

Jill Trehella
Professor Emeritus

31 January 2019

To the wwPDB Leadership Group
John L. Markley, BMRB
Haruki Nakamura, PDBj
Sameer Valenkar, PDBe
Stephen K. Burley, PDB RSCB
Helen Berman, PDB RSCB

Transmitted by email

Dear Colleagues

I write to provide a brief update of work done in preparation for the next phase of work being proposed by the SASvtf that is follow up to you original request in your letters of 18 February, 2017 to:

1. *review the state-of-the-art and develop and promulgate recommendations regarding validation of data and metadata coming from small-angle scattering (SAS) studies of biological macromolecules, and*
2. *review the state-of-the-art and develop and promulgate recommendations regarding validation of integrative/hybrid methods NMR-SAS refined atomic coordinate structures:*

I am pleased to report that our 2017 publication guidelines that includes recommendations for reporting meta data, deposition of data, and model validation tools (<http://scripts.iucr.org/cgi-bin/paper?S2059798317011597>) is at the top of the journals most read list, enjoying downloads approaching 7000 and growing citations that are already well into double digits.

As indicated in our 7 August 2017 letter to you, we also resolved at our May 4 2017 virtual meeting, to form a subgroup to look in detail at modelling scattering profiles from PDB coordinates, as this is a subject of ongoing research. The initial proposal was to use a set of well known, relatively rigid structures to test and bench mark different approaches. A small planning group has worked to develop a detailed proposal that I am about to forward to the broader SASvtf, as well as some additional recruits to the effort, for comment, with a copy to you so that you also have the opportunity to comment.

All feedback on our draft plan is welcome. The project is quite a big undertaking and while it has been evolving only slowly due to the volunteer nature of the work force, it is a very important step for the field and the community. Establishing community agreed standards and model validation tools is an essential step for communities with potential interest in developing repositories and, eventually, joining the envisioned federated resources. It is our hope that the SAS community will be a good partner in best practice in implementing this vision that the wwPDB is leading.



THE UNIVERSITY OF
SYDNEY

I look forward to seeing at least some of you in Baltimore for the workshop on 1 March. I will also be giving a platform talk at the Annual meeting that follows on "Reliable Biomolecular Structural Modelling with Small-Angle Scattering" that will in part reflect on the issues that this project will be specifically addressing.

Yours sincerely,

A handwritten signature in black ink that reads "Jill Trewhella".

Jill Trewhella, PhD

cc SASvtf members
Gaetano Montelione, Michael Nilges, Co-Chairs, NMRvtf