



# Agenda

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|-----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|
| <b>Meeting title:</b> | CCP4 Working Group 1 meeting                                                                                                                                                                                                                                                                                                                                                 |                            |
| <b>Date:</b>          | Wednesday 7 <sup>th</sup> January 2026                                                                                                                                                                                                                                                                                                                                       | <b>Time:</b> 16:00 – 17.30 |
| <b>Location:</b>      | Hybrid: EMC Nottingham and Zoom                                                                                                                                                                                                                                                                                                                                              |                            |
| <b>Circulation:</b>   | ccp4wg2@stfc.ac.uk                                                                                                                                                                                                                                                                                                                                                           |                            |
| <b>Attending:</b>     | Jon Agirre, Charles Ballard, Arnaud Basle, Benjamin Bax, Dave Brown, Tom Burnley, Ivan Campeotto, Chun-Wa Chung, Sandra Eltschkner, Gwyndaf Evans, Vilmos Fulop, Mads Gabrielsen, Elspeth Garman, Dave Hall, Mike Hough, Robbie Joosten, Eugene Krissinel, Ed Lowe, Martin Malý, Peter Moody, Robert Oeffner, Dan Rigden, Paul Roland, Ivo Tews, David Waterman, Martyn Winn |                            |
| <b>Online:</b>        | Airlie Mc Coy, John Helliwell, Yvonne Jones, Jennifer Littlechild, Richard Pickersgill, Randy Read, Paula Salgado, Christian Siebold, Dave Stuart, Keith Wilson                                                                                                                                                                                                              |                            |

1. Chair - report: Ivo Tews
2. Core team report: Eugene Krissinel
3. Finance report: Charles Ballard
4. CCP4 Grant report:
  1. WP1 Data Analysis - Mike Hough
  2. WP2 Refinement - Martin Malý
  3. WP3 Electron Diffraction - David Waterman
  4. WP4 Bioinformatics - Dan Rigden
5. The CCP4 Study Weekend: Arnaud Basle
6. WG2 and ED&I report: Arnaud Basle, Jon Agirre 5'
7. Exec committee – elections
8. AOB

# Minutes

## 1. Chairs report (Ivo Tews)

IT is in office since 01/23. Activities since included:

BBSRC grant “New horizons in computational structural biology with CCP4: multiple states, models and methods, use of AI and validation”. 08/24 – 07/28, £1.92m. Details see individual reports point 4.

EPSRC / STFC for CoSeC Bridging Funding. Award to the new CCP consortium “Digital Research Infrastructure for Integrative Molecular Biology” in the molecular life sciences, includes CCPBioSim, CCP4, CCPN, CCP-EM.

ED&I was strengthened, producing a web presence, best practice documents, and a roadmap for CCP4, see report under point 4. Discussion and integration for fairness in access is taken up in the next two exec meetings that discuss preparation for the next round of grant application. A rough schedule is as follows:

- The midterm report for the present grant will be summer 2026.
- A call for projects for the next grant coincides with the CCP4 Developers Meeting July 2026.
- Suggestion of candidates for the role of chairs and proposal for projects to go into the next grant will happen over autumn 2026.
- A pre-selection of projects together with elections for chairs will be brought to WG1 2027.
- The confirmed projects WP leads will be approved in January by Exec.
- This leads into development of work packages and finally submission of a new grant proposal.

Get in touch: [Ivo.Tews@soton.ac.uk](mailto:Ivo.Tews@soton.ac.uk) (Enquiries on funding), [Arnaud.Basle@newcastle.ac.uk](mailto:Arnaud.Basle@newcastle.ac.uk) (WG2 - Meetings and workshops), [Jon.Agirre@york.ac.uk](mailto:Jon.Agirre@york.ac.uk) (WG2 – Software, ED&I coordinator)

## 2. Core team report: Eugene Krissinel

There are several teamed efforts in the core group, which are (1) Housekeeping (2) Releases & Updates (3) CCP4 Infrastructure (4) CCP4 Cloud (5) Diffraction data analysis (6) Structure analysis and other tools and methods (7) AI/ML methods in MX (8) Education and outreach.

