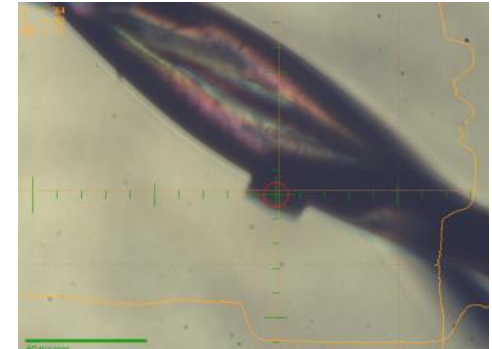
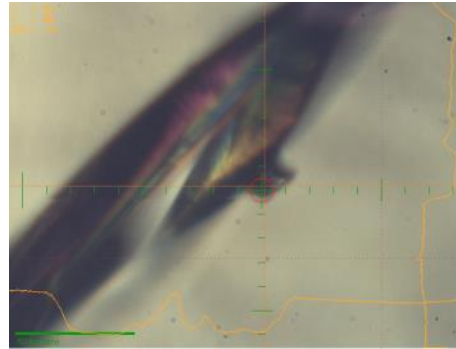


ID23-EH2

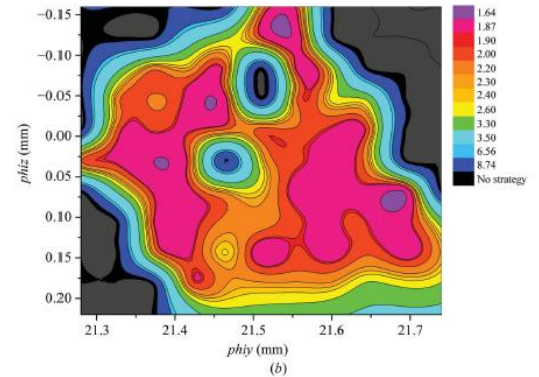
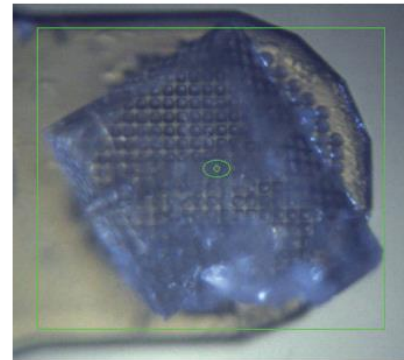
Max Nanao

USE CASES FOR SMALL BEAMS IN MX

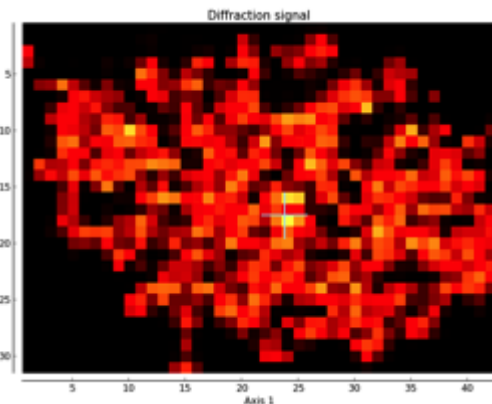
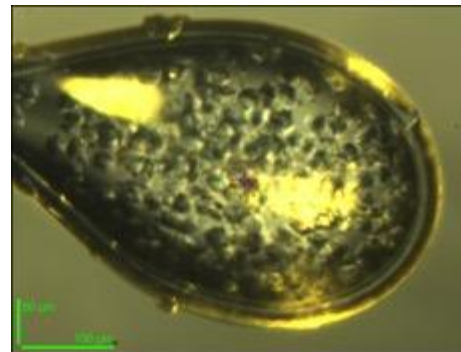
Smaller crystals



