Table A3.6.1.1. *Categories in the mmCIF dictionary*

Numbers in parentheses refer to the section of this chapter in which each category is described in detail.

ATOM group (§3.6.7.1)
- ATOM_SITE (§3.6.7.1.1(*a*))
- ATOM_SITE_ANISOTROP (§3.6.7.1.1(*b*))
- ATOM_SITES (§3.6.7.1.2(*a*))
- ATOM_SITES_ALT (§3.6.7.1.4(*a*))
- ATOM_SITES_ALT_ENS (§3.6.7.1.4(*b*))
- ATOM_SITES_ALT_GEN (§3.6.7.1.4(*c*))
- ATOM_SITES_FOOTNOTE (§3.6.7.1.2(*b*))
- ATOM_TYPE (§3.6.7.1.3)

AUDIT group (§3.6.9.1)
- AUDIT (§3.6.9.1(*a*))
- AUDIT_AUTHOR (§3.6.9.1(*b*))
- AUDIT_CONFORM (§3.6.9.1(*c*))
- AUDIT_CONTACT_AUTHOR (§3.6.9.1(*d*))
- AUDIT_LINK (§3.6.9.2(*c*))

CELL group (§3.6.5.1)
- CELL (§3.6.5.1(*a*))
- CELL_MEASUREMENT (§3.6.5.1(*b*))
- CELL_MEASUREMENT_REFLN (§3.6.5.1(*c*))

CHEM_COMP group (§3.6.7.2.2)
- CHEM_COMP (§3.6.7.2.2(*a*))
- CHEM_COMP_ANGLE (§3.6.7.2.2(*b*))
- CHEM_COMP_ATOM (§3.6.7.2.2(*c*))
- CHEM_COMP_BOND (§3.6.7.2.2(*d*))
- CHEM_COMP_CHIR (§3.6.7.2.2(*e*))
- CHEM_COMP_CHIR_ATOM (§3.6.7.2.2(*f*))
- *CHEM_COMP_LINK* (*see CHEM_LINK group*)
- CHEM_COMP_PLANE (§3.6.7.2.2(*h*))
- CHEM_COMP_PLANE_ATOM (§3.6.7.2.2(*i*))
- CHEM_COMP_TOR (§3.6.7.2.2(*j*))
- CHEM_COMP_TOR_VALUE (§3.6.7.2.2(*k*))

CHEM_LINK group (§3.6.7.2.3)
- CHEM_COMP_LINK (§3.6.7.2.2(*g*))
- CHEM_LINK (§3.6.7.2.3(*a*))
- CHEM_LINK_ANGLE (§3.6.7.2.3(*b*))
- CHEM_LINK_BOND (§3.6.7.2.3(*c*))
- CHEM_LINK_CHIR (§3.6.7.2.3(*d*))
- CHEM_LINK_CHIR_ATOM (§3.6.7.2.3(*e*))
- CHEM_LINK_PLANE (§3.6.7.2.3(*f*))
- CHEM_LINK_PLANE_ATOM (§3.6.7.2.3(*g*))
- CHEM_LINK_TOR (§3.6.7.2.3(*h*))
- CHEM_LINK_TOR_VALUE (§3.6.7.2.3(*i*))
- ENTITY_LINK (§3.6.7.2.3(*j*))

CHEMICAL group (§3.6.7.2)
- CHEMICAL (§3.6.7.2.1(*a*))
- CHEMICAL_CONN_ATOM (§3.6.7.2.1(*b*))
- CHEMICAL_CONN_BOND (§3.6.7.2.1(*c*))
- CHEMICAL_FORMULA (§3.6.7.2.1(*d*))

CITATION group (§3.6.8.1)
- CITATION (§3.6.8.1(*a*))
- CITATION_AUTHOR (§3.6.8.1(*b*))
- CITATION_EDITOR (§3.6.8.1(*c*))

COMPUTING group (§3.6.8.2)
- COMPUTING (§3.6.8.2(*a*))
- SOFTWARE (§3.6.8.2(*b*))

DATABASE group (§§3.6.8.3, 3.6.9.3)
- DATABASE (§3.6.8.3.1(*a*))
- DATABASE_2 (§3.6.8.3.1(*b*))
- *The following also belong to the PDB group*
- DATABASE_PDB_CAVEAT (§3.6.8.3.2(*e*))
- DATABASE_PDB_MATRIX (§3.6.8.3.2(*c*))
- DATABASE_PDB_REMARK (§3.6.8.3.2(*f*))
- DATABASE_PDB_REV (§3.6.8.3.2(*a*))
- DATABASE_PDB_REV_RECORD (§3.6.8.3.2(*b*))
- DATABASE_PDB_TVECT (§3.6.8.3.2(*d*))

