the refinement. Use of **_refln_include_status** to provide more information about each reflection is greatly preferred.

Other data names in this category allow the recording of specific information about each reflection, such as the symmetry reinforcement factor ε, the number of reflections symmetry-equivalent under the Laue symmetry, the d spacing, the mean path length through the crystal $\bar{t}$, the $(\sin\theta)/\lambda$ value and, in the case of Laue experiments, the mean wavelength of the radiation. (For polychromatic radiation, the wavelength information might instead be given by **_refln_wavelength_id**, which is a code identifying a matching entry in the DIFFRN_RADIATION category.)

Other codes provide links to identifiers in other categories. The **_refln_class_code** identifies a set of reflections binned as described by entries in the REFLNS_CLASS category. **_refln_scale_group_code** identifies groups of reflections to which the same structure-factor scaling has been applied.

Note that the values of the Miller indices in this list must correspond to the cell defined by the lengths and angles recorded in the CELL category; they may, however, be different from the Miller indices in the DIFFRN_REFLN list if a transformation of the original cell has taken place. In this case, the transformation matrix is given using the **_diffrn_reflns_transf_matrix_*** items.

The usual use of a CIF as an archive of a completed structure determination implies that the values given in the REFLN list are derived from the final cycle of refinement, but this is not a formal requirement. Care should be taken when preparing a CIF for archiving that the structural model corresponds to the refinement cycle summarized in the accompanying REFLN table, especially if the file is constructed from fragments output from different programs.

3.2.3.2.2. *Groups of reflections*

The data items in these categories are as follows:

(*a*) REFLNS

_reflns_d_resolution_high
_reflns_d_resolution_low
_reflns_Friedel_coverage
_reflns_limit_h_max
_reflns_limit_h_min
_reflns_limit_k_max
_reflns_limit_k_min
_reflns_limit_l_max
_reflns_limit_l_min
_reflns_number_gt
† **_reflns_number_observed**
_reflns_number_total
† **_reflns_observed_criterion**
_reflns_special_details
_reflns_threshold_expression

(*b*) REFLNS_CLASS

• **_reflns_class_code**
_reflns_class_d_res_high
_reflns_class_d_res_low
_reflns_class_description
_reflns_class_number_gt
_reflns_class_number_total
_reflns_class_R_factor_all
_reflns_class_R_factor_gt
_reflns_class_R_Fsqd_factor
_reflns_class_R_I_factor
_reflns_class_wR_factor_all

(*c*) REFLNS_SCALE

• **_reflns_scale_group_code**
_reflns_scale_meas_F
_reflns_scale_meas_F_squared
_reflns_scale_meas_intensity

(*d*) REFLNS_SHELL

• **_reflns_shell_d_res_high**
• **_reflns_shell_d_res_low**
† **_reflns_shell_meanI_over_sigI_all**
† **_reflns_shell_meanI_over_sigI_gt**
† **_reflns_shell_meanI_over_sigI_obs**
_reflns_shell_meanI_over_uI_all
_reflns_shell_meanI_over_uI_gt
_reflns_shell_number_measured_all
_reflns_shell_number_measured_gt
† **_reflns_shell_number_measured_obs**
_reflns_shell_number_possible
_reflns_shell_number_unique_all
_reflns_shell_number_unique_gt
† **_reflns_shell_number_unique_obs**
_reflns_shell_percent_possible_all
_reflns_shell_percent_possible_gt
† **_reflns_shell_percent_possible_obs**
_reflns_shell_Rmerge_F_all
_reflns_shell_Rmerge_F_gt
† **_reflns_shell_Rmerge_F_obs**
_reflns_shell_Rmerge_I_all
_reflns_shell_Rmerge_I_gt
† **_reflns_shell_Rmerge_I_obs**

The bullet (•) *indicates a category key. Where multiple items within a category are marked with a bullet, they must be taken together to form a compound key. The dagger* (†) *indicates a deprecated item, which should not be used in the creation of new CIFs.*

The data items in the REFLNS category describe properties or attributes of the complete set of reflections used in the structure refinement. Several are derivative and may be obtained from the information in the reflections list, but it is convenient to present them separately so that they do not need to be calculated again. They can also be used to check the consistency of the reflections list.

The **_reflns_limit_*** data items define the upper and lower bounds on the Miller indices and on the interplanar d spacings.

The **_reflns_threshold_expression** is a text field describing the criterion applied to mark individual reflections as 'significantly intense' (*i.e.* distinct from the background level). This is typically expressed as a multiple of the standard uncertainty on the quantity used in refinement, *e.g.* `I>2u(I)`.

The number of reflections with values higher than the threshold is reported in **_reflns_number_gt**. The total number of reflections measured is given by **_reflns_number_total**. Although the use of these data names appears to be obvious, different practices have been used in the past to report total numbers (*e.g.* by neglecting symmetry-equivalent reflections) and the definitions in the dictionary should be consulted. Both numbers may contain Friedel-equivalent reflections (those which are symmetry-equivalent under the Laue symmetry but inequivalent under the crystal class).

The proportion of Friedel-related reflections present is reported separately by **_reflns_Friedel_coverage**, defined as $(N_C - N_L)/N_L$, where N_C is the number of reflections obtained on averaging under the symmetry of the crystal class and N_L is the number obtained on averaging under the Laue class. The definition in the dictionary provides examples of how the value of this data name may be used as an indicator of the fraction of the available reciprocal space sampled in the diffraction experiment.

