

Work on imgCIF and CBFlib supported in part by the U. S. Department of Energy (DOE) under grants ER63601-1021466-0009501 and ER64212-1027708-0011962, by the U. S. National Science Foundation (NSF) under grants DBI-0610407, DBI-0315281 and EF-0312612, the U. S. National Institutes of Health (NIH) under grants 1R15GM078077 from NIGMS and 1R13RR023192 from NCRR and funding from the International Union for Crystallographyn (IUCr). The content is solely the responsibility of the authors and does not necessarily represent the official views of DOE, NSF, NIH, NIGMS, NCRR or IUCr.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

			Version History
Version	Date	By	Description
0.1	Apr. 1998	PJE	This was the first CBFlib release. It supported binary CBF files using binary strings.
<u>0.2</u>	Aug. 1998	НЈВ	This release added ascii imgCIF support using MIME-encoded binary sections, added the option of MIME headers for the binary strings was well. MIME code adapted from mpack 1.5. Added hooks needed for DDL1-style names without categories.
<u>0.3</u>	Sep. 1998	PJE	This release cleaned up the changes made for version 0.2, allowing multi-threaded use of the code, and removing dependence on the mpack package.
0.4	Nov. 1998	НЈВ	This release merged much of the message digest code into the general file reading and writing to reduce the number of passes. More consistency checking between the MIME header and the binary header was introduced. The size in the MIME header was adjusted t agree with the version 0.2 documentation.
<u>0.5</u>	Dec. 1998	PJE	This release greatly increased the speed of processing by allowing for deferred digest evaluation.
<u>0.6</u>	Jan. 1999	НЈВ	This release removed the redundant information (binary id, size, compression id) from a binary header when there is a MIME header, removed the unused repeat argument, and made the memory allocation for buffering and tables with many rows sensitive to the current memory allocation already used.
0.6.1	Feb. 2001	HP (per HJB)	This release fixed a memory leak due to misallocation by size of cbf_handle instead of cb handle_struct
0.7	Mar. 2001	PJE	This release added high-level instructions based on the imgCIF dictionary version 1.1.
<u>0.7.1</u>	Mar. 2001	PJE	The high-level functions were revised to permit future expansion to files with multiple images.
0.7.2	Apr. 2001	HJB	This release adjusted cbf_cimple.c to conform to cif_img.dic version 1.1.3
0.7.2.1	May 2001	PJE	This release corrected an if nesting error in the prior mod to cbf_cimple.c.
<u>0.7.3</u>	Oct 2002	PJE	This release modified cbf_simple.c to reorder image data on read so that the indices are always increasing in memory (this behavior was undefined previously).
<u>0.7.4</u>	Jan 2004	НЈВ	This release fixes a parse error for quoted strings, adds code to get and set character string types, and removes compiler warnings
<u>0.7.5</u>	Apr 2006	НЈВ	This release cleans up some compiler warnings, corrects a parse error on quoted strings with a leading blank as adds the new routines for support of aliases, dictionaries and real arrays, higher level routines to get and set pixel sizes, do cell computations, and to set bear centers, improves support for conversion of images, picking up more data from headers.
0.7.6	Jul 2006	нлв	This release reorganizes the kit into two pieces: CBFlib_0.7.6_Data_Files and CBFlib_ 0.7.6. An optional local copy of getopt is added. The 1.4 draft dictionary has been added. cif2cbf updated to support vcif2 validation. convert_image and cif2cbf updated to report to of error messages. convert_image updated to support tag and category aliases, default to adxv images. convert_image and img updated to support row-major images. Support added for binning. API Support added for validation, wide files and line folding. Logic changed beam center reporting. Added new routines: cbf_validate, cbf_get_bin_sizes, cbf_set_bin_
v://local	host/Users/	vava/Г	Desktop/nCBF/CBFlib_bleeding_edge/doc/CBFlib.html 08/07/07 09:2



# In order to work with CBFlib, you need:

- the source code, in the form of a "gzipped" tar, CBFlib\_0.7.8.tar.gz; and
- the test data, in the form of a "gzipped" tar CBFlib\_0.7.8\_Data\_Files.tar.gz

Uncompress both of these files, and unpack them with tar:

- gunzip < CBFlib 0.7.8.tar.gz | tar xvf -
- gunzip < CBFlib\_0.7.8\_Data\_Files.tar.gz | tar xvf -

As with prior releases, to run the test programs, you will also need Paul Ellis's sample MAR345 image, example.mar2300, and Chris Nielsen's sample ADSC Quantum 315 image, mb\_LP\_1\_001.img as sample data. In

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

3

addition there are not various insulin\_pilatus6m sample data files from E. Eikenberry at SLS. All these files will be extracted by the Makefile from CBFlib\_0.7.8\_Data\_Files. Do not download copies into the top level directory.

Thare are various sample Makefiles for common configurations. The Makefile\_LINUX and Makefile\_OSX samples are for systems with gfortran from prior to the release of gcc 4.2. For the most recent gfortran, use Makefile\_LINUX\_gcc42 ot Makfile\_OSX\_gcc42. All the Makefiles come from m4/Makefile.m4.

If necessary, adjust the definition of CC and C++ and other definitions in Makefile to point to your compilers. Set the definition of CFLAGS to an appropriate value for your C and C++ compilers, the definition of F90C to point to your Fortan-90/95 compiler, and the definitions of F90FLAGS and F90LDFLAGS to approvate values for your Fortan-90/95 compilers, and then

make all make tests

We have included <u>examples</u> of CBF/imgCIF files produced by CBFlib, the current best draft of the <u>CBF Extensions</u> <u>Dictionary</u>, and of Andy Hammersley's CBF definition, updated to become a <u>DRAFT CBF/ImgCIF DEFINITION</u>.



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html



• 2.3.68 cbf\_find\_tag, cbf\_find\_local\_tag
file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

• 2.4.46 cbf get inferred pixel size

08/07/07 09:24:51





file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### **CBFlib** Manual

Almost all of the CBFlib functions receive a value of type cbf\_handle (a CBF handle) as the first argument. Several of the high-level CBFlib functions dealing with geometry receive a value of type cbf\_goniometer (a handle for a CBF goniometer object) or cbf detector (a handle for a CBF detector object).

All functions return an integer equal to 0 for success or an error code for failure.

### 2.1.1 CBF handles

CBFlib permits a program to use multiple CBF objects simultaneously. To identify the CBF object on which a function will operate, CBFlib uses a value of type cbf\_handle.

All functions in the library except cbf\_make\_handle expect a value of type cbf\_handle as the first argument.

The function **cbf** make handle creates and initializes a new CBF handle.

The function cbf free handle destroys a handle and frees all memory associated with the corresponding CBF object.

### 2.1.2 CBF goniometer handles

To represent the goniometer used to orient a sample, CBFlib uses a value of type cbf\_goniometer.

A goniometer object is created and initialized from a CBF object using the function cbf\_construct\_goniometer.

The function cbf free goniometer destroys a goniometer handle and frees all memory associated with the corresponding object.

### 2.1.3 CBF detector handles

To represent a detector surface mounted on a positioning system, CBFlib uses a value of type cbf detector.

A goniometer object is created and initialized from a CBF object using one of the functions cbf\_construct\_detector, cbf\_construct\_reference\_detector or cbf\_require\_reference\_detector.

The function cbf\_free\_detector destroys a detector handle and frees all memory associated with the corresponding object.

### 2.1.4 Return values

All of the CBFlib functions return 0 on success and an error code on failure. The error codes are:

CBF_FORMAT	The file format is invalid	
CBF_ALLOC	Memory allocation failed	
CBF_ARGUMENT	Invalid function argument	
CBF_ASCII	The value is ASCII (not binary)	
CBF_BINARY	The value is binary (not ASCII)	
CBF_BITCOUNT	The expected number of bits does	
	not match the actual number written	
CBF_ENDOFDATA	The end of the data was reached	
	before the end of the array	
CBF_FILECLOSE	File close error	
CBF_FILEOPEN	File open error	
CBF_FILEREAD	File read error	
CBF_FILESEEK	File seek error	

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

CBF\_FILETELL CBF\_FILEWRITE CBF\_IDENTICAL CBF\_NOTFOUND CBF\_OVERFLOW

File write error A data block with the new name already exists The data block, category, column or row does not exist The number read cannot fit into the

destination argument. The destination has been set to the nearest value.

CBF\_UNDEFINED The requested number is not defined (e.g. 0/0; new for version 0.7). CBF\_NOTIMPLEMENTED The requested functionality is not yet implemented (New for version 0.7).

If more than one error has occurred, the error code is the logical OR of the individual error codes.

File tell error

2.2 Reading and writing files containing binary sections

### 2.2.1 Reading binary sections

The current version of CBFlib only decompresses a binary section from disk when requested by the program.

When a file containing one or more binary sections is read, CBFlib saves the file pointer and the position of the binary section within the file and then jumps past the binary section. When the program attempts to access the binary data, CBFlib sets the file position back to the start of the binary section and then reads the data.

### For this scheme to work:

1. The file must be a random-access file opened in binary mode (fopen (," rb")).

2. The program must not close the file. CBFlib will close the file using fclose () when it is no longer needed.

At present, this also means that a program cant read a file and then write back to the same file. This restriction will be eliminated in a future version.

When reading an imgCIF vs a CBF, the difference is detected automatically.

### 2.2.2 Writing binary sections

When a program passes CBFlib a binary value, the data is compressed to a temporary file. If the CBF object is subsequently written to a file, the data is simply copied from the temporary file to the output file.

The output file can be of any type. If the program indicates to CBFlib that the file is a random-access and readable, CBFlib will conserve disk space by closing the temporary file and using the output file as the location at which the binary value is stored.

For this option to work:

The file must be a random-access file opened in binary update mode (fopen (, "w+b")).
 The program *must not* close the file. CBFlib will close the file using fclose () when it is no longer needed.

2. The program must not close the me. CBTHD will close the me using relose () when it is no longer need

If this option is not used:

1. CBFlib will continue using the temporary file.

2. CBFlib will not close the file. This is the responsibility of the main program.

### 2.2.3 Summary of reading and writing files containing binary sections

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

0

1. Open disk files to read using the mode "rb".

If possible, open disk files to write using the mode "w+b" and tell CBFlib that it can use the file as a buffer.
 Do not close any files read by CBFlib or written by CBFlib with buffering turned on.
 Do not attempt to read from a file, then write to the same file.

2.3 Low-level function prototypes

2.3.1 cbf\_make\_handle

PROTOTYPE

#include "cbf.h"

int cbf make handle (cbf handle \*handle);

DESCRIPTION

cbf\_make\_handle creates and initializes a new internal CBF object. All other CBFlib functions operating on this object receive the CBF handle as the first argument.

ARGUMENTS

handle Pointer to a CBF handle.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.2 cbf\_free\_handle

### 2.3.2 cbf\_free\_handle

**РКОТОТУРЕ** 

#include "cbf.h"

int cbf\_free\_handle (cbf\_handle handle);

DESCRIPTION

cbf\_free\_handle destroys the CBF object specified by the handle and frees all associated memory.

ARGUMENTS

handle CBF handle to free.

RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.1 cbf make handle

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

2.3.3 cbf\_read\_file

PROTOTYPE

#include "cbf.h"

int cbf\_read\_file (cbf\_handle handle, FILE \*file, int headers); int cbf\_read\_widefile (cbf\_handle handle, FILE \*file, int headers);

### DESCRIPTION

cbf\_read\_file reads the CBF or CIF file *file* into the CBF object specified by *handle*, using the CIF 1.0 convention of 80 character lines. cbf\_read\_widefile reads the CBF or CIF file *file* into the CBF object specified by *handle*, using the CIF 1.1 convention of 2048 character lines. A warning is issued to stderr for ascii lines over the limit. No test is performed on binary sections.

Validation is performed in three ways levels: during the lexical scan, during the parse, and, if a dictionary was converted, against the value types, value enumerations, categories and parent-child relationships specified in the dictionary.

headers controls the interprestation of binary section headers of imgCIF files.

required, see MSG DIGESTNOW, below,

MSG\_ DIGEST: Instructs CBFlib to check that the digest of the binary section matches any header value. If the digests do not match, the call will return CBF\_FORMAT. This evaluation and comparison is delayed (a "lazy" evaluation) to ensure maximal processing efficiency. If an immediately evaluation is

MSG\_ DIGESTNOW:

Instructs CBFlib to check that the digest of the binary section matches any header value. If the digests do not match, the call will return CBF\_FORMAT. This evaluation and comparison is performed during initial parsing of the section to ensure timely error reporting at the expense of processing efficiency. If a more efficient delayed ("lazy") evaluation is required, see MSG\_DIGESTNOW, below.



Do not check the digest (default).

CBFlib defers reading binary sections as long as possible. In the current version of CBFlib, this means that:

1. The file must be a random-access file opened in binary mode (fopen (, "rb")).

2. The program *must not* close the file. CBFlib will close the file using fclose () when it is no longer needed These restrictions may change in a future release.

### ARGUMENTS

- handle CBF handle.
- file Pointer to a file descriptor.
- headers Controls interprestation of binary section headers.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.4 cbf write file

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

11

# 2.3.4 cbf\_write\_file PROTOTYPE

#include "cbf.h"

int cbf\_write\_file (cbf\_handle handle, FILE \*file, int readable, int ciforcbf, int headers, int encoding); int cbf\_write\_widefile (cbf\_handle handle, FILE \*file, int readable, int ciforcbf, int headers, int encoding);

DESCRIPTION

cbf\_write\_file writes the CBF object specified by *handle* into the file *file*, following CIF 1.0 conventions of 80 character lines, cbf\_write\_widefile writes the CBF object specified by *handle* into the file *file*, following CIF 1.1 conventions of 2048 character lines. A warning is issued to stderr for ascii lines over the limit, and an attempt is made to fold lines to fit. No test is performed on binary sections.

If a dictionary has been provided, aliases will be applied on output.

Unlike cbf\_read\_file, the *file* does not have to be random-access.

If the file is random-access and readable, *readable* can be set to non-0 to indicate to CBFlib that the file can be used as a buffer to conserve disk space. If the file is not random-access or not readable, *readable* must be 0.

If *readable* is non-0, CBFlib will close the file when it is no longer required, otherwise this is the responsibility of the program.

ciforcbf selects the format in which the binary sections are written:

CIF Write an imgCIF file.

CBF Write a CBF file (default).

headers selects the type of header used in CBF binary sections and selects whether message digests are generated. The value of headers can be a logical OR of any of:

MIME\_HEADERS Use MIME-type headers (default).

MIME\_NOHEADERS Use a simple ASCII headers.

MSG\_DIGEST Generate message digests for binary data validation.

MSG\_NODIGEST Do not generate message digests (default). *encoding* selects the type of encoding used for binary sections and the type of line-termination in imgCIF files. The value can be a logical OR of any of:

- ENC\_BASE64 Use BASE64 encoding (default).
- ENC\_QP Use QUOTED-PRINTABLE encoding.
- ENC\_BASE8 Use BASE8 (octal) encoding.
- ENC\_BASE10 Use BASE10 (decimal) encoding.
- ENC\_BASE16 Use BASE16 (hexadecimal) encoding.

ENC\_FORWARD For BASE8, BASE10 or BASE16 encoding, map bytes to words forward (1234) (default on little-endian machines).

- ENC\_ Map bytes to words backward (4321) (default on big-endian machines).
- BACKWARD
- ENC\_CRTERM Terminate lines with CR.
- ENC\_LFTERM Terminate lines with LF (default).

### ARGUMENTS

handle CBF handle.

 $file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html$ 

file Pointer to a file descriptor.

*readable* If non-0: this file is random-access and readable and can be used as a buffer.

- Selects the format in which the binary sections are written (CIF/CBF). ciforcbf
- Selects the type of header in CBF binary sections and message digest generation. headers
- encoding Selects the type of encoding used for binary sections and the type of line-termination in imgCIF files.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

SEE ALSO

### 2.3.3 cbf read file

### 2.3.5 cbf\_new\_datablock, cbf\_new\_saveframe

PROTOTYPE

#include "cbf.h"

int cbf new datablock (cbf handle handle, const char \*datablockname); int cbf\_new\_saveframe (cbf\_handle handle, const char \*saveframename);

### DESCRIPTION

cbf new datablock creates a new data block with name datablockname and makes it the current data block. cbf new saveframe creates a new save frame with name saveframename within the current data block and makes the new save frame the current save frame.

If a data block or save frame with this name already exists, the existing data block or save frame becomes the current data block or save frame.

### ARGUMENTS

handle CBF handle. datablockname The name of the new data block. saveframename The name of the new save frame.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.6 cbf force new datablock, cbf force new saveframe 2.3.7 cbf\_new\_category 2.3.8 cbf\_force\_new\_category 2.3.9 cbf new column 2.3.10 cbf\_new\_row 2.3.11 cbf\_insert\_row 2.3.12 cbf set datablockname, cbf\_set\_saveframename 2.3.17 cbf\_remove\_datablock, cbf\_remove\_saveframe

# 2.3.59 cbf require datablock

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

13

### 2.3.60 cbf require category 2.3.61 cbf\_require\_column

### 2.3.6 cbf\_force\_new\_datablock, cbf\_force\_new\_saveframe

PROTOTYPE

#include "cbf.h"

int cbf force new datablock (cbf handle handle, const char \*datablockname); int cbf\_force\_new\_saveframe (cbf\_handle handle, const char \*saveframename);

### DESCRIPTION

cbf\_force\_new\_datablock creates a new data block with name datablockname and makes it the current data block. Duplicate data block names are allowed. cbf\_force\_new\_saveframe creates a new savew frame with name saveframename and makes it the current save frame. Duplicate save frame names are allowed.

Even if a save frame with this name already exists, a new save frame is created and becomes the current save frame.

### ARGUMENTS

handle CBF handle. datablockname The name of the new data block. saveframename The name of the new save frame.

### RETURN VALUE

# SEE ALSO

# 2.3.5 cbf\_new\_datablock, cbf\_new\_saveframe

2.3.8 cbf\_force\_new\_cate

```
2.3.11 cbf_insert_row
2.3.12 cbf set datablockname, cbf set saveframename
2.3.17 cbf_remove_datablock, cbf_remove_saveframe
   .59 cbf require datablock
2.3.60 cbf require category
```

int cbf\_new\_category (cbf\_handle handle, const char \*categoryname);



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

Returns an error code on failure or 0 for success.

2.3.7 cbf\_new\_category

2.3.9 cbf new column



PROTOTYPE #include "cbf.h"

2.3.7 cbf\_new\_category

cbf new category creates a new category in the current data block with name categoryname and makes it the current category.

If a category with this name already exists, the existing category becomes the current category.

# ARGUMENTS handle CBF handle. categoryname The name of the new category. RETURN VALUE Returns an error code on failure or 0 for success. SEE ALSO



### 2.3.8 cbf\_force\_new\_category

PROTOTYPE

#include "cbf.h"

int cbf\_force\_new\_category (cbf\_handle handle, const char \*categoryname);

### DESCRIPTION

cbf\_force\_new\_category creates a new category in the current data block with name categoryname and makes it the current category. Duplicate category names are allowed.

Even if a category with this name already exists, a new category of the same name is created and becomes the current category. The allows for the creation of unlooped tag/value lists drawn from the same category.

### ARGUMENTS

CBF handle. handle categoryname The name of the new category.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.5 cbf\_new\_datablock, cbf\_new\_saveframe 2.3.6 cbf\_force\_new\_datablock, cbf\_force\_new\_saveframe 2.3.7 cbf\_new\_category 2.3.9 cbf\_new\_column

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

15

2.3.10 cbf new row 2.3.11 cbf\_insert\_row 2.3.18 cbf\_remove\_category 2.3.59 cbf\_require\_datablock

### 2.3.9 cbf\_new\_column

### PROTOTYPE

### #include "cbf.h"

int cbf new column (cbf handle handle, const char \*columnname):

### DESCRIPTION

cbf\_new\_column creates a new column in the current category with name columnname and makes it the current column.

If a column with this name already exists, the existing column becomes the current category.

### ARGUMENTS

handle CBF handle columnname The name of the new column.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.5 cbf\_new\_datablock, cbf\_new\_saveframe 2.3.6 cbf\_force\_new\_datablock, cbf\_force\_new\_saveframe 2.3.7 cbf\_new\_category 2.3.8 cbf\_force\_new\_category 2.3.10 cbf\_new\_row 2.3.11 cbf insert row 2.3.19 cbf\_remove\_column 2.3.59 cbf require datablock 2.3.60 cbf require category 2.3.61 cbf require column 2.3.10 cbf\_new\_row

### PROTOTYPE

#include "cbf.h"

DESCRIPTION

int cbf\_new\_row (cbf\_handle handle);

cbf\_new\_row adds a new row to the current category and makes it the current row.

ARGUMENTS

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51





# 2.3.61 cbf require column



### DESCRIPTION

cbf\_insert\_row adds a new row to the current category. The new row is inserted as row *rownumber* and existing rows starting from *rownumber* are moved up by 1. The new row becomes the current row.

If the category has fewer than *rownumber* rows, the function returns CBF\_NOTFOUND.

The row numbers start from 0.

### ARGUMENTS

handle CBF handle.

rownumber The row number of the new row.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

### SEE ALSO



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

### 2.3.60 cbf\_require\_category 2.3.61 cbf\_require\_column

### 2.3.12 cbf\_delete\_row

### PROTOTYPE

#include "cbf.h"

int cbf\_delete\_row (cbf\_handle handle, unsigned int rownumber);

### DESCRIPTION

 $cbf_delete_row deletes a row from the current category. Rows starting from rownumber +1 are moved down by 1. If the current row was higher than rownumber, or if the current row is the last row, it will also move down by 1.$ 

The row numbers start from 0.

### ARGUMENTS

handle CBF handle.

rownumber The number of the row to delete.

**RETURN VALUE** 

### Returns an error code on failure or 0 for success.

SEE ALSO

- 2.3.10 cbf\_new\_row
- 2.3.11 cbf insert row 2.3.17 cbf remove datablock, cbf remove saveframe 2.3.18 cbf remove category 2.3.19 cbf remove column 2.3.20 cbf remove row 2.3.59 cbf require datablock 2.3.60 cbf require category 2.3.61 cbf require column

### 2.3.13 cbf\_set\_datablockname, cbf\_set\_saveframename

PROTOTYPE

#include "cbf.h"

int cbf\_set\_datablockname (cbf\_handle *handle*, const char \**datablockname*); int cbf\_set\_saveframename (cbf\_handle *handle*. const char \**saveframename*);

### DESCRIPTION

cbf\_set\_datablockname changes the name of the current data block to *datablockname*. cbf\_set\_saveframename changes the name of the current save frame to *saveframename*.

If a data block or save frame with this name already exists (comparison is case-insensitive), the function returns CBF\_IDENTICAL.

### ARGUMENTS

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

handleCBF handle.datablocknameThe new data block name.datablocknameThe new save frame name.

### **RETURN VALUE**

### Returns an error code on failure or 0 for success.

SEE ALSO

2.3.5 cbf\_new\_datablock, cbf\_new\_saveframe 2.3.14 cbf\_reset\_datablocks 2.3.15 cbf\_reset\_datablock, cbf\_reset\_saveframe 2.3.17 cbf\_remove\_datablock, cbf\_remove\_saveframe 2.3.24 cbf\_datablock\_name

### 2.3.14 cbf\_reset\_datablocks

### PROTOTYPE

#include "cbf.h"

int cbf\_reset\_datablocks (cbf\_handle handle);

### DESCRIPTION

cbf\_reset\_datablocks deletes all categories from all data blocks.

