#### **Supporting Information**

#### Structural features of a 3' splice site in influenza A

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Figure S1: Equilibria of 19-nt duplex mimics of a portion of the 39-nt hairpin with homodimers of the top strands of their duplexes. (a) If residue 14 of a duplex is a uridine, as in the 39-mer, then a homodimer may form that is more stable than the target heterodimer. (b) If residue 14 of a duplex is a cytidine, then the analogous homodimer is less stable than the target heterodimer.

(a)  
(b)  
(b)  

$$\begin{array}{c}
 & A & G & A^{20} \\
 & A & G & A^{20} \\
 & 5' & C & U & A \\
 & 3' & G & G & G & U \\
 & 3' & 30 & G & G & U \\
\end{array}$$
(b)  
 $\begin{array}{c}
 & 7 & 10 \\
 & 5' & G & C & A \\
 & 3' & G & G & G & U \\
 & 3' & 35 & G & A \\
 & 35 & G & A \\
\end{array}$ 
(b)  
 $\begin{array}{c}
 & 7 & 10 \\
 & 5' & G & C & A \\
 & 1 & 1 & 1 \\
 & 3' & 35 & G & A \\
 & 35 & G & A \\
\end{array}$ 

Figure S2: Fragments of the 39-nt hairpin used for modeling with CS-ROSETTA.<sup>1, 2</sup> (a) The 19-nt hairpin with the A26 bulge and hairpin loop. (b) The 18-nt duplex with the  $2 \times 2$  nt internal loop.



Figure S3: Imino region of 1D proton spectra of the 39-nt hairpin acquired with 0, 5 and 10 mM Mg<sup>2+</sup> at 4 °C. These spectra were acquired on the 39-nt hairpin synthesized with commercial transcription kits and do not have a signal for U39. <sup>†</sup> Chemical exchange peak.



Figure S4: Imino to amino/non-exchangeable proton region of a 2D NOESY spectrum of the 39-nt hairpin. Crosspeaks within base pairs from C amino proton(s) to GH1 and AH2 to UH3 are labeled blue, where the C amino proton or AH2 and GH1 or UH3 corresponds to the first and second residues, respectively. Interresidue H1' to H1/H3 cross-peaks are labeled green, where H1' and H1/H3 correspond to the first and second residues, respectively. The A22H8-G19H1 and A31H2-G11H1 cross-peaks are labeled red. The water signal was suppressed with an S-pulse. The spectrum was acquired at -2 °C with 125 ms mixing time.



Figure S5: H1' to H6/H8 region of a 2D proton NOESY spectrum of the 39-nt hairpin showing sequential proton walks for residues G2 to G10 and U33 to U39. H1' to H6/H8 walk NOEs are labeled blue for residues 2 to 10 and green for residues 33 to 39. Adenine H2 signals are labeled with red dashed lines. H1' to adenine H2 NOEs are labeled red with only the label of the residue for the H1'. Spectrum was acquired at 20 °C and 350 ms mixing time with a WATERGATE pulse to suppress the water signal. In the secondary structure of the 39-nt hairpin., residues whose intraresidue H1' to H6/H8 NOEs were identified in the NOESY walks are labeled blue for residues 2 to 10 and green for residues 33 to 39.



Where x is the concentration of single-stranded RNA in duplex and  $C_{\rm T}$  is the total concentration of strands. The concentration of duplex and hairpin are x/2 and  $C_{\rm T} - x$ , respectively. The value of x at 2 °C, with  $C_{\rm T} = 4$  mM, is  $2.31 \times 10^{-6}$  M. Therefore, the concentration of hairpin is approximately 4 mM. At  $C_{\rm T} = 0.2$  mM, x is  $5.78 \times 10^{-9}$  M. Therefore, the concentration of hairpin is approximately 0.2 mM.

Figure S6: Thermodynamics calculations with the nearest neighbor model showing that the 11-nt hairpin conformation is preferred to a duplex formed by self-dimerization of the RNA sequence.



Figure S7: Imino proton region of the 11-nt hairpin at a strand concentration of 0.2 mM and 4 mM. The  $Mg^{2+}$ concentration was 0.25 mM and 5 mM for the 0.2 mM and 4 mM samples, respectively. The phosphates concentration was the same in the two samples. Spectra were acquired with a 1-1-echo pulse at 2 °C.





13.6 13.4 13.2 13.0 12.8 12.6 12.4 12.2 12.0 11.8 11.6 11.4 11.2 11.0 10.8 ppm Figure S9: Imino region of 1D proton spectra of the 19-nt duplex acquired with 0 and 5 mM  $Mg^{2+}$  at 5 °C. <sup>†</sup> Chemical exchange peak.



Figure S10: Differences in chemical shifts of select non-exchangeable hydrogens of the 11-nt hairpin with and without 5 mM Mg<sup>2+</sup> at -2 °C. Residue numbers on the x-axis align with the middle of each set of two bars in each plot.



Figure S11: Differences in chemical shifts of select non-exchangeable hydrogens of the 19-nt duplex with and without 5 mM  $Mg^{2+}$  at -2 °C. Residue numbers on the x-axis align with the middle of each set of two bars in each plot.



Figure S12: The ensemble of the 10 structures of the 11-nt hairpin modeled in AMBER with the lowest distance restraint violation energies and which agreed with NMR restraints.



Figure S13: The ensemble of the 10 structures of the 19-nt duplex modeled in AMBER with the lowest distance restraint violation energies and which agreed with NMR restraints.



Figure S14: Calculated structure of the hairpin loop of the 11-nt hairpin construct. (a) Model of the GAAA loop and closing AC pair of the 11-nt hairpin construct calculated by AMBER, showing the 3'  $A_3$  stack and an AC pair with a hydrogen bond from the C23 amino group to A18N1. (b) Space-filling model of the A18-C23 pair. (c) Space-filling model of the G19-A22 pair.



Figure S15: H1' to H2' region of a 2D TOCSY spectrum of the 11-nt hairpin. All visible cross-peaks are circled. Cross-peaks circled blue correspond to H1' to H2' cross-peaks for residues labeled with the same color. Cross-peaks circled orange are unassigned artifacts. As expected, the 3' terminal A26 residue has a relatively large H1' to H2' cross-peak. All H1' to H2' cross-peaks are small compared to C or U H5 to H6 cross-peaks in the same spectrum (not shown), indicating weak coupling between these protons and that all residues primarily have a C3' endo sugar pucker. The spectrum was acquired at 20 °C in D<sub>2</sub>O and 5 mM Mg<sup>2+</sup>.



Figure S16: H1' to H2' region of a 2D TOCSY spectrum of the 19-nt duplex. All visible cross-peaks are circled. Cross-peaks circled blue correspond to H1' to H2' cross-peaks for residues labeled with the same color. Cross-peaks circled orange are unassigned artifacts. As expected, terminal residues have a relatively large H1' to H2' cross-peak. All H1' to H2' cross-peaks are small compared to C or U H5 to H6 cross-peaks in the same spectrum (not shown), indicating weak coupling between these protons and that all residues primarily have a C3' endo sugar pucker. The noise at 4.75 ppm is the residual water peak. The spectrum was acquired at 25 °C in D<sub>2</sub>O and 5 mM Mg<sup>2+</sup>.



Figure S17: Calculated structure of the internal loop of the 19-nt duplex construct. (a) G10 is stacked below G11 with an *anti* conformation. (b) G10 flipped out of the helix with an *anti* conformation. (c) Space-filling model of the G11-A31 pair.



Figure S18: Chemical shift differences of the 19-nt duplex between experiment, assigned at 25 °C in the presence of 5 mM  $Mg^{2+}$ , and those predicted by NUCHEMICS for H2/H5, H6/H8, H1' and H2' in an ensemble of 20 structures generated with NMR restraints. Residue numbers on the x-axis align with the middle of each set of two bars in each plot.



Figure S19: Chemical shift differences of the 11-nt hairpin between experiment, assigned at 20 °C in the presence of 5 mM  $Mg^{2+}$ , and those predicted by NUCHEMICS for H2/H5, H6/H8, H1' and H2' in an ensemble of 20 structures generated with NMR restraints. Residue numbers on the x-axis align with the middle of each set of two bars in each plot.



Figure S20: Differences between experimental and NUCHEMICS-predicted chemical shifts of a GAAA hairpin, closed by a GU pair, which consists of a helical region of a group II intron. Residue numbers on the x-axis align with the middle of each set of two bars in each plot. Experimental chemical shifts were obtained from BMRB entry 15859 and 3D structures were obtained from PDB entry  $2K66.^3$ 



Figure S21: Differences between experimental and NUCHEMICS-predicted chemical shifts of a GAAA hairpin, closed by a GC pair, which contains an internal loop from a ribozyme. Residue numbers on the x-axis align with the middle of each set of two bars in each plot. Experimental chemical shifts were obtained from BMRB entry 17292 and 3D structures were obtained from PDB entry 2L5Z.<sup>4</sup>



Figure S22: Differences between experimental and NUCHEMICS-predicted chemical shifts of a GAAA hairpin, closed by an AU pair, which consists of a helical region of a ribozyme. Residue numbers on the x-axis align with the middle of each set of two bars in each plot. Experimental chemical shifts were obtained from BMRB entry 17877 and 3D structures were obtained from PDB entry 2LI4.<sup>5</sup>



Figure S23: Differences between experimental chemical shifts of the 39-nt hairpin, assigned at 20 °C, and those predicted by NUCHEMICS for H2/H5, H6/H8, H1' and H2' in an ensemble of 20 structures of the 19-nt hairpin generated by CS-ROSETTA with chemical shift restraints. Bars colored with light shades belong to terminal helix residues 12 and 30 of the 19-mer that are not at the termini of any helixes of the 39-mer, and thus are in structurally inequivalent regions among the constructs. Residue numbers on the x-axis align with the middle of each set of two bars in each plot.



Figure S24: Differences between experimental chemical shifts of the 39-nt hairpin, assigned at 20 °C, and those predicted by NUCHEMICS for H2/H5, H6/H8, H1' and H2' in an ensemble of 20 structures of the 18-nt duplex generated by CS-ROSETTA with chemical shift restraints. Bars colored with light shades belong to terminal helix residues 7, 15, 27 and 35 of the 18-mer that are not at the termini of any helixes of the 39-mer, and thus are in structurally inequivalent regions among the constructs. Residue numbers on the x-axis align with the middle of each set of two bars in each plot.

$$\begin{array}{c} 267 \\ 5' G A \\ \hline G A \\ \hline G G \\ \hline G A \\ \hline G A \\ \hline G A \\ \hline A$$

Figure S25: Secondary structure of a hairpin with a  $2 \times 2$  internal loop from a group II intron of *Oceanobacillus iheyensis*.<sup>6</sup>

Table S1: Chemical shifts used to model fragments of the segment 7 hairpin with CS-ROSETTA. Chemical shifts
were taken from spectra of the 39-nt hairpin (red), 19-nt duplex (blue) and 11-nt hairpin (green) at 20 °C (39-nt
hairpin and 11-nt hairpin) or 25 °C (19-nt duplex) unless otherwise noted. The spectra for the 39-nt hairpin were
acquired with no $Mg^{2^+}$ and those for the 19-nt duplex and 11-nt hairpin were acquired with 5 mM $Mg^{2^+}$ .

