```
* Stream file for dehydro-amino residues
* If using these parameters please cite:
* Turpin, ER, Mulholland, S, Bonev, BB & Hirst, JD, RSC Adv., 2014, DOI:
10.1039/c4ra09897h
* eleanor.turpin@nottingham.ac.uk SEPTEMBER 2014
********
* Initial toppar stream file generated by
* CHARMM General Force Field (CGenFF) program version 0.9.6 beta
* For use with CGenFF version 2b7
*

read rtf card append
* Initial topology guesses generated by
* CHARMM General Force Field (CGenFF) program version 0.9.6 beta
*
36 1

DECL -C
DECL +N
DEFA FIRS NTER LAST CTER

! Dehydroalanine dipetide
! Initial guess of parameters created by ParamChem website
! ERT Feb 2013

RESI DHAD           0.000 !
GROUP                     !    H4    O3          O9          H1
ATOM C2     CG331  -0.270 !     \    ||  H9      ||  H11    /
ATOM H4     HGA3    0.090 !      \   ||  |       ||  |     /
ATOM H5     HGA3    0.090 ! H5---C2--C4--N8--C6--C5--N10--C1---H2
ATOM H6     HGA3    0.090 !      /           ||            \
GROUP                     !     /            ||             \
ATOM C4     CG2O1   0.400 !    H6            C7              H3
ATOM O3     OG2D1  -0.400 !                 /  \
GROUP                     !               H7    H8
ATOM N8     NG2S1  -0.670 !
ATOM H9     HGP1    0.360 !
ATOM C6     CG2D1O  0.310 !
GROUP
ATOM C7     CG2DC3 -0.420 !
ATOM H7     HGA5    0.210 !
ATOM H8     HGA5    0.210 !
GROUP
ATOM C5     CG2O1   0.635 !
ATOM O9     OG2D1  -0.635 !
GROUP
ATOM N10    NG2S1  -0.500 !
ATOM H11    HGP1    0.335 !
ATOM C1     CG331  -0.105 !
ATOM H1     HGA3    0.090 !
ATOM H2     HGA3    0.090 !
ATOM H3     HGA3    0.090 !

DOUBLE C6   C7
BOND C6   N8
BOND C5   C6
BOND C5   O9
BOND C4   N8
BOND O3   C4
BOND C2   C4
```

```
BOND C5   N10
BOND C1   N10
BOND C1   H1
BOND C1   H2
BOND C1   H3
BOND C2   H4
BOND C2   H5
BOND C2   H6
BOND C7   H7
BOND C7   H8
BOND N8   H9
BOND N10  H11
IMPR C4     C2     N8     O3
IMPR C5     C6     N10    O9
IMPR C6     C7     C5     N8

! Dehydrobutyrine dipetide
! Based on DHAD residue
! ERT Aug 2013

RESI DHBD           0.000 !
GROUP                     !    H4    O3          O9          H1
ATOM C2     CG331  -0.270 !     \    ||  H9      ||  H11    /
ATOM H4     HGA3    0.090 !      \   ||  |       ||  |     /
ATOM H5     HGA3    0.090 ! H5---C2--C4--N8--C6--C5--N10--C1---H2
ATOM H6     HGA3    0.090 !      /           ||            \
GROUP                     !     /            ||             \
ATOM C4     CG2O1   0.400 !    H6            C7  H8          H3
ATOM O3     OG2D1  -0.400 !                 /  \ |
GROUP                     !               H7    C11-H12
ATOM N8     NG2S1  -0.670 !                      |
ATOM H9     HGP1    0.360 !                      H13
ATOM C6     CG2D1O  0.310 !
GROUP
ATOM C7     CG2DC1 -0.150 !
ATOM H7     HGA4    0.150 !
GROUP
ATOM C11    CG331  -0.270 !
ATOM H8     HGA3    0.090 !
ATOM H12    HGA3    0.090 !
ATOM H13    HGA3    0.090 !
GROUP
ATOM C5     CG2O1   0.635 !
ATOM O9     OG2D1  -0.635 !
GROUP
ATOM N10    NG2S1  -0.500 !
ATOM H11    HGP1    0.335 !
ATOM C1     CG331  -0.105 !
ATOM H1     HGA3    0.090 !
ATOM H2     HGA3    0.090 !
ATOM H3     HGA3    0.090 !

DOUBLE C6   C7
BOND C6   N8
BOND C5   C6
BOND C5   O9
BOND C4   N8
BOND O3   C4
BOND C2   C4
BOND C5   N10
```

```
BOND C1   N10
BOND C1   H1
BOND C1   H2
BOND C1   H3
BOND C2   H4
BOND C2   H5
BOND C2   H6
BOND C7   H7
BOND N8   H9
BOND N10  H11
BOND C7   C11
BOND C11  H8
BOND C11  H12
BOND C11  H13
IMPR C4      C2     N8     O3
IMPR C5      C6     N10    O9
IMPR C6      C7     C5     N8

! Dehydroalanine residue

RESI DHAR           0.000 !
 !          O
 !  HN      ||
 !  |       ||
 ! -N--CA--C--
 !     ||
 !     ||
 !     CB
 !    /  \
 !   HB1  HB2
GROUP
ATOM N     NG2S1  -0.670 !
ATOM HN    HGP1    0.360 !
ATOM CA    CG2D1O  0.310 !
GROUP
ATOM CB      CG2DC3 -0.420 !
ATOM HB1     HGA5    0.210 !
ATOM HB2     HGA5    0.210 !
GROUP
ATOM C       CG2O1   0.635 !
ATOM O       OG2D1  -0.635 !

DOUBLE CA   CB
BOND CA   N
BOND CA   C
BOND C    O
BOND C    +N
BOND N    HN
BOND CB HB1 CB HB2
IMPR CA CB  C   N
IMPR C  CA +N   O
DONOR HN N
ACCEPTOR O C

! Dehydrobutyrine residue
! Based on DHAD residue
! ERT Aug 2013

RESI DHBR           0.000 !
!         O
```

```
!  H      ||
!  |      ||
! -N--CA--C-
!     ||
!     ||
!     CB  HG1
!    /  \ |
!   HB    CG-HG2
!         |
!         HG3
!
GROUP                     !
ATOM N     NG2S1  -0.670 !
ATOM HN     HGP1    0.360 !
ATOM CA    CG2D1O  0.310 !
GROUP
ATOM CB     CG2DC1 -0.150 !
ATOM HB     HGA4    0.150 !
GROUP
ATOM CG     CG331  -0.270 !
ATOM HG1    HGA3    0.090 !
ATOM HG2    HGA3    0.090 !
ATOM HG3    HGA3    0.090 !
GROUP
ATOM C     CG2O1   0.635 !
ATOM O     OG2D1  -0.635 !

BOND N HN N CA CA CB CA C C O C +N
BOND CB HB CB CG CG HG1 CG HG2 CG HG3
IMPR C     CA     +N    O
IMPR CA    CB     C     N
DONOR HN N
ACCEPTOR O C

! alpha-aminobutyric acid, needed for nisin
! built by analogy

RESI ABU          0.00  !
