Supporting Information

Figure S1. Mean structure from the Accelerated MD simulations on the Set-1 poses bound with gp120 UNLIG. Overlay of the mean structure. The structures are colored by MD thermal factors. The color scale runs from blue (most stable) to red (least stable). The inset shows that BMS-626529 has nearly converged between the four different simulations with the caveat that the proteins have not. The Set-1:1and 2 simulations show the tightest convergence. Set-1:3 and 4 differ somewhat from each other and from the Set-1:1 and 2 simulations.

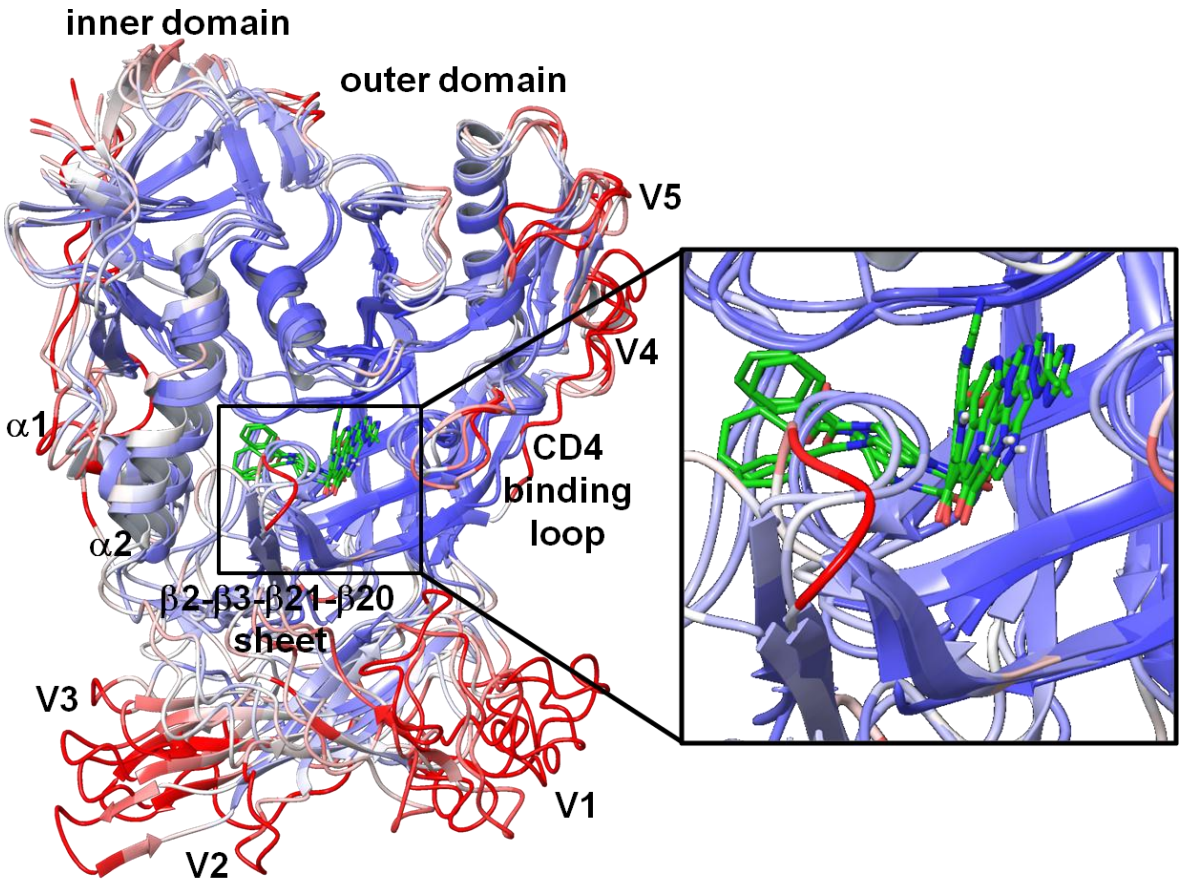
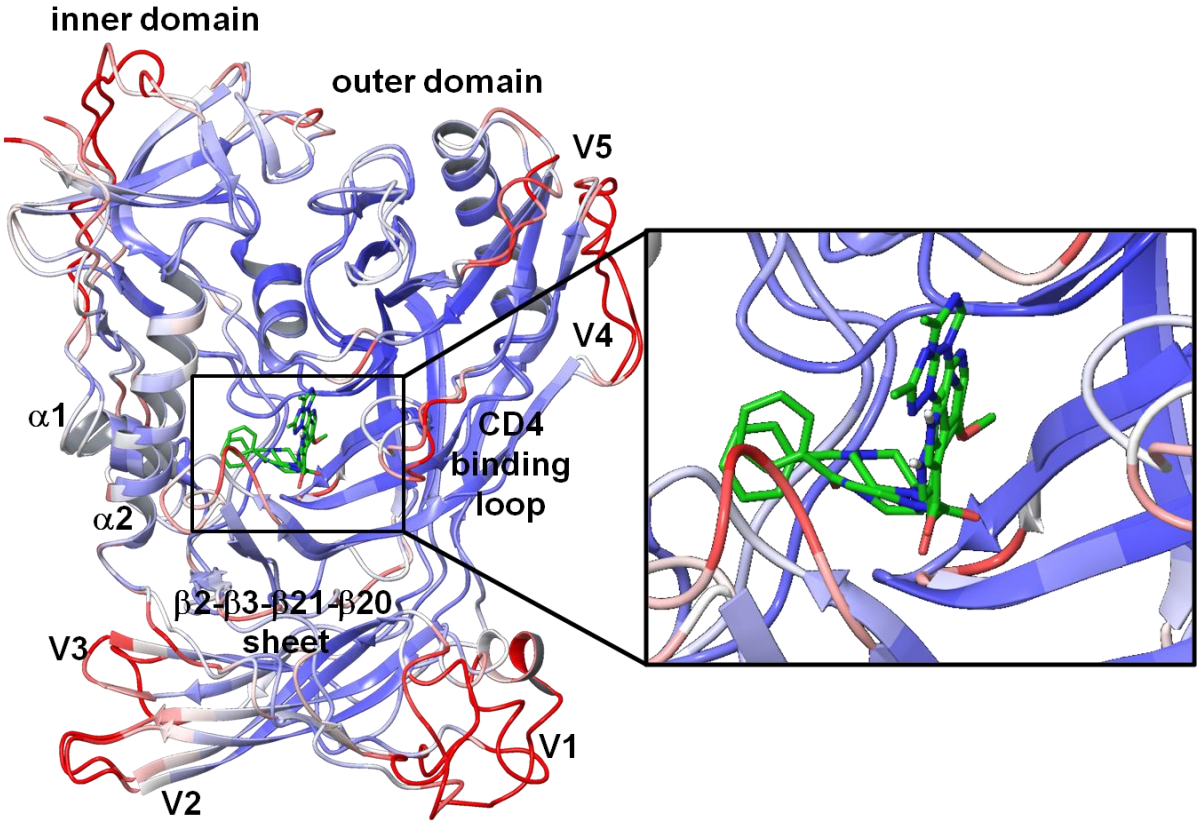


Figure S2: Mean structure from Set-1:1 and 2 simulations. Overlay of the mean structure from each simulation (averaged over 15–110-ns frames). The structures are colored by MD thermal factors. The color scale runs from blue (smallest fluctuation) to red (largest fluctuation). The inset shows that BMS-626529 has nearly converged between the two different simulations with the caveat that the proteins have not. Note that the piperazine ring is nearly flat in one structure and an up-chair in the other. The flat ring is due to averaging over multiple frames where nearly half the frames contain an up-chair while the other half contained the down-chair.



