```
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.

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