Supplementary Material (ESI) for Molecular BioSystems

The Binding of Vitamin B_{12} to Transcobalamin(II); Structural Considerations for Bioconjugate Design – a Molecular Dynamics Study

Damian G. Allis[a], Timothy J. Fairchild[b], and Robert P. Doyle[a]

GROMOS96 Force Field Topologies and employed atomic charges for:

B12 (cobalamin)
LYB (cobalamin with the ribose 5'-hydroxy-amide bond-lysine residue)
BCN (cyanocobalamin, CN-Cbl)
LCB (cyanocobalamin, CN-Cbl with the ribose 5'-hydroxy-amide bond-lysine residue)

```
[ B12 ]
[ atoms ]
C27     C       0.38000     0    ;  from GLN residue
O28     O      -0.38000     0    ;  from GLN residue
N29     NT     -0.83000     0    ;  from GLN residue
HAE     H       0.41500     0    ;  from GLN residue
HAD     H       0.41500     0    ;  from GLN residue
C32     C       0.38000     1    ;  from GLN residue
O34     O      -0.38000     1    ;  from GLN residue
N33     NT     -0.83000     1    ;  from GLN residue
HAG     H       0.41500     1    ;  from GLN residue
HAF     H       0.41500     1    ;  from GLN residue
C38     C       0.38000     2    ;  from GLN residue
O39     O      -0.38000     2    ;  from GLN residue
N40     NT     -0.83000     2    ;  from GLN residue
HAI     H       0.41500     2    ;  from GLN residue
HAH     H       0.41500     2    ;  from GLN residue
C43     C       0.38000     3    ;  from GLN residue
O44     O      -0.38000     3    ;  from GLN residue
N45     NT     -0.83000     3    ;  from GLN residue
HAK     H       0.41500     3    ;  from GLN residue
HAJ     H       0.41500     3    ;  from GLN residue
C50     C       0.38000     4    ;  from GLN residue
O51     O      -0.38000     4    ;  from GLN residue
N52     NT     -0.83000     4    ;  from GLN residue
HAM     H       0.41500     4    ;  from GLN residue
HAL     H       0.41500     4    ;  from GLN residue
C61     C       0.38000     5    ;  from GLN residue
O63     O      -0.38000     5    ;  from GLN residue
N62     NT     -0.83000     5    ;  from GLN residue
HAO     H       0.41500     5    ;  from GLN residue
HAN     H       0.41500     5    ;  from GLN residue
C20     CH3     0.00000     6    ;  methyl group
C25     CH3     0.00000     7    ;  methyl group
C36     CH3     0.00000     8    ;  methyl group
C46     CH3     0.00000     9    ;  methyl group
C47     CH3     0.00000     10   ;  methyl group
C54     CH3     0.00000     11   ;  methyl group
C26     CH2     0.00000     12   ;  non-polar CHn fragments
C30     CH2     0.00000     13   ;  non-polar CHn fragments
C31     CH2     0.00000     13   ;  non-polar CHn fragments
C37     CH2     0.00000     14   ;  non-polar CHn fragments
C41     CH2     0.00000     15   ;  non-polar CHn fragments
C42     CH2     0.00000     15   ;  non-polar CHn fragments
C48     CH2     0.00000     16   ;  non-polar CHn fragments
C49     CH2     0.00000     16   ;  non-polar CHn fragments
C56     CH2     0.00000     17   ;  non-polar CHn fragments
C55     CH2     0.00000     17   ;  non-polar CHn fragments
C60     CH2     0.00000     18   ;  non-polar CHn fragments
C2R     CH1     0.15000     19   ;  C2*-O2*-H2* from ADE
O7R     OA     -0.54800     19   ;  C2*-O2*-H2* from ADE
HAA     H       0.39800     19   ;  C2*-O2*-H2* from ADE
C1R     CH1     0.20000     20   ;  C1*-O4*-C4* from ADE
O6R     OA     -0.36000     20   ;  C1*-O4*-C4* from ADE
C4R     CH1     0.16000     20   ;  C1*-O4*-C4* from ADE
C3R     CH1     0.00000     21   ;  C3* from ADE
C5R     CH2     0.15000     22   ;  C2*-O2*-H2* from ADE
O8R     OA     -0.54800     22   ;  C2*-O2*-H2* from ADE
```

```
 HAB     H        0.39800     22   ;  C2*-O2*-H2* from ADE
 P       P        2.20000     23   ;  PO3+O3* fragment from ADE
 O2      OA      -0.80000     23   ;  PO3+O3* fragment from ADE
 O4      OM      -1.00000     23   ;  PO3+O3* fragment from ADE
 O5      OM      -1.00000     23   ;  PO3+O3* fragment from ADE
 O3      OA      -0.80000     23   ;  PO3+O3* fragment from ADE
 C2P     CH1      0.35000     24   ;  non-polar CHn fragment
 C3P     CH3      0.00000     24   ;  non-polar CHn fragment
 C1P     CH2      0.00000     24   ;  non-polar CHn fragment
 N59     N       -0.28000     25   ;  tempered GLN fragment charges
 HAC     H        0.28000     25   ;  tempered GLN fragment charges
 C57     C        0.38000     25   ;  tempered GLN fragment charges
 O58     O       -0.38000     25   ;  tempered GLN fragment charges
 C5B     C        0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C5M     CH3      0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6B     C        0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6M     CH3      0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C4B     C       -0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H4B     H        0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C7B     C       -0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H7B     H        0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 N3B     NR      -0.55000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 C9B     C        0.20000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 N1B     NR      -0.30000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C8B     C        0.20000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C2B     C        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H2B     H        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C5      C       -0.05000     33   ;  C-CH3 group (non-polar)
 C35     CH3      0.00000     33   ;  C-CH3 group (non-polar)
 C15     C       -0.05000     34   ;  C-CH3 group (non-polar)
 C53     CH3      0.00000     34   ;  C-CH3 group (non-polar)
 FE      FE       0.62000     35   ;  HEMC Fe-N group
 N21     NR      -0.44000     35   ;  HEMC Fe-N group
 N22     NR      -0.50000     35   ;  HEMC Fe-N group
 N23     NR      -0.50000     35   ;  HEMC Fe-N group
 N24     NR      -0.44000     35   ;  HEMC Fe-N group
 C1      CH0      0.22000     36   ;  non-polar HEMC-derived corrin atoms
 C2      CH0      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C3      CH1      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C4      C        0.38000     36   ;  non-polar HEMC-derived corrin atoms
 C6      C        0.29000     37   ;  non-polar HEMC-derived corrin atoms
 C7      CH0      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C8      CH1      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C9      C        0.35000     37   ;  non-polar HEMC-derived corrin atoms
 C16     C        0.38000     38   ;  non-polar HEMC-derived corrin atoms
 C17     CH0      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C18     CH1      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C19     CH1      0.24000     38   ;  non-polar HEMC-derived corrin atoms
 C11     C        0.35000     39   ;  non-polar HEMC-derived corrin atoms
 C12     CH0      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C13     CH1      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C14     C        0.29000     39   ;  non-polar HEMC-derived corrin atoms
 C10     C       -0.24000     40   ;  aromatic C-H from TRP, PHE
 H10     H        0.14000     40   ;  aromatic C-H from TRP, PHE
;
; Since CO is not defined as an atom in GROMOSxx, CO is converted to FE and the HEME
; values are employed.  This is a workaround due for proper implementation.
;
[ bonds ]
;  ai    aj    gromos type
   C26   C27    gb_27   ;  from GLN fragment 0
   C27   O28    gb_5    ;  from GLN
   C27   N29    gb_9    ;  from GLN
   N29   HAE    gb_2    ;  from GLN
   N29   HAD    gb_2    ;  from GLN
   C31   C32    gb_27   ;  from GLN fragment 1
   C32   O34    gb_5    ;  from GLN
   C32   N33    gb_9    ;  from GLN
   N33   HAG    gb_2    ;  from GLN
   N33   HAF    gb_2    ;  from GLN
   C37   C38    gb_27   ;  from GLN fragment 2
   C38   O39    gb_5    ;  from GLN
   C38   N40    gb_9    ;  from GLN
   N40   HAI    gb_2    ;  from GLN
   N40   HAH    gb_2    ;  from GLN
   C42   C43    gb_27   ;  from GLN fragment 3
   C43   O44    gb_5    ;  from GLN
   C43   N45    gb_9    ;  from GLN
   N45   HAK    gb_2    ;  from GLN
   N45   HAJ    gb_2    ;  from GLN
   C49   C50    gb_27   ;  from GLN fragment 4
```

```
C50   O51   gb_5    ;  from GLN
C50   N52   gb_9    ;  from GLN
N52   HAM   gb_2    ;  from GLN
N52   HAL   gb_2    ;  from GLN
C60   C61   gb_27   ;  from GLN fragment 5
C61   O63   gb_5    ;  from GLN
C61   N62   gb_9    ;  from GLN
N62   HAO   gb_2    ;  from GLN
N62   HAN   gb_2    ;  from GLN
FE    N21   gb_35   ;  FE-N bond from HEMC
FE    N22   gb_35   ;  FE-N bond from HEMC
FE    N23   gb_35   ;  FE-N bond from HEMC
FE    N24   gb_35   ;  FE-N bond from HEMC
FE    N3B   gb_37   ;  FE-N3B bond from HEMC not in corrin ring
P     O2    gb_28   ;  from ADE phosphate
P     O4    gb_24   ;  from ADE phosphate
P     O5    gb_24   ;  from ADE phosphate
P     O3    gb_28   ;  from ADE phosphate
N21   C1    gb_21   ;  corrin ring N-CHn bonds
N21   C4    gb_14   ;  corrin ring N-C bonds
N22   C6    gb_14   ;  corrin ring N-C bonds
N22   C9    gb_14   ;  corrin ring N-C bonds
N23   C11   gb_14   ;  corrin ring N-C bonds
N23   C14   gb_14   ;  corrin ring N-C bonds
N24   C16   gb_14   ;  corrin ring N-C bonds
N24   C19   gb_21   ;  corrin ring N-CHn bonds
C30   C31   gb_27   ;  CH2-CH2 bonds
C41   C42   gb_27   ;  CH2-CH2 bonds
C48   C49   gb_27   ;  CH2-CH2 bonds
C55   C56   gb_27   ;  CH2-CH2 bonds
C56   C57   gb_27   ;  CH2-CH2 bonds
N1B   C1R   gb_22   ;  sugar bonds from ADE
C1R   C2R   gb_26   ;  sugar bonds from ADE
C2R   O7R   gb_20   ;  sugar bonds from ADE
O7R   HAA   gb_1    ;  sugar bonds from ADE
C2R   C3R   gb_26   ;  sugar bonds from ADE
C3R   C4R   gb_26   ;  sugar bonds from ADE
C3R   O2    gb_20   ;  sugar bonds from ADE
C4R   C5R   gb_26   ;  sugar bonds from ADE
C5R   O8R   gb_20   ;  sugar bonds from ADE
O8R   HAB   gb_1    ;  sugar bonds from ADE
C4R   O6R   gb_20   ;  sugar bonds from ADE
O6R   C1R   gb_20   ;  sugar bonds from ADE
C1P   N59   gb_9    ;  amide corrin - phosphate linkage
C1P   C2P   gb_27   ;  amide corrin - phosphate linkage
C2P   C3P   gb_27   ;  amide corrin - phosphate linkage
C2P   O3    gb_20   ;  amide corrin - phosphate linkage
N59   HAC   gb_2    ;  amide corrin - phosphate linkage
N59   C57   gb_9    ;  amide corrin - phosphate linkage
C57   O58   gb_5    ;  amide corrin - phosphate linkage
N1B   C2B   gb_10   ;  dimethylbenzimidazole ring
C2B   N3B   gb_10   ;  dimethylbenzimidazole ring
C2B   H2B   gb_3    ;  dimethylbenzimidazole ring
N3B   C9B   gb_10   ;  dimethylbenzimidazole ring
C9B   C4B   gb_16   ;  dimethylbenzimidazole ring
C4B   C5B   gb_16   ;  dimethylbenzimidazole ring
C4B   H4B   gb_3    ;  dimethylbenzimidazole ring
C5B   C6B   gb_16   ;  dimethylbenzimidazole ring
C5B   C5M   gb_27   ;  dimethylbenzimidazole ring
C6B   C7B   gb_16   ;  dimethylbenzimidazole ring
C6B   C6M   gb_27   ;  dimethylbenzimidazole ring
C7B   C8B   gb_16   ;  dimethylbenzimidazole ring
C7B   H7B   gb_3    ;  dimethylbenzimidazole ring
C8B   N1B   gb_10   ;  dimethylbenzimidazole ring
C8B   C9B   gb_16   ;  dimethylbenzimidazole ring
C1    C20   gb_27   ;  corrin ring carbon framework
C1    C2    gb_27   ;  corrin ring carbon framework
C2    C3    gb_27   ;  corrin ring carbon framework
C2    C25   gb_27   ;  corrin ring carbon framework
C2    C26   gb_27   ;  corrin ring carbon framework
C3    C4    gb_27   ;  corrin ring carbon framework
C3    C30   gb_27   ;  corrin ring carbon framework
C4    C5    gb_17   ;  corrin ring carbon framework
C5    C6    gb_17   ;  corrin ring carbon framework
C5    C35   gb_27   ;  corrin ring carbon framework
C6    C7    gb_27   ;  corrin ring carbon framework
C7    C8    gb_27   ;  corrin ring carbon framework
C7    C37   gb_27   ;  corrin ring carbon framework
C7    C36   gb_27   ;  corrin ring carbon framework
C8    C9    gb_27   ;  corrin ring carbon framework
C8    C41   gb_27   ;  corrin ring carbon framework
```

```
   C9    C10    gb_17   ;  corrin ring carbon framework
   C10   C11    gb_17   ;  corrin ring carbon framework
   C11   C12    gb_27   ;  corrin ring carbon framework
   C12   C46    gb_27   ;  corrin ring carbon framework
   C12   C47    gb_27   ;  corrin ring carbon framework
   C12   C13    gb_27   ;  corrin ring carbon framework
   C13   C14    gb_27   ;  corrin ring carbon framework
   C13   C48    gb_27   ;  corrin ring carbon framework
   C14   C15    gb_17   ;  corrin ring carbon framework
   C15   C16    gb_17   ;  corrin ring carbon framework
   C15   C53    gb_27   ;  corrin ring carbon framework
   C16   C17    gb_27   ;  corrin ring carbon framework
   C17   C18    gb_27   ;  corrin ring carbon framework
   C17   C54    gb_27   ;  corrin ring carbon framework
   C17   C55    gb_27   ;  corrin ring carbon framework
   C18   C19    gb_27   ;  corrin ring carbon framework
   C18   C60    gb_27   ;  corrin ring carbon framework
   C19   C1     gb_27   ;  corrin ring carbon framework
   C10   H10    gb_3    ;  corrin ring C10-H10 bond
    [ exclusions ]
;  ai    aj
   FE    C2
   FE    C3
   FE    C5
   FE    C7
   FE    C8
   FE    C10
   FE    C12
   FE    C13
   FE    C15
   FE    C17
   FE    C18
   FE    C20
   N21   C25
   N21   C26
   N21   C30
   N21   C35
   N21   C6
   N21   C9
   N21   C11
   N21   C14
   N21   C16
   N21   C19
   N21   C10
   N22   C1
   N22   C4
   N22   C36
   N22   C37
   N22   C11
   N22   C14
   N22   C16
   N22   C19
   N22   C15
   N23   C16
   N23   C19
   N23   C1
   N23   C4
   N23   C6
   N23   C9
   N23   C46
   N23   C47
   N23   C48
   N23   C5
   N24   C4
   N24   C5
   N24   C6
   N24   C9
   N24   C10
   N24   C11
   N24   C14
   N24   C55
   N24   C54
   N24   C60
   C1R   C7B
   C1R   C9B
   C1R   N3B
   N1B   C6B
   N1B   C4B
   C8B   C5B
   C8B   C5M
   C8B   C6M
```

```
   C7B   C4B
   C7B   N3B
   C7B   C2B
   C2B   C9B
   C5B   C2B
   C5M   C6M
   C1    C30   ;  HEMC-based C framework exclusions
   C1    C5    ;  HEMC-based C framework exclusions
   C2    C5    ;  HEMC-based C framework exclusions
   C3    C35   ;  HEMC-based C framework exclusions
   C3    C6    ;  HEMC-based C framework exclusions
   C4    C26   ;  HEMC-based C framework exclusions
   C4    C7    ;  HEMC-based C framework exclusions
   C30   C26   ;  HEMC-based C framework exclusions
   C30   C5    ;  HEMC-based C framework exclusions
   C5    C8    ;  HEMC-based C framework exclusions
   C5    C9    ;  HEMC-based C framework exclusions
   C5    C36   ;  HEMC-based C framework exclusions
   C5    C37   ;  HEMC-based C framework exclusions
   C35   C7    ;  HEMC-based C framework exclusions
   C6    C41   ;  HEMC-based C framework exclusions
   C6    C10   ;  HEMC-based C framework exclusions
   C7    C10   ;  HEMC-based C framework exclusions
   C8    H10   ;  HEMC-based C framework exclusions
   C8    C11   ;  HEMC-based C framework exclusions
   C9    C36   ;  HEMC-based C framework exclusions
   C9    C37   ;  HEMC-based C framework exclusions
   C9    C12   ;  HEMC-based C framework exclusions
   C36   C41   ;  HEMC-based C framework exclusions
   C37   C10   ;  HEMC-based C framework exclusions
   C10   C13   ;  HEMC-based C framework exclusions
   C10   C14   ;  HEMC-based C framework exclusions
   C10   C46   ;  HEMC-based C framework exclusions
   C10   C47   ;  HEMC-based C framework exclusions
   H10   C12   ;  HEMC-based C framework exclusions
   C11   C48   ;  HEMC-based C framework exclusions
   C11   C15   ;  HEMC-based C framework exclusions
   C12   C15   ;  HEMC-based C framework exclusions
   C13   C53   ;  HEMC-based C framework exclusions
   C13   C16   ;  HEMC-based C framework exclusions
   C14   C46   ;  HEMC-based C framework exclusions
   C14   C47   ;  HEMC-based C framework exclusions
   C14   C17   ;  HEMC-based C framework exclusions
   C46   C48   ;  HEMC-based C framework exclusions
   C47   C48   ;  HEMC-based C framework exclusions
   C48   C15   ;  HEMC-based C framework exclusions
   C15   C18   ;  HEMC-based C framework exclusions
   C15   C19   ;  HEMC-based C framework exclusions
   C15   C54   ;  HEMC-based C framework exclusions
   C15   C55   ;  HEMC-based C framework exclusions
   C53   C17   ;  HEMC-based C framework exclusions
   C16   C60   ;  HEMC-based C framework exclusions
   C19   C54   ;  HEMC-based C framework exclusions
   C19   C55   ;  HEMC-based C framework exclusions
   C54   C60   ;  HEMC-based C framework exclusions
   C55   C60   ;  HEMC-based C framework exclusions
 [ angles ]
;  ai    aj    ak   gromos type
   C2    C26   C27   ga_15   ;  from GLN, fragment 1
   C26   C27   O28   ga_30   ;  from GLN
   C26   C27   N29   ga_19   ;  from GLN
   O28   C27   N29   ga_33   ;  from GLN
   C27   N29   HAE   ga_23   ;  from GLN
   C27   N29   HAD   ga_23   ;  from GLN
   HAE   N29   HAD   ga_24   ;  from GLN
   C30   C31   C32   ga_15   ;  from GLN, fragment 2
   C31   C32   O34   ga_30   ;  from GLN
   C31   C32   N33   ga_19   ;  from GLN
   O34   C32   N33   ga_33   ;  from GLN
   C32   N33   HAG   ga_23   ;  from GLN
   C32   N33   HAF   ga_23   ;  from GLN
   HAG   N33   HAF   ga_24   ;  from GLN
   C7    C37   C38   ga_15   ;  from GLN, fragment 3
   C37   C38   O39   ga_30   ;  from GLN
   C37   C38   N40   ga_19   ;  from GLN
   O39   C38   N40   ga_33   ;  from GLN
   C38   N40   HAI   ga_23   ;  from GLN
   C38   N40   HAH   ga_23   ;  from GLN
   HAI   N40   HAH   ga_24   ;  from GLN
   C41   C42   C43   ga_15   ;  from GLN, fragment 4
   C42   C43   O44   ga_30   ;  from GLN
```

```
C42   C43   N45   ga_19   ;  from GLN
O44   C43   N45   ga_33   ;  from GLN
C43   N45   HAK   ga_23   ;  from GLN
C43   N45   HAJ   ga_23   ;  from GLN
HAK   N45   HAJ   ga_24   ;  from GLN
C48   C49   C50   ga_15   ;  from GLN, fragment 5
C49   C50   O51   ga_30   ;  from GLN
C49   C50   N52   ga_19   ;  from GLN
O51   C50   N52   ga_33   ;  from GLN
C50   N52   HAM   ga_23   ;  from GLN
C50   N52   HAL   ga_23   ;  from GLN
HAM   N52   HAL   ga_24   ;  from GLN
C18   C60   C61   ga_15   ;  from GLN, fragment 6
C60   C61   O63   ga_30   ;  from GLN
C60   C61   N62   ga_19   ;  from GLN
O63   C61   N62   ga_33   ;  from GLN
C61   N62   HAO   ga_23   ;  from GLN
C61   N62   HAN   ga_23   ;  from GLN
HAO   N62   HAN   ga_24   ;  from GLN
N21   FE    N22   ga_2    ;  corrin ring Fe-N angle
N21   FE    N24   ga_2    ;  corrin ring Fe-N angle
N22   FE    N23   ga_2    ;  corrin ring Fe-N angle
N23   FE    N24   ga_2    ;  corrin ring Fe-N angle
N21   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N22   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N23   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N24   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
FE    N21   C1    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N21   C4    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N22   C6    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N22   C9    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N23   C11   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N23   C14   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N24   C16   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N24   C19   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N3B   C9B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
FE    N3B   C2B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
C8B   N1B   C2B   ga_7    ;  angle containing C8B, see minimization issues discussion
N1B   C8B   C9B   ga_7    ;  angle containing C8B, see minimization issues discussion
C8B   C9B   N3B   ga_7    ;  angle containing C8B, see minimization issues discussion
C7B   C8B   N1B   ga_39   ;  angle containing C8B, see minimization issues discussion
C8B   N1B   C1R   ga_37   ;  angle containing C8B, see minimization issues discussion
C4B   C9B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C6B   C7B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C7B   C8B   C9B   ga_27   ;  angle containing C8B, see minimization issues discussion
N21   C1    C2    ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C1    C20   ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C4    C3    ga_33   ;  corrin ring-specific but HEMC-derived angles
C4    N21   C1    ga_6    ;  corrin ring-specific but HEMC-derived angles
C5    C4    N21   ga_33   ;  corrin ring-specific but HEMC-derived angles
C19   C1    N21   ga_13   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C5    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C7    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C9    C8    ga_33   ;  corrin ring-specific but HEMC-derived angles
C9    N22   C6    ga_6    ;  corrin ring-specific but HEMC-derived angles
C10   C9    N22   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C10   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C12   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C14   C13   ga_33   ;  corrin ring-specific but HEMC-derived angles
C14   N23   C11   ga_6    ;  corrin ring-specific but HEMC-derived angles
C15   C14   N23   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C16   C15   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C19   C1    ga_13   ;  corrin ring-specific but HEMC-derived angles
C19   N24   C16   ga_6    ;  corrin ring-specific but HEMC-derived angles
C17   C16   N24   ga_33   ;  corrin ring-specific but HEMC-derived angles
C18   C19   N24   ga_13   ;  corrin ring-specific but HEMC-derived angles
C3R   O2    P     ga_26   ;  phosphate angle from ADE
O2    P     O3    ga_5    ;  phosphate angle from ADE
O2    P     O4    ga_14   ;  phosphate angle from ADE
O2    P     O5    ga_14   ;  phosphate angle from ADE
O3    P     O4    ga_14   ;  phosphate angle from ADE
O3    P     O5    ga_14   ;  phosphate angle from ADE
O4    P     O5    ga_29   ;  phosphate angle from ADE
P     O3    C2P   ga_26   ;  phosphate angle from ADE
O2    C3R   C2R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O2    C3R   C4R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C1P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C3P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
C1    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C3    ga_13   ;  CHn-CHn-CHn angles
```

```
C1    C19   C18   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C19   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C20   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C30   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C3    C30   C31   ga_13   ;  CHn-CHn-CHn angles
C7    C8    C41   ga_13   ;  CHn-CHn-CHn angles
C8    C41   C42   ga_13   ;  CHn-CHn-CHn angles
C12   C13   C48   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C46   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C13   C48   C49   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C19   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C17   C55   C56   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C54   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C19   C1    C20   ga_13   ;  CHn-CHn-CHn angles
C19   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C25   C2    C26   ga_13   ;  CHn-CHn-CHn angles
