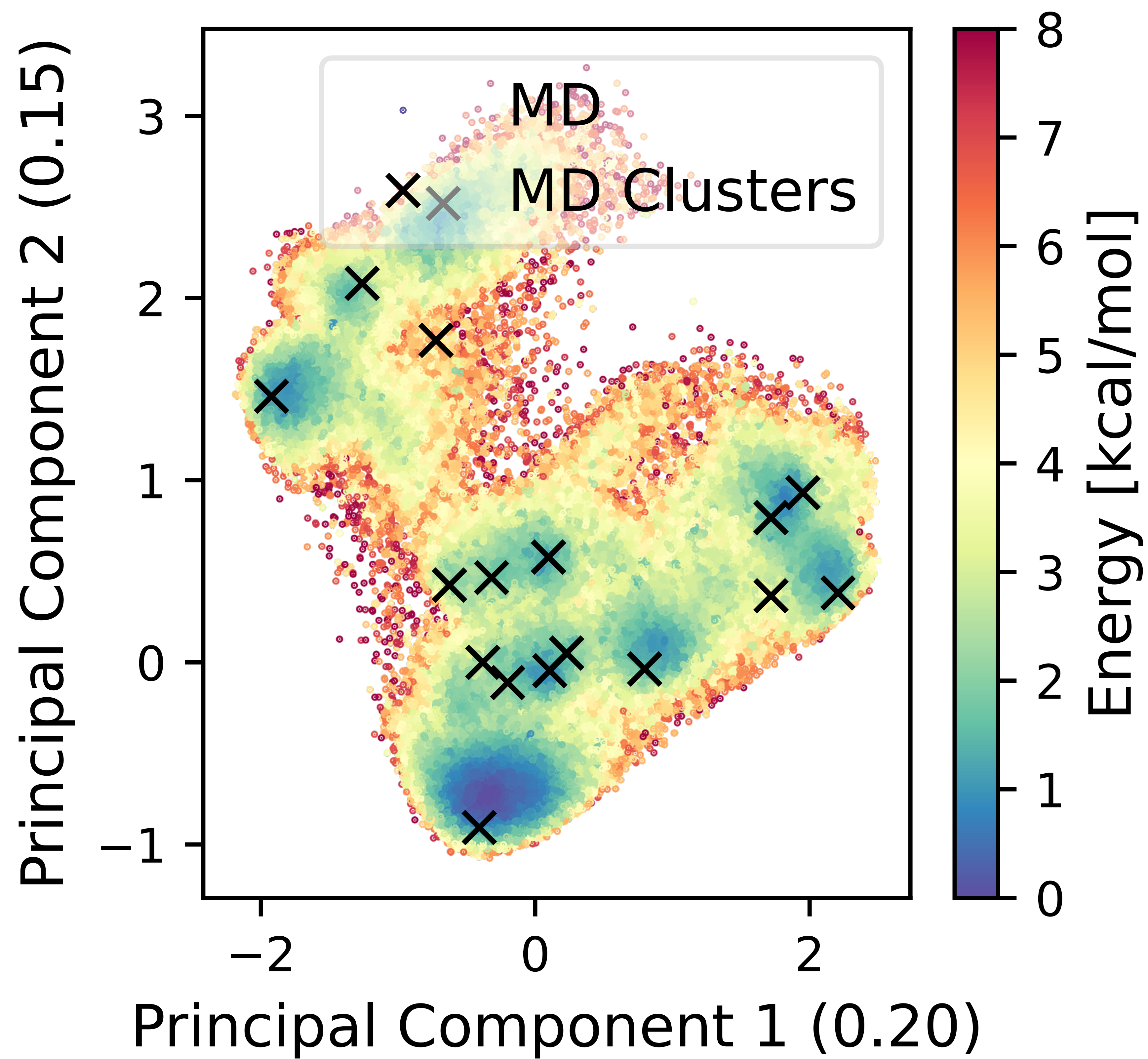
