Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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Exploration of the Conformational and Reactive Dynamics of Biomolecules in Solution using an Extended Version of the Glycine Reactive Force Field

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Force Field Parametrization and Validation

Zijing Lin and co-workers: Amino Acids. The amino acid structures added to the trainset were obtained through systematic quantum mechanical studies carried out at the DFT-B3LYP/6-311++G** level of theory. The authors conducted exhaustive conformational searches building all combinations of internal single-bond rotamers and performed energy optimization of the generated conformations without any constraint. Subsequent checks, comprising harmonic frequencies and single point calculations at a higher level of theory (MP2/6-311G(2df,p)//B3LYP/6-311++G**), allowed for the identification of the lowest energy conformers. **[TRAINSET]**

Kaminsky and Jensen: Dipeptides. Kaminsky and Jensen sampled and optimized, at the DFT and MP2 levels with an augmented double-zeta basis set, the conformational degrees of freedom of glycine, alanine, serine and cysteine. They obtained the best estimate of the relative conformational energies by means of an extrapolation procedure of the MP2 energy results (extrapolation to the basis set limit and CCSD(T) correction - see Reference for details) and used these data as reference to check the performance of eight different force fields. The comparison revealed that only half of the conformations were identified by the force fields based on fixed partial charges, whereas those including multipoles and polarizability, could reproduce most of the structures. These structures, which comprised two Gly, seven Ala, thirty-eight Ser and forty-seven Cys conformations, were not included in ReaxFF training set but were used as test case to check the parameters and assess the validity of the new reactive force field. **[VALIDATION]**

Hobza and co-workers: Oligopeptides. Hobza and co-workers performed theoretical studies on the performance of different levels of theory in comparison with the CCSD(T)/CBS benchmark for Phe-Gly-Phe (FGF), Trp-Gly (WG), Trp-Gly-Gly (WGG), Phe-Gly-Gly (FGG), Gly-Gly-Phe (GGF) and Gly-Phe-Ala (GFA) peptides. On the basis of experimental observations they restricted the benchmark study to fifteen different conformers for each species, which were selected following a procedure defined in earlier investigations [Valdés, H.; Pluhackova, K.; Hobza, P. J. Chem. Theory Comput. 2009, 5, 2248]. Geometry optimizations were performed at the RI-MP2/cc-pVTZ level of theory and also by means of the AMBER ff99 force field with the HF/6-31G* RESP charges. In their conclusion the authors did not recommend the use of this force field for investigations in the gas phase but suggested that a reliable strategy could be to use three different levels of theory, namely tight-binding DFT-D, RI-MP2 or M06-2X, and MP2/CBS for the study of the potential energy surface of the peptide, the reoptimization of selected structures and single-point energy calculations, respectively.
Some of these structures (fifteen WG, fifteen WGG and sixteen GFA conformations), were included in ReaxFF training set, whereas the others (fifteen FGF, fifteen FGG and fifteen GGF conformations) were used as test case to validate the developed parameters. **[TRAINSET]+[VALIDATION]**

Martin Head-Gordon and co-workers : Tetrapeptides, Octapeptides and Hexadecapeptides. A series of polypeptide conformations, made of alanine residues, were employed by Martin Head-Gordon and co-workers [Di Stasio, R. A.; Jung, Y.; Head-Gordon, M. J. Chem. Theory Comput. 2005, 1, 862] to appraise the overall performance of the RI-TRIM MP2 method against other techniques in the prediction of the relative energies of the structures. The main sample consisted of twenty seven different geometries of the alanine tetrapeptide, but octapeptide, and hexadecapeptide structures were also present among

the deposited data. All the conformations were optimized at the HF/6-31G** level and in addition, they also performed single-point energy calculations with higher levels and with different basis sets. The authors concluded that the accurate prediction of the relative energies of the series of tetrapeptides implies calculations with the cc-pVTZ and cc-pVQZ basis sets and then extrapolation to the cc-pV(TQ)Z limit. This data was not part of training set, but it was used for validation. **[VALIDATION]**

Protein Models and Structured Oligopeptides

Crambin. Crambin is a small protein consisting of 46 amino acids, it has been used as test case for a wide variety of simulations mainly for two reasons **1)** its crystal and solution structures have been resolved to a high degree of accuracy (0.48 Å) in the best case [*Schmidt, A.; Teeter, M.; Weckert, E.; Lamzin, V. S. Acta Cryst. 2011, F67, 424*]) **2)** it contains different secondary structure elements (two antiparallel α-helices, a short segment of anti parallel β-sheet and a classical β-turn), hydrophilic and hydrophobic residues, a salt bridge (between Arg10 and the terminal Asn46 carboxyl) and three disulfide bridges that are expected to reduce the overall conformational freedom of the molecule.
The protein is quite hydrophobic and, even though it is small, it presents well defined charged areas. There are two negative regions around the C-terminus and the β-turn, while the preponderant flat surface is positively charged. The protein does not contain reactive residues or a definite active site, thus its role is accomplished by its structure, shape and surface properties.

Tryptophan Cage. TRP-cage is a synthetic miniprotein made of 20 amino acids with a cooperatively folded tertiary structure, a globular shape and a combination of secondary structure motifs and tertiary contacts typical of more complex proteins [*Neidigh, J. W.; Fesinmeyer, R. M.; Andersen, N. H. Nat. Struct. Biol. 2002, 9, 425; Gellman, S. H.; Woolfson, D. N. Nat. Struct. Biol. 2002, 9, 408*]. It was designed by Neidigh and co-workers [*Neidigh, J. W.; Fesinmeyer, R. M.; Andersen, N. H. Nat. Struct. Biol. 2002, 9, 425*] to explore the folding pathways and understand the stability of globular proteins from both an experimental and theoretical point of view. Indeed, this protein is an ideal choice because it is able to fold quickly (in about 4 μs) and spontaneously to a native state where a short α-helix (residues 2-9), a 3_{10} helix (residues 11-14) and a polyproline II helix at the C-terminus are present. All these secondary structure elements are packed against the central tryptophan residue (TRP6) [*Neidigh, J. W.; Fesinmeyer, R. M.; Andersen, N. H. Nat. Struct. Biol. 2002, 9, 425; Qiu, L.; Pabit, S. A.; Roitberg, A. E. J. Am. Chem. Soc. 2002, 124, 12952*] and shield it from the solvent action.
TRP-cage has been well characterized from an experimental point of view and many simulations have been carried out using both implicit and explicit solvent models to disclose the different folding events. However, it was observed that, as in many other cases, solvent effects play a crucial role in conformational dynamics and molecular stability and thus a more realistic representation of the systems should be obtained if explicit solvent molecules are added as a surrounding medium. These models differ from a continuum solvent description as they take into account local effect and specific perturbations to the macromolecular structures.