The current data block does not change.

### ARGUMENTS

handle CBF handle.

**RETURN VALUE** 

Returns an error code on failure or 0 for success. SEE ALSO

# 2.3.15 cbf reset datablock, cbf reset saveframe

2.3.18 cbf\_remove\_category

### 2.3.15 cbf\_reset\_datablock, cbf\_reset\_datablock

PROTOTYPE

#include "cbf.h"

int cbf\_reset\_datablock (cbf\_handle *handle*); int cbf\_reset\_saveframe (cbf\_handle *handle*);

DESCRIPTION

# n An

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

19

08/07/07 09:24:51



# cbf\_reset\_datablock deletes all categories from the current data block. cbf\_reset\_saveframe deletes all categories from the current save frame.



### RETURN VALUE

### Returns an error code on failure or 0 for success.

SEE ALSO 2.3.14 cbf\_reset\_datablocks

2.3.18 cbf\_remove\_category

### 2.3.16 cbf\_reset\_category

PROTOTYPE

#include "cbf.h"

int cbf\_reset\_category (cbf\_handle handle); DESCRIPTION

cbf\_reset\_category deletes all columns and rows from current category.

ARGUMENTS

handle CBF handle.

# RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO 2.3.16 cbf\_reset\_category

2.3.19 cbf\_remove\_column 2.3.20 cbf\_remove\_row

### 2.3.17 cbf\_remove\_datablock, cbf\_remove\_saveframe

### PROTOTYPE

#include "cbf.h"
int cbf\_remove\_datablock (cbf\_handle handle);



cbf\_remove\_datablock deletes the current data block. cbf\_remove\_saveframe deletes the current save frame.

The current data block becomes undefined.

The current data block becomes

ARGUMENTS

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

CBFlib Manual

int cbf\_remove\_column (cbf\_handle handle);

### DESCRIPTION

cbf\_remove\_column deletes the current column.

The current column becomes undefined.

ARGUMENTS

handle CBF handle.

RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

### 2.3.9 cbf new column 2.3.17 cbf remove datablock, cbf remove saveframe 2.3.18 cbf remove category 2.3.20 cbf remove row 2.3.59 cbf require category 2.3.61 cbf require category 2.3.61 cbf require column

### 2.3.20 cbf\_remove\_row

### PROTOTYPE

#include "cbf.h"

int cbf\_remove\_row (cbf\_handle handle);

DESCRIPTION

cbf\_remove\_row deletes the current row in the current category.

If the current row was the last row, it will move down by 1, otherwise, it will remain the same.

ARGUMENTS handle CBF handle. RETURN VALUE Returns an error code on failure or 0 for success. SEE ALSO 2.3.10 cbf new row 2.3.11 cbf insert row 2.3.17 cbf remove datablock, cbf remove saveframe 2.3.18 cbf remove category 2.3.19 cbf remove column 2.3.12 cbf delete row

2.3.59 cbf\_require\_datablock

 $file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html$ 



# 2.3.60 cbf\_require\_category



The current column and row become undefined.
ARGUMENTS
handle CBF handle.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

23

type CBF handle.
RETURN VALUE
Returns an error code on failure or 0 for success.

### SEE ALSO 2.3.21 cbf rewind\_datablock 2.3.19 cbf rewind\_column 2.3.24 cbf rewind\_row 2.3.26 cbf next\_category, cbf next\_saveframe, cbf next\_blockitem

2.3.26 cbl\_next\_category, cbl\_next\_saveIrame, cbl\_next\_bloc

2.3.23 cbf\_rewind\_column

PROTOTYPE

#include "cbf.h"

int cbf\_rewind\_column (cbf\_handle handle);

### DESCRIPTION

cbf\_rewind\_column makes the first column in the current category the current column.

If there are no columns, the function returns CBF\_NOTFOUND.

The current row is not affected.

ARGUMENTS handle CBF handle.

RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.21 cbf rewind\_datablock 2.3.22 cbf rewind\_category, cbf\_rewind\_saveframe, cbf\_rewind\_blockitem 2.3.24 cbf\_rewind\_row 2.3.27 cbf\_next\_column

### 2.3.24 cbf\_rewind\_row

PROTOTYPE

DESCRIPTION

#include "cbf.h"

int cbf\_rewind\_row (cbf\_handle handle);

cbf\_rewind\_row makes the first row in the current category the current row.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51



# DESCRIPTION

cbf\_next\_category makes the category following the current category in the current data block the current category. If there are no more categories, the function returns CBF\_NOTFOUND.

The current column and row become undefined.

### ARGUMENTS

handle CBF handle.

**RETURN VALUE** Returns an error code on failure or 0 for success.

SEE ALSO

2.3.22 cbf rewind\_category, cbf rewind\_saveframe, cbf\_rewind\_blockitem 2.3.25 cbf\_next\_datablock 2.3.27 cbf\_next\_column 2.3.27 cbf\_next\_row

# 2.3.27 cbf\_next\_column

PROTOTYPE

#include "cbf.h"

int cbf\_next\_column (cbf\_handle handle);

DESCRIPTION

cbf\_next\_column makes the column following the current column in the current category the current column.

If there are no more columns, the function returns CBF\_NOTFOUND.

The current row is not affected.

ARGUMENTS handle CBF handle.

# RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.19 cbf rewind column 2.3.25 cbf next\_datablock 2.3.26 cbf next\_category, cbf next\_saveframe, cbf next\_blockitem 2.3.28 cbf next\_row

### 2.3.28 cbf\_next\_row

### PROTOTYPE

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51



#include "cbf.h" int cbf next row (cbf handle handle);

DESCRIPTION

cbf\_next\_row makes the row following the current row in the current category the current row.

If there are no more rows, the function returns CBF\_NOTFOUND.

The current column is not affected.

ARGUMENTS

handle CBF handle.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.24 cbf\_rewind\_row 2.3.25 cbf next datablock 2.3.26 cbf next category, cbf next saveframe, cbf next blockitem .3.27 cbf\_next\_column

### 2.3.29 cbf find datablock

### PROTOTYPE

#include "cbf.h"

int cbf\_find\_datablock (cbf\_handle handle, const char \*datablockname);

### DESCRIPTION

cbf\_find\_datablock makes the data block with name datablockname the current data block.

The comparison is case-insensitive.

If the data block does not exist, the function returns CBF\_NOTFOUND.

The current category becomes undefined.

### ARGUMENTS

handle CBF handle. datablockname The name of the data block to find.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.21 cbf\_rewind\_datablock 2.3.25 cbf next datablock

27

### 2.3.30 cbf\_find\_category, cbf\_find\_saveframe, cbf\_find\_blockitem 2.3.31 cbf\_find\_column .3.32 cbf find row

CBFlib Manual

2.3.42 cbf datablock name 2.3.59 cbf\_require\_datablock 2.3.60 cbf require category

2.3.61 cbf\_require\_column

# 2.3.30 cbf find category PROTOTYPE

#include "cbf.h"

int cbf\_find\_category (cbf\_handle handle, const char \*categoryname);

### DESCRIPTION

cbf\_find\_category makes the category in the current data block with name categoryname the current category.

The comparison is case-insensitive.

If the category does not exist, the function returns CBF\_NOTFOUND.

The current column and row become undefined.

### ARGUMENTS

DESCRIPTION

categoryname The name of the category to find.

### Returns an error code on failure or 0 for success.

2.3.22 cbf\_rewind\_category, cbf\_rewind\_saveframe, cbf\_rewind\_blockitem 2.3.26 cbf\_next\_category, cbf\_next\_saveframe, cbf\_next\_blockitem

### int cbf\_find\_column (cbf\_handle handle, const char \*columnname);



08/07/07 09:24:51

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

handle CBF handle. **RETURN VALUE** SEE ALSO 2.3.29 cbf find datablock 2.3.31 cbf\_find\_column .3.32 cbf find row 2.3.43 cbf\_category\_na 2.3.59 cbf\_require\_databloc .3.60 cbf require category 2.3.61 cbf\_require\_column 2.3.31 cbf find column PROTOTYPE #include "cbf.h"





29

cbf\_find\_column makes the columns in the current category with name columnname the current column.

The comparison is case-insensitive.

### If the column does not exist, the function returns CBF\_NOTFOUND.



Returns an error code on failure or 0 for success.



CBFlib Manual

2.3.24 cbf rewind row 2.3.28 cbf\_next\_row .3.29 cbf find datablock 2.3.30 cbf find category, cbf find saveframe, cbf find blockitem 2.3.31 cbf\_find\_column 2.3.33 cbf find nextrow 2.3.46 cbf\_get\_value, cbf\_require\_value 2.3.48 cbf\_get\_typeofvalue 2.3.33 cbf\_find\_nextrow

### PROTOTYPE

#include "cbf.h"

int cbf find nextrow (cbf handle handle, const char \*value);

### DESCRIPTION

cbf\_find\_nextrow makes the makes the next row in the current column with value value the current row. The search starts from the row following the last row found with cbf find row or cbf find nextrow, or from the current row if the current row was defined using any other function.

The comparison is case-sensitive.

If no more matching rows exist, the function returns CBF\_NOTFOUND.

The current column is not affected.

ARGUMENTS

handle CBF handle.

value the value to search for.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

SEE ALSO



### 2.3.34 cbf\_count\_datablocks



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

### DESCRIPTION

cbf count datablocks puts the number of data blocks in \*datablocks.

ARGUMENTS handle CBF handle. datablocks Pointer to the destination data block count.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.35 cbf count\_categories, cbf count\_saveframes, cbf count\_blockitems 2.3.36 cbf count\_columns 2.3.37 cbf count\_rows 2.3.38 cbf select datablock

### 2.3.35 cbf\_count\_categories

### PROTOTYPE

### #include "cbf.h"

int cbf\_count\_categories (cbf\_handle handle, unsigned int \*categories);

### DESCRIPTION

cbf\_count\_categories puts the number of categories in the current data block in \*categories.

### ARGUMENTS

handle CBF handle.

categories Pointer to the destination category count.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.34 cbf\_count\_datablocks 2.3.36 cbf\_count\_columns

### 2.3.37 cbf count rows 2.3.39 cbf select category, cbf select saveframe, cbf select blockitem



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

31

### DESCRIPTION

cbf\_count\_columns puts the number of columns in the current category in \*columns.

### ARGUMENTS

handle CBF handle.

columns Pointer to the destination column count.

### RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO

### 2.3.34 cbf count datablocks

2.3.35 cbf count categories, cbf count saveframes, cbf count blockitems 2.3.37 cbf count rows 2.3.40 cbf select column

### 2.3.37 cbf\_count\_rows

### PROTOTYPE

#include "cbf.h"

int cbf count rows (cbf handle handle, unsigned int \*rows);

### DESCRIPTION

cbf\_count\_rows puts the number of rows in the current category in \*rows

### ARGUMENTS

handle CBF handle.

rows Pointer to the destination row count.

### RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO

### 2.3.34 cbf\_count\_datablocks

2.3.35 cbf\_count\_categories, cbf\_count\_saveframes, cbf\_count\_blockitems 2.3.36 cbf\_count\_columns 2.3.41 cbf\_select\_row

# 2.3.38 cbf\_select\_datablock PROTOTYPE

#include "cbf.h"

int cbf\_select\_datablock (cbf\_handle handle, unsigned int datablock);

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

DESCRIPTION

cbf select datablock selects data block number datablock as the current data block The first data block is number 0.

If the data block does not exist, the function returns CBF\_NOTFOUND.

### ARGUMENTS

handle CBF handle. datablock Number of the data block to select.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.34 cbf\_count\_datablocks 2.3.39 <u>cbf\_select\_category, cbf\_select\_saveframe, cbf\_select\_blockitem</u> 2.3.40 cbf\_select\_column 2.3.41 cbf\_select\_row

### 2.3.39 cbf\_select\_category

PROTOTYPE

#include "cbf.h"

int cbf\_select\_category (cbf\_handle handle, unsigned int category);

### DESCRIPTION

cbf\_select\_category selects category number category in the current data block as the current category.

The first category is number 0. The current column and row become undefined.

ARGUMENTS

handle CBF handle. category Number of the category to select.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.40 cbf\_select\_column 2.3.41 cbf\_select\_row

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

33

CBFlib Manual

# 2.3.40 cbf select column PROTOTYPE

#include "cbf.h"

int cbf\_select\_column (cbf\_handle handle, unsigned int column);

### DESCRIPTION

cbf\_select\_column selects column number column in the current category as the current column.

The first column is number 0.

The current row is not affected

If the column does not exist, the function returns CBF\_NOTFOUND

### ARGUMENTS

handle CBF handle. column Number of the column to select.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

SEE ALSO

### 2.3.36 cbf\_count\_columns

2.3.38 cbf select datablock 2.3.39 cbf\_select\_category, cbf\_select\_saveframe, cbf\_select\_blockitem 2.3.41 cbf select row

### 2.3.41 cbf select row

PROTOTYPE #include "cbf.h"

int cbf\_select\_row (cbf\_handle handle, unsigned int row);

### DESCRIPTION

cbf\_select\_row selects row number row in the current category as the current row.

The first row is number 0.

The current column is not affected

If the row does not exist, the function returns CBF\_NOTFOUND.

### ARGUMENTS

handle CBF handle.

Number of the row to select. row

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

08/07/07 09:24:51

If the category does not exist, the function returns CBF\_NOTFOUND. 2.3.35 cbf\_count\_categories, cbf\_count\_saveframes, cbf\_count\_blockitems 2.3.38 cbf\_select\_datablock

# RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

### 2.3.37 cbf\_count\_rows 2.3.38 cbf\_select\_datablock 2.3.39 cbf select category, cbf\_select\_saveframe, cbf\_select\_blockitem 2.3.40 cbf\_select\_column

### 2.3.42 cbf\_datablock\_name

### PROTOTYPE

# #include "cbf.h"

int cbf\_datablock\_name (cbf\_handle handle, const char \*\*datablockname);

### DESCRIPTION

cbf\_datablock\_name sets \* datablockname to point to the name of the current data block.

The data block name will be valid as long as the data block exists and has not been renamed.

The name must not be modified by the program in any way.

### ARGUMENTS

handle CBF handle.

datablockname Pointer to the destination data block name pointer.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.29 cbf\_find\_datablock

### 2.3.43 cbf\_category\_name

### PROTOTYPE

#include "cbf.h"

int cbf\_category\_name (cbf\_handle handle, const char \*\*categoryname);

### DESCRIPTION

cbf\_category\_name sets \*categoryname to point to the name of the current category of the current data block.

The category name will be valid as long as the category exists.

The name must not be modified by the program in any way.

### ARGUMENTS

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

35

### handle CBF handle.

categoryname Pointer to the destination category name pointer.

### RETURN VALUE

### Returns an error code on failure or 0 for success.

SEE ALSO 2.3.30 cbf find category, cbf find saveframe, cbf find blockitem

### 2.3.44 cbf\_column\_name

PROTOTYPE

### #include "cbf.h"

int cbf column name (cbf handle handle, const char \*\* columnname);

### DESCRIPTION

cbf\_column\_name sets \*columnname to point to the name of the current column of the current category.

The column name will be valid as long as the column exists.

The name must not be modified by the program in any way.

### ARGUMENTS

handle CBF handle. columnname Pointer to the destination column name pointer.

### RETURN VALUE

Returns an error code on failure or 0 for success.

# SEE ALSO

# 2.3.31 cbf find column

2.3.45 cbf\_row\_number PROTOTYPE

#include "cbf.h"

int cbf row number (cbf handle handle, unsigned int \*row);

### DESCRIPTION

cbf\_row\_number sets \*row to the number of the current row of the current category.

ARGUMENTS

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51









handle CBF handle. Pointer to the destination row number. row

RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO 2.3.41 cbf select row

2.3.46 cbf\_get\_value, cbf\_require\_value

### PROTOTYPE

#include "cbf.h"

int cbf get value (cbf handle handle, const char \*\*value); int cbf\_require\_value (cbf\_handle handle, const char \*\*value, const char \*defaultvalue );

### DESCRIPTION

cbf get value sets \*value to point to the ASCII value of the item at the current column and row. cbf set value sets \*value to point to the ASCII value of the item at the current column and row, creating the data item if necessary and initializing it to a copy of *defaultvalue*.

If the value is not ASCII, the function returns CBF\_BINARY.

The value will be valid as long as the item exists and has not been set to a new value.

The value must not be modified by the program in any way.

ARGUMENTS

### handle CBF handle.

- value Pointer to the destination value pointer.
- value Default value character string.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

# 2.3.47 cbf\_set\_value 2.3.48 cbf\_get\_typeofvalue

2.3.49 cbf\_set\_typeofvalue 2.3.50 cbf\_get\_integervalue, cbf\_require\_integervalue

realarrayparameters\_wdims

### 2.3.55 cbf\_get\_integerarray, cbf\_get\_realarray

2.3.62 cbf require column value 2.3.63 cbf\_require\_column\_integervalue

### 2.3.64 cbf\_require\_column\_doublevalue

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51



37

# 2.3.47 cbf set value PROTOTYPE #include "cbf.h" int cbf set value (cbf handle handle, const char \*value); DESCRIPTION cbf\_set\_value sets the item at the current column and row to the ASCII value value. ARGUMENTS handle CBF handle.

value ASCII value.

defaultvalue default ASCII value.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.46 cbf\_get\_value, cbf\_require\_value

2.3.48 cbf\_get\_typeofvalue 2.3.49 cbf\_set\_typeofvalue .3.51 cbf set integervalue 2.3.53 cbf set doublevalue 2.3.56 cbf\_set\_integerarray, cbf\_set\_integerarray\_wdims, cbf\_set\_realarray, cbf\_set\_realarray\_wdims 2.3.62 cbf require column value 2.3.63 cbf\_require\_column\_integervalue 2.3.64 cbf\_require\_column\_doublevalue

### 2.3.48 cbf\_get\_typeofvalue

### PROTOTYPE

#include "cbf.h"

int cbf\_get\_typeofvalue (cbf\_handle handle, const char \*\*typeofvalue);

### DESCRIPTION

cbf\_get\_value sets \*typeofvalue to point an ASCII descriptor of the value of the item at the current column and row. The strings that may be returned are "null" for a null value indicated by a "." or a "?", "bnry" for a binary value, "word" for an unquoted string, "dblq" for a double-quoted string, "sglq" for a single-quoted string, and "text" for a semicolonquoted text field. A field for which no value has been set sets \*typeofyalue to NULL rather than to the string "null".

The typeofvalue must not be modified by the program in any way.

ARGUMENTS handle CBF handle. typeofvalue Pointer to the destination type-of-value string pointer.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html









### DESCRIPTION

cbf\_set\_typeofvalue sets the type of the item at the current column and row to the type specified by the ASCII character string given by *typeofvalue* sets the type of the term at the current column and you to the typeofvalue sets of the random string given by *typeofvalue*. The strings that may be used are "null" for a null value indicated by a "." or a "?", "word" for an unquoted string, "dblq" for a double-quoted string, "sglq" for a single-quoted string, and "text" for a semicolon-quoted text field. Not all types may be used for all values. No changes may be made to the type of binary values. You may not set the type of a string that contains a single quote followed by a blank or a tab or which contains multiple lines to "sglq". You may not set the type of a string that contains a double quote followed by a blank or a tab or which contains multiple lines to "dblq".



CBF handle. handle

typeofvalue ASCII string for desired type of value.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

### SEE ALSO



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### **CBFlib** Manual

### 2.3.50 cbf get integervalue, cbf require integervalue

### PROTOTYPE

### #include "cbf.h"

int cbf\_get\_integervalue (cbf\_handle handle, int \*number); int cbf\_require\_integervalue (cbf\_handle handle, int \*number, int defaultvalue);

### DESCRIPTION

cbf get integervalue sets \*number to the value of the ASCII item at the current column and row interpreted as a decimal integer. cbf\_require\_integervalue sets \*number to the value of the ASCII item at the current column and row interpreted as a decimal integer, setting it to defaultvalue if necessary.

If the value is not ASCII, the function returns CBF BINARY.

### ARGUMENTS

handle CBF handle.

number pointer to the number. defaultvalue default number value.

### RETURN VALUE

Returns an error code on failure or 0 for success.

SEE ALSO

# 2.3.46 cbf\_get\_value, cbf\_require\_value 2.3.48 cbf\_get\_typeofvalue

2.3.51 cbf\_set\_integervalue

2.3.52 cbf\_get\_doublevalue, cbf\_require\_doublevalue .3.54 cbf\_get\_integerarrayparameters, cbf\_get\_integerarrayparameters\_wdims, cbf\_get\_realarrayparameters, cbf\_get\_

realarrayparameters\_wdims 2.3.55 cbf\_get\_integerarray, cbf\_get\_realarray 2.3.62 cbf require column value

2.3.63 cbf require column integervalue 2.3.64 cbf require\_column\_doublevalue

2.3.51 cbf set integervalue

### PROTOTYPE

#include "cbf.h"

int cbf\_set\_integervalue (cbf\_handle handle, int number);

### DESCRIPTION

cbf set integervalue sets the item at the current column and row to the integer value number written as a decimal ASCII string.

ARGUMENTS

handle CBF handle.

number Integer value.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51



### 2.3.52 cbf get doublevalue, cbf require doublevalue

### PROTOTYPE

#include "cbf.h"

int cbf get doublevalue (cbf handle handle, double \*number); int cbf\_require\_doublevalue (cbf\_handle handle, double \*number, double defaultvalue);

### DESCRIPTION

cbf\_get\_doublevalue sets \*number to the value of the ASCII item at the current column and row interpreted as a decimal floating-point number. cbf\_require\_doublevalue sets \*number to the value of the ASCII item at the current column and row interpreted as a decimal floating-point number, setting it to defaultvalue if necessary.

If the value is not ASCII, the function returns CBF\_BINARY.

### ARGUMENTS

handle CBF handle. number Pointer to the destination number. defaultvalue default number value.

RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO 2.3.46 cbf\_get\_value, cbf\_require\_value 2.3.48 cbf get typeofvalue 2.3.49 cbf\_set\_typeofvalue 2.3.50 cbf get integervalue, cbf require integervalue 2.3.53 cbf set\_doublevalue 2.3.54 cbf get integerarrayparameters, cbf get integerarrayparameters wdims, cbf get realarrayparameters, cbf get realarrayparameters\_wdims 2.3.55 cbf\_get\_integerarray, cbf\_get\_realarray 2.3.62 cbf\_require\_column\_value

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### **CBFlib** Manual



### 2.3.53 cbf\_set\_doublevalue

### PROTOTYPE

#include "cbf.h"

int cbf set doublevalue (cbf handle handle, const char \*format, double number);

### DESCRIPTION

cbf\_set\_doublevalue sets the item at the current column and row to the floating-point value number written as an ASCII string with the format specified by format as appropriate for the printf function.

