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

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

GROMOS96 Force Field Topologies and employed atomic charges for:

B12 (cobalamin)

LYB (cobalamin with the ribose 5'-hydroxy-amide bond-lysine residue)

BCN (cyanocobalamin, CN-Cbl)

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

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[ B12 ]
[ atoms ]
C27   C   0.38000   0 ; from GLN residue
O28   O   -0.38000   0 ; from GLN residue
N29   N   -0.18000   0 ; from GLN residue
HAH   H   0.41500   0 ; from GLN residue
HAD   H   0.41500   0 ; from GLN residue
C32   C   0.38000   1 ; from GLN residue
O34   O   -0.38000   1 ; from GLN residue
N33   N   -0.18000   1 ; from GLN residue
HAG   H   0.41500   1 ; from GLN residue
HAF   H   0.41500   1 ; from GLN residue
C38   C   0.38000   2 ; from GLN residue
O39   O   -0.38000   2 ; from GLN residue
N40   N   -0.18000   2 ; from GLN residue
HAI   H   0.41500   2 ; from GLN residue
HAH   H   0.41500   2 ; from GLN residue
C43   C   0.38000   3 ; from GLN residue
O44   O   -0.38000   3 ; from GLN residue
N45   N   -0.18000   3 ; from GLN residue
HAK   H   0.41500   3 ; from GLN residue
HAH   H   0.41500   3 ; from GLN residue
C50   C   0.38000   4 ; from GLN residue
O51   O   -0.38000   4 ; from GLN residue
N52   N   -0.18000   4 ; from GLN residue
HAN   H   0.41500   4 ; from GLN residue
HAL   H   0.41500   4 ; from GLN residue
C61   C   0.38000   5 ; from GLN residue
O63   O   -0.38000   5 ; from GLN residue
N62   N   -0.18000   5 ; from GLN residue
HAA   H   0.41500   5 ; from GLN residue
HAN   H   0.41500   5 ; from GLN residue
C20   CH3  0.00000   6 ; methyl group
C25   CH3  0.00000   7 ; methyl group
C36   CH3  0.00000   8 ; methyl group
C46   CH3  0.00000   9 ; methyl group
C47   CH3  0.00000  10 ; methyl group
C54   CH3  0.00000  11 ; methyl group
C26   CH2  0.00000  12 ; non-polar CHn fragments
C30   CH2  0.00000  13 ; non-polar CHn fragments
C31   CH2  0.00000  14 ; non-polar CHn fragments
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C48   CH2  0.00000  18 ; non-polar CHn fragments
C49   CH2  0.00000  19 ; non-polar CHn fragments
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C60   CH2  0.00000  22 ; non-polar CHn fragments
C2R   CH1  0.15000  23 ; C2*-O2*-H2* from ADE
O7R   OA   -0.54800  23 ; C2*-O2*-H2* from ADE
HAA   H   0.41500  24 ; from GLN residue
C1R   CH1  0.20000  25 ; C1*-O4*-C4* from ADE
OA    OA   -0.36000  25 ; C1*-O4*-C4* from ADE
C4R   CH1  0.16000  26 ; C1*-O4*-C4* from ADE
C3R   CH1  0.00000  27 ; C3* from ADE
C5R   CH2  0.15000  28 ; C2*-O2*-H2* from ADE
O8R   OA   -0.54800  28 ; C2*-O2*-H2* from ADE
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<th>Atom 1</th>
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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 to proper implementation.

* bonds *

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C50 N52 gb_9 ; from GLN
N52 HAN gb_2 ; from GLN
N52 HAL gb_2 ; from GLN
C60 C61 gb_27 ; from GLN fragment S
C61 O63 gb_5 ; from GLN
C61 N62 gb_9 ; from GLN
N62 HAO gb_2 ; from GLN
N62 NAR gb_2 ; from GLN
FE N21 gb_35 ; FE-N bond from HEMC
FE N22 gb_35 ; FE-N bond from HEMC
FE N23 gb_35 ; FE-N bond from HEMC
FE N24 gb_35 ; FE-N bond from HEMC
FE N3B gb_37 ; FE-N3B bond from HEMC not in corrin ring
P O2 gb_28 ; from ADE phosphate
P O4 gb_24 ; from ADE phosphate
P O5 gb_24 ; from ADE phosphate
P O3 gb_28 ; from ADE phosphate
N21 C1 gb_21 ; corrin ring N-CHn bonds
N21 C4 gb_14 ; corrin ring N-C bonds
N22 C6 gb_14 ; corrin ring N-C bonds
N22 C9 gb_14 ; corrin ring N-C bonds
N23 C11 gb_14 ; corrin ring N-C bonds
N23 C14 gb_14 ; corrin ring N-C bonds
N24 C16 gb_14 ; corrin ring N-C bonds
N24 C19 gb_21 ; corrin ring N-CHn bonds
C30 C31 gb_27 ; CH2-CH2 bonds
C41 C42 gb_27 ; CH2-CH2 bonds
C48 C49 gb_27 ; CH2-CH2 bonds
C55 C56 gb_27 ; CH2-CH2 bonds
C56 C57 gb_27 ; CH2-CH2 bonds
N1B C1R gb_22 ; sugar bonds from ADE
C1R C2R gb_26 ; sugar bonds from ADE
C2R O7R gb_20 ; sugar bonds from ADE
O7R HAA gb_1 ; sugar bonds from ADE
C2R C3R gb_26 ; sugar bonds from ADE
C3R C4R gb_26 ; sugar bonds from ADE
C3R O2 gb_20 ; sugar bonds from ADE
C4R CSR gb_26 ; sugar bonds from ADE
C5R O8R gb_20 ; sugar bonds from ADE
O8R HAB gb_1 ; sugar bonds from ADE
C4R O6R gb_20 ; sugar bonds from ADE
O6R C1R gb_20 ; sugar bonds from ADE
C1P N59 gb_24 ; amide corrin - phosphate linkage
C1P C2P gb_27 ; amide corrin - phosphate linkage
C2P C3P gb_27 ; amide corrin - phosphate linkage
C2P O3 gb_20 ; amide corrin - phosphate linkage
N59 HAC gb_2 ; amide corrin - phosphate linkage
N59 C57 gb_9 ; amide corrin - phosphate linkage
C57 O58 gb_5 ; amide corrin - phosphate linkage
N1B C2B gb_10 ; dimethylbenzimidazole ring
C2B N3B gb_10 ; dimethylbenzimidazole ring
C2B N2B gb_1 ; dimethylbenzimidazole ring
N3B C9B gb_10 ; dimethylbenzimidazole ring
C9B C4B gb_16 ; dimethylbenzimidazole ring
C4B C5B gb_16 ; dimethylbenzimidazole ring
C4B H4B gb_3 ; dimethylbenzimidazole ring
C5B C6B gb_16 ; dimethylbenzimidazole ring
C5B C5M gb_27 ; dimethylbenzimidazole ring
C6B C7B gb_16 ; dimethylbenzimidazole ring
C7B C8B gb_16 ; dimethylbenzimidazole ring
C7B N7B gb_3 ; dimethylbenzimidazole ring
C8B N1B gb_10 ; dimethylbenzimidazole ring
C1 C2O gb_27 ; corrin ring carbon framework
C1 C2 gb_27 ; corrin ring carbon framework
C2 C3 gb_27 ; corrin ring carbon framework
C2 C25 gb_27 ; corrin ring carbon framework
C2 C26 gb_27 ; corrin ring carbon framework
C3 C4 gb_27 ; corrin ring carbon framework
C3 C3O gb_27 ; corrin ring carbon framework
C4 C5 gb_17 ; corrin ring carbon framework
C5 C6 gb_17 ; corrin ring carbon framework
C5 C35 gb_27 ; corrin ring carbon framework
C6 C7 gb_27 ; corrin ring carbon framework
C7 C8 gb_27 ; corrin ring carbon framework
C7 C37 gb_27 ; corrin ring carbon framework
C7 C36 gb_27 ; corrin ring carbon framework
C8 C9 gb_27 ; corrin ring carbon framework
C8 C41 gb_27 ; corrin ring carbon framework
C7B C4B  
C7B N3B  
C7B C2B  
C2B C9B  
C5B C2B  
CSM C6H  

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C1 C5   ;  HBMC-based C framework exclusions  
C2 C5   ;  HBMC-based C framework exclusions  
C1 C35  ;  HBMC-based C framework exclusions  
C3 C6   ;  HBMC-based C framework exclusions  
C4 C26  ;  HBMC-based C framework exclusions  
C4 C7   ;  HBMC-based C framework exclusions  
C30 C26 ;  HBMC-based C framework exclusions  
C30 C5   ;  HBMC-based C framework exclusions  
C5 C8   ;  HBMC-based C framework exclusions  
C5 C9   ;  HBMC-based C framework exclusions  
C5 C36  ;  HBMC-based C framework exclusions  
C5 C37  ;  HBMC-based C framework exclusions  
C35 C7  ;  HBMC-based C framework exclusions  
C6 C41  ;  HBMC-based C framework exclusions  
C6 C10  ;  HBMC-based C framework exclusions  
C7 C10  ;  HBMC-based C framework exclusions  
C8 H10  ;  HBMC-based C framework exclusions  
C9 C11  ;  HBMC-based C framework exclusions  
C9 C36  ;  HBMC-based C framework exclusions  
C9 C37  ;  HBMC-based C framework exclusions  
C9 C12  ;  HBMC-based C framework exclusions  
C36 C41 ;  HBMC-based C framework exclusions  
C10 C13 ;  HBMC-based C framework exclusions  
C10 C14 ;  HBMC-based C framework exclusions  
C10 C46 ;  HBMC-based C framework exclusions  
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H10 C12 ;  HBMC-based C framework exclusions  
C11 C48 ;  HBMC-based C framework exclusions  
C11 C15 ;  HBMC-based C framework exclusions  
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C14 C17 ;  HBMC-based C framework exclusions  
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C54 C60 ;  HBMC-based C framework exclusions  
C55 C60 ;  HBMC-based C framework exclusions  

[ angles ]  
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C26 C27 O28 ga_30  ;  from GLN  
C26 C27 N29 ga_19  ;  from GLN  
O28 C27 N29 ga_33  ;  from GLN  
C27 N29 HAE ga_23  ;  from GLN  
C27 N29 HAD ga_23  ;  from GLN  
HAE N29 HAD ga_24  ;  from GLN  
C30 C31 C32 ga_15  ;  from GLN, fragment 2  
C31 C32 O34 ga_30  ;  from GLN  
C31 C32 N33 ga_19  ;  from GLN  
O34 C32 N33 ga_33  ;  from GLN  
C32 N33 HAG ga_23  ;  from GLN  
C32 N33 HAF ga_23  ;  from GLN  
HAG N33 HAF ga_24  ;  from GLN  
C30 C31 C32 ga_15  ;  from GLN, fragment 3  
C37 C38 O39 ga_30  ;  from GLN  
C37 C38 N40 ga_19  ;  from GLN  
O39 C38 N40 ga_33  ;  from GLN  
C38 N40 HAI ga_23  ;  from GLN  
C38 N40 HAH ga_23  ;  from GLN  
HAI N40 HAH ga_24  ;  from GLN  
C41 C42 C43 ga_15  ;  from GLN, fragment 4  
C42 C43 O44 ga_30  ;  from GLN
| C42  | C43  | N45   | ga_19   | ; from GLN          |
| O44  | C43  | N45   | ga_33   | ; from GLN          |
| C44  | H45  | A45   | ga_23   | ; from GLN          |
| H45  | N45  | A45   | ga_24   | ; from GLN          |
| C44  | C45  | S50   | ga_15   | ; from GLN, fragment 5 |
| C49  | C50  | N51   | ga_30   | ; from GLN          |
| C49  | C50  | N52   | ga_19   | ; from GLN          |
| O51  | C50  | N52   | ga_33   | ; from GLN          |
| C50  | N52  | HAL   | ga_23   | ; from GLN          |
| HAM  | N52  | HAL   | ga_24   | ; from GLN          |
| C60  | C61  | N62   | ga_15   | ; from GLN, fragment 6 |
| C60  | C61  | N63   | ca_19   | ; from GLN          |
| O63  | C61  | N62   | ga_33   | ; from GLN          |
| C61  | N62  | HAO   | ga_23   | ; from GLN          |
| C61  | N62  | HAN   | ga_23   | ; from GLN          |
| HAO  | N62  | HAN   | ga_24   | ; from GLN          |
| N21  | FE   | N22   | ga_2    | ; corrin ring Fe-N angle |
| N21  | FE   | N24   | ga_2    | ; corrin ring Fe-N angle |
| N22  | FE   | N23   | ga_2    | ; corrin ring Fe-N angle |
| N23  | FE   | N24   | ga_2    | ; corrin ring Fe-N angle |
| N21  | FE   | N3B   | ga_2    | ; corrin-Fe-dimethylbenzimidazole |
| N22  | FE   | N3B   | ga_2    | ; corrin-Fe-dimethylbenzimidazole |
| N23  | FE   | N3B   | ga_2    | ; corrin-Fe-dimethylbenzimidazole |
| N24  | FE   | N3B   | ga_2    | ; corrin-Fe-dimethylbenzimidazole |
| N21  | C1   | C2    | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| N21  | C1    | C20   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C4    | N21  | C1    | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| N21  | C4    | N21   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C4    | N21  | C1    | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C5    | C4    | N21   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C9    | C4    | N21   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C10   | C9    | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C11   | C10   | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C12   | C11   | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C13   | C12   | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C14   | C13   | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C15   | C14   | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C16   | C15   | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C17   | C16   | N22   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C18   | C17   | N24   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C18   | C17   | N24   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C18   | C17   | N24   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C18   | C17   | N24   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C19   | C18   | C17   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| C19   | C18   | C17   | ga_13   | ; corrin ring-specific but HEMC-derived angles |
| P     | O2    | P     | ga_26   | ; phosphate angle from ADE |
| O2    | P     | O3    | ga_5    | ; phosphate angle from ADE |
| O2    | P     | O4    | ga_14   | ; phosphate angle from ADE |
| O3    | P     | O4    | ga_14   | ; phosphate angle from ADE |
| O3    | P     | O5    | ga_14   | ; phosphate angle from ADE |
| O4    | P     | O5    | ga_14   | ; phosphate angle from ADE |
| P     | O2    | C2P   | ga_26   | ; phosphate angle from ADE |
| O2    | C3R   | C2R   | ga_9    | ; phosphate oxygen to CHn carbons from ADE |
| O2    | C3R   | C4R   | ga_9    | ; phosphate oxygen to CHn carbons from ADE |
| O2    | C3R   | C5P   | ga_9    | ; phosphate oxygen to CHn carbons from ADE |
| O2    | C3R   | C5P   | ga_9    | ; phosphate oxygen to CHn carbons from ADE |
| O3    | C2P   | C1P   | ga_9    | ; phosphate oxygen to CHn carbons from ADE |
| O3    | C2P   | C3P   | ga_9    | ; phosphate oxygen to CHn carbons from ADE |
| C1    | C2    | C12   | ga_13   | ; CHn-CHn-CHn angles |
| C2    | C2    | C13   | ga_13   | ; CHn-CHn-CHn angles |
| C2    | C2    | C13   | ga_13   | ; CHn-CHn-CHn angles |
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C1    C19   ga_13   ;  CHn-CHn-CHn angles
C1    C19   ga_13   ;  CHn-CHn-CHn angles
C1    C20   ga_13   ;  CHn-CHn-CHn angles
C3    C30   ga_13   ;  CHn-CHn-CHn angles
C7    C8    ga_13   ;  CHn-CHn-CHn angles
C17   C18   ga_13   ;  CHn-CHn-CHn angles
C17   C18   ga_13   ;  CHn-CHn-CHn angles
C17   C18   ga_13   ;  CHn-CHn-CHn angles
C1    C2    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C3    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C7    C8    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C9    C10   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C14   C15   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C5    ga_17   ;  sp2-sp2-sp2 corrin ring carbon angle
C5    C6    ga_17   ;  sp2-sp2-sp2 corrin ring carbon angle
C9    C10   ga_17   ;  sp2-sp2-sp2 corrin ring carbon angle
C17   C18   ga_17   ;  sp2-sp2-sp2 corrin ring carbon angle
C19   C20   ga_17   ;  sp2-sp2-sp2 corrin ring carbon angle
C25   C26   ga_17   ;  sp2-sp2-sp2 corrin ring carbon angle
C5M   C5B   ga_17   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C6M   C6B   ga_17   ;  sp2-sp2-methyl dimethylbenzimidazole angle
C4B   C5B   ga_17   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B   C6B   ga_17   ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
N1B   C1R   ga_19   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C1R   ga_19   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C1R   C2R   ga_19   ;  from ADE sugar angle
C1R   C2R   ga_19   ;  from ADE sugar angle
C1R   O7R   ga_19   ;  from ADE sugar angle
C1R   C3R   ga_19   ;  from ADE sugar angle
C1R   O8R   ga_19   ;  from ADE sugar angle
N3B   O8R   ga_19   ;  from ADE sugar angle
C2R   C3R   ga_19   ;  from ADE sugar angle
C2R   C3R   ga_19   ;  from ADE sugar angle
C3R   C4R   ga_19   ;  from ADE sugar angle
C3R   C4R   ga_19   ;  from ADE sugar angle
C4R   O8R   ga_19   ;  from ADE sugar angle
C5R   O8R   ga_19   ;  from ADE sugar angle
C6R   O8R   ga_19   ;  from ADE sugar angle
C7   C8   ga_19   ;  amide linkage angle
C7   C8   ga_19   ;  amide linkage angle
C7   C8   ga_19   ;  amide linkage angle
C7   C8   ga_19   ;  amide linkage angle
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C57 N59 HAC ga_23 ; from GLN angle
N59 C57 O58 ga_33 ; from GLN angle
C56 N59 ga_19 ; from GLN angle
O58 C57 C56 ga_10 ; from GLN angle
C1P N59 C57 ga_31 ; from force field angle definitions
C1P N59 HAC ga_18 ; from force field angle definitions
C2P C1P N59 ga_14 ; from force field angle definitions
C5B C4B H4B ga_25 ; from PHE C-C-H angle
C9B C4B H4B ga_25 ; from PHE C-C-H angle
C6B C7B H7B ga_25 ; from PHE C-C-H angle
C8B C7B H7B ga_25 ; from PHE C-C-H angle
N1B C2B H2B ga_36 ; from ADE N-H angle
N3B C2B H2B ga_36 ; from ADE N-H angle
C9 C10 H10 ga_25 ; corrin ring C-C10-H angle
C11 C10 H10 ga_20 ; corrin ring C-C10-H angle

