

Worldwide Protein Data Bank Advisory Committee (wwPDB-AC)
Report of September 27th 2013 Meeting
Rutgers, the State University of New Jersey, New Jersey, USA

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wwPDB-AC Mission Statement

To help ensure that the Protein Data Bank is maintained for the public good as a secure, singular global archive for experimental structural biology data that is freely accessible in perpetuity.

Meeting Summary

The Worldwide Protein Data Bank Advisory Committee (wwPDB-AC) to the leadership of the Research Collaboratory for Structural Bioinformatics (RCSB-PDB), the BioMagResBank (BMRB), the Protein Data Bank in Europe (PDBe), and the Protein Data Bank Japan (PDBj) met at Rutgers, the State University of New Jersey, USA on September 27th 2013.

The agenda included

- (1) Overview;
- (2) Deposition and Annotation (D&A) tool;
- (3) Format issues, validation & experimental methods;
- (4) NMR;
- (5) Outreach;
- (6) Matters arising, discussion; and
- (7) Executive session and feedback

Following a welcome talk by S. Burley, an overview of the state of the wwPDB was presented by Helen Berman, followed by a summary of recent activities was subsequently provided by Quesada, Kleywegt, Markley, and Nakamura.

(1) Overview (Helen Berman)

H. Berman provided an overview of the past year.

The wwPDB-AC was pleased to learn of the continuing strong growth of archiving, significant progress on common deposition and annotation system (D&A), and implementation of the new format PDBx during the past 12 months. The four wwPDB partner centers collaborate towards the common goal of providing a stable, state-of-the-art macromolecular structure archive to broad scientific communities. Data depositions have steadily increased, with impressive records of website access and structure downloads reaching a million downloads each day. The PDB continues to serve as an important international archive used by science communities including bioinformatics, structural biology, biochemistry, cell and molecular biology and translational medicine, as well as various areas of industries. The wwPDB continues to expand its scope toward integrative structural biology.

The wwPDB-AC applauds the four data centers for having developed a culture of cooperation among them. The collaborative atmosphere is evident in many areas, e.g. D&A, validation task forces, etc. The biggest concern of the wwPDB-AC remains the sustainable funding of the four centers, which have totally different funding schemes and funding periods. In particular, FY2013-14 has been critically important as some centers apply for major or medium scale funding renewals. The wwPDB-AC is pleased to note that the success of each partner owes a lot to the strong and successful wwPDB collaborations.

The wwPDB-AC endorses the proposal by the four centers regarding global annotation workload balance. Implementing a scheme whereby workload among different centers can be dynamically balanced so that each wwPDB center assumes responsibility for depositions originating from within their respective geographies will be most welcome. To this effect, successful implementation of the common D&A continues to be crucial.

Funding efforts:

Following submission of the RCSB PDB's non-competitive NSF grant renewal for 2014-2018, the site visit to RCSB PDB went well and funding was renewed. This renewal is most welcome since it provides five years of stable funding to support operation of RCSB PDB, a key to the overall capacity of wwPDB.

Post Meeting Addendum: Regrettably, the RCSB PDB's 2014 budget was slightly reduced versus 2013 despite the significant increases in fringe benefits at both RU and UCSD. The RCSB PDB will be seeking additional funding from other sources.

The core funding of PDBe from EMBL is in the last year of the 5 year cycle, and a renewal process will begin in December 2014 for the next 3- or 5-years. PDBe expects flat or slightly reduced funding from EMBL and other funding agencies. The wwPDB-AC is anxious to help whenever needed in terms of longer term sustainability, for example, PDBe expects that they will be invited to apply for another Wellcome Trust grant in 2014.

PDBj's grant renewal with JST was due in October 2013. Funding levels in this next 3-year cycle of JST funding is expected to be slightly reduced compared to the current funding period. The wwPDB-AC understands that there is general support of PDBj's activities in Japan, and hopes the renewal will be successful.

Post Meeting Addendum: Subsequently the wwPDB-AC learned of the success of the grant application.

The wwPDB-AC is particularly pleased to learn that BMRB's R01 funding will start on Dec 1, 2013, and will run for 4 years. Despite a slightly reduced level of funding, this will certainly ensure continued development and support by the BMRB center in the area of NMR structural biology.

wwPDB Foundation

wwPDB-AC recommends considering rescoping for larger scale funding, for example, for expanded outreach and education activities while wwPDB Foundation funds cannot be used to fund PDB operations.

