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.



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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.



-0.15 Gaussian Curvature

0.00

-0.30

-0.30 -0.15 0.00 Gaussian Curvature

Supplementary Figure 2 Continued





trajectory 02





Mean Curvature

trajectory 09



Mean Curvature



trajectory 06

Mean Curvature

trajectory 10









trajectory 07







Mean Curvature

Supplementary Figure 2 Continued



-0.05 -0.30 -0.15 0.00

Gaussian



Gaussian

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 .





tau0

-60 0 40

200

0

tau0

Supplementary Figure 3 Continued





trajectory 02

trajectory 05



trajectory 09





trajectory 06

trajectory 10





trajectory 03



trajectory 07





7





tau4

Supplementary Figure 3 Continued



tau0

tau0

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.



Gaussian

Gaussian

Supplementary Figure 4 Continued





Contraction of the second seco

Supplementary Figure 4 Continued



Gaussian

-0.025

-0.010

Gaussian

-0.010

-0.025

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





trajectory 02

1500

500

0

-0.04

trajectory 06

Count



trajectory 03



trajectory 04

trajectory 07





0.00

Mean

0.04

1500

500

0

-0.04



trajectory 05

trajectory 09

trajectory 10

0.00

Mean

0.04





Supplementary Figure 5 Continued



-0.62 Gaussian

-0.70

-0.04 -0.70 -0.62

Gaussian

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



trajectory 05

1000

500

0

-0.4

Count



trajectory 06

1000

500

0

-0.4

Count

Count

trajectory 02



trajectory 03



trajectory 08

0.4

trajectory 04

trajectory 07

0.0

1000

500

0

-0.4

Count



trajectory 09

0.0

Mean

0.4

0.0

Mean

0.4





Supplementary Figure 6 Continued



-0.75 Gaussian

-0.90

-0.4 -0.60 -0.90 -0.75

Gaussian

-0.60

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.

