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New wwPDB validation pipelines for X-ray, NMR and 3DEM structures

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The Protein Data Bank (PDB) is the single global archive of 3D biomacromolecular structure data. The archive is managed by the Worldwide Protein Data Bank (wwPDB; wwpdb.org) organisation through its partners, the Research Collaboratory for Structural Bioinformatics (RCSB PDB), the Protein Data Bank Japan (PDBj), the Protein Data Bank in Europe and the Biological Magnetic Resonance Bank (BMRB). Analogously, the Electron Microscopy Data Bank (EMDB) is managed by the EMDataBank (emdatbank.org) organisation. A few years ago, realising the needs and opportunities to assess the quality of biomacromolecular structures deposited in the PDB, the wwPDB and EMDataBank partners established Validation Task Forces (VTFs) to advise them on up-to-date and community-agreed methods and standards to validate X-ray, NMR and 3DEM structures and data. All three VTFs have now published their recommendations (1, 2, 3) and these are getting implemented as validation-software pipelines. The pipelines are integrated in the new joint wwPDB deposition and annotation system (<http://deposit.wwpdb.org/deposition/>). In addition, stand-alone servers are provided to allow practising structural biologists to validate models prior to publication and deposition (<http://wwpdb.org/validation-servers.html>). The validation pipelines and the output they produce (human-readable PDF reports and machine-readable XML files) will be described.

[1] Read, R. J. et al. (2011). *Structure*, 19, 1395-1412., **[2]** Montelione G. T. et al. (2013) *Structure* 21, 1563-1570., **[3]** Henderson R. et al. (2012) *Structure* 20: 205-214.

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