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Atomic co-ordinates for yeast phenylalanine tRNA

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ABSTRACT

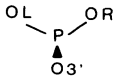
Atomic coordinates are presented for yeast $tRNA^{Phe}$ derived from a wire skeletal model fitted to an electron density map at 2.5 Å resolution obtained by isomorphous replacement.

The crystal structure of the monoclinic form of yeast $tRNA^{Phe}$ has been determined by the method of isomorphous replacement. The first stage of the X-ray analysis was carried out to a resolution of 3Å and the tertiary structure described[1]. We have now extended the resolution of the isomorphous replacement map to 2.5Å, which has enabled a more detailed and more certain interpretation to be made[2]. No serious change in our view of the structure can now be expected and it is unlikely that there will be any large changes in atomic co-ordinates on further refinement.

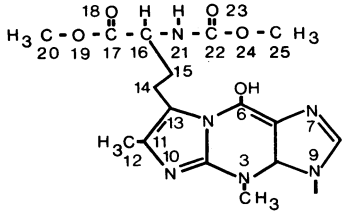
A model of yeast $tRNA^{Phe}$ was built out of Kendrew skeletal parts to fit the 2.5Å map, using a Richards optical comparator[3]. Co-ordinates were measured by hand directly on the model. Bad contacts and major errors of measurement were then removed by the energy refinement method of Levitt[4], to give the co-ordinates listed in Table 1. The final

LEGEND TO TABLE 1 (see following 6 pages)

Atoms in the bases and sugars are numbered in the standard manner. OL and OR refer to the phosphate oxygens.



The Y base[8] is numbered as follows



	X	Y	Z
1 guanosine			
O3'	27.6	5.1	50.7
P	26.3	5.8	51.5
OL	26.6	7.2	51.8
OR	25.1	5.6	50.7
O5'	26.3	5.0	52.9
C5'	25.6	5.6	54.0
C4'	26.0	4.9	55.2
O1'	25.2	3.8	55.4
C3'	27.5	4.4	55.0
C2'	27.5	3.2	55.9
O2'	27.8	3.5	57.2
C1'	26.0	2.7	55.9
N9	25.8	1.6	54.9
C8	25.0	1.6	53.9
N7	25.0	0.5	53.2
C5	26.0	-0.4	53.9
C6	26.4	-1.7	53.6
O6	26.2	-2.2	52.6
N1	27.3	-2.2	54.5
C2	27.8	-1.5	55.5
N2	28.8	-2.0	56.2
N3	27.4	-0.3	55.8
C4	26.4	0.4	54.9
2 cytidine			
O3'	28.4	5.4	55.5
P	29.7	5.6	54.7
OL	29.4	5.7	53.3
OR	30.4	6.8	55.2
O5'	30.6	4.3	55.1
C5'	31.3	4.4	56.3
C4'	32.0	3.0	56.6
O1'	31.0	2.0	56.6
C3'	33.0	2.7	55.5
C2'	33.2	1.2	55.9
O2'	34.0	1.1	57.0
C1'	31.7	0.8	56.1
N1	31.1	0.3	54.9
C2	31.3	-0.9	54.5
O2	32.1	-1.7	55.1
N3	30.7	-1.4	53.3
C4	29.9	-0.6	52.6
N4	29.3	-1.1	51.6
C5	29.7	0.7	53.1
C6	30.3	1.1	54.2
3 guanosine			
O3'	34.2	3.4	55.8
P	35.0	3.9	54.5
OL	34.1	4.2	53.4
OR	35.9	5.0	54.8
O5'	35.9	2.6	54.1
C5'	37.1	2.3	54.9
C4'	37.4	0.8	54.7
O1'	36.3	-0.0	55.0
C3'	37.8	0.5	53.3
C2'	37.5	-1.0	53.2
O2'	38.6	-1.7	53.9
C1'	36.3	-1.1	54.1
N9	35.1	-0.8	53.1
C8	34.4	0.3	53.1
N7	33.5	0.2	52.1
C5	33.7	-1.0	51.5
C6	33.0	-1.6	50.4
O6	31.9	-1.2	50.0
N1	33.4	-2.8	50.0
C2	34.5	-3.4	50.5
N2	34.9	-4.6	50.1
N3	35.1	-2.9	51.6
C4	34.7	-1.7	52.1
4 guanosine			
O3'	39.2	0.7	53.0
P	39.5	1.7	51.8
OL	38.4	1.8	50.8
OR	39.8	3.1	52.4
O5'	40.9	1.1	51.1
C5'	40.8	0.3	50.0
C4'	40.3	-1.1	50.3
O1'	38.9	-1.1	50.6
C3'	40.4	-2.0	49.1
C2'	39.3	-3.0	49.2
O2'	39.8	-4.2	50.0
C1'	38.3	-2.3	50.1
N9	37.1	-1.8	49.2
C8	36.5	-0.7	49.4
N7	35.5	-0.6	48.5
C5	35.5	-1.7	47.7
C6	34.6	-2.2	46.8
O6	33.5	-1.7	46.7
N1	34.9	-3.3	46.2
C2	35.9	-4.1	46.5
N2	36.1	-5.3	46.0
N3	36.8	-3.7	47.5
C4	36.6	-2.5	48.2
5 adenosine			
O3'	41.7	-2.6	49.1
P	42.8	-2.1	48.1
OL	44.1	-1.8	48.7
OR	43.0	-3.1	47.0
O5'	42.1	-0.8	47.5
C5'	42.1	-0.5	46.1
C4'	41.2	-1.5	45.4
O1'	40.1	-1.8	46.2
C3'	40.7	-1.1	44.0
C2'	39.6	-2.2	43.9
O2'	40.2	-3.5	43.6
C1'	39.0	-2.2	45.3
N9	38.1	-1.1	45.4
C8	38.1	-0.0	46.2
N7	37.0	0.7	46.0
C5	36.3	0.2	45.0
C6	35.0	0.4	44.5
N6	34.1	1.2	45.3
N1	34.5	-0.3	43.5
C2	35.2	-1.3	43.0
N3	36.4	-1.6	43.5
C4	37.0	-0.9	44.6
6 uridine			
O3'	41.7	-1.4	43.1
P	42.1	-0.2	42.1
OL	42.3	1.0	42.9
OR	43.3	-0.6	41.3
O5'	40.8	-0.2	41.2
C5'	40.6	-1.3	40.3
C4'	39.3	-1.0	39.5
O1'	38.2	-0.8	40.4
C3'	39.5	0.2	38.7
C2'	38.0	0.5	38.4
O2'	37.6	-0.3	37.2
C1'	37.2	-0.1	39.6
N1	36.6	0.9	40.4
C2	35.4	1.4	40.1
O2	34.9	1.1	39.0
N3	34.8	2.3	40.9
C4	35.4	2.8	41.9
O4	34.7	3.4	42.8
C5	36.7	2.4	42.3
C6	37.3	1.4	41.5
7 uridine			
O3'	40.2	-0.1	37.5
P	41.1	1.1	36.9
OL	41.6	2.0	38.0
OR	42.3	0.5	36.2
O5'	40.1	1.8	35.9
C5'	39.7	1.1	34.8
C4'	38.3	1.7	34.3
O1'	37.6	2.1	35.5
C3'	38.6	2.9	33.5
C2'	38.5	4.1	34.5
O2'	38.1	5.3	33.8
C1'	37.5	3.5	35.4
N1	37.5	4.1	36.8
C2	36.5	4.8	37.2
O2	35.7	5.3	36.4
N3	36.5	5.3	38.5
C4	37.5	5.1	39.3
O4	37.4	5.4	40.5
C5	38.6	4.3	38.9
C6	38.5	3.8	37.6
8 uridine			
O3'	37.5	3.0	32.5
P	37.7	2.3	31.1
OL	38.4	1.0	31.2
OR	36.4	2.2	30.4
O5'	38.6	3.4	30.4
C5'	38.1	4.7	30.3
C4'	39.2	5.6	29.8
O1'	40.3	5.6	30.7
C3'	39.8	5.1	28.5
C2'	41.1	5.8	28.4
O2'	41.0	7.2	28.1
C1'	41.6	5.6	29.9
N1	42.3	4.3	30.1
C2	43.5	4.1	29.6
O2	44.0	5.0	28.9
N3	44.1	3.0	29.8
C4	43.6	2.0	30.6
O4	44.3	1.0	30.9
C5	42.4	2.2	31.2
C6	41.7	3.4	31.0
9 adenosine			
O3'	39.0	5.6	27.4
P	39.0	4.6	26.1
OL	40.4	4.5	25.6
OR	38.6	3.2	26.6
O5'	38.0	5.2	25.0
C5'	38.3	6.4	24.5
C4'	38.2	6.4	22.9
O1'	39.5	6.4	22.4
C3'	37.5	5.1	22.4
C2'	38.7	4.2	22.0
O2'	38.3	3.5	20.8
C1'	39.7	5.3	21.6
N9	41.1	4.7	21.8
C8	41.4	3.6	22.4
N7	42.8	3.5	22.4
C5	43.3	4.6	21.7
C6	44.6	4.9	21.3
N6	45.6	4.1	21.6
N1	44.8	6.0	20.6
C2	43.8	6.8	20.2
N3	42.5	6.5	20.6
C4	42.2	5.3	21.3
10 2m-guanosine			
O3'	36.7	5.4	21.3
P	35.2	5.7	21.6
OL	34.9	5.6	23.1
OR	34.7	7.0	21.1
O5'	34.4	4.5	20.9
C5'	32.9	4.5	21.1
C4'	32.4	3.2	20.6
O1'	32.7	3.0	19.2
C3'	33.0	2.0	21.3
C2'	32.9	0.9	20.2
O2'	31.6	0.3	20.2
C1'	33.2	1.7	19.0
N9	34.6	1.8	18.7
C8	35.4	2.9	18.5
N7	36.7	2.5	18.4
C5	36.8	1.2	18.5
C6	37.8	0.3	18.3
O6	39.0	0.7	18.4
N1	37.6	-1.0	18.4
C2	36.4	-1.5	18.5
N2	36.2	-2.8	18.6
C2M	34.9	-3.4	18.8
N3	35.3	-0.7	18.7
C4	35.5	0.7	18.6
11 cytidine			
O3'	32.1	1.6	22.4
P	32.8	1.3	23.8
OL	34.2	1.8	23.8
OR	32.0	1.9	24.9
O5'	32.8	-0.3	24.0
C5'	33.5	-1.0	22.9
C4'	33.8	-2.5	23.2
O1'	34.5	-3.0	22.1
C3'	34.7	-2.7	24.4
C2'	35.8	-3.7	23.9
O2'	35.2	-5.0	24.1
C1'	35.8	-3.4	22.4
N1	36.9	-2.4	22.2
C2	38.1	-2.8	21.9
O2	38.4	-4.0	21.9
N3	39.1	-1.9	21.6
C4	38.8	-0.6	21.7
N4	39.8	0.3	21.3
C5	37.6	-0.1	21.9
C6	36.6	-1.1	22.2
12 uridine			
O3'	34.1	-3.3	25.5
P	34.7	-3.2	27.0
OL	34.8	-1.7	27.3
OR	33.8	-3.8	28.0
O5'	36.1	-3.9	27.0
C5'	36.1	-5.3	27.5
C4'	37.6	-5.8	27.3
O1'	38.1	-5.5	26.0
C3'	38.6	-5.2	28.3
C2'	39.9	-5.5	27.6
O2'	40.2	-6.9	27.8
C1'	39.5	-5.3	26.1
N1	39.8	-4.0	25.7
C2	41.1	-3.7	25.3
O2	41.9	-4.6	25.2
N3	41.4	-2.5	24.9
C4	40.6	-1.5	25.0
O4	40.8	-0.4	24.5
C5	39.3	-1.7	25.4
C6	38.9	-3.0	25.7
13 cytidine			
O3'	38.6	-6.0	29.5
P	39.3	-5.3	30.8
OL	38.4	-4.5	31.6
OR	39.8	-6.4	31.7
O5'	40.6	-4.5	30.3
C5'	41.8	-4.7	30.9
C4'	43.0	-4.3	30.1
O1'	42.6	-3.6	28.9
C3'	43.8	-3.2	30.9
C2'	44.7	-2.8	29.7
O2'	45.7	-3.8	29.5
C1'	43.8	-2.8	28.5
N1	43.4	-1.4	28.1
C2	44.3	-0.6	27.6
O2	45.4	-0.9	27.5
N3	43.9	0.7	27.3
C4	42.7	1.1	27.4
N4	42.3	2.1	26.6
C5	41.7	0.2	27.9
C6	42.1	-1.1	28.3
14 adenosine			
O3'	44.6	-3.9	31.9
P	45.3	-2.9	32.9
OL	44.7	-1.6	33.0
OR	45.3	-3.6	34.3
O5'	46.8	-2.8	32.4
C5'	47.1	-1.8	31.5
C4'	48.5	-1.9	30.8
O1'	48.4	-1.6	29.4
C3'	49.4	-0.8	31.4
C2'	50.3	-0.5	30.3
O2'	51.3	-1.5	30.1
C1'	49.3	-0.6	29.1

