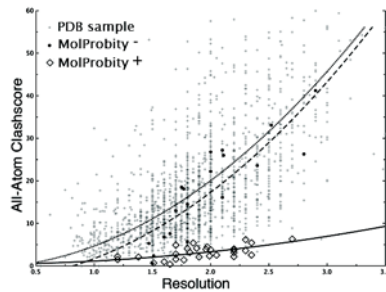


E0027

Checking on Your Mol's Probity and Healing Her Hurts. Jane S. Richardson, Ian W. Davis, W. Bryan Arendall III, Wolfram Tempel¹, & David C. Richardson, Dept. of Biochemistry, Duke Univ., Durham, NC 27710, ¹Dept. of Biochemistry & Molecular Biology, Univ. of Georgia, Athens, GA 30602.

The MolProbity web service at <http://kinemage.biochem.duke.edu> combines hydrogen addition and all-atom contact analysis with updated geometrical validation tools to provide both improved global quality assessments of macromolecular structures and also very sensitive flags of problem areas fit into the wrong local minimum conformation. These outliers are highly resolution and B-factor dependent. Since they are both local and directional, in most cases they indicate changes that can correct the identified problem. The figure plots all-atom clashscore vs resolution for 1784 sample PDB structures (grey crosses, dotted-line fit).



The solid circles are SECSG structures done without MolProbity (note: quality is generally a bit better, not worse, for structural genomics). The open diamonds are SECSG structures that benefited from MolProbity-based diagnosis and corrections during the refinement process. R, Rfree and fit to electron density become better, while clash, rotamer and Ramachandran scores improve by dramatic factors of 5- to 10-fold. You too can get rid of uncomfortable red clash spikes and boost your molecule's accuracy.

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