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

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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 ]
                         0.38000
                                                        from GLN residue
028
            Ω
                       -0.38000
                                                        from GLN residue
            NT
N29
                       -0.83000
                                                        from GLN residue
HAE
                        0.41500
            Η
                                                   : from GLN residue
HAD
            Η
                        0.41500
                                                  ; from GLN residue
; from GLN residue
                                                        from GLN residue
                         0.38000
034
            Ω
                       -0.38000
                                           1
                                                  ; from GLN residue
            NT
                       -0.83000
N33
                                           1
                                                        from GLN residue
HAG
                        0.41500
                                                        from GLN residue
            Η
                                                  ; from GLN residue
; from GLN residue
HAF
                         0.41500
                                                  ; from GLN residue
; from GLN residue
C38
            C
                        0.38000
039
            \cap
                       -0.38000
            NT
                                                  ; from GLN residue
; from GLN residue
; from GLN residue
N40
                       -0.83000
HAI
                        0.41500
HAH
            Η
                         0.41500
C43
            C
                        0.38000
                                                        from GLN residue
                                                  ; from GLN residue
; from GLN residue
044
            0
                       -0.38000
N45
            NT
                       -0.83000
                                                  ; from GLN residue
; from GLN residue
HAK
                        0.41500
HAJ
            Η
                         0.41500
                                           3
                       0.38000
                                                  ; from GLN residue
; from GLN residue
; from GLN residue
C50
            C
051
N52
            NT
                       -0.83000
HAM
                         0.41500
                                                        from GLN residue
HAL
            Н
                        0.41500
                                                  ; from GLN residue
; from GLN residue
C61
            C
063
                       -0.38000
                                                        from GLN residue
                                                  ; from GLN residue
; from GLN residue
N62
            NT
                       -0.83000
                                                 ; from GLN residue
; from GLN residue
; from GLN residue
; methyl group
; non-polar CHn fragments
HAO
            Η
                         0.41500
HAN
                         0.41500
C20
            CH3
                         0.00000
            CH3
                         0.00000
C36
C46
            CH3
                         0.00000
            CH3
                         0.00000
C47
            CH3
                         0.00000
                                           10
C54
            CH3
                         0.00000
C26
            CH2
                         0.00000
C30
            CH2
                         0.00000
                                           13
C31
            CH2
                         0.00000
                                            13
C37
            CH2
                         0.00000
                                                        non-polar CHn fragments
                                                  ; non-polar CHn fragments
; non-polar CHn fragments
; non-polar CHn fragments
C41
                         0.00000
            CH2
C42
            CH2
                         0.00000
                                           15
                                                  ; non-polar CHn fragments ; non-polar CHn fragments
C48
            CH2
                         0.00000
                                           16
C49
                         0.00000
            CH2
                                           16
                                                  ; non-polar CHn fragments
; non-polar CHn fragments
; non-polar CHn fragments
; non-polar CHn fragments
; C2*-O2*-H2* from ADE
; C2*-O2*-H2* from ADE
; C2*-O2*-H2* from ADE
                         0.00000
C55
            CH2
                         0.00000
                                           17
C60
            CH2
                         0.00000
                                           18
C2R
            CH1
                         0.15000
                                           19
O7R
            OA
                       -0.54800
HAA
                         0.39800
                                            19
                                                  ; C2*-O2*-H2* from
                                                       C1*-O4*-C4* from
            CH1
                                                  ; C1*-O4*-C4* from ADE
; C1*-O4*-C4* from ADE
C1R
                         0.20000
                                           2.0
06R
                       -0.36000
                                           20
            OA
C4R
            CH1
                        0.16000
                                                        C1*-O4*-C4*
                                                                          from ADE
C3R
            CH1
                         0.00000
                                                        C3* from ADE
C5R
            CH2
                         0.15000
                                                        C2*-O2*-H2* from ADE
                                                   ; C2*-O2*-H2* from ADE
                       -0.54800
O8R
            OA
```

```
C2*-O2*-H2* from ADE
                                           PO3+O3* fragment
                   2.20000
                                 23
                                                               from
                                           PO3+O3* fragment
02
         OΑ
                  -0.80000
                                 23
                                                               from ADE
                                           PO3+O3*
                                                    fragment
04
         OM
                  -1.00000
                                 23
                                                               from ADE
05
         OM
                  -1.00000
                                           PO3+O3*
                                                    fragment
                                                               from ADE
                                 23
                                           PO3+O3* fragment from ADE
03
         ΟA
                  -0.80000
C2P
         CH1
                   0.35000
                                           non-polar CHn fragment
                                          non-polar CHn fragment non-polar CHn fragment
C3P
         CH3
                   0.00000
                                 24
C1P
                                 24
         CH2
                   0.00000
                  -0.28000
                                           tempered GLN fragment charges
HAC
         Η
                   0.28000
                                           tempered GLN fragment
                                                                     charges
                                           tempered GLN fragment
tempered GLN fragment
                                                                     charges
C57
         C
                   0.38000
                                 25
058
         0
                  -0.38000
                                 25
                                                                     charges
                                           dimethylbenzimidazole
C5B
         C
                   0.00000
                                 26
                                                                     C-CH3 group
C5M
         CH3
                   0.00000
                                                                     C-CH3 group
                                           dimethylbenzimidazole
C6B
                   0.00000
                                 2.7
                                           dimethylbenzimidazole C-CH3 group
                                                                                   (non-polar)
                                           dimethylbenzimidazole C-CH3 group
         CH3
                                 2.7
C6M
                   0.00000
                                                                                   (non-polar)
                                          dimethylbenzimidazole aromatic C-H from TRP, dimethylbenzimidazole aromatic C-H from TRP,
C4B
                  -0.14000
                                 28
H4B
         Η
                   0.14000
C7B
         С
                  -0.14000
                                 29
                                           dimethylbenzimidazole aromatic C-H from
                                          dimethylbenzimidazole aromatic C-H from dimethylbenzimidazole polar aromatic NC
                                                                                          TRP.
H7B
         Н
                   0.14000
                                 29
         NR
                  -0.55000
                                 30
                                                                                          fragment
N<sub>3</sub>B
                   0.20000
                                           dimethylbenzimidazole polar aromatic NC
N1B
         NR
                  -0.30000
                                           dimethylbenzimidazole polar aromatic NC fragment
         C
C
C8B
                   0.20000
                                 31
                                           dimethylbenzimidazole polar aromatic NC fragment
C2B
                   0.23000
                                 32
                                           dimethylbenzimidazole aromatic C-H from TRP,
                   0.23000
                                           dimethylbenzimidazole aromatic C-H from TRP, PHE
H2B
         Н
                                 32
                  -0.05000
                                           C-CH3 group (non-polar)
C35
         CH3
                   0.00000
                                 33
                                           C-CH3 group (non-polar)
                                           C-CH3 group
C15
                  -0.05000
                                 34
                                                         (non-polar)
C53
         CH3
                   0.00000
                                 34
                                           C-CH3 group
                                                         (non-polar)
                                           HEMC Fe-N group
FE
         FE
                   0.62000
                                 35
N21
         NR
                  -0.44000
                                           HEMC Fe-N group
N22
         NR
                  -0.50000
                                 35
                                           HEMC Fe-N group
                                           HEMC Fe-N group
N23
         NR
                  -0.50000
                                 35
                                           HEMC Fe-N
N24
         NR
                  -0.44000
                                                      group
C1
                   0.22000
                                           non-polar HEMC-derived corrin atoms
         CH0
C2
C3
         CHO
                   0.00000
                                 36
                                           non-polar HEMC-derived corrin atoms
                                           non-polar HEMC-derived corrin atoms
                   0.00000
         CH1
                                 36
C4
                   0.38000
                                           non-polar HEMC-derived corrin atoms
                                 36
C6
                                                      HEMC-derived corrin atoms
                   0.29000
                                           non-polar
C7
         CH0
                   0.0000
                                 37
                                           non-polar HEMC-derived corrin atoms
                                          non-polar HEMC-derived corrin atoms
                                 37
         CH1
                   0.00000
                                           non-polar HEMC-derived corrin atoms
C9
                   0.35000
                                 37
C16
                   0.38000
                                 38
                                           non-polar HEMC-derived corrin atoms
         CH0
                   0.00000
                                           non-polar
                                                      {\tt HEMC-derived}
                                                                      corrin atoms
C18
         CH1
                   0.00000
                                 38
                                           non-polar HEMC-derived corrin atoms
C19
         CH1
                   0.24000
                                           non-polar HEMC-derived corrin atoms
                                 38
C11
                   0.35000
                                           non-polar HEMC-derived corrin atoms
                                 39
         CH0
C12
                   0.00000
                                 39
                                           non-polar HEMC-derived
                                                                      corrin atoms
C13
         CH1
                   0.00000
                                 39
                                           non-polar HEMC-derived corrin atoms
C14
                                          non-polar HEMC-derived corrin atoms aromatic C-H from TRP, PHE
         C
                   0.29000
                                 39
         C
                  -0.24000
C10
                                 40
H10
         Η
                                           aromatic C-H from TRP,
                   0.14000
                                 40
Since CO is not defined as an atom in {\tt GROMOSxx}, CO is converted to FE and the HEME values are employed. This is a workaround due for proper implementation.
bonds ]
  ai
C26
         aj
C27
                gromos type
                               from GLN fragment 0
                 qb 27
                 gb_5
  C27
         028
                               from GLN
  C27
         N29
                 gb_9
                               from
                                    GLN
                 gb_2
gb_2
  N29
         HAE
                               from
                                    GLN.
  N29
         HAD
                               from GLN
                  qb 27
                                    GLN fragment 1
  C31
         C32
                               from
                  gb_5
  C32
                               from
                                    GLN
  C32
         N33
                  gb 9
                               from
                                    GLN
                 gb_2
gb_2
gb_27
  N33
         HAG
                               from
                                    GLN
  N33
         HAF
                               from
                                    GLN
  C37
         C38
                               from
                                    \operatorname{GLN}
                                         fragment 2
  C38
         039
                  gb 5
                               from
                                    GLN
  C38
         N40
                  gb_9
                               from
                                    GLN
                 gb_2
qb_2
  N40
         HAT
                               from
                                    GLN.
  N40
         HAH
                               from
                                    GLN
  C42
         C43
                  gb_27
                               from
                                    GLN fragment 3
  C43
         044
                  gb 5
                               from
                                    GLN
  C43
N45
         N4 5
                  gb_9
                               {\tt from}
                                    GLN.
                 gb 2
         HAK
                               from
                                    GLN
                 gb_2
                               from
  N45
         HAJ
                                    GLN
  C49
                               from GLN fragment 4
         C50
```

```
gb_5
gb_9
                            from
C50
       N52
                             from GLN
N52
       HAM
               gb_2
                            from GLN
               gb_2
N52
       HAL
                            from GLN
       C61
               qb 27
                                  GLN fragment 5
C60
                            from
               gb_5
C61
       063
                            {\tt from}
                                  GLN
C61
       N62
               gb_9
                             from
                                  GLN
               gb_2
qb_2
N62
       HAO
                            from GLN
N62
       HAN
                            from
                                  GLN
FΕ
               gb_35
                                  bond from HEMC
FE
       N22
               gb_35
                            FE-N bond from HEMC
FE
       N23
               gb_35
                            FE-N bond from HEMC
               gb_35
gb_37
FE
                            FE-N bond from HEMC
       N24
                            FE-N3B bond from HEMC not in corrin ring
FΕ
       N3B
               gb_28
                             from ADE phosphate
       02
P
       04
               gb 24
                            from ADE phosphate
               gb_24
gb_28
gb_21
Р
       05
                            from ADE phosphate
                            from ADE phosphate
       03
N21
       C1
                            corrin ring N-CHn bonds
N21
       C4
               gb_14
                            corrin ring N-C bonds
               gb_14
gb_14
                            corrin ring N-C bonds corrin ring N-C bonds
N22
       C6
N22
       C9
N23
       C11
               gb 14
                            corrin ring N-C bonds
N23
       C14
               gb_14
                            corrin ring N-C bonds
N24
N24
       C16
C19
               gb_14
gb_21
                            corrin ring N-C bonds
                            corrin ring N-CHn bonds
C30
               gb 27
                            CH2-CH2 bonds
       C31
               gb_27
                            CH2-CH2 bonds
C41
               gb_27
gb_27
gb_27
C48
       C49
                            CH2-CH2 bonds
       C56
C57
C55
                            CH2-CH2 bonds
C56
                            CH2-CH2 bonds
               gb 22
                            sugar bonds from ADE
N1B
       C1R
C1R
       C2R
               gb_26
                            sugar bonds from ADE
C2R
O7R
       O7R
               gb_20
                            sugar bonds from ADE
                            sugar bonds from ADE
       HAA
               qb 1
C2R
       C3R
               gb 26
                                   bonds from
                                                ADE
                            sugar
C3R
       C4R
               gb 26
                            sugar bonds from
C3R
C4R
       02
               gb_20
                            sugar bonds from ADE
       C5R
               gb_26
gb_20
                            sugar bonds from ADE
C5R
                            sugar bonds from ADE
       08R
O8R
       HAB
               gb_1
                            sugar bonds from ADE
               gb_20
gb_20
C4R
       06R
                            sugar bonds from ADE
O6R
       C1R
                            sugar bonds from ADE
                            amide corrin - phosphate linkage
amide corrin - phosphate linkage
C1P
               gb 9
       N59
C1P
       C2P
               gb 27
                            amide corrin - phosphate
amide corrin - phosphate
       C3 P
C2P
               gb_27
                                                          linkage
               gb_20
gb_2
C2P
       03
                                              phosphate
                                                          linkage
N59
       HAC
                            amide corrin - phosphate linkage
                            amide corrin - phosphate linkage
amide corrin - phosphate linkage
N59
       C57
               gb 9
C57
       058
N1B
       C2B
               gb 10
                            dimethylbenzimidazole ring
C2B
C2B
                            dimethylbenzimidazole ring
dimethylbenzimidazole ring
       N3B
               gb_10
       H2B
               qb 3
               gb 10
N3В
       С9В
                            dimethylbenzimidazole ring
С9В
       C4B
               gb_16
                            dimethylbenzimidazole
               gb_16
gb_3
gb_16
C4B
       C5B
                            dimethylbenzimidazole
C4B
       H4B
                            dimethylbenzimidazole
C5B
                            dimethylbenzimidazole
       С6В
C5B
       C5M
               gb_27
                            dimethylbenzimidazole
C6B
       C7B
               gb_16
ab 27
                            dimethylbenzimidazole
C6B
       C6M
                            dimethvlbenzimidazole
С7В
       C8B
               gb 16
                            dimethylbenzimidazole
                                                      ring
C7B
       Н7В
                            dimethylbenzimidazole
               gb_3
C8B
       N1B
               gb 10
                            dimethylbenzimidazole
C8B
       C9B
               gb_16
                            dimethylbenzimidazole ring
               gb 27
C1
       C20
                            corrin ring carbon framework
C1
                            corrin ring carbon framework
C2
       C3
               gb_27
                            corrin ring carbon framework
               gb_27
gb_27
gb_27
C2
       C25
                            corrin ring carbon framework
C2
C3
       C26
                            corrin ring carbon framework
                            corrin ring carbon
                                                   framework
C3
       C30
               gb_27
                            corrin ring carbon
                                                   framework
C4
C5
       C5
               gb_17
                            corrin ring carbon framework
       C6
               qb 17
                            corrin ring carbon framework
C5
               qb 27
       C35
                            corrin ring carbon framework
               gb_27
                            corrin ring carbon framework
C7
C7
C7
               gb_27
gb_27
gb_27
       C8
                            corrin ring
                                          carbon framework
       C37
                            corrin ring carbon framework
       C36
                            corrin ring carbon framework
C8
               gb 27
                            corrin ring carbon framework
                            corrin ring carbon framework
```

corrin ring carbon framework

```
C9
C10
               gb_17
gb_17
       C11
                             corrin ring carbon framework
C11
C12
       C12
C46
               gb_27
gb_27
gb_27
                             corrin ring carbon framework
                             corrin ring carbon framework
C12
       C47
                            corrin ring carbon framework
C12
       C13
               gb_27
                            corrin ring carbon framework
               gb_27
gb_27
gb_17
C13
       C14
                            corrin ring carbon
                                                   framework
C13
       C48
                            corrin ring carbon framework
C14
       C15
                            corrin ring carbon framework
C15
               gb_17
                            corrin ring carbon framework
               gb_17
gb_27
gb_27
gb_27
gb_27
C15
       C53
                            corrin ring carbon framework
C16
C17
       C17
                            corrin ring carbon framework
       C18
                            corrin ring carbon framework
C17
       C54
                            corrin ring carbon framework
C17
       C55
                             corrin ring carbon framework
               gb_27
gb_27
gb_27
gb_27
gb_3
C18
       C19
                            corrin ring carbon framework
C18
       C60
                            corrin ring carbon framework
C19
       C1
                            corrin ring carbon framework
       H10
C10
                            corrin ring C10-H10 bond
 [ exclusions
ai
FE
       C5
       C7
C8
FE
FE
FE
       C10
FE
       C13
FE
       C15
FΕ
       C17
       C18
FΕ
N21
       C25
N21
       C26
N21
       C30
N21
       C35
N21
N21
       C6
C9
       C11
N21
N21
       C16
C19
N21
N21
N21
       C10
N22
       C1
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
C47
N23
N23
       C48
N23
       C5
N24
       C4
N24
       C5
N24
       C6
N24
       C10
N24
       C11
       C14
C55
N24
N24
N24
       C54
N24
       C60
C1R
       C7B
C1R
       C9B
C1R
       N3B
N1B
       C6B
       C4B
C5B
N<sub>1</sub>B
C8B
C8B
       C5M
C8B
```

```
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
                 HEMC-based C
                               framework exclusions
      C5
C3
                 HEMC-based
                                {\tt framework}
                                           exclusions
C3
                 HEMC-based C
                               framework exclusions
                 HEMC-based C framework exclusions
C4
      C26
                 HEMC-based C
C4
                               framework exclusions
      C7
      C26
C30
                 HEMC-based C
                               framework exclusions
C30
                 HEMC-based C
                                framework
C5
      C8
                 HEMC-based C framework exclusions
                 HEMC-based C
C5
      C9
                               framework exclusions
                 HEMC-based C
C5
      C36
                               framework exclusions
C5
      C37
                 HEMC-based C framework exclusions
C35
      C7
                 {\tt HEMC-based}\ {\tt C}
                               {\tt framework}
                                           exclusions
C6
      C41
                 HEMC-based C
                               framework exclusions
C6
      C10
                 HEMC-based
                               framework exclusions
C7
      C10
                 HEMC-based
                                framework
                                           exclusions
C8
      H10
                 HEMC-based C framework exclusions
C8
      C11
C36
                 HEMC-based C HEMC-based C
                               framework exclusions framework exclusions
C9
      C37
                 HEMC-based C
                               framework exclusions
C9
                 HEMC-based
                                framework
                                           exclusions
                HEMC-based C
HEMC-based C
C36
      C41
                               framework exclusions
C37
      C10
                               framework exclusions
C10
      C13
                 HEMC-based C
                               framework exclusions
C10
                 HEMC-based C
                               framework exclusions
      C14
C10
      C46
                 HEMC-based
                             С
                                framework
                                           exclusions
C10
      C47
C12
                 HEMC-based C
                               framework exclusions
H10
                 HEMC-based
                             C
                               framework exclusions
C11
      C48
                 HEMC-based
                               framework
                                           exclusions
C11
      C15
                 HEMC-based C
                               framework
                                           exclusions
C12
      C15
                 HEMC-based C framework exclusions
                 HEMC-based C
C13
                               framework exclusions
      C53
C13
      C16
                 HEMC-based C
                               framework exclusions
C14
      C46
                 {\tt HEMC-based}
                                framework
                                           exclusions
                HEMC-based C
C14
      C47
                               framework exclusions
      C17
                               framework exclusions
C14
C46
                 HEMC-based C
                               framework exclusions
      C48
C47
      C48
                 HEMC-based C
                               framework exclusions
                 HEMC-based
C48
                                framework
                                           exclusions
C15
      C18
                 HEMC-based C framework exclusions
C15
      C19
                 HEMC-based C framework exclusions
C15
                 HEMC-based
                               framework exclusions
      C54
C15
      C55
                 HEMC-based C
                               {\tt framework}
C53
      C17
                 HEMC-based C framework exclusions
C16
                 HEMC-based C
      C60
                               framework exclusions
C19
                 HEMC-based C
                               framework exclusions
      C54
C19
                 HEMC-based C
                               framework exclusions
                HEMC-based C framework exclusions
HEMC-based C framework exclusions
C54
      C60
C55
      C60
angles ]
                   gromos type
ai
      аj
             ak
C2
                    ga_15
                                 from GLN, fragment 1
C26
      C27
             028
                    ga_30
                                 from GLN
C26
      C27
             N29
                    ga 19
                                 from
                                      GLN
028
      C27
             N29
                    ga 33
                                 from
                                      GLN
C27
      N29
                    ga_23
                                 {\tt from}
C27
      N29
             HAD
                       _
23
                                 from
                                      GLN
                    qa
HAE
      N29
             HAD
                    ga_24
                                 from GLN
C30
      C31
                    ga 15
                                      GLN.
                                            fragment 2
             C32
                                 from
C31
                    ga 30
      C32
                                 from
                                      GLN
C31
      C32
             N33
                    ga 19
                                 from
                                      GLN
034
      C32
             N33
                    ga_33
                                 from
                                      GLN
C32
      N33
             HAG
                    ga_23
ga_23
                                 from
                                      GLN
C32
      N33
             HAF
                                 from
                                      GLN
HAG
                    ga_24
      N33
                                 from
                                      GLN
C7
      C37
             C38
                    ga_15
                                 from
                                      GLN,
                                            fragment 3
C37
      C38
             039
                    ga 30
                                 from GLN
                    ga 19
C37
      C38
             N40
                                 from GLN
039
      C38
                    ga_33
                                 {\tt from}
                                      \operatorname{GLN}
C38
      N40
             HAI
                    ga_23
                                 from
                                      GLN
                    ga_23
ga_24
C38
      N40
             НΔН
                                 from
                                      GT.N
HAI
      N40
             HAH
                                 from
                                      GLN
                                 from
C41
      C42
             C43
                    ga 15
                                      GLN,
                                            fragment 4
```

```
ga_19
ga_33
                                 from
044
       C43
              N45
                                 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
                    ga 15
                                 {\tt from}
                                       GLN, fragment 5
C49
       C50
              051
                    ga_30
                                 {\tt from}
                                       GLN
C49
       C50
              N52
                    ga_19
                                 from GLN
051
       C50
                    ga 33
              N52
                                 from
                                       GLN
C50
       N52
                    ga_23
                                 from
                                       GLN
       N52
C50
              HAL
                    ga 23
                                 from
                                       GLN
HAM
       N52
              HAL
                     ga_24
                                 from
                                       GLN
C18
                    ga 15
                                 from GLN, fragment 6
       C60
              C61
C60
       C61
              063
                    ga 30
                                 from GLN
C60
       C61
              N62
                    ga_19
                                 from
                                       GLN
063
       C61
              N62
                    ga 33
                                 from GLN
C61
       N62
              HAO
                    ga_23
                                 from GLN
C61
       N62
              HAN
                    ga 23
                                 from GLN
                    ga_24
HAO
       N62
                                 from GLN
N21
       FE
              N22
                    ga_2
                                 corrin ring Fe-N angle
                    ga_2
qa_2
                                 corrin ring Fe-N angle corrin ring Fe-N angle
N21
       FE
              N24
              N23
N22
       FE
N23
                    ga_2
                                 corrin ring Fe-N angle
N21
       FE
                    ga 2
                                 corrin-Fe-dimethylbenzimidazole
              N3B
                    ga_2
ga_2
N22
N23
       FE
              N<sub>3</sub>B
                                 corrin-Fe-dimethylbenzimidazole
                                 corrin-Fe-dimethylbenzimidazole
       FE
              N<sub>3</sub>B
N24
       FΕ
             N3B
                    ga_2
                                 corrin-Fe-dimethylbenzimidazole
FE
       N21
                    ga_34
                                 corrin Fe-N-C angles (based on HEMC)
                                 corrin Fe-N-C angles corrin Fe-N-C angles
FE
       N21
              C4
                    ga 34
                                                         (based on HEMC)
FE
       N22
              C6
                     ga_34
                                                          (based on HEMC
                                 corrin Fe-N-C angles
              C9
FΕ
                    ga 34
                                                          (based on HEMC
       N22
              C11
                                 corrin Fe-N-C angles
FΕ
       N23
                    ga 34
                                                          (based on HEMC)
                                 corrin Fe-N-C angles (based on HEMC)
corrin Fe-N-C angles (based on HEMC)
corrin Fe-N-C angles (based on HEMC)
                    ga_34
FE
       N23
              C14
FE
       N24
              C16
                     ga_34
              C19
FE
       N24
                    ga 34
FE
       N3B
              С9В
                    ga 34
                                 Fe-dimethylbenzimidazole-N,C angle
              C2B
                    ga 34
                                 Fe-dimethylbenzimidazole-N,C angle
FΕ
       N3B
                    ga_7
CAB
       N1B
              C2B
                                 angle containing C8B, see minimization issues discussion
                    ga_7
                                 angle containing C8B, see minimization
N<sub>1</sub>B
              C9B
       C8B
                                                                              issues discussion
                    ga 7
                                 angle containing C8B, see minimization
       С9В
                                                                              issues discussion
C8B
              изв
С7В
       C8B
                    ga_39
                                 angle containing C8B,
                                                          see minimization
                                                                              issues
C8B
       N1B
                    ga_37
                                 angle containing C8B,
                                                          see minimization
                                                                              issues discussion
              C1R
C4B
       C9B
              C8B
                    ga 27
                                 angle containing
                                                    CSB.
                                                          see minimization
                                                                              issues discussion
       С7В
                    ga 27
C6B
              C8B
                                 angle containing C8B,
                                                          see minimization
                                                                              issues discussion
С7В
       C8B
              С9В
                    ga 27
                                 angle containing C8B, see minimization issues discussion
                                 corrin ring-specific but HEMC-derived angles corrin ring-specific but HEMC-derived angles
N21
       C1
                    ga_13
                    ga_13
N21
       C1
              C20
                                 corrin ring-specific but HEMC-derived angles
N21
       C4
              C3
                    ga 33
              C1
                                                             HEMC-derived angles
C4
       N21
                                 corrin ring-specific but
                    qa 6
C5
              N21
                    ga 33
                                 corrin ring-specific but
                                                             HEMC-derived
C19
       C1
             N21
                    ga 13
                                 corrin ring-specific but HEMC-derived angles
                                 corrin ring-specific but HEMC-derived angles
N22
       C6
              C5
                    ga_33
                                 corrin ring-specific but HEMC-derived angles
       C6
              C7
N22
                    ga 33
                    ga 33
                                                             HEMC-derived angles
N22
              C8
                                 corrin ring-specific but
C9
       N22
              C6
                                 corrin ring-specific but HEMC-derived angles
                                 corrin ring-specific but HEMC-derived angles
C10
       C9
             N22
                    ga_33
                                 \hbox{\tt 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
N23
       C14
              C13
                    ga 33
                                                             HEMC-derived angles
C14
       N23
              C11
                    ga_6
                                 corrin ring-specific but
                                                             HEMC-derived angles
                                 corrin ring-specific but HEMC-derived angles
C15
                    ga 33
       C14
             N23
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
                                 corrin ring-specific but HEMC-derived angles
                    ga_33
C17
       C16
              N24
                                 corrin ring-specific but HEMC-derived angles
C18
       C19
                    ga 13
             N24
                    ga_26
                                 phosphate angle from ADE
02
       Ρ
              03
                    ga_5
                                 phosphate angle from ADE
02
       Р
              04
                    ga_14
                                 phosphate angle from ADE
02
              05
                    ga_14
ga_14
                                 phosphate angle from ADE
03
              04
                                 phosphate angle from
                                                         ADF
03
                    ga 14
       Ρ
              05
                                 phosphate angle from
                                                         ADE
04
              05
                    ga_29
                                 phosphate angle from ADE
                     ga 26
       03
              C2P
                                 phosphate angle from ADE
02
       C3R
              C2R
                    ga 9
                                 phosphate oxygen to CHn carbons from ADE
                    ga_9
                                 phosphate oxygen to CHn carbons from ADE
03
       C2P
              C1P
                    ga 9
                                 phosphate oxygen to CHn carbons from
                                 phosphate oxygen to CHn carbons from ADE CHn-CHn-CHn angles
03
       C2 P
              C3D
                    ga_9
C1
              C26
       C2
                    ga 13
              C25
                    ga 13
                                 CHn-CHn-CHn angles
                                 CHn-CHn-CHn angles
              C3
```

