

ID23-EH2

Max Nanao, Shibom Basu

- **First microfocus beamline dedicated to MX**
- **Fixed energy 14.2 keV, Pilatus3 2M**
- **Operation since 2006**
- **Incremental upgrades: Detector, Multilayer optics**
- **Major upgrade, delivered July 2017**
- **EBS, Spring 2020 (source u23->u20)!**

ID23-2 SAMPLE POSITION

+Variable vertical focus+high flux

+MD3Up diffractometer

+Very fast mesh scans

+Excellent OAV

+Split beamstop

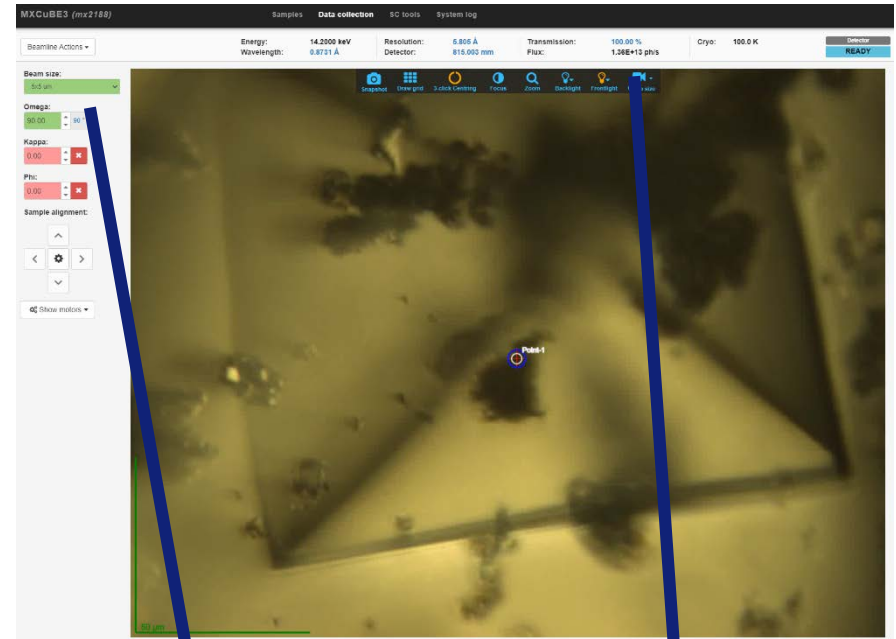
+Apertures

+Excellent beam visualisation

+Mini Kappa goniometry

+Plate Gripper

+New FLEX HCD. UNIPUCKS ONLY,



Transmission: 100.00 %
Flux: 1.38E+13 ph/s



<http://www.raddo.se/>

<https://onlinelibrary.wiley.com/doi/full/10.1002/pro.3922>

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+MD3Up diffractometer

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e.g. 125x150 crystal, 1400
images -> grid scan in 25s
(+preparation and analysis time)

