Supplementary Data

"DSSR: an integrated software tool for dissecting the spatial structure of RNA" by Lu *et al.*

Supplementary Figures

Supplementary Sample Output

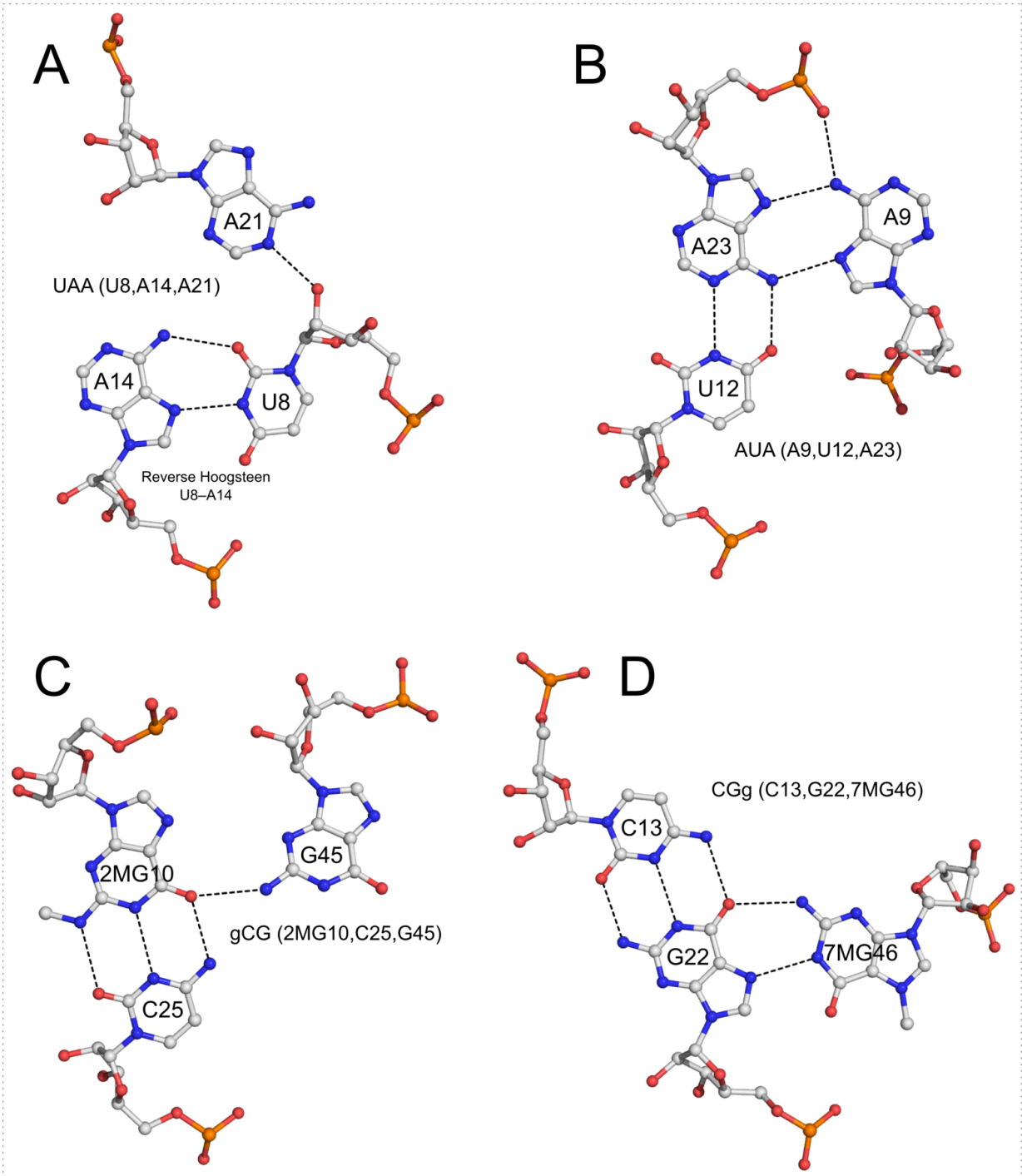

Figure S1: The four base triplets and associated hydrogen bonds (dashed lines) detected by DSSR in yeast tRNA$^{\texttt{Phe}}$ (PDB id: `1ehz`). (**A**) UAA (U8,A14,A21), with a reverse Hoogsteen U8–A14 pair. (**B**) AUA (A9,U12,A23). (**C**) gCG (2MG10,C25,G45). (**D**) CGg (C13,G22,7MG46). Here, the bases in each triplet are listed in sequential order, with the one-letter shorthand form followed by more detailed identifiers in parentheses. In (**C**) and (**D**), the lower case 'g' represents the shortened name for modified guanine nucleotides 2MG10 and 7MG46, respectively. Note that the triplets and hydrogen bonds match those originally reported by Quigley and Rich for yeast tRNA$^{\texttt{Phe}}$.

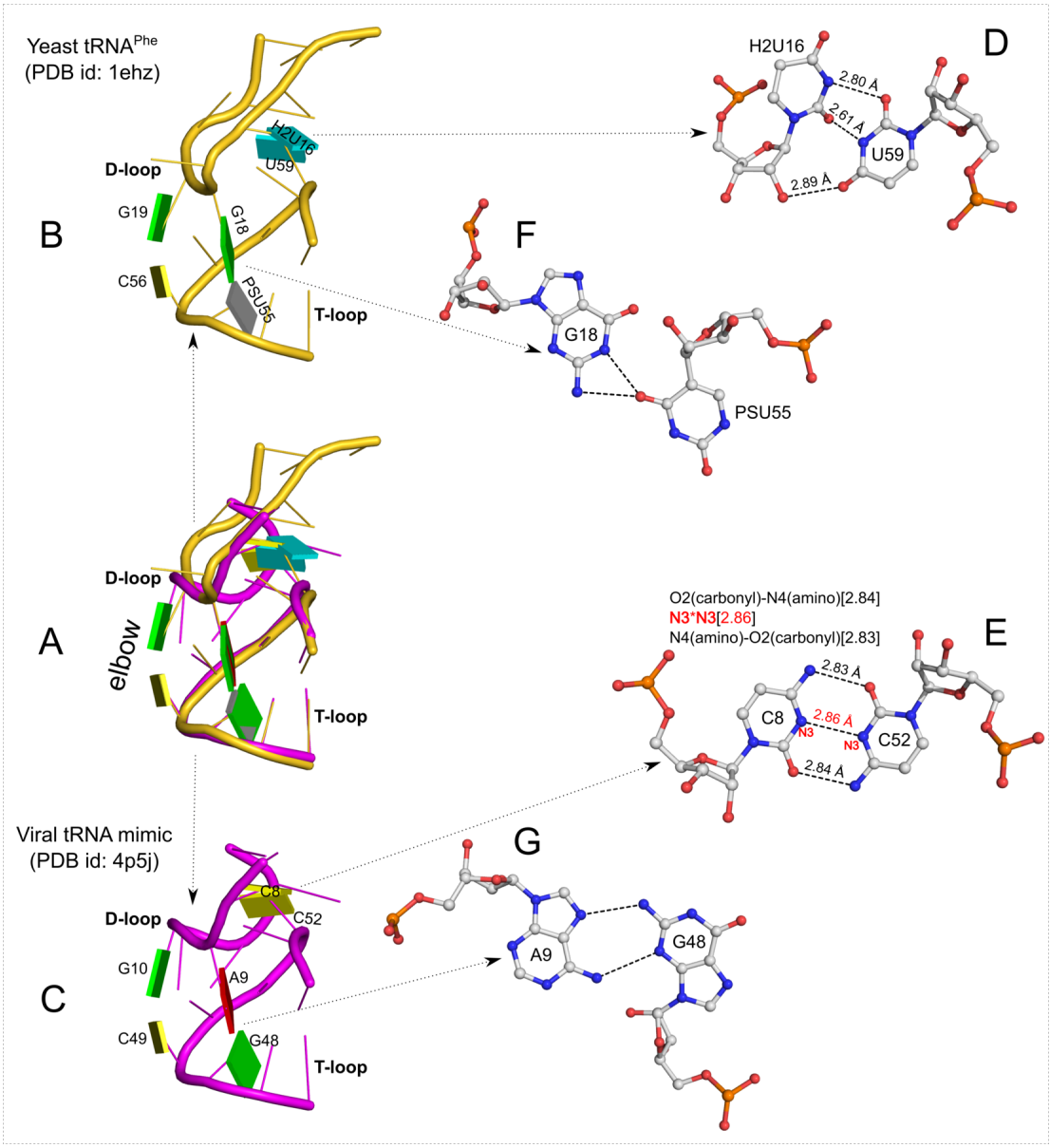

Figure S2: Three similarly positioned base pairs that hold the D- and T-loops of tRNA$^{\text{Phe}}$ (PDB id: `1ehz`, gold) and its viral mimic (PDB id: `4p5j`, magenta) in place. The interacting loops in the two molecules are overlaid on the reference frame of the common elbow G–C pair, which is oriented vertically with its major-groove edge facing the viewer, roughly matching Figures 2 and 3 (**A-C**). Since the two elbow G–C pairs have very similar base-pair parameters, they overlap nearly perfectly. Despite large structural variations between the D-loops, the H2U16+U59 pair in tRNA (**B**, detailed in **D**) is similar to the presumably semi-protonated C8+C52 pair (forming an i-motif) in the mimic (**C**, detailed in **E**). The other two pairs near the elbow (**F** and **G**) are also strikingly alike, despite dramatically different modes of interaction. Note that DSSR identifies the C+C pair (**E**) with the assumed acceptor-acceptor (N3 to N3) hydrogen bond highlighted (red).

