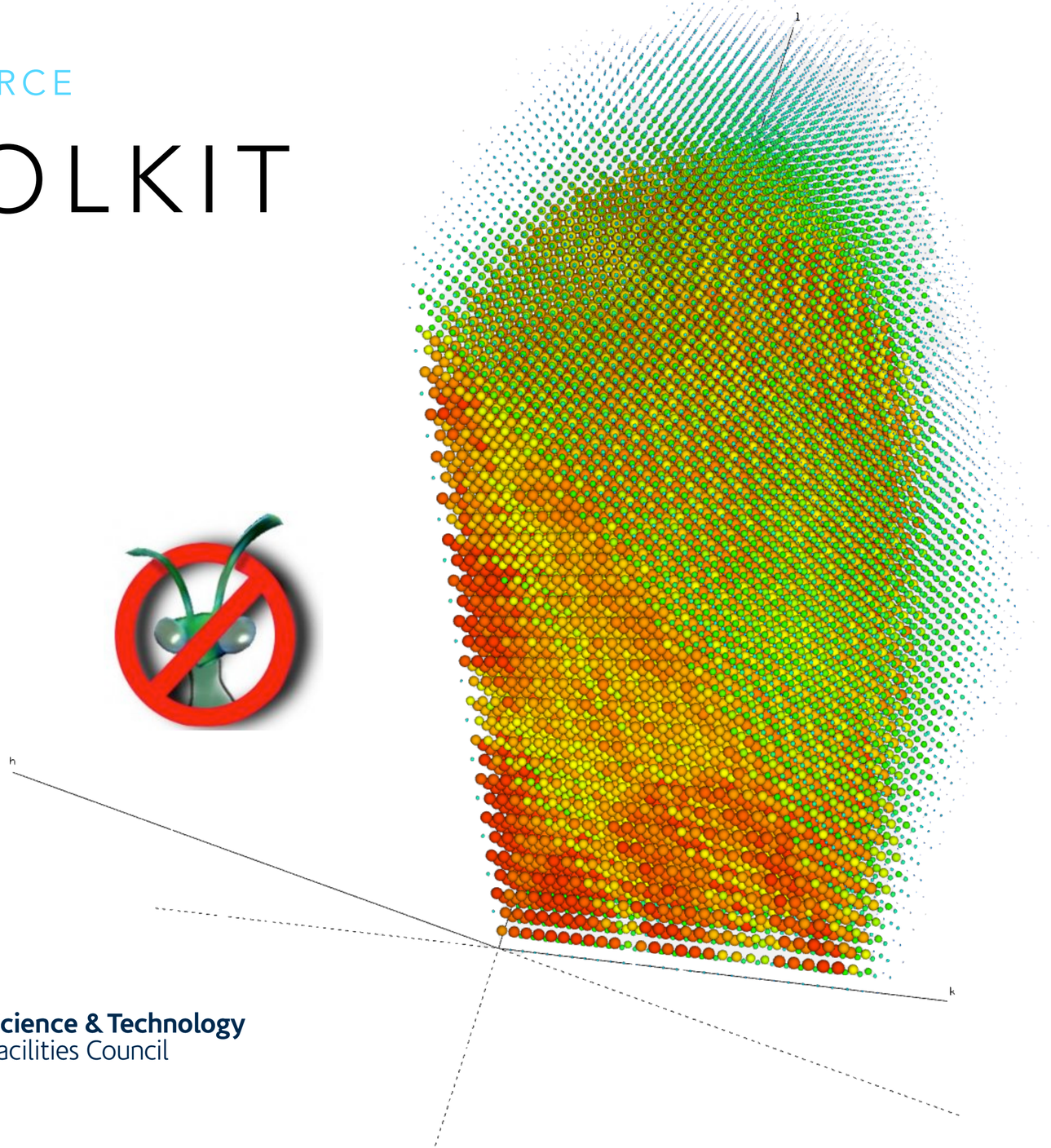
NOBUGS 2022

GRAEME WINTER / DIAMOND LIGHT SOURCE

DIALS AS A TOOLKIT



DIALS
Diffraction Integration for Advanced Light Sources

diamond

CCP4

BERKELEY LAB
Lawrence Berkeley National Laboratory

wellcome

Science & Technology Facilities Council

DIALS
Diffraction Integration for Advanced Light Sources

wellcome

BioStructX

diamond

CCP4

BERKELEY LAB
Lawrence Berkeley National Laboratory

Science & Technology Facilities Council

FP7 Research infrastructures, Grant/Award Number: 283570;
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Wellcome Trust, Grant/Award Numbers: 202933/Z/16/Z, 218270/Z/19/Z

research papers

Acta Crystallographica Section D
Biological Crystallography
ISSN 0907-4449

The integration of macromolecular diffraction data

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The objective of any modern data-processing program is to produce from a set of diffraction images a set of indices (*hkl*s) with their associated intensities (and estimates of their uncertainties), together with an accurate estimate of the crystal unit-cell parameters. This procedure should not only be reliable, but should involve an absolute minimum of user intervention. The process can be conveniently divided into three stages. The first (autoindexing) determines the unit-cell parameters and the orientation of the crystal. The unit-cell parameters may indicate the likely Laue group of the crystal. The second step is to refine the initial estimate of the unit-cell parameters and also the crystal mosaicity using a procedure known as post-refinement. The third step is to integrate the images, which consists of predicting the positions of the Bragg reflections on each image and obtaining an estimate of the intensity of each reflection and its uncertainty. This is carried out while simultaneously refining various detector and crystal parameters. Basic features of the algorithms employed for each of these three separate steps are described, principally with reference to the program *MOSFLM*.

1. Introduction

The collection of macromolecular diffraction data has undergone dramatic advances during the last 15 years with the advent of two-dimensional area detectors such as image plates and CCDs, crystal cryocooling and the availability of intense, monochromatic and highly collimated X-ray beams from

research papers

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XDS

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A version of this paper will be published as a chapter in the new edition of Volume *F* of *International Tables for Crystallography*.

The usage and control of recent modifications of the program package *XDS* for the processing of rotation images are described in the context of previous versions. New features include automatic determination of spot size and reflecting range and recognition and assignment of crystal symmetry. Moreover, the limitations of earlier package versions on the number of correction/scaling factors and the representation of pixel contents have been removed. Large program parts have been restructured for parallel processing so that the quality and completeness of collected data can be assessed soon after measurement.

1. Functional specification

The program package *XDS* (Kabsch, 1988*a*,*b*, 1993, 2010) was developed for the reduction of single-crystal diffraction data recorded on a planar detector by the rotation method using monochromatic X-rays. It includes a set of three programs.

XDS accepts a sequence of adjacent non-overlapping rotation images from a variety of imaging-plate, CCD, pixel and multiwire area detectors, infers crystal symmetry and metrics and produces a list of corrected integrated intensities of the reflections occurring in the images in a nearly automatic way. The program assumes that each image covers the same

research papers

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The finer things in X-ray diffraction data collection

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Received 6 May 1999
Accepted 5 July 1999

X-ray diffraction images from two-dimensional position-sensitive detectors can be characterized as thick or thin, depending on whether the rotation-angle increment per image is greater than or less than the crystal mosaicity, respectively. The expectations and consequences of the processing of thick and thin images in terms of spatial overlap, saturated pixels, X-ray background and $I/\sigma(I)$ are discussed. The *d*TREK* software suite for processing diffraction images is briefly introduced, and results from *d*TREK* are compared with those from another popular package.

1. Introduction

research papers

Acta Crystallographica Section D
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How good are my data and what is the res

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Received 7
Accepted

Following integration of the observed diffraction spots, the process of 'data reduction' initially aims to determine the point-group symmetry of the data and the likely space group. This can be performed with the program *POINTLESS*. The scaling program then puts all the measurements on a common scale, averages measurements of symmetry-related reflections (using the symmetry determined previously) and produces many statistics that provide the first important measures of data quality. A new scaling program, *AIMLESS*, implements scaling models similar to those in *SCALA* but adds some additional analyses. From the analyses, a number of decisions can be made about the quality of the data and whether some measurements should be discarded. The effective 'resolution' of a data set is a difficult and possibly contentious question (particularly with referees of papers) and this is discussed in the light of tests comparing the data-processing statistics with trials of refinement against observed and simulated data, and automated model-building and comparison of maps calculated with different resolution limits. These trials show that adding weak high-resolution data beyond the commonly used limits may make some improvement and does no harm.

Centre National de la Recherche Scientifique
Université Paris-Sud

Laboratoire pour l'Utilisation du Rayonnement Electromagnétique

Proceedings

of the EEC Cooperative Workshop

on Position-Sensitive Detector Software

(Phases I & II)

held at L.U.R.E. from May 26 to June 7, 1986.

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Wellcome Trust, Grant/Award Numbers: 202933/Z/16/Z, 218270/Z/19/Z

The following have contributed to the git repositories (based on their git identities, in first-name alphabetical order) for dxtbx and dials:

Aaron Brewster, Asmit Bhowmick, Ben Williams, Billy Poon, Clemens Weninger, Cody, Daniel Paley, David McDonagh, David Waterman, Derek Mendez, Dorothee Liebschner, Elena Pascal, Graeme Winter, Helen Ginn, Huw Jenkins, Ian Rees, Iris Young, James Beilsten-Edmands, James Parkhurst, Johan Hattne, Katrin Leinweber, Keitaro Yamashita, Kevin Dalton, Lee James O'Riordan, Luis Fuentes-Montero, Marcin Wojdyr, Markus Gerstel, Nathaniel Echols, Nicholas Devenish, Nicholas Sauter, Nigel W. Moriarty, Noemi Frisina, Oliver Zeldin, Robert Bolotovsky, Richard Gildea, Robert Rosca, Tara Michels-Clark, Takanori Nakane, and Viktor Bengtsson.