Diffraction mapping



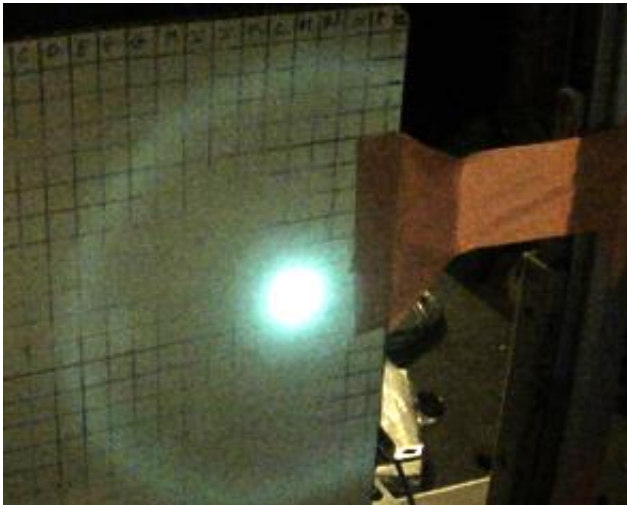
Serial crystallography



ID23-2 REBUILD

Almost a complete rebuild! Work began in October 2016, First users July 2017.

- +Improve focus and flux for existing beam size
- +Install new sample changer
- +Install high performance MD
- +Add new smaller beam size
- +Control software changed to BLISS



+2x flux and smaller beam for normal beam size (6x4 FWHM VxH) $\sim 2 \times 10^{12}$ ph/s

+Variable vertical focus

+New MD3Up diffractometer

+Very fast mesh scans

+Better OAV

+Split beamstop

+Apertures

+Better beam visualisation

+Mini Kappa goniometry

+Plate Gripper

+New FLEX HCD. UNIPUCKS ONLY, double gripper

+Improved thermal stability

+Commissioning smaller beam size (2x2 microns)

+2x flux and smaller beam for normal beam size (6x4 FWHM VxH) $\sim 2 \times 10^{12}$ ph/s

+Variable vertical focus

+New MD3Up diffractometer

+Very fast mesh scans

+Better OAV

+Split beamstop

+Apertures

+Better beam visualisation

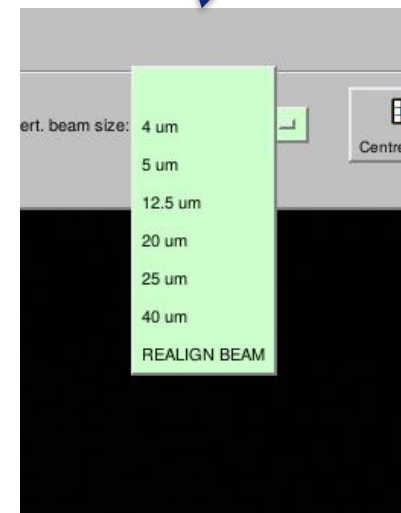
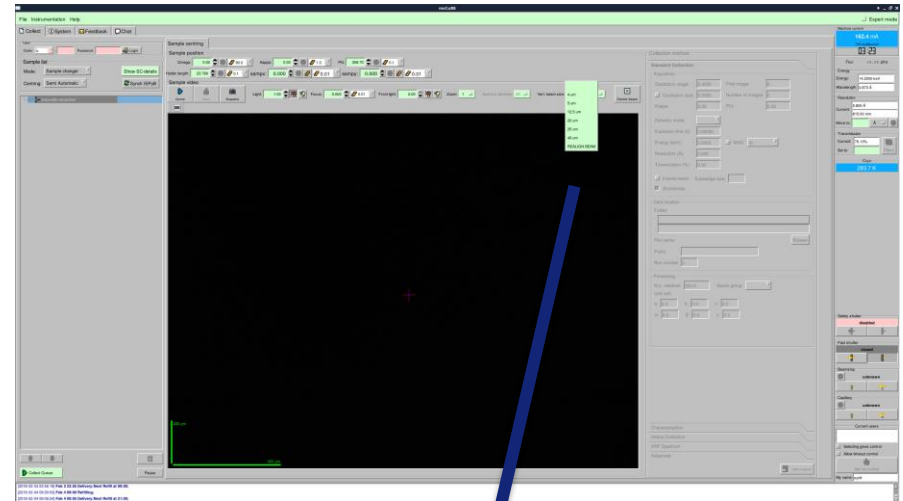
+Mini Kappa goniometry

+Plate Gripper

+New FLEX HCD. UNIPUCKS ONLY, double gripper

+Improved thermal stability

+Commissioning smaller beam size (2x2 microns)



+2x flux and smaller beam for normal beam size (6x4 FWHM VxH) $\sim 2 \times 10^{12}$ ph/s

