Supporting Information

Aryl-fluorosulfate-based Lysine Covalent pan-Inhibitor of Apoptosis Proteins (IAPs) Antagonists with Cellular Efficacy

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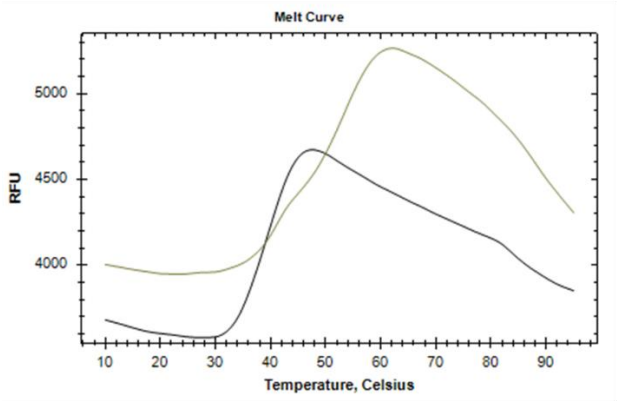
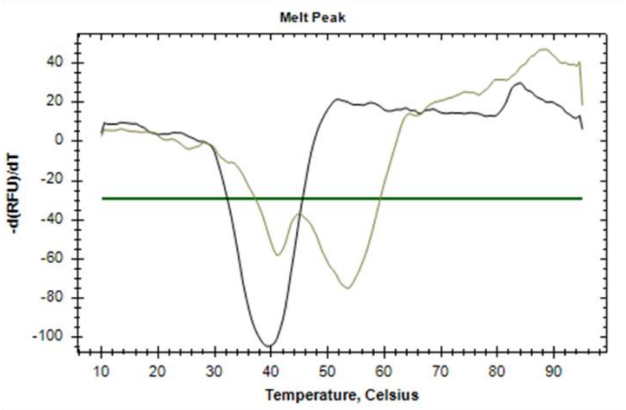
SI content:

Figure S1. Thermal shift data (ΔTm) obtained incubating XIAP-BIR3 and ligands for 2 hours at room temperature or 6 hours at 37°C, respectively

LCL161 2hr

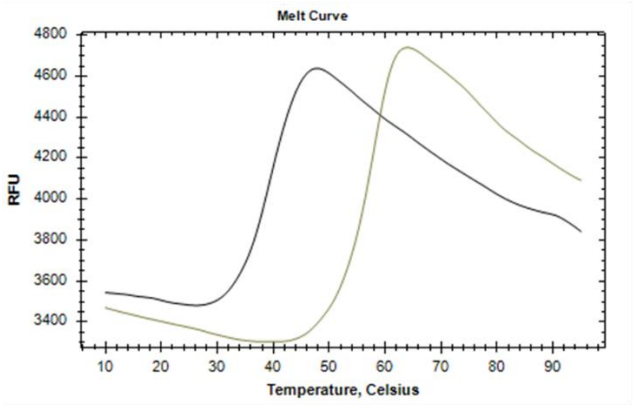


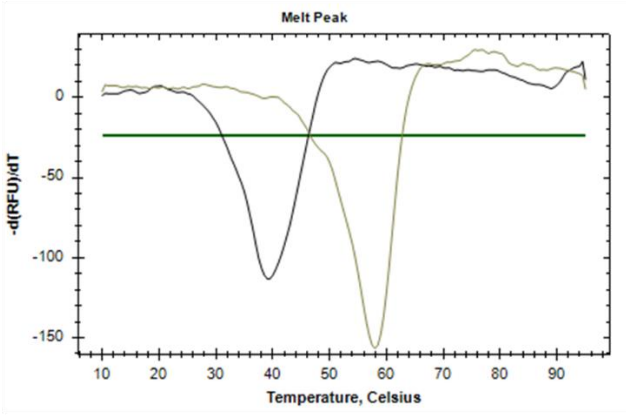


$T_{m\ BIR3\ WT}$= 39.5°C
$T_{m\ LCL161}$= 58°C

ΔT_m = 18.5°C

LCL161 6hr

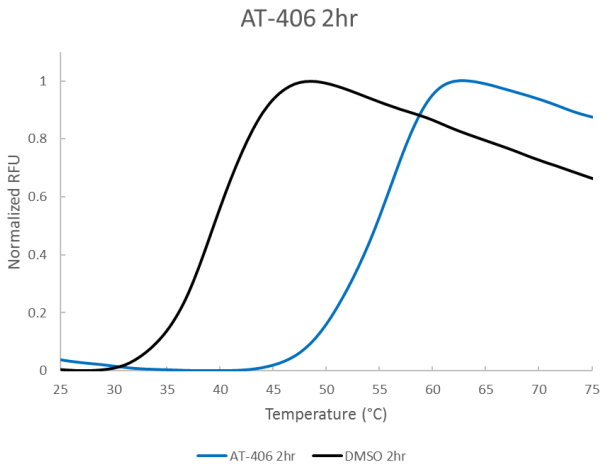


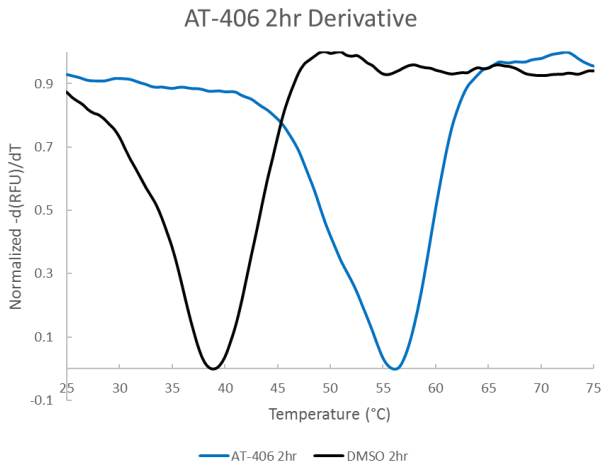


$T_{m\ BIR3\ WT}$= 39.5°C
$T_{m\ LCL161}$= 53.5°C

ΔT_m = 14°C

AT-406 2hr

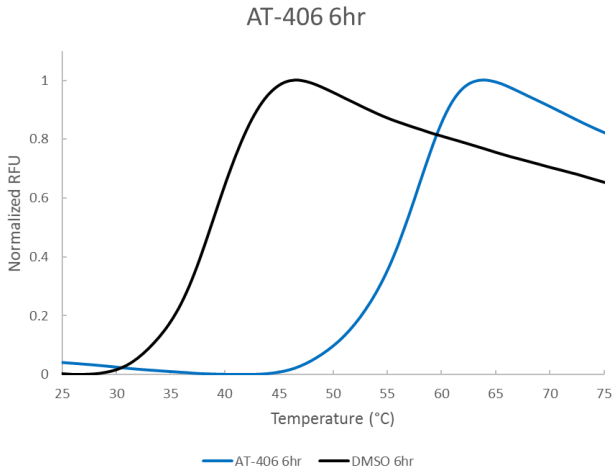


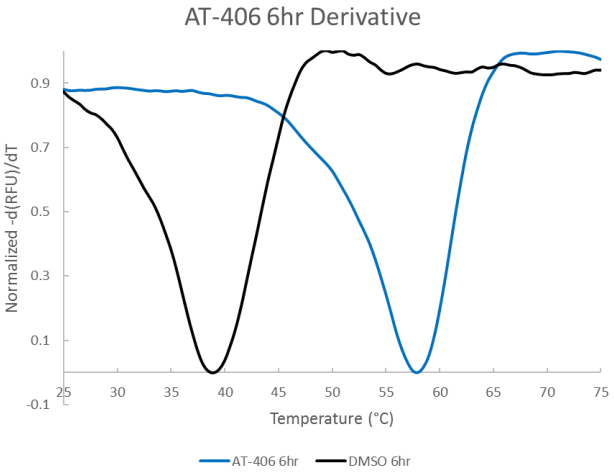


$T_{m\ BIR3}$= 39.0 °C
$T_{m\ AT\text{-}406}$= 56.0 °C

ΔT_m= 17.0 °C

AT-406 6hr

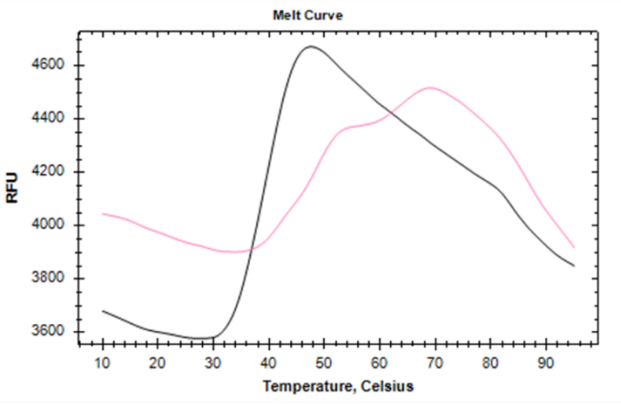


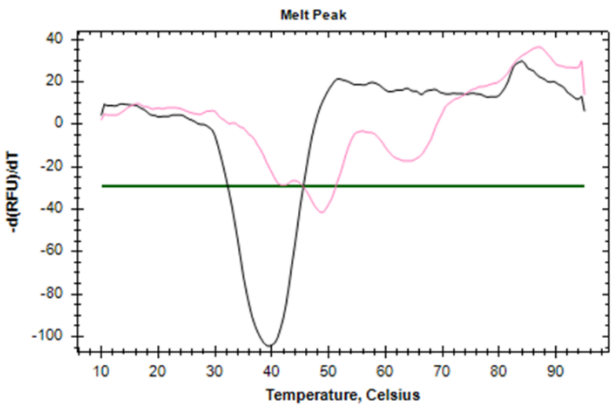


$T_{m\ BIR3}$= 39.0 °C
$T_{m\ AT\text{-}406}$= 58.0 °C

ΔT_m= 19.0 °C

Compound 1 2hr

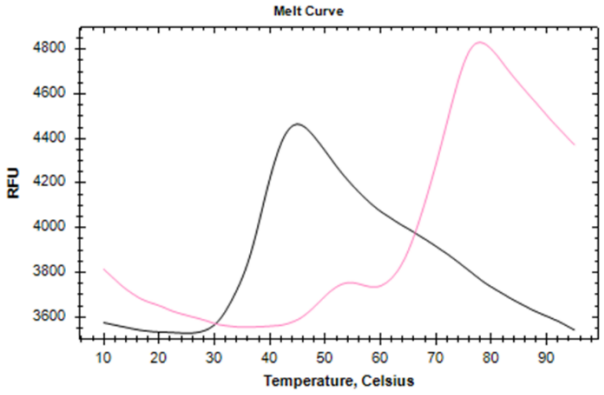


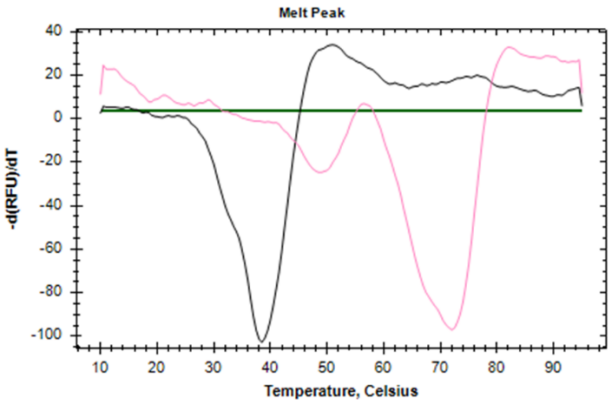


$T_{m\ BIR3\ WT}$= 39.5°C
$T_{m\ 142B12}$= 49°C

ΔT_m = 9.5°C

Compound 1 6hr

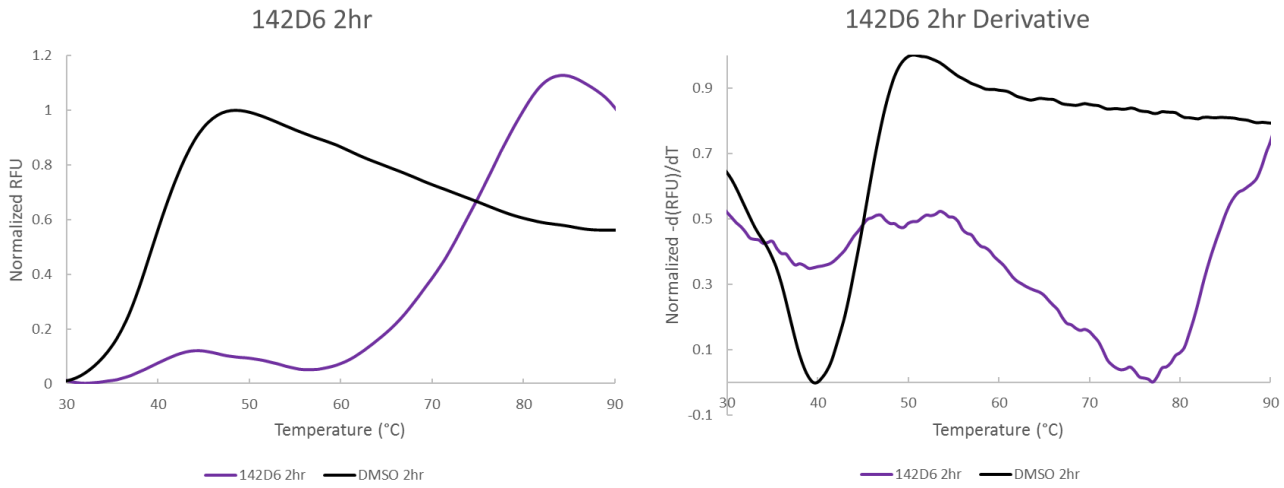




$T_{m\ BIR3\ WT}$= 38.5°C
$T_{m\ 142B12}$= 72°C

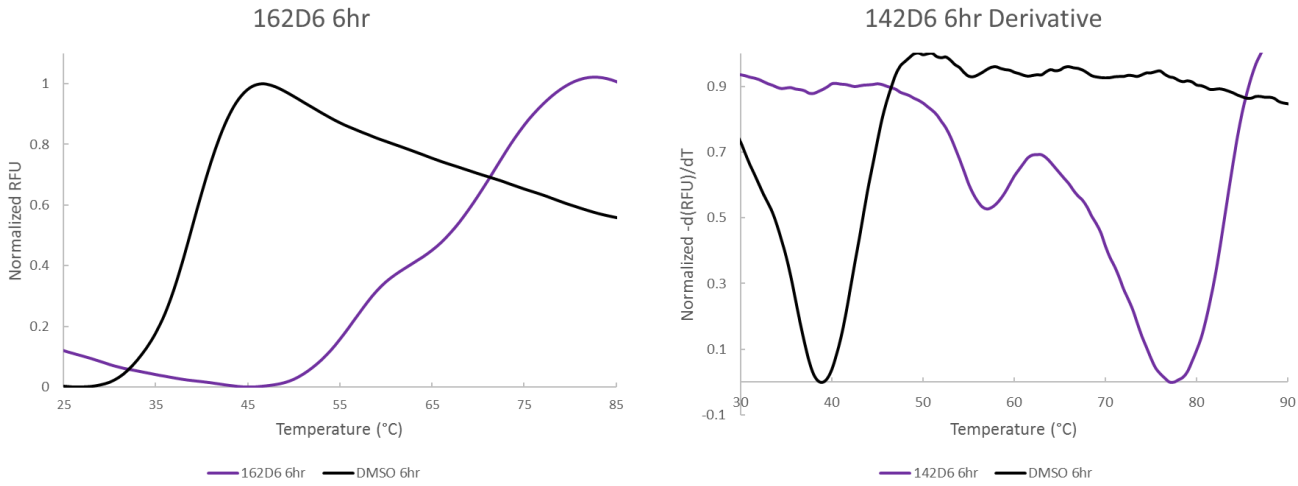
ΔT_m = 33.5°C

Compound 2 2hr



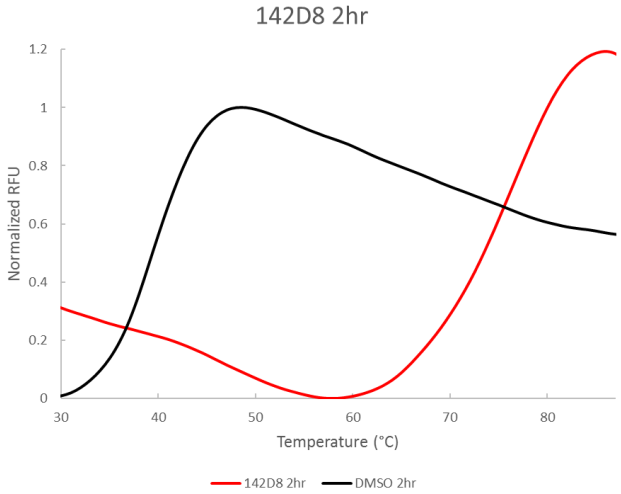
$T_{m\ BIR3}$= 39.5 °C
$T_{m\ 142D6}$= 77.0 °C **ΔT_m= 37.5 °C**

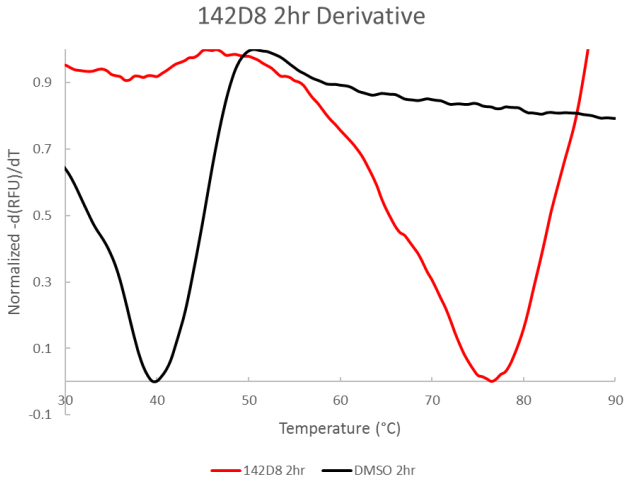
Compound 2 6hr



$T_{m\ BIR3}$= 39.5 °C
$T_{m\ 142D6}$= 77.5 °C **ΔT_m= 38.0 °C**

Compound 3 2hr

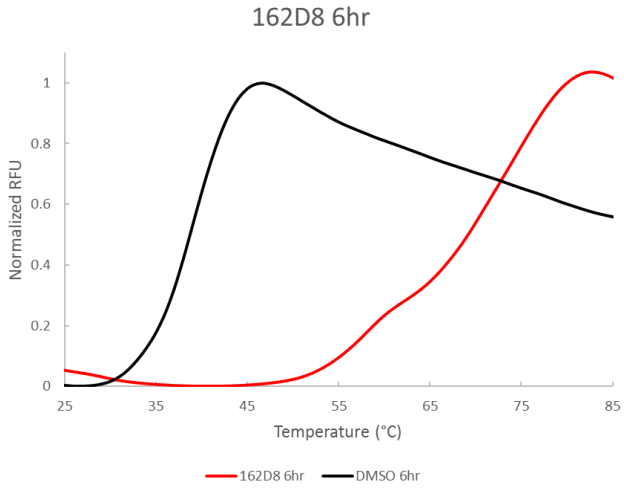


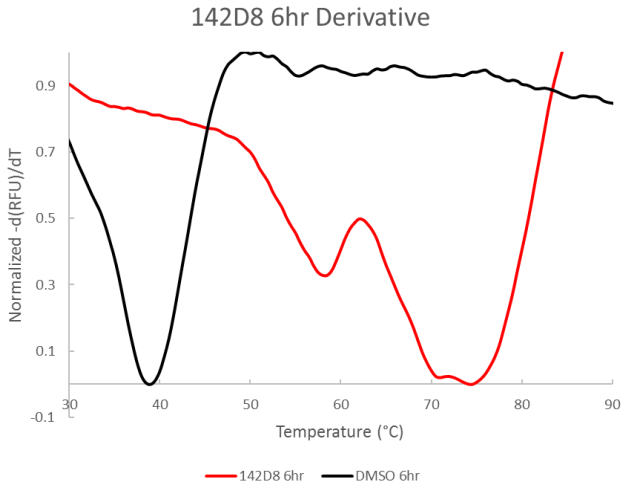


$T_{m\ BIR3}$= 39.0 °C
$T_{m\ 142D8}$= 76.5 °C

ΔT_m= 37.5 °C

Compound 3 6hr



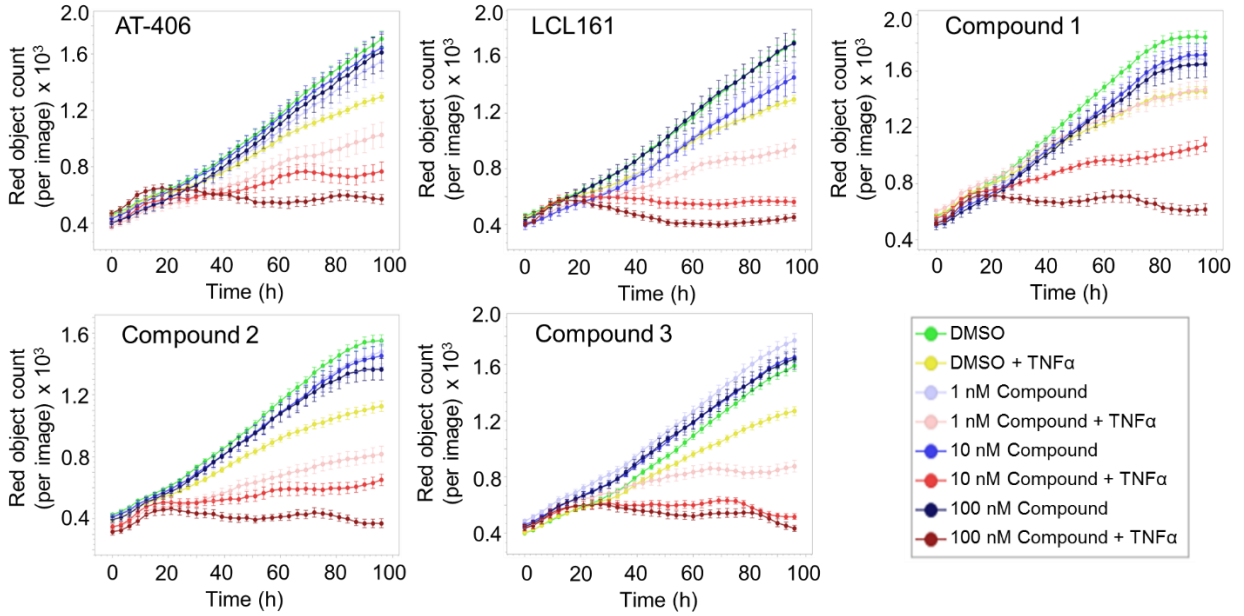


$T_{m\ BIR3}$= 39.0 °C
$T_{m\ 142D8}$= 74.5 °C

ΔT_m= 35.5 °C

Figure S2. SK-MEL-28 NucLight (top) and A549 NucLight (bottom) cells showing red nuclei were plated at 5 x 10^3 cells per well, treated with various compounds and normalized to 1% DMSO (v/v) control in the presence or absence of 1 ng/mL TNFα. Cells were imaged every 3 h for 4 days and analyzed with the IncuCyte S3 live-cell analysis system.

Cell viability SK-MEL-28



Cell viability A549

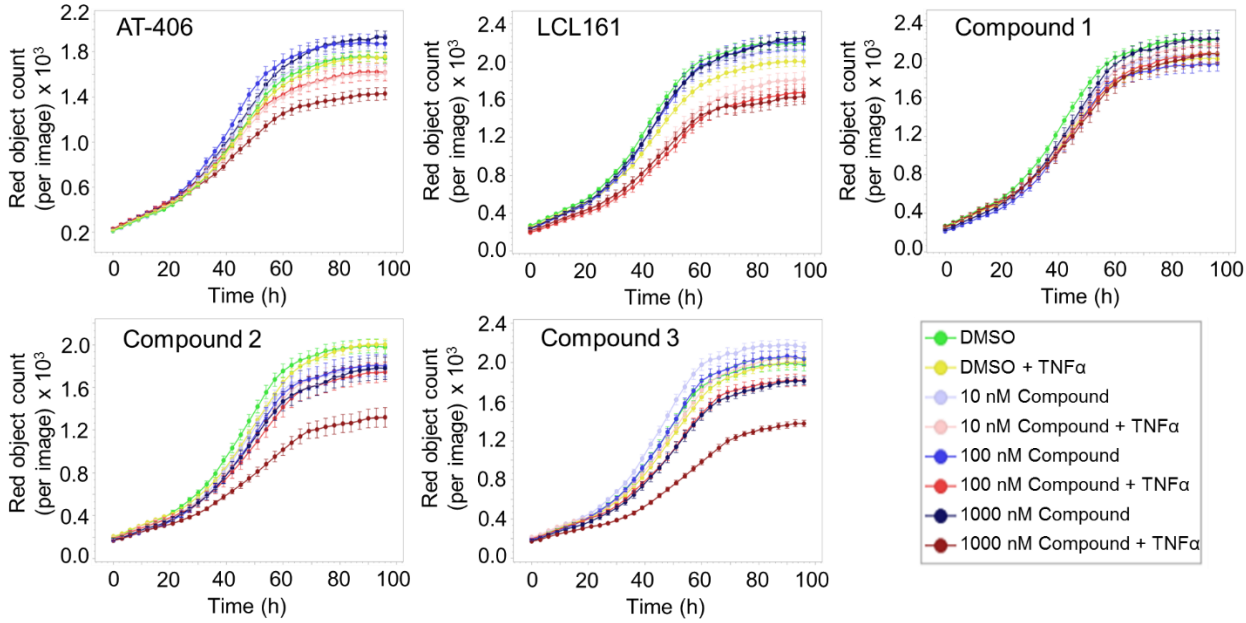
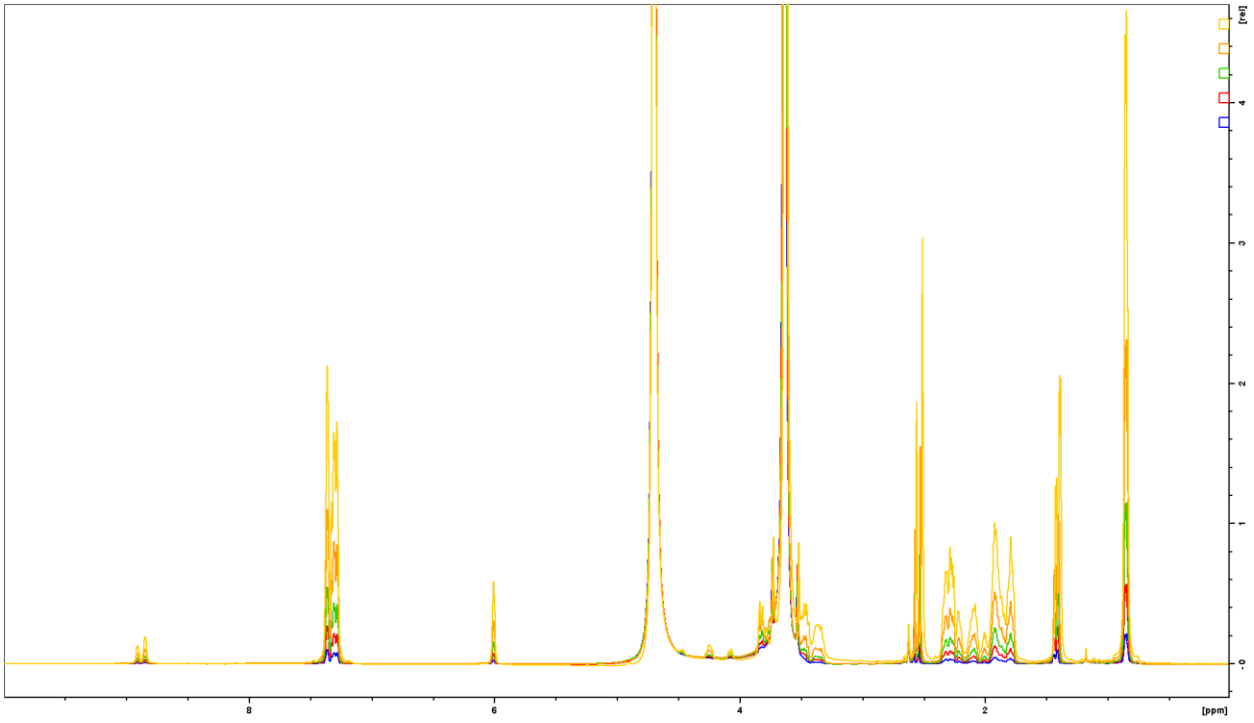


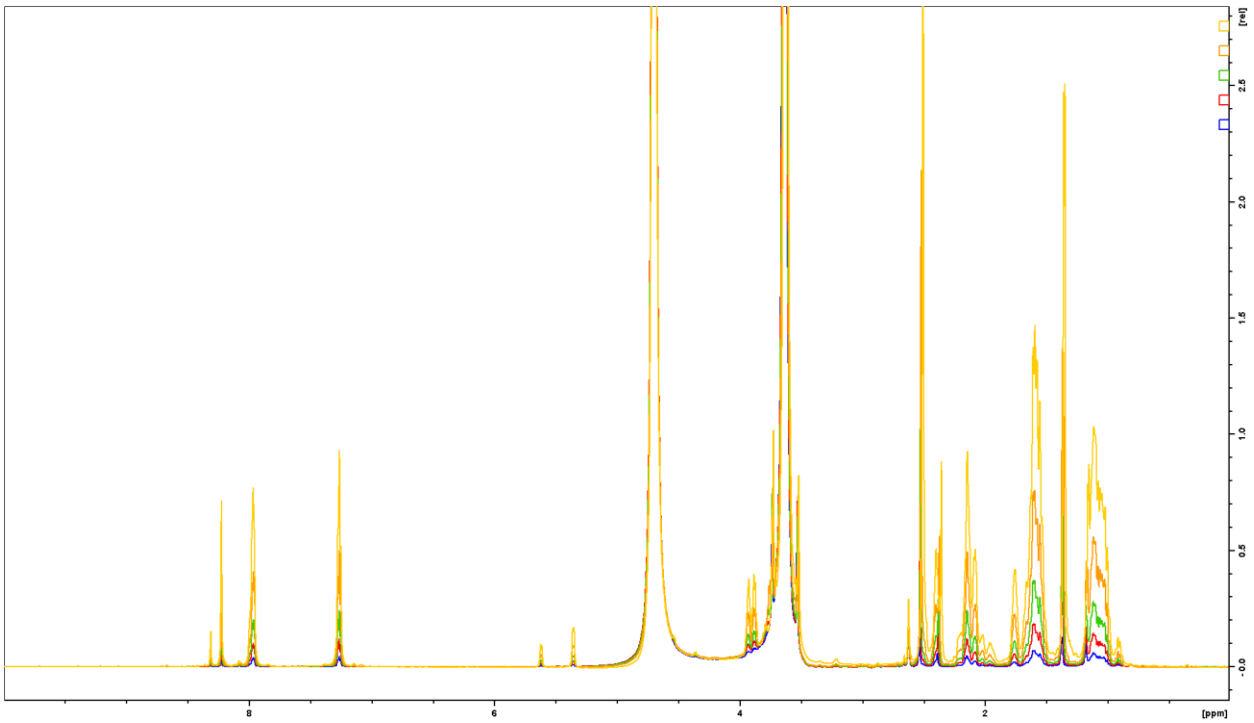
Figure S3

1D ^{1}H NMR based solubility determinations of agents in aqueous buffer. The agents tested were AT-406, LCL161, compound **1**, compound **2**, and compound **3**. For compounds AT-406, LCL161, compound **1**, and compound **2** the spectra were collected at 100 μM, 250 μM, 500 μM, 1 mM, and 2 mM. For compound **3**, spectra were collected at 200 μM, 500 μM, and 1 mM.

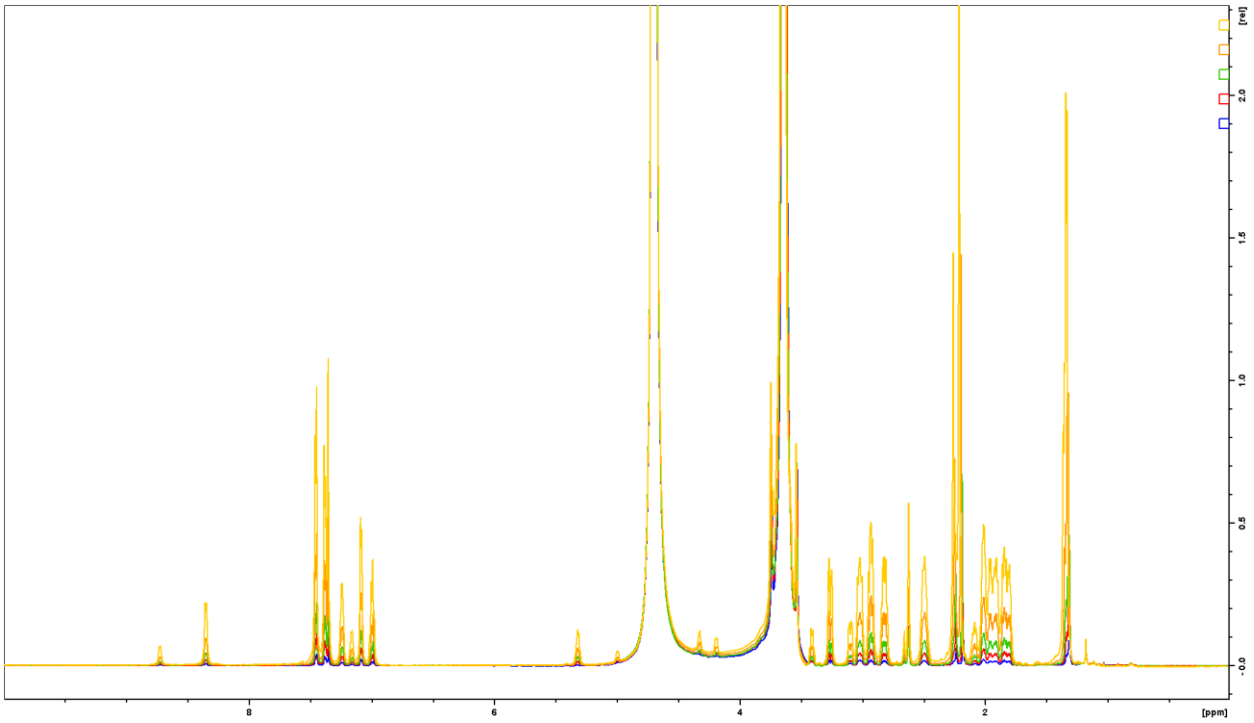
AT-406



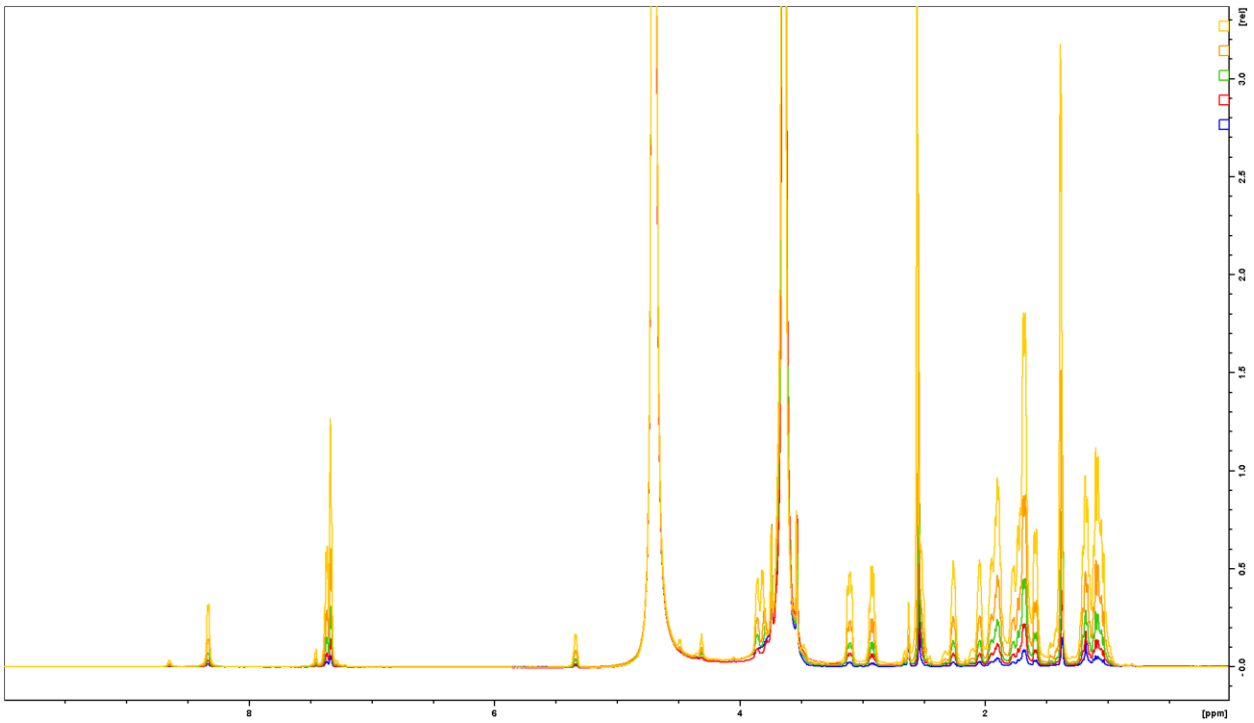
LCL161



Compound 1



Compound 2



Compound 3

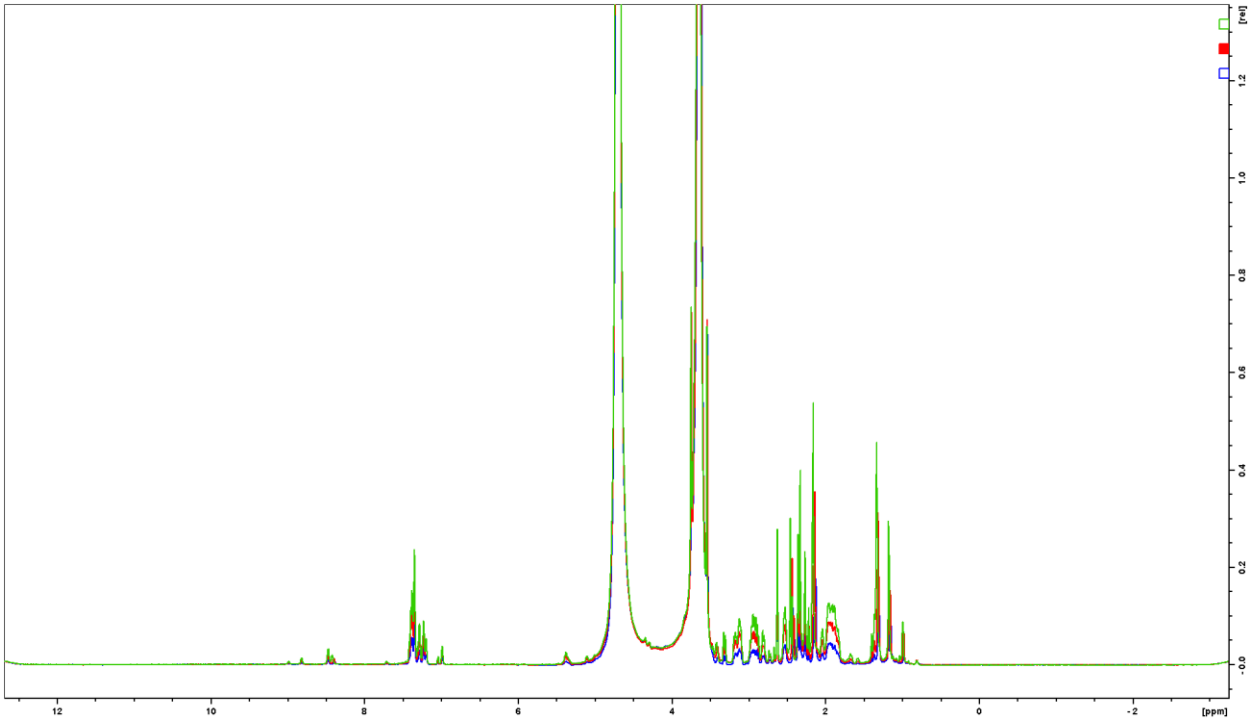
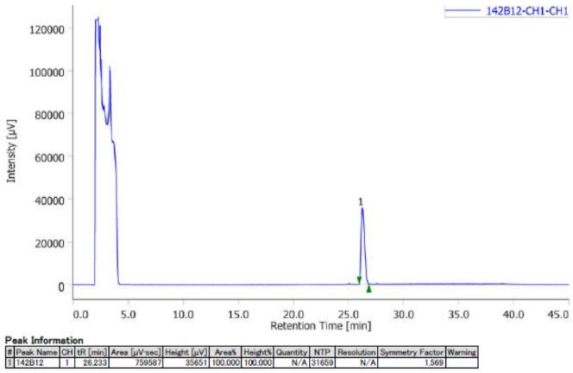


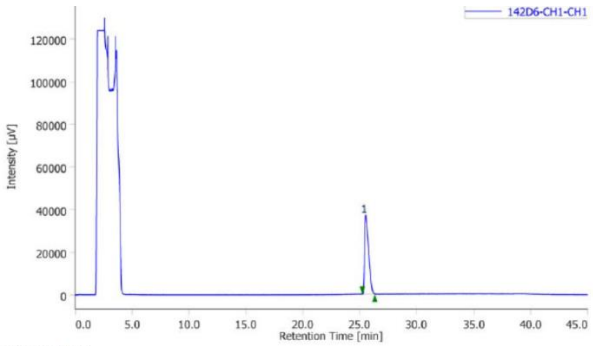
Figure S4. HPLC traces for tested compounds. Purification was accomplished using an Atlantis T3 3µm 4.6x150mm column (H_2O/ACN gradient from 5% to 100% in 45min). All compounds displayed purity >95%.

Compound **1**



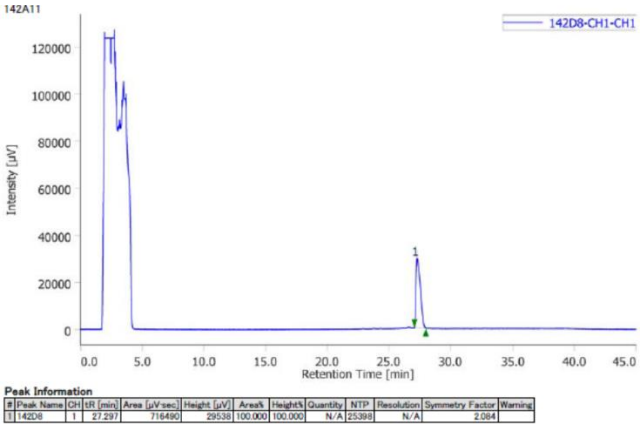
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	142B12	1	26.233	759587	35651	100.000	100.000	N/A	31659	N/A	1.569	

Compound **2**



#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	142D6	1	25.528	936970	37010	100.000	100.000	N/A	21844	N/A	1.990	

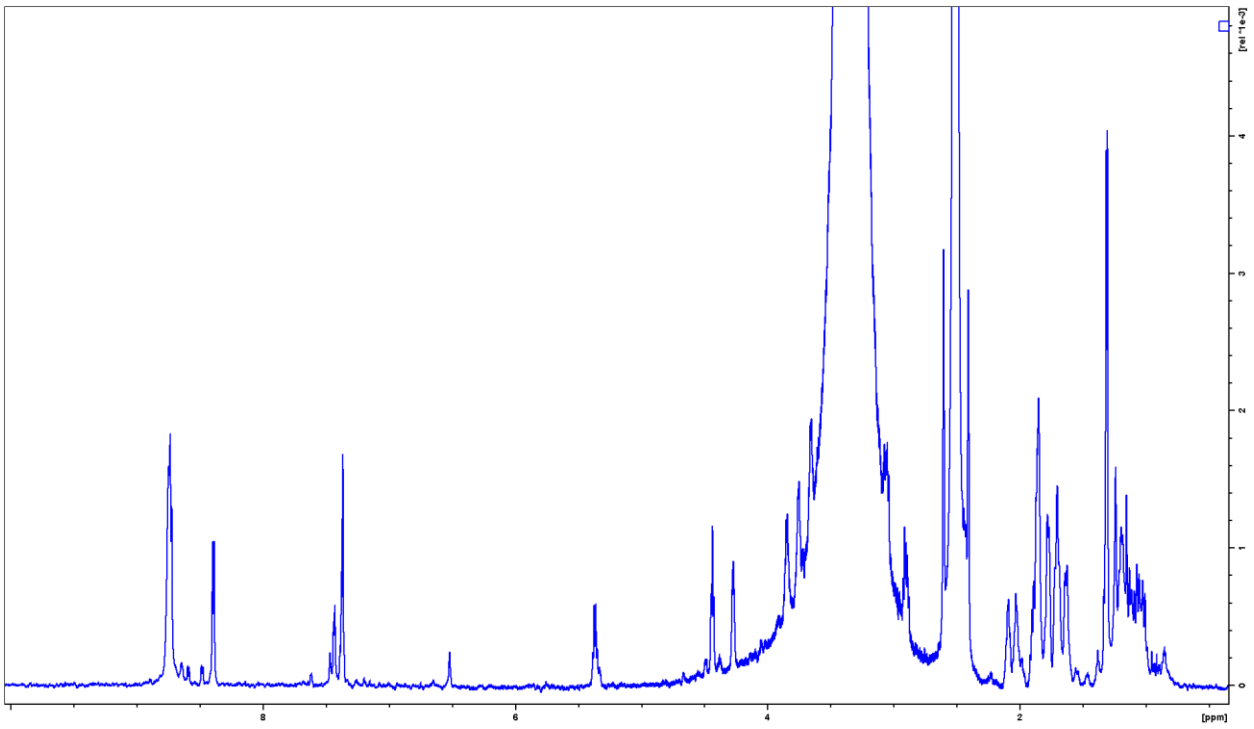
Compound **3**



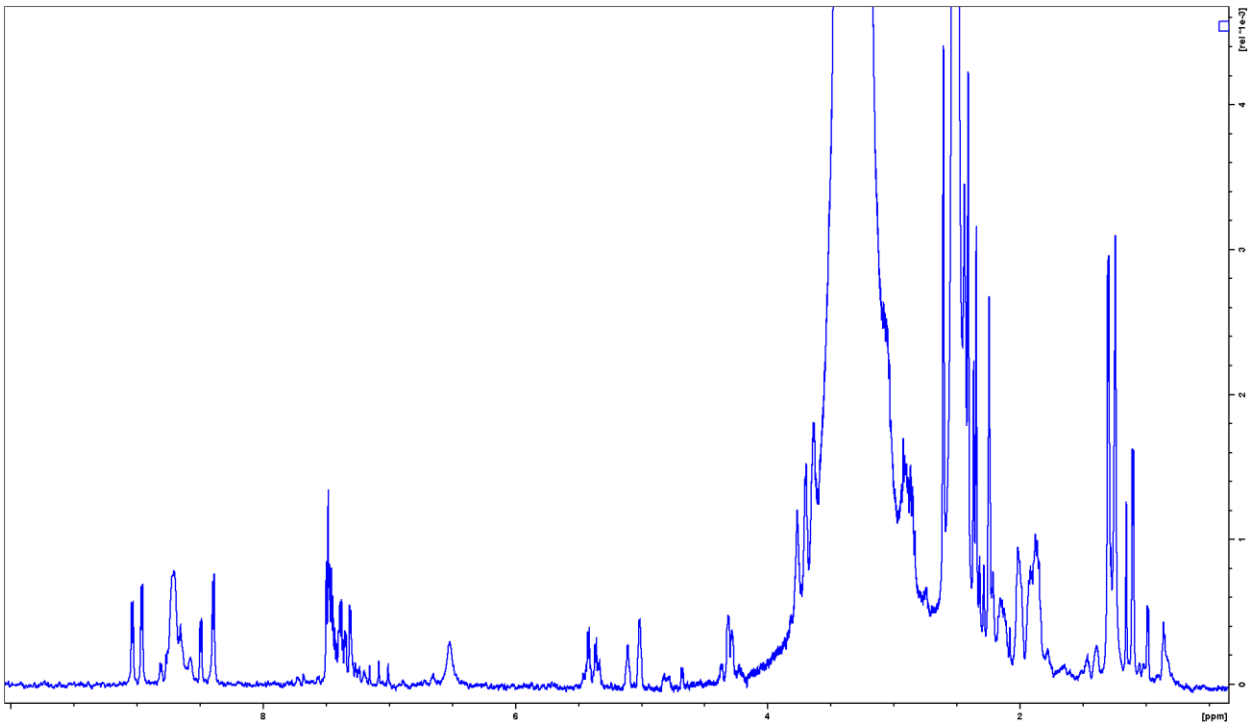
#	Peak Name	CH	tR [min]	Area [µV·sec]	Height [µV]	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor	Warning
1	142D8	1	27.297	716490	29538	100.000	100.000	N/A	25398	N/A	2.084	

Figure S5

1D ^{1}H NMR spectra of **compound 2** and **compound 3** at 100 μM in d6-DMSO.



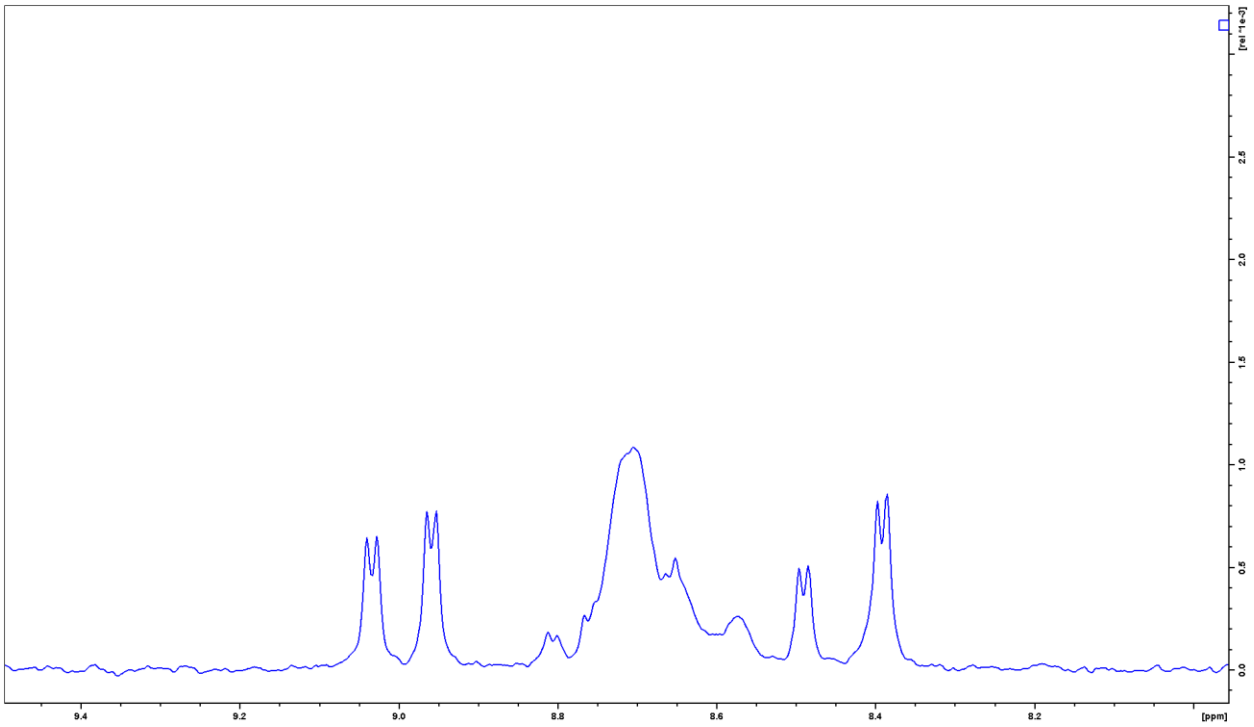
Compound 2: ^{1}H NMR (700 MHz, DMSO-d6): δ 8.74 (m, 3H), 8.1 (d, J = 8.39 Hz, 1H), 7.50-7.35 (m, 2H), 5.36 (m, 1H), 4.44 (t, 1H), 4.27 (t, 1H), 2.13-1.95 (m, 2H), 1.91-1.58 (m, 10H), 1.30 (d, J = 6.4 Hz, 3H), 1.27-0.83 (m, 10H)



Compound 3: 1H NMR (700 MHz, DMSO-d6): δ 9.03 (d, J = 8.42 Hz, 1H), 8.96 (d, J = 8.11 Hz, 1H), 8.78 – 8.60 (m, 6H), 8.49 (d, J = 8.73 Hz, 1H), 8.39 (d, J = 8.73 Hz, 1H), 7.52 – 6.98 (m, 9H), 6.51 (m, 2H), 5.49 – 5.30 (m, 2H), 5.11 (m, 1H), 5.01 (m, 1H), 4.39 – 4.24 (m, 2H), 2.05 – 1.80 (m, 13H), 1.29 (d, J = 6.45 Hz, 6H), 1.24 (s, 6H), 1.15 (s, 1H), 1.10 (d, J = 6.45 Hz, 3H), 0.98 (d, J = 6.7 Hz, 1H).

