SUPPLEMENTARY MATERIALS
xia2: An Expert System for MX Data Reduction

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(Received 0 XXXXXXX 0000; accepted 0 XXXXXXX 0000)

1. Example XIA2 Information File and Output

This is the example xia2 input file used for the TB0541B example described above, which specifies the correct beam centre and image ranges to use for the two wavelengths. The names specified here will be used set the project, crystal and dataset names in the resulting MTZ files, as well as defining the directory hierarchy for the processing.

```
BEGIN PROJECT TB0541B
BEGIN CRYSTAL X12287

BEGIN WAVELENGTH INFL
WAVELENGTH 0.979660
END WAVELENGTH INFL

BEGIN WAVELENGTH LREM
WAVELENGTH 1.000000
END WAVELENGTH LREM

BEGIN SWEEP SWEEP1
WAVELENGTH INFL
DIRECTORY /Volumes/data/jcsg/12287
IMAGE 12287_1_E1_001.img
START_END 1 60
EPOCH 1096203695
BEAM 108.98 105.05
END SWEEP SWEEP1

BEGIN SWEEP SWEEP2
```

```
WAVELENGTH LREM
DIRECTORY /Volumes/data/jcsg/12287
IMAGE 12287_1_E2_001.img
START_END 1 60
EPOCH 1096203943
BEAM 109.00 105.07
END SWEEP SWEEP2

END CRYSTAL X12287
END PROJECT TB0541B
```

The corresponding program output, where the results of the intermediate steps in processing (autoindexing and integration) are summarised with the merging statistics for publication. The list of programs used in the analysis and corresponding references is then given, along with links to the reflection files.

