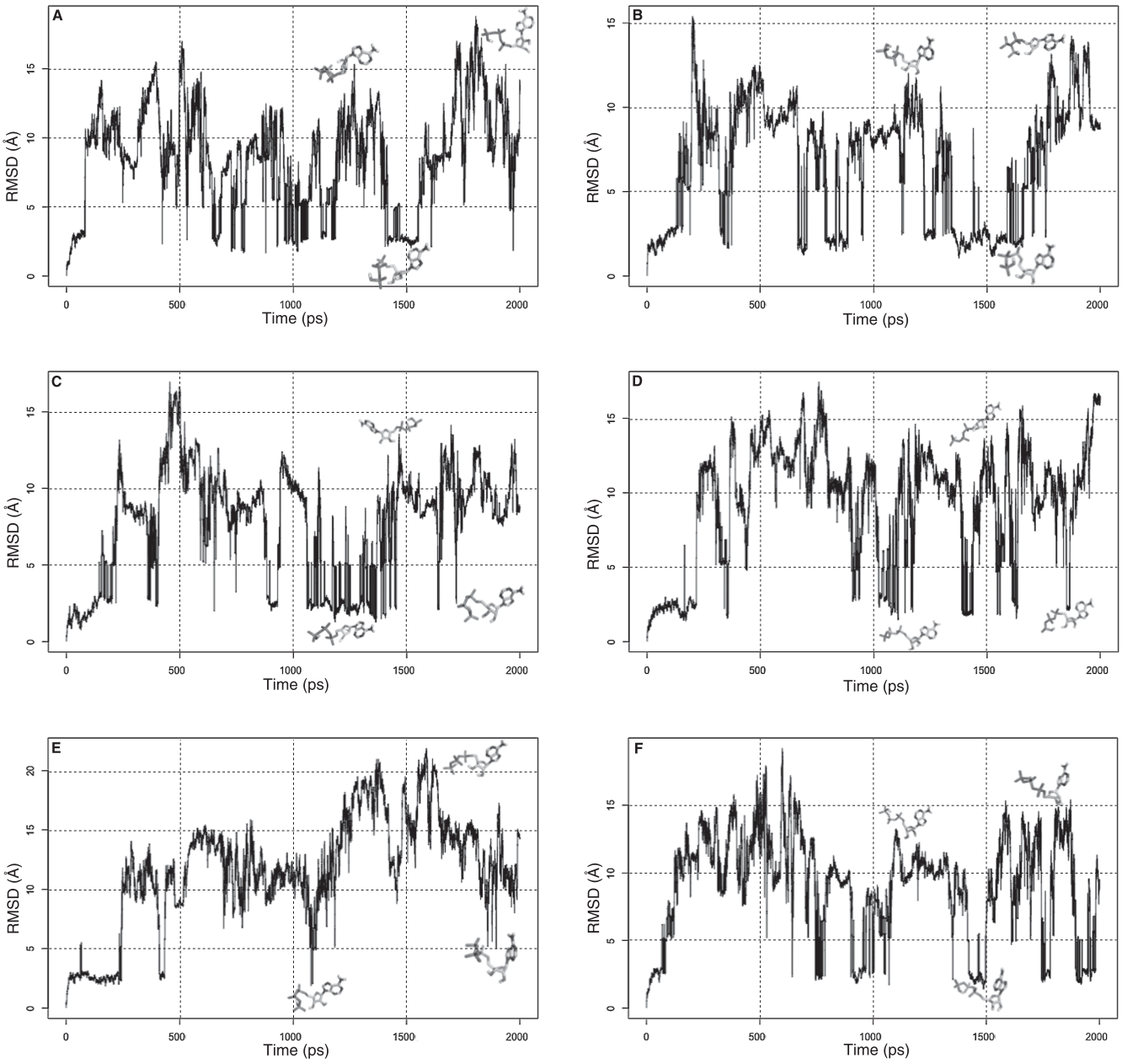
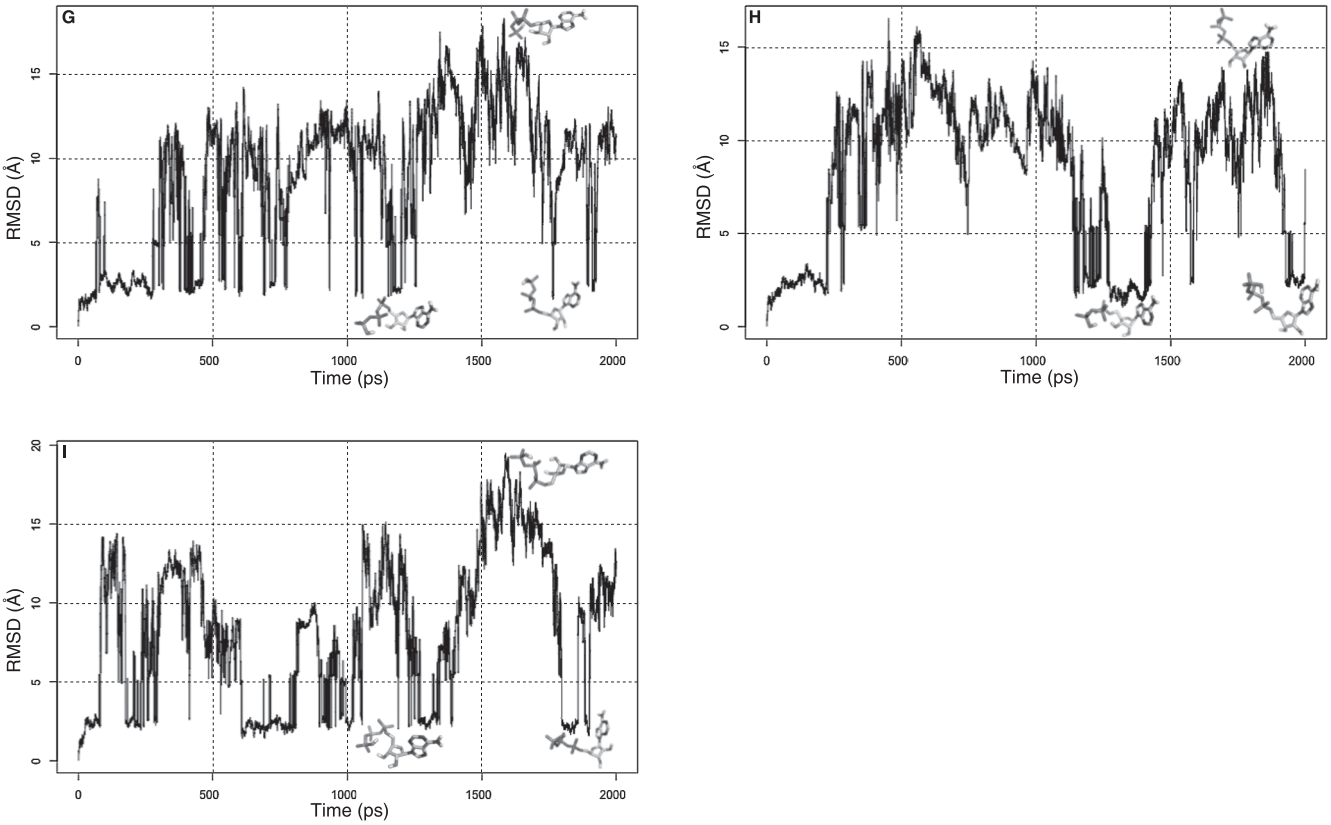
Supplementary Materials

