



# Agenda

|                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                            |
|-----------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------|
| <b>Meeting title:</b>       | CCP4 Working Group 1 meeting                                                                                                                                                                                                                                                                                                                                                                                                                            |                            |
| <b>Date:</b>                | Tuesday 7 <sup>th</sup> January 2025                                                                                                                                                                                                                                                                                                                                                                                                                    | <b>Time:</b> 16:30 – 17.30 |
| <b>Location:</b>            | Hybrid: EMC Nottingham and Zoom                                                                                                                                                                                                                                                                                                                                                                                                                         |                            |
| <b>Circulation:</b>         | ccp4wg1@stfc.ac.uk                                                                                                                                                                                                                                                                                                                                                                                                                                      |                            |
| <b>Attending in-person:</b> | Jon Agirre, Charles Ballard, Arnaud Basle, Benjamin Bax, Dave Brown, Frank von Delft, Paul Emsley, Gwyndaf Evans, Ralf Flaig, Vilmos Fulop, Mads Gabrielsen, Elspeth Garman, Dave Hall, Mike Hough, Ronan Keegan, Eugene Krissinel, Dave Lawson, Andrew Lebedev, Ed Lowe, Martin Malý, Airlie Mc Coy, Peter Moody, Alan Orville, Richard Pickersgill, Randy Read, Dan Rigden, Rachel Tang, Ivo Tews, Adetir Voorspers, Aderick Voorspoels, Martin Walsh |                            |
| <b>Attending by zoom:</b>   | Svetlana Antonyuk, Elspeth Garman, Jenny Littlechild, Airle McCoy, Garib Murshudov, Martin Noble, Mark Roe, Pula Salgado, Johan Turkenburg, Roberto Steiner, Keith Wilson, Martyn Winn                                                                                                                                                                                                                                                                  |                            |

1. Chair - report: Ivo Tews
2. Core team report: Eugene Krissinel
3. Finance report: Charles Ballard
4. CCP4 Grant report:
  1. WP1 Data Analysis (PI Hough): Rachel Tang
  2. WP2 Refinement (PI Murshudov): Martin Malý
  3. WP3 Electron Diffraction (PI Krissinel): Eugene Krissinel
  4. WP4 Bioinformatics (PI Rigden): Aderik Voorspoels
5. ED&I report: ED&I team
6. The CCP4 Study Weekend: Arnaud Basle, Jon Agirre  
SW 2024 Report; SW 2026 Proposals
7. Exec committee – elections
8. AOB

# Minutes

## 1. Chairs report (Ivo Tews)

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

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

Grant submission to 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, to:

- advance key technologies and community building
- provide and develop data exchange
- derive data models to represent the dynamic states in Molecular Biology
- remove bottlenecks in data driven research
- use and validate AI generated information, particularly the fast-growing resource of computed models
- propose development and provision of innovative training in simulation and data processing
- engage widely with the UK computational community and interact with further CCPs
- Identify areas for future development and directing future investment

Awarded are:

- post in crystallography + EM on data format and inter-compatibility
- CoSeC post to scope heterogeneous computing, using MR replacement and computed structures as a test case
- funds for networking, conferences and workshops

The chair explores trends for future development of software:

- ligands and model completion
- force fields in refinement
- quantum crystallography
- EM diffraction and EM joint refinement
- MR replacement, computed structures
- the growing importance of serial and time resolved work

ED&I was strengthened, producing a web presence, best practice documents, and a roadmap for CCP4. Consultation is ongoing.

## 2. Core team report: Eugene Krissinel

There were five new releases since CCP4 9.0 was introduced. With 8+4 staff members the core group is stable. Hardware: refreshed by replacements and new GPU cores for AlphaFold.

Q: Using Amazon (or other) commercial cloud services?

A: STFC does not encourage this, and there is already a CCP4 cloud service in place, which is funded.