C46   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C54   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C36   C7    C37   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C4    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C3    C30   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C8    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C7    C8    C9    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C9    C8    C41   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C13   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C46   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C47   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C12   C13   C14   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C14   C13   C48   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C18   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C54   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C55   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C5    C6    ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
C9    C10   C11   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
C14   C15   C16   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
C3    C4    C5    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C4    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C5    C6    C7    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C6    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C8    C9    C10   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C10   C11   C12   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C13   C14   C15   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C14   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C15   C16   C17   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C16   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C5M   C5B   C4B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C5M   C5B   C6B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C6M   C6B   C5B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C6M   C6B   C7B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C4B   C5B   C6B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B   C4B   C9B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B   C6B   C7B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
N1B   C1R   C2R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C1R   O6R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C2B   N3B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C2B   N1B   C1R   ga_37   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N3B   C9B   C4B   ga_39   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C9B   N3B   C2B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C1R   C2R   C3R   ga_8    ;  from ADE sugar angle
C1R   C2R   O7R   ga_9    ;  from ADE sugar angle
C1R   O6R   C4R   ga_10   ;  from ADE sugar angle
C2R   C1R   O6R   ga_9    ;  from ADE sugar angle
C2R   C3R   C4R   ga_8    ;  from ADE sugar angle
C2R   O7R   HAA   ga_12   ;  from ADE sugar angle
C3R   C2R   O7R   ga_9    ;  from ADE sugar angle
C3R   C4R   C5R   ga_8    ;  from ADE sugar angle
C3R   C4R   O6R   ga_9    ;  from ADE sugar angle
C4R   C5R   O8R   ga_9    ;  from ADE sugar angle
C5R   O8R   HAB   ga_12   ;  from ADE sugar angle
C5R   C4R   O6R   ga_9    ;  from ADE sugar angle
C1P   C2P   C3P   ga_13   ;  amide linkage angle
C57   C56   C55   ga_13   ;  amide linkage angle
```

```
   C57   N59   HAC   ga_23   ;  from GLN angle
   N59   C57   O58   ga_33   ;  from GLN angle
   C56   C57   N59   ga_19   ;  from GLN angle
   O58   C57   C56   ga_30   ;  from GLN angle
   C1P   N59   C57   ga_31   ;  from force field angle definitions
   C1P   N59   HAC   ga_18   ;  from force field angle definitions
   C2P   C1P   N59   ga_15   ;  from force field angle definitions
   C5B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C9B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C6B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   C8B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   N1B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   N3B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   C9    C10   H10   ga_25   ;  corrin ring C-C10-H angle
   C11   C10   H10   ga_20   ;  corrin ring C-C10-H angle
   [ impropers ]
;  ai    aj    ak    al   gromos type
   C1R   C8B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   N1B   C8B   C9B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C7B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C2B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C7B   C6B   C5B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C9B   N3B   C2B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C8B   C9B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C6B   C5B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C6B   C5B   C4B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5B   C4B   C9B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C8B   C7B   C6B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C4B   N3B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   N3B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C2B   N1B   C8B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5M   C4B   C6B   C5B   gi_1    ;  dimethylbenzimidazole methyl groups
   C6M   C7B   C5B   C6B   gi_1    ;  dimethylbenzimidazole methyl groups
   C2B   N1B   N3B   H2B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C4B   C9B   C5B   H4B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C7B   C8B   C6B   H7B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   N3B   FE    C2B   C9B   gi_1    ;  Fe-dimethylbenzimidazole planarity
   N21   C4    C5    C6    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C6    C5    C4    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C9    C10   C11   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C11   C10   C9    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C14   C15   C16   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N24   C16   C15   C14   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C15   C16   C14   C53   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C27   O28   N29   C26   gi_1    ;  from GLN improper torsion definition
   N29   HAE   HAD   C27   gi_1    ;  from GLN improper torsion definition
   C32   O34   N33   C31   gi_1    ;  from GLN improper torsion definition
   N33   HAG   HAF   C32   gi_1    ;  from GLN improper torsion definition
   C38   O39   N40   C37   gi_1    ;  from GLN improper torsion definition
   N40   HAI   HAH   C38   gi_1    ;  from GLN improper torsion definition
   C43   O44   N45   C42   gi_1    ;  from GLN improper torsion definition
   N45   HAK   HAJ   C43   gi_1    ;  from GLN improper torsion definition
   C50   O51   N52   C49   gi_1    ;  from GLN improper torsion definition
   N52   HAM   HAL   C50   gi_1    ;  from GLN improper torsion definition
   C61   O63   N62   C60   gi_1    ;  from GLN improper torsion definition
   N62   HAO   HAN   C61   gi_1    ;  from GLN improper torsion definition
   C57   C56   O58   N59   gi_1    ;  amide linkage C57 planarity
   N59   C57   C1P   HAC   gi_1    ;  amide linkage N59 planarity
   C4    N21   C3    C5    gi_1    ;  corrin ring C sp2 planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring C sp2 planarity
   C6    N22   C5    C7    gi_1    ;  corrin ring C sp2 planarity
   C9    N22   C10   C8    gi_1    ;  corrin ring C sp2 planarity
   C11   N23   C10   C12   gi_1    ;  corrin ring C sp2 planarity
   C14   N23   C15   C13   gi_1    ;  corrin ring C sp2 planarity
   C15   C14   C16   C53   gi_1    ;  corrin ring C sp2 planarity
   C16   N24   C15   C17   gi_1    ;  corrin ring C sp2 planarity
   C10   C9    C11   H10   gi_1    ;  corrin ring C10 planarity
   C18   C17   C19   C60   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C19   N24   C18   C1    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C3    C2    C30   C4    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C8    C9    C7    C41   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C13   C14   C12   C48   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C2P   C1P   O3    C3P   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C1R   N1B   C2R   O6R   gi_2    ;  sugar C atom tetrahedral geometry
   C2R   O7R   C3R   C1R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C5R   O6R   C4R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C2R   O2    C4R   gi_2    ;  sugar C atom tetrahedral geometry
   FE    C1    C4    N21   gi_3    ;  HEMC improper definition
   FE    C6    C9    N22   gi_3    ;  HEMC improper definition
   FE    C11   C14   N23   gi_3    ;  HEMC improper definition
```

```
   FE    C16   C19   N24   gi_3    ;  HEMC improper definition
 [ dihedrals ]
;  ai    aj    ak    al   gromos type
   C3R   O2    P     O3    gd_20   ;  from ADE phosphate definition
   C3R   O2    P     O3    gd_27   ;  from ADE phosphate definition
   C2P   O3    P     O2    gd_20   ;  from ADE phosphate definition
   C2P   O3    P     O2    gd_27   ;  from ADE phosphate definition
   P     O3    C2P   C1P   gd_7    ;  from ADE phosphate definition
   C2R   C3R   O2    P     gd_29   ;  from ADE phosphate definition
   O8R   C5R   C4R   O6R   gd_8    ;  from ADE sugar dihedrals
   O8R   C5R   C4R   O6R   gd_25   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_17   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_34   ;  from ADE sugar dihedrals
   C3R   C4R   O6R   C1R   gd_29   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   C2R   gd_34   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   O2    gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   C2R   gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   O2    gd_18   ;  from ADE sugar dihedrals
   C4R   O6R   C1R   C2R   gd_29   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   O7R   gd_18   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   C4R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   O2    gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   C4R   gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   O2    gd_18   ;  from ADE sugar dihedrals
   C1R   C2R   O7R   HAA   gd_23   ;  from ADE sugar dihedrals
   N1B   C1R   C2R   O7R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   N1B   C8B   gd_16   ;  from ADE sugar dihedrals
   C4R   C5R   O8R   HAB   gd_2    ;  additional ADE-based sugar dihedral
   N1B   C1R   C2R   C3R   gd_17   ;  additional ADE-based sugar dihedral
   N1B   C1R   O6R   C4R   gd_17   ;  additional ADE-based sugar dihedral
   C2    C26   C27   N29   gd_40   ;  from GLN dihedral
   C26   C27   N29   HAD   gd_14   ;  from GLN dihedral
   C30   C31   C32   N33   gd_40   ;  from GLN dihedral
   C31   C32   N33   HAF   gd_14   ;  from GLN dihedral
   C7    C37   C38   N40   gd_40   ;  from GLN dihedral
   C37   C38   N40   HAH   gd_14   ;  from GLN dihedral
   C41   C42   C43   N45   gd_40   ;  from GLN dihedral
   C42   C43   N45   HAJ   gd_14   ;  from GLN dihedral
   C48   C49   C50   N52   gd_40   ;  from GLN dihedral
   C49   C50   N52   HAL   gd_14   ;  from GLN dihedral
   C18   C60   C61   N62   gd_40   ;  from GLN dihedral
   C60   C61   N62   HAN   gd_14   ;  from GLN dihedral
   C5M   C5B   C6B   C6M   gd_33   ;  dimethylbenzimidazole methyl dihedral fix
   C4B   C5B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C8B   C7B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C7B   C6B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C9B   C4B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C35   C5    C4    N21   gd_10   ;  corrin ring methyl planarity
   C35   C5    C6    N22   gd_10   ;  corrin ring methyl planarity
   C53   C15   C14   N23   gd_10   ;  corrin ring methyl planarity
   C53   C1    C16   N24   gd_10   ;  corrin ring methyl planarity
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N21   C4    C5    C6    gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C4    C5    C6    N22   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N22   C9    C10   C11   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C9    C10   C11   N23   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N23   C14   C15   C16   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C14   C15   C16   N24   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C1    C2    C26   C27   gd_40   ;  corrin ring HEMC derived CHn torsions
   C25   C2    C26   C27   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C26   C27   O28   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C3    C30   C31   gd_9    ;  corrin ring HEMC derived CHn torsions
   C3    C30   C31   C32   gd_40   ;  corrin ring HEMC derived CHn torsions
   C30   C31   C32   O34   gd_40   ;  corrin ring HEMC derived CHn torsions
   C6    C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C36   C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C37   C38   O39   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C8    C41   C42   gd_9    ;  corrin ring HEMC derived CHn torsions
   C8    C41   C42   C43   gd_34   ;  corrin ring HEMC derived CHn torsions
   C41   C42   C43   O44   gd_40   ;  corrin ring HEMC derived CHn torsions
   C12   C13   C48   C49   gd_9    ;  corrin ring HEMC derived CHn torsions
   C13   C48   C49   C50   gd_34   ;  corrin ring HEMC derived CHn torsions
   C48   C49   C50   O51   gd_40   ;  corrin ring HEMC derived CHn torsions
   C16   C17   C55   C56   gd_40   ;  corrin ring HEMC derived CHn torsions
   C54   C17   C56   C57   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C55   C56   C57   gd_34   ;  corrin ring HEMC derived CHn torsions
   C55   C56   C57   O58   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C18   C60   C61   gd_9    ;  corrin ring HEMC derived CHn torsions
```

```
C18   C60   C61   O63   gd_34   ;  corrin ring HEMC derived CHn torsions
C18   C17   C55   C56   gd_9    ;  corrin ring HEMC derived CHn torsions
N59   C1P   C2P   O3    gd_34   ;  amide linkage torsion terms
N59   C1P   C2P   C3P   gd_34   ;  amide linkage torsion terms
C2P   C1P   N59   C57   gd_34   ;  amide linkage torsion terms
C56   C57   N59   C1P   gd_14   ;  amide linkage torsion terms
C55   C56   C57   N59   gd_40   ;  amide linkage torsion terms
C17   C55   C56   C57   gd_40   ;  amide linkage torsion terms
C5    C4    N21   C1    gd_14   ;  corrin ring sp3-containing torsions
C10   C9    N22   C6    gd_14   ;  corrin ring sp3-containing torsions
C5    C6    N22   C9    gd_14   ;  corrin ring sp3-containing torsions
C15   C14   N23   C11   gd_14   ;  corrin ring sp3-containing torsions
C10   C11   N23   C14   gd_14   ;  corrin ring sp3-containing torsions
C15   C16   N24   C19   gd_14   ;  corrin ring sp3-containing torsions
C4    N21   C1    C2    gd_40   ;  corrin ring sp3-containing torsions
C18   C19   N24   C16   gd_40   ;  corrin ring sp3-containing torsions
N22   C6    C5    C4    gd_33   ;  corrin ring sp3-containing torsions
N23   C11   C10   C9    gd_33   ;  corrin ring sp3-containing torsions
C19   C18   C17   C55   gd_34   ;  corrin ring sp3-containing torsions
C55   C17   C16   C15   gd_40   ;  corrin ring sp3-containing torsions
C17   C18   C19   C1    gd_34   ;  corrin ring sp3-containing torsions
C18   C19   C1    C2    gd_34   ;  corrin ring sp3-containing torsions
C17   C16   C15   C14   gd_10   ;  corrin ring sp3-containing torsions
C16   C15   C14   C13   gd_10   ;  corrin ring sp3-containing torsions
C15   C14   C13   C12   gd_40   ;  corrin ring sp3-containing torsions
C6    C7    C8    C9    gd_34   ;  corrin ring sp3-containing torsions
C8    C7    C6    C5    gd_34   ;  corrin ring sp3-containing torsions
C30   C3    C2    C1    gd_34   ;  corrin ring sp3-containing torsions
C11   C12   C13   C14   gd_34   ;  corrin ring sp3-containing torsions
C13   C12   C11   C10   gd_34   ;  corrin ring sp3-containing torsions
C10   C9    C8    C7    gd_10   ;  corrin ring sp3-containing torsions
C5    C4    C3    C30   gd_34   ;  corrin ring sp3-containing torsions
C3    C2    C1    C19   gd_34   ;  corrin ring sp3-containing torsions
C9B   N3B   FE    N21   gd_38   ;   THIS IS NEW!!!
N3B   FE    N21   C1    gd_38   ;   THIS IS NEW!!!
N3B   FE    N22   C6    gd_38   ;   THIS IS NEW!!!
N3B   FE    N23   C11   gd_38   ;   THIS IS NEW!!!
N3B   FE    N24   C16   gd_38   ;   THIS IS NEW!!!
```

```
[ LYB ]
 [ atoms ]
 C27      C       0.38000     0    ;  from GLN residue
 O28      O      -0.38000     0    ;  from GLN residue
 N29      NT     -0.83000     0    ;  from GLN residue
 HAE      H       0.41500     0    ;  from GLN residue
 HAD      H       0.41500     0    ;  from GLN residue
 C32      C       0.38000     1    ;  from GLN residue
 O34      O      -0.38000     1    ;  from GLN residue
 N33      NT     -0.83000     1    ;  from GLN residue
 HAG      H       0.41500     1    ;  from GLN residue
 HAF      H       0.41500     1    ;  from GLN residue
 C38      C       0.38000     2    ;  from GLN residue
 O39      O      -0.38000     2    ;  from GLN residue
 N40      NT     -0.83000     2    ;  from GLN residue
 HAI      H       0.41500     2    ;  from GLN residue
 HAH      H       0.41500     2    ;  from GLN residue
 C43      C       0.38000     3    ;  from GLN residue
 O44      O      -0.38000     3    ;  from GLN residue
 N45      NT     -0.83000     3    ;  from GLN residue
 HAK      H       0.41500     3    ;  from GLN residue
 HAJ      H       0.41500     3    ;  from GLN residue
 C50      C       0.38000     4    ;  from GLN residue
 O51      O      -0.38000     4    ;  from GLN residue
 N52      NT     -0.83000     4    ;  from GLN residue
 HAM      H       0.41500     4    ;  from GLN residue
 HAL      H       0.41500     4    ;  from GLN residue
 C61      C       0.38000     5    ;  from GLN residue
 O63      O      -0.38000     5    ;  from GLN residue
 N62      NT     -0.83000     5    ;  from GLN residue
 HAO      H       0.41500     5    ;  from GLN residue
 HAN      H       0.41500     5    ;  from GLN residue
 C20      CH3     0.00000     6    ;  methyl group
 C25      CH3     0.00000     7    ;  methyl group
 C36      CH3     0.00000     8    ;  methyl group
 C46      CH3     0.00000     9    ;  methyl group
 C47      CH3     0.00000     10   ;  methyl group
 C54      CH3     0.00000     11   ;  methyl group
 C26      CH2     0.00000     12   ;  non-polar CHn fragments
 C30      CH2     0.00000     13   ;  non-polar CHn fragments
 C31      CH2     0.00000     13   ;  non-polar CHn fragments
 C37      CH2     0.00000     14   ;  non-polar CHn fragments
 C41      CH2     0.00000     15   ;  non-polar CHn fragments
 C42      CH2     0.00000     15   ;  non-polar CHn fragments
 C48      CH2     0.00000     16   ;  non-polar CHn fragments
 C49      CH2     0.00000     16   ;  non-polar CHn fragments
 C56      CH2     0.00000     17   ;  non-polar CHn fragments
 C55      CH2     0.00000     17   ;  non-polar CHn fragments
 C60      CH2     0.00000     18   ;  non-polar CHn fragments
 C2R      CH1     0.15000     19   ;  C2*-O2*-H2* from ADE
 O7R      OA     -0.54800     19   ;  C2*-O2*-H2* from ADE
 HAA      H       0.39800     19   ;  C2*-O2*-H2* from ADE
 C1R      CH1     0.20000     20   ;  C1*-O4*-C4* from ADE
 O6R      OA     -0.36000     20   ;  C1*-O4*-C4* from ADE
 C4R      CH1     0.16000     20   ;  C1*-O4*-C4* from ADE
 C3R      CH1     0.00000     21   ;  C3* from ADE
 C5R      CH2     0.15000     22   ;  C2*-O2*-H2* from ADE
 O8R      OA     -0.54800     22   ;  C2*-O2*-H2* from ADE
; O8R      OA     -0.54800     22   ;  C2*-O2*-H2* from ADE  ; original from B12
;
;    HAB from B12 is gone in LYB, where the lysine fragment is added via CLB
;    HAB     H       0.39800     22   ;  C2*-O2*-H2* from ADE
;    HAB from B12 is gone in LYB, where the lysine fragment is added via CLB
;
 P        P       2.20000     23   ;  PO3+O3* fragment from ADE
;
; the O2P is a special mod to the PDB file.  The O2 (fine in B12) is a "special" label
; that pdb2gmx has some kind of structure prep issue with.  This, like the CO to FE, is a
; by-hand hack of the PDB file (for now)
;
 O2P      OA     -0.80000     23   ;  PO3+O3* fragment from ADE
 O4       OM     -1.00000     23   ;  PO3+O3* fragment from ADE
 O5       OM     -1.00000     23   ;  PO3+O3* fragment from ADE
 O3       OA     -0.80000     23   ;  PO3+O3* fragment from ADE
 C2P      CH1     0.35000     24   ;  non-polar CHn fragment
 C3P      CH3     0.00000     24   ;  non-polar CHn fragment
 C1P      CH2     0.00000     24   ;  non-polar CHn fragment
 N59      N      -0.28000     25   ;  tempered GLN fragment charges
 HAC      H       0.28000     25   ;  tempered GLN fragment charges
 C57      C       0.38000     25   ;  tempered GLN fragment charges
 O58      O      -0.38000     25   ;  tempered GLN fragment charges
```

```
 C5B      C        0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C5M      CH3      0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6B      C        0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6M      CH3      0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C4B      C       -0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H4B      H        0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C7B      C       -0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H7B      H        0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 N3B      NR      -0.55000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 C9B      C        0.20000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 N1B      NR      -0.30000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C8B      C        0.20000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C2B      C        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H2B      H        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C5       C       -0.05000     33   ;  C-CH3 group (non-polar)
 C35      CH3      0.00000     33   ;  C-CH3 group (non-polar)
 C15      C       -0.05000     34   ;  C-CH3 group (non-polar)
 C53      CH3      0.00000     34   ;  C-CH3 group (non-polar)
 FE       FE       0.62000     35   ;  HEMC Fe-N group
 N21      NR      -0.44000     35   ;  HEMC Fe-N group
 N22      NR      -0.50000     35   ;  HEMC Fe-N group
 N23      NR      -0.50000     35   ;  HEMC Fe-N group
 N24      NR      -0.44000     35   ;  HEMC Fe-N group
 C1       CH0      0.22000     36   ;  non-polar HEMC-derived corrin atoms
 C2       CH0      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C3       CH1      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C4       C        0.38000     36   ;  non-polar HEMC-derived corrin atoms
 C6       C        0.29000     37   ;  non-polar HEMC-derived corrin atoms
 C7       CH0      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C8       CH1      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C9       C        0.35000     37   ;  non-polar HEMC-derived corrin atoms
 C16      C        0.38000     38   ;  non-polar HEMC-derived corrin atoms
 C17      CH0      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C18      CH1      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C19      CH1      0.24000     38   ;  non-polar HEMC-derived corrin atoms
 C11      C        0.35000     39   ;  non-polar HEMC-derived corrin atoms
 C12      CH0      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C13      CH1      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C14      C        0.29000     39   ;  non-polar HEMC-derived corrin atoms
 C10      C       -0.24000     40   ;  aromatic C-H from TRP, PHE
 H10      H        0.14000     40   ;  aromatic C-H from TRP, PHE
;
;    Since CO is not defined as an atom in GROMOSxx, CO is converted to FE and the HEME
;    values are employed.  This is a workaround due for proper implementation.
