Beamline BL13–XALOC: Macromolecular Crystallography

www.cells.es/beamlines/XALOC

Scientists: Jordi Juanhuix and Jordi Benach

Control and Electronics: Guifré Cuní, Julio Lidón (Engineering), Andrej Seljak (Technician)

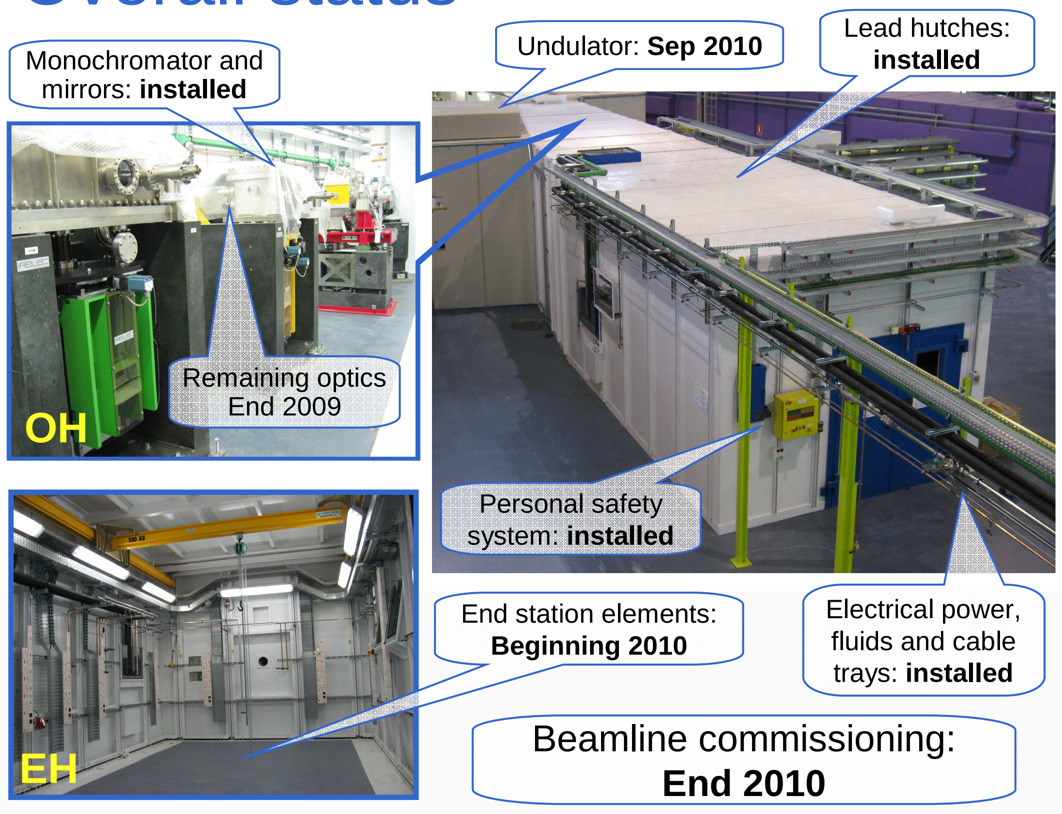
Mechanics: Carles Colldelram, Jonathan McKinlay, Claude Ruget (Engineering), Àlex Enrique (Technician)

Scientific case

The need for 3D atomic information of biological molecules in Biology, Biomedicine, and related disciplines has increased exponentially in the past few decades. X-ray crystallography has emerged as a very effective technique to perform these studies on biomolecules at the atomic level.

In response to this, one of the phase-I beamlines (**XALOC – BL13**) of the third generation **3-GeV synchrotron Alba** will be devoted to Macromolecular Crystallography.