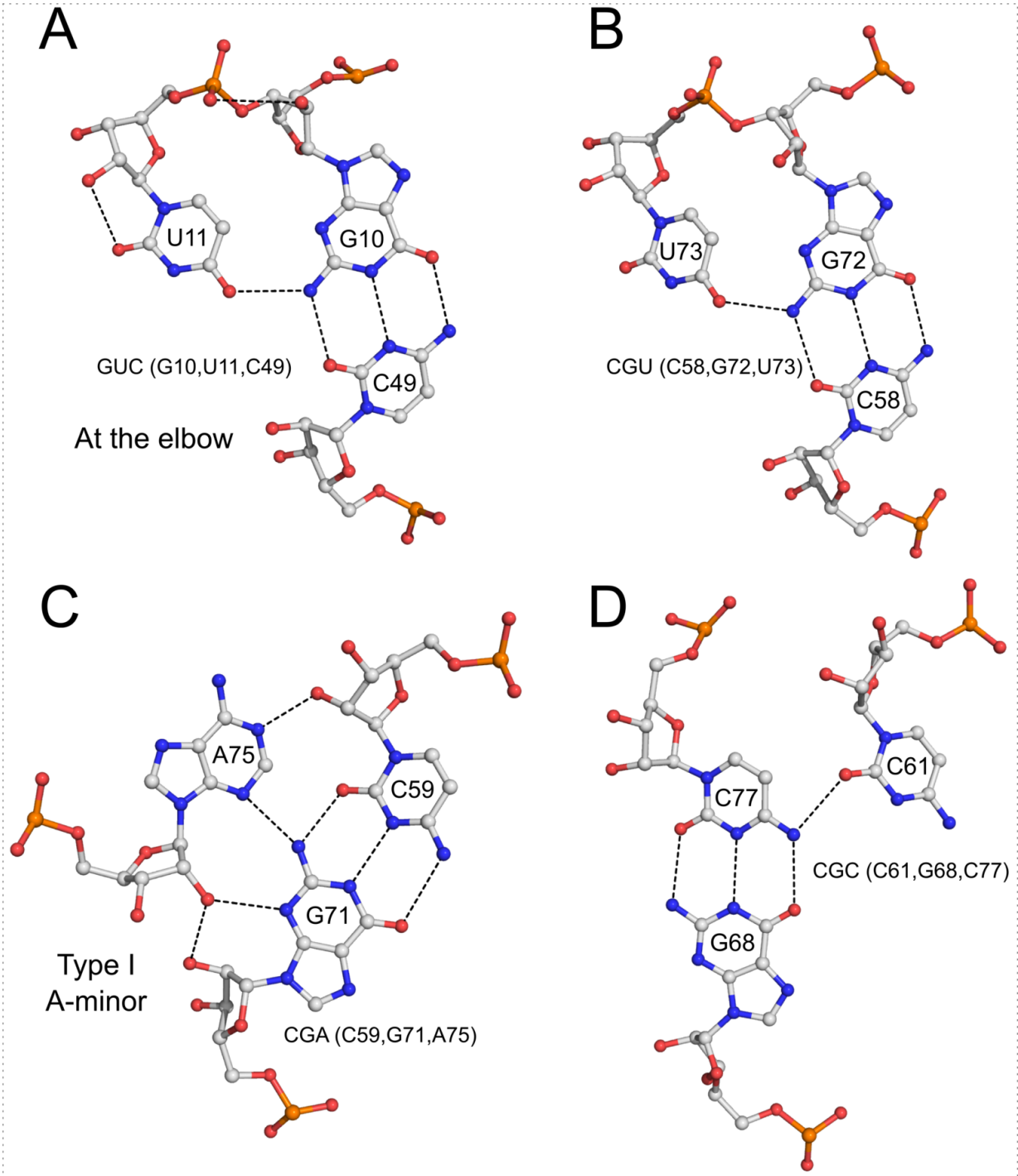

Figure S3: The four base triplets and associated hydrogen bonds (dashed lines) detected by DSSR in the viral tRNA mimic (PDB id: `4p5j`) from turnip yellow mosaic virus. (**A**) GUC (G10,U11,C49) lies at the elbow of the L-shaped tertiary structure, with G10 and U11 forming a GpU dinucleotide platform. (**B**) CGU (C58,G72,U73) includes another GpU (G72 and U73) platform, with a single base-base hydrogen bond. (**C**) CGA (C59,G71,A75) forms a type I A-minor motif. (**D**) CGC (C61,G68,C77) contains a loop nucleotide (C61) from the hairpin-type pseudoknot. The last three triplets (**B**-**D**) are located at the 3′-end of the structure around the hairpin-type pseudoknot.

