```
mass HX  1.008   ! defined by LZ, UIUC
mass HXX  1.008  !defined by LZ, UIUC
mass CX  12.011  !defined by LZ, UIUC
mass CXX  12.011 !defined by LZ, UIUC

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

residue DALA     ! D-ALA ; defined by LZ, UIUC; PDB ligand name is DAL
 group
   atom N   type=NH1 charge=-0.36 end
   atom HN  type=H   charge= 0.26 end
 group
   atom CA  type=CT  charge= 0.00 end
   atom HA  type=HA  charge= 0.10 end
 group
   atom CB  type=CT  charge=-0.30 end
   atom HB1 type=HA  charge= 0.10 end
   atom HB2 type=HA  charge= 0.10 end
   atom HB3 type=HA  charge= 0.10 end
 group
   atom C   type=C   charge= 0.48 end
   atom O   type=O   charge=-0.48 end

 bond N  HN
 bond N  CA    bond CA  HA
 bond CA  CB   bond CB  HB1   bond CB  HB2     bond CB  HB3
 bond CA  C
 bond C   O

 improper HA C N CB   ! change from L-aa: a N c b, to D-aa: a C N b, stereo CA
 improper HB1 HB2 CA HB3  !stereo CB

end


residue ABU   ! define ABU ; defined by LZ, UIUC; PDB ligand name is ABA
 group
   atom N    type=NH1 charge=-0.36 end
   atom HN   type=H   charge= 0.26 end
 group
   atom CA   type=CT  charge= 0.00 end
   atom HA   type=HA  charge= 0.10 end
 group
   atom CB   type=CT  charge=-0.20 end
```

```
   atom HB1   type=HA  charge= 0.10 end
   atom HB2   type=HA  charge= 0.10 end
 group
   atom CG  type=CT  charge=-0.30 end
   atom HG1 type=HA  charge= 0.10 end
   atom HG2 type=HA  charge= 0.10 end
   atom HG3 type=HA  charge= 0.10 end
 group
   atom C    type=C   charge= 0.48 end
   atom O    type=O   charge=-0.48 end

 bond N   HN
 bond N   CA     bond CA  HA
 bond CA  CB     bond CB  HB1   bond CB HB2
 bond CB  CG    bond CG HG1    bond CG HG2    bond CG HG3
 bond CA  C
 bond C   O

 improper HA N C CB         !stereo CA

 improper HB1 HB2 CA CG     !stereo CB, HA HA CT CT: -78.874 methylene
 improper HG1 HG2 CB HG3    !stereo CG, HA HA CT HA: -66.514 methyl

 dihedral CG CB CA  N       ! dihedral X CT CT X kdih 3 0.0 chi1-chi4, where 3=n, multiplicity,
0.0=phase shift, aleady defined in par file as X CT CT X

end

residue DABU   ! define DABU ; defined by LZ, UIUC; PDB ligand name is DBB
 group
   atom N    type=NH1 charge=-0.36 end
   atom HN   type=H   charge= 0.26 end
 group
   atom CA   type=CT  charge= 0.00 end
   atom HA   type=HA  charge= 0.10 end
 group
   atom CB   type=CT  charge=-0.20 end
   atom HB1   type=HA  charge= 0.10 end
   atom HB2   type=HA  charge= 0.10 end
 group
   atom CG  type=CT  charge=-0.30 end
   atom HG1 type=HA  charge= 0.10 end
   atom HG2 type=HA  charge= 0.10 end
   atom HG3 type=HA  charge= 0.10 end
 group
   atom C    type=C   charge= 0.48 end
```

```
   atom O    type=O   charge=-0.48 end

  bond N   HN
  bond N   CA     bond CA  HA
  bond CA  CB     bond CB  HB1   bond CB HB2
  bond CB  CG    bond CG HG1    bond CG HG2    bond CG HG3
  bond CA  C
  bond C   O

  improper HA C N CB         !stereo CA ! change stero from L-ABU to D-ABU: HA N C CB

  improper HB1 HB2 CA CG     !stereo CB
  improper HG1 HG2 CB HG3    !stereo CG

  dihedral CG CB CA  N

end


residue DHB   ! define DHB; defined by LZ, UIUC; PDB ligand name is DBU
  group
    atom N    type=NH1 charge=-0.670 end
    atom HN   type=H   charge= 0.360 end
    atom CA   type=CXX  charge= 0.310 end
 group
    atom CB   type=CXX  charge=-0.15 end
    atom HB   type=HXX  charge= 0.15 end
 group
    atom CG  type=CT  charge=-0.27 end
    atom HG1 type=HA  charge= 0.090 end
    atom HG2 type=HA  charge= 0.090 end
