```
data_atom_site_Cartn_
    loop_ _name                 '_atom_site_Cartn_x'
                                '_atom_site_Cartn_y'
                                '_atom_site_Cartn_z'
    _category                    atom_site
    _type                        numb
    _type_conditions             esd
    _list                        yes
    _list_reference             '_atom_site_label'
    _units                       A
    _units_detail               'angstroms'
    _definition
;   The atom-site coordinates in angstroms specified
    according to a set of orthogonal Cartesian axes
    related to the cell axes as specified by the
    _atom_sites_Cartn_transform_axes description.
;
```

(*a*)

```
save__atom_site.Cartn_x
    _item_description.description
;   The x atom-site coordinate in angstroms
    specified according to a set of orthogonal
    Cartesian axes related to the cell axes as
    specified by the description given in
    _atom_sites.Cartn_transform_axes.
;
    _item.name                  '_atom_site.Cartn_x'
    _item.category_id            atom_site
    _item.mandatory_code         no
    _item_sub_category.id        cartesian_coordinate
    _item_aliases.alias_name    '_atom_site_Cartn_x'
    _item_aliases.dictionary     cif_core.dic
    _item_aliases.version        2.0.1
     loop_
    _item_dependent.dependent_name
                                '_atom_site.Cartn_y'
                                '_atom_site.Cartn_z'
    _item_related.related_name
                               '_atom_site.Cartn_x_esd'
    _item_related.function_code associated_esd
    _item_type.code              float
    _item_type_conditions.code   esd
    _item_units.code             angstroms
     save_
```

(*b*)

Fig. 2.5.4.1. Comparison of DDL versions: (*a*) DDL1, (*b*) DDL2.

3.2–3.5 and presented in full in Chapters 4.1–4.4, respectively, of this volume.

It is helpful to give a brief comparison of the definition capabilities of DDL1 and DDL2. The differences may be best illustrated by simply comparing their application to the definition of the same data item. The two separate definitions of `_atom_site_Cartn_x` are shown in Fig. 2.5.4.1.

Although both DDL versions conform to the syntax of the STAR File (DDL1 conforms to the CIF syntax but DDL2 uses STAR File save frames not permitted in CIF data files) and are composed of similar attributes, there are clear differences. These are summarized in Table 2.5.4.1.

The similarity in the two DDL versions is such that software exists for parsing and validating CIFs against the DDL1 or DDL2 dictionaries interchangeably (*e.g.* see the CIF toolbox software *CIFtbx* described in Chapter 5.4).

2.5.5. The structure of DDL1 definitions

The organization of definitions in a CIF dictionary is straightforward. We are all familiar with how words are described in a

```
data_cell_formula_units_Z
    _name                       '_cell_formula_units_Z'
    _category                    cell
    _type                        numb
    _enumeration_range           1:
    _definition
; The number of the formula units in the unit cell
  as specified by _chemical_formula_structural,
  _chemical_formula_moiety or _chemical_formula_sum.
;
```

Fig. 2.5.5.1. DDL1 definition with a few attributes.

```
data_on_this_dictionary
    _dictionary_name            cif_example.dic
    _dictionary_version         0.0
    _dictionary_update          1999-03-15
    _dictionary_history
;  1999-03-11  Created as a dictionary example
   1999-03-15  Further simplifications
;
data_parameter_ABC
    _name                       '_parameter_ABC'
#        <<<<<<<<<< other data attributes here
data_factor_XYZ
    _name                       '_factor_XYZ'
#        <<<<<<<<<< other data attributes here
data_and_so_on
    _name                       '_and_so_on'
#        <<<<<<<<<< other data attributes here
```

Fig. 2.5.5.2. DDL1 definition showing basic dictionary organization.

spoken-language dictionary. Each defined word is followed by a sequence of attribute descriptions, such as phonetic annotation, grammatical context, word origins, meanings, examples of use and so on. The definition of data items in a CIF dictionary is organized in the same way. Each item description is preceded by the item's unique identifying tag as a datablock code, and is composed of a sequence of attribute items specifying the item's characteristics. A full description of the DDL1 attributes is given in Chapter 4.9.

