Engineering and Physical Sciences Research Council

NRF ANNUAL REPORT

Name: EPSRC National Crystallography Service (NCS)

Director(s): Professor Simon Coles

Co-director(s): Professor Michael Probert

Location(s): University of Southampton / Newcastle University

Grant reference: EP/W02098X/1 & EP/W021129/1

1) Purpose and vision of the NRF

Crystal structure analysis is a cornerstone of chemical and materials research. The NCS provides structural characterisation support which crucially drives research across the range of disciplines performing chemical synthesis and materials characterisation. Decades of expertise and advanced instrumentation make NCS a world-leading, high-powered, high-throughput facility. Its core service provides state-of-the-art crystallisation and structure characterisation, significantly beyond that found in home departments, for chemists, materials scientists and crystallographers in academia and industry. Sample turnaround time is exemplary, meaning that via NCS this technique is often used to progress research, as well as producing the characterisation of its final outputs.

Crystallisation or diffraction quality of a new compound is not predictable and so synthesis chemists need timely recourse to higher-powered facilities, but not for all their samples – thus making a centralised facility the only scalable and financially viable option. This University-based facility provides a highly effective screen for a follow-on service at the Diamond Light Source, making use of this facility as efficient, cost effective and timely as possible. The NCS mission over 4 decades has been to define state of the art in the field – this has been achieved through many X-ray diffraction firsts which are now commonplace and is being continued through pioneering electron diffraction which opens up study of nanocrystals and is becoming the biggest step change for crystal structure analysis in several decades. The NCS greatly enhances the reach of the technique by providing state of the art crystallisation services and in-situ study of dynamic solid-state systems at high temperature, pressure and in different gaseous environments. This underpins developments in strategic research areas e.g., energy, carbon capture, functional and catalyst materials, but requires specialised equipment and extensive experience, often considered the preserve of the expert crystallographer. The NCS broadens the impact of these techniques by making them available to the wider chemistry community.

The NCS is a world leading facility, spreading its expertise by educating, training, facilitating, and empowering non-experts across the community. It increases the levels at which structure characterisation can be carried out in the UK and enables accessibility of the technique to entirely new communities. In its globally leading role, the NCS drives innovation and adoption of novel instrumentation, software, methods, analysis, standards and dissemination.

2) Quality and breadth of research that the facility has enabled

Scientific Excellence and Impact

The NCS provides a service for structural characterisation of crystalline chemical compounds by single crystal diffraction. The exceptional level of publication outputs (averaging around one a week, see below) is testament to the scientific excellence both supported and driven by the NCS. We cover a huge number of research areas, such as molecular organic frameworks, pharmaceuticals, agricultural chemistry, battery and energy storage materials, catalysis and many more, with users in institutions across the country. There are many specific examples of high impact research outcomes and scientific excellence throughout this report.

NCS operates a hub and spoke model with the University of Southampton acting as the central site offering data collection and full crystallographic characterisation experiments on challenging samples that users can't examine locally. Additionally, it offers more advanced single crystal diffraction techniques including gas cell, variable temperature, Crystal Sponge, Quantum Crystallography and structural characterisation by single crystal electron diffraction. The spokes include Diamond Light Source, where the Southampton Hub has regular beamtime (on average 1 visit every 6 weeks) to investigate the most challenging samples and Newcastle University which offers high pressure crystallography studies and ENaCt (Encapsulated Nanodroplet Crystallisation) services.

The University of Warwick can also be considered as a spoke offering electron diffraction, however it is not funded directly by the NRF grant which didn't cover electron diffraction at the most recent 2022 NCS renewal. In 2023 Southampton and Warwick realised that the nascent 3D-ED electron diffraction technique was highly complementary to its X-ray analogue and would be a step change driving the future of structure analysis by single crystal diffraction (it can investigate nanoparticles, while the X-ray method is limited to micro scale crystals). The two institutions partnered in a top-ranked EPSRC Strategic Infrastructure bid which funded electron diffraction equipment at both sites. From the outset it was clear that this technique would be the future of the NCS, so the partnership leveraged the NCS infrastructure and community engagement, instantly enabling national access.

The electron diffraction activities were launched in 2024, where we explored how to deliver a user centric facility at national scale – the first time this had been done anywhere in the world. During this reporting period we have established a stable operation of the electron diffraction services in collaboration with Warwick, with a clear understanding of the modes of access/use, facility capacity and user demand. Access to the service is fully integrated with NCS standard application routes and users are visiting and sending samples to both sites for analysis for structural characterisation. The result of the groundwork of the last two years has led to numerous publications this year, discussed in the section below. Some of this work was also highlighted at a keynote talk at the British Crystallography Association (BCA) Spring Meeting by Prof Simon Coles, Dr Peter Horton and Dr Daniel Rainer discussing problematic datasets for both X-ray and electron diffraction. Electron diffraction has therefore now become a core access route for users requiring crystal structures and accounted for approximately 20% of our successful outputs for 2025. We have also acquired a gas cell holder and air-free transfer holder to perform advanced technique experiments with electrons to bring the technique in line with the types of experiments we are able to offer with X-ray diffraction and work has begun on developing these experimental procedures.

This extension of advanced techniques to electron diffraction was also supported this year via the award of an EPSRC standard grant in collaboration with Ross Forgan (University of Glasgow) to merge the capabilities of the Crystal Sponge and electron diffraction approaches. This successful proposal arose directly out of the Crystal Sponge project work (based purely on X-ray analysis) that NCS ran with Merck (2021-2023). Crystalline sponges are Metal Organic Frameworks into which analytes that do not typically crystallise can be soaked into the pores, where they sit in an ordered site. This allows the analyte to be studied with structural characterisation diffraction techniques. By utilising electron diffraction in the Crystal Sponge approach, the ability to examine powdered sponges enables a larger surface area / volume ratio so that the analytes can soak more readily into the MOF allowing for higher loading, and therefore potentially better diffraction data. This project began during this reporting period and is both developing new electron diffraction-based protocols and new crystalline sponge materials with a long-term view to provide it as a service.

