The collective variable

Here we define a collective variable (d_p, described in the main text) that can distinguish between planar and non-planar geometries of the DNAns. In practice, d_p is obtained from the direction of each of the dsDNA arms in a nanostar. This is done in the following way: First we compute the position, $\mathbf{r}_{core}$, of the DNAns core. This is done by locating the base-pair (bp) closer to the FJC in each arm (three in total) and calculating the centre of mass (COM) using the position of the six nucleotides previously selected. Then, the unitary vectors $(\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_2, \hat{\boldsymbol{e}}_3)$ pointing from the core of the molecule to the COM of the bp closer to the sticky end in each arm, define the direction of the three dsDNA arms.

To compute d_p we find two vectors ($\mathbf{A}$ and $\mathbf{B}$) that connect the end of any two arms, for example:

$$\mathbf{A} = \hat{\boldsymbol{e}}_2 - \hat{\boldsymbol{e}}_1 .$$

$$\mathbf{B} = \hat{\boldsymbol{e}}_3 - \hat{\boldsymbol{e}}_1 . \tag{S3}$$

These vectors define a plane whose normal can be found as the cross product $\mathbf{n} = \mathbf{A} \times \mathbf{B}$. Then, the distance d_p from this plane to the core of the molecule, is given by the projection of any of the three dsDNA arms (for example $\hat{\boldsymbol{e}}_2$) onto the unitary normal vector:

$$d_p = |\hat{\boldsymbol{e}}_2 \cdot \hat{\boldsymbol{n}}| . \tag{S4}$$

The range of our CV is from $d_p = 0$ (for a completely planar DNAns) to $d_p \lesssim 1$. The larger the value of d_p the less planar the molecule. Note that d_p cannot be equal to 1 due to the excluded volume interaction between arms.