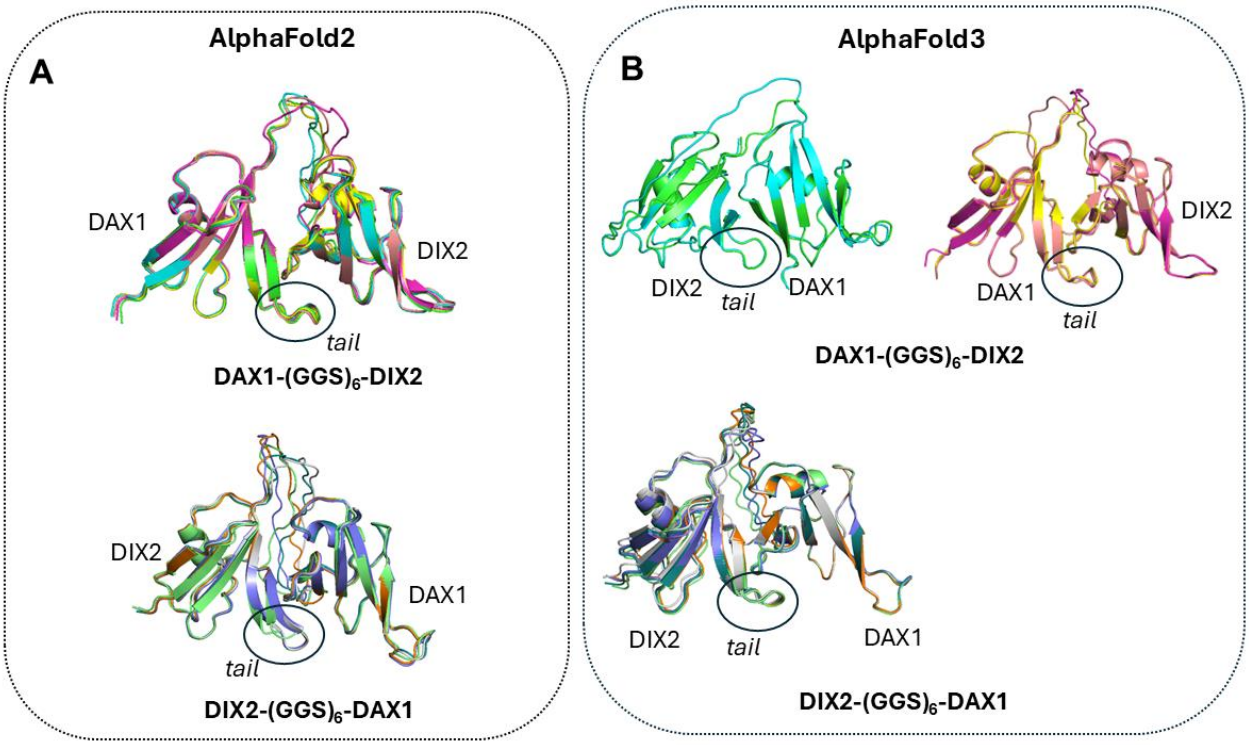

Figure S1. AlphaFold2 and AlphaFold3 predictions of DAX1–DIX2 and DIX2–DAX1 heterodimeric structures. (A) AlphaFold2 predictions of the DAX1–DIX2 and DIX2–DAX1 heterodimers. The predicted models support both tail-to-head arrangements, including the DAX1 tail/DIX2 head and DIX2 tail/DAX1 head interfaces, consistent with the experimental results. **(B)** AlphaFold3 predictions of the same heterodimeric constructs. For DAX1-$(GGS)_6$-DIX2, two heterodimeric arrangements were predicted: the DIX2 tail/DAX1 head structure appeared as the rank 1 and rank 2 models, whereas the DAX1 tail/DIX2 head structure appeared as the rank 3, rank 4, and rank 5 models, differing from the AlphaFold2 prediction. For DIX2-$(GGS)_6$-DAX1, AlphaFold3 predicted the DIX2 tail/DAX1 head structure, consistent with the AlphaFold2 prediction.

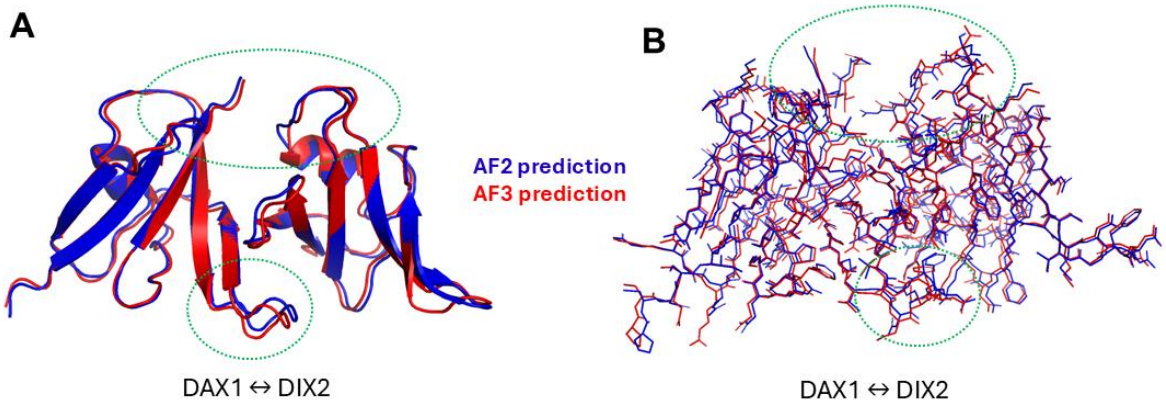

Figure S2. Comparison of AlphaFold2 and AlphaFold3 predictions for the DAX1–DIX2 heterodimer. (A) Superposition of the AlphaFold2 model (blue, rank 1) and the AlphaFold3 model (red, rank 3) for the DAX1–DIX2 heterodimer, shown as cartoon representations. The two predicted structures are highly similar, with an RMSD of 0.715 Å. The green-circled region highlights a local structural difference between the two predictions. **(B)** Comparison of side-chain conformations in the predicted heterodimeric interface (stick model). Although the overall heterodimeric architecture is similar between the AlphaFold2 and AlphaFold3 models, the side chains in the green-circled region do not fully overlap, indicating a local difference in side-chain placement.