communications chemistry

A Nature Portfolio journal

Comment

https://doi.org/10.1038/s42004-025-01519-w

BioStruct-Africa's capacity building workshops as a model for advancing the emerging community of structural biologists in Africa

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Structural biology is crucial in understanding disease mechanisms and in driving drug and vaccine development—applications that are particularly relevant to Africa's challenges—yet Africa faces significant barriers to advancing structural biology. Here, the authors outline a recent capacity building workshop run by BioStruct-Africa, focused on training of artificial intelligence tools such as AlphaFold, designed to foster a highly skilled community of structural biologists in Africa.

The need for capacity-building in structural biology in Africa

Structural biology is crucial in understanding disease mechanisms, driving drug and vaccine development, and advancing fields such as agriculture, biotechnology, food safety, and environmental sustainability. These applications are particularly relevant to Africa's challenges, aligning with the United Nations Sustainable Development Goals (SDGs), including Good Health and Well-being (SDG 3), Zero Hunger (SDG 2), and Clean Water and Sanitation (SDG 6)[1]. The continent faces a disproportionate burden from neglected tropical diseases, droughts, and limited access to clean water. Notably, African researchers contribute to one-third of global publications[2] in tropical medicine.

Despite its importance, Africa faces significant barriers to advancing structural biology. The continent has significantly progressed in the last two decades but contributes less than 8% to global scientific knowledge[2]. Progress is further hampered by inadequate infrastructure, brain drain, and limited funding for research[3,4]. African scientists who remain on the continent and those in the diaspora who consider returning often face daunting resource gaps compared to their peers in more developed regions.

Recent breakthroughs, such as AlphaFold[5], offer a transformative opportunity for the field and democratize access to cutting-edge methods[6,7]. AlphaFold is a state-of-the-art artificial intelligence (AI) tool developed by Google DeepMind for highly accurate protein structure prediction and was co-awarded the 2024 Nobel Prize in Chemistry.

However, unlocking AlphaFold's full potential requires more than access to the tool: scientists must receive proper training to use it effectively. A lack of training and awareness about structural biology tools and techniques in Africa represents a critical bottleneck. This gap impedes the ability of researchers to address the continent's health challenges independently. Capacity-building initiatives in structural biology, focused on training and infrastructure development, are vital for equipping African scientists to lead research on neglected diseases, develop sustainable healthcare solutions, and contribute to global scientific advancements.

The non-profit organization BioStruct-Africa was established in 2017 to address this critical gap. By integrating remote access to specialized facilities with AI-driven techniques, and personal mentoring, its capacity-building workshops foster a highly skilled community of structural biologists in Africa[8,9].

BioStruct-Africa's journey and approach

BioStruct-Africa is a not-for-profit organization registered in Sweden and Ghana. Founded in 2017 by Dr. E. Nji, Dr. D. Traore, and Dr. M. Ndi, it is led by Dr. E. Nji as CEO. Through hands-on workshops at partner institutions and universities, complemented by online mentoring, BioStruct-Africa aims to establish a sustainable community of Africa-based structural biologists. BioStruct-Africa covers participants' travel, accommodation, registration, and visa fees—an essential support given the challenges of free cross-border travel within the continent. A diverse network of scientists and policymakers supports the initiative.

BioStruct-Africa's workshops and activities have received significant support in the form of grants, awards, provision of venue, reagent donations, and expert lectures from esteemed organizations, including the Company of Biologists in the United Kingdom (UK), the Royal Society of Chemistry, Chemical and Biology Division (UK), the Canadian Light Source (Canada),

the African Crystallography Association, Diamond Light Source (UK), the European Synchrotron Radiation Facility (France), Google (Ireland), Google DeepMind (UK), the Swedish Research Council (Sweden), Formas (Sweden), the International Union of Crystallography (UK), Schrödinger in the United State of America (USA), the SBGrid Consortium, Havard Medical School (USA), MiTeGen (USA), University of Ghana (Ghana), Malaria Research and Training Centre (Mali) and the International Livestock Research Institute (Kenya)

Since 2019, BioStruct-Africa has conducted three workshops across Africa, attracting 60 participants selected from close to 300 applicants. Demand for these workshops consistently exceeds availability, with oversubscription rates reaching close to five times the number of available spots in 2024.

The inaugural workshop in 2019, held at the University of Ghana, provided hands-on training in crystallization, cryo-cooling of harvested crystals, and remote data collection via the Diamond Light Source in the United Kingdom[3]. In 2020, two planned workshops— in Rwanda and Malawi—were canceled due to the COVID-19 pandemic. These workshops were intended to cover crystallization, cryo-cooling, and imaging, with data collection at the European Synchrotron Radiation Facility (ESRF)[10]. The 2022 workshop at the Malaria Research and Training Center in Bamako, Mali, expanded on previous programs by incorporating Cryogenic Electron Microscopy (cryo-EM) data collection, complementing synchrotron radiation-based structural analysis[4]. The most recent workshop, held in October 2024, will be detailed in the following sections[8].

Generally speaking, structural biology, with its recent technological advancements, is particularly suited for capacity-building initiatives in Africa. The field has embraced automation and remote experimentation at research infrastructures, such as synchrotron radiation sources, abroad - nearly all located in the Global North. Moreover, AI-powered tools like AlphaFold have enabled researchers to perform complex analyses with minimal physical infrastructure. Combining these tools with bioinformatics, data or visualization software allows advanced research to be conducted with a stable internet connection, reducing dependency on expensive, location-specific facilities[11].

BioStruct-Africa takes a holistic approach in its workshops, guiding participants through the entire process—from formulating research questions to leveraging complementary modeling tools like AlphaFold, conducting experimental validation using remote access to synchrotron light sources, and performing post-experimental data analysis (Fig. 1). When defining research questions, the focus is placed on identifying the specific protein or protein complex under study and determining the primary objective (e.g., functions, interactions, or drug-binding potential). AlphaFold can then generate computational models of protein structures, providing a cost-effective and efficient starting point for structural predictions. These predictions guide experimental designs and hypotheses but often require validation due to limitations with flexible regions or large complexes. Experimental validation using synchrotron techniques follows if needed. High-resolution data collection methods, such as X-ray crystallography or small-angle X-ray scattering (SAXS), provide experimentally verified

