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#
# Hydrogen bond distances were specified for charge-charge and charge-neutral
# hydrogen bonding pairs according to the following:
#
# (+) charge H-bond donor of protein[4]: NR3, NC2, NP, NH3
# neutral H-bond donor of protein [7]: NR1, NH1, NH2, NY, OH1, S, OT [water]
# neutral H-bond acceptor of protein [8]: OH1, S, O, OB, OS, NR2, OT [water], OX
# (-) charge H-bond acceptor of protein [1]: OC
# (+) charge H-bond donor of ligand [5]: NG2P1, NG2R52, NG3P1, NG3P2, NG3P3
# neutral H-bond donor of ligand [13]: NG2S1, NG2S2, NG2S3, NG2R43, NG2R51, NG2R53,
# NG2R61, NG311, NG321, NG331, NG3C51, OG311, SG311
# neutral H-bond acceptor of ligand [29]: NG1T1, NG2D1, NG2S0, NG2R50, NG2R57,
# NG2R60, NG2R62, NG2R67, NG2RC0, NG301, NG3N1, OG2D1, OG2D3, OG2D4, OG2D5, OG2R50,
# OG3R60, OG301, OG302, OG303, OG304, OG311, OG3C31, OG3C51, OG3C61, SG2D1, SG2R50,
# SG311, SG301
# (-) charge H-bond acceptor of ligand [5]: OG2D2, OG2N1, OG2P1, OG312, SG302
# Polar atoms, none of above categories NG3P0, NG2O1, SG302, SG301, SG303
#
#      Atom  element  van der Waals
#      type  number  radius energy_min (absolute value)
# -----
225
1      H      1      0.22450 0.046000 # polar H
2      HC     1      0.22450 0.046000 # N-ter H
3      HA     1      1.32000 0.022000 # nonpolar H
4      HP     1      1.35820 0.030000 # aromatic H
5      HB1    1      1.32000 0.022000 # backbone H
6      HR1    1      0.90000 0.046000 # his he1, (+) his HG,HD2
7      HR2    1      0.70000 0.046000 # (+) his HE1
8      HR3    1      1.46800 0.007800 # neutral his HG, HD2
9      HS     1      0.45000 0.100000 # thiol hydrogen
10     HE1    1      1.25000 0.031000 # for alkene; RHC=CR
...

...
220     ZN     30      1.0900 0.2500  # zinc (II) cation
221     CAD    48      1.3570 0.1200  # cadmium (II) cation
222     CLA    17      2.27   0.150   # Chloride Ion
223     CT     6      2.275  0.020   # TIP3P
224     OT     8      1.7682 0.1521  # TIP3P
225     HT     1      0.2245 0.0460  # TIP3P
#
# Hydrogen bond distances between donor and acceptor
#
# The table cannot be separated
#
# First line: Default distance for all atom and element types
#
# First block:
# element donor
# number  acceptor
# i j      distance
# -----
#
# Second block:
# atom     donor
# type     acceptor
# i j      distance
# -----
#
#
#
#
2.9
9
7      7      3.1
7      8      2.9
7      16     2.9
8      8      2.7
8      16     2.9
16     16     2.9

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