Supplementary Material for Computational Investigation on the Binding Modes of PET Polymer to PETase

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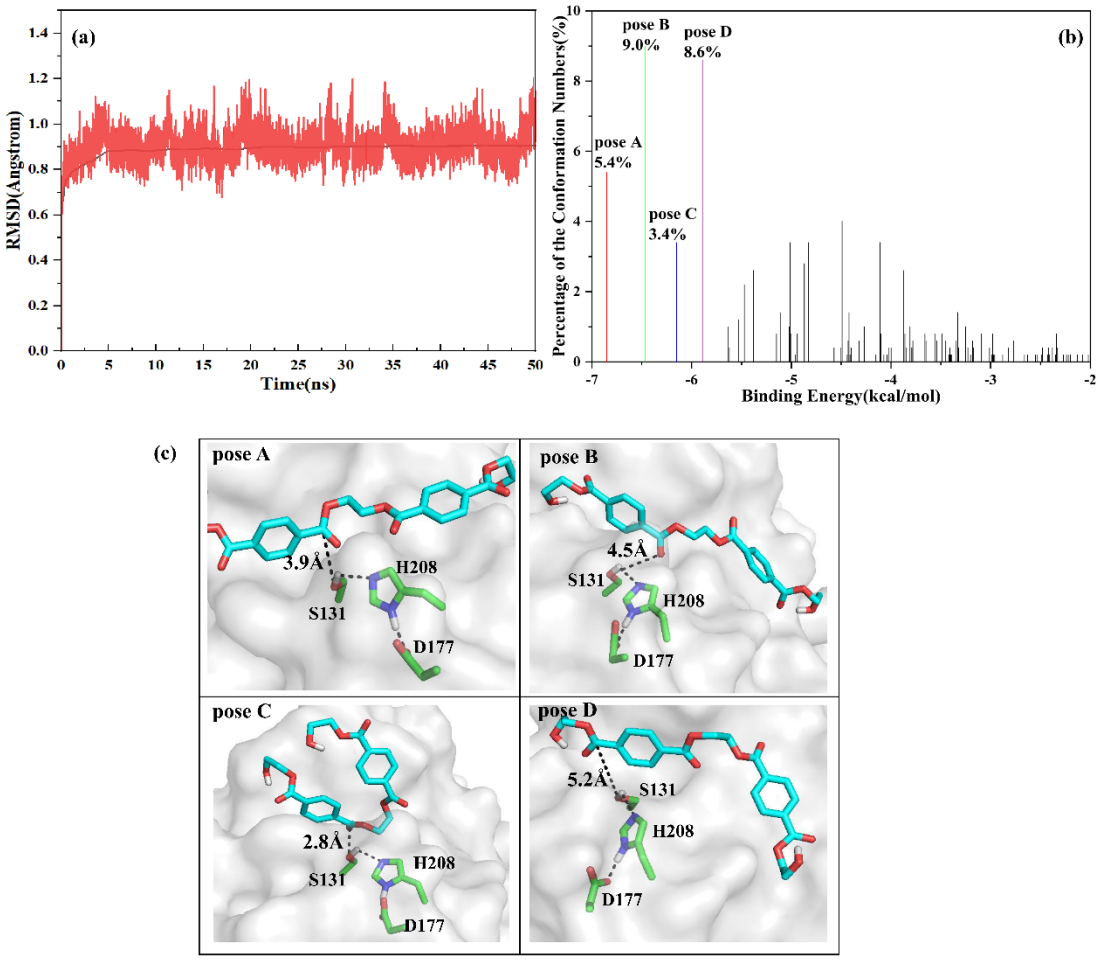

Figure S1. (a) RMSD of backbone heavy atoms of PETase relative to the first structure for 50ns MD simulation. The accumulated average is shown as black line, which elucidates that the system is converged; **(b)** Correlation of percentages of the conformation numbers versus binding energies predicted by Autodock 4.2; **(c)** the docking modes of poses A, B, C, and D respectively.

