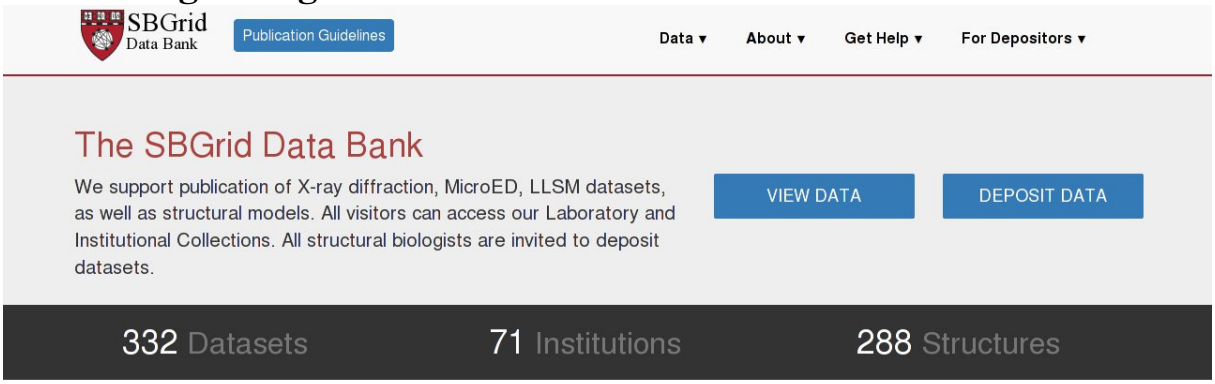
SBDG sbgrid.org



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Facts

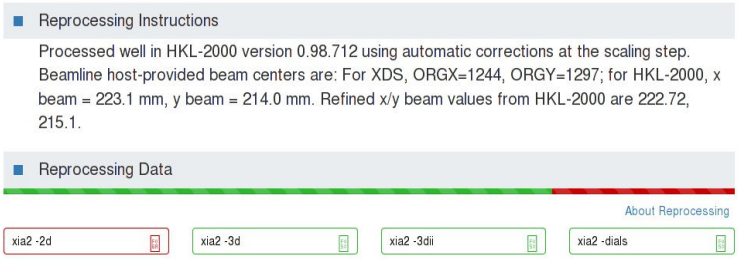
The SBGrid Data Bank has been established in close collaboration between SBGrid and the Dataverse Project. Supported by the Leona M. and Harry B. Helmsley Charitable Trust the joint initiative combines long-standing expertise in data preservation with dedication to providing revolutionary solutions for the scientific community.

Project Team

Piotr Sliz, PhD ***Tale***
Mercè Crosas, PhD
Pete Meyer, PhD
Stephanie Socias
Bill McKinney, JD MLS
Jason Key, PhD
Philip Durbin
Michelle Ottaviano

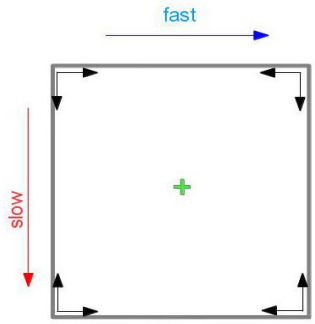
419

5L2E	2016	resolution 4 Å	HKL2000



Beamline: 23-ID-D APS Argonne
Detector: Pilatus 6M
Format: cbf
Header: minicbf

Expert knowledge: spindle axis horizontal
center detector=(1231,1263) pixels
offset of 6 mm in vertical direction



=> Processing with Dirax/EVAL: **succesful**

N.B. Beam offset and directions choosen correctly

```
###CBF: VERSION 1.5, CBFlib v0.7.8 - PILATUS detectors

data_A1_8_00001

_array_data.header_convention "PILATUS_1.2"
_array_data.header_contents
;
# Detector: PILATUS3 6M, S/N 60-0122
# 2016-04-19T00:33:47.179
# Pixel_size 172e-6 m x 172e-6 m
# Silicon sensor, thickness 0.001000 m
# Exposure_time 0.1990400 s
# Exposure_period 0.2000000 s
# Tau = 0 s
# Count_cutoff 1930685 counts
# Threshold_setting: 6000 eV
# Gain_setting: autog (vrf = 1.000)
# N_excluded_pixels = 623
# Excluded_pixels: badpixel_mask.tif
# Flat_field: FF_p60-0122_E11999_T6000_vrf_m0p100.tif
# Trim_file: p60-0122_E11999_T6000.bin
# Image_path: /ramdisk/mnt/beegfs/eozkan/23IDD_2016_04_18/A1/
# Comment: run 8
# Ratecorr_lut_directory: ContinuousStandard_v1.1
# Retrigger_mode: 1
# Wavelength 1.03320 A
# Detector_distance 0.70000 m
# Beam_xy (1243.00, 1298.00) pixels
# Start_angle 42.0000 deg.
# Angle_increment 0.2000 deg.
# Detector_2theta -0.0002 deg.
# Shutter_time 0.2000000 s
;


_array_data.data
;
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
    conversions="x-CBF_BYTE_OFFSET"
Content-Transfer-Encoding: BINARY
X-Binary-Size: 6224257
X-Binary-ID: 1
X-Binary-Element-Type: "signed 32-bit integer"
X-Binary-Element-Byte-Order: LITTLE_ENDIAN
Content-MD5: vbASdqa0niwEiiCPZJae0A==
X-Binary-Number-of-Elements: 6224001
X-Binary-Size-Fastest-Dimension: 2463
X-Binary-Size-Second-Dimension: 2527
X-Binary-Size-Padding: 4095
```

