

## 3.1. GENERAL CONSIDERATIONS WHEN DEFINING A CIF DATA ITEM

Table 3.1.8.1. CIF dictionary register (maintained as a STAR File)

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```

data_validation_dictionaries
loop_
  _cifdic_dictionary.name
  _cifdic_dictionary.version
  _cifdic_dictionary.DDL_compliance
  _cifdic_dictionary.reserved_prefix
  _cifdic_dictionary.URL
  _cifdic_dictionary.description
cif_core.dic . 1.4.1 .
  ftp://ftp.iucr.org/pub/cifdics/cif_core.dic
  'Core CIF Dictionary'
cif_core.dic 1.0 . .
  ftp://ftp.iucr.org/pub/cifdics/cifdic.C91
  'Original Core CIF Dictionary'
cif_core.dic 2.3.1 1.4.1 .
  ftp://ftp.iucr.org/pub/cifdics/cif_core_2.3.1.dic
  'Core CIF Dictionary'
cif_pd.dic . 1.4 .
  ftp://ftp.iucr.org/pub/cifdics/cif_pd.dic
  'Powder CIF Dictionary'
cif_pd.dic 1.0.1 1.4 .
  ftp://ftp.iucr.org/pub/cifdics/cif_pd_1.0.1.dic
  'Powder CIF Dictionary'
cif_ms.dic . 1.4 .
  ftp://ftp.iucr.org/pub/cifdics/cif_ms.dic
  'Modulated structures CIF Dictionary'
cif_ms.dic 1.0.1 1.4 .
  ftp://ftp.iucr.org/pub/cifdics/cif_ms_1.0.1.dic
  'Modulated structures CIF Dictionary'
cif_rho.dic . 1.4 .
  ftp://ftp.iucr.org/pub/cifdics/cif_rho.dic
  'Modulated structures CIF Dictionary'
cif_rho.dic 1.0.1 1.4 .
  ftp://ftp.iucr.org/pub/cifdics/cif_rho_1.0.1.dic
  'Electron density CIF Dictionary'
cif_mm.dic . 2.1.2 .
  ftp://ftp.iucr.org/pub/cifdics/cif_mm.dic
  'Macromolecular CIF Dictionary'
cif_mm.dic 1.0 2.1.2 .
  ftp://ftp.iucr.org/pub/cifdics/cif_mm_1.0.dic
  'Macromolecular CIF Dictionary'
mmcif_std.dic . 2.1.6 .
  ftp://ftp.iucr.org/pub/cifdics/mmcif_std.dic
  'Macromolecular CIF Dictionary'
mmcif_std.dic 2.0.09 2.1.6 .
  ftp://ftp.iucr.org/pub/cifdics/cif_mm_2.0.09.dic
  'Macromolecular CIF Dictionary'
cif_img.dic . 2.1.3 .
  ftp://ftp.iucr.org/pub/cifdics/cif_img.dic
  'Image CIF Dictionary'
cif_img.dic 1.0 2.1.3 .
  ftp://ftp.iucr.org/pub/cifdics/cif_img_1.0.dic
  'Image CIF Dictionary'
cif_img.dic 1.3.2 2.1.3 .
  ftp://ftp.iucr.org/pub/cifdics/cif_img_1.3.2.dic
  'Image CIF Dictionary'
cif_sym.dic . 2.1.3 .
  ftp://ftp.iucr.org/pub/cifdics/cif_sym.dic
  'Symmetry CIF Dictionary'
cif_sym.dic 1.0.1 2.1.3 .
  ftp://ftp.iucr.org/pub/cifdics/cif_sym_1.0.1.dic
  'Symmetry CIF Dictionary'
cif_compat.dic . 1.4 .
  ftp://ftp.iucr.org/pub/cifdics/cif_compat.dic
  'Legacy CIF Dictionary of deprecated terms'
ddl_core.dic . 1.4.1 .
  ftp://ftp.iucr.org/pub/cifdics/ddl_core.dic
  'Non-relational dictionary definition language'
ddl_core_2.1.3.dic . 2.1.3 .
  ftp://ftp.iucr.org/pub/cifdics/ddl_core_2.1.3.dic
  'Relational dictionary definition language'
mmcif_ddl.dic . 2.1.6 .
  ftp://ftp.iucr.org/pub/cifdics/mmcif_ddl.dic
  'Relational dictionary definition language'

```

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Table 3.1.8.1 is an extract from the current register. The latest version of the register will always be available from the URL given above.

The entries for each dictionary include one with the version string set to '.', representing the current version; this is the version that should be retrieved unless a data file specifies otherwise.

Note that the register may also contain locators for local dictionaries constructed by owners of reserved prefixes (Section 3.1.2.2) when the owner has requested that a dictionary of local names be made publicly available. An appropriate name for a local dictionary in the register (`_dictionary_name` or `_dictionary.title` for DDL1 or DDL2 dictionaries, respectively) would be `cif_local_myprefix.dic`, where the string indicated by `myprefix` is one of the prefixes reserved for private use by the author of the dictionary (see Section 3.1.2.2). This scheme complements the naming convention for public dictionaries.

## 3.1.8.3. Locating a dictionary for validation

The following protocol applies to the creation and use of software designed to locate the dictionaries referenced by a data file and validate the data file against them. The protocol is necessary to address the issues that arise because dictionaries evolve through various audited versions, because not all dictionaries referenced by a data file may be accessible, and because data files might not in practice contain pointers to their associated dictionaries.

Software source code for applications that use CIF dictionaries to validate the contents of data files should be distributed with a copy of the most recent version of the register of dictionaries, and with the URL of the master copy hard-coded. Library utilities should be provided that permit local cacheing of the register file and the ability to download and replace the cached register at regular intervals. Individual dictionary files located and retrieved through the use of the register should also be cached locally, to guard against temporary unavailability of network resources.

Each CIF data file should contain a reference to one or more dictionary files against which the file may be validated. At the very least this will be `_audit_conform_dict_name` (`_audit_conform.dict_name` for DDL2 files) ( $N$ ). `*_version` ( $V$ ) and `*_location` ( $L$ ) are optional. In the event that no dictionaries are specified, the default validation dictionary should be that identified as having  $N = \text{cif\_core.dic}$  and  $V = \text{'.'}$  (i.e. the most recent version of the core dictionary). Since dictionaries are intended always to be extended, it is normally enough just to specify the name (and possibly the location).

This default is appropriate for most well formed CIFs, but if it is important to provide formal validation of old CIFs conforming to the earliest printed specification, which used the now-deprecated units extension convention, the dictionary `cif_compat.dic` may also be added to the default list (Section 3.1.5.4.3).

There is a difficulty associated with assuming this default for CIFs containing DDL2 data names. At present, the DDL2 version of the core dictionary does not exist as a separate file. Most existing CIFs built on the DDL2 model conform to the macromolecular (mmCIF) dictionary, and so best current working practice is to assume a default validation dictionary for DDL2-style CIFs with  $N = \text{mmcif\_std.dic}$  and  $V = \text{'.'}$  (i.e. the most recent version of the mmCIF dictionary), since this includes the core data names as a subset. However, to anticipate future developments, it is suggested that applications built to validate DDL2 files first search the register for a default entry with  $N = \text{cif\_core.dic}$ ,  $V = \text{'.'}$  and a value of 2 or higher for the relevant DDL version:

```

loop_
  _cifdic_dictionary.name
  _cifdic_dictionary.version
  _cifdic_dictionary.DDL_compliance
cif_core.dic . 2.1.2

```