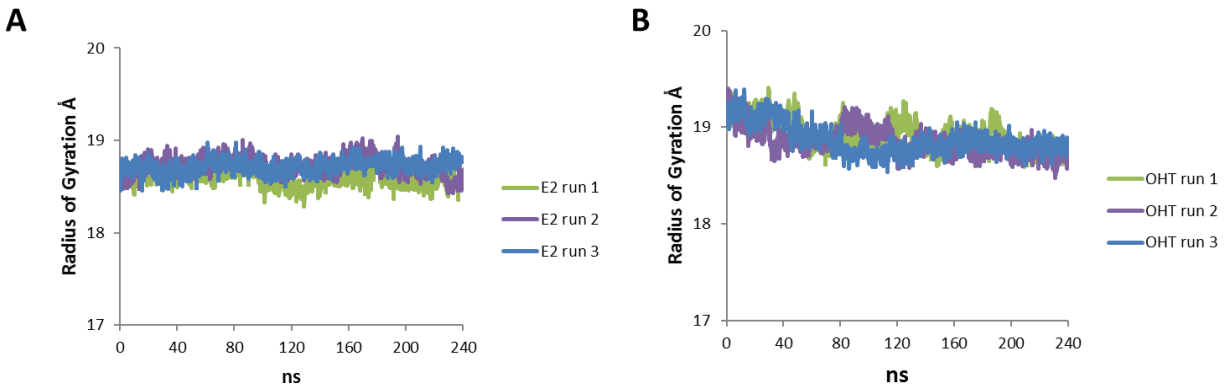
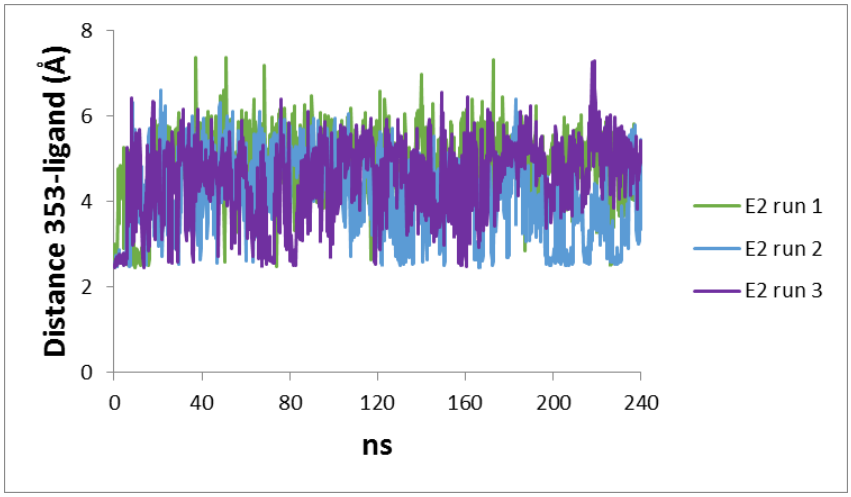
Supplementary data

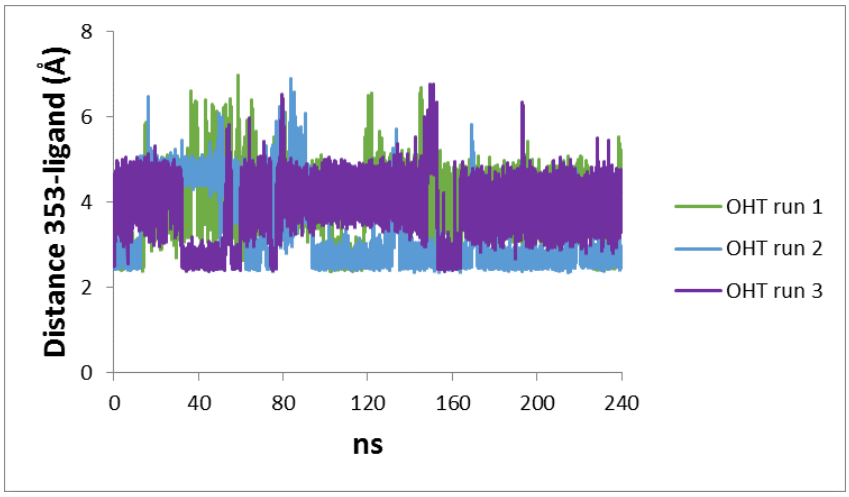


Supplementary Fig. 1. Mass weighted radius of gyration for A) ER-α + E2 and B) ER-α + OHT over the simulation trajectory. Calculations only include non-hydrogen atoms from ER-α.