### ARGUMENTS

handle CBF handle.

format Format for the number.

number Floating-point value.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

SEE ALSO

### 2.3.46 cbf\_get\_value, cbf\_require\_value

.3.63 cbf\_require\_column\_integervalue 2.3.64 cbf require column doublevalue

2.3.47 cbf\_set\_value 2.3.48 cbf get typeofyalue

### 2.3.49 cbf\_set\_typeofvalue

2.3.51 cbf\_set\_integervalue

.3.52 cbf get doublevalue, cbf require doublevalue 2.3.56 cbf set integerarray, cbf set integerarray wdims, cbf set realarray, cbf set realarray wdims

2.3.62 cbf require column value

2.3.54 cbf\_get\_integerarrayparameters, cbf\_get\_integerarrayparameters\_wdims, cbf\_get\_realarrayparameters, cbf\_get\_realarrayparameters\_wdims

### PROTOTYPE

#include "cbf.h"

int cbf\_get\_integerarrayparameters (cbf\_handle handle, unsigned int \*compression, int \*binary\_id, size\_t \*elsize, int \*elsigned, int \*elunsigned, size\_t \*elements, int \*minelement, int \*maxelement); int cbf get integerarrayparameters wdims (cbf handle handle, unsigned int \*compression, int \*binary id, size t \*elsize, int \*elsigned, int \*elunsigned, size\_t \*elements, int \*minelement, int \*maxelement, const char \*\*byteorder, size\_ t\*dim1, size\_t\*dim2, size\_t\*dim3, size\_t\*padding);

int cbf get realarrayparameters (cbf handle handle, unsigned int \*compression, int \*binary id, size t \*elsize, size t \*elements):

int cbf\_get\_realarrayparameters\_wdims (cbf\_handle handle, unsigned int \*compression, int \*binary\_id, size\_t \*elsize, size\_t \*elements, const char \*\*byteorder, size\_t \*dim1, size\_t \*dim2, size\_t \*dim3, size\_t \*padding);

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html 08/07/07 09:24:51

### DESCRIPTION

cbf\_get\_integerarrayparameters sets \*compression, \*binary\_id, \*elsize, \*elsigned, \*elunsigned, \*elements, \*minelement and \*maxelement to values read from the binary value of the item at the current column and row. This provides all the arguments needed for a subsequent call to cbf\_set\_integerarray, if a copy of the array is to be made into another CIF or CBF. cbf\_get\_realarrayparameters sets \*compression, \*binary\_id, \*elsize, \*elements to values read from the binary value of the item at the current column and row. This provides all the arguments needed for a subsequent call to cbf\_set\_ realarray, if a copy of the arry is to be made into another CIF or CBF.

The variants cbf\_get\_integerarrayparameters\_wdims and cbf\_get\_realarrayparameters\_wdims set \*\*byteorder, \*dim1, \*dim2, \*dim3, and \*padding as well, providing the additional parameters needed for a subsequent call to cbf\_set\_integerarray\_wdims or cbf\_set\_realarray\_wdims.

The value returned in *\*byteorder* is a pointer either to the string "little\_endian" or to the string "big\_endian". This should be the byte order of the data, not necessarily of the host machine. No attempt should be made to modify this string. At this time only "little\_endian" will be returned.

The values returned in \**dim1*, \**dim2* and \**dim3* are the sizes of the fastest changing, second fastest changing and third fastest changing dimensions of the array, if specified, or zero, if not specified.

The value returned in *\*padding* is the size of the post-data padding, if any and if specified in the data header. The value is given as a count of octets.

### If the value is not binary, the function returns CBF\_ASCII.

### ARGUMENTS

AKGUMENTS	
handle	CBF handle.
compression	Compression method used.
elsize	Size in bytes of each array element.
binary_id	Pointer to the destination integer binary identifier.
elsigned	Pointer to an integer. Set to 1 if the elements can be read
elunsigned	Pointer to an integer. Set to 1 if the elements can be read
elements	Pointer to the destination number of elements.
minelement	Pointer to the destination smallest element.
maxelement	Pointer to the destination largest element.
byteorder	Pointer to the destination byte order.
diml	Pointer to the destination fastest dimension.
dim2	Pointer to the destination second fastest dimension.
dim3	Pointer to the destination third fastest dimension.
padding	Pointer to the destination padding size.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.46 cbf get value, cbf require value 2.3.48 cbf get typeofvalue 2.3.49 cbf set typeofvalue 2.3.50 cbf get integervalue, cbf require integervalue 2.3.52 cbf get doublevalue, cbf require doublevalue 2.3.55 cbf get integerarray, cbf get realarray



as signed integers

as unsigned integers.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

43

### 2.3.56 cbf set integerarray, cbf set integerarray wdims, cbf set realarray, cbf set realarray wdims

2.3.62 cbf\_require\_column\_value 2.3.63 cbf\_require\_column\_integervalue 2.3.64 cbf\_require\_column\_doublevalue

### 2.3.55 cbf\_get\_integerarray, cbf\_get\_realarray

### PROTOTYPE

#include "cbf.h"

int cbf\_get\_integerarray (cbf\_handle handle, int \*binary\_id, void \*array, size\_t elsize, int elsigned, size\_t elements, size\_t \*elements\_read);

int cbf\_get\_realarray (cbf\_handle handle, int \*binary\_id, void \*array, size\_t elsize, size\_t elements, size\_t \*elements\_ read);

### DESCRIPTION

cbf\_get\_integerarray reads the binary value of the item at the current column and row into an integer array. The array consists of *elements* elements of *elsize* bytes each, starting at *array*. The elements are signed if *elsigned* is non-0 and unsigned otherwise. *\*binary\_idi* is set to the binary section identifier and *\*elements\_read* to the number of elements actually read. cbf\_get\_realarray reads the binary value of the item at the current column and row into a real array. The array consists of *elements* get\_realarray reads the binary section identifier and *\*elements\_read* to the binary section identifier and *\*elements\_read* to the number of elements actually read.

If any element in the integer binary data cant fit into the destination element, the destination is set the nearest possible value.

If the value is not binary, the function returns CBF\_ASCII.

If the requested number of elements cant be read, the function will read as many as it can and then return CBF\_ ENDOFDATA.

Currently, the destination array must consist of chars, shorts or ints (signed or unsigned). If *elsize* is not equal to sizeof (char), sizeof (short) or sizeof (int), for cbf\_get\_integerarray, or sizeof(double) or sizeof(float), for cbf\_get\_realarray the function returns CBF\_ARGUMENT.

An additional restriction in the current version of CBFlib is that values too large to fit in an int are not correctly decompressed. As an example, if the machine with 32-bit ints is reading an array containing a value outside the range  $0 \cdot 2^{\Lambda^3 1} \cdot 1$  (unsigned) or  $-2^{\Lambda^3 1} \cdot 2^{\Lambda^{31} - 1}$  (signed), the array will not be correctly decompressed. This restriction will be removed in a future release. For cbf\_get\_realarray, only IEEE format is supported. No conversion to other floating point formats is done at this time.

ARGUMENTS	
handle	CBF handle.
binary_id	Pointer to the destination integer binary identifier.
array	Pointer to the destination array.
elsize	Size in bytes of each destination array element.
elsigned	Set to non-0 if the destination array elements are signed.
elements	The number of elements to read.
elements_read	Pointer to the destination number of elements actually read.
RETURN VALU	

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.46 cbf\_get\_value, cbf\_require\_value 2.3.48 cbf\_get\_typeofvalue 2.3.49 cbf set typeofvalue 2.3.50 cbf\_get\_integervalue, cbf\_require\_integervalue

2.3.52 cbf\_get\_doublevalue, cbf\_require\_doublevalue 2.3.54 cbf get integerarrayparameters, cbf get integerarrayparameters wdims, cbf get realarrayparameters, cbf get

realarrayparameters\_wdims

2.3.56 cbf\_set\_integerarray, cbf\_set\_integerarray\_wdims, cbf\_set\_realarray, cbf\_set\_realarray\_wdims .3.62 cbf require column value

2.3.63 cbf\_require\_column\_integervalue

2.3.64 cbf require column doublevalue

2.3.56 cbf\_set\_integerarray, cbf\_set\_integerarray\_wdims, cbf\_set\_realarray, cbf\_set\_realarray\_wdims

### PROTOTYPE

#include "cbf.h"

int cbf set integerarray (cbf handle handle, unsigned int compression, int binary id, void \*array, size t elsize, int elsigned, size\_t elements);

int cbf set integerarray wdims (cbf handle handle, unsigned int compression, int binary id, void \*array, size t elsize, int elsigned, size\_t elements, const char \*byteorder, size\_t dim1, size\_t dim2, size\_t dim3, size\_t padding); int cbf\_set\_realarray (cbf\_handle handle, unsigned int compression, int binary\_id, void \*array, size\_t elsize, size\_t elements);

int cbf\_set\_realarray\_wdims (cbf\_handle handle, unsigned int compression, int binary\_id, void \*array, size\_t elsize, size\_t elements, const char \*byteorder, size\_t dim1, size\_t dim2, size\_t dim3, size\_t padding);

### DESCRIPTION

cbf set integerarray sets the binary value of the item at the current column and row to an integer array. The array consists of *elements* elements of *elsize* bytes each, starting at *array*. The elements are signed if *elsigned* is non-0 and unsigned otherwise. *binary\_id* is the binary section identifier. cbf\_set\_realarray sets the binary value of the item at the current column and row to an integer array. The array consists of elements elements of elsize bytes each, starting at array. binary id is the binary section identifier.

The cbf\_set\_integerarray\_wdims and cbf\_set\_realarray\_wdims allow the data header values of byteorder, dim1, dim2, dim3 and padding to be set to the data byte order, the fastest, second fastest and third fastest array dimensions and the size in byte of the post data padding to be used.

The array will be compressed using the compression scheme specifed by compression. Currently, the available schemes



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

**CBFlib** Manual

45

CBF_ CANONICAL	Canonical-code compression (section 3.3.1)	
CBF_PACKED	CCP4-style packing (section 3.3.2)	
CBF_PACKED_	CCP4-style packing, version 2 (section 3.3.2)	
V2 7		
CBF_BYTE_	Simple "byte_offset" compression.	
OFFSET		
CBF_NONE	No compression. NOTE: This scheme is by far t space. It is intended for routine use with small arr	
	be used only for debugging.	

The values compressed are limited to 64 bits. If any element in the array is larger than 64 bits, the value compressed is the nearest 64-bit value.

Currently, the source array must consist of chars, shorts or ints (signed or unsigned), for cbf\_set\_integerarray, or IEEE doubles or floats for cbf\_set\_realarray. If elsize is not equal to sizeof (char), sizeof (short) or sizeof (int), the function returns CBF ARGUMENT.

### ARGUMENTS

handle	CBF handle.
compression	Compression method to use.
binary_id	Integer binary identifier.
array	Pointer to the source array.
elsize	Size in bytes of each source array element.
elsigned	Set to non-0 if the source array elements are sig elements: The number of elements in the array.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

### SEE ALSO





file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

#define cbf\_failnez(f) {int err; err = (f); if (err) return err; }

### DESCRIPTION

cbf\_failnez is a macro used for error propagation throughout CBFlib. cbf\_failnez executes the function f and saves the returned error value. If the error value is non-0, cbf\_failnez executes a return with the error value as argument. If CBFDEBUG is defined, then a report of the error is also printed to the standard error stream, stderr, in the form

CBFlib error f in "symbol"

where f is the decimal value of the error and symbol is the symbolic form.



f Integer error value.

SEE ALSO

2.3.58 cbf\_onfailnez

-

### 2.3.58 cbf\_onfailnez

### DEFINITION

#include "cbf.h"

#define cbf\_onfailnez(f,c) {int err; err = (f); if (err) {{c; }return err; }}

### DESCRIPTION

cbf\_onfailnez is a macro used for error propagation throughout CBFlib. cbf\_onfailnez executes the function f and saves the returned error value. If the error value is non-0, cbf\_failnez executes first the statement c and then a return with the error value as argument. If CBFDEBUG is defined, then a report of the error is also printed to the standard error stream, stderr, in the form

CBFlib error f in "symbol"		
where $f$ is the decimal value of the error and $sy$	<i>ambol</i> is the symbolic form.	
ARGUMENTS f integer function to execute. c statement to execute on failure.		
SEE ALSO		
• <u>2.3.57 cbf_failnez</u>		
2.3.59 cbf_require_datablock		
РКОТОТУРЕ		
#include "cbf.h"		
int cbf_require_datablock (cbf_handle handle,	const char *datablockname);	

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

47

### DESCRIPTION

cbf\_require\_datablock makes the data block with name *datablockname* the current data block, if it exists, or creates it if it does not.

The comparison is case-insensitive.

The current category becomes undefined.

### ARGUMENTS

handle CBF handle.

datablockname The name of the data block to find or create.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

SEE ALSO

2.3.21 cbf\_rewind\_datablock 2.3.25 cbf\_next\_datablock 2.3.29 cbf\_find\_datablock 2.3.30 cbf\_find\_category, cbf\_find\_saveframe, cbf\_find\_blockitem 2.3.31 cbf\_find\_column 2.3.32 cbf\_find\_column 2.3.42 cbf\_find\_row 2.3.42 cbf\_datablock\_name 2.3.60 cbf\_require\_category 2.3.61 cbf\_require\_column

### 2.3.60 cbf\_require\_category

### PROTOTYPE

#include "cbf.h"

int cbf\_require\_category (cbf\_handle handle, const char \*categoryname);

DESCRIPTION

cbf\_rewuire\_category makes the category in the current data block with name *categoryname* the current category, if it exists, or creates the catagory if it does not exist.

The comparison is case-insensitive.

The current column and row become undefined.

### ARGUMENTS

handle CBF handle.

categoryname The name of the category to find.

RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

# 2.3.22 cbf\_rewind\_category, cbf\_rewind\_saveframe, cbf\_rewind\_blockitem 2.3.26 cbf\_next\_category, cbf\_next\_saveframe, cbf\_next\_blockitem .3.29 cbf find datablock 2.3.31 cbf find\_column 2.3.32 cbf\_find\_row 2.3.43 cbf category name 2.3.59 cbf\_require\_datablock 2.3.61 cbf\_require\_column 2.3.61 cbf\_require\_column PROTOTYPE #include "cbf.h"

int cbf\_require\_column (cbf\_handle handle, const char \*columnname);

### DESCRIPTION

cbf\_require\_column makes the columns in the current category with name columnname the current column, if it exists, or creates it if it does not.

The comparison is case-insensitive.

The current row is not affected.

### ARGUMENTS

handle CBF handle.

columnname The name of column to find.

### RETURN VALUE



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

49

cbf require column doublevalue sets \*value to the ASCII item at the current row for the column given with the name given by \*columnname, or to the string given by defaultvalue if the item cannot be found.

# ARGUMENTS

handle CBF handle.

columname Name of the column containing the number. value pointer to the location to receive the value.

# defaultvalue Value to use if the requested column and value cannot be found.

# **RETURN VALUE**

Returns an error code on failure or 0 for success.

SEE ALSO

# 2.3.46 cbf get value, cbf require value 2.3.47 cbf\_set\_value

2.3.48 cbf get typeofvalue 2.3.49 cbf\_set\_typeofvalue .3.51 cbf\_set\_integervalue 2.3.52 cbf get\_doublevalue, cbf\_require\_doublevalue 2.3.56 cbf\_set\_integerarray, cbf\_set\_integerarray\_wdims, cbf\_set\_realarray, cbf\_set\_realarray\_wdims .3.63 cbf require column integervalue 2.3.64 cbf require column doublevalue

### 2.3.63 cbf\_require\_column\_integervalue

### PROTOTYPE

#include "cbf.h"

int cbf\_require\_column\_integervalue (cbf\_handle handle, const char \*columnname, int \*number, const int defaultvalue);

### DESCRIPTION

cbf require column doublevalue sets \*number to the value of the ASCII item at the current row for the column given with the name given by \*columnname, with the value interpreted as an integer number, or to the number given by defaultvalue if the item cannot be found.

### ARGUMENTS

- handle CBF handle.
- columnname Name of the column containing the number. number
- pointer to the location to receive the integer value. defaultvalue Value to use if the requested column and value cannot be found.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

### 2.3.46 cbf\_get\_value, cbf\_require\_value 2.3.47 cbf set value 2.3.48 cbf\_get\_typeofvalue

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

2.3.49 cbf set typeofyalue 2.3.51 cbf\_set\_integervalue 2.3.52 cbf\_get\_doublevalue, cbf\_require\_doublevalue

2.3.56 cbf\_set\_integerarray, cbf\_set\_integerarray\_wdims, cbf\_set\_realarray, cbf\_set\_realarray\_wdims

2.3.62 cbf\_require\_column\_value 2.3.64 cbf require column doublevalue

### 2.3.64 cbf\_require\_column\_doublevalue

### PROTOTYPE

#include "cbf.h"

int cbf require column doublevalue (cbf handle handle, const char \*columnname, double \*number, const double defaultvalue);

### DESCRIPTION

cbf require column doublevalue sets \*number to the value of the ASCII item at the current row for the column given with the name given by \*columnname, with the value interpreted as a decimal floating-point number, or to the number given by defaultvalue if the item cannot be found.

### ARGUMENTS

### handle CBF handle.

columnname Name of the column containing the number.

pointer to the location to receive the floating-point value. number

defaultvalue Value to use if the requested column and value cannot be found.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### SEE ALSO

2.3.46 cbf\_get\_value, cbf\_require\_value

- 2.3.47 cbf\_set\_value
- 2.3.48 cbf\_get\_typeofvalue

2.3.49 cbf\_set\_typeofvalue .3.51 cbf\_set\_integervalue

.3.52 cbf\_get\_doublevalue, cbf\_require\_doublevalue

2.3.56 cbf\_set\_integerarray, cbf\_set\_integerarray\_wdims, cbf\_set\_realarray, cbf\_set\_realarray\_wdims

2.3.62 cbf\_require\_column\_value

2.3.63 cbf require column integervalue

2.3.65 cbf get local integer byte order, cbf get local real byte order, cbf get local real format

### PROTOTYPE

#include "cbf.h"

int cbf\_get\_local\_integer\_byte\_order (char \*\* byte\_order); int cbf get local real byte order (char \*\* byte order); int cbf\_get\_local\_real\_format (char \*\* real\_format );

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### **CBFlib** Manual

51

### DESCRIPTION

cbf get local integer byte order returns the byte order of integers on the machine on which the API is being run in the form of a character string returned as the value pointed to by byte\_order. cbf\_get\_local\_real\_byte\_order returns the byte order of reals on the machine on which the API is being run in the form of a character string returned as the value pointed to by byte order. cbf get local real format returns the format of floats on the machine on which the API is being run in the form of a character string returned as the value pointed to by real\_format. The strings returned must not be modified in any way.

The values returned in byte\_order may be the strings "little\_endian" or "big-endian". The values returned in real\_format may be the strings "ieee 754-1985" or "other". Additional values may be returned by future versions of the API.

### ARGUMENTS

byte\_order pointer to the returned string

real format pointer to the returned string



Returns an error code on failure or 0 for success.

2.3.66 cbf get dictionary, cbf set dictionary, cbf require dictionary

PROTOTYPE

#include "cbf.h"

int cbf\_get\_dictionary (cbf\_handle handle, cbf\_handle \* dictionary); int cbf\_set\_dictionary (cbf\_handle handle, cbf\_handle dictionary\_in); int cbf\_require\_dictionary (cbf\_handle handle, cbf\_handle \* dictionary)

### DESCRIPTION

cbf\_get\_dictionary sets \*dictionary to the handle of a CBF which has been associated with the CBF handle by cbf\_set\_ dictionary. cbf set dictionary associates the CBF handle dictionary in with handle as its dictionary. cbf require\_ dictionary sets \*dictionary to the handle of a CBF which has been associated with the CBF handle by cbf set dictionary or creates a new empty CBF and associates it with handle, returning the new handle in \*dictionary.

### ARGUMENTS

handle CBF handle. dictionary Pointer to CBF handle of dictionary. dictionary\_in CBF handle of dcitionary. RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.3.67 cbf convert dictionary

PROTOTYPE

#include "cbf.h"

int cbf\_convert\_dictionary (cbf\_handle handle, cbf\_handle dictionary)

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### DESCRIPTION

cbf\_convert\_dictionary converts *dictionary* as a DDL1 or DDL2 dictionary to a CBF dictionary of category and item properties for *handle*, creating a new dictionary if none exists or layering the definitions in *dictionary* onto the existing dictionary of *handle* if one exists.

If a CBF is read into *handle* after calling cbf\_convert\_dictionary, then the dictionary will be used for validation of the CBF as it is read.

### ARGUMENTS

handle CBF handle.

dictionary CBF handle of dictionary.

RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.3.68 cbf\_find\_tag, cbf\_find\_local\_tag

### PROTOTYPE

#include "cbf.h"

int cbf\_find\_tag (cbf\_handle handle, const char \*tag)
int cbf\_find\_local\_tag (cbf\_handle handle, const char \*tag)

### DESCRIPTION

cbf\_find\_tag searches all of the CBF *handle* for the CIF tag given by the string *tag* and makes it the current tag. The search does not include the dictionary, but does include save frames as well as categories.

The string *tag* is the complete tag in either DDL1 or DDL2 format, starting with the leading underscore, not just a category or column.

### ARGUMENTS

handle CBF handle.

tag CIF tag. RETURN VALUE

Returns an error code on failure or 0 for success.

2.3.69 cbf\_find\_category\_root, cbf\_set\_category\_root, cbf\_require\_category\_root

### PROTOTYPE

#include "cbf.h"

int cbf\_find\_category\_root (cbf\_handle handle, const char\* categoryname, const char\*\* categoryroot); int cbf\_set\_category\_root (cbf\_handle handle, const char\* categoryname\_in, const char\*categoryroot); int cbf\_require\_category\_root (cbf\_handle handle, const char\*categoryname, const char\*categoryroot);

### DESCRIPTION

cbf\_find\_category\_root sets \*categoryroot to the root category of which categoryname is an alias. cbf\_set\_category\_root sets categoryname\_in as an alias of categoryroot in the dictionary associated with handle, creating the dictionary if

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

53

-----

necessary. cbf\_require\_category\_root sets \*categoryroot to the root category of which categoryname is an alias, if there is one, or to the value of categoryname, if categoryname is not an alias.

A returned categoryroot string must not be modified in any way.

### ARGUMENTS

handle	CBF handle.
categoryname	category name which may be an alias.
categoryroot	pointer to a returned category root name.
categoryroot_in	input category root name.

RETURN VALUE

Returns an error code on failure or 0 for success.

2.3.70 cbf\_find\_tag\_root, cbf\_set\_tag\_root, cbf\_require\_tag\_root

### PROTOTYPE

#include "cbf.h"

int cbf\_find\_tag\_root (cbf\_handle handle, const char\* tagname, const char\*\* tagroot); int cbf\_set\_tag\_root (cbf\_handle handle, const char\* tagname, const char\*tagroot\_in); int cbf\_require\_tag\_root (cbf\_handle handle, const char\* tagname, const char\*\* tagroot);

### DESCRIPTION

cbf\_find\_tag\_root sets \*tagroot to the root tag of which tagname is an alias. cbf\_set\_tag\_root sets tagname as an alias of tagroot\_in in the dictionary associated with handle, creating the dictionary if necessary. cbf\_require\_tag\_root sets \*tagroot to the root tag of which tagname is an alias, if there is one, or to the value of tagname, if tagname is not an alias.

A returned *tagroot* string must not be modified in any way.

### ARGUMENTS

handle CBF handle.

- tagname tag name which may be an alias.
- tagroot pointer to a returned tag root name.

*tagroot\_in* input tag root name. **RETURN VALUE** 

Returns an error code on failure or 0 for success.

### 2.3.71 cbf\_find\_tag\_category, cbf\_set\_tag\_category

PROTOTYPE

#include "cbf.h"

int cbf\_find\_tag\_category (cbf\_handle handle, const char\* tagname, const char\*\* categoryname); int cbf\_set\_tag\_category (cbf\_handle handle, const char\* tagname, const char\* categoryname\_in);

DESCRIPTION

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

cbf find tag category sets categoryname to the category associated with tagname in the dictionary associated with handle. cbf\_set\_tag\_category upddates the dictionary associated with handle to indicated that tagname is in category categoryname in.

