The original Supporting Information, published February 10, 2006, was incorrect. The corrected version was posted March 10, 2006.

Complete ref 26:

26. MacKerell, A. D.; Bashford, D.; Bellott, M.; Dunbrack, R. L.; Evanseck, J. D.; Field, M. J.; Fischer, S.; Gao, J.; Guo, H.; Ha, S.; Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F. T. K.; Mattos, C.; Michnick, S.; Ngo, T.; Nguyen, D. T.; Prodhom, B.; Reiher, W. E.; Roux, B.; Schlenkrich, M.; Smith, J. C.; Stote, R.; Straub, J.; Watanabe, M.; Wiorkiewicz-Kuczera, J.; Yin, D.; Karplus, M. *J. Phys. Chem. B* **1998**, *102*, 3586-3616.

CHARMM topology including Charges for ACh:

```
DEFA FIRS NTER LAST CTER
AUTO ANGLES DIHE

RESI ACH         1.00 ! acetylcholine, D. Zhang
GROUP
ATOM  N1  NH1    0.131
ATOM  C1  CT3   -0.353 !               H11
ATOM  H11 HA     0.186 !                |
ATOM  H12 HA     0.186 !           H12--C1--H13
ATOM  H13 HA     0.186 !       H22      |      H32
ATOM  C2  CT3   -0.353 !          \     |     /
ATOM  H21 HA     0.186 !      H21--C2---N1---C3--H31
ATOM  H22 HA     0.186 !          /     |     \
ATOM  H23 HA     0.186 !       H23      |      H33
ATOM  C3  CT3   -0.353 !           H41-C4-H42
ATOM  H31 HA     0.186 !                |
ATOM  H32 HA     0.186 !           H51-C5-H52
ATOM  H33 HA     0.186 !                |
ATOM  C4  CT2   -0.270 !                O1
ATOM  H41 HA     0.172 !                |
ATOM  H42 HA     0.172 !                C6==O2
ATOM  C5  CT2    0.427 !                |
ATOM  H51 HA     0.014 !           H71--C7--H73
ATOM  H52 HA     0.014 !                |
ATOM  O1  OS    -0.569 !               H72
ATOM  C6  CC     0.937 !
ATOM  O2  O     -0.604 !
ATOM  C7  CT3   -0.525 !
ATOM  H71  HA    0.162 !
ATOM  H72  HA    0.162 !
ATOM  H73  HA    0.162 !
BOND  N1 C1   N1 C2   N1 C3  N1 C4
BOND  C1 H11  C1 H12  C1 H13
BOND  C2 H21  C2 H22  C2 H23
BOND  C3 H31  C3 H32  C3 H33
BOND  C4 H41  C4 H42  C4 C5
BOND  C5 H51  C5 H52  C5 O1
BOND  O1 C6   C6 C7
DOUBLE   C6 O2
BOND  C7 H71  C7 H72  C7 H73
IMPR  C6 O1 O2 C7
ACCEPTOR O2 C6
PATC  FIRS NONE LAST NONE
```

CHARMM parameters for ACh:

```
BONDS
!
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
!atom type Kb          b0
OS   CT2   450.000     1.3300 ! ALLOW   ALC use OC-CT2
                ! ethoxide 6-31+G* geom/freq, adm jr., 6/1/92
OS   CC    525.000     1.2600 ! ALLOW   PEP POL ARO ION use OC-CC
                ! adm jr. 7/23/91, acetic acid
ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!V(Urey-Bradley) = Kub(S - S0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A
!
!atom types     Ktheta    Theta0   Kub     S0
CT2  NH1  CT3      50.000   109.5000 ! ALLOW   ALI PEP POL ARO
                ! NMA Vib Modes (LK)
CT3  NH1  CT3      50.000   109.5000 ! ALLOW   ALI PEP POL ARO
                ! NMA Vib Modes (LK)
CT2  CT2  OS       52.000   108.0000 ! ALLOW   ALI PEP POL ARO
                ! from CT2  CT1  C, for lactams, adm jr.
CT2  OS   CC       40.000    109.60  ! ALLOW  POL PEP
                ! adm jr. 5/02/91, acetic acid pure solvent
O    CC   OS       40.000    110.00  ! guess
CT3  CC   OS       40.000    110.00  ! guess --DZ
DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
!atom types             Kchi    n   delta
!
HA   CT3  NH1  CT3      0.0000  3     0.00 ! ALLOW PEP
                ! LK for autogenerate dihe, sp2-methyl, no dihedral
potential
HA   CT2  NH1  CT3      0.0000  3     0.00 ! ALLOW PEP
CT2  CT2  NH1  CT3      1.8000  1     0.00 ! ALLOW PEP
                ! ala dipeptide update for new C VDW Rmin, adm jr.,
3/3/93c
HA   CT3  NH1  CT2      0.0000  3     0.00
CT2  OS   CC   CT3      0.4000  1     0.00 ! ALLOW PEP PRO
CT2  OS   CC   O        0.4000  1     0.00 ! ALLOW PEP PRO
```