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Supporting Material

All-Atom Contact Model for Understanding Protein Dynamics from Crystallographic B-factors

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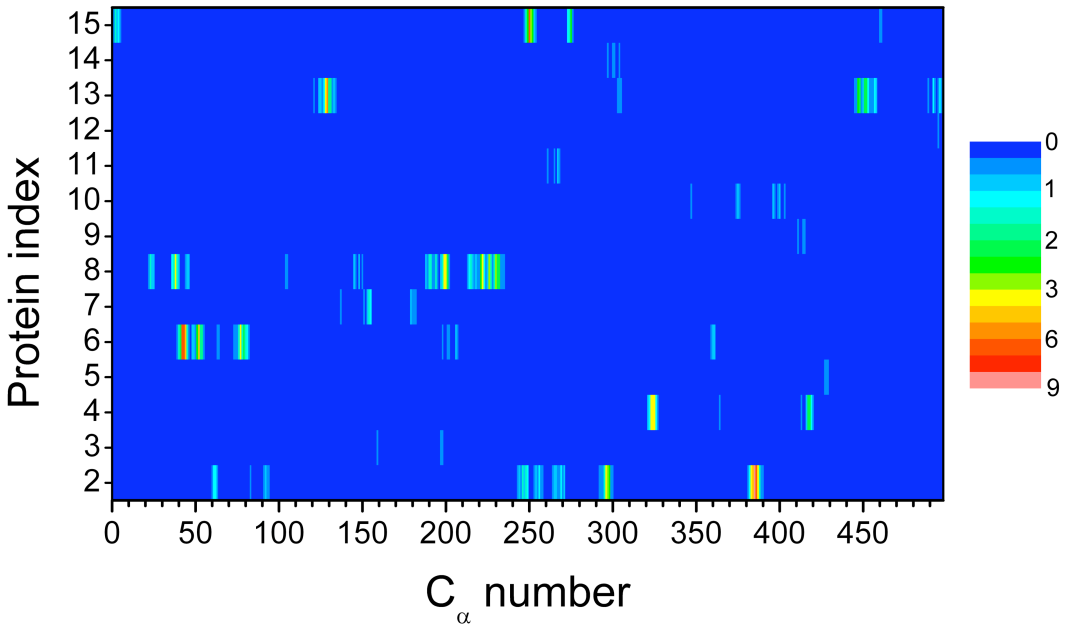

Fig. S1. Contributions to the Cα contact sum by the 14 closest protein neighbors. Note that the color scale is not linear and has two segments. Some Cα atoms have contributions from more than 1 neighboring protein. The surrounding proteins are numbered from 2 - 15.

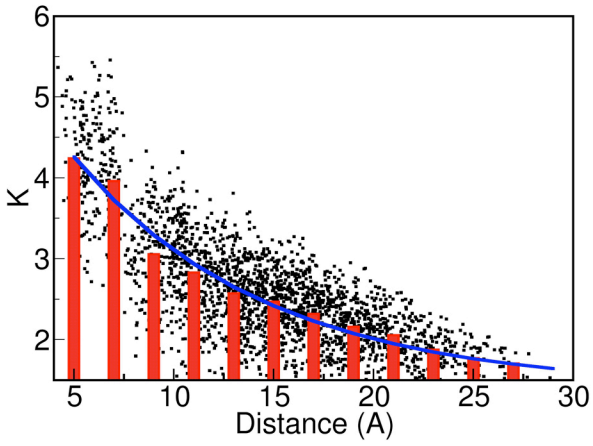

Fig. S2. Force constant K (f_{ij}) as a function of distance r_{ij} between all pairs of Cα atoms of the GNM model applied to Ubiquitin. The black dots are generated from a canonical ensemble using the GNM energy function directly. The red bars are averages over 2 Å distance intervals. The blue is a least-squares fit by the exponential function of Eq. 13.

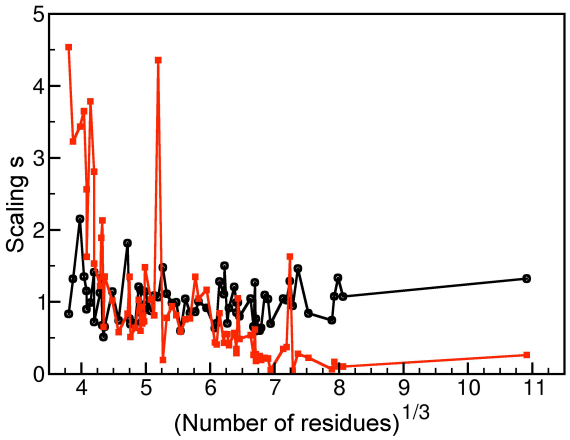

Fig. S3. The overall scaling factor of B-factors as a function of protein size (determined by (number of residues)$^{-1/3}$) for eLCMB (black) and ROM (red).