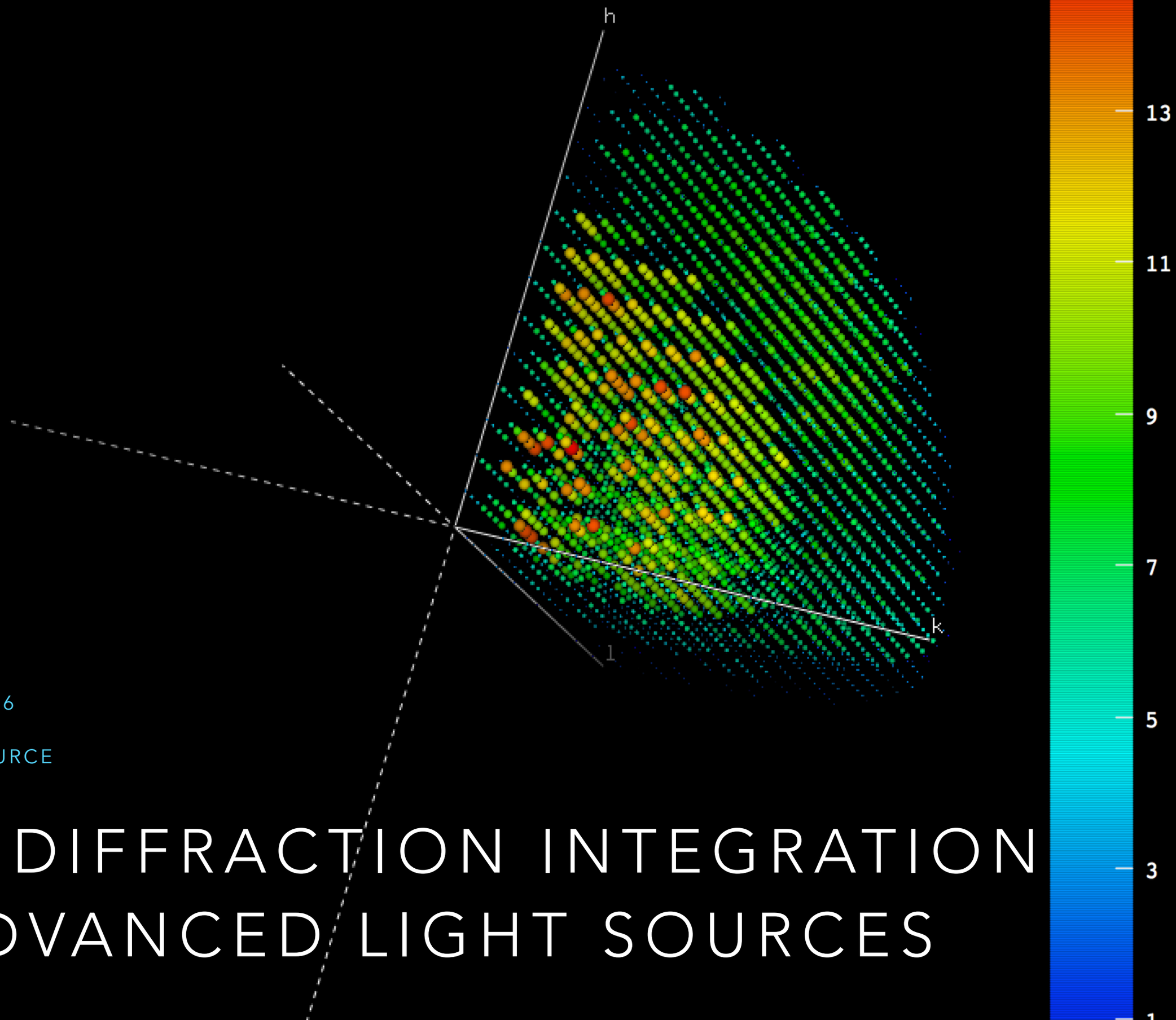


CCP4 DECEMBER 2016
GRAEME WINTER
DIAMOND LIGHT SOURCE

DIALS: DIFFRACTION INTEGRATION FOR ADVANCED LIGHT SOURCES

PROJECT SUPPORT



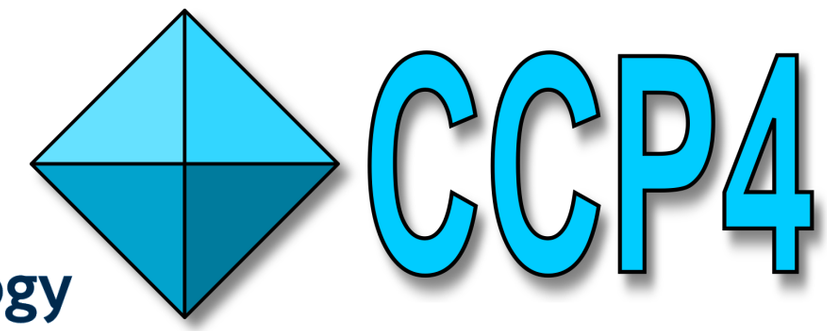








Science & Technology
Facilities Council



EU FP7: #283570 NIH: GM095887 & GM102520


DIALS East
DIALS West
Nunavut Territory
CANADA
ARCTIC CIRCLE
Great Bear Lake
Great Slave Lake
Foxe Basin
Hudson Bay
Southern Indian Lake
Reindeer Lake
Lake Winnipeg
Edmonton
Calgary
Regina
Winnipeg
Vancouver
Seattle
Portland
Salt Lake City
Denver
Kansas City
St Louis
Chicago
Detroit
Pittsburgh
Washington
Ottawa
Montreal
Toronto
Quebec
Boston
New York
Philadelphia
Baltimore
Nova Scotia
Island of Newfoundland
St Pierre and Miquelon (France)
LABRADOR SEA
Davis Strait
Greenland
Gunnbjorn Fjeld
Denmark Strait
ICELAND
Reykjavik
Faroe Islands (Denmark)
Shetland Islands (U.K.)
NORWAY
SWEDEN
Oslo
Stockholm
NORTH SEA
DENMARK
Copenhagen
UNITED KINGDOM
Edinburgh
Belfast
Dublin
IRELAND
Manchester
London
Cardiff
Hamburg
Amsterdam
Berlin
GERMANY
Paris
FRANCE
Munich
Lyon
Milan
Marseille
Monaco
ITALY
Rome
Barcelona
Madrid
PORTUGAL
Lisbon
SPAIN
Seville
Algiers
Tunis
Rabat
Casablanca
Marrakesh
MOROCCO
Atlas Mountains
TUNISIA
MALTA
Tripoli
LIBYA
ALGERIA
WESTERN SAHARA
MAURITANIA
Nouakchott
MALI
NIGER
Niamey
Dakar
SENEGAL
Bamako
GAMBIA
GUINEA-BISSAU
GUINEA
Conakry
Freetown
SIERRA LEONE
Monrovia
LIBERIA
Abidjan
BURKINA
Ouagadougou
COTE D'IVOIRE
GHANA
Accra
TOGO
BENIN
NIGERIA
Abuja
Lagos
CAMEROON
Yaounde
EQUAT. GUINEA
GABON
CONGO
Brazzaville
Libreville
Kinshasa
Luanda
ANGOLA
Praia
CAPE VERDE
Azores (Portugal)
Madeira Islands (Portugal)
Canary Islands (Spain)
Ascension (U.K.)
São Pedro e São Paulo (Brazil)
Fernando de Noronha (Brazil)
Gulf of Guinea
EQUATOR
TROPIC OF CANCER
NORTH ATLANTIC OCEAN
Bermuda (U.K.)
Gulf of Mexico
Miami
BAHAMAS
Havana
CUBA
DOMINICAN REP.
Puerto Rico (U.S.A.)
HAITI
Port-au-Prince
Sto Domingo
ST KITTS AND NEVIS
ANTIGUA AND BARBUDA
DOMINICA
ST LUCIA
BARBADOS
ST VINCENT AND THE GRENADINES
GRENADA
TRINIDAD AND TOBAGO
CARIBBEAN SEA
Caracas
VENEZUELA
Georgetown
Paramaribo
GUYANA
SURINAME
FRENCH GUIANA (France)
Bogotá
COLOMBIA
Medellín
Cali
Quito
ECUADOR
Guayaquil
Chimborazo
Galápagos (Ecuador)
Malpelo Island (Colombia)
Coco Island (Costa Rica)
Cartagena
Panamá
COSTA RICA
NICARAGUA
HONDURAS
GUATEMALA
EL SALVADOR
BELIZE
JAMAICA
Cayman Is. (U.K.)
Mérida
Cancun
Tampico
Guadalajara
Mexico
MEXICO
Acapulco
Monterrey
Ciudad Juárez
Mexicali
Tijuana
San Diego
Los Angeles
San Francisco
Sacramento
Houston
Dallas
New Orleans
San Antonio
Memphis
Atlanta
Guadalupe I. (Mexico)
Revillagigedo Is. (Mexico)
Clipperton (France)
Rio Grande
Colorado
Arkansas
Missouri
Mississippi
Ohio
Lake Michigan
Lake Erie
L. Ontario
L. Huron
Lake Superior
Peace
Columbia
Fraser
Rocky Mountains
Amazon
Rio Negro
Porto Velho
Manaus
Belém
São Luis
Fortaleza
Natal
João Pessoa
Recife
Maceió
Aracaju
Salvador
Teresina
Tocantins
São Francisco
Amazon Basin
BRAZIL
PERU
Trujillo
Nev. Huascarán
Lima
Cusco
Iquitos
Boa Vista
Porto Velho
Manaus
Belém
Fernando de Noronha (Brazil)
Ascension (U.K.)

CORE DEVELOPMENT TEAMS

- DIALS East: PI Gwyndaf Evans; David Waterman, Richard Gildea, James Parkhurst, Markus Gerstel, Luis Fuentes Montero, Graeme Winter - synchrotron rotation data
- DIALS West: PI Nick Sauter; Aaron Brewster, Tara Michels-Clark, Iris Young - X-FEL serial crystallography

ACKNOWLEDGEMENTS

research papers

Acta Crystallographica Section D
Biological Crystallography
ISSN 0907-4449

XDS

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Received 19 August 2009
Accepted 9 November 2009

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

research papers

Acta Crystallographica Section D
Biological Crystallography
ISSN 0907-4449

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

Two-dimensional position-sensitive detectors have been used for many years in X-ray diffraction data collection. In particular, data from crystals of macromolecules such as proteins, oligonucleotides and their complexes are almost always acquired with an area detector such as film (now virtually obsolete), a multi-wire system, an imaging plate or the recently commercialized charge-coupled device (CCD) coupled to a phosphor-coated fiber-optic taper. With all these detectors, the crystal, centered in the X-ray beam, is rotated or oscillated around a single axis through a small angle of 0.1 to ~2.0°, while counts from diffracted photons are accumulated for a specified time. At the end of the small rotation, the detector is read out and the counts are stored as an image: a two-dimensional array with each array element (pixel) related to a distinct position on the detector and the number of

research papers

Acta Crystallographica Section D
Biological Crystallography
ISSN 0907-4449

The integration of macromolecular diffraction data

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Received 19 May 2005
Accepted 24 November 2005

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

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)

WHAT IS DIALS?

- Indexing, refinement and integration programs
- Scope similar to MOSFLM i.e. does *not* include scaling - use POINTLESS/AIMLESS for scaling (work in progress)
- Integration algorithm similar to XDS
- Does *not* currently include a GUI (in development) though does include a range of visual analysis tools
- Also DIALS is a toolkit, so you can do lots more

