|  |
| --- |
|  |
| **Figure 8–figure supplement 2. Model Robustness Analysis.** As with the FRET Network Robustness Analysis, where we analyzed the model dependence on the inclusion of individual variants, here we bootstrapped the dependency of the models on error in the FRET distances using the same framework. For each trial, we introduced a random, artificial error on each of the FRET distances and repeated the classification of structures from DMD into the two basin ensembles. To check the dependence on the magnitude of the error, we used introduced a random error to each variant between 5 and -5% or between 15 and -15% of the original distance. Each condition was repeated 3 times with different random errors. To compare conditions, we measured the change in the center of mass of the surface distribution composed from the individual PDZ3 centers of mass identified by that screen. We found that increasing the distance error did not significantly impact the classification of structures into the two ensembles. The variance in the mean ensemble positions over three repeats increased with increasing error along with small shifts in the mean positions. Notably, +/-15% is greater than the uncertainties in distances obtained via global fitting of fluorescence decays, suggesting that the intrinsic uncertainty in the FRET-derived distances from a single fit (Supplemental file 3D) does not significantly impact the ensemble assignment or their fuzziness. |