Figure S1. Box-and-whisker plots for the BC and FG loops calculated over the whole trajectory for all CYP2D6 variants. The distribution of the data points: the pink boxes indicate the upper - and lower quartile (25% of the data is greater than or less than this value), the caps indicate the greatest and the smallest value excluding outliers. The outliers represent more than or less than 3/2 times the upper or lower quartile, and the red line indicate the median value.