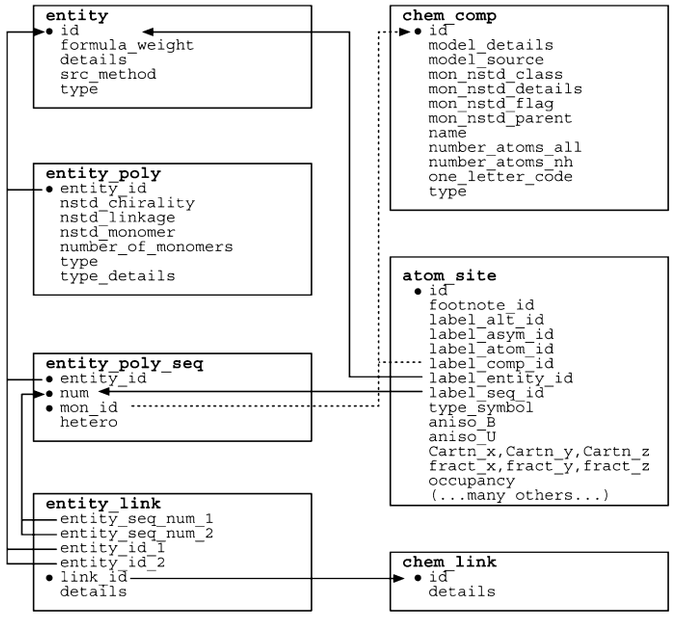

Fig. 3.6.7.6. The family of categories used to describe polymer chemical entities. Boxes surround categories of related data items. Data items that serve as category keys are preceded by a bullet (•). Lines show relationships between linked data items in different categories with arrows pointing at the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

_geom_angle.atom_site_label_comp_id_1
→ _atom_site.label_comp_id
_geom_angle.atom_site_label_seq_id_1
→ _atom_site.label_seq_id
→ _atom_site.id
_geom_angle.atom_site_label_alt_id_2
→ _atom_site.label_alt_id
_geom_angle.atom_site_label_asym_id_2
→ _atom_site.label_asym_id
_geom_angle.atom_site_label_atom_id_2
→ _atom_site.label_atom_id
_geom_angle.atom_site_label_comp_id_2
→ _atom_site.label_comp_id
_geom_angle.atom_site_label_seq_id_2
→ _atom_site.label_seq_id
→ _atom_site.id
_geom_angle.atom_site_label_alt_id_3
→ _atom_site.label_alt_id
_geom_angle.atom_site_label_asym_id_3
→ _atom_site.label_asym_id
_geom_angle.atom_site_label_atom_id_3
→ _atom_site.label_atom_id
_geom_angle.atom_site_label_comp_id_3
→ _atom_site.label_comp_id
_geom_angle.atom_site_label_seq_id_3
→ _atom_site.label_seq_id
_geom_angle.publ_flag
+ _geom_angle.value (∼ _geom_angle)

(*c*) GEOM_BOND
• _geom_bond.atom_site_id_1
(∼ _geom_bond_atom_site_label_1)
• _geom_bond.atom_site_id_2
(∼ _geom_bond_atom_site_label_2)
• _geom_bond.site_symmetry_1
• _geom_bond.site_symmetry_2
_geom_bond.atom_site_auth_asym_id_1
→ _atom_site.auth_asym_id
_geom_bond.atom_site_auth_atom_id_1
→ _atom_site.auth_atom_id
_geom_bond.atom_site_auth_comp_id_1
→ _atom_site.auth_comp_id
_geom_bond.atom_site_auth_seq_id_1
→ _atom_site.auth_seq_id
_geom_bond.atom_site_auth_asym_id_2
→ _atom_site.auth_asym_id
_geom_bond.atom_site_auth_atom_id_2
→ _atom_site.auth_atom_id
_geom_bond.atom_site_auth_comp_id_2
→ _atom_site.auth_comp_id
_geom_bond.atom_site_auth_seq_id_2
→ _atom_site.auth_seq_id
→ _atom_site.id
_geom_bond.atom_site_label_alt_id_1
→ _atom_site.label_alt_id
_geom_bond.atom_site_label_asym_id_1
→ _atom_site.label_asym_id
_geom_bond.atom_site_label_atom_id_1
→ _atom_site.label_atom_id
_geom_bond.atom_site_label_comp_id_1
→ _atom_site.label_comp_id
_geom_bond.atom_site_label_seq_id_1
→ _atom_site.label_seq_id
→ _atom_site.id
_geom_bond.atom_site_label_alt_id_2
→ _atom_site.label_alt_id
_geom_bond.atom_site_label_asym_id_2
→ _atom_site.label_asym_id
_geom_bond.atom_site_label_atom_id_2
→ _atom_site.label_atom_id
_geom_bond.atom_site_label_comp_id_2
→ _atom_site.label_comp_id
_geom_bond.atom_site_label_seq_id_2
→ _atom_site.label_seq_id
+ _geom_bond.dist (∼ _geom_bond_distance)
_geom_bond.publ_flag
_geom_bond.valence

