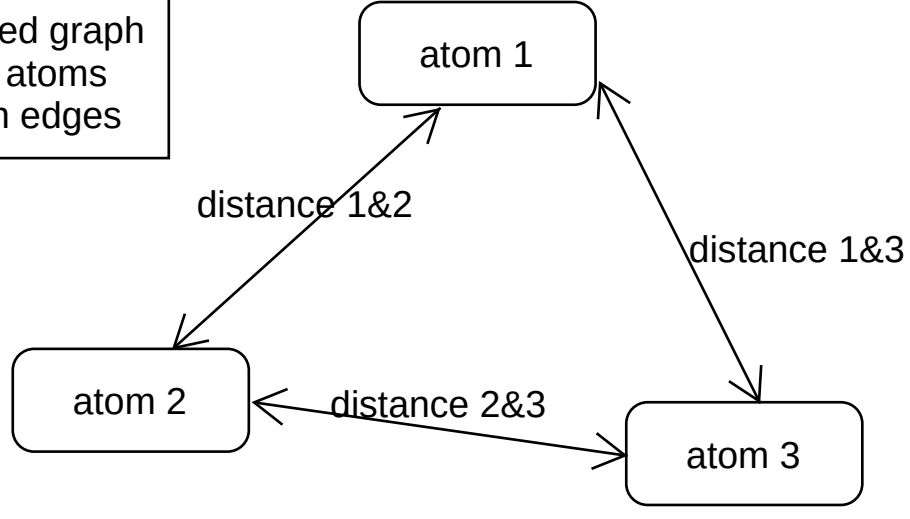
«PDB_fileUtilities»
pdbHandle getPDB_handle(pdbFileName) adjacencyMatrix getAtomDistanceAdjacencyMatrix(pdbHandle)
Provides methods for extracting parameters of a protein PDB file into a useful data structure

Note:
adjacencyMatrix
Represents an
undirected weighted graph
distance between atoms
are the weights on edges



Internal Energy

Lennard-Jones Energy Parameters (Van der Waals Potential Energy)
- Epsilon - Sigma

Coulomb's Law (Electrostatic Force)
- Charge - Dielectric constant

Solvation Energy
- Atomic solvation parameter of an atom - Accessible surface area of atom