Structural insights into the cTAR DNA recognition by the HIV-1 Nucleocapsid protein

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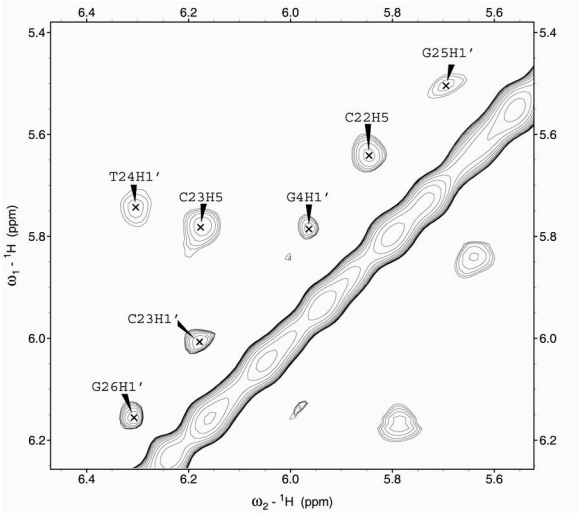
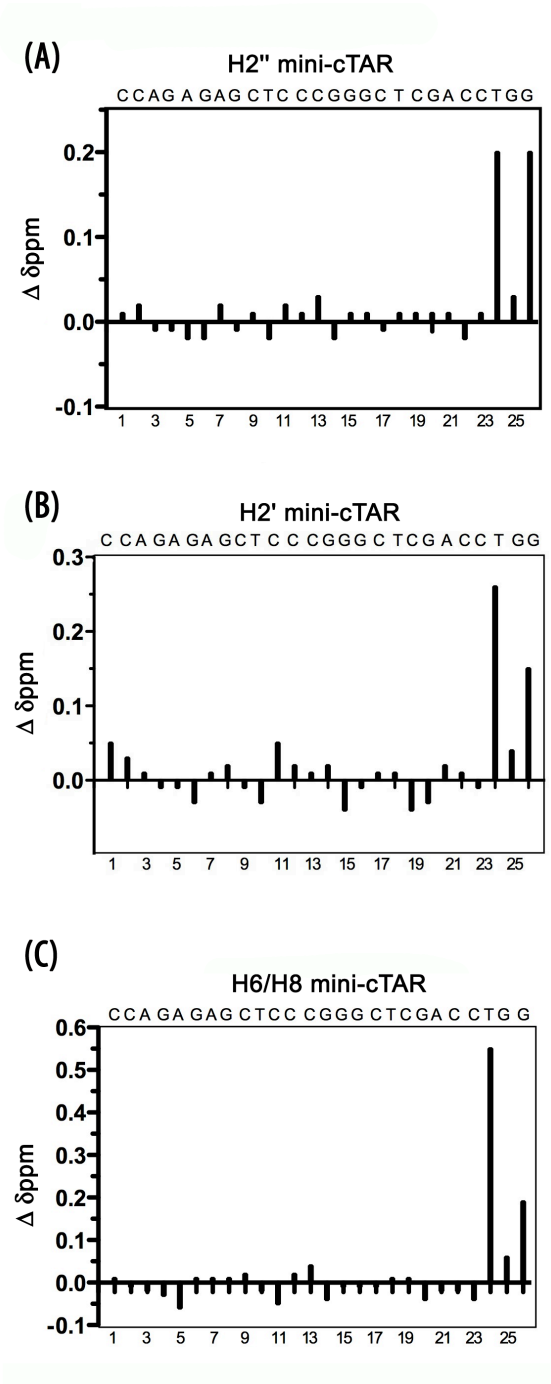
Supplementary Materials

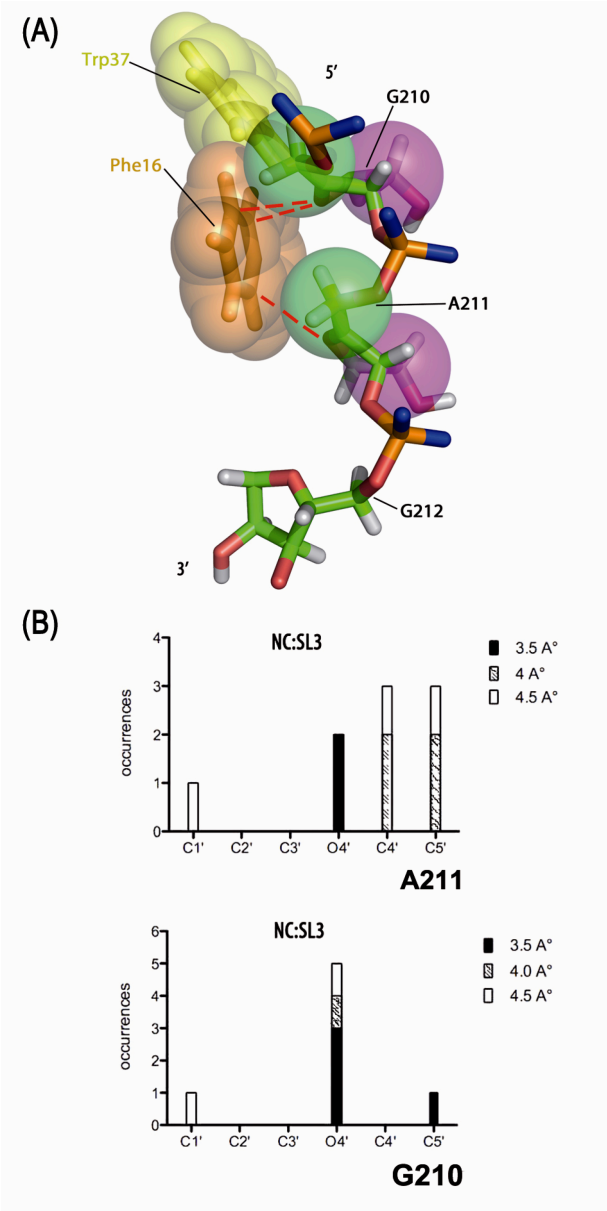
Supplementary Figures



Supplementary Figure S1. Selected region of the TOCSY spectrum recorded at 25°C in H_2O (pH 6.5) for 1 mM of the NC(11-55):mini-cTAR complex showing exchange cross peaks for mini-cTAR in the H1' region.



Supplementary Figure S2. Proton chemical shift changes due to complex formation between mini-cTAR and NC(11-55). **(A)** Chemical shifts changes of H2" proton of mini-cTAR upon NC(11-55) binding. **(B)** Chemical shifts changes of H2' proton of mini-cTAR upon NC(11-55) binding. **(C)** Chemical shifts changes of H6/H8 proton of mini-cTAR upon NC(11-55) binding. The chemical shift differences (in ppm) are obtained by taking the difference between the bound (1:1 complex) and the free forms.



Supplementary Figure S3. **(A)** View of the NC:SL3 complex (50) displaying the contacts involving ribose rings. Protein side chains in close contact with riboses are displayed as spheres. For a better visualization of the contacts, the nucleobases are not represented. In the sugar, the C2' and C5' atoms are displayed as violet and green spheres. Close contacts involving O4' ribose are indicated by dotted red lines**. (B)** Cumulative numbers of protein-nucleic acid contacts involving sugar atoms in the NC:SL3 complex. The contacts with sugars involve atoms C1', C2', O4', C3', C4' and C5'. The contacts were counted within three cutoff distances: 3.5 Å (black areas in the bars), 4.0 Å (hatched areas), and 4.5 Å (white areas).