

**Figure 1.** Monomeric form of LLT1 (PDB code 4QKG) and its crystal contacts.

**Keywords:** LLT1, NK receptor, C-type lectin like

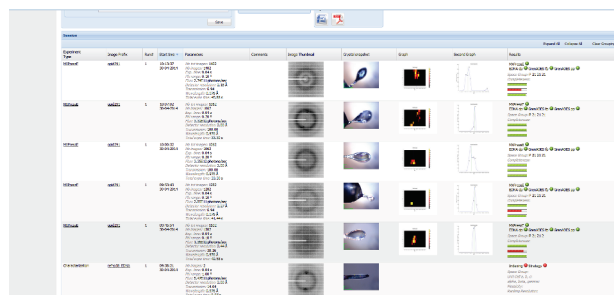
## MS9-P19 MASSIF1: fully automated macromolecular crystallography

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MASSIF1 is a unique facility for the high throughput, fully automatic characterisation and data collection of crystals of macromolecules. The new service is not designed to replace user visits to the synchrotron but rather to do the hard work of screening crystals or collecting data sets through the night, freeing researchers to spend time on more challenging data collection problems and study the underlying biology. Beam time is booked flexibly and samples then enter a queuing system, users interact with the beamline by describing experimental requirements, that are used by the beamline software to set data collection parameters, in a database, ISPyB, where results are also viewed and downloaded. The service is made possible by RoboDiff – a new ESRF-developed sample changer that also acts as a goniometer –, a highly intense X-ray beam ( $3 \times 10^{12}$  ph/sec in  $100 \times 50 \mu\text{m}^2$ ) and complex workflows that fully evaluate samples, centre the best volumes and collect diffraction data sets optimised for maximum resolution with minimised radiation damage. As MASSIF1 is fully automatic, data are collected for the first time in a consistent manner and should allow the accumulation and comparison of a large amount of information that was previously unknown, including the exact dimensions of crystals and deeper information about their quality. Once the beamline has been running for an extended period, it will provide a treasure trove of additional information to feed back into crystallisation experiments and the software used to collect the data. In less than three months of operation more than 6 million diffraction images have been collected from 4272 samples ranging from initial hits from crystallisation experiments to large-scale data collection for drug discovery programmes. The automatic routines developed are often able to locate crystals more effectively than the human eye and in many cases have obtained higher resolution data sets as all positions within a sample can be evaluated for diffraction quality. The routines used on MASSIF-1 have been developed using a workflow tool that is also used to provide a wide variety of complex data acquisition protocols available on all ESRF MX beamlines.



**Figure 1.** Summary page of data collections performed on MASSIF1 as seen in ISPyB showing diffraction quality maps, snapshots and the results of processed data.

**Keywords:** Automation, fragment screening, robotics, workflows