Overall status



Beamline commissioning: **End 2010**

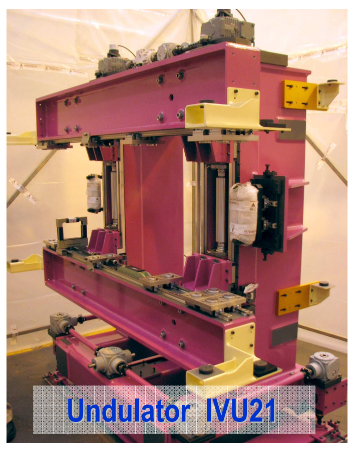
XALOC is a versatile beamline

…for many techniques

- All wavelength-dependent techniques can be performed (MAD, SAD, etc) due to the **full-wavelength tunability** and the high resolution ($\Delta\lambda/\lambda$~2 10^{-4}) of the beam,
- All common **K and L_3 absorption edges** can be reached due to the large wavelength span: 2.4–0.6 Å or 5–21 keV. Covered elements are: V→Mo (K edge); La→ U (L_3 edge).,
- An in-vacuum undulator (IVU21) feeds the beamline with a **high-flux beam** (>10^{12} ph/s in 100×100 μm^2) over the whole wavelength range.

Specifications of the in-vacuum undulator (IVU21)

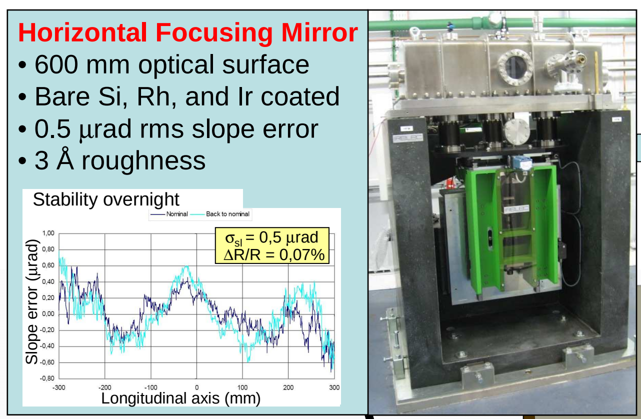
Period (number of periods)	21.6 mm (92)
K (at minimum gap, 5.5 mm)	1.60
Photon source size (h×v, FWHM)	309 × 18 μm^2
Photon source div. (h×v, FWHM)	112 × 30 μrad^2



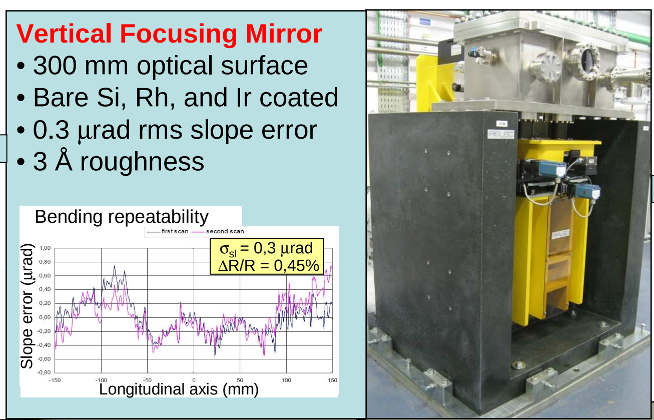
…for many crystal types

- **Small crystals** can be studied by **focusing** the beam down to **~50×10 μm^2** (h×v) where the beam divergence is **0.5 ×0.1 mrad^2**, allowing the study of macromolecules that crystallize only in small crystals,
- **Any medium-sized crystals** can be dealt with by **defocusing** the beam up to **~300×100 μm^2** (h×v),
- **Larger crystals** can be completely exposed to the x-ray beam by **unfocusing** the beam to **~500×500 μm^2** (h×v). This beam is also highly vertically collimated (**0.03 mrad**) and hence it can be used for crystals with **very large unit cells** like protein-protein complexes, viruses, etc.

