

Discussion

Various results of theoretical calculations [23-25] on model systems for amino acids in vacuum have shown that the right-handed α -helix conformation is not stable (with a few exceptions [26]) while the β -sheet conformation is quite stable. This is not consistent with experiment, and hence it has been proposed that the right-handed α -helix must be stabilized by specific nonbond interactions [13]. It has been suggested that the α -helical conformation is destabilized compared to the β -sheet conformation by the dipole moment interaction between the side chain and the backbone [27].

In contrast, the calculations for water show that this unfavorable dipole moment of the α -helix induces a stronger solvent effect in water, leading to an α -helical conformation nearly as stable as the β -sheet conformation in water (the solvation energy is directly related to the dipole moment of the solute). This strong solvent effect in water for the α -helical conformation agrees with earlier thermodynamic studies, which included the solvent effects on an alanine dipeptide [13]. The HF calculations show that proline's α -helix conformation is more stable (4 to 6 kcal/mol) than its β -sheet conformation and for alanine the α -helical conformation (0.501 kcal/mol), is slightly more stable than the β -sheet conformation (0.986 kcal/mol). For glycine the helical conformation is more stable than parallel β -sheet conformation (0.948 kcal/mol) but less stable than the antiparallel β -sheet conformation (0.509 kcal/mol). This becomes clear for the calculations on the 10 nonpolar amino acids for the α -helix and β -sheet conformations. For all 10 relatively hydrophobic amino acids the β -sheet is more stable than the α -helix conformation in vacuum (hydrophobic environment), but in water the

stability of the α -helix conformation becomes very close to that of the β -sheet conformation due to the strong solvent stabilization of the α -helix [28].

These results support the observation that β -sheets usually occur only inside folded proteins. This is because a protein's interior is usually hydrophobic, favoring the β -sheet conformation. These results are also supported by experiments which show: (i) a transition of polylysine from the α -helix to β -sheet conformations by the addition of anesthetics, and (ii) a transition of polylysine from β -sheet to α -helix occurs by applying pressure [29]. The anesthetics induce a partial dehydration of the polypeptide side chains, creating a more hydrophobic environment favorable for β -sheet conformation for the polypeptide [30]. In contrast, the applied pressure seems to push water near the side chains and makes the environment more hydrophilic [31,32].

These results support the observation that hydrophobic residues have high preferences and polar residues have low preferences for the β -sheet secondary structure [5,6]. Hydrophobic residues are more likely to be inside the protein (in a hydrophobic environment) than are hydrophilic residues while hydrophilic residues have relatively high probabilities to be placed on the exterior of proteins compared to the hydrophobic residues. These results also explain the many α -helix models stable in water, making it easy to study the properties of α -helices, while there are very few β -sheet models stable in water, making it difficult to study β -sheets [13,26]. These conclusions are supported by results that show the presence of a hydrophobic core is essential for the formation of a β -sheet [9,10].

Peptides from the prion protein induce conformational transitions due to addition of acetonitrile and/or salts [33]. The added denaturants make the microenvironment around the peptides more hydrophobic, causing a conformational change in the peptides from α -helix to β -sheet. This observation is consistent with our results, thus providing a possible insight into explaining the Creutzfeldt-Jakob disease, the most common human prion disease [35]. These results also show that for the case of alanine and glycine the α -helical conformation is comparable to the β -sheet conformation in water. For the case of proline the α -helical conformation is much more stable than the β -sheet conformations both in water and in vacuum. This seems to contradict the observation that a proline residue tends to destroy the formation of an α -helix. Proline residues destabilize the α -helix because of the pyrrolidine ring attached to the imide nitrogen. Its presence matters only when the succeeding residue is a proline. The steric interactions of a residue are independent of the nature of the predecessor because only the carbonyl group(C=O) of the preceding residue is involved [36]. This is supported by the observation that proline residues are one of the best residues to initiate an α -helix [37]. The QM results show that an α -helix conformation is stabilized by solvation with water, providing insight into understanding the role of interactions between solvents and proteins in guiding protein folding.

Conclusion

We find that solvents have a significant effect on the conformation of polypeptides. We believe that these effects play an important role in protein folding. We report torsional parameters to use in chemical MD calculations.

References

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Appendix A – BUFF Parameters

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PARAMETER FORMAT (11-89)
  233   5   0   0   0   0   0   0   0   0   0   0   0   0   0   0
UFF parameters for all H amino acid case
*
* Parameters Current as of April 27, 2000.
*
FORCEFIELD GENFF
DEFAULTS xxxdataxxx plus comments
LBOND      T          T >> use bond terms
LANGLE     T          T >> use angle terms
ANGX 2 K   F          T >> use true force constants for cosine ang-str cross terms
ANGANGINV  F          T >> use angle-angle inversion terms
LINVERSN   T          T >> use inversion terms
ALL INVER  T          T >> use all possible inversion terms on each center
BNDXANG    F          T >> use bond cross angle terms
ANGXANG    F          T >> use angle cross angle terms
LTIORSION  T          T >> use torsion terms
BNDENDTOR  F          T >> allow coupling of the 1-2 and 3-4 bonds of torsions
ANGANGTOR  F          T >> allow coupling of the 1-2-3 and 2-3-4 angles of torsions
LPITWIST   F          T >> use pi twist terms
TORS SCAL  T          T >> will renormalize torsions (not allow SNGTOR)
ALL TORSN  T          T >> use all possible torsion terms per each central bond
ETOR SCAL  1.0000    exocyclic scaling factor
TORANGSW   F          T >> switch torsion barrier off as angle becomes linear
TORANGR    135. 180. on and off angles for torsion angle switch
UREYBRAD   F          T >> use urey-bradley terms
LNONBOND   T          T >> use nonbond terms
RNB GEOMN  T          T >> use geom mean for nonbond cross terms
NBEXBND    T          T >> exclude 1-2 terms from nonbonds
NBEXANG    T          T >> exclude 1-3 terms from nonbonds
NBEXTOR    F          T >> exclude 1-4 terms from nonbonds
DOALLCOUL  F          T >> do NOT exclude coulomb terms from nonbonds
SCAL NB14  1.0000    factor scale 1-4 nonbonds (1.0 >> full value)
SHRINK CH  F          T >> allow shrunk CH bonds for
SHRINK FC  1.0000    shrink factor for CH bonds
LCOULMB    T          T >> use Coulomb terms
R*EPS      F          T >> use shielded Coulomb 1/(eps*R**2) instead of 1/(eps*R)
DIELECTRIC 1.0000    Dielectric constant, eps
LHBOND     F          T >> use hb interactions
ATM DEFLT  C_3       default atom for FF
MASSZER    F          T >> use zero mass option
POLYENE    F          T >> use polyene option
USRENERGY  F          T >> use user energy expression
*
FFLABEL    ATNO  MODIFD  MS  CHARG  HYB  BND  CPK  #IH  #LP  RES
H_         1      0.00  0   1   8   0   0   0   F
H__A      1      0.00  0   1   8   0   0   0   F
H__O3     1      0.00  0   1   8   0   0   0   F
H__N3     1      0.00  0   1   8   0   0   0   F
H__NR     1      0.00  0   1   8   0   0   0   F
H__N3+    1      0.00  0   1   8   0   0   0   F
H__NR+    1      0.00  0   1   8   0   0   0   F
H__S3     1      0.00  0   1   8   0   0   0   F
C_3       6      0.00  3   4   5   0   0   0   F
C_A       6      0.00  3   4   5   0   0   0   F
C_R       6      0.00  2   3   5   0   0   0   T
C_2       6      0.00  2   3   5   0   0   0   F
N_3       7      0.00  3   3   7   0   0   0   F
N_R       7      0.00  2   3   7   0   0   0   T
N_R2      7      0.00  2   3   7   0   0   0   T
O_3       8      0.00  3   2   2   0   0   0   F
O_2       8      0.00  2   1   2   0   0   0   F
O_2m      8      0.00  2   1   2   0   0   0   F
S_3      16      0.00  3   2   3   0   0   0   F

```

H_F	1	1.0080	0.41	0	0	8	0	0	
O_3F	8	15.9994	-0.82	3	0	2	0	2	F
P_3	15		0.00	3	3	3	0	1	
Cl	17		-1.00	0	1	4	0	3	
Br	35		-1.00	0	1	4	0	3	
Na	11		1.00	0	-6	1	0	0	
Ca	20		2.00	0	-4	1	0	0	
Fe3+2	26		3.00	0	-6	6	0	0	
Fe6+2	26		3.00	0	-6	6	0	0	
Zn	30		2.00	0	-4	1	0	0	
Ru	44		3.00	0	-6	6	0	0	

*

ADDED H HYDROGEN 1IMPLCTH 2IMPLCTH 3IMPLCTH 4IMPLCTH

H_ H_
H__A H_
C_3 H_
C_A H_
C_R H_
C_2 H_
N_3 H_N3+
N_R H_NR
N_R2 H_NR+
O_3 H_O3
O_2 H__A
S_3 H_S3
H_F H_F
O_3F H_F

*

LONE PAIRS

*

VDW AT ITY	RNB	DENB	SCALE	1/R12 fct	1/R6 fct	
*LJ12-6 1	Re	De	not used			
*exp-6 2	Re	De	exp scal	pre-expon	dispersn	exponent
*morse 3	Re	De	exp scal			
*pur exp 5	Re	De	exp scal	pre-expon	not used	exponent

*

* Dreiding NB (Directly from paper. Exp-6)

H_	2	3.19500	0.01520	12.38200	17198.63477	32.33693
H__A	2	3.19500	0.00010	12.00000	113.14890	0.21274
H_O3	2	3.19500	0.00010	12.00000	113.14890	0.21274
H_N3	2	3.19500	0.00010	12.00000	113.14890	0.21274
H_NR	2	3.19500	0.00010	12.00000	113.14890	0.21274
H_N3+	2	3.19500	0.00010	12.00000	113.14890	0.21274
H_NR+	2	3.19500	0.00010	12.00000	113.14890	0.21274
H_S3	2	3.19500	0.00010	12.00000	113.14890	0.21274
C_3	2	3.89830	0.09510	14.03400	1171341.25000	667.51642
C_A	2	3.89830	0.09510	14.03400	1171341.25000	667.51642
C_2	2	3.89830	0.09510	14.03400	1171341.25000	667.51642
C_R	2	3.89830	0.09510	14.03400	1171341.25000	667.51642
N_3	2	3.66210	0.07740	13.84300	450301.56250	373.38098
N_R	2	3.66210	0.07740	13.84300	450301.56250	373.38098
N_R2	2	3.66210	0.07740	13.84300	450301.56250	373.38098
O_3	2	3.40460	0.09570	13.48300	232115.98438	298.08386
O_2	2	3.40460	0.09570	13.48300	232115.98438	298.08386
O_2m	2	3.40460	0.09570	13.48300	232115.98438	298.08386
S_3	2	4.03000	0.34400	12.00000	6312761.00000	2947.26294
P_3	2	4.15000	0.32000	12.00000		
Cl	2	3.95030	0.28330	13.86100		
Br	2	3.95000	0.37000	12.00000		
Na	2	3.14400	0.50000	12.00000		
Ca	2	3.47200	0.05000	12.00000		
Fe3+2	2	4.54000	0.05500	12.00000		
Fe6+2	2	4.54000	0.05500	12.00000		
Zn	2	4.54000	0.05500	12.00000		
Ru	2	4.54000	0.05500	12.00000		

*

* F3C Nonbonds

H_F	1	0.90000	0.01000	12.0000		
O_3F	1	3.55320	0.18480	12.0000		

