Supporting Information

NMR-assisted prediction of secondary structure for RNA: Incorporation of direction-dependent NMR constraints limits folding space

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Spectral analysis of \textit{r(CUGGCUAG)}\textsubscript{2} and \textit{r(AGGC\textsubscript{U}U)}\textsubscript{2}

2D NOESY spectra for \textit{r(CUGGCUAG)}\textsubscript{2} were obtained with mixing times of 100 ms and 400 ms at 5 °C. The G3H1 and U6H3 protons were assigned according to their positions in the imino region of the 100 ms spectrum (Figure S1). Cross-peaks to G3H1 and U6H3 identified the G4H1 resonance while an NOE to A7H2 at around 7.12 ppm was used to identify U2H3. Cross-peaks between amino protons and H5 of C in NOESY spectra were used to differentiate their H5- H6 cross-peaks from those of U. The H5 of the terminal C1 residue is characteristically downfield from that of C5. H1’ to H6 and H8 resonances form a sequential walk, and the assignments of G3H1’ and G8H1’ were confirmed by interstrand and intrastrand NOE contacts, respectively, to A7H2 (Figure S1).

2D NOESY spectra for \textit{r(AGGC\textsubscript{U}U)}\textsubscript{2} were obtained with mixing times of 100 ms and 400 ms at 0 °C and 8 °C, respectively. The longer mixing-time 2D NOESY spectrum was acquired at 8 °C because aromatic peaks were well-resolved at this temperature among a series of 1D 11-echo spectra acquired at different temperatures. The G2H1 and U5H3 wobble pair and G3H1 imino protons were assigned according to their positions in the imino region in the 100 ms spectrum (Figure S2). Among the pyrimidine H5 protons, C4H5 has a cross-peak to C4H41/H42 and U5H5 has a cross-peak to G2H1. U6H5 was thereby assigned through process of elimination. Assignments for aromatic and H1’ peaks were confirmed with a sequential NOESY walk with the 400 ms spectrum (Figure S2). Within this region, G3H8 has a cross-peak to C4H5. H1’ cross-peaks to H2’ in the 400 ms spectrum were larger than those to H3’. Cross-peaks from A1H8 to its own H1’, H2’ and H3’ were used to differentiate A1H8 from A1H2.
Figure S1: 2D imino (top) and NOESY walk (bottom) region spectra of r(CUGCUAG)$_2$. The top spectrum was acquired with 100 ms mixing time at 5 °C and the bottom spectrum was acquired with 400 ms mixing time at 5 °C. Both spectra were acquired with a WATERGATE pulse to suppress water.
Figure S2: 2D imino (top) and NOESY walk (bottom) region spectra of r(AGGCUU)$_{2}$. The top spectrum was acquired with 100 ms mixing time at 0 °C and the bottom spectrum was acquired with 400 ms mixing time at 8 °C. Both spectra were acquired with a WATERGATE pulse to suppress water.
Figure S3: NMR spectra of human HAR1 showing imino proton walks for helix P2 (see Figure 9 for secondary structure). The top spectrum is a $^1$H-$^1$H NOESY spectrum acquired at 25 °C with 125 ms mixing time. Colored lines depict imino proton walks for helix P2 and correspond to base pairs in Figure 9 with the same colors. Colored dots represent base pair type (red is GC). A sequence of dots for the imino proton walk is in the lower right of the spectrum. The red box around the sequence of dots corresponds to the red base pairs in Figure 9. The bottom spectrum is a $^{15}$N-$^1$H HSQC spectrum acquired at 25 °C.
Figure S4: NMR spectra of human HAR1 showing imino proton walks for helix P3 (see Figure 9 for secondary structure). The top spectrum is a $^1$H-$^1$H NOESY spectrum acquired at 25 °C with 125 ms mixing time. Colored lines depict imino proton walks for helix P3 and correspond to base pairs in Figure 9 with the same colors. Colored dots represent base pair type (red is GC, blue is AU, and green is GU). Sequences of dots for imino proton walks are in the lower right of the spectrum. Light blue, orange, and purple boxes around sequences of dots correspond to light blue, orange, and purple base pairs in Figure 9. The bottom spectrum is a $^{15}$N-$^1$H HSQC spectrum acquired at 25 °C.
Figure S5: NMR spectra of human HAR1 showing imino proton walks for helix P4 (see Figure 9 for secondary structure). The top spectrum is a $^1$H-$^1$H NOESY spectrum acquired at 15 °C with 60 ms mixing time. Colored lines depict imino proton walks for helix P4 and correspond to base pairs in Figure 9 with the same colors. Colored dots represent base pair type (blue is AU and green is GU). A sequence of dots for the imino proton walk is in the lower right of the spectrum. The box around the sequences of dots is colored according to the U79:G104 and U80:A103 base pairs in Figure 9. The bottom spectrum is a $^{15}$N-$^1$H HSQC spectrum acquired at 25 °C.
Figure S6: NMR spectra of the 75-nt *B. mori* R2 retrotransposon pseudoknot showing an imino proton walk for base pairs G1:C57 to C5:G53 (see Figure 11 for secondary structure). The top spectrum was acquired at 25 °C with 200 ms mixing time. Colored lines depict imino proton for base pairs G1:C57 to C5:G53 and correspond to base pairs in Figure 11 with the same colors. Colored dots represent base pair type (red is GC). A sequence of dots for the imino proton walk is in the lower right of the spectrum. The box around the sequence of dots is colored according to base pairs G1:C57 to C5:G53 in Figure 11. The bottom is a $^{15}$N-$^1$H HSQC spectrum acquired at 25 °C.
Figure S7: NMR spectra of the 75-nt B. mori R2 retrotransposon pseudoknot showing an imino proton walk for base pairs G10:C29 to C14:G25 and C16:G23 to C17:G22 (see Figure 11 for secondary structure). The top spectrum was acquired at 25 °C with 200 ms mixing time. Colored lines depict imino proton for base pairs G10:C29 to C14:G25 and C16:G23 to C17:G22 and correspond to base pairs in Figure 11 with the same colors. Colored dots represent base pair type (red is GC and blue is AU). Sequences of dots for the imino proton walk is in the lower right of the spectrum. Green, purple, and red boxes around the sequence of dots correspond to green, purple, and red base pairs in Figure 11. The bottom is a $^{15}$N-$^1$H HSQC spectrum acquired at 25 °C.
Figure S8: NMR spectra of the 75-nt *B. mori* R2 retrotransposon pseudoknot showing an imino proton walk for base pairs G32:C75 to U35:G72 (see Figure 11 for secondary structure). The top spectrum was acquired at 25 °C with 200 ms mixing time. Colored lines depict imino proton for base pairs G32:C75 to U35:G72 and correspond to base pairs in Figure 11 with the same colors. Colored dots represent base pair type (red is GC and green is GU). A sequence of dots for the imino proton walk is in the lower right of the spectrum. The box around the sequence of dots is colored according to base pairs G32:C75 to U35:G72 in Figure 11. The bottom is a $^{15}$N-$^1$H HSQC spectrum acquired at 25 °C.
Figure S9: NMR spectra of the 75-nt *B. mori* R2 retrotransposon pseudoknot showing an imino proton walk for base pairs G37:C71 to U42:G66 and A43:U52 to C44:G51, including a connection across coaxially stacked helixes (see Figure 11 for secondary structure). The top spectrum was acquired at 25 °C with 200 ms mixing time. Colored lines depict imino proton for base pairs G37:C71 to U42:G66 and A43:U52 to C44:G51 and correspond to base pairs in Figure 11 with the same colors. Colored dots represent base pair type (red is GC and blue is AU). A sequence of dots for the imino proton walk is in the lower right of the spectrum. The box around the sequence of dots is colored according to base pairs G37:C71 to U42:G66 and A43:U52 to C44:G51 in Figure 11. The bottom is a $^{15}$N-$^1$H HSQC spectrum acquired at 25 °C.
Figure S10: Five structures without pseudoknots used to benchmark NAPSS-CS. Colored base pairs correspond to imino proton walks identified from literature NMR spectra (Tables S25 to S32). The sixth secondary structure, HAR1, is shown in Figure 9.
**K. lactis** telomerase RNA pseudoknot

**Murine leukemia virus recording signal pseudoknot**

Figure S11: Structures that NAPSS-CS failed to predict. Colored base pairs correspond to imino proton walks identified from literature NMR spectra (Tables S33 and S34).

| Table S1: Acquisition parameters used in NMR experiments on HAR1. |
|---|---|---|---|---|
| Experiment | Number of scans | Relaxation delay (s) | Direct | Indirect | Mixing time (s) |
| | | | complex data | complex data | |
| | | | points and spectral | points and spectral | |
| | | | width in t2 dimension | width in t1 dimension | |
| NOESY 60 | 512 | 0.07 | 15000 | 8550 | 0.06 |
| NOESY 125 | 512 | 0.07 | 15000 | 8550 | 0.125 |
| 13N-1H HSQC | 64 | 0.1 | 15000 | 1500 |  |

Table S2: Chemical shift assignments for r(AGGCUU).

