

## Protein hydrogen bond parameters as a new validation tool

**Pavel Afonine<sup>1</sup>, Oleg Sobolev<sup>1</sup>, Nigel Moriarty<sup>1</sup>, Yanting Xu<sup>1,2</sup>, Thomas Terwilliger<sup>3,4</sup>, Paul Adams<sup>1,5</sup>**

<sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, United States of America;

<sup>2</sup>International Center for Quantum and Molecular Structures, Shanghai University, Shanghai 200444, People's Republic of China;

<sup>3</sup>Bioscience Division, Los Alamos National Laboratory, Mail Stop M888, Los Alamos, NM 87545, USA;

<sup>4</sup>New Mexico Consortium, Los Alamos, NM 87544, USA;

<sup>5</sup>Department of Bioengineering, University of California Berkeley, Berkeley, CA 94720, USA;

*pafonine@lbl.gov*

Atomic model refinement and completion at low resolution (cryo-EM or crystallographic) is often a challenging task. This is mostly because the experimental data aren't sufficiently detailed to describe using atomic models. To make refinement practical and ensure a refined model is geometrically meaningful additional *a priori* information about model geometry needs to be used. This information includes restraints on Ramachandran plot distributions or side chain rotameric states. However, using Ramachandran plot or rotameric states as refinement targets diminish the validating power of these tools. Therefore finding additional model validation criteria that are not used or difficult to use as refinement goals is desirable. Hydrogen bonds are one of most important non-covalent interactions that shape and maintain protein structure. These interactions can be characterized by specific geometry of hydrogen donor and acceptor atoms. Systematic analysis of these geometries performed for all quality-filtered high-resolution models of proteins from PDB shows they have distinct and conserved distribution that can be characterized by only two parameters. Here we demonstrate how these two parameters can serve as unique validation metrics and how they can pinpoint severe modeling problems that no other validation tools can detect. This tool is now a part of Phenix model validation suite; guidelines to its use and interpretation will be given.

**Keywords: hydrogen bond, Phenix, crystallography, cryo-EM, validation**