; ai aj ak al gromos type
C1R C8B C2B N1B gl_1 ; dimethylbenzimidazole improper for planarity
N1B C8B C9B N3B gl_1 ; dimethylbenzimidazole improper for planarity
C8B N1B C7B C9B gl_1 ; dimethylbenzimidazole improper for planarity
C8B N1B C2B N3B gl_1 ; dimethylbenzimidazole improper for planarity
C6B C7B C5B C4B gl_1 ; dimethylbenzimidazole improper for planarity
C8B N1B C7B C9B gl_1 ; dimethylbenzimidazole improper for planarity
C9B C8B C7B C6B gl_1 ; dimethylbenzimidazole improper for planarity
C9B N1B C8B C9B gl_1 ; dimethylbenzimidazole improper for planarity
C9B N3B C2B C1B gl_1 ; dimethylbenzimidazole improper for planarity
C2B N1B C8B C9B gl_1 ; dimethylbenzimidazole improper for planarity
C5M C6M C7B C5B gl_1 ; dimethylbenzimidazole methyl groups
C6M C7B C5B C6B gl_1 ; dimethylbenzimidazole methyl groups
C2B N1B C7B H2B gl_1 ; dimethylbenzimidazole H atom-containing planarity
C9B C4B C8B C9B gl_1 ; dimethylbenzimidazole H atom-containing planarity
C7B C8B C1B H7B gl_1 ; dimethylbenzimidazole H atom-containing planarity
C3B FE C2B C9B gl_1 ; Fe-dimethylbenzimidazole planarity
N2B C7B C5B C1B gl_1 ; HEMC-based conjugated corrin ring improper planarity
N2B C6 C5 C4 gl_1 ; HEMC-based conjugated corrin ring improper planarity
N2B C9 C10 C11 gl_1 ; HEMC-based conjugated corrin ring improper planarity
N2B C9 C10 C11 gl_1 ; HEMC-based conjugated corrin ring improper planarity
N2B C14 C15 C16 gl_1 ; HEMC-based conjugated corrin ring improper planarity
N2B C14 C15 C16 gl_1 ; HEMC-based conjugated corrin ring improper planarity
C5 C4 C6 C35 gl_1 ; corrin ring on-Csp2 methyl group improper planarity
C15 C16 C14 C53 gl_1 ; corrin ring on-Csp2 methyl group improper planarity
C27 O28 N29 C26 gl_1 ; from GLN improper torsion definition
N29 HAB HAD C27 gl_1 ; from GLN improper torsion definition
C32 O34 N33 C31 gl_1 ; from GLN improper torsion definition
N33 HAG HAF C32 gl_1 ; from GLN improper torsion definition
C38 O39 N40 C37 gl_1 ; from GLN improper torsion definition
N40 HAK HAH C38 gl_1 ; from GLN improper torsion definition
C43 O44 N45 C42 gl_1 ; from GLN improper torsion definition
N45 HAK HAJ C43 gl_1 ; from GLN improper torsion definition
C50 O51 N52 C49 gl_1 ; from GLN improper torsion definition
N52 HAM HAL C50 gl_1 ; from GLN improper torsion definition
C61 O63 N62 C60 gl_1 ; from GLN improper torsion definition
N62 HAO HAN C61 gl_1 ; from GLN improper torsion definition
C57 C56 O58 N59 gl_1 ; amide linkage C57 planarity
N59 C57 C1P HAC gl_1 ; amide linkage N59 planarity
C4 N21 C3 C5 gl_1 ; corrin ring C sp2 planarity
C5 C4 C6 C35 gl_1 ; corrin ring C sp2 planarity
C6 N22 C5 C7 gl_1 ; corrin ring C sp2 planarity
C9 N22 C10 C8 gl_1 ; corrin ring C sp2 planarity
C11 N23 C10 C12 gl_1 ; corrin ring C sp2 planarity
C14 N23 C15 C13 gl_1 ; corrin ring C sp2 planarity
C15 C14 C16 C53 gl_1 ; corrin ring C sp2 planarity
C11 C14 C17 gl_1 ; corrin ring C sp2 planarity
C10 C9 C11 H10 gl_1 ; corrin ring C10 planarity
C18 C17 C19 C60 gl_2 ; corrin ring C atom sp3 tetrahedral geometry
C19 N24 C18 C1 gl_2 ; corrin ring C atom sp3 tetrahedral geometry
C3 C2 C30 C4 gl_2 ; corrin ring C atom sp3 tetrahedral geometry
C9 C8 C7 C41 gl_2 ; corrin ring C atom sp3 tetrahedral geometry
C13 C12 H48 gl_2 ; corrin ring C atom sp3 tetrahedral geometry
C2P C1P O3 C3P gl_2 ; corrin ring C atom sp3 tetrahedral geometry
C1R N1B C2R O6R gl_2 ; sugar C atom tetrahedral geometry
C2R C1R C7R gl_2 ; sugar C atom tetrahedral geometry
C3R C5R O6R C4R gl_2 ; sugar C atom tetrahedral geometry
C3R C2R O2R C4R gl_2 ; sugar C atom tetrahedral geometry
FC C4 N21 gl_3 ; HEMC improper definition
FC C6 C9 N22 gl_3 ; HEMC improper definition
FC C11 C14 N23 gl_3 ; HEMC improper definition

; ai aj ak al gromos type
C18  C60  C61  O63  gd_34  ;  corrin ring HEMC derived CHn torsions
C18  C17  C55  O56  gd_9  ;  corrin ring HEMC derived CHn torsions
N59  C1P  C2P  O3  gd_34  ;  amide linkage torsion terms
N59  C1P  C2P  C3P  gd_34  ;  amide linkage torsion terms
C2P  C1P  N59  C1P  gd_14  ;  amide linkage torsion terms
C55  C56  C57  N59  gd_40  ;  amide linkage torsion terms
C17  C55  C56  gd_40  ;  amide linkage torsion terms
C5  C4  N21  C1  gd_14  ;  corrin ring sp3-containing torsions
C10  C9  N22  C9  gd_14  ;  corrin ring sp3-containing torsions
C5  C6  N22  C9  gd_14  ;  corrin ring sp3-containing torsions
C15  C14  N23  C11  gd_14  ;  corrin ring sp3-containing torsions
C10  C11  N23  C14  gd_14  ;  corrin ring sp3-containing torsions
C15  C16  N24  C19  gd_14  ;  corrin ring sp3-containing torsions
C4  N21  C1  C2  gd_40  ;  corrin ring sp3-containing torsions
C18  C19  N24  C16  gd_40  ;  corrin ring sp3-containing torsions
N22  C6  C5  C4  gd_33  ;  corrin ring sp3-containing torsions
N23  C11  C10  C9  gd_33  ;  corrin ring sp3-containing torsions
C19  C18  C17  C55  gd_34  ;  corrin ring sp3-containing torsions
C55  C17  C16  C15  gd_40  ;  corrin ring sp3-containing torsions
C17  C18  C19  C1  gd_34  ;  corrin ring sp3-containing torsions
C18  C19  C1  C2  gd_34  ;  corrin ring sp3-containing torsions
C17  C16  C15  C14  gd_10  ;  corrin ring sp3-containing torsions
C16  C15  C14  C13  gd_10  ;  corrin ring sp3-containing torsions
C15  C14  C13  C12  gd_40  ;  corrin ring sp3-containing torsions
C6  C7  C8  C9  gd_34  ;  corrin ring sp3-containing torsions
C8  C7  C6  C5  gd_34  ;  corrin ring sp3-containing torsions
C30  C3  C2  C1  gd_34  ;  corrin ring sp3-containing torsions
C13  C12  C11  C10  gd_34  ;  corrin ring sp3-containing torsions
C10  C9  C8  C7  gd_10  ;  corrin ring sp3-containing torsions
C5  C4  C3  C2  gd_34  ;  corrin ring sp3-containing torsions
C3  C2  C1  C19  gd_34  ;  corrin ring sp3-containing torsions
C9B  N3B  FE  N21  gd_38  ;  THIS IS NEW!!!
N3B  FE  N21  C1  gd_38  ;  THIS IS NEW!!!
N3B  FE  N22  C6  gd_38  ;  THIS IS NEW!!!
N3B  FE  N23  C11  gd_38  ;  THIS IS NEW!!!
N3B  FE  N24  C16  gd_38  ;  THIS IS NEW!!!
[LYB]

[atoms]

c27  c  0.38000  0  ; from gln residue
o28  o  -0.38000  0  ; from gln residue
n29  n  -0.83000  0  ; from gln residue
h2a  h  0.41500  0  ; from gln residue
h2b  h  0.41500  0  ; from gln residue
c32  c  0.38000  1  ; from gln residue
o34  o  -0.38000  1  ; from gln residue
n33  n  -0.83000  1  ; from gln residue
h3a  h  0.41500  1  ; from gln residue
h3b  h  0.41500  1  ; from gln residue
c38  c  0.38000  2  ; from gln residue
o39  o  -0.38000  2  ; from gln residue
n40  n  -0.83000  2  ; from gln residue
h4a  h  0.41500  2  ; from gln residue
h4b  h  0.41500  2  ; from gln residue
c43  c  0.38000  3  ; from gln residue
o44  o  -0.38000  3  ; from gln residue
n45  n  -0.83000  3  ; from gln residue
h5a  h  0.41500  3  ; from gln residue
h5b  h  0.41500  3  ; from gln residue
c50  c  0.38000  4  ; from gln residue
o51  o  -0.38000  4  ; from gln residue
n52  n  -0.83000  4  ; from gln residue
h5a  h  0.41500  4  ; from gln residue
h5b  h  0.41500  4  ; from gln residue
c55  c  0.38000  5  ; from gln residue
o56  o  -0.38000  5  ; from gln residue
n57  n  -0.83000  5  ; from gln residue
h6a  h  0.41500  5  ; from gln residue
h6b  h  0.41500  5  ; from gln residue
c20  ch3  0.00000  6  ; methyl group

; 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)