;
 N        N       -0.31000     41   ;  standard LYS (lysine) atom information
 H        H        0.31000     41   ;  standard LYS (lysine) atom information
 CA       CH1      0.00000     42   ;  standard LYS (lysine) atom information
 CB       CH2      0.00000     42   ;  standard LYS (lysine) atom information
 CG       CH2      0.00000     43   ;  standard LYS (lysine) atom information
 CD       CH2      0.00000     43   ;  standard LYS (lysine) atom information
 CE       CH2      0.00000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
 NZ       NT      -0.34000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
 HZ1      H        0.34000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
; CE       CH2    -0.24000      44   ;  standard LYS (lysine) atom information
; NZ       NT     -0.64000      44   ;  standard LYS (lysine) atom information
; HZ1      H       0.44000      44   ;  standard LYS (lysine) atom information
;
;    this H atom is gone, replaced by the linkage CLB atom.
;    HZ2      H     0.44000      44   ;  standard LYS (lysine) atom information
;    this H atom is gone, replaced by the linkage CLB atom.
;
 C        C        0.20000     45   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
 O        O       -0.20000     45   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
; C        C       0.45000      45   ;  standard LYS (lysine) atom information
; O        O      -0.45000      45   ;  standard LYS (lysine) atom information
;
;  linkage atoms (added new)
;
 CLB      C        0.00000     46   ;  this is the linkage carbon atom between LYS and B12
 OLB      O        0.00000     46   ;  this is the additional =O at the linkage position
;
[ bonds ]
;  ai    aj    gromos type
   C26   C27    gb_27   ;  from GLN fragment 0
   C27   O28    gb_5    ;  from GLN
   C27   N29    gb_9    ;  from GLN
   N29   HAE    gb_2    ;  from GLN
   N29   HAD    gb_2    ;  from GLN
   C31   C32    gb_27   ;  from GLN fragment 1
   C32   O34    gb_5    ;  from GLN
```

```
   C32   N33    gb_9    ;  from GLN
   N33   HAG    gb_2    ;  from GLN
   N33   HAF    gb_2    ;  from GLN
   C37   C38    gb_27   ;  from GLN fragment 2
   C38   O39    gb_5    ;  from GLN
   C38   N40    gb_9    ;  from GLN
   N40   HAI    gb_2    ;  from GLN
   N40   HAH    gb_2    ;  from GLN
   C42   C43    gb_27   ;  from GLN fragment 3
   C43   O44    gb_5    ;  from GLN
   C43   N45    gb_9    ;  from GLN
   N45   HAK    gb_2    ;  from GLN
   N45   HAJ    gb_2    ;  from GLN
   C49   C50    gb_27   ;  from GLN fragment 4
   C50   O51    gb_5    ;  from GLN
   C50   N52    gb_9    ;  from GLN
   N52   HAM    gb_2    ;  from GLN
   N52   HAL    gb_2    ;  from GLN
   C60   C61    gb_27   ;  from GLN fragment 5
   C61   O63    gb_5    ;  from GLN
   C61   N62    gb_9    ;  from GLN
   N62   HAO    gb_2    ;  from GLN
   N62   HAN    gb_2    ;  from GLN
   FE    N21    gb_35   ;  FE-N bond from HEMC
   FE    N22    gb_35   ;  FE-N bond from HEMC
   FE    N23    gb_35   ;  FE-N bond from HEMC
   FE    N24    gb_35   ;  FE-N bond from HEMC
   FE    N3B    gb_37   ;  FE-N3B bond from HEMC not in corrin ring
   P     O2P    gb_28   ;  from ADE phosphate
   P     O4     gb_24   ;  from ADE phosphate
   P     O5     gb_24   ;  from ADE phosphate
   P     O3     gb_28   ;  from ADE phosphate
   N21   C1     gb_21   ;  corrin ring N-CHn bonds
   N21   C4     gb_14   ;  corrin ring N-C bonds
   N22   C6     gb_14   ;  corrin ring N-C bonds
   N22   C9     gb_14   ;  corrin ring N-C bonds
   N23   C11    gb_14   ;  corrin ring N-C bonds
   N23   C14    gb_14   ;  corrin ring N-C bonds
   N24   C16    gb_14   ;  corrin ring N-C bonds
   N24   C19    gb_21   ;  corrin ring N-CHn bonds
   C30   C31    gb_27   ;  CH2-CH2 bonds
   C41   C42    gb_27   ;  CH2-CH2 bonds
   C48   C49    gb_27   ;  CH2-CH2 bonds
   C55   C56    gb_27   ;  CH2-CH2 bonds
   C56   C57    gb_27   ;  CH2-CH2 bonds
   N1B   C1R    gb_22   ;  sugar bonds from ADE
   C1R   C2R    gb_26   ;  sugar bonds from ADE
   C2R   O7R    gb_20   ;  sugar bonds from ADE
   O7R   HAA    gb_1    ;  sugar bonds from ADE
   C2R   C3R    gb_26   ;  sugar bonds from ADE
   C3R   C4R    gb_26   ;  sugar bonds from ADE
   C3R   O2P    gb_20   ;  sugar bonds from ADE
   C4R   C5R    gb_26   ;  sugar bonds from ADE
   C5R   O8R    gb_20   ;  sugar bonds from ADE
;
;  HAB is deleted from B12 for LYB    O8R   HAB    gb_1    ;  sugar bonds from ADE
;
   C4R   O6R    gb_20   ;  sugar bonds from ADE
   O6R   C1R    gb_20   ;  sugar bonds from ADE
   C1P   N59    gb_9    ;  amide corrin - phosphate linkage
   C1P   C2P    gb_27   ;  amide corrin - phosphate linkage
   C2P   C3P    gb_27   ;  amide corrin - phosphate linkage
   C2P   O3     gb_20   ;  amide corrin - phosphate linkage
   N59   HAC    gb_2    ;  amide corrin - phosphate linkage
   N59   C57    gb_9    ;  amide corrin - phosphate linkage
   C57   O58    gb_5    ;  amide corrin - phosphate linkage
   N1B   C2B    gb_10   ;  dimethylbenzimidazole ring
   C2B   N3B    gb_10   ;  dimethylbenzimidazole ring
   C2B   H2B    gb_3    ;  dimethylbenzimidazole ring
   N3B   C9B    gb_10   ;  dimethylbenzimidazole ring
   C9B   C4B    gb_16   ;  dimethylbenzimidazole ring
   C4B   C5B    gb_16   ;  dimethylbenzimidazole ring
   C4B   H4B    gb_3    ;  dimethylbenzimidazole ring
   C5B   C6B    gb_16   ;  dimethylbenzimidazole ring
   C5B   C5M    gb_27   ;  dimethylbenzimidazole ring
   C6B   C7B    gb_16   ;  dimethylbenzimidazole ring
   C6B   C6M    gb_27   ;  dimethylbenzimidazole ring
   C7B   C8B    gb_16   ;  dimethylbenzimidazole ring
   C7B   H7B    gb_3    ;  dimethylbenzimidazole ring
   C8B   N1B    gb_10   ;  dimethylbenzimidazole ring
   C8B   C9B    gb_16   ;  dimethylbenzimidazole ring
```

```
   C1    C20    gb_27   ;  corrin ring carbon framework
   C1    C2     gb_27   ;  corrin ring carbon framework
   C2    C3     gb_27   ;  corrin ring carbon framework
   C2    C25    gb_27   ;  corrin ring carbon framework
   C2    C26    gb_27   ;  corrin ring carbon framework
   C3    C4     gb_27   ;  corrin ring carbon framework
   C3    C30    gb_27   ;  corrin ring carbon framework
   C4    C5     gb_17   ;  corrin ring carbon framework
   C5    C6     gb_17   ;  corrin ring carbon framework
   C5    C35    gb_27   ;  corrin ring carbon framework
   C6    C7     gb_27   ;  corrin ring carbon framework
   C7    C8     gb_27   ;  corrin ring carbon framework
   C7    C37    gb_27   ;  corrin ring carbon framework
   C7    C36    gb_27   ;  corrin ring carbon framework
   C8    C9     gb_27   ;  corrin ring carbon framework
   C8    C41    gb_27   ;  corrin ring carbon framework
   C9    C10    gb_17   ;  corrin ring carbon framework
   C10   C11    gb_17   ;  corrin ring carbon framework
   C11   C12    gb_27   ;  corrin ring carbon framework
   C12   C46    gb_27   ;  corrin ring carbon framework
   C12   C47    gb_27   ;  corrin ring carbon framework
   C12   C13    gb_27   ;  corrin ring carbon framework
   C13   C14    gb_27   ;  corrin ring carbon framework
   C13   C48    gb_27   ;  corrin ring carbon framework
   C14   C15    gb_17   ;  corrin ring carbon framework
   C15   C16    gb_17   ;  corrin ring carbon framework
   C15   C53    gb_27   ;  corrin ring carbon framework
   C16   C17    gb_27   ;  corrin ring carbon framework
   C17   C18    gb_27   ;  corrin ring carbon framework
   C17   C54    gb_27   ;  corrin ring carbon framework
   C17   C55    gb_27   ;  corrin ring carbon framework
   C18   C19    gb_27   ;  corrin ring carbon framework
   C18   C60    gb_27   ;  corrin ring carbon framework
   C19   C1     gb_27   ;  corrin ring carbon framework
   C10   H10    gb_3    ;  corrin ring C10-H10 bond
;
; linker bond from B12 to CLB
;
   O8R   CLB    gb_5    ;  LYS B12 linker (CLB replaces H)
;
;  Lysine bond topology
;
   N     H      gb_2    ;  standard LYS (lysine)
   N     CA     gb_21   ;  standard LYS (lysine)
   CA    CB     gb_27   ;  standard LYS (lysine)
   CA    C      gb_27   ;  standard LYS (lysine)
   CB    CG     gb_27   ;  standard LYS (lysine)
   CG    CD     gb_27   ;  standard LYS (lysine)
   CD    CE     gb_27   ;  standard LYS (lysine)
   CE    NZ     gb_21   ;  standard LYS (lysine)
   NZ    HZ1    gb_2    ;  standard LYS (lysine)
;
; this replaces the HZ2 with CLB for the B12-LYS connection
;
   NZ    CLB    gb_9    ;  standard LYS (lysine)
   C     O      gb_5    ;  standard LYS (lysine)
   C     +N     gb_10   ;  standard LYS (lysine)
;
;  below is the C=O bond on the B12-LYS linkage (OLB is only connected to CLB)
;
   CLB  OLB     gb_27   ;  CLB-OLB linkage bond (previously nowhere in the structure)
    [ exclusions ]
;  ai    aj
   FE    C2
   FE    C3
   FE    C5
   FE    C7
   FE    C8
   FE    C10
   FE    C12
   FE    C13
   FE    C15
   FE    C17
   FE    C18
   FE    C20
   N21   C25
   N21   C26
   N21   C30
   N21   C35
   N21   C6
   N21   C9
```

```
N21   C11
N21   C14
N21   C16
N21   C19
N21   C10
N22   C1
N22   C4
N22   C36
N22   C37
N22   C11
N22   C14
N22   C16
N22   C19
N22   C15
N23   C16
N23   C19
N23   C1
N23   C4
N23   C6
N23   C9
N23   C46
N23   C47
N23   C48
N23   C5
N24   C4
N24   C5
N24   C6
N24   C9
N24   C10
N24   C11
N24   C14
N24   C55
N24   C54
N24   C60
C1R   C7B
C1R   C9B
C1R   N3B
N1B   C6B
N1B   C4B
C8B   C5B
C8B   C5M
C8B   C6M
C7B   C4B
C7B   N3B
C7B   C2B
C2B   C9B
C5B   C2B
C5M   C6M
C1    C30   ;  HEMC-based C framework exclusions
C1    C5    ;  HEMC-based C framework exclusions
C2    C5    ;  HEMC-based C framework exclusions
C3    C35   ;  HEMC-based C framework exclusions
C3    C6    ;  HEMC-based C framework exclusions
C4    C26   ;  HEMC-based C framework exclusions
C4    C7    ;  HEMC-based C framework exclusions
C30   C26   ;  HEMC-based C framework exclusions
C30   C5    ;  HEMC-based C framework exclusions
C5    C8    ;  HEMC-based C framework exclusions
C5    C9    ;  HEMC-based C framework exclusions
C5    C36   ;  HEMC-based C framework exclusions
C5    C37   ;  HEMC-based C framework exclusions
C35   C7    ;  HEMC-based C framework exclusions
C6    C41   ;  HEMC-based C framework exclusions
C6    C10   ;  HEMC-based C framework exclusions
C7    C10   ;  HEMC-based C framework exclusions
C8    H10   ;  HEMC-based C framework exclusions
C8    C11   ;  HEMC-based C framework exclusions
C9    C36   ;  HEMC-based C framework exclusions
C9    C37   ;  HEMC-based C framework exclusions
C9    C12   ;  HEMC-based C framework exclusions
C36   C41   ;  HEMC-based C framework exclusions
C37   C10   ;  HEMC-based C framework exclusions
C10   C13   ;  HEMC-based C framework exclusions
C10   C14   ;  HEMC-based C framework exclusions
C10   C46   ;  HEMC-based C framework exclusions
C10   C47   ;  HEMC-based C framework exclusions
H10   C12   ;  HEMC-based C framework exclusions
C11   C48   ;  HEMC-based C framework exclusions
C11   C15   ;  HEMC-based C framework exclusions
C12   C15   ;  HEMC-based C framework exclusions
C13   C53   ;  HEMC-based C framework exclusions
```

```
   C13   C16   ;  HEMC-based C framework exclusions
   C14   C46   ;  HEMC-based C framework exclusions
   C14   C47   ;  HEMC-based C framework exclusions
   C14   C17   ;  HEMC-based C framework exclusions
   C46   C48   ;  HEMC-based C framework exclusions
   C47   C48   ;  HEMC-based C framework exclusions
   C48   C15   ;  HEMC-based C framework exclusions
   C15   C18   ;  HEMC-based C framework exclusions
   C15   C19   ;  HEMC-based C framework exclusions
   C15   C54   ;  HEMC-based C framework exclusions
   C15   C55   ;  HEMC-based C framework exclusions
   C53   C17   ;  HEMC-based C framework exclusions
   C16   C60   ;  HEMC-based C framework exclusions
   C19   C54   ;  HEMC-based C framework exclusions
   C19   C55   ;  HEMC-based C framework exclusions
   C54   C60   ;  HEMC-based C framework exclusions
   C55   C60   ;  HEMC-based C framework exclusions
 [ angles ]
;  ai    aj    ak   gromos type
   C2    C26   C27   ga_15   ;  from GLN, fragment 1
   C26   C27   O28   ga_30   ;  from GLN
   C26   C27   N29   ga_19   ;  from GLN
   O28   C27   N29   ga_33   ;  from GLN
   C27   N29   HAE   ga_23   ;  from GLN
   C27   N29   HAD   ga_23   ;  from GLN
   HAE   N29   HAD   ga_24   ;  from GLN
   C30   C31   C32   ga_15   ;  from GLN, fragment 2
   C31   C32   O34   ga_30   ;  from GLN
   C31   C32   N33   ga_19   ;  from GLN
   O34   C32   N33   ga_33   ;  from GLN
   C32   N33   HAG   ga_23   ;  from GLN
   C32   N33   HAF   ga_23   ;  from GLN
   HAG   N33   HAF   ga_24   ;  from GLN
   C7    C37   C38   ga_15   ;  from GLN, fragment 3
   C37   C38   O39   ga_30   ;  from GLN
   C37   C38   N40   ga_19   ;  from GLN
   O39   C38   N40   ga_33   ;  from GLN
   C38   N40   HAI   ga_23   ;  from GLN
   C38   N40   HAH   ga_23   ;  from GLN
   HAI   N40   HAH   ga_24   ;  from GLN
   C41   C42   C43   ga_15   ;  from GLN, fragment 4
   C42   C43   O44   ga_30   ;  from GLN
   C42   C43   N45   ga_19   ;  from GLN
   O44   C43   N45   ga_33   ;  from GLN
   C43   N45   HAK   ga_23   ;  from GLN
   C43   N45   HAJ   ga_23   ;  from GLN
   HAK   N45   HAJ   ga_24   ;  from GLN
   C48   C49   C50   ga_15   ;  from GLN, fragment 5
   C49   C50   O51   ga_30   ;  from GLN
   C49   C50   N52   ga_19   ;  from GLN
   O51   C50   N52   ga_33   ;  from GLN
   C50   N52   HAM   ga_23   ;  from GLN
   C50   N52   HAL   ga_23   ;  from GLN
   HAM   N52   HAL   ga_24   ;  from GLN
   C18   C60   C61   ga_15   ;  from GLN, fragment 6
   C60   C61   O63   ga_30   ;  from GLN
   C60   C61   N62   ga_19   ;  from GLN
   O63   C61   N62   ga_33   ;  from GLN
   C61   N62   HAO   ga_23   ;  from GLN
   C61   N62   HAN   ga_23   ;  from GLN
   HAO   N62   HAN   ga_24   ;  from GLN
   N21   FE    N22   ga_2    ;  corrin ring Fe-N angle
   N21   FE    N24   ga_2    ;  corrin ring Fe-N angle
   N22   FE    N23   ga_2    ;  corrin ring Fe-N angle
   N23   FE    N24   ga_2    ;  corrin ring Fe-N angle
   N21   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
   N22   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
   N23   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
   N24   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
   FE    N21   C1    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N21   C4    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N22   C6    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N22   C9    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N23   C11   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N23   C14   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N24   C16   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N24   C19   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
   FE    N3B   C9B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
   FE    N3B   C2B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
   C8B   N1B   C2B   ga_7    ;  angle containing C8B, see minimization issues discussion
   N1B   C8B   C9B   ga_7    ;  angle containing C8B, see minimization issues discussion
```

```
C8B   C9B   N3B   ga_7    ;  angle containing C8B, see minimization issues discussion
C7B   C8B   N1B   ga_39   ;  angle containing C8B, see minimization issues discussion
C8B   N1B   C1R   ga_37   ;  angle containing C8B, see minimization issues discussion
C4B   C9B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C6B   C7B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C7B   C8B   C9B   ga_27   ;  angle containing C8B, see minimization issues discussion
N21   C1    C2    ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C1    C20   ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C4    C3    ga_33   ;  corrin ring-specific but HEMC-derived angles
C4    N21   C1    ga_6    ;  corrin ring-specific but HEMC-derived angles
C5    C4    N21   ga_33   ;  corrin ring-specific but HEMC-derived angles
C19   C1    N21   ga_13   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C5    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C7    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C9    C8    ga_33   ;  corrin ring-specific but HEMC-derived angles
C9    N22   C6    ga_6    ;  corrin ring-specific but HEMC-derived angles
C10   C9    N22   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C10   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C12   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C14   C13   ga_33   ;  corrin ring-specific but HEMC-derived angles
C14   N23   C11   ga_6    ;  corrin ring-specific but HEMC-derived angles
C15   C14   N23   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C16   C15   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C19   C1    ga_13   ;  corrin ring-specific but HEMC-derived angles
C19   N24   C16   ga_6    ;  corrin ring-specific but HEMC-derived angles
C17   C16   N24   ga_33   ;  corrin ring-specific but HEMC-derived angles
C18   C19   N24   ga_13   ;  corrin ring-specific but HEMC-derived angles
C3R   O2P   P     ga_26   ;  phosphate angle from ADE
O2P   P     O3    ga_5    ;  phosphate angle from ADE
O2P   P     O4    ga_14   ;  phosphate angle from ADE
O2P   P     O5    ga_14   ;  phosphate angle from ADE
O3    P     O4    ga_14   ;  phosphate angle from ADE
O3    P     O5    ga_14   ;  phosphate angle from ADE
O4    P     O5    ga_29   ;  phosphate angle from ADE
P     O3    C2P   ga_26   ;  phosphate angle from ADE
O2P   C3R   C2R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O2P   C3R   C4R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C1P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C3P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
C1    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C3    ga_13   ;  CHn-CHn-CHn angles
C1    C19   C18   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C19   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C20   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C30   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C3    C30   C31   ga_13   ;  CHn-CHn-CHn angles
C7    C8    C41   ga_13   ;  CHn-CHn-CHn angles
C8    C41   C42   ga_13   ;  CHn-CHn-CHn angles
C12   C13   C48   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C46   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C13   C48   C49   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C19   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C17   C55   C56   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C54   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C19   C1    C20   ga_13   ;  CHn-CHn-CHn angles
C19   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C25   C2    C26   ga_13   ;  CHn-CHn-CHn angles
C46   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C54   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C36   C7    C37   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C4    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C3    C30   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C8    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C7    C8    C9    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C9    C8    C41   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C13   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C46   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C47   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C12   C13   C14   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C14   C13   C48   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C18   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
```

```
   C16   C17   C54   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C16   C17   C55   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C4    C5    C6    ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
   C9    C10   C11   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
   C14   C15   C16   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
   C3    C4    C5    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C4    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C5    C6    C7    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C6    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C8    C9    C10   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C10   C11   C12   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C13   C14   C15   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C14   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C15   C16   C17   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C16   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C5M   C5B   C4B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C5M   C5B   C6B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C6M   C6B   C5B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C6M   C6B   C7B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C4B   C5B   C6B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
   C5B   C4B   C9B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
   C5B   C6B   C7B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
   N1B   C1R   C2R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   N1B   C1R   O6R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   N1B   C2B   N3B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   C2B   N1B   C1R   ga_37   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   N3B   C9B   C4B   ga_39   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   C9B   N3B   C2B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   C1R   C2R   C3R   ga_8    ;  from ADE sugar angle
   C1R   C2R   O7R   ga_9    ;  from ADE sugar angle
   C1R   O6R   C4R   ga_10   ;  from ADE sugar angle
   C2R   C1R   O6R   ga_9    ;  from ADE sugar angle
   C2R   C3R   C4R   ga_8    ;  from ADE sugar angle
   C2R   O7R   HAA   ga_12   ;  from ADE sugar angle
   C3R   C2R   O7R   ga_9    ;  from ADE sugar angle
   C3R   C4R   C5R   ga_8    ;  from ADE sugar angle
   C3R   C4R   O6R   ga_9    ;  from ADE sugar angle
   C4R   C5R   O8R   ga_9    ;  from ADE sugar angle
;
;  HAB angle is gone from B12 for LYB  C5R O8R HAB ga_12 ;  from ADE sugar angle
;
   C5R   C4R   O6R   ga_9    ;  from ADE sugar angle
   C1P   C2P   C3P   ga_13   ;  amide linkage angle
   C57   C56   C55   ga_13   ;  amide linkage angle
   C57   N59   HAC   ga_23   ;  from GLN angle
   N59   C57   O58   ga_33   ;  from GLN angle
   C56   C57   N59   ga_19   ;  from GLN angle
   O58   C57   C56   ga_30   ;  from GLN angle
   C1P   N59   C57   ga_31   ;  from force field angle definitions
   C1P   N59   HAC   ga_18   ;  from force field angle definitions