```

*H_F      6   3.19500   0.00000   0.00000
*O_3F     6   3.40460   0.00000   0.00000
*
NONBOND-OFF
*IIII-JJJJ
*LJ12-6    1       Re       De   not used   1/R12 fct   1/R6 fct
*exp-6    2       Re       De   exp scal   pre-expon   dispersn   exponent
*morse    3       Re       De   exp scal
*pur exp  5       Re       De   exp scal   pre-expon   not used   exponent
*LJ12-10  7       Re       De   not used   1/R12 fct   1/R10 fct
*
* F3C off-diagonal
*O_3F -H_F    1   3.29800   0.03800  12.93250
O_3F -O_3F    1   3.57237   0.15047   0.00000
*
* SDG Nylon pure repulsive H-bonding term
O_2 -H__A    5   3.01696   0.02800  12.00000
O_2m -H__A   5   3.01696   0.02800  12.00000
O_3 -H__A    5   3.01696   0.02800  12.00000
N_R -H__A    5   3.01696   0.02800  12.00000
N_R2 -H__A   5   3.01696   0.02800  12.00000
*
* BUFF H__O3 donors
O_3 -H__O3    3   2.00000   1.50000  10.60000
H__O3-H__O3   2   3.50000   0.20000   9.76000
O_2 -H__O3    3   2.20000   0.83400   8.86000
O_2m -H__O3   3   2.29000   2.90000   6.86000
N_R -H__O3    3   2.37000   1.86000   7.51000
N_R2 -H__O3   3   2.37000   1.86000   7.51000
*
* BUFF H_N3+ donors
O_3 -H_N3+    5   3.16000   0.10000   8.00000
O_2 -H_N3+    3   2.00000   2.90000   6.60000
O_2m -H_N3+   5   2.36000   3.45000   5.39000
N_R -H_N3+    3   2.20000   4.25000   5.70000
N_R2 -H_N3+   3   2.20000   4.25000   5.70000
*
* BUFF H_NR+ donors
O_3 -H_NR+    3   2.50000   3.51000   5.84000
O_2 -H_NR+    3   3.66000   0.21400   7.95000
O_2m -H_NR+   3   2.09000   3.68000   6.22000
N_R -H_NR+    3   3.24000   0.61000   7.46000
N_R2 -H_NR+   3   3.24000   0.61000   7.46000
*
* BUFF H__N3 donors
* Not implemented yet since H__N3 is rare in proteins...
* H__N3 is usually charged and thus H_N3+
O_3 -H__N3    5   3.01696   0.02800  12.00000
O_2 -H__N3    5   3.01696   0.02800  12.00000
O_2m -H__N3   5   3.01696   0.02800  12.00000
N_R -H__N3    5   3.01696   0.02800  12.00000
N_R2 -H__N3   5   3.01696   0.02800  12.00000
*
* BUFF H__NR donors
O_3 -H__NR    3   2.63000   0.29100   6.77000
O_2 -H__NR    3   2.58000   0.18600  10.00000
O_2m -H__NR   3   2.34000   2.41000   6.27000
N_R -H__NR    3   3.73000   1.35000   5.27000
N_R2 -H__NR   3   3.73000   1.35000   5.27000
*
* BUFF H__S3 donors
O_3 -H__S3    3   2.52000   0.76000   8.26000
O_2 -H__S3    3   3.07000   0.07700  10.63000
O_2m -H__S3   3   1.80000   8.44000   4.62000
N_R -H__S3    3   2.44000   3.31000   8.00000
N_R2 -H__S3   3   2.44000   3.31000   8.00000
*
BONDSTRICH TYPE
* morse      2 FORC CNST  BND DIST  BOND E

```

