Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information for "A hybrid all-atom/coarse grain model for multiscale simulations of DNA"

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Helical parameters for systems S_{AA2} and S_{H2}

Structural parameters at the AA region of S_{H2} (base pairs G_8 to C_{13}) show a good match against those of S_{AA2}, in close analogy with the results found for S_{H1} and S_{AA1} (Figure S1). Notably, the sequence specific behavior in Twist, Roll or Shift is well reproduced in the atomistic region of S_{H2}. There are differences in both S_{H2} and S_{AA2} respect to experimental values for Twist and Slide. Such departures are always related to pyrimidine-purine steps (TG, CA), which show a higher dispersion in the experimental data set[2].

References

1 S. Arnott, P. J. Campbell-Smith and R. Chandrasekaran, in Handbook of biochemistry and molecular biology, ed. Nucleic Acids, CRC Press, Cleveland, 3rd edn., 1976, vol. II, pp. 411-422.

2 A. Pérez, F. Lankas, F. J. Luque and M. Orozco, *Nucleic Acids Res.*, 2008, **36**, 2379-2394.

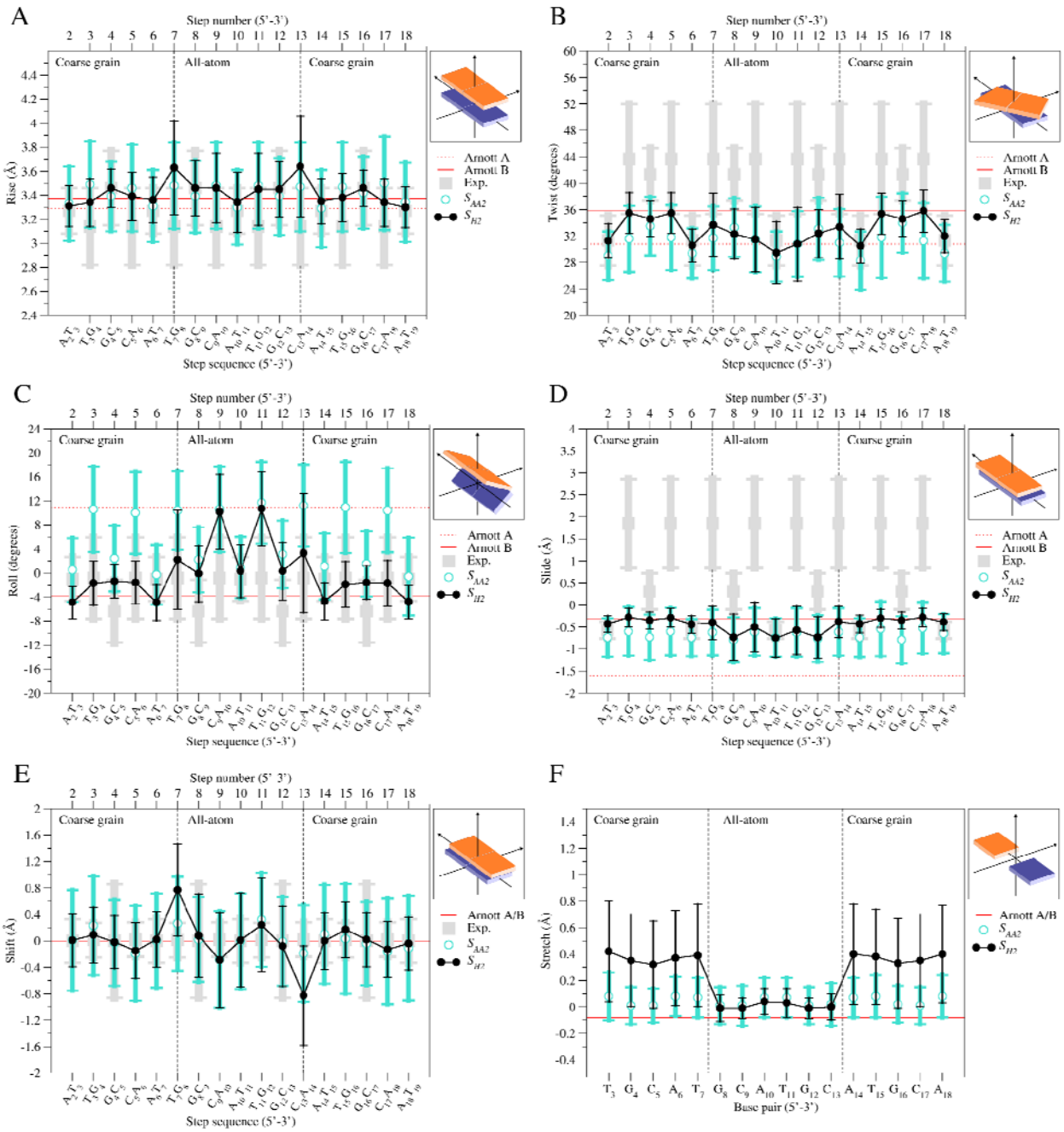

Figure S1. Comparison of DNA helical parameters for systems S_{AA2} and S_{H2}. A) Rise, B) Twist, C) Roll, D) Slide, E) Shift and F) Stretch. The vertical dashed lines indicate the AA/CG frontiers in S_{H2}. The canonical values for A and B DNA forms according to Arnott et al.[1] are indicated with dashed and continuous red lines, respectively. Filled and open circles represent data for systems S_{H2} and S_{AA2}, respectively. Squares correspond to averaged experimental data taken form reference 2. Standard deviations are reported as error bars.