	X	Y	Z
N9	48.6	0.7	29.1
C8	47.3	0.9	29.5
N7	47.0	2.2	29.2
C5	48.1	2.9	28.7
C6	48.4	4.2	28.2
N6	47.4	5.0	28.1
N1	49.5	4.5	27.7
C2	50.5	3.6	27.6
N3	50.3	2.3	28.0
C4	49.1	1.9	28.6

15 guanosine

O3'	50.2	-1.4	32.5
P	50.6	-0.3	33.6
OL	49.4	0.0	34.4
OR	51.7	-0.9	34.5
O5'	51.2	0.9	32.8
C5'	51.6	2.0	33.6
C4'	51.7	3.3	32.8
O1'	50.7	3.1	31.8
C3'	51.3	4.5	33.6
C2'	50.7	5.4	32.5
O2'	51.8	6.2	31.9
C1'	50.2	4.4	31.5
N9	48.7	4.5	31.7
C8	48.0	3.5	32.2
N7	46.7	3.9	32.2
C5	46.6	5.2	31.7
C6	45.6	6.1	31.5
O6	44.5	6.0	32.1
N1	45.9	7.3	31.0
C2	47.1	7.6	30.6
N2	47.4	8.8	30.1
N3	48.1	6.8	30.8
C4	47.9	5.5	31.3

16 dihydrouridine

O3'	52.4	5.2	34.2
P	52.0	5.8	35.6
OL	50.6	6.3	35.6
OR	52.0	4.7	36.6
O5'	53.0	7.0	36.0
C5'	54.4	6.8	36.1
C4'	55.0	7.1	37.4
O1'	54.4	6.4	38.5
C3'	56.5	6.7	37.5
C2'	56.7	6.2	38.9
O2'	56.8	7.4	39.8
C1'	55.3	5.6	39.2
N1	55.4	4.2	38.6
C2	55.4	3.2	39.5
O2	55.6	3.4	40.7
N3	55.5	1.9	39.0
C4	55.5	1.6	37.7
O4	55.2	0.5	37.3
C5	55.6	2.7	36.7
C6	54.8	3.9	37.3

17 dihydrouridine

O3'	57.4	7.8	37.2
P	59.0	7.4	37.3
OL	59.5	7.6	38.7
OR	59.2	6.0	36.8
O5'	59.7	8.4	36.2
C5'	59.2	9.7	36.0
C4'	59.2	10.5	37.3
O1'	60.5	11.0	37.5
C3'	58.3	11.7	37.0
C2'	59.3	12.6	36.2
O2'	58.9	14.0	36.4
C1'	60.6	12.3	37.0
N1	61.8	12.5	36.1
C2	62.6	13.6	36.4
O2	62.3	14.4	37.3
N3	63.7	13.8	35.6
C4	64.0	12.9	34.7
O4	65.1	13.1	34.0
C5	63.3	11.7	34.5
C6	61.8	11.9	34.8

	X	Y	Z

18 guanosine

O3'	57.8	12.3	38.2
P	56.5	11.7	38.8
OL	56.6	10.2	39.0
OR	56.2	12.3	40.1
O5'	55.4	12.0	37.7
C5'	54.5	13.0	38.0
C4'	53.8	13.5	36.8
O1'	52.9	14.6	37.1
C3'	54.9	14.0	35.9
C2'	55.0	15.4	36.5
O2'	55.6	16.3	35.5
C1'	53.6	15.8	36.8
N9	53.5	16.7	37.9
C8	54.3	16.6	39.0
N7	54.1	17.6	39.8
C5	53.1	18.4	39.2
C6	52.5	19.6	39.6
O6	52.8	20.2	40.7
N1	51.6	20.2	38.8
C2	51.3	19.6	37.6
N2	50.5	20.3	36.8
N3	51.8	18.5	37.2
C4	52.7	17.8	38.0

19 guanosine

O3'	54.4	14.0	34.6
P	55.6	14.1	33.5
OL	56.9	14.2	34.2
OR	55.5	12.9	32.6
O5'	55.3	15.4	32.6
C5'	54.1	15.4	31.8
C4'	54.1	16.5	30.8
O1'	54.6	17.7	31.4
C3'	55.2	16.2	29.7
C2'	56.5	16.7	30.3
O2'	57.3	17.1	29.2
C1'	55.9	18.0	31.0
N9	56.7	18.3	32.2
C8	57.5	17.5	32.9
N7	58.0	18.2	33.9
C5	57.5	19.6	33.9
C6	57.6	20.6	34.7
O6	57.9	20.5	35.9
N1	56.9	21.8	34.4
C2	56.3	21.9	33.2
N2	55.6	23.0	32.9
N3	56.2	20.8	32.4
C4	56.8	19.6	32.7