GROUP                   !            HG1
ATOM N    NH1    -0.47  !     |      |
ATOM HN   H       0.31  !  HN-N      CG-HG2
ATOM CA   CT1     0.07  !     |     / \
ATOM HA   HB1     0.09  !     |    /   HG3
GROUP                   !  HA-CA--CB
ATOM CB   CT2    -0.18  !     |   / \
ATOM HB1  HA2     0.09  !     | HB1 HB2
ATOM HB2  HA2     0.09  !   O=C
GROUP                   !     |
ATOM CG   CT3    -0.27  !
ATOM HG1  HA3     0.09  !
ATOM HG2  HA3     0.09  !
ATOM HG3  HA3     0.09  !
GROUP                   !
ATOM C    C       0.51  !
ATOM O    O      -0.51  !

BOND CB CA  N  HN  N  CA
BOND C  CA  C  +N  CA HA  CB HB1  CB HB2
BOND CB CG CG HG1 CG HG2 CG HG2 CG HG3
DOUBLE O  C
```

```
IMPR N -C CA HN  C CA +N O
CMAP -C  N  CA  C   N  CA  C  +N
DONOR HN N
ACCEPTOR O C

!Pacth to change charge on C+
PRES  DHCC     0.00
GROUP
ATOM   C   C    0.635
ATOM   O   O   -0.635

!Patch to connect thioether rings, where first res is ALA
PRES THIA       0.00
DELETE ATOM 1HB1
DELETE ATOM 2HG1
GROUP
ATOM 1CB  CT2  -0.135
ATOM 1HB2 HA2   0.09
ATOM 1HB3 HA2   0.09
ATOM 2SG  S    -0.09
ATOM 2CB  CT2  -0.135
ATOM 2HB1 HA2   0.09
ATOM 2HB2 HA2   0.09
BOND 1CB 2SG

!Patch to connect thioether rings, where first res is ABU
PRES THIB       0.00
DELETE ATOM 1HB1
DELETE ATOM 2HG1
GROUP
ATOM 1CB  CT2  -0.09
ATOM 1HB2 HA2   0.09
ATOM 2SG  S    -0.09
ATOM 2CB  CT2  -0.09
ATOM 2HB1 HA2   0.09
ATOM 2HB2 HA2   0.09
BOND 1CB 2SG

END

read param card flex append
* Initial parameter guess generated by analogy by
* CHARMM General Force Field (CGenFF) program version 0.9.6 beta
*

BONDS
CG2D1O CG2DC3  440.00     1.3400 ! Molecule , from CG2D2O CG2DC2,
CG2D1O CG2O1   440.00     1.4890 ! Molecule , from CG2DC1 CG2O1,
CG2D1O NG2S1   370.00     1.390  ! edited by ERT
CG2D1O CG2DC2  440.00     1.3400 ! Molecule , from CG2D2O CG2DC2,
C      NG2S1   370.000     1.3450 ! joining protein & cgenff sets
CG2O1  NH1     370.000     1.3450 ! joining protein & cgenff sets


ANGLES
CG2DC3 CG2D1O CG2O1    60.00    120.00 ! Molecule , from CG2DC3 CG2DC1 CG2O4,
CG2DC3 CG2D1O NG2S1    80.00    128.00 ! Molecule , from CG2D2 CG2D1O NG321,
CG2O1  CG2D1O NG2S1    80.00    110.00 ! ERT
CG2D1O CG2DC3 HGA5     45.00    120.50 ! Molecule , from CG2DC1 CG2DC3 HGA5,
CG2D1O CG2O1  NG2S1    80.00    116.50 ! Molecule , from CG2DC1 CG2O1 NG2S1,
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CG2D1O CG2O1  OG2D1    80.00    122.50 ! Molecule , from CG2DC1 CG2O1 OG2D1,
CG2D1O NG2S1  CG2O1    50.00    120.00 ! Molecule , from CG2O1 NG2S1 CG2R61,
CG2D1O NG2S1  HGP1     34.00    117.00 ! Molecule , from CG2R61 NG2S1 HGP1,
CG2DC1 CG2D1O NG2S1    80.00    128.00 ! Molecule , from CG2D2 CG2D1O NG321,
CG2DC1 CG2D1O CG2O1    60.00    120.00 ! Molecule , from CG2DC3 CG2DC1 CG2O4,
CG2D1O CG2DC1 CG331    43.50    126.50 ! ERT from CG2D1O CG2DC1 CG321
! For linking protein and CGenFF parameter sets; analogy w/ prot set
CT1    C      NG2S1     80.000   116.5000
O      C      NG2S1     80.000   122.5000
C      NG2S1  HGP1      34.000   123.0000
C      NG2S1  CG2D1O    50.00    120.00
CG2D1O CG2O1  NH1       80.00    116.50
OG2D1  CG2O1  NH1       80.000   122.5000
CG2O1  NH1    H         34.000   123.0000
CG2O1  NH1    CT1       50.00    120.00
CG2O1  NH1    CTD1      50.00    120.00

CT2    S      CT2       34.000   95.0000 ! from MET CT3 S CT2

DIHEDRALS
CG2O1  CG2D1O CG2DC3 HGA5       3.2000  2   180.00 ! Molecule , from CG2O4
CG2DC1 CG2DC3 HGA5,
NG2S1  CG2D1O CG2DC3 HGA5       5.0000  2   180.00 ! Molecule , from CG2DC2
CG2DC1 CG2DC3 HGA5,
CG2DC3 CG2D1O NG2S1  HGP1       2.5000  2   180.00 ! Molecule , from CG2DC1
CG2O1 NG2S1 HGP1,
CG2O1  CG2D1O NG2S1  HGP1       2.5000  2   180.00 ! Molecule , from CG2R61
CG2O1 NG2S1 HGP1,
CG2D1O CG2O1  NG2S1  HGP1       2.5000  2   180.00 ! Molecule , from CG2DC1
CG2O1 NG2S1 HGP1,


CG2DC1  CG2D1O    NG2S1    CG2O1     0.50  1    180.0
CG2DC1  CG2D1O    NG2S1    CG2O1     0.50  2      0.0
CG2DC1  CG2D1O    NG2S1    CG2O1     0.20  3    180.0

NG2S1    CG2D1O   CG2DC1   HGA4      3.0000  2   180.00 !dhb
NG2S1    CG2D1O   CG2DC1   CG331     3.5000  2   180.00 !dhb  c11c7c6n8
NG2S1    CG2D1O   CG2DC1   CG331     1.700  1    180.00
NG2S1    CG2D1O   CG2DC1   CG331     0.500  3    180.00
HGP1     NG2S1    CG2D1O   CG2DC1    2.5000  2   180.00  !dhb
CG2D1O   CG2DC1   CG331    HGA3      0.3000  3   180.00 !dhb
CG2DC1   CG2D1O    CG2O1    OG2D1     0.57  1      0.0 !dhb
CG2DC1   CG2D1O    CG2O1    OG2D1     0.59  2      0.0 !dhb
CG2DC1   CG2D1O    CG2O1    OG2D1     2.96  3      0.0 !dhb
CG2DC1   CG2D1O    CG2O1    NG2S1     2.10  1    180.0 !dhb
CG2DC1   CG2D1O    CG2O1    NG2S1     2.88  2      0.0 !dhb
CG2DC1   CG2D1O    CG2O1    NG2S1     2.00  3      0.0 !dhb
HGA4     CG2DC1   CG2D1O   CG2O1     3.2000  2   180.00 !dhb
CG331    CG2DC1   CG2D1O   CG2O1     3.5000  2   180.00 !dhb c11c7c6c5
CG331    CG2DC1   CG2D1O   CG2O1     1.700  1     0.00
CG331    CG2DC1   CG2D1O   CG2O1     0.500  3     0.00
CG2DC2   CG2D1O    CG2O1    NG2S1     2.10  1    180.0 !c7c6c5n10
CG2DC2   CG2D1O    CG2O1    NG2S1     2.88  2    180.0
CG2DC2   CG2D1O    CG2O1    NG2S1     2.00  3    180.0
CG2D1O    NG2S1    CG2O1    CG331     2.29  1    180.0 !c2c4n8c6
CG2D1O    NG2S1    CG2O1    CG331     3.48  2    180.0
