MS107.P02

Gemmi – new GΦL+CCP4 project for handling (mm)CIF files

Marcin Wojdyr[1]

[1]*CCP4 / Global Phasing Ltd, Didcot, United Kingdom*
E-mail: wojdyr@gmail.com

CCP4 and Global Phasing Ltd started in January 2017 a joint open-source project, named Gemmi, to create a new software library that will be used by both organizations.

In the first year of the development we focus on handling mmCIF files and monomer library files (ligand CIFs). We started from the lowest level - parsing CIF files and validating them with DDL dictionaries. Next, we will provide interface to manipulate the structure in terms of models, chains, residues and atoms. On top of it we will provide a collection of algorithms, primarily for use in macromolecular refinement programs. Finally, the library will be integrated with BUSTER and Refmac.

This presentation will describe the state of the project as of August 2017.