Crystallography News

British Crystallographic Association

Issue No. 175 December 2025
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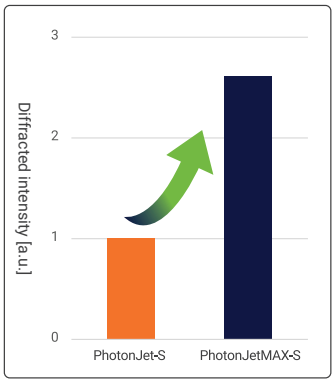

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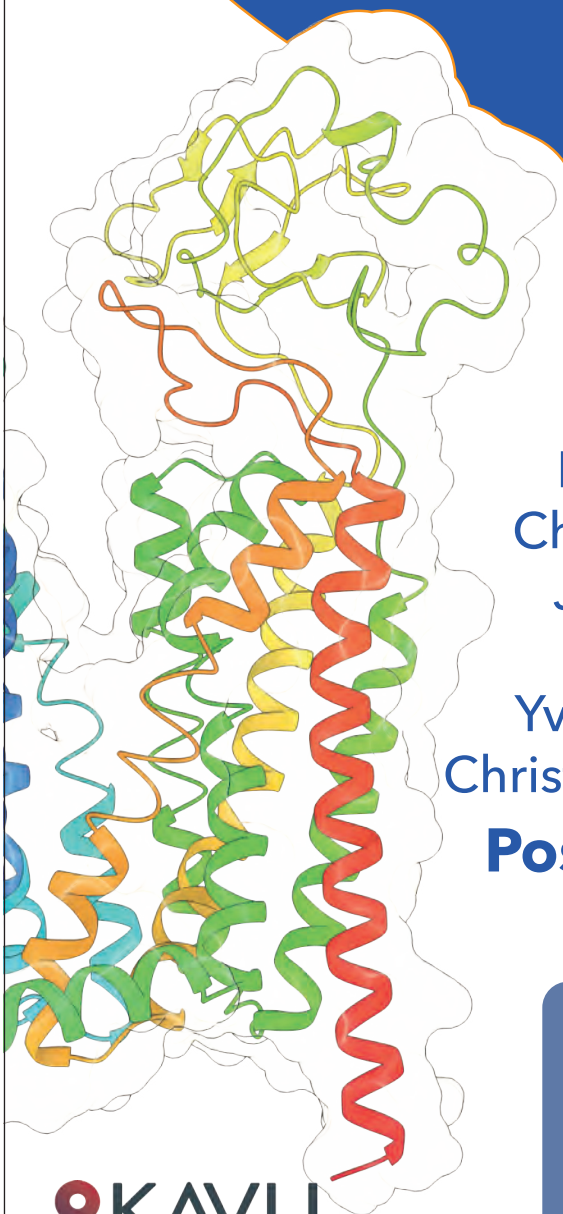
BIOLOGICAL STRUCTURES GROUP

Winter Meeting 2025

New Advances and Future Directions in Structural Biology



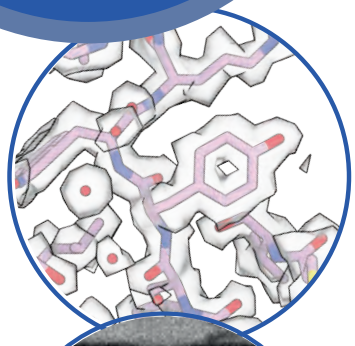
Friday 12th December 2025

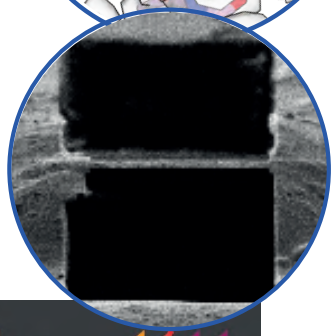
10:30-18:00

Confirmed Speakers:

Neil Ranson (Leeds)
Chun-wa Chung (GSK)
Josie Ferreira (UCL)
Chris Hill (York)
Yvonne Jones (Oxford)
Christos Pliotas (Manchester)

Poster Talks & Prizes available





KAVLI INSTITUTE FOR NANOSCIENCE DISCOVERY

department of BIOCHEMISTRY 1923 - 2023

UNIVERSITY OF OXFORD

QR code

Registration
Programme

Dorothy Crowfoot Hodgkin Building

Organisers:

Simon Newstead
Jo Parker
Rachael Wilkinson

BCA Corporate Membership

The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis and includes the following benefits:

- Up to 10 free BCA memberships for your employees.
- 10% discount on exhibition stands at the annual BCA Spring meeting.
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- Corporate Members will be listed in every Crystallography News and on the BCA website with clickable links to your organisation's website.

Corporate Membership is currently **£850** for one year.

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Douglas Instruments: https://www.douglas.co.uk/

International Centre for Diffraction Data (ICDD): https://www.icdd.com/

Oxford Cryosystems: https://oxcryo.com

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Benefits of Individual BCA Membership:

- The professional organisation for crystallographers in the UK
- A broad range of meetings organised by the BCA and its subject groups
- Preferential members' rates for such meetings
- Eligibility of students and postdocs for an Arnold Beevers Bursary award
- A copy of Crystallography News every quarter
- Optional E-mail notifications of news items and meeting information
- Influence on the development of crystallography and the BCA

For current rates, and to join, please see **www.crystallography.org.uk/membership/**

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Applications are invited for fellow membership of the BCA via the members area of https://www.crystallography.org.uk/.

Fellows of the BCA shall have an established career in crystallographic teaching or research and must hold one other class of membership. Fellows will normally have been members for at least five years, but the BCA shall consider exceptions such as those with an established career abroad or members who have taken recent career breaks.

In addition to recognising an established career, fellow membership provides a simple way to support the association. The current rates for fellow membership are set at double those of the member's normal renewal price.

Contents

This month's cover:

Recent crystallography meetings in the UK and abroad: SWSBC, ECM35 Posnan and the Bernal lecture at Birkbeck, London

BCA Administrative Office,
4 Dragon Road
Harrogate HG1 5DF
Tel: +44 (0)1423 529 333
e-mail: bca@hg3.co.uk

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Text should preferably be sent electronically as MSword documents (any version – .docx, .doc, .rtf or .txt files). Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, .png or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the March 2026 issue are sent to the Editor to arrive before 25 January 2026.

Editor: Jon Cooper
University College London,
Gower Street, WC1E 6BT
e-mail: jon.cooper@ucl.ac.uk

Deputy Editor, Dave Allan
e-mail: dave.allan@diamond.ac.uk

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These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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Unit 8, Malton Enterprise Park, 17 Cherry Farm Close,
Malton, North Yorkshire YO17 6AS
Tel: 01653 697261
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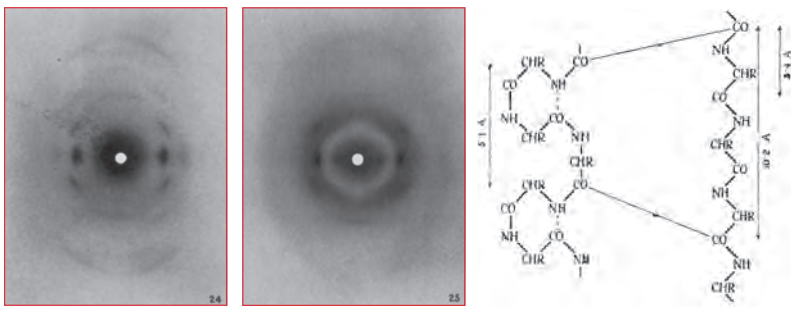
From the President

WELCOME to the final Crystallography News of the year, I hope all is going smoothly in the build-up to the holidays, or if not then at least progressing steadily towards a quieter period! At the safe remove of early November I still have the vain hope that I will be in the former status when I read this issue in print… In any case, right now I have the pleasure to be attending the PCG/SCMPG-CCG-ISIS-Diamond Winter Crystallography Meeting, which is always a combination of a welcome end-of-year gathering with friends and colleagues and an inspiring collection of new results and discoveries.

We have recently received the news that **James Watson**, 1962 Nobel Laureate along with **Francis Crick** and **Maurice Wilkins** for his role in the historic discovery of the helical structure of DNA, has passed away. A key part of one of the formative advances and triumphs of X-ray crystallography, he was nevertheless a highly controversial figure in more recent years due to his documented racist and sexist beliefs. I recommend some of the published obituaries, such as the one available on the *Nature* website as I write, to give a suitably considered and detailed picture of Watson.

I took the opportunity upon hearing the news to remind myself of the magnitude of the challenges that were undertaken in the early years of X-ray crystallography. Many of us, for example, can recognise by sight that a diffraction pattern generated by our chosen radiation and technique comes from a material with a perovskite structure (apologies to those who are not part of the perovskite-obsessed portion of the membership – please swap in your favourite standard chemical construct instead!), and the structure-pattern relationship feels very natural. I am reminded, however, when I read once more about the discovery of the helical structure of DNA that many of the materials studied in the early years of X-ray crystallography were not so simple*, and the relationship not so tractable. For example, natural fibres such as wool and hair were studied via X-ray diffraction in the early 1930s by **William Astbury** and others. These fibres, in common with DNA, had structures dependent on hydration levels and physical perturbations such as stretching, adding another layer of complexity to both measurement and analysis. They certainly weren't afraid of a difficult problem in those days!



Diffraction patterns of unstretched silk (left) and stretched human hair (right). The similarity allowed deduction of the fact that both fibroin (in silk) and β-keratin (in stretched hair) have similar structures of extended chains of polypeptides. α-keratin (in unstretched hair) has a shorter, folded structure, seen in the diagram alongside its β-form. Reproduced from Astbury and Woods, Philos. Trans. R. Soc., A, 232, 333 (1934).

I am very glad to see in the current issue of CN how those far better qualified than I are passing on the essence of other parts of the past century or so of crystallography through forums such as the Bernal Lecture and the Kathleen Lonsdale Lecture, and through the pages of this magazine (see e.g. notes on the Precession Camera in the *Crystallographic Forteana* section courtesy of **Jon Cooper**). That the BCA continues to value and treasure this rich history is wonderful.

Heading towards the other end of the time spectrum we come to the near future in the form of the Spring Meeting. Please do take a look at the programme later in the issue and put some thoughts to abstract submission, which is now open. This year's BSG plenary will look at some of the intricacies of cell cycle regulation. As a naïve solid-state materials chemist the fact that biological crystallographers can tackle such a problem, even with modern technology, is to be honest equally astounding as the work of the early pioneers! I am very much looking forward to being re-astounded by the details as I sit there in a few months' time.

If you are lucky enough to find a few minutes of free time over the holidays I can recommend a couple of crystallography-related distractions. The first is www.crystallify.com, thanks to **Jon Cooper** for bringing it to my attention. This website provides an excellent and highly enjoyable way to explore space groups and their symmetry, along with visualising Miller planes – I will certainly be using it in my teaching. Another item is the *Science in the Making* online archive of the Royal Society (https://makingscience.royalsociety.org), which has a huge collection of historical referee reports which make entertaining and informative reading. The reviews of Astbury and Street's 'X-ray studies of the structure of hair, wool, and related fibres.- I. General' are by **W. L. Bragg** and **F. W. Aston** (RR/41/10 and RR/41/11 respectively) and are concise in the extreme – almost a perfect set of plain yes's and no's! Coming back full circle to DNA, I would also highlight **Dorothy Hodgkin**'s review of the Crick and Watson paper 'The complementary structure of deoxyribonucleic acid' (RR/79/230). This one is not quite so brief (but still extremely concise by modern standards) and a model of well-mannered, constructive reviewing.

With that positive ending I hope you all have a great festive season and wish you all a Happy New Year when it comes!

* Here I use simple in the facile sense of perovskites being materials formed of simple arrangements of atoms constituting a small unit cell, which are generally robust to changes in ambient conditions and other perturbations. I do not dare to suggest that they are simple on a true scientific level, please don't get out the pitchforks!

Alex Gibbs
St Andrews

BCA Council 2025

COUNCIL OFFICERS

President (2027)
Dr Alexandra Gibbs
School of Chemistry,
University of St Andrews,
North Haugh, St Andrews,
Fife, KY16 9ST
president@crystallography.org.uk

Vice President (2025)
Dr Suzanna Ward
Cambridge Crystallographic
Data Centre,
12 Union Road, Cambridge,
CB2 1EZ
ward@ccdc.cam.ac.uk

Secretary (2028)
Dr Lauren Hatcher
School of Chemistry,
Cardiff University Main
Building, Park Place,
Cardiff, CF10 3AT
secretary@crystallography.org.uk

Treasurer (2026)
Dr Claire Naylor
Thermo Fisher Scientific
treasurer@crystallography.org.uk

ORDINARY MEMBERS

Dr Lucy Saunders (2028)
Diamond Light Source,
Harwell Science and
Innovation Campus,
Didcot,
Oxford, OX11 0DE
lucy.saunders@diamond.ac.uk

Dr Briony Yorke (2026)
School of Chemistry,
University of Leeds,
Woodhouse Lane, Leeds,
LS2 9JT
B.A.Yorke@leeds.ac.uk

Dr Jeremiah Tidey (2027)
Department of Chemistry,
University of Warwick,
Gibbet Hill, Coventry,
CV4 7AL
Jere.Tidey@warwick.ac.uk

EDUCATION & OUTREACH

Dr Ilaria Gimondi (2027)
Cambridge Crystallographic
Data Centre,
12 Union Road, Cambridge,
CB2 1EZ

GROUP REPRESENTATIVES

Biological Structures
Dr Mark Montgomery
Syngenta
Jealott's Hill International
Research Centre,
Bracknell, Berkshire
RG42 6EY, UK
mark.montgomery@syngenta.com

Chemical Crystallography
Dr Natalie Pridmore
School of Chemistry,
Cantock's Close,
Bristol, BS8 1TS
n.pridmore@bristol.ac.uk

Industrial
Dr Helen Blade
AstraZeneca,
Macclesfield Campus,
Macclesfield,
Cheshire, SK10 2NA
Helen.Blade@astrazeneca.com

Physical Crystallography
Dr Helen Playford
Building R3, Room 1.22
STFC ISIS Facility,
Rutherford Appleton
Laboratory,
Didcot, OX11 0QX
Tel: 01235 446890
helen.playford@stfc.ac.uk

Early Stage Crystallographers
Dr Thomas Hitchings
School of Chemistry
and Forensic Science,
University of Kent,
Canterbury, CT2 7NH
tjh55@kent.ac.uk

CO-OPTED MEMBERS

Programme Chair (2025)
Prof Katharina Edkins
Strathclyde Institute
of Pharmacy and
Biomedical Sciences,
161 Cathedral Street,
Glasgow, G4 0RE
katharina.edkins@strath.ac.uk

Programme Chair (2026)
Dr Lewis Owen
Department of Materials
Science and Engineering,
University of Sheffield
lewis.owen@sheffield.ac.uk

GROUP CHAIRS

Biological Structures
Prof Simon Newstead
Department of
Biochemistry,
University of Oxford,
South Parks Road,
Oxford, OX1 3QU
simon.newstead@bioch.ox.ac.uk

Chemical Crystallography
Dr Hamish Yeung
School of Chemistry,
University of Birmingham,
Birmingham, B15 2TT
chair@ccg.crystallography.org.uk

Industrial
Luca Russo
GSK Medicines Research
Centre, Gunnels Wood
Road, Stevenage,
Hertfordshire, SG1 2NY, UK
luca.x.russo@gsk.com

Physical Crystallography
Dr Lewis Owen
Department of Materials
Science and Engineering,
University of Sheffield
lewis.owen@sheffield.ac.uk

Early Stage Crystallographers
Dr Thomas Hitchings
School of Chemistry and
Forensic Science,
University of Kent,
Canterbury, CT2 7NH
tjh55@kent.ac.uk

EX-OFFICIO MEMBERS

BCA Administrative Officer
Nicola Hardaker
Hg3 Ltd
4 Dragon Road,
Harrogate, HG1 5DF
bca@hg3.co.uk

Webmaster
Dr Ben Coulcon
Diamond Light Source Ltd,
Harwell Science &
Innovation Campus, Didcot,
Oxfordshire, OX11 0DE
ben.coulson@diamond.ac.uk

Editor "Crystallography News" **Prof Jon Cooper**
University College London,
Gower Street, London,
WC1E 6BT
jon.cooper@ucl.ac.uk

Past President
Prof Richard Cooper
Chemistry Research
Laboratory, Mansfield Road,
Oxford, OX1 3TA
richard.cooper@chem.ox.ac.uk

(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website
www.crystallography.org.uk

From the Editor

IT is that time of year when we rapidly approach the season of good cheer, so I take this opportunity to wish members a really great Christmas as well as a productive and happy new year.

In this issue we have more details of the programme for the 2026 Spring Meeting which looks really fascinating. By way of an erratum, I must apologise for a couple of typographical errors in the last issue which could have caused confusion about the duration of the early career stage crystallographers group meeting with respect to the main meeting. It was simply a subtitle which became duplicated twice unnecessarily and I did not spot that while doing a last-minute proof read of that section. I can only recommend that members read the current version of the programme which follows in this issue for the latest and best version available to date.

We then have a report by **Gary Nichol** (Edinburgh) on the excellent ECM35 meeting which was held in Poznań back in the Summer and an account of the very recent CCG Autumn Meeting by **David Cordes** (St Andrews). It does sound like these were superb meetings so I do recommend that you read these great articles which are followed by a report on the South West Structural Biology Consortium meeting in Sussex in July.

