Supplementary material III:

Normal Mode Analysis was carried out using the Elastic Network model developed by Tirion (Tirion, 1996) and further implemented by Tama and Sanejouand (Tama and Sanejouand,2001). The last version of the program was downloaded at the following address: http://ecole.modelisation.free.fr/modes.html. (package 3.73).. Calculations were preformed using default parameters, *i.e.* Cα calculations with 10Å cutoff and an interaction force constant equal to 1. Analysis tools were used to generate trajectories along the hundred lowest-frequencies modes and to compute B-factors (predicted B-factors). Correlations between experimental and predicted B-factors were obtained for the corresponding output. Two sets of 3D structures were examined, the MD dataset that contains ~40 proteins smaller than 200 residues and a set of ~40 proteins larger than 200 residues.

We observed that the relationship between X-Ray B-factors and ENM predicted B-factors (ENM-Bfac) or ENM predicted RMSF (ENM-RMSF) was stronger on average than with MD-RMSF. The average correlation on a per-protein basis (ρ value) between the B-factors and ENM-Bfac reached 0. 66. The values were similar with ENM-RMSF, *i.e.* 0.68, a value larger than observed with MD-RMSF. Depending on the protein, the correlation can range from 0.36 to 0.92. The average correlation between MD-RMSF and ENM-BFac was quite similar but decreased when the simulation was lengthened (0.55). The correlation between ENM B-Factors and MD RMSF equaled 0.68, but decreased with longer simulations or when larger proteins were examined with ρ equal to 0.57 and 0.54 respectively.

References:

Tirion M.M. (1996) "Large amplitude elastic motions in proteins from a single-parameter, atomic analysis", Phys. Rev. letters vol.77(9), p1905-1908

Tama F. and Sanejouand (2001) Y.H. "Conformational change of proteins arising from normal mode calculations" Protein Engineering.**14**, p1-6.