   C2P   C1P   N59   ga_15   ;  from force field angle definitions
   C5B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C9B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C6B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   C8B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   N1B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   N3B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   C9    C10   H10   ga_25   ;  corrin ring C-C10-H angle
   C11   C10   H10   ga_20   ;  corrin ring C-C10-H angle
   C5R   O8R   CLB   ga_12   ;  for LYS-B12 bridge (just replaces O8R H atom with CLB)
;
;  standard Lysine angle topology
;
   -C    N     H     ga_32   ;  Standard LYS (lysine)
   -C    N     CA    ga_31   ;  Standard LYS (lysine)
   H     N     CA    ga_18   ;  Standard LYS (lysine)
   N     CA    CB    ga_13   ;  Standard LYS (lysine)
   N     CA    C     ga_13   ;  Standard LYS (lysine)
   CB    CA    C     ga_13   ;  Standard LYS (lysine)
   CA    CB    CG    ga_15   ;  Standard LYS (lysine)
   CB    CG    CD    ga_15   ;  Standard LYS (lysine)
   CG    CD    CE    ga_15   ;  Standard LYS (lysine)
   CD    CE    NZ    ga_15   ;  Standard LYS (lysine)
   CE    NZ    HZ1   ga_11   ;  Standard LYS (lysine)
   CE    NZ    CLB   ga_6    ;  Modification from LYS (CLB from NZ H atom)
   HZ1   NZ    CLB   ga_23   ;  Modification from LYS (CLB from NZ H atom)
   CA    C     O     ga_30   ;  Standard LYS (lysine)
   CA    C     +N    ga_19   ;  Standard LYS (lysine)
   O     C     +N    ga_33   ;  Standard LYS (lysine)
;
; additional CLB-OLB angle linkages
```

```
;
   OLB   CLB   O8R   ga_33   ;  new OLB-CLB linkage angles
   OLB   CLB   NZ    ga_33   ;  new OLB-CLB linkage angles
   O8R   CLB   NZ    ga_33   ;  new OLB-CLB linkage angles
   [ impropers ]
;  ai    aj    ak    al   gromos type
   C1R   C8B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   N1B   C8B   C9B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C7B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C2B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C7B   C6B   C5B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C9B   N3B   C2B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C8B   C9B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C6B   C5B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C6B   C5B   C4B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5B   C4B   C9B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C8B   C7B   C6B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C4B   N3B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   N3B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C2B   N1B   C8B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5M   C4B   C6B   C5B   gi_1    ;  dimethylbenzimidazole methyl groups
   C6M   C7B   C5B   C6B   gi_1    ;  dimethylbenzimidazole methyl groups
   C2B   N1B   N3B   H2B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C4B   C9B   C5B   H4B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C7B   C8B   C6B   H7B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   N3B   FE    C2B   C9B   gi_1    ;  Fe-dimethylbenzimidazole planarity
   N21   C4    C5    C6    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C6    C5    C4    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C9    C10   C11   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C11   C10   C9    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C14   C15   C16   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N24   C16   C15   C14   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C15   C16   C14   C53   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C27   O28   N29   C26   gi_1    ;  from GLN improper torsion definition
   N29   HAE   HAD   C27   gi_1    ;  from GLN improper torsion definition
   C32   O34   N33   C31   gi_1    ;  from GLN improper torsion definition
   N33   HAG   HAF   C32   gi_1    ;  from GLN improper torsion definition
   C38   O39   N40   C37   gi_1    ;  from GLN improper torsion definition
   N40   HAI   HAH   C38   gi_1    ;  from GLN improper torsion definition
   C43   O44   N45   C42   gi_1    ;  from GLN improper torsion definition
   N45   HAK   HAJ   C43   gi_1    ;  from GLN improper torsion definition
   C50   O51   N52   C49   gi_1    ;  from GLN improper torsion definition
   N52   HAM   HAL   C50   gi_1    ;  from GLN improper torsion definition
   C61   O63   N62   C60   gi_1    ;  from GLN improper torsion definition
   N62   HAO   HAN   C61   gi_1    ;  from GLN improper torsion definition
   C57   C56   O58   N59   gi_1    ;  amide linkage C57 planarity
   N59   C57   C1P   HAC   gi_1    ;  amide linkage N59 planarity
   C4    N21   C3    C5    gi_1    ;  corrin ring C sp2 planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring C sp2 planarity
   C6    N22   C5    C7    gi_1    ;  corrin ring C sp2 planarity
   C9    N22   C10   C8    gi_1    ;  corrin ring C sp2 planarity
   C11   N23   C10   C12   gi_1    ;  corrin ring C sp2 planarity
   C14   N23   C15   C13   gi_1    ;  corrin ring C sp2 planarity
   C15   C14   C16   C53   gi_1    ;  corrin ring C sp2 planarity
   C16   N24   C15   C17   gi_1    ;  corrin ring C sp2 planarity
   C10   C9    C11   H10   gi_1    ;  corrin ring C10 planarity
   C18   C17   C19   C60   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C19   N24   C18   C1    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C3    C2    C30   C4    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C8    C9    C7    C41   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C13   C14   C12   C48   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C2P   C1P   O3    C3P   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C1R   N1B   C2R   O6R   gi_2    ;  sugar C atom tetrahedral geometry
   C2R   O7R   C3R   C1R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C5R   O6R   C4R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C2R   O2P   C4R   gi_2    ;  sugar C atom tetrahedral geometry
   FE    C1    C4    N21   gi_3    ;  HEMC improper definition
   FE    C6    C9    N22   gi_3    ;  HEMC improper definition
   FE    C11   C14   N23   gi_3    ;  HEMC improper definition
   FE    C16   C19   N24   gi_3    ;  HEMC improper definition
;
; standard Lysine improper torsions
;
   N     -C    CA    H     gi_1    ;  Standard LYS (lysine)
   CA    N     C     CB    gi_2    ;  Standard LYS (lysine)
   C     CA    +N    O     gi_1    ;  Standard LYS (lysine)
   CLB   O8R   OLB   NZ    gi_1    ;  Linkage improper torsion to maintain planarity at CLB
 [ dihedrals ]
;  ai    aj    ak    al   gromos type
   C3R   O2P   P     O3    gd_20   ;  from ADE phosphate definition
```

```
   C3R   O2P   P     O3    gd_27   ;  from ADE phosphate definition
   C2P   O3    P     O2P   gd_20   ;  from ADE phosphate definition
   C2P   O3    P     O2P   gd_27   ;  from ADE phosphate definition
   P     O3    C2P   C1P   gd_7    ;  from ADE phosphate definition
   C2R   C3R   O2P   P     gd_29   ;  from ADE phosphate definition
   O8R   C5R   C4R   O6R   gd_8    ;  from ADE sugar dihedrals
   O8R   C5R   C4R   O6R   gd_25   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_17   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_34   ;  from ADE sugar dihedrals
   C3R   C4R   O6R   C1R   gd_29   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   C2R   gd_34   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   O2P   gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   C2R   gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   O2P   gd_18   ;  from ADE sugar dihedrals
   C4R   O6R   C1R   C2R   gd_29   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   O7R   gd_18   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   C4R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   O2P   gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   C4R   gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   O2P   gd_18   ;  from ADE sugar dihedrals
   C1R   C2R   O7R   HAA   gd_23   ;  from ADE sugar dihedrals
   N1B   C1R   C2R   O7R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   N1B   C8B   gd_16   ;  from ADE sugar dihedrals
;
;  HAB-based torsion gone for LYB  C4R C5R O8R HAB gd_2 ;  additional ADE-based sugar dihedral
;
   N1B   C1R   C2R   C3R   gd_17   ;  additional ADE-based sugar dihedral
   N1B   C1R   O6R   C4R   gd_17   ;  additional ADE-based sugar dihedral
   C2    C26   C27   N29   gd_40   ;  from GLN dihedral
   C26   C27   N29   HAD   gd_14   ;  from GLN dihedral
   C30   C31   C32   N33   gd_40   ;  from GLN dihedral
   C31   C32   N33   HAF   gd_14   ;  from GLN dihedral
   C7    C37   C38   N40   gd_40   ;  from GLN dihedral
   C37   C38   N40   HAH   gd_14   ;  from GLN dihedral
   C41   C42   C43   N45   gd_40   ;  from GLN dihedral
   C42   C43   N45   HAJ   gd_14   ;  from GLN dihedral
   C48   C49   C50   N52   gd_40   ;  from GLN dihedral
   C49   C50   N52   HAL   gd_14   ;  from GLN dihedral
   C18   C60   C61   N62   gd_40   ;  from GLN dihedral
   C60   C61   N62   HAN   gd_14   ;  from GLN dihedral
   C5M   C5B   C6B   C6M   gd_33   ;  dimethylbenzimidazole methyl dihedral fix
   C4B   C5B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C8B   C7B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C7B   C6B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C9B   C4B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C35   C5    C4    N21   gd_10   ;  corrin ring methyl planarity
   C35   C5    C6    N22   gd_10   ;  corrin ring methyl planarity
   C53   C15   C14   N23   gd_10   ;  corrin ring methyl planarity
   C53   C1    C16   N24   gd_10   ;  corrin ring methyl planarity
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N21   C4    C5    C6    gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C4    C5    C6    N22   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N22   C9    C10   C11   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C9    C10   C11   N23   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N23   C14   C15   C16   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C14   C15   C16   N24   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C1    C2    C26   C27   gd_40   ;  corrin ring HEMC derived CHn torsions
   C25   C2    C26   C27   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C26   C27   O28   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C3    C30   C31   gd_9    ;  corrin ring HEMC derived CHn torsions
   C3    C30   C31   C32   gd_40   ;  corrin ring HEMC derived CHn torsions
   C30   C31   C32   O34   gd_40   ;  corrin ring HEMC derived CHn torsions
   C6    C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C36   C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C37   C38   O39   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C8    C41   C42   gd_9    ;  corrin ring HEMC derived CHn torsions
   C8    C41   C42   C43   gd_34   ;  corrin ring HEMC derived CHn torsions
   C41   C42   C43   O44   gd_40   ;  corrin ring HEMC derived CHn torsions
   C12   C13   C48   C49   gd_9    ;  corrin ring HEMC derived CHn torsions
   C13   C48   C49   C50   gd_34   ;  corrin ring HEMC derived CHn torsions
   C48   C49   C50   O51   gd_40   ;  corrin ring HEMC derived CHn torsions
   C16   C17   C55   C56   gd_40   ;  corrin ring HEMC derived CHn torsions
   C54   C17   C56   C57   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C55   C56   C57   gd_34   ;  corrin ring HEMC derived CHn torsions
   C55   C56   C57   O58   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C18   C60   C61   gd_9    ;  corrin ring HEMC derived CHn torsions
   C18   C60   C61   O63   gd_34   ;  corrin ring HEMC derived CHn torsions
   C18   C17   C55   C56   gd_9    ;  corrin ring HEMC derived CHn torsions
```

```
   N59   C1P   C2P   O3    gd_34   ;  amide linkage torsion terms
   N59   C1P   C2P   C3P   gd_34   ;  amide linkage torsion terms
   C2P   C1P   N59   C57   gd_34   ;  amide linkage torsion terms
   C56   C57   N59   C1P   gd_14   ;  amide linkage torsion terms
   C55   C56   C57   N59   gd_40   ;  amide linkage torsion terms
   C17   C55   C56   C57   gd_40   ;  amide linkage torsion terms
   C5    C4    N21   C1    gd_14   ;  corrin ring sp3-containing torsions
   C10   C9    N22   C6    gd_14   ;  corrin ring sp3-containing torsions
   C5    C6    N22   C9    gd_14   ;  corrin ring sp3-containing torsions
   C15   C14   N23   C11   gd_14   ;  corrin ring sp3-containing torsions
   C10   C11   N23   C14   gd_14   ;  corrin ring sp3-containing torsions
   C15   C16   N24   C19   gd_14   ;  corrin ring sp3-containing torsions
   C4    N21   C1    C2    gd_40   ;  corrin ring sp3-containing torsions
   C18   C19   N24   C16   gd_40   ;  corrin ring sp3-containing torsions
   N22   C6    C5    C4    gd_33   ;  corrin ring sp3-containing torsions
   N23   C11   C10   C9    gd_33   ;  corrin ring sp3-containing torsions
   C19   C18   C17   C55   gd_34   ;  corrin ring sp3-containing torsions
   C55   C17   C16   C15   gd_40   ;  corrin ring sp3-containing torsions
   C17   C18   C19   C1    gd_34   ;  corrin ring sp3-containing torsions
   C18   C19   C1    C2    gd_34   ;  corrin ring sp3-containing torsions
   C17   C16   C15   C14   gd_10   ;  corrin ring sp3-containing torsions
   C16   C15   C14   C13   gd_10   ;  corrin ring sp3-containing torsions
   C15   C14   C13   C12   gd_40   ;  corrin ring sp3-containing torsions
   C6    C7    C8    C9    gd_34   ;  corrin ring sp3-containing torsions
   C8    C7    C6    C5    gd_34   ;  corrin ring sp3-containing torsions
   C30   C3    C2    C1    gd_34   ;  corrin ring sp3-containing torsions
   C11   C12   C13   C14   gd_34   ;  corrin ring sp3-containing torsions
   C13   C12   C11   C10   gd_34   ;  corrin ring sp3-containing torsions
   C10   C9    C8    C7    gd_10   ;  corrin ring sp3-containing torsions
   C5    C4    C3    C30   gd_34   ;  corrin ring sp3-containing torsions
   C3    C2    C1    C19   gd_34   ;  corrin ring sp3-containing torsions
;
; standard Lysine torsion topology
;
   -CA   -C    N     CA    gd_14   ;  Standard LYS (lysine)
   -C    N     CA    C     gd_39   ;  Standard LYS (lysine)
   N     CA    CB    CG    gd_34   ;  Standard LYS (lysine)
   N     CA    C     +N    gd_40   ;  Standard LYS (lysine)
   CA    CB    CG    CD    gd_34   ;  Standard LYS (lysine)
   CB    CG    CD    CE    gd_34   ;  Standard LYS (lysine)
   CG    CD    CE    NZ    gd_34   ;  Standard LYS (lysine)
   CD    CE    NZ    HZ1   gd_29   ;  Standard LYS (lysine)
   C4R   C5R   O8R   CLB   gd_23   ;  LYS-B12 linkage dihedral terms
   C5R   O8R   CLB   OLB   gd_12   ;  LYS-B12 linkage dihedral terms
   O8R   CLB   NZ    CE    gd_14   ;  LYS-B12 linkage dihedral terms
   OLB   CLB   NZ    CE    gd_14   ;  LYS-B12 linkage dihedral terms
   C9B   N3B   FE    N21   gd_38   ;   THIS IS NEW!!!
   N3B   FE    N21   C1    gd_38   ;   THIS IS NEW!!!
   N3B   FE    N22   C6    gd_38   ;   THIS IS NEW!!!
   N3B   FE    N23   C11   gd_38   ;   THIS IS NEW!!!
   N3B   FE    N24   C16   gd_38   ;   THIS IS NEW!!!
;
; Use of LYB, which employs the pdb2gmx method for sewing the peptide chain together,
; requires the addition of this very new, bulky amino acid to aminoacids.dat.
```

```
[ BCN ]
;
; cyanocobalamin based on the HEMC CO parameters
;
 [ atoms ]
 C27      C        0.38000     0    ;  from GLN residue
 O28      O       -0.38000     0    ;  from GLN residue
 N29      NT      -0.83000     0    ;  from GLN residue
 HAE      H        0.41500     0    ;  from GLN residue
 HAD      H        0.41500     0    ;  from GLN residue
 C32      C        0.38000     1    ;  from GLN residue
 O34      O       -0.38000     1    ;  from GLN residue
 N33      NT      -0.83000     1    ;  from GLN residue
 HAG      H        0.41500     1    ;  from GLN residue
 HAF      H        0.41500     1    ;  from GLN residue
 C38      C        0.38000     2    ;  from GLN residue
 O39      O       -0.38000     2    ;  from GLN residue
 N40      NT      -0.83000     2    ;  from GLN residue
 HAI      H        0.41500     2    ;  from GLN residue
 HAH      H        0.41500     2    ;  from GLN residue
 C43      C        0.38000     3    ;  from GLN residue
 O44      O       -0.38000     3    ;  from GLN residue
 N45      NT      -0.83000     3    ;  from GLN residue
 HAK      H        0.41500     3    ;  from GLN residue
 HAJ      H        0.41500     3    ;  from GLN residue
 C50      C        0.38000     4    ;  from GLN residue
 O51      O       -0.38000     4    ;  from GLN residue
 N52      NT      -0.83000     4    ;  from GLN residue
 HAM      H        0.41500     4    ;  from GLN residue
 HAL      H        0.41500     4    ;  from GLN residue
 C61      C        0.38000     5    ;  from GLN residue
 O63      O       -0.38000     5    ;  from GLN residue
 N62      NT      -0.83000     5    ;  from GLN residue
 HAO      H        0.41500     5    ;  from GLN residue
 HAN      H        0.41500     5    ;  from GLN residue
 C20      CH3      0.00000     6    ;  methyl group
 C25      CH3      0.00000     7    ;  methyl group
 C36      CH3      0.00000     8    ;  methyl group
 C46      CH3      0.00000     9    ;  methyl group
 C47      CH3      0.00000     10   ;  methyl group
 C54      CH3      0.00000     11   ;  methyl group
 C26      CH2      0.00000     12   ;  non-polar CHn fragments
 C30      CH2      0.00000     13   ;  non-polar CHn fragments
 C31      CH2      0.00000     13   ;  non-polar CHn fragments
 C37      CH2      0.00000     14   ;  non-polar CHn fragments
 C41      CH2      0.00000     15   ;  non-polar CHn fragments
 C42      CH2      0.00000     15   ;  non-polar CHn fragments
 C48      CH2      0.00000     16   ;  non-polar CHn fragments
 C49      CH2      0.00000     16   ;  non-polar CHn fragments
 C56      CH2      0.00000     17   ;  non-polar CHn fragments
 C55      CH2      0.00000     17   ;  non-polar CHn fragments
 C60      CH2      0.00000     18   ;  non-polar CHn fragments
 C2R      CH1      0.15000     19   ;  C2*-O2*-H2* from ADE
 O7R      OA      -0.54800     19   ;  C2*-O2*-H2* from ADE
 HAA      H        0.39800     19   ;  C2*-O2*-H2* from ADE
 C1R      CH1      0.20000     20   ;  C1*-O4*-C4* from ADE
 O6R      OA      -0.36000     20   ;  C1*-O4*-C4* from ADE
 C4R      CH1      0.16000     20   ;  C1*-O4*-C4* from ADE
 C3R      CH1      0.00000     21   ;  C3* from ADE
 C5R      CH2      0.15000     22   ;  C2*-O2*-H2* from ADE
 O8R      OA      -0.54800     22   ;  C2*-O2*-H2* from ADE
 HAB      H        0.39800     22   ;  C2*-O2*-H2* from ADE
 P        P        2.20000     23   ;  PO3+O3* fragment from ADE
 O2       OA      -0.80000     23   ;  PO3+O3* fragment from ADE
 O4       OM      -1.00000     23   ;  PO3+O3* fragment from ADE
 O5       OM      -1.00000     23   ;  PO3+O3* fragment from ADE
 O3       OA      -0.80000     23   ;  PO3+O3* fragment from ADE
 C2P      CH1      0.35000     24   ;  non-polar CHn fragment
 C3P      CH3      0.00000     24   ;  non-polar CHn fragment
 C1P      CH2      0.00000     24   ;  non-polar CHn fragment
 N59      N       -0.28000     25   ;  tempered GLN fragment charges
 HAC      H        0.28000     25   ;  tempered GLN fragment charges
 C57      C        0.38000     25   ;  tempered GLN fragment charges
 O58      O       -0.38000     25   ;  tempered GLN fragment charges
 C5B      C        0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C5M      CH3      0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6B      C        0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6M      CH3      0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C4B      C       -0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H4B      H        0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C7B      C       -0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
```

```
 H7B     H        0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 N3B     NR      -0.55000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 C9B     C        0.20000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 N1B     NR      -0.30000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C8B     C        0.20000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C2B     C        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H2B     H        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C5      C       -0.05000     33   ;  C-CH3 group (non-polar)
 C35     CH3      0.00000     33   ;  C-CH3 group (non-polar)
 C15     C       -0.05000     34   ;  C-CH3 group (non-polar)
 C53     CH3      0.00000     34   ;  C-CH3 group (non-polar)
 FE      FE       1.00000     35   ;  HEMC Fe-N group
 N21     NR      -0.44000     35   ;  HEMC Fe-N group
 N22     NR      -0.50000     35   ;  HEMC Fe-N group
 N23     NR      -0.50000     35   ;  HEMC Fe-N group
 N24     NR      -0.44000     35   ;  HEMC Fe-N group
 C1      CH0      0.22000     36   ;  non-polar HEMC-derived corrin atoms
 C2      CH0      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C3      CH1      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C4      C        0.38000     36   ;  non-polar HEMC-derived corrin atoms
 C6      C        0.29000     37   ;  non-polar HEMC-derived corrin atoms
 C7      CH0      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C8      CH1      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C9      C        0.35000     37   ;  non-polar HEMC-derived corrin atoms
 C16     C        0.38000     38   ;  non-polar HEMC-derived corrin atoms
 C17     CH0      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C18     CH1      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C19     CH1      0.24000     38   ;  non-polar HEMC-derived corrin atoms
 C11     C        0.35000     39   ;  non-polar HEMC-derived corrin atoms
 C12     CH0      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C13     CH1      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C14     C        0.29000     39   ;  non-polar HEMC-derived corrin atoms
 C10     C       -0.24000     40   ;  aromatic C-H from TRP, PHE
 H10     H        0.14000     40   ;  aromatic C-H from TRP, PHE
;
; cyano group addition to the original B12 topology
;
 C1N     C        0.04000     41   ;  CN group on Fe
 N1C     N       -0.42000     41   ;  CN group on Fe
;
; Since CO is not defined as an atom in GROMOSxx, CO is converted to FE and the HEME
; values are employed.  This is a workaround due for proper implementation.