+Variable vertical focus

MD3Up diffractometer

+Very fast mesh scans

+Excellent OAV

+Split beamstop

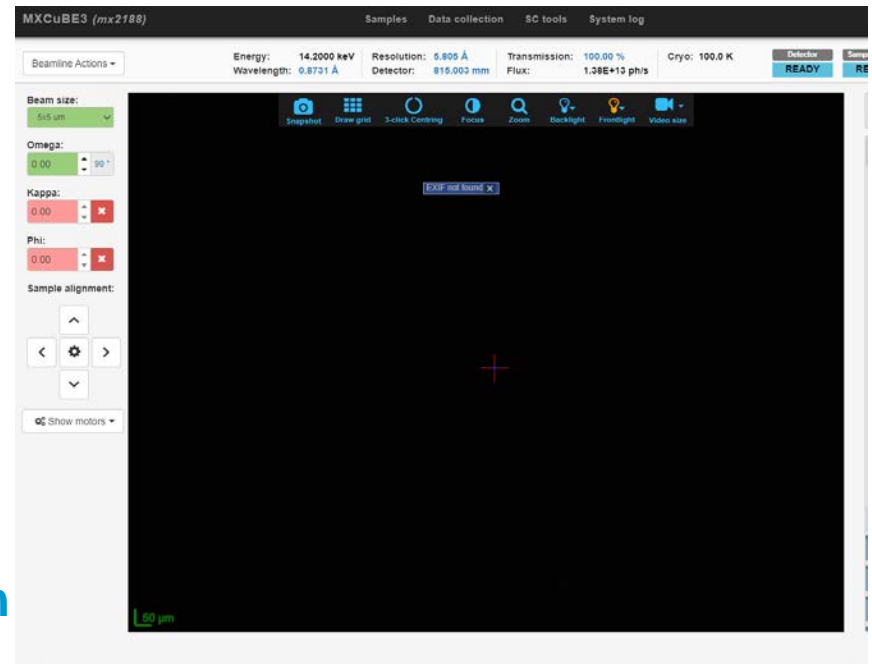
+Apertures

+Excellent beam visualisation

+Mini Kappa goniometry

+Plate Gripper

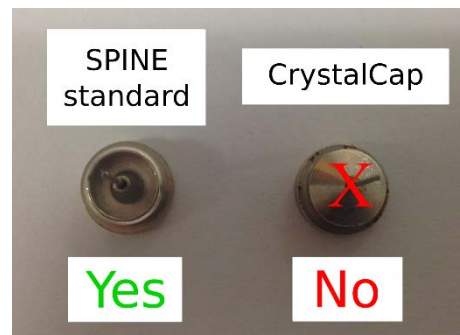
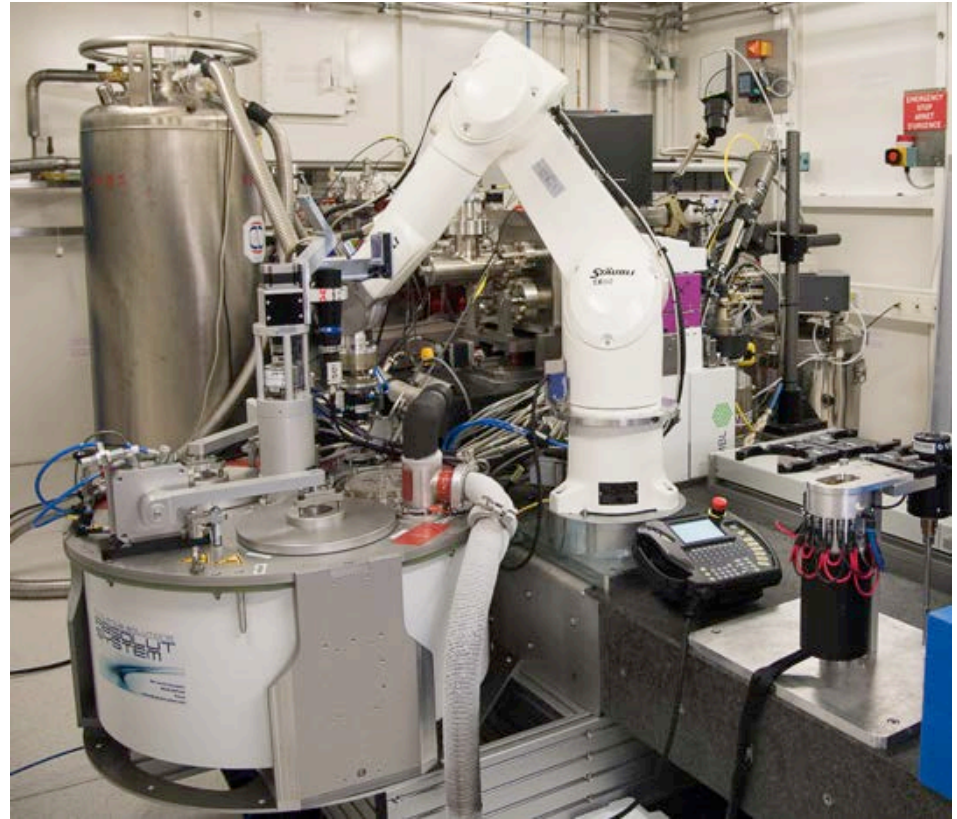
+New FLEX HCD. UNIPUCKS ONLY,



