

Supplementary material

Table S1. Root mean square deviations between the conformational snapshots drawn from the MD simulation of the TBP-DNA complex and the experimental crystallographic structure (PDB: 1CDW) <sup>1</sup>. The last column shows interface areas calculated with the program Intervor <sup>2</sup>.

<b>RMSD ( Å )</b>	<b>MD1</b>	<b>MD2</b>	<b>MD3</b>	<b>MD4</b>	<b>Interface area ( Å<sup>2</sup>)</b>
1CDW	1.73	2.54	2.92	2.50	2005
MD1		1.79	2.37	1.82	2024
MD2			1.39	1.47	2118
MD3				1.63	2034
MD4					2072

n.b. Values are calculated for all non-hydrogen atoms of DNA and for all non-hydrogen backbone atoms of the protein. RMSD values for DNA alone are 1.36 - 3.59 Å, and for TBP alone are 0.74 - 1.49 Å

Table S2. Root mean square deviations between the conformational snapshots drawn from the MD simulation of the SRY-DNA complex with respect to the experimental NMR structure (PDB:1J46) <sup>3</sup>. The last column shows interface areas calculated with the program Intervor <sup>2</sup>.

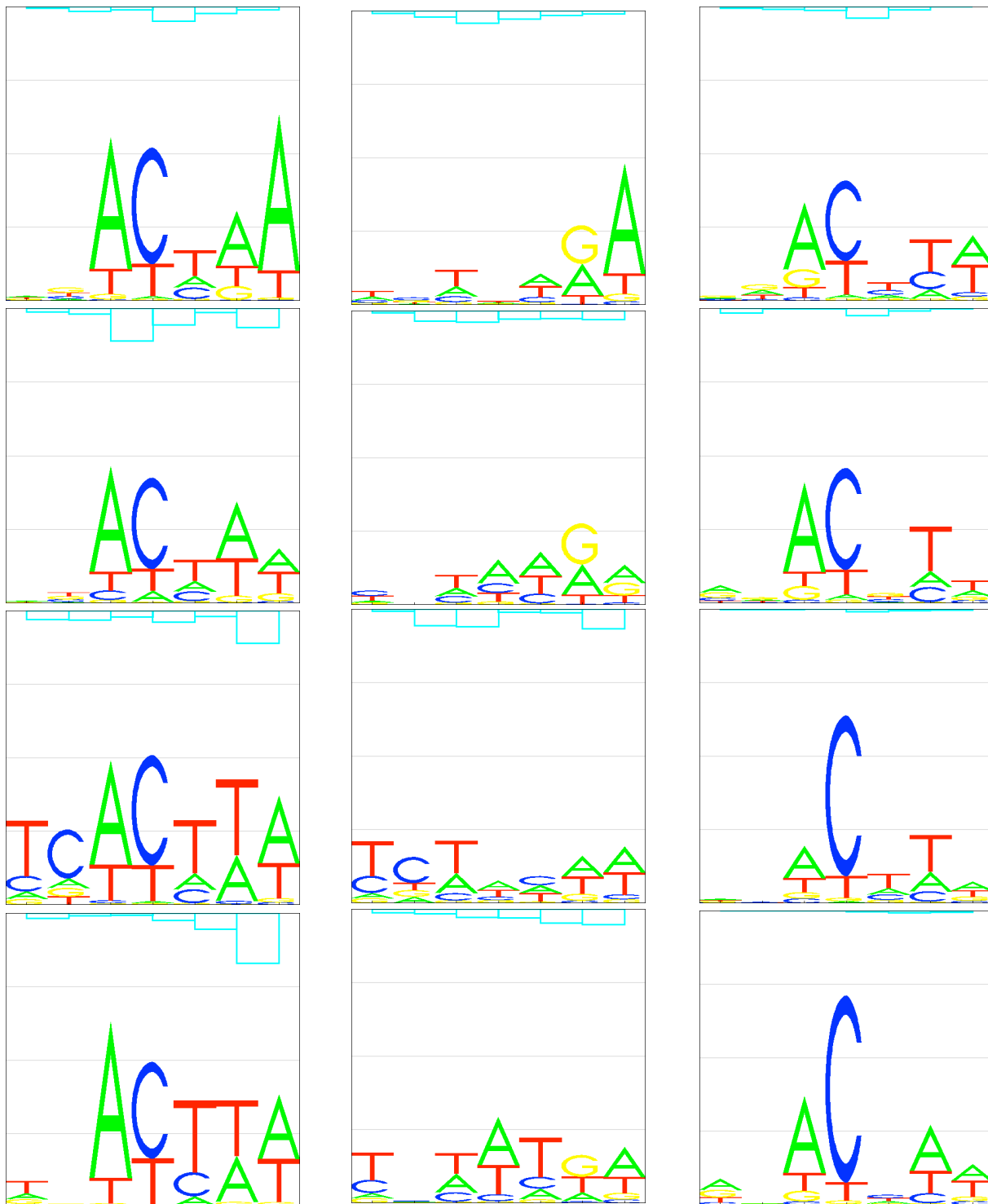
<b>RMSD ( Å )</b>	<b>MD1</b>	<b>MD2</b>	<b>MD3</b>	<b>MD4</b>	<b>Interface area ( Å<sup>2</sup>)</b>
1J46	2.26	2.56	2.84	2.56	2241
MD1		1.32	1.45	1.73	2322
MD2			1.50	1.79	2368
MD3				1.20	2366
MD4					2377

n.b. Values are calculated for all non-hydrogen atoms of DNA and for all non-hydrogen backbone atoms of the protein. RMSD values for DNA alone are 1.03 - 2.53 Å, and for SRY alone are 1.33 - 2.91 Å.

Figure S1. Binding selectivity logos for the TBP-DNA complex derived from four snapshots taken at regular intervals during a 10 ns molecular dynamics trajectory. The results for the four conformations of the protein complex are shown in the four sets of images, with the time axis increasing from top to bottom of the figure. Each set of three horizontal windows shows the total binding selectivity (left), the selectivity due to DNA deformation (center) and that due to protein-DNA interaction (right).



Figure S2. Binding selectivity logos for the SRY-DNA complex derived from four snapshots taken at regular intervals during a 10 ns molecular dynamics trajectory. The results for the four conformations of the protein complex are shown in the four sets of images, with the time axis increasing from top to bottom of the figure. Each set of three horizontal windows shows the total binding selectivity (left), the selectivity due to DNA deformation (center) and that due to protein-DNA interaction (right).



## References

- 1 D.B. Nikolov, H. Chen, E.D. Halay, A. Hoffman, R.G. Roeder, S.K. Burley, *Proc Natl Acad Sci U S A*, 1996,**93**, 4862.
- 2 B. Bouvier, R. Grünberg, M. Nilges, F. Cazals, *Proteins*, 2009,**76**, 677.
- 3 E.C. Murphy, V.B. Zhurkin, J.M. Louis, G. Cornilescu, G.M. Clore, *J Mol Biol*, 2001,**312**, 481.