Videos S3, S4, and S5 portray the last 10 ns of the MD simulations of BMS-626529 bound to the gp120 "closed" UNLIG state, models Set-1:1, Set-1:2, and Set-2:3, respectively. PDB files were extracted in 500 ps intervals from the MD simulation and morphed from one another by creating three intermediate frames through linear interpolation using a Python script. The frames were rendered in PyMol (The PyMol Molecular Graphics System Version 1.5.0.4, Schrödinger LLC) and saved as PNG files. The PNG files were assembled into the video using MPlayer (MPlayer Version 1.1.0 MPlayer Team). Inner domain (orange), outer domain (green), V1/V2 (yellow), V3 (pink), β3–β2 sheet (light blue), β20–β21 (blue), CD4 binding loop (red), BMS-626529 (maroon). Yellow dotted lines depict hydrogen bonds.

Table S1: BMS-626529.pdb, BMS-626529.rtf, BMS-626529.prm files.

```
ATOM      1  C14 L0      1      -0.874  -1.932   8.836  1.00  0.00         L0
ATOM      2  H13 L0      1      -0.471  -1.880   7.828  1.00  0.00         L0
ATOM      3  C15 L0      1      -0.280  -1.194   9.855  1.00  0.00         L0
ATOM      4  H14 L0      1       0.610  -0.603   9.655  1.00  0.00         L0
ATOM      5  C16 L0      1      -0.833  -1.218  11.130  1.00  0.00         L0
ATOM      6  H15 L0      1      -0.352  -0.675  11.939  1.00  0.00         L0
ATOM      7  C17 L0      1      -2.004  -1.937  11.376  1.00  0.00         L0
ATOM      8  H16 L0      1      -2.472  -1.893  12.356  1.00  0.00         L0
ATOM      9  C18 L0      1      -2.574  -2.712  10.367  1.00  0.00         L0
ATOM     10  H17 L0      1      -3.472  -3.291  10.566  1.00  0.00         L0
ATOM     11  C19 L0      1      -1.988  -2.743   9.098  1.00  0.00         L0
ATOM     12  C13 L0      1      -2.544  -3.633   8.020  1.00  0.00         L0
ATOM     13  O3  L0      1      -3.731  -3.532   7.703  1.00  0.00         L0
ATOM     14  N2  L0      1      -1.674  -4.469   7.399  1.00  0.00         L0
ATOM     15  C12 L0      1      -0.365  -4.880   7.937  1.00  0.00         L0
ATOM     16  C10 L0      1       0.731  -4.366   6.979  1.00  0.00         L0
ATOM     17  H7  L0      1       1.708  -4.743   7.291  1.00  0.00         L0
ATOM     18  H8  L0      1       0.749  -3.273   6.982  1.00  0.00         L0
ATOM     19  H11 L0      1      -0.323  -5.970   8.006  1.00  0.00         L0
ATOM     20  H12 L0      1      -0.227  -4.450   8.932  1.00  0.00         L0
ATOM     21  C11 L0      1      -1.963  -5.048   6.085  1.00  0.00         L0
ATOM     22  H9  L0      1      -2.973  -4.776   5.769  1.00  0.00         L0
ATOM     23  H10 L0      1      -1.879  -6.137   6.127  1.00  0.00         L0
ATOM     24  C9  L0      1      -0.913  -4.458   5.120  1.00  0.00         L0
ATOM     25  H6  L0      1      -0.991  -3.368   5.098  1.00  0.00         L0
ATOM     26  H18 L0      1      -1.064  -4.851   4.111  1.00  0.00         L0
ATOM     27  N1  L0      1       0.426  -4.852   5.613  1.00  0.00         L0
ATOM     28  C8  L0      1       1.247  -5.580   4.803  1.00  0.00         L0
ATOM     29  O2  L0      1       0.944  -5.989   3.681  1.00  0.00         L0
ATOM     30  C7  L0      1       2.698  -5.909   5.345  1.00  0.00         L0
ATOM     31  O1  L0      1       3.024  -7.096   5.366  1.00  0.00         L0
ATOM     32  C1  L0      1       3.606  -4.868   5.848  1.00  0.00         L0
ATOM     33  C   L0      1       4.642  -5.169   6.712  1.00  0.00         L0
ATOM     34  H   L0      1       4.919  -6.123   7.144  1.00  0.00         L0
ATOM     35  N   L0      1       5.365  -4.056   7.010  1.00  0.00         L0
ATOM     36  H1  L0      1       6.163  -4.013   7.629  1.00  0.00         L0
ATOM     37  C3  L0      1       4.849  -2.974   6.339  1.00  0.00         L0
ATOM     38  C2  L0      1       3.709  -3.436   5.590  1.00  0.00         L0
ATOM     39  C5  L0      1       3.022  -2.465   4.818  1.00  0.00         L0
ATOM     40  O   L0      1       1.977  -2.899   4.034  1.00  0.00         L0
ATOM     41  C6  L0      1       0.961  -1.974   3.660  1.00  0.00         L0
ATOM     42  H3  L0      1       0.222  -2.492   3.044  1.00  0.00         L0
ATOM     43  H4  L0      1       1.409  -1.156   3.091  1.00  0.00         L0
ATOM     44  H5  L0      1       0.483  -1.579   4.560  1.00  0.00         L0
ATOM     45  C4  L0      1       3.483  -1.144   4.862  1.00  0.00         L0
ATOM     46  H2  L0      1       2.974  -0.366   4.297  1.00  0.00         L0
