Ligand Validation for the Protein Data Bank

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The Protein Data Bank (PDB) is the global repository for experimentally-determined 3D structures of biological macromolecules. It is managed by the Worldwide Protein Data Bank (wwPDB, wwpdb.org). In addition to biopolymer structure data, the PDB Chemical Component Dictionary (CCD) catalogues small molecule ligands, encompassing IUPAC atom nomenclature for standard amino acids and nucleotides, stereo-chemical assignments, bond order assignments, experimental model and computed ideal coordinates, systematic names, and chemical descriptors. Precise knowledge of interactions between macromolecules and small ligands is central to our understanding of biological function, drug action, mechanisms of drug resistance, and drug-drug interactions.

The wwPDB OneDep system supports PDB data deposition, validation, and biocuration. OneDep produces Validation Reports using standards developed with expert task forces. For X-ray structures, the fit of the ligand to electron density difference maps is assessed quantitatively using real-space R-factors (RSR and RSR Z-scores). Within OneDep, 3D electron density difference maps are produced for expert review. For released structures, precomputed electron density difference maps for bound ligands and wwPDB Validation Reports can be accessed from RCSB PDB Structure Summary pages (e.g., http://www.rcsb.org/structure/1VOL for PDB ID 1vol).

The 2015 Ligand Validation Workshop generated community recommendations aimed at further improving validation of ligand structures in the PDB (Adams *et al*. 2016; *Structure 24*, 502-508). Progress towards implementation of these recommendations will be reported together with ongoing enhancements to the CCD and wwPDB Validation Report.

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