ARGUMENTS handle CBF handle.

tag name. tagname

categoryname pointer to a returned category name.

categoryname\_in input category name.

### RETURN VALUE

Returns an error code on failure or 0 for success.

2.4 High-level function prototypes

2.4.1 cbf\_read\_template

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_read\_template (cbf\_handle handle, FILE \*file);

### DESCRIPTION

cbf\_read\_template reads the CBF or CIF file file into the CBF object specified by handle and selects the first datablock as the current datablock.

### ARGUMENTS

handle Pointer to a CBF handle.

file Pointer to a file descriptor.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.4.2 cbf\_get\_diffrn\_id, cbf\_require\_diffrn\_id

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_diffrn\_id (cbf\_handle handle, const char \*\*diffrn\_id); int cbf\_require\_diffrn\_id (cbf\_handle handle, const char \*\* diffrn\_id, const char \* default\_id)

### DESCRIPTION

cbf\_get\_diffrn\_id sets \*diffrn\_id to point to the ASCII value of the "diffrn.id" entry. cbf\_require\_diffrn\_id also sets \*diffrn\_id to point to the ASCII value of the "diffrn.id" entry, but, if the "diffrn.id" entry does not exist, it sets the value in the CBF and in\**diffrn\_id* to the character string given by *default\_id*, creating the category and column is necessary.

The *diffrn* id will be valid as long as the item exists and has not been set to a new value.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### **CBFlib** Manual

The diffrn\_id must not be modified by the program in any way.

ARGUMENTS

handle CBF handle.

diffrn id Pointer to the destination value pointer. default\_id Character string default value.

### RETURN VALUE

### Returns an error code on failure or 0 for success.

2.4.3 cbf\_set\_diffrn\_id

PROTOTYPE

#include "cbf\_simple.h"

int cbf\_set\_diffrn\_id (cbf\_handle handle, const char \*diffrn\_id);

### DESCRIPTION

cbf set diffrn id sets the "diffrn.id" entry of the current datablock to the ASCII value diffrn id.

This function also changes corresponding "diffrn\_id" entries in the "diffrn\_source", "diffrn\_radiation", "diffrn\_detector and "diffrn\_measurement" categories.

# RETURN VALUE

Returns an error code on failure or 0 for success.

2.4.4 cbf\_get\_crystal\_id PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_crystal\_id (cbf\_handle handle, const char \*\*crystal\_id);

DESCRIPTION

cbf\_get\_crystal\_id sets \*crystal\_id to point to the ASCII value of the "diffrn.crystal\_id" entry.

If the value is not ASCII, the function returns CBF BINARY.

The value will be valid as long as the item exists and has not been set to a new value.

The value must not be modified by the program in any way.

### ARGUMENTS

CBF handle. handle

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51





56









file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

int cbf\_set\_wavelength (cbf\_handle *handle*, double *wavelength*); DESCRIPTION

cbf\_set\_wavelength sets the current wavelength in Å to wavelength.

ARGUMENTS handle CBF handle. wavelength Wavelength in Å.

RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.4.8 cbf\_get\_polarization

PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_polarization (cbf\_handle handle, double \*polarizn\_source\_ratio, double \*polarizn\_source\_norm);

cbf\_get\_polarization sets \*polarizn\_source\_ratio and \*polarizn\_source\_norm to the corresponding source polarization parameters.

Either destination pointer may be NULL.

### ARGUMENTS

DESCRIPTION

handle CBF handle.

polarizn\_source\_ratio Pointer to the destination polarizn\_source\_ratio.

polarizn\_source\_norm Pointer to the destination polarizn\_source\_norm.

### RETURN VALUE

Returns an error code on failure or 0 for success.

2.4.9 cbf\_set\_polarization PROTOTYPE #include "cbf\_simple.h" int cbf\_set\_polarization (cbf\_handle handle, double polarizn\_source\_ratio, double polarizn\_source\_norm); DESCRIPTION cbf\_set\_polarization sets the source polarization to the values specified by polarizn\_source\_ratio and polarizn\_source\_ norm. ARGUMENTS handle CBF handle. polarizn\_source\_ratio New value of polarizn\_source\_ratio.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

polarizn\_source\_norm New value of polarizn\_source\_norm.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

# 2.4.10 cbf\_get\_divergence

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_divergence (cbf\_handle handle, double \*div\_x\_source, double \*div\_y\_source, double \*div\_xy\_source);

### DESCRIPTION

cbf\_get\_divergence sets \**div\_x\_source*, \**div\_y\_source* and \**div\_x\_y\_source* to the corresponding source divergence parameters.

Any of the destination pointers may be NULL.

### ARGUMENTS

handle CBF handle.

div_x_source	Pointer to the destination div_x_source.
div_y_source	Pointer to the destination div_y_source.
div_x_y_source	Pointer to the destination div_x_y_source.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.4.11 cbf\_ set\_divergence

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_set\_divergence (cbf\_handle handle, double div\_x\_source, double div\_y\_source, double div\_xy\_source);

### DESCRIPTION

cbf\_set\_divergence sets the source divergence parameters to the values specified by *div\_x\_source*, *div\_y\_source* and *div\_x\_y\_source*.

### ARGUMENTS

handle	CBF handle.
div_x_source	New value of div_x_source.
div_y_source	New value of div_y_source.
div_x_y_source	New value of div_x_y_source.

### **RETURN VALUE**

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

59

Returns an error code on failure or 0 for success.



element\_id Pointer to the destination.

### RETURN VALUE

Returns an error code on failure or 0 for success.

2.4.14 cbf\_get\_gain

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

### PROTOTYPE

#include "cbf simple.h"

int cbf\_get\_gain (cbf\_handle handle, unsigned int element\_number, double \*gain, double \*gain\_esd);

### DESCRIPTION

cbf\_get\_gain sets \*gain and \*gain\_esd to the corresponding gain parameters for element number element\_number.

Either of the destination pointers may be NULL.

### ARGUMENTS

### 

### RETURN VALUE

Returns an error code on failure or 0 for success.



### CBFlib Manual

int cbf\_get\_overload (cbf\_handle handle, unsigned int element\_number, double \*overload);

# DESCRIPTION

cbf\_get\_overload sets \*overload to the overload value for element number element\_number.

### ARGUMENTS

### handle CBF handle.

*element\_* The number of the detector element counting from 0 by order of appearance in the "diffrn\_data\_ *number* frame" category.

overload Pointer to the destination overload.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

### 2.4.17 cbf\_ set\_overload

PROTOTYPE

### #include "cbf\_simple.h"

int cbf\_set\_overload (cbf\_handle handle, unsigned int element\_number, double overload);

### DESCRIPTION

cbf\_set\_overload sets the overload value of element number *element\_number* to overload.

# ARGUMENTS

handle CBF handle. element\_ The number of the detector element counting from 0 by order of appearance in the "diffrn\_data\_

number frame" category.

overload New overload value.

### RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.4.18 cbf\_get\_integration\_time

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_integration\_time (cbf\_handle handle, unsigned int reserved, double \*time);

### DESCRIPTION

cbf\_get\_integration\_time sets \*time to the integration time in seconds. The parameter reserved is presently unused and should be set to 0.

# ARGUMENTS

handle CBF handle.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

CBI

*reserved* Unused. Any value other than 0 is invalid. *time* Pointer to the destination time.

**RETURN VALUE** 

Returns an error code on failure or 0 for success.

### 2.4.19 cbf\_set\_integration\_time

### PROTOTYPE

#include "cbf\_simple.h"

int cbf set integration time (cbf handle handle, unsigned int reserved, double time);

### DESCRIPTION

cbf\_set\_integration\_time sets the integration time in seconds to the value specified by *time*. The parameter *reserved* is presently unused and should be set to 0.

# ARGUMENTS handle CBF handle. reserved Unused. Any value other than 0 is invalid. time Integration time in seconds. RETURN VALUE Returns an error code on failure or 0 for success.

### 2.4.20 cbf\_get\_timestamp

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_timestamp (cbf\_handle handle, unsigned int reserved, double \*time, int \*timezone);

### DESCRIPTION

cbf\_get\_timestamp sets \*time to the collection timestamp in seconds since January 1 1970. \*timezone is set to timezone difference from UTC in minutes. The parameter reserved is presently unused and should be set to 0.

### Either of the destination pointers may be NULL.

### ARGUMENTS

- handleCBF handle.reservedUnused. Any value other than 0 is invalid.
- *time* Pointer to the destination collection timestamp.
- timezone Pointer to the destination timezone difference.

### RETURN VALUE

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

63

Returns an error code on failure or 0 for success.

### 2.4.21 cbf\_set\_timestamp

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_set\_timestamp (cbf\_handle handle, unsigned int reserved, double time, int timezone, double precision);

### DESCRIPTION

cbf\_set\_timestamp sets the collection timestamp in seconds since January 1 1970 to the value specified by *time*. The timezone difference from UTC in minutes is set to *timezone*. If no timezone is desired, *timezone* should be CBF\_NOTIM EZONE. The parameter *reserved* is presently unused and should be set to 0.

The precision of the new timestamp is specified by the value *precision* in seconds. If *precision* is 0, the saved timestamp is assumed accurate to 1 second.

### ARGUMENTS

- handle CBF handle.
- reserved Unused. Any value other than 0 is invalid.
- time Timestamp in seconds since January 1 1970.
- timezone Timezone difference from UTC in minutes or CBF\_NOTIMEZONE.
- precision Timestamp precision in seconds.

### RETURN VALUE

Returns an error code on failure or 0 for success.

# 2.4.22 cbf\_get\_datestamp

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_datestamp (cbf\_handle, unsigned int reserved, int \*year, int \*month, int \*day, int \*hour, int \*minute, double \*second, int \*timezone);

### DESCRIPTION

cbf\_get\_datestamp sets \*year, \*month, \*day, \*hour, \*minute and \*second to the corresponding values of the collection timestamp. \*timezone is set to timezone difference from UTC in minutes. The parameter < i>reserved is presently unused and should be set to 0.

- Any of the destination pointers may be NULL.
- ARGUMENTS
- handle CBF handle.
- reserved Unused. Any value other than 0 is invalid.
- year Pointer to the destination timestamp year.
- month Pointer to the destination timestamp month (1-12).

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51



Pointer to the destination timestamp day (1-31). day hour Pointer to the destination timestamp hour (0-23). Pointer to the destination timestamp minute (0-59). minute

second Pointer to the destination timestamp second (0-60.0).

timezone Pointer to the destination timezone difference from UTC in minutes.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

# 2.4.23 cbf\_set\_datestamp

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_set\_datestamp (cbf\_handle handle, unsigned int reserved, int year, int month, int day, int hour, int minute, double second, int timezone, double precision);

### DESCRIPTION

cbf\_set\_datestamp sets the collection timestamp in seconds since January 1 1970 to the value specified by time. The timezone difference from UTC in minutes is set to timezone. If no timezone is desired, timezone should be CBF NOTIM EZONE. The parameter reserved is presently unused and should be set to 0.

The precision of the new timestamp is specified by the value precision in seconds. If precision is 0, the saved timestamp is assumed accurate to 1 second.

### ARGUMENTS

handle CBF handle.

reserved Unused. Any value other than 0 is invalid.

Timestamp in seconds since January 1 1970. time

timezone Timezone difference from UTC in minutes or CBF NOTIMEZONE

precision Timestamp precision in seconds.

### RETURN VALUE

Returns an error code on failure or 0 for success.

# 2.4.24 cbf\_set\_current\_timestamp

PROTOTYPE

#include "cbf simple.h"

int cbf set current timestamp (cbf handle handle, unsigned int reserved, int timezone)

### DESCRIPTION



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### **CBFlib** Manual

65

cbf set current timestamp sets the collection timestamp to the current time. The timezone difference from UTC in minutes is set to timezone. If no timezone is desired, timezone should be CBF\_NOTIMEZONE. If no timezone is used,

the timest amp will be UTC. The parameter reserved is presently unused and should be set to 0.

The new timestamp will have a precision of 1 second.

### ARGUMENTS

handle CBF handle.

reserved Unused. Any value other than 0 is invalid.

timezone Timezone difference from UTC in minutes or CBF NOTIMEZONE

RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.4.25 cbf\_get\_image\_size, cbf\_get\_3d\_image\_size

### PROTOTYPE

#include "cbf simple.h"

int cbf\_get\_image\_size (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, size\_t\*ndim1, size\_t \*ndim2):

int cbf\_get\_3d\_image\_size (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, size\_t \*ndim1, size t\*ndim2, size t\*ndim3);

### DESCRIPTION

cbf\_get\_image\_size sets \*ndim1 and \*ndim2 to the slow and fast dimensions of the image array for element number element number. If the array is 1-dimensional, \*ndim1 will be set to the array size and \*ndim2 will be set to 1. If the array is 3-dimensional an error code will be returned. cbf\_get\_3d\_image\_size sets \**hdim1*, \**ndim2* and \**ndim3* to the slowest, next fastest and fastest dimensions, respectively, of the 3D image array for element number *element\_number*. If the array is 1-dimensional, \*ndim1 will be set to the array size and \*ndim2 and \*ndim3 will be set to 1. If the array is 2dimensional \*ndim1 and \*ndim2 will be set as for a call to cbf\_get\_image\_size and \*ndim3 will be set to 1.

Note that the ordering of dimensions is specified by values of the tag \_array\_structure\_list.precedence with a precedence of 1 for the fastest dimension, 2 for the next slower, etc., which is opposite to the ordering of the dimension arguments for these functions.

Any of the destination pointers may be NULL.

The parameter reserved is presently unused and should be set to 0.

handle	CBF handle.
reserved	Unused. Any value other than 0 is invalid.
element_ number	The number of the detector element counting from 0 by order of appearance in the "diffrn_data_ frame" category.
ndim1	Pointer to the destination slowest dimension.
ndim2	Pointer to the destination next faster dimension.
ndim3	Pointer to the destination fastest dimension.
RETURN VA	

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51





Returns an error code on failure or 0 for success.

### 2.4.26 cbf\_get\_image, cbf\_get\_real\_image, cbf\_get\_3d\_image, cbf\_get\_real\_3d\_image

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_image (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, void \*array, size\_t elsize, int elsign, size\_t ndim1, size\_t ndim2);

int cbf\_get\_real\_image (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, void \*array, size\_t elsize, size\_t ndim1, size\_t ndim2);

int cbf\_get\_3d\_image (cbf\_handle *handle*, unsigned int *reserved*, unsigned int *element\_number*, void \**array*, size\_t *elsize*, int *elsign*, size\_t *ndim1*, size\_t *ndim2*, size\_t *ndim3*);

int cbf\_get\_real\_3d\_image (cbf\_handle *handle*, unsigned int *reserved*, unsigned int *element\_number*, void \**array*, size\_t *elsize*, size\_t *ndim1*, size\_t *ndim3*, size\_t *ndim3*);

### DESCRIPTION

cbf\_get\_image reads the image array for element number *element\_number* into an *array*. The array consists of *ndim1xndim2* elements of *elsize* bytes each, starting at *array*. The elements are signed if *elsign* is non-0 and unsigned otherwise. cbf\_get\_real\_image reads the image array of IEEE doubles or floats for element number *element\_number* into an *array*. A real array is always signed. cbf\_get\_image reads the 3D image array for element number *element\_number into* an *array*. The array consists of *ndim1xndim3* elements of *elsize* bytes each, starting at *array*. The elements are signed if *elsign* is non-0 and unsigned otherwise. cbf\_get\_real\_3d\_image reads the 3D image array of IEEE doubles or floats for element number *element\_number* into an *array*. The signed if *elsign* is non-0 and unsigned otherwise. cbf\_get\_real\_3d\_image reads the 3D image array of IEEE doubles or floats for element number *element\_number* into an *array*. A real array is always signed.

The structure of the array as a 1-, 2- or 3-dimensional array should agree with the structure of the array given in the ARRAY\_STRUCTURE\_LIST category. If the array is 1-dimensional, *ndim1* should be the array size and *ndim2* and, for the 3D calls, *ndim3*, should be set to 1 both in the call and in the imgCIF data being processed. If the array is 2- dimensional and a 3D calls is used, *ndim1* and *ndim2* should be the array dimensions and *ndim3* should be set to 1 both in the call and in the imgCIF data being processed.

If any element in the binary data canOt fit into the destination element, the destination is set the nearest possible value.

If the value is not binary, the function returns CBF\_ASCII.

If the requested number of elements canOt be read, the function will read as many as it can and then return CBF\_ ENDOFDATA.

Currently, the destination *array* must consist of chars, shorts or ints (signed or unsigned) for cbf\_get\_image, or IEEE doubles or floats for cbf\_get\_real\_image. If *elsize* is not equal to sizeof (char), sizeof (short), sizeof (int), sizeof(double) or sizeof(float), the function returns CBF\_ARGUMENT.

The parameter reserved is presently unused and should be set to 0.

### ARGUMENTS

handle	CBF handle.
reserved	Unused. Any value other than 0 is invalid.
element_ number	The number of the detector element counting from 0 by order of appearance in the "diffrn_data_ frame" category.
array	Pointer to the destination array.
elsize	Size in bytes of each destination array element.
elsigned	Set to non-0 if the destination array elements are signed.
ndim1	Slowest array dimension.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

CBFlib Manual

67

08/07/07 09:24:51

 ndim2
 Next faster array dimension.

 ndim3
 Fastest array dimension.

 RETURN VALUE
 Returns an error code on failure or 0 for success.



### 2.4.27 cbf\_set\_image, cbf\_set\_real\_image, cbf\_set\_3d\_image, cbf\_set\_real\_3d\_image

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_set\_image (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, unsigned int compression, void \*array, size t elsize, int elsign, size\_t ndim1, size\_t ndim2); int cbf\_set\_real\_image (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, unsigned int compression, void \*array, size\_t elsize, size\_t ndim1, size\_t ndim2); int cbf\_set\_3d\_image (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, unsigned int compression, void \*array, size\_t elsize, size\_t ndim1, size\_t ndim2, size\_t ndim2=3); int cbf\_set\_real\_3d\_image (cbf\_handle handle, unsigned int reserved, unsigned int element\_number, unsigned int compression, void \*array, size\_t telsize, size\_t ndim1, size\_t ndim2, size\_t ndim2=3);

### DESCRIPTION

cbf\_set\_image writes the image array for element number *element\_number*. The *array* consists of *ndim1×ndim2* elements of *elsize* bytes each, starting at *array*. The elements are signed if *elsign* is non-0 and unsigned otherwise. cbf\_set\_real\_image writes the image array for element number *element\_number*. The *array* consists of *ndim1×ndim2* IEEE double or float elements of *elsize* bytes each, starting at *array*. cbf\_set\_3d\_image writes the 3D image array for element number *element\_number*. The *array* consists of *ndim1×ndim2* is elements are signed if *elsign* is non-0 and unsigned otherwise. cbf\_set\_3d\_image writes the 3D image array for element number *element\_number*. The *array* consists of *ndim1×ndim2×ndim3* elements of *elsize* bytes each, starting at *array*. The elements are signed if *elsign* is non-0 and unsigned otherwise. cbf\_set\_real\_3d\_image writes the 3D image array for element number *element\_number*. The *array* consists of *ndim1×ndim2×ndim3* IEEE double or float elements of *elsize* bytes each, starting at *array*.

If the array is 1-dimensional, *ndim1* should be the array size and *ndim2* and, for the 3D calls, *ndim3*, should be set to 1. If the array is 2-dimensional and the 3D calls are used, *ndim1* and *ndim2* should be used for the array dimensions and *ndim3* should be set to 1.

The array will be compressed using the compression scheme specifed by compression. Currently, the available schemes are:

CBF_CANONICAL	Canonical-code compression (section 3.3.1)	
CBF_PACKED	CCP4-style packing (section 3.3.2)	
CBF_PACKED_V2	CCP4-style packing, version 2 (section 3.3.2)	
CBF_BYTE_OFFSET	Simple "byte_offset" compression.	
CBF_NONE	No compression.	

The values compressed are limited to 64 bits. If any element in the array is larger than 64 bits, the value compressed is the nearest 64-bit value.

Currently, the source *array* must consist of chars, shorts or ints (signed or unsigned)for cbf\_set\_image, or IEEE doubles or floats for cbf\_set\_real\_image. If *elsize* is not equal to sizeof (short), sizeof (int), sizeof(double) or sizeof(float), the function returns CBF ARGUMENT.

The parameter *reserved* is presently unused and should be set to 0.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

# ARGUMENTS

CBF handle. handle reserved Unused. Any value other than 0 is invalid. element\_ The number of the detector element counting from 0 by order of appearance in the "diffrn\_data\_ frame" category. number Compression type. compression array Pointer to the image array. Size in bytes of each image array element. elsize Set to non-0 if the image array elements are signed. elsigned ndim1 Slow array dimension. Fast array dimension. ndim2

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

### 2.4.28 cbf\_get\_axis\_setting

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_axis\_setting (cbf\_handle *handle*, unsigned int *reserved*, const char \**axis\_id*, double \**start*, double \**increment*);

### DESCRIPTION

cbf\_get\_axis\_setting sets \*start and \*increment to the corresponding values of the axis axis\_id.

Either of the destination pointers may be NULL.

The parameter reserved is presently unused and should be set to 0.

### ARGUMENTS

handleCBF handle.reservedUnused. Any value other than 0 is invalid.

axis\_id Axis id.

start Pointer to the destination start value.

increment Pointer to the destination increment value.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

69

int cbf\_set\_axis\_setting (cbf\_handle *handle*, unsigned int *reserved*, const char *\*axis\_id*, double *start*, double *increment*);

# DESCRIPTION

cbf\_set\_axis\_setting sets the starting and increment values of the axis axis\_id to start and increment.

The parameter *reserved* is presently unused and should be set to 0.

### ARGUMENTS

- handle CBF handle.
- reserved Unused. Any value other than 0 is invalid.

axis\_id Axis id.

start Start value. increment Increment value

# RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.4.30 cbf\_construct\_goniometer

PROTOTYPE #include "cbf\_simple.h"

int cbf\_construct\_goniometer (cbf\_handle handle, cbf\_goniometer \*goniometer);

### DESCRIPTION

cbf\_construct\_goniometer constructs a goniometer object using the description in the CBF object handle and initialises the goniometer handle \*goniometer.

### ARGUMENTS

goniometer Pointer to the destination goniometer handle.

RETURN VALUE

handle

Returns an error code on failure or 0 for success.

CBF handle.

### 2.4.31 cbf\_free\_goniometer

PROTOTYPE

#include "cbf simple.h"

int cbf\_free\_goniometer (cbf\_goniometer goniometer);



cbf\_free\_goniometer destroys the goniometer object specified by *goniometer* and frees all associated memory. ARGUMENTS

 $file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html$ 

goniometer Goniometer handle to free.

Returns an error code on failure or 0 for success.

# 2.4.32 cbf\_get\_rotation\_axis

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_rotation\_axis (cbf\_goniometer goniometer, unsigned int reserved, double \*vector1, double \*vector2, double vector3);

### DESCRIPTION

cbf\_get\_rotation\_axis sets \*vector1, \*vector2, and \*vector3 to the 3 components of the goniometer rotation axis used for the exposure.

Any of the destination pointers may be NULL.

The parameter reserved is presently unused and should be set to 0.

### ARGUMENTS

goniometer Goniometer handle.

- reserved Unused. Any value other than 0 is invalid.
- *vector1* Pointer to the destination x component of the rotation axis.
- *vector2* Pointer to the destination y component of the rotation axis.
- *vector3* Pointer to the destination z component of the rotation axis.

### **RETURN VALUE**

Returns an error code on failure or 0 for success.