ATOM     47  N3  L0      1       4.553  -0.729   5.576  1.00  0.00         L0
ATOM     48  C20 L0      1       5.264  -1.632   6.296  1.00  0.00         L0
ATOM     49  N5  L0      1       6.436  -1.172   6.949  1.00  0.00         L0
ATOM     50  N4  L0      1       7.427  -1.996   7.320  1.00  0.00         L0
ATOM     51  C21 L0      1       8.327  -1.174   7.811  1.00  0.00         L0
ATOM     52  C23 L0      1       9.651  -1.681   8.331  1.00  0.00         L0
ATOM     53  H20 L0      1      10.127  -2.341   7.603  1.00  0.00         L0
ATOM     54  H21 L0      1       9.501  -2.243   9.255  1.00  0.00         L0
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ATOM     57  C22 L0      1       6.825   0.104   7.265  1.00  0.00         L0
ATOM     58  H19 L0      1       6.209   0.968   7.071  1.00  0.00         L0
END

* AMBER   ! Force Field for organic molecules
* Wang J, Wolf RM, Caldwell JW, Kollman PA, Case DA. Development and testing
* of a general amber force field. J Comput Chem 2004;25:1157-1174.
* Converted into CHARMM format
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* David R. Langley, Feb. 3, 2006
*
   22    0

AUTOGENERATE ANGLES DIHE
DEFA FIRS NONE LAST NONE

RESI L0       0.00
GROUP
ATOM   C14    gca    -0.10772
ATOM   H13    gha    0.13831
ATOM   C15    gca    -0.13266
ATOM   H14    gha    0.13743
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ATOM   H15    gha    0.13587
ATOM   C17    gca    -0.13256
ATOM   H16    gha    0.13793
ATOM   C18    gca    -0.09041
ATOM   H17    gha    0.14654
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ATOM   H8     gh1    0.05167
ATOM   H11    gh1    0.06040
ATOM   H12    gh1    0.07036
ATOM   C11    gc3    0.05818
ATOM   H9     gh1    0.05548
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ATOM   C9     gc3    0.06105
ATOM   H6     gh1    0.06441
ATOM   H18    gh1    0.06219
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ATOM   O2     go     -0.57646
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ATOM   H5     gh1    0.02774
ATOM   C4     gca    0.33916
ATOM   H2     gh4    0.03706
ATOM   N3     gnb    -0.66193
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ATOM   N5     gna    -0.09800
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ATOM   C23    gc3    -0.11818
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ATOM   H21    ghc    0.05781
ATOM   H22    ghc    0.05808
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ATOM   H19    gh5    0.09396
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BOND   N      H1
BOND   N      C3
BOND   C1     C2
BOND   C1     C7
BOND   C2     C3
BOND   C2     C5
BOND   C3     C20
BOND   C4     H2
BOND   C4     C5
BOND   C4     N3
BOND   C5     O
BOND   O      C6
BOND   C6     H3
BOND   C6     H4
BOND   C6     H5
BOND   C7     O1
BOND   C7     C8
BOND   C8     O2
BOND   C8     N1
BOND   N1     C9
BOND   N1     C10
BOND   C9     H6
BOND   C9     C11
BOND   C9     H18
BOND   C10    H7
BOND   C10    H8
BOND   C10    C12
BOND   C11    H9
BOND   C11    H10
BOND   C11    N2
BOND   C12    H11
BOND   C12    H12
BOND   C12    N2
BOND   N2     C13
BOND   C13    O3
BOND   C13    C19
BOND   C14    H13
BOND   C14    C15
BOND   C14    C19
BOND   C15    H14
BOND   C15    C16
BOND   C16    H15
BOND   C16    C17
BOND   C17    H16
BOND   C17    C18
BOND   C18    H17
BOND   C18    C19
BOND   N3     C20
BOND   C20    N5
BOND   C21    N4
BOND   C21    N6
BOND   C21    C23
BOND   N4     N5
BOND   C22    H19
BOND   C22    N5
BOND   C22    N6
BOND   C23    H20
BOND   C23    H21
BOND   C23    H22
IMPH   C19    C15    C14    H13
IMPH   C14    C16    C15    H14
IMPH   C15    C17    C16    H15
IMPH   C18    C16    C17    H16
IMPH   C19    C17    C18    H17
IMPH   C13    C18    C19    C14
IMPH   C19    N2     C13    O3
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IMPH   C8     C1     C7     O1
IMPH   C7     C2     C1     C
IMPH   C1     H      C      N
IMPH   C3     C      N      H1
IMPH   C2     C20    C3     N
IMPH   C3     C5     C2     C1
IMPH   C2     C4     C5     O
IMPH   C5     H2     C4     N3
IMPH   C3     N5     C20    N3
IMPH   C20    C22    N5     N4
IMPH   C23    N6     C21    N4
IMPH   H19    N5     C22    N6
IMPH    C8      C9      N1      C10 !DRL
IMPH    C13     C11     N2      C12 !DRL
END

* AMBER   ! Force Field for organic molecules
* Wang J, Wolf RM, Caldwell JW, Kollman PA, Case DA. Development and testing * of a
general amber force field. J Comput Chem 2004;25:1157-1174.
