Appendix

This appendix is essentially a visual representation of the information encoded in the coarse-grain .cgc files, showing how each of the amino acids as well as a POPC lipid is divided into coarse-grained beads. Excerpts from the standard CHARMM topology file are shown with the Martini bead assignments overlaid.

```
RESI ALA          0.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !     |      HB1
ATOM HA   HB      0.09  !     |     /
GROUP                   !  HA-CA--CB-HB2
ATOM CB   CT3    -0.27  !     |     \
ATOM HB1  HA      0.09  !     |      HB3
ATOM HB2  HA      0.09  !   O=C
ATOM HB3  HA      0.09  !     |
GROUP                   !
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  N  HN  N  CA
BOND C  CA  C  +N  CA HA  CB HB1  CB HB2  CB HB3
DOUBLE O  C
```

BAS = P4

```
RESI ARG          1.00
GROUP
ATOM N    NH1    -0.47  !     |                    HH11
ATOM HN   H       0.31  !  HN-N                     |
ATOM CA   CT1     0.07  !     |      HB1 HG1 HD1 HE    NH1-HH12
ATOM HA   HB      0.09  !     |      |   |   |   |   //(+)
GROUP                   !  HA-CA--CB--CG--CD--NE--CZ
ATOM CB   CT2    -0.18  !     |      |   |   |     \
ATOM HB1  HA      0.09  !     |      HB2 HG2 HD2      NH2-HH22
ATOM HB2  HA      0.09  !   O=C                       |
GROUP                   !     |                      HH21
ATOM CG   CT2    -0.18
ATOM HG1  HA      0.09
ATOM HG2  HA      0.09
GROUP
ATOM CD   CT2     0.20
ATOM HD1  HA      0.09
ATOM HD2  HA      0.09
ATOM NE   NC2    -0.70
ATOM HE   HC      0.44
ATOM CZ   C       0.64
ATOM NH1  NC2    -0.80
ATOM HH11 HC      0.46
ATOM HH12 HC      0.46
ATOM NH2  NC2    -0.80
ATOM HH21 HC      0.46
ATOM HH22 HC      0.46
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA  CG  CB  CD CG  NE CD  CZ NE
BOND NH2 CZ  N  HN  N  CA
BOND C   CA  C  +N  CA HA  CB HB1
BOND CB  HB2 CG  HG1 CG HG2 CD HD1 CD HD2
BOND NE  HE  NH1 HH11  NH1 HH12  NH2 HH21  NH2 HH22
DOUBLE O  C    CZ  NH1
```

SI1 = N0r

BAS = P5

SI2 = Qdr

```
RESI ASN          0.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !     |      HB1 OD1    HD21 (cis to OD1)
ATOM HA   HB      0.09  !     |      |   ||    /
GROUP                   !  HA-CA--CB--CG--ND2
ATOM CB   CT2    -0.18  !     |      |         \
ATOM HB1  HA      0.09  !     |      HB2        HD22 (trans to OD1)
ATOM HB2  HA      0.09  !   O=C
GROUP                   !     |
ATOM CG   CC      0.55
ATOM OD1  O      -0.55
GROUP
ATOM ND2  NH2    -0.62
ATOM HD21 H       0.32
ATOM HD22 H       0.30
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  CG CB   ND2 CG
BOND N  HN  N  CA   C   CA   C +N
BOND CA HA  CB HB1  CB  HB2  ND2 HD21  ND2 HD22
DOUBLE C  O   CG  OD1
```

SID = P5n

BAS = P5

```
RESI ASP         -1.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !     |      HB1   OD1
ATOM HA   HB      0.09  !     |      |     //
GROUP                   !  HA-CA--CB--CG
ATOM CB   CT2    -0.28  !     |      |     \
ATOM HB1  HA      0.09  !     |      HB2   OD2(-)
ATOM HB2  HA      0.09  !   O=C
ATOM CG   CC      0.62  !     |
ATOM OD1  OC     -0.76
ATOM OD2  OC     -0.76
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  CG CB  OD2 CG
BOND N  HN  N  CA   C   CA  C +N
BOND CA HA  CB HB1  CB HB2
DOUBLE  O   C   CG  OD1
```