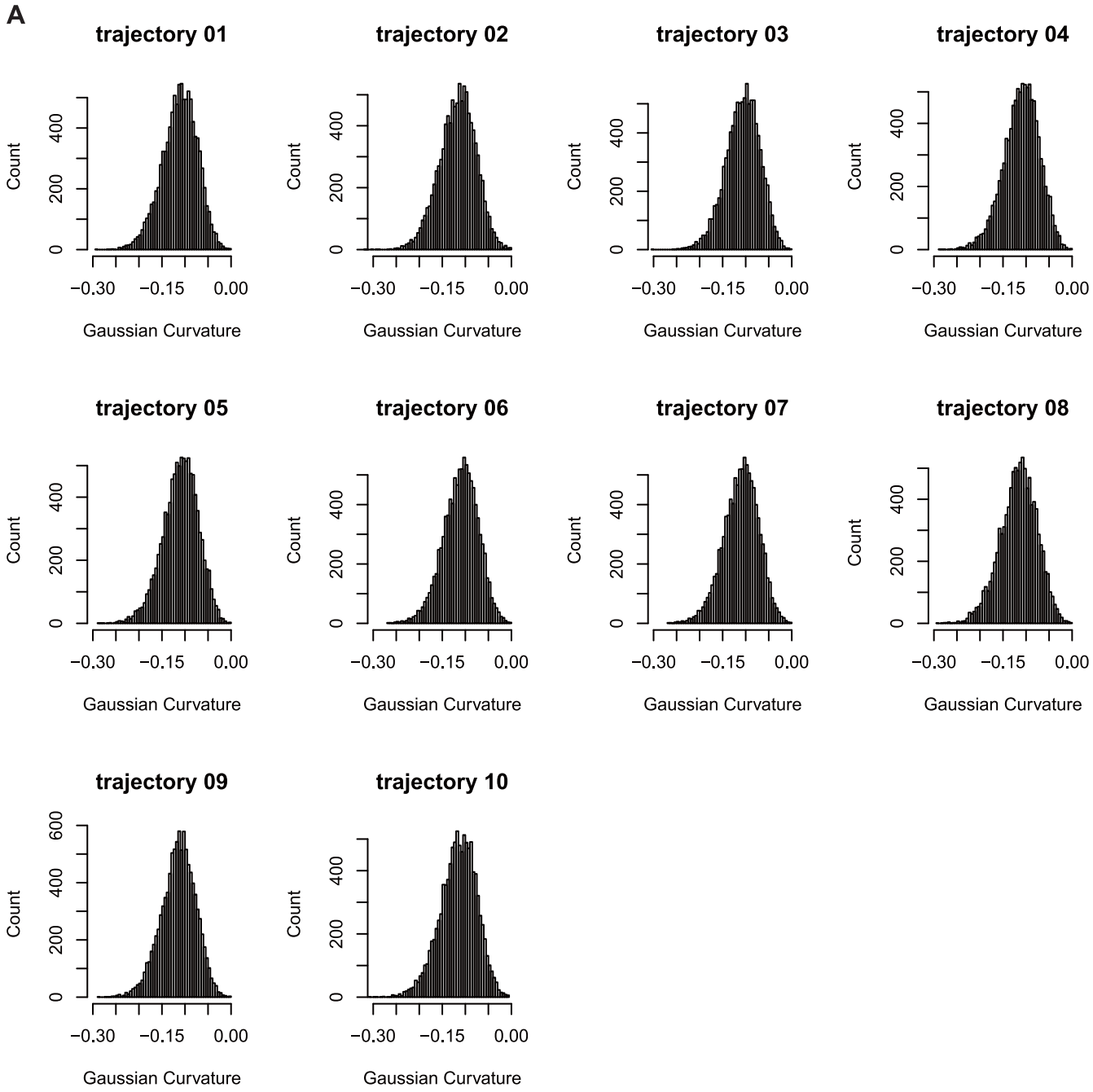
Supplementary Figure 1 RMSD of ATP during the different nine runs of simulation. The calculation was done between the initial structure and structures of every 0.1 ps. All 36 atoms including hydrogen atoms were used in the calculation. In each trajectory, three snap shot structures were drawn in the graph. **A.** Trajectory 02: from left to right, conformations of 1,270 ps, 1,500 ps and 1,722 ps. **B.** Trajectory 03: conformations of 1,148 ps, 1,515 ps and 1,783 ps. **C.** Trajectory 04: conformations of 1,207 ps, 1,418 ps and 1,720 ps. **D.** Trajectory 05: conformations of 1,111 ps, 1,500 ps and 1,853 ps. **E.** Trajectory 06: conformations of 1,088 ps, 1,583 ps and 1,878 ps. **F.** Trajectory 07: conformations of 1,104 ps, 1,496 ps and 1,872 ps. **G.** Trajectory 08: conformations of 1,174 ps, 1,504 ps and 1,722 ps. **H.** Trajectory 09: conformations of 1,221 ps, 1,810 ps and 1,960 ps. **I.** Trajectory10: conformations of 1,307 ps, 1,588 ps and 1,843 ps.