20 guanosine

O3'	54.8	17.0	28.6
P	53.3	16.9	28.0
OL	52.8	15.5	28.3
OR	52.4	17.9	28.7
O5'	53.4	17.1	26.5
C5'	52.4	16.5	25.7
C4'	53.0	15.4	24.9
O1'	54.0	14.6	25.6
C3'	52.0	14.3	24.3
C2'	53.0	13.2	24.0
O2'	53.7	13.5	22.8
C1'	54.0	13.3	25.2
N9	53.4	12.4	26.2
C8	53.5	12.7	27.5
N7	52.9	11.7	28.2
C5	52.5	10.7	27.3
C6	52.0	9.4	27.4
O6	51.6	9.0	28.5
N1	51.8	8.7	26.3
C2	52.1	9.1	25.1
N2	52.2	8.3	24.1
N3	52.6	10.4	25.0
C4	52.9	11.2	26.1

21 adenosine

O3'	51.5	14.8	23.0
P	50.1	15.6	22.9
OL	49.8	16.5	24.1
OR	50.1	16.4	21.7
O5'	48.9	14.6	22.8
C5'	48.2	14.0	23.9
C4'	48.7	12.6	24.2
O1'	47.8	12.1	25.1
C3'	48.6	11.8	22.9
C2'	47.1	11.4	23.1
O2'	46.7	10.2	22.4
C1'	47.0	11.1	24.5
N9	45.6	11.2	24.9
C8	44.8	12.1	24.5
N7	43.7	12.0	25.2
C5	43.8	10.9	26 0
C6	43.0	10.4	27.1
N6	41.8	10.9	27.3
N1	43.4	9.3	27.7
C2	44.5	8.7	27.4
N3	45.3	9.1	26.4
C4	45.0	10.3	25.7

22 guanosine

O3'	50.1	10.8	22.7
P	49.7	10.1	21.2
OL	50.8	10.4	20.2
OR	48.5	10.7	20.7
O5'	49.6	8.5	21.4
C5'	50.7	7.7	21.2
C4'	50.7	6.4	22.0
O1'	50.2	6.5	23.3
C3'	49.8	5.3	21.3
C2'	49.9	4.3	22.5
O2'	51.1	3.6	22.4
C1'	49.8	5.2	23.7
N9	48.4	5.2	24.2
C8	47.6	6.2	24.1
N7	46.4	5.9	24.6
C5	46.5	4.5	25.0
C6	45.5	3.7	25.6
O6	44.4	4.1	25.8
N1	45.9	2.4	25.9
C2	47.1	2.0	25.6
N2	47.4	0.8	26.0
N3	48.0	2.8	25.1
C4	47.7	4.1	24.7

23 adenosine

O3'	50.4	4.7	20.2
P	49.5	3.8	19.3
OL	48.1	4.4	19.2
OR	50.1	3.5	18.0
O5'	49.4	2.4	20.1
C5'	50.6	1.6	20.1
C4'	50.5	0.4	21.0
O1'	50.0	0.7	22.3
C3'	49.5	-0.7	20.4
C2'	49.2	-1.5	21.7
O2'	50.3	-2.4	21.9
C1'	49.2	-0.4	22.7
N9	47.8	0.1	22.7
C8	47.4	1.3	22.3
N7	46.1	1.4	22.5
C5	45.6	0.2	23.1
C6	44.4	-0.2	23.7
N6	43.3	0.6	23.5
N1	44.3	-1.4	24.2
C2	45.3	-2.2	24.3
N3	46.5	-1.9	23.8
C4	46.7	-0.6	23.2

24 guanosine

O3'	50.2	-1.5	19.5
P	49.9	-1.4	17.9
OL	49.3	-0.1	17.6
OR	51.0	-1.7	17.1
O5'	48.8	-2.6	17.8
C5'	49.3	-3.9	17.7
C4'	48.4	-4.8	18.6
O1'	48.1	-4.1	19.8
C3'	47.1	-5.0	17.9
C2'	46.3	-5.5	19.2
O2'	46.7	-6.8	19.5
C1'	46.8	-4.6	20.3
N9	46.0	-3.4	20.2
C8	46.3	-2.1	19.9
N7	45.3	-1.3	20.0
C5	44.2	-2.0	20.5
C6	42.9	-1.7	21.0
O6	42.5	-0.5	20.8
N1	42.1	-2.6	21.4
C2	42.5	-3.9	21.4
N2	41.5	-4.9	21.5
N3	43.7	-4.3	21.1
C4	44.6	-3.4	20.6

25 cytidine

O3'	47.2	-6.2	17.1
P	46.1	-6.3	15.9
OL	46.3	-5.1	15.0
OR	46.4	-7.6	15.1
O5'	44.7	-6.3	16.5
C5'	44.0	-7.6	16.5
C4'	42.5	-7.5	16.8
O1'	42.3	-6.9	18.0
C3'	41.7	-6.8	15.7
C2'	40.4	-6.7	16.5
O2'	39.8	-8.0	16.6
C1'	40.9	-6.3	17.9
N1	41.0	-4.9	18.0
C2	39.9	-4.1	18.2
O2	38.8	-4.7	18.4
N3	40.0	-2.8	18.3
C4	41.1	-2.2	18.0
N4	41.2	-0.9	18.2
C5	42.3	-2.9	17.8
C6	42.2	-4.3	17.7

26 2,2dim-guanosine

O3'	41.4	-7.7	14.6
P	40.9	-7.1	13.2
OL	42.1	-6.5	12.6
OR	40.3	-8.1	12.3
O5'	39.8	-6.0	13.5
C5'	38.5	-6.3	13.8
C4'	37.8	-5.1	14.3
O1'	38.8	-4.4	15.1
C3'	37.6	-4.1	13.2
C2'	37.6	-2.8	13.9
O2'	36.2	-2.5	14.4
C1'	38.5	-3.0	15.1
N9	39.7	-2.2	14.9
C8	40.9	-2.6	14.6
N7	41.8	-1.5	14.5
C7M	41.0	-0.4	14.7
C5	41.2	1.0	14.6
C6	42.3	1.4	14.2
O6	40.2	1.8	14.8
N1	38.9	1.4	15.0
N2	37.9	2.2	15.0
C2M1	36.5	1.5	15.0
C2M2	38.0	3.6	14.8
N3	38.7	0.1	15.1
C4	39.7	-0.9	14.9

27 cytidine

O3'	36.3	-4.3	12.6
P	36.2	-3.9	11.0
OL	37.4	-4.4	10.3
OR	34.9	-4.5	10.5
O5'	36.1	-2.3	11.1
C5'	34.8	-1.8	11.2
C4'	34.8	-0.2	11.1
O1'	35.6	0.4	12.0
C3'	35.4	0.2	9.7
C2'	35.7	1.7	10.0
O2'	34.4	2.4	10.1
C1'	36.3	1.5	11.5
N1	37.7	1.2	11.4

	X	Y	Z
C2	38.6	2.2	11.1
O2	38.2	3.3	10.6
N3	39.9	1.9	11.0
C4	40.4	0.7	11.2
N4	41.7	0.5	11.4
C5	39.5	-0.3	11.5
C6	38.1	-0.0	11.6

28 cytidine

O3'	34.4	0.2	8.7
P	34.5	-0.9	7.5
OL	35.2	-2.1	8.0
OR	33.2	-1.3	7.0
O5'	35.4	-0.1	6.4
C5'	34.7	0.8	5.6
C4'	35.6	1.9	5.2
O1'	36.3	2.3	6.4
C3'	36.7	1.5	4.2
C2'	37.7	2.6	4.5
O2'	37.3	3.8	3.8
C1'	37.6	2.8	6.0
N1	38.6	1.9	6.6
C2	39.9	2.3	6.5
O2	40.2	3.4	6.1
N3	40.9	1.6	7.1
C4	40.6	0.4	7.7
N4	41.6	-0.3	8.2
C5	39.3	0.0	7.9
C6	38.3	0.8	7.3

