```
+ _atom_site.aniso_B[1][2]
        ⇌ _atom_site_anisotrop.B[1][2]
+ _atom_site.aniso_B[1][3]
        ⇌ _atom_site_anisotrop.B[1][3]
+ _atom_site.aniso_B[2][2]
        ⇌ _atom_site_anisotrop.B[2][2]
+ _atom_site.aniso_B[2][3]
        ⇌ _atom_site_anisotrop.B[2][3]
+ _atom_site.aniso_B[3][3]
        ⇌ _atom_site_anisotrop.B[3][3]
  _atom_site.aniso_ratio
        ⇌ _atom_site_anisotrop.ratio
+ _atom_site.aniso_U[1][1]
        ⇌ _atom_site_anisotrop.U[1][1]
+ _atom_site.aniso_U[1][2]
        ⇌ _atom_site_anisotrop.U[1][2]
+ _atom_site.aniso_U[1][3]
        ⇌ _atom_site_anisotrop.U[1][3]
+ _atom_site.aniso_U[2][2]
        ⇌ _atom_site_anisotrop.U[2][2]
+ _atom_site.aniso_U[2][3]
        ⇌ _atom_site_anisotrop.U[2][3]
+ _atom_site.aniso_U[3][3]
        ⇌ _atom_site_anisotrop.U[3][3]
  _atom_site.attached_hydrogens
  _atom_site.auth_asym_id
  _atom_site.auth_atom_id
  _atom_site.auth_comp_id
  _atom_site.auth_seq_id
+ _atom_site.B_equiv_geom_mean
+ _atom_site.B_iso_or_equiv
  _atom_site.calc_attached_atom
  _atom_site.calc_flag
+ _atom_site.Cartn_x
+ _atom_site.Cartn_y
+ _atom_site.Cartn_z
  _atom_site.chemical_conn_number
        → _chemical_conn_atom.number
  _atom_site.constraints
  _atom_site.details (~ _atom_site_description)
  _atom_site.disorder_assembly
  _atom_site.disorder_group
  _atom_site.footnote_id
+ _atom_site.fract_x
+ _atom_site.fract_y
+ _atom_site.fract_z
  _atom_site.group_PDB
  _atom_site.label_alt_id
        → _atom_sites_alt.id
  _atom_site.label_asym_id
        → _struct_asym.id
  _atom_site.label_atom_id
        → _chem_comp_atom.atom_id
  _atom_site.label_comp_id
        → _chem_comp.id
  _atom_site.label_entity_id
        → _entity.id
  _atom_site.label_seq_id
        → _entity_poly_seq.num
+ _atom_site.occupancy
  _atom_site.refinement_flags
  _atom_site.refinement_flags_adp
  _atom_site.refinement_flags_occupancy
  _atom_site.refinement_flags_posn
  _atom_site.restraints
  _atom_site.symmetry_multiplicity
  _atom_site.thermal_displace_type
  _atom_site.type_symbol
        → _atom_type.symbol
+ _atom_site.U_equiv_geom_mean
+ _atom_site.U_iso_or_equiv
  _atom_site.Wyckoff_symbol
```

(*b*) ATOM_SITE_ANISOTROP

```
• _atom_site_anisotrop.id
+ _atom_site_anisotrop.B[1][1] (~ _atom_site_aniso_B_11)
+ _atom_site_anisotrop.B[1][2] (~ _atom_site_aniso_B_12)
+ _atom_site_anisotrop.B[1][3] (~ _atom_site_aniso_B_13)
+ _atom_site_anisotrop.B[2][2] (~ _atom_site_aniso_B_22)
+ _atom_site_anisotrop.B[2][3] (~ _atom_site_aniso_B_23)
+ _atom_site_anisotrop.B[3][3] (~ _atom_site_aniso_B_33)
  _atom_site_anisotrop.ratio (~ _atom_site_aniso_ratio)
        → _atom_site.id
  _atom_site_anisotrop.type_symbol
        (~ _atom_site_aniso_type_symbol)
        → _atom_type.symbol
+ _atom_site_anisotrop.U[1][1] (~ _atom_site_aniso_U_11)
+ _atom_site_anisotrop.U[1][2] (~ _atom_site_aniso_U_12)
+ _atom_site_anisotrop.U[1][3] (~ _atom_site_aniso_U_13)
+ _atom_site_anisotrop.U[2][2] (~ _atom_site_aniso_U_22)
+ _atom_site_anisotrop.U[2][3] (~ _atom_site_aniso_U_23)
+ _atom_site_anisotrop.U[3][3] (~ _atom_site_aniso_U_33)
```

