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For this assignment I selected and downloaded 3 lipase enzymes from PDB, with accessions **1W52**, **2BYE**, and **2BYF**. To align these enzymes, I loaded them into PyMOL 1.3 and used the **align** command to do the 9 structural alignments (3 pairs of enzymes, and for each pair: one overall alignment, one C^{α} alignment, one active site alignment). For the overall alignments, I used the command `align 1W52, 2BYE`. For the C^{α} alignments and active site alignments, I simply used the **n.** and **i.** qualifiers to specify atom types and active residues (respectively). Graphics of aligned enzymes are attached to this homework submission.

For each pair of atoms, there was not much difference between the overall alignment and the C^{α} alignment, either spatially or in terms of RMSD. However, in each case, aligning based on active site residues made a significant difference. The relative orientation was quite different, and there was a significant increase in RMSD. Forcing the actively relevant residues to align properly caused other parts of the structural alignment to diverge, thus the increase in RMSD.

One way this information could be used to improve protein sequence alignments is to look at spatially homologous active residues from a set of structural alignments. Building a table of frequencies based on these residues in active sites may help alignment algorithms to align functionally relevant residues correctly, even if the overall alignment is not as optimal.