29 adenosine

O3'	36.2	1.7	2.8
P	37.0	1.2	1.6
OL	37.5	-0.2	1.9
OR	36.2	1.3	0.3
O5'	38.3	2.1	1.4
C5'	38.2	3.2	0.5
C4'	39.6	4.0	0.5
O1'	40.0	4.3	1.8
C3'	40.7	3.1	-0.1
C2'	41.9	4.0	0.5
O2'	41.9	5.2	-0.3
C1'	41.4	4.3	1.9
N9	41.8	3.1	2.6
C8	40.9	2.1	3.1
N7	41.7	1.2	3.7
C5	43.0	1.5	3.6
C6	44.2	0.9	4.0
N6	44.1	-0.3	4.6
N1	45.4	1.5	3.8
C2	45.4	2.7	3.2
N3	44.3	3.3	2.8
C4	43.1	2.7	3.0

30 guanosine

O3'	40.8	3.1	-1.5
P	41.7	2.0	-2.2
OL	41.2	0.7	-1.7
OR	41.7	2.1	-3.6
O5'	43.2	2.2	-1.6
C5'	44.0	3.3	-2.2
C4'	45.5	3.1	-1.9
O1'	45.8	3.0	-0.5
C3'	46.0	1.8	-2.5
C2'	47.3	1.7	-1.7
O2'	48.3	2.5	-2.3
C1'	46.9	2.2	-0.3
N9	46.5	1.0	0.4
C8	45.2	0.6	0.6
N7	45.2	-0.5	1.3
C5	46.5	-0.9	1.6
C6	47.0	-2.0	2.3
O6	46.3	-2.7	3.0
N1	48.3	-2.1	2.4
C2	49.2	-1.2	1.8
N2	50.5	-1.5	1.7
N3	48.7	-0.2	1.1
C4	47.3	0.0	1.0

31 adenosine

O3'	46.2	1.9	-3.9
P	46.2	0.6	-4.8
OL	44.8	-0.0	-4.6
OR	46.4	0.9	-6.2
O5'	47.3	-0.3	-4.2
C5'	48.7	0.1	-4.4
C4'	49.6	-0.8	-3.6
O1'	49.1	-1.0	-2.3
C3'	49.7	-2.2	-4.2
C2'	50.2	-3.0	-3.0
O2'	51.7	-2.8	-3.0
C1'	49.6	-2.2	-1.8
N9	48.5	-3.0	-1.3
C8	47.2	-2.9	-1.5
N7	46.5	-3.8	-0.8
C5	47.4	-4.5	-0.1
C6	47.3	-5.5	0.9
N6	46.0	-5.9	1.3
N1	48.3	-6.1	1.5
C2	49.6	-5.7	1.2
N3	49.8	-4.7	0.3
C4	48.7	-4.1	-0.4

32 2'Om-cytidine

O3'	50.7	-2.2	-5.2
P	50.9	-3.4	-6.2
OL	49.9	-3.3	-7.3
OR	52.2	-3.5	-6.7
O5'	50.6	-4.8	-5.4
C5'	51.6	-5.8	-5.6
C4'	51.3	-7.1	-4.9
O1'	50.7	-7.0	-3.6
C3'	50.3	-8.0	-5.7
C2'	50.1	-9.0	-4.6
O2'	51.3	-9.8	-4.6
C2M	51.2	-10.8	-3.6
C1'	50.0	-8.2	-3.3
N1	48.6	-7.9	-3.0
C2	47.8	-8.9	-2.6
O2	48.3	-9.9	-2.2
N3	46.5	-8.6	-2.3
C4	46.0	-7.4	-2.5
N4	44.7	-7.2	-2.3
C5	46.8	-6.4	-3.0
C6	48.2	-6.7	-3.3

33 uridine

O3'	50.9	-8.5	-6.9
P	50.0	-8.3	-8.2
OL	49.5	-7.0	-8.3
OR	50.8	-8.7	-9.4
O5'	48.8	-9.4	-8.0
C5'	49.2	-10.8	-7.8
C4'	48.0	-11.4	-7.0
O1'	47.7	-10.6	-5.9
C3'	46.8	-11.6	-7.8
C2'	45.8	-11.8	-6.7
O2'	45.9	-13.1	-6.2
C1'	46.3	-10.8	-5.6
N1	45.6	-9.5	-5.8
C2	44.4	-9.4	-5.3
O2	44.0	-10.2	-4.5
N3	43.7	-8.2	-5.3
C4	44.3	-7.1	-5.9
O4	43.8	-6.0	-5.6
C5	45.6	-7.2	-6.4
C6	46.2	-8.5	-6.3

34 2'Om-guanosine

O3'	46.8	-12.8	-8.6
P	46.6	-12.5	-10.2
OL	46.8	-11.1	-10.5
OR	47.4	-13.4	-11.0
O5'	45.0	-12.9	-10.4
C5'	44.6	-12.4	-11.7
C4'	43.1	-12.8	-11.9
O1'	42.9	-14.1	-12.4
C3'	42.3	-12.6	-10.6
C2'	41.2	-13.6	-10.8
O2'	40.2	-13.0	-11.6
C2M	39.1	-14.0	-11.8
C1'	41.9	-14.7	-11.6
N9	42.6	-15.7	-10.8
C8	43.9	-16.0	-11.0
N7	44.2	-17.0	-10.1
C5	43.1	-17.5	-9.5
C6	42.8	-18.5	-8.7
O6	43.8	-19.2	-8.3
N1	41.6	-18.8	-8.2
C2	40.6	-18.0	-8.6
N2	39.4	-18.2	-8.0
N3	40.8	-17.0	-9.4
C4	42.0	-16.6	-9.9

35 adenosine

O3'	41.7	-11.3	-10.6
P	42.3	-10.1	-9.7
OL	43.8	-10.3	-9.4
OR	42.0	-8.8	-10.2
O5'	41.4	-10.4	-8.4
C5'	40.1	-9.9	-8.5
C4'	39.2	-10.9	-7.8
O1'	39.4	-12.2	-8.2
C3'	39.5	-10.9	-6.3
C2'	38.7	-12.1	-5.9
O2'	37.3	-11.8	-6.0
C1'	39.1	-13.1	-7.1
N9	40.2	-13.9	-6.7
C8	41.5	-13.7	-7.1
N7	42.3	-14.6	-6.6
C5	41.5	-15.5	-5.9
C6	41.8	-16.7	-5.2
N6	43.0	-17.2	-5.1
N1	40.8	-17.3	-4.6
C2	39.5	-16.9	-4.6
N3	39.2	-15.8	-5.3
C4	40.2	-15.0	-6.0

36 adenosine

O3'	38.9	-9.7	-5.8
P	39.6	-9.0	-4.5
OL	39.4	-7.6	-4.5
OR	41.1	-9.3	-4.5
O5'	38.9	-9.7	-3.3
C5'	37.5	-9.6	-3.2
C4'	37.0	-10.9	-2.5
O1'	37.5	-12.1	-3.2
C3'	37.5	-10.9	-1.1
C2'	37.5	-12.4	-0.9
O2'	36.2	-12.8	-0.5
C1'	37.9	-13.0	-2.2
N9	39.3	-13.2	-2.3
C8	40.2	-12.4	-3.0
N7	41.4	-12.9	-3.0
C5	41.4	-14.1	-2.2
C6	42.3	-15.1	-2.0
N6	43.6	-14.8	-2.2
N1	42.0	-16.1	-1.3
C2	40.8	-16.3	-0.8
N3	39.8	-15.4	-1.0
C4	40.1	-14.2	-1.8

37 Y

O3'	36.6	-10.3	-0.3
P	37.1	-9.8	1.1
OL	38.2	-8.9	0.9
OR	36.0	-9.1	1.9
O5'	37.6	-11.1	1.8
C5'	39.0	-11.1	2.1
C4'	39.4	-12.4	2.6
O1'	39.9	-13.2	1.6
C3'	40.6	-12.2	3.5
C2'	41.0	-13.7	3.6
O2'	40.0	-14.4	4.5
C1'	40.8	-14.1	2.2
N9	42.2	-14.0	1.6
C8	42.6	-13.1	0.8
N7	43.9	-13.3	0.5
C5	44.3	-14.4	1.2
C6	45.6	-15.0	1.4
O6	46.4	-14.8	0.6
N1	45.6	-16.1	2.2
C2	44.5	-16.6	2.8
N3	43.2	-16.1	2.6
C3M	42.1	-17.1	2.5
C4	43.2	-15.0	1.8
N10	44.8	-17.7	3.6
C11	46.1	-17.8	3.5
C12M	46.9	-18.7	4.4
C13	46.7	-16.8	2.7
C14	48.1	-16.5	2.3
C15	48.6	-17.7	1.5
C16	50.0	-17.4	1.0
C17	50.5	-18.6	0.2
O18	50.2	-18.8	-1.0
O19	51.2	-19.4	0.8
C20M	51.5	-19.1	2.1
N21	49.7	-16.3	-0.0
C22	50.7	-15.5	-0.3
O23	51.8	-15.6	0.2
O24	50.5	-14.6	-1.2
C25M	51.7	-13.8	-1.3

