3	23.3	19.0	53.9
C2	22.5	19.2	52.9
O2	22.1	18.4	52.2
69 URIDINE			
P	17.1	21.1	53.9
O1P	17.9	21.7	55.1
O2P	15.7	21.5	53.8
O5'	17.3	19.5	53.9
C5'	16.6	18.6	52.9
C4'	17.0	17.2	53.1
O1'	18.5	17.1	52.9
C1'	19.0	16.1	53.8
C3'	16.7	16.5	54.4
C2'	17.8	15.4	54.5
O2'	17.4	14.3	53.7
O3'	15.4	16.1	54.5
N1	20.0	16.7	54.8
C6	20.1	18.1	55.1
C5	21.0	18.6	56.0
C4	21.9	17.7	56.6
O4	22.8	18.0	57.3
N3	21.8	16.4	56.3
C2	20.9	15.9	55.4
O2	20.9	14.7	55.3
70 CYTIDINE			
P	14.6	15.8	55.9
O1P	14.9	16.9	56.9
O2P	13.2	15.6	55.7
O5'	15.4	14.5	56.4
C5'	15.2	13.2	55.8
C4'	16.1	12.1	56.4
O1'	17.5	12.5	56.1
C1'	18.3	12.1	57.3
C3'	16.0	12.0	57.9
C2'	17.3	11.4	58.3
O2'	17.4	10.0	58.1
O3'	14.9	11.3	58.3
N1	19.0	13.3	57.9
C6	18.5	14.7	57.9
C5	19.2	15.7	58.4
C4	20.4	15.3	59.1
N4	21.1	16.3	59.6
N3	20.9	14.1	59.1
C2	20.2	13.1	58.6
O2	20.6	11.9	58.6
71 GUANOSINE			
P	14.1	11.8	59.7
O1P	14.0	13.3	59.7
O2P	12.8	11.1	59.7
O5'	15.1	11.3	60.8
C5'	15.4	9.9	61.0
C4'	16.6	9.6	61.9
O1'	17.8	10.1	61.3
C1'	18.7	10.6	62.3
C3'	16.6	10.3	63.2
C2'	18.0	10.3	63.6
O2'	18.4	9.0	64.0
O3'	15.7	9.7	64.2
N9	19.0	12.1	62.2
C8	18.4	13.1	61.5
N7	18.9	14.2	61.7
C5	19.9	14.0	62.6
C6	20.8	14.9	63.1
N1	21.7	14.3	64.0
C2	21.7	13.0	64.4
N2	22.6	12.6	65.2
N3	20.8	12.1	63.8
C4	20.0	12.7	62.9
72 CYTIDINE			
P	15.1	10.6	65.4
O1P	14.5	11.9	64.9
O2P	14.1	9.8	66.2
O5'	16.4	10.9	66.3
C5'	17.2	9.8	66.9
C4'	18.4	10.3	67.6
O1'	19.3	11.0	66.7
C1'	19.9	12.1	67.5
C3'	18.1	11.3	68.7
C2'	19.4	11.9	68.9
O2'	20.2	11.1	69.7
O3'	17.5	10.7	69.8
N1	19.6	13.5	66.9
C6	18.5	13.8	66.1
C5	18.3	15.0	65.6
C4	19.3	16.0	66.0
N4	19.1	17.2	65.4
N3	20.3	15.8	66.8
C2	20.5	14.6	67.3
O2	21.5	14.4	68.0
73 ADENOSINE			
P	16.1	11.3	70.4
O1P	15.2	11.7	69.2
O2P	15.5	10.2	71.2
O5'	16.7	12.5	71.2
C5'	17.6	12.3	72.3
C4'	18.6	13.4	72.5
O1'	19.2	13.8	71.2
C1'	19.4	15.2	71.2
C3'	18.1	14.7	73.1
C2'	19.1	15.7	72.6
O2'	20.3	15.6	73.4
O3'	18.0	14.7	74.5
N9	18.6	16.0	70.1
C8	17.6	15.5	69.3
N7	17.1	16.5	68.5
C5	17.7	17.6	68.9
C6	17.7	18.9	68.4
N6	16.8	19.3	67.5
N1	18.5	19.8	69.0
C2	19.3	19.4	69.9
N3	19.5	18.2	70.4
C4	18.7	17.4	69.8
74 CYTIDINE			
P	16.7	15.4	75.2
O1P	15.4	14.9	74.7
O2P	16.8	15.2	76.7
O5'	16.9	16.9	74.8
C5'	18.1	17.7	75.3
C4'	17.9	19.2	74.9
O1'	18.1	19.2	73.4
C1'	17.2	20.3	72.9
C3'	16.6	19.9	75.1
C2'	16.6	21.0	74.1
O2'	17.4	22.0	74.5
O3'	16.4	20.4	76.4
N1	16.2	19.7	71.9
C6	15.6	18.4	72.0
C5	14.7	18.0	71.1
C4	14.3	18.9	70.1
N4	13.4	18.6	69.2
N3	14.8	20.2	70.0
C2	15.7	20.6	70.9
O2	16.2	21.7	70.9
75 CYTIDINE			
P	15.5	19.5	77.5
O1P	14.3	18.8	76.7
O2P	16.4	18.5	78.1
O5'	15.1	20.7	78.5
C5'	13.7	21.1	78.6
C4'	13.4	22.4	77.9
O1'	13.9	22.3	76.5
C1'	13.0	23.0	75.6
C3'	11.9	22.7	77.7
C2'	11.9	23.6	76.5
O2'	12.3	24.9	76.8
O3'	11.2	23.4	78.7
N1	12.5	22.0	74.5
C6	12.2	20.7	74.7
C5	11.8	19.9	73.7
C4	11.6	20.5	72.4
N4	11.2	19.8	71.3
N3	11.9	21.8	72.2
C2	12.3	22.6	73.2
O2	12.6	23.8	73.1
76 ADENOSINE			
P	11.4	23.1	80.3
O1P	11.4	21.7	80.7
O2P	12.5	23.9	80.9
O5'	10.0	23.8	80.9
C5'	8.7	23.2	80.6
C4'	7.7	23.7	81.7
O1'	8.3	23.3	83.0
C1'	8.0	24.3	83.9
C3'	7.4	25.1	81.8
C2'	6.9	25.2	83.2
O2'	5.7	24.7	83.4
O3'	6.4	25.5	80.8
N9	9.3	24.8	84.5
C8	9.8	24.7	85.8
N7	11.0	25.2	86.0
C5	11.3	25.8	84.8
C6	12.5	26.5	84.4
N6	13.5	26.7	85.2
N1	12.5	26.9	83.1
C2	11.5	26.7	82.3
N3	10.4	26.0	82.6
C4	10.4	25.6	83.9

