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{ALA}                                ! Alanine
[info]
    SYBYLtype  RESIDUE      !SYBYL substructure type
[atoms]
    1 N        NH1          -0.470 !At. no., name, type, charge
    2 HN       H            0.310 !At. no., name, type, charge
    3 CA       CT1          0.070 !At. no., name, type, charge
    4 HA       HB           0.090 !At. no., name, type, charge
    5 CB       CT3          -0.270 !At. no., name, type, charge
    6 HB1      HA           0.090 !At. no., name, type, charge
    7 HB2      HA           0.090 !At. no., name, type, charge
    8 HB3      HA           0.090 !At. no., name, type, charge
    9 C        C            0.510 !At. no., name, type, charge
    10 O       O            -0.510 !At. no., name, type, charge
[bonds]
    CB  CA
    N   HN
    N   CA
    O   C
    C   CA
    CA  HA
    CB  HB1
    CB  HB2
    CB  HB3
[connections] !how to bond to previous and next
    head      N
    tail      C
[impropers]
    N      -C      CA      HN
    C      CA      +N      O
[charge_groups] !charge groups, with switch atom first
    N      HN      CA      HA
    CB      HB1     HB2     HB3
    C      O

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