| Residue | H1' | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---|---|---|---|---|---|
| A1 | 5.927 | 7.706 | 8.337 | - | |
| G2 | 5.677 | - | 7.487 | 11.04 | |
| G3 | 5.682 | - | 7.434 | 13.53 | |
| C4 | 5.583 | 5.227 | 7.577 | - | 8.553, 7.024 |
| U5 | 5.751 | 5.721 | 7.821 | 12.00 | |
| U6 | 5.768 | 5.675 | 7.858 | - | |

H1', H6 and H8 resonances were assigned in 400 ms spectra at 8°C. Other resonances were assigned in 100 ms spectra at 0°C.  *Assigned in 400 ms spectra at 8°C.*
Table S3: Chemical shift assignments for r(AGUCGAUU)$_2$.

| Residue | H1'   | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|-------|-------|-------|-------|---------------|
| A1      | 6.031 | 7.859 | 8.391 | -     |               |
| G2      | 5.731 | -     | 7.713 | 11.75 |               |
| U3      | 5.521 | 5.290 | 7.772 | 14.44 |               |
| C4      | 5.624 | 5.590 | 7.900 | -     | 8.200, 6.905  |
| G5      | 5.650 | -     | 7.529 | 12.00 |               |
| A6      | 5.910 | 7.757 | 7.690 | -     |               |
| U7      | 5.368 | 5.334 | 7.468 | 11.75 |               |
| U8      | 5.823 | 5.580 | 7.790 | -     |               |

H1’, H6 and H8 resonances were assigned in 400 ms spectra at 12°C. Other resonances were assigned in 100 ms spectra at 1°C unless otherwise noted. * Assigned in 400 ms spectra at 12°C.

Table S4: Chemical shift assignments for r(CUGGCUAG)$_2$.

| Residue | H1’   | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|-------|-------|-------|-------|---------------|
| C1      | 5.515 | 6.012 | 8.108 | -     | 8.280, 7.274  |
| U2      | 5.773 | 5.548 | 8.056 | 14.01 |               |
| G3      | 5.810 | -     | 7.759 | 10.24 |               |
| G4      | 5.664 | -     | 7.308 | 13.41 |               |
| C5      | 5.518 | 5.195 | 7.497 | -     | 8.429, 7.019  |
| U6      | 5.649 | 5.741 | 7.807 | 11.68 |               |
| A7      | 5.871 | 7.124 | 8.267 | -     |               |
| G8      | 5.729 | -     | 7.351 | -     |               |

H1’, H6 and H8 resonances were assigned in 400 ms spectra at 5°C. Other resonances were assigned in 100 ms spectra at 5°C.

Table S5: Chemical shift assignments for r(CAGUCGAUUG)$_2$.

| Residue | H1’   | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|-------|-------|-------|-------|---------------|
| C1      | 5.490 | 6.004 | 8.133 | -     | 8.370, 7.212  |
| A2      | 6.079 | 7.186 | 8.270 | -     |               |
| G3      | 5.638 | -     | 7.040 | 11.74 |               |
| U4      | 5.460 | 5.115 | 7.655 | 14.42 |               |
| C5      | 5.578 | 5.584 | 7.877 | -     | 8.251, 6.837  |
| G6      | 5.626 | -     | 7.518 | 11.98 |               |
| A7      | 5.905 | 7.749 | 7.731 | -     |               |
| U8      | 5.266 | 5.375 | 7.553 | 11.74 |               |
| U9      | 5.574 | 5.525 | 7.943 | 14.00 |               |
| G10     | 5.869 | -     | 7.706 | 12.66 |               |

H1’, H6 and H8 resonances were assigned in 400 ms spectra at 5°C. Other resonances were assigned in 100 ms spectra at 5°C.
Table S6: Chemical shift assignments for r(CCGAAUUUGG)$_2$.

| Residue | H1' | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|-----|-------|-------|-------|---------------|
| C1      | 5.518 | 5.950 | 8.109 | -     | 8.346, 7.162  |
| C2      | 5.686 | 5.572 | 7.944 | -     | 8.545, 6.892  |
| G3      | 5.704 | -     | 7.516 | 9.990 |               |
| A4      | 5.842 | 7.211 | 7.726 | -     |               |
| A5      | 5.895 | 7.731 | 7.713 | -     |               |
| U6      | 5.479 | 5.003 | 7.557 | 14.04 |               |
| U7      | 5.596 | 5.466 | 7.809 | 13.76 |               |
| U8      | 5.495 | 5.743 | 7.871 | 11.53 |               |
| G9      | 5.656 | -     | 7.897 | 12.61 |               |
| G10     | 5.800 | -     | 7.323 | 13.34 |               |

H1', H6 and H8 resonances were assigned in 400 ms spectra at 20°C. Other resonances were assigned in 100 ms spectra at 5°C.

Table S7: Chemical shift assignments for r(CGGAAUUUCG)$_2$.

| Residue | H1' | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|-----|-------|-------|-------|---------------|
| C1      | 5.615 | 5.967 | 8.060 | -     | 8.169, 7.131  |
| G2      | 5.856 | -     | 7.829 | 12.53 |               |
| G3      | 5.746 | -     | 7.217 | 10.46 |               |
| A4      | 5.889 | 7.252 | 7.714 | -     |               |
| A5      | 5.867 | 7.727 | 7.692 | -     |               |
| U6      | 5.483 | 4.993 | 7.553 | 14.03 |               |
| U7      | 5.613 | 5.500 | 7.836 | 13.71 |               |
| U8      | 5.460 | 5.764 | 7.997 | 11.95 |               |
| C9      | 5.488 | 5.626 | 7.833 | -     | 8.380, 6.833  |
| G10     | 5.762 | -     | 7.585 | -     |               |

H1', H6 and H8 resonances were assigned in 400 ms spectra at 20°C. Other resonances were assigned in 100 ms spectra at 5°C.

Table S8: Chemical shift assignments for r(CGGAUAUUCG)$_2$.

| Residue | H1' | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|-----|-------|-------|-------|---------------|
| C1      | 5.577 | 5.949 | 8.060 | -     | 8.169, 7.070  |
| G2      | 5.859 | -     | 7.850 | 12.56 |               |
| G3      | 5.750 | -     | 7.228 | 10.51 |               |
| A4      | 5.938 | 7.797 | 7.834 | -     |               |
| U5      | 5.470 | 5.088 | 7.654 | 13.28 |               |
| A6      | 6.005 | 7.074 | 8.123 | -     |               |
| U7      | 5.401 | 5.008 | 7.524 | 13.97 |               |
| U8      | 5.513 | 5.700 | 7.966 | 11.95 |               |
| C9      | 5.500 | 5.625 | 7.818 | -     | 8.366, 6.795  |
| G10     | 5.763 | -     | 7.588 | -     |               |

H1', H6 and H8 resonances were assigned in 400 ms spectra at 20°C. Other resonances were assigned in 100 ms spectra at 5°C.
Table S9: Chemical shift assignments for r(CGUGAUUACG)$_2$.

| Residue | H1'  | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|------|-------|-------|-------|---------------|
| C1      | 5.169| 5.851 | 7.877 | -     | 8.219, 6.983  |
| G2      | 5.749| -     | 7.724 | 13.03 |
| U3      | 5.579| 5.157 | 7.713 | 13.74 |
| G4      | 5.737| -     | 7.609 | 9.884 |
| A5      | 5.801| 7.722 | 7.760 | -     |
| U6      | 5.387| 4.965 | 7.439 | 14.01 |
| U7      | 5.423| 5.735 | 7.912 | 11.56 |
| A8      | 5.802| 7.158 | 8.383 | -     |
| C9      | 5.323| 5.195 | 7.468 | -     | 8.197, 6.839  |
| G10     | 5.748| -     | 7.485 | -     |

All resonances were assigned in 100 ms spectra at 0°C.

Table S10: Chemical shift assignments for r(CUGGAUUCAG)$_2$.

| Residue | H1'  | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|------|-------|-------|-------|---------------|
| C1      | 5.550| 6.011 | 8.137 | -     | 8.201, 7.272  |
| U2      | 5.648| 5.487 | 8.090 | 13.93 |
| G3      | 5.881| -     | 7.773 | 11.87 |
| G4      | 5.659| -     | 7.139 | 10.48 |
| A5      | 5.918| 7.844 | 7.753 | -     |
| U6      | 5.459| 5.008 | 7.482 | 14.09 |
| U7      | 5.514| 5.750 | 7.954 | 11.92 |
| C8      | 5.680| 5.680 | 7.896 | -     | 8.358, 6.891  |
| A9      | 5.806| 7.154 | 7.959 | -     |
| G10     | 5.704| -     | 7.289 | 13.59 |

H1’, H6 and H8 resonances were assigned in 400 ms spectra at 20°C. Other resonances were assigned in 100 ms spectra at 5°C.

