

Supplementary Information

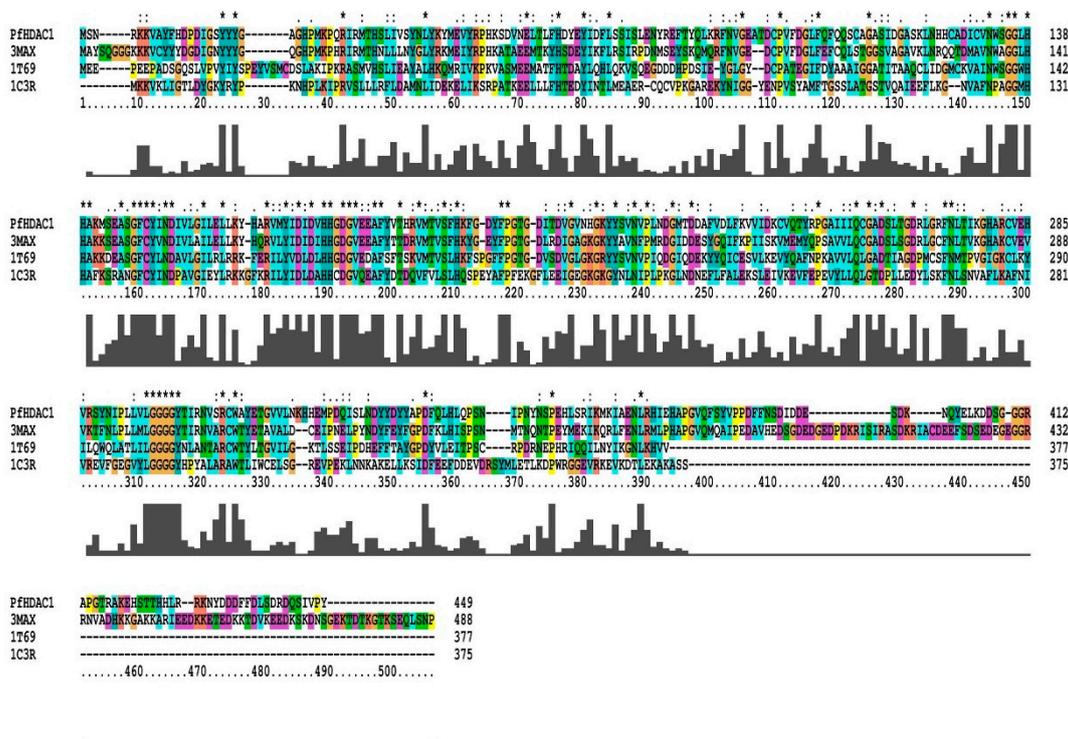


Figure S1. Multiple sequence alignment of *Pf*HDAC-1 with the templates selected to build the homology model in this study (3MAX) and previous studies (1T69 and 1C3R). Color codes as in ClustalX [26].