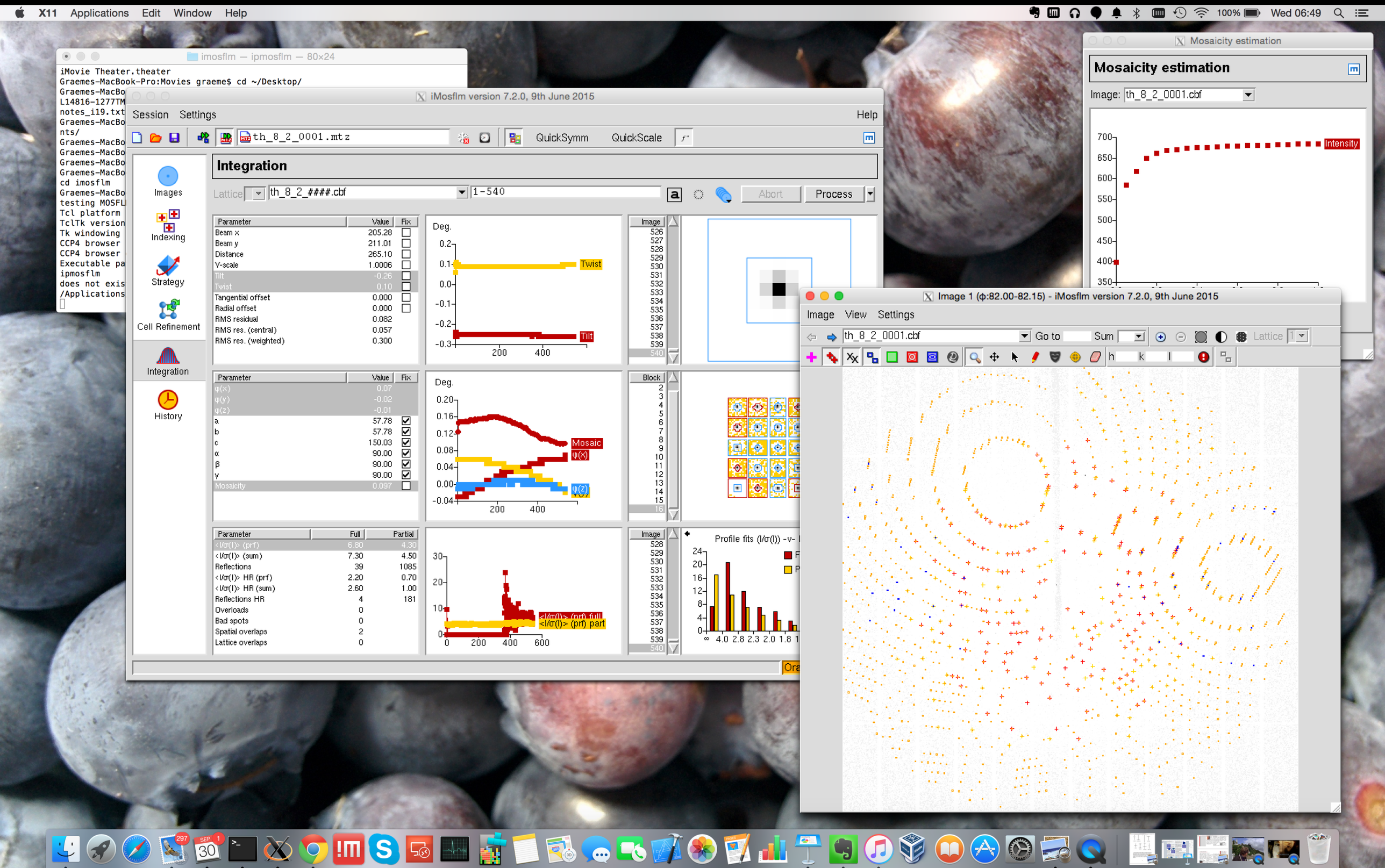
PHILOSOPHY

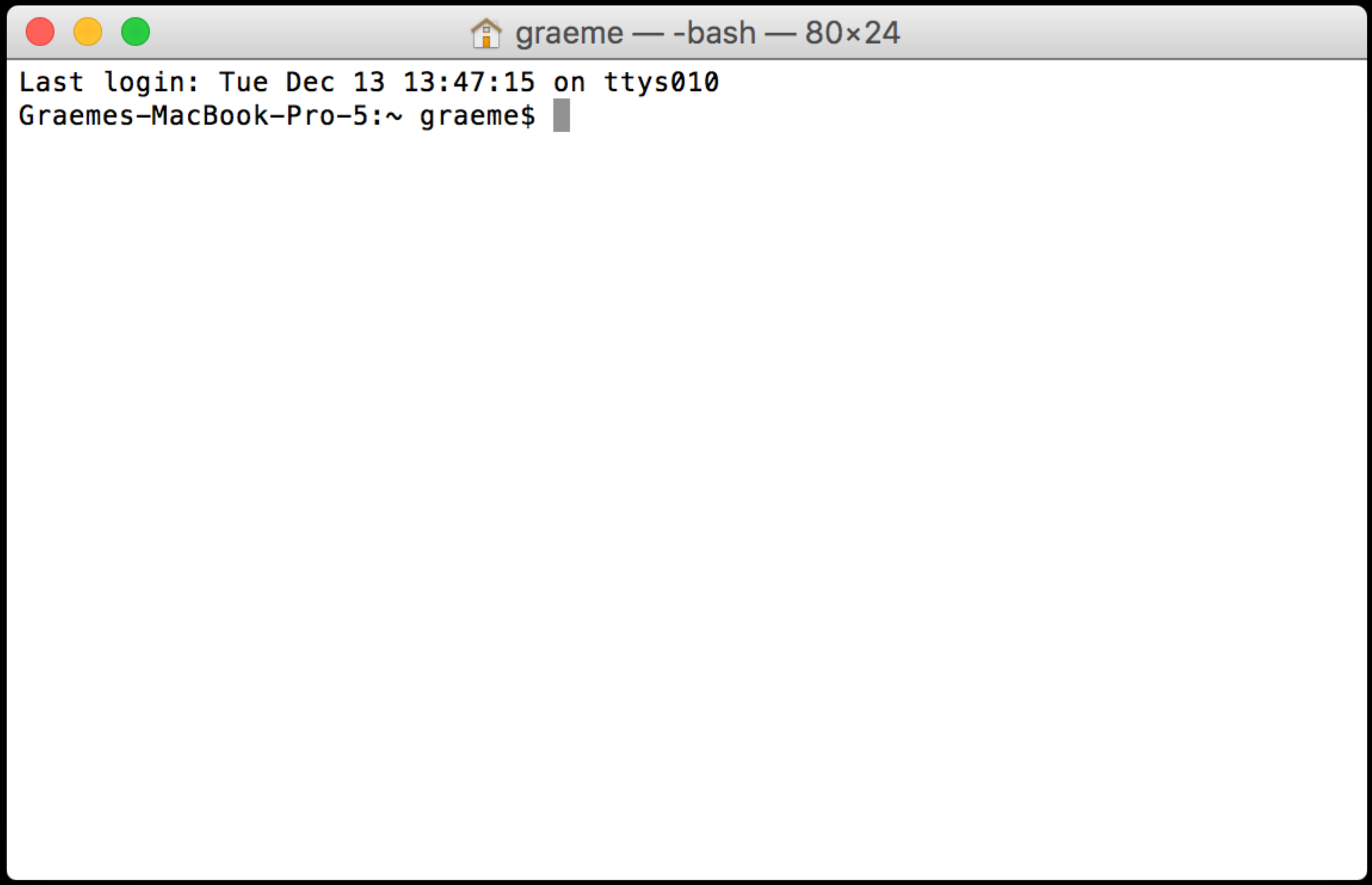
- Global analysis and model - take data from every image in your data set
- No assumptions made about experimental geometry - completely general / vectorial description
- Treat data as 3D volume not 2D “frames”
- Toolkit - for data processing but you can do fun experiments with a little code

USING DIALS

- Automatic: xia2 (nothing to learn here, though *is* primary UI)
- Manual: *via* command-line steps (still relatively automatic)

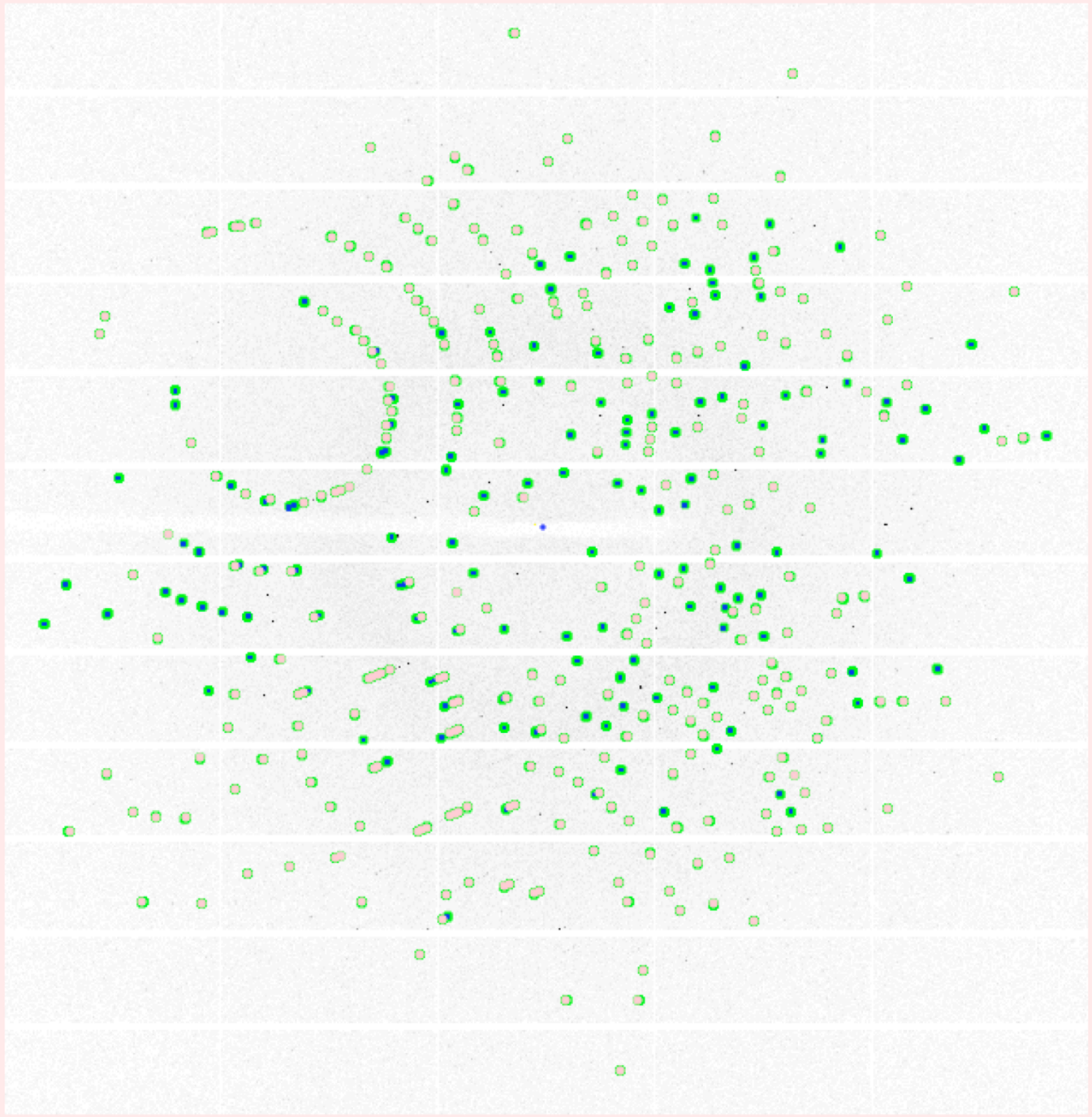
MISSING USER INTERFACE




graeme — -bash — 80×24
Last login: Tue Dec 13 13:47:15 on ttys010
Graemes-MacBook-Pro-5:~ graeme$

/Users/graeme/data/i04-bag-training/th_8_2_0001.cbf.gz

Load file Save As... Image: th_8_2_0001.cbf.gz [1] Previous Next Jump to image: 1



Click and drag to pan; middle-click and drag to plot intensity profile, right-click to zoom

Reflection data viewer

High resolution: 2.00

Min Z 0

Max Z 540

Show rotation axis

Show beam vector

Invert rotation axis

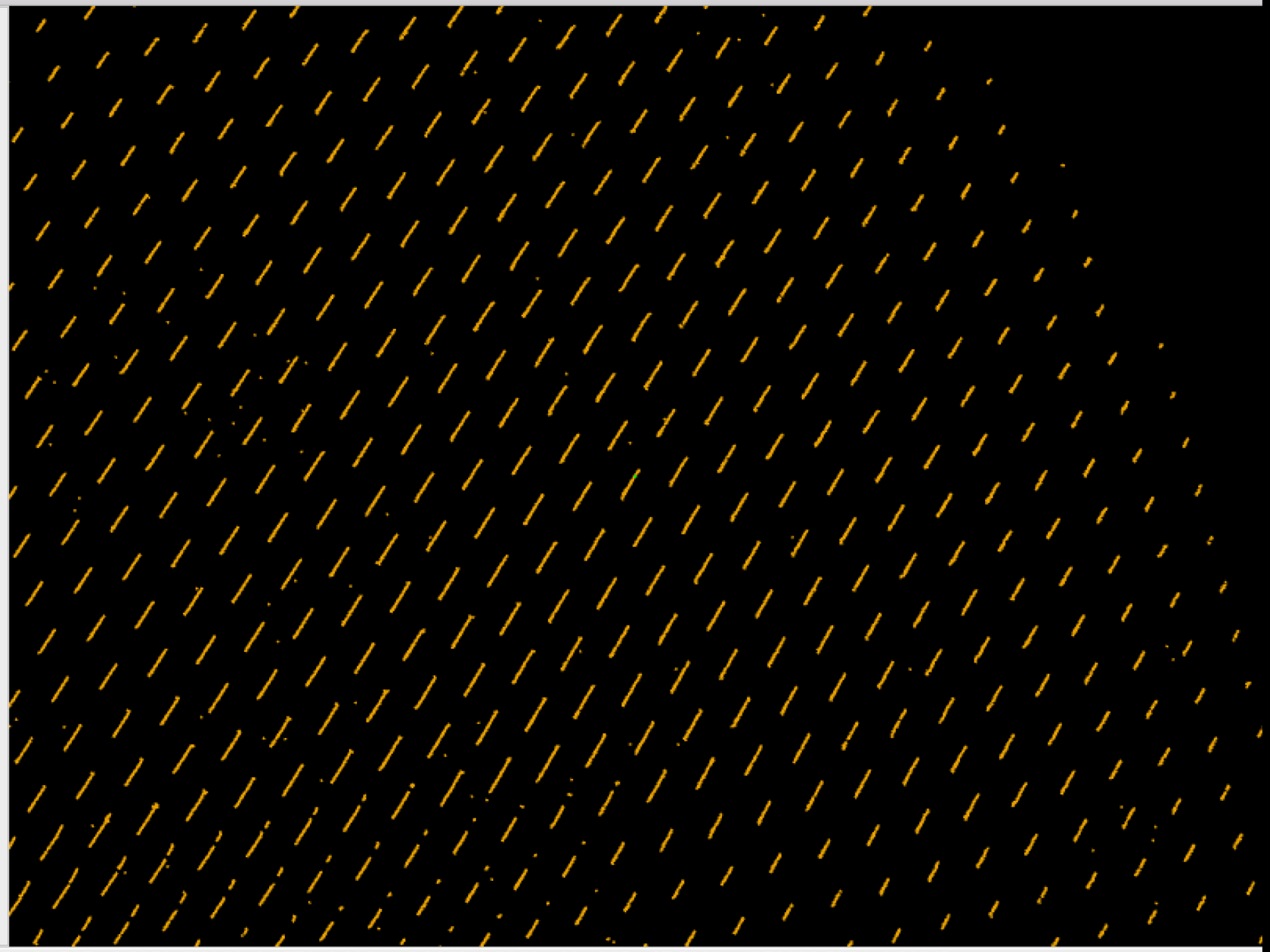
Beam fast 210.76

Beam slow 205.28

Marker size: 5

all | indexed | unindexed | integrated

all | inliers | outliers



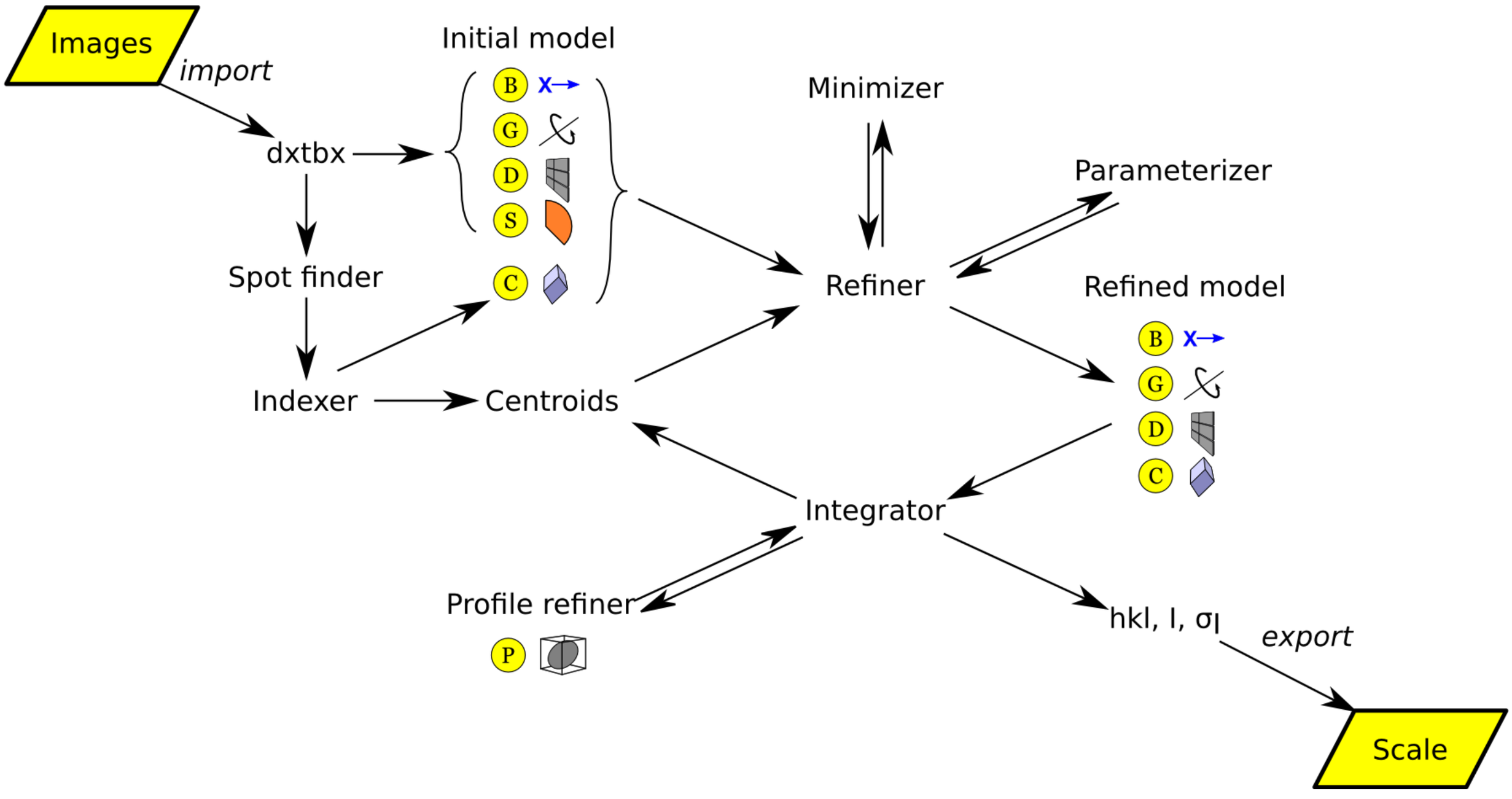
Model view matrix: [0.2768, 0.3511, 0.8945, 0.0000, 0.9592, -0.1567, -0.2353, 0.0000, 0.0576, 0.9231, -0.3802, 0.0000, -26.1067, -17.7981, -1873323.5000, 1.0000]