38 adenosine

O3'	40.2	-11.7	4.8
P	40.6	-10.2	5.1
OL	40.8	-9.4	3.8
OR	39.6	-9.5	5.9
O5'	42.0	-10.3	5.8
C5'	42.1	-11.0	7.1
C4'	43.1	-12.1	6.9
O1'	43.2	-12.4	5.5
C3'	44.5	-11.8	7.2
C2'	45.2	-12.9	6.5
O2'	45.1	-14.1	7.3
C1'	44.4	-13.1	5.3
N9	45.1	-12.5	4.2
C8	44.7	-11.5	3.3
N7	45.7	-11.2	2.5
C5	46.8	-11.9	2.8
C6	48.1	-12.0	2.3
N6	48.5	-11.1	1.4
N1	49.0	-12.8	2.9
C2	48.7	-13.5	3.9
N3	47.5	-13.5	4.4
C4	46.5	-12.7	3.9

39 pseudouridine

O3'	44.8	-12.1	8.6
P	46.0	-11.5	9.4
OL	45.8	-10.1	9.8
OR	46.3	-12.3	10.6
O5'	47.3	-11.5	8.4
C5'	48.5	-11.0	9.1
C4'	49.8	-11.0	8.2
O1'	49.5	-11.5	6.8
C3'	50.4	-9.6	8.1
C2'	51.0	-9.7	6.8
O2'	52.3	-10.3	6.9
C1'	50.1	-10.6	5.9
C5	49.0	-9.8	5.3
C4	49.3	-9.0	4.2
O4	50.5	-8.7	3.8
N3	48.3	-8.3	3.6
C2	47.0	-8.5	4.0
O2	46.1	-8.0	3.3
N1	46.8	-9.3	5.1
C6	47.7	-9.9	5.7

40 5m-cytidine

O3'	51.4	-9.5	9.1
P	51.6	-8.1	9.7
OL	50.3	-7.5	10.2
OR	52.6	-8.1	10.8
O5'	52.2	-7.2	8.5
C5'	53.6	-7.1	8.3

	X	Y	Z
C4'	53.9	-6.1	7.2
O1'	53.2	-6.5	6.0
C3'	53.4	-4.7	7.5
C2'	53.4	-4.2	6.1
O2'	54.7	-3.9	5.7
C1'	52.8	-5.3	5.3
N1	51.4	-5.2	5.2
C2	50.8	-4.3	4.3
O2	51.6	-3.6	3.7
N3	49.5	-4.2	4.2
C4	48.7	-4.9	5.0
N4	47.4	-4.7	4.9
C5	49.2	-5.8	5.9
C5M	48.3	-6.4	6.9
C6	50.6	-5.9	6.0

41 uridine

O3'	54.3	-4.0	8.3
P	53.7	-2.7	9.0
OL	52.5	-3.1	9.9
OR	54.7	-2.0	9.8
O5'	53.1	-1.7	7.9
C5'	54.1	-1.0	7.1
C4'	53.5	0.0	6.2
O1'	52.6	-0.6	5.2
C3'	52.6	0.9	7.0
C2'	51.9	1.6	5.8
O2'	52.9	2.5	5.2
C1'	51.7	0.4	4.9
N1	50.3	-0.0	5.2
C2	49.2	0.6	4.6
O2	49.4	1.5	3.9
N3	48.0	0.1	4.9
C4	47.8	-0.9	5.7
O4	46.6	-1.3	5.9
C5	48.8	-1.5	6.3
C6	50.1	-1.1	6.0

42 guanosine

O3'	53.3	1.9	7.8
P	52.6	2.5	9.0
OL	52.0	1.5	9.9
OR	53.4	3.5	9.7
O5'	51.4	3.4	8.3
C5'	51.8	4.5	7.5
C4'	50.6	5.0	6.7
O1'	49.9	3.9	6.0
C3'	49.6	5.5	7.7
C2'	48.4	5.6	6.8
O2'	48.5	6.7	5.9
C1'	48.5	4.3	6.0
N9	47.7	3.2	6.7
C8	48.2	2.3	7.4
N7	47.2	1.5	7.8
C5	46.0	2.0	7.4
C6	44.7	1.6	7.4
O6	44.4	0.4	7.7
N1	43.7	2.3	6.9
C2	44.0	3.5	6.3
N2	43.0	4.3	5.9
N3	45.3	3.9	6.1
C4	46.3	3.2	6.7

43 guanosine

O3'	50.0	6.8	8.2
P	49.5	7.1	9.6
OL	49.5	5.9	10.5
OR	50.3	8.2	10.2
O5'	48.0	7.7	9.4
C5'	47.9	8.9	8.7
C4'	46.5	9.0	8.2
O1'	46.1	7.9	7.5
C3'	45.5	9.1	9.4
C2'	44.2	8.7	8.6
O2'	43.7	9.9	7.8
C1'	44.7	7.6	7.7
N9	44.7	6.3	8.5
C8	45.7	5.7	9.0
N7	45.3	4.6	9.6
C5	44.0	4.5	9.5
C6	43.0	3.5	9.9
O6	43.4	2.4	10.3
N1	41.7	3.7	9.7
C2	41.3	4.8	9.1
N2	40.0	5.1	9.1
N3	42.2	5.8	8.7
C4	43.5	5.6	8.9

44 adenosine

O3'	45.4	10.5	9.8
P	45.2	10.8	11.4
OL	45.8	9.7	12.2
OR	45.7	12.1	11.8
O5'	43.6	10.7	11.6
C5'	42.8	11.7	11.0
C4'	41.4	11.1	10.8
O1'	41.4	10.0	10.0
C3'	40.8	10.7	12.1
C2'	39.8	9.7	11.6
O2'	38.7	10.5	11.0
C1'	40.6	9.0	10.6
N9	41.4	8.0	11.3
C8	42.7	8.0	11.3
N7	43.2	7.0	12.0
C5	42.1	6.2	12.4
C6	41.9	4.9	12.9
N6	43.0	4.1	13.1
N1	40.7	4.4	13.1
C2	39.7	5.1	12.7
N3	39.7	6.3	12.1
C4	41.0	6.9	11.9

45 guanosine

O3'	40.2	11.8	12.8
P	40.8	12.1	14.3
OL	42.2	11.7	14.4
OR	40.6	13.5	14.7
O5'	39.9	11.1	15.1
C5'	38.5	11.4	15.2
C4'	37.8	10.1	15.5
O1'	38.3	9.1	14.6
C3'	38.0	9.6	16.9
C2'	37.7	8.1	16.7
O2'	36.3	7.9	16.6
C1'	38.4	7.8	15.4
N9	39.8	7.5	15.6
C8	40.8	8.2	15.3
N7	42.0	7.5	15.7
C5	41.6	6.4	16.3
C6	42.2	5.3	16.9
O6	43.5	5.3	16.9
N1	41.6	4.3	17.4
C2	40.2	4.3	17.5
N2	39.6	3.4	18.2
N3	39.5	5.3	17.0
C4	40.2	6.4	16.3

46 7m-guanosine

O3'	37.0	10.1	17.8
P	36.8	11.6	18.3
OL	36.5	12.5	17.2
OR	35.8	11.6	19.3
O5'	38.3	12.0	19.0
C5'	39.1	11.1	19.7
C4'	38.5	10.4	20.9
O1'	39.5	9.6	21.5
C3'	38.2	11.5	21.9
C2'	39.7	11.8	22.4
O2'	39.6	12.4	23.7
C1'	40.1	10.4	22.5
N9	41.6	10.3	22.6
C8	42.4	11.2	22.1
N7	43.7	10.8	22.4
C7M	44.8	11.3	21.6
C5	43.6	9.6	23.0
C6	44.6	8.6	23.4
O6	45.6	8.5	22.7
N1	44.2	7.5	24.1
C2	42.9	7.3	24.3
N2	42.6	6.2	25.1
N3	42.0	8.1	23.9
C4	42.3	9.3	23.2

47 uridine

O3'	37.5	11.0	23.0
P	36.2	11.7	23.4
OL	35.4	12.1	22.2
OR	35.4	10.9	24.4
O5'	36.7	13.0	24.2
C5'	37.3	12.8	25.5
C4'	36.9	14.0	26.3
O1'	35.4	14.2	26.3
C3'	37.2	13.8	27.8
C2'	36.2	14.7	28.5
O2'	36.8	16.0	28.7
C1'	35.1	14.8	27.5
N1	33.8	14.3	27.9
C2	33.2	14.8	29.0
O2	33.6	15.7	29.6
N3	32.0	14.2	29.4
C4	31.4	13.3	28.7
O4	30.2	12.9	29.0
C5	32.0	12.8	27.6
C6	33.2	13.3	27.2

