Histidine (protonated, neutral, deprotonated) Extended description of residue
Overall residue properties section:
3-letters residue name
| Residue type (0=Amino Acid, 1=Sugar, 2=Nucleic Acid, 3=Heme, 4=Phosphate, 5=Co-factor, 6=Ion, 7=Detergent, 8=Other)
| | Residue anhydrous molecular volume (Å^3)
| | | Maximum accessible surface area (Å^2)
| | | | Number of atoms in residue
| | | | | Number of beads for residue
| | | | | | Residue partial specific volume (cm^3/g)
| | | | | | | Partial specific volume (repeated for potential pH-dependence, not implemented)
| | | | | | | | Selected atom pK1 (order is automatically sorted, lowest-->highest)
| | | | | | | | | Additional partial specific volume (repeated again, as above), needed if a second pK is present
| | | | | | | | | | Selected atom pK2 (order is automatically sorted, lowest-->highest)
↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓
HIS 0 160 193 10 2 0.668 0.668 6.54 0.668 11.5
Residue atoms properties section:
Atom identifier as in PDB
| Hybridization (at pH=0, if it applies)
| | Atom molecular weight (hybridization-linked, pH=0, if it applies)
| | | Atom van der Waals radius (hybridization-linked; at pH=0, if it applies)
| | | | Atom assignment to bead #
| | | | | Atom determines bead position (0=no, 1=yes)
| | | | | | Atom progressive number
| | | | | | | Number of atom-associated water molecules (at pH=0, if it applies)
| | | | | | | | Order of pK application in the computations with multiple pKs (automatically sorted)
| | | | | | | | | Hybridization at pH=14
↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ | | Atom molecular weight (hybridization-linked, at pH=14)
N N3H1 15.02 1.64 0 0 0 1 | | | Atom van der Waals radius (hybridization-linked; at pH=14)
CA C4H1 13.02 1.88 0 0 1 0 | | | | Atom assignment to bead #
C C3H0 12.01 1.61 0 1 2 0 | | | | | Atom determines bead position (0=no, 1=yes)
O O1H0 16 1.42 0 1 3 0 | | | | | | Atom progressive number
CB C4H2 14.03 1.88 1 0 4 0 | | | | | | | N. of atom-associated water molecules at pH=14
CG C3H0 12.01 1.61 1 0 5 0 ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓
ND1 N3H1 15.02 1.64 1 1 6 1 2 N2H0- 14.01 1.64 1 1 6 4
CD2 C3H1 13.02 1.76 1 0 7 0
CE1 C3H1 13.02 1.76 1 0 8 0
NE2 N3H1+ 15.02 1.64 1 1 9 2 1 N2H0 14.01 1.64 1 1 9 0
Beads properties section:
Number of bead-associated water molecules at pH=7, used in the generation of the hydrated bead volume (it is overridden if pH-dependence applies)
| Bead "color" (from 0 to 15; 0, 6, 7, 8 are reserved and thus never used in this file)
| | Bead positioning method (0=CM of included atoms, 1=farthest atom from CM, 2=no positioning)
| | | Bead belongs to 0=main chain, 1=side chain
| | | | Bead anhydrous volume
↓ ↓ ↓ ↓ ↓
1 1 0 0 64.9
3 4 0 1 95.1