Supplementary information

Table 1: The ^{1}H, ^{13}C chemical shifts of the *H. hal.* 29-mer RNA based on the assignment of the exchangeable protons (measured at 2ºC) and non-exchangeable proton, carbon resonances (measured at 25ºC). A mark "~" indicates that the chemical shift was not obtained during assignment.

Table 2: Table giving information on the five groups of NOEs and the parameters used in CcpNmr Analysis to produce the NOE based distance constraints.

Table 3: Table indicating the approximate value of the $^3J_{H1',H2'}$ for each residue and how the ribose of the residue was constrained based on this information. The final column indicates how the glycosic torsion angle (χ) was constrained.

Table 4: Table giving the imino proton chemical shifts and whether they were constrained as Watson-Crick base pairs in the structure determination.

Table 5: The Table shows the base pairs observed in the NMR structure of *H. hal.* 29mer RNA; whether they are standard Watson-Crick base pairs, their hydrogen bonds and their distances. The mark "---" indicates that the particular field is not relevant to the particular base pair.

Table 6: The Table shows the local base pair step parameters and the form of the RNA at a given step. A mark "~" indicates that the information could not be given.

Table 7.1 – 7.6: Additional helical parameters and dihedral angles for the *H. hal.* 29-mer NMR solution structure. The local step parameters are shown in Table 7.1 and the local base pair parameters are shown in Table 7.2. The ribose dihedral angles of the base paired residues, their sugar pucker, the amplitude of pseudorotation of the sugar ring and the phase angle of pseudorotation of the sugar ring are shown in Tables 7.3 and 7.4. Tables 7.5 and 7.6 show the backbone and glycosidic torsion angles of all the base paired residues.

Left panel

	C8	C6	C5	C2	C5'	C4'	C3'	C2'	C1'	H5b	H5a	H4'	H3'	H2'	H1'	H2	H8	H6	H5	H42	H41	H22	H21	H62	H61	Imino
C1		145.10	98.57		61.74					3.91	4.05	4.33		4.48	5.52			6.12	6.01							
C2		141.85	97.42						90.64					4.48	5.61			7.99	5.62		8.37					
C3		141.31	97.65						92.94					4.35	5.49			7.78	5.56		8.39					
U4		141.79	103.67					–						–	5.62	7.02	8.01	7.82	5.42							13.22
A6	141.24		103.98	152.87					92.94				4.33	4.63	5.90		8.10	7.25	5.22					6.37	7.61	10.91
A7				152.88									4.47	4.11	5.08	6.92	7.24									
G8														4.60	5.83		8.03							6.37		13.22
A9				153.39									4.47	4.60	5.53	7.42	7.33									
G10													4.46	4.79	5.97											13.50
C11		140.98	97.18						92.61				4.38	4.38	5.60			7.57	5.20							
U12		142.19	103.72						94.36				4.35	4.40	5.61			7.86	5.38							14.01
U13		142.91	104.11										4.38	4.29	5.83			7.93	5.66							13.82
U14		143.58	104.51									4.20	4.24	4.14	5.64			7.80	5.68							

Right panel

	C8	C6	C5	C2	C8'	C4'	C3'	C2'	C1'	H5b	H5a	H4'	H3'	H2'	H1'	H2	H8	H6	H5	H42	H41	H22	H21	H62	H61	Imino
A21	142.33			153.92	63.18				91.76	3.88	3.80	4.33	4.61	4.65	5.75	7.65	8.19									
A22	140.46			153.39					90.82				4.53	4.72	5.80	7.42	8.08								6.54	
A23	139.63			153.40										4.67	5.87	7.58	7.83							7.87	7.87	
G24	135.73								92.68				4.47	–	5.54		7.13									13.50
C25		141.00	97.29						94.24				4.37	4.29	5.46			7.48	5.17							
U26		142.00	104.16						98.19					4.36	5.84	7.72	7.75		5.40							13.62
A27	141.33			154.66										–	5.97		8.29									
C28		97.67							93.86					4.48	5.42			7.49	5.53							
C29		95.58											4.39	4.20	5.64			7.86	5.95			6.07				
U30		103.76							98.88					4.26	5.30			7.79	5.54							12.99
U31		104.16		152.74										4.63	5.64	6.91	8.21	7.92	5.71							13.95
G33									98.13				4.44	4.58	5.93		7.23							7.59		12.99
G34													4.37	4.53	5.63		7.06									12.76
G35	137.17												4.21	4.05	5.87		7.30									12.56