The return of early autumn and the run-up to the start of term saw a couple of very interesting one day meetings of a crystallographic nature. One in Leeds which was dedicated to the life and work of Kathleen Lonsdale and another at Birkbeck in London which was held in memory of Alan Mackay who very sadly passed away in the early months of this year. The expertly written report on the Leeds meeting is by **Jake Hill** (Leeds) and the report on the Bernal Lecture which was given by **John Finney** (UCL) at Birkbeck is, like the SWSBC report, by none other than the editor of this very newsletter. All of this reminds me to appeal to members to please keep me posted with notices of future meetings and reports or copies of your notes on meetings which have already been held. A very big thank you to those who have already done so.

We then have our regular news features from the CCDC and the wwPDB before two reviews of the excellent new textbook “Mathematics for Biosciences” co-authored by the former BCA president **Elspeth Garman** (Oxford). Indeed reading another, albeit much older, book on crystallography prompted me to write some notes summarising the introductory chapter, initially for myself, but on thinking they might even be useful for members, I have spruced them up a bit with some diagrams and they are reproduced towards the end of this issue.

This issue sees the return of our occasional series on *Crystallographic Forteana* in the form of an article which briefly analyses the phenomenon of precession as applied in various realms of physics, chemistry, celestial mechanics and, of course, crystallography. We delve into the ancient art of precession photography which was mainly used to characterise crystals prior to data collection, although I believe that in some cases screenless precession photography was actually used for data collection, but I would need to do my homework to confirm that.# For small molecule work, another form of X-ray photography, known as the Weissenberg method, was generally the preferred approach. However, for macromolecular crystallography, the precession camera was a firm favourite for determining unit cell parameters and crystal symmetry, as far as one can from diffraction intensities. As we look back into the past in this section we also meet the remit of another occasional series which is due for a return to these hallowed pages and that is our semi- regular section on crystallographic memorabilia - Down Memory Lane.

We then have our regular Puzzle Corner and the section on future meetings. Finally, please note that corporate member profiles will return in a future issue.

Jon Cooper
UCL

Well, I have now done some homework and indeed screenless precession photography was developed, mainly by the San Diego group in the US, as a means of data collection up until about 50 years ago and here are some references to really great papers on the subject.

- Xuong, N.-H., Kraut, J., Seely, O., Freer, S. T. & Wright, C. S. (1968). Rapid measurement of large numbers of reflection intensities for proteins. *Acta Crystallogr. B* **24,** 289-290.
- Xuong, N.-H. & Freer, S. T. (1971). Reflection intensity measurement by screenless precession photography. *Acta Crystallogr. B* **27,** 2380-2387.
- Leijonmarck, M., Ronnquist, O. & Werner, P.-E. (1973). Prediction of partially recorded reflexions on screenless precession photographs. *Acta Crystallogr. A* **29,** 461-463.

However the advantage of slightly greater data collection efficiency over the single-axis rotation or oscillation method which is now the universal standard in macromolecular work, at least, is offset by a number of issues which are described in the below paper.

- Arndt, U. W., Champness, J. M., Phizackerley, R. P. & Wonacott, A. J. (1973). A single-crystal oscillation camera for large unit cells. *J. Appl. Crystallogr.* **6,** 457-463.

Probably the most significant disadvantage of the screenless precession method is that partially recorded reflections are not recorded contiguously on adjacent diffraction images, as they are in the rotation method. With fine-slicing, all of the reflections are partially recorded, so turning the crystal around on only one axis, as we do in the rotation method, makes a lot of sense!

2026 Spring Meeting Programme

University of Leeds

Monday 30th March 2026

EARLY STAGE CRYSTALLOGRAPHERS GROUP (ESCG)

11:00-18:00 **Rupert Beckett Lecture Theatre, Michael Sadler Building**

The ESCG satellite meeting is an opportunity for all early-stage crystallography researchers, from across the BSG, CCG, PCG and IG, to present their work in a supportive and friendly environment, which will be run by fellow early career scientists.

11:00-11:30 **ESCG Opening Plenary:**

Session Chair: Sam Lewis (Cardiff University / Diamond Light Source)

Speaker: Ines Collings (Natural History Museum)

Salt hydrates on icy moons: Structures and properties under extreme conditions

11:30-12:15 **ESCG Research Session 1**

Contributed talks from the ESCG community

12:15-12:45 **Flash Poster Presentations**

Researchers have an opportunity to present an overview of their poster in 30 seconds with one PowerPoint slide.

13:45-16:00 **ESCG Research Session 2&3**

Contributed talks from the ESCG community

16:00-16:30 **ESCG Annual General Meeting**

16:45-17:15 **ESCG Research Session 4**

Contributed talks from the ESCG community

17:15-17:45 **Parkin Lecture**

The Parkin Prize and Lecture is awarded annually and is intended to honour the outstanding achievements of the late Dr Andrew Parkin as scientist and teacher and his contribution to the ESCG.

MAIN MEETING

Room: Rupert Beckett Lecture Theatre, Michael Sadler Building

18:00-18:45 **Lonsdale Lecture**

Session Chair: ***TBC***

Speaker: Samantha Chong

18:45-19:00 **Exhibitor Talks**

19:00 **Poster Session with Dinner and Wine**

21:00 **Evening Concludes**

Tuesday 31st March 2026

BCA 2026 MAIN MEETING PROGRAMME

08:30-09:15 **IG Plenary**

Room: **Rupert Beckett Lecture Theatre, Michael Sadler Building**

Session Chair: **Tony Bell *(Sheffield Hallam University)***

Speaker: **John Helliwell *(University of Manchester)***

Open Science and Industry

09:15-10:00 **BSG Plenary**

Room: Rupert Beckett Lecture Theatre, Michael Sadler Building

Session Chair: ***TBC***

Speaker: **Basil Gerber *(The Institute of Cancer Research)***

Mechanistic insight into the function of the human CDK-activating kinase

10:30-12:00 **Parallel Sessions**

BSG: Structure-Based Drug Discovery

Session Chair: Daren Fearon *(Diamond Light Source)* and Blake Balcomb *(Diamond Light Source)*

Keynote: ***TBC***

How are disease insights feeding into structural biology, and how are structural insights informing clinical strategy? This session focusses on relating patient benefit to biological structure determination and welcomes contributions from industry and academia.

CCG/ESCG/IG: Crystal Formation (Crystallisation/Crystal prediction/Crystal Engineering

Session Chair: Andrea Laybourn *(Leeds)* and Sam Lewis *(Cardiff University and Diamond Light Source)*

Keynote: Sarah (Sally) L Price *(University College London)*

What is needed for the ideal organic crystal structure prediction code?

The session is interested in all areas of crystal formation, including crystallisation, crystal prediction and crystal engineering.

PCG: Energy materials

Session Chair: Ashok Menon *(University of Warwick)*

Keynote: Julia Payne *(University of St Andrews)*

Physical crystallography plays an important role in the transition to a more sustainable society. This session is intended to cover a range of materials with applications within any aspects of energy storage, harvesting and sustainability.

12:00-12:30 **AGMs**
BSG Annual General Meeting
CG Annual General Meeting
PCG Annual General Meeting

13:30-15:00 **Parallel Sessions**
BSG: Complex structures
Session Chair: Olivia Gittins
(Durham University)
Keynote: Mohinder Pal ***(University of Kent)***
Cryo-electron microscopy, tomography and related techniques are allowing for unprecedented detail in our visualization of large structures. This session highlights how these techniques are offering insight into biological machinery.

Commemorative session for George Sheldrick: his life and impact
Session Chair: Judith Howard
(Durham University)
Keynote: ***Bill Clegg (University of Newcastle)***
Sheldrick the legend, George the man
The crystallographic world is mourning the loss of George Sheldrick and the BCA will pay its respects and honour him in this session at the 2026 Spring Meeting. George's SHELX software has had a huge impact, initially in chemical crystallography but later expanding with great success and popularity for larger biological structures. We will reflect on his legacy in both scientific and personal arenas.

PCG: Quantum Materials
Session Chair: Nicola Kelly
(University of Cambridge)
Keynote: Lucy Clark
(University of Birmingham)
Tackling Synthesis-Dependent Structure and Properties in Quantum Materials
A session dedicated to materials where quantum effects, in a general sense, are relevant for the behaviour. This can include various forms of magnetism, spin-orbit coupling, and unusual electronic effects

15:30-17:00 **Parallel Sessions**
BSG/IG: Complementary techniques
Session Chair: Natalie Johnson ***(CCDC)***
Keynote: ***TBC***
Structure determination from diffraction data alone is not always enough to build a full picture of a material and its properties. Complementary techniques, either experimental (e.g. NMR, mass spectrometry) or computational, can provide additional structural information or help in the solution of more challenging structures. In this session we welcome contributions using additional techniques alongside experimental crystallography to gain further structural understanding.

CCG: Open Session (all talks 20 minutes)
Session Chair: Fanny Nascimento Costa
(University of Leeds)
An opportunity to showcase the wide range of research that falls under the general area of chemical crystallography.

PCG/CCG: Functional materials
Session Chair: Ines Collings
(Natural History Museum)
Keynote: Euan Brechin
(University of Edinburgh)
Molecular Iron Oxides
An opportunity to show research related to the crystallography of all compounds that can reasonably be described as functional

17:10-17:55 **PCG Plenary**
Room: Rupert Beckett Lecture Theatre, Michael Sadler Building
Session Chair: Lewis Owen
(University of Sheffield)
Speaker: Abbie McLaughlin
(University of Aberdeen)
Hexagonal Perovskite Derivatives: A New Platform for the Discovery of Fast Oxide Ion Conductors

18:00-19:00 **BCA Annual General Meeting**

19:30-00:00 **Conference Dinner, Networking & Ceilidh**

Wednesday 1st April 2026

BCA 2026 Main Meeting Programme

09:00-09:45 **CCG Plenary**
Room: Rupert Beckett Lecture Theatre, Michael Sadler Building
Speaker: Neil Champness
(University of Birmingham)
Session Chair: Hamish Yeung
(University of Birmingham)
Talk Title: TBC

09:45-10:30 **Exhibitor Talks**

10:30-12:00 **Parallel Sessions**
BSG: Open Session
Session Chair: ***TBC***
Nowadays, we use a variety of techniques to investigate biological structures. This open session captures aspects of the modern crystallographer: a multidisciplinary scientist using the right tools to answer important biological questions.

CCG: Advanced Techniques for Molecular Crystals
Session Chair: Lauren Hatcher
(Cardiff University)
Keynote: Florian Kleemis
(RWTH Aachen University)
Broadly themed around the investigation of molecular crystals using advanced techniques. Whether this is through quantum crystallography, in-situ techniques, 3D ED, serial crystallography or other emerging techniques.

PCG: Open Session
Session Chair: Ben Tragheim
(University of Sheffield)
This session is intended for all aspects of physical crystallography in the broadest sense.

13:00-14:10 **Parallel Sessions**

BSG: Protein Design Workshop

Session Chair: Natalie Tatum ***(Newcastle University)***

Keynote: ***TBC***

Advances in tools for de novo protein design and sequence optimisation, hand-in-hand with structure prediction, have made bespoke proteins accessible for many applications. This session will showcase some of the research questions being answered with targeted protein design, and serve as a primer to those new to the concept.

CCG: Workshop: Micro crystals analysis

Session Chair: Daniel Rainer ***(NCS Southampton)***

Keynote: Arianna Lanza ***(University of Copenhagen)***

Electron crystallography: how a wild beam can be tamed to become a reliable multipurpose tool

An informative and educational session on what can be achieved from small crystals, showcasing the current possibilities of different methods, radiation types, experimental setups, etc. Intended to increase awareness of possibilities, pitfalls, advantages and limitations of the different methods and how they are all complementary. As well as talks from the three speakers, the session will include a panel Q&A with all the speakers.

IG/PCG: PDF Workshop

Session Chair: Tony Bell ***(Sheffield Hallam University)***

Keynote: Dave Keen ***(ISIS)***

PDF is an increasing popular and accessible technique and this session will give an overview of PDF, including its history, development and best practices.

14:40-15:45 **BCA Prize Lecture**

Speaker: ***TBC***

Session Chair: ***TBC***

15:35-16:45 **Early Career Prize Lectures**

Biological Structures Group Early Career Prize

The BSG will award a prize to someone who has had an impact in the field of Structural Biology (with an emphasis on crystallography) and recently obtained a personal fellowship, a lectureship or equivalent position.

Chemical Crystallography Group Prize for Younger Scientists

The CCG will award a prize to a younger scientist who has performed original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry.

Physical Crystallography Group Early Career Prize

The Physical Crystallography Prize is awarded for the best recently published work by a person in the early stages of their career, working in the field of Physical Crystallography, whose research is expected to make a significant impact in the field.

17:05-17:20 **Poster prizes and close**

Room: Rupert Beckett Lecture Theatre, Michael Sadler Building

Session Chair: TBC

CLOSE OF CONFERENCE

ECM35 Poznań 2025

I try not to fly too much these days so my journey to the 2025 European Crystallographic Meeting went something like this: Fort William – London – Brussels – Dresden – Wroclaw – Poznań. One Interrail pass, two consecutive nights on sleeper trains (spaced by a decent lunch on Eurostar) and a journey in a 6-person train compartment made my arrival in Poznań feel something like the start of a novel by Agatha Christie. However, there was no mystery about this meeting, my second ECM; I enjoyed last year's in Padua so much I thought I'd come back for more. Despite the E in the meeting's name, attendance was from all over the world and it was really nice, and unexpected, to bump into old friends from my days of working in the USA.

My conference started with a day-long workshop on Quantum Crystallography which, I naively assumed, was to be held at the handsome campus of Adam Mickiewicz University, Collegium Minus, located approximately half way between my hotel and the conference centre. Instead, a chance encounter with arriving CCDC colleagues as I wandered the town on the Sunday afternoon revealed it was actually at a new campus, to the north of the city, beyond the end of a tram line, and it started at 8 in the morning. I am not sure how much I enjoy a conference if I have to set my alarm clock for an earlier time than I do when at home. The workshop was one of several satellites all taking place in the Faculty of Chemistry (excellent catering, by the way!), was well-received and, if I may bend the ear of other conference organisers, I think we need more workshops like this to share the knowledge of how to use quantum crystallography in everyday refinements.

Later that afternoon we transferred to the main conference centre (handily our conference badges apparently doubled as a local transport pass, though they didn't look particularly official to me and I'm quite glad I did not have to attempt to explain to an inspector why a piece of printed card on a lanyard exempted me from buying a ticket) for the conference opening ceremony.

This ECM ought to have taken place in Ukraine, hosted in Lviv, but was moved to Poznań for obvious reasons. The opening ceremony, however, paid more than a nod to our original hosts: the Ukrainian Ambassador to Poland gave an address, as did Poznań's mayor. Following two opening lectures, by the always entertaining **Sven Lidin** (Lund) and Perutz Prize winner **Gilberto Artoli** (Padova) we were then treated to a superb performance by Lira, a female voice folk choir made up primarily of students from Lviv university. Hearing Leonard Cohen's *Hallelujah* sung in Ukrainian was a personal favourite.

The following morning started with a reflective look from **Isabel Uson** (CSIC – IBMB, Barcelona) at the enormous contribution to the field made by George Sheldrick, who died earlier this year. She traced his life from childhood in Yorkshire (the motto of his school, "Success for All", being the subtitle of her talk), through education and his early time at Cambridge to his career in Goettingen from where he became the crystallography laboratory equivalent of a household name.

Starting the *Supramolecular interactions behind crystal engineering* session **Susan Bourne** (Cape Town) described the influence and roles of silver-halogen interactions in benzoate complexes, followed later in the session by **Louise Dawe** (Wilfrid Laurier), whose discussion of aminopyrazole systems included some completely unexpected proper, covalent bond-forming, organic chemistry which they'd not quite figured out. Seated as I was at the rear of the room it was quite amusing to see more than one audience member proceed to waggle a finger in the air, pushing imaginary curly arrows in order to effect a possible mechanism.

The *Potential of online courses in crystallography* is the sort of session title where one feels one will definitely come out inspired and with ideas, regardless of career stage or knowledge and this was the case in this afternoon session which started with a good overview by **Ilaria Gimondi** (CCDC) of the various workshops, teaching subsets and other hosted online content made freely available by CCDC. I also enjoyed the talk by **Stefano Canossa** (ETH Zurich) on how we can find, with the help of our phones, Fourier transforms in everyday life. The day ended as it began, with several personal reflections from former students and colleagues of George Sheldrick, followed by the Sheldrick Prize lecture given down the line from Switzerland by **Lauren Hatcher** (Cardiff), a whistle stop tour from time-resolved photocrystallography to developing serial methods of data collection for chemical crystallography at synchrotron beamlines.

A concert at Adam Mickiewicz University, Collegium Minus this time, was organised for our evening entertainment and I recommend you seek out a recording of Juliusz Zarębski's excellent Piano Quintet in G minor.

How to... successfully apply for funding is another of those microsymposia topics where you feel everyone will be able to contribute and take something away. Personal reflections by **Anna Krawczuk** (Goettingen) – generating much discussion along the way – were followed by thoughts from **Mattia Gaboardi** (Rome Tor Vergata) on applying for, and successfully obtaining, time at central facilities, something particularly close to my heart at that point with a big deadline for Diamond looming! Following this, I nipped out and into another session to hear **Andy Maloney** (CCDC) describe their implementation of the FIDEL method for powder diffraction pattern matching. Nipping between sessions at this venue was slightly complicated by one room being labelled differently from what was written in the programme (A became E, if memory serves) and some rooms had additional doors which led directly into a service corridor of sorts, adding a touch of "not sure I'm supposed to be here" primary school energy to the place. The early evening saw the return of the Science Slam and after Bill Clegg's heroic Flanders & Swann pastiche in Padua this year's competitors

studiously avoided singing, with **Sam Horrell** (Imperial) – who was later recognised, in the street and from behind, as "the synchrotron mug guy" – taking the honours.

