**Table S3.** MFPTs and numbers of transitions (in parenthesis) between conformational sub-states of the NCBD/ACTR complex computed from the production Langevin simulations. The state assignment criteria are provided in the main text, and the transitions shown are from the one in the row to that in the column. All MFPTs are given in ns.

|  |  |  |  |
| --- | --- | --- | --- |
| **w/o charge****w/charge+0.05M salt****w/charge** | **U** | **CC** | **B** |
| **U** | - | 7.71 (2282)3.50 (2161)1.26 (181) | 11.06 (5)27.20 (2)22.60 (1) |
| **CC** | 1.57 (2287)2.95 (2160)22.10 (180) | - | 8.14 (16)13.13 (52)44.56 (108) |
| **B** | 1420.5 (1)368.77 (3)165.00 (2) | 818.89 (21)274.24 (51)190.80 (108) | - |