48 cytidine

O3'	38.6	14.3	27.9
P	39.4	14.2	29.3
OL	40.7	15.0	29.1
OR	38.7	14.8	30.4
O5'	39.8	12.7	29.5
C5'	38.8	11.7	29.8
C4'	39.5	10.4	30.2
O1'	40.7	10.3	29.5
C3'	39.8	10.4	31.7
C2'	41.2	11.0	31.8
O2'	41.9	10.5	32.9
C1'	41.8	10.3	30.5
N1	43.0	11.0	30.0
C2	44.1	10.5	30.2
O2	44.2	9.3	30.5
N3	45.3	11.1	29.8
C4	45.2	12.3	29.2
N4	46.3	12.7	28.5
C5	44.0	12.9	29.1
C6	42.9	12.3	29.5

49 5m-cytidine

O3'	39.8	9.1	32.3
P	39.1	8.9	33.6
OL	39.8	7.9	34.5
OR	39.0	10.2	34.3
O5'	37.7	8.3	33.2
C5'	36.8	9.0	32.3
C4'	35.6	9.6	33.0
O1'	35.3	8.8	34.1
C3'	36.0	10.9	33.7
C2'	34.7	11.0	34.5
O2'	33.6	11.3	33.6
C1'	34.6	9.6	35.0
N1	35.2	9.5	36.4
C2	34.5	10.0	37.4
O2	33.4	10.5	37.3
N3	35.1	10.0	38.7
C4	36.3	9.5	38.9
N4	36.8	9.5	40.1
C5	37.0	9.0	37.8
C5M	38.4	8.5	37.9
C6	36.4	9.0	36.5

50 uridine

O3'	36.1	12.1	32.8
P	37.0	13.2	33.3
OL	37.3	13.1	34.8
OR	38.3	13.2	32.6
O5'	36.2	14.6	33.1
C5'	34.8	14.5	32.8
C4'	33.9	14.7	34.1
O1'	34.0	13.7	35.1
C3'	34.1	16.0	34.8
C2'	33.3	15.7	36.1
O2'	31.9	16.0	35.7
C1'	33.5	14.2	36.3
N1	34.4	13.9	37.4
C2	34.1	14.1	38.6
O2	33.1	14.6	39.0
N3	35.0	13.8	39.6
C4	36.2	13.3	39.3
O4	36.9	12.7	40.2
C5	36.5	13.0	38.0
C6	35.6	13.4	37.0

51 guanosine

O3'	33.6	17.1	34.1
P	34.5	18.4	34.0
OL	35.9	18.0	33.7
OR	34.0	19.4	33.1
O5'	34.4	18.9	35.5
C5'	33.2	19.5	35.9
C4'	33.0	19.5	37.4
O1'	33.2	18.2	38.0
C3'	34.1	20.4	38.1
C2'	33.9	19.9	39.5
O2'	32.8	20.6	40.1
C1'	33.6	18.4	39.3
N9	34.9	17.7	39.5
C8	35.5	17.1	38.5
N7	36.7	16.5	39.0
C5	36.7	16.8	40.4
C6	37.6	16.5	41.4
O6	38.4	15.5	41.3
N1	37.4	17.0	42.6
C2	36.4	17.8	42.9
N2	36.1	18.1	44.2
N3	35.5	18.1	42.0
C4	35.6	17.6	40.7

52 uridine

O3'	33.7	21.8	38.0
P	34.8	22.9	37.7
OL	35.6	22.3	36.6
OR	34.1	24.1	37.3
O5'	35.6	23.0	39.1
C5'	35.1	24.1	39.9
C4'	35.7	23.9	41.3
O1'	35.6	22.5	41.7
C3'	37.1	24.2	41.5
C2'	37.3	23.6	42.9
O2'	36.6	24.4	43.9
C1'	36.6	22.3	42.7
N1	37.6	21.3	42.1
C2	38.5	20.8	42.9
O2	38.5	21.1	44.1
N3	39.4	20.0	42.4
C4	39.4	19.6	41.2
O4	40.3	18.8	40.7
C5	38.4	20.1	40.3
C6	37.5	21.0	40.9

53 guanosine

O3'	37.4	25.6	41.8
P	38.8	26.2	41.6
OL	39.2	26.0	40.2
OR	38.9	27.7	41.9
O5'	39.8	25.4	42.6
C5'	40.1	26.0	43.8
C4'	41.1	25.2	44.6
O1'	40.9	23.8	44.4
C3'	42.6	25.4	44.3
C2'	43.2	24.2	44.8
O2'	43.4	24.4	46.2
C1'	42.1	23.1	44.7
N9	42.4	22.3	43.5
C8	41.7	22.3	42.3
N7	42.3	21.4	41.5
C5	43.3	20.7	42.2

	X	Y	Z
C6	44.1	19.7	41.9
O6	43.8	18.9	41.0
N1	45.1	19.3	42.8
C2	45.2	19.9	44.0
N2	46.1	19.4	44.8
N3	44.4	20.9	44.3
C4	43.4	21.3	43.5

54 ribosylthymine

	X	Y	Z
O3'	43.1	26.5	45.0
P	44.5	27.2	44.7
OL	44.5	27.7	43.3
OR	44.8	28.3	45.6
O5'	45.6	26.1	44.9
C5'	46.1	25.8	46.2
C4'	47.1	24.7	46.1
O1'	46.5	23.5	45.6
C3'	48.3	24.9	45.1
C2'	48.8	23.6	45.0
O2'	49.6	23.2	46.1
C1'	47.5	22.7	44.9
N1	47.2	22.6	43.5
C2	47.7	21.6	42.8
O2	48.4	20.8	43.3
N3	47.4	21.5	41.5
C4	46.4	22.2	40.9
O4	45.9	21.9	39.9
C5	45.9	23.2	41.7
C5M	44.7	24.1	41.1
C6	46.2	23.4	43.0

55 pseudouridine

	X	Y	Z
O3'	49.3	25.7	45.7
P	50.1	26.7	44.7
OL	49.1	27.7	44.2
OR	51.2	27.3	45.4
O5'	50.6	25.7	43.5
C5'	51.7	24.9	43.8
C4'	52.0	24.1	42.5
O1'	50.9	23.3	42.0
C3'	52.2	25.1	41.3
C2'	52.2	24.1	40.2
O2'	53.4	23.3	40.2
C1'	51.0	23.2	40.6
C5	49.8	23.7	39.9
C6	49.2	23.0	38.9
O4	49.3	21.8	38.9
N3	48.1	23.5	38.3
C2	47.6	24.7	38.7
O2	46.5	25.0	38.2
N1	48.1	25.3	39.8
C6	49.1	24.9	40.4

56 cytidine

	X	Y	Z
O3'	53.5	25.8	41.5
P	53.4	27.3	41.0
OL	52.1	27.9	41.6
OR	54.5	28.1	41.5
O5'	53.3	27.3	39.5
C5'	52.9	28.5	38.9
C4'	53.3	28.5	37.4
O1'	54.7	28.3	37.2
C3'	52.6	27.3	36.7
C2'	53.5	27.2	35.5
O2'	53.2	28.3	34.5
C1'	54.9	27.5	36.1
N1	55.6	26.3	36.5
C2	55.7	25.2	35.7
O2	55.6	25.3	34.5
N3	56.4	24.1	36.2
C4	56.9	24.0	37.4
N4	57.5	22.9	37.8
C5	56.9	25.1	38.2
C6	56.2	26.3	37.7

57 guanosine

	X	Y	Z
O3'	51.3	27.7	36.2
P	50.2	26.8	36.7
OL	50.4	26.4	38.1
OR	48.8	27.4	36.6
O5'	50.3	25.5	35.8
C5'	49.7	25.6	34.5
C4'	50.1	24.5	33.5
O1'	51.5	24.4	33.4
C3'	49.6	23.1	34.0
C2'	50.6	22.2	33.2
O2'	50.1	22.2	31.8
C1'	51.9	23.0	33.3
N9	52.5	22.7	34.6
C8	52.7	23.5	35.6
N7	53.4	22.8	36.6
C5	53.6	21.5	36.1
C6	54.5	20.5	36.6
O6	55.1	20.7	37.6
N1	54.6	19.4	35.9
C2	53.9	19.2	34.7
N2	53.9	18.0	34.2
N3	53.2	20.2	34.2
C4	53.0	21.4	34.9

