XDS.INP input file for data collected on Rigaku FR-X with EIGER 4M

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! Example file XDS.INP for the EIGER 4M pixel detector, IGBMC CBI
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! Last edit: Alastair McEwen, 2017/07/06
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!============================ JOB CONTROL PARAMETERS
============================!
JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT
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 MAXIMUM_NUMBER_OF_PROCESSORS=4

!====================== GEOMETRICAL PARAMETERS
==================================!
 ORGX=1010.21  ORGY=831.47        !Detector origin (pixels)
 DETECTOR_DISTANCE= 61            !(mm) (range = 61 - 280)
 OSCILLATION_RANGE=0.25           !degrees (>0)
 X-RAY_WAVELENGTH=1.54178         !Angstroem (do not change)
 STARTING_ANGLE=-68               !degrees

!======================= CRYSTAL PARAMETERS
=====================================!
 SPACE_GROUP_NUMBER=0   !0 for unknown crystals; cell constants are ignored.
 UNIT_CELL_CONSTANTS= 77.7 77.7 77.7 90 90 90
!REIDX=   0  0 -1  0  0 -1  0  0 -1  0  0  0
 FRIEDEL'S_LAW=FALSE !Default is TRUE

!=================== SELECTION OF DATA IMAGES
==================================!
 NAME_TEMPLATE_OF_DATA_FRAMES=path-to/Image_????.img
 STARTING_FRAME=101      !Number of first image
 DATA_RANGE=1 720        !Numbers of first and last data image collected
!BACKGROUND_RANGE=1  40  !rather use defaults (first 5 degrees of rotation)
 SPOT_RANGE=1 360        !First and last data image number for finding spots
!REFERENCE_DATA_SET=./XDS_ASCII.HKL

!================ PARAMETERS CONTROLLING REFINEMENTS
============================!
 REFINE(IDXREF)=CELL BEAM ORIENTATION AXIS !DISTANCE POSITION
 REFINE(INTEGRATE)=DISTANCE POSITION BEAM ORIENTATION ! AXIS CELL
!REFINE(CORRECT)=CELL BEAM ORIENTATION AXIS DISTANCE POSITION !Default is:
refine everything
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!======================== DETECTOR AND GENERATOR PARAMETERS
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 DETECTOR=EIGER
 MINIMUM_VALID_PIXEL_VALUE=0  OVERLOAD=2147483647
 SENSOR_THICKNESS=0.45
 NX=2070 NY=2167 QX=0.075 QY=0.075
 DIRECTION_OF_DETECTOR_X-AXIS=0.927184 0 0.374607 !cos(2theta) 0 sin(2theta)
 DIRECTION_OF_DETECTOR_Y-AXIS=0.0 1.0 0.0
 ROTATION_AXIS=0 -1 0
 INCIDENT_BEAM_DIRECTION=0.0 0.0 1.0
 POLARIZATION_PLANE_NORMAL=1 0 0
 FRACTION_OF_POLARIZATION=0.50 !default=0.5 for unpolarized beam
 TRUSTED_REGION=0.0 1.2 ! partially use corners of detector (0 1.4143: use
all pixels)

 UNTRUSTED_RECTANGLE= 1030 1041    0 2168
 UNTRUSTED_RECTANGLE=    0 2071  514  552
 UNTRUSTED_RECTANGLE=    0 2071 1065 1103
 UNTRUSTED_RECTANGLE=    0 2071 1616 1654

!====================== INDEXING PARAMETERS
====================================!
 STRONG_PIXEL=4           ! COLSPOT: only use strong reflections (default is
3)
 MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=3 ! default of 6 is sometimes too high

!============== DECISION CONSTANTS FOR FINDING CRYSTAL SYMMETRY
==================!
!Decision constants for detection of lattice symmetry (IDXREF, CORRECT)
 MAX_CELL_AXIS_ERROR=0.03 ! Maximum relative error in cell axes tolerated
 MAX_CELL_ANGLE_ERROR=2.0 ! Maximum cell angle error tolerated

!Decision constants for detection of space group symmetry (CORRECT).
!Resolution range for accepting reflections for space group determination in
!the CORRECT step. It should cover a sufficient number of strong
reflections.
 TEST_RESOLUTION_RANGE=8.0 4.5
 MIN_RFL_Rmeas= 50 ! Minimum #reflections needed for calculation of Rmeas
 MAX_FAC_Rmeas=2.0 ! Sets an upper limit for acceptable Rmeas

!================== CRITERIA FOR ACCEPTING REFLECTIONS
==========================!
 VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 6000. 30000. !Used by DEFPIX
                   !for excluding shaded parts of the detector.

 INCLUDE_RESOLUTION_RANGE=50.0 1.5 !Angstroem; used by
DEFPIX,INTEGRATE,CORRECT

!used by CORRECT to exclude ice-reflections
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!EXCLUDE_RESOLUTION_RANGE= 3.93 3.87 !ice-ring at 3.897 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 3.70 3.64 !ice-ring at 3.669 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 3.47 3.41 !ice-ring at 3.441 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 2.70 2.64 !ice-ring at 2.671 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 2.28 2.22 !ice-ring at 2.249 Angstrom
!EXCLUDE_RESOLUTION_RANGE= 2.102 2.042 !ice-ring at 2.072 Angstrom - strong
!EXCLUDE_RESOLUTION_RANGE= 1.978 1.918 !ice-ring at 1.948 Angstrom - weak
!EXCLUDE_RESOLUTION_RANGE= 1.948 1.888 !ice-ring at 1.918 Angstrom - strong
!EXCLUDE_RESOLUTION_RANGE= 1.913 1.853 !ice-ring at 1.883 Angstrom - weak
!EXCLUDE_RESOLUTION_RANGE= 1.751 1.691 !ice-ring at 1.721 Angstrom - weak

!============== INTEGRATION AND PEAK PROFILE PARAMETERS
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 NUMBER_OF_PROFILE_GRID_POINTS_ALONG_ALPHA/BETA=13!used by: INTEGRATE
!NUMBER_OF_PROFILE_GRID_POINTS_ALONG_GAMMA= 9     !used by: INTEGRATE
```