Supporting Information S3 Fig. Proteins’ backbone. A) Ca root-mean-square-deviations (RMSDs) of hA2AR across the three systems are plotted as a function of the simulated time. The RMSD values for the full lengths hA2AR (residue 1-329), hA2AR without histidine tag [1] (residue 1-317) and truncated hA2AR (residue 1-291) are represented in red, blue and green, respectively. A dotted black line indicates where RMSDs start to oscillate around averaged values. B) Superposition between representative receptor structures obtained by clustering procedure [2] of the three MD simulations (yellow) and the CFF/hA2AR complex X-ray structure [1] (cyan).

Supporting references