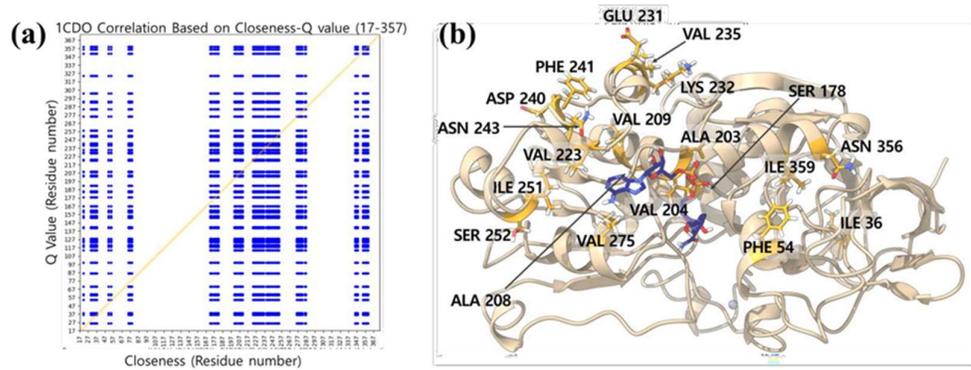
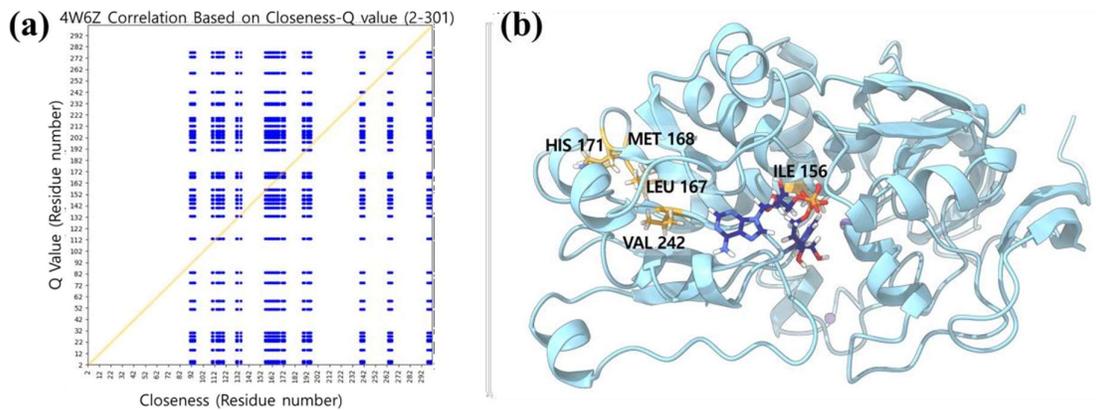


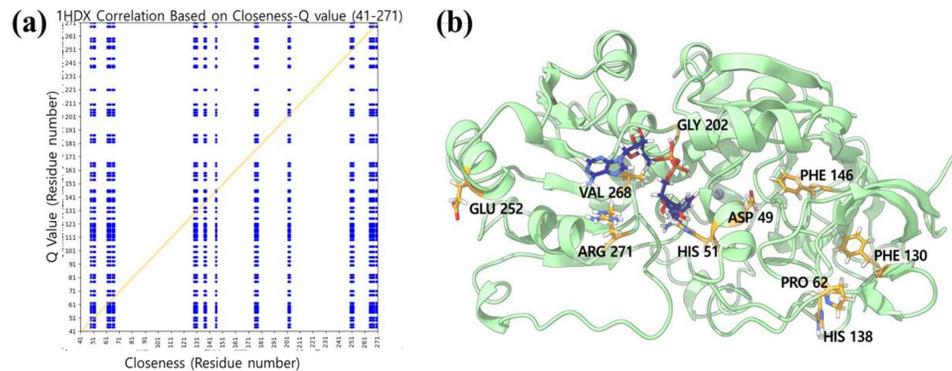
**Figure S2.** Root mean square fluctuation (RMSF) graphs during 100 ns MD simulations repeated three times for three PDB structures. (a) RMSF values during 100 ns MD simulations for 1CDO. (b) RMSF values during 100 ns MD simulations for 1HDX. (c) RMSF values during 100 ns MD simulations for 4W6Z.



**Figure S3.** Correlation between Q-value and centrality measure for fish ADH1/ADH3 divergence (ADH1: 1CDO). (a) Q value plotted against closeness centrality values. (b) Key residues with matching closeness centrality and Q-value are highlighted and labelled.



**Figure S4.** Correlation between Q-value and centrality measure for fungi ADH1/ADH5 divergence (ADH1: 4W6Z). (a) Q value plotted against closeness centrality values. (b) Key residues with matching closeness centrality and Q-value are highlighted and labelled.



**Figure S5.** Correlation between Q-value and centrality measure for the Mammalia ADH1/ADH4 divergence (ADH1: 1HDX). (a) Q value plotted against closeness centrality values. (b) Key residues with matching closeness centrality and Q-value are highlighted and labelled.