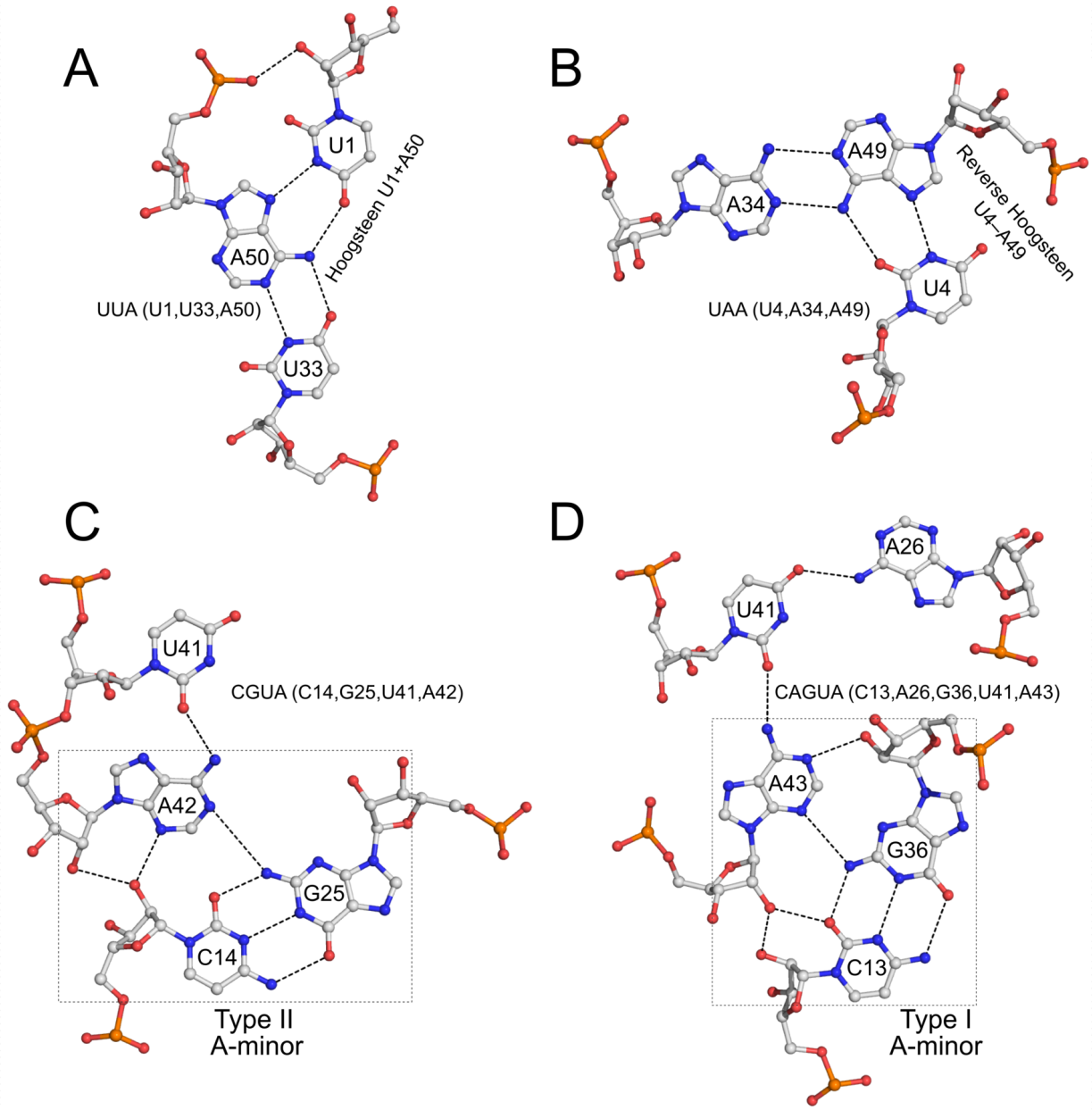

Figure S4: The four base multiplets and associated hydrogen bonds (dashed lines) detected by DSSR in the *env22* twister ribozyme (chain A, PDB id: `4rge`). (**A**) Triplet UUA (U1,U33,A50) where U1 and A50 form a Hoogsteen pair (U1+A50). (**B**) Triplet UAA (U4,A34,A49) where U4 and A49 form a reverse Hoogsteen pair (U4–A49). (**C**) Quadruplet CGUA (C14,G25,U41,A42) which includes a type II A-minor motif. (**D**) Pentaplet CAGUA (C13,A26,G36,U41,A43) which contains a type I A-minor motif. The two neighboring A-minor motifs (in **C** and **D**) are part of a larger structural framework involving U41 and A26 (see Figure 4).

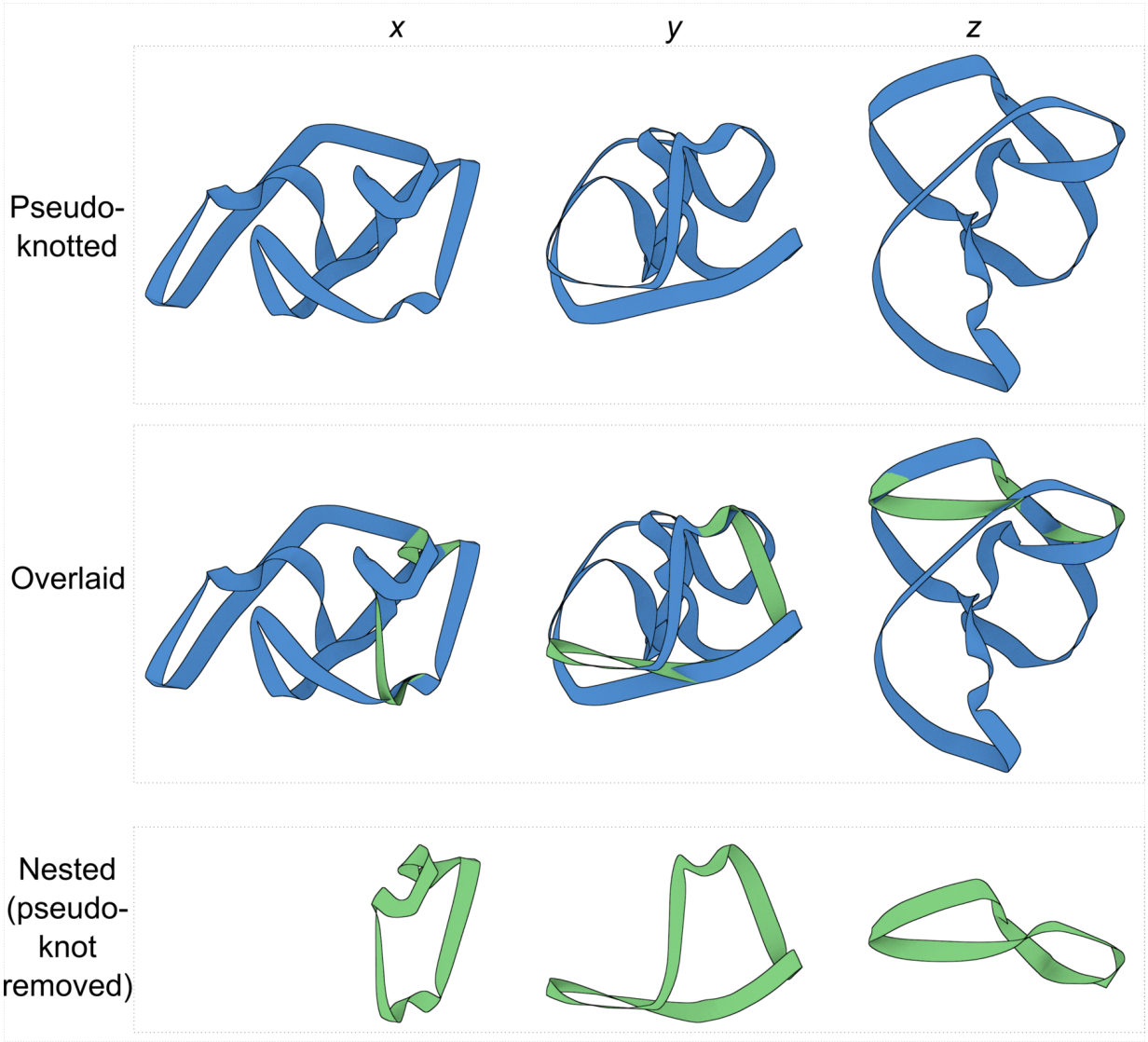

Figure S5: Ribbon representations of the junction loop in the *env22* twister ribozyme (PDB id: `4rge`). The ribbons are defined in terms of the C1′ and P atoms of the nucleotides that make up the junction loop. Inclusion of pseudoknots in the analysis of the structure reveals a [4,2,2,0,1,3,0,0,1,1] ten-way junction and a ribbon that follows a supercoiled pathway, with a linking number of three (blue, top row). Upon pseudoknot removal, only a [2,1,3] three-way junction and a ribbon with a simple relaxed circular configuration remain (green, bottom row). The overlap of the two junction loops in the middle row clearly shows that the over-simplified three-way junction spans only a small portion of the ten-way loop. The ribbons are shown in three projections: down the x-axis (left column), the y-axis (middle column), and the z-axis (right column). The images were kindly generated by Dr. Nicolas Clauvelin using the approach described in ref. 52.

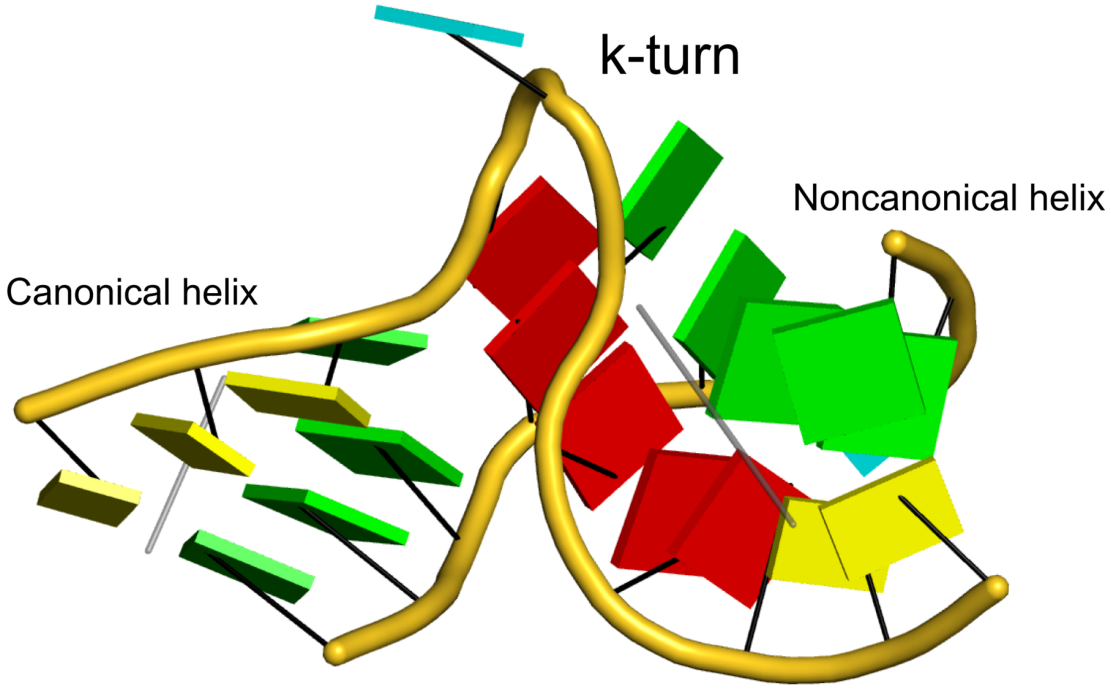

Figure S6: The k-turn identified by DSSR in the SAM-I riboswitch (PDB id: `2gis`). Base-stacking interactions are interrupted around the k-turn even though the backbone is continuous along each strand. Thus DSSR assigns two helices (depicted by gray lines), the canonical helix on the left, and the noncanonical one on the right.