ID23-2 SAMPLE CHANGER

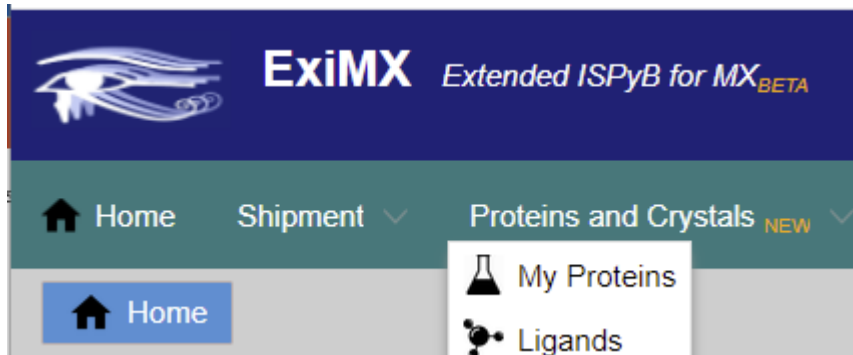
- +Variable vertical focus
- +MD3Up diffractometer
 - +Very fast mesh scans
 - +Excellent OAV
 - +Split beamstop
 - +Apertures
 - +Excellent beam visualisation
 - +Mini Kappa goniometry
 - +Plate Gripper

+FLEX HCD. UNIPUCKS ONLY



- +New queuing system (SLURM) used
- +Proposal for more compute machines in progress
- +Multiple alternate MR models and complexes
- +Automation of Mesh and Collect data analysis
- +SDF files with multiple ligands for automatic ligand fitting

tinyurl.com/iiqgypj9



NOTIFICATION THAT PHASING WAS SUCCESSFUL

ExiMX Extended ISPyB for MX₂ESRF

Version: 0.9.5 Released: 2016/12/22

Home | Shipment | Proteins and Crystals | Prepare Experiment | Data Explorer | Offline Data Analysis | Help

search by protein accession

Log out | @nanao

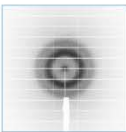
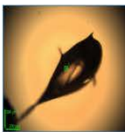
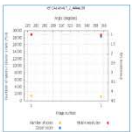
New Tab

Flux start: 2.37e+11 ph/sec | Flux end: 2.39e+11 ph/sec | Alpha: 90 | Beta: 104.4 | Gamma: 90

Run #3: Characterisation Dec 12, 2016 10:04:47 PM

Summary | Beamline Parameters | Data Collection (1) | Sample | Results | Workflow (1)

Workflow	Characterisation	Type	Characterization	Resolution	0.2	Mobility	0.2
Protein		Res. (corner)	1.16 Å (0.98 Å)	Space Group	P2		
Sample		Wavelength	0.973 Å	Plan. Res.	1.14 Å	Exp. Time	0.02 s
Prefix		Omega range	1°	Images	1300	Total rotation	0.1°
Images	2	Omega start (total)	450° (180°)	Transmission	5.496		
Transmission	100	Exposure Time	0.05 s	cell A	cell B	cell C	
Flux start	2.46e+12 ph/sec	Flux end	2.43e+12 ph/sec	Alpha	Beta	Gamma	
				90	104.52	90	

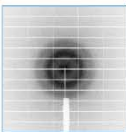
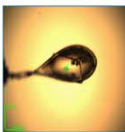
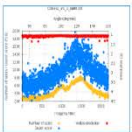




Run #2: OSC Dec 12, 2016 9:59:29 PM

Summary | Beamline Parameters | Data Collection (1) | Sample | Results (10) | Workflow | Phasing (37)

Workflow		Type	OSC	#1 211	Completeness	74%	Res.	Resolution	4.9	2.1
Protein		Res. (corner)	1.16 Å (0.98 Å)	Overall	65%	1.1	30.0			
Sample		Wavelength	0.973 Å	Overall	60%	1.1	2.7			
Prefix		Omega range	0.05°	cell A	cell B	cell C				
Images	2100	Omega start (total)	180° (180°)	42.0	41.2	72				
Transmission	4.9048	Exposure Time	0.02 s	Alpha	Beta	Gamma				
Flux start	1.49e+11 ph/sec	Flux end	1.54e+11 ph/sec	90	104.3	90				




Automatic SAD appears to have worked with the space group P1211

Run #1: Characterisation Dec 12, 2016 9:57:01 PM

Summary | Beamline Parameters | Data Collection (1) | Sample | Results | Workflow (1)

Workflow	Characterisation	Type	Characterization	Resolution	0.16	Mobility	0.16
Protein		Res. (corner)	1.19 Å (1 Å)	Space Group	P2		
Sample		Wavelength	0.973 Å	Plan. Res.	1.16 Å	Exp. Time	0.02 s
Prefix		Omega range	1°	Images	2100	Total rotation	0.05°