373

5K70	2013	Resolution 2.70 Å	iMOSFLM

Reprocessing Instructions

none

Reprocessing Data

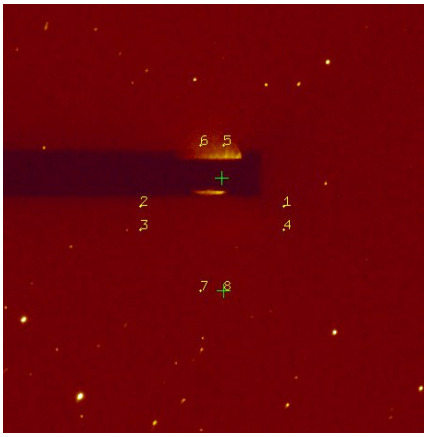
About Reprocessing

xia2 -2d | xia2 -3d | xia2 -3dii | xia2 -dials

	cell						distance	Rmerge
xia2-3dii (xds)	110.4	116.3	125.9	76.8	68.5	63.8	397.7	0.87
xia2-dials	110.9	111.6	111.6	61.2	72.2	72.2	390.8	1.06
literature	**110.8**	**113.4**	**185.9**	**90**	**103.7**	**90**		0.10
Dirax	110	111	111	60	72	72		P1
	192	112	110	90	110	90	395.5	C2 0.09
	110.8	112.7	186.6	90	103.9	90		I2

Beamline: 24-ID-E APS Argonne
Detector: ADSC (Quantum-315)
Format: img
Header: ADSC

Expert knowledge: spindle axis horizontal



1) beam manually picked

==>Processing with Dirax/EVAL: successful

ALIGNDETID adsc916
! Displacements in mm
DETZEROX 0.092003
DETZEROY 1.03755
DETZEROZ 4.378124
! Rotations in degrees
DETROTX -0.021253
DETROTY 0.274627
DETROTZ 0.022829

HEADER_BYTES= 1024;
DIM=2;
BYTE_ORDER=little_endian;
TYPE=unsigned_short;
SIZE1=1024;
SIZE2=1024;
PIXEL_SIZE=0.10259;
BIN=2x2;
ADC=slow;
DETECTOR_SN=916;
COLLECT_MODE=RUN;
BEAMLINE=24_ID_E;
DATE=Fri Jul 19 12:00:19 2013;
TIME=1.00;
DISTANCE=395.600;
OSC_RANGE=1.000;
SWEEPS=1;
PHI=0.000;
OSC_START=0.000;
TWOTHETA=0.000;
TWOTHETADIST=395.60;
AXIS=phi;
WAVELENGTH=0.97913;
BEAM_CENTER_X=156.335;
BEAM_CENTER_Y=165.501;
TRANSMISSION=18.387;
PUCK=A;
SAMPLE=2;
RING_CUR=93.9;
RING_MODE=0+324x1;
MD2_APERTURE=50;
MD2_PRG_EXP=1.000000;
MD2_NET_EXP=000;
CREV=0;
CCD=TH7899;
BIN_TYPE=HW;
ACC_TIME=1885;
UNIF_PED=1500;
SIZE1=1024;
SIZE2=1024;
IMAGE_PEDESTAL=40;
CCD_IMAGE_SATURATION=65535;
SIZE1=3072;
SIZE2=3072;
CCD_IMAGE_SATURATION=65535;

254

5EO9	2013	Resolution 2.3 Å	HKL2000

Reprocessing Instructions

HKL2000 beam center parameters should be x beam, y beam = 216.76, 212.26. XDS beam center parameters are in the header.

Reprocessing Data

About Reprocessing

xia2 -2d | xia2 -3d | xia2 -3dii | xia2 -dials

	cell						spgr	Rmerge
xia2-dials	49.5	54.9	130.8	90.0	90.0	89.9	P1	0.046
literature	**49.3**	**54.7**	**130.3**	**90**	**90.0**	**90**	$P2_12_12_1$	0.082
Dirax/EVAL	49.5	54.5	130.0	90	90	90		0.087

Beamline: 11-1 SSRL SLAC
Detector: Pilatus 6M
Format: cbf
Header: minicbf

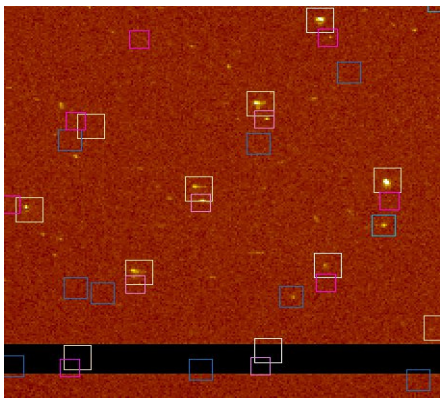
Expert knowledge: badpixels -1 and 0
Expert knowledge: rotation-axis phi, horizontal

Beam_xy is center of detector => Beam center not given

Dirax finds:
cell 49.5 55.1 128.2 92.7 90.0 91.9 <= inaccurate.
less than 50% of peaks fit

Peakref refines beam offset to: (0.24,0.60) mm

Dirax finds two additional matrices: rotated over 10° and 19°, and still only 50% of the reflections are indexed=> fragmented crystal



Only 3% overlap. Integration OK, though radiation damage.

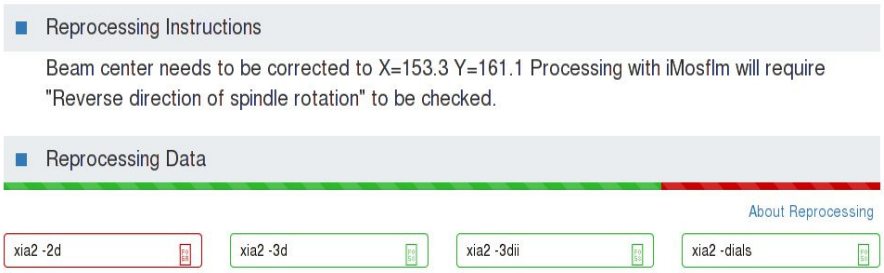
```
###CBF: VERSION 1.5, CBFlib v0.7.8 - PILATUS detectors

data_1368912431_00000

_array_data.header_convention "PILATUS_1.2"
_array_data.header_contents
;
# Detector: PILATUS 6M, S/N 60-0113,
# 2013-05-18T14:27:14.027
# Pixel_size 172e-6 m x 172e-6 m
# Silicon sensor, thickness 0.000320 m
# Exposure_time 1.5093928 s
# Exposure_period 1.5116928 s
# Tau = 199.1e-09 s
# Count_cutoff 1233917 counts
# Threshold_setting: 5300 eV
# Gain_setting: mid gain (vrf = -0.200)
# N_excluded_pixels = 454
# Excluded_pixels: badpix_mask.tif
# Flat_field: (nil)
# Trim_file: p6m0113_E10600_T5300_vrf_m0p20.bin
# Image_path: /home/det/p2_det/images/
# Wavelength 0.97945 A
# Detector_distance 0.55019 m
# Beam_xy (1231.50, 1263.50) pixels
# Start_angle 0.0000 deg.
# Angle_increment 0.2000 deg.
# Phi 0.0000 deg.
;

_array_data.data
;
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
    conversions="x-CBF_BYTE_OFFSET"
Content-Transfer-Encoding: BINARY
X-Binary-Size: 6224483
X-Binary-ID: 1
X-Binary-Element-Type: "signed 32-bit integer"
X-Binary-Element-Byte-Order: LITTLE_ENDIAN
Content-MD5: ntjYdWN4Ahuc2sm47R62AA==
X-Binary-Number-of-Elements: 6224001
X-Binary-Size-Fastest-Dimension: 2463
X-Binary-Size-Second-Dimension: 2527
X-Binary-Size-Padding: 4095
```

