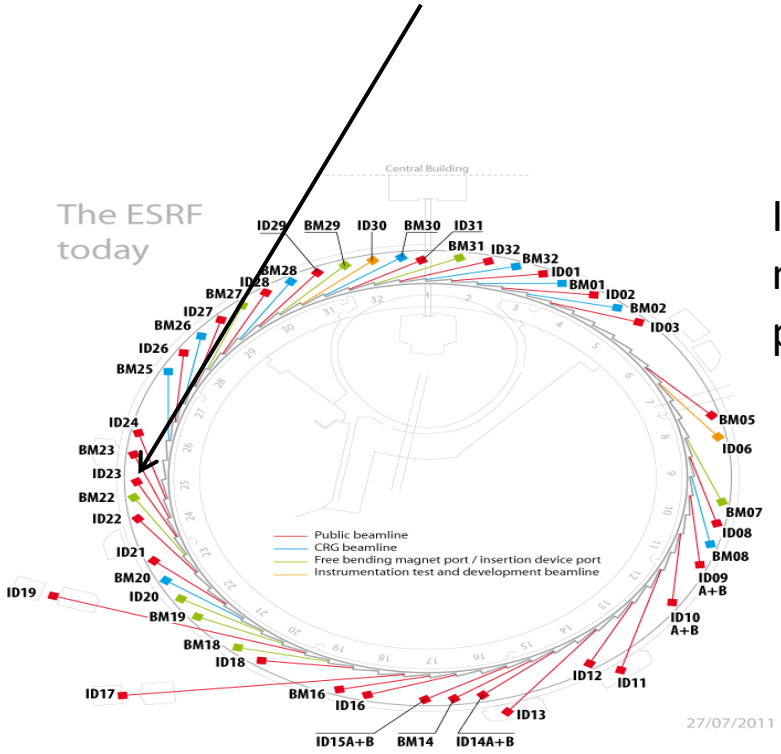
ID23-1 MX beamline news

Alexander Popov

ESRF, MX group



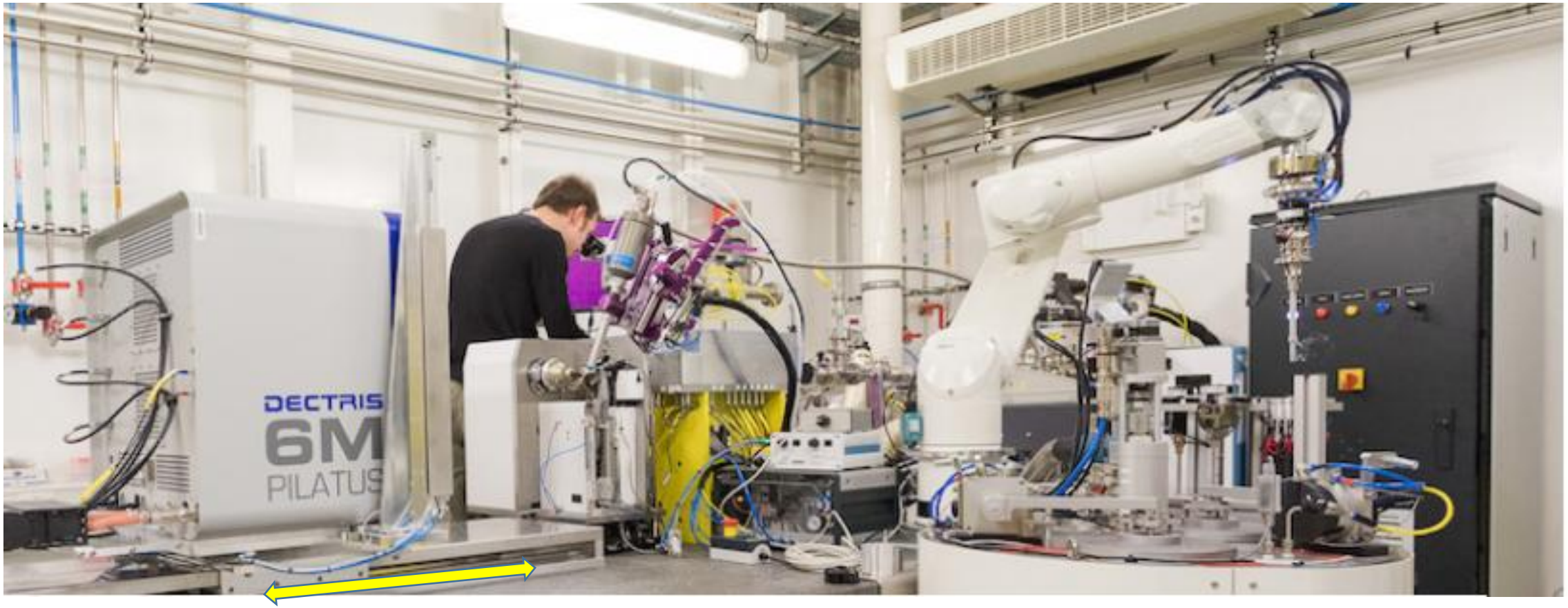
ID23-1 offers the opportunity to make highly efficient monochromatic measurements at energies from 5 Kev to 20 Kev with a flux of ~1-4 E12 photons/second and a variable beam size from 0.05 to 0.001 mm^2.

- ✓**Fast crystal best position screening**
- ✓**X-ray centering**
- ✓**Crystal cartography**
- ✓**Helical Data Collection**
- ✓**X-ray diffraction protein crystal detection**

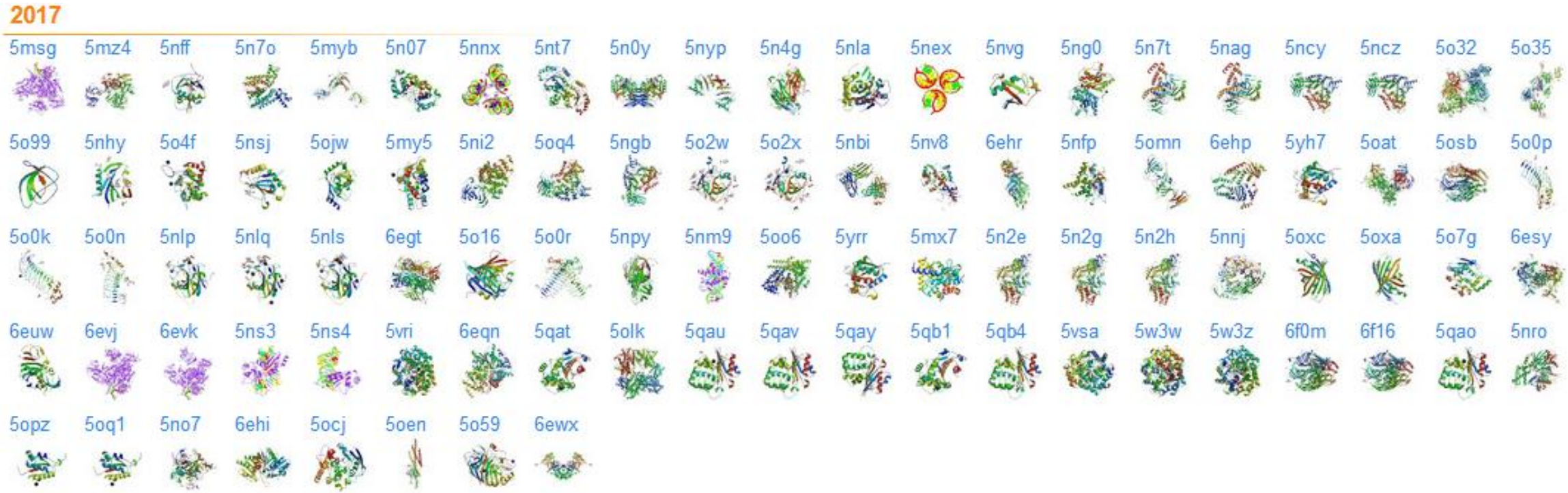
MD2M mini-diffractometer and Rapid Exchanger (ReX) for automated exchange between HC1 humidifier nozzle and cryo-stream nozzle. Including mechanical support system with alignment axes

FlexHCD sample changer

new YAG with SC



PDB Structures for which data was collected from beamline ID23-1 at ESRF (total = 92)



Total publications in 2017: 199

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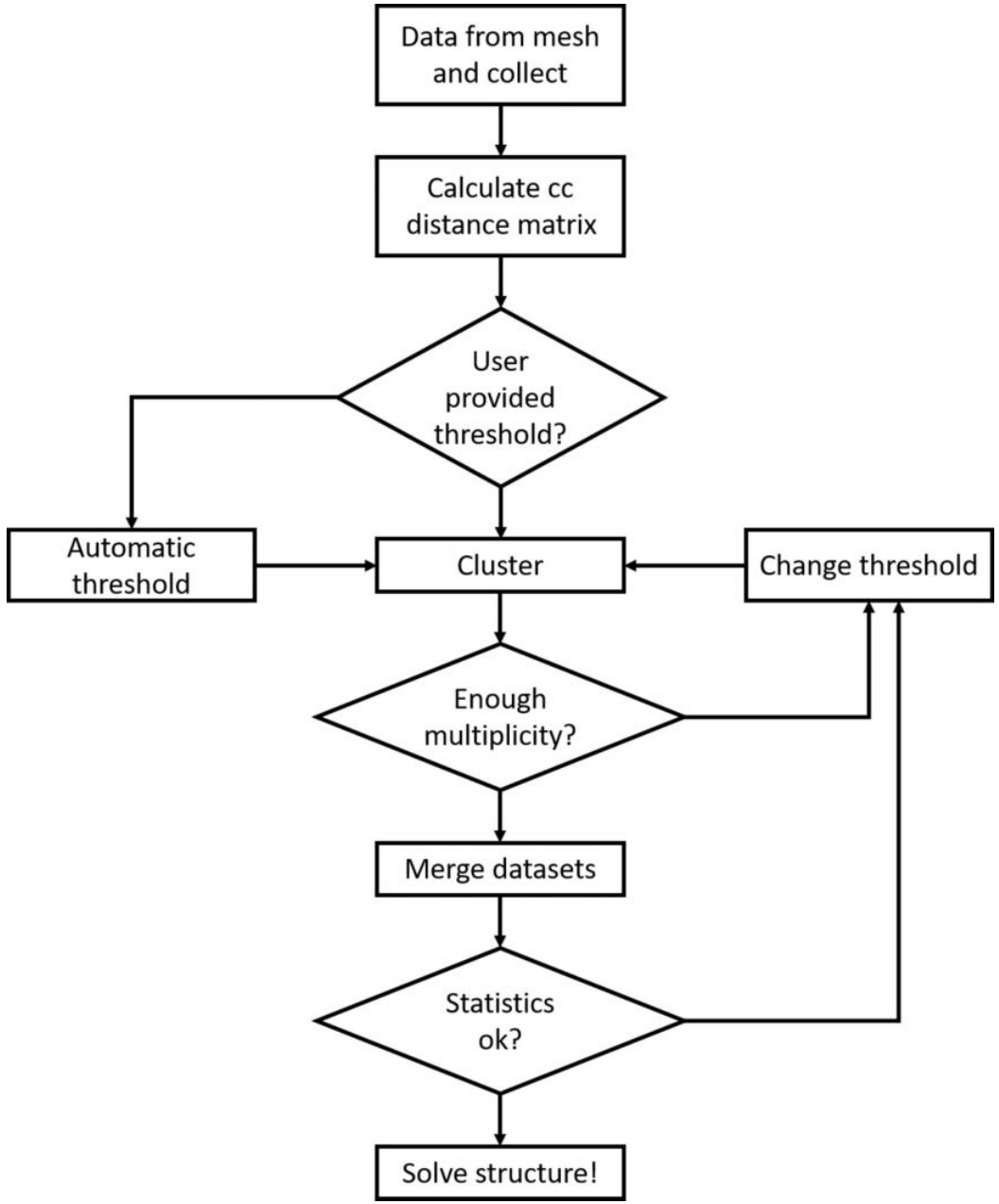
Hierarchical clustering for multiple-crystal macromolecular crystallography experiments: the *ccCluster* program

