



Agenda

Meeting title:	CCP4 Working Group 2 meeting (chaired by Arnaud Basle)		
Date:	Wednesday 2 nd March 2023	Time:	9:30 – 11.30
Location:	Zoom	Zoom:	link see email
Circulation:	ccp4wg2@stfc.ac.uk		
Online:	Jon Agirre, Svetlana Antonyuk, Charles Ballard, Arnaud Basle, Ben Bax, Paul Bond, Paul Emsley, Ralf Flaig, Vilmos Fulop, Robbie Joosten, Maria Fando, Petr Kolenko, Luiso Fuentes Montero, Ronan Keegan, Andrey Lebedev, Martin Malý, Karen McIntyre, Stuart McNicholas, Peter Moody, Andy Purkiss, Dan Rigden, Alan Roseman, Adam Simpkin, Roberto Steiner, Ville Uski, David Waterman, Keith Wilson, Briony Yorke.		
Apologies	Ed Lowe, Pietro Roversi, Sameer Velankar		

1. Approval of minutes from the last WG2 meeting (08-02-2023)
2. Update from CCP4 SW 2023 organisers (David Waterman on behalf of the team)
3. CCP4 Core Team Update (Eugene Krissinel and Charles Ballard)
4. Next CCP4 SW: topic and potential organisers
5. Next CCP4 WG2 meeting
6. AOB

Minutes

1. Approval of minutes from the online WG2 meeting 12/1/23 (Ivo Tews)

The minutes from the last WG2 meeting 08/02/2023 were approved.

2. Update from organisers of CCP4 SW 2023 (David Waterman)

The special issue is coming along nicely. One paper has been already submitted and is under review (Marjan Hadian-Jazi), and while some five papers are going to be review-type, many others are going to be research articles. Only four or five presenters have declined to submit a paper. Expecting 19 contributions.

3. Update from CCP4 Core Team

Eugene discusses the new software included in the latest update of CCP4. The Israel workshop that was meant to happen after the DLS workshop was cancelled due to lack of interest. Charles (chat): Melbourne is 2 days shared between CCP4 and CCP-EM.

The 009 update includes new versions of CCP4 cloud, CCP4i2, cbuccaneerNN (new model building program), Paired 1.3.11, CCIF, Refmac5, Pandda, some new monomers for the monomer library, and Morda.

Martin Maly: I am a developer, how should I tell CCP4 what's new in my software whenever there is a new release?

Charles: use the tracker. Raise a ticket, add what's new in the ticket description.

4. Next study weekend.

Proposed topic: automated vs manual. A discussion starts on where we should be doing the Study Weekends, as current numbers suggest some 200 attendees in person, and the East Midlands is getting expensive because it holds 400. It is a difficult decision, because the current economic deficit is basically the annual cost of one post. One of the challenges is that students don't pay, and they are the majority of the attendance.

Dan Rigden: Perhaps we could charge the students a little fee?

Arnaud: good idea, for CCP4exec to discuss.

Chairs to discuss and come up with suitable options for the next executive meeting.

5. Next WG2 meeting (Refinement)

We have a few confirmed speakers, including Keitaro Yamashita (MRC-LMB) on Servalcat, which is being pitched for inclusion in CCP4. Here is a short description of what Servalcat does:

Macromolecular refinement uses experimental data together with prior chemical knowledge (usually digested into geometrical restraints) to optimally fit an atomic structural model into experimental data, while ensuring that the model is chemically plausible. In the CCP4 suite that chemical knowledge is stored in a Monomer Library, which comprises a set of restraint dictionaries. To use restraints in refinement, the model is analysed and template restraints from the dictionary are used to infer: (1) restraints between concrete atoms; and (2) positions for riding hydrogen atoms. Recently, this process was delegated to GEMMI and the whole procedure is controlled by Servalcat. This was also an opportunity to enhance the Monomer Library with new features, resulting in a small improvement of REFMAC5 refinement. Importantly, the overhaul of this part of CCP4 has increased flexibility and eased experimentation, opening up new possibilities.

Luiso mentions that he wants to demonstrate the use of the newest DUI. Other people suggested: Kiarash Jamali (Model angelo), Paul Bond (Modelcraft).

6. AOB