```

* uff      8      Ke0      Re0 elec dRe      Ren      Ken
*simp harm 1 FORC CNST BND DIST
* (Put in using harmonic bonstretch.)
N_R -H__A 1 1030.9469 1.053000 -0.0096 1.0434 1059.5963 0.0000
N_R -H__NR 1 1030.9469 1.053000 -0.0096 1.0434 1059.5963 0.0000
N_R -H__NR+ 1 1030.9469 1.053000 -0.0096 1.0434 1059.5963 0.0000
N_R -C_3 1 1046.4963 1.456000 -0.0059 1.4501 1059.3770 0.0000
N_R -C_A 1 1046.4963 1.456000 -0.0059 1.4501 1059.3770 0.0000
N_R -H_ 1 1030.9469 1.053000 -0.0096 1.0434 1059.5963 0.0000
N_R2 -H__A 1 1030.9469 1.053000 -0.0096 1.0434 1059.5963 0.0000
N_3 -H__A 1 1028.0154 1.054000 -0.0096 1.0444 1056.5662 0.0000
N_R2 -H__NR 1 1030.9469 1.053000 -0.0096 1.0434 1059.5963 0.0000
N_R2 -H__NR+ 1 1030.9469 1.053000 -0.0096 1.0434 1059.5963 0.0000
N_3 -H__N3 1 1028.0154 1.054000 -0.0096 1.0444 1056.5662 0.0000
N_3 -H__N3+ 1 1028.0154 1.054000 -0.0096 1.0444 1056.5662 0.0000
C_3 -C_3 1 699.5920 1.514000 0.0000 1.5140 699.5920 0.0000
C_3 -C_A 1 699.5920 1.514000 0.0000 1.5140 699.5920 0.0000
C_3 -C_R 1 739.8881 1.486000 0.0000 1.4860 739.8881 0.0000
C_A -C_R 1 739.8881 1.486000 0.0000 1.4860 739.8881 0.0000
C_3 -H_ 1 659.7507 1.111000 -0.0016 1.1094 662.6080 0.0000
C_A -H_ 1 659.7507 1.111000 -0.0016 1.1094 662.6080 0.0000
C_3 -C_2 1 735.4249 1.489000 0.0000 1.4890 735.4249 0.0000
C_3 -S_3 1 568.4460 1.821000 -0.0073 1.8137 575.2924 0.0000
C_A -N_3 1 1044.3430 1.457000 -0.0059 1.4511 1057.1967 0.0000
C_3 -N_3 1 1044.3430 1.457000 -0.0059 1.4511 1057.1967 0.0000
C_3 -O_3 1 1030.7742 1.415000 -0.0212 1.3938 1078.4241 0.0000
C_2 -O_3 1 1087.3977 1.390000 -0.0212 1.3938 1078.4241 0.0000
C_2 -O_2 1 1610.4080 1.217000 -0.0204 1.2195 1610.4076 0.0000
C_2 -O_2m 1 1610.4080 1.217000 -0.0204 1.2195 1610.4076 0.0000
C_2 -N_R 1 1284.9920 1.360000 -0.0058 1.3597 1284.9924 0.0000
C_2 -C_2 1 773.7474 1.464000 -0.0058 1.3597 1284.9924 0.0000
C_R -C_2 1 778.5236 1.461000 0.0000 1.3793 925.3104 0.0000
C_R -C_R 1 938.6990 1.373000 0.0000 1.3793 925.3104 0.0000
C_R -H_ 1 712.2570 1.083000 -0.0016 1.0814 715.3873 0.0000
C_2 -H_ 1 706.3705 1.086000 -0.0016 1.0814 715.3873 0.0000
C_R -O_2 1 1621.0470 1.217000 -0.0204 1.3426 1206.6206 0.0000
C_R -O_2m 1 1621.0470 1.217000 -0.0204 1.3426 1206.6206 0.0000
C_2 -N_3 1 1100.0002 1.432000 -0.0204 1.3426 1206.6206 0.0000
*
* Metal bonding (from UFF)
Zn -N_R 1 326.3616 1.892000 0.0000 0.0000 0.0000 0.0000
Zn -O_2 1 327.6860 1.827000 0.0000 0.0000 0.0000 0.0000
Zn -O_3 1 315.1042 1.851000 0.0000 0.0000 0.0000 0.0000
Fe3+2-N_R 1 549.4361 1.955000 0.0000 0.0000 0.0000 0.0000
Fe3+2-S_3 1 343.1248 2.334000 0.0000 0.0000 0.0000 0.0000
Fe6+2-N_R 1 487.8706 2.034000 0.0000 0.0000 0.0000 0.0000
Fe6+2-N_R2 1 487.8706 2.034000 0.0000 0.0000 0.0000 0.0000
Fe6+2-S_3 1 315.9832 2.399000 0.0000 0.0000 0.0000 0.0000
Ru -N_R 1 557.0706 2.177000 0.0000 0.0000 0.0000 0.0000
*
* CR-NR is backbone type NR
C_R -N_R 1 1293.1050 1.357000 -0.0058 1.3568 1293.1053 0.0000
* Arg (outter 2 N), His, Trp type NR
C_R -N_R2 1 1364.3630 1.330000 -0.0058 1.3568 1293.1053 0.0000
*
C_R -O_3 1 1094.4690 1.387000 -0.0207 1.3663 1144.9427 0.0000
O_3 -H__A 1 1050.0039 1.012000 -0.0217 0.9903 1120.7078 0.0000
S_3 -H__A 1 448.6317 1.418000 -0.0107 1.4073 458.9131 0.0000
O_3 -H__O3 1 1050.0039 1.012000 -0.0217 0.9903 1120.7078 0.0000
S_3 -H__S3 1 448.6317 1.418000 -0.0107 1.4073 458.9131 0.0000
S_3 -S_3 1 503.6175 2.128000 0.0000 2.1280 503.6175 0.0000
*
* F3C bondstretch
O_3F -H_F 1 500.0000 1.000000 0.0000 0.0000 0.0000 0.0000
*
ANGLE-(L-C-R) TYPE
*simple cossthet 1 FORC CNST EQUIL ANG
*
H_ -C_3 -H_ 1 75.2779 109.4710 0.0000 0.0000 0.0000 0.0000 0.2233 0.0000 0.0000
H_ -C_A -H_ 1 75.2779 109.4710 0.0000 0.0000 0.0000 0.0000 0.2233 0.0000 0.0000
H_ -C_R -H_ 1 64.1310 120.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000

```

H_	-N_R	-H_	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
H_	-C_2	-H_	1	63.6010	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-C_2	-H_	1	102.2140	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_R	-C_2	-C_3	1	181.9801	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-C_2	-C_3	1	181.4303	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-C_2	-C_2	1	186.1347	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
N_R	-C_2	-C_3	1	268.1890	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
O_3	-C_2	-C_3	1	240.1350	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0825	3.0000	53.5392
C_3	-C_2	-C_3	1	176.9158	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0825	3.0000	53.5392
O_2	-C_2	-C_3	1	262.5995	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0825	3.0000	53.5392
O_2m	-C_2	-C_3	1	262.5995	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0825	3.0000	53.5392
O_2	-C_2	-N_R	1	434.1630	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0879	3.0000	75.8849
O_2	-C_2	-O_2	1	399.3190	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0944	3.0000	73.6727
O_2	-C_2	-O_3	1	322.9095	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0944	3.0000	73.6727
O_2m	-C_2	-O_2m	1	399.3190	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0944	3.0000	73.6727
N_R	-C_3	-C_2	1	311.5480	109.4710	0.0000	0.0000	0.0000	0.0000	0.0959	0.0000	0.0000
C_2	-C_3	-C_2	1	225.1782	109.4710	0.0000	0.0000	0.0000	0.0000	0.0882	0.0000	0.0000
C_3	-C_3	-C_3	1	214.2065	109.4710	0.0000	0.0000	0.0000	0.0000	0.0882	0.0000	0.0000
C_3	-C_3	-C_A	1	214.2065	109.4710	0.0000	0.0000	0.0000	0.0000	0.0882	0.0000	0.0000
C_2	-C_3	-C_3	1	219.5725	109.4710	0.0000	0.0000	0.0000	0.0000	0.0904	0.0000	0.0000
C_R	-C_3	-C_3	1	220.2246	109.4710	0.0000	0.0000	0.0000	0.0000	0.0907	0.0000	0.0000
C_R	-C_3	-C_A	1	220.2246	109.4710	0.0000	0.0000	0.0000	0.0000	0.0907	0.0000	0.0000
C_R	-C_A	-C_3	1	220.2246	109.4710	0.0000	0.0000	0.0000	0.0000	0.0907	0.0000	0.0000
S_3	-C_3	-C_3	1	224.7200	109.4710	0.0000	0.0000	0.0000	0.0000	0.0650	0.0000	0.0000
S_3	-C_3	-C_A	1	224.7200	109.4710	0.0000	0.0000	0.0000	0.0000	0.0650	0.0000	0.0000
O_3	-C_3	-C_3	1	290.0060	109.4710	0.0000	0.0000	0.0000	0.0000	0.0973	0.0000	0.0000
