

CCP4/APS School in Macromolecular Crystallography: From Data Collection to Structure Refinement and Beyond

Argonne National Laboratory

June 22 Monday, 2026 - July 7-14, 2026

Chicago Time (CDT)

Virtual Day (Mon June 22): Cryocrystallography and Bioinformatics (zoom link)

9:00 AM	0:30	Introduction: Outline resources and SLACK Arrangements	Charles Ballard
9:30 AM	0:45	Cryo-crystallography	Elspeth Garman
10:15 AM	0:45	Radiation Damage	Elspeth Garman
11:00 AM	0:15	Break	
11:15 AM	0:45	Bioinformatics	Dan Rigden
12:00 PM	1:00	Lunch Break	
1:00 PM	1:00	Introduction to CCP4 and CCP4 Cloud	Charles Ballard / Maria Fando
2:00 PM	1:00	Access to APS and beyond	NECAT & GMCA
3:00 PM	1:00	How to Collect the Best Macromolecular Diffraction Data - Dectris	
4:00 PM	1:00	Enabling Crystallography with Developments from MiTeGen	Joyce Frank/Mitegen

Day 1 (Tue July 7): Data Collection and Processing

8:30 AM	0:05	Welcome and Introduction	Qingping Xu
8:35 AM	0:40	Introduction to the Upgraded APS and MX Capabilities	Bob Fischetti
9:15 AM	1:00	Basic Diffraction Theory	Kamel El Omari
10:15 AM	0:15	Break	
10:30 AM	1:00	Data Collection Concepts and Tips	Graeme Winter
11:30 AM	1:00	Assessing Diffraction Data Quality	Kay Diederich
12:30 PM	1:00	Lunch break	
1:30 PM	1:15	Data Processing with XDS - demo-lecture	Kay Diederichs
2:45 PM	1:15	Data Processing with DIALS - demo-lecture	Graeme Winter
4:00 PM	0:15	Break	
4:15 PM	1:45	GMCA and NECAT Beamline Tour	NECAT & GMCA
6:00 PM	1:30	Data Processing with HKL3000 - demo-lecture	
7:30 PM	1:00	Dinner Break	
8:30 PM	1:30	TBA	

Day 2 (Wed July 8): Data Collection and Processing at GMCA & NECAT

8:30 AM	1:30	Scaling and Merging the Data (Multi-crystal Data)	Graeme Winter
10:00 AM	2:30	Data Collection (coffee available from 10:30 am)	NECAT/GMCA
12:30 PM	1:00	Lunch Break	
1:30 PM	3:00	Data Collection (coffee available from 4 pm)	NECAT/GMCA
4:30 PM	3:00	Data Collection	NECAT/GMCA
7:30 PM	1:00	Dinner Break	
8:30 PM	2:00	Data Collection	NECAT/GMCA

Day 3 (Thu July 9): Data Processing and Experimental Phasing

8:30 AM	1:00	Symmetry	Charles
9:30 AM	1:00	Twinning and Other Pathologies lecture + demo	Andrey Lebedev (Virtual)
10:30 AM	0:15	Break	
10:45 AM	0:30	Tutorial in Dealing with Twinning	Andrey Lebedev (Virtual)
11:15 AM	1:15	Phase Problem and Experimental Phasing (Long Wavelength, Soaks, Identification of Metals)	Kamel El'Omari
12:30 PM	1:00	Lunch Break	
1:30 PM	0:30	Phasing Demo EP	Kamel or Charles
2:00 PM	4:00	Processing Data (coffee available from 4pm)	
6:00 PM	1:30	Student Presentations Part 1	Students
7:30 PM	1:00	Dinner Break	
8:30 PM	1:30	Student Presentations Part 2	Students
10:00 PM		Dataset of the Day and Practical Session	

Day 4 (Fri July 10): Molecular Replacement

8:30 AM	1:00	Molecular Replacement - basics	Randy Read (Virtual) / Airlie
9:30 AM	1:00	Phaser, model prep, docking into CryoEM lectures	Randy Read (Virtual) /Airlie
10:30 AM	0:15	Break	
10:45 AM	0:45	Generating your models	Adam Simpkin
11:30 AM	1:00	Arcimboldo, Shelx for MR	Josep Triviño
12:30 PM	1:00	Lunch Break	
1:30 PM	1:00	Phasing in Phenix	Dorothee Liebschner
2:30 PM	1:00	MR in CCP4 Talk/Demo	Adam Simpkin
3:30 PM	4:00	Practical Session (coffee available from 4pm)	
7:30 PM	1:00	Dinner Break	
8:30 PM	1:30	Dataset of the Day and Practical Session	

Day 5 (Sat July 11): Model Building

8:30 AM	1:30	Introduction to model building and model building in COOT	Lucrezia Capatoni
10:00 AM	0:30	Model Building in Phenix (1)	Dorothee Liebschner
10:30 AM	0:15	Break	
10:45 AM	0:45	Model Building in Phenix (2)	Dorothee Liebschner
11:30 AM	1:00	Automatic model building in CCP4: Modelcraft + Nautilus + DNA	Paul Bond
12:30 PM	1:00	Lunch	
1:30 PM		Free time (afternoon and evening)	

Day 6 (Sun July 12): Refinement and Ligands

8:30 AM	1:00	Introduction to Refinement with CCP4	Rob Nicholls
9:30 AM	1:00	Model-building errors, the quiz	Robbie Joosten
10:30 AM	0:15	Break	
10:45 AM	0:45	Modelling ligands in CCP4	Rob Nicholls
11:30 AM	1:00	Refinement against cryoEM reconstructions	Rob Nicholls
12:30 PM	1:00	Lunch Break	
1:30 PM	1:00	CryoEM: model building and validation	Genki Terashi/Daisuke Kihara - Purdue
2:30 PM	1:30	Phenix-refine	Pavel Afonine
4:00 PM	0:15	Break	
4:15 PM	3:15	Practical Session (coffee available from 4pm)	
7:30 PM	1:00	Dinner Break	
8:30 PM	1:30	Dataset of the Day and Practical Session	

Day 7 (Mon July 13): Other Macromolecules, Ligands, Validation

8:30 AM	1:00	Carbohydrates (demo and lecture)	Jon Agirre (Virtual)
9:30 AM	1:00	Metals / Check my metal; Model completion and Validation -1	Robbie Joosten
10:30 AM	0:15	Break	
10:45 AM	0:45	Model completion and Validation - 2	Robbie Joosten
11:30 AM	1:00	Coot advanced including DNA/RNA and ligands	Lucrezia Capatoni
12:30 PM	1:00	Lunch Break	
1:30 PM	1:00	Validation in Phenix	Pavel Afonine
2:30PM	0:45	TBC	TBC
3:15 PM	4:15	Practical Session (coffee available from 4pm)	
7:30 PM	1:00	Dinner Break	
8:30 PM	1:30	Dataset of the Day and Practical Session	

Day 8 (Tue July 14): Structure Analysis and Deposition

8:30 AM	0:40	Use of PDB	TBC
9:10 AM	0:40	CryoEM: Tools in Phenix	Pavel Afonine
9:50 AM	0:40	RCSB PDB deposition, validation and resources	Gregg Crichlow (Virtual)
10:30 AM	0:15	Break	
10:45 AM	0:45	RCSB PDB tools and development	TBC
11:30 AM	1:00	Structural Analysis & Macromolecular Complexes	Eugene Krissinel (Virtual)
12:30 PM	1:00	Lunch Break	
1:30 PM	2:30	The last hands on and backup	
4:00 PM		Au revoir	