Table S11: Chemical shift assignments for r(GAGAGCUUUC)$_2$.

| Residue | H1'  | H2/H5 | H6/H8 | H1/H3 | H41, H42 amino |
|---------|------|-------|-------|-------|---------------|
| G1      | 5.670| -     | 8.015 | -     |
| A2      | 6.129| 7.408 | 8.091 | -     |
| G3      | 5.665| -     | 6.934 | 10.62 |
| A4      | 5.887| 7.509 | 7.628 | -     |
| G5      | 5.665| -     | 7.205 | 13.43 |
| C6      | 5.527| 5.147 | 7.607 | -     | 8.561, 6.906  |
| U7      | 5.561| 5.423 | 7.789 | 14.04 |
| U8      | 5.470| 5.789 | 8.003 | 11.76 |
| U9      | 5.529| 5.629 | 8.106 | 14.49 |
| C10     | 5.806| 5.681 | 7.724 | -     | 8.221, 7.026  |

H1’, H6 and H8 resonances were assigned in 400 ms spectra at 20°C. Other resonances were assigned in 100 ms spectra at 5°C.
Table S12: Chemical shift assignments for r(GAGGAUCUUC)$_2$.

| Residue | H1'  | H2/H5 | H6/H8 | H1/H3 | amino |
|---------|------|-------|-------|-------|-------|
| G1      | 5.695| -     | 8.028 | 12.32 |
| A2      | 6.147| 7.525 | 8.098 | -     |
| G3      | 5.628| -     | 6.914 | 10.92 |
| G4      | 5.709| -     | 7.191 | 12.56 |
| A5      | 5.982| 7.799 | 7.743 | -     |
| U6      | 5.531| 5.038 | 7.630 | 14.10 |
| C7      | 5.570| 5.570 | 7.705 | -     | 8.360, 6.955 |
| U8      | 5.606| 5.674 | 7.867 | 11.75 |
| U9      | 5.555| 5.631 | 8.085 | 14.40 |
| C10     | 5.838| 5.702 | 7.728 | -     | 8.241, 7.070 |

H1’, H6 and H8 resonances were assigned in 400 ms spectra at 25°C. Other resonances were assigned in 100 ms spectra at 5°C.

Table S13: Chemical shift assignments for r(GUGAAUUUAC)$_2$.

| Residue | H1'  | H2/H5 | H6/H8 | H1/H3 | amino |
|---------|------|-------|-------|-------|-------|
| G1      | 5.708| -     | 8.048 | -     |
| U2      | 5.776| 5.163 | 7.949 | 14.11 |
| G3      | 5.789| -     | 7.725 | 9.885 |
| A4      | 5.769| 7.156 | 7.713 | -     |
| A5      | 5.880| 7.716 | 7.742 | -     |
| U6      | 5.480| 4.965 | 7.580 | 14.02 |
| U7      | 5.595| 5.480 | 7.834 | 13.70 |
| U8      | 5.386| 5.780 | 7.966 | 11.56 |
| A9      | 5.857| 7.342 | 8.369 | -     |
| C10     | 5.645| 5.239 | 7.369 | -     | 8.175, 7.030 |

H1’, H6 and H8 resonances were assigned in 400 ms spectra at 12°C. Other resonances were assigned in 100 ms spectra at 5°C.
| Residue | H1/H3  | H2  | N1/N3 |
|---------|--------|-----|-------|
| G2      | 12.82  |     |       |
| G3      | 13.15  | 149.1|
| U4      | 13.52  | 162.6|
| G5      | 11.64  | 146.9|
| A6      |        | 6.99 |       |
| A7      |        | 7.08 |       |
| A8      |        | 7.72 |       |
| G11     | 11.71  | 147.2|
| A12     |        | 7.35 |       |
| G13     | 12.68  | 148.3|
| G14     | 12.27  | 147.9|
| G19/G30 | 13.10/12.65 | 149.0/148.0 |
| G36     | 12.83  | 148.3|
| U38     | 11.52  | 158.7|
| G44     | 11.57  | 146.5|
| A45     |        | 7.68 |       |
| U46     | 11.26  | 158.9|
| G49/G51 | 13.16/12.61 | 149.1/148.7 |
| G57     | 12.90  | 148.4|
| G61     | 11.15  | 145.0|
| U62     | 14.20  | 163.5|
| G67     | 10.32  | 143.5|
| G68     | 13.18  | 149.1|
| U79     | 11.68b | 158.8|
| U80     | 14.05b |       |
| A103    |        | 7.18b|
| G104    | 10.55b | 143.5|
| U112    | 13.82  | 163.0|
| G116    | 12.93  | 148.6|
| U117    | 14.09  | 163.0|
| U118    | 13.79  | 163.3|
| U119    | 13.63  | 163.4|
| A121    |        | 7.34 |       |

1H chemical shifts were assigned at 25 °C unless otherwise noted. 15N chemical shifts were assigned at 20 °C. "Ambiguous. Assigned at 15 °C. Residue numbering in the structure reported in this work is shifted by three residues relative to the consensus sequence."
Table S15: Assigned $^1$H and $^{15}$N chemical shifts for the 75-nt *B. mori* R2 retrotransposon pseudoknot.

| Residue | $^{1}$H/H3 | H2  | $^{15}$N/N3 |
|---------|------------|-----|------------|
| G1      | 12.04      | 146.2 |           |
| G2      | 12.88      | 147.9 |           |
| G9      | 12.31      | 148.4 |           |
| G10     | 11.96      | 147.0 |           |
| A11     | 7.62       |      |           |
| G13     | 12.34      | 146.6 |           |
| G14     | 12.63      | 148.0 |           |
| G22     | 12.46      | 147.4 |           |
| G23     | 12.66      | 147.9 |           |
| G27     | 12.83      | 147.4 |           |
| U28     | 14.64      | 163.4 |           |
| A30     | 7.54       |      |           |
| G32     | 12.92      | 148.9 |           |
| U35     | 11.93      | 158.0 |           |
| G37     | 12.57      | 148.0 |           |
| A39     | 7.01       |      |           |
| G40     | 12.82      | 147.4 |           |
| G41     | 13.16      | 147.6/148.4$^a$ |       |
| U42     | 13.23      | 160.8 |           |
| A43     | 6.94       |      |           |
| G49     | 10.15      | 143.8 |           |
| G50     | 13.05      | 147.6 |           |
| G51     | 13.12      | 148.8 |           |
| U52     | 14.14      | 163.1 |           |
| G53     | 12.97      | 147.4 |           |
| G54     | 13.51      | 148.8 |           |
| G55     | 13.30      | 149.1 |           |
| A66     | 7.54       |      |           |
| U69     | 13.32      | 162.0 |           |
| G70     | 12.45      | 146.9 |           |
| G72     | 10.42      | 143.3 |           |
| G73     | 13.14      | 148.4/147.6$^a$ |       |
| G74     | 13.31      | 148.5 |           |

$^1$H and $^{15}$N chemical shifts were assigned at 25 °C. $^a$ Ambiguous.
Notes for Tables S16 to S34: Colors correspond to those in the secondary structure of Error! Reference source not found. and the imino proton walks shown in Error! Reference source not found.. Chemical shifts are submitted to NAPSS-CS as shown on the left and base pairs predicted by NAPSS-CS are shown on the right. Integers 5, 6, and 7 represent AU, GC, and GU pairs, respectively. Numbers in parentheses are chemical shifts for imino protons, respectively. For GU pairs, numbers in parentheses are chemical shifts of GH1, UH3, and UH5, respectively. For AU pairs, numbers in parentheses are chemical shifts of AH2, UH3, and UH5, respectively. For GC pairs, the first number in parentheses is the chemical shift of GH1. For GU and AU pairs, zero means an unavailable chemical shift. For GC pairs, the second two zeros are placeholders for absent chemical shift constraints.

Table S16: NMR constraints used to predict the structure of B. mori R2 retrotransposon pseudoknot (74-nt).

| Constraints | Sequence of base pairs predicted by NAPSS-CS |
|-------------|---------------------------------------------|
| 66(12.93 0 0)6(13.29 0 0)6(13.50 0 0)6 | G1:C57, G2:C56, C3:G55, C4:G54, C5:G53 |
| 65(7.547 14.39 0)6(12.75 0 0)6(12.34 0 0)6 | G10:C29, A11:U28, C12:G27, G13:C26, G14:C25 |
| 66 | G22:C17, G23:C16 |
| 66(12.43 0 0)5(6.927 13.27 0)6(12.80 0 0)6(13.07 0 0)5(7.558 13.33 0)5(6.874 14.25 0)6 | G37:C71, C38:G70, A39:U69, G40:C68, G41:C67, U42:A66, A43:U52, C44:G51 |

Chemical shifts (Table S15) are from this work.