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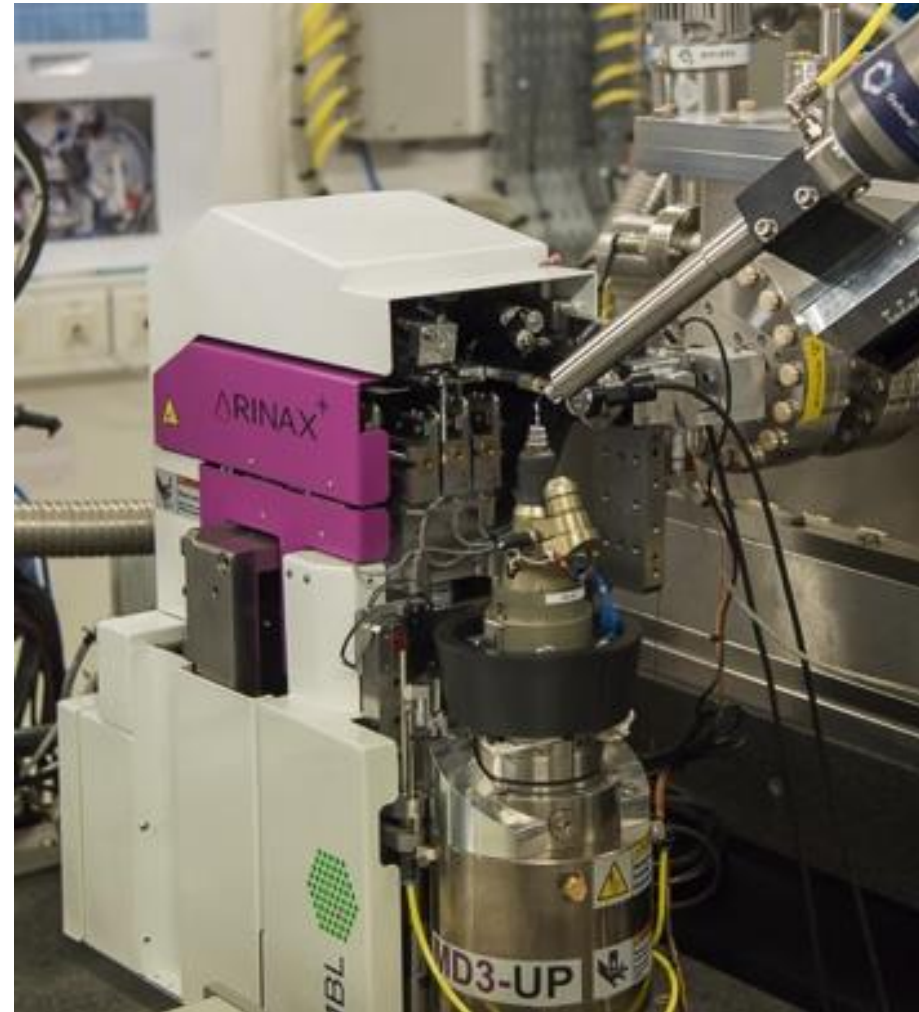
+Mini Kappa goniometry

+Plate Gripper

+New FLEX HCD. UNIPUCKS ONLY, double gripper

+Improved thermal stability

+Commissioning smaller beam size (2x2 microns)



+2x flux and smaller beam for normal beam size (6x4 FWHM VxH) $\sim 2 \times 10^{12}$ ph/s

