## SUPPLEMENTARY INFORMATION

# Structural basis for the dual U4 and U4atac snRNA-binding specificity of spliceosomal protein hPrp31

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**Running Head**

Dual RNA-binding specificity of hPrp31

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# SUPPLEMENTAL FIGURE LEGENDS

## SUPPLEMENTAL FIGURE 1

Final $2F_o$-$F_c$ electron densities (gray meshes) contoured at the 1σ level. (**A**) Monomeric complex. (**B**) Dimeric complex.

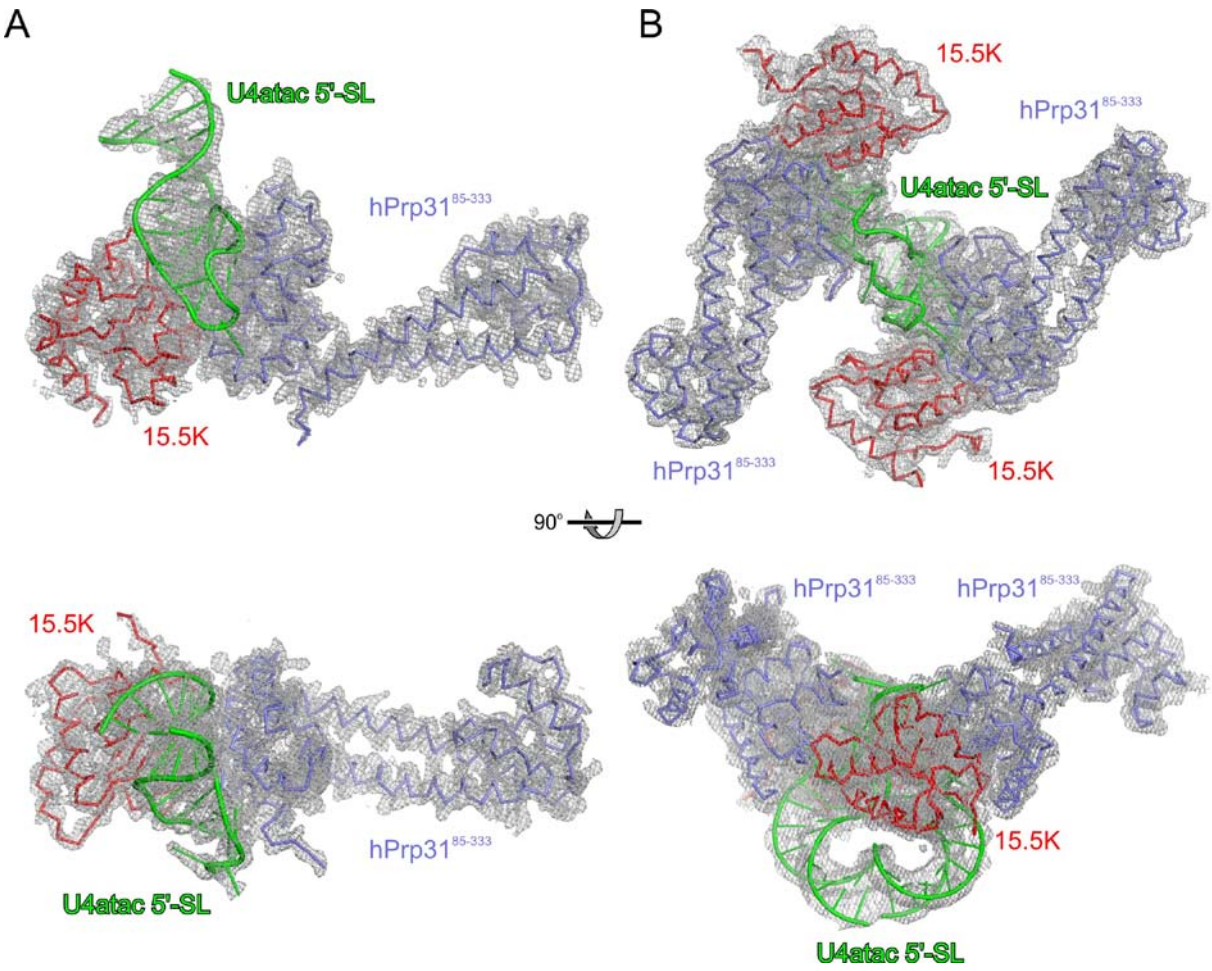
## SUPPLEMENTAL FIGURE 2

15.5K-RNA and 15.5K-Prp31 interactions. (**A**, **B**) Stereo ribbon plots showing the interaction of 15.5K with the K-turns of U4atac 5'SL (**A**) and U4 5'SL (**B**). Three RNA-binding loops in 15.5K (between strand β1 and helix α2, between strand β2 and helix α3 and between helix α4 and strand β4) are shown in cyan. RNA regions are color-coded. Stem I – beige; K-turn – green (U4atac) or gold (U4); stem II – brown; pentaloop – gray. Glu61 (15.5K) and the bulged U36 (U4atac) and U31 (U4), which engage in hydrogen bonding interactions, are shown as sticks and are colored by