Figure S6

1D ^{1}H NMR spectra of the amide region of **compound 3** at 100 μM in d6-DMSO. The presence of 4 amide signals indicate the presence of the 2 diasteroisomer, both at almost half concentration compared to other agents. The ratio between the two diasteroisomer is close to 1:1.



XIAP-BIR3 + compound 1 .mol2 file

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@<TRIPOS>MOLECULE
3HL5.B
1466 1495 91 0 0
BIOPOLYMER
USER_CHARGES


@<TRIPOS>ATOM
   1 N         2.1170    -0.3132    -4.3406 N.3     1 LEU256  -0.9900
BACKBONE
   2 H1        2.0332    -0.5642    -5.3153 H       1 LEU256   0.3600
   3 H2        1.3268    -0.6796    -3.8295 H       1 LEU256   0.3600
   4 CA        2.1479     1.1767    -4.2103 C.3     1 LEU256   0.2510
BACKBONE
   5 HA        3.0279     1.5350    -4.7445 H       1 LEU256   0.0800
   6 C         2.2746     1.6066    -2.7445 C.2     1 LEU256   0.5690
BACKBONE
   7 O         1.5872     1.0512    -1.8812 O.2     1 LEU256  -0.5700
BACKBONE
   8 CB        0.8991     1.8054    -4.8442 C.3     1 LEU256  -0.1600
   9 HB2       0.0372     1.3970    -4.3165 H       1 LEU256   0.0800
  10 HB3       0.9600     2.8788    -4.6646 H       1 LEU256   0.0800
  11 CG        0.6313     1.6198    -6.3444 C.3     1 LEU256  -0.0800
  12 HG        0.4927     0.5526    -6.5172 H       1 LEU256   0.0800
  13 CD1      -0.6274     2.3690    -6.7515 C.3     1 LEU256  -0.2400
  14 HD11     -0.4872     3.4359    -6.5782 H       1 LEU256   0.0800
  15 HD12     -1.4701     2.0122    -6.1592 H       1 LEU256   0.0800
  16 HD13     -0.8273     2.1958    -7.8089 H       1 LEU256   0.0800
  17 CD2       1.8066     2.0728    -7.2003 C.3     1 LEU256  -0.2400
  18 HD21      1.9743     3.1396    -7.0519 H       1 LEU256   0.0800
  19 HD22      1.5860     1.8824    -8.2506 H       1 LEU256   0.0800
  20 HD23      2.7008     1.5208    -6.9110 H       1 LEU256   0.0800
  21 N         3.1508     2.5933    -2.4523 N.am    2 PRO257  -0.2548
BACKBONE
  22 CA        4.0107     3.3225    -3.3975 C.3     2 PRO257  -0.0266
BACKBONE
  23 HA        3.4546     3.6609    -4.2717 H       2 PRO257   0.0641
  24 C         5.1380     2.4535    -3.9503 C.2     2 PRO257   0.5896
BACKBONE
  25 O         5.6310     1.5678    -3.2440 O.2     2 PRO257  -0.5748
BACKBONE
  26 CB        4.5894     4.4593    -2.5470 C.3     2 PRO257  -0.0070
  27 HB2       5.6165     4.6738    -2.8422 H       2 PRO257   0.0253
  28 HB3       3.9857     5.3609    -2.6510 H       2 PRO257   0.0253
  29 CG        4.5421     3.9585    -1.1516 C.3     2 PRO257   0.0189
  30 HG2       4.4457     4.7910    -0.4547 H       2 PRO257   0.0213
  31 HG3       5.4466     3.3953    -0.9217 H       2 PRO257   0.0213
  32 CD        3.3368     3.0654    -1.0656 C.3     2 PRO257   0.0192
  33 HD2       2.4641     3.6222    -0.7242 H       2 PRO257   0.0391
  34 HD3       3.5205     2.2287    -0.3915 H       2 PRO257   0.0391
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  35 N        5.5373     2.7138    -5.1965 N.am   3 ARG258  -0.3479
BACKBONE
  36 H        5.0834     3.4563    -5.7092 H      3 ARG258   0.2747
  37 CA       6.6169     1.9557    -5.8494 C.3    3 ARG258  -0.2637
BACKBONE
  38 HA       6.3002     0.9130    -5.8252 H      3 ARG258   0.1560
  39 C        7.9501     2.0638    -5.1019 C.2    3 ARG258   0.7341
BACKBONE
  40 O        8.7036     1.0902    -5.0371 O.2    3 ARG258  -0.5894
BACKBONE
  41 CB       6.8112     2.3870    -7.3111 C.3    3 ARG258  -0.0007
  42 HB2      7.1412     3.4258    -7.3126 H      3 ARG258   0.0327
  43 HB3      7.5886     1.7582    -7.7451 H      3 ARG258   0.0327
  44 CG       5.5701     2.2860    -8.2057 C.3    3 ARG258   0.0390
  45 HG2      5.7377     2.8993    -9.0911 H      3 ARG258   0.0285
  46 HG3      4.7172     2.6756    -7.6501 H      3 ARG258   0.0285
  47 CD       5.2356     0.8745    -8.6618 C.3    3 ARG258   0.0486
  48 HD2      5.0617     0.2462    -7.7883 H      3 ARG258   0.0687
  49 HD3      6.0711     0.4748    -9.2363 H      3 ARG258   0.0687
  50 NE       4.0340     0.8819    -9.4982 N.pl3  3 ARG258  -0.5295
  51 HE       3.7693     1.7587    -9.9241 H      3 ARG258   0.3456
  52 CZ       3.2621    -0.1760    -9.7421 C.cat  3 ARG258   0.8076
  53 NH1      3.5506    -1.3644    -9.2255 N.pl3  3 ARG258  -0.8627
  54 HH12     4.3673    -1.4767    -8.6419 H      3 ARG258   0.4478
  55 HH11     2.9533    -2.1563    -9.4160 H      3 ARG258   0.4478
  56 NH2      2.1866    -0.0402   -10.5072 N.pl3  3 ARG258  -0.8627
  57 HH21     1.9574     0.8612   -10.9008 H      3 ARG258   0.4478
  58 HH22     1.5972    -0.8384   -10.6960 H      3 ARG258   0.4478
  59 N        8.2364     3.2494    -4.5601 N.am   4 ASN259  -0.4157
BACKBONE
  60 H        7.6021     4.0196    -4.7165 H      4 ASN259   0.2719
  61 CA       9.4365     3.4791    -3.7456 C.3    4 ASN259   0.0143
BACKBONE
  62 HA       9.8697     2.4984    -3.5488 H      4 ASN259   0.1048
  63 C        9.1202     4.0968    -2.3725 C.2    4 ASN259   0.5973
BACKBONE
  64 O        9.1271     5.3237    -2.2168 O.2    4 ASN259  -0.5679
BACKBONE
  65 CB      10.4723     4.3243    -4.5116 C.3    4 ASN259  -0.2041
  66 HB2     10.0943     5.3429    -4.5989 H      4 ASN259   0.0797
  67 HB3     10.6020     3.8984    -5.5065 H      4 ASN259   0.0797
  68 CG      11.8361     4.3665    -3.8161 C.2    4 ASN259   0.7130
  69 OD1     12.0019     3.8675    -2.7009 O.2    4 ASN259  -0.5931
  70 ND2     12.8182     4.9674    -4.4817 N.am   4 ASN259  -0.9191
  71 HD22    12.6413     5.3639    -5.3936 H      4 ASN259   0.4196
  72 HD21    13.7408     5.0273    -4.0752 H      4 ASN259   0.4196
  73 N        8.8499     3.2402    -1.3667 N.am   5 PRO260  -0.2548
BACKBONE
  74 CA       8.5077     3.6981    -0.0188 C.3    5 PRO260  -0.0266
BACKBONE
  75 HA       7.6949     4.4235    -0.0567 H      5 PRO260   0.0641
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  76 C        9.6204     4.4645     0.6988 C.2    5 PRO260   0.5896
BACKBONE
  77 O        9.3231     5.2518     1.5944 O.2    5 PRO260  -0.5748
BACKBONE
  78 CB       8.1613     2.4026     0.7269 C.3    5 PRO260  -0.0070
  79 HB2      8.5400     2.4369     1.7484 H      5 PRO260   0.0253
  80 HB3      7.0823     2.2489     0.7445 H      5 PRO260   0.0253
  81 CG       8.8247     1.3261    -0.0348 C.3    5 PRO260   0.0189
  82 HG2      8.2779     0.3898     0.0775 H      5 PRO260   0.0213
  83 HG3      9.8493     1.1923     0.3121 H      5 PRO260   0.0213
  84 CD       8.8127     1.7697    -1.4715 C.3    5 PRO260   0.0192
  85 HD2      7.9062     1.4361    -1.9766 H      5 PRO260   0.0391
  86 HD3      9.6854     1.3930    -2.0049 H      5 PRO260   0.0391
  87 N       10.8775     4.2642     0.2986 N.am   6 SER261  -0.4157
BACKBONE
  88 H       11.0655     3.5803    -0.4205 H      6 SER261   0.2719
  89 CA      11.9940     5.0199     0.8844 C.3    6 SER261  -0.0249
BACKBONE
  90 HA      11.8913     4.9441     1.9669 H      6 SER261   0.0843
  91 C       11.9440     6.5045     0.5179 C.2    6 SER261   0.5973
BACKBONE
  92 O       12.6204     7.3400     1.1377 O.2    6 SER261  -0.5679
BACKBONE
  93 CB      13.3392     4.4190     0.4683 C.3    6 SER261   0.2117
  94 HB2     13.2591     3.3319     0.4714 H      6 SER261   0.0352
  95 HB3     14.1029     4.7290     1.1816 H      6 SER261   0.0352
  96 OG      13.7137     4.8496    -0.8235 O.3    6 SER261  -0.6546
  97 HG      13.0309     4.5628    -1.4344 H      6 SER261   0.4275
  98 N       11.1394     6.8260    -0.4911 N.am   7 MET262  -0.4157
BACKBONE
  99 H       10.6134     6.0933    -0.9456 H      7 MET262   0.2719
 100 CA      10.9885     8.1923    -0.9646 C.3    7 MET262  -0.0237
BACKBONE
 101 HA      11.7148     8.8132    -0.4401 H      7 MET262   0.0880
 102 C        9.6016     8.7667    -0.6376 C.2    7 MET262   0.5973
BACKBONE
 103 O        9.2073     9.7906    -1.1885 O.2    7 MET262  -0.5679
BACKBONE
 104 CB      11.2723     8.2554    -2.4717 C.3    7 MET262   0.0342
 105 HB2     10.8918     9.2041    -2.8502 H      7 MET262   0.0241
 106 HB3     10.7420     7.4334    -2.9525 H      7 MET262   0.0241
 107 CG      12.7558     8.1515    -2.8453 C.3    7 MET262   0.0018
 108 HG2     12.8324     7.9804    -3.9190 H      7 MET262   0.0440
 109 HG3     13.1902     7.3067    -2.3108 H      7 MET262   0.0440
 110 SD      13.6938     9.6393    -2.4306 S.3    7 MET262  -0.2737
 111 CE      14.6453     9.0852    -1.0172 C.3    7 MET262  -0.0536
 112 HE1     15.2704     9.9024    -0.6570 H      7 MET262   0.0684
 113 HE2     15.2770     8.2467    -1.3105 H      7 MET262   0.0684
 114 HE3     13.9675     8.7694    -0.2241 H      7 MET262   0.0684
 115 N        8.8778     8.1134     0.2737 N.am   8 ALA263  -0.4157
BACKBONE
 116 H        9.2613     7.2841     0.7042 H      8 ALA263   0.2719
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 117 CA       7.5399     8.5686     0.6660 C.3    8 ALA263   0.0337
BACKBONE
 118 HA       6.9897     8.7381    -0.2595 H      8 ALA263   0.0823
 119 C        7.5615     9.8953     1.4145 C.2    8 ALA263   0.5973
BACKBONE
 120 O        6.6315    10.6916     1.2919 O.2    8 ALA263  -0.5679
BACKBONE
 121 CB       6.8096     7.4972     1.4828 C.3    8 ALA263  -0.1825
 122 HB1      7.3500     7.3177     2.4122 H      8 ALA263   0.0603
 123 HB2      6.7597     6.5728     0.9073 H      8 ALA263   0.0603
 124 HB3      5.7997     7.8389     1.7098 H      8 ALA263   0.0603
 125 N        8.6279    10.1320     2.1739 N.am   9 ASP264  -0.5163
BACKBONE
 126 H        9.3555     9.4332     2.2226 H      9 ASP264   0.2936
 127 CA       8.7850    11.3685     2.9414 C.3    9 ASP264   0.0381
BACKBONE
 128 HA       7.7908    11.6511     3.2874 H      9 ASP264   0.0880
 129 C        9.3467    12.4930     2.0842 C.2    9 ASP264   0.5366
BACKBONE
 130 O       10.3692    12.3231     1.4154 O.2    9 ASP264  -0.5819
BACKBONE
 131 CB       9.7048    11.1547     4.1498 C.3    9 ASP264  -0.0303
 132 HB2      9.9371    12.1260     4.5865 H      9 ASP264  -0.0122
 133 HB3     10.6248    10.6809     3.8074 H      9 ASP264  -0.0122
 134 CG       9.0788    10.2804     5.2189 C.2    9 ASP264   0.7994
 135 OD1      7.8382    10.1066     5.2178 O.co2  9 ASP264  -0.8014
 136 OD2      9.8389     9.7748     6.0712 O.co2  9 ASP264  -0.8014
 137 N        8.6745    13.6399     2.1284 N.am  10 TYR265  -0.4157
BACKBONE
 138 H        7.8218    13.6739     2.6688 H     10 TYR265   0.2719
 139 CA       9.1072    14.8617     1.4320 C.3   10 TYR265  -0.0014
BACKBONE
 140 HA       9.0172    14.6627     0.3641 H     10 TYR265   0.0876
 141 C       10.5738    15.2136     1.7021 C.2   10 TYR265   0.5973
BACKBONE
 142 O       11.3083    15.5788     0.7790 O.2   10 TYR265  -0.5679
BACKBONE
 143 CB       8.2047    16.0435     1.8211 C.3   10 TYR265  -0.0152
 144 HB2      7.2250    15.8840     1.3706 H     10 TYR265   0.0295
 145 HB3      8.1082    16.0528     2.9067 H     10 TYR265   0.0295
 146 CG       8.7110    17.4083     1.3800 C.ar  10 TYR265  -0.0011
 147 CD1      8.5093    17.8654     0.0750 C.ar  10 TYR265  -0.1906
 148 HD1      7.9818    17.2419    -0.6317 H     10 TYR265   0.1699
 149 CD2      9.3972    18.2377     2.2718 C.ar  10 TYR265  -0.1906
 150 HD2      9.5612    17.9031     3.2855 H     10 TYR265   0.1699
 151 CE1      8.9841    19.1282    -0.3323 C.ar  10 TYR265  -0.2341
 152 HE1      8.8301    19.4689    -1.3456 H     10 TYR265   0.1656
 153 CE2      9.8746    19.4881     1.8801 C.ar  10 TYR265  -0.2341
 154 HE2     10.4134    20.1067     2.5826 H     10 TYR265   0.1656
 155 CZ       9.6557    19.9335     0.5885 C.ar  10 TYR265   0.3226
 156 OH      10.1302    21.1700     0.2157 O.3   10 TYR265  -0.5579
 157 HH      10.5955    21.6506     0.9043 H     10 TYR265   0.3992
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 158 N       10.9904    15.1212     2.9649 N.am  11 GLU266  -0.5163
BACKBONE
 159 H       10.3512    14.7940     3.6751 H     11 GLU266   0.2936
 160 CA      12.3627    15.4867     3.3427 C.3   11 GLU266   0.0397
BACKBONE
 161 HA      12.5375    16.4978     2.9752 H     11 GLU266   0.1105
 162 C       13.4009    14.5788     2.6777 C.2   11 GLU266   0.5366
BACKBONE
 163 O       14.4579    15.0435     2.2487 O.2   11 GLU266  -0.5819
BACKBONE
 164 CB      12.5339    15.5014     4.8643 C.3   11 GLU266   0.0560
 165 HB2     12.1618    14.5560     5.2589 H     11 GLU266  -0.0173
 166 HB3     13.5967    15.5951     5.0873 H     11 GLU266  -0.0173
 167 CG      11.7912    16.6440     5.5727 C.3   11 GLU266   0.0136
 168 HG2     11.8894    17.5434     4.9647 H     11 GLU266  -0.0425
 169 HG3     12.2622    16.8076     6.5421 H     11 GLU266  -0.0425
 170 CD      10.2976    16.3810     5.8030 C.2   11 GLU266   0.8054
 171 OE1      9.8163    15.2430     5.5654 O.co2 11 GLU266  -0.8188
 172 OE2      9.5990    17.3252     6.2379 O.co2 11 GLU266  -0.8188
 173 N       13.0802    13.2888     2.5869 N.am  12 ALA267  -0.4157
BACKBONE
 174 H       12.2203    12.9696     3.0098 H     12 ALA267   0.2719
 175 CA      13.9309    12.3172     1.8951 C.3   12 ALA267   0.0337
BACKBONE
 176 HA      14.9248    12.3725     2.3393 H     12 ALA267   0.0823
 177 C       14.0759    12.6500     0.4119 C.2   12 ALA267   0.5973
BACKBONE
 178 O       15.1694    12.5557    -0.1413 O.2   12 ALA267  -0.5679
BACKBONE
 179 CB      13.3940    10.9009     2.0857 C.3   12 ALA267  -0.1825
 180 HB1     12.3991    10.8274     1.6466 H     12 ALA267   0.0603
 181 HB2     13.3391    10.6734     3.1503 H     12 ALA267   0.0603
 182 HB3     14.0605    10.1908     1.5962 H     12 ALA267   0.0603
 183 N       12.9770    13.0601    -0.2233 N.am  13 ARG268  -0.3479
BACKBONE
 184 H       12.1023    13.1090     0.2795 H     13 ARG268   0.2747
 185 CA      13.0165    13.4406    -1.6358 C.3   13 ARG268  -0.2637
BACKBONE
 186 HA      13.4515    12.6150    -2.1991 H     13 ARG268   0.1560
 187 C       13.8949    14.6715    -1.8337 C.2   13 ARG268   0.7341
BACKBONE
 188 O       14.6837    14.7353    -2.7792 O.2   13 ARG268  -0.5894
BACKBONE
 189 CB      11.6055    13.6867    -2.1754 C.3   13 ARG268  -0.0007
 190 HB2     11.1498    14.4879    -1.5938 H     13 ARG268   0.0327
 191 HB3     11.6848    13.9945    -3.2180 H     13 ARG268   0.0327
 192 CG      10.6965    12.4610    -2.1025 C.3   13 ARG268   0.0390
 193 HG2     10.3448    12.3431    -1.0775 H     13 ARG268   0.0285
 194 HG3     11.2682    11.5800    -2.3941 H     13 ARG268   0.0285
 195 CD       9.4832    12.5950    -3.0311 C.3   13 ARG268   0.0486
 196 HD2      8.9789    11.6299    -3.0801 H     13 ARG268   0.0687
 197 HD3      9.8384    12.8701    -4.0242 H     13 ARG268   0.0687
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198	NE	8.5132	13.6025	-2.5906	N.pl3	13 ARG268	-0.5295
199	HE	8.5659	14.5189	-3.0119	H	13 ARG268	0.3456
200	CZ	7.5676	13.3969	-1.6754	C.cat	13 ARG268	0.8076
201	NH1	7.4643	12.2239	-1.0583	N.pl3	13 ARG268	-0.8627
202	HH12	8.0997	11.4737	-1.2899	H	13 ARG268	0.4478
203	HH11	6.7503	12.0829	-0.3579	H	13 ARG268	0.4478
204	NH2	6.7268	14.3758	-1.3628	N.pl3	13 ARG268	-0.8627
205	HH21	6.8051	15.2737	-1.8187	H	13 ARG268	0.4478
206	HH22	6.0088	14.2226	-0.6692	H	13 ARG268	0.4478
207	N	13.7640	15.6378	-0.9260	N.am	14 ILE269	-0.4157
BACKBONE							
208	H	13.0965	15.5170	-0.1778	H	14 ILE269	0.2719
209	CA	14.5546	16.8683	-0.9764	C.3	14 ILE269	-0.0597
BACKBONE							
210	HA	14.3069	17.3607	-1.9167	H	14 ILE269	0.0869
211	C	16.0528	16.5835	-0.9818	C.2	14 ILE269	0.5973
BACKBONE							
212	O	16.7998	17.1958	-1.7527	O.2	14 ILE269	-0.5679
BACKBONE							
213	CB	14.1873	17.8288	0.1839	C.3	14 ILE269	0.1303
214	HB	14.0907	17.2391	1.0955	H	14 ILE269	0.0187
215	CG1	12.8403	18.5115	-0.0905	C.3	14 ILE269	-0.0430
216	HG12	12.1184	17.7404	-0.3595	H	14 ILE269	0.0236
217	HG13	12.5186	19.0064	0.8259	H	14 ILE269	0.0236
218	CG2	15.2962	18.8629	0.4232	C.3	14 ILE269	-0.3204
219	HG21	15.4222	19.4740	-0.4706	H	14 ILE269	0.0882
220	HG22	16.2308	18.3483	0.6462	H	14 ILE269	0.0882
221	HG23	15.0230	19.5007	1.2638	H	14 ILE269	0.0882
222	CD1	12.8628	19.5578	-1.2154	C.3	14 ILE269	-0.0660
223	HD11	13.1823	19.0856	-2.1444	H	14 ILE269	0.0186
224	HD12	13.5583	20.3558	-0.9555	H	14 ILE269	0.0186
225	HD13	11.8639	19.9743	-1.3444	H	14 ILE269	0.0186
226	N	16.4767	15.6401	-0.1386	N.am	15 PHE270	-0.4157
BACKBONE							
227	H	15.8018	15.1849	0.4592	H	15 PHE270	0.2719
228	CA	17.8862	15.2378	-0.0457	C.3	15 PHE270	-0.0024
BACKBONE							
229	HA	18.4213	16.1573	0.1915	H	15 PHE270	0.0978
230	C	18.4932	14.7205	-1.3490	C.2	15 PHE270	0.5973
BACKBONE							
231	O	19.7029	14.8509	-1.5587	O.2	15 PHE270	-0.5679
BACKBONE							
232	CB	18.0875	14.2018	1.0657	C.3	15 PHE270	-0.0343
233	HB2	17.2425	13.5135	1.0503	H	15 PHE270	0.0295
234	HB3	19.0068	13.6532	0.8609	H	15 PHE270	0.0295
235	CG	18.1885	14.7989	2.4476	C.ar	15 PHE270	0.0118
236	CD1	19.1286	15.7927	2.7295	C.ar	15 PHE270	-0.1256
237	HD1	19.7853	16.1426	1.9469	H	15 PHE270	0.1330
238	CD2	17.3609	14.3488	3.4711	C.ar	15 PHE270	-0.1256
239	HD2	16.6377	13.5727	3.2687	H	15 PHE270	0.1330
240	CE1	19.2299	16.3386	4.0076	C.ar	15 PHE270	-0.1704
241	HE1	19.9576	17.1104	4.2105	H	15 PHE270	0.1430

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 242 CE2     17.4524    14.8870     4.7578 C.ar  15 PHE270  -0.1704
 243 HE2     16.8008    14.5312     5.5422 H     15 PHE270   0.1430
 244 CZ      18.3891    15.8856     5.0242 C.ar  15 PHE270  -0.1072
 245 HZ      18.4632    16.3072     6.0157 H     15 PHE270   0.1297
 246 N       17.6641    14.1433    -2.2209 N.am  16 THR271  -0.4157
BACKBONE
 247 H       16.6743    14.1199    -2.0213 H     16 THR271   0.2719
 248 CA      18.1616    13.5412    -3.4654 C.3   16 THR271  -0.0389
BACKBONE
 249 HA      19.0048    12.9309    -3.1419 H     16 THR271   0.1007
 250 C       18.6545    14.5720    -4.4787 C.2   16 THR271   0.5973
BACKBONE
 251 O       19.5097    14.2746    -5.3109 O.2   16 THR271  -0.5679
BACKBONE
 252 CB      17.1125    12.6360    -4.1618 C.3   16 THR271   0.3654
 253 HB      17.5904    12.1637    -5.0201 H     16 THR271   0.0043
 254 OG1     16.0044    13.4251    -4.6190 O.3   16 THR271  -0.6761
 255 HG1     15.6149    13.8506    -3.8516 H     16 THR271   0.4102
 256 CG2     16.6286    11.5294    -3.2297 C.3   16 THR271  -0.2438
 257 HG21    16.1449    11.9731    -2.3595 H     16 THR271   0.0642
 258 HG22    17.4789    10.9292    -2.9061 H     16 THR271   0.0642
 259 HG23    15.9163    10.8954    -3.7575 H     16 THR271   0.0642
 260 N       18.1128    15.7816    -4.4012 N.am  17 PHE272  -0.4157
BACKBONE
 261 H       17.4977    16.0003    -3.6306 H     17 PHE272   0.2719
 262 CA      18.3891    16.8017    -5.4081 C.3   17 PHE272  -0.0024
BACKBONE
 263 HA      18.3381    16.3076    -6.3782 H     17 PHE272   0.0978
 264 C       19.8001    17.3779    -5.3258 C.2   17 PHE272   0.5973
BACKBONE
 265 O       20.4606    17.5375    -6.3553 O.2   17 PHE272  -0.5679
BACKBONE
 266 CB      17.3292    17.8997    -5.3515 C.3   17 PHE272  -0.0343
 267 HB2     17.2187    18.2205    -4.3156 H     17 PHE272   0.0295
 268 HB3     17.6688    18.7395    -5.9577 H     17 PHE272   0.0295
 269 CG      15.9895    17.4593    -5.8579 C.ar  17 PHE272   0.0118
 270 CD1     15.0848    16.8220    -5.0115 C.ar  17 PHE272  -0.1256
 271 HD1     15.3494    16.6522    -3.9782 H     17 PHE272   0.1330
 272 CD2     15.6255    17.6852    -7.1824 C.ar  17 PHE272  -0.1256
 273 HD2     16.3141    18.1859    -7.8469 H     17 PHE272   0.1330
 274 CE1     13.8468    16.4025    -5.4805 C.ar  17 PHE272  -0.1704
 275 HE1     13.1587    15.8982    -4.8183 H     17 PHE272   0.1430
 276 CE2     14.3886    17.2749    -7.6590 C.ar  17 PHE272  -0.1704
 277 HE2     14.1199    17.4528    -8.6898 H     17 PHE272   0.1430
 278 CZ      13.4963    16.6347    -6.8078 C.ar  17 PHE272  -0.1072
 279 HZ      12.5315    16.3175    -7.1755 H     17 PHE272   0.1297
 280 N       20.2653    17.6603    -4.1082 N.am  18 GLY273  -0.4157
BACKBONE
 281 H       19.6928    17.4494    -3.3033 H     18 GLY273   0.2719
 282 CA      21.5825    18.2675    -3.9045 C.3   18 GLY273  -0.0252
BACKBONE
 283 HA2     21.7477    18.4080    -2.8362 H     18 GLY273   0.0698
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 284 HA3     22.3467    17.6020    -4.3059 H     18 GLY273   0.0698
 285 C       21.6814    19.6129    -4.6021 C.2   18 GLY273   0.5973
BACKBONE
 286 O       20.7486    20.4162    -4.5375 O.2   18 GLY273  -0.5679
BACKBONE
 287 N       22.8062    19.8520    -5.2746 N.am  19 THR274  -0.4157
BACKBONE
 288 H       23.5501    19.1696    -5.2395 H     19 THR274   0.2719
 289 CA      23.0006    21.0697    -6.0625 C.3   19 THR274  -0.0389
BACKBONE
 290 HA      22.6648    21.9176    -5.4655 H     19 THR274   0.1007
 291 C       22.1834    20.9701    -7.3495 C.2   19 THR274   0.5973
BACKBONE
 292 O       22.5439    20.2266    -8.2667 O.2   19 THR274  -0.5679
BACKBONE
 293 CB      24.4954    21.3040    -6.4062 C.3   19 THR274   0.3654
 294 HB      24.7913    20.5759    -7.1615 H     19 THR274   0.0043
 295 OG1     25.2993    21.1328    -5.2300 O.3   19 THR274  -0.6761
 296 HG1     26.2140    21.2847    -5.4789 H     19 THR274   0.4102
 297 CG2     24.7085    22.7104    -6.9690 C.3   19 THR274  -0.2438
 298 HG21    24.4159    23.4486    -6.2224 H     19 THR274   0.0642
 299 HG22    24.1011    22.8392    -7.8648 H     19 THR274   0.0642
 300 HG23    25.7604    22.8454    -7.2207 H     19 THR274   0.0642
 301 N       21.0829    21.7153    -7.4053 N.am  20 TRP275  -0.4157
BACKBONE
 302 H       20.8996    22.3761    -6.6638 H     20 TRP275   0.2719
 303 CA      20.1287    21.6046    -8.5126 C.3   20 TRP275  -0.0275
BACKBONE
 304 HA      20.3426    20.6806    -9.0499 H     20 TRP275   0.1123
 305 C       20.2867    22.7473    -9.5130 C.2   20 TRP275   0.5973
BACKBONE
 306 O       19.9565    23.9039    -9.2247 O.2   20 TRP275  -0.5679
BACKBONE
 307 CB      18.6960    21.5354    -7.9722 C.3   20 TRP275  -0.0050
 308 HB2     18.6940    20.8858    -7.0970 H     20 TRP275   0.0339
 309 HB3     18.3945    22.5410    -7.6790 H     20 TRP275   0.0339
 310 CG      17.6817    21.0080    -8.9501 C.2   20 TRP275  -0.1415
 311 CD1     16.6384    21.7012    -9.5007 C.2   20 TRP275  -0.1638
 312 HD1     16.4104    22.7374    -9.2990 H     20 TRP275   0.2062
 313 CD2     17.6036    19.6767    -9.4825 C.ar  20 TRP275   0.1243
 314 NE1     15.9214    20.8883   -10.3486 N.pl3 20 TRP275  -0.3418
 315 HE1     15.1093    21.1666   -10.8805 H     20 TRP275   0.3412
 316 CE2     16.4875    19.6398   -10.3545 C.ar  20 TRP275   0.1380
 317 CE3     18.3636    18.5111    -9.3071 C.ar  20 TRP275  -0.2387
 318 HE3     19.2187    18.5053    -8.6475 H     20 TRP275   0.1700
 319 CZ2     16.1121    18.4810   -11.0486 C.ar  20 TRP275  -0.2601
 320 HZ2     15.2568    18.4752   -11.7080 H     20 TRP275   0.1572
 321 CZ3     17.9926    17.3579   -10.0026 C.ar  20 TRP275  -0.1972
 322 HZ3     18.5730    16.4550    -9.8827 H     20 TRP275   0.1447
 323 CH2     16.8726    17.3541   -10.8584 C.ar  20 TRP275  -0.1134
 324 HH2     16.6068    16.4443   -11.3762 H     20 TRP275   0.1417
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 325 N       20.7913    22.4042   -10.6930 N.am  21 ILE276  -0.4157
BACKBONE
 326 H       20.9383    21.4251   -10.8926 H     21 ILE276   0.2719
 327 CA      21.1420    23.3911   -11.7140 C.3   21 ILE276  -0.0597
BACKBONE
 328 HA      21.0805    24.3772   -11.2537 H     21 ILE276   0.0869
 329 C       20.1431    23.3719   -12.8812 C.2   21 ILE276   0.5973
BACKBONE
 330 O       20.4884    23.7000   -14.0222 O.2   21 ILE276  -0.5679
BACKBONE
 331 CB      22.6106    23.1987   -12.2083 C.3   21 ILE276   0.1303
 332 HB      22.7917    23.9141   -13.0105 H     21 ILE276   0.0187
 333 CG1     22.8269    21.7877   -12.7750 C.3   21 ILE276  -0.0430
 334 HG12    22.9679    21.1030   -11.9386 H     21 ILE276   0.0236
 335 HG13    21.9333    21.5034   -13.3305 H     21 ILE276   0.0236
 336 CG2     23.5955    23.4715   -11.0688 C.3   21 ILE276  -0.3204
 337 HG21    23.4223    22.7606   -10.2609 H     21 ILE276   0.0882
 338 HG22    23.4497    24.4859   -10.6976 H     21 ILE276   0.0882
 339 HG23    24.6159    23.3623   -11.4364 H     21 ILE276   0.0882
 340 CD1     24.0301    21.6561   -13.7072 C.3   21 ILE276  -0.0660
 341 HD11    24.9371    21.9360   -13.1714 H     21 ILE276   0.0186
 342 HD12    23.8978    22.3139   -14.5662 H     21 ILE276   0.0186
 343 HD13    24.1137    20.6245   -14.0490 H     21 ILE276   0.0186
 344 N       18.8974    23.0076   -12.5782 N.am  22 TYR277  -0.4157
BACKBONE
 345 H       18.6419    22.8788   -11.6097 H     22 TYR277   0.2719
 346 CA      17.8906    22.7900   -13.6206 C.3   22 TYR277  -0.0014
BACKBONE
 347 HA      18.3362    23.1116   -14.5619 H     22 TYR277   0.0876
 348 C       16.6521    23.6763   -13.5033 C.2   22 TYR277   0.5973
BACKBONE
 349 O       16.5084    24.4211   -12.5391 O.2   22 TYR277  -0.5679
BACKBONE
 350 CB      17.5597    21.2976   -13.7285 C.3   22 TYR277  -0.0152
 351 HB2     17.0700    20.9725   -12.8106 H     22 TYR277   0.0295
 352 HB3     16.8893    21.1401   -14.5734 H     22 TYR277   0.0295
 353 CG      18.8164    20.4845   -13.9346 C.ar  22 TYR277  -0.0011
 354 CD1     19.3722    19.7499   -12.8877 C.ar  22 TYR277  -0.1906
 355 HD1     18.8859    19.7458   -11.9234 H     22 TYR277   0.1699
 356 CD2     19.4813    20.4973   -15.1619 C.ar  22 TYR277  -0.1906
 357 HD2     19.0756    21.0748   -15.9795 H     22 TYR277   0.1699
 358 CE1     20.5425    19.0233   -13.0673 C.ar  22 TYR277  -0.2341
 359 HE1     20.9549    18.4466   -12.2526 H     22 TYR277   0.1656
 360 CE2     20.6570    19.7791   -15.3496 C.ar  22 TYR277  -0.2341
 361 HE2     21.1594    19.7948   -16.3055 H     22 TYR277   0.1656
 362 CZ      21.1767    19.0437   -14.2984 C.ar  22 TYR277   0.3226
 363 OH      22.3403    18.3299   -14.4758 O.3   22 TYR277  -0.5579
 364 HH      22.6402    17.8445   -13.7037 H     22 TYR277   0.3992
 365 N       15.7769    23.5878   -14.5058 N.am  23 SER278  -0.4157
BACKBONE
 366 H       15.7911    22.7588   -15.0827 H     23 SER278   0.2719
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 367 CA      14.7949    24.6332   -14.8133 C.3   23 SER278  -0.0249
BACKBONE
 368 HA      15.3681    25.5592   -14.7698 H     23 SER278   0.0843
 369 C       13.6683    24.8358   -13.7994 C.2   23 SER278   0.5973
BACKBONE
 370 O       13.1058    25.9268   -13.7098 O.2   23 SER278  -0.5679
BACKBONE
 371 CB      14.1971    24.3909   -16.2053 C.3   23 SER278   0.2117
 372 HB2     13.5506    25.2284   -16.4676 H     23 SER278   0.0352
 373 HB3     13.6118    23.4716   -16.1882 H     23 SER278   0.0352
 374 OG      15.2210    24.2721   -17.1767 O.3   23 SER278  -0.6546
 375 HG      14.7993    24.1223   -18.0260 H     23 SER278   0.4275
 376 N       13.3402    23.7754   -13.0639 N.am  24 VAL279  -0.4157
BACKBONE
 377 H       13.8351    22.9098   -13.2251 H     24 VAL279   0.2719
 378 CA      12.3015    23.7978   -12.0356 C.3   24 VAL279  -0.0875
BACKBONE
 379 HA      11.8233    24.7768   -12.0031 H     24 VAL279   0.0969
 380 C       12.9712    23.4834   -10.6997 C.2   24 VAL279   0.5973
BACKBONE
 381 O       13.7035    22.5013   -10.5980 O.2   24 VAL279  -0.5679
BACKBONE
 382 CB      11.1908    22.7517   -12.3484 C.3   24 VAL279   0.2985
 383 HB      11.6621    21.7699   -12.3934 H     24 VAL279  -0.0297
 384 CG1     10.1315    22.7177   -11.2456 C.3   24 VAL279  -0.3192
 385 HG11     9.6439    23.6904   -11.1799 H     24 VAL279   0.0791
 386 HG12    10.6063    22.4841   -10.2927 H     24 VAL279   0.0791
 387 HG13     9.3892    21.9542   -11.4783 H     24 VAL279   0.0791
 388 CG2     10.5409    23.0504   -13.6950 C.3   24 VAL279  -0.3192
 389 HG21    10.0664    24.0311   -13.6599 H     24 VAL279   0.0791
 390 HG22     9.7897    22.2910   -13.9124 H     24 VAL279   0.0791
 391 HG23    11.3018    23.0425   -14.4755 H     24 VAL279   0.0791
 392 N       12.7437    24.3178    -9.6854 N.am  25 ASN280  -0.4157
BACKBONE
 393 H       12.0875    25.0773    -9.7981 H     25 ASN280   0.2719
 394 CA      13.4407    24.1400    -8.4050 C.3   25 ASN280   0.0143
BACKBONE
 395 HA      14.4769    23.9320    -8.6717 H     25 ASN280   0.1048
 396 C       12.9591    22.9247    -7.6085 C.2   25 ASN280   0.5973
BACKBONE
 397 O       11.8143    22.4775    -7.7542 O.2   25 ASN280  -0.5679
BACKBONE
 398 CB      13.4374    25.4192    -7.5510 C.3   25 ASN280  -0.2041
 399 HB2     13.8431    26.2362    -8.1477 H     25 ASN280   0.0797
 400 HB3     14.0711    25.2566    -6.6792 H     25 ASN280   0.0797
 401 CG      12.0521    25.8102    -7.0751 C.2   25 ASN280   0.7130
 402 ND2     11.7161    25.6457    -5.9010 N.am  25 ASN280  -0.9191
 403 HD22    12.3677    25.2471    -5.2403 H     25 ASN280   0.4196
 404 HD21    10.7889    25.9096    -5.5994 H     25 ASN280   0.4196
 405 OD1     11.2428    26.3269    -7.9842 O.2   25 ASN280  -0.5931
 406 N       13.8563    22.3994    -6.7772 N.am  26 LYS281  -0.3479
BACKBONE
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 407 H       14.7088    22.9103    -6.5971 H     26 LYS281   0.2747
 408 CA      13.6553    21.1093    -6.1137 C.3   26 LYS281  -0.2400
BACKBONE
 409 HA      13.4817    20.4086    -6.9304 H     26 LYS281   0.1426
 410 C       12.4144    21.0134    -5.2328 C.2   26 LYS281   0.7341
BACKBONE
 411 O       11.8008    19.9559    -5.1577 O.2   26 LYS281  -0.5894
BACKBONE
 412 CB      14.9008    20.7000    -5.3212 C.3   26 LYS281  -0.0094
 413 HB2     14.7206    19.7095    -4.9033 H     26 LYS281   0.0362
 414 HB3     15.7392    20.6541    -6.0162 H     26 LYS281   0.0362
 415 CG      15.2927    21.6263    -4.1762 C.3   26 LYS281   0.0187
 416 HG2     15.5798    22.5982    -4.5777 H     26 LYS281   0.0103
 417 HG3     14.4453    21.7478    -3.5015 H     26 LYS281   0.0103
 418 CD      16.4596    21.0296    -3.4176 C.3   26 LYS281  -0.0479
 419 HD2     17.2694    20.8290    -4.1192 H     26 LYS281   0.0621
 420 HD3     16.1386    20.0954    -2.9568 H     26 LYS281   0.0621
 421 CE      16.9696    21.9587    -2.3351 C.3   26 LYS281  -0.0143
 422 HE2     16.3848    21.8174    -1.4263 H     26 LYS281   0.1135
 423 HE3     16.8796    22.9927    -2.6681 H     26 LYS281   0.1135
 424 NZ      18.4011    21.6434    -2.0631 N.4   26 LYS281  -0.3854
 425 HZ3     18.4823    20.6845    -1.7562 H     26 LYS281   0.3400
 426 HZ1     18.7502    22.2584    -1.3419 H     26 LYS281   0.3400
 427 HZ2     18.9408    21.7736    -2.9069 H     26 LYS281   0.3400
 428 N       12.0555    22.1101    -4.5651 N.am  27 GLU282  -0.5163
BACKBONE
 429 H       12.5855    22.9612    -4.6862 H     27 GLU282   0.2936
 430 CA      10.9082    22.1008    -3.6614 C.3   27 GLU282   0.0397
BACKBONE
 431 HA      11.0399    21.2671    -2.9716 H     27 GLU282   0.1105
 432 C        9.5975    21.8643    -4.4139 C.2   27 GLU282   0.5366
BACKBONE
 433 O        8.7593    21.0835    -3.9707 O.2   27 GLU282  -0.5819
BACKBONE
 434 CB      10.8492    23.3901    -2.8437 C.3   27 GLU282   0.0560
 435 HB2     10.8821    24.2336    -3.5331 H     27 GLU282  -0.0173
 436 HB3      9.9068    23.4047    -2.2963 H     27 GLU282  -0.0173
 437 CG      11.9932    23.5487    -1.8351 C.3   27 GLU282   0.0136
 438 HG2     12.2510    22.5619    -1.4505 H     27 GLU282  -0.0425
 439 HG3     11.6442    24.1779    -1.0165 H     27 GLU282  -0.0425
 440 CD      13.2546    24.1805    -2.4242 C.2   27 GLU282   0.8054
 441 OE1     13.2063    24.7406    -3.5439 O.co2 27 GLU282  -0.8188
 442 OE2     14.3062    24.1178    -1.7509 O.co2 27 GLU282  -0.8188
 443 N        9.4293    22.5323    -5.5543 N.am  28 GLN283  -0.4157
BACKBONE
 444 H       10.1322    23.1958    -5.8468 H     28 GLN283   0.2719
 445 CA       8.2453    22.3244    -6.3937 C.3   28 GLN283  -0.0031
BACKBONE
 446 HA       7.3737    22.5285    -5.7719 H     28 GLN283   0.0850
 447 C        8.1519    20.8812    -6.8852 C.2   28 GLN283   0.5973
BACKBONE
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 448 O        7.0716    20.2860    -6.8687 O.2   28 GLN283  -0.5679
BACKBONE
 449 CB       8.2302    23.2908    -7.5833 C.3   28 GLN283  -0.0036
 450 HB2      9.1610    23.1660    -8.1365 H     28 GLN283   0.0171
 451 HB3      7.3885    23.0296    -8.2247 H     28 GLN283   0.0171
 452 CG       8.0978    24.7612    -7.1957 C.3   28 GLN283  -0.0645
 453 HG2      9.0382    25.0941    -6.7562 H     28 GLN283   0.0352
 454 HG3      7.2985    24.8597    -6.4611 H     28 GLN283   0.0352
 455 CD       7.7773    25.6419    -8.3857 C.2   28 GLN283   0.6951
 456 NE2      8.6129    26.4277    -8.8343 N.am  28 GLN283  -0.9407
 457 HE22     9.5239    26.4963    -8.4037 H     28 GLN283   0.4251
 458 HE21     8.3871    27.0035    -9.6328 H     28 GLN283   0.4251
 459 OE1      6.5659    25.5098    -8.9105 O.2   28 GLN283  -0.6086
 460 N        9.2871    20.3121    -7.2918 N.am  29 LEU284  -0.4157
BACKBONE
 461 H       10.1440    20.8463    -7.2678 H     29 LEU284   0.2719
 462 CA       9.3180    18.9273    -7.7731 C.3   29 LEU284  -0.0518
BACKBONE
 463 HA       8.5233    18.8109    -8.5100 H     29 LEU284   0.0922
 464 C        9.0445    17.9453    -6.6343 C.2   29 LEU284   0.5973
BACKBONE
 465 O        8.2114    17.0416    -6.7722 O.2   29 LEU284  -0.5679
BACKBONE
 466 CB      10.6520    18.6127    -8.4741 C.3   29 LEU284  -0.1102
 467 HB2     11.4622    18.9253    -7.8153 H     29 LEU284   0.0457
 468 HB3     10.7060    17.5353    -8.6305 H     29 LEU284   0.0457
 469 CG      10.8498    19.3014    -9.8319 C.3   29 LEU284   0.3531
 470 HG      10.4597    20.3166    -9.7600 H     29 LEU284  -0.0361
 471 CD1     12.3291    19.3961   -10.1806 C.3   29 LEU284  -0.4121
 472 HD11    12.7486    18.3932   -10.2597 H     29 LEU284   0.1000
 473 HD12    12.8518    19.9482    -9.3995 H     29 LEU284   0.1000
 474 HD13    12.4456    19.9147   -11.1322 H     29 LEU284   0.1000
 475 CD2     10.0652    18.5751   -10.9295 C.3   29 LEU284  -0.4121
 476 HD21    10.4343    17.5539   -11.0248 H     29 LEU284   0.1000
 477 HD22    10.1960    19.0985   -11.8766 H     29 LEU284   0.1000
 478 HD23     9.0072    18.5561   -10.6680 H     29 LEU284   0.1000
 479 N        9.7151    18.1481    -5.4992 N.am  30 ALA285  -0.4157
BACKBONE
 480 H       10.3458    18.9342    -5.4331 H     30 ALA285   0.2719
 481 CA       9.5587    17.2575    -4.3458 C.3   30 ALA285   0.0337
BACKBONE
 482 HA       9.7373    16.2460    -4.7106 H     30 ALA285   0.0823
 483 C        8.1436    17.2840    -3.7708 C.2   30 ALA285   0.5973
BACKBONE
 484 O        7.6134    16.2340    -3.4006 O.2   30 ALA285  -0.5679
BACKBONE
 485 CB      10.5850    17.5721    -3.2622 C.3   30 ALA285  -0.1825
 486 HB1     10.4192    18.5819    -2.8869 H     30 ALA285   0.0603
 487 HB2     11.5889    17.5003    -3.6808 H     30 ALA285   0.0603
 488 HB3     10.4804    16.8588    -2.4446 H     30 ALA285   0.0603
 489 N        7.5340    18.4725    -3.7049 N.am  31 ARG286  -0.3479
BACKBONE
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 490 H        8.0380    19.3053    -3.9740 H     31 ARG286   0.2747
 491 CA       6.1465    18.5851    -3.2485 C.3   31 ARG286  -0.2637
BACKBONE
 492 HA       6.1321    18.1954    -2.2307 H     31 ARG286   0.1560
 493 C        5.1940    17.7561    -4.1027 C.2   31 ARG286   0.7341
BACKBONE
 494 O        4.2190    17.1956    -3.5870 O.2   31 ARG286  -0.5894
BACKBONE
 495 CB       5.6725    20.0377    -3.2335 C.3   31 ARG286  -0.0007
 496 HB2      5.9679    20.5028    -4.1740 H     31 ARG286   0.0327
 497 HB3      4.5855    20.0412    -3.1521 H     31 ARG286   0.0327
 498 CG       6.2363    20.8671    -2.0963 C.3   31 ARG286   0.0390
 499 HG2      7.2500    21.1785    -2.3480 H     31 ARG286   0.0285
 500 HG3      6.2564    20.2641    -1.1885 H     31 ARG286   0.0285
 501 CD       5.3768    22.1031    -1.8581 C.3   31 ARG286   0.0486
 502 HD2      5.7017    22.5813    -0.9341 H     31 ARG286   0.0687
 503 HD3      4.3369    21.7914    -1.7598 H     31 ARG286   0.0687
 504 NE       5.4738    23.0765    -2.9496 N.pl3 31 ARG286  -0.5295
 505 HE       4.8138    22.9951    -3.7099 H     31 ARG286   0.3456
 506 CZ       6.3711    24.0629    -3.0117 C.cat 31 ARG286   0.8076
 507 NH1      7.2762    24.2207    -2.0480 N.pl3 31 ARG286  -0.8627
 508 HH12     7.2880    23.5911    -1.2583 H     31 ARG286   0.4478
 509 HH11     7.9509    24.9699    -2.1066 H     31 ARG286   0.4478
 510 NH2      6.3647    24.8983    -4.0477 N.pl3 31 ARG286  -0.8627
 511 HH21     5.6825    24.7849    -4.7837 H     31 ARG286   0.4478
 512 HH22     7.0421    25.6457    -4.0980 H     31 ARG286   0.4478
 513 N        5.4844    17.6906    -5.4022 N.am  32 ALA287  -0.4157
BACKBONE
 514 H        6.3015    18.1780    -5.7413 H     32 ALA287   0.2719
 515 CA       4.6650    16.9393    -6.3595 C.3   32 ALA287   0.0337
BACKBONE
 516 HA       3.6445    16.9710    -5.9780 H     32 ALA287   0.0823
 517 C        5.0199    15.4511    -6.4491 C.2   32 ALA287   0.5973
BACKBONE
 518 O        4.5687    14.7569    -7.3568 O.2   32 ALA287  -0.5679
BACKBONE
 519 CB       4.7112    17.6029    -7.7386 C.3   32 ALA287  -0.1825
 520 HB1      5.7309    17.5725    -8.1225 H     32 ALA287   0.0603
 521 HB2      4.3855    18.6397    -7.6540 H     32 ALA287   0.0603
 522 HB3      4.0499    17.0689    -8.4210 H     32 ALA287   0.0603
 523 N        5.8080    14.9620    -5.4899 N.am  33 GLY288  -0.4157
BACKBONE
 524 H        6.2179    15.5997    -4.8226 H     33 GLY288   0.2719
 525 CA       6.0987    13.5303    -5.3722 C.3   33 GLY288  -0.0252
BACKBONE
 526 HA2      6.1241    13.2803    -4.3115 H     33 GLY288   0.0698
 527 HA3      5.2884    12.9838    -5.8549 H     33 GLY288   0.0698
 528 C        7.4074    13.0676    -5.9919 C.2   33 GLY288   0.5973
BACKBONE
 529 O        7.7941    11.9043    -5.8362 O.2   33 GLY288  -0.5679
BACKBONE
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 530 N        8.0827    13.9752    -6.6912 N.am  34 PHE289  -0.4157
BACKBONE
 531 H        7.7448    14.9269    -6.7032 H     34 PHE289   0.2719
 532 CA       9.3010    13.6503    -7.4475 C.3   34 PHE289  -0.0024
BACKBONE
 533 HA       9.1666    12.6133    -7.7551 H     34 PHE289   0.0978
 534 C       10.5923    13.7074    -6.6283 C.2   34 PHE289   0.5973
BACKBONE
 535 O       10.7541    14.5526    -5.7404 O.2   34 PHE289  -0.5679
BACKBONE
 536 CB       9.4478    14.5682    -8.6688 C.3   34 PHE289  -0.0343
 537 HB2      9.4853    15.6000    -8.3197 H     34 PHE289   0.0295
 538 HB3     10.3821    14.3210    -9.1730 H     34 PHE289   0.0295
 539 CG       8.3309    14.4465    -9.6601 C.ar  34 PHE289   0.0118
 540 CD1      8.2469    13.3391   -10.5059 C.ar  34 PHE289  -0.1256
 541 HD1      8.9940    12.5617   -10.4445 H     34 PHE289   0.1330
 542 CD2      7.3616    15.4410    -9.7527 C.ar  34 PHE289  -0.1256
 543 HD2      7.4185    16.3037    -9.1055 H     34 PHE289   0.1330
 544 CE1      7.2092    13.2267   -11.4284 C.ar  34 PHE289  -0.1704
 545 HE1      7.1527    12.3663   -12.0786 H     34 PHE289   0.1430
 546 CE2      6.3242    15.3370   -10.6662 C.ar  34 PHE289  -0.1704
 547 HE2      5.5766    16.1140   -10.7264 H     34 PHE289   0.1430
 548 CZ       6.2473    14.2260   -11.5085 C.ar  34 PHE289  -0.1072
 549 HZ       5.4405    14.1434   -12.2217 H     34 PHE289   0.1297
 550 N       11.5067    12.7992    -6.9486 N.am  35 TYR290  -0.4157
BACKBONE
 551 H       11.2606    12.0802    -7.6138 H     35 TYR290   0.2719
 552 CA      12.8521    12.7943    -6.3814 C.3   35 TYR290  -0.0014
BACKBONE
 553 HA      13.0301    13.7354    -5.8611 H     35 TYR290   0.0876
 554 C       13.8562    12.6450    -7.5231 C.2   35 TYR290   0.5973
BACKBONE
 555 O       13.5199    12.1013    -8.5796 O.2   35 TYR290  -0.5679
BACKBONE
 556 CB      13.0223    11.6849    -5.3232 C.3   35 TYR290  -0.0152
 557 HB2     14.0297    11.7629    -4.9144 H     35 TYR290   0.0295
 558 HB3     12.2942    11.8617    -4.5316 H     35 TYR290   0.0295
 559 CG      12.8304    10.2644    -5.8262 C.ar  35 TYR290  -0.0011
 560 CD1     13.9216     9.4967    -6.2487 C.ar  35 TYR290  -0.1906
 561 HD1     14.9133     9.9233    -6.2197 H     35 TYR290   0.1699
 562 CD2     11.5624     9.6801    -5.8627 C.ar  35 TYR290  -0.1906
 563 HD2     10.7063    10.2483    -5.5300 H     35 TYR290   0.1699
 564 CE1     13.7509     8.1912    -6.7061 C.ar  35 TYR290  -0.2341
 565 HE1     14.6031     7.6133    -7.0319 H     35 TYR290   0.1656
 566 CE2     11.3831     8.3781    -6.3204 C.ar  35 TYR290  -0.2341
 567 HE2     10.3944     7.9445    -6.3489 H     35 TYR290   0.1656
 568 CZ      12.4796     7.6399    -6.7398 C.ar  35 TYR290   0.3226
 569 OH      12.2950     6.3526    -7.1907 O.3   35 TYR290  -0.5579
 570 HH      12.9272     6.0595    -7.8510 H     35 TYR290   0.3992
 571 N       15.0752    13.1308    -7.3049 N.am  36 ALA291  -0.4157
BACKBONE
 572 H       15.2998    13.4877    -6.3872 H     36 ALA291   0.2719
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 573 CA      16.1039    13.1671    -8.3475 C.3   36 ALA291   0.0337
BACKBONE
 574 HA      15.5762    13.2976    -9.2923 H     36 ALA291   0.0823
 575 C       16.8878    11.8646    -8.4752 C.2   36 ALA291   0.5973
BACKBONE
 576 O       17.1733    11.1833    -7.4837 O.2   36 ALA291  -0.5679
BACKBONE
 577 CB      17.0535    14.3513    -8.1273 C.3   36 ALA291  -0.1825
 578 HB1     17.5821    14.2224    -7.1828 H     36 ALA291   0.0603
 579 HB2     16.4791    15.2773    -8.0989 H     36 ALA291   0.0603
 580 HB3     17.7742    14.3958    -8.9439 H     36 ALA291   0.0603
 581 N       17.2385    11.5332    -9.7132 N.am  37 LEU292  -0.4157
BACKBONE
 582 H       16.9858    12.1460   -10.4753 H     37 LEU292   0.2719
 583 CA      17.9779    10.3102   -10.0032 C.3   37 LEU292  -0.0518
BACKBONE
 584 HA      17.8862     9.6634    -9.1306 H     37 LEU292   0.0922
 585 C       19.4808    10.5389   -10.1839 C.2   37 LEU292   0.5973
BACKBONE
 586 O       20.2359     9.5906   -10.3946 O.2   37 LEU292  -0.5679
BACKBONE
 587 CB      17.3649     9.6040   -11.2175 C.3   37 LEU292  -0.1102
 588 HB2     17.4193    10.2815   -12.0696 H     37 LEU292   0.0457
 589 HB3     17.9535     8.7104   -11.4255 H     37 LEU292   0.0457
 590 CG      15.8989     9.1819   -11.0314 C.3   37 LEU292   0.3531
 591 HG      15.3166    10.0802   -10.8266 H     37 LEU292  -0.0361
 592 CD1     15.3590     8.5389   -12.2961 C.3   37 LEU292  -0.4121
 593 HD11    15.9301     7.6372   -12.5175 H     37 LEU292   0.1000
 594 HD12    15.4491     9.2391   -13.1266 H     37 LEU292   0.1000
 595 HD13    14.3104     8.2788   -12.1523 H     37 LEU292   0.1000
 596 CD2     15.7451     8.2366    -9.8408 C.3   37 LEU292  -0.4121
 597 HD21    16.3196     7.3282   -10.0216 H     37 LEU292   0.1000
 598 HD22    14.6931     7.9817    -9.7128 H     37 LEU292   0.1000
 599 HD23    16.1129     8.7256    -8.9388 H     37 LEU292   0.1000
 600 N       19.9076    11.7964   -10.0966 N.am  38 GLY293  -0.4157
BACKBONE
 601 H       19.2306    12.5367    -9.9796 H     38 GLY293   0.2719
 602 CA      21.3261    12.1375   -10.1650 C.3   38 GLY293  -0.0252
BACKBONE
 603 HA2     21.4553    13.1467    -9.7740 H     38 GLY293   0.0698
 604 HA3     21.8784    11.4334    -9.5427 H     38 GLY293   0.0698
 605 C       21.9032    12.0912   -11.5640 C.2   38 GLY293   0.5973
BACKBONE
 606 O       23.0968    11.8496   -11.7438 O.2   38 GLY293  -0.5679
BACKBONE
 607 N       21.0515    12.3315   -12.5554 N.am  39 GLU294  -0.5163
BACKBONE
 608 H       20.0823    12.5081   -12.3330 H     39 GLU294   0.2936
 609 CA      21.4650    12.3489   -13.9460 C.3   39 GLU294   0.0397
BACKBONE
 610 HA      22.5341    12.5490   -14.0173 H     39 GLU294   0.1105
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 611 C       20.6891    13.4417   -14.6598 C.2    39 GLU294   0.5366
BACKBONE
 612 O       19.5257    13.2552   -15.0142 O.2    39 GLU294  -0.5819
BACKBONE
 613 CB      21.2005    10.9888   -14.5942 C.3    39 GLU294   0.0560
 614 HB2     21.6231    10.2167   -13.9512 H      39 GLU294  -0.0173
 615 HB3     20.1218    10.8502   -14.6676 H      39 GLU294  -0.0173
 616 CG      21.7954    10.8289   -15.9823 C.3    39 GLU294   0.0136
 617 HG2     22.8807    10.8968   -15.9070 H      39 GLU294  -0.0425
 618 HG3     21.4242    11.6342   -16.6162 H      39 GLU294  -0.0425
 619 CD      21.4345     9.5006   -16.6222 C.2    39 GLU294   0.8054
 620 OE1     21.2387     8.5057   -15.8848 O.co2  39 GLU294  -0.8188
 621 OE2     21.3437     9.4524   -17.8689 O.co2  39 GLU294  -0.8188
 622 N       21.3328    14.5863   -14.8611 N.am   40 GLY295  -0.4157
BACKBONE
 623 H       22.3160    14.6498   -14.6384 H      40 GLY295   0.2719
 624 CA      20.6401    15.7550   -15.3999 C.3    40 GLY295  -0.0252
BACKBONE
 625 HA2     21.3271    16.6008   -15.4275 H      40 GLY295   0.0698
 626 HA3     20.2936    15.5354   -16.4098 H      40 GLY295   0.0698
 627 C       19.4460    16.1040   -14.5220 C.2    40 GLY295   0.5973
BACKBONE
 628 O       19.5210    15.9903   -13.2903 O.2    40 GLY295  -0.5679
BACKBONE
 629 N       18.3442    16.5063   -15.1515 N.am   41 ASP296  -0.5163
BACKBONE
 630 H       18.3457    16.5565   -16.1603 H      41 ASP296   0.2936
 631 CA      17.1276    16.8790   -14.4208 C.3    41 ASP296   0.0381
BACKBONE
 632 HA      17.4561    17.1397   -13.4147 H      41 ASP296   0.0880
 633 C       16.1274    15.7297   -14.2457 C.2    41 ASP296   0.5366
BACKBONE
 634 O       14.9699    15.9498   -13.8771 O.2    41 ASP296  -0.5819
BACKBONE
 635 CB      16.4512    18.1060   -15.0654 C.3    41 ASP296  -0.0303
 636 HB2     17.2119    18.8667   -15.2406 H      41 ASP296  -0.0122
 637 HB3     15.7043    18.4920   -14.3716 H      41 ASP296  -0.0122
 638 CG      15.7617    17.7955   -16.3955 C.2    41 ASP296   0.7994
 639 OD1     15.8640    16.6623   -16.9287 O.co2  41 ASP296  -0.8014
 640 OD2     15.0978    18.7168   -16.9138 O.co2  41 ASP296  -0.8014
 641 N       16.5854    14.5097   -14.5178 N.am   42 LYS297  -0.3479
BACKBONE
 642 H       17.5536    14.4053   -14.7856 H      42 LYS297   0.2747
 643 CA      15.7480    13.3168   -14.4457 C.3    42 LYS297  -0.2400
BACKBONE
 644 HA      14.9185    13.4475   -15.1407 H      42 LYS297   0.1426
 645 C       15.1569    13.1208   -13.0473 C.2    42 LYS297   0.7341
BACKBONE
 646 O       15.8912    13.0227   -12.0585 O.2    42 LYS297  -0.5894
BACKBONE
 647 CB      16.5684    12.0877   -14.8395 C.3    42 LYS297  -0.0094
 648 HB2     17.3141    12.3963   -15.5722 H      42 LYS297   0.0362
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 649 HB3     17.0694    11.7123   -13.9472 H     42 LYS297   0.0362
 650 CG      15.7595    10.9611   -15.4355 C.3   42 LYS297   0.0187
 651 HG2     14.8645    10.8144   -14.8308 H     42 LYS297   0.0103
 652 HG3     15.4713    11.2355   -16.4503 H     42 LYS297   0.0103
 653 CD      16.5389     9.6489   -15.4846 C.3   42 LYS297  -0.0479
 654 HD2     15.8651     8.8559   -15.8089 H     42 LYS297   0.0621
 655 HD3     16.9078     9.4256   -14.4835 H     42 LYS297   0.0621
 656 CE      17.7250     9.7007   -16.4400 C.3   42 LYS297  -0.0143
 657 HE2     18.4488    10.4287   -16.0738 H     42 LYS297   0.1135
 658 HE3     17.3765    10.0004   -17.4284 H     42 LYS297   0.1135
 659 NZ      18.3815     8.3588   -16.5353 N.4   42 LYS297  -0.3854
 660 HZ3     18.7084     8.0783   -15.6218 H     42 LYS297   0.3400
 661 HZ1     19.1641     8.4113   -17.1716 H     42 LYS297   0.3400
 662 HZ2     17.7148     7.6813   -16.8770 H     42 LYS297   0.3400
 663 N       13.8276    13.0782   -12.9780 N.am  43 VAL298  -0.4157
BACKBONE
 664 H       13.2930    13.2377   -13.8200 H     43 VAL298   0.2719
 665 CA      13.1101    12.8095   -11.7304 C.3   43 VAL298  -0.0875
BACKBONE
 666 HA      13.8753    12.5079   -11.0151 H     43 VAL298   0.0969
 667 C       12.0999    11.6727   -11.8905 C.2   43 VAL298   0.5973
BACKBONE
 668 O       11.7757    11.2702   -13.0131 O.2   43 VAL298  -0.5679
BACKBONE
 669 CB      12.3909    14.0733   -11.1563 C.3   43 VAL298   0.2985
 670 HB      11.8724    13.7701   -10.2467 H     43 VAL298  -0.0297
 671 CG1     13.3967    15.1595   -10.7759 C.3   43 VAL298  -0.3192
 672 HG11    13.9338    15.4853   -11.6667 H     43 VAL298   0.0791
 673 HG12    14.1053    14.7604   -10.0501 H     43 VAL298   0.0791
 674 HG13    12.8685    16.0072   -10.3396 H     43 VAL298   0.0791
 675 CG2     11.3402    14.6067   -12.1277 C.3   43 VAL298  -0.3192
 676 HG21    11.8258    14.9203   -13.0519 H     43 VAL298   0.0791
 677 HG22    10.8293    15.4584   -11.6787 H     43 VAL298   0.0791
 678 HG23    10.6156    13.8223   -12.3460 H     43 VAL298   0.0791
 679 N       11.6020    11.1747   -10.7589 N.am  44 LYS299  -0.3479
BACKBONE
 680 H       11.8882    11.5913    -9.8844 H     44 LYS299   0.2747
 681 CA      10.6654    10.0592   -10.7204 C.3   44 LYS299  -0.2400
BACKBONE
 682 HA      10.0576    10.0362   -11.6248 H     44 LYS299   0.1426
 683 C        9.7608    10.2257    -9.4966 C.2   44 LYS299   0.7341
BACKBONE
 684 O       10.2114    10.6745    -8.4399 O.2   44 LYS299  -0.5894
BACKBONE
 685 CB      11.4560     8.7549   -10.6079 C.3   44 LYS299  -0.0094
 686 HB2     12.3196     8.8325   -11.2686 H     44 LYS299   0.0362
 687 HB3     11.7952     8.6606    -9.5763 H     44 LYS299   0.0362
 688 CG      10.7183     7.4922   -10.9648 C.3   44 LYS299   0.0187
 689 HG2      9.7252     7.5046   -10.5155 H     44 LYS299   0.0103
 690 HG3     10.6261     7.4113   -12.0479 H     44 LYS299   0.0103
 691 CD      11.5140     6.3138   -10.4252 C.3   44 LYS299  -0.0479
 692 HD2     11.0742     6.0009    -9.4782 H     44 LYS299   0.0621
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693	HD3	12.5425	6.6346	-10.2598	H	44 LYS299	0.0621
694	CE	11.5224	5.1343	-11.3659	C.3	44 LYS299	-0.0143
695	HE2	10.4915	4.8595	-11.5894	H	44 LYS299	0.1135
696	HE3	12.0224	4.2999	-10.8741	H	44 LYS299	0.1135
697	NZ	12.2270	5.4241	-12.6473	N.4	44 LYS299	-0.3854
698	HZ3	11.7683	6.1912	-13.1178	H	44 LYS299	0.3400
699	HZ1	12.2032	4.6047	-13.2374	H	44 LYS299	0.3400
700	HZ2	13.1869	5.6727	-12.4550	H	44 LYS299	0.3400
701	N	8.4906	9.8600	-9.6339	N.am	45 CYS300	-0.4157
BACKBONE							
702	H	8.1563	9.5392	-10.5314	H	45 CYS300	0.2719
703	CA	7.5739	9.9178	-8.4988	C.3	45 CYS300	-0.0351
BACKBONE							
704	HA	7.8588	10.7688	-7.8800	H	45 CYS300	0.0508
705	C	7.6759	8.6640	-7.6302	C.2	45 CYS300	0.5973
BACKBONE							
706	O	7.7141	7.5453	-8.1471	O.2	45 CYS300	-0.5679
BACKBONE							
707	CB	6.1511	10.1178	-8.9840	C.3	45 CYS300	-0.2413
708	HB2	5.9515	9.3738	-9.7551	H	45 CYS300	0.1122
709	HB3	6.0808	11.1162	-9.4156	H	45 CYS300	0.1122
710	SG	4.8729	9.9668	-7.7222	S.3	45 CYS300	-0.8844
711	N	7.7213	8.8629	-6.3120	N.am	46 PHE301	-0.4157
BACKBONE							
712	H	7.6542	9.8079	-5.9620	H	46 PHE301	0.2719
713	CA	7.8651	7.7611	-5.3471	C.3	46 PHE301	-0.0024
BACKBONE							
714	HA	8.7349	7.1927	-5.6764	H	46 PHE301	0.0978
715	C	6.6745	6.8072	-5.3269	C.2	46 PHE301	0.5973
BACKBONE							
716	O	6.8035	5.6538	-4.8933	O.2	46 PHE301	-0.5679
BACKBONE							
717	CB	8.0764	8.3127	-3.9337	C.3	46 PHE301	-0.0343
718	HB2	8.5409	7.5349	-3.3276	H	46 PHE301	0.0295
719	HB3	8.7444	9.1715	-3.9968	H	46 PHE301	0.0295
720	CG	6.8053	8.7493	-3.2523	C.ar	46 PHE301	0.0118
721	CD1	6.1146	7.8704	-2.4141	C.ar	46 PHE301	-0.1256
722	HD1	6.4981	6.8736	-2.2529	H	46 PHE301	0.1330
723	CD2	6.2967	10.0271	-3.4509	C.ar	46 PHE301	-0.1256
724	HD2	6.8209	10.7152	-4.0975	H	46 PHE301	0.1330
725	CE1	4.9348	8.2663	-1.7829	C.ar	46 PHE301	-0.1704
726	HE1	4.4069	7.5773	-1.1403	H	46 PHE301	0.1430
727	CE2	5.1173	10.4322	-2.8251	C.ar	46 PHE301	-0.1704
728	HE2	4.7286	11.4260	-2.9915	H	46 PHE301	0.1430
729	CZ	4.4420	9.5470	-1.9831	C.ar	46 PHE301	-0.1072
730	HZ	3.5350	9.8597	-1.4873	H	46 PHE301	0.1297
731	N	5.5148	7.2908	-5.7649	N.am	47 HIS302	-0.4157
BACKBONE							
732	H	5.4859	8.1957	-6.2125	H	47 HIS302	0.2719
733	CA	4.2880	6.5248	-5.6033	C.3	47 HIS302	-0.0581
BACKBONE							
734	HA	4.4598	5.7962	-4.8111	H	47 HIS302	0.1360

