HICCuP was designed to allow users of the Cambridge Structural Database (Allen, 2002) to check structures intended for deposition in the database and therefore included a range of additional content checks specific to this purpose. These could, however, be disabled by the user.

5.3.3.3.1. *Interactive use of the program*

5.3.3.3.1.1. *The control window*

Because *HICCuP* was designed as an interactive tool, upon invocation it presented to the user a *control window* from which CIFs could be selected for analysis and in which summary results of the program's operations were logged. Fig. 5.3.3.8 shows an example of the control window after a single CIF has been loaded.

In the large frame below the file-entry field are listed the data blocks found by the program. The names are highlighted in various colours according to the highest level of severity of errors found within the corresponding data block.

Because the utility was designed for processing large amounts of CIF data for structural databases, it was considered useful to supply a compact visual indicator of the progress of the program through a large file. This takes the form of a grid of rectangular cells, one column for each data block present. Each column contains three cells, which monitor the performance of checks on the file syntax, conformance against a CIF dictionary, and other checks specific to the requirements of the Cambridge Crystallographic Data Centre. As each data block was checked, the corresponding cells were coloured according to the types of error found. Different colours were used to indicate: no errors; structure errors in the initial syntax tests; dictionary errors; or a deviation from certain conventions used by journals and databases in naming datablocks.

The large frame at the bottom of the control window provides a text summary of the same information, listing the number of errors found.

Check boxes and an 'Options…' button allowed some configurability of checks by the user.

5.3.3.3.1.2. *The report frame and edit window*

The user could get more details of the reported errors by clicking on the name of the data block of interest in the control window. The text of the CIF would appear in a new window positioned at the point where the program has detected the first error and a terse statement of the type of error, with a longer explanation of its nature and possible cause, would be given.

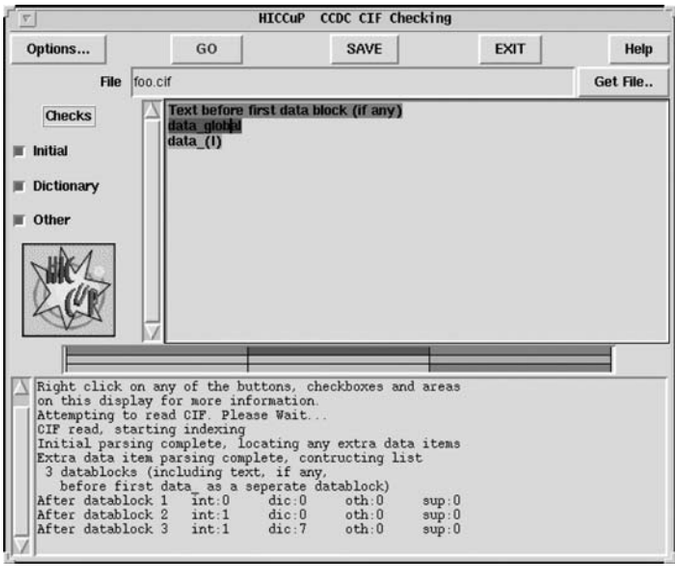

Fig. 5.3.3.8. Control window of the *HICCuP* application.

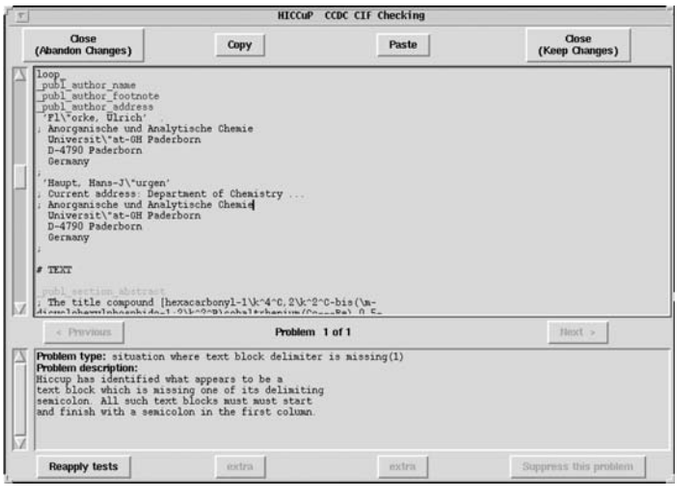

Fig. 5.3.3.9. *HICCuP* edit window and error description.

In the example of Fig. 5.3.3.9, the program has detected that there is a missing text delimiter (a semicolon character), and positions the text in the upper frame at the likely location of the error. The program has attempted to localize the region where the error may have occurred. Because a text field might contain arbitrary contents, including extracts of CIF content, it is impossible to be sure on purely syntactic grounds of the nature of the error. Nonetheless, some heuristic rules serve to identify the author's likely intent in the majority of cases. So, in this example, the user may scan the file contents in the vicinity of the line highlighted by the program and find the error within a few lines (in this example an incorrectly terminated `_publ_author_footnote` entry beginning 'Current address:').

For this example, the more literal *vcif* error analysis provides only the message

```
ERROR: Text field at end of file does not terminate
```

The upper frame in this window is an editable window, so that the user could modify the text and revalidate the current data block. Only when a satisfactorily 'clean' data block was obtained were the changes saved, and the modified data block written back into the original file.

5.3.3.3.1.3. *Dictionary browsing*

An additional useful feature of the program was its interactive link to a CIF dictionary file (Fig. 5.3.3.10). The browser window contains the definition section of the dictionary referring to

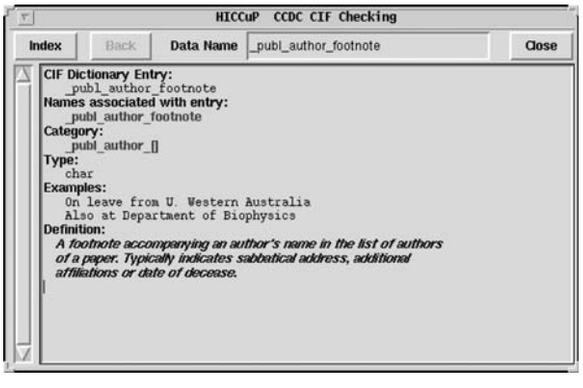

Fig. 5.3.3.10. *HICCuP* dictionary browser window.

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