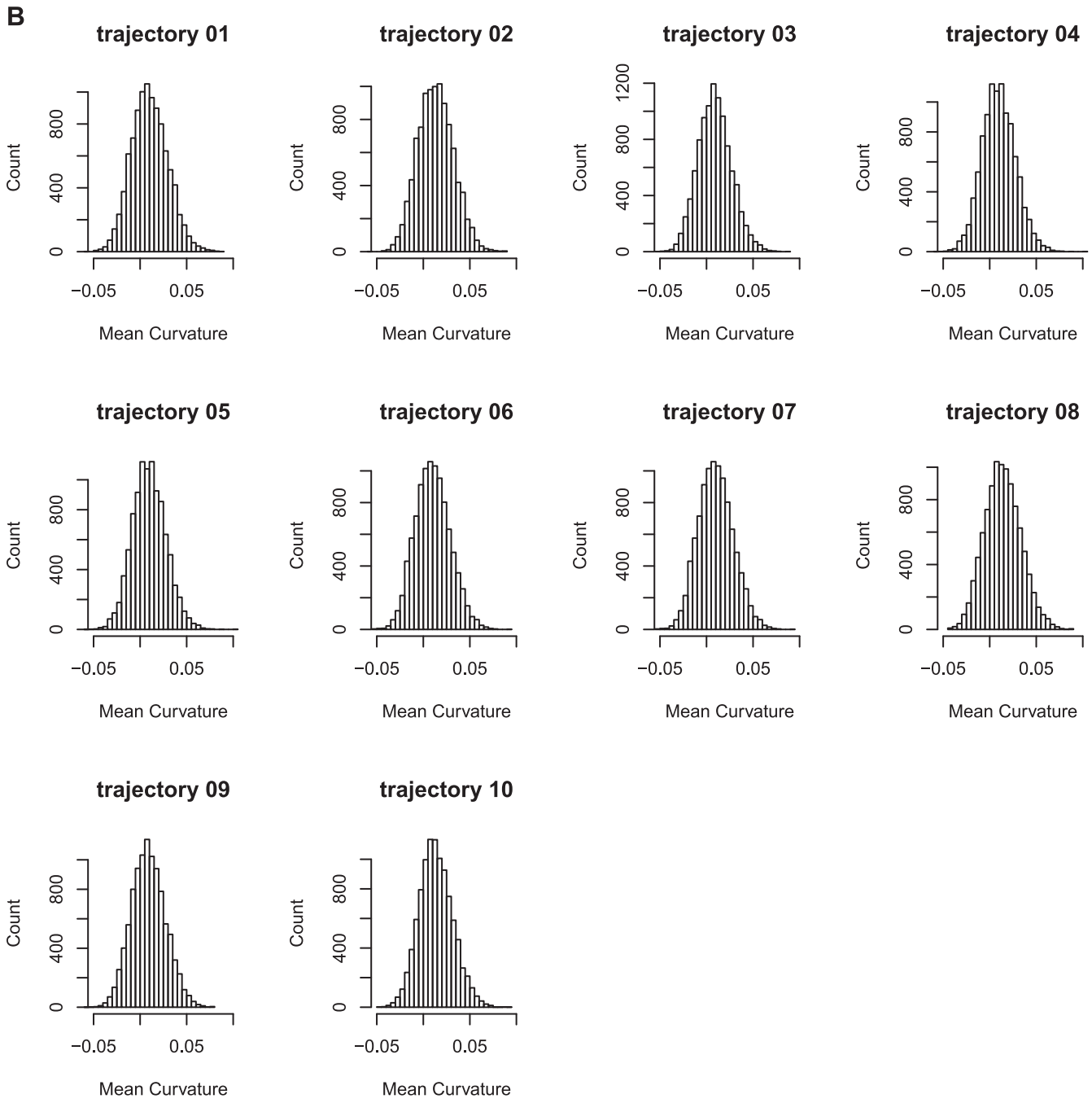
Supplementary Figure 1 Continued



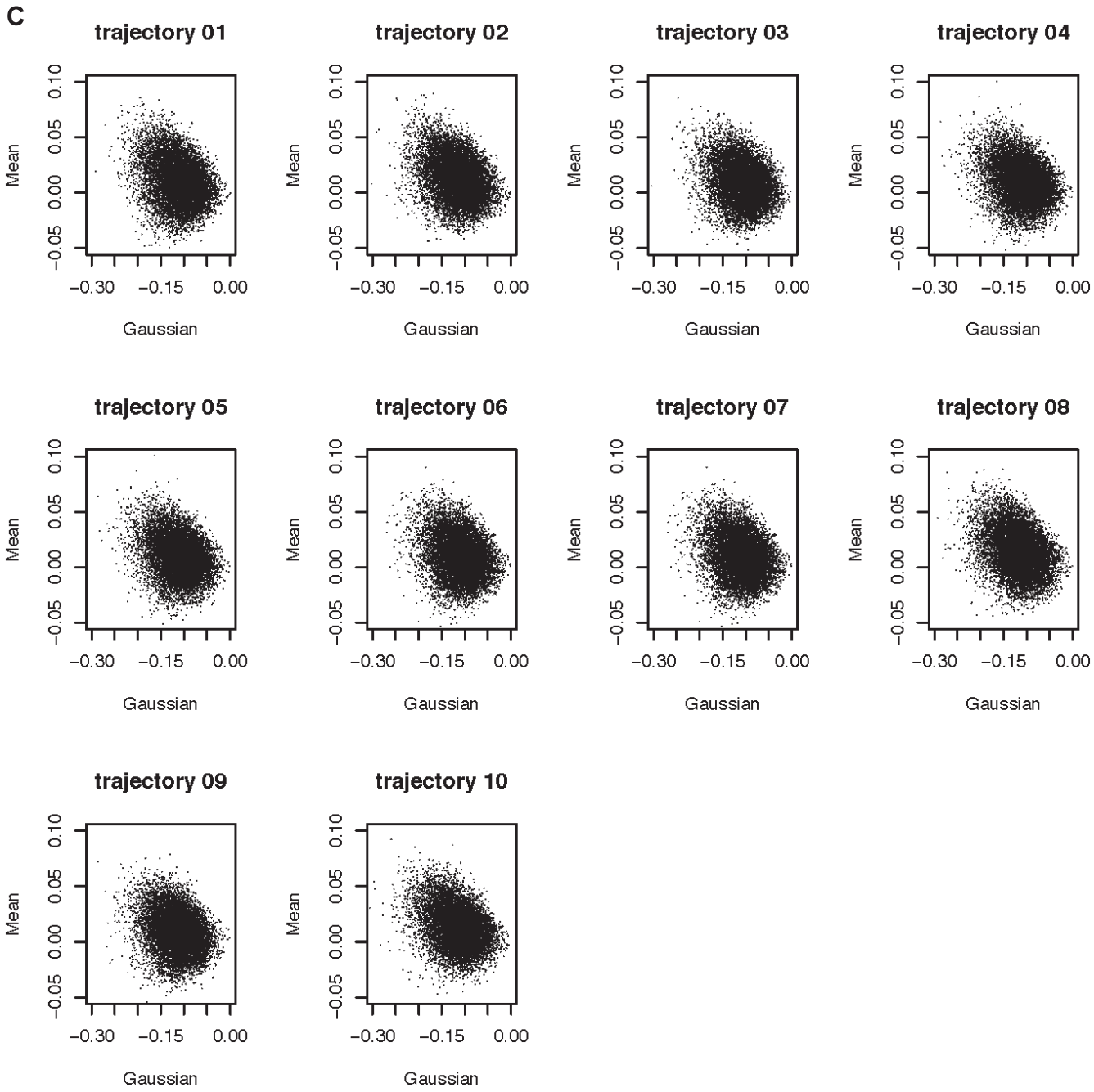
Supplementary Figure 2 Ribose curvature in the conformations from each trajectory of ten runs of molecular dynamics simulation. **A.** The histograms of Gaussian curvature. **B.** The histograms of mean curvature. **C.** Relationship between the Gaussian and mean curvatures.