### 2.4.33 cbf\_get\_rotation\_range

### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_rotation\_range (cbf\_goniometer goniometer, unsigned int reserved, double \*start, double \*increment);

### DESCRIPTION

cbf\_get\_rotation\_range sets \*start and \*increment to the corresponding values of the goniometer rotation axis used for the exposure.

Either of the destination pointers may be NULL.

The parameter reserved is presently unused and should be set to 0.

### ARGUMENTS

goniometer Goniometer handle.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

### CBFlib Manual

71

 reserved
 Unused. Any value other than 0 is invalid.

 start
 Pointer to the destination start value.

 increment
 Pointer to the destination increment value.

### RETURN VALUE

Returns an error code on failure or 0 for success.

# 2.4.34 cbf\_rotate\_vector

PROTOTYPE

#include "cbf\_simple.h"

int cbf\_rotate\_vector (cbf\_goniometer goniometer, unsigned int reserved, double ratio, double initial1, double initial2, double initial3, double \*final1, double \*final2, double \*final3);

### DESCRIPTION

cbf\_rotate\_vector sets \*final1, \*final2, and \*final3 to the 3 components of the of the vector (*initial1*, *initial2*, *initial3*) after reorientation by applying the goniometer rotations. The value ratio specifies the goniometer setting and varies from 0.0 at the beginning of the exposure to 1.0 at the end, irrespective of the actual rotation range.

Any of the destination pointers may be NULL.

The parameter reserved is presently unused and should be set to 0.

### ARGUMENTS

goniometer Goniometer handle.

- reserved Unused. Any value other than 0 is invalid.
- ratio Goniometer setting. 0 = beginning of exposure, 1 = end.
- *initial1* x component of the initial vector.
- *initial2* y component of the initial vector.
- *initial3* z component of the initial vector.
- *vector1* Pointer to the destination x component of the final vector.
- *vector2* Pointer to the destination y component of the final vector.
- vector3 Pointer to the destination z component of the final vector.

# RETURN VALUE

Returns an error code on failure or 0 for success.

### 2.4.35 cbf\_get\_reciprocal

PROTOTYPE

### #include "cbf\_simple.h"

int cbf\_get\_reciprocal (cbf\_goniometer goniometer, unsigned int reserved, double ratio, double wavelength, double real1, double real2, double real3, double \*reciprocal1, double \*reciprocal2, double \*reciprocal3);

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html
## DESCRIPTION

cbf\_get\_reciprocal sets \**reciprocal1*, \* *reciprocal2*, and \* *reciprocal3* to the 3 components of the of the reciprocal-space vector corresponding to the real-space vector (*real1*, *real2*, *real3*). The reciprocal-space vector is oriented to correspond to the goniometer setting with all axes at 0. The value *wavelength* is the wavlength in Å and the value *ratio* specifies the current goniometer setting and varies from 0.0 at the beginning of the exposure to 1.0 at the end, irrespective of the actual rotation range.

Any of the destination pointers may be NULL.

#### The parameter reserved is presently unused and should be set to 0.

#### ARGUMENTS

goniometer Goniometer handle.

reserved Unused. Any value other than 0 is invalid.

*ratio* Goniometer setting. 0 = beginning of exposure, 1 = end.

wavelength Wavelength in Å.

reall x component of the real-space vector.

*real2* y component of the real-space vector.

*real3* z component of the real-space vector.

reciprocall Pointer to the destination x component of the reciprocal-space vector.

*reciprocal2* Pointer to the destination y component of the reciprocal-space vector. *reciprocal3* Pointer to the destination z component of the reciprocal-space vector.

#### RETURN VALUE

Returns an error code on failure or 0 for success.

2.4.36 cbf construct detector, cbf construct reference detector, cbf require reference detector

#### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_construct\_detector (cbf\_handle handle, cbf\_detector \*detector, unsigned int element\_number);

int cbf\_construct\_reference\_detector (cbf\_handle handle, cbf\_detector \*detector, unsigned int element\_number);

int cbf require reference detector (cbf handle handle, cbf detector \* detector, unsigned int element number);

#### DESCRIPTION

cbf\_construct\_detector constructs a detector object for detector element number *element\_number* using the description in the CBF object handle and initialises the detector handle \**detector*.

cbf\_construct\_reference\_detector constructs a detector object for detector element number *element\_number* using the description in the CBF object handle and initialises the detector handle \**detector* using the reference settings of the axes. cbf\_require\_reference\_detector is similar, but try to force the creations of missing intermediate categories needed to construct a detector object.

#### ARGUMENTS handle CBF handle.

detector Pointer to the destination detector handle.

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

73

08/07/07 09:24:51

#### CBFlib Manual

*element\_* The number of the detector element counting from 0 by order of appearance in the "diffrn\_data\_ *number* frame" category.

## RETURN VALUE

Returns an error code on failure or 0 for success.

## 2.4.37 cbf free detector

PROTOTYPE

#include "cbf\_simple.h"

int cbf\_free\_detector (cbf\_detector detector);

DESCRIPTION

cbf\_free\_detector destroys the detector object specified by detector and frees all associated memory.

ARGUMENTS detector Detector handle to free.

RETURN VALUE

Returns an error code on failure or 0 for success.

#### 2.4.38 cbf\_get\_beam\_center, cbf\_set\_beam\_center, set\_reference\_beam\_center

#### PROTOTYPE

#include "cbf simple.h"

int cbf\_get\_beam\_center (cbf\_detector detector, double \*index1, double \*index2, double \*center1, double \*center2);

int cbf\_set\_beam\_center (cbf\_detector detector, double \*index1, double \*index2, double \*center1, double \*center2);

int cbf\_set\_reference\_beam\_center (cbf\_detector *detector*, double \**index1*, double \**index2*, double \**center1*, double \**center2*);

#### DESCRIPTION

cbf\_get\_beam\_center sets \**center1* and \**center2* to the displacements in mm along the detector axes from pixel (0, 0) to the point at which the beam intersects the detector and \**index1* and \**index2* to the corresponding indices. cbf\_set\_ beam\_center sets the offsets in the axis category for the detector element axis with precedence 1 to place the beam center at the position given in mm by \**center1* and \**center2* as the displacements in mm along the detector axes from pixel (0, 0) to the point at which the beam intersects the detector at the indices given \**index1* and \**index2*. cbf\_set\_ reference\_beam\_center sets the reference offsets in the axis category for the the detector element axis with precedence 1 to place the beam center at the position given in mm by \**center1* and \**center2* as the displacements in mm along the detector axes from pixel (0, 0) to the point at which the beam intersects the detector at the indices given \**index1* and \**index2*. In order to achieve consistent results, a reference detector should be used for *detector* to have all axes at their reference settings.

Any of the destination pointers may be NULL for getting the beam center. For setting the beam axis, either the indices of the center must not be NULL.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

The indices are non-negative for beam centers within the detector surface, but the center for an axis with a negative increment will be negative for a beam center within the detector surface.

For cbf\_set\_beam\_center if the diffrn\_data\_frame category exists with a row for the corresponding element id, the values will be set for \_diffrn\_data\_frame.center\_fast and \_diffrn\_data\_frame.center\_slow in millimetres and the value of \_diffrn\_data\_frame.center\_units will be set to 'mm'.

For cbf\_set\_reference\_beam\_center if the diffrm\_detector\_element category exists with a row for the corresponding element id, the values will be set for \_diffrm\_detector\_element.reference\_center\_fast and \_diffrm\_detector\_ element.reference\_center\_fast and \_diffrm\_detector\_ element.reference\_center\_slow in millimetres and the value of \_diffrm\_detector\_element.reference\_units will be set to 'mm'.

## ARGUMENTS

- *detector* Detector handle. *index1* Pointer to the destination slow index.
- *index2* Pointer to the destination fast index.
- *center1* Pointer to the destination displacement along the slow axis.
- center2 Pointer to the destination displacement along the fast axis.

#### **RETURN VALUE**

Returns an error code on failure or 0 for success.

#### 2.4.39 cbf\_get\_detector\_distance

#### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_detector\_distance (cbf\_detector detector, double \*distance);

#### DESCRIPTION

cbf\_get\_detector\_distance sets \*distance to the nearest distance from the sample position to the detector plane.

#### ARGUMENTS

*detector* Detector handle. *distance* Pointer to the destination distance.

**RETURN VALUE** 

## Returns an error code on failure or 0 for success.

2.4.40 cbf\_get\_detector\_normal

#### PROTOTYPE

#include "cbf\_simple.h"



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

## CBFlib Manual

75

cbf\_get\_detector\_normal sets \*normal1, \*normal2, and \*normal3 to the 3 components of the of the normal vector to the detector plane. The vector is normalized.

Any of the destination pointers may be NULL.

#### ARGUMENTS

*detector* Detector handle.

*normal1* Pointer to the destination x component of the normal vector. *normal2* Pointer to the destination y component of the normal vector. *normal3* Pointer to the destination z component of the normal vector.

RETURN VALUE

Returns an error code on failure or 0 for success.

#### 2.4.41 cbf get pixel coordinates

PROTOTYPE

#### #include "cbf\_simple.h"

int cbf\_get\_pixel\_coordinates (cbf\_detector *detector*, double *index1*, double *index2*, double *\*coordinate1*, double *\*coordinate3*, double *\*coordinate3*);

## DESCRIPTION

cbf\_get\_pixel\_coordinates sets \*coordinate1, \*coordinate2, and \*coordinate3 to the vector position of pixel (*index1*, *index2*) on the detector surface. If *index1* and *index2* are integers then the coordinates correspond to the center of a pixel.

Any of the destination pointers may be NULL.

#### ARGUMENTS

detector Detector handle.

index1 Slow index.

index2 Fast index.

coordinate1 Pointer to the destination x component.

coordinate2 Pointer to the destination y component.

coordinate3 Pointer to the destination z component.

#### RETURN VALUE

Returns an error code on failure or 0 for success.



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html



CDI no Mandai

int cbf\_get\_pixel\_normal (cbf\_detector detector, double index1, double index2, double \*normal1, double \*normal2, double \*normal3);

## DESCRIPTION

cbf\_get\_detector\_normal sets \*normal1, \*normal2, and \*normal3 to the 3 components of the of the normal vector to the pixel at (*index1*, *index2*). The vector is normalized.

Any of the destination pointers may be NULL.

#### ARGUMENTS

*detector* Detector handle. *index1* Slow index.

index2 Fast index.

normall Pointer to the destination x component of the normal vector.

normal2 Pointer to the destination y component of the normal vector.

normal3 Pointer to the destination z component of the normal vector.

#### RETURN VALUE

Returns an error code on failure or 0 for success.

2.4.43 cbf\_get\_pixel\_area

INGIGINIE

#include "cbf\_simple.h"

int cbf\_get\_pixel\_area (cbf\_detector detector, double index1, double index2, double \*area, double \*projected\_area);

## DESCRIPTION

cbf\_get\_pixel\_area sets \*area to the area of the pixel at (*index1*, *index2*) on the detector surface and \*projected\_area to the apparent area of the pixel as viewed from the sample position.



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

## CBFlib Manual

77

#include "cbf\_simple.h"

int cbf\_get\_pixel\_size (cbf\_handle handle, unsigned int element\_number, unsigned int axis\_number, double \*psize);

## DESCRIPTION

cbf\_get\_pixel\_size sets \**psize* to point to the double value in millimeters of the axis *axis\_number* of the detector element *element\_number*. The *axis\_number* is numbered from 1, starting with the fastest axis.

If the pixel size is not given explcitly in the "array\_element\_size" category, the function returns CBF\_NOTFOUND.

#### ARGUMENTS

handle	CBF handle.
element_	The number of the detector element counting from 0 by order of appearance in the "diffrn_data_
number	frame" category.
axis_number	The number of the axis, fastest first, starting from 1.
psize	Pointer to the destination pixel size.

## RETURN VALUE

Returns an error code on failure or 0 for success.

## 2.4.45 cbf\_set\_pixel\_size

PROTOTYPE

#include "cbf\_simple.h"

int cbf\_set\_pixel\_size (cbf\_handle handle, unsigned int element\_number, unsigned int axis\_number, double psize);

## DESCRIPTION

cbf\_set\_pixel\_size sets the item in the &quote;size&quote; column of the "array\_structure\_list" category at the row which matches axis *axis\_number* of the detector element *element\_number* converting the double pixel size *psize* from meters to millimeters in storing it in the "size" column for the axis *axis\_number* of the detector element *element\_number*. The *axis\_number* is numberd from 1, starting with the fastest axis.

If the "array\_structure\_list" category does not already exist, it is created.

If the appropriate row in the "array\_structure\_list" catgeory does not already exist, it is created.

If the pixel size is not given explcitly in the "array\_element\_size category", the function returns CBF\_NOTFOUND.

ARGUMENTS handle CBF handle. The number of the detector element counting from 0 by order of appearance in the "diffrn\_data\_ element number frame" category. axis\_number The number of the axis, fastest first, starting from 1. The pixel size in millimeters. psize **RETURN VALUE** Returns an error code on failure or 0 for success.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html



cbf\_get\_unit\_cell sets cell[0:2] to the double values of the cell edge lengths a, b and c in Ångstroms, cell[3:5] to the double values of the cell angles  $\alpha$ ,  $\beta$  and  $\gamma$  in degrees, cell\_esd[0:2] to the double values of the estimated strandard deviations of the cell edge lengths a, b and c in Ångstroms, cell\_esd[3:5] to the double values of the estimated standard deviations of the the cell angles  $\alpha$ ,  $\beta$  and  $\gamma$  in degrees.

The values returned are retrieved from the first row of the "cell" category. The value of "\_cell.entry\_id" is ignored.

cell or cell\_esd may be NULL.

If cell is NULL, the cell parameters are not retrieved.

If cell\_esd is NULL, the cell parameter esds are not retrieved.

If the "cell" category is present, but some of the values are missing, zeros are returned for the missing values.

#### ARGUMENTS

handle CBF handle.

cellPointer to the destination array of 6 doubles for the cell parameters.

cell\_esd Pointer to the destination array of 6 doubles for the cell parameter esds.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

#### **CBFlib** Manual

79

**RETURN VALUE** 

Returns an error code on failure or 0 for success. No errors is returned for missing values if the "cell" category exists.

#### SEE ALSO

2.4.48 cbf\_set\_unit\_cell 2.4.49 cbf get reciprocal cel .4.50 cbf set reciprocal\_cell 2.4.51 cbf\_compute\_cell\_volur 2.4.52 cbf compute reciprocal cell



## 2.4.48 cbf set unit cell

PROTOTYPE

#include "cbf simple.h"

int cbf set unit cell (cbf handle handle, double cell[6], double cell esd[6]).

#### DESCRIPTION

cbf\_set\_unit\_cell sets the cell parameters to the double values given in cell[0:2] for the cell edge lengths a, b and c in Ångstroms, the double values given in cell[3:5] for the cell angles  $\alpha$ ,  $\beta$  and  $\gamma$  in degrees, the double values given in cell\_esd[0:2] for the estimated strandard deviations of the cell edge lengths a, b and c in Ångstroms, and the double values given in *cell\_esd*[3:5] for the estimated standard deviations of the the cell angles  $\alpha$ ,  $\beta$  and  $\gamma$  in degrees.

The values are placed in the first row of the "cell" category. If no value has been given for "\_cell.entry\_id", it is set to the value of the "diffrn.id" entry of the current data block.

cell or cell\_esd may be NULL.

If cell is NULL, the cell parameters are not set.

If cell\_esd is NULL, the cell parameter esds are not set.

If the "cell" category is not present, it is created. If any of the necessary columns are not present, they are created.

#### ARGUMENTS

- handle CBF handle.
- cell Pointer to the array of 6 doubles for the cell parameters.

cell\_esd Pointer to the array of 6 doubles for the cell parameter esds.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

#### **RETURN VALUE**

Returns an error code on failure or 0 for success.

SEE ALSO

#### 2.4.47 cbf get unit cel 2.4.49 cbf\_get\_reciproca 2.4.50 cbf\_set\_reciprocal\_cell

.4.51 cbf compute cell volum 4.52 cbf compute reciprocal ce

## SEE ALSO

## 2.4.49 cbf\_get\_reciprocal\_cell

PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_reciprocal\_cell (cbf\_handle handle, double cell[6], double cell\_esd[6]);

## DESCRIPTION

cbf\_get\_reciprocal\_cell sets *cell*[0:2] to the double values of the reciprocal cell edge lengths  $a^*$ ,  $b^*$  and  $c^*$  in Ångstroms<sup>-1</sup>, *cell*[3:5] to the double values of the reciprocal cell angles  $\alpha^*$ ,  $\beta^*$  and  $\gamma^*$  in degrees, *cell\_esd*[0:2] to the double values of the reciprocal cell edge lengths  $a^*$ ,  $b^*$  and  $c^*$  in Ångstroms<sup>-1</sup>, *cell\_esd*[3:5] to the double values of the estimated standard deviations of the the reciprocal cell angles  $\alpha^*$ ,  $\beta^*$  and  $\gamma^*$  in degrees.

The values returned are retrieved from the first row of the "cell" category. The value of "\_cell.entry\_id" is ignored.

cell or cell\_esd may be NULL.

If cell is NULL, the reciprocal cell parameters are not retrieved.

If *cell\_esd* is NULL, the reciprocal cell parameter esds are not retrieved.

If the "cell" category is present, but some of the values are missing, zeros are returned for the missing values.

## ARGUMENTS

handle CBF handle.

*cell* Pointer to the destination array of 6 doubles for the reciprocal cell parameters.

cell\_esd Pointer to the destination array of 6 doubles for the reciprocal cell parameter esds.

## **RETURN VALUE**

Returns an error code on failure or 0 for success. No errors is returned for missing values if the "cell" category exists.

#### SEE ALSO



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

#### CBFlib Manual

81

cbf\_set\_reciprocal\_cell sets the reciprocal cell parameters to the double values given in *cell*[0:2] for the reciprocal cell edge lengths  $a^*$ ,  $b^*$  and  $c^*$  in Ångstroms<sup>-1</sup>, the double values given in *cell*[3:5] for the reciprocal cell angles  $\alpha^*$ ,  $\beta^*$  and  $\gamma^*$  in degrees, the double values given in *cell\_esd*[0:2] for the estimated strandard deviations of the reciprocal cell edge lengths  $a^*$ ,  $b^*$  and  $c^*$  in Ångstroms, and the double values given in *cell\_esd*[3:5] for the estimated standard deviations of the reciprocal cell angles  $\alpha^*$ ,  $\beta^*$  and  $\gamma^*$  in degrees.

The values are placed in the first row of the "cell" category. If no value has been given for "\_cell.entry\_id", it is set to the value of the "diffrn.id" entry of the current data block.

cell or cell\_esd may be NULL.

If cell is NULL, the reciprocal cell parameters are not set.

If cell\_esd is NULL, the reciprocal cell parameter esds are not set.

If the "cell" category is not present, it is created. If any of the necessary columns are not present, they are created.

## ARGUMENTS

- handle CBF handle.
- *cell* Pointer to the array of 6 doubles for the reciprocal cell parameters. *cell\_esd* Pointer to the array of 6 doubles for the reciprocal cell parameter esds.

RETURN VALUE

#### Returns an error code on failure or 0 for success.

SEE ALSO

2.4.47 cbf get unit cell 2.4.48 cbf set unit cell 2.4.50 cbf get reciprocal cell 2.4.51 cbf compute cell volume 2.4.52 cbf compute reciprocal cell

## 2.4.51 cbf\_compute\_cell\_volume

## PROTOTYPE

#include "cbf\_simple.h"

int cbf\_compute\_cell\_volume ( double cell[6], double \*volume );

## DESCRIPTION

cbf\_compute\_cell\_volume sets \*volume to point to the volume of the unit cell computed from the double values in cell [0:2] for the cell edge lengths a, b and c in Angstroms and the double values given in cell[3:5] for the cell angles  $\alpha$ ,  $\beta$  and  $\gamma$  in degrees.

## ARGUMENTS

cell Pointer to the array of 6 doubles giving the cell parameters.

volume Pointer to the doubles for cell volume.

## **RETURN VALUE**

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

Returns an error code on failure or 0 for success.

SEE ALSO 2.4.46 cbf get unit cell 2.4.47 cbf set unit cell 2.4.50 cbf get reciprocal cell 2.4.50 cbf set reciprocal cell 2.4.52 cbf compute reciprocal cell

#### 2.4.52 cbf compute reciprocal cell

#### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_compute\_reciprocal\_cell ( double cell[6], double rcell[6]);

#### DESCRIPTION

cbf\_compute\_reciprocal\_cell sets *rcell* to point to the array of reciprocal cell parameters computed from the double values *cell*[0:2] giving the cell edge lengths a, b and c in Ångstroms, and the double values *cell*[3:5] giving the cell angles  $\alpha$ ,  $\beta$  and  $\gamma$  in degrees. The double values *rcell*[0:2] will be set to the reciprocal cell lengths a<sup>\*</sup>, b<sup>\*</sup> and c<sup>\*</sup> in Ångstroms<sup>-1</sup> and the double values *rcell*[3:5] will be set to the reciprocal cell angles  $\alpha^*$ ,  $\beta^*$  and  $\gamma^*$  in degrees.

#### ARGUMENTS

- cell Pointer to the array of 6 doubles giving the cell parameters.
- *rcell* Pointer to the destination array of 6 doubles giving the reciprocal cell parameters.
- *volume* Pointer to the doubles for cell volume.

#### **RETURN VALUE**

Returns an error code on failure or 0 for success.

#### SEE ALSO



#### 2.4.53 cbf\_get\_orientation\_matrix, cbf\_set\_orientation\_matrix

#### PROTOTYPE

#include "cbf\_simple.h"

int cbf\_get\_orientation\_matrix (cbf\_handle *handle*, double *ub\_matrix*[9]); int cbf\_set\_orientation\_matrix (cbf\_handle *handle*, double *ub\_matrix*[9]);

#### DESCRIPTION

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

#### CBFlib Manual

83

cbf\_get\_orientation\_matrix sets ub\_matrix to point to the array of orientation matrix entries in the "diffrn" category in the order of columns:



cbf\_set\_orientation\_matrix sets the values in the "diffrn" category to the values pointed to by ub\_matrix.

#### ARGUMENTS

#### handle CBF handle.

ubmatric Source or destination array of 9 doubles giving the orientation matrix parameters.

#### **RETURN VALUE**

Returns an error code on failure or 0 for success.



## 2.4.54 cbf\_get\_bin\_sizes, cbf\_set\_bin\_sizes

PROTOTYPE

#include "cbf\_simple.h"

DESCRIPTION

int cbf\_get\_bin\_sizes(cbf\_handle handle, unsigned int element\_number, double \* slowbinsize, double \* fastbinsize); int cbf\_set\_bin\_sizes(cbf\_handle handle, unsigned int element\_number, double slowbinsize\_in,double fastbinsize\_in);

cbf\_get\_bin\_sizes sets *slowbinsize* to point to the value of the number of pixels composing one array element in the dimension that changes at the second-fastest rate and *fastbinsize* to point to the value of the number of pixels composing one array element in the dimension that changes at the fastest rate for the detector element with the ordinal *element\_number*. cbf\_set\_bin\_sizes sets the the pixel bin sizes in the "array\_intensities" category to the values of *slowbinsize\_in* for the number of pixels composing one array element in the dimension that changes at the second-fastest rate and *fastbinsize\_in* for the number of pixels composing one array element in the dimension that changes at the fastest rate for the detector element with the ordinal *element\_number*.

In order to allow for software binning involving fractions of pixels, the bin sizes are doubles rather than ints.