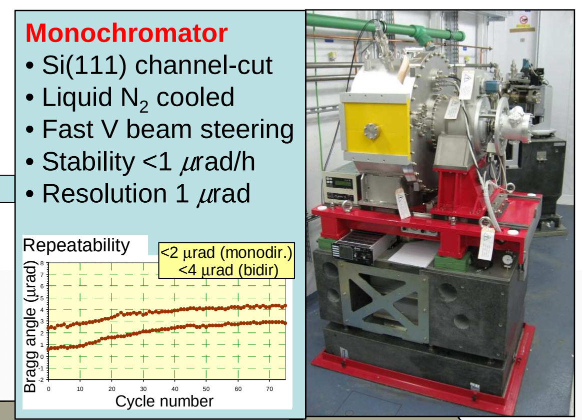
Horizontal Focusing Mirror
- 600 mm optical surface
- Bare Si, Rh, and Ir coated
- 0.5 μrad rms slope error
- 3 Å roughness

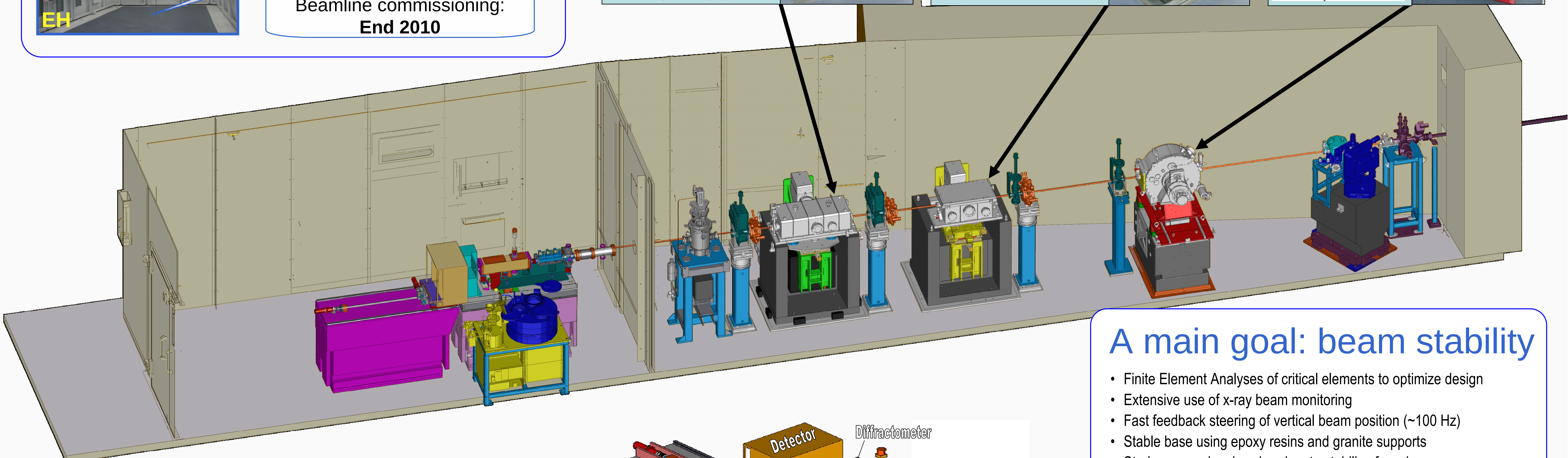


Vertical Focusing Mirror
- 300 mm optical surface
- Bare Si, Rh, and Ir coated
- 0.3 μrad rms slope error
- 3 Å roughness



Monochromator
- Si(111) channel-cut
- Liquid N_2 cooled
- Fast V beam steering
- Stability <1 μrad/h
- Resolution 1 μrad