O_3	-C_3	-C_A	1	290.0060	109.4710	0.0000	0.0000	0.0000	0.0000	0.0973	0.0000	0.0000
N_3	-C_3	-C_3	1	303.2690	109.4710	0.0000	0.0000	0.0000	0.0000	0.0933	0.0000	0.0000
N_3	-C_A	-C_3	1	303.2690	109.4710	0.0000	0.0000	0.0000	0.0000	0.0933	0.0000	0.0000
N_R	-C_3	-C_3	1	303.5660	109.4710	0.0000	0.0000	0.0000	0.0000	0.0934	0.0000	0.0000
N_R	-C_3	-C_A	1	303.5660	109.4710	0.0000	0.0000	0.0000	0.0000	0.0934	0.0000	0.0000
N_3	-C_A	-C_R	1	303.5660	109.4710	0.0000	0.0000	0.0000	0.0000	0.0934	0.0000	0.0000
N_R	-C_A	-C_3	1	303.5660	109.4710	0.0000	0.0000	0.0000	0.0000	0.0934	0.0000	0.0000
N_R	-C_3	-C_R	1	312.5190	109.4710	0.0000	0.0000	0.0000	0.0000	0.0962	0.0000	0.0000
N_R	-C_A	-C_R	1	312.5190	109.4710	0.0000	0.0000	0.0000	0.0000	0.0962	0.0000	0.0000
S_3	-C_3	-H_	1	112.5440	109.4710	0.0000	0.0000	0.0000	0.0000	0.0871	0.0000	0.0000
C_3	-C_3	-H_	1	117.3990	109.4710	0.0000	0.0000	0.0000	0.0000	0.1296	0.0000	0.0000
C_3	-C_A	-H_	1	117.3990	109.4710	0.0000	0.0000	0.0000	0.0000	0.1296	0.0000	0.0000
C_A	-C_3	-H_	1	117.3990	109.4710	0.0000	0.0000	0.0000	0.0000	0.1296	0.0000	0.0000
C_2	-C_3	-H_	1	121.3740	109.4710	0.0000	0.0000	0.0000	0.0000	0.1340	0.0000	0.0000
C_R	-C_3	-H_	1	121.8610	109.4710	0.0000	0.0000	0.0000	0.0000	0.1345	0.0000	0.0000
C_R	-C_A	-H_	1	121.8610	109.4710	0.0000	0.0000	0.0000	0.0000	0.1345	0.0000	0.0000
N_R	-C_3	-H_	1	170.1120	109.4710	0.0000	0.0000	0.0000	0.0000	0.1400	0.0000	0.0000
N_R	-C_A	-H_	1	170.1120	109.4710	0.0000	0.0000	0.0000	0.0000	0.1400	0.0000	0.0000
N_3	-C_3	-H_	1	168.8850	109.4710	0.0000	0.0000	0.0000	0.0000	0.1398	0.0000	0.0000
N_3	-C_A	-H_	1	168.8850	109.4710	0.0000	0.0000	0.0000	0.0000	0.1398	0.0000	0.0000
O_3	-C_3	-H_	1	165.8800	109.4710	0.0000	0.0000	0.0000	0.0000	0.1479	0.0000	0.0000
O_2	-C_R	-C_3	1	281.0080	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0830	3.0000	53.8777
O_2m	-C_R	-C_3	1	281.0080	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0830	3.0000	53.8777
O_2	-C_R	-C_A	1	281.0080	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0830	3.0000	53.8777
O_2m	-C_R	-C_A	1	281.0080	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0830	3.0000	53.8777
N_R	-C_R	-C_3	1	273.1685	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0777	3.0000	55.8001
N_R	-C_R	-C_A	1	273.1685	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0777	3.0000	55.8001
C_R	-C_R	-C_3	1	199.5395	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0754	3.0000	40.6878
C_A	-C_R	-C_3	1	199.5395	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0754	3.0000	40.6878
C_A	-C_R	-C_A	1	199.5395	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0754	3.0000	40.6878
*(mjc)												
O_3	-C_R	-C_R	1	271.5450	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0835	3.0000	54.1926
C_R	-C_R	-C_R	1	226.2168	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0776	3.0000	41.8760
N_R2	-C_R	-C_3	1	273.1685	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0777	3.0000	55.8001
N_R2	-C_R	-C_R	1	214.9725	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0801	3.0000	57.4616
N_R2	-C_R	-H_	1	162.3270	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1186	3.0000	31.7273
N_R2	-C_R	-N_R	1	436.6740	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0826	3.0000	78.8955
N_R2	-C_R	-N_R2	1	436.6740	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0826	3.0000	78.8955
N_R	-C_R	-C_R	1	214.9725	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0801	3.0000	57.4616
N_R	-C_R	-H_	1	162.3270	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1186	3.0000	31.7273
C_R	-C_R	-H_	1	115.6673	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1140	3.0000	22.9257
O_2	-C_R	-H_	1	140.6971	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1140	3.0000	22.9257
O_2m	-C_R	-H_	1	140.6971	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1140	3.0000	22.9257
N_R	-C_R	-N_R	1	436.6740	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0826	3.0000	78.8955
O_2	-C_R	-N_R	1	436.9620	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0885	3.0000	76.3751
O_2	-C_R	-O_2	1	401.9570	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0950	3.0000	74.1603
O_2m	-C_R	-N_R	1	436.9620	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0885	3.0000	76.3751
O_2m	-C_R	-O_2m	1	401.9570	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0950	3.0000	74.1603
C_3	-N_3	-C_3	1	260.8690	106.7000	0.0000	0.0000	0.0000	0.0000	0.1574	0.0000	0.0000
C_A	-N_3	-C_3	1	260.8690	106.7000	0.0000	0.0000	0.0000	0.0000	0.1574	0.0000	0.0000
C_3	-N_3	-H_N3+	1	144.7980	106.7000	0.0000	0.0000	0.0000	0.0000	0.1574	0.0000	0.0000
C_A	-N_3	-H_N3+	1	144.7980	106.7000	0.0000	0.0000	0.0000	0.0000	0.1574	0.0000	0.0000
H_N3	-N_3	-H_N3	1	97.1150	106.7000	0.0000	0.0000	0.0000	0.0000	0.2804	0.0000	0.0000
C_3	-N_3	-H_N3+	1	144.7980	106.7000	0.0000	0.0000	0.0000	0.0000	0.1574	0.0000	0.0000
C_3	-N_3	-H_N3	1	144.7980	106.7000	0.0000	0.0000	0.0000	0.0000	0.1574	0.0000	0.0000
H_N3	-N_3	-H_N3	1	97.1150	106.7000	0.0000	0.0000	0.0000	0.0000	0.2804	0.0000	0.0000
H_N3	-N_R	-H_N3	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
H_NR	-N_R	-H_NR	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
H_NR	-N_R2	-H_NR	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
H_NR	-N_R2	-H_NR	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
C_3	-N_R	-C_3	1	191.5490	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0779	3.0000	42.0488
C_A	-N_R	-C_3	1	191.5490	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0779	3.0000	42.0488
C_A	-N_R	-C_A	1	191.5490	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0779	3.0000	42.0488
C_R	-N_R	-C_3	1	210.9740	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0802	3.0000	43.2802
C_R	-N_R	-C_A	1	210.9740	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0802	3.0000	43.2802
C_2	-N_R	-C_3	1	2								

C_3	-N_R	-H_	1	108.4940	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1178	3.0000	23.6902
C_2	-N_R	-H_A	1	122.6710	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1218	3.0000	24.4966
C_3	-N_R	-H_A	1	108.4940	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1178	3.0000	23.6902
