Supplemental Information:

Thermodynamic and Structural Determinants of Differential Pdx1 Binding to Elements from the Insulin and IAPP Promoters

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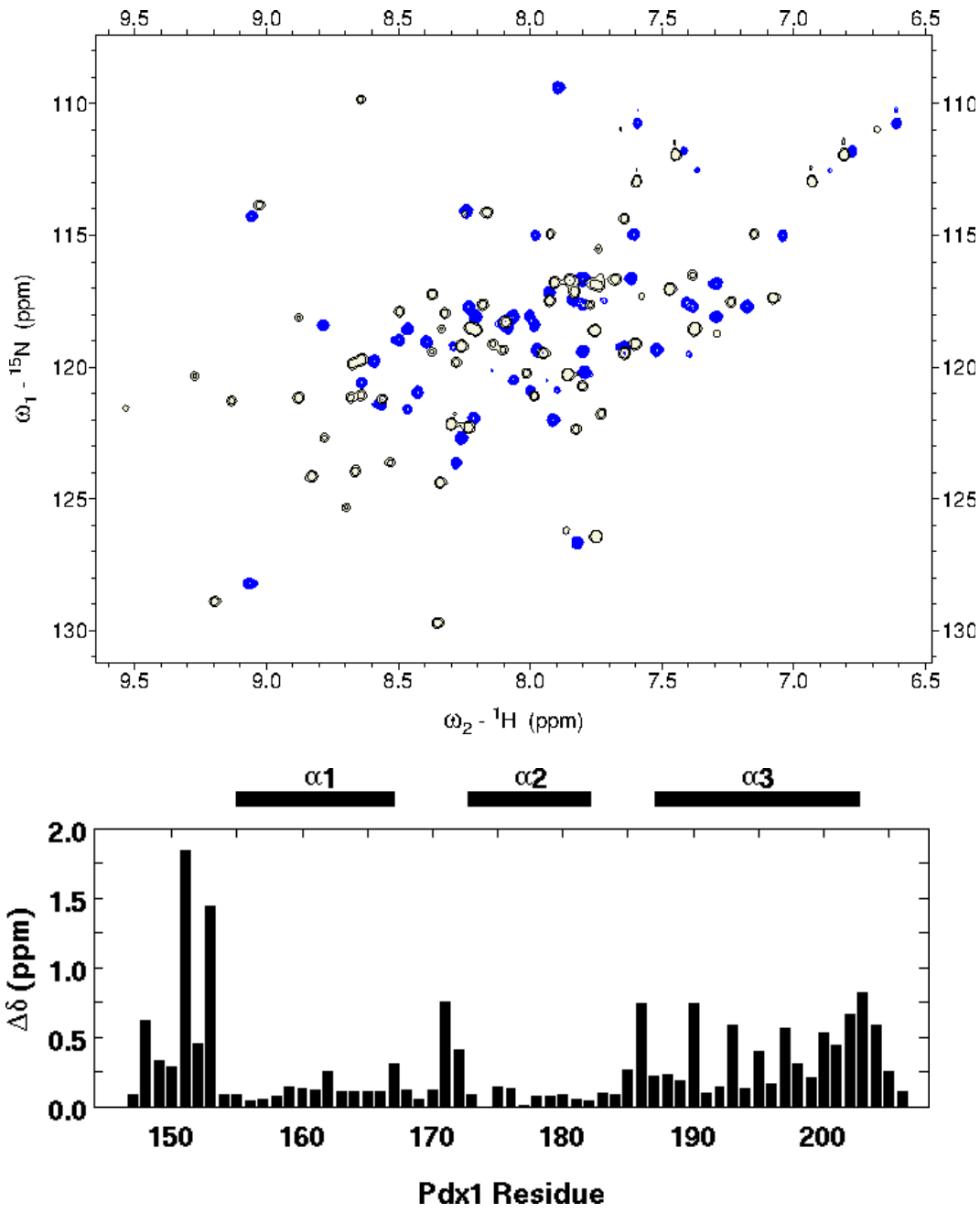

