a space-filling molecular representation, and the drop-down menu indicates some of the options available to modify the appearance of the graphics. The molecular-graphics library used by the program is part of the larger database interface software package developed at the Cambridge Crystallographic Data Centre. In the present version, the visualizer is run only upon initial parsing of the input CIF, and therefore does not provide an ability to track visually the molecular changes associated with direct modification of the contents of the file.

5.3.3.2. *CIFEDIT*

The *CIFEDIT* program (Toby, 2003) is written in Tcl/Tk (Ousterhout, 1994) and provides an application for viewing and editing CIFs. The code is written in such a way that it can be embedded into larger programs to provide a CIF-editing interface within larger application suites.

The current version of the program is able to validate CIFs against both DDL1 and DDL2 dictionaries, although the DDL2 validation is currently less complete than for DDL1. For example, numeric values are checked against permitted enumeration ranges only for DDL1. Dictionaries are accessed through index files, each of which contains Tcl data structures that point to the location of the definitions in the dictionary file itself and store information such as units and enumeration ranges that can be used for data validation. A utility provided with the program allows a user to generate new index files when new versions of the dictionaries become available. It is intended that dictionary indexing will be incorporated within the main application in the next program release, so that interactive dictionary selection will be possible.

When a CIF is opened, the contents are parsed and validated against one or more user-selected dictionaries. Errors are displayed in a pop-up window and may be written to a file or viewed within the application. The main program window displays the contents of the CIF in two primary panes (Fig. 5.3.3.6). In the left-hand pane, a tree structure shows the data blocks in the file and the data names present in each block. The data blocks may be expanded or collapsed by the user, to present an overview or a detailed view of the data structure of the file. Underneath the icon representing the data block, non-looped data items are listed alphabetically. The figure demonstrates how a single value may be selected in the left-hand pane (`_cell_length_a`) and displayed in the main window. Physical units for the selected quantity are extracted from the corresponding dictionary definition and presented alongside the numeric value. The dictionary definition may also be displayed in a separate pop-up window using the 'Show CIF Definitions' button.

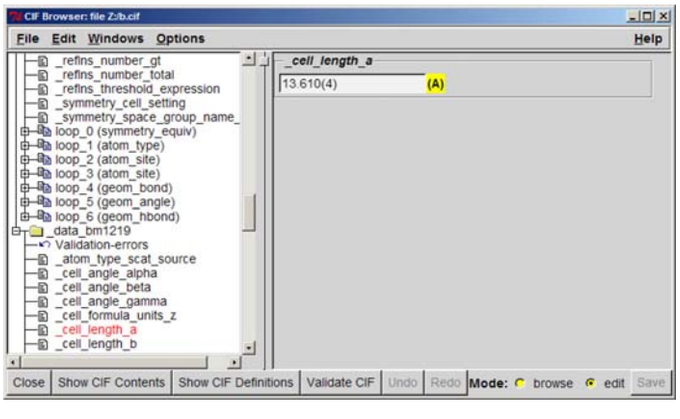

Fig. 5.3.3.6. The use of *CIFEDIT* to display and alter the contents of a CIF; here a non-looped data item is shown.

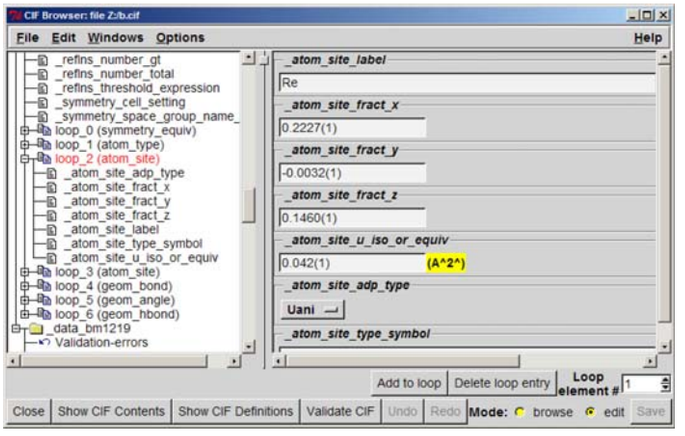

Fig. 5.3.3.7. Row-based loop editing with *CIFEDIT*; here loop_2 (comprising the ATOM_SITE category) has been selected by the user; the editing cursor begins at row 1 of the loop.

The program may be run in two modes: a 'browse' mode, where the selected value is displayed in the main pane, but may not be altered; and an 'edit' mode (as in the example) where the value appears in an editable text widget.

Data loops in the CIF are displayed after the alphabetical list of non-looped items. The loops are numbered sequentially from zero and an indication of the loop category is given in parentheses in the tree-view window. The loop 'branches' of the tree may be expanded or collapsed as the user wishes.

Loops may be viewed and edited in two ways: by row or by column. If the user selects the loop title node in the hierarchical view pane, the loop is presented by row, starting in sequence at row 1 (Fig. 5.3.3.7). Other rows may be selected by using the address box in the lower-right-hand part of the window. Alternatively, if the user selects an individual data name within the loop representation in the hierarchical view, all instances of that data item within the loop are displayed in the main pane. (In practice the number of values shown is constrained to a maximum number that the user may choose, so that the application does not run out of memory if there are very large loops.)

For items with a restricted set of permitted values in the dictionary, the editing function allows the user to select only one of the permitted options *via* a drop-down menu.

While the application is intended to be used in this structured and itemized mode, there is an option to open the entire CIF in a text-editing window if there are errors that cannot be handled in the normal mode. This is not recommended, but is occasionally convenient. While this free-text editing mode is in operation, the ability to modify the file through the structured editing pane is suspended to avoid conflicting changes.

After any change has been made, the user may revalidate the file. This is strongly recommended after making changes in the free-text editing mode.

5.3.3.3. *HICCuP*

The program *HICCuP* (Edgington, 1997) was an early graphical utility developed at the Cambridge Crystallographic Data Centre for interactive editing and validation of a CIF. It is no longer supported, having been replaced by *enCIFer* (Section 5.3.3.1). Nevertheless, it contained some interesting features and is of potential interest to developers using multiple-platform scripting languages. It was implemented in the Python language (van Rossum, 1991) and required that Tcl/Tk (Ousterhout, 1994) be also available on the host computer. The name of the program is an acronym for 'High-Integrity CIF Checking using Python'.