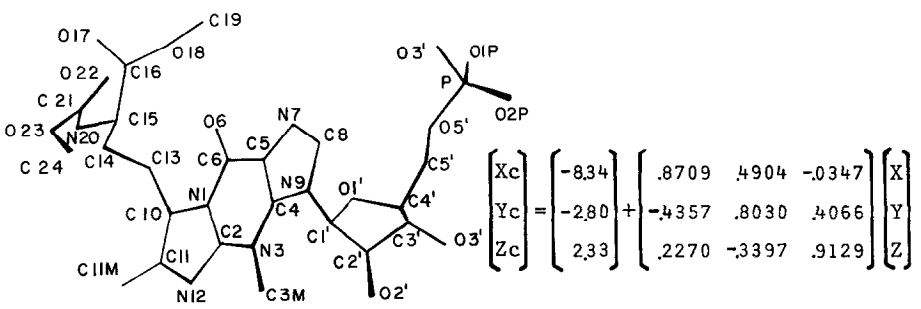

Table Legend: Atomic coordinates of yeast $tRNA^{PHE}$ in the orthorhombic crystal form on an orthogonal axis system. The Y axis was chosen to be approximately perpendicular to the molecular plane. The key for the atomic numbering, using the Y nucleotide as an example, and the conversion matrix to the crystallographic coordinates are given at the end of the table. All the atoms are listed except hydrogens, tightly bound metal ions and water molecules.