Demand for the Encapsulated Nanodroplet Crystallisation Service at Newcastle University has continued to grow throughout the year. A total of 43 crystallisation studies were performed with publications resulting from work with Sheffield and Durham, and publications in progress with Edinburgh, York, Manchester and through some internal projects. Following discussions with the Strategy and Allocations Panel (SAP), several successful projects used ENaCt to produce nanocrystalline material which was then analysed by Electron Diffraction at the University of Southampton. Given the materials that are typically sent for crystallisation services typically do not form large crystals, this pairing of techniques forms a perfectly synergistic analytical pipeline, which has already led to the elucidation of around 10 structures. This collaboration has led to discussions between the sites, alongside the SAP, about how we can best ensure that samples submitted to our X-ray single crystal service that are not suitable as they are too small, can be appropriately assigned to one or more other NCS techniques to maximise the structural services and outputs for users. The University of Newcastle also continues to perform high pressure studies for the community with two projects (four samples) leading to two manuscripts in progress with the universities of Birmingham and Surrey.

Publications

The NCS fundamentally supports, drives and contributes to a high volume of publications across three categories:

- Data Collection Only (collect data for users who analyse/publish it independently),
- Full Structure Analysis (collect, solve & analyse data, co-authoring publications with users),
- Crystallography-led studies (NCS driven research e.g. advanced structural studies or method development).

The total number of publications for the reporting period are compared with previous years in Table 1 both showing that the higher level of outputs of recent years has been sustained.

Year	2020	2021	2022	2023	2024	2025
No. of publications	38	28	37	47	45	43

Table 1. Total number of NCS publications.

The following selected publication highlights illustrate the strength of science supported.

- Crystallizing the Uncrystallizable: Insights from Extensive Screening of PROTACs – https://pubs.acs.org/doi/10.1021/jacs.5c07977

In this study, researchers from Durham University worked with our ENaCt crystallisation service to form crystals of three polymorphs of a PROTAC drug molecule. PROTACs are very difficult to crystallise due to their long flexible structures and poor aqueous solubility. ENaCt crystallisation is performed in 96 well plates with 16 different solvents with very small quantities of a compound, allowing for hundreds, or even thousands, of crystallisation attempts to be performed very quickly. This process led to crystals that were suitable to be studied in Southampton with the electron diffractometer. This body of work is an excellent example of the synergy between the techniques between NCS sites, with Newcastle producing crystals of traditionally uncrystallisable materials and Southampton able to study crystals smaller than 100 nm.

- Structure–property relationships in disodium anthracene dicarboxylate for sodium-ion storage via 3D electron diffraction - https://pubs.rsc.org/en/content/articlelanding/2025/cc/d5cc03175c

Researchers at the University of St Andrews evaluated the use of highly conjugated disodium anthracene-9,10-carboxylate (Na_2ADC), synthesised using rapid microwave-assisted heating, as a potential anode material in sodium-ion batteries. Research into potential battery materials, especially organic based materials as a sustainable alternative, is a topic of particular current importance. The structure of the material was confirmed by electron diffraction at the University of Southampton by Dr Daniel Rainer. The researchers commented in the publication that "*Owing to their high ionic character, materials such as sodium carboxylates can be harder to grow as large single crystals that do not contain any lattice solvent molecules. This makes traditional single-crystal X-ray diffraction challenging, but can be overcome by employing electron diffraction, which can be used for single crystallites that are considerably smaller in size.*" This paper demonstrates the ability to apply structural characterisation to whole new areas of chemistry, such as battery materials, to give better understanding of how these materials are structured and lead to better material design. "*In this pursuit the effective use of 3D ED offers a new frontier for battery materials, especially OEMs, to have a better handle on structure–property correlation.*"

- A Bis-Perylene Diimide Macrocycle Chiroptical Switch - https://doi.org/10.1002/anie.202501122

This paper covers the synthesis and characterisation of a bis-perylene diimide macrocycle, which acts as a discrete molecular model for a chiral supramolecular assembly. The chirality is switchable dependent on the solvent system and can be 'switched off' with the binding of a polycyclic aromatic hydrocarbons. This behaviour has important implications for the design of high fidelity supramolecular chiroptical switches. The single crystal X-ray diffraction data was collected at the NCS and it is a great example of some of our data collection only work, where access to our instruments is provided for the purposes of data collection but the analysis is performed by the submitting research group.

Case studies

In this period, we generated two case studies. The first was a collaboration with researchers in the Planas group at Imperial College London. They synthesised the first stable, crystalline subvalent indium hydride compound, supported by a bis(NHC)borate ligand scaffold, showing how careful steric design, noncovalent interactions and zwitterionic charge distribution can stabilise previously unknown low-valent heavy main group hydride species. The crystallography was all performed at the National Crystallography Service, and analysed by Dr Graham Tizzard.

- https://www.ncs.ac.uk/ncs/wp-content/uploads/sites/426/2026/02/Planas-case-study.pdf

The second case study was a collaboration between one of our electron diffraction facility sites and the Parsons group at the University of Edinburgh. This case study focussed on *in situ* studies of relatively unexplored Metal Organic Polyhedra. The analysis was performed by Dr Jere Tidey at the University of Warwick, with a PhD student of Prof Simon Parsons' (Mr Calum Sangster). Simon said of the collaboration *"The structure would have been inaccessible from powder methods, partly because of size broadening, but also simply because of its complexity. I'd also like to mention the importance of the in-person training, approved by the NCS panel and delivered by Jere, given to our student, Calum Sangster. This has been a key part of Calum's PhD research, but, more generally, is really important for ensuring that expertise in a new and developing technique is disseminated into the research community."*

- https://www.ncs.ac.uk/ncs/wp-content/uploads/sites/426/2026/02/Parsons-case-study.pdf

We also highlight two publicity case studies that were undertaken to advertise various aspects of the service. Professor Simon Coles and the NCS were the subject of a Rigaku case study on the advocacy for the use of rotating anodes in crystallography. The NCS was the first chemical crystallography laboratory to adopt this technology in 1989 and has been demonstrating its value and developing its potential ever since. The case study, entitled 'Revolutionizing Crystallography: The Impact of Modern Rotating Anode X-ray Sources', took the form of a professionally created YouTube video interview and facility tour (https://www.youtube.com/watch?v=rVeMb7ULtTc) and subsequent related social media campaign eg

- https://www.linkedin.com/posts/rigaku-single-crystal-diffraction_revolutionizing-crystallography-the-impact-activity-7351368319565750272-aYB6
- https://www.facebook.com/RigakuCorp/videos/why-did-simon-coles-adopt-rotating-anodes-for-the-national-crystallography-servi/613986641325782/
- https://www.facebook.com/100063557081043/videos/1390346958745112/?__so__=permalink
- https://bsky.app/profile/rigakuoxfordxrd.bsky.social/post/3ltxbilanjc2x

Secondly, Mr Owen Hewitt was interviewed for technicians.org as part of their push to showcase stories of technicians throughout the UK. Owen has been a great success story for apprentice technicians in the field od analytical chemistry and in this showcase he talks about his love for crystallography and the team of crystallographers he works alongside.

