

## 3. CIF DATA DEFINITION AND CLASSIFICATION

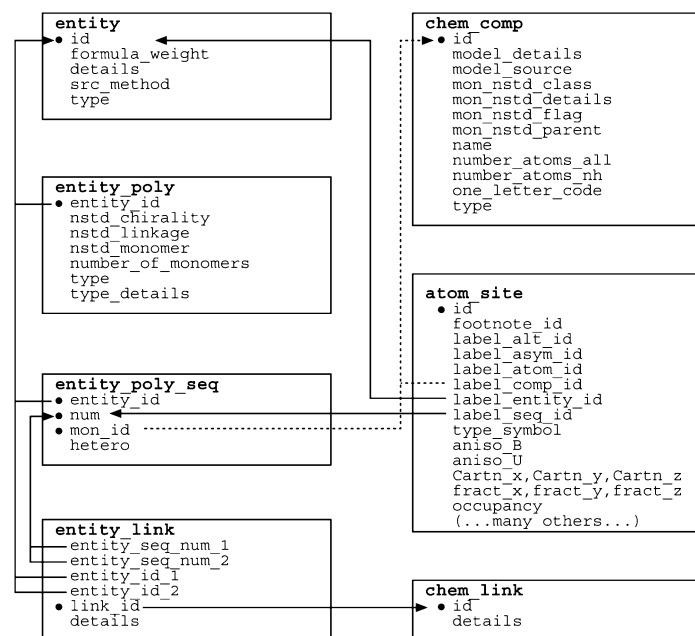


Fig. 3.6.7.6. The family of categories used to describe polymer chemical entities. Boxes surround categories of related data items. Data items that serve as category keys are preceded by a bullet (•). Lines show relationships between linked data items in different categories with arrows pointing at the parent data items.

Example 3.6.7.7. An example of both polymer and non-polymer entities in a drug–DNA complex (NDB DDF040) described with data items in the ENTITY, ENTITY\_KEYWORDS, ENTITY\_NAME\_COM, ENTITY\_POLY and ENTITY\_POLY\_SEQ categories (Narayana et al., 1991).

```

loop_
_entity.id
_entity.type
_entity.src_method
  1 polymer man
  2 non-polymer man
  3 water .

loop_
_entity_keywords.entity_id
_entity_keywords.text
  1 'nucleic acid'
  2 'drug'

loop_
_entity_name_com.entity_id
_entity_name_com.name
  2 adriamycin
  3 water

loop_
_entity_poly.entity_id
_entity_poly.number_of_monomers
_entity_poly.type
  1 8 'polydeoxyribonucleotide'

loop_
_entity_poly_seq.entity_id
_entity_poly_seq.mon_id
_entity_poly_seq.num
  1 T 1
  1 G 2
  1 G 3
  1 C 4
  1 C 5
  1 A 6
# - - - abbreviated - - -
  
```

by the assigned type is indicated by assigning a value of yes to the data item `_entity_poly.nstd_chirality`. A value of yes for `_entity_poly.nstd_linkage` indicates the presence of monomer-to-monomer links different from those implied by the assigned

type and a value of yes for `_entity_poly.nstd_monomer` indicates the presence of one or more nonstandard monomer components.

Data items in the ENTITY\_POLY\_SEQ category describe the sequence of monomers in a polymer. By including `_entity_poly_seq.mon_id` in the category key, it is possible to allow for sequence heterogeneity by allowing a given sequence number to be correlated with more than one monomer ID. Sequence heterogeneity is shown in the example of crambin in Section 3.6.3.

## 3.6.7.4. Molecular or packing geometry

The categories describing geometry are as follows:

GEOM group

GEOM  
GEOM\_ANGLE  
GEOM\_BOND  
GEOM\_CONTACT  
GEOM\_HBOND  
GEOM\_TORSION

The categories within the GEOM group are used in the core CIF dictionary to describe the geometry of the model that results from the structure determination, and can be used to select values that will be published in a report describing the structure. The complexity of macromolecular structures means that a different approach to presenting the results of a structure determination is needed. The STRUCT family of categories was created to meet this need. The GEOM categories are retained in the mmCIF dictionary, but only for consistency with the core CIF dictionary.

The data items in the categories in the GEOM group are:

(a) GEOM

```

• _geom.entry_id
  → _entry.id
  _geom.details (~ _geom_special_details)
  
```

(b) GEOM\_ANGLE

```

• _geom_angle.atom_site_id_1
  (~ _geom_angle_atom_site_label_1)
• _geom_angle.atom_site_id_2
  (~ _geom_angle_atom_site_label_2)
• _geom_angle.atom_site_id_3
  (~ _geom_angle_atom_site_label_3)
• _geom_angle.site_symmetry_1
• _geom_angle.site_symmetry_2
• _geom_angle.site_symmetry_3
  _geom_angle.atom_site_auth_asym_id_1
  → _atom_site.auth_asym_id
  _geom_angle.atom_site_auth_atom_id_1
  → _atom_site.auth_atom_id
  _geom_angle.atom_site_auth_comp_id_1
  → _atom_site.auth_comp_id
  _geom_angle.atom_site_auth_seq_id_1
  → _atom_site.auth_seq_id
  _geom_angle.atom_site_auth_asym_id_2
  → _atom_site.auth_asym_id
  _geom_angle.atom_site_auth_atom_id_2
  → _atom_site.auth_atom_id
  _geom_angle.atom_site_auth_comp_id_2
  → _atom_site.auth_comp_id
  _geom_angle.atom_site_auth_seq_id_2
  → _atom_site.auth_seq_id
  _geom_angle.atom_site_auth_asym_id_3
  → _atom_site.auth_asym_id
  _geom_angle.atom_site_auth_atom_id_3
  → _atom_site.auth_atom_id
  _geom_angle.atom_site_auth_comp_id_3
  → _atom_site.auth_comp_id
  _geom_angle.atom_site_auth_seq_id_3
  → _atom_site.auth_seq_id
  → _atom_site.id
  _geom_angle.atom_site_label_alt_id_1
  → _atom_site.label_alt_id
  _geom_angle.atom_site_label_asym_id_1
  → _atom_site.label_asym_id
  _geom_angle.atom_site_label_atom_id_1
  → _atom_site.label_atom_id
  
```