58 1m-adenosine

	X	Y	Z
O3'	48.3	22.9	33.4
P	47.3	21.8	34.0
OL	47.3	21.8	35.5
OR	46.0	22.0	33.4
O5'	47.8	20.3	33.5
C5'	48.8	19.7	34.3
C4'	48.5	18.2	34.5
O1'	49.0	17.8	35.8
C3'	46.9	18.0	34.7
C2'	46.8	18.2	36.2
O2'	45.6	17.5	36.6
C1'	48.0	17.5	36.7
N9	48.3	17.9	38.1
C8	47.8	19.0	38.7
N7	48.3	19.1	39.9
C5	49.2	18.0	40.1
C6	50.0	17.7	41.2
N6	50.1	18.5	42.2
N1	50.8	16.6	41.1
C1M	51.8	16.4	42.2
C2	50.7	15.8	40.0
N3	49.9	16.1	39.0
C4	49.1	17.2	39.0

59 uridine

	X	Y	Z
O3'	46.5	16.8	34.3
P	46.5	16.4	32.7
OL	45.4	17.3	32.1
OR	47.8	16.6	32.0
O5'	46.0	14.9	32.7
C5'	44.6	14.7	33.1
C4'	44.4	13.2	33.5
O1'	45.1	12.4	32.6
C3'	45.1	13.0	34.8
C2'	45.1	11.5	34.8
O2'	43.8	11.0	35.1
C1'	45.4	11.2	33.3
N1	46.7	10.7	33.1
C2	47.1	9.5	33.6
O2	46.3	8.7	33.9
N3	48.4	9.1	33.5
C4	49.3	9.9	32.8
O4	50.4	9.4	32.6
C5	48.9	11.1	32.4
C6	47.6	11.5	32.6

60 cytidine

	X	Y	Z
O3'	44.3	13.3	35.9
P	45.0	13.6	37.3
OL	45.9	14.8	37.2
OR	44.0	13.8	38.4
O5'	45.8	12.3	37.6
C5'	45.3	11.4	38.5
C4'	46.5	10.8	39.4
O1'	47.5	10.4	38.5
C3'	47.1	11.9	40.3
C2'	48.1	12.5	39.4
O2'	49.2	12.9	40.3
C1'	48.7	11.2	38.8
N1	49.6	11.3	37.6
C2	50.1	12.5	37.2
O2	50.5	13.3	38.1
N3	50.9	12.5	36.1
C4	51.2	11.4	35.4
N4	52.0	11.4	34.4
C5	50.7	10.1	35.9
C6	49.8	10.1	37.0

61 cytidine

	X	Y	Z
O3'	47.9	11.3	41.3
P	47.3	10.3	42.4
OL	46.0	10.7	42.9
OR	47.3	8.9	41.8
O5'	48.5	10.5	43.5
C5'	49.5	11.4	43.2
C4'	49.6	12.5	44.3
O1'	50.0	13.7	43.6
C3'	48.4	12.8	45.0
C2'	48.6	14.2	45.5
O2'	49.6	14.1	46.6
C1'	49.3	14.8	44.3
N1	48.2	15.3	43.4
C2	47.7	16.5	43.5
O2	48.0	17.2	44.6
N3	46.8	17.0	42.7
C4	46.3	16.3	41.7
N4	45.7	16.9	40.7
C5	46.9	15.1	41.5
C6	47.8	14.6	42.3

62 adenosine

	X	Y	Z
O3'	48.3	11.9	46.2
P	46.9	11.6	46.9
OL	46.0	11.1	45.8
OR	47.0	10.7	48.0
O5'	46.4	13.0	47.4
C5'	47.1	13.6	48.5
C4'	46.5	15.0	48.8
O1'	46.6	15.8	47.7
C3'	45.0	14.8	49.1
C2'	44.5	16.2	48.8
O2'	44.6	17.1	49.9
C1'	45.4	16.7	47.7
N9	44.8	16.5	46.4
C8	45.1	15.6	45.5
N7	44.2	15.8	44.4
C5	43.4	16.8	44.7
C6	42.3	17.4	44.0
N6	42.1	17.1	42.7
N1	41.7	18.5	44.5
C2	42.0	18.9	45.7
N3	43.0	18.4	46.4
C4	43.7	17.3	45.9

63 cytidine

	X	Y	Z
O3'	44.8	14.6	50.5
P	43.6	13.6	50.9
OL	43.8	12.3	50.2
OR	43.5	13.5	52.4
O5'	42.3	14.4	50.3
C5'	41.8	15.5	51.1
C4'	40.6	16.2	50.4
O1'	41.0	16.6	49.1
C3'	39.4	15.2	50.2
C2'	38.6	16.1	49.2
O2'	37.8	17.1	49.9
C1'	39.7	16.9	48.4
N1	39.8	16.2	47.1
C2	39.0	16.6	46.1
O2	38.2	17.5	46.3
N3	39.1	16.1	44.9
C4	39.9	15.1	44.7
N4	40.1	14.6	43.4
C5	40.8	14.6	45.7
C6	40.7	15.2	46.9

64 adenosine

	X	Y	Z
O3'	38.6	15.1	51.3
P	37.7	13.8	51.4
OL	38.5	12.6	51.0
OR	37.1	13.6	52.8
O5'	36.5	14.1	50.4
C5'	35.3	14.5	50.9
C4'	34.3	15.1	49.9
O1'	35.1	15.8	48.9
C3'	33.4	14.1	49.2
C2'	33.1	15.0	47.9
O2'	32.0	15.9	48.3
C1'	34.4	15.8	47.7
N9	35.2	15.0	46.8
C8	36.3	14.3	47.1
N7	36.8	13.7	46.0
C5	36.1	14.1	44.9
C6	36.2	13.9	43.5
N6	37.1	13.0	43.1
N1	35.3	14.4	42.7
C2	34.3	15.2	43.2
N3	34.2	15.5	44.5
C4	35.1	14.9	45.4

65 guanosine

	X	Y	Z
O3'	32.2	13.9	49.9
P	31.3	12.7	49.6
OL	32.1	11.4	49.7
OR	30.1	12.7	50.5
O5'	30.8	12.9	48.1
C5'	29.7	13.8	47.8
C4'	29.6	14.0	46.3
O1'	30.8	14.4	45.7
C3'	29.2	12.7	45.6
C2'	29.6	13.1	44.2
O2'	28.5	14.0	43.7
C1'	30.8	13.9	44.4
N9	31.9	13.0	44.3
C8	32.7	12.5	45.3
N7	33.6	11.7	44.7
C5	33.4	11.6	43.3
C6	34.2	11.1	42.3
O6	35.3	10.7	42.5
N1	33.7	11.2	41.0
C2	32.6	11.9	40.8
N2	32.1	11.8	39.6
N3	31.9	12.5	41.7
C4	32.3	12.4	43.1

66 adenosine

	X	Y	Z
O3'	27.9	12.4	45.7
P	27.5	10.8	45.7
OL	28.2	10.2	46.9
OR	26.0	10.6	45.9
O5'	28.0	10.2	44.3
C5'	27.1	10.5	43.2
C4'	27.8	10.1	41.9
O1'	29.2	10.4	41.9
C3'	27.7	8.6	41.6
C2'	28.7	8.6	40.4
O2'	28.0	9.1	39.2
C1'	29.8	9.6	40.9
N9	30.9	8.9	41.4
C8	31.3	8.8	42.7
N7	32.5	8.2	42.8
C5	32.9	7.8	41.5
C6	34.0	7.1	41.0
N6	35.0	6.8	41.8
N1	34.1	6.9	39.7
C2	33.1	7.3	38.9
N3	32.0	7.9	39.3
C4	31.9	8.2	40.6

67 adenosine

	X	Y	Z
O3'	26.4	8.2	41.1
P	25.6	7.1	42.0
OL	26.3	6.9	43.2
OR	24.2	7.5	42.1
O5'	25.7	5.7	41.1

	X	Y	Z
C5'	24.7	5.5	40.0
C4'	25.4	4.8	38.8
O1'	26.5	5.5	38.3
C3'	25.9	3.3	39.2
C2'	27.0	3.2	38.1
O2'	26.4	2.9	36.8
C1'	27.6	4.6	38.0
N9	28.6	4.7	39.1
C8	28.4	5.5	40.2
N7	29.5	5.4	41.0
C5	30.4	4.6	40.4
C6	31.7	4.2	40.7
N6	32.2	4.5	41.9
N1	32.4	3.4	39.9
C2	31.8	2.9	38.8
N3	30.6	3.3	38.4
C4	29.8	4.1	39.2

68 uridine

O3'	24.9	2.4	38.8
P	25.0	0.9	39.4
OL	24.7	1.0	40.9
OR	24.0	0.0	38.7
O5'	26.5	0.4	39.2
C5'	26.8	-0.1	37.9
C4'	28.2	-0.7	38.0
O1'	29.2	0.2	38.4
C3'	28.3	-1.9	39.0
C2'	29.8	-1.9	39.2
O2'	30.3	-2.7	38.0
C1'	30.2	-0.5	39.0
N1	30.5	0.1	40.4
C2	31.7	-0.1	41.0
O2	32.5	-0.9	40.5
N3	31.9	0.5	42.2
C4	31.0	1.2	42.8
O4	31.4	2.0	43.7
C5	29.8	1.4	42.2
C6	29.5	0.9	41.0