(*d*) GEOM_CONTACT
• _geom_contact.atom_site_id_1
(∼ _geom_contact_atom_site_label_1)
• _geom_contact.atom_site_id_2
(∼ _geom_contact_atom_site_label_2)
• _geom_contact.site_symmetry_1
• _geom_contact.site_symmetry_2
_geom_contact.atom_site_auth_asym_id_1
→ _atom_site.auth_asym_id
_geom_contact.atom_site_auth_atom_id_1
→ _atom_site.auth_atom_id
_geom_contact.atom_site_auth_comp_id_1
→ _atom_site.auth_comp_id
_geom_contact.atom_site_auth_seq_id_1
→ _atom_site.auth_seq_id
_geom_contact.atom_site_auth_asym_id_2
→ _atom_site.auth_asym_id
_geom_contact.atom_site_auth_atom_id_2
→ _atom_site.auth_atom_id
_geom_contact.atom_site_auth_comp_id_2
→ _atom_site.auth_comp_id
_geom_contact.atom_site_auth_seq_id_2
→ _atom_site.auth_seq_id
→ _atom_site.id
_geom_contact.atom_site_label_alt_id_1
→ _atom_site.label_alt_id
_geom_contact.atom_site_label_asym_id_1
→ _atom_site.label_asym_id
_geom_contact.atom_site_label_atom_id_1
→ _atom_site.label_atom_id
_geom_contact.atom_site_label_comp_id_1
→ _atom_site.label_comp_id
_geom_contact.atom_site_label_seq_id_1
→ _atom_site.label_seq_id
→ _atom_site.id
_geom_contact.atom_site_label_alt_id_2
→ _atom_site.label_alt_id
_geom_contact.atom_site_label_asym_id_2
→ _atom_site.label_asym_id
_geom_contact.atom_site_label_atom_id_2
→ _atom_site.label_atom_id
_geom_contact.atom_site_label_comp_id_2
→ _atom_site.label_comp_id
_geom_contact.atom_site_label_seq_id_2
→ _atom_site.label_seq_id
+ _geom_contact.dist (∼ _geom_contact_distance)
_geom_contact.publ_flag