* Converted into CHARMM format
* David R. Langley, Feb. 3, 2006
*

BOND
 gc  gc    290.1   1.550
 gc  gn    478.2   1.345
 gc  go    648.0   1.214
 gc gc3    328.3   1.508
 gc gca    349.7   1.487
 gc gcc    377.4   1.462
 gc gcd    377.4   1.462
 gc gha    325.1   1.101
 gc gnc    438.8   1.371
 gc gnd    438.8   1.371
 gc gos    411.3   1.343
 gn  gn    469.7   1.390
 gn  go    646.6   1.264
 gn gna    486.8   1.379
 gn gnc    532.1   1.352
 gn gnd    532.1   1.352
 gn gos    372.3   1.429
 go  go    384.3   1.430
 go gos    306.3   1.504
gc3  gn    330.6   1.460
gc3  go    422.6   1.335
gc3 gc3    303.1   1.535
gc3 gca    323.5   1.513
gc3 gcc    337.3   1.499
gc3 gcd    337.3   1.499
gc3 gh1    335.9   1.093
gc3 ghc    337.3   1.092
gc3 gna    334.7   1.456
gc3 gnc    334.7   1.456
gc3 gnd    334.7   1.456
gc3 gos    301.5   1.439
gca  gn    372.3   1.422
gca  go    519.7   1.275
gca gca    478.4   1.387
gca gcc    411.7   1.434
gca gcd    411.7   1.434
gca gh4    342.9   1.088
gca gh5    347.2   1.085
gca gha    344.3   1.087
gca gna    470.3   1.350
gca gnb    483.1   1.342
gca gnc    492.9   1.336
gca gnd    492.9   1.336
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gcc gcc    418.3   1.429
gcc gcd    504.0   1.371
gcc gh4    350.1   1.083
gcc gh5    356.0   1.079
gcc gha    347.2   1.085
gcc gna    438.8   1.371
gcc gnc    431.6   1.376
gcc gnd    494.6   1.335
gcc gos    376.1   1.370
gcd  gn    426.0   1.380
gcd gcd    418.3   1.429
gcd gh4    350.1   1.083
gcd gh5    356.0   1.079
gcd gha    347.2   1.085
gcd gna    438.8   1.371
gcd gnc    494.6   1.335
gcd gnd    431.6   1.376
gcd gos    376.1   1.370
ghn  gn    410.2   1.009
ghn gna    406.6   1.011
gna  go    644.3   1.265
gna gna    453.3   1.401
gna gnc    535.7   1.350
gna gnd    535.7   1.350
gna gos    355.2   1.444
gnb gnb    550.2   1.342
gnc gnc    486.8   1.379
gnc gnd    602.9   1.315
gnc gos    414.9   1.395
gnd gnd    486.8   1.379
gnd gos    414.9   1.395
gos gos    343.6   1.466

ANGLE
 gc  gc  gc   62.300 111.680
 gc  gc  gn   69.900 104.810
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 gc  gc gc3   61.700 116.860
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 gc  gc gcd   64.000 111.670
 gc  gc gha   44.800 115.430
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 gc  gn  gc   67.400 119.630
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 gc  gn  go   71.600 118.900
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 gc  gn gna   68.200 119.200
 gc  gn gnc   68.600 120.310
 gc  gn gnd   68.600 120.310
 gc  gn gos   69.100 113.140
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 gc gca gca   64.600 120.140
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 gc gca gnd   64.400 130.800
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 gc gcc gcd   65.700 119.920
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 gc gcc gnc   64.300 130.800
 gc gcc gnd   70.100 112.910
 gc gcd  gn   68.200 116.060
 gc gcd gc3   64.900 112.750
 gc gcd gca   63.600 122.950
 gc gcd gcc   65.700 119.920
 gc gcd gcd   63.700 122.690
 gc gcd gha   47.000 117.020
 gc gcd gnc   70.100 112.910
 gc gcd gnd   64.300 130.800
 gc gna  gc   64.700 126.400
 gc gna  gn   66.300 124.660
 gc gna gc3   64.700 117.600
 gc gna gca   65.300 125.200
 gc gna ghn   48.800 118.000
 gc gnc gca   66.600 120.660
 gc gnc gcd   67.000 119.250
 gc gnd gca   66.600 120.660
 gc gnd gcc   67.000 119.250
 gc gos  gc   64.000 122.650
 gc gos gc3   63.600 115.140
 gc gos gca   64.600 117.610
 gc gos gcc   64.200 119.620
 gc gos gcd   64.200 119.620
 gn  gc  gn   75.400 111.700
 gn  gc  go   75.800 122.030
 gn  gc gnc   73.000 116.840
 gn  gc gnd   73.000 116.840
 gn  gc gos   74.700 115.250
 gn  gn  gn   69.900 114.620
 gn gc3  gn   68.800 113.810
 gn gca gnc   69.700 123.860
 gn gca gnd   69.700 123.860
 gn gcc  gc   68.200 116.060
 gn gcc gnd   70.900 123.860
 gn gcd gnc   70.900 123.860
 gn gna  gn   67.800 123.800
 gn gna gnc   69.600 119.850
 gn gna gnd   69.600 119.850
 gn gna gos   72.300 104.710
 gn gos  gn   67.200 108.310
 go  gc  go   79.100 127.330
 go  gc gos   76.200 122.430
 go  gn  go   73.400 128.610
 go gc3  go   73.400 122.300
 go gca  go   75.500 126.820
 go gna  go   74.000 126.200
 go gna gos   70.800 118.390
 go gos  go   62.800 114.680