Figure S1. Chemical shift change between apo-Pdx1 and the Pdx1-DNA complex. Overlaying the $^{1}H,^{15}N$-HSQC (top) of apo-Pdx1 (blue) and the Pdx1-DNA complex (black and tan) reveals that resonances are well resolved and the lines are sharp in both spectra. Change in chemical shift between the two states is recorded as a function of residue number (bottom) by taking the weighted average chemical ^{1}H and ^{15}N chemical shift change as $\Delta\delta = SQRT((\Delta H)^2 + (\alpha\ \Delta N)^2)$, where $\alpha = 0.1$ normalizes the ^{1}H and ^{15}N chemical shift ranges. Secondary structure assignments from the crystal structure of Pdx1 are reported above the graph for clarity. Experimental conditions for both samples were 20 mM cacodylate, pH 6.5, 100 mM KCl, 298K.

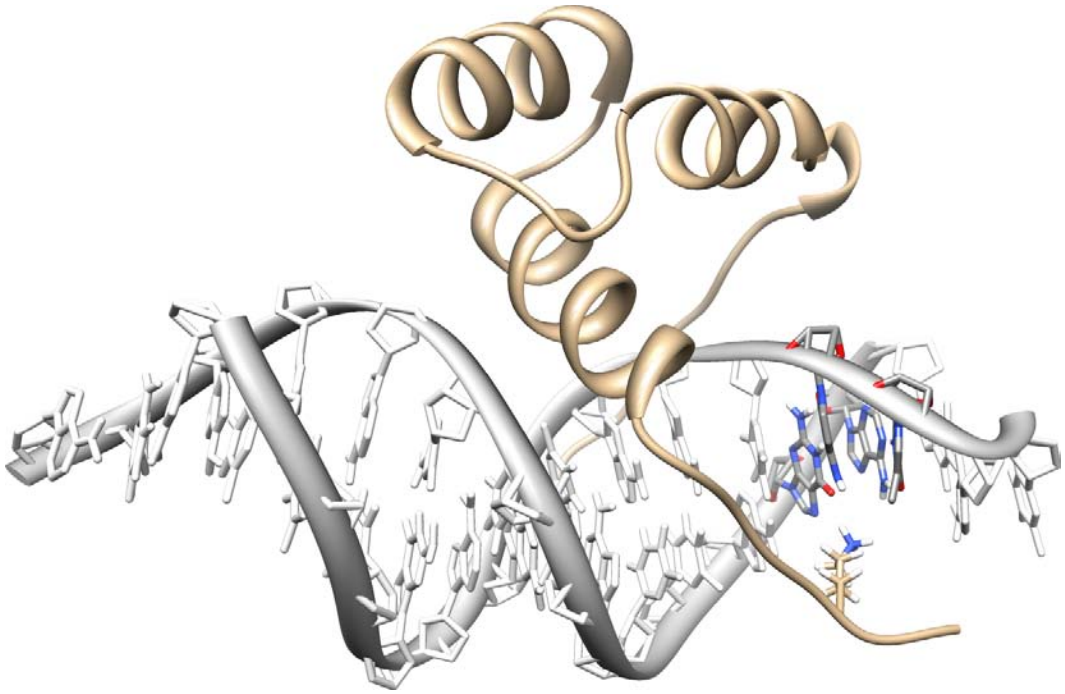

Figure S2. Representative snapshot from the Pdx1-DNA_{CON} simulation, showing the C-terminal tail of Pdx1 inserted into the major groove of the DNA. The side chain of Lys-203 is shown interacting with nucleobases from the T·A and C·G base pairs in the 3´-positions relative to the core TAAT motif. The atoms corresponding to these four bases are indicated in color, whereas all other nucleobases are represented in white for clarity.