SID = Qad

BAS = P5

```
RESI CYS          0.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !     |      HB1
ATOM HA   HB      0.09  !     |      |
GROUP                   !  HA-CA--CB--SG
ATOM CB   CT2    -0.11  !     |      |     \
ATOM HB1  HA      0.09  !     |      HB2    HG1
ATOM HB2  HA      0.09  !   O=C
ATOM SG   S      -0.23  !     |
ATOM HG1  HS      0.16
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA   SG CB   N HN  N  CA
BOND C  CA   C +N  CA HA  CB HB1
BOND CB HB2  SG HG1
DOUBLE O  C
```

SID = C5c

BAS = P5

```
RESI GLN          0.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  !  HN-N
ATOM CA   CT1     0.07  !     |      HB1 HG1 OE1   HE21 (cis to OE1)
ATOM HA   HB      0.09  !     |      |   |   ||    /
GROUP                   !  HA-CA--CB--CG--CD--NE2
ATOM CB   CT2    -0.18  !     |      |   |         \
ATOM HB1  HA      0.09  !     |      HB2 HG2       HE22 (trans to OE1)
ATOM HB2  HA      0.09  !   O=C
GROUP                   !     |
ATOM CG   CT2    -0.18
ATOM HG1  HA      0.09
ATOM HG2  HA      0.09
GROUP
ATOM CD   CC      0.55
ATOM OE1  O      -0.55
GROUP
ATOM NE2  NH2    -0.62
ATOM HE21 H       0.32
ATOM HE22 H       0.30
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  CG  CB   CD  CG   NE2 CD
BOND N  HN  N   CA   C   CA
BOND C  +N  CA  HA   CB  HB1  CB  HB2  CG HG1
BOND CG HG2 NE2 HE21 NE2 HE22
DOUBLE O  C    CD  OE1
```

BAS = P5

SID = P4q

```
RESI GLU          -1.00
GROUP
ATOM N    NH1    -0.47  !      |
ATOM HN   H       0.31  !   HN-N
ATOM CA   CT1     0.07  !      |      HB1 HG1   OE1
ATOM HA   HB      0.09  !      |      |   |    //
GROUP                   !   HA-CA--CB--CG--CD
ATOM CB   CT2    -0.18  !      |      |   |    \
ATOM HB1  HA      0.09  !      |      HB2 HG2   OE2(-)
ATOM HB2  HA      0.09  !    O=C
GROUP                   !      |
ATOM CG   CT2    -0.28
ATOM HG1  HA      0.09
ATOM HG2  HA      0.09
ATOM CD   CC      0.62
ATOM OE1  OC     -0.76
ATOM OE2  OC     -0.76
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  CG CB  CD CG  OE2 CD
BOND N  HN  N  CA C   CA
BOND C  +N  CA HA  CB HB1 CB  HB2 CG  HG1
BOND CG HG2
DOUBLE O  C   CD  OE1
```

BAS = P5

SID = Qae

```
RESI GLY          0.00
GROUP
ATOM N    NH1    -0.47  !      |
ATOM HN   H       0.31  !      N-H
ATOM CA   CT2    -0.02  !      |
ATOM HA1  HB      0.09  !      |
ATOM HA2  HB      0.09  !   HA1-CA-HA2
GROUP                   !      |
ATOM C    C       0.51  !      |
ATOM O    O      -0.51  !      C=O
                        !      |
BOND N HN  N  CA  C CA
BOND C +N  CA HA1 CA HA2
DOUBLE O  C
```