The final day started with a moving keynote talk by **Ilias Shcherbakov** (Kharkiv) of how research in Ukraine continues amidst ongoing shelling and frequent interruptions to work by air raid alarms. Despite this, new research programmes have started and new laboratories have been opened over the last couple of years though access to literature and to replacement parts for equipment remains an ongoing problem. *Exploiting crystallographic databases in solving, refining, and validating crystal structures* started with an examination by **Natalie Johnson** (CCDC) of how the data-rich Cambridge Structural Database is much more than a tool for checking unit cell parameters, followed by a suite of speakers, all also drawing on the database in one form or another. **Diane Dickie** (Virginia) perhaps unwittingly outed herself as a modern-day Dick Marsh in describing how she uncovered several egregious entries (some innocent, others less so) in the course of preparing material for undergraduate practical classes while **Bill Clegg** (Newcastle) showed how prior knowledge mined from the CSD can be used to help in modelling particularly tricky boron cluster structures. Incidentally, in a city whose mascots are a pair of goats, Bill showed that he is indeed the GOAT coming as he did top of the CCDC leaderboard and providing me with some motivation to publish more structures containing niche f-block elements in order to progress beyond silver.

After another deliciously carb-heavy lunch – **Sally Price** (UCL) declared it "the best conference food" she'd ever eaten – I wandered into the *Publishing Crystallography* session where **Louise Jones** (IUCr) took us through the mechanics of publishing work in one of the IUCr's suite of journals. This was followed by an absorbing take on ethical publication by **Manfred Weiss** (Berlin) illustrated with examples from the macromolecular world where authors of somewhat questionable work had been challenged: some doubled down, others quietly retracted, none openly took responsibility. Next up, your Edinburgh correspondent describing how we use university-funded undergraduate internships' CSD Communications to keep a check on our ever-rising pile of unpublished structures, a problem which will continue to grow as data collection times continue to decrease, and a presentation of the alternative, and entirely complementary, Crystallography Open Database by **Saulius Gražulis** (Vilnius). The session closed with an audience discussion picking up on some of the issues raised by all four previous speakers.

The conference ended with a twilight guided tour of Poznań, two hours strolling the historic centre and finishing off, as so many other evenings did, with a pint or two of good local beer at Brovaria and thoughts turning to the next meeting, in Prague, in 2027. I hope to make it three in a row!

Gary Nichol, Edinburgh

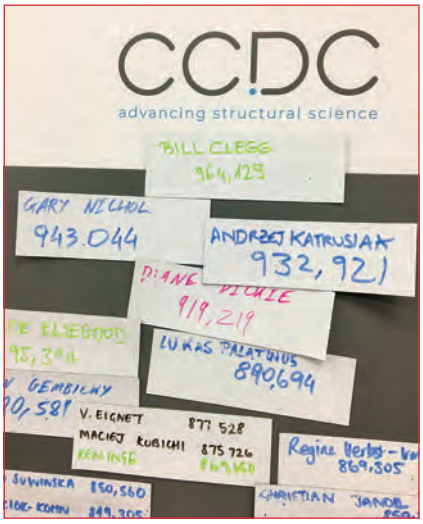
A "double helix" at Dresden railway station en route to Poznań is a stack of Ritter Sport chocolate bars. I thought it a harbinger of a good meeting to come.

The two crosses tied with rope is a sculpture in memory to those who died in food riots.

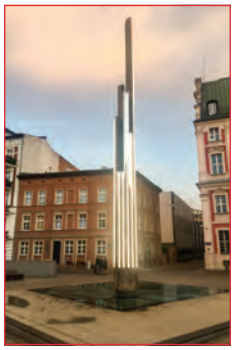


Two goats make up the mascot of the city of Poznań.

The obelisk with numbers is a memorial to Polish Enigma code crackers.

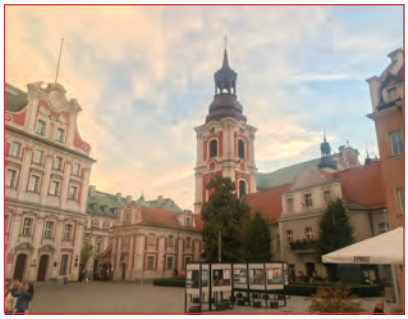
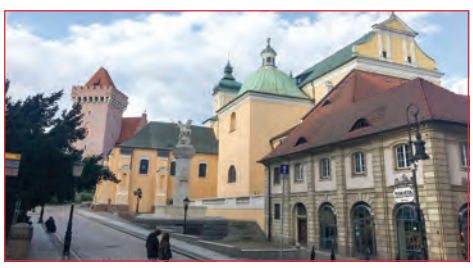


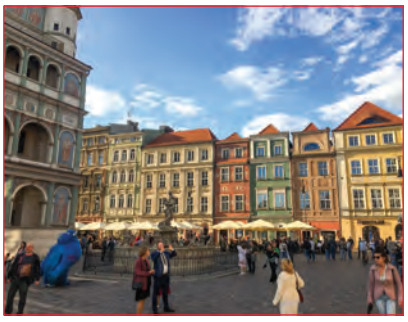
At the conference!









Photos of Poznań taken during the day and during the evening guided tour.

Suzanna Ward (CCDC) speaking at the ECM35 in Poznań on "Breaking boundaries, creating connections: the CSD at 60."

Patrick Shaw Stewart (Douglas Instruments) presented on "Using phase diagrams with microseeding to prepare crystal samples for advanced data collection techniques."

Jeremy Cockcroft (UCL) speaking on the subject of "Exploring non-covalent interactions in simple binary adducts by a combination of DSC and variable temperature powder and single-crystal X-ray diffraction."

Representatives of Molecular Dimensions and ThermoFisher Scientific.

The photos on this page are by Grzegorz Dutkiewicz and permission to use them here has very kindly been granted by the ECM35 secretariat. Photos on previous pages of this meeting report are by the author, Gary Nichol (Edinburgh).

CCG Autumn Meeting

THE online CCG Autumn Meeting returned this year with a theme of *Advances in Chemical Crystallography*. Held on Wednesday 22nd October 2025 the meeting featured ten interesting talks, from people at various career stages, across a broad range of crystallographic topics and showcasing a wide range of advancements in the field to a great turnout of over 60 attendees. Barring a couple of minor technical hitches at the start, the online meeting went very smoothly, with several participants remarking on how enjoyable it was!

The morning started with a celebration of 60 years of the Cambridge Structural Database and how it has influenced structural science, through a talk from **Natalie Johnson** (CCDC). This was followed by **Karen Robertson** (Nottingham) who introduced us to her recent work on structural characterisation of crystals under flow conditions, including the apparatus for collecting single- crystal data on samples in a flow system. **Adam Michalchuk** (Birmingham) took us (carefully!) through his structural and theoretical work, using the structures of energetic materials to gain an understanding of underlying properties such as phonon scattering, and then using this to build a predictive model for their impact sensitivity.

The second session started with **Lauren Hatcher** (Cardiff) describing how her work on photocrystallography has led to the development of small-molecule-suitable serial synchrotron crystallography, and how this is now moving towards small-molecule serial techniques suitable for use at XFELs. Then the presentation by **Andy Brown** (Leeds) took us in a rather different direction, introducing us to scanning electron diffraction, and how this technique, which combines aspects of SEM and ED, can be used to get structural information on beam-sensitive materials. **Sudeshna Roy** (Leeds) finished the session, telling us about her work on the preparation and ageing behaviours of co-amorphous materials, and how process factors can influence these.

The last session of the day began with a talk from **Michael Bodensteiner** (Regensberg) reminding us that atomic scattering factors include anomalous dispersion components which can influence structures to a surprising extent. We were introduced to the idea that refining these anomalous components can be done and be useful for particularly heavy-element structures. The next presentation, from **Giovanna Barrionuevo Martins** (Newcastle), demonstrated a new variation of the ENaCt nanoscale crystallisation technique. This involves the addition of designed reagents to the crystallisations to functionalise the compounds being crystallised, leading to a higher likelihood of forming crystals. This was followed by a talk and demonstration by **Horst Puschmann** (OlexSys) on the use of non-spherical atomic scattering factors in the refinement of routine structures, using NoSpherA2 within Olex2. The final talk of the meeting was by **Jere Tidey** (Warwick) on some of the practicalities of 3D ED, as experienced in the National Electron Diffraction Facility, and what structures you can and cannot obtain from crystalline dust.

Thank you to all the speakers and attendees for a brilliant day!

David Cordes, St Andrews

South West Structural Biology Consortium

THE 22nd SWSBC meeting was held in Sussex from the 21st to the 22nd July 2025 and was organised by Antony Oliver (Sussex), Mark Roe (Sussex) and Luke Yates (Sussex). The meeting was generously sponsored by CCP4, Cytiva, Bruker, Molecular Dimensions, Douglas Instruments and iLAB. Attendees were also given the option of an interesting tour of the local X-ray laboratory.

The first session was chaired by **Antony Oliver** (Sussex) and began with a lecture by **Biniam Haile** (Sussex) entitled "MOKCa-3D database: functional and structural analysis of missense mutations in cancer." The speaker explained the classification of cancer-associated mutations in terms of gain-of-function (GOF) and loss-of-function (LOF) changes and mentioned how some 3 million such mutations have been reported. These are publicly available in the COSMIC database maintained by the Sanger Centre in Cambridge. By mapping these mutations to AlphaFold structures a pipeline has been created for calculating the impact of these mutations at the level of protein 3D structure. Effects include the breakage of hydrogen bonds, conformational perturbations due to glycine and proline mutations, changes to catalytic residues and disruption of the protein's stability through the introduction of steric clashes as well as changes affecting hydrophobicity, disulphide bridges and charges. A MySQL database has been created which allows the user to search for cancer-associated mutations in specific genes and extract information from it such the tissue location, etc. The speaker outlined how tumor formation begins with driver mutations and is followed by numerous passenger mutations during evolution of the tumor, the key issue being to identify the driver mutations which lead to the disease. The structural impact of these mutations is assessed by secondary structure prediction. The speaker outlined studies of residues at or in the immediate vicinity of phosphorylation sites, observing that GOF mutations are generally less disruptive structurally than LOF changes and that the effect of driver mutations is context dependent. Machine learning is being used to predict pathogenic mutations. The database provides visualisation tools for inspecting the structural context of mutation sites, including ligand- and protein-protein binding sites, domain boundaries and post-translational modifications. It is available at the following URL: https://bioinformaticslab.sussex.ac.uk/MOKCa-3D/ and provides a very useful source of information about all genes, not just those implicated in cancer.

The next lecture was given by **Michael Beer** (Bristol) and was entitled "Mechanism, dynamics and inhibition of class A β-lactamases through computation and experiment." The speaker introduced the subject of antibiotic resistance stemming from the action of the β-lactamase enzymes and the range of structural and computational chemistry tools being used to mitigate the problem. The β-lactam antibiotics constitute something like 52 % of all prescriptions and fall into four major classes: penicillins, cephalosporins, carbapenems and monobactams. Crystallographic studies of these enzyme benefit from the fact that atomic resolution data can be collected on a short time scale, enabling reliable classical Newtonian molecular mechanics (MM) and quantum mechanics (QM) simulations of the reaction to be undertaken. Specifically the project involved studies of carbapenem resistance by analysis of acyl enzyme complexes which the enzyme either can or cannot hydrolyse, the latter being an ideal characteristic for an inhibitor. This work revealed the roles of regions distal to the active site. In the QM/MM approach the active site is treated by QM while the rest of the enzyme is handled by the less computationally intensive MM theory. Specifically treating the active site Ser, Glu and Lys residues along with a water molecule by QM and the remainder of the structure by MM allowed a 180 picosecond simulation of the reaction to be completed in 9 days of computer time. In one crystal structure, the observed electron density for the intermediate did not allow discrimination between a trans-enamine, a cis-enamine or an imine. Consequently the QM/MM approach was used to optimise them and this suggested that the trans-enamine was the most likely interpretation. The speaker described how dynamical non-equilibrium molecular dynamics (D-NEMD) is being used to identify distal regions of the structure which affect the catalytic activity.

The next lecture was given by **Mahjoobeh Ehsani** (Southampton) who spoke on the subject of "Structural dynamics analysis of cancer-associated BCL-2 mutants using HDX-MS." The B-cell lymphoma-2 (BCL-2) family of proteins are known for their ability to regulate apoptosis in cancer cells, some being pro-apoptotic and others being pro-survival. Cancer associated mutants of BCL-2 arise spontaneously in lymphomas or as a result of treatment with the chronic lymphocytic leukemia (CLL) drug venetoclax, which binds to pro-survival BCL-2's and inhibits their action. The speaker covered the structure and function of the BCL-2 protein domains. A number of mutant forms of BCL-2 were analysed by hydrogen-deuterium exchange mass spectrometry (HDX-MS). The experiments were based on H-D exchange at neutral pH followed by quenching at low pH, pepsinolysis and then MS. The work showed how the mutations alter the mobility of the protein as well as its stability and drug-binding ability, often in regions distant from the mutated residue. The mutations G101V, A113G, R129L, R139L and V156D were found to alter the dynamics of the drug-binding site. Circular dichroism (CD) has been used to determine the Tm's of the mutants and microscale thermophoresis to determine their K_d's, ultimately showing that many have markedly reduced affinity for the drug.

After lunch, the second session was chaired by **Laurence Pearl** (Sussex) and began with a lecture by **Jack Stubbs** (Southampton / DLS) entitled "Droplet microfluidics for uniform micro-crystallisation and rapid mixing." Jack covered

the evolving field of macromolecular crystallography as applied to microcrystals which are specifically required for serial crystallography. Optimally for work of this nature, the crystals should be small and of uniform size, typically 2 – 3 microns, to allow rapid mixing across a range of tuneable delivery times. The speaker emphasised how microfluidics now allows working on volume scales as small of nL, pL and fL with crystal growth being achieved on the second timescale, at least in the case of lysozyme. A highly compact lattice of crystallisation droplets can be made by encapsulating them under oil and phase diagrams to optimise crystallisation and seeding conditions for the experiment can be obtained. The reliability of this approach allows growth of typically one crystal per pL volume droplet under oil and the addition of detergent then yields a stream of crystals suitable for time-resolved data collection. Microfluidics allows convective-diffusive mixing of nanodroplets on timescales as short as 2 milliseconds and the droplets travel through the chip so fast that special cells are required to slow them down. In the actual delivery of crystals to the beam, there is a significant problem of sedimentation which can be circumvented by rocking the syringe. Jack emphasised that the techniques described are very much work in progress.

The next lecture was given by **Adam Cutts** (Cardiff) and was entitled "The long and short of it – distinct natural crystal packing strategies of Cry toxins from *Bacillus thuringiensis* using serial femtosecond crystallography." The speaker described how this bacterium is a Gram-positive, sporulating microorganism which expresses parasporal crystals of Cry proteins as inclusion bodies and these have a protective insecticidal function, allowing the bacteria to be used agriculturally as a pesticide. Structural studies have shown that all of the Cry proteins contain 3 domains, with some possessing an additional 4 domains which facilitate crystallisation. Indeed the crystals from the bacteria are suitable for serial crystallography. The speaker presented a 1.6 Å resolution structure for the Cry1 protein determined using serial data, demonstrating that the crystallisation domains are disulphide-rich with some of the intermolecular disulphide-bridges forming lattice contacts. In contrast, the 2.2 Å resolution structure of Cry8, also determined using serial data, shows that this protein possesses no disulphides but has an unusual projecting region, affectionately called "the peg", that interdigitates with other molecules in the lattice. One of the structures had a non-proline cis-peptide which was involved in forming an ion binding site. In summary, four novel seven-domain Cry structures have been determined by serial femtosecond work at EuXFEL.

The next presentation was given by **Mathew McLaren** (Exeter) who described how "Cryo-EM resolves the structure of the archaeal dsDNA virus HFTV1 from head to tail." Haloferax tailed virus 1 (HFTV1) is found in Lake Retba in Senegal which has a salt content of up to 40 % and is known for its pink colour due to the presence of halophilic algae. HFTV1 has many morphological similarities with the tailed bacterial phages suggesting a common evolutionary origin. Initially, the viral capsid of this phage binds the S-layer of the target bacterium (*Haloferax gibbonsii LR2-5*) prior to a reorientation such that the tail can deliver the genomic material. The eBIC facility at DLS was used for cryo-EM data collection with a pre-processing correction which summed the movies into single frames. AlphaFold models of proteins present within the virus were used for sequence assignment of the map. Structure solution by symmetry-averaging proceeded from the capsid to the tail followed by the baseplate and then on to the DNA within the tail. The *T*=7 icosahedral capsid was found to be covered with turrets which have a hexameric base and a trimeric head. The latter have putative polysaccharide deacetylase activity against the S-layer of target bacteria which may account for the initial binding of the capsid to the cell-surface. The portal protein between the capsid and the tail was also resolved while the base plate of the tail was found to have three spikes. The double-stranded DNA within the capsid was found to be arranged in 10 concentric shells with its termini close to the portal.

Next came an exhibitor presentation by **John Hinks** (Cytiva) entitled "Optimisation and troubleshooting of purification strategies for structural biology." John described the ÄKTA pure micro system which aims to reduce dilution of the sample during purification and has a fraction collector capable of collecting µl volumes. The system allows analytical size-exclusion chromatography and is well-suited for preparative EM work. John then moved on to describe the ÄKTA go system which, amongst many other things, allows automated peak-to-loop elution of proteins of interest. **Paul Driver** (Calibre Scientific) then gave a presentation demonstrating the Proteus X-Spinner which features specially designed pressure caps that allow protein solutions to be concentrated without a centrifuge. Paul then described the RAMP crystal screen which incorporates a mixture of lipids for membrane protein crystallisation before moving on to the ANTcryo holey support film for cryo-EM which is made from amorphous nickel-titanium alloy. These films allow higher particle densities to be achieved and improved resolution of the final analysis.