A series of example definitions will be used to introduce the basic structure of the dictionary and definitions. The definitions are of familiar crystallographic data items, extracted from the core CIF dictionary in Chapter 4.1. Note that, in some cases, the text part of the definitions has been abbreviated for conciseness.

2.5.5.1. Definition example 1: formula units per cell (*Z*)

A definition for formula units in a crystal unit cell (*Z*) is shown in Fig. 2.5.5.1. The definition includes only the attributes `_name`, `_category`, `_type`, `_enumeration_range` and `_definition`. These identify the item's unique properties and enable its validation. The `_category` attribute indicates the class of the defined data item. Since lists may contain only items of one category type, this attribute is critical to data items appearing in lists (see Section 2.5.5.5). The attribute `_enumeration_range` has the value '`1:`' which stipulates that the item must be 'one or a higher number'.

2.5.5.2. Definition example 2: dictionary audit information

A CIF dictionary file contains, in addition to the data definitions, information about the nature of the dictionary. Fig. 2.5.5.2 shows the typical organization of definitions in a dictionary. Each dictionary starts with the audit information giving its version and creation history. This is followed by definitions in separate data

```
data_cell_length_
    loop_ _name                 '_cell_length_a'
                                '_cell_length_b'
                                '_cell_length_c'
    _category                    cell
    _type                        numb
    _type_conditions             esd
    _enumeration_range           0.0:
    _units                       A
    _units_detail               'angstroms'
    _definition
;   Unit-cell lengths in angstroms corresponding to
    the structure reported.
;
```

Fig. 2.5.5.3. DDL1 definition of irreducible data items.

```
data_atom_site_attached_hydrogens
_name             '_atom_site_attached_hydrogens'
    _category              atom_site
    _type                  numb
    _list                  yes
    _list_reference        '_atom_site_label'
    _enumeration_range     0:8
    _enumeration_default   0
    _definition
;   The number of hydrogen atoms attached to the atom
    at this site excluding any hydrogen atoms for
    which coordinates (measured or calculated) are
    given.
;
```

Fig. 2.5.5.4. DDL1 definition of a 'list' data item.

blocks. The name of a data block matches the defined data name or the initial portion thereof. Each definition data block contains a sequence of data declarations, one for each attribute. The attributes within a data block constitute the total definition information, and only those attributes appropriate to a given defined item need be specified.

2.5.5.3. Definition example 3: irreducible data items

Some data items are closely related to other data items. Fig. 2.5.5.3 shows the definition of the length components `_cell_length_a`, `*_b` and `*_c` of the crystal unit-cell metric tensor. Because of their different enumeration and units attributes, the definition blocks for cell lengths and angles are specified separately. This definition shows how data items closely related in function may be defined in the same data block. The `loop_` command is used to list the multiple `_name` values. The attribute `_type_conditions` is used to indicate that these values are measurements and can have a standard uncertainty ('s.u.') value appended in parentheses *e.g.* 7.254(2). (The label 'esd' reflects the historical but inaccurate terminology 'estimated standard deviation'.) The `_units` and `_units_detail` attributes stipulate that the measurement unit of length is ångströms.

2.5.5.4. Definition example 4: list data

The definition of the number of hydrogen atoms attached to an atom site is shown in Fig. 2.5.5.4. The attributes `_list` and `_list_reference` signal whether the item is used in a list and what key item is in that list. As described in Chapters 2.1 and 2.2, a CIF list is a two-dimensional table where data items are in the columns (headed by the data names) and the values are the rows. The attribute `_list` is `yes` if a data item may be used in a list. The attribute `_list_reference` specifies the key item as `_atom_site_label`. Each value of a key item must be unique so that the row of associated items can be accessed unambiguously. The attribute `_enumeration_default` specifies a default value for the defined item if it is absent from the data file.