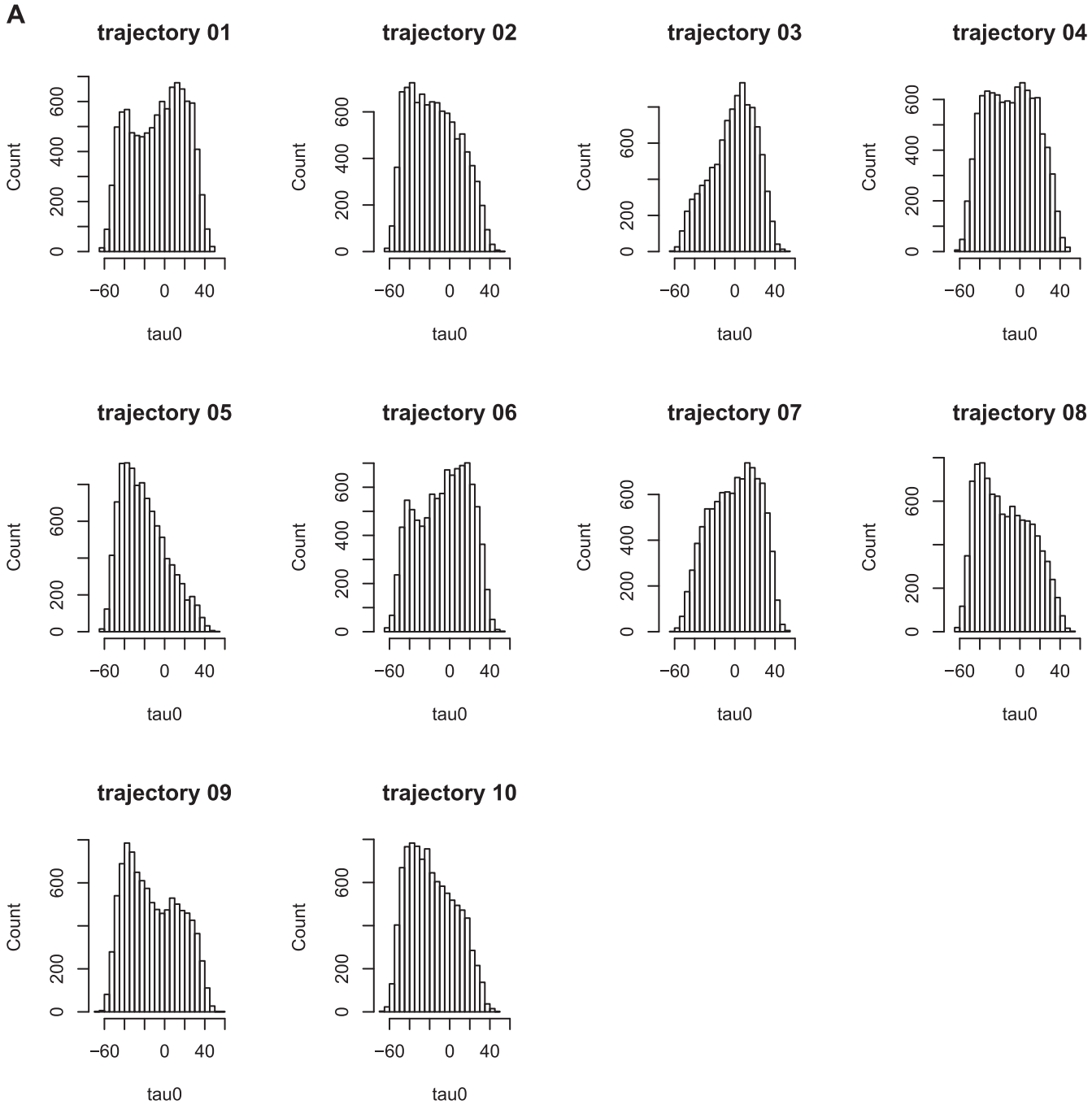
Supplementary Figure 2 Continued



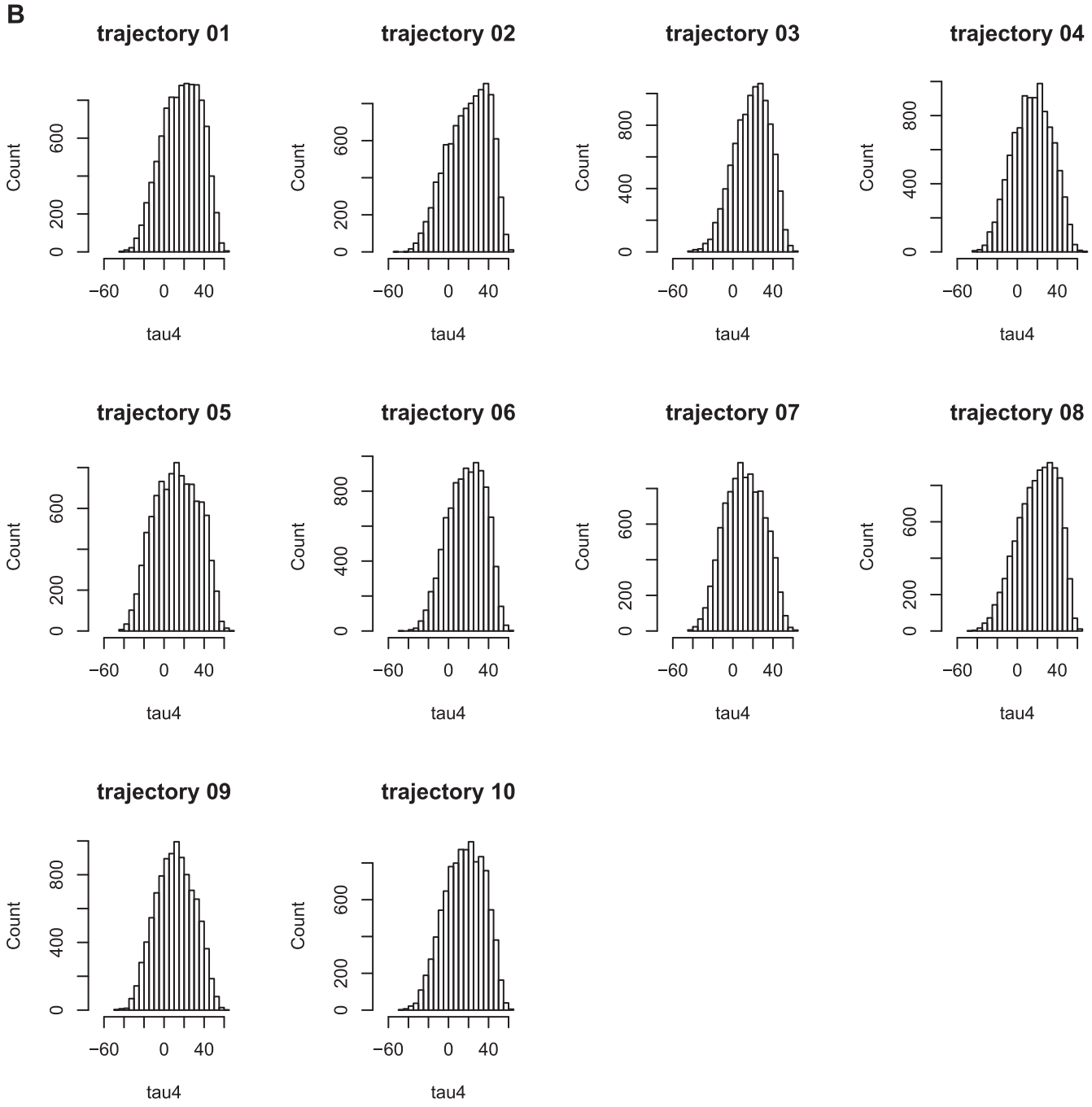
Supplementary Figure 2 Continued



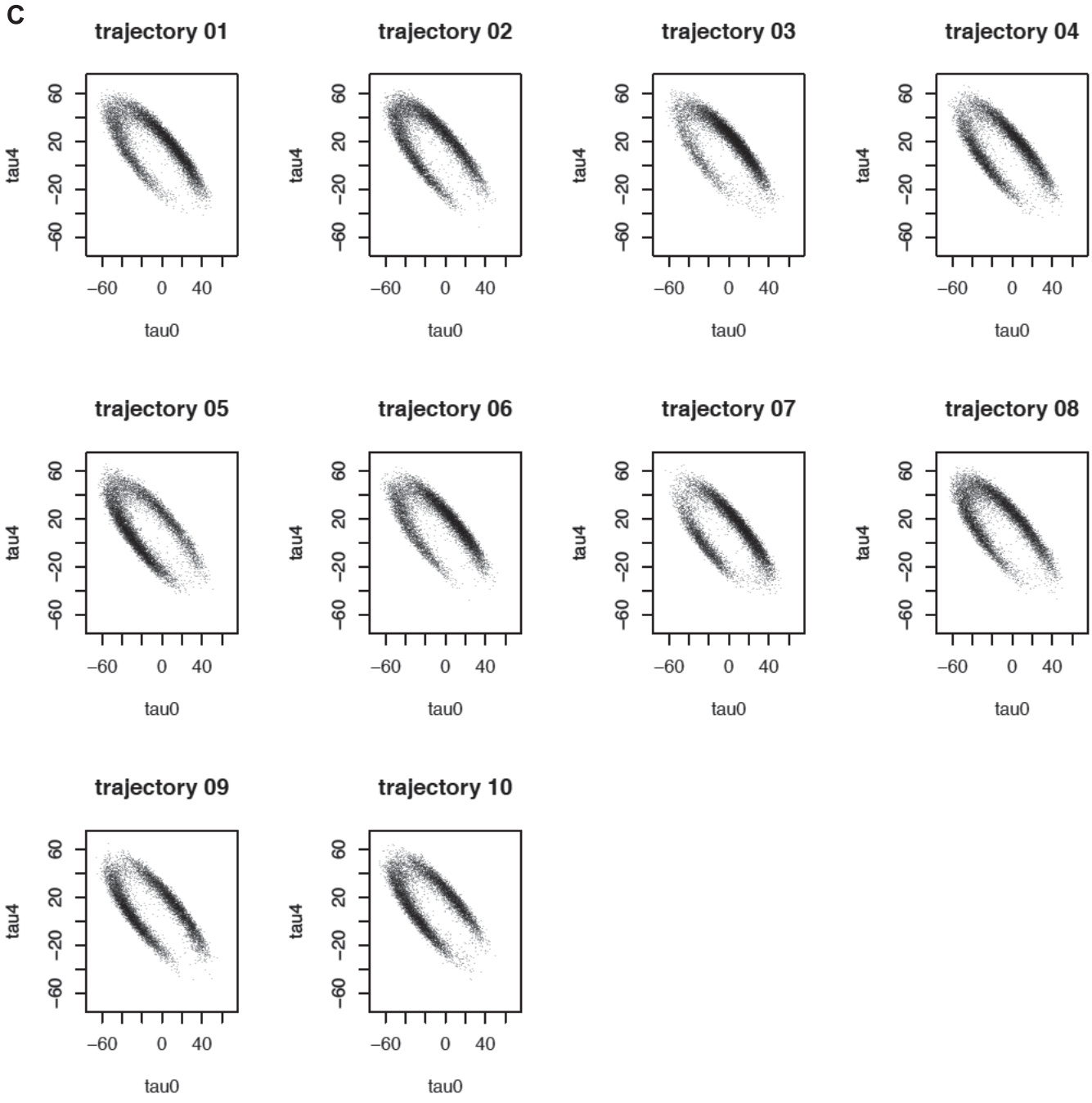
Supplementary Figure 3 Ribose torsion angles τ_0 and τ_4 in the conformations from each trajectory of ten runs of molecular dynamics simulation. **A.** The histograms of torsion angle τ_0. **B.** The histograms of torsion angle τ_4. **C.** Relationship between the torsion angles τ_0 and τ_4.