Table S17: NMR constraints used to predict the structure of B. mori R2 retrotransposon pseudoknot (75-nt).

| Constraints | Sequence of base pairs predicted by NAPSS-CS |
|-------------|---------------------------------------------|
| 66(12.88 0 0)6(13.30 0 0)6(13.51 0 0)6 | G1:C57, G2:C56, C3:G55, C4:G54, C5:G53 |
| 65(7.618 14.64 0)6 | G10:C29, A11:U28, C12:G27 |
| 66 | G13:C26, G14:C25 |
| 66 | G22:C17, G23:C16 |
| 66(13.31 0 0)6(13.14 0 0)7 | G32:C75, C33:G74, C34:G73, U35:G72 |
| 66(12.45 0 0)5(7.012 13.32 0)6(12.82 0 0)6(13.16 0 0)5(7.540 13.23 0)5(6.937 14.14 0)6 | G37:C71, C38:G70, A39:U69, G40:C68, G41:C67, U42:A66, A43:U52, C44:G51 |

Table S18: NMR constraints used to predict the structure of E. coli tmRNA pseudoknot.

| Constraints | Sequence of base pairs predicted by NAPSS-CS |
|-------------|---------------------------------------------|
| 65(13.4 0 0)6 | G2:C18, A3:U17, G4:C16, G5:C15 |
| 66(13.1 0 0)6(12.2 0 0)6(13.6 0 0)7 | G7:C30, C8:G29, G9:C28, G10:C27, U11:G26 |

Table S19: NMR constraints used to predict the structure of human hepatitis delta virus ribozyme pseudoknot.

| Constraints | Sequence of base pairs predicted by NAPSS-CS |
|-------------|---------------------------------------------|
| 76(13.40 0 0)6(13.21 0 0)56 | G2:U37, G3:C36, G4:C35, U5:A34, C6:G33 |
| 67(11.60 11.94 0)56(12.40 0 0)6 | G12:C63, G13:U62, U14:A61, C15:G60, C16:G59 |
| 66(12.67 0 0)6 | G18:C30, C19:G29, C20:G28 |
| 556 | A42:U51, U43:A50, C44:G49 |
| Table S20: NMR constraints used to predict the structure of mouse mammary tumor virus modified frameshifting pseudoknot. |
| Constraints | Sequence of base pairs predicted by NAPSS-CS |
| 66(13.13 0 0)6 | G1:C19, G2:C18, C3:G17 |
| 66 | G4:C16, C5:G15 |
| 66(12.60 0 0)6 | G9:C32, G10:C31, G11:C30 |

| Table S21: NMR constraints used to predict the structure of pea enation mosaic virus pseudoknot. |
| Constraints | Sequence of base pairs predicted by NAPSS-CS |
| 66(12.97 0 0)6(12.81 0 0)6 | C6:G19, C7:G18, G8:C17, G9:C16 |
| 65(7.69 14.25 4.81)6 | G12:C21, A13:U30, C14:G29 |

| Table S22: NMR constraints used to predict the structure of S. pneumoniae preQ1-II riboswitch. |
| Constraints | Sequence of base pairs predicted by NAPSS-CS |
| 66(13.485 0 0)5(7.369 13.937 5.308)5(6.683 13.099 5.55)6(11.922 0 0)6(13.172 0 0)5(7.087 14.117 5.032)6 | G1:C28, C2:G27, U3:A26, U4:A25, G5:C24, G6:C23, U7:A22, G8:C21 |
| 55(7.41 14.362 5.377)6(12.759 0 0)7(10.463 11.972)5(7.55 13.865 5.359)6 | G38:C49, C39:G48, G40:C47 |
| A52:U19, A53:U18, G54:C17, G55:U16, A56:U15, G57:C14 |

| Table S23: NMR constraints used to predict the structure of simian retrovirus k1 mutant frameshifting pseudoknot. |
| Constraints | Sequence of base pairs predicted by NAPSS-CS |
| 66(12.5 0 0)6(12.6 0 0)6(13.2 0 0)6(13.3 0 0)6 | G3:C21, G4:C20, G5:C19, G6:C18, C7:G17, C8:G16 |
| 66(13.0 0 0)6(12.25 0 0)6(12.6 0 0)6 | G10:C39, C11:G38, G12:C37, G13:C36, G14:C35 |

| Table S24: NMR constraints used to predict the structure of simian retrovirus k1 wild type frameshifting pseudoknot. |
| Constraints | Sequence of base pairs predicted by NAPSS-CS |
| 66(12.5 0 0)6(12.6 0 0)6(13.2 0 0)6 | G3:C21, G4:C20, G5:C19, G6:C18, C7:G17 |
| 66(13.25 0 0)6(12.6 0 0)6(12.6 0 0)6 | G10:C39, C11:G38, G12:C37, C13:G36, C14:G35 |

| Table S25: NMR constraints used to predict the structure of B. subtilis pbuE adenine riboswitch aptamer mutant. |
| Constraints | Sequence of base pairs predicted by NAPSS-CS |
| 66(12.95 0 0)6(11.94 0 0)5(7.35 13.96 0)6(13.31 0 0)5(7.11 13.57 0)5 | G1:C67, C2:G66, G3:C65, A4:U64, G5:C63, U6:A62, A7:U61 |
| 66(12.64 0 0)5(7.29 13.95 0)6(11.47 0 0)5(7.57 12.91 0)5 | C11:G31, C12:G30, U13:A29, C14:G28, A15:U27, A16:U26 |
| 65(7.07 13.90 0)6(12.92 0 0)6(12.40 0 0)5 | C40:G58, A41:U57, G42:C56, G43:C55, A44:U54 |
| Table S26: NMR constraints used to predict the structure of *B. subtilis* tRNA<sup>Trp</sup>.<sup>1</sup> | Constraints | Sequence of base pairs predicted by NAPSS-CS |
|---|---|---|
| 66 | G4:C67, G5:C66 |
| 6557 | G10:C24, U11:A23, U12:A22, U13:G21 |
| 656(12.86 0 0)6 | G26:C42, A27:U41, G28:C40, G29:C39 |
| 657(10.00 11.33 0)6(12.68 0 0)6 | G47:C63, U48:A62, G49:U61, G50:C60, G51:C59 |

| Table S27: NMR constraints used to predict the structure of bovine tRNA<sup>Trp</sup>.<sup>2</sup> | Constraints | Sequence of base pairs predicted by NAPSS-CS |
|---|---|---|
| 656(13.16 0 0)6(12.72 0 0)7(10.61 11.83 0)6(12.76 0 0)6 | G1:C71, A2:U70, C3:G69, C4:G68, U5:G67, C6:G66, G7:G65 |
| 66(13.22 0 0)6(12.96 0 0)6 | G10:C24, C11:G23, G12:C22, C13:G21 |
| 656 | C27:G41, U28:A40, G29:C39 |
| 76(12.91 0 0)6(12.65 0 0)56 | G48:U64, C49:G63, G50:C62, U51:A61, G52:C60 |

| Table S28: NMR constraints used to predict the structure of influenza A segment 7 multibranch loop.<sup>3</sup> | Constraints | Sequence of base pairs predicted by NAPSS-CS |
|---|---|---|
| 67 | G2:C59, G3:U58 |
| 67(10.92 12.24 0)6 | C6:G55, U7:G54, C8:G53 |
| 66(12.15 0 0)5 | G11:C36, G12:C35, A13:U34 |
| 66(12.02 0 0)6(13.08 0 0)5 | G16:C31, G17:C30, U18:C29, C19:G28, U20:A27 |

| Table S29: NMR constraints used to predict the structure of Medaka telomerase RNA CR4/5 domain multibranch loop.<sup>4</sup> | Constraints | Sequence of base pairs predicted by NAPSS-CS |
|---|---|---|
| 65(7.119 13.69 5.614)5(7.148 13.81 5.643)5(7.795 14.29 5.179)6 | G2:C52, A3:U51, A4:U50, A5:U49, C6:G48 |
| 66(12.77 0 0)7(10.64 11.95 5.758)6 | G10:C29, C11:G28, G12:U27, G13:C26 |
| 65 | A16:U24, G17:C23 |
| 65(7.629 14.22 5.486)6 | G33:C43, A34:U42, G35:C41 |

| Table S30: NMR constraints used to predict the structure of moloney murine leukemia virus core encapsidation signal multibranch loop.<sup>5</sup> | Constraints | Sequence of base pairs predicted by NAPSS-CS |
|---|---|---|
| 76 | G2:U29, C3:G28 |
| 76 | G4:U27, G5:C26 |
| 56(13.382 0 0)5(7.874 14.336 5.072)5 | A10:U21, G11:C20, U12:A19, U13:A18 |
| 66(12.718 0 0)6(13.162 0 0)5(7.759 13.883 5.213)6 | G43:C71, G45:C70, G46:C69, U47:A68, G48:C67 |
| 65(7.234 13.814 5.647)5(7.871 14.366 5.153)6(13.419 0 0)5 | G49:C62, A50:U61, A51:U60, C52:G59, U53:A58 |
| 65(7.028 13.4 5.779)6(11.913 0 0)6(12.558 0 0)6 | C82:G97, U83:A96, G84:C95, G85:C94, G86:C93 |
| Table S31: NMR constraints used to predict the structure of *S. cerevisiae* group II intron Sc.ai5γ domain 1 κ-ζ multibranch loop. |
|-----------------------------------------------|
| **Constraints**                             | **Sequence of base pairs predicted by NAPSS-CS** |
| 65(7.16 13.77 0)5                            | G2:C48, A3:U47, A4:U46 |
| 66(13.474 0 0)5(7.571 14.37 0)6(12.526 0 0)5(7.562 14.108 0)6(11.596 0 0)5 | G8:C41, C9:G40, U10:A39, C11:G38, U24:A37, C25:G36, A26:U35 |
| 56                                            | A13:U20, C14:G19 |