COMPLETE VIEW OF ALL PHASING TRIALS

ExiMX Extended ISPyB for MX_{data}

Home | Shipment | Proteins and Crystals | Prepare Experiment | Data Explorer | Offline Data Analysis | Help

search by protein accession

Log out MX1841@nanao

Version: 0.5.8
Released: 201612/22

ESRF

Transmission: 100 | Exposure Time: 0.05 s | cell A: 42.54 | cell B: 41.5 | cell C: 72.83
Flux start: 2.46e+12 ph/sec | Flux end: 2.43e+12 ph/sec | Alpha: 90 | Beta: 104.52 | Gamma: 90

Run #3 Dec 12, 2016 9:59:29 PM

Summary | Beamline Parameters | Data Collections (1) | Sample | Results (18) | Workflow | Phasing (32)

Phasing	PREPARE	SUBSTRUCTURE	PHASING	MODEL	Download	Program	Method	Resolution	Solvent	Chain Count	Residues Count	Average Fragment Length	CC of partial model	Electron Density	PDB
P1211	✓	✓	✓	✓	📄	shelx	SAD	2.71 - 60.0	0.37	10	208	20	38.04	🔍	🔍
						shelx	SAD	2.71 - 60.0	0.37	9	198	22	34.35	🔍	🔍
						shelx	SAD	2.71 - 60.0	0.62	8	198	25	33.22	🔍	🔍
						shelx	SAD	2.71 - 60.0	0.42	11	198	18	32.82	🔍	🔍
						shelx	SAD	2.71 - 60.0	0.42	14	208	15	31.52	🔍	🔍
						shelx	SAD	2.71 - 60.0	0.47	9	208	23	30.42	🔍	🔍
						shelx	SAD	2.71 - 60.0	0.47	10	183	18	29.3	🔍	🔍
						shelx	SAD	2.71 - 60.0	0.53	12	188	13	28.28	🔍	🔍
P121	✓	✓	✓	✗	📄	shelx	SAD	2.71 - 60.0	0.62				5.88		
						shelx	SAD	2.71 - 60.0	0.67				6.81		
						shelx	SAD	2.71 - 60.0	0.42				5.54		
						shelx	SAD	2.71 - 60.0	0.47				5.45		
						shelx	SAD	2.71 - 60.0	0.47				4.79		
						shelx	SAD	2.71 - 60.0	0.42				4.48		
						shelx	SAD	2.71 - 60.0	0.37				4.44		
						shelx	SAD	2.71 - 60.0	0.67				4.08		

PNG snapshot of PDB

Interactive density viewer (UglyMol)