Residue	Atom	Chemical	Residue	Atom	Chemical	Residue	Atom	Chemical
		shift (ppm)			shift (ppm)			Shift (ppm)
<b>G</b> 7	H1′	5.681	C17	H2′	4.178	U27	H2′	4.401
G7	H2′	4.415	C17	H5	5.365	U27	H5	5.262
G7	H8	7.677	C17	H6	7.596	U27	H6	7.479
C8	H1'	5.504	A18	H1'	5.980	G28	H1'	5.769
C8	H2′	4.316	A18	H2	7.670	G28	H2′	4.719
C8	H3'	4.605	A18	H2′	4.474	G28	H8	7.700
C8	H4′	4.461	A18	H3'	4.848	G29	H1'	5.745
C8	H5	5.273	A18	H8	8.184	G29	H2′	4.560
C8	H6	7.835	G19	H1'	5.563	G29	H3'	4.504
A9	H1'	5.878	G19	H2′	4.352	G29	H4'	4.507
A9	H2	7.198	G19	H3′	4.607	G29	H8	7.329
A9	H2′	4.491	G19	H4′	4.366	G30	H1'	5.660
A9	H3′	4.852	G19	H8	7.335	G30	H2′	4.169
A9	H4′	4.391	A20	H1'	5.681	G30	H3′	4.647
A9	H8	8.045	A20	H2	7.726	G30	H4′	4.420
G10	H1'	6.038	A20	H2′	4.680	G30	H8	7.264
G10	H2′	4.500	A20	H3′	4.475	A31	H1'	6.104
G10	H3′	4.716	A20	H4′	4.250	A31	H2	7.948
G10	H4′	4.491	A20	H8	8.210	A31	H2′	4.842
G10	H8	7.679	A21	H1'	5.515	A31	H3′	4.678
G11	H1′	5.567	A21	H2	7.610	A31	H4′	4.480
G11	H2′	4.583	A21	H2′	4.558	A31	H8	8.078
G11	H3'	4 353	A21	H3'	4 655	G32	H1'	$5.370^{a}$
G11	H8	$7369^{a}$	A21	H4'	4 410	G32	H2'	4 358
C12	H1'	5 523	A21	H8	7 888	G32	H3'	4 229
C12	H2'	4 239	A22	H1'	5 850	G32	H8	7 100
C12	H3'	4 451	A22	H2	8 082	U33	H1'	5 518
C12	H5	5 208	A22	H2'	4 675	1133	H2'	4 600
C12	H6	7 512	Δ22	H3'	4.620	1133	H3'	4.533
C12 C13	H17	5 367	Δ22	H4'	4.020	1133	HA'	4 422
C13	нт н2	4 200	A22	ня Н8	7 030	1133	H5	5.040
C13	112 112'	4.290	C23	По Ц1/	1.950	1122	П5 Ц6	7 722
C13		4.403	$C_{23}$	нн цэ/	4.830	G34	П0 Ц1/	5 745
C13	114 115	5 422	C23	112 Ц27	4.414	G34	нт цэ	J.745 A A15
C13	П5 Ц6	J.423 7 927	C23	115 115	4.338	G24	112 LI21	4.415
		7.037 5.516	C23	П.) Ц6	J.385 7 720	G24	ПЭ ЦЛ/	4.556
U14 U14	111 ЦЭ/	4.252	C23		5 5 2 9	G24	114 LIQ	7.602
U14 U14	П2 115	4.232	G24 C24	П1 112/	3.320	C25	П0 Ц1/	7.095
U14	П.) 116	3.730	G24 C24		4.098	C35		3.337
014		7.802	G24 C25		7.390	C35	П2 112/	4.303
A15	HI	5.959	G25 C25		5.040	C35		4.370
A15		/.41/	G25	H2 112/	4.391	C35	H4 115	4.550
A15	H2'	4.519	G25	110	4.304	C35	НЭ	5.1/U 7.429
AIS	H5'	4.013	625		/.30/	035	Hb	1.438
AI5	H8	8.250	A26	HI'	5.924			
CI6	HI'	5.139	A26	H2	7.960			
Cl6	H5	5.360	A26	H2′	4.387			
C16	H6	7.421	A26	H8	8.036			
<u>C17</u>	HI'	5.302	U27	Hl'	5.598			
" Assigned	at −2 °C	•						

Dosiduo	U1/	<u>ц</u> 2/	U2/U5	U6/U9	U1/U2	H21/41/61, H22/42/62
Residue	пі	Π2	Π2/Π3	П0/По	П1/П <b>5</b>	amino
G2	5.78	4.76	N/A	7.89	-	-
A3	5.88	4.71	7.88	8.38	N/A	-
U4	5.54	4.56	5.14	7.60	14.14	N/A
U5	5.48	-	5.51	7.93	11.92	N/A
U6	5.47	4.56	5.53	7.94	13.51	N/A
G7	5.68	4.42	N/A	7.68	12.41	6.25
C8	5.32		5.17	7.61	N/A	8.28, 6.87
A9	5.78	4.47	7.06	7.90	N/A	-
G10	5.88	-	N/A	7.60	$10.79^{a}$	-
G11	5.51	4.58	N/A	-	13.08	5.88
C12	5.52	4.26	5.13	7.50	N/A	8.42, 6.98
C13	5.35	4.51	5.37	7.67	N/A	8.22, 6.91
U14	5.52	4.25	5.74	7.80	11.66	N/A
A15	5.94	4.52	7.42	8.25	N/A	-
C16	5.14	-	5.36	7.42	N/A	$8.10, 6.92^{b}$
C17	5.30	4.18	5.37	7.60	N/A	8.22, 6.93
A18	5.82	4.36	7.43	8.00	N/A	-
G19	5.45	4.36	N/A	7.34	10.46	7.02
A20	5.67	4.62	7.78	8.16	N/A	-
A21	5.57	4.55	7.73	7.96	N/A	-
A22	5.81	4.64	-	7.98	N/A	-
C23	-	-	5.60	7.64	N/A	-
G24	5.53	4.70	N/A	7.60	11.92	-
G25	5.64	4.39	N/A	7.31	$12.41^{b}$	-
A26	5.92	4.39	7.96	8.04	N/A	-
U27	5.60	4.40	5.26	7.48	12.23	N/A
G28	5.77	4.72	N/A	7.70	10.30	6.30
G29	5.62	4.51	N/A	7.10	12.70	$6.17^{b}$
G30	5.65	4.23	N/A	7.16	12.49	-
A31	6.06	4.86	-	8.03	N/A	-
G32	-	4.37	N/A	-	$10.79^{a}$	-
U33	5.49	4.60	4.99	7.68	13.39	N/A
G34	5.71	4.37	N/A	7.68	12.69/12.41 <sup>c</sup>	-
C35	5.32	4.36	5.19	7.61	N/A	8.31, 6.86
A36	5.91	4.59	6.81	7.92	N/A	
G37	5.48	4.61	N/A	6.87	10.67	6.34
A38	5.89	4.34	7.88	7.71	N/A	-
U39	5.71	4.10	5.08	7.45	13.66	N/A

Table S2: Assigned chemical shifts of the 39-nt 3' splice site segment 7 hairpin construct.

Exchangeable proton chemical shifts were assigned in a -2 °C spectrum. Non-exchangeable proton chemical shifts were assigned in a 20 °C spectrum. Exceptions are noted. <sup>*a*</sup> Ambiguous. <sup>*b*</sup> Assigned in a 20 °C spectrum. <sup>*c*</sup> Minor conformation.

										H21/41/61,	
Residue	H1'	H2′	H3′	H4'	H5′	H5″	H2/H5	H6/H8	H1/H3	H22/42/62	$\mathbf{P}^{a}$
										amino	
C16	5.62	4.50	4.46	4.40	4.12	3.94	6.04	8.13	N/A	8.55, 7.10	
C17	5.43	4.28	4.68	4.41	4.58	4.16	5.53	7.82	N/A	8.49, 6.93	-4.10
A18	5.98	4.47	4.85	-	4.52	4.18	7.67	8.18	N/A	-	-3.98
G19	5.56	4.35	4.61	4.37	4.42	4.11	N/A	7.34	10.49	7.16	-3.47
A20	5.68	4.68	4.48	4.25	4.26	3.95	7.73	8.21	N/A	-	-2.12
A21	5.52	4.56	4.66	4.41	4.30	4.02	7.61	7.89	N/A	-	-3.21
A22	5.85	4.68	4.62	4.47	4.58	4.21	8.08	7.93	N/A	-	-4.16
C23	4.85	4.41	4.34	4.30 <sup><i>a</i></sup>	4.36	4.13	5.58	7.73	N/A	7.72, 6.58	-3.95
G24	5.59	4.72	4.33	-	4.25	4.10	N/A	7.58	11.97	5.87, 7.39	-3.56
G25	5.69	4.52	4.57	4.42	4.50	4.07	N/A	7.30	12.80	8.18	-4.07
A26	5.96	4.10	4.29	4.26	4.43	4.06	7.91	7.85	N/A	-	-3.86

Table S3: Assigned chemical shifts of the 11-nt hairpin construct.

Exchangeable proton chemical shifts were assigned in a -1 °C spectrum in H<sub>2</sub>O. Non-exchangeable proton chemical shifts were assigned in a 20 °C spectrum in D<sub>2</sub>O. All chemical shifts were assigned in spectra obtained with 5 mM Mg<sup>2+</sup>. Exceptions are noted. <sup>*a*</sup> Assigned in a 20 °C spectrum without Mg<sup>2+</sup>.

Desides	111/	110/	112/	114/	1151	11511	110/115	117/110	111/112	H21/41/61,	л
Residue	HI	$HZ^{r}$	H3	H4	HO	HS	H2/H3	H6/H8	HI/H3	H22/42/62	Р
										amino	
G7	5.87	4.79	4.56	4.44	4.13	3.95	N/A	8.13	12.67	-	
C8	5.50	4.32	4.61	4.46	-	4.17	5.27	7.84	N/A	8.54, 6.82	-4.34
A9	5.88	4.49	4.85	4.39	-	4.19	7.20	8.05	N/A	-	-4.02
G10	6.04	4.50	4.72	4.49	-	-	N/A	7.68	10.86 <sup><i>a</i></sup>	-	
G11	5.57	4.58	4.35	-	-	-	N/A	$7.37^{b}$	13.08	5.91	-3.93
C12	5.52	4.24	4.45	-	-	4.10	5.21	7.51	N/A	8.47, 7.06	-4.49
C13	5.37	4.29	4.49	4.36	-	4.05	5.42	7.84	N/A	8.42, 6.96	-4.54
C14	5.41	4.32	4.47	4.34	-	4.05	5.43	7.64	N/A	8.25, 6.97	-4.07
A15	5.98	4.08	4.31	4.24	-	4.09	7.46	8.03	N/A	-	-3.94
U27	5.77	4.62	4.63	4.37	4.00	3.90	5.85	8.01	-	N/A	
G28	5.91	4.79	4.69	4.56	-	-	N/A	8.02	12.16	-	-3.74
G29	5.75	4.56	4.50	4.51	4.51	4.14	N/A	7.33	12.81	-	-3.69
G30	5.66	4.17	4.65	4.42	4.54	4.09	N/A	7.26	12.57	-	
A31	6.10	4.84	4.68	4.48	-	-	7.95	8.08	N/A	-	
G32	$5.37^{b}$	4.36	4.23	-	-	-	N/A	7.10	10.86 <sup><i>a</i></sup>	-	-4.00
U33	5.52	4.60	4.53	4.42	-	4.09	5.04	7.73	13.31	N/A	-4.85
G34	5.75	4.42	4.56	4.44	-	4.11	N/A	7.69	12.91	-	-4.05
C35	5.36	4.30	4.37	4.33	-	4.04	5.17	7.44	N/A	8.07, 6.91	-4.23
A36	5.97	4.03	4.27	4.21	4.40	4.03	7.41	8.01	N/A	-	-3.85

Table S4: Assigned chemical shifts of the 19-nt duplex construct.

