Alternate Locations vs. Singletons and Occupancies in PDB Files

by Eric Martz, September 10, 2023

Atoms are marked with alternate location codes in PDB files primarily to indicate **multiple locations** for these atoms. In such cases, typically each location is assigned an occupancy **< 100%**, such that the occupancies of all locations for a given atom **sum to 100%**. But there are many exceptions.

25 PDB entries were arbitrarily selected for testing in FirstGlance its handling of atoms with alternate location codes (**altlocs**). These were released 1988-2022, median 2009, average 2009. 24 were from X-ray diffraction, and 1 from NMR (5i1r). X-ray resolutions were 1.0-3.2 Å, median 1.6, average 1.7. (The median X-ray resolution in the PDB is 2.0 Å.) Analysis was done with FirstGlance version 4.2. The data are in altloc-singleton-occupancy.xlsx

Singleton-AltLocs

Singleton-altlocs are common. Most have occupancies <100%, but not all.

12/25 (**48%**) have atoms marked with altloc codes, but only **one location/atom** (average release in 2012). Singletons are atoms of protein, ligands, nucleotides, and water. Singleton counts range from 3 to 7,243 per entry. Most singletons have occupancies <100%, but in 4/12 (33% of entries with

singletons), the highest occupancy for ligand (1bxo), nucleotides (7ucr), or water (3eoj, 4nia) is **100%**. In 6ucy, the highest occupancy for singleton water is **99%**.

100% Occupancy AltLocs

Atoms with altloc codes but 100% occupancy are fairly common, and mostly singletons.

5/25 entries (20%) have 3-35 altloc atoms/entry with 100% occupancy. These are mostly protein and nucleotide atoms, plus some water atoms. These atoms are mostly singletons, with the exception of 7s99, which has 8 atoms of Thr88 with 2 locations each, %A occupancy 100%, %B occupancy 0%.

Partial occupancy without altloc codes

Atoms with partial occupancy but no altloc codes are common, and include water, ligands, and protein.

13/25 entries (**52%**) have atoms with partial occupancy but no altloc codes. These atoms are often water, also ligands, also protein (1zir, 8a3h). Atoms having partial occupancies without altloc codes are:
- Water: 30-99%.
- Ligands: 45-87%.
- Protein: 0-75%. (2 amino acids in 1zir have 0%.)

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(The End)