Gianluca Santoni, Ulrich Zander, Christoph Mueller-Dieckmann, Gordon Leonard and Alexander Popov

J. Appl. Cryst. (2017). **50**, 1844–1851



ccCluster: distance definitions

Based on correlation coefficient

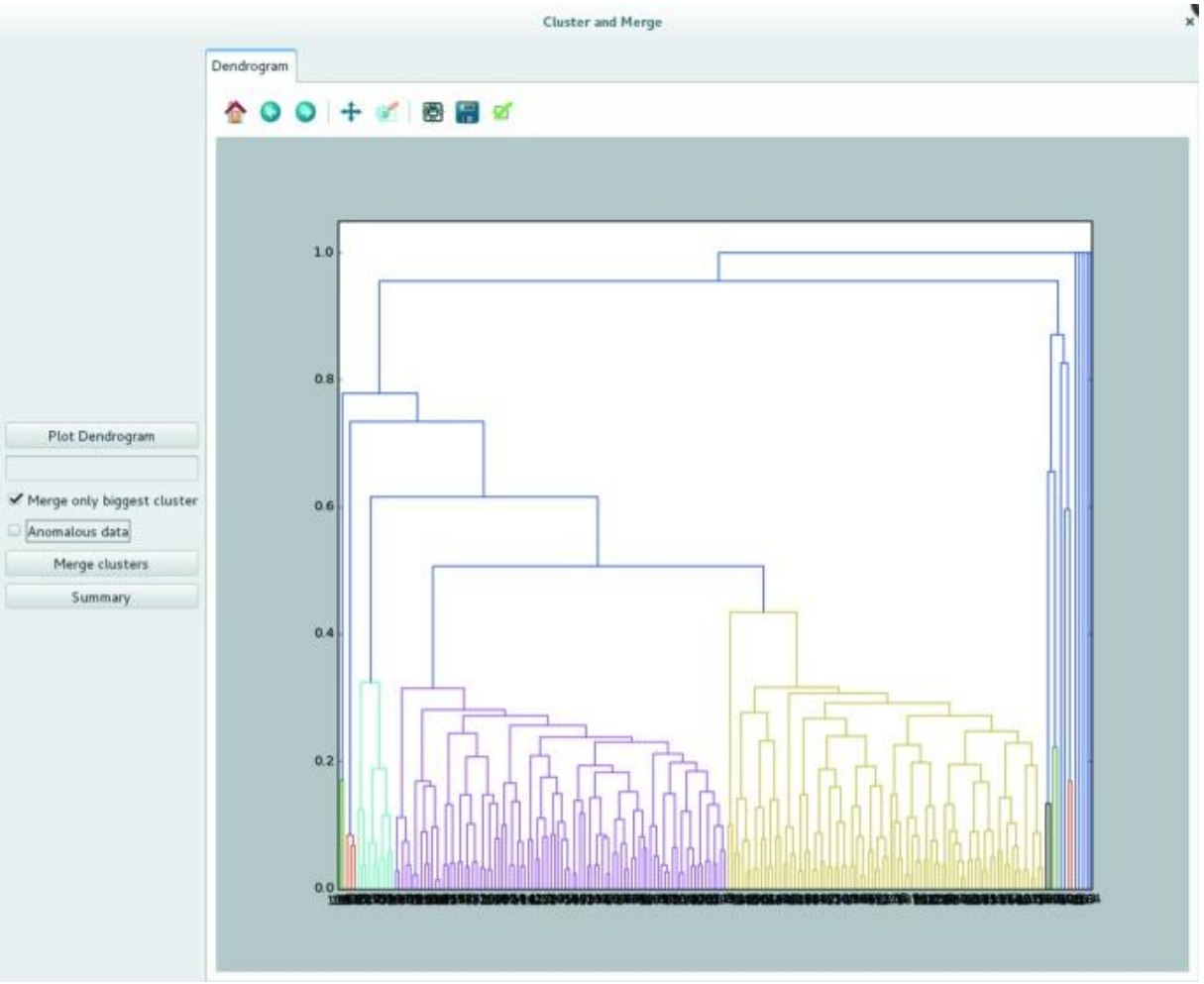
$$D(a,b) = \sqrt{1 - cc_{a,b}^2}$$

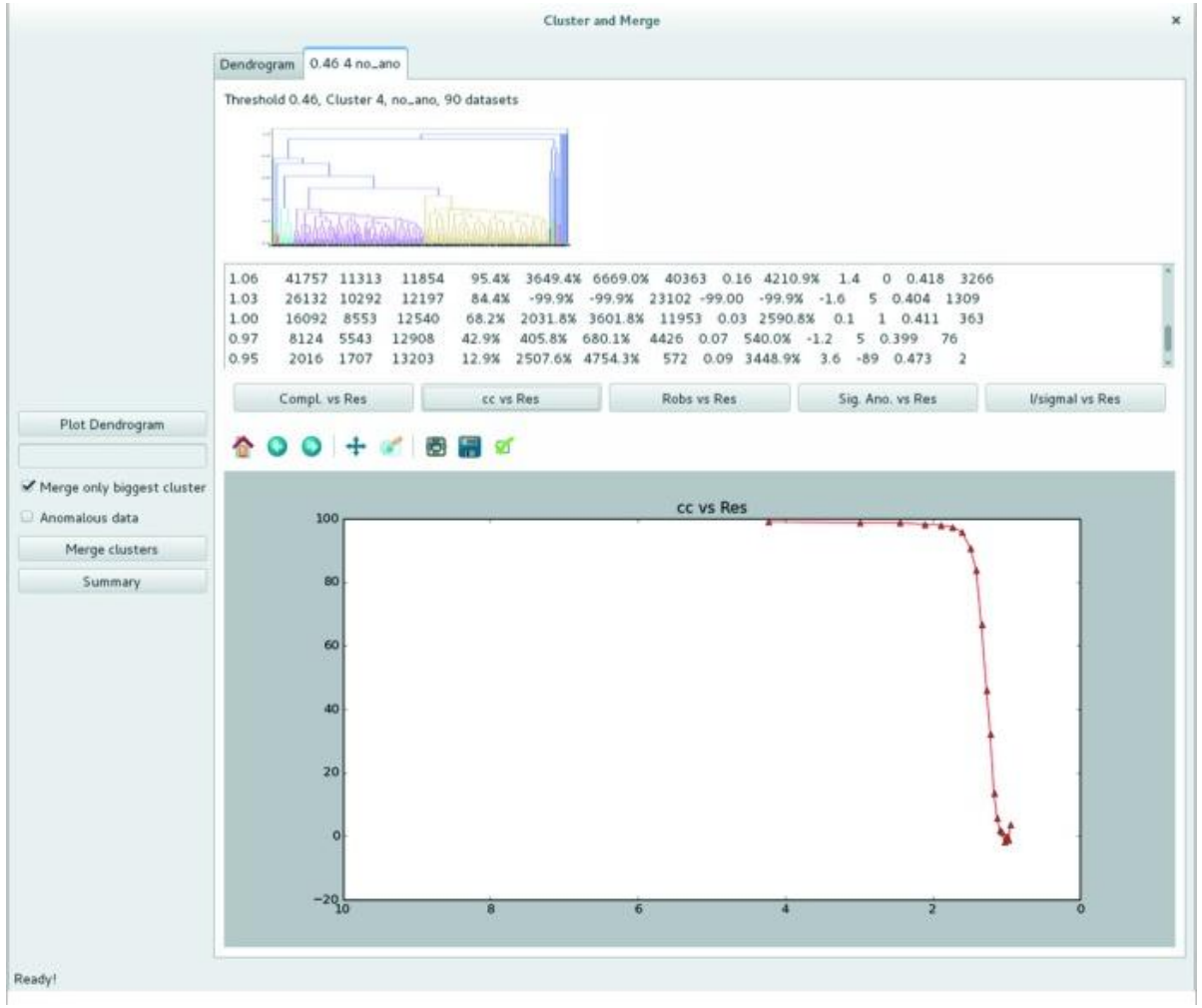
Giordano, R et al. (2012). *Acta D* **68**, 649–658.