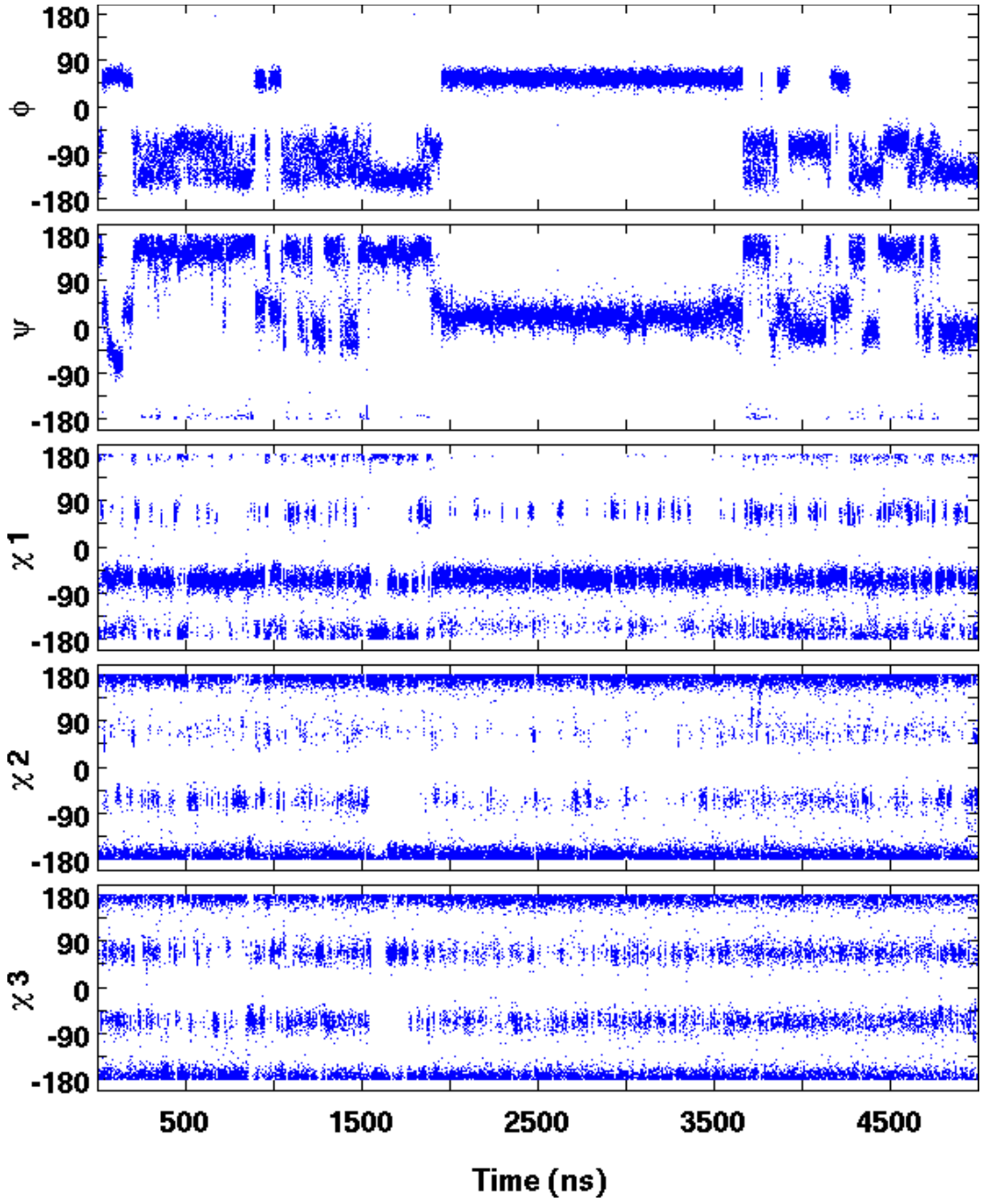

Figure S3: Torsion angle values for Arg-150 in apo-Pdx1 plotted as a function of time during the course of the 5 μs trajectory. Data points are reported once per 200 ps of simulation time.