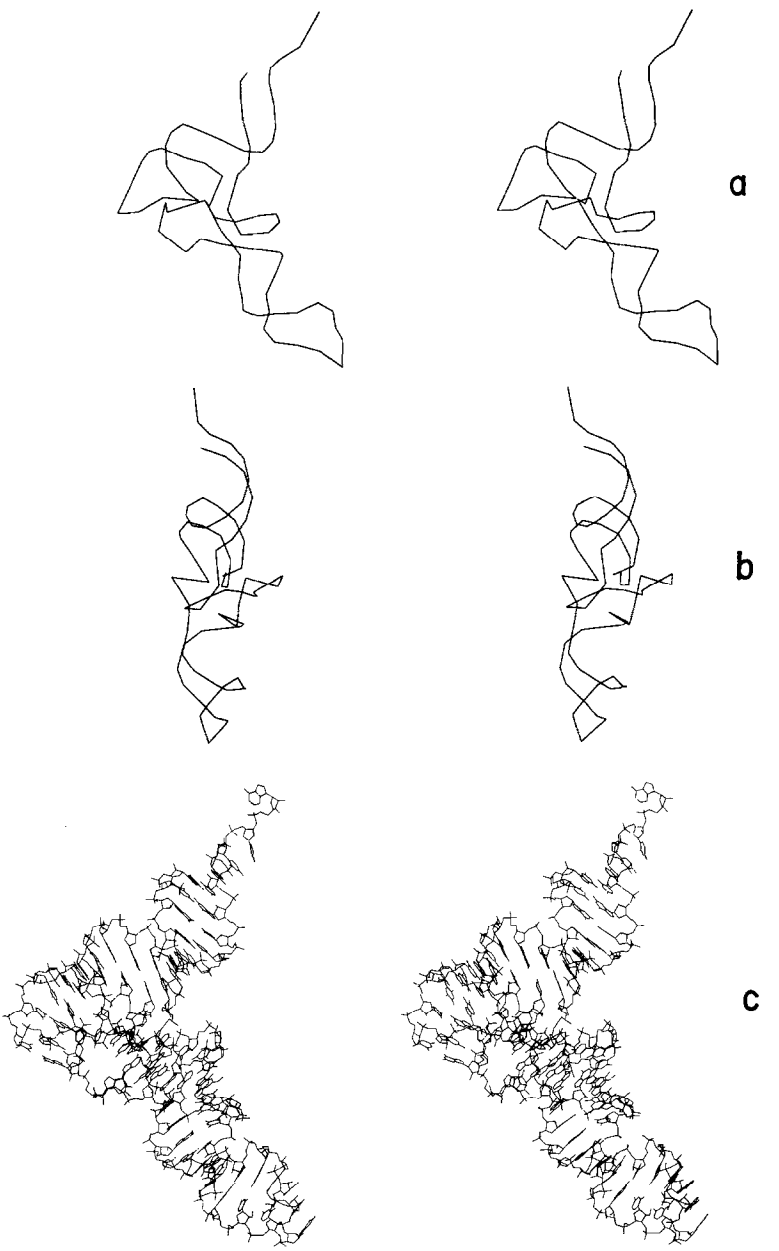

Figure Legend: Stereo views of yeast $tRNA^{PHE}$ in the orthorhombic crystal form. C1'-backbone structure viewed along the Y axis (a) and the X axis (b). The complete atomic structure viewed along the Y axis (c). The pseudo twofold axis relating the double helical stems (see ref. 9) is parallel to the X axis. The views along the Y axis, (a) and (c), are similar to the schematic drawings shown earlier (Fig. 3 of ref. 2 and Fig. 1 of ref. 9).

lengths, torsion angles, and the target positions in the electron density and a term for non-bonded interaction energy. At the current stage of refinement, the crystallographic residual index is 0.39 and the correlation coefficient (7) is 0.74. The average deviations from "standard" bond lengths and angles are 0.02 Å and 1.5° respectively, and there are no non-bonded contact distances shorter than the expected van der Waals distances by 0.1 Å.

All the riboses are in the 3'-endo conformation except those from residues 7, 9, 17, 19, 21, 46, 48, and 60, which are in the 2'-endo conformation. Most of the bases are in the anti conformation with respect to their riboses, with the following exceptions: the base of residue 19 is near the borderline between syn and anti; the bases for pyrimidine residues 17 and 60 (both have 2'-endo riboses) in the loop regions can be interpreted as either anti or syn; the base for residue 76 is tentatively assigned to be in the syn conformation. The electron densities for the last residue at the 3' end and for the side chain of the Y base are weak.

A comparison of the structures in the orthorhombic and monoclinic crystal form (8) shows that the structures in both crystal forms are essentially the same, except for a few differences. They are the positions of residues 16 and 76, the sugar conformations of residues 18 and 58, and the base conformation of residue 19. The root mean square and the average deviations (for the center positions of the phosphates, riboses and bases) between this structure and the one in the monoclinic crystal form (8) are 1.34 Å and 1.10 Å respectively, while these values between the two sets of coordinates for the orthorhombic crystal form (Duke and M.I.T.) are 1.20 Å and 0.99 Å.

Although we are continuing the refinement of this structure and the collection of higher resolution data in order to locate the tightly bound metal ions and water molecules, the coordinates presented here are sufficiently accurate for comparison, model building, drawing, designing new experiments, and interpreting other experimental results.

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