The much-needed afternoon coffee break was followed by a drug design-themed session which was chaired by **Susan Crennell** (Bath) and began with a presentation by **Kirsty Goudar** (Bristol) entitled "Cracking the code: structural & functional insights into class D β-lactamases and their inhibitors." The speaker began by introducing the field of antimicrobials and the problem of antibiotic resistance due to the action of β-lactamase enzymes which is reported to result in millions of deaths worldwide. These enzymes are the subject of numerous multidisciplinary studies by kinetics, crystallography, simulation and mass-spectrometry which are aimed at tackling *E. coli*, klebsiella and pneumococcus infections. The speaker mentioned that the time from discovery of a novel antibiotic to the appearance of resistance in the bacterial population is around 10 years or less, with carbapenen resistant and 3rd generation cephalosporin resistant bacteria being the worst. The speaker described the serine- and metallo- classes of the β-lactamases, the former possessing an active site serine (Ser 70) and a carbamylated lysine residue (Lys 73). Kirsty described studies of the OXA-48 carbapenemase and how the β-lactamase inhibitors avibactam and nacubactam act on it and a number of active site variants (OXA-163 and OXA-405). Enterobacterales possessing OXA-48 are responsible for seriously intransigent infections. Nacubactam was found to be not as good as avibactam towards OXA-48, but this difference reduces in OXA-163 and OXA-405. Crystal structures and molecular dynamics simulations were employed to study this effect, revealing electrostatic repulsion between nacubactam and Arg 214 of the OXA-48 β5 – β6 active-site loop, but not with avibactam. These

effects are absent in OXA-163 and OXA-405 which lack Arg 214. Crystallographic and mass spectrometry data demonstrate that all three enzymes facilitate desulphation of the bound inhibitors over a 16 hour period.

Freddie Munns (Portsmouth) was the next speaker on the subject of "DNA Ligases: novel drug targets in the fight against antimicrobial resistance." The speaker began by emphasising that by 2050 it is estimated that antimicrobial resistance will be responsible for around 2 million deaths. Freddie mentioned that whilst current antibiotics target cell wall synthesis, ribosomes and DNA gyrase, there is much potential for development of inhibitors to DNA ligase - an enzyme involved in DNA replication, recombination and repair. The ligase uses AMP to seal nicks in the DNA substrate, with prokaryotes generating the AMP from NAD+ and eukaryotes generating it from ATP. This difference might be exploitable for development of antibiotics. The speaker described how the prokaryotic and eukaryotic enzymes have differences in their domain sizes. AlphaFold has been used to derive models of the enzyme from the most multidrug resistant strains of bacteria. The speaker described the expression of the enzyme from several such bacteria, with CD being used to confirm correct folding and an assay using fluorescein-labelled DNA. This work showed that polycyclic ruthenium organometallic compounds which intercalate between the DNA base pairs were effective inhibitors with IC_{50}'s in the 5 μM range. Future work will target the enzyme moiety for drug design.

The next lecture was entitled "Structure guided drug design of novel antibiotics targeting DNA gyrase" and was given by **Harry Morgan** (Cardiff) who began by describing the spiropyrimidinetrione antibiotic zoliflodacin which is a gyrase inhibitor. As with the fluoroquinolone moxifloxacin, bacterial resistance arises from overexpression of efflux pumps and other effects. The specific aim of the project has been to determine the structure of the zoliflodacin-stabilised *S. aureus* DNA gyrase DNA-cleavage complex, and this remains the subject of ongoing work. Sitting drop crystallisation facilitated a successful structure analysis of the enzyme at 2 Å resolution and has allowed an XChem fragment screen to be undertaken at DLS with around 30 interesting hits having been obtained from around 500 compounds tested.

Last but not least, the concluding lecture of the day was presented by **Ryan Lawrence** (Southampton) and had a title of "Structural insights into multidrug resistance by the anaerobic efflux pump MdtF." Efflux pumps are huge multi-protein active transporters which span the inner and outer bacterial membranes of Gram negative bacteria and consist mainly of TolC and MdtF, the latter being a homologue of AcrB. With collaborators at UCB Biopharma, the cryo-EM structure of MdtF bound to rhodamine 6G was determined at 3.6 Å resolution in styrene maleic acid lipid particles which mimic the native lipid environment of the protein. The system has also been studied by fluorescence polarisation and molecular dynamics to gain an improved understanding of drug efflux and bacterial detoxification in acidic and anaerobic conditions as well as in biofilms.

The first day of the conference then concluded with a combined poster and exhibition session followed by the conference dinner which was held in the open air on what turned out to be an extremely pleasant evening.

The following day began early with a session chaired by **Eamonn Reading** (Southampton) in which the first talk was given by **Georgios Kontellas** (Exeter) on the subject of "Sustainable degradation of keratin waste using thermophilic enzymes (ThermoK)." The speaker began by discussing the issue of feather waste from poultry farming and biofriendly ways in which this potentially valuable source of materials for the agricultural, cosmetics and pharmaceutical sectors could be processed more effectively rather than by merely burning or dumping in landfill sites. The work is funded by the EU consortium project ThermoK which has partners in Norway, France, South Africa and the UK. The speaker mentioned how the anaerobic and thermophilic fervidobacteria express keratinases and other enzymes which degrade the β-keratin present in feathers. Georgios described the expression of a number of enzymes involved in this process, including the serine peptidases S8 and DoP, the pyrrolidone carboxypeptidase PcP and the disulphide reductase DSR. Intriguingly PcP is a cysteine proteinase which is capable of removing pyroglutamic acid from the N-termini of proteins possessing this modification, which are abundant in feather material. The structures of these microbial keratinases were initially modelled using AlphaFold. Mass-spectrometric assays of peptides produced from degradation of feathers showed that combinations of these enzymes were successful, with the best cocktail possessing all three! Indeed crystals of DoP and DSR have already been obtained and thermal stability studies of these enzymes, which seem to be optimally active around 65 °C, are in progress.

The next lecture was given by **John Spencer** (Sussex) and was entitled "Degrader collapse rationalised by structural studies." The speaker covered the acetylation of lysine residues in histones and how bromodomains are able to detect this post-translational modification and promote gene expression. PHIP(2) is an atypical bromodomain which is implicated in metastatic lung cancer and melanoma. The speaker described a wide range of studies of this protein by fragment screening, hit elaboration and follow-up crystal structure determination studies at DLS which have yielded inhibitors with 5 μM affinity. The speaker then moved on to the subject of proteolysis-targetting chimeras, or PROTACs for short, which are drugs consisting of a moiety that binds to E3 ubiquitin ligase and another group which binds the protein of interest or POI, both moieties being joined by a linker region. This leads to the POI being polyubiquitinated and ultimately degraded by the proteasome. John described the compound ISOX-DUAL that was designed to target BRD4 and CBP/EP300 although it presented some problems in the synthesis which were overcome. John mentioned the importance of getting the length of the linker region right and how this work allowed structures of a number of potent compounds bound to the bromodomain to be determined. However these compounds were not found to cause ubiquitination of the POI and the crystallography revealed that the region of the PROTAC that should have targetted E3 ligase was actually binding within the bromodomain – an effect referred to as degrader collapse.

The concluding talk of the first session was given by **Joe Ball** (Portsmouth) and was entitled "The expression and characterisation of novel PET-degrading enzymes." The speaker explained that PET stands for polyethylene terephthalate which is the most common polyester used for manufacturing clothing materials, food containers and glass fibre products. It can also be aluminised to reduce

its permeability for certain applications. Environmental dumping of plastics is a serious issue on both land and at sea, and microplastic deposits in the kidney, liver and brain are increasingly recognised as an age-related human health problem. Enzymic degradation of plastics would provide an environmentally friendly solution to many of these pollution problems. Suitable candidate enzymes are known as PETases although currently these struggle to degrade crystalline regions of the plastic and therefore engineered thermostable forms that could work close the glass-transition temperature of PET are needed. Bioinformatics screening was used to identify suitable candidate enzymes of the polyesterase-lipase-cutinase family, such as dienelactone hydrolase, which occur naturally in microbes for degradation of the waxy coating on leaves. Candidate genes were then cloned and expressed for characterisation of activity and thermostability. Joe reported that a number of the recombinant enzymes suffered from insolubility and therefore refolding with urea was attempted and this was successful in one case.

After the morning coffee break, the next session was chaired by **John Spencer** (Sussex) and began with a lecture on how "Structure-guided disulfide engineering restricts antibody conformation to elicit TNFR agonism in anti-cancer therapeutics" which was given by **Isabel Elliott** (Southampton). The speaker began by outlining the structure of antibody molecules, their antigen-binding or Fab arms, antigen specificity and effector functions. Agonist antibodies that activate cellular signalling pathways have emerged as promising therapeutic agents. For example, activation of immune signalling pathways through the use of antibodies that target co-stimulatory receptors, such as tumour necrosis factor receptors (TNFRs) can enhance the immune response towards tumours, resulting in powerful anti-cancer effects. Agonist antibodies cause clustering of the target receptor at the cell surface and restricting antibody conformation through disulphide modification further enhances the signalling effect. Thus the project focusses on studying the effects of disulphide exchange in the vicinity of the hinge region of IgG2 to join the two Fab regions. This work involves structure-guided disulphide engineering of other IgG variants including IgG1. Experimental work involves the use of the long-wavelength beamline at DLS to enhance visibility of the electron-rich sulphur atoms and SAXS is used to study the effect of disulphide swaps on the overall shape of the molecule. Use of Kratky plots to determine radii of gyration (R_G) demonstrated that the disulphide mutants are more compact. These studies were complemented by SAXS-weighted MD simulations and confocal microscopy to study receptor clustering, B-cell activation markers and proliferation. Isabel concluded by describing studies of a double mutant with enhanced compactness and improved co-stimulatory effects.

The next lecture was given by **Rebekah Cooke** (Cardiff) who spoke on the subject of "C5 inhibition by mAbs: there's many ways to skin a cat!" Rebecca began by outlining the innate immune system and its involvement in many diseases such as haemolysis. This has led to the concept of complement immunotherapeutics which involves monoclonal antibodies being used as drugs to target and inhibit enzymes in the complement cascade. Crovalimab and eculizumab are examples of drugs in this category which are made by hybridoma technology. The project involved AlphaFold modelling of the 3D structures of a number of monoclonals which were developed in house to inhibit complement activation. Rebekah described studies of their effectiveness by a wide range of laboratory assay techniques including surface plasmon resonance (SPR). The project led to the discovery of four epitopes on the complement protein C5 which can be occupied simultaneously by antibodies and several different mechanisms of inhibition.

In the last lecture before lunch, **Malek Hawela**, (Southampton) spoke on "Regulation of bacterial biofilm dispersal by multi-domain redox sensing proteins." Concentrating on the major hospital pathogen *Pseudomonas aeruginosa* which is well-known for its antibiotic resistance and biofilm-forming abilities, Malek described how neutrophils destroy and disperse biofilms by production of reactive oxygen species as well as nitric oxide. The speaker described how the bacterial secondary messenger cyclic diguanylate monophosphate (c-di-GMP) upregulates biofilm formation. This process is also regulated by the linearised degradation product of c-di-GMP which is known as pGpG. The project is based on analysing a number of membrane proteins which are involved in sensing nitric oxide and triggering c-di-GMP production. These proteins possess PAS sensing domains which sense nitric oxide and deletion of these domains was found to affect biofilm dispersal. The project involves crystal violet staining with confocal microscopy, numerous cell culture and assay techniques as well as crystallography. Improved understanding of biofilm dispersal mechanisms should aid targeting of these systems to improve the efficacy of antibiotics.

The concluding session of the meeting was chaired by **Jon Cooper** (UCL) and began with a presentation by **Charles Ballard** (CCP4) on the CCP4 program suite. Charles mentioned that whilst the UK collaborative computing projects (CCP's) to some extent, come and go, the protein crystallography project (CCP4) which was founded in 1979 and the equivalent groups for EM (CCPEM) and NMR (CCPN) are going from strength to strength. The CCP4 core group is based at the Harwell campus with additional splinter groups in Cambridge, York and Newcastle doing their respective things, alongside a number of overseas collaborators. The work of the group can be broadly split into automation of tasks currently done by various discrete programs within the suite and fundamental research on developing new approaches to solving specific crystallographic problems. The speaker mentioned how the package consists of in excess of 100 programs and occupies 5 Gb of storage with operation being possible from the command line or from one of two GUI's, namely CCP4i which dates from the late 90's and CCP4i2 which was released in 2016. It has also been possible to run the programme suite in the cloud since 2019. Charles mentioned that the 2026 study weekend will be focussed on handling ligands in protein structures whilst a number of Summer and Autumn schools are run annually. Charles spoke about the application of AlphaFold models in molecular replacement and the need to split them into separate domains as well as the benefits of jelly-body refinement in this approach. Charles concluded by outlining a number of new developments in the suite including the programs Modelcraft, Buccaneer, Webcoot/Moorhen and Slice'n'Dice.

Next, **Kieran Hartwell** (Cardiff) spoke on the subject of "Engineering a copper-dependent fluorescent protein association system" with the well-known green fluorescent protein firmly in mind. This molecule has been shown to consist of 11 β-strands with an α-helix passing through the centre of the barrel. The helix carries the covalently bonded chromophore which is formed by a spontaneous reaction involving a Ser-Tyr-Gly sequence in the presence of oxygen that is catalysed by specific residues of the inner surface of the barrel (Wikipedia, the free encyclopedia). It has numerous biotechnological applications in sensing trace metals and protein-protein interactions. Indeed the aim of this project is to engineer a GFP capable of sensing dimerisation of a protein in response to trace metal ions. In-silico design suggested that the residue His 148 could be mutated to Cys so that a disulphide might form on dimerisation of the GFP molecule when coupled with a leucine zipper protein. Covalent dimer formation in the presence of copper sulphate is accompanied by a change in the fluorescence from 400 nm to 490 nm. The system has promising potential for detection of both copper I and copper II ions, the different oxidising effects of which cause the GFP dimer to form on very different timescales. The aim of the project is to develop an in-cell copper probe.

Following on, **James Geraets** (Sussex) began his talk on the subject of "Cryo-EM at the University of Sussex" by asking the audience for a show of hands to canvas their experience with electron microscopy, electron tomography and in situ structural biology in general. James mentioned that his own interests in these techniques stem from his work on virology and amyloids. In his role as a facility manager, James overseas a JEOL Cryo ARM 200 and a JEOL 1400+ equipped with Gatan K2 and Gatan OneView detectors, respectively. The facility provides training and technical assistance to both faculty and external users, as well as consultation on project development and optimisation of workflows to address research questions. James has research interests in structural biology and software development. James briefly described a new automated freeze-plunger for cryo-EM grids – the Cryogenium (Linkham), which offers improved control of sample vitrification as well as greater reproducibility and efficiency.

There followed an interesting lecture by **Eamonn Reading** (Southampton) entitled "The backbone of multidrug efflux within RND-type pumps" who described the AcrAB-TolC system which is a member of the resistance-nodulation-cell-division (RND) family of active transporters present in the cytoplasmic membrane, mainly in Gram-negative bacteria. Eamonn mentioned how there is a significant amount of structural movement within the transporter in order for it to pump substrates and this flexibility renders the system amenable to H/D exchange (HDX) mass spectrometry (MS). HDX is sensitive to pH, temperature, sequence, pressure and ionic strength, and as an MS technique it allows breathing motions and flexible regions of proteins to be studied. The speaker described studies of the fluoroquinolone ciprofloxacin and other antibiotics as well as studies of an efflux pump inhibitor bound to AcrA, the protein component which connects AcrB and TolC in the efflux pump. The compound was found to rigidify the whole structure. In practice deuteration studies of cells actively pumping out drugs has improved to the point where an analysis which previously required 4 weeks can now be completed in 2 days. The speaker then described the SpyTag and SpyCatcher system for studying protein-protein interactions as well as a 'lemon-catcher' system for covalent capture in MS work. Fusing the gene of interest with a short piece of DNA encoding the SpyTag peptide allows it to be specifically conjugated with the SpyCatcher protein or another protein recombinantly fused with the catcher protein. The spy peptide and the catcher protein recognise each other with high specificity and become covalently linked by an isopeptide bond on a short timescale. This relatively new technology can be used for vaccine production, stabilising multi-protein complexes and for studying membrane protein localisation and topology.

Last, but by no means least, the final lecture of the meeting was given by **Kamel El Omari** (DLS) on the subject of "Light atoms identification and location by anomalous scattering." Kamel started by citing a recent study in which it was found that over 50% of metal ions in protein structures had been misidentified (Grime *et al*., 2020) and how this long-running concern has led to various efforts such as the CheckMyMetal website (https://cmm.minorlab.org/) to improve the situation. Kamel mentioned how the use of anomalous data can significantly improve the accuracy of the assignment of metals. However, there are stringent requirements for collection of accurate and truly redundant diffraction data, necessitating 360° crystal rotation as well as minimising the amount of solvent surrounding the crystal by optimising the loop size. With a suitable crystal an X-ray fluorescence spectrum will reveal potential metal absorption edges and diffraction data can be collected at three wavelengths, one above the absorption edge, another below and one right on the edge itself. Changes in the anomalous difference Fourier peak heights at these wavelengths should reveal nature and locations of the relevant metal ions in the structure. Many of the lighter metals present in proteins have long absorption edges and this therefore requires that long wavelengths are used.

Accordingly, the in-vacuum beamline I23 at DLS is designed for working in the wavelength range of 1.1 to 5.9 Å and has a large semi-cylindrical detector. This allows measurement of a large range of diffraction angles and a multi-axis goniometer is available for crystal alignment and orientation. Laser-shaping of the crystal is also an option to reduce the amount of surrounding material present in the beam. Kamel then outlined studies on specific proteins such as phosphoenolpyruvate carboxykinase (PEPCK) which revealed the presence of a manganese ion and the LeuT transporter (a Na/Leu symporter) which revealed the location of sodium, although the long absorption wavelength of this element does not allow edge datasets to be collected. Long wavelength studies have also been used to pin-point fragment orientations and for studies of the Φ8 phage P2 RNA-dependent RNA polymerase.