The Foundation charter is not about operations, however; each site can raise money in any way it chooses independent of the Foundation. The wwPDB-AC also welcomes the new chair Anthony Nicholls, who will lead the Foundation members, the directors of the four centers, and the Foundation secretary and treasurer.

(2) Deposition and Annotation (D&A) tool (Martha Quesada)

The D&A project has progressed rapidly during the last 12 months. The committee was impressed by the demonstration of the D&A by Jasmine Young during the meeting. There was a suggestion from the RCSB of adding an option for depositors to add their citation. This would be as an additional option to having the depositor enter the communication module and let the annotator know that their publication has come out.

For smooth launching of D&A tools, the wwPDB-AC recommends soliciting more feedback on the D&A from Validation Task Forces and software developers worldwide. To spread the use of D&A tools rapidly we recommend more efforts will be given to its advertisement in Asia and Oceania.

Timeline for NMR and EM.

The NMR validation tools are in internal testing, and the expectation is that NMR deposition will be available for public testing within the D&A system in early 2014. Completion of the development of the EM functionality for D&A is expected to take place in Q1 of 2014. An updated timeline for completion of these components should be provided to the wwPDB-AC at the 2014 meeting.

(3) Format issues, validation & experimental methods (Gerard Kleywegt)

Uptake of validation reports by journals

Starting Aug 1, 2013 all depositors of X-ray crystal structures have received the new Validation Report PDF, which will be made available for all depositors in 2014. The Committee finds the uptake of validation reports at the time of manuscript submissions has been good, including IUCr journals, NSMB, JBC *etc.* The efforts by the four wwPDB centers are to be commended.

Ligand density

There was a question of whether the density for ligands can be provided as a snapshot in the validation report. It appears very challenging due to the number of variables and that the wwPDB validation report is produced automatically while visualization of the density requires user manipulation of the image for useful review. Nevertheless, there is need for development of better methods for assessing the local ligand density fit by the crystallographic community so that these methods can be adopted by the wwPDB.

According to the Validation TF, there is a requirement that for each structure there would be a clear representation of the validation report. For example, the PDB FTP site will have the validation reports. They will also be presented on each wwPDB website in their own ways since data out is the competitive portion of the wwPDB relationships.

The validation tools will be used to validate historic structures; all structures in the archive will be run through the pipeline with validation reports created for each.

The Committee also learned that the stand-alone X-ray validation server would become available to the public in several weeks and further validation tools will be developed for RNA and DNA.

Hybrid data

In light of future directions of structural biology research around the world, wwPDB-AC emphasizes the importance of making stronger efforts on the incorporation of hybrid data into PDB. The committee sees the importance of defining a process of updating the VTF membership, and in particular, recommends assembling a Hybrid Methods Task Force that includes members from the VTFs as well as experts in the relevant methodologies. In the area of NMR, the Committee notes that it is worth considering including models generated from sparse NMR data such as residual dipole coupling and chemical shifts. The NMR community requests that this be taken into consideration in defining/reassessing how validation is defined. There will be a meeting in 2014 to discuss hybrid methods broadly. Overall, the committee strongly recommends to develop a strategy for a much bigger scale of hybrid methods beyond cryoEM, CLEM, mass spec, cross linking etc.

(4) NMR (John Markley)

As described above securing the R01 grant from NIGMS is an important milestone for the Center. The agencies now prefer 4-year rather than 5-year awards. BMRB expects to be able to hire one more staff member, in addition to Vincent Chen who is currently working with the NMR facility.

(5) Outreach (Haruki Nakamura)

International Year of Crystallography 2014

Ted Baker, wwPDB, IUCr representative is asked to promote the wwPDB calendar to be distributed at the opening ceremony of the year of crystallography in January 2014 in Paris. Hard copies of the IYCr 2014 calendar were shown to the wwPDB-AC members. The committee recommends that printable and slide show versions to be made available for larger audience.

BSR2016 Stanford

The announcement was made regarding the next Biology and Synchrotron Radiation will be held in Stanford in late August 2016, to be organized by S. Wakatsuki (Stanford/SLAC) and S.K. Burley (Rutgers/RCSB) in collaboration with the light source facilities in the northern USA and Canada.

(6) Matters arising (Helen Berman):

Responses to the Letters to Editor in Acta Cryst D.

Timely deposition of PDB entries.

The wwPDB-AC discussed the PDB centers' response to R. Joosten whose letter to the Editor was to be published in Acta Cryst D:

“Timely deposition of macromolecular structures is necessary for peer review.”