WORKFLOW

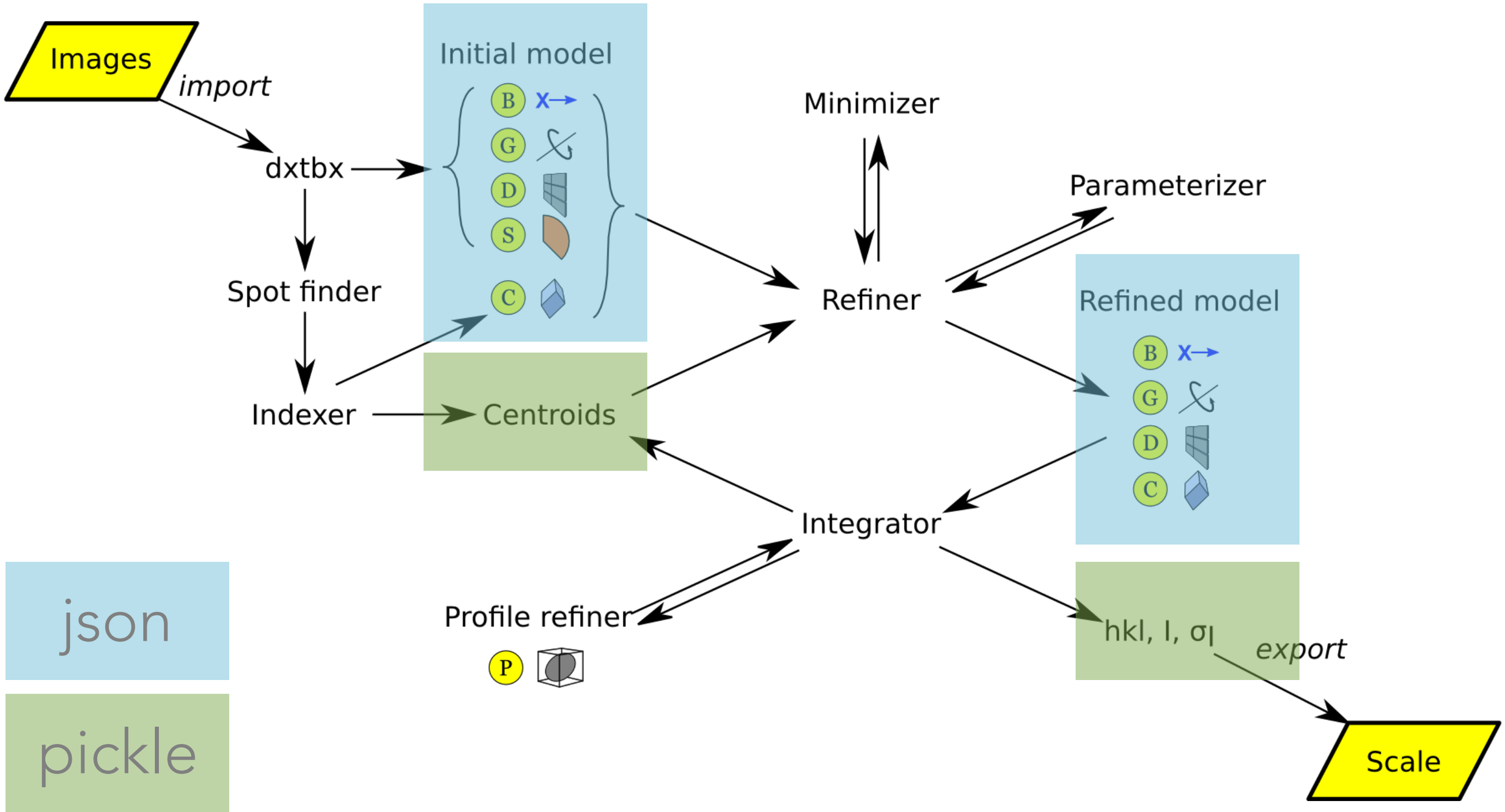


- import - read headers, construct model of experiment
- find_spots - find spots on every image; 3D if rotation data
- index - index the reflection list (may be > 1 sweep) in P1 & perform static refinement
- refine_bravais_settings - consider / refine indexed spots in all possible lattices
- reindex - reindex the indexed spot list
- refine - actually refine the model, usually with scan varying model
- integrate - actually integrate the data
- export_mtz - export an MTZ file for scaling with pointless & aimless (CCP4)

DIALS


Images
import
dxtbx
Initial model
B
G
D
S
C
Minimizer
Parameterizer
Refiner
Refined model
Spot finder
Indexer
Centroids
Integrator
Profile refiner
P
hkl, I, σI
export
Scale