5TP3	2015	resolution 1.87 Å	iMOSFLM



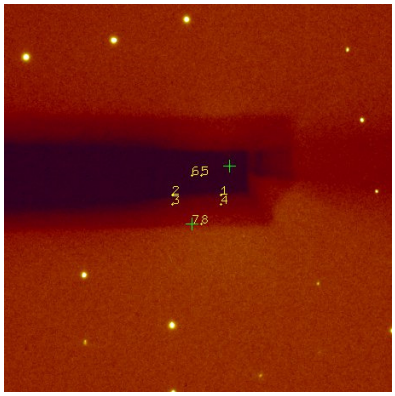
Beamline: 19-ID APS Argonne
Detector: ADSC Quantum-315
Format: img
Header: ADSC + extended 19-ID

Expert knowledge: spindle axis horizontal

At first: Dirax found no solution

center detector=(1536,1536) pixels

BEAM_CENTER=(1541.5,1564.5)



1) rotation direction had to be reversed
2) beam center manually picked

==>Processing with Dirax/EVAL: succesful

HEADER_BYTES= 6656;
DIM=2;
BYTE_ORDER=big_endian;
TYPE=unsigned_short;
BIN=2x2;
BIN_TYPE=HW;
PIXEL_SIZE=0.102400;
DETECTOR_SN=458;
DATE=Thu Nov 5 21:36:34 2015;
BYTE_ORDER=little_endian;
CREV=1;
CCD=TH7899;
BIN_TYPE=HW;
ACC_TIME=1641;
UNIF_PED=1500;
IMAGE_PEDESTAL=40;
SCAN_IMAGES=360;
ADC=fast;
TIME= 1.00;
DISTANCE=274.39;
OSC_RANGE= 0.50;
PHI=-90.00;
OSC_START=-90.00;
AXIS=phi;
WAVELENGTH= 0.9792909;
BEAM_CENTER_X=157.800;
BEAM_CENTER_Y=160.200;
LOGNAME=user19id;
SCAN_SEQ_INFO=1 1 1;
WAVELENGTH= 0.9792909;
SCAN_WAVELENGTH= 0.9792909;
SCAN_TEMPLATE=/net/data/idgup/user19id/McLellanLab/Collect/Nb4Alone_X2/Nb4_X2.????;
CRYSTAL_GONIO_VALUES=0.000 0.000 0.000;
SOURCE_WAVELENGTH=1.0000 0.97929092640;
SCAN_ROTATION=-90.000 90.000 0.500 1.000 0.0 0.0 0.0 100.0 0.0 0.0;
ROTATION=-90.000 -89.500 0.500 1.000 0.0 0.0 0.0 100.0 0.0 0.0;
ROTATION_START=-90.00;
ROTATION_END=-89.50;
SCAN_INCREMENT= 0.50;
SCAN_EXPOSURE_TIME= 1.00;
FILENAME=/net/data/idgup/user19id/McLellanLab/Collect/Nb4Alone_X2/Nb4_X2.0001;
SOURCE_INTENSITY=0.025639;
BEAMLINE_NAME=ID19_;
.
.
.
SIZE1=3072;
SIZE2=3072;
CCD_IMAGE_SATURATION=65535;

ID19_SCAN_EXPOSURE_MODE=ScanOpen;
ID19_SCAN_EXPOSURE_TIME=1.000;
ID19_SCAN_RELZERO_OMEGA=0.000;
ID19_SCAN_AXIS=Omega;
ID19_SCAN_START=-90.000;
ID19_SCAN_INCREMENT= 0.50;
ID19_SCAN_IMAGES=360;
ID19_ROTATION_SERIAL_NUM=1;
ID19_ROTATION_START=-90.00;
ID19_ROTATION_END=-89.50;
.
.
DETECTOR_NAMES=ADSC914_;
ADSC914_DETECTOR_SIZE=315.16 315.16;
ADSC914_DETECTOR_VECTORS=1 0 0 0 1 0;
ADSC914_NONUNF_INFO=$(FirstScanImage);
ADSC914_NONUNF_TYPE=None;
ADSC914_SPATIAL_DISTORTION_TYPE=Simple_spatial;
ADSC914_SPATIAL_DISTORTION_VECTORS=-1 0 0 -1;
ADSC914_DETECTOR_DESCRIPTION=ADSC Quantum 315 at SBC 19ID;
ADSC914_GONIO_DESCRIPTION=A simple detector goniostat;
ADSC914_GONIO_NAMES=RotZ RotX/Swing RotY TransX TransY TransZ/Dist;
ADSC914_GONIO_NUM_VALUES=6;
ADSC914_GONIO_UNITS=deg deg deg mm mm mm;
ADSC914_GONIO_VECTORS=0 0 1 1 0 0 0 1 0 1 0 0 0 1 0 0 0 -1;
ROTATION_AXIS_NAME=Omega;
ROTATION_VECTOR=-1.0 0.0 0.0;
SOURCE_CROSSFIRE=0.0002 0.0002 0.0 0.0;
SOURCE_POLARZ=0.99 0 1 0;
SOURCE_SIZE=0.0 0.0 0.0 0.0;
SOURCE_SPECTRAL_DISPERSION=0.0002 0.0002;
SOURCE_VECTORS=0.0 0.0 1.0 1 0 0 0 1 0;
ADSC914_DETECTOR_REFINE_FLAGS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
SOURCE_REFINE_FLAGS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
ADSC914_GONIO_VALUES=0.000 0.00 0.000 0.000 0.01 274.39;
ADSC914_DETECTOR_DIMENSIONS=3072 3072;
ADSC914_SPATIAL_DISTORTION_INFO=1563.2 1562.3 0.10259 0.10259;
ADSC914_SPATIAL_BEAM_POSITION=1563.2 1562.3;