Based on unit cell parameters

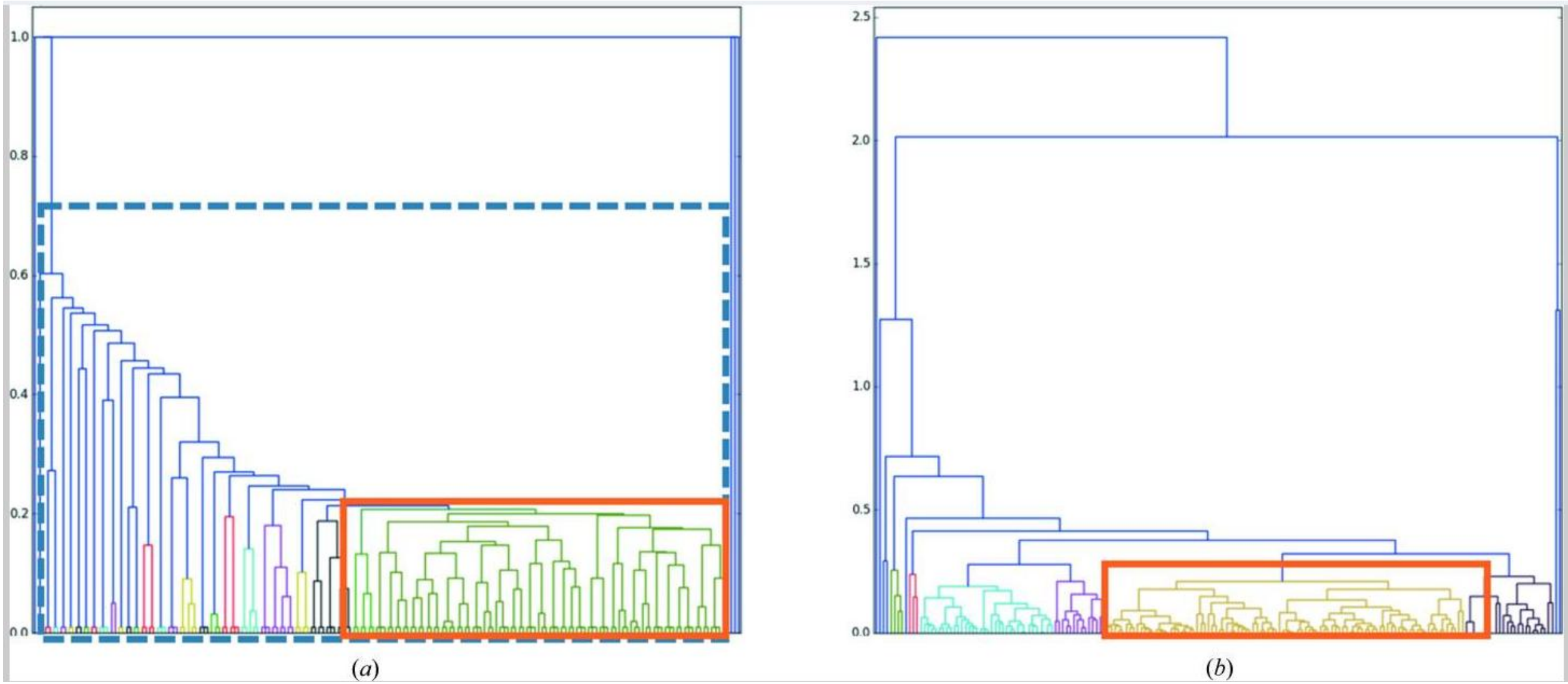
$$D(a,b) = max\left(\frac{|A_a - A_b|}{min(A_a,A_b)}, \frac{|B_a - B_b|}{min(B_a,B_b)}, \frac{|C_a - C_b|}{min(C_a,C_b)}\right)$$

- D=0 means identical crystals (cc=1)
- D=1 means uncorrelated crystals (cc=0)





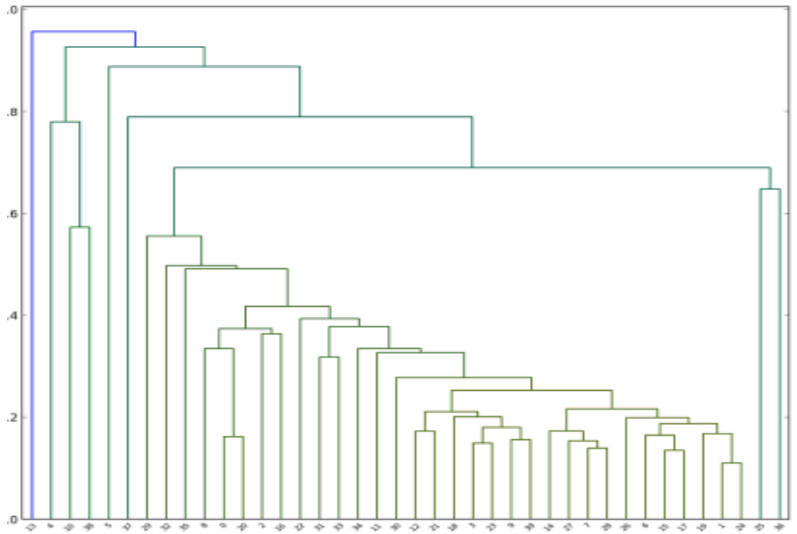
Main features of the *ccCluster* GUI. (*a*) Main panel. The dendrogram is coloured according to the chosen clustering thresholds. Blue branches represent nodes above the thresholds chosen, meaning that they will not be used during the merging step. On the left, buttons allow the user to launch the merging procedure. (*b*) Results panel. A tab is produced for each merged group of datasets, allowing the plotting of statistics calculated using *XSCALE*. Each tab code corresponds to the name of the folder containing the output of merging.



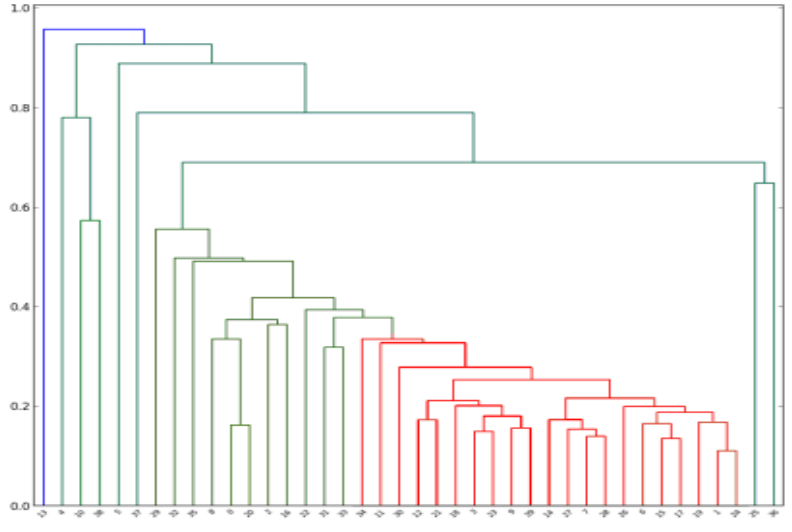
Dendrograms representing the clustering of 184 2° wedges collected from different thaumatin crystals. (*a*) Clustering according to correlation coefficient. The orange rectangle represents the cluster at a threshold of 0.21 and the blue dashed rectangle the cluster at 0.8. (*b*) Clustering based on variation of unit-cell parameters. The selected cluster (orange rectangle) comprises 90 datasets at a threshold of 0.27.

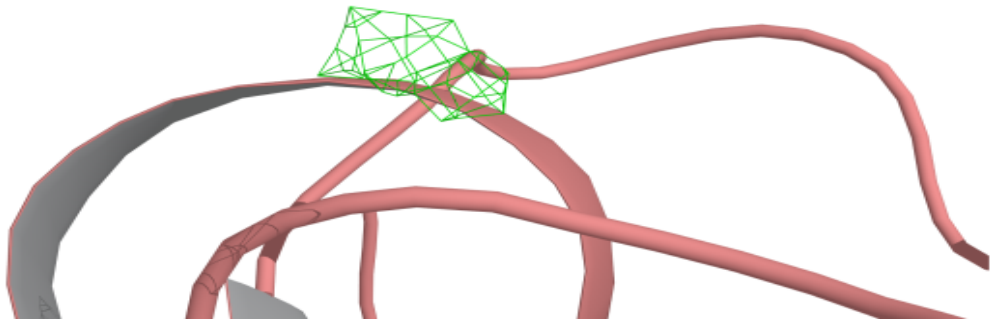
effect of clustering threshold

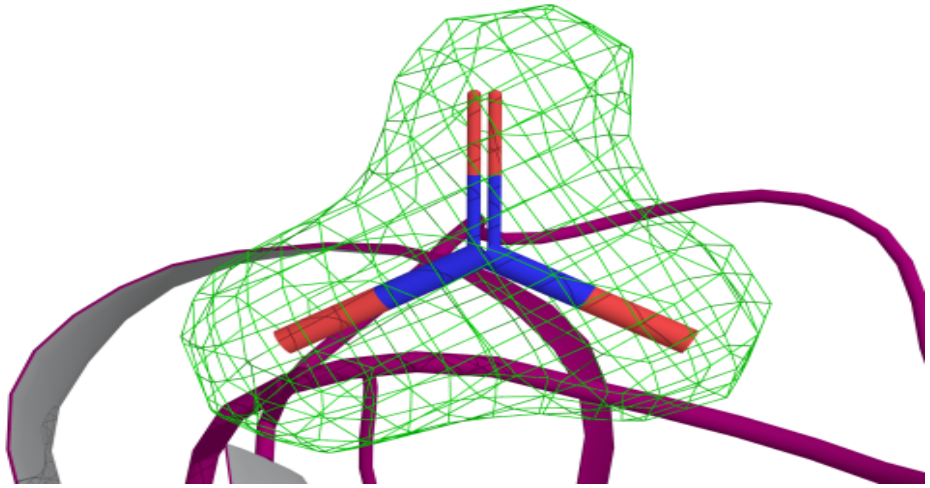
Big cluster: 39 data sets



Small cluster: 21 data sets







The complex analysis of X-ray mesh scans for macromolecular crystallography

Authors

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[a] European Synchrotron Radiation Facility, BP 220, Grenoble, 38043, France

