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Structural Properties of DNA Base Pair Mismatches with Molecular Dynamics ADELAIDE KINGSLAND, LUTZ MAIBAUM, University of Washington — Mismatches in DNA can have disastrous consequences, yet little theoretical study has been done to elucidate the mechanics of DNA mismatches. Further, the exact mechanism by which mismatches are repaired is unknown. Both matched and mismatched DNA sequences were studied using molecular dynamics in biased and unbiased simulation. Significant differences were found between matched and mismatched pairs in structure, hydrogen bonding, and base flip. Mismatched pairs show greater movement in the x-y plane and a lower free energy barrier for base flip than do matched pairs. This supports experimental findings that the primary mechanism utilized by mismatch repair enzymes is to fully flip the base into the active site. Because the free energy of base flip is lower for mismatched systems, mismatch repair enzymes should show an enhanced preference for mismatched pairs.

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