New projects and collaborations are Software for Fragment Screening (CCP4-Diamond K04-Dundee), AI/ML ready PDB depositions (CCP4-CCPEM-GPhL-PDBe-Phenix-PDB), Integrative Research Framework for SB (CCP4-CCPEM-PDBe-UCL)

The last year(s) did see significant grant success for the core team, including ALC: 6 (STFC), CoSec: 1 (STFC), DRI: 2 (EBI-CCP4-CCPEM), BBR24: 1 (CCP4-CCPEM-EBI-UCL), BBSRC: 2 (CCP4 & EBI-CCP4), BBSRC/NSF: 1 (PDB-EBI-CCP4-CCPEM-Phenix-GPhL).

Similarly, the core group have a strong publication record (10+ publications over the past two years).

## 3. Finance report: Charles Ballard

Overall licenses are stable. Most licenses were renewed.

| Year                | 2021-22      | 2022-23       | 2023-24      | 2024-25       | 2025-26   |
|---------------------|--------------|---------------|--------------|---------------|-----------|
| <b>Main (£12k)</b>  | 132 (+16/-3) | 151 (+33/-14) | 161 (+17/-7) | 160 (+20/-21) | (+15/-16) |
| <b>Subs (£8.7k)</b> | 50 (+2/-1)   | 51 (+1/-0)    | 52 (+1/-0)   | 50 (+1/-3)    | (+3/-5)   |
| <b>Ac (£3.5k)</b>   | 3 (+1/-0)    | 4 (+1/-0)     | 7 (+3/-0)    | 4 (+0/-3)     | (0/-1)    |
| <b>Total</b>        | <b>185</b>   | <b>206</b>    | <b>220</b>   | <b>214</b>    |           |

| Year               | 2021-22 | 2022-23 | 2023-24 | 2024-25 | 2025-26 |
|--------------------|---------|---------|---------|---------|---------|
| <b>Income</b>      | 1,705 k | 1,988 k | 2,148 k | 2,420k  | 2,400   |
| <b>Expenditure</b> | 1,654 k | 1,680 k | 1,957 k | 2,256k  | 2,190   |
| <b>+/-</b>         | -51 k   | -308 k  | -191 k  | -164k   | -210    |

- Price increase in 2026/27:
  - £13,000 for main sites, £9,000 for subsidiary sites
- Price increase in 2024/25 (first since 2018)
  - £10,500 to £12,000 for main sites
  - £7,550 to £8,000 for subsidiary sites

Projected to underspend by £200k - defensive reallocation of resources.

#### 4. CCP4 grant report

##### WP1 Data Analysis – Mike Hough

We are investigating how to identify changes in structure without proceeding to full datasets and maps, addressing the question: how much data are needed to resolve a change. We use (a series of) diffraction images at a particular timepoint along a reaction coordinate, a dose-point, etc.

Deliverables D1.1 (Measures of non-/isomorphism) and 1.2 (Identification of the pairwise differences) are being conducted in parallel. D1.1 provides a solid foundation (expected complete Aug 2026), with D1.2 following quickly after. D1.4 (Capture of all relevant metadata) is underway and in discussion with beamline and DAQ teams. Methods employed are Naïve Bayes classification, PCA on features in intensity data, Gaussian process regression (GPR) and max-likelihood approaches.

NB. There was a team change, as Graeme Winter is now at the APS, and James Beilsten Edmands leads DIALS and is now on the grant.

##### WP2 Refinement - Martin Malý

Input unmerged data

- Merging in groups of selected batches
- Calculation of correlation between intensities to assess isomorphism
- Automatic refinement and analysis
- Scaled difference maps

Uncertainties from resampled data sets

- To provide any feature of structure model parameters with its uncertainty (e.g. distance between non-covalently interacting atoms with standard deviation)
- Average density maps - work in progress
- Planned to be submitted to a journal in 2026

The features are implemented in Multixem software pipeline, depending on GEMMI and Servalcat. Identify

Robert Öffner: Do these weights really represent random structures?

Peter Moody: how do you insure this is not self full-filling, as the distribution from the assigned errors is used to determine the error of the structure?

