```
! BONDS ! based on Turpin paper: RSC Adv 2014, 4, 48621-48631

 bond     CXX  HX            $kbon     1.08   ! defined for DHB and DHA by LZ, UIUC
 bond     CXX  HXX           $kbon     1.08   ! defined for DHB and DHA by LZ, UIUC
 bond     CXX  CT            $kbon     1.509  ! defined for DHB by LZ, UIUC
 bond     CXX  CXX           $kbon     1.40   ! defined for DHB and DHA by LZ, UIUC
 bond     CXX  NH1           $kbon     1.410  ! defined for DHB and DHA by LZ, UIUC
 bond     CXX  C             $kbon     1.510  ! defined for DHB and DHA by LZ, UIUC

! ANGLES

! based on Turpin paper: RSC Adv 2014, 4, 48621-48631
! New CHARMM force field parameters for dehydrated amnio acid resdies, the key to Lantibiotic Molecular
! dynamic simulation
! added 5/14/2017, L Zhu

 angle    CXX  CXX   C          60.00     120.0   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  CXX   NH1        80.00     128.0   ! defined for DHA and DHB by LZ, UIUC
 angle    C    CXX   NH1        80.00     110.0   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  CXX   HX         45.00     120.5   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  CXX   HXX        45.00     120.5   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  C     NH1        80.00     116.5   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  C     O          80.00     122.5   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  C     N          80.0      119.0   ! defined for DHB-Pro link by LZ, UIUC
 angle    CXX  NH1   C          50.00     120.0   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  NH1   H          34.00     117.0   ! defined for DHA and DHB by LZ, UIUC
 angle    CXX  CXX   CT         43.50     126.5   ! defined for DHB by LZ, UIUC
 angle    HXX  CXX   CT         43.50     118.0   ! defined for DHB by LZ, UIUC
 angle    HX   CXX   HXX        43.50     118.0   ! defined for DHA by LZ, UIUC
 angle    CXX  CT    HA         80.0      109.5   ! defined for DHB by LZ, UIUC

! IMPROPERS based on Turpin paper: RSC Adv 2014, 4, 48621-48631
```

```
! For dihedrals and impropers, the following convention was adopted:
! All dihedral terms maintaining planarity (esp. omega) have been
! converted into impropers. The only dihedrals left are around
! rotatable bonds.

 improper  C    CXX  +NH1  O      $kpla    0    180.0     ! defined for DHA and DHB by LZ, UIUC
 improper  C    CXX  N  O        $kpla    0    180.0     ! defined for DHA and DHB by LZ, UIUC
 improper  CXX  C    NH1  CT      $kpla    0    180.0     ! defined for DHA and DHB, backbone to next resid, by LZ, UIUC
 improper  CXX  C    N    CT     $kback   0    180.0     ! NH peptide planarity, DHB link to PRO, by LZ, UIUC
 improper  HA   HA   CXX  HA     $kchi    0    -66.514     ! defined for DHB by LZ, UIUC
 improper  O    C    NH1  CXX     $kpla     0    0.0      ! CO peptide planarity, front; defined for DHA and DHB by LZ, UIUC
 improper  CT   C    NH1  CXX     $kpla     0    180.0    ! new trans peptide bond; defined for DHA and DHB by LZ, UIUC
 improper  H    NH1  C    CXX     $kpla     0    0.0      ! NH peptide planarity; defined for DHA and DHB by LZ, UIUC
 improper  C    CXX  CXX  CT      $kpla     0    -180.0    ! defined for DHB by LZ, UIUC
 improper  CXX  CXX  C  N     $kpla     0    0.0          ! defined for DHB by LZ, UIUC
 improper  NH1  CXX  CXX  CT       $kpla     0    0.0       ! defined for DHB by LZ, UIUC
 improper  C    CXX  CXX  HX       $kpla     0    -180.0     ! defined for DHA by LZ, UIUC
 improper  C    CXX  CXX  HXX     $kpla     0    0.0       ! defined for DHB by LZ, UIUC
 improper  NH1    CXX  CXX  HX    $kpla     0    0.0       ! defined for DHB by LZ, UIUC
 improper  NH1    CXX  CXX  HXX $kpla     0    180.0      ! defined for DHB by by LZ, UIUC
 improper  CXX  CXX   CT    HXX      $kpla  0   180.0  !defined for DHB by LZ, UIUC
 improper  CXX  CXX   C     O       $kpla  0   180.0  ! defined for DHB and DHA by by LZ, UIUC

! based on Turpin paper: RSC Adv 2014, 4, 48621-48631

 dihedral  H    NH1   CXX    CXX     2.5000  2   180.0  ! defined for DHB and DHA by LZ, UIUC
 dihedral  CXX  CXX   NH1    H       2.5000  2   180.0  ! defined for DHA and DHB by LZ, UIUC
 dihedral  C    CXX   NH1    H      2.5000  2   180.0  ! defined for DHA and DHB by LZ, UIUC
 dihedral  CXX  C     NH1    H      2.5000  2   180.0  ! defined for DHA and DHB by LZ, UIUC
 dihedral  CXX  CXX   NH1    C       0.5000  1   180.0  ! defined for DHA and DHB by LZ, UIUC
 dihedral  CXX  CXX   NH1    C       0.5000  2   0.0    ! defined for DHA and DHB by LZ, UIUC
 dihedral  CXX  CXX   NH1    C       0.2000  3   180.0  ! defined for DHA and DHB by LZ, UIUC
```

```
 improper  C     CXX  NH1  O        120.000  0    0.0     ! defined for DHA and DHB CO peptide planarity, self; by LZ, UIUC
 improper  CXX   CXX  C    NH1      72.000   0     0.0    ! CA chirality, self; defined by LZ, UIUC
 improper  HA   CT   S   CT       $kchi    0   65.977     ! CB chirality; for L-Abu in CyllL/S of ABUS linker (R at CB); defined by LZ,
UIUC
 improper  HA   S   CT   CT       $kchi    0   -65.977    ! CB chirality; for D-Abu of ABS linker (S at CB); defined by LZ, UIUC

 dihedral  CT    CT   S    CT      0.2400   1    180.0  ! chi1 - chi4 defined for ALAS and ABUS; defined by LZ, UIUC
 dihedral  CT    CT   S    CT      0.3700   3    0.0    ! chi1 - chi4 defined for ALAS and ABUS; defined by LZ, UIUC
 dihedral  CT    S    CT   CT      0.2400   1    180.0  ! chi1 - chi4 defined for ALAS and ABUS; defined by LZ, UIUC
 dihedral  CT    S    CT   CT      0.3700   3    0.0    ! chi1 - chi4 defined for ALAS and ABUS; defined by LZ, UIUC
 dihedral  CT    S    CT   HA      0.2800   3    0.0    ! chi1 - chi4 defined for ALAS and ABUS; defined by LZ, UIUC

 dihedral  CT   CT   CT   NH1      $kdih    3    0.0  ! chi1 - chi4, defined for ABU; defined by LZ, UIUC


 NONBonded  CXX      0.1450   3.2072      0.1450   3.2072  ! LZ

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

! NONBONDED

! MolProbity vdw radii.
! (Table 1 in [Word et. al (1999) J. Mol. Biol. 285:1711].)



 nonbonded  HX       0.0045   $S_HH      0.0045   $S_HH   ! defined for DHB and DHA by LZ, UIUC
 nonbonded  HXX      0.0045   $S_HH      0.0045   $S_HH   ! defined for DHB and DHA by LZ, UIUC

!===============================================================================
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