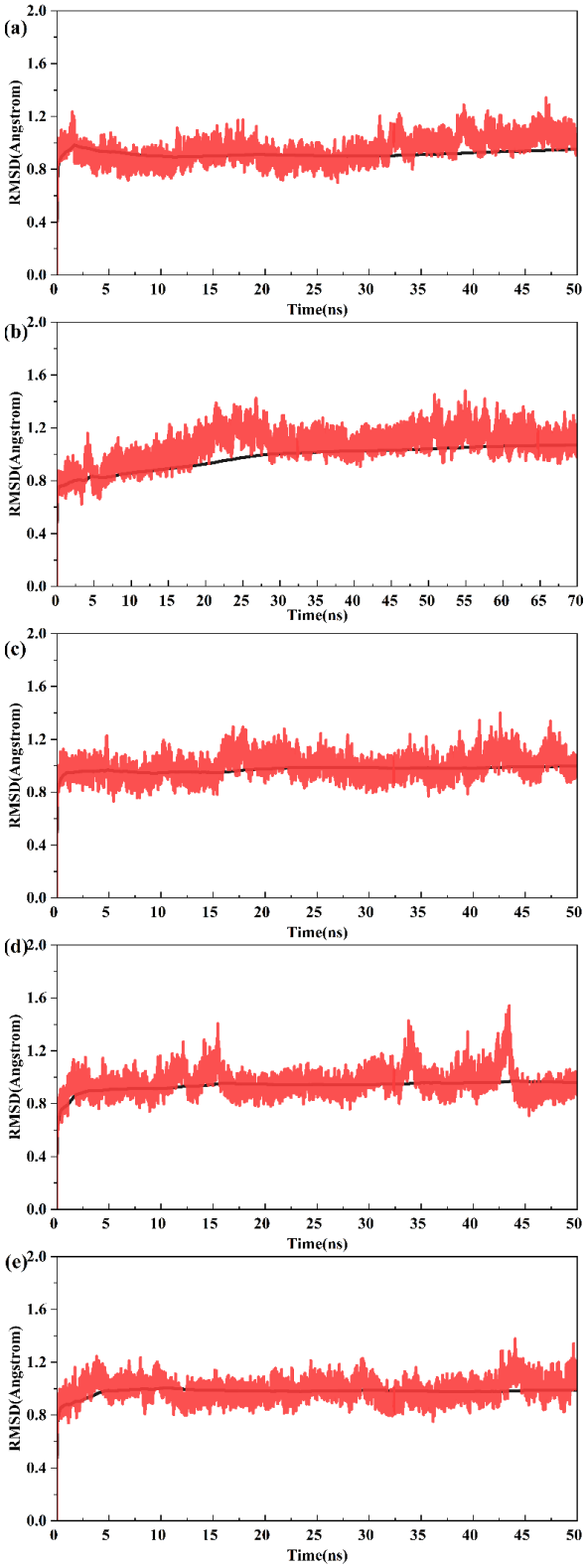

Figure S2. RMSD of backbone heavy atoms of PETase relative to the first structure in complex with **(a)** 2PET, **(b)** 4PET, **(c)** 6PET, **(d)** 7PET, and **(e)** 8PET for 50ns MD simulation. The accumulated averages are shown as black lines, which elucidate that the system is converged.

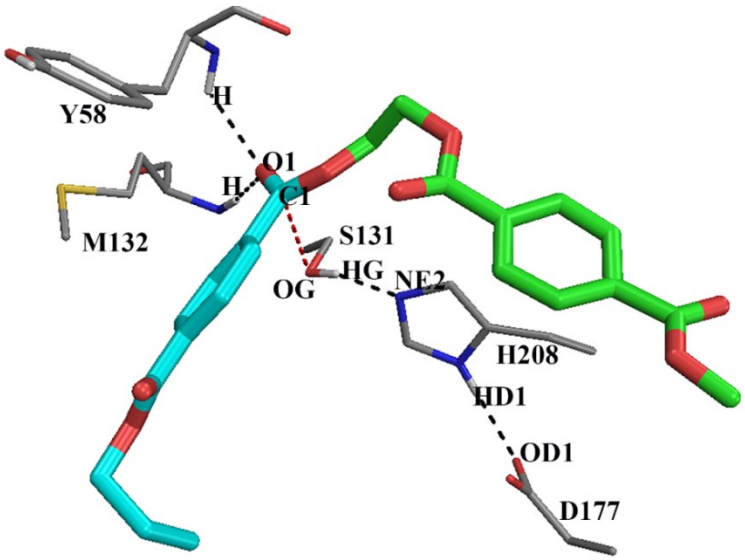

Figure S3. Stick representation of important residues in the active site. Atom names for some important atoms are also labeled.

