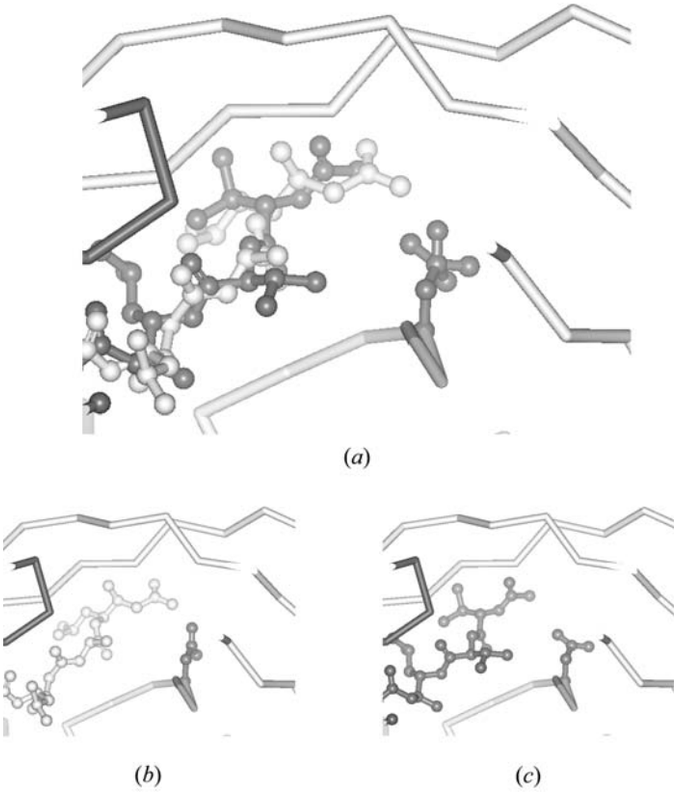

Fig. 3.6.7.2. Alternative conformations in an HIV-1 protease structure (PDB 5HVP) to be described with data items in the ATOM_SITES_ALT, ATOM_SITES_ALT_ENS and ATOM_SITES_ALT_GEN categories. (*a*) Complete structure, (*b*) ensemble 1, (*c*) ensemble 2.

3.6.7.1.4. *Alternative conformations*

The data items in these categories are as follows:

(*a*) ATOM_SITES_ALT

- **_atom_sites_alt.id**
  _atom_sites_alt.details

(*b*) ATOM_SITES_ALT_ENS

- **_atom_sites_alt_ens.id**
  _atom_sites_alt_ens.details

(*c*) ATOM_SITES_ALT_GEN

- **_atom_sites_alt_gen.alt_id**
  → **_atom_sites_alt.id**
- **_atom_sites_alt_gen.ens_id**
  → **_atom_sites_alt_gen.ens_id**

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 arrow (→) is a reference to a parent data item.

Biological macromolecules are often very flexible, and as the resolution of a structure determination increases, it becomes increasingly possible to model reliably the alternative conformations that the structure adopts. Typically, partial occupancies are assigned to atom sites within the alternative conformations to indicate the relative frequency of occurrence of each conformation. It can, however, be difficult to deduce the possible different conformations of the whole structure from inspection of the atom-site occupancies alone. For instance, a segment of protein main chain might adopt one of three slightly different conformations, and within each conformation a particular side chain might adopt one of two possible conformations, one of which sterically distorts an adjacent residue sequence, while the other does not. The data model in the mmCIF dictionary allows these kinds of correlations in positions to be described.

The relationships between the categories used to describe alternative conformations are shown in Fig. 3.6.7.1.

In the core CIF dictionary, alternative conformations are indicated by using the **_atom_site.disorder_assembly** and ***.disorder_group** data items. Aliases to these data items are present in the mmCIF dictionary, but it is not intended that they should be used to describe disorder in a macromolecular structure.

The model for describing alternative conformations in mmCIF uses the ATOM_SITES_ALT family of categories. Ensembles of correlated alternative conformations can be identified using the category ATOM_SITES_ALT_ENS. Each ensemble is generated from one or more of the alternative conformations given in the list of alternative sites in the ATOM_SITES_ALT category. Data items in the

Example 3.6.7.3. *Alternative conformations in an HIV-1 protease structure (PDB 5HVP) described with data items in the ATOM_SITES_ALT, ATOM_SITES_ALT_ENS and ATOM_SITES_ALT_GEN categories.*

```
loop_
_atom_sites_alt.id
_atom_sites_alt.details
  .
; Atom sites with the alternative ID set to null are
  not modelled in alternative conformations
;
  1
; Atom sites with the alternative ID set to 1 have
  been modelled in alternative conformations with
  respect to atom sites marked with alternative
  ID 2. The conformations of amino-acid side chains
  with alternative ID set to 1 correlate with the
  conformation of the inhibitor marked with
  alternative ID 1. Atoms in these side chains have
  been given an occupancy of 0.58 to match the
  occupancy assigned to the inhibitor.
;
  2
; Atom sites with the alternative ID set to 2 have
  been modelled in alternative conformations with
  respect to atom sites marked with alternative
  ID 1. The conformations of amino-acid side chains
  with alternative ID set to 2 correlate with the
  conformation of the inhibitor marked with
  alternative ID 2. Atoms in these side chains have
  been given an occupancy of 0.42 to match the
  occupancy assigned to the inhibitor.
;

loop_
_atom_sites_alt_ens.id
_atom_sites_alt_ens.details
  'Ensemble 1'
; The inhibitor binds to the enzyme in two, roughly
  twofold symmetric, alternative conformations.

  This conformational ensemble includes the more-
  populated conformation of the inhibitor (ID=1) and
  the amino-acid side chains that correlate with this
  inhibitor conformation.
;
  'Ensemble 2'
; The inhibitor binds to the enzyme in two, roughly
  twofold symmetric, alternative conformations.

  This conformational ensemble includes the less-
  populated conformation of the inhibitor (ID=2) and
  the amino-acid side chains that correlate with this
  inhibitor conformation.
;

loop_
_atom_sites_alt_gen.ens_id
_atom_sites_alt_gen.alt_id
   'Ensemble 1'  .
   'Ensemble 1'  1
   'Ensemble 2'  .
   'Ensemble 2'  2
```