Supplemental materials for:

Bacterial denitrifying nitric oxide reductases and aerobic respiratory terminal oxidases use similar delivery pathways for their molecular substrates

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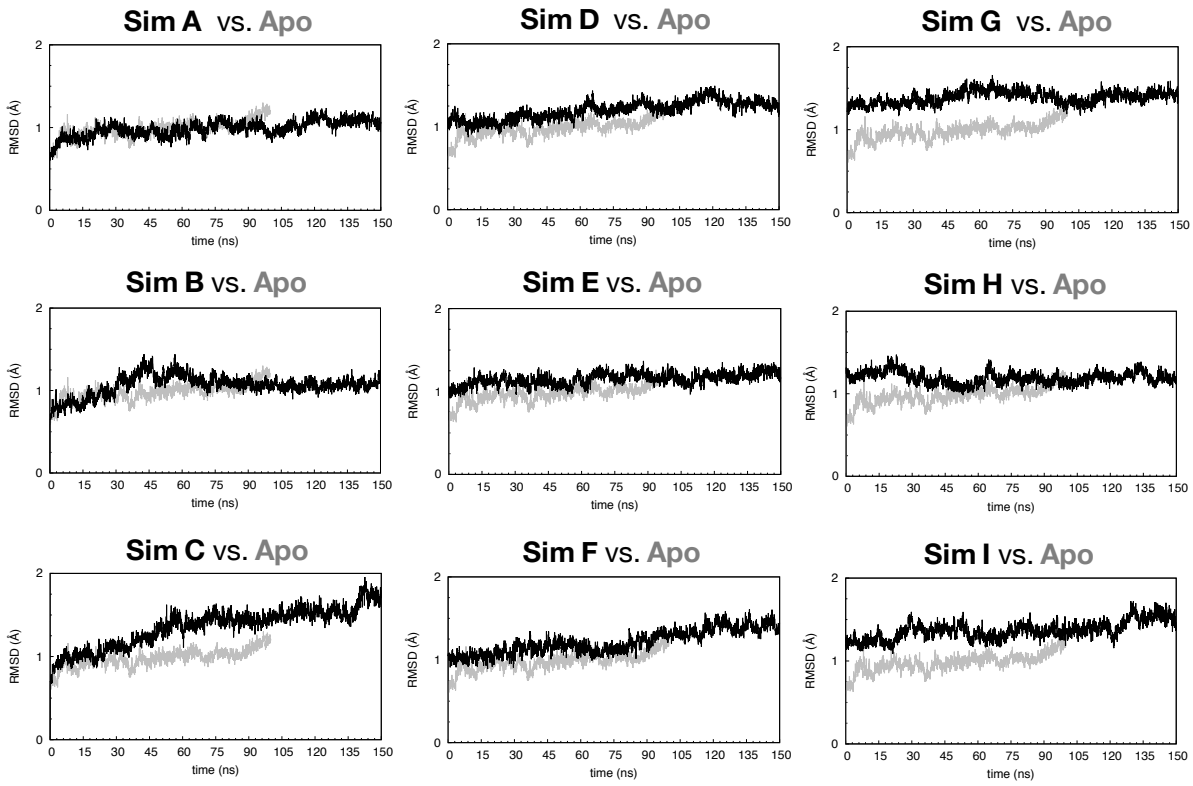

Fig. S1: Overall conformational dynamics of the NorB subunit of cNOR in the presence (black) and absence (gray) of 100 NO molecules quantified by RMSD. The final structure of the 20-ns relaxation step of the simulation was used as the reference. Sims A-C of the flooding simulations and the 100-ns apo simulation started the 20-ns relaxation step. Sims D-F and Sims G-H started from the 50-ns and 100-ns time points of the apo simulation. Low and comparable RMSD values in the apo and flooding simulations indicate that the presence of 100 NO molecules does not perturb the structure the protein.