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+Very fast mesh scans

+Better OAV

+Split beamstop

+Apertures

+Better beam visualisation

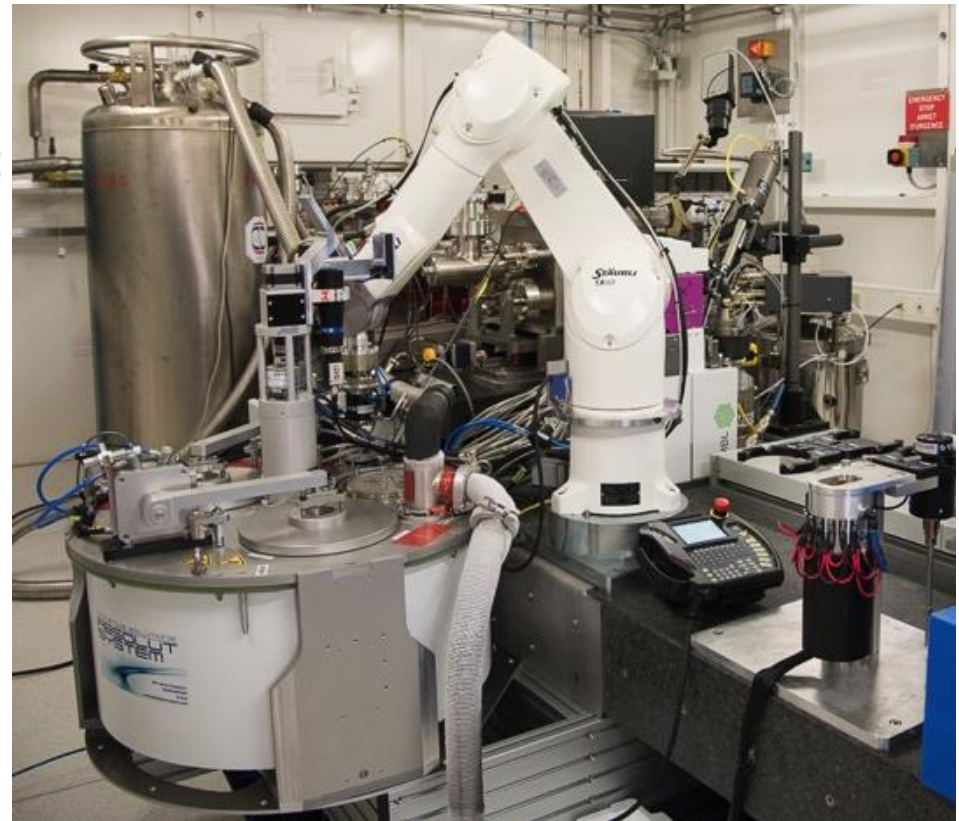
+Mini Kappa goniometry

+Plate Gripper

+New FLEX HCD. UNIPUCKS ONLY, double gripper

+Improved thermal stability

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+2x flux and smaller beam for normal beam size (6x4 FWHM VxH) $\sim 2 \times 10^{12}$ ph/s