```
ga_13
ga_13
                                 CHn-CHn-CHn angles
C2
C2
C2
       C1
              C19
                                 CHn-CHn-CHn angles
       C1
             C20
                    ga_13
                                 CHn-CHn-CHn angles
                                 CHn-CHn-CHn angles
       C3
             C30
                    ga 13
C3
                                 CHn-CHn-CHn angles
       C2
             C25
                    ga 13
C3
       C2
                    ga 13
                                 CHn-CHn-CHn angles
C3
       C30
             C31
                    ga_13
                                 CHn-CHn-CHn angles
                                 CHn-CHn-CHn angles
C7
       C8
             C41
                    ga_13
C8
             C42
                                 CHn-CHn-CHn angles
       C41
                    ga 13
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
             C49
                                 CHn-CHn-CHn angles
       C48
                    ga 13
             C19
                    ga_13
C17
       C18
                                 CHn-CHn-CHn angles
C17
                                 CHn-CHn-CHn angles
       C18
             C60
                    ga_13
C17
       C55
             C56
                    ga 13
                                 CHn-CHn-CHn angles
C18
      C17
             C54
                    ga 13
                                 CHn-CHn-CHn angles
C18
             C55
                                 CHn-CHn-CHn angles
       C17
                    ga 13
                    ğa_13
C19
       C1
              C20
                                 CHn-CHn-CHn angles
C19
       C18
             C60
                    ga_13
                                 CHn-CHn-CHn angles
             C26
C47
                    ga_13
ga_13
C25
       C2
                                 CHn-CHn-CHn angles
C46
      C12
                                 CHn-CHn-CHn angles
C54
       C17
                    ga 13
                                 CHn-CHn-CHn angles
C36
       C7
             C37
                    ga 13
                                 CHn-CHn-CHn angles
C2
C4
                                sp3-sp3-sp2
sp3-sp3-sp2
                                                      ring carbon angle
       C3
             C4
                    ga_15
                                              corrin
             C30
       C3
                    ga 15
                                              corrin ring
                                                            carbon
                                                                    angle
                    ga 15
                                 sp3-sp3-sp2
                                              corrin ring carbon
C6
       C7
             C8
                                                                    angle
                    ga_15
                                 sp3-sp3-sp2
                                              corrin ring
                                                            carbon
                                                                    angle
C6
             C37
                    ga 15
                                 sp3-sp3-sp2 corrin ring
                                                            carbon angle
                                              corrin ring
                                                                   angle
C7
       C8
             C9
                    ga_15
                                 sp3-sp3-sp2
                                                            carbon
                                sp3-sp3-sp2
C8
       C7
             C36
                    ga 15
                                              corrin ring
                                                            carbon
                                                                   angle
             C37
                    ga 15
                                 sp3-sp3-sp2
                                                                   angle
C8
                                              corrin ring
                                                            carbon
                    ga_15
C9
       C8
             C41
                                 sp3-sp3-sp2
                                              corrin ring
                                                            carbon
C11
       C12
             C13
                    ga 15
                                 sp3-sp3-sp2
                                              corrin ring
                                                            carbon angle
                                sp3-sp3-sp2
C11
                    ga 15
      C12
             C46
                                              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
                                                            carbon angle
C14
       C13
             C48
                    ga_15
                                 sp3-sp3-sp2 corrin ring
C16
      C17
             C18
                                 sp3-sp3-sp2
                    ga 15
                                              corrin ring
                                                            carbon
                                                                    angle
                    ga 15
                                 sp3-sp3-sp2 corrin ring
C16
      C17
             C54
                                                            carbon
                                                                   angle
C16
       C17
             C55
                    ga_15
                                 sp3-sp3-sp2 corrin ring
                                                            carbon
                                                                   angle
                    ga_27
ga_27
C4
       C5
                                 sp2-sp2-sp2
                                              corrin ring
                                                            carbon angle
C9
       C10
             C11
                                 sp2-sp2-sp2 corrin ring
                                                            carbon angle
                    ga 27
                                 sp2-sp2-sp2
C14
             C16
      C15
                                              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
                                                            carbon angle
C5
       C6
             C7
                    ga_37
                                 sp3-sp2-sp2 corrin ring
                                 sp3-sp2-sp2 corrin ring
C6
       C5
             C35
                    ga 37
                                                            carbon angle
C8
             C10
                                 sp3-sp2-sp2
       C9
                    ga 37
                                              corrin ring
                                                            carbon angle
C10
       C11
             C12
                    ga 37
                                 sp3-sp2-sp2
                                              corrin ring
                                                            carbon
C13
       C14
             C15
                    ga 37
                                 sp3-sp2-sp2
                                              corrin ring
                                                            carbon angle
             C53
C14
       C15
                    ga 37
                                 sp3-sp2-sp2
                                              corrin ring carbon angle
                                sp3-sp2-sp2 corrin ring carbon angle
C15
             C17
                    ga 37
       C16
                    ga 37
C16
       C15
                                 sp3-sp2-sp2 corrin ring carbon angle
C5M
       C5B
             C4B
                    ga_37
                                 sp2-sp2-methyl dimethylbenzimidazole
                    ga_37
ga_37
C5M
       C5B
             C6B
                                 sp2-sp2-methyl dimethylbenzimidazole
                                                                          angle
                                 sp2-sp2-methyl dimethylbenzimidazole
C6M
       C6B
             C5B
                                                                          angle
                                 sp2-sp2-methyl dimethylbenzimidazole
C6M
       С6В
             С7В
                    ga 37
                                                                          angle
C4B
       C5B
              C6B
                    ga_27
                                 Csp2-Csp2-Csp2 dimethylbenzimidazole
C5B
C5B
       C4B
             C9B
                    ga_27
                                Csp2-Csp2-Csp2 dimethylbenzimidazole angle Csp2-Csp2-Csp2 dimethylbenzimidazole angle
             C7B
                    ga 27
       C6B
N1B
       C1R
              C2R
                    ga_9
                                 from ADE Nsp2-containing dimethylbenzimidazole angle
N1B
       C1R
                    ga_9
                                 from ADE Nsp2-containing dimethylbenzimidazole
             06R
N<sub>1</sub>B
       C2B
             N3B
                    ga 7
                                 from ADE Nsp2-containing dimethylbenzimidazole
                    ga_37
C2B
      N<sub>1</sub>B
             C1R
                                 from ADE Nsp2-containing dimethylbenzimidazole angle
                                          Nsp2-containing dimethylbenzimidazole angle
Nsp2-containing dimethylbenzimidazole angle
N<sub>3</sub>B
      C9B
             C4B
                                 from ADE
                    ga 39
                    ga_7
С9В
      изв
                                 from ADE
                                          sugar angle
C1R
       C2R
             C3R
                    ga 8
                                 from ADE
C1R
       C2R
             O7R
                    ga_9
                                 from ADE
                                          sugar angle
                    ga_10
ga_9
C1R
      06R
             C4R
                                 from ADE
                                           sugar angle
C2R
                                          sugar
       C1R
             06R
                                 from
                                      ADE
                                                 angle
C2R
       C3R
                    ga 8
              C4R
                                 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
                    ga_9
                                 from ADE
                                          sugar angle
C4R
       C5R
             08R
                    ga 9
                                      ADE
                                 from
                                           sugar angle
                    ga_12
ga_9
CSR
       ORR
             HAR
                                 from ADE sugar angle
C5R
                                 from ADE sugar angle
       C4R
             06R
C1P
       C2P
             C3P
                    ga 13
                                 amide linkage angle
                                 amide linkage angle
C57
       C56
             C55
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ga_23
ga_33
                                    from GLN angle
N59
       C57
               058
                                    from GLN angle
C56
       C57
              N59
                      ga_19
                                    from GLN angle
058
       C57
               C56
                      ga_30
                                    from GLN angle
C1P
                                          force field angle definitions
       N59
               C57
                      ga 31
                                    from
                      ga_18
                                          force field angle definitions
C1P
       N59
                                    from
C2P
       C1P
               N59
                      ga_15
                                    from
                                          force field angle definitions
C5B
                                    from PHE C-C-H angle
       C4B
               H<sub>4</sub>B
                      ga_25
                                    from PHE C-C-H angle
C9B
       C4B
                      ga 25
               H4B
C6B
                      ga_25
                                    from PHE C-C-H angle
C8B
       C7B
               Н7В
                      ga 25
                                    from PHE C-C-H angle
                                    from ADE N-C-H angle
N<sub>1</sub>B
       C2B
               H2B
                      ga_36
                                    from ADE N-C-H angle
corrin ring C-C10-H angle
       C2B
                      ga 36
N<sub>3</sub>B
               H<sub>2</sub>B
                      ga_25
C9
       C10
               H10
C11
                      ga_20
                                    corrin ring C-C10-H angle
       C10
               H10
[ impropers
              1
ai
       аj
               ak
                      al
                            gromos type
                                            dimethylbenzimidazole improper for planarity
       C8B
C1R
               C2B
                      N1B
                              gi_1
gi 1
N1B
       C8B
               С9В
                      N3B
                                            dimethylbenzimidazole improper for planarity
C8B
       N1B
               C7B
                      С9В
                              gi_1
                                            dimethylbenzimidazole improper for
                                                                                       planarity
       N1B
C7B
                              gi_1
gi_1
                                            dimethylbenzimidazole improper for planarity dimethylbenzimidazole improper for planarity
C8B
               C2B
                      N<sub>3</sub>B
C8B
               C6B
                      C5B
C8B
       С9В
                              gi 1
                                            dimethylbenzimidazole improper
                                                                                  for planarity
С7В
       C8B
               С9В
                      C4B
                              gi_1
                                            dimethylbenzimidazole improper for planarity
                      C4B
C9B
                                            dimethylbenzimidazole improper for planarity dimethylbenzimidazole improper for planarity
C7B
       C6B
               C5B
C6B
               C4B
       C5B
                              gi_1
gi_1
                                            dimethylbenzimidazole improper for planarity
C5B
       C4B
               С9В
                      C8B
С9В
       C8B
               C7B
                              gi_1
                                            dimethylbenzimidazole improper for planarity
C9B
       C4B
              N3B
                      C8B
                                            dimethylbenzimidazole improper for planarity
C9B
       N3B
               C2B
                      N<sub>1</sub>B
                                            dimethylbenzimidazole improper for planarity
                                            dimethylbenzimidazole improper for planarity dimethylbenzimidazole methyl groups
                              gi_1
gi_1
C2B
               C8B
       N1B
                      C9B
C5M
                      C5B
       C4B
               C6B
C6M
       C7B
               C5B
                      C6B
                              gi_1
                                            dimethylbenzimidazole methyl groups
C2B
       N<sub>1</sub>B
               N<sub>3</sub>B
                      H2B
                              gi_1
                                            dimethylbenzimidazole H atom-containing planarity
C4B
                                            dimethylbenzimidazole H atom-containing planarity
       C9B
               C5B
                      H<sub>4</sub>B
                              gi 1
C7B
       C8B
               C6B
                      Н7В
                                            dimethylbenzimidazole H atom-containing planarity
                              qi 1
N3B
       FE
               C2B
                      С9В
                                            Fe-dimethylbenzimidazole planarity
N21
       C4
               C5
                      C6
                              gi_1
                                           HEMC-based conjugated corrin ring improper planarity
                                            HEMC-based conjugated corrin ring improper planarity
               C5
N22
       C6
                      C4
                              gi_1
                      C11
                                            HEMC-based conjugated corrin ring
N22
       C9
               C10
                                                                                      improper planarity
                              ai 1
N23
       C11
               C10
                              gi_1
                                            HEMC-based conjugated corrin ring improper planarity
                              gi_1
gi_1
              C15
                      C16
C14
N23
       C14
                                            HEMC-based conjugated corrin ring improper planarity
       C16
                                           HEMC-based conjugated corrin ring improper planarity
N24
                                            corrin ring on-Csp2 methyl group improper planarity corrin ring on-Csp2 methyl group improper planarity
                      C35
C5
       C4
               C6
                              gi_1
gi_1
C15
       C16
               C14
                      C53
       028
               N29
                              gi_1
                                            from GLN improper torsion definition
N29
       HAE
               HAD
                      C27
                              gi_1
                                            from GLN improper torsion definition
                      C31
C32
       034
                                            from GLN improper torsion definition
               N33
                              gi 1
       HAG
               HAF
                      C32
                                            from GLN improper torsion definition
N33
                              gi_1
gi_1
C38
       039
                      C37
                                            from GLN improper torsion definition
               N40
N40
       HAI
              HAH
                      C38
                              gi 1
                                            from GLN improper torsion definition
                      C42
C43
       044
               N45
                              gi_1
                                            from GLN improper torsion definition
N45
                                            from GLN improper torsion definition
       HAK
                      C43
               HAJ
                              gi 1
C50
       051
                              gi 1
                                            from GLN improper torsion definition
N52
       HAM
               HAL
                      C50
                                            from GLN improper torsion definition
C61
       063
               N62
                      C60
                              gi_1
                                            from GLN improper torsion definition
                                           from GLN improper amide linkage C57
       HAO
                                                                  torsion definition
N62
               HAN
                      C61
                              gi_1
gi_1
C57
       C56
               058
                      N59
                                                                  planarity
N59
       C57
               C1P
                      HAC
                              gi_1
                                            amide linkage N59
                                                                  planarity
                                           corrin ring C sp2 planarity corrin ring C sp2 planarity
C4
C5
       N21
               C3
                      C5
                              gi_1
gi_1
                      C35
               C6
       C4
                                            corrin ring C sp2 planarity
C6
       N22
               C5
                      C7
                              gi 1
C9
               C10
                      C8
                                            corrin ring C sp2 planarity
       N22
                              gi_1
                                           corrin ring C sp2 planarity
corrin ring C sp2 planarity
C11
       N23
               C10
                      C12
               C15
                      C13
C14
       N23
                              gi_1
                                            corrin ring C sp2 planarity
                      C53
C15
       C14
               C16
                              gi_1
gi_1
C16
                                            corrin ring C sp2 planarity
C10
       C9
               C11
                      H10
                              gi_1
                                            corrin ring C10 planarity
       C17
C18
               C19
                      C60
                              gi_2
                                            corrin ring C atom sp3 tetrahedral geometry
                                           corrin ring C atom sp3 tetrahedral geometry
corrin ring C atom sp3 tetrahedral geometry
                              gi_2
gi_2
C19
       N24
               C18
                      C1
C3
               C30
       C2
C8
       C9
               C7
                      C41
                              gi 2
                                            corrin ring C atom sp3 tetrahedral geometry
                                            corrin ring C atom sp3 tetrahedral geometry corrin ring C atom sp3 tetrahedral geometry sugar C atom tetrahedral geometry
C13
       C14
               C12
                      C48
                              gi_2
C2P
                      C3P
       C1P
               03
                              gi 2
C1R
       N1B
               C2R
                      06R
C2R
       07R
               C3R
                      C1R
                              gi_2
                                            sugar C atom tetrahedral geometry
                                            sugar C atom tetrahedral geometry
sugar C atom tetrahedral geometry
HEMC improper definition
C3R
       C5R
               06R
                      C4R
                              gi_2
gi_3
C3B
       C2R
               02
                      C4R
       C1
                      N21
FΕ
               C4
                              gi_3
gi_3
FΕ
       C6
               C9
                                            HEMC improper definition
                                            HEMC improper definition
       C11
               C14
```

```
N24
                                      ; HEMC improper definition
                             gi 3
[ dihedrals ]
  ai
        аj
                ak
                      аl
                            gromos type
                                          from ADE phosphate definition
  C3R
        02
                      03
                             gd_20
                             qd 27
                                          from ADE phosphate definition
  C3R
        02
                      03
                             gd_20
  C2P
         03
                      02
                                          from ADE phosphate definition
                             gd_27
gd_7
  C2P
        03
               Р
                      02
                                          from ADE phosphate definition
               C2P
        03
                      C1P
                                          from ADE phosphate definition
                             gd 29
  C2R
        C3R
               02
                                          from ADE phosphate definition
  O8R
                                          from ADE sugar dihedrals
                             gd_25
  O8R
         C5R
               C4R
                      06R
                                          from ADE sugar dihedrals
  O8R
         CSR
               C4R
                      C3R
                             gd_17
                                          from ADE sugar dihedrals
                      C3R
                                          from ADE sugar dihedrals
  08R
         C5R
               C4R
                             qd 34
                      C1R
                             gd 29
  C3R
         C4R
               06R
                                          from ADE sugar dihedrals
  C5R
               C3R
                      C2R
                                          from ADE sugar dihedrals
         C4R
  C5R
         C4R
               C3R
                      02
                             gd 17
                                          from ADE sugar dihedrals
               C3R
                      C2R
                             gd 17
  06R
         C4R
                                          from ADE sugar dihedrals
                                          from ADE sugar dihedrals
  06R
         C4R
               C3R
                      02
                             gd_18
qd_29
  C4R
         06R
               C1R
                      C2R
                                          from ADE sugar dihedrals
  06R
         C1R
               C2R
                      O7R
                             gd 18
                                          from ADE sugar dihedrals
               C2R
C2R
                             gd_17
qd_34
  06R
         C1R
                      C3R
                                          from ADE sugar dihedrals
                      C3R
                                          from ADE sugar dihedrals
  06R
         C1R
  C1R
         C2R
                      C4R
                                          from ADE sugar dihedrals
  C1R
         C2R
               C3R
                      02
                             gd 17
                                          from ADE sugar dihedrals
                             gd_17
gd_18
               C3R
C3R
                      C4R
O2
                                          from ADE sugar dihedrals from ADE sugar dihedrals
  O7R
         C2R
  07R
         C2R
  C1R
         C2R
               O7R
                      HAA
                             gd 23
                                          from ADE sugar dihedrals
  N<sub>1</sub>B
               C2R
                                          from ADE sugar dihedrals
  06R
         C1R
               N1B
                      CAB
                             gd 16
                                          from ADE sugar dihedrals
                             gd_2
gd_17
                                          additional ADE-based sugar dihedral additional ADE-based sugar dihedral
  C4R
         C5R
               O8R
                      HAB
  N1B
         C1R
               C2R
                      C3R
                      C4R
                                          additional ADE-based sugar dihedral
  N1B
         C1R
               06R
  C2
         C26
                C27
                      N29
                             gd_40
                                          from GLN dihedral
  C26
         C27
               N29
                      HAD
                             gd_14
                                          from GLN dihedral
  C30
                                          from GLN dihedral
        C31
               C32
                      N33
                             qd 40
  C31
         C32
               N33
                      HAF
                                          from GLN dihedral
                             qd 14
  C7
         C37
               C38
                             gd 40
                                          from GLN dihedral
                      N40
                             gd_14
  C37
        C38
               N40
                      HAH
                                          from GLN dihedral
  C41
                      N45
                                          from GLN dihedral
         C42
               C43
                             ad 40
  C42
                             gd 14
         C43
               N45
                      HAJ
                                          from GLN dihedral
  C48
         C49
                             gd_40
                                          from GLN dihedral
  C49
         C50
               N52
                      HAL
                             gd_14
                                          from GLN dihedral
                             gd 40
                                          from GLN dihedral
  C18
         C60
               C61
                      N62
  C60
         C61
                      HAN
                                          from GLN dihedral
               N62
                             qd 14
  C5M
         C5B
               С6В
                      C6M
                             gd 33
                                          dimethylbenzimidazole methyl dihedral fix
  C4B
         C5B
                      C6M
                                          dimethylbenzimidazole methyl dihedral
                             gd_10
  C8B
         C7B
               C6B
                      C6M
                                          dimethylbenzimidazole methyl dihedral
                                                                                     fix
  C7B
                      C5M
        C6B
               C5B
                                          dimethylbenzimidazole methyl dihedral
                             qd 10
  С9В
         C4B
               C5B
                      C5M
                                          dimethylbenzimidazole methyl dihedral fix
                             gd 10
                                          corrin ring methyl planarity
corrin ring methyl planarity
  C35
         C5
                C4
                      N21
                             gd 10
  C35
         C5
               C6
                      N22
                             gd 10
                                         corrin ring methyl planarity corrin ring methyl planarity
  C53
        C15
               C14
                      N23
                             gd 10
  C53
               C16
                             qd 10
        C1
                      N24
                                          corrin ring but HEMC-derived N,C torsions
  N24
         C19
               C1
                                          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
                             qd 15
                                                            HEMC-derived N,C
         C5
                      N22
  C4
               C6
                             qd 15
                                          corrin ring but
                                                                                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
                                         corrin ring but HEMC-derived N,C torsions corrin ring but HEMC-derived N,C torsions
  N23
         C14
               C15
C16
                      C16
                             gd_15
ad 15
  C14
        C15
                      N24
  C1
         C2
               C26
                      C27
                             gd 40
                                          corrin ring HEMC derived CHn torsions
  C25
                      C27
                                          corrin ring HEMC derived CHn torsions
                C26
  C2
         C26
               C27
                      028
                             gd 34
                                          corrin ring HEMC derived CHn torsions
  C2
         C3
               C30
                      C31
                             gd 9
                                          corrin ring HEMC derived CHn torsions
                      C32
                             gd_40
gd_40
        C30
  C3
               C31
                                          corrin ring HEMC
                                                             derived
                                                                      CHn torsions
  C30
         C31
                                          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
                                          corrin ring HEMC
  C7
         C37
               C38
                      039
                             gd_40
gd_9
                                                             derived
                                                                      CHn torsions
  C7
               C41
                      C42
                                          corrin ring HEMC
                                                             derived
                                                                      CHn torsions
  C8
               C42
                      C43
                             gd 34
                                                       HEMC
                                                             derived
         C41
                                          corrin ring
                                                                      CHn torsions
  C41
         C42
               C43
                      044
                             gd_40
                                          corrin ring HEMC
                                                             derived CHn torsions
  C12
         C13
               C48
                      C49
                             ad 9
                                          corrin ring HEMC
                                                             derived
                                                                      CHn torsions
  C13
         C48
               C49
                      C50
                             qd 34
                                          corrin ring HEMC
                                                             derived
                                                                      CHn torsions
  C48
         C49
               C50
                      051
                                          corrin ring HEMC
                                                             derived
                                                                      CHn torsions
                                          corrin ring
                                                             {\tt derived}
  C16
         C17
               C55
                      C56
                             gd 40
                                                       HEMC
                                                                      CHn torsions
  C54
C17
                      C57
                             gd_40
gd_34
         C17
               C56
                                          corrin ring HEMC
                                                             derived
                                                                      CHn torsions
               C56
                      C57
                                                                      CHn torsions
        C55
                                          corrin ring HEMC
                                                             derived
  C55
         C56
                      058
                             gd 40
                                          corrin ring HEMC
                                                             derived
                                                                      CHn torsions
  C17
                                         corrin ring HEMC derived CHn torsions
         C18
               C60
```

```
gd_34
gd_9
gd_34
                                        corrin ring HEMC derived CHn torsions
                                        corrin ring HEMC derived CHn torsions
C18
       C17
             C55
                    C56
N59
      C1P
             C2P
                    03
                                        amide linkage torsion terms
N59
             C2P
      C1P
                    C3P
                                        amide linkage torsion terms
                           gd_34
C2P
      C1P
                    C57
                           gd_3^4
                                        amide linkage torsion terms
             N59
C56
       C57
                    C1P
                           gd_14
                                        amide linkage torsion terms
C55
       C56
             C57
                    N59
                           gd_40
                                        amide linkage torsion terms
C17
                           gd_40
gd_14
      C55
             C56
                    C57
                                        amide linkage torsion terms
                    C1
C5
             N21
      C4
                                        corrin ring sp3-containing torsions
C10
       C9
                    C6
                                        corrin ring sp3-containing
                                                                       torsions
                                                                       torsions
C5
       С6
             N22
                    C9
                           gd_14
                                        corrin ring sp3-containing
C15
                    C11
C14
      C14
             N23
                           gd_14
                                        corrin ring sp3-containing
                                                                       torsions
C10
      C11
                                        corrin ring sp3-containing
             N23
                           qd 14
                                                                       torsions
C15
                    C19
                           gd 14
       C16
             N24
                                        corrin ring sp3-containing
                                                                       torsions
C4
      N21
                           gd_40
                                        corrin ring sp3-containing
C18
      C19
             N24
                    C16
                           gd 40
                                        corrin ring sp3-containing
                                                                       torsions
                    C4
N22
      C6
             C5
                           gd 33
                                        corrin ring sp3-containing
                                                                       torsions
                           gd_33
gd_34
N23
      C11
             C10
                    C9
                                        corrin ring sp3-containing
                                                                       torsions
C19
       C18
             C17
                    C55
                                        corrin ring sp3-containing
C55
       C17
             C16
                    C15
                           gd_40
                                        corrin ring sp3-containing
                                                                       torsions
C17
C18
             C19
C1
                    C1
C2
                           gd_34
gd_34
                                       corrin ring sp3-containing corrin ring sp3-containing
      C18
                                                                       torsions
      C19
                                                                       torsions
C17
       C16
             C15
                    C14
                           gd 10
                                        corrin ring sp3-containing
                                                                       torsions
C16
       C15
             C14
                    C13
                           gd_10
                                        corrin ring sp3-containing
C15
C6
      C14
C7
             C13
C8
                    C12
C9
                           gd_40
gd_34
                                        corrin ring sp3-containing
                                                                       torsions
                                        corrin ring sp3-containing
                                                                       torsions
                    C5
C8
      C7
             C6
                           gd 34
                                        corrin ring sp3-containing
                                                                       torsions
C30
       C3
                    C1
                           gd_34
                                        corrin ring sp3-containing
                                                                       torsions
                    C14
C10
C11
      C12
             C13
                           gd_34
                                        corrin ring sp3-containing
                                                                       torsions
             C11
C13
      C12
                           gd_34
                                        corrin ring sp3-containing
                                                                       torsions
C10
             C8
                    C7
      C9
                           qd 10
                                        corrin ring sp3-containing
                                                                      torsions
C5
       C4
             C3
                    C30
                           gd 34
                                        corrin ring sp3-containing torsions
C3
       C2
              C1
                    C19
                                        corrin ring sp3-containing torsions
C9B
      N3B
             FE
                    N21
                           gd_38
                                         THIS IS NEW!!!
THIS IS NEW!!!
N<sub>3</sub>B
      FΕ
             N21
                    C1
                           qd 38
N3B
       FE
             N22
                    C6
                           gd_38
                                         THIS IS NEW!!!
N3B
             N23
                    C11
                           gd_38
                                         THIS IS NEW!!!
N3B
      FE
             N24
                    C16
                           gd_38
                                         THIS IS NEW!!!
```

```
[ atoms C27
         C
                   0.38000
                                          from GLN residue
                                          from GLN residue
028
         0
                  -0.38000
                                 0
N29
         NT
                  -0.83000
                                          from GLN residue
                   0.41500
                                          from GLN residue
HAD
         Η
                   0.41500
                                 0
                                          from GLN residue
C32
         C
                   0.38000
                                          from GLN residue
034
         0
                  -0.38000
                                          from GLN residue
                                 1
         NT
                  -0.83000
                                          from GLN residue
HAG
         Η
                   0.41500
                                 1
                                          from GLN residue
HAF
         Η
                   0.41500
                                 1
                                          from GLN residue
                   0.38000
                                          from GLN residue
C38
         C
                  -0.38000
         0
                                          from GLN residue
N40
         NT
                 -0.83000
                                          from GLN residue
HAI
         Η
                   0.41500
                                          from GLN residue
                                 2
HAH
         Η
                   0.41500
                                          from GLN residue
C43
         C
                   0.38000
                                          from GLN residue
044
         Ó
                  -0.38000
                                          from GLN residue
N45
         NT
                 -0.83000
                                 3
                                          from GLN residue
                   0.41500
0.41500
HAK
         Н
                                 3
                                          from GLN residue
                                 3
HAJ
                                          from GLN residue
         Η
                   0.38000
                                          from GLN residue
051
         0
                  -0.38000
                                          from GLN residue
N52
         NT
                 -0.83000
                                 4
                                          from GLN residue
                                          from GLN residue
HAM
                   0.41500
         Η
HAL
         Н
                   0.41500
                                          from GLN residue
                                          from GLN residue
                   0.38000
063
         Ω
                  -0.38000
                                          from GLN residue
         NT
                                 5
N62
                  -0.83000
                                          from GLN residue
HAO
                   0.41500
                                          from GLN residue
         Η
                   0.41500
                                          from GLN residue
HAN
C20
         CH3
                   0.00000
                                          methyl group
C25
         CH3
                   0.00000
                                          methyl group
                   0.00000
                                          methyl group
C36
         CH3
                                 8
                                     ; methyl group
; methyl group
; methyl group
; methyl group
; non-polar CHn fragments
C46
         CH3
                   0.00000
C47
         СНЗ
                   0.00000
                                 10
C54
         CH3
                   0.00000
                                 11
C26
         CH2
                   0.00000
C30
         CH2
                   0.00000
                                          non-polar CHn fragments
                                 13
                   0.00000
C31
         CH2
                                          non-polar CHn fragments
C37
         CH2
                   0.00000
                                          non-polar CHn fragments
C41
                                          non-polar CHn fragments
         CH<sub>2</sub>
                   0.00000
                                 15
                   0.00000
                                          non-polar CHn fragments
         CH2
                                 15
C42
C48
         CH2
                   0.00000
                                 16
                                          non-polar CHn fragments
         CH2
                   0.00000
                                          non-polar CHn fragments
C56
         CH2
                   0.00000
                                 17
                                          non-polar CHn fragments
                                          non-polar CHn fragments
C55
         CH2
                   0.00000
                                 17
                                          non-polar CHn fragments
C2*-O2*-H2* from ADE
C2*-O2*-H2* from ADE
         CH2
                   0.00000
C60
                                 18
C2R
         CH1
                   0.15000
                                 19
O7R
         OA
                  -0.54800
                                 19
                                          C2*-O2*-H2* from ADE
                   0.39800
HAA
         Н
                                 19
                                          C1*-O4*-C4* from ADE
         CH1
C1R
                   0.20000
                                 20
                                          C1*-O4*-C4* from ADE
C1*-O4*-C4* from ADE
06R
         OA
                  -0.36000
C4R
         CH1
                   0.16000
                                 20
                                          C3* from ADE
C3R
         CH1
                   0.00000
                                 21
                                          C2*-O2*-H2* from ADE
C2*-O2*-H2* from ADE
C2*-O2*-H2* from ADE
                                 22
C5R
         CH2
                   0.15000
08R
                  -0.54800
                                 22
         OA
                   -0.54800
                                                                     ; 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
                   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)
02P
                  -0.80000
                                          PO3+O3* fragment from ADE
04
         OM
                  -1.00000
                                 23
                                          PO3+O3* fragment from ADE
05
         OM
                  -1.00000
                                 23
                                          PO3+O3* fragment from ADE PO3+O3* fragment from ADE
                                 23
03
         OA
                  -0.80000
C2P
         CH1
                   0.35000
                                 24
                                          non-polar CHn fragment
C3P
         CH3
                   0.00000
                                          non-polar CHn fragment
C1P
         CH2
                   0.00000
                                 24
                                          non-polar CHn fragment
                                          tempered GLN fragment charges
tempered GLN fragment charges
N59
         M
                  -0.28000
                  0.28000
                                 25
HAC
         Η
                                          tempered GLN fragment charges
                   0.38000
                                          tempered GLN fragment charges
                  -0.38000
```