Oligopeptides. The selected short structured oligopeptides are the C-terminal β-hairpin of G protein [*Blanco, F. J.; Rivas, G.; Serrano, L. Nat. Struct. Biol. 1994, 1, 584*] (**protG**), the synthetic EK α_R-helix [*Scholtz, J. M.; Barrick, D.; York, E. J.; Stewart, J. M.; Baldwin, R. L. Proc. Natl. Acad. Sci.U.S.A. 1995, 92, 185*] (**EK**), the helical C peptide of ribonuclease A [*Bierzynski, A.; Kim, P. S.; Baldwin, R. L. Proc. Natl. Acad. Sci. U.S.A. 1982, 79, 2470]* (**Baldwin**) and the synthetic trpzip2 hairpin [*Cochran, A. G.; Skelton, N. J.; Starovasnik, M. A. Proc. Natl. Acad. Sci. U.S.A. 2001, 98, 5578*] (**trpzip2**).

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Briefly, **protG** has a β-hairpin conformation which is stabilized by four salt bridges, and hydrophobic interactions between the Tyr/Phe and Trp/Val residue pairs. The polar nature of **EK**, which contains two AEAAKA segments, confers to the molecule an α-helical conformation; **Baldwin** is a 13-amino acid helix partially stabilized by a salt bridge and **trpzip2** consists of 12 residues arranged as a hairpin due to the interactions between the side chains of its Trp residues (stacking complexes) and a salt bridge between Glu5 and Lys8 charged side chains.

```
Reactive MD-force field: prot_ff + GFA WGG WG Hobza_DB. March20 2012
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
    1.6725 !Valency angle conjugation parameter
    1.7224 !Triple bond stabilisation parameter
    6.8702 !Triple bond stabilisation parameter
   60.4850 !C2-correction
    1.0588 !Undercoordination parameter
    4.6000 !Triple bond stabilisation parameter
   12.1176 !Undercoordination parameter
   13.3056 !Undercoordination parameter
  -40.0000 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    6.0891 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.3989 !Double bond/angle parameter: overcoord
    3.9954 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.7796 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.9487 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1645 !Conjugation
    1.5591 !vdWaals shielding
    0.1000 !Cutoff for bond order (*100)
    1.7602 !Valency angle conjugation parameter
    0.6991 !Overcoordination parameter
   50.0000 !Overcoordination parameter
    1.8512 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    0.7903 !Valency angle conjugation parameter
 11    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
            alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
            cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
            ov/un;val1;n.u.;val3,vval4
 C     1.3817   4.0000  12.0000   1.8903   0.1838   0.6387   1.1341   4.0000
       9.7559   2.1346   4.0000  34.9350  79.5548   4.9218   6.0000   0.0000
       1.2114   0.0000 202.2908   8.9539  34.9289  13.5366   0.8563   0.0000
      -2.8983   2.5000   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
 H     0.8930   1.0000   1.0080   1.3550   0.0930   0.8203  -0.1000   1.0000
       8.2230  33.2894   1.0000   0.0000 121.1250   3.7248   9.6093   1.0000
      -0.1000   0.0000  55.1878   3.0408   2.4197   0.0003   1.0698   0.0000
     -19.4571   4.2733   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
 O     1.2450   2.0000  15.9990   2.3890   0.1000   1.0898   1.0548   6.0000
       9.7300  13.8449   4.0000  37.5000 116.0768   8.5000   8.3122   2.0000
       0.9049   0.4056  68.0152   3.5027   0.7640   0.0021   0.9745   0.0000
      -3.5500   2.9000   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
 N     1.2333   3.0000  14.0000   2.1294   0.1322   1.0000   1.1748   5.0000
      10.0056  10.8657   4.0000  30.9146 100.0000   6.4603   7.0317   2.0000
       1.0433   4.7941 119.9837   0.6005   7.9731   2.2800   0.9745   0.0000
      -4.6366   4.0000   1.0183   4.0000   2.8793   0.0000   0.0000   0.0000
 S     1.9673   2.0000  32.0600   2.1729   0.3000   1.0336   1.5359   6.0000
      10.3008   4.9055   4.0000  52.9998 112.1416   6.5000   8.2545   2.0000
       1.4601   9.7177  71.1843   5.7487  23.2859  12.7147   0.9745   0.0000
     -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
 Mg    1.8315   2.0000  24.3050   2.2464   0.1806   0.5020   1.0000   2.0000
      10.9186  27.1205   3.0000  38.0000   0.0000   0.9499   5.6130   0.0000
      -1.3000   0.0000 220.0000  49.9248   0.3370   0.0000   0.0000   0.0000
      -1.0823   2.3663   1.0564   6.0000   2.9663   0.0000   0.0000   0.0000
```

```
P    1.5994   3.0000  30.9738   1.7000   0.1743   1.0000   1.3000   5.0000
     9.1909  14.2932   5.0000   0.0000   0.0000   1.8292   7.2520   0.0000
    -1.0000  10.2596   1.5000   0.2205  16.7429  15.9629   0.0000   0.0000
    -2.5000   1.6114   1.0338   5.0000   2.8793   0.0000   0.0000   0.0000
Na   2.0300   1.0000  22.9898   2.3334   0.1481   0.8765  -1.0000   1.0000
    11.0000   9.8000   1.0000   0.0000   0.0000  -3.8501   5.9459   0.0000
    -1.0000   0.0000  67.5458 100.0000  10.0000   0.2500   0.8563   0.0000
    -2.5766   2.5000   1.0338   6.0000   2.5791   0.0000   0.0000   0.0000
Cu   1.9202   2.0000  63.5460   1.9221   0.2826   1.0000   0.1000   1.0000
    10.9889 100.0000   1.0000   0.0000   0.0000   2.7875   6.0000   0.0000
