2. CONCEPTS AND SPECIFICATIONS

The attributes `_list_mandatory` and `_list_reference` are also connected to each other. The former signals (with values of `yes` or `no`) whether the presence of a data item is essential to preserving the validity of a list of items. The latter attribute identifies the data item in the list that provides the unique key value to each packet or row of items in a list. A packet is made up of listed values, one for each item in the name list (*i.e.* the packet size matches the number of data names at the head of the list). The `_list_reference` attribute identifies items that are the keys to specific packets in the list. In Example 2 of Fig. 2.5.5.5 the key item is `_atom_site_label` and the listed labels S1, S2, N1 and C1 must be unique.

The attribute `_list_uniqueness` is used to identify items that must be unique for a list to be valid and accessible. This attribute is similar to `_list_reference` except that it appears only in a definition in which `_list_mandatory` is set to `yes`. This simplifies validation because it may be used as the placeholder for all items that jointly identify the uniqueness of a list packet. This is in contrast to the attribute `_list_reference`, which appears in the definition of every item dependent on this item.

Relational attributes are used to link equivalent data. The `_related_item` attribute identifies items related to the defined data item. The nature of this relationship is specified with the `_related_function` attribute according to the restricted value states of `alternate`, `convention`, `conversion` and `replace`. The definition of these states is detailed in Chapter 4.9. Relational attributes are used to provide equivalent data items, to replace definitions when definitions are superseded or to change access pathways. These facilities are for archives, because they enable old data to be accessed and the associated definitions to remain in a dictionary even when superseded by new definitions. The old and new definitions are linked by these attributes so that all related data items can be validated and accessed.

2.5.6.5. Dictionary registration attributes

This class of attributes is used to register the dictionary version and audit information. They are

```
_dictionary_history
_dictionary_name
_dictionary_update
_dictionary_version
```

Dictionary attributes are used to record the creation and update history of a dictionary. The attribute `_dictionary_history` specifies the entry and update information of the dictionary, and `_dictionary_name` specifies the generic name of the electronic file containing the dictionary (the actual name of the file can vary from site to site). The attributes `_dictionary_version` and `_dictionary_update` specify the version number and the date of the last change in the dictionary. Both items represent important external reference information. An example application of these attributes is shown in Fig. 2.5.5.2.

References

Allen, F. H., Barnard, J. M., Cook, A. F. P. & Hall, S. R. (1995). *The Molecular Information File (MIF): core specifications of a new standard format for chemical data. J. Chem. Inf. Comput. Sci.* **35**, 412–427.

Bourne, P. E., Berman, H. M., McMahon, B., Watenpaugh, K. D., Westbrook, J. D. & Fitzgerald, P. M. D. (1997). *Macromolecular Crystallographic Information File. Methods Enzymol.* **277**, 571–590.

Gray, P. M. D., Kulkarni, K. G. & Paton, N. W. (1992). *Object oriented databases*. New York: Prentice Hall.

Hall, S. R. (1991). *The STAR File: a new format for electronic data transfer and archiving. J. Chem. Inf. Comput. Sci.* **31**, 326–333.

Hall, S. R., Allen, F. H. & Brown, I. D. (1991). *The Crystallographic Information File (CIF): a new standard archive file for crystallography. Acta Cryst.* A**47**, 655–685.

Hall, S. R. & Cook, A. P. F. (1995). *STAR dictionary definition language: initial specification. J. Chem. Inf. Comput. Sci.* **35**, 819–825.

Hall, S. R. & Spadaccini, N. (1994). *The STAR File: detailed specifications. J. Chem. Inf. Comput. Sci.* **34**, 505–508.

IEEE (1991). *IEEE Standard for Information Technology – Portable Operating System Interface (POSIX) – Part 2: Shell and utilities*, Vol. 1, IEEE Standard 1003.2-1992. New York: The Institute of Electrical and Electronic Engineers, Inc.

Kim, W. (1990). *Introduction to object oriented databases*. Boston: MIT Press.

Westbrook, J. D. & Hall, S. R. (1995). *A dictionary description language for macromolecular structure*. http://ndbserver.rutgers.edu/mmcif/ddl/.

references