The meeting was wrapped-up by **Luke Yates** (Sussex) who thanked all of the speakers for giving such excellent presentations as well as the generous sponsors and exhibitors. Luke also presented the organisers **Antony Oliver** (Sussex) and **Mark Rowe** (Sussex) with a special reward for their hard work. Luke then invited **Anastasya Shilova** (Bruker) and **Michael Carr** (Bruker) to the stage for presenting the following speaker and poster prizes.

- Best talk: **Michael Beer** (Bristol)
- Runner up: **Rebekah Cooke** (Cardiff)
- Best poster: **Joe Hoff** (Bristol)
- Runner up: **Polina Heatley** (Southampton)
- Special commendations: **Chris Slack** (Cardiff) and **Vishwanath Bhat Kumble** (Sussex).

Just before the meeting closed, Luke emphasised that, as evidenced by the strength and volume of the work presented at the meeting, there clearly remains a role for structural biology in the post-AlphaFold era. Luke also encouraged everyone to attend the 2026 SWSBC which Cardiff have very kindly offered to host next year.

Jon Cooper, UCL

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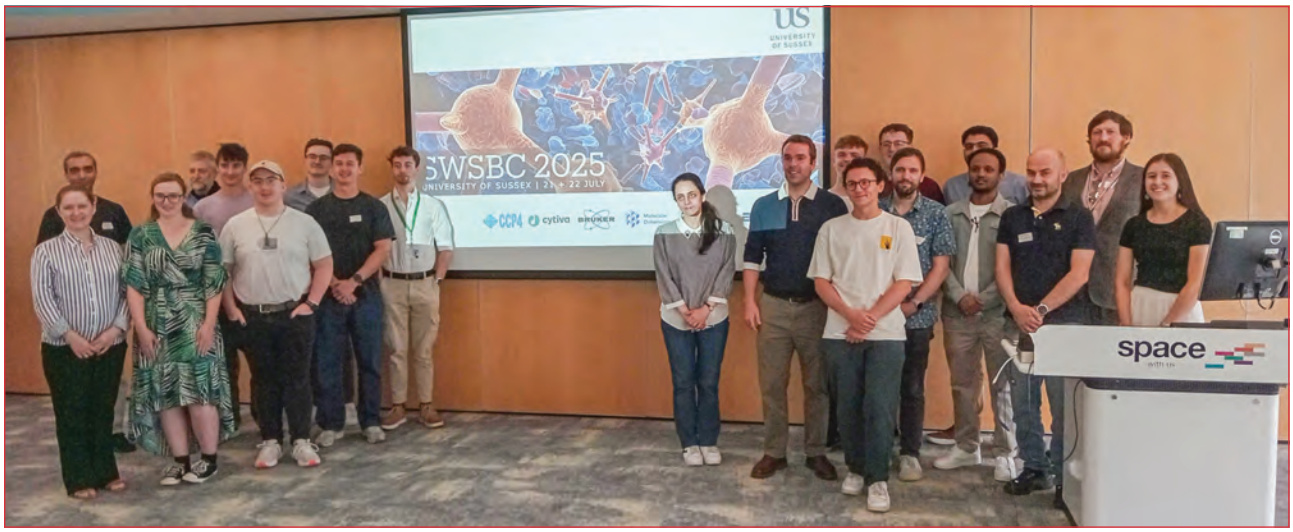
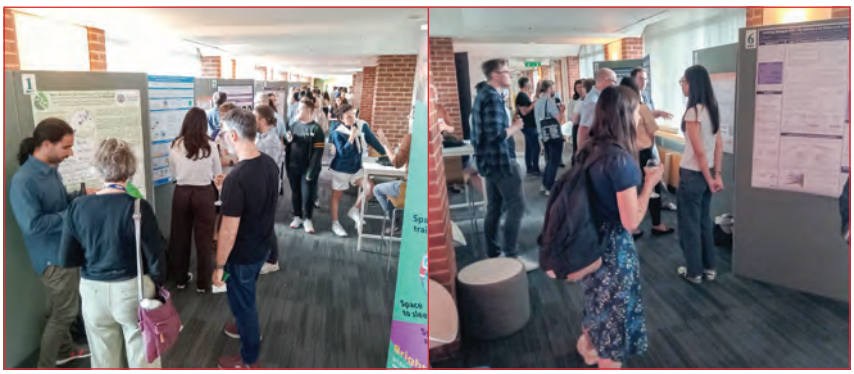


Speakers at the SWSBC, Sussex, 21st-22nd July 2025.

***Eamonn Reading** (Southampton) speaking on "The backbone of multidrug efflux within RND-type pumps."*



Intense poster judging in progress.

A relatively peaceful moment for the exhibitors at the SWSBC.

Winners of the speaker and poster prizes which were kindly sponsored by Bruker.

Kathleen Lonsdale Public Lecture

ON 10th September 2025, as part of the Royal Institution (Ri) and Royal Society of Chemistry (RSC) bicentennial celebrations of Michael Faraday's discovery of benzene, the University of Leeds School of Chemistry hosted a public lecture. The event was held to commemorate the two centuries since the discovery of benzene and, particularly to discuss the pioneering work of Dame Kathleen Lonsdale; who a century later definitively established its planar structure. The day brought together a diverse audience, including students, academics, and even members of Kathleen Lonsdale's family. The series of talks offered both historical insights into Lonsdale's work and a showcase of the current state of crystallography and structural science.

The event commenced with a welcome address by **Colin Fishwick** (Leeds), who provided a historical overview of the notable structural work carried out at Leeds, initially by the Braggs and later by Lonsdale and Christopher Ingold, who pioneered the work on benzene's structure. This was followed by an insightful and inspiring introduction to the life of Kathleen Lonsdale by **Jocelyn Bell Burnell** (Oxford). She drew parallels with her own life and Lonsdale's experiences as a woman in science. For instance, Lonsdale attended a local boys' school as the girls' school did not offer maths or science, while Bell Burnell was the sole woman in her undergraduate class. Both Quakers, Lonsdale was a source of inspiration in many ways, and Bell Burnell highlighted her status as an icon of resilience, noting her principled pacifism which led to her imprisonment and subsequent prison reform advocacy.

Following this, presentations by **Briony Yorke** (Leeds) and **Fanny Costa** (Leeds) demonstrated the contemporary relevance of crystallographic techniques. Dr Yorke covered her work on the lens protein crystallin, focusing on how it interacts with antioxidants and its role in the formation of cataracts. She showcased the use of pump-probe experiments to understand protein dynamics and photochemistry across timescales, including transient disulfides recently captured using an XFEL. Dr Costa's discussion on polyamorphism in pharmaceuticals highlighted its critical importance in drug development, noting that different crystal forms of the same compound can have drastically different properties. She explained that this was an underappreciated phenomenon for many years, only gaining real traction with the widely reported recall of Ritonavir due to an unexpected polymorph. Dr Costa explored some open questions regarding amorphous states and the use of pair distribution function analysis to help decipher them.

Arwen Pearson (Hamburg) then provided a concise history of crystallography, tracing its origins from the 1660s through the work of Bravais, Röntgen, and Laue, to the contributions of the Braggs and ultimately, Lonsdale. After constructing a diffractometer with Bragg in London, Lonsdale moved to Leeds and built her own diffractometer on a budget of £150 (the equivalent of approximately £8000 today). Professor Pearson then guided us through Lonsdale's pivotal 1929 paper, detailing how she first calculated the most likely symmetry and diffraction patterns before comparing them to her experimental measurements. She further highlighted what is perhaps Lonsdale's most enduring legacy: her instrumental role in the establishment of the International Union of Crystallography (IUCr) and in standardizing the notation and space groups that are now fundamental to the field. Finally, Arwen looked to the future and asked what might be left to do in the field of macromolecular crystallography. Drawing inspiration from Lonsdale, who wrote that "nowadays X-ray crystallographers . . . study the dynamics of crystals; but only because they must. To the early research workers, as also to the crystallographer-physicist of today, the interest is in the dynamics itself," she showed how a diverse set of approaches, including trapping, time-resolved, and high-resolution techniques, can all be combined to 'see' chemistry as it happens. Lonsdale famously compared crystallographers to Walter de la Mare's wizards in her inaugural UCL lecture, saying they are "a flock of crazy prophets who by staring at a crystal can fill it with more wonders than are herrings in the sea." Arwen rounded off the talk with a peek at some proof-of-concept work applying electric fields to crystals to mimic the potential difference across a membrane receptor.

The event concluded with closing remarks from **Richard Catlow** (UCL), who offered a thoughtful reflection on Lonsdale as an individual. He drew compelling parallels between Lonsdale and Faraday, noting that both were versatile experimentalists driven by deep personal principles. The day's lectures presented a rich array of views, showcasing Lonsdale's pioneering work and its enduring relevance today, both in science and in the collegiate and collaborative nature of crystallography. The event was supported by the Ri, the RSC and the BCA.

Jake Hill, Leeds

Bernal Lecture, Birkbeck

The harvest of an eclectic mind. Alan Mackay and the rewriting of the book of crystallography

THE 2025 Bernal Lecture at Birkbeck, London, was given by John Finney (UCL) on 23rd September. The lecture was opened by the Head of the School of Natural Sciences, Katherine Thompson (Birkbeck) who introduced the Vice Chancellor Sally Wheeler (Birkbeck) to the audience. Sally described how the Bernal lectures are held approximately annually in honour of the pioneering crystallographer John Desmond Bernal FRS (1901-1971) who wrote extensively on science and society as well as the history of science. He was made the chair of crystallography in 1963. Sally mentioned that members of the Bernal and Mackay families were present for the occasion before introducing the main speaker, John Finney, who, like Bernal, studied natural sciences in Cambridge. John then moved to Birkbeck in the mid-1960s to study for a PhD with Bernal in the Department of Crystallography. In 1988 he was seconded to the ISIS neutron and muon source at the Rutherford Appleton Laboratory before becoming Quain Professor of Physics at UCL in 1993.

John began his lecture with a quote from the ancient Greek pre-Socratic philosopher Democritus who wrote on ethics, aesthetics and physics as well as famously conjecturing that "there exists only atoms and empty space." This line was one of Alan Mackay's own favourites. John mentioned how Alan published a Dictionary of Scientific Quotations in 1969 (CRC Press) which has now gone into several editions.

John described how Alan was brought up in Wolverhampton and studied as an undergraduate in Cambridge and as a post-graduate with Prof J. D. Bernal at Birkbeck, starting in 1949. Immediately prior to that he had spent 2 years working as a volunteer on the Bosnia Youth Railway Project in Yugoslavia. His PhD thesis was on the structure of calcium phosphate – a material of great interest in bone structure and repair. Other early studies include silicates and corrosion as well as electron microscopy. His work on establishing phase diagrams of iron oxides and hydroxides was followed by studies of silicate minerals.

A review of Mackay's publications suggests that throughout the 50s and 60s his work falls mainly within the domain of conventional crystallography, including diffractometry and X-ray photography. In subsequent decades there is a significant increase in work on packing of spheres, icosahedra and generalised periodic geometries. During this period he focussed on post-classical aspects of symmetry, antisymmetry, colour groups and antiferromagnetism. He recognised that whilst traditional crystallographic symmetry (as encapsulated for example in the International Tables) is key for X-ray diffraction to work, it cannot easily deal with defects, dislocations, twinning and variable composition of real-world materials.

Mackay's work on 3D polyhedra, most notably the Mackay icosahedron which he published in 1962, represents one of his biggest scientific impacts [1]. In pioneering studies he modelled the close packing of spheres arranged in shells around a single central particle and found that they can be organised into 20 distorted tetrahedra. John emphasised how terms such as Mackay, anti- Mackay, double-Mackay, pseudo-Mackay and Mackay nanoclusters have since arisen and now pepper the entire field. In fact most icosahedra observed in metal clusters and nanoparticles are of the Mackay type [2].

Much of Alan's later work on five-fold symmetry stemmed from the fundamental truth that one cannot tessellate pentagons by strict crystallographic symmetry. However he realised that packing five pentagons around a central one makes a larger pentagon and these can be recursively packed in structures of ever increasing size in a quasi-crystallographic manner. These studies led to a number of pivotal publications and by the very early 1980s an optical diffraction pattern of his pentagonal tiling scheme revealing 10-fold symmetry had been obtained and published in a Russian journal for Boris Vainshtein's 60th birthday [3]. A few years later, Dan Schechtman (Technion, Israel) discovered the icosahedral phase of aluminium-transition metal alloys, thus placing quasi-crystallography on a firm experimental footing. Schechtman received the 2011 Nobel Prize for Chemistry and Mackay the 2010 Buckley Prize of the American Physical Society, along with Dov Levine and Paul Steinhardt.

Alan was elected to the Royal Society in 1988 for this and other work on non-Euclidean crystallography, and for his key work on the crystallographic use of quaternions. John described how Alan saw connections between disparate areas of science and was an ambassador for Bernal's scientific and sociological ideas. His eclectic nature meant that he was always seeking alternative descriptors for phenomena, such as his coining of the novel phrase flexi-crystallography. Alan continued work long into retirement on novel systems such as the periodic minimal surfaces and geometric designs uncovered in ancient art.

Alan was always interested in science and society. A notable reflection of this was his publication of the book "The science of science" in 1964 (Souvenir Press) which was co-edited by Maurice Goldsmith. This book is collection of 15 essays by eminent scientists, including the well-known author C. P. Snow, who reflect on Bernal's own decisively important work "The social function of science" which was published in 1939 (Routledge). Their conclusion was that an astonishing number of Bernal's conclusions, recommendations and prophecies indeed became fact.

John reflected on how Alan often published on esoteric subjects such as his intriguing paper on "The molecular basis of morality" in the journal Philosophy and Social Action in 2005. At Birkbeck Alan ran a small research group which he modelled on Bernal's non-intrusive management style and, as one of the family members confirmed after the lecture,

he kept an open house for scientific visitors from across the globe. Prophetically, Alan always attributed his interest in electron microscopy as a structural technique to its ability to allow one to move away from the crystal lattice. Always non-conformist and mischievous but profoundly workaholic, he was a citizen of science and the world as well as the epitome of the socially and politically conscious scientist.

A recording of the lecture is available at:
https://www.youtube.com/watch?v=EMMnG2Tb4Fs

I am grateful to John Finney for commenting on this article. We think the painting of Alan Mackay which can be seen in the meeting photographs is by Carol Tarn.

Jon Cooper, UCL

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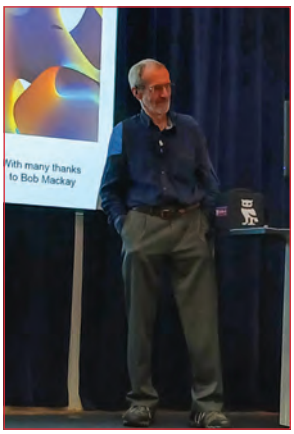
*The 2025 Bernal lecture in honour of the late Alan Mackay FRS (Birkbeck) held at Birkbeck on 23rd September was given by **John Finney** (UCL).*

*Alan Mackay's sons (Bob and Andrew) speaking with **John Finney** (UCL) on the right.*

Members of the Mackay and Bernal families were present.

The above photos were very kindly provided by **Mark Nakasone** (Birkbeck) and are released under creative commons (the most permissive). The following photos were very kindly provided by **Shabir Najmudin** (City St Georges).



*The 2025 Bernal lecturer **John Finney** (UCL).*

More scenes from the post-lecture reception in the Clore Management Centre, Birkbeck.

Nominations Open for the CCDC Chemical Crystallography Prize for Younger Scientists 2026

The Chemical Crystallography Prize for Younger Scientists is sponsored by the Cambridge Crystallographic Data Centre (CCDC) and is awarded by the Chemical Crystallography Group (CCG) of the British Crystallographic Association (BCA) annually to an outstanding early career researcher who has made significant contribution to chemical crystallography and its community.

The call for nominations will be open from Monday 1st December 2025 until 12:00 (GMT) on Friday 30th January 2026.

The award is principally based on original published research within the scientific field of interest of the CCDC and Chemical Crystallography Group of the BCA.

More details, including full eligibility rules and the nomination form, can be found online:
https://ccg.crystallography.org.uk/young-crystallographer-prize/

CCDC Publications 2025

The CCDC team regularly publish the results of their research, often in collaboration with other academic and industrial scientists.

You can explore the full list of our publications on our website. Below are the most recent papers published in 2025.

