Supplementary material for "The natural DNA bending angle in the lac repressor headpiece - O1 operator complex is determined by protein-DNA contacts and water release", by Daniel Barr and Arjan van der Vaart

Supplementary Figure S1. Convergence of the variance-covariance matrix for the unrestrained and restrained protein-DNA simulations (see text).
Supplementary Figure S2. Hotspot analysis for the system at (A) the unrestrained angle, as well as for the restrained simulations at angles of (B) 27°, (C) 29°, (D) 30°, (E) 34°, (F) 39°, (G) 42°, (H) 47°, (I) 51°, and (J) 55°. Secondary structure elements are labeled as in Fig. 4 and 5. The intensity of color for any pairwise interaction represents the intensity of energetic coupling between those residues.
**Supplementary Figure S3.** Distortion energy of the DNA throughout the restrained angle simulations for (A) 27°, (B) 29°, (C) 30°, (D) 34°, (E) 39°, (F) 42°, (G) 47°, (H) 51°, and (I) 55°.
Supplementary Figure S4. (A) total distortion energy of DNA, and (B) the total contact occupancy of all base-specific protein-DNA contacts.
Supplementary Figure S5. Number of interstitial waters in the protein-DNA interface for (A) the left (black) and right (gray) sites, and (B) the polar (black) and nonpolar (gray) surfaces of the complex.