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+Better beam visualisation

+Mini Kappa goniometry

+Plate Gripper

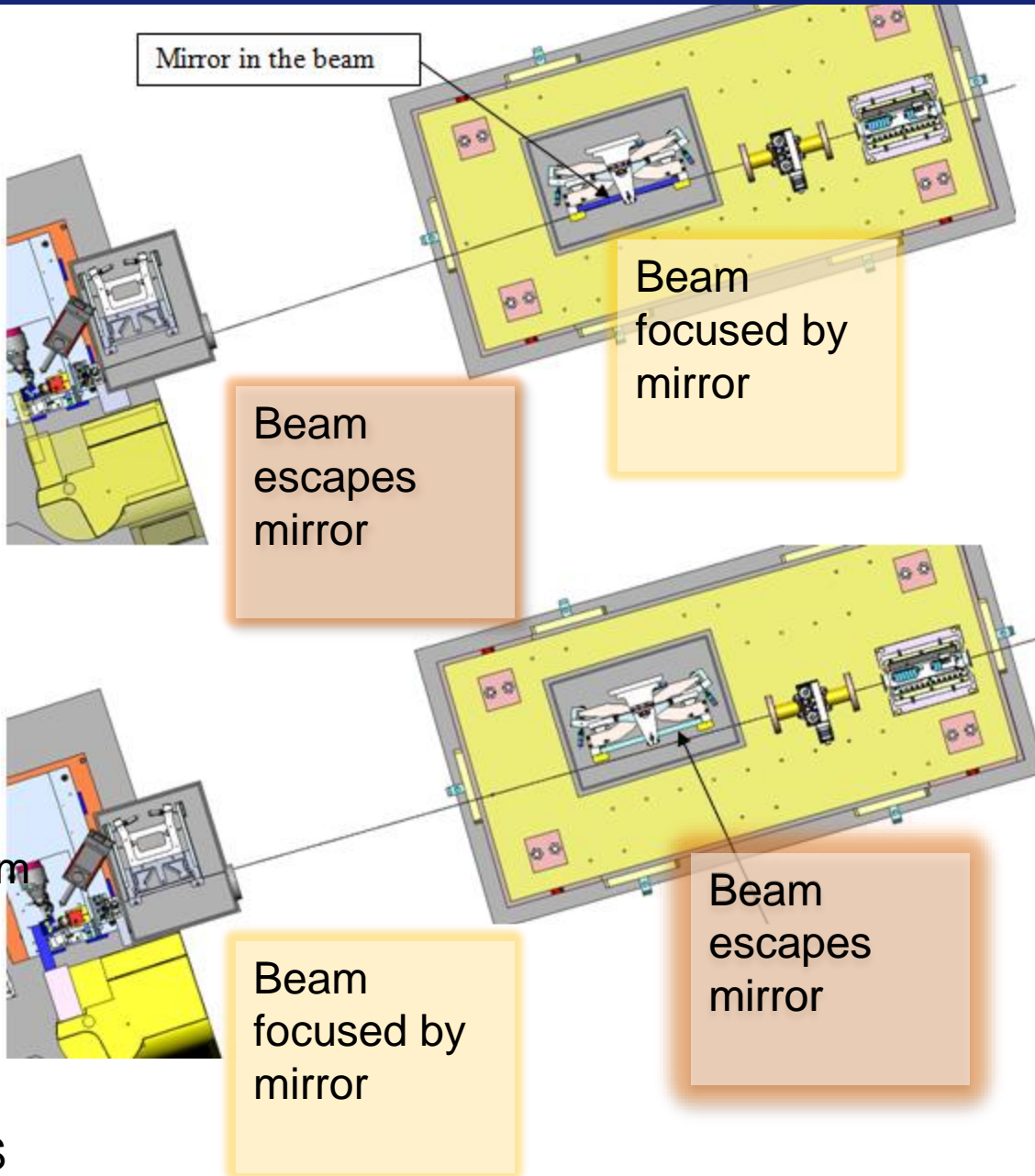
+New FLEX HCD. UNIPUCKS ONLY, double gripper

+Improved thermal stability

+Commissioning smaller beam size (2x2 microns)



OPTICAL LAYOUT



Optical design:

Vertical focus with transfoctors

Horizontal focus with mirrors.

Continue small beam comissioning
Install software for MxCube for plate gripper

Better ISPyB integration of automatic SAD phasing

Higher performance – more nodes, improved queuing system

Automatic MR on user supplied PDB

Ligand fitting of SMILES ligand

Automatic SAD on samples with anomalous signal (even on fixed energy beamlines)

NOTIFICATION THAT PHASING WAS SUCCESSFUL

ExiMX Extended ISPyB for MX₂EX

Version: 2.9.5
Released: 2016/12/22

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

search by protein acronym

Log out | nnaao

New Tab

Flux start: 2.37e+11 ph/sec | Flux end: 2.35e+11 ph/sec | Alpha: 99 | Beta: 104.4 | Gamma: 90

Run #3 Character121210 Dec 12, 2016 10:04:47 PM

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

Workflow: Characterisation

Type: Characterization

Protein: Res. (open) 1.16 Å (0.98 Å)

Sample: Wavelength: 0.973 Å

Prefix: Omega range: 1°

Images: 2 | Omega start (total): 450° (180°)

Transmission: 100 | Exposure Time: 0.05 s

Flux start: 2.46e+12 ph/sec | Flux end: 2.43e+12 ph/sec

Resolution: 1.16 Å

Space Group: P2

Plan. Res: 1.16 Å | Exp. Time: 0.02 s

Images: 1300 | Total rotation: 0.1°

Transmission: 5.496

cell A	cell B	cell C
42.54	41.5	72.93
Alpha	Beta	Gamma
99	104.52	90

Automatic SAD appears to have worked with the space group P1211

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

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

Workflow: OSC

Type: OSC

Protein: Res. (open) 1.18 Å (0.98 Å)

Sample: Wavelength: 0.973 Å

Prefix: Omega range: 0.05°

Images: 2199 | Omega start (total): 180° (180°)