415

5ELI	2012	Resolution 3.3 Å	HKL2000

Reprocessing Instructions

Used HKL2000

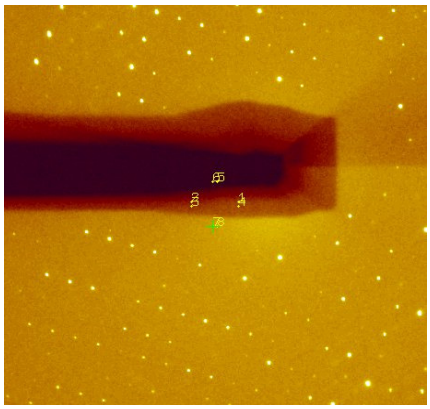
Reprocessing Data

About Reprocessing

xia2 -2d | xia2 -3d | xia2 -3dii | xia2 -dials

	cell						distance	Rmerge
xia2-3d (xds)	124.2	125.9	180.8	89.7	89.9	61.8	240.3	0.03
xia2-3dii (xds)	125.6	125.6	183.4	90.0	90.0	120.0	250.3	0.13
xia2-dials	129.4	221.4	186.6	90	90	90	255.2	0.99
literature	125.7	125.7	183.6	90.0	90.0	120.0		
Dirax/EVAL	125.6	125.6	183.5	90.0	90.0	120.0	250.1	0.11

Beamline: 19-ID APS Argonne
Detector: ADSC Quantum-315
Format: img
Header: ADSC + extended 19-ID



BEAM_CENTER=(1538.2,1561.6)

1) rotation direction had to be reversed
2) beam center manually picked

==>Processing with Dirax/EVAL: succesful

HEADER_BYTES= 6144;
DIM=2;
BYTE_ORDER=big_endian;
TYPE=unsigned_short;
BIN=2x2;
BIN_TYPE=HW;
PIXEL_SIZE=0.102588;
DETECTOR_SN=914;
DATE=Sun Jul 1 21:57:19 2012;
BYTE_ORDER=little_endian;
CREV=1;
CCD=TH7899;
BIN_TYPE=HW;
ACC_TIME=8922;
UNIF_PED=1500;
IMAGE_PEDESTAL=40;
SCAN_IMAGES=120;
ADC=fast;
TIME=7.000;
DISTANCE=249.9430;
OSC_RANGE=1.000;
PHI=-90.000;
OSC_START=-90.000;
AXIS=phi;
WAVELENGTH= 0.9792611;
BEAM_CENTER_X=157.800; <== (same as 426 in 2015)
BEAM_CENTER_Y=160.200;
LOGNAME=user16id;
SCAN_SEQ_INFO=1 1 1;
WAVELENGTH= 0.9792611;
SCAN_WAVELENGTH= 0.9792611;
SCAN_TEMPLATE=/net/data/idgup/user16id/tjb_trem2_9.????;
CRYSTAL_GONIO_VALUES=-90.000 -0.000 -0.018;
.
.
BEAMLINE_NAME=ID19_;
.
.
DETECTOR_NAMES=ADSC914_;
ADSC914_DETECTOR_SIZE=315.16 315.16;
.
.
ADSC914_SPATIAL_BEAM_POSITION=1563.2 1562.3;
SIZE1=3072;
SIZE2=3072;
CCD_IMAGE_SATURATION=65535;