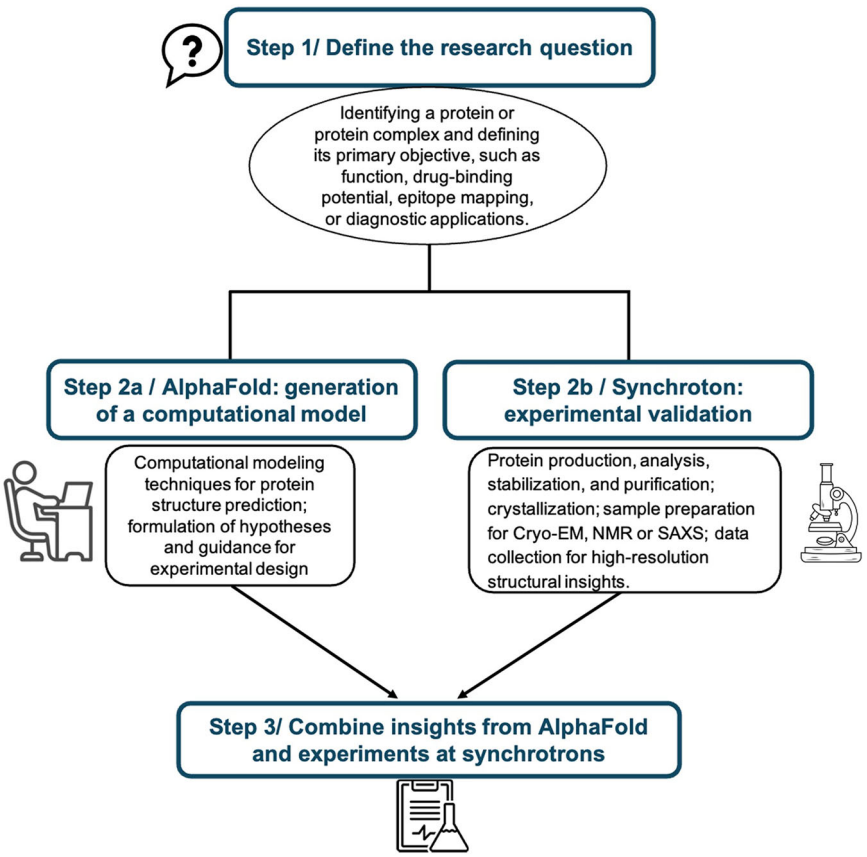

Fig. 1 | Workflow for protein structure determination and validation. (Step 1) Definition of the research question: Identification of the protein/protein complex and its primary objective. (Step 2a) Computational modeling using AlphaFold for structure prediction and hypothesis generation. (Step 2b) Experimental validation using synchrotron-based techniques, including X-ray Crystallography, Cryo-EM, and SAXS. (Step 3) Integration of computational and experimental insights for structural analysis.

structural insights. Protein samples are prepared, data is collected (often remotely), and structures are refined to achieve accurate models, particularly for active and binding sites or dynamic regions. Finally, the integrated data is analyzed in the context of the research question, advancing understanding of protein function, informing drug design, and exploring molecular mechanisms or evolutionary relationships. This comprehensive training equips African scientists to independently tackle pressing research challenges and contribute effectively to global scientific progress.

Design of BioStruct-Africa's fifth workshop

BioStruct-Africa's fifth workshop was held from 7 to 11 October 2024 in Douala, Cameroon. Building on the experience of previous workshops, this edition refined its structure, extended its duration, and broadened its outreach to a more diverse and interdisciplinary participant pool. The framework of this workshop can highlight a replicable model for capacity building in structural biology across the continent.

The primary objectives of the workshop included equipping participants with cutting-edge techniques and tools, fostering cross-border collaboration among African scientists, and enabling participants to apply their skills to practical contexts, including drug discovery, disease research, and structural biology capacity building.

The participant selection process emphasized diversity in geographical location, scientific discipline, and professional background. Applications were reviewed rigorously, and motivational letters were analyzed to align participants' research interests, professional backgrounds, and personal motivation with the workshop's goals.

The workshop's structure was deliberately extended to ensure deeper engagement with its theoretical and practical components. The agenda comprised three primary segments: expert lectures, hands-on training sessions, and a live demonstration of remote data collection.

First, two expert lectures (30 min each) on the principles and significance of structural biology provided participants with a strong theoretical base. The lectures traced the history of fundamental discoveries, from the identification of amino acids to ground-breaking advancements in protein crystallography and Deoxyribonucleic acid (DNA) structure elucidation. Techniques such as X-ray crystallography, Cryo-EM, nuclear magnetic resonance (NMR) spectroscopy, and SAXS were highlighted for their roles in determining macromolecular structures, emphasizing their applications in drug design and understanding biological mechanisms.

Second, hands-on training sessions offered practical experience with advanced tools and platforms. AlphaFold: An overview of AlphaFold's impact on molecular prediction and key limitations was presented by Google DeepMind, as well as the advancements in AlphaFold3[12], which now supports a broader range of molecular predictions and a dedicated server for life scientists. Participants received hands-on training using the AlphaFold2 database[5] and the AlphaFold3 web server[12] for protein structure prediction. The sessions focused on guiding attendees through the workflow, including input preparation, structure prediction, and result interpretation. The sessions emphasized understanding key metrics essential for structural prediction studies, including pLDDT (predicted Local Distance Difference Test), PAE (Predicted Aligned Error), pTM (Predicted Template Modeling), and ipTM (Interfaced Predicted Template Modeling) (Fig. 2). pLDDT measures local confidence, scaled from 0 to 100, with a color gradient output where blue indicates high confidence (Fig. 2). PAE evaluates confidence in the relative position of two residues, while pTM and ipTM assess the overall quality of predicted complexes (Fig. 2). An ipTM score of 0.8 or higher

