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* Generated by Kong Lesheng, Bioinformatics Centre, National Univeristy
of Singapore
*
MASS    30 N     14.00700 N
MASS    20 CP1   12.01100 C
MASS     6 HB     1.00800 H
MASS    23 CC    12.01100 C
MASS    44 O     15.99900 O
MASS    21 CP2   12.01100 C
MASS     3 HA     1.00800 H
MASS    13 CT1   12.01100 C
MASS    47 OH1   15.99900 O
MASS     1 H      1.00800 H
MASS    22 CP3   12.01100 C
MASS    15 CT3   12.01100 C
MASS    11 C     12.01100 C
MASS    35 NH2   14.00700 N
DECL -N
DECL +C

AUTO ANGLES DIHE




RESI HYP        0.00000
GROUP                    !       HD1 HD2
ATOM N    N    -0.2900   !     |   \ /
ATOM CA   CP1   0.0200   !     N---CD   HG
ATOM HA   HB    0.0900   !     |     \  /
GROUP                    !     |      CG
ATOM C    CC    0.5300   !     |     /  \
ATOM O    O    -0.5300   !  HA-CA--CB   OG2--HG2
GROUP                    !     |   / \
ATOM CB   CP2  -0.1800   !     | HB1 HB2
ATOM HB1  HA    0.0900   !   O=C
ATOM HB2  HA    0.0900   !     |
GROUP
ATOM CG   CT1   0.1400
ATOM HG   HA    0.0900
ATOM OG2  OH1  -0.6600
ATOM HG2  H     0.4300
GROUP
ATOM CD   CP3   0.1800
ATOM HD1  HB    0.0000
ATOM HD2  HB    0.0000
BOND N    CA      N    CD      CA   HA      CA   CB      CA   C
BOND C    O       CB   HB1     CB   HB2     CB   CG      CG   HG
BOND CG   OG2     CG   CD      CD   HD1     CD   HD2     N    +C
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BOND C    N       OG2  HG2
IMPH N    CA   CD   +C       C    CA   N    O
DONOR HG2  OG2
ACCEPTOR O    C
IC CD   N    CA   CB    1.4468  114.9587  -11.2918  101.8808  1.5360
IC CD   N    CA   HA    1.4468  114.9587 -129.2290  110.5162  1.0924
IC CD   N    CA   C     1.4468  114.9587  109.5875  111.6376  1.5380
IC HA   CA   N    +C     1.0924  110.5162   50.0429  122.5076  1.3162
IC CD   +C    *N    CA    1.4468  122.5296 -179.2170  122.5076  1.4550
IC CA   N    CD   CG    1.4550  114.9587  -11.8599  102.4794  1.5305
IC CA   N    CD   HD1   1.4550  114.9587 -131.8901  111.1069  1.0924
IC CA   N    CD   HD2   1.4550  114.9587  106.0401  109.5406  1.0925
IC N    CA   CB   CG    1.4550  101.8808   29.6080  103.6605  1.5362
IC N    CA   CB   HB1   1.4550  101.8808  152.0681  112.9350  1.0925
IC N    CA   CB   HB2   1.4550  101.8808  -86.5729  108.9663  1.0930
IC N    CA   C    O     1.4550  111.6376  149.4002  120.4223  1.2316
IC N    CA   C    N     1.4550  111.6376  -31.0428  120.0469  1.3161
IC N    CA   *C    O     1.3161  120.0469 -179.5571  120.4223  1.2316
IC CA   CB   CG   OG2   1.5360  103.6605 -158.7449  112.5784  1.4300
IC CA   CB   CG   HG    1.5360  103.6605   79.0616  109.5554  1.0926
IC CD   CG   OG2  HG2   1.5305  112.2089   31.3937  109.5000  1.0300
IC N    CD   CG   CB    1.4468  102.4794   29.9288  103.3139  1.5362
PATCHING FIRS PROP


END
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