441

4JDK	2012	Resolution 2.4 Å	HKL2000

Reprocessing Instructions

none

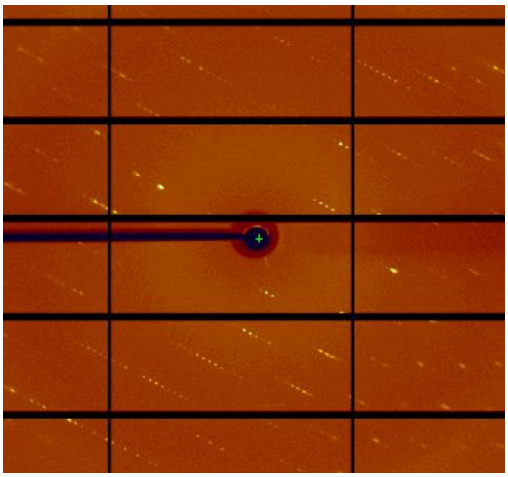
Reprocessing Data

About Reprocessing

xia2 -2d | xia2 -3d | xia2 -3dii | xia2 -dials

Beamline: NLSL X25
Detector: Pilatus 6M
Format: cbf
Header: minicbf

Detector in Literature, SBgrid and PDB: **ADSC Q315**



Detector position asymetric: beam_xy OK

==>Processing with Dirax/EVAL: straightforward

```
###CBF: VERSION 1.5, CBFlib v0.7.8 - PILATUS detectors

data_BHH-63P15_3_00001

_array_data.header_convention "PILATUS_1.2"
_array_data.header_contents
;
# Detector: PILATUS 6M, S/N 60-0107, BNL
# 2012-03-29T22:49:53.410
# Pixel_size 172e-6 m x 172e-6 m
# Silicon sensor, thickness 0.000320 m
# Exposure_time 1.9976000 s
# Exposure_period 2.0000000 s
# Tau = 199.1e-09 s
# Count_cutoff 1179367 counts
# Threshold_setting: 6000 eV
# Gain_setting: mid gain (vrf = -0.200)
# N_excluded_pixels = 300
# Excluded_pixels: badpix_mask.tif
# Flat_field: (nil)
# Trim_file: p6m0107_E12000_T6000_vrf_m0p20.bin
# Image_path: /img12/data1/pxuser/boggon/px11-0139/BHH-63P15/3/
# Wavelength 1.10000 A
# Energy_range (0, 0) eV
# Detector_distance 0.40000 m
# Detector_Voffset 0.00000 m
# Beam_xy (1285.00, 1305.00) pixels
# Flux 0.0000
# Filter_transmission 0.0000
# Start_angle 0.0000 deg.
# Angle_increment 1.0000 deg.
# Detector_2theta 0.0000 deg.
# Polarization 0.000    ????
# Alpha 0.0000 deg.
# Kappa 0.0000 deg.
# Phi 0.0000 deg.
# Chi 0.0000 deg.
# Oscillation_axis X, CW    ????
# N_oscillations 135777226
;
_array_data.data
;
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
    conversions="x-CBF_BYTE_OFFSET"
Content-Transfer-Encoding: BINARY
X-Binary-Size: 6225851
X-Binary-ID: 1
X-Binary-Element-Type: "signed 32-bit integer"
X-Binary-Element-Byte-Order: LITTLE_ENDIAN
Content-MD5: uzOY25tctuB2Z8ICUcSjrg==
X-Binary-Number-of-Elements: 6224001
X-Binary-Size-Fastest-Dimension: 2463
X-Binary-Size-Second-Dimension: 2527
X-Binary-Size-Padding: 4095
```

405

5DT6	2014	Resolution 1.6 Å	HKL2000

Reprocessing Instructions

Detector MAR 300 CCD, x beam 150.011, y beam 144.093, distance 200.18, wavelength 1.00000

Reprocessing Data

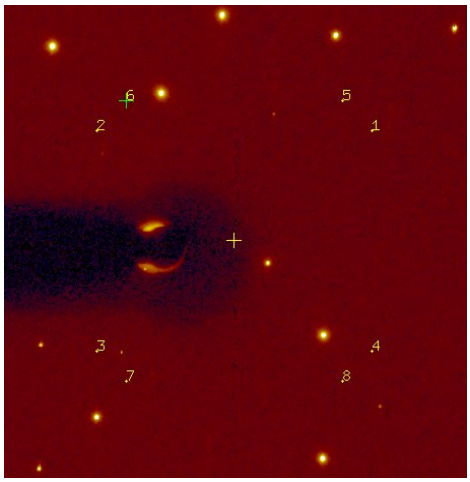
About Reprocessing

xia2 -2d | xia2 -3d | xia2 -3dii | xia2 -dials

Beamline: APS ID22
Detector: Mar CCD
Format: mccd
Header: binary

Problems with reprocessing:
1) Binary header?
2) omega-scan?
3) beam center?

Expert knowledge: binary header info
Expert knowledge: horizontal rotation axis



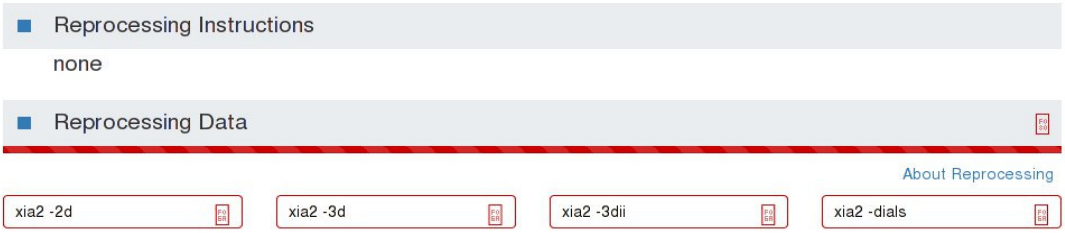
only after manual picking of beam position:
==>Processing with Dirax/EVAL: straightforward

Rmerge=0.073 to resolution 1.54 Å

header_type 2
header_byte_order 1234
header_block 4096 bytes
==>
ImhNx=4096 ImhNy=4096 ImhNOverflow=0 ImhNBytes=8192
ImhCircular=false
ImhDxStart=0.0 **Beamx=1941.8 Beamy=1912.3** ImhBeamInPixels=on
ImhIntegrationtime=1.62 ImhExposuretime=1.0 ImhReadOut=1
twotheta (1) 0.0 0.0 omega (2) 25.0 26.0 chi (3) 180.0 180.0 kappa (4)
0.0 0.0 phi (5) 0.0 0.0 delta (6) 0.0 0.0 gamma (7) 0.0 0.0 dx (8)
200.0 200.0 rotationaxis 2 rotationrange 1.0 DetRotX 0.0 DetRotY 0.0
DetRotZ 0.0
ImhDxStart=0. **Set to 200.0**
ImhThetaStart=0.0 ImhPhiStart=0.0 ImhOmegaStart=25.0
ImhChiStart=180.0 **ImhOmegaRange=1.0**
ImhPixelXSize 73.242 ImhPixelYSize 73.242 ImhAdded 10
ImhAlpha1 1.0
ImhDetectorId=marccd7 ImhDetGain=2.0
.
.