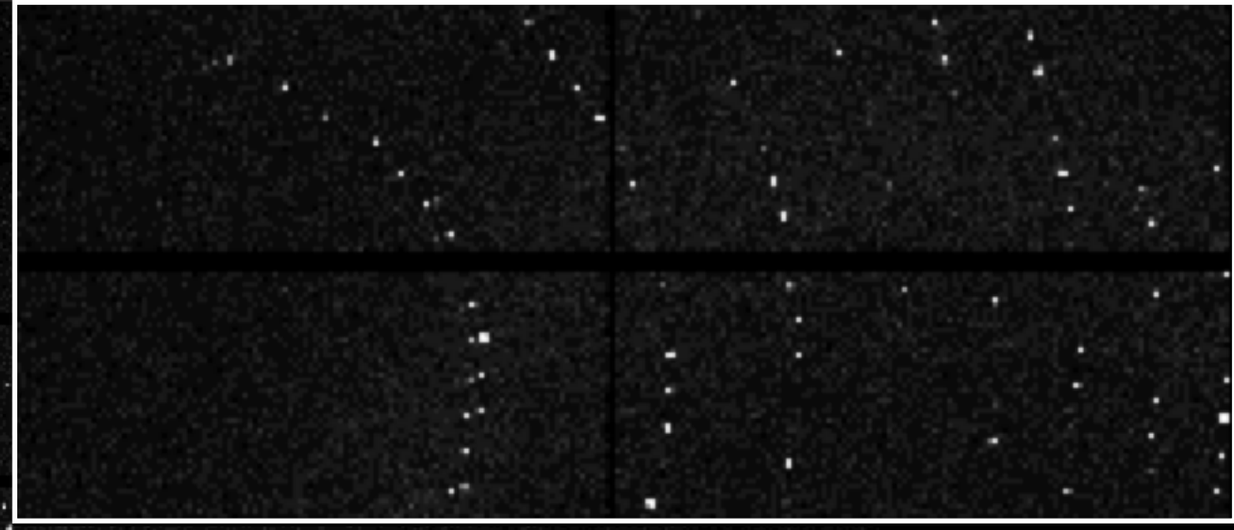
DIALS, FILES, ARCANE NAMES



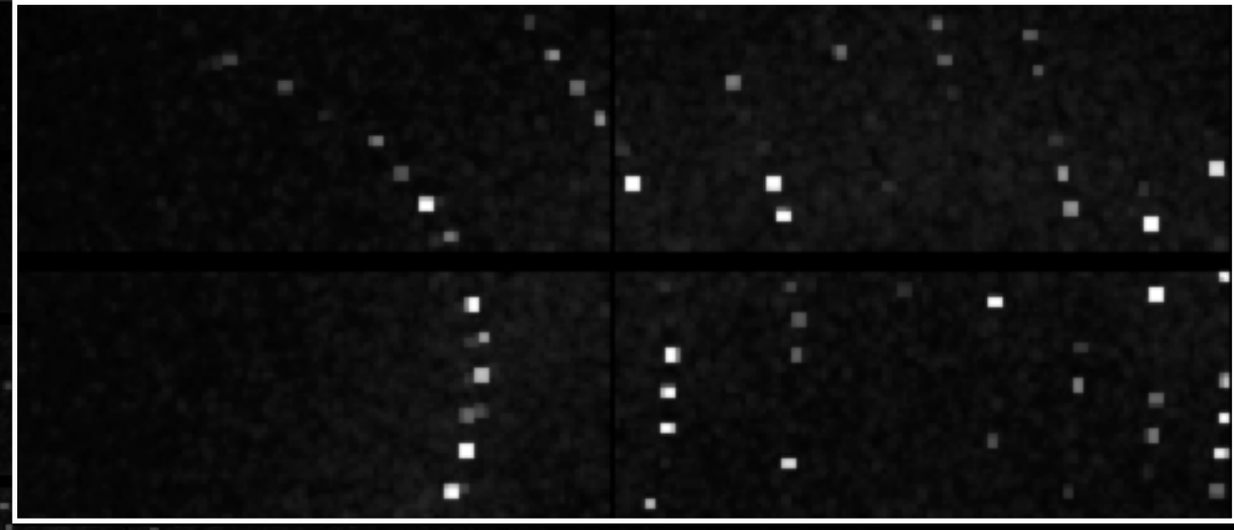
ALGORITHMS

SPOT FINDING

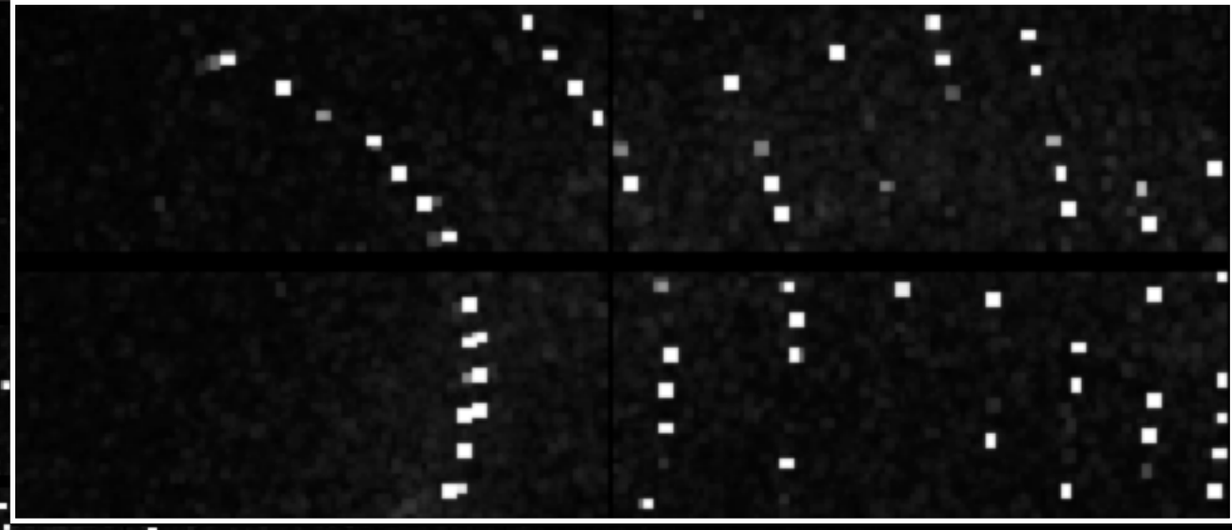
SPOT FINDING



SPOT FINDING



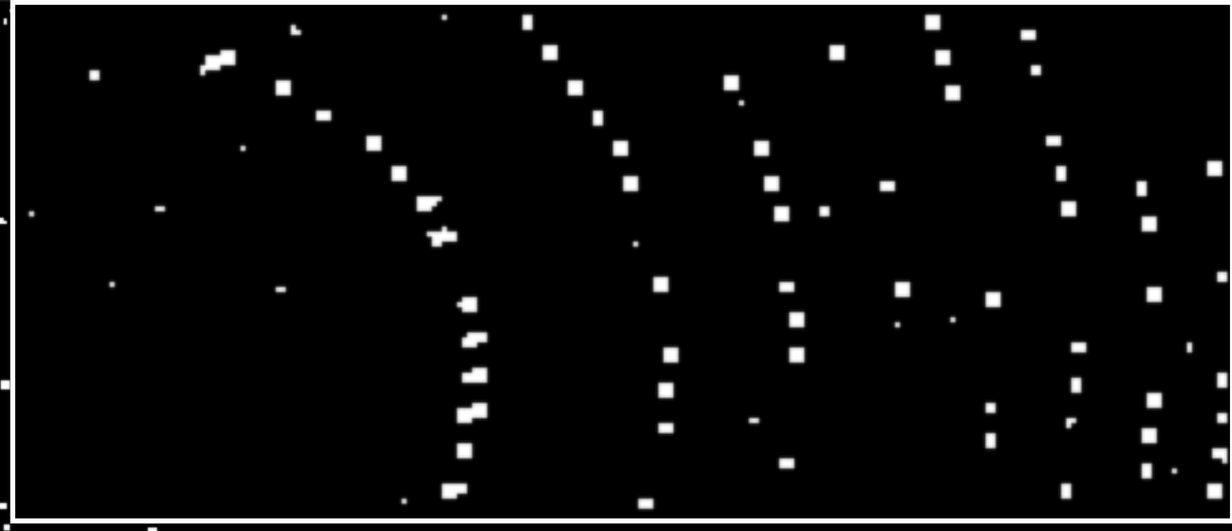
SPOT FINDING



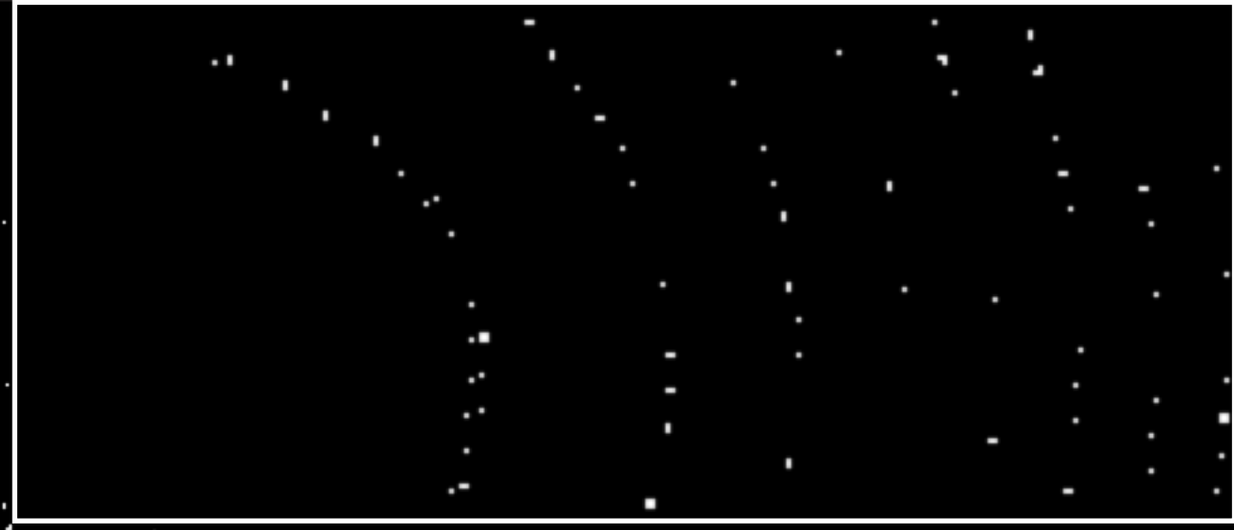
SPOT FINDING



SPOT FINDING



SPOT FINDING

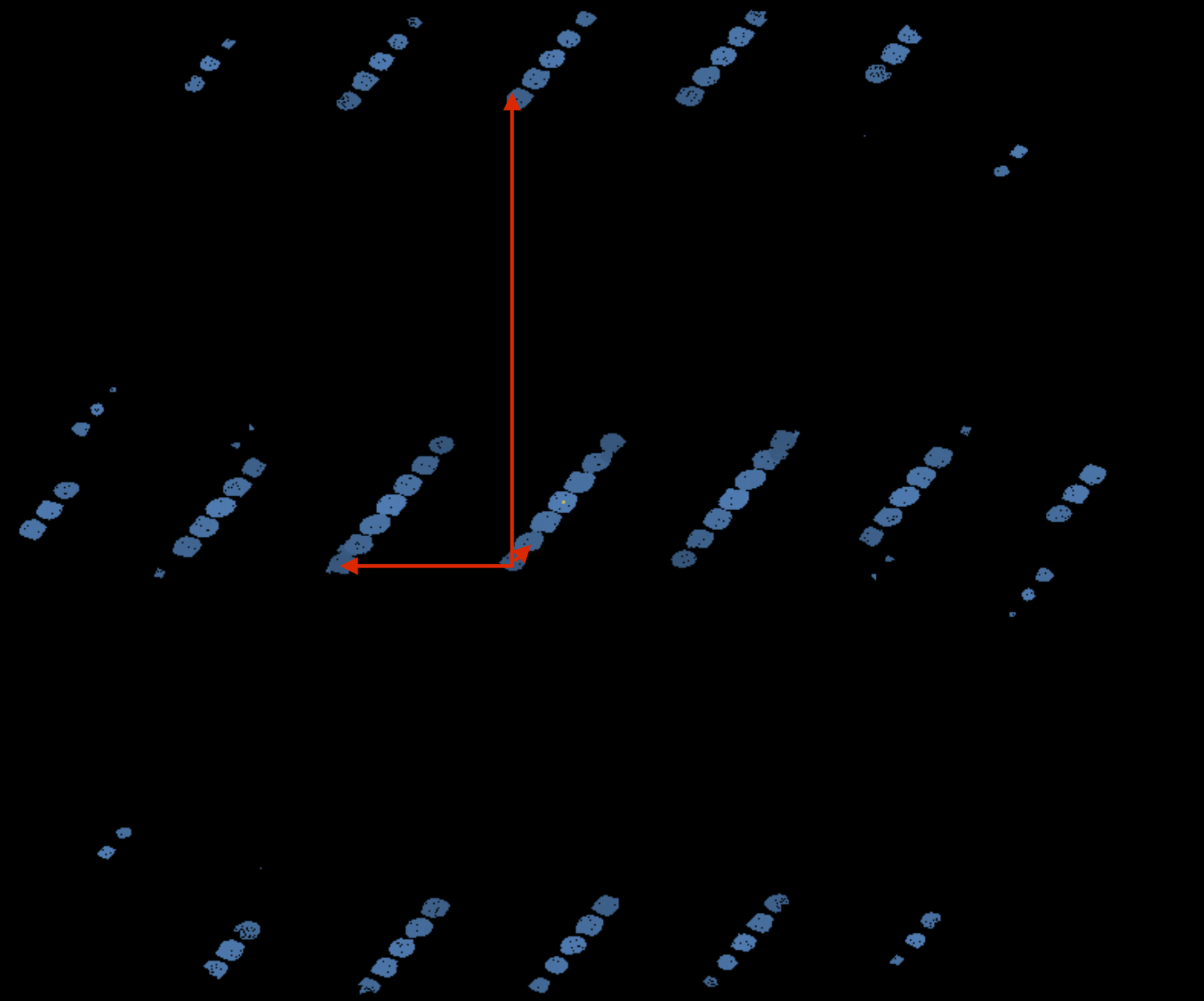


INDEXING

INDEXING



INDEXING



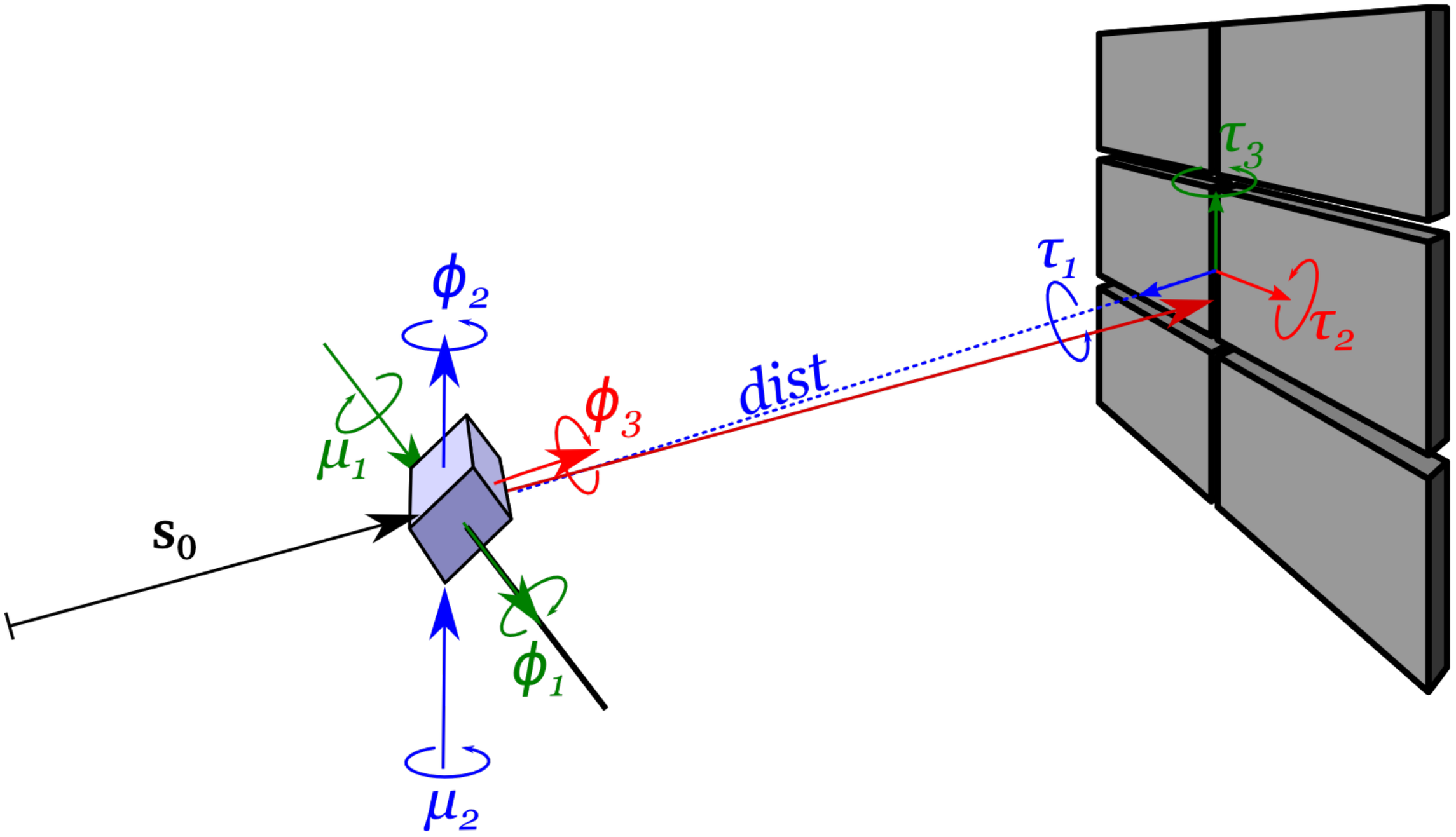
SOLUTION PICKING

Solution	Metric fit	rmsd	min/max cc	#spots	lattice	unit_cell						volume	cb_op
9	1.1465	0.655	0.490/0.650	18000	tI	79.27	79.27	68.72	90.00	90.00	90.00	431793	a+c,a+b,b+c
8	1.1465	0.665	0.487/0.650	18000	oF	68.75	112.00	112.28	90.00	90.00	90.00	864603	b+c,-b+c,2*a+b+c
7	1.1465	0.540	0.487/0.487	18000	mI	65.34	112.03	66.09	90.00	117.08	90.00	430757	a,-b+c,-a-b-c
6	1.1330	0.544	0.493/0.493	18000	mI	64.98	111.74	65.74	90.00	116.83	90.00	425978	-b,-2*a-b-c,-c
5	1.0311	0.392	0.650/0.884	18000	oI	68.51	78.60	79.44	90.00	90.00	90.00	427759	b+c,a+c,a+b
4	1.0310	0.395	0.716/0.716	18000	mI	68.52	78.62	79.46	90.00	89.95	90.00	428065	-b-c,a+c,-a-b
3	1.0311	0.417	0.650/0.650	18000	mI	78.58	68.52	79.43	90.00	90.19	90.00	427706	a+c,b+c,-a-b
2	0.0165	0.056	0.884/0.884	18000	mI	67.96	79.16	77.97	90.00	91.03	90.00	419397	b+c,a+b,-a-c
1	0.0000	0.055	-/-	18000	aP	64.76	64.74	65.48	117.10	106.47	104.64	209642	a,b,c

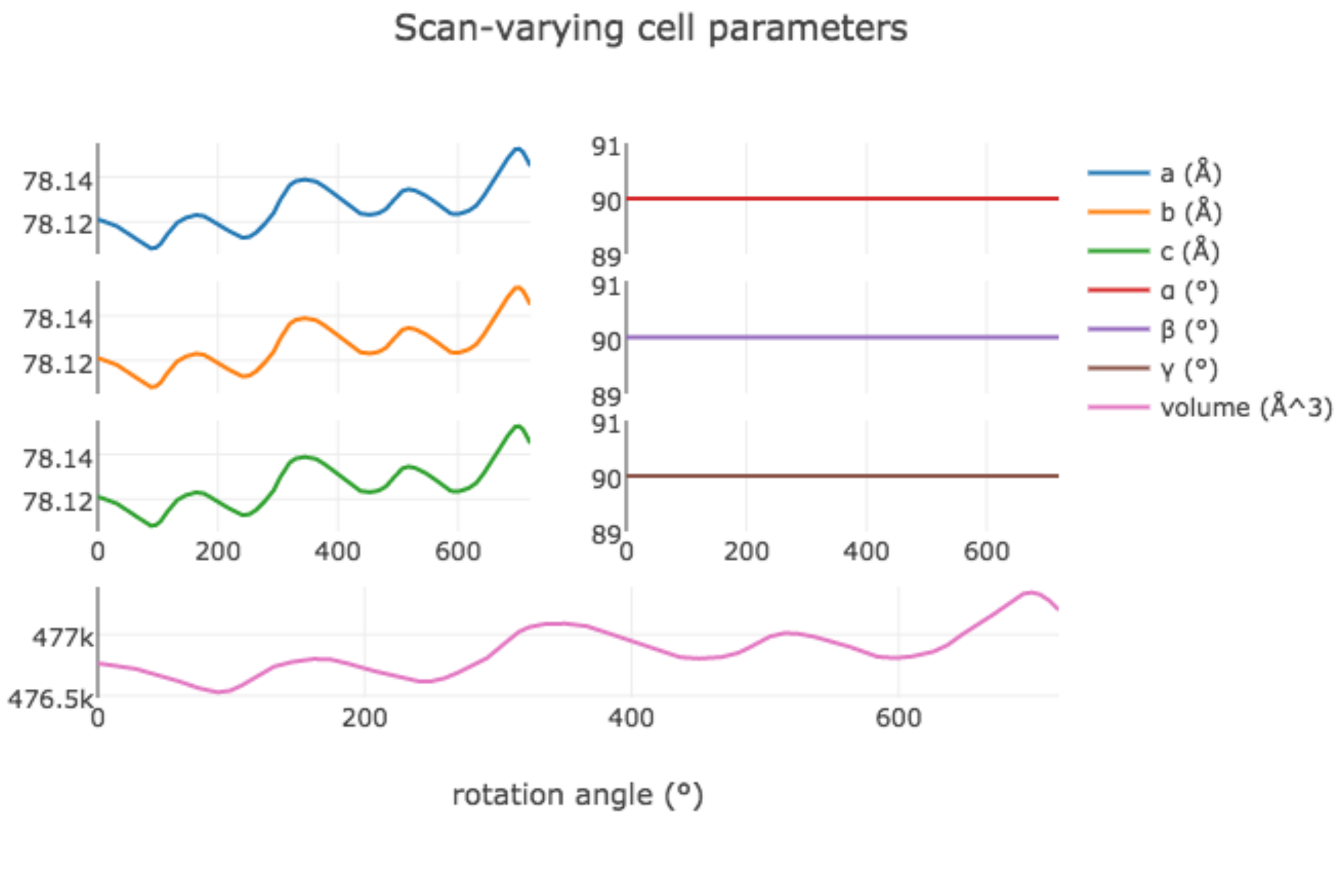
SOLUTION PICKING

Solution	Metric fit	rmsd	min/max cc	#spots	lattice		
9	1.1465	0.655	0.490/0.650	18000	tI	79.27	7
8	1.1465	0.665	0.487/0.650	18000	oF	68.75	11
7	1.1465	0.540	0.487/0.487	18000	mI	65.34	11
6	1.1330	0.544	0.493/0.493	18000	mI	64.98	11
5	1.0311	0.392	0.650/0.884	18000	oI	68.51	7
4	1.0310	0.395	0.716/0.716	18000	mI	68.52	7
3	1.0311	0.417	0.650/0.650	18000	mI	78.58	6
2	0.0165	0.056	0.884/0.884	18000	mI	67.96	7
1	0.0000	0.055	-/-	18000	aP	64.76	6