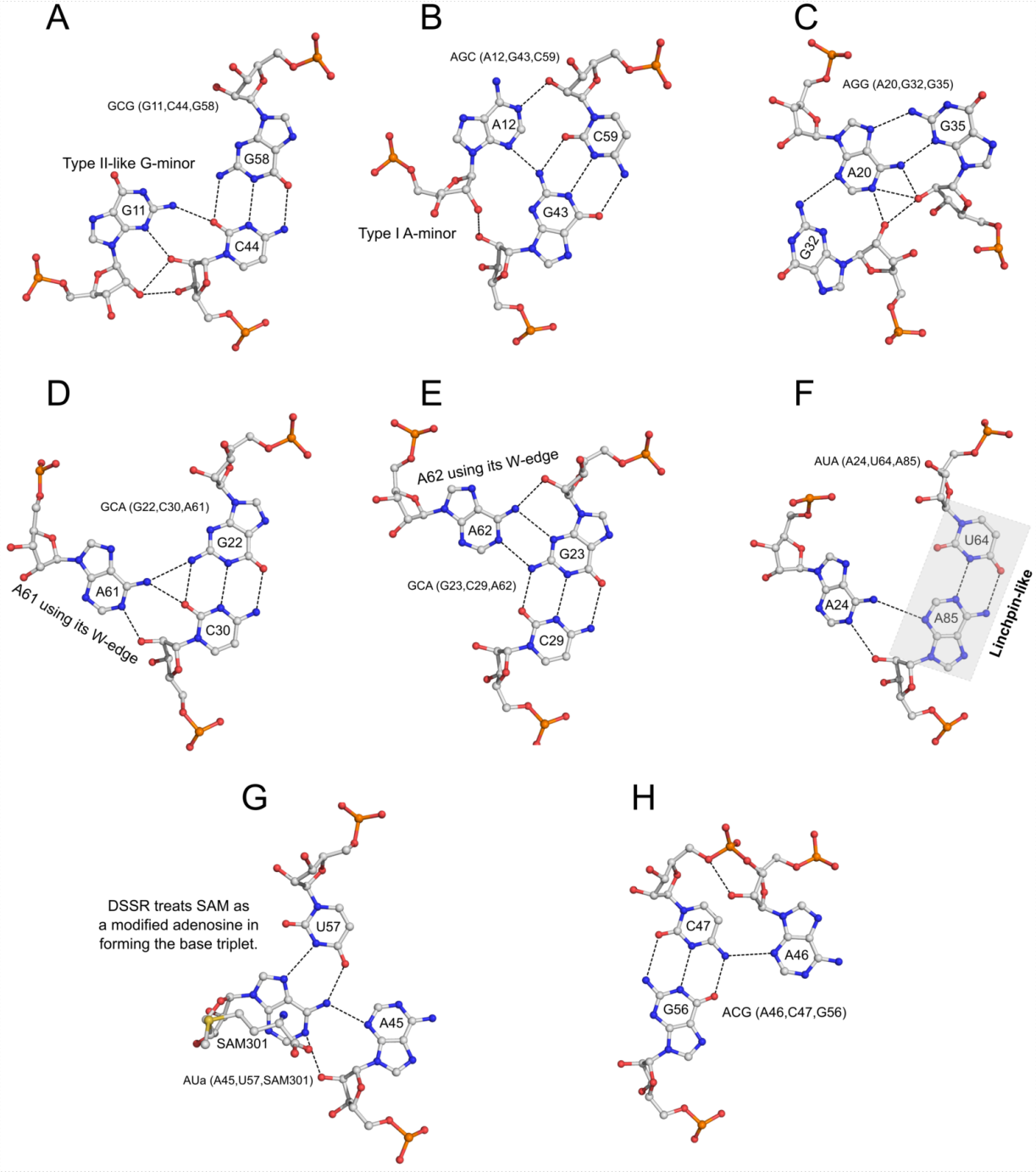

Figure S7: The eight base triplets and associated hydrogen bonds (dashed lines) detected by DSSR in the SAM-I riboswitch (PDB id: `2gis`). (**A**) GCG (G11,C44,G58), with G11 in a similar position and orientation as in a type II A-minor motif. (**B**) AGC (A12,G43,C59), a type I A-minor motif. (**C**) AGG (A20,G32,G35). (**D**) GCA (G22,C30,A61). (**E**) GCA (G23,C29,A62). (**F**) AUA (A24,U64,A85), with the isolated, linchpin-like U64-A85 pair. (**G**) AUa (A45,U57,SAM301), with the SAM adenosine moiety taken as a modified base in forming the triplet. (**H**) ACG (A46,C47,G56). Note that in (**D**) and (**E**), A61 and A62 employ their **W**atson-Crick edges, rather than the minor-groove edges as in A-minor motifs, to interact with the minor-groove edges of the two consecutive G–C pairs.

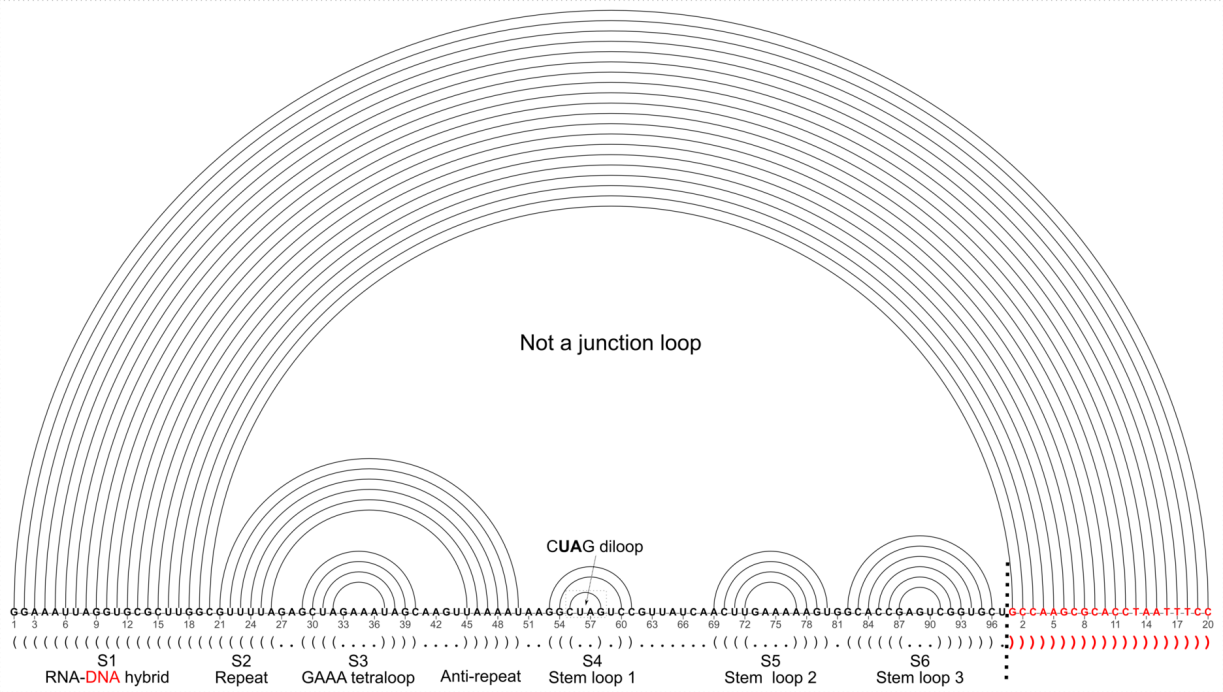

Figure S8: The linear (arc) secondary structure diagram of the RNA-DNA hybrid structure in the CRISPR Cas9-sgRNA-DNA ternary complex (PDB id: `4oo8`), annotated with DSSR-derived dot-bracket notation and key structural elements. The target DNA base sequence is colored red, and the chain switch from sgRNA to DNA is marked by the dotted vertical line. DSSR detects no junction loops in this hybrid structure because of the chain break.

