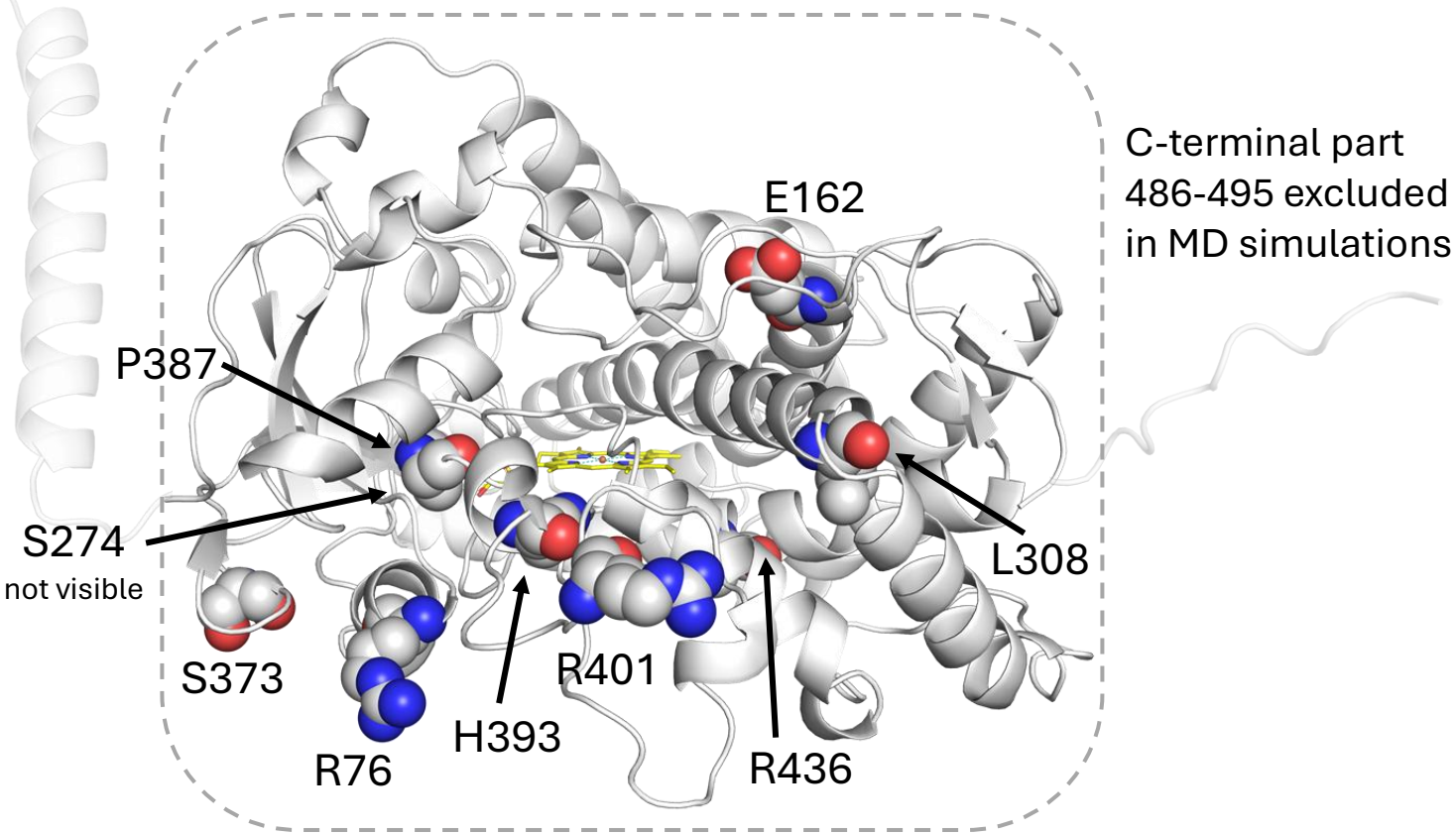
N-terminal part 1-29 excluded in MD simulations



C-terminal part 486-495 excluded in MD simulations

MD setup for CYP21A2 WT: 456 residues, heme group,15806 water molecules, 2 sodium ions, 54835 atoms in total