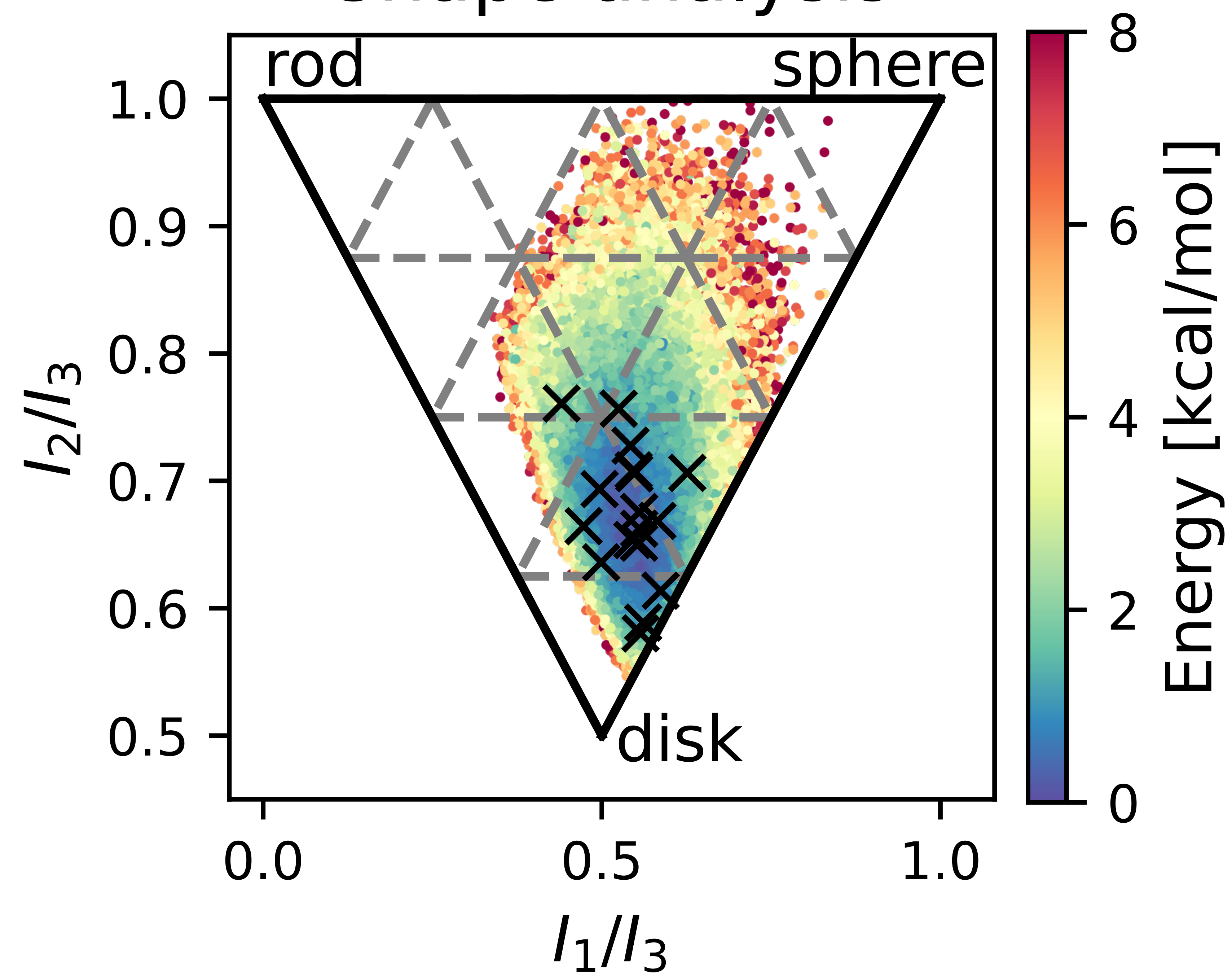