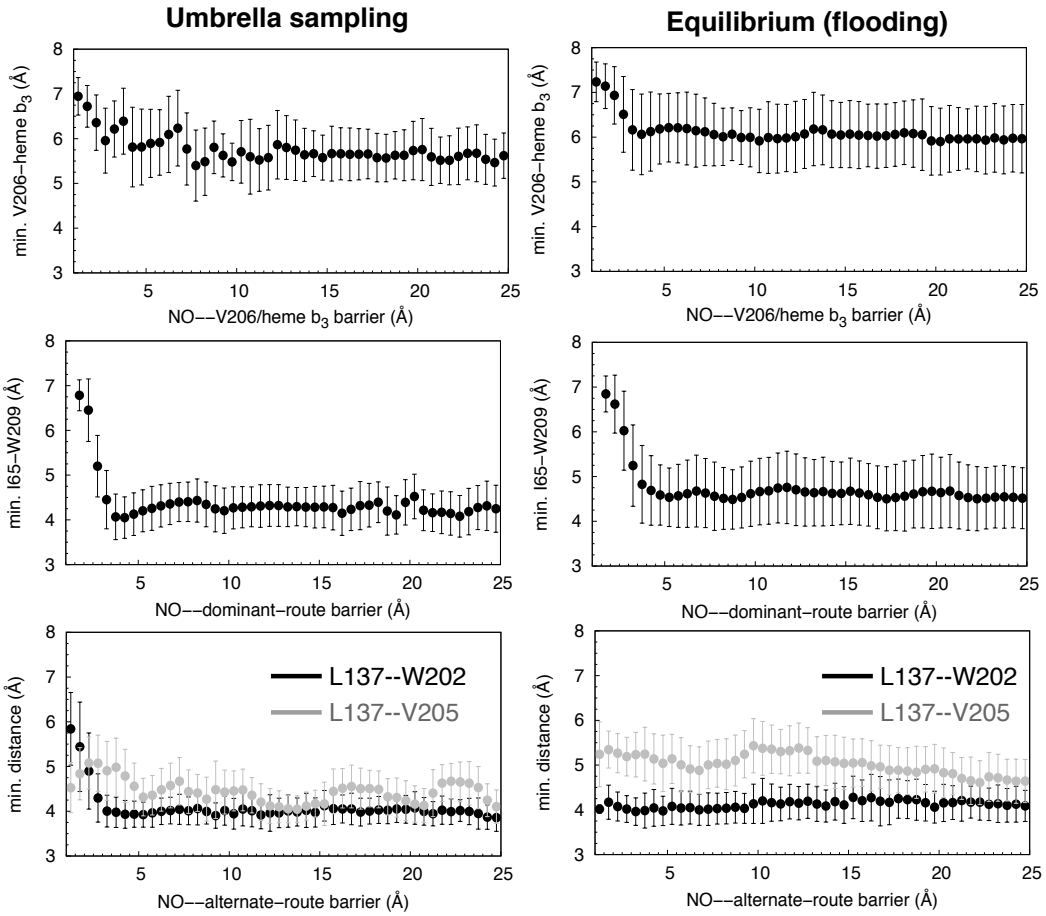

Figure S2: Dynamics of bottleneck residues along the delivery pathway upon the localization of NO. The barrier at V206 and heme b_3 is defined by the center of mass between the sidechain of V206 and the methyl group of heme b_3 D-ring. The main barrier of the dominant route is defined by the center of mass of I65 and W209 side chains. In both equilibrium (unconstrained) and umbrella sampling simulations, the pairwise distances of the residues at a barrier region increased (e.g., from 4 to 7 Å) when an NO molecule was localized within 3Å of that region, indicating a partial opening of the pathway. The main barrier of the alternate route is defined by the center of mass of L137, W202 and V205 side chains.