Transmission: 4.9048 | Exposure Time: 0.02 s

Flux start: 1.49e+11 ph/sec | Flux end: 1.54e+11 ph/sec

Resolution: 1.18 Å

Space Group: P2

Plan. Res: 1.18 Å | Exp. Time: 0.02 s

Images: 2180 | Total rotation: 0.05°

Transmission: 5.496

Overall: 74% | 45% | 60%

cell A: 42.54 | cell B: 41.5 | cell C: 72.93

Alpha: 99 | Beta: 104.5 | Gamma: 90

Run #1 Character121210 Dec 12, 2016 9:57:01 PM

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

Workflow: Characterisation

Type: Characterization

Protein: Res. (open) 1.19 Å (1 Å)

Sample: Wavelength: 0.973 Å

Prefix: Omega range: 1°

Images: 2 | Omega start (total): 450° (180°)

Transmission: 100 | Exposure Time: 0.05 s

Flux start: 2.46e+12 ph/sec | Flux end: 2.43e+12 ph/sec

Resolution: 1.19 Å

Space Group: P2

Plan. Res: 1.19 Å | Exp. Time: 0.02 s

Images: 1300 | Total rotation: 0.1°

Transmission: 5.496

cell A	cell B	cell C
42.54	41.5	72.93
Alpha	Beta	Gamma
99	104.52	90

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 acronym

Logout MX1841@jnanao

Version: 0.5.8
Released: 20161202

ESRF

Transmission: 100, Exposure Time: 0.05 s, cell A: 42.54, cell B: 41.5, cell C: 72.83, Fluor start: 2.43e+12 ph/sec, Fluor 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	2.71-80.0	0.37	10	220	23	38.04	🔍	🔍
						shelx	SAD	2.71-80.0	0.37	9	198	22	34.35	🔍	🔍
						shelx	SAD	2.71-80.0	0.62	8	198	25	33.22	🔍	🔍
						shelx	SAD	2.71-80.0	0.42	11	198	18	32.82	🔍	🔍
						shelx	SAD	2.71-80.0	0.42	14	208	15	31.52	🔍	🔍
						shelx	SAD	2.71-80.0	0.47	9	208	23	30.42	🔍	🔍
						shelx	SAD	2.71-80.0	0.47	10	183	18	29.3	🔍	🔍
						shelx	SAD	2.71-80.0	0.52	12	198	13	28.25	🔍	🔍
P121	✓	✓	✓	✗	📄	shelx	SAD	2.71-80.0	0.62				6.88	🔍	🔍
						shelx	SAD	2.71-80.0	0.67				6.81	🔍	🔍
						shelx	SAD	2.71-80.0	0.42				6.54	🔍	🔍
						shelx	SAD	2.71-80.0	0.47				6.45	🔍	🔍
						shelx	SAD	2.71-80.0	0.47				4.75	🔍	🔍
						shelx	SAD	2.71-80.0	0.42				4.48	🔍	🔍
						shelx	SAD	2.71-80.0	0.37				4.44	🔍	🔍
						shelx	SAD	2.71-80.0	0.67				4.08	🔍	🔍

PNG snapshot of PDB

Interactive density viewer (UglyMol)

PNG CARTOON OF SHELXE MODEL

ExiMX Extended ISPyB for MX₃

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

New Tab

Transmission: 100 | Exposure Time: 0.05 s | cell A: 42.54 Alpha 80
Flux start: 2.48e+12 ph/sec | Flux end: 2.43e+12 ph/sec

Run #1 000 Dec 12, 2016 9:59:29 PM

Phasing	PREPARE	SUBSTRUCTURE	PHASING	MODEL	Download	Phase
P1211	✓	✓	✓	✓	ⓐ	phasing
P121	✓	✓	✓	✗	ⓐ	phasing