| Table S32: NMR constraints used to predict the structure of tobacco ringspot virus adenine-dependent hairpin ribozyme. |
|-----------------------------------------------|
| **Constraints**                             | **Sequence of base pairs predicted by NAPSS-CS** |
| 66(12.3 0 0)5556(12.3 0 0)56                  | G2:C79, C3:G78, A4:U77, A5:U76, A6:U75, C7:G74, A8:U73, G9:C72 |
| 656                                           | G14:C67, U15:A66, C16:G65 |
| 66(11.8 0 0)5                                | C19:G56, C20:G55, A21:U54 |
| 656                                           | C30:G43, A31:U42, C32:G41 |
| 66                                            | G33:C40, C34:G39 |

| Table S33: NMR constraints used to predict the structure of *K. lactis* telomerase RNA pseudoknot. |
|-----------------------------------------------|
| **Constraints**                             | **Sequence of base pairs predicted by NAPSS-CS** |
| 65(7.976 14.53 5.09)5(7.153 13.78 5.548)5    | G2:C27, U3:A26, U4:A25, U5:A24 |
| 75                                            | G13:U46, U14:A45 |
| 65                                            | G15:C44, A16:U43 |
| 55(7.043 13.59 5.559)5(7.183 13.23 5.53)5(7.064 13.51 5.459)5(7.141 13.42 5.365)6(12.15 0 0)6 | U17:A42, U18:A41, U19:A40, U20:A39, U21:A38, C22:G36, C23:G34 |

| Table S34: NMR constraints used to predict the structure of murine leukemia virus recording signal pseudoknot. |
|-----------------------------------------------|
| **Constraints**                             | **Sequence of base pairs predicted by NAPSS-CS** |
| 66(12.861 0 0)6(12.792 0 0)5(7.8316 13.744 4.975)6(11.948 0 0)5(7.077 13.688 5.466)6(13.066 0 0)6(12.488 0 0)6(11.771 0 0)6(12.392 0 0)6(13.054 0 0)6(12.288 0 0)6(12.446 0 0)6 | G9:C33, G10:C32, G11:C31, U12:A30, C13:G28, A14:U27, G15:C26, G16:C25, G52:C24, G53:C23, G54:C22, G55:C21, G56:C20, G57:C19 |
Plasmid insert design for *in vitro* transcription of the 75-nt *B. mori* R2 retrotransposon pseudoknot by T7 RNA polymerase.

Cloning vector: pUC19

Intended sequence of the 75-nt pseudoknot:
5′GGCCCGAUUGGACGGACCGGACCGGACCGGUCAAGCCUAGGUACCUCUUCCGUGG GCCUUGC GAUACCUGCGGCC3′

Sequence of the insert:
5′GAATTCTAATACGACTCACTATAGGCCCGATGGACGGACCCGAGGACCGGACCGGAGGACGCGTCAAGCTAGCA GGTACCTTCGCGGTGGCCCTTCGGATACCTGCGGCCGCGCTAGCAAGCTT3′

Reverse complement of the insert:
5′AAGCTTGCTAGCGCCCGCAGGTATCGCAAGGCCAACCGAAGGTACCTGCTAGGCTTGACG GTCCTCGGCGTCGCTCCATCGGGCCTATAAGTAGTGACGTGTAGTAAGCTC3′

Notation:
EcoRI recognition sequence: 5′GAATTC3′
HindIII recognition sequence: 5′AAGCTT3′
NheI recognition sequence: 5′GCTAGC3′
RNA pseudoknot sequence
T7 RNA polymerase promoter
Accession codes and primary references from which direction-dependent chemical shift constraints were derived.

| BMRB ID | Structure                                      | Ref. |
|---------|------------------------------------------------|------|
| 4125    | *E. coli* RNase P 31-mer domain                | 19   |
| 4135    | r(5’CGACUCAGG/3’CCUGCGUCG)                     | 20   |
| 4175    | HIV-1 SL3 hairpin                              | 21   |
| 4226    | Leadzyme                                       | 22   |
| 4247    | r(GCAGUGGC)-r(GCCA)d(CTGC) duplex             | 23   |
| 4250    | TYMV pseudoknot 3’ hairpin                    | 24   |
| 4253    | Bacteriophage T2 gene 32 mRNA pseudoknot      | 25   |
| 4345    | *S. cerevisiae* L30 and its regulatory pre-mRNA complex | 26   |
| 4346    | *S. cerevisiae* L30 regulatory pre-mRNA        | 27   |
| 4745    | RNA duplex with bulged adenosine              | 28   |
| 4750    | Conserved internal loop in *E. coli* SRP       | 29   |
| 4780    | HIV-1 SL2 of Ψ packaging signal               | 30   |
| 4816    | Influenza A virus promoter                     | 31   |
| 4867    | Nucleolin recognition element                 | 32   |
| 5007    | *Neurospora* VS ribozyme stem-loop substrate | 33   |
| 5046    | HCV IRES stem-loop IIIc                        | 34   |
| 5170    | RNA binding site for histone stem-loop binding protein | 35   |
| 5256    | *E. coli* tRNA\textsuperscript{Phe} unmodified anticodon stem-loop | 36   |
| 5278    | PEMV-1 P1-P2 frameshifting pseudoknot          | 37   |
| 5321    | Human SRP RNA SRP19 binding site               | 38   |
| 5371    | *S. cerevisiae* U6-A62G 3SL RNA               | 39   |
| 5394    | r(5’GGUGψAGUA/3’UACUAACACC)                   | 40   |
| 5395    | r(5’GGUGUAGUA/3’UACUAACACC)                   | 41   |
| 5528    | Influenza A cRNA promoter                      | 42   |
| 5530    | Yeast ASL\textsuperscript{Phe}-C\textsubscript{32,Gm\textsubscript{14,mC}}\textsubscript{40} | 43   |
| 5553    | Influenza A promoter, U4C mutant               | 44   |
| 5586    | r(GGCPAGCCU)\textsubscript{2}                | 45   |
| 5587    | r(GGCAPGCCU)\textsubscript{2}                | 46   |
| 5588    | r(GGCPPGCCU)\textsubscript{2}                | 47   |
| 5614    | r(GGCAAGCCU)\textsubscript{2}                | 48   |
| 5632    | Human telomerase RNA P2b hairpin               | 49   |
| 5655    | *S. cerevisiae* U6 ISL stem-loop, U80G        | 50   |
| 5703    | *S. cerevisiae* U6 ISL stem-loop, S\textsubscript{r}-ISL | 51   |
| 5705    | 14-mer hairpin with cUUCGg tetraloop          | 52   |
| 5834    | HIV-1 frameshifting inducing stem-loop RNA     | 53   |
| 5852    | *Neurospora* VS ribozyme SL1’ hairpin         | 54   |
| 5919    | *S. oleracia* 5S rRNA loop E region           | 55   |
| 5932    | Human telomerase RNA DCloop mutant P2b hairpin | 56   |
| 5962    | *S. cerevisiae* group II intron Sc.ai5γ domain 5 | 57   |
Accession codes and primary references from which direction-dependent chemical shift constraints were derived (continued).

| BMRB ID | Structure                                                      | Ref. |
|---------|----------------------------------------------------------------|------|
| 5980    | GBV-B IRES stem-loop IIc                                       | 55   |
| 6042    | Coxsackievirus stem-loop D                                     | 55   |
| 6062    | RSV residues 907-929                                           | 54   |
| 6076    | Enterovirus IRES stem-loop IV domain, WT34                    | 55   |
| 6077    | Enterovirus IRES stem-loop IV domain, 10U                      | 55   |
| 6094    | MLV core encapsidation signal                                  | 2    |
| 6115    | HRV-14 internal cis-acting replication element                 | 56   |
| 6239    | VS ribozyme stem-loop VI                                       | 57   |
| 6300    | S. cerevisiae extended U6 ISL                                  | 58   |
| 6477    | Human telomerase RNA P2h-P3 pseudoknot                         | 59   |
| 6485    | Human GluR-B R/G central loop                                  | 60   |
| 6509    | SLYLV pseudoknot                                               | 61   |
| 6543    | HIV-1 frameshift inducing element                              | 62   |
| 6562    | BEV1 cloverleaf 1 apical D-loop                                | 63   |
| 6563    | HIV-1 frameshifting signal                                     | 64   |
| 6565    | GAAA tetraloop-receptor complex                                 | 65   |
| 6756    | Domain 6 of a group II intron                                  | 66   |
| 6814    | Class I GTP aptamer                                            | 67   |
| 6979    | r(5'GGUGAAGGCUC/3'PCCGAAGCCG)                                  | 68   |
| 7090    | Human PGY/MDR1 hairpin                                         | 69   |
| 7098    | HIV-1 SL1 dimer                                                | 70   |
| 7230    | r(5'GGCUAAGAC/3'CCGAAGCUG)                                     | 71   |
| 7403    | Human telomerase RNA CR7 3′ terminal hairpin                   | 72   |
| 7404    | Human telomerase RNA U64 H/ACA snoRNA 3′ terminal hairpin      | 72   |
| 7405    | Human telomerase RNA U85 C/D-H/ACA scaRNA 5′ terminal hairpin  | 72   |
| 10014   | P. furiosus SRP RNA helix 6 tetraloop                          | 73   |
| 10018   | Eel UnaL2 LINE36 hairpin                                       | 74   |
| 11014   | HIV-1 TAR and aptamer complex                                  | 75   |
| 15080   | S. cerevisiae U2 snRNA stem I                                  | 76   |
| 15319   | E. coli tRNA^{Val}_{UAC} unmodified anticodon stem-loop        | 77   |
| 15331   | E. coli tRNA^{Val}_{UAC} anticodon stem-loop, cmo5U34 and M6A37| 77   |
| 15342   | E. coli tRNA^{Val}_{UAC} anticodon stem-loop, cmo5U34          | 77   |
| 15362   | E. coli tRNA^{Val}_{UAC} anticodon stem-loop M6A37             | 77   |
| 15417   | SIV frameshift-inducing stem-loop                              | 78   |
| 15538   | Anti-NF-κB aptamer                                             | 79   |
| 15571   | r(5'GCAGAGAGCG/3'CGUCUCUCGC)                                   | 80   |
| 15572   | r(5'GCAGAGAGCG/3'CGUCUCUCGC)                                   | 80   |
Accession codes and primary references from which direction-dependent chemical shift constraints were derived (continued).