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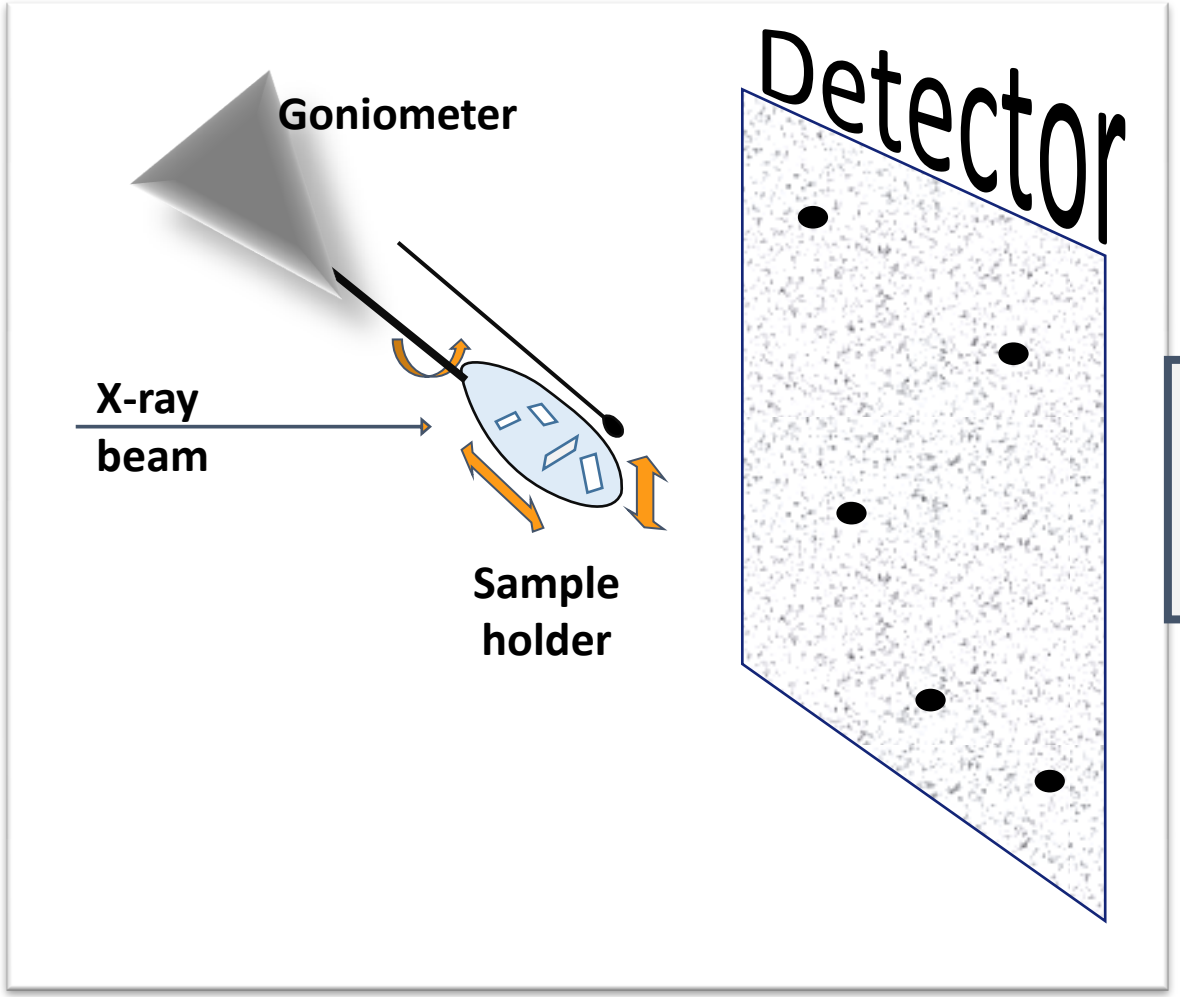
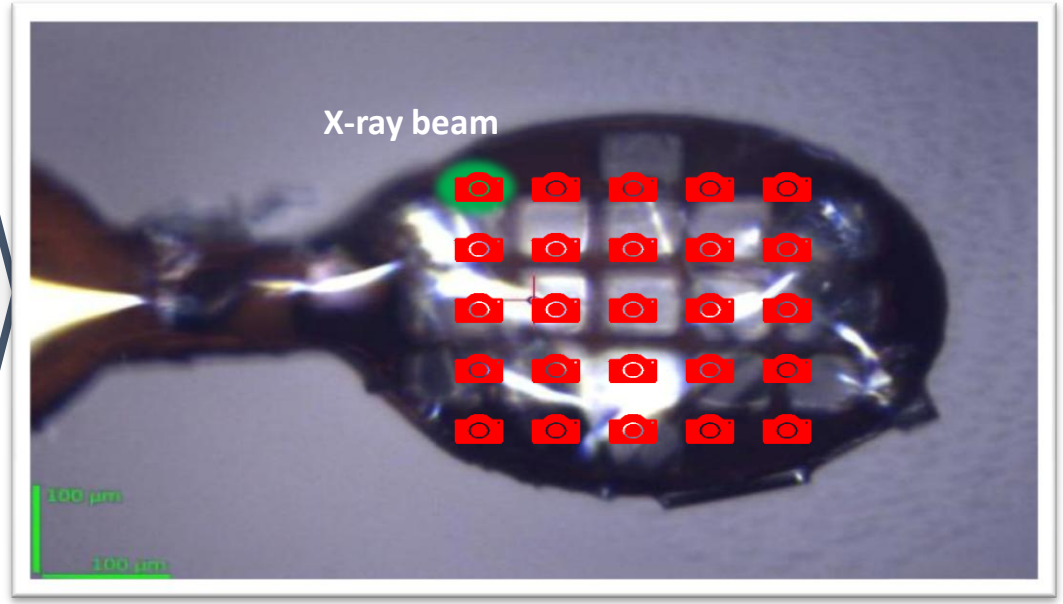
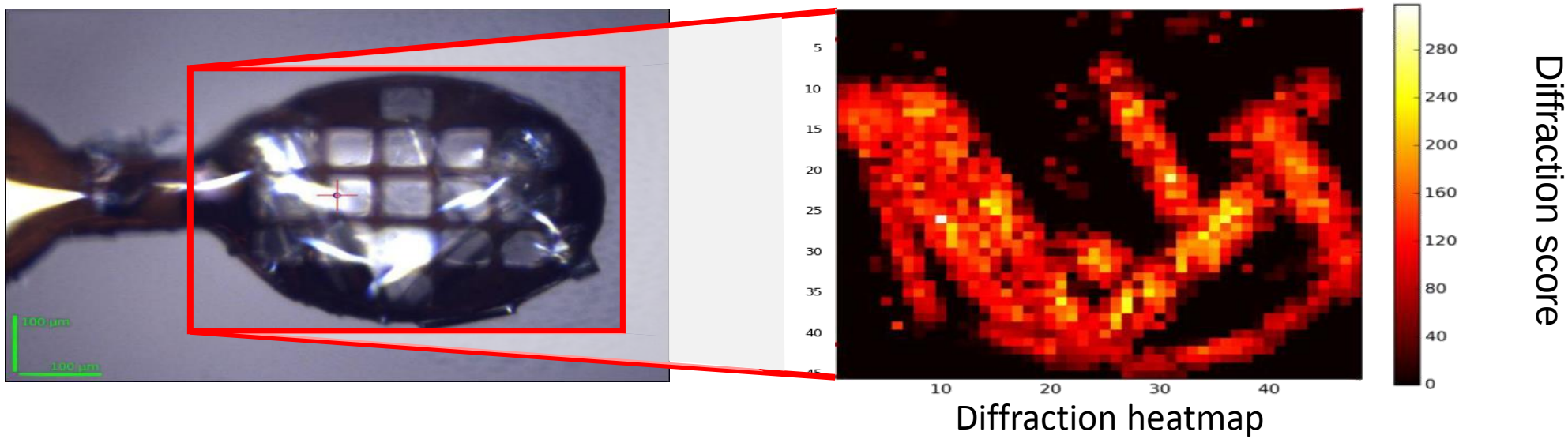
X-ray mesh scanS