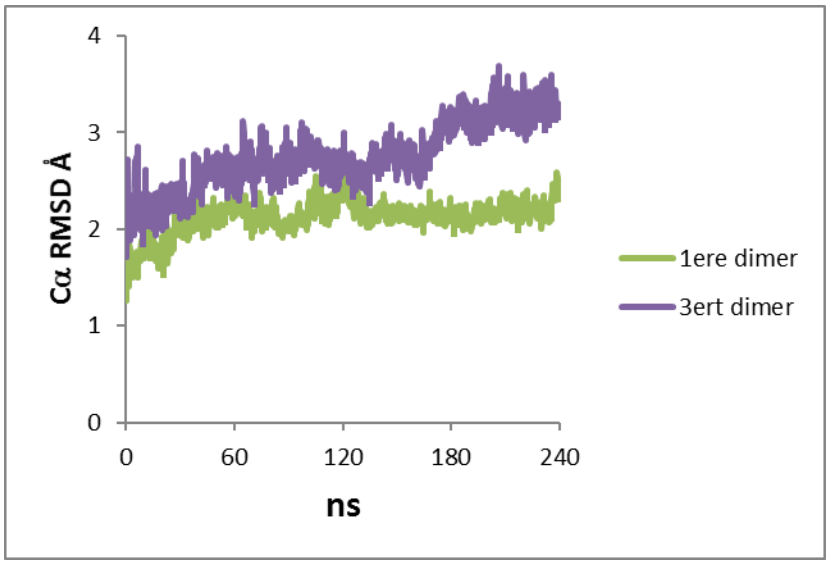
A)



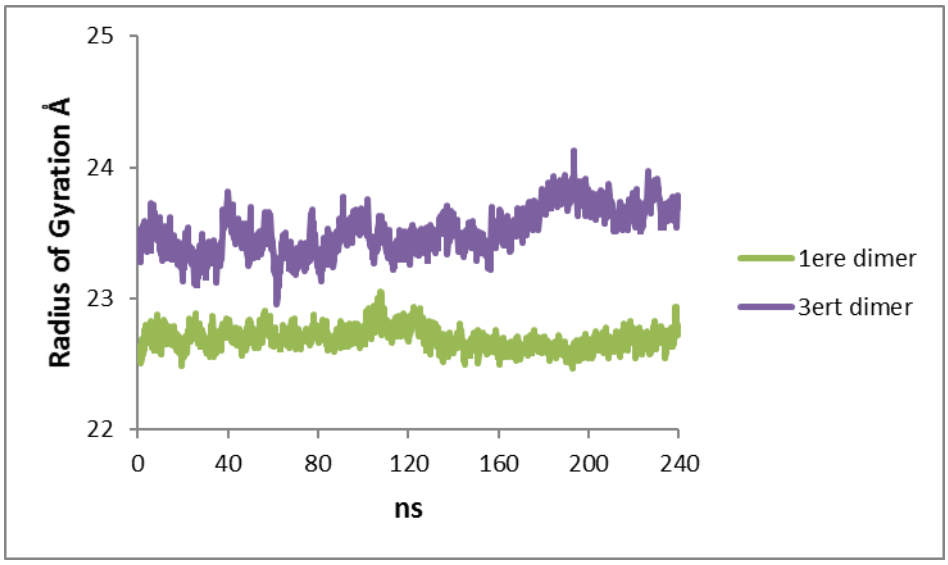
B)