#### ARGUMENTS

handle	CBF handle.
element_	The number of the detector element counting from 0 by order of appearance in the "diffrn_data
number	frame" category.
slowbinsize	Pointer to the returned number of pixels composing one array element in the dimension that changes at the second-fastest rate.
fastbinsize	Pointer to the returned number of pixels composing one array element in the dimension that changes at the fastest rate.
slowbinsize_in	The number of pixels composing one array element in the dimension that changes at the second-fastest rate.
fastbinsize_in	The number of pixels composing one array element in the dimension that changes at the fastest rate.
RETURN VALU	

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

# Returns an error code on failure or 0 for success.

#### 2.5 F90 function interfaces

At the suggestion of W. Kabsch, Fortran 90/95 routines have been added to CBFlib. As of this writing code has been written to allow the reading of CBF\_BYTE\_OFFSET, CBF\_PACKED and CBF\_PACKED\_V2 binary images. This code has been gather into FCBlib (Fortran Crystallographic Binary library) as lib/libfcb.

In general, most of the FCBlib functions return 0 for normal completion and a non-zero value in case of an error. In a few cases, such as FCB\_ATOL\_WCNT and FCB\_NBLEN\_ARRAY in order to conform to the conventions for commonly used C-equivalent functions, the function return is the value being computed.

For each function, an interface is given to be included in the declarations of your Fortran 90/95 code. Some functions in FCBIIB are not intended for external use and are subject to change: FCB\_UPDATE\_JPA\_POINTERS\_12, FCB\_UPDATE\_JPA\_POINTERS\_14, FCB\_UPDATE\_JPA\_POINTERS\_3D\_12, FCB\_UPDATE\_JPA\_POINTERS\_3D\_14 and CNT2PIX. These names should not be used for user routines.

The functions involving reading of a CBF have been done strictly in Fortran without the use of C code. This has required some compromises and the use of direct access I/O. Rather than putting the buffer and its control variables into COMMON these are passed as local arguments to make the routines inherently threadsafe' in a parallel programming environment. Note also, that a reading error could occur for the last record if it does not fill a full block. The code is written to recover from end-of-record and end-of-file errors, if possible. On many modern system, no special action is required, but on some systems it may be necessary to make use of the padding between the end of binary data and the terminal MIME boundary marker in binary sections. To ensure maximum portability of CBF files, a padding of 4095 bytes is recommended. Existing files without padding can be converted to files with padding by use of the new -p4 option for cif2cbf.

#### 2.5.1 FCB\_ATOL\_WCNT

INTERFACE		
INTEGER(8) FUNCTION FCB ATOL WCNT(ARRAY,	Ν.	CNT)
INTEGER(1), INTENT(IN):: ARRAY(N)		. ,
INTEGER, INTENT(IN):: N		
INTEGER, INTENT(OUT):: CNT		
END FUNCTION		
END INTERFACE		

FCB\_ATOL\_WCNT converts INTEGER(1) bytes in *ARRAY* of *N* bytes to an INTEGER(8) value returned as the function value. The number of bytes of *ARRAY* actually used before encountering a character not used to form the number is returned in *CNT*.

The scan stops at the first byte in ARRAY that cannot be properly parsed as part of the integer result.

ARGUMENTS ARRAY The array of INTEGER(1) bytes to be scanned

- N The INTEGER size of ARRAY
- *CNT* The INTEGER size of the portion of *ARRAY* scanned.

#### **RETURN VALUE**

Returns the INTEGER(8) value derived from the characters ARRAY(1:CNT) scanned.

#### 2.5.2 FCB\_CI\_STRNCMPARR

#### INTERFACE

INTEGER FUNCTION FCB CI\_STRNCMPARR(STRING>, ARRAY, N, LIMIT) CHARACTER(LEN=\*),INTENT(IN):: STRING>

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

## CBFlib Manual

85



The function FCB\_CI\_STRNCMPARR compares up to *LIMIT* characters of character string *STRING* and INTEGER(1) byte array *ARRAY* of dimension *N* in a case-insensitive manner, returning 0 for a match.

#### ARGUMENTS

STRING A character string

- ARRAY The array of INTEGER(1) bytes to be scanned
- N The INTEGER size of ARRAY
- N The INTEGER limit on the number of characters to consider in the comparison

#### **RETURN VALUE**

Returns 0 if the string and array match, a non-zero value otherwise.

#### 2.5.3 FCB\_EXIT\_BINARY



The function FCB\_EXIT\_BINARY is used to skip from the end of a binary section past any padding to the end of the text section that encloses the binary section. The values of the arguments must be consistent with those in the last call to FCB\_NEXT\_BINARY

ARGUMENTS	
TAPIN	The INTEGER Fortran device unit number assigned to image file.
LAST_CHAR	The last character (as an INTEGER(1) byte) read.
FCB_BYTES_IN_	The INTEGER number of bytes in a record.
REC	
BYTE_IN_FILE	The INTEGER byte (counting from 1) of the byte to read.
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.
BUFFER	The INTEGER(1) array of length FCB_BYTES_IN_REC to hold the appropriate record from TAPIN
PADDING	The INTEGER(8) number of bytes of padding after the binary data and before the closing MIME boundary.
RETURN VALUE	
Returns 0 if the funct necessary next line ca	tion is successful. Returns whatever non-zero error value is reported by <u>FCB_READ_LINE</u> if a annot be read.

#### SEE ALSO

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

#### CDFIID Mailuai

87

2.5.5 FCB\_NEXT\_BINARY 2.5.6 FCB\_OPEN\_CIFIN 2.5.9 FCB\_READ\_BYTE 2.5.11 FCB\_READ\_LINE

#### 2.5.4 FCB\_NBLEN\_ARRAY

INTERFACE
INTEGER FUNCTION FCB NBLEN ARRAY (ARRAY, ARRAYLEN)
INTEGER, INTENT(IN):: ARRAYLEN
INTEGER(1), INTENT(IN):: ARRAY(ARRAYLEN)
END FUNCTION
END INTERFACE

The function FCB\_NBLEN\_ARRAY returns the trimmed length of the INTEGER(1) byte array ARRAY of dimension ARRAYLEN after removal of trailing ASCII blanks, horizontal tabs (Z'09'), newlines (Z'0A') and carriage returns (Z'0D'). The resulting length may be zero.

The INTEGER trimmed length is returned as the function value.

#### ARGUMENTS

ARRAY The array of bytes for which the trimmed length is required ARRAYLEN The dimension of the array of bytes to be scanned.

#### **RETURN VALUE**

Returns the trimmed length of the array ARRAY.

#### 2.5.5 FCB\_NEXT\_BINARY



The function FCB\_NEXT\_BINARY skips to the start of the next binary section in the image file on unit *TAPIN* leaving the file positioned for a subsequent read of the image data. The skip may prior to the text field that contains the binary section. When the text filed is reached, it will be scanned for a MIME boundary marker, and, if it is found the subsequence MIME headers will be used to populate the arguments *ENCODING*, *SIZE*, *ID*, *DIGEST*, *COMPRESSION*, *BITS*, *VORZEICHEN*, *REELL*, *BYTEORDER*, *DIMOVER*, *DIM1*, *DIM2*, *DIM3*, *PADDING*.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

#### CBFlib Manual

The value returned in *ENCODING* is taken from the MIME header Content-Transfer-Encoding as an INTEGER. It is returned as 0 if not specified. The reported value is one of the integer values ENC\_NONE (Z'0001') for BINARY encoding, ENC\_BASE64 (Z'0002') for BASE64 encoding, ENC\_BASE32K (Z'0004') for X-BASE32K encoding, ENC\_QP (Z'0008') for QUOTED-PRINTABLE encoding, ENC\_BASE10 (Z'0010') for BASE10 encoding, ENC\_BASE16 (Z'0020') for BASE16 encoding or ENC\_BASE8 (Z'0040') for BASE8 encoding. At this time FCBlib only supports ENC\_NONE BINARY encoding.

The value returned in *SIZE* is taken from the MIME header X-Binary-Size as an INTEGER. It is returned as 0 if not specified.

The value returned in *ID* is taken from the MIME header X-Binary-ID as an INTEGER. It is returned as 0 if not specified.

The value returned in *DIGEST* is taken from the MIME header Content-MD5. It is returned as a character string. If no digest is given, an empty string is returned.

The value returned in *COMPRESSION* is taken from the MIME header Content-Type in the conversions parameter. The reported value is one of the INTEGER values CBF\_CANONICAL (Z'0050'), CBF\_PACKED (Z'0060'), CBF\_PACKED\_V2 (Z'0090'), CBF\_BYTE\_OFFSET (Z'0070'), CBF\_PREDICTOR (Z'0080'), CBF\_NONE (Z'0040'). Two flags may be combined with CBF\_PACKED or CBF\_PACKED\_V2: CBF\_UNCORRELATED\_SECTIONS (Z'0100') or CBF\_FLAT\_IMAGE (Z'0200'). At this time FCBlib does not support CBF\_PREDICTOR or CBF\_NONE compression.

The values returned in *BITS*, *VORZEICHEN* and *REELL* are the parameters of the data types of the elements. These values are taken from the MIME header X-Binary-Element-Type, which has values of the form "signed *BITS*-bit integer", "unsigned *BITS*-bit integer", "signed *BITS*-bit real IEEE" or "signed *BITS*-bit complex IEEE". If no value is given, *REELL* is reported as -1. If the value in one of the integer types, *REELL* is reported as 0. If the value is one of the real or complex types, *REELL* is reported as 1. In the current release of FCBlib only the integer types for *BITS* equal to 16 or 32 are supported.

The value returned in *BYTEORDER* is the byte order of the data in the image file as reported in the MIME header. The value, if specified, will be either the character string "LITTLE\_ENDIAN" or the character string "BIG\_ENDIAN". If no byte order is specified, "LITTLE\_ENDIAN" reported. This value is taken from the MIME header X-Binary-Element-Byte-Order. As of this writing, CBFlib will not generate "BIG\_ENDIAN" byte-order files. However, both CBFlib and FCBlib read "LITTLE\_ENDIAN" byte-order files, even on big-endian machines.

The value returned in *DIMOVER* is the overall number of elements in the image array, if specified, or zero, if not specified. This value is taken from the MIME header X-Binary-Number-of-Elements. The values returned in *DIM1*, *DIM2* and *DIM3* are the sizes of the fastest changing, second fastest changing and third fastest changing dimensions of the array, if specified, or zero, if not specified. These values are taken from the MIME header X-Binary-Size-Fastest-Dimension, X-Binary-Size-Second-Dimension and X-Binary-Size-Third-Dimension respectively.

The value returned in *PADDING* is the size of the post-data padding, if any, if specified or zero, if not specified. The value is given as a count of octets. This value is taken from the MIME header X-Binary-Size-Padding.

ARGUMENTS	
TAPIN	The INTEGER Fortran device unit number assigned to image file.
LAST_CHAR	The last character (as an INTEGER(1) byte) read.
FCB_BYTES_IN_	The INTEGER number of bytes in a record.
REC	
BYTE_IN_FILE	The INTEGER byte (counting from 1) of the byte to read.
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.
BUFFER	The INTEGER(1) array of length FCB_BYTES_IN_REC to hold the appropriate record from
	TAPIN
ENCODING	INTEGER type of encoding for the binary section as reported in the MIME header.

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html



file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

08/07/07 09:24:51

END FUNCTION			
END INTERFACE			
INTERFACE			
INTEGER FUNCTION FCB_DECOMPF		,NELEM,NELEM_READ, &	
ELSIGN, COMPRESSION, DIM1,			
TAPIN, FCB_BYTES_IN_REC, BY	TE_IN_FILE,	&	
REC_IN_FILE, BUFFER)			
INTEGER(4), INTENT(OUT):: .			
INTEGER(8), INTENT(OUT):: .			
INTEGER(8), INTENT(IN)::			
INTEGER, INTENT(IN)::			
INTEGER(8), INTENT(IN)::			
	TAPIN, FCB_BYTES_IN_REC		
INTEGER, INTENT(INOUT):: J			
INTEGER(1), INTENT(INOUT)::	BUFFER(FCB_BYTES_IN_REC)		
END FUNCTION			
END INTERFACE			

The functions FCB\_DECOMPRESS\_PACKED\_12, FCB\_DECOMPRESS\_PACKED\_14, FCB\_DECOMPRESS\_PACKED\_3D\_12 and FCB\_DECOMPRESS\_PACKED\_3D\_14, decompress images compress according the the CBF\_PACKED or CBF\_PACKED\_V2 compression described in section <u>3.3.2</u> on J. P. Abrahams CCP4 packed compression.

The relevant function should be called immediately after a call to <u>FCB\_NEXT\_BINARY</u>, using the values returned by <u>FCB\_NEXT\_BINARY</u> to select the appropriate version of the function.

#### ARGUMENTS

ARRAY	The array to receive the image	
NELEM	The INTEGER(8) number of elements to be read	
NELEM_READ	The INTEGER(8) returned value of the number of elements actually read	
ELSIGN	The INTEGER value of the flag for signed (1) OR unsigned (0) data	
<b>COMPRESSION</b>	The compression of the image	
DIMI	The INTEGER(8) value of the fastest dimension of ARRAY	
DIM2	The INTEGER(8) value of the second fastest dimension	
DIM3	The INTEGER(8) value of the third fastest dimension	
TAPIN	The INTEGER Fortran device unit number assigned to image file.	
FCB_BYTES_IN_	The INTEGER number of bytes in a record.	
REC		
BYTE_IN_FILE	The INTEGER byte (counting from 1) of the byte to read.	
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.	
BUFFER	The INTEGER(1) array of length FCB_BYTES_IN_REC to hold the appropriate record from TAPIN	

#### RETURN VALUE



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

#### CBFlib Manual

91

#### 2.5.8 FCB\_READ\_BITS

INTEGER FC		BITS(TAPIN, FCB_BYTES_IN_REC , BYTE IN FILE, BCOUNT, BBYTE,	
	BITCOUNT, II.		
INTEGER,		TAPIN, FCB BYTES IN REC	
		REC IN FILE, BYTE IN FILE	
		BUFFER(FCB BYTES IN REC)	
	INTENT(INOUT)::		
	, INTENT (INOUT) ::		
	INTENT(IN)::		
INTEGER,	INTENT (IN)::	LINT	
INTEGER (4	, INTENT(OUT)::	IINT(LINT)	
END FUNCTI	ON		
END INTERN	ACE		

The function FCB\_READ\_BITS gets the integer value starting at *BYTE\_IN\_FILE* from file TAPIN continuing through BITCOUNT bits, with sign extension. *BYTE\_IN\_FILE* is left at the entry value and not incremented. The resulting, sign-extended integer value is stored in the INTEGER(4) array *IINT* of dimension *LINT* with the least significant portion in *IINT*(1).

ARGUMENTS	
TAPIN	The INTEGER Fortran device unit number assigned to image file.
FCB_BYTES_IN_ REC	The INTEGER number of bytes in a record.
BUFFER	The INTEGER(1) array of length <i>FCB_BYTES_IN_REC</i> to hold the appropriate record from <i>TAPIN</i>
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.
BYTE_IN_FILE	The INTEGER byte (counting from 1) of the byte to read.
BCOUNT	The INTEGER count of bits remaining unused from the last call to FCB_READ_BITS.
BBYTE	The INTEGER(1) byte containing the unused bits from the last call to FCB_READ_BITS.
BITCOUNT	The INTEGER count of the number of bits to be extracted from the image file.
IINT	The INTEGER(4) array into which to store the value extracted from the image file.
LINT	The INTEGER length of the array <i>IINT</i> .

#### **RETURN VALUE**

Returns 0 if the function is successful. Because of the use of direct access I/O in blocks of size FCB\_BYTES\_IN\_REC the precise location of the end of file may not be detected.

SEE ALSO

```
2.5.3 FCB EXIT BINARY
2.5.5 FCB NEXT BINARY
2.5.6 FCB OPEN CIFIN
2.5.9 FCB READ BYTE
2.5.11 FCB READ LINE
```

#### 2.5.9 FCB\_READ\_BYTE

#### INTERFACE

INTEGER FUNCTION FCB\_READ\_BYTE(TAPIN,FCB\_BYTES\_IN\_REC, BUFFER, REC\_IN\_FILE,BYTE\_IN\_FILE,IBYTE) INTEGER, INTENT(IN):: TAPIN,FCB\_BYTES\_IN\_REC INTEGER, INTENT(INOUT):: REC\_IN\_FILE,BYTE\_IN\_FILE INTEGER(1),INTENT(INOUT):: BUFFER[FCB\_BYTES\_IN\_REC)

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

INTEGER(1), INTENT(OUT):: IBYTE END FUNCTION END INTERFACE

The function FCB\_READ\_BYTE reads the byte at the position  $BYTE_IN_FILE$  in the image file TAPIN. The first byte in the file is at  $BYTE_IN_FILE = 1$ .  $BYTE_IN_FILE$  should be set to the desired value before the call to the function and is not incremented within the function.

The function attempts to suppress the error caused by a read of a short last record, and in most systems cannot determine the exact location of the end of the image file, returning zero bytes until the equivalent of a full final record has been read.

#### ARGUMENTS

TAPIN	The INTEGER Fortran device unit number assigned to image file.		
FCB_BYTES_IN_	The INTEGER number of bytes in a record.		
REC			
BUFFER	The INTEGER(1) array of length FCB_BYTES_IN_REC to hold the appropriate record from TAPIN		
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.		
BYTE_IN_FILE	<i>LE</i> The INTEGER byte (counting from 1) of the byte to read.		
IBYTE	The INTEGER(1) byte found in the image file at the byte position BYTE_IN_FILE.		
RETURN VALUE			
Detume 0 if the functi	ing is an approximately provide the use of dimentioners 1/0 in blacks of size ECB, BYTES, IN, BEC,		

Returns 0 if the function is successful. Because of the use of direct access I/O in blocks of size FCB\_BYTES\_IN\_REC the precise location of the end of file may not be detected.

SEE ALSO



2.5.10 FCB\_READ\_IMAGE\_12, FCB\_READ\_IMAGE\_14, FCB\_READ\_IMAGE\_3D\_12, FCB\_READ\_IMAGE\_3D\_14



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

93

**CBFlib** Manual

#### ELSIGN, COMPRESSION, DIM1, DIM2, PADDING, TAPIN, FCB BYTES IN REC, BYTE IN FILE, REC IN FILE BUFFER INTEGER(4), INTENT(OUT):: ARRAY(DIM1,DIM2) INTEGER(8), INTENT (OUT) :: NELEM READ INTEGER(8), INTENT(IN):: NELEM INTEGER . INTENT(IN):: ELSIGN INTEGER . INTENT(OUT):: COMPRESSION INTEGER(8), INTENT(IN):: DIM1, DIM2 INTEGER(8), INTENT (OUT) :: PADDING INTENT (IN):: TAPIN, FCB BYTES IN REC INTENT (INOUT):: REC IN FILE, BYTE IN FILE INTEGER INTEGER . INTEGER(1), INTENT(INOUT):: BUFFER(FCB BYTES IN REC) END FUNCTION END INTERFACE INTERFACE INTEGER FUNCTION FCB READ IMAGE 3D 12(ARRAY, NELEM, NELEM READ, ELSIGN, COMPRESSION, DIM1, DIM2, DIM3, PADDING, TAPIN, FCB\_BYTES\_IN\_REC, BYTE\_IN\_FILE, REC\_IN\_FILE, BUFFER) \_\_\_\_\_\_ INTEGER(2), INTENT(OUT):: ARRAY(DIM1,DIM2,DIM3) INTENT(OUT):: NELEM READ INTEGER(8), INTEGER(8), INTENT(IN):: NELEM INTEGER, INTENT(IN):: ELSIGN INTENT(OUT):: COMPRESSION INTEGER . INTEGER(8), INTENT(IN):: DIM1, DIM2, DIM3 INTEGER(8), INTENT(OUT):: PADDING INTEGER, INTENT(IN):: TAPIN, FCB\_BYTES\_IN\_REC INTEGER, INTENT(INOUT):: REC\_IN\_FILE, BYTE\_IN\_FILE INTEGER(1), INTENT(INOUT):: BUFFER(FCB\_BYTES\_IN\_REC) END FUNCTION END INTERFACE INTERFACE INTEGER FUNCTION FCB READ IMAGE 3D I4 (ARRAY, NELEM, NELEM READ, ELSIGN, COMPRESSION, DIM1, DIM2, DIM3, PADDING, TAPIN, FCB BYTES IN REC, BYTE IN FILE REC\_IN\_FILE, BUFFER) INTEGER (4), INTENT (OUT):: ARRAY(DIM1,DIM2,DIM3) INTEGER(8), INTENT (OUT) :: NELEM READ INTENT (IN) :: NELEM INTEGER(8), INTEGER, INTENT(IN):: ELSIGN INTEGER, INTENT(OUT):: COMPRESSION INTENT(IN):: DIM1, DIM2, DIM3 INTEGER(8). INTEGER(8), INTENT (OUT) :: PADDING INTENT(IN):: TAPIN, FCB\_BYTES\_IN\_REC INTEGER. INTEGER, INTENT(INOUT):: REC IN FILE, BYTE IN FILE INTEGER(1), INTENT(INOUT):: BUFFER(FCB\_BYTES\_IN\_REC)

The function FCB\_READ\_IMAGE\_I2 reads a 16-bit twos complement INTEGER(2) 2D image. The function FCB\_ READ\_IMAGE\_I4 read a 32-bit twos complement INTEGER(4) 2D image. The function FCB\_READ\_IMAGE\_3D\_I4 reads a 32-bit twos reads a 16-bit twos complement INTEGER(2) 3D image. The function FCB\_READ\_IMAGE\_3D\_I4 reads a 32-bit twos complement INTEGER(4) 3D image. In each case the image is compressed either by a BYTE\_OFFSET algorithm by W. Kabsch based on a proposal by A. Hammersley or by a PACKED algorithm by J. P. Abrahams as used in CCP4, with modifications by P. Ellis and H. J. Bernstein.

The relevant function automatically first calls <u>FCB\_NEXT\_BINARY</u> to skip to the next binary section and then starts to read. An error return will result if the parameters of this call are inconsistent with the values in MIME header.