The bullet (•) indicates a category key. The arrow (→) is a reference to a parent data item. Items in italics have aliases in the core CIF dictionary formed by changing the full stop (.) to an underscore (_) except where indicated by the ~ symbol. Data items marked with a plus (+) have companion data names for the standard uncertainty in the reported value, formed by appending the string **_esd** *to the data name listed. The double arrow (⇌) indicates alternative names in a distinct category.*

The refined coordinates of the atoms in the crystallographic asymmetric unit are stored in the ATOM_SITE category. Atom positions and their associated uncertainties may be given using either Cartesian or fractional coordinates, and anisotropic displacement factors and occupancies may be given for each position.

The relationships between categories describing atom sites are shown in Fig. 3.6.7.1.

Several of the mmCIF data names arise from the need to associate atom sites with residues and chains. As in the core CIF dictionary, the identifier for the atom site is the data item **_atom_site_label**. To accommodate standard practice in macromolecular crystallography, the mmCIF atom identifier is the aggregate of **_atom_site.label_alt_id**, ***.label_asym_id**, ***.label_atom_id**, ***.label_comp_id** and ***.label_seq_id**. For the two types of files to be compatible, the data item **_atom_site.id**, which is independent of the different modes of identifying atoms (discussed below), was introduced. The mmCIF identifier **_atom_site.id** is aliased to the core CIF identifier **_atom_site_label**.

Since the identifier does not need to be a number, it is quite possible (although it is not recommended) to use a complex label with an internal structure corresponding to the label components that the mmCIF dictionary provides as separate data items. This scheme is described in Section 3.2.4.1.1. However, normal practice in mmCIFs should be to label sites with the functional components available and to assign a simple numeric sequence to the values of **_atom_site.id** (see Example 3.6.7.1).

In addition to labelling information, each entry in the ATOM_SITE list must contain a value for the data item **_atom_site.type_symbol**, which is a pointer to the table of element symbols in the ATOM_TYPE category. All other data items in the ATOM_SITE category are optional, but it is normal practice to

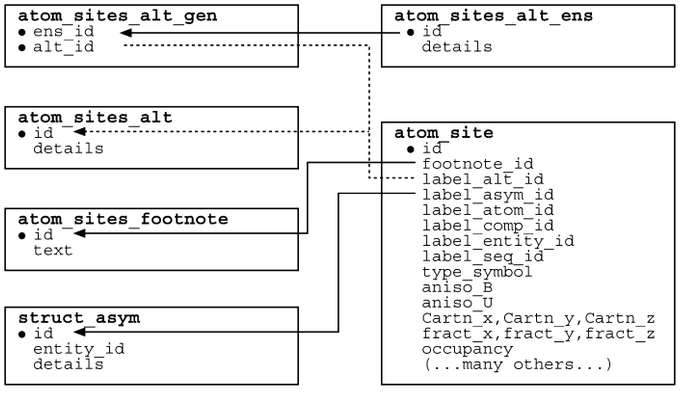

Fig. 3.6.7.1. The family of categories used to describe atom sites. Boxes surround categories of related data items. Data items that serve as category keys are preceded by a bullet (•). Lines show relationships between linked data items in different categories with arrows pointing at the parent data items.

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