Supplementary material

Table 1: Comparison of distances between the crystal structure, the NMR structure by Van Melckebeke *et al*. and the model by Beaurain et al. *(1,2)*. Differences in comparison to the crystal structure are indicated in bracket.

Geometric parameters	X-Ray	NMR	Molecular Dynamics
Turns			
C5(P)-U7(P)	5.73	5.25 ± 0.08 *(-0.48)*	5.47 *(-0.26)*
C5(P)-G8(P)	10.35	9.37 ± 0.12 *(-0.98)*	8.42 *(-1.93)*
G5*(P)-C7*(P)	5.72	9.61 ± 0.38 *(+3.89)*	5.35 *(-0.37)*
G5*(P)-C8*(P)	10.58	14.32 ± 0.47 *(+3.74)*	9.4 *(-1.18)*
G5*(P)-A12*(P)	18.59	20.76 ± 0.18 *(+2.17)*	18.29 *(-0.30)*
U6*(P)-A11(P)	17.17	21.00 ± 0.18 *(+3.83)*	17.4 *(-0.23)*
G5*•A12* pair			
N1(G*)-N1(A*)	2.91	2.83 ± 0.01 *(-0.09)*	3.15 *(+0.19)*
O6(G*)-N6(A*)	2.99	2.57 ± 0.04 *(-0.42)*	2.85 *(-0.14)*
C1'(G*)-C1'(A*)	12.74	12.60 ± 0.01 *(-0.14)*	13.06 *(+0.17)*
Hydrogen bonds			
G5*(O2')-C5(O3')	3.38	2.60 ± 0.11 *(-0.78)*	5.55 *(+2.17)*
G5*(O2')-C6(O5')	4.69	2.23 ± 0.01 *(-2.42)*	4.55 *(-0.14)*
G5*(O2')-C6(O1p)	4.47	4.13 ± 0.06 *(-0.34)*	3.61 *(-0.86)*
G5*(O2')-C6(O2p)	2.57	2.86 ± 0.14 *(+0.29)*	5.79 *(+3.22)*
C5(O2')-U6*(O1p)	3.30	3.37 ± 0.57 *(+0.07)*	4.18 *(+0.88)*
C5(O2')-U6*(O2p)	2.79	5.04 ± 0.19 *(+2.25)*	5.55 *(+2.76)*

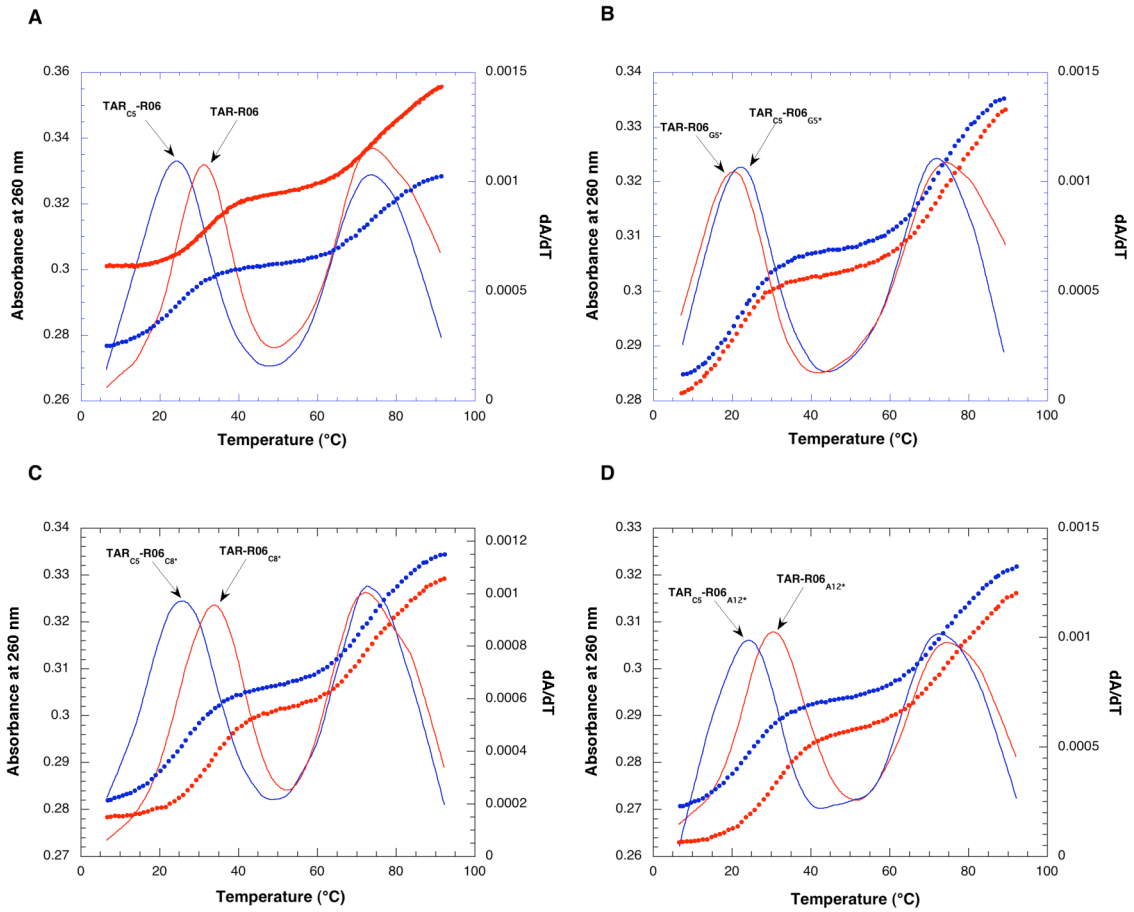

Figure 1: Melting transitions and first derivative curves for TAR-R06 modified complexes. The experiments were performed at 1 μM or each RNA in a 10 mM sodium phosphate buffer, pH 7.2 at 20 °C, containing 140 mM potassium chloride, 20 mM sodium chloride and 0.3 mM magnesium. Denaturation of the samples was achieved by increasing the temperature at a 0.4 °C/min rate from 5 °C to 95 °C and was followed at 260 nm. A) Thermal denaturation of TAR-R06 (red curves) and TAR_{C5}-R06 (blue curves) complexes. B) Thermal denaturation of TAR-$R06_{G5*}$ (red curves) and TAR_{C5}-$R06_{G5*}$ (blue curves) complexes. C) Thermal denaturation of TAR-$R06_{C8*}$ (red curves) and TAR_{C5}-$R06_{C8*}$ (blue curves) complexes. D) Thermal denaturation of TAR-$R06_{A12*}$ (red curves) and TAR_{C5}-$R06_{A12*}$ (blue curves) complexes. Subscripts refer to 2'-O-methyl residues at the indicated positions (see Figure 1A).

1. Beaurain, F., Di Primo, C., Toulmé, J.J. and Laguerre, M. (2003) Molecular dynamics reveals the stabilizing role of loop closing residues in kissing interactions: comparison between TAR-TAR* and TAR-aptamer. *Nucleic Acids Res*, **31**, 4275-4284.

2. Van Melckebeke, H., Devany, M., Di Primo, C., Beaurain, F., Toulmé, J.J., Bryce, D.L. and Boisbouvier, J. (2008) Liquid-crystal NMR structure of HIV TAR RNA bound to its SELEX RNA aptamer reveals the origins of the high stability of the complex. *Proc. Natl. Acad. Sci USA*, **105**, 9210-9215.