C_R	-N_R	-H_A	1	128.4833	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1223	3.0000	24.5955
C_2	-N_R	-H_NNR	1	122.6710	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1218	3.0000	24.4966
C_3	-N_R	-H_NNR	1	108.4940	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1178	3.0000	23.6902
C_A	-N_R	-H_NNR	1	108.4940	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1178	3.0000	23.6902
C_R	-N_R	-H_NNR	1	128.4833	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1223	3.0000	24.5955
C_R	-N_R2	-C_R	1	246.6940	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0826	3.0000	44.5711
C_R	-N_R2	-H_A	1	128.4833	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1223	3.0000	24.5955
C_3	-O_3	-H_A	1	174.2860	104.5100	0.0000	0.0000	0.0000	0.0000	0.1830	0.0000	0.0000
C_R	-O_3	-H_A	1	181.7360	104.5100	0.0000	0.0000	0.0000	0.0000	0.1908	0.0000	0.0000
C_2	-O_3	-H_O3	1	180.9220	104.5100	0.0000	0.0000	0.0000	0.0000	0.1908	0.0000	0.0000
C_R	-N_R2	-H_NNR	1	128.4833	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1223	3.0000	24.5955
C_3	-O_3	-H_O3	1	174.2860	104.5100	0.0000	0.0000	0.0000	0.0000	0.1830	0.0000	0.0000
C_R	-O_3	-H_O3	1	181.7360	104.5100	0.0000	0.0000	0.0000	0.0000	0.1908	0.0000	0.0000
C_3	-S_3	-C_3	1	201.9560	92.1000	0.0000	0.0000	0.0000	0.0000	0.0822	0.0000	0.0000
S_3	-S_3	-C_3	1	217.9600	92.1000	0.0000	0.0000	0.0000	0.0000	0.0632	0.0000	0.0000
C_3	-S_3	-H_A	1	102.0450	92.1000	0.0000	0.0000	0.0000	0.0000	0.1111	0.0000	0.0000
C_3	-S_3	-H_S3	1	102.0450	92.1000	0.0000	0.0000	0.0000	0.0000	0.1111	0.0000	0.0000
C_2	-N_R	-H_NNR+	1	122.6710	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1218	3.0000	24.4966
C_3	-N_R	-H_NNR+	1	108.4940	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1178	3.0000	23.6902
C_R	-N_R	-H_NNR+	1	128.4833	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1223	3.0000	24.5955
C_R	-N_R2	-H_NNR+	1	128.4833	120.0000	0.0000	0.0000	0.0000	-1.0000	0.1223	3.0000	24.5955
H_N3+	-N_3	-H_N3+	1	97.1150	106.7000	0.0000	0.0000	0.0000	0.0000	0.2804	0.0000	0.0000
H_A	-N_R	-H_A	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
H_NNR+	-N_R	-H_NNR+	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
H_A	-N_R2	-H_A	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
H_NNR+	-N_R2	-H_NNR+	1	71.3950	120.0000	0.0000	0.0000	0.0000	-1.0000	0.2060	3.0000	15.4366
Zn	-N_R	-C_R	1	86.4530	120.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
Zn	-O_2	-C_2	1	100.4620	120.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
Zn	-O_3F	-H_F	1	64.1760	104.5100	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
O_3	-Zn	-N_R	1	187.7090	109.4710	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
N_R	-Zn	-N_R	1	197.4920	109.4710	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
O_2	-Zn	-O_3	1	182.2370	109.4710	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
O_2	-Zn	-N_R	1	191.2200	109.4710	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
O_2	-Zn	-O_2	1	185.8360	109.4710	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
* Stuff for Heme group												
N_R	-Fe3+2-N_R		1	188.3380	109.4710	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
N_R	-Fe6+2-N_R		1	289.5630	90.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
N_R2	-Fe6+2-N_R		1	289.5630	90.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
C_2	-N_R	-C_2	1	291.3030	111.3000	0.0000	0.0000	0.0000	-1.0000	0.0800	3.0000	43.1465
N_R	-C_2	-C_2	1	279.4170	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
N_R	-C_2	-C_R	1	280.3450	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-C_2	-C_R	1	186.7077	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-C_R	-C_2	1	187.2837	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-C_R	-H_	1	102.9250	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
Fe3+2-N_R	-C_2		1	198.2260	111.3000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
Fe3+2-S_3	-C_3		1	171.0890	92.1000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
S_3	-Fe3+2-N_R		1	148.3640	109.4710	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
S_3	-Fe6+2-N_R		1	217.2056	90.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
S_3	-Fe6+2-N_R2		1	217.2056	90.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
Fe6+2-N_R	-C_2		1	151.0240	120.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
Fe6+2-N_R2	-C_R		1	137.5332	120.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
Fe6+2-S_3	-C_3		1	199.5525	92.1000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366

* P450 Ru Linker params.

N_R	-Ru	-N_R	1	238.6410	90.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
Ru	-N_R	-C_R	1	188.2300	120.0000	0.0000	0.0000	0.0000	0.0000	0.0000	3.0000	15.4366
N_3	-C_2	-C_3	1	249.3046	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
O_2	-C_2	-N_3	1	240.9266	120.0000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-N_3	-C_3	1	267.6580	106.7000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570
C_2	-N_3	-H_N3	1	147.3000	106.7000	0.0000	0.0000	0.0000	-1.0000	0.0773	3.0000	55.4570

* F3C angle

H_F	-O_3F	-H_F	21	120.0000	109.4700	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
-----	-------	------	----	----------	----------	--------	--------	--------	--------	--------	--------	--------

*
TORSION CASE BARRIER PERIOD CISMIN(1) ANGANG BNDTOR MPHI B-B
POLY

*must have angang etc on last one

* Taken from UFF and placed in Cos expansion form.

TORSION FOURIER

*LLLL-CCCC-CCCC-RRRRR	CASE	v0	v1	v2	v3	v4	v5	v6		
v7	v8	v9	v10	v11	v12					
X	-N_R	-C_3	-X	1	1.0000	0.0000	0.0000	1.0000		
X	-C_3	-C_3	-X	1	1.0595	0.0000	0.0000	1.0595		
X	-C_3	-C_R	-X	1	0.5000	0.0000	0.0000	0.0000	0.0000	-0.5000
X	-N_R	-C_R	-X	1	14.1644	0.0000	-14.1644			
X	-N_R2	-C_R	-X	1	14.1644	0.0000	-14.1644			
X	-S_3	-C_3	-X	1	0.5064	0.0000	0.0000	0.5064		
X	-N_R	-C_2	-X	1	12.1810	0.0000	-12.1810			
X	-C_2	-C_3	-X	1	0.5000	0.0000	0.0000	0.0000	0.0000	-0.5000
X	-C_R	-C_R	-X	1	14.2069	0.0000	-14.2069			
X	-C_2	-C_R	-X	8	5.0000	0.0000	-5.0000			
X	-C_2	-C_2	-X	8	5.0000	0.0000	-5.0000			
X	-C_2	-O_3	-X	8	5.0000	0.0000	-5.0000			