- https://www.technicians.org.uk/stories/owen-hewitt/

3) Usage, user focus and non-scientific impacts

Statistics on usage and the range of users

NCS users fall into seven categories: a) Research Group Principal Investigators. We do not record the number of students for each PI accessing the NCS, however an accepted estimation is that an average user has 2-3 students (some groups are much more); b) UK service crystallographers. As 'gateway' users, this access mode supports large numbers of researchers, as departmental crystallographers access the NCS to analyse difficult samples from across their entire user base; c) Collaborators using Advanced Techniques; d) Commercial Users. Mainly from the pharmaceutical sector, but now also engaging agrichemicals; e) International Collaborations. Not the focus of this section but some key examples give in Additional Information section below; f) People accessing the training programme.

Prospective academic users (categories a-c above) must make an application in response to a six-monthly call to access the NCS. This application must estimate an allocation of expected samples that will require the NCS facilities i.e., there is great uncertainty as to how many new compounds will be made, how many of these can be crystallised and how many of these will be of lesser quality and therefore not examinable with local facilities. Furthermore, departmental service crystallographers (category b above) apply on behalf of several academics in their department, further increasing the uncertainty around the likely number of samples that will be produced. On application these users are asked to identify academics they are submitting on behalf of, however no information on numbers of students, PhD candidates or PDRAs is requested from category a-c users due to the significant additional requirements that would be placed on users to gather this information for an application relating to speculative samples. We cannot therefore report on the level of granularity of users as requested. It should also be noted that industry users are counted as companies, not individuals, and within each company there are generally many research scientists who use our services but through a gateway user - again we do not request this level of information of our clients. The user information presented in the table below is therefore that which is most appropriate for the NCS and which we are currently able to gather.

This year has seen a further increase on the number of users, with a healthy mix of returning and new users. This is partly attributed to users engaging with our advanced techniques, particularly ENaCt and 3DED, but we are also increasing the amount of single crystal x-ray diffraction work we are undertaking. These techniques have been rolled out as a standard part of the NCS application process and so it is easy for traditional single crystal x-ray users to apply for these techniques and we are also seeing those who are onboarded through wanting these techniques then also going on to apply for routine x-ray work. NCS users in this period originated from 47 different institutions. Approximately 85% of users are based in chemistry departments, while the remaining 15% originate from chemical engineering, natural science, materials science, defence materials, pharmacy, and biochemistry departments. The geographic spread of users is even and touches all regions of the UK. The most common research areas include catalysis, chemical structure, synthetic chemistry (organic, supramolecular, organometallic, inorganic etc.), carbon capture, energy storage, small molecule activation, materials for energy applications. Table 2 details the breakdown of user types, comparing with previous years.

N.B. The NCS has a large number of international collaborations, both for structural characterisation and to advance the technique. Not being eligible to independently apply to EPSRC, nor a formal requirement herein, we do not provide extensive details here, but provide a list of some key strategic collaborations as an annex.

Year	**Unique academic users**			**Repeat academic users**	**Total inc. repeat**	**Industry**
	% internal	**% external**	**Total excl. repeat**			
2020	**3**	**97**	**11**	**56**	**67(+48)****	**7**
2021	**3**	**97**	**12**	**62**	**74 (+63)****	**6**

2022	**3**	**97**	**10**	**57**	**67 (+70)****	**6**
2023	**2**	**98**	**23**	**68**	**91 (+ 50)****	**7**
2024	**4**	**96**	**29**	**64**	**93 (+ 64)****	**8**
2025	**3**	**97**	**24**	**87**	**111(+ 71)****	**10**

Table 2: Breakdown of Users **Some academic users are departmental crystallographers who apply and submit samples on behalf of others in their department (number indicated in brackets).

Service Demand

The NCS processes a high volume of *samples*, each requiring a relatively short timescale for analysis when compared to the *project* type studies typically undertaken by many of the NRFs (which can often take weeks or months). Single Crystal XRD (SCXRD) data collection times range from minutes to two days depending on crystal quality. Due to this variability our capacity is somewhat dynamic, as to some extent we can adjust data collection times to match demand. This also means we cannot allocate 'time on instruments' to users, as we do not know how long a sample will take until it is on the instrument, so instead we deal in terms of allocations comprising several samples. There are two ways of accessing the SCXRD service: Data Collection Only (DCO) and Full Structure Analysis (FSA). DCO serves experienced users requiring access to the instrumentation but who can process and solve their own datasets. FSA supports users unfamiliar with structural analysis or those with particularly challenging samples, where we would collect data and then process and analyse it. This significantly increases staff time required to process a sample. The speed of these advanced SCXRD instruments means they can collect data significantly faster than it can be processed. Accordingly, the biggest demand on resources has shifted towards a need for staff time.

Users apply for an allocation every six months, although rapid access is available throughout the year. It is worth mentioning that these applications are speculative, based on previous usage. Applicants do not usually apply for analysis of samples they immediately have to hand, but rather for the number of samples they expect to generate in a 6-month period. On application, single crystal X-ray diffraction allocations are prioritised into high, medium and low categories. On receipt, a sample is logged into the Portal system with 'time until data collection' Service Levels of 10, 20 and 30 days for High, Medium and Low priority samples respectively (this prioritisation is regardless of whether a sample is FSA or DCO as the system is based on scientific merit). If applicants request a particularly large allocation or require rapid access at a period when the facility is reaching capacity, there is the ability to assign 'reserved' samples, which allows users to submit excess samples that can be examined should there be spare capacity. This means if a user requests access, we are always able to accommodate it.