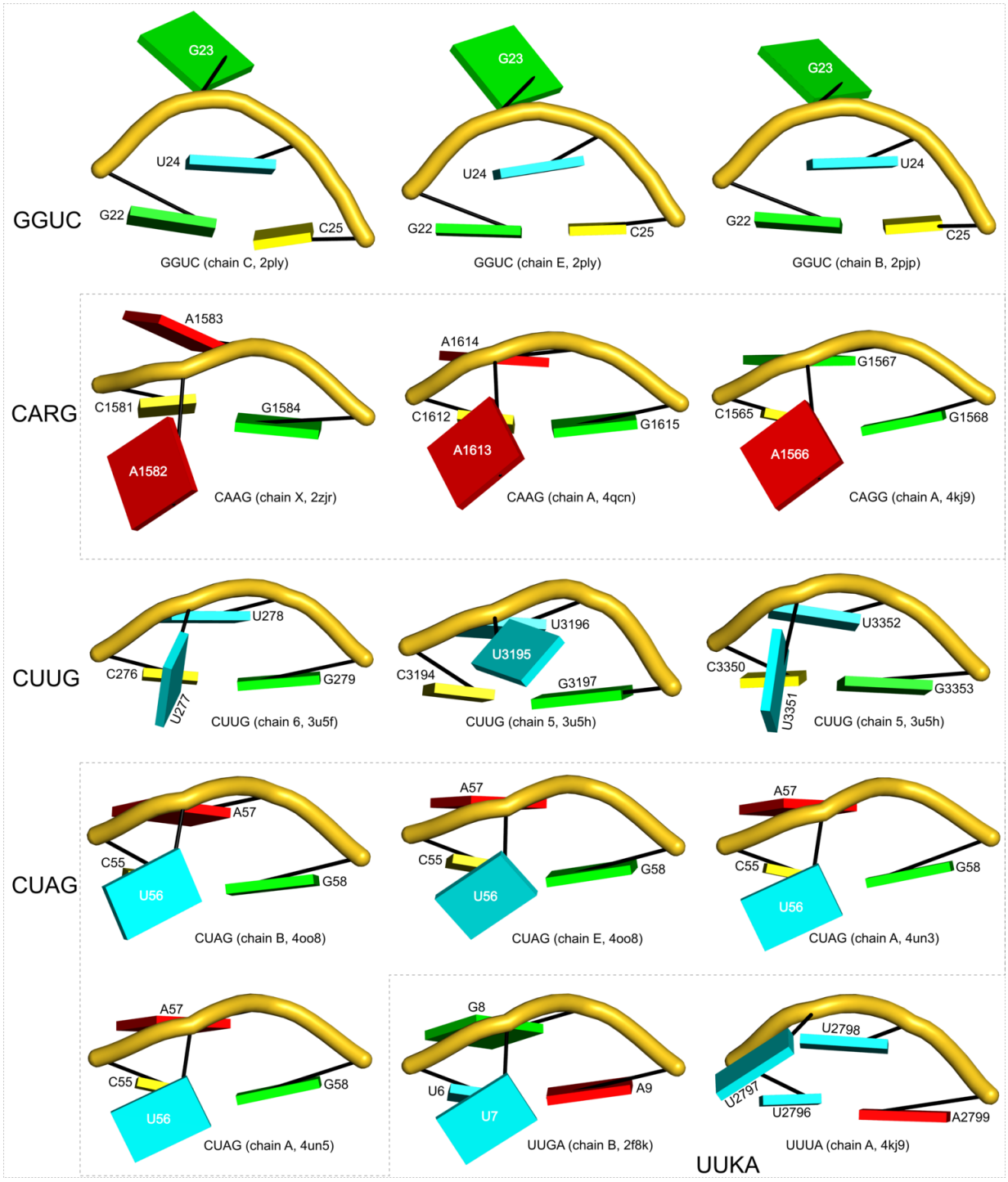

Figure S9: Images of 15 diloops (GGUC, CARG, CUUG, CUAG, and UUKA) identified by DSSR in the NR3A-dataset. The diloops can be categorized into five groups by base sequence: GGUC, where the second position G is flipped away from the closing pair; CARG, where the second position A is extruded into the minor-groove side of the closing pair; CUUG, which shows structural variations in the three crystallographic examples and differences from their NMR solution counterpart (PDB id: `1rng`, Figure 6C); CUAG, where all four cases occur in Cas9 complexes either without (PDB id: `4oo8`) or with (PDB ids: `4un3` and `4un5`) a protospacer adjacent motif; and UUKA, where the two cases are quite distinct.

