

**Fig S3.** Coordination of the intra-membrane sodium ion in  $\beta$ 1-AR The sodium ion (gray sphere) is coordinated by 3 water molecules (red spheres), the  $\gamma$ -hydroxyl of Ser128 and a carboxylate oxygen of Asp87. Helices H2 and H3 are shown in ribbon representation. 2Fo-Fc density (sharpened by a B factor of -20 and contoured at 1 Å) is shown for the two side chains, the sodium ion and the coordinating waters. Sodium coordination distances are in Å.