gc3  gc  gn   67.900 115.150
gc3  gc  go   68.000 123.110
gc3  gc gc3   62.800 116.050
gc3  gc gca   62.300 119.530
gc3  gc gcc   67.200 104.510
gc3  gc gcd   67.200 104.510
gc3  gc gha   46.000 115.220
gc3  gc gos   69.300 111.960
gc3  gn gc3   64.000 112.620
gc3  gn gca   62.400 121.150
gc3  gn gcc   63.300 121.170
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gc3  gn gcd   63.300 121.170
gc3  gn ghn   46.000 116.780
gc3 gc3  gn   65.900 112.130
gc3 gc3 gc3   63.200 110.630
gc3 gc3 gca   62.500 114.610
gc3 gc3 gcc   64.700 108.100
gc3 gc3 gcd   64.700 108.100
gc3 gc3 gh1   46.400 110.070
gc3 gc3 ghc   46.400 110.050
gc3 gc3 gna   65.800 112.590
gc3 gc3 gos   67.800 108.420
gc3 gca gc3   62.400 116.800
gc3 gca gca   63.800 120.630
gc3 gcc gca   64.100 117.810
gc3 gcc gcc   64.700 115.970
gc3 gcc gcd   64.800 119.450
gc3 gcc gha   45.100 121.520
gc3 gcc gna   65.500 122.800
gc3 gcc gnc   65.800 121.440
gc3 gcc gnd   66.400 121.960
gc3 gcc gos   67.800 115.890
gc3 gcd gca   64.100 117.810
gc3 gcd gcc   64.800 119.450
gc3 gcd gcd   64.700 115.970
gc3 gcd gha   45.100 121.520
gc3 gcd gna   65.500 122.800
gc3 gcd gnc   66.400 121.960
gc3 gcd gnd   65.800 121.440
gc3 gcd gos   67.800 115.890
gc3 gna gc3   60.700 125.590
gc3 gna gca   63.100 124.360
gc3 gna gcc   62.600 125.090
gc3 gna gcd   62.600 125.090
gc3 gna gnc   65.700 120.460
gc3 gna gnd   65.700 120.460
gc3 gna gos   68.900 104.390
gc3 gnc gcd   67.600 109.510
gc3 gnd gcc   67.600 109.510
gc3 gos  gn   65.300 108.570
gc3 gos  go   65.600 103.000
gc3 gos gc3   62.100 113.410
gc3 gos gca   62.400 117.600
gc3 gos gcc   63.100 115.180
gc3 gos gcd   63.100 115.180
gc3 gos gna   64.500 109.910
gc3 gos gnc   64.800 112.730
gc3 gos gnd   64.800 112.730
gc3 gos gos   65.900 105.010
gca  gc  gn   69.400 112.030
gca  gc  go   68.700 123.440
gca  gc gca   62.800 119.530
gca  gc gcc   64.800 114.090
gca  gc gcd   64.800 114.090
gca  gc gha   46.800 114.120
gca  gc gos   68.800 115.540
gca  gn gca   64.500 116.800
gca  gn gcc   65.000 118.420
gca  gn gcd   65.000 118.420
gca  gn ghn   47.600 114.590
gca  gn gna   66.800 117.570
gca  gn gnc   68.800 113.030
gca  gn gnd   68.800 113.030
gca gc3 gca   63.600 112.470
gca gc3 gcc   65.200 108.080
gca gc3 gcd   65.200 108.080
gca gc3 gh1   46.800 110.950
gca gc3 ghc   47.000 110.150
gca gc3 gnc   68.200 106.510
```

```
gca gc3 gnd   68.200 106.510
gca gc3 gos   67.700 110.510
gca gca  gn   68.000 119.890
gca gca  go   70.900 123.430
gca gca gca   67.200 119.970
gca gca gcc   66.000 120.100
gca gca gcd   66.000 120.100
gca gca gh4   48.200 121.090
gca gca gha   48.500 120.010
gca gca gna   70.200 118.340
gca gca gnb   69.200 122.630
gca gca gnc   70.100 119.720
gca gca gnd   70.100 119.720
gca gca gos   69.800 119.200
gca gcc  gn   72.500 104.870
gca gcc gcc   67.700 111.040
gca gcc gcd   68.200 113.510
gca gcc gh4   45.600 128.660
gca gcc gha   46.400 124.040
gca gcc gnd   70.200 115.050
gca gcc gos   69.500 116.240
gca gcd  gn   72.500 104.870
gca gcd gcc   68.200 113.510
gca gcd gcd   67.700 111.040
gca gcd gh4   45.600 128.660
gca gcd gha   46.400 124.040
gca gcd gnc   70.200 115.050
gca gcd gos   69.500 116.240
gca gna  gn   67.300 122.000
gca gna  go   70.900 120.680
gca gna gca   67.100 119.800
gca gna gcc   68.500 113.150
gca gna gcd   68.500 113.150
gca gna ghn   48.200 122.770
gca gna gna   66.300 123.760
gca gna gnc   69.300 117.850
gca gna gnd   69.300 117.850
gca gna gos   69.700 109.460
gca gnb gca   68.600 115.860
gca gnb gnb   69.400 118.890
gca gnc  gn   73.800 104.690
gca gnc gca   70.700 109.950
gca gnc gcd   71.100 108.820
gca gnc gna   74.100 104.160
gca gnc gos   73.100 104.340
gca gnd  gn   73.800 104.690
gca gnd gca   70.700 109.950
gca gnd gcc   71.100 108.820
gca gnd gna   74.100 104.160
gca gnd gos   73.100 104.340
gca gos gca   63.600 118.960
gca gos gcc   66.200 109.770
gca gos gcd   66.200 109.770
gca gos gna   66.500 108.240
gca gos gnc   66.100 113.680
gca gos gnd   66.100 113.680
gcc  gc  gn   70.200 111.860
gcc  gc  go   68.900 125.710
gcc  gc gcc   65.300 114.450
gcc  gc gcd   65.700 112.790
gcc  gc gos   70.500 112.300
gcc  gn  gn   66.500 121.370
gcc  gn  go   70.100 120.540
gcc  gn gcc   68.800 108.920
gcc  gn ghn   47.500 121.520
gcc  gn gna   67.900 117.570
gcc  gn gnc   69.900 113.030