Exchangeable proton chemical shifts were assigned in a 0 °C spectrum in H<sub>2</sub>O. Non-exchangeable proton and phosphorus chemical shifts were assigned in a 25 °C spectrum in D<sub>2</sub>O. All chemical shifts were assigned in spectra obtained with 5 mM Mg<sup>2+</sup>. Exceptions are noted. <sup>*a*</sup> Ambiguous. <sup>*b*</sup> Assigned in a –2 °C spectrum.

# Plasmid insert design for *in vitro* transcription of the 39-nt 3' segment 7 mRNA hairpin by T7 RNA polymerase

Cloning vector: pUC18 (Fermentas)

Intended sequence of the 39-nt RNA hairpin: 5 'GGAUUUGCAGGCCUACCAGAAACGGAUGGGAGUGCAGAU3 '

Sequence of the insert: 5 'GACGAAGCTT<u>TAATACGACTCACTATA</u>GGATTTGCAGGCCTACCAGAAACGGATGGGAGTGC AGATATCGAATTCGAGC3 '

Reverse complement of the insert: 5 'GCTCGAATTCGATATCTGCACTCCCATCCGTTTCTGGTAGGCCTGCAAATCCTATAGTGAGT CGTATTAAAGCTTCGTC3 '

Notation: EcoR1 recognition sequence: 5 'GAATTC3 ' EcoRV recognition sequence: 5 'GATATC3 '<sup>a</sup> HindIII recognition sequence: 5 'AAGCTT3 ' RNA hairpin sequence T7 RNA polymerase promoter

<sup>*a*</sup> Bases that are part of the RNA hairpin sequence are labeled red.

assign	(residue	17	and	name	H1'	)	(residue	17	and	name	H6	)	4.00	0.84	1.04 !
assign	(residue	17	and	name	H2'	)	(residue	17	and	name	H6	)	3.69	0.77	0.96 !
assign	(residue	17	and	name	H2'	)	(residue	18	and	name	H1'	)	4.70	0.99	1.22 !
assign	(residue	17	and	name	H2'	)	(residue	18	and	name	H8	)	2.47	0.52	0.64 !
assign	(residue	17	and	name	H3'	)	(residue	17	and	name	H1'	)	3.69	0.78	0.96 !
assign	(residue	17	and	name	H3'	)	(residue	18	and	name	H8	)	3.11	0.65	0.81 !
assign	(residue	18	and	name	H1'	)	(residue	18	and	name	H8	)	4.27	0.90	1.11 !
assign	(residue	18	and	name	H2'	)	(residue	18	and	name	H8	)	3.46	0.73	0.90 !
assign	(residue	18	and	name	H3'	)	(residue	18	and	name	H1'	)	4.46	0.94	1.16 !
assign	(residue	18	and	name	H3'	)	(residue	18	and	name	H8	)	2.64	0.55	0.69 !
assign	(residue	19	and	name	H1'	)	(residue	18	and	name	H2	)	5.03	1.06	1.31 !
assign	(residue	19	and	name	H2'	)	(residue	19	and	name	H1'	)	2.82	0.59	0.73 !
assign	(residue	19	and	name	H3'	)	(residue	19	and	name	H8	)	2.72	0.57	0.71 !
assign	(residue	19	and	name	H4'	)	(residue	19	and	name	H1'	)	3.15	0.66	0.82 !
assign	(residue	20	and	name	H1'	)	(residue	20	and	name	Н8	)	3.85	0.81	1.00 !
assign	(residue	20	and	name	H2'	Ś	(residue	20	and	name	H8	ý	3.79	0.80	0.98 !
assign	(residue	20	and	name	H2'	Ś	(residue	21	and	name	H1'	ý	3.45	0.72	0.90 !
assign	(residue	20	and	name	H2'	ý	(residue	21	and	name	Н8	ý	2.77	0.58	0.72 !
assign	(residue	20	and	name	Н3'	Ś	(residue	20	and	name	Н8	Ś	3.28	0.69	0.85 !
assign	(residue	20	and	name	H3'	Ś	(residue	21	and	name	H8	Ś	2.59	0.54	0.67 !
assign	(residue	21	and	name	H1'	Ś	(residue	20	and	name	H2	Ś	3.25	0.68	0.85 !
assign	(residue	21	and	name	H1'	Ś	(residue	21	and	name	H8	ś	4.47	0.94	1.16 !
assign	(residue	21	and	name	H2'	Ś	(residue	22	and	name	H1'	ś	5.01	1.05	1.30
assign	(residue	21	and	name	нз'	Ś	(residue	21	and	name		Ś	2 90	0 61	0 75 I
assign	(residue	22	and	name	H1'	Ś	(residue	21	and	name	Н2	Ś	4 02	0.01	1 05 1
assign	(residue	22	and	name	н4'	Ś	(residue	22	and	name	H1 '	Ś	3 72	0.04	0 97 I
assign	(residue	23	and	name	H2'	Ś	(residue	23	and	name	Н6	Ś	3 60	0.76	0 94 I
assign	(residue	25	and	name	H3'	Ś	(residue	25	and	name	ня	Ś	3 10	0.70	0.94 . 0.81 I
accion	(residue	17	and	name	нз'	Ś	(residue	17	and	name	нб	Ś	2 60	0.05	0.62
assign	(residue	18	and	name	H2'	Ś	(residue	18	and	name	н1 '	Ś	2.00	0.55	0.00 1
assign	(residue	18	and	name	H2'	Ś	(residue	19	and	name	нт.	Ś	3 69	0.55	0.00
assign	(residue	18	and	name	H2'	Ś	(residue	19	and	name	HS	Ś	3 02	0.70	0.00 ! 0.79
assign	(nesidue	10	and	name	יב <u>וו</u>	~	(residue	21	and	name	цо	~	2 00	0.05	1 01 1
assign	(residue	10	anu	name	יכם		(residue	10	anu	name	по ⊔1 '	{	1 00	0.02	1 06 1
assign	(residue	20	anu	name	רח יגם	Ś	(residue	20	anu	name	пт 111		4.09	0.00	1.00 !
assign	(residue	20	anu	name	ח-4- וינים		(residue	20	anu	name	пт 111	{	2.4/ 2.72	0.75	0.90 !
assign	(residue	21	anu	name	יכוו	Ś	(residue	21	anu	name		Ś	2.12	0.57	
assign	(residue	21	anu	name	כח	Ś	(resture	21	anu	name			2.00	0.77	0.95 !
assign	(residue	21	anu	name	П4 112 I	Ś	(residue	21	anu	name		)	2.02	0.70	0.94 !
assign	(residue	22	anu	name	п∠ 112 '	Ś	(residue	22	anu	name	пт	)	2.0/	0.00	0.75 !
assign	(residue	22	anu	name		Ś	(residue	25	anu	name		~	2.00	0.59	0.75 !
assign	(residue	22	and	name	H3	)	(residue	23	and	name	Hb	)	2.63	0.55	0.68 !
assign	(residue	23	and	name	HZ	)	(residue	24	and	name	HI	)	3.13	0.66	0.82 !
assign	(residue	1/	and	name	H41	)	(residue	24	and	name	HI	)	2.33	0.93	0.93 !
assign	(residue	18	and	name	H1.	)	(residue	24	and	name	N2	)	2.62	1.05	2.05 !
assign	(residue	22	and	name	H8	)	(residue	19	and	name	H21	)	2.88	1.15	1.15 !
assign	(residue	23	and	name	N4	)	(residue	18	and	name	H2	)	2.70	1.08	2.08 !
assign	(residue	25	and	name	H1'	)	(residue	24	and	name	N2	)	2.77	1.11	2.11 !
assign	(residue	8	and	name	H2'	)	(residue	8	and	name	H1'	)	2.60	0.55	0.68 !
assign	(residue	8	and	name	H3'	)	(residue	8	and	name	H6	)	2.42	0.51	0.63 !
assign	(residue	8	and	name	H4 '	)	(residue	8	and	name	H1'	)	2.75	0.58	0.71 !
assign	(residue	9	and	name	H2'	)	(residue	9	and	name	H1'	)	2.62	0.55	0.68 !
assign	(residue	9	and	name	H2'	)	(residue	10	and	name	H8	)	1.80	0.00	3.20 !
assign	(residue	9	and	name	H3'	)	(residue	9	and	name	H8	)	3.05	0.64	0.79 !