```

X  -N_3  -C_3  -X      1  0.4882  0.0000  0.0000  0.4882
X  -O_3  -C_3  -X      1  0.0976  0.0000  0.0000  0.0976
X  -O_3  -C_R  -X      1  5.0000  0.0000 -5.0000
X  -S_3  -S_3  -X      1  0.2420  0.0000  0.2420
X  -Zn   -N_R  -X      1  0.5000  0.0000  0.0000  0.0000  0.0000  0.0000 -0.5000
X  -Zn   -O_2  -X      1  0.5000  0.0000  0.0000  0.0000  0.0000  0.0000 -0.5000
X  -Ru   -N_R  -X     41  0.0000
X  -N_3  -C_2  -X      1  1.0000  0.0000  0.0000  1.0000
* Fe - N_R torsion zero rather than 1 since N_R is N_2 actually.
X  -Fe3+2-N_R  -X     44  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
X  -Fe3+2-S_3  -X      1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
X  -Fe6+2-N_R  -X     44  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
X  -Fe6+2-N_R2 -X     44  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
X  -Fe6+2-S_3  -X      1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
*
* The following zeroed to make sure phi/psi/proline torsions work out correctly..
X  -C_3  -C_A  -X      1  0.0000  0.0000  0.0000  0.0000
X  -N_3  -C_A  -X      1  0.0000  0.0000  0.0000  0.0000
X  -N_R  -C_A  -X      1  0.0000  0.0000  0.0000  0.0000
X  -C_A  -C_R  -X      1  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000  0.0000
*
* Modified torsions as per CMP/MJC/WAG torsion paper of tripeptides (12/10/99)
* *** Multiplied by 6 to get correct barriers... ***
*phi (CNCC)  psi (NCCN)  (CCCN is Cbeta torsion (psi + 120), CCNC is Cb (phi -120) )
*
*PHI*
C_R  -N_R  -C_A  -C_R      0  0.0000  0.0000  0.0000 -2.7000  0.0000  0.0000  0.0000
*PSI*
N_R  -C_R  -C_A  -N_R      0  0.0000  0.0000-15.0000 -1.2000  0.0000  0.0000  0.0000
*(added for Nterminal N_3)
N_R  -C_R  -C_A  -N_3      0  0.0000  0.0000-15.0000 -1.2000  0.0000  0.0000  0.0000
*
*
*"C-b phi"
C_R  -N_R  -C_A  -C_3      0  0.0000 -6.0000 -6.0000-14.4000 -9.0000
*"C-beta psi"
N_R  -C_R  -C_A  -C_3      0  0.0000  3.6000  1.8000 -3.0000
*
*
INVERSION (CENT AT 1ST) TYPE  FRC CNST  EQU ANGL          D          E          F
*CCCC-JJJJJ-KKKKK-LLLLL  TYPE=1 FOR CHARMM,TYPE=2 FOR SPECTROSCOPIC, TYPE=3 FOR AMBER
C_R  -X    -X    -X        2    6.0000    0.0000
C_R  -O_2  -X    -X        2   50.0000    0.0000
C_R  -X    -X    -O_2      2   50.0000    0.0000
C_2  -O_2  -X    -X        2   50.0000    0.0000
C_2  -X    -X    -O_2      2   50.0000    0.0000
C_3  -X    -X    -X        2    0.0000    0.0000
C_2  -X    -X    -X        2    6.0000    0.0000
C_R  -O_2m -X    -X        2   50.0000    0.0000
C_R  -X    -X    -O_2m     2   50.0000    0.0000
C_2  -O_2m -X    -X        2   50.0000    0.0000
C_2  -X    -X    -O_2m     2   50.0000    0.0000
N_R  -X    -X    -X        2    6.0000    0.0000
N_R2 -X    -X    -X        2    6.0000    0.0000
N_3  -X    -X    -X        2    0.0000    61.2230
S_3  -X    -X    -X        2    0.0000    0.0000
*
END OF DATA

```

Appendix B – BUFF Conversion File

