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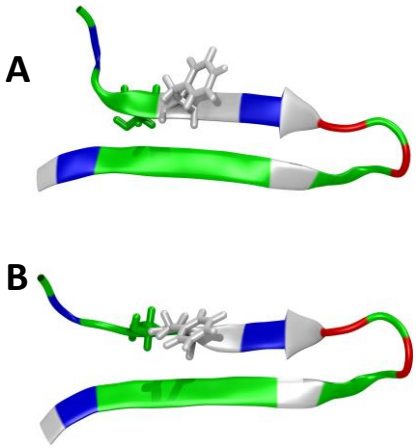
Supplemental Figure 1



Supplemental Figure 1: Snapshots of the loop E at t=1ns (A) and t=500ns (B), before and after the change in the structure of the loop (at t~300ns). Here, despite the changes in the structure of the loop, i.e., losing the secondary structure of the S144 and F145 residues, the general structure of the loop E remained in the β-sheet configuration. S144 is in green and F145 is in white. The β-sheet is colored by residue type. PBD File: Hco-UNC-49

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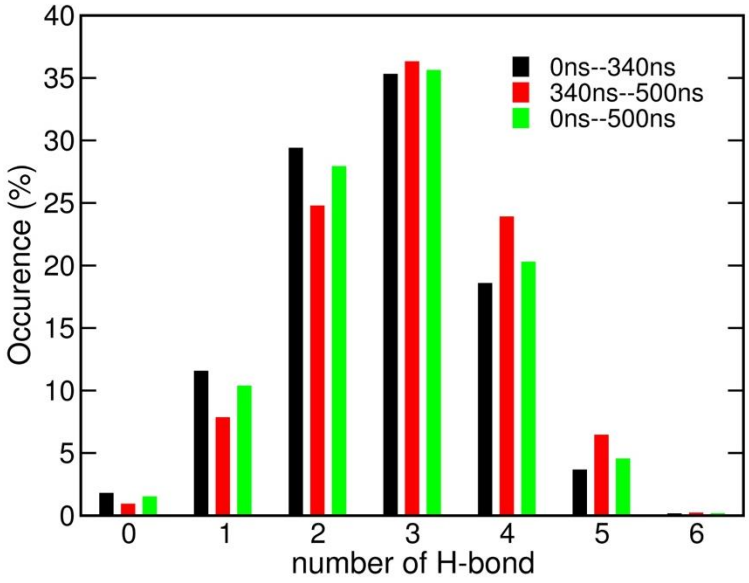
Supplemental Figure 2



Supplemental Figure 2: Histogram of number of H-bonds between the GABA molecules and the nearby residues for different time frames of the simulation. The default values (d<3.0Å and θ<20°) are used to determine the H-bonds. These results indicate that the GABA could form up to 6 H-bond with residues around it. PBD File: Hco-UNC-49

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Supplemental Table 1

Supplemental Table 1. Percentage of H-bond occurrence between GABA and residues on the loop E of the protein during different time frames of the simulation. Occurrences above 10% are reported.

Residue	H-bond percentage (%) 0ns–340ns	H-bond percentage (%) 340ns–500ns	H-bond percentage (%) 0ns–500ns
Y155 (donor)	48.22	64.30	53.36
S157 (donor)	72.23	78.55	74.25

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PDB File: Hco-UNC-49B homodimer