During these application periods, users are also able to apply for our advanced techniques including high pressure studies, ENaCt and crystal sponge crystallisation services, and electron diffraction. This period saw four high pressure studies from two groups including Surrey and Birmingham, with three publications currently in draft for this work. There were 43 total samples studied by ENaCt, submitted by 8 separate groups from 7 institutions, generating two publications, with a further two in progress. This also led to the exploration of the synergy between the Newcastle and Southampton sites using ENaCt for crystallisation and 3DED for analysis of small crystals, as described in the publications section. Between the Southampton and Warwick electron diffraction facilities, users submitted 140 samples, leading to 87 successfully determined structures – given this is the first fully established year of operation, we will use these metrics as an initial baseline going forward.

Operating Capacity. Due to the nature of service operations, as described above, it is difficult to ascribe a capacity for the service and a demand outside of the theoretical. The figures for the number of samples processed by the NCS in an annual reporting period are presented below.

	2021-2022	2022-2023	2023-2024	2024-2025
Low	125	150	99	146
Medium	290	289	265	319
High	149	192	183	217
Total	572	631	547	682

Table 3. Single Crystal X-ray Diffraction samples processed across all prioritisation types

Data Collection Only samples processed during this period accounted for 62% of the core service and Full Structure Analysis the remaining 38%. Relative to previous years this is a typical and healthy balance for the NCS, as Full Structure Analysis samples are much more labour intensive and require a lot more attention, expertise and time. There was a substantial increase in the number of single crystal X-ray diffraction samples submitted this year over previous years. This illustrates that alongside the advanced techniques we have been developing, there is still a strong community need for structure characterisation X-ray datasets on demanding samples.

Training, outreach, skills and non-scientific impacts

Recognising that samples suitable for electron diffraction differ markedly from those typically prepared for single-crystal X-ray diffraction, we have placed strong emphasis this year on targeted training for the user community. Our experience has shown that many of the challenges and least understood aspects encountered in electron diffraction arise at the sample preparation and selection stage, and that these are best addressed through direct, hands-on engagement rather than providing written guidance or classroom-based training. We have therefore encouraged users to bring their own samples to the facility and work alongside our crystallographers during data collection. This collaborative, in-facility training model allows users to develop a practical understanding of crystal size, thickness, crystallinity and stability requirements specific to electron diffraction, while also enabling rapid feedback and troubleshooting. As a result, users gain a clearer sense of what constitutes a “good” electron diffraction sample. This has essentially meant that every electron diffraction shift that has been run this period has been run as a training opportunity for the crystallographic community. It has taken a significant amount of resourcing but is worth the investment to ensure the sample quality that we receive leads to good results, and we believe that in due course a proportion of these users may be able to shift to postal/remote access due to their deeper understanding of the process and its challenges.

We also hosted two summer interns, providing them with valuable hands-on experience in the facility and the opportunity to develop new technical and laboratory skills. One placement was funded by the Technology Specialists Network (TSN ROKS, £5k awarded to our RTP Dr James Orton to oversee), focussing on broadening practical technician competencies in a research environment. An NCS internship similarly supported skills development and career progression, and the Southampton student (Alice Saxton) has since secured a position on the Science and Analytical Chemistry Graduate Programme with Babcock International Group.

We continue to actively promote our services through engagement at both specialist crystallography meetings and broader chemistry conferences, ensuring strong visibility within the research community. This included significant involvement in ICDM10 (International Charge Density Meeting) at Durham University, a specialist conference on Quantum Crystallography organised by Prof Simon Coles and attended by Dr Graham Tizzard and Dr Robert Bannister. Dr Bannister also contributed to European-scale cross-facility dialogue by presenting a talk on the NCS as a best practice example of core facility management at the inaugural Materials Science Core Facility Synergy Forum in Bremen, and by presenting a poster on electron diffraction at the biennial RSC Dalton Conference in Warwick. The group maintained a strong presence at the British Crystallography Association Spring Meeting where Prof Coles, Dr Peter Horton and Dr Daniel Rainer delivered a joint Keynote presentation on problematic datasets, and Owen Hewitt presented a poster highlighting the role of technicians (winning a poster prize). In addition, Owen represented the facility at the Solutions in Science (SinS) conference in Brighton, giving a talk focused on apprenticeships in science and facility management. Dr Daniel Rainer attended the prestigious Erice Summer School in Electron Diffraction and presented recent developments in Electron Diffraction at a Rigaku User Meeting (Frankfurt) and to facility users at the ISIS Neutron Facility.

We have continued our strong presence at Southampton Science and Engineering Festival (SOTSEF). Alongside established activities such as crystal gardens, painting with salt crystals, making slime and learning about radiation, we expanded the programme through collaboration with the RSC local section to introduce a new stand, Chemistry Makes Scents, exploring volatile compounds and the chemistry behind smell. This work was recognised with a Dean's Award for Dr Robert Bannister and led to an invitation to contribute to a follow up Public Engagement Celebration event highlighting exemplar activities from SOTSEF and across Southampton. Building on this success, these activities are a core component of the School of Chemistry's successful bid to host a chemistry hub during the British Science Festival at Southampton in September 2026. At this national scale event we will deliver two days of engagement with ca 3000 expected visitors aged 16+, including coordinated schools visits. The established Spectroscopy in a Suitcase (SIAS) outreach activity takes analytical chemistry into schools and colleges and reached ca 130 Year 11 to Year 13 students across four institutions—Cantell School (Southampton), St Gabriel's School and St Bartholomew's College (Newbury), and Sir William Perkins School (Chertsey). The activity is now managed and delivered by our apprentice technician, Owen Hewitt, and a crystallography group PhD student. Owen also presented on the technical apprentice career path and sat on an expert panel at Horsham Girls School, which was filmed for BBC Bitesize.

The NCS strives to be a leader in the development of technical and post-doctoral staff and in the reporting period three staff members (Dr Robert Bannister, Dr Peter Horton and Dr Daniel Rainer) promotion applications were successful. Robert and Peter are now Senior Enterprise Fellows and Daniel a Senior Research Technician. Dr Alexandra Longcake, NCS ENaCt scientist in Newcastle, undertook extensive electron diffraction training in Southampton, pioneering the combination of the two techniques, which set her up ideally to be recruited to manage the new electron diffraction – X-ray facility in Liverpool. Other technical training undertaken included Project Management (RDB) who successfully completed his PRINCE2 training. Owen Hewitt completed his apprenticeship course at Fareham College and is now embarking on a degree level apprenticeship aimed at a wider role incorporating other analytical techniques as part of the new Materials Characterisation Hub.