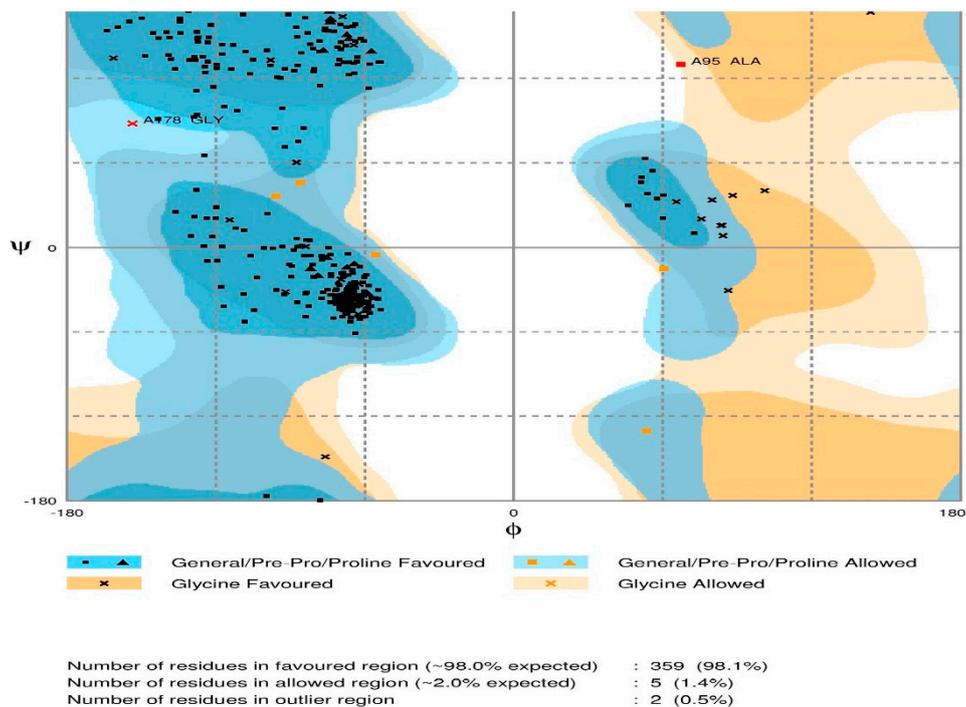


Figure S2. Ramachandran plot of (ϕ, ψ) dihedral angles distribution for *Pf*HDAC-1 residues.

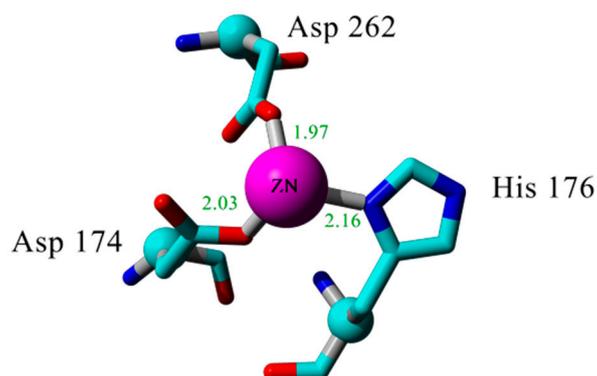


Figure S3. Zinc coordination in ligand free *Pf*HDAC-1, coordination distances in Å are shown in green.

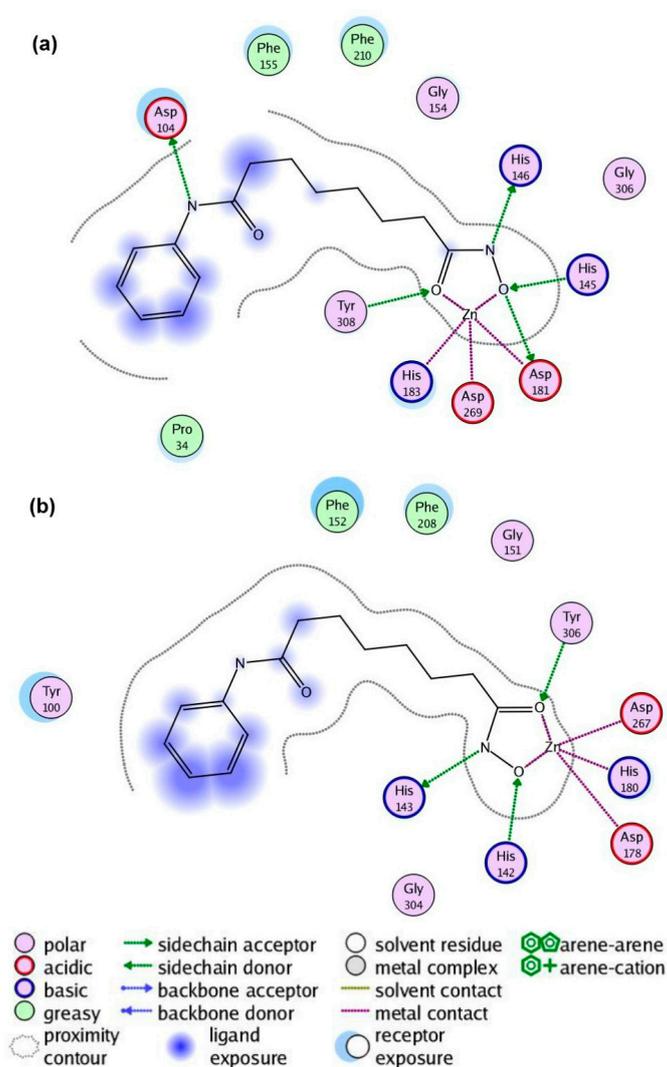


Figure S4. Hydroxamate derivative interaction in solvated structures of HDAC homologues. (a) SAHA interactions in crystal structure of T311M HDAC8 (PDB: 4QA0) [55]; and (b) SAHA interactions in crystal structure of human HDAC (PDB: 4LXZ) [56].