DIALS East PI - **Gwyndaf Evans**
DIALS West PI - **Nick Sauter**

TARGET AUDIENCE

- Single-crystal X-ray diffraction people - users, beamline staff, support groups
- Anyone using a pixel array detector may find some of this useful

BACKGROUND ON THE DIALS PROJECT

- Tools for analysis of X-ray diffraction data
- Also designed to allow extension / modification / abuse in entertaining ways (aim: motivated researcher should be able to abuse, extend and contribute)
- Based on CCTBX and written in mix of C++ and Python
- Design inspired by d*TREK e.g. collection of tools rather than a monolithic program

GENERAL CAPABILITIES

- Minimal assumptions about experiment
- Optimised for PAD
- Only really useful for single*-crystal diffraction

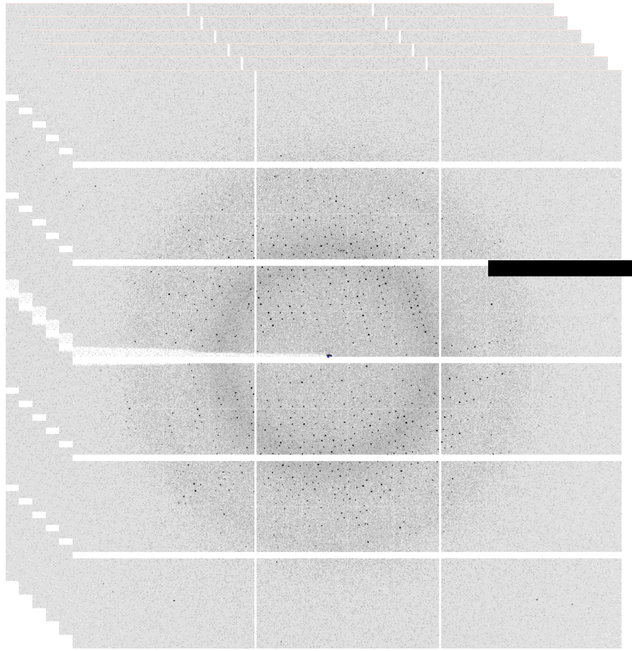
*or small N samples in the beam at once**
**OK not powder diffraction or small angle scattering

OVERVIEW

- Automated processing
- Common command-line data analysis
- Advanced command-line tools
- Python API

AUTOMATIC PROCESSING

- Diffraction data go in, MTZ files come out
- Can use DIALS or XDS for "processing engine"
- Set up to do all the decision making for you
- Workhorse for data processing at Diamond



xia2

DIALS
Diffraction Integration for Advanced Light Sources

```
OPENED INPUT MTZ FILE
Logical Name: HKLIN   Filename: scaled.mtz

* Title:

From dials.export

* Base dataset:

       0 HKL_base
         HKL_base
         HKL_base

* Number of Datasets = 1

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

       1 DIALS
         XTAL
         FROMDIALS
            77.8825   77.8825   77.8825   90.0000   90.0000   90.0000
            0.91808
```

USAGE

```
xia2 /directory
xia2.small_molecule /directory  <- small molecule mode

xia2 image=/directory/filename_0001.cbf or filename.h5

xia2 image=/directory/filename.h5:1:1800

xia2 image=A image=B image=C
```

ADDITIONAL

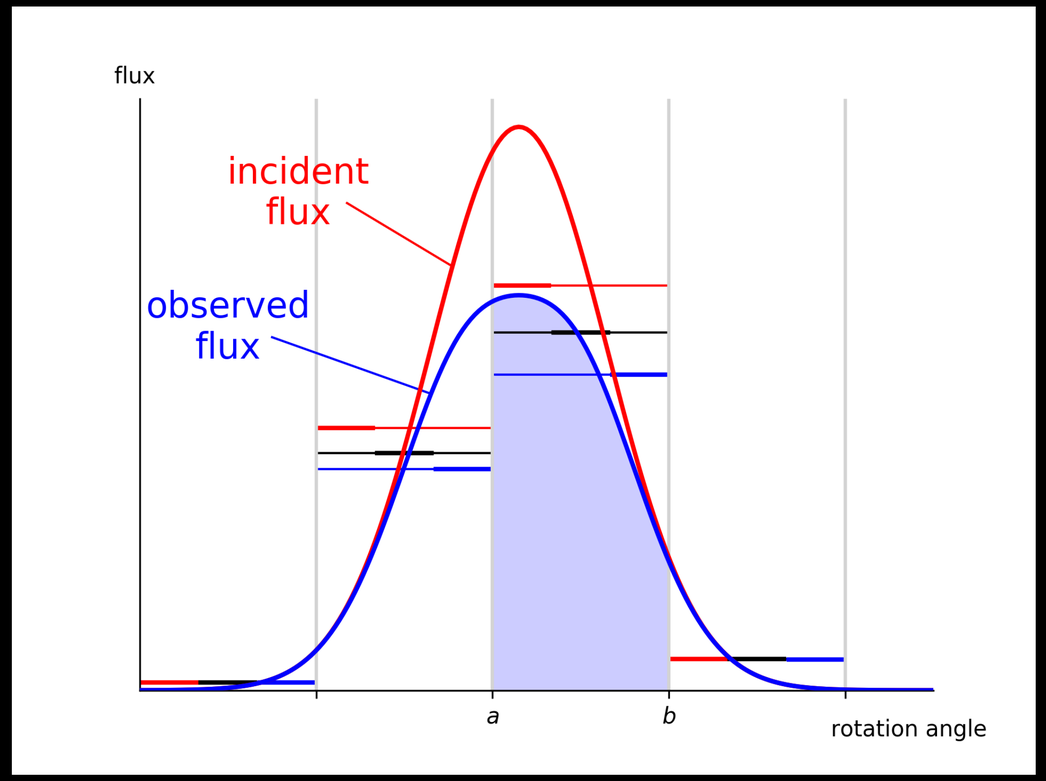
- Can index all sweeps together -> multi_sweep_index=true - nice for multi-axis experiments, critical for e.g. absolute structure experiments, default for “small molecule” mode
- Can adjust the extent of expected absorption etc - useful for longer wavelength experiments

OTHER XIA2 TOOLS

- screen19 - estimation of data collection parameters for small molecule data collection
- xia2.multiplex - automated combination of multi-crystal data sets

SCREEN 19

- Prevent data exceeding PAD instantaneous count rate limit
- Performs profile fitting on small data sets to estimate peak rate, not strongest pixel
- Provides recommendations of data collection parameters to use
- Targets small molecules / i19 @ DLS



MULTIPLEX

- Automated composition of data from multiple samples
- Uses results of DIALS integration
- Derives crystal symmetry and resolves indexing ambiguity in parallel
- Can be used to also provide sub-clusters for comparison

research papers

Acta Cryst D STRUCTURAL BIOLOGY

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xia2.multiplex: a multi-crystal data-analysis pipeline

Richard J. Gildea,[a]* James Beilsten-Edmands,[a] Danny Axford,[a] Sam Horrell,[a,b] Pierre Aller,[a] James Sandy,[a] Juan Sanchez-Weatherby,[a] C. David Owen,[a,b] Petra Lukacik,[a,b] Claire Strain-Damerell,[a,b] Robin L. Owen,[a] Martin A. Walsh[a,b] and Graeme Winter[a]

[a]Diamond Light Source Ltd, Diamond House, Harwell Science and Innovation Campus, Didcot OX11 0DE, United Kingdom, and [b]Research Complex at Harwell, Harwell Science and Innovation Campus, Didcot OX11 0FA, United Kingdom. *Correspondence e-mail: richard.gildea@diamond.ac.uk

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Keywords: *xia2.multiplex*; multi-crystal data sets; data processing; data analysis; partial data sets; SARS-CoV-2.