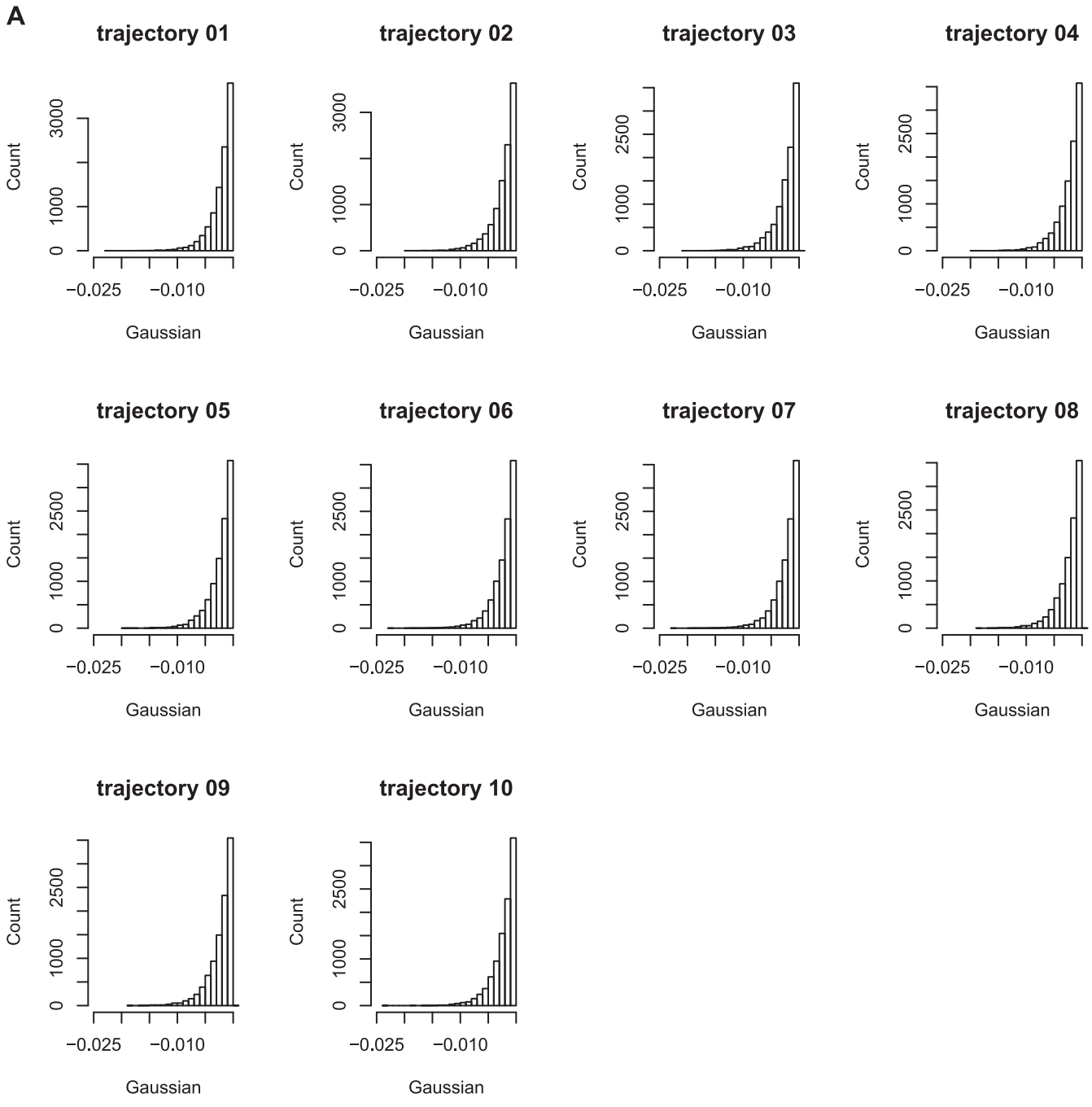
Supplementary Figure 3 Continued



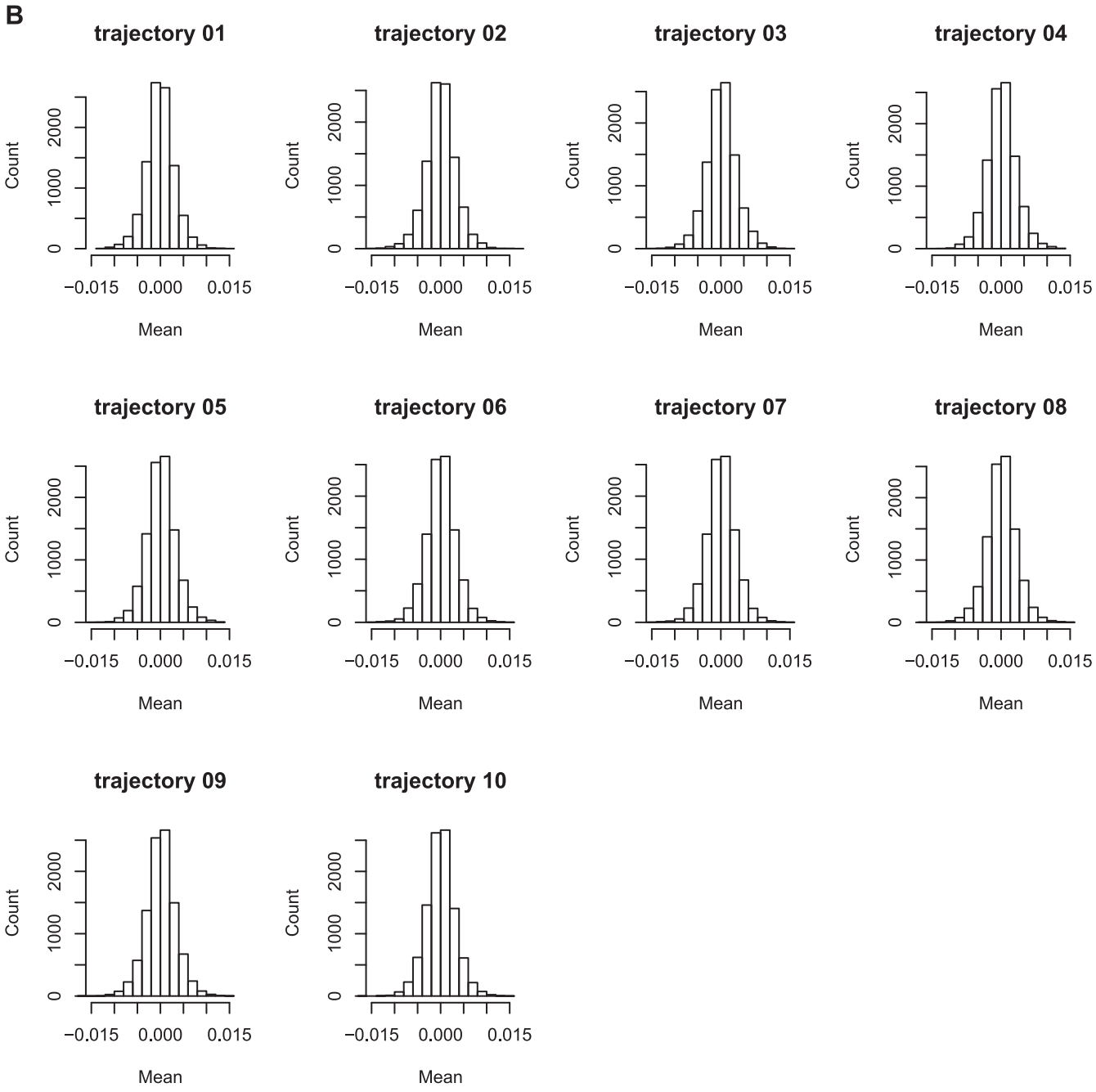
Supplementary Figure 3 Continued



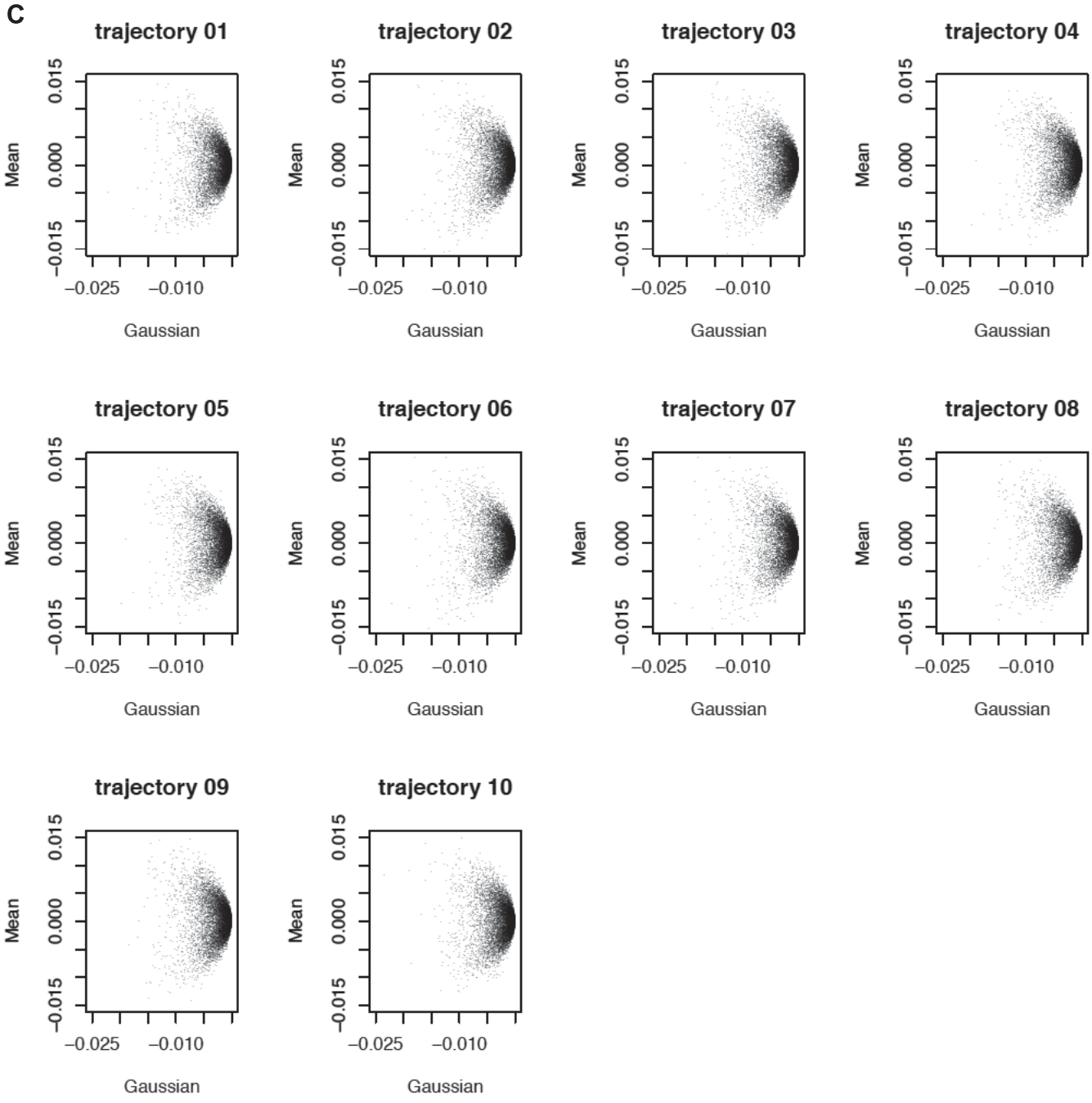
Supplementary Figure 4 Adenine five-membered ring curvature in the conformations from each trajectory of ten runs of molecular dynamics simulation. **A.** The histograms of Gaussian curvature. **B.** The histograms of mean curvature. **C.** Relationship between the Gaussian and mean curvatures.