CG2D1O    NG2S1    CG2O1    CG331     0.63  3      0.0
CG2O1   CG2D1O    NG2S1    CG2O1     2.50  1      0.0
CG2O1   CG2D1O    NG2S1    CG2O1     1.50  2    180.0
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CG2O1   CG2D1O    NG2S1    CG2O1     0.30  3      0.0
CG2O1   CG2D1O    NG2S1    CG2O1     0.75  5      0.0
CG2DC3  CG2D1O    NG2S1    CG2O1     0.50  1    180.0
CG2DC3  CG2D1O    NG2S1    CG2O1     0.50  2      0.0
CG2DC3  CG2D1O    NG2S1    CG2O1     0.20  3    180.0
CG2D1O  CG2O1     NG2S1    CG331     2.37  1      0.0
CG2D1O  CG2O1     NG2S1    CG331     0.50  2      0.0
CG2DC3   CG2D1O    CG2O1     NG2S1     2.10  1    180.0 !c7c6c5n10
CG2DC3   CG2D1O    CG2O1     NG2S1     2.88  2      0.0
CG2DC3   CG2D1O    CG2O1     NG2S1     2.00  3      0.0
CG2DC3   CG2D1O    CG2O1     OG2D1     0.57  1      0.0 !c7c6c5o9o9
CG2DC3   CG2D1O    CG2O1     OG2D1     0.59  2      0.0
CG2DC3   CG2D1O    CG2O1     OG2D1     2.96  3      0.0
NG2S1   CG2D1O    CG2O1     NG2S1     1.53  1    180.0 !n8c6c5n10
NG2S1   CG2D1O    CG2O1     NG2S1     3.63  2    180.0
NG2S1   CG2D1O    CG2O1     NG2S1     0.10  3    180.0
NG2S1   CG2D1O    CG2O1     OG2D1     0.79  1    180.0 !n8c6c5o9
NG2S1   CG2D1O    CG2O1     OG2D1     2.85  2    180.0
NG2S1   CG2D1O    CG2O1     OG2D1     1.49  3      0.0
CG2D1O    NG2S1    CG2O1     OG2D1     2.45  1    180.0 !o3c4n8c6
CG2D1O    NG2S1    CG2O1     OG2D1     0.69  2      0.0
CG2D1O    NG2S1    CG2O1     OG2D1     1.09  3      0.0
! For joining protein and CGen sets
NH1      CT1      C        NG2S1       0.6000  1     0.00
CT1      C        NG2S1    HGP1        2.5000  2   180.00
CT1      C        NG2S1    CG2D1O      1.6000  1     0.00
CT1      C        NG2S1    CG2D1O      2.5000  2   180.00
HB1      CT1      C        NG2S1       0.0000  1     0.00
CT3      CT1      C        NG2S1       0.0000  1     0.00
C        NG2S1    CG2D1O   CG2DC3      0.50  1    180.0
C        NG2S1    CG2D1O   CG2DC3      0.50  2      0.0
C        NG2S1    CG2D1O   CG2DC3      0.20  3    180.0
C        NG2S1    CG2D1O   CG2O1       2.50  1      0.0
C        NG2S1    CG2D1O   CG2O1       1.50  2    180.0
C        NG2S1    CG2D1O   CG2O1       0.30  3      0.0
C        NG2S1    CG2D1O   CG2O1       0.75  5      0.0
O        C        NG2S1    HGP1        2.5000  2   180.00
O        C        NG2S1    CG2D1O      2.5000  2   180.00
NG2S1    CG2D1O   CG2O1    NH1         0.6000  1     0.00
CG2D1O   CG2O1    NH1      H           2.5000  2   180.00
CG2D1O   CG2O1    NH1      CT1         1.6000  1     0.00
CG2D1O   CG2O1    NH1      CT1         2.5000  2   180.00
CG2DC3   CG2D1O   CG2O1    NH1         2.10  1    180.0
CG2DC3   CG2D1O   CG2O1    NH1         2.88  2      0.0
CG2DC3   CG2D1O   CG2O1    NH1         2.00  3      0.0
CG2O1    NH1      CT1      HB1         0.0000  1     0.0
CG2O1    NH1      CT1      CT3         1.8000  1     0.00
CG2O1    NH1      CT1      C           0.2000  1   180.00
OG2D1    CG2O1    NH1      H           2.5000  2   180.00
OG2D1    CG2O1    NH1      CT1         2.5000  2   180.00
C        NG2S1    CG2D1O   CG2DC1      0.50  1    180.0
C        NG2S1    CG2D1O   CG2DC1      0.50  2      0.0
C        NG2S1    CG2D1O   CG2DC1      0.20  3    180.0
CG2DC1   CG2D1O   CG2O1    NH1         2.10  1    180.0
CG2DC1   CG2D1O   CG2O1    NH1         2.88  2      0.0
CG2DC1   CG2D1O   CG2O1    NH1         2.00  3      0.0
CT1      CT1      C        NG2S1       0.0000  1     0.00
CG2D1O   CG2O1    NH1      CTD1        1.6000  1     0.00
CG2D1O   CG2O1    NH1      CTD1        2.5000  2   180.00
CG2O1    NH1      CTD1     HB1         0.0000  1     0.0
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```
CG2O1    NH1      CTD1     CT3          1.8000  1     0.00
CG2O1    NH1      CTD1     C            0.2000  1   180.00
OG2D1    CG2O1    NH1      CTD1         2.5000  2   180.00
CG2O1    NH1      CT1      CT2          1.8000  1     0.00
NH3      CT1      C        NG2S1        0.6000  1     0.00
CG2O1    NH1      CT1      CC           0.2000  1   180.00
CG2O1    NH1      CTD1     CT2          1.8000  1     0.00

CTD1     CT2      S       CT2      0.2400  1   180.00 ! from CT3  CT2  S    CT3
CTD1     CT2      S       CT2      0.3700  3     0.00 ! from CT3  CT2  S    CT3
CT2      S        CT2     CT1      0.2400  1   180.00 ! from CT3  CT2  S    CT3
CT2      S        CT2     CT1      0.3700  3     0.00 ! from CT3  CT2  S    CT3
CT2      S        CT2     HA2      0.2800  3     0.00 ! from HA2  CT2  S    CT3
CT3      CT2      S       CT2      0.2400  1   180.00 ! from CT3  CT2  S    CT3
CT3      CT2      S       CT2      0.3700  3     0.00 ! from CT3  CT2  S    CT3

IMPROPERS
CG2D1O CG2DC3 CG2O1  NG2S1     72.0000  0     0.00 ! Molecule , from CG2O5 CG2O3
CG2R61 OG2D3
CG2O1  CG2D1O NG2S1  OG2D1    120.0000  0     0.00 ! Molecule , from CG2O1
CG2DC1 NG2S1 OG2D1
CG2D1O CG2DC1 CG2O1  NG2S1     72.0000  0     0.00 ! Molecule , from CG2O5 CG2O3
CG2R61 OG2D3
CG2O1  CG2D1O NH1    OG2D1    120.0000  0     0.00

CMAP
!! CMAP terms to allow DHAR and DHAB to be included in the peptide chain. CMAP
is not applied to the
!! non-standard residues, but definition of phi and psi is changed for
neighborous due to different atom
!! type names in CGEN and protein parameter sets.
