

Selection of input parameters:

For SAAMBE webserver, 1BRS.pdb is used for example.

Download the protein 1BRS.pdb, and use it for training purposes.

For example:

Partner 1: A

Partner 2: D

Position: 80

Chain: D

Original Amino Acid (One letter abbreviation): E

Mutated Amino Acid (One letter abbreviation): A

The change of binding energy due to mutation from SAAMBE and experimental results are 0.46708 kcal/mol and 0.48415 kcal/mol respectively. Note that this change is mutant minus wild-type binding free energies. Thus, positive change implies mutation destabilizes the protein-protein interaction.

Be aware that NAMD energy minimization does not result in identical structures, if repeated several times on the same file. Because of that, if you run the same mutation via SAAMBE, the results may be slightly different.