

5. APPLICATIONS

character string is put. The *logical* function is returned as `.true.` if the data name passes any requested dictionary validation checks.

`pnumb_` puts the specified data name *name*, single-precision number *numb* and an appended standard uncertainty *sdev* into the output CIF. The *logical* function is returned as `.true.` if the data name passes any requested dictionary validation checks.

`pnumd_` puts the specified data name *name*, double-precision number *numb* and an appended standard uncertainty *sdev* into the output CIF. The *logical* function is returned as `.true.` if the data name passes any requested dictionary validation checks.

`ptext_` puts the specified data name *name* and text string *string* into the output CIF. The data name will only be inserted on the first invocation of a sequence. The *logical* function is returned as `.true.` if the data name passes any requested dictionary validation checks. This command must be invoked repeatedly until the text is finished. The terminal semicolon character ';' is placed in the output CIF when the next call to `pchar_`, `pnumb_` or `pnumd_` is made, or if a call is made to `ptext_` for a different data name.

`pcmnt_` puts the specified comment string *string* into the output CIF. The *logical* function is always returned as `.true.`. The comment character '#' should not be included in the string. A blank comment is presented as a blank line without the leading '#'. The string `char(0)//char(0)` can be used to produce an empty comment with the leading '#'. The string `char(0)//char(0)` can be used to produce an empty comment with the leading '#'.

`prefix_` prefixes the specified string *strg* of length *lstrg* to subsequent lines of the output CIF. The total line length is still limited to the value given by the variable `line_` (the default is 80 characters). This function is useful when embedding a CIF into another text document, such as a PDB REMARK. The *logical* function is always returned as `.true.`.

`close_` closes the output CIF only. This command *must* be used if `pfile_` is used. This a subroutine call.

5.4.6. Variables

The *CIFtbx* library also contains a large number of variables declared in the common blocks in the file `ciftbx.cmn` that provide signals to the programmer on various aspects of the data reading and writing processes. These variables are described below in four broad categories, as shown in Table 5.4.6.1: general monitor variables, general control variables, input monitor variables and output control variables.

Note that for all but special applications only the basic variables `list_`, `loop_`, `strg_`, `text_` and `type_` are usually used. These variables supplement the argument lists of the various commands, providing essential status information.

5.4.6.1. General monitor variables

These variables are returned by *CIFtbx* and provide information about the general status of processing.

`file_`: *character string* containing the file name of the current input file.

`longf_`: *integer variable* containing the length of the file name in `file_`.

`precn_`: *integer variable* containing the line number (starting from 1) of the last line written to the output CIF.

`recn_`: *integer variable* containing the line number (starting from 1) of the last line read from the input CIF.

`tbxver_`: *character*32 variable* that is the *CIFtbx* version and date in the form 'CIFtbx version N.N.N DD MMM YYYY' (some older versions of *CIFtbx* use a two-digit year and have a comma after the version number).

Table 5.4.6.1. *CIFtbx* variables

General monitor	General control	Input monitor	Output control
	alias_		aliaso_ align_
	append_	bloc_ decp_ diccat_ dicname_ dictype_ dicver_	pdecp_ esdlim_
file_		glob_	globo_
	line_	list_ long_	
longf_		loop_ lzero_	plzero_ nblanko_
	nblank_	posdec_ posend_ posnam_ posval_	pposdec_ pposend_ pposnam_ pposval_
precn_		quote_	pquote_
	recbeg_ recend_		
recn_		save_ strg_	saveo_ tabl_ ptabx_
	tabx_	tagname_	
tbxver_		text_ type_	xmlout_ xmlong_

5.4.6.2. General control variables

These variables control *CIFtbx* commands. The user may accept the default values or may store new values into these variables to change the behaviour of the commands.

`alias_`: *logical variable* to control the use of data-name aliases for input items. If set to `.true.`, aliases from the input dictionary may be used (see Section 5.4.7). The default is `.true.`.

`append_`: *logical variable* to control reuse of the direct-access file. If set to `.true.`, it will cause each call to `ocif_` to append the information found to the current CIF. The default is `.false.`.

`line_`: *integer variable* to set the input/output line limit for processing a CIF. The default value is 80 characters. This limit counts the visible printable characters of the line, not the system-dependent line terminators.

`nblank_`: *logical variable* to control the treatment of input blank strings. If set to `.true.`, `char_` or `test_`, it will return the type as 'null' rather than 'char' when encountering a quoted blank.

`recbeg_`: *integer variable* to give the record number of the first record to be used. May be changed by the user to restrict access to a CIF.

`recend_`: *integer variable* to give the record number of the last record to be used. May be changed by the user to restrict access to a CIF.

`tabx_`: *logical variable* is set to `.true.` for tab stops to be expanded to blanks during the reading of a CIF. The default is `.true.`