### **WP3 Electron Diffraction - David Waterman**

Deliverables D3.1 is use of ML to correct for correct effects of dynamical electron diffraction. This started on test data for 1,3,5-Triphenylbenzene TPB (4 datasets) and Paracetamol (764 datasets). We used the open source abTEM package which uses both Multislice and Bloch wave methods to extract unit cell rotation from experimental data. This is useful for later stages in D3.2 (Electron Diffraction in presence of crystal defects and solvent) and D3.3 (Assessment of ED data suitability for structure solution). abTEM will be explored to predict chirality, and for data generation. Collaborative publication in Ultramicroscopy 281 (2026), 114298.

ITs: is there enough protein diffraction data as yet?

DW: more test data needed.

### **WP4 Bioinformatics – Dan Rigden**

Good progress has been made against grant objectives. Work on RNA structure validation has been done first due to the background of the post-doc Aderik Voorspoels. Two methods for validation of RNA structure based on contacts, distograms and DL-based predictions have been developed: one based on contact map alignment and another using an SVM. Much lower-level development of Conkit and GESAMT was necessary as a prerequisite. The two approaches will be applied PDB-wide and the results published. 4 publications suitable for ResearchFish so far.

Q from Robbie Joosten around SVM descriptors for RNA analogous to the DSSP states used in the original protein validation work. DNATCO classes were suggested as possibly useful and will be explored.

## **5. The CCP4 Study Weekend: Arnaud Basle**

The topic for the 2027 study weekend shall be discussed in the plenum this year, at the end of the study weekend. A change for 2027 is that we will allow sponsors. WG2:

- coordinates Study Weekend and two regional meetings (Southwest and Northeast)
- held 4 online meetings (2 hours) last year, plus 2 hybrid ones (11am-5pm) in Cambridge (summer) and York (winter), with 15-20 in-person attendees. Online meetings focus on Study Weekend preparation, whereas the hybrid ones evaluate (i) new software for the suite; and (ii) new functionality already in the suite.
- Minutes of WG2 meeting recorded and published on CCP4 website
- WG2 is a mailing list.

## **6. WG2 and ED&I report: Arnaud Basle and Jon Agirre**

Please see our Web Page. Roadmap in preparation. Best practice in hiring becoming available for download.

To address the lack of diversity in the methods development community, our main aims are to:

- Attract, retain and develop a diverse pool of talented individuals.
- Make the route to senior levels more equitable.
- Enhance the representation of speakers from underrepresented groups at CCP4 events.
- Improve transparency of funding support allocation within CCP4.
- Create an even more welcoming and inclusive community.

We have developed a roadmap to support our goals to turn our goals into actionable steps. Inspiration has been drawn from the BBSRC Equity, Diversity and Inclusion Action Plan:

- “Investing in early career programmes and pilots to support underrepresented and disadvantaged groups.” We aim to support more events aimed at early career researchers, the CCP4 Northern Meeting, and a coding bootcamp.

- “Sharing and promoting good practice by facilitating networking and collaboration.” We have developed guidance documents, including best practices for hiring processes, and promoting transparency for funding allocation.
- “Routinely gathering and analysing EDI data.” We are collecting and analysing ED&I statistics at CCP4 events.

## 7. Exec committee – elections

Project leads: WG1 thanks Gwyndaf Evans for his long-time work for CCP4 as a Diamond Rep, notably binging CCP4 and DLS interests into synergy. Mike Hough was proposed by the DLS, confirmed by Exec, and elected confirmed as Diamond Light Source Representative by WG1.

### Elected Grant

Ivo Tews 2023-28 Chair  
Jon Agirre 2024-28 WG2 Chair, ED&I coordinator  
Arnaud Basle 2024-28 WG2 Chair

### Elected

Helen Walden 2022-28  
Helen Ginn 2024-26  
Briony Yorke 2025-28  
Dave Brown 2024-26 Industry  
Judit Debreczeni 2017-26 Industry  
Keith Wilson Secretary -2026

### Grant 2024-28

|                  |             |
|------------------|-------------|
| Mike Hough       | Grant WP PI |
| Garib Murshudov  | Grant WP PI |
| Eugene Krissinel | Grant WP PI |
| Dan Rigden       | Grant WP PI |

### Project leads and Reps

|                  |                   |
|------------------|-------------------|
| Eugene Krissinel | Head of core team |
| Martin Noble     | i2 lead           |
| Airlie McCoy     | Phaser/Phenix     |
| Martyn Winn      | STFC Rep          |
| Mike Hough       | Diamond Rep       |

## 8. AOB

None.