assign	(residue	9	and	name	H4'	)	(residue	9	and	name	H1'	)	3.19	0.67	0.83 !
assign	(residue	11	and	name	H2'	ś	(residue	11	and	name	H1 '	ś	2.90	0.61	0.75 I
assign	(residue	11	and	name	н2'	Ś	(residue	12	and	name		Ś	2 51	0.53	0 65 1
assign	(residue	12	and	name	H2'	Ś	(residue	12	and	name	н1'	Ś	2.51	0.55	0.05 . 0 71 I
assign	(residue	12	and	name	H2'	Ś	(residue	12	and	name	Н6	Ś	4 05	0.37	1 05 1
assign	(residue	12	and	name	H2'	Ś	(residue	13	and	name	Нб	Ś	2 32	0.05	0 60 I
accion	(residue	12	and	name	нз'	Ś	(residue	12	and	name	нб	Ś	2.52	0.45	0.00
assign	(nociduo	12	and	name	יכם		(residue	12	and	name	110 LI1 I	~	2.04	0.55	0.00 : 0.01 I
assign	(nociduo	12	and	name	יכם		(residue	12	and	name	ш <u>с</u>	~	2.11	0.05	0.01 :
assign	(nociduo	12	and	name	יגם		(residue	12	and	name	110 LI1 I	~	2.55	0.45	0.01 :
assign	(residue	20	and	name	ח-4- נים		(residue	20	and	name	по	~	2.62	0.04	0.75
assign	(residue	20	anu	name	п <u>∠</u> 112 !	Ś	(residue	20	anu	name		~	2.00	0.77	1 1 2 1
assign	(residue	20	anu	name		Ż	(residue	29	anu	name	пт	,	4.55	0.91	1.12 !
assign	(residue	28	and	name	HZ	)	(residue	29	and	name	Hð	)	2.48	0.52	0.65 !
assign	(residue	28	and	name	H3	)	(residue	28	and	name	HI	)	3.21	0.6/	0.84 !
assign	(residue	28	and	name	H3 '	)	(residue	28	and	name	H8	)	2.89	0.61	0.75 !
assign	(residue	28	and	name	H3 '	)	(residue	29	and	name	H8	)	3.28	0.69	0.85 !
assign	(residue	28	and	name	H4 '	)	(residue	28	and	name	H1'	)	3.18	0.67	0.83 !
assign	(residue	29	and	name	H2'	)	(residue	29	and	name	H8	)	4.42	0.93	1.15 !
assign	(residue	29	and	name	H2'	)	(residue	30	and	name	H1'	)	4.37	0.92	1.14 !
assign	(residue	29	and	name	H2'	)	(residue	30	and	name	H8	)	2.48	0.52	0.64 !
assign	(residue	29	and	name	H3'	)	(residue	29	and	name	H8	)	2.81	0.59	0.73 !
assign	(residue	29	and	name	H3'	)	(residue	30	and	name	H8	)	3.38	0.71	0.88 !
assign	(residue	30	and	name	H2'	)	(residue	30	and	name	H1'	)	2.77	0.58	0.72 !
assign	(residue	30	and	name	H2'	)	(residue	31	and	name	H8	)	2.49	0.52	0.65 !
assign	(residue	30	and	name	H3'	)	(residue	30	and	name	H1'	)	3.99	0.84	1.04 !
assign	(residue	30	and	name	H3'	)	(residue	30	and	name	H8	)	2.88	0.61	0.75 !
assign	(residue	30	and	name	H3'	)	(residue	31	and	name	Н8	)	3.74	0.79	0.97 !
assign	(residue	30	and	name	H4'	)	(residue	30	and	name	H1'	)	3.47	0.73	0.90 !
assign	(residue	31	and	name	H2'	ý	(residue	31	and	name	H1'	)	2.61	0.55	0.68 !
assign	(residue	31	and	name	H3'	ý	(residue	31	and	name	H1'	ý	3.82	0.80	0.99 !
assign	(residue	31	and	name	H3'	ý	(residue	31	and	name	H8	ý	2.78	0.58	0.72 !
assign	(residue	31	and	name	H4'	ý	(residue	31	and	name	H1'	ý	3.34	0.70	0.87 !
assign	(residue	32	and	name	H2'	Ś	(residue	33	and	name	H6	Ś	2.44	0.51	0.63 !
assign	(residue	32	and	name	Н3'	Ś	(residue	33	and	name	H6	Ś	3.21	0.67	0.83 !
assign	(residue	33	and	name	H2'	Ś	(residue	34	and	name	H1'	Ś	3.64	0.76	0.95 !
assign	(residue	33	and	name	H2'	Ś	(residue	34	and	name	H8	ś	2.34	0.49	0.61 !
assign	(residue	33	and	name	H3'	Ś	(residue	33	and	name	H1'	ś	2.50	0.00	2.00 !
assign	(residue	33	and	name	H3'	ś	(residue	33	and	name	H6	ś	2.43	0.51	0.63
assign	(residue	34	and	name	H2'	ś	(residue	34	and	name	HR	ś	3.51	0.74	0.91
assign	(residue	34	and	name	H2'	Ś	(residue	35	and	name	H1 '	Ś	3.71	0.78	0.96
assign	(residue	34	and	name	H2'	Ś	(residue	35	and	name	H6	Ś	2 44	0.70	0.50
assign	(residue	34	and	name	нз'	Ś	(residue	34	and	name	ня	Ś	2.44	0.51	0.05
assign	(residue	35	and	namo	цз'		(residue	35	and	namo	на	Ś	2.55	0.55	0.00 I
assign	(residue	2	and	name	ц1 '		(residue	2	and	name	на		2 83	0.55	
assign	(nociduo	0	and	name	111 112 1		(residue	0	and	name	110 LI1 I	~	2 10	0.00	0.99 :
assign	(residue	10	anu	name	רח י נו		(residue	10	anu	name	пт	~	2.13	0.07	0.05 :
assign	(residue	11	anu	name			(residue	11	anu	name	110	~	2.02	0.05	0.70 !
assign	(nesture	17	and	name	П⊥ ⊔1 '	,	(nesture	11 12	and	name		)	5.20 2 20	0.00	0.00!
assign	(nestane	12 12	anu	name	ПТ П1 і	)	(nestane	12 12	anu	name	טח ער	)	J.20	0.00	1 17 !
assign	(nesidue	20	and	name	חד יכי	)	(nesidue	20	and	name	רוט וינ⊔	)	4.4ð	0.94 0 F1	T'T\
assign	(nesidue	29	and	name	ח∠ יינו	ļ	(nesidue	29	and	name	ח⊥ י י⊔	)	2.45	0.00	2 00 1
assign	(nesidue	29	and	name	п3 1121	)	(nesidue	29	and	name	UT UT	)	2.50	0.00	2.00 !
assign	(residue	31	and	name	HZ'	) )	(residue	32 21	and	name	HX	)	3.1/	0.6/	0.82 !
assign	(residue	32	and	name	HI.	)	(residue	31	and	name	H2	)	3.51	0./4	0.91 !

accion	(rociduo	3/	and	name	H1'	)	(recidue	Q	and	name	Н2	)	1 10	0 86	1 07 I
assign	(nociduo	24	and	name	יכם	~	(nosiduo	21	and	name	11Z	~	2 20	0.00	0 62 1
assign	(residue	34	and	name	11Z		(residue	34	and	name	нт ПП	~	2.55	0.50	0.02 :
assign	(residue	24	and	name	רו י בים		(residue	25	and	name	п <u>т</u> ЦС	~	3 00	0.05	0.01 !
assign	(residue	24	anu	name	п <u>э</u> ⊔1 '	~	(residue	22	anu	name		~	2 04	0.05	1 00 1
assign	(residue	22	anu	name	112	~	(residue	22	anu	name		Ś	2.04	1 02	1 02 1
assign	(residue	9	anu	name			(residue	>> >∢	anu	name		)	2.5/	1.05	1.05 !
assign	(residue	12	and	name	HZ	)	(residue	34	and	name	HI	)	4.19	1.68	1.68 !
assign	(residue	12	and	name	HI	)	(residue	11	and	name	HI	)	3.55	1.42	1.42 !
assign	(residue	12	and	name	H41	)	(residue	30	and	name	HI	)	2.15	0.86	0.86 !
assign	(residue	13	and	name	HI	)	(residue	30	and	name	HI	)	4.41	1.76	1.76 !
assign	(residue	30	and	name	H1.	)	(residue	29	and	name	H1	)	3.42	1.3/	1.3/ !
assign	(residue	31	and	name	H2	)	(residue	11	and	name	H1	)	2.77	1.11	1.11 !
assign	(residue	11	and	name	H22	)	(residue	31	and	name	H2	)	1.80	0.00	1.50 !
assign	(residue	5	and	name	H1'	)	(residue	4	and	name	H3	)	5.25	2.10	2.10 !
assign	(residue	6	and	name	H5	)	(residue	5	and	name	H3	)	5.66	2.27	2.27 !
assign	(residue	28	and	name	Η1	)	(residue	14	and	name	H3	)	2.29	0.92	0.92 !
assign	(residue	37	and	name	H1	)	(residue	5	and	name	H3	)	3.10	1.24	1.24 !
assign	(residue	37	and	name	N2	)	(residue	5	and	name	H3	)	3.00	0.00	3.00 !
assign	(residue	3	and	name	H2	)	(residue	39	and	name	H3	)	4.01	1.60	1.60 !
assign	(residue	5	and	name	H3	)	(residue	4	and	name	H3	)	4.07	1.63	1.63 !
assign	(residue	5	and	name	H3	)	(residue	6	and	name	H3	)	4.54	1.81	1.81 !
assign	(residue	6	and	name	H1'	)	(residue	37	and	name	H1	)	3.81	1.52	1.52 !
assign	(residue	7	and	name	H1	)	(residue	6	and	name	H3	)	5.07	2.03	2.03 !
assign	(residue	7	and	name	H1'	)	(residue	6	and	name	H3	)	3.00	0.00	5.00 !
assign	(residue	7	and	name	N2	)	(residue	6	and	name	H3	)	3.00	0.00	4.00 !
assign	(residue	14	and	name	H1'	)	(residue	14	and	name	H3	)	4.84	1.94	1.94 !
assign	(residue	14	and	name	H1'	)	(residue	28	and	name	H1	)	4.86	1.94	1.94 !
assign	(residue	14	and	name	H1'	)	(residue	29	and	name	H1	)	3.49	1.40	1.40 !
assign	(residue	14	and	name	H3	)	(residue	29	and	name	H1	)	4.08	1.63	1.63 !
assign	(residue	15	and	name	H1'	)	(residue	14	and	name	H3	)	4.73	1.89	1.89 !
assign	(residue	15	and	name	H1'	)	(residue	28	and	name	H1	)	3.59	1.44	1.44 !
assign	(residue	15	and	name	H2	)	(residue	14	and	name	H3	)	5.65	2.26	2.26 !
assign	(residue	15	and	name	H2	)	(residue	28	and	name	H1	)	5.16	2.06	2.06 !
assign	(residue	28	and	name	H1	ý	(residue	14	and	name	H3	Ś	2.76	1.10	1.10 !
assign	(residue	28	and	name	H1	ý	(residue	29	and	name	H1	Ś	4.58	1.83	1.83 !
assign	(residue	28	and	name	N2	Ś	(residue	14	and	name	H3	Ś	3.00	0.00	3.00 !
assign	(residue	28	and	name	N2	Ś	(residue	29	and	name	H1	Ś	3.00	0.00	4.00 !
assign	(residue	29	and	name	H1'	ý	(residue	14	and	name	H3	Ś	3.00	0.00	5.00 !
assign	(residue	35	and	name	N4	ý	(residue	6	and	name	H3	Ś	4.31	1.72	2.72 !
assign	(residue	36	and	name	H1'	ś	(residue	6	and	name	H3	ś	3.00	0.00	5.00 !
assign	(residue	37	and	name	H1	ś	(residue	4	and	name	H3	ś	5.52	2.21	2.21
assign	(residue	37	and	name	H1	Ś	(residue	6	and	name	НЗ	ś	4.37	1.75	1.75
assign	(residue	37	and	name	H1'	ś	(residue	6	and	name	H3	ś	4.51	1.80	1.80
assign	(residue	39	and	name	H1'	Ś	(residue	4	and	name	НЗ	ś	5.08	2.03	2.03
assign	(residue	3	and	name	H1'	ś	(residue	ג	and	name	НЯ	ś	5 00	2 00	2 00 1
assign	(residue	3	and	name	H2'	Ś	(residue	3	and	name	H1 '	Ś	3 26	1 31	1 31 1
assign	(residue	2	and	name	H2'	Ś	(residue	2	and	name	ня	Ś	2 00	a aa	2 50 1
assign	(residue	7	and	name	H1'		(residue	2	and	name	H2	Ś	2.00	0.00 0 00	3 00 1
accion	(residue	-+ Л	and	name	нт.		(residue	ر ۸	and	name	HA	Ś	2.00	0.00 0 00	3 00 1
accion	(residue	ч Л	and	name	H2'		(residue	ч Л	and	name	H1 '	Ś	2.00	1 29	1 29 1
accion	(residue	-+ 5	and	name	H1'		(residue	<del>י</del> קצ	and	name	H2	Ś	J.2J Z //Z	1 27	1 27 1
accian	(nociduo	7	and	name	нт Ц1 '		(nociduo	36	and	name	11Z		2 50	1 /2	1 /2 !
assign	(nociduo	7	and	name	רוב יכו		(nociduo	00	and	name		~	1 00	1.45 0 00	1.45 ! 2.70 !
asstRij	(Lesture	/	anu	name	ΠZ	)	(Lesture	0	anu	name	110	)	T.00	0.00	2.70 !

