3.6.7.1.2. *Collections of atom sites*

The data items in these categories are as follows:

(*a*) ATOM_SITES

- **_atom_sites.entry_id**
  → **_entry.id**
  _atom_sites.Cartn_transf_matrix[1][1]
  (∼ **_atom_sites_Cartn_tran_matrix_11**)
  _atom_sites.Cartn_transf_matrix[1][2]
  (∼ **_atom_sites_Cartn_tran_matrix_12**)
  _atom_sites.Cartn_transf_matrix[1][3]
  (∼ **_atom_sites_Cartn_tran_matrix_13**)
  _atom_sites.Cartn_transf_matrix[2][1]
  (∼ **_atom_sites_Cartn_tran_matrix_21**)
  _atom_sites.Cartn_transf_matrix[2][2]
  (∼ **_atom_sites_Cartn_tran_matrix_22**)
  _atom_sites.Cartn_transf_matrix[2][3]
  (∼ **_atom_sites_Cartn_tran_matrix_23**)
  _atom_sites.Cartn_transf_matrix[3][1]
  (∼ **_atom_sites_Cartn_tran_matrix_31**)
  _atom_sites.Cartn_transf_matrix[3][2]
  (∼ **_atom_sites_Cartn_tran_matrix_32**)
  _atom_sites.Cartn_transf_matrix[3][3]
  (∼ **_atom_sites_Cartn_tran_matrix_33**)
  _atom_sites.Cartn_transf_vector[1]
  (∼ **_atom_sites_Cartn_tran_vector_1**)
  _atom_sites.Cartn_transf_vector[2]
  (∼ **_atom_sites_Cartn_tran_vector_2**)
  _atom_sites.Cartn_transf_vector[3]
  (∼ **_atom_sites_Cartn_tran_vector_3**)
  _atom_sites.Cartn_transform_axes
  _atom_sites.fract_transf_matrix[1][1]
  (∼ **_atom_sites_fract_tran_matrix_11**)
  _atom_sites.fract_transf_matrix[1][2]
  (∼ **_atom_sites_fract_tran_matrix_12**)
  _atom_sites.fract_transf_matrix[1][3]
  (∼ **_atom_sites_fract_tran_matrix_13**)
  _atom_sites.fract_transf_matrix[2][1]
  (∼ **_atom_sites_fract_tran_matrix_21**)
  _atom_sites.fract_transf_matrix[2][2]
  (∼ **_atom_sites_fract_tran_matrix_22**)
  _atom_sites.fract_transf_matrix[2][3]
  (∼ **_atom_sites_fract_tran_matrix_23**)
  _atom_sites.fract_transf_matrix[3][1]
  (∼ **_atom_sites_fract_tran_matrix_31**)
  _atom_sites.fract_transf_matrix[3][2]
  (∼ **_atom_sites_fract_tran_matrix_32**)
  _atom_sites.fract_transf_matrix[3][3]
  (∼ **_atom_sites_fract_tran_matrix_33**)
  _atom_sites.fract_transf_vector[1]
  (∼ **_atom_sites_fract_tran_vector_1**)
  _atom_sites.fract_transf_vector[2]
  (∼ **_atom_sites_fract_tran_vector_2**)
  _atom_sites.fract_transf_vector[3]
  (∼ **_atom_sites_fract_tran_vector_3**)
  _atom_sites.solution_hydrogens
  _atom_sites.solution_primary
  _atom_sites.solution_secondary
  _atom_sites.special_details

(*b*) ATOM_SITES_FOOTNOTE

- **_atom_sites_footnote.id**
  _atom_sites_footnote.text

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.*

The ATOM_SITES category of the core dictionary, which is used to record information that applies collectively to all the atom sites in the model of the structure, is incorporated without change into the mmCIF dictionary, and Section 3.2.4.1.2 can be consulted for details.

In practice, the data names in the PHASING categories are preferred to the aliases to the core CIF data items **_atom_sites.solution_primary**, ***_secondary** and ***_hydrogens**. The data items in the mmCIF PHASING categories are designed to allow a much more detailed description of how a macromolecular structure was solved.

Example 3.6.7.2. *Footnotes for particular groups of atom sites in an HIV-1 protease structure (PDB 5HVP) using data items in the ATOM_SITES_FOOTNOTE category.*

```
loop_
  _atom_sites_footnote.id
  _atom_sites_footnote.text
     3
; The positions of these water molecules correlate
  with the alternative orientations of the
  inhibitor. Water molecules with alternative ID
  "1" and occupancy 0.58 correlate with
  inhibitor orientation "1". Water molecules with
  alternative ID "2" and occupancy 0.42 correlate
  with inhibitor orientation "2".
;
     4
; Side chains of these residues adopt alternative
  orientations that do not correlate with the
  alternative orientation of the inhibitor.
;
```

The data item **_atom_sites.entry_id** has been added to the ATOM_SITES category to provide the formal category key required by the DDL2 data model.

The ATOM_SITES_FOOTNOTE category can be used to note something about a group of sites in the ATOM_SITE coordinate list, each of which is flagged with the same value of **_atom_site.footnote_id**. For example, an author may wish to note atoms for which the electron density is very weak, or atoms for which static disorder has been modelled. Example 3.6.7.2 shows how an author has used these data items to describe alternative orientations in part of a structure. However, the very large number of data names describing specific structural characteristics in the mmCIF dictionary mean that these rather general data names are rarely needed.

3.6.7.1.3. *Atom types*

The data items in this category are as follows:

ATOM_TYPE

- **_atom_type.symbol**
  _atom_type.analytical_mass_percent
  (∼ **_atom_type_analytical_mass_%**)
  _atom_type.description
  _atom_type.number_in_cell
  _atom_type.oxidation_number
  _atom_type.radius_bond
  _atom_type.radius_contact
  _atom_type.scat_Cromer_Mann_a1
  _atom_type.scat_Cromer_Mann_a2
  _atom_type.scat_Cromer_Mann_a3
  _atom_type.scat_Cromer_Mann_a4
  _atom_type.scat_Cromer_Mann_b1
  _atom_type.scat_Cromer_Mann_b2
  _atom_type.scat_Cromer_Mann_b3
  _atom_type.scat_Cromer_Mann_b4
  _atom_type.scat_Cromer_Mann_c
  _atom_type.scat_dispersion_imag
  _atom_type.scat_dispersion_real
  _atom_type.scat_dispersion_source
  _atom_type.scat_length_neutron
  _atom_type.scat_source
  _atom_type.scat_versus_stol_list

The bullet (•) *indicates a category key. 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.*

The ATOM_TYPE category, which provides information about the atomic species associated with each atom site in the model of the structure, is used in the same way in the mmCIF dictionary as in the core CIF dictionary. See Section 3.2.4.1.3 for details.