Table 1

NOE group	Reference intensity	Reference distance	Upper/ lower fractional error	Distance function	Number of constraints generated
Exchangeable	7.99×10^6	3.2	1.00/1.00	$i^{-1/4}$	35
Non-overlapped	7.65×10^5	3.7	0.30/0.30	$i^{-1/6}$	53
Overlapped	7.65×10^5	3.7	0.60/0.30	$i^{-1/6}$	55
Very overlapped	7.65×10^5	3.7	0.90/0.30	$i^{-1/6}$	77
Very, very overlapped	7.65×10^5	3.7	1.20/0.30	$i^{-1/6}$	36
Total number of NOE constraints					256

Table 2

Residue	Approximate $^3J_{H1',H2'}$ (Hz)	Ribose constrained as	Glycosidic angle constrained as
C1	Small	$C_{3'}$-endo	Unconstrained
C2	Small	$C_{3'}$-endo	anti
C3	Small	$C_{3'}$-endo	anti
U4	Small	$C_{3'}$-endo	anti
A5	Small	$C_{3'}$-endo	Unconstrained
U6	Small	Unconstrained	Unconstrained
A7	Small	Unconstrained	Unconstrained
G8	Large	Unconstrained	Unconstrained
A9	Small	Unconstrained	Unconstrained
G10	Small	$C_{3'}$-endo	anti
C11	Small	$C_{3'}$-endo	anti
U12	Small	Unconstrained	anti
U13	Large	$C_{2'}$-endo	anti
U14	Large	$C_{2'}$-endo	Unconstrained
A21	Large	$C_{2'}$-endo	Unconstrained
A22	Small	$C_{3'}$-endo	anti
A23	Small	Unconstrained	anti
G24	Small	$C_{3'}$-endo	anti
C25	Small	$C_{3'}$-endo	anti

U26	Large	Unconstrained	Unconstrained
A27	Large	Unconstrained	Unconstrained
C28	Small	Unconstrained	Unconstrained
C29	Small	Unconstrained	Unconstrained
U30	Small	Unconstrained	Unconstrained
U31	Small	Unconstrained	*anti*
A32	Large	Unconstrained	*anti*
G33	Small	$C_{3'}$-*endo*	*anti*
G34	Small	$C_{3'}$-*endo*	*anti*
G35	Large	$C_{2'}$-*endo*	Unconstrained

Table 3

Base pair	Imino chemical shift (δ, ppm)	Base pair constrained?
C1-G35	12.56	Yes
C2-G34	12.76	Yes
C3-G33	12.99	Yes
U4-A32	13.22	Yes
A5-U31	13.95	Yes
A7-U30	12.99	No
G8-C29	13.22	No
A9-U26	13.62	No
G10-C25	13.50	Yes
C11-G24	13.50	Yes
U12-A23	14.01	Yes
U13-A22	13.92	Yes
U14-A21	~	Yes

