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Evaluation of Target Residues for Crystallization by Surface Entropy Reduction. David R. Cooper¹, Tomasz Boczek^{1,3}, Katarzyna Grelewska^{1,3}, Malgorzata Pinkowska^{1,3}, Michal Zawadzki^{1,3}, Lukasz Goldschmidt^{2,3}, David Eisenberg^{2,3}, Zygmunt Derewenda^{1,3}, ¹Dept. of Molecular Physiology and Biological Physics, Univ. of Virginia, Charlottesville, VA 22908, ²Dept. of Chemistry and Biochemistry, Univ. of California, Los Angeles, Los Angeles, CA 90095, ³PSI Center for Structure and Function Innovation.

The fact that crystallization remains a bottleneck for the structure determination of even well-behaved, soluble proteins is leading more laboratories to use mutagenesis to facilitate crystallization. The Surface Entropy Reduction (SER) approach that our lab has focused on has shown to be quite successful. Although intuitively alanine is a good target amino acid and has proven to aid crystallization, preliminary successes with other residues have led us to perform a more extensive examination of the role of the target residue. Nine sets of mutations were chosen for a model protein, and five target residues (A, S, T, H, & Y) were systematically examined for their ability to facilitate crystallization. We also evaluated the use of alternate reservoirs for crystallization. Although no one target residue stands out as the magic bullet, this study suggests a crystallization strategy that can dramatically increase the chances of obtaining crystals of difficult proteins.