2.5.5.5. Definition example 5: category information

Each CIF dictionary also contains example applications of defined data items, grouped according to category. Fig. 2.5.5.5 shows these for the category ATOM_SITE, as defined in the core dictionary (see Chapter 3.2). A `_type` attribute with a value of `null` specifies that a data block contains no definition information. The particular examples shown here illustrate that the reference key for the ATOM_SITE category is `_atom_site_label`. This data item is present in both examples shown, and in each packet the label is unique.

2.5.5.6. Definition example 6: mandatory and linked items

The example definition in Fig. 2.5.5.6 shows the attributes for the item `_atom_site_label`. As illustrated in Section 2.5.5.5, this item is the reference key to a list of items belonging to the category ATOM_SITE. The attribute `_list_mandatory`, which is set to a value of `yes`, specifies that this item is a mandatory item to a list of category ATOM_SITE items. The attribute `_list_link_child` identifies items in other categories that are 'linked' by derivation to this item and therefore share the same data values. This dependency is known as a child dependency. The definition shows that data items describing the labels of atom sites in a list of angular geometry, *i.e.* `_geom_angle_atom_site_label_1` and `_geom_angle_atom_site_label_2`, are the same labels described by `_atom_site_label` in the atom-site list. This is because the geometry is derived directly from the atom-site data. Note that this dependency requires that the ATOM_SITE list be present in the same CIF as the GEOM_ANGLE list, otherwise the molecular geometry information cannot be linked to the three-dimensional structural information.

2.5.5.7. Definition example 7: joinable lists

In the example definition shown in Fig. 2.5.5.7, the key item `_atom_site_aniso_label` is shown to have a special relationship with the key item `_atom_site_label`. This is because the data items in the list category ATOM_SITE_ANISO may be merged with (*i.e.* joined to) items in the list category ATOM_SITE. If this happens, the item `_atom_site_label` assumes the role as the key to the merged packets and this is signalled using the attribute `_list_link_parent`. When these two categories appear in separate lists, the category ATOM_SITE_ANISO data require the category ATOM_SITE data to be present in the data instantiation, but not *vice versa*. Note that the parent relationship, unlike that in the example of Section 2.5.5.6 arising from a derivation dependency, is because ATOM_SITE_ANISO is a subcategory of ATOM_SITE.

2.5.5.8. Definition example 8: equivalent items

As with the preceding example definition, this example concerns anisotropic atomic displacement parameters. Fig. 2.5.5.8 shows the definition of the component items `_atom_site_aniso_U_` that comprise an irreducible set of matrix elements. The key item in a list of ATOM_SITE_ANISO items is `_atom_site_aniso_label`. This definition illustrates how the attributes `_related_item` and `_related_function` are used to identify the similar data items `_atom_site_aniso_B_` that are atomic displacement parameters related by a simple conversion factor. Other attributes used to specify data relationships are described in Section 2.5.6 below.

```
################
## ATOM_SITE ##
################
data_atom_site_[]
    _name                      '_atom_site_[]'
    _category                    category_overview
    _type                        null
    loop_ _example
          _example_detail
# - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 1 - based on data set TOZ of Willis,
    Beckwith & Tozer [Acta Cryst. (1991), C47,
    2276-2277].
;
;   loop_
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_adp_type
    _atom_site_calc_flag
    _atom_site_calc_attached_atom
O1   .4154(4)  .5699(1)  .3026(0)  .060(1)  Uani  ? ?
C2   .5630(5)  .5087(2)  .3246(1)  .060(2)  Uani  ? ?
C3   .5350(5)  .4920(2)  .3997(1)  .048(1)  Uani  ? ?
N4   .3570(3)  .5558(1)  .4167(0)  .039(1)  Uani  ? ?
# - - - - data truncated for brevity - - - -
H321C  .04(1)  .318(3)   .320(2)   .14000   Uiso  ? ?
H322A  .25(1)  .272(4)   .475(3)   .19000   Uiso  ? ?
H322B  .34976  .22118    .40954    .19000   Uiso
                                             calc C322
;
# - - - - - - - - - - - - - - - - - - - - - - - - -
;   Example 2 - based on data set DPTD of Yamin,
    Suwandi, Fun, Sivakumar & bin Shawkataly
    [Acta Cryst. (1996), C52, 951-953].
;
;   loop_
    _atom_site_label
    _atom_site_chemical_conn_number
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
S1  1  0.74799(9)  -0.12482(11) 0.27574(9) 0.0742(3)
S2  2  1.08535(10)  0.16131(9)  0.34061(9) 0.0741(3)
N1  3  1.0650(2)   -0.1390(2)   0.2918(2)  0.0500(5)
C1  4  0.9619(3)   -0.0522(3)   0.3009(2)  0.0509(6)
# - - - - data truncated for brevity - - - -
;
    _definition
;    Data items in the ATOM_SITE category record
     details about the atom sites in a crystal
     structure, such as the positional
     coordinates, atomic displacement parameters,
     and magnetic moments and directions.
;
```