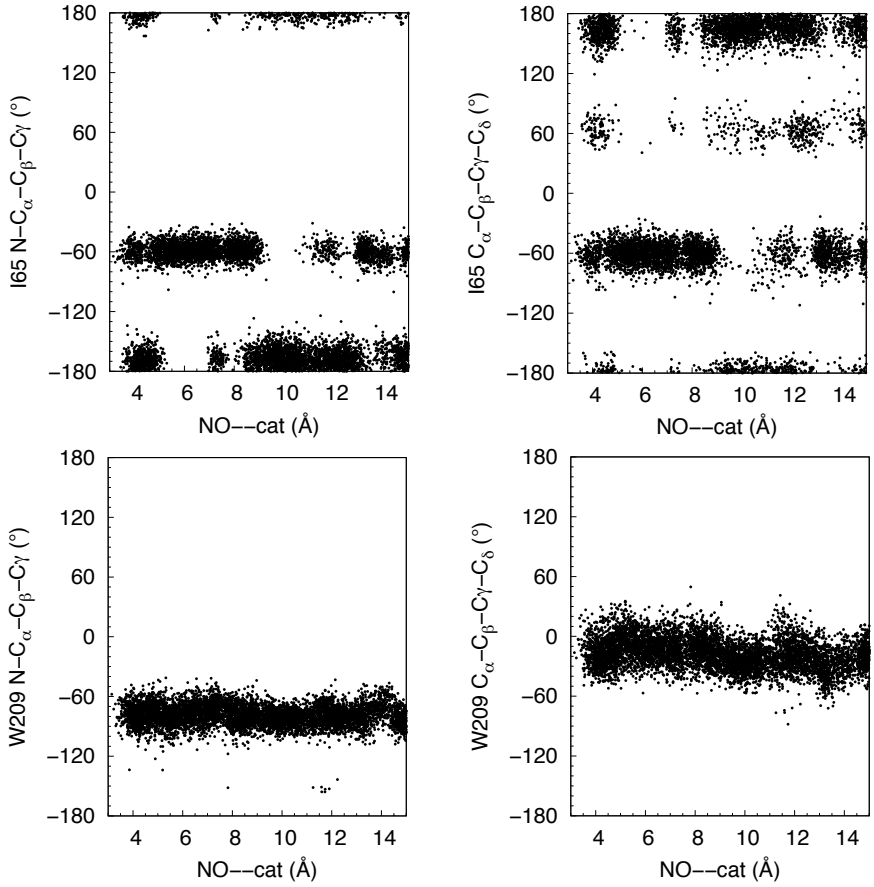

Fig. S3: Conformational dynamics of I65 and W209 projected as the function of the position of an NO molecule in the dominant route of the NO delivery pathway. These results were obtained from the US simulations. I65 and W209 are located at the distance of ~13Å.