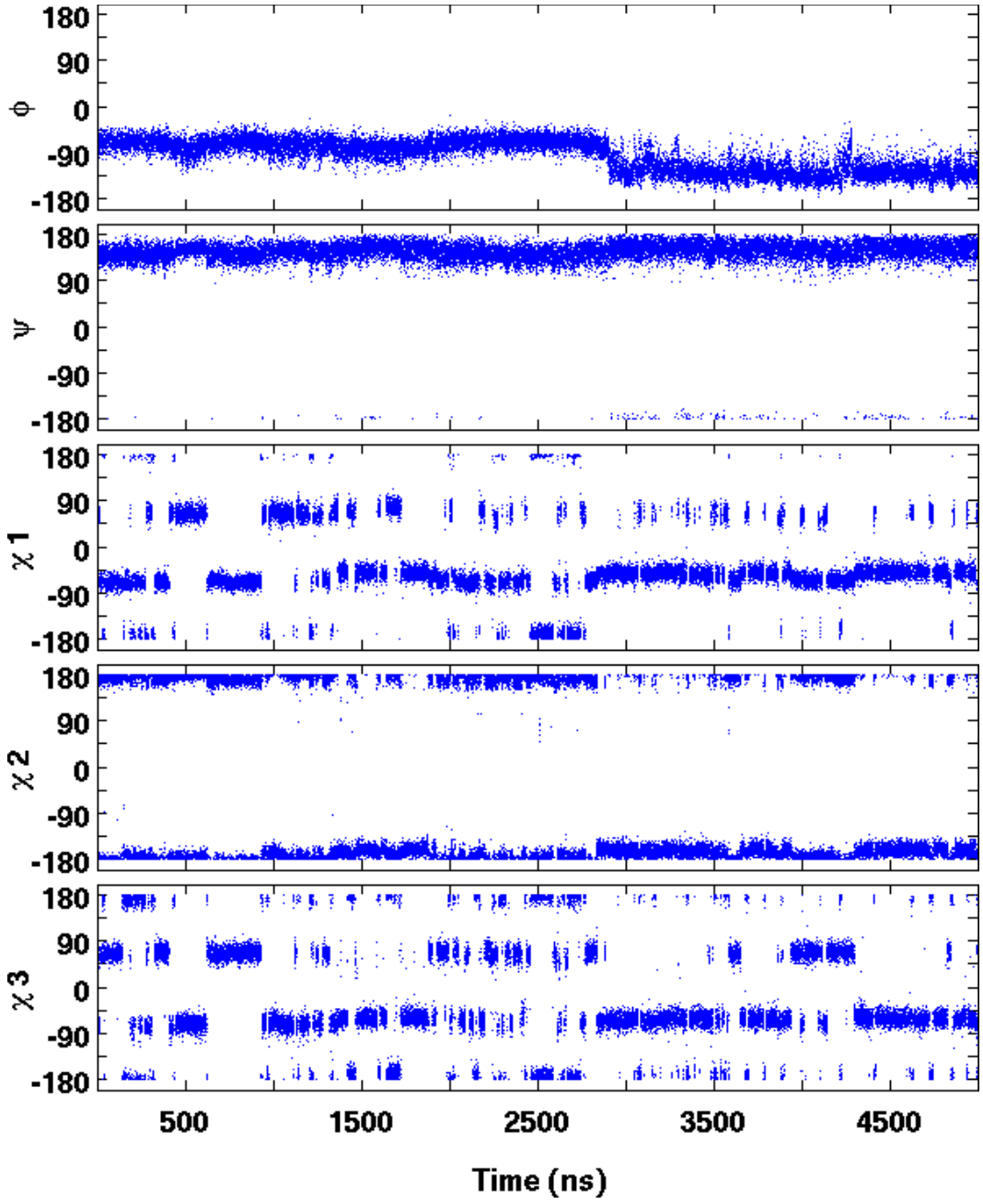

Figure S4: Torsion angle values for Arg-150 in the Pdx1-DNA$_{CON}$ complex, plotted as a function of time during the course of the 5 μs trajectory. Data points are reported once per 200 ps of simulation time.