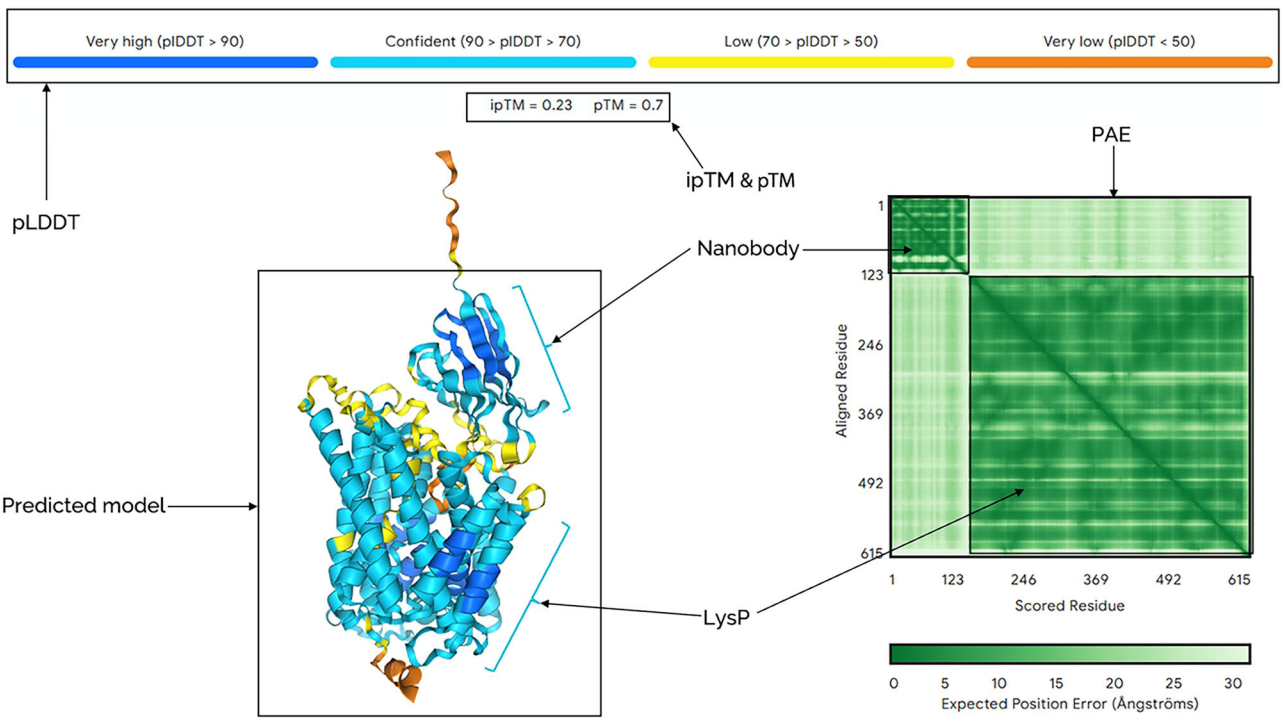

Fig. 2 | Structural prediction of the *Pseudomonas aeruginosa* lysine-specific permease (LysP) in complex with a LysP-specific nanobody, based on amino acid sequences and performed using the AlphaFold3 web server. A snapshot from the AlphaFold3 Server showing important metrics: pLDDT, pTM, ipTM, PAE and the predicted model of the LysP-nanobody complex.

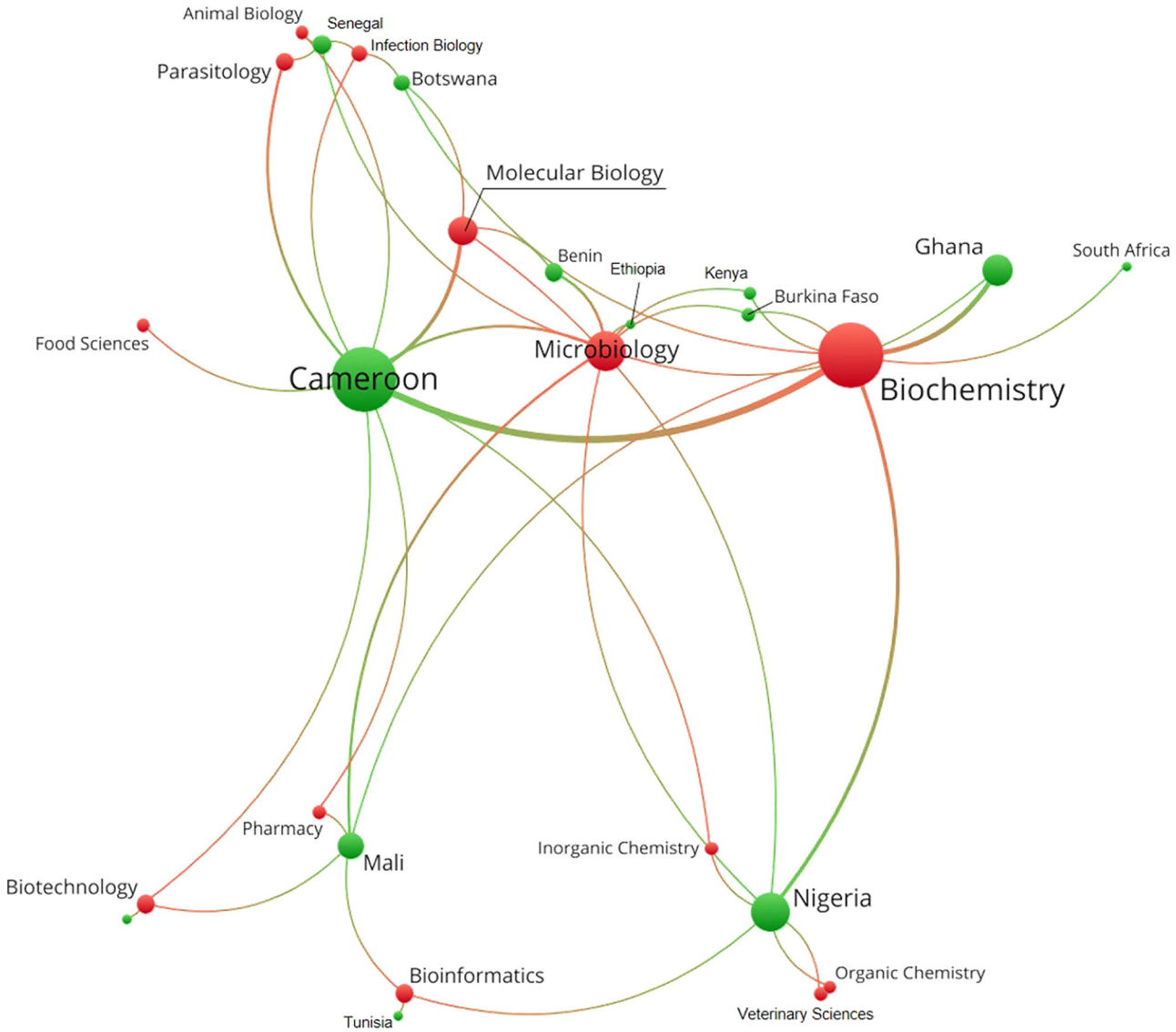

Fig. 3 | Bipartite network of countries of institutional affiliations and scientific disciplines. This network visualization displays two node types: scientific disciplines (red) and countries of institutional affiliation (green). Edges indicate connections formed through applicants, linking specific disciplines to affiliated countries. The network highlights a concentration in biochemistry and strong representation from West African institutions, while also reflecting a broader pan-African engagement across scientific fields.

indicates a high-quality structure, while values below 0.6 suggest a failed prediction. Scores between 0.6 and 0.8 require cautious interpretation. During the training, participants also conducted an experiment comparing AlphaFold2/3 predicted structures of an amino acid transporter to the experimentally determined cryo-EM structure[13]. Using the abovementioned metrics, they assessed the quality of the predicted models. Additionally, they practiced fitting the AlphaFold3 model into the cryo-EM density map of the protein, gaining hands-on experience in integrating computational predictions with experimental data.