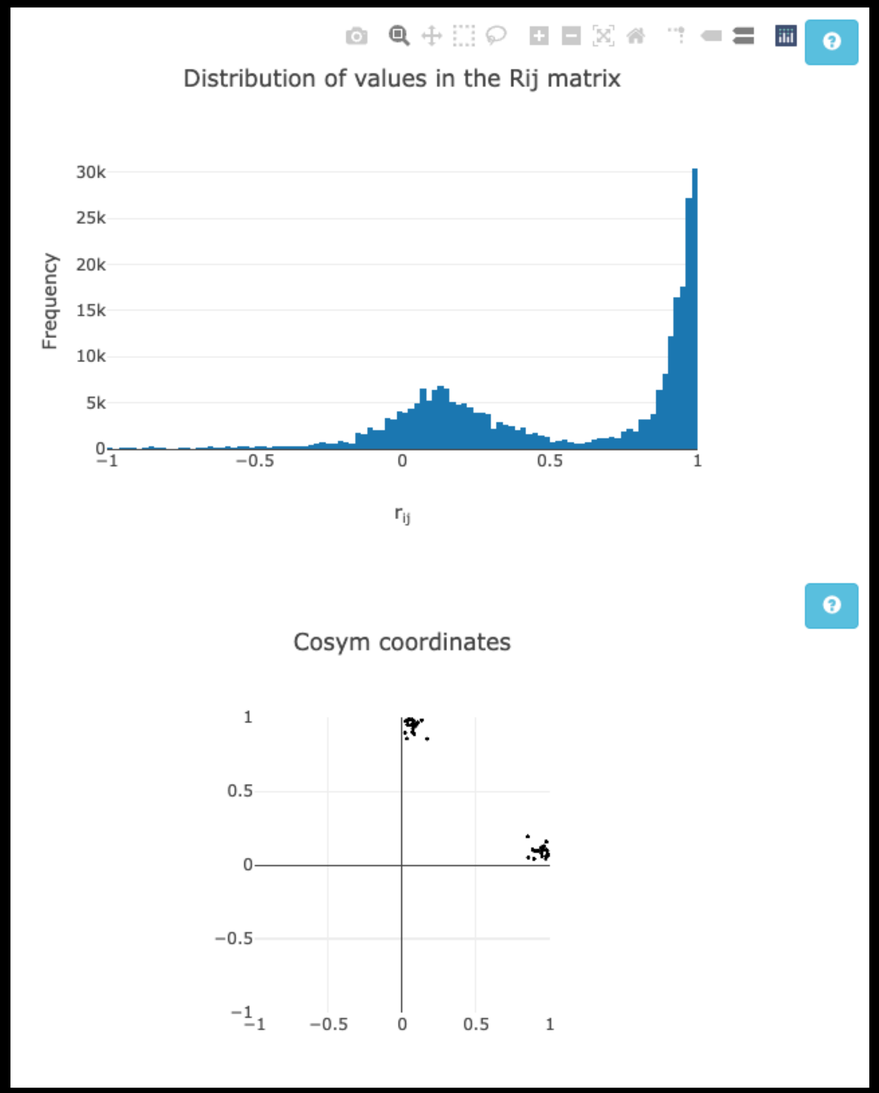
PDB references: SARS-CoV-2 main protease, complex with Z31792168, 7qt5; complex with Z1367324110, 7qt6; complex with Z4439011520, 7qt7; complex with ABT-957, 7qt8; complex with Z4439011584, 7qt9

Supporting information: this article has supporting information at journals.iucr.org/d

In macromolecular crystallography, radiation damage limits the amount of data that can be collected from a single crystal. It is often necessary to merge data sets from multiple crystals; for example, small-wedge data collections from micro-crystals, *in situ* room-temperature data collections and data collection from membrane proteins in lipidic mesophases. Whilst the indexing and integration of individual data sets may be relatively straightforward with existing software, merging multiple data sets from small wedges presents new challenges. The identification of a consensus symmetry can be problematic, particularly in the presence of a potential indexing ambiguity. Furthermore, the presence of non-isomorphous or poor-quality data sets may reduce the overall quality of the final merged data set. To facilitate and help to optimize the scaling and merging of multiple data sets, a new program, *xia2.multiplex*, has been developed which takes data sets individually integrated with *DIALS* and performs symmetry analysis, scaling and merging of multi-crystal data sets. *xia2.multiplex* also performs analysis of various pathologies that typically affect multi-crystal data sets, including non-isomorphism, radiation damage and preferential orientation. After the description of a number of use cases, the benefit of *xia2.multiplex* is demonstrated within a wider autoprocessing framework in facilitating a multi-crystal experiment collected as part of *in situ* room-temperature fragment-screening experiments on the SARS-CoV-2 main protease.

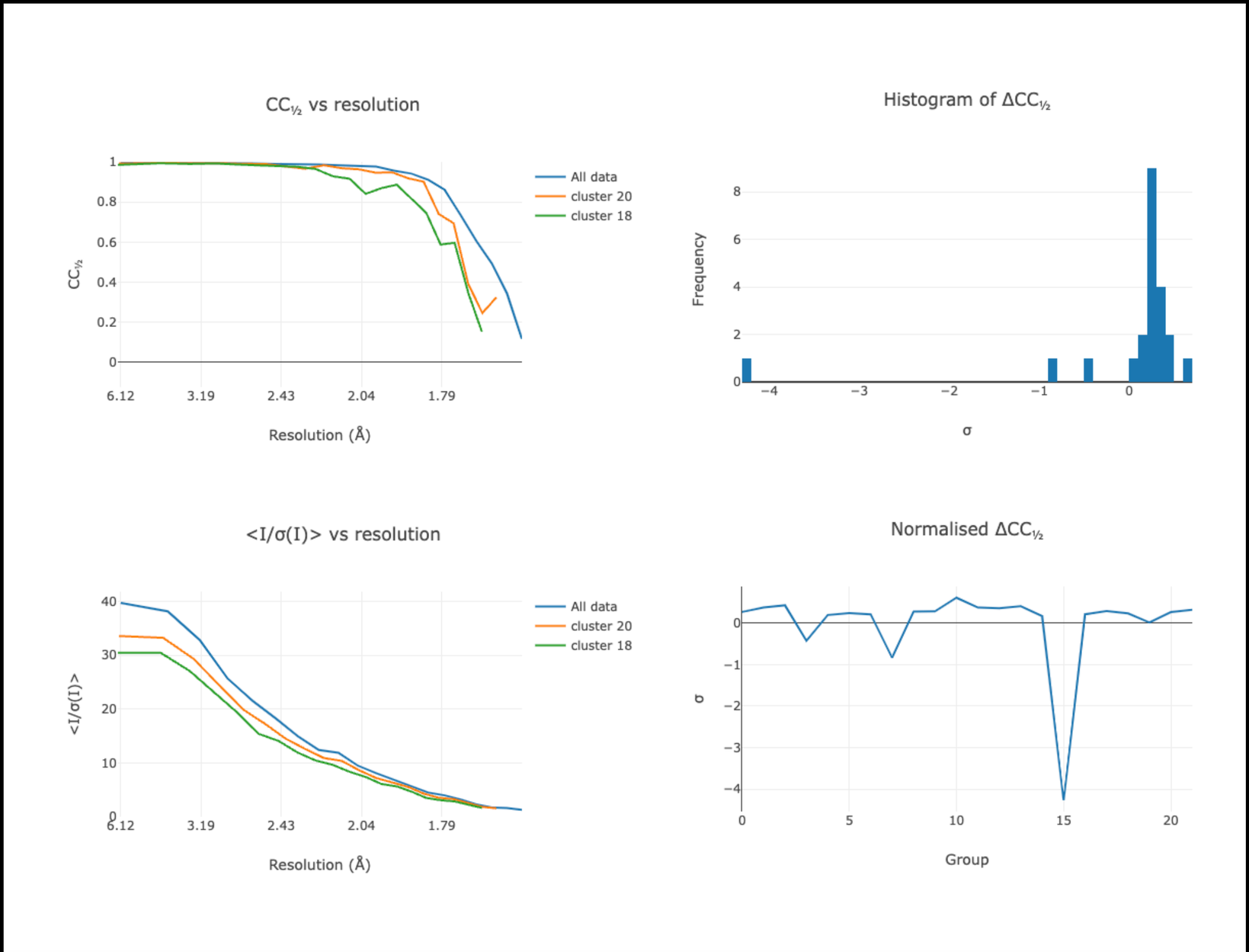
MULTIPLEX

- Resolve symmetry and indexing ambiguity
- If ambiguity will see multiple clusters
- Size of “clump” gives sense of internal variation



MULTIPLEX

- Sub-clusters can be compared (generate by setting e.g. min_completeness=0.99)
- Contributions of individual data sets also



DIALS ON THE COMMAND LINE

THE COMMAND LINE TOOLS (YES THIS SCRIPT MOSTLY WORKS)

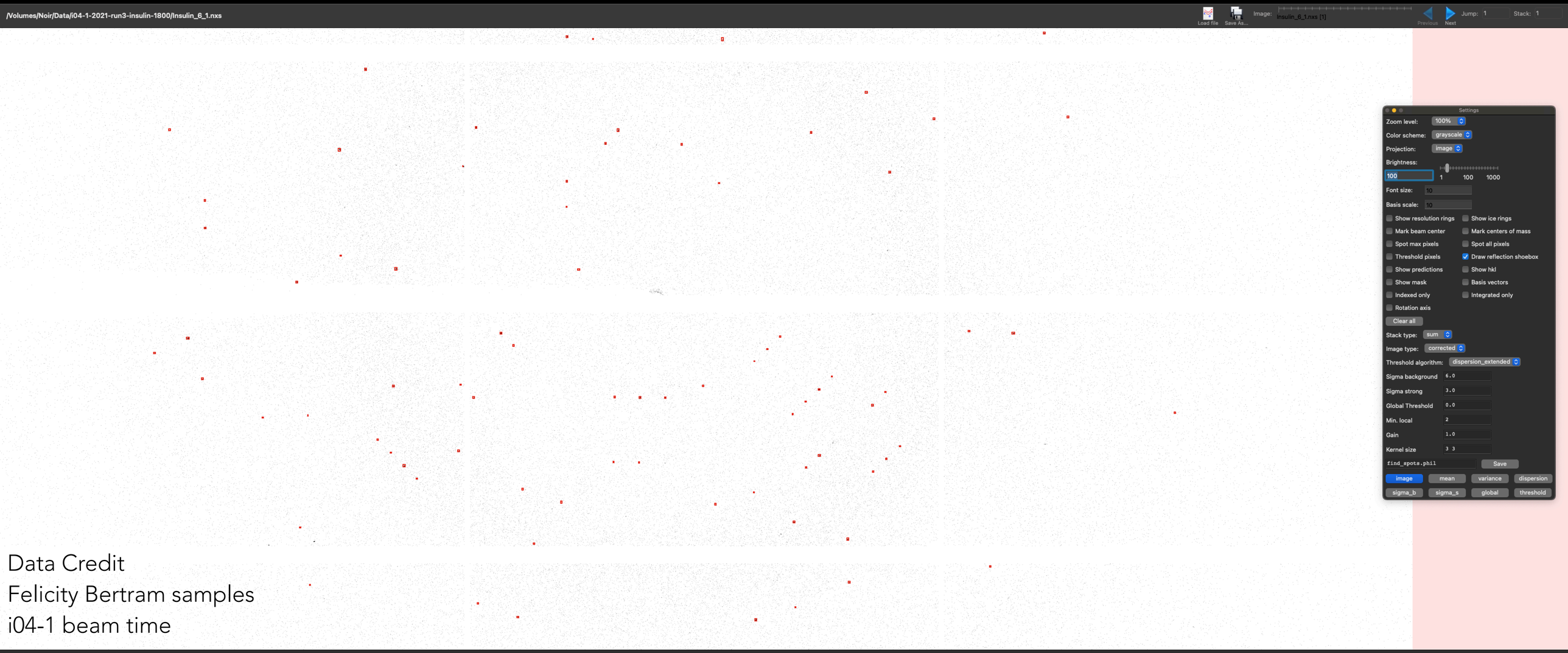
```
dials.import ../data.nxs
dials.find_spots imported.expt
dials.index imported.expt strong.refl
dials.refine indexed.expt indexed.refl
dials.integrate refined.expt refined.refl
dials.symmetry integrated.expt integrated.refl
dials.scale symmetrized.expt symmetrized.refl \
    anomalous=true absorption_level=medium
```

