# Base Flipping Mechanism of DNA Repair Enzyme Fpg Examined via Nudged Elastic Band Simulations

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A central mechanism of 8-oxoguanine repair by the glycosylase Fpg concerns the path by which the damaged base is everted from an intrahelical position to an extrahelical position in the active site of the enzyme. To elucidate the effect of a wedge residue mutation, which confers a loss of function, on the Fpg-DNA complex, we present a study of the conformational changes which occur during this base eversion process as described using the nudged elastic band (NEB) model. The NEB model determines the minimum potential energy pathway of a conformational transition based on endpoint configurations. Decoupling of the forces applied to each image on the chain results in a minimum energy path. The implementation of the NEB model on the fully solvated Fpg-DNA system (60000+ atoms), will be discussed.