; p  p  2.20000  23  ; po3*po3* fragment from ade
; h2b from b12 is in lyb, where the lysine fragment is added via clb
; h2b from b12 is in lyb, where the lysine fragment is added via clb
; c2*-o2*-h2* from ade
; c2*-o2*-h2* from ade
; c1*-o4*-c4* from ade
; c1*-o4*-c4* from ade
; c2*-o2*-h2* from ade
; c2*-o2*-h2* from ade
C5B  C     0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
C5M  CH3    0.00000     26   ;  dimethylbenzimidazole C-CH3 group (non-polar)
C6B  C     0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
C6M  CH3    0.00000     27   ;  dimethylbenzimidazole C-CH3 group (non-polar)
C4B  C     -0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
H4B  H      0.14000     28   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
C7B  C     -0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
H7B  H      0.14000     29   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
N3B  NR    -0.55000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
C9B  C      0.20000     30   ;  dimethylbenzimidazole polar aromatic NC fragment
N1B  NR    -0.30000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
C8B  C      0.20000     31   ;  dimethylbenzimidazole polar aromatic NC fragment
C2B  C      0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
H2B  H      0.23000     32   ;  dimethylbenzimidazole aromatic C-H from TRP, PHE
N21  NR    -0.44000     35   ;  HEMC Fe-N group
N22  NR    -0.50000     35   ;  HEMC Fe-N group
N23  NR    -0.50000     35   ;  HEMC Fe-N group
N24  NR    -0.44000     35   ;  HEMC Fe-N group
C1  CH0    0.22000     36   ;  non-polar HEMC-derived corrin atoms
C2  CH0    0.00000     36   ;  non-polar HEMC-derived corrin atoms
C3  CH1    0.00000     36   ;  non-polar HEMC-derived corrin atoms
C4  C      0.38000     36   ;  non-polar HEMC-derived corrin atoms
C6  C      0.29000     37   ;  non-polar HEMC-derived corrin atoms
C7  CH0    0.00000     37   ;  non-polar HEMC-derived corrin atoms
C8  CH1    0.00000     37   ;  non-polar HEMC-derived corrin atoms
C9  C      0.35000     37   ;  non-polar HEMC-derived corrin atoms
C16  C     0.38000     38   ;  non-polar HEMC-derived corrin atoms
C17  CH0    0.00000     38   ;  non-polar HEMC-derived corrin atoms
C18  CH1    0.00000     38   ;  non-polar HEMC-derived corrin atoms
C19  CH1    0.24000     38   ;  non-polar HEMC-derived corrin atoms
C11  C     0.35000     39   ;  non-polar HEMC-derived corrin atoms
C12  CH0    0.00000     39   ;  non-polar HEMC-derived corrin atoms
C13  CH1    0.00000     39   ;  non-polar HEMC-derived corrin atoms
C14  C      0.29000     39   ;  non-polar HEMC-derived corrin atoms
C10  C    -0.24000     40   ;  aromatic C-H from TRP, PHE
H10  H     0.14000     40   ;  aromatic C-H from TRP, PHE
; Since CO is not defined as an atom in GROMOSxx, CO is converted to FE and the HEME
; values are employed. This is a workaround due for proper implementation.
; N     N     -0.31000     41   ;  standard LYS (lysine) atom information
H     H      0.31000     41   ;  standard LYS (lysine) atom information
CA    CH1    0.00000     42   ;  standard LYS (lysine) atom information
CB    CH2    0.00000     42   ;  standard LYS (lysine) atom information
CG    CH2    0.00000     43   ;  standard LYS (lysine) atom information
CD    CH2    0.00000     43   ;  standard LYS (lysine) atom information
CE    CH2    0.00000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
NZ    NT    -0.34000     44   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
HZ1   H      0.44000     44   ;  standard LYS (lysine) atom information
; CE    CH2    -0.24000     44   ;  standard LYS (lysine) atom information
; NZ    NT    -0.64000     44   ;  standard LYS (lysine) atom information
; HZ1   H      0.44000     44   ;  standard LYS (lysine) atom information
; this H atom is gone, replaced by the linkage CLB atom.
; HZ2   H      0.44000     44   ;  standard LYS (lysine) atom information
; this H atom is gone, replaced by the linkage CLB atom.
C      C      0.20000     45   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
O      O     -0.20000     45   ;  NEW CHARGE FROM B12 standard LYS (lysine) atom information
C      C      0.45000     45   ;  standard LYS (lysine) atom information
O      O     -0.45000     45   ;  standard LYS (lysine) atom information
; linkage atoms (added new)
CLB    C     0.00000     46   ;  this is the linkage carbon atom between LYS and B12
OLB    O     0.00000     46   ;  this is the additional -O at the linkage position
}
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C1 C20 gb_27 ; corrin ring carbon framework
C1 C2 gb_27 ; corrin ring carbon framework
C2 C3 gb_27 ; corrin ring carbon framework
C2 C25 gb_27 ; corrin ring carbon framework
C2 C26 gb_27 ; corrin ring carbon framework
C2 C4 gb_27 ; corrin ring carbon framework
C3 C30 gb_27 ; corrin ring carbon framework
C4 C5 gb_17 ; corrin ring carbon framework
C5 C6 gb_17 ; corrin ring carbon framework
C5 C3 gb_27 ; corrin ring carbon framework
C6 C7 gb_27 ; corrin ring carbon framework
C7 C8 gb_27 ; corrin ring carbon framework
C7 C37 gb_27 ; corrin ring carbon framework
C7 C26 gb_27 ; corrin ring carbon framework
C8 C9 gb_27 ; corrin ring carbon framework
C8 C41 gb_27 ; corrin ring carbon framework
C9 C10 gb_17 ; corrin ring carbon framework
C10 C11 gb_17 ; corrin ring carbon framework
C11 C12 gb_27 ; corrin ring carbon framework
C12 C46 gb_27 ; corrin ring carbon framework
C12 C47 gb_27 ; corrin ring carbon framework
C12 C13 gb_27 ; corrin ring carbon framework
C13 C14 gb_27 ; corrin ring carbon framework
C13 C48 gb_27 ; corrin ring carbon framework
C14 C15 gb_17 ; corrin ring carbon framework
C15 C16 gb_17 ; corrin ring carbon framework
C15 C53 gb_27 ; corrin ring carbon framework
C16 C17 gb_27 ; corrin ring carbon framework
C17 C4 gb_27 ; corrin ring carbon framework
C17 C54 gb_27 ; corrin ring carbon framework
C17 C55 gb_27 ; corrin ring carbon framework
C18 C19 gb_27 ; corrin ring carbon framework
C18 C60 gb_27 ; corrin ring carbon framework
C19 C1 gb_27 ; corrin ring carbon framework
C10 H10 gb_3 ; corrin ring C10-H10 bond
;
; linker bond from B12 to CLB
;
O8R CLB gb_5 ; LYS B12 linker (CLB replaces H)
;
; Lysine bond topology
;
N H gb_2 ; standard LYS (lysine)
N CA gb_21 ; standard LYS (lysine)
CA CB gb_27 ; standard LYS (lysine)
CA C gb_27 ; standard LYS (lysine)
CB CG gb_27 ; standard LYS (lysine)
CG CD gb_27 ; standard LYS (lysine)
CD CE gb_27 ; standard LYS (lysine)
CE NZ gb_21 ; standard LYS (lysine)
NZ HZ2 gb_2 ; standard LYS (lysine)
;
; this replaces the HZ2 with CLB for the B12-lysine connection
;
NZ CLB gb_9 ; standard LYS (lysine)
C O gb_5 ; standard LYS (lysine)
C +N gb_10 ; standard LYS (lysine)
;
; below is the C=O bond on the B12-lysine linkage (OLB is only connected to CLB)
;
CLB OLB gb_27 ; CLB-OLB linkage bond (previously nowhere in the structure)
[
; exclusions
; ai aj
FE C2
FE C3
FE C5
FE C7
FE C8
FE C10
FE C12
FE C13
FE C15
FE C17
FE C18
FE C20
N21 C25
N21 C26
N21 C30
N21 C35
N21 C6
N21 C9
]
N21 C11
N21 C14
N21 C16
N21 C19
N21 C10
N22 C1
N22 C4
N22 C36
N22 C37
N22 C15
N23 C16
N23 C19
N23 C1
N23 C4
N23 C6
N23 C9
N23 C46
N23 C47
N23 C5
N24 C5
N24 C6
N24 C9
N24 C11
N24 C14
N24 C55
N24 C54
N24 C60
C1R C7B
C1R C9B
C1R N3B
N1B C6B
N1B C4B
C4B C5B
C4B C5M
C4B C6M
C7B C4B
C7B N3B
C7B C2B
C2B C9B
C5B C2B
C5M C6M
C1 C30 ; HEMC-based C framework exclusions
C1 C5 ; HEMC-based C framework exclusions
C2 C5 ; HEMC-based C framework exclusions
C3 C35 ; HEMC-based C framework exclusions
C3 C6 ; HEMC-based C framework exclusions
C4 C26 ; HEMC-based C framework exclusions
C4 C7 ; HEMC-based C framework exclusions
C10 C26 ; HEMC-based C framework exclusions
C5 C8 ; HEMC-based C framework exclusions
C5 C55 ; HEMC-based C framework exclusions
C5 C36 ; HEMC-based C framework exclusions
C5 C37 ; HEMC-based C framework exclusions
C35 C7 ; HEMC-based C framework exclusions
C6 C41 ; HEMC-based C framework exclusions
C6 C10 ; HEMC-based C framework exclusions
C7 C10 ; HEMC-based C framework exclusions
C8 H10 ; HEMC-based C framework exclusions
C8 C11 ; HEMC-based C framework exclusions
C9 C36 ; HEMC-based C framework exclusions
C9 C37 ; HEMC-based C framework exclusions
C9 C12 ; HEMC-based C framework exclusions
C36 C41 ; HEMC-based C framework exclusions
C37 C10 ; HEMC-based C framework exclusions
C10 C13 ; HEMC-based C framework exclusions
C10 C14 ; HEMC-based C framework exclusions
C10 C46 ; HEMC-based C framework exclusions
C10 C47 ; HEMC-based C framework exclusions
C11 C12 ; HEMC-based C framework exclusions
C11 C48 ; HEMC-based C framework exclusions
C11 C15 ; HEMC-based C framework exclusions
C12 C15 ; HEMC-based C framework exclusions
C13 C53 ; HEMC-based C framework exclusions
C13 C16 ; HEMC-based C framework exclusions
C14 C46 ; HEMC-based C framework exclusions
C14 C47 ; HEMC-based C framework exclusions
C14 C17 ; HEMC-based C framework exclusions
C46 C48 ; HEMC-based C framework exclusions
C47 C48 ; HEMC-based C framework exclusions
C48 C15 ; HEMC-based C framework exclusions
C15 C18 ; HEMC-based C framework exclusions
C15 C19 ; HEMC-based C framework exclusions
C15 C44 ; HEMC-based C framework exclusions
C15 C55 ; HEMC-based C framework exclusions
C37 C17 ; HEMC-based C framework exclusions
C60 C60 ; HEMC-based C framework exclusions
C19 C54 ; HEMC-based C framework exclusions
C19 C55 ; HEMC-based C framework exclusions
C40 C60 ; HEMC-based C framework exclusions
C56 C60 ; HEMC-based C framework exclusions
[ angles ]
ai aj ak gromos type
C2 C26 C27 ga_15 ; from GLN, fragment 1
C26 C27 O28 ga_30 ; from GLN
C26 C27 N29 ga_19 ; from GLN
O28 C27 N29 ga_33 ; from GLN
C27 N29 HAE ga_23 ; from GLN
HAE N29 HAD ga_24 ; from GLN
C30 C31 C32 ga_15 ; from GLN, fragment 2
C31 C32 O34 ga_30 ; from GLN
C31 C32 N33 ga_19 ; from GLN
O34 C32 N33 ga_33 ; from GLN
C32 N33 HAG ga_23 ; from GLN
C32 N33 HAF ga_24 ; from GLN
C7 C37 C38 ga_15 ; from GLN, fragment 3
C37 C38 O39 ga_30 ; from GLN
C37 C38 N40 ga_19 ; from GLN
O34 C32 N33 ga_33 ; from GLN
C32 N33 HAG ga_23 ; from GLN
C32 N33 HAF ga_24 ; from GLN
C48 C49 C50 ga_15 ; from GLN, fragment 5
C49 C50 O51 ga_30 ; from GLN
C49 C50 N52 ga_19 ; from GLN
O51 C50 N52 ga_33 ; from GLN
C50 N52 HAM ga_23 ; from GLN
C50 N52 HAL ga_24 ; from GLN
C18 C60 C61 ga_15 ; from GLN, fragment 6
C60 C61 O63 ga_30 ; from GLN
C60 C61 N62 ga_19 ; from GLN
O63 C61 N62 ga_33 ; from GLN
C61 N62 HAO ga_23 ; from GLN
C61 N62 HAN ga_23 ; from GLN
N21 FE N22 ga_2 ; corrin ring Pe-N angle
N21 FE N24 ga_2 ; corrin ring Pe-N angle
N22 FE N23 ga_2 ; corrin ring Pe-N angle
N23 FE N24 ga_2 ; corrin ring Pe-N angle
N21 FE N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
N21 FE N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
N23 FE N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
N24 FE N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
FE N21 C1 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N21 C4 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N22 C6 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N22 C9 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N23 C11 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N23 C14 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N24 C16 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N24 C19 ga_34 ; corrin Pe-N-C angles (based on HEMC)
FE N38 C9B ga_34 ; Pe-dimethylbenzimidazole-N,C angle
C8B N1B C2B ga_7 ; angle containing C8B, see minimization issues discussion
N1B C8B C9B ga_7 ; angle containing C8B, see minimization issues discussion
C8B C9B N3B ga_7 ; angle containing C8B, see minimization issues discussion
C7B C8B N1B ga_39 ; angle containing C8B, see minimization issues discussion
C8B N1B C1R ga_37 ; angle containing C8B, see minimization issues discussion
C4B C9B C8B ga_27 ; angle containing C8B, see minimization issues discussion
C6B C7B C8B ga_27 ; angle containing C8B, see minimization issues discussion
N21 C1 C20 ga_13 ; corrin ring-specific but HEMC-derived angles
N21 C4 C3 ga_33 ; corrin ring-specific but HEMC-derived angles
N22 C6 C5 ga_33 ; corrin ring-specific but HEMC-derived angles
N22 C6 C7 ga_33 ; corrin ring-specific but HEMC-derived angles
N22 C6 C9 ga_33 ; corrin ring-specific but HEMC-derived angles
C4 C5 N21 ga_33 ; corrin ring-specific but HEMC-derived angles
N22 C9 C8 ga_33 ; corrin ring-specific but HEMC-derived angles
C8 N22 C6 ga_33 ; corrin ring-specific but HEMC-derived angles
C19 C1 N21 ga_13 ; corrin ring-specific but HEMC-derived angles
C14 N23 C11 ga_6 ; corrin ring-specific but HEMC-derived angles
N23 C11 C10 ga_33 ; corrin ring-specific but HEMC-derived angles
N23 C11 C12 ga_33 ; corrin ring-specific but HEMC-derived angles
C15 C14 N23 ga_33 ; corrin ring-specific but HEMC-derived angles
N24 C16 C15 ga_33 ; corrin ring-specific but HEMC-derived angles
N24 C19 C11 ga_13 ; corrin ring-specific but HEMC-derived angles
C17 C12 C47 ga_13 ; corrin ring-specific but HEMC-derived angles
C17 C12 C46 ga_13 ; corrin ring-specific but HEMC-derived angles
C17 C12 C47 ga_13 ; corrin ring-specific but HEMC-derived angles
C17 C18 C19 ga_13 ; corrin ring-specific but HEMC-derived angles
C25 C26 C27 ga_13 ; CHn-CHn-CHn angles
C2 C3 C26 ga_13 ; CHn-CHn-CHn angles
C1 C2 C26 ga_13 ; CHn-CHn-CHn angles
C1 C2 C3 ga_13 ; CHn-CHn-CHn angles
C1 C19 C18 ga_13 ; CHn-CHn-CHn angles
C1 C19 C18 ga_13 ; CHn-CHn-CHn angles
C1 C19 C18 ga_13 ; CHn-CHn-CHn angles
C7 C8 C41 ga_13 ; CHn-CHn-CHn angles
C6 C7 C41 ga_13 ; CHn-CHn-CHn angles
C12 C13 C48 ga_13 ; CHn-CHn-CHn angles
C13 C12 C46 ga_13 ; CHn-CHn-CHn angles
C13 C12 C47 ga_13 ; CHn-CHn-CHn angles
C13 C12 C47 ga_13 ; CHn-CHn-CHn angles
C17 C18 C19 ga_13 ; CHn-CHn-CHn angles
C17 C18 C60 ga_13 ; CHn-CHn-CHn angles
C17 C55 C56 ga_13 ; CHn-CHn-CHn angles
C17 C55 C56 ga_13 ; CHn-CHn-CHn angles
C17 C55 C56 ga_13 ; CHn-CHn-CHn angles
C17 C55 C56 ga_13 ; CHn-CHn-CHn angles
C18 C17 C55 ga_13 ; CHn-CHn-CHn angles
C19 C18 C60 ga_13 ; CHn-CHn-CHn angles
C19 C18 C60 ga_13 ; CHn-CHn-CHn angles
C25 C2C26 ga_13 ; CHn-CHn-CHn angles
C25 C2C26 ga_13 ; CHn-CHn-CHn angles
C25 C2C26 ga_13 ; CHn-CHn-CHn angles
C46 C12 C47 ga_13 ; CHn-CHn-CHn angles
C46 C12 C47 ga_13 ; CHn-CHn-CHn angles
C46 C12 C47 ga_13 ; CHn-CHn-CHn angles
C46 C12 C47 ga_13 ; CHn-CHn-CHn angles
C54 C17 C55 ga_13 ; CHn-CHn-CHn angles
C54 C17 C55 ga_13 ; CHn-CHn-CHn angles
C36 C7 C37 ga_13 ; CHn-CHn-CHn angles
C4 C3 C30 ga_15 ; sp3-sp2 corrin ring carbon angle
C4 C3 C30 ga_15 ; sp3-sp2 corrin ring carbon angle
C6 C7 C8 ga_15 ; sp3-sp2 corrin ring carbon angle
C6 C7 C8 ga_15 ; sp3-sp2 corrin ring carbon angle
C6 C7 C8 ga_15 ; sp3-sp2 corrin ring carbon angle
C6 C7 C8 ga_15 ; sp3-sp2 corrin ring carbon angle
C8 C7 C8 ga_15 ; sp3-sp2 corrin ring carbon angle
C8 C7 C8 ga_15 ; sp3-sp2 corrin ring carbon angle
C9 C8 C41 ga_15 ; sp3-sp2 corrin ring carbon angle
C11 C12 C13 ga_15 ; sp3-sp2 corrin ring carbon angle
C11 C12 C13 ga_15 ; sp3-sp2 corrin ring carbon angle
C11 C12 C13 ga_15 ; sp3-sp2 corrin ring carbon angle
C11 C12 C13 ga_15 ; sp3-sp2 corrin ring carbon angle
C16 C17 C18 ga_15 ; sp3-sp2 corrin ring carbon angle
C16 C17 C18 ga_15 ; sp3-sp2 corrin ring carbon angle
C16  C17  C54  ga_15  ;  sp3-sp3-sp2 corrin ring carbon angle
C16  C17  C55  ga_15  ;  sp3-sp3-sp2 corrin ring carbon angle
C9   C10  C11  ga_27  ;  sp2-sp2-sp2 corrin ring carbon angle
C14  C15  C16  ga_27  ;  sp2-sp2-sp2 corrin ring carbon angle
C4   C5   C35  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C4   C5   C35  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C5   C6   C7   ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C6   C7   C8   ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C14  C15  C16  ga_27  ;  sp2-sp2-sp2 corrin ring carbon angle
C3   C4   C5   ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C4   C5   C35  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C5   C6   C7   ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C9   C10  C11  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C14  C15  C16  ga_27  ;  sp2-sp2-sp2 corrin ring carbon angle
C3   C4   C5   ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C4   C5   C35  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C5   C6   C7   ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C6   C7   C8   ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C14  C15  C53  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C15  C16  C17  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C16  C15  C53  ga_37  ;  sp3-sp2-sp2 corrin ring carbon angle
C5M  C5B  C4B  ga_37  ;  sp2-sp2-methyl dimethylbenzimidazole angle
C5M  C5B  C6B  ga_37  ;  sp2-sp2-methyl dimethylbenzimidazole angle
C6M  C6B  C5B  ga_37  ;  sp2-sp2-methyl dimethylbenzimidazole angle
C6M  C6B  C7B  ga_37  ;  sp2-sp2-methyl dimethylbenzimidazole angle
C4B  C5B  C6B  ga_27  ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B  C4B  C9B  ga_27  ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
C5B  C6B  C7B  ga_27  ;  Csp2-Csp2-Csp2 dimethylbenzimidazole angle
N1B  C1R  C2R  ga_9   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B  C1R  O6R  ga_9   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B  C2B  N3B  ga_9   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C9B  N3B  C2B  ga_7   ;  from ADE Nsp2-containing dimethylbenzimidazole angle
C1R  C2R  C3R  ga_8   ;  from ADE sugar angle
C1R  C2R  O7R  ga_9   ;  from ADE sugar angle
C1R  O6R  C4R  ga_10  ;  from ADE sugar angle
C2R  O6R  C4R  ga_9   ;  from ADE sugar angle
C2R  C3R  C4R  ga_8   ;  from ADE sugar angle
C2R  O7R  H3A  ga_12  ;  from ADE sugar angle
C3R  C2R  O7R  ga_9   ;  from ADE sugar angle
C3R  C4R  C5R  ga_8   ;  from ADE sugar angle
C3R  C4R  O6R  ga_9   ;  from ADE sugar angle
C4R  C5R  O8R  ga_9   ;  from ADE sugar angle
C1P  C2P  C3P  ga_13  ;  amide linkage angle
C57  C56  C55  ga_13  ;  amide linkage angle
C57  N59  HAC  ga_23  ;  from GLN angle
N59  C57  O58  ga_33  ;  from GLN angle
C56  C57  N59  ga_19  ;  from GLN angle
O58  C57  C56  ga_30  ;  from GLN angle
C1P  N59  C57  ga_31  ;  from force field angle definitions
C1P  N59  HAC  ga_18  ;  from force field angle definitions
C1P  N59  N59  ga_15  ;  from force field angle definitions
C5B  C4B  C4B  ga_25  ;  from PHE C-C-H angle
C9B  C4B  C4B  ga_25  ;  from PHE C-C-H angle
C6B  C7B  C7B  ga_25  ;  from PHE C-C-H angle
C8B  C7B  C7B  ga_25  ;  from PHE C-C-H angle
N1B  C2B  H2B  ga_36  ;  from ADE N-C-H angle
N3B  C2B  H2B  ga_36  ;  from ADE N-C-H angle
C9  C10  C10  ga_25  ;  corrin ring C-C10-H angle
C11  C10  H10  ga_20  ;  corrin ring C-C10-H angle
C5R  O8R  CLB  ga_12  ;  for LYS-B12 bridge (just replaces O8R H atom with CLB)