assign	(residue	13	and	name	H2'	)	(	residue	14	and	name	H6	)	2.29	0.92	0.92
assign	(residue	14	and	name	H1'	)	Ì	residue	14	and	name	H6	)	3.33	1.33	1.33
assign	(residue	14	and	name	H2'	ý	Ì	residue	14	and	name	H6	ý	3.05	1.22	1.22
assign	(residue	14	and	name	H2'	Ś	ì	residue	15	and	name	H8	Ś	2.18	0.87	0.87
assign	(residue	14	and	name	H5	Ś	ì	residue	13	and	name	H6	ś	3.74	1.50	1.50
assign	(residue	15	and	name	HR	ś	ì	residue	14	and	name	H6	ś	4.52	1.81	1.81
assign	(residue	15	and	name	н1'	Ś	ì	residue	15	and	name	ня	Ś	3 87	1 55	1 55
accion	(residue	15	and	name	н1'	Ś	ì	racidua	28	and	name	N2	Ś	2 00	0 00	2 00
assign	(residue	15	and	name	н <u>л</u>			rociduo	15	and	name	и <u>г</u>	~	2.00	0.00	1 50
assign	(residue	15	and	name	11Z			rociduo	15	and	name	ЦΩ	{	2.00	0.00	2 50
assign	(residue	15	and	name	יכם יכם			nociduo	16	and	name	110	{	2.00	0.00	2.50
assign	(resture	10	anu	name		Ś		restuue	10	anu	name		,	2.00	1 20	1 20
assign	(resture	10	anu	name		Ś		restaue	12	anu	name		)	2.01	1.20	2.20
assign	(residue	1/	and	name	HI	)	(	residue	26	and	name	HZ	)	3.00	0.00	2.50
assign	(residue	23	and	name	H5	)	(	residue	18	and	name	H2	)	3.66	1.46	2.46
assign	(residue	25	and	name	H2	)	(	residue	27	and	name	H6	)	4.00	0.00	99.00
assign	(residue	26	and	name	H1'	)	(	residue	26	and	name	H8	)	4.38	1.75	1.75
assign	(residue	26	and	name	H2'	)	(	residue	26	and	name	H1'	)	2.71	1.08	1.08
assign	(residue	27	and	name	H1'	)	(	residue	27	and	name	H6	)	3.37	1.35	1.35
assign	(residue	27	and	name	H2'	)	(	residue	27	and	name	H1'	)	2.00	0.00	1.50
assign	(residue	27	and	name	H5	)	(	residue	26	and	name	H8	)	4.07	1.63	1.63
assign	(residue	26	and	name	H8	)	(	residue	27	and	name	H6	)	4.07	1.63	1.63
assign	(residue	28	and	name	H1'	)	(	residue	15	and	name	H2	)	3.19	1.28	1.28
assign	(residue	29	and	name	H1'	)	(	residue	28	and	name	N2	)	2.00	0.00	2.00
assign	(residue	35	and	name	H2'	)	(	residue	36	and	name	H8	)	1.80	0.00	2.70
assign	(residue	36	and	name	H1'	)	(	residue	36	and	name	H8	)	4.24	1.70	1.70
assign	(residue	36	and	name	H2'	)	(	residue	36	and	name	H1'	)	2.45	0.98	0.98
assign	(residue	36	and	name	H2'	)	Ì	residue	37	and	name	Н8	)	2.53	1.01	1.01
assign	(residue	37	and	name	H1'	ý	Ì	residue	36	and	name	H2	ý	4.62	1.85	1.85
assign	(residue	38	and	name	H1'	ý	ì	residue	37	and	name	N2	Ś	2.00	0.00	2.00
assign	(residue	38	and	name	H2'	Ś	ì	residue	39	and	name	H6	Ś	2.00	0.00	2.50
assign	(residue	39	and	name	H1'	Ś	ì	residue	39	and	name	H6	Ś	4.02	1.61	1.61
assign	(residue	39	and	name	H2'	Ś	ì	residue	39	and	name	H1'	Ś	3.26	1.30	1.30
assign	(residue	39	and	name	H2'	ś	ì	residue	39	and	name	н6	ś	2 99	0 00	2 50
ussign	(1031000	22	unu	manic	112	)	(	I CSIUUC	55	unu	manic	110	,	2.00	0.00	2.50
assign	(resid 3	and	d nar	ne N1	)	(res	si	d 39 and	d na	ame H	H3)	2.1	0.3	3 0.3		
assign	(resid 3	and	d nar	ne H61	L)	(re	es	id 39 ar	nd r	name	04	) 2.1	0.3	3 0.3		
assign	(resid 4	and	d nar	ne H3	)	(res	si	d 38 and	d na	ame N	V1 )	2.1	0.3	3 0.3		
assign	(resid 4	and	d nar	ne 04	)	(res	si	d 38 and	d na	ame H	161	) 2.1	0.3	3 0.3		
assign	(resid 5	and	d nar	ne H3	)	(res	si	d 37 and	d na	ame (	) )	2.1	0.3	3 0.3		
assign	(resid 5	and	d nar	ne 02	)	(res	si	d 37 and	d na	ame H	-11 )	2.1	0.3	0.3		
assign	(resid 6	and	d nar	ne H3	) (	(res	si	d 36 and	d na	ame N	v1 )	2.1	0.3	3 0.3		
assign	(resid 6	and	d nar	ne 04	ý	(res	si	d 36 and	d na	ame H	-161 É	) 2.1	0.3	3 0.3		
assign	(resid 7	and	d nar	ne H1	Ś	、 (res	si	d 35 and	d na	ame N	νз ) <sup>΄</sup>	2.1	0.3	3 0.3		
assign	(resid 7	and	d nar	ne 06	j,	(res	si	d 35 and	d na	ame H	41	) 2.1	0.3	3 0.3		
assign	(resid 7	and	d nar	ne H22	$\gamma$	(re	5	id 35 ar	nd r	name	02	2.1	0.3	3 0.3		
assign	(resid 8	and	d nar	ne N3	- ví	(req	:i	d 34 and	d na	ame H	ں <sub>1</sub>	2.1	0.3	3 0.3		
assion	(resid &	and	d nar	ne H/11	, '∖ ⊢`\	(n4	 	id 34 ar	nd r	name	06	) 2 1	а :	- 0.J - 0		
assign	(resid Q	and	d nor	ne ∩?	- /	(rod		d 34 an	1 n:	ame 4	422	, <u>-</u> .1 ) ) 1	a :	- 0 - 0 -		
accian	(resid 0	and	d ner	ης 02 ης Ν1		( n = 3	, T	d 33 and	1 110		י <i>בב</i> אז י	, <u>2</u> .1 ) 1	Q	20.2		
accian	(resid 0	and	d ner	ης ΝΙ ης μεί	ייי ריי	( ) E3	<u>э</u> с	id 32 on	nd r	2000 I 1900		2.1 \	Q	20.2		
assign	(resid 12	ant יב (	nd n	- 101 - Ma	- / 2 \	(n	:3 20	יר גר אי זר גר איר	nd r	name	и Н1	/ <u>2</u> .1 \	1 0	20.2		
assign	(nocid 12	aı הר (	nd nr		, ) 11 '	۲. (۱۳	:5	- 02 JU -	nu i and	name	- UC	, <u>2</u> . \	1 0	ς.ος.		
assign	(nocid 12	_ ai	nu ile		+⊥ ,	) (1 /~-	2	14 20	anu ad -		= 00 1122	) 2.	10			
asstRu	(LESTO T	_ di	iu Ila	anie Uz	- )	(1.6	:5	ם שכ חד	iu r	alle	ΠΖΖ	) 2.	тØ	.5 0.3		

assign	(resid	13	and	name	N3	) (resid 29 and name H1 ) 2.1 0.3 0.3
assign	(resid	13	and	name	H41	) (resid 29 and name O6 ) 2.1 0.3 0.3
assign	(resid	13	and	name	02	) (resid 29 and name H22 ) 2.1 0.3 0.3
assign	(resid	14	and	name	H3	) (resid 28 and name 06 ) 2.1 0.3 0.3
assign	(resid	14	and	name	02	) (resid 28 and name H1 ) 2.1 0.3 0.3
assign	(resid	15	and	name	N1	) (resid 27 and name H3 ) 2.1 0.3 0.3
assign	(resid	15	and	name	H61	) (resid 27 and name O4 ) 2.1 0.3 0.3
assign	(resid	16	and	name	N3	) (resid 25 and name H1 ) 2.1 0.3 0.3
assign	(resid	16	and	name	H41	) (resid 25 and name O6 ) 2.1 0.3 0.3
assign	(resid	16	and	name	02	) (resid 25 and name H22 ) 2.1 0.3 0.3
assign	(resid	17	and	name	N3	) (resid 24 and name H1 ) 2.1 0.3 0.3
assign	(resid	17	and	name	H41	) (resid 24 and name 06 ) 2.1 0.3 0.3
assign	(resid	17	and	name	02	) (resid 24 and name H22 $$ ) 2.1 0.3 0.3 $$

# Dihedral restraints for AMBER modeling of 39-nt hairpin

2	GUA	ALPHA	-155.0	25.0	18	ADE	GAMMA	0.0	120.0
3	ADF	ΑΙ ΡΗΑ	-155.0	25.0	28	GUA	GAMMA	0.0	120.0
4	URA		-155.0	25.0	29	GUA	GAMMA	0.0	120.0
5			-155 0	25.0	30	GUA	GAMMA	0.0 0 0	120.0
6			-155 0	25.0	34	GUA	GAMMA	0.0 0 0	120.0
7	GUA		-155 0	25.0	25	CVT	GAMMA	0.0 0 0	120.0
, 0	CVT		155.0	25.0	26		CAMMA	0.0	120.0
0			155.0	25.0	0C 7C		CAMMA	0.0	120.0
12			155.0	25.0	) ( ) (		CAMMA	0.0	120.0
10			155.0	25.0	ەد مد			0.0	120.0
14			-155.0	25.0	59	UKA		0.0	115 0
1/			-155.0	25.0	1	GUA		45.0	115.0
18	ADE	ALPHA	-155.0	25.0	2	GUA	DELTA	45.0	115.0
28	GUA	ALPHA	-155.0	25.0	3	ADE	DELTA	45.0	115.0
29	GUA	ALPHA	-155.0	25.0	4	URA	DELIA	45.0	115.0
30	GUA	ALPHA	-155.0	25.0	5	URA	DELTA	45.0	115.0
34	GUA	ALPHA	-155.0	25.0	6	URA	DELTA	45.0	115.0
35	CYT	ALPHA	-155.0	25.0	7	GUA	DELTA	45.0	115.0
36	ADE	ALPHA	-155.0	25.0	8	CYT	DELTA	45.0	115.0
37	GUA	ALPHA	-155.0	25.0	9	ADE	DELTA	45.0	115.0
38	ADE	ALPHA	-155.0	25.0	12	CYT	DELTA	45.0	115.0
39	URA	ALPHA	-155.0	25.0	13	CYT	DELTA	45.0	115.0
2	GUA	BETA	90.0	240.0	14	URA	DELTA	45.0	115.0
3	ADE	BETA	90.0	240.0	15	ADE	DELTA	45.0	115.0
4	URA	BETA	90.0	240.0	16	CYT	DELTA	45.0	115.0
5	URA	BETA	90.0	240.0	17	СҮТ	DELTA	45.0	115.0
6	URA	BETA	90.0	240.0	18	ADE	DELTA	45.0	115.0
7	GUA	BETA	90.0	240.0	23	CYT	DELTA	45.0	115.0
8	СҮТ	BETA	90.0	240.0	26	ADE	DELTA	45.0	115.0
9	ADE	BETA	90.0	240.0	27	URA	DELTA	45.0	115.0
13	СҮТ	BETA	90.0	240.0	28	GUA	DELTA	45.0	115.0
14	URA	вета	90.0	240.0	29	GUA	DELTA	45.0	115.0
17	CYT	BETA	90.0	240.0	30	GUA	DELTA	45.0	115.0
18	ADF	BETA	90.0	240.0	31	ADF	DELTA	45.0	115.0
28	GUA	BETA	90.0	240.0	33	LIRA		45.0	115.0
29	GUA	BETA	90.0	240 0	34	GUA		45 0	115 0
30	GUA	BETA	90.0	240.0	35	CVT		45.0	115 0
3/	GUA	RETA	90.0	240.0	36			45.0	115 0
35	CVT	BETA	90.0	240.0	37	GUA		45.0	115 0
36		RETA	90.0	240.0	38			45.0	115 0
37		BETA	90.0	240.0	30			45.0	115 0
20		BETA	90.0	240.0	1	GUA		-240 0	10 0
20		DETA	90.0	240.0	1	CUA		240.0	10.0
29			90.0	120.0	2		EPSILN	-240.0	10.0
1 2	GUA	GAMMA	0.0	120.0	3		EPSILN	-240.0	10.0
2	GUA	GAMMA	0.0	120.0	4		EPSILN	-240.0	10.0
3	ADE	GAMMA	0.0	120.0	5	URA	EPSILN	-240.0	10.0
4	URA	GAMMA	0.0	120.0	6	UKA	EPSILN	-240.0	10.0
5	URA	GAMMA	0.0	120.0	7	GUA	EPSILN	-240.0	10.0
6	URA	GAMMA	0.0	120.0	8	CYT	EPSILN	-240.0	10.0
7	GUA	GAMMA	0.0	120.0	12	CYT	EPSILN	-240.0	10.0
8	CYT	GAMMA	0.0	120.0	13	CYT	EPSILN	-240.0	10.0
9	ADE	Gamma	0.0	120.0	14	URA	EPSILN	-240.0	10.0
13	CYT	Gamma	0.0	120.0	16	CYT	EPSILN	-240.0	10.0
14	URA	Gamma	0.0	120.0	17	CYT	EPSILN	-240.0	10.0
17	CYT	GAMMA	0.0	120.0	27	URA	EPSILN	-240.0	10.0