6

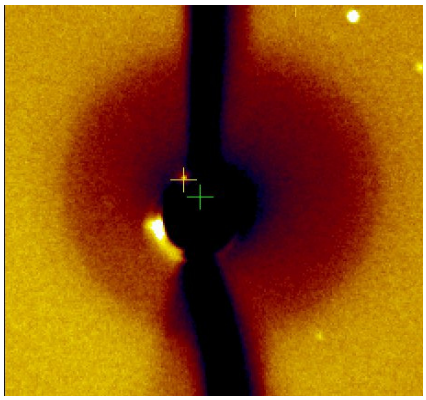
1YVJ	2004	Resolution 2.55 Å	DENZO



Beamline: in house Rigaku RU-300
Detector: Mar345 imageplate
Format: mar2300
Header: binary

Beam_xy not given
Spindle axis not given

Expert knowledge/guess:
datatype=u16
orientation spindle axis (euler)
axis=3
Rotation direction: -1.0
Beam_xy => center of detector



Manual tweeking to find the correct beam and detector position

==>Processing with Dirax/EVAL: succesful

==>
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GoniostatType=euler GoniostatId=mar IntegrationTime=-9999.9
nx=2300 ny=2300 Binned=no Theta=0.0 Omega=0.0 Chi=0.0 Phi=15.0
Interval=1.0 **Dx=200.0** RadiationType=XRAY
PixelXsize=150.0 PixelYsize=150.0 Detgain=1.0 DataType=u16
Alpha=1.54179 Polarisation=SYNCHROTRON BeamHor=0.0
BeamVer=0.0 Circular Swing=0.0
Dist=200.0 Axis=3 RotAxis=Phi **StartPos=0.0 0.0 15.0** EndPos=0.0 0.0 16.0 MeanPos=0.0 0.0 15.5 Goniostat=0.0 0.0 0.0
RotStart=15.0 **RotInc=1.0** RotEnd=16.0 RotValue=15.5
OverflowLevel=131070 DoSwapHeader=off DoSwapData=on No AdcZero correction
fast=right slow=down

383

5HV4	2014	Resolution 2.35 Å	XDS

Reprocessing Instructions

This dataset was indexed in C2221 and processed with XDS at 2.35 A resolution.

Reprocessing Data

About Reprocessing

xia2 -2d | xia2 -3d | xia2 -3dii | xia2 -dials

Beamline: 4.2.2 ALS
Detector: CMOS_8M RDI
Format: img
Header: ADSC

Assumed: Euler goniostat with χ=90º

Beam_center: OK

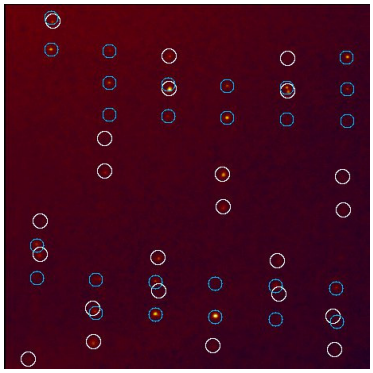
manually set: phi-range = 0.2

Monoclinic:
42.6 75.2 76.5 90 106.2 90

C-centered orthorhombic
42.6 146.4 75.2 90 90 90

Dirax finds two matrices

Problems with reprocessing:
1) offset of omega-axis (~1°)
2) twin 177.6° rotation around
(0,1,-2) in orthorhombic lattice



23% deconvoluted
15% overlapping

Re-analysis in progress

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SIZE2=2820;
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DATE=Sun Mar 02 2014 18:06:53.191944;
ZEROOFFSET=1;
COMPRESSION=None;
DTDISPLAY_ORIENTATION=+X+Y;
DETECTOR_NUMBER=1;
DETECTOR_NAMES=RDI1_;
RDI1_DETECTOR_DESCRIPTION=CMOS-1 MBC Detector;
RDI1_DETECTOR_DIMENSIONS=2952 2820;
RDI1_DETECTOR_SIZE=295.50 282.28;
RDI1_DETECTOR_VECTORS= -1 0 0 0 -1 0;
RDI1_GONIO_DESCRIPTION=Larry Rock detector support;
RDI1_GONIO_NAMES=RotZ RotX/Swing RotY TransX TransY TransZ/Dist;
RDI1_GONIO_NUM_VALUES=6;
RDI1_GONIO_UNITS=deg deg deg mm mm mm;
RDI1_GONIO_VECTORS=0.0 0.0 1.0 -1.0 0.0 0.0 0.0 1.0 0.0 1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 -1.0 ;
RDI1_NONUNF_TYPE=None;
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RDI1_TITLE=CMOS1 MBC Data Collection;
CRYSTAL_DESCRIPTION=unknown;
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CRYSTAL_GONIO_NAMES=Omega Kappa Phi;
CRYSTAL_GONIO_NUM_VALUES=3;
CRYSTAL_GONIO_UNITS=deg deg deg;
CRYSTAL_GONIO_VECTORS= 1.0 0.0 0.0 -0.5000000 0.8660254 0.0000000 -1.0 0.0 0.0;
CRYSTAL_MOSAICITY=0.5000 0.0000 0.0000;
ROTATION_AXIS_NAME=Omega;
ROTATION_LIMITS=-120.000 120.000 1000.000;
ROTATION_VECTOR= 1.000 0.000 0.000;
SATURATED_VALUE=14000;
SCAN_TITLE=start end inc time nOsc nDark nDup nDlim NDC nDCup;
SCAN_ROTATION_AXIS_NAME=Omega;
SCAN_ROTATION_LIMITS=-120.000 120.000 360.000;
SCAN_ROTATION_VECTOR= 1.000 0.000 0.000;

SCAN_SEQ_INFO= 1 1 1;SOURCE_CROSSFIRE=0.0002 0.0002 0.0000 0.0000;
SOURCE_POLARZ=0.9900 0.0000 1.0000 0.0000;
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SOURCE_VECTORS=0.000 0.000 1.000 0.000 1.000 0.000 1.000 0.000 0.000;
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AXIS=omega;
PIXEL_SIZE=0.1001;
CCD_IMAGE_SATURATION=14000;
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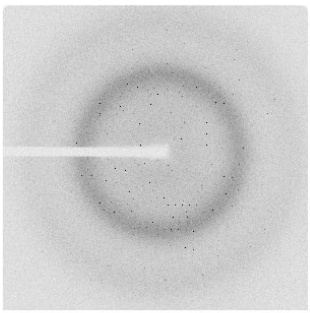
SCAN_TEMPLATE=D:/data/iowa2/030214/4-2-bap/4-2-bap_????.img;
OMEGA=0.000000;
BEAM_CENTER_X=1468.000000;
BEAM_CENTER_Y=1409.000000;
WAVELENGTH=1.000060;
ENERGY=12397.679535;
OMEGA_DELTA=0.200000;
NUMBER_OF_FRAMES=900;
DISTANCE=300.000000;
ZERO_OFFSET=20.000000;
INTENSITY=50;
EXPOSE=0.500000;
SCAN_ROTATION= 0.00 0.20 0.20 1.000 1.000 1.000 1.000 1.000 1.000 300.00;
ROTATION= 0.00 0.20 0.20 1.000 1.000 1.000 1.000 1.000 1.000 300.00;
SPATIAL_BEAM_POSITION=1468.0 1409.0;
SOURCE_WAVELENGTH=1.000 1.000;
RDI1_GONIO_VALUES=0.000 0.000 0.000 0.000 0.000 300;