; standard lysine angle topology
-C  N  H  ga_32  ;  Standard LYS (lysine)
-C  N  CA  ga_31  ;  Standard LYS (lysine)
H  N  CA  ga_18  ;  Standard LYS (lysine)
N  CA  CB  ga_13  ;  Standard LYS (lysine)
N  CA  C  ga_13  ;  Standard LYS (lysine)
CB  CA  C  ga_13  ;  Standard LYS (lysine)
CA  CB  CD  ga_15  ;  Standard LYS (lysine)
CB  CG  CD  ga_15  ;  Standard LYS (lysine)
CG  CD  CE  ga_15  ;  Standard LYS (lysine)
CD  CE  NZ  ga_15  ;  Standard LYS (lysine)
CE  NZ  H21  ga_11  ;  Standard LYS (lysine)
CE  NZ  CLB  ga_6  ;  Modification from LYS (CLB from NZ H atom)
H2B  CLB  ga_13  ;  Modification from LYS (CLB from NZ H atom)
CA  C  O  ga_30  ;  Standard LYS (lysine)
CA  C  +N  ga_19  ;  Standard LYS (lysine)
O  C  +N  ga_33  ;  Standard LYS (lysine)

; additional CLB-OLB angle linkages
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; OLBR CLBR OR8 ga_33 ; new OLBR-CLBR linkage angles
; OLBR N2 ga_33 ; new OLBR-CLBR linkage angles
; OR8 CLBR N2 ga_33 ; new OLBR-CLBR linkage angles
[ impropers ]
; ai aj ak al gromos type
C3R C8B C2B N1B gi_1 ; dimethylbenzimidazole improper for planarity
N1B C8B C9B N3B gi_1 ; dimethylbenzimidazole improper for planarity
C9B N1B C7B C9B gi_1 ; dimethylbenzimidazole improper for planarity
C8B C7B C6B C5B gi_1 ; dimethylbenzimidazole improper for planarity
C8B C9B N3B C2B gi_1 ; dimethylbenzimidazole improper for planarity
C7B C9B C4B C8B gi_1 ; dimethylbenzimidazole improper for planarity
C7B C6B C5B C4B gi_1 ; dimethylbenzimidazole improper for planarity
C6B C5B C4B C9B gi_1 ; dimethylbenzimidazole improper for planarity
C5B C4B N3B C8B gi_1 ; dimethylbenzimidazole improper for planarity
C9B C8B C7B C6B gi_1 ; dimethylbenzimidazole improper for planarity
N1B C8B C9B gi_1 ; dimethylbenzimidazole improper for planarity
N3B C2B C1B gi_1 ; dimethylbenzimidazole improper for planarity
C2B N1B C9B gi_1 ; dimethylbenzimidazole improper for planarity
C5B C4B C6B C5B gi_1 ; dimethylbenzimidazole improper for planarity
C6C C7B C8B C6B gi_1 ; dimethylbenzimidazole improper methyl groups
C7B C8B C6B gi_1 ; HEMC improper definition
C8B C9B C5B H4B gi_1 ; HEMC improper definition
C7B C8B C6B H7B gi_1 ; HEMC improper definition
N22 C9 C10 C11 gi_1 ; HEMC-based conjugated corrin ring improper planarity
N23 C11 C10 C9 gi_1 ; HEMC-based conjugated corrin ring improper planarity
N24 C14 C15 C16 gi_1 ; HEMC-based conjugated corrin ring improper planarity
C5 C4 C3 C5 gi_1 ; core ring on-Csp2 methyl group improper planarity
C16 C15 C14 C13 gi_1 ; HEMC-based conjugated corrin ring improper planarity
C11 C15 C14 C10 gi_1 ; HEMC-based conjugated corrin ring improper planarity
N22 C10 C9 C8 gi_1 ; HEMC-based conjugated corrin ring improper planarity
N23 C11 C10 C9 gi_1 ; HEMC-based conjugated corrin ring improper planarity
N24 C14 C15 C16 gi_1 ; HEMC-based conjugated corrin ring improper planarity

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N59 C1P C2P C3 gd_34 ; amide linkage torsion terms
N59 C1P C2P C3P gd_34 ; amide linkage torsion terms
C2P C1P N59 C57 gd_34 ; amide linkage torsion terms
C56 C57 N59 C1P gd_14 ; amide linkage torsion terms
C55 C56 C57 N59 gd_40 ; amide linkage torsion terms
C17 C55 C56 C57 gd_40 ; amide linkage torsion terms
C5 C4 N21 C1 gd_14 ; corrin ring sp3-containing torsions
C10 C9 N22 C6 gd_14 ; corrin ring sp3-containing torsions
C5 C6 N22 C9 gd_14 ; corrin ring sp3-containing torsions
C15 C14 N23 C11 gd_14 ; corrin ring sp3-containing torsions
C10 C11 N23 C14 gd_14 ; corrin ring sp3-containing torsions
C15 C16 N24 C19 gd_14 ; corrin ring sp3-containing torsions
C4 N21 C1 C2 gd_40 ; corrin ring sp3-containing torsions
C18 C19 N24 C16 gd_40 ; corrin ring sp3-containing torsions
N22 C6 C5 C4 gd_33 ; corrin ring sp3-containing torsions
N23 C11 C10 C9 gd_33 ; corrin ring sp3-containing torsions
C19 C18 C17 C55 gd_34 ; corrin ring sp3-containing torsions
C55 C17 C16 C15 gd_40 ; corrin ring sp3-containing torsions
C17 C16 C15 C14 gd_10 ; corrin ring sp3-containing torsions
C16 C15 C14 C13 gd_10 ; corrin ring sp3-containing torsions
C15 C14 C13 C12 gd_40 ; corrin ring sp3-containing torsions
C6 C7 C8 C9 gd_34 ; corrin ring sp3-containing torsions
C9 C7 C6 C5 gd_34 ; corrin ring sp3-containing torsions
C30 C3 C2 C1 gd_34 ; corrin ring sp3-containing torsions
C11 C12 C13 C14 gd_34 ; corrin ring sp3-containing torsions
C13 C12 C11 C10 gd_34 ; corrin ring sp3-containing torsions
C10 C9 C8 C7 gd_10 ; corrin ring sp3-containing torsions
C5 C4 C3 C30 gd_34 ; corrin ring sp3-containing torsions
C3 C2 C1 C19 gd_34 ; corrin ring sp3-containing torsions

; standard lysine torsion topology

-CA -C N CA gd_14 ; Standard LYS (lysine)
-C N CA C gd_39 ; Standard LYS (lysine)
N CA CB CG gd_34 ; Standard LYS (lysine)
N CA C +N gd_40 ; Standard LYS (lysine)
CA CB CO CD gd_34 ; Standard LYS (lysine)
CB CG CD CE gd_34 ; Standard LYS (lysine)
CA CB CE NZ gd_34 ; Standard LYS (lysine)
CD CE NZ HE1 gd_29 ; Standard LYS (lysine)
C4R C5R O8R CLB gd_23 ; LYS-B12 linkage dihedral terms
O8R CLB NZ CE gd_14 ; LYS-B12 linkage dihedral terms
CLB CLB NZ CE gd_14 ; LYS-B12 linkage dihedral terms
C9B N3B FE N21 gd_38 ; THIS IS NEW!!!
N3B FE N21 C1 gd_38 ; THIS IS NEW!!!
N3B FE N22 C6 gd_38 ; THIS IS NEW!!!
N3B FE N23 C11 gd_38 ; THIS IS NEW!!!
N3B FE N24 C16 gd_38 ; THIS IS NEW!!!

; Use of LYB, which employs the pdb2gmx method for sewing the peptide chain together,
; requires the addition of this very new, bulky amino acid to aminoacids.dat.

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[ BCN ]
;
; cyanocobalamin based on the HEMC CO parameters
;
[ atoms ]
C27  C      0.38000  0 ; from GLN residue
O28  O      -0.38000  0 ; from GLN residue
N29  NT     -0.83000  0 ; from GLN residue
HAE   H      0.41500  0 ; from GLN residue
HAD   H      0.41500  0 ; from GLN residue
C32  C      0.38000  1 ; from GLN residue
O34  O      -0.38000  1 ; from GLN residue
N33  NT     -0.83000  1 ; from GLN residue
HAG   H      0.41500  1 ; from GLN residue
HAF   H      0.41500  1 ; from GLN residue
C38  C      0.38000  2 ; from GLN residue
O39  O      -0.38000  2 ; from GLN residue
N40  NT     -0.83000  2 ; from GLN residue
HAI   H      0.41500  2 ; from GLN residue
HAH   H      0.41500  2 ; from GLN residue
C43  C      0.38000  3 ; from GLN residue
O44  O      -0.38000  3 ; from GLN residue
N45  NT     -0.83000  3 ; from GLN residue
HAK   H      0.41500  3 ; from GLN residue
HAJ   H      0.41500  3 ; from GLN residue
C50  C      0.38000  4 ; from GLN residue
O51  O      -0.38000  4 ; from GLN residue
N52  NT     -0.83000  4 ; from GLN residue
HAM   H      0.41500  4 ; from GLN residue
HAL   H      0.41500  4 ; from GLN residue
C61  C      0.38000  5 ; from GLN residue
O63  O      -0.38000  5 ; from GLN residue
N62  NT     -0.83000  5 ; from GLN residue
HAI   H      0.41500  5 ; from GLN residue
HAI   H      0.41500  5 ; from GLN residue
C20  CH3    0.00000  6 ; methyl group
C25  CH3    0.00000  7 ; methyl group
C36  CH3    0.00000  8 ; methyl group
C46  CH3    0.00000  9 ; methyl group
C47  CH3    0.00000 10 ; methyl group
C54  CH3    0.00000 11 ; methyl group
C42  CH2    0.00000 12 ; non-polar CHn fragments
C30  CH2    0.00000 13 ; non-polar CHn fragments
C31  CH2    0.00000 14 ; non-polar CHn fragments
C37  CH2    0.00000 15 ; non-polar CHn fragments
C41  CH2    0.00000 16 ; non-polar CHn fragments
C42  CH2    0.00000 17 ; non-polar CHn fragments
C45  CH2    0.00000 18 ; non-polar CHn fragments
C49  CH2    0.00000 19 ; non-polar CHn fragments
C56  CH2    0.00000 20 ; non-polar CHn fragments
C60  CH2    0.00000 21 ; non-polar CHn fragments
C41  CH1    0.15000 12 ; C2*-O2*-H2* from ADE
O7R   OA     -0.54800 13 ; C2*-O2*-H2* from ADE
HAA   H      0.39800 14 ; C2*-O2*-H2* from ADE
C1R   CH1    0.20000 15 ; C1*-O4*-C4* from ADE
O6R   OA     -0.36000 16 ; C1*-O4*-C4* from ADE
C4R   CH1    0.16000 17 ; C1*-O4*-C4* from ADE
C3R   CH1    0.00000 18 ; C3* from ADE
C5R   CH2    0.15000 19 ; C2*-O2*-H2* from ADE
O8R   OA     -0.54800 20 ; C2*-O2*-H2* from ADE
HAB   H      0.39800 21 ; C2*-O2*-H2* from ADE
P      P      2.20000 22 ; PO3+O3* fragment from ADE
O2    OA     -0.80000 23 ; PO3+O3* fragment from ADE
O4    OM     -1.00000 24 ; PO3+O3* fragment from ADE
O5    OM     -1.00000 25 ; PO3+O3* fragment from ADE
O3    OA     -0.80000 26 ; PO3+O3* fragment from ADE
C2P   CH1    0.35000 27 ; non-polar CHn fragments
C3P   CH3    0.00000 28 ; non-polar CHn fragments
C3P   CH3    0.00000 29 ; non-polar CHn fragments
N59   N      -0.28000 25 ; tempered GLN fragment charges
HAC   H      0.28000 26 ; tempered GLN fragment charges
C57   C      0.38000 25 ; tempered GLN fragment charges
O58   O      -0.38000 25 ; tempered GLN fragment charges
C5B   C      0.00000 26 ; dimethylbenzimidazole C-CH3 group (non-polar)
C5M   CH3    0.00000 27 ; dimethylbenzimidazole C-CH3 group (non-polar)
C6B   C      0.00000 28 ; dimethylbenzimidazole C-CH3 group (non-polar)
C6M   CH3    0.00000 29 ; dimethylbenzimidazole C-CH3 group (non-polar)
C4R   CH2    0.14000 28 ; dimethylbenzimidazole aromatic C-H from TRP, PHE
C4B   CH2    0.14000 29 ; dimethylbenzimidazole aromatic C-H from TRP, PHE
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H7B H 0.14000 29 ; dimethylbenzimidazole aromatic C-H from TRP, PHE
N3B NR -0.55000 30 ; dimethylbenzimidazole polar aromatic NC fragment
C9B C 0.20000 30 ; dimethylbenzimidazole polar aromatic NC fragment
N1B NR -0.30000 31 ; dimethylbenzimidazole polar aromatic NC fragment
C8B C 0.20000 31 ; dimethylbenzimidazole polar aromatic NC fragment
H2B H 0.20000 32 ; dimethylbenzimidazole aromatic C-H from TRP, PHE
C5 C -0.05000 33 ; C-CH3 group (non-polar)
C15 C -0.05000 34 ; C-CH3 group (non-polar)
C35 CH3 0.00000 33 ; C-CH3 group (non-polar)
C15 CH0 0.20000 35 ; HEMC Fe-N group
C1 CH0 0.22000 36 ; non-polar HEMC-derived corrin atoms
C2 CH0 0.00000 36 ; non-polar HEMC-derived corrin atoms
C3 CH1 0.00000 36 ; non-polar HEMC-derived corrin atoms
C4 C 0.38000 36 ; non-polar HEMC-derived corrin atoms
C6 C 0.29000 37 ; non-polar HEMC-derived corrin atoms
C7 CH1 0.00000 37 ; non-polar HEMC-derived corrin atoms
C8 CH1 0.00000 37 ; non-polar HEMC-derived corrin atoms
C9 C 0.35000 37 ; non-polar HEMC-derived corrin atoms
C16 C 0.38000 38 ; non-polar HEMC-derived corrin atoms
C17 CH0 0.00000 38 ; non-polar HEMC-derived corrin atoms
C18 CH1 0.00000 38 ; non-polar HEMC-derived corrin atoms
C19 CH1 0.24000 38 ; non-polar HEMC-derived corrin atoms
C11 C 0.35000 39 ; non-polar HEMC-derived corrin atoms
C12 CH0 0.00000 39 ; non-polar HEMC-derived corrin atoms
C13 CH1 0.00000 39 ; non-polar HEMC-derived corrin atoms
C14 C 0.24000 39 ; non-polar HEMC-derived corrin atoms
C10 C -0.24000 40 ; aromatic C-H from TRP, PHE
H10 H 0.14000 40 ; aromatic C-H from TRP, PHE

