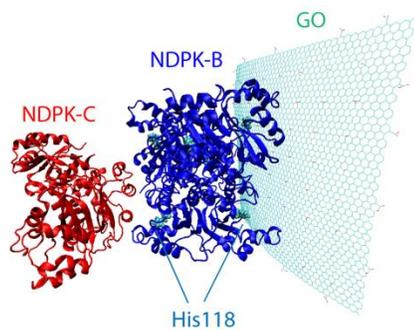
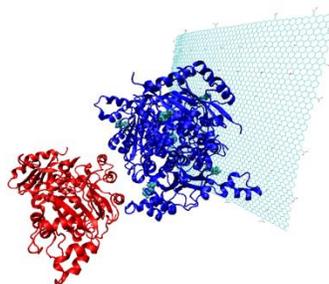


Figure S1. Screenshots of the NDPK-BC system at four points throughout the simulation: (a) 0 ns; (b) 75 ns; (c) 150 ns; (d) 250 ns. The position of the observer remains the same for all four screenshots.

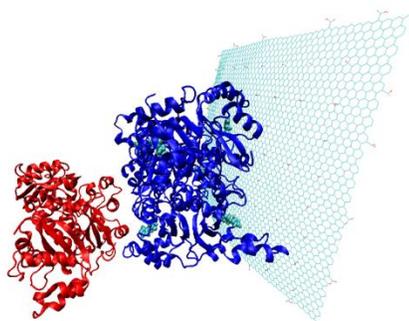
a 0 ns



c 150 ns



b 75 ns



d 250 ns

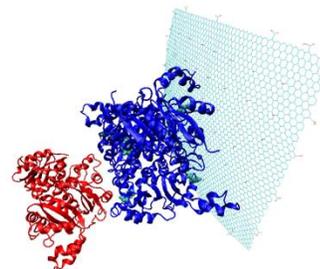


Figure S2. Screenshots of the NDPK-BC system in the presence of GO at four points throughout the simulation: (a) 0 ns; (b) 75 ns; (c) 150 ns; (d) 250 ns. The position of the observer remains the same for all four screenshots.

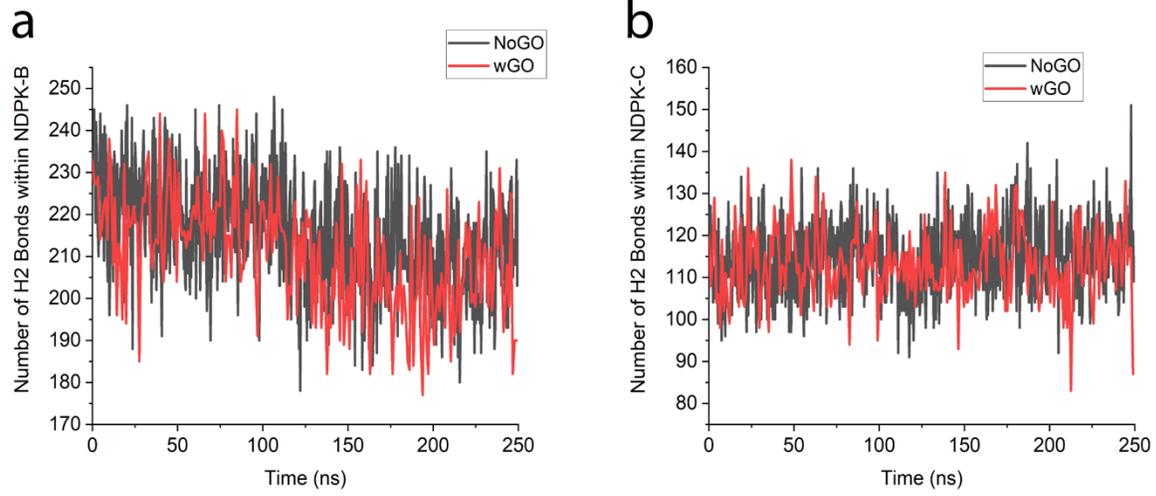


Figure S3. Number of intramolecular hydrogen bonds within: (a) NDPK-B; (b) NDPK-C.

