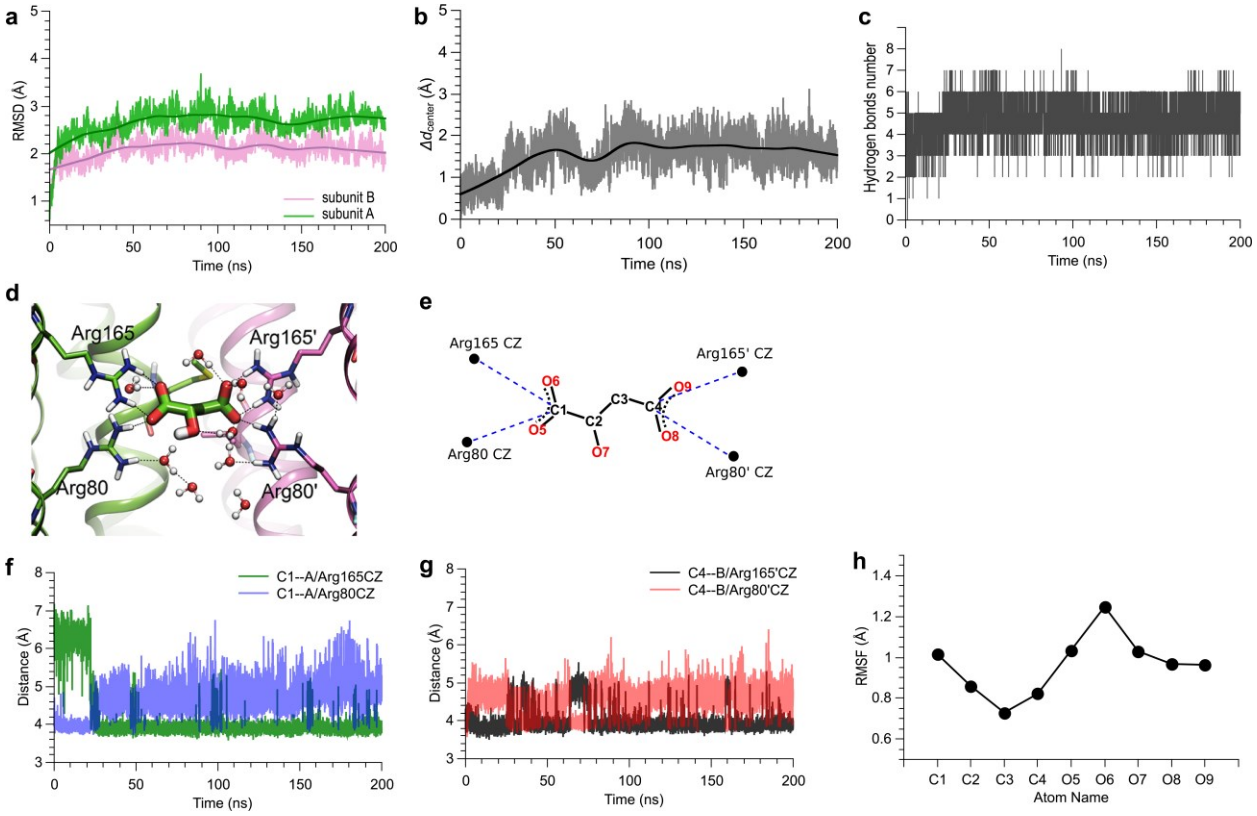

Fig. S7 Molecular dynamic simulation of ALMT1$_{malate/pH7.5}$.

a, The RMSD of the backbone of the two subunits during the simulation. Both subunits were equilibrated after 50 ns, with RMSD values converging at < 3.0 Å. **b,** Deviations of the malate mass center from its original coordinate (Δd_{center}) during MD simulation. **c,** The hydrogen bond numbers between the malate and the four Arg residues. Five hydrogen bonds are formed between the malate and Arg80, Arg165 from two subunits. **d,** The representative conformation of the biggest cluster of malate. Dashed lines represent hydrogen bonds. **e,** The atom names in the malate structure for the simulation. The blue dashed lines are for the measurement of the distance between carboxylate carbon atoms (C1/C4) and the zeta carbon (CZ) of the Arg80/Arg165 from each subunit. **f,** The distances between malate C1 and CZ of the two Arg residues from subunit A during the simulation. **g,** The distances between malate C4 and CZ of the two Arg residues from subunit B during the simulation. **h,** The root-mean-square-fluctuation (RMSF) values of the nine atoms of the malate for the 200 ns MD simulation.