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 735 C        3.9421     5.7436    -6.8648 C.2   47 HIS302   0.5973
BACKBONE
 736 O        3.8412     4.5193    -6.8225 O.2   47 HIS302  -0.5679
BACKBONE
 737 CB       3.1266     7.4244    -5.1643 C.3   47 HIS302  -0.0074
 738 HB2      2.6270     7.8016    -6.0566 H     47 HIS302   0.0367
 739 HB3      3.5343     8.2601    -4.5955 H     47 HIS302   0.0367
 740 CG       2.1098     6.7226    -4.3127 C.2   47 HIS302   0.1868
 741 ND1      1.4155     5.6115    -4.7439 N.2   47 HIS302  -0.5432
 742 CD2      1.6799     6.9692    -3.0520 C.2   47 HIS302  -0.2207
 743 HD2      2.0149     7.7661    -2.4046 H     47 HIS302   0.1862
 744 CE1      0.5997     5.2061    -3.7878 C.2   47 HIS302   0.1635
 745 HE1     -0.0667     4.3580    -3.8434 H     47 HIS302   0.1435
 746 NE2      0.7372     6.0147    -2.7512 N.pl3 47 HIS302  -0.2795
 747 HE2      0.2318     5.9429    -1.8797 H     47 HIS302   0.3339
 748 N        3.7738     6.4409    -7.9860 N.am  48 CYS303  -0.4157
BACKBONE
 749 H        3.8860     7.4445    -7.9727 H     48 CYS303   0.2719
 750 CA       3.4266     5.7643    -9.2421 C.3   48 CYS303  -0.0351
BACKBONE
 751 HA       2.8073     4.9128    -8.9601 H     48 CYS303   0.0508
 752 C        4.6387     5.1892    -9.9877 C.2   48 CYS303   0.5973
BACKBONE
 753 O        4.4834     4.3211   -10.8498 O.2   48 CYS303  -0.5679
BACKBONE
 754 CB       2.6251     6.6956   -10.1614 C.3   48 CYS303  -0.2413
 755 HB2      1.7471     7.0381    -9.6139 H     48 CYS303   0.1122
 756 HB3      2.3090     6.1214   -11.0323 H     48 CYS303   0.1122
 757 SG       3.5254     8.1503   -10.7451 S.3   48 CYS303  -0.8844
 758 N        5.8356     5.6697    -9.6532 N.am  49 GLY304  -0.4157
BACKBONE
 759 H        5.8960     6.3643    -8.9225 H     49 GLY304   0.2719
 760 CA       7.0694     5.2232   -10.3114 C.3   49 GLY304  -0.0252
BACKBONE
 761 HA2      7.9077     5.4365    -9.6482 H     49 GLY304   0.0698
 762 HA3      7.0002     4.1479   -10.4751 H     49 GLY304   0.0698
 763 C        7.3371     5.8951   -11.6524 C.2   49 GLY304   0.5973
BACKBONE
 764 O        8.2753     5.5292   -12.3601 O.2   49 GLY304  -0.5679
BACKBONE
 765 N        6.5060     6.8724   -12.0035 N.am  50 GLY305  -0.4157
BACKBONE
 766 H        5.7625     7.1324   -11.3712 H     50 GLY305   0.2719
 767 CA       6.6337     7.5808   -13.2723 C.3   50 GLY305  -0.0252
BACKBONE
 768 HA2      6.7697     6.8452   -14.0651 H     50 GLY305   0.0698
 769 HA3      5.7145     8.1394   -13.4487 H     50 GLY305   0.0698
 770 C        7.7978     8.5494   -13.3132 C.2   50 GLY305   0.5973
BACKBONE
 771 O        7.9163     9.4297   -12.4517 O.2   50 GLY305  -0.5679
BACKBONE
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 772 N        8.6423     8.3972   -14.3313 N.am  51 GLY306  -0.4157
BACKBONE
 773 H        8.4898     7.6415   -14.9839 H     51 GLY306   0.2719
 774 CA       9.7833     9.2884   -14.5353 C.3   51 GLY306  -0.0252
BACKBONE
 775 HA2     10.0373     9.7482   -13.5803 H     51 GLY306   0.0698
 776 HA3     10.6265     8.6946   -14.8882 H     51 GLY306   0.0698
 777 C        9.5157    10.3920   -15.5449 C.2   51 GLY306   0.5973
BACKBONE
 778 O        8.7475    10.2032   -16.4932 O.2   51 GLY306  -0.5679
BACKBONE
 779 N       10.1455    11.5481   -15.3355 N.am  52 LEU307  -0.4157
BACKBONE
 780 H       10.6838    11.6617   -14.4884 H     52 LEU307   0.2719
 781 CA      10.0864    12.6617   -16.2889 C.3   52 LEU307  -0.0518
BACKBONE
 782 HA       9.8394    12.2388   -17.2627 H     52 LEU307   0.0922
 783 C       11.4332    13.3700   -16.3819 C.2   52 LEU307   0.5973
BACKBONE
 784 O       12.1136    13.5828   -15.3702 O.2   52 LEU307  -0.5679
BACKBONE
 785 CB       8.9950    13.6702   -15.9096 C.3   52 LEU307  -0.1102
 786 HB2      9.1467    13.9320   -14.8624 H     52 LEU307   0.0457
 787 HB3      9.1420    14.5542   -16.5301 H     52 LEU307   0.0457
 788 CG       7.5274    13.2437   -16.0646 C.3   52 LEU307   0.3531
 789 HG       7.3984    12.3239   -15.4941 H     52 LEU307  -0.0361
 790 CD1      6.5781    14.2930   -15.4811 C.3   52 LEU307  -0.4121
 791 HD11     6.6850    15.2268   -16.0331 H     52 LEU307   0.1000
 792 HD12     6.8226    14.4610   -14.4322 H     52 LEU307   0.1000
 793 HD13     5.5506    13.9386   -15.5623 H     52 LEU307   0.1000
 794 CD2      7.1761    12.9262   -17.5233 C.3   52 LEU307  -0.4121
 795 HD21     7.2933    13.8247   -18.1291 H     52 LEU307   0.1000
 796 HD22     6.1439    12.5807   -17.5816 H     52 LEU307   0.1000
 797 HD23     7.8415    12.1475   -17.8961 H     52 LEU307   0.1000
 798 N       11.7977    13.7418   -17.6035 N.am  53 THR308  -0.4157
BACKBONE
 799 H       11.1750    13.5552   -18.3766 H     53 THR308   0.2719
 800 CA      13.0652    14.4097   -17.8659 C.3   53 THR308  -0.0389
BACKBONE
 801 HA      13.4545    14.7736   -16.9150 H     53 THR308   0.1007
 802 C       12.8696    15.6079   -18.7965 C.2   53 THR308   0.5973
BACKBONE
 803 O       11.8099    15.7508   -19.4108 O.2   53 THR308  -0.5679
BACKBONE
 804 CB      14.0916    13.4201   -18.4733 C.3   53 THR308   0.3654
 805 HB      14.0463    12.4939   -17.9005 H     53 THR308   0.0043
 806 OG1     15.4060    13.9823   -18.3964 O.3   53 THR308  -0.6761
 807 HG1     15.4000    14.8034   -18.8938 H     53 THR308   0.4102
 808 CG2     13.7615    13.0989   -19.9325 C.3   53 THR308  -0.2438
 809 HG21    13.8014    14.0137   -20.5239 H     53 THR308   0.0642
 810 HG22    12.7611    12.6705   -19.9929 H     53 THR308   0.0642
 811 HG23    14.4871    12.3837   -20.3202 H     53 THR308   0.0642
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 812 N       13.8959    16.4581   -18.8870 N.am  54 ASP309  -0.5163
BACKBONE
 813 H       14.6940    16.3137   -18.2851 H     54 ASP309   0.2936
 814 CA      13.9201    17.5934   -19.8200 C.3   54 ASP309   0.0381
BACKBONE
 815 HA      14.8261    18.1698   -19.6326 H     54 ASP309   0.0880
 816 C       12.7433    18.5402   -19.5704 C.2   54 ASP309   0.5366
BACKBONE
 817 O       11.9096    18.7954   -20.4482 O.2   54 ASP309  -0.5819
BACKBONE
 818 CB      14.0038    17.1154   -21.2797 C.3   54 ASP309  -0.0303
 819 HB2     13.9572    17.9851   -21.9350 H     54 ASP309  -0.0122
 820 HB3     13.1551    16.4620   -21.4823 H     54 ASP309  -0.0122
 821 CG      15.2956    16.3473   -21.5750 C.2   54 ASP309   0.7994
 822 OD1     16.2737    16.4903   -20.8107 O.co2 54 ASP309  -0.8014
 823 OD2     15.3403    15.5998   -22.5724 O.co2 54 ASP309  -0.8014
 824 N       12.6956    19.0453   -18.3424 N.am  55 TRP310  -0.4157
BACKBONE
 825 H       13.4168    18.7795   -17.6872 H     55 TRP310   0.2719
 826 CA      11.6562    19.9637   -17.8911 C.3   55 TRP310  -0.0275
BACKBONE
 827 HA      10.7045    19.6180   -18.2947 H     55 TRP310   0.1123
 828 C       11.9207    21.3772   -18.3787 C.2   55 TRP310   0.5973
BACKBONE
 829 O       13.0667    21.8330   -18.3865 O.2   55 TRP310  -0.5679
BACKBONE
 830 CB      11.6316    19.9865   -16.3688 C.3   55 TRP310  -0.0050
 831 HB2     12.6511    20.1444   -16.0170 H     55 TRP310   0.0339
 832 HB3     11.0052    20.8210   -16.0538 H     55 TRP310   0.0339
 833 CG      11.1085    18.7490   -15.7264 C.2   55 TRP310  -0.1415
 834 CD1     11.7429    17.5417   -15.6135 C.2   55 TRP310  -0.1638
 835 HD1     12.7266    17.3212   -16.0010 H     55 TRP310   0.2062
 836 CD2      9.8494    18.6039   -15.0715 C.ar  55 TRP310   0.1243
 837 NE1     10.9430    16.6477   -14.9328 N.pl3 55 TRP310  -0.3418
 838 HE1     11.1780    15.6878   -14.7243 H     55 TRP310   0.3412
 839 CE2      9.7778    17.2771   -14.5868 C.ar  55 TRP310   0.1380
 840 CE3      8.7705    19.4686   -14.8426 C.ar  55 TRP310  -0.2387
 841 HE3      8.7977    20.4898   -15.1929 H     55 TRP310   0.1700
 842 CZ2      8.6623    16.7917   -13.8941 C.ar  55 TRP310  -0.2601
 843 HZ2      8.6242    15.7733   -13.5365 H     55 TRP310   0.1572
 844 CZ3      7.6640    18.9824   -14.1542 C.ar  55 TRP310  -0.1972
 845 HZ3      6.8224    19.6354   -13.9754 H     55 TRP310   0.1447
 846 CH2      7.6202    17.6578   -13.6870 C.ar  55 TRP310  -0.1134
 847 HH2      6.7463    17.3147   -13.1531 H     55 TRP310   0.1417
 848 N       10.8574    22.0742   -18.7708 N.am  56 LYS311  -0.3479
BACKBONE
 849 H        9.9531    21.6246   -18.7850 H     56 LYS311   0.2747
 850 CA      10.9625    23.4699   -19.1806 C.3   56 LYS311  -0.2400
BACKBONE
 851 HA      11.9892    23.6814   -19.4795 H     56 LYS311   0.1426
 852 C       10.5956    24.3760   -18.0053 C.2   56 LYS311   0.7341
BACKBONE
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 853 O        9.8119    23.9746   -17.1372 O.2   56 LYS311  -0.5894
BACKBONE
 854 CB      10.1613    23.5927   -20.5529 C.3   56 LYS311  -0.0094
 855 HB2      9.2363    24.1057   -20.2877 H     56 LYS311   0.0362
 856 HB3     10.6980    24.2913   -21.1947 H     56 LYS311   0.0362
 857 CG       9.6945    22.3622   -21.4724 C.3   56 LYS311   0.0187
 858 HG2      9.5131    21.5054   -20.8368 H     56 LYS311   0.0103
 859 HG3      8.7123    22.6643   -21.8387 H     56 LYS311   0.0103
 860 CD      10.4123    21.7591   -22.7469 C.3   56 LYS311  -0.0479
 861 HD2     11.2335    21.1271   -22.4022 H     56 LYS311   0.0621
 862 HD3     10.8286    22.5703   -23.3429 H     56 LYS311   0.0621
 863 CE       9.4526    20.8930   -23.6725 C.3   56 LYS311  -0.0143
 864 HE2      8.7547    21.5603   -24.1803 H     56 LYS311   0.1135
 865 HE3      8.8705    20.2388   -23.0215 H     56 LYS311   0.1135
 866 NZ      10.1910    20.0210   -24.7125 N.4   56 LYS311  -0.3854
 867 HZ2     10.8578    19.4739   -24.0816 H     56 LYS311   0.0000
 868 HZ3     10.8021    20.7063   -25.2638 H     56 LYS311   0.0000
 869 N       11.1602    25.5995   -17.9586 N.am  57 PRO312  -0.2548
BACKBONE
 870 CA      10.8998    26.4799   -16.8073 C.3   57 PRO312  -0.0266
BACKBONE
 871 HA      11.1036    25.9522   -15.8756 H     57 PRO312   0.0641
 872 C        9.4416    26.9246   -16.6400 C.2   57 PRO312   0.5896
BACKBONE
 873 O        9.0555    27.3723   -15.5516 O.2   57 PRO312  -0.5748
BACKBONE
 874 CB      11.8014    27.6900   -17.0790 C.3   57 PRO312  -0.0070
 875 HB2     11.3141    28.6115   -16.7606 H     57 PRO312   0.0253
 876 HB3     12.7536    27.5842   -16.5594 H     57 PRO312   0.0253
 877 CG      12.0030    27.6865   -18.5390 C.3   57 PRO312   0.0189
 878 HG2     12.9329    28.1933   -18.7969 H     57 PRO312   0.0213
 879 HG3     11.1697    28.1789   -19.0404 H     57 PRO312   0.0213
 880 CD      12.0687    26.2344   -18.9287 C.3   57 PRO312   0.0192
 881 HD2     13.0825    25.8462   -18.8306 H     57 PRO312   0.0391
 882 HD3     11.7198    26.0851   -19.9505 H     57 PRO312   0.0391
 883 N        8.6497    26.7982   -17.7022 N.am  58 SER313  -0.4157
BACKBONE
 884 H        9.0403    26.4275   -18.5566 H     58 SER313   0.2719
 885 CA       7.2310    27.1759   -17.6820 C.3   58 SER313  -0.0249
BACKBONE
 886 HA       7.1441    28.0432   -17.0276 H     58 SER313   0.0843
 887 C        6.3379    26.0743   -17.1169 C.2   58 SER313   0.5973
BACKBONE
 888 O        5.1482    26.2964   -16.8695 O.2   58 SER313  -0.5679
BACKBONE
 889 CB       6.7635    27.5198   -19.0974 C.3   58 SER313   0.2117
 890 HB2      7.3666    28.3420   -19.4827 H     58 SER313   0.0352
 891 HB3      5.7166    27.8214   -19.0643 H     58 SER313   0.0352
 892 OG       6.8979    26.4006   -19.9599 O.3   58 SER313  -0.6546
 893 HG       6.5931    26.6668   -20.8304 H     58 SER313   0.4275
 894 N        6.9109    24.8959   -16.9054 N.am  59 GLU314  -0.5163
BACKBONE
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 895 H        7.9147    24.8128   -16.9805 H     59 GLU314   0.2936
 896 CA       6.1187    23.7174   -16.5663 C.3   59 GLU314   0.0397
BACKBONE
 897 HA       5.1268    23.8824   -16.9871 H     59 GLU314   0.1105
 898 C        5.8875    23.5327   -15.0738 C.2   59 GLU314   0.5366
BACKBONE
 899 O        6.8147    23.6341   -14.2634 O.2   59 GLU314  -0.5819
BACKBONE
 900 CB       6.7328    22.4666   -17.1976 C.3   59 GLU314   0.0560
 901 HB2      7.7422    22.3341   -16.8081 H     59 GLU314  -0.0173
 902 HB3      6.1244    21.6022   -16.9316 H     59 GLU314  -0.0173
 903 CG       6.7999    22.5736   -18.7112 C.3   59 GLU314   0.0136
 904 HG2      7.4357    23.4208   -18.9682 H     59 GLU314  -0.0425
 905 HG3      5.7923    22.7478   -19.0887 H     59 GLU314  -0.0425
 906 CD       7.3535    21.3423   -19.3835 C.2   59 GLU314   0.8054
 907 OE1      8.2950    20.7229   -18.8410 O.co2 59 GLU314  -0.8188
 908 OE2      6.8530    21.0088   -20.4773 O.co2 59 GLU314  -0.8188
 909 N        4.6287    23.2819   -14.7231 N.am  60 ASP315  -0.5163
BACKBONE
 910 H        3.9175    23.2662   -15.4401 H     60 ASP315   0.2936
 911 CA       4.2403    23.0296   -13.3449 C.3   60 ASP315   0.0381
BACKBONE
 912 HA       4.9182    23.5469   -12.6660 H     60 ASP315   0.0880
 913 C        4.3132    21.5299   -13.0898 C.2   60 ASP315   0.5366
BACKBONE
 914 O        3.6995    20.7541   -13.8263 O.2   60 ASP315  -0.5819
BACKBONE
 915 CB       2.8297    23.5638   -13.0791 C.3   60 ASP315  -0.0303
 916 HB2      2.1279    23.0296   -13.7196 H     60 ASP315  -0.0122
 917 HB3      2.8074    24.6260   -13.3226 H     60 ASP315  -0.0122
 918 CG       2.4002    23.3879   -11.6366 C.2   60 ASP315   0.7994
 919 OD1      1.8323    22.3267   -11.3094 O.co2 60 ASP315  -0.8014
 920 OD2      2.6227    24.3128   -10.8272 O.co2 60 ASP315  -0.8014
 921 N        5.0862    21.1130   -12.0654 N.am  61 PRO316  -0.2548
BACKBONE
 922 CA       5.2239    19.6959   -11.7326 C.3   61 PRO316  -0.0266
BACKBONE
 923 HA       5.6754    19.1424   -12.5559 H     61 PRO316   0.0641
 924 C        3.8962    18.9525   -11.5230 C.2   61 PRO316   0.5896
BACKBONE
 925 O        3.7605    17.8180   -11.9787 O.2   61 PRO316  -0.5748
BACKBONE
 926 CB       6.0704    19.7179   -10.4508 C.3   61 PRO316  -0.0070
 927 HB2      5.4348    19.7598    -9.5663 H     61 PRO316   0.0253
 928 HB3      6.7134    18.8395   -10.3949 H     61 PRO316   0.0253
 929 CG       6.8774    20.9565   -10.5813 C.3   61 PRO316   0.0189
 930 HG2      7.7348    20.7928   -11.2340 H     61 PRO316   0.0213
 931 HG3      7.2234    21.2975    -9.6055 H     61 PRO316   0.0213
 932 CD       5.9248    21.9525   -11.1890 C.3   61 PRO316   0.0192
 933 HD2      6.4608    22.7072   -11.7646 H     61 PRO316   0.0391
 934 HD3      5.3242    22.4399   -10.4211 H     61 PRO316   0.0391
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 935 N        2.9212    19.5891   -10.8738 N.am  62 TRP317  -0.4157
BACKBONE
 936 H        3.0844    20.5204   -10.5185 H     62 TRP317   0.2719
 937 CA       1.6154    18.9548   -10.6689 C.3   62 TRP317  -0.0275
BACKBONE
 938 HA       1.8240    17.9670   -10.2580 H     62 TRP317   0.1123
 939 C        0.8378    18.7502   -11.9730 C.2   62 TRP317   0.5973
BACKBONE
 940 O        0.1866    17.7231   -12.1531 O.2   62 TRP317  -0.5679
BACKBONE
 941 CB       0.7642    19.7472    -9.6703 C.3   62 TRP317  -0.0050
 942 HB2      0.9769    20.8071    -9.8102 H     62 TRP317   0.0339
 943 HB3     -0.2854    19.5548    -9.8926 H     62 TRP317   0.0339
 944 CG       1.0059    19.4081    -8.2208 C.2   62 TRP317  -0.1415
 945 CD1      1.2492    20.2881    -7.2058 C.2   62 TRP317  -0.1638
 946 HD1      1.3108    21.3605    -7.3188 H     62 TRP317   0.2062
 947 CD2      1.0045    18.1002    -7.6265 C.ar  62 TRP317   0.1243
 948 NE1      1.4047    19.6111    -6.0184 N.pl3 62 TRP317  -0.3418
 949 HE1      1.5942    20.0355    -5.1217 H     62 TRP317   0.3412
 950 CE2      1.2610    18.2680    -6.2487 C.ar  62 TRP317   0.1380
 951 CE3      0.8262    16.8027    -8.1278 C.ar  62 TRP317  -0.2387
 952 HE3      0.6379    16.6394    -9.1787 H     62 TRP317   0.1700
 953 CZ2      1.3334    17.1862    -5.3589 C.ar  62 TRP317  -0.2601
 954 HZ2      1.5272    17.3375    -4.3073 H     62 TRP317   0.1572
 955 CZ3      0.8971    15.7244    -7.2404 C.ar  62 TRP317  -0.1972
 956 HZ3      0.7562    14.7199    -7.6112 H     62 TRP317   0.1447
 957 CH2      1.1485    15.9284    -5.8753 C.ar  62 TRP317  -0.1134
 958 HH2      1.1978    15.0751    -5.2152 H     62 TRP317   0.1417
 959 N        0.9102    19.7337   -12.8694 N.am  63 GLU318  -0.5163
BACKBONE
 960 H        1.4501    20.5582   -12.6487 H     63 GLU318   0.2936
 961 CA       0.2313    19.6562   -14.1644 C.3   63 GLU318   0.0397
BACKBONE
 962 HA      -0.8133    19.4089   -13.9756 H     63 GLU318   0.1105
 963 C        0.8221    18.5518   -15.0350 C.2   63 GLU318   0.5366
BACKBONE
 964 O        0.0844    17.7964   -15.6687 O.2   63 GLU318  -0.5819
BACKBONE
 965 CB       0.2810    21.0061   -14.8903 C.3   63 GLU318   0.0560
 966 HB2      1.3208    21.3281   -14.9485 H     63 GLU318  -0.0173
 967 HB3     -0.1144    20.8709   -15.8970 H     63 GLU318  -0.0173
 968 CG      -0.5272    22.1037   -14.1964 C.3   63 GLU318   0.0136
 969 HG2     -0.1384    22.2321   -13.1862 H     63 GLU318  -0.0425
 970 HG3     -1.5688    21.7864   -14.1472 H     63 GLU318  -0.0425
 971 CD      -0.4658    23.4469   -14.9107 C.2   63 GLU318   0.8054
 972 OE1      0.2186    23.5561   -15.9517 O.co2 63 GLU318  -0.8188
 973 OE2     -1.1125    24.3993   -14.4244 O.co2 63 GLU318  -0.8188
 974 N        2.1509    18.4677   -15.0593 N.am  64 GLN319  -0.4157
BACKBONE
 975 H        2.6934    19.1633   -14.5675 H     64 GLN319   0.2719
 976 CA       2.8509    17.4013   -15.7747 C.3   64 GLN319  -0.0031
BACKBONE
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 977 HA       2.4870    17.4015   -16.8022 H     64 GLN319   0.0850
 978 C        2.5499    16.0240   -15.1738 C.2   64 GLN319   0.5973
BACKBONE
 979 O        2.3285    15.0531   -15.9062 O.2   64 GLN319  -0.5679
BACKBONE
 980 CB       4.3604    17.6608   -15.7812 C.3   64 GLN319  -0.0036
 981 HB2      4.6694    17.9094   -14.7659 H     64 GLN319   0.0171
 982 HB3      4.8634    16.7483   -16.1008 H     64 GLN319   0.0171
 983 CG       4.7951    18.8014   -16.7101 C.3   64 GLN319  -0.0645
 984 HG2      5.8483    19.0170   -16.5304 H     64 GLN319   0.0352
 985 HG3      4.1993    19.6851   -16.4820 H     64 GLN319   0.0352
 986 CD       4.6122    18.4559   -18.1728 C.2   64 GLN319   0.6951
 987 OE1      5.1539    17.4658   -18.6630 O.2   64 GLN319  -0.6086
 988 NE2      3.8397    19.2698   -18.8772 N.am  64 GLN319  -0.9407
 989 HE22     3.4146    20.0717   -18.4342 H     64 GLN319   0.4251
 990 HE21     3.6759    19.0883   -19.8571 H     64 GLN319   0.4251
 991 N        2.5479    15.9476   -13.8445 N.am  65 HIS320  -0.4157
BACKBONE
 992 H        2.7668    16.7743   -13.3071 H     65 HIS320   0.2719
 993 CA       2.2384    14.7026   -13.1360 C.3   65 HIS320   0.0188
BACKBONE
 994 HA       2.9970    13.9645   -13.3966 H     65 HIS320   0.0881
 995 C        0.8654    14.1717   -13.5611 C.2   65 HIS320   0.5973
BACKBONE
 996 O        0.7175    12.9887   -13.8569 O.2   65 HIS320  -0.5679
BACKBONE
 997 CB       2.2689    14.9234   -11.6198 C.3   65 HIS320  -0.0462
 998 HB2      1.2865    15.2753   -11.3047 H     65 HIS320   0.0402
 999 HB3      3.0158    15.6860   -11.3992 H     65 HIS320   0.0402
1000 CG       2.6033    13.6961   -10.8337 C.2   65 HIS320  -0.0266
1001 ND1      3.2445    13.7466    -9.6130 N.pl3 65 HIS320  -0.3811
1002 HD2      3.5574    14.6488    -9.1085 H     65 HIS320   0.3649
1003 CD2      2.4024    12.3827   -11.0988 C.2   65 HIS320   0.1292
1004 HD2      1.9228    11.9718   -11.9749 H     65 HIS320   0.1147
1005 CE1      3.4155    12.5181    -9.1583 C.2   65 HIS320   0.2057
1006 HE1      3.8795    12.2507    -8.2205 H     65 HIS320   0.1392
1007 NE2      2.9223    11.6717   -10.0460 N.2   65 HIS320  -0.5727
1008 N       -0.1236    15.0600   -13.6161 N.am  66 ALA321  -0.4157
BACKBONE
1009 H        0.0753    16.0263   -13.3999 H     66 ALA321   0.2719
1010 CA      -1.4907    14.6828   -13.9797 C.3   66 ALA321   0.0337
BACKBONE
1011 HA      -1.7082    13.7514   -13.4569 H     66 ALA321   0.0823
1012 C       -1.6547    14.3998   -15.4716 C.2   66 ALA321   0.5973
BACKBONE
1013 O       -2.4667    13.5597   -15.8607 O.2   66 ALA321  -0.5679
BACKBONE
1014 CB      -2.4634    15.7505   -13.5404 C.3   66 ALA321  -0.1825
1015 HB1     -2.2433    16.6805   -14.0647 H     66 ALA321   0.0603
1016 HB2     -2.3691    15.9082   -12.4660 H     66 ALA321   0.0603
1017 HB3     -3.4801    15.4339   -13.7733 H     66 ALA321   0.0603
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1018 N      -0.8989   15.1170  -16.3009 N.am  67 LYS322  -0.3479
BACKBONE
1019 H      -0.2832   15.8185  -15.9149 H     67 LYS322   0.2747
1020 CA     -0.9285   14.9248  -17.7550 C.3   67 LYS322  -0.2400
BACKBONE
1021 HA     -1.9571   15.0333  -18.0989 H     67 LYS322   0.1426
1022 C      -0.4598   13.5197  -18.1304 C.2   67 LYS322   0.7341
BACKBONE
1023 O      -1.1416   12.8050  -18.8690 O.2   67 LYS322  -0.5894
BACKBONE
1024 CB     -0.0642   15.9922  -18.4437 C.3   67 LYS322  -0.0094
1025 HB2    -0.5404   16.9603  -18.2879 H     67 LYS322   0.0362
1026 HB3     0.9158   15.9884  -17.9666 H     67 LYS322   0.0362
1027 CG      0.1434   15.8086  -19.9396 C.3   67 LYS322   0.0187
1028 HG2     0.3326   14.7557  -20.1487 H     67 LYS322   0.0103
1029 HG3    -0.7549   16.1282  -20.4679 H     67 LYS322   0.0103
1030 CD      1.3380   16.6422  -20.4247 C.3   67 LYS322  -0.0479
1031 HD2     2.2287   16.3310  -19.8790 H     67 LYS322   0.0621
1032 HD3     1.1376   17.6945  -20.2230 H     67 LYS322   0.0621
1033 CE      1.5901   16.4670  -21.9191 C.3   67 LYS322  -0.0143
1034 HE2     2.4144   17.1172  -22.2122 H     67 LYS322   0.1135
1035 HE3     0.6893   16.7558  -22.4607 H     67 LYS322   0.1135
1036 NZ      1.9366   15.0643  -22.2843 N.4   67 LYS322  -0.3854
1037 HZ3     2.7753   14.7863  -21.7948 H     67 LYS322   0.3400
1038 HZ1     2.0927   15.0045  -23.2804 H     67 LYS322   0.3400
1039 HZ2     1.1768   14.4514  -22.0252 H     67 LYS322   0.3400
1040 N       0.6966   13.1268  -17.5959 N.am  68 TRP323  -0.4157
BACKBONE
1041 H       1.1478   13.7259  -16.9195 H     68 TRP323   0.2719
1042 CA      1.3347   11.8643  -17.9512 C.3   68 TRP323  -0.0275
BACKBONE
1043 HA      1.0771   11.6701  -18.9924 H     68 TRP323   0.1123
1044 C       0.8320   10.7036  -17.1106 C.2   68 TRP323   0.5973
BACKBONE
1045 O       0.6762    9.5880  -17.6192 O.2   68 TRP323  -0.5679
BACKBONE
1046 CB      2.8500   11.9670  -17.7888 C.3   68 TRP323  -0.0050
1047 HB2     3.0619   12.3279  -16.7824 H     68 TRP323   0.0339
1048 HB3     3.2752   10.9713  -17.9147 H     68 TRP323   0.0339
1049 CG      3.5135   12.8887  -18.7681 C.2   68 TRP323  -0.1415
1050 CD1     3.8932   14.1828  -18.5507 C.2   68 TRP323  -0.1638
1051 HD1     3.7545   14.7202  -17.6242 H     68 TRP323   0.2062
1052 CD2     3.8978   12.5757  -20.1137 C.ar  68 TRP323   0.1243
1053 NE1     4.4778   14.7027  -19.6828 N.pl3 68 TRP323  -0.3418
1054 HE1     4.8324   15.6433  -19.7813 H     68 TRP323   0.3412
1055 CE2     4.5009   13.7361  -20.6554 C.ar  68 TRP323   0.1380
1056 CE3     3.7891   11.4297  -20.9166 C.ar  68 TRP323  -0.2387
1057 HE3     3.3348   10.5285  -20.5322 H     68 TRP323   0.1700
1058 CZ2     4.9928   13.7857  -21.9671 C.ar  68 TRP323  -0.2601
1059 HZ2     5.4464   14.6830  -22.3614 H     68 TRP323   0.1572
1060 CZ3     4.2789   11.4785  -22.2187 C.ar  68 TRP323  -0.1972
1061 HZ3     4.2008   10.6045  -22.8483 H     68 TRP323   0.1447
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1062 CH2      4.8769    12.6528   -22.7311 C.ar  68 TRP323  -0.1134
1063 HH2      5.2499    12.6576   -23.7447 H     68 TRP323   0.1417
1064 N        0.5855    10.9624   -15.8272 N.am  69 TYR324  -0.4157
BACKBONE
1065 H        0.5865    11.9198   -15.5055 H     69 TYR324   0.2719
1066 CA       0.3136     9.8866   -14.8762 C.3   69 TYR324  -0.0014
BACKBONE
1067 HA       0.1088     8.9866   -15.4561 H     69 TYR324   0.0876
1068 C       -0.9436    10.1317   -14.0281 C.2   69 TYR324   0.5973
BACKBONE
1069 O       -0.8636    10.2198   -12.8020 O.2   69 TYR324  -0.5679
BACKBONE
1070 CB       1.5455     9.6533   -13.9878 C.3   69 TYR324  -0.0152
1071 HB2      1.6526    10.5096   -13.3221 H     69 TYR324   0.0295
1072 HB3      1.3744     8.7532   -13.3974 H     69 TYR324   0.0295
1073 CG       2.8536     9.4790   -14.7555 C.ar  69 TYR324  -0.0011
1074 CD1      3.9643    10.2789   -14.4764 C.ar  69 TYR324  -0.1906
1075 HD1      3.8981    11.0304   -13.7036 H     69 TYR324   0.1699
1076 CD2      2.9725     8.5149   -15.7629 C.ar  69 TYR324  -0.1906
1077 HD2      2.1256     7.8865   -15.9963 H     69 TYR324   0.1699
1078 CE1      5.1660    10.1200   -15.1860 C.ar  69 TYR324  -0.2341
1079 HE1      6.0177    10.7464   -14.9654 H     69 TYR324   0.1656
1080 CE2      4.1537     8.3500   -16.4666 C.ar  69 TYR324  -0.2341
1081 HE2      4.2224     7.6006   -17.2413 H     69 TYR324   0.1656
1082 CZ       5.2461     9.1483   -16.1743 C.ar  69 TYR324   0.3226
1083 OH       6.4116     8.9631   -16.8820 O.3   69 TYR324  -0.5579
1084 HH       7.1334     9.5457   -16.6346 H     69 TYR324   0.3992
1085 N       -2.1166    10.2107   -14.6821 N.am  70 PRO325  -0.2548
BACKBONE
1086 CA      -3.3459    10.5777   -13.9772 C.3   70 PRO325  -0.0266
BACKBONE
1087 HA      -3.1876    11.4631   -13.3616 H     70 PRO325   0.0641
1088 C       -3.8494     9.5315   -12.9775 C.2   70 PRO325   0.5896
BACKBONE
1089 O       -4.7560     9.8205   -12.2000 O.2   70 PRO325  -0.5748
BACKBONE
1090 CB      -4.3525    10.7437   -15.1151 C.3   70 PRO325  -0.0070
1091 HB2     -5.3542    10.4635   -14.7894 H     70 PRO325   0.0253
1092 HB3     -4.3622    11.7721   -15.4760 H     70 PRO325   0.0253
1093 CG      -3.8586     9.8104   -16.1803 C.3   70 PRO325   0.0189
1094 HG2     -4.2406    10.0996   -17.1593 H     70 PRO325   0.0213
1095 HG3     -4.1520     8.7830   -15.9648 H     70 PRO325   0.0213
1096 CD      -2.3693     9.9665   -16.1188 C.3   70 PRO325   0.0192
1097 HD2     -2.0392    10.8113   -16.7232 H     70 PRO325   0.0391
1098 HD3     -1.8666     9.0601   -16.4559 H     70 PRO325   0.0391
1099 N       -3.2763     8.3308   -13.0149 N.am  71 GLY326  -0.4157
BACKBONE
1100 H       -2.5530     8.1546   -13.6976 H     71 GLY326   0.2719
1101 CA      -3.6600     7.2634   -12.1020 C.3   71 GLY326  -0.0252
BACKBONE
1102 HA2     -4.7100     7.3974   -11.8421 H     71 GLY326   0.0698
1103 HA3     -3.5318     6.3112   -12.6169 H     71 GLY326   0.0698
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1104 C      -2.8553     7.2212   -10.8191 C.2   71 GLY326   0.5973
BACKBONE
1105 O      -3.0700     6.3429    -9.9816 O.2   71 GLY326  -0.5679
BACKBONE
1106 N      -1.9333     8.1719   -10.6580 N.am  72 CYS327  -0.4157
BACKBONE
1107 H      -1.8142     8.8729   -11.3753 H     72 CYS327   0.2719
1108 CA     -1.0945     8.2185    -9.4665 C.3   72 CYS327  -0.0351
BACKBONE
1109 HA     -0.6295     7.2382    -9.3620 H     72 CYS327   0.0508
1110 C      -1.9124     8.4998    -8.2107 C.2   72 CYS327   0.5973
BACKBONE
1111 O      -2.7181     9.4343    -8.1774 O.2   72 CYS327  -0.5679
BACKBONE
1112 CB     -0.0220     9.2810    -9.6139 C.3   72 CYS327  -0.2413
1113 HB2    -0.5067    10.2382    -9.8059 H     72 CYS327   0.1122
1114 HB3     0.6117     9.0182   -10.4610 H     72 CYS327   0.1122
1115 SG      1.0169     9.4487    -8.1525 S.3   72 CYS327  -0.8844
1116 N      -1.6800     7.7011    -7.1739 N.am  73 LYS328  -0.3479
BACKBONE
1117 H      -0.9531     7.0033    -7.2425 H     73 LYS328   0.2747
1118 CA     -2.4495     7.8081    -5.9396 C.3   73 LYS328  -0.2400
BACKBONE
1119 HA     -3.4604     8.0938    -6.2304 H     73 LYS328   0.1426
1120 C      -1.9396     8.9046    -5.0131 C.2   73 LYS328   0.7341
BACKBONE
1121 O      -2.6984     9.4046    -4.1794 O.2   73 LYS328  -0.5894
BACKBONE
1122 CB     -2.5090     6.4605    -5.2117 C.3   73 LYS328  -0.0094
1123 HB2    -1.4937     6.1668    -4.9456 H     73 LYS328   0.0362
1124 HB3    -3.1010     6.5840    -4.3048 H     73 LYS328   0.0362
1125 CG     -3.1360     5.3375    -6.0530 C.3   73 LYS328   0.0187
1126 HG2    -2.4733     5.1095    -6.8879 H     73 LYS328   0.0103
1127 HG3    -3.2523     4.4514    -5.4290 H     73 LYS328   0.0103
1128 CD     -4.5018     5.7390    -6.6013 C.3   73 LYS328  -0.0479
1129 HD2    -4.3988     6.6632    -7.1700 H     73 LYS328   0.0621
1130 HD3    -5.1860     5.8995    -5.7682 H     73 LYS328   0.0621
1131 CE     -5.0697     4.6604    -7.5078 C.3   73 LYS328  -0.0143
1132 HE2    -4.9222     3.6901    -7.0336 H     73 LYS328   0.1135
1133 HE3    -4.5372     4.6850    -8.4585 H     73 LYS328   0.1135
1134 NZ     -6.5336     4.8521    -7.7694 N.4   73 LYS328  -0.3854
1135 HZ3    -7.0384     4.8243    -6.8950 H     73 LYS328   0.3400
1136 HZ1    -6.8668     4.1150    -8.3741 H     73 LYS328   0.3400
1137 HZ2    -6.6817     5.7462    -8.2153 H     73 LYS328   0.3400
1138 N      -0.6635     9.2704    -5.1533 N.am  74 TYR329  -0.4157
BACKBONE
1139 H      -0.0486     8.7255    -5.7407 H     74 TYR329   0.2719
1140 CA     -0.1474    10.4523    -4.4646 C.3   74 TYR329  -0.0014
BACKBONE
1141 HA     -0.4010    10.3793    -3.4070 H     74 TYR329   0.0876
1142 C      -0.8008    11.7013    -5.0585 C.2   74 TYR329   0.5973
BACKBONE
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1143 O      -1.2381    12.5938    -4.3274 O.2   74 TYR329  -0.5679
BACKBONE
1144 CB      1.3826    10.5357    -4.5363 C.3   74 TYR329  -0.0152
1145 HB2     1.7997     9.6475    -4.0617 H     74 TYR329   0.0295
1146 HB3     1.6787    10.5603    -5.5849 H     74 TYR329   0.0295
1147 CG      1.9527    11.7650    -3.8450 C.ar  74 TYR329  -0.0011
1148 CD1     1.8711    11.9114    -2.4569 C.ar  74 TYR329  -0.1906
1149 HD1     1.4008    11.1369    -1.8691 H     74 TYR329   0.1699
1150 CD2     2.5515    12.7877    -4.5815 C.ar  74 TYR329  -0.1906
1151 HD2     2.6166    12.7012    -5.6561 H     74 TYR329   0.1699
1152 CE1     2.3861    13.0396    -1.8164 C.ar  74 TYR329  -0.2341
1153 HE1     2.3188    13.1355    -0.7428 H     74 TYR329   0.1656
1154 CE2     3.0682    13.9219    -3.9504 C.ar  74 TYR329  -0.2341
1155 HE2     3.5298    14.7047    -4.5339 H     74 TYR329   0.1656
1156 CZ      2.9856    14.0374    -2.5729 C.ar  74 TYR329   0.3226
1157 OH      3.4930    15.1606    -1.9582 O.3   74 TYR329  -0.5579
1158 HH      3.8822    15.8071    -2.5516 H     74 TYR329   0.3992
1159 N      -0.8793    11.7400    -6.3860 N.am  75 LEU330  -0.4157
BACKBONE
1160 H      -0.4361    11.0050    -6.9184 H     75 LEU330   0.2719
1161 CA     -1.5797    12.8008    -7.1061 C.3   75 LEU330  -0.0518
BACKBONE
1162 HA     -1.1025    13.7514    -6.8677 H     75 LEU330   0.0922
1163 C      -3.0462    12.9021    -6.6641 C.2   75 LEU330   0.5973
BACKBONE
1164 O      -3.5440    13.9988    -6.3867 O.2   75 LEU330  -0.5679
BACKBONE
1165 CB     -1.4781    12.5611    -8.6183 C.3   75 LEU330  -0.1102
1166 HB2    -0.4276    12.6715    -8.8874 H     75 LEU330   0.0457
1167 HB3    -1.7933    11.5334    -8.7987 H     75 LEU330   0.0457
1168 CG     -2.2797    13.4483    -9.5761 C.3   75 LEU330   0.3531
1169 HG     -3.3038    13.5139    -9.2085 H     75 LEU330  -0.0361
1170 CD1    -1.7274    14.8671    -9.6193 C.3   75 LEU330  -0.4121
1171 HD11   -0.7001    14.8462    -9.9832 H     75 LEU330   0.1000
1172 HD12   -1.7492    15.2962    -8.6174 H     75 LEU330   0.1000
1173 HD13   -2.3375    15.4744   -10.2879 H     75 LEU330   0.1000
1174 CD2    -2.2892    12.8279   -10.9618 C.3   75 LEU330  -0.4121
1175 HD21   -1.2678    12.7591   -11.3361 H     75 LEU330   0.1000
1176 HD22   -2.8815    13.4488   -11.6339 H     75 LEU330   0.1000
1177 HD23   -2.7252    11.8302   -10.9102 H     75 LEU330   0.1000
1178 N      -3.7234    11.7575    -6.5886 N.am  76 LEU331  -0.4157
BACKBONE
1179 H      -3.2634    10.8979    -6.8527 H     76 LEU331   0.2719
1180 CA     -5.1116    11.7080    -6.1351 C.3   76 LEU331  -0.0518
BACKBONE
1181 HA     -5.6960    12.3274    -6.8156 H     76 LEU331   0.0922
1182 C      -5.2856    12.2982    -4.7286 C.2   76 LEU331   0.5973
BACKBONE
1183 O      -6.1700    13.1316    -4.5060 O.2   76 LEU331  -0.5679
BACKBONE
1184 CB     -5.6441    10.2712    -6.1902 C.3   76 LEU331  -0.1102
1185 HB2    -5.4893     9.9064    -7.2057 H     76 LEU331   0.0457
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1186	HB3	-5.0490	9.6776	-5.4963	H	76 LEU331	0.0457
1187	CG	-7.1183	10.0387	-5.8416	C.3	76 LEU331	0.3531
1188	HG	-7.3036	10.4310	-4.8417	H	76 LEU331	-0.0361
1189	CD1	-8.0397	10.7923	-6.8066	C.3	76 LEU331	-0.4121
1190	HD11	-7.8819	10.4254	-7.8208	H	76 LEU331	0.1000
1191	HD12	-7.8144	11.8580	-6.7666	H	76 LEU331	0.1000
1192	HD13	-9.0784	10.6296	-6.5190	H	76 LEU331	0.1000
1193	CD2	-7.4262	8.5455	-5.8405	C.3	76 LEU331	-0.4121
1194	HD21	-7.2459	8.1366	-6.8347	H	76 LEU331	0.1000
1195	HD22	-8.4699	8.3899	-5.5675	H	76 LEU331	0.1000
1196	HD23	-6.7829	8.0425	-5.1186	H	76 LEU331	0.1000
1197	N	-4.4355	11.8741	-3.7971	N.am	77 GLU332	-0.5163
BACKBONE							
1198	H	-3.7169	11.2139	-4.0575	H	77 GLU332	0.2936
1199	CA	-4.5052	12.3324	-2.4019	C.3	77 GLU332	0.0397
BACKBONE							
1200	HA	-5.5162	12.1310	-2.0478	H	77 GLU332	0.1105
1201	C	-4.2790	13.8431	-2.2671	C.2	77 GLU332	0.5366
BACKBONE							
1202	O	-5.0231	14.5287	-1.5605	O.2	77 GLU332	-0.5819
BACKBONE							
1203	CB	-3.5023	11.5595	-1.5378	C.3	77 GLU332	0.0560
1204	HB2	-3.6120	10.4972	-1.7557	H	77 GLU332	-0.0173
1205	HB3	-2.4976	11.8841	-1.8085	H	77 GLU332	-0.0173
1206	CG	-3.6805	11.7599	-0.0332	C.3	77 GLU332	0.0136
1207	HG2	-4.7203	11.5550	0.2216	H	77 GLU332	-0.0425
1208	HG3	-3.4449	12.7966	0.2074	H	77 GLU332	-0.0425
1209	CD	-2.7903	10.8551	0.8082	C.2	77 GLU332	0.8054
1210	OE1	-2.0061	10.0625	0.2348	O.co2	77 GLU332	-0.8188
1211	OE2	-2.8784	10.9360	2.0556	O.co2	77 GLU332	-0.8188
1212	N	-3.2667	14.3535	-2.9647	N.am	78 GLN333	-0.4157
BACKBONE							
1213	H	-2.7704	13.7565	-3.6108	H	78 GLN333	0.2719
1214	CA	-2.8475	15.7486	-2.8289	C.3	78 GLN333	-0.0031
BACKBONE							
1215	HA	-2.9556	15.9897	-1.7715	H	78 GLN333	0.0850
1216	C	-3.7220	16.7356	-3.5947	C.2	78 GLN333	0.5973
BACKBONE							
1217	O	-3.9616	17.8530	-3.1219	O.2	78 GLN333	-0.5679
BACKBONE							
1218	CB	-1.3937	15.9078	-3.2752	C.3	78 GLN333	-0.0036
1219	HB2	-1.3081	15.5423	-4.2984	H	78 GLN333	0.0171
1220	HB3	-1.1409	16.9677	-3.2456	H	78 GLN333	0.0171
1221	CG	-0.3935	15.1549	-2.4146	C.3	78 GLN333	-0.0645
1222	HG2	0.5934	15.2438	-2.8688	H	78 GLN333	0.0352
1223	HG3	-0.6843	14.1050	-2.3802	H	78 GLN333	0.0352
1224	CD	-0.3238	15.6838	-0.9999	C.2	78 GLN333	0.6951
1225	NE2	-0.0469	16.8614	-0.7782	N.am	78 GLN333	-0.9407
1226	HE22	0.1360	17.4906	-1.5468	H	78 GLN333	0.4251
1227	HE21	-0.0023	17.1993	0.1726	H	78 GLN333	0.4251
1228	OE1	-0.5721	14.8165	-0.0356	O.2	78 GLN333	-0.6086

