

Supporting Information

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Evidence that Electrostatic Interactions Dictate the Ligand-Induced Arrest of RNA Global Flexibility**

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Figure S1. Correlation plot between one bond C1'H1', C2H2, C5H5, C6H6, C8H8, N1H1, and N3H3 RDCs measured using NMR frequency experiments in which splitting are measured along the direct $({}^{1}\text{H})$ or indirect $({}^{1}\text{C}/{}^{15}\text{N})$ dimension (see ref 7d) for a) TAR-NeoB and b) TAR-AcP.

Figure S2. Correlation plot between measured RDCs and values back-calculated using the best fit order tensor for a) TAR-NeoB using NMR model 10 (PDB code 1QD3) and an idealized helix for domains I and II respectively and b) for TAR-AcP using idealized A-form helices for both domains I and II respectively.

Figure S3. Best-fit ϑ values for domains I and II in TAR-AcP determined using idealized A-form helices as input structures in which ~20% of the input RDC data is randomly omitted from the ϑ calculations. Twenty-five such reiterations are shown.

Table S1. RDCs (in Hz) measured in the TAR-NeoB complex (1:2 molar ratios).

Table S2. RDCs (in Hz) measured in the TAR-AcP complex (1:2 molar ratios).





Supporting Figure 3 Pitt et al.



	τ, γ. υ <u>υ</u>
Residue(Stem1)	RDC(Hz)
C19(C5H5)	-10.5
C19(C6H6)	16.5
A20(C1'H1')	-60.2
A20(C2H2)	-5.9
A20(C8H8)	4.6
G21(C1'H1')	-40.9
G21(C8H8)	25.1
G21(N1H1)	-11.8
A22(C2H2)	22.8
A22(C8H8)	31.3
U40(C5H5)	26.7
U40(C6H6)	29.0
C41(C5H5)	36.4
C41(C6H6)	24.4
U42(C1'H1')	38.6
U42(C6H6)	7.9
U42(N3H3)	-7.1
G43(C1'H1')	21.9
G43(C8H8)	1.9
G43(N1H1)	2.8

Residue(Stem2)	RDC(Hz)
G26(C1'H1')	-2.5
G26(C8H8)	35.9
G26(N1H1)	-12.8
A27(C1'H1')	31.7
A27(C2H2)	35.6
A27(C8H8)	25.5
G28(C1'H1')	27.6
G28(C8H8)	15.9
G28(N1H1)	-7.6
C29(C6H6)	18.8
G36(C1'H1')	-57.2
G36(C8H8)	23.2
G36(N1H1)	-8.6
C37(C6H6)	19.9
U38(C6H6)	19.1
U38(N3H3)	-10.0
C39(C5H5)	18.0
C39(C6H6)	33.1

Table S1 TAR-NeoB (1:2) Phage RDCs

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Residue(Stem1)	RDC(Hz)
G18(C1'H1')	-47.1
G18(C8H8)	2.0
G18(N1H1)	-7.5
C19(C6H6)	23.7
A20(C2H2)	22.7
A20(C8H8)	26.6
G21(C8H8)	20.7
G21(N1H1)	-6.3
A22 (C2H2)	18.1
A22(C8H8)	17.3
U40(C5H5)	20.0
C41(C5H5)	16.7
C41(C6H6)	18.7
U42(C1'H1')	27.3
U42(C5H5)	10.5
U42(C6H6)	19.2
U42(N3H3)	-8.2
G43(N1H1)	-10.5
G43(C8H8)	29.1
C44(C5H5)	17.5
C44(C6H6)	8.6

Residue(Stem2)	RDC(Hz)
G26(C1'H1')	-37.9
G26(N1H1)	-14.5
G26(C8H8)	35.9
A27(C1'H1')	-31.8
A27(C2H2)	33.1
A27(C8H8)	27.6
G28(C1'H1')	-26.2
G28(C8H8)	25.2
C29(C6H6)	37.3
G36(C8H8)	43.1
C37(C5H5)	39.1
C37(C6H6)	32.5
U38(C1'H1')	-0.8
U38(N3H3)	-14.5
U38(C5H5)	41.6
U38(C6H6)	27.8
C39(C1'H1')	2.0
C39(C5H5)	28.9
C39(C6H6)	24.0