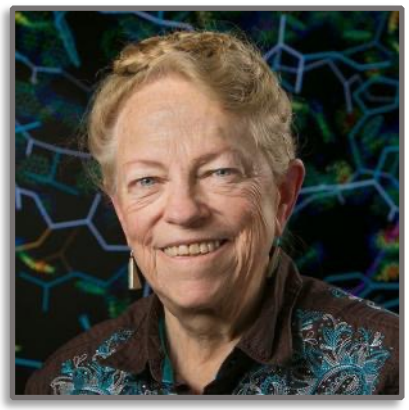

Jane Shelby Richardson, MA
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New Problems and Answers for Atomic Models at >2.5Å - Pernicious Overfitting vs Good Analytics and Predictions

Jane Richardson and her husband David have worked together for over 50 years on research to understand the 3D structure of protein and RNA molecules. They were early pioneers in protein crystallography, protein de novo design, and molecular graphics. They developed a method that calculates hydrogen-atom contacts to quantify the details of modeled packing interactions, widely used on their MolProbity website and elsewhere to improve the accuracy of macromolecular structures by crystallography, cryoEM, and now AI predictions.

Jane developed the ribbon representation of protein structures, described many common features of overall protein folds and local motifs (Greek key beta barrels, helix caps, etc.), and works to spread molecular 3D literacy at Duke and around the world. From a Swarthmore B.A. in philosophy she has become a biophysicist, a MacArthur Fellow, a member of the National Academies of Sciences & of Medicine, Hollaender Award in Biophysics, and has three honorary degrees. For details, see Ann. Rev. Biophysics 4:1-28.

More recently she and Dave have been busy responding to the CryoEM Resolution Revolution, 3D structures of SARS CoV-2 macromolecules, and AlphaFold structure predictions including what happens when they fail.