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1229 N       -4.1849    16.3328    -4.7768 N.am  79 LYS334  -0.3479
BACKBONE
1230 H       -4.0423    15.3746    -5.0625 H     79 LYS334   0.2747
1231 CA      -4.8960    17.2483    -5.6712 C.3   79 LYS334  -0.2400
BACKBONE
1232 HA      -4.8380    18.2199    -5.1804 H     79 LYS334   0.1426
1233 C       -6.3812    16.9425    -5.8412 C.2   79 LYS334   0.7341
BACKBONE
1234 O       -7.1731    17.8536    -6.0924 O.2   79 LYS334  -0.5894
BACKBONE
1235 CB      -4.2189    17.3085    -7.0491 C.3   79 LYS334  -0.0094
1236 HB2     -4.3255    16.3309    -7.5194 H     79 LYS334   0.0362
1237 HB3     -4.7380    18.0578    -7.6467 H     79 LYS334   0.0362
1238 CG      -2.7257    17.6663    -7.0328 C.3   79 LYS334   0.0187
1239 HG2     -2.1905    16.8994    -6.4728 H     79 LYS334   0.0103
1240 HG3     -2.3618    17.6867    -8.0600 H     79 LYS334   0.0103
1241 CD      -2.4447    19.0305    -6.3865 C.3   79 LYS334  -0.0479
1242 HD2     -1.3754    19.1132    -6.1923 H     79 LYS334   0.0621
1243 HD3     -2.9907    19.0920    -5.4452 H     79 LYS334   0.0621
1244 CE      -2.8705    20.1843    -7.2742 C.3   79 LYS334  -0.0143
1245 HE2     -3.9507    20.1439    -7.4148 H     79 LYS334   0.1135
1246 HE3     -2.3747    20.0903    -8.2403 H     79 LYS334   0.1135
1247 NZ      -2.5097    21.4942    -6.6705 N.4   79 LYS334  -0.3854
1248 HZ3     -2.9695    21.5909    -5.7763 H     79 LYS334   0.3400
1249 HZ1     -2.8055    22.2404    -7.2836 H     79 LYS334   0.3400
1250 HZ2     -1.5091    21.5413    -6.5414 H     79 LYS334   0.3400
1251 N       -6.7527    15.6696    -5.7291 N.am  80 GLY335  -0.4157
BACKBONE
1252 H       -6.0487    14.9663    -5.5569 H     80 GLY335   0.2719
1253 CA      -8.1528    15.2602    -5.8484 C.3   80 GLY335  -0.0252
BACKBONE
1254 HA2     -8.3193    14.4161    -5.1792 H     80 GLY335   0.0698
1255 HA3     -8.7800    16.0969    -5.5408 H     80 GLY335   0.0698
1256 C       -8.5682    14.8452    -7.2480 C.2   80 GLY335   0.5973
BACKBONE
1257 O       -7.9217    15.2083    -8.2346 O.2   80 GLY335  -0.5679
BACKBONE
1258 N       -9.6606    14.0871    -7.3235 N.am  81 GLN336  -0.4157
BACKBONE
1259 H      -10.1543    13.8695    -6.4697 H     81 GLN336   0.2719
1260 CA     -10.1814    13.5531    -8.5854 C.3   81 GLN336  -0.0031
BACKBONE
1261 HA      -9.3738    12.9806    -9.0416 H     81 GLN336   0.0850
1262 C      -10.5687    14.6466    -9.5812 C.2   81 GLN336   0.5973
BACKBONE
1263 O      -10.3300    14.5014   -10.7779 O.2   81 GLN336  -0.5679
BACKBONE
1264 CB     -11.3818    12.6394    -8.3164 C.3   81 GLN336  -0.0036
1265 HB2    -11.0948    11.9248    -7.5451 H     81 GLN336   0.0171
1266 HB3    -12.2011    13.2587    -7.9512 H     81 GLN336   0.0171
1267 CG     -11.8890    11.8496    -9.5288 C.3   81 GLN336  -0.0645
1268 HG2    -11.0854    11.2049    -9.8849 H     81 GLN336   0.0352
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1269 HG3    -12.1637    12.5547   -10.3132 H     81 GLN336   0.0352
1270 CD     -13.1056    10.9802    -9.2057 C.2   81 GLN336   0.6951
1271 NE2    -13.1437    10.2972    -8.1802 N.am  81 GLN336  -0.9407
1272 HE22   -12.3659    10.3095    -7.5360 H     81 GLN336   0.4251
1273 HE21   -13.9528     9.7254    -7.9842 H     81 GLN336   0.4251
1274 OE1    -14.0997    11.0031   -10.0888 O.2   81 GLN336  -0.6086
1275 N      -11.1675    15.7296    -9.0850 N.am  82 GLU337  -0.5163
BACKBONE
1276 H      -11.3005    15.8019    -8.0864 H     82 GLU337   0.2936
1277 CA     -11.6409    16.8237    -9.9500 C.3   82 GLU337   0.0397
BACKBONE
1278 HA     -12.2470    16.3481   -10.7211 H     82 GLU337   0.1105
1279 C      -10.5087    17.5577   -10.6628 C.2   82 GLU337   0.5366
BACKBONE
1280 O      -10.6463    17.9175   -11.8262 O.2   82 GLU337  -0.5819
BACKBONE
1281 CB     -12.5210    17.8171    -9.1765 C.3   82 GLU337   0.0560
1282 HB2    -11.9772    18.1306    -8.2855 H     82 GLU337  -0.0173
1283 HB3    -12.7003    18.6816    -9.8157 H     82 GLU337  -0.0173
1284 CG     -13.8769    17.2592    -8.7366 C.3   82 GLU337   0.0136
1285 HG2    -14.4752    18.0785    -8.3378 H     82 GLU337  -0.0425
1286 HG3    -13.7091    16.5181    -7.9552 H     82 GLU337  -0.0425
1287 CD     -14.6548    16.5990    -9.8713 C.2   82 GLU337   0.8054
1288 OE1    -14.7720    17.2083   -10.9606 O.co2 82 GLU337  -0.8188
1289 OE2    -15.1502    15.4656    -9.6707 O.co2 82 GLU337  -0.8188
1290 N       -9.3994    17.7723    -9.9595 N.am  83 TYR338  -0.4157
BACKBONE
1291 H       -9.3815    17.5041    -8.9860 H     83 TYR338   0.2719
1292 CA      -8.2024    18.3835   -10.5455 C.3   83 TYR338  -0.0014
BACKBONE
1293 HA      -8.4844    19.3693   -10.9154 H     83 TYR338   0.0876
1294 C       -7.6727    17.5592   -11.7276 C.2   83 TYR338   0.5973
BACKBONE
1295 O       -7.3944    18.1005   -12.8092 O.2   83 TYR338  -0.5679
BACKBONE
1296 CB      -7.1003    18.5359    -9.4820 C.3   83 TYR338  -0.0152
1297 HB2     -7.4454    19.2431    -8.7277 H     83 TYR338   0.0295
1298 HB3     -6.9321    17.5637    -9.0187 H     83 TYR338   0.0295
1299 CG      -5.7825    19.0351   -10.0386 C.ar  83 TYR338  -0.0011
1300 CD1     -5.5472    20.4018   -10.1956 C.ar  83 TYR338  -0.1906
1301 HD1     -6.3124    21.1087    -9.9106 H     83 TYR338   0.1699
1302 CD2     -4.7742    18.1430   -10.4207 C.ar  83 TYR338  -0.1906
1303 HD2     -4.9373    17.0807   -10.3148 H     83 TYR338   0.1699
1304 CE1     -4.3411    20.8694   -10.7140 C.ar  83 TYR338  -0.2341
1305 HE1     -4.1745    21.9303   -10.8286 H     83 TYR338   0.1656
1306 CE2     -3.5636    18.6018   -10.9354 C.ar  83 TYR338  -0.2341
1307 HE2     -2.7922    17.9008   -11.2184 H     83 TYR338   0.1656
1308 CZ      -3.3563    19.9657   -11.0819 C.ar  83 TYR338   0.3226
1309 OH      -2.1663    20.4333   -11.5898 O.3   83 TYR338  -0.5579
1310 HH      -2.1022    21.3887   -11.6592 H     83 TYR338   0.3992
1311 N       -7.5309    16.2552   -11.5047 N.am  84 ILE339  -0.4157
BACKBONE
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1312 H       -7.7839    15.8914   -10.5972 H     84 ILE339   0.2719
1313 CA      -7.0246    15.3218   -12.5156 C.3   84 ILE339  -0.0597
BACKBONE
1314 HA      -6.0471    15.6915   -12.8252 H     84 ILE339   0.0869
1315 C       -7.9605    15.2651   -13.7252 C.2   84 ILE339   0.5973
BACKBONE
1316 O       -7.5178    15.4029   -14.8680 O.2   84 ILE339  -0.5679
BACKBONE
1317 CB      -6.8655    13.8891   -11.9386 C.3   84 ILE339   0.1303
1318 HB      -7.8419    13.5478   -11.5946 H     84 ILE339   0.0187
1319 CG1     -5.9212    13.8880   -10.7330 C.3   84 ILE339  -0.0430
1320 HG12    -4.9005    14.0072   -11.0967 H     84 ILE339   0.0236
1321 HG13    -6.1800    14.7320   -10.0937 H     84 ILE339   0.0236
1322 CG2     -6.3813    12.9177   -13.0265 C.3   84 ILE339  -0.3204
1323 HG21    -5.4041    13.2365   -13.3892 H     84 ILE339   0.0882
1324 HG22    -7.0922    12.9140   -13.8528 H     84 ILE339   0.0882
1325 HG23    -6.3041    11.9138   -12.6090 H     84 ILE339   0.0882
1326 CD1     -5.9867    12.6185    -9.8991 C.3   84 ILE339  -0.0660
1327 HD11    -5.7306    11.7613   -10.5217 H     84 ILE339   0.0186
1328 HD12    -6.9957    12.4937    -9.5061 H     84 ILE339   0.0186
1329 HD13    -5.2809    12.6905    -9.0716 H     84 ILE339   0.0186
1330 N       -9.2502    15.0711   -13.4570 N.am  85 ASN340  -0.4157
BACKBONE
1331 H       -9.5426    14.9927   -12.4934 H     85 ASN340   0.2719
1332 CA     -10.2588    14.9676   -14.5146 C.3   85 ASN340   0.0143
BACKBONE
1333 HA      -9.9117    14.1969   -15.2028 H     85 ASN340   0.1048
1334 C      -10.4002    16.2588   -15.3226 C.2   85 ASN340   0.5973
BACKBONE
1335 O      -10.5104    16.2111   -16.5421 O.2   85 ASN340  -0.5679
BACKBONE
1336 CB     -11.6152    14.5458   -13.9351 C.3   85 ASN340  -0.2041
1337 HB2    -12.3692    14.6296   -14.7177 H     85 ASN340   0.0797
1338 HB3    -11.8670    15.2175   -13.1145 H     85 ASN340   0.0797
1339 CG     -11.6157    13.1131   -13.4095 C.2   85 ASN340   0.7130
1340 OD1    -10.6428    12.3670   -13.5739 O.2   85 ASN340  -0.5931
1341 ND2    -12.7121    12.7270   -12.7688 N.am  85 ASN340  -0.9191
1342 HD22   -13.4839    13.3687   -12.6568 H     85 ASN340   0.4196
1343 HD21   -12.7745    11.7915   -12.3932 H     85 ASN340   0.4196
1344 N      -10.3746    17.4027   -14.6420 N.am  86 ASN341  -0.4157
BACKBONE
1345 H      -10.2807    17.3726   -13.6369 H     86 ASN341   0.2719
1346 CA     -10.4787    18.7051   -15.3081 C.3   86 ASN341   0.0143
BACKBONE
1347 HA     -11.3766    18.6546   -15.9239 H     86 ASN341   0.1048
1348 C       -9.3210    18.9960   -16.2614 C.2   86 ASN341   0.5973
BACKBONE
1349 O       -9.5053    19.6658   -17.2761 O.2   86 ASN341  -0.5679
BACKBONE
1350 CB     -10.6402    19.8385   -14.2855 C.3   86 ASN341  -0.2041
1351 HB2    -10.2840    20.7657   -14.7343 H     86 ASN341   0.0797
1352 HB3    -10.0372    19.6044   -13.4082 H     86 ASN341   0.0797
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1353 CG     -12.0904    20.0361   -13.8425 C.2   86 ASN341   0.7130
1354 ND2    -12.3533    20.6102   -12.7801 N.am  86 ASN341  -0.9191
1355 HD22   -11.6063    20.9486   -12.1906 H     86 ASN341   0.4196
1356 HD21   -13.3152    20.7409   -12.5014 H     86 ASN341   0.4196
1357 OD1    -13.0363    19.5701   -14.6575 O.2   86 ASN341  -0.5931
1358 N       -8.1331    18.4907   -15.9336 N.am  87 ILE342  -0.4157
BACKBONE
1359 H       -8.0258    18.0399   -15.0362 H     87 ILE342   0.2719
1360 CA      -6.9753    18.5664   -16.8311 C.3   87 ILE342  -0.0597
BACKBONE
1361 HA      -6.8428    19.6089   -17.1203 H     87 ILE342   0.0869
1362 C       -7.2212    17.7537   -18.1097 C.2   87 ILE342   0.5973
BACKBONE
1363 O       -6.8432    18.1717   -19.2072 O.2   87 ILE342  -0.5679
BACKBONE
1364 CB      -5.6682    18.1193   -16.1115 C.3   87 ILE342   0.1303
1365 HB      -5.9085    17.2881   -15.4484 H     87 ILE342   0.0187
1366 CG1     -5.1168    19.2856   -15.2787 C.3   87 ILE342  -0.0430
1367 HG12    -4.8822    20.1054   -15.9577 H     87 ILE342   0.0236
1368 HG13    -5.8935    19.6014   -14.5823 H     87 ILE342   0.0236
1369 CG2     -4.6124    17.5977   -17.1066 C.3   87 ILE342  -0.3204
1370 HG21    -4.3370    18.3960   -17.7957 H     87 ILE342   0.0882
1371 HG22    -5.0250    16.7594   -17.6680 H     87 ILE342   0.0882
1372 HG23    -3.7287    17.2689   -16.5596 H     87 ILE342   0.0882
1373 CD1     -3.8801    18.9674   -14.4859 C.3   87 ILE342  -0.0660
1374 HD11    -3.0871    18.6482   -15.1623 H     87 ILE342   0.0186
1375 HD12    -4.0980    18.1675   -13.7783 H     87 ILE342   0.0186
1376 HD13    -3.5584    19.8557   -13.9424 H     87 ILE342   0.0186
1377 N       -7.8797    16.6101   -17.9564 N.am  88 HIS343  -0.4157
BACKBONE
1378 H       -8.2331    16.3649   -17.0425 H     88 HIS343   0.2719
1379 CA      -8.1061    15.6981   -19.0743 C.3   88 HIS343  -0.0581
BACKBONE
1380 HA      -7.3465    15.9380   -19.8183 H     88 HIS343   0.1360
1381 C       -9.4274    15.9002   -19.8114 C.2   88 HIS343   0.5973
BACKBONE
1382 O       -9.5614    15.5051   -20.9729 O.2   88 HIS343  -0.5679
BACKBONE
1383 CB      -7.9362    14.2567   -18.6110 C.3   88 HIS343  -0.0074
1384 HB2     -8.3093    13.5945   -19.3923 H     88 HIS343   0.0367
1385 HB3     -8.5211    14.1126   -17.7026 H     88 HIS343   0.0367
1386 CG      -6.5144    13.8997   -18.3233 C.2   88 HIS343   0.1868
1387 ND1     -5.5878    13.6863   -19.3220 N.2   88 HIS343  -0.5432
1388 CD2     -5.8487    13.7526   -17.1531 C.2   88 HIS343  -0.2207
1389 HD2     -6.2618    13.8619   -16.1612 H     88 HIS343   0.1862
1390 CE1     -4.4156    13.4060   -18.7796 C.2   88 HIS343   0.1635
1391 HE1     -3.5053    13.1882   -19.3185 H     88 HIS343   0.1435
1392 NE2     -4.5474    13.4379   -17.4666 N.pl3 88 HIS343  -0.2795
1393 HE2     -3.8106    13.2596   -16.7992 H     88 HIS343   0.3339
1394 N      -10.3956    16.5098   -19.1368 N.am  89 LEU344  -0.4157
BACKBONE
1395 H      -10.2651    16.7055   -18.1546 H     89 LEU344   0.2719
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1396 CA     -11.6420    16.9026   -19.7818 C.3   89 LEU344  -0.0518
BACKBONE
1397 HA     -11.8273    16.2852   -20.6608 H     89 LEU344   0.0922
1398 C      -11.5063    18.3653   -20.2129 C.2   89 LEU344   0.5973
BACKBONE
1399 O      -11.8663    19.2868   -19.4758 O.2   89 LEU344  -0.5679
BACKBONE
1400 CB     -12.8450    16.6749   -18.8525 C.3   89 LEU344  -0.1102
1401 HB2    -12.7605    17.3849   -18.0298 H     89 LEU344   0.0457
1402 HB3    -13.7460    16.8900   -19.4270 H     89 LEU344   0.0457
1403 CG     -13.0150    15.2751   -18.2367 C.3   89 LEU344   0.3531
1404 HG     -12.0645    15.0310   -17.7621 H     89 LEU344  -0.0361
1405 CD1    -14.1060    15.2644   -17.1674 C.3   89 LEU344  -0.4121
1406 HD11   -15.0653    15.5069   -17.6247 H     89 LEU344   0.1000
1407 HD12   -13.8713    16.0036   -16.4015 H     89 LEU344   0.1000
1408 HD13   -14.1598    14.2751   -16.7131 H     89 LEU344   0.1000
1409 CD2    -13.2852    14.2031   -19.2894 C.3   89 LEU344  -0.4121
1410 HD21   -14.2314    14.4137   -19.7879 H     89 LEU344   0.1000
1411 HD22   -13.3375    13.2264   -18.8082 H     89 LEU344   0.1000
1412 HD23   -12.4796    14.2036   -20.0237 H     89 LEU344   0.1000
1413 N      -10.9547    18.5587   -21.4092 N.am  90 THR345  -0.7301
BACKBONE
1414 H      -10.7380    17.7510   -21.9755 H     90 THR345   0.3700
1415 CA     -10.6471    19.8898   -21.9431 C.3   90 THR345   0.2811
BACKBONE
1416 HA     -10.0811    20.3931   -21.1592 H     90 THR345   0.0800
1417 C      -11.8945    20.7427   -22.2127 C.2   90 THR345   0.4490
BACKBONE
1418 H      -11.7859    21.8057   -22.3694 H     90 THR345   0.0600
1419 O      -13.0193    20.2362   -22.2537 O.2   90 THR345  -0.5700
BACKBONE
1420 CB      -9.7722    19.8020   -23.2240 C.3   90 THR345   0.2000
1421 HB      -8.9305    19.1441   -23.0079 H     90 THR345   0.0800
1422 OG1     -9.2985    21.1076   -23.5792 O.3   90 THR345  -0.6800
1423 HG1     -8.7638    21.0168   -24.3714 H     90 THR345   0.4000
1424 CG2    -10.5560    19.2120   -24.3998 C.3   90 THR345  -0.2400
1425 HG21   -11.4036    19.8569   -24.6316 H     90 THR345   0.0800
1426 HG22   -10.9173    18.2187   -24.1335 H     90 THR345   0.0800
1427 HG23    -9.9049    19.1403   -25.2710 H     90 THR345   0.0800
1428 C        8.3416    16.6475   -18.2357 C.3   91 <91>     0.0300
1429 C        8.2367    18.3180   -21.6858 C.3   91 <91>    -0.2400
1430 C        7.9733    17.2102   -20.6578 C.3   91 <91>     0.2510
1431 C        8.2561    15.7827   -21.2368 C.2   91 <91>     0.5690
1432 N        8.7081    17.5139   -19.3854 N.3   91 <91>    -0.9000
1433 O        7.5464    15.3088   -22.1196 O.2   91 <91>    -0.5700
1434 C        9.7796    13.7353   -21.3667 C.3   91 <91>     0.2810
1435 C        9.8062    12.6463   -20.2477 C.2   91 <91>     0.5690
1436 N        9.3442    15.0727   -20.9312 N.am  91 <91>    -0.7300
1437 O       10.4585    12.8594   -19.2269 O.2   91 <91>    -0.5700
1438 C       11.0795    13.8046   -22.1869 C.3   91 <91>    -0.0160
1439 N        9.2210    11.4371   -20.4140 N.am  91 <91>    -0.6600
1440 C        8.4256    11.1467   -21.5979 C.3   91 <91>     0.1400
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1441 C        7.5395     9.9714   -21.2048 C.3   91 <91>    -0.1600
1442 C        8.4632     9.1888   -20.2748 C.3   91 <91>    -0.1600
1443 C        9.2059    10.2824   -19.4929 C.3   91 <91>     0.2810
1444 C       10.5875     9.7577   -18.9933 C.2   91 <91>     0.5690
1445 N       11.7322    10.2402   -19.4692 N.am  91 <91>    -0.7300
1446 C       13.0891     9.8634   -19.1131 C.3   91 <91>     0.3640
1447 O       10.6708     8.8465   -18.1789 O.2   91 <91>    -0.5700
1448 C       13.0090     9.3345   -17.7119 C.ar  91 <91>    -0.1440
1449 C       12.8927     7.9636   -17.7022 C.ar  91 <91>    -0.1440
1450 C       12.8796     7.3851   -19.0894 C.3   91 <91>    -0.0160
1451 C       13.4304     8.5801   -19.9124 C.3   91 <91>    -0.1600
1452 C       13.0281    10.0545   -16.5177 C.ar  91 <91>    -0.1500
1453 C       12.9293     9.3771   -15.2984 C.ar  91 <91>    -0.1500
1454 C       12.8090     7.9867   -15.2802 C.ar  91 <91>    -0.1500
1455 C       12.7902     7.2982   -16.4883 C.ar  91 <91>     0.1900
1456 F       12.6684     5.9480   -16.4747 F     91 <91>    -0.1900
1457 C       10.7997    14.7280   -23.3564 C.ar  91 <91>    -0.1440
1458 C       11.0871    16.0910   -23.2499 C.ar  91 <91>    -0.1500
1459 C       10.8928    16.9352   -24.3376 C.ar  91 <91>    -0.1500
1460 C       10.4146    16.4029   -25.5293 C.ar  91 <91>     0.0820
1461 C       10.0888    15.0530   -25.6433 C.ar  91 <91>    -0.1500
1462 C       10.2891    14.2166   -24.5505 C.ar  91 <91>    -0.1500
1463 O       10.0543    17.5084   -26.3708 O.3   91 <91>    -0.2660
1464 S        9.1629    18.8216   -25.8835 S.o2  91 <91>     1.6830
1465 O        8.0672    18.3622   -25.1193 O.2   91 <91>    -0.6500
1466 O        8.7789    19.5906   -27.0076 O.2   91 <91>    -0.6500
@<TRIPOS>BOND
   1    1    2  1
   2    1    3  1
   3    1    4  1   BACKBONE
   4    4    5  1
   5    4    6  1   BACKBONE
   6    4    8  1
   7    6    7  2   BACKBONE
   8    6   21  am  BACKBONE|INTERRES
   9    8    9  1
  10    8   10  1
  11    8   11  1
  12   11   12  1
  13   11   13  1
  14   11   17  1
  15   13   14  1
  16   13   15  1
  17   13   16  1
  18   17   18  1
  19   17   19  1
  20   17   20  1
  21   21   22  1   BACKBONE
  22   21   32  1
  23   22   23  1
  24   22   24  1   BACKBONE
  25   22   26  1
```

26	24	25	2	BACKBONE
27	24	35	am	BACKBONE|INTERRES
28	26	27	1	
29	26	28	1	
30	26	29	1	
31	29	30	1	
32	29	31	1	
33	29	32	1	
34	32	33	1	
35	32	34	1	
36	35	36	1	
37	35	37	1	BACKBONE
38	37	38	1	
39	37	39	1	BACKBONE
40	37	41	1	
41	39	40	2	BACKBONE
42	39	59	am	BACKBONE|INTERRES
43	41	42	1	
44	41	43	1	
45	41	44	1	
46	44	45	1	
47	44	46	1	
48	44	47	1	
49	47	48	1	
50	47	49	1	
51	47	50	1	
52	50	51	1	
53	50	52	ar	
54	52	53	ar	
55	52	56	ar	
56	53	54	1	
57	53	55	1	
58	56	57	1	
59	56	58	1	
60	59	60	1	
61	59	61	1	BACKBONE
62	61	62	1	
63	61	63	1	BACKBONE
64	61	65	1	
65	63	64	2	BACKBONE
66	63	73	am	BACKBONE|INTERRES
67	65	66	1	
68	65	67	1	
69	65	68	1	
70	68	69	2	
71	68	70	am	
72	70	71	1	
73	70	72	1	
74	73	74	1	BACKBONE
75	73	84	1	
76	74	75	1	
77	74	76	1	BACKBONE

78	74	78	1	
79	76	77	2	BACKBONE
80	76	87	am	BACKBONE|INTERRES
81	78	79	1	
82	78	80	1	
83	78	81	1	
84	81	82	1	
85	81	83	1	
86	81	84	1	
87	84	85	1	
88	84	86	1	
89	87	88	1	
90	87	89	1	BACKBONE
91	89	90	1	
92	89	91	1	BACKBONE
93	89	93	1	
94	91	92	2	BACKBONE
95	91	98	am	BACKBONE|INTERRES
96	93	94	1	
97	93	95	1	
98	93	96	1	
99	96	97	1	
100	98	99	1	
101	98	100	1	BACKBONE
102	100	101	1	
103	100	102	1	BACKBONE
104	100	104	1	
105	102	103	2	BACKBONE
106	102	115	am	BACKBONE|INTERRES
107	104	105	1	
108	104	106	1	
109	104	107	1	
110	107	108	1	
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114	111	112	1	
115	111	113	1	
116	111	114	1	
117	115	116	1	
118	115	117	1	BACKBONE
119	117	118	1	
120	117	119	1	BACKBONE
121	117	121	1	
122	119	120	2	BACKBONE
123	119	125	am	BACKBONE|INTERRES
124	121	122	1	
125	121	123	1	
126	121	124	1	
127	125	126	1	
128	125	127	1	BACKBONE
129	127	128	1	

```
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131  127  131  1
132  129  130  2   BACKBONE
133  129  137  am  BACKBONE|INTERRES
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135  131  133  1
136  131  134  1
137  134  135  ar
138  134  136  ar
139  137  138  1
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141  139  140  1
142  139  141  1   BACKBONE
143  139  143  1
144  141  142  2   BACKBONE
145  141  158  am  BACKBONE|INTERRES
146  143  144  1
147  143  145  1
148  143  146  1
149  146  147  ar
150  146  149  ar
151  147  148  1
152  147  151  ar
153  149  150  1
154  149  153  ar
155  151  152  1
156  151  155  ar
157  153  154  1
158  153  155  ar
159  155  156  1
160  156  157  1
161  158  159  1
162  158  160  1   BACKBONE
163  160  161  1
164  160  162  1   BACKBONE
165  160  164  1
166  162  163  2   BACKBONE
167  162  173  am  BACKBONE|INTERRES
168  164  165  1
169  164  166  1
170  164  167  1
171  167  168  1
172  167  169  1
173  167  170  1
174  170  171  ar
175  170  172  ar
176  173  174  1
177  173  175  1   BACKBONE
178  175  176  1
179  175  177  1   BACKBONE
180  175  179  1
181  177  178  2   BACKBONE
```

```
182  177  183  am  BACKBONE|INTERRES
183  179  180  1
184  179  181  1
185  179  182  1
186  183  184  1
187  183  185  1   BACKBONE
188  185  186  1
189  185  187  1   BACKBONE
190  185  189  1
191  187  188  2   BACKBONE
192  187  207  am  BACKBONE|INTERRES
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194  189  191  1
195  189  192  1
196  192  193  1
197  192  194  1
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204  200  201  ar
205  200  204  ar
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211  207  209  1   BACKBONE
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216  211  226  am  BACKBONE|INTERRES
217  213  214  1
218  213  215  1
219  213  218  1
220  215  216  1
221  215  217  1
222  215  222  1
223  218  219  1
224  218  220  1
225  218  221  1
226  222  223  1
227  222  224  1
228  222  225  1
229  226  227  1
230  226  228  1   BACKBONE
231  228  229  1
232  228  230  1   BACKBONE
233  228  232  1
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```
234  230  231  2   BACKBONE
235  230  246  am  BACKBONE|INTERRES
236  232  233  1
237  232  234  1
238  232  235  1
239  235  236  ar
240  235  238  ar
241  236  237  1
242  236  240  ar
243  238  239  1
244  238  242  ar
245  240  241  1
246  240  244  ar
247  242  243  1
248  242  244  ar
249  244  245  1
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256  250  260  am  BACKBONE|INTERRES
257  252  253  1
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260  254  255  1
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262  256  258  1
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265  260  262  1   BACKBONE
266  262  263  1
267  262  264  1   BACKBONE
268  262  266  1
269  264  265  2   BACKBONE
270  264  280  am  BACKBONE|INTERRES
271  266  267  1
272  266  268  1
273  266  269  1
274  269  270  ar
275  269  272  ar
276  270  271  1
277  270  274  ar
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279  272  276  ar
280  274  275  1
281  274  278  ar
282  276  277  1
283  276  278  ar
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```

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290  285  286  2   BACKBONE
291  285  287  am  BACKBONE|INTERRES
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311  305  306  2   BACKBONE
312  305  325  am  BACKBONE|INTERRES
313  307  308  1
314  307  309  1
315  307  310  1
316  310  311  2
317  310  313  1
318  311  312  1
319  311  314  1
320  313  316  ar
321  313  317  ar
322  314  315  1
323  314  316  1
324  316  319  ar
325  317  318  1
326  317  321  ar
327  319  320  1
328  319  323  ar
329  321  322  1
330  321  323  ar
331  323  324  1
332  325  326  1
333  325  327  1   BACKBONE
334  327  328  1
335  327  329  1   BACKBONE
336  327  331  1
337  329  330  2   BACKBONE
```

```
338  329  344  am  BACKBONE|INTERRES
339  331  332  1
340  331  333  1
341  331  336  1
342  333  334  1
343  333  335  1
344  333  340  1
345  336  337  1
346  336  338  1
347  336  339  1
348  340  341  1
349  340  342  1
350  340  343  1
351  344  345  1
352  344  346  1   BACKBONE
353  346  347  1
354  346  348  1   BACKBONE
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356  348  349  2   BACKBONE
357  348  365  am  BACKBONE|INTERRES
358  350  351  1
359  350  352  1
360  350  353  1
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362  353  356  ar
363  354  355  1
364  354  358  ar
365  356  357  1
366  356  360  ar
367  358  359  1
368  358  362  ar
369  360  361  1
370  360  362  ar
371  362  363  1
372  363  364  1
373  365  366  1
374  365  367  1   BACKBONE
375  367  368  1
376  367  369  1   BACKBONE
377  367  371  1
378  369  370  2   BACKBONE
379  369  376  am  BACKBONE|INTERRES
380  371  372  1
381  371  373  1
382  371  374  1
383  374  375  1
384  376  377  1
385  376  378  1   BACKBONE
386  378  379  1
387  378  380  1   BACKBONE
388  378  382  1
389  380  381  2   BACKBONE
```

```
390  380  392  am  BACKBONE|INTERRES
391  382  383  1
392  382  384  1
393  382  388  1
394  384  385  1
395  384  386  1
396  384  387  1
397  388  389  1
398  388  390  1
399  388  391  1
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403  394  396  1   BACKBONE
404  394  398  1
405  396  397  2   BACKBONE
406  396  406  am  BACKBONE|INTERRES
407  398  399  1
408  398  400  1
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410  401  402  am
411  401  405  2
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420  410  428  am  BACKBONE|INTERRES
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440  430  434  1
441  432  433  2   BACKBONE
```

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442  432  443  am  BACKBONE|INTERRES
443  434  435  1
444  434  436  1
445  434  437  1
446  437  438  1
447  437  439  1
448  437  440  1
449  440  441  ar
450  440  442  ar
451  443  444  1
452  443  445  1   BACKBONE
453  445  446  1
454  445  447  1   BACKBONE
455  445  449  1
456  447  448  2   BACKBONE
457  447  460  am  BACKBONE|INTERRES
458  449  450  1
459  449  451  1
460  449  452  1
461  452  453  1
462  452  454  1
463  452  455  1
464  455  456  am
465  455  459  2
466  456  457  1
467  456  458  1
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469  460  462  1   BACKBONE
470  462  463  1
471  462  464  1   BACKBONE
472  462  466  1
473  464  465  2   BACKBONE
474  464  479  am  BACKBONE|INTERRES
475  466  467  1
476  466  468  1
477  466  469  1
478  469  470  1
479  469  471  1
480  469  475  1
481  471  472  1
482  471  473  1
483  471  474  1
484  475  476  1
485  475  477  1
486  475  478  1
487  479  480  1
488  479  481  1   BACKBONE
489  481  482  1
490  481  483  1   BACKBONE
491  481  485  1
492  483  484  2   BACKBONE
493  483  489  am  BACKBONE|INTERRES
```

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496  485  488  1
497  489  490  1
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499  491  492  1
500  491  493  1   BACKBONE
501  491  495  1
502  493  494  2   BACKBONE
503  493  513  am  BACKBONE|INTERRES
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512  501  504  1
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514  504  506  ar
515  506  507  ar
516  506  510  ar
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524  515  517  1   BACKBONE
525  515  519  1
526  517  518  2   BACKBONE
527  517  523  am  BACKBONE|INTERRES
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529  519  521  1
530  519  522  1
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533  525  526  1
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536  528  529  2   BACKBONE
537  528  530  am  BACKBONE|INTERRES
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541  532  534  1   BACKBONE
542  532  536  1
543  534  535  2   BACKBONE
544  534  550  am  BACKBONE|INTERRES
545  536  537  1
```

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565  554  571  am  BACKBONE|INTERRES
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587  575  581  am  BACKBONE|INTERRES
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595  583  587  1
596  585  586  2   BACKBONE
597  585  600  am  BACKBONE|INTERRES
```

```
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614  602  605  1   BACKBONE
615  605  606  2   BACKBONE
616  605  607  am  BACKBONE|INTERRES
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618  607  609  1   BACKBONE
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620  609  611  1   BACKBONE
621  609  613  1
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623  611  622  am  BACKBONE|INTERRES
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625  613  615  1
626  613  616  1
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628  616  618  1
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631  619  621  ar
632  622  623  1
633  622  624  1   BACKBONE
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635  624  626  1
636  624  627  1   BACKBONE
637  627  628  2   BACKBONE
638  627  629  am  BACKBONE|INTERRES
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640  629  631  1   BACKBONE
641  631  632  1
642  631  633  1   BACKBONE
643  631  635  1
644  633  634  2   BACKBONE
645  633  641  am  BACKBONE|INTERRES
646  635  636  1
647  635  637  1
648  635  638  1
649  638  639  ar
```

