# Supplementary Material

## Predicting the effect of ions on the conformation of the H-NS dimerization domain

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| System | Origin | Number of atoms | Time (ns) |
|---|---|---|---|
| *ap – wt – 2-47* | 1NI8 | 46604 | 8x40 |
| *p – wt – 2-47* | 1LR1, S21C mutation, deletion of 48-58 | 21628 | 8x10 |
| *ap – C21S – 2-47* | 2-47ap, C21S mutation | 46604 | 8x10 |
| *p – wt – 2-58* | 1LR1, S21C mutation | 45484 | 8x40 |
| *ap – wt – 2-58* | 1NI8, addition of 48-58 from 1LR1 | 99176 | 8x10 |
| *p – C21S – 2-58* | 1LR1 | 45484 | 8x40 |
| Starting from anti-parallel | 1NI8, monomer A | 25064 | 8x10 |
| Starting from parallel | 1LR1, monomer A | 44316 | 8x10 |
| *23-43m* | cut from 1NI8, monomer A | 23137 | 8x10 |
| *ap – wt – 23-43* | cut from 1NI8 | 31904 | 8x10 |
| *p – wt – 23-43* | cut from 1LR1 | 19788 | 8x10 |

Table S1 - List of systems, their origin, the total number of atoms and the simulation time. We indicated the different systems by their orientation (anti-parallel – ap; parallel – p), wild type or mutation and the length of the sequence. The system *ap – C21S – 2-47* contains a complex in the anti-parallel conformation of two monomers of length 2-47 with a mutation at position 21 of cysteine to serine. The label *m* indicates that the system contains a monomer, not a dimer.

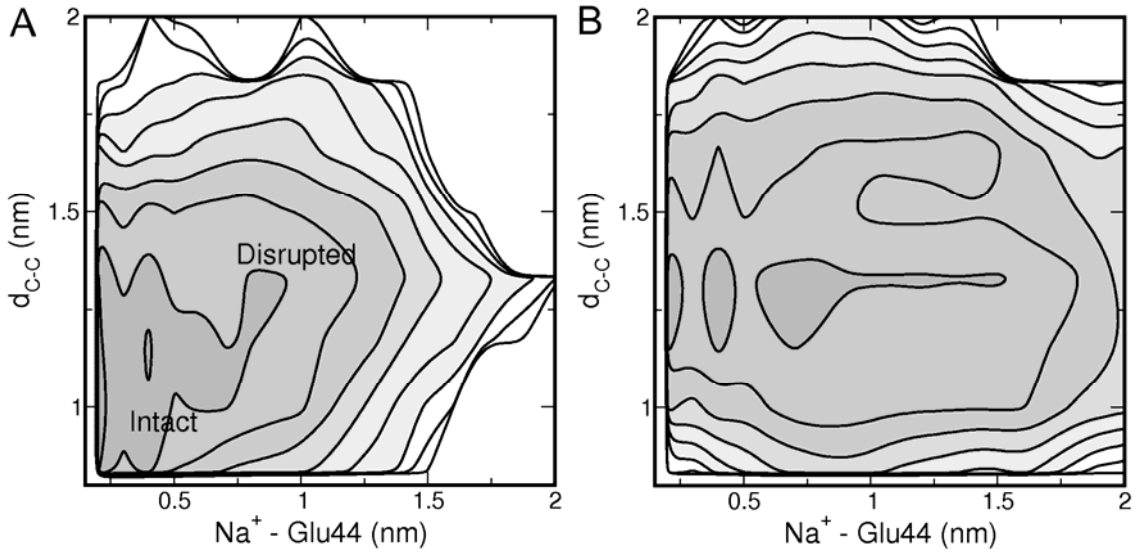


Figure S1
Log-probability plots as a function of the minimum distance between the sidechain of Glu44 and a sodium ion and the distance between C-terminal ends $d_{C-C}$ for (A) the parallel wild type conformation and (B) the parallel C21S mutant.

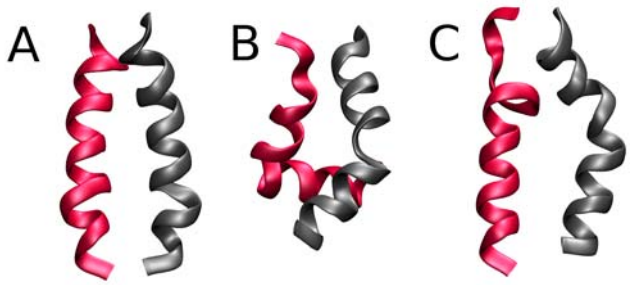


Figure S2
Snapshots of the disrupted parallel trigger sequence complex in ribbon representation. (A) Intact complex (B,C) Disrupted complex.