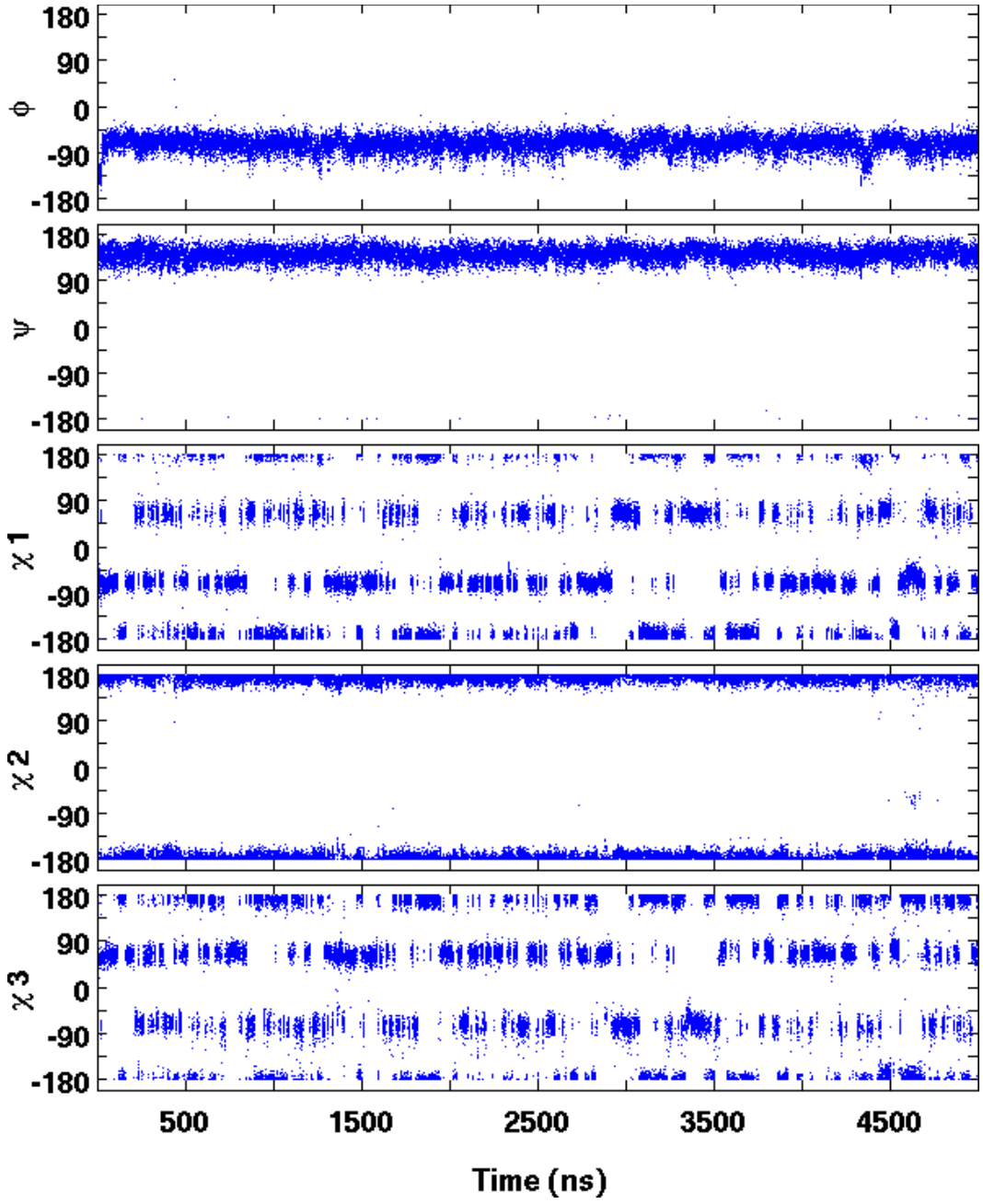

Figure S5: Torsion angle values for Arg-150 in the Pdx1-DNA(TTAAT) complex, plotted as a function of time during the course of the 5 μs trajectory. Data points are reported once per 200 ps of simulation time.