C    NH1  CT1  C    NH1  CT1  C    NG2S1   24
! phi = -180.0
     0.126790      0.768700      0.971260      1.250970      2.121010
     2.720430      2.089440      1.789790      0.780870     -0.688474
     1.001130     -2.200520     -4.827670     -4.821447     -4.913223
    -3.591106     -2.766446     -2.784200     -2.454589     -2.346991
    -2.335350     -1.522656     -0.951542     -0.036650

! phi = -165.0
    -0.127133      1.377090      1.577020      1.872290      2.398990
     2.486630      2.436754      1.929070      1.086456      0.643400
     0.258676     -2.800440     -4.009477     -4.135306     -3.420090
    -2.602140     -2.299128     -1.501241     -1.101780     -0.861434
    -0.640168     -0.207701     -1.076344     -1.122030

! phi = -150.0
     0.084069      1.420317      1.624350      2.047200      2.653910
     2.716410      2.321416      1.985454      1.557466      2.463293
    -0.225720     -1.815886     -2.583256     -3.006154     -2.551995
    -1.890683     -1.354215     -0.727243      0.068512     -0.225016
    -0.765479     -1.283444     -1.293226     -0.816303

! phi = -135.0
     0.927992      1.521370      2.242218      2.546305      3.111384
     2.918410      2.460813      2.187970      2.058314      1.852278
     0.115935     -1.183897     -1.995479     -2.278329     -1.959136
    -1.340467     -0.932949      0.021790      0.313725     -0.517358
    -1.152891     -0.983285     -0.566518     -0.442565
```

```
! phi = -120.0
     1.357468      1.959160      2.698894      3.037857      3.698960
     3.558453      2.639296      2.773853      2.719664      1.627997
     0.705667     -0.785637     -2.118268     -2.628489     -1.803113
    -0.425969     -0.062320      0.439040      0.910952     -0.546994
    -0.968118     -0.856791     -0.250116      0.449309

! phi = -105.0
     2.045006      2.544424      2.818030      3.088582      3.370620
     3.551568      3.073520      2.903794      2.956634      2.124759
     0.906487     -0.823628     -2.090819     -2.241579     -1.456524
     0.206160      0.082195      0.771710      1.040241     -0.124647
    -0.316550     -0.164333      0.314474      0.733747

! phi = -90.0
     1.451735      2.748481      2.738185      3.156796      3.450028
     3.344157      3.180200      3.898724      3.335030      2.440579
     0.912671     -0.606502     -1.511772     -1.620864     -0.962798
    -0.020653      0.415153      0.908250      0.459433      0.145910
    -0.071054      0.017622      0.280839      0.748823

! phi = -75.0
     1.378160      3.345958      2.352424      3.063543      3.814070
     3.700796      3.580310      4.212293      3.536425      1.693809
     0.095172     -0.682452     -0.123614     -0.427765     -0.598368
     0.226352      0.423308      0.301999      0.551890      0.191719
    -0.253585     -0.190548     -0.253412      0.468922

! phi = -60.0
     0.237754      1.229980      1.716960      3.168570      4.208190
     4.391860      4.276080      3.673107      2.272295     -0.482789
    -0.406695     -0.038919     -0.357600     -0.823341     -0.173146
     0.139806      0.267796      0.322420      0.309664     -0.666399
    -0.948631     -1.534365     -1.479968     -0.204264

! phi = -45.0
    -1.184837      0.078060      2.347410      4.211350      5.376000
     5.389940      4.380200      2.461506      1.123713      0.107016
     0.007574     -0.149443     -0.797230     -0.582210      0.082910
     0.271580     -0.045570      0.379430      0.247770     -0.890956
    -1.582430     -1.954532     -1.980965     -2.000433

! phi = -30.0
    -1.174720      1.067030      4.180460      6.741610      6.070770
     4.806470      2.783340      1.320806      0.765978     -0.008448
     0.276860     -0.707140      1.314360      1.522590      1.915550
     2.223490      0.194290      0.534000      0.331780     -1.595147
    -2.849141     -3.550465     -3.277369     -2.655135

! phi = -15.0
     0.293590      5.588070      3.732620      3.217620      3.272450
     2.517320      1.588700      1.381760      0.856410      0.655170
     1.616970      0.846920      0.511070      0.740760      1.021020
     1.616580     -0.342400      0.181770     -0.613920     -2.558037
    -3.786839     -3.807325     -3.155346     -1.749204

! phi =   0.0
     2.832310      0.787990      0.323280      0.479230      0.628600
     0.976330      1.238750      1.671950      1.645480      2.520340
     1.606970      0.776350      0.119780      0.070390      0.121170
```

```
    -1.569230     -1.213010     -1.846360     -2.744510     -3.792530
    -3.934880     -3.615930     -2.675750     -0.924170

! phi =  15.0
    -0.778340     -1.912680     -2.052140     -1.846280     -1.047430
     0.183400      1.682950      2.223500      1.358370      2.448660
     1.436920      0.678570     -0.237060     -0.535320     -0.790380
    -2.182580     -3.251140     -4.195110     -4.269270     -3.908210
    -3.455620     -2.773970      1.755370      0.313410

! phi =  30.0
    -2.963810     -3.483730     -3.441809     -2.400349     -1.125083
     0.336200      1.428450      1.394630      0.970370      2.462720
     1.522430      0.553620     -0.407380     -1.482950     -3.613920
    -4.159810     -4.709721     -4.496271     -3.764540     -2.959140
    -1.963850     -1.071260     -1.599580     -2.445320

! phi =  45.0
    -4.021496     -3.836549     -3.365327     -2.334377     -0.984725
     0.362000      0.814380      0.754110      0.502370      1.903420
     0.770220     -0.416420     -3.286310     -3.875270     -4.611550
    -5.287977     -5.146239     -4.038627     -2.865450     -2.368170
    -2.860490     -3.416560     -3.666490     -3.595217

! phi =  60.0
    -3.353683     -2.984416     -2.317412     -1.240143     -0.257890
     0.722610      0.668070      0.438130      2.395330      1.632470
    -2.041450     -3.218100     -3.915080     -4.568574     -5.096776
    -5.526955     -5.005312     -3.777879     -2.840678     -3.508820
    -3.756430     -3.640810     -3.451845     -3.342810

! phi =  75.0
    -2.248733     -1.641080     -1.010583      0.039656      0.636063
     0.823710      0.517140     -0.013120     -0.370910     -1.192809
    -2.305650     -3.420580     -4.484960     -5.597237     -5.601264
    -5.727739     -4.740525     -3.819378     -3.685150     -4.151360
    -4.170739     -3.725589     -3.736732     -2.620673

! phi =  90.0
    -1.720840     -1.177830     -0.428430      0.277730      0.807900
     0.803260      0.482510     -0.336900     -0.786270     -1.774070
    -2.793220     -3.828560     -5.211800     -6.294328     -6.617221
    -5.763953     -5.072995     -3.911450     -4.158306     -4.473413
    -4.099325     -3.769822     -3.157300     -2.651694

! phi = 105.0
    -1.850640     -1.092420     -0.445020      0.128490      1.005520
     0.884820      0.485850     -0.218470     -0.857670     -1.682330