REFINEMENT



REFINEMENT


Scan-varying cell parameters
78.14
78.12
78.14
78.12
78.14
78.12
0
200
400
600
91
90
89
91
90
89
0
200
400
600
477k
476.5k
0
200
400
600
a (Å)
b (Å)
c (Å)
α (°)
β (°)
γ (°)
volume (Å^3)
rotation angle (°)

INTEGRATION

3.4. Intensity estimation

If an expected intensity distribution $\{p_i | i \in D_0\}$ of the observed profile is given in a domain D_0, the reflection intensity I can be estimated as

$$I = \frac{\sum_{i \in D} (c_i - b_i) p_i / v_i}{\sum_{i \in D} p_i^2 / v_i},$$

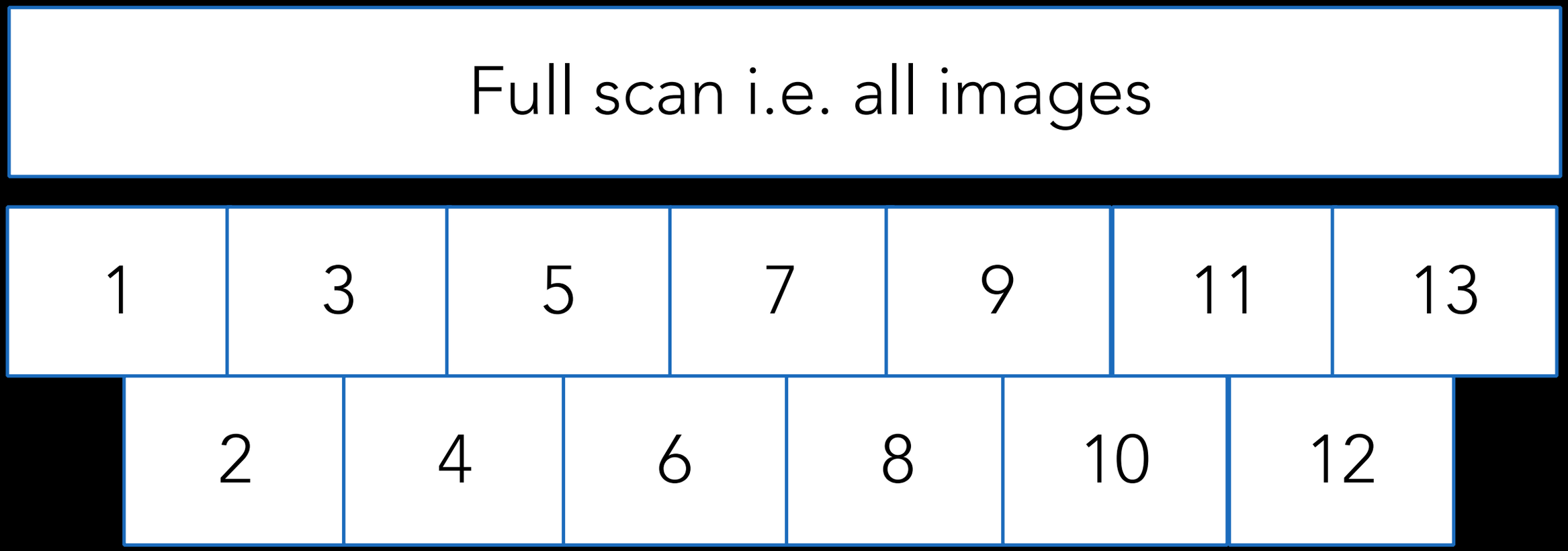
which minimizes the function

$$\psi(I) = \sum_{i \in D} (c_i - I \cdot p_i - b_i)^2 / v_i, \quad \sum_{i \in D_0} p_i = 1.$$

b_i, c_i, v_i $(i \in D)$ are the background, contents and variance of pixels observed in a subdomain $D \subseteq D_0$ of the expected distribution. The background b_i underneath a diffraction spot is often assumed to be a constant which is estimated from the neighbourhood around the reflection.

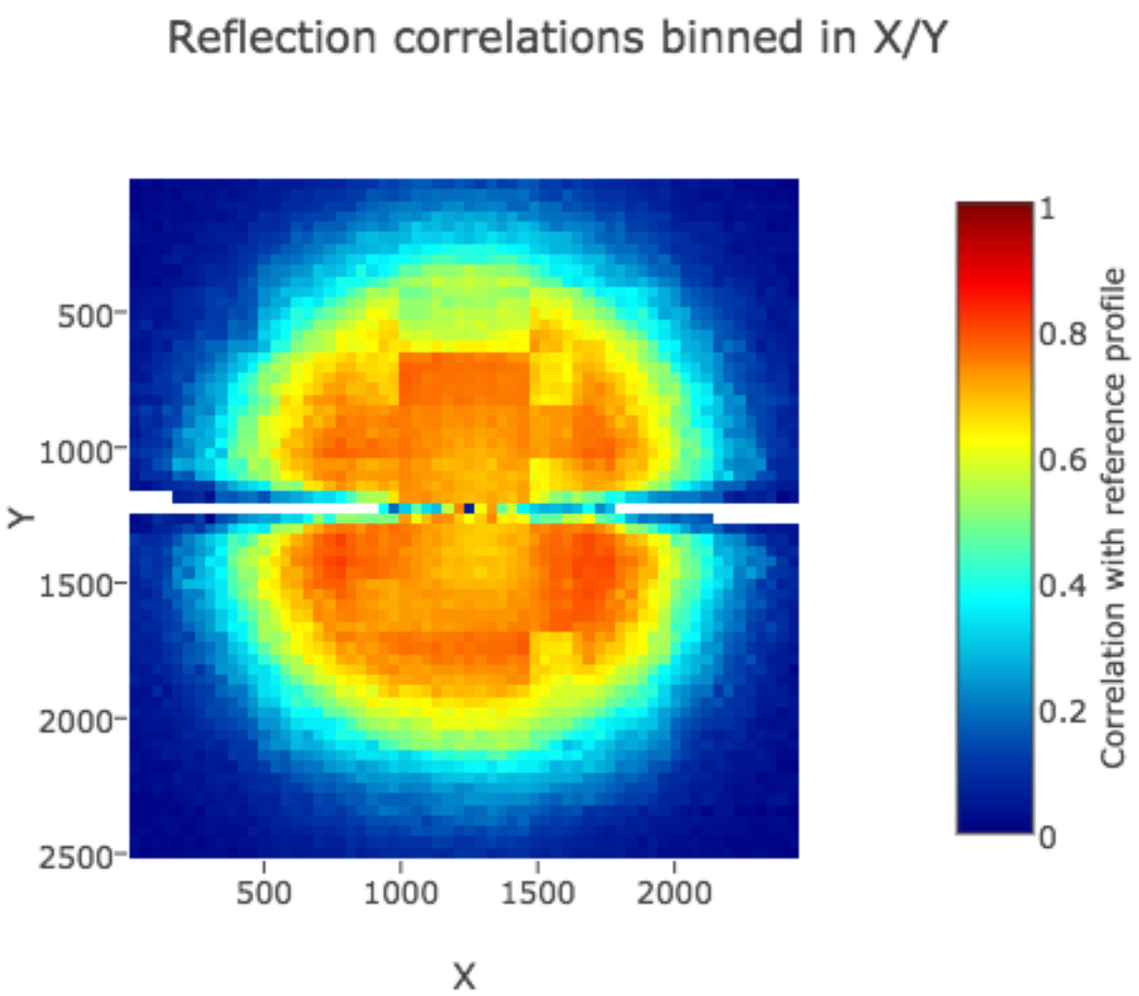
```
/**
 * Evaluate the next intensity iteration.
 * @ returns The estimate of the intensity
 */
vec2<double>
estimate_intensity(const af::const_ref<FloatType, af::c_grid<3> > &p,
                   const af::const_ref<bool, af::c_grid<3> > &m,
                   const af::const_ref<FloatType, af::c_grid<3> > &c,
                   const af::const_ref<FloatType, af::c_grid<3> > &b,
                   double I) const {
  double sum1 = 0.0;
  double sum2 = 0.0;
  double sumv = 0.0;
  for (std::size_t i = 0; i < p.size(); ++i) {
    if (m[i]) {
      double v = std::abs(b[i]) + std::abs(I * p[i]);
      sumv += v;
      if (v > 0) {
        sum1 += (c[i] - b[i]) * p[i] / v;
        sum2 += p[i] * p[i] / v;
      }
    }
  }
  return vec2<double>(sum2 != 0 ? sum1 / sum2 : 0.0, sumv);
```

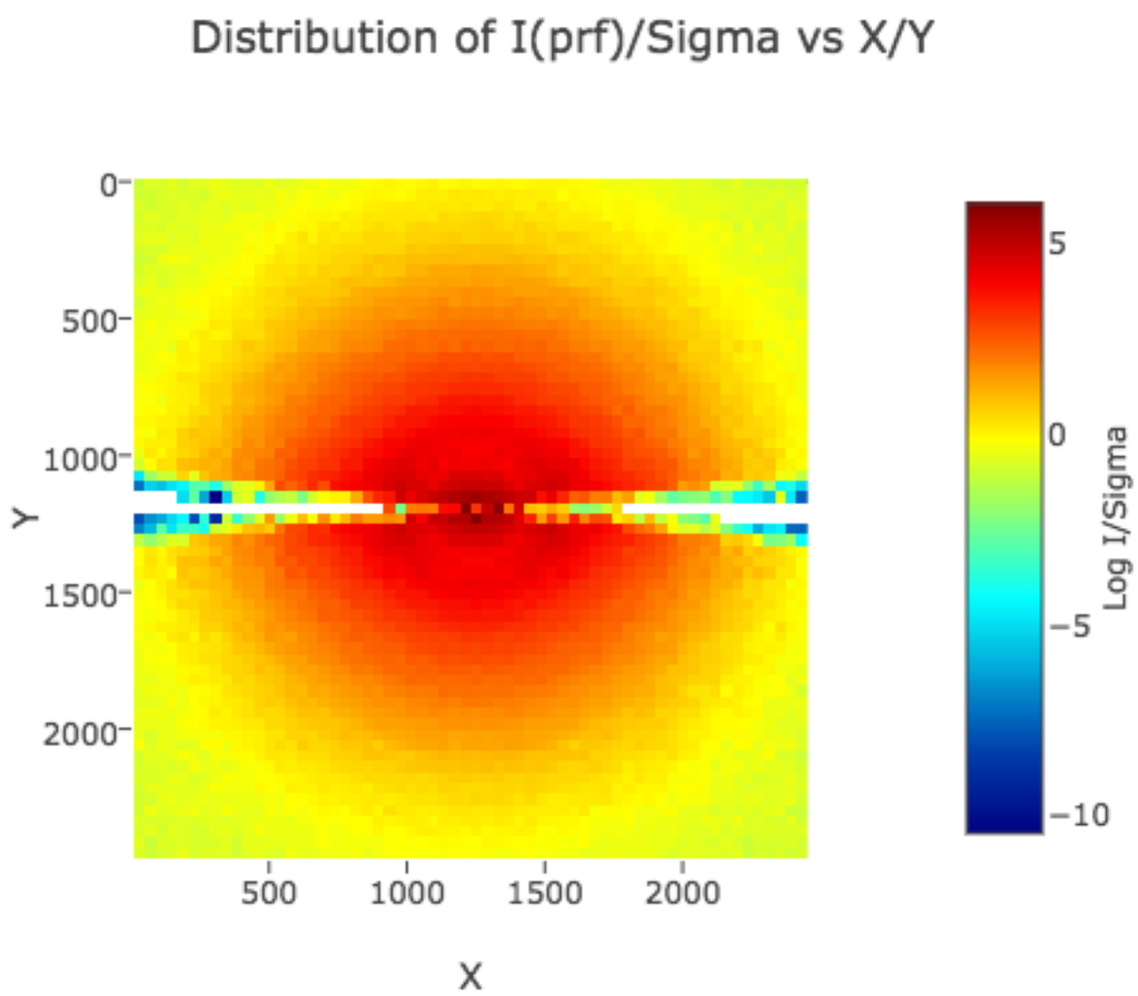
REFLECTION PROFILES



Profile for reflection at position x derived from average of strong reflections in block with centre nearest x

INTEGRATION

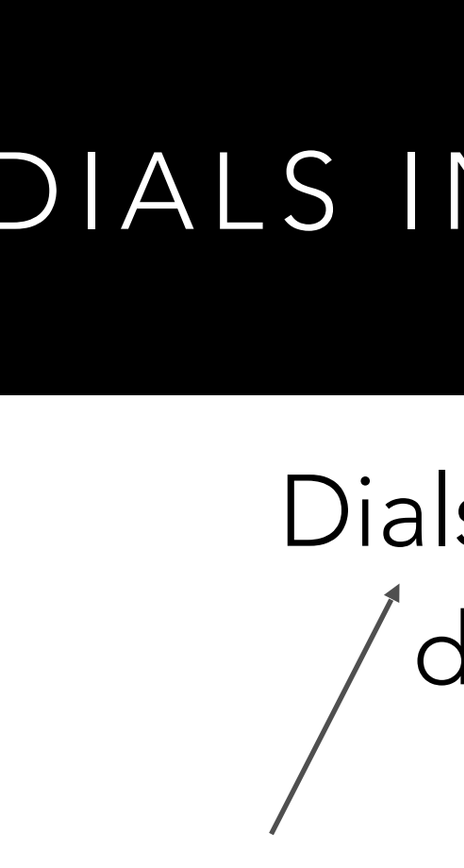




START DEMONSTRATION

DIALS IN XIA2

DialsIndexer = dials.import + dials.find_spots +
dials.index + dials.refine_bravais_settings