69 uridine

O3'	27.8	-3.1	38.4
P	27.5	-4.3	39.4
OL	26.6	-3.8	40.5
OR	26.8	-5.4	38.6
O5'	28.9	-4.8	39.9
C5'	29.7	-5.6	39.0
C4'	31.1	-5.7	39.7
O1'	31.6	-4.4	40.0
C3'	31.0	-6.4	41.1
C2'	32.3	-6.0	41.6
O2'	33.4	-6.7	40.9
C1'	32.4	-4.5	41.2
N1	31.8	-3.7	42.3
C2	32.5	-3.2	43.3
O2	33.5	-3.9	43.6
N3	32.0	-2.4	44.2
C4	30.7	-2.0	44.2
O4	30.3	-1.2	45.0
C5	29.9	-2.5	43.1
C6	30.5	-3.3	42.2

70 cytidine

O3'	30.8	-7.7	40.9
P	29.5	-8.3	41.7
OL	28.4	-7.3	41.6
OR	29.1	-9.6	41.2
O5'	30.0	-8.4	43.2
C5'	31.0	-9.4	43.4
C4'	32.0	-8.8	44.4
O1'	32.0	-7.4	44.4
C3'	31.5	-9.1	45.9
C2'	32.5	-8.2	46.5
O2'	33.8	-8.9	46.5
C1'	32.6	-7.0	45.6
N1	31.9	-5.8	46.2
C2	32.5	-5.1	47.1
O2	33.5	-5.5	47.7
N3	31.9	-4.1	47.7
C4	30.6	-3.7	47.3
N4	30.1	-2.6	47.7
C5	30.0	-4.5	46.3
C6	30.6	-5.6	45.8

71 guanosine

O3'	31.7	-10.4	46.2
P	30.6	-11.0	47.2
OL	29.3	-10.4	47.0
OR	30.5	-12.5	47.1
O5'	31.2	-10.6	48.7
C5'	32.1	-11.5	49.3
C4'	32.9	-10.7	50.3
O1'	33.4	-9.5	49.8
C3'	32.1	-10.4	51.5
C2'	32.9	-9.2	52.1
O2'	34.1	-9.8	52.8
C1'	33.4	-8.5	50.8
N9	32.4	-7.5	50.5
C8	31.5	-7.6	49.5
N7	30.8	-6.5	49.5
C5	31.2	-5.7	50.6
C6	30.8	-4.4	51.1
O6	29.9	-3.8	50.5
N1	31.4	-3.9	52.1
C2	32.4	-4.6	52.7
N2	33.0	-4.0	53.8
N3	32.8	-5.8	52.3
C4	32.3	-6.4	51.2

72 cytidine

O3'	32.1	-11.4	52.5
P	30.8	-11.5	53.5
OL	29.6	-11.4	52.7
OR	30.9	-12.7	54.3
O5'	31.0	-10.2	54.4
C5'	32.0	-10.2	55.4
C4'	32.0	-8.8	56.0
O1'	32.0	-7.8	55.0
C3'	30.7	-8.6	56.7
C2'	30.7	-7.1	56.8
O2'	31.6	-6.6	57.9
C1'	31.3	-6.7	55.4
N1	30.2	-6.3	54.5
C2	29.7	-5.1	54.7
O2	30.2	-4.3	55.3
N3	28.6	-4.8	53.9
C4	28.2	-5.6	52.9
N4	27.4	-5.1	51.9
C5	28.7	-6.8	52.8
C6	29.8	-7.2	53.6

73 adenosine

O3'	30.7	-9.1	58.0
P	29.6	-10.2	58.3
OL	29.5	-11.1	57.2
OR	29.9	-11.0	59.6
O5'	28.3	-9.4	58.5
C5'	28.0	-8.8	59.8
C4'	27.2	-7.5	59.6
O1'	27.7	-6.9	58.4
C3'	25.7	-7.6	59.4
C2'	25.4	-6.3	58.7
O2'	25.5	-5.3	59.7
C1'	26.6	-6.2	57.8
N9	26.2	-6.8	56.5
C8	26.7	-8.0	56.1
N7	26.1	-8.3	54.9
C5	25.2	-7.3	54.6
C6	24.3	-7.1	53.5
N6	24.0	-8.1	52.7
N1	23.5	-6.0	53.5
C2	23.6	-5.1	54.5
N3	24.4	-5.2	55.5
C4	25.3	-6.3	55.6

74 cytidine

O3'	25.0	-7.6	60.6
P	23.5	-7.9	60.7
OL	23.3	-9.4	60.3
OR	22.9	-7.7	62.1
O5'	22.7	-7.0	59.7
C5'	22.2	-5.7	60.0
C4'	21.3	-5.3	58.9
O1'	21.9	-5.4	57.6
C3'	20.1	-6.3	58.9
C2'	19.6	-6.0	57.5
O2'	18.9	-4.7	57.4
C1'	20.9	-5.8	56.7
N1	21.3	-7.2	56.2
C2	20.7	-7.7	55.1
O2	19.9	-7.1	54.5
N3	21.1	-8.9	54.7
C4	22.1	-9.6	55.3
N4	22.7	-10.6	54.6
C5	22.7	-9.1	56.4
C6	22.3	-7.9	56.8

75 cytidine

O3'	19.1	-6.0	59.8
P	18.9	-7.1	61.0
OL	19.8	-8.3	60.7
OR	19.2	-6.5	62.3
O5'	17.4	-7.4	60.8
C5'	16.5	-6.4	61.1
C4'	15.1	-6.7	60.4
O1'	15.2	-6.4	59.0
C3'	14.6	-8.1	60.6
C2'	13.8	-8.3	59.3
O2'	12.4	-7.8	59.6
C1'	14.5	-7.4	58.3
N1	15.4	-8.1	57.5
C2	15.0	-8.8	56.4
O2	13.8	-8.8	56.2
N3	15.9	-9.5	55.7
C4	17.2	-9.5	56.0
N4	18.1	-9.8	55.1
C5	17.6	-8.8	57.1
C6	16.7	-8.1	57.8

76 adenosine

O3'	13.6	-8.1	61.7
P	13.9	-7.4	63.1
OL	12.8	-7.9	64.0
OR	15.2	-7.8	63.6
O5'	13.7	-5.9	62.8
C5'	12.7	-5.4	62.0
C4'	11.9	-4.2	62.5
O1'	10.9	-4.6	63.4
C3'	12.8	-3.2	63.2
C2'	11.9	-2.6	64.2
O2'	11.1	-1.6	63.5
C1'	11.0	-3.7	64.5
N9	11.5	-4.5	65.7
C8	12.7	-5.1	65.6
N7	12.9	-5.8	66.8
C5	11.8	-5.6	67.6
C6	11.5	-5.9	68.9
N6	12.3	-6.7	69.6
N1	10.3	-5.6	69.4
C2	9.5	-4.8	68.8
N3	9.8	-4.4	67.5
C4	10.9	-4.8	66.9
OH3'	13.2	-2.2	62.2

X	Y	Z

crystallographic discrepancy index, R, was 39%, a value which compares well with that for most proteins at this stage of the analysis.

The co-ordinates are given in Å on a Cartesian reference system whose x, y and z axes are parallel to the crystallographic directions a^*, b, c. The placing of the molecule in the unit cell is shown in earlier diagrams (Fig. 2a of ref. 7, see also Fig. 5 of ref. 1), and the origin of x and z co-ordinates is at the upper right hand corner of the unit cell shown there. The origin of x lies outside the molecular body, and the bulk of the model (apart from the CCA end) will occupy a slab x = 25 to 65Å, y = -20 to 29Å, z = -13 to 53Å.

All bases are anti with respect to their sugars and the sugar conformation is C3'-endo for all but ten where it is of the C2'-endo type. These ten are the sugars of residues 7, 9, 17, 18, 19, 21, 46, 48, 58 and 60.

A similar model has been proposed by Kim et al. for the closely related orthorhombic form[5]. Apart from several differences about precise H-bonding schemes, the tertiary structure appears to be essentially the same as that found for the monoclinic crystal studied here. A paradox nevertheless remains because in the revised interpretation[5] of the 3Å map of the orthorhombic crystal[6] it is stated that the nucleotide assignment previously made to peaks in the map of a stem region was incorrect by one nucleotide. We have shown[7] that the assignment in one strand of the crucial D stem and loop was in error by two nucleotides, in the other strand by one, and also that assignments in other helical stems were incorrect. It therefore remains to be seen by a comparison of atomic co-ordinates whether there is still a real difference between the two models.

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