atom type. Carbon and phosphorus – as the respective molecule; nitrogen – blue; oxygen – red. Rotated 180° about the vertical axis compared to Fig. 1B. (**C**, **D**) Ribbon plots showing the conserved interactions between proteins 15.5K and hPrp31 in the U4atac (**C**) and U4 (**D**) complexes. Coloring as before. Selected residues engaging in interactions are shown as sticks, colored by atom type and labeled. Dashed lines indicate hydrogen bonds or salt bridges. Rotated 90° about the horizontal axis compared to Fig. 1B.

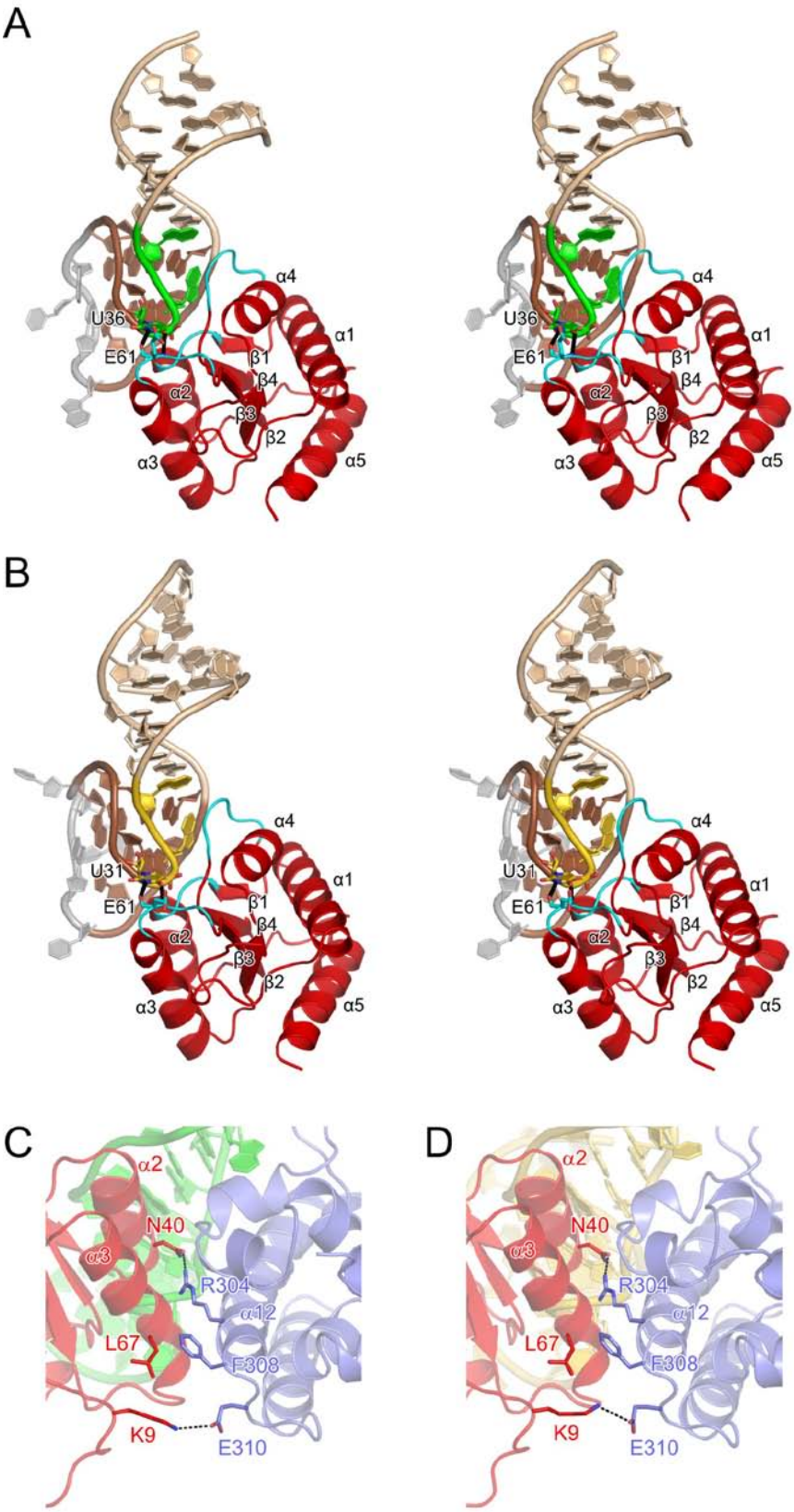
## SUPPLEMENTAL FIGURE 3

RNA domain swap. (**A**) Elution profile a of hPrp31$^{85\text{-}333}$-15.5K-U4atac 5'SL complex separated by gel filtration. Two distinct peak fractions were observed, which correspond to monomeric (Low-MW) and dimeric (High-MW) complexes, respectively. The gel was first stained with Coomassie and subsequently with silver. Below the gel is a schematic representation of the dimeric and monomeric assemblies, illustrating the domain swap in the RNA of the dimeric complex. (**B**) Stereo ribbon plot showing an overlay of the U4atac snRNA