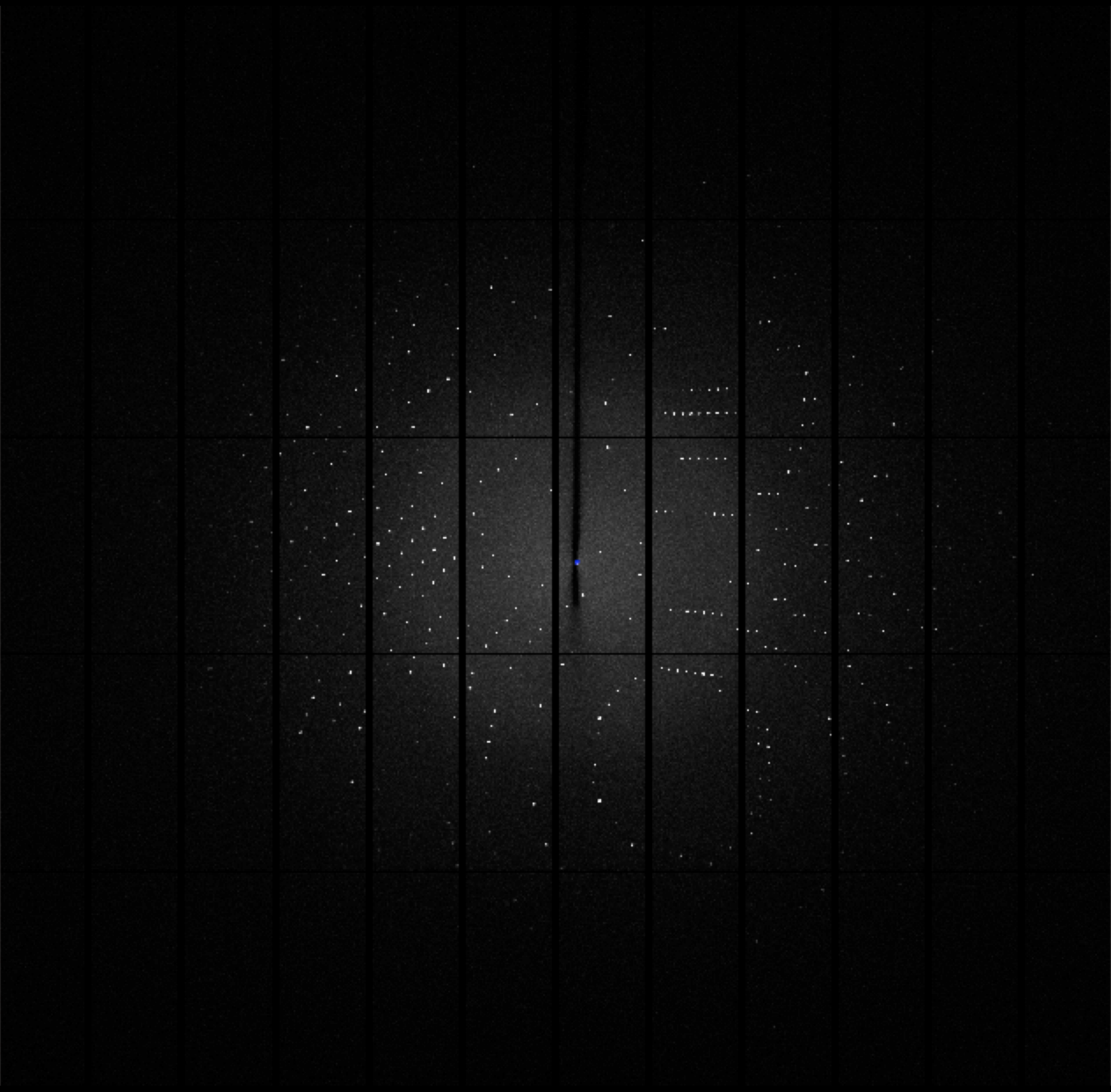


DialsRefiner = dials.refine

DialsIntegrater = dials.integrate + dials.export_mtz

Then scale with POINTLESS / AIMLESS

3-sweep beta lactamase



```
xia2 atom=Zn /Volumes/GraemeData/how_to/beta-lactamase/C2_s4
```

C2_dials — gw56@cs03r-sc-serv-16:/dls/tmp/gw56 — less xia2.txt — 80×24

```
------------------- Spotfinding SWEEP1 --------------------
103745 spots found on 3600 images (max 1954 / bin)
****                        **  *****                          ****** *
*********              ****************************************
************       *****************************************
**************   *******************************************
*************************************************************
*************************************************************
*************************************************************
*************************************************************
*************************************************************
*************************************************************
1                            image                          3600
------------------- Autoindexing SWEEP1 --------------------
All possible indexing solutions:
mC  53.22  61.29  69.28  90.00  93.03  90.00
aP  40.60  40.58  69.29  91.93  92.04  98.07
Indexing solution:
mC  53.22  61.29  69.28  90.00  93.03  90.00
-------------------- Integrating SWEEP1 --------------------
Processed batches 1 to 3600
Standard Deviation in pixel range: 0.31 0.58
Integration status per image (60/record):
:
```

```
xia2 atom=Zn /Volumes/GraemeData/how_to/beta-lactamase/C2_s4
```

C2_dials — gw56@cs03r-sc-serv-16:/dls/tmp/gw56 — less xia2.txt — 80×24

```
------------------- Integrating SWEEP1 --------------------
Processed batches 1 to 3600
Standard Deviation in pixel range: 0.31 0.58
Integration status per image (60/record):
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:
```

```
xia2 atom=Zn /Volumes/GraemeData/how_to/beta-lactamase/C2_s4
```

C2_dials — gw56@cs03r-sc-serv-16:/dls/tmp/gw56 — less xia2.txt — 80×24

```
-------------------- Spotfinding SWEEP2 --------------------
52523 spots found on 1800 images (max 972 / bin)
** *                                          * ** ****  * *
******* ****** * *** ***  ************** ********************
**************************************************************
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**************************************************************
1                          image                          1800
-------------------- Autoindexing SWEEP2 --------------------
All possible indexing solutions:
mC  53.21  61.22  69.29  90.00  93.03  90.00
aP  40.56  40.55  69.30  91.97  92.01  98.02
Indexing solution:
mC  53.21  61.22  69.29  90.00  93.03  90.00
-------------------- Integrating SWEEP2 --------------------
Processed batches 1 to 1800
Standard Deviation in pixel range: 0.29 0.58
Integration status per image (60/record):
:
```

```
xia2 atom=Zn /Volumes/GraemeData/how_to/beta-lactamase/C2_s4
```

C2_dials — gw56@cs03r-sc-serv-16:/dls/tmp/gw56 — less xia2.txt — 80×24

```
-------------------- Spotfinding SWEEP3 --------------------
52378 spots found on 1800 images (max 996 / bin)
*** ****                                          **** **** **
************** *                            **************************
********************** **       ********************************
**************************************************************
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**************************************************************
1                           image                          1800
-------------------- Autoindexing SWEEP3 --------------------
All possible indexing solutions:
mC  53.23  61.32  69.29  90.00  93.02  90.00
aP  40.60  40.60  69.30  92.03  91.93  98.07
Indexing solution:
mC  53.23  61.32  69.29  90.00  93.02  90.00
-------------------- Integrating SWEEP3 --------------------
Processed batches 1 to 1800
Standard Deviation in pixel range: 0.31 0.59
Integration status per image (60/record):
:
```

```
xia2 atom=Zn /Volumes/GraemeData/how_to/beta-lactamase/C2_s4
```

C2_dials — gw56@cs03r-sc-serv-16:/dls/tmp/gw56 — less xia2.txt — 80×24

```
------------------- Preparing DEFAULT --------------------
Likely spacegroups:
C 1 2 1
Reindexing to first spacegroup setting: C 1 2 1 (h,k,l)
--------------------- Scaling DEFAULT ---------------------
Resolution limit for SAD/SWEEP1:  1.32
Resolution limit for SAD/SWEEP2:  1.35
Resolution limit for SAD/SWEEP3:  1.36
--------------------- Scaling DEFAULT ---------------------
Resolution limit for SAD/SWEEP1:  1.32
Resolution limit for SAD/SWEEP2:  1.35
Resolution limit for SAD/SWEEP3:  1.36
------------------- Unit cell refinement -------------------
SAD:  53.21  61.28  69.27  90.00  93.03  90.00
Overall twinning score: 2.37
Your data do not appear twinned
Project: AUTOMATIC
Crystal: DEFAULT
Sequence:
Wavelength name: SAD
Wavelength 1.23985
Sweeps:
SWEEP SWEEP1 [WAVELENGTH SAD]
:
```

```
xia2 atom=Zn /Volumes/GraemeData/how_to/beta-lactamase/C2_s4
```

C2_dials — gw56@cs03r-sc-serv-16:/dls/tmp/gw56 — less xia2.txt — 80×24

For AUTOMATIC/DEFAULT/SAD	Overall	Low	High
High resolution limit	1.32	3.58	1.32
Low resolution limit	40.15	40.16	1.34
Completeness	97.6	100.0	67.1
Multiplicity	11.7	13.4	3.4
I/sigma	15.6	58.7	1.1
Rmerge(I)	0.071	0.042	0.717
Rmerge(I+/-)	0.064	0.036	0.605
Rmeas(I)	0.074	0.043	0.843
Rmeas(I+/-)	0.069	0.039	0.807
Rpim(I)	0.021	0.012	0.433
Rpim(I+/-)	0.027	0.015	0.527
CC half	0.999	0.999	0.743
Wilson B factor	12.471		
Anomalous completeness	96.4	100.0	2.8
Anomalous multiplicity	6.0	7.0	1.9
Anomalous correlation	0.459	0.513	0.037
Anomalous slope	1.163		
dF/F	0.071		
dI/s(dI)	1.210		
Total observations	597099	35974	5854
Total unique	50984	2692	1741

Assuming spacegroup: C 1 2 1

:

```
xia2 atom=Zn /Volumes/GraemeData/how_to/beta-lactamase/C2_s4
```

C2_dials — gw56@cs03r-sc-serv-16:/dls/tmp/gw56 — less xia2.txt — 80×24

```
Unit cell (with estimated std devs):
53.20942(16) 61.2818(2) 69.27089(17)
90.0          93.0325(2) 90.0
mtz format:
Scaled reflections: /Users/graeme/Projects/biochemical-society/nice_example/C2_d
ials/DataFiles/AUTOMATIC_DEFAULT_free.mtz
mtz_unmerged format:
Scaled reflections (SAD): /Users/graeme/Projects/biochemical-society/nice_exampl
e/C2_dials/DataFiles/AUTOMATIC_DEFAULT_scaled_unmerged.mtz
sca format:
Scaled reflections (SAD): /Users/graeme/Projects/biochemical-society/nice_exampl
e/C2_dials/DataFiles/AUTOMATIC_DEFAULT_scaled.sca
sca_unmerged format:
Scaled reflections (SAD): /Users/graeme/Projects/biochemical-society/nice_exampl
e/C2_dials/DataFiles/AUTOMATIC_DEFAULT_scaled_unmerged.sca
Processing took 00h 39m 00s
XIA2 used... aimless, ccp4, dials, pointless, xia2
Here are the appropriate citations (BIBTeX in xia2-citations.bib.)
Evans, P. (2006) Acta Cryst. D62, 72-82.
Evans, P. R. and Murshudov, G. N. (2013) Acta Cryst. D69, 1204-1214.
Winn, M. D. et al. (2011) Acta Cryst. D67, 235-242.
Winter, G. (2010) J. Appl. Cryst. 43, 186-190.
Status: normal termination
(END)
```

