

Supporting Information for Phillips, C.M., Schreiter, E.R., Stultz, C.M., and Drennan, C.L. Manuscript Entitled: “Structural Basis of Low Affinity Nickel Binding to the Nickel-Responsive Transcription Factor NikR from *Escherichia coli*”

Figure S1. Low affinity nickel site 4 is stabilized by a crystallographically-related DNA molecule. NikR-DNA crystal structure shown in Figure 2 is again shown in color with nickel anomalous maps for orientation. The grey NikR-DNA molecule is a crystallographically related molecule whose DNA helps stabilize site 4 on the neighboring NikR-DNA complex. DNA and H48 are in stick form for reference (inset), the rest of the structure is represented in cartoon form.

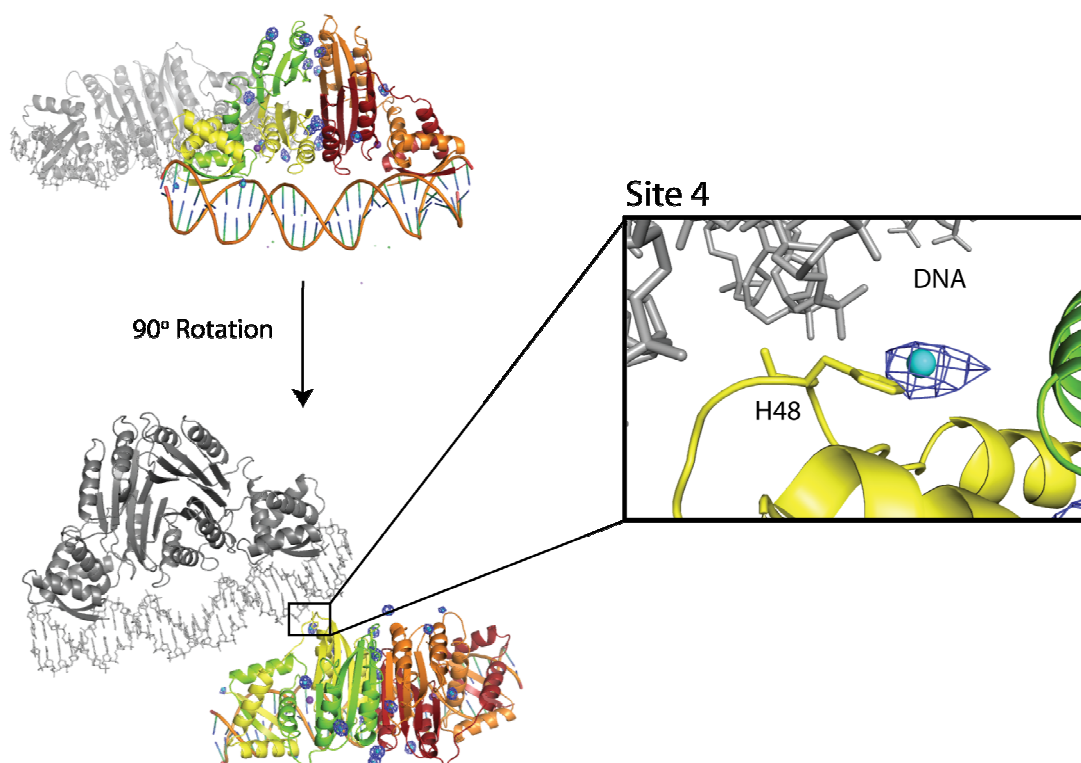


Figure S2. Representative composite omit density in the NikR structure with excess nickel. The NikR structure with excess nickel ions is shown on the left and a close up of one of the four high affinity nickel sites is shown on the right. The dimer from the asu is shown in green and yellow with the composite omit map contoured at $1.0\ \sigma$ in pink. The crystallographically related dimer in orange and red is shown for orientation. The composite omit map around the high affinity nickel site and four coordinating ligands is also contoured at $1.0\ \sigma$ (inset). Coloring is the same as in Figures 2 and 3 with the detergent molecule shown in stick form with magenta bonds (left).