The deprecated data names **_reflns_observed_criterion** and **_reflns_number_observed** reflect the old use of 'observed' as a term describing significantly intense reflections. They should not be used in the creation of new CIFs, but are retained to ensure that the information can be extracted from old CIFs.

The free-text field **_reflns_special_details** can be used to discuss any aspects of the reflections list not covered by other data names. It is recommended that information about the averaging of symmetry-equivalent reflections (including Friedel pairs) should be given here.

Example 3.2.3.3. *Description of subsets of the reflection list.*

```
loop_
  _reflns_class_number_gt
  _reflns_class_code
  _reflns_class_description
      584    'Main'   'm=0; main reflections'
      226    'Sat1'   'm=1; first-order satellites'
      50     'Sat2'   'm=2; second-order satellites'
```

The REFLNS_CLASS category is used to summarize the properties of subsets of the reflection list. The data names are analogous to several in the REFLNS and REFINE categories, but are applied to individual classes of reflections labelled by **_reflns_class_code** and described by **_reflns_class_description** (see Example 3.2.3.3).

Individual reflections in the structure-factor listing can be recognized through the matching value of **_refln_class_code** as belonging to a particular class labelled by **_reflns_class_code**.

Although classes can be assigned according to arbitrary criteria, the specific case for which the REFLNS_CLASS category was designed was the partitioning of the reflection list into contributions from different components in incommensurately modulated structures. However, the formalism is general and other binning strategies can be described. Note, however, that the specific case of processing of reflections by shells of resolution (in macromolecular crystallography, for example) is handled explicitly by the REFLNS_SHELL category.

The category REFLNS_SCALE provides a listing of the scale factors applied to individual reflections sharing a common value of **_refln_scale_group_code**. Each value is indexed by the matching identifier **_reflns_scale_group_code** of this category.

The REFLNS_SHELL category describes the properties of separate resolution shells of reflections and is a special case of the binning of reflections into classes (compare REFLNS_CLASS above).

Each shell is defined by an upper and lower resolution limit (**_reflns_shell_d_res_high** and ***_low**), and for each shell there are data names for the number of reflections measured and exceeding a threshold of significance, for the percentage of geometrically possible reflections collected, and for the ratios of the mean intensities to their standard uncertainties.

$R_{\rm merge}$ values are also defined for each shell of resolution (both for all measured reflections and for significantly intense ones).

This category also contains a number of deprecated data names reflecting older terminology and notation. Such data names should not be used in creating new CIFs, but will need to be recognized by CIF-reading software in order to process old CIFs.

3.2.4. Atomicity, chemistry and structure

The core CIF dictionary provides many data names for describing the structural model.

The categories describing the atom sites handle these in a general way as sites of significant electron density which might be contributed to by more than one element species. The chemical identification of the compound under study, and where appropriate a model of the molecular connectivity and bonding, are handled separately by the chemistry-related categories. The geometry-related categories are purely derivative, given knowledge of the positions of the atom sites and the crystallographic symmetry; but as with other examples of derived data, they are given their own data names to provide convenient listings and to check the consistency of information provided by other categories. The symmetry-related data names in the core dictionary are restricted to those essential for the construction of a geometric model; Chapter 3.8 describes a symmetry extension dictionary suitable for a more complete description of crystal symmetry.

3.2.4.1. Atom sites

The categories describing atom sites are as follows:

ATOM group

Individual atom sites (§3.2.4.1.1)

ATOM_SITE

Collections of atom sites (§3.2.4.1.2)

ATOM_SITES

Atom types (§3.2.4.1.3)

ATOM_TYPE

These categories permit the traditional interpretation of regular concentrations of electron density in a crystalline lattice as atom sites containing one or more chemical elements, with complete or partial occupancy, and with a spatial distribution affected by thermal displacement or disorder.

Lists of atom-site coordinates and anisotropic displacement factors are covered by data items in the ATOM_SITE category. Identification of the chemical species occupying each site is handled by data items in the ATOM_TYPE category and data items in the ATOM_SITES category record collective information common to all sites.

While the ATOM_SITE category formally contains the data items describing both positions and atomic displacements, the anisotropic displacement parameters are often given in a separate looped list. In the version of the core dictionary embedded in the macromolecular CIF dictionary, which uses the DDL2 formalism, this is recognized by the creation of a separate, but overlapping, ATOM_SITE_ANISOTROP category.

3.2.4.1.1. *Individual atom sites*

The data items in this category are as follows:

ATOM_SITE

```
• _atom_site_label
  _atom_site_adp_type
  _atom_site_aniso_B_11
  _atom_site_aniso_B_12
  _atom_site_aniso_B_13
  _atom_site_aniso_B_22
  _atom_site_aniso_B_23
  _atom_site_aniso_B_33
  _atom_site_aniso_label
        → _atom_site_label
  _atom_site_aniso_ratio
  _atom_site_aniso_type_symbol
        → _atom_site_type_symbol
  _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
  _atom_site_attached_hydrogens
  _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_description
  _atom_site_disorder_assembly
  _atom_site_disorder_group
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_label_component_0
  _atom_site_label_component_1
```