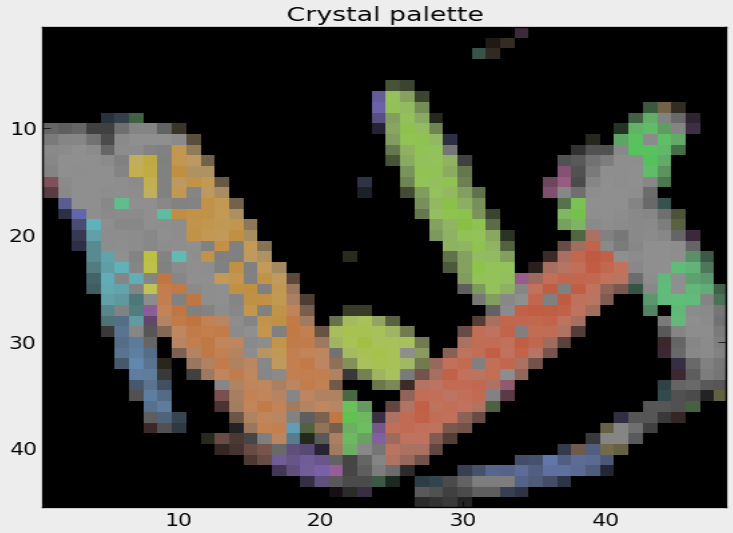


Diffraction quality evaluation

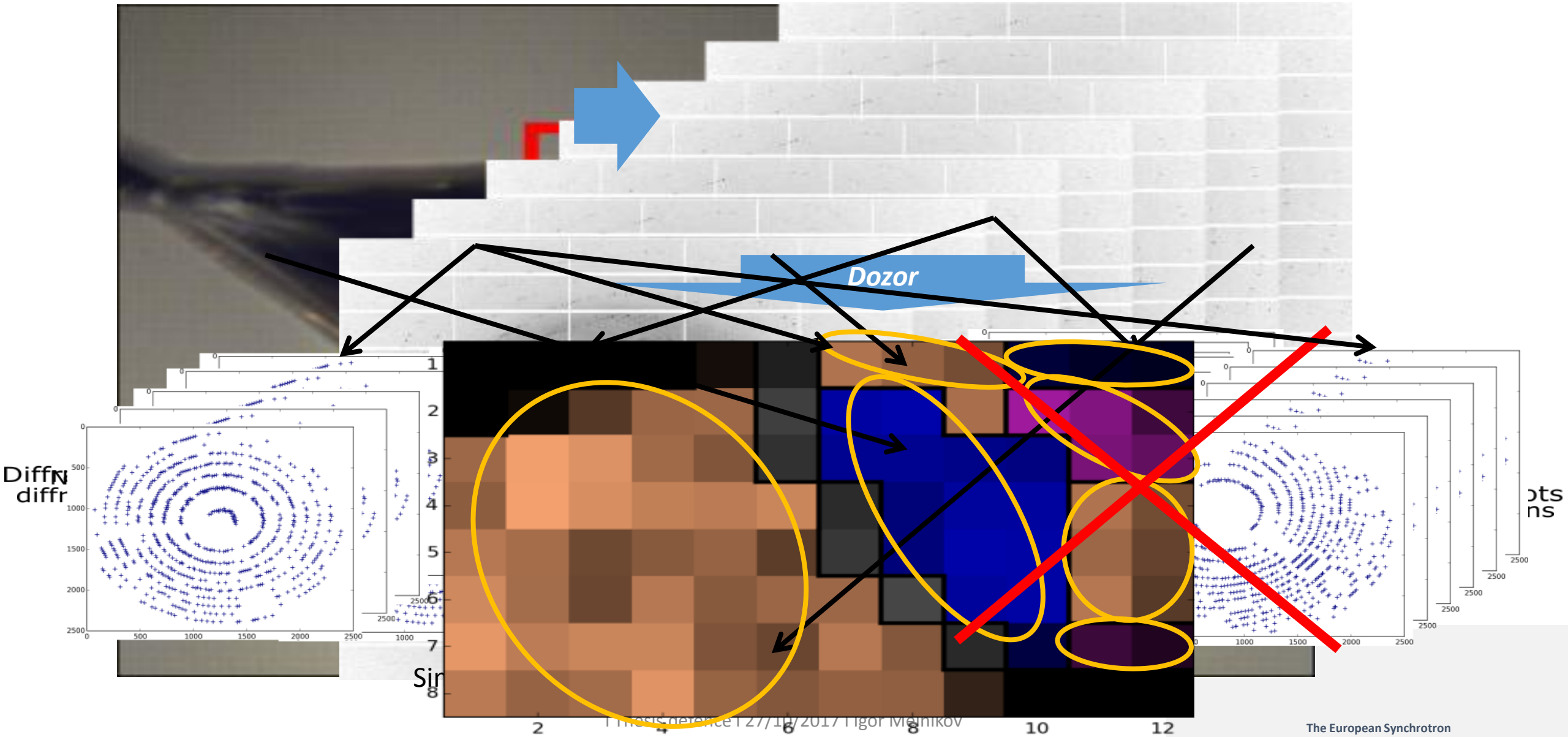
Dozor



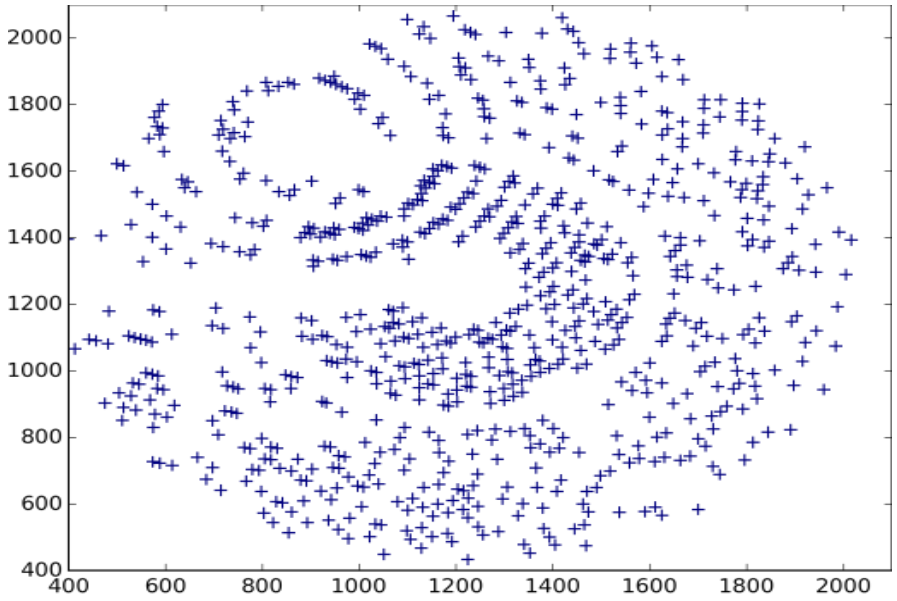
But, the analysis should go further

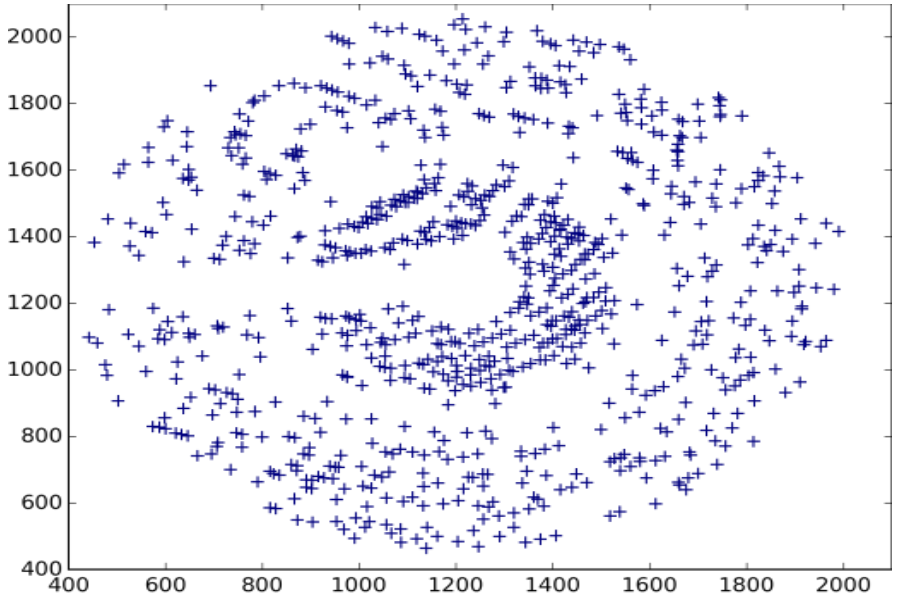


Meshbest – A program to analyse mesh scans

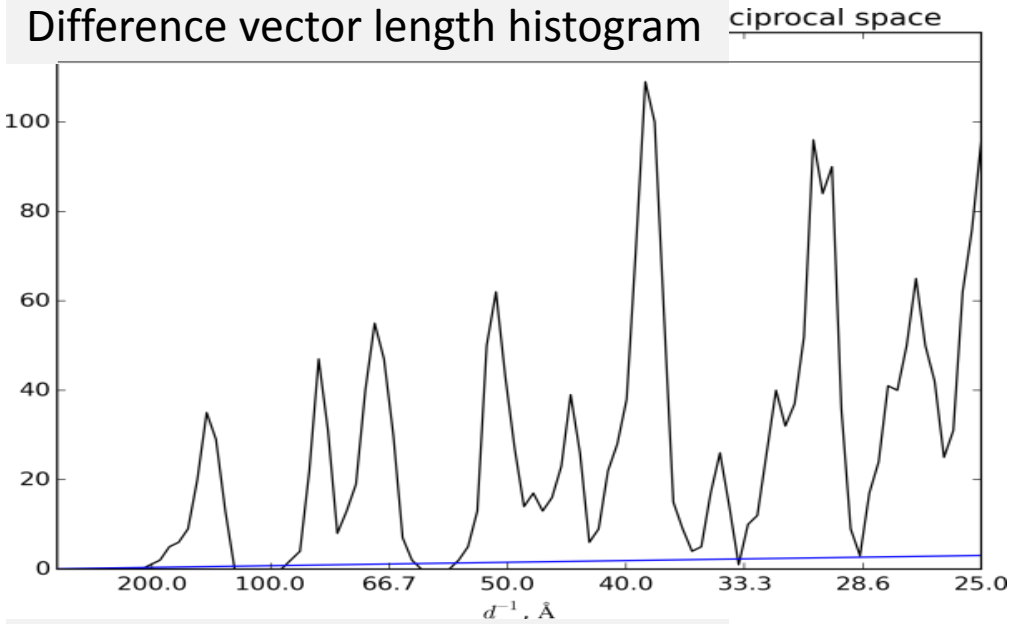


DVL histogram

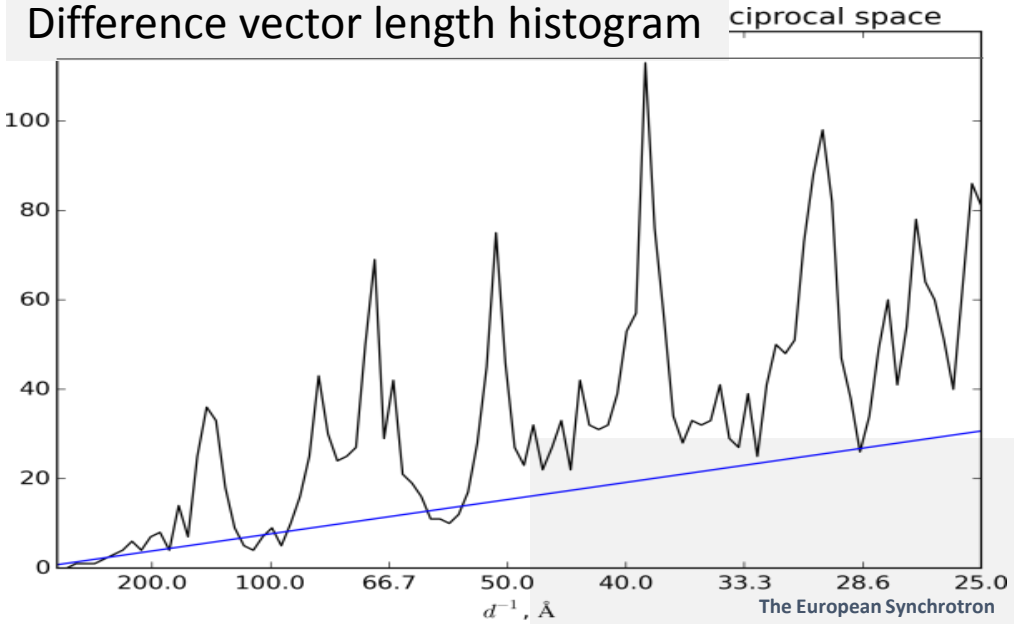




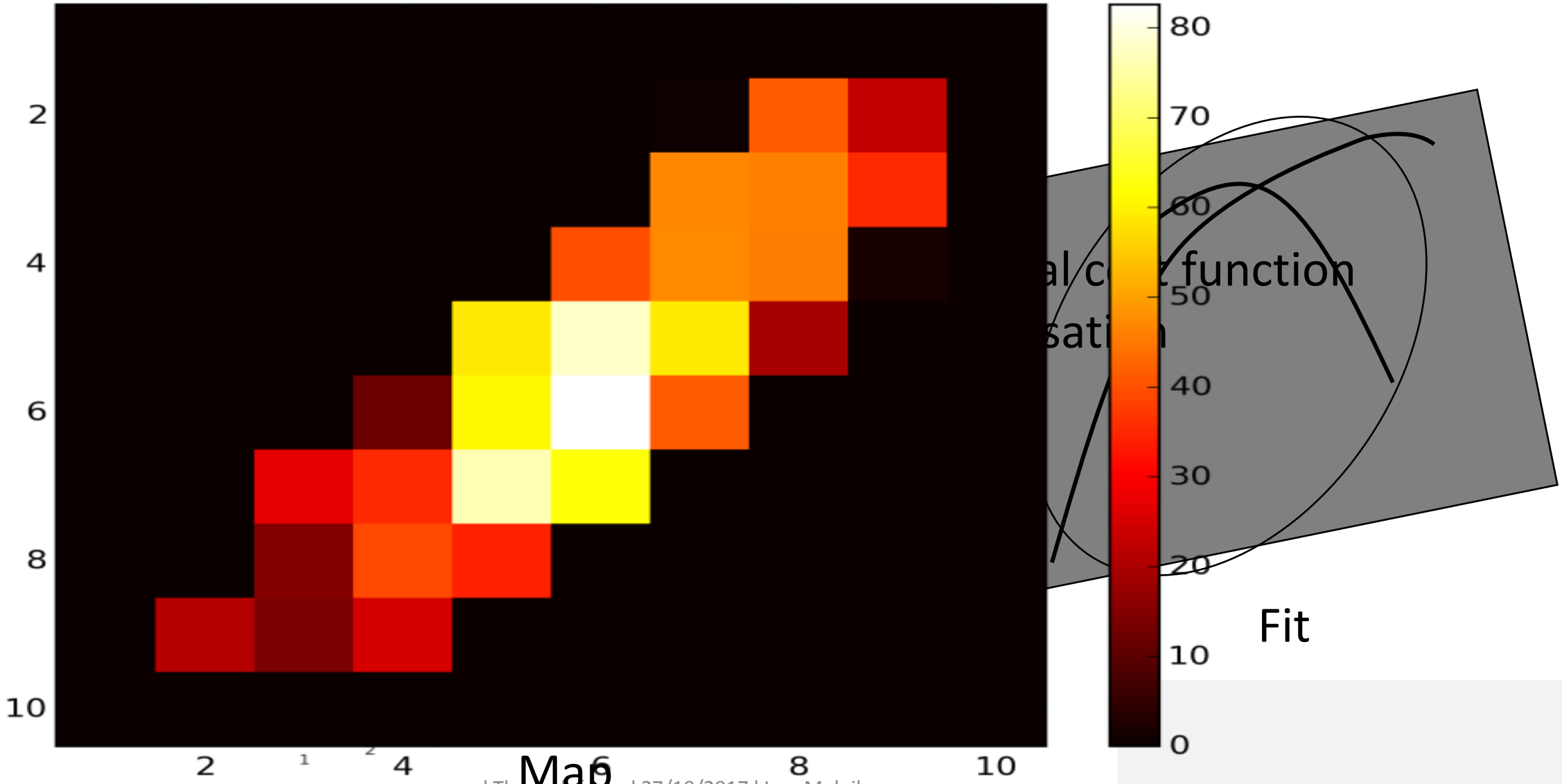
Difference vector length histogram