| BMRB ID | Structure | Ref. |
|---------|-----------|-----|
| 15656   | Duck HBV ε apical stem-loop | 81  |
| 15697   | GVB B IRES | 82  |
| 15745   | HBV post-transcriptional regulatory element stem-loop α | 83  |
| 15780   | r(5’GUCGAGCUG/3’CAGCCGAC) | 84  |
| 15781   | r(5’GUCGUGCU3’CAGCCGAC) | 84  |
| 15786   | Duck HBV ε primer loop | 85  |
| 15858   | S. cerevisiae group II intron Sc.ai5γ d3’ hairpin, including EBS1/IBS1 | 86  |
| 15859   | S. cerevisiae group II intron Sc.ai5γ d3’ hairpin closed by GAAA tetraloop | 86  |
| 15869   | HIV-2 TAR | 87  |
| 15915   | Human tRNA\textsuperscript{Lys} anticodon fragment bound to HIV-1 genome loop I | 88  |
| 16431   | HIV-2 TAR | 89  |
| 16479   | B. subtilis xpt-pbuX-mRNA guanine sensing riboswitch | 90  |
| 16714   | Xist RNA A-repeat AUCG tetraloop | 91  |
| 16950   | r(GACAAGUGUCA)\textsubscript{2} | 92  |
| 16951   | r(GACGAGCGUCA)\textsubscript{2} | 92  |
| 16952   | r(GACUAGAGUCA)\textsubscript{2} | 92  |
| 16953   | r(GGUAGGCCA)\textsubscript{2} | 92  |
| 17188   | Human telomerase RNA P2ab | 95  |
| 17292   | Neurospora VS ribozyme A730 loop | 94  |
| 17309   | Coronavirus SL2 | 95  |
| 17316   | B. subtilis tyrS T-box leader specifier domain | 96  |
| 17326   | P. fluourescens hcnA Shine-Dalgarno sequence | 97  |
| 17406   | r(5’GUGAAGGCCGU/3’CGGAGGACACU) | 98  |
| 17449   | Human tRNA\textsuperscript{Lys} UUU ASL | 99  |
| 17566   | TASL1 22-nt artificial stem-loop | 97  |
| 17567   | TASL2 26-nt artificial stem-loop | 97  |
| 17568   | TASL3 30-nt artificial stem-loop | 97  |
| 17601   | MLV read-through pseudoknot signal | 10  |
| 17671   | HIV-1 exon splicing silencer 3 | 100 |
| 17682   | E. coli 16S rRNA helix 27 | 101 |
| 17860   | Chimpanzee HAR1 helix h1 (c37) | 102 |
| 17901   | U6 snRNA 5’ stem-loop 30-nt construct | d |
| 17921   | GAAA tetraloop receptor variant | b |
| 17941   | CVB-3 IRES subdomain IV-B | c |

\textsuperscript{a} Butcher, S. E. and Clos, L. Unpublished.
\textsuperscript{b} Vander Muelen, K., Davis, J., Clos, L., and Butcher, S. E. Unpublished.
\textsuperscript{c} Ihle, Y., Zell, R., and Goerlach, M. Unpublished.
Accession codes and primary references from which direction-dependent chemical shift constraints were derived (continued).

| BMRB ID | Structure                                      | Ref. |
|---------|------------------------------------------------|------|
| 17972   | *S. cerevisiae* U2/U6 complex helix I           | 103  |
| 18239   | BMV subgenomic stem-loop, WT                   | 104  |
| 18240   | BMV subgenomic stem-loop, del-A                | 104  |
| 18336   | *B. subtilis* phage φ29 pRNA hairpin           | 105  |
| 18503   | *S. cerevisiae* group II intron Sc.ai5γ K-ζ region | 106  |
| 18515   | Human HAR1 helix h1 (h37)                      | 102  |
| 18838   | *S. cerevisiae* group II intron Sc.ai5γ domain I ID3 stem-loop | 107  |
| 18881   | *S. cerevisiae* group II intron Sc.ai5γ d3′ hairpin, including EBS1:dIBS1 complex | 108  |
| 18891   | *T. thermophila* telomerase RNA stem-loop IV   | 109  |
| 18892   | *T. thermophila* telomerase RNA helix II template boundary element | 110  |
| 18974   | *E. coli* 23S rRNA H69, modified               | 111  |
| 18975   | *E. coli* 23S rRNA H69, unmodified            | 111  |
| 19081   | CPEB3 ribozyme P4 domain                      | 112  |
| 19260   | *K. lactis* telomerase RNA pseudoknot          | 113  |
| 19634   | Medaka telomerase RNA CR4/5 domain             | 114  |
| 19692   | *Neurospora* VS ribozyme SLVI                 | 115  |
| 19887   | miR-21 stem-loop                               | 116  |
| 25163   | *Neurospora* VS ribozyme III-IV-V junction    | 117  |
| 25164   | *Neurospora* VS ribozyme III-IV-V junction, PRE | 118  |
|         | - HCV IRES IIIId fragment                      | 119  |
|         | - HIV-1 packaging signal SL4                   | 120  |
|         | - *E. coli* 23S rRNA helix 42 lower stem       | 121  |
|         | - *E. coli* 16S rRNA hairpin                   | 122  |
|         | - r(GACGAGUGUCA)2                              | 123  |
|         | - Hairpin with 5’GG/3’UU motif                  | 124  |
|         | - TYMV pseudoknot                              | 125  |
|         | - Bacteriophages T2 and T6 gene 32 pseudoknot  | 126  |
|         | - r(GAGGUCUC)2                                 | 127  |
|         | - *E. coli* 5S rRNA helix I                    | 128  |
|         | - RNA I                                       | 129  |
|         | - CUUG hairpin                                 | 130  |
|         | - Hammerhead ribozyme-substrate complex        | 131  |
|         | - *T. Thermophila* group II intron P5 helix    | 132  |
|         | - *T. Thermophila* group II intron P5 helix with Co(NH3)6 ++ | 133  |
|         | - sTRSV hairpin ribozyme loop A                | 134  |
|         | - MMTV frameshifting pseudoknot                | 135  |
|         | - Group I intron P4/P6 domain                  | 136  |

*d* Hart, J. M. Unpublished.
Accession codes and primary references from which direction-dependent chemical shift constraints were derived (continued).

| BMRB ID | Structure                                      | Ref. |
|---------|------------------------------------------------|------|
|         | *Bacillus* RNase P P5.1 hairpin                 | 129  |
|         | EIAV TAR                                        | 130  |
|         | HIV-1 TAR CUGGGA loop                           | 131  |
|         | r(GAGUGCUC)₂                                    | 132  |
|         | r(GGCGUCUC)₂                                    | 132  |
|         | r(5′GAGGAAGGCGA/3′PCUCUAUUGCU)                   | e    |

* Znosko, B. M. Unpublished.
Accession codes and primary references of PDB NMR structures in which distances between imino protons of adjacent base pairs were measured.