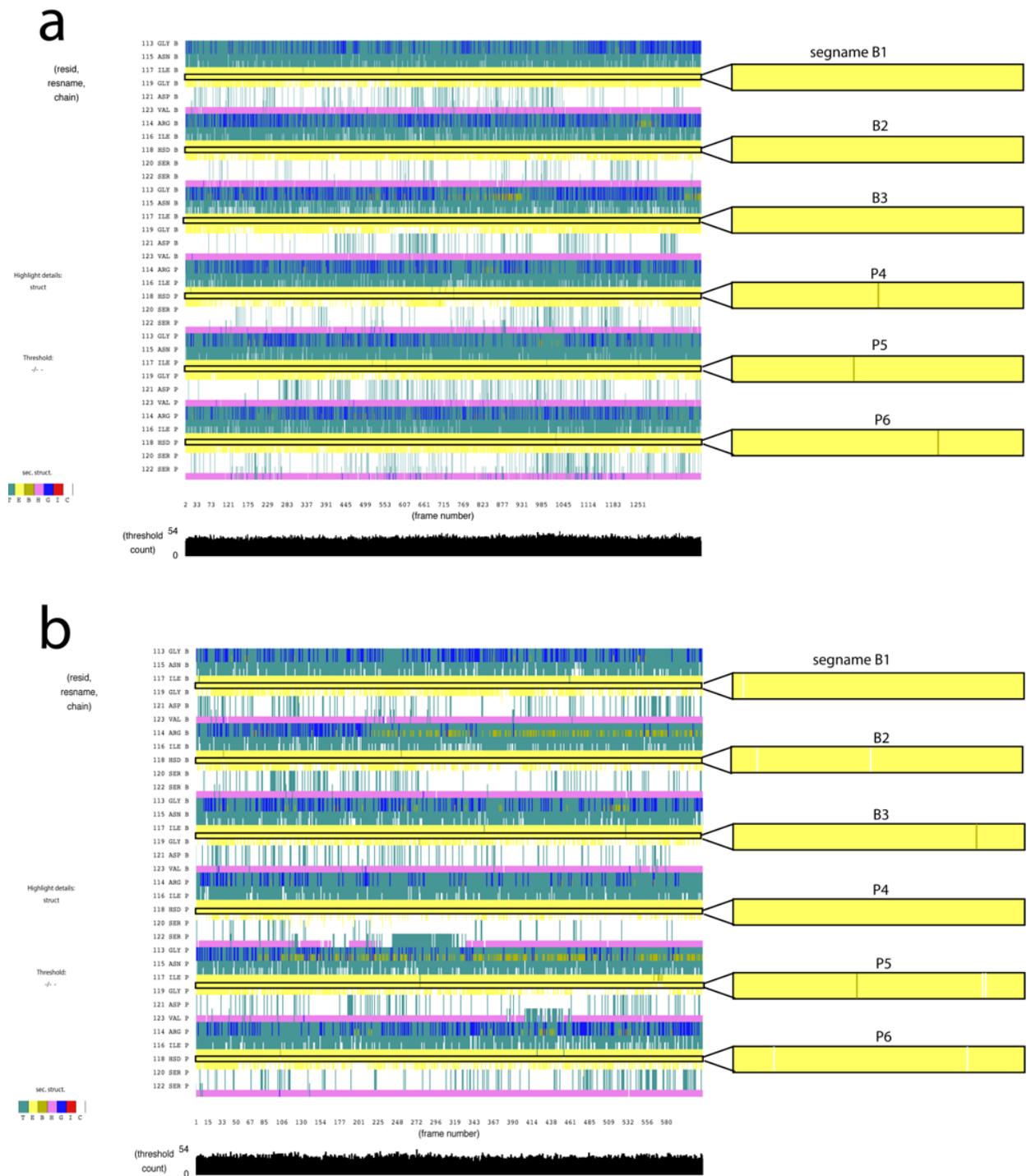


Figure S4. Secondary structure analysis of six His118 residues of NDPK-B measured along with 5 residues in vicinity, zoomed in on His118: (a) in the absence of GO; (b) in the presence of GO.

Table S1. Intramolecular salt bridges within NDPK-B

Salt bridge type	Without GO	With GO
<i>Broken</i>	98	82
<i>Formed</i>	61	71
<i>Sustained</i>	14	19
<i>Weak</i>	31	22

Table S2. Intramolecular salt bridges within NDPK-C

Salt bridge type	Without GO	With GO
<i>Broken</i>	38	41
<i>Formed</i>	31	39
<i>Sustained</i>	13	10
<i>Weak</i>	21	16