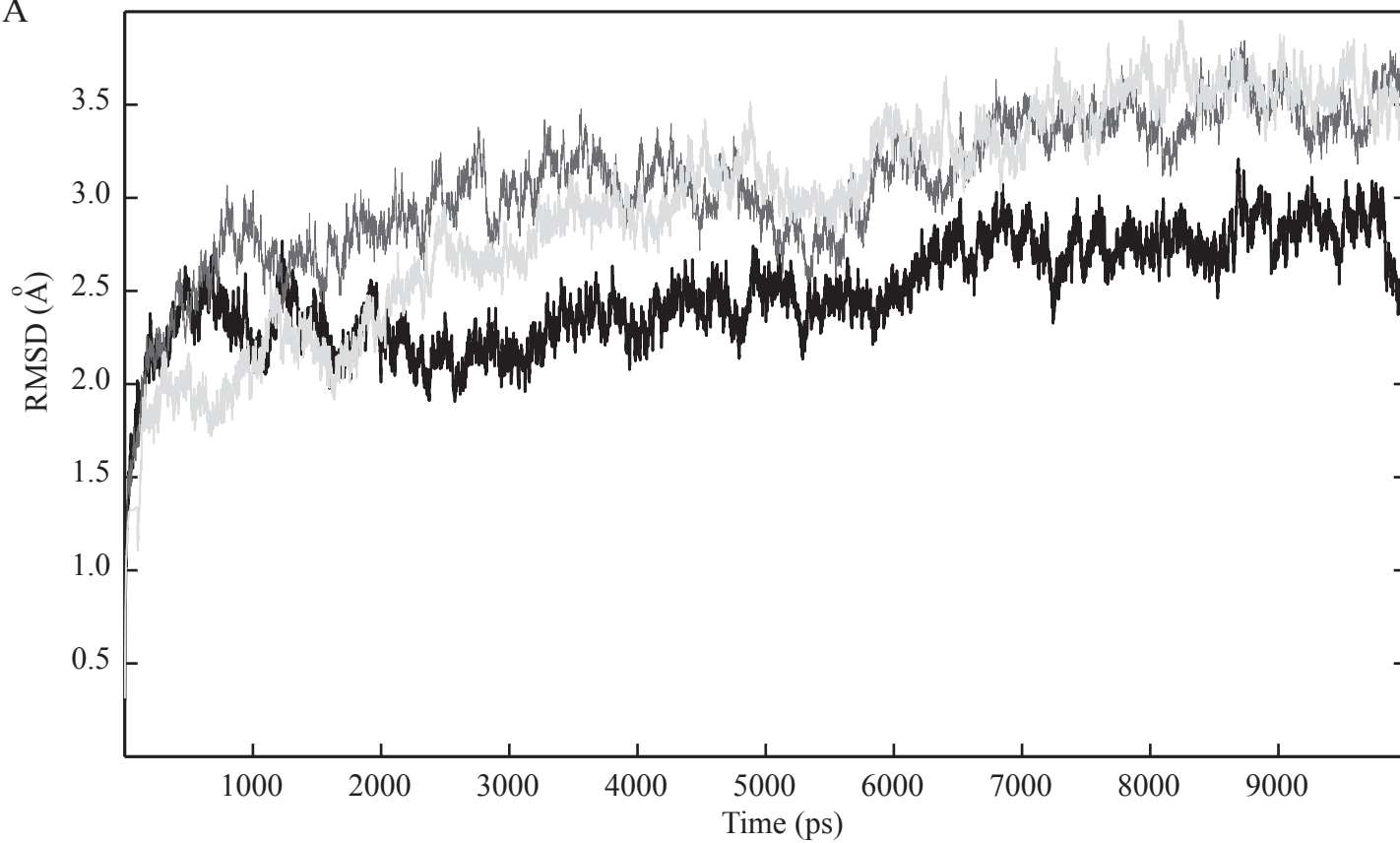


## SUPPLEMENTAL DATA

**Figure S1. Analysis of MD trajectories.** (A) Time evolution of average RMSD (with respect to the starting conformation) in C $\alpha$ -coordinates for three runs MD1 (black), MD2 (dark gray) and MD3 (light gray). (B) Motions along essential modes, illustrated for modes 1, 2, 4 and 16 evaluated for MD1, after excluding the equilibration period of 1500 ps.

**Figure S2. Cumulative correlations between mode spectra obtained from GNM and MD.** (A) Cumulative squared cosines  $\{\sigma^2(k)\}_{l_{tot}}$  between  $l_{tot}$  essential modes from MD simulations and each GNM mode (k) for  $l_{tot} = 10$  (black), 20 (gray) and 30 (white). (B)  $\{\sigma^2(l)\}_{k_{tot}}$  between top-ranking  $k_{tot} = 10$  (black), 20 (gray) and 30 (white) GNM modes with the MD modes (l) listed along the abscissa. Note, the dominant contribution of the slowest modes to the low frequency end of the spectrum, in each case, followed by the larger contribution of intermediate frequency, and then higher frequency modes, indicate the consistency between the two sets of mode spectra.

A



B