    atom HG3 type=HA  charge= 0.090 end
 group
    atom C    type=C   charge= 0.635 end
    atom O    type=O   charge=-0.635 end

  bond N   HN
  bond N   CA
  bond CA  CB     bond CB  HB
  bond CB  CG    bond CG HG1    bond CG HG2    bond CG HG3
  bond CA  C
  bond C   O

  improper C CA CB CG
  improper N CA CB CG
  improper N CA CB HB
```

```
  improper C CA CB HB

  DONOR       HN N
  ACCEPTOR O C

end

residue DHA   ! define DHA ; defined by LZ, UIUC
  group
    atom N    type=NH1 charge=-0.670 end
    atom HN   type=H   charge= 0.360 end
    atom CA   type=CXX  charge= 0.310 end
 group
    atom CB   type=CXX  charge=-0.420 end
    atom HB1   type=HX  charge= 0.210 end
    atom HB2   type=HXX  charge= 0.21 end
 group
    atom C    type=C   charge= 0.635 end
    atom O    type=O   charge=-0.635 end

!  double CA CB
  bond N   HN
  bond N   CA
  bond CA  CB     bond CB  HB1  bond CB HB2
  bond CA  C
  bond C   O
!  bond C   +N

  !improper CA CB C N        !stereo CA, Zhu 5/10/2017, based on Turpin's paper
  !improper CA CB C N        !stereo CA, Zhu 5/10/2017, based on Turpin's paper
!  improper C CA +N O        !stereo CA, Zhu 5/10/2017, based on Turpin's paper

  improper N CA CB HB1       !added 6/28/19
  improper N CA CB HB2       !added 6/28/19
  improper C CA CB HB1
  improper C CA CB HB2

  DONOR       HN N
  ACCEPTOR O C

end

presidue ABUS               ! S-link between HB1 of ABU and CYS  ...ABU - S - CYS...
         ! defined by LZ, UIUC
  group
    delete    atom 1HB1             end
```

```
   modify    atom 1CB  charge= 0.10 end  ! to make the new bond charge to zero
  group
   delete    atom 2HG              end
   modify    atom 2SG  charge=-0.10 end   ! make the net charge to zero for the new bond

  add bond 1CB 2SG

  add angle 1CA 1CB 2SG
  add angle 1CB 2SG 2CB
  add angle 1HB2 1CB 2SG  ! 5/9/2017

  add dihedral 1CA 1CB 2SG 2CB  ! Zhu 5/9/2017
  add dihedral 1CB 2SG 2CB 2CA

  !!  add improper LZ  5/8/2020 fix CB stereochemistry of L-LABU to (R)
  improper 1HB2 1CA 2SG 1CG       !!stereo CB for former Ser/Thr residue that is R at CA and
R at CB

end

presidue ABS               ! S-link between HB1 of ABU and CYS  ...ABU - S - CYS...
         ! added by Zhu, L based on DISU 1/2/2015
  group
   delete    atom 1HB1              end
   modify    atom 1CB  charge= 0.10 end  ! to make the new bond charge to zero
  group
   delete    atom 2HG              end
   modify    atom 2SG  charge=-0.10 end   ! make the net charge to zero for the new bond

  add bond 1CB 2SG

  add angle 1CA 1CB 2SG
  add angle 1CB 2SG 2CB
  add angle 1HB2 1CB 2SG  ! 5/9/2017

  add dihedral 1CA 1CB 2SG 2CB  ! Zhu 5/9/2017
  add dihedral 1CB 2SG 2CB 2CA


!!  add improper LZ  5/8/2020 fix CB stereochemistry of D-ABU to (S)
  improper 1HB2 2SG 1CG 1CA       !!stereo CB for former Ser/Thr residue that is S at CA and S
at CB

end

presidue ALAS              ! S-link bet. S link between ALA and CYS with a single -C-S-C-...
```

```
                ! defined by LZ, UIUC
  group
    delete    atom 1HB1              end
    modify    atom 1CB  charge= 0.20 end

  group
    delete    atom 2HG               end
    modify    atom 2SG  charge=-0.20 end

  add bond 1CB 2SG

  add angle 1CB 2SG 2CB
  add angle 1CA 1CB 2SG
  add angle 1HB2 1CB 2SG
  add angle 1HB3 1CB 2SG  ! 5/9/2017

  add dihedral 1CA 1CB 2SG 2CB  ! Zhu 5/9/2017
  add dihedral 1CB 2SG 2CB 2CA

end

!================================================================================
====
```