Atom types for atoms in 20 standard amino acids.

- **1st code- Element (C,N,O,S)**
- **2nd code- SP2, SP3, resonating/conjugated, aromatic, allylic/benzylic/enolizable, Dative (2,3,C,A,L,D)**
- **3rd code- partial positive, partial negative, nonpolar, variable, charged (O,E,N,V,C)**

Peptide backbone except CA

- N- NCO
- C- CCO
  - this carbon is in a resonating bond. To distinguish between carbons of the backbone and carbons of the residues that would otherwise have the same descriptor, C (conjugated/resonating) will be used to describe resonating carbons in the backbone and 2 (sp2) will be used to describe resonating carbons in residues. Both terms are valid.
- O- OCE
- OXT- OCC
  - OXT designates the Carboxy terminus of a peptide chain. If this appears then both OXT and O of the indicated residue are OCC.
  - The N following an OXT is the amino terminus of the next chain. This N is N3C.
  - CA for carboxy and amino terminus?

Alanine

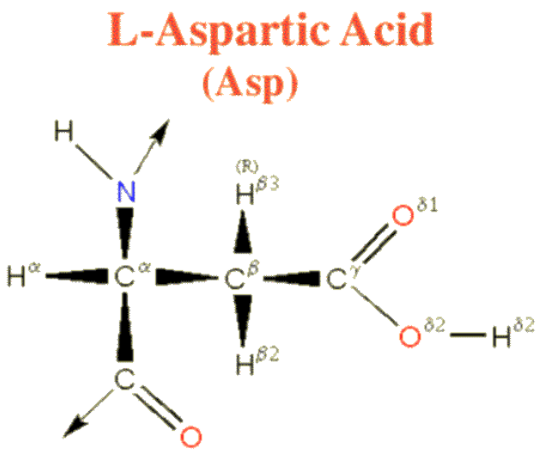
- CA- C3O
- CB- C3N

Cysteine

- CA- C3O
- CB- C3O
- SG- S3E

Aspartic Acid

- CA- C3O
- CB- CLN
- CG- C2O
- OD1- OCC
- OD2- OCC



Glutamic Acid

- CA- C3O
- CB- C3N
- CG- CLN

- CD- C2O
- OE1- OCC
- OE2- OCC

Phenylalanine

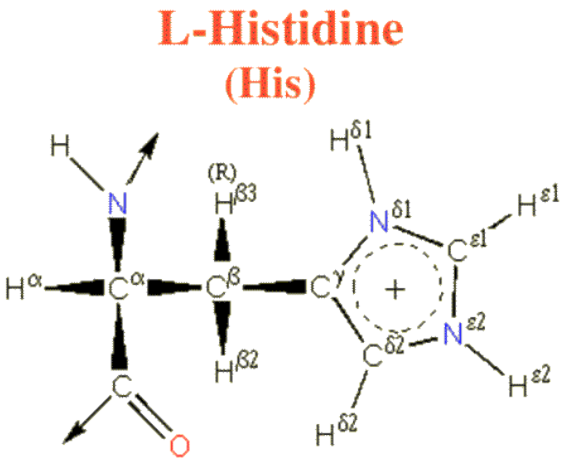
- CA- C3O
- CB- CLN
- CG- CAN
- CD1- CAN
- CD2- CAN
- CE1- CAN
- CE2- CAN

Glycine

- CA- C3O

Histidine

- CA- C3O
- CB- CLN
- CG- CAO
    - The carbons directly adjacent to the N of his and trp are labeled as having a partial positive charge. While these C do participate in a delocalized pi bond, they also have a sigma bond that is polar.
- ND1- NAV
- CD2- CAO
- CE1- CAO
- NE2- NAV



Isoleucine

- CA- C3O
- CB- C3N
- CG1- C3N
- CG2- C3N
- CD- C3N

Lysine

- CA- C3O
- CB- C3N
- CG- C3N
- CD- C3N
- CE- C3O
- NZ- N3C

Leucine

- CA- C3O
- CB- C3N
- CG- C3N
- CD1- C3N
- CD2- C3N

Methionine

- CA- C3O
- CB- C3N
- CG- C3O
- SD- S3N
    - Methionine's sulfur is labeled N (neutral) to distinguish it from the sulfur in cysteine

Asparagine

- CA- C3O
- CB- CLN
- CG- C2O
- OD1- O2E
- ND2- N3O
    - The nitrogen and oxygen in Asn and Gln are not labeled C(conjugated/resonating) to distinguish from the N and O of the backbone. If the atom type descriptors were based purely of the organic chem the amide groups of both would have the same code.

Proline

- CA- C3O
- CB- C3N
- CG- C3N
- CD- C3O

Glutamine

- CA- C3O
- CB- C3N
- CG- CLN
- CD- C2O
- OE1- O2E
- NE2- N3O

Arginine

- CA- C3O
- CB- C3N
- CG- C3N
- CD- CLO
- NE- NCC
- CZ- C2O

- NH1- NCC
- NH2- NCC

Serine

- CA- C3O
- CB- C3O
- OG- O3E

Threonine

- CA- C3O
- CB- C3O
- OG1- O3E
- CG2- C3N

Valine

- CA- C3O
- CB- C3N
- CG1- C3N
- CG2- C3N

Tryptophan

- CA- C3O
- CB- CLN
- CG- CAN
- CD1- CAO
- CD2- CAN
- NE1- NAV
- CE2- CAO
- CE3- CAN
- CZ2- CAN
- CZ3- CAN
- CH2- CAN

Tyrosine

- CA- C3O
- CB- CLN
- CG- CAN
- CD1- CAN
- CD2- CAN
- CE1- CAN
- CE2- CAN
- CZ- CAO
- OH- OLE