#### ARGUMENTS

END FUNCTION

ARRAY	The array to receive the image
NELEM	The INTEGER(8) number of elements to be read
NELEM_READ	The INTEGER(8) returned value of the number of elements actually read
ELSIGN	The INTEGER value of the flag for signed (1) OR unsigned (0) data

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

COMPRESSION	The actual communication of the image	BUFFER The INTEGER(1) array of length FCB BYTES IN REC to hold the appropria	to more of C
COMPRESSION DIM1	The actual compression of the image The INTEGER(8) value of the fastest dimension of <i>ARRAY</i>	BUFFER The INTEGER(1) array of length FCB_BYTES_IN_REC to hold the appropria TAPIN.	te record fi
DIMI DIM2	The INTEGER(8) value of the fastest dimension	LINE The INTEGER(1) array of length N to hold the line to be read from TAPIN.	
DIM2 DIM3	The INTEGER(8) value of the third fastest dimension	<i>N</i> The INTEGER dimension of <i>LINE</i> .	
TAPIN	The INTEGER Fortran device unit number assigned to image file.	LINELEN The INTEGER number of characters read into LINE.	
FCB_BYTES_IN_	The INTEGER number of bytes in a record.		
REC	The INTEGER humber of bytes in a fectral.	RETURN VALUE	
BYTE_IN_FILE	The INTEGER byte (counting from 1) of the byte to read.	Returns 0 if the function is successful.	
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.	SEE ALSO	
BUFFER	The INTEGER(1) array of length FCB_BYTES_IN_REC to hold the appropriate record from		
	TAPIN	2.5.3 FCB_EXIT_BINARY 2.5.5 FCB_NEXT_BINARY	
RETURN VALUE		2.5.6 FCB OPEN CIFIN	
ALIUKIN VALUE		2.5.7 FCB_DECOMPRESS: FCB_DECOMPRESS_PACKED_12, FCB_DECOMPRESS_PACKED_14	4, FCB_
Returns 0 if the funct	tion is successful.	DECOMPRESS_PACKED_3D_12, FCB_DECOMPRESS_PACKED_3D_14 2.5.9 FCB_READ_BYTE	
SEE ALSO		2.5.12 FCB_READ_XDS_12	
2.5.3 FCB_EXIT_BI		INTERFACE	
2.5.5 FCB_NEXT_B 2.5.6 FCB_OPEN_C		INTEGER FUNCTION FCB READ XDS 12(FILNAM, TAPIN, NX, NY, IFRAME, JFRAME)	
	PRESS: FCB_DECOMPRESS_PACKED_12, FCB_DECOMPRESS_PACKED_14, FCB_	CHARACTER(len=*), INTENT(IN) :: FILNAM INTEGER, INTENT(IN) :: TAPIN, NX, NY	
DECOMPRESS PAG	CKED 3D I2, FCB DECOMPRESS PACKED 3D I4	INTEGER(2), INTENT(OUT):: IFRAME(NX*NY) INTEGER(4), INTENT(OUT):: JFRAME(NX,NY)	
2.5.9 FCB_READ_B 2.5.11 FCB_READ_		END FUNCTION	
		END INTERFACE	
2.5.11 FCB_READ	TINE	The function FCB_READ_XDS_I2 read a 32-bit integer twos complement image into a 16-bit INTEGE using the CBF_BYTE_OFFSET, CBF_PACKED or CBF_PACKED_V2 compressions for the 32-bit da	ER(2) XDS
2.5.11 FCD_READ_		OFFSET algorithm is a variant of the September 2006 version by W. Kabsch which was based on a sug	
INTERFACE	CTION FCB_READ_LINE(TAPIN, LAST_CHAR, FCB_BYTES_IN_REC, &	Hammersley and which was further modified by H. Bernstein.	J) (
	BYTE IN FILE, REC IN FILE, BUFFER, LINE, N, LINELEN)	The file named FILNAM is opened on the logical unit TAPIN and FCB_NEXT_BINARY is used to skip	to the nex
	INTENT (IN):: TAPIN, FCB BYTES IN REC, N INTENT (INOUT):: BYTE_IN_FILE, REC_IN_FILE	binary image. The binary image is then decompressed to produce an XDS 16-bit integer image array IF	
INTEGER, INTEGER(1),	INTENT(OUT):: LINELEN INTENT(INOUT):: LAST_CHAR, BUFFER, (FCB_BYTES_IN_REC)	NX by NY. The dimensions must agree with the dimensions specified in MIME header.	
INTEGER(1), END FUNCTION	INTENT(OUT):: LINE(N)	The conversion from a 32-bit integer I32 to 16-bit XDS pixel I16 is done as per W. Kabsch as follows: T	
END FUNCTION END INTERFA		limited to the range $-1023 \le 132 \le 1048576$ . If 132 is outside that range it is truncated to the closer boun	dary. The
The function FCB_R	EAD_LINE reads successive bytes into the INTEGER(1) byte array LINE of dimension N),	generate II6, the 16-bit result, if I32 > 32767, it is divided by 32 (producing a number between 1024 an then negated (producing a number between -1024 and -32768).	ia 32768),
stopping at N bytes o	or the first error or the first CR (Z'0D') or LF (Z'0A'), whichever comes first. It discards an LF after a		
CR. The variable LA.	<i>ST_CHAR</i> is checked for the last character from the previous line to make this determination.	For CBF_BYTE_OFFSET this conversion can be done on the fly directly into the target array <i>IFRAME</i> CBF_PACKED or CBF_PACKED_V2, the full 32 bit precision is needed during the decompression, for	, but for the
The actual number of	f bytes read into the line, not including any terminal CR or LF is stored in LINELEN.	an intermediate INTEGER(4) array <i>JFRAME</i> to hold the 32-bit image in that case.	neing the
ARGUMENTS		The image file is closed after reading one image.	
TAPIN	The INTEGER Fortran device unit number assigned to image file.	ARGUMENTS	
LAST_CHAR	The INTEGER(1) byte holding the ASCII value of the last character read for each line read.	FILNAM The character string name of the image file to be opened.	
FCB_BYTES_IN_	The INTEGER number of bytes in a record.	TAPIN The INTEGER Fortran device unit number assigned to image file.	
REC		NX The INTEGER fast dimension of the image array.	
BYTE_IN_FILE	The INTEGER byte (counting from 1) of the byte to read.	<i>NY</i> The INTEGER slow dimension of the image array.	
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.	<i>IFRAME</i> The INTEGER(2) XDS image array.	
		in found The invited Ex(2) ADO image allay.	

97

JFRAME The INTEGER(4) 32-bit image scratch array needed for CBF PACKED or CBF PACKED V2 images.

## RETURN VALUE

Returns 0 if the function is successful, CBF FORMAT (=1) if it cannot handle this CBF format (not implemented), -1 if it cannot determine endian architecture of this machine, -2: if it cannot open the image file, -3: if it finds the wrong image format and -4 if it cannot read the image.

#### 2.5.13 FCB SKIP WHITESPACE

#### INTERFACE

INTEGER FUNCTION FCB SKIP WHITESPACE (TAPIN, LAST CHAR,	&
FCB BYTES IN REC, BYTE IN FILE, REC IN FILE, BUFFER, &	
LINE, N, LINELEN, ICUR, FRESH LINE)	
INTEGER, INTENT(IN):: TAPIN, FCB BYTES IN REC, N	
INTEGER, INTENT(INOUT):: BYTE IN FILE, REC IN FILE, LINELEN, ICUR,	&
FRESH LINE	
INTEGER(1), INTENT(INOUT):: BUFFER(FCB BYTES IN REC), LINE(N),	&
LAST CHAR	
END INTERFACE	

The function FCB\_SKIP\_WHITESPACE skips forward on the current INTEGER(1) byte array LINE of size N with valid data in LINE(1:LINELEN) from the current position ICUR moving over MIME header whitespace and comments, reading new lines into LINE if needed. The flag FRESH\_LINE indicates that a fresh line should be read on entry.

## ARGUMENTS

TAPIN	The INTEGER Fortran device unit number assigned to image file.
LAST_CHAR	The INTEGER(1) byte holding the ASCII value of the last character read for each line read.
FCB_BYTES_IN_	The INTEGER number of bytes in a record.
REC	
BYTE_IN_FILE	The INTEGER byte (counting from 1) of the byte to read.
REC_IN_FILE	The INTEGER record number (counting from 1) of next record to read.
BUFFER	The INTEGER(1) array of length <i>FCB_BYTES_IN_REC</i> to hold the appropriate record from <i>TAPIN</i> .
LINE	The INTEGER(1) array of length N to hold the line to be read from TAPIN.
Ν	The INTEGER dimension of LINE.
LINELEN	The INTEGER number of characters read into LINE.
ICUR	The INTEGER position within the line.
FRESH_LINE	The INTEGER flag that a fresh line is needed.
RETURN VALUE	
Returns 0 if the function	n is successful.
SEE ALSO	
2.5.6 FCB OPEN CIF 2.5.7 FCB DECOMPR	ARY IN ESS: FCB_DECOMPRESS_PACKED_12, FCB_DECOMPRESS_PACKED_14, FCB (ED_3D_12, FCB_DECOMPRESS_PACKED_3D_14
file://localhost/Users/yay	/a/Desktop/nCBF/CBFlib_bleeding_edge/doc/CBFlib.html 08/07/07 09:24:51

#### CBFlib Manual

## 3. File format

#### 3.1 General description

With the exception of the binary sections, a CBF file is an mmCIF-format ASCII file, so a CBF file with no binary sections is a CIF file. An imgCIF file has any binary sections encoded as CIF-format ASCII strings and is a CIF file whether or not it contains binary sections. In most cases, CBFlib can also be used to access normal CIF files as well as CBF and imgCIF files.

#### 3.2 Format of the binary sections

Before getting to the binary data itself, there are some preliminaries to allow a smooth transition from the conventions of CIF to those of raw or encoded streams of "octets" (8-bit bytes). The binary data is given as the essential part of a specially formatted semicolon-delimited CIF multi-line text string. This text string is the value associated with the tag \_array\_data.data".

The specific format of the binary sections differs between an imgCIF and a CBF file.

#### 3.2.1 Format of imgCIF binary sections

Each binary section is encoded as a semicolon-delimited string. Within the text string, the conventions developed for transmitting email messages including binary attachments are followed. There is secondary ASCII header information. formatted as Multipurpose Internet Mail Extensions (MIME) headers (see RFCs 2045-49 by Freed, et al.). The boundary marker for the beginning of all this is the special string

--CIF-BINARY-FORMAT-SECTION--

at the beginning of a line. The initial "--" says that this is a MIME boundary. We cannot put "###" in front of it and conform to MIME conventions. Immediately after the boundary marker are MIME headers, describing some useful information we will need to process the binary section. MIME headers can appear in different orders, and can be very confusing (look at the raw contents of a email message with attachments), but there is only one header which is has to be understood to process an imgCIF: "Content-Transfer-Encoding". If the value given on this header is "BINARY", this is a CBF and the data will be presented as raw binary, containing a count (in the header described in 3.2.2 Format of CBF binary sections) so that we'll know when to start looking for more information.

If the value given for "Content-Transfer-Encoding" is one of the real encodings: "BASE64", "QUOTED-PRINTABLE", "X-BASE8", "X-BASE10" or "X-BASE16", the file is an imgCIF, and we'll need some other headers to process the encoded binary data properly. It is a good practice to give headers in all cases. The meanings of various encodings is given in the CBF extensions dictionary, cif img 1.5.3.dic, as one html file, or as separate pages for each defintion.

For certain compressions (e.g. CBF PACKED) MIME headers are essential to determine the parameters of the compression. The full list of MIME headers recognized by and generated by CBFlib is:

- Content-Type:
- Content-Transfer-Encoding:
- Content-MD5:
- X-Binary-Size:
- X-Binary-ID:
- X-Binary-Element-Type:
- X-Binary-Element-Byte-Order:
- X-Binary-Number-of-Elements:
- X-Binary-Size-Fastest-Dimension: X-Binary-Size-Second-Dimension:
- X-Binary-Size-Third-Dimension:
- X-Binary-Size-Padding:

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

Content-Type:

The "Content-Type" header tells us what sort of data we have (currently always "application/octet-stream" for a miscellaneous stream of binary data) and, optionally, the conversions that were applied to the original data. The default is to compress the data with the "CBF-PACKED" algorithm. The Content-Type may be any of the discrete types permitted in RFC 2045; "application/octet-stream" is recommended. If an octet stream was compressed, the compression should be specified by the parameter 'conversions="X-CBF\_PACKED" or the parameter 'conversions="X-CBF\_CANONICAL"" or t

If the parameter 'conversions="**X**-CBF\_PACKED" or 'conversions="**X**-CBF\_PACKED\_V2"' is given it may be further modified with the parameters "uncorrelated\_sections"' or "flat"

If the "uncorrelated\_sections" parameter is given, each section will be compressed without using the prior section for averaging. If the "flat" parameter is given, each the image will be treated as one long row.

Content-Transfer-Encoding:

The "Content-Transfer-Encoding" may be 'BASE64', 'Quoted-Printable', 'X-BASE8', 'X-BASE10', 'X-BASE16' or 'X-BASE32K', for an imgCIF or 'BINARY' for a CBF. The octal, decimal and hexadecimal transfer encodings are provided for convenience in debugging and are not recommended for archiving and data interchange.

In a CIF, one of the parameters 'charset=us-ascii', 'charset=utf-8' or 'charset=utf-16' may be used on the Content-Transfer-Encoding to specify the character set used for the external presentation of the encoded data. If no charset parameter is given, the character set of the enclosing CIF is assumed. In any case, if a BOM flag is detected (FE FF for big-endian UTF-16, FF EF for little-endian UTF-16 or EF BB BF for UTF-8) is detected, the indicated charset will be assumed until the end of the encoded data or the detection of a different BOM. The charset of the Content-Transfer-Encoding is not the character set of the encoded data, only the character set of the presentation of the encoded data and should be respecified for each distinct STAR string.

In an imgCIF file, the encoded binary data begins after the empty line terminating the header. In an imgCIF file, the encoded binary data ends with the terminating boundary delimiter 'n-CIF-BINARY-FORMAT-SECTION----' in the currently effective charset or with the 'n; ' that terminates the STAR string.

In a CBF, the raw binary data begins after an empty line terminating the header and after the sequence:

Octet	Hex	Decimal	Purpose
0	0C	12	(ctrl-L) Page break
1	1A	26	(ctrl-Z) Stop listings in MS-DOS
2	04	04	(Ctrl-D) Stop listings in UNIX
3	D5	213	Binary section begins

None of these octets are included in the calculation of the message size or in the calculation of the message digest.

• Content-MD5:

An MD5 message digest may, optionally, be used. The 'RSA Data Security, Inc. MD5 Message-Digest Algorithm' should be used. No portion of the header is included in the calculation of the message digest. The optional "Content-MD5" header provides a much more sophisticated check on the integrity of the binary data than size checks alone can provide.

• X-Binary-Size:

The "X-Binary-Size" header specifies the size of the equivalent binary data in octets. This is the size **after** any compressions, but before any ascii encodings. This is useful in making a simple check for a missing portion of this file. The 8 bytes for the Compression type (see below) are not counted in this field, so the value of "X-Binary-Size" is 8 less than the quantity in bytes 12-19 of the raw binary data (3.2.2 Format of CBF binary sections).

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

08/07/07 09:24:51

#### CBFlib Manual

90

- X-Binary-ID: The "X-Binary-ID" header should contain the same value as was given for "\_array\_data.binary\_id".
- X-Binary-Element-Type:

The "X-Binary-Element-Type" header specifies the type of binary data in the octets, using the same descriptive phrases as in <u>array structure encoding type</u>. The default value is 'unsigned 32-bit integer'.

• X-Binary-Element-Byte-Order:

The "X-Binary-Element-Byte-Order" can specify either "BIG\_ENDIAN" or "LITTLE\_ENDIAN" byte order of the image data. CBFlib only writes "LITTLE\_ENDIAN", and in general can only process LITTLE\_ENDIAN even on machines that are BIG\_ENDIAN.

• X-Binary-Number-of-Elements:

The "X-Binary-Number-of-Elements" specifies the number of elements (not the number of octets) in the decompressed, decoded image.

• X-Binary-Size-Fastest-Dimension:

The optional "X-Binary-Size-Fastest-Dimension" specifies the number of elements (not the number of octets) in one row of the fastest changing dimension of the binary data array. This information must be in the MIME header for proper operation of some of the decompression algorithms.

X-Binary-Size-Second-Dimension:

The optional "X-Binary-Size-Second-Dimension" specifies the number of elements (not the number of octets) in one column of the second-fastest changing dimension of the binary data array. This information must be in the MIME header for proper operation of some of the decompression algorithms.

• X-Binary-Size-Third-Dimension:

The optional "X-Binary-Size-Third-Dimension" specifies the number of sections for the third-fastest changing dimension of the binary data array.

X-Binary-Size-Padding:

The optional "X-Binary-Size-Padding" specifies the size in octets of an optional padding after the binary array data and before the closing flags for a binary section. CBFlib always writes this padding as zeros, but this information should be in the MIME header for a binary section that uses padding, especially if non-zero padding is used.

A blank line separator immediately precedes the start of the encoded binary data. Blank spaces may be added prior to the preceding "line separator" if desired (e.g. to force word or block alignment).

Because CBFLIB may jump forward in the file from the MIME header, the length of encoded data cannot be greater than the value defined by "X-Binary-Size" (except when "X-Binary-Size" is zero, which means that the size is unknown), unless "X-Binary-Size-Padding" is specified to allow for the padding. At exactly the byte following the full binary section as defined by the length and padding values is the end of binary section identifier. This consists of the line-termination sequence followed by:

--CIF-BINARY-FORMAT-SECTION----

with each of these lines followed by a line-termination sequence. This brings us back into a normal CIF environment. This identifier is, in a sense, redundant because the binary data length value tells the a program how many bytes to jump

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

over to the end of the binary data. This redundancy has been deliberately added for error checking, and for possible file recovery in the case of a corrupted file and this identifier must be present at the end of every block of binary data.

#### 3.2.2 Format of CBF binary sections

In a CBF file, each binary section is encoded as a :-delimited string, starting with an arbitrary number of pure-ASCII characters.

Note: For historical reasons, CIFlib has the option of writing simple header and footer sections: "START OF BINARY SECTION" at the start of a binary section and "END OF BINARY SECTION" at the end of a binary section, or writing MIME-type header and footer sections (3.2.1 Format of imgCIF binary sections). If the simple header is used, the actual ASCII text is ignored when the binary section is read. Use of the simple binary header is deprecated.

#### The MIME header is recommended.

Between the ASCII header and the actual CBF binary data is a series of bytes ("octets") to try to stop the listing of the header, bytes which define the binary identifier which should match the "binary\_id" defined in the header, and bytes which define the length of the binary section.



NOTE: When a MIME header is used, only bytes 5 through 5+n-1 are considered in computing the size and the message digest, and only these bytes are encoded for the equivalent imgCIF file using the indicated Content-Transfer-Encoding.

If no MIME header has been requested (a deprecated use), then bytes 5 through 28 are used for three 8-byte words to hold the binary id, the size and the compression type:



#### file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

#### CBFlib Manual

101

The binary data then follows in bytes 29 through 29+n-1.

The binary characters serve specific purposes:

- The Control-L (from-feed) will terminate printing of the current page on most operating systems.
- The Control-Z will stop the listing of the file on MS-DOS type operating systems.
- The Control-D will stop the listing of the file on Unix type operating systems.
- The unsigned byte value 213 (decimal) is binary 11010101. (Octal 325, and hexadecimal D5). This has the eighth bit set so can be used for error checking on 7-bit transmission. It is also asymmetric, but with the first bit also set in the case that the bit order could be reversed (which is not a known concern).
- (The carriage return, line-feed pair before the START\_OF\_BIN and other lines can also be used to check that the file has not been corrupted e.g. by being sent by ftp in ASCII mode.)

At present four compression schemes are implemented are defined: CBF\_NONE (for no compression), CBF\_ CANONICAL (for and entropy-coding scheme based on the canonical-code algorithm described by Moffat, et al. (International Journal of High Speed Electronics and Systems, Vol 8, No 1 (1997) 179-231)), CBF PACKED or CBF\_PACKED\_V2 for J. P. Abrahams CCP4-style packing schemes and CBF\_BYTE\_OFFSET for a simple byte\_offset compression scheme. Other compression schemes will be added to this list in the future.

For historical reasons, CBFlib can read or write a binary string without a MIME header. The structure of a binary string with simple headers is:

Byte	ASCII symbol	Decimal value	Description
1	; na	59	Initial ; delimiter
2	carriage-return	13	
3	line-feed	10	The CBF new-line code is carriage-return, line-feed
4	S	83	
5	T	84	
6	A	65	
7	R	83	
8	Т	84	
9		32	
10	0	79	
11	F	70	
12		32	
13	В	66	
14	ILE	73	
15	N	78	
16	A	65	
17	R	83	
18	Y	89	
19		32	
20	SI	83	

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

CBFlib Manual

103

82 + n;

3.3 Compression schemes

Two schemes for lossless compression of integer arrays (such as images) have been implemented in this version of CBFlib:

Final ; delimiter

1. An entropy-encoding scheme using canonical coding 2. A CCP4-style packing scheme.

59

Both encode the difference (or error) between the current element in the array and the prior element. Parameters required for more sophisticated predictors have been included in the compression functions and will be used in a future version of the library.

#### 3.3.1 Canonical-code compression

The canonical-code compression scheme encodes errors in two ways: directly or indirectly. Errors are coded directly using a symbol corresponding to the error value. Errors are coded indirectly using a symbol for the number of bits in the (signed) error, followed by the error iteslf.

At the start of the compression, CBFlib constructs a table containing a set of symbols, one for each of the  $2^{A^n}$  direct codes from  $-2^{A(n-1)}$ .  $2^{A(n-1)}$ . 1, one for a stop code, and one for each of the *maxbits* -n indirect codes, where n is chosen at compress time and *maxbits* is the maximum number of bits in an error. CBFlib then assigns to each symbol a bit-code, using a shorter bit code for the more common symbols and a longer bit code for the less common symbols. The bit-code lengths are calculated using a Huffman-type algorithm, and the actual bit-codes are constructed using the canonical-code algorithm described by Moffat, *et al.* (*International Journal of High Speed Electronics and Systems*, Vol 8, No 1 (1997) 179-231).

The structure of the compressed data is: Byte Value 1..8 Number of elements (64-bit little-endian number) 9..16 Minimum element 17..24 Maximum element 25..32 (reserved for future use) 33 Number of bits directly coded, n 34 Maximum number of bits encoded, maxbits Number of bits in each direct code 35 .. 35+2^n-1 Number of bits in the stop code 35+2^n Number of bits in each indirect code  $35+2^{n}+1 \dots 35+2^{n}+maxbits-n$ Coded data  $35+2^{n}+maxbits-n+1$ ...

### 3.3.2 CCP4-style compression

Starting with CBFlib 0.7.7, CBFlib supports three variations on CCP4-style compression: the "flat" version supported in versions of CBFlib prior to release 0.7.7, as well as both version 1 and version 2 of J. P. Abrahams "pack\_c" compression.

The CBF\_PACKED and CBF\_PACKED\_V2 compression and decompression code incorporated in CBFlib is derived in large part from the J. P. Abrahams pack\_c.c compression code in CCP4. This code is incorporated in CBFlib under the GPL and the LGPL with both the permission Jan Pieter Abrahams, the original author of pack\_c.c (email from Jan Pieter

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

Abrahams of 15 January 2007) and of the CCP4 project (email from Martyn Winn on 12 January 2007). The cooperation of J. P. Abrahams and of the CCP4 project is gratefully acknowledged.

The basis for all three versions is a scheme to pack offsets (differences from a base value) into a small-endian bit stream. The stream is organized into blocks. Each block begins with a header of 6 bits in the flat packed version and version 1 of J. P. Abrahams compression, and 7 bits in version 2 of J. P. Abrahams compression. The header gives the number of offsets that follow and the number of bits in each offset. Each offset is a signed, 2's complement integer.

The first 3 bits in the header gives the logarithm base 2 of the numer of offsets that follow the header. For example, if a header has a zero in bits, only one offset follows the header. If those same bits contain the number n, the number of offsets in the block is 2<sup>n</sup>.

The following 3 bits (flat and version 1) or 4 bits (version 2) contains a number giving an index into a table of bit-lengths for the offsets. All offsets in a given block are of the same length.



The value "max" is determined by the compression version and the element size. If the compression used is "flat", then "max" is 65. If the compression is version 1 or version 2 of the JPA compression, then "max" is the number of bits in each element, i.e. 8, 16, 32 or 64 bits.

The major difference between the three variants of packed compression is the choice of the base value from which the offset is measured. In all cases the first offset is measured from zero, i.e. the first offset is the value of the first pixel of the image. If "flat" is chosen or if the dimensions of the data array are not given, then the remaining offset are measure against the prior value, making it similar in approach to the "byte offset" compression described in section 3.3.3 Byte offset compression, but with a more efficient representation of the offsets.

