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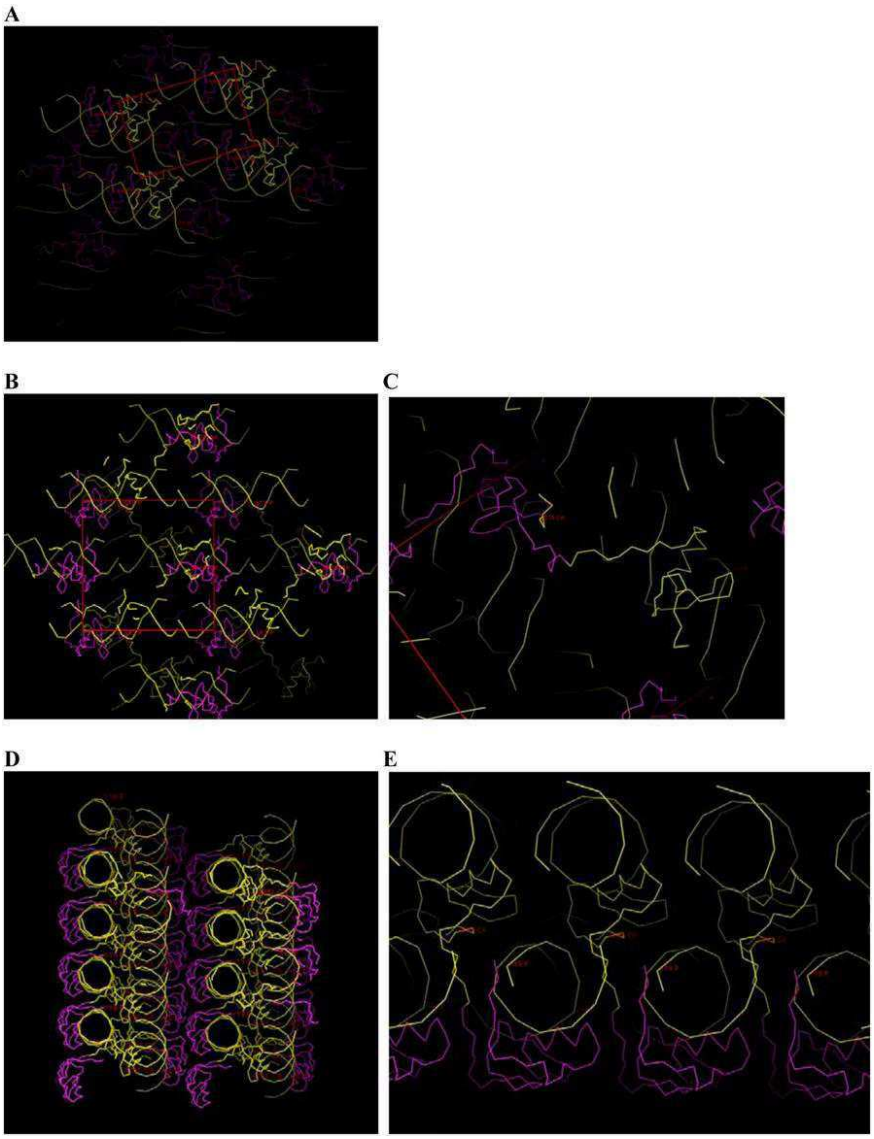

Figure S1. Crystal Packing of Different GATA3/DNA Complexes, Related to Figure 1

(A) Complex 1. The crystal belongs to the $P2_1$ space group. Each asymmetric unit contains one GATA3 DBD bound to a palindromic dsDNA substrate. The DNA molecules form a pseudo-continuous helix along the diagonal of the *ab* plane of the unit cell. Two layers of DNA follow two crossing diagonals of the *ab* plane.

(B and C) Complex 2. The crystal belongs to the $P2_1$ space group, with two copies of GATA3 DBD and two dsDNA substrates in each asymmetric unit. The DNA molecules form a pseudo-continuous helix along the *a* and *b* axes of the unit cell, which explains why the unit cell axes *a* and *b* have lengths that are approximately equal to the length of 20-mer dsDNA (65 Å). The two layers of DNA molecules run perpendicularly to each other. The N-finger (yellow) and C-finger (magenta) of GATA3 bridge separated DNA fragments arranged in parallel within the same plane, not between the layers.

(D and E) Complex 3. The crystal belongs to the C_2 space group, with one GATA3 DBD and one dsDNA molecule in each asymmetric unit. The DNA molecules also form a pseudo-continuous helix but do not align with any major unit cell axis. The axes of DNA in alternating layers run across each other at an angle of ~30°. The packings of different layers of DNA are mediated by the N-finger and C-finger, respectively. The N-finger layer is sandwiched by DNA layers and therefore is densely packed, whereas the C-finger layer is formed by protein–protein interactions between symmetry-related C-fingers. The N-finger and C-finger of the same GATA DBD bind to sites on separated DNA molecules from different DNA layers that sandwich the N-finger.

