Supplementary Material to

“Principal component analysis of molecular dynamics: On the use of Cartesian vs. internal coordinates”

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FIG. S1: Free energy landscape of HP35 along the first two principal components of a cPCA. Compared are the results of different rotational fitting procedures, including (a) a single-reference fit to the native-like metastable state $N_2$ identified in the dynamical clustering analysis of Ref. 1, (b) a multi-reference fit$^2$ against the crystal structure, and (c) a min(Var+Prev) fit according to Ref. 3.
FIG. S2: Convergence of the cumulative fluctuations of various PCAs for BPTI. Shown are results for a dPCA (blue), a cPCA with standard fitting (red), and a cPCA with min(Var+NN) fitting (cyan). Interestingly, we find a quite similar convergence for the dPCA and the cPCA/min(Var+NN), which both were found to describe the conformational distribution of BPTI similarly well (see Fig.4 in the main text). The cPCA with standard fitting, on the other hand, exhibits a dominant first component, which presumably partially reflects overall motion of the system.
FIG. S3: Free energy curves along the first six principal components of a cPCA of BPTI after standard fitting.
FIG. S4: Free energy curves along the first six principal components of a cPCA of BPTI after min(Var+NN) fitting with NN=25.
FIG. S5: Free energy curves along the first six principal components of a dPCA of BPTI.
FIG. S6: Free energy curves along the principal components seven to twelve of a dPCA of BPTI.
FIG. S7: Dendrogram showing the splitting of conformational states of BPTI at different metastabilities $Q_{\text{min}}$, as obtained from the most probable path clustering. Choosing $Q_{\text{min}} = 0.98$ (dashed line), we found eight distinct metastable states of BPTI. Two of these states were found to be only minor populated and were therefore lumped with their neighbor states. This results in the six metastable states shown in Fig. 4 of the main text.
FIG. S8: Conformational states of BPTI obtained from the most probable path clustering using $Q_{\text{min}} = 0.95$, projected on the first two principal components from the dPCA.