Output

Data files can be found in

```
DataFiles
```

Log files to look at can be found in …

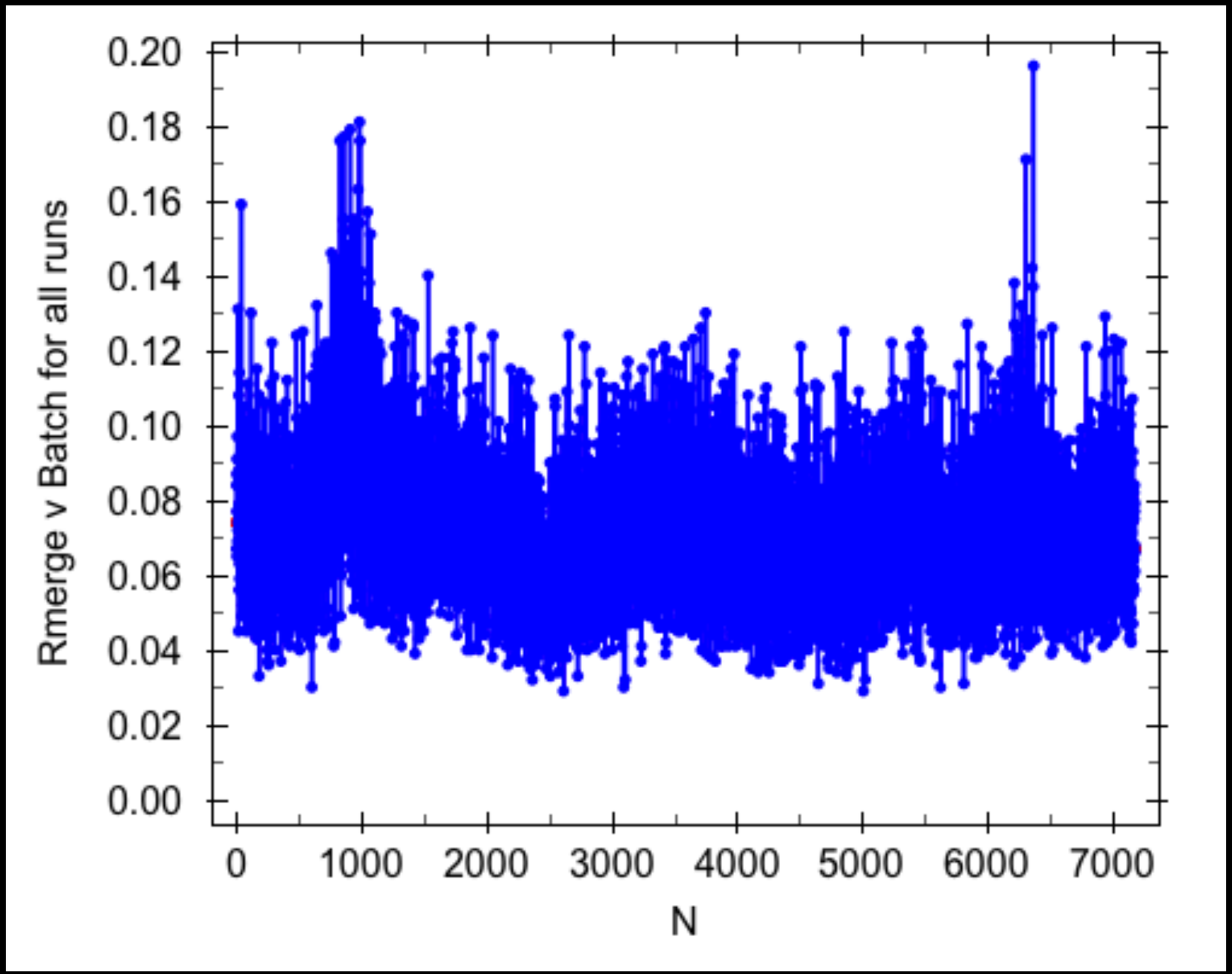
```
LogFiles
```

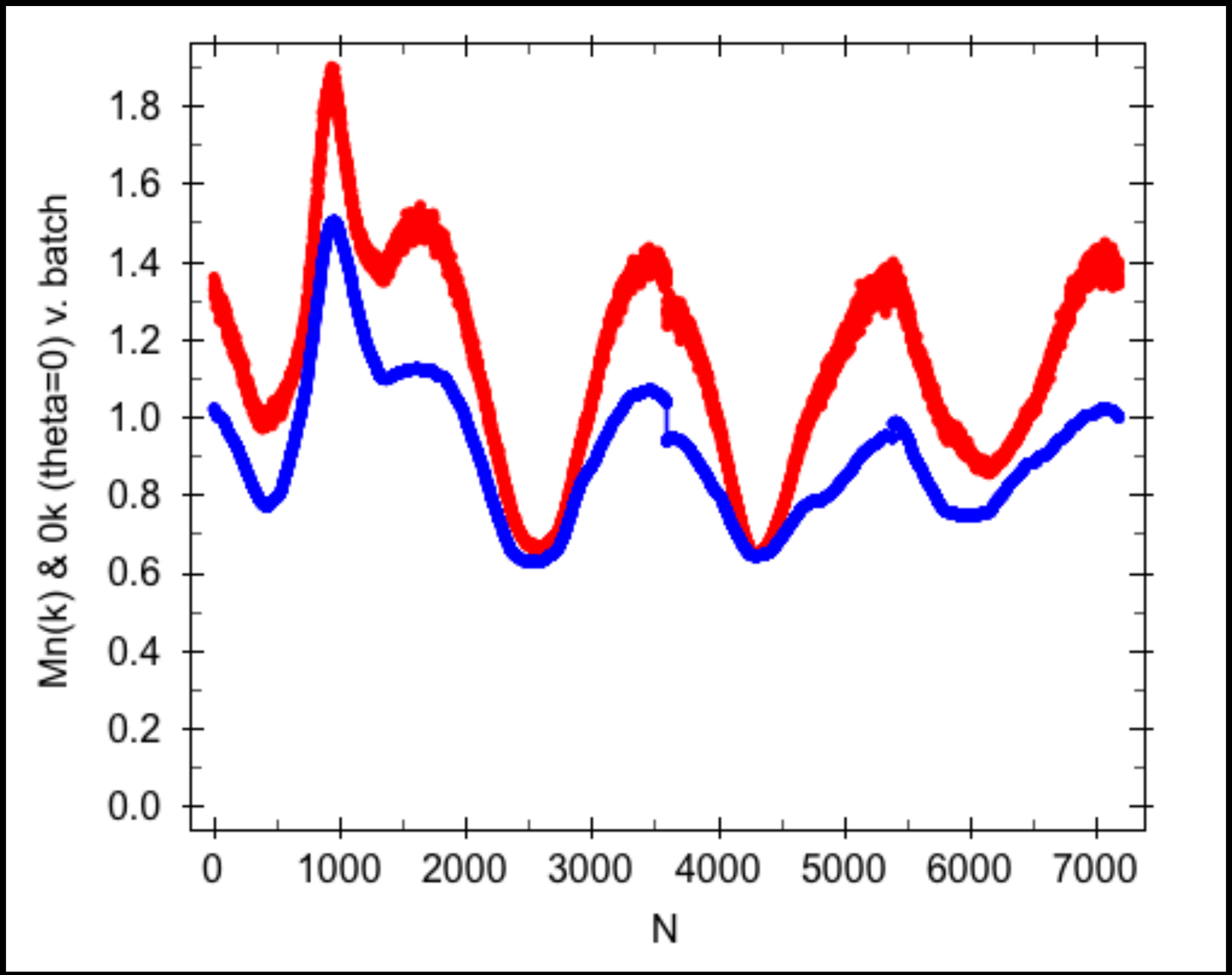
Worth trying e.g.

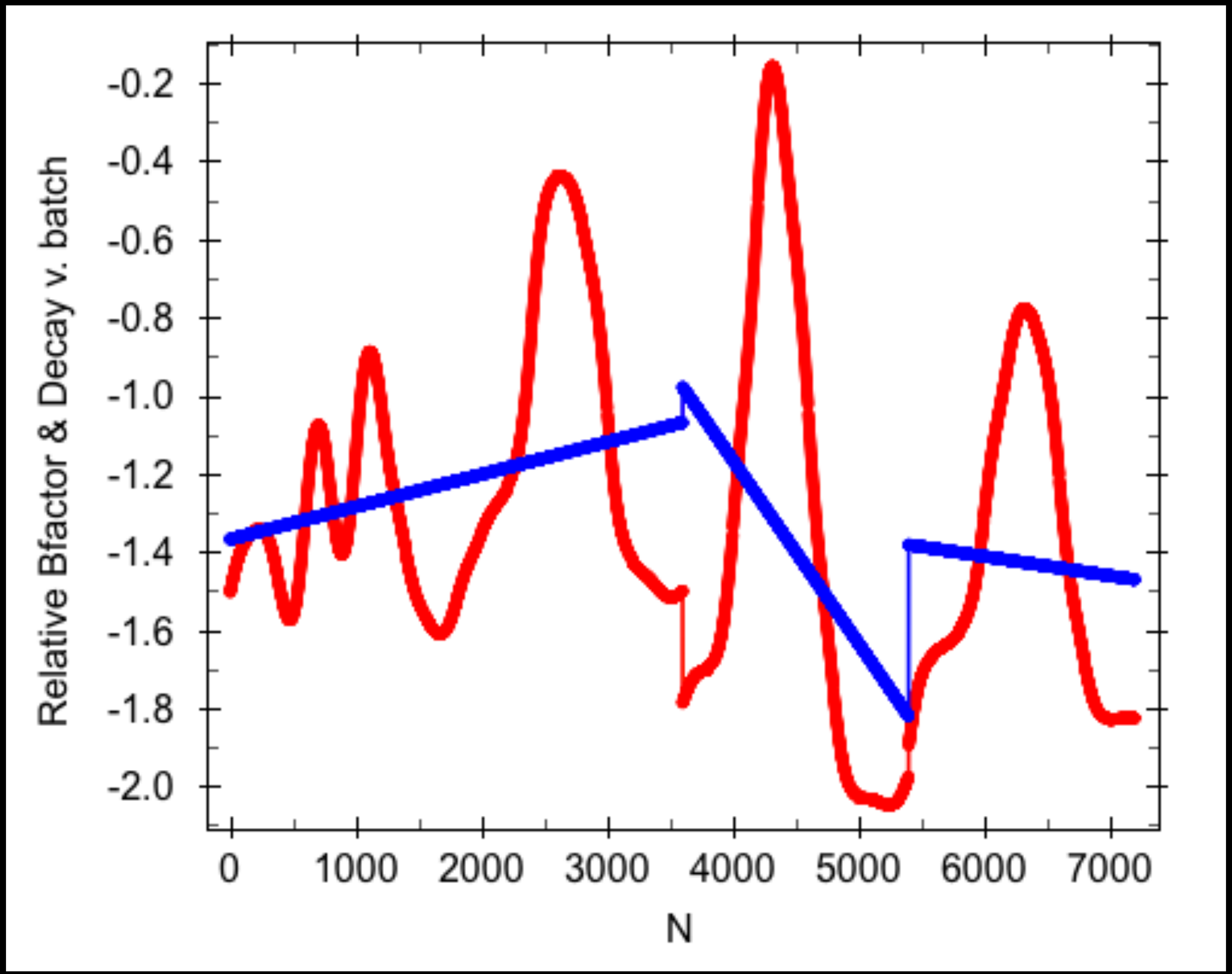
```
loggraph LogFiles/*aimless*.log
```

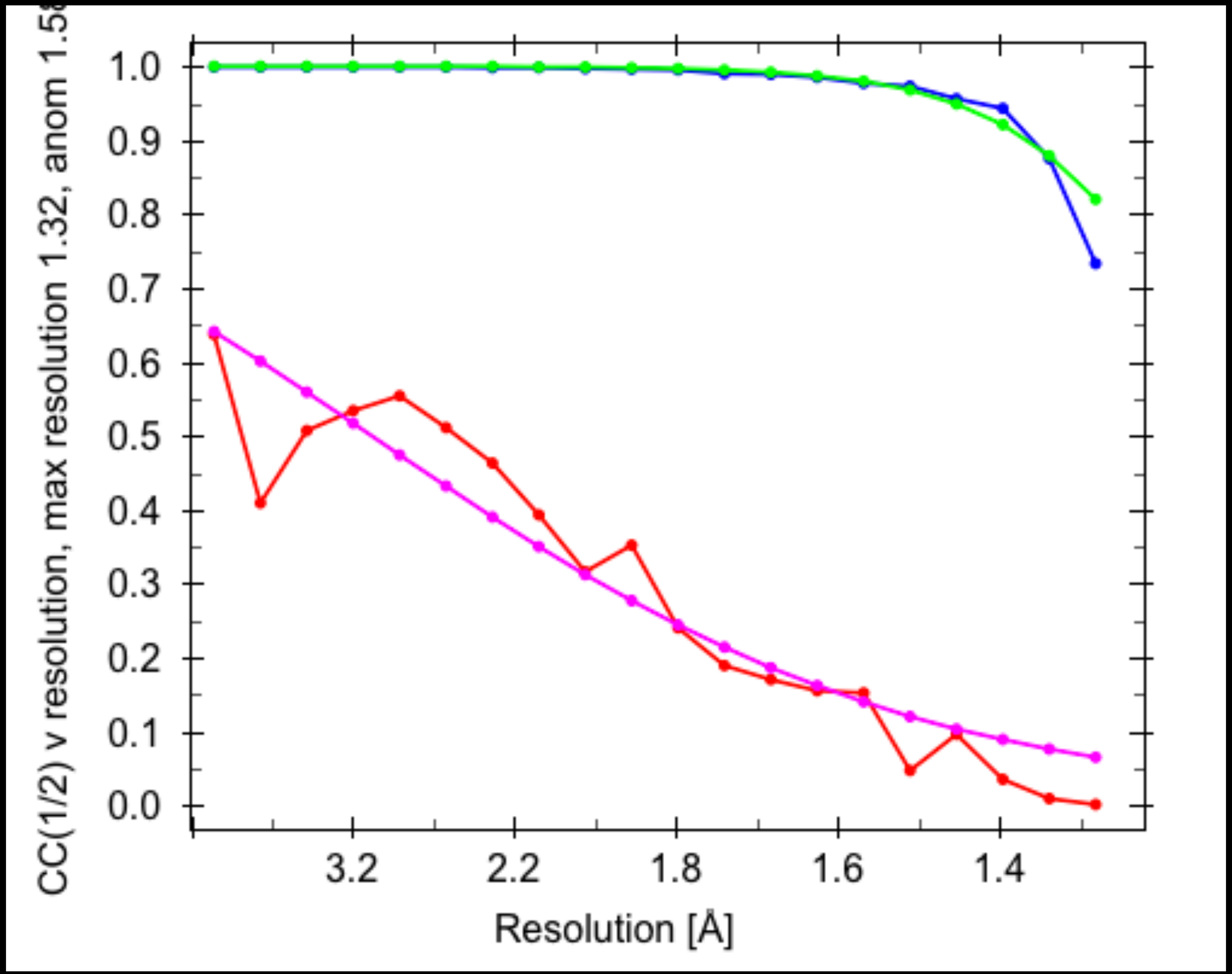
Also

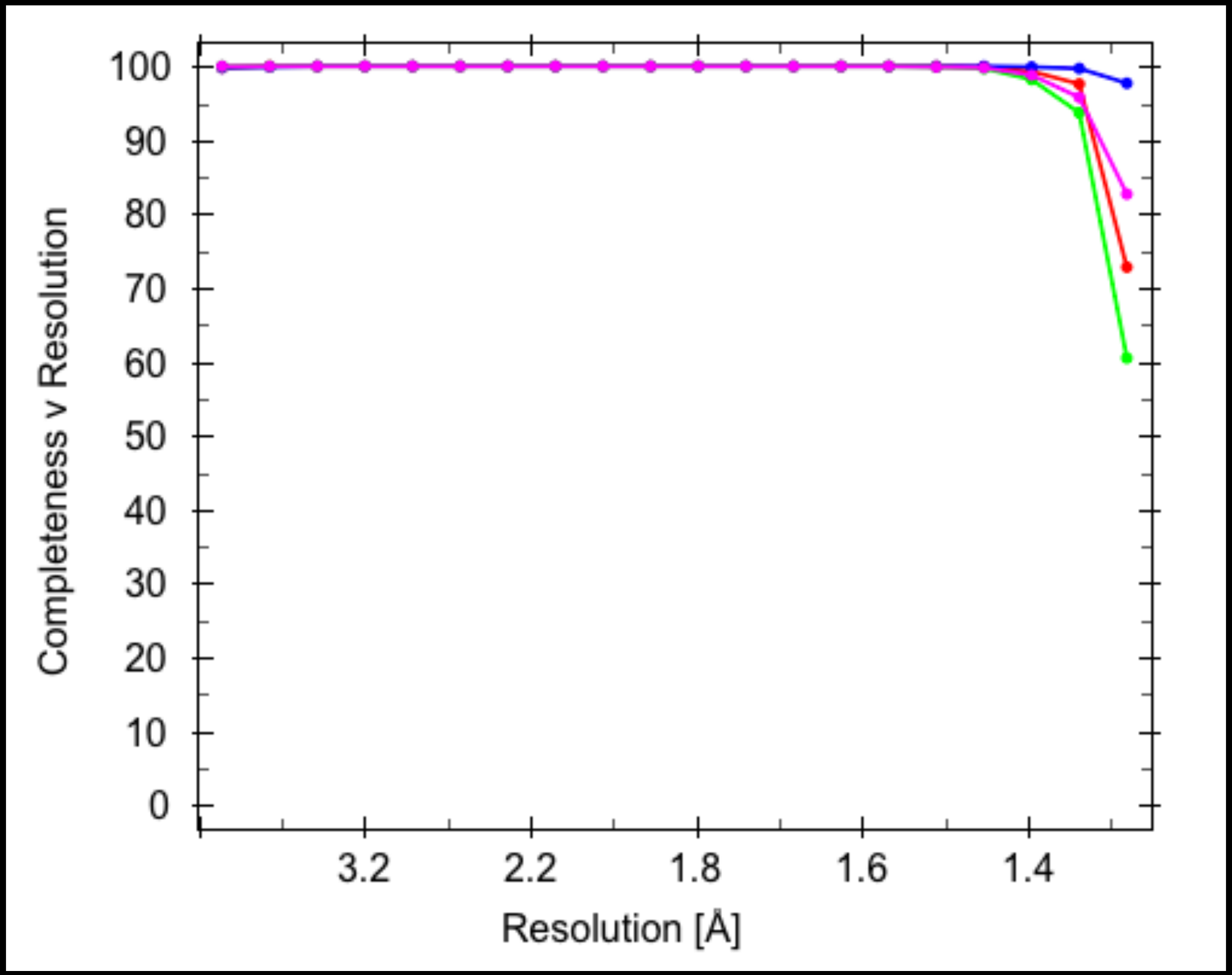
```
firefox *html
```


Rmerge v Batch for all runs
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0
1000
2000
3000
4000
5000
6000
7000
N


Mn(k) & 0k (theta=0) v. batch
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
1000
2000
3000
4000
5000
6000
7000
N


Relative Bfactor & Decay v. batch
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-1.4
-1.6
-1.8
-2.0
0
1000
2000
3000
4000
5000
6000
7000
N