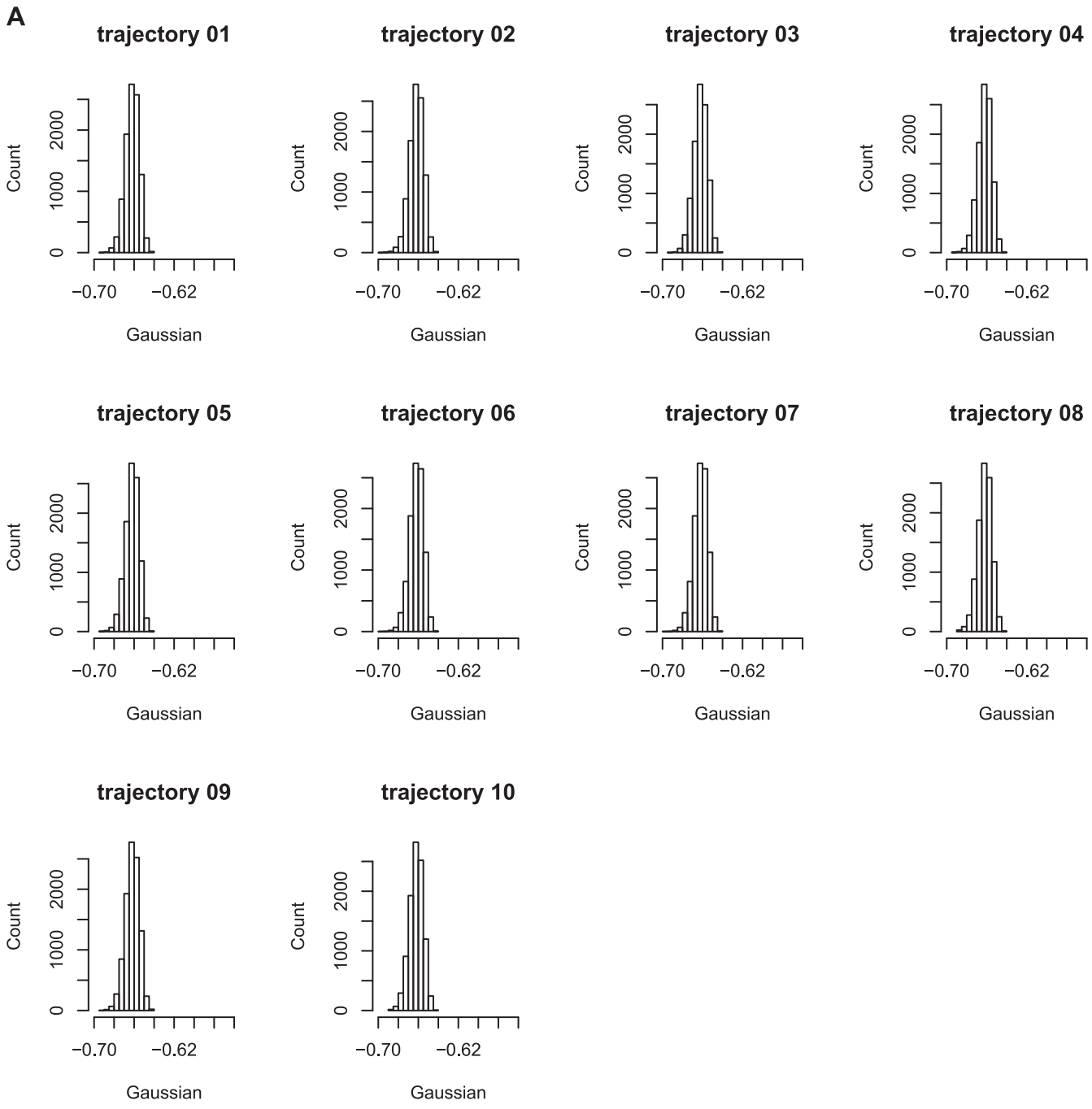
Supplementary Figure 4 Continued



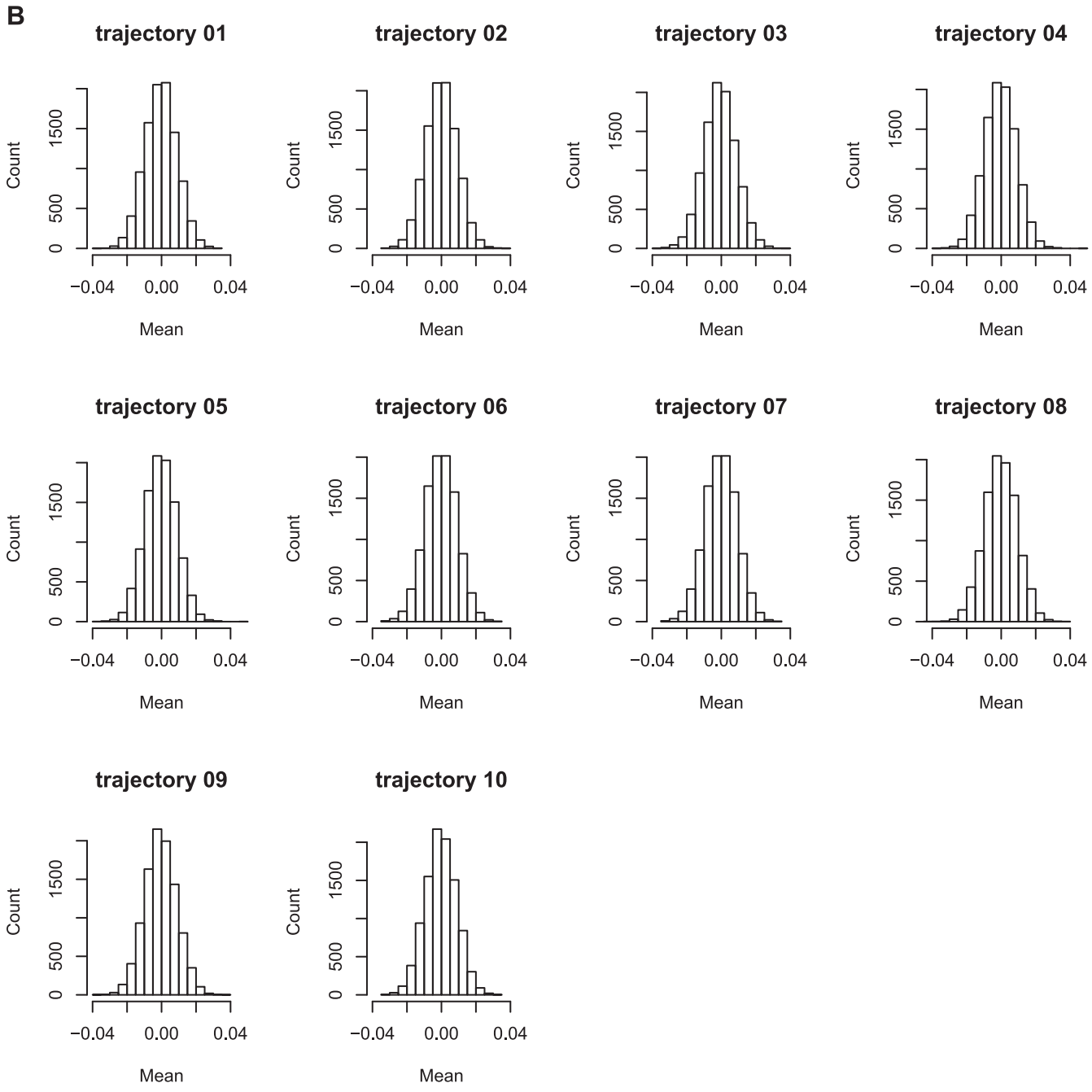
Supplementary Figure 4 Continued



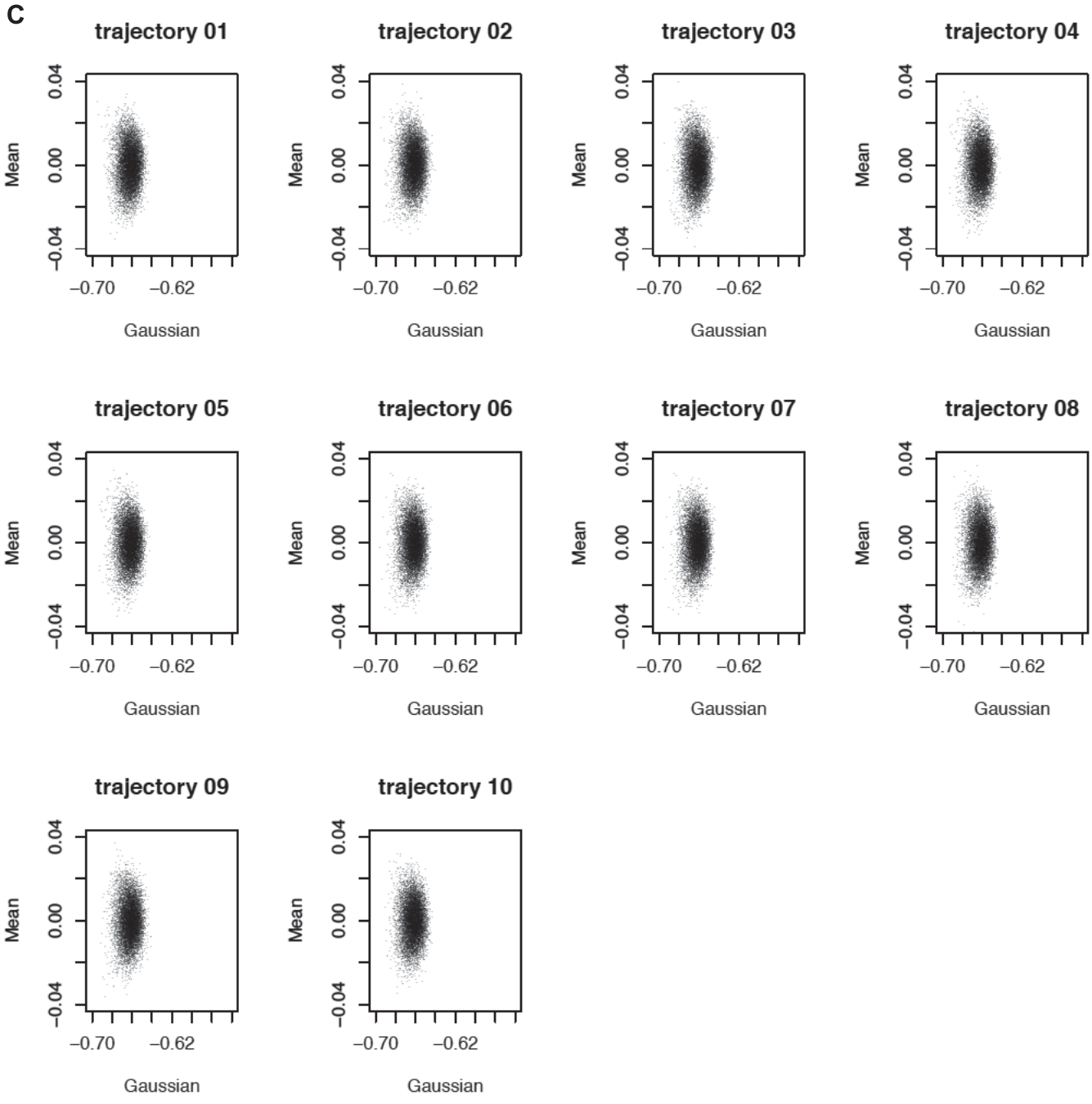
Supplementary Figure 5 Adenine six-membered ring curvature in the conformations from each trajectory of ten runs of molecular dynamics simulation. **A.** The histograms of Gaussian curvature. **B.** The histograms of mean curvature. **C.** Relationship between the Gaussian and mean curvatures.