```

C Record format is 1X,A3, 1X,A7, 1X,A7, 1X,I2, 1X,I2, 1X,F8.4 and
C corresponds to:
C
C RES OLDTYP NEWTYP MB NL CHARGE
C
C where RES      = residue name
C      OLDTYP = old atom type (type on input data file)
C      NEWTYP = new atom type (type used in calculations)
C      MB      = maximum number of covalent connections
C      NL      = number of lone pairs at MB (for H-bond acceptors)
C      CHARGE  = charge on atom (used in electrostatic calculation)
*
* Common hydrogens in amino acids.
*(These will be wrong in BUFF charge model if not explicit in file.)
*
*** HN      H__NR      1 0  0.0000
*** H       H__NR      1 0  0.0000
*** H       H__NR      1 0  0.0000
*** #H      H__A       1 0  0.0000
*** #D      H__A       1 0  0.0000
*** HA      H_         1 0  0.0000
*** DA      H_         1 0  0.0000
*** #HB     H_         1 0  0.0000
*** #DB     H_         1 0  0.0000
*** HB1     H_         1 0  0.0000
*** HB2     H_         1 0  0.0000
*** HB3     H_         1 0  0.0000
*** H       H__A       1 0  0.0000
*** #H      H__A       1 0  0.0000
*
C Amino acid conversions to BUFF atom types with LMP2 charges
*
ALA N       N_R        2 1 -0.8570
ALA HN      H__NR      1 0  0.3420
ALA CA      C_A        4 0  0.4870
ALA HCA     H_         1 0  0.0110
ALA HA      H_         1 0  0.0110
ALA C       C_R        3 0  0.7260
ALA O       O_2        1 2 -0.6500
ALA OXT     O_2        1 2 -0.6500
ALA CB      C_3        4 0 -0.3950
ALA H       H__NR      1 0  0.3420
ALA #H      H__NR      1 0  0.3420
ALA HCB     H_         1 0  0.1120
ALA #HB     H_         1 0  0.1120
ALA HB      H_         1 0  0.1120
* *ALA Done*
ARG N       N_R        2 1 -0.7390
ARG H       H__NR      1 0  0.3340

```

ARG #H	H__NR	1	0	0.3340
ARG HN	H__NR	1	0	0.3340
ARG CA	C_A	4	0	0.0290
ARG HCA	H_	1	0	0.1300
ARG HA	H_	1	0	0.1300
ARG C	C_R	3	0	0.8770
ARG O	O_2	1	2	-0.6990
ARG OXT	O_2	1	2	-0.6990
ARG CB	C_3	4	0	-0.2210
ARG HCB	H_	1	0	0.0850
ARG #HB	H_	1	0	0.0850
ARG HB	H_	1	0	0.0850
ARG CG	C_3	4	0	0.1720
ARG HCG	H_	1	0	0.0360
ARG #HG	H_	1	0	0.0360
ARG #DG	H_	1	0	0.0360
ARG HG1	H_	1	0	0.0360
ARG HG2	H_	1	0	0.0360
ARG CD	C_3	4	0	-0.0750
ARG HCD	H_	1	0	0.1070
ARG #HD	H_	1	0	0.1070
ARG #DD	H_	1	0	0.1070
ARG HD1	H_	1	0	0.1070
ARG HD2	H_	1	0	0.1070
ARG NE	N_R	2	1	-0.6240
ARG HNE	H__NR	1	0	0.3820
ARG HE	H__NR	1	0	0.3820
ARG #HE	H__NR	1	0	0.3820
ARG #DE	H__NR	1	0	0.3820
ARG CZ	C_R	3	0	1.1000
ARG NH1	N_R2	3	0	-1.0930
ARG HNH1	H_NR+	1	0	0.5160
ARG HN11	H_NR+	1	0	0.5160
ARG HN12	H_NR+	1	0	0.5160
ARG HH11	H_NR+	1	0	0.5160
ARG NH2	N_R2	3	0	-1.0930
ARG HNH2	H_NR+	1	0	0.5160
ARG HN21	H_NR+	1	0	0.5160
ARG HN22	H_NR+	1	0	0.5160
ARG HH21	H_NR+	1	0	0.5160
ARG HH22	H_NR+	1	0	0.5160
ARG #HH1	H_NR+	1	0	0.5160
ARG #DH1	H_NR+	1	0	0.5160
ARG #HH2	H_NR+	1	0	0.5160
ARG #DH2	H_NR+	1	0	0.5160
* *ARG done*				
ASN N	N_R	2	1	-0.7760
ASN HN	H__NR	1	0	0.3290
ASN H	H__NR	1	0	0.3290
ASN #H	H__NR	1	0	0.3290
ASN CA	C_A	4	0	0.2590
ASN HCA	H_	1	0	0.0880
ASN HA	H_	1	0	0.0880
ASN C	C_R	3	0	0.8040
ASN O	O_2	1	2	-0.6580

ASN	OXT	O_2	1	2	-0.6580
ASN	CB	C_3	4	0	-0.4180
ASN	HCB	H_	1	0	0.1440
ASN	#HB	H_	1	0	0.1440
ASN	HB	H_	1	0	0.1440
ASN	CG	C_R	3	0	0.9380
ASN	OD1	O_2	1	2	-0.7280
ASN	AD1	O_2	1	2	-0.7280
ASN	ND2	N_R	2	1	-1.0200
ASN	AD2	N_R	2	1	-1.0200
ASN	HND1	H__NR	1	0	0.4470
ASN	HND2	H__NR	1	0	0.4470
ASN	HD21	H__NR	1	0	0.4470
ASN	HD22	H__NR	1	0	0.4470
ASN	HAD2	H__NR	1	0	0.4470
ASN	#HD2	H__NR	1	0	0.4470
ASN	#DD2	H__NR	1	0	0.4470
* *ASN done*					
ASP	N	N_R	2	1	-0.8800
ASP	HN	H__NR	1	0	0.3760
ASP	CA	C_A	4	0	0.1300
ASP	HCA	H_	1	0	0.0860
ASP	HA	H_	1	0	0.0860
ASP	C	C_R	3	0	0.9140
ASP	O	O_2	1	2	-0.7290
ASP	OXT	O_2	1	2	-0.7290
ASP	CB	C_3	4	0	-0.0960
ASP	HCB	H_	1	0	0.0330
ASP	#HB	H_	1	0	0.0330
ASP	HB	H_	1	0	0.0330
ASP	H	H__NR	1	0	0.3760
ASP	#H	H__NR	1	0	0.3760
ASP	CG	C_R	3	0	0.9150
ASP	OD1	O_2m	1	2	-0.8910
ASP	OD2	O_2m	1	2	-0.8910
* *ASP done using h2o optimized geometry for charges*					
CYS	N	N_R	2	1	-0.9160
CYS	HN	H__NR	1	0	0.3860
CYS	CA	C_A	4	0	0.4020
CYS	HCA	H_	1	0	0.0700
CYS	HA	H_	1	0	0.0700
CYS	C	C_R	3	0	0.8120
CYS	O	O_2	1	2	-0.6360
CYS	OXT	O_2	1	2	-0.6360
CYS	CB	C_3	4	0	-0.4080
CYS	HCB	H_	1	0	0.1990
CYS	#HB	H_	1	0	0.1990
CYS	HB	H_	1	0	0.1990
CYS	H	H__NR	1	0	0.3860
CYS	#H	H__NR	1	0	0.3860
CYS	SG	S_3	2	2	-0.1080
CYS	S1	S_3	2	2	-0.1080
* (for no disulfide)					
* CYS	SG	S_3	2	2	-0.3850
* (If you have no disulfide, SG needs to be changed to -0.385)					

CYS HSG	H__S3	1	0	0.2770
CYS HG	H__S3	1	0	0.2770
CYS HG	H__S3	1	0	0.2770
CYS DG	H__S3	1	0	0.2770
*				
* If no disulfide, SG needs to be -0.3850				
* *CYS done*				
GLU N	N_R	2	1	-0.7680
GLU HN	H__NR	1	0	0.3210
GLU CA	C_A	4	0	0.1040
GLU HCA	H_	1	0	0.0810
GLU HA	H_	1	0	0.0810
GLU C	C_R	3	0	0.8710
GLU O	O_2	1	2	-0.6800
GLU OXT	O_2	1	2	-0.6800
GLU CB	C_3	4	0	-0.0250
GLU HCB	H_	1	0	0.0260
GLU #HB	H_	1	0	0.0260
GLU HB	H_	1	0	0.0260
GLU H	H__NR	1	0	0.3210
GLU #H	H__NR	1	0	0.3210
GLU CG	C_3	4	0	-0.1470
GLU HCG	H_	1	0	0.0470
GLU #HG	H_	1	0	0.0470
GLU #DG	H_	1	0	0.0470
GLU HG1	H_	1	0	0.0470
GLU HG2	H_	1	0	0.0470
GLU CD	C_R	3	0	0.9510
GLU OE1	O_2m	1	2	-0.9270
GLU OE2	O_2m	1	2	-0.9270
* *GLU done*				
GLN N	N_R	2	1	-0.7240
GLN HN	H__NR	1	0	0.3160
GLN CA	C_A	4	0	0.1480
GLN HCA	H_	1	0	0.0770
GLN HA	H_	1	0	0.0770
GLN C	C_R	3	0	0.7920
GLN O	O_2	1	2	-0.6690
GLN OXT	O_2	1	2	-0.6690
GLN CB	C_3	4	0	-0.0060
GLN HCB	H_	1	0	0.0320
GLN #HB	H_	1	0	0.0320
GLN HB	H_	1	0	0.0320
GLN H	H__NR	1	0	0.3160
GLN #H	H__NR	1	0	0.3160
GLN CG	C_3	4	0	-0.2460
GLN HCG	H_	1	0	0.1000
GLN #HG	H_	1	0	0.1000
GLN #DG	H_	1	0	0.1000
GLN HG1	H_	1	0	0.1000
GLN HG2	H_	1	0	0.1000
GLN CD	C_R	3	0	0.9340
GLN OE1	O_2	1	2	-0.7410
GLN AE1	O_2	1	2	-0.7410
GLN NE2	N_R	2	1	-1.1230

GLN	AE2	N_R	2	1	-1.1230
GLN	HNE1	H__NR	1	0	0.4890
GLN	HNE2	H__NR	1	0	0.4890
GLN	HE21	H__NR	1	0	0.4890
GLN	HE22	H__NR	1	0	0.4890
GLN	HAE2	H__NR	1	0	0.4890
GLN	#HE2	H__NR	1	0	0.4890
GLN	#DE2	H__NR	1	0	0.4890
* *GLN done*					
GLY	N	N_R	2	1	-0.6540
GLY	HN	H__NR	1	0	0.2970
GLY	CA	C_A	4	0	0.0010
GLY	HCA	H_	1	0	0.1000
GLY	HA	H_	1	0	0.1000
GLY	C	C_R	3	0	0.8360
GLY	O	O_2	1	2	-0.6800
GLY	OXT	O_2	1	2	-0.6800
GLY	#HA	H_	1	0	0.1000
GLY	HA1	H_	1	0	0.1000
GLY	HA2	H_	1	0	0.1000
GLY	H	H__NR	1	0	0.2970
GLY	#H	H__NR	1	0	0.2970
* *GLY done*					
HIS	N	N_R	2	1	-0.9440
HIS	HN	H__NR	1	0	0.3590
HIS	CA	C_A	4	0	0.7570
HIS	HCA	H_	1	0	-0.0440
HIS	HA	H_	1	0	-0.0440
HIS	C	C_R	3	0	0.6380
HIS	O	O_2	1	2	-0.6240
HIS	OXT	O_2	1	2	-0.6240
HIS	CB	C_3	4	0	-0.5280
HIS	HCB	H_	1	0	0.1630
HIS	#HB	H_	1	0	0.1630
HIS	HB	H_	1	0	0.1630
HIS	H	H__NR	1	0	0.3590
HIS	#H	H__NR	1	0	0.3590
HIS	CG	C_R	3	0	0.0790
HIS	ND1	N_R2	3	0	-0.3440
HIS	AD1	N_R2	3	0	-0.3440
HIS	HND1	H__NR	1	0	0.3240
HIS	HD1	H__NR	1	0	0.3240
HIS	HAD1	H__NR	1	0	0.3240
HIS	HD1	H__NR	1	0	0.3240
HIS	DD1	H__NR	1	0	0.3240
HIS	CD2	C_R	3	0	0.2180
HIS	AD2	C_R	3	0	0.2180
HIS	HCD2	H_	1	0	0.0910
HIS	HD2	H_	1	0	0.0910
HIS	DD2	H_	1	0	0.0910
HIS	CE1	C_R	3	0	0.3930
HIS	AE1	C_R	3	0	0.3930
HIS	HCE1	H_	1	0	0.1080
HIS	HE1	H_	1	0	0.1080
HIS	DE1	H_	1	0	0.1080