; cyano group addition to the original B12 topology
;
C1N C 0.04000 41 ; CN group on Fe
N1C N -0.42000 41 ; CN group on Fe

; Since CO is not defined as an atom in GROMOSxx, CO is converted to FE and the HEME values are employed. This is a workaround due for proper implementation.

[ bonds ]
; ai aj gromos type
C26 C27 gb_27 ; from GLN fragment 0
C27 O28 gb_5 ; from GLN
C27 N29 gb_9 ; from GLN
N29 HAB gb_2 ; from GLN
N29 HAD gb_2 ; from GLN
C31 C32 gb_27 ; from GLN fragment 1
C32 O34 gb_5 ; from GLN
C32 N33 gb_9 ; from GLN
N33 HAG gb_2 ; from GLN
N33 HAF gb_2 ; from GLN
C37 C38 gb_27 ; from GLN fragment 2
C38 O39 gb_5 ; from GLN
C38 N40 gb_9 ; from GLN
N40 HAO gb_2 ; from GLN
N40 HAN gb_2 ; from GLN
C42 C43 gb_27 ; from GLN fragment 3
C43 O44 gb_5 ; from GLN
C43 N45 gb_9 ; from GLN
N45 HAK gb_2 ; from GLN
N45 HAJ gb_2 ; from GLN
C49 C50 gb_27 ; from GLN fragment 4
C50 O51 gb_5 ; from GLN
C50 N52 gb_9 ; from GLN
N52 HAH gb_2 ; from GLN
N52 HAJ gb_2 ; from GLN
C60 C61 gb_27 ; from GLN fragment 5
C61 O63 gb_5 ; from GLN
C61 N62 gb_9 ; from GLN
N62 HAO gb_2 ; from GLN
N62 HAN gb_2 ; from GLN
FR N21 gb_35 ; FE-N bond from HEMC
FR N22 gb_35 ; FE-N bond from HEMC
FR N23 gb_35 ; FE-N bond from HEMC
FR N24 gb_35 ; FE-N bond from HEMC
FR N3B gb_37 ; FE-N3b bond from HEMC not in corrin ring
P O2 gb_28 ; from ADE phosphate
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P O4 gb_24; from ADE phosphate
P O5 gb_24; from ADE phosphate
P O3 gb_28; from ADE phosphate
N21 C1 gb_21; corrin ring N-CHn bonds
N21 C4 gb_14; corrin ring N-C bonds
N22 C6 gb_14; corrin ring N-C bonds
N22 C9 gb_14; corrin ring N-C bonds
N23 C11 gb_14; corrin ring N-C bonds
N23 C14 gb_14; corrin ring N-C bonds
N24 C16 gb_14; corrin ring N-C bonds
N24 C19 gb_21; corrin ring N-CHn bonds
C30 C31 gb_27; CH2-CH2 bonds
C41 C42 gb_27; CH2-CH2 bonds
C48 C49 gb_27; CH2-CH2 bonds
C55 C56 gb_27; CH2-CH2 bonds
N1B C1R gb_22; sugar bonds from ADE
C1R C2R gb_26; sugar bonds from ADE
C2R O7R gb_20; sugar bonds from ADE
O7R HAA gb_1; sugar bonds from ADE
C2R C3R gb_26; sugar bonds from ADE
C2R C4R gb_26; sugar bonds from ADE
C3R O2 gb_20; sugar bonds from ADE
C4R C5R gb_26; sugar bonds from ADE
C5R O8R gb_20; sugar bonds from ADE
O8R HAB gb_1; sugar bonds from ADE
C4R O6R gb_20; sugar bonds from ADE
O6R C1R gb_20; sugar bonds from ADE
C1P N59 gb_9; amide corrin - phosphate linkage
C1P C2P gb_27; amide corrin - phosphate linkage
C2P C3P gb_27; amide corrin - phosphate linkage
C2P O3 gb_20; amide corrin - phosphate linkage
N59 HAC gb_2; amide corrin - phosphate linkage
N59 C57 gb_9; amide corrin - phosphate linkage
C87 C68 gb_6; amide corrin - phosphate linkage
N1B C2B gb_10; dimethylbenzimidazole ring
C2B N3B gb_10; dimethylbenzimidazole ring
C2B H2B gb_3; dimethylbenzimidazole ring
N3B C9B gb_10; dimethylbenzimidazole ring
C9B C4B gb_16; dimethylbenzimidazole ring
C6B C7B gb_16; dimethylbenzimidazole ring
C6B H4B gb_3; dimethylbenzimidazole ring
C5B C6B gb_16; dimethylbenzimidazole ring
C6B C7B gb_16; dimethylbenzimidazole ring
C6B C6M gb_27; dimethylbenzimidazole ring
C7B C8B gb_16; dimethylbenzimidazole ring
C7B H7B gb_3; dimethylbenzimidazole ring
C8B N1B gb_10; dimethylbenzimidazole ring
C9B C9B gb_16; dimethylbenzimidazole ring
C1 C2 gb_27; corrin ring carbon framework
C1 C2 gb_27; corrin ring carbon framework
C2 C3 gb_27; corrin ring carbon framework
C2 C25 gb_27; corrin ring carbon framework
C2 C26 gb_27; corrin ring carbon framework
C3 C4 gb_27; corrin ring carbon framework
C3 C20 gb_27; corrin ring carbon framework
C4 C5 gb_17; corrin ring carbon framework
C5 C6 gb_17; corrin ring carbon framework
C5 C35 gb_27; corrin ring carbon framework
C6 C7 gb_27; corrin ring carbon framework
C7 C8 gb_27; corrin ring carbon framework
C7 C37 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C36 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
C8 C9 gb_27; corrin ring carbon framework
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C18   C19    gb_27   ;  corrin ring carbon framework
C18   C60    gb_27   ;  corrin ring carbon framework
C19   C1     gb_27   ;  corrin ring carbon framework
C10   H10    gb_3    ;  corrin ring C10-H10 bond

;  cyano group addition to the original B12 topology
;
FE   C1N    gb_30    ;  cyano group on the Fe
C1N   N1C    gb_4     ;  cyano group on the Fe

[ exclusions ]
;
ai    aj
FE    N1C   ;  new add
FE    C1    ;  new add
FE    C2
FE    C3
FE    C5
FE    C7
FE    C8
FE    C10
FE    C12
FE    C13
FE    C15
FE    C17
FE    C18
FE    C20
N21   C24
N21   C26
N21   C30
N21   C35
N21   C6
N21   C9
N21   C11
N21   C14
N21   C16
N21   C19
N21   C10
N22   C1
N22   C4
N22   C6
N22   C9
N22   C46
N22   C47
N23   C16
N23   C19
N23   C1
N23   C4
N23   C6
N23   C9
N23   C46
N23   C47
N24   C4
N24   C5
N24   C6
N24   C9
N24   C10
N24   C11
N24   C14
N24   C55
N24   C54
N24   C60
C1R   C7B
C1R   C9B
C1R   N3B
N1B   C6B
N1B   C4B
C8B   C5B
C8B   C5N
C8B   C6M
C7B   C4B
C7B   N3B
C7B   C2B
C2B   C9B
C5B   C2B
C5M   C6N
C1   C30   ;  HEMC-based C framework exclusions
C1   C5    ;  HEMC-based C framework exclusions
HAG N33 HAP ga_24 ; from GLN
C7 C37 C38 ga_15 ; from GLN, fragment 3
C37 C38 C39 ga_30 ; from GLN
C37 C38 N40 ga_19 ; from GLN
O39 C38 C38 ga_15 ; from GLN, fragment 3
C37 C38 O39 ga_30 ; from GLN
C37 C38 N40 ga_19 ; from GLN
O39 C38 N40 ga_33 ; from GLN
C38 N40 HAI ga_23 ; from GLN
C38 N40 HAH ga_23 ; from GLN
HAI N40 HAH ga_24 ; from GLN
C41 C42 C43 ga_15 ; from GLN, fragment 4
C42 C43 C44 ga_30 ; from GLN
C42 C43 N45 ga_19 ; from GLN
O44 C43 C43 ga_30 ; from GLN
C42 C43 N45 ga_33 ; from GLN
C43 N45 HAK ga_23 ; from GLN
C43 N45 HAJ ga_23 ; from GLN
HAK N45 HAJ ga_24 ; from GLN
C48 C49 C50 ga_15 ; from GLN, fragment 5
C49 C50 O51 ga_30 ; from GLN
C49 C50 N52 ga_19 ; from GLN
O52 C50 N52 ga_33 ; from GLN
C50 N52 HAM ga_23 ; from GLN
C50 N52 HAL ga_23 ; from GLN
HAL N52 HAL ga_24 ; from GLN
C18 C60 C61 ga_15 ; from GLN, fragment 6
C60 C61 O63 ga_30 ; from GLN
C60 C61 N62 ga_19 ; from GLN
O63 C61 N62 ga_33 ; from GLN
C61 N62 HAO ga_23 ; from GLN
C61 N62 HAN ga_23 ; from GLN
HAO N62 HAO ga_24 ; from GLN
C18 C60 C61 ga_15 ; from GLN, fragment 6
C60 C61 O63 ga_30 ; from GLN
C60 C61 N62 ga_19 ; from GLN
O63 C61 N62 ga_33 ; from GLN
C61 N62 HAO ga_23 ; from GLN
C61 N62 HAN ga_23 ; from GLN
HAO N62 HAO ga_24 ; from GLN
N21 FE N22 ga_2 ; corrin ring Fe-N angle
N21 FE N24 ga_2 ; corrin ring Fe-N angle
N23 FE N23 ga_2 ; corrin ring Fe-N angle
N23 FE N24 ga_2 ; corrin ring Fe-N angle
N21 FE N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
N21 N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
N23 N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
N23 FE N38 ga_2 ; corrin-Fe-dimethylbenzimidazole
FE N21 C1 ga_34 ; corrin Fe-N-C angles (based on HEMC)
FE N21 C4 ga_34 ; corrin Fe-N-C angles (based on HEMC)
FE N22 C6 ga_34 ; corrin Fe-N-C angles (based on HEMC)
FE N22 C9 ga_34 ; corrin Fe-N-C angles (based on HEMC)
FE N23 C11 ga_34 ; corrin Fe-N-C angles (based on HEMC)
FE N23 C14 ga_34 ; corrin Fe-N-C angles (based on HEMC)
FE N24 C19 ga_34 ; corrin Fe-N-C angles (based on HEMC)
FE N38 C9B ga_34 ; Fe-dimethylbenzimidazole-N,C angle
FE N3B C9B ga_34 ; Fe-dimethylbenzimidazole-N,C angle
C8B C9B ga_7 ; angle containing C8B, see minimization issues discussion
N1B C8B C9B ga_7 ; angle containing C8B, see minimization issues discussion
C8B C9B N1B ga_7 ; angle containing C8B, see minimization issues discussion
C7B C8B N1B ga_39 ; angle containing C8B, see minimization issues discussion
C8B N1B C1R ga_37 ; angle containing C8B, see minimization issues discussion
C4B C8B N1B ga_27 ; angle containing C8B, see minimization issues discussion
C6B C8B N1B ga_27 ; angle containing C8B, see minimization issues discussion
C7B C8B C9B ga_27 ; angle containing C8B, see minimization issues discussion
N21 C1 C2 ga_13 ; corrin ring-specific but HEMC-derived angles
N22 C2 C3 ga_13 ; corrin ring-specific but HEMC-derived angles
N21 C4 C3 ga_33 ; corrin ring-specific but HEMC-derived angles
N21 C4 C3 ga_33 ; corrin ring-specific but HEMC-derived angles
C4 N21 C1 ga_6 ; corrin ring-specific but HEMC-derived angles
C5 C4 C3 ga_33 ; corrin ring-specific but HEMC-derived angles
C9 C9 N21 ga_6 ; corrin ring-specific but HEMC-derived angles
N22 C6 C5 ga_33 ; corrin ring-specific but HEMC-derived angles
N22 C6 C5 ga_33 ; corrin ring-specific but HEMC-derived angles
N22 C6 C5 ga_33 ; corrin ring-specific but HEMC-derived angles
N22 C6 C5 ga_33 ; corrin ring-specific but HEMC-derived angles
C9 C9 N22 ga_6 ; corrin ring-specific but HEMC-derived angles
C10 C9 N22 ga_33 ; corrin ring-specific but HEMC-derived angles
N23 C11 C12 ga_33 ; corrin ring-specific but HEMC-derived angles
N23 C11 C12 ga_33 ; corrin ring-specific but HEMC-derived angles
N23 C11 C12 ga_33 ; corrin ring-specific but HEMC-derived angles
N24 C16 C15 ga_33 ; corrin ring-specific but HEMC-derived angles
C14 N24 C16 ga_6 ; corrin ring-specific but HEMC-derived angles
C14 N24 C16 ga_6 ; corrin ring-specific but HEMC-derived angles
C14 N24 C16 ga_6 ; corrin ring-specific but HEMC-derived angles
C17 C16 N24 ga_33 ; corrin ring-specific but HEMC-derived angles
C14 N24 ga_33 ; corrin ring-specific but HEMC-derived angles
C14 N24 ga_33 ; corrin ring-specific but HEMC-derived angles
C13 O2 P ga_26 ; phosphate angle from ADE
O2 P O3 ga_5 ; phosphate angle from ADE
O2 P O4 ga_14 ; phosphate angle from ADE
O2 P O5 ga_14 ; phosphate angle from ADE
O3 P O4 ga_14 ; phosphate angle from ADE
O3    P     O5    ga_14   ;  phosphate angle from ADE
O4    P     O5    ga_29   ;  phosphate angle from ADE
P     O3    C2P   ga_26   ;  phosphate angle from ADE
O2    P     O3    ga_9    ;  phosphate oxygen to CHn carbons from ADE
O4    P     O3    ga_29   ;  phosphate angle from ADE
C2    P     C3P   ga_9    ;  phosphate oxygen to CHn carbons from ADE
C1    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C1    C2    C3    ga_13   ;  CHn-CHn-CHn angles
C1    C19   C18   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C19   ga_13   ;  CHn-CHn-CHn angles
C2    C1    C20   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C30   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C25   ga_13   ;  CHn-CHn-CHn angles
C3    C2    C26   ga_13   ;  CHn-CHn-CHn angles
C3    C30   C31   ga_13   ;  CHn-CHn-CHn angles
C7    C8    C41   ga_13   ;  CHn-CHn-CHn angles
C8    C41   C42   ga_13   ;  CHn-CHn-CHn angles
C12   C13   C48   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C46   ga_13   ;  CHn-CHn-CHn angles
C13   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C13   C48   C49   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C19   ga_13   ;  CHn-CHn-CHn angles
C17   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C17   C55   C56   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C54   ga_13   ;  CHn-CHn-CHn angles
C18   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C19   C18   C60   ga_13   ;  CHn-CHn-CHn angles
C25   C26   C2   ga_13   ;  CHn-CHn-CHn angles
C46   C12   C47   ga_13   ;  CHn-CHn-CHn angles
C54   C17   C55   ga_13   ;  CHn-CHn-CHn angles
C36   C7    C37   ga_13   ;  CHn-CHn-CHn angles
C2    C3    C4    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C3    C30   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C8    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C7    C8    C9    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C36   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C8    C7    C37   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C9    C8    C41   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C13   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C46   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C47   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C12   C13   C14   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C14   C15   C16   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C18   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C16   C17   C54   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C17   C18   C55   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C18   C19   C14   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4    C5    C6    ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C9    C10   C11   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C11   C12   C13   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C5M   C5B   C4B   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C5M   C5B   C6B   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6M   C6B   C5B   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C6M   C6B   C7B   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C4B   C5B   C6B   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C5B   C4B   C9B   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
C5B   C6B   C7B   ga_15   ;  sp3-sp3-sp2 corrin ring carbon angle
N1B   C1R   C2R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C1R   O6R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C2R   O6R   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1B   C2B   N3B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N2B   N3B   C4B   ga_9    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N2B   N3B   C2B   ga_7    ;  from ADE Nsp2-containing dimethylbenzimidazole angle
N1R   C2R   C3R   ga_8    ;  from ADE sugar angle
C1R   C2R   O7R   ga_9    ;  from ADE sugar angle
C1R   O6R   C4R   ga_10   ;  from ADE sugar angle
C2R   C1R   O6R   ga_9    ;  from ADE sugar angle
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C2R  C3R  C4R  ga_8 ; from ADE sugar angle
C2R  O7R  HAA  ga_12 ; from ADE sugar angle
C3R  O7R  O9R  ga_9 ; from ADE sugar angle
C3R  C4R  C5R  ga_8 ; from ADE sugar angle
C3R  C4R  O6R  ga_9 ; from ADE sugar angle
C4R  C5R  O9R  ga_9 ; from ADE sugar angle
C5R  O8R  HAB  ga_12 ; from ADE sugar angle
C5R  C4R  O6R  ga_9 ; from ADE sugar angle
C1P  C2P  C3P  ga_13 ; amide linkage angle
C57  N59  HAC  ga_23 ; from GLN angle
N59  C57  O58  ga_33 ; from GLN angle
C57  N59  ga_19 ; from GLN angle
C57  C56  O58  N59  ga_1 ; from GLN angle
N62  HAO  HAN  C61  ga_1 ; from GLN improper torsion definition
C61  O63  N62  C60  ga_1 ; from GLN improper torsion definition
N52  HAM  HAL  C50  ga_1 ; from GLN improper torsion definition
C50  O51  N52  C49  ga_1 ; from GLN improper torsion definition
N45  HAK  HAJ  C43  ga_1 ; from GLN improper torsion definition
C43  O44  N45  C42  ga_1 ; from GLN improper torsion definition
N40  HAI  HAH  C38  ga_1 ; from GLN improper torsion definition
C38  O39  N40  C37  ga_1 ; from GLN improper torsion definition
N33  HAG  HAF  C32  ga_1 ; from GLN improper torsion definition
C32  O33  N34  C31  ga_1 ; from GLN improper torsion definition
N29  HAE  HAD  C26  ga_1 ; from GLN improper torsion definition
C26  O28  N29  C28  ga_1 ; from GLN improper torsion definition
C15  C16  C14  C53  ga_1 ; from ADE sugar angle
C15  C16  C14  C53  ga_1 ; from ADE sugar angle
C22  C5  C7  ga_1 ; from ADE sugar angle
C6  N22  C5  C7  ga_1 ; from ADE sugar angle