Schrödinger LLC (New York, USA) including Glide, Prime, FEP +, PyMOL. Senior scientists from Schrödinger delivered a presentation of their computational chemistry platform, which integrates physics-based modeling and machine learning to accelerate drug discovery. Schrödinger offers solutions across the drug discovery process, from target validation and hit identification to lead optimization and preclinical development. Key components of their platform are Glide[14] for small-molecule docking, Prime[14] for protein structure prediction and refinement, and Free Energy Pertubation (FEP +)[14] for predicting protein-ligand binding affinity at an accuracy matching experimental methods. Together with the rest of the Schrödinger software suite, these products facilitate efficient, multi-parameter optimization of drug candidates, addressing issues such as potency, solubility, and selectivity. In addition, Schrödinger demonstrated Python Based Molecular Graphic (PyMOL)[15], guiding users through steps ranging from downloading and preparing Protein Data Bank (PDB) files to manipulating molecular representations within PyMOL's user interface.

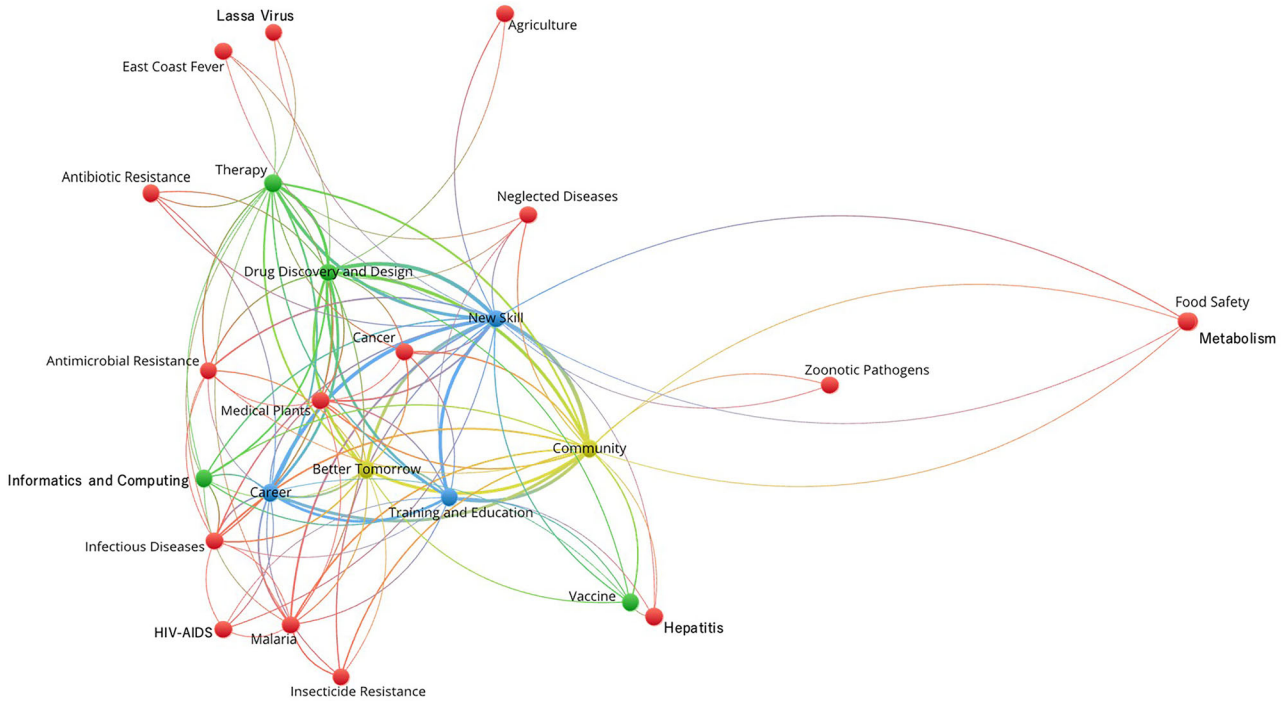

Fig. 4 | Thematic network of applicants' motivational letters. This network visualization categorizes key themes (colored nodes) from applicants' letters, illustrating their interconnections. A qualification triangle (blue) links themes related to skill acquisition, training, and career aspirations. Other clusters highlight research interests such as infectious diseases, antibiotic resistance, and neglected diseases. The figure emphasizes the diverse motivations and focal areas of the applicants.

The participants were taught how to identify and highlight specific protein residues that interact with ligands, generate different representations of molecules and create images suitable for publication. The practical exercises provided an understanding of protein-ligand interactions, structural alignments, and in-silico mutagenesis. The instructors also walked the participants through recent updates of Maestro[16] and how to carry out docking studies and compound library screening. Then, they introduced Glide with Electrostatic Map (GlideEM)[17], a variant of Glide that docks small molecules into electron density maps, and Phenix/Optimized Potential for Liquid Simulations 3e (Phenix/OPLS3e)[18], a technology for structure refinement that combines Schrödinger's OPLS3e forcefield with experimental density data to improve structure quality and reduce overfitting.

ChimeraX. Participants explored University of California, San Francisco's (UCSF) ChimeraX[19], a software tool optimized for molecular visualization, handling large datasets, and integrating with AlphaFold. During this session, they learned how to load structural data, use advanced visualization tools, fit AlphaFold models into cryo-EM maps, and create high-quality molecular images and movies. The demonstration of Chimera X was made possible through a collaborative partnership, the SBGrid Consortium at Harvard Medical School and Meharry Medical College (MMC), that organizes workshops that demonstrate the array of structural biology software, mainly focusing on ChimeraX and cryo-EM data processing software (e.g., CryoSPARC and Relion), for new and continuing structural biology mentors. A part of the US-American National Institutes of Health National Institute of General Medical Sciences (NIH NIGMS) Innovative Programs for Enhancing Research Training (IPERT), this program aims to increase access to advanced structural biology tools and research, particularly among faculty at small and Minority-Serving Institutions (MSIs). As part of this funded program, participants received hands-on training on how to visualize protein structure and manage data using ChimeraX in the easy-to-use SBGrid software environment, which supports access to over 500 scientific applications. With ChimeraX being completely free, all participants could download the software and run the exercises on their laptops.

Coot and Phenix. Coot[20] and Phenix[21], two widely used protein structure analysis and refinement programs, were introduced to participants. The workshop's practical sessions utilized these tools to help participants gain protein modeling and validation proficiency. Participants used Coot to visualize electron density maps generated from cryo-EM data. The workshop taught participants how to manipulate protein structures within these maps by fitting amino acid residues, adjusting side chains, and correcting structural errors. In practical exercises, participants built and refined protein models, enhancing their experience interpreting electron density data and improving model accuracy. The Phenix software, on the other hand, was used as a tool for refining and validating the protein structures constructed by participants. The software helped automate many aspects of the refinement process, ensuring that the experimental data fit the atomic models accurately. It was particularly helpful in improving the precision of model fitting, making them suitable for further biological interpretation and research applications.