A survey of crystallographic quality metrics from CIFs in the Cambridge Structural Database. Clare A. Tovee, Seth B. Wiggin, Natalie T. Johnson, Philip I. Andrews and Matthew P. Lightfoot. DOI 10.1107/S2052252525007134

FAIRSpec-ready spectroscopic data collections – advice for researchers, authors, and data managers (IUPAC Technical Report). Mark Archibald, Ian Bruno, Stuart Chalk, Antony N. Davies, Robert M. Hanson, Stefan Kuhn, Robert J. Lancashire and Henry S. Rzepa. DOI 10.1515/pac-2025-0409

Exploring data curation and management in physical sciences: a report from the PSDI roadshow in Cambridge and Southampton. Agnes Jasinska, Ian Bruno, Cian Dingle, Cerys Willoughby and Nicola Knight. DOI 10.5281/zenodo.17078903

Data-driven generation of conformational ensembles and ternary complexes for PROTAC and other chimera systems. Fabio Montisci, Laura Friggeri, Kepa K. Burusco-Goni, Patrick McCabe, Bojana Popovic and Jason C. Cole. DOI 10.1021/acs.jcim.5c00880

Collaborative development and sustainability of digital chemical data standards. Leah McEwen* (Chair), Ian Bruno, Ilia Dorokhov, Richard Hartshorn, Simon Hodson, Carsten Kettner, Sarah Kilz, Oliver Koepler, Steffen Neuman, Wendy Patterson, John Rumble and Dana Vanderwall. DOI 10.1021/acs.jcim.5c00880

Advances in structural science: education, outreach and research applications. Charles Bou-Nader, Jamaine Davis, Louise N. Dawe, David S. Goodsell, James Kaduk, Bart Kahr, Helen Maynard-Casely, Brandon Q. Mercado, Beata E. Mierzwa, Olayinka Olatunji-Ojo, Allen Oliver, Christine Zardecki, and Shao- Liang Zheng. DOI 10.1063/4.0000304

Progress in the understanding of traditional and nontraditional molecular interactions. Robin Taylor and Jason C. Cole. DOI 10.1016/B978-0-443-29808-0.00013-3

Prediction of enzyme inhibition (IC_{50}) using a combination of protein-ligand docking and semiempirical quantum mechanics. Robert C. Glen, Jason C. Cole and James J. P. Stewart. DOI 10.1007/s00894-025-06423-7

Recent computational advances in the identification of cryptic binding sites for drug discovery. Dorota Gašparíková, Rupesh Chikhale, Jason Cole and Ehmke Pohl. DOI 10.1093/bioadv/vbaf156

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Combining experiment and prediction to explore surface chemistry and dissolution. Andrew G. P. Maloney. DOI 10.1107/S2052252525001782

CSD Communications 2025

CSD Communications is a way to share small molecule crystal structures directly in the Cambridge Structural Database (CSD) without requiring an associated scientific publication.

Each entry includes author and crystallographer details, an ISSN, and a full CCDC citation with DOI and publication year, ensuring proper credit for data contributors.

The goal is to expand public access to crystallographic data. Around 5,000 structures are shared annually that might otherwise remain unpublished. Previously known as Private Communications, CSD Communications helps make valuable scientific data widely available.

It's a community-driven effort, with datasets contributed by researchers from around the world. Check out how the CSD has grown over the years.

Explore structures published as CSD Communications in our online access structures service by searching Journal = CSD Communications.

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New Training and Learning Resources Launched in 2025

New Videos

- **How To: Use Cambridge Structural Database Subsets**

  In this 5-minute video, you will learn about the different CSD subsets available, how to view and search them in ConQuest and how to access them in Mercury. You can also find out about CSD classifiers as a complementary way to uncover entries belonging to different chemical classes.

- **How to: Use Filters and Selections in Mercury for CSD Data Analysis**

  Learn how to select and filter data in Mercury's Data Analysis module, using results from ConQuest searches. You'll learn how to apply numerical and text filters to explore and save datasets. These tools are useful for crystallographers, chemists and materials scientists working with complex data and can also support teaching core chemistry concepts.

- **How to: Search Scientific Literature with the Cambridge Structural Database (CSD)**

  With this tutorial, you'll learn how to search using WebCSD and download data, making it ideal for enhancing literature reviews and research. It's a great starting point for students and researchers looking to explore, contextualise results and support scientific writing.

- **How to: Build and combine searches in ConQuest**

  This video tutorial shows you how to create different query types (Substructure and Elements) and combine them in a single search in ConQuest. You can also see how to view search results and information, how to export results and how to save search sessions.

- **How to: Search and visualize 3D structural data using WebCSD**

  Explore, search and view 3D structures in WebCSD. Watch this tutorial to learn how to draw substructure queries, set 3D constraints like distances and angles and explore structural data using built-in tools.

Self-guided Workshop

- **Analysing the Molecular Geometry of Disordered Structures using Mogul and the CSD Python API (MOG-003)**

  Explore molecular geometry with Mogul in our new self-guided workshop! You will learn how to assess disordered structures using the Mogul Geometry Check in Mercury and the CSD Python API. It's a practical way to deepen your understanding of 3D disorder data in over 300,000 CSD entries.

CSD60 Frontier Panel Webinars – Watch On Demand

This year, we hosted four panel webinars to celebrate the 60th anniversary of the CCDC and the Cambridge Structural Database (CSD). Each session brought together experts from our community to explore key themes: Data, Education, Drug Discovery and Metal-Organic Frameworks (MOFs).

Together, they reflected on progress made in these areas and shared inspiring insights into the many opportunities still ahead for the scientific community.

All webinars are available to watch on demand.

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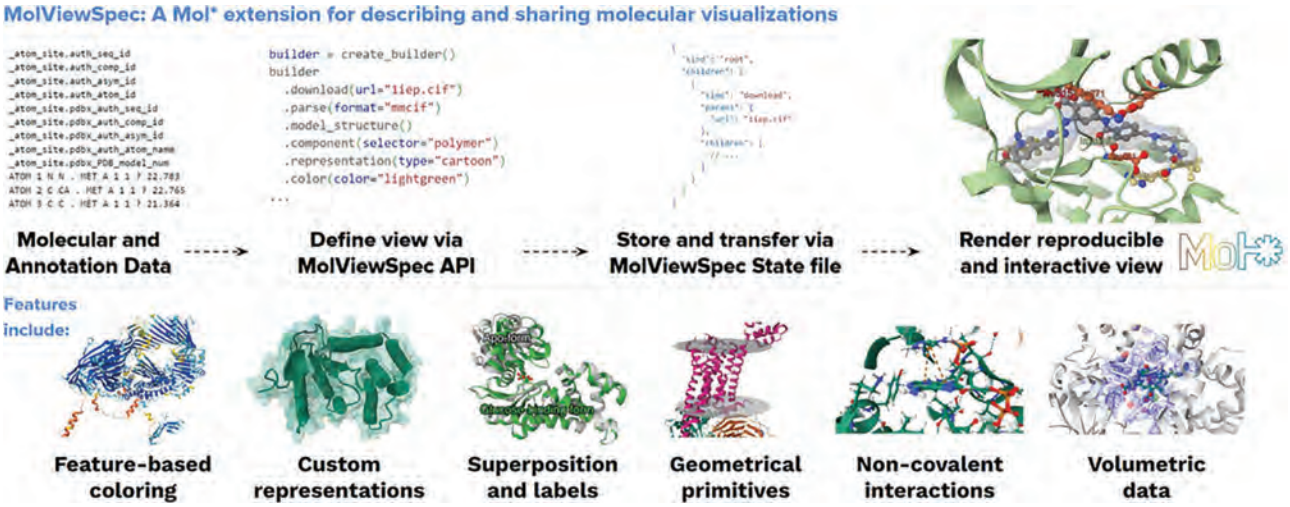
News from the wwPDB

MolViewSpec: describe, share, and reproduce Mol* molecular scenes



MolViewSpec is a new Mol* extension to create molecular scenes that allows users to:

- Describe molecular scenes. What to load (structures, maps, annotations) and how to show it (representations, colours, labels, measurements, custom 3D shapes…). You can mix data types (structural, volumetric, annotations) in one scene with consistent styling.
- Share. To use the scenes, simply open the spec in Mol* in the browser or use the standalone Python package for scripted workflows.
- Reproduce. Scenes make visuals reproducible across browsers, collaborators and notebooks. No more "how did you make that figure?"
- Automate figure creation and analysis by generating specs from Python pipelines.

Learn more and try examples at **molstar.org**

Read more: "MolViewSpec: a Mol* extension for describing and sharing molecular visualizations." Adam Midlik, Sebastian Bittrich, Jennifer R Fleming, Sreenath Nair, Sameer Velankar, Stephen K Burley, Jasmine Y Young, Brinda Vallat & David Sehnal. (2025). *Nucl. Acids Res.* **53**, W408–W414 10.1093/nar/gkaf370

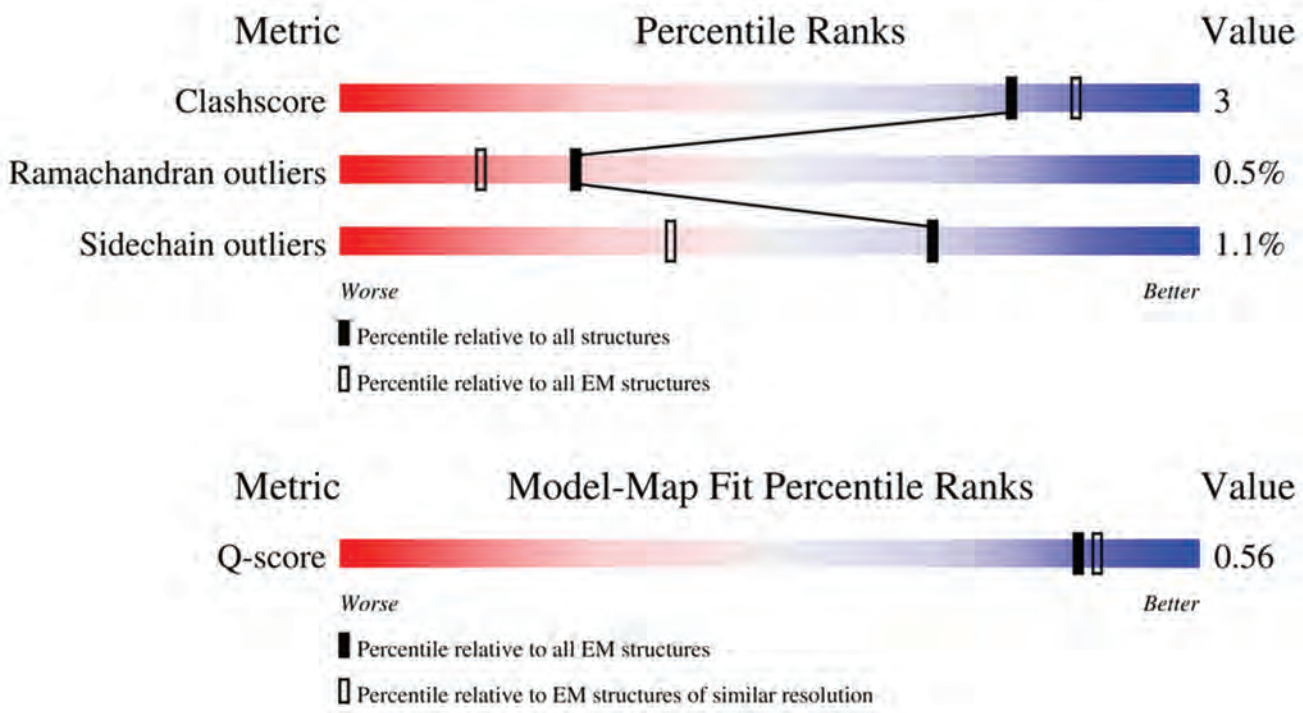
Introducing the first 3DEM model-map percentile slider to the wwPDB validation report

The wwPDB is continuing to improve and expand our validation offerings with a new addition to the wwPDB - PDF validation reports. Building on the success of the coordinate -model percentile sliders, which help depositors, reviewers and archive users assess PDB model quality in the context of the PDB archive, we are now extending this section to include a Q-score percentile slider. The new slider is the first to empower users of this report to assess model-map quality at a glance relative to the EMDB/PDB archives.

Starting October 01, newly released 3DEM entries will include the Q-score percentile slider in its own section below the current sliders under "Overall quality at a glance." The slider compares an entry's average Q-score against both the entire EMDB/PDB archive and a resolution-similar subset. Because Q-score correlates strongly with resolution between 1–10 Å, the percentile helps check whether a reported global resolution is reasonable; unusually low values can flag model–map fit or map quality issues. A dedicated Q-score section supports deeper review with residue-level mapping to the coordinate model and per-chain tables.

In the near future, wwPDB will re-generate validation reports with Q-score slider for all existing entries in the PDB archive.

We are excited for our users to get their hands on this new validation metric. If you have any queries or feedback please let us know at **info@wwpdb.org**.



3DEM Model-Map percentile slider from the wwPDB validation report

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Book review

"Mathematics for Biosciences: From Theory to Worked Examples and Applications" by Elspeth F. Garman and Nicola Laurieri. (2025). World Scientific Publishing Europe Ltd., 426 pp.

I always feel a bit of trepidation when asked to review a book written by someone I know. I have had some real clunkers come across my desk. The fact that I am writing this review should tell you: Mathematics for Biosciences is a good book. Being an American, some of the British colloquialisms required some thinking on my part. For example, I learned to "solve for y" rather than "make y the subject of the equation."

The book is divided into nine chapters covering basic tools, basic algebra, graphs, basic functions, differentiation, exponential and log functions, trigonometric functions and complex numbers, integration and differential equations. Each chapter has a brief introduction, a clear explanation of the topic, numerous real-world examples from biology, biochemistry, chemistry and medicine. Finally, exercises reinforce the subject matter. At the end of each chapter, there is an answer key. Each chapter is well written and sufficiently detailed for an advanced high school or college student to grasp. Differential equations were my bane as a second-year student, and the authors did a great job of simplifying a complex subject into a single, accessible chapter. The book effectively integrates the basic concepts of mathematics and the sciences, a feature often overlooked in general math texts.

There is one deficiency, especially given the nature of bioscience: a chapter on statistics. I hope the second edition will address this area. Despite this, Mathematics for Biosciences is an accessible, well-structured resource that I would confidently recommend to students and instructors alike.

Joseph D. Ferrara, Rigaku

This book is aimed at first year undergraduates in Biochemistry, Biology, Chemistry or Medicine, (the content well summarised by the diagram on the cover). Mathematical topics are presented in a logical order to build on one another through the book, presumably the same order as introduced in the Maths course taken by first year Biochemistry students at Oxford, the teaching materials for which were the starting point for the book.

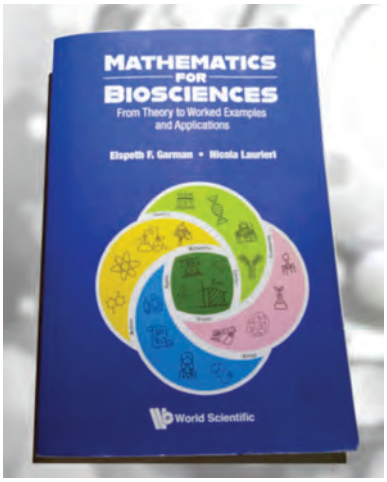
Many mathematical tools that undergraduate Bioscientists will find valuable in their future study are covered, from basic algebra, graphs and functions through to calculus, not surprisingly with a focus on Biochemical interests such as kinetics in the examples. One omission appears to be treatment of vectors, although complex numbers do appear in the trigonometry chapter.

The chapters on each topic are well structured, with each new mathematical concept stated, then demonstrated in an example with a worked solution. The chapters also contain a sprinkling of examples of how the mathematical concept might be used in the Biosciences. These enable the student to see how the mathematical technique can be used in interpreting data to which they can relate. Each chapter ends with a good number of example questions, with answers, which would be useful for staff delivering such a course, less so for a student working through the book as they are not worked solutions.

Each chapter starts with a preamble, written in approachable language, explaining how the concepts covered in the chapter can be used in science. However following these first few paragraphs, the language is dry, mathematically precise, using terminology which although correct, is likely to be off-putting for the target audience. The impression that these sections are written by a mathematician is rather reinforced by the explanation of the use of a microscope in chapter 1, which is knowledge that could be assumed in the target audience. By contrast, the language of the examples is more like that of the preamble, interesting and relevant to a first year bioscientist with some chemistry training. The language is the main hurdle to accessibility for the target audience of this book.

Although well written for a mathematically-interested reader, for those that are Maths-averse, for instance those who decided against post-16 study in mathematics, the formal use of mathematical terms will mean that this book is not readily perused. However, although it is not suitable as a stand-alone training for most diverse cohorts of 1st year undergraduate bioscientists it could be an excellent textbook for use alongside a course where these mathematical processes are taught to the class where this serves as the reference text. For students with post-16 qualifications in mathematics, also for postgraduate students or postdoctoral researchers, who are interested in revising their mathematics, this book will prove an approachable refresher of these fundamental mathematical concepts.

Susan Crennell, Bath

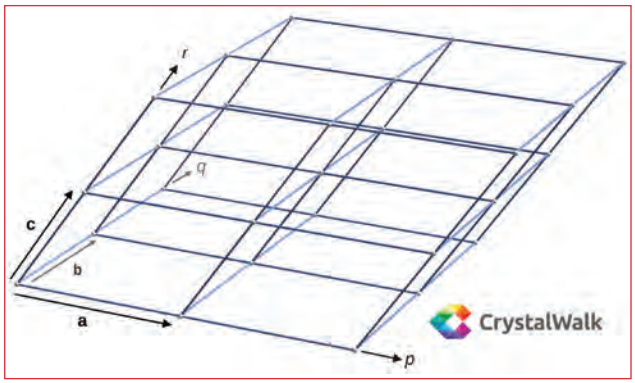


"Mathematics for Biosciences: From Theory to Worked Examples and Applications" is by Elspeth F. Garman and Nicola Laurieri. (2025). World Scientific.

A crystallography revision card

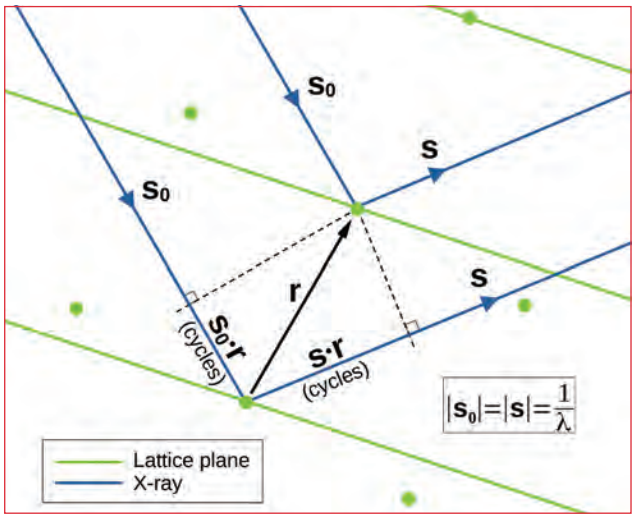
I recently started reading "The determination of Crystal Structures" by H. Lipson and W. Cochran (Bell, 3rd ed. 1966) which is the third volume of a series edited by Lawrence Bragg entitled "The Crystalline State." I decided to write some notes for my own use and then thought they might be useful revision for members! So here they are. The only prerequisites for understanding this article are a basic understanding of the dot and cross products of vectors, complex numbers and complex exponentials.