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650  638  640  ar
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653  643  644  1
654  643  645  1   BACKBONE
655  643  647  1
656  645  646  2   BACKBONE
657  645  663  am  BACKBONE|INTERRES
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659  647  649  1
660  647  650  1
661  650  651  1
662  650  652  1
663  650  653  1
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673  663  664  1
674  663  665  1   BACKBONE
675  665  666  1
676  665  667  1   BACKBONE
677  665  669  1
678  667  668  2   BACKBONE
679  667  679  am  BACKBONE|INTERRES
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681  669  671  1
682  669  675  1
683  671  672  1
684  671  673  1
685  671  674  1
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687  675  677  1
688  675  678  1
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690  679  681  1   BACKBONE
691  681  682  1
692  681  683  1   BACKBONE
693  681  685  1
694  683  684  2   BACKBONE
695  683  701  am  BACKBONE|INTERRES
696  685  686  1
697  685  687  1
698  685  688  1
699  688  689  1
700  688  690  1
701  688  691  1
```

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709  697  699  1
710  697  700  1
711  701  702  1
712  701  703  1   BACKBONE
713  703  704  1
714  703  705  1   BACKBONE
715  703  707  1
716  705  706  2   BACKBONE
717  705  711  am  BACKBONE|INTERRES
718  707  708  1
719  707  709  1
720  707  710  1
721  711  712  1
722  711  713  1   BACKBONE
723  713  714  1
724  713  715  1   BACKBONE
725  713  717  1
726  715  716  2   BACKBONE
727  715  731  am  BACKBONE|INTERRES
728  717  718  1
729  717  719  1
730  717  720  1
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741  729  730  1
742  731  732  1
743  731  733  1   BACKBONE
744  733  734  1
745  733  735  1   BACKBONE
746  733  737  1
747  735  736  2   BACKBONE
748  735  748  am  BACKBONE|INTERRES
749  737  738  1
750  737  739  1
751  737  740  1
752  740  741  1
753  740  742  2
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754  741  744  2
755  742  743  1
756  742  746  1
757  744  745  1
758  744  746  1
759  746  747  1
760  748  749  1
761  748  750  1   BACKBONE
762  750  751  1
763  750  752  1   BACKBONE
764  750  754  1
765  752  753  2   BACKBONE
766  752  758  am  BACKBONE|INTERRES
767  754  755  1
768  754  756  1
769  754  757  1
770  758  759  1
771  758  760  1   BACKBONE
772  760  761  1
773  760  762  1
774  760  763  1   BACKBONE
775  763  764  2   BACKBONE
776  763  765  am  BACKBONE|INTERRES
777  765  766  1
778  765  767  1   BACKBONE
779  767  768  1
780  767  769  1
781  767  770  1   BACKBONE
782  770  771  2   BACKBONE
783  770  772  am  BACKBONE|INTERRES
784  772  773  1
785  772  774  1   BACKBONE
786  774  775  1
787  774  776  1
788  774  777  1   BACKBONE
789  777  778  2   BACKBONE
790  777  779  am  BACKBONE|INTERRES
791  779  780  1
792  779  781  1   BACKBONE
793  781  782  1
794  781  783  1   BACKBONE
795  781  785  1
796  783  784  2   BACKBONE
797  783  798  am  BACKBONE|INTERRES
798  785  786  1
799  785  787  1
800  785  788  1
801  788  789  1
802  788  790  1
803  788  794  1
804  790  791  1
805  790  792  1
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806  790  793  1
807  794  795  1
808  794  796  1
809  794  797  1
810  798  799  1
811  798  800  1   BACKBONE
812  800  801  1
813  800  802  1   BACKBONE
814  800  804  1
815  802  803  2   BACKBONE
816  802  812  am  BACKBONE|INTERRES
817  804  805  1
818  804  806  1
819  804  808  1
820  806  807  1
821  808  809  1
822  808  810  1
823  808  811  1
824  812  813  1
825  812  814  1   BACKBONE
826  814  815  1
827  814  816  1   BACKBONE
828  814  818  1
829  816  817  2   BACKBONE
830  816  824  am  BACKBONE|INTERRES
831  818  819  1
832  818  820  1
833  818  821  1
834  821  822  ar
835  821  823  ar
836  824  825  1
837  824  826  1   BACKBONE
838  826  827  1
839  826  828  1   BACKBONE
840  826  830  1
841  828  829  2   BACKBONE
842  828  848  am  BACKBONE|INTERRES
843  830  831  1
844  830  832  1
845  830  833  1
846  833  834  2
847  833  836  1
848  834  835  1
849  834  837  1
850  836  839  ar
851  836  840  ar
852  837  838  1
853  837  839  1
854  839  842  ar
855  840  841  1
856  840  844  ar
857  842  843  1
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858  842  846  ar
859  844  845  1
860  844  846  ar
861  846  847  1
862  848  849  1
863  848  850  1   BACKBONE
864  850  851  1
865  850  852  1   BACKBONE
866  850  854  1
867  852  853  2   BACKBONE
868  852  869  am  BACKBONE|INTERRES
869  854  855  1
870  854  856  1
871  854  857  1
872  857  858  1
873  857  859  1
874  857  860  1
875  860  861  1
876  860  862  1
877  860  863  1
878  863  864  1
879  863  865  1
880  863  866  1
881  866  867  1
882  866  868  1
883  866 1464  1   INTERRES
884  869  870  1   BACKBONE
885  869  880  1
886  870  871  1
887  870  872  1   BACKBONE
888  870  874  1
889  872  873  2   BACKBONE
890  872  883  am  BACKBONE|INTERRES
891  874  875  1
892  874  876  1
893  874  877  1
894  877  878  1
895  877  879  1
896  877  880  1
897  880  881  1
898  880  882  1
899  883  884  1
900  883  885  1   BACKBONE
901  885  886  1
902  885  887  1   BACKBONE
903  885  889  1
904  887  888  2   BACKBONE
905  887  894  am  BACKBONE|INTERRES
906  889  890  1
907  889  891  1
908  889  892  1
909  892  893  1
```

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910  894  895  1
911  894  896  1   BACKBONE
912  896  897  1
913  896  898  1   BACKBONE
914  896  900  1
915  898  899  2   BACKBONE
916  898  909  am  BACKBONE|INTERRES
917  900  901  1
918  900  902  1
919  900  903  1
920  903  904  1
921  903  905  1
922  903  906  1
923  906  907  ar
924  906  908  ar
925  909  910  1
926  909  911  1   BACKBONE
927  911  912  1
928  911  913  1   BACKBONE
929  911  915  1
930  913  914  2   BACKBONE
931  913  921  am  BACKBONE|INTERRES
932  915  916  1
933  915  917  1
934  915  918  1
935  918  919  ar
936  918  920  ar
937  921  922  1   BACKBONE
938  921  932  1
939  922  923  1
940  922  924  1   BACKBONE
941  922  926  1
942  924  925  2   BACKBONE
943  924  935  am  BACKBONE|INTERRES
944  926  927  1
945  926  928  1
946  926  929  1
947  929  930  1
948  929  931  1
949  929  932  1
950  932  933  1
951  932  934  1
952  935  936  1
953  935  937  1   BACKBONE
954  937  938  1
955  937  939  1   BACKBONE
956  937  941  1
957  939  940  2   BACKBONE
958  939  959  am  BACKBONE|INTERRES
959  941  942  1
960  941  943  1
961  941  944  1
```

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 962  944  945  2
 963  944  947  1
 964  945  946  1
 965  945  948  1
 966  947  950  ar
 967  947  951  ar
 968  948  949  1
 969  948  950  1
 970  950  953  ar
 971  951  952  1
 972  951  955  ar
 973  953  954  1
 974  953  957  ar
 975  955  956  1
 976  955  957  ar
 977  957  958  1
 978  959  960  1
 979  959  961  1   BACKBONE
 980  961  962  1
 981  961  963  1   BACKBONE
 982  961  965  1
 983  963  964  2   BACKBONE
 984  963  974  am  BACKBONE|INTERRES
 985  965  966  1
 986  965  967  1
 987  965  968  1
 988  968  969  1
 989  968  970  1
 990  968  971  1
 991  971  972  ar
 992  971  973  ar
 993  974  975  1
 994  974  976  1   BACKBONE
 995  976  977  1
 996  976  978  1   BACKBONE
 997  976  980  1
 998  978  979  2   BACKBONE
 999  978  991  am  BACKBONE|INTERRES
1000  980  981  1
1001  980  982  1
1002  980  983  1
1003  983  984  1
1004  983  985  1
1005  983  986  1
1006  986  987  2
1007  986  988  am
1008  988  989  1
1009  988  990  1
1010  991  992  1
1011  991  993  1   BACKBONE
1012  993  994  1
1013  993  995  1   BACKBONE
```