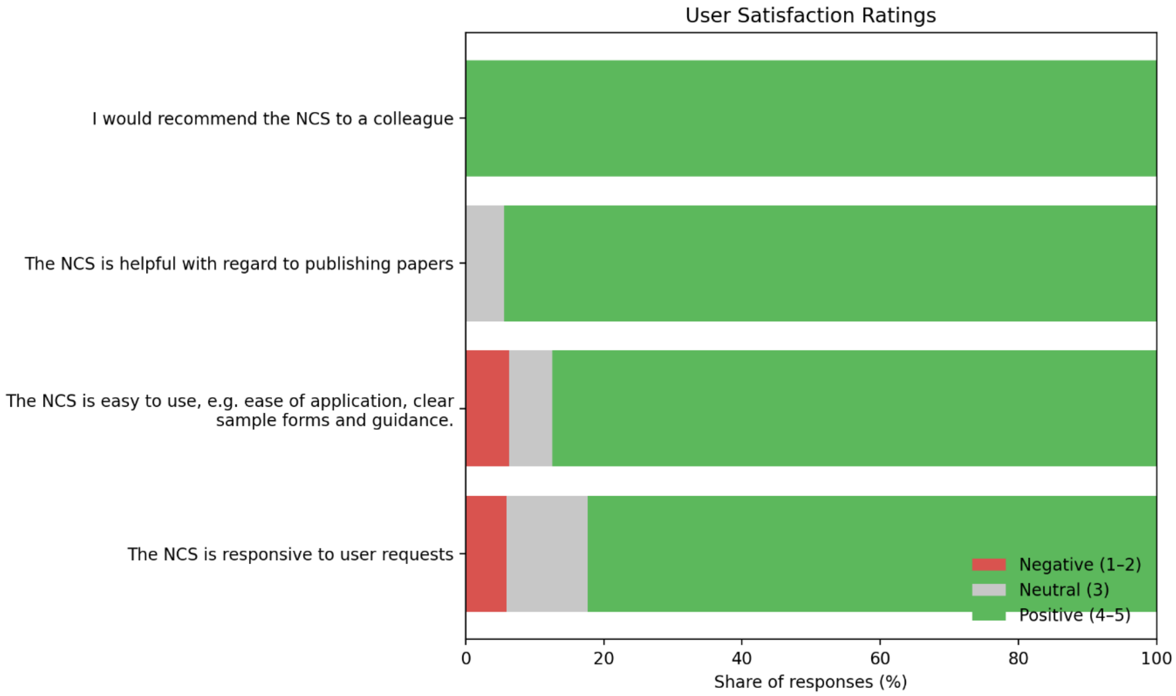
The NCS website is available at https://www.ncs.ac.uk/. The website was refreshed in 2021, moving from our old format to a new WordPress site. This gives us greater control over the content and the ability to make changes. We do not closely monitor usage of the website, as all our user interaction occurs either through email or via our Portal system but in this reporting period Google Analytics reports 2,300 active visitors with a total of 3200 sessions. Both our Single Crystal X-ray and Electron Diffraction services have been included in the new Southampton Chemistry and Chemical Engineering Enterprise Solutions (CChES, https://cches.co.uk/). This new research consultancy service is a way to offer analytical and research solutions to wider chemical industry, with greater cost recovery implications outlined below.

User Satisfaction

Our annual user feedback survey was sent to all 50 user groups with an active allocation. Responses demonstrate that the NCS is in a healthy position, with some very positive feedback and one or two suggestions for improvement. User feedback is not mandatory and we do not currently have a way to ensure users fill in the feedback survey so responses can be difficult to obtain. The survey used a Likert scale (strongly agree to strongly disagree) for the following questions:

1. The NCS is easy to use, e.g. ease of application, clear sample forms and guidance.
2. The NCS is responsive to user requests, e.g. rapid turnaround, additional data collections etc.
3. The NCS is helpful with regard to publication, e.g. all data necessary provided, assistance with crystallography sections etc. as per type of service requested.
4. I would recommend the NCS to a colleague.

The results are presented below. In summary the feedback we received was overwhelmingly positive, scoring 5/5 (or strongly agree) from most people for most questions. Our lowest score was for 'The NCS is easy to use' with one user answering 'Strongly disagree' and the comments for this question are largely around confusions about interacting with our Portal2 software and how the applications process works. We have taken this into account and will develop better resources on our website and give better instructions during our call periods, as well as detailed instructions to new users on how to submit samples once they have an allocation. We received one Strongly disagree response for 'the NCS is responsive to user requests', but from the comments this seems to be because the user has not yet submitted a sample but left the following comment "*Communication is prompt and polite; everything is well explained; procedures for co-authorship are explained clearly up-front. We have not yet had data back, but I am sure this will be a positive experience too, hence my 5-star rating."* It should have been made more clear in the feedback that responses to all questions were not mandatory and in future a N/A answer will be made available.



Feedback comments were overwhelmingly positive and some representative quotes include:

"I couldn't have done my research without the expertise of Dr Graham J Tizzard and Prof Simon J Coles. They have been extremely supportive, provided detailed reports of each XRD structure measured, and were exceptionally helpful during the review process of papers published with them."

"The NCS continues to be a fantastic service, without which, I would struggle to publish my work. They are efficient, effective and very friendly. They often go above and beyond, especially when producing journal papers."

"An extension of my research team, so friendly, approachable and helpful. Also, experts in difficult to get structures!"

There were some comments on areas to improve: *"Mostly great and couldn't do without this service. It is a chore having to trawl through papers, structures included, and funding information during the applications process. We see why this is done and are not sure how this could be made simpler, but that part is very time-consuming."* The NCS consults the Strategy and Allocations Panel on this topic regularly and over the years has made changes to make outcomes reporting easier for NCS users, however this data is fundamentally required for the NCS to report back to EPSRC and so the situation is unlikely to change significantly in the near future.

A further important point was made: *"Proposal system a bit opaque to use. Rules around raw data are challenging for crystallographically tricky materials where collaborative analysis would be beneficial."* This point refers to the availability of raw data from electron diffraction studies. As an emergent technique with many aspects that require highly specific expert input to obtain a trustworthy result, the NCS has been wary about releasing all data to users at such an early stage of development. The simplest and clearest approach to ensuring no reputational damage (to the NCS, but also to the technique as a whole) and ensuring trustworthy structures are published was to implement a blanket policy that raw data was not made available. The technique and our experience in delivering this service is developing rapidly and we can now review this policy, which will be tabled at the next Strategy and Allocations Panel meeting.

