|  |
| --- |
|  |
| **Figure 9–figure supplement 1. Principal Component Analysis of COM and AV Data.** In order to visualize the conformational landscape of the PSG supramodule within PSD95, we performed principal component analysis using the distances between the domain’s centers of mass (COM) and the simulated for PDZ3 to SH3 and PDZ3 to GuK (Figure 8-Figure Supplement 1). Data were analyzed using scikit-learn (sklearn) in Python. Data were first standardized such that each set of inter-COM and AV-derived interdye distances had mean 0 and unit variance using the sklearn.preprocessing.StandardScaler. Principal components were calculated using sklearn.decomposition.PCA with two components. The surface depth corresponds to the relative number of structures from DMD simulations which occupy some region of the principal component (PC) space. PCA results in basins α and β separated along PC1, which explains 65% of the standardized dataset variance. The variance along PC2 (16% explained variance ratio) mostly corresponds to apparent heterogeneity in basin α. Additionally, there is an apparent saddle point corresponding to the transition pathway between the two basins along PC1. This suggests that the motions corresponding to heterogeneity in basin α are distinct from those corresponding to interdomain transitions as observed by FRET. This surface was rescaled for Figure 9 such that the integrated volume of the two basins were equivalent to the population fractions for states A and B obtained from seTCSPC analysis. |