BAS = P5

```
RESI HSD          0.00  ! neutral HIS, proton on ND1
GROUP
ATOM N    NH1    -0.47  !      |          HD1    HE1
ATOM HN   H       0.31  !   HN-N           |     /
ATOM CA   CT1     0.07  !      |      HB1   ND1--CE1
ATOM HA   HB      0.09  !      |      |     /     ||
GROUP                   !   HA-CA--CB--CG      ||
ATOM CB   CT2    -0.09  !      |      ||\\     ||
ATOM HB1  HA      0.09  !      |      HB2   CD2--NE2
ATOM HB2  HA      0.09  !    O=C             |
ATOM ND1  NR1    -0.36  !      |             HD2
ATOM HD1  H       0.32
ATOM CG   CPH1   -0.05
GROUP
ATOM CE1  CPH2    0.25
ATOM HE1  HR1     0.13
ATOM NE2  NR2    -0.70
ATOM CD2  CPH1    0.22
ATOM HD2  HR3     0.10
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG  CB   ND1 CG   CE1 ND1
BOND NE2 CD2  N   HN   N   CA
BOND C   CA   C   +N   CA  HA   CB  HB1
BOND CB  HB2  ND1 HD1  CD2 HD2  CE1 HE1
DOUBLE O  C   CG  CD2   CE1  NE2
```

SI3 = SP1h

SI1 = SC4h

BAS = P5

SI2 = SP1h

```
RESI HSE          0.00  ! neutral His, proton on NE2
GROUP
ATOM N    NH1    -0.47  !      |          HE1
ATOM HN   H       0.31  !   HN-N           __  /
ATOM CA   CT1     0.07  !      |      HB1   ND1--CE1
ATOM HA   HB      0.09  !      |      |     /     ||
GROUP                   !   HA-CA--CB--CG      ||
ATOM CB   CT2    -0.08  !      |      ||\\     ||
ATOM HB1  HA      0.09  !      |      HB2   CD2--NE2
ATOM HB2  HA      0.09  !    O=C             |
ATOM ND1  NR2    -0.70  !      |             HD2    HE2
ATOM CG   CPH1    0.22
ATOM CE1  CPH2    0.25
ATOM HE1  HR1     0.13
GROUP
ATOM NE2  NR1    -0.36
ATOM HE2  H       0.32
ATOM CD2  CPH1   -0.05
ATOM HD2  HR3     0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG  CB   ND1 CG
BOND NE2 CD2  N   HN   N   CA
BOND C   CA   C   +N   NE2 CE1  CA  HA   CB HB1
BOND CB  HB2  NE2 HE2  CD2 HD2  CE1 HE1
DOUBLE   O   C   CD2 CG   CE1 ND1
```

SI3 = SP1h

SI1 = SC4h

BAS = P5

SI2 = SP1h

```
RESI HSP          1.00  ! Protonated His
GROUP
ATOM N    NH1    -0.47  !      |          HD1    HE1
ATOM HN   H       0.31  !   HN-N           |     /
ATOM CA   CT1     0.07  !      |      HB1   ND1--CE1
ATOM HA   HB      0.09  !      |      |     /     ||
GROUP                   !   HA-CA--CB--CG      ||
ATOM CB   CT2    -0.05  !      |      ||\\     ||
ATOM HB1  HA      0.09  !      |      HB2   CD2--NE2(+)
ATOM HB2  HA      0.09  !    O=C             |
ATOM CD2  CPH1    0.19  !      |             HD2    HE2
ATOM HD2  HR1     0.13
ATOM CG   CPH1    0.19
GROUP
ATOM NE2  NR3    -0.51
ATOM HE2  H       0.44
ATOM ND1  NR3    -0.51
ATOM HD1  H       0.44
ATOM CE1  CPH2    0.32
ATOM HE1  HR2     0.18
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG  CB   ND1 CG   CE1 ND1
BOND NE2 CD2  N   HN   N   CA
BOND C   CA   C   +N  CA  HA  CB HB1
BOND CB  HB2  ND1 HD1  NE2 HE2  CD2 HD2 CE1 HE1
DOUBLE  O   C   CD2 CG     NE2 CE1
```