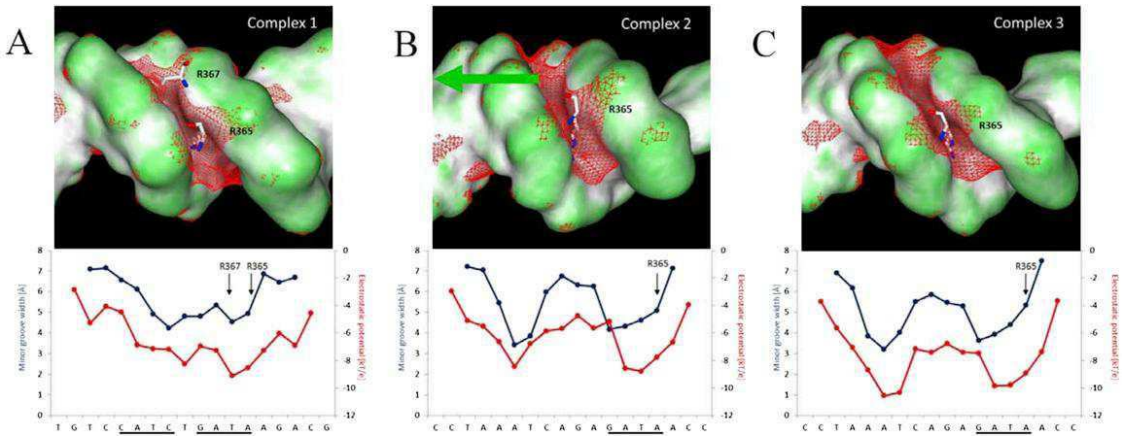

Figure S2. Protein–DNA Interactions Representing the Shape Readout between GATA Arginine Residues and the Shape-Dependent Negative Electrostatic Potential in the Minor Groove, Related to Figure 2

The DNA shape is shown in green and dark gray for convex and concave surfaces, respectively. The red mesh represents a −5 kT/e isopotential surface. The plots below show the correlation between minor groove width (blue plots) and electrostatic potential (red plots), which attracts arginine contacts.

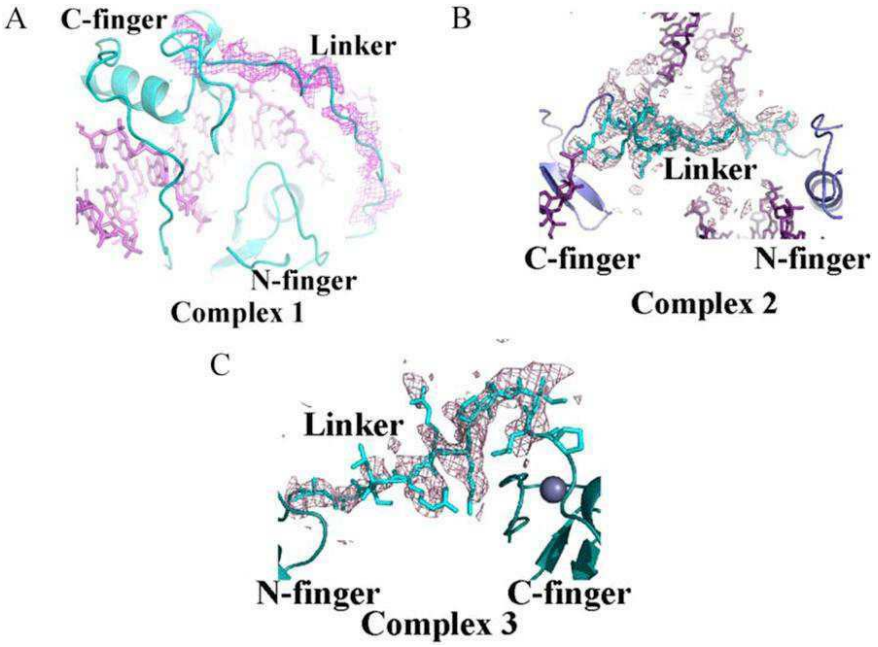

Figure S3. Electron Density Maps of Linker Regions, Related to Figure 4

(A) Complex 1. (B) Complex 2. (C) Complex 3.

It is apparent in this figure that although the protein side chains cannot be resolved due to flexibility, the backbone of the linker can be correctly traced. The electron density is calculated from composite omit map.

Figure S4. Sequence Alignment between the GATA3 N-finger and C-finger, Related to Figure 4

The homology is indicated according to standard convention below the sequence alignment.