

Abstract Submitted  
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**Thermodynamics of the Beta-hairpin to Coil Transition using a Distance Constraint Model**<sup>1</sup> OLEG VOROV, DONALD JACOBS, DENNIS LIVESAY, University of North Caroline, Charlotte — The configuration partition function is calculated exactly [1] for a distance constraint protein model that describes the beta-hairpin to coil transition. The model employs a Gaussian backbone chain of  $N$  atoms in which bonds may form to crosslink pairs of atoms in close proximity along the chain, represented by fluctuating distance constraints. Each distinct pattern of cross-linking bonds defines a constant energy over all atomic geometries that are consistent with the constraint topology. This geometrical degeneracy factor is directly calculated from configuration space integrals for each accessible constraint topology. All constraint topologies consistent with no pair of bonds that link two backbone atoms are themselves crossed are enumerated, leading to an analytical closed form expression for the configuration partition function. The phase diagram for the beta-hairpin to coil transition as a function of chain length has been studied.

[1] O.K.Vorov, D.J.Jacobs, D.R.Livesay, subm. to Phys.Rev.Lett., 2006, in preparation.

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