    -1.0000   0.0000  80.7000  34.9555   0.4988   0.0000   0.8563   0.0000
    -5.1872   3.1491   1.0000   4.0000   2.5791   0.0000   0.0000   0.0000
Cl   1.7140   1.0000  35.4500   1.9139   0.2000   0.3837  -1.0000   7.0000
    11.5345  10.1330   1.0000   0.0000   0.0000   9.9614   6.5316   0.0000
    -1.0000   3.5750 143.1770   6.2293   5.2294   0.1542   0.8563   0.0000
   -10.2080   2.9867   1.0338   6.2998   2.5791   0.0000   0.0000   0.0000
X   -0.0998   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000   0.0000
    -0.1000   0.0000  -2.3700   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   4.0000   2.8793   0.0000   0.0000   0.0000
43      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                       pbe2;pbo3;pbo4;Etrip;pbo1;pbo2;ovcorr
 1  1 158.2004  99.1897  78.0000  -0.7738  -0.4550   1.0000  37.6117   0.4147
       0.4590  -0.1000   9.1628   1.0000  -0.0777   6.7268   1.0000   0.0000
 1  2 169.4760   0.0000   0.0000  -0.6083   0.0000   1.0000   6.0000   0.7652
       5.2290   1.0000   0.0000   1.0000  -0.0553   6.9316   0.0000   0.0000
 2  2 153.3934   0.0000   0.0000  -0.4600   0.0000   1.0000   6.0000   0.7300
       6.2500   1.0000   0.0000   1.0000  -0.0790   6.0552   0.0000   0.0000
 1  3 115.3161 127.1562  61.7072   0.5141  -0.3474   1.0000  18.9948   0.9954
       1.5618  -0.3414   8.9489   1.0000  -0.1628   5.6821   0.0000   0.0000
 3  3 142.2858 145.0000  50.8293   0.2506  -0.1000   1.0000  29.7503   0.6051
       0.3451  -0.1055   9.0000   1.0000  -0.1225   5.5000   1.0000   0.0000
 1  4 164.1304 141.3380 102.0464  -1.8021  -0.5696   1.0000  27.6095   0.2487
       0.3953  -0.3663   7.1330   1.0000  -0.2557   4.6940   1.0000   0.0000
 3  4 128.8596 167.8643  40.0000   0.3819  -0.1539   1.0000  34.9972   0.1900
       1.0110  -0.3716   7.0805   1.0000  -0.1265   6.8843   1.0000   0.0000
 4  4 160.1592  82.5526 153.9884   0.4110  -0.0934   1.0000  12.4304   0.5899
       0.1538  -0.1473  11.9187   1.0000  -0.0753   5.4371   1.0000   0.0000
 2  3 160.0000   0.0000   0.0000  -0.5725   0.0000   1.0000   6.0000   0.5626
       1.1150   1.0000   0.0000   0.0000  -0.0920   4.2790   0.0000   0.0000
 2  4 211.6032   0.0000   0.0000  -0.3415   0.0000   1.0000   6.0000   0.4726
       2.7198   1.0000   0.0000   1.0000  -0.1744   5.6399   0.0000   0.0000
 1  5 150.8132  59.3363  55.2528  -0.0628  -0.5211   1.0000  18.9617   0.3219
       0.3317  -0.2289   7.5946   1.0000  -0.1946   5.9455   1.0000   0.0000
 2  5 143.4377   0.0000   0.0000  -0.2944   0.0000   1.0000   6.0000   0.6034
       9.5627   1.0000   0.0000   1.0000  -0.0516   7.0960   1.0000   0.0000
 3  5   0.0000   0.0000   0.0000   0.5563  -0.4038   1.0000  49.5611   0.6000
       0.4259  -0.4577  12.7569   1.0000  -0.1100   7.1145   1.0000   0.0000
 4  5   0.0000   0.0000   0.0000   0.4438  -0.2034   1.0000  40.3399   0.6000
       0.3296  -0.3153   9.1227   1.0000  -0.1805   5.6864   1.0000   0.0000
 5  5 140.8887  84.9350  68.6860  -0.4111  -0.4781   1.0000  17.8574  -0.1336
       0.2881  -0.2494   9.8436   1.0000  -0.1806   7.4732   1.0000   0.0000
 2  6  58.6896   0.0000   0.0000  -0.0203  -0.1418   1.0000  13.1260   0.0230
       8.2136  -0.1310   0.0000   1.0000  -0.2692   6.4254   0.0000  24.4461
 3  6  87.0227   0.0000  43.3991   0.0030  -0.3000   1.0000  36.0000   0.0250
       0.0087  -0.2500  12.0000   1.0000  -0.0439   6.6073   1.0000  24.4461
 6  6  32.3808   0.0000   0.0000  -0.0076  -0.2000   0.0000  16.0000   0.2641
       4.8726  -0.2000  10.0000   1.0000  -0.0729   4.6319   0.0000   0.0000
 1  7 110.0000  92.0000   0.0000   0.2171  -0.1418   1.0000  13.1260   0.6000
       0.3601  -0.1310  10.7257   1.0000  -0.0869   5.3302   1.0000   0.0000
 2  7   0.1466   0.0000   0.0000   0.2250  -0.1418   1.0000  13.1260   0.6000
       0.3912  -0.1310   0.0000   1.0000  -0.1029   9.3302   0.0000   0.0000
 3  7 202.5868 164.1808   0.0000   0.5506  -0.5000   1.0000  25.0000   0.4300
       0.0912  -0.1285  16.0342   1.0000  -0.2008   6.2678   1.0000   0.0000
 4  7 130.0000   0.0000   0.0000   0.2171  -0.1418   1.0000  13.1260   0.6000
       0.3601  -0.1310  10.7257   1.0000  -0.0869   5.3302   1.0000   0.0000
 6  7   0.1000   0.0000   0.0000   0.2500  -0.5000   1.0000  35.0000   0.6000
       0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000   0.0000
 7  7   0.0000   0.0000   0.0000   0.2171  -0.5000   1.0000  35.0000   0.6000
```

```
          0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000   0.0000
  2   8   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000   0.7000
         10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000   0.0000
  3   8  76.0753   0.0000   0.0000  -0.4452  -0.3000   1.0000  36.0000   0.6433
          5.6834  -0.3500  25.0000   1.0000  -0.0539   8.0273   1.0000   0.0000
  4   8   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000   0.7000
         10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000   0.0000
  6   8   0.1000   0.0000   0.0000   0.2500  -0.5000   1.0000  35.0000   0.6000
          0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000   0.0000
  7   8   0.1000   0.0000   0.0000   0.2500  -0.5000   1.0000  35.0000   0.6000
