Assigned chemical shift ambiguity codes and definitions

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| **Table 4.** Assigned chemical shift ambiguity codes and definitions | |
| **Ambiguity code** | **Definition** |
| 1 | Unique (including isolated methyl protons, geminal atoms, and geminal methyl groups with identical chemical shifts) (e.g. ILE HD11, HD12, HD13 protons) |
| 2 | Ambiguity of geminal atoms or geminal methyl proton groups (e.g. ASP HB2 and HB3 protons, LEU CD1 and CD2 carbons, or LEU HD11, HD12, HD13 and HD21, HD22, HD23 methyl protons) |
| 3 | Experimental ambiguity in aromatic atoms on opposite sides of symmetrical rings (e.g. TYR and PHE HD1/HD2, CD1/CD2, HE1/HE2, and CE1/CE2 protons). The ambiguity results from a lack of experimental data required to unambiguously assign the chemical shift to a specific atom. |
| 4 | Intraresidue ambiguities (e.g. LYS HG and HD protons or TRP HZ2 and HZ3 protons) |
| 5 | Interresidue ambiguities (LYS 12 vs. LYS 27) |
| 6 | Intermolecular ambiguities (e.g. ASP 31 CA in monomer 1 and ASP 31 CA in monomer 2 of an asymmetrical homodimer, duplex DNA assignments, or other assignments that may apply to atoms in one or more molecule in the molecular assembly) |
| 9 | Ambiguous, specific ambiguity not defined (essentially an unassigned chemical shift) |
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