| PDB Code | Structure | Ref. |
|----------|-----------|------|
| 17RA     | RNA I     | 123  |
| 1A60     | TYMV pseudoknot | 133  |
| 1BN0     | HIV-1 SL3 hairpin | 211 |
| 1BYX     | r(GCAGUGGGC)-r(GCCA)d(CTGC) duplex | 25 |
| 1C4L     | r(5′CGACUCAGG/3′CCUGCGUCG) | 20 |
| 1CQL     | E. coli SRP domain IV | 154 |
| 1EKA     | r(5′GAGUGCUC) | 132 |
| 1EKD     | r(5′GGCGUGGCC) | 132 |
| 1F6U     | HIV-1 SL2 of Ψ packaging signal | 29 |
| 1GUC     | r(5′GAGGUGUCUC) | 121 |
| 1HWQ     | Neurospora VS ribozyme stem-loop substrate | 52 |
| 1JO7     | Influenza A virus promoter | 50 |
| 1JOX     | Bacillus RNase P P5.1 hairpin | 129 |
| 1JTW     | HIV-1 packaging signal SL4 | 116 |
| 1JU7     | RNA binding site for histone stem-loop binding protein | 54 |
| 1K5I     | E. coli 16S rRNA hairpin | 118 |
| 1K8S     | RNA duplex with bulged adenosine | 27 |
| 1KKA     | E. coli tRNA\(^{\text{unmodified}}\) anticodon stem-loop | 55 |
| 1L1W     | Human SRP RNA SRP19 binding site | 56 |
| 1LC6     | S. cerevisiae U6-A62G ISL RNA | 57 |
| 1LDZ     | Leadzyme | 135 |
| 1LMV     | r(5′GGUGUAGUA/3′UACUAACACC) | 38 |
| 1LPW     | r(5′GGUGψAGUA/3′UACUAACACC) | 38 |
| 1M82     | Influenza A cRNA promoter | 59 |
| 1MNX     | S. oleracea 5S rRNA loop E region | 20 |
| 1N8X     | HIV-1 Ψ packaging signal SL1 | 130 |
| 1NA2     | Human temolerase RNA P2b hairpin | 44 |
| 1NC0     | S. cerevisiae U6 ISL stem-loop, U80G | 45 |
| 1NZ1     | S. cerevisiae U6 ISL stem-loop, U80 | 46 |
| 1OW9     | Neurospora VS ribozyme SL1′ hairpin | 49 |
| 1PJY     | HIV-1 framesshifting inducing stem-loop RNA | 48 |
| 1Q75     | Human telomerase RNA DCloop mutant P2b hairpin | 51 |
| 1QES     | r(5′GGAGUUC) | 15/ |
| 1QET     | r(5′GGAGUUGCC) | 15/ |
| 1R2P     | S. cerevisiae group II intron Sc.ai5γ domain 5 | 52 |
| 1R7W     | Enterovirus IRES stem-loop IV domain, WT34 | 55 |
| 1R7Z     | Enterovirus IRES stem-loop IV domain, 10U | 55 |
| 1RFR     | Coxackievirus stem-loop D | 53 |
| 1S2F     | RSV splicing suppressor pseudo-5′ splice site | 54 |
| 1S34     | RSV residues 907-929 | 54 |
Accession codes and primary references of PDB NMR structures in which distances between imino protons of adjacent base pairs were measured (continued).

| PDB  | Structure                                               | Ref. |
|------|---------------------------------------------------------|------|
| 1S9S | MLV core encapsidation signal                          | 2    |
| 1SCL | *E. coli* 28S rRNA sarcin/ricin loop                    | 138  |
| 1SY4 | *S. cerevisiae* U6 ISL stem-loop                        | 46   |
| 1T28 | HRV-14 internal cis-acting replication element          | 26   |
| 1TJZ | VS ribozyme stem-loop VI                                | 57   |
| 1XHP | *S. cerevisiae* extended U6 ISL                         | 58   |
| 1YG3 | ScYLV pseudoknot                                        | 61   |
| 1YMO | Human telomerase RNA P2b-P3 pseudoknot                  | 59   |
| 1YSV | Human GluR-B R/G central loop                           | 60   |
| 1Z2J | HIV-1 frameshift inducing element                       | 62   |
| 1Z30 | BEV1 cloverleaf 1 apical D-loop                         | 65   |
| 1ZC5 | HIV-1 frameshifting signal                              | 64   |
| 28SR | Conserved internal loop in *E. coli* SRP                | 28   |
| 2ADT | GAAA tetraloop-receptor complex                          | 65   |
| 2AHT | Domain 6 of a group II intron                            | 66   |
| 2AU4 | Class I GTP aptamer                                     | 67   |
| 2B7G | *D. melanogaster* Smaug recognition element             | 139  |
| 2D17 | HIV-1 bulge34 stem-bulge-stem region                    | 140  |
| 2D18 | HIV-1 loop25 extended-duplex dimer                       | 140  |
| 2D19 | HIV-1 loop25 kissing-loop dimer                          | 140  |
| 2D1A | HIV-1 DIS-39 extended-duplex dimer                       | 140  |
| 2D1B | HIV-1 DIS-39 kissing loop dimer                          | 140  |
| 2F87 | *P. furiosus* SRP RNA helix 6 tetraloop                 | 75   |
| 2FDT | Eel UnaL2 LINE36 hairpin                                | 74   |
| 2GM0 | HIV-1 SL1 dimer                                         | 70   |
| 2GVO | Human PGY/MDR1 hairpin                                  | 69   |
| 2IHX | RSV µΨ RNA packaging signal                             | 141  |
| 2IXY | HBV encapsidation signal apical stem-loop               | 142  |
| 2JR4 | *E. coli* tRNA\(^{\text{Val}}\)\(_{UC}\) unmodified anticodon stem-loop | ///  |
| 2JRG | *E. coli* tRNA\(^{\text{Val}}\)\(_{UC}\) anticodon stem-loop, cmo5U34 and M6A37 | ///  |
| 2JRQ | *E. coli* tRNA\(^{\text{Val}}\)\(_{UC}\) anticodon stem-loop, cmo5U34 | ///  |
| 2JSG | *E. coli* tRNA\(^{\text{Val}}\)\(_{UC}\) anticodon stem-loop M6A37 | ///  |
| 2JTP | SIV frameshift-induced stem-loop                         | 78   |
| 2JWV | Anti-NF-κB aptamer                                       | 79   |
| 2JXQ | r(5’GCAGAGAGCG/3’CGUCUCUCGC)                            | 80   |
| 2JXS | r(5’GCAGAGAGCG/3’CGUCUCUCGC)                            | 80   |
| 2JYM | HBV post-transcriptional regulatory element stem-loop α | 85   |
| 2K3Z | r(5’GUCGAGCGUG/3’CAGCCGAC)                              | 84   |
| 2K41 | r(5’GUCGUGCGUG/3’CAGCCGAC)                              | 84   |
| 2K5Z | Duck HBV e apical stem-loop                             | 143  |
### Accession codes and primary references of PDB NMR structures in which distances between imino protons of adjacent base pairs were measured (continued).

| PDB  | Structure                                                                 | Ref. |
|------|---------------------------------------------------------------------------|------|
| 2K65 | *S. cerevisiae* group II intron *Sc.ai5γ* d3' hairpin, including EBS1/IBS1 | 86   |
| 2K66 | *S. cerevisiae* group II intron *Sc.ai5γ* d3' hairpin closed by GAAA tetraloop | 86   |
| 2K7E | Human tRNA\textsuperscript{Lys\textsubscript{Lyk}}\textsuperscript{Lys\textsubscript{Lyk}} anticodon fragment bound to HIV-1 genome loop 1 | 88   |
| 2KOC | 14-mer hairpin with cUUCGg tetraloop                                     | 144  |
| 2KRL | RBSE in 3' UTR of TCV                                                     | 145  |
| 2KXZ | r(GACAAGUGUCU)\textsubscript{2}                                            | 92   |
| 2KY0 | r(GACGAGCGUCA)\textsubscript{2}                                           | 92   |
| 2KY1 | r(GACUAGAGUCA)\textsubscript{2}                                           | 92   |
| 2KYD | 16-mer A-form RNA                                                         | 146  |
| 2KZL | *B. subtilis* tyrS T-box leader specifier domain                          | 96   |
| 2L1F | MoMuLV Ψ\textsuperscript{C,ES} site                                      | 147  |
| 2L3E | Human telomerase RNA P2ab                                                | 95   |
| 2L5Z | *Neurospora* VS ribozyme A730 loop                                       | 94   |
| 2L6I | Coronavirus SL2                                                           | 95   |
| 2L8H | HIV-1 TAR and small molecule complex                                      | 148  |
| 2L8U | r(CGCUGCGG)\textsubscript{2}                                             | 149  |
| 2L9E | Human tRNA\textsuperscript{Lys\textsubscript{Lyk}}\textsuperscript{Lys\textsubscript{Lyk}} anticodon stem | 99   |
| 2LA9 | *B. subtilis* \(\psi_{39}\)-tRNA\textsuperscript{1yr}                   | 150  |
| 2LAC | *B. subtilis* unmodified tRNA\textsuperscript{1yr}                       | 150  |
| 2LBJ | *B. subtilis* tRNA\textsuperscript{Gly,GCC} anticodon stem-loop          | 151  |
| 2LBK | *S. epidermidis* tRNA\textsuperscript{Gly,UCC} anticodon stem-loop       | 151  |
| 2LBL | *B. subtilis* tRNA\textsuperscript{Gly,UCC} anticodon stem-loop          | 151  |
| 2LBQ | *B. subtilis* \(i6A_{37}\)-tRNA\textsuperscript{1yr} anticodon arm       | 150  |
| 2LBR | *B. subtilis* \(i6A_{37}, \psi_{39}\)-tRNA\textsuperscript{1yr} anticodon arm | 150  |
| 2LC8 | MLV read-through pseudoknot signal                                        | 10   |
| 2LDL | HIV-1 exon splicing silencer 3                                            | 100  |
| 2LDT | *E. coli* 16S rRNA helix 27                                               | 101  |
| 2LHP | Chimpanzee HAR1 helix h1 (c37)                                            | 102  |
| 2L14 | *Y. enterocolitica* mgtA riboswitch antiterminator loop C, lower part     | 152  |
| 2LJJ | CVB-3 IRES subdomain IV-B                                                | \(\textsuperscript{a}\) |
| 2LK3 | *S. cerevisiae* U2/U6 complex helix I                                    | 103  |
| 2LP9 | BMV subgenomic stem-loop, wild type                                      | 104  |
| 2LPA | BMV subgenomic stem-loop, del-A                                          | 104  |
| 2LQZ | *B. subtilis* phage φ29 pRNA hairpin                                     | 105  |
| 2LU0 | *S. cerevisiae* group II intron *Sc.ai5γ* K-ζ region                     | \(\textsuperscript{a}\) |