28	GUA	EPSILN	-240.0	10.0
29	GUA	EPSILN	-240.0	10.0
33	URA	EPSILN	-240.0	10.0
34	GUA	EPSILN	-240.0	10.0
35	CYT	EPSILN	-240.0	10.0
36	ADE	EPSILN	-240.0	10.0
37	GUA	EPSILN	-240.0	10.0
38	ADE	EPSILN	-240.0	10.0
1	GUA	ZETA	-160.0	20.0
2	GUA	ZETA	-160.0	20.0
3	ADE	ZETA	-160.0	20.0
4	URA	ZETA	-160.0	20.0
5	URA	7FTA	-160.0	20.0
6	URA	7FTA	-160.0	20.0
7	GUA	7FTA	-160.0	20.0
, 8	СУТ	<b>ΖΕ</b> ΤΛ 7ΕΤΔ	-160.0	20.0
12	СУТ	7674	-160.0	20.0
12	CVT		-160.0	20.0
1/			-160.0	20.0
14	CVT		160.0	20.0
17	CVT		160.0	20.0
1/ 27			160.0	20.0
2/			100.0	20.0
28	GUA		-160.0	20.0
29	GUA		-160.0	20.0
33	UKA	ZETA	-160.0	20.0
34	GUA	ZETA	-160.0	20.0
35	CYI	ZETA	-160.0	20.0
36	ADE	ZETA	-160.0	20.0
37	GUA	ZETA	-160.0	20.0
38	ADE	ZETA	-160.0	20.0
1	GUA	CHI	170.0	340.0
2	GUA	CHI	170.0	340.0
3	ADE	CHI	170.0	340.0
4	URA	CHI	170.0	340.0
5	URA	CHI	170.0	340.0
6	URA	CHI	170.0	340.0
7	GUA	CHI	170.0	340.0
8	CYT	CHI	170.0	340.0
9	ADE	CHI	170.0	340.0
11	GUA	CHI	170.0	340.0
12	CYT	CHI	170.0	340.0
13	CYT	CHI	170.0	340.0
14	URA	CHI	170.0	340.0
15	ADE	CHI	170.0	340.0
16	CYT	CHI	170.0	340.0
17	CYT	CHI	170.0	340.0
18	ADE	CHI	170.0	340.0
19	GUA	CHI	170.0	340.0
20	ADE	CHI	170.0	340.0
21	ADE	CHI	170.0	340.0
22	ADE	CHI	170.0	340.0
23	CYT	CHT	170.0	340.0
24	GUA	CHT	170.0	340.0
25	GUA	CHI	170.0	340.0

26	ADE	CHI	170.0	340.0
27	URA	CHI	170.0	340.0
28	GUA	CHI	170.0	340.0
29	GUA	CHI	170.0	340.0
30	GUA	CHI	170.0	340.0
31	ADE	CHI	170.0	340.0
32	GUA	CHI	170.0	340.0
33	URA	CHI	170.0	340.0
34	GUA	CHI	170.0	340.0
35	CYT	CHI	170.0	340.0
36	ADE	CHI	170.0	340.0
37	GUA	CHI	170.0	340.0
38	ADE	CHI	170.0	340.0
39	URA	CHI	170.0	340.0

# Distance restraints for AMBER modeling of 11-nt hairpin

accion	(residue	16	and	name	H1'	)	(residue	16	and	name	H6	)	3 68	Q 77	Q 96
assign	(nosiduo	16	and	name	111 111		(nosiduo	26	and	name	цр		2 96	0.77	1 00
assign	(residue	17	and	name	11 <u>1</u>	~	(residue	17	and	name		~	1 00	0.01	1 04
assign	(residue	17	anu	name	יכח	Ś	(residue	17	anu	name		~	2 60	0.04	0.04
assign	(residue	17	anu	name	п <u>∠</u>	,	(residue	10	anu	name		,	2.09	0.77	1 22
assign	(residue	17	anu	name		Ś	(residue	10	anu	name		Ś	4.70	0.99	1.22
assign	(residue	17	anu	name	HZ	)	(residue	12	and	name	Πð	)	2.4/	0.52	0.64
assign	(residue	17	and	name	H3	)	(residue	1/	and	name	HI	)	3.69	0.78	0.96
assign	(residue	1/	and	name	H3	)	(residue	18	and	name	H8	)	3.11	0.65	0.81
assign	(residue	18	and	name	H1'	)	(residue	18	and	name	H8	)	4.27	0.90	1.11
assign	(residue	18	and	name	H2 '	)	(residue	18	and	name	H8	)	3.46	0.73	0.90
assign	(residue	18	and	name	H3 '	)	(residue	18	and	name	H1'	)	4.46	0.94	1.16
assign	(residue	18	and	name	H3'	)	(residue	18	and	name	H8	)	2.64	0.55	0.69
assign	(residue	19	and	name	H1'	)	(residue	18	and	name	H2	)	5.03	1.06	1.31
assign	(residue	19	and	name	H2'	)	(residue	19	and	name	H1'	)	2.82	0.59	0.73
assign	(residue	19	and	name	H3'	)	(residue	19	and	name	H8	)	2.72	0.57	0.71
assign	(residue	19	and	name	H4'	)	(residue	19	and	name	H1'	)	3.15	0.66	0.82
assign	(residue	20	and	name	H1'	)	(residue	20	and	name	H8	)	3.85	0.81	1.00
assign	(residue	20	and	name	H2'	)	(residue	20	and	name	H8	)	3.79	0.80	0.98
assign	(residue	20	and	name	H2'	)	(residue	21	and	name	H1'	)	3.45	0.72	0.90
assign	(residue	20	and	name	H2'	)	(residue	21	and	name	H8	)	2.77	0.58	0.72
assign	(residue	20	and	name	H3'	ý	(residue	20	and	name	Н8	)	3.28	0.69	0.85
assign	(residue	20	and	name	H3'	Ś	(residue	21	and	name	Н8	ý	2.59	0.54	0.67
assign	(residue	21	and	name	H1'	Ś	(residue	20	and	name	H2	Ś	3.25	0.68	0.85
assign	(residue	21	and	name	H1'	Ś	(residue	21	and	name	Н8	ś	4.47	0.94	1.16
assign	(residue	21	and	name	H2'	ś	(residue	22	and	name	H1'	ś	5.01	1.05	1.30
assign	(residue	21	and	name	НЗ'	Ś	(residue	21	and	name		Ś	2.90	0.61	0.75
assign	(residue	22	and	name	H1'	Ś	(residue	21	and	name	H2	Ś	4 02	0.01	1 05
assign	(residue	22	and	name	H4'	Ś	(residue	22	and	name	H1'	Ś	3 72	0.04 0.78	A 97
accion	(residue	22	and	name	H2'	Ś	(residue	22	and	name	НА	Ś	3 60	0.70 0.76	0.9/ 0 9/
assign	(residue	22	and	name	H2'	Ś	(residue	27	and	name	ня		3 17	0.70	0.24
assign	(residue	27	and	name	11Z 112'		(residue	27	and	name	ЦΩ	~	2 52	0.07	0.05
assign	(residue	24	and	name	11Z		(residue	27	and	name	ц1 '	~	3 00	0.55	0.05
assign	(residue	24	and	name	יכו		(residue	24	and	name	пт ПО	~	2.09	0.05	0.00
assign	(residue	24	anu	name	יכם יכם	~	(residue	24	anu	name	по	~	2.90	0.01	0.75
assign	(residue	24	anu	name	ПЭ 111 1	,	(residue	25	anu	name		,	2.05	0.04	1 10
assign	(residue	25	anu	name	п <u>т</u>	Ś	(residue	25	anu	name		)	4.4/	0.94	1.10
assign	(residue	25	and	name	HZ	Ś	(residue	25	and	name		)	2.66	0.50	0.69
assign	(residue	25	and	name	HZ	)	(residue	26	and	name	HI	)	4.54	0.95	1.18
assign	(residue	25	and	name	H3	)	(residue	25	and	name	H8	)	3.10	0.65	0.81
assign	(residue	26	and	name	HI	)	(residue	26	and	name	HZ	)	5.58	1.1/	1.45
assign	(residue	26	and	name	H1	)	(residue	26	and	name	H8	)	4.29	0.90	1.12
assign	(residue	17	and	name	H3	)	(residue	17	and	name	H6	)	2.60	0.55	0.68
assign	(residue	18	and	name	H2'	)	(residue	18	and	name	H1'	)	2.60	0.55	0.68
assign	(residue	18	and	name	H2'	)	(residue	19	and	name	H1'	)	3.69	0.78	0.96
assign	(residue	18	and	name	H2'	)	(residue	19	and	name	H8	)	3.02	0.63	0.79
assign	(residue	19	and	name	H2'	)	(residue	21	and	name	H8	)	3.90	0.82	1.01
assign	(residue	19	and	name	H3'	)	(residue	19	and	name	H1'	)	4.09	0.86	1.06
assign	(residue	20	and	name	H4'	)	(residue	20	and	name	H1'	)	3.47	0.73	0.90
assign	(residue	21	and	name	H2'	)	(residue	21	and	name	H1'	)	2.72	0.57	0.71
assign	(residue	21	and	name	H3'	)	(residue	21	and	name	H1'	)	3.66	0.77	0.95
assign	(residue	21	and	name	H4'	)	(residue	21	and	name	H1'	)	3.62	0.76	0.94
assign	(residue	22	and	name	H2'	)	(residue	22	and	name	H1'	)	2.87	0.60	0.75
assign	(residue	22	and	name	H2'	)	(residue	23	and	name	H6	)	2.80	0.59	0.73
assign	(residue	22	and	name	H3'	)	(residue	23	and	name	H6	)	2.63	0.55	0.68