    -3.014400     -4.481110     -6.053510     -6.865400     -6.871130
    -5.728240     -3.912230     -4.802110     -5.034640     -4.715990
    -4.600554     -4.086721     -3.274630     -2.410940

! phi = 120.0
    -1.969230     -1.116650     -0.540250     -0.150330      0.763520
     1.038890      0.758480      0.313530     -0.333050     -1.872770
    -3.366270     -5.008260     -6.124810     -7.034830     -6.724320
    -3.700200     -4.510620     -5.185650     -5.361620     -4.847490
    -4.444320     -4.004260     -3.415720     -2.751230

! phi = 135.0
```

```
   -2.111250     -1.168960     -0.322790     -0.006920      0.316660
    1.086270      0.939170      0.625340     -0.166360     -1.830310
   -3.469470     -4.946030     -6.112560     -1.915580     -4.047310
   -4.996740     -4.996730     -4.842690     -4.886620     -4.300540
   -4.494620     -4.442210     -4.163570     -3.183510

! phi = 150.0
   -1.757590     -0.403620      0.023920      0.362390      0.634520
    1.264920      1.361360      0.948420     -0.073680     -1.483560
   -3.152820      1.835120     -1.762860     -5.093660     -5.744830
   -5.390070     -4.783930     -4.190630     -4.115420     -4.042280
   -4.125570     -4.028550     -4.026100     -2.937910

! phi = 165.0
   -0.810590     -0.071500      0.378890      0.543310      1.277880
    1.641310      1.698840      1.519950      0.631950     -1.088670
   -2.736530     -0.735240     -4.563830     -6.408350     -5.889450
   -5.141750     -4.194970     -3.666490     -3.843450     -3.555000
   -3.548722     -3.246995     -2.751289     -1.814368

CG2O1 NH1 CT1 C NH1 CT1 C NH1 24

! phi = -180.0
    0.126790      0.768700      0.971260      1.250970      2.121010
    2.720430      2.089440      1.789790      0.780870     -0.688474
    1.001130     -2.200520     -4.827670     -4.821447     -4.913223
   -3.591106     -2.766446     -2.784200     -2.454589     -2.346991
   -2.335350     -1.522656     -0.951542     -0.036650

! phi = -165.0
   -0.127133      1.377090      1.577020      1.872290      2.398990
    2.486630      2.436754      1.929070      1.086456      0.643400
    0.258676     -2.800440     -4.009477     -4.135306     -3.420090
   -2.602140     -2.299128     -1.501241     -1.101780     -0.861434
   -0.640168     -0.207701     -1.076344     -1.122030

! phi = -150.0
    0.084069      1.420317      1.624350      2.047200      2.653910
    2.716410      2.321416      1.985454      1.557466      2.463293
   -0.225720     -1.815886     -2.583256     -3.006154     -2.551995
   -1.890683     -1.354215     -0.727243      0.068512     -0.225016
   -0.765479     -1.283444     -1.293226     -0.816303

! phi = -135.0
    0.927992      1.521370      2.242218      2.546305      3.111384
    2.918410      2.460813      2.187970      2.058314      1.852278
    0.115935     -1.183897     -1.995479     -2.278329     -1.959136
   -1.340467     -0.932949      0.021790      0.313725     -0.517358
   -1.152891     -0.983285     -0.566518     -0.442565

! phi = -120.0
    1.357468      1.959160      2.698894      3.037857      3.698960
    3.558453      2.639296      2.773853      2.719664      1.627997
    0.705667     -0.785637     -2.118268     -2.628489     -1.803113
   -0.425969     -0.062320      0.439040      0.910952     -0.546994
   -0.968118     -0.856791     -0.250116      0.449309

! phi = -105.0
    2.045006      2.544424      2.818030      3.088582      3.370620
    3.551568      3.073520      2.903794      2.956634      2.124759
```

```
     0.906487     -0.823628     -2.090819     -2.241579     -1.456524
     0.206160      0.082195      0.771710      1.040241     -0.124647
    -0.316550     -0.164333      0.314474      0.733747

! phi = -90.0
     1.451735      2.748481      2.738185      3.156796      3.450028
     3.344157      3.180200      3.898724      3.335030      2.440579
     0.912671     -0.606502     -1.511772     -1.620864     -0.962798
    -0.020653      0.415153      0.908250      0.459433      0.145910
    -0.071054      0.017622      0.280839      0.748823

! phi = -75.0
     1.378160      3.345958      2.352424      3.063543      3.814070
     3.700796      3.580310      4.212293      3.536425      1.693809
     0.095172     -0.682452     -0.123614     -0.427765     -0.598368
     0.226352      0.423308      0.301999      0.551890      0.191719
    -0.253585     -0.190548     -0.253412      0.468922

! phi = -60.0
     0.237754      1.229980      1.716960      3.168570      4.208190
     4.391860      4.276080      3.673107      2.272295     -0.482789
    -0.406695     -0.038919     -0.357600     -0.823341     -0.173146
     0.139806      0.267796      0.322420      0.309664     -0.666399
    -0.948631     -1.534365     -1.479968     -0.204264

! phi = -45.0
    -1.184837      0.078060      2.347410      4.211350      5.376000
     5.389940      4.380200      2.461506      1.123713      0.107016
     0.007574     -0.149443     -0.797230     -0.582210      0.082910
     0.271580     -0.045570      0.379430      0.247770     -0.890956
    -1.582430     -1.954532     -1.980965     -2.000433

! phi = -30.0
    -1.174720      1.067030      4.180460      6.741610      6.070770
     4.806470      2.783340      1.320806      0.765978     -0.008448
     0.276860     -0.707140      1.314360      1.522590      1.915550
     2.223490      0.194290      0.534000      0.331780     -1.595147
    -2.849141     -3.550465     -3.277369     -2.655135

! phi = -15.0
     0.293590      5.588070      3.732620      3.217620      3.272450
     2.517320      1.588700      1.381760      0.856410      0.655170
     1.616970      0.846920      0.511070      0.740760      1.021020
     1.616580     -0.342400      0.181770     -0.613920     -2.558037
    -3.786839     -3.807325     -3.155346     -1.749204

! phi =   0.0
     2.832310      0.787990      0.323280      0.479230      0.628600
     0.976330      1.238750      1.671950      1.645480      2.520340
     1.606970      0.776350      0.119780      0.070390      0.121170
    -1.569230     -1.213010     -1.846360     -2.744510     -3.792530
    -3.934880     -3.615930     -2.675750     -0.924170

! phi =  15.0
    -0.778340     -1.912680     -2.052140     -1.846280     -1.047430
     0.183400      1.682950      2.223500      1.358370      2.448660
     1.436920      0.678570     -0.237060     -0.535320     -0.790380
    -2.182580     -3.251140     -4.195110     -4.269270     -3.908210
    -3.455620     -2.773970      1.755370      0.313410
```

```
! phi =  30.0
    -2.963810      -3.483730      -3.441809      -2.400349      -1.125083
     0.336200       1.428450       1.394630       0.970370       2.462720
     1.522430       0.553620      -0.407380      -1.482950      -3.613920
    -4.159810      -4.709721      -4.496271      -3.764540      -2.959140
    -1.963850      -1.071260      -1.599580      -2.445320

! phi =  45.0