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1014  993  997  1
1015  995  996  2   BACKBONE
1016  995 1008  am  BACKBONE|INTERRES
1017  997  998  1
1018  997  999  1
1019  997 1000  1
1020 1000 1001  1
1021 1000 1003  2
1022 1001 1002  1
1023 1001 1005  1
1024 1003 1004  1
1025 1003 1007  1
1026 1005 1006  1
1027 1005 1007  2
1028 1008 1009  1
1029 1008 1010  1   BACKBONE
1030 1010 1011  1
1031 1010 1012  1   BACKBONE
1032 1010 1014  1
1033 1012 1013  2   BACKBONE
1034 1012 1018  am  BACKBONE|INTERRES
1035 1014 1015  1
1036 1014 1016  1
1037 1014 1017  1
1038 1018 1019  1
1039 1018 1020  1   BACKBONE
1040 1020 1021  1
1041 1020 1022  1   BACKBONE
1042 1020 1024  1
1043 1022 1023  2   BACKBONE
1044 1022 1040  am  BACKBONE|INTERRES
1045 1024 1025  1
1046 1024 1026  1
1047 1024 1027  1
1048 1027 1028  1
1049 1027 1029  1
1050 1027 1030  1
1051 1030 1031  1
1052 1030 1032  1
1053 1030 1033  1
1054 1033 1034  1
1055 1033 1035  1
1056 1033 1036  1
1057 1036 1037  1
1058 1036 1038  1
1059 1036 1039  1
1060 1040 1041  1
1061 1040 1042  1   BACKBONE
1062 1042 1043  1
1063 1042 1044  1   BACKBONE
1064 1042 1046  1
1065 1044 1045  2   BACKBONE
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1066 1044 1064  am  BACKBONE|INTERRES
1067 1046 1047  1
1068 1046 1048  1
1069 1046 1049  1
1070 1049 1050  2
1071 1049 1052  1
1072 1050 1051  1
1073 1050 1053  1
1074 1052 1055  ar
1075 1052 1056  ar
1076 1053 1054  1
1077 1053 1055  1
1078 1055 1058  ar
1079 1056 1057  1
1080 1056 1060  ar
1081 1058 1059  1
1082 1058 1062  ar
1083 1060 1061  1
1084 1060 1062  ar
1085 1062 1063  1
1086 1064 1065  1
1087 1064 1066  1   BACKBONE
1088 1066 1067  1
1089 1066 1068  1   BACKBONE
1090 1066 1070  1
1091 1068 1069  2   BACKBONE
1092 1068 1085  am  BACKBONE|INTERRES
1093 1070 1071  1
1094 1070 1072  1
1095 1070 1073  1
1096 1073 1074  ar
1097 1073 1076  ar
1098 1074 1075  1
1099 1074 1078  ar
1100 1076 1077  1
1101 1076 1080  ar
1102 1078 1079  1
1103 1078 1082  ar
1104 1080 1081  1
1105 1080 1082  ar
1106 1082 1083  1
1107 1083 1084  1
1108 1085 1086  1   BACKBONE
1109 1085 1096  1
1110 1086 1087  1
1111 1086 1088  1   BACKBONE
1112 1086 1090  1
1113 1088 1089  2   BACKBONE
1114 1088 1099  am  BACKBONE|INTERRES
1115 1090 1091  1
1116 1090 1092  1
1117 1090 1093  1
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1118 1093 1094  1
1119 1093 1095  1
1120 1093 1096  1
1121 1096 1097  1
1122 1096 1098  1
1123 1099 1100  1
1124 1099 1101  1   BACKBONE
1125 1101 1102  1
1126 1101 1103  1
1127 1101 1104  1   BACKBONE
1128 1104 1105  2   BACKBONE
1129 1104 1106  am  BACKBONE|INTERRES
1130 1106 1107  1
1131 1106 1108  1   BACKBONE
1132 1108 1109  1
1133 1108 1110  1   BACKBONE
1134 1108 1112  1
1135 1110 1111  2   BACKBONE
1136 1110 1116  am  BACKBONE|INTERRES
1137 1112 1113  1
1138 1112 1114  1
1139 1112 1115  1
1140 1116 1117  1
1141 1116 1118  1   BACKBONE
1142 1118 1119  1
1143 1118 1120  1   BACKBONE
1144 1118 1122  1
1145 1120 1121  2   BACKBONE
1146 1120 1138  am  BACKBONE|INTERRES
1147 1122 1123  1
1148 1122 1124  1
1149 1122 1125  1
1150 1125 1126  1
1151 1125 1127  1
1152 1125 1128  1
1153 1128 1129  1
1154 1128 1130  1
1155 1128 1131  1
1156 1131 1132  1
1157 1131 1133  1
1158 1131 1134  1
1159 1134 1135  1
1160 1134 1136  1
1161 1134 1137  1
1162 1138 1139  1
1163 1138 1140  1   BACKBONE
1164 1140 1141  1
1165 1140 1142  1   BACKBONE
1166 1140 1144  1
1167 1142 1143  2   BACKBONE
1168 1142 1159  am  BACKBONE|INTERRES
1169 1144 1145  1
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1170 1144 1146  1
1171 1144 1147  1
1172 1147 1148  ar
1173 1147 1150  ar
1174 1148 1149  1
1175 1148 1152  ar
1176 1150 1151  1
1177 1150 1154  ar
1178 1152 1153  1
1179 1152 1156  ar
1180 1154 1155  1
1181 1154 1156  ar
1182 1156 1157  1
1183 1157 1158  1
1184 1159 1160  1
1185 1159 1161  1   BACKBONE
1186 1161 1162  1
1187 1161 1163  1   BACKBONE
1188 1161 1165  1
1189 1163 1164  2   BACKBONE
1190 1163 1178  am  BACKBONE|INTERRES
1191 1165 1166  1
1192 1165 1167  1
1193 1165 1168  1
1194 1168 1169  1
1195 1168 1170  1
1196 1168 1174  1
1197 1170 1171  1
1198 1170 1172  1
1199 1170 1173  1
1200 1174 1175  1
1201 1174 1176  1
1202 1174 1177  1
1203 1178 1179  1
1204 1178 1180  1   BACKBONE
1205 1180 1181  1
1206 1180 1182  1   BACKBONE
1207 1180 1184  1
1208 1182 1183  2   BACKBONE
1209 1182 1197  am  BACKBONE|INTERRES
1210 1184 1185  1
1211 1184 1186  1
1212 1184 1187  1
1213 1187 1188  1
1214 1187 1189  1
1215 1187 1193  1
1216 1189 1190  1
1217 1189 1191  1
1218 1189 1192  1
1219 1193 1194  1
1220 1193 1195  1
1221 1193 1196  1
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1222 1197 1198  1
1223 1197 1199  1   BACKBONE
1224 1199 1200  1
1225 1199 1201  1   BACKBONE
1226 1199 1203  1
1227 1201 1202  2   BACKBONE
1228 1201 1212  am  BACKBONE|INTERRES
1229 1203 1204  1
1230 1203 1205  1
1231 1203 1206  1
1232 1206 1207  1
1233 1206 1208  1
1234 1206 1209  1
1235 1209 1210  ar
1236 1209 1211  ar
1237 1212 1213  1
1238 1212 1214  1   BACKBONE
1239 1214 1215  1
1240 1214 1216  1   BACKBONE
1241 1214 1218  1
1242 1216 1217  2   BACKBONE
1243 1216 1229  am  BACKBONE|INTERRES
1244 1218 1219  1
1245 1218 1220  1
1246 1218 1221  1
1247 1221 1222  1
1248 1221 1223  1
1249 1221 1224  1
1250 1224 1225  am
1251 1224 1228  2
1252 1225 1226  1
1253 1225 1227  1
1254 1229 1230  1
1255 1229 1231  1   BACKBONE
1256 1231 1232  1
1257 1231 1233  1   BACKBONE
1258 1231 1235  1
1259 1233 1234  2   BACKBONE
1260 1233 1251  am  BACKBONE|INTERRES
1261 1235 1236  1
1262 1235 1237  1
1263 1235 1238  1
1264 1238 1239  1
1265 1238 1240  1
1266 1238 1241  1
1267 1241 1242  1
1268 1241 1243  1
1269 1241 1244  1
1270 1244 1245  1
1271 1244 1246  1
1272 1244 1247  1
1273 1247 1248  1
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1274 1247 1249  1
1275 1247 1250  1
1276 1251 1252  1
1277 1251 1253  1   BACKBONE
1278 1253 1254  1
1279 1253 1255  1
1280 1253 1256  1   BACKBONE
1281 1256 1257  2   BACKBONE
1282 1256 1258  am  BACKBONE|INTERRES
1283 1258 1259  1
1284 1258 1260  1   BACKBONE
1285 1260 1261  1
1286 1260 1262  1   BACKBONE
1287 1260 1264  1
1288 1262 1263  2   BACKBONE
1289 1262 1275  am  BACKBONE|INTERRES
1290 1264 1265  1
1291 1264 1266  1
1292 1264 1267  1
1293 1267 1268  1
1294 1267 1269  1
1295 1267 1270  1
1296 1270 1271  am
1297 1270 1274  2
1298 1271 1272  1
1299 1271 1273  1
1300 1275 1276  1
1301 1275 1277  1   BACKBONE
1302 1277 1278  1
1303 1277 1279  1   BACKBONE
1304 1277 1281  1
1305 1279 1280  2   BACKBONE
1306 1279 1290  am  BACKBONE|INTERRES
1307 1281 1282  1
1308 1281 1283  1
1309 1281 1284  1
1310 1284 1285  1
1311 1284 1286  1
1312 1284 1287  1
1313 1287 1288  ar
1314 1287 1289  ar
1315 1290 1291  1
1316 1290 1292  1   BACKBONE
1317 1292 1293  1
1318 1292 1294  1   BACKBONE
1319 1292 1296  1
1320 1294 1295  2   BACKBONE
1321 1294 1311  am  BACKBONE|INTERRES
1322 1296 1297  1
1323 1296 1298  1
1324 1296 1299  1
1325 1299 1300  ar
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1326 1299 1302  ar
1327 1300 1301  1
1328 1300 1304  ar
1329 1302 1303  1
1330 1302 1306  ar
1331 1304 1305  1
1332 1304 1308  ar
1333 1306 1307  1
1334 1306 1308  ar
1335 1308 1309  1
1336 1309 1310  1
1337 1311 1312  1
1338 1311 1313  1   BACKBONE
1339 1313 1314  1
1340 1313 1315  1   BACKBONE
1341 1313 1317  1
1342 1315 1316  2   BACKBONE
1343 1315 1330  am  BACKBONE|INTERRES
1344 1317 1318  1
1345 1317 1319  1
1346 1317 1322  1
1347 1319 1320  1
1348 1319 1321  1
1349 1319 1326  1
1350 1322 1323  1
1351 1322 1324  1
1352 1322 1325  1
1353 1326 1327  1
1354 1326 1328  1
1355 1326 1329  1
1356 1330 1331  1
1357 1330 1332  1   BACKBONE
1358 1332 1333  1
1359 1332 1334  1   BACKBONE
1360 1332 1336  1
1361 1334 1335  2   BACKBONE
1362 1334 1344  am  BACKBONE|INTERRES
1363 1336 1337  1
1364 1336 1338  1
1365 1336 1339  1
1366 1339 1340  2
1367 1339 1341  am
1368 1341 1342  1
1369 1341 1343  1
1370 1344 1345  1
1371 1344 1346  1   BACKBONE
1372 1346 1347  1
1373 1346 1348  1   BACKBONE
1374 1346 1350  1
1375 1348 1349  2   BACKBONE
1376 1348 1358  am  BACKBONE|INTERRES
1377 1350 1351  1
```

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1378 1350 1352  1
1379 1350 1353  1
1380 1353 1354  am
1381 1353 1357  2
1382 1354 1355  1
1383 1354 1356  1
1384 1358 1359  1
1385 1358 1360  1   BACKBONE
1386 1360 1361  1
1387 1360 1362  1   BACKBONE
1388 1360 1364  1
1389 1362 1363  2   BACKBONE
1390 1362 1377  am  BACKBONE|INTERRES
1391 1364 1365  1
1392 1364 1366  1
1393 1364 1369  1
1394 1366 1367  1
1395 1366 1368  1
1396 1366 1373  1
1397 1369 1370  1
1398 1369 1371  1
1399 1369 1372  1
1400 1373 1374  1
1401 1373 1375  1
1402 1373 1376  1
1403 1377 1378  1
1404 1377 1379  1   BACKBONE
1405 1379 1380  1
1406 1379 1381  1   BACKBONE
1407 1379 1383  1
1408 1381 1382  2   BACKBONE
1409 1381 1394  am  BACKBONE|INTERRES
1410 1383 1384  1
1411 1383 1385  1
1412 1383 1386  1
1413 1386 1387  1
1414 1386 1388  2
1415 1387 1390  2
1416 1388 1389  1
1417 1388 1392  1
1418 1390 1391  1
1419 1390 1392  1
1420 1392 1393  1
1421 1394 1395  1
1422 1394 1396  1   BACKBONE
1423 1396 1397  1
1424 1396 1398  1   BACKBONE
1425 1396 1400  1
1426 1398 1399  2   BACKBONE
1427 1398 1413  am  BACKBONE|INTERRES
1428 1400 1401  1
1429 1400 1402  1
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1430 1400 1403  1
1431 1403 1404  1
1432 1403 1405  1
1433 1403 1409  1
1434 1405 1406  1
1435 1405 1407  1
1436 1405 1408  1
1437 1409 1410  1
1438 1409 1411  1
1439 1409 1412  1
1440 1413 1414  1
1441 1413 1415  1   BACKBONE
1442 1415 1416  1
1443 1415 1417  1   BACKBONE
1444 1415 1420  1
1445 1417 1418  1
1446 1417 1419  2   BACKBONE
1447 1420 1421  1
1448 1420 1422  1
1449 1420 1424  1
1450 1422 1423  1
1451 1424 1425  1
1452 1424 1426  1
1453 1424 1427  1
1454 1428 1432  1
1455 1429 1430  1
1456 1430 1431  1
1457 1430 1432  1
1458 1431 1433  2
1459 1431 1436  am
1460 1434 1435  1
1461 1434 1436  1
1462 1434 1438  1
1463 1435 1437  2
1464 1435 1439  am
1465 1438 1457  1
1466 1439 1440  1
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  1 LEU256    4 RESIDUE 4 B1 LEU  1
  2 PRO257   22 RESIDUE 4 B1 PRO  2
  3 ARG258   37 RESIDUE 4 B1 ARG  2
  4 ASN259   61 RESIDUE 4 B1 ASN  2
  5 PRO260   74 RESIDUE 4 B1 PRO  2
  6 SER261   89 RESIDUE 4 B1 SER  2
  7 MET262  100 RESIDUE 4 B1 MET  2
  8 ALA263  117 RESIDUE 4 B1 ALA  2
  9 ASP264  127 RESIDUE 4 B1 ASP  2
 10 TYR265  139 RESIDUE 4 B1 TYR  2
 11 GLU266  160 RESIDUE 4 B1 GLU  2
 12 ALA267  175 RESIDUE 4 B1 ALA  2
 13 ARG268  185 RESIDUE 4 B1 ARG  2
 14 ILE269  209 RESIDUE 4 B1 ILE  2
 15 PHE270  228 RESIDUE 4 B1 PHE  2
 16 THR271  248 RESIDUE 4 B1 THR  2
 17 PHE272  262 RESIDUE 4 B1 PHE  2
 18 GLY273  282 RESIDUE 4 B1 GLY  2
 19 THR274  289 RESIDUE 4 B1 THR  2
 20 TRP275  303 RESIDUE 4 B1 TRP  2
 21 ILE276  327 RESIDUE 4 B1 ILE  2
 22 TYR277  346 RESIDUE 4 B1 TYR  2
 23 SER278  367 RESIDUE 4 B1 SER  2
 24 VAL279  378 RESIDUE 4 B1 VAL  2
 25 ASN280  394 RESIDUE 4 B1 ASN  2
 26 LYS281  408 RESIDUE 4 B1 LYS  2
 27 GLU282  430 RESIDUE 4 B1 GLU  2
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 29 LEU284  462 RESIDUE 4 B1 LEU  2
 30 ALA285  481 RESIDUE 4 B1 ALA  2
 31 ARG286  491 RESIDUE 4 B1 ARG  2
 32 ALA287  515 RESIDUE 4 B1 ALA  2
 33 GLY288  525 RESIDUE 4 B1 GLY  2
 34 PHE289  532 RESIDUE 4 B1 PHE  2
 35 TYR290  552 RESIDUE 4 B1 TYR  2
 36 ALA291  573 RESIDUE 4 B1 ALA  2
 37 LEU292  583 RESIDUE 4 B1 LEU  2
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38 GLY293  602 RESIDUE 4 B1 GLY  2
39 GLU294  609 RESIDUE 4 B1 GLU  2
40 GLY295  624 RESIDUE 4 B1 GLY  2
41 ASP296  631 RESIDUE 4 B1 ASP  2
42 LYS297  643 RESIDUE 4 B1 LYS  2
43 VAL298  665 RESIDUE 4 B1 VAL  2
44 LYS299  681 RESIDUE 4 B1 LYS  2
45 CYS300  703 RESIDUE 4 B1 CYS  2
46 PHE301  713 RESIDUE 4 B1 PHE  2
47 HIS302  733 RESIDUE 4 B1 HIS  2
48 CYS303  750 RESIDUE 4 B1 CYS  2
49 GLY304  760 RESIDUE 4 B1 GLY  2
50 GLY305  767 RESIDUE 4 B1 GLY  2
51 GLY306  774 RESIDUE 4 B1 GLY  2
52 LEU307  781 RESIDUE 4 B1 LEU  2
53 THR308  800 RESIDUE 4 B1 THR  2
54 ASP309  814 RESIDUE 4 B1 ASP  2
55 TRP310  826 RESIDUE 4 B1 TRP  2
56 LYS311  850 RESIDUE 4 B1 LYS  3
57 PRO312  870 RESIDUE 4 B1 PRO  2
58 SER313  885 RESIDUE 4 B1 SER  2
59 GLU314  896 RESIDUE 4 B1 GLU  2
60 ASP315  911 RESIDUE 4 B1 ASP  2
61 PRO316  922 RESIDUE 4 B1 PRO  2
62 TRP317  937 RESIDUE 4 B1 TRP  2
63 GLU318  961 RESIDUE 4 B1 GLU  2
64 GLN319  976 RESIDUE 4 B1 GLN  2
65 HIS320  993 RESIDUE 4 B1 HIS  2
66 ALA321 1010 RESIDUE 4 B1 ALA  2
67 LYS322 1020 RESIDUE 4 B1 LYS  2
68 TRP323 1042 RESIDUE 4 B1 TRP  2
69 TYR324 1066 RESIDUE 4 B1 TYR  2
70 PRO325 1086 RESIDUE 4 B1 PRO  2
71 GLY326 1101 RESIDUE 4 B1 GLY  2
72 CYS327 1108 RESIDUE 4 B1 CYS  2
73 LYS328 1118 RESIDUE 4 B1 LYS  2
74 TYR329 1140 RESIDUE 4 B1 TYR  2
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76 LEU331 1180 RESIDUE 4 B1 LEU  2
77 GLU332 1199 RESIDUE 4 B1 GLU  2
78 GLN333 1214 RESIDUE 4 B1 GLN  2
79 LYS334 1231 RESIDUE 4 B1 LYS  2
80 GLY335 1253 RESIDUE 4 B1 GLY  2
81 GLN336 1260 RESIDUE 4 B1 GLN  2
82 GLU337 1277 RESIDUE 4 B1 GLU  2
83 TYR338 1292 RESIDUE 4 B1 TYR  2
84 ILE339 1313 RESIDUE 4 B1 ILE  2
85 ASN340 1332 RESIDUE 4 B1 ASN  2
86 ASN341 1346 RESIDUE 4 B1 ASN  2
87 ILE342 1360 RESIDUE 4 B1 ILE  2
88 HIS343 1379 RESIDUE 4 B1 HIS  2
89 LEU344 1396 RESIDUE 4 B1 LEU  2
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 90 THR345 1415 RESIDUE 4 B1 THR  1
 91 ****   1435 GROUP   4 B2 **** 1

# MOE 2019.01 (io_trps.svl 2018.10)
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XIAP-BIR3 + compound 2 .mol2 file

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@<TRIPOS>MOLECULE
COVALENT_142D6_3HL5_XIAP.A
1570 1601 94 0 0
BIOPOLYMER
USER_CHARGES


@<TRIPOS>ATOM
   1 N       -0.8904     2.4146   -11.0087 N.3    1 SER253  -0.3650
BACKBONE
   2 CA      -2.0137     3.1422   -10.4199 C.3    1 SER253   0.1280
BACKBONE
   3 C       -2.4644     2.5385    -9.1021 C.2    1 SER253   0.2007
BACKBONE
   4 O       -3.6299     2.6852    -8.7594 O.2    1 SER253  -0.3948
BACKBONE
   5 CB      -3.1695     3.1056   -11.4592 C.3    1 SER253   0.0792
   6 OG      -3.7021     1.7711   -11.5336 O.3    1 SER253  -0.3908
   7 H       -0.9771     1.4234   -11.1354 H      1 SER253   0.1394
   8 HA      -1.7352     4.1906   -10.2199 H      1 SER253   0.0759
   9 HB3     -2.7838     3.4097   -12.4465 H      1 SER253   0.0601
  10 HB2     -3.9667     3.8080   -11.1755 H      1 SER253   0.0601
  11 HG      -4.4079     1.6673   -12.1677 H      1 SER253   0.2097
  12 NCAP    -0.1014     2.9244   -11.3720 H      1 SER253   0.1394
  13 N       -1.5708     1.8689    -8.3420 N.am   2 HIS254  -0.2622
BACKBONE
  14 CA      -1.9988     1.1380    -7.1402 C.3    2 HIS254   0.1421
BACKBONE
  15 C       -1.9946     2.0367    -5.9113 C.2    2 HIS254   0.2060
BACKBONE
  16 O       -1.4665     3.1334    -5.9896 O.2    2 HIS254  -0.3942
BACKBONE
  17 CB      -1.0458    -0.0753    -6.9298 C.3    2 HIS254   0.0427
  18 CG      -1.6463    -1.2223    -6.1446 C.2    2 HIS254   0.0561
  19 ND1     -2.3456    -2.1918    -6.6858 N.pl3  2 HIS254  -0.2623
  20 CD2     -1.5503    -1.4195    -4.8161 C.2    2 HIS254  -0.0276
  21 CE1     -2.7175    -3.0341    -5.7798 C.2    2 HIS254   0.0875
  22 NE2     -2.2925    -2.6450    -4.6635 N.2    2 HIS254  -0.3437
  23 H       -0.5974     1.8711    -8.5813 H      2 HIS254   0.1885
  24 HA      -3.0160     0.7413    -7.2885 H      2 HIS254   0.0824
  25 HB3     -0.1169     0.2668    -6.4444 H      2 HIS254   0.0491
  26 HB2     -0.7686    -0.4939    -7.9106 H      2 HIS254   0.0491
  27 HD1     -2.5635    -2.2843    -7.6913 H      2 HIS254   0.2386
  28 HD2     -1.0615    -0.8315    -4.0474 H      2 HIS254   0.0324
  29 HE1     -3.3027    -3.9429    -5.9366 H      2 HIS254   0.1149
  30 N       -2.5641     1.5959    -4.7636 N.am   3 MET255  -0.2636
BACKBONE
  31 CA      -2.5157     2.3870    -3.5196 C.3    3 MET255   0.1317
BACKBONE
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  32 C       -1.3160     2.0300    -2.6514 C.2    3 MET255   0.2039
BACKBONE
  33 O       -1.3997     2.2163    -1.4481 O.2    3 MET255  -0.3944
BACKBONE
  34 CB      -3.7939     2.0950    -2.6788 C.3    3 MET255  -0.0034
  35 CG      -5.1082     2.4841    -3.4033 C.3    3 MET255  -0.0024
  36 SD      -5.3884     4.2796    -3.2303 S.o    3 MET255  -0.1639
  37 CE      -7.1425     4.4041    -3.7022 C.3    3 MET255  -0.0181
  38 H       -3.0118     0.7009    -4.7288 H      3 MET255   0.1883
  39 HA      -2.4745     3.4716    -3.7128 H      3 MET255   0.0800
  40 HB3     -3.7744     2.6265    -1.7111 H      3 MET255   0.0320
  41 HB2     -3.8057     1.0121    -2.4649 H      3 MET255   0.0320
  42 HG3     -5.9398     1.9575    -2.9063 H      3 MET255   0.0378
  43 HG2     -5.0963     2.2065    -4.4690 H      3 MET255   0.0378
  44 LPD2    -5.2866     4.4876    -2.5920 LP     3 MET255   0.0000
  45 LPD1    -4.9913     4.6357    -3.6505 LP     3 MET255   0.0000
  46 HE3     -7.2330     4.3531    -4.7955 H      3 MET255   0.0340
  47 HE2     -7.5312     5.3703    -3.3488 H      3 MET255   0.0340
  48 HE1     -7.7360     3.5941    -3.2513 H      3 MET255   0.0340
  49 N       -0.1870     1.5137    -3.1863 N.am   4 LEU256  -0.2637
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  50 CA       0.9549     1.1474    -2.3363 C.3    4 LEU256   0.1314
BACKBONE
  51 C        2.1448     1.8111    -2.9933 C.2    4 LEU256   0.2064
BACKBONE
  52 O        2.3768     1.4677    -4.1428 O.2    4 LEU256  -0.3942
BACKBONE
  53 CB       1.1235    -0.3993    -2.3003 C.3    4 LEU256  -0.0101
  54 CG       2.3165    -0.9258    -1.4406 C.3    4 LEU256  -0.0425
  55 CD1      2.0790    -0.7453     0.0870 C.3    4 LEU256  -0.0625
  56 CD2      2.5430    -2.4397    -1.7274 C.3    4 LEU256  -0.0625
  57 H       -0.0813     1.3861    -4.1723 H      4 LEU256   0.1883
  58 HA       0.8042     1.4932    -1.3070 H      4 LEU256   0.0800
  59 HB3      1.2615    -0.7264    -3.3435 H      4 LEU256   0.0315
  60 HB2      0.1942    -0.8524    -1.9165 H      4 LEU256   0.0315
  61 HG       3.2333    -0.3800    -1.7277 H      4 LEU256   0.0298
  62 HD13     1.9812     0.3094     0.3706 H      4 LEU256   0.0232
  63 HD12     2.9293    -1.1607     0.6507 H      4 LEU256   0.0232
  64 HD11     1.1639    -1.2722     0.4000 H      4 LEU256   0.0232
  65 HD23     1.6475    -3.0225    -1.4582 H      4 LEU256   0.0232
  66 HD22     3.3940    -2.8231    -1.1426 H      4 LEU256   0.0232
  67 HD21     2.7612    -2.6082    -2.7935 H      4 LEU256   0.0232
  68 N        2.9092     2.7659    -2.4125 N.am   5 PRO257  -0.2498
BACKBONE
  69 CA       3.9056     3.4335    -3.2315 C.3    5 PRO257   0.1338
BACKBONE
  70 C        4.9932     2.5128    -3.7345 C.2    5 PRO257   0.2041
BACKBONE
  71 O        5.4021     1.6204    -3.0077 O.2    5 PRO257  -0.3944
BACKBONE
  72 CB       4.4625     4.4725    -2.2324 C.3    5 PRO257  -0.0104
  73 CG       4.0889     3.9172    -0.8387 C.3    5 PRO257  -0.0281
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74	CD	2.7068	3.2605	-1.0551	C.3	5 PRO257	0.0369
75	HA	3.3826	3.9096	-4.0768	H	5 PRO257	0.0802
76	HB3	3.9483	5.4341	-2.3753	H	5 PRO257	0.0313
77	HB2	5.5481	4.6109	-2.3467	H	5 PRO257	0.0313
78	HG2	4.8167	3.1354	-0.5622	H	5 PRO257	0.0287
79	HG3	4.0779	4.6947	-0.0566	H	5 PRO257	0.0287
80	HD2	2.5387	2.5030	-0.2763	H	5 PRO257	0.0524
81	HD3	1.9010	4.0139	-1.0493	H	5 PRO257	0.0524
82	N	5.4895	2.7098	-4.9784	N.am	6 ARG258	-0.2637
BACKBONE							
83	CA	6.5226	1.8023	-5.4676	C.3	6 ARG258	0.1311
BACKBONE							
84	C	7.8520	2.0161	-4.7815	C.2	6 ARG258	0.2040
BACKBONE							
85	O	8.6375	1.0817	-4.8015	O.2	6 ARG258	-0.3944
BACKBONE							
86	CB	6.7368	1.8954	-7.0015	C.3	6 ARG258	-0.0092
87	CG	5.4867	1.4341	-7.7970	C.3	6 ARG258	-0.0156
88	CD	5.7521	1.2952	-9.3195	C.3	6 ARG258	0.0627
89	NE	6.6629	0.1697	-9.6028	N.pl3	6 ARG258	-0.2723
90	CZ	7.9659	0.2594	-9.7853	C.cat	6 ARG258	0.2882
91	NH1	8.6421	1.3797	-9.6783	N.pl3	6 ARG258	-0.2849
92	NH2	8.6303	-0.8339	-10.0849	N.pl3	6 ARG258	-0.2849
93	H	5.1809	3.4683	-5.5674	H	6 ARG258	0.1883
94	HA	6.2223	0.7669	-5.2295	H	6 ARG258	0.0800
95	HB3	7.5760	1.2321	-7.2565	H	6 ARG258	0.0313
96	HB2	7.0047	2.9288	-7.2719	H	6 ARG258	0.0313
97	HG3	4.6702	2.1546	-7.6306	H	6 ARG258	0.0301
98	HG2	5.1538	0.4546	-7.4216	H	6 ARG258	0.0301
99	HD3	6.0144	2.2546	-9.7701	H	6 ARG258	0.0689
100	HD2	4.7777	1.0469	-9.7756	H	6 ARG258	0.0689
101	HE	6.2158	-0.7508	-9.6942	H	6 ARG258	0.2642
102	HH11	8.1874	2.2519	-9.4188	H	6 ARG258	0.2615
103	HH12	9.6590	1.4011	-9.8264	H	6 ARG258	0.2615
104	HH21	8.1606	-1.7418	-10.1774	H	6 ARG258	0.2615
105	HH22	9.6527	-0.8151	-10.2336	H	6 ARG258	0.2615
106	N	8.1574	3.1874	-4.1775	N.am	7 ASN259	-0.2616
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107	CA	9.4359	3.3248	-3.4723	C.3	7 ASN259	0.1478
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108	C	9.2404	3.8978	-2.0833	C.2	7 ASN259	0.2088
BACKBONE							
109	O	9.4655	5.0870	-1.9074	O.2	7 ASN259	-0.3940
BACKBONE							
110	CB	10.3923	4.2039	-4.3135	C.3	7 ASN259	0.0773
111	CG	11.7742	4.2215	-3.7086	C.2	7 ASN259	0.1780
112	OD1	12.0123	3.5220	-2.7360	O.2	7 ASN259	-0.3970
113	ND2	12.7225	4.9971	-4.2608	N.am	7 ASN259	-0.3007
114	H	7.5401	3.9825	-4.2150	H	7 ASN259	0.1885
115	HA	9.9499	2.3586	-3.3502	H	7 ASN259	0.0826
116	HB3	9.9964	5.2267	-4.3832	H	7 ASN259	0.0551
117	HB2	10.4629	3.7848	-5.3293	H	7 ASN259	0.0551

118	HD21	12.5293	5.5590	-5.0632	H	7 ASN259	0.1814
119	HD22	13.6375	4.9950	-3.8571	H	7 ASN259	0.1814
120	N	8.8385	3.1024	-1.0589	N.am	8 PRO260	-0.2497
BACKBONE							
121	CA	8.7091	3.6537	0.2826	C.3	8 PRO260	0.1338
BACKBONE							
122	C	9.8787	4.4987	0.7336	C.2	8 PRO260	0.2042
BACKBONE							
123	O	9.6528	5.4968	1.4008	O.2	8 PRO260	-0.3944
BACKBONE							
124	CB	8.5938	2.3407	1.0956	C.3	8 PRO260	-0.0104
125	CG	7.8599	1.3862	0.1251	C.3	8 PRO260	-0.0281
126	CD	8.5324	1.6874	-1.2358	C.3	8 PRO260	0.0369
127	HA	7.7708	4.2261	0.3379	H	8 PRO260	0.0802
128	HB3	8.0661	2.4764	2.0535	H	8 PRO260	0.0313
129	HB2	9.5983	1.9325	1.2964	H	8 PRO260	0.0313
130	HG2	7.9335	0.3259	0.4171	H	8 PRO260	0.0287
131	HG3	6.7955	1.6691	0.0822	H	8 PRO260	0.0287
132	HD2	9.4600	1.0996	-1.3364	H	8 PRO260	0.0524
133	HD3	7.8503	1.4715	-2.0730	H	8 PRO260	0.0524
134	N	11.1386	4.1531	0.3854	N.am	9 SER261	-0.2616
BACKBONE							
135	CA	12.2572	4.9723	0.8593	C.3	9 SER261	0.1539
BACKBONE							
136	C	12.1485	6.4041	0.3793	C.2	9 SER261	0.2062
BACKBONE							
137	O	12.6959	7.2702	1.0431	O.2	9 SER261	-0.3943
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138	CB	13.6400	4.4030	0.4464	C.3	9 SER261	0.0843
139	OG	13.8056	4.5202	-0.9771	O.3	9 SER261	-0.3903
140	H	11.3228	3.3740	-0.2196	H	9 SER261	0.1884
141	HA	12.2157	4.9915	1.9615	H	9 SER261	0.0823
142	HB3	13.7014	3.3465	0.7612	H	9 SER261	0.0606
143	HB2	14.4398	4.9682	0.9563	H	9 SER261	0.0606
144	HG	14.6209	4.1434	-1.2935	H	9 SER261	0.2097
145	N	11.4484	6.6931	-0.7436	N.am	10 MET262	-0.2636
BACKBONE							
146	CA	11.2444	8.0856	-1.1609	C.3	10 MET262	0.1317
BACKBONE							
147	C	9.8421	8.5718	-0.8331	C.2	10 MET262	0.2039
BACKBONE							
148	O	9.3987	9.5760	-1.3757	O.2	10 MET262	-0.3944
BACKBONE							
149	CB	11.6235	8.2090	-2.6633	C.3	10 MET262	-0.0034
150	CG	13.1467	8.0166	-2.8780	C.3	10 MET262	-0.0024
151	SD	14.0413	9.4723	-2.2409	S.o	10 MET262	-0.1639
152	CE	15.7526	8.9152	-2.5054	C.3	10 MET262	-0.0181
153	H	10.9984	5.9674	-1.2768	H	10 MET262	0.1883
154	HA	11.8859	8.7850	-0.6025	H	10 MET262	0.0800
155	HB3	11.3344	9.1908	-3.0655	H	10 MET262	0.0320
156	HB2	11.0913	7.4342	-3.2350	H	10 MET262	0.0320
157	HG3	13.3747	7.9232	-3.9505	H	10 MET262	0.0378

158	HG2	13.4933	7.1087	-2.3600	H	10 MET262	0.0378
159	LPD2	13.8996	10.0325	-2.5974	LP	10 MET262	0.0000
160	LPD1	13.9098	9.5827	-1.5840	LP	10 MET262	0.0000
161	HE3	15.9144	7.9436	-2.0156	H	10 MET262	0.0340
162	HE2	16.4423	9.6522	-2.0701	H	10 MET262	0.0340
163	HE1	15.9477	8.8204	-3.5841	H	10 MET262	0.0340
164	N	9.1099	7.8976	0.0840	N.am	11 ALA263	-0.2640
BACKBONE							
165	CA	7.8212	8.4360	0.5116	C.3	11 ALA263	0.1282
BACKBONE							
166	C	8.0403	9.6884	1.3229	C.2	11 ALA263	0.2037
BACKBONE							
167	O	7.2912	10.6421	1.1616	O.2	11 ALA263	-0.3944
BACKBONE							
168	CB	7.0064	7.4096	1.3400	C.3	11 ALA263	-0.0244
169	H	9.4487	7.0700	0.5427	H	11 ALA263	0.1883
170	HA	7.2351	8.7343	-0.3652	H	11 ALA263	0.0797
171	HB3	7.5622	7.1204	2.2459	H	11 ALA263	0.0277
172	HB2	6.8161	6.5107	0.7347	H	11 ALA263	0.0277
173	HB1	6.0392	7.8419	1.6420	H	11 ALA263	0.0277
174	N	9.0650	9.7165	2.1984	N.am	12 ASP264	-0.2622
BACKBONE							
175	CA	9.2760	10.9171	2.9985	C.3	12 ASP264	0.1423
BACKBONE							
176	C	9.5822	12.1044	2.0992	C.2	12 ASP264	0.2057
BACKBONE							
177	O	10.4490	12.0250	1.2421	O.2	12 ASP264	-0.3943
BACKBONE							
178	CB	10.3850	10.7184	4.0594	C.3	12 ASP264	0.0406
179	CG	10.5895	11.9545	4.8866	C.2	12 ASP264	0.0393
180	OD1	9.9215	12.9931	4.6222	O.co2	12 ASP264	-0.5688
181	OD2	11.4415	11.8926	5.8062	O.co2	12 ASP264	-0.5688
182	H	9.6885	8.9415	2.3079	H	12 ASP264	0.1884
183	HA	8.3496	11.0892	3.5701	H	12 ASP264	0.0819
184	HB3	11.3328	10.4713	3.5639	H	12 ASP264	0.0478
185	HB2	10.1172	9.8850	4.7284	H	12 ASP264	0.0478
186	N	8.8784	13.2423	2.2849	N.am	13 TYR265	-0.2620
BACKBONE							
187	CA	9.2231	14.4608	1.5527	C.3	13 TYR265	0.1390
BACKBONE							
188	C	10.6561	14.8549	1.8260	C.2	13 TYR265	0.2057
BACKBONE							
189	O	11.3387	15.2861	0.9064	O.2	13 TYR265	-0.3942
BACKBONE							
190	CB	8.2952	15.6175	2.0120	C.3	13 TYR265	0.0163
191	CG	8.7890	16.9907	1.5300	C.ar	13 TYR265	-0.0493
192	CD1	8.5524	17.4153	0.2257	C.ar	13 TYR265	-0.0685
193	CD2	9.4810	17.8367	2.4139	C.ar	13 TYR265	-0.0685
194	CE1	8.8930	18.7254	-0.1524	C.ar	13 TYR265	-0.0398
195	CE2	9.8077	19.1354	2.0428	C.ar	13 TYR265	-0.0398
196	CZ	9.4564	19.6026	0.7633	C.ar	13 TYR265	0.0805
197	OH	9.6605	20.9428	0.4350	O.3	13 TYR265	-0.3376

198	H	8.2129	13.2906	3.0325	H	13 TYR265	0.1885
199	HA	9.1105	14.2981	0.4691	H	13 TYR265	0.0821
200	HB2	8.2513	15.6348	3.1133	H	13 TYR265	0.0453
201	HB3	7.2728	15.4422	1.6405	H	13 TYR265	0.0453
202	HD1	8.1036	16.7459	-0.5005	H	13 TYR265	0.0530
203	HD2	9.7637	17.4765	3.3993	H	13 TYR265	0.0530
204	HE1	8.7053	19.0517	-1.1675	H	13 TYR265	0.0525
205	HE2	10.3323	19.7894	2.7334	H	13 TYR265	0.0525
206	HH	10.2159	20.9975	-0.3407	H	13 TYR265	0.2458
207	N	11.1303	14.7152	3.0828	N.am	14 GLU266	-0.2635
BACKBONE							
208	CA	12.4999	15.1308	3.3760	C.3	14 GLU266	0.1325
BACKBONE							
209	C	13.4703	14.2873	2.5654	C.2	14 GLU266	0.2040
BACKBONE							
210	O	14.4198	14.7943	1.9831	O.2	14 GLU266	-0.3944
BACKBONE							
211	CB	12.8301	15.0740	4.8913	C.3	14 GLU266	-0.0008
212	CG	11.9924	16.1009	5.7065	C.3	14 GLU266	0.0044
213	CD	12.2181	17.5195	5.2452	C.2	14 GLU266	0.0350
214	OE1	13.3790	17.8526	4.8869	O.co2	14 GLU266	-0.5690
215	OE2	11.2392	18.3142	5.2272	O.co2	14 GLU266	-0.5690
216	H	10.5757	14.2927	3.8149	H	14 GLU266	0.1883
217	HA	12.5926	16.1785	3.0705	H	14 GLU266	0.0801
218	HB3	13.8998	15.3016	5.0321	H	14 GLU266	0.0330
219	HB2	12.6468	14.0539	5.2623	H	14 GLU266	0.0330
220	HG3	12.2748	16.0461	6.7692	H	14 GLU266	0.0433
221	HG2	10.9210	15.8611	5.6295	H	14 GLU266	0.0433
222	N	13.2416	12.9584	2.4899	N.am	15 ALA267	-0.2640
BACKBONE							
223	CA	14.0943	12.1303	1.6363	C.3	15 ALA267	0.1282
BACKBONE							
224	C	14.0560	12.6401	0.2120	C.2	15 ALA267	0.2036
BACKBONE							
225	O	15.0730	12.6018	-0.4637	O.2	15 ALA267	-0.3944
BACKBONE							
226	CB	13.6530	10.6424	1.6231	C.3	15 ALA267	-0.0244
227	H	12.4689	12.5462	2.9768	H	15 ALA267	0.1883
228	HA	15.1327	12.1959	2.0023	H	15 ALA267	0.0797
229	HB3	12.6216	10.5530	1.2492	H	15 ALA267	0.0277
230	HB2	13.7034	10.2252	2.6406	H	15 ALA267	0.0277
231	HB1	14.3148	10.0517	0.9687	H	15 ALA267	0.0277
232	N	12.8933	13.1209	-0.2808	N.am	16 ARG268	-0.2637
BACKBONE							
233	CA	12.8609	13.6281	-1.6490	C.3	16 ARG268	0.1311
BACKBONE							
234	C	13.5304	14.9789	-1.7553	C.2	16 ARG268	0.2039
BACKBONE							
235	O	14.2828	15.1605	-2.6968	O.2	16 ARG268	-0.3944
BACKBONE							
236	CB	11.4302	13.7345	-2.2393	C.3	16 ARG268	-0.0092
237	CG	10.7238	12.3523	-2.2429	C.3	16 ARG268	-0.0156

238 CD	9.4531	12.3627	-3.1347	C.3	16	ARG268	0.0627
239 NE	8.4568	13.3025	-2.6168	N.pl3	16	ARG268	-0.2723
240 CZ	7.6686	13.0364	-1.6005	C.cat	16	ARG268	0.2882
241 NH1	7.7188	11.9143	-0.9224	N.pl3	16	ARG268	-0.2849
242 NH2	6.7924	13.9477	-1.2555	N.pl3	16	ARG268	-0.2849
243 H	12.0651	13.1688	0.2854	H	16	ARG268	0.1883
244 HA	13.4245	12.9301	-2.2937	H	16	ARG268	0.0800
245 HB3	11.5237	14.1138	-3.2700	H	16	ARG268	0.0313
246 HB2	10.8323	14.4560	-1.6606	H	16	ARG268	0.0313
247 HG3	10.4725	12.0886	-1.2097	H	16	ARG268	0.0301
248 HG2	11.4081	11.5752	-2.6069	H	16	ARG268	0.0301
249 HD3	9.0410	11.3525	-3.2602	H	16	ARG268	0.0689
250 HD2	9.7492	12.6599	-4.1500	H	16	ARG268	0.0689
251 HE	8.3745	14.2210	-3.1012	H	16	ARG268	0.2642
252 HH11	8.3801	11.1515	-1.1439	H	16	ARG268	0.2615
253 HH12	7.1071	11.7498	-0.1039	H	16	ARG268	0.2615
254 HH21	6.7160	14.8446	-1.7698	H	16	ARG268	0.2615
255 HH22	6.1403	13.7915	-0.4753	H	16	ARG268	0.2615
256 N	13.3040	15.9662	-0.8598	N.am	17	ILE269	-0.2635
BACKBONE							
257 CA	14.0059	17.2431	-1.0505	C.3	17	ILE269	0.1335
BACKBONE							
258 C	15.5052	17.0115	-1.0358	C.2	17	ILE269	0.2043
BACKBONE							
259 O	16.2191	17.6115	-1.8265	O.2	17	ILE269	-0.3944
BACKBONE							
260 CB	13.5812	18.3825	-0.0751	C.3	17	ILE269	-0.0037
261 CG1	14.0116	19.8014	-0.5612	C.3	17	ILE269	-0.0491
262 CG2	14.1742	18.1750	1.3424	C.3	17	ILE269	-0.0582
263 CD1	13.3211	20.2590	-1.8714	C.3	17	ILE269	-0.0648
264 H	12.6843	15.8285	-0.0766	H	17	ILE269	0.1883
265 HA	13.7333	17.5854	-2.0536	H	17	ILE269	0.0803
266 HB	12.4789	18.3560	0.0014	H	17	ILE269	0.0345
267 HG13	15.1053	19.8531	-0.6919	H	17	ILE269	0.0267
268 HG12	13.7284	20.5229	0.2250	H	17	ILE269	0.0267
269 HG23	13.9982	17.1509	1.6640	H	17	ILE269	0.0235
270 HG22	13.6936	18.8485	2.0702	H	17	ILE269	0.0235
271 HG21	15.2603	18.3528	1.3563	H	17	ILE269	0.0235
272 HD13	13.7427	19.7793	-2.7677	H	17	ILE269	0.0230
273 HD12	13.4402	21.3467	-1.9848	H	17	ILE269	0.0230
274 HD11	12.2506	20.0275	-1.8076	H	17	ILE269	0.0230
275 N	16.0023	16.1238	-0.1444	N.am	18	PHE270	-0.2619
BACKBONE							
276 CA	17.4476	15.8886	-0.0527	C.3	18	PHE270	0.1404
BACKBONE							
277 C	18.1023	15.6163	-1.3929	C.2	18	PHE270	0.2060
BACKBONE							
278 O	19.1760	16.1297	-1.6731	O.2	18	PHE270	-0.3942
BACKBONE							
279 CB	17.6894	14.6597	0.8643	C.3	18	PHE270	0.0214
280 CG	19.1773	14.3038	0.9605	C.ar	18	PHE270	-0.0386
281 CD1	20.0030	14.9815	1.8621	C.ar	18	PHE270	-0.0601

282	CD2	19.7171	13.2925	0.1561	C.ar	18 PHE270	-0.0601
283	CE1	21.3420	14.6094	2.0082	C.ar	18 PHE270	-0.0686
284	CE2	21.0537	12.9156	0.3050	C.ar	18 PHE270	-0.0686
285	CZ	21.8651	13.5659	1.2382	C.ar	18 PHE270	-0.0687
286	H	15.3862	15.6258	0.4807	H	18 PHE270	0.1885
287	HA	17.9265	16.7776	0.3883	H	18 PHE270	0.0823
288	HB3	17.1294	13.7969	0.4727	H	18 PHE270	0.0474
289	HB2	17.3037	14.8697	1.8746	H	18 PHE270	0.0474
290	HD1	19.6064	15.7990	2.4561	H	18 PHE270	0.0557
291	HD2	19.0999	12.7946	-0.5849	H	18 PHE270	0.0557
292	HE1	21.9756	15.1283	2.7202	H	18 PHE270	0.0599
293	HE2	21.4625	12.1149	-0.3039	H	18 PHE270	0.0599
294	HZ	22.8990	13.2626	1.3657	H	18 PHE270	0.0559
295	N	17.4679	14.7965	-2.2539	N.am	19 THR271	-0.2612
BACKBONE							
296	CA	18.0971	14.4387	-3.5296	C.3	19 THR271	0.1565
BACKBONE							
297	C	18.2754	15.6599	-4.4022	C.2	19 THR271	0.2066
BACKBONE							
298	O	19.1526	15.6542	-5.2520	O.2	19 THR271	-0.3943
BACKBONE							
299	CB	17.1742	13.4593	-4.2952	C.3	19 THR271	0.0924
300	OG1	15.9256	14.1724	-4.3312	O.3	19 THR271	-0.3874
301	CG2	17.0797	12.0933	-3.5621	C.3	19 THR271	-0.0346
302	H	16.5324	14.4840	-2.0602	H	19 THR271	0.1884
303	HA	19.0868	13.9883	-3.3516	H	19 THR271	0.0826
304	HB	17.5435	13.2740	-5.3184	H	19 THR271	0.0639
305	HG1	15.1510	13.6618	-4.5038	H	19 THR271	0.2101
306	HG22	16.3542	11.4475	-4.0773	H	19 THR271	0.0257
307	HG21	16.7598	12.2112	-2.5166	H	19 THR271	0.0257
308	HG23	18.0584	11.5865	-3.5717	H	19 THR271	0.0257
309	N	17.4698	16.7290	-4.2137	N.am	20 PHE272	-0.2619
BACKBONE							
310	CA	17.6758	17.9429	-4.9984	C.3	20 PHE272	0.1404
BACKBONE							
311	C	18.6770	18.8858	-4.3515	C.2	20 PHE272	0.2058
BACKBONE							
312	O	18.7003	20.0518	-4.7226	O.2	20 PHE272	-0.3942
BACKBONE							
313	CB	16.3174	18.6647	-5.1744	C.3	20 PHE272	0.0214
314	CG	15.3050	17.8452	-5.9867	C.ar	20 PHE272	-0.0386
315	CD1	14.2616	17.1596	-5.3637	C.ar	20 PHE272	-0.0601
316	CD2	15.4029	17.7897	-7.3817	C.ar	20 PHE272	-0.0601
317	CE1	13.2883	16.5029	-6.1183	C.ar	20 PHE272	-0.0686
318	CE2	14.4692	17.0817	-8.1404	C.ar	20 PHE272	-0.0686
319	CZ	13.4130	16.4222	-7.5108	C.ar	20 PHE272	-0.0687
320	H	16.7634	16.7355	-3.4982	H	20 PHE272	0.1885
321	HA	18.0629	17.7053	-6.0035	H	20 PHE272	0.0823
322	HB3	16.4837	19.6033	-5.7136	H	20 PHE272	0.0474
323	HB2	15.9093	18.9153	-4.1827	H	20 PHE272	0.0474
324	HD1	14.2016	17.1382	-4.2850	H	20 PHE272	0.0557
325	HD2	16.2135	18.3016	-7.8739	H	20 PHE272	0.0557

326	HE1	12.4354	16.0590	-5.6208	H	20 PHE272	0.0599
327	HE2	14.5707	17.0438	-9.2212	H	20 PHE272	0.0599
328	HZ	12.6969	15.8513	-8.0924	H	20 PHE272	0.0559
329	N	19.5189	18.4404	-3.3881	N.am	21 GLY273	-0.2663
BACKBONE							
330	CA	20.4671	19.3644	-2.7657	C.3	21 GLY273	0.1201
BACKBONE							
331	C	21.1563	20.2687	-3.7652	C.2	21 GLY273	0.2008
BACKBONE							
332	O	21.1514	21.4763	-3.5758	O.2	21 GLY273	-0.3947
BACKBONE							
333	H	19.4817	17.4989	-3.0318	H	21 GLY273	0.1881
334	HA2	21.2605	18.8120	-2.2354	H	21 GLY273	0.0763
335	HA3	19.9267	19.9763	-2.0275	H	21 GLY273	0.0763
336	N	21.7523	19.6873	-4.8316	N.am	22 THR274	-0.2616
BACKBONE							
337	CA	22.5054	20.4725	-5.8146	C.3	22 THR274	0.1565
BACKBONE							
338	C	21.7329	20.5886	-7.1148	C.2	22 THR274	0.2066
BACKBONE							
339	O	22.3167	20.5002	-8.1827	O.2	22 THR274	-0.3943
BACKBONE							
340	CB	23.8594	19.7408	-6.0368	C.3	22 THR274	0.0924
341	OG1	23.5422	18.3789	-6.3862	O.3	22 THR274	-0.3874
342	CG2	24.7166	19.7537	-4.7432	C.3	22 THR274	-0.0346
343	H	21.6980	18.6953	-4.9833	H	22 THR274	0.1884
344	HA	22.7085	21.5001	-5.4734	H	22 THR274	0.0826
345	HB	24.4283	20.2353	-6.8463	H	22 THR274	0.0639
346	HG1	24.3130	17.8595	-6.5929	H	22 THR274	0.2101
347	HG22	25.6584	19.2070	-4.9113	H	22 THR274	0.0257
348	HG21	24.1725	19.2664	-3.9184	H	22 THR274	0.0257
349	HG23	24.9586	20.7878	-4.4503	H	22 THR274	0.0257
350	N	20.3998	20.7916	-7.0736	N.am	23 TRP275	-0.2626
BACKBONE							
351	CA	19.6464	20.8773	-8.3319	C.3	23 TRP275	0.1352
BACKBONE							
352	C	19.9850	22.1435	-9.0932	C.2	23 TRP275	0.2052
BACKBONE							
353	O	19.8958	23.2043	-8.4958	O.2	23 TRP275	-0.3942
BACKBONE							
354	CB	18.1353	20.8626	-8.0039	C.3	23 TRP275	0.0042
355	CG	17.1565	20.7877	-9.1462	C.2	23 TRP275	-0.0418
356	CD1	16.2953	21.7447	-9.5433	C.2	23 TRP275	0.0167
357	CD2	16.9154	19.5955	-10.0276	C.ar	23 TRP275	-0.0214
358	NE1	15.5470	21.2869	-10.5045	N.pl3	23 TRP275	-0.2890
359	CE2	15.8575	20.0078	-10.8145	C.ar	23 TRP275	0.0603
360	CE3	17.4877	18.3222	-10.1552	C.ar	23 TRP275	-0.0747
361	CZ2	15.2704	19.1573	-11.7490	C.ar	23 TRP275	-0.0443
362	CZ3	16.9001	17.4598	-11.0866	C.ar	23 TRP275	-0.0792
363	CH2	15.7998	17.8644	-11.8563	C.ar	23 TRP275	-0.0768
364	H	19.9260	20.8794	-6.1905	H	23 TRP275	0.1884
365	HA	19.8776	19.9868	-8.9397	H	23 TRP275	0.0815

366	HB3	17.9013	21.7430	-7.3872	H	23 TRP275	0.0397
367	HB2	17.9693	19.9619	-7.4025	H	23 TRP275	0.0397
368	HD1	16.2218	22.7465	-9.1137	H	23 TRP275	0.0795
369	HE1	14.7860	21.8344	-10.9557	H	23 TRP275	0.2216
370	HE3	18.3389	18.0236	-9.5557	H	23 TRP275	0.0540
371	HZ2	14.4411	19.4839	-12.3670	H	23 TRP275	0.0541
372	HZ3	17.3048	16.4592	-11.2163	H	23 TRP275	0.0510
373	HH2	15.3485	17.1639	-12.5516	H	23 TRP275	0.0530
374	N	20.3615	22.0642	-10.3940	N.am	24 ILE276	-0.2634
BACKBONE							
375	CA	20.6856	23.2697	-11.1688	C.3	24 ILE276	0.1335
BACKBONE							
376	C	19.6765	23.5474	-12.2640	C.2	24 ILE276	0.2043
BACKBONE							
377	O	19.9371	24.4323	-13.0636	O.2	24 ILE276	-0.3944
BACKBONE							
378	CB	22.1139	23.1698	-11.7999	C.3	24 ILE276	-0.0037
379	CG1	22.2014	22.0627	-12.9010	C.3	24 ILE276	-0.0491
380	CG2	23.1732	22.9673	-10.6817	C.3	24 ILE276	-0.0582
381	CD1	23.5350	22.0764	-13.6955	C.3	24 ILE276	-0.0648
382	H	20.4160	21.1810	-10.8590	H	24 ILE276	0.1883
383	HA	20.6619	24.1731	-10.5366	H	24 ILE276	0.0803
384	HB	22.3385	24.1359	-12.2877	H	24 ILE276	0.0345
385	HG13	21.3912	22.2080	-13.6343	H	24 ILE276	0.0267
386	HG12	22.0849	21.0599	-12.4622	H	24 ILE276	0.0267
387	HG23	23.0402	23.7145	-9.8834	H	24 ILE276	0.0235
388	HG22	24.1923	23.0838	-11.0792	H	24 ILE276	0.0235
389	HG21	23.0779	21.9643	-10.2408	H	24 ILE276	0.0235
390	HD13	23.7306	23.0775	-14.1108	H	24 ILE276	0.0230
391	HD12	23.4803	21.3596	-14.5315	H	24 ILE276	0.0230
392	HD11	24.3797	21.7820	-13.0555	H	24 ILE276	0.0230
393	N	18.5371	22.8272	-12.3682	N.am	25 TYR277	-0.2621
BACKBONE							
394	CA	17.6574	23.0260	-13.5225	C.3	25 TYR277	0.1390
BACKBONE							
395	C	16.5817	24.0451	-13.2224	C.2	25 TYR277	0.2058
BACKBONE							
396	O	16.3385	24.3486	-12.0668	O.2	25 TYR277	-0.3942
BACKBONE							
397	CB	17.0631	21.6750	-13.9934	C.3	25 TYR277	0.0163
398	CG	18.2297	20.7301	-14.3155	C.ar	25 TYR277	-0.0493
399	CD1	18.6254	19.7487	-13.4056	C.ar	25 TYR277	-0.0685
400	CD2	18.9206	20.8529	-15.5278	C.ar	25 TYR277	-0.0685
401	CE1	19.7179	18.9180	-13.6806	C.ar	25 TYR277	-0.0398
402	CE2	20.0114	20.0275	-15.8033	C.ar	25 TYR277	-0.0398
403	CZ	20.4198	19.0562	-14.8798	C.ar	25 TYR277	0.0805
404	OH	21.5218	18.2495	-15.1778	O.3	25 TYR277	-0.3376
405	H	18.2559	22.1736	-11.6658	H	25 TYR277	0.1885
406	HA	18.2363	23.4147	-14.3767	H	25 TYR277	0.0821
407	HB2	16.4380	21.8007	-14.8914	H	25 TYR277	0.0453
408	HB3	16.4234	21.2650	-13.1998	H	25 TYR277	0.0453
409	HD1	18.0917	19.6241	-12.4750	H	25 TYR277	0.0530

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 410 HD2     18.6117    21.5938   -16.2589 H     25 TYR277   0.0530
 411 HE1     20.0092    18.1705   -12.9494 H     25 TYR277   0.0525
 412 HE2     20.5518    20.1328   -16.7376 H     25 TYR277   0.0525
 413 HH      21.6300    17.5240   -14.5707 H     25 TYR277   0.2458
 414 N       15.9245    24.6039   -14.2621 N.am  26 SER278  -0.2614
BACKBONE
 415 CA      14.9744    25.6944   -14.0252 C.3   26 SER278   0.1539
BACKBONE
 416 C       13.7945    25.2901   -13.1706 C.2   26 SER278   0.2062
BACKBONE
 417 O       13.2854    26.1230   -12.4371 O.2   26 SER278  -0.3943
BACKBONE
 418 CB      14.4171    26.2283   -15.3722 C.3   26 SER278   0.0843
 419 OG      13.5799    27.3773   -15.1476 O.3   26 SER278  -0.3903
 420 H       16.1149    24.3161   -15.2025 H     26 SER278   0.1884
 421 HA      15.4938    26.5258   -13.5195 H     26 SER278   0.0823
 422 HB3     13.8431    25.4262   -15.8684 H     26 SER278   0.0606
 423 HB2     15.2630    26.5169   -16.0201 H     26 SER278   0.0606
 424 HG      13.2271    27.7480   -15.9506 H     26 SER278   0.2097
 425 N       13.3013    24.0348   -13.2424 N.am  27 VAL279  -0.2634
BACKBONE
 426 CA      12.0721    23.7245   -12.5132 C.3   27 VAL279   0.1333
BACKBONE
 427 C       12.3108    23.7198   -11.0157 C.2   27 VAL279   0.2043
BACKBONE
 428 O       13.3414    23.2403   -10.5653 O.2   27 VAL279  -0.3944
BACKBONE
 429 CB      11.3981    22.4101   -12.9924 C.3   27 VAL279  -0.0063
 430 CG1     10.1554    22.0544   -12.1375 C.3   27 VAL279  -0.0584
 431 CG2     10.9446    22.5462   -14.4699 C.3   27 VAL279  -0.0584
 432 H       13.7539    23.3227   -13.7787 H     27 VAL279   0.1883
 433 HA      11.3605    24.5364   -12.7379 H     27 VAL279   0.0802
 434 HB      12.1290    21.5868   -12.9049 H     27 VAL279   0.0343
 435 HG13    10.4094    21.9668   -11.0730 H     27 VAL279   0.0234
 436 HG12     9.7543    21.0892   -12.4807 H     27 VAL279   0.0234
 437 HG11     9.3806    22.8267   -12.2550 H     27 VAL279   0.0234
 438 HG23    10.2877    23.4171   -14.6179 H     27 VAL279   0.0234
 439 HG22    10.3729    21.6528   -14.7516 H     27 VAL279   0.0234
 440 HG21    11.8195    22.6473   -15.1282 H     27 VAL279   0.0234
 441 N       11.3537    24.2647   -10.2252 N.am  28 ASN280  -0.2616
BACKBONE
 442 CA      11.5991    24.4481    -8.7974 C.3   28 ASN280   0.1476
BACKBONE
 443 C       11.7031    23.1301    -8.0459 C.2   28 ASN280   0.2063
BACKBONE
 444 O       10.8028    22.3060    -8.1214 O.2   28 ASN280  -0.3942
BACKBONE
 445 CB      10.5015    25.3250    -8.1413 C.3   28 ASN280   0.0773
 446 CG      10.7432    25.3936    -6.6561 C.2   28 ASN280   0.1780
 447 OD1     10.0720    24.6709    -5.9398 O.2   28 ASN280  -0.3970
 448 ND2     11.6872    26.2034    -6.1410 N.am  28 ASN280  -0.3007
 449 H       10.4807    24.5839   -10.5992 H     28 ASN280   0.1885
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 450 HA      12.5415    25.0136    -8.7116 H     28 ASN280   0.0826
 451 HB3      9.5223    24.8631    -8.3259 H     28 ASN280   0.0551
 452 HB2     10.4861    26.3341    -8.5810 H     28 ASN280   0.0551
 453 HD21    12.2176    26.8316    -6.7088 H     28 ASN280   0.1814
 454 HD22    11.8741    26.1392    -5.1519 H     28 ASN280   0.1814
 455 N       12.8060    22.9153    -7.2919 N.am  29 LYS281  -0.2636
BACKBONE
 456 CA      12.9620    21.6640    -6.5536 C.3   29 LYS281   0.1310
BACKBONE
 457 C       11.9156    21.4486    -5.4837 C.2   29 LYS281   0.2039
BACKBONE
 458 O       11.4484    20.3289    -5.3220 O.2   29 LYS281  -0.3944
BACKBONE
 459 CB      14.3793    21.5096    -5.9399 C.3   29 LYS281  -0.0122
 460 CG      14.7660    22.5552    -4.8557 C.3   29 LYS281  -0.0440
 461 CD      16.2420    22.3739    -4.4070 C.3   29 LYS281  -0.0124
 462 CE      16.6543    23.3560    -3.2783 C.3   29 LYS281  -0.0354
 463 NZ      18.0989    23.2088    -2.9670 N.4   29 LYS281   0.2185
 464 H       13.5392    23.5917    -7.2422 H     29 LYS281   0.1883
 465 HA      12.8458    20.8447    -7.2751 H     29 LYS281   0.0800
 466 HB3     15.1171    21.5319    -6.7590 H     29 LYS281   0.0312
 467 HB2     14.3908    20.5173    -5.4673 H     29 LYS281   0.0312
 468 HG3     14.1098    22.4181    -3.9877 H     29 LYS281   0.0269
 469 HG2     14.6377    23.5843    -5.2218 H     29 LYS281   0.0269
 470 HD3     16.9008    22.5319    -5.2747 H     29 LYS281   0.0317
 471 HD2     16.3906    21.3507    -4.0328 H     29 LYS281   0.0317
 472 HE3     16.0448    23.1408    -2.3823 H     29 LYS281   0.0813
 473 HE2     16.4277    24.3910    -3.5914 H     29 LYS281   0.0813
 474 HZ3     18.3626    22.1988    -2.6802 H     29 LYS281   0.1994
 475 HZ2     18.4015    23.8597    -2.1567 H     29 LYS281   0.1994
 476 HZ1     18.7405    23.4427    -3.8071 H     29 LYS281   0.1994
 477 N       11.5307    22.4938    -4.7242 N.am  30 GLU282  -0.2636
BACKBONE
 478 CA      10.5355    22.2805    -3.6789 C.3   30 GLU282   0.1325
BACKBONE
 479 C        9.2690    21.7723    -4.3362 C.2   30 GLU282   0.2040
BACKBONE
 480 O        8.6985    20.7873    -3.8922 O.2   30 GLU282  -0.3944
BACKBONE
 481 CB      10.2633    23.5437    -2.8118 C.3   30 GLU282  -0.0008
 482 CG      11.4837    23.9573    -1.9386 C.3   30 GLU282   0.0044
 483 CD      12.7089    24.3345    -2.7305 C.2   30 GLU282   0.0350
 484 OE1     12.5604    24.7171    -3.9279 O.co2 30 GLU282  -0.5690
 485 OE2     13.8330    24.2362    -2.1691 O.co2 30 GLU282  -0.5690
 486 H       11.8976    23.4237    -4.8628 H     30 GLU282   0.1883
 487 HA      10.8895    21.4861    -3.0105 H     30 GLU282   0.0801
 488 HB3      9.4160    23.3260    -2.1393 H     30 GLU282   0.0330
 489 HB2      9.9744    24.3887    -3.4555 H     30 GLU282   0.0330
 490 HG3     11.7380    23.1342    -1.2524 H     30 GLU282   0.0433
 491 HG2     11.2162    24.8344    -1.3288 H     30 GLU282   0.0433
 492 N        8.8162    22.4246    -5.4252 N.am  31 GLN283  -0.2636
BACKBONE
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493	CA	7.6143	21.9586	-6.1114	C.3	31 GLN283	0.1330
BACKBONE							
494	C	7.8146	20.5252	-6.5686	C.2	31 GLN283	0.2040
BACKBONE							
495	O	6.9251	19.7098	-6.3735	O.2	31 GLN283	-0.3944
BACKBONE							
496	CB	7.2579	22.8636	-7.3233	C.3	31 GLN283	0.0045
497	CG	6.8444	24.3070	-6.9124	C.3	31 GLN283	0.0412
498	CD	6.6840	25.2147	-8.1087	C.2	31 GLN283	0.1737
499	OE1	7.0652	24.8420	-9.2076	O.2	31 GLN283	-0.3973
500	NE2	6.1331	26.4315	-7.9423	N.am	31 GLN283	-0.3009
501	H	9.3327	23.2031	-5.7902	H	31 GLN283	0.1883
502	HA	6.7717	21.9833	-5.4028	H	31 GLN283	0.0801
503	HB3	6.4137	22.4124	-7.8703	H	31 GLN283	0.0337
504	HB2	8.1299	22.8971	-7.9944	H	31 GLN283	0.0337
505	HG3	7.5986	24.7703	-6.2619	H	31 GLN283	0.0504
506	HG2	5.8933	24.2740	-6.3588	H	31 GLN283	0.0504
507	HE21	5.8268	26.7549	-7.0476	H	31 GLN283	0.1814
508	HE22	6.0248	27.0195	-8.7446	H	31 GLN283	0.1814
509	N	8.9726	20.1772	-7.1752	N.am	32 LEU284	-0.2637
BACKBONE							
510	CA	9.1799	18.7837	-7.5865	C.3	32 LEU284	0.1312
BACKBONE							
511	C	9.0355	17.8388	-6.4067	C.2	32 LEU284	0.2039
BACKBONE							
512	O	8.3153	16.8531	-6.4970	O.2	32 LEU284	-0.3944
BACKBONE							
513	CB	10.5730	18.5642	-8.2497	C.3	32 LEU284	-0.0101
514	CG	10.6694	19.1362	-9.6958	C.3	32 LEU284	-0.0425
515	CD1	12.1473	19.3656	-10.1189	C.3	32 LEU284	-0.0625
516	CD2	10.0051	18.1939	-10.7387	C.3	32 LEU284	-0.0625
517	H	9.6962	20.8607	-7.3345	H	32 LEU284	0.1883
518	HA	8.3899	18.5196	-8.3007	H	32 LEU284	0.0800
519	HB3	10.8095	17.4931	-8.2906	H	32 LEU284	0.0315
520	HB2	11.3294	19.0294	-7.6043	H	32 LEU284	0.0315
521	HG	10.1520	20.1060	-9.7105	H	32 LEU284	0.0298
522	HD13	12.6392	20.1142	-9.4845	H	32 LEU284	0.0232
523	HD12	12.1872	19.7325	-11.1541	H	32 LEU284	0.0232
524	HD11	12.7169	18.4284	-10.0595	H	32 LEU284	0.0232
525	HD23	10.5142	17.2219	-10.7279	H	32 LEU284	0.0232
526	HD22	10.0857	18.6164	-11.7521	H	32 LEU284	0.0232
527	HD21	8.9436	18.0240	-10.5320	H	32 LEU284	0.0232
528	N	9.7184	18.1106	-5.2748	N.am	33 ALA285	-0.2640
BACKBONE							
529	CA	9.5975	17.2027	-4.1296	C.3	33 ALA285	0.1282
BACKBONE							
530	C	8.1826	17.1816	-3.5766	C.2	33 ALA285	0.2036
BACKBONE							
531	O	7.6936	16.1181	-3.2061	O.2	33 ALA285	-0.3944
BACKBONE							
532	CB	10.6135	17.5983	-3.0292	C.3	33 ALA285	-0.0244
533	H	10.2949	18.9375	-5.2087	H	33 ALA285	0.1883

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 534 HA       9.8390    16.1807    -4.4581 H     33 ALA285   0.0797
 535 HB3     10.4492    18.6441    -2.7376 H     33 ALA285   0.0277
 536 HB2     11.6375    17.5027    -3.4203 H     33 ALA285   0.0277
 537 HB1     10.5097    16.9552    -2.1417 H     33 ALA285   0.0277
 538 N        7.5084    18.3567    -3.5216 N.am  34 ARG286  -0.2637
BACKBONE
 539 CA       6.1101    18.3799    -3.0854 C.3   34 ARG286   0.1311
BACKBONE
 540 C        5.2550    17.6224    -4.0781 C.2   34 ARG286   0.2039
BACKBONE
 541 O        4.3194    16.9656    -3.6506 O.2   34 ARG286  -0.3944
BACKBONE
 542 CB       5.5090    19.8084    -2.9241 C.3   34 ARG286  -0.0092
 543 CG       6.1830    20.7046    -1.8420 C.3   34 ARG286  -0.0156
 544 CD       5.9456    20.2615    -0.3678 C.3   34 ARG286   0.0627
 545 NE       6.8132    21.0025     0.5602 N.pl3 34 ARG286  -0.2723
 546 CZ       6.8964    20.7592     1.8497 C.cat 34 ARG286   0.2882
 547 NH1      6.1623    19.8552     2.4469 N.pl3 34 ARG286  -0.2849
 548 NH2      7.7523    21.4429     2.5687 N.pl3 34 ARG286  -0.2849
 549 H        7.9348    19.2132    -3.8402 H     34 ARG286   0.1883
 550 HA       6.0282    17.8332    -2.1344 H     34 ARG286   0.0800
 551 HB3      4.4362    19.7309    -2.6821 H     34 ARG286   0.0313
 552 HB2      5.5976    20.3082    -3.9026 H     34 ARG286   0.0313
 553 HG3      5.8036    21.7353    -1.9515 H     34 ARG286   0.0301
 554 HG2      7.2616    20.7371    -2.0263 H     34 ARG286   0.0301
 555 HD3      6.1845    19.1923    -0.2818 H     34 ARG286   0.0689
 556 HD2      4.8796    20.4146    -0.1256 H     34 ARG286   0.0689
 557 HE       7.4233    21.7326     0.1558 H     34 ARG286   0.2642
 558 HH11     5.4719    19.2964     1.9342 H     34 ARG286   0.2615
 559 HH12     6.2574    19.6741     3.4565 H     34 ARG286   0.2615
 560 HH21     8.3728    22.1460     2.1385 H     34 ARG286   0.2615
 561 HH22     7.8541    21.2824     3.5811 H     34 ARG286   0.2615
 562 N        5.5437    17.6580    -5.3986 N.am  35 ALA287  -0.2640
BACKBONE
 563 CA       4.7542    16.8594    -6.3421 C.3   35 ALA287   0.1282
BACKBONE
 564 C        5.0808    15.3788    -6.3564 C.2   35 ALA287   0.2034
BACKBONE
 565 O        4.6555    14.7050    -7.2856 O.2   35 ALA287  -0.3944
BACKBONE
 566 CB       4.7768    17.4983    -7.7506 C.3   35 ALA287  -0.0244
 567 H        6.3123    18.2046    -5.7515 H     35 ALA287   0.1883
 568 HA       3.7042    16.8729    -6.0422 H     35 ALA287   0.0797
 569 HB3      5.8119    17.4862    -8.1096 H     35 ALA287   0.0277
 570 HB2      4.4254    18.5397    -7.6852 H     35 ALA287   0.0277
 571 HB1      4.1400    16.9579    -8.4682 H     35 ALA287   0.0277
 572 N        5.7921    14.8404    -5.3345 N.am  36 GLY288  -0.2664
BACKBONE
 573 CA       6.0443    13.4027    -5.2713 C.3   36 GLY288   0.1201
BACKBONE
 574 C        7.3414    13.0182    -5.9344 C.2   36 GLY288   0.2009
BACKBONE
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 575 O       7.6760    11.8436    -5.8934 O.2   36 GLY288  -0.3947
BACKBONE
 576 H       6.1829    15.3981    -4.6005 H     36 GLY288   0.1881
 577 HA2     5.2357    12.8316    -5.7519 H     36 GLY288   0.0763
 578 HA3     6.0895    13.0717    -4.2224 H     36 GLY288   0.0763
 579 N       8.0982    13.9471    -6.5631 N.am  37 PHE289  -0.2622
BACKBONE
 580 CA      9.2413    13.5028    -7.3547 C.3   37 PHE289   0.1404
BACKBONE
 581 C      10.5484    13.4856    -6.6059 C.2   37 PHE289   0.2061
BACKBONE
 582 O      10.7231    14.2704    -5.6900 O.2   37 PHE289  -0.3942
BACKBONE
 583 CB      9.4769    14.4109    -8.5823 C.3   37 PHE289   0.0214
 584 CG      8.3324    14.3000    -9.5862 C.ar  37 PHE289  -0.0386
 585 CD1     8.1421    13.1099   -10.3004 C.ar  37 PHE289  -0.0601
 586 CD2     7.4781    15.3847    -9.8140 C.ar  37 PHE289  -0.0601
 587 CE1     7.1180    12.9995   -11.2325 C.ar  37 PHE289  -0.0686
 588 CE2     6.4902    15.3021   -10.7884 C.ar  37 PHE289  -0.0686
 589 CZ      6.2897    14.0998   -11.4772 C.ar  37 PHE289  -0.0687
 590 H       7.9032    14.9342    -6.5327 H     37 PHE289   0.1885
 591 HA      9.0469    12.4957    -7.7355 H     37 PHE289   0.0823
 592 HB3    10.3881    14.1008    -9.1042 H     37 PHE289   0.0474
 593 HB2     9.6223    15.4456    -8.2458 H     37 PHE289   0.0474
 594 HD1     8.8012    12.2669   -10.1357 H     37 PHE289   0.0557
 595 HD2     7.5922    16.2917    -9.2328 H     37 PHE289   0.0557
 596 HE1     6.9641    12.0688   -11.7736 H     37 PHE289   0.0599
 597 HE2     5.8828    16.1723   -11.0145 H     37 PHE289   0.0599
 598 HZ      5.5037    14.0142   -12.2061 H     37 PHE289   0.0559
 599 N      11.5007    12.6176    -7.0173 N.am  38 TYR290  -0.2620
BACKBONE
 600 CA     12.8706    12.7210    -6.5180 C.3   38 TYR290   0.1390
BACKBONE
 601 C      13.8448    12.7050    -7.6797 C.2   38 TYR290   0.2057
BACKBONE
 602 O      13.5605    12.0168    -8.6487 O.2   38 TYR290  -0.3942
BACKBONE
 603 CB     13.1518    11.6078    -5.4792 C.3   38 TYR290   0.0163
 604 CG     13.0173    10.1861    -6.0347 C.ar  38 TYR290  -0.0493
 605 CD1    14.1564     9.4650    -6.4121 C.ar  38 TYR290  -0.0685
 606 CD2    11.7574     9.5889    -6.1443 C.ar  38 TYR290  -0.0685
 607 CE1    14.0542     8.1098    -6.7394 C.ar  38 TYR290  -0.0398
 608 CE2    11.6511     8.2775    -6.6159 C.ar  38 TYR290  -0.0398
 609 CZ     12.7957     7.5024    -6.8198 C.ar  38 TYR290   0.0805
 610 OH     12.6655     6.1363    -7.0901 O.3   38 TYR290  -0.3376
 611 H      11.3102    11.9045    -7.6992 H     38 TYR290   0.1885
 612 HA     13.0161    13.6824    -6.0019 H     38 TYR290   0.0821
 613 HB2    12.4394    11.7302    -4.6536 H     38 TYR290   0.0453
 614 HB3    14.1619    11.7055    -5.0661 H     38 TYR290   0.0453
 615 HD1    15.1296     9.9490    -6.4442 H     38 TYR290   0.0530
 616 HD2    10.8608    10.1377    -5.8655 H     38 TYR290   0.0530
 617 HE1    14.9565     7.5353    -6.9252 H     38 TYR290   0.0525
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 618 HE2     10.6801     7.8542    -6.8312 H     38 TYR290   0.0525
 619 HH      13.4675     5.7497    -7.4277 H     38 TYR290   0.2458
 620 N       14.9728    13.4576    -7.6247 N.am  39 ALA291  -0.2639
BACKBONE
 621 CA      15.9308    13.4306    -8.7312 C.3   39 ALA291   0.1282
BACKBONE
 622 C       16.6437    12.0975    -8.7856 C.2   39 ALA291   0.2036
BACKBONE
 623 O       16.9363    11.5686    -7.7246 O.2   39 ALA291  -0.3944
BACKBONE
 624 CB      17.0169    14.5308    -8.5906 C.3   39 ALA291  -0.0244
 625 H       15.1952    14.0334    -6.8365 H     39 ALA291   0.1883
 626 HA      15.4003    13.6243    -9.6714 H     39 ALA291   0.0797
 627 HB3     17.6009    14.3812    -7.6693 H     39 ALA291   0.0277
 628 HB2     16.5545    15.5244    -8.5517 H     39 ALA291   0.0277
 629 HB1     17.7016    14.5082    -9.4505 H     39 ALA291   0.0277
 630 N       16.9588    11.5475    -9.9834 N.am  40 LEU292  -0.2637
BACKBONE
 631 CA      17.7704    10.3257   -10.0349 C.3   40 LEU292   0.1312
BACKBONE
 632 C       19.2518    10.6190   -10.1682 C.2   40 LEU292   0.2037
BACKBONE
 633 O       20.0209     9.6725   -10.1961 O.2   40 LEU292  -0.3944
BACKBONE
 634 CB      17.3283     9.4098   -11.2089 C.3   40 LEU292  -0.0101
 635 CG      15.8424     8.9448   -11.1339 C.3   40 LEU292  -0.0425
 636 CD1     15.5589     7.9869   -12.3215 C.3   40 LEU292  -0.0625
 637 CD2     15.5202     8.2141    -9.8016 C.3   40 LEU292  -0.0625
 638 H       16.7035    11.9904   -10.8538 H     40 LEU292   0.1883
 639 HA      17.6914     9.7412    -9.1043 H     40 LEU292   0.0800
 640 HB3     17.9728     8.5151   -11.2240 H     40 LEU292   0.0315
 641 HB2     17.4927     9.9555   -12.1530 H     40 LEU292   0.0315
 642 HG      15.1838     9.8276   -11.2239 H     40 LEU292   0.0298
 643 HD13    15.8429     8.4737   -13.2589 H     40 LEU292   0.0232
 644 HD12    14.4958     7.7185   -12.3824 H     40 LEU292   0.0232
 645 HD11    16.1488     7.0639   -12.2252 H     40 LEU292   0.0232
 646 HD23    16.2614     7.4258    -9.5979 H     40 LEU292   0.0232
 647 HD22    14.5277     7.7450    -9.8403 H     40 LEU292   0.0232
 648 HD21    15.5164     8.9317    -8.9699 H     40 LEU292   0.0232
 649 N       19.7164    11.8846   -10.2529 N.am  41 GLY293  -0.2664
BACKBONE
 650 CA      21.1490    12.1139   -10.4476 C.3   41 GLY293   0.1201
BACKBONE
 651 C       21.5700    11.9451   -11.8888 C.2   41 GLY293   0.2007
BACKBONE
 652 O       22.7561    11.7607   -12.1096 O.2   41 GLY293  -0.3947
BACKBONE
 653 H       19.1068    12.6746   -10.2330 H     41 GLY293   0.1881
 654 HA2     21.7402    11.4214    -9.8263 H     41 GLY293   0.0763
 655 HA3     21.4285    13.1377   -10.1528 H     41 GLY293   0.0763
 656 N       20.6523    12.0224   -12.8828 N.am  42 GLU294  -0.2639
BACKBONE
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 657 CA      21.0526    11.8774   -14.2836 C.3   42 GLU294   0.1324
BACKBONE
 658 C       20.3833    12.9701   -15.0951 C.2   42 GLU294   0.2038
BACKBONE
 659 O       19.1921    12.8804   -15.3486 O.2   42 GLU294  -0.3944
BACKBONE
 660 CB      20.6788    10.4498   -14.7676 C.3   42 GLU294  -0.0008
 661 CG      21.1940    10.1891   -16.2098 C.3   42 GLU294   0.0044
 662 CD      21.0180     8.7616   -16.6488 C.2   42 GLU294   0.0350
 663 OE1     21.0859     7.8529   -15.7805 O.co2 42 GLU294  -0.5690
 664 OE2     20.8316     8.5427   -17.8742 O.co2 42 GLU294  -0.5690
 665 H       19.6767    12.1617   -12.7010 H     42 GLU294   0.1883
 666 HA      22.1435    11.9752   -14.3995 H     42 GLU294   0.0801
 667 HB3     19.5872    10.3013   -14.7306 H     42 GLU294   0.0330
 668 HB2     21.1449     9.7258   -14.0774 H     42 GLU294   0.0330
 669 HG3     22.2743    10.3887   -16.2710 H     42 GLU294   0.0433
 670 HG2     20.6721    10.8581   -16.9123 H     42 GLU294   0.0433
 671 N       21.1023    14.0378   -15.5129 N.am  43 GLY295  -0.2664
BACKBONE
 672 CA      20.4317    15.0970   -16.2691 C.3   43 GLY295   0.1201
BACKBONE
 673 C       19.3836    15.7376   -15.3930 C.2   43 GLY295   0.2008
BACKBONE
 674 O       19.6634    15.9408   -14.2210 O.2   43 GLY295  -0.3947
BACKBONE
 675 H       22.0690    14.1515   -15.2842 H     43 GLY295   0.1881
 676 HA2     19.9720    14.6630   -17.1718 H     43 GLY295   0.0763
 677 HA3     21.1289    15.8891   -16.5852 H     43 GLY295   0.0763
 678 N       18.1789    16.0469   -15.9266 N.am  44 ASP296  -0.2624
BACKBONE
 679 CA      17.0692    16.4632   -15.0743 C.3   44 ASP296   0.1423
BACKBONE
 680 C       16.1481    15.2777   -14.8596 C.2   44 ASP296   0.2056
BACKBONE
 681 O       14.9656    15.4812   -14.6284 O.2   44 ASP296  -0.3943
BACKBONE
 682 CB      16.3478    17.6892   -15.7020 C.3   44 ASP296   0.0406
 683 CG      15.8834    17.4129   -17.1094 C.2   44 ASP296   0.0393
 684 OD1     16.4951    16.5243   -17.7652 O.co2 44 ASP296  -0.5688
 685 OD2     14.9204    18.0769   -17.5843 O.co2 44 ASP296  -0.5688
 686 H       17.9455    15.9296   -16.9036 H     44 ASP296   0.1884
 687 HA      17.4099    16.7595   -14.0698 H     44 ASP296   0.0819
 688 HB3     17.0680    18.5162   -15.7640 H     44 ASP296   0.0478
 689 HB2     15.5010    18.0163   -15.0794 H     44 ASP296   0.0478
 690 O        9.3860    12.0831   -19.6903 O.2   45 LYS297  -0.3942
BACKBONE
 691 C        8.5493    12.0913   -20.5799 C.2   45 LYS297   0.2067
BACKBONE
 692 N        7.6579    11.0614   -20.6747 N.am  45 LYS297  -0.2498
BACKBONE
 693 C        7.8175     9.8742   -19.8375 C.3   45 LYS297   0.1338
BACKBONE
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 694 H        7.5690    10.1410   -18.8049 H     45 LYS297   0.0802
 695 C        9.1769     9.2182   -19.9469 C.2   45 LYS297   0.2038
BACKBONE
 696 N        9.9408     9.0959   -18.8435 N.am  45 LYS297  -0.2719
BACKBONE
 697 H        9.5981     9.3844   -17.9496 H     45 LYS297   0.1879
 698 C       11.3067     8.5958   -18.9554 C.3   45 LYS297   0.0721
BACKBONE
 699 H       11.8343     9.0931   -19.7892 H     45 LYS297   0.0703
 700 C       12.0402     8.9087   -17.6678 C.ar  45 LYS297  -0.0244
BACKBONE
 701 C       12.4541     7.7851   -16.9923 C.ar  45 LYS297  -0.0075
BACKBONE
 702 C       11.9741     6.5271   -17.6886 C.3   45 LYS297  -0.0199
BACKBONE
 703 H       12.7728     5.7794   -17.8183 H     45 LYS297   0.0389
 704 H       11.1566     6.0992   -17.0867 H     45 LYS297   0.0389
 705 C       11.4394     7.0496   -19.0530 C.3   45 LYS297  -0.0141
BACKBONE
 706 H       12.1848     6.8031   -19.8262 H     45 LYS297   0.0326
 707 H       10.4863     6.5755   -19.3319 H     45 LYS297   0.0326
 708 C       13.2051     7.9039   -15.8087 C.ar  45 LYS297   0.1169
BACKBONE
 709 C       13.3024     9.1587   -15.2163 C.ar  45 LYS297  -0.0440
BACKBONE
 710 H       13.6917     9.2877   -14.2125 H     45 LYS297   0.0468
 711 C       12.8969    10.3040   -15.9239 C.ar  45 LYS297  -0.0838
BACKBONE
 712 H       13.0771    11.2798   -15.5069 H     45 LYS297   0.0515
 713 C       12.2745    10.1921   -17.1608 C.ar  45 LYS297  -0.0756
BACKBONE
 714 H       11.9540    11.0583   -17.7199 H     45 LYS297   0.0448
 715 O       13.8241     6.7848   -15.2502 O.3   45 LYS297  -0.1878
BACKBONE
 716 S       15.0736     6.2955   -15.9611 S.o2  45 LYS297   0.0426
 717 O       16.1887     6.5258   -15.0695 O.2   45 LYS297  -0.1587
BACKBONE
 718 O       14.8331     4.9126   -16.3475 O.2   45 LYS297  -0.1587
BACKBONE
 719 N1      15.2469     7.2290   -17.3244 N.am  45 LYS297  -0.5394
 720 O        9.5596     8.8077   -21.0304 O.2   45 LYS297  -0.3944
BACKBONE
 721 C        6.7084     8.9484   -20.3956 C.3   45 LYS297  -0.0104
BACKBONE
 722 H        7.0782     8.3668   -21.2564 H     45 LYS297   0.0313
 723 H        6.3116     8.2500   -19.6379 H     45 LYS297   0.0313
 724 C        5.6587     9.9552   -20.9113 C.3   45 LYS297  -0.0281
BACKBONE
 725 H        5.1338    10.3729   -20.0351 H     45 LYS297   0.0287
 726 H        4.9201     9.5057   -21.5954 H     45 LYS297   0.0287
 727 C        6.5119    11.0654   -21.5742 C.3   45 LYS297   0.0369
BACKBONE
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 728 H        5.9296    11.9964   -21.5795 H     45 LYS297   0.0524
 729 H        6.8222    10.7903   -22.5948 H     45 LYS297   0.0524
 730 C        8.6052    13.2750   -21.5383 C.3   45 LYS297   0.1339
BACKBONE
 731 H        7.6442    13.3517   -22.0600 H     45 LYS297   0.0803
 732 N        8.7846    14.5402   -20.7909 N.am  45 LYS297  -0.2641
BACKBONE
 733 H        9.6945    14.7805   -20.4461 H     45 LYS297   0.1883
 734 C        7.7366    15.3712   -20.5540 C.2   45 LYS297   0.1952
BACKBONE
 735 C        7.9608    16.7464   -19.9406 C.3   45 LYS297   0.0951
BACKBONE
 736 H        8.7720    17.2330   -20.5109 H     45 LYS297   0.0700
 737 N        6.7435    17.6046   -19.9950 N.3   45 LYS297  -0.2998
BACKBONE
 738 H        6.8930    18.5164   -19.4150 H     45 LYS297   0.1245
 739 C        6.2464    17.9784   -21.3332 C.3   45 LYS297  -0.0133
BACKBONE
 740 H        6.9717    18.6185   -21.8627 H     45 LYS297   0.0390
 741 H        6.0284    17.1034   -21.9609 H     45 LYS297   0.0390
 742 H        5.3090    18.5421   -21.2005 H     45 LYS297   0.0390
 743 C        8.4032    16.6123   -18.4619 C.3   45 LYS297  -0.0322
BACKBONE
 744 H        7.5800    16.2004   -17.8599 H     45 LYS297   0.0269
 745 H        9.2816    15.9580   -18.3762 H     45 LYS297   0.0269
 746 H        8.6700    17.5991   -18.0529 H     45 LYS297   0.0269
 747 O        6.5975    15.0410   -20.8403 O.2   45 LYS297  -0.3952
BACKBONE
 748 C        9.6453    13.0311   -22.7025 C.3   45 LYS297  -0.0006
BACKBONE
 749 H        9.1017    12.8869   -23.6553 H     45 LYS297   0.0348
 750 C       10.5947    14.2418   -22.9177 C.3   45 LYS297  -0.0460
BACKBONE
 751 H       10.0086    15.1684   -23.0414 H     45 LYS297   0.0270
 752 H       11.2456    14.3354   -22.0369 H     45 LYS297   0.0270
 753 C       11.5228    14.0483   -24.1446 C.3   45 LYS297  -0.0526
BACKBONE
 754 H       12.1688    14.9354   -24.2644 H     45 LYS297   0.0265
 755 H       10.9213    13.9440   -25.0625 H     45 LYS297   0.0265
 756 C       12.4008    12.7872   -23.9405 C.3   45 LYS297  -0.0530
BACKBONE
 757 H       13.0589    12.9295   -23.0688 H     45 LYS297   0.0265
 758 H       13.0434    12.6334   -24.8238 H     45 LYS297   0.0265
 759 C       11.5006    11.5439   -23.7177 C.3   45 LYS297  -0.0526
BACKBONE
 760 H       12.1350    10.6623   -23.5185 H     45 LYS297   0.0265
 761 H       10.9269    11.3461   -24.6382 H     45 LYS297   0.0265
 762 C       10.5167    11.7507   -22.5317 C.3   45 LYS297  -0.0460
BACKBONE
 763 H       11.0909    11.8283   -21.5979 H     45 LYS297   0.0270
 764 H        9.8696    10.8604   -22.4718 H     45 LYS297   0.0270
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765 N	16.6348	14.0087	-14.8991	N.am	45	LYS297	-0.2636
BACKBONE							
766 CA	15.7025	12.8963	-14.6881	C.3	45	LYS297	0.1310
BACKBONE							
767 C	15.1351	12.9445	-13.2695	C.2	45	LYS297	0.2039
BACKBONE							
768 O	15.9070	12.9190	-12.3173	O.2	45	LYS297	-0.3944
BACKBONE							
769 CB	16.2815	11.4489	-14.8675	C.3	45	LYS297	-0.0124
770 CG	16.2930	10.8719	-16.3131	C.3	45	LYS297	-0.0502
771 CD	16.4201	9.3108	-16.3189	C.3	45	LYS297	-0.0687
772 CE	15.7714	8.6022	-17.5512	C.3	45	LYS297	-0.1233
773 H	17.6024	13.7916	-15.0702	H	45	LYS297	0.1883
774 HA	14.8878	13.0052	-15.4263	H	45	LYS297	0.0800
775 HB3	15.6156	10.8003	-14.2680	H	45	LYS297	0.0312
776 HB2	17.2881	11.4140	-14.4068	H	45	LYS297	0.0312
777 HG3	17.1033	11.3333	-16.9019	H	45	LYS297	0.0267
778 HG2	15.3407	11.1333	-16.7900	H	45	LYS297	0.0267
779 HD3	15.8465	8.9067	-15.4826	H	45	LYS297	0.0251
780 HD2	17.4720	9.0005	-16.1766	H	45	LYS297	0.0251
781 HE3	16.4949	8.6140	-18.3993	H	45	LYS297	0.0062
782 HE2	14.9267	9.2318	-17.9086	H	45	LYS297	0.0062
783 N	13.7873	12.8980	-13.1113	N.am	46	VAL298	-0.2635
BACKBONE							
784 CA	13.2118	12.6947	-11.7833	C.3	46	VAL298	0.1332
BACKBONE							
785 C	12.2489	11.5350	-11.7848	C.2	46	VAL298	0.2041
BACKBONE							
786 O	11.8258	11.1268	-12.8558	O.2	46	VAL298	-0.3944
BACKBONE							
787 CB	12.4747	13.9705	-11.2867	C.3	46	VAL298	-0.0063
788 CG1	13.3105	15.2529	-11.5333	C.3	46	VAL298	-0.0584
789 CG2	11.0779	14.1147	-11.9585	C.3	46	VAL298	-0.0584
790 H	13.1505	12.9843	-13.8867	H	46	VAL298	0.1883
791 HA	13.9917	12.4011	-11.0671	H	46	VAL298	0.0802
792 HB	12.3565	13.8667	-10.1970	H	46	VAL298	0.0343
793 HG13	14.3160	15.1670	-11.0978	H	46	VAL298	0.0234
794 HG12	12.8062	16.1194	-11.0796	H	46	VAL298	0.0234
795 HG11	13.4090	15.4332	-12.6128	H	46	VAL298	0.0234
796 HG23	11.1805	14.2135	-13.0483	H	46	VAL298	0.0234
797 HG22	10.5619	15.0029	-11.5708	H	46	VAL298	0.0234
798 HG21	10.4309	13.2490	-11.7613	H	46	VAL298	0.0234
799 N	11.8657	11.0112	-10.5931	N.am	47	LYS299	-0.2637
BACKBONE							
800 CA	10.9042	9.9061	-10.5484	C.3	47	LYS299	0.1310
BACKBONE							
801 C	9.8669	10.0051	-9.4466	C.2	47	LYS299	0.2039
BACKBONE							
802 O	10.2030	10.5139	-8.3894	O.2	47	LYS299	-0.3944
BACKBONE							
803 CB	11.7293	8.6025	-10.4359	C.3	47	LYS299	-0.0122
804 CG	10.9066	7.3290	-10.7569	C.3	47	LYS299	-0.0440

805	CD	11.8228	6.0749	-10.7384	C.3	47 LYS299	-0.0124
806	CE	11.1044	4.7818	-11.2169	C.3	47 LYS299	-0.0354
807	NZ	10.6886	4.8412	-12.6410	N.4	47 LYS299	0.2185
808	H	12.2779	11.3189	-9.7301	H	47 LYS299	0.1883
809	HA	10.3321	9.9117	-11.4805	H	47 LYS299	0.0800
810	HB3	12.1580	8.5475	-9.4242	H	47 LYS299	0.0312
811	HB2	12.5549	8.6764	-11.1603	H	47 LYS299	0.0312
812	HG3	10.4706	7.4646	-11.7554	H	47 LYS299	0.0269
813	HG2	10.0894	7.2067	-10.0284	H	47 LYS299	0.0269
814	HD3	12.1876	5.9288	-9.7086	H	47 LYS299	0.0317
815	HD2	12.6993	6.2398	-11.3846	H	47 LYS299	0.0317
816	HE3	10.2357	4.5928	-10.5630	H	47 LYS299	0.0813
817	HE2	11.8098	3.9413	-11.0797	H	47 LYS299	0.0813
818	HZ3	9.8707	5.5240	-12.8275	H	47 LYS299	0.1994
819	HZ2	10.3022	3.8931	-12.9887	H	47 LYS299	0.1994
820	HZ1	11.4989	5.1118	-13.3059	H	47 LYS299	0.1994
821	N	8.6042	9.5583	-9.6788	N.am	48 CYS300	-0.2629
BACKBONE							
822	CA	7.5656	9.6627	-8.6484	C.3	48 CYS300	0.1406
BACKBONE							
823	C	7.7076	8.5401	-7.6373	C.2	48 CYS300	0.2049
BACKBONE							
824	O	7.6313	7.3879	-8.0326	O.2	48 CYS300	-0.3943
BACKBONE							
825	CB	6.1439	9.6281	-9.2726	C.3	48 CYS300	0.0443
826	SG	4.8855	9.7613	-7.9666	S.3	48 CYS300	-0.0882
827	H	8.3536	9.1306	-10.5560	H	48 CYS300	0.1884
828	HA	7.6319	10.6342	-8.1443	H	48 CYS300	0.0808
829	HB3	5.9938	8.6811	-9.7994	H	48 CYS300	0.0432
830	HB2	5.9815	10.4538	-9.9811	H	48 CYS300	0.0432
831	LPG2	4.9546	9.2682	-7.5049	LP	48 CYS300	0.0000
832	LPG1	4.9120	10.3655	-7.6580	LP	48 CYS300	0.0000
833	N	7.9069	8.8043	-6.3231	N.am	49 PHE301	-0.2619
BACKBONE							
834	CA	8.0236	7.6885	-5.3714	C.3	49 PHE301	0.1404
BACKBONE							
835	C	6.8170	6.7822	-5.3680	C.2	49 PHE301	0.2061
BACKBONE							
836	O	6.9553	5.5898	-5.1286	O.2	49 PHE301	-0.3942
BACKBONE							
837	CB	8.2239	8.1509	-3.9013	C.3	49 PHE301	0.0214
838	CG	6.9093	8.5611	-3.2155	C.ar	49 PHE301	-0.0386
839	CD1	6.2373	7.6421	-2.3884	C.ar	49 PHE301	-0.0601
840	CD2	6.3597	9.8332	-3.3770	C.ar	49 PHE301	-0.0601
841	CE1	5.0791	8.0143	-1.7085	C.ar	49 PHE301	-0.0686
842	CE2	5.1843	10.2033	-2.7259	C.ar	49 PHE301	-0.0686
843	CZ	4.5424	9.2897	-1.8745	C.ar	49 PHE301	-0.0687
844	H	7.9800	9.7519	-5.9961	H	49 PHE301	0.1885
845	HA	8.8797	7.0658	-5.6684	H	49 PHE301	0.0823
846	HB3	8.9457	8.9774	-3.8786	H	49 PHE301	0.0474
847	HB2	8.6586	7.3208	-3.3227	H	49 PHE301	0.0474
848	HD1	6.6388	6.6456	-2.2647	H	49 PHE301	0.0557

849	HD2	6.8477	10.5554	-4.0159	H	49 PHE301	0.0557
850	HE1	4.5915	7.3158	-1.0311	H	49 PHE301	0.0599
851	HE2	4.7621	11.1917	-2.8700	H	49 PHE301	0.0599
852	HZ	3.6381	9.5769	-1.3500	H	49 PHE301	0.0559
853	N	5.6190	7.3625	-5.5920	N.am	50 HIS302	-0.2617
BACKBONE							
854	CA	4.3981	6.5799	-5.4843	C.3	50 HIS302	0.1421
BACKBONE							
855	C	4.1384	5.8079	-6.7575	C.2	50 HIS302	0.2060
BACKBONE							
856	O	4.2621	4.5912	-6.7362	O.2	50 HIS302	-0.3942
BACKBONE							
857	CB	3.2123	7.4704	-5.0302	C.3	50 HIS302	0.0427
858	CG	2.1348	6.6248	-4.3971	C.2	50 HIS302	0.0561
859	ND1	1.4686	5.6836	-5.0202	N.pl3	50 HIS302	-0.2623
860	CD2	1.7293	6.7094	-3.1158	C.2	50 HIS302	-0.0276
861	CE1	0.6426	5.1181	-4.2035	C.2	50 HIS302	0.0875
862	NE2	0.7401	5.6642	-3.0772	N.2	50 HIS302	-0.3437
863	H	5.5419	8.3342	-5.8098	H	50 HIS302	0.1885
864	HA	4.5577	5.8554	-4.6770	H	50 HIS302	0.0824
865	HB3	2.7991	8.0732	-5.8509	H	50 HIS302	0.0491
866	HB2	3.6021	8.1624	-4.2699	H	50 HIS302	0.0491
867	HD1	1.5880	5.4182	-6.0113	H	50 HIS302	0.2386
868	HD2	2.0538	7.3696	-2.3129	H	50 HIS302	0.0324
869	HE1	-0.0382	4.2976	-4.4212	H	50 HIS302	0.1149
870	N	3.7741	6.4812	-7.8727	N.am	51 CYS303	-0.2627
BACKBONE							
871	CA	3.5433	5.7720	-9.1253	C.3	51 CYS303	0.1406
BACKBONE							
872	C	4.8198	5.2684	-9.7657	C.2	51 CYS303	0.2045
BACKBONE							
873	O	4.7284	4.3865	-10.6062	O.2	51 CYS303	-0.3944
BACKBONE							
874	CB	2.7066	6.6305	-10.1189	C.3	51 CYS303	0.0443
875	SG	3.4367	8.2233	-10.6584	S.3	51 CYS303	-0.0882
876	H	3.6637	7.4797	-7.9072	H	51 CYS303	0.1884
877	HA	2.9402	4.8737	-8.9049	H	51 CYS303	0.0808
878	HB3	1.7481	6.8542	-9.6407	H	51 CYS303	0.0432
879	HB2	2.5075	6.0488	-11.0321	H	51 CYS303	0.0432
880	LPG2	4.1018	8.1532	-10.7759	LP	51 CYS303	0.0000
881	LPG1	3.1299	8.4480	-11.2209	LP	51 CYS303	0.0000
882	N	6.0279	5.7773	-9.4294	N.am	52 GLY304	-0.2664
BACKBONE							
883	CA	7.2260	5.3360	-10.1463	C.3	52 GLY304	0.1201
BACKBONE							
884	C	7.4121	5.9788	-11.5018	C.2	52 GLY304	0.2005
BACKBONE							
885	O	8.4200	5.7030	-12.1375	O.2	52 GLY304	-0.3947
BACKBONE							
886	H	6.1313	6.4945	-8.7307	H	52 GLY304	0.1881
887	HA2	7.1873	4.2561	-10.3286	H	52 GLY304	0.0763
888	HA3	8.1249	5.5282	-9.5426	H	52 GLY304	0.0763

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 889 N        6.4673     6.8178   -11.9767 N.am  53 GLY305  -0.2666
BACKBONE
 890 CA       6.6256     7.4729   -13.2699 C.3   53 GLY305   0.1201
BACKBONE
 891 C        7.9045     8.2712   -13.3332 C.2   53 GLY305   0.2005
BACKBONE
 892 O        8.2444     8.9077   -12.3478 O.2   53 GLY305  -0.3947
BACKBONE
 893 H        5.6311     7.0050   -11.4677 H     53 GLY305   0.1881
 894 HA2      5.8068     8.1932   -13.4276 H     53 GLY305   0.0763
 895 HA3      6.5679     6.7141   -14.0649 H     53 GLY305   0.0763
 896 N        8.6173     8.2640   -14.4835 N.am  54 GLY306  -0.2666
BACKBONE
 897 CA       9.8094     9.0978   -14.6433 C.3   54 GLY306   0.1201
BACKBONE
 898 C        9.5200    10.2770   -15.5406 C.2   54 GLY306   0.2007
BACKBONE
 899 O        8.7347    10.0880   -16.4592 O.2   54 GLY306  -0.3947
BACKBONE
 900 H        8.3198     7.7385   -15.2844 H     54 GLY306   0.1881
 901 HA2     10.5911     8.5047   -15.1369 H     54 GLY306   0.0763
 902 HA3     10.2205     9.4287   -13.6878 H     54 GLY306   0.0763
 903 N       10.1459    11.4651   -15.3373 N.am  55 LEU307  -0.2640
BACKBONE
 904 CA       9.9782    12.5738   -16.2867 C.3   55 LEU307   0.1312
BACKBONE
 905 C       11.2844    13.3033   -16.5473 C.2   55 LEU307   0.2040
BACKBONE
 906 O       12.0550    13.4822   -15.6159 O.2   55 LEU307  -0.3944
BACKBONE
 907 CB       8.9909    13.6465   -15.7631 C.3   55 LEU307  -0.0101
 908 CG       7.5049    13.2023   -15.6947 C.3   55 LEU307  -0.0425
 909 CD1      6.6825    14.3099   -14.9836 C.3   55 LEU307  -0.0625
 910 CD2      6.8871    12.9458   -17.0966 C.3   55 LEU307  -0.0625
 911 H       10.7580    11.6130   -14.5506 H     55 LEU307   0.1883
 912 HA       9.6400    12.1883   -17.2550 H     55 LEU307   0.0800
 913 HB3      9.0545    14.5535   -16.3825 H     55 LEU307   0.0315
 914 HB2      9.3361    13.8985   -14.7509 H     55 LEU307   0.0315
 915 HG       7.4568    12.2799   -15.0938 H     55 LEU307   0.0298
 916 HD13     7.0895    14.4883   -13.9798 H     55 LEU307   0.0232
 917 HD12     5.6229    14.0220   -14.8947 H     55 LEU307   0.0232
 918 HD11     6.7499    15.2511   -15.5464 H     55 LEU307   0.0232
 919 HD23     6.9414    13.8460   -17.7255 H     55 LEU307   0.0232
 920 HD22     5.8333    12.6577   -16.9902 H     55 LEU307   0.0232
 921 HD21     7.3944    12.1305   -17.6192 H     55 LEU307   0.0232
 922 N       11.5410    13.7442   -17.8054 N.am  56 THR308  -0.2613
BACKBONE
 923 CA      12.7991    14.4243   -18.1247 C.3   56 THR308   0.1565
BACKBONE
 924 C       12.6236    15.4467   -19.2275 C.2   56 THR308   0.2066
BACKBONE
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 925 O       11.5250    15.5469   -19.7550 O.2   56 THR308  -0.3943
BACKBONE
 926 CB      13.8652    13.3922   -18.5780 C.3   56 THR308   0.0924
 927 OG1     15.1058    14.0914   -18.7653 O.3   56 THR308  -0.3874
 928 CG2     13.4767    12.6751   -19.8975 C.3   56 THR308  -0.0346
 929 H       10.8993    13.6016   -18.5641 H     56 THR308   0.1884
 930 HA      13.1827    14.9722   -17.2472 H     56 THR308   0.0826
 931 HB      13.9666    12.6544   -17.7694 H     56 THR308   0.0639
 932 HG1     15.8412    13.5196   -18.9625 H     56 THR308   0.2101
 933 HG22    14.2799    11.9918   -20.2146 H     56 THR308   0.0257
 934 HG21    13.3198    13.4183   -20.6918 H     56 THR308   0.0257
 935 HG23    12.5572    12.0905   -19.7671 H     56 THR308   0.0257
 936 N       13.7073    16.1855   -19.5736 N.am  57 ASP309  -0.2621
BACKBONE
 937 CA      13.6214    17.2516   -20.5765 C.3   57 ASP309   0.1423
BACKBONE
 938 C       12.5654    18.2283   -20.1185 C.2   57 ASP309   0.2057
BACKBONE
 939 O       11.6227    18.5379   -20.8319 O.2   57 ASP309  -0.3943
BACKBONE
 940 CB      13.3646    16.7337   -22.0130 C.3   57 ASP309   0.0406
 941 CG      13.5409    17.8195   -23.0448 C.2   57 ASP309   0.0393
 942 OD1     14.2549    18.8389   -22.8228 O.co2 57 ASP309  -0.5688
 943 OD2     12.9431    17.7695   -24.1537 O.co2 57 ASP309  -0.5688
 944 H       14.5908    16.0433   -19.0997 H     57 ASP309   0.1884
 945 HA      14.5719    17.8144   -20.5885 H     57 ASP309   0.0819
 946 HB3     12.3242    16.3890   -22.0898 H     57 ASP309   0.0478
 947 HB2     14.0562    15.9063   -22.2374 H     57 ASP309   0.0478
 948 N       12.7073    18.7275   -18.8758 N.am  58 TRP310  -0.2626
BACKBONE
 949 CA      11.7248    19.6828   -18.3844 C.3   58 TRP310   0.1352
BACKBONE
 950 C       11.8808    21.0027   -19.1108 C.2   58 TRP310   0.2052
BACKBONE
 951 O       12.9924    21.3391   -19.4910 O.2   58 TRP310  -0.3942
BACKBONE
 952 CB      11.9053    19.9215   -16.8701 C.3   58 TRP310   0.0042
 953 CG      11.4701    18.7342   -16.0516 C.2   58 TRP310  -0.0418
 954 CD1     12.1963    17.6565   -15.6977 C.2   58 TRP310   0.0167
 955 CD2     10.1027    18.5423   -15.4613 C.ar  58 TRP310  -0.0214
 956 NE1     11.4687    16.8578   -14.9721 N.pl3 58 TRP310  -0.2890
 957 CE2     10.2260    17.3516   -14.7733 C.ar  58 TRP310   0.0603
 958 CE3      8.9032    19.2635   -15.4841 C.ar  58 TRP310  -0.0747
 959 CZ2      9.1804    16.8339   -14.0168 C.ar  58 TRP310  -0.0443
 960 CZ3      7.8524    18.7638   -14.7085 C.ar  58 TRP310  -0.0792
 961 CH2      7.9804    17.5569   -14.0033 C.ar  58 TRP310  -0.0768
 962 H       13.5128    18.4884   -18.3150 H     58 TRP310   0.1884
 963 HA      10.7120    19.2820   -18.5648 H     58 TRP310   0.0815
 964 HB3     11.2667    20.7711   -16.6156 H     58 TRP310   0.0397
 965 HB2     12.9499    20.1915   -16.6442 H     58 TRP310   0.0397
 966 HD1     13.2335    17.4733   -15.9731 H     58 TRP310   0.0795
 967 HE1     11.8016    15.9536   -14.5997 H     58 TRP310   0.2216
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968	HE3	8.8026	20.1613	-16.0798	H	58 TRP310	0.0540
969	HZ2	9.2872	15.9155	-13.4558	H	58 TRP310	0.0541
970	HZ3	6.9273	19.3312	-14.6601	H	58 TRP310	0.0510
971	HH2	7.1458	17.1610	-13.4343	H	58 TRP310	0.0530
972	N	10.7838	21.7703	-19.3098	N.am	59 LYS311	-0.2636
BACKBONE							
973	CA	10.8755	23.0132	-20.0776	C.3	59 LYS311	0.1312
BACKBONE							
974	C	10.6855	24.2287	-19.1904	C.2	59 LYS311	0.2064
BACKBONE							
975	O	10.1909	24.0588	-18.0862	O.2	59 LYS311	-0.3942
BACKBONE							
976	CB	9.8625	22.9503	-21.2574	C.3	59 LYS311	-0.0122
977	CG	10.0334	21.6826	-22.1478	C.3	59 LYS311	-0.0440
978	CD	11.4413	21.5856	-22.7952	C.3	59 LYS311	-0.0124
979	CE	11.5490	20.3714	-23.7583	C.3	59 LYS311	-0.0354
980	NZ	12.9287	20.1845	-24.2560	N.4	59 LYS311	0.2185
981	H	9.8777	21.5039	-18.9507	H	59 LYS311	0.1883
982	HA	11.8824	23.1222	-20.4942	H	59 LYS311	0.0800
983	HB3	9.9522	23.8451	-21.8939	H	59 LYS311	0.0312
984	HB2	8.8435	22.9395	-20.8390	H	59 LYS311	0.0312
985	HG3	9.2691	21.7129	-22.9439	H	59 LYS311	0.0269
986	HG2	9.8451	20.7788	-21.5431	H	59 LYS311	0.0269
987	HD3	12.1963	21.4343	-22.0118	H	59 LYS311	0.0317
988	HD2	11.6717	22.5211	-23.3284	H	59 LYS311	0.0317
989	HE3	10.8545	20.5145	-24.6060	H	59 LYS311	0.0813
990	HE2	11.2253	19.4666	-23.2091	H	59 LYS311	0.0813
991	HZ3	13.2689	20.9938	-24.8835	H	59 LYS311	0.1994
992	HZ2	13.0435	19.2654	-24.8309	H	59 LYS311	0.1994
993	HZ1	13.6739	20.1459	-23.4651	H	59 LYS311	0.1994
994	N	11.0585	25.4838	-19.5610	N.am	60 PRO312	-0.2498
BACKBONE							
995	CA	10.8711	26.5728	-18.6131	C.3	60 PRO312	0.1338
BACKBONE							
996	C	9.4351	26.7637	-18.1764	C.2	60 PRO312	0.2042
BACKBONE							
997	O	8.5334	26.4534	-18.9376	O.2	60 PRO312	-0.3944
BACKBONE							
998	CB	11.3666	27.7795	-19.4476	C.3	60 PRO312	-0.0104
999	CG	12.3647	27.1405	-20.4413	C.3	60 PRO312	-0.0281
1000	CD	11.6625	25.8226	-20.8492	C.3	60 PRO312	0.0369
1001	HA	11.5334	26.3913	-17.7498	H	60 PRO312	0.0802
1002	HB3	11.8134	28.5752	-18.8287	H	60 PRO312	0.0313
1003	HB2	10.5288	28.2034	-20.0279	H	60 PRO312	0.0313
1004	HG2	12.6008	27.7896	-21.3018	H	60 PRO312	0.0287
1005	HG3	13.2991	26.9106	-19.9005	H	60 PRO312	0.0287
1006	HD2	10.8780	26.0288	-21.5936	H	60 PRO312	0.0524
1007	HD3	12.4079	25.1301	-21.2654	H	60 PRO312	0.0524
1008	N	9.1953	27.2794	-16.9511	N.am	61 SER313	-0.2616
BACKBONE							
1009	CA	7.8208	27.5334	-16.5137	C.3	61 SER313	0.1539
BACKBONE							

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1010 C        6.9176    26.3179   -16.4605 C.2   61 SER313   0.2062
BACKBONE
1011 O        5.7262    26.5339   -16.3081 O.2   61 SER313  -0.3943
BACKBONE
1012 CB       7.1822    28.6692   -17.3598 C.3   61 SER313   0.0843
1013 OG       8.0529    29.8187   -17.3400 O.3   61 SER313  -0.3903
1014 H        9.9471    27.5419   -16.3415 H     61 SER313   0.1884
1015 HA       7.8426    27.9025   -15.4746 H     61 SER313   0.0823
1016 HB3      6.1967    28.9408   -16.9424 H     61 SER313   0.0606
1017 HB2      7.0309    28.3213   -18.3949 H     61 SER313   0.0606
1018 HG       7.7131    30.5463   -17.8530 H     61 SER313   0.2097
1019 N        7.3845    25.0505   -16.5554 N.am  62 GLU314  -0.2636
BACKBONE
1020 CA       6.4480    23.9340   -16.3831 C.3   62 GLU314   0.1325
BACKBONE
1021 C        6.1361    23.7074   -14.9169 C.2   62 GLU314   0.2041
BACKBONE
1022 O        6.9901    23.9647   -14.0823 O.2   62 GLU314  -0.3944
BACKBONE
1023 CB       6.9642    22.5884   -16.9613 C.3   62 GLU314  -0.0008
1024 CG       6.9123    22.5663   -18.5077 C.3   62 GLU314   0.0044
1025 CD       7.3128    21.2042   -19.0073 C.2   62 GLU314   0.0350
1026 OE1      8.4625    20.7851   -18.7122 O.co2 62 GLU314  -0.5690
1027 OE2      6.4888    20.5367   -19.6858 O.co2 62 GLU314  -0.5690
1028 H        8.3576    24.8500   -16.6889 H     62 GLU314   0.1883
1029 HA       5.5016    24.1743   -16.8949 H     62 GLU314   0.0801
1030 HB3      6.3357    21.7594   -16.5956 H     62 GLU314   0.0330
1031 HB2      7.9953    22.4158   -16.6141 H     62 GLU314   0.0330
1032 HG3      7.5911    23.3343   -18.9018 H     62 GLU314   0.0433
1033 HG2      5.8931    22.7918   -18.8574 H     62 GLU314   0.0433
1034 N        4.9189    23.2069   -14.5871 N.am  63 ASP315  -0.2622
BACKBONE
1035 CA       4.5812    22.9127   -13.1932 C.3   63 ASP315   0.1425
BACKBONE
1036 C        4.7215    21.4168   -12.9408 C.2   63 ASP315   0.2081
BACKBONE
1037 O        4.1475    20.6433   -13.6971 O.2   63 ASP315  -0.3941
BACKBONE
1038 CB       3.1399    23.3567   -12.8446 C.3   63 ASP315   0.0406
1039 CG       2.8130    22.8472   -11.4664 C.2   63 ASP315   0.0393
1040 OD1      3.0612    23.5638   -10.4626 O.co2 63 ASP315  -0.5688
1041 OD2      2.3242    21.6925   -11.3727 O.co2 63 ASP315  -0.5688
1042 H        4.2358    22.9691   -15.2807 H     63 ASP315   0.1884
1043 HA       5.1899    23.5295   -12.5182 H     63 ASP315   0.0819
1044 HB3      2.4395    22.9307   -13.5719 H     63 ASP315   0.0478
1045 HB2      3.0401    24.4532   -12.8862 H     63 ASP315   0.0478
1046 N        5.4579    20.9277   -11.9098 N.am  64 PRO316  -0.2497
BACKBONE
1047 CA       5.4415    19.4973   -11.6192 C.3   64 PRO316   0.1338
BACKBONE
1048 C        4.1126    18.8126   -11.3973 C.2   64 PRO316   0.2042
BACKBONE
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1049 O        3.9532    17.6742   -11.8166 O.2   64 PRO316  -0.3944
BACKBONE
1050 CB       6.1983    19.5111   -10.2732 C.3   64 PRO316  -0.0104
1051 CG       7.1897    20.6763   -10.4346 C.3   64 PRO316  -0.0281
1052 CD       6.3139    21.7731   -11.0820 C.3   64 PRO316   0.0369
1053 HA       6.0154    18.9752   -12.3939 H     64 PRO316   0.0802
1054 HB3      6.6688    18.5423   -10.0664 H     64 PRO316   0.0313
1055 HB2      5.5221    19.7750    -9.4457 H     64 PRO316   0.0313
1056 HG2      7.6699    20.9855    -9.4966 H     64 PRO316   0.0287
1057 HG3      7.9656    20.3524   -11.1422 H     64 PRO316   0.0287
1058 HD2      5.7101    22.3235   -10.3402 H     64 PRO316   0.0524
1059 HD3      6.9693    22.4617   -11.6390 H     64 PRO316   0.0524
1060 N        3.1459    19.4643   -10.7195 N.am  65 TRP317  -0.2627
BACKBONE
1061 CA       1.8647    18.8051   -10.4947 C.3   65 TRP317   0.1352
BACKBONE
1062 C        1.2124    18.6120   -11.8387 C.2   65 TRP317   0.2052
BACKBONE
1063 O        0.7119    17.5305   -12.1207 O.2   65 TRP317  -0.3942
BACKBONE
1064 CB       0.9048    19.6186    -9.5876 C.3   65 TRP317   0.0042
1065 CG       1.3986    19.6463    -8.1727 C.2   65 TRP317  -0.0418
1066 CD1      1.9961    20.6455    -7.4998 C.2   65 TRP317   0.0167
1067 CD2      1.2833    18.4815    -7.2305 C.ar  65 TRP317  -0.0214
1068 NE1      2.2260    20.2539    -6.2742 N.pl3 65 TRP317  -0.2890
1069 CE2      1.8035    18.9914    -6.0582 C.ar  65 TRP317   0.0603
1070 CE3      0.8095    17.1775    -7.3478 C.ar  65 TRP317  -0.0747
1071 CZ2      1.8381    18.2231    -4.8931 C.ar  65 TRP317  -0.0443
1072 CZ3      0.9045    16.3781    -6.2022 C.ar  65 TRP317  -0.0792
1073 CH2      1.4119    16.8924    -5.0018 C.ar  65 TRP317  -0.0768
1074 H        3.2353    20.4437   -10.4888 H     65 TRP317   0.1884
1075 HA       2.0329    17.8158   -10.0419 H     65 TRP317   0.0815
1076 HB3     -0.0811    19.1304    -9.5721 H     65 TRP317   0.0397
1077 HB2      0.7626    20.6467    -9.9459 H     65 TRP317   0.0397
1078 HD1      2.2390    21.6206    -7.9324 H     65 TRP317   0.0795
1079 HE1      2.6901    20.8351    -5.5572 H     65 TRP317   0.2216
1080 HE3      0.3973    16.8094    -8.2785 H     65 TRP317   0.0540
1081 HZ2      2.1925    18.6383    -3.9564 H     65 TRP317   0.0541
1082 HZ3      0.5893    15.3436    -6.2486 H     65 TRP317   0.0510
1083 HH2      1.4932    16.2278    -4.1485 H     65 TRP317   0.0530
1084 N        1.2238    19.6728   -12.6762 N.am  66 GLU318  -0.2635
BACKBONE
1085 CA       0.5891    19.5461   -13.9780 C.3   66 GLU318   0.1325
BACKBONE
1086 C        1.1928    18.3775   -14.7202 C.2   66 GLU318   0.2040
BACKBONE
1087 O        0.4621    17.5373   -15.2255 O.2   66 GLU318  -0.3944
BACKBONE
1088 CB       0.6655    20.8123   -14.8709 C.3   66 GLU318  -0.0008
1089 CG      -0.1772    21.9845   -14.2991 C.3   66 GLU318   0.0044
1090 CD      -0.0962    23.2134   -15.1619 C.2   66 GLU318   0.0350
1091 OE1      0.6848    23.2141   -16.1513 O.co2 66 GLU318  -0.5690
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1092 OE2     -0.8272    24.1889   -14.8456 O.co2 66 GLU318  -0.5690
1093 H        1.6630    20.5460   -12.4160 H     66 GLU318   0.1883
1094 HA      -0.4612    19.3300   -13.7771 H     66 GLU318   0.0801
1095 HB3      0.2652    20.5690   -15.8696 H     66 GLU318   0.0330
1096 HB2      1.7186    21.1102   -14.9915 H     66 GLU318   0.0330
1097 HG3      0.1602    22.2585   -13.2898 H     66 GLU318   0.0433
1098 HG2     -1.2368    21.6918   -14.2417 H     66 GLU318   0.0433
1099 N        2.5386    18.3006   -14.7989 N.am  67 GLN319  -0.2636
BACKBONE
1100 CA       3.1348    17.2009   -15.5568 C.3   67 GLN319   0.1330
BACKBONE
1101 C        2.9199    15.8640   -14.8607 C.2   67 GLN319   0.2044
BACKBONE
1102 O        2.6575    14.8787   -15.5363 O.2   67 GLN319  -0.3944
BACKBONE
1103 CB       4.6278    17.4558   -15.8966 C.3   67 GLN319   0.0045
1104 CG       4.8387    18.7265   -16.7700 C.3   67 GLN319   0.0412
1105 CD       4.0705    18.6750   -18.0713 C.2   67 GLN319   0.1737
1106 OE1      3.8723    17.5984   -18.6222 O.2   67 GLN319  -0.3973
1107 NE2      3.6137    19.8215   -18.6093 N.am  67 GLN319  -0.3009
1108 H        3.1215    18.9809   -14.3345 H     67 GLN319   0.1883
1109 HA       2.6091    17.1366   -16.5159 H     67 GLN319   0.0801
1110 HB3      5.0187    16.6008   -16.4681 H     67 GLN319   0.0337
1111 HB2      5.1854    17.5265   -14.9506 H     67 GLN319   0.0337
1112 HG3      5.9030    18.8181   -17.0368 H     67 GLN319   0.0504
1113 HG2      4.5555    19.6229   -16.1988 H     67 GLN319   0.0504
1114 HE21     3.7899    20.7130   -18.1886 H     67 GLN319   0.1814
1115 HE22     3.1101    19.7837   -19.4690 H     67 GLN319   0.1814
1116 N        3.0080    15.7814   -13.5115 N.am  68 HIS320  -0.2587
BACKBONE
1117 CA       2.7431    14.4981   -12.8390 C.3   68 HIS320   0.1612
BACKBONE
1118 C        1.3749    14.0005   -13.2535 C.2   68 HIS320   0.2098
BACKBONE
1119 O        1.2411    12.8302   -13.5744 O.2   68 HIS320  -0.3939
BACKBONE
1120 CB       2.8136    14.6202   -11.2830 C.3   68 HIS320   0.1055
1121 CG       2.9694    13.3759   -10.4054 C.2   68 HIS320   0.1973
1122 ND1      3.3158    13.4872    -9.1336 N.pl3 68 HIS320  -0.1586
1123 CD2      2.8018    12.0773   -10.7234 C.2   68 HIS320   0.1263
1124 CE1      3.3666    12.3074    -8.5910 C.cat 68 HIS320   0.1842
1125 NE2      3.0905    11.4542    -9.4601 N.2   68 HIS320  -0.2010
1126 H        3.2253    16.6071   -12.9733 H     68 HIS320   0.1888
1127 HA       3.4643    13.7561   -13.2051 H     68 HIS320   0.0867
1128 HB3      1.9233    15.1667   -10.9335 H     68 HIS320   0.0803
1129 HB2      3.6785    15.2535   -11.0470 H     68 HIS320   0.0803
1130 HD1      3.5364    14.3564    -8.6189 H     68 HIS320   0.2700
1131 HD2      2.5300    11.5752   -11.6503 H     68 HIS320   0.1326
1132 HE1      3.6020    12.0213    -7.5732 H     68 HIS320   0.1885
1133 N        0.3527    14.8762   -13.2574 N.am  69 ALA321  -0.2636
BACKBONE
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1134 CA      -0.9650    14.4122   -13.6863 C.3   69 ALA321   0.1282
BACKBONE
1135 C       -1.0124    14.1911   -15.1820 C.2   69 ALA321   0.2036
BACKBONE
1136 O       -1.4733    13.1416   -15.5912 O.2   69 ALA321  -0.3944
BACKBONE
1137 CB      -2.0621    15.4335   -13.3160 C.3   69 ALA321  -0.0244
1138 H        0.4756    15.8508   -13.0174 H     69 ALA321   0.1883
1139 HA      -1.1888    13.4414   -13.2313 H     69 ALA321   0.0797
1140 HB3     -1.8931    16.3610   -13.8767 H     69 ALA321   0.0277
1141 HB2     -2.0261    15.6782   -12.2446 H     69 ALA321   0.0277
1142 HB1     -3.0641    15.0466   -13.5691 H     69 ALA321   0.0277
1143 N       -0.5512    15.1467   -16.0007 N.am  70 LYS322  -0.2637
BACKBONE
1144 CA      -0.6684    14.9713   -17.4494 C.3   70 LYS322   0.1310
BACKBONE
1145 C       -0.1298    13.6255   -17.8948 C.2   70 LYS322   0.2040
BACKBONE
1146 O       -0.7120    13.0281   -18.7858 O.2   70 LYS322  -0.3944
BACKBONE
1147 CB       0.1095    16.0885   -18.1828 C.3   70 LYS322  -0.0122
1148 CG       0.0344    15.9963   -19.7313 C.3   70 LYS322  -0.0440
1149 CD       0.6517    17.2768   -20.3604 C.3   70 LYS322  -0.0124
1150 CE       0.7404    17.2146   -21.9098 C.3   70 LYS322  -0.0354
1151 NZ       1.8600    16.3566   -22.3729 N.4   70 LYS322   0.2185
1152 H       -0.1582    15.9951   -15.6361 H     70 LYS322   0.1883
1153 HA      -1.7334    15.0224   -17.7256 H     70 LYS322   0.0800
1154 HB3      1.1669    16.0159   -17.8923 H     70 LYS322   0.0312
1155 HB2     -0.2824    17.0636   -17.8511 H     70 LYS322   0.0312
1156 HG3     -1.0161    15.9017   -20.0490 H     70 LYS322   0.0269
1157 HG2      0.5755    15.0961   -20.0576 H     70 LYS322   0.0269
1158 HD3      1.6565    17.4524   -19.9475 H     70 LYS322   0.0317
1159 HD2      0.0175    18.1328   -20.0737 H     70 LYS322   0.0317
1160 HE3      0.9010    18.2410   -22.2869 H     70 LYS322   0.0813
1161 HE2     -0.2260    16.8626   -22.3118 H     70 LYS322   0.0813
1162 HZ3      2.8150    16.6975   -21.9919 H     70 LYS322   0.1994
1163 HZ2      1.9454    16.3514   -23.4521 H     70 LYS322   0.1994
1164 HZ1      1.7476    15.3213   -22.0855 H     70 LYS322   0.1994
1165 N        0.9783    13.1366   -17.3007 N.am  71 TRP323  -0.2627
BACKBONE
1166 CA       1.5147    11.8390   -17.7209 C.3   71 TRP323   0.1352
BACKBONE
1167 C        1.0728    10.6702   -16.8649 C.2   71 TRP323   0.2053
BACKBONE
1168 O        1.0837     9.5697   -17.3920 O.2   71 TRP323  -0.3942
BACKBONE
1169 CB       3.0562    11.9217   -17.7496 C.3   71 TRP323   0.0042
1170 CG       3.4814    12.9087   -18.8062 C.2   71 TRP323  -0.0418
1171 CD1      4.0041    14.1344   -18.6235 C.2   71 TRP323   0.0167
1172 CD2      3.4063    12.6877   -20.2937 C.ar  71 TRP323  -0.0214
1173 NE1      4.2770    14.6696   -19.7808 N.pl3 71 TRP323  -0.2890
1174 CE2      3.9610    13.8467   -20.8014 C.ar  71 TRP323   0.0603
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1175 CE3	2.9481	11.6619	-21.1252	C.ar	71	TRP323	-0.0747
1176 CZ2	4.1370	14.0361	-22.1728	C.ar	71	TRP323	-0.0443
1177 CZ3	3.0999	11.8507	-22.5049	C.ar	71	TRP323	-0.0792
1178 CH2	3.6857	13.0162	-23.0204	C.ar	71	TRP323	-0.0768
1179 H	1.4425	13.6532	-16.5718	H	71	TRP323	0.1884
1180 HA	1.1908	11.5940	-18.7458	H	71	TRP323	0.0815
1181 HB3	3.4921	10.9409	-17.9989	H	71	TRP323	0.0397
1182 HB2	3.4200	12.2170	-16.7539	H	71	TRP323	0.0397
1183 HD1	4.1800	14.5924	-17.6495	H	71	TRP323	0.0795
1184 HE1	4.7401	15.5926	-19.9016	H	71	TRP323	0.2216
1185 HE3	2.5012	10.7616	-20.7185	H	71	TRP323	0.0540
1186 HZ2	4.6119	14.9307	-22.5621	H	71	TRP323	0.0541
1187 HZ3	2.7595	11.0750	-23.1862	H	71	TRP323	0.0510
1188 HH2	3.7975	13.1285	-24.0959	H	71	TRP323	0.0530
1189 N	0.7005	10.8226	-15.5749	N.am	72	TYR324	-0.2620
BACKBONE							
1190 CA	0.3172	9.6473	-14.7819	C.3	72	TYR324	0.1392
BACKBONE							
1191 C	-0.9878	9.9029	-14.0534	C.2	72	TYR324	0.2082
BACKBONE							
1192 O	-0.9992	9.8866	-12.8311	O.2	72	TYR324	-0.3940
BACKBONE							
1193 CB	1.4792	9.2916	-13.8222	C.3	72	TYR324	0.0164
1194 CG	2.7905	9.1399	-14.6114	C.ar	72	TYR324	-0.0493
1195 CD1	3.7261	10.1752	-14.6377	C.ar	72	TYR324	-0.0685
1196 CD2	3.0656	7.9598	-15.3171	C.ar	72	TYR324	-0.0685
1197 CE1	4.9446	10.0105	-15.3106	C.ar	72	TYR324	-0.0398
1198 CE2	4.2725	7.8041	-16.0007	C.ar	72	TYR324	-0.0398
1199 CZ	5.2365	8.8232	-15.9811	C.ar	72	TYR324	0.0805
1200 OH	6.4666	8.6249	-16.6203	O.3	72	TYR324	-0.3376
1201 H	0.6987	11.7185	-15.1162	H	72	TYR324	0.1885
1202 HA	0.1658	8.7414	-15.3872	H	72	TYR324	0.0821
1203 HB2	1.2686	8.3608	-13.2693	H	72	TYR324	0.0453
1204 HB3	1.5670	10.0959	-13.0839	H	72	TYR324	0.0453
1205 HD1	3.5192	11.1154	-14.1369	H	72	TYR324	0.0530
1206 HD2	2.3339	7.1579	-15.3335	H	72	TYR324	0.0530
1207 HE1	5.6603	10.8191	-15.2970	H	72	TYR324	0.0525
1208 HE2	4.4761	6.8916	-16.5507	H	72	TYR324	0.0525
1209 HH	7.0711	9.3630	-16.5504	H	72	TYR324	0.2458
1210 N	-2.1372	10.1330	-14.7367	N.am	73	PRO325	-0.2497
BACKBONE							
1211 CA	-3.3458	10.4883	-14.0009	C.3	73	PRO325	0.1338
BACKBONE							
1212 C	-3.7888	9.4199	-13.0268	C.2	73	PRO325	0.2039
BACKBONE							
1213 O	-4.5391	9.7377	-12.1194	O.2	73	PRO325	-0.3944
BACKBONE							
1214 CB	-4.3507	10.6612	-15.1668	C.3	73	PRO325	-0.0104
1215 CG	-3.7523	9.8254	-16.3212	C.3	73	PRO325	-0.0281
1216 CD	-2.2275	10.0521	-16.1926	C.3	73	PRO325	0.0369
1217 HA	-3.2052	11.4310	-13.4469	H	73	PRO325	0.0802
1218 HB3	-4.3732	11.7132	-15.4849	H	73	PRO325	0.0313

1219	HB2	-5.3756	10.3537	-14.9044	H	73 PRO325	0.0313
1220	HG2	-3.9773	8.7614	-16.1379	H	73 PRO325	0.0287
1221	HG3	-4.1508	10.1114	-17.3090	H	73 PRO325	0.0287
1222	HD2	-1.6854	9.2211	-16.6690	H	73 PRO325	0.0524
1223	HD3	-1.9318	11.0013	-16.6631	H	73 PRO325	0.0524
1224	N	-3.3570	8.1468	-13.1507	N.am	74 GLY326	-0.2664
BACKBONE							
1225	CA	-3.7228	7.1670	-12.1287	C.3	74 GLY326	0.1201
BACKBONE							
1226	C	-2.8826	7.2439	-10.8697	C.2	74 GLY326	0.2008
BACKBONE							
1227	O	-3.1631	6.4449	-9.9834	O.2	74 GLY326	-0.3947
BACKBONE							
1228	H	-2.7443	7.8721	-13.8930	H	74 GLY326	0.1881
1229	HA2	-3.6123	6.1496	-12.5339	H	74 GLY326	0.0763
1230	HA3	-4.7792	7.2906	-11.8429	H	74 GLY326	0.0763
1231	N	-1.8736	8.1513	-10.7700	N.am	75 CYS327	-0.2631
BACKBONE							
1232	CA	-1.0232	8.1916	-9.5745	C.3	75 CYS327	0.1406
BACKBONE							
1233	C	-1.8689	8.4546	-8.3423	C.2	75 CYS327	0.2047
BACKBONE							
1234	O	-2.6857	9.3630	-8.3643	O.2	75 CYS327	-0.3944
BACKBONE							
1235	CB	0.1566	9.2051	-9.6995	C.3	75 CYS327	0.0443
1236	SG	1.2255	9.1885	-8.2138	S.3	75 CYS327	-0.0882
1237	H	-1.6730	8.8137	-11.5010	H	75 CYS327	0.1884
1238	HA	-0.5796	7.1905	-9.4804	H	75 CYS327	0.0808
1239	HB3	-0.2127	10.2283	-9.8427	H	75 CYS327	0.0432
1240	HB2	0.7710	8.9602	-10.5771	H	75 CYS327	0.0432
1241	LPG2	1.0539	9.6801	-7.7781	LP	75 CYS327	0.0000
1242	LPG1	1.2033	8.5879	-7.8978	LP	75 CYS327	0.0000
1243	N	-1.7285	7.6704	-7.2457	N.am	76 LYS328	-0.2637
BACKBONE							
1244	CA	-2.6026	7.8786	-6.0894	C.3	76 LYS328	0.1310
BACKBONE							
1245	C	-2.0831	8.9905	-5.2131	C.2	76 LYS328	0.2040
BACKBONE							
1246	O	-2.8871	9.8115	-4.8083	O.2	76 LYS328	-0.3944
BACKBONE							
1247	CB	-2.9090	6.5667	-5.3189	C.3	76 LYS328	-0.0122
1248	CG	-3.6481	5.5327	-6.2223	C.3	76 LYS328	-0.0440
1249	CD	-5.0746	5.9880	-6.6627	C.3	76 LYS328	-0.0124
1250	CE	-5.8463	4.9061	-7.4669	C.3	76 LYS328	-0.0354
1251	NZ	-5.2066	4.6537	-8.7812	N.4	76 LYS328	0.2185
1252	H	-1.0332	6.9516	-7.1918	H	76 LYS328	0.1883
1253	HA	-3.5674	8.2631	-6.4325	H	76 LYS328	0.0800
1254	HB3	-3.5349	6.7970	-4.4404	H	76 LYS328	0.0312
1255	HB2	-1.9613	6.1408	-4.9487	H	76 LYS328	0.0312
1256	HG3	-3.7537	4.5906	-5.6610	H	76 LYS328	0.0269
1257	HG2	-3.0106	5.3329	-7.0967	H	76 LYS328	0.0269
1258	HD3	-5.0393	6.8729	-7.3151	H	76 LYS328	0.0317

1259	HD2	-5.6546	6.2480	-5.7616	H	76 LYS328	0.0317
1260	HE3	-6.8828	5.2582	-7.6247	H	76 LYS328	0.0813
1261	HE2	-5.8991	3.9737	-6.8771	H	76 LYS328	0.0813
1262	HZ3	-5.0004	5.5372	-9.3750	H	76 LYS328	0.1994
1263	HZ2	-5.7660	3.9439	-9.3751	H	76 LYS328	0.1994
1264	HZ1	-4.2520	4.1828	-8.6482	H	76 LYS328	0.1994
1265	N	-0.7722	9.0968	-4.9233	N.am	77 TYR329	-0.2621
BACKBONE							
1266	CA	-0.2959	10.2761	-4.1885	C.3	77 TYR329	0.1390
BACKBONE							
1267	C	-0.8899	11.5448	-4.7753	C.2	77 TYR329	0.2057
BACKBONE							
1268	O	-1.3552	12.4224	-4.0629	O.2	77 TYR329	-0.3942
BACKBONE							
1269	CB	1.2456	10.3590	-4.3173	C.3	77 TYR329	0.0163
1270	CG	1.8245	11.6180	-3.6590	C.ar	77 TYR329	-0.0493
1271	CD1	1.8930	11.6893	-2.2656	C.ar	77 TYR329	-0.0685
1272	CD2	2.2997	12.6857	-4.4305	C.ar	77 TYR329	-0.0685
1273	CE1	2.5785	12.7421	-1.6523	C.ar	77 TYR329	-0.0398
1274	CE2	2.9806	13.7379	-3.8151	C.ar	77 TYR329	-0.0398
1275	CZ	3.1670	13.7410	-2.4289	C.ar	77 TYR329	0.0805
1276	OH	3.9397	14.7320	-1.8280	O.3	77 TYR329	-0.3376
1277	H	-0.1307	8.3870	-5.2188	H	77 TYR329	0.1885
1278	HA	-0.5978	10.1842	-3.1314	H	77 TYR329	0.0821
1279	HB2	1.5521	10.3129	-5.3750	H	77 TYR329	0.0453
1280	HB3	1.6752	9.4909	-3.8023	H	77 TYR329	0.0453
1281	HD1	1.4224	10.9243	-1.6544	H	77 TYR329	0.0530
1282	HD2	2.1453	12.6980	-5.5055	H	77 TYR329	0.0530
1283	HE1	2.6548	12.7813	-0.5699	H	77 TYR329	0.0525
1284	HE2	3.3635	14.5594	-4.4092	H	77 TYR329	0.0525
1285	HH	3.3806	15.2522	-1.2516	H	77 TYR329	0.2458
1286	N	-0.8863	11.6406	-6.1195	N.am	78 LEU330	-0.2636
BACKBONE							
1287	CA	-1.5454	12.7637	-6.7873	C.3	78 LEU330	0.1312
BACKBONE							
1288	C	-3.0181	12.8218	-6.4396	C.2	78 LEU330	0.2039
BACKBONE							
1289	O	-3.5013	13.8776	-6.0575	O.2	78 LEU330	-0.3944
BACKBONE							
1290	CB	-1.3617	12.5687	-8.3161	C.3	78 LEU330	-0.0101
1291	CG	-2.2194	13.4681	-9.2448	C.3	78 LEU330	-0.0425
1292	CD1	-1.7453	14.9428	-9.2007	C.3	78 LEU330	-0.0625
1293	CD2	-2.1179	12.8905	-10.6803	C.3	78 LEU330	-0.0625
1294	H	-0.4647	10.9131	-6.6657	H	78 LEU330	0.1883
1295	HA	-1.0798	13.7024	-6.4593	H	78 LEU330	0.0800
1296	HB3	-1.6726	11.5412	-8.5340	H	78 LEU330	0.0315
1297	HB2	-0.2920	12.6634	-8.5668	H	78 LEU330	0.0315
1298	HG	-3.2795	13.4218	-8.9480	H	78 LEU330	0.0298
1299	HD13	-1.7522	15.3083	-8.1654	H	78 LEU330	0.0232
1300	HD12	-2.4189	15.5775	-9.7941	H	78 LEU330	0.0232
1301	HD11	-0.7264	15.0321	-9.6071	H	78 LEU330	0.0232
1302	HD23	-1.0601	12.8456	-10.9809	H	78 LEU330	0.0232

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1303 HD22    -2.6736    13.5146   -11.3862 H     78 LEU330   0.0232
1304 HD21    -2.5418    11.8746   -10.7286 H     78 LEU330   0.0232
1305 N       -3.7564    11.6993    -6.5758 N.am  79 LEU331  -0.2637
BACKBONE
1306 CA      -5.1802    11.7141    -6.2290 C.3   79 LEU331   0.1312
BACKBONE
1307 C       -5.3537    12.1335    -4.7844 C.2   79 LEU331   0.2039
BACKBONE
1308 O       -6.2310    12.9277    -4.4853 O.2   79 LEU331  -0.3944
BACKBONE
1309 CB      -5.7924    10.2941    -6.4171 C.3   79 LEU331  -0.0101
1310 CG      -7.3384    10.1965    -6.2540 C.3   79 LEU331  -0.0425
1311 CD1     -8.0845    10.8932    -7.4234 C.3   79 LEU331  -0.0625
1312 CD2     -7.7672     8.7019    -6.1919 C.3   79 LEU331  -0.0625
1313 H       -3.3287    10.8430    -6.8816 H     79 LEU331   0.1883
1314 HA      -5.6826    12.4505    -6.8721 H     79 LEU331   0.0800
1315 HB3     -5.3366     9.6404    -5.6586 H     79 LEU331   0.0315
1316 HB2     -5.5161     9.9107    -7.4129 H     79 LEU331   0.0315
1317 HG      -7.6374    10.6757    -5.3052 H     79 LEU331   0.0298
1318 HD13    -7.8942    11.9746    -7.4242 H     79 LEU331   0.0232
1319 HD12    -9.1680    10.7399    -7.3178 H     79 LEU331   0.0232
1320 HD11    -7.7678    10.4712    -8.3894 H     79 LEU331   0.0232
1321 HD23    -7.4601     8.1743    -7.1083 H     79 LEU331   0.0232
1322 HD22    -8.8601     8.6144    -6.0888 H     79 LEU331   0.0232
1323 HD21    -7.3058     8.2031    -5.3254 H     79 LEU331   0.0232
1324 N       -4.5160    11.5994    -3.8738 N.am  80 GLU332  -0.2636
BACKBONE
1325 CA      -4.6449    11.9038    -2.4515 C.3   80 GLU332   0.1325
BACKBONE
1326 C       -4.3208    13.3601    -2.2024 C.2   80 GLU332   0.2040
BACKBONE
1327 O       -5.0447    14.0034    -1.4592 O.2   80 GLU332  -0.3944
BACKBONE
1328 CB      -3.6782    11.0084    -1.6234 C.3   80 GLU332  -0.0008
1329 CG      -4.0764     9.5054    -1.6892 C.3   80 GLU332   0.0044
1330 CD      -2.9542     8.5809    -1.3013 C.2   80 GLU332   0.0350
1331 OE1     -1.8900     9.0673    -0.8324 O.co2 80 GLU332  -0.5690
1332 OE2     -3.1390     7.3473    -1.4791 O.co2 80 GLU332  -0.5690
1333 H       -3.7672    11.0063    -4.1712 H     80 GLU332   0.1883
1334 HA      -5.6792    11.7083    -2.1244 H     80 GLU332   0.0801
1335 HB3     -3.6638    11.3255    -0.5674 H     80 GLU332   0.0330
1336 HB2     -2.6619    11.1450    -2.0245 H     80 GLU332   0.0330
1337 HG3     -4.3723     9.2156    -2.7075 H     80 GLU332   0.0433
1338 HG2     -4.9320     9.3133    -1.0233 H     80 GLU332   0.0433
1339 N       -3.2356    13.9112    -2.7918 N.am  81 GLN333  -0.2636
BACKBONE
1340 CA      -2.8899    15.3056    -2.5025 C.3   81 GLN333   0.1330
BACKBONE
1341 C       -3.7177    16.2928    -3.3001 C.2   81 GLN333   0.2040
BACKBONE
1342 O       -4.1443    17.2841    -2.7292 O.2   81 GLN333  -0.3944
BACKBONE
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1343 CB      -1.3880    15.5881    -2.7831 C.3   81 GLN333   0.0045
1344 CG      -1.0056    17.0694    -2.4871 C.3   81 GLN333   0.0412
1345 CD      -1.2075    17.4804    -1.0523 C.2   81 GLN333   0.1737
1346 OE1     -1.2044    16.6280    -0.1794 O.2   81 GLN333  -0.3973
1347 NE2     -1.3660    18.7823    -0.7504 N.am  81 GLN333  -0.3009
1348 H       -2.6598    13.3725    -3.4186 H     81 GLN333   0.1883
1349 HA      -3.0702    15.4997    -1.4312 H     81 GLN333   0.0801
1350 HB3     -1.1753    15.3664    -3.8426 H     81 GLN333   0.0337
1351 HB2     -0.7729    14.9136    -2.1653 H     81 GLN333   0.0337
1352 HG3     -1.5560    17.7456    -3.1597 H     81 GLN333   0.0504
1353 HG2      0.0648    17.2212    -2.6723 H     81 GLN333   0.0504
1354 HE21    -1.3705    19.4929    -1.4530 H     81 GLN333   0.1814
1355 HE22    -1.4939    19.0371     0.2093 H     81 GLN333   0.1814
1356 N       -3.9343    16.0934    -4.6194 N.am  82 LYS334  -0.2637
BACKBONE
1357 CA      -4.6623    17.0935    -5.4098 C.3   82 LYS334   0.1310
BACKBONE
1358 C       -6.1195    16.7397    -5.6261 C.2   82 LYS334   0.2037
BACKBONE
1359 O       -6.8648    17.6406    -5.9801 O.2   82 LYS334  -0.3944
BACKBONE
1360 CB      -3.9810    17.3052    -6.7894 C.3   82 LYS334  -0.0122
1361 CG      -2.4914    17.7514    -6.6949 C.3   82 LYS334  -0.0440
1362 CD      -2.2419    19.1979    -6.1709 C.3   82 LYS334  -0.0124
1363 CE      -2.7117    20.2973    -7.1696 C.3   82 LYS334  -0.0354
1364 NZ      -2.2539    21.6542    -6.7778 N.4   82 LYS334   0.2185
1365 H       -3.6122    15.2569    -5.0752 H     82 LYS334   0.1883
1366 HA      -4.6744    18.0725    -4.9047 H     82 LYS334   0.0800
1367 HB3     -4.5516    18.0449    -7.3679 H     82 LYS334   0.0312
1368 HB2     -4.0385    16.3475    -7.3325 H     82 LYS334   0.0312
1369 HG3     -2.0474    17.6871    -7.7016 H     82 LYS334   0.0269
1370 HG2     -1.9564    17.0382    -6.0463 H     82 LYS334   0.0269
1371 HD3     -1.1545    19.3169    -6.0306 H     82 LYS334   0.0317
1372 HD2     -2.7119    19.3409    -5.1861 H     82 LYS334   0.0317
1373 HE3     -3.8127    20.2898    -7.2489 H     82 LYS334   0.0813
1374 HE2     -2.3004    20.0631    -8.1656 H     82 LYS334   0.0813
1375 HZ3     -2.6274    21.9421    -5.8038 H     82 LYS334   0.1994
1376 HZ2     -2.5878    22.4167    -7.4719 H     82 LYS334   0.1994
1377 HZ1     -1.1741    21.7338    -6.7409 H     82 LYS334   0.1994
1378 N       -6.5781    15.4811    -5.4381 N.am  83 GLY335  -0.2664
BACKBONE
1379 CA      -7.9936    15.1866    -5.6658 C.3   83 GLY335   0.1201
BACKBONE
1380 C       -8.2880    14.8961    -7.1201 C.2   83 GLY335   0.2007
BACKBONE
1381 O       -7.4766    15.1840    -7.9843 O.2   83 GLY335  -0.3947
BACKBONE
1382 H       -5.9809    14.7192    -5.1667 H     83 GLY335   0.1881
1383 HA2     -8.6309    16.0263    -5.3476 H     83 GLY335   0.0763
1384 HA3     -8.2909    14.3074    -5.0715 H     83 GLY335   0.0763
1385 N       -9.4672    14.3125    -7.4302 N.am  84 GLN336  -0.2638
BACKBONE
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1386 CA -9.7576 13.9618 -8.8217 C.3 84 GLN336 0.1330
BACKBONE
1387 C -10.0347 15.1890 -9.6638 C.2 84 GLN336 0.2040
BACKBONE
1388 O -9.5605 15.2524 -10.7874 O.2 84 GLN336 -0.3944
BACKBONE
1389 CB -10.9892 13.0183 -8.9116 C.3 84 GLN336 0.0045
1390 CG -11.1321 12.4068 -10.3297 C.3 84 GLN336 0.0412
1391 CD -12.4150 11.6299 -10.4800 C.2 84 GLN336 0.1737
1392 OE1 -12.9507 11.1620 -9.4872 O.2 84 GLN336 -0.3973
1393 NE2 -12.9450 11.4624 -11.7059 N.am 84 GLN336 -0.3009
1394 H -10.1445 14.1086 -6.7208 H 84 GLN336 0.1883
1395 HA -8.8846 13.4408 -9.2464 H 84 GLN336 0.0801
1396 HB3 -11.9016 13.5844 -8.6606 H 84 GLN336 0.0337
1397 HB2 -10.8899 12.2001 -8.1822 H 84 GLN336 0.0337
1398 HG3 -10.2917 11.7258 -10.5357 H 84 GLN336 0.0504
1399 HG2 -11.1155 13.2151 -11.0703 H 84 GLN336 0.0504
1400 HE21 -12.5102 11.8432 -12.5260 H 84 GLN336 0.1814
1401 HE22 -13.7973 10.9459 -11.7902 H 84 GLN336 0.1814
1402 N -10.8128 16.1711 -9.1596 N.am 85 GLU337 -0.2636
BACKBONE
1403 CA -11.1679 17.3318 -9.9865 C.3 85 GLU337 0.1325
BACKBONE
1404 C -9.9331 17.9028 -10.6576 C.2 85 GLU337 0.2041
BACKBONE
1405 O -9.9055 18.0369 -11.8726 O.2 85 GLU337 -0.3944
BACKBONE
1406 CB -11.9663 18.3497 -9.1199 C.3 85 GLU337 -0.0008
1407 CG -12.3895 19.6247 -9.8950 C.3 85 GLU337 0.0044
1408 CD -11.2199 20.5430 -10.1277 C.2 85 GLU337 0.0350
1409 OE1 -10.3898 20.7031 -9.1921 O.co2 85 GLU337 -0.5690
1410 OE2 -11.1236 21.1125 -11.2456 O.co2 85 GLU337 -0.5690
1411 H -11.1721 16.1007 -8.2276 H 85 GLU337 0.1883
1412 HA -11.8331 16.9835 -10.7912 H 85 GLU337 0.0801
1413 HB3 -11.3792 18.6337 -8.2313 H 85 GLU337 0.0330
1414 HB2 -12.8815 17.8447 -8.7648 H 85 GLU337 0.0330
1415 HG3 -13.1268 20.1896 -9.3017 H 85 GLU337 0.0433
1416 HG2 -12.8603 19.3442 -10.8508 H 85 GLU337 0.0433
1417 N -8.8740 18.2004 -9.8778 N.am 86 TYR338 -0.2621
BACKBONE
1418 CA -7.6208 18.6698 -10.4758 C.3 86 TYR338 0.1390
BACKBONE
1419 C -7.1635 17.7936 -11.6304 C.2 86 TYR338 0.2057
BACKBONE
1420 O -6.6637 18.2995 -12.6245 O.2 86 TYR338 -0.3942
BACKBONE
1421 CB -6.5108 18.6309 -9.3904 C.3 86 TYR338 0.0163
1422 CG -5.1626 19.1376 -9.9251 C.ar 86 TYR338 -0.0493
1423 CD1 -4.9311 20.5132 -10.0346 C.ar 86 TYR338 -0.0685
1424 CD2 -4.1559 18.2409 -10.2971 C.ar 86 TYR338 -0.0685
1425 CE1 -3.6981 20.9904 -10.4849 C.ar 86 TYR338 -0.0398
1426 CE2 -2.9098 18.7177 -10.7171 C.ar 86 TYR338 -0.0398

1427 CZ	-2.6784	20.0907	-10.8212	C.ar	86	TYR338	0.0805
1428 OH	-1.4335	20.5415	-11.2611	O.3	86	TYR338	-0.3376
1429 H	-8.9524	18.1176	-8.8828	H	86	TYR338	0.1885
1430 HA	-7.7651	19.7018	-10.8362	H	86	TYR338	0.0821
1431 HB2	-6.4141	17.5975	-9.0199	H	86	TYR338	0.0453
1432 HB3	-6.8046	19.2622	-8.5366	H	86	TYR338	0.0453
1433 HD1	-5.7126	21.2191	-9.7699	H	86	TYR338	0.0530
1434 HD2	-4.3384	17.1717	-10.2641	H	86	TYR338	0.0530
1435 HE1	-3.5373	22.0596	-10.5712	H	86	TYR338	0.0525
1436 HE2	-2.1155	18.0240	-10.9722	H	86	TYR338	0.0525
1437 HH	-1.4061	21.4634	-11.4941	H	86	TYR338	0.2458
1438 N	-7.3173	16.4555	-11.5216	N.am	87	ILE339	-0.2633
BACKBONE							
1439 CA	-6.8804	15.5680	-12.6027	C.3	87	ILE339	0.1335
BACKBONE							
1440 C	-7.8479	15.7225	-13.7567	C.2	87	ILE339	0.2043
BACKBONE							
1441 O	-7.4173	15.8551	-14.8954	O.2	87	ILE339	-0.3944
BACKBONE							
1442 CB	-6.8172	14.0703	-12.1606	C.3	87	ILE339	-0.0037
1443 CG1	-5.8985	13.8951	-10.9119	C.3	87	ILE339	-0.0491
1444 CG2	-6.3434	13.1748	-13.3430	C.3	87	ILE339	-0.0582
1445 CD1	-5.9286	12.4597	-10.3229	C.3	87	ILE339	-0.0648
1446 H	-7.8171	16.0700	-10.7422	H	87	ILE339	0.1883
1447 HA	-5.8751	15.8740	-12.9371	H	87	ILE339	0.0803
1448 HB	-7.8341	13.7444	-11.8839	H	87	ILE339	0.0345
1449 HG13	-6.2191	14.5709	-10.1071	H	87	ILE339	0.0267
1450 HG12	-4.8685	14.1722	-11.1714	H	87	ILE339	0.0267
1451 HG23	-6.9994	13.2974	-14.2183	H	87	ILE339	0.0235
1452 HG22	-6.3681	12.1096	-13.0715	H	87	ILE339	0.0235
1453 HG21	-5.3162	13.4430	-13.6334	H	87	ILE339	0.0235
1454 HD13	-6.9659	12.1172	-10.1963	H	87	ILE339	0.0230
1455 HD12	-5.4378	12.4376	-9.3401	H	87	ILE339	0.0230
1456 HD11	-5.3961	11.7550	-10.9731	H	87	ILE339	0.0230
1457 N	-9.1699	15.7017	-13.4665	N.am	88	ASN340	-0.2616
BACKBONE							
1458 CA	-10.1504	15.8930	-14.5324	C.3	88	ASN340	0.1476
BACKBONE							
1459 C	-9.8378	17.1764	-15.2685	C.2	88	ASN340	0.2064
BACKBONE							
1460 O	-9.8049	17.1757	-16.4889	O.2	88	ASN340	-0.3942
BACKBONE							
1461 CB	-11.6052	16.0458	-14.0076	C.3	88	ASN340	0.0773
1462 CG	-12.1131	14.8412	-13.2565	C.2	88	ASN340	0.1780
1463 OD1	-11.5710	13.7570	-13.4060	O.2	88	ASN340	-0.3970
1464 ND2	-13.1748	14.9836	-12.4377	N.am	88	ASN340	-0.3007
1465 H	-9.4977	15.5758	-12.5231	H	88	ASN340	0.1885
1466 HA	-10.0931	15.0443	-15.2340	H	88	ASN340	0.0826
1467 HB3	-12.2824	16.2089	-14.8606	H	88	ASN340	0.0551
1468 HB2	-11.6696	16.9237	-13.3487	H	88	ASN340	0.0551
1469 HD21	-13.6420	15.8616	-12.3282	H	88	ASN340	0.1814
1470 HD22	-13.5132	14.1882	-11.9352	H	88	ASN340	0.1814

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1471 N       -9.6104    18.2913   -14.5377 N.am  89 ASN341  -0.2615
BACKBONE
1472 CA      -9.3663    19.5602   -15.2232 C.3   89 ASN341   0.1476
BACKBONE
1473 C       -8.2174    19.4163   -16.1988 C.2   89 ASN341   0.2063
BACKBONE
1474 O       -8.2918    19.9078   -17.3139 O.2   89 ASN341  -0.3942
BACKBONE
1475 CB      -9.0517    20.6919   -14.2104 C.3   89 ASN341   0.0773
1476 CG      -8.8867    21.9933   -14.9550 C.2   89 ASN341   0.1780
1477 OD1     -9.8512    22.4401   -15.5574 O.2   89 ASN341  -0.3970
1478 ND2     -7.7056    22.6404   -14.9618 N.am  89 ASN341  -0.3007
1479 H       -9.6137    18.2660   -13.5282 H     89 ASN341   0.1885
1480 HA     -10.2776    19.8335   -15.7792 H     89 ASN341   0.0826
1481 HB3     -8.1531    20.4360   -13.6271 H     89 ASN341   0.0551
1482 HB2     -9.8939    20.8047   -13.5094 H     89 ASN341   0.0551
1483 HD21    -6.9020    22.2939   -14.4784 H     89 ASN341   0.1814
1484 HD22    -7.6425    23.4978   -15.4729 H     89 ASN341   0.1814
1485 N       -7.1230    18.7361   -15.8017 N.am  90 ILE342  -0.2633
BACKBONE
1486 CA      -5.9867    18.6043   -16.7196 C.3   90 ILE342   0.1335
BACKBONE
1487 C       -6.3185    17.7337   -17.9100 C.2   90 ILE342   0.2043
BACKBONE
1488 O       -5.7729    17.9861   -18.9733 O.2   90 ILE342  -0.3944
BACKBONE
1489 CB      -4.7259    18.1122   -15.9484 C.3   90 ILE342  -0.0037
1490 CG1     -4.2774    19.3016   -15.0459 C.3   90 ILE342  -0.0491
1491 CG2     -3.5989    17.6213   -16.9077 C.3   90 ILE342  -0.0582
1492 CD1     -3.2476    18.8794   -13.9844 C.3   90 ILE342  -0.0648
1493 H       -7.0949    18.2988   -14.8955 H     90 ILE342   0.1883
1494 HA      -5.7590    19.5975   -17.1474 H     90 ILE342   0.0803
1495 HB      -5.0113    17.2510   -15.3185 H     90 ILE342   0.0345
1496 HG13    -5.1397    19.7255   -14.5034 H     90 ILE342   0.0267
1497 HG12    -3.8392    20.1009   -15.6688 H     90 ILE342   0.0267
1498 HG23    -3.9566    16.7945   -17.5390 H     90 ILE342   0.0235
1499 HG22    -2.7361    17.2320   -16.3523 H     90 ILE342   0.0235
1500 HG21    -3.2604    18.4422   -17.5579 H     90 ILE342   0.0235
1501 HD13    -3.6618    18.1059   -13.3197 H     90 ILE342   0.0230
1502 HD12    -2.9518    19.7561   -13.3934 H     90 ILE342   0.0230
1503 HD11    -2.3693    18.4950   -14.5046 H     90 ILE342   0.0230
1504 N       -7.2009    16.7185   -17.7912 N.am  91 HIS343  -0.2619
BACKBONE
1505 CA      -7.5644    15.9257   -18.9694 C.3   91 HIS343   0.1421
BACKBONE
1506 C       -8.8785    16.4347   -19.5152 C.2   91 HIS343   0.2060
BACKBONE
1507 O       -9.6445    15.6528   -20.0491 O.2   91 HIS343  -0.3942
BACKBONE
1508 CB      -7.5907    14.4127   -18.6130 C.3   91 HIS343   0.0427
1509 CG      -6.2026    13.9732   -18.2194 C.2   91 HIS343   0.0561
1510 ND1     -5.6043    14.3354   -17.1160 N.pl3 91 HIS343  -0.2623
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1511 CD2     -5.3976    13.1616   -18.9393 C.2   91 HIS343  -0.0276
1512 CE1     -4.4231    13.8195   -17.0796 C.2   91 HIS343   0.0875
1513 NE2     -4.2251    13.1106   -18.1036 N.2   91 HIS343  -0.3437
1514 H       -7.6936    16.5636   -16.9255 H     91 HIS343   0.1885
1515 HA      -6.8387    16.0300   -19.7909 H     91 HIS343   0.0824
1516 HB3     -7.9405    13.8364   -19.4964 H     91 HIS343   0.0491
1517 HB2     -8.3117    14.2411   -17.7889 H     91 HIS343   0.0491
1518 HD1     -5.9991    14.9284   -16.3732 H     91 HIS343   0.2386
1519 HD2     -5.6007    12.6838   -19.9061 H     91 HIS343   0.0324
1520 HE1     -3.7034    13.9718   -16.2754 H     91 HIS343   0.1149
1521 N       -9.1736    17.7475   -19.4055 N.am  92 LEU344  -0.2636
BACKBONE
1522 CA     -10.4586    18.2511   -19.8963 C.3   92 LEU344   0.1312
BACKBONE
1523 C      -10.4716    18.3435   -21.4063 C.2   92 LEU344   0.2040
BACKBONE
1524 O      -11.5068    18.0870   -21.9997 O.2   92 LEU344  -0.3944
BACKBONE
1525 CB     -10.7489    19.6215   -19.2152 C.3   92 LEU344  -0.0101
1526 CG     -12.1147    20.2752   -19.5852 C.3   92 LEU344  -0.0425
1527 CD1    -12.6339    21.1258   -18.3913 C.3   92 LEU344  -0.0625
1528 CD2    -12.0022    21.1832   -20.8430 C.3   92 LEU344  -0.0625
1529 H       -8.5378    18.3939   -18.9767 H     92 LEU344   0.1883
1530 HA     -11.2546    17.5450   -19.5969 H     92 LEU344   0.0800
1531 HB3     -9.9341    20.3332   -19.4240 H     92 LEU344   0.0315
1532 HB2    -10.7371    19.4065   -18.1358 H     92 LEU344   0.0315
1533 HG     -12.8547    19.4791   -19.7787 H     92 LEU344   0.0298
1534 HD13   -12.8048    20.4928   -17.5069 H     92 LEU344   0.0232
1535 HD12   -13.5869    21.6102   -18.6491 H     92 LEU344   0.0232
1536 HD11   -11.9033    21.9046   -18.1249 H     92 LEU344   0.0232
1537 HD23   -11.3151    22.0210   -20.6513 H     92 LEU344   0.0232
1538 HD22   -12.9895    21.5973   -21.0962 H     92 LEU344   0.0232
1539 HD21   -11.6344    20.6341   -21.7187 H     92 LEU344   0.0232
1540 N       -9.3523    18.7080   -22.0688 N.am  93 THR345  -0.2613
BACKBONE
1541 CA      -9.3884    18.8729   -23.5263 C.3   93 THR345   0.1564
BACKBONE
1542 C       -9.4040    17.5635   -24.2907 C.2   93 THR345   0.2044
BACKBONE
1543 O       -9.5365    17.6338   -25.5021 O.2   93 THR345  -0.3944
BACKBONE
1544 CB      -8.2015    19.7804   -23.9655 C.3   93 THR345   0.0924
1545 OG1     -8.1730    20.8949   -23.0513 O.3   93 THR345  -0.3874
1546 CG2     -8.3267    20.3223   -25.4172 C.3   93 THR345  -0.0346
1547 H       -8.5003    18.9025   -21.5789 H     93 THR345   0.1884
1548 HA     -10.3135    19.4086   -23.7913 H     93 THR345   0.0826
1549 HB      -7.2671    19.1986   -23.8722 H     93 THR345   0.0639
1550 HG1     -7.4421    21.4873   -23.1965 H     93 THR345   0.2101
1551 HG22    -7.5320    21.0586   -25.6156 H     93 THR345   0.0257
1552 HG21    -9.3000    20.8186   -25.5589 H     93 THR345   0.0257
1553 HG23    -8.2211    19.5181   -26.1595 H     93 THR345   0.0257
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1554 N       -9.2815    16.3674   -23.6651 N.am  94 HIS346  -0.2881
BACKBONE
1555 CA      -9.2849    15.1234   -24.4394 C.3   94 HIS346   0.0164
BACKBONE
1556 C       -9.9333    14.0078   -23.6656 C.2   94 HIS346  -0.1856
BACKBONE
1557 O       -9.8916    12.8616   -24.0849 O.2   94 HIS346  -0.7200
BACKBONE
1558 CB      -7.8341    14.7541   -24.8449 C.3   94 HIS346   0.0174
1559 CG      -6.8790    14.7660   -23.6745 C.2   94 HIS346   0.0535
1560 ND1     -5.7104    15.3700   -23.6979 N.pl3 94 HIS346  -0.2624
1561 CD2     -7.0565    14.1789   -22.4726 C.2   94 HIS346  -0.0277
1562 CE1     -5.1083    15.2153   -22.5600 C.2   94 HIS346   0.0875
1563 NE2     -5.8346    14.5325   -21.8005 N.2   94 HIS346  -0.3437
1564 H       -9.1721    16.2842   -22.6730 H     94 HIS346   0.1855
1565 HA      -9.9087    15.2212   -25.3453 H     94 HIS346   0.0497
1566 HB3     -7.5119    15.4965   -25.5920 H     94 HIS346   0.0464
1567 HB2     -7.8118    13.7609   -25.3242 H     94 HIS346   0.0464
1568 HD1     -5.3265    15.8905   -24.4956 H     94 HIS346   0.2386
1569 HD2     -7.8907    13.5890   -22.0961 H     94 HIS346   0.0324
1570 HE1     -4.1224    15.6092   -22.2961 H     94 HIS346   0.1149
@<TRIPOS>BOND
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   2    1    7  1
   3    1   12  1
   4    2    3  1   BACKBONE
   5    2    5  1
   6    2    8  1
   7    3    4  2   BACKBONE
   8    3   13  am  BACKBONE|INTERRES
   9    5    6  1
  10    5    9  1
  11    5   10  1
  12    6   11  1
  13   13   14  1   BACKBONE
  14   13   23  1
  15   14   15  1   BACKBONE
  16   14   17  1
  17   14   24  1
  18   15   16  2   BACKBONE
  19   15   30  am  BACKBONE|INTERRES
  20   17   18  1
  21   17   25  1
  22   17   26  1
  23   18   19  1
  24   18   20  2
  25   19   21  1
  26   19   27  1
  27   20   22  1
  28   20   28  1
  29   21   22  2
  30   21   29  1
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32   30   38  1
33   31   32  1   BACKBONE
34   31   34  1
35   31   39  1
36   32   33  2   BACKBONE
37   32   49  am  BACKBONE|INTERRES
38   34   35  1
39   34   40  1
40   34   41  1
41   35   36  1
42   35   42  1
43   35   43  1
44   36   37  1
45   36   44  1
46   36   45  1
47   37   46  1
48   37   47  1
49   37   48  1
50   49   50  1   BACKBONE
51   49   57  1
52   50   51  1   BACKBONE
53   50   53  1
54   50   58  1
55   51   52  2   BACKBONE
56   51   68  am  BACKBONE|INTERRES
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58   53   59  1
59   53   60  1
60   54   55  1
61   54   56  1
62   54   61  1
63   55   62  1
64   55   63  1
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66   56   65  1
67   56   66  1
68   56   67  1
69   68   69  1   BACKBONE
70   68   74  1
71   69   70  1   BACKBONE
72   69   72  1
73   69   75  1
74   70   71  2   BACKBONE
75   70   82  am  BACKBONE|INTERRES
76   72   73  1
77   72   76  1
78   72   77  1
79   73   74  1
80   73   78  1
81   73   79  1
82   74   80  1
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85	82	93	1	
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87	83	86	1	
88	83	94	1	
89	84	85	2	BACKBONE
90	84	106	am	BACKBONE|INTERRES
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92	86	95	1	
93	86	96	1	
94	87	88	1	
95	87	97	1	
96	87	98	1	
97	88	89	1	
98	88	99	1	
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100	89	90	ar	
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102	90	91	ar	
103	90	92	ar	
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105	91	103	1	
106	92	104	1	
107	92	105	1	
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110	107	108	1	BACKBONE
111	107	110	1	
112	107	115	1	
113	108	109	2	BACKBONE
114	108	120	am	BACKBONE|INTERRES
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116	110	116	1	
117	110	117	1	
118	111	112	2	
119	111	113	am	
120	113	118	1	
121	113	119	1	
122	120	121	1	BACKBONE
123	120	126	1	
124	121	122	1	BACKBONE
125	121	124	1	
126	121	127	1	
127	122	123	2	BACKBONE
128	122	134	am	BACKBONE|INTERRES
129	124	125	1	
130	124	128	1	
131	124	129	1	
132	125	126	1	
133	125	130	1	
134	125	131	1	

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140  135  138  1
141  135  141  1
142  136  137  2   BACKBONE
143  136  145  am  BACKBONE|INTERRES
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145  138  142  1
146  138  143  1
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153  147  148  2   BACKBONE
154  147  164  am  BACKBONE|INTERRES
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156  149  155  1
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172  166  167  2   BACKBONE
173  166  174  am  BACKBONE|INTERRES
174  168  171  1
175  168  172  1
176  168  173  1
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183  176  186  am  BACKBONE|INTERRES
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195  188  207  am  BACKBONE|INTERRES
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201  192  194  ar
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217  209  222  am  BACKBONE|INTERRES
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225  213  215  ar
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231  224  225  2   BACKBONE
232  224  232  am  BACKBONE|INTERRES
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320  311  329  am  BACKBONE|INTERRES
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328  316  318  ar
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330  317  319  ar
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332  318  319  ar
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341  331  336  am  BACKBONE|INTERRES
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348  338  350  am  BACKBONE|INTERRES
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362  352  374  am  BACKBONE|INTERRES
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498  482  491  1
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515  498  500  am
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549  539  540  1   BACKBONE
550  539  542  1
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553  540  562  am  BACKBONE|INTERRES
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566  546  548  ar
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577  564  572  am  BACKBONE|INTERRES
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587  574  579  am  BACKBONE|INTERRES
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594  581  599  am  BACKBONE|INTERRES
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599  584  586  ar
600  585  587  ar
601  585  594  1
602  586  588  ar
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611  600  601  1   BACKBONE
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613  600  612  1
614  601  602  2   BACKBONE
615  601  620  am  BACKBONE|INTERRES
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617  603  613  1
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620  604  606  ar
621  605  607  ar
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623  606  608  ar
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625  607  609  ar
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627  608  609  ar
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636  622  623  2   BACKBONE
637  622  630  am  BACKBONE|INTERRES
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647  632  649  am  BACKBONE|INTERRES
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653  635  642  1
654  636  643  1
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662  650  651  1   BACKBONE
663  650  654  1
664  650  655  1
665  651  652  2   BACKBONE
666  651  656  am  BACKBONE|INTERRES
667  656  657  1   BACKBONE
668  656  665  1
669  657  658  1   BACKBONE
670  657  660  1
671  657  666  1
672  658  659  2   BACKBONE
673  658  671  am  BACKBONE|INTERRES
674  660  661  1
675  660  667  1
676  660  668  1
677  661  662  1
678  661  669  1
679  661  670  1
680  662  663  ar
681  662  664  ar
682  671  672  1   BACKBONE
683  671  675  1
684  672  673  1   BACKBONE
685  672  676  1
686  672  677  1
687  673  674  2   BACKBONE
688  673  678  am  BACKBONE|INTERRES
689  678  679  1   BACKBONE
690  678  686  1
691  679  680  1   BACKBONE
692  679  682  1
693  679  687  1
694  680  681  2   BACKBONE
695  680  765  am  BACKBONE|INTERRES
696  682  683  1
697  682  688  1
698  682  689  1
699  683  684  ar
700  683  685  ar
701  690  691  2   BACKBONE
702  691  692  am  BACKBONE
703  691  730  1   BACKBONE
704  692  693  1   BACKBONE
705  692  727  1   BACKBONE
706  693  694  1
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707  693  695  1   BACKBONE
708  693  721  1   BACKBONE
709  695  696  am  BACKBONE
710  695  720  2   BACKBONE
711  696  697  1
712  696  698  1   BACKBONE
713  698  699  1
714  698  700  1   BACKBONE
715  698  705  1   BACKBONE
716  700  701  ar  BACKBONE
717  700  713  ar  BACKBONE
718  701  702  1   BACKBONE
719  701  708  ar  BACKBONE
720  702  703  1
721  702  704  1
722  702  705  1   BACKBONE
723  705  706  1
724  705  707  1
725  708  709  ar  BACKBONE
726  708  715  1   BACKBONE
727  709  710  1
728  709  711  ar  BACKBONE
729  711  712  1
730  711  713  ar  BACKBONE
731  713  714  1
732  715  716  1
733  716  717  2
734  716  718  2
735  716  719  am
736  719  772  1
737  721  722  1
738  721  723  1
739  721  724  1   BACKBONE
740  724  725  1
741  724  726  1
742  724  727  1   BACKBONE
743  727  728  1
744  727  729  1
745  730  731  1
746  730  732  1   BACKBONE
747  730  748  1   BACKBONE
748  732  733  1
749  732  734  am  BACKBONE
750  734  735  1   BACKBONE
751  734  747  2   BACKBONE
752  735  736  1
753  735  737  1   BACKBONE
754  735  743  1   BACKBONE
755  737  738  1
756  737  739  1   BACKBONE
757  739  740  1
758  739  741  1
```