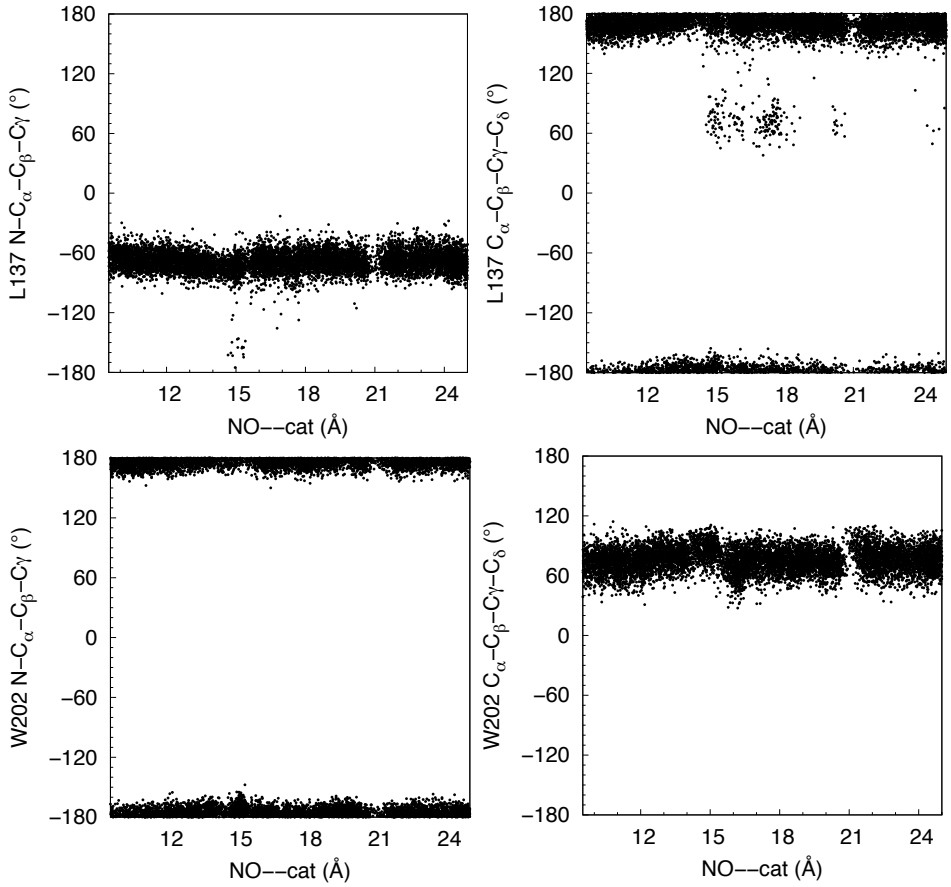

Fig. S4: Conformational dynamics of L137 and W202 projected as the function of the position of an NO molecule in the alternate route of the NO delivery pathway. These results were obtained from the US simulations.

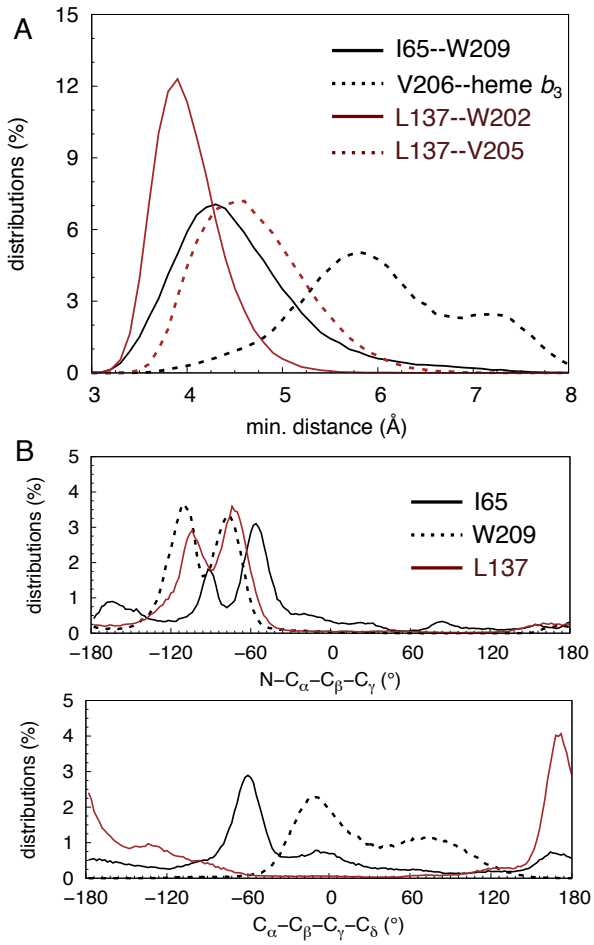

Fig. S5: Conformational dynamics of bottleneck residues along the pathway observed during the unconstrained (flooding and apo) simulations characterized by the distributions of minimum pairwise distances (A) and dihedral angles of the side chains (B).