IRRMC Integrated Resource for Reproducibility in Macrmolecular Crystallography

National Institutes of Health
Office of the Director
Data Science at NIH

Integrated Resource for Reproducibility in Macromolecular Crystallography

This project is being funded by the Targeted Software Development award 1 U01 HG008424-01 as part of the BD2K (Big Data to Knowledge) program of the National Institute of Health. The project is developing tools for "wrangling" data from protein diffraction experiments. We are also creating a growing repository of diffraction experiments used to determine protein structures in the PDB, contributed by the CSGID, SSGCID, JCSG, MCSG, SGC, and other large-scale projects, as well as individual research laboratories.



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research papers

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A public database of macromolecular diffraction experiments

Marek Grabowski,[a]‡ Karol M. Langner,[a]‡§ Marcin Cymborowski,[a] Przemyslaw J. Porebski,[a,b] Piotr Sroka,[a] Heping Zheng,[a] David R. Cooper,[a] Matthew D. Zimmerman,[a] Marc-André Elsliger,[c] Stephen K. Burley[d,e] and Wladek Minor[a]*

[a]Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, VA 22904, USA, [b]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Niezapominajek 8, 30-239 Cracow, Poland, [c]Department of Integrative Structural and Computational Biology, The Scripps Research Institute, La Jolla, CA 90237, USA, [d]RCSB Protein Data Bank; Center for Integrative Proteomics Research; Institute for Quantitative Biomedicine; Rutgers Cancer Institute of New Jersey; Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA, and [e]San Diego Supercomputer Center and Skaggs School of Pharmacological Sciences, University of California, San Diego, La Jolla, CA 92093, USA. *Correspondence e-mail: wladek@iwonka.med.virginia.edu

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‡ The first two authors contributed equally.
§ Present address: Google Inc., Mountain View, CA 94043, USA.

Keywords: diffraction experiment; protein crystallography; repository; data; metadata; IRRMC.

The low reproducibility of published experimental results in many scientific disciplines has recently garnered negative attention in scientific journals and the general media. Public transparency, including the availability of 'raw' experimental data, will help to address growing concerns regarding scientific integrity. Macromolecular X-ray crystallography has led the way in requiring the public dissemination of atomic coordinates and a wealth of experimental data, making the field one of the most reproducible in the biological sciences. However, there remains no mandate for public disclosure of the original diffraction data. The Integrated Resource for Reproducibility in Macromolecular Crystallography (IRRMC) has been developed to archive raw data from

BJP1_3m8t

3M8T	2008	Resolution 1.33 Å	MOSFLM

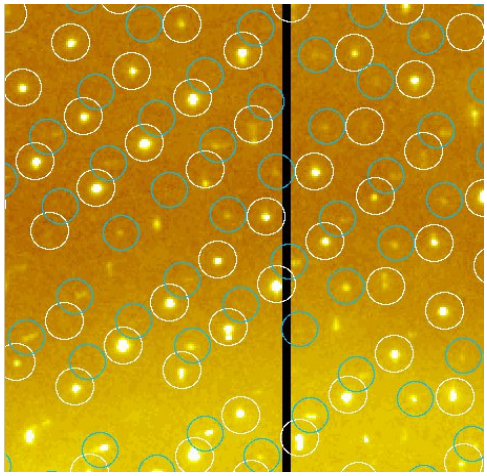
Beamline: ESRF ID14-1
Detector: ADSC Quantum 210
Format: img
Header: ADSC

Expert knowledge: spindle axis horizontal phi

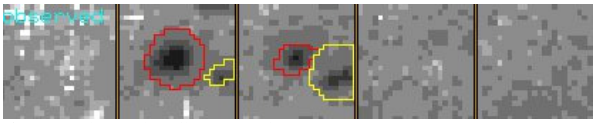
Beam_center: OK

Dirax finds cell: 47.2 45.2 77.4 100.9 89.8 118.1
apparent C-centering: 79.7 42.7 77.4 90 102.3 90
but symmetry not present

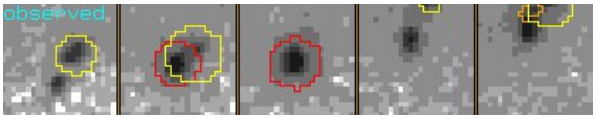
second fragment visible at frame 100



Second fragment:



5% overlap with first matrix



=> Processing with Dirax/EVAL: straightforward

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BYTE_ORDER=little_endian;
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PIXEL_SIZE=0.1024;
BIN=2x2;
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DETECTOR_SN=444;
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OSC_START=0.000;
TWOTHETA=0.000;
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WAVELENGTH=0.9340;
BEAM_CENTER_X=105.026;
BEAM_CENTER_Y=105.091;
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CCD=TH7899;
BIN_TYPE=HW;
ACC_TIME=2235;
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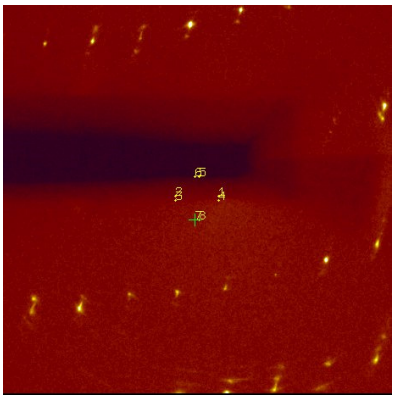
IMAGE_PEDESTAL=20;
SIZE1=2048;
SIZE2=2048;
CCD_IMAGE_SATURATION=65535;