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759  739  742  1
760  743  744  1
761  743  745  1
762  743  746  1
763  748  749  1
764  748  750  1   BACKBONE
765  748  762  1   BACKBONE
766  750  751  1
767  750  752  1
768  750  753  1   BACKBONE
769  753  754  1
770  753  755  1
771  753  756  1   BACKBONE
772  756  757  1
773  756  758  1
774  756  759  1   BACKBONE
775  759  760  1
776  759  761  1
777  759  762  1   BACKBONE
778  762  763  1
779  762  764  1
780  765  766  1   BACKBONE
781  765  773  1
782  766  767  1   BACKBONE
783  766  769  1
784  766  774  1
785  767  768  2   BACKBONE
786  767  783  am  BACKBONE|INTERRES
787  769  770  1
788  769  775  1
789  769  776  1
790  770  771  1
791  770  777  1
792  770  778  1
793  771  772  1
794  771  779  1
795  771  780  1
796  772  781  1
797  772  782  1
798  783  784  1   BACKBONE
799  783  790  1
800  784  785  1   BACKBONE
801  784  787  1
802  784  791  1
803  785  786  2   BACKBONE
804  785  799  am  BACKBONE|INTERRES
805  787  788  1
806  787  789  1
807  787  792  1
808  788  793  1
809  788  794  1
810  788  795  1
```

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811  789  796  1
812  789  797  1
813  789  798  1
814  799  800  1   BACKBONE
815  799  808  1
816  800  801  1   BACKBONE
817  800  803  1
818  800  809  1
819  801  802  2   BACKBONE
820  801  821  am  BACKBONE|INTERRES
821  803  804  1
822  803  810  1
823  803  811  1
824  804  805  1
825  804  812  1
826  804  813  1
827  805  806  1
828  805  814  1
829  805  815  1
830  806  807  1
831  806  816  1
832  806  817  1
833  807  818  1
834  807  819  1
835  807  820  1
836  821  822  1   BACKBONE
837  821  827  1
838  822  823  1   BACKBONE
839  822  825  1
840  822  828  1
841  823  824  2   BACKBONE
842  823  833  am  BACKBONE|INTERRES
843  825  826  1
844  825  829  1
845  825  830  1
846  826  831  1
847  826  832  1
848  833  834  1   BACKBONE
849  833  844  1
850  834  835  1   BACKBONE
851  834  837  1
852  834  845  1
853  835  836  2   BACKBONE
854  835  853  am  BACKBONE|INTERRES
855  837  838  1
856  837  846  1
857  837  847  1
858  838  839  ar
859  838  840  ar
860  839  841  ar
861  839  848  1
862  840  842  ar
```