Assume a lattice of point scatterers having indices (p, q, r) and unit cell vectors **a**, **b** and **c**. The position vector of any lattice point is given by the equation $\mathbf{r}= p\,\mathbf{a} + q\,\mathbf{b} + r\,\mathbf{c}$, noting importantly that the symbol for the position vector **r** is distinct from that of the lattice index r.



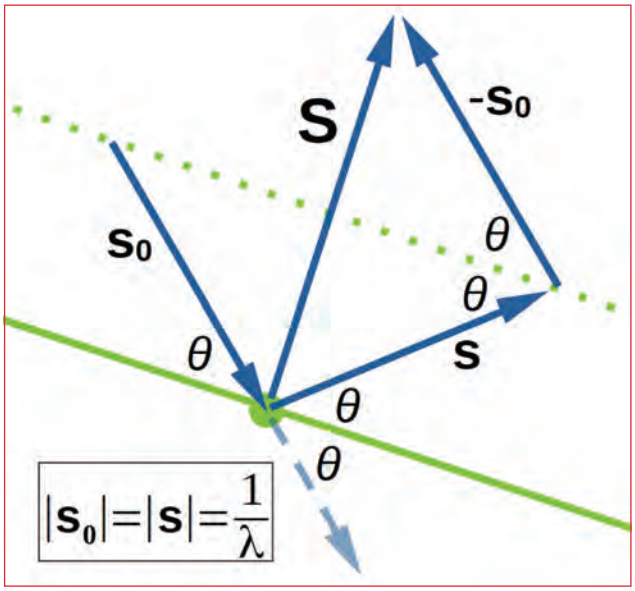
The incident and scattered wave vectors ($\mathbf{s_0}$ and **s**, respectively) obey $|\mathbf{s_0}|=|\mathbf{s}|=1/\lambda$

The path difference between the waves scattered by points separated by vector **r** is $\lambda(\mathbf{s}\cdot\mathbf{r}-\mathbf{s_0}\cdot\mathbf{r})=\lambda(\mathbf{S}\cdot\mathbf{r})$ where the scattering vector $\mathbf{S}=\mathbf{s}-\mathbf{s_0}$ and the phase difference is $\mathbf{S}\cdot\mathbf{r}$ cycles.



In the example shown above, since $\mathbf{s_0}\cdot\mathbf{r}$ is negative, $\mathbf{s}\cdot\mathbf{r}-\mathbf{s_0}\cdot\mathbf{r}$ can be seen to be the total number of wavelengths by which the two scattered waves differ in phase. Lipson and Cochran also point out that "**s** is not necessarily in the same plane as $\mathbf{s_0}$ and **r**" but the scattering vector **S** will be coplanar with **s** and $\mathbf{s_0}$. In fact it is perpendicular to the group of parallel planes which are said to be reflecting the X-rays and it bisects the angle between **s** and $\mathbf{s_0}$.

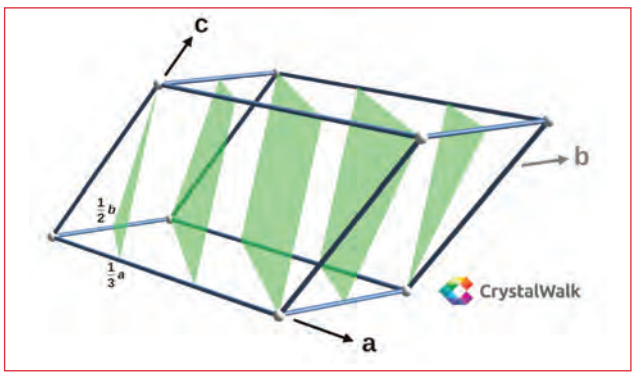
In the following diagram, from basic trigonometry we see that $|\mathbf{S}|=(2\sin\theta)/\lambda$ and from Bragg's law ($\lambda=2d\sin\theta$) it follows that $|\mathbf{S}|=\frac{1}{d}$ where d is the inter-planar spacing. Note also that the diffracted beam is at an angle of 2θ from the incident beam direction, where θ is the angle of incidence or reflection with respect to the reflecting plane.



For constructive interference to occur $\mathbf{S}\cdot\mathbf{r}$ must be an integer and for any point in the real lattice the following $\mathbf{S}\cdot(p\,\mathbf{a}+q\,\mathbf{b}+r\,\mathbf{c})$ must be an integral number. Since p, q and r are all integers, for $\mathbf{S}\cdot\mathbf{r}$ to be integral, then considering the axial lattice points like (p, 0, 0), (0, q, 0) and (0, 0, r) allows us to see that the individual dot products $\mathbf{S}\cdot\mathbf{a}$, $\mathbf{S}\cdot\mathbf{b}$ and $\mathbf{S}\cdot\mathbf{c}$ must also be integral. Hence:

$\mathbf{S}\cdot\mathbf{a}=h$, $\mathbf{S}\cdot\mathbf{b}=k$ and $\mathbf{S}\cdot\mathbf{c}=l$

where h, k and l are integers that correspond to families of lattice planes (h, k, l). These are known as the Laue equations.



This figure shows an example of the (3, 2, 1) family of lattice planes i.e. $h=3$, $k=2$, $l=1$. The plane closest to the origin (far left) cuts **a** at ⅓ of its length, **b** at ½ of its length and **c** at its extremity.

The Laue equations can be used to confirm that **S** is perpendicular to the family of lattice planes (*h*, *k*, *l*). Rearranging them gives:

$$\mathbf{S}\cdot\left(\frac{\mathbf{a}}{h}\right)=1,\ \mathbf{S}\cdot\left(\frac{\mathbf{b}}{k}\right)=1 \text{ and } \mathbf{S}\cdot\left(\frac{\mathbf{c}}{l}\right)=1$$

and subtracting them in pairs gives: =0

$$\mathbf{S}\cdot\left(\frac{\mathbf{a}}{h}-\frac{\mathbf{b}}{k}\right)=0,\ \mathbf{S}\cdot\left(\frac{\mathbf{a}}{h}-\frac{\mathbf{c}}{l}\right)=0 \text{ and } \mathbf{S}\cdot\left(\frac{\mathbf{b}}{k}-\frac{\mathbf{c}}{l}\right)=0$$

The resultant vectors given by the bracketed terms all lie in the zeroth layer of the family of lattice planes (*h*, *k*, *l*) and for the dot products to be zero, **S** must be perpendicular to this plane. This is important in view of the rearranged form of the Laue equations e.g. the first one.

$$\mathbf{S}\cdot\left(\frac{\mathbf{a}}{h}\right)=1$$

Since **S** is normal to the (*h*, *k*, *l*) plane, we know that the projection of (**a**/*h*) onto **S** is the inter-planar distance d_{hkl}, and the same is true for the projections of (**b**/*k*) and (**c**/*l*) onto **S**. Therefore:

$$|\mathbf{S}|=\frac{1}{d_{hkl}}$$

The first Laue equation (**S**·**a**=*h*) also means that the tip of the **S** vector can only lie in evenly-spaced planes which are perpendicular to **a**. The other two equations mean that allowed **S** vectors must also have their tips in groups of planes perpendicular to **b** and **c**. This leads to the concept of the reciprocal lattice since the allowed values of **S** occur only at points where the three groups of planes intersect. The reciprocal lattice is defined by vectors **a***, **b*** and **c*** with the points being indexed by *h*, *k* and *l*.

$$\mathbf{S}=h\,\mathbf{a}^*+k\,\mathbf{b}^*+l\,\mathbf{c}^*$$

X-rays reflected by the family of planes containing **b** and **c** will have their scattering vector **S** perpendicular to this group of planes, for which *k* and *l* are zero. In this case **S** will be parallel with the reciprocal lattice vector **a*** and for the first order reflection (*h*=1) **S**=**a***. It follows from the Laue equations that **a***·**a**=1 and since **a*** is perpendicular to **b** and **c** we see that **a***·**b**=0 and **a***·**c**=0. In summary for all of the reciprocal lattice vectors we may state:

a*·**a**=1	**a***·**b**=0	**a***·**c**=0
b*·**a**=0	**b***·**b**=1	**b***·**c**=0
c*·**a**=0	**c***·**b**=0	**c***·**c**=1

Since **a*** is perpendicular to **b** and **c**, and by definition similar relationships must exist for the other reciprocal lattice vectors **b*** and **c***, we can say:

$$\mathbf{a}^*=\zeta\,(\mathbf{b}\wedge\mathbf{c}),\ \mathbf{b}^*=\phi\,(\mathbf{c}\wedge\mathbf{a}) \text{ and } \mathbf{c}^*=\psi(\mathbf{a}\wedge\mathbf{b})$$

where ζ, ϕ and ψ are constants to be determined. Substituting into $\mathbf{S}=h\,\mathbf{a}^*+k\,\mathbf{b}^*+l\,\mathbf{c}^*$ gives:

$$\mathbf{S}=h\zeta\,(\mathbf{b}\wedge\mathbf{c})+k\,\phi\,(\mathbf{c}\wedge\mathbf{a})+l\,\psi(\mathbf{a}\wedge\mathbf{b})$$

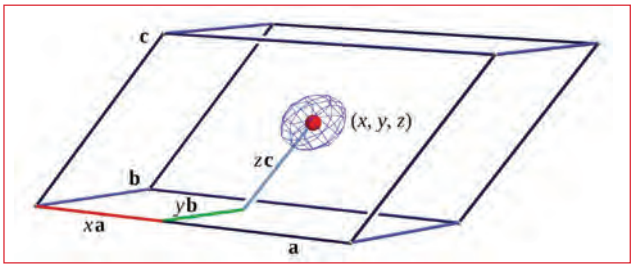
and use of the first Laue equation gives us:

$$\mathbf{S}\cdot\mathbf{a}=h\,\zeta\,(\mathbf{a}\cdot\mathbf{b}\wedge\mathbf{c})+k\,\phi\,(\mathbf{a}\cdot\mathbf{c}\wedge\mathbf{a})+l\,\psi(\,\mathbf{a}\cdot\mathbf{a}\wedge\mathbf{b})=h$$

Since **a**·**c**∧**a** and **a**·**a**∧**b** are by definition zero, we have $h\zeta\,(\mathbf{a}\cdot\mathbf{b}\wedge\mathbf{c})=h$ or $\zeta\,(\mathbf{a}\cdot\mathbf{b}\wedge\mathbf{c}\,)=1$ and since **a**·**b**∧**c** is the volume of the unit cell (*V*) we arrive at $\zeta=1/V$. Similarly for the second and third Laue equations we arrive at the same answer for ϕ and ψ . Hence:

$$\mathbf{a}^*=\left(\frac{1}{V}\right)\mathbf{b}\wedge\mathbf{c},\ \mathbf{b}^*=\left(\frac{1}{V}\right)\mathbf{c}\wedge\mathbf{a} \text{ and } \mathbf{c}^*=\left(\frac{1}{V}\right)\mathbf{a}\wedge\mathbf{b}$$

The position vector of the n^{th} atom in the unit cell $\mathbf{r}_n$ is given by the equation $\mathbf{r}_n=x_n\,\mathbf{a}+y_n\,\mathbf{b}+z_n\,\mathbf{c}$ where x_n, y_n and z_n are fractional axial coordinates, as indicated for a single atom below. The phase of a wave scattered by this atom relative to one on the origin (lower left corner) is $\mathbf{S}\cdot\mathbf{r}_n=x_n\,\mathbf{S}\cdot\mathbf{a}+y_n\,\mathbf{S}\cdot\mathbf{b}+z_n\,\mathbf{S}\cdot\mathbf{c}$ which reduces to $h\,x_n+k\,y_n+l\,z_n$ following substitution of the Laue equations.



The X-ray scattering ability of an atom, referred to as the scattering factor *f,* is directly proportional to its atomic number at a given θ angle and is expressed relative to that of a single electron. Since each atom in the unit cell contributes a scattered wave with a phase of $h\,x_n+k\,y_n+l\,z_n$ relative to the origin of the unit cell, the combined scattering effect, or structure factor F_{hkl}, is given by the sum of the wave equations for each atom:

$$F_{hkl}=\sum_n f_n \exp(2\,\pi\,i\,(h\,x_n+k\,y_n+l\,z_n))$$

Even in perfect crystals, atoms are not point scatterers due to the finite size of the electron cloud and thermal motion. Instead they are better represented by a continuous electron density function $\rho(x, y, z)$ which can be contoured in 3D, as shown by the pale blue mesh in the above figure. The equation for F_{hkl} can be expressed in terms of $\rho(x, y, z)$ by integrating it over the whole unit cell volume (*V*).

$$F_{hkl}=V\iiint_{x\,y\,z}\rho(x, y, z)\exp(2\pi i(hx+k\,y+lz))dx\,dy\,dz$$

This equation can be rearranged by a Fourier transform that, in principle, allows the electron density distribution to be calculated from the structure factors.

$$\rho(x, y, z)=\frac{1}{V}\sum_h\sum_k\sum_l F_{hkl}exp(-2\,\pi\,i\,(hx+k\,y+l\,z))$$

The transform is named after Joseph Fourier (1768-1830) whose work on trigonometric series was based on earlier studies of waves in vibrating strings by Euler, Bernoulli, d'Alembert and Lagrange [1, 2]. However, it took mathematicians the best part of a century to prove it rigorously, so that is not something we will try here!

Name some of the many other things that have been left out of this article.

Jon Cooper, UCL

Unit cell figures were prepared with the Crystal Walk website: https://crystalwalk.herokuapp.com/.

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[2] Wayne, R. P. (1987). Fourier transformed. *Chemistry in Britain* **23**, 440-446.

Down Memory Lane

Processing precession

THE precession camera was an ingenious device which allowed an undistorted photograph of the reciprocal lattice of a crystal to be recorded. The design was originally conceived by Martin J. Buerger (1903-1986) around 1940 and is described in detail in his book entitled "The precession method in X-ray crystallography" (Wiley, 1964). The camera provided a way of measuring precise lattice parameters, determining the symmetry of the crystal, quantitatively measuring diffraction intensities and, for many protein crystallography PhD students and post-docs, a means of screening for heavy atom derivatives. Indeed many such folk dedicated significant chunks of their lives to using these instruments.

The crystal had to be pre-aligned with one major axis precisely parallel with the beam and usually one of the other principal axes parallel to the rotation axis. This entailed taking a number of alignment shots, both still and low-angle precession, the result being that much time was spent in the dark room processing your precession photographs. At Birkbeck, for example, a range of precession camera models from different manufacturers were available, some considerably more sophisticated in appearance than others, so you chose your camera carefully! Of course, these instruments became obsolete with the advent of area detectors which allowed data to be collected from randomly oriented crystals, indexed, integrated and any heavy atom sites located in downstream processing.

In the precession method the crystal rotates slowly around an axis much like the wobbling of a spinning top, although the axis of precession is horizontal rather than vertical. The device is engineered so that the orientation of the X-ray film changes continuously to follow the movement of the crystal precisely. One complication is that to photograph individual layers of the reciprocal lattice requires the use of an annular metal screen and this too has to follow the rotation of the crystal. Unlike the Weissenberg method which uses a cylindrical X-ray film that completely surrounds the crystal, the precession camera uses a flat piece of film, typically 10 cm from the crystal. This does restrict the resolution of the data which can be obtained by precession photography but, since the diffraction spots are relatively far apart, this method can be used on crystals which have large unit cells - hence it became the protein crystallographer's firm favourite.

Planetary precession, also known as axial precession, refers to the slow change in orientation of a planet's rotation axis. For example, the north star Polaris now coincides approximately with the earth's rotation axis, but this axis itself will turn around in a circle, much like the rotation axis of a spinning top or gyroscope as it wobbles slightly. The earth will continue rotating on its axis once every 24 hours but very, very slowly the axis itself rotates and other stars will take it in turn to be 'The North Star' until around 26,000 years from now when Polaris will return again to its pride of place. This rate of precession is equivalent to about 1 degree of rotation every 72 years as the earth's polar axis slowly moves in a circle of about 23 degrees angular radius [1]. Yes, this does impact the climate but that is outside our remit here.

Nuclear precession, also known as Larmor precession, refers to the rotation of the magnetic moment of an particle in an applied magnetic field. The angular frequency of the precessing nucleus is referred to as the Larmor frequency and this is independent of the angle between the applied field and the dipole moment of the nucleus [1]. It is a very important concept in the application of nuclear magnetic resonance (and electron spin resonance) in structural chemistry and biochemistry since the resonance frequency of each NMR-active nucleus depends on its chemical environment.

Oak processionary moth has nothing to do with precession apart from the fact that the creature is very commonly misspelt as such. Processionary moths are so called because the larvae form a long nose-to-tail procession following a single leader, the purpose of which is probably to find new sources of food and/or somewhere for the larvae to pupate safely [1]. They cause significant damage to trees and are covered with a large number of long fragile bristles which become airborne, causing dermatitis and asthma. In the UK, the oak processionary moth has become a significant concern and the Forestry Commission requests that all sightings of the larvae be reported to them for eradication.

In Southern Europe it is the pine processionary moth which poses a greater threat because there the oak moth has a number of effective natural predators which do not exist in the UK. The pine moth larvae progress in single file whereas the oak moth larvae line up side-by-side in rows in their processions.