DIFFRN group (§3.6.5.2)
- DIFFRN (§3.6.5.2(*a*))
- DIFFRN_ATTENUATOR (§3.6.5.2(*b*))
- DIFFRN_DETECTOR (§3.6.5.2(*c*))
- DIFFRN_MEASUREMENT (§3.6.5.2(*d*))
- DIFFRN_ORIENT_MATRIX (§3.6.5.2(*e*))
- DIFFRN_ORIENT_REFLN (§3.6.5.2(*f*))
- DIFFRN_RADIATION (§3.6.5.2(*g*))
- DIFFRN_RADIATION_WAVELENGTH (§3.6.5.2(*h*))
- DIFFRN_REFLN (§3.6.5.2(*i*))
- DIFFRN_REFLNS (§3.6.5.2(*j*))
- DIFFRN_REFLNS_CLASS (§3.6.5.2(*k*))
- DIFFRN_SCALE_GROUP (§3.6.5.2(*l*))
- DIFFRN_SOURCE (§3.6.5.2(*m*))
- DIFFRN_STANDARD_REFLN (§3.6.5.2(*n*))
- DIFFRN_STANDARDS (§3.6.5.2(*o*))

ENTITY group (§3.6.7.3)
- ENTITY (§3.6.7.3.1(*a*))
- ENTITY_KEYWORDS (§3.6.7.3.1(*b*))
- *ENTITY_LINK* (*see CHEM_LINK group*)
- ENTITY_NAME_COM (§3.6.7.3.1(*c*))
- ENTITY_NAME_SYS (§3.6.7.3.1(*d*))
- ENTITY_POLY (§3.6.7.3.2(*a*))
- ENTITY_POLY_SEQ (§3.6.7.3.2(*b*))
- ENTITY_SRC_GEN (§3.6.7.3.1(*e*))
- ENTITY_SRC_NAT (§3.6.7.3.1(*f*))

ENTRY group (§3.6.9.2)
- ENTRY (§3.6.9.2(*a*))
- ENTRY_LINK (§3.6.9.2(*b*))

EXPTL group (§3.6.5.3)
- EXPTL (§3.6.5.3.1(*a*))
- EXPTL_CRYSTAL (§3.6.5.3.1(*b*))
- EXPTL_CRYSTAL_FACE (§3.6.5.3.1(*c*))
- EXPTL_CRYSTAL_GROW (§3.6.5.3.2(*a*))
- EXPTL_CRYSTAL_GROW_COMP (§3.6.5.3.2(*b*))

GEOM group (§3.6.7.4)
- GEOM (§3.6.7.4(*a*))
- GEOM_ANGLE (§3.6.7.4(*b*))
- GEOM_BOND (§3.6.7.4(*c*))
- GEOM_CONTACT (§3.6.7.4(*d*))
- GEOM_HBOND (§3.6.7.4(*e*))
- GEOM_TORSION (§3.6.7.4(*f*))

IUCR group (§3.6.8.4)
- JOURNAL (§3.6.8.4.1(*a*))
- JOURNAL_INDEX (§3.6.8.4.1(*b*))
- PUBL (§3.6.8.4.2(*a*))
- PUBL_AUTHOR (§3.6.8.4.2(*b*))
- PUBL_BODY (§3.6.8.4.2(*c*))
- PUBL_MANUSCRIPT_INCL (§3.6.8.4.2(*d*))

PHASING group (§3.6.6.1)
- PHASING (§3.6.6.1.1)
- PHASING_AVERAGING (§3.6.6.1.2)
- PHASING_ISOMORPHOUS (§3.6.6.1.3)
- PHASING_MAD (§3.6.6.1.4(*a*))
- PHASING_MAD_CLUST (§3.6.6.1.4(*b*))
- PHASING_MAD_EXPT (§3.6.6.1.4(*c*))
- PHASING_MAD_RATIO (§3.6.6.1.4(*d*))
- PHASING_MAD_SET (§3.6.6.1.4(*e*))
- PHASING_MIR (§3.6.6.1.5(*a*))
- PHASING_MIR_DER (§3.6.6.1.5(*c*))
- PHASING_MIR_DER_REFLN (§3.6.6.1.5(*d*))
- PHASING_MIR_DER_SHELL (§3.6.6.1.5(*e*))
- PHASING_MIR_DER_SITE (§3.6.6.1.5(*f*))
- PHASING_MIR_SHELL (§3.6.6.1.5(*b*))
- PHASING_SET (§3.6.6.1.6(*a*))
- PHASING_SET_REFLN (§3.6.6.1.6(*b*))
- PUBL (*see IUCR group*)
- PUBL_AUTHOR (*see IUCR group*)
- PUBL_BODY (*see IUCR group*)
- PUBL_MANUSCRIPT_INCL (*see IUCR group*)

