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#
# global directories for PDB files and the correspondig .pkl models
# this is relative to the proteusPy package folder hierarchy!
#

PDB_DIR = '../pdb/'
MODEL_DIR = f'{PDB_DIR}models/'
DATA_DIR = '../data/'

# global for initialization of dihedrals and energies

ORIENT_BACKBONE = 2
ORIENT_SIDECHAIN = 1

# Cα Cβ Sγ X1 - X5 X

#/* atoms_covalent.inc - covalent radii used by atoms.inc */
#/* from Pauling and CAChe S/W */
# /* 5/4/94 -egs- */

N_RAD_COV = 0.74
C_RAD_COV = 0.77
O_RAD_COV = 0.73
P_RAD_COV = 1.10
S_RAD_COV = 1.04
CA_RAD_COV = 1.74
H_RAD_COV = .35
FE_RAD_COV = 1.17

ATOM_RADII_COVALENT = {"N": N_RAD_COV, "C": C_RAD_COV, "CA": CA_RAD_COV,
"O": O_RAD_COV, "S": S_RAD_COV, "SG": S_RAD_COV, "H": H_RAD_COV, "CB":
C_RAD_COV}

# /* atoms_cpk.inc - CPK radii for atoms, used by atoms.inc */

N_RAD_CPK = 1.54
C_RAD_CPK = 1.7
O_RAD_CPK = 1.4
P_RAD_CPK = 1.9
S_RAD_CPK = 1.8
CA_RAD_CPK = 1.274
H_RAD_CPK = 1.2

ATOM_RADII_CPK = {"N": N_RAD_CPK, "C": C_RAD_CPK, "CA": CA_RAD_CPK, "O":
O_RAD_CPK, "SG": S_RAD_CPK, "S": S_RAD_CPK, "H": H_RAD_CPK, "CB": C_RAD_CPK
ATOM_COLORS = {'O': [1.0, 0.0, 0.0], 'C': [.5, .5, .5], 'N': [0.0, 0.0,
1.0], 'S': 'y', 'H': 'white', 'SG': 'yellow', 'CB': 'grey'}

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BOND_RADIUS = .25


```