```

HIS  NE2    N_R2    2  1  -0.8090
HIS  AE2    N_R2    2  1  -0.8090
*  *HIS done*  -> assume "HSD" is deprotonated
*                and "HSP" is protonated form.
*  HIS has no proton on outter most nitrogen...
*
HSD  N      N_R      2  1  -1.1790
HSD  HN     H__NR    1  0   0.4120
HSD  CA     C_A     4  0   1.0990
HSD  HCA    H_      1  0  -0.0990
HSD  HA     H_      1  0  -0.0990
HSD  C      C_R     3  0   0.5540
HSD  O      O_2     1  2  -0.6300
HSD  OXT    O_2     1  2  -0.6300
HSD  CB     C_3     4  0  -0.8520
HSD  HCB    H_      1  0   0.1950
HSD  #HB    H_      1  0   0.1950
HSD  HB     H_      1  0   0.1950
HSD  H      H__NR    1  0   0.4120
HSD  #H     H__NR    1  0   0.4120
HSD  CG     C_R     3  0   0.2900
HSD  ND1    N_R2    2  1  -0.6270
HSD  AD1    N_R2    2  1  -0.6270
HSD  CD2    C_R     3  0   0.0580
HSD  AD2    C_R     3  0   0.0580
HSD  HCD2   H_      1  0   0.0810
HSD  HD2    H_      1  0   0.0810
HSD  HAD2   H_      1  0   0.0810
HSD  CE1    C_R     3  0   0.4070
HSD  AE1    C_R     3  0   0.4070
HSD  HCE1   H_      1  0   0.0320
HSD  HE1    H_      1  0   0.0320
HSD  HAE1   H_      1  0   0.0320
HSD  NE2    N_R2    3  0  -0.9360
HSD  AE2    N_R2    3  0  -0.9360
*  *HSD Done.*  Assumed HSD had charge -1, no HN hydrogens.*
HSP  N      N_R      2  1  -0.8980
HSP  HN     H__NR    1  0   0.4080
HSP  H      H__NR    1  0   0.4080
HSP  #H     H__NR    1  0   0.4080
HSP  CA     C_A     4  0   0.2970
HSP  HCA    H_      1  0   0.1300
HSP  HA     H_      1  0   0.1300
HSP  C      C_R     3  0   0.8650
HSP  O      O_2     1  2  -0.6810
HSP  OXT    O_2     1  2  -0.6810
HSP  CB     C_3     4  0  -0.6540
HSP  HCB    H_      1  0   0.2150
HSP  #HB    H_      1  0   0.2150
HSP  HB     H_      1  0   0.2150
HSP  CG     C_R     3  0   0.4130
HSP  ND1    N_R2    3  0  -0.2410
HSP  AD1    N_R2    3  0  -0.2410
HSP  HND1   H__NR+   1  0   0.3710
HSP  HD1    H__NR+   1  0   0.3710

```

HSP HAD1	H_NR+	1	0	0.3710
HSP CD2	C_R	3	0	-0.2710
HSP AD2	C_R	3	0	-0.2710
HSP HCD2	H_	1	0	0.2640
HSP HD2	H_	1	0	0.2640
HSP HAD2	H_	1	0	0.2640
HSP CE1	C_R	3	0	0.1280
HSP AE1	C_R	3	0	0.1280
HSP HCE1	H_	1	0	0.2440
HSP HE1	H_	1	0	0.2440
HSP HAE1	H_	1	0	0.2440
HSP NE2	N_R2	3	0	-0.2380
HSP AE2	N_R2	3	0	-0.2380
HSP HNE2	H_NR+	1	0	0.4330
HSP HE2	H_NR+	1	0	0.4330
HSP HAE2	H_NR+	1	0	0.4330

* *HSP done* Used +1 total net charge, 2 NH hydrogens
 * *Used H2O solvent optimized geometry to get charges*
 * (H_NR in HSP may need special plus hydrogen terms...)
 *

ILE N	N_R	2	1	-0.6820
ILE HN	H_NR	1	0	0.2830
ILE H	H_NR	1	0	0.2830
ILE #H	H_NR	1	0	0.2830
ILE CA	C_A	4	0	0.0380
ILE HCA	H_	1	0	0.1090
ILE HA	H_	1	0	0.1090
ILE C	C_R	3	0	0.8600
ILE O	O_2	1	2	-0.7080
ILE OXT	O_2	1	2	-0.7080
ILE CB	C_3	4	0	0.1600
ILE HCB	H_	1	0	0.0080
ILE #HB	H_	1	0	0.0080
ILE HB	H_	1	0	0.0080
ILE CG1	C_3	4	0	0.0500
ILE HCG1	H_	1	0	0.0290
ILE #HG1	H_	1	0	0.0290
ILE #DG1	H_	1	0	0.0290
ILE HG1	H_	1	0	0.0290
ILE CG2	C_3	4	0	-0.3880
ILE HCG2	H_	1	0	0.1000
ILE #HG2	H_	1	0	0.1000
ILE #DG2	H_	1	0	0.1000
ILE HG2	H_	1	0	0.1000
ILE CD1	C_3	4	0	-0.3640
ILE HCD1	H_	1	0	0.0920
ILE #HD1	H_	1	0	0.0920
ILE #DD1	H_	1	0	0.0920
ILE HD1	H_	1	0	0.0920
ILE HD2	H_	1	0	0.0920
ILE HD3	H_	1	0	0.0920

* *ILE done* *H's need to be double checked.*
 * *removed HD4 through HD6 since unspecified.*

LEU N	N_R	2	1	-0.7070
LEU HN	H_NR	1	0	0.2970

LEU H	H__NR	1	0	0.2970
LEU #H	H__NR	1	0	0.2970
LEU CA	C_A	4	0	0.3160
LEU HCA	H_	1	0	0.0530
LEU HA	H_	1	0	0.0530
LEU C	C_R	3	0	0.6760
LEU O	O_2	1	2	-0.6510
LEU OXT	O_2	1	2	-0.6510
LEU CB	C_3	4	0	-0.3170
LEU HCB	H_	1	0	0.0800
LEU #HB	H_	1	0	0.0800
LEU HB	H_	1	0	0.0800
LEU CG	C_3	4	0	0.5390
LEU HCG	H_	1	0	-0.0480
LEU HG	H_	1	0	-0.0480
LEU DG	H_	1	0	-0.0480
LEU CD1	C_3	4	0	-0.5160
LEU HCD1	H_	1	0	0.1190
LEU #HD1	H_	1	0	0.1190
LEU #DD1	H_	1	0	0.1190
LEU CD2	C_3	4	0	-0.5160
LEU HCD2	H_	1	0	0.1190
LEU #HD2	H_	1	0	0.1190
LEU #DD2	H_	1	0	0.1190
LEU HD1	H_	1	0	0.1190
LEU HD2	H_	1	0	0.1190
LEU HD3	H_	1	0	0.1190
LEU HD4	H_	1	0	0.1190
LEU HD5	H_	1	0	0.1190
LEU HD6	H_	1	0	0.1190
* *LEU done*				
LYS N	N_R	2	1	-0.7090
LYS HN	H__NR	1	0	0.3230
LYS CA	C_A	4	0	0.0030
LYS HCA	H_	1	0	0.1120
LYS HA	H_	1	0	0.1120
LYS C	C_R	3	0	0.8720
LYS O	O_2	1	2	-0.6920
LYS OXT	O_2	1	2	-0.6920
LYS CB	C_3	4	0	-0.0380
LYS HCB	H_	1	0	0.0400
LYS #HB	H_	1	0	0.0400
LYS HB	H_	1	0	0.0400
LYS H	H__NR	1	0	0.3230
LYS #H	H__NR	1	0	0.3230
LYS CG	C_3	4	0	0.0360
LYS HCG	H_	1	0	0.0200
LYS #HG	H_	1	0	0.0200
LYS #DG	H_	1	0	0.0200
LYS HG1	H_	1	0	0.0200
LYS HG2	H_	1	0	0.0200
LYS CD	C_3	4	0	-0.1640
LYS HCD	H_	1	0	0.0680
LYS #HD	H_	1	0	0.0680
LYS #DD	H_	1	0	0.0680