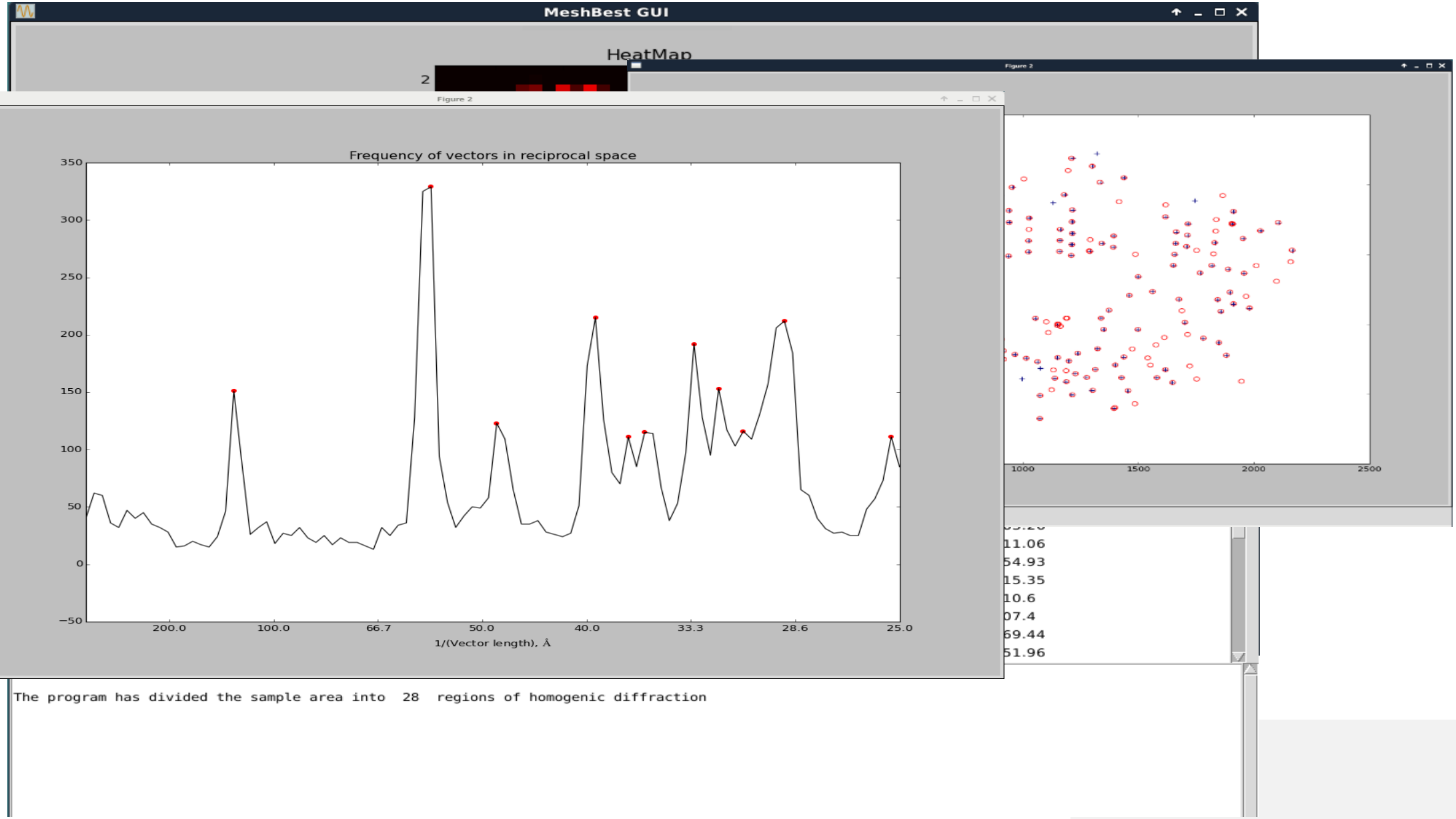
Difference vector length histogram



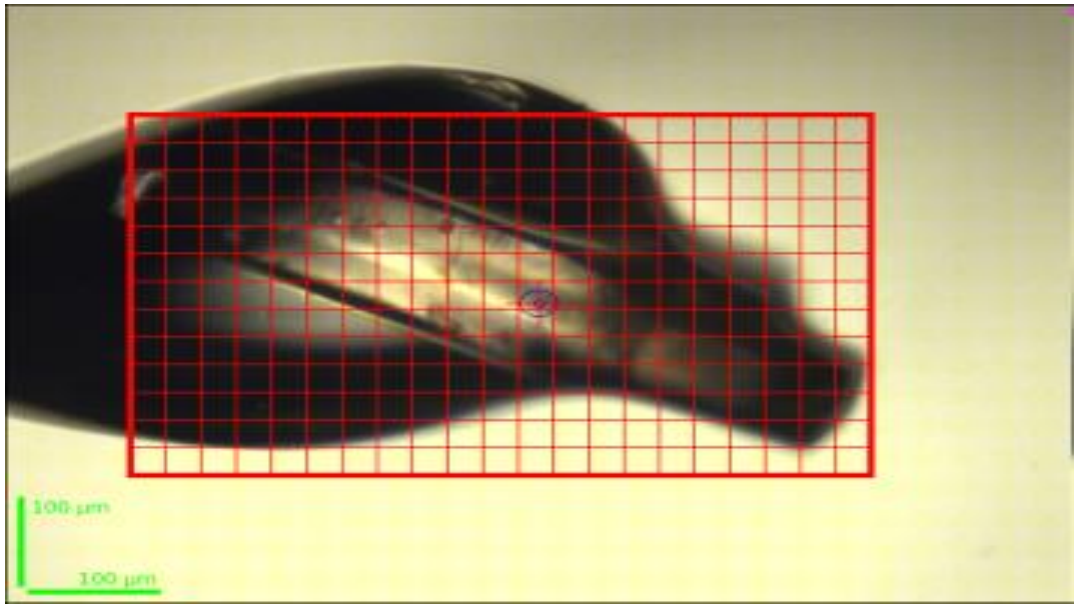
fit to the crystal shape

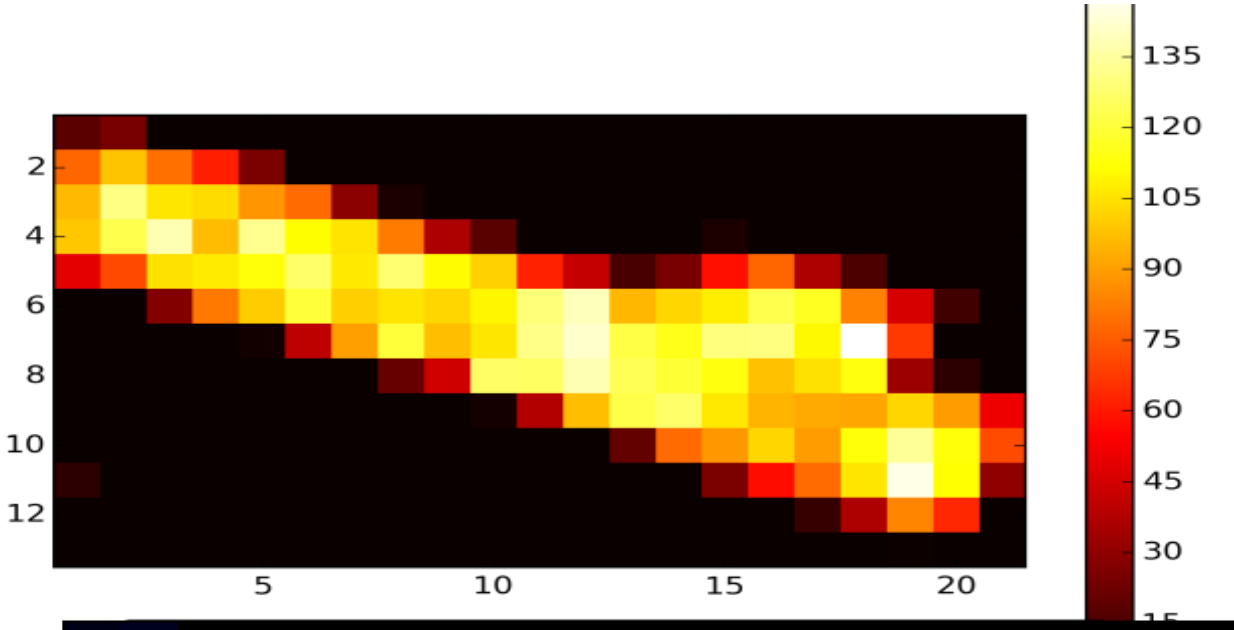


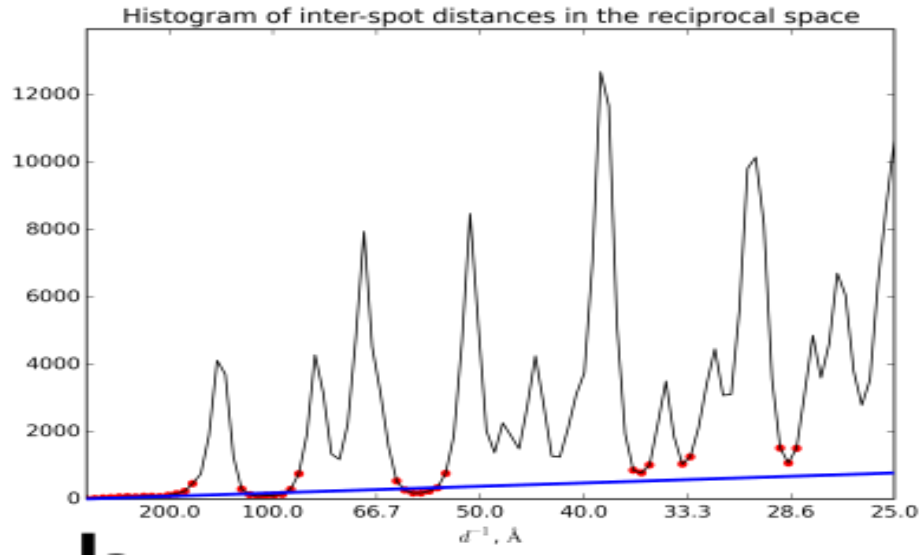
MeshBest GUI

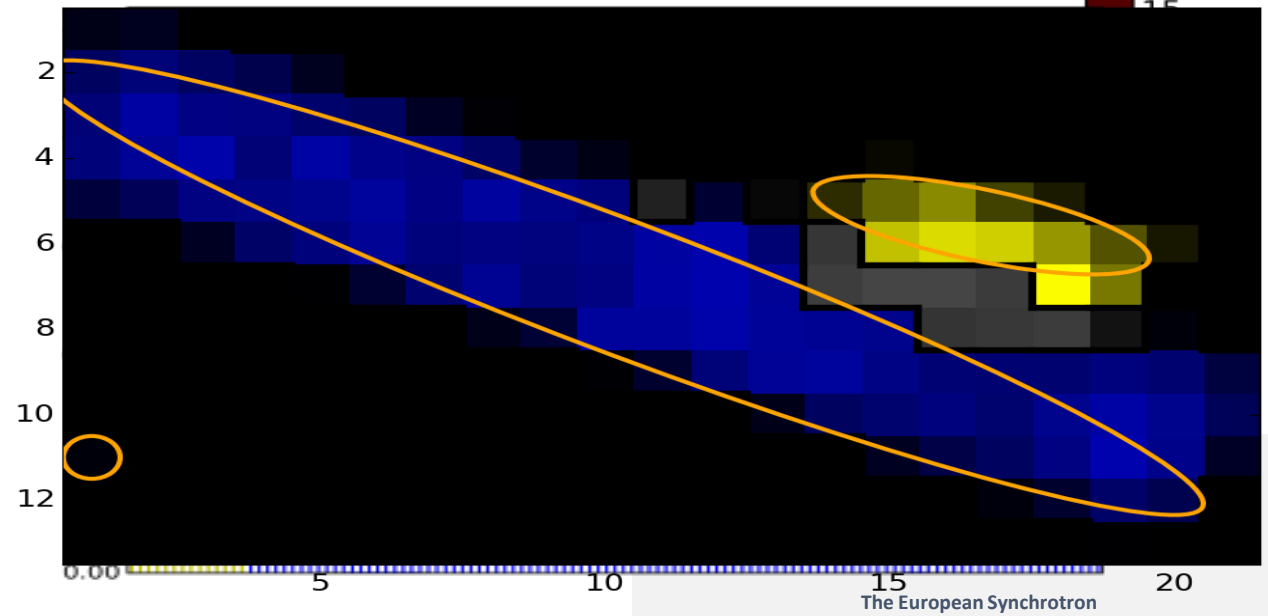


A large crystal with A SMALL Satellite

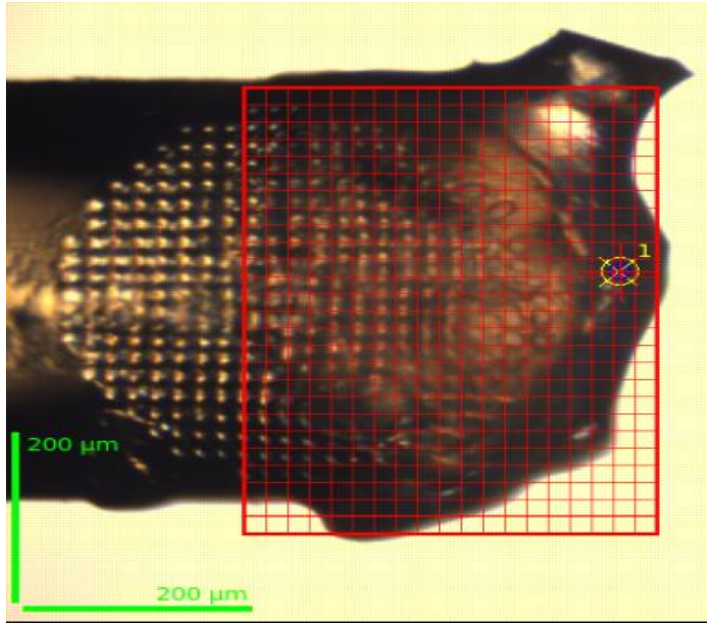


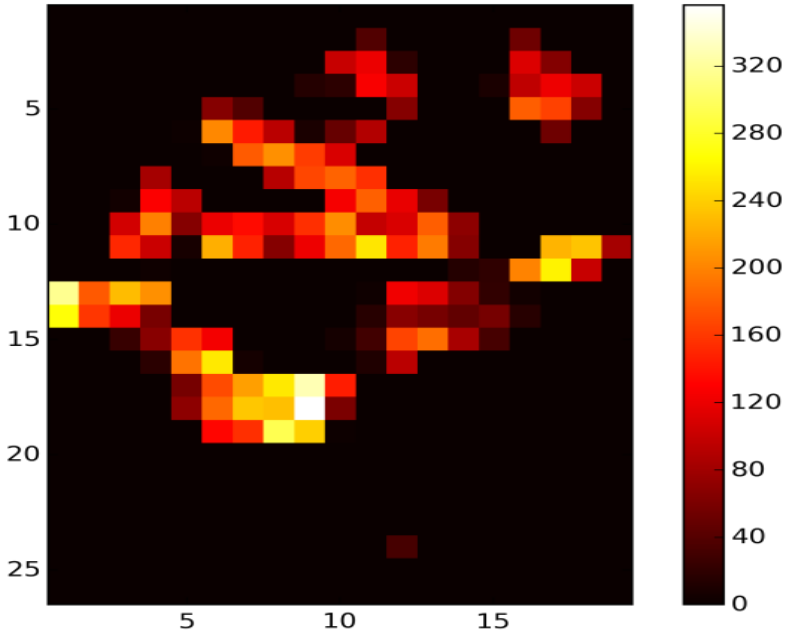




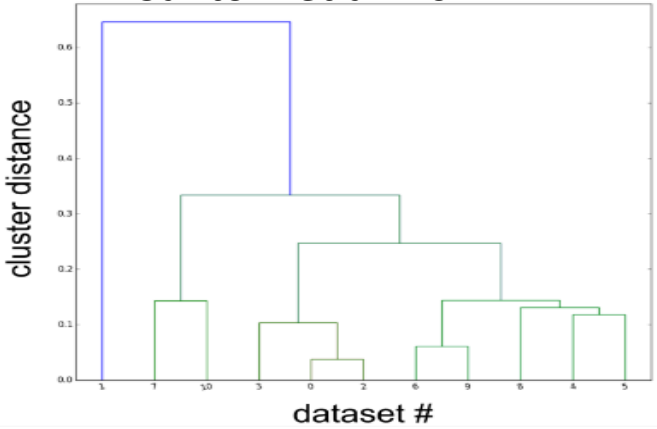