          0.5000  -0.5000  20.0000   1.0000  -0.2000  10.0000   1.0000   0.0000
  8   8  27.8052   0.0000   0.0000   0.4022   0.3000   0.0000  25.0000   0.4894
          0.6222  -0.4000  12.0000   1.0000  -0.0500   5.3362   0.0000   0.0000
  4   6   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000   0.7000
         10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000   0.0000
  1   9   0.0000   0.0000   0.0000   0.2000  -0.1418   1.0000  13.1260   0.5000
          0.5000  -0.2000  20.0000   1.0000  -0.1000   9.0000   0.0000   0.0000
  2   9   0.0000   0.0000   0.0000   0.2000  -0.1418   1.0000  13.1260   0.5000
          0.5000  -0.2000  20.0000   1.0000  -0.1000   9.0000   0.0000   0.0000
  3   9  81.4346   0.0000   0.0000  -0.1594  -0.3000   1.0000  36.0000   0.0025
          0.2904  -0.2500  12.0000   1.0000  -0.0742   9.3638   0.0000   0.0000
  4   9  96.5322   0.0000   0.0000   0.9970  -0.3000   1.0000  36.0000   0.5095
          0.7247  -0.2500  12.0000   1.0000  -0.1175   9.9985   0.0000   0.0000
  9   9  73.6263   0.0000   0.0000   0.0209  -0.2000   0.0000  16.0000   0.3414
          0.4703  -0.2000  15.0000   1.0000  -0.1319   5.9254   0.0000   0.0000
  2  10 109.1686   0.0000   0.0000  -0.1657  -0.2000   0.0000  16.0000   1.2500
          2.8463  -0.2000  15.0000   1.0000  -0.1111   5.2687   0.0000   0.0000
  3  10   0.0000   0.0000   0.0000   0.5000  -0.2000   0.0000  16.0000   0.5000
          1.0001  -0.2000  15.0000   1.0000  -0.1000  10.0000   0.0000   0.0000
  9  10 118.3052   0.0000   0.0000  -0.1168  -0.2000   0.0000  16.0000   0.0697
          2.9176  -0.2000  15.0000   1.0000  -0.1316   5.3624   0.0000   0.0000
 10  10   0.2500   0.0000   0.0000   0.1803  -0.2000   0.0000  16.0000   0.3356
          0.9228  -0.2000  15.0000   1.0000  -0.1178   5.6715   0.0000   0.0000
  1   8   0.0000   0.0000   0.0000  -1.0000  -0.3000   1.0000  36.0000   0.7000
         10.1151  -0.3500  25.0000   1.0000  -0.1053   8.2003   1.0000   0.0000
  1  10   0.0000   0.0000   0.0000   0.5000  -0.2000   0.0000  16.0000   0.5000
          1.0001  -0.2000  15.0000   1.0000  -0.1000  10.0000   0.0000   0.0000
  4  10   0.0000   0.0000   0.0000   0.5000  -0.2000   0.0000  16.0000   0.5000
          1.0001  -0.2000  15.0000   1.0000  -0.1000  10.0000   0.0000   0.0000
 22     ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
  1   2   0.1239   1.4004   9.8467   1.1210  -1.0000  -1.0000
  2   3   0.0283   1.2885  10.9190   0.9215  -1.0000  -1.0000
  2   4   0.1664   1.3100   9.6406   1.0569  -1.0000  -1.0000
  1   3   0.0503   1.8006  10.2114   1.3492   1.1992   1.0506
  1   4   0.1771   1.8995   9.6891   1.3428   1.2492   1.1154
  3   4   0.2000   1.8388   9.5137   1.4587   1.0933   1.1826
  1   5   0.1618   1.7943  10.1042   1.7489   1.3150   1.4031
  2   5   0.0764   1.5838  10.1462   1.4206  -1.0000  -1.0000
  3   5   0.1022   1.9887  10.0605   1.5799   1.4000  -1.0000
  4   5   0.1505   1.9000  10.5104   1.8000   1.4000  -1.0000
  2   6   0.0100   1.6000  13.2979   1.8670  -1.0000  -1.0000
  3   6   0.0809   1.7000  11.4606   1.5177  -1.0000  -1.0000
  3   7   0.0611   1.7624  10.2685   1.7989   1.4523  -1.0000
  6   7   0.1801   1.8566   9.8498   0.1000  -1.0000  -1.0000
  3   8   0.1592   1.8283  11.7256   1.6655  -1.0000  -1.0000
  1   9   0.0500   1.7500  12.3500   0.1000  -1.0000  -1.0000
  2   9   0.0300   1.5200  12.5000   0.1000  -1.0000  -1.0000
  3   9   0.0348   1.7637  12.3562   1.7228  -1.0000  -1.0000
  4   9   0.0478   1.7704  12.8051   1.6100  -1.0000  -1.0000
  2  10   0.0568   1.6740   9.6297   1.2200  -1.0000  -1.0000
  3  10   0.1927   2.2551  11.2308  -1.0000  -1.0000  -1.0000
  9  10   0.1402   2.1604  10.9786   1.7505  -1.0000  -1.0000
104     ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2
  1   1   1  59.0573  30.7029   0.7606   0.0000   0.7180   6.2933   1.1244
  1   1   2  65.7758  14.5234   6.2481   0.0000   0.5665   0.0000   1.6255
  2   1   2  70.2607  25.2202   3.7312   0.0000   0.0050   0.0000   2.7500
  1   2   2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
  1   2   1   0.0000   3.4110   7.7350   0.0000   0.0000   0.0000   1.0400
  2   2   2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
```

1	1	3	54.7427	21.1992	1.0613	0.0000	2.9950	58.6562	1.1232
3	1	3	78.6632	16.3065	6.3613	-19.9300	1.5183	0.0000	2.2234
1	1	4	78.9895	29.7448	1.4146	0.0000	1.1834	0.0000	2.4298
3	1	4	74.5431	30.9283	1.2618	0.0000	1.1019	0.0000	1.0888
4	1	4	90.0000	15.9388	0.5081	0.0000	1.1155	0.0000	2.5891
2	1	3	50.0000	12.9103	2.5311	0.0000	0.1000	0.0000	1.0000
2	1	4	73.8008	28.9565	1.9450	0.0000	0.2000	0.0000	2.9066
1	2	4	0.0000	0.0019	6.3000	0.0000	0.0000	0.0000	1.0400
1	3	1	71.6401	45.0000	1.2667	0.0000	2.8294	0.0000	1.0000
1	3	3	76.3686	44.8665	1.9461	0.0000	1.0572	68.1072	1.8676
1	3	4	70.4701	35.0124	2.2286	0.0000	2.9000	0.0000	2.4754
3	3	3	89.9293	15.8855	2.0229	0.0000	2.9881	0.0000	1.0237
3	3	4	84.0202	31.3592	1.0534	0.0000	2.9000	0.0000	1.4406
4	3	4	72.3904	15.0722	5.0227	0.0000	3.0072	0.0000	1.0000
1	3	2	90.0000	6.6459	5.2255	0.0000	1.3111	0.0000	3.0000
2	3	3	75.6935	50.0000	2.0000	0.0000	1.0000	0.0000	1.1680
2	3	4	68.4187	33.4407	7.5000	0.0000	0.1000	0.0000	1.0000