In version 1 and version 2 of the J. P. Abrahams compression, the offsets are measured against an average of earlier pixels. If there is only one row only the prior pxiel is used, starting with the same offsets for that row as for "flat". After the first row, three pixels from the prior row are used in addition to using the immediately prior pixel. If there are multiple sections, and the sections are marked as correlated, after the first section, 4 pixels from the prior section are included in the average. The CBFlib code differs from the pack\_c code in the handling of the beginnings and ends of

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

**CBFlib** Manual

rows and sections. The pack c code will use pixels from the other side of the image in doing the averaging. The CBFlib code drops pixels from the other side of the image from the pool. The details follow.

After dealing with the special case of the first pixel. The algorithm uses an array of pointers, trail char data. The assignment of pixels to the pool to be averaged begins with trail\_char\_data[0] points to the pixel immediately prior to the next pixel to be processed, either in the same row (fastest index) or, at the end of the prior row if the next data element to be processed is at the end of a row. The location of the pixel pointed to by trail\_char\_data[0] is used to compute the locations of the other pixels in the pool. It will be dropped from the pool before averaging if it is on the opposite side of the image. The pool will consist of 1, 2, 4 or 8 pixels.

Assume ndim1, ndim2, ndim3 are the indices of the same pixel as trail char data[0] points to. These indices are incremented to be the indices of the next pixel to be processed before populating trail char data.

On exit, trail char data[0, 7] will have been populated with pointers to the pixels to be used in forming the average. Pixels that will not be used will be set to NULL. Note that trail char data[0] may be set to NULL.

If we mark the next element to be processed with a "\*" and the entries in trail\_char\_data with their array indices 0 .. 7, the possible patterns of settings in the general case are:



If there is no prior section (i.e. ndim3 is 0, or the CBF\_UNCORRELATED\_SECTIONS flag is set to indicate discontinuous sections), the values for trail\_char\_data[4..7] will all be NULL. When there is a prior section, trail\_char\_ data[5..7] are pointers to the pixels immediately below the elements pointed to by trail\_char\_data[1..3], except trail\_ char data[4] is one element further along its row to be directly below the next element to be processed.

The first element of the first row of the first section is a special case, with no averaging.

In the first row of the first section (ndim2 = 0, and ndim3 = 0), after the first element (ndim1 > 0), only trail char data [0] is used

current section.

0 \*



file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

08/07/07 09:24:51

For subsequent rows of the first section (ndim 2 > 0, and ndim 3 = 0), for the first element (ndim 1 = 0), two elements from the prior row are used:

105

107

while for element after the first element, but before the last element of the row, a full set of 4 elements is used



For sections after the first section, provided the CBF UNCORRELATED SECTIONS flag is not set in the compression, for each non-NULL entry in trail char data [0..3] an entry is made in trail char data [4..7], except for the first element of the first row of a section. In that case an entry is made in trail\_char\_data[4].

The structure of the compressed data is:



#### 3.3.3 Byte offset compression

Starting with CBFlib 0.7.7, CBFlib supports a simple and efficient "byte\_offset" algorithm originally proposed by Andy Hammerley and modified by Wolgang Kabsch and Herbert Bernstein. The original proposal was called "byte\_offsets". We distinguish this variant by calling it "byte\_offset". The major differences are that the "byte\_offsets" algorithm started with explicit storage of the first element of the array as a 4-byte signed two's integer, and checked for image edges to changes the selection of prior pixel. The CBFlib "byte\_offset" alogorithm starts with an assumed zero before the first pixel and represents the value of the first pixel as an offset of whatever number of size is needed to hold the value, and for speed, treats the entire image as a simple linear array, allowing use of the last pixel of one row as the base against which to compute the offset for the first element of the next row.

The algorithm is simple and easily implemented. This algorithm can never achieve better than a factor of two compression relative to 16-bit raw data or 4 relative to 32-bit raw data, but for most diffraction data the compression will indeed be very close to these ideal values. It also has the advantage that integer values up to 32 bits (or 31 bits and sign) may be stored efficiently without the need for special over-load tables. It is a fixed algorithm which does not need to calculate any image statistics, so is fast.

The algorithm works because of the following property of almost all diffraction data and much other image data: The value of one element tends to be close to the value of the adjacent elements, and the vast majority of the differences use little of the full dynamic range. However, noise in experimental data means that run-length encoding is not useful (unless the image is separated into different bit-planes). If a variable length code is used to store the differences, with the number of bits used being inversely proportional to the probability of occurrence, then compression ratios of 2.5 to 3.0 may be achieved. However, the optimum encoding becomes dependent of the exact properties of the image, and in

**CBFlib** Manual

particular on the noise. Here a lower compression ratio is achieved, but the resulting algorithm is much simpler and more robust.

The "byte offset" compression algorithm is the following:

- 1. Start with a base pixel value of 0.
- 2. Compute the difference delta between the next pixel value and the base pixel value.
- 3. If  $-127 \le delta \le 127$ , output delta as one byte, make the current pixel value the base pixel value and return to step
- 4. Otherwise output -128 (F0 hex).
- 5. We still have to output delta. If  $-32767 \le \text{delta} \le 32767$ , output delta as a little\_endian 16-bit quantity, make the current pixel value the base pixel value and return to step 2.
- 6. Otherwise output -32768 (F000 hex, little\_endian, i.e. 00 then F0)
- 7. We still have to output delta. If  $-2147483647 \le delta \le 2147483647$ , output delta as a little endian 32 bit quantity. make the current pixel value the base pixel value and return to step 2.
- 8. Otherwise output -2147483648 (F0000000 hex, little endian, i.e. 00, then 00, then 00, then F0) and then output the pixel value as a little-endian 64 bit quantity, make the current pixel value the base pixel value and return to step 2.

The "byte\_offset" decompression algorithm is the following:

- 1. Start with a base pixel value of 0.
- 2. Read the next byte as delta
- 3. If  $-127 \le delta \le 127$ , add delta to the base pixel value, make that the new base pixel value, place it on the output array and return to step 2.
- 4. If delta is F0 hex, read the next two bytes as a little\_endian 16-bit number and make that delta.
- 5. If  $-32767 \le delta \le 32767$ , add delta to the base pixel value, make that the new base pixel value, place it on the output array and return to step 2.
- 6. If delta is F000 hex, read the next 4 bytes as a little endian 32-bit number and make that delta
- 7. If  $-2147483647 \le delta \le 2147483647$ , add delta to the base pixel value, make that the new base pixel value, place it on the output array and return to step 2.
- 8. If delta is F0000000 hex, read the next 4 bytes as a little\_endian 32-bit number and make that delta, read the next 8 bytes as a little endia 64-bit number and make that delta, add delta to the base pixel value, make that the new base pixel value, place it on the output array and return to step 2.

Let us look at an example, of two 1000 x 1000 flat field images presented as a mimimal imgCIF file. The first image uses 32-bit unsigned integers and the second image uses 16-bit unsigned integers.

The imgCIF file begins with some identifying comments (magic numbers) to track the version of the dictionary and library:

###CBF: VERSION 1.5 # CBF file written by CBFlib v0.7.7

This is followed by the necessary syntax to start a CIF data block and by whatever tags and values are appropriate to describe the experiment. The minimum is something like

data testflat

eventually we come to the actual binary data, which begins the loop header for the array\_data category

1000 \_array\_data.data

with any additional tags needed, and then the data itself, which starts with the mini-header:

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

08/07/07 09:24:51

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

08/07/07 09:24:51

--CIF-BINARY-FORMAT-SECTION--Content-Type: application/octet-stream; conversions="x-CBF\_BYTE\_OFFSET" Content-Transfer-Encoding: BINARY X-Binary-Size: 1000002 X-Binary-ID: 1 X-Binary-Element-Type: "unsigned 32-bit integer" X-Binary-Element-Byte-Order: LITTLE ENDIAN Content-MD5: +FqUJGxXhvCijXMFHC0kaA== X-Binary-Number-of-Elements: 1000000 X-Binary-Size-Fastest-Dimension: 1000 X-Binary-Size-Second-Dimension: 1000 X-Binary-Size-Padding: 4095

followed by an empty line and then the sequence of characters:

^L^Z^D<D5>

followed immediately by the compressed data.

The binary data begins with the hex byte 80 to flag the need for a value that will not fit in one byte. That is followed by the small\_endian hex value 3E8 saying that the first delta is 1000. Then 999,999 bytes of zero follow, since this is a flat field, with all values equal to zero. That gives us our entire 1000x1000 compressed flat field. However, because we asked for 4095 bytes of padding, there is an additional 4095 bytes of zero that are not part of the compressed field. They are just pad and can be ignored. Finally, after the pad, the CIF text field that began with

; --CIF-BINARY-FORMAT-SECTION--

is completed with

--CIF-BINARY-FORMAT-SECTION----

notice the extra --

The second flat field then follows, with a very similar mini-header:

--CIF-BINARY-FORMAT-SECTION--Content-Type: application/octet-stream; conversions="x-CBF BYTE OFFSET" Content-Transfer-Encoding: BINARY X-Binary-Size: 1000002 X-Binary-ID: 2 X-Binary-Element-Type: "unsigned 16-bit integer" X-Binary-Element-Byte-Order: LITTLE ENDIAN Content-MD5: +FqUJGxXhvCijXMFHC0kaA= X-Binary-Number-of-Elements: 1000000 X-Binary-Size-Fastest-Dimension: 1000 X-Binary-Size-Second-Dimension: 1000 X-Binary-Size-Padding: 4095

^L^Z^D<D5>

The only difference is that we have declared this array to be 16-bit and have chosen a different binary id (2 instead of 1). Even the checksum is the same.

4. Installation

CBFlib should be built on a disk with at least 200 megabytes of free space. CBFlib.tar.gz is a "gzipped" tar of the code as it now stands. Place the gzipped tar in the directory that is intended to contain a new directory, named CBFlib 0.7.5 (the "top-level" directory) and uncompress it with gunzip and unpack it with tar:

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

109

08/07/07 09:24:51

**CBFlib** Manual

and the

make

gunzip CBFlib.tar.gz tar xvf CBFLIB.tar

As with prior releases, to run the test programs, you will also need Paul Ellis's sample MAR345 image, example.mar2300, and Chris Nielsen's sample ADSC Quantum 315 image, mb\_LP\_1\_001.img as sample data. Both these files will be extracted by the Makefile from CBFlib\_0.7.7\_Data\_Files. Do not download copies into the top level directory.

After unpacking the archive, the top-level directory should contain a makefile:

	Makefile Makefile for unix
e subdirectories:	
src/	CBFLIB source files
include/	CBFLIB header files
m4/	CBFLIB m4 macro files (used to build .f90 files)
examples/	Example program source files
doc/	Documentation
lib/	Compiled CBFLIB library
bin/	Executable example programs
html_images/	JPEG images used in rendering the HTML files

For instructions on compiling and testing the library, go to the top-level directory and type:

The CBFLIB source and header files are in the "src" and "include" subdirectories. The FCBLIB source and m4 files are in the "src" and "m4" subdirectories. The files are:

src/	include/ m4/	Description
cbf.c	cbf.h	CBFLIB API fu
cbf_alloc.c	cbf_alloc.h	Memory allocat
cbf_ascii.c	cbf_ascii.h	Function for wr
cbf_binary.c	cbf_binary.h	Functions for bi
cbf_byte_offset.c	cbf_byte_offset.h	Byte-offset com
cbf_canonical.c	cbf_canonical.h	Canonical-code
cbf_codes.c	cbf_codes.h	Encoding and m
cbf_compress.c	cbf_compress.h	General compre
cbf_context.c	cbf_context.h	Control of temp
cbf_file.c	cbf_file.h	File in/out funct
cbf_lex.c	cbf_lex.h	Lexical analyse
cbf_packed.c	cbf_packed.h	CCP4-style pack
cbf_predictor.c	cbf_predictor.h	Predictor-Huffn
cbf_read_binary.c	cbf_read_binary.h	Read binary hea
cbf_read_mime.c	cbf_read_mime.h	Read MIME-en
cbf_simple.c	cbf_simple.h	Higher-level CE
cbf_string.c	cbf_string.h	Case-insensitive

unctions tion functions riting ASCII values inary values npression e compression nessage digest functions ession routines porary files tions er king compression man compression (not implemented) eaders ncoded binary sections BFlib functions e string comparisons

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

cbf stx.c cbf stx.h cbf tree.c cbf tree.h cbf uncompressed.c / cbf\_ uncompressed.h cbf\_write.c cbf write.h cbf write binary.c cbf write binary.h cbf.stx.y md5.h md5c.c global.h fcb atol wcnt.f90 fcb ci strncmparr.f90 fcb\_nblen\_array.f90 fcb\_read\_byte.f90 fcb read line.f90 fcb skip whitespace.f90

array header fcb\_exit\_ binary.m4 field fcb next Function to skip to the next binary binary.m4 fcb\_open\_ cifin.m4 fcb packed.m4 fcb read 3D I4 format image.m4 fcb read xds i2.m4 fcblib defines.m4 In the "examples" subdirectory, there are 2 additional files used by the example programs (section 5) for reading MAR300, MAR345 or ADSC CCD images:

img.c img.h Simple image library

and the example programs themselves:

makecbf.c Make a CBF file from an image	
img2cif.c Make an imgCIF or CBF from an image	
cif2cbf.c Copy a CIF/CBF to a CIF/CBF	
convert_ Convert an image file to a cbf using a templa	te file
image.c	

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

Parser (generated from cbf.stx.y) CBF tree-structure functions

Uncompressed binary sections

Functions for writing Write binary sections bison grammar to define cbf stx.c (see WARNING) RSA message digest software from mpack

## Function to convert a string to an integer Function to do a case-insensitive comparison of a string to a byte array Function to determine the non-blank length of a byte Function to read a single byte Function to read a line into a byte array

Function to skip whitespace and comments in a MIME Function to skip past the end of the current binary text

Function to open a CBF file for reading

Functions to read a JPA CCP4 compressed image fcb read bits.m4 Functions to read nay number of bits as an integer Functions to read the next image in I2, I4, 3D\_I2 and

Function to read a single xds image.

General m4 macro file for FCBLIB routines.

08/07/07 09:24:51

111

**CBFlib** Manual

cif2c.c Convert a template cbf file into a function to produce the same template in an internal cbf data structure

testcell.C Exercise the cell functions

as well as three template files: template adscouantum4 2304x2304.cbf, template mar345 2300x2300.cbf, and template\_adscquantum315\_3072x3072.cbf.

Two additional examples (test\_fcb\_read\_image.f90 and test\_xds\_binary.f90) are created from two files (test\_fcb\_read\_image.m4 and test\_xds\_binary.m4) in the m4 directory.

The documentation files are in the "doc" subdirectory:

CBFlib.html	This document (HTML)
CBFlib.txt	This document (ASCII)
CBFlib_NOTICES.html	Important NOTICES PLEASE READ
CBFlib_NOTICES.txt	Important NOTICES PLEASE READ
gpl.txt	GPL PLEASE READ
lgpl.txt	LGPL PLEASE READ
cbf_definition_rev.txt	Draft CBF/ImgCIF definition (ASCII)
cbf_definition_rev.html	Draft CBF/ImgCIF definition (HTML)
cif_img.html	CBF/ImgCIF extensions dictionary (HTML)
cif_img.dic	CBF/ImgCIF extensions dictionary (ASCII)
ChangeLog,html	Summary of change history (HTML)
ChangeLog	Summary of change history (ASCII)

## 5. Example programs

The example programs makecbf.c, img2cif.c and convert\_image.c read an image file from a MAR300, MAR345 or ADSC CCD detector and then uses CBFlib to convert it to CBF format (makecbf) or either imgCIF or CBF format (img2cif). makecbf writes the CBF-format image to disk, reads it in again, and then compares it to the original. img2cif just writes the desired file. makecbf works only from stated files on disk, so that random I/O can be used. img2cif includes code to process files from stdin and to stdout. convert\_image reads a template as well as the image file and produces a complete CBF. The program convert\_minicbf reads a minimal CBF file with just and image and some lines of text specifying the parameters of the data collection as done at SLS and combines the result with a template to produce a full CBF. The program cif2cbf can be used to convert among carious compression and encoding schemes. The program sauter\_test.C is a C++ test program contributed by Nick Sauter to help in resolving a memory leak he found.

makecbf.c is a good example of how many of the CBFlib functions can be used. To compile makecbf and the other example programs use the Makefile in the top-level directory:

make all

This will place the programs in the bin directory.

To run makecbf with the example image, type:

./bin	/makecbf example.mar2300 test.cbf		
The program	n img2cif has the following command line interface:		
img2cif	<pre>[-i input_image] [-o output_cif] [-c {p[acked]]c[annonical] [n[one]}] [-m {h[eaders] n[oheaders]}]</pre>		

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

The remaining options specify the characteristics of the output cbf. The characteristics of the input cif are derived

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

from context.



08/07/07 09:24:51

## CBFlib Manual

- -c compression scheme (packed, canonical, byte offset,
- -m [no]headers (default headers for cifs, noheaders for cbfs) selects MIME (N. Freed, N. Borenstein, RFC 2045, November 1996) headers within binary data value text fields.
- -d [no]digest (default md5 digest [R. Rivest, RFC 1321, April 1992 using "RSA Data Security, Inc. MD5 Message-Digest Algorithm"] when MIME headers are selected)
- -e encoding (base64, quoted-printable or none, default base64) specifies one of the standard MIME encodings for an ascii cif
- -b byte order (forward or backwards, default forward (1234) on little-endian machines, backwards (4321) on big-endian machines
- -p K of padding (0, 1, 2, 4) for no padding after binary data 1023, 2047 or 4095 bytes of padding after binary data
- -v dictionary specifies a dictionary to be used to validate the input cif and to apply aliases to the output cif. This option may be specified multiple times, with dictionaries

The program convert\_image requires two arguments: imagefile and cbffile. Those are the primary input and output. The detector type is extracted from the image file or from the command line, converted to lower case and used to construct the name of a template cbf file to use for the copy. The template file name is of the form template name columnsxrows.

convert\_image [-i input\_img] [-o output\_cbf] [-p template\_cbf] [-d detector name] - m [x|y]x=y] [-z distance] [-c category\_alias=category\_root]\* [-t tag\_alias=tag\_root]\* [-F] [-R]

the input file as an image in smv, mar300, or mar345 format. If input\_img is not specified or is given as "-", it is copied

- the template for the final cbf to be produced. If template cbf is not specified the name is constructed from the first token
- the output cbf combining the image and the template. If the output cbf is not specified or is given as "-", it is written

when writing packed compression, treat the entire image as one line with no averaging

-m [x|y|x=y] (default x=y, square arrays only) mirror the array in the x-axis (y -> -y)

file://localhost/Users/vava/Desktop/nCBF/CBFlib bleeding edge/doc/CBFlib.html

08/07/07 09:24:51

**CBFlib** Manual 115 **CBFlib** Manual in the y-axis  $(x \rightarrow -x)$ or in x=y ( x -> y, y-> x) -r n rotate the array n times 90 degrees counter clockwise  $x \rightarrow y$ ,  $y \rightarrow -x$  for each rotation, n = 1, 2 or 3 -R-R if setting a beam center, set reference values of axis settings as well as standard settings -z distance -z distance detector distance along Z-axis -c category\_alias=category\_root -t tag alias=tagroot map the given alias to the given root, so that instead of outputting the alias, the root will be presented in the times as needed. output cbf instead. These options may be repeated as many times as needed. The program convert minicbf requires two arguments: minicbf and cbffile. Those are the primary input and output. The detector type is extracted from the image file or from the command line, converted to lower case and used to construct the name of a template cbf file to use for the copy. The template file name is of the form template\_name\_columnsxrows. The full set of options is: convert\_minicbf [-i input\_cbf] [-o output\_cbf] [-p template\_cbf]\ [-q] [-c convention] [-d detector name] -m [x]y]x=y] [-z distance] [-c category\_alias=category\_root]\* [-t tag\_alias=tag\_root]\* [-F] [-R] [input\_obf] [output\_off] pixels set to 1000. pixels set to 1000. the options are: -i input\_cbf (default: stdin) the input file as a CBF with at least an image. -p template\_cbf the template for the final cbf to be produced. If template cbf is not specified the name is constructed from the first token of the detector name and the image size as template <type> <columns>x<rows>.cbf -o output\_cbf (default: stdout ) the output cbf combining the image and the template. If the output cbf is not specified or is given as "-", it is written to stdout. -q exit quickly with just the miniheader expanded after the data. No template is used. as in: exit quickly with just the miniheader unexpanded before the data. No template is used. -C convention convert the comment form of miniheader into the array\_data.header\_convention convention array\_data.header\_convents overriding any existing values -d detectorname a detector name to be used if none is provided in the image header. when writing packed compression, treat the entire image as one line with no averaging -m [x|y|x=y] (default x=y, square arrays only)

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51



The example programs testfals, testfal and testfalapacked compression. Each is run without any arguments. testreals will read real images from the data file testrealin.cbf and write a file with real images in testrealout.cbf, which should be identical to testrealin.cbf. testflat and testflatpacked read 4 1000x1000 2D images and one 50x60x70 3D image and produce an output file that should be identical to the input. testflat reads testflatin.cbf and produces testflatout.cbf using CBF\_BYTE\_OFFSET compression. testflatpacked reads testflatpackedin.cbf and produces testflatpackedout.cbf. The images are:

- A 1000 x 1000 array of 32-bit integers forming a flat field with all pixels set to 1000.
- A 1000 x 1000 array of 16-bit integers forming a flat field with all pixels set to 1000.
- A 1000 x 1000 array of 32-bit integers forming a flat field with all pixels set to 1000, except for -3 along the main diagonal and its transpose.
- A 1000 x 1000 array of 16-bit integers forming a flat field with all pixels set to 1000, except for -3 along the main diagonal and its transpose.
- A 50 x 60 x 70 array of 32-bit integers in a flat field of 1000, except for -3 along the main diagonal and the values i+j+k (counting from zero) every 1000th pixel

The example programs test fcb\_read\_image and test xds\_binary are designed read the output of testflat and testflatpacked using the FCBlib routines in lib/libfob. test\_xds\_binary reads only the first image and closes the file immediately. test\_fcb\_read\_image reads all 5 images from the input file. The name of the input file should be provided on stdin, as in:

- echo testflatout.cbf | bin/test\_xds\_binary
- echo testflatpackedout.cbf | bin/test\_xds\_binary
- echo testflatout.cbf | bin/test\_fcb\_read\_image
- echo testflatpackedout.cbf | bin/test\_fcb\_read\_image

In order to compile these programs correctly for the G95 compiler it is important to set the record size for reading to be no larger

file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html

08/07/07 09:24:51

117

than the padding after binary images. This in controlled in Makefile by the line

M4FLAGS = -Dfcb\_bytes\_in\_rec=131072

which provides good performance for gfortran. For g95, this line must be changed to

#### M4FLAGS = -Dfcb\_bytes\_in\_rec=4096

The program sauter test.C is a C++ test program contributed by Nick Sauter to help in resolving a memory leak he found. The program is run as bin/sauter\_test and should run long enough to allow a check with top to ensure that it has constant memory demands. In addition, starting with release 0.7.8.1, the addition of -DCBFLIB\_MEM DEBUG to the compiler flags will cause detailed reports on memory use to stderr to be reported.



file://localhost/Users/yaya/Desktop/nCBF/CBFlib\_bleeding\_edge/doc/CBFlib.html