DATA FILE TYPES

- reflections - refl - currently serialised as message pack (spots, integrated intensities, scaled data etc.)
- experiments - expt - currently serialised as JSON (metadata, description of experiment etc.)

SPOT FINDING - VIEWER CAN ...

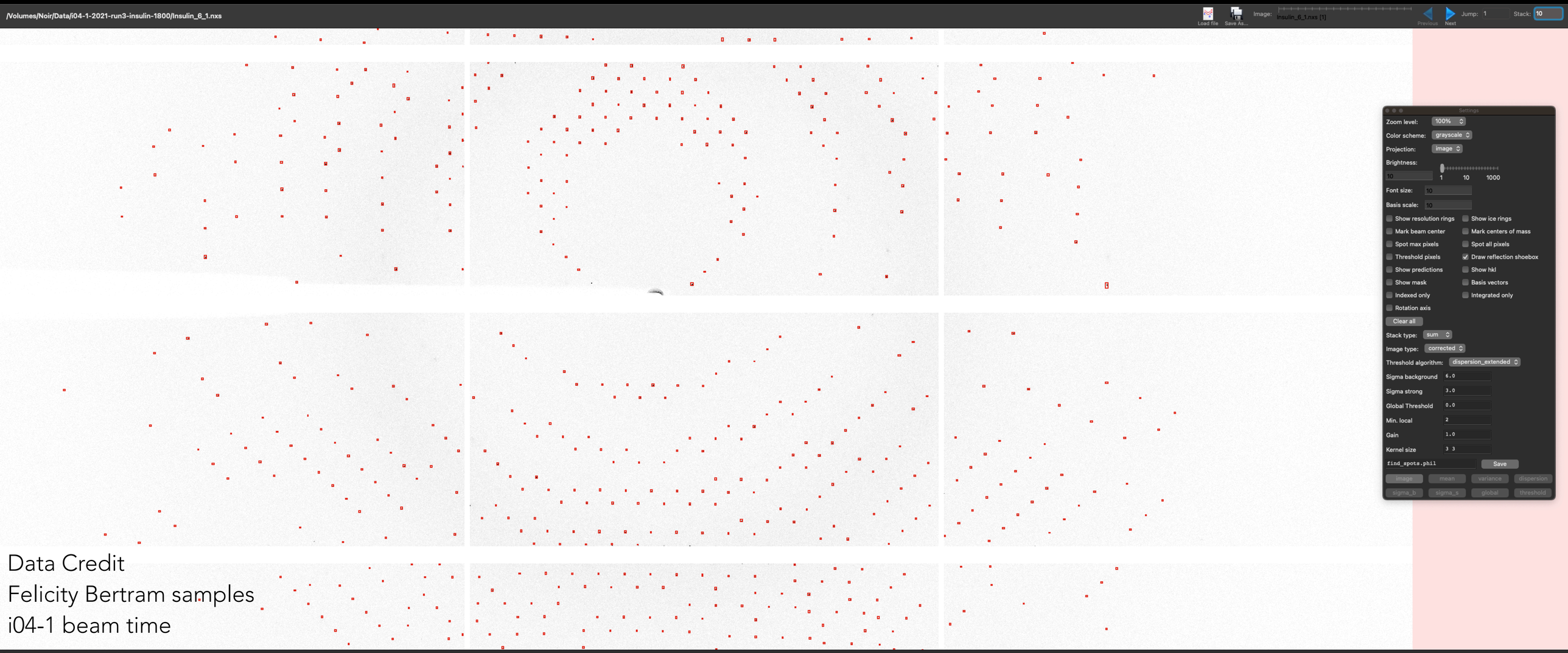
```
dials.image_viewer indexed.*
```



Data Credit
Felicity Bertram samples
i04-1 beam time

SPOT FINDING - VIEWER CAN … SUM

```
dials.image_viewer indexed.*
```



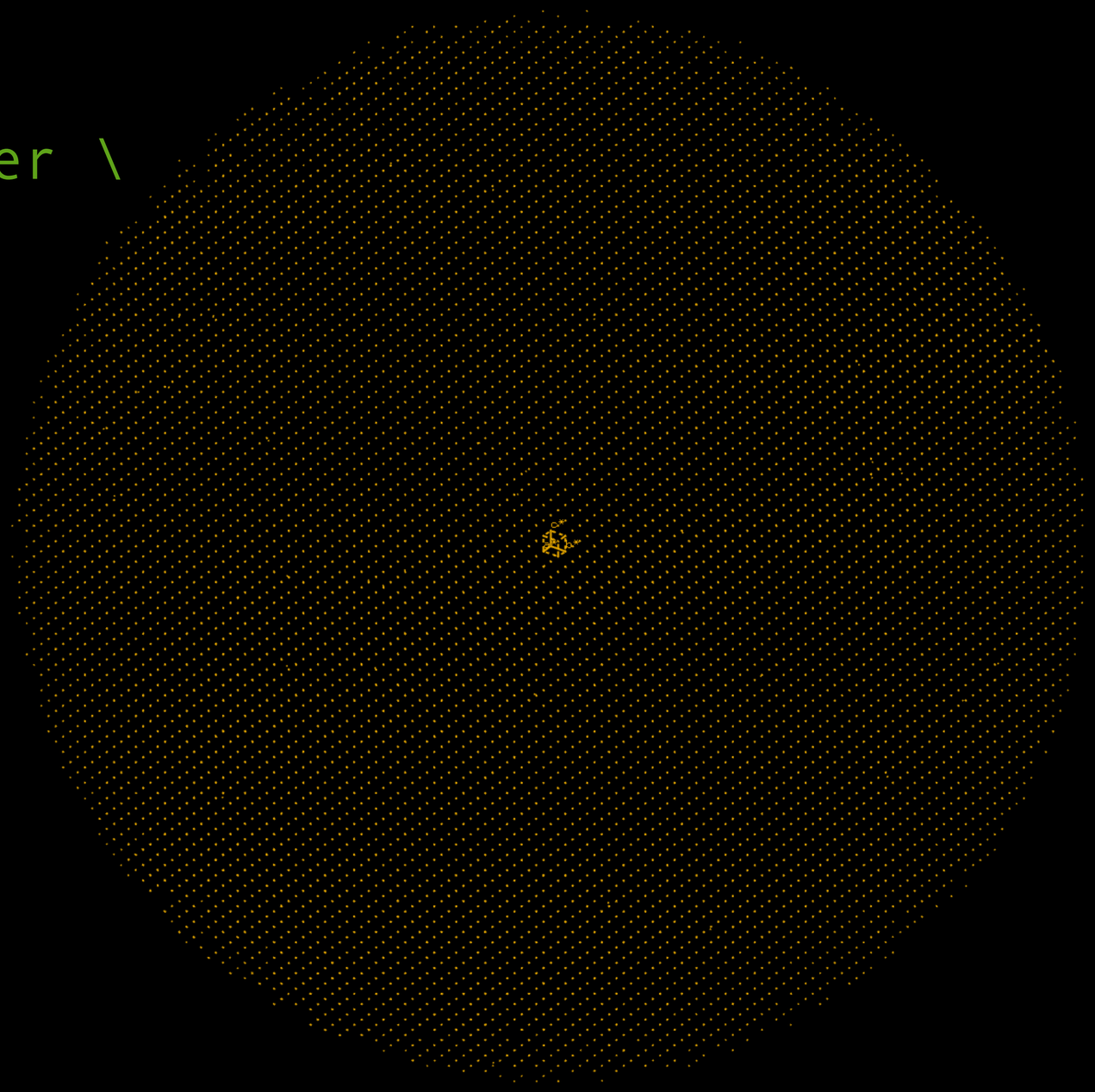
Data Credit
Felicity Bertram samples
i04-1 beam time