```
dimethylbenzimidazole C-CH3 group
                                                                                       (non-polar)
                    0.00000
 C5M
           CH3
                                             dimethylbenzimidazole C-CH3 group
                                             dimethylbenzimidazole C-CH3 group
C6B
           C
                    0.00000
                                   27
                                                                                        (non-polar)
                                             dimethylbenzimidazole C-CH3 group
           CH3
                                   2.7
C6M
                    0.00000
                                                                                       (non-polar)
 C4B
                                             dimethylbenzimidazole aromatic C-H from TRP, PHE
                    -0.14000
                                   28
                                             dimethylbenzimidazole aromatic C-H from TRP,
 H4B
                    0.14000
 C7B
           C
                   -0.14000
                                             dimethylbenzimidazole aromatic C-H from
                                             dimethylbenzimidazole aromatic C-H from
H7B
          Н
                    0.14000
                                   29
                                                                                              TRP.
                   -0.55000
                                                                                              fragment
N3B
          NR
                                   30
                                             dimethylbenzimidazole polar aromatic NC
                    0.20000
                                             dimethylbenzimidazole polar aromatic NC
N1B
          NR
                   -0.30000
                                             dimethylbenzimidazole polar aromatic NC fragment
          C
C
 C8B
                    0.20000
                                   31
                                             dimethylbenzimidazole polar aromatic NC fragment
 C2B
                    0.23000
                                             dimethylbenzimidazole aromatic C-H from TRP,
                                   32
                                             dimethylbenzimidazole aromatic C-H from TRP, PHE
 H2B
          Η
                    0.23000
           C
                   -0.05000
                                             C-CH3 group (non-polar)
 C35
          CH3
                    0.00000
                                   33
                                             C-CH3 group (non-polar)
                                             C-CH3 group (non-polar)
 C15
           C
                   -0.05000
                                   34
           СНЗ
                                             C-CH3 group (non-polar)
 C53
                    0.00000
                                   34
 FE
                    0.62000
                                             HEMC Fe-N group
N21
          NR
                   -0.44000
                                   35
                                             HEMC Fe-N group
N22
          NR
                   -0.50000
                                   35
                                             HEMC Fe-N group
                                             HEMC Fe-N group
N23
                   -0.50000
          NR
                                   35
N24
          NR
                    -0.44000
                                             HEMC Fe-N group
           CH0
                    0.22000
                                             non-polar HEMC-derived corrin atoms
 C1
 C2
C3
                                             non-polar HEMC-derived corrin atoms non-polar HEMC-derived corrin atoms
           CH<sub>0</sub>
                    0.00000
                                   36
           CH1
                     0.00000
                                   36
                                             non-polar HEMC-derived corrin atoms
 C4
                    0.38000
                                   36
 C6
                                             non-polar HEMC-derived corrin atoms
                     0.29000
 C7
           CH<sub>0</sub>
                    0.00000
                                   37
                                             non-polar HEMC-derived corrin atoms
                                             non-polar HEMC-derived corrin atoms
 C8
           CH1
                    0.00000
                                   37
 Ċ9
                                             non-polar HEMC-derived corrin atoms
                    0.35000
                                   37
                                             non-polar HEMC-derived corrin atoms
 C16
                     0.38000
 C17
           CHO
                    0.00000
                                             non-polar HEMC-derived corrin atoms
                                             non-polar HEMC-derived corrin atoms
 C18
           CH1
                    0.00000
                                   38
                                             non-polar HEMC-derived corrin atoms
 C19
          CH1
                    0.24000
                                   38
 C11
                    0.35000
                                             non-polar HEMC-derived corrin atoms
                                   39
 C12
           CH0
                     0.00000
                                             non-polar HEMC-derived corrin atoms
                                   39
 C13
          CH1
                    0.00000
                                   39
                                             non-polar HEMC-derived corrin atoms
                                             non-polar HEMC-derived corrin atoms
aromatic C-H from TRP, PHE
 C14
          C
                    0.29000
                                   39
 C10
          C
                    -0.24000
                                   40
H10
                                             aromatic C-H from TRP, PHE
                    0.14000
      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.
                                             standard LYS
                                                             (lysine) atom information
                                             standard LYS (lysine) atom information standard LYS (lysine) atom information
          Η
                    0.31000
                                   41
CA
          CH1
                    0.00000
                                   42
 СВ
           CH2
                    0.00000
                                             standard LYS
                                   42
                                                                        atom information
                                                             (lysine)
                                             standard LYS (lysine) atom information standard LYS (lysine) atom information
 CG
           CH2
                     0.00000
                                   43
 CD
           CH2
                    0.00000
                                   43
                                             NEW CHARGE FROM B12 standard LYS (lysine) atom information
NEW CHARGE FROM B12 standard LYS (lysine) atom information
 CE
           CH2
                    0.00000
                                   44
                    -0.34000
NZ.
          NT
                                   44
          Η
                    0.34000
                                             NEW CHARGE FROM B12 standard LYS (lysine) atom information
                                         ; standard LYS (lysine) atom information
; standard LYS (lysine) atom information
            CH2
                     -0.24000
                                    44
 CE
 NZ.
            NT
                     -0.64000
                                     44
  HZ1
                      0.44000
                                    44
                                              standard LYS (lysine) atom information
      this H atom is gone, replaced by the linkage CLB atom.
      {
m HZ2} H 0.44000 44 ; standard LYS (lysine this H atom is gone, replaced by the linkage CLB atom.
                       0.44000
                                               standard LYS (lysine) atom information
                    0.20000
                                             NEW CHARGE FROM B12 standard LYS (lysine) atom information NEW CHARGE FROM B12 standard LYS (lysine) atom information
0
          0
                   -0.20000
                                   45
; C
            C
                                    4.5
                                             standard LYS (lysine) atom information standard LYS (lysine) atom information
                      0.45000
            0
                     -0.45000
                                    45
  linkage atoms (added new)
 CLB
                    0.00000
                                             this is the linkage carbon atom between LYS and B12 this is the additional =0 at the linkage position \,
           C
                                   46
                    0.00000
 OLB
  bonds ]
          aj
C27
   аi
                  gromos type
   C26
                   qb 27
                                 from GLN fragment 0
   C27
           028
                   gb_5
                                 from GLN
   C27
          N29
                   gb_9
                                 from
                                       GLN
                   gb_2
gb_2
   M29
          HAE
                                 from GLN
   N29
          HAD
                                 from
                                       GLN
   C31
           C32
                   gb 27
                                 from GLN fragment 1
   C32
          034
```

```
gb_9
gb_2
                               from
N33
        HAG
                                from GLN
N33
C37
        HAF
                 gb_2
                               from GLN
                 gb_27
        C38
                               from GLN fragment 2
                 qb 5
C38
        039
                               from GLN
C38
        N40
                 gb_9
                               {\tt from}
                                      GLN
N40
        HAI
                 gb_2
                                from
                                     GLN
                 gb_2
gb_27
N40
        HAH
                               from GLN
C42
        C43
                                     GLN fragment 3
                               from
C43
        044
                 gb_5
                                from
                                     GLN
C43
        N45
                 gb 9
                               {\tt from}
                                     GLN
                 gb_2
gb_2
N45
N45
        HAK
                               {\tt from}
                                     GLN
        HAJ
                                     GLN
                               from
C49
        C50
                 gb 27
                               {\tt from}
                                     GLN fragment 4
C50
        051
                 gb_5
                                from
                                     GLN
                 gb_9
C50
        N52
                               from GLN
                 gb_2
gb_2
gb_27
N52
        HAM
                               from GLN
        HAL
N52
                               from GLN
C60
        C61
                               from
                                     GLN fragment 5
C61
        063
                 gb_5
                                from GLN
                 gb_9
qb_2
                               from GLN from GLN
C61
        N62
N62
        HAO
N62
        HAN
                 gb_2
                               from
                                     GLN
FΕ
        N21
                 gb_35
                               FE-N bond from HEMC
                 gb_35
gb_35
                                     bond from HEMC bond from HEMC
FE
        N22
                               FE-N
FE
        N23
                               FE-N bond
                 gb 35
                               FE-N bond from HEMC
FΕ
        N24
                 gb_37
                               FE-N3B bond from HEMC not in corrin ring
        N3B
        02P
                 gb_28
                               from ADE phosphate
                               from ADE phosphate
from ADE phosphate
from ADE phosphate
                 gb_24
gb_24
Р
        04
        05
                 gb 28
        03
N21
        C1
                               corrin ring N-CHn bonds
                               corrin ring N-C bonds
corrin ring N-C bonds
N21
        C4
                 gb_14
N22
        C6
                 qb 14
N22
        C9
                 gb 14
                               corrin ring N-C bonds
N23
        C11
                 gb 14
                               corrin ring N-C bonds
                               corrin ring N-C bonds
corrin ring N-C bonds
corrin ring N-CHn bonds
N23
        C14
                 gb_14
N24
        C16
                 gb_14
qb_21
N24
        C19
                 gb_27
C30
        C31
                               CH2-CH2 bonds
                 gb_27
gb_27
        C42
C49
C41
                               CH2-CH2 bonds
C48
                               CH2-CH2 bonds
                 gb_27
C55
        C56
                               CH2-CH2
                                         bonds
C56
        C57
                 gb 27
                               CH2-CH2 bonds
N1B
        C1R
                 gb_22
                               sugar bonds from
                               sugar bonds from ADE
sugar bonds from ADE
C1R
C2R
        C2R
                 gb_26
        07R
                 gb 20
O7R
        HAA
                                                     ADE
                               sugar bonds from
                 qb 1
C2R
        C3R
                               sugar bonds from
C3R
        C4R
                 gb 26
                               sugar bonds from
                                                     ADE
C3R
                 gb_20
        02P
                               sugar bonds from ADE
                 qb 26
                               sugar bonds from ADE
C4R
        C5R
C5R
        O8R
                 gb 20
                               sugar bonds from ADE
HAB is deleted from B12 for LYB
                                                     HAB
                                             08R
                                                               gb_1
                                                                         ; sugar bonds from ADE
C4R
        06R
                 gb_20
                               sugar bonds from ADE
                               sugar bonds from ADE
06R
        C1R
                 gb_20
                               amide corrin - phosphate linkage amide corrin - phosphate linkage
C1P
C1P
        N59
                 gb_9
ab_27
        C2P
C2P
        C3P
                 gb 27
                               amide corrin - phosphate linkage
                               amide corrin - phosphate linkage
amide corrin - phosphate linkage
C2P
        03
                 gb_20
                 gb_2
gb_9
N59
        HAC
                               amide corrin - phosphate linkage
amide corrin - phosphate linkage
amide corrin - phosphate linkage
N59
        C57
C57
        058
                 gb 5
                 gb 10
                               dimethylbenzimidazole ring
N1B
C2B
        N3B
                 gb_10
                               dimethylbenzimidazole ring
C2B
        H2B
                 gb_3
                               dimethylbenzimidazole ring
N<sub>3</sub>B
        C9B
                 gb_10
gb_16
                               dimethylbenzimidazole ring
dimethylbenzimidazole ring
C9B
        C4B
C4B
        C5B
                 gb_16
                               dimethylbenzimidazole
C4B
        H4B
                 gb_3
                               {\tt dimethylbenzimidazole}
C5B
                 gb_16
qb_27
        C6B
                               dimethylbenzimidazole
                               dimethylbenzimidazole
C5B
        C5M
                                                            ring
C6B
        С7В
                 gb_16
                                dimethylbenzimidazole
C6B
        C6M
                 gb_27
                               dimethylbenzimidazole
                               dimethylbenzimidazole ring dimethylbenzimidazole ring
C7B
        CAR
                 gb_16
C7B
        Н7В
                 gb 3
C8B
        N1B
                 gb 10
                               dimethylbenzimidazole ring
C8B
                               dimethylbenzimidazole ring
        C9B
```

```
corrin ring carbon framework
 C1
       C2
               gb_27
                           corrin ring carbon
                                                framework
C2
C2
               gb_27
gb_27
       C3
                           corrin ring carbon framework
       C25
                           corrin ring carbon framework
 C2
               qb 27
       C26
                           corrin ring carbon framework
 C3
               gb_27
                           corrin ring carbon framework
 C3
       C30
               gb_27
                           corrin ring
                                        carbon
                                                framework
 C4
               gb_17
ab_17
       C5
                           corrin ring carbon framework
 C5
       C6
                           corrin ring carbon framework
       C35
               gb_27
                           corrin ring carbon framework
               gb_27
gb_27
gb_27
gb_27
gb_27
 C6
                           corrin ring carbon framework
 C:7
       CB
                           corrin ring
                                        carbon framework
 C7
       C37
                           corrin ring carbon framework
 C7
       C36
                           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
               gb_17
gb_27
                           corrin ring carbon framework
       C11
 C11
       C12
                           corrin ring carbon framework
 C12
       C46
               gb_27
                           corrin ring carbon framework
C12
C12
       C47
C13
               gb_27
qb_27
                           corrin ring carbon framework
                           corrin ring carbon framework
 C13
       C14
               gb 27
                           corrin ring carbon framework
 C13
       C48
               gb_27
                           corrin ring carbon framework
C14
C15
       C15
               gb_17
                           corrin ring carbon framework
               gb 17
       C16
                           corrin ring carbon framework
               gb 27
 C15
       C53
                           corrin ring carbon framework
 C16
               gb_27
                           corrin ring carbon framework
               gb_27
gb_27
gb_27
 C17
       C18
                           corrin ring carbon framework
 C17
       C54
                           corrin ring carbon framework
 C17
       C55
                           corrin ring carbon framework
 C18
               gb 27
       C19
                           corrin ring carbon framework
 C18
       C60
               gb_27
                           corrin ring carbon
                                                framework
 C19
       C1
               gb_27
                           corrin ring carbon framework
       H10
                           corrin ring C10-H10 bond
 C10
               qb 3
linker bond from B12 to CLB
                      ; LYS B12 linker (CLB replaces H)
 O8R
      CLB
               gb_5
 Lysine bond topology
                           standard LYS (lysine)
               gb_2
               gb_21
gb_27
       CA
                           standard LYS
                                          (lysine)
 CA
       СВ
                           standard LYS
                                          (lysine)
               gb_27
gb_27
gb_27
                           standard LYS
                                          (lysine)
       CG
 CB
                           standard LYS
                                          (lysine)
 CG
       CD
                           standard LYS
                                          (lysine)
               gb_27
 CD
       CE
                           standard LYS
                                          (lysine)
 CE
       NZ
               gb_21
                           standard LYS
 NZ
       HZ1
               gb 2
                           standard LYS (lysine)
this replaces the HZ2 with CLB for the B12-LYS connection
               gb_9
gb_5
 NZ
       \mathtt{CLB}
                           standard LYS (lysine)
 C
                           standard LYS (lysine)
       +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 ]
 FE
 FE
       C3
 FE
       C5
 FΕ
       C8
 FE
       C10
 FE
       C12
 FΕ
       C13
       C15
 FE
       C17
 FE
       C18
 FΕ
       C20
 N21
       C26
 N21
       C30
       C35
 N21
 N21
       C6
 N21
       C9
```

```
N21
       C14
N21
N21
       C16
       C19
N21
       C10
       C1
N22
       C4
N22
       C36
N22
       C37
N22
N22
       C14
N22
       C16
N22
       C19
N22
       C15
N23
       C16
N23
       C19
N23
       C1
N23
       C4
N23
       C6
N23
       C9
N23
N23
       C46
       C47
N23
       C48
N23
       C5
N24
N24
       C4
C5
N24
       C6
N24
N24
       C10
N24
       C11
N24
       C14
N24
       C55
N24
       C54
N24
C1R
       C60
       С7В
C1R
       С9В
C1R
       N3B
N1B
       C6B
N<sub>1</sub>B
       C4B
       C5B
C8B
C8B
C8B
C7B
       C6M
       C4B
C7B
       N3B
С7В
       C2B
C2B
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
                 HEMC-based C framework exclusions
       C6
C4
                 HEMC-based C
       C26
                                framework exclusions
C4
       C7
                 HEMC-based C framework exclusions
                 HEMC-based C framework exclusions
C30
       C26
C30
                 HEMC-based C framework exclusions
       C5
C5
                 HEMC-based C framework exclusions
       C8
C5
       C9
                 HEMC-based C framework exclusions
C5
C5
       C36
                 HEMC-based C framework exclusions
HEMC-based C framework exclusions
       C37
                 HEMC-based C framework exclusions
C35
       C7
       C41
                 HEMC-based C framework exclusions
C6
       C10
                 HEMC-based C framework exclusions
                 HEMC-based C framework exclusions
C7
       C10
C8
                 HEMC-based C framework exclusions
       H10
                 HEMC-based C framework exclusions
C9
       C36
                 HEMC-based C framework exclusions
C9
       C37
                 {\tt HEMC\text{-}based} C framework exclusions
       C12
                 HEMC-based C framework exclusions
C9
C36
       C41
                 HEMC-based C framework exclusions
C37
       C10
                 HEMC-based C framework exclusions
C10
       C13
                 HEMC-based C framework exclusions
HEMC-based C framework exclusions
C10
       C14
                 HEMC-based C
                                framework exclusions
C10
       C46
C10
       C47
                 HEMC-based C framework exclusions
H10
       C12
                 {\tt HEMC\text{-}based} C framework exclusions
                 HEMC-based C framework exclusions
C11
C11
       C48
       C15
                 HEMC-based C
                                framework exclusions
C12
       C15
                 HEMC-based C
                                framework exclusions
                 HEMC-based C framework exclusions
C13
```

framework exclusions

HEMC-based C

```
C14
         C46
                    HEMC-based C
                                    framework
 C14
C14
         C47
                    HEMC-based C
                                   framework exclusions
                                 C
         C17
                    HEMC-based
                                   framework
                                               exclusions
  C46
                    HEMC-based
                                    framework
         C48
                                               exclusions
  C47
                                               exclusions
         C48
                    HEMC-based
                                    {\tt framework}
  C48
         C15
                    HEMC-based
                                 C
                                   framework
                                               exclusions
                    HEMC-based C
  C15
         C18
                                   framework exclusions
  C15
                    HEMC-based
                                 C
                                   framework exclusions
         C19
  C15
         C54
                    HEMC-based
                                    framework exclusions
                    HEMC-based C HEMC-based C
  C15
         C55
                                   framework exclusions
  C53
         C17
                                   framework exclusions
                    HEMC-based C
  C16
                                   framework exclusions
         C60
                                   framework exclusions
  C19
         C54
                    HEMC-based C
  C19
         C55
                    HEMC-based C
                                   framework exclusions
                   HEMC-based C framework exclusions
HEMC-based C framework exclusions
  C54
         C60
  C55
         C60
Γ
 angles ]
                      gromos type
  C2
         C26
                C27
                       ga_15
                                     from GLN, fragment 1
         C27
                       ga_30
ga_19
  C26
                028
                                     from GLN
  C26
                N29
                                     from
                                           GLN
  028
         C27
                       ga 33
                                     from
                                           GLN
  C27
         N29
                       ga_23
                                     from
                                           GLN
                HAE
                       ga_23
ga_24
  C27
         N29
                HAD
                                     {\tt from}
                                           GLN
  HAE
         N29
                                     from
                                           GLN
                HAD
  C30
         C31
                C32
                       ga 15
                                     from
                                           GLN,
                                                 fragment 2
  C31
         C32
                       ga_30
                                     {\tt from}
                                           GLN
  C31
         C32
                N33
                       ga 19
                                     from
                                           GLN
  034
         C32
                N33
                        ga_33
                                     from
                                           GLN
  C32
         N33
                       ga 23
                                           GLN
                HAG
                                     from
  C32
                       ga 23
         N33
                HAF
                                     from
                                           GLN
  HAG
         N33
                HAF
                       ga_24
                                     from
                                           GLN
  C7
         C37
                C38
                       ga_15
                                     from
                                           GLN.
                                                 fragment 3
  C37
         C38
                       ga 30
                039
                                     from
                                           GLN
  C37
         C38
                N40
                       ga 19
                                           GLN
                                     from
  039
         C38
                N40
                       ga 33
                                     from
  C38
         N40
                HAI
                       ga_23
                                     from
                                           GLN
  C38
                       ga_23
                                           GLN
         N40
                HAH
                                     from
  HAI
         N40
                       ga 24
                                     from
                                           GLN
                HAH
  C41
         C42
                C43
                       ga_15
                                     from
                                           GLN,
                                                 fragment 4
  C42
         C43
                044
                       ga_30
                                     from
                                           GLN
         C43
  C42
                N45
                       ga 19
                                     from
                                           GLN
         C43
                       ga 33
                                           GLN
  044
                N45
                                     from
  C43
         N45
                HAK
                       ga 23
                                     from
                                           GLN
                       ga_23
                                     {\tt from}
                                           GLN
                        ga_24
  HAK
         N45
                HAJ
                                     from
                                           GLN
  C48
         C49
                C50
                       ga 15
                                     from
                                           GLN.
                                                 fragment 5
  C49
                       ga 30
                                           GLN
         C50
                051
                                     from
  C49
         C50
                N52
                       ga_19
                                     from
                                           GLN
  051
         C50
                N52
                       ga 33
                                     from
                                           GLN
  C50
         N52
                                     from GLN
                HAM
                       ga_23
  C50
         N52
                HAL
                       ga 23
                                     from
                                           GLN
                       ga 24
  HAM
         N52
                HAL
                                     from
                                           GLN
  C18
         C60
                       ga_15
                                     {\tt from}
                                           GLN,
                                                fragment 6
                C61
  C60
         C61
                063
                       ga_30
                                     from GLN
  C60
         C61
                N62
                       ga_19
                                     from GLN
  063
         C61
                N62
                       ga 33
                                     from
                                           GLN
                HAO
                       ga_23
  C61
         N62
                                     from
                                           GLN
  C61
         N62
                HAN
                       ga_23
                                     from GLN
  HAO
                       ga 24
         N62
                HAN
                                     from GLN
  N21
         FE
                N22
                       ga 2
                                     corrin ring Fe-N angle
  N21
                       ga_2
                                     corrin ring Fe-N angle
  N22
         FE
                N23
                       ga 2
                                     corrin ring Fe-N angle
                       ga_2
                                    corrin ring Fe-N angle corrin-Fe-dimethylbenzimidazole
  N23
         FE
                N24
                       ga_2
  N21
         FE
                N<sub>3</sub>B
                       ga_2
                                     corrin-Fe-dimethylbenzimidazole
  N23
         FΕ
                N3B
                       ga 2
                                     corrin-Fe-dimethylbenzimidazole
  N24
         FE
                N3B
                        ga_2
                                     corrin-Fe-dimethylbenzimidazole
                       ga_34
ga_34
                                    corrin Fe-N-C angles (based on HEMC) corrin Fe-N-C angles (based on HEMC)
  FE
         N21
                C1
                C4
  FΕ
         N21
                C6
                       ga_34
                                     corrin Fe-N-C angles
                                                               (based on
  FΕ
         N22
                                                                          HEMC
                                     corrin Fe-N-C angles
corrin Fe-N-C angles
corrin Fe-N-C angles
  FE
         N22
                C9
                       ga_34
                                                               (based on HEMC)
                C11
  FE
         N23
                        ga 34
                                                               (based on HEMC
                       ga 34
  FE
         N23
                C14
                                                              (based on HEMC)
                C16
                       ga_34
                                     corrin Fe-N-C angles
                                                              (based on HEMC)
  FE
         N24
                C19
                       ga 34
                                     corrin Fe-N-C angles
                                                              (based on HEMC)
                       ga_34
ga_34
                                     Fe-dimethylbenzimidazole-N,C angle Fe-dimethylbenzimidazole-N,C angle
  FE
         M3B
                COR
                C2B
  FE
         N3B
         N1B
  C8B
                C2B
                       ga 7
                                     angle containing C8B, see minimization issues discussion
                                     angle containing C8B, see minimization issues discussion
  N<sub>1</sub>B
         C8B
                C9B
```

```
angle containing C8B, see minimization issues discussion
                   ga_7
ga_39
C7B
      C8B
             N1B
                               angle containing C8B, see minimization
                                                                         issues
                                                                                 discussion
C8B
      N1B
             C1R
                   ga_37
                               angle containing C8B,
                                                       see minimization issues discussion
                   ga_27
C4B
      C9B
             C8B
                               angle containing C8B, see minimization
                                                                         issues discussion
C6B
                   ga 27
                               angle containing C8B, see minimization
      C7B
             C8B
                                                                         issues discussion
                   ga_27
                               angle containing C8B, see minimization issues discussion
С7В
      C8B
             С9В
N21
      C1
             C2
                   ga_13
                               corrin ring-specific but HEMC-derived angles
                               corrin ring-specific but HEMC-derived angles
             C20
                   ga_13
N21
      C1
N21
                   ga 33
                               corrin ring-specific but
                                                          HEMC-derived angles
      C4
             C3
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
                                                          HEMC-derived angles
                               corrin ring-specific but
N22
      C6
             C5
                   ga 33
                               corrin ring-specific but HEMC-derived angles
N22
      C6
             C7
                   ga 33
      C9
                               corrin ring-specific but
                                                          HEMC-derived angles
N22
             C8
                   ga_33
C9
      N22
             C6
                   ga 6
                               corrin ring-specific but HEMC-derived angles
                               corrin ring-specific but HEMC-derived angles
C10
             N22
      C9
                   ga 33
                                                          HEMC-derived angles
N23
      C11
             C10
                   ga_33
ga_33
                               corrin ring-specific but
N23
      C11
             C12
                               corrin ring-specific but HEMC-derived angles
N23
      C14
             C13
                   ga_33
                               corrin ring-specific but HEMC-derived angles
                               corrin ring-specific but HEMC-derived angles
C14
      N23
             C11
                   ga_6
C15
                               corrin ring-specific but HEMC-derived angles
      C14
             N23
                   ga 33
N24
      C16
             C15
                   ga 33
                               corrin ring-specific
                                                     but
                                                          HEMC-derived angles
N24
      C19
             C1
                   ga 13
                               corrin ring-specific but HEMC-derived angles
                   ga_6
ga_33
C19
C17
      N24
             C16
                               corrin ring-specific but HEMC-derived angles
                               corrin ring-specific but
                                                          HEMC-derived angles
             N24
      C16
                               corrin ring-specific but HEMC-derived angles
C18
      C19
             N24
                   ga 13
                   ga_26
C3R
      02P
                               phosphate angle from ADE
                   ga_5
02P
      Ρ
             03
                               phosphate angle from ADE
                   ga_14
02 P
      Р
             04
                               phosphate angle from ADE
02P
             05
                               phosphate angle from ADE
                   ga 14
                   ga 14
03
             04
                               phosphate angle from ADE
                   ga_14
03
      Р
             05
                               phosphate angle
                                                from
                                                      ADE
04
      Р
             05
                   ga_29
                               phosphate angle from ADE
             C2P
                   ga 26
                               phosphate angle from ADE
      03
02P
      C3R
             C2R
                   ga_9
                               phosphate oxygen to CHn carbons from ADE
02 P
      C3R
             C4R
                   ga_9
                               phosphate oxygen to CHn carbons from ADE
03
      C2P
             C1P
                   ga_9
                               phosphate oxygen to CHn carbons from ADE
             C3P
03
      C2P
                   ga_9
                               phosphate oxygen to CHn carbons from ADE CHn-CHn-CHn angles
C1
             C26
                   ga 13
      C2
C1
      C2
             C25
                   ga_13
                               CHn-CHn-CHn angles
C1
                               CHn-CHn-CHn angles
C1
             C18
      C19
                   ga 13
                               CHn-CHn-CHn angles
C2
             C19
                               CHn-CHn-CHn angles
      C1
                   ga 13
C2
      C1
             C20
                   ga 13
                               CHn-CHn-CHn angles
C2
                   ga_13
                               CHn-CHn-CHn angles
                   ga_13
C3
      C2
             C25
                               CHn-CHn-CHn angles
C3
      C2
             C26
                   ga 13
                               CHn-CHn-CHn angles
C3
             C31
                               CHn-CHn-CHn angles
      C30
                   ga 13
C7
      C8
             C41
                               CHn-CHn-CHn angles
C8
      C41
             C42
                   ga 13
                               CHn-CHn-CHn angles
             C48
C12
      C13
                   ga 13
                               CHn-CHn-CHn angles
C13
             C46
                               CHn-CHn-CHn angles
      C12
                   ga 13
C13
      C12
                   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
                               CHn-CHn-CHn angles
      C18
             C60
                   ga 13
                   ga 13
C17
      C55
             C56
                               CHn-CHn-CHn angles
C18
      C17
             C54
                   ga 13
                               CHn-CHn-CHn angles
C18
      C17
             C55
                   ga_13
                               CHn-CHn-CHn angles
C19
             C20
                               CHn-CHn-CHn angles
      C1
                   ga 13
C19
      C18
             C60
                   ga 13
                               CHn-CHn-CHn angles
C25
                               CHn-CHn-CHn angles
                   ga_13
                   ga_13
C46
      C12
             C47
                               CHn-CHn-CHn angles
C54
      C17
             C55
                   ga_13
                               CHn-CHn-CHn angles
C36
      C7
             C37
                   ga 13
                               CHn-CHn-CHn angles
                   ğa_15
C2
                               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
C:6
      C7
             C36
                   ga_15
ga_15
                               sp3-sp3-sp2
                                            corrin ring carbon angle
C6
             C37
                               sp3-sp3-sp2
                                            corrin ring
                                                         carbon
                                                                 angle
                               sp3-sp3-sp2 corrin ring
C7
             C9
                   ga 15
      C8
                                                         carbon
C8
      C7
             C36
                   ga_15
                               sp3-sp3-sp2 corrin ring
                                                         carbon angle
                   ga 15
C8
      C7
             C37
                               sp3-sp3-sp2
                                            corrin ring
                                                         carbon
                                                                angle
                   ga 15
                               sp3-sp3-sp2 corrin ring carbon angle
C9
      C8
             C41
C11
             C13
                   ga_15
                               sp3-sp3-sp2 corrin ring
                                                         carbon angle
C11
      C12
             C46
                   ga 15
                               sp3-sp3-sp2 corrin ring
                                                         carbon angle
                   ga_15
ga_15
C11
      C12
             C47
                               sp3-sp3-sp2
                                            corrin ring
                                                         carbon angle
C12
      C13
             C14
                               sp3-sp3-sp2
                                            corrin ring carbon angle
C14
      C13
             C48
                   ga 15
                               sp3-sp3-sp2 corrin ring carbon angle
                   ga 15
                               sp3-sp3-sp2 corrin ring carbon angle
C16
      C17
             C18
```