gcc  gn gos   67.600 115.560
```

```
gcc gc3 gcc   65.500 107.990
gcc gc3 gcd   67.300 102.350
gcc gc3 gh1   47.000 111.620
gcc gc3 ghc   47.200 110.860
gcc gc3 gnc   68.400 107.040
gcc gc3 gos   67.800 111.280
gcc gca gnb   66.900 126.210
gcc gcc  gn   67.900 119.890
gcc gcc gcc   67.900 110.700
gcc gcc gcd   68.200 114.190
gcc gcc gh4   45.600 129.470
gcc gcc gha   46.600 123.740
gcc gcc gna   72.200 106.800
gcc gcc gnc   70.000 113.420
gcc gcc gnd   71.100 112.560
gcc gcc gos   68.400 120.430
gcc gcd  gn   70.700 115.520
gcc gcd gcc   69.300 115.510
gcc gcd gcd   68.200 114.190
gcc gcd gh4   47.200 129.110
gcc gcd gha   48.400 122.890
gcc gcd gna   72.900 109.420
gcc gcd gnd   71.000 114.980
gcc gcd gos   70.000 120.300
gcc gna  gn   66.500 123.190
gcc gna  go   69.000 125.210
gcc gna gcc   68.900 109.900
gcc gna gcd   63.900 128.010
gcc gna ghn   47.200 124.660
gcc gna gna   65.900 123.430
gcc gna gnc   70.200 113.020
gcc gna gos   67.300 115.740
gcc gnc gcc   68.600 110.190
gcc gnc gcd   70.500 107.470
gcc gnc gna   73.400 102.970
gcc gnc gnd   72.500 107.940
gcc gnd  gn   74.000 104.150
gcc gnd gcd   70.500 107.470
gcc gnd gna   74.200 103.730
gcc gnd gnd   71.400 109.510
gcc gnd gos   72.200 106.990
gcc gos gcc   66.500 109.170
gcc gos gcd   62.700 122.990
gcc gos gna   65.500 111.660
gcc gos gnc   68.100 107.230
gcc gos gos   66.300 108.470
gcd  gc  gn   70.200 111.860
gcd  gc  go   68.900 125.710
gcd  gc gcd   65.300 114.450
gcd  gc gos   70.500 112.300
gcd  gn  gn   66.500 121.370
gcd  gn  go   70.100 120.540
gcd  gn gcd   68.800 108.920
gcd  gn ghn   47.500 121.520
gcd  gn gna   67.900 117.570
gcd  gn gnd   69.900 113.030
gcd  gn gos   67.600 115.560
gcd gc3 gcd   65.500 107.990
gcd gc3 gh1   47.000 111.620
gcd gc3 ghc   47.200 110.860
gcd gc3 gnd   68.400 107.040
gcd gc3 gos   67.800 111.280
gcd gca gnb   66.900 126.210
gcd gcc  gn   70.700 115.520
gcd gcc gcd   69.300 115.510
gcd gcc gh4   47.200 129.110
gcd gcc gha   48.400 122.890
gcd gcc gna   72.900 109.420
```

```
gcd gcc gnc   71.000 114.980
gcd gcc gos   70.000 120.300
gcd gcd  gn   67.900 119.890
gcd gcd gcd   67.900 110.700
gcd gcd gh4   45.600 129.470
gcd gcd gha   46.600 123.740
gcd gcd gna   72.200 106.800
gcd gcd gnc   71.100 112.560
gcd gcd gnd   70.000 113.420
gcd gcd gos   68.400 120.430
gcd gna  gn   66.500 123.190
gcd gna  go   69.000 125.210
gcd gna gcd   68.900 109.900
gcd gna ghn   47.200 124.660
gcd gna gna   65.900 123.430
gcd gna gnd   70.200 113.020
gcd gna gos   67.300 115.740
gcd gnc  gn   74.000 104.150
gcd gnc gna   74.200 103.730
gcd gnc gnc   71.400 109.510
gcd gnc gos   72.200 106.990
gcd gnd gcd   68.600 110.190
gcd gnd gna   73.400 102.970
gcd gnd gnc   72.500 107.940
gcd gos gcd   66.500 109.170
gcd gos gna   65.500 111.660
gcd gos gnd   68.100 107.230
gcd gos gos   66.300 108.470
gh1 gc3  gn   49.800 109.320
gh1 gc3  go   52.000 117.190
gh1 gc3 gh1   39.200 109.550
gh1 gc3 gna   49.900 109.450
gh1 gc3 gnc   50.100 108.570
gh1 gc3 gnd   50.100 108.570
gh1 gc3 gos   50.800 108.820
gh4 gca  gn   49.500 116.020
gh4 gca gna   51.900 114.650
gh4 gca gnb   51.800 115.940
gh4 gca gnc   51.500 118.360
gh4 gca gnd   51.500 118.360
gh4 gca gos   52.300 111.150
gh4 gcc  gn   50.400 117.620
gh4 gcc gna   50.200 119.660
gh4 gcc gnc   50.000 120.030
gh4 gcc gnd   51.400 119.110
gh4 gcc gos   52.300 111.890
gh4 gcd  gn   50.400 117.620
gh4 gcd gna   50.200 119.660
gh4 gcd gnc   51.400 119.110
gh4 gcd gnd   50.000 120.030
gh4 gcd gos   52.300 111.890
gh5 gca gnb   51.800 116.350
gh5 gca gnc   50.700 122.110
gh5 gca gnd   50.700 122.110
gh5 gcc gna   49.800 122.100
gh5 gcc gnc   49.300 123.700
gh5 gcc gnd   50.100 125.380
gh5 gcc gos   51.300 116.330
gh5 gcd gna   49.800 122.100
gh5 gcd gnc   50.100 125.380
gh5 gcd gnd   49.300 123.700
gh5 gcd gos   51.300 116.330
gha  gc  gn   52.400 112.370
gha  gc  go   54.300 121.940
gha  gc gha   37.900 115.610
gha  gc gos   53.200 110.340
gha gcc gna   49.800 121.500
gha gcc gnc   50.700 116.540
```

```
gha gcc gnd   51.400 118.880
gha gcc gos   52.500 110.860
gha gcd gna   49.800 121.500
gha gcd gnc   51.400 118.880
gha gcd gnd   50.700 116.540
gha gcd gos   52.500 110.860
ghc  gc  gn   51.100 120.000
ghc  gc  go   55.400 120.000
ghc  gc ghc   39.300 115.680
ghc  gc gos   52.900 113.580