SPOT FINDING - VIEWER CAN … SHOW HKL

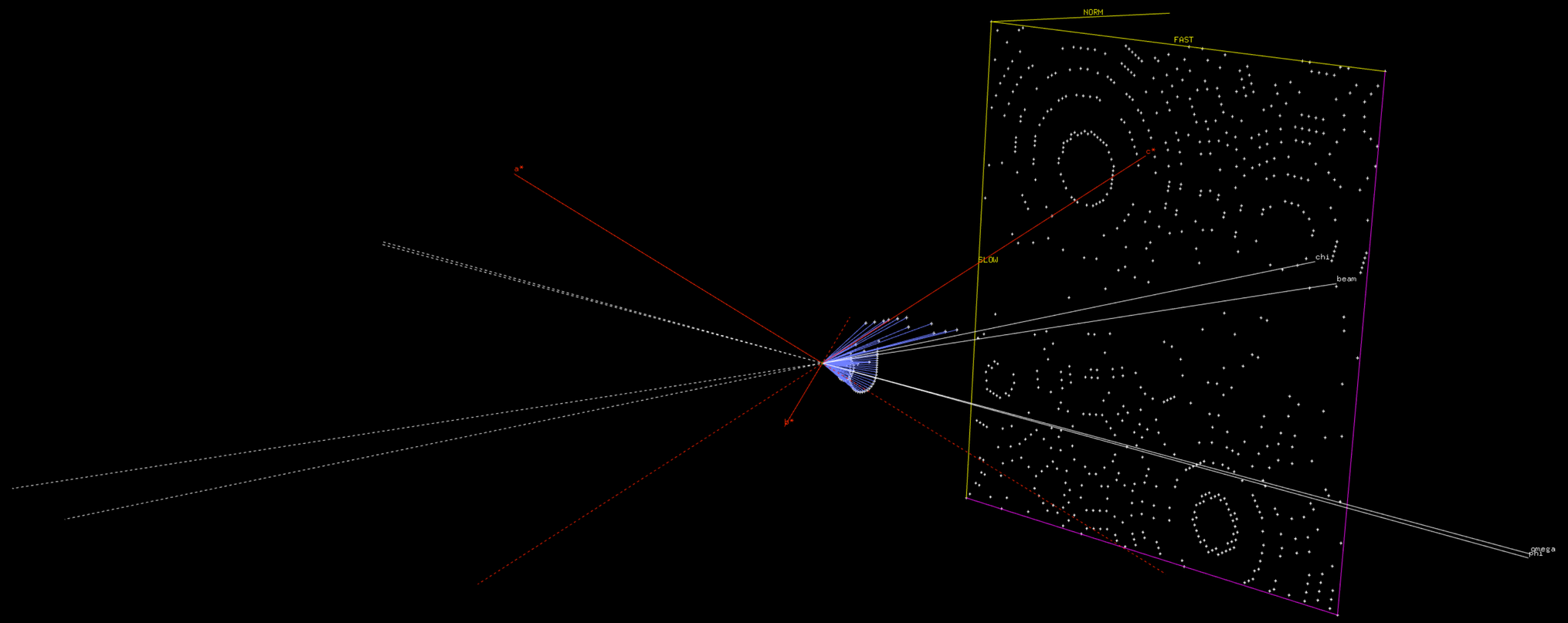
```
dials.image_viewer indexed.*
```

INDEXING

```
dials.reciprocal_lattice_viewer \
    indexed.*
```



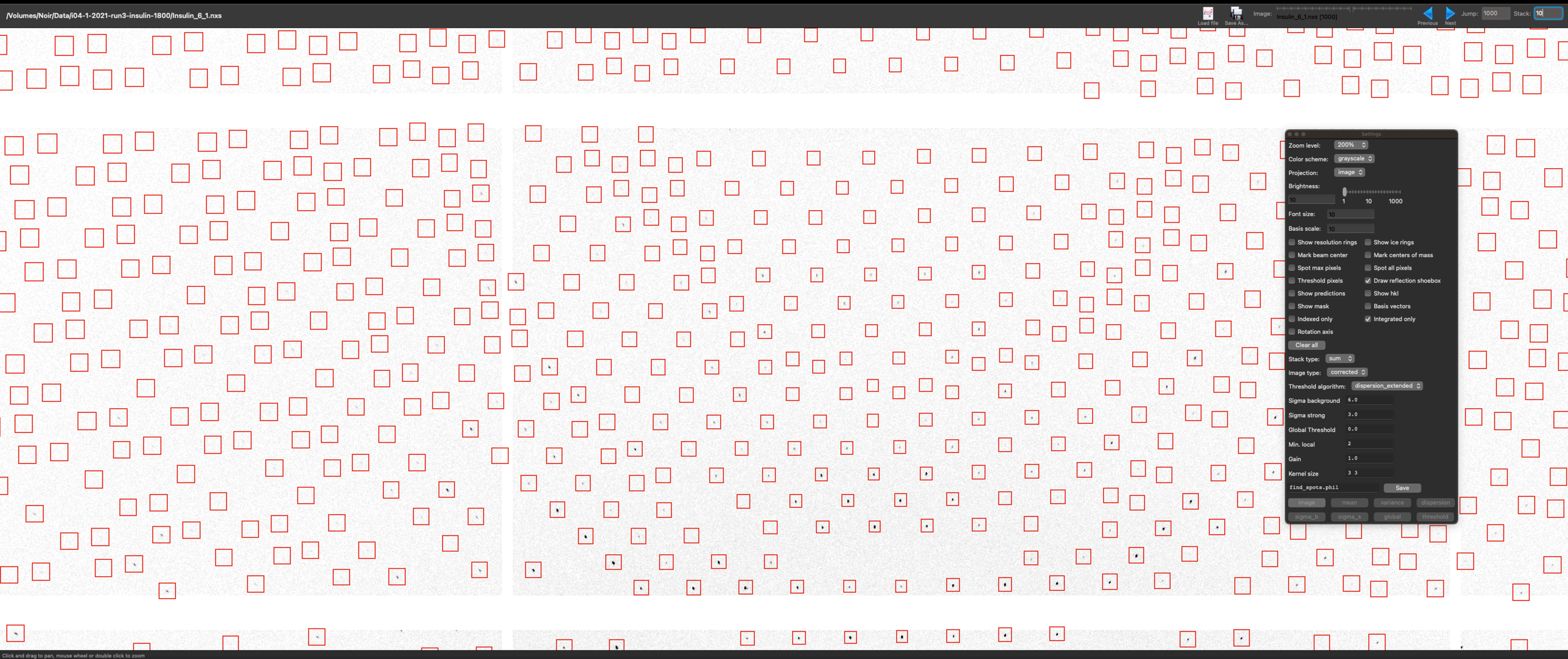
REFINEMENT




```
dials.geometry_viewer indexed.* predict=true
```