2	3	2	85.8000	9.8453	2.2720	0.0000	2.8635	0.0000	1.5800
1	4	1	81.2266	17.5379	1.2324	0.0000	2.8702	0.0000	1.0000
1	4	3	73.8735	39.1639	1.0445	0.0000	2.8701	0.0000	1.7008
1	4	4	71.3629	18.4874	2.3468	0.0000	2.8701	0.0000	1.8255
3	4	3	74.9086	21.9109	2.5904	-18.0069	3.0701	0.0000	1.0000
3	4	4	77.8757	28.9944	1.2740	-0.9193	3.0117	0.0000	1.0000
4	4	4	76.1795	29.2290	1.6529	0.0000	2.9983	0.0000	2.4525
1	4	2	69.0828	11.0941	2.4635	0.0000	0.2025	0.0000	2.3768
2	4	3	77.7697	23.7768	2.7987	0.0000	0.3956	0.0000	3.0000
2	4	4	74.3012	42.0419	1.2591	0.0000	0.5437	0.0000	1.1369
2	4	2	84.3282	13.8208	4.6573	0.0000	0.1000	0.0000	1.0000
1	2	3	0.0000	16.7302	1.1143	0.0000	0.0000	0.0000	1.0000
1	2	4	0.0000	14.7285	3.8173	0.0000	0.0000	0.0000	2.1043
1	2	5	0.0000	15.0000	3.0000	0.0000	0.0000	0.0000	1.0400
3	2	3	0.0000	15.0000	2.8900	0.0000	0.0000	0.0000	2.8774
3	2	4	0.0000	1.4986	0.1000	0.0000	0.0000	0.0000	3.0000
4	2	4	0.0000	2.4033	0.1000	0.0000	0.0000	0.0000	1.8653
2	2	3	0.0000	8.5744	3.0000	0.0000	0.0000	0.0000	1.0421
2	2	4	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
1	1	5	74.4180	33.4273	1.7018	0.1463	0.5000	0.0000	1.6178
1	5	1	79.7037	28.2036	1.7073	0.1463	0.5000	0.0000	1.6453
2	1	5	63.3289	29.4225	2.1326	0.0000	0.5000	0.0000	3.0000
1	5	2	85.9449	38.3109	1.2492	0.0000	0.5000	0.0000	1.1000
1	5	5	80.0000	25.0000	2.0000	0.0000	0.5000	0.0000	1.3830
2	5	2	85.0000	15.1317	2.0000	0.0000	0.5000	0.0000	2.0000
2	5	5	97.0064	32.1121	2.0242	0.0000	0.5000	0.0000	2.8568
2	2	5	0.0000	0.0019	6.0000	0.0000	0.0000	0.0000	1.0400
5	4	5	62.0000	33.4273	1.7018	0.1463	0.5000	0.0000	1.0500
3	5	3	77.0699	39.4349	2.1313	-30.0000	0.9567	0.0000	1.1483
1	5	3	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
1	5	4	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
3	5	4	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
5	1	7	70.0000	35.0000	3.4223	0.0000	1.3550	0.0000	1.2002
1	3	5	73.0990	33.8942	1.2098	0.0000	0.8161	0.0000	1.1776
3	3	5	83.9753	31.0715	3.5590	0.0000	0.8161	0.0000	1.1776
2	3	5	76.9521	20.0000	2.0903	0.0000	1.0000	0.0000	1.0400
2	6	2	0.0000	49.8261	0.2093	0.0000	2.0870	0.0000	2.2895
2	2	6	0.0000	39.7818	3.1505	0.0000	1.1296	0.0000	1.1110
6	2	6	0.0000	0.5047	0.8000	0.0000	0.8933	0.0000	4.6650
2	6	6	0.0000	8.7037	0.0827	0.0000	3.5597	0.0000	1.1198
3	6	3	0.0000	9.2317	0.1000	0.0000	1.0000	0.0000	1.0920
6	3	6	0.0008	25.0000	8.0000	0.0000	1.0000	0.0000	3.0000
2	3	6	66.0423	5.0000	1.0000	0.0000	1.0000	0.0000	1.2500
2	6	3	0.0000	0.5000	0.1000	0.0000	1.0000	0.0000	3.0000
3	3	6	70.0000	20.0000	1.0000	0.0000	1.0000	0.0000	1.2500
3	7	3	88.6293	18.2614	0.8145	0.0000	-0.1780	0.0000	2.3661
2	3	7	75.0000	7.8005	0.9394	0.0000	1.3523	0.0000	1.0400
3	3	7	60.0000	40.0000	4.0000	0.0000	1.0000	0.0000	1.0400
3	2	7	0.0000	10.0000	1.0000	0.0000	1.0000	0.0000	1.0400
6	3	7	41.7798	3.5596	7.5000	0.0000	-0.2621	0.0000	1.0400
7	3	7	50.6740	13.3258	0.1000	0.0000	1.0718	0.0000	1.1254
1	3	7	76.8677	5.4250	3.1105	0.0000	-0.0827	0.0000	2.1396

```
 2  7  3  75.0000  25.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 3  7  7  70.0000  25.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 3  9  3  96.2265   4.5610  12.0000   0.0000   0.3211   0.0000   1.5204
 3  9  3   0.0000   9.1552   7.9919   0.0000   0.1660   0.0000   1.5386
 9  3  9 100.0000  10.1065   6.0000   0.0000   1.0000   0.0000   3.6601
 2  3  9  55.0417   3.5032   3.9979   0.0000   1.5171   0.0000   1.0400
 3  3  9  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 3  9  9  66.7783  14.3146   0.7911   0.0000   1.0000   0.0000   1.2333
 3  9 10  96.6924   9.4823   5.7883   0.0000   0.2248   0.0000   2.2640
 3  9 10   0.0000   3.8549   3.7230   0.0000   0.1482   0.0000   1.0400
 9 10  9   0.0000  11.2336   6.8851   0.0000   1.0000   0.0000   1.0893
 9  9 10  90.0000   5.0811   5.2147   0.0000   1.0000   0.0000   1.8538
10  9 10   0.0100  21.1482   0.3506   0.0000   1.0000   0.0000   1.4361
 3  2 10   0.0000   0.0100   0.5211   0.0000   0.0000   0.0000   1.3859
 3  9  4 100.0000  28.1532  12.0000   0.0000   0.2932   0.0000   1.6489
 3  9  4   0.0000  22.7457   2.9039   0.0000   0.5593   0.0000   1.9764
 4  9  4  87.0081  27.6432   3.9735   0.0000   4.0000   0.0000   1.4578
 4  9  4   0.0000  22.8998   3.1077   0.0000   3.0000   0.0000   1.0696
 9  4  9 100.0000  10.1065   6.0000   0.0000   1.0000   0.0000   3.6601
 2  4  9  80.0000   3.5601   3.3645   0.0000   1.5171   0.0000   1.0400
 3  4  9  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 4  3  9  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 4  4  9  70.0000  30.0000   2.0000   0.0000   1.0000   0.0000   1.2500
 4  9  9  66.7783  14.3146   0.7911   0.0000   1.0000   0.0000   1.2333
 4  9 10  95.2122   5.7090  12.0000   0.0000   0.2248   0.0000   2.8936
 4  9 10   0.0000   9.0054   7.9511   0.0000   0.1482   0.0000   1.6245
 4  2 10   0.0000  15.0000   2.8900   0.0000   0.0000   0.0000   2.8774
 1  3  9  55.0000  15.0000   1.0000   0.0000   1.0000   0.0000   1.5000
 1  4  9  55.0000  15.0000   1.0000   0.0000   1.0000   0.0000   1.5000
64    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1  1  1  1  -0.2500  34.7453   0.0288  -6.3507  -1.6000   0.0000   0.0000
 1  1  1  2  -0.2500  29.2131   0.2945  -4.9581  -2.1802   0.0000   0.0000
