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Computational Biology Homework 8

1. Group 1, which has larger ASA and small B-factor, is composed of LEU6, ALA19, and LEU29. These residues are hydrophobic, short-chain, and uncharged. The small B-factor is because of their short carbon chains and because their exposure to polar solvent doesn’t cause electronic interactions, thus low fluctuations in the electronic distribution, resulting in low B-factor.

On the other hand, Group 2, which has larger ASA and a large B-factor, is composed of ARG20, LYS46, GLU49, ARG53. These residues are hydrophilic, long-chain, polar, and charged. The high B-factor is explained by their longer carbon chains, and the exposure to polar solvent causes electronic interactions leading to fluctuations in the electronic distribution, or high B-factor.

2. The apparent limitation in flexibility is caused by hydrogen bonding (3 H-bonds) between the two residues since they are located on antiparallel strands of a beta sheet. This limits the electronic distribution, so we have a low-B-factor.