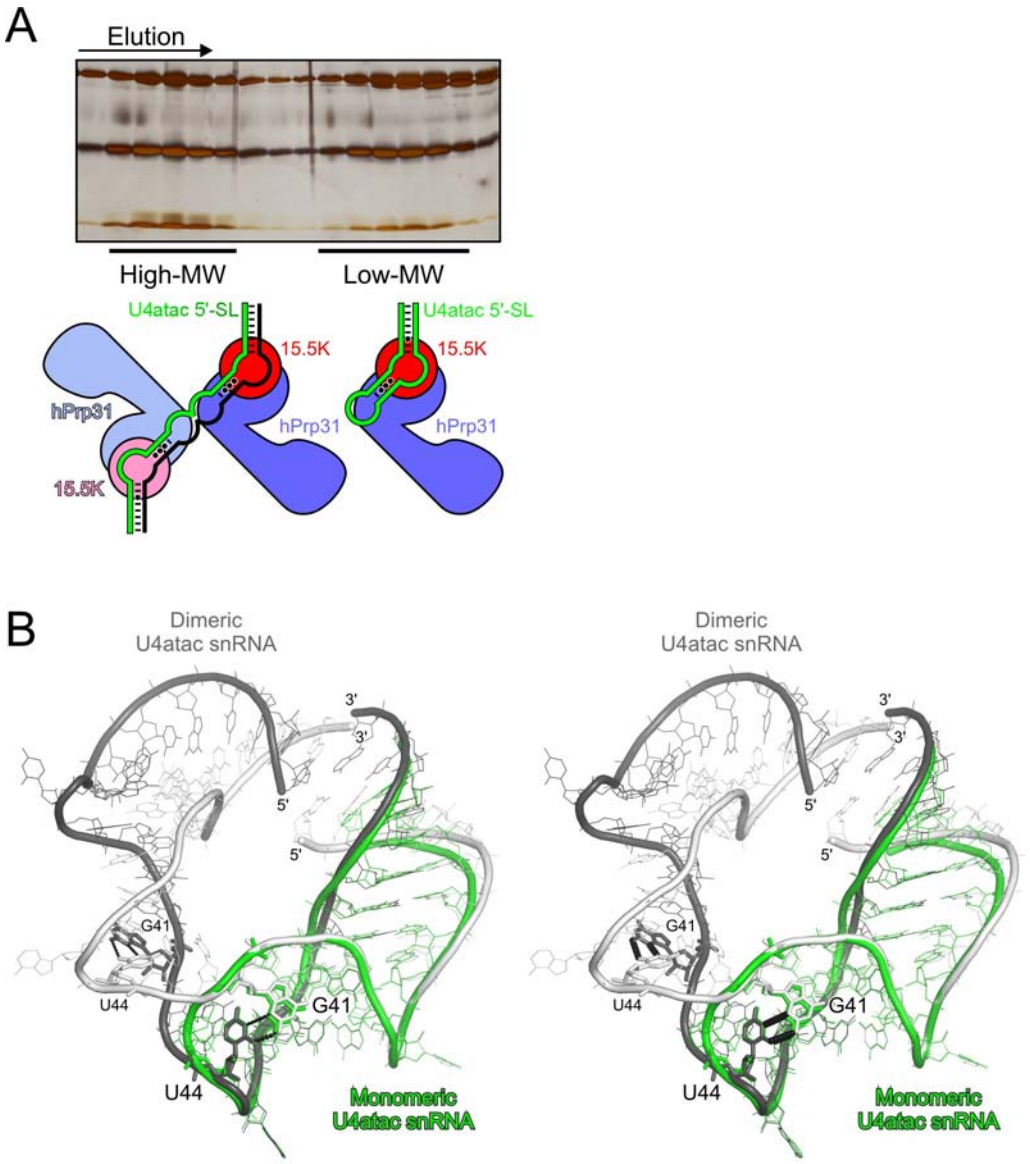
of the monomeric complex (green) and of the dimeric complex (light and dark gray). Nucleotides are shown by fine lines. The non-canonical base pairs between G41 and U44 nucleotides, which are present in the monomeric RNA as well as in the domain-swapped dimeric RNA, are shown as sticks with hydrogen bonds indicated by dashed lines. RNA termini are labeled. The monomeric RNA is rotated 90° about the vertical axis compared to Fig. 1B.




Supplemental Figure 1




Supplemental Figure 2




Supplemental Figure 3