



**Supplementary Figure 1** Overall charge distribution of the NBD dimer. **(a)** Different views of the NBD dimer (surface electrostatic potential) bound to two DNA molecules (gray stick model) are shown. Rotating the complex in the top panel by  $90^\circ$  shows that the helix axes of the two DNA molecules are offset by 30 degrees. Both sides of the NBD dimer are highly electropositive (blue) and favor DNA binding. **(b)** A side view of one of the NBD-DNA interfaces highlights the electrostatic and conformational complementarity between the NBD and DNA. **(c)** A close-up view of the GGRPR motif in the minor groove. The tract of five thymines in the nonamer is highlighted in yellow.