Output of a sample DSSR run on yeast tRNA^{Phe} (PDB id: `1ehz`)

```
****************************************************************************
               DSSR: an Integrated Software Tool for
              Dissecting the Spatial Structure of RNA
               v1.2.8-2015jun15 by xiangjun@x3dna.org

   This program is being actively maintained and developed. As always,
   I greatly appreciate your feedback! Please report all DSSR-related
   issues on the 3DNA Forum (forum.x3dna.org). I strive to respond
   *promptly* to *any questions* posted there.

****************************************************************************
Note: Each nucleotide is identified by model:chainId.name#, where the
      'model:' portion is omitted if no model number is available (as
      is often the case for x-ray crystal structures in the PDB). So a
      common example would be B.A1689, meaning adenosine #1689 on
      chain B. One-letter base names for modified nucleotides are put
      in lower case (e.g., 'c' for 5MC). For further information about
      the output notation, please refer to the DSSR User Manual.
      Questions and suggestions are always welcome on the 3DNA Forum.

Command: x3dna-dssr -i=1ehz.pdb --u-turn --non-pair --po4 -o=1ehz.out
Date and time: Tue Jul 14 06:36:37 2015
File name: 1ehz.pdb
    no. of DNA/RNA chains: 1 [A=76]
    no. of nucleotides:    76
    no. of atoms:          1821
    no. of waters:         160
    no. of metals:         9 [Mg=6,Mn=3]

****************************************************************************
List of 11 types of 14 modified nucleotides
      nt    count  list
   1 1MA-a    1    A.1MA58
   2 2MG-g    1    A.2MG10
   3 5MC-c    2    A.5MC40,A.5MC49
   4 5MU-t    1    A.5MU54
   5 7MG-g    1    A.7MG46
   6 H2U-u    2    A.H2U16,A.H2U17
   7 M2G-g    1    A.M2G26
   8 OMC-c    1    A.OMC32
   9 OMG-g    1    A.OMG34
  10 PSU-P    2    A.PSU39,A.PSU55
  11 YYG-g    1    A.YYG37

****************************************************************************
List of 34 base pairs
      nt1            nt2           bp  name         Saenger    LW  DSSR
   1 A.G1           A.C72          G-C WC           19-XIX     cWW  cW-W
   2 A.C2           A.G71          C-G WC           19-XIX     cWW  cW-W
   3 A.G3           A.C70          G-C WC           19-XIX     cWW  cW-W
   4 A.G4           A.U69          G-U Wobble       28-XXVIII  cWW  cW-W
   5 A.A5           A.U68          A-U WC           20-XX      cWW  cW-W
   6 A.U6           A.A67          U-A WC           20-XX      cWW  cW-W
   7 A.U7           A.A66          U-A WC           20-XX      cWW  cW-W
   8 A.U8           A.A14          U-A rHoogsteen   24-XXIV    tWH  tW-M
   9 A.U8           A.A21          U+A --           n/a        tSW  tm+W
  10 A.A9           A.A23          A+A --           02-II      tHH  tM+M
  11 A.2MG10        A.C25          g-C WC           19-XIX     cWW  cW-W
  12 A.2MG10        A.G45          g+G --           n/a        cHS  cM+m
  13 A.C11          A.G24          C-G WC           19-XIX     cWW  cW-W
```

```
  14 A.U12          A.A23          U-A WC           20-XX     cWW  cW-W
  15 A.C13          A.G22          C-G WC           19-XIX    cWW  cW-W
  16 A.G15          A.C48          G+C rWC          22-XXII   tWW  tW+W
  17 A.H2U16        A.U59          u+U --           n/a       tSW  tm+W
  18 A.G18          A.PSU55        G+P --           n/a       tWS  tW+m
  19 A.G19          A.C56          G-C WC           19-XIX    cWW  cW-W
  20 A.G22          A.7MG46        G-g --           07-VII    tHW  tM-W
  21 A.M2G26        A.A44          g-A Imino        08-VIII   cWW  cW-W
  22 A.C27          A.G43          C-G WC           19-XIX    cWW  cW-W
  23 A.C28          A.G42          C-G WC           19-XIX    cWW  cW-W
  24 A.A29          A.U41          A-U WC           20-XX     cWW  cW-W
  25 A.G30          A.5MC40        G-c WC           19-XIX    cWW  cW-W
  26 A.A31          A.PSU39        A-P --           n/a       cWW  cW-W
  27 A.OMC32        A.A38          c-A --           n/a       c.W  c.-W
  28 A.U33          A.A36          U-A --           n/a       tSH  tm-M
  29 A.5MC49        A.G65          c-G WC           19-XIX    cWW  cW-W
  30 A.U50          A.A64          U-A WC           20-XX     cWW  cW-W
  31 A.G51          A.C63          G-C WC           19-XIX    cWW  cW-W
  32 A.U52          A.A62          U-A WC           20-XX     cWW  cW-W
  33 A.G53          A.C61          G-C WC           19-XIX    cWW  cW-W
  34 A.5MU54        A.1MA58        t-a rHoogsteen   24-XXIV   tWH  tW-M

*****************************************************************************
List of 4 multiplets
   1 nts=3 UAA A.U8,A.A14,A.A21
   2 nts=3 AUA A.A9,A.U12,A.A23
   3 nts=3 gCG A.2MG10,A.C25,A.G45
   4 nts=3 CGg A.C13,A.G22,A.7MG46

*****************************************************************************
List of 2 helices
  Note: a helix is defined by base-stacking interactions, regardless of bp
        type and backbone connectivity, and may contain more than one stem.
      helix#number[stems-contained] bps=number-of-base-pairs in the helix
      bp-type: '|' for a canonical WC/wobble pair, '.' otherwise
      helix-form: classification of a dinucleotide step comprising the bp
        above the given designation and the bp that follows it. Types
        include 'A', 'B' or 'Z' for the common A-, B- and Z-form helices,
        '.' for an unclassified step, and 'x' for a step without a
        continuous backbone.
      ------------------------------------------------------------------
  helix#1[2] bps=15
      strand-1 5'-GCGGAUUcUGUGtPC-3'
       bp-type    ||||||||||||..|
      strand-2 3'-CGCUUAAGACACaGG-5'
      helix-form  AA....xAAAAxx.
   1 A.G1           A.C72          G-C WC           19-XIX    cWW  cW-W
   2 A.C2           A.G71          C-G WC           19-XIX    cWW  cW-W
   3 A.G3           A.C70          G-C WC           19-XIX    cWW  cW-W
   4 A.G4           A.U69          G-U Wobble       28-XXVIII cWW  cW-W
   5 A.A5           A.U68          A-U WC           20-XX     cWW  cW-W
   6 A.U6           A.A67          U-A WC           20-XX     cWW  cW-W
   7 A.U7           A.A66          U-A WC           20-XX     cWW  cW-W
   8 A.5MC49        A.G65          c-G WC           19-XIX    cWW  cW-W
   9 A.U50          A.A64          U-A WC           20-XX     cWW  cW-W
  10 A.G51          A.C63          G-C WC           19-XIX    cWW  cW-W
  11 A.U52          A.A62          U-A WC           20-XX     cWW  cW-W
  12 A.G53          A.C61          G-C WC           19-XIX    cWW  cW-W
  13 A.5MU54        A.1MA58        t-a rHoogsteen   24-XXIV   tWH  tW-M
  14 A.PSU55        A.G18          P+G --           n/a       tSW  tm+W
  15 A.C56          A.G19          C-G WC           19-XIX    cWW  cW-W
  ------------------------------------------------------------------------
  helix#2[2] bps=15
```

```
      strand-1 5'-AAPcUGGAgCUCAGu-3'
       bp-type    ...||||.||||...
      strand-2 3'-UcAGACCgCGAGUCU-5'
      helix-form  x..AAAAxAA.xxx
   1 A.A36          A.U33          A-U --           n/a       tHS  tM-m
   2 A.A38          A.OMC32        A-c --           n/a       cW.  cW-.
   3 A.PSU39        A.A31          P-A --           n/a       cWW  cW-W
   4 A.5MC40        A.G30          c-G WC           19-XIX    cWW  cW-W
   5 A.U41          A.A29          U-A WC           20-XX     cWW  cW-W
   6 A.G42          A.C28          G-C WC           19-XIX    cWW  cW-W
   7 A.G43          A.C27          G-C WC           19-XIX    cWW  cW-W
   8 A.A44          A.M2G26        A-g Imino        08-VIII   cWW  cW-W
   9 A.2MG10        A.C25          g-C WC           19-XIX    cWW  cW-W
  10 A.C11          A.G24          C-G WC           19-XIX    cWW  cW-W
  11 A.U12          A.A23          U-A WC           20-XX     cWW  cW-W
  12 A.C13          A.G22          C-G WC           19-XIX    cWW  cW-W
  13 A.A14          A.U8           A-U rHoogsteen   24-XXIV   tHW  tM-W
  14 A.G15          A.C48          G+C rWC          22-XXII   tWW  tW+W
  15 A.H2U16        A.U59          u+U --           n/a       tSW  tm+W

************************************************************************
List of 4 stems
  Note: a stem is defined as a helix consisting of only canonical WC/wobble
        pairs, with a continuous backbone.
      stem#number[#helix-number containing this stem]
      Other terms are defined as in the above Helix section.
      ------------------------------------------------------------------
  stem#1[#1] bps=7
      strand-1 5'-GCGGAUU-3'
       bp-type    |||||||
      strand-2 3'-CGCUUAA-5'
      helix-form  AA....
   1 A.G1           A.C72          G-C WC           19-XIX    cWW  cW-W
   2 A.C2           A.G71          C-G WC           19-XIX    cWW  cW-W
   3 A.G3           A.C70          G-C WC           19-XIX    cWW  cW-W
   4 A.G4           A.U69          G-U Wobble       28-XXVIII cWW  cW-W
   5 A.A5           A.U68          A-U WC           20-XX     cWW  cW-W
   6 A.U6           A.A67          U-A WC           20-XX     cWW  cW-W
   7 A.U7           A.A66          U-A WC           20-XX     cWW  cW-W
  ------------------------------------------------------------------------
  stem#2[#2] bps=4
      strand-1 5'-gCUC-3'
       bp-type    ||||
      strand-2 3'-CGAG-5'
      helix-form  AA.
   1 A.2MG10        A.C25          g-C WC           19-XIX    cWW  cW-W
   2 A.C11          A.G24          C-G WC           19-XIX    cWW  cW-W
   3 A.U12          A.A23          U-A WC           20-XX     cWW  cW-W
   4 A.C13          A.G22          C-G WC           19-XIX    cWW  cW-W
  ------------------------------------------------------------------------
  stem#3[#2] bps=4
      strand-1 5'-CCAG-3'
       bp-type    ||||
      strand-2 3'-GGUc-5'
      helix-form  AAA
   1 A.C27          A.G43          C-G WC           19-XIX    cWW  cW-W
   2 A.C28          A.G42          C-G WC           19-XIX    cWW  cW-W
   3 A.A29          A.U41          A-U WC           20-XX     cWW  cW-W
   4 A.G30          A.5MC40        G-c WC           19-XIX    cWW  cW-W
  ------------------------------------------------------------------------
  stem#4[#1] bps=5
      strand-1 5'-cUGUG-3'
       bp-type    |||||
```

```
      strand-2 3'-GACAC-5'
      helix-form  AAAA
   1 A.5MC49        A.G65          c-G WC           19-XIX    cWW  cW-W
   2 A.U50          A.A64          U-A WC           20-XX     cWW  cW-W
   3 A.G51          A.C63          G-C WC           19-XIX    cWW  cW-W
   4 A.U52          A.A62          U-A WC           20-XX     cWW  cW-W
   5 A.G53          A.C61          G-C WC           19-XIX    cWW  cW-W

*************************************************************************
List of 1 isolated WC/wobble pair
  Note: isolated WC/wobble pairs are assigned negative indices to