;
[ bonds ]
;  ai    aj    gromos type
   C26   C27    gb_27   ;  from GLN fragment 0
   C27   O28    gb_5    ;  from GLN
   C27   N29    gb_9    ;  from GLN
   N29   HAE    gb_2    ;  from GLN
   N29   HAD    gb_2    ;  from GLN
   C31   C32    gb_27   ;  from GLN fragment 1
   C32   O34    gb_5    ;  from GLN
   C32   N33    gb_9    ;  from GLN
   N33   HAG    gb_2    ;  from GLN
   N33   HAF    gb_2    ;  from GLN
   C37   C38    gb_27   ;  from GLN fragment 2
   C38   O39    gb_5    ;  from GLN
   C38   N40    gb_9    ;  from GLN
   N40   HAI    gb_2    ;  from GLN
   N40   HAH    gb_2    ;  from GLN
   C42   C43    gb_27   ;  from GLN fragment 3
   C43   O44    gb_5    ;  from GLN
   C43   N45    gb_9    ;  from GLN
   N45   HAK    gb_2    ;  from GLN
   N45   HAJ    gb_2    ;  from GLN
   C49   C50    gb_27   ;  from GLN fragment 4
   C50   O51    gb_5    ;  from GLN
   C50   N52    gb_9    ;  from GLN
   N52   HAM    gb_2    ;  from GLN
   N52   HAL    gb_2    ;  from GLN
   C60   C61    gb_27   ;  from GLN fragment 5
   C61   O63    gb_5    ;  from GLN
   C61   N62    gb_9    ;  from GLN
   N62   HAO    gb_2    ;  from GLN
   N62   HAN    gb_2    ;  from GLN
   FE    N21    gb_35   ;  FE-N bond from HEMC
   FE    N22    gb_35   ;  FE-N bond from HEMC
   FE    N23    gb_35   ;  FE-N bond from HEMC
   FE    N24    gb_35   ;  FE-N bond from HEMC
   FE    N3B    gb_37   ;  FE-N3B bond from HEMC not in corrin ring
   P     O2     gb_28   ;  from ADE phosphate
```

```
P     O4     gb_24   ;  from ADE phosphate
P     O5     gb_24   ;  from ADE phosphate
P     O3     gb_28   ;  from ADE phosphate
N21   C1     gb_21   ;  corrin ring N-CHn bonds
N21   C4     gb_14   ;  corrin ring N-C bonds
N22   C6     gb_14   ;  corrin ring N-C bonds
N22   C9     gb_14   ;  corrin ring N-C bonds
N23   C11    gb_14   ;  corrin ring N-C bonds
N23   C14    gb_14   ;  corrin ring N-C bonds
N24   C16    gb_14   ;  corrin ring N-C bonds
N24   C19    gb_21   ;  corrin ring N-CHn bonds
C30   C31    gb_27   ;  CH2-CH2 bonds
C41   C42    gb_27   ;  CH2-CH2 bonds
C48   C49    gb_27   ;  CH2-CH2 bonds
C55   C56    gb_27   ;  CH2-CH2 bonds
C56   C57    gb_27   ;  CH2-CH2 bonds
N1B   C1R    gb_22   ;  sugar bonds from ADE
C1R   C2R    gb_26   ;  sugar bonds from ADE
C2R   O7R    gb_20   ;  sugar bonds from ADE
O7R   HAA    gb_1    ;  sugar bonds from ADE
C2R   C3R    gb_26   ;  sugar bonds from ADE
C3R   C4R    gb_26   ;  sugar bonds from ADE
C3R   O2     gb_20   ;  sugar bonds from ADE
C4R   C5R    gb_26   ;  sugar bonds from ADE
C5R   O8R    gb_20   ;  sugar bonds from ADE
O8R   HAB    gb_1    ;  sugar bonds from ADE
C4R   O6R    gb_20   ;  sugar bonds from ADE
O6R   C1R    gb_20   ;  sugar bonds from ADE
C1P   N59    gb_9    ;  amide corrin - phosphate linkage
C1P   C2P    gb_27   ;  amide corrin - phosphate linkage
C2P   C3P    gb_27   ;  amide corrin - phosphate linkage
C2P   O3     gb_20   ;  amide corrin - phosphate linkage
N59   HAC    gb_2    ;  amide corrin - phosphate linkage
N59   C57    gb_9    ;  amide corrin - phosphate linkage
C57   O58    gb_5    ;  amide corrin - phosphate linkage
N1B   C2B    gb_10   ;  dimethylbenzimidazole ring
C2B   N3B    gb_10   ;  dimethylbenzimidazole ring
C2B   H2B    gb_3    ;  dimethylbenzimidazole ring
N3B   C9B    gb_10   ;  dimethylbenzimidazole ring
C9B   C4B    gb_16   ;  dimethylbenzimidazole ring
C4B   C5B    gb_16   ;  dimethylbenzimidazole ring
C4B   H4B    gb_3    ;  dimethylbenzimidazole ring
C5B   C6B    gb_16   ;  dimethylbenzimidazole ring
C5B   C5M    gb_27   ;  dimethylbenzimidazole ring
C6B   C7B    gb_16   ;  dimethylbenzimidazole ring
C6B   C6M    gb_27   ;  dimethylbenzimidazole ring
C7B   C8B    gb_16   ;  dimethylbenzimidazole ring
C7B   H7B    gb_3    ;  dimethylbenzimidazole ring
C8B   N1B    gb_10   ;  dimethylbenzimidazole ring
C8B   C9B    gb_16   ;  dimethylbenzimidazole ring
C1    C20    gb_27   ;  corrin ring carbon framework
C1    C2     gb_27   ;  corrin ring carbon framework
C2    C3     gb_27   ;  corrin ring carbon framework
C2    C25    gb_27   ;  corrin ring carbon framework
C2    C26    gb_27   ;  corrin ring carbon framework
C3    C4     gb_27   ;  corrin ring carbon framework
C3    C30    gb_27   ;  corrin ring carbon framework
C4    C5     gb_17   ;  corrin ring carbon framework
C5    C6     gb_17   ;  corrin ring carbon framework
C5    C35    gb_27   ;  corrin ring carbon framework
C6    C7     gb_27   ;  corrin ring carbon framework
C7    C8     gb_27   ;  corrin ring carbon framework
C7    C37    gb_27   ;  corrin ring carbon framework
C7    C36    gb_27   ;  corrin ring carbon framework
C8    C9     gb_27   ;  corrin ring carbon framework
C8    C41    gb_27   ;  corrin ring carbon framework
C9    C10    gb_17   ;  corrin ring carbon framework
C10   C11    gb_17   ;  corrin ring carbon framework
C11   C12    gb_27   ;  corrin ring carbon framework
C12   C46    gb_27   ;  corrin ring carbon framework
C12   C47    gb_27   ;  corrin ring carbon framework
C12   C13    gb_27   ;  corrin ring carbon framework
C13   C14    gb_27   ;  corrin ring carbon framework
C13   C48    gb_27   ;  corrin ring carbon framework
C14   C15    gb_17   ;  corrin ring carbon framework
C15   C16    gb_17   ;  corrin ring carbon framework
C15   C53    gb_27   ;  corrin ring carbon framework
C16   C17    gb_27   ;  corrin ring carbon framework
C17   C18    gb_27   ;  corrin ring carbon framework
C17   C54    gb_27   ;  corrin ring carbon framework
C17   C55    gb_27   ;  corrin ring carbon framework
```

```
   C18   C19    gb_27   ;  corrin ring carbon framework
   C18   C60    gb_27   ;  corrin ring carbon framework
   C19   C1     gb_27   ;  corrin ring carbon framework
   C10   H10    gb_3    ;  corrin ring C10-H10 bond
;
; cyano group addition to the original B12 topology
;
   FE   C1N    gb_30    ;  cyano group on the Fe
  C1N   N1C    gb_4     ;  cyano group on the Fe
    [ exclusions ]
;  ai    aj
   FE    N1C   ;   new add
   FE    C1    ;   new add
   FE    C2
   FE    C3
   FE    C5
   FE    C7
   FE    C8
   FE    C10
   FE    C12
   FE    C13
   FE    C15
   FE    C17
   FE    C18
   FE    C20
   N21   C25
   N21   C26
   N21   C30
   N21   C35
   N21   C6
   N21   C9
   N21   C11
   N21   C14
   N21   C16
   N21   C19
   N21   C10
   N22   C1
   N22   C4
   N22   C36
   N22   C37
   N22   C11
   N22   C14
   N22   C16
   N22   C19
   N22   C15
   N23   C16
   N23   C19
   N23   C1
   N23   C4
   N23   C6
   N23   C9
   N23   C46
   N23   C47
   N23   C48
   N23   C5
   N24   C4
   N24   C5
   N24   C6
   N24   C9
   N24   C10
   N24   C11
   N24   C14
   N24   C55
   N24   C54
   N24   C60
   C1R   C7B
   C1R   C9B
   C1R   N3B
   N1B   C6B
   N1B   C4B
   C8B   C5B
   C8B   C5M
   C8B   C6M
   C7B   C4B
   C7B   N3B
   C7B   C2B
   C2B   C9B
   C5B   C2B
   C5M   C6M
   C1    C30   ;  HEMC-based C framework exclusions
   C1    C5    ;  HEMC-based C framework exclusions
```

```
   C2    C5    ;  HEMC-based C framework exclusions
   C3    C35   ;  HEMC-based C framework exclusions
   C3    C6    ;  HEMC-based C framework exclusions
   C4    C26   ;  HEMC-based C framework exclusions
   C4    C7    ;  HEMC-based C framework exclusions
   C30   C26   ;  HEMC-based C framework exclusions
   C30   C5    ;  HEMC-based C framework exclusions
   C5    C8    ;  HEMC-based C framework exclusions
   C5    C9    ;  HEMC-based C framework exclusions
   C5    C36   ;  HEMC-based C framework exclusions
   C5    C37   ;  HEMC-based C framework exclusions
   C35   C7    ;  HEMC-based C framework exclusions
   C6    C41   ;  HEMC-based C framework exclusions
   C6    C10   ;  HEMC-based C framework exclusions
   C7    C10   ;  HEMC-based C framework exclusions
   C8    H10   ;  HEMC-based C framework exclusions
   C8    C11   ;  HEMC-based C framework exclusions
   C9    C36   ;  HEMC-based C framework exclusions
   C9    C37   ;  HEMC-based C framework exclusions
   C9    C12   ;  HEMC-based C framework exclusions
   C36   C41   ;  HEMC-based C framework exclusions
   C37   C10   ;  HEMC-based C framework exclusions
   C10   C13   ;  HEMC-based C framework exclusions
   C10   C14   ;  HEMC-based C framework exclusions
   C10   C46   ;  HEMC-based C framework exclusions
   C10   C47   ;  HEMC-based C framework exclusions
   H10   C12   ;  HEMC-based C framework exclusions
   C11   C48   ;  HEMC-based C framework exclusions
   C11   C15   ;  HEMC-based C framework exclusions
   C12   C15   ;  HEMC-based C framework exclusions
   C13   C53   ;  HEMC-based C framework exclusions
   C13   C16   ;  HEMC-based C framework exclusions
   C14   C46   ;  HEMC-based C framework exclusions
   C14   C47   ;  HEMC-based C framework exclusions
   C14   C17   ;  HEMC-based C framework exclusions
   C46   C48   ;  HEMC-based C framework exclusions
   C47   C48   ;  HEMC-based C framework exclusions
   C48   C15   ;  HEMC-based C framework exclusions
   C15   C18   ;  HEMC-based C framework exclusions
   C15   C19   ;  HEMC-based C framework exclusions
   C15   C54   ;  HEMC-based C framework exclusions
   C15   C55   ;  HEMC-based C framework exclusions
   C53   C17   ;  HEMC-based C framework exclusions
   C16   C60   ;  HEMC-based C framework exclusions
   C19   C54   ;  HEMC-based C framework exclusions
   C19   C55   ;  HEMC-based C framework exclusions
   C54   C60   ;  HEMC-based C framework exclusions
   C55   C60   ;  HEMC-based C framework exclusions
;
; cyano group addition to the original B12 topology
;
   N21   N1C   ;  cyano exclusions from HEMC CO group
   N22   N1C   ;  cyano exclusions from HEMC CO group
   N23   N1C   ;  cyano exclusions from HEMC CO group
   N24   N1C   ;  cyano exclusions from HEMC CO group
   C1    C1N   ;  cyano exclusions from HEMC CO group
   C4    C1N   ;  cyano exclusions from HEMC CO group
   C6    C1N   ;  cyano exclusions from HEMC CO group
   C9    C1N   ;  cyano exclusions from HEMC CO group
   C11   C1N   ;  cyano exclusions from HEMC CO group
   C14   C1N   ;  cyano exclusions from HEMC CO group
   C16   C1N   ;  cyano exclusions from HEMC CO group
   C19   C1N   ;  cyano exclusions from HEMC CO group
   N3B   N1C   ;  cyano exclusion unique to 6-coordinate iron
   C1N   C9B   ;  additional cyano exclusion at Fe 6-center
   C1N   C2B   ;  additional cyano exclusion at Fe 6-center
 [ angles ]
;  ai    aj    ak   gromos type
   C2    C26   C27   ga_15   ;  from GLN, fragment 1
   C26   C27   O28   ga_30   ;  from GLN
   C26   C27   N29   ga_19   ;  from GLN
   O28   C27   N29   ga_33   ;  from GLN
   C27   N29   HAE   ga_23   ;  from GLN
   C27   N29   HAD   ga_23   ;  from GLN
   HAE   N29   HAD   ga_24   ;  from GLN
   C30   C31   C32   ga_15   ;  from GLN, fragment 2
   C31   C32   O34   ga_30   ;  from GLN
   C31   C32   N33   ga_19   ;  from GLN
   O34   C32   N33   ga_33   ;  from GLN
   C32   N33   HAG   ga_23   ;  from GLN
   C32   N33   HAF   ga_23   ;  from GLN
```

```
HAG   N33   HAF   ga_24   ;  from GLN
C7    C37   C38   ga_15   ;  from GLN, fragment 3
C37   C38   O39   ga_30   ;  from GLN
C37   C38   N40   ga_19   ;  from GLN
O39   C38   N40   ga_33   ;  from GLN
C38   N40   HAI   ga_23   ;  from GLN
C38   N40   HAH   ga_23   ;  from GLN
HAI   N40   HAH   ga_24   ;  from GLN
C41   C42   C43   ga_15   ;  from GLN, fragment 4
C42   C43   O44   ga_30   ;  from GLN
C42   C43   N45   ga_19   ;  from GLN
O44   C43   N45   ga_33   ;  from GLN
C43   N45   HAK   ga_23   ;  from GLN
C43   N45   HAJ   ga_23   ;  from GLN
HAK   N45   HAJ   ga_24   ;  from GLN
C48   C49   C50   ga_15   ;  from GLN, fragment 5
C49   C50   O51   ga_30   ;  from GLN
C49   C50   N52   ga_19   ;  from GLN
O51   C50   N52   ga_33   ;  from GLN
C50   N52   HAM   ga_23   ;  from GLN
C50   N52   HAL   ga_23   ;  from GLN
HAM   N52   HAL   ga_24   ;  from GLN
C18   C60   C61   ga_15   ;  from GLN, fragment 6
C60   C61   O63   ga_30   ;  from GLN
C60   C61   N62   ga_19   ;  from GLN
O63   C61   N62   ga_33   ;  from GLN
C61   N62   HAO   ga_23   ;  from GLN
C61   N62   HAN   ga_23   ;  from GLN
HAO   N62   HAN   ga_24   ;  from GLN
N21   FE    N22   ga_2    ;  corrin ring Fe-N angle
N21   FE    N24   ga_2    ;  corrin ring Fe-N angle
N22   FE    N23   ga_2    ;  corrin ring Fe-N angle
N23   FE    N24   ga_2    ;  corrin ring Fe-N angle
N21   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N22   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N23   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N24   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
FE    N21   C1    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N21   C4    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N22   C6    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N22   C9    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N23   C11   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N23   C14   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N24   C16   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N24   C19   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N3B   C9B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
FE    N3B   C2B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
C8B   N1B   C2B   ga_7    ;  angle containing C8B, see minimization issues discussion
N1B   C8B   C9B   ga_7    ;  angle containing C8B, see minimization issues discussion
C8B   C9B   N3B   ga_7    ;  angle containing C8B, see minimization issues discussion
C7B   C8B   N1B   ga_39   ;  angle containing C8B, see minimization issues discussion
C8B   N1B   C1R   ga_37   ;  angle containing C8B, see minimization issues discussion
C4B   C9B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C6B   C7B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C7B   C8B   C9B   ga_27   ;  angle containing C8B, see minimization issues discussion
N21   C1    C2    ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C1    C20   ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C4    C3    ga_33   ;  corrin ring-specific but HEMC-derived angles
C4    N21   C1    ga_6    ;  corrin ring-specific but HEMC-derived angles
C5    C4    N21   ga_33   ;  corrin ring-specific but HEMC-derived angles
C19   C1    N21   ga_13   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C5    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C7    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C9    C8    ga_33   ;  corrin ring-specific but HEMC-derived angles
C9    N22   C6    ga_6    ;  corrin ring-specific but HEMC-derived angles
C10   C9    N22   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C10   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C12   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C14   C13   ga_33   ;  corrin ring-specific but HEMC-derived angles
C14   N23   C11   ga_6    ;  corrin ring-specific but HEMC-derived angles
C15   C14   N23   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C16   C15   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C19   C1    ga_13   ;  corrin ring-specific but HEMC-derived angles
C19   N24   C16   ga_6    ;  corrin ring-specific but HEMC-derived angles
C17   C16   N24   ga_33   ;  corrin ring-specific but HEMC-derived angles
C18   C19   N24   ga_13   ;  corrin ring-specific but HEMC-derived angles
C3R   O2    P     ga_26   ;  phosphate angle from ADE
O2    P     O3    ga_5    ;  phosphate angle from ADE
O2    P     O4    ga_14   ;  phosphate angle from ADE
O2    P     O5    ga_14   ;  phosphate angle from ADE
O3    P     O4    ga_14   ;  phosphate angle from ADE
```

```
O3    P     O5    ga_14   ;  phosphate angle from ADE
O4    P     O5    ga_29   ;  phosphate angle from ADE
P     O3    C2P   ga_26   ;  phosphate angle from ADE
O2    C3R   C2R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O2    C3R   C4R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C1P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C3P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
C1    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C3    ga_13   ;  CHn-CHn-CHn angles
C1    C19   C18   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C19   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C20   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C30   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C3    C30   C31   ga_13   ;  CHn-CHn-CHn angles
C7    C8    C41   ga_13   ;  CHn-CHn-CHn angles
C8    C41   C42   ga_13   ;  CHn-CHn-CHn angles
C12   C13   C48   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C46   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C13   C48   C49   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C19   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C17   C55   C56   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C54   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C19   C1    C20   ga_13   ;  CHn-CHn-CHn angles
C19   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C25   C2    C26   ga_13   ;  CHn-CHn-CHn angles
C46   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C54   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C36   C7    C37   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C4    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C3    C30   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C8    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C7    C8    C9    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C9    C8    C41   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C13   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C46   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C47   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C12   C13   C14   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C14   C13   C48   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C18   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C54   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C55   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C5    C6    ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
C9    C10   C11   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
C14   C15   C16   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
C3    C4    C5    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C4    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C5    C6    C7    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C6    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C8    C9    C10   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C10   C11   C12   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C13   C14   C15   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C14   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C15   C16   C17   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C16   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
C5M   C5B   C4B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C5M   C5B   C6B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C6M   C6B   C5B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C6M   C6B   C7B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C4B   C5B   C6B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B   C4B   C9B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B   C6B   C7B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
N1B   C1R   C2R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C1R   O6R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C2B   N3B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C2B   N1B   C1R   ga_37   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N3B   C9B   C4B   ga_39   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C9B   N3B   C2B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C1R   C2R   C3R   ga_8    ;  from ADE sugar angle
C1R   C2R   O7R   ga_9    ;  from ADE sugar angle
C1R   O6R   C4R   ga_10   ;  from ADE sugar angle
C2R   C1R   O6R   ga_9    ;  from ADE sugar angle
```

```
   C2R   C3R   C4R   ga_8    ;  from ADE sugar angle
   C2R   O7R   HAA   ga_12   ;  from ADE sugar angle
   C3R   C2R   O7R   ga_9    ;  from ADE sugar angle
   C3R   C4R   C5R   ga_8    ;  from ADE sugar angle
   C3R   C4R   O6R   ga_9    ;  from ADE sugar angle
   C4R   C5R   O8R   ga_9    ;  from ADE sugar angle
   C5R   O8R   HAB   ga_12   ;  from ADE sugar angle
   C5R   C4R   O6R   ga_9    ;  from ADE sugar angle
   C1P   C2P   C3P   ga_13   ;  amide linkage angle
   C57   C56   C55   ga_13   ;  amide linkage angle
   C57   N59   HAC   ga_23   ;  from GLN angle
   N59   C57   O58   ga_33   ;  from GLN angle
   C56   C57   N59   ga_19   ;  from GLN angle
   O58   C57   C56   ga_30   ;  from GLN angle
   C1P   N59   C57   ga_31   ;  from force field angle definitions
   C1P   N59   HAC   ga_18   ;  from force field angle definitions
   C2P   C1P   N59   ga_15   ;  from force field angle definitions