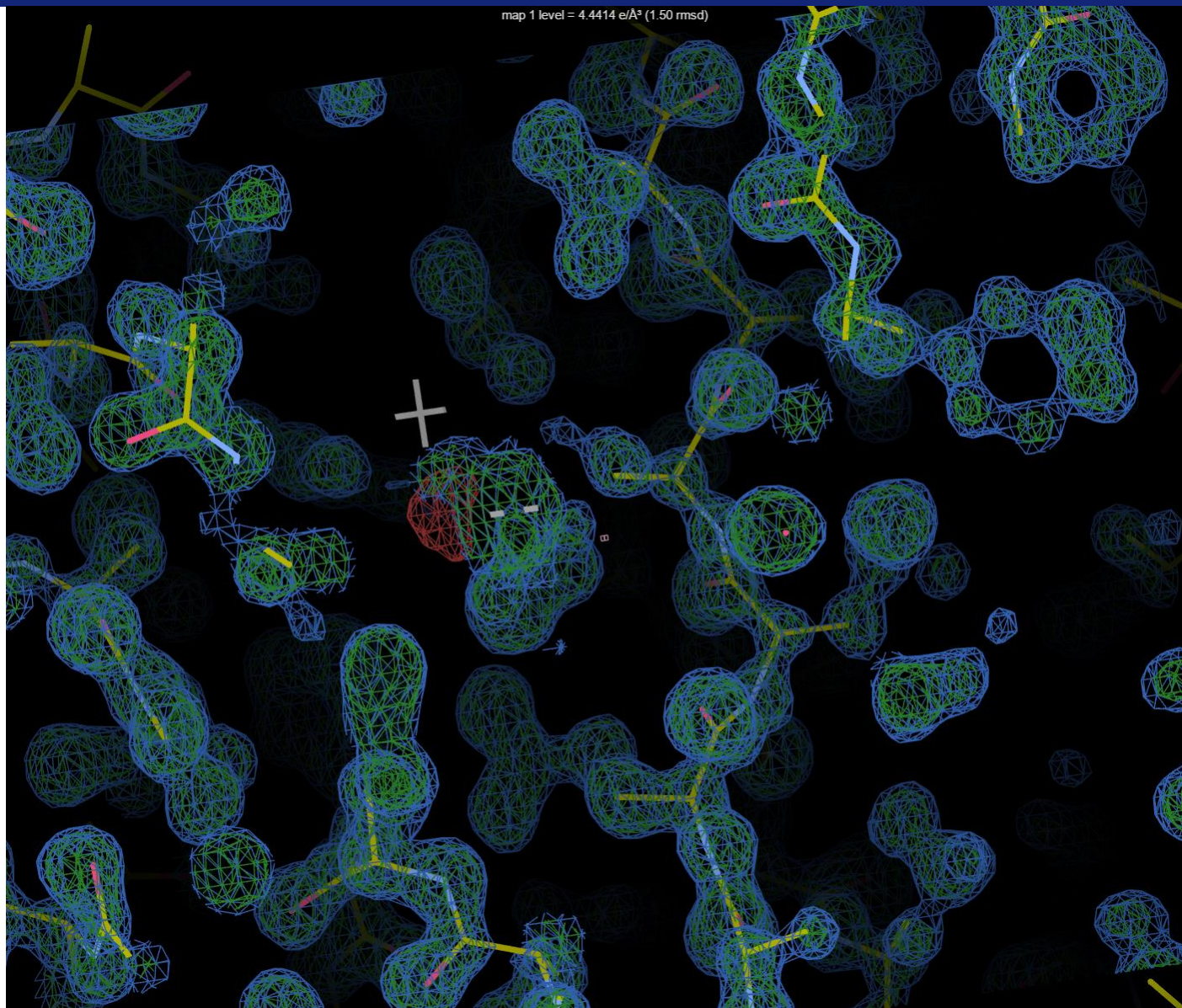
MODELBUILDING : P1211
image 1 of 8

Average Fragment Length	CC of partial model
23	38.04
22	34.35
25	33.22
18	32.52
15	31.52
23	30.42
18	29.50
13	28.28
5.88	5.88
5.81	5.81
5.54	5.54
5.49	5.49
4.78	4.78
4.48	4.48
4.44	4.44
4.08	4.08