Table 4

Base pair	W-C type?	First hydrogen bond	Distance (Å)	Second hydrogen bond	Distance (Å)	Third hydrogen bond	Distance (Å)	Fourth hydrogen bond	Distance (Å)
1C-G35	Yes	O2 - N2	2.99	N3 - N1	2.78	N4 - O6	2.92	---	---
2C-G34	Yes	O2 - N2	2.40	N3 - N1	2.37	N4 - O6	2.35	---	---
3C-G33	Yes	O2 - N2	2.72	N3 - N1	2.62	N4 - O6	2.55	---	---
4U-A32	Yes	N3 - N1	2.82	O4 - N6	2.58	---	---	---	---
5A-U31	Yes	N1 - O2	2.40	N1 - N3	2.60	---	---	---	---
6U-U30	No	N3 - O2	4.24	O4-N3	4.46	---	---	---	---
7A-C29	No	N1 - N3	3.33	N1-N4	3.31	N6-N4	3.16	---	---
8G-C28	No	N1 - N3	3.50	O6 - N3	2.76	---	---	---	---
9A-A27	No	N3 - N1	3.39	N1 - N3	3.93	N6 - N7	4.15	N7-N6	4.43
10G-C25	Yes	N2 - O2	3.01	N1 - N3	2.77	O6 - N4	2.50	---	---
11C-G24	Yes	O2 - N2	2.25	N3 - N1	2.33	N4 - O6	2.33	---	---
12U-A23	Yes	O2 - N1	2.72	N3 - N1	2.67	---	---	---	---
13U-A22	Yes	N3 - N1	2.64	O4 - N6	2.75	---	---	---	---
14U-A21	Yes	N3 - N1	2.49	O4 - N6	2.94	---	---	---	---

Table 5

Step	Shift (Dx)	Slide (Dy)	Rise (Dz)	Tilt (τ)	Roll (ρ)	Twist (Ω)	Form
C1-C2/G34-G35	0.73	-1.35	3.83	-13.84	12.24	27.74	A
C2-C3/G33-G34	0.15	-1.41	3.60	15.13	7.21	27.42	A
C3-U4/A32-G33	-1.45	-1.13	3.80	-5.84	4.24	29.32	A
U4-A5/U31-A32	0.22	-1.78	3.23	-3.91	4.45	29.12	A
A5-U6/U30-U31	0.58	-1.35	3.16	6.48	0.77	34.27	A
U6-G8/C29-U30	-0.96	-1.41	5.91	16.73	3.26	46.73	~
G8-A9/A27-C29	-0.46	0.18	5.55	-12.35	13.56	67.04	~
A9-G10/C25-A27	3.37	-1.98	5.07	-22.34	5.28	30.30	A
G10-C11/G24-C25	0.01	-2.12	4.55	-1.59	9.24	26.97	A
C11-U12/A23-G24	-0.40	-1.64	3.63	6.55	13.55	24.49	~
U12-U13/A22-A23	1.39	-0.83	3.92	-3.19	-7.32	31.30	~
U13-U14/A21-A22	0.32	-1.36	4.31	-10.39	-11.27	27.92	~

Table 6

Step	X-displacement	Y-displacement	Inclination	Tip
C1-C2/G34-G35	-4.53	-1.92	23.90	15.16
C2-C3/G33-G34	-6.02	3.94	20.48	-16.39
C3-U4/A32-G33	-3.29	-0.74	2.34	6.95
U4-A5/U31-A32	-5.40	-1.25	13.52	10.93
A5-U6/U30-U31	-1.81	-2.19	-2.22	-12.72
U6-A7/C29-U30	-1.06	2.94	2.62	-22.29
A7-G8/C28-A27	-4.06	5.18	31.01	11.55
G8-A9/A27-C28	-1.91	-3.26	3.35	2.11
A9-G10/C25-A27	-2.58	-6.04	8.15	36.67
G10-C11/G24-C25	-7.77	-0.67	25.44	-0.23
C11-U12/A23-G24	-5.60	3.29	26.47	-19.61
U12-U13/A22-A23	-0.84	-0.96	-5.20	4.36
U13-U14/A21-A22	1.04	-5.37	-19.27	16.97

Table 7.1: Shows the local base pair step parameters of the *H. hal.* 29-mer NMR solution structure.