assign (residue 23 and name H2' ) 3.13 0.66 0.82 ) (residue 24 and name H1' assign (residue 17 and name H41 ) (residue 24 and name H1 ) 2.33 0.93 0.93 assign (residue 18 and name H1' ) (residue 24 and name N2 ) 2.62 1.05 2.05 assign (residue 22 and name H8 ) (residue 19 and name H21 ) 2.88 1.15 1.15 assign (residue 23 and name N4 ) (residue 18 and name H2 ) 2.70 1.08 2.08 assign (residue 25 and name H1' ) (residue 24 and name N2 ) 2.77 1.11 2.11 assign (resid 16 and name N3  $\,$  ) (resid 25 and name H1  $\,$  )  $\,$  2.1 0.3 0.3  $\,$ assign (resid 16 and name H41 ) (resid 25 and name 06 ) 2.1 0.3 0.3 assign (resid 16 and name O2 ) (resid 25 and name H22 ) 2.1 0.3 0.3 assign (resid 17 and name N3 ) (resid 24 and name H1 ) 2.1 0.3 0.3 assign (resid 17 and name H41 ) (resid 24 and name 06 ) 2.1 0.3 0.3 assign (resid 17 and name O2 ) (resid 24 and name H22 ) 2.1 0.3 0.3 assign (resid 19 and name H1 ) (resid 19 and name H22 ) 1.8 0 0.7 assign (resid 24 and name H1  $\,$  ) (resid 24 and name H22  $\,$  ) 1.8 0 0.7  $\,$ assign (resid 25 and name H1 ) (resid 25 and name H22 ) 1.8 0 0.7

#### Dihedral restraints for AMBER modeling of 11-nt hairpin

17	CYT	ALPHA	-155.0	25.0
18	ADE	ALPHA	-155.0	25.0
17	CYT	BETA	90.0	240.0
18	ADE	BETA	90.0	240.0
17	CYT	GAMMA	0.0	120.0
18	ADE	GAMMA	0.0	120.0
16	CYT	DELTA	45.0	115.0
17	CYT	DELTA	45.0	115.0
18	ADE	DELTA	45.0	115.0
23	CYT	DELTA	45.0	115.0
26	ADE	DELTA	45.0	115.0
16	CYT	EPSILN	-240.0	10.0
17	CYT	EPSILN	-240.0	10.0
17 16	CYT CYT	EPSILN CHI	-240.0 170.0	10.0 340.0
17 16 17	CYT CYT CYT	EPSILN CHI CHI	-240.0 170.0 170.0	10.0 340.0 340.0
17 16 17 18	CYT CYT CYT ADE	EPSILN CHI CHI CHI	-240.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0
17 16 17 18 19	CYT CYT CYT ADE GUA	EPSILN CHI CHI CHI CHI	-240.0 170.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0 340.0
17 16 17 18 19 20	CYT CYT ADE GUA ADE	EPSILN CHI CHI CHI CHI CHI	-240.0 170.0 170.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0 340.0 340.0
17 16 17 18 19 20 21	CYT CYT ADE GUA ADE ADE	EPSILN CHI CHI CHI CHI CHI CHI	-240.0 170.0 170.0 170.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0 340.0 340.0 340.0
17 16 17 18 19 20 21 22	CYT CYT ADE GUA ADE ADE ADE	EPSILN CHI CHI CHI CHI CHI CHI CHI	-240.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0
17 16 17 18 19 20 21 22 23	CYT CYT ADE GUA ADE ADE ADE CYT	EPSILN CHI CHI CHI CHI CHI CHI CHI CHI	-240.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0
17 16 17 18 19 20 21 22 23 24	CYT CYT ADE GUA ADE ADE CYT GUA	EPSILN CHI CHI CHI CHI CHI CHI CHI CHI CHI	-240.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0
17 16 17 18 20 21 22 23 24 25	CYT CYT ADE GUA ADE ADE ADE CYT GUA GUA	EPSILN CHI CHI CHI CHI CHI CHI CHI CHI CHI CHI	-240.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0 170.0	10.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0 340.0

# Distance restraints for AMBER modeling of 19-nt duplex

assign	(residue	8	and	name	H1'	)	(residue	7	and	name	H1	)	3.93	1.57	1.57
assign	(residue	9	and	name	H2	Ś	(residue	33	and	name	H3	Ś	2.57	1.03	1.03
assign	(residue	9	and	name	H2	Ś	(residue	34	and	name	H1	ś	4.19	1.68	1.68
assign	(residue	12	and	name	н1'	Ś	(residue	11	and	name	H1	ś	3 55	1 42	1 42
assign	(residue	12	and	name	H41	Ś	(residue	30	and	name	H1	ś	2 15	0 86	0 86
assign	(residue	13	and	name	H1'	Ś	(residue	30	and	name	H1	Ś	<i>L</i> .13	1 76	1 76
assign	(residue	1/	and	namo	ц1'	~	(residue	20	and	name	н <u>т</u>	Ś	3 03	1 57	1 57
assign	(residue	14	anu	name		Ś	(residue	29	anu	name		~	2.22 2 20	1.J/ 0.01	0 01
assign	(residue	20	anu	name		Ś	(residue	20	anu	name		,	2.20	1 27	1 27
assign	(residue	50 71	anu	name	пт Т	Ś	(residue	29	anu	name		Ś	5.4Z	1.5/	1.5/
assign	(residue	31	and	name	HZ	Ś	(residue	11	and	name	HI	)	2.//	1.11	1.11
assign	(residue	35	and	name	H41	)	(residue	/	and	name	HI	)	2.10	0.84	0.84
assign	(residue	36	and	name	H1.	)	(residue	/	and	name	H1	)	3.5/	1.43	1.43
assign	(residue	11	and	name	H22	)	(residue	31	and	name	H2	)	1.80	0.00	1.50
assign	(residue	7	and	name	H2'	)	(residue	8	and	name	H6	)	2.44	0.51	0.64
assign	(residue	7	and	name	H3'	)	(residue	7	and	name	H8	)	3.45	0.72	0.90
assign	(residue	7	and	name	H4'	)	(residue	7	and	name	H1'	)	3.18	0.67	0.83
assign	(residue	8	and	name	H2'	)	(residue	8	and	name	H1'	)	2.60	0.55	0.68
assign	(residue	8	and	name	H3'	)	(residue	8	and	name	H6	)	2.42	0.51	0.63
assign	(residue	8	and	name	H4'	)	(residue	8	and	name	H1'	)	2.75	0.58	0.71
assign	(residue	9	and	name	H2'	)	(residue	9	and	name	H1'	)	2.62	0.55	0.68
assign	(residue	9	and	name	H2'	)	(residue	10	and	name	H8	)	1.80	0.00	3.20
assign	(residue	9	and	name	H3'	Ś	(residue	9	and	name	H8	ý	3.05	0.64	0.79
assign	(residue	9	and	name	H4'	Ś	(residue	9	and	name	H1'	Ś	3.19	0.67	0.83
assign	(residue	11	and	name	H2'	Ś	(residue	11	and	name	H1'	ś	2.90	0.61	0.75
assign	(residue	11	and	name	H2'	Ś	(residue	12	and	name	Н6	ś	2.51	0.53	0.65
assign	(residue	12	and	name	H2'	Ś	(residue	12	and	name	H1'	ś	2 71	0.55	0 71
assign	(residue	12	and	name	H2'	Ś	(residue	12	and	name	Н6	Ś	4 05	0.97	1 05
accion	(residue	12	and	name	H2'	Ś	(residue	13	and	name	Н6	Ś	2 22	0.0J 0 /9	0 60
assign	(residue	12	and	namo	<u>цзі</u>	~	(residue	12	and	name	не	Ś	2.52	0.45	0.00
assign	(residue	12	and	name	יכם	{	(nociduo	11	and	name	ПО ЦС	~	2.54	0.55	0.00
assign	(residue	10	anu	name	112	Ś	(residue	17	anu	name		(	2.41 2 11	0.51	0.05
assign	(residue	10	anu	name	כחיכוו	Ś	(residue	10	anu	name		,	2.11	0.05	0.01
assign	(resture	12	anu	name		Ś	(residue	12	anu	name		)	2.55	0.49	0.01
assign	(residue	13	and	name	H4	,	(residue	13	and	name	HI	)	3.05	0.64	0.79
assign	(residue	14	and	name	HZ	)	(residue	14	and	name	HI	)	2.5/	0.54	0.6/
assign	(residue	14	and	name	H3	)	(residue	15	and	name	H8	)	3.08	0.65	0.80
assign	(residue	27	and	name	H4 '	)	(residue	27	and	name	H1'	)	3.08	0.65	0.80
assign	(residue	28	and	name	H2'	)	(residue	28	and	name	H8	)	3.68	0.77	0.96
assign	(residue	28	and	name	H2'	)	(residue	29	and	name	H1'	)	4.33	0.91	1.13
assign	(residue	28	and	name	H2'	)	(residue	29	and	name	H8	)	2.48	0.52	0.65
assign	(residue	28	and	name	H3'	)	(residue	28	and	name	H1'	)	3.21	0.67	0.84
assign	(residue	28	and	name	H3'	)	(residue	28	and	name	H8	)	2.89	0.61	0.75
assign	(residue	28	and	name	H3'	)	(residue	29	and	name	H8	)	3.28	0.69	0.85
assign	(residue	28	and	name	H4'	)	(residue	28	and	name	H1'	)	3.18	0.67	0.83
assign	(residue	29	and	name	H2'	)	(residue	29	and	name	H8	)	4.42	0.93	1.15
assign	(residue	29	and	name	H2'	)	(residue	30	and	name	H1'	)	4.37	0.92	1.14
assign	(residue	29	and	name	H2'	)	(residue	30	and	name	H8	)	2.48	0.52	0.64
assign	(residue	29	and	name	H3'	)	(residue	29	and	name	H8	)	2.81	0.59	0.73
assign	(residue	29	and	name	H3'	ý	(residue	30	and	name	H8	ý	3.38	0.71	0.88
assign	(residue	30	and	name	H2'	ý	(residue	30	and	name	H1'	Ś	2.77	0.58	0.72
assign	(residue	30	and	name	H2'	ý	(residue	31	and	name	H8	Ś	2.49	0.52	0.65
assign	(residue	30	and	name	H3'	ý	(residue	30	and	name	H1 '	ś	3.99	0.84	1.04
assign	(residue	30	and	name	НЗ'	ì	(residue	30	and	name	HR	Ś	2.88	0.61	0.75
assion	(residue	30	and	name	нз'	)	(residue	31	and	name	ня	Ś	3 74	0 79	0 97
assten	(I COTUNE	50	unu	nume			( COTURE	71	unu	nume	10	)	2.74	0.75	0.57