   C5B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C9B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C6B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   C8B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   N1B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   N3B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   C9    C10   H10   ga_25   ;  corrin ring C-C10-H angle
   C11   C10   H10   ga_20   ;  corrin ring C-C10-H angle
;
; cyano group addition to the original B12 topology
;
   N21   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   N22   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   N23   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   N24   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   FE    C1N   N1C   ga_41   ;  cyano group from HEMC CO group
   N3B   FE    C1N   ga_41   ;  cyano group from HEMC CO group (found during pdb2gmx)
   [ impropers ]
;  ai    aj    ak    al   gromos type
   C1R   C8B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   N1B   C8B   C9B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C7B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C2B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C7B   C6B   C5B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C9B   N3B   C2B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C8B   C9B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C6B   C5B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C6B   C5B   C4B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5B   C4B   C9B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C8B   C7B   C6B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C4B   N3B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   N3B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C2B   N1B   C8B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5M   C4B   C6B   C5B   gi_1    ;  dimethylbenzimidazole methyl groups
   C6M   C7B   C5B   C6B   gi_1    ;  dimethylbenzimidazole methyl groups
   C2B   N1B   N3B   H2B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C4B   C9B   C5B   H4B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C7B   C8B   C6B   H7B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   N3B   FE    C2B   C9B   gi_1    ;  Fe-dimethylbenzimidazole planarity
   N21   C4    C5    C6    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C6    C5    C4    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C9    C10   C11   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C11   C10   C9    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C14   C15   C16   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N24   C16   C15   C14   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C15   C16   C14   C53   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C27   O28   N29   C26   gi_1    ;  from GLN improper torsion definition
   N29   HAE   HAD   C27   gi_1    ;  from GLN improper torsion definition
   C32   O34   N33   C31   gi_1    ;  from GLN improper torsion definition
   N33   HAG   HAF   C32   gi_1    ;  from GLN improper torsion definition
   C38   O39   N40   C37   gi_1    ;  from GLN improper torsion definition
   N40   HAI   HAH   C38   gi_1    ;  from GLN improper torsion definition
   C43   O44   N45   C42   gi_1    ;  from GLN improper torsion definition
   N45   HAK   HAJ   C43   gi_1    ;  from GLN improper torsion definition
   C50   O51   N52   C49   gi_1    ;  from GLN improper torsion definition
   N52   HAM   HAL   C50   gi_1    ;  from GLN improper torsion definition
   C61   O63   N62   C60   gi_1    ;  from GLN improper torsion definition
   N62   HAO   HAN   C61   gi_1    ;  from GLN improper torsion definition
   C57   C56   O58   N59   gi_1    ;  amide linkage C57 planarity
   N59   C57   C1P   HAC   gi_1    ;  amide linkage N59 planarity
   C4    N21   C3    C5    gi_1    ;  corrin ring C sp2 planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring C sp2 planarity
   C6    N22   C5    C7    gi_1    ;  corrin ring C sp2 planarity
```

```
   C9    N22   C10   C8    gi_1    ;  corrin ring C sp2 planarity
   C11   N23   C10   C12   gi_1    ;  corrin ring C sp2 planarity
   C14   N23   C15   C13   gi_1    ;  corrin ring C sp2 planarity
   C15   C14   C16   C53   gi_1    ;  corrin ring C sp2 planarity
   C16   N24   C15   C17   gi_1    ;  corrin ring C sp2 planarity
   C10   C9    C11   H10   gi_1    ;  corrin ring C10 planarity
   C18   C17   C19   C60   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C19   N24   C18   C1    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C3    C2    C30   C4    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C8    C9    C7    C41   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C13   C14   C12   C48   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C2P   C1P   O3    C3P   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C1R   N1B   C2R   O6R   gi_2    ;  sugar C atom tetrahedral geometry
   C2R   O7R   C3R   C1R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C5R   O6R   C4R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C2R   O2    C4R   gi_2    ;  sugar C atom tetrahedral geometry
   FE    C1    C4    N21   gi_3    ;  HEMC improper definition
   FE    C6    C9    N22   gi_3    ;  HEMC improper definition
   FE    C11   C14   N23   gi_3    ;  HEMC improper definition
   FE    C16   C19   N24   gi_3    ;  HEMC improper definition
 [ dihedrals ]
;  ai    aj    ak    al   gromos type
   C3R   O2    P     O3    gd_20   ;  from ADE phosphate definition
   C3R   O2    P     O3    gd_27   ;  from ADE phosphate definition
   C2P   O3    P     O2    gd_20   ;  from ADE phosphate definition
   C2P   O3    P     O2    gd_27   ;  from ADE phosphate definition
   P     O3    C2P   C1P   gd_7    ;  from ADE phosphate definition
   C2R   C3R   O2    P     gd_29   ;  from ADE phosphate definition
   O8R   C5R   C4R   O6R   gd_8    ;  from ADE sugar dihedrals
   O8R   C5R   C4R   O6R   gd_25   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_17   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_34   ;  from ADE sugar dihedrals
   C3R   C4R   O6R   C1R   gd_29   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   C2R   gd_34   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   O2    gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   C2R   gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   O2    gd_18   ;  from ADE sugar dihedrals
   C4R   O6R   C1R   C2R   gd_29   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   O7R   gd_18   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   C4R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   O2    gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   C4R   gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   O2    gd_18   ;  from ADE sugar dihedrals
   C1R   C2R   O7R   HAA   gd_23   ;  from ADE sugar dihedrals
   N1B   C1R   C2R   O7R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   N1B   C8B   gd_16   ;  from ADE sugar dihedrals
   C4R   C5R   O8R   HAB   gd_2    ;  additional ADE-based sugar dihedral
   N1B   C1R   C2R   C3R   gd_17   ;  additional ADE-based sugar dihedral
   N1B   C1R   O6R   C4R   gd_17   ;  additional ADE-based sugar dihedral
   C2    C26   C27   N29   gd_40   ;  from GLN dihedral
   C26   C27   N29   HAD   gd_14   ;  from GLN dihedral
   C30   C31   C32   N33   gd_40   ;  from GLN dihedral
   C31   C32   N33   HAF   gd_14   ;  from GLN dihedral
   C7    C37   C38   N40   gd_40   ;  from GLN dihedral
   C37   C38   N40   HAH   gd_14   ;  from GLN dihedral
   C41   C42   C43   N45   gd_40   ;  from GLN dihedral
   C42   C43   N45   HAJ   gd_14   ;  from GLN dihedral
   C48   C49   C50   N52   gd_40   ;  from GLN dihedral
   C49   C50   N52   HAL   gd_14   ;  from GLN dihedral
   C18   C60   C61   N62   gd_40   ;  from GLN dihedral
   C60   C61   N62   HAN   gd_14   ;  from GLN dihedral
   C5M   C5B   C6B   C6M   gd_33   ;  dimethylbenzimidazole methyl dihedral fix
   C4B   C5B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C8B   C7B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C7B   C6B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C9B   C4B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C35   C5    C4    N21   gd_10   ;  corrin ring methyl planarity
   C35   C5    C6    N22   gd_10   ;  corrin ring methyl planarity
   C53   C15   C14   N23   gd_10   ;  corrin ring methyl planarity
   C53   C1    C16   N24   gd_10   ;  corrin ring methyl planarity
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N21   C4    C5    C6    gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C4    C5    C6    N22   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N22   C9    C10   C11   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C9    C10   C11   N23   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N23   C14   C15   C16   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C14   C15   C16   N24   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C1    C2    C26   C27   gd_40   ;  corrin ring HEMC derived CHn torsions
```

```
   C25   C2    C26   C27   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C26   C27   O28   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C3    C30   C31   gd_9    ;  corrin ring HEMC derived CHn torsions
   C3    C30   C31   C32   gd_40   ;  corrin ring HEMC derived CHn torsions
   C30   C31   C32   O34   gd_40   ;  corrin ring HEMC derived CHn torsions
   C6    C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C36   C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C37   C38   O39   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C8    C41   C42   gd_9    ;  corrin ring HEMC derived CHn torsions
   C8    C41   C42   C43   gd_34   ;  corrin ring HEMC derived CHn torsions
   C41   C42   C43   O44   gd_40   ;  corrin ring HEMC derived CHn torsions
   C12   C13   C48   C49   gd_9    ;  corrin ring HEMC derived CHn torsions
   C13   C48   C49   C50   gd_34   ;  corrin ring HEMC derived CHn torsions
   C48   C49   C50   O51   gd_40   ;  corrin ring HEMC derived CHn torsions
   C16   C17   C55   C56   gd_40   ;  corrin ring HEMC derived CHn torsions
   C54   C17   C56   C57   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C55   C56   C57   gd_34   ;  corrin ring HEMC derived CHn torsions
   C55   C56   C57   O58   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C18   C60   C61   gd_9    ;  corrin ring HEMC derived CHn torsions
   C18   C60   C61   O63   gd_34   ;  corrin ring HEMC derived CHn torsions
   C18   C17   C55   C56   gd_9    ;  corrin ring HEMC derived CHn torsions
   N59   C1P   C2P   O3    gd_34   ;  amide linkage torsion terms
   N59   C1P   C2P   C3P   gd_34   ;  amide linkage torsion terms
   C2P   C1P   N59   C57   gd_34   ;  amide linkage torsion terms
   C56   C57   N59   C1P   gd_14   ;  amide linkage torsion terms
   C55   C56   C57   N59   gd_40   ;  amide linkage torsion terms
   C17   C55   C56   C57   gd_40   ;  amide linkage torsion terms
   C5    C4    N21   C1    gd_14   ;  corrin ring sp3-containing torsions
   C10   C9    N22   C6    gd_14   ;  corrin ring sp3-containing torsions
   C5    C6    N22   C9    gd_14   ;  corrin ring sp3-containing torsions
   C15   C14   N23   C11   gd_14   ;  corrin ring sp3-containing torsions
   C10   C11   N23   C14   gd_14   ;  corrin ring sp3-containing torsions
   C15   C16   N24   C19   gd_14   ;  corrin ring sp3-containing torsions
   C4    N21   C1    C2    gd_40   ;  corrin ring sp3-containing torsions
   C18   C19   N24   C16   gd_40   ;  corrin ring sp3-containing torsions
   N22   C6    C5    C4    gd_33   ;  corrin ring sp3-containing torsions
   N23   C11   C10   C9    gd_33   ;  corrin ring sp3-containing torsions
   C19   C18   C17   C55   gd_34   ;  corrin ring sp3-containing torsions
   C55   C17   C16   C15   gd_40   ;  corrin ring sp3-containing torsions
   C17   C18   C19   C1    gd_34   ;  corrin ring sp3-containing torsions
   C18   C19   C1    C2    gd_34   ;  corrin ring sp3-containing torsions
   C17   C16   C15   C14   gd_10   ;  corrin ring sp3-containing torsions
   C16   C15   C14   C13   gd_10   ;  corrin ring sp3-containing torsions
   C15   C14   C13   C12   gd_40   ;  corrin ring sp3-containing torsions
   C6    C7    C8    C9    gd_34   ;  corrin ring sp3-containing torsions
   C8    C7    C6    C5    gd_34   ;  corrin ring sp3-containing torsions
   C30   C3    C2    C1    gd_34   ;  corrin ring sp3-containing torsions
   C11   C12   C13   C14   gd_34   ;  corrin ring sp3-containing torsions
   C13   C12   C11   C10   gd_34   ;  corrin ring sp3-containing torsions
   C10   C9    C8    C7    gd_10   ;  corrin ring sp3-containing torsions
   C5    C4    C3    C30   gd_34   ;  corrin ring sp3-containing torsions
   C3    C2    C1    C19   gd_34   ;  corrin ring sp3-containing torsions
;
;  cyano group dihedral.  imidazole-Fe-CN group torsion
;
   C9B   N3B   FE    N21   gd_38   ;   THIS IS NEW!!!
   N3B   FE    N21   C1    gd_38   ;   THIS IS NEW!!!
   N3B   FE    N22   C6    gd_38   ;   THIS IS NEW!!!
   N3B   FE    N23   C11   gd_38   ;   THIS IS NEW!!!
   N3B   FE    N24   C16   gd_38   ;   THIS IS NEW!!!
   N3B   FE    C1N   N1C   gd_38   ;  corrin ring sp3-containing torsions
```

```
[ LCB ]
;
; lysine-cyanocobalamin residue file based on the HEMC CO parameters
;
 [ atoms ]
 C27      C       0.38000     0    ;  from GLN residue
 O28      O      -0.38000     0    ;  from GLN residue
 N29      NT     -0.83000     0    ;  from GLN residue
 HAE      H       0.41500     0    ;  from GLN residue
 HAD      H       0.41500     0    ;  from GLN residue
 C32      C       0.38000     1    ;  from GLN residue
 O34      O      -0.38000     1    ;  from GLN residue
 N33      NT     -0.83000     1    ;  from GLN residue
 HAG      H       0.41500     1    ;  from GLN residue
 HAF      H       0.41500     1    ;  from GLN residue
 C38      C       0.38000     2    ;  from GLN residue
 O39      O      -0.38000     2    ;  from GLN residue
 N40      NT     -0.83000     2    ;  from GLN residue
 HAI      H       0.41500     2    ;  from GLN residue
 HAH      H       0.41500     2    ;  from GLN residue
 C43      C       0.38000     3    ;  from GLN residue
 O44      O      -0.38000     3    ;  from GLN residue
 N45      NT     -0.83000     3    ;  from GLN residue
 HAK      H       0.41500     3    ;  from GLN residue
 HAJ      H       0.41500     3    ;  from GLN residue
 C50      C       0.38000     4    ;  from GLN residue
 O51      O      -0.38000     4    ;  from GLN residue
 N52      NT     -0.83000     4    ;  from GLN residue
 HAM      H       0.41500     4    ;  from GLN residue
 HAL      H       0.41500     4    ;  from GLN residue
 C61      C       0.38000     5    ;  from GLN residue
 O63      O      -0.38000     5    ;  from GLN residue
 N62      NT     -0.83000     5    ;  from GLN residue
 HAO      H       0.41500     5    ;  from GLN residue
 HAN      H       0.41500     5    ;  from GLN residue
 C20      CH3     0.00000     6    ;  methyl group
 C25      CH3     0.00000     7    ;  methyl group
 C36      CH3     0.00000     8    ;  methyl group
 C46      CH3     0.00000     9    ;  methyl group
 C47      CH3     0.00000     10   ;  methyl group
 C54      CH3     0.00000     11   ;  methyl group
 C26      CH2     0.00000     12   ;  non-polar CHn fragments
 C30      CH2     0.00000     13   ;  non-polar CHn fragments
 C31      CH2     0.00000     13   ;  non-polar CHn fragments
 C37      CH2     0.00000     14   ;  non-polar CHn fragments
 C41      CH2     0.00000     15   ;  non-polar CHn fragments
 C42      CH2     0.00000     15   ;  non-polar CHn fragments
 C48      CH2     0.00000     16   ;  non-polar CHn fragments
 C49      CH2     0.00000     16   ;  non-polar CHn fragments
 C56      CH2     0.00000     17   ;  non-polar CHn fragments
 C55      CH2     0.00000     17   ;  non-polar CHn fragments
 C60      CH2     0.00000     18   ;  non-polar CHn fragments
 C2R      CH1     0.15000     19   ;  C2*-O2*-H2* from ADE
 O7R      OA     -0.54800     19   ;  C2*-O2*-H2* from ADE
 HAA      H       0.39800     19   ;  C2*-O2*-H2* from ADE
 C1R      CH1     0.20000     20   ;  C1*-O4*-C4* from ADE
 O6R      OA     -0.36000     20   ;  C1*-O4*-C4* from ADE
 C4R      CH1     0.16000     20   ;  C1*-O4*-C4* from ADE
 C3R      CH1     0.00000     21   ;  C3* from ADE
 C5R      CH2     0.15000     22   ;  C2*-O2*-H2* from ADE
 O8R      OA     -0.54800     22   ;  C2*-O2*-H2* from ADE
; O8R      OA     -0.54800     22   ;  C2*-O2*-H2* from ADE
;
;    HAB from B12 is gone in LYB, where the lysine fragment is added via CLB
;    HAB      H       0.39800     22   ;  C2*-O2*-H2* from ADE
;    HAB from B12 is gone in LYB, where the lysine fragment is added via CLB
;
 P        P       2.20000     23   ;  PO3+O3* fragment from ADE
;
; the O2P is a special mod to the PDB file.  The O2 (fine in B12) is a "special" label
; that pdb2gmx has some kind of structure prep issue with.  This, like the CO to FE, is a
; by-hand hack of the PDB file (for now)
;
 O2P      OA     -0.80000     23   ;  PO3+O3* fragment from ADE
 O4       OM     -1.00000     23   ;  PO3+O3* fragment from ADE
 O5       OM     -1.00000     23   ;  PO3+O3* fragment from ADE
 O3       OA     -0.80000     23   ;  PO3+O3* fragment from ADE
 C2P      CH1     0.35000     24   ;  non-polar CHn fragment
 C3P      CH3     0.00000     24   ;  non-polar CHn fragment
 C1P      CH2     0.00000     24   ;  non-polar CHn fragment
 N59      N      -0.28000     25   ;  tempered GLN fragment charges
```

```
 HAC      H        0.28000     25   ;  tempered GLN fragment charges
 C57      C        0.38000     25   ;  tempered GLN fragment charges
 O58      O       -0.38000     25   ;  tempered GLN fragment charges
 C5B      C        0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C5M      CH3      0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6B      C        0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C6M      CH3      0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
 C4B      C       -0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H4B      H        0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C7B      C       -0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H7B      H        0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 N3B      NR      -0.55000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 C9B      C        0.20000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
 N1B      NR      -0.30000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C8B      C        0.20000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
 C2B      C        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 H2B      H        0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
 C5       C       -0.05000     33   ;  C-CH3 group (non-polar)
 C35      CH3      0.00000     33   ;  C-CH3 group (non-polar)
 C15      C       -0.05000     34   ;  C-CH3 group (non-polar)
 C53      CH3      0.00000     34   ;  C-CH3 group (non-polar)
 FE       FE       1.00000     35   ;  HEMC Fe-N group
 N21      NR      -0.44000     35   ;  HEMC Fe-N group
 N22      NR      -0.50000     35   ;  HEMC Fe-N group
 N23      NR      -0.50000     35   ;  HEMC Fe-N group
 N24      NR      -0.44000     35   ;  HEMC Fe-N group
 C1       CH0      0.22000     36   ;  non-polar HEMC-derived corrin atoms
 C2       CH0      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C3       CH1      0.00000     36   ;  non-polar HEMC-derived corrin atoms
 C4       C        0.38000     36   ;  non-polar HEMC-derived corrin atoms
 C6       C        0.29000     37   ;  non-polar HEMC-derived corrin atoms
 C7       CH0      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C8       CH1      0.00000     37   ;  non-polar HEMC-derived corrin atoms
 C9       C        0.35000     37   ;  non-polar HEMC-derived corrin atoms
 C16      C        0.38000     38   ;  non-polar HEMC-derived corrin atoms
 C17      CH0      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C18      CH1      0.00000     38   ;  non-polar HEMC-derived corrin atoms
 C19      CH1      0.24000     38   ;  non-polar HEMC-derived corrin atoms
 C11      C        0.35000     39   ;  non-polar HEMC-derived corrin atoms
 C12      CH0      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C13      CH1      0.00000     39   ;  non-polar HEMC-derived corrin atoms
 C14      C        0.29000     39   ;  non-polar HEMC-derived corrin atoms
 C10      C       -0.24000     40   ;  aromatic C-H from TRP, PHE
 H10      H        0.14000     40   ;  aromatic C-H from TRP, PHE
;
;    Since CO is not defined as an atom in GROMOSxx, CO is converted to FE and the HEME
;    values are employed.  This is a workaround due for proper implementation.
