



Fig S2. The PC modes that best match the dynamics variables of ubiquitin.

(A) The Pearson correlation coefficient between the anisotropic displacement parameters (ADP) profile assembled from all the PC modes higher or equal to a specific mode with the experimental ADP profile (PDB: 2GBJ) is shown in red crosses. Blue circles give correlation coefficients between RMSF profile derived from covariance comprising PC modes higher or equal to a given mode (Eq S8) and RMSF derived from a set of NMR-determined conformers (PDB: 1G6J). In (A), the PC modes are calculated using only $C\alpha$ atoms (coarse-grained). (B) Pearson correlation coefficient between experimental NMR order parameters and order parameters estimated from the PCA of heavy-atoms with the backbone nitrogen's hydrogen atom. The black arrow indicates the PC mode with the highest correlation.