```
sp3-sp3-sp2 corrin ring carbon angle
 C16
        C17
               C55
                      ga_15
                                   sp3-sp3-sp2
                                                corrin ring
                                                              carbon angle
 C4
C9
        C5
               C6
                      ga_27
                                   sp2-sp2-sp2
                                                corrin ring carbon angle
                      ga_27
        C10
               C11
                                   sp2-sp2-sp2
                                                corrin ring
                                                              carbon angle
 C14
                      ga 27
                                   sp2-sp2-sp2
        C15
               C16
                                                corrin ring carbon angle
 C3
                      ga_37
                                   sp3-sp2-sp2
                                                corrin ring carbon angle
 C4
        C5
               C35
                      ga_37
                                   sp3-sp2-sp2
                                                corrin ring
                                                              carbon
                     ga_37
ga_37
 C5
        C6
               C7
                                   sp3-sp2-sp2 corrin ring carbon angle
                                  sp3-sp2-sp2
        C5
               C35
 C6
                                                corrin ring carbon angle
 C8
               C10
                      ga_37
                                   sp3-sp2-sp2 corrin ring carbon angle
        C11
 C10
               C12
                      ga 37
                                   sp3-sp2-sp2 corrin ring
                                                              carbon angle
                                  sp3-sp2-sp2 corrin ring carbon angle
sp3-sp2-sp2 corrin ring carbon angle
 C13
        C14
               C15
                      ga_37
 C14
               C53
        C15
                      ga 37
                                   sp3-sp2-sp2 corrin ring carbon angle
 C15
        C16
               C17
                      ga 37
                      ga_37
 C16
               C53
        C15
                                   sp3-sp2-sp2 corrin ring carbon angle
 C5M
        C5B
               C4B
                      ga 37
                                  sp2-sp2-methyl dimethylbenzimidazole angle
                                  sp2-sp2-methyl dimethylbenzimidazole angle
                      ga_37
 C5M
        C5B
               C6B
                                  sp2-sp2-methyl dimethylbenzimidazole
 C6M
        C6B
               C5B
                     ga_37
ga_37
               C7B
                                   sp2-sp2-methyl dimethylbenzimidazole angle
 C6M
        C6B
 C4B
        C5B
               C6B
                      ga_27
                                   Csp2-Csp2-Csp2 dimethylbenzimidazole angle
                      ga_27
ga_27
                                  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
Csp2-Csp2-Csp2 dimethylbenzimidazole angle
 C5B
        C4B
               C9B
 C5B
        C6B
               С7В
 N1B
        C1R
               C2R
                      ga_9
                                   from ADE Nsp2-containing dimethylbenzimidazole angle
 N1B
        C1R
               06R
                      ga 9
                                   from ADE Nsp2-containing dimethylbenzimidazole angle
                                   from ADE Nsp2-containing dimethylbenzimidazole angle from ADE Nsp2-containing dimethylbenzimidazole angle
 N1B
        C2B
               N3B
                      ga_7
                      ga_37
 C2B
        N<sub>1</sub>B
               C1R
                                   from ADE Nsp2-containing dimethylbenzimidazole angle
 N3B
        С9В
               C4B
                      ga 39
                      ga_7
                                   from ADE Nsp2-containing dimethylbenzimidazole angle
 C9B
        N<sub>3</sub>B
 C1R
        C2R
               C3R
                      ga 8
                                   from ADE sugar angle
 C1R
        C2R
               O7R
                      ga_9
                                   from ADE
                                             sugar angle
                      ga_10
 C1R
        06R
               C4R
                                   from ADE
                                             sugar angle
                     ga_9
 C2R
        C1R
               06R
                                   from ADE
                                             sugar angle
 C2R
        C3R
               C4R
                      ga_8
                                   from
                                        ADE
                                             sugar
                                                    angle
 C2R
        O7R
               HAA
                      ga_12
                                   from ADE sugar angle
 C3R
                      ga 9
        C2R
               O7R
                                   from ADE
                                             sugar angle
 C3R
        C4R
               C5R
                      ga 8
                                   from ADE
                                             sugar angle
 C3R
        C4R
                      ga_9
               06R
                                   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
                      ga_9
ga_13
                                   from ADE sugar angle
 C5R
        C2P
 C1P
               C3P
                                  amide linkage angle
               C55
                     ga_13
ga_23
                                   amide linkage angle
        C56
 C57
 C57
        N59
               HAC
                                   from GLN angle
 N59
        C57
                      ga_33
                                   from GLN angle
 C56
        C57
               N59
                      ga_19
                                   from GLN angle
 058
        C57
                      ga 30
                                   from GLN angle
               C56
 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
                                   from PHE C-C-H angle
 C5B
                      ga_25
        C4B
               H4B
                                   from PHE C-C-H angle
 C9B
        C4B
               H<sub>4</sub>B
                      ga 25
                      ga 25
                                   from PHE C-C-H angle
 C6B
        С7В
 C8B
        С7В
               Н7В
                      ga_25
                                   from PHE C-C-H angle
 N<sub>1</sub>B
        C2B
               H2B
                      ga_36
                                   from ADE N-C-H angle
                                   from ADE N-C-H angle
                      ga_36
 N<sub>3</sub>B
        C2B
               H2B
                                  corrin ring C-C10-H angle corrin ring C-C10-H angle
                      ga 25
 C9
        C10
               H10
                      ga_20
 C11
        C10
               H10
 C5R
        O8R
               CLB
                     ga_12
                                  for LYS-B12 bridge (just replaces O8R H atom with CLB)
 standard Lysine angle topology
 - C
                      ga 32
                                   Standard LYS (lysine)
                     ga_31
ga_18
ga_13
 -C
        Ν
               CA
                                   Standard LYS
                                                  (lysine)
 Η
                                   Standard LYS
        Ν
               CA
                                                  (lvsine)
        CA
               СВ
                                   Standard LYS
                                                  (lysine)
 Ν
        CA
               C
                      ga 13
                                   Standard LYS
                                                  (lysine)
               С
 CB
        CA
                      ga_13
                                  Standard LYS
                                                  (lysine)
               CG
 CA
        CB
                     ga_15
ga_15
                                  Standard LYS
                                                  (lysine)
               CD
 СВ
        CG
                                  Standard LYS
                                                  (lysine)
               CE
                      ga 15
                                   Standard LYS
 CG
        CD
                                                  (lysine)
 CD
        CE
               NZ
                      ga_15
                                   Standard LYS
                                                  (lysine)
                      ga 11
 CE
        NZ
               HZ1
                                   Standard LYS
                                                  (lysine)
 CE
        NZ
               CLB
                      ga 6
                                  Modification from LYS
                                                            (CLB from NZ H atom)
 HZ1
               CLB
                      ga_23
                                   Modification from LYS
                                                            (CLB from NZ H atom)
 CA
               0
                      ga_30
                                   Standard LYS
        С
                                                  (lysine)
               +N
 CA
        C
                      ga_19
                                   Standard LYS
                                                  (lysine)
        Č
                      ga_33
                                  Standard LYS (lysine)
               +N
additional CLB-OLB angle linkages
```

```
OLB
        CLB
               08R
                       ga_33
                                     new OLB-CLB linkage angles
                                 ;
OLB
        CLB
               NZ
                       ga_33
                                    new OLB-CLB linkage angles
                                    new OLB-CLB linkage angles
O8R
        CLB
               NZ
                       ga_33
 [ impropers
               1
ai
               ak
                             gromos type
 C1R
        C8B
               C2B
                       N<sub>1</sub>B
                              gi_1
                                            dimethylbenzimidazole improper for planarity
                              gi_1
gi_1
N<sub>1</sub>R
        CAB
               C9B
                       N3B
                                            dimethylbenzimidazole improper for planarity
                                            dimethylbenzimidazole improper for planarity
 C8B
        N1B
               С7В
                       C9B
 C8B
        N1B
                              gi_1
                                            dimethylbenzimidazole improper
                                                                                  for planarity
 C8B
        C7B
               C6B
                       C5B
                              gi_1
                                            dimethylbenzimidazole improper for
                                                                                       planarity
                                                                                       planarity
C8B
        C9R
               N<sub>3</sub>B
                       C2B
                                            dimethylbenzimidazole improper for
                              gi_1
gi_1
 C7B
        C8B
                       C4B
                                            dimethylbenzimidazole improper for planarity
               C9B
 C7B
               C5B
                                            dimethylbenzimidazole improper for planarity
        C6B
                       C4B
                              gi_1
gi_1
 C6B
        C5B
                       С9В
                                            dimethylbenzimidazole improper
                                                                                       planarity
                C4B
                                                                                  for
 C5B
        C4B
               C9B
                       C8B
                                            dimethylbenzimidazole improper for planarity
               C7B
C9B
        C8B
                       C6B
                               gi_1
                                            dimethylbenzimidazole improper for planarity
                                            dimethylbenzimidazole improper for planarity
 C9B
        C4B
               N<sub>3</sub>B
                       C8B
                              gi_1
gi_1
 С9В
        изв
               C2B
                                            dimethylbenzimidazole improper for planarity
                       N<sub>1</sub>B
 C2B
        N1B
               C8B
                       C9B
                                            dimethylbenzimidazole improper for planarity
        C4B
C7B
               C6B
C5B
                              gi_1
gi_1
                                            dimethylbenzimidazole methyl groups dimethylbenzimidazole methyl groups
 C5M
                       C5B
 C6M
                       C6B
 C2B
        N1B
               N3В
                              gi
                                            dimethylbenzimidazole H atom-containing planarity
 C4B
        С9В
               C5B
                                            dimethylbenzimidazole H atom-containing planarity
                       H4B
 C7B
        C8B
               C6B
                       H7B
                                            dimethylbenzimidazole H atom-containing planarity
                              gi_1
gi_1
                                            Fe-dimethylbenzimidazole planarity
HEMC-based conjugated corrin ring improper planarity
N3B
        FE
               C2B
                       C9B
N21
        C4
               C5
                       C6
                                            HEMC-based conjugated corrin ring
N22
                C5
                              gi_1
                                                                                      improper planarity
N22
        C9
               C10
                       C11
                                            HEMC-based conjugated corrin ring
                                                                                      improper planarity
N23
        C11
               C10
                       C9
                                            HEMC-based conjugated corrin ring
                                                                                      improper planarity
                                            HEMC-based conjugated corrin ring improper planarity
N23
        C14
               C15
                       C16
                              gi_1
gi_1
               C15
                       C14
                                            HEMC-based conjugated corrin ring improper planarity
N24
        C16
                                            corrin ring on-Csp2 methyl group improper planarity corrin ring on-Csp2 methyl group improper planarity from GLN improper torsion definition
 C5
                       C35
                              gi_1
 C15
        C16
               C14
                       C53
                               gi_1
C27
                       C26
        028
               N29
                              gi 1
N29
        HAE
               HAD
                       C27
                                            from GLN improper torsion definition
                              qi
 C32
        034
                       C31
                                            from GLN improper torsion definition
N33
        HAG
               HAF
                       C32
                              gi_1
                                            from GLN improper torsion definition
                       C37
                                            from GLN improper torsion definition
 C38
        039
                              gi_1
gi_1
               N40
                                            from GLN improper torsion definition
N40
        HAI
                       C38
               HAH
 C43
        044
                       C42
                              gi_1
                                            from GLN improper torsion definition
                              gi_1
gi_1
                       C43
C49
N45
        HAK
                                            from GLN improper torsion definition
               HAJ
        051
 C50
               N52
                                            from GLN improper torsion definition
N52
        HAM
               HAL
                       C50
                                            from GLN improper torsion definition
                              gi_1
gi_1
 C61
        063
               N62
                       C60
                                            from GLN improper
                                                                  torsion definition
N62
        HAO
               HAN
                              gi_1
                                            from GLN improper
                                                                  torsion definition
                                            amide linkage C57 planarity
amide linkage N59 planarity
                                                                  planarity
 C57
        C56
               058
                       N59
                               gi_1
N59
        C57
               C1P
                       HAC
                              gi 1
                                            corrin ring C sp2 planarity
corrin ring C sp2 planarity
               C3
                              gi_1
gi_1
 C4
        N21
                       C5
 C5
               C6
                       C35
                       C7
C8
                                            corrin ring C sp2 planarity
corrin ring C sp2 planarity
C6
        N22
               C5
                               gi 1
               C10
C9
        N22
                              gi_1
                                            corrin ring C sp2 planarity
C11
               C10
                       C12
        N23
                              gi 1
                                            corrin ring C sp2 planarity
corrin ring C sp2 planarity
                       C13
 C14
        N23
               C15
                              gi
 C15
        C14
               C16
                       C53
                                            corrin ring C sp2 planarity
C16
        N24
               C15
                       C17
                              gi_1
                                            corrin ring C 10 planarity
corrin ring C10 planarity
corrin ring C atom sp3 tetrahedral geometry
C10
               C11
        C9
                       H10
                              gi_1
gi_2
        C17
 C18
               C19
                       C60
 C19
        N24
               C18
                       C1
                                            corrin ring C atom sp3 tetrahedral geometry
                                            corrin ring C atom sp3 tetrahedral geometry corrin ring C atom sp3 tetrahedral geometry
 C3
        C2
C9
               C30
C7
                       C4
                              gi_2
gi_2
                       C41
C8
                              gi_2
                                            corrin ring C atom sp3 tetrahedral geometry
 C13
        C14
               C12
                       C48
 C2P
        C1P
                       C3P
                              gi_2
                                            corrin ring C atom sp3 tetrahedral geometry
               03
                                            sugar C atom tetrahedral geometry sugar C atom tetrahedral geometry
C1R
        N1B
               C2R
                       06R
C2R
        O7R
               C3R
                       C1R
                               gi
                                            sugar C atom tetrahedral geometry
                       C4R
C3R
        C5R
               06R
                              qi
                                            sugar C atom tetrahedral geometry
 C3R
        C2R
                              gi
 FΕ
        C1
               C4
                       N21
                              gi_3
                                            HEMC improper definition
FE
        C6
               C9
                       N22
                               gi_3
                                            HEMC improper definition
 FE
        C11
               C14
                       N23
                              gi_3
gi_3
                                            HEMC improper definition HEMC improper definition
               C19
        C16
standard Lysine improper torsions
Ν
        - C
                       Η
                              qi 1
                                            Standard LYS (lysine)
               CA
                              gi_2
gi_1
 CA
        Ν
               С
                       СВ
                                            Standard LYS (lysine)
        CA
                +N
                       Ω
                                            Standard LYS (lysine)
 CT.B
                       NZ
        OAR
               OLB
                                            Linkage improper torsion to maintain planarity at CLB
dihedrals ]
               ak
                       al
ai
        аj
                             gromos type
C3R
                                       ; from ADE phosphate definition
        02P
                              gd_20
```

```
gd_27
gd_20
                                       from ADE phosphate definition
C2P
      03
                    02P
                                       from ADE
                                                 phosphate definition
                           gd_27
gd_7
C2P
      03
             P
                    02P
                                       from ADE phosphate definition
             C2P
                    C1P
      03
                                       from ADE
                                                 phosphate definition
C2R
      C3R
                                       from ADE
                                                 phosphate definition
             02P
                           ad 29
                    06R
                           gd 8
08R
      C5R
                                       from ADE
                                                 sugar dihedrals
O8R
      C5R
             C4R
                    06R
                                       from ADE sugar dihedrals
                           gd_17
qd_34
ORR
      C5R
             C4R
                    C3R
                                       from ADE sugar dihedrals
08R
      C5R
             C4R
                    C3R
                                       from ADE sugar dihedrals
C3R
      C4R
             06R
                    C1R
                                       from ADE
                                                 sugar dihedrals
C5R
      C4R
             C3R
                    C2R
                           gd 34
                                       from ADE sugar dihedrals
                           gd_17
CSR
      C4R
             C3B
                    02P
                                       from ADE sugar dihedrals
06R
      C4R
             C3R
                    C2R
                                       from ADE sugar dihedrals
                           ad 17
06R
      C4R
             C3R
                    02 P
                           gd 18
                                       from ADE sugar dihedrals
C4R
                                       from ADE
      06R
             C1R
                    C2R
                                                 sugar dihedrals
06R
      C1R
             C2R
                    O7R
                           gd 18
                                       from ADE sugar dihedrals
                    C3R
06R
      C1R
             C2R
                           gd 17
                                       from ADE sugar dihedrals
                                       from ADE sugar dihedrals
06R
             C2R
                    C3R
                           gd_34
qd_34
      C1R
C1R
      C2R
             C3R
                    C4R
                                       from ADE sugar dihedrals
C1R
      C2R
             C3R
                    02P
                           gd_17
                                       from ADE sugar dihedrals
                           gd_17
qd_18
O7R
      C2R
             C3R
                    C4R
                                       from ADE sugar dihedrals
07R
      C2R
             C3R
                    02P
                                       from ADE sugar dihedrals
C1R
      C2R
             O7R
                    HAA
                           gd 23
                                       from ADE sugar dihedrals
N1B
      C1R
             C2R
                    O7R
                           gd 17
                                       from ADE sugar dihedrals
06R
      C1R
             N<sub>1</sub>B
                    C8B
                           gd_16
                                       from ADE sugar dihedrals
HAB-based torsion gone for LYB C4R C5R O8R HAB gd 2 ; additional ADE-based sugar dihedral
                                       additional ADE-based sugar dihedral additional ADE-based sugar dihedral
             C2R
                           gd_17
N1B
      C1R
                    C3R
                           gd_17
N1B
      C1R
             06R
                    C4R
C2
      C26
             C27
                    N29
                           gd 40
                                       from GLN dihedral
                                       from GLN dihedral
C26
      C27
                           gd 14
             N29
                    HAD
      C31
                    N33
C30
             C32
                           gd_40
                                       from GLN dihedral
C31
      C32
             N33
                    HAF
                           gd 14
                                       from GLN dihedral
                                       from GLN dihedral
C7
      C37
             C38
                    N40
                           qd 40
C37
      C38
             N40
                    HAH
                                       from GLN dihedral
                           qd 14
C41
      C42
             C43
                           gd 40
                                       from GLN dihedral
                    N45
C42
      C43
             N45
                    HAJT
                           gd_14
                                       from GLN dihedral
C48
      C49
                                       from GLN dihedral
             C50
                    N52
                           ad 40
C49
                           qd 14
      C50
             N52
                                       from GLN dihedral
                    HAL
C18
      C60
                           gd_40
                                       from GLN dihedral
C60
      C61
                    HAN
                           gd_14
                                       from GLN dihedral
             N62
                           gd 33
C5M
                                       dimethylbenzimidazole methyl dihedral fix
      C5B
             C6B
                    C6M
C4B
      C5B
                    C6M
                                       dimethylbenzimidazole methyl dihedral fix
             C6B
                           qd 10
C8B
      С7В
             C6B
                    C6M
                           gd 10
                                       dimethylbenzimidazole methyl dihedral fix
C7B
      C6B
                    C5M
                                       dimethylbenzimidazole methyl dihedral
                           gd_10
C9B
      C4B
             C5B
                    C5M
                                       dimethylbenzimidazole methyl dihedral fix
C35
                                       corrin ring methyl planarity
      C5
             C4
                    N21
                           qd 10
C35
      C5
                                       corrin ring methyl planarity corrin ring methyl planarity
             C6
                    N22
                           gd_10
gd_10
C53
      C15
             C14
                    N23
C53
      C1
             C16
                    N24
                           gd 10
                                       corrin ring methyl planarity
                                       corrin ring but HEMC-derived N,C torsions
N24
      C19
             C1
                    N21
                           gd_34
                                                         HEMC-derived N,C
N24
             C1
      C19
                    N21
                                       corrin ring but
                           qd 34
                                                                            torsions
                                                         HEMC-derived N,C
N21
      C4
                           gd 15
                                       corrin ring but
                                                                            torsions
C4
      C5
             C6
                    N22
                           gd_15
                                       corrin ring but
                                                         HEMC-derived N,C torsions
                           gd_15
                                                         HEMC-derived N.C torsions
N22
      C9
             C10
                    C11
                                       corrin ring but
                                                         HEMC-derived N,C
C9
      C10
             C11
                    N23
                           qd 15
                                       corrin ring but
                                                                            torsions
                                       corrin ring but HEMC-derived N,C torsions
N23
      C14
             C15
                    C16
                           gd 15
C14
      C15
             C16
                    N24
                           gd 15
                                       corrin ring
                                                    but HEMC-derived N,C torsions
C1
      C2
             C26
                    C27
C27
                           gd_40
ad 34
                                       corrin ring HEMC derived CHn torsions corrin ring HEMC derived CHn torsions
C25
      C2
             C26
C2
      C26
             C27
                    028
                           gd 34
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C2
             C30
      C3
                    C31
                           gd_9
                                       corrin ring HEMC
                                                          derived CHn torsions
C3
      C30
             C31
                    C32
                           gd 40
                                       corrin ring
                                                    HEMC
                                                          derived
                                                                   CHn torsions
             C32
C30
      C31
                    034
                           gd_40
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C6
      C7
             C37
                    C38
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
                           qd 40
                           gd 40
C36
                                       corrin ring HEMC
                                                          derived
                                                                   CHn
                                                                        torsions
C7
      C37
             C38
                    039
                           gd 40
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C7
      C8
             C41
                    C42
                           gd_9
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
                           gd_34
gd_40
                                       corrin ring HEMC
C8
      C41
             C42
                    C43
                                                          derived
                                                                   CHn torsions
C41
             C43
                                       corrin ring HEMC
      C42
                    044
                                                          derived
                                                                   CHn torsions
C12
      C13
             C48
                    C49
                                                    HEMC
                                       corrin ring
                                                          derived
                                                                   CHn torsions
C13
      C48
             C49
                    C50
                           gd_34
                                       corrin ring HEMC
                                                          derived CHn torsions
C48
      C49
             C50
                    051
                           ad 40
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C16
                           qd 40
      C17
             C55
                    C56
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C54
      C17
             C56
                    C57
                           ad 40
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
                                       corrin ring
                                                          derived
C17
      C55
             C56
                    C57
                                                    HEMC
                                                                   CHn torsions
                           qd 34
C55
      C56
             C57
                    058
                           gd_40
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C17
      C18
             C60
                    C61
                           ad 9
                                       corrin ring HEMC
                                                                   CHn torsions
                                                          derived
C18
             C61
                    063
                           gd 34
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
      C60
                           gd 9
                                       corrin ring HEMC derived CHn torsions
C18
      C17
             C55
```