    -4.021496      -3.836549      -3.365327      -2.334377      -0.984725
     0.362000       0.814380       0.754110       0.502370       1.903420
     0.770220      -0.416420      -3.286310      -3.875270      -4.611550
    -5.287977      -5.146239      -4.038627      -2.865450      -2.368170
    -2.860490      -3.416560      -3.666490      -3.595217

! phi =  60.0
    -3.353683      -2.984416      -2.317412      -1.240143      -0.257890
     0.722610       0.668070       0.438130       2.395330       1.632470
    -2.041450      -3.218100      -3.915080      -4.568574      -5.096776
    -5.526955      -5.005312      -3.777879      -2.840678      -3.508820
    -3.756430      -3.640810      -3.451845      -3.342810

! phi =  75.0
    -2.248733      -1.641080      -1.010583       0.039656       0.636063
     0.823710       0.517140      -0.013120      -0.370910      -1.192809
    -2.305650      -3.420580      -4.484960      -5.597237      -5.601264
    -5.727739      -4.740525      -3.819378      -3.685150      -4.151360
    -4.170739      -3.725589      -3.736732      -2.620673

! phi =  90.0
    -1.720840      -1.177830      -0.428430       0.277730       0.807900
     0.803260       0.482510      -0.336900      -0.786270      -1.774070
    -2.793220      -3.828560      -5.211800      -6.294328      -6.617221
    -5.763953      -5.072995      -3.911450      -4.158306      -4.473413
    -4.099325      -3.769822      -3.157300      -2.651694

! phi = 105.0
    -1.850640      -1.092420      -0.445020       0.128490       1.005520
     0.884820       0.485850      -0.218470      -0.857670      -1.682330
    -3.014400      -4.481110      -6.053510      -6.865400      -6.871130
    -5.728240      -3.912230      -4.802110      -5.034640      -4.715990
    -4.600554      -4.086721      -3.274630      -2.410940

! phi = 120.0
    -1.969230      -1.116650      -0.540250      -0.150330       0.763520
     1.038890       0.758480       0.313530      -0.333050      -1.872770
    -3.366270      -5.008260      -6.124810      -7.034830      -6.724320
    -3.700200      -4.510620      -5.185650      -5.361620      -4.847490
    -4.444320      -4.004260      -3.415720      -2.751230

! phi = 135.0
    -2.111250      -1.168960      -0.322790      -0.006920       0.316660
     1.086270       0.939170       0.625340      -0.166360      -1.830310
    -3.469470      -4.946030      -6.112560      -1.915580      -4.047310
    -4.996740      -4.996730      -4.842690      -4.886620      -4.300540
    -4.494620      -4.442210      -4.163570      -3.183510

! phi = 150.0
    -1.757590      -0.403620       0.023920       0.362390       0.634520
     1.264920       1.361360       0.948420      -0.073680      -1.483560
    -3.152820       1.835120      -1.762860      -5.093660      -5.744830
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    -5.390070     -4.783930     -4.190630     -4.115420     -4.042280
    -4.125570     -4.028550     -4.026100     -2.937910

! phi = 165.0
    -0.810590     -0.071500      0.378890      0.543310      1.277880
     1.641310      1.698840      1.519950      0.631950     -1.088670
    -2.736530     -0.735240     -4.563830     -6.408350     -5.889450
    -5.141750     -4.194970     -3.666490     -3.843450     -3.555000
    -3.548722     -3.246995     -2.751289     -1.814368

CG2O1    NH1      CT1      C NH1      CT1      C        NG2S1 24


! phi = -180.0
     0.126790      0.768700      0.971260      1.250970      2.121010
     2.720430      2.089440      1.789790      0.780870     -0.688474
     1.001130     -2.200520     -4.827670     -4.821447     -4.913223
    -3.591106     -2.766446     -2.784200     -2.454589     -2.346991
    -2.335350     -1.522656     -0.951542     -0.036650

! phi = -165.0
    -0.127133      1.377090      1.577020      1.872290      2.398990
     2.486630      2.436754      1.929070      1.086456      0.643400
     0.258676     -2.800440     -4.009477     -4.135306     -3.420090
    -2.602140     -2.299128     -1.501241     -1.101780     -0.861434
    -0.640168     -0.207701     -1.076344     -1.122030

! phi = -150.0
     0.084069      1.420317      1.624350      2.047200      2.653910
     2.716410      2.321416      1.985454      1.557466      2.463293
    -0.225720     -1.815886     -2.583256     -3.006154     -2.551995
    -1.890683     -1.354215     -0.727243      0.068512     -0.225016
    -0.765479     -1.283444     -1.293226     -0.816303

! phi = -135.0
     0.927992      1.521370      2.242218      2.546305      3.111384
     2.918410      2.460813      2.187970      2.058314      1.852278
     0.115935     -1.183897     -1.995479     -2.278329     -1.959136
    -1.340467     -0.932949      0.021790      0.313725     -0.517358
    -1.152891     -0.983285     -0.566518     -0.442565

! phi = -120.0
     1.357468      1.959160      2.698894      3.037857      3.698960
     3.558453      2.639296      2.773853      2.719664      1.627997
     0.705667     -0.785637     -2.118268     -2.628489     -1.803113
    -0.425969     -0.062320      0.439040      0.910952     -0.546994
    -0.968118     -0.856791     -0.250116      0.449309

! phi = -105.0
     2.045006      2.544424      2.818030      3.088582      3.370620
     3.551568      3.073520      2.903794      2.956634      2.124759
     0.906487     -0.823628     -2.090819     -2.241579     -1.456524
     0.206160      0.082195      0.771710      1.040241     -0.124647
    -0.316550     -0.164333      0.314474      0.733747

! phi = -90.0
     1.451735      2.748481      2.738185      3.156796      3.450028
     3.344157      3.180200      3.898724      3.335030      2.440579
     0.912671     -0.606502     -1.511772     -1.620864     -0.962798
    -0.020653      0.415153      0.908250      0.459433      0.145910
```

```
     -0.071054      0.017622      0.280839      0.748823

! phi = -75.0
      1.378160      3.345958      2.352424      3.063543      3.814070
      3.700796      3.580310      4.212293      3.536425      1.693809
      0.095172     -0.682452     -0.123614     -0.427765     -0.598368
      0.226352      0.423308      0.301999      0.551890      0.191719
     -0.253585     -0.190548     -0.253412      0.468922

! phi = -60.0
      0.237754      1.229980      1.716960      3.168570      4.208190
      4.391860      4.276080      3.673107      2.272295     -0.482789
     -0.406695     -0.038919     -0.357600     -0.823341     -0.173146
      0.139806      0.267796      0.322420      0.309664     -0.666399
     -0.948631     -1.534365     -1.479968     -0.204264

! phi = -45.0
     -1.184837      0.078060      2.347410      4.211350      5.376000
      5.389940      4.380200      2.461506      1.123713      0.107016
      0.007574     -0.149443     -0.797230     -0.582210      0.082910
      0.271580     -0.045570      0.379430      0.247770     -0.890956
     -1.582430     -1.954532     -1.980965     -2.000433

