



Extended Data Figure 6 | Comparison between the GCGR–NNC1702 structure and the GCGR–glucagon model derived from molecular dynamics simulations. **a**, Extracellular view of the transmembrane helical bundle. The GCGR–NNC1702 structure is shown in cartoon representation and coloured blue (GCGR) and red (NNC1702). The GCGR–glucagon model derived from molecular dynamics simulations is shown in cartoon representation and coloured orange (GCGR) and yellow (glucagon). The green arrows indicate shifts of helices VI and VII.

b, Close-up view of the interaction between H1 of glucagon and D385^{7.42b} of GCGR in the molecular dynamics simulations. The NNC1702 residue S2, the glucagon residues H1 and S2 and the GCGR residue D385^{7.42b} in both the GCGR–NNC1702 structure and the GCGR–glucagon model are shown as sticks. The hydrogen bond formed by H1 and D385^{7.42b} in the molecular dynamics simulations is displayed as a red dashed line. **c**, Intracellular view of the transmembrane helical bundle. The green arrows indicate shifts of helices V and VI.