```
gd_34
gd_34
                                        amide linkage torsion terms
N59
       C1P
              C2P
                     C3P
                                         amide linkage
                                                        torsion
C2P
       C1P
              N59
                     C57
                            gd_34
                                        amide linkage torsion terms
                     C1P
C56
       C57
              N59
                            gd 14
                                        amide linkage
                                                        torsion
                                                                 terms
C55
                            qd 40
       C56
              C57
                     N59
                                        amide linkage torsion terms
 C17
                            gd_40
                                        amide linkage torsion terms
       C55
                     C57
 C5
       C4
              N21
                     C1
                            gd_14
                                        corrin ring sp3-containing torsions
C10
                            gd_14
gd_14
       C9
              N22
                     C6
                                        corrin ring sp3-containing
                                                                       torsions
C5
                     C9
                                        corrin ring sp3-containing
       C6
              N22
                                                                       torsions
 C15
       C14
                     C11
                            gd_14
                                        corrin ring sp3-containing
                                                                       torsions
C10
       C11
              N23
                     C14
                            gd_14
                                        corrin ring sp3-containing
                                                                       torsions
                     C19
C2
C15
       C16
              N24
                            gd_14
                                        corrin ring sp3-containing
                                                                       torsions
C4
                            gd_40
gd_40
       N21
              C1
                                        corrin ring sp3-containing
                                                                       torsions
                     C16
 C18
       C19
              N24
                                        corrin ring sp3-containing
                                                                       torsions
N22
              C5
                     C4
                                        corrin ring sp3-containing
                                                                       torsions
N23
       C11
              C10
                     C9
                            gd 33
                                        corrin ring sp3-containing
                                                                       torsions
              C17
                     C55
C19
       C18
                            gd_34
                                        corrin ring sp3-containing
                                                                       torsions
                            gd_40
gd_34
C55
              C16
                     C15
                                        corrin ring sp3-containing
       C17
                                                                       torsions
 C17
       C18
              C19
                     C1
                                        corrin ring sp3-containing
C18
       C19
              C1
                     C2
                            gd_34
                                        corrin ring sp3-containing
                                                                       torsions
                            gd_10
gd_10
C17
       C16
              C15
                     C14
                                        corrin ring sp3-containing
                                                                       torsions
C16
              C14
                     C13
       C15
                                        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
       C7
C3
              C6
C2
C8
                     C5
                            gd_34
                                        corrin ring sp3-containing
                                                                       torsions
C30
                     C1
                                        corrin ring sp3-containing
                            gd 34
                                                                       torsions
C11
       C12
              C13
                     C14
                            gd 34
                                        corrin ring sp3-containing
                                                                       torsions
 C13
       C12
              C11
                     C10
                            gd_34
                                        corrin ring sp3-containing
                                                                       torsions
                     C7
C30
                                                                       torsions
C10
       C9
              С8
                            gd_10
                                        corrin ring sp3-containing
C5
       C4
              C3
                            gd_34
                                        corrin ring sp3-containing
                                                                       torsions
C3
                                        corrin ring sp3-containing torsions
       C2
              C1
                     C19
                            gd_3^4
standard Lysine torsion topology
        -C
                            gd_14
gd_39
gd_34
                                        Standard LYS (lysine)
 -CA
                     CA
 -C
       N
              CA
                                        Standard LYS
                                                        (lysine)
Ν
       CA
              СВ
                     CG
                                        Standard LYS
                                                        (lysine)
Ν
       CA
              C
                     +N
                            gd_40
                                        Standard LYS
                                                        (lysine)
              CG
 CA
       CB
                                        Standard LYS
                     CD
                            gd_34
                                                        (lysine)
 СВ
                     CE
                                        Standard LYS
       CG
              CD
                            ad 34
                                                        (lvsine)
 CG
       CD
              CE
                     NZ
                            gd_34
                                        Standard LYS
                                                        (lysine)
                            gd_29
gd_23
 CD
       CE
              NZ
                     HZ1
                                        Standard LYS
                                                       (lysine)
C4R
       C5R
              OSR
                     CLB
                                        LYS-B12 linkage dihedral terms
                                        LYS-B12 linkage dihedral terms
 C5R
       08R
              CLB
                     OLB
                            qd 12
O8R
       CLB
              NZ
                     CE
                            gd 14
                                        LYS-B12 linkage dihedral terms
 OLB
       CLB
                     CE
                            gd_14
                                        LYS-B12 linkage dihedral terms
                                         THIS IS NEW!!!
THIS IS NEW!!!
 C9B
       N3B
              FE
                     N21
                            gd_38
N<sub>3</sub>B
              N21
                     C1
       FE
                            qd 38
                            gd_38
gd_38
N3B
       FE
                     C6
              N22
                                         THIS IS NEW!!!
N3B
       FE
              N23
                     C11
                                         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.

```
cyanocobalamin based on the HEMC CO parameters
[ atoms ]
                   0.38000
                                       ; from GLN residue
028
         0
                 -0.38000
                                 0
                                          from GLN residue
         NТ
N29
                 -0.83000
                                 Ω
                                          from GLN residue
HAE
                   0.41500
                                          from GLN residue
         Η
                                 0
                   0.41500
                                          \quad \hbox{from $\operatorname{GLN}$}
                                                     residue
C32
         С
                   0.38000
                                          from GLN residue
034
         \cap
                 -0.38000
                                          from GLN residue
         NT
                 -0.83000
                                          from GLN residue
N33
HAG
         Η
                 0.41500
                                          from GLN residue
HAF
                   0.41500
                                          from GLN residue
C38
         С
                   0.38000
                                          from GLN residue
                                 2
         0
                 -0.38000
039
                                          from GLN residue
                 -0.83000
N40
         NT
                                          from GLN residue
                   0.41500
                                          from GLN residue
HAH
         Η
                   0.41500
                                 2
                                          from GLN residue
                 0.38000
C43
         C
                                          from GLN residue
         Ö
044
                                          from GLN residue
         NT
                 -0.83000
                                          from GLN residue
HAK
         Н
                   0.41500
                                          from GLN residue
HAJ
C50
                  0.41500
0.38000
         H
C
                                 3
                                          from GLN residue
                                          from GLN residue
051
         0
                 -0.38000
                                          from GLN residue
         NT
                 -0.83000
N52
                                          from GLN residue
HAM
         Η
                   0.41500
                                 4
                                          from GLN residue
                  0.41500
0.38000
HAL
         Η
                                 4
5
                                          from GLN residue
         C
                                          from GLN residue
C61
                  -0.38000
063
                                          from GLN residue
N62
         NT
                 -0.83000
                                          from GLN residue
HAO
         Η
                   0.41500
                                          from GLN residue
HAN
                   0.41500
                                 5
                                          from GLN residue
         Η
C20
         CH3
                   0.00000
                                          methyl group
C25
         СНЗ
                   0.00000
                                          methyl group
C36
         CH3
                   0.00000
                                 8
                                          methyl group
C46
                   0.00000
                                          methyl group
         CH3
C47
                                          methyl group
         СНЗ
                   0.00000
                                 10
                   0.00000
                                          methyl group
C26
         CH2
                   0.00000
                                          non-polar CHn fragments
C30
                                          non-polar CHn fragments
         CH<sub>2</sub>
                   0.00000
                                 13
                   0.00000
C31
         CH2
                                          non-polar CHn fragments
                                 13
C37
         CH2
                                          non-polar CHn fragments
         CH2
                   0.00000
                                          non-polar
                                                      CHn
                                                           fragments
C42
         CH2
                   0.00000
                                 15
                                          non-polar CHn fragments
C48
         CH2
                   0.00000
                                          non-polar CHn fragments
                                 16
C49
         CH2
                   0.00000
                                          non-polar CHn fragments
                                 16
C56
         CH2
                   0.00000
                                 17
                                          non-polar CHn fragments
C55
         CH2
                   0.00000
                                 17
                                          non-polar CHn fragments
C60
                   0.00000
                                          non-polar CHn fragments
C2*-O2*-H2* from ADE
         CH2
                                 18
C2R
         CH1
                   0.15000
                                 19
O7R
                                          C2*-O2*-H2* from ADE
         OA
                  -0.54800
                                          C2*-O2*-H2* from ADE
HAA
                   0.39800
                                 19
                                          C1*-O4*-C4* from ADE
         CH1
C1R
                   0.20000
                                 2.0
                                          C1*-O4*-C4* from ADE
                  -0.36000
06R
         OΑ
                                 20
         CH1
                                          C1*-O4*-C4* from ADE
C4R
                   0.16000
C3R
         CH1
                   0.00000
                                          C3* from ADE
                                          C2*-O2*-H2* from ADE
C2*-O2*-H2* from ADE
C5R
         CH2
                   0.15000
                                 22
22
08R
                  -0.54800
         OA
                   0.39800
                                          C2*-O2*-H2* from ADE
HAB
         Н
                   2.20000
                                          PO3+O3* fragment
                                                               from
02
                                          PO3+O3* fragment
         OA
                  -0.80000
                                                               from ADE
                                          PO3+O3* fragment
PO3+O3* fragment
04
                                 23
         OM
                 -1.00000
                                                               from ADE
05
         OM
                  -1.00000
                                 23
                                                               from ADE
                  -0.80000
                                          PO3+O3* fragment from ADE
C2P
         CH1
                   0.35000
                                          non-polar CHn fragment
C3P
         CH3
                   0.00000
                                 24
                                          non-polar CHn fragment
                   0.00000
                                          non-polar CHn fragment
tempered GLN fragment charges
C1P
         CH2
                  -0.28000
HAC
         Η
                   0.28000
                                          tempered GLN fragment charges
                                          tempered GLN fragment charges tempered GLN fragment charges
C57
         C
                   0.38000
058
         0
                 -0.38000
                                          dimethylbenzimidazole C-CH3 group
dimethylbenzimidazole C-CH3 group
C5B
                   0.00000
                                                                                   (non-polar)
         CH3
                   0.00000
                                                                                   (non-polar)
                                          dimethylbenzimidazole C-CH3 group (non-polar) dimethylbenzimidazole C-CH3 group (non-polar) dimethylbenzimidazole aromatic C-H from TRP, PHE
C6B
                   0.00000
         CH3
C6M
                   0.00000
C4B
         C
                 -0.14000
                                 28
                                          dimethylbenzimidazole aromatic C-H from TRP,
H4B
                   0.14000
                 -0.14000
                                          dimethylbenzimidazole aromatic C-H from TRP,
```

```
0.14000
                                          dimethylbenzimidazole aromatic C-H from TRP, PHE
N3B
         NR
                  -0.55000
                                 30
                                          dimethylbenzimidazole polar aromatic NC fragment
C9B
         C
                  0.20000
                                 3.0
                                          dimethylbenzimidazole polar aromatic NC fragment
                                          dimethylbenzimidazole polar aromatic NC fragment
N<sub>1</sub>B
         NR
                  -0.30000
                                 31
                                          dimethylbenzimidazole polar aromatic NC fragment
C8B
         C
                  0.20000
                                 31
                  0.23000
                                          dimethylbenzimidazole aromatic C-H from TRP, PHE
H2B
         Η
                  0.23000
                                          dimethylbenzimidazole aromatic C-H from TRP,
                                          C-CH3 group (non-polar)
C-CH3 group (non-polar)
C-CH3 group (non-polar)
C5
         C
                  -0.05000
                                 33
C35
         CH3
                  0.00000
                                 33
                  -0.05000
C53
         CH3
                  0.00000
                                          C-CH3 group
                                                        (non-polar)
FE
         ਸਬ
                  1.00000
                                 35
                                          HEMC Fe-N group
                                          HEMC Fe-N group
HEMC Fe-N group
N21
                                 35
         NR
                  -0.44000
                  -0.50000
N22
                                 35
         NR
                                          HEMC Fe-N group
                  -0.50000
N23
         NR
N24
         NR
                  -0.44000
                                 35
                                          HEMC Fe-N group
                                          non-polar HEMC-derived corrin atoms non-polar HEMC-derived corrin atoms
C1
         CH<sub>0</sub>
                  0.22000
                                 36
C2
                  0.00000
         CH0
                                 36
                                          non-polar HEMC-derived corrin atoms
C3
                   0.00000
         CH1
C4
                  0.38000
                                 36
                                          non-polar HEMC-derived corrin atoms
C6
C7
                  0.29000
                                 37
                                          non-polar HEMC-derived corrin atoms
                                          non-polar HEMC-derived corrin atoms
         CH<sub>0</sub>
                  0.00000
                                 37
C8
         CH1
                  0.00000
                                          non-polar HEMC-derived corrin atoms
C9
                   0.35000
                                 37
                                          non-polar HEMC-derived corrin atoms
C16
C17
                                          non-polar HEMC-derived corrin atoms non-polar HEMC-derived corrin atoms
                  0.38000
                                 38
         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
C11
                  0.35000
                                 39
                                          non-polar HEMC-derived corrin atoms
                                          non-polar HEMC-derived corrin atoms
         CH0
C12
                  0.00000
                                 39
                                          non-polar HEMC-derived corrin atoms
C13
                  0.00000
                                 39
         CH1
                  0.29000
C14
                                          non-polar HEMC-derived corrin atoms
                                 39
                                          aromatic C-H from TRP,
aromatic C-H from TRP,
C10
         С
                  -0.24000
                                 40
H10
         Η
                  0.14000
                                 40
 cyano group addition to the original B12 topology
                  0.04000
C1N
         C
                                 41
                                          CN group on Fe
N1C
                 -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 ]
                gromos type
  ai
         аj
                 gb_27
gb_5
                               from GLN fragment 0
         C27
  C27
         028
                              from GLN
  C27
         N29
                 gb_9
                              from
                                    GLN
  N29
                                    GLN
         HAE
                 qb 2
                              from
  N29
         HAD
                 gb_2
                               from
                                    GLN
  C31
         C32
                  gb_27
                              from
                                    GLN fragment 1
                  gb_5
                              from GLN
  C32
         034
  C32
                 qb 9
         N33
                              from
                                    GLN
  N33
         HAG
                 gb 2
                               from
                                    GLN
  N33
         HAF
                  gb_2
                              {\tt from}
                                    GLN
                 gb_27
gb_5
  C37
         C38
                              from GLN fragment 2
  C38
         039
                              from GLN
                 gb 9
  C38
         N40
                              from
                                    GLN
                  gb_2
  N40
         HAI
                               from
                                    GLN
  N40
         HAH
                 gb_2
gb_27
                              from GLN
  C42
                                    GLN fragment 3
         C43
                              from
                 gb 5
  C43
         044
                              from
                                    GLN
  C43
         N45
                 gb_9
                               from
                                    GLN
                 gb_2
gb_2
  N45
         HAK
                              {\tt from}
                                    GLN
  N45
         HAJ
                              from GLN
  C49
                 qb 27
                                    GLN fragment 4
         C50
                              from
  C50
                 gb_5
                               from
                                    GLN
  C50
         N52
                 gb 9
                              from
                                    GLN
                 gb_2
gb_2
gb_27
  N52
         HAM
                              from
                                    GLN
                              from GLN
  N52
         HAL
  C60
         C61
                              from
                                    GLN fragment 5
  C61
         063
                  gb 5
                               from
                                    GLN
  C61
         N62
                  gb_9
                              {\tt from}
                                    GLN
                 gb_2
qb_2
  N62
         HAO
                              from
                                    GI<sub>1</sub>N
  N62
         HAN
                              from
                                    GLN
  FΕ
                 gb_35
                                    bond from HEMC
  FE
         N22
                 gb_35
                              FE-N
                                    bond from HEMC
                 gb_35
gb_35
  FE
         M23
                              FE-N bond from HEMC
                              FE-N bond from HEMC
  FΕ
         N24
         N3B
                 gb 37
                              FE-N3B bond from HEMC not in corrin ring
                              from ADE phosphate
```

```
from ADE phosphate
       05
                           from ADE phosphate
       03
               gb_28
                           from ADE phosphate
N21
               gb_21
                           corrin ring N-CHn bonds
       C1
N21
                           corrin ring N-C bonds
       C4
               ab 14
              gb_14
                           corrin ring N-C bonds
N22
       C9
               gb_14
                           corrin ring N-C bonds
              gb_14
ab_14
                           corrin ring N-C bonds
N23
       C11
N23
       C14
                           corrin ring N-C
                                             bonds
N24
       C16
               gb_14
                           corrin ring N-C bonds
              gb_21
gb_27
gb_27
N24
       C19
                           corrin ring N-CHn bonds
C30
       C31
                           CH2-CH2 bonds
C41
                           CH2-CH2 bonds
       C42
C48
       C49
              gb 27
                           CH2-CH2 bonds
C55
       C56
                           CH2-CH2
                                   bonds
C56
       C57
               gb 27
                           CH2-CH2 bonds
N1B
               gb_22
                           sugar bonds from ADE
       C1R
                           sugar bonds from ADE
C1R
       C2R
              gb_26
qb_20
C2R
       07R
                           sugar bonds from ADE
              gb_1
O7R
      HAA
                           sugar bonds from ADE
C2R
C3R
              gb_26
qb_26
       C3R
                           sugar bonds from ADE
       C4R
                           sugar bonds from ADE
C3R
       02
              gb 20
                           sugar
                                 bonds from ADE
C4R
       C5R
              gb_26
                           sugar bonds from ADE
C5R
       O8R
               gb_20
                           sugar bonds from ADE
08R
      HAB
                           sugar bonds from ADE
              ab 1
                           sugar bonds from ADE
C4R
      06R
              gb 20
06R
              gb_20
                           sugar bonds from ADE
                           amide corrin - phosphate linkage
amide corrin - phosphate linkage
C1P
      N59
              gb_9
              gb_27
gb_27
C1P
      C2P
                           amide corrin - phosphate linkage
C2P
       C3P
C2P
              gb 20
                           amide corrin - phosphate linkage
       03
              gb_2
gb_9
N59
      HAC
                           amide corrin -
                                           phosphate
                           amide corrin - phosphate linkage
N59
       C57
                           amide corrin - phosphate linkage
C57
      058
              gb 5
N1B
       C2B
              gb 10
                           dimethylbenzimidazole ring
C2B
      N3B
               gb 10
                           dimethylbenzimidazole ring
C2B
      H2B
               gb_3
                           dimethylbenzimidazole ring
N3B
              gb_10
gb_16
       C9B
                           dimethylbenzimidazole ring
                           dimethylbenzimidazole
С9В
       C4B
       C5B
              gb_16
                           dimethylbenzimidazole ring
C4B
C4B
C5B
      H4B
                           dimethylbenzimidazole
               gb_16
       C6B
                           dimethylbenzimidazole
C5B
       C5M
              gb_27
                           dimethylbenzimidazole
C6B
       С7В
              gb 16
                           dimethylbenzimidazole
C6B
               gb_27
                           dimethylbenzimidazole
C7B
C7B
       C8B
               gb_16
                           dimethylbenzimidazole
                                                   ring
      Н7В
                           dimethylbenzimidazole ring
              qb 3
C8B
              gb_10
                           dimethylbenzimidazole ring
      N1B
C8B
       С9В
               gb_16
                           dimethylbenzimidazole ring
              gb_27
gb_27
gb_27
C1
       C20
                           corrin ring carbon framework
C1
       C2
                           corrin ring carbon framework
C2
                           corrin ring carbon framework
       C3
C2
              gb 27
                           corrin ring carbon framework
C2
       C26
               gb_27
                           corrin ring
                                        carbon framework
              gb_27
gb_27
C3
       C4
                           corrin ring carbon framework
C3
       C30
                           corrin ring carbon framework
              gb 17
C4
       C5
                           corrin ring carbon
                                                framework
C5
       C6
               gb_17
                           corrin ring carbon
                                                framework
       C35
C5
C6
              gb_27
ab_27
                           corrin ring carbon framework
       C7
                           corrin ring carbon framework
              gb 27
C7
       C8
                           corrin ring carbon framework
C7
       C37
              gb_27
                           corrin ring carbon framework
              gb_27
gb_27
gb_27
C7
       C36
                           corrin ring
                                        carbon framework
C8
       C9
                           corrin ring carbon framework
C8
      C41
                           corrin ring carbon framework
                           corrin ring carbon framework
C10
       C11
              gb 17
                           corrin ring carbon framework
              gb_27
gb_27
gb_27
C11
       C12
                           corrin ring carbon framework
      C46
C47
C12
                           corrin ring carbon framework
C12
                           corrin ring carbon
                                                framework
C12
       C13
                           corrin ring carbon
                                                framework
C13
       C14
               gb_27
                           corrin ring carbon framework
C13
              gb_27
gb_17
       C48
                           corrin ring carbon framework
C14
       C15
                           corrin ring carbon framework
C15
       C16
              gb_17
                           corrin ring carbon framework
              gb_27
gb_27
gb_27
C15
       C53
                           corrin ring
                                        carbon framework
C16
C17
       C17
                           corrin ring carbon framework
      C18
                           corrin ring carbon framework
C17
       C54
              gb 27
                           corrin ring carbon framework
C17
       C55
                          corrin ring carbon framework
```

```
gb_27
gb_27
gb_27
gb_3
 C18
C18
                              corrin ring carbon framework
        C60
                              corrin ring carbon framework
 C19
C10
        C1
                             corrin ring carbon framework
        H10
                         ; corrin ring C10-H10 bond
cyano group addition to the original B12 topology
                         ; cyano group on the Fe; cyano group on the Fe
    C1N gb_30
N1C gb_4
exclusions ]
 FE
C1N
        N1C
 FE
                    new add
                   new add
 FE
        C1
 FE
        C2
 FE
        C3
        C5
C7
 FE
 FE
 FE
        C8
        C10
 FE
        C12
        C13
C15
 FE
 FE
        C17
 FE
        C18
        C20
C25
 FE
 N21
 N21
        C26
 N21
        C35
        C6
C9
 N21
 N21
 N21
        C11
 N21
        C14
 N21
        C16
 N21
        C19
 N21
        C10
 N22
        C1
 N22
        C4
 N22
        C36
        C37
 N22
 N22
        C11
        C14
C16
 N22
 N22
 N22
        C19
 N22
        C15
 N23
 N23
        C19
 N23
        C1
 N23
        C4
 N23
        C6
 N23
        C9
 N23
        C46
        C47
 N23
 N23
        C48
 N23
        C5
        C4
 N24
 N24
        C5
 N24
        C6
 N24
        C9
 N24
        C10
C11
 N24
 N24
        C14
 N24
        C55
 N24
        C54
 N24
        C60
 C1R
        С7В
 C1R
 C1R
        N3B
 N1B
        C6B
 N<sub>1</sub>B
        C4B
 C8B
        C5B
 C8B
        C5M
 C8B
        C6M
 C7B
        C4B
 C7B
        N3B
 С7В
        C2B
 C2B
        С9В
 C5B
        C2B
 C5M
        C6M
 C1
        C30
                  HEMC-based C framework exclusions
                  HEMC-based C framework exclusions
 C1
        C5
```

```
C2
C3
                 HEMC-based C
                               framework exclusions
       C35
                 HEMC-based C
                                framework
C3
       C6
                 HEMC-based C
                               framework
                                          exclusions
C4
                             C
       C26
                 HEMC-based
                                framework
                                          exclusions
C4
                 HEMC-based
                                framework
       C7
                                          exclusions
 C30
       C26
                 HEMC-based
                                {\tt framework}
                                          exclusions
 C30
       C5
                 HEMC-based
                             C
                                framework
                                          exclusions
                 HEMC-based C
 C5
       C8
                               framework exclusions
 C5
                 HEMC-based
                             C
                               framework exclusions
       C9
 C5
                 HEMC-based
                                {\tt framework}
                                          exclusions
 C5
       C37
                 {\tt HEMC-based}\ {\tt C}
                               framework exclusions
                 HEMC-based C
C35
       C7
                               framework exclusions
                 HEMC-based C
C6
       C41
                               framework exclusions
 C6
       C10
                 HEMC-based
                               framework exclusions
 C7
                 HEMC-based
                             С
       C10
                                framework
                                          exclusions
C8
       H10
                 HEMC-based C
                               framework exclusions
                 HEMC-based C
C8
       C11
                               framework exclusions
C9
                 HEMC-based C
                               framework
       C36
                                          exclusions
 C9
       C37
                 HEMC-based C
                               framework
                                          exclusions
 C9
       C12
                 {\tt HEMC-based}\ {\tt C}
                               {\tt framework}
                                          exclusions
C36
       C41
                 HEMC-based C
                               framework exclusions
C37
       C10
                 HEMC-based
                               framework exclusions
 C10
       C13
                 HEMC-based
                                framework
                                          exclusions
 C10
       C14
                 HEMC-based C
                               framework exclusions
C10
C10
       C46
C47
                               framework framework
                 HEMC-based C
                                          exclusions
                             C
                 HEMC-based
                                          exclusions
H10
       C12
                 HEMC-based
                               framework
                                          exclusions
 C11
                 HEMC-based
                                framework
                                          exclusions
                 HEMC-based C HEMC-based C
C11
       C15
                               framework exclusions
C12
       C15
                               framework exclusions
C13
                 HEMC-based
                                framework
       C53
                                          exclusions
                 HEMC-based
 C13
       C16
                               framework
                                          exclusions
 C14
       C46
                 HEMC-based
                             С
                                framework
                                          exclusions
C14
       C47
                 HEMC-based C
                               framework exclusions
                 HEMC-based
                             C
                               framework exclusions
C14
       C17
 C46
       C48
                 HEMC-based
                                framework
                                          exclusions
 C47
       C48
                 HEMC-based C
                               framework
                                          exclusions
C48
       C15
                 HEMC-based C
                               framework exclusions
                 HEMC-based C
C15
                               framework exclusions
       C18
 C15
                 HEMC-based
                               framework exclusions
       C19
 C15
                 HEMC-based
                                framework
                                          exclusions
       C55
                 HEMC-based C
 C15
                               framework exclusions
 C53
                               framework exclusions
       C17
C16
                 HEMC-based C
                               framework exclusions
       C60
 C19
       C54
                 HEMC-based
                               framework exclusions
                 HEMC-based C
HEMC-based C
 C19
       C55
                                framework exclusions
 C54
       C60
                               framework exclusions
                 HEMC-based C framework exclusions
C55
       C60
cyano group addition to the original B12 topology
N21
       N1C
                 cyano exclusions from HEMC CO group
                 cvano exclusions from HEMC
N22
       N1C
                                               CO
                                                  group
N23
       N1C
                 cyano exclusions
                                    from
                                                  group
N24
       N1C
                 cyano exclusions from
                                         HEMC
                                               CO
                                                  group
C1
       C1N
                 cyano exclusions
                                    from
                                         HEMC
                                               CO
                                                  group
                                         HEMC
 C4
       C1N
                 cyano exclusions from
                                               CO
                                                  group
 C6
                 cyano exclusions
                                    from
                                         HEMC
                                               CO
       C1N
                                                  group
 C9
       C1N
                 cyano exclusions
                                    from
                                         HEMC
                                               CO
                                                  group
C11
       C1N
                 cyano exclusions from HEMC
                                               CO group
C14
                 cvano exclusions from HEMC
                                               CO group
       C1N
 C16
       C1N
                 cyano exclusions from HEMC
                                               CO group
 C19
       C1N
                 cyano exclusions from HEMC CO group
N<sub>3</sub>B
       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 ]
              ak
                   gromos type
                                from GLN, fragment 1
C2
       C26
              C27
                    ga_15
                    ga_30
ga_19
C26
       C2.7
              028
                                 from GLN
 C26
       C27
                                 from
                                      GLN
028
       C27
                    ga_33
                                 from
                                      GLN
 C27
       N29
              HAE
                    ga_23
                                 from
                                      GLN
 C27
       N29
              HAD
                     ga 23
                                 from
                                      GLN
                    ga 24
HAE
       N29
              HAD
                                 from
                                      GLN
 C30
       C31
              C32
                    ga_15
                                 from
                                      GLN,
                                            fragment 2
 C31
       C32
              034
                    ga 30
                                 from
                                      GLN
                    ga_19
ga_33
C31
       C32
              M33
                                 from
                                      GT.N
034
       C32
              N33
                                 from
                                      GLN
                                 from
 C32
       N33
                    ga 23
                                      GLN
              HAG
 C32
                    ga 23
       N33
```

from GLN

```
C7
       C37
             C38
                    ga_15
                                 from GLN,
                                            fragment 3
C37
       C38
             039
                    ga_30
                                 from GLN
C37
       C38
             N40
                    ga 19
                                 from
                                      GLN
039
       C38
             N40
                    ga 33
                                 from
                                      GLN
                    ga 23
C38
      N40
                                 {\tt from}
                                      GLN
C38
      N40
             HAH
                    ga_23
                                 from
                                      GLN
HAT
      N40
             HAH
                    ga_24
                                 from
                                      GLN.
C41
       C42
                                      GLN, fragment 4
             C43
                    ga 15
                                 from
C42
       C43
                    ga_30
                                 from
                                      GLN
C42
       C43
             N45
                    ga 19
                                 from
                                      GLN
044
       C43
             N45
                    ga_33
                                 from
                                      GLN
C43
      N45
             HAK
                                      GLN
                    ga 23
                                 from
C43
                    ga 23
      N45
             HAJ
                                 from
                                      GLN
HAK
                    ga_24
      N45
             HAJ
                                 from
                                      GLN
C48
       C49
             C50
                    ga 15
                                 from GLN,
                                           fragment 5
C49
       C50
             051
                    ga 30
                                 from GLN
C49
       C50
             N52
                    ga 19
                                 from GLN
                    ğa_33
051
       C50
                                 from
C50
      N52
             HAM
                    ga_23
                                 from
                                      \operatorname{GLN}
                    ga_23
ga_24
C50
      N52
             HAL
                                 from GLN
HAM
      N52
             HAL
                                 from
                                      GLN
C18
       C60
             C61
                    ga 15
                                 from
                                      GLN, fragment 6
C60
       C61
             063
                    ga 30
                                 from
                                      GLN
C60
O63
      C61
             N62
                    ga_19
                                 from GLN
                    ga 33
             N62
                                 from
                                      GLN
                    ga 23
C61
      N62
             HAO
                                 from
                                      GLN
C61
       N62
             HAN
                    ga_23
                                 from GLN
HAO
      N62
             HAN
                    ga 24
                                 from GLN
                    ga_2
ga_2
N21
       FE
             N22
                                 corrin ring Fe-N angle
N21
       FΕ
                                corrin ring Fe-N angle
             N24
                    ga 2
N22
                                 corrin ring Fe-N angle
                                 corrin ring Fe-N angle
N23
       FE
             N24
                    ga_2
N21
       FE
             N<sub>3</sub>B
                    ga_2
                                corrin-Fe-dimethylbenzimidazole
                    ga<sup>2</sup>
                                corrin-Fe-dimethylbenzimidazole
N22
       FE
             N<sub>3</sub>B
N23
       FE
             N3B
                    ga<sup>2</sup>
                                corrin-Fe-dimethylbenzimidazole
N24
                    ga 2
                                 corrin-Fe-dimethylbenzimidazole
       FΕ
             N3B
FE
      N21
             C1
                    ga_34
                                corrin Fe-N-C angles (based on HEMC)
                                corrin Fe-N-C angles
             C4
FE
      N21
                                                         (based on HEMC)
                    ga 34
                                corrin Fe-N-C angles
             С6
                                                         (based on HEMC
FE
      N22
                    ga 34
                                corrin Fe-N-C angles
                    ga_34
                                                         (based on HEMC)
                                corrin Fe-N-C angles
corrin Fe-N-C angles
             C11
C14
      N23
                    ga_34
                                                         (based on HEMC)
FE
FE
      N23
                    ga 34
                                                         (based on HEMC
                                corrin Fe-N-C angles
FE
             C16
                    ga 34
                                                         (based on HEMC)
      N24
FΕ
      N24
             C19
                    ga 34
                                 corrin Fe-N-C angles (based on HEMC
                                Fe-dimethylbenzimidazole-N,C angle Fe-dimethylbenzimidazole-N,C angle
                    ga_34
FE
      N3B
             C2B
                    ga_34
C8B
             C2B
                    ga 7
                                angle containing C8B, see minimization issues discussion
      N<sub>1</sub>B
N1B
                    ga 7
                                 angle containing C8B, see minimization
       C8B
             C9B
                                                                            issues discussion
C8B
       С9В
             N3B
                    ga_7
                                 angle containing
                                                   С8В,
                                                         see minimization
                                                                                    discussion
C7B
       C8B
             N1B
                    ga 39
                                 angle containing C8B,
                                                         see minimization
                                                                            issues discussion
C8B
      N<sub>1</sub>B
             C1R
                    ga 37
                                 angle containing C8B,
                                                         see minimization
                                                                            issues discussion
C4B
                                                                            issues discussion
                                angle containing
                                                   C8B, see minimization
      C9B
             C8B
                    ga 27
                    ga 27
C6B
       С7В
                                 angle containing C8B,
                                                         see minimization
                                                                            issues discussion
С7В
       C8B
             С9В
                    ga_27
                                 angle containing C8B,
                                                         see minimization issues discussion
N21
       C1
             C2
                    ga_13
                                 corrin ring-specific but HEMC-derived angles
                                                             HEMC-derived angles
             C20
                    ga 13
N21
       C1
                                corrin ring-specific but
                    ga 33
N21
       C4
             C3
                                corrin ring-specific
                                                        but HEMC-derived angles
                                 corrin ring-specific but
C4
      N21
             C1
                    ga 6
                                                             HEMC-derived
C5
       C4
             N21
                    ga_33
                                 corrin ring-specific but
                                                             HEMC-derived angles
C19
                                corrin ring-specific but HEMC-derived angles
      C1
                    ga 13
             N21
                                                             HEMC-derived angles
N22
       C6
             C5
                    ga 33
                                corrin ring-specific but
N22
             C7
                                 corrin ring-specific but HEMC-derived angles
       C6
                    ga_33
N22
       C9
             C8
                    ga 33
                                 corrin ring-specific but HEMC-derived angles
                                corrin ring-specific but HEMC-derived angles
C9
      N22
             C6
                    ga_6
                                corrin ring-specific but HEMC-derived angles
             N22
C10
      C9
                    ga 33
                                 corrin ring-specific but
                                                             HEMC-derived angles
       C11
                    ga 33
N23
       C11
             C12
                    ga 33
                                 corrin ring-specific but
                                                             HEMC-derived angles
N23
       C14
             C13
                    ga_33
                                corrin ring-specific but HEMC-derived angles
                                                             HEMC-derived angles
                                corrin ring-specific but corrin ring-specific but
C14
      N23
             C11
                    ga_6
                    ga_33
C15
             N23
                                                             HEMC-derived angles
       C14
N24
       C16
             C15
                    ga 33
                                 corrin ring-specific but
                                                             HEMC-derived angles
N24
       C19
             C1
                    ga_13
                                 corrin ring-specific but HEMC-derived angles
             C16
                    ga 6
                                 corrin ring-specific but HEMC-derived angles
C19
      N24
C17
       C16
             N24
                    ga 33
                                 corrin ring-specific but HEMC-derived angles
C18
       C19
                    ga_13
                                 corrin ring-specific but HEMC-derived angles
      02
C3R
                    ga 26
                                phosphate angle from ADE
             03
02
       P
                    ga_5
                                 phosphate angle from ADE
02
       P
                    ga 14
                                 phosphate angle from ADE
             04
02
             05
                    ga 14
                                phosphate angle from ADE
                    ga 14
                                phosphate angle from ADE
```

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ga_14
ga_29
                                phosphate angle from ADE
04
             05
                                phosphate angle from ADE
P
      03
             C2P
                    ga_26
                                phosphate angle from ADE
02
       C3R
             C2R
                    ga 9
                                phosphate oxygen to CHn carbons from ADE
02
                    ga 9
       C3R
             C4R
                                phosphate oxygen to CHn carbons from ADE
                    ga 9
03
       C2P
             C1P
                                phosphate oxygen to CHn carbons
                                                                    from
03
       C2P
             C3P
                    ga_9
                                phosphate oxygen to CHn carbons from
C1
       C2
             C26
                    ga_13
                                CHn-CHn-CHn angles
C1
       C2
             C25
                                CHn-CHn-CHn angles
                    ga 13
C1
             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
             C20
                                CHn-CHn-CHn angles
       C1
                    ga 13
                    ga_13
C2
       C3
             C30
                                CHn-CHn-CHn angles
C3
                                CHn-CHn-CHn angles
       C2
             C25
                    ga_13
C3
       C2
             C26
                    ga 13
                                CHn-CHn-CHn angles
C3
       C30
             C31
                    ga 13
                                CHn-CHn-CHn angles
C7
             C41
                                CHn-CHn-CHn angles
       C8
                    ga 13
                    ğa_13
                                CHn-CHn-CHn angles
C8
             C42
C12
       C13
             C48
                    ga_13
                                CHn-CHn-CHn angles
C13
      C12
C12
                    ga_13
ga_13
             C46
                                CHn-CHn-CHn angles
             C47
                                CHn-CHn-CHn angles
C13
       C48
             C49
                    ga 13
                                CHn-CHn-CHn angles
C17
       C18
             C19
                    ga 13
                                CHn-CHn-CHn angles
C17
             C60
C56
                    ga_13
       C18
                                CHn-CHn-CHn angles
                                CHn-CHn-CHn angles
       C55
                    ga 13
                    ga 13
C18
       C17
             C54
                                CHn-CHn-CHn angles
C18
                    ga_13
       C17
             C55
                                CHn-CHn-CHn angles
                                CHn-CHn-CHn angles
C19
       C1
             C20
                    ga 13
C19
       C18
             C60
                    ga 13
                                CHn-CHn-CHn angles
C25
       C2
             C26
                                CHn-CHn-CHn angles
                    ga 13
      C12
                                CHn-CHn-CHn angles
C46
                    ga 13
             C47
C54
       C17
             C55
                    ga_13
                                CHn-CHn-CHn angles
C36
       C7
             C37
                    ga_13
                                CHn-CHn-CHn angles
C2
                    ga 15
                                sp3-sp3-sp2
                                             corrin ring carbon angle
      C3
             C4
C4
       C3
             C30
                    ga 15
                                sp3-sp3-sp2
                                             corrin ring carbon angle
C6
             C8
                    ga 15
                                sp3-sp3-sp2
                                             corrin ring
                                                           carbon
                                             corrin ring
                                                           carbon angle
C6
       C7
             C36
                    ga_15
                                sp3-sp3-sp2
C6
       C7
             C37
                                sp3-sp3-sp2
                    ga 15
                                             corrin ring
                                                           carbon
                                                                   angle
                    ga 15
                                sp3-sp3-sp2 corrin ring
C7
             C9
       C8
                                                           carbon
                                                                   angle
C8
             C36
                    ga_15
                                sp3-sp3-sp2 corrin ring
                                                           carbon
                                                                   angle
C8
             C37
                    ga_15
                                sp3-sp3-sp2 corrin ring
                                                           carbon
                                                                   angle
C9
       C8
             C41
                    ga 15
                                sp3-sp3-sp2 corrin ring
                                                           carbon
                                sp3-sp3-sp2
C11
             C13
      C12
                    ga 15
                                             corrin ring
                                                           carbon
                                                                   angle
C11
       C12
             C46
                    ga_15
                                sp3-sp3-sp2 corrin ring
                                                           carbon
                                                                   angle
C11
                    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
             C18
                                sp3-sp3-sp2
       C17
                    ga 15
                                             corrin ring
                                                           carbon
                                                                   angle
C16
       C17
             C54
                    ga 15
                                sp3-sp3-sp2
                                             corrin ring
                                                           carbon
                                             corrin ring
                                                           carbon
C16
       C17
             C55
                    ga 15
                                sp3-sp3-sp2
                                                                   angle
C4
C9
                    ga_27
       C5
             C6
                                sp2-sp2-sp2
                                             corrin ring
                                                           carbon angle
                    ga 27
                                sp2-sp2-sp2 corrin ring
      C10
             C11
                                                           carbon
                                                                   angle
                    ga 27
C14
       C15
             C16
                                sp2-sp2-sp2
                                             corrin ring
                                                           carbon
                                                                   angle
C3
       C4
             C5
                    ga_37
                                sp3-sp2-sp2 corrin ring
                                                           carbon
                                                                   angle
                    ga_37
ga_37
                                                                   angle
C4
       C5
             C35
                                sp3-sp2-sp2 corrin ring
                                                           carbon
C5
             C7
                                sp3-sp2-sp2 corrin ring
       C6
                                                           carbon
                                                                   angle
                                sp3-sp2-sp2 corrin ring
C6
       C5
             C35
                    ga 37
                                                           carbon angle
C8
       C9
             C10
                    ga 37
                                sp3-sp2-sp2 corrin ring
                                                           carbon
C10
       C11
             C12
                    ga_37
                                sp3-sp2-sp2 corrin ring
                                                           carbon angle
C13
      C14
             C15
                    ga 37
                                sp3-sp2-sp2 corrin ring
                                                           carbon angle
                                sp3-sp2-sp2 corrin ring carbon angle
C14
       C15
             C53
                    ga 37
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
             C4B
                                sp2-sp2-methyl dimethylbenzimidazole
sp2-sp2-methyl dimethylbenzimidazole
       C5B
                    ga_37
C5M
       C5B
             C6B
                    ga 37
                                                                         angle
                    ga 37
                                sp2-sp2-methyl dimethylbenzimidazole
C6M
       C6B
C6M
       C6B
             C7B
                    ga 37
                                sp2-sp2-methyl dimethylbenzimidazole
C4B
       C5B
             C6B
                    ga_27
                                Csp2-Csp2-Csp2 dimethylbenzimidazole angle
                    ga_27
ga_27
                                Csp2-Csp2-Csp2 dimethylbenzimidazole angle Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B
       C4B
             C9B
C5B
       C6B
             C7B
N1B
       C1R
             C2R
                    ga_9
                                from ADE Nsp2-containing dimethylbenzimidazole angle
                    ga_9
ga_7
N1B
       C1R
             06R
                                from ADE Nsp2-containing dimethylbenzimidazole angle
                                from ADE Nsp2-containing dimethylbenzimidazole
N<sub>1</sub>B
       C2B
             N3B
                                          Nsp2-containing dimethylbenzimidazole angle
C2B
      N1B
             C1R
                    ga 37
                                from ADE
изв
       С9В
                    ga_39
                                from
                                     ADE
                                          Nsp2-containing dimethylbenzimidazole angle
С9В
      N3B
             C2B
                                      ADE
                                          Nsp2-containing dimethylbenzimidazole angle
                                from
C1R
       C2R
             C3B
                    ga_8
                                from ADE
                                          sugar angle
C1R
       C2R
             O7R
                    ga<sup>-</sup>9
                                      ADE
                                from
                                          sugar angle
       06R
             C4R
                    ga 10
                                from ADE sugar angle
C1R
                    ga 9
C2R
       C1R
                                from ADE sugar angle
```

