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1: Biopolymers 1996;40(5):553-9

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Structure and dynamics of the DNA binding protein HU from *Bacillus stearothermophilus* by NMR spectroscopy.

Boelens R, Vis H, Vorgias CE, Wilson KS, Kaptein R.

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The DNA-binding protein HU from *Bacillus stearothermophilus* (HUBst) is a dimer with a molecular weight of 195 kDa that is capable of bending DNA. An x-ray structure has been determined previously [Tanaka et al. 1984] *Nature*, vol. 310, pp. 376-381], but no structure could be established for a large part of the supposed DNA-binding beta-arms. Distance geometry and restrained molecular dynamics using nmr restraints were used to generate a set of 25 structures. These structures display a backbone rms deviation (RMSD) of 0.36 Å for the well-defined region (residues 2-54 and 75-90). The structure of the core is very similar to that observed in the x-ray structure, with a pairwise RMSD of 1.06 Å. The structure of the beta-hairpin arm contains a double flip-over at the prolines in the two strands of the beta-arm. Heteronuclear ¹⁵N relaxation measurements indicate that the beta-arm and the tip of the beta-arm is flexible. This explains the disorder observed in the solution and x-ray structures of the beta-arm with respect to the core of the protein. Overlaid onto itself the beta-arm is better defined, with a backbone RMSD of 1.0 Å calculated for residues 54-59 and 69-74. The tip of the arm adopts a well-defined 4 : 6 beta-hairpin conformation. Changes in amide ¹⁵N and ¹H chemical shifts upon titrating DNA are most pronounced for the residues in the beta-hairpin arm and for the residues in the second half of the third alpha-helix. Heteronuclear ¹⁵N relaxation data for free and complexed HUBst show that that the arms become structured upon

DNA binding. Together with chemically induced nuclear polarization measurements on a mutant HUBst (M69Y; V76Y) this shows that the beta-hairpin arm is involved in direct DNA interaction.

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