BAS = P5

SID = AC1i

```
RESI ILE          0.00
GROUP
ATOM N    NH1    -0.47  !      |      HG21 HG22
ATOM HN   H       0.31  !   HN-N       | /
ATOM CA   CT1     0.07  !      |      CG2--HG23
ATOM HA   HB      0.09  !      |     /
GROUP                   !   HA-CA--CB-HB    HD1
ATOM CB   CT1    -0.09  !      |      \       /
ATOM HB   HA      0.09  !      |      CG1--CD--HD2
GROUP                   !    O=C     / \     \
ATOM CG2  CT3    -0.27  !      |    HG11 HG12  HD3
ATOM HG21 HA      0.09
ATOM HG22 HA      0.09
ATOM HG23 HA      0.09
GROUP
ATOM CG1  CT2    -0.18
ATOM HG11 HA      0.09
ATOM HG12 HA      0.09
GROUP
ATOM CD   CT3    -0.27
ATOM HD1  HA      0.09
ATOM HD2  HA      0.09
ATOM HD3  HA      0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG1 CB   CG2 CB   CD  CG1
BOND N   HN   N   CA    C   CA   C   +N
BOND CA  HA   CB  HB   CG1 HG11 CG1 HG12 CG2 HG21
BOND CG2 HG22 CG2 HG23 CD  HD1  CD  HD2  CD  HD3
DOUBLE  O   C
```

```
RESI LEU          0.00
GROUP
ATOM N    NH1    -0.47  !     |          HD11 HD12
ATOM HN   H       0.31  ! HN-N            | /
ATOM CA   CT1     0.07  !    |    HB1   CD1--HD13
ATOM HA   HB      0.09  !    |    |    /
GROUP                   ! HA-CA--CB--CG-HG
ATOM CB   CT2    -0.18  !    |    |    \
ATOM HB1  HA      0.09  !    |    HB2   CD2--HD23
ATOM HB2  HA      0.09  !  O=C              | \
GROUP                   !    |          HD21 HD22
ATOM CG   CT1    -0.09
ATOM HG   HA      0.09
GROUP
ATOM CD1  CT3    -0.27
ATOM HD11 HA      0.09
ATOM HD12 HA      0.09
ATOM HD13 HA      0.09
GROUP
ATOM CD2  CT3    -0.27
ATOM HD21 HA      0.09
ATOM HD22 HA      0.09
ATOM HD23 HA      0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG  CB   CD1 CG   CD2 CG
BOND N   HN   N   CA    C   CA   C +N
BOND CA  HA   CB  HB1  CB  HB2  CG  HG   CD1 HD11
BOND CD1 HD12 CD1 HD13 CD2 HD21 CD2 HD22 CD2 HD23
DOUBLE   O   C
```

BAS = P5

SID = AC1l

```
RESI LYS          1.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  ! HN-N
ATOM CA   CT1     0.07  !    |    HB1 HG1 HD1 HE1    HZ1
ATOM HA   HB      0.09  !    |    |   |   |   |     /
GROUP                   ! HA-CA--CB--CG--CD--CE--NZ--HZ2
ATOM CB   CT2    -0.18  !    |    |   |   |   |     \
ATOM HB1  HA      0.09  !    |    HB2 HG2 HD2 HE2    HZ3
ATOM HB2  HA      0.09  !  O=C
GROUP                   !    |
ATOM CG   CT2    -0.18
ATOM HG1  HA      0.09
ATOM HG2  HA      0.09
GROUP
ATOM CD   CT2    -0.18
ATOM HD1  HA      0.09
ATOM HD2  HA      0.09
GROUP
ATOM CE   CT2     0.21
ATOM HE1  HA      0.05
ATOM HE2  HA      0.05
ATOM NZ   NH3    -0.30
ATOM HZ1  HC      0.33
ATOM HZ2  HC      0.33
ATOM HZ3  HC      0.33
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA   CG CB   CD CG   CE CD   NZ CE
BOND N  HN   N  CA    C  CA
BOND C  +N   CA HA   CB HB1  CB HB2  CG HG1
BOND CG HG2  CD HD1  CD HD2  CE HE1  CE HE2
DOUBLE   O  C
BOND NZ HZ1  NZ HZ2  NZ HZ3
```