4) Effective Management

Cost Recovery

The NCS has operated for >40 years as an NRF (or equivalent) that is free at the point of access for users. The driving reason for this is the nature of the work we do – it is a sample focussed service, not a project focussed one. We therefore have a high throughput, working with a lot of samples that can't be examined on users home systems or that require expert handling/interpretation. Users will often submit several samples in a period that originate from different projects and at the time of application these samples generally don't exist (ie application is prior to successful/final crystallisation of a material, sometimes even without synthesis completed) – the NCS therefore needs to be timely with a quick turnaround time.

Therefore, for core X-ray work the only route for cost recovery is to provide a service to industry. We have been doing this for over 15 years and it is relatively successful however the market is relatively small, unchanging and saturated with potential solutions. This year saw a marked increase in commercial activity for the single crystal Xray diffraction service, generating £46,565 in income, representing a significant uplift compared with previous years. We also launched a new commercial 3D electron diffraction (3DED) service, which has already generated £24,500 and represents a strong foundation for a new revenue stream with clear potential for growth and long-term sustainability. Notably, this income was derived from just nine commercial 3DED samples, compared with 54 samples required to generate the single crystal Xray service income, highlighting both the efficiency and high value of the technique. As electron diffraction can address structural problems that are not possible to solve with conventional single crystal X-ray methods, and therefore often open up structure characterisation to entirely new classes of chemical compounds, we anticipate increasing industry demand for the technique and a rise in commercial income in future years.-crystal X-ray diffraction service, generating £46,565 in income, representing a significant uplift compared with previous years. -term sustainability. Notably, this income was derived from just -crystal X-ray service income, highlighting both the efficiency and high value of the technique. As electron diffraction can address structural problems that are -crystal methods, we anticipate increasing demand for 3DED and a

This year the University of Southampton School of Chemistry launched the Chemistry and Chemical Engineering Enterprise Solutions (CChES) consulting services. CChES is a way for the department at Southampton to advertise and provide services for commercial clients through an expedited process. The NCS was heavily involved in the development, marketing and launch of this research consultancy service and both the Single Crystal X-ray Diffraction and 3DED services are available through them as advertised on their website - https://cches.co.uk/.

We plan to explore costing of facilities access into users grant proposals for the increasing amount of project-type (advanced techniques) work we do and intend to expand in the future. This has recently become viable as we begin to establish our range of advanced techniques. Further, much electron diffraction work is rather more involved than X-ray work and lends itself to a project-like approach, and we expect this type of costed access to increase as the technique becomes more established and key to certain areas of research – the first successful proposal with this type of access included was this year (£9k as a component of a 5 year Programme Grant at Durham University).

Cost recovery figures for this period, and relation to previous periods, is given in Table 4 below.

Year	Running Costs	Grants	Other Academic	Students	Industry	Other*	%
2020	£465,000	£12,000			£36,000		10.3
2021	£518,000	£48,000			£33,000		15.6
2022	£426,000	£31,000			£24,000		12.9
2023	£511,000				£23,000		4.5
2024	£515,000	£1000			£30,500		6.2
2025	£585,800	£19,000			£66,065		14.5

Table 4. Cost recovery breakdown.

N.B. The ENaCt service delivered by Newcastle University was an inclusion at the last NCS renewal. Accordingly, it was in a start-up/lead-in phase for the initial reporting phases of this grant and has not been included in the regular cost recovery reporting. However, in this period a £20,000 cost recovery income from facilities access on grants was made – this has not been reported in the table above to avoid skewing the year-on-year comparison.

Risks

N.B. The full Risk Register and Equipment Risk Register are provided as appendices to this report.

NCS is embedded in School of Chemistry and Chemical Engineering strategy, with the Head of Department attending OMT (Operations & Management Team) once a quarter and SAP (Strategy and Allocations Panel) twice a year. The Newcastle operation is similarly embedded in its department strategy. This ensures a two-way understanding of high-level general risks with the host institution. Examples of these risks and how they are considered include:

- Disaster recovery e.g. fire, pandemic – covered by Departmental policy and mitigation/recovery measures put in place,
- Host institution issues e.g. infrastructure failure – reporting channels clear, close two-way interaction with School Facilities Manager,
- Financial e.g. planning and management - regular review to ensure no overspend, contingency plans if funding renewal doesn't occur,
- Safety e.g. compliance and safe working environment - regular safety inspections and staff training, with a system to review and ensure these are adhered to.

At the facility operations level risks are regularly assessed by the OMT, which passes concerns or strategic requirements to the SAP. This is driven by a Risk Register (included separately). Further to this an understanding of risk relating to the capital equipment (>£10k) is further considered with its own register (also included). A general mitigation against equipment failure is that the apprentice technician's principal role is its monitoring and preventative maintenance.
In this period the following risks were graded either Amber or Red and so are elaborated here:

Risk 2 (Equipment Failure, graded Red); High *Likelihood, Maximum Impact*.
Risk 3 (Equipment Obsolescence, graded Red); *High Likelihood, Maximum Impact*.
In general, and due to recent Core Equipment grants and Crystal Sponge collaboration with Rigaku), the equipment base is less than 5 years old. However, these two risks are related in that the clear exception is that both the rotating anode X-ray generators were installed in 2011 and nearing end-of-life. The 007 (Cu) generator has had less heavy use and is still a model sold, supported and under service by Rigaku. However, the FR-E+ is no longer sold and Rigaku consider it to be beyond service

life and are warning that parts for the FR-E+ are now incredibly rare. In fact, an electronics failure because of the 2025 Christmas shutdown resulted in an extensive exercise to source the replacement part which was eventually shipped from Japan but resulted in a 3-week outage. Failure of either of these units would be pivotal with the FR-E+ in particular, as the most powerful Mo X-ray generator in the country (if not the world), having an immense impact. As this would be incredibly disruptive to the operation of the NCS the following mitigating considerations have been made.
1) There is redundancy in that there are two generators and an assessment of capacity indicated that should one fail, measures could be taken such that the core structure analysis work could still be covered [reduction in some time-consuming advanced techniques; more efficient scheduling and longer lab working hours, evenings and weekends; make more use of Diamond facilities; use Newcastle facilities as a backup].
2) A thorough analysis by Rigaku Service Engineers was performed. They concluded that the units are in good condition and should be able to operate until the end of the current NCS funding period (June 2027); Rigaku have put aside what essential spares they have to cover this period; we purchased a second hand FR-E+ generator that had been decommissioned and Rigaku engineers stripped it of all useful components (which are now stored at Southampton); Rigaku have committed to a service contract with NCS to take us to the end of the current funding period.
3) A more thorough and regular monitoring process has been drawn up and is conducted by the NCS apprentice.
4) Options for funding a replacement have been assessed and specifications drawn up with Rigaku. An EPSRC Strategic Infrastructure proposal has been supported by the University of Southampton and an outline proposal submitted to EPSRC in December 2025 – if invited, a full proposal would be due mid 2026 which, if successful, would enable a replacement to be installed in the laboratory around the summer 2027 end of life time.