PyRx and open Babel. Docking helps researchers to identify and optimize compounds that interact specifically with target macromolecules, thereby accelerating the development of new drugs in the early stages. This session covered practical aspects of setting up docking simulations, preparing receptor and ligand files, and analyzing docking results. The focus was on

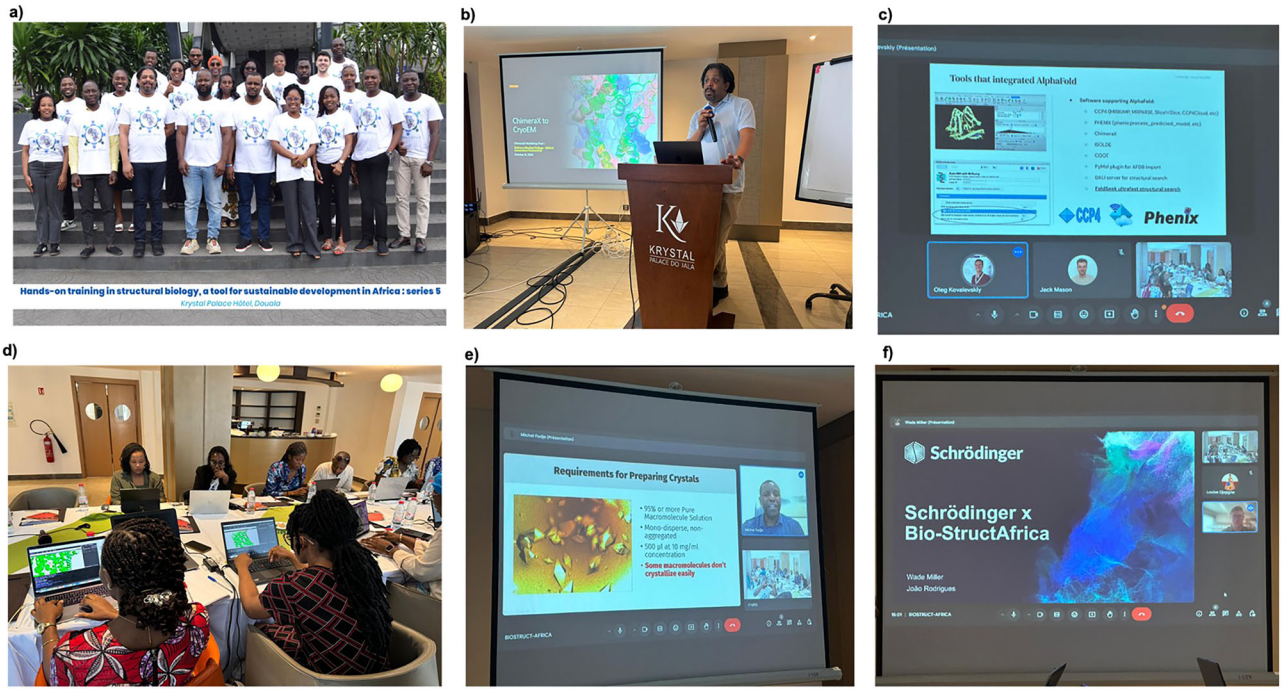

Fig. 5 | Snapshots of key moments reflecting the workshop's interactive, hybrid, and interdisciplinary approach. a Group photograph of participants and facilitators. **b** Presenter delivering a session on structural biology techniques, showcasing the integration of tools like ChimeraX and CryoEM. **c** Virtual presentation featuring tools integrated with AlphaFold. **d** Hands-on session with participants actively engaging in computational exercises. **e** Presentation on requirements for preparing crystals, addressing practical challenges in macromolecular crystallization. **f** Collaborative session by Schrödinger and BioStruct-Africa, demonstrating cutting-edge software applications in structural biology and drug discovery. The authors affirm that informed consent for publication of the images in this Figure was obtained from the identifiable individuals.

binding affinities and interactions between binding sites. Participants used PyRx[22], which integrates tools such as AutoDock Vina[23] and Open Babel[24] and helps to simplify complex docking workflows, making multiple compounds easily screenable against macromolecular targets. Participants first used Open Babel to prepare the proper extension for molecules to create a chemical screening workflow on the provided amino acid transporter structure. This workflow provided the ease and flexibility to screen through 300 compounds and to compare their energy-binding affinities and poses.

Third, the workshop participants received a live demonstration of a remote data collection experiment at a synchrotron beamline and a lecture on various methods for preparing and shipping samples for synchrotron macromolecular X-ray crystallography. A remote connection to the Canadian Light Source Macromolecular Crystallography Facility (CMCF) enabled participants to see all aspects of the synchrotron data collection process, including sample alignment, data collection and processing.

Finally, collaborative discussions encouraged knowledge sharing and fostered a sense of community, enabling participants to discuss how their training applied in their respective fields. The integration of customized learning pathways with post-monitoring and mentoring ensured that the workshop remained accessible and relevant to all participants, regardless of their prior experience.

Impact and added value of the workshop

Although previous workshops also gathered participant feedback, this fifth workshop in Cameroon was the first time a comprehensive assessment of the impact and added value was conducted, incorporating qualitative and quantitative analysis of the participants' applications and feedback.

The participants constituted a cross-border community of African researchers who identify with similar academic fields and share scientific interests. We observed a connected network with common professional expertise by examining the relationship between applicants' countries of institutional affiliation (green nodes, Fig. 3) and their scientific disciplines (red nodes, Fig. 3). Within this network, biochemistry is the dominant discipline with strong ties to applicants from Cameroon, Ghana, Burkina Faso, Kenya or South Africa. The high number of applicants from West African countries is unsurprising, given that the workshop was held in Cameroon. While there is a strong emphasis on West African countries, the pool of applicants also included individuals from Ethiopia, Egypt, Kenya, or South Africa, highlighting interest from across the continent. By leveraging its location, the workshop in Cameroon strategically attracted a significant number of participants from West Africa while maintaining a pan-African focus.

