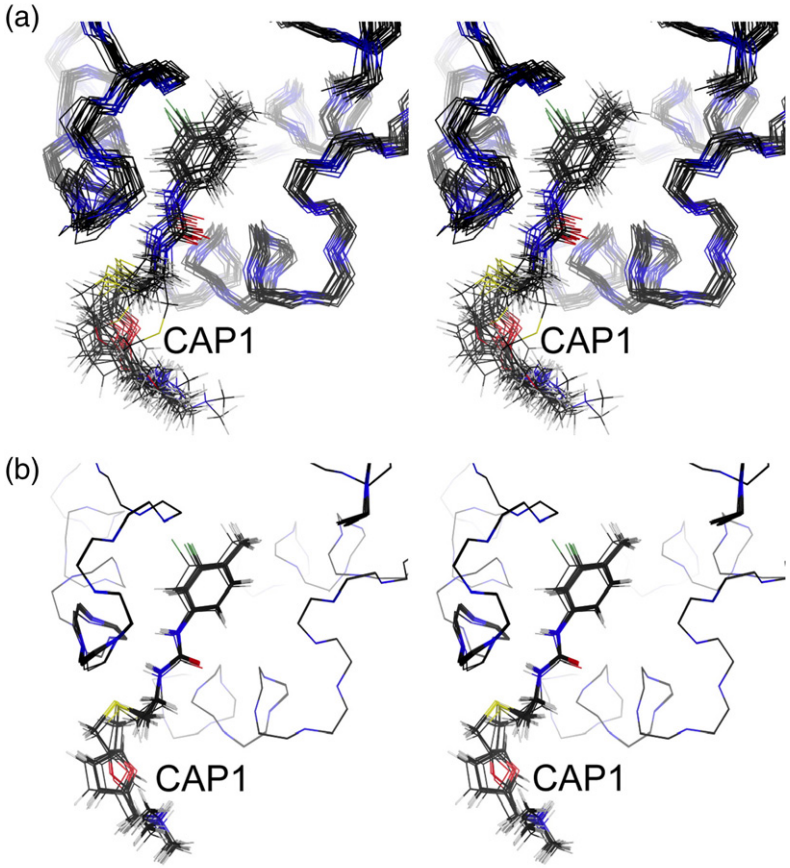

Figure 3. CAP-1:CA^N structures calculated by restrained molecular dynamics with AMBER using the hybrid X-ray/NMR approach. (a) Ensemble of 20 structures calculated after equilibration at 350 K using NOESY NMR-derived distance restraints. The positions of CA^N atoms with well-defined electron density were restrained to coordinates of the crystal structure. (b) Ensemble of 20 refined models obtained by energy minimization after cooling to 0 K.

been derived by docking high resolution CA^N and CA^C structures into EM reconstructions of *in vitro* assembled CA tubes[14] and 2D crystalline sheets (M. Yeager, personal communication). A crystal structure of Moloney murine leukaemia virus (MLV) CA^N also revealed a hexameric assembly[17] that allows construction of a HIV-1 CA^N hexamer by homology modelling (Figure 6). The MLV and HIV-1 CA^N hexamers are stabilized by intermolecular packing interactions between helices H1, H2, and H3, and perhaps also by weak interactions between the six N-terminal β-hairpins at the top of the

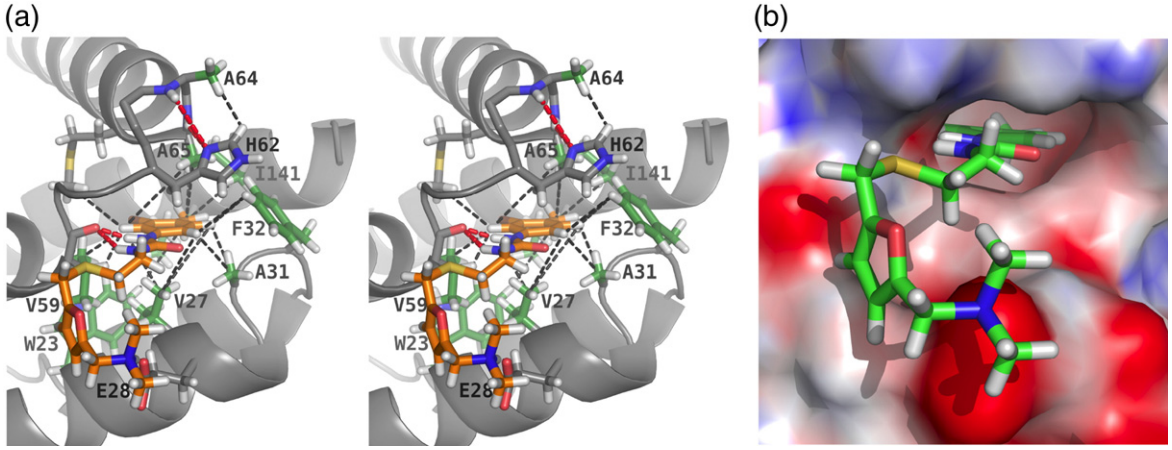

Figure 4. Representative CAP-1:CA^N structure calculated by restrained molecular dynamics using the hybrid X-ray/NMR approach. (a) Stereo view of the CAP-1 binding with observed NOEs (broken black lines) and potential hydrogen bonds (broken red lines) labeled. The side-chain of Phe32, which is displaced from the core upon CAP-1 binding, is also shown. (b) Electrostatic surface representation of the CAP-1 binding site showing the insertion of the CAP-1 aromatic ring into the pocket vacated by Phe32.