 2  1  1  2  -0.2500  31.2081   0.4539  -4.8923  -2.2677   0.0000   0.0000
 1  1  1  3  -2.5000  25.4016   1.0000  -4.4850  -1.1000   0.0000   0.0000
 2  1  1  3  -0.9763  59.4161   1.0000  -7.7414  -1.0978   0.0000   0.0000
 3  1  1  3  -2.5000  52.7614  -1.0000  -4.0134  -0.8614   0.0000   0.0000
 1  1  3  1  -1.9125  80.0000  -1.0000  -4.5626  -0.9000   0.0000   0.0000
 1  1  3  2   0.6154   8.3019  -0.4870  -2.9336  -0.9000   0.0000   0.0000
 2  1  3  1  -2.5000  80.0000   0.9658  -4.4935  -0.9000   0.0000   0.0000
 2  1  3  2  -1.0000  31.8695   1.0000  -2.6151  -1.1000   0.0000   0.0000
 1  1  3  3   0.7514  34.1941   0.5669  -5.5360  -2.0544   0.0000   0.0000
 2  1  3  3   2.5000  80.0000   1.0000  -2.6841  -2.8274   0.0000   0.0000
 3  1  3  1   0.2515  79.1495  -0.6263  -4.3647  -3.0437   0.0000   0.0000
 3  1  3  2   1.0000  37.1243   1.0000  -2.5000  -3.0476   0.0000   0.0000
 3  1  3  3  -1.0092  41.0504   0.3915  -6.0913  -2.7174   0.0000   0.0000
 1  3  3  1  -1.6378 -11.8357   0.3815  -3.2104  -2.7536   0.0000   0.0000
 1  3  3  2  -2.5000  -9.2805   0.3063  -5.9187  -2.9498   0.0000   0.0000
 2  3  3  2   0.2732 -21.6925  -1.0000  -2.5000  -0.9921   0.0000   0.0000
 1  3  3  3   2.5000 -17.6041   1.0000  -2.5000  -0.9972   0.0000   0.0000
 2  3  3  3  -2.5000  78.0855  -0.8750  -7.8902  -1.2407   0.0000   0.0000
 3  3  3  3  -2.5000 -25.0000   1.0000  -2.5000  -0.9000   0.0000   0.0000
 1  1  4  2   1.4427  31.7903   0.2054  -8.0000  -1.9825   0.0000   0.0000
 2  1  4  2  -1.0000  64.2008   0.3037  -7.5233  -2.1051   0.0000   0.0000
 3  1  4  2   1.0000  29.1410   1.0000  -3.2244  -2.5261   0.0000   0.0000
 3  1  1  4  -1.0000  65.1457   0.2433  -4.9542  -0.9511   0.0000   0.0000
 4  1  1  4   1.0000  87.8413   0.3817  -3.7479  -1.7241   0.0000   0.0000
 1  1  4  1   1.0000  12.2873   0.7438  -3.5510  -1.6589   0.0000   0.0000
 3  1  4  1  -1.0000  -0.2183   1.0000  -3.5014  -1.8038   0.0000   0.0000
 2  1  1  4   1.0000  23.7736   0.4235  -2.7665  -1.9000   0.0000   0.0000
 4  1  4  2   1.0000  96.1436   1.0000  -6.9528  -2.0202   0.0000   0.0000
 2  1  4  1  -1.0000  88.5527  -0.3433  -7.9806  -1.5996   0.0000   0.0000
 0  1  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  2  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
 0  2  3  0   0.0000   0.1000   0.0200  -2.5415   0.0000   0.0000   0.0000
 0  1  1  0   0.0000  50.0000   0.3000  -4.0000  -2.0000   0.0000   0.0000
 0  3  3  0   0.5511  25.4150   1.1330  -5.1903  -1.0000   0.0000   0.0000
 0  1  4  0   0.2176  40.4126   0.3535  -3.9875  -2.0051   0.0000   0.0000
 0  2  4  0   0.0000   0.1032   0.3000  -5.0965   0.0000   0.0000   0.0000
 0  3  4  0   1.1397  61.3225   0.5139  -3.8507  -2.7831   0.0000   0.0000
```

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0  4  4  0   0.7265  44.3155   1.0000  -4.4046  -2.0000   0.0000   0.0000
4  1  4  4  -0.0949   8.7582   0.3310  -7.9430  -2.0000   0.0000   0.0000
0  1  5  0   0.8251  92.1468   0.7176  -4.2341   0.0000   0.0000   0.0000
0  5  5  0   0.1291  -5.0000   0.9649  -5.0903   0.0000   0.0000   0.0000
0  2  5  0   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
0  6  6  0   0.0000   0.0000   0.1200  -2.4426   0.0000   0.0000   0.0000
0  2  6  0   0.0000   0.0000   0.1200  -2.4847   0.0000   0.0000   0.0000
0  3  6  0   0.0000   0.0000   0.1200  -2.4703   0.0000   0.0000   0.0000
1  1  3  3  -0.0002  20.1851   0.1601  -9.0000  -2.0000   0.0000   0.0000
1  3  3  1   0.0002  80.0000  -1.5000  -4.4848  -2.0000   0.0000   0.0000
3  1  3  3  -0.1583  20.0000   1.5000  -9.0000  -2.0000   0.0000   0.0000
1  1  1  7   0.0000  19.3871   0.0103 -25.5765  -1.7255   0.0000   0.0000
7  1  1  7   0.0000  80.5586   0.1104  -8.0928  -1.7255   0.0000   0.0000
0  1  7  0   4.0000  45.8264   0.9000  -4.0000   0.0000   0.0000   0.0000
0  7  7  0   4.0000  45.8264   0.9000  -4.0000   0.0000   0.0000   0.0000
2  1  3  7  -1.5000  13.7486   0.1710  -3.7686   0.0000   0.0000   0.0000
2  3  7  3  -0.3120  -1.7990   0.2371  -3.2710   0.0000   0.0000   0.0000
1  3  7  3  -1.5000  -2.5000   0.6794  -2.5000   0.0000   0.0000   0.0000
7  3  7  3  -1.5000   7.4600  -0.9075  -9.0000   0.0000   0.0000   0.0000
2  3  9  3  -1.5000   6.8333  -0.1978  -1.4683   0.0000   0.0000   0.0000
2  3  9  4  -0.6181   7.1542  -0.0047  -1.6577   0.0000   0.0000   0.0000
2  4  9  3  -1.5000   1.7820  -1.0000  -5.4916   0.0000   0.0000   0.0000
2  4  9  4  -0.1959   2.3626  -1.0000  -3.0702   0.0000   0.0000   0.0000
2  1  4  9   0.0000  10.0000   0.3000  -6.0000  -1.0000   0.0000   0.0000
2  3  9 10   0.1589  12.5000   0.4388  -1.5000   0.0000   0.0000   0.0000
9    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
3  2  3   2.1200  -3.5800   1.4500  19.5000
3  2  4   2.0985  -4.5000   1.4500  19.5000
4  2  3   1.7500  -1.5000   1.4500  19.5000
4  2  4   1.9893  -3.2987   1.4500  19.5000
3  2  5   1.5000  -2.0000   1.4500  19.5000
4  2  5   1.5000  -2.0000   1.4500  19.5000
5  2  3   1.5000  -2.0000   1.4500  19.5000
5  2  4   1.5000  -2.0000   1.4500  19.5000
5  2  5   1.5000  -2.0000   1.4500  19.5000
```

Table 1: ReaxFF parameters for the protein force field – units are in Ångstrom, degrees and kcal/mol, unless mentioned otherwise.