SI1 = C3k

SI2 = Qdk

BAS = P5

```
RESI MET          0.00
GROUP
ATOM N    NH1    -0.47  !     |
ATOM HN   H       0.31  ! HN-N
ATOM CA   CT1     0.07  !    |    HB1 HG1     HE1
ATOM HA   HB      0.09  !    |    |   |       |
GROUP                   ! HA-CA--CB--CG--SD--CE--HE3
ATOM CB   CT2    -0.18  !    |    |   |       |
ATOM HB1  HA      0.09  !    |    HB2 HG2     HE2
ATOM HB2  HA      0.09  !  O=C
GROUP                   !    |
ATOM CG   CT2    -0.14
ATOM HG1  HA      0.09
ATOM HG2  HA      0.09
ATOM SD   S      -0.09
ATOM CE   CT3    -0.22
ATOM HE1  HA      0.09
ATOM HE2  HA      0.09
ATOM HE3  HA      0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA   CG CB   SD CG   CE SD
BOND N  HN   N  CA    C  CA   C  +N
BOND CA HA   CB HB1  CB HB2  CG HG1  CG HG2
BOND CE HE1  CE HE2  CE HE3
DOUBLE   O  C
```

BAS = P5

SID = C5m

```
RESI PRO          0.00
GROUP                   !       HD1 HD2
ATOM N    N      -0.29  !     |   \ /
ATOM CD   CP3     0.00  !    N---CD   HG1
ATOM HD1  HA      0.09  !    |     \  /
ATOM HD2  HA      0.09  !    |      CG
ATOM CA   CP1     0.02  !    |     /  \
ATOM HA   HB      0.09  ! HA-CA--CB   HG2
GROUP                   !    |    / \
ATOM CB   CP2    -0.18  !    |  HB1 HB2
ATOM HB1  HA      0.09  ! O=C
ATOM HB2  HA      0.09  !   |
GROUP
ATOM CG   CP2    -0.18
ATOM HG1  HA      0.09
ATOM HG2  HA      0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND C  CA  C   +N
BOND N  CA  CA  CB  CB  CG  CG  CD  N   CD
BOND HA CA  HG1 CG  HG2 CG  HD1 CD  HD2 CD  HB1 CB  HB2 CB
DOUBLE   O  C
```

SID = AC2p

BAS = P5

```
RESI PHE          0.00
GROUP
ATOM N    NH1    -0.47  !     |          HD1  HE1
ATOM HN   H       0.31  ! HN-N            |    |
ATOM CA   CT1     0.07  !    |    HB1  CD1--CE1
ATOM HA   HB      0.09  !    |    |   //      \\
GROUP                   ! HA-CA--CB--CG        CZ--HZ
ATOM CB   CT2    -0.18  !    |    |   \\      //
ATOM HB1  HA      0.09  !    |    HB2  CD2--CE2
ATOM HB2  HA      0.09  !  O=C             |    |
GROUP                   !    |           HD2  HE2
ATOM CG   CA      0.00
GROUP
ATOM CD1  CA     -0.115
ATOM HD1  HP      0.115
GROUP
ATOM CE1  CA     -0.115
ATOM HE1  HP      0.115
GROUP
ATOM CZ   CA     -0.115
ATOM HZ   HP      0.115
GROUP
ATOM CD2  CA     -0.115
ATOM HD2  HP      0.115
GROUP
ATOM CE2  CA     -0.115
ATOM HE2  HP      0.115
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG CB   CD2 CG   CE1 CD1
BOND CZ  CE2  N   HN
BOND N   CA    C   CA   C   +N   CA  HA
BOND CB  HB1  CB HB2  CD1 HD1  CD2 HD2  CE1 HE1
DOUBLE   O  C    CD1 CG  CZ CE1   CE2 CD2
BOND CE2 HE2  CZ HZ
```