```
from ADE sugar angle
                      ga_8
ga_12
 C2R
        O7R
               HAA
                                   from ADE sugar angle
 C3R
        C2R
               O7R
                      ga_9
                                   from ADE sugar angle
 C3R
        C4R
               C5R
                      ga 8
                                   from ADE
                                             sugar angle
 C3R
                                   from ADE
        C4R
               06R
                      ga 9
                                             sugar angle
                      ga 9
 C4R
        C5R
                                   from ADE
                                             sugar angle
 C5R
        08R
               HAB
                      ga_12
                                   from ADE sugar angle
                      ga_9
 C5R
        C4R
               O6R
                                   from ADE sugar angle
 C1P
        C2P
               C3P
                      ga 13
                                   amide linkage angle
 C57
        C56
                      ga_13
                                   amide linkage angle
 C57
        N59
               HAC
                      ga 23
                                   from GLN angle
 N59
        C57
               058
                      ga_33
                                   from GLN angle
 C56
        C57
                                   from GLN angle
               N59
                      ga 19
                                   from GLN angle
 058
        C57
               C56
                      ga 30
 C1P
        N59
                                         force field angle definitions
               C57
                      ga_31
                                   from
 C1P
        N59
               HAC
                      ga 18
                                   from force field angle definitions
 C2P
        C1P
               N59
                      ga 15
                                   from force field angle definitions
                                   from PHE C-C-H angle from PHE C-C-H angle
 C5B
        C4B
                      ga 25
               H<sub>4</sub>B
                      ga_25
 С9В
        C4B
 C6B
        C7B
               Н7В
                      ga_25
                                   from PHE C-C-H angle
                      ga_25
ga_36
                                   from PHE C-C-H angle
 C8B
        C7B
               H7B
                                   from ADE N-C-H angle
               H<sub>2</sub>B
 N<sub>1</sub>B
        C2B
 N3B
        C2B
               H2B
                      ga 36
                                   from ADE N-C-H angle
 C9
        C10
                      ga 25
                                   corrin ring C-C10-H angle
               H10
 C11
        C10
               H10
                      ga_20
                                   corrin ring C-C10-H angle
cyano group addition to the original B12 topology
               C1N
 N21
        ਸ਼ਸ਼
                                   cyano group from HEMC CO group
 N22
        FE
               C1N
                      ga_1
                                   cyano group from HEMC
                                                             CO group
 N23
        FΕ
               C1N
                                                 from HEMC
                                                             CO
                      ga 1
                                   cyano group
                                                                 group
               C1N
                      ga 1
 N24
        FE
                                   cyano group from HEMC
                                                             CO group
                      ga_41
 FE
        C1N
               N1C
                                   cyano group
                                                 from HEMC
                                                             CO group
 N<sub>3</sub>B
        FE
               ClN
                      ga_41
                                   cyano group from HEMC CO group (found during pdb2gmx)
 [ impropers
               1
               ak
                      al
                            gromos type
 ai
        аi
 C1R
        C8B
                      N1B
                                          dimethylbenzimidazole improper for planarity
               C2B
                             gi 1
 N<sub>1</sub>B
        CSB
               C9B
                      N3B
                             gi_1
                                          dimethylbenzimidazole improper for planarity
               C7B
        N<sub>1</sub>B
                      C9B
                             gi_1
gi_1
 C8B
                                          dimethylbenzimidazole improper for planarity
                                          dimethylbenzimidazole improper
               C2B
                      N3B
                                                                               for planarity
 C8B
        N1B
 C8B
        С7В
                             gi_1
                                          dimethylbenzimidazole improper
                                                                               for planarity
                             gi_1
gi_1
                                          dimethylbenzimidazole
 C8B
        С9В
                      C2B
                                                                    improper for
               N3B
                      C4B
 C7B
        CAB
               C9B
                                          dimethylbenzimidazole improper for planarity
 С7В
               C5B
                      C4B
                             gi_1
                                          dimethylbenzimidazole improper for planarity
        C6B
 C6B
        C5B
               C4B
                      С9В
                             gi 1
                                          dimethylbenzimidazole improper for planarity
 C5B
        C4B
                             gi_1
                                          dimethylbenzimidazole
                                                                    improper
                                                                               for planarity
 C9B
        C8B
               C7B
                      C6B
                             gi_1
                                          dimethylbenzimidazole improper for planarity
                      C8B
 C9B
        C4B
               N3B
                                          dimethylbenzimidazole improper for planarity
                             gi 1
                                          dimethylbenzimidazole improper for planarity dimethylbenzimidazole improper for planarity
 С9В
                      N1B
        N<sub>3</sub>B
               C2B
                             gi_1
gi_1
 C2B
        N1B
               C8B
                      С9В
 C5M
        C4B
               C6B
                      C5B
                             gi 1
                                          dimethylbenzimidazole methyl groups
                                          dimethylbenzimidazole methyl groups
dimethylbenzimidazole H atom-containing planarity
 C6M
        C7B
                      C6B
               C5B
                             gi_1
 C2B
        N1B
                      H2B
               N<sub>3</sub>B
                             gi 1
 C4B
        С9В
                      H4B
                             gi 1
                                          dimethylbenzimidazole H atom-containing planarity
 С7В
        C8B
               C6B
                      Н7В
                                          dimethylbenzimidazole H atom-containing planarity
 N3B
        FE
               C2B
                      C9B
                             gi_1
                                          Fe-dimethylbenzimidazole planarity
                      C6
                                          HEMC-based conjugated corrin ring improper planarity
 N21
        C4
               C5
                             gi_1
                             gi 1
                                          HEMC-based conjugated corrin ring improper planarity
 N22
               C5
                      C4
        C6
                                                                                  improper
 N22
        C9
               C10
                      C11
                             gi_1
                                          HEMC-based conjugated corrin ring
                                                                                             planarity
 N23
        C11
               C10
                      C9
                             gi_1
gi_1
                                          HEMC-based conjugated corrin ring
                                                                                  improper planarity
                      C16
        C14
               C15
                                          HEMC-based conjugated corrin ring improper planarity
 N23
 N24
        C16
               C15
                      C14
                             gi 1
                                          HEMC-based conjugated corrin ring improper planarity
                                          corrin ring on-Csp2 methyl group improper planarity corrin ring on-Csp2 methyl group improper planarity
                      C35
 C5
        C4
                             gi_1
 C15
        C16
               C14
                      C53
                                          from GLN improper torsion definition from GLN improper torsion definition
                      C26
 C2.7
        028
               N29
                             gi_1
                      C27
 N29
        HAE
                             gi_1
gi_1
               HAD
                                                     improper torsion definition
                                           from GLN
 N33
        HAG
               HAF
                      C32
                             gi_1
                                          from GLN improper torsion definition
 C38
        039
               N40
                      C37
                             gi_1
                                          from GLN improper torsion definition
 N40
        HAI
               HAH
                      C38
                             gi_1
gi_1
                                          from GLN improper torsion definition from GLN improper torsion definition
 C43
                      C42
        044
 N45
        HAK
                      C43
                             gi_1
               HAJ
                                          from GLN
                                                     improper torsion definition
 C50
        051
               N52
                      C49
                             gi_1
                                          from GLN improper torsion definition
                      C50
 N52
        MAH
               HAT
                                          from GLN improper torsion definition
                             gi 1
 C61
        063
               N62
                      C60
                                          from GLN improper torsion definition
 N62
        HAO
                      C61
                             gi_1
                                          from GLN improper torsion definition
        C56
 C57
               058
                      N59
                                          amide linkage C57
                                                               planarity
                                          amide linkage N59 planarity
corrin ring C sp2 planarity
 N59
        C57
               C1P
                      HAC
                             gi_1
               C3
        N21
 C4
                      C5
                             gi_1
                             gi_1
                                          corrin ring C sp2 planarity
 C5
               С6
                      C35
        C4
        N22
                      C7
                                          corrin ring C sp2 planarity
               C5
```

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sp2 planarity
                                         corrin ring C
                            gi_1
gi_1
C11
       N23
              C10
                     C12
                                         corrin ring
                                                          sp2
                                                              planarity
                     C13
C53
C14
       N23
              C15
                             gi_1
                                         corrin ring C
                                                          sp2 planarity
C15
                                         corrin ring C
              C16
                            gi_1
gi_1
gi_1
       C14
                                                          sp2 planarity
                                         corrin ring C
C16
              C15
                     C17
                                                          sp2 planarity
       N24
C10
              C11
                                         corrin ring C10 planarity
       C9
                     H10
       C1.7
                                         corrin ring C atom sp3 tetrahedral geometry corrin ring C atom sp3 tetrahedral geometry
C18
              C19
                     C60
                     C1
                            gi_2
gi_2
C19
       N24
              C18
C3
                                         corrin ring C atom sp3 tetrahedral geometry
       C2
              C30
                     C4
C8
       C9
                            gi_2
                                         corrin ring C
                                                          atom sp3
                                                                    tetrahedral
                                                                                  geometry
                                         corrin ring C atom sp3 tetrahedral geometry corrin ring C atom sp3 tetrahedral geometry
C13
       C14
              C12
                     C48
C2P
       C1 P
              03
                     C3P
C1R
                                         sugar C atom tetrahedral geometry
sugar C atom tetrahedral geometry
              C2R
                     06R
                            gi_2
       N<sub>1</sub>B
                            gi_2
C2R
       O7R
              C3R
                     C1R
C3R
       C5R
              06R
                     C4R
                            gi_2
                                         sugar C atom tetrahedral geometry
                                         sugar C atom tetrahedral geometry
C3R
       C2R
              02
                     C4R
                             gi 2
FE
       C1
              C4
                     N21
                             gi_3
                                         HEMC improper definition
                                         HEMC improper definition
FE
       C6
              C9
                     N22
                            gi_3
gi_3
       C11
              C14
                     N23
                                         HEMC improper definition
FE
       C16
              C19
                     N24
                            gi_3
                                         HEMC improper definition
dihed
      rals 1
              ak
                     al
                           gromos type
ai
       аi
C3R
       02
                     03
                            gd 20
                                         from ADE phosphate definition
C3R
              Ρ
                     03
                            gd 27
                                         from ADE phosphate definition
       02
                                                    phosphate definition
C2P
C2P
                     02
02
                            gd_20
gd_27
       03
              Р
                                         from ADE
       03
              P
                                         from ADE phosphate definition
                            gd_7
                                         from ADE phosphate definition
       03
              C2P
                     C1P
                                         from ADE phosphate definition
C2R
       C3R
              02
                            gd_29
O8R
       C5R
              C4R
                     06R
                            gd 8
                                         from ADE sugar dihedrals
O8R
       C5R
              C4R
                     06R
                             gd_25
                                         from ADE sugar dihedrals
08R
       C5R
              C4R
                     C3R
                            qd^{-}17
                                         from ADE sugar dihedrals
       C5R
              C4R
                     C3R
                            gd 34
08R
                                         from ADE
                                                    sugar dihedrals
                                                    sugar dihedrals
C3R
       C4R
              06R
                     C1R
                            gd_29
                                         from ADE
C5R
       C4R
              C3R
                     C2R
                             gd_34
                                         from ADE sugar dihedrals
C5R
       C4R
              C3R
                            qd 17
                                         from ADE sugar dihedrals
                     02
06R
       C4R
              C3R
                     C2R
                            gd_17
                                         from ADE sugar dihedrals
06R
       C4R
              C3R
                            gd 18
                                         from ADE sugar dihedrals
                     02
C4R
       06R
              C1R
                     C2R
                            gd_29
                                         from ADE sugar dihedrals
              C2R
                            gd 18
                                         from ADE sugar dihedrals
06R
       C1R
                     O7R
06R
              C2R
                     C3R
                                         from ADE sugar dihedrals
       C1R
                            ad 17
06R
       C1R
                     C3R
                            gd_34
                                         from ADE sugar dihedrals
C1R
              C3R
                     C4R
                                         from ADE sugar dihedrals
       C2R
                             gd 17
C1R
       C2R
              C3R
                     02
                                         from ADE sugar dihedrals
O7R
                                         from ADE sugar dihedrals
       C2R
              C3R
                     C4R
                            qd 17
O7R
       C2R
              C3R
                     02
                            gd 18
                                         from ADE sugar dihedrals
                                          from ADE sugar dihedrals
C1R
              O7R
                     HAA
N<sub>1</sub>B
       C1R
              C2R
                     O7R
                             gd_17
                                         from ADE sugar dihedrals
                     C8B
06R
       C1R
              N1B
                            qd 16
                                         from ADE sugar dihedrals
C4R
                     HAB
                                         additional ADE-based sugar dihedral
       C5R
              O8R
                            gd_2
gd_17
N1B
       C1R
              C2R
                     C3R
                                         additional ADE-based sugar dihedral
N1B
       C1R
              06R
                     C4R
                             gd 17
                                         additional ADE-based sugar dihedral
                            gd_40
gd_14
                                         from GLN dihedral
C2
       C26
              C27
                     N29
C26
                                         from GLN dihedral
       C27
                     HAD
              N29
C30
       C31
                            gd 40
                                         from GLN dihedral
C31
       C32
              N33
                     HAF
                            gd_14
                                         from GLN dihedral
C7
       C37
              C38
                     N40
                             gd_40
                                         from GLN dihedral
C37
                                         from GLN dihedral
       C38
              N40
                     HAH
                            gd_14
gd_40
C41
       C42
              C43
                     N45
                                         from GLN dihedral
C42
       C43
              N45
                     HAJ
                            gd 14
                                         from GLN dihedral
C48
C49
       C49
              C50
                     N52
                            gd_40
ad 14
                                         from GLN dihedral
       C50
              N52
                     HAL
                                         from GLN dihedral
C18
       C60
              C61
                     N62
                            gd 40
                                         from GLN dihedral
C60
                                         from GLN dihedral
       C61
              N62
C5M
       C5B
              C6B
                     C6M
                             gd 33
                                         dimethylbenzimidazole methyl dihedral fix
C4B
       C5B
              C6B
                     C6M
                             gd_10
                                         dimethylbenzimidazole methyl dihedral fix
C8B
                                         dimethylbenzimidazole methyl dihedral
       C7B
              C6B
                     C6M
                            ad 10
                                         dimethylbenzimidazole methyl dihedral
       C6B
С9В
       C4B
              C5B
                     C5M
                            gd 10
                                         dimethylbenzimidazole methyl dihedral fix
C35
       C5
              C4
                     N21
                             gd_10
                                         corrin ring methyl planarity
                                         corrin ring methyl planarity corrin ring methyl planarity
C35
       C5
              C6
                     N22
                            gd_10
gd_10
C53
       C15
              C14
                     N23
C53
       C1
              C16
                                         corrin ring methyl planarity
                     N24
                            qd 10
                                         corrin ring but HEMC-derived N,C torsions corrin ring but HEMC-derived N,C torsions corrin ring but HEMC-derived N,C torsions
N24
       C19
              C1
                     N21
                            gd_34
N24
       C19
              C1
                     N21
                             qd 34
N21
       C4
              C5
                     C6
                            qd 15
C4
       C5
                            qd 15
                                         corrin ring but
                                                            HEMC-derived N,C
                                                                                torsions
                                         corrin ring
                                                       but
N22
       C9
              C10
                     C11
                                                            HEMC-derived N,C
                            qd 15
                                                                                torsions
C9
       C10
              C11
                     N23
                             gd_15
                                         corrin ring but
                                                            HEMC-derived N,C
                                                                                torsions
N23
       C14
              C15
                                         corrin ring but HEMC-derived N,C
                     C16
                            qd 15
                                                                                torsions
                     N24
C14
       C15
              C16
                            gd 15
                                         corrin ring but HEMC-derived N,C torsions
                            gd 40
                                         corrin ring HEMC derived CHn torsions
              C26
```

```
gd_34
gd_34
                                       corrin ring HEMC
                                                          derived CHn torsions
C2
C2
C3
       C26
             C27
                    028
                                       corrin ring
                                                    HEMC
                                                          derived
                                                                   CHn
                    C31
C32
       C3
             C30
                           gd_9
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
                           gd_40
       C30
             C31
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C30
                                       corrin ring HEMC
      C31
             C32
                    034
                           ad 40
                                                          derived
                                                                   CHn
                                                                        torsions
                           gd_40
C6
             C37
                    C38
                                       corrin ring HEMC
                                                          derived
                                                                    CHn
                                                                        torsions
C36
       C7
             C37
                    C38
                           gd_40
                                       corrin ring
                                                    HEMC
                                                          derived
                                                                    CHn
                                                                        torsions
       C37
                           gd_40
gd_9
C7
             C38
                    039
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C7
                    C42
       C8
             C41
                                       corrin ring HEMC
                                                                   CHn torsions
                                                          derived
C8
       C41
             C42
                    C43
                           gd_34
                                       corrin ring
                                                    HEMC
                                                          derived
                                                                    CHn
                                                                        torsions
                                                                   CHn torsions
C41
       C42
             C43
                    044
                           gd 40
                                       corrin ring
                                                    HEMC
                                                          derived
                                       corrin ring
C12
       C13
             C48
                    C49
                           gd_9
                                                    HEMC
                                                          derived
                                                                   CHn torsions
C13
             C49
                    C50
                           gd 34
                                       corrin ring HEMC
       C48
                                                          derived
                                                                   CHn torsions
                           gd 40
C48
       C49
             C50
                    051
                                       corrin ring
                                                    HEMC
                                                          derived
                                                                   CHn
                                                                        torsions
C16
       C17
             C55
                    C56
                                                     HEMC
                                       corrin ring
                                                          derived
                                                                    CHn
C54
       C17
             C56
                    C57
                           gd 40
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
C17
                    C57
       C55
             C56
                           gd 34
                                       corrin ring HEMC
                                                          derived
                                                                   CHn torsions
                           gd_40
gd_9
                                       corrin ring HEMC
C55
       C56
             C57
                    058
                                                          derived
                                                                   CHn torsions
C17
       C18
             C60
                    C61
                                       corrin ring HEMC derived
                                                                   CHn torsions
C18
       C60
             C61
                    063
                           gd_34
                                       corrin ring HEMC derived
                                                                   CHn torsions
      C17
C1P
                           gd_9
qd_34
                                       corrin ring HEMC derived CHn torsions amide linkage torsion terms
C18
             C55
                    C56
N59
             C2P
                    03
N59
       C1P
                    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
                           gd^{-}40
       C56
             C57
                    N59
                                       amide linkage torsion terms
                                       amide linkage torsion terms
C17
       C55
             C56
                    C57
                           gd 40
C5
             N21
                    C1
                           gd_14
                                       corrin ring sp3-containing
                                                                      torsions
                                                                      torsions
C10
       C9
             N22
                    С6
                           gd 14
                                       corrin ring sp3-containing
                           gd_14
C5
       C6
             N22
                    C9
                                       corrin ring sp3-containing
                                                                      torsions
C15
       C14
                    C11
                                       corrin ring sp3-containing
             N23
                           qd 14
                                                                      torsions
C10
                    C14
                           gd 14
       C11
             N23
                                       corrin ring sp3-containing
                                                                      torsions
                                       corrin ring sp3-containing
C15
       C16
             N24
                    C19
C4
C18
      N21
             C1
                    C2
                           gd_40
                                       corrin ring sp3-containing
                                                                      torsions
                    C16
                           qd 40
      C19
             N24
                                       corrin ring sp3-containing
                                                                      torsions
N22
             C5
                    C4
                                       corrin ring sp3-containing
       C6
                           qd 33
                                                                      torsions
N23
       C11
             C10
                    C9
                                       corrin ring sp3-containing
C19
      C18
             C17
                    C55
                           gd_34
                                       corrin ring sp3-containing
                                                                      torsions
                    C15
C55
             C16
       C17
                           gd 40
                                       corrin ring sp3-containing
                                                                      torsions
C17
             C19
                    C1
                           qd 34
      C18
                                       corrin ring sp3-containing
                                                                      torsions
C18
       C19
             C1
                           gd_34
                                       corrin ring sp3-containing
                                                                      torsions
                    C14
C13
C17
       C16
             C15
                           gd_10
                                       corrin ring sp3-containing
                                                                      torsions
C16
             C14
      C15
                           qd 10
                                       corrin ring sp3-containing
                                                                      torsions
                    C12
C15
             C13
                           ad 40
      C14
                                       corrin ring sp3-containing
                                                                      torsions
C6
       C7
             C8
                    C9
                           gd 34
                                       corrin ring sp3-containing
                                                                      torsions
C8
                    C5
                           gd_34
                                       corrin ring sp3-containing
                                                                      torsions
C30
       C3
             C2
                    C1
                           gd_34
                                       corrin ring sp3-containing
                                                                      torsions
C11
      C12
             C13
                    C14
                           qd 34
                                       corrin ring sp3-containing
                                                                      torsions
C13
       C12
             C11
                    C10
                           gd_34
gd_10
                                       corrin ring sp3-containing
                                                                      torsions
C10
       C9
             C8
                    C7
                                       corrin ring sp3-containing
C5
       C4
             C3
                    C30
                           gd 34
                                       corrin ring sp3-containing
                                                                      torsions
C3
             C1
       C2
                    C19
                           gd_34
                                       corrin ring sp3-containing torsions
cyano group dihedral.
                          imidazole-Fe-CN group torsion
C9B
      N3B
                    N21
                           gd_38
                                         THIS IS NEW!!!
                           gd_38
gd_38
N<sub>3</sub>B
       FE
             N21
                    C1
                                         THIS IS NEW!!!
       FE
             N22
                    C6
                                         THIS IS NEW!!!
N3B
N3B
       FΕ
             N23
                    C11
                           gd_38
                                              IS NEW!!!
N<sub>3</sub>B
       FE
             N24
                    C16
                           gd_38
                                        THIS IS NEW!!!
                           ad 38
                                       corrin ring sp3-containing torsions
N<sub>3</sub>B
      FE
             C1N
                    N1C
```

```
; lysine-cyanocobalamin residue file based on the HEMC CO parameters
 [ atoms ]
                                               ; from GLN residue
                       0.38000
028
            0
                      -0.38000
                                        0
                                                    from GLN residue
            NT
N29
                     -0.83000
                                        Ω
                                                   from GLN residue
HAE
                      0.41500
                                                   from GLN residue
            Η
                                        0
                       0.41500
                                                    from GLN residue
 C32
            С
                       0.38000
                                                   from GLN residue
034
            \cap
                      -0.38000
                                        1
                                                   from GLN residue
            NT
                     -0.83000
                                                   from GLN residue
N33
 HAG
            Η
                      0.41500
                                                   from GLN residue
                       0.41500
HAF
                                                    from GLN residue
            Η
                                              ; from GLN residue
; from GLN residue
 C38
            С
                      0.38000
                                        2
                                        2
                     -0.38000
039
            0
                                               ; from GLN residue
                                                   from GLN residue
N40
            NT
                     -0.83000
                                              ; from GLN residue
; from GLN residue
            Н
                       0.41500
HAH
            Η
                       0.41500
                                        2
                                                   from GLN residue
                      0.38000
 C43
            C
                                              ; from GLN residue
; from GLN residue
                                        3
044
            0
N45
            NT
                      -0.83000
                                                   from GLN residue
HAK
            Н
                       0.41500
                                                   from GLN residue
HAJ
C50
                       0.41500
0.38000
            Η
                                        3
                                              ; from GLN residue
; from GLN residue
; from GLN residue
                                                   from GLN residue
            C
 051
            0
                      -0.38000
                                                   from GLN residue
            NT
                      -0.83000
 N52
                                              ; from GLN residue
; from GLN residue
HAM
            Η
                       0.41500
                                        4
                       0.41500
0.38000
HAL
            Η
                                        4
5
                                                   from GLN residue
            C
                                                   from GLN residue
 C61
                                              ; from GLN residue
; from GLN residue
                      -0.38000
 063
                                              ; from GLN residue
; from GLN residue
; from GLN residue
 N62
            NT
                      -0.83000
 HAO
            Η
                       0.41500
                       0.41500
                                        5
HAN
            Η
                                              ; methyl group
; methyl group
; methyl group
 C20
            CH3
                       0.00000
 C25
            СНЗ
                       0.00000
 C36
            CH3
                       0.00000
                                        8
                                             ; methyl group
; methyl group
; methyl group
; non-polar CHn fragments
; non-polar CHn fragments
 C46
            CH3
                       0.00000
 C47
            CH3
                       0.00000
                                        10
                       0.00000
            CH3
                                        11
 C26
            CH2
                       0.00000
 C30
            CH<sub>2</sub>
                       0.00000
                                        13
                                              ; non-polar CHn fragments
; non-polar CHn fragments
                       0.00000
 C31
            CH2
                                        13
 C37
            CH2
                       0.00000
                                              ; non-polar CHn fragments
; non-polar CHn fragments
; non-polar CHn fragments
            CH2
                       0.00000
 C42
            CH2
                       0.00000
                                        15
 C48
            CH2
                       0.00000
                                        16
                                             ; non-polar CHn fragments
; C2*-O2*-H2* from ADE
; C2*-O2*-H2* from ADE
 C49
            CH2
                       0.00000
                                        16
 C56
            CH2
                       0.00000
                                        17
 C55
            CH2
                       0.00000
                                        17
 C60
                       0.00000
            CH2
                                        18
 C2R
            CH1
                       0.15000
                                        19
 O7R
            OA
                      -0.54800
                                                   C2*-O2*-H2* from ADE
 HAA
                       0.39800
                                        19
                                                   C1*-O4*-C4* from ADE
 C1R
            CH1
                       0.20000
                                        2.0
                                                   C1*-O4*-C4* from ADE
                      -0.36000
                                        20
 06R
            OA
            CH1
                                                    C1*-O4*-C4* from ADE
 C4R
                      0.16000
                                        20
 C3R
            CH1
                       0.00000
                                        21
                                                    C3* from ADE
                                                   C2*-O2*-H2* from ADE
C2*-O2*-H2* from ADE
 CSR
            CH2
                       0.15000
                                        22
22
08R
            OA
                      -0.54800
                                                    C2*-O2*-H2* from ADE
                        -0.54800
      HAB from B12 is gone in LYB, where the lysine fragment is added via CLB HAB _{\rm H} 0.39800 22 ; C2*-O2*-H2* from ADE HAB from B12 is gone in LYB, where the lysine fragment is added via CLB
Ρ
                       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)
02P
                      -0.80000
-1.00000
                                                   PO3+O3* fragment from ADE
            OA
            OM
                                        23
                                                    PO3+O3* fragment from ADE
 04
            OM
                      -1.00000
                                        23
                                                    PO3+O3* fragment from ADE
 03
            OA
                      -0.80000
                                        23
                                                   PO3+O3* fragment from ADE
                       0.35000
                                        24
                                                   non-polar CHn fragment non-polar CHn fragment
 C2P
            CH1
 C3P
                                        24
            CH3
                                                   non-polar CHn fragment
            CH2
                       0.00000
                      -0.28000
                                               ; tempered GLN fragment charges
```

```
tempered GLN fragment charges
C57
          C
                   0.38000
                                 25
                                           tempered GLN fragment charges
058
          Ω
                  -0.38000
                                 25
                                           tempered GLN fragment charges
C5B
          C
                   0.00000
                                 26
                                           dimethylbenzimidazole
                                                                    C-CH3 group
                                                                                   (non-polar)
          CH3
                   0.00000
                                           dimethylbenzimidazole C-CH3 group
C5M
                                 26
                                                                                   (non-polar)
                                                                    C-CH3 group
                   0.00000
                                           dimethylbenzimidazole
                                                                                   (non-polar)
                                           dimethylbenzimidazole C-CH3 group
 C6M
          CH3
                   0.00000
                                                                                   (non-polar)
                                           dimethylbenzimidazole aromatic C-H from TRP, PHE dimethylbenzimidazole aromatic C-H from TRP, PHE
C4B
          C
                  -0.14000
                                 2.8
                   0.14000
H4B
          Η
                                 28
                  -0.14000
                                           dimethylbenzimidazole aromatic C-H from
Н7В
          Η
                   0.14000
                                           dimethylbenzimidazole aromatic C-H from
                                 29
                                                                                          TRP.
                                                                                         fragment
N3B
          NR
                  -0.55000
                                 3.0
