(*j*) ENTITY_LINK

```
• _entity_link.link_id
        → _chem_link.id
  _entity_link.details
  _entity_link.entity_id_1
        → _entity.id
  _entity_link.entity_id_2
        → _entity.id
  _entity_link.entity_seq_num_1
        → _entity_poly_seq.num
  _entity_link.entity_seq_num_2
        → _entity_poly_seq.num
```

*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. 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.*

The geometry of the links between chemical components or entities can be described in the CHEM_LINK group of categories. Chemical components may be linked together according to the type of the component; defining the linking according to the type of the component rather than by each component in turn allows a type of polymer link for all the monomers in a polymer to be specified (*e.g.* L-peptide linking). The geometry of the links can be specified in the remaining CHEM_LINK categories. The relationships between categories used to describe links between chemical components are shown in Fig. 3.6.7.4, which also shows how information about the links is passed to the CHEM_COMP and CHEM_LINK categories. For simplicity, the categories CHEM_COMP_PLANE, CHEM_COMP_PLANE_ATOM, CHEM_COMP_CHIR, CHEM_COMP_CHIR_ATOM and ENTITY_LINK are not included in Fig. 3.6.7.4.

Note that this category group can be used to describe the links that connect the monomers within a macromolecular polymer (using the CHEM_LINK categories) and also the intramolecular links between separate molecules in the whole complex (using the ENTITY_LINK category). Intramolecular links, for example a covalent bond formed between a bound ligand and an amino-acid side chain, are usually discovered as a result of the structure determination, and it would therefore seem more appropriate to describe them in the STRUCT_CONN category. However, since one of the roles of the CHEM_LINK category group is to record target values used for restraints or constraints during the refinement of the model of the structure, ideal values for the geometry of any entity-to-entity links should be given here.

Data items in the CHEM_LINK category are used to assign a unique identifier to each link and allow the author to record any unusual aspects of each link. The other categories in the CHEM_LINK category group describe the geometric model of each link, and are closely analogous to the similarly named categories in the CHEM_COMP group.

The relationships among these categories are complex (see Fig. 3.6.7.4). Each atom that participates in an aspect of the link (for example, a bond, an angle, a chiral centre, a torsion angle or a plane) must be identified and it must also be specified whether the atom is in the first or second of the components that form the link.

Data items in the CHEM_LINK_BOND category describe the bonds between atoms participating in an intermolecular link between chemical components. Bond restraints may be described by the distance between the bonded atoms, the bond order or both.

An angle at a link may be described in the CHEM_LINK_ANGLE category as either an angle at the vertex atom or as a distance between the atoms attached to the vertex. For data items in both the CHEM_LINK_BOND and CHEM_LINK_ANGLE categories, a target value and its associated standard uncertainty may be specified (Example 3.6.7.5).

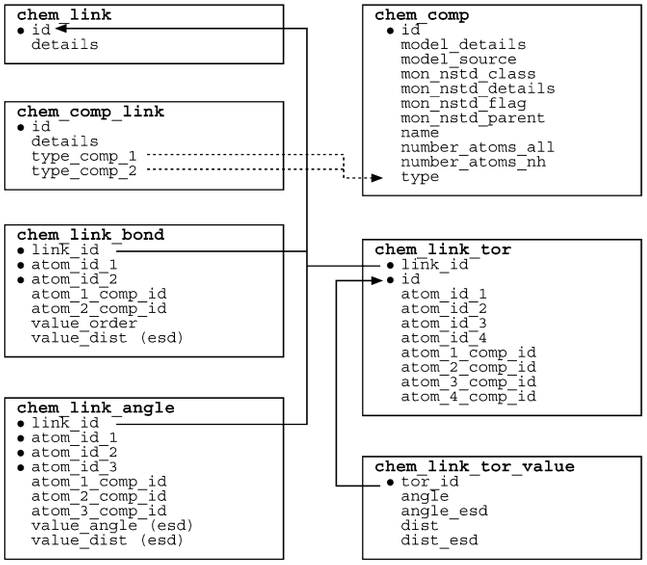


Fig. 3.6.7.4. The family of categories used to describe the links between chemical components. Boxes surround categories of related data items. Data items that serve as category keys are preceded by a bullet (•). Lines show relationships between linked data items in different categories with arrows pointing at the parent data items.

Data items in the CHEM_LINK_CHIR category can be used to describe the conformation of chiral centres in a link between two chemical components. The absolute configuration and the chiral volume may be specified, as well as the total number of atoms and the number of non-hydrogen atoms bonded to the chiral centre. There is also a flag to indicate whether a restrained chiral volume should match the target value in sign as well as in magnitude. Because chiral centres can involve a variable number of atoms, a separate list of the atoms should be given in CHEM_LINK_CHIR_ATOM.

Data items in the CHEM_LINK_PLANE category can be used to list planes defined across a link between two chemical components. Because planes can involve a variable number of atoms, a separate list of the atoms should be given in CHEM_LINK_PLANE_ATOM.

Data items in the CHEM_LINK_TOR category can be used to give details of the torsion angles across a link between two chemical

Example 3.6.7.5. *A peptide bond described with data items in the CHEM_LINK_BOND and CHEM_LINK_ATOM categories.*

```
loop_
  _chem_link_bond.link_id
  _chem_link_bond.value_dist
  _chem_link_bond.value_dist_esd
  _chem_link_bond.atom_id_1
  _chem_link_bond.atom_1_comp_id
  _chem_link_bond.atom_id_2
  _chem_link_bond.atom_2_comp_id
    PEPTIDE  1.329  0.014  C  1  N  2

loop_
  _chem_link_angle.link_id
  _chem_link_angle.value_angle
  _chem_link_angle.value_angle_esd
  _chem_link_angle.atom_id_1
  _chem_link_angle.atom_1_comp_id
  _chem_link_angle.atom_id_2
  _chem_link_angle.atom_2_comp_id
  _chem_link_angle.atom_id_3
  _chem_link_angle.atom_3_comp_id
    PEPTIDE  116.2  2.0  CA 1  C  1  N  2
    PEPTIDE  123.0  1.6  O  1  C  1  N  2
    PEPTIDE  121.7  1.8  C  1  N  2  CA 2
```





references