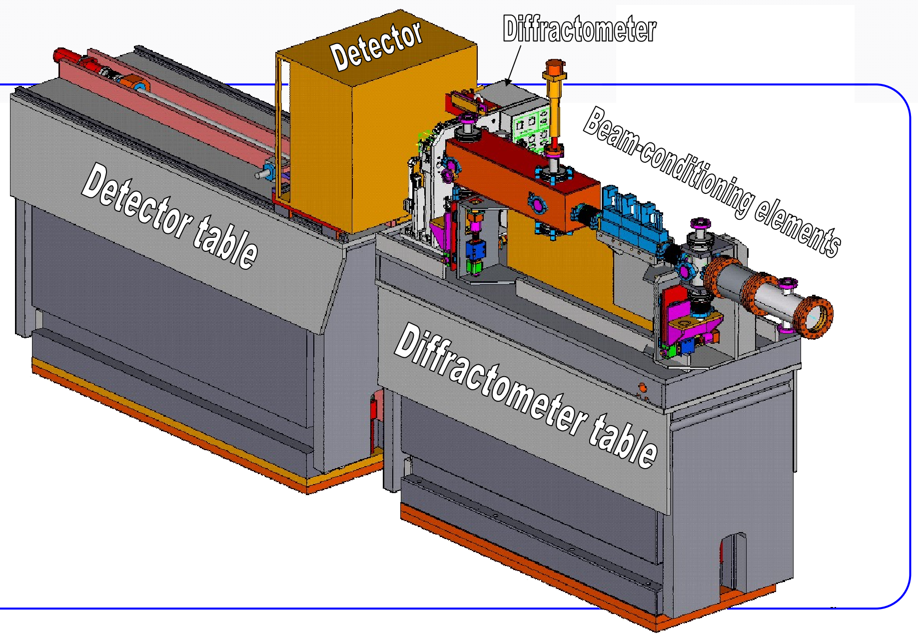


A main goal: beam stability

- Finite Element Analyses of critical elements to optimize design
- Extensive use of x-ray beam monitoring
- Fast feedback steering of vertical beam position (~100 Hz)
- Stable base using epoxy resins and granite supports
- Strain gauges in mirror benders to stabilize focusing
- Seismographs close to optical surfaces to deal with vibrations

End Station: the concept

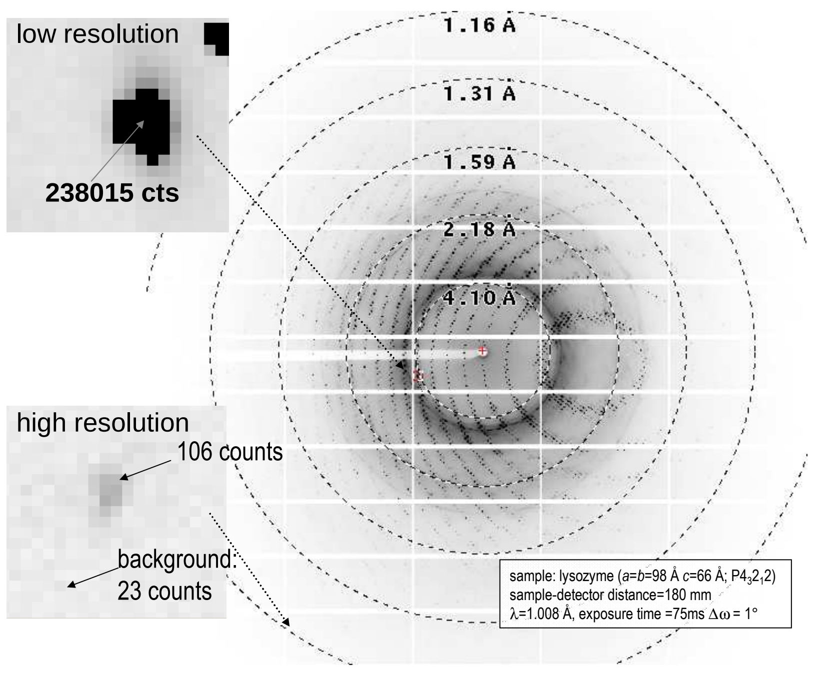
The End station consists of two in-house developed translation/rotation tables that support the diffractometer and the detector, and to guarantee stability they sit on a granite base. The tables are adjustable in X,Y,Z to 1 μm resolution and repeatability. An automatic sample changer stands on a nearby table for automatic sample mounting and allows easy access to manual sample mounting.