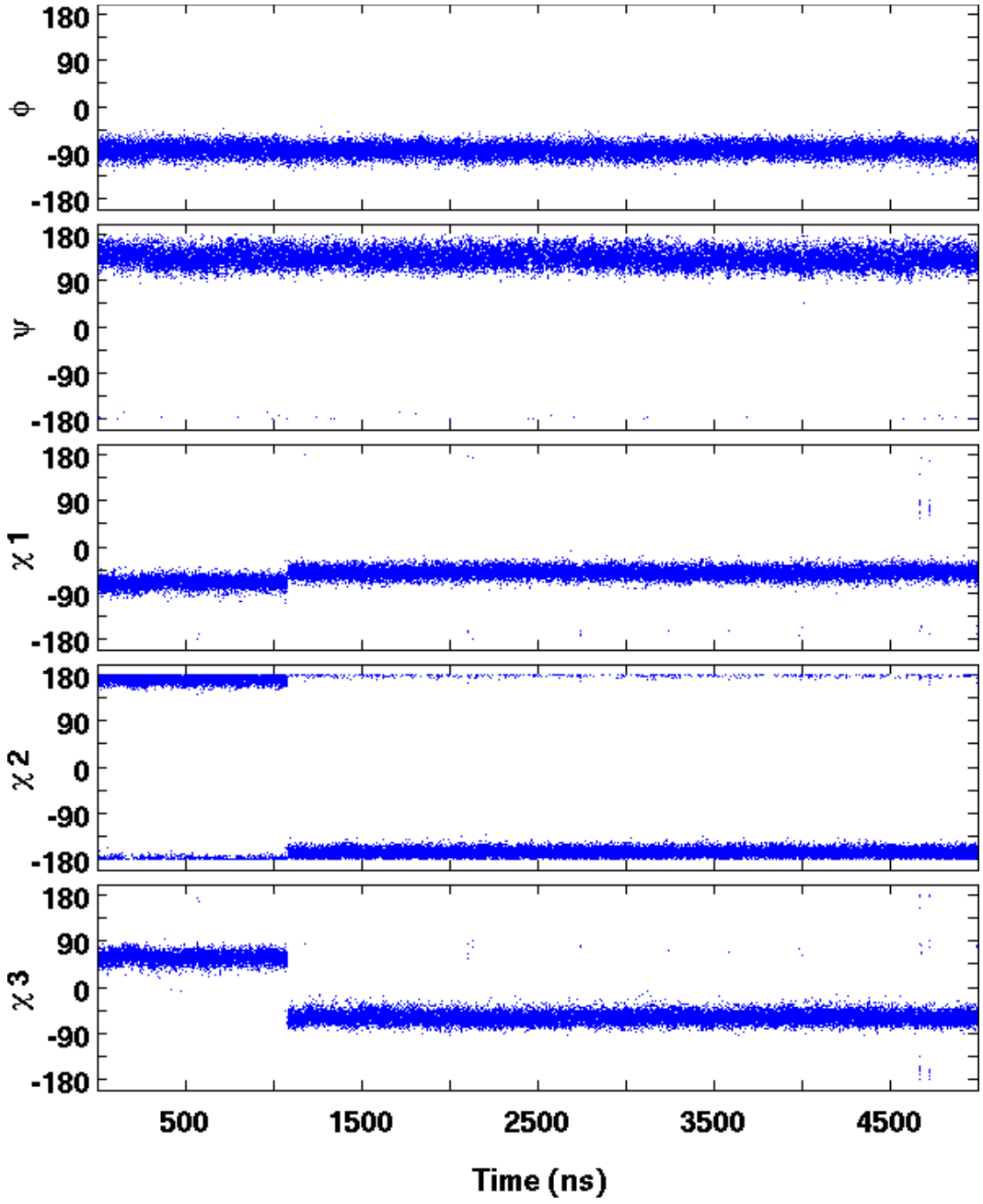

Figure S6: Torsion angle values for Arg-150 in the Pdx1-DNA(GTAAT) complex, plotted as a function of time during the course of the 5 μs trajectory. Data points are reported once per 200 ps of simulation time.

