

Microsymposium

MS099.005

wwPDB onedep validation services

John Westbrook¹, John Markley², Haruki Nakamura³, Sameer Velankar⁴, Stephen Burley¹

¹Rutgers, The State University Of NJ, Piscataway, United States, ²University of Wisconsin-Madison, Madison, United States, ³Osaka University, Suita, Osaka, Japan, ⁴European Molecular Biology Laboratory, European Bioinformatics Institute, Hinxton, United Kingdom

E-mail: jwest@rcsb.rutgers.edu

The Protein Data Bank (PDB) is the single global data resource for experimental biomacromolecular structure data (Berman et al., 2003). The PDB archive is managed by the Worldwide Protein Data Bank (wwPDB; <http://www.wwpdb.org>) organization through its partners: Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB, <http://rcsb.org>), Biological Magnetic Resonance Bank (BMRB, <http://bmr.org>), Protein Data Bank Japan (PDBj, <http://pdbj.org>), and Protein Data Bank in Europe (PDBe, <http://pdbe.org>). Through this global collaboration, the wwPDB has developed the OneDep platform for deposition, biocuration, and validation of 3D biological macromolecules experimentally determined by X-ray crystallography, NMR spectroscopy, and 3D electron microscopy (Young et al., 2017).

The content of validation reports produced by the OneDep system has been informed by recommendations from expert task forces representing the respective experimental communities (<http://wwpdb.org/task/validation-task-forces>). These reports include a variety of metrics useful in the assessment of the quality of the experimental data, the structural model, and the fit between them. Validation reports are provided across the life cycle of a PDB structure entry. Prior to deposition, PDB Depositors may access OneDep validation services using an anonymous stand-alone webserver and using a programmatically accessible web-service. Following biocuration, the wwPDB validation report can be made available to manuscript reviewers. wwPDB validation reports are released with each PDB entry and become a permanent part of the archived structure deposition. Validation reports resident in the PDB archive are recalculated annually using the latest validation tools and with updated comparative statistics. This talk will present an overview of the content of the wwPDB reports along with a description of the available validation services.

wwPDB Members: RCSB PDB (supported by NSF DBI-1338415, NIH, and DOE); PDBe (EMBL-EBI, Wellcome Trust, BBSRC, EU, and MRC); PDBj (JST-NBDC); and BMRB (NIGMS).

Berman, H. M., Henrick, K. & Nakamura, H. (2003). *Nat Struct Biol* 10, 980.

Young, J., Westbrook, J. D., Feng, Z., Sala, R., Peisach, E., Oldfield, T. J., Sen, S., Gutmanas, A., Armstrong, D. R., Berrisford, J. M., Chen, L., Chen, M., Di Costanzo, L., Dimitropoulos, D., Gao, G., Ghosh, S., Gore, S., Guranovic, V., Hendrickx, P. M. S., Hudson, B. P., Igarashi, R., Ikegawa, Y., Kobayashi, N., Lawson, C. L., Liang, Y., Mading, S., Mak, L., Mir, M. S., Mukhopadhyay, A., Patwardhan, A., Persikova, I., Rinaldi, L., Sanz-Garcia, E., Sekharan, M. R., Shao, C., Swaminathan, G. J., Tan, L., Ulrich, E. L., Van Ginkel, G., Yamashita, R., Yang, H., Zhuravleva, M. A., Quesada, M., Kleywegt, G. J., Berman, H. M., Markley, J. L., Nakamura, H., Velankar, S. & Burley, S. K. (2017). *Structure* <http://dx.doi.org/10.1016/j.str.2017.01.004>.

Keywords: [wwPDB](#), [structure data archive](#), [validation](#)