

Supporting information for

Computational identification of slow conformational fluctuations in proteins

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Table S1: Summary of starting PDB structures used for detailed molecular dynamics simulations. These crystal structures were chosen for showing diverse binding partners and also having sufficient structural diversity. RMSD was computed for the backbone of each of the structures to 1UBQ (base structure). The summary of structural changes describes areas highly flexible from the ensemble, as observed by structural overlaps against 1UBQ.

Structure	Chain	RMSD (Å)	Regions with structural changes
1UBQ	A	-	-
1P3Q	U	0.417	β 1- β 2, β 3- β 4
1S1Q	B	0.501	β 1- β 2, β 3- β 4, β 2- α 1
1TBE	B	0.528	α 1- β 3, β 1- β 2, β 3- β 4
1YIW	A	0.574	α 1- β 3, β 1- β 2, β 3- β 4
2D3G	A	0.380	β 1- β 2, β 3- β 4
2FCQ	B	0.568	β 1- β 2, β 3- β 4
2G45	B	0.570	β 1- β 2, β 3- β 4

Animation movies

The following movies are available with this document in MPEG format: Animation movies of Modes 1, 2 and 3 (corresponding to lowest eigenvalue, second lowest eigenvalue and third lowest eigenvalue) computed from QHA_{0.5μs}, NMR and X-ray ensembles.