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C9    N22   C10   C8    gi_1    ;  corrin ring C sp2 planarity
C11   N23   C10   C12   gi_1    ;  corrin ring C sp2 planarity
C14   N23   C15   C13   gi_1    ;  corrin ring C sp2 planarity
C15   C14   C16   C53   gi_1    ;  corrin ring C sp2 planarity
C16   N24   C15   C17   gi_1    ;  corrin ring C sp2 planarity
C10   C9    C11   H10   gi_1    ;  corrin ring C10 planarity
C18   C17   C19   C60   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
C19   N24   C18   C1    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
C3    C2    C30   C4    gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
C8    C9    C7    C41   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
C13   C14   C12   C48   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
C2P   C1P   O3    C3P   gi_2    ;  corrin ring C atom sp3 tetrahedral geometry
C1R   N1B   C2R   O6R   gi_2    ;  sugar C atom tetrahedral geometry
C2R   O7R   C3R   C1R   gi_2    ;  sugar C atom tetrahedral geometry
C3R   C5R   O6R   C4R   gi_2    ;  sugar C atom tetrahedral geometry
C3R   C2R   O2    C4R   gi_2    ;  sugar C atom tetrahedral geometry
FE    C1    C4    N21   gi_3    ;  HEMC improper definition
FE    C6    C9    N22   gi_3    ;  HEMC improper definition
FE    C11   C14   N23   gi_3    ;  HEMC improper definition
FE    C16   C19   N24   gi_3    ;  HEMC improper definition

[ dihedrals ]
;  ai    aj    ak    al   gromos type
C3R   O2    P     O3    gd_20   ;  from ADE phosphate definition
C3R   O2    P     O3    gd_27   ;  from ADE phosphate definition
C2P   O3    P     O2    gd_20   ;  from ADE phosphate definition
C2P   O3    P     O2    gd_27   ;  from ADE phosphate definition
P     O3    C2P   C1P   gd_7    ;  from ADE phosphate definition
C2R   C3R   O2    P     gd_29   ;  from ADE sugar dihedrals
O8R   C5R   C4R   O6R   gd_8    ;  from ADE sugar dihedrals
O8R   C5R   C4R   O6R   gd_25   ;  from ADE sugar dihedrals
O8R   C5R   C4R   C3R   gd_17   ;  from ADE sugar dihedrals
O8R   C5R   C4R   C3R   gd_34   ;  from ADE sugar dihedrals
C3R   C4R   O6R   C1R   gd_29   ;  from ADE sugar dihedrals
C5R   C4R   C3R   C2R   gd_34   ;  from ADE sugar dihedrals
C5R   C4R   C3R   O2    gd_17   ;  from ADE sugar dihedrals
O6R   C1R   C2R   O7R   gd_18   ;  from ADE sugar dihedrals
O6R   C1R   C2R   C3R   gd_17   ;  from ADE sugar dihedrals
O6R   C1R   C2R   C3R   gd_34   ;  from ADE sugar dihedrals
C1R   C2R   C3R   C4R   gd_34   ;  from ADE sugar dihedrals
C1R   C2R   C3R   O2    gd_17   ;  from ADE sugar dihedrals
O7R   C2R   C3R   C4R   gd_17   ;  from ADE sugar dihedrals
O7R   C2R   C3R   O2    gd_18   ;  from ADE sugar dihedrals
C1R   C2R   O7R   HAA   gd_23   ;  from ADE sugar dihedrals
N1B   C1R   C2R   O7R   gd_17   ;  from ADE sugar dihedrals
N1B   C1R   O6R   C4R   gd_17   ;  from ADE sugar dihedrals
C2    C26   C27   N29   gd_40   ;  from GLN dihedral
C26   C27   N29   HAD   gd_14   ;  from GLN dihedral
C30   C31   C32   N33   gd_40   ;  from GLN dihedral
C31   C32   N33   HAF   gd_14   ;  from GLN dihedral
C7    C37   C38   N40   gd_40   ;  from GLN dihedral
C37   C38   N40   HAH   gd_14   ;  from GLN dihedral
C42   C43   N45   HAB   gd_2    ;  additional ADE-based sugar dihedral
C2    C26   C27   N29   gd_40   ;  from GLN dihedral
C26   C27   N29   HAD   gd_14   ;  from GLN dihedral
C30   C31   C32   N33   gd_40   ;  from GLN dihedral
C31   C32   N33   HAF   gd_14   ;  from GLN dihedral
C7    C37   C38   N40   gd_40   ;  from GLN dihedral
C37   C38   N40   HAH   gd_14   ;  from GLN dihedral
C42   C43   N45   HAB   gd_2    ;  additional ADE-based sugar dihedral
C2   C26   C27   N29   gd_40   ;  from GLN dihedral
N1B   C1R   C2R   O7R   gd_17   ;  from ADE sugar dihedrals
O6R   C1R   N1B   C8B   gd_16   ;  from ADE sugar dihedrals
C4R   C5R   O8R   HAB   gd_2    ;  additional ADE-based sugar dihedral
N1B   C1R   C2R   C3R   gd_17   ;  from ADE sugar dihedrals
N1B   C1R   C2R   O8R   gd_17   ;  from ADE sugar dihedrals
C2   C26   C27   N29   gd_40   ;  from GLN dihedral
C26   C27   N29   HAD   gd_14   ;  from GLN dihedral
C30   C31   C32   N33   gd_40   ;  from GLN dihedral
C31   C32   N33   HAF   gd_14   ;  from GLN dihedral
C7    C37   C38   N40   gd_40   ;  from GLN dihedral
C37   C38   N40   HAH   gd_14   ;  from GLN dihedral
C42   C43   N45   HAB   gd_2    ;  additional ADE-based sugar dihedral
C4    C5    C26   C27   gd_40   ;  from GLN dihedral
C5    C6    HAN   gd_14   ;  from GLN dihedral
C5M   C5B   C6B   C6M   gd_33   ;  dimethylbenzimidazole methyl dihedral fix
C4B   C5B   C6B   C6M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
C7B   C6B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
C9B   C4B   C5B   C5M   gd_10   ;  dimethylbenzimidazole methyl dihedral fix
C3S   C4    C5    C6    gd_10   ;  corrin ring methyl planarity
C3S   C4    C5    C6    gd_10   ;  corrin ring methyl planarity
C5S   C4    C5    C6    gd_10   ;  corrin ring methyl planarity
C3S   C4    C5    C6    gd_10   ;  corrin ring methyl planarity
C3S   C4    C5    C6    gd_10   ;  corrin ring methyl planarity
C3S   C4    C5    C6    gd_10   ;  corrin ring methyl planarity
C25 C2 C26 C27 gd_34 ; corrin ring HEMC derived CHn torsions
C2 C26 C27 C28 gd_34 ; corrin ring HEMC derived CHn torsions
C3 C30 C31 C32 gd_40 ; corrin ring HEMC derived CHn torsions
C30 C31 C32 C34 gd_40 ; corrin ring HEMC derived CHn torsions
C6 C7 C37 C38 gd_40 ; corrin ring HEMC derived CHn torsions
C36 C7 C37 C38 gd_40 ; corrin ring HEMC derived CHn torsions
C7 C37 C38 C39 gd_40 ; corrin ring HEMC derived CHn torsions
C7 C8 C41 C42 gd_9 ; corrin ring HEMC derived CHn torsions
C8 C41 C42 C43 gd_34 ; corrin ring HEMC derived CHn torsions
C41 C42 C43 C44 gd_40 ; corrin ring HEMC derived CHn torsions
C12 C13 C48 C49 gd_9 ; corrin ring HEMC derived CHn torsions
C13 C48 C49 C50 gd_34 ; corrin ring HEMC derived CHn torsions
C48 C49 C50 C51 gd_40 ; corrin ring HEMC derived CHn torsions
C16 C17 C55 C56 gd_40 ; corrin ring HEMC derived CHn torsions
C17 C55 C56 C57 gd_34 ; corrin ring HEMC derived CHn torsions
C17 C55 C56 C57 gd_40 ; corrin ring HEMC derived CHn torsions
C18 C60 C61 C63 gd_9 ; corrin ring HEMC derived CHn torsions
C18 C60 C61 C63 gd_34 ; corrin ring HEMC derived CHn torsions
N59 C1P C2P C3 gd_34 ; amide linkage torsion terms
N59 C1P C2P C3 gd_34 ; amide linkage torsion terms
N59 C1P C2P C3P gd_34 ; amide linkage torsion terms
C56 C57 C58 C59 gd_40 ; corrin ring sp3-containing torsions
C15 C14 C13 C12 gd_34 ; corrin ring sp3-containing torsions
C17 C18 C19 C1 gd_34 ; corrin ring sp3-containing torsions
C17 C18 C19 C1 gd_34 ; corrin ring sp3-containing torsions
C5 C4 N21 C1 gd_14 ; corrin ring sp3-containing torsions
C10 C9 N22 C6 gd_14 ; corrin ring sp3-containing torsions
C6 C9 C57 N59 gd_33 ; corrin ring sp3-containing torsions
C19 C18 C17 C55 gd_34 ; corrin ring sp3-containing torsions
C55 C17 C16 C15 gd_34 ; corrin ring sp3-containing torsions
C17 C18 C19 C1 gd_34 ; corrin ring sp3-containing torsions
C17 C18 C19 C1 gd_34 ; corrin ring sp3-containing torsions
C4 N21 C1 C2 gd_40 ; corrin ring sp3-containing torsions
C18 C19 C20 C16 gd_34 ; corrin ring sp3-containing torsions
C18 C19 C20 C16 gd_34 ; corrin ring sp3-containing torsions
C15 C16 C19 C1 gd_34 ; corrin ring sp3-containing torsions
C15 C16 C19 C1 gd_34 ; corrin ring sp3-containing torsions
C4 N21 C1 C2 gd_40 ; corrin ring sp3-containing torsions
C18 C19 C20 C16 gd_34 ; corrin ring sp3-containing torsions
C11 C10 C9 C8 gd_33 ; corrin ring sp3-containing torsions
C10 C9 C8 C7 gd_33 ; corrin ring sp3-containing torsions
C5 C4 C3 C2 gd_34 ; corrin ring sp3-containing torsions
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C8 C7 C6 C5 gd_34 ; corrin ring sp3-containing torsions
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C18 C19 C17 C16 gd_34 ; corrin ring sp3-containing torsions
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C10 C9 C8 C7 gd_10 ; corrin ring sp3-containing torsions
C5 C4 C3 C2 gd_34 ; corrin ring sp3-containing torsions
C11 C10 C9 C8 gd_33 ; corrin ring sp3-containing torsions
C4 C3 C2 C1 gd_34 ; corrin ring sp3-containing torsions
C18 C19 C17 C16 gd_34 ; corrin ring sp3-containing torsions
C9B N3B FE N21 gd_38 ; THIS IS NEW!!!
N3B FE N21 C1 gd_38 ; THIS IS NEW!!!
N3B FE N22 C6 gd_38 ; THIS IS NEW!!!
N3B FE N23 C11 gd_38 ; THIS IS NEW!!!
N3B FE N24 C16 gd_38 ; THIS IS NEW!!!
N3B FE C1N N1C gd_38 ; corrin ring sp3-containing torsions

