

5.3. SYNTACTIC UTILITIES FOR CIF

5.3.2.1.3. Limitations of *vcif*

Because the program is testing certain properties of character strings within logical lines of a file, it stores a line at a time for further internal processing. If a line contains a null character (an ASCII character with integer value zero), this will be taken as the termination of the string currently being processed, according to the normal conventions in the C programming language for marking the end of a text string. In this case, subsequent error messages may not reflect the real problem. The null character, of course, is not allowed in a CIF.

vcif also interprets syntax rules literally, so a misplaced semicolon might mean that a large section of the file is regarded as a text field and too many or too few error messages are generated. This can make a correct interpretation of the causative errors difficult for a novice user.

5.3.3. Editors with graphical user interfaces

A useful class of editing tool is the graphical editor, where different types of access can be provided through icons, windows or frames, menus and other graphical representations. The availability of standard instructions through drop-down menus makes such tools particularly suitable for users who are not expert on the fine details of the file format. The ability within the program to restrict access to particular regions of the file makes it easier to modify the contents of a CIF without breaking the syntax rules. A small but growing number of such editors are becoming available, such as those described here.

5.3.3.1. *enCIFer*

The program *enCIFer* (Allen *et al.*, 2004) has been developed as a graphical utility designed to indicate clearly to a novice user where errors are present in a CIF, to permit interactive editing and revalidation of the file, and to allow visualization of three-dimensional structures described in the file. In its early releases, it was targeted at the community of small-molecule crystallographers interested in publishing structures or depositing them directly in a structure database. Version 1.0 depended on a compiled version of the CIF core dictionary, but subsequent versions allow external CIF dictionaries to be imported. At the time of publication (2005), development is concentrating on support for DDL1 dictionaries.

Given its target user base, the purpose of the program is to permit the following operations within single- or multi-block CIFs:

- (i) Location and reporting of syntax and/or format violations using the current CIF dictionary.
- (ii) Correction of these syntax and/or format violations.
- (iii) Editing of existing individual data items or looped data items.
- (iv) Addition of new individual data items or looped data items.
- (v) Addition of some standard additional information *via* two data-entry utilities prompting the user for required input ('wizards'): the *publication wizard*, for entering the basic bibliographic information required by most journals and databases that accept CIFs for publication or deposition; and the *chemical and crystal data wizard*, for entering chemical and physical property information in a CIF for publication in a journal or deposition in a database.
- (vi) Visualization of the structure(s) in the CIF.

In all cases where data are edited or added, *enCIFer* can be used to check the format integrity of the amended file.

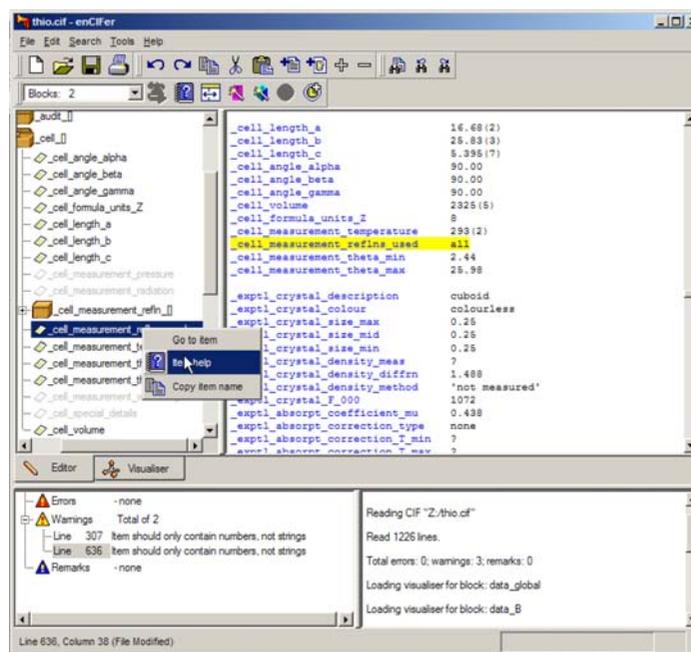


Fig. 5.3.3.1. The *enCIFer* graphical user interface.

5.3.3.1.1. The main graphical window

Fig. 5.3.3.1 is an example of the use of *enCIFer* to read and modify a CIF. The figure shows the components of the main window after a file has been opened. Beneath the standard toolbar that provides access to operating-system utilities and to the main functions of the program itself is a task bar (here split over two lines) providing rapid access to a subset of the program's features. Under this are two large panes. The pane on the right is the editing window, where the content of the CIF is displayed and may be modified. The left-hand pane is a user-selectable view by category of the data names stored in the CIF dictionary against which the file is to be validated. At the bottom are two smaller panes. The one on the right logs the session activities and displays informational messages. The left-hand pane lists errors and warning notices generated by the validation system. Errors are labelled by line number, and selection of a specific message (by a mouse double-click) scrolls the content of the main text-editing window to that line number.

Tabs in the middle of the display allow the user to switch rapidly between the editing mode and a visualization of the three-dimensional structures described in the CIF.

These components are described more fully below, followed by a description of the other windows that may be created by a user: the help viewer, the loop editor and the data-entry wizards.

5.3.3.1.2. The interface toolbar

This toolbar provides menus labelled 'File', 'Edit', 'Search', 'Tools' and 'Help' that provide the expected functionality of graphical interfaces: the ability to open, close and save files, store a list of recently accessed files, spawn help and other windows, allow searching for strings within the document, allow the user to modify aspects of the behaviour or the look and feel of the program, and provide entry points for specific modes of operation. The most useful of these utilities can also be accessed from icons on the task bar. They are discussed in more detail in the following section.

This main menu is structured in a way familiar to users of popular applications designed for the Microsoft Windows operating