Electronic Supplementary Material (ESI) for Chemical Science. This journal is © The Royal Society of Chemistry 2024

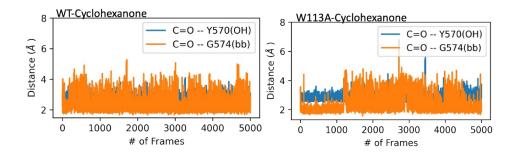


Figure S11. The hydrogen bonding in the wild type CDH and W113A in complex with cyclohexanone. The interatomic distance between the carbonyl oxygen of the cyclohexanone and the side chain of Y570 and the backbone of G574 residue for the 500 ns trajectory.