S9 Table. Average RMSDs to the starting structure (homology model) of MD snapshots of the D_2R and 5-$HT_{2A}R$.

State (template)[a]	MD Trajectory[b]	RMSD (Å)[c]		
		TMBB	BSBB	Ligand
		D_2R		
Apo (D_3R)	1	1.8 ± 0.3	1.9 ± 0.4	-
	2	1.9 ± 0.2	1.9 ± 0.3	-
	3	1.6 ± 0.1	1.6 ± 0.2	-
Apo (Rho)	1	2.4 ± 0.2	2.4 ± 0.1	-
	2	2.3 ± 0.1	2.4 ± 0.2	-
	3	2.4 ± 0.2	2.3 ± 0.2	-
Holo (D_3R)	1	1.3 ± 0.1	1.2 ± 0.2	1.2 ± 0.3
	2	1.6 ± 0.2	1.2 ± 0.2	1.0 ± 0.2
	3	1.4 ± 0.1	1.6 ± 0.3	1.2 ± 0.2
		5-$HT_{2A}R$		
Apo (5-$HT_{2C}R$)	1	1.7 ± 0.2	1.4 ± 0.1	-
	2	2.2 ± 0.3	1.6 ± 0.2	-
	3	1.7 ± 0.2	1.3 ± 0.1	-
Apo (Rho)	1	3.4 ± 0.4	3.8 ± 0.4	-
	2	3.4 ± 0.4	3.9 ± 0.4	-
	3	3.2 ± 0.2	3.6 ± 0.2	-
Holo (5-$HT_{2C}R$)	1	2.2 ± 0.3	1.4 ± 0.2	1.1 ± 0.2
	2	2.1 ± 0.2	1.4 ± 0.2	1.0 ± 0.2
	3	2.0 ± 0.3	1.3 ± 0.1	1.0 ± 0.2

[a] MD simulations were carried out in the absence (apo) and presence (holo) of orthosteric ligand. The template used to create the homology model is shown in parenthesis.
[b] Three MD simulation trajectories of 100 ns were carried out for each homology model.
[c] RMSD ± standard deviation (1000 snapshots from 100 ns) for the TM backbone (TMBB), BS backbone (BSBB), and orthosteric ligand.