Supplemental Data

Pliable DNA Conformation of Response Elements Bound to Transcription Factor p63

Chen Chen, Natalia Gorlatova, and Osnat Herzberg

From the W.M. Keck Laboratory for Structural Biology, Institute for Bioscience and Biotechnology Research and the Department of Chemistry and Biochemistry, University of Maryland, 9600 Gudelsky Drive, Rockville, Maryland 20850

Corresponding author: Osnat Herzberg, Institute for Bioscience and Biotechnology Research 9600 Gudelsky Drive, Rockville, MD 20850, Tel: 240-314-6245, Fax: 240-314-6255, E-mail: osnat@umd.edu

SUPPLEMENTAAL FIGURE LEGENDS

Supplemental Figure S1. A. Crystal packing of p63DBD/22-GC structure. The view is down the unique *b* axis, which is perpendicular to the a/c plane. The protein molecules are colored in green and the DNA in blue. One asymmetric unit (colored in red) contains two p63DBD molecules and a single DNA strand. The DNA double helix and the protein tetramer are generated by the crystallographic 2-fold symmetry axis at the origin (with the protein and DNA in the other asymmetric unit colored in magenta). B. Stereo representation of the electron density map associated with the 22bp-GC DNA. The $2F_o$ - F_c composite omit map is contoured at 1.5 σ . The DNA is shown in a multi-color stick model, and the map is colored in light blue.

Supplemental Figure S2. Similarity and difference between the p63DBD/22bp-AT and p63DBD/22bp-TA structures. A. The structure of p63DBD/22bp-AT (colored in green) is almost the same as that of p63DBD/22bp-TA (colored in gray), with an exception due to the spacer sequence difference. In both structures the two dimers do not contact one another, as indicated by the surface representation. B. Zooming into the region around the 2-bp DNA spacers, outlined in the grey square in panel A.

Supplemental Figure S3. The type III interface of the p63DBD/22bp-GC structure generated by crystallographic symmetry operator across biological units. Two equivalent molecules are colored green and cyan, respectively. This interface involves interdigitating loops L2B, S5/S6, and S7/S8 and a sole hydrogen bond network involving water molecules is shown in dashed lines.



В

Figure S2



В





