

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.

pcmt_ 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 ‘#’.

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
	<i>alias_</i>		<i>aliaso_</i> <i>align_</i>
	<i>append_</i>	<i>bloc_</i> <i>dec_</i> <i>diccat_</i> <i>dicname_</i> <i>dictype_</i> <i>dicver_</i>	<i>pdec_</i> <i>esdlm_</i>
<i>file_</i>	<i>line_</i>	<i>glob_</i>	<i>globo_</i>
		<i>list_</i> <i>long_</i>	
<i>longf_</i>		<i>loop_</i> <i>lzero_</i>	<i>plzero_</i> <i>nblanko_</i>
	<i>nblank_</i>	<i>posdec_</i> <i>posend_</i> <i>posnam_</i> <i>posval_</i>	<i>pposdec_</i> <i>pposend_</i> <i>pposnam_</i> <i>pposval_</i>
<i>precn_</i>		<i>quote_</i>	<i>pquote_</i>
	<i>recbeg_</i> <i>recend_</i>		
<i>recn_</i>		<i>save_</i> <i>strg_</i>	<i>saveo_</i> <i>tabl_</i> <i>ptabx_</i>
	<i>tabx_</i>	<i>tagname_</i>	
<i>tbxver_</i>		<i>text_</i> <i>type_</i>	<i>xmlout_</i> <i>xmlong_</i>

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.*