energy minimization. Initial CAP-1 coordinates and the associated force field library were generated with X-Leap,[60] which was then used to manually dock the CAP-1 model into the vacant pocket of the X-ray structure. The resulting initial complex was subjected to restrained molecular dynamics at 350 K (50 ps). Atoms of the crystal structure with well-defined electron density were restrained to initial reference coordinates with a 1.0 kcal/mol-Å^2 potential. Other atoms of the crystal structure were unrestrained. Intermolecular NOEs with strong, medium and weak intensities were used to assign upper-limit distance restraints of 2.7, 3.3 and 5.0 Å, respectively, and were implemented with a 20 kcal/mol-Å^2 potential. Restraints involving methyl pseudo-atoms were increased by 0.5 Å.

Atomic coordinates

The atomic coordinates have been deposited in the Protein Data Bank‖. PDB ID codes: 2pxr, CA^N crystallized in the presence of CAP-1; 2pwm, CA^N A92E true cell; 2pwo, CA^N A92E pseudo cell; 2jpr, CAP-1:CAN complex determined by the hybrid NMR/Xray crystallography approach.

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Supplementary Data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.jmb.2007.07.070

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