ghc gc3  gn   49.800 109.500
ghc gc3 ghc   39.400 108.350
ghc gc3 gna   49.900 109.500
ghc gc3 gos   50.900 108.700
ghn  gn  gn   50.100 113.120
ghn  gn  go   53.800 116.320
ghn  gn ghn   39.700 117.850
ghn  gn gna   50.400 113.550
ghn  gn gos   50.100 108.900
ghn gna ghn   39.800 116.800
ghn gna gnc   50.000 119.610
ghn gna gnd   50.000 119.610
ghn gna gos   51.400 101.410
gna  gc  go   75.000 122.850
gna  gc gna   73.200 115.400
gna  gn gna   69.600 117.380
gna gc3 gna   69.100 113.490
gna gc3 gos   71.200 109.190
gna gca gna   74.500 113.320
gna gca gnb   70.200 128.560
gna gcc gnc   69.700 125.320
gna gcc gnd   74.800 112.020
gna gcd gnc   74.800 112.020
gna gcd gnd   69.700 125.320
gna gna gna   66.800 123.600
gna gna gnc   69.100 119.640
gna gna gnd   69.100 119.640
gna gna gos   70.200 109.470
gna gnc gnd   76.000 105.470
gna gnd gnc   76.000 105.470
gna gos gna   66.100 109.590
gnb gca gnb   71.200 125.840
gnb gca gnc   71.100 126.500
gnb gca gnd   71.100 126.500
gnb gnb gnb   70.400 121.040
gnc  gc  go   73.900 125.290
gnc  gn gnc   71.300 116.410
gnc gc3 gnc   70.000 110.610
gnc gc3 gos   69.300 115.410
gnc gca gnc   70.700 128.740
gnc gcc gnd   72.500 118.690
gnc gcd gnd   72.500 118.690
gnc gcd gos   73.000 119.140
gnc gna  go   72.000 122.790
gnc gna gnc   71.200 117.080
gnc gna gos   68.300 119.650
gnc gnc gnd   73.200 111.150
gnc gnd gnd   73.200 111.150
gnc gnd gos   74.400 107.220
gnc gos gnc   68.200 110.400
gnd  gc  go   73.900 125.290
gnd  gn gnd   71.300 116.410
gnd gc3 gnd   70.000 110.610
gnd gc3 gos   69.300 115.410
gnd gca gnd   70.700 128.740
gnd gcc gos   73.000 119.140
gnd gna  go   72.000 122.790
gnd gna gnd   71.200 117.080
```

```
gnd gna gos   68.300 119.650
gnd gnc gos   74.400 107.220
gnd gos gnd   68.200 110.400
gos  gc gos   77.800 107.490
gos  gn gos   71.300 106.530
gos gc3 gos   71.700 110.240
gos gca gos   74.000 113.730
gos gna gos   71.300 104.450

DIHE
  X   gc  gc   X  0.3000000000 2   180.0
  X   gc  gn   X  2.5000000000 2   180.0
  X   gc gc3   X  0.0000000000 2   180.0
  X   gc gca   X  3.6250000000 2   180.0
  gn  gc gca gca  0.6250000000 2   180.0 !DRL
  go  gc gca gca  0.6250000000 2   180.0 !DRL
  X   gc gcc   X  2.8750000000 2   180.0
  X   gc gcd   X  2.8750000000 2   180.0
  X   gc gna   X  0.3500000000 4   180.0
  X   gc gna   X  1.4500000000 2   180.0
  X   gc gnc   X  4.0000000000 2   180.0
  X   gc gnd   X  4.0000000000 2   180.0
  X   gc gos   X  2.7000000000 2   180.0
  X   gn  gn   X  1.1500000000 2     0.0
  X   gn gcc   X  1.6500000000 2   180.0
  X   gn gcd   X  1.6500000000 2   180.0
  X   gn gna   X  0.7000000000 2     0.0
  X   gn gnc   X  4.8000000000 2   180.0
  X   gn gnd   X  4.8000000000 2   180.0
  X   gn gos   X  1.1000000000 2     0.0
  X  gc3  gn   X  0.0000000000 2     0.0
  X  gc3 gc3   X  0.1555555556 3     0.0
  X  gc3 gca   X  0.0000000000 2     0.0
  X  gc3 gcc   X  0.0000000000 3     0.0
  X  gc3 gcd   X  0.0000000000 3     0.0
  X  gc3 gna   X  0.0000000000 2     0.0
  X  gc3 gos   X  0.3833333333 3     0.0
  X  gca  gn   X  0.4500000000 2   180.0
  X  gca gca   X  3.6250000000 2   180.0
  X  gca gna   X  1.1000000000 2   180.0 !DRL
  X  gca gnb   X  4.8000000000 2   180.0
  X  gca gnc   X  4.8000000000 2   180.0
  X  gca gnd   X  4.8000000000 2   180.0
  X  gca gos   X  0.9000000000 2   180.0
  X  gcc gcc   X  4.0000000000 2   180.0
  X  gcc gcd   X  4.0000000000 2   180.0
  X  gcc gna   X  1.7000000000 2   180.0
  X  gcc gnc   X  4.7500000000 2   180.0
  X  gcc gnd   X  4.7500000000 2   180.0
  X  gcd gcd   X  4.0000000000 2   180.0
  X  gcd gna   X  1.7000000000 2   180.0
  X  gcd gnc   X  4.7500000000 2   180.0
  X  gcd gnd   X  4.7500000000 2   180.0
  X  gna gna   X  0.9000000000 2     0.0
  X  gna gnc   X  4.8000000000 2   180.0
  X  gna gnd   X  4.8000000000 2   180.0
  X  gna gos   X  0.6500000000 2     0.0
  X  gnc gnc   X  4.0000000000 2   180.0
  X  gnc gnd   X  4.0000000000 2   180.0
  X  gnc gos   X  4.8000000000 2   180.0
  X  gnd gnd   X  4.0000000000 2   180.0
  X  gos gos   X  1.0000000000 1     0.0
 gc  gn gc3  gc 0.8000000000 1     0.0
 gc  gn gc3  gc 0.8500000000 2   180.0
 gc gcd gca gca 2.5500000000 2   180.0
 gn gc3  gc  gn 1.7000000000 1   180.0
 gn gc3  gc  gn 2.0000000000 2   180.0
 go  gc gos gc3 1.4000000000 1   180.0
