

EMBL Hamburg Unit Review 25 - 27 February 2019

The EMBL Hamburg Unit was reviewed on 25 to 27 February 2019 by a panel of 15 international experts, including five members of the Scientific Advisory Committee (SAC). The review was chaired by Poul Nissen, Interdisciplinary Nanoscience Center, Aarhus (DK).

Evaluation Summary

The overall performance of EMBL Hamburg was rated as outstanding by the panel, based on the quality of the unit's research and services as well as the training and development of young scientists. The panel applauded the unit's capacity to facilitate outstanding research programmes and projects, both locally and across the world. This is being achieved through the excellent running of the synchrotron beamlines, sample preparation and characterisation facility, software programmes and governance. Since the previous review, the unit has consolidated and further developed its position at the forefront of X-ray sciences, structural biology and life sciences. Research programmes and projects of the unit address a broad range of important questions in structural biology and infection biology. These include elucidating the structures of a wide-range of membrane proteins, understanding complex biological networks and pathways such as the influenza virus infection cycle, and advanced modelling based on core principles of protein structure and dynamics. The results are disseminated with high recognition from the community. The current beamlines P12, P13 and P14, for which EMBL Hamburg is fully responsible, provide a robust, high-end service to a large and growing user community. Alongside the latest software and database developments, these services are of immense importance to the structural biology community and mail-in and remote access user support must also be encouraged. These achievements are made possible by the strong leadership and vision of the Head of Unit Matthias Wilmanns and the Joint Heads of Research Infrastructures Dmitri Svergun and Thomas Schneider.

The panel discussed many of the unit's excellent research highlights, including the development of a time-resolved pump-probe protein crystallography station at P14 with Arwen Pearson's group from the University of Hamburg. This development highlights a very important transition to "4D structural biology" and has the potential to attract a growing user community focussing on cutting-edge research problems of structural biology and biocatalysis. A novel analysis method which allows the "soft" refinement of high-resolution protein structures guided by agreement with small angle X-ray scattering data was also highlighted by the panel. There was a recommendation that excellent work such as this must adhere to EMBL's open source policy of software.

The panel noted that EMBL Hamburg is tightly integrated into a complex, local research structure, not least with the newly opened Centre for Structural Systems Biology (CSSB), on the German Synchrotron (DESY) campus, with contributions of ten research partners including EMBL. The panel recommended that EMBL Hamburg and CSSB should improve coherence and establish a joint scientific culture and community. Additionally, it was recommended that a partnership between EMBL Hamburg and the European X-Ray Free-Electron Laser Facility Biology Infrastructure (European XFEL XBI) should be further explored, and an XFEL-oriented group leader recruitment could be a wise strategy. Further afield, EMBL Hamburg has fruitful collaborations to ensure complementing expertise with EMBL Grenoble and integrates exceptionally well into the European life science research community.

Looking into the future, the Hamburg Advanced Research Centre for Bioorganic Chemistry (HARBOR) initiative, specialising in time-resolved studies using X-ray and imaging infrastructures, is under construction, and plans for a PETRA IV upgrade have been launched. The panel recommended that, prior to transition to PETRA IV, EMBL carefully evaluates the potential for biological X-ray imaging as well as considering that administrative burdens of general user support and beamtime allocation is released from the responsibility of the beamline managers and better transferred to the administrative support team of the Hamburg Unit. The panel welcomes further steps (including a symposium) to explore the possibilities for research in X-ray imaging of biological samples at PETRA IV. The panel noted that the recruitment of a small-angle X-ray scattering (SAXS) group or team leader must be carefully considered in light of highly dynamic developments in structural biology. In addition to the



PETRA IV upgrade, it was recommended that the unit should join other EMBL units in applying cryoelectron microscopy (cryo-EM) as a core method in structural biology, and a potential target for method development.

The review panel engaged in wide-ranging discussions with predoctoral and postdoctoral fellows over many aspects of research, training, mentoring and work/life balance at EMBL Hamburg. On the whole training and development of young scientists is maintained to an outstanding level at the unit. In the context of training, some students expressed concern that they are not given sufficient time to write their thesis, and the review panel felt that a mentor outside of the thesis committee would be beneficial. Mentoring was also recommended for young group leaders to ensure future career progression. Combined with general EMBL procedures and structures, the young scientists overall have great opportunities to leave the unit well prepared for a future career.

Response to the Panel's Recommendations

I would like to begin by thanking the review panel for their detailed evaluation of the activities of EMBL Hamburg. I am delighted with their overwhelmingly positive report of the unit's performance. The review panel were very positive about the leadership and research performance of the unit management team and this opinion reflects my own. I would like to congratulate them for leading by example and creating a stimulating research and service environment.

Several recommendations were made by the panel. Concerning the future transition to PETRA IV on the DESY campus, EMBL will carefully evaluate the potential implications and opportunities that PETRA IV will bring for biological research and in particular X-ray imaging. Part of the brainstorming around this will involve the organisation of a workshop to explore these possibilities.

Another point raised concerned the European XFEL XBI partnership which is currently being explored, and an XFEL-oriented group leader recruitment was suggested to be a wise strategy. This consideration will be balanced alongside skills needed for the upcoming PETRA IV upgrade, to prioritise resources in the best interest of EMBL and the external research community.

Several points were raised by the panel concerning the future of SAXS at EMBL Hamburg, particularly in the context of the upcoming retirement of Dmitri Svergun. After discussion with the unit leadership, and given the success of SAXS, it is considered important that this activity is maintained and a call will be launched in the near future.

Another point raised in the context of SAXS concerned possible transfer of the Small Angle Scattering Biological Data Bank (SASBDB) standardisation and development to EMBL-EBI. SASBDB is still being refined by the Svergun group and its curation requires active expert interactions with the depositors, which would be more difficult if the curation was moved elsewhere. As of July 2019, a postdoctoral fellow, funded by the German Federal Ministry of Education and Research (BMBF), will curate and further develop SASBDB, and this will help to free internal resources. These funds will also go towards identifying and implementing a forward-looking solution to ensure long-term sustainability of SASBDB, in cooperation with Protein Data Bank in Europe (PDBe) hosted at EMBL-EBI.

The panel also raised the general issue of EMBL open source policy of software and models for the commercialisation of open source software. In-line with EMBL's founding principles, the Laboratory endeavours to publish or otherwise make generally available its results and developed software. This is in line with established general Open Access principles. I agree that it is critical to ensure that software developments remain accessible ideally with options for further developments, for example, when an individual leaves EMBL. To ensure this, I will create a small working group to formulate a forward-looking EMBL-wide solution.

The panel strongly recommends the construction of a new building, possibly as a new wing of the CSSB, which would host EMBL. I am keen to take on this project on board with high priority for timely realisation, to unify the activities of the unit.



The recommendation that the unit should consider cryo-EM as a core method and a potential target for method development at the same level as other techniques has been taken on board. This will be weighed up against other methods that are available and will be part of more general discussions concerning the development of the DESY campus.

Finally, the review panel recommended that the general user support and beamtime allocation should be released from the responsibility of the beamline managers and transferred to administrative support. This has been discussed with the unit leadership and efforts will be made to find the appropriate balance between beamline and administrative support. Furthermore, mail-in and remote access user support will be encouraged for outside users.

In summary, I would like to congratulate the Unit leaders and members for their performance over the last review period and give credit to Matthias Wilmanns for providing visionary leadership.

Professor Edith Heard, FRS Director General

12 June 2019