Atom	r_o	χ_{EEM}(eV)	η_{EEM}(eV)	γ_{EEM}	r_{vdW}	ε_{vdW}	α_{vdW}	γ_{vdW}
	r_π	$r_{\pi\pi}$						
C	1.3817	6.0000	4.9218	0.6387	1.8903	0.1838	9.7559	2.1346
	1.1341	1.2114						
H	0.8930	9.6093	3.7248	0.8203	1.3550	0.0930	8.2230	33.2894
	–	–						
O	1.2450	8.3122	8.5000	1.0898	2.3890	0.1000	9.7300	13.8449
	1.0548	0.9049						
N	1.2333	7.0317	6.4603	1.0000	2.1294	0.1322	10.0056	10.8657
	1.1748	1.0433						
S	1.9673	8.2545	6.5000	1.0336	2.1729	0.3000	10.3008	4.9055
	1.5359	1.4601						

Bond	□	$p_{be,1}$	$p_{ovun,1}$	$p_{be,2}$	$p_{bo,1}$	$p_{bo,2}$
	□	$p_{bo,3}$	$p_{bo,4}$	□	$p_{bo,5}$	$p_{bo,6}$
C-C	158.2004	-0.7738	0.4147	0.4590	-0.0777	6.7268
	99.1897	-0.1000	9.1628	78.0000	-0.4550	37.6117
C-H	169.4760	-0.6083	0.7652	5.2290	-0.0553	6.9316
	0.0000	–	–	0.0000	–	–
H-H	153.3934	-0.4600	0.7300	6.2500	-0.0790	6.0552
	0.0000	–	–	0.0000	–	–
C-O	115.3161	0.5141	0.9954	1.5618	-0.1628	5.6821
	127.1562	-0.3414	8.9489	61.7072	-0.3474	18.9948
O-O	142.2858	0.2506	0.6051	0.3451	-0.1225	5.5000
	145.0000	-0.1055	9.0000	50.8293	-0.1000	29.7503
C-N	164.1304	-1.8021	0.2487	0.3953	-0.2557	4.6940
	141.3380	-0.3663	7.1330	102.0464	-0.5696	27.6095
O-N	128.8596	0.3819	0.1900	1.0110	-0.1265	6.8843
	167.8643	-0.3716	7.0805	40.0000	-0.1539	34.9972
N-N	160.1592	0.4110	0.5899	0.1538	-0.0753	5.4371
	82.5526	-0.1473	11.9187	153.9884	-0.0934	12.4304
H-O	160.0000	-0.5725	0.5626	1.1150	-0.0920	4.2790
	0.0000	–	–	0.0000	–	–
H-N	211.6032	-0.3415	0.4726	2.7198	-0.1744	5.6399
	0.0000	–	–	0.0000	–	–
C-S	150.8132	-0.0628	0.3219	0.3317	-0.1946	5.9455
	59.3363	-0.2289	7.5946	55.2528	-0.5211	18.9617
H-S	143.4377	-0.2944	0.6034	9.5627	-0.0516	7.0960
	0.0000	–	–	0.0000	–	–

O-S	0.0000	0.5563	0.6000	0.4259	-0.1100	7.1145
	0.0000	-0.4577	12.7569	0.0000	–	–
N-S	0.0000	0.4438	0.6000	0.3296	-0.1805	5.6864
	0.0000	-0.3153	9.1227	0.0000	–	–
S-S	140.8887	-0.4111	-0.1336	0.2881	-0.1806	7.4732
	84.9350	-0.2494	9.8436	68.6860	-0.4781	17.8574
Off-Diagonal	r^{σ}	r^{π}	$r^{\pi\pi}$	r_{vdW}	α_{vdW}	ε_{vdW}
C-H	1.1210	–	–	1.4004	9.8467	0.1239
H-O	0.9215	–	–	1.2885	10.9190	0.0283
H-N	1.0569	–	–	1.3100	9.6406	0.1664
C-O	1.3492	1.1992	1.0506	1.8006	10.2114	0.0503
C-N	1.3428	1.2492	1.1154	1.8995	9.6891	0.1771
O-N	1.4587	1.0933	1.1826	1.8388	9.5137	0.2000
C-S	1.7489	1.3150	1.4031	1.7943	10.1042	0.1618
H-S	1.4206	–	–	1.5838	10.1462	0.0764
O-S	1.5799	1.4000	–	1.9887	10.0605	0.1022
N-S	1.8000	1.4000	–	1.9000	10.5104	0.1505
Valence Angle	θ_o	k_a	k_b	$p_{val,1}$	$p_{val,2}$	
C-C-C	59.0573	30.7029	0.7606	0.7180	1.1244	
C-C-H	65.7758	14.5234	6.2481	0.5665	1.6255	
H-C-H	70.2607	25.2202	3.7312	0.0050	2.7500	
C-H-H	0.0000	0.0000	6.0000	0.0000	1.0400	
C-H-C	0.0000	3.4110	7.7350	0.0000	1.0400	
H-H-H	0.0000	27.9213	5.8635	0.0000	1.0400	
C-C-O	54.7427	21.1992	1.0613	2.9950	1.1232	
O-C-O	78.6632	16.3065	6.3613	1.5183	2.2234	
C-C-N	78.9895	29.7448	1.4146	1.1834	2.4298	
O-C-N	74.5431	30.9283	1.2618	1.1019	1.0888	
N-C-N	90.0000	15.9388	0.5081	1.1155	2.5891	
H-C-O	50.0000	12.9103	2.5311	0.1000	1.0000	
H-C-N	73.8008	28.9565	1.9450	0.2000	2.9066	
C-H-N	0.0000	0.0019	6.3000	0.0000	1.0400	
C-O-C	71.6401	45.0000	1.2667	2.8294	1.0000	
C-O-O	76.3686	44.8665	1.9461	1.0572	1.8676	
C-O-N	70.4701	35.0124	2.2286	2.9000	2.4754	
O-O-O	89.9293	15.8855	2.0229	2.9881	1.0237	
O-O-N	84.0202	31.3592	1.0534	2.9000	1.4406	
N-O-N	72.3904	15.0722	5.0227	3.0072	1.0000	
C-O-H	90.0000	6.6459	5.2255	1.3111	3.0000	
H-O-O	75.6935	50.0000	2.0000	1.0000	1.1680	

H-O-N	68.4187	33.4407	7.5000	0.1000	1.0000
H-O-H	85.8000	9.8453	2.2720	2.8635	1.5800
C-N-C	81.2266	17.5379	1.2324	2.8702	1.0000
C-N-O	73.8735	39.1639	1.0445	2.8701	1.7008
C-N-N	71.3629	18.4874	2.3468	2.8701	1.8255
O-N-O	74.9086	21.9109	2.5904	3.0701	1.0000
O-N-N	77.8757	28.9944	1.2740	3.0117	1.0000
N-N-N	76.1795	29.2290	1.6529	2.9983	2.4525
C-N-H	69.0828	11.0941	2.4635	0.2025	2.3768
