

```
!*****
! File XDS.INP containing named arguments for running XDS (arbitrary order).
! For further explanations of the meaning of these parameters see xds.man.
! Characters in a line to the right of an exclamation mark are comment.
!*****
```

```
DETECTOR=ADSC MINIMUM_VALID_PIXEL_VALUE=1 OVERLOAD=65000
DIRECTION_OF_DETECTOR_X-AXIS= 1.0 0.0 0.0
DIRECTION_OF_DETECTOR_Y-AXIS= 0.0 1.0 0.0
ROFF=0.0 TOFF=0.0!Radial & tangential offset for spiral read-out scanners
```

```
MAXIMUM_NUMBER_OF_PROCESSORS=16!<25;ignored by single cpu version of xds
```

```
!===== JOB CONTROL PARAMETERS =====
```

```
! JOB= ALL !XYCORR INIT COLSPOT IDXREF DEFPIX XPLAN INTEGRATE CORRECT
JOB= XYCORR INIT COLSPOT IDXREF
! JOB= IDXREF
! JOB= DEFPIX
! JOB= CORRECT
```

```
!===== GEOMETRICAL PARAMETERS =====
```

```
NX=3072 NY=3072 QX=0.102592 QY=0.102592 !ADSC Q315 version
ORGX=1539.81 ORGY=1534.30 !Detector origin (pixels).
DETECTOR_DISTANCE=141.025000 !Distance of detector from crystal (mm)
```

```
ROTATION_AXIS= -1.0 0.0 0.0
OSCILLATION_RANGE=1.000000 !degrees (>0)
```

```
X-RAY_WAVELENGTH=0.979263 !Angstroem
INCIDENT_BEAM_DIRECTION=0.0 0.0 1.0
FRACTION_OF_POLARIZATION=0.95 !default=0.5 for unpolarized beam
POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0
AIR=0.001 !Air absorption coefficient of x-rays
```

```
!===== CRYSTAL PARAMETERS =====
```

```
!If you do not know the space group, you may comment out the next two lines
! SPACE_GROUP_NUMBER=0 !0 for unknown crystals; cell constants are ignored.
! UNIT_CELL_CONSTANTS= 0 0 0 0 0 0
!Optional reindexing transformation to apply reflection indices
! REIDX= 0 0 -1 0 0 -1 0 0 -1 0 0 0
```

```
!===== DATA COLLECTION STRATEGY (XPLAN) =====
```

```
! !!! Warning !!!
! If you processed your data for a crystal with unknown cell constants and
! space group symmetry, XPLAN will report the results for space group P1.
!FRIEDEL'S_LAW=FALSE !Default is TRUE.
```

```
!===== SELECTION OF DATA IMAGES =====
```

```
!Generic file name, access, and format of data images
NAME_TEMPLATE_OF_DATA_FRAMES=../img/prefix_1_?????.img
DATA_RANGE=1 180 !Numbers of first and last data image collected
```

```
BACKGROUND_RANGE=1 5 !Numbers of first and last data image for background
```

```
SPOT_RANGE=1 10 !First and last data image number for finding spots
SPOT_RANGE=91 100 !First and last data image number for finding spots
!Up to 20 SPOT_RANGE= parameters can be specified
```

```
!===== INDEXING PARAMETERS =====
```

```
!Never forget to check this, since the default 0 0 0 is almost always correct!
INDEX_ORIGIN= 0 0 0 ! used by IDXREF to add an index offset
```

```
!===== CRITERIA FOR ACCEPTING REFLECTIONS =====
```

```
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 7000 30000 !Used by DEFPIX
!for excluding shaded parts of the detector.
```

```
TRUSTED_REGION= 0.0 1.41
```

```
INCLUDE_RESOLUTION_RANGE=50.0 0.0 !Angstroem; used by DEFPIX,INTEGRATE,CORRECT
```

```
!used by CORRECT to exclude ice-reflections
```

```
!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
```

```
!===== INTEGRATION AND PEAK PROFILE PARAMETERS =====
```

```
!Parameters that are refined during the INTEGRATE step.
```

!Refinement is turned off if none of the keywords is supplied.

REFINE( INTEGRATE)=DISTANCE BEAM ORIENTATION CELL !AXIS

DELPHI= 5.000000 !controls the number of reference profiles and scaling factors

\*\*\*\*\*

Most important things to know about XDS.INP (the rest can be found in the documentation, where the exhaustive list of input parameters are described, if needed)

Everything written after a ! is comment, i.e. not taken into account

#### Highlighted in cyan:

Input parameters describing the experimental setup. In principle, they do not require editing, since they should reflect the actual setup.

#### Highlighted in yellow:

Input parameters defining the use of the different detector regions. In principle, no editing is required.

#### Highlighted in green:

Parameters to be possibly edited. See comments for each input parameters for more informations.