Miscellaneous quotes regarding lennard jones potential and coulombic partial charges of amino acids.

As with proteins, many features of the current force fields, including partial atomic charges, Lennard-Jones parameters, and most bond and angle terms, date back to force fields developed in the 1990’s, and overviews of this work are available.

<http://ambermd.org/doc12/Amber14.pdf>

Brad:

It seems the most popular force field library is AMBER FF14SP force field library. The library is used by UCSF chimera (UCSF) and is cited by many publications.

UCSF Computer Graphics Laboratory <https://www.cgl.ucsf.edu/chimera/docs/ContributedSoftware/addcharge/addcharge.html>

Brad:

AMBER FF14SP force field parameters are separated into three libraries consisting of one for topologies and charges for amino acids, one for N-terminal amino acids, and the other for C-terminal amino acids. (AMBER 30)

AMBER <http://ambermd.org/doc12/Amber14.pdf>

Amber is designed to work with several simple types of force fields, although it is most commonly used with parametrizations developed by Peter Kollman and his co-workers and “descendents”. The traditional parametrization uses fixed partial charges, centered on atoms. The current recommended force field for proteins and nucleic acids is ff14SB. (AMBER 29)

AMBER <http://ambermd.org/doc12/Amber14.pdf>

As in previous versions of GLYCAM, the atomic partial charges were determined using the RESP formalism, with a weighting factor of 0.01,[43, 52] from a wavefunction computed at the HF/6-31G(d) level. To reduce artifactual fluctuations in the charges on aliphatic hydrogen atoms, and on the adjacent saturated carbon atoms, charges on aliphatic hydrogens (types HC, H1, H2, and H3) were set to zero while the partial charges were fit to the remaining atoms. (AMBER 37)

AMBER <http://ambermd.org/doc12/Amber14.pdf>

Transferring parameters from one force field to another must respect the underlying functional form, the units in which parameters are expressed in the parameter files, and also the exact procedures on how individual parameters were obtained. In addition, attention must be paid to the methods used to deduce partial charges. Force fields are self-consistent, i.e., all terms are interrelated and their actual values depend on the way they were derived. Therefore, any parameter transfer between different force fields is dangerous, even when the functional form is the same (or looks as if it were...). (AMBER 225)

AMBER <http://ambermd.org/doc12/Amber14.pdf>

The electrostatic contribution to the solvation free energy is calculated with a numerical solver for the Poisson-Boltzmann (PB) method, for example, as implemented in the pbsa program[140] or by generalized Born (GB) methods implemented in sander. Previous MM\_PBSA applications were mostly performed with a numerical PB solver in the widely used DelPhi program,[143] which has been shown by Amber developers to be numerically consistent with the pbsa program. The nonpolar contribution to the solvation free energy has been determined with solvent-accessible-surface-area-dependent terms.[137] The surface area is computed with Paul Beroza’s molsurf program, which is based on analytical ideas primarily developed by Mike Connolly. (AMBER 593)

AMBER <http://ambermd.org/doc12/Amber14.pdf>