Figure 4 illustrates the network derived from analysing the applicants' motivational letters, which were categorized into thematic tags. On the one hand, Fig. 4 highlights a qualification triangle (blue), linking thematic tags such as "new skill", "training and education" and "career". Most applicants expressed that participating in the workshop would enable them to expand their knowledge, acquire new skills, and enhance their professional portfolios as researchers. Additionally, many applicants emphasized their intention to apply these skills and knowledge in practical contexts, such as therapy, drug discovery, and design. On the other hand, this focus on career

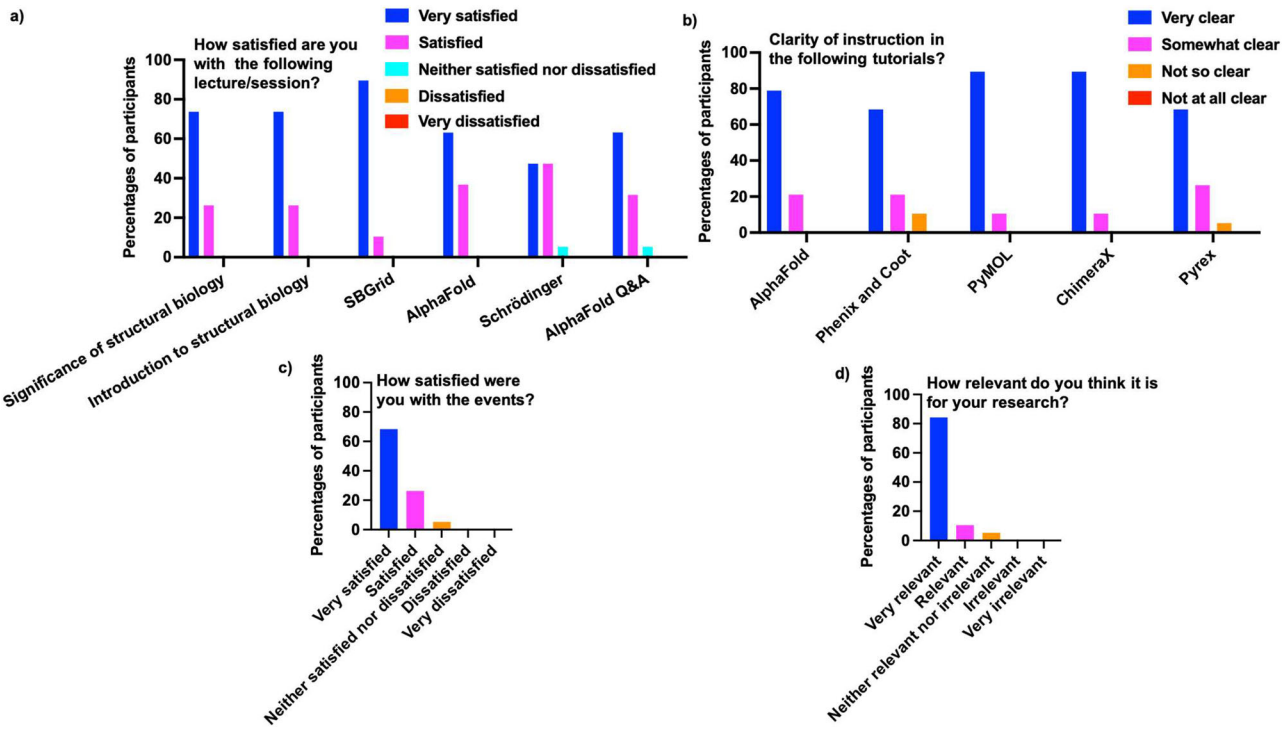

Fig. 6 | Participant feedback on lectures, tutorials, events, and research relevance. **a** Satisfaction levels with various lectures/sessions. **b** Clarity of instruction in tutorial sessions. **c** Overall satisfaction with event organization. **d** Perceived relevance of the event to participants' research. Results indicate a predominantly positive response across all aspects.

advancement and professional qualification was often tied to a broader, community-centered narrative (yellow). One applicant stated being

> "[…] determined to using the information and skills I obtained from this program to solve major challenges in Africa and to help the scientific community enhance health and well-being across the continent".

Similarly, another one expressed the wish to

> "[…] play a vital role in improving the lives of individuals, communities, and the entire continent of Africa."

Applicants frequently stated their desire to contribute to the collective development of structural biology in Africa by sharing their skills and experiences ("community"). The applicants often envisioned themselves as part of a motivated workforce and a new generation of highly skilled researchers, aiming to make a lasting impact on the continent's future and the health and well-being of its population, striving for a better and sustainable future ("better tomorrow").

While the community shared a common motivation for joining the workshop, their research areas and applications are thematically diverse. At the network's periphery (Fig. 4, red nodes), we observed a wide range of research specializations, reflecting the community's broad expertise, spanning topics such as agriculture, food safety, antibiotic resistance or neglected diseases. At the same time, these diverse specialties also underline Africa's unique and urgent health challenges, such as research on neglected diseases, Lassa virus, East Coast fever, and the enhanced use of medicinal plants for alternative drug development.

The workshop participants represent the foundation of an emergent scientific community of African structural biologists, united by shared interests, professional development, and skills. Figure 5a–f illustrates key moments reflecting the interactive, hybrid, and interdisciplinary approach of the workshop. This collaborative network illustrates the cross-disciplinary nature of structural biology and its ability to transcend national boundaries. They are motivated to enhance their skills, expand their knowledge, and contribute to forming a continent-wide scientific community. Scholarship in the social sciences has identified such dynamics as critical for developing strong scientific capacities. The successful construction and operation of a future African Light Source (AfLS), the first on the continent, will depend on the strength of robust scientific networks and ecosystems. These infrastructures are collaborative hubs, providing researchers with cutting-edge technology and fostering knowledge exchange to drive scientific advancements. However, without a well-established community of skilled researchers, these facilities may struggle to realize their full potential[25,26]. Second, emerging scientific networks provide the foundation for breakthroughs and significant scientific advances. Well-connected scientific communities foster the exchange of ideas, mentorship, and interdisciplinary collaboration—key drivers of innovation[27].