## 3. Finance report: Charles Ballard

Overall licenses are stable. Most licenses were renewed. We lost a few licences, and gained six new licences (one of them a major site); there are 240 licences in total.

| Year          | 2021-22      | 2022-23       | 2023-24      | 2024-25*      |
|---------------|--------------|---------------|--------------|---------------|
| Main (£10.5k) | 132 (+16/-3) | 151 (+33/-14) | 161 (+17/-7) | 160 (+20/-21) |
| Subs (£7.55k) | 50 (+2/-1)   | 51 (+1/-0)    | 52 (+1/-0)   | 50 (+1/-3)    |
| Ac (£3.5k)    | 3 (+1/-0)    | 4 (+1/-0)     | 7 (+3/-0)    | 4 (+0/-3)     |
| Total         | 185          | 206           | 220          | 214           |

| Year        | 2021-22 | 2022-23 | 2023-24 | 2024-25*   |
|-------------|---------|---------|---------|------------|
| Income      | 1,705 k | 1,988 k | 2,148 k | est 2,410k |
| Expenditure | 1,654 k | 1,680 k | 1,957 k | est 2,325k |
| +/-         | -51 k   | -308 k  | -191 k  | est -95k   |

- Price increase in 2024/25 (first since 2018)
  - £10,500 to £12,000 for main sites
  - £7,550 to £8,000 for subsidiary sites
- WG1 recommended adjustments (in the 2024 meeting):
  - £13,000 for main sites, £9,000 for subsidiary sites
- EXEC has green lit this recommendation
  - Confirm by Exec decision following this WG1 (8.1.25)
  - A further increase of £1,000 (and pro-rata) for 2026/27
  - Mails to license holders will go out before the end of this financial year (March 2025)

Projected to underspend by £100k - defensive reallocation of resources. A problem that remains: funds allocated to year, staff turnover and delays in filling positions.

AB: There is a financial pressure at Diamond – CCP4 sponsored a meeting to host the Diamond satellite.

EG: Can we consider bursaries for retired people

#### 4. CCP4 grant report

##### WP1 Data Analysis (PI Hough): Rachel Tang

- Identify change in serial crystallography data from intensities without need for full datasets and data analysis
- Use this to identify that a process has initiated and what intermediates are present
- Apply to serial tr-MX, dose series, ligand binding etc...
- Appropriately handle metadata and link to WP2

##### WP2 Refinement (PI Murshudov): Martin Malý

Refine several structures simultaneously at the same time using a common coordinate frame. Combination of crystallography and cryo EM. Joint refinement using *servalcat*.

##### WP3 Electron Diffraction (PI Krissinel): Eugene Krissinel

- Using Machine Learning approach, develop a method for extracting the most likely structure factor amplitudes from ED data with significant dynamic component
- Investigate the effect of experimental imperfections on the manifestation and scale of multiple scattering in ED data, using ED simulation tools that we developed in the previous grant period (2019-2024)
- Develop a Machine Learning procedure for detecting patterns in ED data indicative of the overall suitability for structure determination

Simulated electron diffraction: primitive model not successful; plan to use machine learning to get the most likely structure factor. Intensities (dynamic theory) → Intensities (kinematic theory), multiple scattering flattens intensity distribution unevenly in respect to hkl. Tarik Drevon has resigned, with no new candidate identified. Potential redeployment from the core group (would adversely affect delivery of the suite).

## WP4 Bioinformatics (PI Rigden): Aderik Voorspoels

Machine learning – nucleic acid structure prediction and validation (ConKit). Errors in PDB database were investigated.