Base pair	Shear	Stretch	Stagger	Buckle	Propeller	Opening
C1-G35	-0.37	-0.38	-0.86	-3.81	29.95	-10.85
C2-G34	-0.10	-0.67	0.19	13.09	11.35	-0.03
C3-G33	-0.32	-0.98	-1.67	3.99	7.42	-11.22
U4-A32	0.14	-0.31	-0.62	1.51	-2.76	-8.36
A5-U31	0.22	-1.02	1.43	0.72	-17.19	-10.66
U6-U30	-1.87	-0.48	1.30	-7.40	-26.19	12.37
A7-C29	0.96	-0.34	-2.07	-7.35	-6.18	-1.92
G8-C28	-0.07	-0.62	-2.33	-7.86	-21.46	-52.50
A9-A27	1.06	-0.14	-0.89	-21.26	10.74	-25.28
G10-C25	0.19	-0.28	0.02	12.03	14.60	-8.98
C11-G24	0.02	-0.71	-0.23	0.23	5.81	-1.55
U12-A23	0.14	-0.89	-1.71	6.95	7.04	-10.68
U13-A22	0.02	-0.80	-1.68	14.84	12.68	-10.37
U14-A21	0.35	-0.56	0.69	-0.98	30.60	14.97

Table 7.2: Shows the local base pair parameters of the *H. hal.* 29-mer NMR solution structure.

Residue	v_0	v_1	v_2	v_3	v_4	tm	P	Puckering
C1	-14.2	-9.1	27.0	-36.6	31.8	36.0	41.5	$C_{4'}$-*exo*
C2	-6.2	-17.3	32.3	-37.4	27.5	36.7	28.4	$C_{3'}$-*endo*
C3	-15.5	-8.4	27.1	-37.3	33.2	37.0	43.0	$C_{4'}$-*exo*
U4	-6.6	-15.0	29.7	-34.8	25.7	34.2	29.7	$C_{3'}$-*endo*
A5	-1.7	-20.1	32.5	-35.1	23.2	35.0	21.7	$C_{3'}$-*endo*
U6	-0.4	-23.8	37.1	-38.7	24.7	39.4	19.3	$C_{3'}$-*endo*
A7	-17.0	-1.9	18.4	-29	28.8	30.0	52.2	$C_{4'}$-*exo*
G8	-24.4	6.9	11.3	-26	31.7	31.1	68.6	$C_{4'}$-*exo*
A9	-18.7	-2.6	21.1	-32.8	31.9	33.7	51.3	$C_{4'}$-*exo*
G10	-7.1	-16.1	31.4	-37	27.7	36.3	29.9	$C_{3'}$-*endo*
C11	-18.6	-5.5	25.7	-37.8	35.3	38.0	47.4	$C_{4'}$-*exo*
U12	-32.8	23.6	-6.5	-12.7	28.6	32.4	101.5	$O_{4'}$-*endo*
U13	-28.4	33.0	-25.4	9.5	11.9	32.8	140.8	$C_{1'}$-*exo*
U14	-26.9	36.2	-31.2	16.5	6.3	35.6	151.1	$C_{2'}$-*endo*

Table 7.3: Shows the ribose dihedral angles,v_0 to v_4, the amplitude of *pseudorotation* of the sugar ring, tm, the phase angle of pseudorotation of the sugar ring, P, and the resultant type of puckering of the first strand of the *H. hal.* 29-mer NMR solution structure.

Residue	v_0	v_1	v_2	v_3	v_4	tm	P	Puckering
G35	-29.4	43.8	-40.3	24.6	2.8	43.6	157.5	$C_{2'}$-endo
G34	-20.9	-3.0	23.8	-37.2	36.2	38.0	51.2	$C_{4'}$-exo
G33	-23.6	-1.2	23.6	-38.4	38.9	40.1	54.0	$C_{4'}$-exo
A32	-13.8	-10.8	29.4	-38.8	32.9	38.1	39.5	$C_{4'}$-exo
U31	5.6	-27.7	37.5	-36.0	19.2	38.2	10.8	$C_{3'}$-endo
U30	-12.4	-10.3	27.3	-35.6	30.0	35.0	38.8	$C_{4'}$-exo
C29	-16.1	6.7	4.3	-13.9	18.9	18.6	76.6	$O_{4'}$-endo
C28	-24.2	0.2	21.5	-36.4	38.3	38.7	56.3	$C_{4'}$-exo
A27	-21.4	13.6	-1.5	-11.0	20.3	21.6	93.9	$O_{4'}$-endo
C25	-22.5	-1.2	22.5	-36.7	37.0	38.1	53.9	$C_{4'}$-exo
G24	-8.8	-14.9	31.1	-37.7	29.2	36.9	32.4	$C_{3'}$-endo
A23	-5.0	-18.2	32.6	-37.1	26.6	36.5	26.6	$C_{3'}$-endo
A22	-3.6	-19.3	33.4	-37.0	25.4	36.6	24.4	$C_{3'}$-endo
A21	9.2	5.9	-17.7	23.7	-20.6	23.5	221.2	$C_{4'}$-endo

