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Global Phasing Limited

Status Report for Global Phasing Ltd.

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Global Phasing Ltd, Cambridge, UK

MXCuBE-ISPyB Meeting, 8-9 December 2022, ESRF

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Summary of Main Activities

- Active participation in developers' meetings for MXCuBE (and MXCuBE3) frequently including the writing up and broadcasting of Minutes (Rasmus Fogh).
- Participation in the refactoring of the MXCuBE code (Rasmus Fogh): important aspects to be dealt with at the SC/DC meeting this afternoon.
- Continued development and deployment of the GPhL Workflow and its associated autoPROC-essing at MXCuBE synchrotron beamlines (Rasmus Fogh, Peter Keller, Claus Flensburg, Clemens Vonrhein), especially
  - on P14 at EMBL-HH (Gleb Bourenkov) with MPI Göttingen projects (A. Chari)
  - on MASSIF-1 at ESRF/EMBL-GR (Olof Svensson, Matthew Bowler)
- Details in this afternoon's talk by Rasmus, and on the next slide.

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The Global Phasing Workflow on P14 after 1.5 year of routine operation

Overview

- ~ 1250 high-quality datasets collected
- Numerous crystal types, with asymmetric unit contents ranging from 21 kDa to 2.5 MDa
- Various ligand soaks and reaction intermediates
- Resolutions ranging from 3.2 Å to ... 0.59 Å !!
- Work reported at the GRC on Diffraction Methods 2022

Some projects require pushing various frontiers:

- Overcoming pseudosymmetry/pseudocentring problems
- Handling of huge files (e.g. MTZ with 440M unmerged reflections), pushed as an update to the CCP4 MTZ library.
- Reliable high-quality data processing
- Speeding up scaling
- Efficient and accurate model building, esp. AltConf networks
- Automated and standardised model refinement protocols

Courtesy of Ashwin Chari (MPI Gottingen)