! phi = -30.0
     -1.174720      1.067030      4.180460      6.741610      6.070770
      4.806470      2.783340      1.320806      0.765978     -0.008448
      0.276860     -0.707140      1.314360      1.522590      1.915550
      2.223490      0.194290      0.534000      0.331780     -1.595147
     -2.849141     -3.550465     -3.277369     -2.655135

! phi = -15.0
      0.293590      5.588070      3.732620      3.217620      3.272450
      2.517320      1.588700      1.381760      0.856410      0.655170
      1.616970      0.846920      0.511070      0.740760      1.021020
      1.616580     -0.342400      0.181770     -0.613920     -2.558037
     -3.786839     -3.807325     -3.155346     -1.749204

! phi =   0.0
      2.832310      0.787990      0.323280      0.479230      0.628600
      0.976330      1.238750      1.671950      1.645480      2.520340
      1.606970      0.776350      0.119780      0.070390      0.121170
     -1.569230     -1.213010     -1.846360     -2.744510     -3.792530
     -3.934880     -3.615930     -2.675750     -0.924170

! phi =  15.0
     -0.778340     -1.912680     -2.052140     -1.846280     -1.047430
      0.183400      1.682950      2.223500      1.358370      2.448660
      1.436920      0.678570     -0.237060     -0.535320     -0.790380
     -2.182580     -3.251140     -4.195110     -4.269270     -3.908210
     -3.455620     -2.773970      1.755370      0.313410

! phi =  30.0
     -2.963810     -3.483730     -3.441809     -2.400349     -1.125083
      0.336200      1.428450      1.394630      0.970370      2.462720
      1.522430      0.553620     -0.407380     -1.482950     -3.613920
     -4.159810     -4.709721     -4.496271     -3.764540     -2.959140
     -1.963850     -1.071260     -1.599580     -2.445320

! phi =  45.0
     -4.021496     -3.836549     -3.365327     -2.334377     -0.984725
```

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      0.362000      0.814380      0.754110      0.502370      1.903420
      0.770220     -0.416420     -3.286310     -3.875270     -4.611550
     -5.287977     -5.146239     -4.038627     -2.865450     -2.368170
     -2.860490     -3.416560     -3.666490     -3.595217

! phi =  60.0
     -3.353683     -2.984416     -2.317412     -1.240143     -0.257890
      0.722610      0.668070      0.438130      2.395330      1.632470
     -2.041450     -3.218100     -3.915080     -4.568574     -5.096776
     -5.526955     -5.005312     -3.777879     -2.840678     -3.508820
     -3.756430     -3.640810     -3.451845     -3.342810

! phi =  75.0
     -2.248733     -1.641080     -1.010583      0.039656      0.636063
      0.823710      0.517140     -0.013120     -0.370910     -1.192809
     -2.305650     -3.420580     -4.484960     -5.597237     -5.601264
     -5.727739     -4.740525     -3.819378     -3.685150     -4.151360
     -4.170739     -3.725589     -3.736732     -2.620673

! phi =  90.0
     -1.720840     -1.177830     -0.428430      0.277730      0.807900
      0.803260      0.482510     -0.336900     -0.786270     -1.774070
     -2.793220     -3.828560     -5.211800     -6.294328     -6.617221
     -5.763953     -5.072995     -3.911450     -4.158306     -4.473413
     -4.099325     -3.769822     -3.157300     -2.651694

! phi = 105.0
     -1.850640     -1.092420     -0.445020      0.128490      1.005520
      0.884820      0.485850     -0.218470     -0.857670     -1.682330
     -3.014400     -4.481110     -6.053510     -6.865400     -6.871130
     -5.728240     -3.912230     -4.802110     -5.034640     -4.715990
     -4.600554     -4.086721     -3.274630     -2.410940

! phi = 120.0
     -1.969230     -1.116650     -0.540250     -0.150330      0.763520
      1.038890      0.758480      0.313530     -0.333050     -1.872770
     -3.366270     -5.008260     -6.124810     -7.034830     -6.724320
     -3.700200     -4.510620     -5.185650     -5.361620     -4.847490
     -4.444320     -4.004260     -3.415720     -2.751230

! phi = 135.0
     -2.111250     -1.168960     -0.322790     -0.006920      0.316660
      1.086270      0.939170      0.625340     -0.166360     -1.830310
     -3.469470     -4.946030     -6.112560     -1.915580     -4.047310
     -4.996740     -4.996730     -4.842690     -4.886620     -4.300540
     -4.494620     -4.442210     -4.163570     -3.183510

! phi = 150.0
     -1.757590     -0.403620      0.023920      0.362390      0.634520
      1.264920      1.361360      0.948420     -0.073680     -1.483560
     -3.152820      1.835120     -1.762860     -5.093660     -5.744830
     -5.390070     -4.783930     -4.190630     -4.115420     -4.042280
     -4.125570     -4.028550     -4.026100     -2.937910

! phi = 165.0
     -0.810590     -0.071500      0.378890      0.543310      1.277880
      1.641310      1.698840      1.519950      0.631950     -1.088670
     -2.736530     -0.735240     -4.563830     -6.408350     -5.889450
     -5.141750     -4.194970     -3.666490     -3.843450     -3.555000
     -3.548722     -3.246995     -2.751289     -1.814368
```

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CG2O1  NH1  CTD1  C    NH1  CTD1  C    NH1   24
!-180
      0.318000       0.161300      -0.741600      -1.303800      -2.114700
     -2.129330      -2.239660      -2.572520      -2.555440      -3.375000
     -4.686760      -4.591700      -4.627070      -2.004200       1.196740
     -0.505800       0.958820       1.968850       2.270310       2.902970
      2.303900       1.436500       1.159000       0.957800

!-165
     -0.602100      -1.593500      -2.518600      -3.010270      -3.315480
     -3.326870      -3.621140      -3.447370      -3.971900      -4.909480
     -5.645370      -6.183050      -4.382570      -0.544900      -2.544430
     -0.901520       0.815600       1.702920       1.882240       1.826490
      1.464090       0.732300       0.572900       0.128200

!-150
     -1.550010      -2.719240      -3.799900      -3.804440      -3.908390
     -3.834080      -3.912760      -3.989630      -4.580850      -5.180800
     -5.551653      -4.939713      -1.574530       2.019030      -2.977770
     -1.303570       0.104220       1.125620       1.539620       1.443750
      0.814930       0.545220       0.212300      -0.206550

!-135
     -1.919560      -2.986620      -3.966600      -4.249090      -4.309170
     -4.120940      -4.711580      -4.670431      -4.825664      -4.833039
     -3.895350      -1.748976      -5.944140      -4.773780      -3.285510
     -1.651960       0.008830       0.799790       1.114040       1.261370
      0.491610       0.169660      -0.143000      -0.983360

!-120
     -1.792360      -2.574640      -3.240070      -3.832430      -4.278530
     -4.687260      -5.205396      -5.031707      -4.359533      -3.545746
     -6.568035      -6.863508      -5.928660      -4.813000      -3.172860
     -1.681690      -0.146590       0.496930       0.939250       1.216890