        differentiate them from the stem numbers, which are positive.
        ---------------------------------------------------------------
[#1]     -1 A.G19          A.C56          G-C WC           19-XIX    cWW  cW-W

*************************************************************************
List of 2 coaxial stacks
   1 Helix#1 contains 2 stems: [#1,#4]
   2 Helix#2 contains 2 stems: [#3,#2]

*************************************************************************
List of 92 non-pairing interactions
   1 A.G1           A.C2           stacking: 5.4(2.6)--pm(>>,forward) H-bonds[1]: "OP2*OP2
     ↪ [2.99]"
   2 A.G1           A.A73          stacking: 2.4(1.2)--mm(<>,outward)
   3 A.C2           A.G3           stacking: 0.5(0.0)--pm(>>,forward)
   4 A.G3           A.G4           stacking: 3.2(1.8)--pm(>>,forward)
   5 A.G3           A.G71          stacking: 2.6(0.3)--mm(<>,outward)
   6 A.G4           A.A5           stacking: 5.6(3.5)--pm(>>,forward)
   7 A.A5           A.U6           stacking: 5.9(4.3)--pm(>>,forward)
   8 A.U6           A.U7           stacking: 0.6(0.0)--pm(>>,forward)
   9 A.U7           A.5MC49        stacking: 1.2(0.0)--pm(>>,forward) H-bonds[1]: "O2'(
     ↪ hydroxyl)-OP2[2.68]"
  10 A.U8           A.C13          stacking: 2.0(0.0)--pp(><,inward)
  11 A.U8           A.G15          stacking: 0.5(0.0)--mm(<>,outward)
  12 A.A9           A.C11          H-bonds[1]: "O2'(hydroxyl)-N4(amino)[2.90]"
  13 A.A9           A.C13          H-bonds[1]: "OP2-N4(amino)[3.01]"
  14 A.A9           A.G22          stacking: 0.1(0.0)--mp(<<,backward)
  15 A.A9           A.G45          stacking: 1.6(0.5)--pp(><,inward)
  16 A.A9           A.7MG46        stacking: 1.6(0.7)--mm(<>,outward) H-bonds[1]: "O5'-N2(
     ↪ amino)[3.34]"
  17 A.2MG10        A.C11          stacking: 4.2(1.3)--pm(>>,forward)
  18 A.2MG10        A.M2G26        stacking: 1.0(0.0)--mm(<>,outward)
  19 A.C11          A.U12          stacking: 0.9(0.0)--pm(>>,forward)
  20 A.U12          A.C13          stacking: 1.3(0.3)--pm(>>,forward)
  21 A.A14          A.G15          stacking: 2.4(0.8)--pm(>>,forward)
  22 A.A14          A.G22          stacking: 1.9(0.1)--mm(<>,outward)
  23 A.G15          A.H2U16        stacking: 0.4(0.0)--pm(>>,forward)
  24 A.G15          A.U59          stacking: 0.4(0.0)--pm(>>,forward)
  25 A.H2U16        A.C60          stacking: 1.4(0.0)--pm(>>,forward) H-bonds[1]: "O2'(
     ↪ hydroxyl)-N3[3.46]"
  26 A.H2U17        A.G18          H-bonds[1]: "O2'(hydroxyl)-OP1[2.97]"
  27 A.G18          A.G57          stacking: 4.3(1.5)--pp(><,inward) H-bonds[3]: "O3'-N2(
     ↪ amino)[3.29],O2'(hydroxyl)-N1(imino)[3.04],O2'(hydroxyl)-N2(amino)[2.71]"
  28 A.G18          A.1MA58        stacking: 8.3(3.6)--mm(<>,outward) H-bonds[2]: "N2(
     ↪ amino)-O5'[3.22],N2(amino)-O4'[3.11]"
  29 A.G19          A.G57          stacking: 3.3(0.9)--mm(<>,outward) H-bonds[1]: "O4'-N2(
     ↪ amino)[3.17]"
  30 A.G19          A.C60          H-bonds[1]: "OP1-N4(amino)[3.27]"
  31 A.G20          A.A21          H-bonds[1]: "OP1*OP2[2.74]"
  32 A.G20          A.G22          H-bonds[1]: "N2(amino)-O4'[3.24]"
  33 A.A21          A.G22          H-bonds[1]: "O2'(hydroxyl)-O4'[3.44]"
  34 A.A21          A.7MG46        stacking: 5.0(2.1)--pp(><,inward)
```

```
  35 A.A21           A.C48           stacking: 5.9(2.9)--mm(<>,outward)
  36 A.G22           A.A23           stacking: 1.1(0.1)--pm(>>,forward)
  37 A.A23           A.G24           stacking: 4.1(3.3)--pm(>>,forward)
  38 A.G24           A.C25           stacking: 7.5(4.2)--pm(>>,forward)
  39 A.C25           A.M2G26         stacking: 2.0(1.0)--pm(>>,forward)
  40 A.M2G26         A.C27           stacking: 6.8(3.6)--pm(>>,forward)
  41 A.C27           A.C28           stacking: 0.9(0.1)--pm(>>,forward)
  42 A.C28           A.G43           stacking: 0.2(0.0)--mm(<>,outward)
  43 A.A29           A.G30           stacking: 2.4(2.2)--pm(>>,forward)
  44 A.A29           A.G42           stacking: 2.8(1.6)--mm(<>,outward)
  45 A.G30           A.A31           stacking: 6.3(3.5)--pm(>>,forward)
  46 A.G30           A.U41           stacking: 0.8(0.0)--mm(<>,outward)
  47 A.A31           A.OMC32         stacking: 6.2(4.1)--pm(>>,forward)
  48 A.OMC32         A.U33           stacking: 3.6(1.3)--pm(>>,forward)
  49 A.U33           A.A35           H-bonds[1]: "O2'(hydroxyl)-N7[2.37]"
  50 A.U33           A.YYG37         H-bonds[1]: "O2'(hydroxyl)-O22[3.41]"
  51 A.OMG34         A.A35           stacking: 6.0(4.1)--pm(>>,forward) H-bonds[1]: "O2'(
      ↪ hydroxyl)-O4'[3.33]"
  52 A.A35           A.A36           stacking: 4.7(2.1)--pm(>>,forward)
  53 A.A36           A.YYG37         stacking: 5.3(3.9)--pm(>>,forward) H-bonds[4]: "O2'(
      ↪ hydroxyl)-O4'[2.49],N6(amino)-O17[3.25],N6(amino)*N20[2.94],N6(amino)-O22[3.25]"
  54 A.YYG37         A.A38           stacking: 7.7(3.5)--pm(>>,forward)
  55 A.A38           A.PSU39         stacking: 5.9(4.1)--pm(>>,forward)
  56 A.PSU39         A.5MC40         stacking: 5.4(1.1)--pm(>>,forward)
  57 A.G42           A.G43           stacking: 3.3(1.8)--pm(>>,forward)
  58 A.G43           A.A44           stacking: 4.7(2.9)--pm(>>,forward)
  59 A.A44           A.G45           stacking: 5.4(2.5)--pm(>>,forward)
  60 A.7MG46         A.C48           H-bonds[1]: "O2'(hydroxyl)-OP2[3.55]"
  61 A.U47           A.5MC49         H-bonds[1]: "O2'(hydroxyl)-O3'[3.21]"
  62 A.U47           A.U50           H-bonds[1]: "O2'(hydroxyl)-OP1[2.71]"
  63 A.C48           A.5MC49         H-bonds[1]: "O2'(hydroxyl)-OP1[3.13]"
  64 A.C48           A.U59           H-bonds[1]: "O2'(hydroxyl)-O2'(hydroxyl)[3.07]"
  65 A.U50           A.G51           stacking: 0.4(0.0)--pm(>>,forward)
  66 A.U50           A.G65           stacking: 0.4(0.0)--mm(<>,outward)
  67 A.G51           A.U52           stacking: 6.8(4.0)--pm(>>,forward)
  68 A.G51           A.A64           stacking: 2.5(1.1)--mm(<>,outward)
  69 A.G53           A.5MU54         stacking: 7.9(3.4)--pm(>>,forward)
  70 A.G53           A.A62           stacking: 4.2(2.0)--mm(<>,outward)
  71 A.5MU54         A.PSU55         stacking: 5.7(2.2)--pm(>>,forward)
  72 A.PSU55         A.G57           H-bonds[1]: "O2'(hydroxyl)-N7[2.72]"
  73 A.PSU55         A.1MA58         H-bonds[1]: "N3-OP2[2.77]"
  74 A.C56           A.G57           stacking: 1.9(1.2)--pm(>>,forward)
  75 A.1MA58         A.C60           H-bonds[1]: "O2'(hydroxyl)-OP2[2.42]"
  76 A.1MA58         A.C61           stacking: 4.8(1.3)--pm(>>,forward)
  77 A.U59           A.C60           stacking: 6.7(4.2)--pm(>>,forward)
  78 A.C60           A.C61           H-bonds[1]: "OP1-N4(amino)[3.12]"
  79 A.A62           A.C63           stacking: 4.7(3.0)--pm(>>,forward)
  80 A.C63           A.A64           stacking: 0.6(0.0)--pm(>>,forward)
  81 A.A64           A.G65           stacking: 4.0(2.9)--pm(>>,forward)
  82 A.G65           A.A66           stacking: 3.3(1.7)--pm(>>,forward)
  83 A.A66           A.A67           stacking: 4.7(3.9)--pm(>>,forward)
  84 A.A67           A.U68           stacking: 4.5(3.1)--pm(>>,forward)
  85 A.U68           A.U69           stacking: 2.6(1.0)--pm(>>,forward)
  86 A.U69           A.C70           stacking: 0.4(0.0)--pm(>>,forward) H-bonds[1]: "O2'(
      ↪ hydroxyl)-O4'[3.16]"
  87 A.C70           A.G71           stacking: 1.4(0.2)--pm(>>,forward)
  88 A.G71           A.C72           stacking: 7.4(4.2)--pm(>>,forward)
  89 A.C72           A.A73           stacking: 0.3(0.1)--pm(>>,forward)
  90 A.A73           A.C74           stacking: 6.0(4.0)--pm(>>,forward)
  91 A.C74           A.C75           stacking: 4.8(2.5)--pm(>>,forward)
  92 A.C75           A.A76           H-bonds[1]: "O5'*OP1[3.27]"

*************************************************************************
```

```
List of 11 stacks
  Note: a stack is an ordered list of nucleotides assembled together via
        base-stacking interactions, regardless of backbone connectivity.
        Stacking interactions within a stem are *not* included.
        ------------------------------------------------------------------
   1 nts=2 Uc A.U7,A.5MC49
   2 nts=2 UC A.U8,A.C13
   3 nts=2 GA A.G65,A.A66
   4 nts=3 CgC A.C25,A.M2G26,A.C27
   5 nts=3 gAC A.7MG46,A.A21,A.C48
   6 nts=3 GtP A.G53,A.5MU54,A.PSU55
   7 nts=4 GACC A.G1,A.A73,A.C74,A.C75
   8 nts=4 GAcU A.G30,A.A31,A.OMC32,A.U33
   9 nts=5 GGGaC A.G19,A.G57,A.G18,A.1MA58,A.C61
  10 nts=7 gAAgAPc A.OMG34,A.A35,A.A36,A.YYG37,A.A38,A.PSU39,A.5MC40
  11 nts=9 GAGAGAGUC A.G43,A.A44,A.G45,A.A9,A.G22,A.A14,A.G15,A.U59,A.C60
     ------------------------------------------------------------------
  Nucleotides not involved in stacking interactions
     nts=4 uGUA A.H2U17,A.G20,A.U47,A.A76

****************************************************************************
Note: for the various types of loops listed below, numbers within the first
      set of brackets are the number of loop nts, and numbers in the second
      set of brackets are the identities of the stems (positive number) or
      isolated WC/wobble pairs (negative numbers) to which they are linked.

****************************************************************************
List of 3 hairpin loops
   1 hairpin loop: nts=10; [8]; linked by [#2]
     nts=10 CAGuuGGGAG A.C13,A.A14,A.G15,A.H2U16,A.H2U17,A.G18,A.G19,A.G20,A.A21,A.G22
       nts=8 AGuuGGGA A.A14,A.G15,A.H2U16,A.H2U17,A.G18,A.G19,A.G20,A.A21
   2 hairpin loop: nts=11; [9]; linked by [#3]
     nts=11 GAcUgAAgAPc A.G30,A.A31,A.OMC32,A.U33,A.OMG34,A.A35,A.A36,A.YYG37,A.A38,A.
         ↪ PSU39,A.5MC40
       nts=9 AcUgAAgAP A.A31,A.OMC32,A.U33,A.OMG34,A.A35,A.A36,A.YYG37,A.A38,A.PSU39
   3 hairpin loop: nts=9; [7]; linked by [#4]
     nts=9 GtPCGaUCC A.G53,A.5MU54,A.PSU55,A.C56,A.G57,A.1MA58,A.U59,A.C60,A.C61
       nts=7 tPCGaUC A.5MU54,A.PSU55,A.C56,A.G57,A.1MA58,A.U59,A.C60

****************************************************************************
List of 1 junction
   1 4-way junction: nts=16; [2,1,5,0]; linked by [#1,#2,#3,#4]
     nts=16 UUAgCgCGAGgUCcGA A.U7,A.U8,A.A9,A.2MG10,A.C25,A.M2G26,A.C27,A.G43,A.A44,A.G45,
         ↪ A.7MG46,A.U47,A.C48,A.5MC49,A.G65,A.A66
       nts=2 UA A.U8,A.A9
       nts=1 g A.M2G26
       nts=5 AGgUC A.A44,A.G45,A.7MG46,A.U47,A.C48
       nts=0

****************************************************************************
List of 1 non-loop single-stranded segment
   1 nts=4 ACCA A.A73,A.C74,A.C75,A.A76

****************************************************************************
List of 1 kissing loop interaction
   1 isolated-pair #-1 between hairpin loops #1 and #3

****************************************************************************
List of 2 U-turns
   1  A.U33-A.A36 H-bonds[1]: "N3(imino)-OP2[2.80]" nts=6 cUgAAg A.OMC32,A.U33,A.OMG34,A.
       ↪ A35,A.A36,A.YYG37
   2  A.PSU55-A.1MA58 H-bonds[1]: "N3-OP2[2.77]" nts=6 tPCGaU A.5MU54,A.PSU55,A.C56,A.G57,
       ↪ A.1MA58,A.U59
```