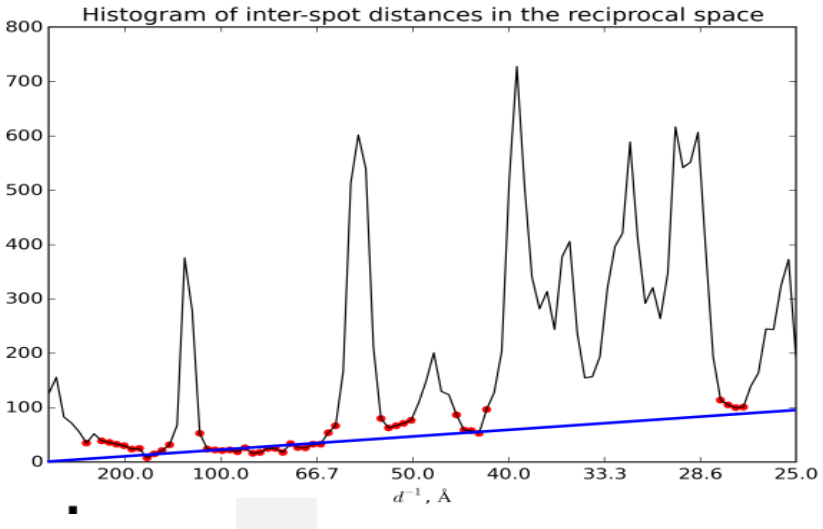
meshbest in SSX pipeline

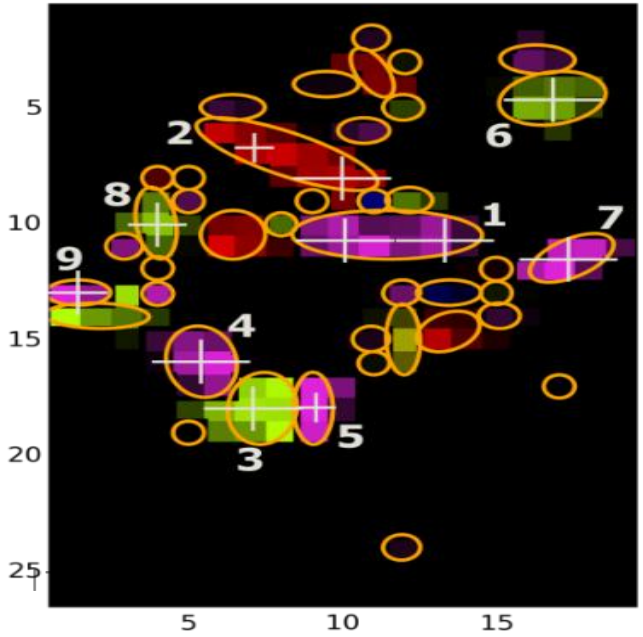




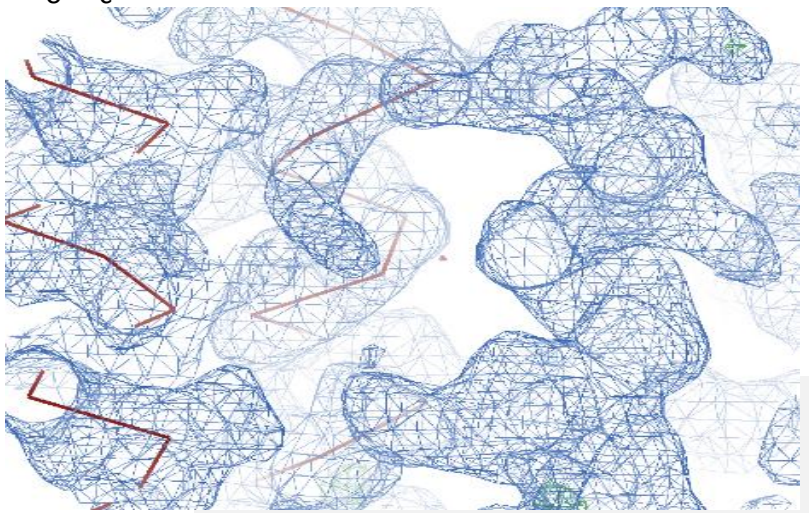
Santoni et al. 2017



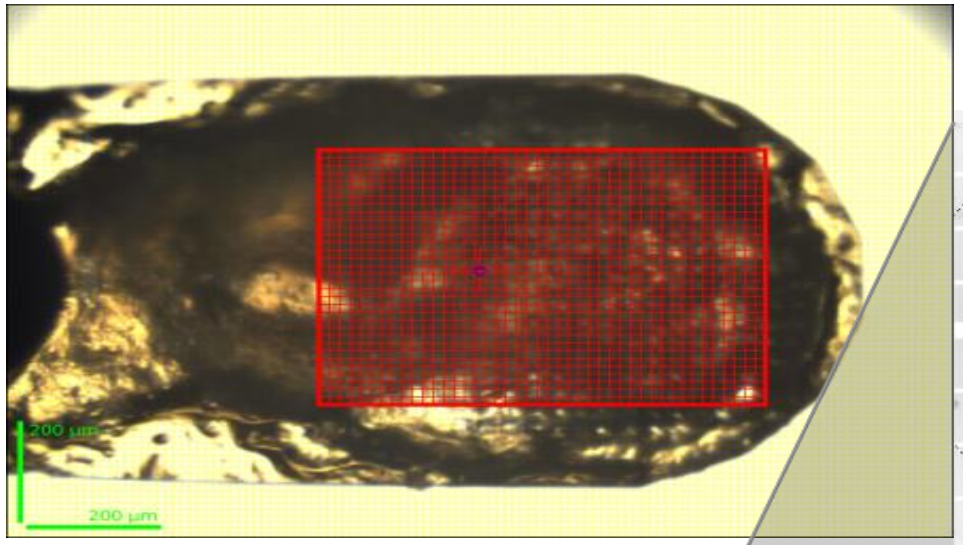


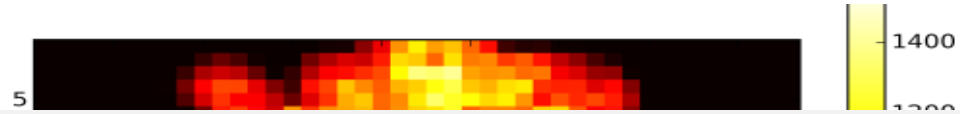


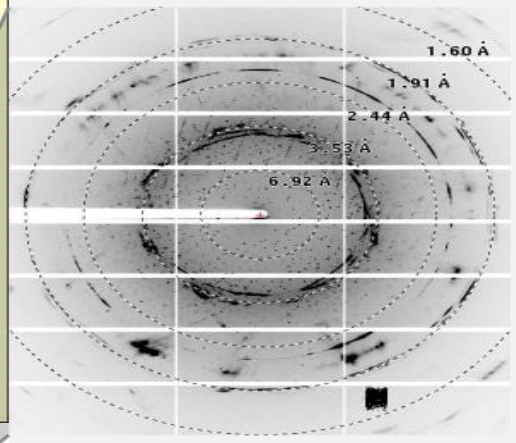
$2F_o$-F_c, contoured at 1.2σ

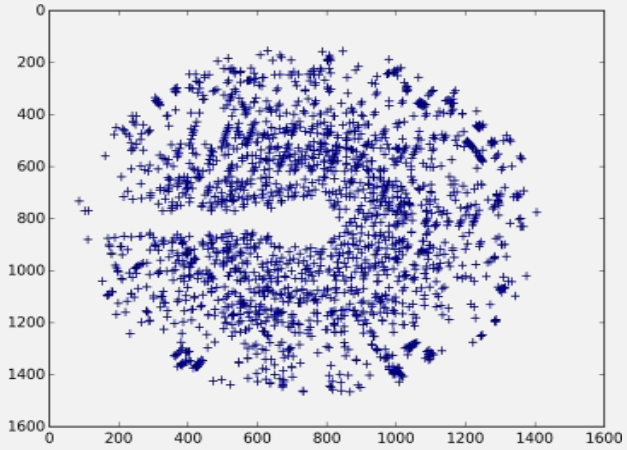


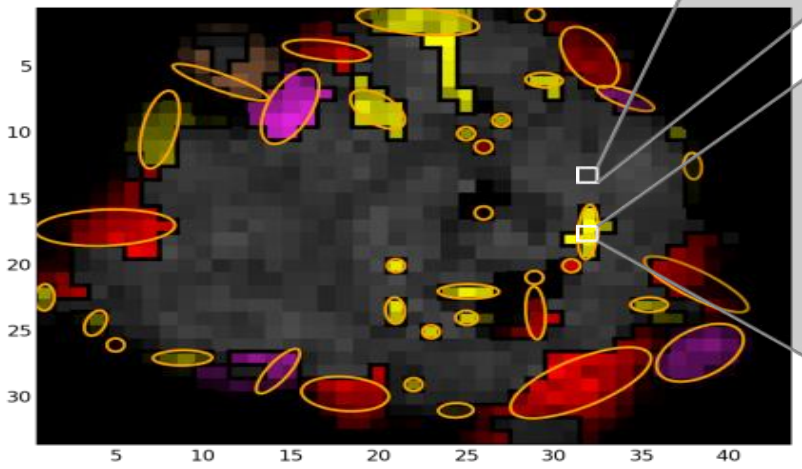
crystal mess

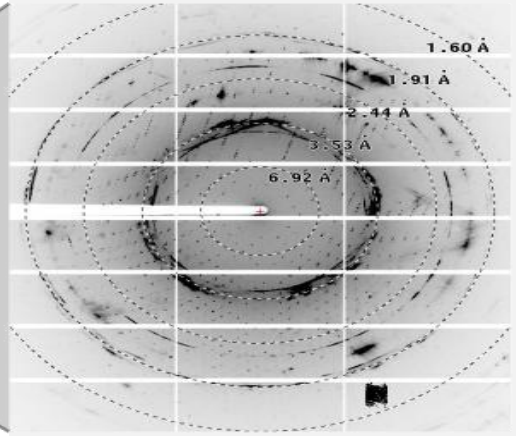