; cyano group dihedral. imidazole-Fe-CN group torsion
; C9B N3B N21 C6 gd_38 ; THIS IS NEW!!!
N3B FE N21 C1 gd_38 ; THIS IS NEW!!!
N3B FE N22 C6 gd_38 ; THIS IS NEW!!!
N3B FE N23 C11 gd_38 ; THIS IS NEW!!!
N3B FE N24 C16 gd_38 ; THIS IS NEW!!!
N3B FE C1N N1C gd_38 ; corrin ring sp3-containing torsions
[ LCB ]

; lysine-cyanocobalamin residue file based on the HEMC CO parameters

; [ atoms ]
C27  C  0.38000  0  ; from GLN residue
O28  O  -0.38000  0  ; from GLN residue
N29  NT -0.83000  0  ; from GLN residue
H23  H  0.41500  0  ; from GLN residue
C32  C  0.38000  1  ; from GLN residue
O34  O  -0.38000  1  ; from GLN residue
N33  NT -0.83000  1  ; from GLN residue
H27  H  0.41500  1  ; from GLN residue
H28  H  0.41500  1  ; from GLN residue
C38  C  0.38000  2  ; from GLN residue
O39  O  -0.38000  2  ; from GLN residue
N40  NT -0.83000  2  ; from GLN residue
H32  H  0.41500  2  ; from GLN residue
H33  H  0.41500  2  ; from GLN residue
C43  C  0.38000  3  ; from GLN residue
O44  O  -0.38000  3  ; from GLN residue
N45  NT -0.83000  3  ; from GLN residue
H37  H  0.41500  3  ; from GLN residue
H38  H  0.41500  3  ; from GLN residue
C48  C  0.38000  4  ; from GLN residue
O49  O  -0.38000  4  ; from GLN residue
N50  NT -0.83000  4  ; from GLN residue
H43  H  0.41500  4  ; from GLN residue
H44  H  0.41500  4  ; from GLN residue
C50  C  0.38000  5  ; from GLN residue
O51  O  -0.38000  5  ; from GLN residue
N52  NT -0.83000  5  ; from GLN residue
H48  H  0.41500  5  ; from GLN residue
H49  H  0.41500  5  ; from GLN residue
C61  C  0.38000  6  ; methyl group
O63  O  -0.38000  6  ; methyl group
N59  N  -0.28000  6  ; tempered GLN fragment charges

C20  CH3  0.00000  7  ; methyl group
C25  CH3  0.00000  8  ; methyl group
C36  CH3  0.00000  9  ; methyl group
C46  CH3  0.00000 10  ; methyl group
C47  CH3  0.00000 11  ; methyl group
C54  CH3  0.00000 12  ; methyl group
C26  CH2  0.00000 13  ; non-polar CHn fragments
C30  CH2  0.00000 14  ; non-polar CHn fragments
C31  CH2  0.00000 15  ; non-polar CHn fragments
C37  CH2  0.00000 16  ; non-polar CHn fragments
C41  CH2  0.00000 17  ; non-polar CHn fragments
C42  CH2  0.00000 18  ; non-polar CHn fragments
C48  CH2  0.00000 19  ; non-polar CHn fragments
C49  CH2  0.00000 20  ; non-polar CHn fragments
C55  CH2  0.00000 21  ; non-polar CHn fragments
C56  CH2  0.00000 22  ; non-polar CHn fragments
C50  CH2  0.00000 23  ; non-polar CHn fragments
C60  CH2  0.00000 24  ; non-polar CHn fragments
C2R  CH1  0.15000 25  ; non-polar CHn fragments
O7R  OA  -0.54800 26  ; non-polar CHn fragments
H2A  H  0.39800 27  ; non-polar CHn fragments
C1R  CH1  0.20000 28  ; non-polar CHn fragments
O6R  OA  -0.36000 29  ; non-polar CHn fragments
C4R  CH1  0.16000 30  ; non-polar CHn fragments
C3R  CH1  0.00000 31  ; non-polar CHn fragments
C5R  CH1  0.00000 32  ; non-polar CHn fragments
C42  CH2  0.00000 33  ; non-polar CHn fragments
C49  CH2  0.00000 34  ; non-polar CHn fragments
C55  CH2  0.00000 35  ; non-polar CHn fragments
P  P  2.20000 36  ; PO3*O3* fragment from ADE
O2P  O  -0.80000 37  ; PO3*O3* fragment from ADE
O4  OM  -1.00000 38  ; PO3*O3* fragment from ADE
O5  OM  -1.00000 39  ; PO3*O3* fragment from ADE
O3  OA  -0.80000 40  ; PO3*O3* fragment from ADE
C2P  CH1  0.35000 41  ; non-polar CHn fragment
C3P  CH1  0.00000 42  ; non-polar CHn fragment
C1P  CH2  0.00000 43  ; non-polar CHn fragment
N59  N  -0.28000 44  ; tempered GLN fragment charges
### Table 1: Atom Information

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<th>Atom</th>
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<th>Z</th>
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<td>CN group on Fe</td>
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<tr>
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<td>Standard LYS (lysine) atom information</td>
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<td>Standard LYS (lysine) atom information</td>
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<tr>
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<td>aromatic C-H from TRP, PHE</td>
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<td>OLB</td>
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<td>this is the linkage carbon atom between LYS and B12</td>
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<tr>
<td>CN</td>
<td>0.04000</td>
<td>41</td>
<td></td>
<td>CN group on Fe</td>
</tr>
</tbody>
</table>

### Notes
- **bonds**
- CO is not defined as an atom in GROMOSxx, CO is converted to FE and the HEME.
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; ai   aj   gromos type
C26  C27  gb_27 ; from GLN fragment 0
C27  O28  gb_5  ; from GLN
C27  N29  gb_9  ; from GLN
N29  HAB  gb_2  ; from GLN
C31  C32  gb_27 ; from GLN fragment 1
C32  O34  gb_5  ; from GLN
C32  N33  gb_9  ; from GLN
N33  HAF  gb_2  ; from GLN
N33  HAE  gb_2  ; from GLN
C37  C38  gb_27 ; from GLN fragment 2
C38  O39  gb_5  ; from GLN
C38  N40  gb_9  ; from GLN
N40  HAG  gb_2  ; from GLN
N40  HAH  gb_2  ; from GLN
C42  C43  gb_27 ; from GLN fragment 3
C43  O44  gb_5  ; from GLN
C43  N45  gb_9  ; from GLN
N45  HAF  gb_2  ; from GLN
N45  HAE  gb_2  ; from GLN
C49  C50  gb_27 ; from GLN fragment 4
C50  O51  gb_5  ; from GLN
C50  N52  gb_9  ; from GLN
N52  HAF  gb_2  ; from GLN
N52  HAE  gb_2  ; from GLN
C60  C61  gb_27 ; from GLN fragment 5
C61  O63  gb_5  ; from GLN
C61  N62  gb_9  ; from GLN
N62  HAF  gb_2  ; from GLN
N62  HAE  gb_2  ; from GLN
FE    N21  gb_35 ; FE-N bond from HEMC
FE    N22  gb_35 ; FE-N bond from HEMC
FE    N23  gb_35 ; FE-N bond from HEMC
FE    N24  gb_35 ; FE-N bond from HEMC
FE    N3B  gb_37 ; FE-N3B bond from HEMC not in corrin ring
P     O2P  gb_28 ; from ADE phosphate
P     O4   gb_24 ; from ADE phosphate
P     O5   gb_24 ; from ADE phosphate
P     O3   gb_28 ; from ADE phosphate
N21  C1   gb_21 ; corrin ring N-CHn bonds
N21  C4   gb_14 ; corrin ring N-C bonds
N22  C6   gb_14 ; corrin ring N-C bonds
N22  C9   gb_14 ; corrin ring N-C bonds
N23  C11  gb_14 ; corrin ring N-C bonds
N23  C14  gb_14 ; corrin ring N-C bonds
N24  C16  gb_14 ; corrin ring N-C bonds
C19  gb_21 ; corrin ring N-CHn bonds
C30  C31  gb_27 ; CH2-CH2 bonds
C41  C42  gb_27 ; CH2-CH2 bonds
C48  C49  gb_27 ; CH2-CH2 bonds
C55  C56  gb_27 ; CH2-CH2 bonds
C56  C57  gb_27 ; CH2-CH2 bonds
N1B  C1R  gb_22 ; sugar bonds from ADE
C1R  C2R  gb_26 ; sugar bonds from ADE
C2R  O7R  gb_20 ; sugar bonds from ADE
O7R  HAA  gb_1  ; sugar bonds from ADE
C2R  C3R  gb_26 ; sugar bonds from ADE
C3R  C4R  gb_26 ; sugar bonds from ADE
C3R  O2P  gb_20 ; sugar bonds from ADE
C4R  C5R  gb_26 ; sugar bonds from ADE
C5R  O8R  gb_20 ; sugar bonds from ADE
C4R  O6R  gb_20 ; sugar bonds from ADE
O6R  gb_20 ; sugar bonds from ADE
C1P  N59  gb_9 ; amide corrin - phosphate linkage
C1P  C2P  gb_27 ; amide corrin - phosphate linkage
C2P  C3P  gb_27 ; amide corrin - phosphate linkage
C2P  O3  gb_20 ; amide corrin - phosphate linkage
N59  HAC  gb_2 ; amide corrin - phosphate linkage
N59  C57  gb_9 ; amide corrin - phosphate linkage
C57  O58  gb_5 ; amide corrin - phosphate linkage
N1B  C2B  gb_10 ; dimethylbenzimidazole ring
C2B  N3B  gb_10 ; dimethylbenzimidazole ring
C2B  H2B  gb_3 ; dimethylbenzimidazole ring
N3B  C9B  gb_10 ; dimethylbenzimidazole ring
C9B  C4B  gb_16 ; dimethylbenzimidazole ring
C4B  C5B  gb_16 ; dimethylbenzimidazole ring
C4B  H4B  gb_3 ; dimethylbenzimidazole ring
C5B  C6B   gb_16  ;  dimethylbenzimidazole ring
C5B  C5N   gb_27  ;  dimethylbenzimidazole ring
C6B  C7B   gb_16  ;  dimethylbenzimidazole ring
C6B  C6N   gb_27  ;  dimethylbenzimidazole ring
C7B  C8B   gb_16  ;  dimethylbenzimidazole ring
C7B  H7B   gb_3   ;  dimethylbenzimidazole ring
C8B  N1B   gb_10  ;  dimethylbenzimidazole ring
C8B  C9B   gb_16  ;  dimethylbenzimidazole ring
C1  C20   gb_27  ;  corrin ring carbon framework
C1  C2    gb_27  ;  corrin ring carbon framework
C2  C3     gb_27  ;  corrin ring carbon framework
C2  C25    gb_27  ;  corrin ring carbon framework
C2  C26    gb_27  ;  corrin ring carbon framework
C3  C4     gb_27  ;  corrin ring carbon framework
C3  C30    gb_27  ;  corrin ring carbon framework
C4  C5     gb_17  ;  corrin ring carbon framework
C5  C6     gb_17  ;  corrin ring carbon framework
C5  C35    gb_27  ;  corrin ring carbon framework
C6  C7     gb_27  ;  corrin ring carbon framework
C7  C8     gb_27  ;  corrin ring carbon framework
C8  C9     gb_27  ;  corrin ring carbon framework
C8  C41    gb_27  ;  corrin ring carbon framework
C9  C10    gb_17  ;  corrin ring carbon framework
C10  C11   gb_17  ;  corrin ring carbon framework
C11  C12   gb_27  ;  corrin ring carbon framework
C11  C47   gb_27  ;  corrin ring carbon framework
C12  C46   gb_27  ;  corrin ring carbon framework
C12  C13   gb_27  ;  corrin ring carbon framework
C13  C14   gb_27  ;  corrin ring carbon framework
C13  C48   gb_27  ;  corrin ring carbon framework
C14  C15   gb_17  ;  corrin ring carbon framework
C14  C16   gb_17  ;  corrin ring carbon framework
C15  C17   gb_27  ;  corrin ring carbon framework
C15  C53   gb_27  ;  corrin ring carbon framework
C16  C17   gb_27  ;  corrin ring carbon framework
C16  C37   gb_27  ;  corrin ring carbon framework
C16  C38   gb_27  ;  corrin ring carbon framework
C17  C18   gb_27  ;  corrin ring carbon framework
C17  C54   gb_27  ;  corrin ring carbon framework
C17  C55   gb_27  ;  corrin ring carbon framework
C18  C19   gb_27  ;  corrin ring carbon framework
C18  C60   gb_27  ;  corrin ring carbon framework
C19  C1    gb_27  ;  corrin ring carbon framework
C19  H10   gb_3   ;  corrin ring C10-H10 bond

; linker bond from B12 to CLB
O8R  CLB   gb_5   ;  LYS B12 linker (CLB replaces H)
N     H      gb_2    ;  standard LYS (lysine)
N     CA     gb_21   ;  standard LYS (lysine)
CA    CB     gb_27   ;  standard LYS (lysine)
CA    C      gb_27   ;  standard LYS (lysine)
CB    CG     gb_27   ;  standard LYS (lysine)
CG    CD     gb_27   ;  standard LYS (lysine)
CD    CE     gb_27   ;  standard LYS (lysine)
CE    NZ     gb_21   ;  standard LYS (lysine)
NZ    HZ1    gb_2    ;  standard LYS (lysine)
NZ    CLB    gb_9    ;  standard LYS (lysine)
C     O      gb_5    ;  standard LYS (lysine)
C     +N     gb_10   ;  standard LYS (lysine)

; this replaces the HZ2 with CLB for the B12-LYS connection

; below is the C=O bond on the B12-LYS linkage (OLB is only connected to CLB)
CLB  OLB    gb_27  ;  CLB-OLB linkage bond (previously nowhere in the structure)

; cyano group addition to the original B12 topology
FE   C1N    gb_30  ;  cyano group on the Fe
C1N  N1C    gb_4   ;  cyano group on the Fe

[ exclusions ]
al  4j
FE
C2
FE
C3
FE
C5
FE
C7
FE
C8
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C9 - C37, HEMC-based C framework exclusions
C9 - C12, HEMC-based C framework exclusions
C36 - C41, HEMC-based framework exclusions
C10 - C13, HEMC-based C framework exclusions
C11 - C47, HEMC-based C framework exclusions
N10 - C12, HEMC-based C framework exclusions
C11 - C48, HEMC-based C framework exclusions
C12 - C13, HEMC-based C framework exclusions
C13 - C63, HEMC-based C framework exclusions
C14 - C16, HEMC-based C framework exclusions
C46 - C47, HEMC-based C framework exclusions
C47 - C48, HEMC-based C framework exclusions
C48 - C15, HEMC-based C framework exclusions
C48 - C15, C75, HEMC-based C framework exclusions
C15 - C55, HEMC-based C framework exclusions
C53 - C17, HEMC-based C framework exclusions
C16 - C60, HEMC-based C framework exclusions
C19 - C54, HEMC-based C framework exclusions
C54 - C60, HEMC-based C framework exclusions
C55 - C60, HEMC-based C framework exclusions

; cyano group addition to the original B12 topology

N21 - N1C, cyano exclusions from HEMC CO group
N22 - N1C, cyano exclusions from HEMC CO group
N23 - N1C, cyano exclusions from HEMC CO group
C11 - C1N, cyano exclusions from HEMC CO group
C4 - C1N, cyano exclusions from HEMC CO group
C6 - C1N, cyano exclusions from HEMC CO group
C5 - C1N, cyano exclusions from HEMC CO group
C15 - C1N, cyano exclusions from HEMC CO group
C14 - C1N, cyano exclusions from HEMC CO group
C15 - C1N, cyano exclusions from HEMC CO group
N3B - N1C, cyano exclusion unique to 6-coordinate iron
C1N - C9B, additional cyano exclusion at Fe 6-center
C1N - C9B, additional cyano exclusion at Fe 6-center

[ angles ]