assign	(residue	30	and	name	H4'	)	(residue	30	and	name	H1'	)	3.47	0.73	0.90
assign	(residue	31	and	name	H2'	)	(residue	31	and	name	H1'	)	2.61	0.55	0.68
assign	(residue	31	and	name	H3'	)	(residue	31	and	name	H1'	)	3.82	0.80	0.99
assign	(residue	31	and	name	H3'	)	(residue	31	and	name	H8	)	2.78	0.58	0.72
assign	(residue	31	and	name	H4'	)	(residue	31	and	name	H1'	)	3.34	0.70	0.87
assign	(residue	32	and	name	H2'	)	(residue	33	and	name	H6	)	2.44	0.51	0.63
assign	(residue	32	and	name	H3'	ý	(residue	33	and	name	H6	)	3.21	0.67	0.83
assign	(residue	33	and	name	H2'	ý	(residue	34	and	name	H1'	ý	3.64	0.76	0.95
assign	(residue	33	and	name	H2'	Ś	(residue	34	and	name	Н8	Ś	2.34	0.49	0.61
assign	(residue	33	and	name	Н3'	Ś	(residue	33	and	name	H1'	Ś	2.50	0.00	2.00
assign	(residue	33	and	name	H3'	Ś	(residue	33	and	name	H6	Ś	2.43	0.51	0.63
assign	(residue	34	and	name	H2'	ś	(residue	34	and	name	H8	ś	3.51	0.74	0.91
assign	(residue	34	and	name	H2'	Ś	(residue	35	and	name	H1 '	Ś	3 71	0 78	0.96
assign	(residue	34	and	name	H2'	Ś	(residue	35	and	name	Н6	Ś	2 44	0.70	0.50
assign	(residue	34	and	name	<u>цз</u> ,	Ś	(residue	3/	and	name	цо	``	2.44	0.51	0.05
assign	(residue	25	and	name	цз'		(residue	25	and	name	НС		2.55	0.55	0.00
assign	(residue	7	and	name	нэ ц1 '		(residue	7	and	name	ЦΩ		1 05	0.55	1 05
assign	(residue	, 0	and	name	пт Ц1 і		(residue	0	and	name	по Ц6	~	2 02	0.05	1.05
assign	(residue	0	and	name	יכח		(residue	0	and	name	по ⊔1 '		2.02 2 10	0.00	0.99
assign	(residue	10	anu	name	1111		(residue	10	anu	name		,	2.13	0.07	0.05
assign	(residue	10	anu	name			(residue	10	anu	name		)	5.02	0.05	0.70
assign	(residue	11	and	name	HI		(residue	11	and	name	Hð	)	3.20	0.00	0.90
assign	(residue	12	and	name	HI	)	(residue	12	and	name	H6	)	3.20	0.00	0.90
assign	(residue	13	and	name	HI	)	(residue	13	ana	name	H6	)	4.48	0.94	1.1/
assign	(residue	15	and	name	H1'	)	(residue	15	and	name	H8	)	3.79	0.80	0.98
assign	(residue	29	and	name	H2'	)	(residue	29	and	name	H1'	)	2.45	0.51	0.64
assign	(residue	29	and	name	H3 '	)	(residue	29	and	name	H1'	)	2.50	0.00	2.00
assign	(residue	31	and	name	H2'	)	(residue	32	and	name	H8	)	3.17	0.67	0.82
assign	(residue	32	and	name	H1'	)	(residue	31	and	name	H2	)	3.51	0.74	0.91
assign	(residue	34	and	name	H1'	)	(residue	9	and	name	H2	)	4.10	0.86	1.07
assign	(residue	34	and	name	H2'	)	(residue	34	and	name	H1'	)	2.39	0.50	0.62
assign	(residue	34	and	name	H3'	)	(residue	34	and	name	H1'	)	3.10	0.65	0.81
assign	(residue	34	and	name	H3'	)	(residue	35	and	name	H6	)	3.00	0.63	0.78
assign	(residue	35	and	name	H1'	)	(residue	35	and	name	H6	)	3.84	0.81	1.00
assign	(residue	36	and	name	H1'	)	(residue	36	and	name	H8	)	4.10	0.86	1.07
accian	(nocid 7	200	1 10 21	no ∐1	``	(noc	id 25 and	4		ND 1	2 1	0	202		
assign	(resid 7	200	l nar			(nes	$\frac{1}{2}$	סוו ג ימ 1	anne i Smo i	⊔⊿1 <sup>°</sup>	2.1 \ 2.1	_ 0.	20.2		
assign	(resid 7	and	l IIdi l nor			(res		, ne		⊓41 	) 2.1		2 0.2		
assign	(resid /	and	l nar		<u>د د</u>	(1.6	2510 55 di	י גו ה			) Z.1 2 1	0.	20.2		
assign	(resid 8	and	i nar		, )	(res	510 34 and	ina.	ame i		2.1 2.1	. 0.	5 0.5		
assign	(resid 8	and	i nar	ne H4.	т )	(re	2s10 34 ar	ו גר	name	06	) 2.1	. 0.	3 0.3		
assign	(resid 8	and	i nar	ne U2	)	(res	510 34 and	i na	ame i		) 2.1	. 0.	5 0.5		
assign	(resid 9	and	nar	ne NI	)	(res	510 33 and	na	ame I	H3)	2.1	. 0.	3 0.3		
assign	(resid 9	and	d nar	ne H61	1)	(re	esid 33 an	nd i	name	04	) 2.1	. 0.	3 0.3		
assign	(resid 12	2 ar	nd na	ame N3	3)	(re	esid 30 an	nd r	name	H1	) 2.	10	.3 0.3		
assign	(resid 12	2 ar	nd na	ame H4	41	) (r	resid 30 a	and	name	e 06	) 2.	10	.3 0.3		
assign	(resid 12	2 ar	nd na	ame O2	2)	(re	esid 30 an	nd r	name	H22	) 2.	10	.3 0.3		
assign	(resid 13	3 ar	nd na	ame Na	3)	(re	esid 29 an	nd r	name	H1	) 2.	10	.3 0.3		
assign	(resid 13	3 ar	nd na	ame H4	41	) (r	resid 29 a	and	name	e 06	) 2.	10	.3 0.3		
assign	(resid 13	3 ar	nd na	ame O2	2)	(re	esid 29 an	nd i	name	H22	) 2.	10	.3 0.3		
assign	(resid 14	4 ar	nd na	ame N3	3)	(re	esid 28 an	nd i	name	H1	) 2.	10	.3 0.3		
assign	(resid 14	4 ar	nd na	ame H4	41	) (r	resid 28 a	and	name	e 06	) 2.	10	.3 0.3		
assign	(resid 14	4 ar	nd na	ame O2	2)	(re	esid 28 an	nd r	name	H22	) 2.	1 0	.3 0.3		
assign	(resid 1	5 ar	nd na	ame Ni	1)	(re	esid 27 an	nd r	name	H3	) 2.	1 0	.3 0.3		

assign (resid 15 and name H61 ) (resid 27 and name O4 ) 2.1 0.3 0.3

#### Dihedral restraints for AMBER modeling of 19-nt duplex (continued)

8	CYT	ALPHA	-155.0	25.0	7 GUA EPSILN -24	0.0 10.0
9	ADE	ALPHA	-155.0	25.0	8 CYT EPSILN -24	0.0 10.0
13	CYT	ALPHA	-155.0	25.0	12 CYT EPSILN -24	0.0 10.0
14	CYT	ALPHA	-155.0	25.0	13 CYT EPSILN -24	0.0 10.0
15	ADE	ALPHA	-155.0	25.0	14 CYT EPSILN -24	0.0 10.0
28	GUA	ALPHA	-155.0	25.0	27 URA EPSILN -24	0.0 10.0
29	GUA	ALPHA	-155.0	25.0	28 GUA EPSILN -24	0.0 10.0
30	GUA	ALPHA	-155.0	25.0	29 GUA EPSILN -24	0.0 10.0
34	GUA	ALPHA	-155.0	25.0	33 URA EPSILN -24	0.0 10.0
35	CYT	ALPHA	-155.0	25.0	34 GUA EPSILN -24	0.0 10.0
36	ADE	ALPHA	-155.0	25.0	35 CYT EPSILN -24	0.0 10.0
8	CYT	BETA	90.0	240.0	7 GUA ZETA -16	0.0 20.0
9	ADE	BETA	90.0	240.0	8 CYT ZETA -16	0.0 20.0
13	CYT	BETA	90.0	240.0	12 CYT ZETA -16	0.0 20.0
14	CYT	BETA	90.0	240.0	13 CYT ZETA -16	0.0 20.0
15	ADE	BETA	90.0	240.0	14 CYT ZETA -16	0.0 20.0
28	GUA	BETA	90.0	240.0	27 URA ZETA -16	0.0 20.0
29	GUA	BETA	90.0	240.0	28 GUA ZETA -16	0.0 20.0
30	GUA	BETA	90.0	240.0	29 GUA ZETA -16	0.0 20.0
34	GUA	BETA	90.0	240.0	33 URA ZETA -16	0.0 20.0
35	CYT	BETA	90.0	240.0	34 GUA ZETA -16	6.0 20.0
36	ADE	BETA	90.0	240.0	35 CYT ZETA -16	6.0 20.0
7	GUA	GAMMA	0.0	120.0	7 GUA CHI 17	'0.0  340.0
8	СҮТ	Gamma	0.0	120.0	8 CYT CHI 17	'0.0 340.0
9	ADE	Gamma	0.0	120.0	9 ADE CHI 17	'0.0 340.0
13	CYT	GAMMA	0.0	120.0	12 CYT CHI 17	'0.0 340.0
14	CYT	GAMMA	0.0	120.0	13 CYT CHI 17	0.0 340.0
15	ADE	Gamma	0.0	120.0	14 CYT CHI 17	'0.0 340.0
27	URA	GAMMA	0.0	120.0	15 ADE CHI 17	'0.0 340.0
28	GUA	GAMMA	0.0	120.0	27 URA CHI 17	0.0 340.0
29	GUA	GAMMA	0.0	120.0	28 GUA CHI 17	0.0 340.0
30	GUA	GAMMA	0.0	120.0	29 GUA CHI 17	'0.0 340.0
34	GUA	GAMMA	0.0	120.0	30 GUA CHI 17	'0.0 340.0
35	CYI	GAMMA	0.0	120.0	31 ADE CHI 17	'0.0 340.0
36	ADE	GAMMA	0.0	120.0	32 GUA CHI 17	'0.0 340.0
/	GUA	DELTA	45.0	115.0	33 URA CHI 17	'0.0 340.0
8	CYI	DELTA	45.0	115.0	34 GUA CHI 17	'0.0 340.0
10	ADE	DELTA	45.0	115.0	35 CY1 CHI 17	<sup>7</sup> 0.0 340.0
10	GUA	DELTA	45.0	115.0	36 ADE CHI 17	0.0 340.0
11	GUA	DELTA	45.0	115.0		
12		DELTA	45.0	115.0		
13		DELTA	45.0	115.0		
14			45.0	115.0		
12		DELTA	45.0	115.0		
27	UKA	DELTA	45.0	115.0		
28	GUA	DELTA	45.0	115.0		
29	GUA		45.0	115.0		
30	GUA		45.0	115.0		
31	ADE		45.0	112.0		
32	GUA		45.0	115.0		
33	UKA		45.0	112.0		
34	GUA	DELIA	45.0	115.0		
35	CYT	DELTA	45.0	115.0		
36	ADE	DELTA	45.0	115.0		

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