A

Dihedral PCA

**B**

Shape analysis

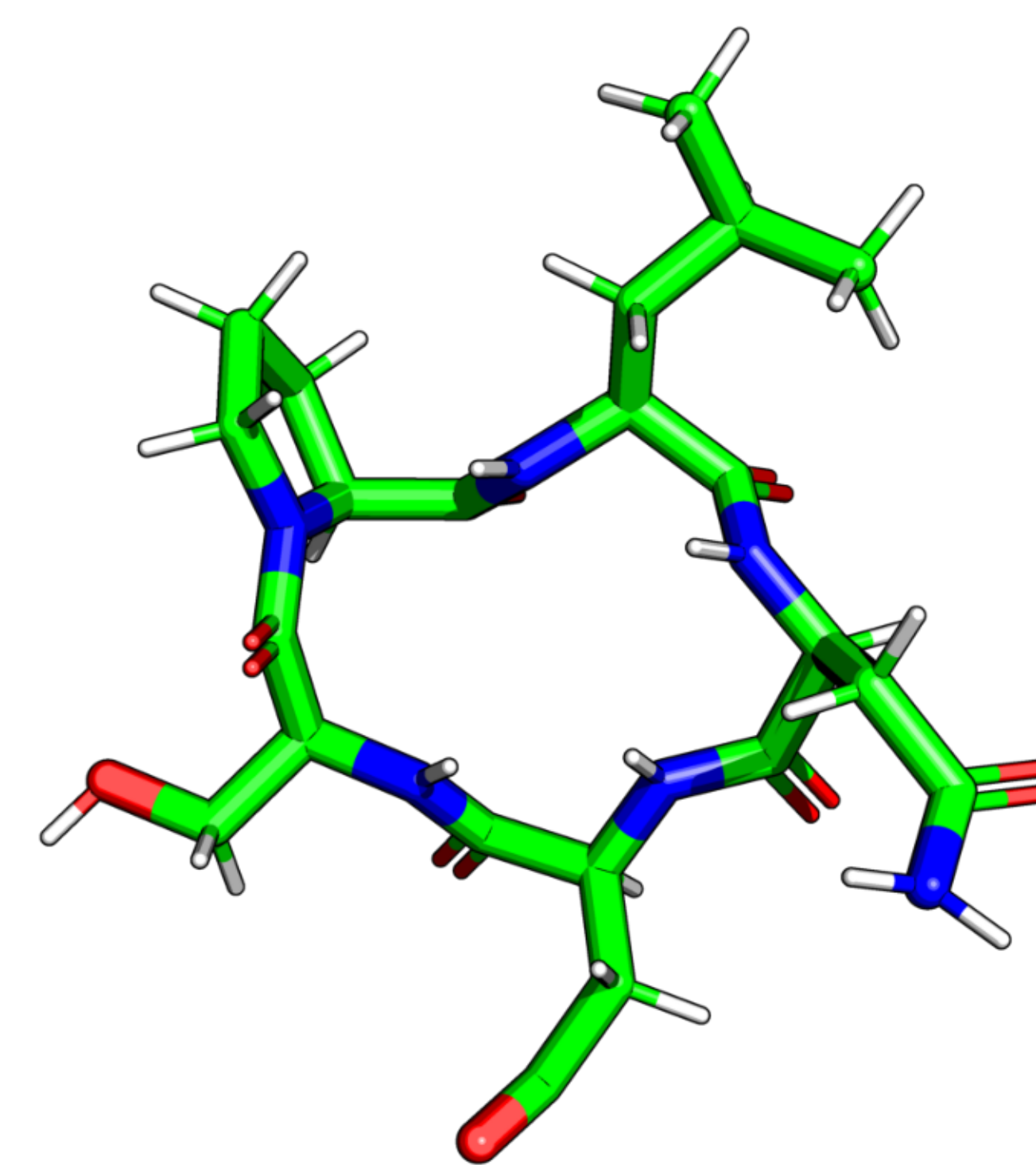
