Dichlorodiphenyltrichloroethane (DDT) is ubiquitous in the environment, and the exposure to DDT and its related pesticides has long been linked to endocrine disruption. The mechanism of endocrine disruption toward targeted receptors, however, remains unclear. Probing the molecular recognition of DDT analogs by targeted receptors at the atomic level is critical for deciphering this mechanism. Molecular dynamics (MD) simulations were applied to probe the molecular recognition process of DDT and its five analogs, including dichlordiphenyldichloroethylene (DDE), dichlorodiphenyldichloroethane (DDD), methoxychlor (MXC), *p*,*p*′-hydroxy-DDT (HPTE), and dicofol by human estrogen receptor (ER) α and human ER-related receptor (ERR) γ. Van der Waals interactions mainly drive the interactions of DDT analogs with ERα ligand-binding domain (LBD) and ERRγ LBD. Minor structural changes of DDT analogs in the number and position of chlorine and phenolic hydroxyl moiety cause differences in binding modes through aromatic stacking and hydrogen bonding and thus affect differently conformational changes of ERα LBD and ERRγ LBD. The binding of DDT analogs affects the helix 12 orientation of ERα LBD but causes no rearrangement of helix 12 of ERRγ LBD. These results extend our understanding of how DDT analogs exert their estrogen-disrupting effects toward different receptors via multiple mechanisms.