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

Summary | Beamline Parameters

INTERACTIVE ELECTRON DENSITY



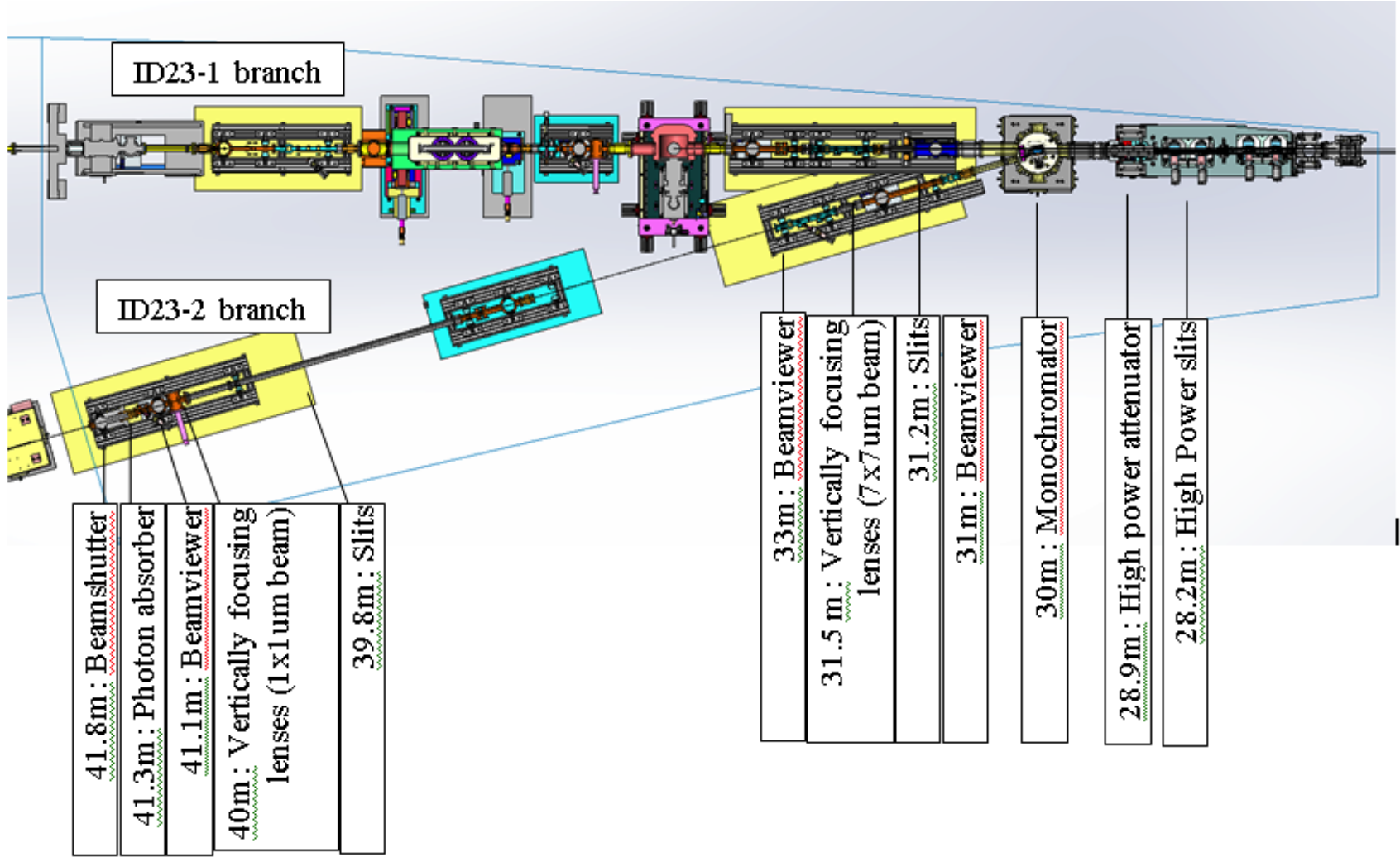
PEOPLE

Olof Svensson
Alejandro de Maria
Daniele de Sanctis
Matias Guijarro
Thomas Boeglin
Stephanie Monaco
Antonia Beteva
Solange Delageniere
Darren Spruce
Marjolaine Bodin
Matthew Bowler
Didier Nurizzo
Gordon Leonard
Andrew McCarthy

Carole Clavel
Ray Barrett
John Surr
Thierry Giraud
Pierre Pinel
Florent Cipriani
Franck Felisaz
Ulrich Zander
Hugo Caserotto
Handling Group
Vacuum Group
Pascal Theveneau
David Flot
Amparo Vivo
Christian Morawe
Fabien Dobias
Francois Torrecillas
Bob Baker
Alexis Van der Kleij



Mario Lentini
October shutdown



Distance from the source for OH1 components, ID23-2 branch