Risk 4 (Portal Administrative System and User Interface, Graded Amber); Medium *Likelihood, Medium impact*

A multi-user, multi-technique high throughput facility cannot be effectively operated without the ability to track and manage users, access, samples and data choreographed with the scheduling and load balancing of numerous machines and staff. The NCS was the first NRF to fully realise this and develop a bespoke system (as part of the e-Science programme 20 years ago). However, technology moves on, as well as the facility, how it is used and how it is operated. The 'Portal' system was completely reworked to address this change and obsolescence. However, it is now clear that this is a perpetually on-going process as systems need maintaining, bugs appear and new functionality is required – and Portal is key to the operation of the facility. Whilst a bespoke system is necessary, obsolescence risks have been addressed by using a modern technology stack that is familiar to many developers. Also, we have used the University of Southampton Research Software Group (RSG) to develop the system and thereby maximise the retention of knowledge and ability to support the system. However, times move quickly and developing new functionality and support/maintenance tasks require more attention, yet the necessary software developer time is not accounted for in the grant. Accordingly, we are investigating a new support model approach with the RSG team, but this can only be fully accounted for at the next funding renewal. We are in close contact with the RSG and despite the fact the original developer has moved on, they are providing support as and when necessary and we are devising approaches to enable NCS administration to perform some tasks independently of the system.

Key Performance Indicators (KPIs) and Service Level (SLs)

This was a strong year for the NCS. We increased the number of unique users, signed up many new users and generated record cost recovery, both through grant income and commercial clients. This growing demand is partly attributable to an interest in advanced techniques, but it is important to note that there has also been an increase in the number of single crystal X-ray diffraction users. Also, it is worthy of note that for the first time in many years all SLs have a 'green' status.

Type	Description	Time for Performance	Green	Amber	Red	1st Sep 2024 - 31st Aug 2025	Directors Comments
RMI	Total number of all Users	Period associated with specific report	N/A	N/A	N/A	111 Academic service users (+71*). 10 Industrial clients.	*Additional users who use NCS via departmental crystallographer
RMI	Spectrum of user types	Period associated with specific report	N/A	N/A	N/A	101 individual users and 10 service crystallographers	
RMI	Number of University / Research Groups Involved	Period associated with specific report	N/A	N/A	N/A	182 Research groups	
RMI	Percentage of Access Requests Accepted	Period associated with specific report	N/A	N/A	N/A	100	
RMI	Percentage of equipment time dedicated to different access modes	Period associated with specific report	N/A	N/A	N/A	60 % Standard NCS time, 10% Commercial clients, 20% Host institution, 10% advanced techniques	
RMI	Completed samples		N/A	N/A	N/A	682	
SL	Percentage of User enquiries responded to within Stated Window	2 working days	95% and above	>90% but <95%	90% or less	100%	
SL	Percentage of Access Requests Responded to within Stated Window	2 working days	95% and above	>90% but <95%	90% or less	100%	

Engineering and Physical Sciences Research Council

SL	Percentage of Training Requests Responded to within Stated Window	2 working days	95% and above	>90% but <95%	90% or less	100%	
SL	Percentage of Training Requests Delivered within 3 months	3 months	95% and above	>90% but <95%	90% or less	100%	
SL	Complaints (expressed as a percentage of the Number of Approvals)	Period associated with specific report	Less than 5%	5-10%	Over 10%	0%	
SL	Customer complaints resolved within Stated Window.	Period associated with specific report	95% and above	>90% but <95%	90% or less	N/A	
SL	Uptime /Downtime	Period associated with specific report	95% and above	>90% but <95%	90% or less	98.0%	Assumed 250 working days. 5 days downtime in Dec24/Jan25
SL	Percentage of Access Costs recovered	Period associated with specific report	10	6	2	14.5%	
SL	Number of Publications	1 year	30	20	10	43	
SL	Publicity Activities	1 year	10	8	6	12	
SL	Time from arrival logging in on Portal	within 2 working days	95% and above	>90% but <95%	90% or less	100%	
SL	The time a sample is in the queue	High Priority DCO (15 days)	95% and above	>90% but <95%	90% or less	97.7%	
SL	The time a sample is in the queue	Medium Priority DCO (25 days)	95% and above	>90% but <95%	90% or less	96.2%	
SL	The time a sample is in the queue	Low Priority DCO (35 days)	95% and above	>90% but <95%	90% or less	97.5%	

SL	The time a sample is in the queue	High Priority FSA (30 days)	95% and above	>90% but <95%	90% or less	97.7%	
SL	The time a sample is in the queue	Medium Priority FSA (40 days)	95% and above	>90% but <95%	90% or less	96.2%	
SL	The time a sample is in the queue	Low Priority FSA (50 days)	95% and above	>90% but <95%	90% or less	95.3%	

Improvements and future plans

The two X-ray generators are now 15 years old and while the copper source (Rigaku 007) is still supported and is less high-powered, the molybdenum source (Rigaku FR-E+) is at end of life – these are no longer manufactured and are also at end of service life. Rigaku have agreed to honour a service contract until the end of our current funding period (June 2027), but thereafter it will be unworkable. This X-ray source is the basis for the unique, world leading NCS offering and so replacement is now a major concern. Replacement with a comparable but even more powerful generator will cost around £1M and so is outside the bounds of Core Equipment funding so other funding routes need to be considered. Accordingly, an EPSRC Strategic Infrastructure outline has been prepared and submitted – with the main case being around moving from using just a high-flux molybdenum source to a 'dual source' solution, which can both act as a replacement and provide new capabilities. The second source proposed is a silver target, which is particularly useful for in-situ cell measurements and Quantum Crystallography work – being on an ultra-high flux generator (and with a tailored detector) would make this world-unique. Further, with a machine upgrade scheduled towards the end of this decade, Diamond Light Source will go 'dark' a considerable period meaning access will be unavailable for around 2 years – this instrument will provide an ideal alternative/stop gap for the current user community, ensuring that a large amount of on-going science can continue.

