

5.6. *CBFlib*: AN ANSI C LIBRARY FOR MANIPULATING IMAGE DATA

```

###CBF: VERSION 1.1

data_image_1

# category DIFFRN
loop_
_diffrn.id
_diffrn.crystal_id
DIFFRN_ID DIFFRN_CRYSTAL_ID

# category DIFFRN_SOURCE
loop_
_diffrn_source.diffrn_id
_diffrn_source.source
_diffrn_source.current
_diffrn_source.type
DIFFRN_ID synchrotron 100.0 'SSRL beamline 1-5'

# category DIFFRN_DETECTOR_ELEMENT
loop_
_diffrn_detector_element.id
_diffrn_detector_element.detector_id
ELEMENT1 ADSCQ4

# category DIFFRN_RADIATION
loop_
_diffrn_radiation.diffrn_id
_diffrn_radiation.wavelength_id
_diffrn_radiation.probe
_diffrn_radiation.monochromator
_diffrn_radiation.polarizn_source_ratio
_diffrn_radiation.polarizn_source_norm
_diffrn_radiation.div_x_source
_diffrn_radiation.div_y_source
_diffrn_radiation.div_x_y_source
_diffrn_radiation.collimation
DIFFRN_ID WAVELENGTH1 x-ray 'Si 111' 0.8 0.0 0.08
0.01 0.00 '0.20 mm x 0.20 mm'

# category DIFFRN_RADIATION_WAVELENGTH
loop_
_diffrn_radiation_wavelength.id
_diffrn_radiation_wavelength.wavelength
_diffrn_radiation_wavelength.wt
WAVELENGTH1 0.98 1.0

# category DIFFRN_DETECTOR
loop_
_diffrn_detector.diffrn_id
_diffrn_detector.id
_diffrn_detector.type
_diffrn_detector.details
_diffrn_detector.number_of_axes
DIFFRN_ID ADSCQ4 'ADSC QUANTUM4' 'slow mode' 4

# category DIFFRN_DETECTOR_AXIS
loop_
_diffrn_detector_axis.detector_id
_diffrn_detector_axis.axis_id
ADSCQ4 DETECTOR_X
ADSCQ4 DETECTOR_Y
ADSCQ4 DETECTOR_Z
ADSCQ4 DETECTOR_PITCH

# category DIFFRN_DATA_FRAME
loop_
_diffrn_data_frame.id
_diffrn_data_frame.detector_element_id
_diffrn_data_frame.array_id
_diffrn_data_frame.binary_id
FRAME1 ELEMENT1 ARRAY1 1

```

Fig. 5.6.4.1. Template imgCIF for use with an ADSC Quantum 4 detector.

```

# category DIFFRN_MEASUREMENT
loop_
_diffrn_measurement.diffrn_id
_diffrn_measurement.id
_diffrn_measurement.number_of_axes
_diffrn_measurement.method
_diffrn_measurement.details
DIFFRN_ID GONIOMETER 3 rotation
; i0=1.000 i1=1.000 i2=1.000 ib=1.000 beamstop=20 mm
0% attenuation
;

# category DIFFRN_MEASUREMENT_AXIS
loop_
_diffrn_measurement_axis.measurement_id
_diffrn_measurement_axis.axis_id
GONIOMETER GONIOMETER_PHI
GONIOMETER GONIOMETER_KAPPA
GONIOMETER GONIOMETER_OMEGA

# category DIFFRN_SCAN
loop_
_diffrn_scan.id
_diffrn_scan.frame_id_start
_diffrn_scan.frame_id_end
_diffrn_scan.frames
SCAN1 FRAME1 FRAME1 1

# category DIFFRN_SCAN_AXIS
loop_
_diffrn_scan_axis.scan_id
_diffrn_scan_axis.axis_id
_diffrn_scan_axis.angle_start
_diffrn_scan_axis.angle_range
_diffrn_scan_axis.angle_increment
_diffrn_scan_axis.displacement_start
_diffrn_scan_axis.displacement_range
_diffrn_scan_axis.displacement_increment
SCAN1 GONIOMETER_OMEGA 0.0 0.0 0.0 0.0 0.0 0.0
SCAN1 GONIOMETER_KAPPA 0.0 0.0 0.0 0.0 0.0 0.0
SCAN1 GONIOMETER_PHI 0.0 0.0 0.0 0.0 0.0 0.0
SCAN1 DETECTOR_Z 0.0 0.0 0.0 0.0 0.0 0.0
SCAN1 DETECTOR_Y 0.0 0.0 0.0 0.0 0.0 0.0
SCAN1 DETECTOR_X 0.0 0.0 0.0 0.0 0.0 0.0
SCAN1 DETECTOR_PITCH 0.0 0.0 0.0 0.0 0.0 0.0

# category DIFFRN_SCAN_FRAME
loop_
_diffrn_scan_frame.frame_id
_diffrn_scan_frame.frame_number
_diffrn_scan_frame.integration_time
_diffrn_scan_frame.scan_id
_diffrn_scan_frame.date
FRAME1 1 0.0 SCAN1 1997-12-04T10:23:48

# category DIFFRN_SCAN_FRAME_AXIS
loop_
_diffrn_scan_frame_axis.frame_id
_diffrn_scan_frame_axis.axis_id
_diffrn_scan_frame_axis.angle
_diffrn_scan_frame_axis.displacement
FRAME1 GONIOMETER_OMEGA 0.0 0.0
FRAME1 GONIOMETER_KAPPA 0.0 0.0
FRAME1 GONIOMETER_PHI 0.0 0.0
FRAME1 DETECTOR_Z 0.0 0.0
FRAME1 DETECTOR_Y 0.0 0.0
FRAME1 DETECTOR_X 0.0 0.0
FRAME1 DETECTOR_PITCH 0.0 0.0

```

Fig. 5.6.4.1. (cont.)