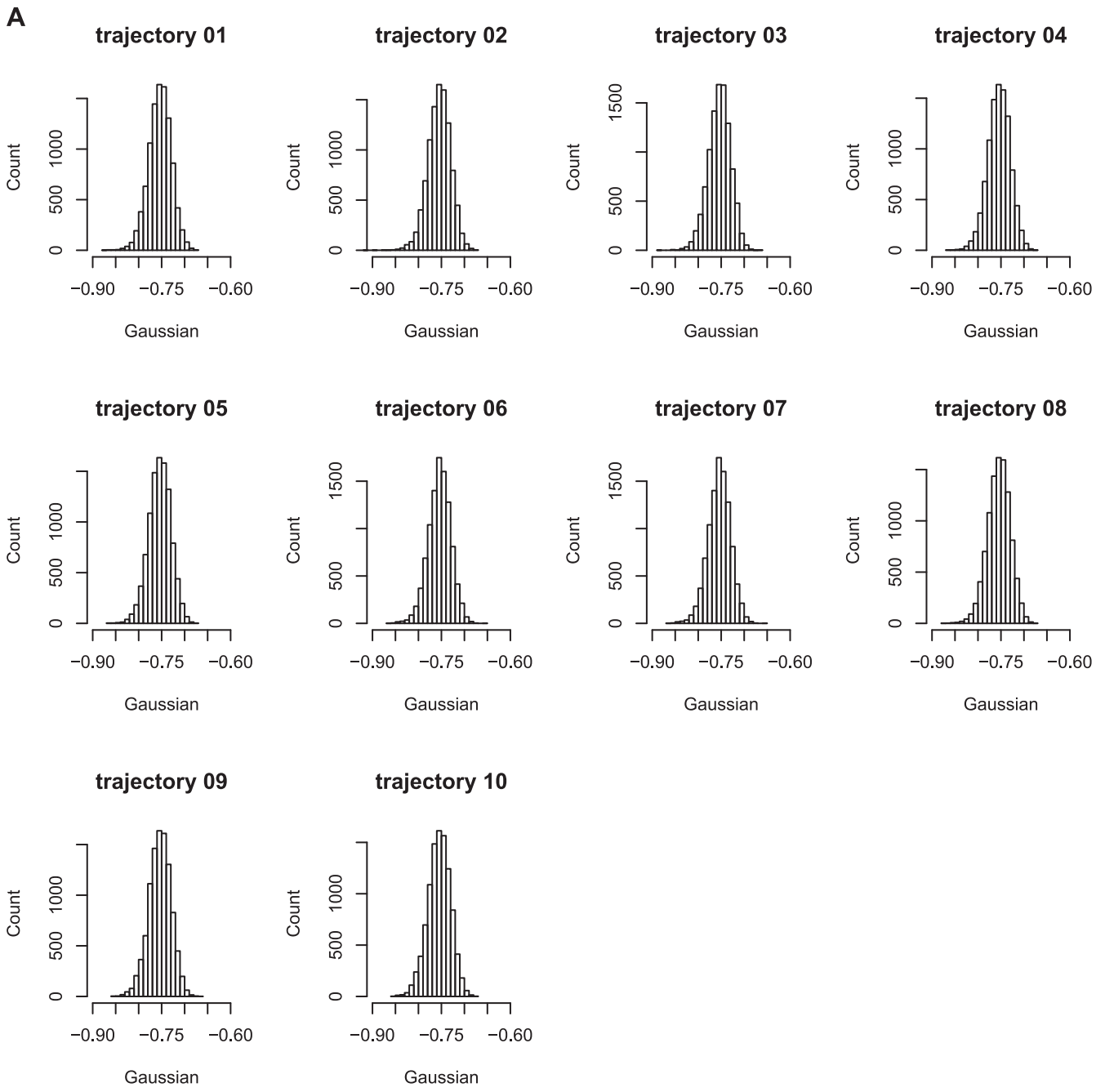
Supplementary Figure 5 Continued



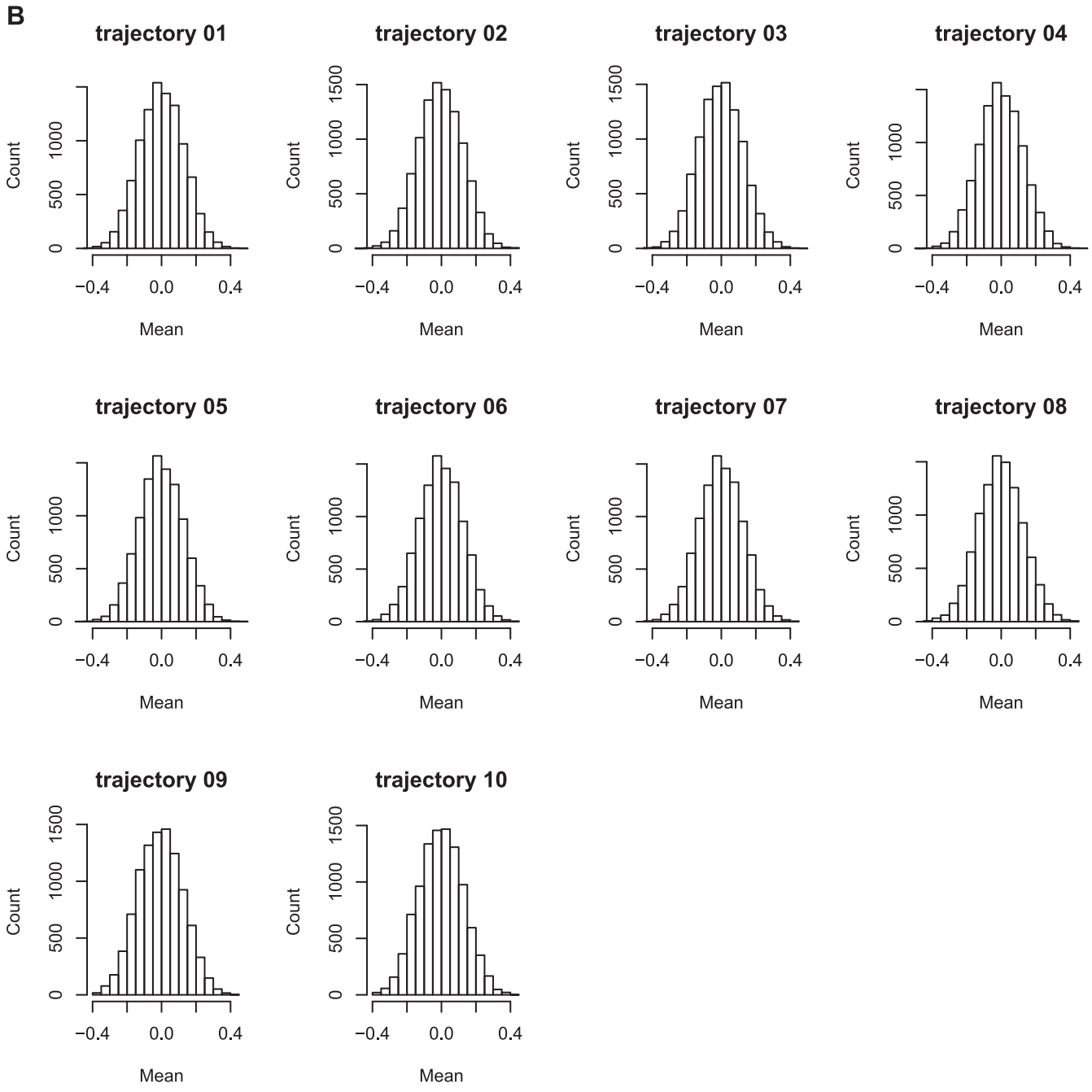
Supplementary Figure 5 Continued



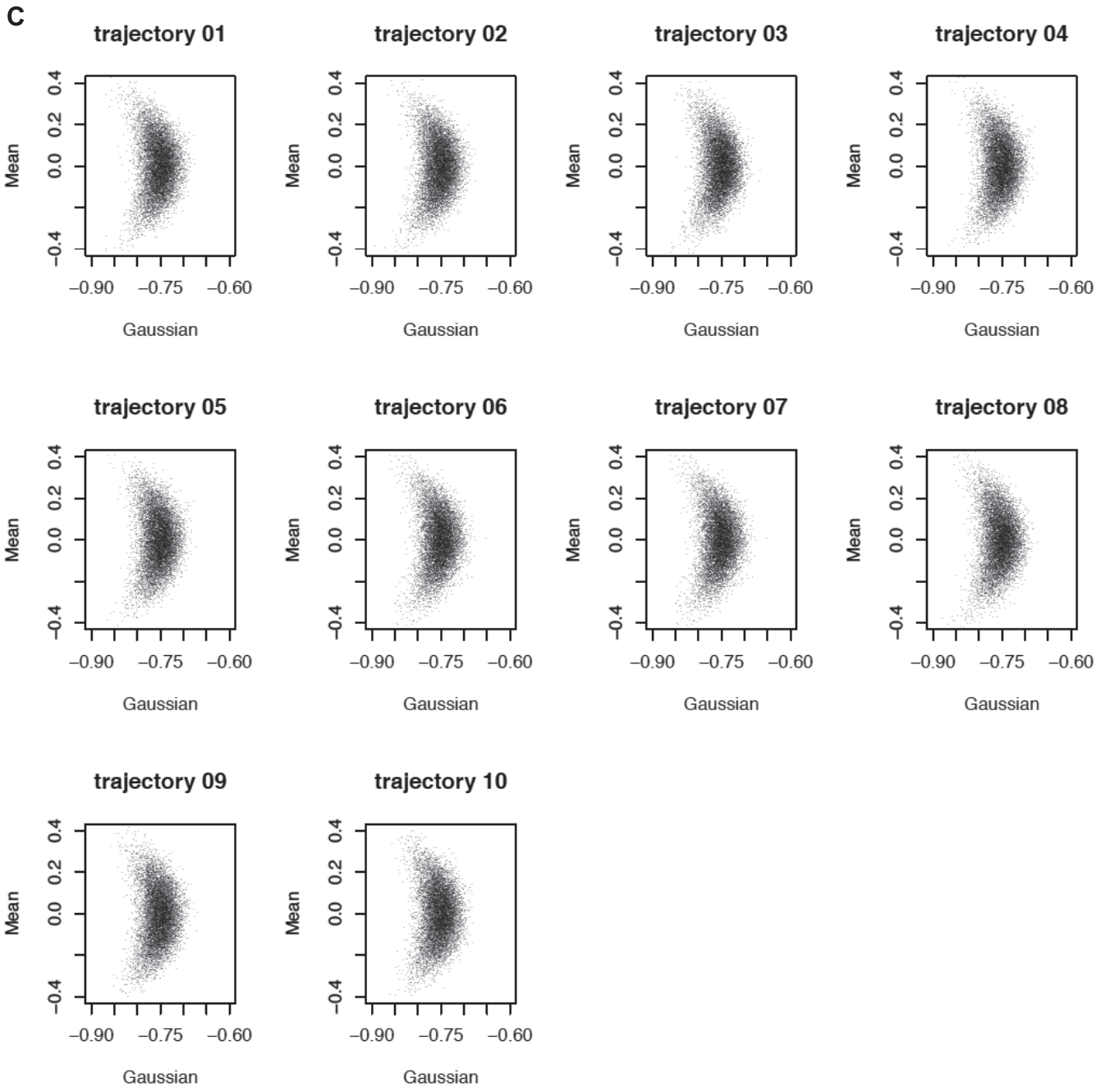
Supplementary Figure 6 Adenine hinge conformations from each trajectory of ten runs of molecular dynamics simulation. **A.** The histograms of Gaussian curvature. **B.** The histograms of mean curvature. **C.** Relationship between the Gaussian and mean curvatures.



Supplementary Figure 6 Continued



Supplementary Figure 6 Continued



Supplementary Figure 7 Probability density function map of the torsion angles γ and χ in each trajectory. The probability is depicted in rainbow colour scheme from blue to red in ascending order as shown in the colour bar.