**Table S1. Atom type mapping and the electron counts for the 20 common residues.**

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| --- | --- |
| Residue | Atom types |
| GLY | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, OXT: O\_intermediate |
| ALA | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, OXT: O\_intermediate |
| VAL | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG1: C\_single, CG2: C\_single, OXT: O\_intermediate |
| LEU | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_single, CD1: C\_single, CD2: C\_single, OXT: O\_intermediate |
| ILE | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG1: C\_single, CG2: C\_single, CD1: C\_single, OXT: O\_intermediate |
| MET | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_single, SD: S\_single, CE: C\_single, OXT: O\_intermediate |
| PHE | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_intermediate, CD1: C\_intermediate, CD2: C\_intermediate, CE1: C\_intermediate, CE2: C\_intermediate, CZ: C\_intermediate, OXT: O\_intermediate |
| TRP | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_intermediate, CD1: C\_intermediate, CD2: C\_intermediate, NE1: N\_intermediate, CE2: C\_intermediate, CE3: C\_intermediate, CZ2: C\_intermediate, CZ3: C\_intermediate, CH2: C\_intermediate, OXT: O\_intermediate |
| PRO | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_single, CD: C\_single, OXT: O\_intermediate |
| SER | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, OG: O\_single, OXT: O\_intermediate |
| THR | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, OG1: O\_single, CG2: C\_single, OXT: O\_intermediate |
| CYS | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, SG: S\_single, OXT: O\_intermediate |
| TYR | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_intermediate, CD1: C\_intermediate, CD2: C\_intermediate, CE1: C\_intermediate, CE2: C\_intermediate, CZ: C\_intermediate, OH: O\_single, OXT: O\_intermediate |
| ASN | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_double, OD1: O\_double, ND2: N\_single, OXT: O\_intermediate, |
| GLN | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_single, CD: C\_double, OE1: O\_double, NE2: N\_single, OXT: O\_intermediate |
| ASP | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_double, OD1: O\_intermediate, OD2: O\_intermediate, OXT: O\_intermediate |
| GLU | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_single, CD: C\_double, OE1: O\_intermediate, OE2: O\_intermediate, OXT: O\_intermediate |
| LYS | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_single, CD: C\_single, CE: C\_single, NZ: N\_single, OXT: O\_intermediate |
| ARG | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_single, CD: C\_single, NE: N\_intermediate, CZ: C\_double, NH1: N\_intermediate, NH2: N\_intermediate, OXT: O\_intermediate |
| HIS | N: N\_single\_bb, CA: C\_single\_bb, C: C\_double\_bb, O: O\_double\_bb, CB: C\_single, CG: C\_intermediate, ND1: N\_intermediate, CD2: C\_intermediate, CE1: C\_intermediate, NE2: N\_intermediate, OXT: O\_intermediate |