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| **Figure 10–figure supplement 1. Docking of Neuroligin to PDZ3 and the PSG Supramodule in α-basin. (A)** Docked conformationof NL10 peptide bound to the PDZ3. The NL10 peptide is shown in black with the three histidine residues shown in blue. When protonated, these histidine residues extend towards E331, D332, and E334 in PDZ3, which may explain the higher binding affinity at low pH. At physiological pH, the negatively charged residues will inhibit binding of uncharged histidines. **(B-C)** Representative conformationsof NL10 peptide binding to PDZ3 within the PSG α-basin. In the context of PSG, positively charged residues in the SH3 HOOK insertion form salt-bridges with the negatively charged residues in PDZ3. These electrostatic interactions sequester these negative charges to stabilize the binding of NL10 at physiological pH. |