The workshop participants evaluated the expert lectures, tools, presentations, and facilitators as part of the assessment. To measure the impacts and achievements of the hands-on training, they completed a pre-test at the beginning and a post-test at the end of the workshop. The participants' evaluations across various aspects of the training were analyzed and broken

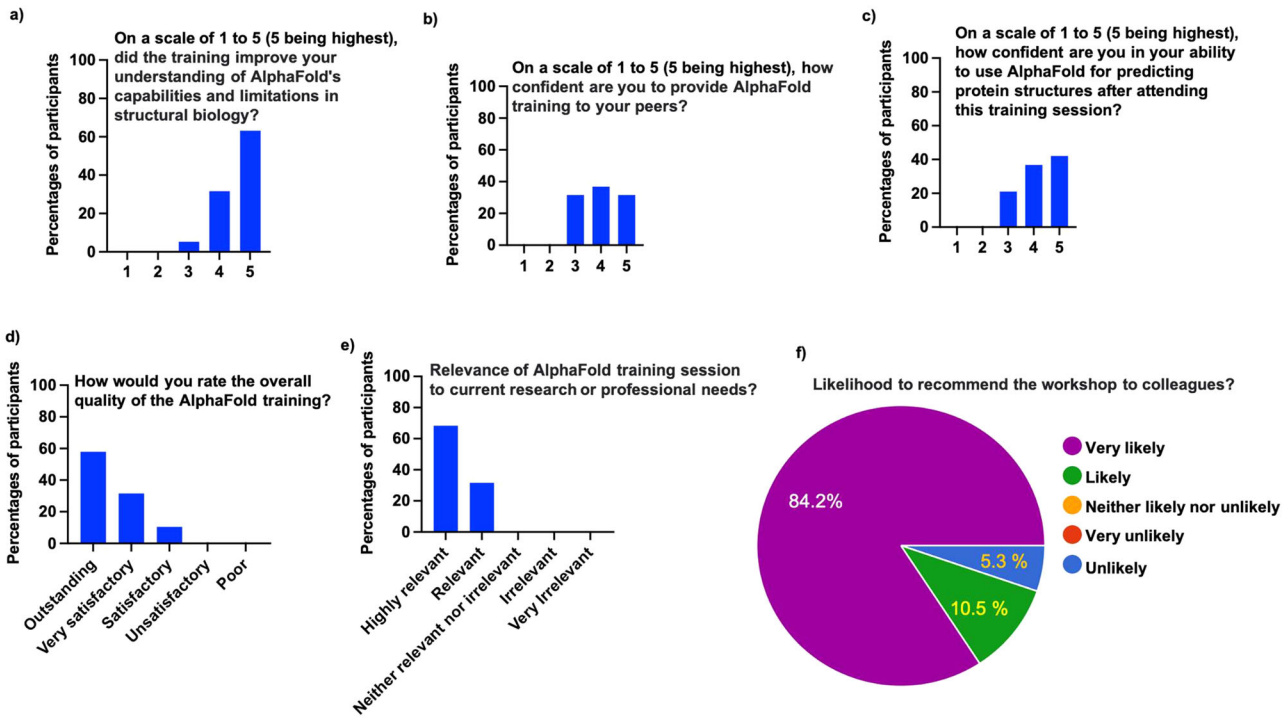

Fig. 7 | Evaluation of workshop participants' feedback on AlphaFold training. **a** improvement in understanding AlphaFold's capabilities and limitations. **b** confidence in providing AlphaFold training to peers. **c** improved confidence and ability to use AlphaFold for predicting protein structures. **d** overall quality of the AlphaFold training. **e** relevance of the training to their current research or professional needs. **f** The likelihood of participants recommending the workshop to colleagues.

down by categories of lectures/sessions, tutorials and tools/techniques. Most participants showed great satisfaction with the expert lectures (Fig. 6a). This helped provide a strong theoretical background for the subsequent hands-on training sessions.

The SBGrid session highlighted sample structural biology workflows on the SBGrid platform, thereby bridging the background theoretical sessions with the hands-on sections. Analysis showed that the session received highly positive feedback, with the majority of participants expressing strong satisfaction in understanding the structural biology workflow provided by the consortium (Fig. 6a).

Other sessions and tutorials rated high by the participants include the AlphaFold and Schrödinger software suite, indicating strong interest and satisfaction in learning protein structure prediction and applications in drug discovery (Fig. 6a, b). The tools for structural determination and refinement (Phenix and Coot) also scored well, with some variability among participants, suggesting a mix of experiences or confidence levels (Fig. 6b). Structure visualization and analysis tools including ChimeraX and PyMOL were also rated positively (Fig. 6b).

It is worth noting that the majority of participants were very satisfied (Fig. 6c) and rated the tools and techniques learned as highly relevant to their current and future research (Fig. 6d). This indicates the workshop's general effectiveness in addressing the participants' research needs. Overall, the evaluation by the participants suggests that the workshop was well-received, with practical and theoretical components effectively covering essential techniques in structural biology.

Evaluation of the participant's feedback on AlphaFold reflects the overall effectiveness and relevance of the AlphaFold training session as depicted in Fig. 7. There was an improvement in the participants' understanding of the capabilities and limitations of AlphaFold in structural biology (Fig. 7a). The confidence and ability of the participants to use and provide training on AlphaFold to peers was enhanced (Fig. 7b, c). Furthermore, most participants rated the training as outstanding and demonstrated strong relevance to the training to their current research or professional needs (Fig. 7d, e) as most participants are willing to recommend the workshop to others (Fig. 7f).

High relevance ratings and strong recommendations affirm the training's alignment with participants' needs. Confidence ratings indicate the development of teaching skills, empowering participants to disseminate their learning. This aligns with the goal of BioStruct-Africa, which is geared towards empowering Africa-based scientists through education, structural biology knowledge transfer, and mentoring. A lower rating of a few participants of their confidence or the relevance of the training suggests areas for improvement and the need for follow-up support.

Future directions for capacity building in structural biology in Africa

The fifth BioStruct-Africa workshop in Cameroon in October 2024 can be a model for designing impactful structural biology training programs. Combining theoretical knowledge, hands-on experience, and community-building efforts, it addressed the needs of African scientists while fostering collaboration and capacity building. Moving forward, the integration of systematic impact assessment and community monitoring, enhanced inclusivity, and scalable practices will be pivotal in strengthening structural biology capacity-building across the continent. This approach will ensure

African researchers are well-positioned to make meaningful contributions to global scientific progress.

Several recommendations are proposed to guide future initiatives: First, future workshops should incorporate follow-up support mechanisms, such as online mentorship programs, collaborative forums, or video tutorials, to reinforce learning and address participants' confidence gaps. Second, efforts should continue to ensure broader representation by including participants from underrepresented regions, institutions, and disciplines. This will help create a more equitable distribution of structural biology expertise across Africa. Third, workshops should integrate real-world case studies or projects to demonstrate the practical applications of training in fields such as drug discovery, disease research, and biotechnology. Fourth, to ensure sustainability, best practices from these workshops should be documented and shared widely. This will facilitate replicating successful models in other regions and institutions across the continent.

Funding remains a critical and persistent challenge. Capacity building in African structural biology still largely depends on public funding, primarily from major European and U.S.-based organizations. These funds are vital in supporting individuals, research communities, and institutions, facilitating expertise development and infrastructure growth. However, securing sustainable funding sources within Africa will be essential for long-term progress. Equally important is the need for long-term monitoring, which should become a cornerstone of BioStruct-Africa's efforts. Implementing systematic methods to track training initiatives' scientific and socio-economic impacts over time will provide valuable insights. By regularly assessing workshop outcomes—such as career advancements, research productivity, and the expansion of collaboration networks—it will be possible to measure their contributions to strengthening African structural biology capacity. Additionally, these insights can help refine and enhance workshop content and methodologies, ensuring continuous improvement and more significant impact.