Detector

Status	Call for tender issued
Delivery	End of 2010

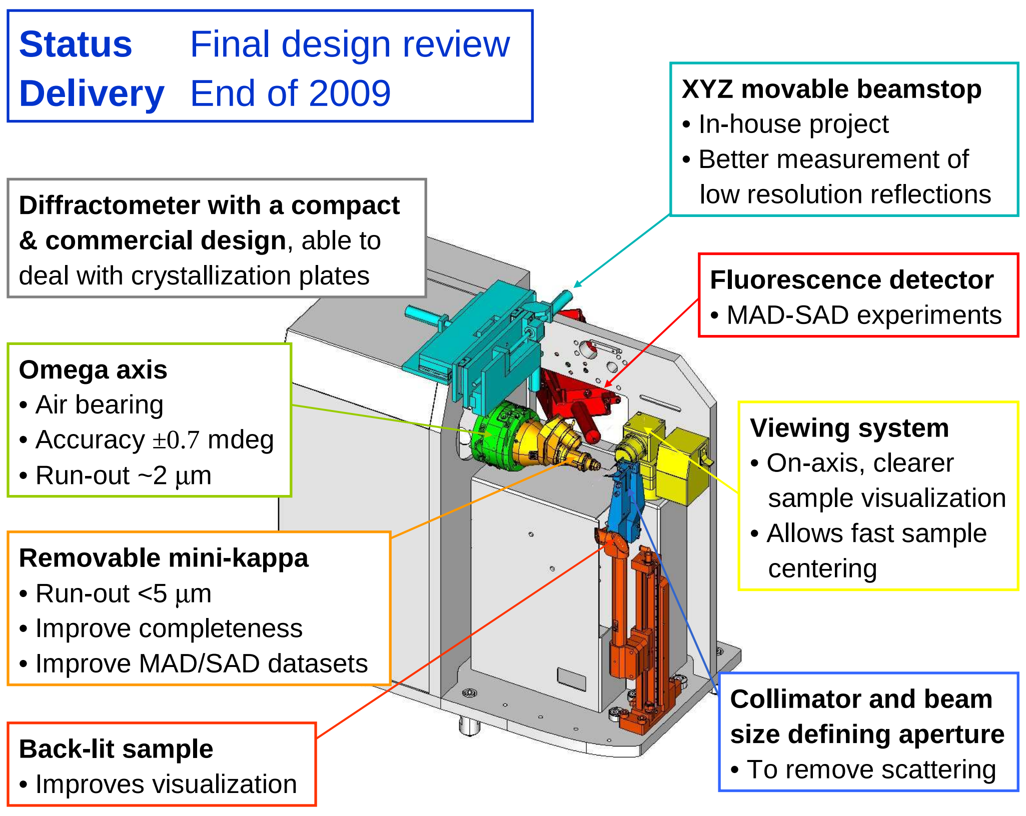
- **High dynamic range** (1 million): collection of low and high resolution data on the same frame
- Extremely **low background noise** : better data
- Very **fast read-out**: shutterless operation, minimizing mechanical systematic errors
- **Thin ω-slicing** which often results in better data, specifically in high-resolution data and large unit cell crystals
- **Extremely fast frame collection** (80ms): a 360º 1.1 Å resolution dataset can be collected in 33 seconds



frame collected at the SLS beamline X06SA (courtesy Clemens Schulze-Briese)

Diffractometer

Status	Final design review
Delivery	End of 2009



Automatic Sample changer

Status	Final design review
Delivery	Early 2010