PNG CARTOON OF SHELXE MODEL

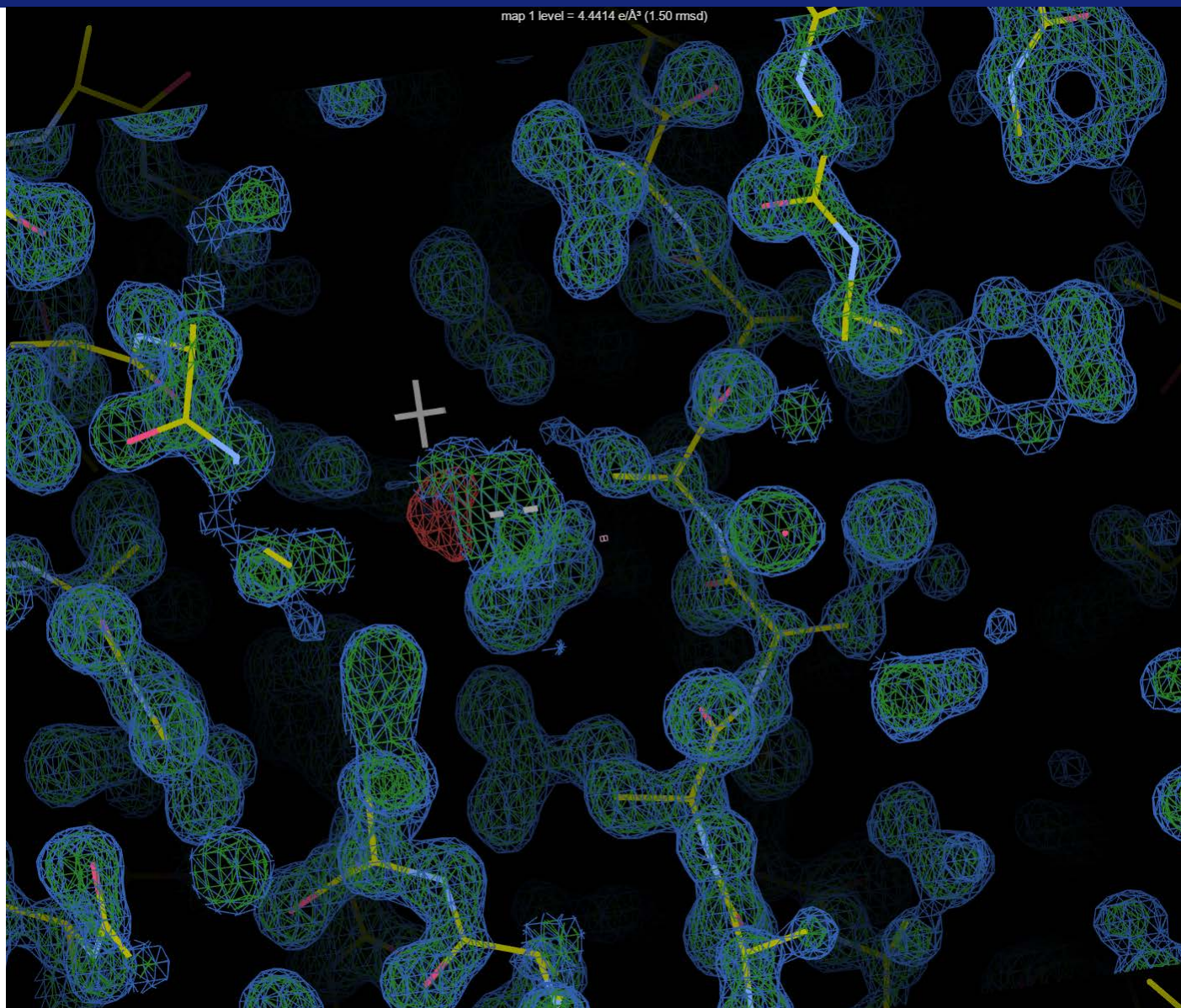
The screenshot displays the ExiMX software interface. At the top, there is a navigation menu with options: Home, Reports, Planning and Control, Prepare Experiments, Data Explorer, and Other Tools. Below the menu, there is a 'How To' section and a table with columns: Parameters, ID, Species Type, and others. The table contains data for 'P1211' and 'P1212'. A central window titled 'MODELBUILDING : P1211' shows a 3D ribbon model of a protein structure in green. The model is a complex, multi-domain protein with several alpha-helices and beta-strands. The background of the interface is dark, and the overall layout is clean and professional.

Parameters	ID	Species Type	Species	Species Type	Species
P1211	1.00e+02 phases	Forward	2.00e+02 phases	Reverse	2.00e+02 phases
P1212	1.00e+02 phases	Forward	2.00e+02 phases	Reverse	2.00e+02 phases

MODELBUILDING : P1211
Image 1 of 8

Chain	Residue	B-factor	Occupancy	Displacement	Temperature Factor
chain	240	2.71	0.99	0.45	16
chain	241	2.71	0.99	0.41	1
chain	242	2.71	0.99	0.37	181
chain	243	2.71	0.99	0.30	11
chain	244	2.71	0.99	0.32	108
chain	245	2.71	0.99	0.37	108
chain	246	2.71	0.99	0.42	108
chain	247	2.71	0.99	0.47	108
chain	248	2.71	0.99	0.47	108
chain	249	2.71	0.99	0.42	108
chain	250	2.71	0.99	0.37	108
chain	251	2.71	0.99	0.37	108
chain	252	2.71	0.99	0.42	108
chain	253	2.71	0.99	0.37	108
chain	254	2.71	0.99	0.37	108
chain	255	2.71	0.99	0.37	108
chain	256	2.71	0.99	0.37	108
chain	257	2.71	0.99	0.37	108
chain	258	2.71	0.99	0.37	108
chain	259	2.71	0.99	0.37	108
chain	260	2.71	0.99	0.37	108

INTERACTIVE ELECTRON DENSITY



PEOPLE

Ray Barrett
Shibom Basu
Antonia Beteva
Hugo Caserotto
Florent Cipriani
Carole Clavel
Fabien Dobias
Franck Felisaz
David Flot
Nicolas Foos
Thierry Giraud
Matias Guijarro
Mario Lentini
Gordon Leonard
Christian Morawe
Didier Nurizzo
Marcus Oskarsson
Thomas Roth
Jeremy Sinoir
John Surr
Olof Svensson
Pascale Thevenaut
Amparo Vivo
Ulrich Zander