REFINE group (§3.6.6.2)
- REFINE (§3.6.6.2.1(*a*))
- REFINE_ANALYZE (§3.6.6.2.2)
- REFINE_B_ISO (§3.6.6.2.4(*a*))
- REFINE_FUNCT_MINIMIZED (§3.6.6.2.1(*b*))
- REFINE_HIST (§3.6.6.2.5)
- REFINE_LS_RESTR (§3.6.6.2.3(*a*))
- REFINE_LS_RESTR_NCS (§3.6.6.2.3(*b*))
- REFINE_LS_CLASS (§3.6.2.2.3(*e*))
- REFINE_LS_RESTR_TYPE (§3.6.6.2.3(*c*))
- REFINE_LS_SHELL (§3.6.6.2.3(*d*))
- REFINE_OCCUPANCY (§3.6.6.2.4(*b*))

REFLN group (§3.6.6.3)
- REFLN (§3.6.6.3.1(*a*))
- REFLN_SYS_ABS (§3.6.6.3.1(*b*))
- REFLNS (§3.6.6.3.2(*a*))
- REFLNS_CLASS (§3.6.6.3.2(*d*))
- REFLNS_SCALE (§3.6.6.3.2(*b*))
- REFLNS_SHELL (§3.6.6.3.2(*c*))

- *SOFTWARE* (*see COMPUTING group*)
- *SPACE_GROUP* (*see SYMMETRY group*)
- *SPACE_GROUP_SYMOP* (*see SYMMETRY group*)

STRUCT group (§3.6.7.5)
- STRUCT (§3.6.7.5.1(*a*))
- STRUCT_ASYM (§3.6.7.5.1(*b*))
- STRUCT_BIOL (§3.6.7.5.1(*c*))
- STRUCT_BIOL_GEN (§3.6.7.5.1(*d*))
- STRUCT_BIOL_KEYWORDS (§3.6.7.5.1(*e*))
- STRUCT_BIOL_VIEW (§3.6.7.5.1(*f*))
- STRUCT_CONF (§3.6.7.5.2(*b*))
- STRUCT_CONF_TYPE (§3.6.7.5.2(*a*))
- STRUCT_CONN (§3.6.7.5.3(*b*))
- STRUCT_CONN_TYPE (§3.6.7.5.3(*a*))
- STRUCT_KEYWORDS (§3.6.7.5.1(*g*))
- STRUCT_MON_DETAILS (§3.6.7.5.4(*a*))
- STRUCT_MON_NUCL (§3.6.7.5.4(*b*))
- STRUCT_MON_PROT (§3.6.7.5.4(*c*))
- STRUCT_MON_PROT_CIS (§3.6.7.5.4(*d*))
- STRUCT_NCS_DOM (§3.6.7.5.5(*c*))
- STRUCT_NCS_DOM_LIM (§3.6.7.5.5(*d*))
- STRUCT_NCS_ENS (§3.6.7.5.5(*a*))
- STRUCT_NCS_ENS_GEN (§3.6.7.5.5(*b*))
- STRUCT_NCS_OPER (§3.6.7.5.5(*e*))
- STRUCT_REF (§3.6.7.5.6(*a*))
- STRUCT_REF_SEQ (§3.6.7.5.6(*b*))
- STRUCT_REF_SEQ_DIF (§3.6.7.5.6(*c*))
- STRUCT_SHEET (§3.6.7.5.7(*a*))
- STRUCT_SHEET_HBOND (§3.6.7.5.7(*e*))
- STRUCT_SHEET_ORDER (§3.6.7.5.7(*d*))
- STRUCT_SHEET_RANGE (§3.6.7.5.7(*c*))
- STRUCT_SHEET_TOPOLOGY (§3.6.7.5.7(*b*))
- STRUCT_SITE (§3.6.7.5.8(*a*))
- STRUCT_SITE_GEN (§3.6.7.5.8(*c*))
- STRUCT_SITE_KEYWORDS (§3.6.7.5.8(*b*))
- STRUCT_SITE_VIEW (§3.6.7.5.8(*d*))

SYMMETRY group (§3.6.7.6)
- SPACE_GROUP (§3.6.7.6(*c*))
- SPACE_GROUP_SYMOP (§3.6.7.6(*d*))
- SYMMETRY (§3.6.7.6(*a*))
- SYMMETRY_EQUIV (§3.6.7.6(*b*))

VALENCE group (§3.6.7.7)
- VALENCE_PARAM group (§3.6.7.7(*a*))
- VALENCE_REF group (§3.6.7.7(*b*))

and the model number. These have been added to the mmCIF category ATOM_SITE (as `_atom_site.pdbx_PDB_ins_code` and `_atom_site.pdbx_PDB_model_num`) and to all related categories that include atom nomenclature.

The convention for defining the hydrogen bonding in β-sheets differs between the PDB and mmCIF representations. Because the PDB model is fundamentally different from that found in mmCIF, a new category was created to hold the PDB data: PDBX_STRUCT_SHEET_HBOND. The correspondence between the PDB and mmCIF formats is tabulated at http://deposit.pdb.org/mmCIF/dictionaries/pdb-correspondence/pdb2mmcif.html.

references