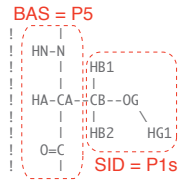
SI1 = SC4f

SI3 = SC4f

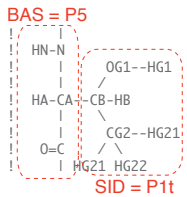
SI2 = SC4f

BAS = P5

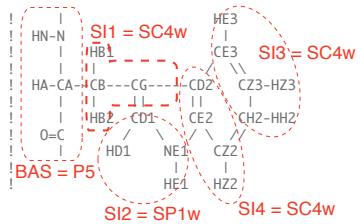
```
RESI SER          0.00
GROUP
ATOM N    NH1    -0.47  !
ATOM HN   H       0.31  !
ATOM CA   CT1     0.07  !
ATOM HA   HB      0.09  !
GROUP                   !
ATOM CB   CT2     0.05  !
ATOM HB1  HA      0.09  !
ATOM HB2  HA      0.09  !
ATOM OG   OH1    -0.66  !
ATOM HG1  H       0.43
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA   OG CB  N HN  N  CA
BOND C  CA  C +N  CA HA  CB HB1
BOND CB HB2  OG HG1
DOUBLE   O  C
```



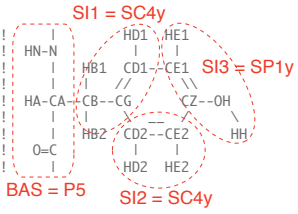

```
RESI THR          0.00
GROUP
ATOM N    NH1    -0.47  !
ATOM HN   H       0.31  !
ATOM CA   CT1     0.07  !
ATOM HA   HB      0.09  !
GROUP                   !
ATOM CB   CT1     0.14  !
ATOM HB   HA      0.09  !
ATOM OG1  OH1    -0.66  !
ATOM HG1  H       0.43  !
GROUP
ATOM CG2  CT3    -0.27
ATOM HG21 HA      0.09
ATOM HG22 HA      0.09
ATOM HG23 HA      0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB CA  OG1 CB   CG2 CB    N   HN
BOND N  CA    C   CA    C   +N    CA  HA
BOND CB HB  OG1 HG1  CG2 HG21  CG2 HG22  CG2 HG23
DOUBLE  O   C
```



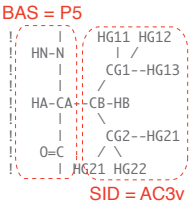

```
RESI TRP          0.00
GROUP
ATOM N    NH1    -0.47  !
ATOM HN   H       0.31  !
ATOM CA   CT1     0.07  !
ATOM HA   HB      0.09  !
GROUP                   !
ATOM CB   CT2    -0.18  !
ATOM HB1  HA      0.09  !
ATOM HB2  HA      0.09  !
GROUP                   !
ATOM CG   CY     -0.03  !
ATOM CD1  CA      0.035 !
ATOM HD1  HP      0.115
ATOM NE1  NY     -0.61
ATOM HE1  H       0.38
ATOM CE2  CPT     0.13
ATOM CD2  CPT    -0.02
GROUP
ATOM CE3  CA     -0.115
ATOM HE3  HP      0.115
GROUP
ATOM CZ3  CA     -0.115
ATOM HZ3  HP      0.115
GROUP
ATOM CZ2  CA     -0.115
ATOM HZ2  HP      0.115
GROUP
ATOM CH2  CA     -0.115
ATOM HH2  HP      0.115
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG  CB   CD2 CG   NE1 CD1
BOND CZ2 CE2
BOND N   HN   N   CA    C   CA   C   +N
BOND CZ3 CH2  CD2 CE3  NE1 CE2  CA  HA   CB  HB1
BOND CB  HB2  CD1 HD1  NE1 HE1  CE3 HE3  CZ2 HZ2
BOND CZ3 HZ3  CH2 HH2
DOUBLE  O   C   CD1 CG   CE2 CD2  CZ3 CE3  CH2 CZ2
```