;
 N        N       -0.31000     41   ;  standard LYS (lysine) atom information
 H        H        0.31000     41   ;  standard LYS (lysine) atom information
 CA       CH1      0.00000     42   ;  standard LYS (lysine) atom information
 CB       CH2      0.00000     42   ;  standard LYS (lysine) atom information
 CG       CH2      0.00000     43   ;  standard LYS (lysine) atom information
 CD       CH2      0.00000     43   ;  standard LYS (lysine) atom information
 CE       CH2      0.00000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
 NZ       NT      -0.34000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
 HZ1      H        0.34000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
; CE       CH2     -0.24000     44   ;  standard LYS (lysine) atom information
; NZ       NT      -0.64000     44   ;  standard LYS (lysine) atom information
; HZ1      H        0.44000     44   ;  standard LYS (lysine) atom information
;
;    this H atom is gone, replaced by the linkage CLB atom.
;    HZ2      H      0.44000     44   ;  standard LYS (lysine) atom information
;    this H atom is gone, replaced by the linkage CLB atom.
;
 C        C        0.20000     45   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
 O        O       -0.20000     45   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
; C        C        0.45000     45   ;  standard LYS (lysine) atom information
; O        O       -0.45000     45   ;  standard LYS (lysine) atom information
;
;  linkage atoms (added new)
;
 CLB      C        0.00000     46   ;  this is the linkage carbon atom between LYS and B12
 OLB      O        0.00000     46   ;  this is the additional =O at the linkage position
;
; cyano group addition to the original B12 topology
;
 C1N      C        0.04000     41   ;  CN group on Fe
 N1C      N       -0.42000     41   ;  CN group on Fe
;
[ bonds ]
```

```
;  ai    aj    gromos type
   C26   C27    gb_27   ;  from GLN fragment 0
   C27   O28    gb_5    ;  from GLN
   C27   N29    gb_9    ;  from GLN
   N29   HAE    gb_2    ;  from GLN
   N29   HAD    gb_2    ;  from GLN
   C31   C32    gb_27   ;  from GLN fragment 1
   C32   O34    gb_5    ;  from GLN
   C32   N33    gb_9    ;  from GLN
   N33   HAG    gb_2    ;  from GLN
   N33   HAF    gb_2    ;  from GLN
   C37   C38    gb_27   ;  from GLN fragment 2
   C38   O39    gb_5    ;  from GLN
   C38   N40    gb_9    ;  from GLN
   N40   HAI    gb_2    ;  from GLN
   N40   HAH    gb_2    ;  from GLN
   C42   C43    gb_27   ;  from GLN fragment 3
   C43   O44    gb_5    ;  from GLN
   C43   N45    gb_9    ;  from GLN
   N45   HAK    gb_2    ;  from GLN
   N45   HAJ    gb_2    ;  from GLN
   C49   C50    gb_27   ;  from GLN fragment 4
   C50   O51    gb_5    ;  from GLN
   C50   N52    gb_9    ;  from GLN
   N52   HAM    gb_2    ;  from GLN
   N52   HAL    gb_2    ;  from GLN
   C60   C61    gb_27   ;  from GLN fragment 5
   C61   O63    gb_5    ;  from GLN
   C61   N62    gb_9    ;  from GLN
   N62   HAO    gb_2    ;  from GLN
   N62   HAN    gb_2    ;  from GLN
   FE    N21    gb_35   ;  FE-N bond from HEMC
   FE    N22    gb_35   ;  FE-N bond from HEMC
   FE    N23    gb_35   ;  FE-N bond from HEMC
   FE    N24    gb_35   ;  FE-N bond from HEMC
   FE    N3B    gb_37   ;  FE-N3B bond from HEMC not in corrin ring
   P     O2P    gb_28   ;  from ADE phosphate
   P     O4     gb_24   ;  from ADE phosphate
   P     O5     gb_24   ;  from ADE phosphate
   P     O3     gb_28   ;  from ADE phosphate
   N21   C1     gb_21   ;  corrin ring N-CHn bonds
   N21   C4     gb_14   ;  corrin ring N-C bonds
   N22   C6     gb_14   ;  corrin ring N-C bonds
   N22   C9     gb_14   ;  corrin ring N-C bonds
   N23   C11    gb_14   ;  corrin ring N-C bonds
   N23   C14    gb_14   ;  corrin ring N-C bonds
   N24   C16    gb_14   ;  corrin ring N-C bonds
   N24   C19    gb_21   ;  corrin ring N-CHn bonds
   C30   C31    gb_27   ;  CH2-CH2 bonds
   C41   C42    gb_27   ;  CH2-CH2 bonds
   C48   C49    gb_27   ;  CH2-CH2 bonds
   C55   C56    gb_27   ;  CH2-CH2 bonds
   C56   C57    gb_27   ;  CH2-CH2 bonds
   N1B   C1R    gb_22   ;  sugar bonds from ADE
   C1R   C2R    gb_26   ;  sugar bonds from ADE
   C2R   O7R    gb_20   ;  sugar bonds from ADE
   O7R   HAA    gb_1    ;  sugar bonds from ADE
   C2R   C3R    gb_26   ;  sugar bonds from ADE
   C3R   C4R    gb_26   ;  sugar bonds from ADE
   C3R   O2P    gb_20   ;  sugar bonds from ADE
   C4R   C5R    gb_26   ;  sugar bonds from ADE
   C5R   O8R    gb_20   ;  sugar bonds from ADE
;
;  HAB is deleted from B12 for LYB    O8R   HAB    gb_1    ;  sugar bonds from ADE
;
   C4R   O6R    gb_20   ;  sugar bonds from ADE
   O6R   C1R    gb_20   ;  sugar bonds from ADE
   C1P   N59    gb_9    ;  amide corrin - phosphate linkage
   C1P   C2P    gb_27   ;  amide corrin - phosphate linkage
   C2P   C3P    gb_27   ;  amide corrin - phosphate linkage
   C2P   O3     gb_20   ;  amide corrin - phosphate linkage
   N59   HAC    gb_2    ;  amide corrin - phosphate linkage
   N59   C57    gb_9    ;  amide corrin - phosphate linkage
   C57   O58    gb_5    ;  amide corrin - phosphate linkage
   N1B   C2B    gb_10   ;  dimethylbenzimidazole ring
   C2B   N3B    gb_10   ;  dimethylbenzimidazole ring
   C2B   H2B    gb_3    ;  dimethylbenzimidazole ring
   N3B   C9B    gb_10   ;  dimethylbenzimidazole ring
   C9B   C4B    gb_16   ;  dimethylbenzimidazole ring
   C4B   C5B    gb_16   ;  dimethylbenzimidazole ring
   C4B   H4B    gb_3    ;  dimethylbenzimidazole ring
```

```
   C5B   C6B    gb_16   ;  dimethylbenzimidazole ring
   C5B   C5M    gb_27   ;  dimethylbenzimidazole ring
   C6B   C7B    gb_16   ;  dimethylbenzimidazole ring
   C6B   C6M    gb_27   ;  dimethylbenzimidazole ring
   C7B   C8B    gb_16   ;  dimethylbenzimidazole ring
   C7B   H7B    gb_3    ;  dimethylbenzimidazole ring
   C8B   N1B    gb_10   ;  dimethylbenzimidazole ring
   C8B   C9B    gb_16   ;  dimethylbenzimidazole ring
   C1    C20    gb_27   ;  corrin ring carbon framework
   C1    C2     gb_27   ;  corrin ring carbon framework
   C2    C3     gb_27   ;  corrin ring carbon framework
   C2    C25    gb_27   ;  corrin ring carbon framework
   C2    C26    gb_27   ;  corrin ring carbon framework
   C3    C4     gb_27   ;  corrin ring carbon framework
   C3    C30    gb_27   ;  corrin ring carbon framework
   C4    C5     gb_17   ;  corrin ring carbon framework
   C5    C6     gb_17   ;  corrin ring carbon framework
   C5    C35    gb_27   ;  corrin ring carbon framework
   C6    C7     gb_27   ;  corrin ring carbon framework
   C7    C8     gb_27   ;  corrin ring carbon framework
   C7    C37    gb_27   ;  corrin ring carbon framework
   C7    C36    gb_27   ;  corrin ring carbon framework
   C8    C9     gb_27   ;  corrin ring carbon framework
   C8    C41    gb_27   ;  corrin ring carbon framework
   C9    C10    gb_17   ;  corrin ring carbon framework
   C10   C11    gb_17   ;  corrin ring carbon framework
   C11   C12    gb_27   ;  corrin ring carbon framework
   C12   C46    gb_27   ;  corrin ring carbon framework
   C12   C47    gb_27   ;  corrin ring carbon framework
   C12   C13    gb_27   ;  corrin ring carbon framework
   C13   C14    gb_27   ;  corrin ring carbon framework
   C13   C48    gb_27   ;  corrin ring carbon framework
   C14   C15    gb_17   ;  corrin ring carbon framework
   C15   C16    gb_17   ;  corrin ring carbon framework
   C15   C53    gb_27   ;  corrin ring carbon framework
   C16   C17    gb_27   ;  corrin ring carbon framework
   C17   C18    gb_27   ;  corrin ring carbon framework
   C17   C54    gb_27   ;  corrin ring carbon framework
   C17   C55    gb_27   ;  corrin ring carbon framework
   C18   C19    gb_27   ;  corrin ring carbon framework
   C18   C60    gb_27   ;  corrin ring carbon framework
   C19   C1     gb_27   ;  corrin ring carbon framework
   C10   H10    gb_3    ;  corrin ring C10-H10 bond
;
; linker bond from B12 to CLB
;
   O8R   CLB    gb_5    ;  LYS B12 linker (CLB replaces H)
;
;  Lysine bond topology
;
   N     H      gb_2    ;  standard LYS (lysine)
   N     CA     gb_21   ;  standard LYS (lysine)
   CA    CB     gb_27   ;  standard LYS (lysine)
   CA    C      gb_27   ;  standard LYS (lysine)
   CB    CG     gb_27   ;  standard LYS (lysine)
   CG    CD     gb_27   ;  standard LYS (lysine)
   CD    CE     gb_27   ;  standard LYS (lysine)
   CE    NZ     gb_21   ;  standard LYS (lysine)
   NZ    HZ1    gb_2    ;  standard LYS (lysine)
;
; this replaces the HZ2 with CLB for the B12-LYS connection
;
   NZ    CLB    gb_9    ;  standard LYS (lysine)
   C     O      gb_5    ;  standard LYS (lysine)
   C     +N     gb_10   ;  standard LYS (lysine)
;
;  below is the C=O bond on the B12-LYS linkage (OLB is only connected to CLB)
;
   CLB  OLB     gb_27   ;  CLB-OLB linkage bond (previously nowhere in the structure)
;
; cyano group addition to the original B12 topology
;
   FE   C1N    gb_30    ;  cyano group on the Fe
  C1N   N1C    gb_4     ;  cyano group on the Fe
    [ exclusions ]
;  ai    aj
   FE    C2
   FE    C3
   FE    C5
   FE    C7
   FE    C8
```

```
FE    C10
FE    C12
FE    C13
FE    C15
FE    C17
FE    C18
FE    C20
N21   C25
N21   C26
N21   C30
N21   C35
N21   C6
N21   C9
N21   C11
N21   C14
N21   C16
N21   C19
N21   C10
N22   C1
N22   C4
N22   C36
N22   C37
N22   C11
N22   C14
N22   C16
N22   C19
N22   C15
N23   C16
N23   C19
N23   C1
N23   C4
N23   C6
N23   C9
N23   C46
N23   C47
N23   C48
N23   C5
N24   C4
N24   C5
N24   C6
N24   C9
N24   C10
N24   C11
N24   C14
N24   C55
N24   C54
N24   C60
C1R   C7B
C1R   C9B
C1R   N3B
N1B   C6B
N1B   C4B
C8B   C5B
C8B   C5M
C8B   C6M
C7B   C4B
C7B   N3B
C7B   C2B
C2B   C9B
C5B   C2B
C5M   C6M
C1    C30   ;  HEMC-based C framework exclusions
C1    C5    ;  HEMC-based C framework exclusions
C2    C5    ;  HEMC-based C framework exclusions
C3    C35   ;  HEMC-based C framework exclusions
C3    C6    ;  HEMC-based C framework exclusions
C4    C26   ;  HEMC-based C framework exclusions
C4    C7    ;  HEMC-based C framework exclusions
C30   C26   ;  HEMC-based C framework exclusions
C30   C5    ;  HEMC-based C framework exclusions
C5    C8    ;  HEMC-based C framework exclusions
C5    C9    ;  HEMC-based C framework exclusions
C5    C36   ;  HEMC-based C framework exclusions
C5    C37   ;  HEMC-based C framework exclusions
C35   C7    ;  HEMC-based C framework exclusions
C6    C41   ;  HEMC-based C framework exclusions
C6    C10   ;  HEMC-based C framework exclusions
C7    C10   ;  HEMC-based C framework exclusions
C8    H10   ;  HEMC-based C framework exclusions
C8    C11   ;  HEMC-based C framework exclusions
C9    C36   ;  HEMC-based C framework exclusions
```

```
   C9    C37   ;  HEMC-based C framework exclusions
   C9    C12   ;  HEMC-based C framework exclusions
   C36   C41   ;  HEMC-based C framework exclusions
   C37   C10   ;  HEMC-based C framework exclusions
   C10   C13   ;  HEMC-based C framework exclusions
   C10   C14   ;  HEMC-based C framework exclusions
   C10   C46   ;  HEMC-based C framework exclusions
   C10   C47   ;  HEMC-based C framework exclusions
   H10   C12   ;  HEMC-based C framework exclusions
   C11   C48   ;  HEMC-based C framework exclusions
   C11   C15   ;  HEMC-based C framework exclusions
   C12   C15   ;  HEMC-based C framework exclusions
   C13   C53   ;  HEMC-based C framework exclusions
   C13   C16   ;  HEMC-based C framework exclusions
   C14   C46   ;  HEMC-based C framework exclusions
   C14   C47   ;  HEMC-based C framework exclusions
   C14   C17   ;  HEMC-based C framework exclusions
   C46   C48   ;  HEMC-based C framework exclusions
   C47   C48   ;  HEMC-based C framework exclusions
   C48   C15   ;  HEMC-based C framework exclusions
   C15   C18   ;  HEMC-based C framework exclusions
   C15   C19   ;  HEMC-based C framework exclusions
   C15   C54   ;  HEMC-based C framework exclusions
   C15   C55   ;  HEMC-based C framework exclusions
   C53   C17   ;  HEMC-based C framework exclusions
   C16   C60   ;  HEMC-based C framework exclusions
   C19   C54   ;  HEMC-based C framework exclusions
   C19   C55   ;  HEMC-based C framework exclusions
   C54   C60   ;  HEMC-based C framework exclusions
   C55   C60   ;  HEMC-based C framework exclusions
;
; cyano group addition to the original B12 topology
;
   N21   N1C   ;  cyano exclusions from HEMC CO group
   N22   N1C   ;  cyano exclusions from HEMC CO group
   N23   N1C   ;  cyano exclusions from HEMC CO group
   N24   N1C   ;  cyano exclusions from HEMC CO group
   C1    C1N   ;  cyano exclusions from HEMC CO group
   C4    C1N   ;  cyano exclusions from HEMC CO group
   C6    C1N   ;  cyano exclusions from HEMC CO group
   C9    C1N   ;  cyano exclusions from HEMC CO group
   C11   C1N   ;  cyano exclusions from HEMC CO group
   C14   C1N   ;  cyano exclusions from HEMC CO group
   C16   C1N   ;  cyano exclusions from HEMC CO group
   C19   C1N   ;  cyano exclusions from HEMC CO group
   N3B   N1C   ;  cyano exclusion unique to 6-coordinate iron
   C1N   C9B   ;  additional cyano exclusion at Fe 6-center
   C1N   C2B   ;  additional cyano exclusion at Fe 6-center
 [ angles ]
;  ai    aj    ak   gromos type
   C2    C26   C27   ga_15   ;  from GLN, fragment 1
   C26   C27   O28   ga_30   ;  from GLN
   C26   C27   N29   ga_19   ;  from GLN
   O28   C27   N29   ga_33   ;  from GLN
   C27   N29   HAE   ga_23   ;  from GLN
   C27   N29   HAD   ga_23   ;  from GLN
   HAE   N29   HAD   ga_24   ;  from GLN
   C30   C31   C32   ga_15   ;  from GLN, fragment 2
   C31   C32   O34   ga_30   ;  from GLN
   C31   C32   N33   ga_19   ;  from GLN
   O34   C32   N33   ga_33   ;  from GLN
   C32   N33   HAG   ga_23   ;  from GLN
   C32   N33   HAF   ga_23   ;  from GLN
   HAG   N33   HAF   ga_24   ;  from GLN
   C7    C37   C38   ga_15   ;  from GLN, fragment 3
   C37   C38   O39   ga_30   ;  from GLN
   C37   C38   N40   ga_19   ;  from GLN
   O39   C38   N40   ga_33   ;  from GLN
   C38   N40   HAI   ga_23   ;  from GLN
   C38   N40   HAH   ga_23   ;  from GLN
   HAI   N40   HAH   ga_24   ;  from GLN
   C41   C42   C43   ga_15   ;  from GLN, fragment 4
   C42   C43   O44   ga_30   ;  from GLN
   C42   C43   N45   ga_19   ;  from GLN
   O44   C43   N45   ga_33   ;  from GLN
   C43   N45   HAK   ga_23   ;  from GLN
   C43   N45   HAJ   ga_23   ;  from GLN
   HAK   N45   HAJ   ga_24   ;  from GLN
   C48   C49   C50   ga_15   ;  from GLN, fragment 5
   C49   C50   O51   ga_30   ;  from GLN
   C49   C50   N52   ga_19   ;  from GLN
```

```
O51   C50   N52   ga_33   ;  from GLN
C50   N52   HAM   ga_23   ;  from GLN
C50   N52   HAL   ga_23   ;  from GLN
HAM   N52   HAL   ga_24   ;  from GLN
C18   C60   C61   ga_15   ;  from GLN, fragment 6
C60   C61   O63   ga_30   ;  from GLN
C60   C61   N62   ga_19   ;  from GLN
O63   C61   N62   ga_33   ;  from GLN
C61   N62   HAO   ga_23   ;  from GLN
C61   N62   HAN   ga_23   ;  from GLN
HAO   N62   HAN   ga_24   ;  from GLN
N21   FE    N22   ga_2    ;  corrin ring Fe-N angle
N21   FE    N24   ga_2    ;  corrin ring Fe-N angle
N22   FE    N23   ga_2    ;  corrin ring Fe-N angle
N23   FE    N24   ga_2    ;  corrin ring Fe-N angle
N21   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N22   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N23   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
N24   FE    N3B   ga_2    ;  corrin-Fe-dimethylbenzimidazole
FE    N21   C1    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N21   C4    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N22   C6    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N22   C9    ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N23   C11   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N23   C14   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N24   C16   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N24   C19   ga_34   ;  corrin Fe-N-C angles (based on HEMC)
FE    N3B   C9B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
FE    N3B   C2B   ga_34   ;  Fe-dimethylbenzimidazole-N,C angle
C8B   N1B   C2B   ga_7    ;  angle containing C8B, see minimization issues discussion
N1B   C8B   C9B   ga_7    ;  angle containing C8B, see minimization issues discussion
C8B   C9B   N3B   ga_7    ;  angle containing C8B, see minimization issues discussion
C7B   C8B   N1B   ga_39   ;  angle containing C8B, see minimization issues discussion
C8B   N1B   C1R   ga_37   ;  angle containing C8B, see minimization issues discussion
C4B   C9B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C6B   C7B   C8B   ga_27   ;  angle containing C8B, see minimization issues discussion
C7B   C8B   C9B   ga_27   ;  angle containing C8B, see minimization issues discussion
N21   C1    C2    ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C1    C20   ga_13   ;  corrin ring-specific but HEMC-derived angles
N21   C4    C3    ga_33   ;  corrin ring-specific but HEMC-derived angles
C4    N21   C1    ga_6    ;  corrin ring-specific but HEMC-derived angles
C5    C4    N21   ga_33   ;  corrin ring-specific but HEMC-derived angles
C19   C1    N21   ga_13   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C5    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C6    C7    ga_33   ;  corrin ring-specific but HEMC-derived angles
N22   C9    C8    ga_33   ;  corrin ring-specific but HEMC-derived angles
C9    N22   C6    ga_6    ;  corrin ring-specific but HEMC-derived angles
C10   C9    N22   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C10   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C11   C12   ga_33   ;  corrin ring-specific but HEMC-derived angles
N23   C14   C13   ga_33   ;  corrin ring-specific but HEMC-derived angles
C14   N23   C11   ga_6    ;  corrin ring-specific but HEMC-derived angles
C15   C14   N23   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C16   C15   ga_33   ;  corrin ring-specific but HEMC-derived angles
N24   C19   C1    ga_13   ;  corrin ring-specific but HEMC-derived angles
C19   N24   C16   ga_6    ;  corrin ring-specific but HEMC-derived angles
C17   C16   N24   ga_33   ;  corrin ring-specific but HEMC-derived angles
C18   C19   N24   ga_13   ;  corrin ring-specific but HEMC-derived angles
C3R   O2P   P     ga_26   ;  phosphate angle from ADE
O2P   P     O3    ga_5    ;  phosphate angle from ADE
O2P   P     O4    ga_14   ;  phosphate angle from ADE
O2P   P     O5    ga_14   ;  phosphate angle from ADE
O3    P     O4    ga_14   ;  phosphate angle from ADE
O3    P     O5    ga_14   ;  phosphate angle from ADE
O4    P     O5    ga_29   ;  phosphate angle from ADE
P     O3    C2P   ga_26   ;  phosphate angle from ADE
O2P   C3R   C2R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O2P   C3R   C4R   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C1P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
O3    C2P   C3P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
C1    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C3    ga_13   ;  CHn-CHn-CHn angles
C1    C19   C18   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C19   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C20   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C30   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C3    C30   C31   ga_13   ;  CHn-CHn-CHn angles
C7    C8    C41   ga_13   ;  CHn-CHn-CHn angles
```

```
   C8    C41   C42   ga_13   ;  CHn-CHn-CHn angles
   C12   C13   C48   ga_13   ;  CHn-CHn-CHn angles
   C13   C12   C46   ga_13   ;  CHn-CHn-CHn angles
   C13   C12   C47   ga_13   ;  CHn-CHn-CHn angles
   C13   C48   C49   ga_13   ;  CHn-CHn-CHn angles
   C17   C18   C19   ga_13   ;  CHn-CHn-CHn angles
   C17   C18   C60   ga_13   ;  CHn-CHn-CHn angles
   C17   C55   C56   ga_13   ;  CHn-CHn-CHn angles
   C18   C17   C54   ga_13   ;  CHn-CHn-CHn angles
   C18   C17   C55   ga_13   ;  CHn-CHn-CHn angles
   C19   C1    C20   ga_13   ;  CHn-CHn-CHn angles
   C19   C18   C60   ga_13   ;  CHn-CHn-CHn angles
   C25   C2    C26   ga_13   ;  CHn-CHn-CHn angles
   C46   C12   C47   ga_13   ;  CHn-CHn-CHn angles
   C54   C17   C55   ga_13   ;  CHn-CHn-CHn angles
   C36   C7    C37   ga_13   ;  CHn-CHn-CHn angles