INTEGRATION

```
dials.image_viewer integrated.*
```



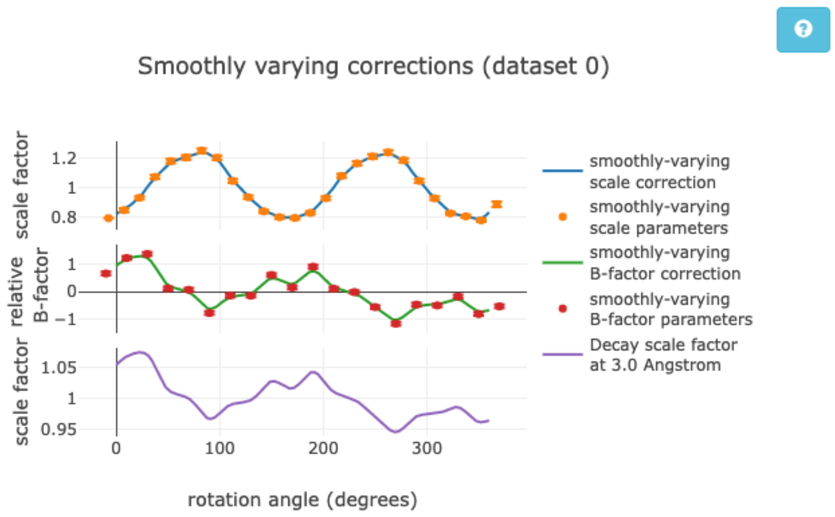
SYMMETRY*

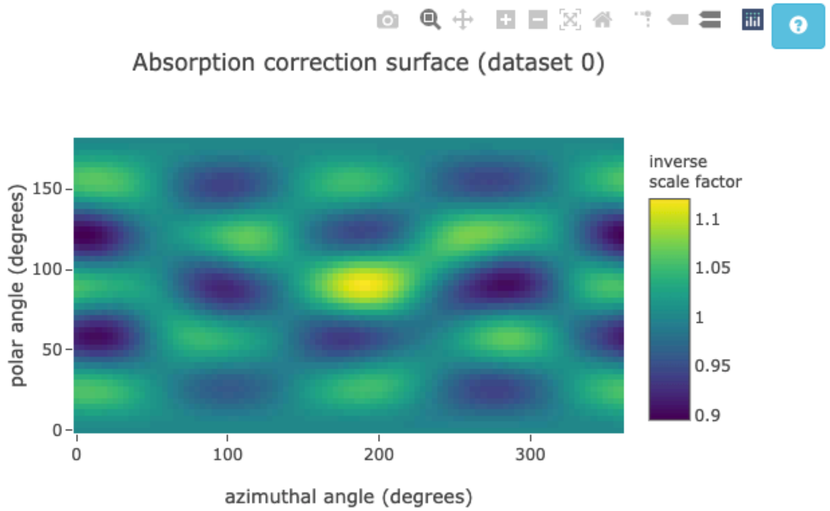
```
Normalising intensities for dataset 1

ML estimate of overall B_cart value:
  12.62, -0.52,  0.19
         14.38,  0.08
                14.56
ML estimate of  -log of scale factor:
  -5.20

--------------------------------------------------------------------------------

Estimation of resolution for Laue group analysis

Removing 51 Wilson outliers with E^2 >= 16.0
Resolution estimate from <I>/<σ(I)> > 4.0 : 3.27
Resolution estimate from CC½ > 0.60: 2.10
High resolution limit set to: 2.10
Selecting 593448 reflections with d > 2.10

Input crystal symmetry:
Unit cell: (128.202, 128.2, 128.21, 119.996, 90.0039, 120)
Space group: P 1 (No. 1)
Change of basis op to minimum cell: x-y,-x+z,-z
Crystal symmetry in minimum cell:
Unit cell: (128.2, 128.202, 128.205, 60.0035, 89.9993, 60.0007)
Space group: P 1 (No. 1)
Lattice point group: F m -3 m (x-y+z,-2*z,x+y+z)

Overall CC for 20000 unrelated pairs: 0.310
Estimated expectation value of true correlation coefficient E(CC) = 0.906
Estimated sd(CC) = 0.668 / sqrt(N)
Estimated E(CC) of true correlation coefficient from identity = 0.946
```

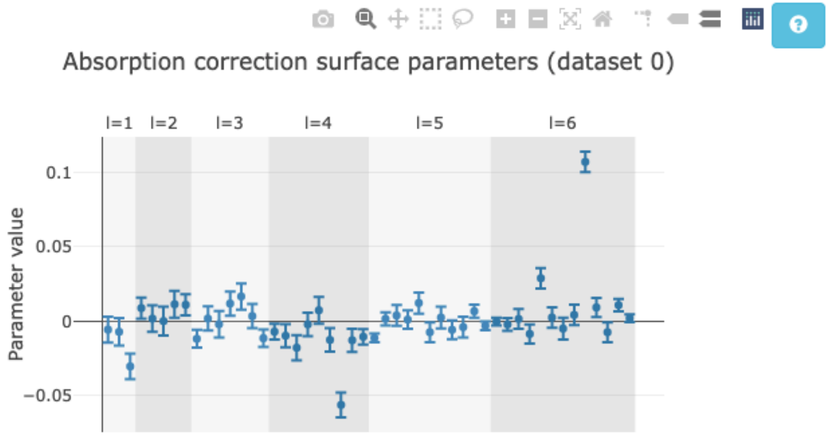
```
Scoring individual symmetry elements

+--------------+--------+------+---------+-----+----------------+
|   likelihood |   Z-CC |   CC |       N |     | Operator       |
|--------------+--------+------+---------+-----+----------------|
|        0.917 |   9.85 | 0.98 |  589492 | *** | 1 |(0, 0, 0)   |
|        0.917 |   9.71 | 0.97 | 1157058 | *** | 4 |(1, 0, 1)   |
|        0.917 |   9.72 | 0.97 | 1157348 | *** | 4 |(-1, 0, 1)  |
|        0.916 |   9.67 | 0.97 | 1157274 | *** | 4 |(1, -2, 1)  |
|        0.917 |   9.75 | 0.97 | 1157140 | *** | 3 |(-1, 2, 1)  |
|        0.917 |   9.74 | 0.97 | 1157094 | *** | 3 |(-1, -2, 1) |
|        0.917 |   9.7  | 0.97 | 1157214 | *** | 3 |(1, -2, 3)  |
|        0.917 |   9.7  | 0.97 | 1157180 | *** | 3 |(3, -2, 1)  |
|        0.917 |   9.78 | 0.98 |  578720 | *** | 2 |(1, 0, 0)   |
|        0.916 |   9.67 | 0.97 |  578600 | *** | 2 |(0, 1, 0)   |
|        0.917 |   9.78 | 0.98 |  578612 | *** | 2 |(0, 0, 1)   |
|        0.917 |   9.73 | 0.97 |  578586 | *** | 2 |(-1, 1, 0)  |
|        0.916 |   9.69 | 0.97 |  578556 | *** | 2 |(1, 0, 1)   |
|        0.916 |   9.65 | 0.96 |  579424 | *** | 2 |(-1, 0, 1)  |
|        0.917 |   9.75 | 0.98 |  578680 | *** | 2 |(0, -1, 1)  |
|        0.917 |   9.77 | 0.98 |  578684 | *** | 2 |(1, -1, 1)  |
|        0.917 |   9.76 | 0.98 |  578584 | *** | 2 |(1, -2, 1)  |
+--------------+--------+------+---------+-----+----------------+
```

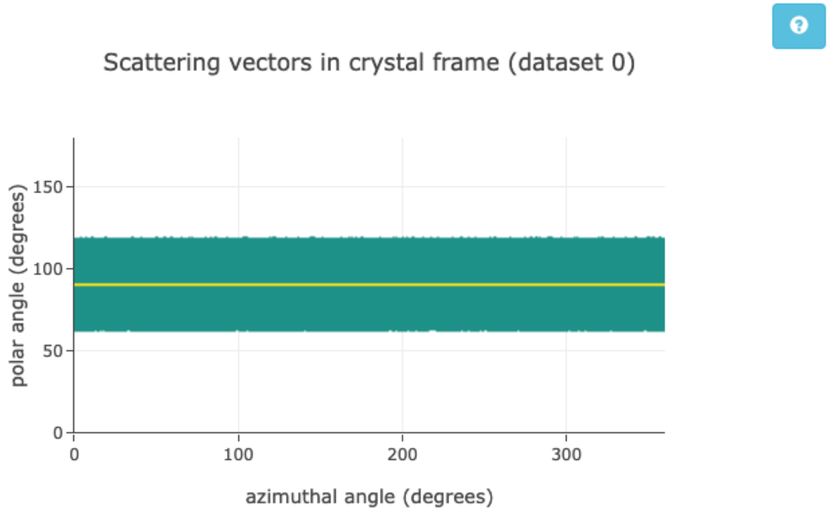
```
Best solution: F m -3 m
Unit cell:
Reindex operator: -a-2*b-c,-a-c,a-c
Laue group probability: 1.000
Laue group confidence: 1.000

+--------------------+--------------------------+
| Patterson group    | Corresponding MX group   |
|--------------------+--------------------------|
| F m -3 m           | F 4 3 2                  |
+--------------------+--------------------------+
```

SCALING*

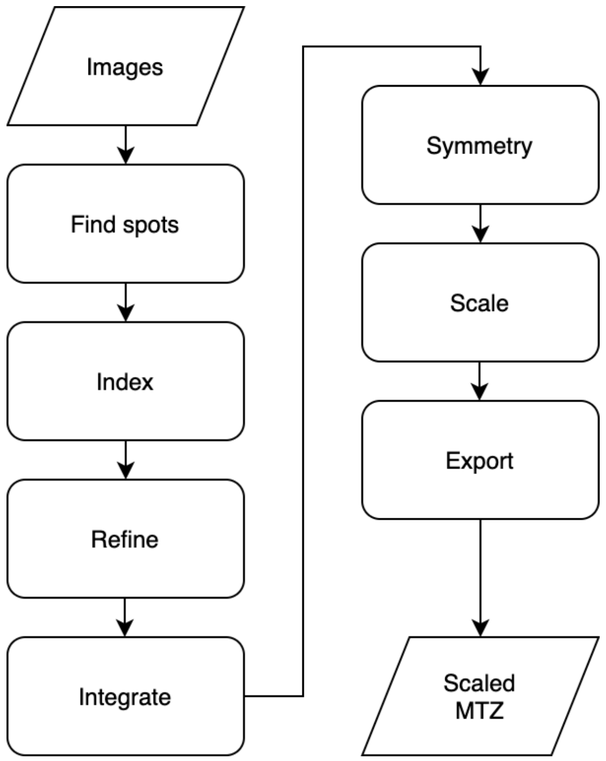

Smoothly varying corrections (dataset 0)
scale factor
relative B-factor
scale factor
1.2
1
0.8
1
0
−1
1.05
1
0.95
0
100
200
300
rotation angle (degrees)
smoothly-varying scale correction
smoothly-varying scale parameters
smoothly-varying B-factor correction
smoothly-varying B-factor parameters
Decay scale factor at 3.0 Angstrom