      0.939030       0.024420      -0.364730      -0.940250

!-105
     -1.676510      -2.239220      -3.105060      -3.921610      -4.441700
     -4.561879      -4.882414      -4.649232      -3.754099      -5.566184
     -6.683430      -6.663330      -5.848020      -4.271050      -2.796960
     -1.461650      -0.643270      -0.013500       0.682650       1.073420
      1.188540       0.308530      -0.266340      -0.915370

!-90
     -1.545490      -2.479890      -2.989360      -3.607340      -3.943710
     -4.322090      -4.006360      -3.753650      -4.908200      -5.583350
     -6.423640      -6.093210      -5.004050      -3.607860      -2.557550
     -1.542900      -0.569000      -0.126800       0.685300       0.998100
      0.995970       0.462260      -0.246420      -0.998620

!-75
     -2.073750      -2.446160      -3.565280      -3.562650      -4.017330
     -4.003830      -3.535470      -3.663780      -4.577080      -5.554240
     -5.420920      -5.414150      -4.293180      -3.212010      -2.092400
     -0.995800      -0.189500       0.168400       0.701600       1.007800
      0.817400       0.219300      -0.831880      -1.463780

!-60
     -3.152770      -3.137590      -3.251010      -3.455590      -3.593703
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     -3.356621     -2.687230     -3.623970     -4.846670     -5.363020
     -4.930860     -4.397530     -3.728840     -3.020230     -1.844300
      1.819200      2.580400      0.625100      0.854200      0.907700
     -0.073900     -1.054400     -2.127020     -2.788900

!-45
     -3.770150     -3.342460     -3.435857     -3.233680     -2.697704
     -2.206907     -2.705960     -3.879900     -4.985030     -5.124630
     -4.443270     -3.700260     -3.097500     -0.220130      0.969900
      2.113150      0.716400      0.961900      1.015200      0.560500
     -0.783400     -2.123570     -3.139530     -3.594750

!-30
     -2.695470     -2.217380     -1.439010     -0.914050     -1.800940
     -2.792774     -3.600060     -4.332720     -4.547400     -3.999100
     -3.448410     -1.305800     -0.219190      0.752670      1.727130
      2.668630      1.173190      1.589820      1.620230      0.534230
     -0.915690     -2.172410     -3.190240     -3.214490

!-15
     -0.577690      0.468040      1.911320     -2.603130     -3.261575
     -3.724230     -4.092000     -4.025430     -3.089640     -2.017270
     -0.620850     -0.355680     -0.052690      0.865190      1.624910
      2.635730      1.539850      2.399590      1.862800      0.373900
     -0.840940     -1.616660     -1.795490     -1.652460

!0
      2.983660     -0.731340     -2.449770     -3.374620     -3.714280
     -3.587390     -2.552950     -1.668870     -1.037370     -1.389120
      0.305970      0.254170      0.301930      0.955800      1.783820
      2.694860      1.815380      1.838200      1.412000      1.158560
      0.826180      0.701570      0.549430      0.944190

!15
      0.516980     -1.453141     -2.871540     -3.554290     -3.554230
     -2.340490     -0.408410      0.382550     -0.135960      1.830730
      1.229850      0.941560      0.702980      1.028110      1.797600
      0.830350      1.023040      1.546780      1.757890      2.690890
      3.459170      3.410046      3.899220      5.776320

!30
     -0.862960     -2.353690     -3.002680     -3.299920     -2.614530
     -1.371160      0.552350      0.761870      0.431270      2.449210
      2.135430      1.728890      1.507040     -0.517670      0.466670
      0.169940      0.932780      1.487640      2.948260      4.980480
      6.256220      6.939911      4.394500      1.306322

!45
     -0.888920     -1.727400     -1.736220     -1.725400     -1.359300
     -0.668800      0.476000      0.617900      0.194000      0.496600
      0.296100     -0.384200     -0.607670      0.044310      0.189700
      0.275600      1.289210      2.626790      4.550970      5.572150
      5.571590      4.423240      2.600280      0.373350

!60
      0.477650      0.015200     -1.274500     -1.332300     -0.746600
     -0.459700      0.522600      0.536700      0.480700      0.347700
      0.027200     -0.632100     -0.174500      0.136700     -0.239500
     -0.322300      2.427630      3.838230      4.445790      4.572180
      4.408980      3.392150      1.959630      1.483230
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!75
      1.564200      0.652600     -0.071900     -0.009100     -0.071100
      0.376500      0.736900      0.484900      0.605400      0.412600
     -0.412200     -0.252200      0.044600     -0.518700      0.253000
      1.845200      3.690420      4.370540      3.741090      3.869090
      3.993580      3.251780      2.549500      3.542540

!90
      1.624000      0.922100      0.454500      0.192500      0.105500
      0.324700      0.640500      1.090200      0.601400      0.169800
     -0.777900     -1.448000     -1.345400     -0.443700      1.071200
      2.597020      3.488740      4.051840      3.335460      3.503140
      3.612780      3.323710      2.909250      2.919700

!105
      2.216200      0.905700      0.488100      0.010900     -0.138900
      0.056000      1.225000      0.963200      0.276600      0.397500
     -1.274200     -2.066100     -1.919700     -0.656900      1.070000
      2.284170      3.112630      3.058460      3.229440      3.710040
      3.531610      3.252290      2.985200      2.715100

!120
      1.530400      0.622100     -0.075800     -0.680200     -0.789200
     -0.366900      1.095800      0.627100      0.126200     -0.240800
     -1.624000     -2.452600     -1.945500     -0.616400      0.870830
      1.789390      2.878530      2.931690      2.798480      3.719400
      3.862340      3.203840      2.868200      2.130900

!135
      1.101400     -0.269000     -0.391000     -0.804800     -0.972800
     -0.337200      0.496800      0.205700     -0.750400     -1.160500
     -1.781500     -2.101700     -1.820130     -1.014040      0.280910
      2.019040      2.221130      2.349690      2.623870      3.083140
      3.277890      2.715500      2.414300      1.696300

!150
      0.255900     -0.642300     -1.115500     -1.103100     -0.583400
     -0.041400      0.253100     -0.544200     -1.173200     -1.711300
     -2.372180     -2.824240     -2.404170     -1.646520     -0.051970
      2.636860      1.722010      2.149900      2.486900      2.883800
      2.822900      2.218200      1.798300      1.594400

!165
      0.046900     -0.944200     -0.893100     -0.016800     -0.444100
     -0.665900     -0.907900     -1.309920     -2.110050     -2.412550
     -3.225790     -3.937160     -3.819750     -2.622840      0.443660
      0.817160      1.255900      2.097480      2.606750      2.658300
      2.572300      2.046800      1.753200      1.552400


END
RETURN
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