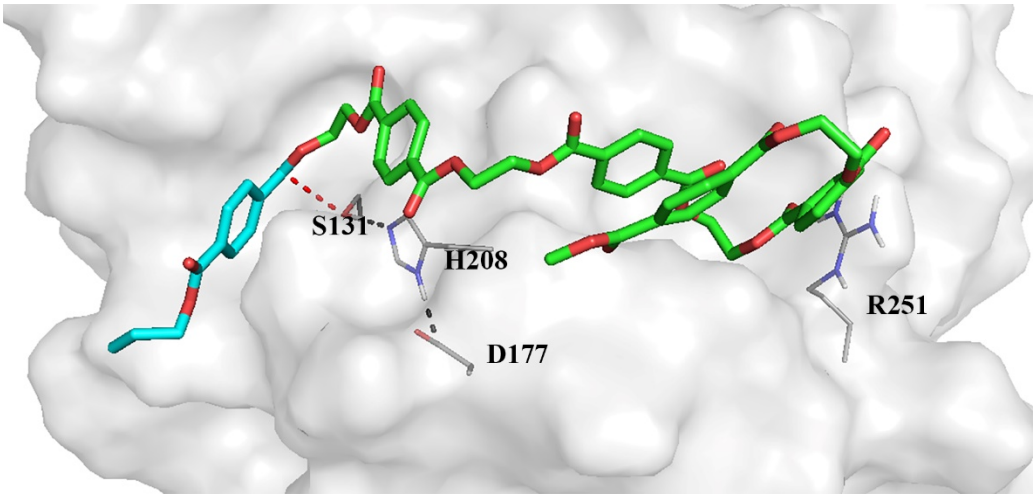

Figure S4. The MD representative snapshot for 5PET bound to PETase. The PETase is presented in surface model, and binding site residues of PETase are highlighted by line model. The HE-terminal of 5PET is shown as green-colored sticks while the TPA-terminal of 5PET is shown as cyan-colored sticks.

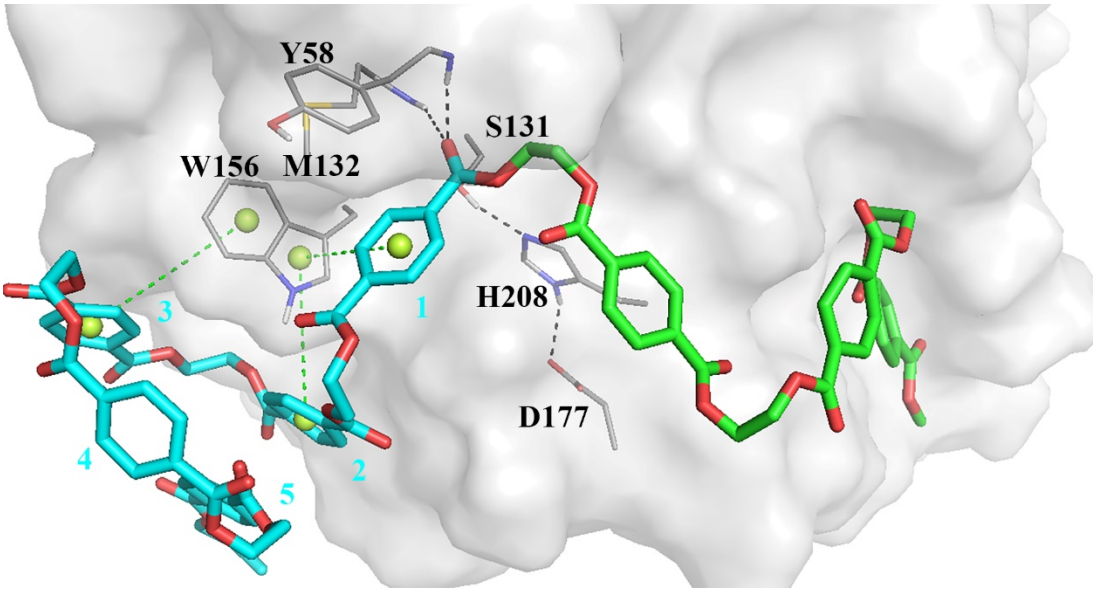

Figure S5. The MD representative snapshot for 8PET bound to PETase. The PETase is presented in surface model, and binding site residues of PETase are highlighted by line model. The HE-terminal of 8PET is shown as green-colored sticks while the TPA-terminal of 8PET is shown as cyan-colored sticks. Yellow lines show the three π-π interactions formed between Trp156 residue and 3 units of 8PET, which sequence numbers are also labeled. The centroids of phenyl groups are highlighted by yellow spheres.