Table 7.4: Shows the ribose dihedral angles, v_0 to v_4, the amplitude of *pseudorotation* of the sugar ring, tm, the phase angle of *pseudorotation* of the sugar ring, P, and the resultant type of puckering of the second strand of the *H. hal.* 29-mer NMR solution structure.

Residue	alpha	beta	gamma	delta	epsilon	zeta	chi
C1	---	---	53.6	81.7	-156.7	-75.5	-157.8
C2	-65.3	171.2	53.1	81.8	-156.5	-71.8	-156.8
C3	-64.0	171.9	53.5	81.7	-158.5	-73.1	-157.1
U4	-61.2	171.3	54.7	82.2	-165.4	-77.9	-156.5
A5	157.7	-158.1	177.1	86.8	-144.4	-67.3	-170.3
U6	-64.7	161.1	62.2	82.5	-156.0	-67.6	-161.7
A7	-66.9	165.3	60.9	87.3	-167.8	-93.4	-145.8
G8	-64.8	174.5	51.9	98.6	-153.5	-68.5	-151.9
A9	-66.1	165.3	56.9	85.3	-158.1	-67.0	-157.8
G10	-64.1	179.1	53.1	82.6	-156.0	-66.3	-158.5
C11	-64.0	179.9	53.5	82.4	-156.4	-69.2	-158.0
U12	-64.7	-179.0	51.4	109.6	-178.5	-89.4	-125.1
U13	-62.7	-177.4	51.7	131.5	-166.5	-100.8	-118.7
U14	-60.8	175.3	62.9	136.6	---	---	-130.0

Table 7.5: Shows the backbone dihedral angles, for the base paired residues of the first strand of the *H. hal.* 29-mer NMR solution structure. The mark "---" indicates that the particular dihedral angle is not applicable to the particular residue.

Residue	alpha	beta	gamma	delta	epsilon	zeta	chi
G35	-64.3	-176.4	50.9	142.6	---	---	-108.2
G34	-64.0	179.4	52.9	82.4	-157.3	-70.7	-158.3
G33	-61.8	172.3	53.9	82.0	-156.6	-69.5	-157.7
A32	-64.0	170.2	53.9	82.1	-157.1	-66.8	-158.6
U31	-67.7	172.1	53.3	82.3	-154.6	-61.3	-157.9
U30	-64.8	172.1	55.8	82.3	-161.1	-91.0	-157.1
C29	-65.1	170.7	51.4	110.0	-175.7	-66.1	-132.7
A27	-58.6	171.6	54.7	83.3	-155.0	-62.0	-149.1
U26	-66.6	173.8	51.8	112.1	177.5	-96.2	-123.8
C25	-63.6	-179.3	53.5	82.0	-157.9	-74.4	-157.9
G24	-64.1	178.0	53.9	82.4	-156.5	-68.1	-157.5
A23	-63.3	171.9	53.4	82.4	-156.0	-67.6	-155.8
A22	-106.9	159.0	91.0	83.1	-155.9	-74.0	-164.1
A21	---	---	51.9	143.5	176.8	-95.3	-120.0

Table 7.6: Shows the backbone dihedral angles, for the base paired residues of the second strand of the
H. hal. 29-mer NMR solution structure. The mark "---" indicates that the particular dihedral angle is
not applicable to the particular residue.