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Received: 23 December 2024; Accepted: 8 April 2025;
Published online: 19 April 2025

References

1. Morton, S., Pencheon, D. & Squires, N. Sustainable Development Goals (SDGs), and their implementation: a national global framework for health, development and equity needs a systems approach at every level. *Br. Med. Bull.* **124**, 81–90 (2017).
2. Sooryamoorthy, R. Science in Africa: contemporary trends in research. *J. Scientometr. Res.* **10**, 366–372 (2022).
3. Nji, E., Traore, D. A. K., Ndi, M., Joko, C. A. & Doyle, D. A. BioStruct-Africa: empowering Africa-based scientists through structural biology knowledge transfer and mentoring - recent advances and future perspectives. *J. Synchrotron Radiat.* **26**, 1843–1850 (2019).
4. Ouologuem, D. T. et al. Hands-on training in structural biology, a tool for sustainable development in Africa series 4. *Biol. Open* **11**, bio059487 (2022).
5. Jumper, J. et al. Highly accurate protein structure prediction with AlphaFold. *Nature* **596**, 583–589 (2021).
6. Subramaniam, S. & Kleywegt, G. J. A paradigm shift in structural biology. *Nat. Methods* **19**, 20–23 (2022).
7. Yang, Z., Zeng, X., Zhao, Y. & Chen, R. AlphaFold2 and its applications in the fields of biology and medicine. *Signal Transduct. Target. Ther.* **8**, 1–14 (2023).
8. Nji, E. et al. Supporting structural biologists in Africa requires resources and capacity building. *Nat. Struct. Mol. Biol.* **31**, 1814–1815 (2024).
9. Nji, E. et al. Leveraging AlphaFold for innovation and sustainable health research in Africa. *Nat. Commun.* **16**, 1334 (2025).
10. Cancelled Workshops, 2020. *BioStruct-Africa* https://www.biostructafrica.org/cancelled-workshops-2020.
11. Mulder, N. J. et al. The development of computational biology in South Africa: successes achieved and lessons learnt. *PLoS Comput. Biol.* **12**, e1004395 (2016).
12. Abramson, J. et al. Accurate structure prediction of biomolecular interactions with AlphaFold 3. *Nature* **630**, 493–500 (2024).
13. Bicer, D. et al. *Structural insights into Pseudomonas aeruginosa lysine-specific uptake mechanism for extremely low pH regulation* https://doi.org/10.1101/2024.05.17.594718 (2024).

14. Bhachoo, J. & Beuming, T. Investigating Protein-Peptide Interactions Using the Schrödinger Computational Suite. *Methods Mol. Biol. Clifton NJ* **1561**, 235–254 (2017).
15. PyMOL | pymol.org. https://www.pymol.org/.
16. Bell, J. et al. PrimeX and the Schrödinger computational chemistry suite of programs. in 534–538 (2012). https://doi.org/10.1107/97809553602060000864.
17. Glide. *Schrödinger* https://www.schrodinger.com/platform/products/glide/.
18. van Zundert, G. C. P., Moriarty, N. W., Sobolev, O. V., Adams, P. D. & Borrelli, K. W. Macromolecular refinement of X-ray and cryo-electron microscopy structures with Phenix/OPLS3e for improved structure and ligand quality. *Struct. Lond. Engl.* **29**, 913–921.e4 (2021).
19. Meng, E. C. et al. UCSF ChimeraX: tools for structure building and analysis. *Protein Sci. Publ. Protein Soc.* **32**, e4792 (2023).
20. Emsley, P. & Cowtan, K. Coot: model-building tools for molecular graphics. *Acta Crystallogr. D Biol. Crystallogr.* **60**, 2126–2132 (2004).
21. Adams, P. D. et al. PHENIX: a comprehensive Python-based system for macromolecular structure solution. *Acta Crystallogr. D Biol. Crystallogr.* **66**, 213–221 (2010).
22. Dallakyan, S. & Olson, A. J. Small-molecule library screening by docking with PyRx. *Chem. Biol. Methods Protoc.* (eds. Hempel, J. E., Williams, C. H. & Hong, C. C.) 243–250 (Springer). https://doi.org/10.1007/978-1-4939-2269-7_19 (2015).
23. Trott, O. & Olson, A. J. AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading. *J. Comput. Chem.* **31**, 455–461 (2010).
24. O'Boyle, N. M. et al. Open Babel: an open chemical toolbox. *J. Cheminform.* **3**, 33 (2011).
25. Wagner, C. *The New Invisible College: Science for Development* (Brookings Institution Press, 2008).
26. Marjanovic, S., Hanlin, R., Diepeveen, S. & Chataway, J. Research capacity-building in Africa: networks, institutions and local ownership. *J. Int. Dev.* **25**, 936–946 (2013).
27. Powell, W. W. & Grodal, S. Networks of Innovators. in *The Oxford Handbook of Innovation* (eds. Fagerberg, J. & Mowery, D. C.) 0 (Oxford University Press). https://doi.org/10.1093/oxfordhb/9780199286805.003.0003 (2006).

Acknowledgements
We acknowledged Wellcome Trust grant number 222999/Z/21/Z and the Google award for "Support for Socially Impactful Research Enabled by AlphaFold in 2024" to E.N. We also thank the Swedish Research Council (grant number 2022-02985 to J.J.G.) and Formas (grant number 2022-02341 to J.J.G.) for sponsoring the workshop. We are grateful to J. Mason, O. Kovalevskiy, and R. Evans from Google DeepMind for delivering lectures and hosting the Q&A session. We also appreciate W. Miller and J. Rodrigues from Schrödinger LLC for their lectures and demonstrations on small-molecule screening. Finally, we sincerely thank S. Tata and the entire staff at Krystal Palace Hotel, Douala, Cameroon, where the workshop took place.

Author contributions
E.N. conceptualized the paper, led the workshop and wrote the manuscript with assistance from S.S., F.G.F., W.H., O.M.O., K.M., I.M., E.A.A., A.T., C.T.F., J.T.J., C.V.T., V.M.T.T-N., D.T.T., B.L.K., T-K.K-A., I.N., T.S.D.S., R.M.N.K., M.F.M.K., Y.C.G., A.F.A.M., K.C.C., N.V.R., L.D., P.S., J.D., M.N.F., and J.J.G.

Competing interests
The authors declare no competing interests.

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Peer review information The manuscript was considered suitable for publication without review.

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