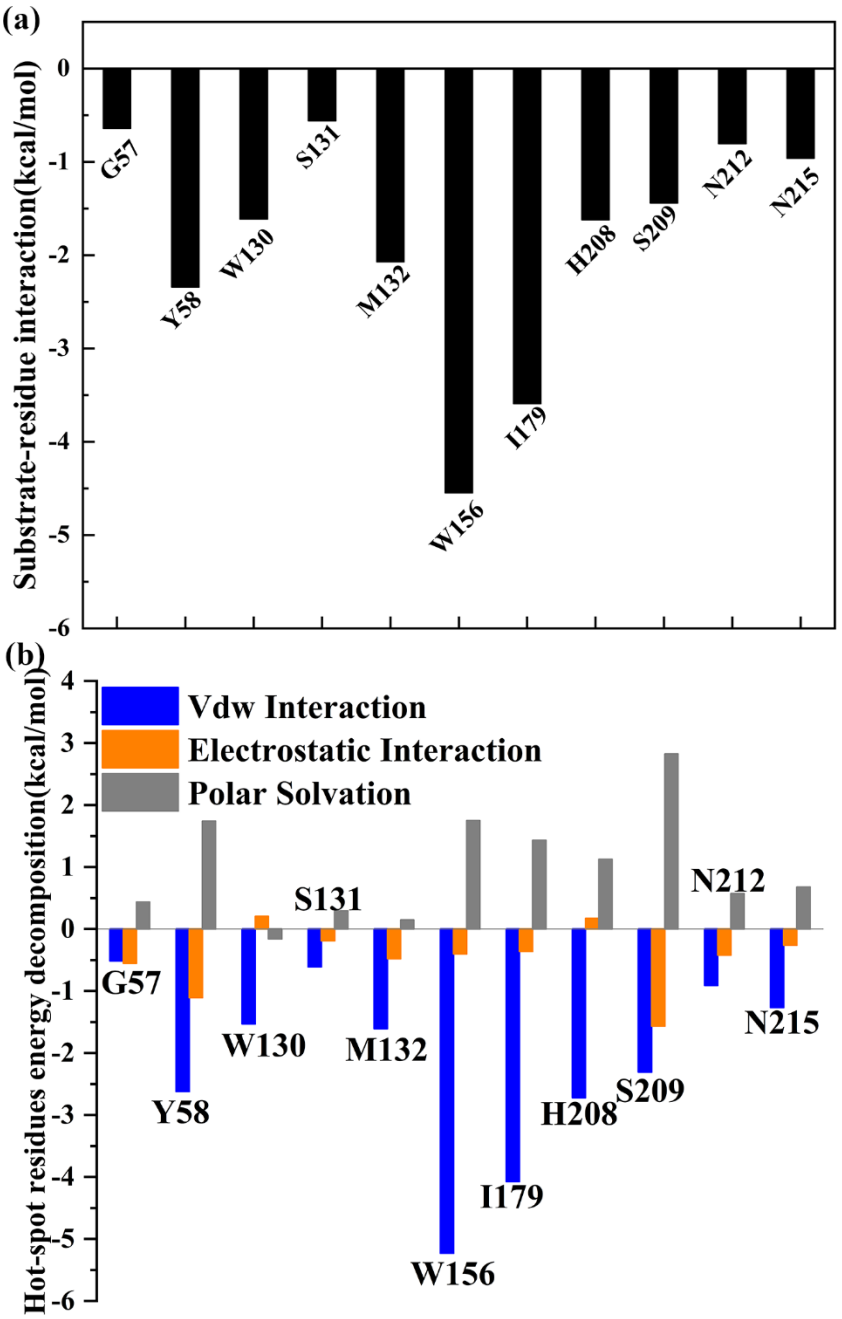

Figure S6. a) Per-residue contribution of binding energies (|contribution|≥0.5 kcal/mol) and b) components from the van der Waals energy, electrostatic interaction in the gas phase, and polar solvation interaction for key residues of PETase for 8PET.