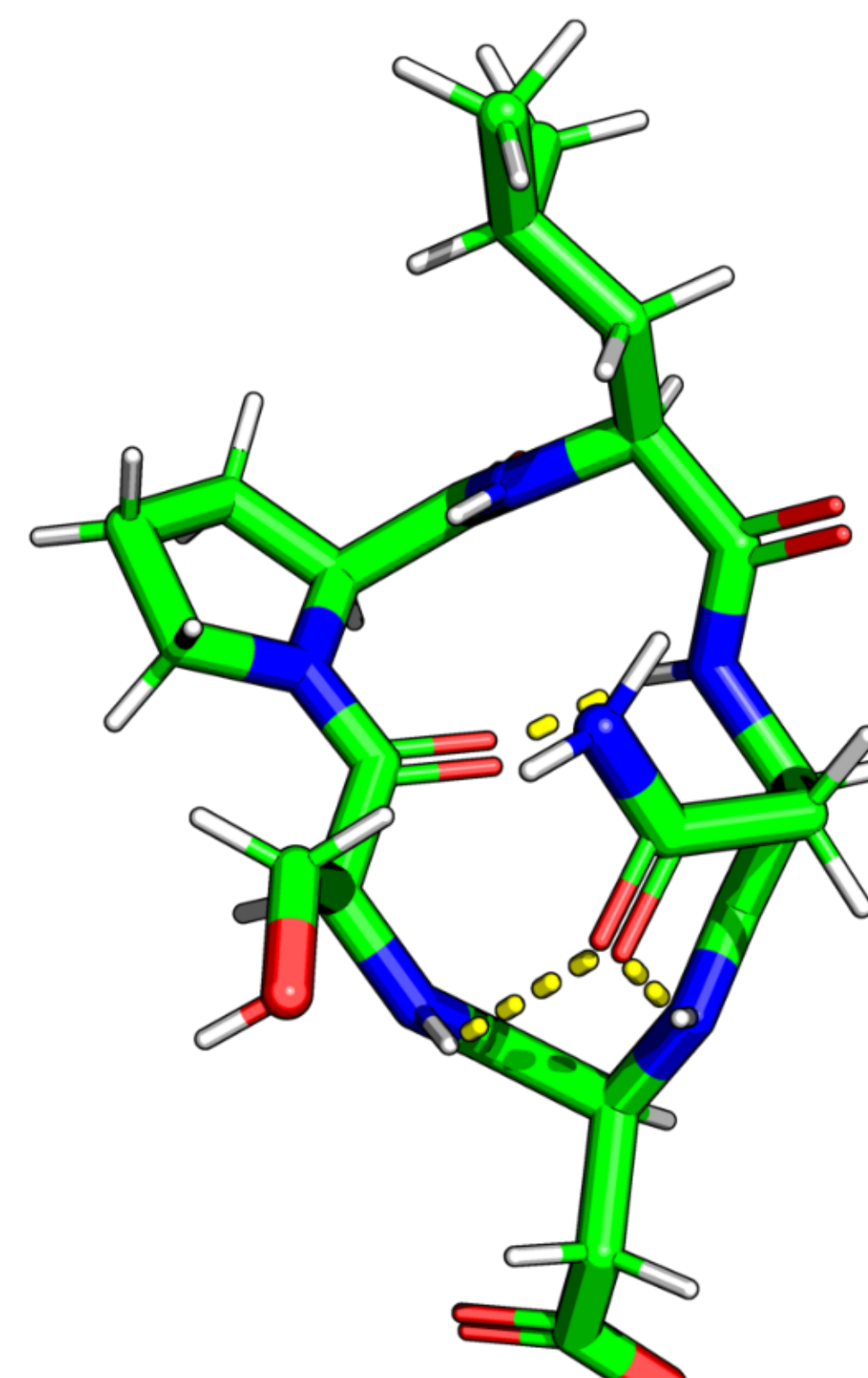
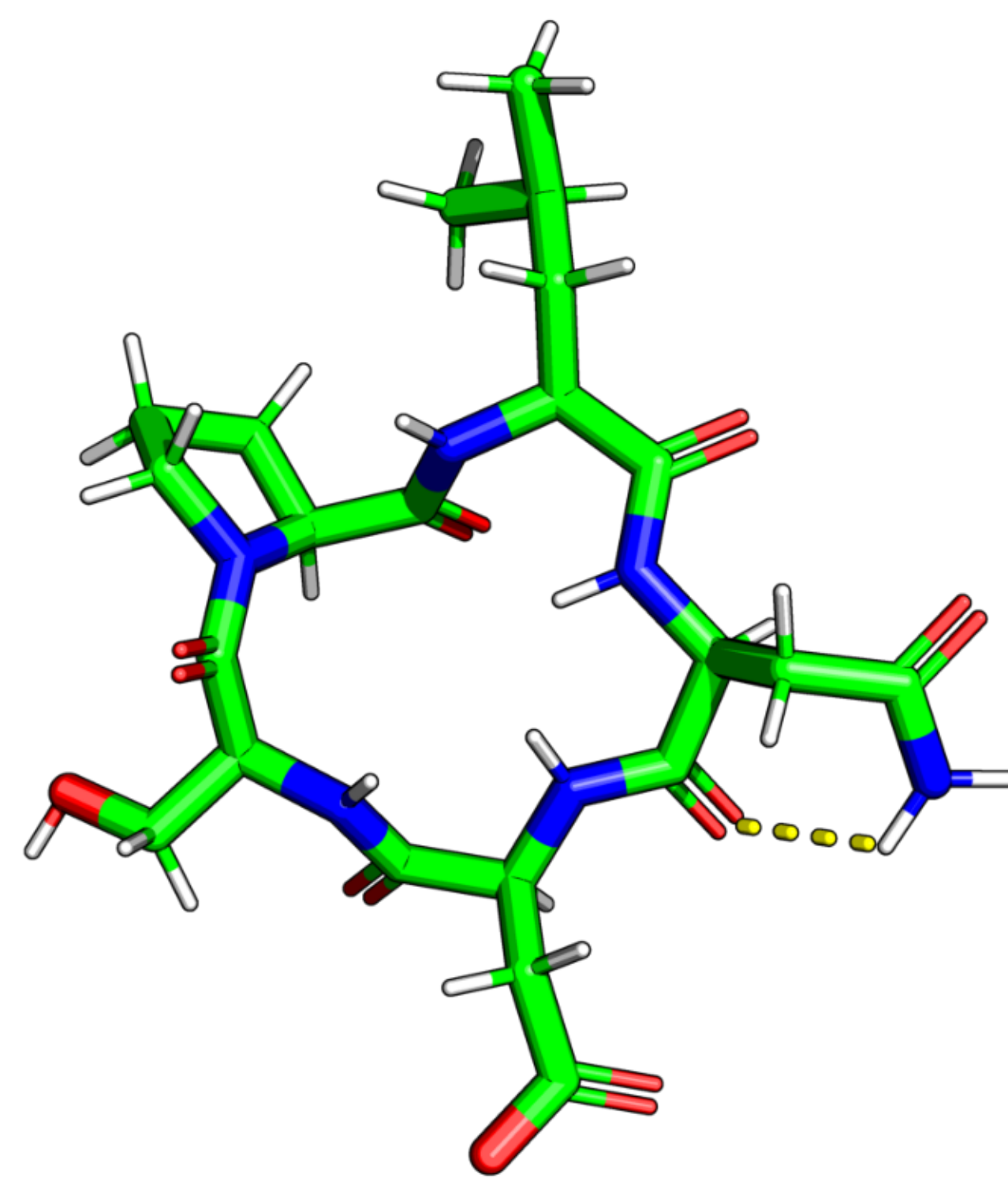
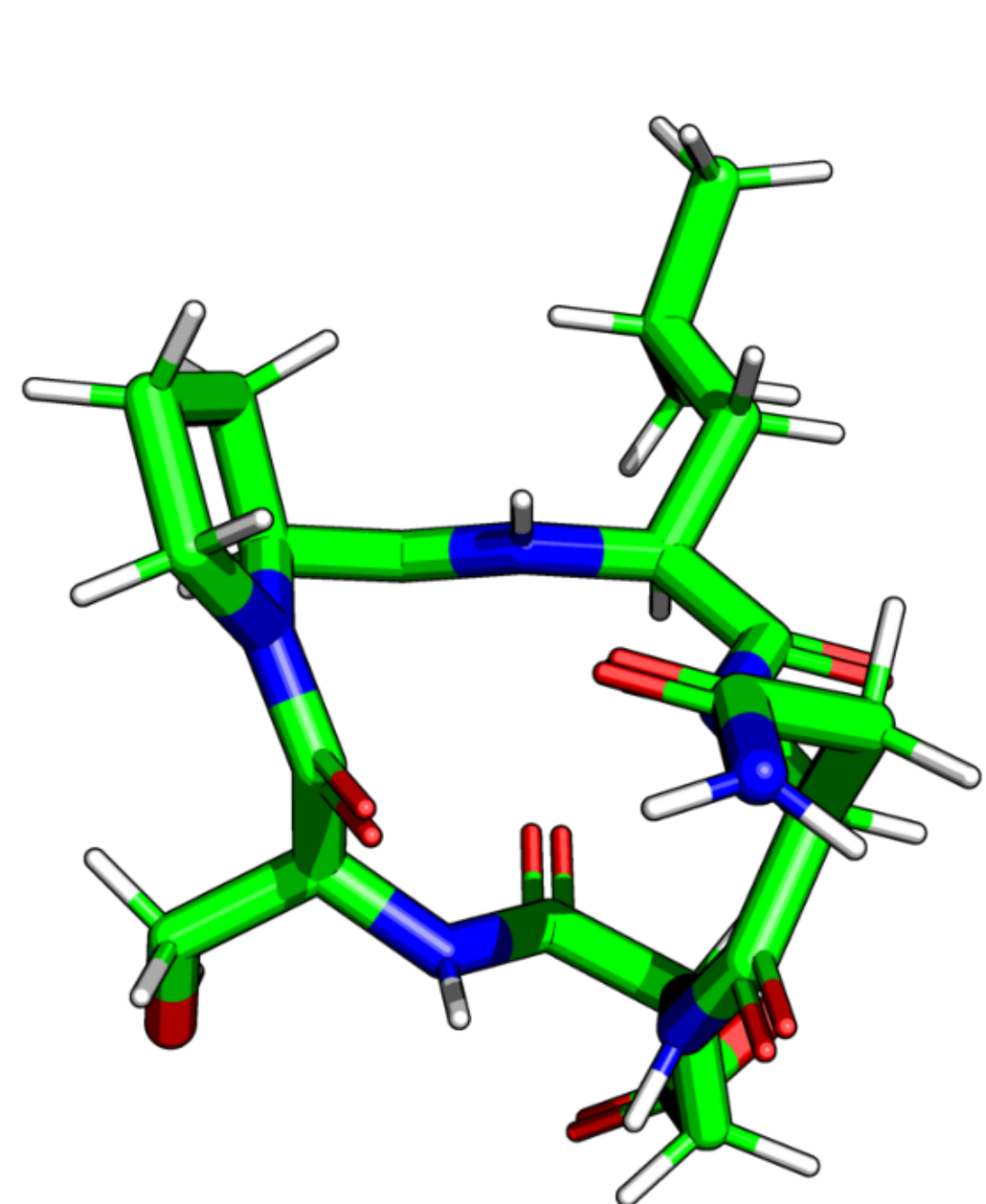
**C**

most spherical

most disk-like

most rod-like

most pop. cluster

**D**

MD - NMR(exp): distance / Å

x deviation

— NMR upper bound

— MD upper bound

— MD lower bound