   C2    C3    C4    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C4    C3    C30   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C6    C7    C8    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C6    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C6    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C7    C8    C9    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C8    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C8    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C9    C8    C41   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C11   C12   C13   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C11   C12   C46   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C11   C12   C47   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C12   C13   C14   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C14   C13   C48   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C16   C17   C18   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C16   C17   C54   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C16   C17   C55   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
   C4    C5    C6    ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
   C9    C10   C11   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
   C14   C15   C16   ga_27   ;  sp2-sp2-sp2 corrin ring carbon angle
   C3    C4    C5    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C4    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C5    C6    C7    ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C6    C5    C35   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C8    C9    C10   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C10   C11   C12   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C13   C14   C15   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C14   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C15   C16   C17   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C16   C15   C53   ga_37   ;  sp3-sp2-sp2 corrin ring carbon angle
   C5M   C5B   C4B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C5M   C5B   C6B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C6M   C6B   C5B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C6M   C6B   C7B   ga_37   ;  sp2-sp2-methyl dimethylbenzimidazole angle
   C4B   C5B   C6B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
   C5B   C4B   C9B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
   C5B   C6B   C7B   ga_27   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
   N1B   C1R   C2R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   N1B   C1R   O6R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   N1B   C2B   N3B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   C2B   N1B   C1R   ga_37   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   N3B   C9B   C4B   ga_39   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   C9B   N3B   C2B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
   C1R   C2R   C3R   ga_8    ;  from ADE sugar angle
   C1R   C2R   O7R   ga_9    ;  from ADE sugar angle
   C1R   O6R   C4R   ga_10   ;  from ADE sugar angle
   C2R   C1R   O6R   ga_9    ;  from ADE sugar angle
   C2R   C3R   C4R   ga_8    ;  from ADE sugar angle
   C2R   O7R   HAA   ga_12   ;  from ADE sugar angle
   C3R   C2R   O7R   ga_9    ;  from ADE sugar angle
   C3R   C4R   C5R   ga_8    ;  from ADE sugar angle
   C3R   C4R   O6R   ga_9    ;  from ADE sugar angle
   C4R   C5R   O8R   ga_9    ;  from ADE sugar angle
;
;  HAB angle is gone from B12 for LYB  C5R O8R HAB ga_12 ;  from ADE sugar angle
;
   C5R   C4R   O6R   ga_9    ;  from ADE sugar angle
   C1P   C2P   C3P   ga_13   ;  amide linkage angle
   C57   C56   C55   ga_13   ;  amide linkage angle
   C57   N59   HAC   ga_23   ;  from GLN angle
   N59   C57   O58   ga_33   ;  from GLN angle
   C56   C57   N59   ga_19   ;  from GLN angle
   O58   C57   C56   ga_30   ;  from GLN angle
   C1P   N59   C57   ga_31   ;  from force field angle definitions
   C1P   N59   HAC   ga_18   ;  from force field angle definitions
```

```
   C2P   C1P   N59   ga_15   ;  from force field angle definitions
   C5B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C9B   C4B   H4B   ga_25   ;  from PHE C-C-H angle
   C6B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   C8B   C7B   H7B   ga_25   ;  from PHE C-C-H angle
   N1B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   N3B   C2B   H2B   ga_36   ;  from ADE N-C-H angle
   C9    C10   H10   ga_25   ;  corrin ring C-C10-H angle
   C11   C10   H10   ga_20   ;  corrin ring C-C10-H angle
   C5R   O8R   CLB   ga_12   ;  for LYS-B12 bridge (just replaces O8R H atom with CLB)
;
;  standard Lysine angle topology
;
   -C    N     H     ga_32   ;  Standard LYS (lysine)
   -C    N     CA    ga_31   ;  Standard LYS (lysine)
   H     N     CA    ga_18   ;  Standard LYS (lysine)
   N     CA    CB    ga_13   ;  Standard LYS (lysine)
   N     CA    C     ga_13   ;  Standard LYS (lysine)
   CB    CA    C     ga_13   ;  Standard LYS (lysine)
   CA    CB    CG    ga_15   ;  Standard LYS (lysine)
   CB    CG    CD    ga_15   ;  Standard LYS (lysine)
   CG    CD    CE    ga_15   ;  Standard LYS (lysine)
   CD    CE    NZ    ga_15   ;  Standard LYS (lysine)
   CE    NZ    HZ1   ga_11   ;  Standard LYS (lysine)
   CE    NZ    CLB   ga_6    ;  Modification from LYS (CLB from NZ H atom)
   HZ1   NZ    CLB   ga_23   ;  Modification from LYS (CLB from NZ H atom)
   CA    C     O     ga_30   ;  Standard LYS (lysine)
   CA    C     +N    ga_19   ;  Standard LYS (lysine)
   O     C     +N    ga_33   ;  Standard LYS (lysine)
;
; additional CLB-OLB angle linkages
;
   OLB   CLB   O8R   ga_33   ;  new OLB-CLB linkage angles
   OLB   CLB   NZ    ga_33   ;  new OLB-CLB linkage angles
   O8R   CLB   NZ    ga_33   ;  new OLB-CLB linkage angles
;
; cyano group addition to the original B12 topology
;
   FE    C1N   N1C   ga_41   ;  cyano group from HEMC CO group
   N21   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   N22   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   N23   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   N24   FE    C1N   ga_1    ;  cyano group from HEMC CO group
   N3B   FE    C1N   ga_1    ;  cyano group from HEMC CO group (found during pdb2gmx)
;   N3B   FE    C1N   ga_41   ;  cyano group from HEMC CO group (found during pdb2gmx)
   [ impropers ]
;  ai    aj    ak    al   gromos type
   C1R   C8B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   N1B   C8B   C9B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C7B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   N1B   C2B   N3B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C7B   C6B   C5B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C8B   C9B   N3B   C2B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C8B   C9B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C7B   C6B   C5B   C4B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C6B   C5B   C4B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5B   C4B   C9B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C8B   C7B   C6B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   C4B   N3B   C8B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C9B   N3B   C2B   N1B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C2B   N1B   C8B   C9B   gi_1    ;  dimethylbenzimidazole improper for planarity
   C5M   C4B   C6B   C5B   gi_1    ;  dimethylbenzimidazole methyl groups
   C6M   C7B   C5B   C6B   gi_1    ;  dimethylbenzimidazole methyl groups
   C2B   N1B   N3B   H2B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C4B   C9B   C5B   H4B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   C7B   C8B   C6B   H7B   gi_1    ;  dimethylbenzimidazole H atom-containing planarity
   N3B   FE    C2B   C9B   gi_1    ;  Fe-dimethylbenzimidazole planarity
   N21   C4    C5    C6    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C6    C5    C4    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N22   C9    C10   C11   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C11   C10   C9    gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N23   C14   C15   C16   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   N24   C16   C15   C14   gi_1    ;  HEMC-based conjugated corrin ring improper planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C15   C16   C14   C53   gi_1    ;  corrin ring on-Csp2 methyl group improper planarity
   C27   O28   N29   C26   gi_1    ;  from GLN improper torsion definition
   N29   HAE   HAD   C27   gi_1    ;  from GLN improper torsion definition
   C32   O34   N33   C31   gi_1    ;  from GLN improper torsion definition
   N33   HAG   HAF   C32   gi_1    ;  from GLN improper torsion definition
   C38   O39   N40   C37   gi_1    ;  from GLN improper torsion definition
   N40   HAI   HAH   C38   gi_1    ;  from GLN improper torsion definition
```

```
   C43   O44   N45   C42   gi_1    ;  from GLN improper torsion definition
   N45   HAK   HAJ   C43   gi_1    ;  from GLN improper torsion definition
   C50   O51   N52   C49   gi_1    ;  from GLN improper torsion definition
   N52   HAM   HAL   C50   gi_1    ;  from GLN improper torsion definition
   C61   O63   N62   C60   gi_1    ;  from GLN improper torsion definition
   N62   HAO   HAN   C61   gi_1    ;  from GLN improper torsion definition
   C57   C56   O58   N59   gi_1    ;  amide linkage C57 planarity
   N59   C57   C1P   HAC   gi_1    ;  amide linkage N59 planarity
   C4    N21   C3    C5    gi_1    ;  corrin ring C sp2 planarity
   C5    C4    C6    C35   gi_1    ;  corrin ring C sp2 planarity
   C6    N22   C5    C7    gi_1    ;  corrin ring C sp2 planarity
   C9    N22   C10   C8    gi_1    ;  corrin ring C sp2 planarity
   C11   N23   C10   C12   gi_1    ;  corrin ring C sp2 planarity
   C14   N23   C15   C13   gi_1    ;  corrin ring C sp2 planarity
   C15   C14   C16   C53   gi_1    ;  corrin ring C sp2 planarity
   C16   N24   C15   C17   gi_1    ;  corrin ring C sp2 planarity
   C10   C9    C11   H10   gi_1    ;  corrin ring C10 planarity
   C18   C17   C19   C60   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C19   N24   C18   C1    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C3    C2    C30   C4    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C8    C9    C7    C41   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C13   C14   C12   C48   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C2P   C1P   O3    C3P   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
   C1R   N1B   C2R   O6R   gi_2    ;  sugar C atom tetrahedral geometry
   C2R   O7R   C3R   C1R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C5R   O6R   C4R   gi_2    ;  sugar C atom tetrahedral geometry
   C3R   C2R   O2P   C4R   gi_2    ;  sugar C atom tetrahedral geometry
   FE    C1    C4    N21   gi_3    ;  HEMC improper definition
   FE    C6    C9    N22   gi_3    ;  HEMC improper definition
   FE    C11   C14   N23   gi_3    ;  HEMC improper definition
   FE    C16   C19   N24   gi_3    ;  HEMC improper definition
;
; standard Lysine improper torsions
;
   N     -C    CA    H     gi_1    ;  Standard LYS (lysine)
   CA    N     C     CB    gi_2    ;  Standard LYS (lysine)
   C     CA    +N    O     gi_1    ;  Standard LYS (lysine)
   CLB   O8R   OLB   NZ    gi_1    ;  Linkage improper torsion to maintain planarity at CLB
 [ dihedrals ]
;  ai    aj    ak    al   gromos type
   C3R   O2P   P     O3    gd_20   ;  from ADE phosphate definition
   C3R   O2P   P     O3    gd_27   ;  from ADE phosphate definition
   C2P   O3    P     O2P   gd_20   ;  from ADE phosphate definition
   C2P   O3    P     O2P   gd_27   ;  from ADE phosphate definition
   P     O3    C2P   C1P   gd_7    ;  from ADE phosphate definition
   C2R   C3R   O2P   P     gd_29   ;  from ADE phosphate definition
   O8R   C5R   C4R   O6R   gd_8    ;  from ADE sugar dihedrals
   O8R   C5R   C4R   O6R   gd_25   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_17   ;  from ADE sugar dihedrals
   O8R   C5R   C4R   C3R   gd_34   ;  from ADE sugar dihedrals
   C3R   C4R   O6R   C1R   gd_29   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   C2R   gd_34   ;  from ADE sugar dihedrals
   C5R   C4R   C3R   O2P   gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   C2R   gd_17   ;  from ADE sugar dihedrals
   O6R   C4R   C3R   O2P   gd_18   ;  from ADE sugar dihedrals
   C4R   O6R   C1R   C2R   gd_29   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   O7R   gd_18   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   C2R   C3R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   C4R   gd_34   ;  from ADE sugar dihedrals
   C1R   C2R   C3R   O2P   gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   C4R   gd_17   ;  from ADE sugar dihedrals
   O7R   C2R   C3R   O2P   gd_18   ;  from ADE sugar dihedrals
   C1R   C2R   O7R   HAA   gd_23   ;  from ADE sugar dihedrals
   N1B   C1R   C2R   O7R   gd_17   ;  from ADE sugar dihedrals
   O6R   C1R   N1B   C8B   gd_16   ;  from ADE sugar dihedrals
;
;  HAB-based torsion gone for LYB  C4R C5R O8R HAB gd_2 ;  additional ADE-based sugar dihedral
;
   N1B   C1R   C2R   C3R   gd_17   ;  additional ADE-based sugar dihedral
   N1B   C1R   O6R   C4R   gd_17   ;  additional ADE-based sugar dihedral
   C2    C26   C27   N29   gd_40   ;  from GLN dihedral
   C26   C27   N29   HAD   gd_14   ;  from GLN dihedral
   C30   C31   C32   N33   gd_40   ;  from GLN dihedral
   C31   C32   N33   HAF   gd_14   ;  from GLN dihedral
   C7    C37   C38   N40   gd_40   ;  from GLN dihedral
   C37   C38   N40   HAH   gd_14   ;  from GLN dihedral
   C41   C42   C43   N45   gd_40   ;  from GLN dihedral
   C42   C43   N45   HAJ   gd_14   ;  from GLN dihedral
   C48   C49   C50   N52   gd_40   ;  from GLN dihedral
   C49   C50   N52   HAL   gd_14   ;  from GLN dihedral
```

```
   C18   C60   C61   N62   gd_40   ;  from GLN dihedral
   C60   C61   N62   HAN   gd_14   ;  from GLN dihedral
   C5M   C5B   C6B   C6M   gd_33   ;  dimethylbenzimidazole methyl dihedral fix
   C4B   C5B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C8B   C7B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C7B   C6B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C9B   C4B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
   C35   C5    C4    N21   gd_10   ;  corrin ring methyl planarity
   C35   C5    C6    N22   gd_10   ;  corrin ring methyl planarity
   C53   C15   C14   N23   gd_10   ;  corrin ring methyl planarity
   C53   C1    C16   N24   gd_10   ;  corrin ring methyl planarity
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N24   C19   C1    N21   gd_34   ;  corrin ring but HEMC-derived N,C torsions
   N21   C4    C5    C6    gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C4    C5    C6    N22   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N22   C9    C10   C11   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C9    C10   C11   N23   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   N23   C14   C15   C16   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C14   C15   C16   N24   gd_15   ;  corrin ring but HEMC-derived N,C torsions
   C1    C2    C26   C27   gd_40   ;  corrin ring HEMC derived CHn torsions
   C25   C2    C26   C27   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C26   C27   O28   gd_34   ;  corrin ring HEMC derived CHn torsions
   C2    C3    C30   C31   gd_9    ;  corrin ring HEMC derived CHn torsions
   C3    C30   C31   C32   gd_40   ;  corrin ring HEMC derived CHn torsions
   C30   C31   C32   O34   gd_40   ;  corrin ring HEMC derived CHn torsions
   C6    C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C36   C7    C37   C38   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C37   C38   O39   gd_40   ;  corrin ring HEMC derived CHn torsions
   C7    C8    C41   C42   gd_9    ;  corrin ring HEMC derived CHn torsions
   C8    C41   C42   C43   gd_34   ;  corrin ring HEMC derived CHn torsions
   C41   C42   C43   O44   gd_40   ;  corrin ring HEMC derived CHn torsions
   C12   C13   C48   C49   gd_9    ;  corrin ring HEMC derived CHn torsions
   C13   C48   C49   C50   gd_34   ;  corrin ring HEMC derived CHn torsions
   C48   C49   C50   O51   gd_40   ;  corrin ring HEMC derived CHn torsions
   C16   C17   C55   C56   gd_40   ;  corrin ring HEMC derived CHn torsions
   C54   C17   C56   C57   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C55   C56   C57   gd_34   ;  corrin ring HEMC derived CHn torsions
   C55   C56   C57   O58   gd_40   ;  corrin ring HEMC derived CHn torsions
   C17   C18   C60   C61   gd_9    ;  corrin ring HEMC derived CHn torsions
   C18   C60   C61   O63   gd_34   ;  corrin ring HEMC derived CHn torsions
   C18   C17   C55   C56   gd_9    ;  corrin ring HEMC derived CHn torsions
   N59   C1P   C2P   O3    gd_34   ;  amide linkage torsion terms
   N59   C1P   C2P   C3P   gd_34   ;  amide linkage torsion terms
   C2P   C1P   N59   C57   gd_34   ;  amide linkage torsion terms
   C56   C57   N59   C1P   gd_14   ;  amide linkage torsion terms
   C55   C56   C57   N59   gd_40   ;  amide linkage torsion terms
   C17   C55   C56   C57   gd_40   ;  amide linkage torsion terms
   C5    C4    N21   C1    gd_14   ;  corrin ring sp3-containing torsions
   C10   C9    N22   C6    gd_14   ;  corrin ring sp3-containing torsions
   C5    C6    N22   C9    gd_14   ;  corrin ring sp3-containing torsions
   C15   C14   N23   C11   gd_14   ;  corrin ring sp3-containing torsions
   C10   C11   N23   C14   gd_14   ;  corrin ring sp3-containing torsions
   C15   C16   N24   C19   gd_14   ;  corrin ring sp3-containing torsions
   C4    N21   C1    C2    gd_40   ;  corrin ring sp3-containing torsions
   C18   C19   N24   C16   gd_40   ;  corrin ring sp3-containing torsions
   N22   C6    C5    C4    gd_33   ;  corrin ring sp3-containing torsions
   N23   C11   C10   C9    gd_33   ;  corrin ring sp3-containing torsions
   C19   C18   C17   C55   gd_34   ;  corrin ring sp3-containing torsions
   C55   C17   C16   C15   gd_40   ;  corrin ring sp3-containing torsions
   C17   C18   C19   C1    gd_34   ;  corrin ring sp3-containing torsions
   C18   C19   C1    C2    gd_34   ;  corrin ring sp3-containing torsions
   C17   C16   C15   C14   gd_10   ;  corrin ring sp3-containing torsions
   C16   C15   C14   C13   gd_10   ;  corrin ring sp3-containing torsions
   C15   C14   C13   C12   gd_40   ;  corrin ring sp3-containing torsions
   C6    C7    C8    C9    gd_34   ;  corrin ring sp3-containing torsions
   C8    C7    C6    C5    gd_34   ;  corrin ring sp3-containing torsions
   C30   C3    C2    C1    gd_34   ;  corrin ring sp3-containing torsions
   C11   C12   C13   C14   gd_34   ;  corrin ring sp3-containing torsions
   C13   C12   C11   C10   gd_34   ;  corrin ring sp3-containing torsions
   C10   C9    C8    C7    gd_10   ;  corrin ring sp3-containing torsions
   C5    C4    C3    C30   gd_34   ;  corrin ring sp3-containing torsions
   C3    C2    C1    C19   gd_34   ;  corrin ring sp3-containing torsions
;
;  standard Lysine torsion topology
;
   -CA   -C    N     CA    gd_14   ;  Standard LYS (lysine)
   -C    N     CA    C     gd_39   ;  Standard LYS (lysine)
   N     CA    CB    CG    gd_34   ;  Standard LYS (lysine)
   N     CA    C     +N    gd_40   ;  Standard LYS (lysine)
   CA    CB    CG    CD    gd_34   ;  Standard LYS (lysine)
   CB    CG    CD    CE    gd_34   ;  Standard LYS (lysine)
```

```
   CG    CD    CE    NZ    gd_34   ;  Standard LYS (lysine)
   CD    CE    NZ    HZ1   gd_29   ;  Standard LYS (lysine)
   C4R   C5R   O8R   CLB   gd_23   ;  LYS-B12 linkage dihedral terms
   C5R   O8R   CLB   OLB   gd_12   ;  LYS-B12 linkage dihedral terms
   O8R   CLB   NZ    CE    gd_14   ;  LYS-B12 linkage dihedral terms
   OLB   CLB   NZ    CE    gd_14   ;  LYS-B12 linkage dihedral terms
;
; Use of LYB, which employs the pdb2gmx method for sewing the peptide chain together,
; requires the addition of this very new, bulky amino acid to aminoacids.dat.
;
;  cyano group dihedral.  imidazole-Fe-CN group torsion
;
   C9B   N3B   FE    N21   gd_38   ;   THIS IS NEW!!!
   N3B   FE    N21   C1    gd_38   ;   THIS IS NEW!!!
   N3B   FE    N22   C6    gd_38   ;   THIS IS NEW!!!
   N3B   FE    N23   C11   gd_38   ;   THIS IS NEW!!!
   N3B   FE    N24   C16   gd_38   ;   THIS IS NEW!!!
   N3B   FE    C1N   N1C   gd_38   ;  imidazole-Fe-CN torsion to 0
```