(*e*) GEOM_HBOND
• _geom_hbond.atom_site_id_A
→ _atom_site.id
• _geom_hbond.atom_site_id_D
→ _atom_site.id
• _geom_hbond.atom_site_id_H
→ _atom_site.id
• _geom_hbond.site_symmetry_A
• _geom_hbond.site_symmetry_D
• _geom_hbond.site_symmetry_H
+ _geom_hbond.angle_DHA
_geom_hbond.atom_site_auth_asym_id_A
→ _atom_site.auth_asym_id
_geom_hbond.atom_site_auth_atom_id_A
→ _atom_site.auth_atom_id
_geom_hbond.atom_site_auth_comp_id_A
→ _atom_site.auth_comp_id
_geom_hbond.atom_site_auth_seq_id_A
→ _atom_site.auth_seq_id
_geom_hbond.atom_site_auth_asym_id_D
→ _atom_site.auth_asym_id
_geom_hbond.atom_site_auth_atom_id_D
→ _atom_site.auth_atom_id
_geom_hbond.atom_site_auth_comp_id_D
→ _atom_site.auth_comp_id
_geom_hbond.atom_site_auth_seq_id_D
→ _atom_site.auth_seq_id
_geom_hbond.atom_site_auth_asym_id_H
→ _atom_site.auth_asym_id
_geom_hbond.atom_site_auth_atom_id_H
→ _atom_site.auth_atom_id
_geom_hbond.atom_site_auth_comp_id_H
→ _atom_site.auth_comp_id
_geom_hbond.atom_site_auth_seq_id_H
→ _atom_site.auth_seq_id
_geom_hbond.atom_site_label_alt_id_A
→ _atom_site.label_alt_id
_geom_hbond.atom_site_label_asym_id_A
→ _atom_site.label_asym_id

_geom_hbond.atom_site_label_atom_id_A
→ _atom_site.label_atom_id
_geom_hbond.atom_site_label_comp_id_A
→ _atom_site.label_comp_id
_geom_hbond.atom_site_label_seq_id_A
→ _atom_site.label_seq_id
_geom_hbond.atom_site_label_alt_id_D
→ _atom_site.label_alt_id
_geom_hbond.atom_site_label_asym_id_D
→ _atom_site.label_asym_id
_geom_hbond.atom_site_label_atom_id_D
→ _atom_site.label_atom_id
_geom_hbond.atom_site_label_comp_id_D
→ _atom_site.label_comp_id
_geom_hbond.atom_site_label_seq_id_D
→ _atom_site.label_seq_id
_geom_hbond.atom_site_label_alt_id_H
→ _atom_site.label_alt_id
_geom_hbond.atom_site_label_asym_id_H
→ _atom_site.label_asym_id
_geom_hbond.atom_site_label_atom_id_H
→ _atom_site.label_atom_id
_geom_hbond.atom_site_label_comp_id_H
→ _atom_site.label_comp_id
_geom_hbond.atom_site_label_seq_id_H
→ _atom_site.label_seq_id
\+ *_geom_hbond.dist_DA* (∼ *_geom_hbond_distance_DA*)
\+ *_geom_hbond.dist_DH* (∼ *_geom_hbond_distance_DH*)
\+ *_geom_hbond.dist_HA* (∼ *_geom_hbond_distance_HA*)
_geom_hbond.publ_flag