                                           dimethylbenzimidazole polar aromatic NC
C9B
                   0.20000
                                           dimethylbenzimidazole polar aromatic NC
          C
                                 30
                                                                                          fragment
                                           dimethylbenzimidazole polar aromatic NC fragment
N1B
          NR
                  -0.30000
                                 31
                                           dimethylbenzimidazole polar aromatic NC fragment
C8B
                   0.20000
C2B
          C
                   0.23000
                                 32
                                           dimethylbenzimidazole aromatic C-H from TRP, PHE
H2B
          Η
                   0.23000
                                 32
                                           dimethylbenzimidazole aromatic C-H from TRP, PHE
                  -0.05000
                                           C-CH3 group (non-polar)
C-CH3 group (non-polar)
C5
                                 33
 C35
          СНЗ
                   0.00000
                                           C-CH3 group
C15
                  -0.05000
                                 34
                                                         (non-polar)
          CH3
                                           C-CH3 group (non-polar)
HEMC Fe-N group
C53
                   0.00000
                                 34
FE
                   1.00000
          FΕ
                                 35
N21
          NR
                  -0.44000
                                           HEMC Fe-N group
                  -0.50000
                                           HEMC Fe-N group
N22
          NR
                                           HEMC Fe-N group
HEMC Fe-N group
non-polar HEMC-derived corrin atoms
N23
          NR
                  -0.50000
                                 35
                                 35
          NR
                  -0.44000
N24
 C1
          CH0
                   0.22000
                                 36
 C2
                                                      HEMC-derived corrin atoms
          CH<sub>0</sub>
                   0.00000
                                           non-polar
 C3
          CH1
                   0.0000
                                           non-polar HEMC-derived corrin atoms
                                 36
C4
C6
                                           non-polar HEMC-derived corrin atoms
          C
                   0.38000
                                 36
                                 37
                                           non-polar HEMC-derived corrin atoms
                   0.29000
                                           non-polar HEMC-derived corrin atoms
 C7
                   0.00000
          CH<sub>0</sub>
 C8
          CH1
                   0.00000
                                 37
                                           non-polar HEMC-derived corrin atoms
                                           non-polar HEMC-derived corrin atoms
 C9
                   0.35000
                                 37
C16
          С
                                           non-polar HEMC-derived corrin atoms
                   0.38000
                                 38
 C17
          CH0
                   0.00000
                                           non-polar HEMC-derived corrin atoms
                                 38
 C18
          CH1
                   0.00000
                                           non-polar HEMC-derived corrin atoms
C19
          CH1
                   0.24000
                                 3.8
                                           non-polar HEMC-derived corrin atoms
                                           non-polar HEMC-derived corrin atoms
C11
                   0.35000
          C
                                 39
          CH0
                                           non-polar HEMC-derived corrin atoms
C12
                   0.00000
                                 39
                                           non-polar HEMC-derived corrin atoms
 C13
          CH1
                   0.00000
                                 39
C14
C10
                                           non-polar HEMC-derived corrin atoms aromatic C-H from TRP, PHE
                   0.29000
                                 39
          C
                  -0.24000
                                 40
                                           aromatic C-H from TRP, PHE
H10
          Η
                   0.14000
                                 40
     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.
Ν
                                           standard LYS
                  -0.31000
                                                         (lysine) atom information
                   0.31000
                                 41
                                           standard LYS (lysine)
                                                                    atom information
CA
          CH1
                   0.00000
                                 42
                                           standard LYS
                                                          (lysine) atom information
                   0.00000
CB
          CH2
                                 42
                                           standard LYS (lysine)
                                                                    atom information
CG
                   0.00000
                                           standard LYS (lysine) atom information
          CH<sub>2</sub>
                                 43
 CD
                   0.00000
                                 43
                                           standard LYS
                                                          (lysine) atom information
                                          NEW CHARGE FROM B12 standard LYS (lysine) atom information
NEW CHARGE FROM B12 standard LYS (lysine) atom information
 CE
          CH2
                   0.00000
                                 44
NZ.
          NТ
                  -0.34000
                                 44
                                           NEW CHARGE FROM B12 standard LYS (lysine) atom information
HZ1
          Η
                   0.34000
                                 44
                                        ; standard LYS (lysine) atom information
; standard LYS (lysine) atom information
           CH2
; CE
                   -0.24000
                                  44
                                  44
 NZ
           NT
                    -0.64000
 HZ1
           Η
                    0.44000
                                   44
                                           standard LYS (lysine) atom information
     this H atom is gone, replaced by the linkage CLB atom.
                      0.44000
                                            standard LYS (lysine) atom information
     this H atom is gone, replaced by the linkage CLB atom.
                   0.20000
                                           NEW CHARGE FROM B12 standard LYS (lysine) atom information
          Ó
                                           NEW CHARGE FROM B12 standard LYS (lysine) atom information
                                 45
           С
                    0.45000
                                  45
                                           standard LYS (lysine) atom information
           0
                    -0.45000
                                   45
                                            standard LYS (lysine) atom information
   linkage atoms (added new)
CLB
                   0.00000
                                           this is the linkage carbon atom between LYS and \ensuremath{\operatorname{B12}}
OLB
          Ω
                   0.00000
                                 46
                                           this is the additional =0 at the linkage position
 cyano group addition to the original B12 topology
C1N
                   0 04000
                                           CN group on Fe
                                          CN group on Fe
N1C
                  -0.42000
                                 41
[bonds]
```

```
gromos type
ai
C26
       aj
C27
                              from GLN fragment 0
C27
       028
                gb_5
                              from GLN
       N29
                gb_9
                              from GLN
N29
       HAE
                ab 2
                              from
                                    GLN
N29
       HAD
                gb_2
                              {\tt from}
                                    GLN
C31
       C32
                gb_27
                              from
                                    GLN fragment 1
C32
       034
                gb_5
                              from GLN
C32
       N33
                gb 9
                              from
                                    GLN
N33
       HAG
                gb_2
                              from
                                    GLN
N33
       HAF
                gb_2
                              {\tt from}
                                    GLN
                gb_27
gb_5
gb_9
C37
       C38
                              {\tt from}
                                    GLN fragment 2
C38
       039
                              from GLN
C38
       N40
                              {\tt from}
                                    GLN
N40
                gb_2
                              from
                                    GLN
                gb_2
gb_27
gb_5
N40
       HAH
                              from GLN
C42
C43
       C43
                              from GLN fragment 3
       044
                              from GLN
C43
       N45
                gb 9
                              from
                                    GLN
N45
       HAK
                gb_2
                              from
                                    GLN
N45
C49
       HAJ
C50
                gb_2
qb_27
                              from GLN
                                    GLN fragment 4
                              from
C50
       051
                gb 5
                              from
                                    GLN
C50
       N52
                gb_9
                              from
                                    GLN
N52
N52
       HAM
HAL
                gb_2
gb_2
                              from
                                    GLN
                              from
                                    GLN
                gb 27
C60
       C61
                              from
                                    GLN fragment 5
C61
                gb_5
                              from GLN
C61
       N62
                gb_9
                              from GLN
                gb_2
gb_2
N62
       HAO
                              from GLN
       HAN
                                    GLN
N62
                              from
FE
       N21
                gb 35
                              FE-N bond from HEMC
FΕ
       N22
                gb_35
                              FE-N
                                    bond from HEMC
FE
       N23
                gb_35
                              {\tt FE-N} bond from {\tt HEMC}
                gb_35
gb_37
                              FE-N bond from HEMC
FE
       N24
FΕ
       N3B
                              FE-N3B bond from HEMC not in corrin ring
       02P
                gb 28
                              from ADE phosphate
P
       04
                gb_24
                              from ADE phosphate
                gb_24
gb_28
                              from ADE phosphate from ADE phosphate
       05
       03
N21
                gb_21
       C1
                              corrin ring N-CHn bonds
                              corrin ring N-C bonds
corrin ring N-C bonds
N21
                gb_14
N22
       C6
                qb 14
                              corrin ring N-C bonds
N22
       C9
                gb 14
N23
       C11
                gb 14
                              corrin ring N-C bonds
                              corrin ring N-C bonds corrin ring N-C bonds
N23
                gb_14
N24
       C16
                gb_14
                gb 21
N24
       C19
                              corrin ring N-CHn bonds
                              CH2-CH2 bonds
CH2-CH2 bonds
C30
                gb 27
       C31
C41
       C42
                gb_27
                gb_27
gb_27
gb_27
C48
       C49
                              CH2-CH2 bonds
C55
       C56
                              CH2-CH2
                                        bonds
C56
       C57
                              CH2-CH2 bonds
                gb 22
N1B
       C1R
                              sugar bonds from ADE
C1R
       C2R
                gb_26
                              sugar bonds from ADE
C2R
       O7R
                gb_20
                              sugar bonds from
                                                   ADE
07R
       HAA
                qb 1
                              sugar bonds from
                                                   ADE
C2R
       C3R
                gb 26
                              sugar bonds
                                             from
                                                   ADE
                              sugar bonds
C3R
       C4R
                gb_26
                                                   ADE
                              sugar bonds from ADE sugar bonds from ADE
C3R
       O2P
C5R
                gb_20
gb_26
C4R
C5R
       08R
                gb 20
                              sugar bonds from
                                                   ADE
HAB is deleted from B12 for LYB
                                            08R
                                                    HAB
                                                            gb 1
                                                                       ; sugar bonds from ADE
C4R
       06R
                gb_20
gb_20
                              sugar bonds from ADE
                              sugar bonds from ADE
06R
C1P
       N59
                gb_9
                              amide corrin - phosphate linkage
                gb_27
gb_27
gb_20
C1P
C2P
       C2P
                              amide corrin -
                                                 phosphate linkage
                              amide corrin - phosphate linkage
amide corrin - phosphate linkage
       C3P
C2P
       03
N59
       HAC
                              amide corrin - phosphate linkage
                              amide corrin -
                              amide corrin - phosphate linkage
amide corrin - phosphate linkage
dimethylbenzimidazole ring
N59
       C57
                gb_9
C57
       058
                qb 5
N1B
       C2B
                qb 10
C2B
       N3B
                gb_10
                              dimethylbenzimidazole ring
C2B
       H2B
                              dimethylbenzimidazole ring
                gb_10
gb_16
                              dimethylbenzimidazole ring dimethylbenzimidazole ring
N3B
       C9R
C9B
       C4B
C4B
       C5B
                gb_16
                              dimethylbenzimidazole ring
C4B
                              dimethylbenzimidazole ring
```

```
dimethylbenzimidazole ring
 C5B
       C5M
               gb_27
                           dimethylbenzimidazole ring
 C6B
       C7B
               gb_16
                           dimethylbenzimidazole ring
               gb_27
 C6B
       C6M
                           dimethylbenzimidazole ring
       C8B
                           dimethylbenzimidazole ring
 C7B
               ab 16
 С7В
       Н7В
               gb_3
                           dimethylbenzimidazole ring
 C8B
       N1B
               gb_10
                           dimethylbenzimidazole ring
               gb_16
qb_27
 C8B
       C9B
                           dimethylbenzimidazole ring
       C20
 C1
                           corrin ring carbon framework
 C1
       C2
               gb_27
                           corrin ring carbon framework
       C3
               gb_27
gb_27
gb_27
 C2
                           corrin ring carbon framework
 C2
       C25
                           corrin ring carbon framework
 C2
       C26
                           corrin ring carbon framework
               gb 27
 C3
                           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
qb_27
                           corrin ring carbon framework
 C6
                           corrin ring carbon framework
 C7
       C8
               gb_27
                           corrin ring carbon
                                               framework
               gb_27
qb_27
 C7
       C37
                           corrin ring carbon framework
 C7
       C36
                           corrin ring carbon framework
 C8
               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
                                               framework
                           corrin ring carbon
               gb 27
 C11
       C12
                           corrin ring carbon framework
 C12
               gb_27
                           corrin ring carbon framework
               gb_27
gb_27
gb_27
 C12
       C47
                           corrin ring carbon framework
 C12
       C13
                           corrin ring carbon framework
 C13
       C14
                           corrin ring carbon framework
 C13
               gb 27
       C48
                           corrin ring carbon framework
 C14
       C15
               gb_17
                           corrin ring carbon
                                               framework
 C15
       C16
               gb_17
                           corrin ring carbon framework
               gb_27
 C15
                          corrin ring carbon framework
       C53
 C16
       C17
               gb 27
                           corrin ring carbon framework
 C17
       C18
               gb 27
                           corrin ring carbon framework
 C17
       C54
               gb_27
gb_27
                           corrin ring
                                       carbon framework
       C55
 C17
                           corrin ring carbon framework
 C18
               qb 27
                           corrin ring carbon framework
       C19
 C18
       C60
               gb_27
                           corrin ring carbon framework
                           corrin ring carbon framework
 C19
       C1
               gb_27
       H10
 C10
               qb<sup>3</sup>
                           corrin ring C10-H10 bond
linker bond from B12 to CLB
                     ; LYS B12 linker (CLB replaces H)
 08R
       CLB
               gb_5
Lysine bond topology
               gb 2
                          standard LYS (lysine)
 Ν
       CA
               gb_21
                           standard LYS
                                         (lysine)
               qb 27
 CA
       CB
                          standard LYS
                                         (lvsine)
 CA
               gb 27
                           standard LYS
                                         (lysine)
 СВ
       CG
               gb_27
                           standard LYS
                                         (lysine)
               gb_27
gb_27
 CG
       CD
                          standard LYS
                                         (lysine)
 CD
       CE
                          standard LYS
                                         (lysine)
 CE
       NZ
               gb 21
                          standard LYS
                                         (lysine)
 NZ
               gb 2
                          standard LYS (lysine)
this replaces the HZ2 with CLB for the B12-LYS connection
 NZ
                           standard LYS (lysine)
                           standard LYS
 C
                                         (lysine)
       +N
               gb_10
                        ; standard LYS (lysine)
 below is the C=O bond on the B12-LYS linkage (OLB is only connected to CLB)
               gb_27 ; CLB-OLB linkage bond (previously nowhere in the structure)
 CLB OLB
cyano group addition to the original B12 topology
 FE
              gb_30
                           cyano group on the Fe
    N1C gb_4 exclusions ]
C1N
                           cyano group on the Fe
 FE
 FE
       C3
       C5
 FE
       C7
```

```
FE
FE
       C12
       C13
C15
FE
FE
       C17
FE
       C18
FE
N21
       C25
       C26
N21
N21
       C30
N21
       C35
N21
N21
       C6
C9
N21
       C11
N21
N21
       C16
N21
       C19
N21
       C10
N22
       C1
N22
       C4
N22
N22
       C36
C37
N22
       C11
N22
       C14
N22
N22
       C16
C19
N22
       C15
N23
       C16
N23
       C19
N23
       C1
N23
       C4
N23
       C6
N23
       C9
N23
       C46
C47
N23
N23
       C48
N23
       C5
N24
N24
       C4
       C5
       C6
N24
N24
       C10
C11
N24
N24
N24
       C14
N24
       C55
N24
N24
C1R
       C60
C7B
C1R
       С9В
C1R
       N3B
N1B
       C6B
N1B
       C4B
C5B
C8B
C8B
       C5M
C8B
       C6M
C7B
       C4B
C7B
       N3B
C7B
       C2B
C2B
       С9В
C5B
C5M
       C2B
       C6M
C1
                  HEMC-based C framework exclusions
       C30
C1
                  HEMC-based C framework exclusions
C2
C3
C3
C4
                  HEMC-based C framework exclusions
HEMC-based C framework exclusions
       C5
       C35
                  HEMC-based C framework exclusions
       C6
       C26
                  HEMC-based C framework exclusions
C4
       C7
                  HEMC-based C framework exclusions
C3 0
C3 0
C5
       C26
                  HEMC-based C framework exclusions
                  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 HEMC-based C framework exclusions
C5
       C37
C7
C35
                  HEMC-based C framework exclusions
                  HEMC-based C framework exclusions
                  HEMC-based C framework exclusions
HEMC-based C framework exclusions
C6
       C10
C7
C8
       C10
       H10
                  HEMC-based C framework exclusions
                  HEMC-based C framework exclusions
       C11
       C36
                  HEMC-based C framework exclusions
```

```
HEMC-based C
                                 framework exclusions
  C9
        C12
                   HEMC-based C
                                  framework
  C36
        C41
                   HEMC-based C
                                 framework exclusions
  C37
                   HEMC-based C
        C10
                                 framework
                                             exclusions
  C10
                   HEMC-based
                                  framework
        C13
                                             exclusions
  C10
                                             exclusions
        C14
                   HEMC-based
                                  {\tt framework}
  C10
        C46
                   HEMC-based
                               C
                                 framework
                                             exclusions
                   HEMC-based C
  C10
        C47
                                 framework exclusions
                   HEMC-based
                               C
                                 framework exclusions
  H10
        C12
  C11
        C48
                   HEMC-based
                                  framework exclusions
  C11
        C15
                   HEMC-based C
                                 framework exclusions
                   HEMC-based C
  C12
        C15
                                 framework exclusions
                   HEMC-based C
  C13
                                 framework exclusions
        C53
  C13
        C16
                   HEMC-based C
                                 framework exclusions
  C14
                   HEMC-based C
                                  framework
  C14
        C47
                   HEMC-based C framework exclusions
                   HEMC-based C
  C14
        C17
                                 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
                                 framework exclusions
  C15
        C54
                   HEMC-based
                                 framework exclusions
  C15
        C55
                   HEMC-based C framework exclusions
                                 framework exclusions framework exclusions
  C53
        C17
                   HEMC-based C
  C16
                   HEMC-based C
        C60
  C19
        C54
                   HEMC-based C
                                 framework exclusions
  C19
        C55
                   HEMC-based C
                                 framework exclusions
                  HEMC-based C framework exclusions
HEMC-based C framework exclusions
  C54
        C60
  C55
        C60
 cyano group addition to the original B12 topology
  N21
        N1C
                   cyano exclusions from HEMC
                                                 CO group
  N22
        N1C
                   cvano exclusions from HEMC
                                                 CO
                                                     group
  N23
        N1C
                   cyano exclusions from HEMC
                                                 CO
                                                     group
  N24
        N1C
                   cyano exclusions from HEMC
                                                     group
                   cyano exclusions from HEMC
  C1
        C1N
                                                 CO
                                                     group
                                           HEMC
  C4
        C1N
                   cyano exclusions from
                                                 CO
                                                     group
                                           HEMC
  C6
                   cyano exclusions from
                                                 CO
        C1N
                                                     group
  C9
        C1N
                   cyano exclusions from HEMC
                                                     group
  C11
        C1N
                   cyano exclusions from HEMC
                   cyano exclusions from HEMC
                                                 CO
  C14
        C1N
                                                     group
  C16
                   cyano exclusions from HEMC
                                                 CO group
        C1N
  C19
        C1N
                   cyano exclusions from HEMC CO group
  N3В
        N<sub>1</sub>C
                   cyano exclusion unique to 6-coordinate iron
                  additional cyano exclusion at Fe 6-center additional cyano exclusion at Fe 6-center
  C1N
        C9B
  C1N
        C2B
[
 angles ]
                     gromos type
  C2
        C26
               C27
                      ga 15
                                   from GLN, fragment 1
                      ga_30
ga_19
                                   from GLN
  C26
        C27
               028
  C26
        C27
               N29
                                   from
                                        GLN
  028
                      ga 33
                                        GLN
                                   from
  C27
        N29
               HAE
                      ga_23
                                   {\tt from}
                                        GLN
  C2.7
        N29
               HAD
                      ga_23
                                   from
                                        GLN.
  HAE
                      ga_24
        N29
               HAD
                                   from
                                        GLN
  C30
        C31
                      ga 15
                                   from
                                        GLN,
                                              fragment 2
               C32
               034
                      ga_30
  C31
        C32
                                   from
                                        GLN
  C31
        C32
               N33
                      ga_19
                                   from GLN
  034
               N33
                      ga 33
                                   from
                                        GLN
  C32
        N33
               HAG
                      ga 23
                                   from
                                        GLN
  C32
        N33
                      ga_23
                                   {\tt from}
                                        GLN
  HAG
        N33
               HAF
                      ga 24
                                   from
                                        GLN
  C7
        C37
               C38
                      ga_15
                                   from GLN,
                                             fragment 3
  C37
        C38
               039
                      ga 30
                                        GLN
                                   from
                      ğa_19
  C37
        C38
                                   from
  039
        C38
               N40
                      ga 33
                                   from
                                        GLN
  C38
        N40
               HAI
                      ga_23
                                   from
                                        GLN
                      ga_23
ga_24
  C38
        N40
               HAH
                                   from GLN
  HAI
        N40
               HAH
                                   from
                                        GLN
  C41
        C42
                      ga_15
                                        GLN
                                              fragment 4
               C43
                                   from
  C42
        C43
               044
                      ga_30
                                   from
                                        GLN
  C42
        C43
               N45
                      ga 19
                                   from
                                        GLN
  044
        C43
               N45
                      ga 33
                                   from
                                        GLN
  C43
        N45
                      ga_23
                                   {\tt from}
                                        GLN
  C43
        N45
               HAJ
                      ga 23
                                   from
                                        GLN
                      ga_24
ga_15
  HAK
        N4 5
               HAJ
                                   from
                                        GLN.
  C48
        C49
               C50
                                   from
                                        GLN,
                                              fragment 5
                                   from
  C49
        C50
               051
                      ga 30
                                        GLN
  C49
        C50
```

```
ga_33
ga_23
                                  from
C50
      N52
              HAM
                                  from
                                       GLN
C50
      N52
             HAL
                     ga_23
                                 from
                                       GLN
HAM
      N52
              HAL
                     ga 24
                                  from
                                       GLN
C18
                     ga 15
                                             fragment 6
       C60
              C61
                                  from
                                       GLN.
                     ga_30
C60
       C61
                                  from
                                       GLN
C60
       C61
              N62
                     ga_19
                                  from
                                       GLN
                    ga_33
ga_23
063
       C61
              N62
                                 from GLN
C61
      N62
                                       GLN
              HAO
                                 from
C61
       N62
              HAN
                     ga_23
                                  from
                                       GLN
HAO
      N62
              HAN
                     ga 24
                                 from GLN
                     ga_2
ga_2
N21
       FE
              N22
                                 corrin ring Fe-N angle
                                 corrin ring Fe-N angle
N21
       FE
              N24
                     ga 2
N22
       FE
              N23
                                 corrin ring Fe-N angle
                     ga_2
N23
       FE
                                 corrin ring Fe-N angle
N21
      FE
             N3B
                     ga 2
                                 corrin-Fe-dimethylbenzimidazole
                     ga_2
N22
       FE
              N<sub>3</sub>B
                                 corrin-Fe-dimethylbenzimidazole
N23
       FE
                     ga 2
                                 corrin-Fe-dimethylbenzimidazole
              N<sub>3</sub>B
N24
                     qa 2
                                 corrin-Fe-dimethylbenzimidazole
FE
      N21
              C1
                     ga_34
                                 corrin Fe-N-C angles (based on HEMC)
                                 corrin Fe-N-C angles corrin Fe-N-C angles
FE
      N21
              C4
                     ga_34
                                                          (based on HEMC)
FE
      N22
              C6
                     ga 34
                                                          (based on HEMC
FE
      N22
                     ga 34
                                 corrin Fe-N-C angles
                                                          (based on HEMC)
              C11
                     ga 34
                                 corrin Fe-N-C angles
                                                          (based on HEMC)
FE
      N23
                                 corrin Fe-N-C angles (based on HEMC) corrin Fe-N-C angles (based on HEMC) corrin Fe-N-C angles (based on HEMC)
             C14
C16
FE
      N23
                     ga_34
                     ga 34
FE
      N24
FΕ
      N24
              C19
                     ga 34
       N<sub>3</sub>B
              C9B
                     ga_34
                                 Fe-dimethylbenzimidazole-N,C angle
                     ga_34
ga_7
FE
      N3B
              C2B
                                 Fe-dimethylbenzimidazole-N,C angle
                                 angle containing C8B, see minimization issues discussion angle containing C8B, see minimization issues discussion
C8B
      N<sub>1</sub>B
              C2B
                     ga_7
              С9В
N<sub>1</sub>B
       C8B
       С9В
                                 angle containing C8B, see minimization
C8B
              N3B
                     ga 7
                                                                               issues
                     ga_39
C7B
       C8B
              N<sub>1</sub>B
                                 angle containing
                                                     C8B,
                                                           see minimization
                                                                               issues
                                                                                       discussion
C8B
      N<sub>1</sub>B
              C1R
                     ga 37
                                 angle containing C8B,
                                                           see minimization
                                                                               issues
                                                                                       discussion
C4B
                     ga 27
                                                                               issues discussion
      C9B
              C8B
                                 angle containing C8B,
                                                           see minimization
C6B
       С7В
              C8B
                     ga 27
                                                     C8B,
                                 angle containing
                                                           see minimization
                                                                               issues
                                                                                       discussion
С7В
       C8B
              С9В
                     ga 27
                                 angle containing C8B,
                                                           see minimization issues discussion
N21
       C1
              C2
                     ga_13
                                 corrin ring-specific but HEMC-derived angles
                                                              HEMC-derived angles
              C20
                                 corrin ring-specific but
N21
       C1
                     ga 13
                     ga 33
                                 corrin ring-specific but HEMC-derived angles
N21
       C4
              C3
                                 corrin ring-specific but HEMC-derived angles
C4
      N21
              C1
                     ga_6
                                 corrin ring-specific but HEMC-derived angles corrin ring-specific but HEMC-derived angles
             N21
C5
       C4
C19
       C1
             N21
                     ga 13
                                 corrin ring-specific but
                                                              HEMC-derived angles
N22
       C6
                     ga 33
              C5
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
                                 corrin ring-specific but HEMC-derived angles
      C9
             N22
                     ga 33
              C10
                                 corrin ring-specific but
                                                              HEMC-derived angles
N23
       C11
                     qa 33
N23
       C11
              C12
                     ga 33
                                 corrin ring-specific but
                                                              HEMC-derived
N23
       C14
              C13
                     ga 33
                                 corrin ring-specific but HEMC-derived angles
                                                              HEMC-derived angles
              C11
C14
      N23
                     ga_6
                                 corrin ring-specific but
                                 corrin ring-specific but
                                                              HEMC-derived angles
C15
                     ga 33
      C14
              N23
                                                              HEMC-derived angles
N24
       C16
              C15
                     ga 33
                                 corrin ring-specific
                                                          but
N24
       C19
              C1
                     ga_13
                                 corrin ring-specific but
                                                              HEMC-derived angles
C19
      N24
              C16
                     ga_6
                                 corrin ring-specific but HEMC-derived angles
                     ga_33
                                 corrin ring-specific but
                                                              HEMC-derived angles
C17
       C16
              N24
                     ga 13
C18
      C19
              N24
                                 corrin ring-specific but HEMC-derived angles
C3R
       02P
                     ga 26
                                 phosphate angle from ADE
02P
       Р
              03
                     ga_5
                                 phosphate angle from ADE
02P
      Ρ
                     ga 14
                                 phosphate angle from ADE
              04
02P
              05
                     ga 14
                                 phosphate angle from ADE
03
       Ρ
                     ga_14
                                 phosphate angle from
03
      Р
              05
                     ga 14
                                 phosphate angle from ADE
04
       Р
              05
                     ga_29
                                 phosphate angle from ADE
      03
              C2P
                     ga 26
                                 phosphate angle from ADE
                     ga_9
02 P
                                 phosphate oxygen to CHn carbons from ADE
                                 phosphate oxygen to CHn carbons from ADE
02P
       C3R
              C4R
                     ga 9
03
       C2P
              C1P
                     ga_9
                                 phosphate oxygen to CHn carbons from ADE
                     ga_9
03
       C2P
              C3P
                                 phosphate oxygen to CHn carbons from ADE CHn-CHn-CHn angles
C1
              C26
       C2
                     ga 13
C1
       C2
              C25
                                 CHn-CHn-CHn angles
                     ga 13
C1
       C2
              C3
                     ga_13
                                  CHn-CHn-CHn angles
C1
                     ga 13
       C19
              C18
                                 CHn-CHn-CHn angles
C2
       C1
              C19
                     ga 13
                                 CHn-CHn-CHn angles
                     ga_13
                                  CHn-CHn-CHn angles
C2
       C3
              C30
                     ga 13
                                 CHn-CHn-CHn angles
                     ga_13
ga_13
C3
       C2
              C25
                                  CHn-CHn-CHn angles
C3
       C2
              C26
                                 CHn-CHn-CHn angles
C3
       C30
              C31
                    ga 13
                                 CHn-CHn-CHn angles
                                 CHn-CHn-CHn angles
```

```
ga_13
ga_13
                                 CHn-CHn-CHn angles
C12
       C13
             C48
                                 CHn-CHn-CHn angles
C13
C13
       C12
             C46
                    ga_13
                                CHn-CHn-CHn angles
       C12
                                CHn-CHn-CHn angles
             C47
                    ga 13
C13
                                CHn-CHn-CHn angles
       C48
             C49
                    ga 13
C17
                    ga 13
       C18
             C19
                                CHn-CHn-CHn angles
C17
       C18
             C60
                    ga_13
                                CHn-CHn-CHn angles
                                CHn-CHn-CHn angles
C17
       C55
             C56
                    ga_13
C18
             C54
                                CHn-CHn-CHn angles
      C17
                    ga 13
C18
       C17
                    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
                                CHn-CHn-CHn angles
      C2
             C26
                    ga 13
                    ga_13
C46
       C12
             C47
                                CHn-CHn-CHn angles
C54
             C55
       C17
                    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
                                sp3-sp3-sp2
       C3
             C30
                    ga 15
                                              corrin ring carbon angle
                    ğa_15
C6
             C8
                                sp3-sp3-sp2 corrin ring carbon angle
C6
       C7
             C36
                    ga_15
                                sp3-sp3-sp2 corrin ring
                                                            carbon
                                                                   angle
             C37
C9
                    ga_15
ga_15
                                sp3-sp3-sp2 corrin ring
sp3-sp3-sp2 corrin ring
                                                            carbon angle
C6
       C7
C7
       C8
                                                           carbon angle
C8
                    ga 15
                                sp3-sp3-sp2 corrin ring
                                                            carbon angle
C8
             C37
                    ga 15
                                sp3-sp3-sp2 corrin ring
                                                            carbon angle
             C41
C13
                                sp3-sp3-sp2
sp3-sp3-sp2
                                                            carbon
C9
       C8
                    ga_15
                                              corrin ring
                                                                   angle
C11
      C12
                    ga 15
                                              corrin ring
                                                            carbon
                                                                   angle
                    ga 15
                                sp3-sp3-sp2 corrin ring
C11
       C12
             C46
                                                           carbon angle
C11
                    ga_15
                                sp3-sp3-sp2 corrin ring
                                                            carbon
                                                                   angle
C12
       C13
             C14
                    ga 15
                                sp3-sp3-sp2 corrin ring
                                                            carbon angle
                                                                   angle
C14
       C13
             C48
                    ga 15
                                sp3-sp3-sp2 corrin ring
                                                            carbon
                                sp3-sp3-sp2
C16
       C17
             C18
                    ga 15
                                              corrin ring
                                                            carbon
                                                                   angle
C16
             C54
                    ga 15
                                sp3-sp3-sp2 corrin ring
                                                            carbon angle
       C17
             C55
C16
       C17
                    ga_15
                                sp3-sp3-sp2
                                              corrin ring
                                                            carbon
                    ga_27
C4
       C5
             C6
                                sp2-sp2-sp2 corrin ring
                                                            carbon angle
C9
      C10
                    ga 27
                                sp2-sp2-sp2 corrin ring
             C11
                                                            carbon
                                                                   angle
C14
       C15
             C16
                    ga 27
                                sp2-sp2-sp2
                                              corrin ring
                                                            carbon
                                                                   angle
C3
             C5
                    ga 37