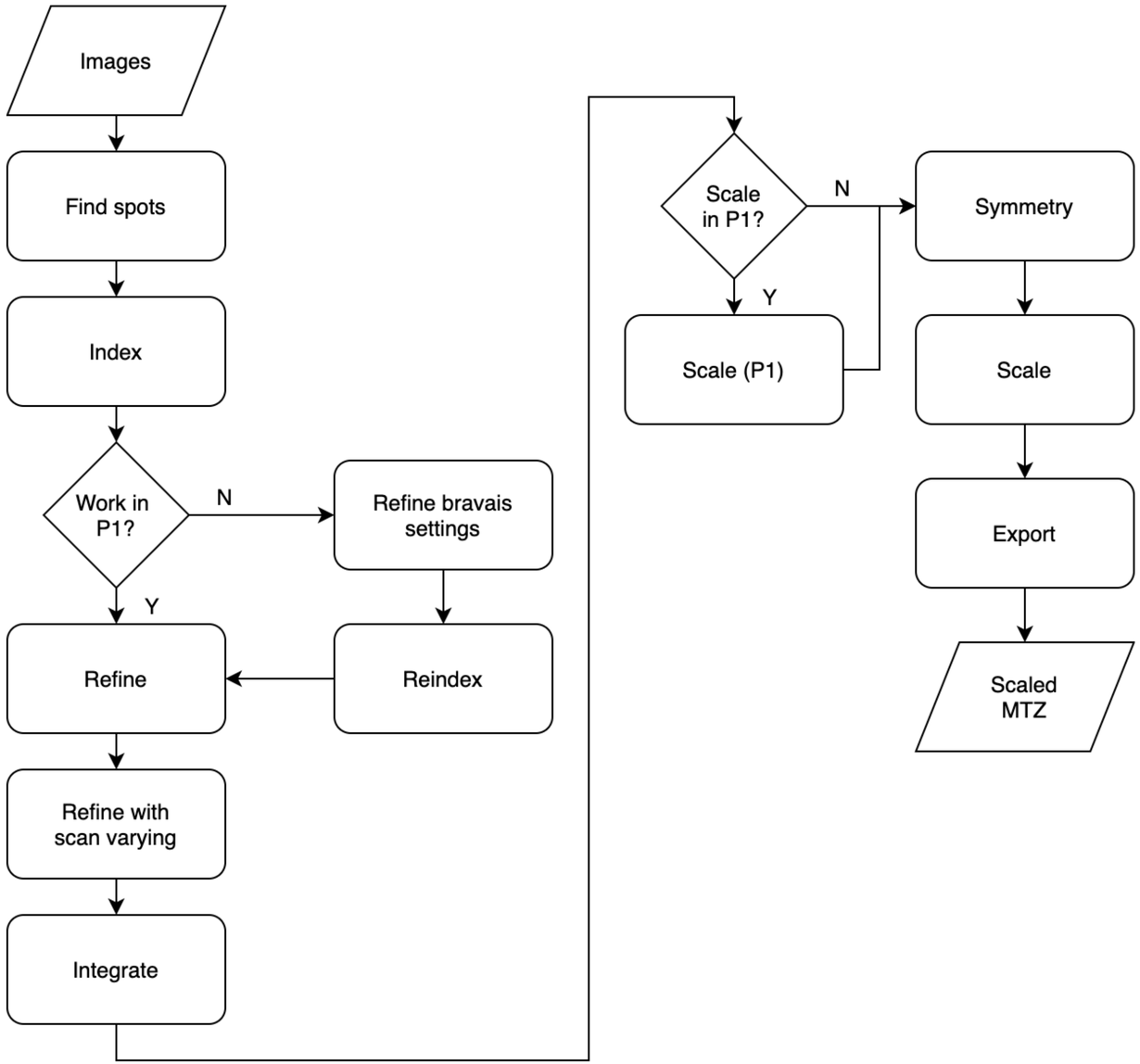

Absorption correction surface (dataset 0)
polar angle (degrees)
150
100
50
0
0
100
200
300
azimuthal angle (degrees)
inverse scale factor
1.1
1.05
1
0.95
0.9


Absorption correction surface parameters (dataset 0)
l=1
l=2
l=3
l=4
l=5
l=6
Parameter value
0.1
0.05
0
−0.05


Scattering vectors in crystal frame (dataset 0)
polar angle (degrees)
150
100
50
0
0
100
200
300
azimuthal angle (degrees)

WORKFLOWS


Images
Find spots
Index
Refine
Integrate
Symmetry
Scale
Export
Scaled MTZ


Images
Find spots
Index
Work in P1?
N
Y
Refine bravais settings
Reindex
Refine
Refine with scan varying
Integrate
Scale in P1?
N
Y
Scale (P1)
Symmetry
Scale
Export
Scaled MTZ

ENSEMBLE PROCESSING

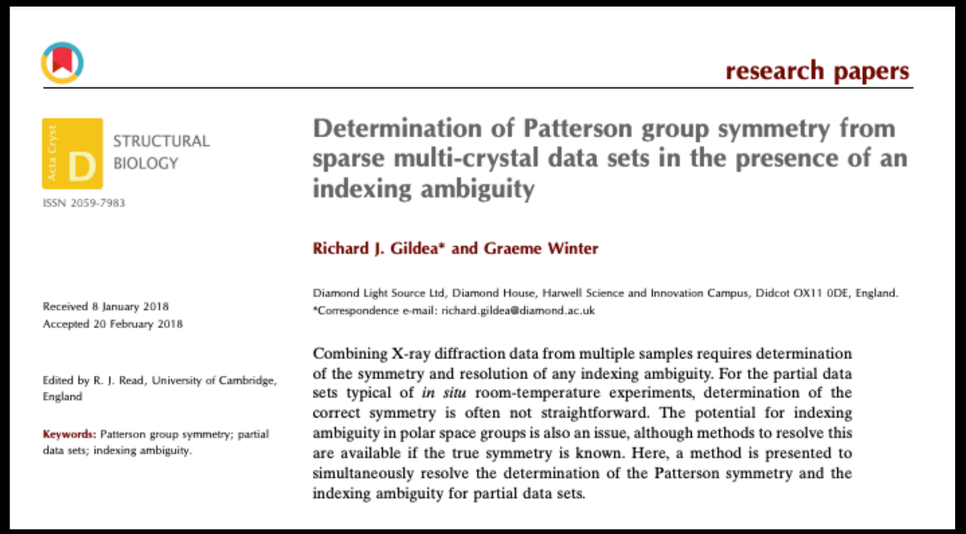
```
dials.import ../data*.nxs
dials.find_spots imported.expt
dials.index imported.expt strong.refl
dials.refine indexed.expt indexed.refl
dials.integrate refined.expt refined.refl
dials.cosym integrated.expt integrated.refl
dials.scale symmetrized.expt symmetrized.refl \
    anomalous=true absorption_level=medium
```

COSYM

- Decide symmetry
- Align crystals in reciprocal space
- Re-index data across many sweeps resolving indexing ambiguity

ANCILLARY TOOLS

- cosym - resolve symmetry and indexing ambiguity simultaneously
- ∂CC1/2 - identify data sets which do not contribute to final result



research papers

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Determination of Patterson group symmetry from sparse multi-crystal data sets in the presence of an indexing ambiguity

Richard J. Gildea* and Graeme Winter

Diamond Light Source Ltd, Diamond House, Harwell Science and Innovation Campus, Didcot OX11 0DE, England. *Correspondence e-mail: richard.gildea@diamond.ac.uk

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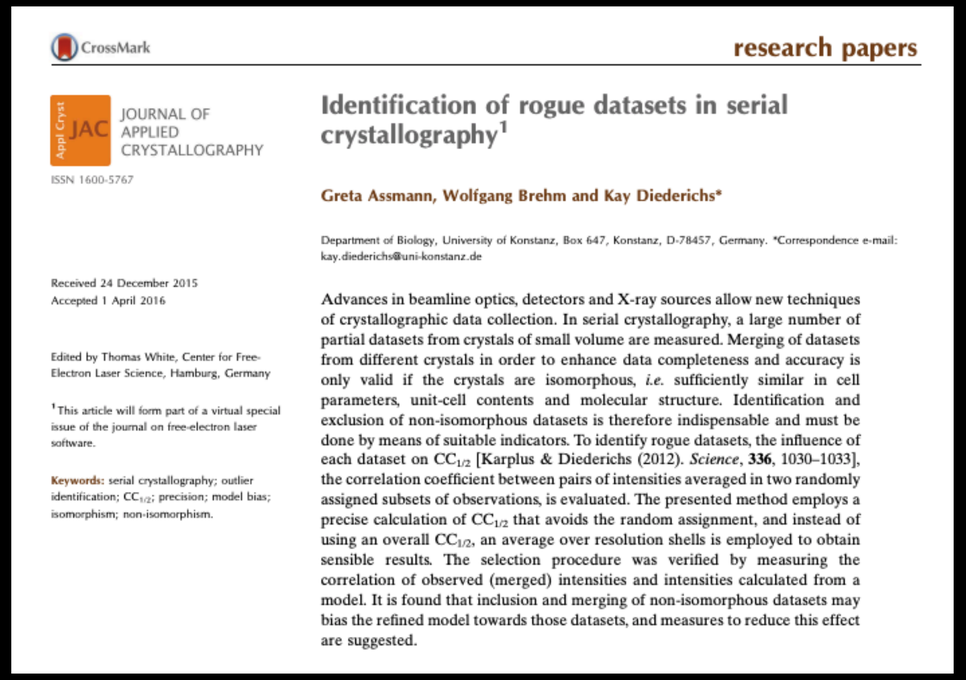
Keywords: Patterson group symmetry; partial data sets; indexing ambiguity.

Combining X-ray diffraction data from multiple samples requires determination of the symmetry and resolution of any indexing ambiguity. For the partial data sets typical of *in situ* room-temperature experiments, determination of the correct symmetry is often not straightforward. The potential for indexing ambiguity in polar space groups is also an issue, although methods to resolve this are available if the true symmetry is known. Here, a method is presented to simultaneously resolve the determination of the Patterson symmetry and the indexing ambiguity for partial data sets.