;  ai  aj  ak  gromos type
C2  C26  C27  ga_15, from GLN, fragment 1
C26  C27  O28  ga_30, from GLN
C26  C27  N29  ga_19, from GLN
O28  C27  N29  ga_33, from GLN
C27  N29  HAE  ga_23, from GLN
C27  N29  HAD  ga_23, from GLN
HAE  N29  HAD  ga_24, from GLN
C30  C31  C32  ga_15, from GLN, fragment 2
C31  C32  O34  ga_30, from GLN
C31  C32  N33  ga_19, from GLN
O34  C32  N33  ga_33, from GLN
C32  N33  HAG  ga_23, from GLN
C32  N33  HAF  ga_23, from GLN
HAG  N33  HAF  ga_24, from GLN
C7  C37  C38  ga_15, from GLN, fragment 3
C37  C38  O39  ga_30, from GLN
C37  C38  N40  ga_19, from GLN
O39  C38  N40  ga_33, from GLN
C38  N40  HAI  ga_23, from GLN
C38  N40  HAHI ga_24, from GLN
C41  C42  C43  ga_15, from GLN, fragment 4
C42  C43  O44  ga_30, from GLN
C42  C43  N45  ga_19, from GLN
O44  C43  N45  ga_33, from GLN
C43  N45  HAK  ga_23, from GLN
C43  N45  HAJ  ga_23, from GLN
HAK  N45  HAJ  ga_24, from GLN
C49  C49  C50  ga_15, from GLN, fragment 5
C49  C50  O51  ga_30, from GLN
C49  C50  N52  ga_19, from GLN
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O51  C50  N52  ga_33  ;  from GLN
C50  N52  HAM  ga_23  ;  from GLN
C50  N52  HAL  ga_23  ;  from GLN
HAM  N52  HAL  ga_24  ;  from GLN
C18  C60  C61  ga_15  ;  from GLN, fragment 6
C60  C61  O63  ga_30  ;  from GLN
C60  C61  N62  ga_19  ;  from GLN
O63  C61  N62  ga_33  ;  from GLN
C61  N62  HAO  ga_23  ;  from GLN
C61  N62  HAN  ga_23  ;  from GLN
N21  FE  N22  ga_2  ;  corrin ring Fe-N angle
N21  FE  N23  ga_6  ;  corrin ring Fe-N angle
N21  FE  N24  ga_6  ;  corrin ring Fe-N angle
N22  FE  N23  ga_2  ;  corrin ring Fe-N angle
N23  FE  N24  ga_2  ;  corrin ring Fe-N angle
N24  FE  N3B  ga_2  ;  corrin-Fe-dimethylbenzimidazole
N21  FE  C1    ga_6  ;  corrin Fe-N-C angles (based on HEMC)
N21  FE  C4    ga_6  ;  corrin Fe-N-C angles (based on HEMC)
N22  FE  C6    ga_6  ;  corrin Fe-N-C angles (based on HEMC)
C4    N21  C1    ga_6  ;  corrin ring-specific but HEMC-derived angles
C19   C1    N21   ga_6  ;  corrin ring-specific but HEMC-derived angles
C2    C1    N21   ga_6  ;  corrin ring-specific but HEMC-derived angles
C2    C3    C30   ga_13  ;  CHn-CHn-CHn angles
C5    C2    C25   ga_13  ;  CHn-CHn-CHn angles
C3    C2    C26   ga_13  ;  CHn-CHn-CHn angles
C7    C8    C41   ga_13  ;  CHn-CHn-CHn angles
C1    C2    C26   ga_13  ;  CHn-CHn-CHn angles
C1    C2    C25   ga_13  ;  CHn-CHn-CHn angles
C1    C3    C19   ga_13  ;  CHn-CHn-CHn angles
C1    C3    C18   ga_13  ;  CHn-CHn-CHn angles
C2    C1    C19   ga_13  ;  CHn-CHn-CHn angles
C2    C1    C18   ga_13  ;  CHn-CHn-CHn angles
C2    C3    C30   ga_13  ;  CHn-CHn-CHn angles
C2    C3    C19   ga_13  ;  CHn-CHn-CHn angles
C2    C3    C18   ga_13  ;  CHn-CHn-CHn angles
C3    C2    C25   ga_13  ;  CHn-CHn-CHn angles
C3    C2    C26   ga_13  ;  CHn-CHn-CHn angles
C3    C3    C31   ga_13  ;  CHn-CHn-CHn angles
C7    C8    C41   ga_13  ;  CHn-CHn-CHn angles

3B   N3B   C9B   ga_34  ;  Fe-dimethylbenzimidazole-N,C angle
3B   N3B   C2B   ga_34  ;  Fe-dimethylbenzimidazole-N,C angle
C8B  N1B   C2B   ga_7  ;  angle containing C8B, see minimization issues discussion
N1B  C8B  C9B   ga_7  ;  angle containing C8B, see minimization issues discussion
C8B  N1B  C1R   ga_7  ;  angle containing C8B, see minimization issues discussion
C8B  C1B  C1R   ga_7  ;  angle containing C8B, see minimization issues discussion
C8B  N1B  C9B   ga_7  ;  angle containing C8B, see minimization issues discussion
C8B  C9B  C2B   ga_7  ;  angle containing C8B, see minimization issues discussion
C8B  C9B  C3B   ga_7  ;  angle containing C8B, see minimization issues discussion
N21  C1    C2    ga_13  ;  corrin ring-specific but HEMC-derived angles
N21  C1    C20   ga_13  ;  corrin ring-specific but HEMC-derived angles
N21  C4    C3    ga_33  ;  corrin ring-specific but HEMC-derived angles
N21  C4    C20   ga_13  ;  corrin ring-specific but HEMC-derived angles
C4    N21  C1    ga_6  ;  corrin ring-specific but HEMC-derived angles
C4    N21  C20   ga_13  ;  corrin ring-specific but HEMC-derived angles
C5    C4    N21   ga_6  ;  corrin ring-specific but HEMC-derived angles
C5    C4    N20   ga_6  ;  corrin ring-specific but HEMC-derived angles
C19  C1    N21   ga_6  ;  corrin ring-specific but HEMC-derived angles
C19  C1    N20   ga_6  ;  corrin ring-specific but HEMC-derived angles
C2    C1    N20   ga_6  ;  corrin ring-specific but HEMC-derived angles
C2    C1    C19   ga_6  ;  corrin ring-specific but HEMC-derived angles
C2P  C1P  N59  ga_15  ;  from force field angle definitions
C5B  C4B  H4B  ga_25  ;  from PHE C-C-H angle
C9B  C4B  H4B  ga_25  ;  from PHE C-C-H angle
C6B  C7B  H7B  ga_25  ;  from PHE C-C-H angle
C8B  C7B  H7B  ga_25  ;  from PHE C-C-H angle
N1B  C2B  H2B  ga_16  ;  from ADE N-C-H angle
N2B  C2B  H2B  ga_16  ;  from ADE N-C-H angle
C9  C10  H10  ga_25  ;  corrin ring C-C10-H angle
C11  C10  H10  ga_20  ;  corrin ring C-C10-H angle
N1B  C2B  H2B  ga_36  ;  Standard LYS (lysine)
N3B  C2B  H2B  ga_36  ;  Standard LYS (lysine)
C9  C10  H10  ga_25  ;  corrin ring C-C10-H angle
C11  C10  H10  ga_20  ;  corrin ring C-C10-H angle
N1B  C2B  H2B  ga_36  ;  Standard LYS (lysine)
N3B  C2B  H2B  ga_36  ;  Standard LYS (lysine)
C9  C10  H10  ga_25  ;  corrin ring C-C10-H angle
C11  C10  H10  ga_20  ;  corrin ring C-C10-H angle
C5R  O8R  CLB  ga_12  ;  for LYS-B12 bridge (just replaces O8R H atom with CLB)
-C    N     H     ga_32  ;  Standard LYS (lysine)
-C    N     CA    ga_31  ;  Standard LYS (lysine)
H     N     CA    ga_18  ;  Standard LYS (lysine)
N1    C2    H2    ga_16  ;  Standard LYS (lysine)
N3    C2    H2    ga_16  ;  Standard LYS (lysine)
C9    C10   H10   ga_25  ;  corrin ring C-C10-H angle
C11   C10   H10   ga_20  ;  corrin ring C-C10-H angle

[ impropers ]
N1B  C8B  C9B  N3B  gi_1  ;  dimethylbenzimidazole improper for planarity
N1B  C8B  C9B  N3B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C6B  C7B  C8B  C9B  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
C5R  O8R  CLB  gi_1  ;  dimethylbenzimidazole improper for planarity
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C43 O44 N45 C42 gi_1 ; from GLN improper torsion definition
N45 HAK HAJ C43 gi_1 ; from GLN improper torsion definition
C50 O51 N52 C49 gi_1 ; from GLN improper torsion definition
N52 HAM HAL C50 gi_1 ; from GLN improper torsion definition
C61 O63 N62 C60 gi_1 ; from GLN improper torsion definition
N62 HAO HAN C61 gi_1 ; from GLN improper torsion definition
C57 C56 O58 N59 gi_1 ; amide linkage C57 planarity
N59 C57 C1P HAC gi_1 ; amide linkage N59 planarity
C4 N21 C3 C5 gi_1 ; corrin ring C sp2 planarity
C5 C4 C6 C35 gi_1 ; corrin ring C sp2 planarity
C6 N22 C7 C5 gi_1 ; corrin ring C sp2 planarity
C9 N22 C10 C8 gi_1 ; corrin ring C sp2 planarity
C11 N23 C12 C48 gi_1 ; corrin ring C sp2 planarity
C14 N23 C15 C13 gi_1 ; corrin ring C sp2 planarity
C15 C14 C16 C53 gi_1 ; corrin ring C sp2 planarity
C10 C9 H10 C10 gi_1 ; corrin ring C10 planarity
C18 C17 C19 C60 gi_2 ; corrin ring C atom sp3 tetrahedral geometry
C19 N24 C18 C1 gi_2 ; corrin ring C atom sp3 tetrahedral geometry
C3 C27 C30 C4 gi_2 ; corrin ring C atom sp3 tetrahedral geometry
C8 C7 C6 C41 gi_2 ; corrin ring C atom sp3 tetrahedral geometry
C13 C14 C12 C49 gi_1 ; corrin ring C atom sp3 tetrahedral geometry
C2P C1P O3 C3P gi_2 ; from ADE phosphate definition
C2R O7R C3R C1R gi_2 ; from ADE phosphate definition
C3R O6R C4R C2R gi_2 ; from ADE phosphate definition
FE C1 C4 N21 gi_3 ; HEMC improper definition
FE C6 C9 N23 gi_3 ; HEMC improper definition
FE C11 C14 N23 gi_3 ; HEMC improper definition
FE C16 C19 N24 gi_3 ; HEMC improper definition

; standard lysine improper torsions
;
N -C CA H gi_1 ; Standard LYS (lysine)
CA N C CB gi_2 ; Standard LYS (lysine)
C CA +N O gi_1 ; Standard LYS (lysine)
CLB O8R OLB NZ gi_1 ; Linkage improper torsion to maintain planarity at CLB

[ dihedrals ]
; ai aj ak al gromos type
C2R C3R O2P P gi_2 ; from ADE phosphate definition
C3R O2P P O3 gi_2 ; from ADE phosphate definition
C2P O3 P O2P gi_2 ; from ADE phosphate definition
C2P O3 P O2P gi_2 ; from ADE phosphate definition
P O3 C2P C1P gi_2 ; from ADE phosphate definition
C2R C3R O2P P gi_2 ; from ADE phosphate definition
O8R C5R C4R O6R gi_2 ; from ADE sugar dihedrals
O8R C5R C4R O6R gi_2 ; from ADE sugar dihedrals
C5R C4R C3R O8R gi_2 ; from ADE sugar dihedrals
C5R C4R C3R O8R gi_2 ; from ADE sugar dihedrals
O6R C4R C3R O8R gi_2 ; from ADE sugar dihedrals
O6R C4R C3R O8R gi_2 ; from ADE sugar dihedrals
O6R C4R C3R O8R gi_2 ; from ADE sugar dihedrals
C4R O6R C1R C2R gi_2 ; from ADE sugar dihedrals
C4R O6R C1R C2R gi_2 ; from ADE sugar dihedrals
C4R O6R C1R C2R gi_2 ; from ADE sugar dihedrals
C4R O6R C1R C2R gi_2 ; from ADE sugar dihedrals
C1R C2R C3R C4R gi_2 ; from ADE sugar dihedrals
C1R C2R C3R C4R gi_2 ; from ADE sugar dihedrals
C1R C2R C3R C4R gi_2 ; from ADE sugar dihedrals
O7R C2R C3R O2P gi_2 ; from ADE sugar dihedrals
C2R O7R C3R O2P gi_2 ; from ADE sugar dihedrals
C2R O7R C3R O2P gi_2 ; from ADE sugar dihedrals
C2R O7R HAA gi_2 ; from ADE sugar dihedrals
N1B C1R C2R O7R gi_2 ; from ADE sugar dihedrals
O6R C1R OBB gi_2 ; from ADE sugar dihedrals

; HAB-based torsion gone for LYB C4R C5R O8R HAB gi_2 ; additional ADE-based sugar dihedral
;
N1B C1R C2R C3R gi_2 ; additional ADE-based sugar dihedral
N1B C1R O6R C4R gi_2 ; additional ADE-based sugar dihedral
C2 C26 C27 N29 C40 gi_2 ; from GLN dihedral
C26 C27 N29 HAD gi_2 ; from GLN dihedral
C30 C31 C32 N33 gi_2 ; from GLN dihedral
C31 C32 N33 HAP gi_2 ; from GLN dihedral
C27 C31 C32 C44 gi_2 ; from GLN dihedral
C3 C27 C31 C32 gi_2 ; from GLN dihedral
C41 C42 C43 C44 gi_2 ; from GLN dihedral
C42 C43 C44 N45 gi_2 ; from GLN dihedral
C48 C49 C50 N52 gi_2 ; from GLN dihedral
C49 C50 N52 HAL gi_2 ; from GLN dihedral
CB    CG    CD    CE    gd_34   ;  Standard LYS (lysine)
N     CA    C     +N    gd_40   ;  Standard LYS (lysine)
N     CA    CB    CG    gd_34   ;  Standard LYS (lysine)
-C    N     CA    C     gd_39   ;  Standard LYS (lysine)
N     CA    CB    CG    gd_34   ;  Standard LYS (lysine)
N     C     +N    CA    gd_40   ;  Standard LYS (lysine)
CA    CB    CG    CD    gd_34   ;  Standard LYS (lysine)
CB    CG    CD    CE    gd_34   ;  Standard LYS (lysine)
-C    N     CA    C     gd_39   ;  Standard LYS (lysine)
N     CA    CB    CG    gd_34   ;  Standard LYS (lysine)
N     C     +N    CA    gd_40   ;  Standard LYS (lysine)
CA    CB    CG    CD    gd_34   ;  Standard LYS (lysine)
CB    CG    CD    CE    gd_34   ;  Standard LYS (lysine)
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CG    CD    CE    NZ    gd_34   ; Standard LYS (lysine)
CD    CE    NZ    H21   gd_29   ; Standard LYS (lysine)
C4R   C5R   O8R   CLB   gd_23   ; LYS-B12 linkage dihedral terms
C5R   O8R   CLB   OLB   gd_12   ; LYS-B12 linkage dihedral terms
O8R   CLB   N2    CE    gd_14   ; LYS-B12 linkage dihedral terms
OLB   CLB   N2    CE    gd_14   ; LYS-B12 linkage dihedral terms

; Use of LYB, which employs the pdb2gmx method for sewing the peptide chain together,
; requires the addition of this very new, bulky amino acid to aminoacids.dat.
; cyano group dihedral. imidazole-Fe-CN group torsion
;
C9B   N3B   FE    N21   gd_38   ; THIS IS NEW!!!
N3B   FE    N21   C1    gd_38   ; THIS IS NEW!!!
N3B   FE    N22   C6    gd_38   ; THIS IS NEW!!!
N3B   FE    N23   C11   gd_38   ; THIS IS NEW!!!
N3B   FE    N24   C16   gd_38   ; THIS IS NEW!!!
N3B   FE    C1N   N1C   gd_38   ; imidazole-Fe-CN torsion to 0