H-N-O	77.7697	23.7768	2.7987	0.3956	3.0000
H-N-N	74.3012	42.0419	1.2591	0.5437	1.1369
H-N-H	84.3282	13.8208	4.6573	0.1000	1.0000
C-H-O	0.0000	16.7302	1.1143	0.0000	1.0000
C-H-N	0.0000	14.7285	3.8173	0.0000	2.1043
C-H-S	0.0000	15.0000	3.0000	0.0000	1.0400
O-H-O	0.0000	15.0000	2.8900	0.0000	2.8774
O-H-N	0.0000	1.4986	0.1000	0.0000	3.0000
N-H-N	0.0000	2.4033	0.1000	0.0000	1.8653
H-H-O	0.0000	8.5744	3.0000	0.0000	1.0421
H-H-N	0.0000	0.0019	6.0000	0.0000	1.0400
C-C-S	74.4180	33.4273	1.7018	0.5000	1.6178
C-S-C	79.7037	28.2036	1.7073	0.5000	1.6453
H-C-S	63.3289	29.4225	2.1326	0.5000	3.0000
C-S-H	85.9449	38.3109	1.2492	0.5000	1.1000
C-S-S	80.0000	25.0000	2.0000	0.5000	1.3830
H-S-H	85.0000	15.1317	2.0000	0.5000	2.0000
H-S-S	97.0064	32.1121	2.0242	0.5000	2.8568
H-H-S	0.0000	0.0019	6.0000	0.0000	1.0400
S-N-S	62.0000	33.4273	1.7018	0.5000	1.0500
O-S-O	77.0699	39.4349	2.1313	0.9567	1.1483
C-S-O	70.0000	35.0000	3.4223	1.3550	1.2002
C-S-N	70.0000	35.0000	3.4223	1.3550	1.2002
N-C-S	60.0000	35.0000	3.0223	2.3550	1.2002
O-S-N	70.0000	35.0000	3.4223	1.3550	1.2002
C-O-S	73.0990	33.8942	1.2098	0.8161	1.1776
O-O-S	83.9753	31.0715	3.5590	0.8161	1.1776
H-O-S	76.9521	20.0000	2.0903	1.0000	1.0400

Torsion Angle	V_1	V_2	V_3	$p_{tor,1}$	$p_{tor,2}$
C-C-C-C	-0.2500	34.7453	0.0288	-6.3507	-1.6000
C-C-C-H	-0.2500	29.2131	0.2945	-4.9581	-2.1802

H-C-C-H	-0.2500	31.2081	0.4539	-4.8923	-2.2677
C-C-C-O	-2.5000	25.4016	1.0000	-4.4850	-1.1000
H-C-C-O	-0.9763	59.4161	1.0000	-7.7414	-1.0978
O-C-C-O	-2.5000	52.7614	-1.0000	-4.0134	-0.8614
C-C-O-C	-1.9125	80.0000	-1.0000	-4.5626	-0.9000
C-C-O-H	0.6154	8.3019	-0.4870	-2.9336	-0.9000
H-C-O-C	-2.5000	80.0000	0.9658	-4.4935	-0.9000
H-C-O-H	-1.0000	31.8695	1.0000	-2.6151	-1.1000
C-C-O-O	0.7514	34.1941	0.5669	-5.5360	-2.0544
H-C-O-O	2.5000	80.0000	1.0000	-2.6841	-2.8274
O-C-O-C	0.2515	79.1495	-0.6263	-4.3647	-3.0437
O-C-O-H	1.0000	37.1243	1.0000	-2.5000	-3.0476
O-C-O-O	-1.0092	41.0504	0.3915	-6.0913	-2.7174
C-O-O-C	-1.6378	-11.8357	0.3815	-3.2104	-2.7536
C-O-O-H	-2.5000	-9.2805	0.3063	-5.9187	-2.9498
H-O-O-H	0.2732	-21.6925	-1.0000	-2.5000	-0.9921
C-O-O-O	2.5000	-17.6041	1.0000	-2.5000	-0.9972
H-O-O-O	-2.5000	78.0855	-0.8750	-7.8902	-1.2407
O-O-O-O	-2.5000	-25.0000	1.0000	-2.5000	-0.9000
C-C-N-H	1.4427	31.7903	0.2054	-8.0000	-1.9825
H-C-N-H	-1.0000	64.2008	0.3037	-7.5233	-2.1051
O-C-N-H	1.0000	29.1410	1.0000	-3.2244	-2.5261
O-C-C-N	-1.0000	65.1457	0.2433	-4.9542	-0.9511
N-C-C-N	1.0000	87.8413	0.3817	-3.7479	-1.7241
C-C-N-C	1.0000	12.2873	0.7438	-3.5510	-1.6589
O-C-N-C	-1.0000	-0.2183	1.0000	-3.5014	-1.8038
H-C-C-N	1.0000	23.7736	0.4235	-2.7665	-1.9000
N-C-N-H	1.0000	96.1436	1.0000	-6.9528	-2.0202
H-C-N-C	-1.0000	88.5527	-0.3433	-7.9806	-1.5996
X-C-H-X	0.0000	0.0000	0.0000	0.0000	0.0000
X-H-H-X	0.0000	0.0000	0.0000	0.0000	0.0000
X-H-O-X	0.0000	0.1000	0.0200	-2.5415	0.0000
X-C-C-X	0.0000	50.0000	0.3000	-4.0000	-2.0000
X-O-O-X	0.5511	25.4150	1.1330	-5.1903	-1.0000
X-C-N-X	0.2176	40.4126	0.3535	-3.9875	-2.0051
X-H-N-X	0.0000	0.1032	0.3000	-5.0965	0.0000
X-O-N-X	1.1397	61.3225	0.5139	-3.8507	-2.7831
X-N-N-X	0.7265	44.3155	1.0000	-4.4046	-2.0000
N-C-N-N	-0.0949	8.7582	0.3310	-7.9430	-2.0000
X-C-S-X	0.8251	92.1468	0.7176	-4.2341	0.0000

X-S-S-X	0.1291	-5.0000	0.9649	-5.0903	0.0000
X-H-S-X	0.0000	0.0000	0.0000	0.0000	0.0000
C-C-O-O	-0.0002	20.1851	0.1601	-9.0000	-2.0000
C-O-O-C	0.0002	80.0000	-1.5000	-4.4848	-2.0000
O-C-O-O	-0.1583	20.0000	1.5000	-9.0000	-2.0000

H-Bond	r_{hb}	D_e	$p_{hb,1}$	$p_{hb,2}$
O-H-O	2.1200	-3.5800	1.4500	19.5000
O-H-N	2.0985	-4.5000	1.4500	19.5000
N-H-O	1.7500	-1.5000	1.4500	19.5000
N-H-N	1.9893	-3.2987	1.4500	19.5000
O-H-S	1.5000	-2.0000	1.4500	19.5000
N-H-S	1.5000	-2.0000	1.4500	19.5000
S-H-O	1.5000	-2.0000	1.4500	19.5000
S-H-N	1.5000	-2.0000	1.4500	19.5000
S-H-S	1.5000	-2.0000	1.4500	19.5000