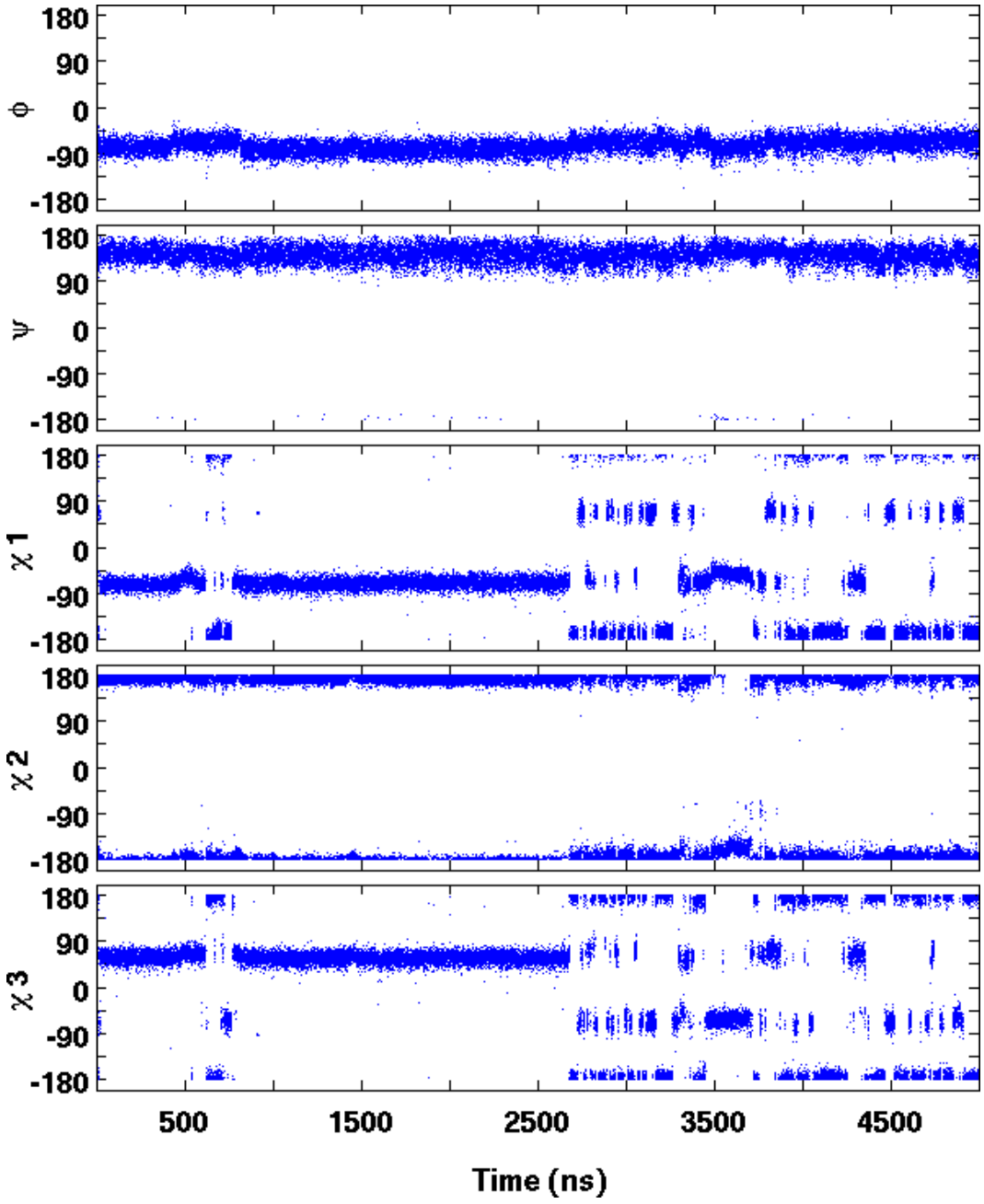

Figure S7: Torsion angle values for Arg-150 in the Pdx1-DNA(ATAAT) complex, plotted as a function of time during the course of the 5 μs trajectory. Data points are reported once per 200 ps of simulation time.