IDP90557_4i08

4I08	2011	Resolution 2.06 Å	HKL3000

Beamline: ID-19 APS
Detector: ADSC Quantum 315
Format: img
Header: ADSC

Expert knowledge: spindle axis phi horizontal



1) rotation direction had to be reversed
2) beam center manually picked

==>Processing with Dirax/EVAL: straightforward

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BIN_TYPE=HW;
PIXEL_SIZE=0.102588;
DETECTOR_SN=914;
DATE=Sat Mar 19 00:57:39 2011;
BYTE_ORDER=little_endian;
CREV=1;
CCD=TH7899;
BIN_TYPE=HW;
ACC_TIME=1828;
UNIF_PED=1500;
IMAGE_PEDESTAL=40;
SCAN_IMAGES=200;
ADC=fast;
TIME=1.000;
DISTANCE=310.0029;
OSC_RANGE=0.500;
PHI=33.500;
OSC_START=33.500;
AXIS=phi;
WAVELENGTH= 0.9791830;
BEAM_CENTER_X=157.800; <= again!
BEAM_CENTER_Y=160.200;
LOGNAME=user20id;
SCAN_SEQ_INFO=1 1 1;
WAVELENGTH= 0.9791830;
SCAN_WAVELENGTH= 0.9791830;
SCAN_TEMPLATE=/net/data/idgup/user20id/UVA/IDP90557_J-2-1/IDP90557_J-2-1_1_????.img;
CRYSTAL_GONIO_VALUES=-65.000 -0.000 -0.018;
SOURCE_WAVELENGTH=1.0000 0.97918296484;
SCAN_ROTATION=-65.000 35.000 0.500 1.000 0.0 0.0 0.0 100.0 0.0 0.0;
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FILENAME=/net/data/idgup/user20id/UVA/IDP90557_J-2-1/IDP90557_J-2-1_1_0198;
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ID19_SCAN_EXPOSURE_TIME=1.000;
ID19_SCAN_RELZERO_OMEGA=0.000;
ID19_SCAN_AXIS=Omega;
ID19_SCAN_START=-65.000;
.
.
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ADSC914_GONIO_DESCRIPTION=A simple;

Detector goniostat
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ADSC914_GONIO_VECTORS=0 0 1 1 0 0 0 1 0 1 0 0 0 1 0 0 0 -1;
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ROTATION_VECTOR=-1.0 0.0 0.0;
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SOURCE_POLARZ=0.99 0 1 0;
SOURCE_SIZE=0.0 0.0 0.0 0.0;
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SOURCE_VECTORS=0.0 0.0 1.0 1 0 0 0 1 0;
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SOURCE_REFINE_FLAGS=0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0;
ADSC914_GONIO_VALUES=0.000 -0.000829 0.000 0.000 0.000633 310.003000;
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ADSC914_SPATIAL_BEAM_POSITION=1563.2 1562.3;
SIZE1=3072;
SIZE2=3072;
CCD_IMAGE_SATURATION=65535;

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The 8 most recent public experiments

The crystal structure of a homodimeric Pseudomonas glyoxalase I enzyme reveals asymmetric metallation commensurate with half-of-sites activity

5th November 2015 2 720

Rohan Bythell-Douglas, Charles Bond

Download data as .tar

The Zn inactive class of glyoxalase I (Glo1) enzymes are metalloenzymes that are typically homodimeric with two metal-dependent active sites. While the two active sites share identical amino acid composition, this class of enzyme is optimally active with only one metal per homodimer. We have determined the X-ray crystal structure of GloA2, one of the Zn inactive Glo1 enzymes from Pseudomonas aeruginosa. The presented structures exhibit an unprecedented metal-binding arrangement consistent with half-of-sites activity: one active site contains a single activating Ni2+ ion while the other contains two inactivating Zn2+ ions. Students from UWA CHEM3007 Undergraduate Unit helped with some of the data collection.

The most recent datasets in this experiment

Raw data for D3_2

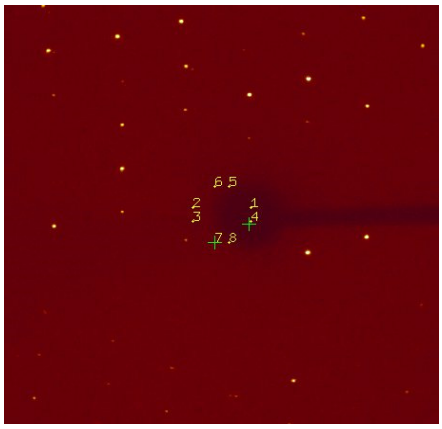
Raw data for D3_1

4mts

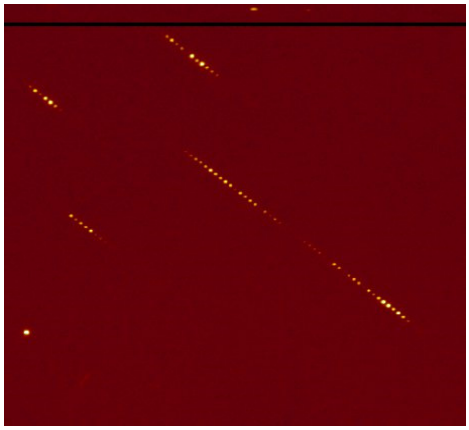
4mts	2015	Resolution 1.8 Å	MOSFLM or XDS

Beamline: MX2 Australian Synchrotron
Detector: ADSC Quantum 315
Format: img
Header: ADSC

1) rotation direction had to be reversed
2) beam center manually picked (or number 4)



Fine tuning peak search because of long axis
cell 50.5 50.5 326.4 90 90 120



==>Processing with Dirax/EVAL: straightforward

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DISTANCE=220.000090;
PHI=0.000000;
OSC_START=0.000000;
OSC_RANGE=0.500000;
WAVELENGTH=0.953696;
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BEAM_CENTER_Y=160.705172;
ACC_TIME=1890;
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