For further detail, the final log files from the key steps are included in the LogFiles directory for off-line inspection.

```
Environment configuration...
XIA2_ROOT => /home/gw56/CVS/xia2
XIA2CORE_ROOT => /home/gw56/CVS/xia2core
CCP4 => /scratch/xtal/ccp4/ccp4-6.1.1
CLIBD => /scratch/xtal/ccp4/ccp4-6.1.1/lib/data
BINSORT_SCR => /tmp/tmppNIYC2
Host: ws050
XIA2 0.3.0.6
------------------- Autoindexing SWEEP1 --------------------
All possible indexing solutions:
tP  51.80  51.80 158.18  90.00  90.00  90.00
oC  73.23  73.34 158.18  90.00  90.00  90.00
oP  51.79  51.84 158.18  90.00  90.00  90.00
mC  73.34  73.23 158.19  90.00  89.95  90.00
mP  51.80 158.18  51.86  90.00  89.91  90.00
aP  51.81  51.86 158.20  89.95  89.98  89.91
Indexing solution:
tP  51.80  51.80 158.18  90.00  90.00  90.00
Sweep epoch: 1096203695
-------------------- Integrating SWEEP1 --------------------
Processed batches 1 to 60
Integration status per image:
ooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooo
"o" => ok          "%" => iffy rmsd "!" => bad rmsd
"O" => overloaded  "#" => many bad  "." => blank
Need to rerun the integration...
-------------------- Integrating SWEEP1 --------------------
Processed batches 1 to 60
Integration status per image:
ooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooo
"o" => ok          "%" => iffy rmsd "!" => bad rmsd
"O" => overloaded  "#" => many bad  "." => blank
```

```
Stored integration parameters for crystal X12287
------------------- Autoindexing SWEEP2 --------------------
All possible indexing solutions:
tP  51.84  51.84 158.23  90.00  90.00  90.00
oC  73.22  73.51 158.27  90.00  90.00  90.00
oP  51.82  51.89 158.24  90.00  90.00  90.00
mC  73.51  73.22 158.28  90.00  89.93  90.00
mP  51.85 158.28  51.94  90.00  89.77  90.00
aP  51.86  51.95 158.28  89.93  89.97  89.77
Indexing solution:
tP  51.84  51.84 158.23  90.00  90.00  90.00
Using integration parameters for crystal X12287
Sweep epoch: 1096203943
-------------------- Integrating SWEEP2 --------------------
Processed batches 1 to 60
Integration status per image:
oooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooooo
"o" => ok          "%" => iffy rmsd "!" => bad rmsd
"O" => overloaded  "#" => many bad  "." => blank
---------------------- Preparing X12287 ----------------------
Likely spacegroups:
P 41 21 2
P 43 21 2
Reindexing to first spacegroup setting: P 41 21 2 (h,k,l)
---------------------- Scaling X12287 ----------------------
Resolution limit for INFL:  1.64
Resolution limit for LREM:  1.64
Optimised SD corrections (A, B) found to be:
Full:       0.03   12.0
Partial:    0.02   12.0
Computed average unit cell (will use in all files)
51.65  51.65 157.70  90.00  90.00  90.00
Overall twinning score: 2.13
Your data do not appear to be twinned

Inter-wavelength B and R-factor analysis:
INFL   0.0 0.00 (ok)
LREM   0.0 0.08 (ok)

Project: TB0541B
Crystal: X12287
Sequence:
Wavelength name: INFL
Wavelength 0.97966
Sweeps:
SWEEP SWEEP1 [WAVELENGTH INFL]
TEMPLATE 12287_1_E1_###.img
DIRECTORY /scratch/gw56/data/jcsg/als1/8.2.1/20040926/collection/TB0541B/12287
DETECTOR adsc
EXPOSURE TIME 5.100000
PHI WIDTH 1.00
IMAGES (USER) 1 to 60
MTZ file: /scratch/gw56/paper/12287/2d/X12287/INFL/SWEEP1/integrate/12287_1_E1__001.mtz
Wavelength name: LREM
Wavelength 1.00000
Sweeps:
```

```
SWEEP SWEEP2 [WAVELENGTH LREM]
TEMPLATE 12287_1_E2_###.img
DIRECTORY /scratch/gw56/data/jcsg/als1/8.2.1/20040926/collection/TB0541B/12287
DETECTOR adsc
EXPOSURE TIME 5.100000
PHI WIDTH 1.00
IMAGES (USER) 1 to 60
MTZ file: /scratch/gw56/paper/12287/2d/X12287/LREM/SWEEP2/integrate/12287_1_E2__001.mtz
For TB0541B/X12287/LREM
High resolution limit                    1.64 7.33 1.64
Low resolution limit                     52.57 52.57 1.68
Completeness                             95.7 98.2 71.8
Multiplicity                             4.2 3.3 2.6
I/sigma                                  13.9 27.2 2.2
Rmerge                                   0.053 0.032 0.354
Rmeas(I)                                 0.067 0.04 0.528
Rmeas(I+/-)                              0.069 0.041 0.489
Rpim(I)                                  0.032 0.021 0.31
Rpim(I+/-)                               0.043 0.026 0.336
Wilson B factor                          18.959
Partial bias                             0.005 -0.028 0.009
Anomalous completeness                   94.3 98.9 67.7
Anomalous multiplicity                   2.3 2.2 1.4
Anomalous correlation                    -0.234 -0.524 -0.021
Anomalous slope                          0.869 0.0 0.0
Total observations                       108108.0 1247.0 3576.0
Total unique                             25995.0 375.0 1383.0

For TB0541B/X12287/INFL
High resolution limit                    1.64 7.33 1.64
Low resolution limit                     52.57 52.57 1.68
Completeness                             97.4 98.0 79.8
Multiplicity                             4.2 3.3 2.8
I/sigma                                  12.8 24.9 2.1
Rmerge                                   0.057 0.031 0.38
Rmeas(I)                                 0.097 0.068 0.582
Rmeas(I+/-)                              0.073 0.041 0.513
Rpim(I)                                  0.045 0.035 0.328
Rpim(I+/-)                               0.046 0.026 0.342
Wilson B factor                          19.244
Partial bias                             -0.007 -0.04 0.011
Anomalous completeness                   96.2 99.4 74.0
Anomalous multiplicity                   2.3 2.2 1.5
Anomalous correlation                    0.654 0.823 0.119
Anomalous slope                          1.558 0.0 0.0
Total observations                       111923.0 1248.0 4218.0
Total unique                             26437.0 374.0 1526.0

Assuming spacegroup: P 41 21 2
Other likely alternatives are:
P 43 21 2
Unit cell:
51.649  51.649 157.697
90.000  90.000  90.000
mtz format:
Scaled reflections: /scratch/gw56/paper/12287/2d/X12287/scale/TB0541B_X12287_free.mtz
```

```
sca format:
Scaled reflections (INFL): /scratch/gw56/paper/12287/2d/X12287/scale/TB0541B_X12287_scaled_INFL.sca
Scaled reflections (LREM): /scratch/gw56/paper/12287/2d/X12287/scale/TB0541B_X12287_scaled_LREM.sca
sca_unmerged format:
Scaled reflections (INFL): /scratch/gw56/paper/12287/2d/X12287/scale/TB0541B_X12287_unmerged_INFL.sca
Scaled reflections (LREM): /scratch/gw56/paper/12287/2d/X12287/scale/TB0541B_X12287_unmerged_LREM.sca
Processing took 00h 16m 48s
XIA2 used...  ccp4 distl labelit mosflm pointless scala
Here are the appropriate citations (BIBTeX in xia-citations.bib.)
(1994) Acta Cryst. D 50, 760--763
Evans, P.R. (1997) Proceedings of CCP4 Study Weekend
Evans, Philip (2006) Acta Cryst. D62, 72--82
Leslie, AGW (1992) Joint CCP4 and ESFEACMB Newsletter on Protein Crystallography 26
Leslie, Andrew G. W. (2006) Acta Cryst. D62, 48--57
Sauter, Nicholas K., Grosse-Kunstleve, Ralf W. and Adams, Paul D. (2004) J. Appl. Cryst. 37, 399--409
Zhang, Z., Sauter, N.K., van den Bedem, H., Snell, G. and Deacon, A.M. (2006) J. Appl. Cryst 39, 112--119
Status: normal termination
```