Example 3.6.6.11. *An example of one cycle of refinement described with data items in the* REFINE_HIST *category.*

```
_refine_hist.cycle_id                 C134
_refine_hist.d_res_high               1.85
_refine_hist.d_res_low                20.0
_refine_hist.number_atoms_solvent      217
_refine_hist.number_atoms_total        808
_refine_hist.number_reflns_all        6174
_refine_hist.number_reflns_obs        4886
_refine_hist.number_reflns_R_free      476
_refine_hist.number_reflns_R_work     4410
_refine_hist.R_factor_all             .265
_refine_hist.R_factor_obs             .195
_refine_hist.R_factor_R_free          .274
_refine_hist.R_factor_R_work          .160
_refine_hist.details
; Add majority of solvent molecules. B factors
  refined by group. Continued to remove
  misplaced water molecules.
;
```

Data items in the REFINE_B_ISO category can be used to record details of the treatment of isotropic B (displacement) factors during refinement. There is no formal link between the classes identified by `_refine_B_iso.class` and individual atom sites, although relationships may be inferred if the class names are carefully chosen. The category allows the treatment of the atoms in each class (isotropic, anisotropic or fixed) and the value assigned for fixed isotropic B factors to be recorded. Any special details can be given in a free-text field.

Data items in the REFINE_OCCUPANCY category can be used to record details of the treatment of occupancies of groups of atom sites during refinement. As with the treatment of displacement factors in the REFINE_B_ISO category, the classes itemized by `_refine_occupancy.class` are not formally linked to the individual atom sites, but the relationships may be deduced if the class names are chosen carefully.

3.6.6.2.5. *History of the refinement*

The data items in this category are as follows:

REFINE_HIST

- `_refine_hist.cycle_id`
  `_refine_hist.details`
  `_refine_hist.d_res_high`
  `_refine_hist.d_res_low`
  `_refine_hist.number_atoms_solvent`
  `_refine_hist.number_atoms_total`
  `_refine_hist.number_reflns_all`
  `_refine_hist.number_reflns_obs`
  `_refine_hist.number_reflns_R_free`
  `_refine_hist.number_reflns_R_work`
  `_refine_hist.R_factor_all`
  `_refine_hist.R_factor_obs`
  `_refine_hist.R_factor_R_free`
  `_refine_hist.R_factor_R_work`

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

Data items in the REFINE_HIST category can be used to record details about the various steps in the refinement of the structure. They do not provide as thorough a description of the refinement as can be given in other categories for the final model, but instead allow a summary of the progress of the refinement to be given and supported by a small set of representative statistics.

The category is sufficiently compact that a large number of cycles could be summarized, but it is not expected that every cycle of refinement would be routinely reported. Example 3.6.6.11 shows an entry for a single cycle of refinement. It is likely that an author would present a representative sequence of entries in a looped list.

3.6.6.3. Reflection measurements

The categories describing the reflections used in the refinement are as follows:

REFLN group

Individual reflections (§3.6.6.3.1)

REFLN

REFLN_SYS_ABS

Groups of reflections (§3.6.6.3.2)

REFLNS

REFLNS_SCALE

REFLNS_SHELL

REFLNS_CLASS

Data items in the REFLN category can be used to give information about the individual reflections that were used to derive the final model. The related category REFLN_SYS_ABS allows the reflections that should be systematically absent for the space group in which the structure was refined to be tabulated. Data items in the REFLNS category can be used to record information that applies to all of the reflections. Scale factors can be listed in the REFLNS_SCALE category, while the data items in REFLNS_SHELL can be used to record information about the reflection set by shells of resolution. The core CIF dictionary category REFLNS_CLASS, which can be used for a general classification of reflection groups according to criteria other than resolution shell, is not expected to be used in mmCIF applications.

3.6.6.3.1. *Individual reflections*

The data items in these categories are as follows:

(*a*) REFLN

- ***`_refln.index_h`***
- ***`_refln.index_k`***
- ***`_refln.index_l`***

  `_refln.A_calc`
  `_refln.A_calc_au`
  `_refln.A_meas`
  `_refln.A_meas_au`
  `_refln.B_calc`
  `_refln.B_calc_au`
  `_refln.B_meas`
  `_refln.B_meas_au`
  `_refln.class_code`
  `_refln.crystal_id`
  → `_exptl_crystal.id`
  `_refln.d_spacing`
  `_refln.F_calc`
  `_refln.F_calc_au`
  `_refln.F_meas`
  `_refln.F_meas_au`
  `_refln.F_meas_sigma` (∼ ***`_refln_F_sigma`***)
  `_refln.F_meas_sigma_au`
  `_refln.F_squared_calc`
  `_refln.F_squared_meas`
  `_refln.F_squared_sigma`
  `_refln.fom`
  `_refln.include_status`
  `_refln.intensity_calc`
  `_refln.intensity_meas`
  `_refln.intensity_sigma`
  `_refln.mean_path_length_tbar`
  `_refln.phase_calc`
  `_refln.phase_meas`
  `_refln.refinement_status`
  `_refln.scale_group_code`
  → `_reflns_scale.group_code`
  `_refln.sint_over_lambda` (∼ ***`_refln_sint/lambda`***)
  `_refln.status` (∼ ***`_refln_observed_status`***)
  `_refln.symmetry_epsilon`
  `_refln.symmetry_multiplicity`
  `_refln.wavelength`