

**Jill Trehella**  
Professor Emeritus

09 August 2017

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

Dear Colleagues

I write to provide an update on outcomes and current activities of the SASvtf, in particular relating to your letters of 18 February.

1. *With regard to your request to the SASvtf to 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:*

As you are aware the SASvtf met virtually on May 4 to review and discuss the draft manuscript that provides an agreed set of guidelines, including specific, implementable recommendations for both data and model validation, which we would formally recommend as the SASvtf. This manuscript now accepted in *Acta Crystallographica D*. With 22 authors from multiple institutions across the US, Europe, and Asia who are leaders in their field, this work constitutes a significant contribution to the field. The quality of the end result is a testament to the strong and active engagement of the entire group.

At our May 4 meeting, the SASvtf also resolved to invite nominations for a subgroup to look in detail at modelling scattering profiles from PDB coordinates as this is a subject of ongoing research. The initial proposal is to use a set of well known, relatively rigid structures to test with exemplar data to bench mark different approaches. I am consulting with an initial set of volunteers to develop a proposal for consideration by the broader SASvtf regarding an approach, time-line for reporting, and participants.

2. *With regard to your request that the SASvtf and NMRvtf to review the state-of-the-art and develop and promulgate recommendations regarding validation of integrative/hybrid methods NMR-SAS refined atomic coordinate structures:*

The NMRvtf met June 16, 2017 and I called in to the meeting from Sweden to provide a summary report on the recommendations from the SASvtf for data and model validation. I also spoke about the proposed subgroup to be focused on modelling scattering profiles from PDB coordinates as this is a topic of significant importance for the co-refinement of NMR and SAS data for structure determination. I will be consulting with the co-Chairs of the NMRvtf in regard to membership of this subgroup.

In regard to items 1 and 2 above, importantly for the wwPDB, Dr John Westbrook has indicated that he sees no issues moving the recommended guidelines into the sasCIF, and similarly integrating with the multi-scale data model in the IHM dictionary.

There are a number of events at the upcoming IUCr Congress and Assembly in Hyderabad that relate to the above work. They include:

- **Open meeting Commission on Small-Angle Scattering (CSAS)**  
Monday the 23<sup>rd</sup> (13.05 - 14:55) , OCM-3 Room MR 2.06 Boardroom 18  
The guidelines paper will be on the agenda of this meeting for discussion
- **CSAS Report to the General Assembly**  
As the outgoing Chair of the CSAS, I will present our triennial report either the First Session of the General Assembly on Tuesday 22 August or the Second Session on Wednesday 23 August. A significant proportion of the work of the CSAS during my tenure as Chair, has been focused on supporting the development of publication guidelines, including data and model validation. This work has been tightly coordinated with the work of the SASvtf, facilitated by the fact that I Chaired both committees and that Dmitri Svergun is a Consultant of CSAS and member of the SASvtf.
- **MS-125: Small-Angle Scattering data formats, standards and repositories**  
Chaired by Cy Jeffries and Manfred Roessle, Monday 28<sup>th</sup> (14:55 – 17:30)  
My colleague J. Mitchell Guss will present a talk in this session in regard to the development of the guidelines through the coordinated efforts of the IUCr CSAS and SASvtf (abstract attached).

Given my tenure as Chair of CSAS ends with the Hyderabad meeting, I suggest that it is important to have a wwPDB liaison on the CSAS. It would be helpful to have the thoughts of the wwPDB leadership on this before the meetings in Hyderabad. Dmitri Svergun and I will be continuing as Consultants on the CSAS, and I will be happy to share with you the full slate of members and consultants once affirmed by the IUCr Executive.

Finally, as you will recall from the discussion at the 4 May virtual meeting, an unresolvable difficulty has been identified with regard to the legacy SAS models transferred from the PDB with the intent of their being deposited in the SASBDB. The SASBDB is organised with the SAS data as the primary deposition item, consistent with the recommendation contained in the first SASvtf report that archived SAS models should be accompanied by their supporting data. This recommendation was affirmed at the May 4 SASvtf meeting. The fact that these legacy models have no accompanying data means that there is no pathway for them to be deposited in SASBDB. In my capacity as Chair of the task force, I am happy to be involved in discussions as to options for the legacy models going forward, but perhaps the most appropriate contribution from the SASvtf is to draft a communication to the depositor explaining the situation. I will await your advice on this matter.

It has been an extremely satisfying project to work with my colleagues on the guidelines for data and model validation, and the SASvtf has played a vital role. I also would like to especially thank John Westbrook for his participation in the guidelines paper, and especially for his work on the development of the sasCIF which is key to our goals.

Yours sincerely,



Jill Trewhella, PhD

cc: SASvtf members

Gaetano Montelione, Michael Nilges, Co-Chairs, NMRvtf

Attachments: Accepted Guidelines Manuscript  
IUCr Abstract