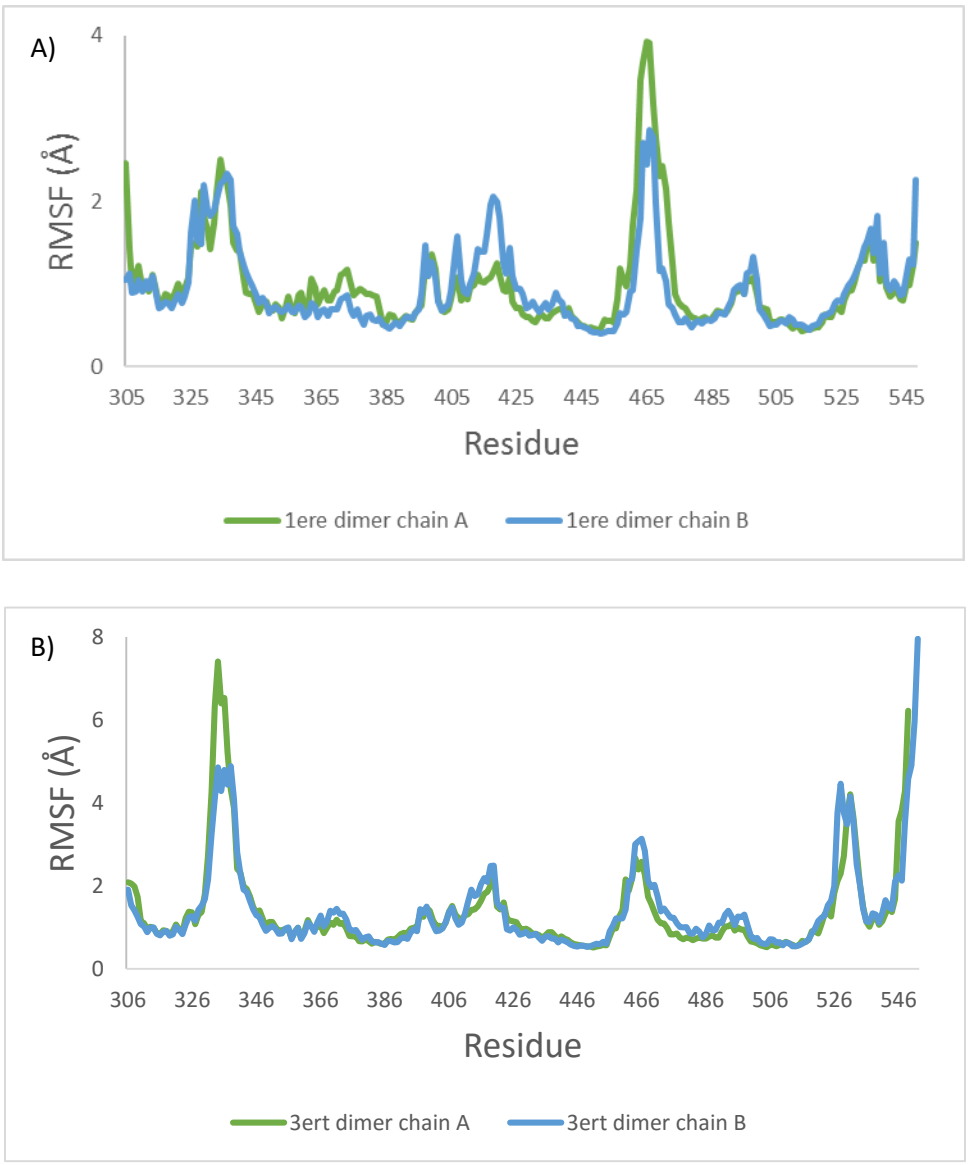
Supplementary Fig. 2. Distance from ER-α Glu353 OE2 to A) E2 and B) OHT over the simulation trajectories.



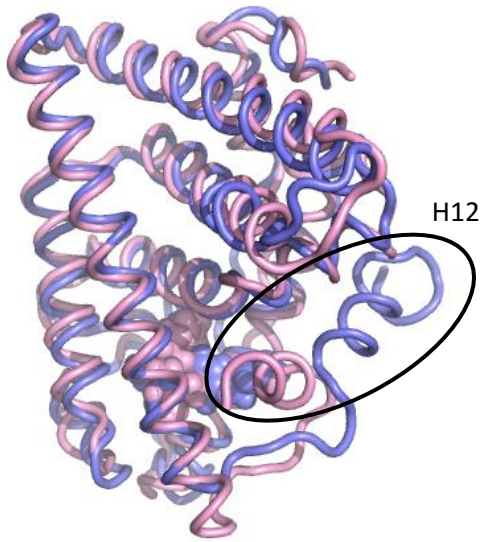
Supplementary Fig 3. RMSD for Cα atoms throughout the MD simulations of ER-α dimer with E2 (pdb 1ere) and OHT (pdb 3ert).



Supplementary Fig 4. Mass weighted radius of gyration for dimers of ER-α + E2 (pdb 1ere) and ER-α + OHT (pdb 3ert) over the simulation trajectory. Calculations only include non-hydrogen atoms from ER-α.



Supplementary Fig. 5. RMSF per residue for Cα atoms throughout the MD simulations of ER-α dimer with (A) E2 (pdb 1ere) and (B) OHT (pdb 3ert).



Supplementary Fig. 6. Superposition of structures of ER-α bound to agonist E2 (pink) and antagonist OH2 (blue) after 240 ns of molecular dynamics simulations. Helix H12 is circled. Structures are taken from run 1 of the three independent trajectories for E2 and OHT.