Fig. 2.5.5.5. DDL1 overview of a category of items.

2.5.5.9. Definition example 9: enumeration states

The last example, in Fig. 2.5.5.9, shows the definition of an item whose value is restricted to a predictable set of values known as enumeration states. The attributes `_enumeration` and `_enumeration_detail` are used to specify which enumeration states are permitted for the defined data item. Only one of these states may appear as the value for the defined item in a CIF. The attribute `_enumeration_default` specifies the state value that is used if an item is not instantiated.

```
data_atom_site_label
    _name                      '_atom_site_label'
    _category                    atom_site
    _type                        char
    _list                        yes
    _list_mandatory              yes
    loop_ _list_link_child
                  '_atom_site_aniso_label'
                  '_geom_angle_atom_site_label_1'
                  '_geom_angle_atom_site_label_2'
                  '_geom_angle_atom_site_label_3'
                  '_geom_bond_atom_site_label_1'
                  '_geom_bond_atom_site_label_2'

    loop_ _example    C12     Ca3g28     Fe3+17
                      H*251  boron2a  C_a_phe_83_a_0
                      Zn_Zn_301_A_0
    _definition
;    The _atom_site_label is a unique identifier for
     a particular site in the crystal.
;
```

Fig. 2.5.5.6. DDL1 definition of a 'mandatory' data item.

```
data_atom_site_aniso_label
    _name                     '_atom_site_aniso_label'
    _category                   atom_site
    _type                       char
    _list                       yes
    _list_link_parent         '_atom_site_label'
    _definition
;   Anisotropic atomic displacement parameters are
    usually looped in a separate list. If this is the
    case, this code must match the _atom_site_label
    of the associated atom in the atom coordinate
    list and conform with the same rules described
    in _atom_site_label.
;
```

Fig. 2.5.5.7. DDL1 definition of a 'parent' data item.

```
data_atom_site_aniso_U_
    loop_ _name                '_atom_site_aniso_U_11'
                               '_atom_site_aniso_U_12'
                               '_atom_site_aniso_U_13'
                               '_atom_site_aniso_U_22'
                               '_atom_site_aniso_U_23'
                               '_atom_site_aniso_U_33'
    _category                   atom_site
    _type                       numb
    _type_conditions            su
    _list                       yes
    _list_reference           '_atom_site_aniso_label'
    _related_item             '_atom_site_aniso_B_'
    _related_function           conversion
    _units                     A^2^
    _units_detail             'angstroms squared'
    _definition
;   These are the standard anisotropic atomic
    displacement components in angstroms squared.
;
```

Fig. 2.5.5.8. DDL1 definition showing 'related' data items.

2.5.6. DDL1 attribute descriptions

This section provides an overview of the different attributes that make up the core data dictionary language DDL1. A more detailed description of attributes is given in the DDL1 dictionary in Chapter 4.9. In this dictionary the attributes are used to define themselves!