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362
363 ****************************************************************************
364 List of 18 phosphate interactions
365    1 A.U7             OP1-hbonds[1]: "MG@A.MG580[2.60]"
366    2 A.A9             OP2-hbonds[1]: "N4@A.C13[3.01]"
367    3 A.A14            OP2-hbonds[1]: "MG@A.MG580[1.93]"
368    4 A.H2U16          OP2-cap: "A.H2U16"
369    5 A.G18            OP1-hbonds[1]: "O2'@A.H2U17[2.97]"
370    6 A.G19            OP1-hbonds[2]: "N4@A.C60[3.27],MN@A.MN530[2.19]"
371    7 A.G20            OP1-hbonds[1]: "MG@A.MG540[2.07]"
372    8 A.A21            OP2-hbonds[1]: "MG@A.MG540[2.11]"
373    9 A.A23            OP2-hbonds[1]: "N6@A.A9[3.12]"
374   10 A.A35            OP2-cap: "A.U33"
375   11 A.A36            OP2-hbonds[1]: "N3@A.U33[2.80]"
376   12 A.YYG37          OP2-hbonds[1]: "MG@A.MG590[2.53]"
377   13 A.C48            OP2-hbonds[1]: "O2'@A.7MG46[3.55]"
378   14 A.5MC49          OP1-hbonds[1]: "O2'@A.C48[3.13]" OP2-hbonds[1]: "O2'@A.U7[2.68]"
379   15 A.U50            OP1-hbonds[1]: "O2'@A.U47[2.71]"
380   16 A.G57            OP2-cap: "A.PSU55"
381   17 A.1MA58          OP2-hbonds[1]: "N3@A.PSU55[2.77]"
382   18 A.C60            OP1-hbonds[1]: "N4@A.C61[3.12]" OP2-hbonds[1]: "O2'@A.1MA58[2.42]"
383
384 ****************************************************************************
385 This structure contains 1-order pseudoknot
386    o You may want to run DSSR again with the '--nested' option which removes
387      pseudoknots to get a fully nested secondary structure representation.
388
389 ****************************************************************************
390 Secondary structures in dot-bracket notation (dbn) as a whole and per chain
391 >1ehz nts=76 [whole]
392 GCGGAUUUAgCUCAGuuGGGAGAGCgCCAGAcUgAAgAPcUGGAGgUCcUGUGtPCGaUCCACAGAAUUCGCACCA
393 (((((((..((((.....[..)))).((((.........)))).....((((((..]....)))))))))))....
394 >1ehz-A #1 nts=76 [chain] RNA
395 GCGGAUUUAgCUCAGuuGGGAGAGCgCCAGAcUgAAgAPcUGGAGgUCcUGUGtPCGaUCCACAGAAUUCGCACCA
396 (((((((..((((.....[..)))).((((.........)))).....((((((..]....)))))))))))....
397
398 ****************************************************************************
399 List of 12 additional files
400    1 dssr-stems.pdb -- an ensemble of stems
401    2 dssr-helices.pdb -- an ensemble of helices (coaxial stacking)
402    3 dssr-pairs.pdb -- an ensemble of base pairs
403    4 dssr-multiplets.pdb -- an ensemble of multiplets
404    5 dssr-hairpins.pdb -- an ensemble of hairpin loops
405    6 dssr-junctions.pdb -- an ensemble of junctions (multi-branch)
406    7 dssr-2ndstrs.bpseq -- secondary structure in bpseq format
407    8 dssr-2ndstrs.ct -- secondary structure in connect table format
408    9 dssr-2ndstrs.dbn -- secondary structure in dot-bracket notation
409   10 dssr-torsions.txt -- backbone torsion angles and suite names
410   11 dssr-Uturns.pdb -- an ensemble of U-turn motifs
411   12 dssr-stacks.pdb -- an ensemble of stacks
```