```

```
 go  gc gos gc3 2.7000000000 2   180.0
gc3 gc3  gc  gn 0.0700000000 2     0.0
gc3 gc3  gc  gn 0.1000000000 4     0.0
gc3 gc3  gn  gc 0.1500000000 3   180.0
gc3 gc3  gn  gc 0.5000000000 4   180.0
gc3 gc3  gn  gc 0.5300000000 1     0.0
gc3 gc3 gc3 gc3 0.1800000000 3     0.0
gc3 gc3 gc3 gc3 0.2000000000 1   180.0
gc3 gc3 gc3 gc3 0.2500000000 2   180.0
gc3 gc3 gos  gc 0.3830000000 3     0.0
gc3 gc3 gos  gc 0.8000000000 1   180.0
gc3 gc3 gos gc3 0.1000000000 2   180.0
gc3 gc3 gos gc3 0.3830000000 3     0.0
gc3 gos gc3 gna 0.3830000000 3     0.0
gc3 gos gc3 gna 0.6500000000 2     0.0
gc3 gos gc3 gos 0.1000000000 3     0.0
gc3 gos gc3 gos 0.8500000000 2   180.0
gc3 gos gc3 gos 1.3500000000 1   180.0
gca gca gna gnd 1.5000000000 2   180.0 !DRL
gcc gcd gca gca 2.5500000000 2   180.0
gh1 gc3  gc  go 0.0800000000 3   180.0
gh1 gc3  gc  go 0.8000000000 1     0.0
gh1 gc3 gc3 gos 0.2500000000 1     0.0
ghc gc3  gc  go 0.0800000000 3   180.0
ghc gc3  gc  go 0.8000000000 1     0.0
ghc gc3 gc3 gc3 0.1600000000 3     0.0
ghc gc3 gc3 ghc 0.1500000000 3     0.0
ghc gc3 gc3 gos 0.2500000000 1     0.0
ghn  gn  gc  go 2.0000000000 1     0.0
ghn  gn  gc  go 2.5000000000 2   180.0
gnb gca gna gnd 1.5000000000 2   180.0 !DRL
gos gc3 gc3 gos 0.1440000000 3     0.0
gos gc3 gc3 gos 1.1750000000 2     0.0
gc3  gn gc3 gc3 0.7          3     0.0 !DRL

IMPR
  X   X  gc  go     10.500   2   180
  X   X  gn ghn      1.100   2   180
  X   X gca gha      1.100   2   180
  X   X gca ghc      1.100   2   180
  X   X gna ghn      1.100   2   180
  X   X  gn gc3     10.500   2   180
  X  go  gc  go     10.500   2   180
  X gc3  gn gc3     10.500   2   180
 gc gc3  gn  go      1.100   2   180
 gc gc3  gn ghn      1.100   2   180
 gc gca gca gc3      1.100   2   180
 gc gca gca gca      1.100   2   180
 gc gca gcd gcc      1.100   2   180
X X gc gos 1.100 2 180
X X gca gca 1.100 2 180
X X gca gcc 1.100 2 180
X X gca gcd 1.100 2 180
X X gca gn 1.100 2 180
X X gca gna 1.100 2 180
X X gca gnb 1.100 2 180
X X gca gnc 1.100 2 180
X X gca gnd 1.100 2 180
X X gca gos 1.100 2 180
X X gcc gcd 1.100 2 180
X X gcc gha 1.100 2 180
X X gcc gn 1.100 2 180
X X gcc gna 1.100 2 180
X X gcc gnc 1.100 2 180
X X gcc gnd 1.100 2 180
X X gcc go 1.100 2 180
X X gcc gos 1.100 2 180
X X gcd gcc 1.100 2 180
```

```
X X gcd gcd 1.100 2 180
X X gcd gha 1.100 2 180
X X gcd gn 1.100 2 180
X X gcd gna 1.100 2 180
X X gcd gnc 1.100 2 180
X X gcd gnd 1.100 2 180
X X gcd go 1.100 2 180
X X gcd gos 1.100 2 180
X X gn gc 1.100 2 180
X X gn gca 1.100 2 180
X X gn gcc 1.100 2 180
X X gn gcd 1.100 2 180
X X gn gn 1.100 2 180
X X gna gca 1.100 2 180
X X gna gcc 1.100 2 180
X X gna gcd 1.100 2 180
X X gna gnc 1.100 2 180
X X gna gnd 1.100 2 180
gc3 gca gca gna      1.100   2   180
gc3 gnc gcc gnd      1.100   2   180
gca  gc gca gc3      1.100   2   180
gca gca gca gc3      1.100   2   180
gca gca gca gcd      1.100   2   180
gca gca gca gna      1.100   2   180
gca gca gca gos      1.100   2   180
gca gca gna gc3      1.100   2   180
gca gcd gna gnd      1.100   2   180
gca gh4 gca gnb      1.100   2   180
gca ghc  gc  go      1.100   2   180
gca gna gca gnb      1.100   2   180
gcd gh4 gcc gna      1.100   2   180
gh5 gna gcd gnc      1.100   2   180
ghc  go  gc gos      1.100   2   180

 NONBONDED  NBXMOD 5  FSHIFT VSWITCH CDIEL -
     CUTNB 14.0  CTOFNB 12.0  CTONNB 10.0  EPS 1.0  E14FAC 0.83333333  WMIN 1.4

 gc   0  -0.08600  1.90800   0 -0.04300  1.90800
 gn   0  -0.17000  1.82400   0 -0.08500  1.82400
 go   0  -0.21000  1.66120   0 -0.10500  1.66120
gc3   0  -0.10940  1.90800   0 -0.05470  1.90800
gca   0  -0.08600  1.90800   0 -0.04300  1.90800
gcc   0  -0.08600  1.90800   0 -0.04300  1.90800
gcd   0  -0.08600  1.90800   0 -0.04300  1.90800
gh1   0  -0.01570  1.38700   0 -0.00785  1.38700
gh4   0  -0.01500  1.40900   0 -0.00750  1.40900
gh5   0  -0.01500  1.35900   0 -0.00750  1.35900
gha   0  -0.01500  1.45900   0 -0.00750  1.45900
ghc   0  -0.01570  1.48700   0 -0.00785  1.48700
ghn   0  -0.01570  0.60000   0 -0.00785  0.60000
gna   0  -0.17000  1.82400   0 -0.08500  1.82400
gnb   0  -0.17000  1.82400   0 -0.08500  1.82400
gnc   0  -0.17000  1.82400   0 -0.08500  1.82400
gnd   0  -0.17000  1.82400   0 -0.08500  1.82400
gos   0  -0.17000  1.68370   0 -0.08500  1.68370
```