areas concentrated upon in the wwPDB remediation efforts are

a) Improving the detailed chemical description of non-polymer and monomer chemical components.
b) Standardizing atom nomenclature.
c) Updating sequence database references and taxonomies.
d) Resolving any remaining differences between chemical and macromolecular sequences.
e) Improving the representation of viruses.
f) Verifying primary citation assignments.
g) Ensuring consistency between beamline and synchrotron facility names with BioSync.

A complete release of remediated data files is available from a dedicated ftp site. This area is separated from the original archive of deposited data files, which will continue to be available as previously. The details of the remediation process as well as its impact on end-users and developers of software will be discussed along with new features in PDB format 3.1.

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The determination of protonation states in proteins J R Helliwell[a,b], H U Ahmed[a], M Blakeley[c], M Cianci[b,@], J A Hubbard[d], S Fisher [a], L Govada[e], N E Chayen[e], E Carpenter[e] and J Squire[e] [a]*School of Chemistry, Brunswick street, The University of Manchester, M13 9PL. UK,* [b]*CCLRC Daresbury Laboratory, Warrington, Cheshire WA4 4AD, UK,* [c]*EMBL Grenoble Outstation, BP 156, 38042, Grenoble, Cedex 9, France* [d]*Computational, Analytical & Structural Sciences, GlaxoSmithKline, Gunnels Wood Road, Stevenage, Hertfordshire, SG1 2NY. UK,* [e]*Sir Alexander Fleming Building, Imperial College of Science, Medicine and Technology, South Kensington, London SW7 2BZ, UK, @ Current address:PETRA III Project, EMBL Outstation, DESY Laboratory, Hamburg, Germany.* E-mail: john.helliwell@manchester.ac.uk

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Biology rests on chemical reactions. Many chemical reactions involve hydrogens or protons. The determination of hydrogens, as is well known, is particularly challenging for protein crystallography. For X-rays as the probe, even with the best possible brilliance synchrotron radiation beamline, mobility of a hydrogen can render the diffraction signal invisible and that of a proton is by definition not visible to X-rays. For neutrons as the probe the issues are technical to do with converting hydrogens to deuteriums, by soaking in D_2O or perdeuteration biological expression, and/or the need for big crystals to be used with weak neutron fluxes. The protonation states of aspartic acids and glutamic acids as well as histidine are investigated in three X-ray cases; Ni, Ca concanavalin A at 0.94Å, a thrombin-hirugen binary complex at 1.26Å resolution and a cardiac myosin binding protein 'C1 domain' at tested resolutions of both 1.2 and 1.3 Å. The truncation of the Ni, Ca concanavalin A data at various test resolutions between 0.94 and 1.50Å provided a test comparator for the thrombin-hirugen and 'mycC0', 'unknown', carboxylate bond lengths. The complementary technique of using neutron protein crystallography has provided evidence of the protonation states of histidine and acidic residues in concanavalin A, and also the correct orientations of asparagine and glutamine side chains. Again the truncation of the neutron data at various test resolutions between 2.5 and 3.0Å, even 3.25 and 3.75Å resolution, examines the limits of the neutron probe. These studies indicate a widening of the scope of both X-ray and neutron probes in certain circumstances to elucidate the protonation states in proteins, and which will have basic and applied (ie Pharma-industrial) research potential.