The harmful effect of the bristles was originally attributed to a protein called thaumetopoein but recent work using proteomics and transcriptomics of the bristles (setae) along with AlphaFold modelling suggests that the situation is considerably more complex with a large number of enzymes and inhibitors being involved [2, 3].

Jon Cooper, UCL

References

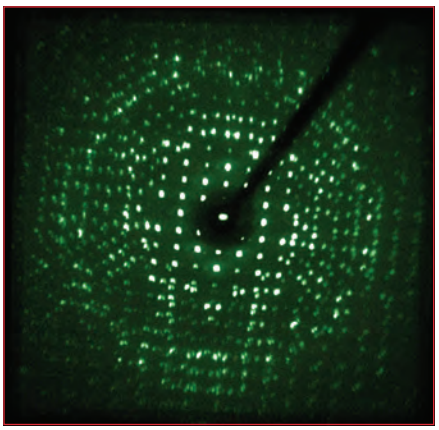
[1] Wikipedia, the free encyclopedia.

[2] Seldeslachts, A., Maurstad, M. F., Øyen, J. P., Undheim, E. A. B., Peigneur, S., & Tytgat, J. (2024). Exploring oak processionary caterpillar induced lepidopterism (Part 1): unveiling molecular insights through transcriptomics and proteomics. *Cell. Molec. Life Sci.* **81**, 311. https://doi.org/10.1007/s00018-024-05330-z

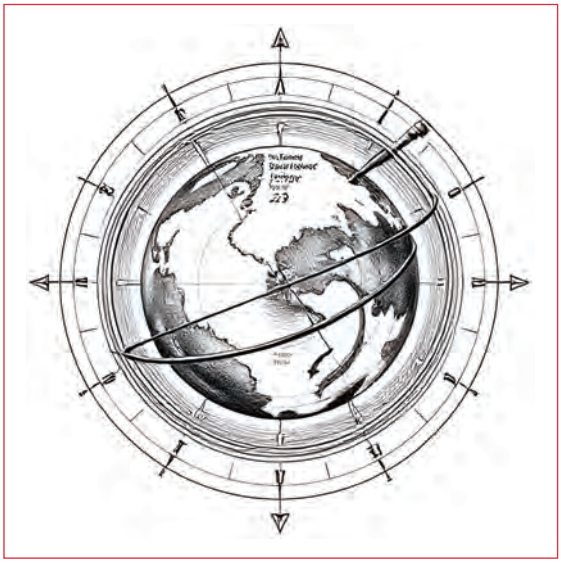
[3] Seldeslachts, A., Undheim, E. A. B., Vriens, J., Tytgat, J., & Peigneur, S. (2024). Exploring oak processionary caterpillar induced lepidopterism (part 2): ex vivo bio-assays unmask the role of TRPV1. *Cell. Molec. Life Sci*. **81**, 281. https://doi.org/10.1007/s00018-024-05318-9

A historic X-ray precession camera. Thankfully the majority of workers who used these devices would have had the good fortune of using a more modern instrument. This photograph was very kindly provided by **John Lisgarten** (London).

The editor's firm favourite was the Huber precession camera, mainly due to its simplicity and reliability. Note the annular metal screen in front of the black film cassette which, if set correctly, ensures that only one layer of the reciprocal lattice is recorded. This photograph was very kindly provided by **Wolfgang Donner** (Darmstadt). The instrument shown has a silver X-ray tube (λ = 0.56 Å) and a graphite monochromator, the film of old being replaced by a modern image plate. This precession camera is used both for educational purposes and for overview scans of diffuse scattering.



Another picture very kindly provided by **Wolfgang Donner** (Darmstadt) showing a precession photograph of rock candy from which students are required to derive the metric of the unit cell of sucrose.



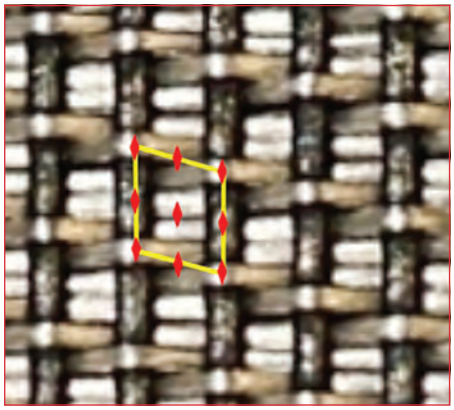
A surreal, AI-generated impression of planetary precession (deepai.org).

The oak processionary moth (*Thaumetopoea processionea*). This image is adapted very slightly from one on Wikipedia (the free encyclopedia) and is available under a Creative Commons Attribution-Share Alike 3.0 Unported license.

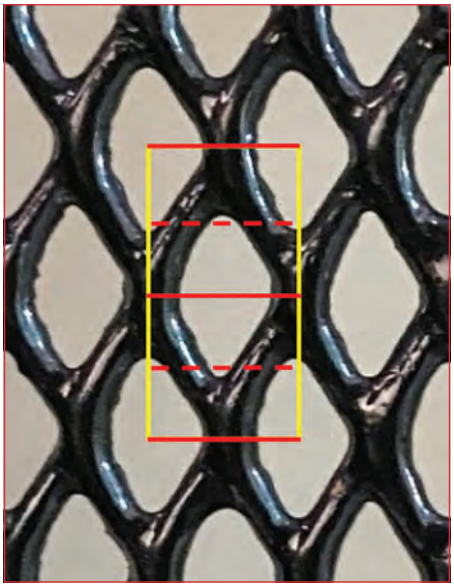
Puzzle Corner

IN the last issue we had a selection of photographs by John Lisgarten (London) for members to attempt to identify their plane group symmetry. I have had a stab at producing some answers which are below. All of them are based on the plane groups in the International Tables for X-ray Crystallography (3rd edition, IUCr, 1969).

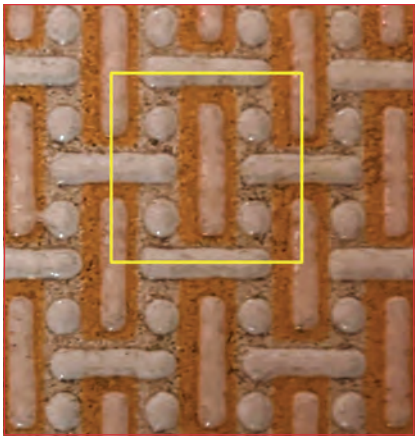
(a) I think this one is *p*2. It is not a perfect match but given that this is a woven pattern that appears to be made with metal strips which presumably can bend a bit and seem to have a different colour depending on the angle from which we look at them, *p*2 is my best bet. This is how the pattern looks after using lunapic.com to remove some of the perspective effect and I have drawn on a *p*2 cell. It is probable that layer groups come into this but that is something I have not graduated to yet.



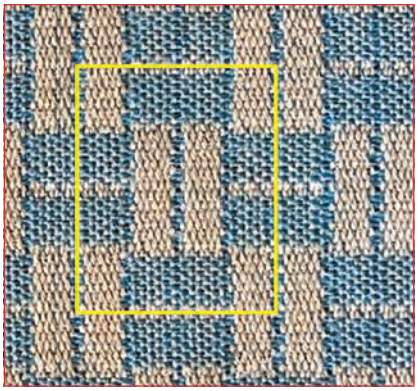
(b) After removing some perspective again I think this one is oblique *p*1.



(c) I think this one is *cm* and I have marked the mirror and glide lines in red, the glide lines being dashed.

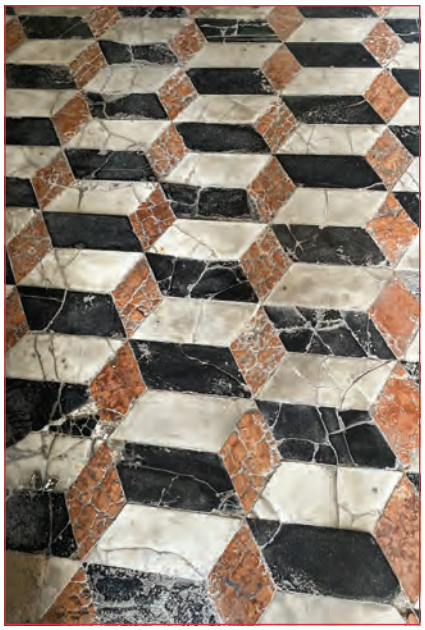


(d) I am pretty sure this is *pmm* with mirror lines along the cell edges and running horizontally and vertically through the middle of the cell (which I have not drawn).

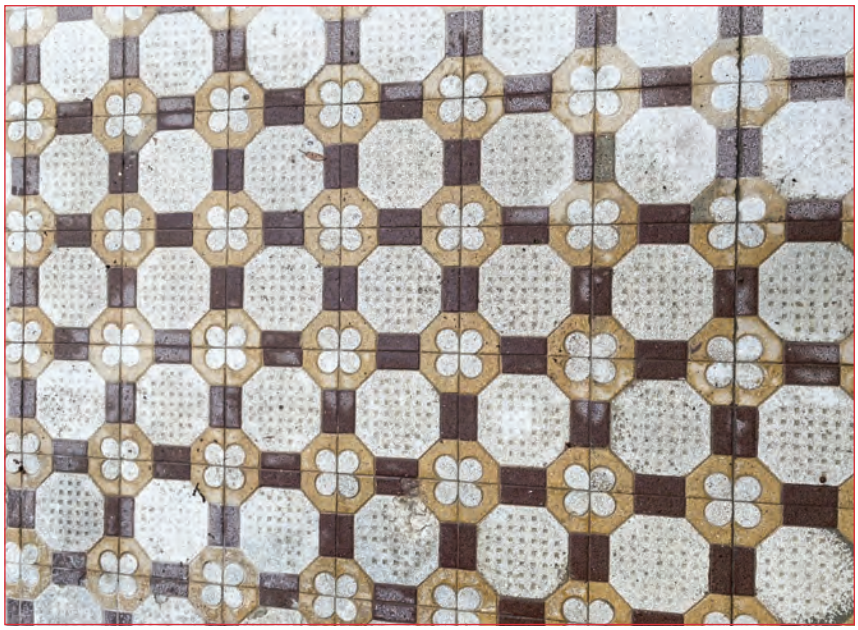


(e) I think this one is *cmm* which has mirror lines along the cell edges and through the middle as well as intervening glide lines. There are lots of 2-fold axes as well so please see the International Tables for more info.

For this issue we have five new patterns from John for plane group identification.



(a)



(b)

(c)

(d)

(e)

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Meetings of Interest

Where possible, information on the following meetings has been abstracted from the conference websites, where further details may be obtained.

Assistance from the IUCr website is also gratefully acknowledged.

If you have news of any meetings to add to future lists, please send them to the Editor, **jon.cooper@ucl.ac.uk**.

34th Annual Meeting of the German Crystallographic Society (DGK)

Lübeck, Germany, 25th-28th February 2026

The aim of the DGK is to bring together all those active in the field of crystallography in order to foster the exchange of scientific experience and ideas as well as further training on a national and international level and to promote crystallography in teaching, research and industrial practice and in the public. For more details please visit: **https://dgk-conference.de/**.

Instruct-ERIC Biennial Structural Biology Conference

Brussels, Belgium, 27th-29th May 2026

The IBSBC showcases the latest in integrative structural biology from leading scientists across the world. For more information on the 2026 conference which is entitled "From structure to new molecules" please visit: **https://instruct-eric.org/ibsbc2026**.

International School Of Crystallography

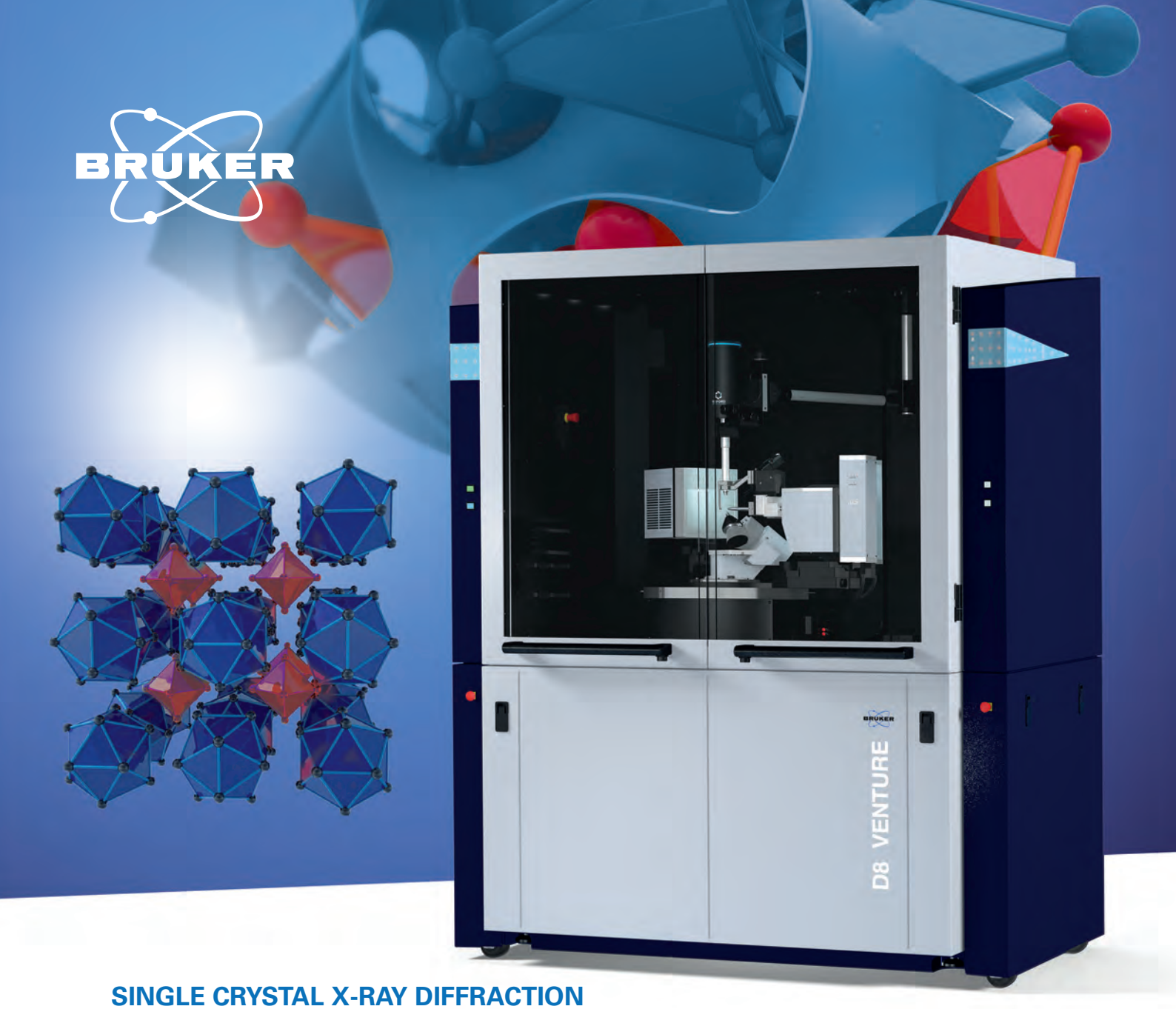
From structural biology to structural cell biology with the aid of machine learning, Erice, Italy, 29th May-6th June 2026

Structural biology has long provided atomic-resolution insights into macromolecular function, but traditional approaches, such as X-ray crystallography and single-particle cryo-EM, require the purification of molecules, removing them from their native cellular environment. This reductionist approach has been crucial for determining structures, yet it often fails to capture how macromolecular assemblies function dynamically within the cell. Machine learning methods are now playing a key role in improving structural classification, denoising, and segmentation in cryo-ET datasets, making them an essential tool for modern structural biologists. This course will train the next generation of researchers in these cutting-edge integrative approaches, ensuring that they are equipped with both experimental and computational skills to tackle the challenges of structural cell biology. For more information please visit: **https://crystalerice.org/2026/**.

Twenty-Seventh Congress and General Assembly of the International Union of Crystallography

Calgary, Canada, 11th-18th August 2026

IUCr2026 is set to be held in the magnificent city of Calgary, located in the heart of Alberta, Canada, from 11th to 18th August 2026. Calgary, a city renowned for its breathtaking natural beauty and warm hospitality, has been chosen as the host for this remarkable occasion. Nestled amidst stunning landscapes and boasting a rich cultural heritage, this vibrant metropolis promises to provide an unforgettable experience for all attendees. More details and registration are available at **https://www.iucr2026.org/**.



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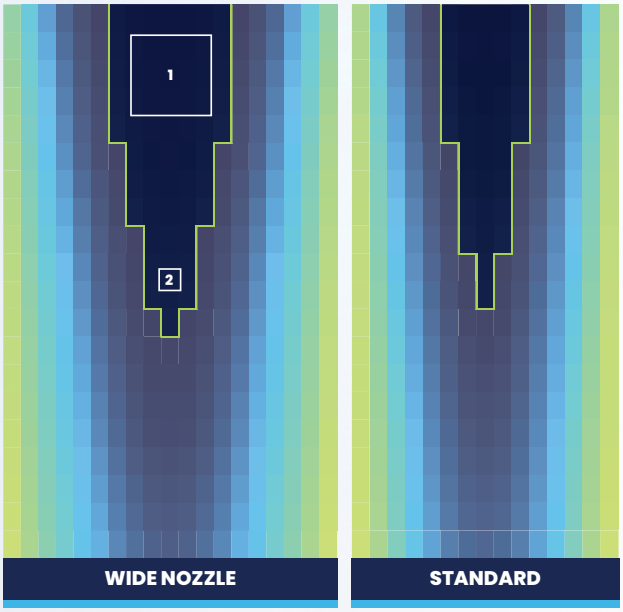

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