(*f*) GEOM_TORSION

• *_geom_torsion.atom_site_id_1*
(∼ *_geom_torsion_atom_site_label_1*)
• *_geom_torsion.atom_site_id_2*
(∼ *_geom_torsion_atom_site_label_2*)
• *_geom_torsion.atom_site_id_3*
(∼ *_geom_torsion_atom_site_label_3*)
• *_geom_torsion.atom_site_id_4*
(∼ *_geom_torsion_atom_site_label_4*)
• *_geom_torsion.site_symmetry_1*
• *_geom_torsion.site_symmetry_2*
• *_geom_torsion.site_symmetry_3*
• *_geom_torsion.site_symmetry_4*
_geom_torsion.atom_site_auth_asym_id_1
→ _atom_site.auth_asym_id
_geom_torsion.atom_site_auth_atom_id_1
→ _atom_site.auth_atom_id
_geom_torsion.atom_site_auth_comp_id_1
→ _atom_site.auth_comp_id
_geom_torsion.atom_site_auth_seq_id_1
→ _atom_site.auth_seq_id
_geom_torsion.atom_site_auth_asym_id_2
→ _atom_site.auth_asym_id
_geom_torsion.atom_site_auth_atom_id_2
→ _atom_site.auth_atom_id
_geom_torsion.atom_site_auth_comp_id_2
→ _atom_site.auth_comp_id
_geom_torsion.atom_site_auth_seq_id_2
→ _atom_site.auth_seq_id
_geom_torsion.atom_site_auth_asym_id_3
→ _atom_site.auth_asym_id
_geom_torsion.atom_site_auth_atom_id_3
→ _atom_site.auth_atom_id
_geom_torsion.atom_site_auth_comp_id_3
→ _atom_site.auth_comp_id
_geom_torsion.atom_site_auth_seq_id_3
→ _atom_site.auth_seq_id
_geom_torsion.atom_site_auth_asym_id_4
→ _atom_site.auth_asym_id
_geom_torsion.atom_site_auth_atom_id_4
→ _atom_site.auth_atom_id
_geom_torsion.atom_site_auth_comp_id_4
→ _atom_site.auth_comp_id
_geom_torsion.atom_site_auth_seq_id_4
→ _atom_site.auth_seq_id
→ _atom_site.id
_geom_torsion.atom_site_label_alt_id_1
→ _atom_site.label_alt_id
_geom_torsion.atom_site_label_asym_id_1
→ _atom_site.label_asym_id
_geom_torsion.atom_site_label_atom_id_1
→ _atom_site.label_atom_id
_geom_torsion.atom_site_label_comp_id_1
→ _atom_site.label_comp_id
_geom_torsion.atom_site_label_seq_id_1
→ _atom_site.label_seq_id
→ _atom_site.id
_geom_torsion.atom_site_label_alt_id_2
→ _atom_site.label_alt_id
_geom_torsion.atom_site_label_asym_id_2
→ _atom_site.label_asym_id
_geom_torsion.atom_site_label_atom_id_2
→ _atom_site.label_atom_id
_geom_torsion.atom_site_label_comp_id_2
→ _atom_site.label_comp_id
_geom_torsion.atom_site_label_seq_id_2
→ _atom_site.label_seq_id
→ _atom_site.id
_geom_torsion.atom_site_label_alt_id_3
→ _atom_site.label_alt_id
_geom_torsion.atom_site_label_asym_id_3
→ _atom_site.label_asym_id
_geom_torsion.atom_site_label_atom_id_3
→ _atom_site.label_atom_id
_geom_torsion.atom_site_label_comp_id_3
→ _atom_site.label_comp_id
_geom_torsion.atom_site_label_seq_id_3
→ _atom_site.label_seq_id
→ _atom_site.id
_geom_torsion.atom_site_label_alt_id_4
→ _atom_site.label_alt_id
_geom_torsion.atom_site_label_asym_id_4
→ _atom_site.label_asym_id
_geom_torsion.atom_site_label_atom_id_4
→ _atom_site.label_atom_id
_geom_torsion.atom_site_label_comp_id_4
→ _atom_site.label_comp_id
_geom_torsion.atom_site_label_seq_id_4
→ _atom_site.label_seq_id
_geom_torsion.publ_flag
\+ *_geom_torsion.value* (∼ *_geom_torsion*)

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. 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. Data items marked with a plus* (+) *have companion data names for the standard uncertainty in the reported value, formed by appending the string* **_esd** *to the data name listed.*

3.6.7.5. Molecular structure

The categories describing molecular structure are as follows:

STRUCT group

Higher-level macromolecular structure (§3.6.7.5.1)
- STRUCT
- STRUCT_ASYM
- STRUCT_BIOL
- STRUCT_BIOL_GEN
- STRUCT_BIOL_KEYWORDS
- STRUCT_BIOL_VIEW

Secondary structure (§3.6.7.5.2)
- STRUCT_CONF
- STRUCT_CONF_TYPE

Structural interactions (§3.6.7.5.3)
- STRUCT_CONN
- STRUCT_CONN_TYPE

Structural features of monomers (§3.6.7.5.4)
- STRUCT_MON_DETAILS
- STRUCT_MON_NUCL
- STRUCT_MON_PROT
- STRUCT_MON_PROT_CIS

Noncrystallographic symmetry (§3.6.7.5.5)
- STRUCT_NCS_DOM
- STRUCT_NCS_DOM_LIM
- STRUCT_NCS_ENS