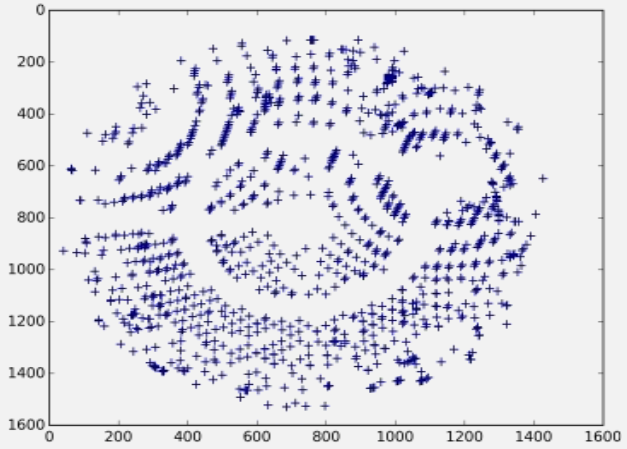












- A method to analyse mesh scans and to localise individual protein crystals in a sample holder has been developed

- The algorithms have been implemented in the program *MeshBest* now installed on the ESRF MX beamlines

- The method yields a crystal map in which individual crystals are color-coded. It also shows areas of multi-crystal diffraction

- Crystal shapes and sizes are assessed by elliptical shape approximation