**SCREAMing Sidechains in Proteins**

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The placement of protein sidechains has important applications in structural biology, ranging from protein-protein recognition to enzyme catalysis. We have been developing a program called SCREAM (*SideChain Rotamer ExcitAtion Method*) that positions sidechains with an emphasis on accuracy of the placement.

Every sidechain placement program has at least three important components: the rotamer library, the scoring function, and the placement algorithm. SCREAM users can specify the fineness of the rotamer library to be used, depending on the nature of the application. SCREAM uses an all-atom potential (modified DREIDIING) to score the sidechains, with a novel van der waals potential that is coupled with the fineness of the rotamer library employed. The placement algorithm is where the program got its name—rotamer excitation. This method allows us to sidestep the combinatorial nature of the problem and arrive at solutions at close to linear time with respect to number of sidechains for a problem that, in computer science parlance, is NP-hard.

Illustration: Designing Mutants