Computer simulations of the adenosine A2a receptor using molecular dynamics have been carried out for 200 nanoseconds and principal component analysis (PCA) have been performed on the molecular motions. The aims are: (i) to study the behaviour of the receptor in the absence and presence of a ligand; (ii) to assess the validity and reliability of these simulations through looking at convergence and reproducibility between replicate simulations; (iii) to evaluate the usefulness of the protein structures derived from these simulations in drug design. Both apo and liganded models were constructed based on the 3EML crystal structure and they were embedded in fully-solvated membrane bilayers. PCA which have been carried out to study the whole protein, transmembrane region, interhelical and intrahelical protein motions have shown that on this timescale, convergence is not readily evident and dependent on the types of the protein motions considered. Helix IV has been found to be the most stable helix while the behaviour of other helices are less predictable and are affected by ligand binding. Protein structures from the liganded simulations have also been found to produce better docking results than the apo simulations. To conclude, some published literature have based results on a single “equilibrated” simulation system over tens to hundreds of nanoseconds. Results shown here suggest that convergence in membrane-protein simulations is difficult to achieve over such timescales.