                                sp3-sp2-sp2 corrin ring
                                                            carbon
                                                            carbon angle
C4
       C5
             C35
                    ga_37
                                sp3-sp2-sp2 corrin ring
             C7
C5
                                sp3-sp2-sp2
       C6
                    ga 37
                                              corrin ring
                                                            carbon angle
                                sp3-sp2-sp2 corrin ring
             C35
                    ga 37
C6
       C5
                                                           carbon angle
C8
             C10
                    ga_37
                                sp3-sp2-sp2 corrin ring carbon angle
C10
                    ga 37
                                sp3-sp2-sp2 corrin ring
             C12
                                                            carbon angle
                                                           carbon angle
       C14
             C15
C13
                    ga 37
                                sp3-sp2-sp2 corrin ring
             C53
                    ga 37
                                sp3-sp2-sp2
C14
       C15
                                              corrin ring carbon angle
C15
       C16
             C17
                    ga 37
                                sp3-sp2-sp2 corrin ring carbon angle
C16
                    ga_37
                                sp3-sp2-sp2 corrin ring
                                                            carbon angle
                    ga_37
                                sp2-sp2-methyl dimethylbenzimidazole sp2-sp2-methyl dimethylbenzimidazole
C5M
       C5B
             C4B
                                                                          angle
C5M
      C5B
                    ga 37
             C6B
                                                                          angle
C6M
                                sp2-sp2-methyl dimethylbenzimidazole
       C6B
             C5B
                    ga 37
                                                                          angle
C6M
       C6B
             С7В
                    ga 37
                                sp2-sp2-methyl dimethylbenzimidazole
C4B
       C5B
             C6B
                    ga 27
                                Csp2-Csp2-Csp2 dimethylbenzimidazole angle
                                Csp2-Csp2-Csp2 dimethylbenzimidazole angle Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B
       C4B
             C9B
                    ga 27
C5B
      C6B
             C7B
                    ga 27
                    ga_9
N1B
       C1R
             C2R
                                 from ADE Nsp2-containing dimethylbenzimidazole angle
N1B
       C1R
             06R
                    ga_9
                                from ADE Nsp2-containing dimethylbenzimidazole
N<sub>1</sub>B
       C2B
             N<sub>3</sub>B
                    ga_7
                                from ADE Nsp2-containing dimethylbenzimidazole angle
                    ga_37
C2B
      N<sub>1</sub>B
             C1R
                                from ADE
                                          Nsp2-containing dimethylbenzimidazole
                                                                                     angle
                                          Nsp2-containing dimethylbenzimidazole angle
N3B
       С9В
             C4B
                    ga 39
                                from ADE
С9В
      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
       06R
             C4R
                    ga 10
                                from ADE sugar angle
C2R
       C1R
                    ga_9
             06R
                                 from
                                      ADE
                                          sugar angle
C2R
       C3R
             C4R
                    ga_8
                                from
                                      ADE
                                          sugar angle
                    ga_12
C2R
      O7R
             HAA
                                from ADE
                                          sugar angle
C3R
      C2R
             O7R
                    ga 9
                                from ADE
                                          sugar angle
                    ga_8
C3R
       C4R
                                 from ADE
                                          sugar angle
C3R
       C4R
             06R
                    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
             06R
                                from ADE sugar angle
                    ga_13
ga_13
C1P
      C2P
             C3P
                                amide linkage angle
             C55
                                amide linkage angle
C57
       C56
C57
      N59
                    ga_23
                                from GLN angle
N59
       C57
             058
                    ga 33
                                from GLN angle
                    ga_19
ga_30
                                from GLN angle
C56
       C57
             N59
058
       C57
             C56
                                from GLN angle
C1P
      N59
                    ga 31
                                 from force field angle definitions
                                from force field angle definitions
C1P
```

```
from force field angle definitions
                                      from PHE C-C-H angle
from PHE C-C-H angle
 C5B
        C4B
                H4B
                        ga_25
 C9B
        C4B
                H4B
                        ga_25
                                      from PHE C-C-H angle
        C7B
                       ga_25
 C6B
                H7B
                                      from PHE C-C-H angle
 C8B
        C7B
                Н7В
                       ga 25
                                      from ADE N-C-H angle
 N1B
        C2B
                       ga_36
 N3B
        C2B
                H<sub>2</sub>B
                       ga_36
                                      from ADE N-C-H angle
                       ga_25
ga_20
                                     corrin ring C-C10-H angle corrin ring C-C10-H angle for LYS-B12 bridge (just replaces O8R H atom with CLB)
 C9
        C10
                H10
 C11
        C10
                H10
        08R
                CLB
                       ga_12
 standard Lysine angle topology
                       ga 32
                                      Standard LYS
                                                      (lysine)
 -C
                                      Standard LYS
        Ν
                       ga_31
                                                       (lysine)
 Н
        N
                CA
                       ga_18
                                      Standard LYS
                                                       (lysine)
 Ν
        CA
                CB
                       ga_13
                                      Standard LYS
                                                       (lysine)
                       ga_13
ga_13
                                      Standard LYS
 Ν
        CA
                C
                                                       (lvsine)
 СВ
                                      Standard LYS
                                                       (lysine)
        CA
 CA
        СВ
                CG
                       ga_15
                                      Standard LYS
                                                       (lysine)
                       ga_15
ga_15
 CB
        CG
                CD
                                     Standard LYS
                                                       (lysine)
                                     Standard LYS
 CG
        CD
                CE
                                                       (lysine)
 CD
        CE
                ΝZ
                       ga 15
                                      Standard LYS
                                                       (lysine)
 CE
        NZ
                       ga 11
                                      Standard LYS
                                                      (lysine)
                HZ1
                       ga_6
ga_23
                                                      from LYS
                                                                  (CLB from NZ H atom)
(CLB from NZ H atom)
 CE
        NZ
                CLB
                                      Modification
                                     Modification
 HZ1
                CLB
        NZ
 CA
        С
                       ga 30
                                      Standard LYS
                                                      (lysine)
                0
        C
                +N
 CA
                       ga_19
                                      Standard LYS
                                                       (lysine)
        С
                +N
                       ga 33
                                     Standard LYS (lysine)
 0
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
                                     new OLB-CLB linkage angles
 08R
        CLB
                NZ
                       ga 33
                                  ;
cyano group addition to the original B12 topology
 FE
        C1N
                N<sub>1</sub>C
                       ga_41
ga_1
                                      cyano group from HEMC CO group
                                     cyano group from HEMC CO group
 N21
                C1N
        FΕ
                       ga_1
 N22
        FΕ
                C1N
                                      cyano group from HEMC CO group
                C1N
                                                                 CO group
 N23
                                      cyano group from HEMC
        FE
                       ga_1
                C1N
                        ga_1
                                     cyano group from HEMC CO group
 N24
        FE
                                ; cyano group from HEMC CO group (found during pdb2gmx)
 N3B
        FΕ
                C1N
                       ga 1
  N3B
         FE
                 C1N
                        ga 41
                                      cyano group from HEMC CO group (found during pdb2gmx)
 [ impropers
 ai
                ak
                        al
                              gromos type
 C1R
        C8B
                C2B
                       N1B
                                             dimethylbenzimidazole improper for planarity
                               gi 1
        C8B
                               gi_1
gi_1
gi_1
                                             dimethylbenzimidazole improper for planarity
 N<sub>1</sub>B
                C9B
                       N<sub>3</sub>B
 C8B
        N1B
                С7В
                        С9В
                                              dimethylbenzimidazole
                                                                        improper for
 C8B
        N1B
                C2B
                       N3B
                                             dimethylbenzimidazole improper for planarity
                                             dimethylbenzimidazole improper for planarity dimethylbenzimidazole improper for planarity
 C8B
        C7B
                C6B
                       C5B
                               gi_1
        С9В
                        C2B
 C8B
                N<sub>3</sub>B
                               gi_1
                               gi 1
                                                                                    for
 C7B
        C8B
                        C4B
                                             dimethylbenzimidazole improper
                                                                                         planarity
 С7В
        C6B
                C5B
                        C4B
                                             dimethylbenzimidazole improper for
                                                                                          planarity
 C6B
        C5B
                C4B
                       C9B
                               gi_1
                                             dimethylbenzimidazole improper for planarity
                        C8B
                                             dimethylbenzimidazole improper for planarity
 C5B
        C4B
                C9B
                               gi_1
gi_1
 С9В
        C8B
                С7В
                        C6B
                                             dimethylbenzimidazole improper for planarity
 С9В
        C4B
                N3B
                        C8B
                               gi_1
                                             dimethylbenzimidazole improper for planarity
 C9B
        N3B
                C2B
                       N<sub>1</sub>B
                               gi_1
gi_1
                                             dimethylbenzimidazole improper for planarity
                                             dimethylbenzimidazole improper for planarity dimethylbenzimidazole methyl groups dimethylbenzimidazole methyl groups
 C2B
                       C9B
        N<sub>1</sub>B
                C8B
                               gi 1
 C5M
        C4B
                C6B
                        C5B
 C6M
        С7В
                C5B
                        C6B
                               gi_1
 C2B
        N1B
                N3B
                       H2B
                               gi
                                             dimethylbenzimidazole H atom-containing planarity
                                             dimethylbenzimidazole H atom-containing planarity dimethylbenzimidazole H atom-containing planarity
C4B
C7B
        C9B
                C5B
                       H4B
                               gi_1
                               gi_1
gi_1
gi_1
        C8B
                C6B
                       Н7В
 N<sub>3</sub>B
                                              Fe-dimethylbenzimidazole planarity
 N21
                C5
                        C6
                                             HEMC-based conjugated corrin ring improper planarity
        C4
 N22
        C6
                C5
                       C4
                               gi_1
                                             HEMC-based conjugated corrin ring improper planarity
                                             HEMC-based conjugated corrin ring improper planarity HEMC-based conjugated corrin ring improper planarity
 N22
        C9
                C10
                        C11
                               gi_1
gi_1
                C10
                        C9
 N23
        C11
        C14
                C15
                        C16
                               gi_1
                                             HEMC-based conjugated corrin ring improper planarity
 N23
                                             HEMC-based conjugated corrin ring improper planarity corrin ring on-Csp2 methyl group improper planarity corrin ring on-Csp2 methyl group improper planarity
 N24
        C16
                C15
                        C14
                               gi_1
                       C35
                               gi_1
gi_1
 C5
        C4
                C6
 C15
        C16
                C14
                        C53
 C27
        028
                N29
                        C26
                               gi_1
                                             from GLN improper torsion definition
 N29
        HAE
                HAD
                        C27
                               gi_1
                                             from GLN improper torsion definition
                                             from GLN improper torsion definition from GLN improper torsion definition
                        C31
 C32
        034
                M33
                               gi_1
                       C32
                HAF
 N33
        HAG
                               gi_1
 C38
        039
                N40
                        C37
                               gi 1
                                             from GLN improper torsion definition
 N40
                       C38
                                             from GLN improper torsion definition
```

```
from GLN improper torsion definition
                              gi_1
gi_1
                                                      improper torsion definition
N45
        HAK
               HAJ
                       C43
                                            from GLN
C50
        051
               N52
                       C49
                              gi_1
                                           from GLN improper torsion definition
                       C50
N52
                              gi_1
gi_1
gi_1
        HAM
               HAL
                                           from GLN improper torsion definition
        063
                       C60
                                           from GLN improper
                                                                 torsion definition
C61
               N62
N62
        HAO
               HAN
                       C61
                                           from GLN improper
                                                                 torsion definition
 C57
        C56
               058
                      N59
                                           amide linkage C57 planarity
                              gi_1
gi_1
N59
        C57
               C1P
                      HAC
                                           amide linkage N59 planarity
                                           corrin ring C
        N21
               C3
                       C5
                                                            sp2 planarity
C4
 C5
        C4
               C6
                       C35
                              gi_1
                                           corrin ring C
                                                            sp2 planarity
                                           corrin ring C sp2 planarity
corrin ring C sp2 planarity
corrin ring C sp2 planarity
 C6
        N22
               C5
                       C7
                              gi_1
C9
        N22
               C10
                       C8
                      C12
                              gi_1
gi_1
C11
               C10
        N23
               C15
                       C13
                                           corrin ring C
                                                            sp2 planarity
 C14
        N23
 C15
               C16
                       C53
                                           corrin ring C sp2 planarity
        C14
                              gi_1
C16
        N24
               C15
                       C17
                              gi 1
                                           corrin ring C sp2 planarity
                                           corrin ring C10 planarity
C10
        C9
               C11
                      H10
                              gi_1
                                           corrin ring C atom sp3 tetrahedral geometry corrin ring C atom sp3 tetrahedral geometry
                              gi_2
gi_2
        C17
C18
               C19
                       C60
 C19
        N24
               C18
                       C1
 C3
        C2
               C30
                       C4
                              gi_2
                                           corrin ring C atom sp3 tetrahedral geometry
                              gi_2
gi_2
                                           corrin ring C atom sp3 tetrahedral geometry corrin ring C atom sp3 tetrahedral geometry
C8
        C9
               C7
                       C41
               C12
                       C48
C13
        C14
 C2P
        C1P
               03
                              gi
                                           corrin ring C atom sp3 tetrahedral geometry
 C1R
        N1B
               C2R
                       06R
                              gi 2
                                           sugar C atom tetrahedral geometry
                              gi_2
gi_2
                                           sugar C atom tetrahedral geometry
sugar C atom tetrahedral geometry
sugar C atom tetrahedral geometry
C2R
C3R
                      C1R
C4R
        O7R
               C3R
        C5R
               06R
                       C4R
 C3R
        C2R
               02P
                              gi 2
 FE
        C1
                      N21
                              gi_3
                                           HEMC improper definition
 FE
        С6
               C9
                      N22
                              gi_3
                                           HEMC improper definition
                                           HEMC improper definition HEMC improper definition
               C14
FE
        C11
                      N23
        C16
               C19
                      N24
standard Lysine improper
                              torsions
        -C
                              gi_1
                                           Standard LYS (lysine)
                      Η
                              gi_2
gi_1
 CA
        Ν
               C
                      СВ
                                           Standard LYS (lysine)
        CA
                +N
                       0
                                           Standard LYS (lysine)
 CLB
        OBR
               OLB
                      NZ
                              gi_1
                                           Linkage improper torsion to maintain planarity at CLB
dihedrals ]
                      al
               ak
ai
                            gromos type
        аi
        02P
 C3R
               Ρ
                      03
                              gd_20
                                           from ADE phosphate definition
 C3R
        02P
               P
P
                      03
                              gd_27
gd_20
                                           from ADE phosphate definition
C2P
        03
                      O2P
                                           from ADE phosphate definition
                              gd_27
gd_7
C2P
        03
               Ρ
                      02P
                                           from ADE phosphate definition
               C2P
                      C1P
                                           from ADE phosphate definition
        03
                                                      phosphate definition
 C2R
               02P
                              gd_29
                                            from
                                                 ADE
                              gd 8
                                           from ADE sugar dihedrals
from ADE sugar dihedrals
O8R
        C5R
               C4R
                      06R
08R
        C5R
               C4R
                      06R
                              qd 25
08R
                       C3R
                              gd_17
gd_34
                                           from ADE sugar dihedrals
        C5R
               C4R
 O8R
        C5R
               C4R
                       C3R
                                           from ADE
                                                      sugar dihedrals
C3R
        C4R
               06R
                      C1R
                              gd 29
                                           from ADE sugar dihedrals
                              gd_34
gd_17
 C5R
                       C2R
        C4R
               C3R
                                           from ADE sugar dihedrals
C5R
        C4R
               C3R
                                           from ADE sugar dihedrals
                      02P
 06R
        C4R
                       C2R
                              gd 17
                                           from ADE sugar dihedrals
 06R
        C4R
               C3R
                       02P
                              gd_18
                                           from ADE sugar dihedrals
C4R
        06R
               C1R
                      C2R
                              gd_29
                                           from ADE sugar dihedrals
                                           from ADE sugar dihedrals
06R
        C1R
               C2R
                      O7R
                              qd 18
                              gd 17
06R
        C1R
               C2R
                       C3R
                                           from ADE sugar dihedrals
                                                      sugar dihedrals
06R
        C1R
               C2R
                       C3R
                              gd_34
                                           from ADE
C1R
        C2R
               C3R
                       C4R
                              gd_34
ad_17
                                           from ADE sugar dihedrals
C1R
        C2R
               C3R
                      02P
                                           from ADE sugar dihedrals
O7R
        C2R
               C3R
                       C4R
                              gd 17
                                           from ADE sugar dihedrals
 O7R
        C2R
               C3R
                       02P
                              gd_18
                                           from ADE sugar dihedrals
 C1R
        C2R
               O7R
                      HAA
                              gd_23
                                           from ADE sugar dihedrals
N<sub>1</sub>B
        C1R
               C2R
                      O7R
                              gd 17
                                           from ADE sugar dihedrals
                      C8B
                                           from ADE sugar dihedrals
06R
        C1R
               N<sub>1</sub>B
                              gd 16
HAB-based torsion gone for LYB
                                       C4R C5R O8R HAB gd_2 ; additional ADE-based sugar dihedral
N1B
        C1R
               C2R
                       C3R
                              gd_17
gd_17
                                           additional ADE-based sugar dihedral
                       C4R
                                           additional ADE-based sugar dihedral
N1B
        C1R
               06R
        C26
               C27
                      N29
                              gd 40
                                           from GLN dihedral
 C2
 C26
        C27
               N29
                      HAD
                              gd_14
                                           from GLN dihedral
                              qd^{-}40
C30
        C31
               C32
                      N33
                                           from GLN dihedral
                              qd 14
 C31
        C32
               N33
                      HAF
                                           from GLN dihedral
 C7
        C37
               C38
                              gd 40
                                           from GLN dihedral
        C38
 C37
               N40
                      HAH
                              gd 14
                                           from GLN dihedral
C41
C42
                              gd_40
gd_14
        C42
               C43
                      N45
                                           from GLN dihedral
                      HAJ
                                           from GLN dihedral
        C43
               N45
 C48
        C49
                      N52
                              gd 40
                                           from GLN dihedral
        C50
               N52
                                           from GLN dihedral
```

```
gd_40
gd_14
                                        from GLN dihedral
 C60
        C61
              N62
                     HAN
                                         from GLN dihedral
 C5M
       C5B
              C6B
                     C6M
                            gd_33
                                        dimethylbenzimidazole methyl dihedral fix
 C4B
       C5B
              C6B
                     C6M
                            qd 10
                                        dimethylbenzimidazole methyl dihedral fix
 C8B
                                        dimethylbenzimidazole methyl dihedral
                                                                                   fix
       C7B
              C6B
                     C6M
                            ad 10
 C7E
       C6B
                     C5M
                            qd 10
                                        dimethylbenzimidazole methyl dihedral
 C9B
       C4B
              C5B
                     C5M
                            gd 10
                                        dimethylbenzimidazole methyl dihedral
 C35
       C5
              C4
                     N21
                            gd_10
                                        corrin ring methyl planarity
                                        corrin ring methyl planarity
 C35
       C5
              C6
                     N22
                            qd 10
 C53
       C15
              C14
                                        corrin ring methyl planarity
                     N24
 C53
       C1
              C16
                            gd 10
                                        corrin ring methyl planarity
                            gd_34
                                        corrin ring but HEMC-derived N,C torsions corrin ring but HEMC-derived N,C torsions
N24
       C19
              C1
                     N21
N24
              C1
       C19
                     N21
                            ad 34
                                                          HEMC-derived N,C
N21
       C4
              C5
                     C6
                            gd 15
                                        corrin ring
                                                     but
                                                                              torsions
       C5
                                        corrin ring
                                                          HEMC-derived N,C
              C6
                                                      but
                                                     but HEMC-derived N,C
but HEMC-derived N,C
N22
       C9
              C10
                     C11
                            gd 15
                                        corrin ring but
                                                                              torsions
C9
       C10
              C11
                     N23
                            gd 15
                                        corrin ring
                                                                              torsions
                                                          HEMC-derived N,C
N23
              C15
                     C16
       C14
                            ad 15
                                        corrin ring but
                                                                              torsions
                                        corrin ring
 C14
       C15
              C16
                     N24
                            qd 15
                                                     but HEMC-derived N,C torsions
 C1
       C2
              C26
                     C27
                            gd_40
                                        corrin ring
                                                     HEMC derived CHn torsions
              C26
C27
                     C27
O28
                            gd_34
qd_34
C25
       C2
                                        corrin ring HEMC derived CHn torsions
 C2
                                                     HEMC
       C26
                                        corrin ring
                                                           derived
                                                                    CHn torsions
 C2
       C3
                     C31
                            gd 9
                                        corrin ring
                                                     HEMC
                                                           derived
                                                                    CHn torsions
 C3
       C30
              C31
                     C32
                            gd 40
                                        corrin ring
                                                     HEMC derived
                                                                    CHn torsions
                            gd_40
gd_40
C30
       C31
C7
              C32
                     034
                                        corrin ring
                                                     HEMC
                                                           derived
                                                                    CHn torsions
                                                     HEMC
                     C38
                                                                    CHn
                                        corrin ring
                                                           derived
                                                                         torsions
 C36
       C7
              C37
                     C38
                            gd 40
                                        corrin ring
                                                     HEMC
                                                           derived
                                                                    CHn
                                                                         torsions
 C7
       C37
              C38
                     039
                            gd_40
                                        corrin ring
                                                      HEMC
                                                            derived
                                                                     CHn
                                                                         torsions
 C7
       C8
              C41
                     C42
                            gd 9
                                        corrin ring
                                                     HEMC
                                                           derived
                                                                    CHn torsions
                            gd_34
                                        corrin ring
                     C43
 C8
       C41
              C42
                                                     HEMC
                                                           derived
                                                                    CHn
                                                                         torsions
 C41
       C42
              C43
                                                     HEMC
                                                                    CHn
                     044
                            qd 40
                                        corrin ring
                                                            derived
                                                                         torsions
                            gd 9
 C12
       C13
              C48
                     C49
                                        corrin ring
                                                     HEMC
                                                            derived
                                                                    CHn
                                                                         torsions
 C13
       C48
              C49
                     C50
                                        corrin ring
                                                      HEMC
                                                            derived
                                                                     CHn
                                                                         torsions
                            gd_40
gd_40
C48
C16
       C49
              C50
                     051
                                        corrin ring
                                                     HEMC
                                                           derived
                                                                    CHn
                                                                         torsions
              C55
                     C56
       C17
                                        corrin ring
                                                     HEMC
                                                           derived
                                                                    CHn torsions
 C54
       C17
              C56
                     C57
                            gd 40
                                                     HEMC
                                                           derived
                                                                    CHn
                                        corrin ring
                                                                         torsions
 C17
       C55
              C56
                     C57
                                        corrin ring
                                                      HEMC
                                                           derived
                                                                    CHn
                                                                         torsions
                            gd_40
                                        corrin ring
 C55
       C56
              C57
                     058
                                                     HEMC
                                                           derived
                                                                    CHn
                                                                         torsions
 C17
                     C61
                                        corrin ring HEMC
       C18
              C60
                            qd 9
                                                           derived
                                                                    CHn torsions
 C18
                            qd 34
                                        corrin ring HEMC
                                                           derived
                                                                    CHn torsions
       C60
              C61
                     063
 C18
       C17
                     C56
                            gd_9
                                        corrin ring HEMC derived CHn torsions
                                        amide linkage torsion terms amide linkage torsion terms
N59
                     03
       C1P
              C2P
                            gd 34
                     C3P
N59
       C1P
              C2P
C2P
                     C57
       C1P
              N59
                            qd 34
                                        amide linkage
                                                        torsion terms
 C56
       C57
              N59
                     C1P
                            gd 14
                                        amide linkage torsion
                                                                 terms
 C55
        C56
                     N59
                            gd_40
                                        amide linkage
                                                        torsion
 C17
       C55
              C56
                     C57
                            gd_40
                                        amide linkage torsion terms
                     C1
C5
              N21
                            qd 14
       C4
                                        corrin ring sp3-containing torsions
 C10
       C9
                     C6
                            gd 14
                                        corrin ring sp3-containing
              N22
                                                                       torsions
 C5
       C6
                     C9
                                        corrin ring sp3-containing
              N22
C15
       C14
              N23
                     C11
                            gd 14
                                        corrin ring sp3-containing
                                                                       torsions
                     C14
C10
       C11
              N23
                            gd_14
                                        corrin ring sp3-containing
                                                                       torsions
                     C19
C15
       C16
              N24
                                        corrin ring sp3-containing
                            qd 14
                                                                       torsions
 C4
       N21
                            gd 40
                                        corrin ring sp3-containing
                                                                       torsions
 C18
       C19
              N24
                     C16
                            gd_40
                                        corrin ring sp3-containing
                                                                       torsions
                            gd_33
N22
       C6
              C5
                     C4
                                        corrin ring sp3-containing
                                                                       torsions
N23
              C10
                     C9
                                        corrin ring sp3-containing
       C11
                            ad 33
                                                                       torsions
                            gd 34
 C19
       C18
              C17
                     C55
                                        corrin ring sp3-containing
                                                                       torsions
 C55
       C17
              C16
                     C15
                            gd 40
                                        corrin ring sp3-containing
                                                                       torsions
 C17
       C18
              C19
                     C1
C2
                            gd_34
                                        corrin ring sp3-containing
                                                                       torsions
C18
       C19
              C1
                            ad 34
                                        corrin ring sp3-containing
                                                                       torsions
 C17
       C16
              C15
                     C14
                            gd 10
                                        corrin ring sp3-containing
                                                                       torsions
 C16
              C14
                     C13
       C15
                            gd_10
                                        corrin ring sp3-containing
                                                                       torsions
 C15
       C14
              C13
                     C12
                            gd 40
                                        corrin ring
                                                     sp3-containing
                                                                       torsions
              C8
                     C9
 C6
       C7
                            gd_34
                                        corrin ring sp3-containing
                                                                       torsions
       C7
              C6
                     C5
C8
                            ad 34
                                        corrin ring sp3-containing
                                                                       torsions
 C30
                            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
gd_34
                                        corrin ring sp3-containing
                                                                       torsions
 C5
              C3
                     C30
       C4
                                        corrin ring sp3-containing
                                                                       torsions
 C3
              C1
                     C19
                            gd 34
       C2
                                        corrin ring sp3-containing
standard Lysine torsion topology
                                        Standard LYS
                                                       (lysine)
                            gd_39
gd_34
gd_40
 - C
       Ν
                                        Standard LYS
              CA
                                                       (lysine)
M
              CB
C
                     CG
       CA
                                        Standard LYS
                                                       (lysine)
Ν
       CA
                     +N
                                        Standard
                                                  LYS
                                                       (lysine)
 CA
       CB
              CG
                     CD
                            gd 34
                                        Standard LYS
                                                       (lysine)
              CD
                                        Standard LYS
                                                       (lysine)
```

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gd_34
gd_29
gd_23
gd_12
gd_14
 CG
CD
                                                      Standard LYS (lysine)
Standard LYS (lysine)
           CE
                   NZ
                             HZ1
 C4R
C5R
                                                      LYS-B12 linkage dihedral terms
LYS-B12 linkage dihedral terms
LYS-B12 linkage dihedral terms
          C5R
                   08R
                             CLB
                   CLB
                            OLB
          08R
 08R
          CLB
                   NZ
                             CE
 OLB
          CLB
                                                      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
                                     gd_38
gd_38
gd_38
gd_38
gd_38
gd_38
 С9В
          N3B
                            N21
                                                        THIS IS NEW!!!
                   FE
 N3B
          FE
                   N21
                             C1
                                                        THIS IS NEW!!!
 N3B
          FE
                   N22
                             С6
                                                        THIS IS NEW!!!
                            C11
C16
 N3B
          FE
                   N23
                                                        THIS IS NEW!!!
          FE
                                                        THIS IS NEW!!!
 N3B
                   N24
          FE
                            N1C
                                                      imidazole-Fe-CN torsion to 0
 N3B
                   C1N
```