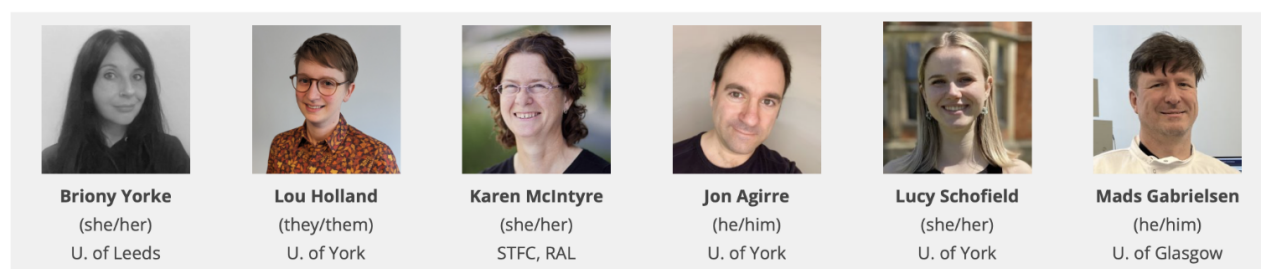
## 5. ED&I report: ED&I team.

### Equity, diversity & inclusion

A diverse and inclusive community is able to offer and harness more viewpoints and experiences, leading to increased creativity in solving difficult problems. The CCP4 Equity, Diversity and Inclusion (ED&I) team strives to counter biases and remove barriers that are currently hindering truly diverse participation in the development of the CCP4 suite and the science that supports it.

### People involved

The ED&I team gets together every 2 months to discuss progress on the implementation of CCP4's ED&I roadmap. Please get in touch if you would like to get involved – email [jon.agirre@york.ac.uk](mailto:jon.agirre@york.ac.uk) to join.



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

## 6. The CCP4 Study Weekend: Arnaud Basle

The SW may be moving to more flexible and general topics. In the last years: 210 participants, it was 2x more before covid, it was above. Over 1000 when only online in 2021 and 2022. Many early career researchers during last years. Networking aspect is affected by being hybrid – many people are online. How do we get back the spirit before covid, attract better in person attendance, and senior PIs?

### Comments:

- many WG1 members don't know they are in WG1
- WG1 members should more encourage students to come to SW
- can we do more outreach, some extra activities, EDI should be improved
- WG1 and SW should be more open. We can consider to get sponsors.
- Engage the whole community
- Is CCP4BB sufficient – we may need social media and other ways for advertising,
- is the decrease in attendance due to lower overseas participation

Should the topics for CCP4SW2025 go along the topics explored by the chair (see point 1)?

BB comment: validation

FvD comment: fast phasing and validation, variations of structures

RP: Ligands, model completion & validation  
 GM: Modelling and validation  
 Comment from Leicester: Sample preparation  
 CB: We have two days, we don't have to have only a single topic  
 RR: Structures which AlphaFold can't solve – at least a session  
 AO: Think on new generation of structure biologists  
 RT: We can give recognised awards for short student talks.

Further comments:

When a topic more specific and less general, more Pis may come.  
 Coordinate CCP4 and Diamond satellite better

The consensus found from discussion was ... (ARNAUD). This will be further explored by WG2 who make the decision on the detailed programme and organiser team.

## 7. Exec committee – elections

James Murray retires from the executive.

Helen Walden was confirmed by vote for a second term

Helen Ginn was elected on to the executive.

Project leads: Randy Read retires. Airlie McCoy was elected.

Keith Wilson was elected as scientific secretary.

### Elected

|                         |                                        |
|-------------------------|----------------------------------------|
| <b>Ivo Tews</b>         | <b>2023-28 Chair</b>                   |
| <b>Helen Walden</b>     | <b>2022-27</b>                         |
| <b>James Murray</b>     | <b>2022-24</b>                         |
| <b>Briony Yorke</b>     | <b>2024-26</b>                         |
| <b>Dave Brown</b>       | <b>2024-26 Industry</b>                |
| <b>Judit Debreczeni</b> | <b>2017-26 Industry</b>                |
| <b>Jon Agirre</b>       | <b>WG2 Chair, ED&amp;I coordinator</b> |
| <b>Arnaud Basle</b>     | <b>WG2 Chair</b>                       |
| <b>Keith Wilson</b>     | <b>Secretary -2026</b>                 |

### 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          |
| Gwyndaf Evans    | Diamond Rep       |

### **AOB**

None.