**Integrative/Hybrid (I/H) methods meeting summary, Thursday April 6th, 2017**

We held a "large" I/H methods virtual meeting with representatives from the laboratories of the members of the I/H methods task force and the wwPDB partners. Seventeen participants from various research groups attended the meeting. Meeting invites were sent to representatives from the following groups.

*I/H methods task force representation and validation sub-group members*

Andrej Sali (UCSF, USA) sali@salilab.org

Torsten Schwede (SIB, Switzerland) torsten.schwede@unibas.ch

Gerhard Hummer (MPI, Germany) gerhard.hummer@biophys.mpg.de

Jens Meiler (Vanderbilt, USA) jens.meiler@vanderbilt.edu

Frank DiMaio (U. Washington, USA) dimaio@u.washington.edu

Emad Tajkhorshid (UIUC, USA) emad@life.illinois.edu

*wwPDB partners*

RCSB PDB (Rutgers, USA) <http://www.rcsb.org/>

PDBe (EBI, UK) <https://www.ebi.ac.uk/pdbe/>

PDBj (Osaka U, Japan) <https://pdbj.org/>

BMRB (U. Wisconsin) <http://www.bmrb.wisc.edu/>

**Meeting Attendees (representatives from the above groups)**

Ben Webb (UCSF, USA) ben@salilab.org

Tom Goddard (UCSF, USA) goddard@cgl.ucsf.edu

Kumaran Baskaran (BMRB, USA) kbaskaran2@wisc.edu

Emad Tajkhorshid (UIUC, USA) emad@life.illinois.edu

Ryan McGreevy (UIUC, USA) ryanmcgreevy@ks.uiuc.edu

John Stone (UIUC, USA) johns@ks.uiuc.edu

Rocco Moretti (Vanderbilt, USA) rmorettiase@gmail.com

John Westbrook (RCSB PDB, USA) john.westbrook@rcsb.org

Brinda Vallat (RCSB, USA) brinda.vallat@rcsb.org

Oliver Smart (PDBe, UK) oliver.smart@ebi.ac.uk

Aleksandras Gutmanas (PDBe, UK) gutmanas@ebi.ac.uk

John Berrisford (PDBe, UK) jmb@ebi.ac.uk

Juergen Haas (SIB, Switzerland) juergen.haas@unibas.ch

Juergen Koefinger (MPI, Germany) juergen.koefinger@biophys.mpg.de

Hirofumi Suzuki (PDBj, Japan) hirofumi@protein.osaka-u.ac.jp

Gert-Jan Bekker (PDBj, Japan) gertjan.bekker@protein.osaka-u.ac.jp

Maggie Gabanyi (RCSB, USA) – Scribe Maggie.gabanyi@rcsb.org

**Meeting Agenda**

1. Overview of the current I/H methods dictionary and documentation. Please follow the links below to access the dictionary and associated documentation on Github.

<https://github.com/ihmwg/IHM-dictionary>

<https://github.com/ihmwg/IHM-dictionary/blob/master/dictionary_documentation/documentation.md>

Our goal is to gather feedback regarding the I/H methods dictionary.

2. Examples of I/H models from IMP (<https://github.com/ihmwg/IHM-dictionary/tree/master/examples> and <https://pdb-dev.rcsb.rutgers.edu/>)

3. Introduce the modeling dictionary, also available on Github ([https://github.com/JuergenHaasSIB/modeling\_dictionary)](https://github.com/JuergenHaasSIB/modeling_dictionary%29)

4. Open discussion

**Meeting Summary**

1. Brinda Vallat started with an overview of the dictionary and documentation on the Github site. The following aspects were highlighted:
* Organization of input datasets in integrative modeling; references to data in the primary data repositories (EMDB, EMPIAR, BMRB, SASBDB, PRIDE); referencing data via DOI for those with no primary data repositories.
* Information regarding starting structural models (references to models PDB, PDB-Dev, Model Archive)
* Descriptions of spatial restraints derived from experiments (2DEM, 3DEM, CX-MS, SAS)
* Modeling of multi-scale, multi-state, time-ordered ensembles
* Definitions of preliminary validation metrics
* A high-level description of the modeling workflow and protocols
1. Ben Webb provided an overview of the three IMP examples in PDB-Dev ([https://pdb-dev.rcsb.rutgers.edu](https://pdb-dev.rcsb.rutgers.edu/)). The nup-84 sub-complex, the mediator complex and the exosome complex. These are in PDBx/mmCIF format and are compliant with the current dictionary (IMP has been extended to support the mmCIF format). These are all coarse-grained models and are not toy systems, they are actual modeling applications from IMP. These examples are purely from IMP and we need more examples from the community so that we can ensure that the dictionary is general enough to work with I/H models generated by other methods and to remove any assumptions that only worked for IMP.
2. Tom Goddard gave a brief overview of visualizing the I/H models with ChimeraX (<https://www.cgl.ucsf.edu/chimera/data/site-visit-nov2016/chimerax_demo.html>). ChimeraX supports the I/H methods extensions to the mmCIF dictionary and visualizes all of the data defined in the dictionary. This includes the multi-scale models (atomistic and coarse-grained), spatial restraints (EM maps, crosslink distances) and starting structural models (comparative and experimental). The multi-scale model of the Nup84 sub-complex visualized using ChimeraX was shown as an example. The 7 sub-units in the coarse-grained models, the red and green crosslinks (violated and satisfied respectively), the starting comparative models, the 2DEM class average image and the localization densities of good-scoring ensembles can all be visualized in ChimeraX.
3. Juergen Haas presented an overview of the modeling dictionary that is being developed in parallel as an extension to the PDBx/mmCIF dictionary. This dictionary defines the data content for *in silico* models to be archived in the Model Archive such as template information, multiple sequence alignments, restraints from co-evolution data and modeling protocols. Feedback on the dictionary is required to proceed.
4. Finally, we had an open round table discussion to address questions or concerns from each attendee. We had enthusiastic response from all participants. Many participants emphasized the fact that we need more examples that cover a wide range of experimental data and modeling methods to make further progress. There were questions regarding how to deposit structures to PDB-Dev, how to visualize these structures on ChimeraX, how to generate dictionary-compliant mmCIF files for deposition and whether the dictionary distinguishes primary and derived data. All participants indicated that this was a very interesting and informative meeting. The next meeting will be held in a month (date and time to be decided at a later time) and the we plan to include a live demo of using ChimeraX to visualize I/H models.