In the last two years we have transformed two new electron diffraction laboratories into an efficient user-facing unified facility and promoted it to the academic crystallography user community, established governance, developed an access mechanism that has seen considerable use, and begun to publish high quality outputs from it. There are several areas where the electron diffraction facility is pioneering advances in the technique which we ultimately expect to become routine service offerings. We are leading the development of Energy Dispersive X-ray Spectroscopy to analyse particle composition and correlated it with structure determination – this is now routine in our laboratory, however some integration work (at the software level) is still required for it to be operated seamlessly. Development of sample preparation protocols for different samples e.g. air sensitive, hygroscopic, 'charged', and their phase e.g. wet, lumpy, powder, etc. is on-going. We have an associated PhD studentship developing a gas cell holder for electron diffraction, however this is a long-term project and will take some time before routinely available as a service offering. However, following the concept of the development of sample environments for electron diffraction, we recently purchased two air-free sample holders. These are being commissioned at the time of writing, however this is progressing very well and we soon expect to be one of the only electron diffraction facilities in the world that can routinely offer the handling of highly air sensitive samples.

As the current NCS funding period comes towards its end, we have been reflecting on the outstanding success of the electron diffraction operation. There is no doubt this technique is pushing the frontiers and enabling the generation of crystal structures from samples in a whole new size regime an order of magnitude smaller. This capability has been funded by two coupled EPSRC Strategic Equipment grants, now at an end, but been made accessible throughout the country by leveraging the philosophy and existing processes of the NCS. The demand is high and increasing number of outputs are of significant impact and therefore the inclusion of this step change in crystallography into the NCS is a clear route that must be taken. Further, we lead the advancement of the technique in the sense of making it widely available and developing methodologies to address the requirements of chemistry and materials science communities eg developing routine air sensitive equipment and methods. The case and plans for this unified facility capability are well advanced, have been shared with the EPSRC secretariat and will form the basis of the next generation NCS.

The establishment of a commercial electron diffraction service has been touched on elsewhere in this report, with thorough planning and the taster days being very successful. During the coming period the service will ramp up and enable an exploration of the level of service we can provide, the size of the potential market, and the requirements of the market/different sectors (some may simply require structure analysis, while others might require more advanced methods or 'project-level' support). We are ideally placed with the new Southampton CChES research consultancy to understand and capitalise on the market to develop a thriving new component of the NCS. The industry interactions we have already initiated, which have produced income already comparable to the X-ray service, illustrate the potential. Further, this area of activity aligns to industry strategy, and so we fully expect to develop more, stronger partnerships and leverage new funding opportunities.

Additional Information

During this period Prof Joke Hadermann (Univeristy of Antwerp), Dr Tanya Ronson (University of Cambridge) and Dr Royston Copley (GSK) joined the SAP as international representative, supramolecular chemistry representative and industrial representative respectively.

NCS has key strategic collaborations and partnerships with numerous *Organisations* and *Facilities*:

- Newcastle University deliver the ENaCt crystallisation service, as well as dedicated high pressure and ultra-low temperature facilities.
- Diamond, through beamline I19 (EH1) are formally key partners in delivering the NCS.
- University of Warwick partners in the delivery of the NEDF facility.
- SJC is also the Director of the Physical Sciences Data-science Service (PSDS). A parallel activity, the Physical Sciences Data Infrastructure (PSDI) is also led by Simon.
- SJC advised on establishing the NXCT NRF and sits on management advisory panel of the Southampton site. Through Simon, PSDI is connecting with NRFs, most notably HarwellXPS and NXCT, to support data management needs.
- A collaboration with the ISIS neutron source to streamline access to the SXD beamline.
- SJC leads the Quantum Crystallography community EPSRC funded QuantumBox project in partnership with Durham University.
- SJC chairs the IUCr Committee on Data and is a founding editor of IUCr 'Raw Data Letters'.
- SJC leads the EPSRC funded Crystal Sponge by Electron Diffraction project in partnership with the University of Glasgow

NCS participates in student exchange, training and collaborative projects/papers with the following *international* institutions:

- X-TechLab (Benin): in-part built on the NCS model and SJC acted as an advisor. The service manager visited NCS for a 3-month residential training and NCS has provided training courses in Benin twice and resulted in a Royal Society International Exchange Grant.
- University of Ghana and KNUST: SJC ran training workshops (Leverhume and Royal Society) and helped organise the Pan-african Conference on Crystallography in Accra.
- UCAD Senegal: Ibrahima Thiam training visit in 2021, 15 papers published.
- Yaounde University (Cameroon): SJC provided a training course, resulting in several papers.
- University of Cagliari: 25-year collaboration with >50 joint papers and several exchange visits (SJC visiting Prof providing training in Cagliari and to visitors to NCS over 2 decades).
- Zonguldak & Gebze (Turkey): SJC visiting academic, providing training both in Istanbul and through researchers visiting the NCS - continual stream of papers and training visits.
- University of Salahaddin (Kurdistan, Iraq): two papers published.
- Electron Diffraction is causing many international approaches, which we evaluate carefully on our demand/capacity, strength of the science and potential to develop methods. Of particular note is a collaboration with the crystallographer at Kings College London, Lygia Silva de Moraes, who has just been awarded a grant from their national funding agency in collaboration with NCS to provide a modest amount of access to the Southampton NEDF site for Brazilian researchers (https://sites.google.com/view/difracaoeletrons/p%C3%A1gina-inicial). Lygia will conduct the experiments, effectively optimising effective instrument use.
- NCS aims to be an international driving force moving Electron Diffraction forward. We have established connections with the main groups building software e.g. DIALS (STFC/CCP4), CrysAlisPro (Rigaku), Olex2 (Durham) & PETS/Jana (Prague) and driven the formation of a user community with others that now have the same instrumentation (Warwick, Glasgow, Liverpool, Catalunya, Copenhagen, NorthWestern, Yale and Lille).