5. APPLICATIONS

```
# category AXIS
loop_
_axis.id
_axis.type
_axis.equipment
_axis.depends_on
_axis.vector[1] _axis.vector[2] _axis.vector[3]
_axis.offset[1] _axis.offset[2] _axis.offset[3]
GONIOMETER_OMEGA rotation goniometer
. 1 0 0 . . .
GONIOMETER_KAPPA rotation goniometer
GONIOMETER_OMEGA 0.64279 0 0.76604 . . .
GONIOMETER_PHI rotation goniometer
GONIOMETER_KAPPA 1 0 0 . . .
SOURCE general source . 0 0 1 . . .
GRAVITY general gravity . 0 -1 0 . . .
DETECTOR_Z translation detector
. 0 0 -1 0 0 0
DETECTOR_Y translation detector
DETECTOR_Z 0 1 0 0 0 0
DETECTOR_X translation detector
DETECTOR_Y 1 0 0 0 0 0
DETECTOR_PITCH rotation detector
DETECTOR_X 0 1 0 0 0 0
ELEMENT_X translation detector
DETECTOR_PITCH 1 0 0 -94.0032 94.0032 0
ELEMENT_Y translation detector
ELEMENT_X 0 1 0 0 0 0

# category ARRAY_STRUCTURE_LIST
loop_
_array_structure_list.array_id
_array_structure_list.index
_array_structure_list.dimension
_array_structure_list.precedence
_array_structure_list.direction
_array_structure_list.axis_set_id
ARRAY1 1 2304 1 increasing ELEMENT_X
ARRAY1 2 2304 2 increasing ELEMENT_Y

# category ARRAY_STRUCTURE_LIST_AXIS
loop_
_array_structure_list_axis.axis_set_id
_array_structure_list_axis.axis_id
_array_structure_list_axis.displacement
_array_structure_list_axis.displacement_increment
ELEMENT_X ELEMENT_X 0.0408 0.0816
ELEMENT_Y ELEMENT_Y -0.0408 -0.0816

# category ARRAY_INTENSITIES
loop_
_array_intensities.array_id
_array_intensities.binary_id
_array_intensities.linearity
_array_intensities.gain
_array_intensities.gain_esd
_array_intensities.overload
_array_intensities.undefined_value
ARRAY1 1 linear 0.23 0.03 65000 0

# category ARRAY_STRUCTURE
loop_
_array_structure.id
_array_structure.encoding_type
_array_structure.compression_type
_array_structure.byte_order
ARRAY1 "signed 32-bit integer" packed little_endian
```

Fig. 5.6.4.1. (cont.)

```
# category ARRAY_DATA
loop_
_array_data.array_id
_array_data.binary_id
_array_data.data
ARRAY1 1 ?
```

Fig. 5.6.4.1. (cont.)

```
loop_
_axis.id
_axis.type
_axis.equipment
_axis.depends_on
_axis.vector[1] _axis.vector[2] _axis.vector[3]
_axis.offset[1] _axis.offset[2] _axis.offset[3]
GONIOMETER_OMEGA rotation goniometer
. 1 0 0 . . .
GONIOMETER_KAPPA rotation goniometer
GONIOMETER_OMEGA 0.64279 0 0.76604 . . .
GONIOMETER_PHI rotation goniometer
GONIOMETER_KAPPA 1 0 0 . . .
SOURCE general source
. 0 0 1 . . .
GRAVITY general gravity
. 0 -1 0 . . .
DETECTOR_Z translation detector
. 0 0 -1 0 0 0
DETECTOR_Y translation detector
DETECTOR_Z 0 1 0 0 0 0
DETECTOR_X translation detector
DETECTOR_Y 1 0 0 0 0 0
DETECTOR_PITCH rotation detector
DETECTOR_X 0 1 0 0 0 0
ELEMENT_X translation detector
DETECTOR_PITCH 1 0 0 -172.5 172.5 0
ELEMENT_Y translation detector
ELEMENT_X 0 1 0 0 0 0

loop_
_array_structure_list.array_id
_array_structure_list.index
_array_structure_list.precedence
_array_structure_list.direction
_array_structure_list.axis_set_id
ARRAY1 1 2300 1 increasing ELEMENT_X
ARRAY1 2 2300 2 increasing ELEMENT_Y

loop_
_array_structure_list_axis.axis_set_id
_array_structure_list_axis.axis_id
_array_structure_list_axis.displacement
_array_structure_list_axis.displacement_increment
ELEMENT_X ELEMENT_X 0.075 0.150
ELEMENT_Y ELEMENT_Y -0.075 -0.150

loop_
_array_intensities.array_id
_array_intensities.binary_id
_array_intensities.linearity
_array_intensities.gain
_array_intensities.gain_esd
_array_intensities.overload
_array_intensities.undefined_value
ARRAY1 1 linear 1.15 0.2 240000 0
```

Fig. 5.6.4.2. Part of the template file for a MAR345 detector. Values that differ from those in Fig. 5.6.4.1 are underlined.