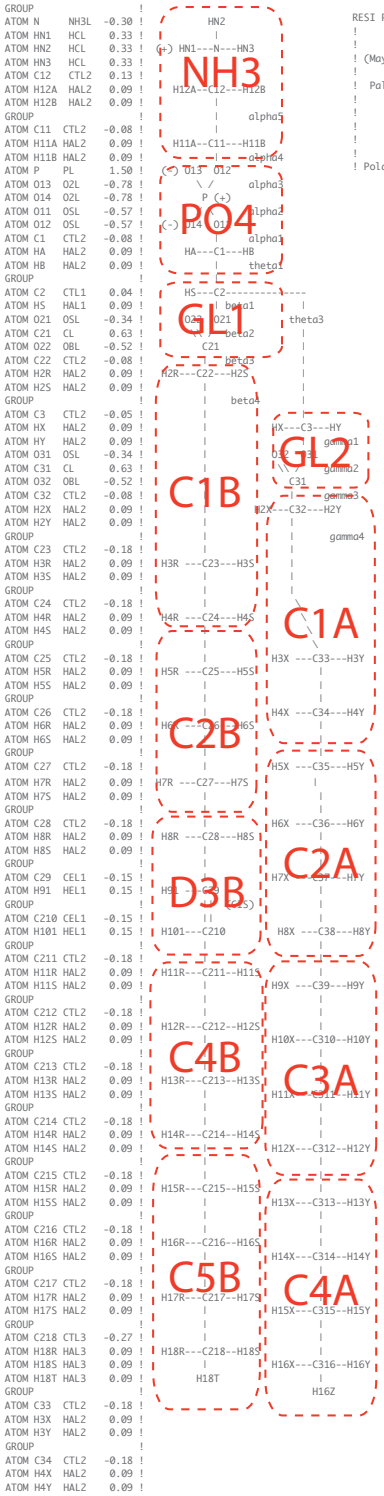



```
RESI TYR          0.00
GROUP
ATOM N    NH1    -0.47  !
ATOM HN   H       0.31  !
ATOM CA   CT1     0.07  !
ATOM HA   HB      0.09  !
GROUP                   !
ATOM CB   CT2    -0.18  !
ATOM HB1  HA      0.09  !
ATOM HB2  HA      0.09  !
GROUP                   !
ATOM CG   CA      0.00
GROUP
ATOM CD1  CA     -0.115
ATOM HD1  HP      0.115
GROUP
ATOM CE1  CA     -0.115
ATOM HE1  HP      0.115
GROUP
ATOM CZ   CA      0.11
ATOM OH   OH1    -0.54
ATOM HH   H       0.43
GROUP
ATOM CD2  CA     -0.115
ATOM HD2  HP      0.115
GROUP
ATOM CE2  CA     -0.115
ATOM HE2  HP      0.115
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA   CG  CB   CD2 CG   CE1 CD1
BOND CZ  CE2  OH  CZ
BOND N   HN   N   CA    C   CA   C   +N
BOND CA  HA   CB  HB1  CB  HB2  CD1 HD1  CD2 HD2
BOND CE1 HE1  CE2 HE2  OH  HH
DOUBLE   O   C   CD1 CG  CE1  CZ  CE2 CD2
```




```
RESI VAL          0.00
GROUP
ATOM N    NH1    -0.47  !
ATOM HN   H       0.31  !
ATOM CA   CT1     0.07  !
ATOM HA   HB      0.09  !
GROUP                   !
ATOM CB   CT1    -0.09  !
ATOM HB   HA      0.09  !
GROUP                   !
ATOM CG1  CT3    -0.27  !
ATOM HG11 HA      0.09
ATOM HG12 HA      0.09
ATOM HG13 HA      0.09
GROUP
ATOM CG2  CT3    -0.27
ATOM HG21 HA      0.09
ATOM HG22 HA      0.09
ATOM HG23 HA      0.09
GROUP
ATOM C    C       0.51
ATOM O    O      -0.51
BOND CB  CA    CG1 CB    CG2 CB    N   HN
BOND N   CA     C   CA    C   +N    CA HA
BOND CB  HB    CG1 HG11  CG1 HG12  CG1 HG13  CG2 HG21
BOND CG2 HG22  CG2 HG23
DOUBLE   O   C
```






```
RESI POPE         0.00 ! 1-palmytoil-2-oleoyl-sn-glycero-
!                        3-Phosphatidylethanolamine
!
! (May 14, 1999 Carlos F. Lopez)
!
!  Palmytoil - CH2
!              |
!      Oleyl - CH
!              |
!              CH2 - PO4 - CH2 - CH2 - NH3
!
! Polar Head and glycerol backbone
```