Supplemental Information for Carbinolamine Formation and Dehydration in a DNA Repair Enzyme Active Site

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Analytical and other software

Most analyses described here were carried out with Perl scripts developed in-house. The statistics described by Gore, *et al.* [1] were calculated as described in file S4.pdf. As a final step, many of the Perl scripts wrote programs in the Gri graphics language (Gri language for scientific illustration; Dan Kelley, Department of Oceanography, Dalhousie University, Halifax, NS B3H 4J1). The Gri programs generated the graphs in the body of the text. These Perl scripts will be made available upon emailed request, but with no further support. Molecular graphics were prepared with MOLSCRIPT [2] and Raster3D [3] directly from PDB files of the quantum region written by AMBER. The orientation matrices for the desired view of the quantum region were generated with VMD [4].

References

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