Joosten RP, Soueidan H, Wessels LF, Perrakis A.

Acta Crystallogr D Biol Crystallogr. 2013 Dec;69(Pt 12):2293-5. doi:

10.1107/S0907444913024621. Epub 2013 Nov 19.

In this letter the authors analyzed the statistics of elapsed time between manuscript submission/publication and PDB deposition. Manuscripts are often submitted to journals prior to deposition. Journals should be re-encouraged about not accepting manuscripts without PDB ID's. They propose to journals to take necessary measures for timely PDB depositions. The wwPDB-AC discussed the Centers' response, proposing to add an option to suppress titles until the time of PDB entry release, which is not the default currently although titles can be suppressed currently by sending an email to one of the wwPDB centers. On the other hand, sequences can be suppressed at the time of deposition. The wwPDB-AC agrees that the suppression of a title should be made an option at the time of deposition.

The committee also recognizes the importance of publicizing the usefulness of releasing the information early to the community, in particular that sequences are released to modeling groups on Friday prior to full release on Wednesday.

C. Wolberger has made an additional proposal to suppress the full author list as an option during the pre-release, limiting the requirement to the depositor's name only. On release full list must be disclosed. Although there is a need for some clarification of details the wwPDB endorses the proposal of options to suppress the full author list at the time of deposition until release.

Response to M. Jaskolski – On the propagation of errors

The committee also discussed another issue raised by another Acta D Letter to Editor, on the propagation of errors by M. Jakolski:

On the propagation of errors. Jaskolski M.

Acta Crystallogr D Biol Crystallogr. 2013 Oct;69(Pt 10):1865-6. doi:

10.1107/S090744491301528X. Epub 2013 Sep 20.

The Committee agrees with the wwPDB Center directors that the new validation tools will help identify out these issues and improve the quality of data deposited in the archive.

Accepting unmerged intensities

The committee notes the value of accepting unmerged intensities to PDB and recommends that X-ray VTF and PDBx/mmCIF Working Group propose and follow detailed paths on how this might be done.

Accepting DOIs or URLs for raw data deposition

The wwPDB-AC considers that depositing raw data is not really needed for the purpose of detecting errors or possible fraud as long as appropriate validation protocols are in place. John Westbrook of RCSB is going to write an article on the implications of storing raw data. And the Committee recommends that wwPDB centers continue to follow these discussions in the community.

Remediation of carbohydrates

Remediation of carbohydrates in the PDB archive is an issue that the software developers come across often. wwPDB-AC suggests PDB centers address this by involving the software development community, and charge a focused group, for example the PDBx/mmCIF Working Group headed by Paul Adams, to help develop and review a plan. It is also to be coordinated with changes in restraints libraries.

Improving IUCr-wwPDB interactions

While the IUCr and wwPDB have a long history of collaboration, it has been noted that the IUCr and wwPDB organizations could benefit from having more frequent communication and interaction. A possibility to explore would be to nominate points of contact from both sides to initiate communication on relevant issues.

Terms of reference (TOR)

A new version of terms of reference was implemented in 2013 with 3 year terms of membership renewable to a total of 6 years, which also applies to chairperson. With the new TOR in place, all the current members are entering their first of three years according to the new TOR. Members are able to send a letter of resignation if necessary. While recognizing the 3 year term of wwPDB-AC membership, it is worthwhile noting the importance of a rolling turnover so that all members do not exit at the same time.

wwPDB webpage

wwPDB webpage visibility can be improved and we are pleased to learn about the ongoing discussions towards transitioning to a new website, PDB.ORG.

The next wwPDB AC meeting will be held in Hinxton, UK on Friday October 10, 2014.

Appendix: PDB Metrics

In aggregate, 9972 (10,700*) depositions were processed between January 1st and December 31st 2012 with a two-week average turnaround (* 2013 projection).

Breakdown of depositions by discipline in calendar year 2012:

X-ray: 9,273 (93%, up from 8,550 in 2011)

NMR: 586 (~6%, up from 583 in 2011)

EM: 101 (~1%, up from 89 in 2011)

Other: 12 (~0.1%)

Breakdown of depositions processed by wwPDB centers in calendar year 2012:

RCSB PDB: 6409 (64%)

PDBj: 1887 (19%)

PDBe: 1676 (17%)

Breakdown of depositions by geography in calendar year 2012:

41.6% North America

28.7% Europe

17.8% Asia

8.1% Industry

1.0% South America

2.6% Oceania

<0.1% Africa