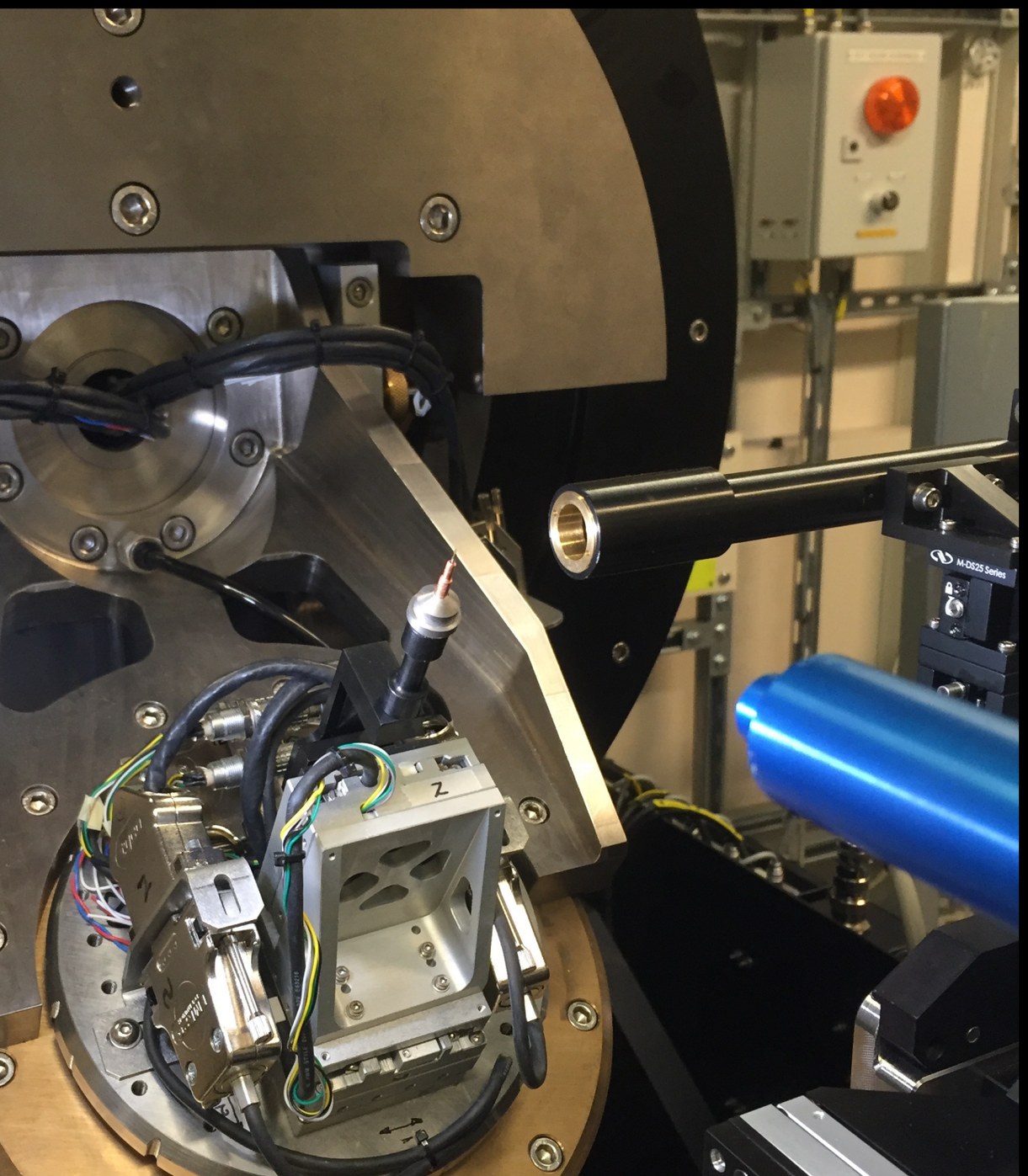

CC(1/2) v resolution, max resolution 1.32, anom 1.58
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
3.2
2.2
1.8
1.6
1.4
Resolution [Å]

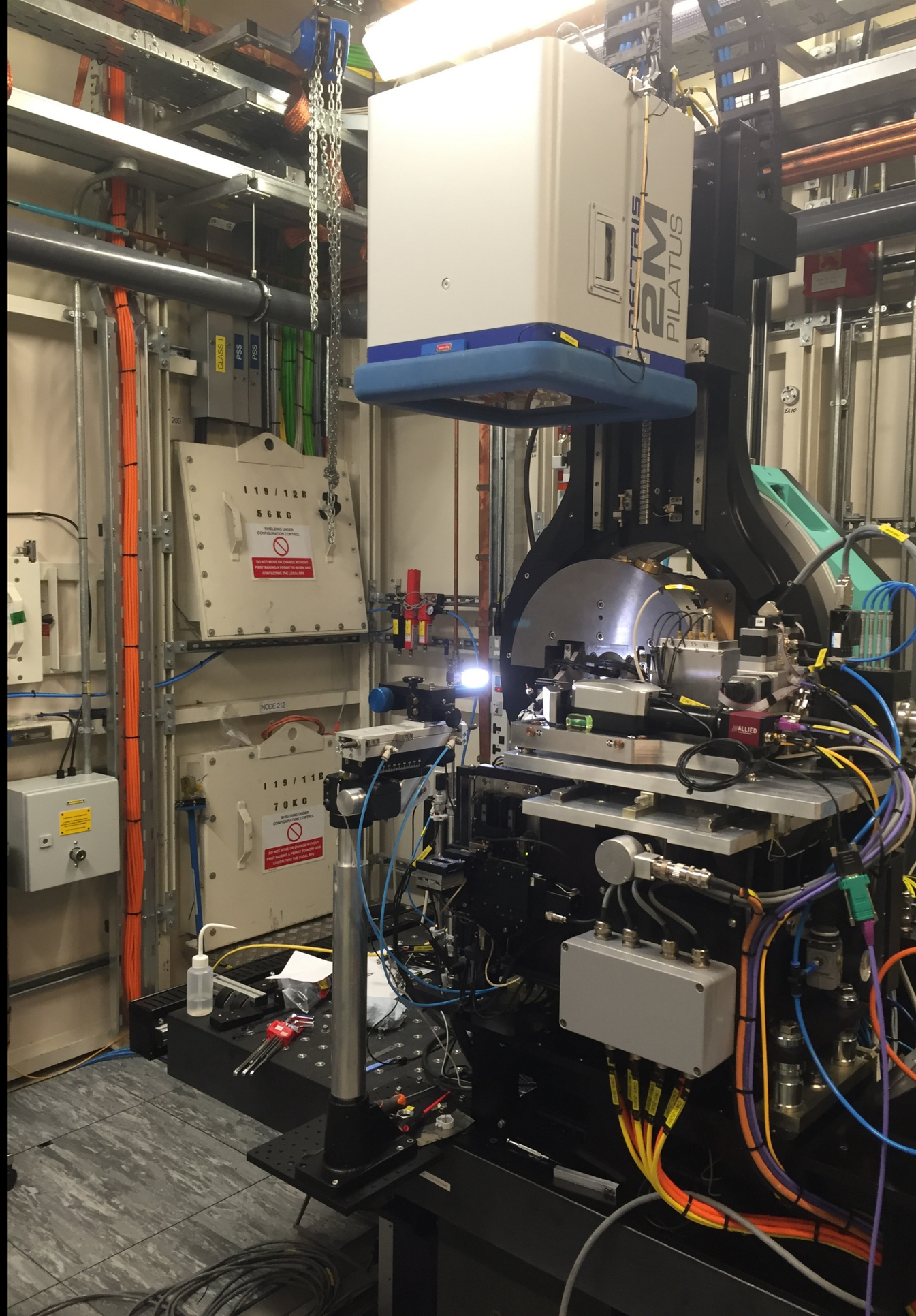

Completeness v Resolution
100
90
80
70
60
50
40
30
20
10
0
3.2
2.2
1.8
1.6
1.4
Resolution [Å]

Data from xia2 + sequence put into Crank2 via CCP4i:
25/27% R/Rfree

NOT JUST MX...

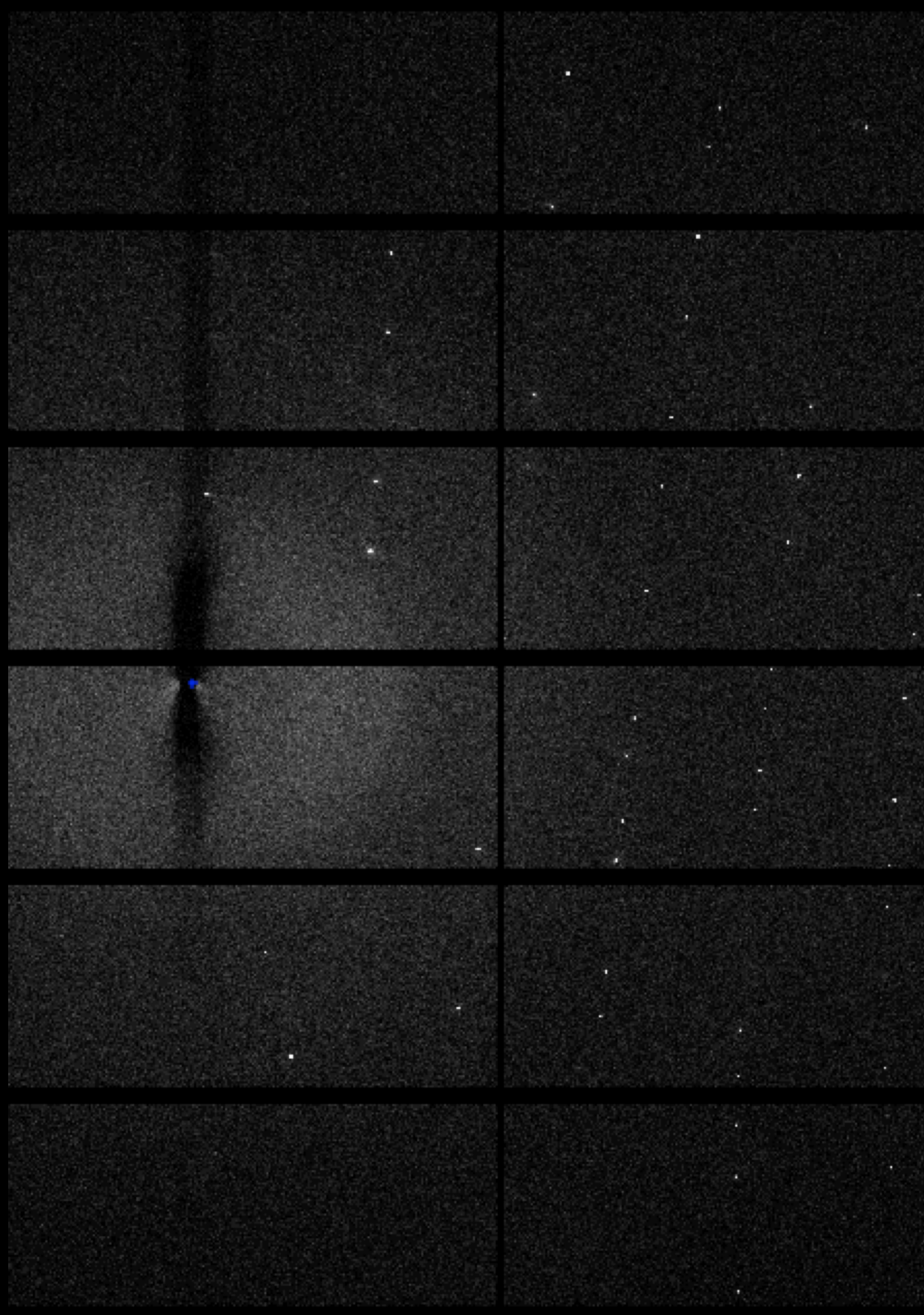
DIAMOND
I19-1





CHEMICAL CRYSTALLOGRAPHY

- “Small molecule” crystallography
- Highly absorbing samples
- High energy data collection => DQE important
- More complex experimental geometry



centre — gw56@cs03r-sc-serv-16:/dls/mx-scratch/gw56/ccp4_2016/xia2-lic-...

```
Command line: xia2 small_molecule=true /Users/graeme/data/i19-1/l-cyst
-------------------- Spotfinding SWEEP1 --------------------
3418 spots found on 1800 images (max 78 / bin)
                      *                          *
           *   *  *  *   *   *                   *    *
  *  * *  *   *  * **   * * *  *  ** *   *** ** * *     *  *
  *  *** ************** ** *** ******** ******** ****    ** *
**** ********************** ************************************
**************************************************************
**************************************************************
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**************************************************************
1                            image                          1800
-------------------- Spotfinding SWEEP2 --------------------
3705 spots found on 1700 images (max 78 / bin)
                                    *  *
*    *               * * ***    *  * **   * ** *  *         *
* * *****  **** **  * ***** ** *  * ** *** ** **** ***   ***
**************** ** ************************ ******************
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:
```

centre — gw56@cs03r-sc-serv-16:/dls/mx-scratch/gw56/ccp4_2016/xia2-lic-...

```
IMAGES (USER) 1 to 1700
MTZ file: /Users/graeme/Projects/centre/DEFAULT/NATIVE/SWEEP4/integrate/dials_in
tegrated.mtz
For AUTOMATIC/DEFAULT/NATIVE
```

	Overall	Low	High
High resolution limit	0.59	1.58	0.59
Low resolution limit	6.01	6.01	0.60
Completeness	96.9	100.0	48.0
Multiplicity	7.5	11.6	1.3
I/sigma	28.4	59.8	6.1
Rmerge(I)	0.034	0.027	0.077
Rmerge(I+/-)	0.032	0.027	0.068
Rmeas(I)	0.035	0.028	0.101
Rmeas(I+/-)	0.035	0.028	0.097
Rpim(I)	0.011	0.008	0.064
Rpim(I+/-)	0.014	0.010	0.068
CC half	1.000	1.000	0.978
Anomalous completeness	91.6	100.0	0.4
Anomalous multiplicity	4.5	8.2	1.1
Anomalous correlation	-0.196	-0.364	0.000
Anomalous slope	0.854		
Total observations	11718	1229	47
Total unique	1560	106	36

```
Assuming spacegroup: P 21 21 21
:
```

USEFUL RESULTS



STATUS

- DIALS now used routinely at Diamond Light Source for automated data processing *via* xia2 - will be in CCP4 7.0
- xia2 is the "friendly" DIALS user interface for synchrotron data, and is bundled with DIALS
- Tools developed using DIALS framework for image inspection, strategy evaluation on I19, detector metrology, …

ACKNOWLEDGEMENTS

- Gwyndaf Evans, David Waterman, James Parkhurst, Luis Fuentes-Montero, Richard Gildea, Markus Gerstel, Alun Ashton

- Andrew Leslie, Harry Powell, Phil Evans, Garib Murshudov

- Nick Sauter, Aaron Brewster, Nat Echols, Ian Rees, Nigel Moriarty, Ralf Grosse-Kunstleve, …

- Software users & Diamond scientists

HTTP://DIALS.DIAMOND.AC.UK

CURRENTLY: 2 POSITIONS

AVAILABLE @ DIALS EAST