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research papers

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Identification of rogue datasets in serial crystallography[1]

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[1] This article will form part of a virtual special issue of the journal on free-electron laser software.

Keywords: serial crystallography; outlier identification; $CC_{1/2}$; precision; model bias; isomorphism; non-isomorphism.

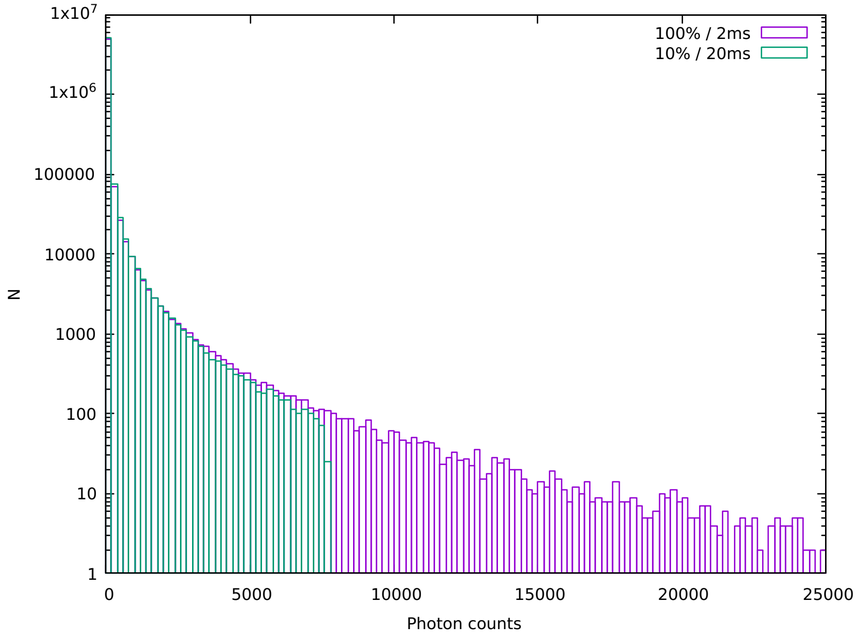
Advances in beamline optics, detectors and X-ray sources allow new techniques of crystallographic data collection. In serial crystallography, a large number of partial datasets from crystals of small volume are measured. Merging of datasets from different crystals in order to enhance data completeness and accuracy is only valid if the crystals are isomorphous, *i.e.* sufficiently similar in cell parameters, unit-cell contents and molecular structure. Identification and exclusion of non-isomorphous datasets is therefore indispensable and must be done by means of suitable indicators. To identify rogue datasets, the influence of each dataset on $CC_{1/2}$ [Karplus & Diederichs (2012). *Science*, **336**, 1030–1033], the correlation coefficient between pairs of intensities averaged in two randomly assigned subsets of observations, is evaluated. The presented method employs a precise calculation of $CC_{1/2}$ that avoids the random assignment, and instead of using an overall $CC_{1/2}$, an average over resolution shells is employed to obtain sensible results. The selection procedure was verified by measuring the correlation of observed (merged) intensities and intensities calculated from a model. It is found that inclusion and merging of non-isomorphous datasets may bias the refined model towards those datasets, and measures to reduce this effect are suggested.

PYTHON API

DETECTION OF OVERLOADED REFLECTIONS

- Assess fraction of count rate used on absolute pixel values
- Find spots with excessively high limit, then analyse pixels found

```
# run dials.find_spots with maximum_trusted=50000 or similar

import sys
from dials.array_family import flex

data = flex.reflection_table.from_file(sys.argv[1])
boxes = data["shoebox"]
nn = boxes.size()
h0 = flex.histogram(flex.double(), data_min=0, data_max=50000, n_slots=50000)

for j in range(nn):
    h1 = flex.histogram(
        boxes[j].data.as_double().as_1d(), data_min=0, data_max=50000, n_slots=50000
    )
    h0.update(h1)

for c, v in zip(h0.slot_centers(), h0.slots()):
    print(c, v)
```



DETECTING BAD PIXELS

- Unreliable pixels => higher than expected probability of recording signal
- Use spot finding algorithms, count how frequently pixel is “signal”

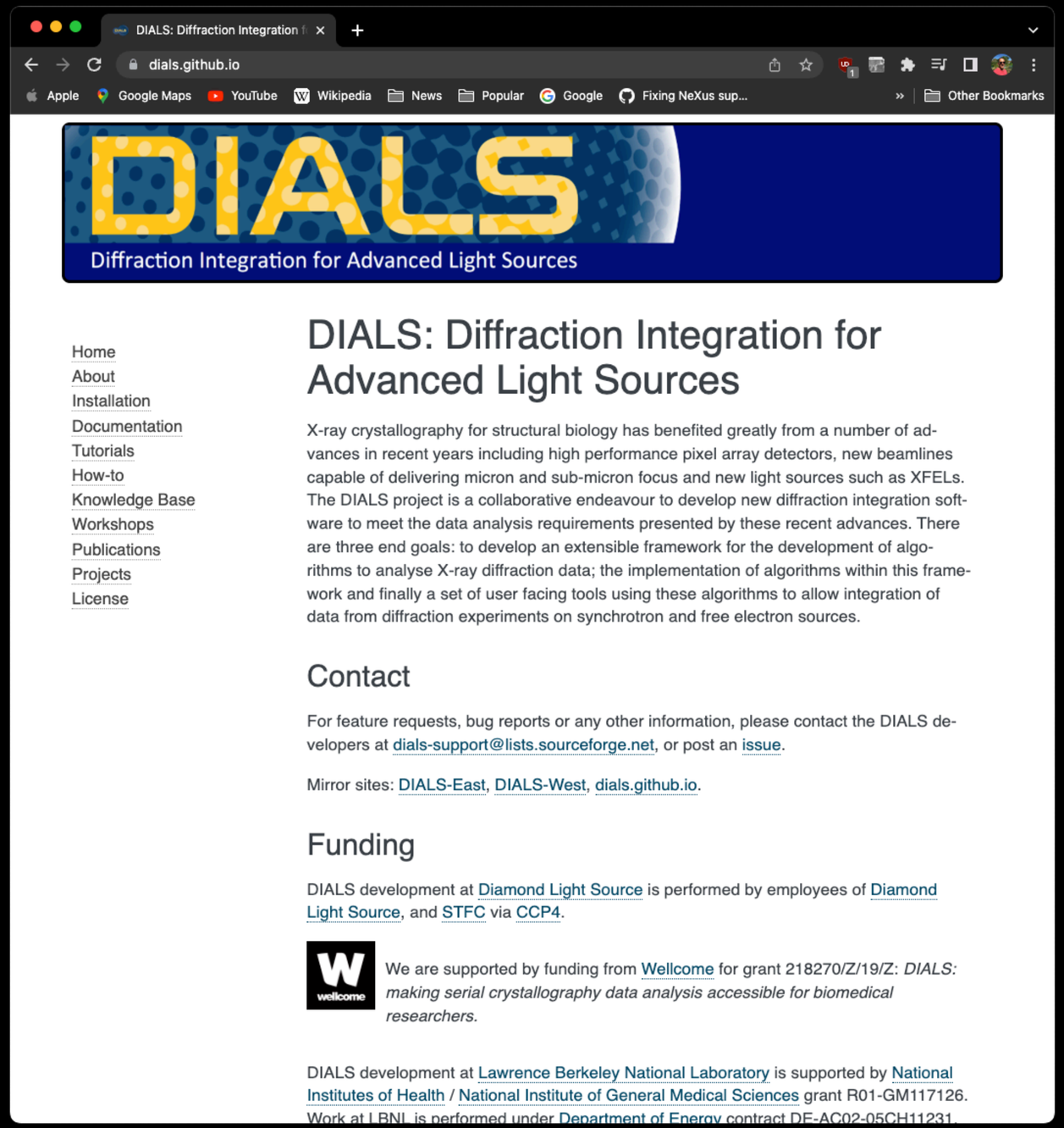
```
detector = imageset.get_detector()[0]
trusted = detector.get_trusted_range()

total = None

for idx in range(100):
    pixels = imageset.get_raw_data(idx - 1)
    known_mask = imageset.get_mask(idx - 1)

    # apply known mask
    for pixel, panel, mask in zip(pixels, panels, known_mask):
        pixel.set_selected(~mask, -1)
        for f0, s0, f1, s1 in panel.get_mask():
            blank = flex.int(flex.grid(s1 - s0, f1 - f0), 0)
            pixel.matrix_paste_block_in_place(blank, s0, f0)

        data = pixels[0]

        negative = data < int(round(trusted[0]))
        hot = data > int(round(trusted[1]))
        bad = negative | hot

        data = data.as_double()

        p = spot_phil.fetch(
            source=iotbx.phil.parse("min_spot_size=1")
        ).extract()
        threshold_function = SpotFinderFactory.configure_threshold(p)
        peak_pixels = threshold_function.compute_threshold(data, ~bad)

        if total is None:
            total = peak_pixels.as_1d().as_int()
        else:
            total += peak_pixels.as_1d().as_int()
```

EXTENSION TO OTHER TECHNIQUES

- Neutron diffraction - time of flight - David Mcdonagh presentation
- Electron diffraction / microED / 3DED - very much work in progress, particular interest at sites at Diamond

GETTING DIALS

- dials.github.io -> installation
- conda install dials
- github.com/dials/dials for code / issues / pull requests etc.
- Tutorials and documentation online



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