\(\textsuperscript{a}\) Ihle et al. Unpublished.
Accession codes and primary references of PDB NMR structures in which distances between imino protons of adjacent base pairs were measured (continued).

| PDB  | Structure                                                                 | Ref. |
|------|---------------------------------------------------------------------------|------|
| 2LUB | Human HAR1 helix h1 (h37)                                                 | 102  |
| 2M12 | *S. cerevisiae* group II intron Sc.ai5γ domain 1 ID3 stem-loop             | 106  |
| 2M10 | *S. cerevisiae* group II intron Sc.ai5γ domain 1 ID3 stem                  | 106  |
| 2M1V | *S. cerevisiae* group II intron Sc.ai5γ d3’ hairpin, including EBS1:dIBS1 complex | 107  |
| 2M21 | *T. thermophila* telomerase RNA stem-loop IV                               | 108  |
| 2M22 | *T. thermophila* telomerase RNA helix II template boundary element         | 109  |
| 2M23 | *S. cerevisiae* group II intron Sc.ai5γ d3’ hairpin, including EBS1        | 86   |
| 2M24 | *S. cerevisiae* group II intron Sc.ai5γ d3’ hairpin, including EBS1        | 86   |
| 2M5U | CPEB3 ribozyme P4 domain                                                  | 111  |
| 2M8K | *K. lactis* telomerase RNA pseudoknot                                     | 9    |
| 2MEQ | *E. coli* 23S rRNA H69, unmodified                                         | 110  |
| 2MER | *E. coli* 23S rRNA H69, modified                                           | 110  |
| 2MHI | Medaka telomerase RNA CR4/5 domain                                         | 6    |
| 2MIS | *Neurospora* VS ribozyme SLVI                                             | 112  |
| 2MNC | miR-21 stem-loop                                                          | 113  |
| 2MTJ | *Neurospora* VS ribozyme III-IV-V junction                                | 114  |
| 2MTK | *Neurospora* VS ribozyme III-IV-V junction, PRE                           | 114  |
| 2QH2 | Human telomerase RNA CR7 3’ terminal hairpin                              | 72   |
| 2QH3 | Human telomerase RNA U64 H/ACA snoRNA 3’ terminal hairpin                 | 72   |
| 2QH4 | Human telomerase RNA U85 C/D-H/ACA scaRNA 5’ terminal hairpin             | 72   |
| 2RN1 | HIV-1 TAR and aptamer complex                                              | 75   |
| 2TPK | Bacteriophage T2 gene 32 mRNA pseudoknot                                  | 25   |
| 2Y95 | Xist RNA A-repeat AUCG tetraloop                                           | 91   |
| 3PHP | TYMV pseudoknot 3’ hairpin                                                | 24   |
| 4A4R | r(GGACCCGGCUAACGCUGGGGUCC)                                                 | 153  |
| 4A4S | r(GGACCCGGCUACGCUGGGGUCC)                                                  | 153  |
| 4A4T | r(GGACCCGGCUUACGCUGGGGUCC)                                                 | 153  |
| 4A4U | r(GGACCCGGCUACGCUGGGGUCC)                                                 | 153  |
Accession codes and primary references of PDB x-ray structures in which distances between imino protons of adjacent base pairs were measured.

| PDB   | Structure / Ref.                                      |
|-------|-------------------------------------------------------|
| 157D  | r(CGCGAAUUAGCG)_2                                    |
| 259D  | r(CCCCGGGG)_2                                        |
| 377D  | r(CGUA)_2                                             |
| 397D  | HIV-1 TAR RNA stem                                    |
| 406D  | r(CACCGGAUGGU^{38}UGGUG)_2                           |
| 420D  | r(GCAGAGUUAAUCUGC)_2                                 |
| 434D  | r(5’GGGGCUA/3’CCUCGAU)                                |
| 435D  | r(5’GGGGCUA/3’CCCCGAU)                                |
| 437D  | BWYV pseudoknot                                       |
| 439D  | r(5’CUGGGCGG/3’GGUCCGCC)                              |
| 464D  | r(5’GGGGGUA/3’CCUCGAU)                                |
| 466D  | r(5’GGGGCUA/3’CCUCGAU)                                |
| 472D  | r(5’GUGUUUAC/3’CACCGAUG)                              |
| 480D  | *E. coli* 23S rRNA sarcin/ricin domain                |
| 1CSL  | HIV-1 RRE high affinity binding site                 |
| 1D4R  | HSR particle helix 6                                  |
| 1DQH  | r(5’GCCACCCUG/3’CGGCUGGAC)                            |
| 1EHZ  | Yeast tRNA^{phe}                                      |
| 1L2X  | BWYV pseudoknot                                       |
| 1MSY  | *E. coli* 23S rRNA sarcin/ricin domain GUAA tetraloop mutant |
| 1NLC  | HIV-1 DIS(Mal) duplex                                 |
| 1NUJ  | Leadzyme                                             |
| 1Q96  | Rat 28S rRNA sarcin/ricin domain mutant               |
| 1QC0  | ColE1 plasmid 19-mer duplex                           |
| 1QC1  | ColE1 plasmid 18-mer duplex                           |
| 1RXB  | r(CCCCGGGG)_2                                        |
| 1T0E  | 2-aminopurine labeled bacterial decoding site RNA     |
| 1XE   | HIV-1 subtype B genomic RNA DIS                       |
| 1ZCI  | HIV-1 DIS RNA subtype F- monoclinic form              |
| 2A43  | Luteoviral RNA pseudoknot                             |
| 2G3S  | r(GGCGUGGC)_2                                        |
| 2G91  | r(GGUGC^cc)_2                                        |
| 2G92  | r(CG(NF2)AAUUAGCG)_2                                 |
| 2OEU  | Hammerhead ribozyme with Mn^{2+} bound                |
| 2O1Y  | HIV-1(Lai) DIS duplex form                            |
| 2QEK  | HIV-1 subtype F DIS RNA duplex form                   |
| 2R20  | r(GCGUUUUGAAACGC)_2                                  |
| 2R22  | r(GCGUUUUGAAACGC)_2                                  |
| 2V6W  | *E. coli* tRNA^{ser} acceptor stem                    |

\(^a\) Shi, K., Pan, B., and Sundaralingam, M. Unpublished.
Accession codes and primary references of PDB x-ray structures in which distances between imino protons of adjacent base pairs were measured (continued).

| PDB     | Structure                                      | Ref. |
|---------|------------------------------------------------|------|
| 2V7R    | Human tRNA<sup>Gly</sup> microhelix           | 187  |
| 2VAL    | *E. coli* tRNA<sup>Gly</sup> microhelix       | 188  |
| 2VUQ    | Human tRNA<sup>Gly</sup> microhelix           | 189  |
| 2W89    | *E. coli* tRNA<sup>Arg</sup> isoacceptor stem | 190  |
| 2XSL    | *T. Thermophilus* tRNA<sup>Gly</sup> acceptor stem microhelix | 191  |
| 2ZY6    | *E. coli* Thl truncated tRNA substrate        | 192  |
| 3CGP    | Pseudouridylated yeast spliceosomal U2 snRNA-intron branch site duplex | 193  |
| 3CGS    | Pseudouridylated U2 snRNA and mammalian intron branch site sequences | 193  |
| 3GVN    | *E. coli* tRNA<sup>Ser</sup> acceptor stem microhelix | 194  |
| 3MEI    | Human thymidylate synthase mRNA regulatory motif | 195  |
| 3RG5    | Mouse tRNA<sup>Sec</sup>                      | 196  |
| 3SJ2    | Fragile X syndrome model of repeating r(CGG) transcript | 197  |
| 3SYW    | Myotonic dystrophy triplet repeat with a 1 x 1 nucleotide UU internal loop | 198  |
| 4E5C    | 19-mer RNA duplex containing CUG/C GG-repeats | 199  |
| 4E6B    | 19-mer RNA duplex p(CGG)<sub>3</sub>C(CUG)<sub>3</sub> | 199  |
| 4FNJ    | CUG helix attached to GAAA tetraloop/receptor | 200  |
| 4J50    | Expanded RNA CAG repeat                        | 201  |
| 4MSB    | 10-mer duplex with two 2'-5' -linkages         | 202  |
| 4NFO    | r(GCAGACUUAAGUCUGC)<sub>2</sub>               | 203  |
| 4P5J    | TYMV TLS                                       | 204  |
| 4PCJ    | CUG repeat expansions with Ψ modification    | 205  |
| 4U37    | r(5'UAGCUCC/3'AUCGAGG)                        | 206  |
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