

Data collection report from measurement on ID29 24.7.2013

During measurement on the beamline ID29 we were able to test 41 crystal with 4 testing images for the diffraction quality of every crystal and several datasets were collected later on with EDNA assistance.

We applied **2D mesh** (20x50) in order to find the best diffraction area for the WrbA protein crystal (“noname”) with 0.04s ex. time, 293.97 mm detector dist., 0.02 oscillation range, and 1.4 Å detector resolution.

Also, 2D mesh was performed for WrbA crystal with “W1” name (0.04s ex. time, 242.2mm detector dist., 0.02 oscillation range, 46.9 starting angle and 1.4 Å detector resolution) as well as for LinB86 (“B6”) with 0.04s ex. time, 0.02 oscillation range, and 2.54 Å detector resolution.

Diffraction data for flavoprotein **WrbA wt** from *E. coli* protein in complex with **benzoquinone** “noname_1” with 1500img (start. angle 143, 0.05s ex. time, 469.6mm detector dist., 0.2 oscillation, and 2.35 resolution at edge) were collected.

For **WrbA wt** crystal named “W11” 4000img were collected with 100-1.52Å resolution and 96.6% completeness for *P212121* space group with following data collection parameters: start. angle 24, 0.037s ex. time, 310mm detector dist., 0.1 oscillation.

For **DmxA wt** from *Marinobacter* sp.ELB17 protein crystals (with different additives supplied during crystallization procedure) we were able to collect several data sets:

1. “D1” 2600img with 100-1.49Å resolution and 99.6% completeness for *C222* space group with following data collection parameters: start. angle 138, 0.037s ex. time, 272.8mm detector dist., 0.05 oscillation.

2a. “D3” 3000img with 50-2.24Å resolution and 84.8% completeness for *P1* space group with following data collection parameters: start. angle 19, 0.037s ex. time, 290.3mm detector dist., 0.05 oscillation.

2b. “D3” 3000img with 100-1.45Å resolution and 99.7% completeness for *P212121* space group with following data collection parameters: start. angle 19, 0.037s ex. time, 265.2mm detector dist., 0.05 oscillation.

3. “D6” 3000img with 100-1.58Å resolution and 95.3% completeness for *C222* space group with following data collection parameters: start. angle 5, 0.037s ex. time, 317.3mm detector dist., 0.05 oscillation.

For **DmxAwt** in complex with **brombutan** named “D8” 3000img were collected with 100-1.72A resolution and 99.8% completeness for *P21212* space group with following data collection parameters: start. angle 18, 0.037s ex. time, 305.1mm detector dist., 0.05 oscillation.

For **LinB86 variant** enzyme from *Sphingomonas paucimobilis* UT26 (“B1”) 2000img were collected with 100-3.02A resolution and 99.8% completeness for *H32* space group with following data collection parameters: start. angle 27, 0.037s ex. time, 593.6mm detector dist., 0.05 oscillation.

As well, as “B7_1” dataset of 3000img was collected with 100-2.76A resolution and 99.9% completeness for *H32* space group with following data collection parameters: start. angle 63, 0.037s ex. time, 465mm detector dist., 0.1 oscillation, and “B7_2” 3000img with 100-2.41A resolution and 99.8% completeness for *H32* space group with following data collection parameters: start. angle 156, 0.037s ex. time, 512.7mm detector dist., 0.1 oscillation.

“B8” (LinB86) 3000img were collected with 50-2.34A resolution and 99.5% completeness for *H32* space group with following data collection parameters: start. angle 18, 0.037s ex. time, 510.5mm detector dist., 0.1 oscillation.

Four tested crystals of **DbeA3** mutant variant from *Bradyrhizobium elkanii* USDA94 did not diffract.

Lysozyme (“L13”) crystal complex with **1-Butyl-2,3-dimethylimidazolium tetrafluoroborate** (18th condition from “Additive ionic liquid screen” from HR) diffracted to 100-1.07A resolution with 99.9% completeness for *P4212* space group with following data collection parameters: start. angle 58, 0.037s ex. time, 168.5mm detector dist., 0.05 oscillation. We also applied XRF spectrum with detection of 3 peaks: S, Cl, Ti.

We have collected several datasets for **AHP2+CKI1**:

1. (“A7”) of 2600img at resolution of 3A (start. angle 107, 0.09s ex. time, 615.9mm detector dist., 0.15 oscillation).
2. “A5_1” 3000img dataset at 3.1A resolution and 97.7% completeness for *P622* space group with following data collection parameters: start. angle 36, 0.037s ex. time, 831.8mm detector dist., 0.05 oscillation.
3. “A5_2” 3000img dataset was collected with detector resolution 3.98A (start. angle 61, 0.04s ex. time, 292.5mm detector dist., 0.1 oscillation).

Obtained datasets were automatically processed on the beamline with XDS program.
The structure determination and refinement are being in progress.