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863  840  849  1
864  841  843  ar
865  841  850  1
866  842  843  ar
867  842  851  1
868  843  852  1
869  853  854  1   BACKBONE
870  853  863  1
871  854  855  1   BACKBONE
872  854  857  1
873  854  864  1
874  855  856  2   BACKBONE
875  855  870  am  BACKBONE|INTERRES
876  857  858  1
877  857  865  1
878  857  866  1
879  858  859  1
880  858  860  2
881  859  861  1
882  859  867  1
883  860  862  1
884  860  868  1
885  861  862  2
886  861  869  1
887  870  871  1   BACKBONE
888  870  876  1
889  871  872  1   BACKBONE
890  871  874  1
891  871  877  1
892  872  873  2   BACKBONE
893  872  882  am  BACKBONE|INTERRES
894  874  875  1
895  874  878  1
896  874  879  1
897  875  880  1
898  875  881  1
899  882  883  1   BACKBONE
900  882  886  1
901  883  884  1   BACKBONE
902  883  887  1
903  883  888  1
904  884  885  2   BACKBONE
905  884  889  am  BACKBONE|INTERRES
906  889  890  1   BACKBONE
907  889  893  1
908  890  891  1   BACKBONE
909  890  894  1
910  890  895  1
911  891  892  2   BACKBONE
912  891  896  am  BACKBONE|INTERRES
913  896  897  1   BACKBONE
914  896  900  1
```

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915  897  898  1   BACKBONE
916  897  901  1
917  897  902  1
918  898  899  2   BACKBONE
919  898  903  am  BACKBONE|INTERRES
920  903  904  1   BACKBONE
921  903  911  1
922  904  905  1   BACKBONE
923  904  907  1
924  904  912  1
925  905  906  2   BACKBONE
926  905  922  am  BACKBONE|INTERRES
927  907  908  1
928  907  913  1
929  907  914  1
930  908  909  1
931  908  910  1
932  908  915  1
933  909  916  1
934  909  917  1
935  909  918  1
936  910  919  1
937  910  920  1
938  910  921  1
939  922  923  1   BACKBONE
940  922  929  1
941  923  924  1   BACKBONE
942  923  926  1
943  923  930  1
944  924  925  2   BACKBONE
945  924  936  am  BACKBONE|INTERRES
946  926  927  1
947  926  928  1
948  926  931  1
949  927  932  1
950  928  933  1
951  928  934  1
952  928  935  1
953  936  937  1   BACKBONE
954  936  944  1
955  937  938  1   BACKBONE
956  937  940  1
957  937  945  1
958  938  939  2   BACKBONE
959  938  948  am  BACKBONE|INTERRES
960  940  941  1
961  940  946  1
962  940  947  1
963  941  942  ar
964  941  943  ar
965  948  949  1   BACKBONE
966  948  962  1
```

967	949	950	1	BACKBONE
968	949	952	1	
969	949	963	1	
970	950	951	2	BACKBONE
971	950	972	am	BACKBONE|INTERRES
972	952	953	1	
973	952	964	1	
974	952	965	1	
975	953	954	2	
976	953	955	1	
977	954	956	1	
978	954	966	1	
979	955	957	ar	
980	955	958	ar	
981	956	957	1	
982	956	967	1	
983	957	959	ar	
984	958	960	ar	
985	958	968	1	
986	959	961	ar	
987	959	969	1	
988	960	961	ar	
989	960	970	1	
990	961	971	1	
991	972	973	1	BACKBONE
992	972	981	1	
993	973	974	1	BACKBONE
994	973	976	1	
995	973	982	1	
996	974	975	2	BACKBONE
997	974	994	am	BACKBONE|INTERRES
998	976	977	1	
999	976	983	1	
1000	976	984	1	
1001	977	978	1	
1002	977	985	1	
1003	977	986	1	
1004	978	979	1	
1005	978	987	1	
1006	978	988	1	
1007	979	980	1	
1008	979	989	1	
1009	979	990	1	
1010	980	991	1	
1011	980	992	1	
1012	980	993	1	
1013	994	995	1	BACKBONE
1014	994	1000	1	
1015	995	996	1	BACKBONE
1016	995	998	1	
1017	995	1001	1	
1018	996	997	2	BACKBONE

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1019  996 1008  am  BACKBONE|INTERRES
1020  998  999  1
1021  998 1002  1
1022  998 1003  1
1023  999 1000  1
1024  999 1004  1
1025  999 1005  1
1026 1000 1006  1
1027 1000 1007  1
1028 1008 1009  1   BACKBONE
1029 1008 1014  1
1030 1009 1010  1   BACKBONE
1031 1009 1012  1
1032 1009 1015  1
1033 1010 1011  2   BACKBONE
1034 1010 1019  am  BACKBONE|INTERRES
1035 1012 1013  1
1036 1012 1016  1
1037 1012 1017  1
1038 1013 1018  1
1039 1019 1020  1   BACKBONE
1040 1019 1028  1
1041 1020 1021  1   BACKBONE
1042 1020 1023  1
1043 1020 1029  1
1044 1021 1022  2   BACKBONE
1045 1021 1034  am  BACKBONE|INTERRES
1046 1023 1024  1
1047 1023 1030  1
1048 1023 1031  1
1049 1024 1025  1
1050 1024 1032  1
1051 1024 1033  1
1052 1025 1026  ar
1053 1025 1027  ar
1054 1034 1035  1   BACKBONE
1055 1034 1042  1
1056 1035 1036  1   BACKBONE
1057 1035 1038  1
1058 1035 1043  1
1059 1036 1037  2   BACKBONE
1060 1036 1046  am  BACKBONE|INTERRES
1061 1038 1039  1
1062 1038 1044  1
1063 1038 1045  1
1064 1039 1040  ar
1065 1039 1041  ar
1066 1046 1047  1   BACKBONE
1067 1046 1052  1
1068 1047 1048  1   BACKBONE
1069 1047 1050  1
1070 1047 1053  1
```

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1071 1048 1049  2   BACKBONE
1072 1048 1060  am  BACKBONE|INTERRES
1073 1050 1051  1
1074 1050 1054  1
1075 1050 1055  1
1076 1051 1052  1
1077 1051 1056  1
1078 1051 1057  1
1079 1052 1058  1
1080 1052 1059  1
1081 1060 1061  1   BACKBONE
1082 1060 1074  1
1083 1061 1062  1   BACKBONE
1084 1061 1064  1
1085 1061 1075  1
1086 1062 1063  2   BACKBONE
1087 1062 1084  am  BACKBONE|INTERRES
1088 1064 1065  1
1089 1064 1076  1
1090 1064 1077  1
1091 1065 1066  2
1092 1065 1067  1
1093 1066 1068  1
1094 1066 1078  1
1095 1067 1069  ar
1096 1067 1070  ar
1097 1068 1069  1
1098 1068 1079  1
1099 1069 1071  ar
1100 1070 1072  ar
1101 1070 1080  1
1102 1071 1073  ar
1103 1071 1081  1
1104 1072 1073  ar
1105 1072 1082  1
1106 1073 1083  1
1107 1084 1085  1   BACKBONE
1108 1084 1093  1
1109 1085 1086  1   BACKBONE
1110 1085 1088  1
1111 1085 1094  1
1112 1086 1087  2   BACKBONE
1113 1086 1099  am  BACKBONE|INTERRES
1114 1088 1089  1
1115 1088 1095  1
1116 1088 1096  1
1117 1089 1090  1
1118 1089 1097  1
1119 1089 1098  1
1120 1090 1091  ar
1121 1090 1092  ar
1122 1099 1100  1   BACKBONE
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1123 1099 1108  1
1124 1100 1101  1   BACKBONE
1125 1100 1103  1
1126 1100 1109  1
1127 1101 1102  2   BACKBONE
1128 1101 1116  am  BACKBONE|INTERRES
1129 1103 1104  1
1130 1103 1110  1
1131 1103 1111  1
1132 1104 1105  1
1133 1104 1112  1
1134 1104 1113  1
1135 1105 1106  2
1136 1105 1107  am
1137 1107 1114  1
1138 1107 1115  1
1139 1116 1117  1   BACKBONE
1140 1116 1126  1
1141 1117 1118  1   BACKBONE
1142 1117 1120  1
1143 1117 1127  1
1144 1118 1119  2   BACKBONE
1145 1118 1133  am  BACKBONE|INTERRES
1146 1120 1121  1
1147 1120 1128  1
1148 1120 1129  1
1149 1121 1122  1
1150 1121 1123  2
1151 1122 1124  ar
1152 1122 1130  1
1153 1123 1125  1
1154 1123 1131  1
1155 1124 1125  1
1156 1124 1132  1
1157 1133 1134  1   BACKBONE
1158 1133 1138  1
1159 1134 1135  1   BACKBONE
1160 1134 1137  1
1161 1134 1139  1
1162 1135 1136  2   BACKBONE
1163 1135 1143  am  BACKBONE|INTERRES
1164 1137 1140  1
1165 1137 1141  1
1166 1137 1142  1
1167 1143 1144  1   BACKBONE
1168 1143 1152  1
1169 1144 1145  1   BACKBONE
1170 1144 1147  1
1171 1144 1153  1
1172 1145 1146  2   BACKBONE
1173 1145 1165  am  BACKBONE|INTERRES
1174 1147 1148  1
```

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1175 1147 1154  1
1176 1147 1155  1
1177 1148 1149  1
1178 1148 1156  1
1179 1148 1157  1
1180 1149 1150  1
1181 1149 1158  1
1182 1149 1159  1
1183 1150 1151  1
1184 1150 1160  1
1185 1150 1161  1
1186 1151 1162  1
1187 1151 1163  1
1188 1151 1164  1
1189 1165 1166  1   BACKBONE
1190 1165 1179  1
1191 1166 1167  1   BACKBONE
1192 1166 1169  1
1193 1166 1180  1
1194 1167 1168  2   BACKBONE
1195 1167 1189  am  BACKBONE|INTERRES
1196 1169 1170  1
1197 1169 1181  1
1198 1169 1182  1
1199 1170 1171  2
1200 1170 1172  1
1201 1171 1173  1
1202 1171 1183  1
1203 1172 1174  ar
1204 1172 1175  ar
1205 1173 1174  1
1206 1173 1184  1
1207 1174 1176  ar
1208 1175 1177  ar
1209 1175 1185  1
1210 1176 1178  ar
1211 1176 1186  1
1212 1177 1178  ar
1213 1177 1187  1
1214 1178 1188  1
1215 1189 1190  1   BACKBONE
1216 1189 1201  1
1217 1190 1191  1   BACKBONE
1218 1190 1193  1
1219 1190 1202  1
1220 1191 1192  2   BACKBONE
1221 1191 1210  am  BACKBONE|INTERRES
1222 1193 1194  1
1223 1193 1203  1
1224 1193 1204  1
1225 1194 1195  ar
1226 1194 1196  ar
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1227 1195 1197  ar
1228 1195 1205  1
1229 1196 1198  ar
1230 1196 1206  1
1231 1197 1199  ar
1232 1197 1207  1
1233 1198 1199  ar
1234 1198 1208  1
1235 1199 1200  1
1236 1200 1209  1
1237 1210 1211  1   BACKBONE
1238 1210 1216  1
1239 1211 1212  1   BACKBONE
1240 1211 1214  1
1241 1211 1217  1
1242 1212 1213  2   BACKBONE
1243 1212 1224  am  BACKBONE|INTERRES
1244 1214 1215  1
1245 1214 1218  1
1246 1214 1219  1
1247 1215 1216  1
1248 1215 1220  1
1249 1215 1221  1
1250 1216 1222  1
1251 1216 1223  1
1252 1224 1225  1   BACKBONE
1253 1224 1228  1
1254 1225 1226  1   BACKBONE
1255 1225 1229  1
1256 1225 1230  1
1257 1226 1227  2   BACKBONE
1258 1226 1231  am  BACKBONE|INTERRES
1259 1231 1232  1   BACKBONE
1260 1231 1237  1
1261 1232 1233  1   BACKBONE
1262 1232 1235  1
1263 1232 1238  1
1264 1233 1234  2   BACKBONE
1265 1233 1243  am  BACKBONE|INTERRES
1266 1235 1236  1
1267 1235 1239  1
1268 1235 1240  1
1269 1236 1241  1
1270 1236 1242  1
1271 1243 1244  1   BACKBONE
1272 1243 1252  1
1273 1244 1245  1   BACKBONE
1274 1244 1247  1
1275 1244 1253  1
1276 1245 1246  2   BACKBONE
1277 1245 1265  am  BACKBONE|INTERRES
1278 1247 1248  1
```

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1279 1247 1254  1
1280 1247 1255  1
1281 1248 1249  1
1282 1248 1256  1
1283 1248 1257  1
1284 1249 1250  1
1285 1249 1258  1
1286 1249 1259  1
1287 1250 1251  1
1288 1250 1260  1
1289 1250 1261  1
1290 1251 1262  1
1291 1251 1263  1
1292 1251 1264  1
1293 1265 1266  1   BACKBONE
1294 1265 1277  1
1295 1266 1267  1   BACKBONE
1296 1266 1269  1
1297 1266 1278  1
1298 1267 1268  2   BACKBONE
1299 1267 1286  am  BACKBONE|INTERRES
1300 1269 1270  1
1301 1269 1279  1
1302 1269 1280  1
1303 1270 1271  ar
1304 1270 1272  ar
1305 1271 1273  ar
1306 1271 1281  1
1307 1272 1274  ar
1308 1272 1282  1
1309 1273 1275  ar
1310 1273 1283  1
1311 1274 1275  ar
1312 1274 1284  1
1313 1275 1276  1
1314 1276 1285  1
1315 1286 1287  1   BACKBONE
1316 1286 1294  1
1317 1287 1288  1   BACKBONE
1318 1287 1290  1
1319 1287 1295  1
1320 1288 1289  2   BACKBONE
1321 1288 1305  am  BACKBONE|INTERRES
1322 1290 1291  1
1323 1290 1296  1
1324 1290 1297  1
1325 1291 1292  1
1326 1291 1293  1
1327 1291 1298  1
1328 1292 1299  1
1329 1292 1300  1
1330 1292 1301  1
```

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1331 1293 1302  1
1332 1293 1303  1
1333 1293 1304  1
1334 1305 1306  1   BACKBONE
1335 1305 1313  1
1336 1306 1307  1   BACKBONE
1337 1306 1309  1
1338 1306 1314  1
1339 1307 1308  2   BACKBONE
1340 1307 1324  am  BACKBONE|INTERRES
1341 1309 1310  1
1342 1309 1315  1
1343 1309 1316  1
1344 1310 1311  1
1345 1310 1312  1
1346 1310 1317  1
1347 1311 1318  1
1348 1311 1319  1
1349 1311 1320  1
1350 1312 1321  1
1351 1312 1322  1
1352 1312 1323  1
1353 1324 1325  1   BACKBONE
1354 1324 1333  1
1355 1325 1326  1   BACKBONE
1356 1325 1328  1
1357 1325 1334  1
1358 1326 1327  2   BACKBONE
1359 1326 1339  am  BACKBONE|INTERRES
1360 1328 1329  1
1361 1328 1335  1
1362 1328 1336  1
1363 1329 1330  1
1364 1329 1337  1
1365 1329 1338  1
1366 1330 1331  ar
1367 1330 1332  ar
1368 1339 1340  1   BACKBONE
1369 1339 1348  1
1370 1340 1341  1   BACKBONE
1371 1340 1343  1
1372 1340 1349  1
1373 1341 1342  2   BACKBONE
1374 1341 1356  am  BACKBONE|INTERRES
1375 1343 1344  1
1376 1343 1350  1
1377 1343 1351  1
1378 1344 1345  1
1379 1344 1352  1
1380 1344 1353  1
1381 1345 1346  2
1382 1345 1347  am
```

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1383 1347 1354  1
1384 1347 1355  1
1385 1356 1357  1   BACKBONE
1386 1356 1365  1
1387 1357 1358  1   BACKBONE
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  6 ARG258   83 RESIDUE 4 A ARG 2
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 12 ASP264  175 RESIDUE 4 A ASP 2
 13 TYR265  187 RESIDUE 4 A TYR 2
 14 GLU266  208 RESIDUE 4 A GLU 2
 15 ALA267  223 RESIDUE 4 A ALA 2
 16 ARG268  233 RESIDUE 4 A ARG 2
 17 ILE269  257 RESIDUE 4 A ILE 2
 18 PHE270  276 RESIDUE 4 A PHE 2
 19 THR271  296 RESIDUE 4 A THR 2
 20 PHE272  310 RESIDUE 4 A PHE 2
 21 GLY273  330 RESIDUE 4 A GLY 2
 22 THR274  337 RESIDUE 4 A THR 2
 23 TRP275  351 RESIDUE 4 A TRP 2
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 25 TYR277  394 RESIDUE 4 A TYR 2
 26 SER278  415 RESIDUE 4 A SER 2
 27 VAL279  426 RESIDUE 4 A VAL 2
 28 ASN280  442 RESIDUE 4 A ASN 2
 29 LYS281  456 RESIDUE 4 A LYS 2
 30 GLU282  478 RESIDUE 4 A GLU 2
 31 GLN283  493 RESIDUE 4 A GLN 2
 32 LEU284  510 RESIDUE 4 A LEU 2
 33 ALA285  529 RESIDUE 4 A ALA 2
 34 ARG286  539 RESIDUE 4 A ARG 2
 35 ALA287  563 RESIDUE 4 A ALA 2
 36 GLY288  573 RESIDUE 4 A GLY 2
 37 PHE289  580 RESIDUE 4 A PHE 2
 38 TYR290  600 RESIDUE 4 A TYR 2
 39 ALA291  621 RESIDUE 4 A ALA 2
 40 LEU292  631 RESIDUE 4 A LEU 2
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42 GLU294  657 RESIDUE 4 A GLU 2
43 GLY295  672 RESIDUE 4 A GLY 2
44 ASP296  679 RESIDUE 4 A ASP 2
45 LYS297  766 RESIDUE 4 A LYS 2
46 VAL298  784 RESIDUE 4 A VAL 2
47 LYS299  800 RESIDUE 4 A LYS 2
48 CYS300  822 RESIDUE 4 A CYS 2
49 PHE301  834 RESIDUE 4 A PHE 2
50 HIS302  854 RESIDUE 4 A HIS 2
51 CYS303  871 RESIDUE 4 A CYS 2
52 GLY304  883 RESIDUE 4 A GLY 2
53 GLY305  890 RESIDUE 4 A GLY 2
54 GLY306  897 RESIDUE 4 A GLY 2
55 LEU307  904 RESIDUE 4 A LEU 2
56 THR308  923 RESIDUE 4 A THR 2
57 ASP309  937 RESIDUE 4 A ASP 2
58 TRP310  949 RESIDUE 4 A TRP 2
59 LYS311  973 RESIDUE 4 A LYS 2
60 PRO312  995 RESIDUE 4 A PRO 2
61 SER313 1009 RESIDUE 4 A SER 2
62 GLU314 1020 RESIDUE 4 A GLU 2
63 ASP315 1035 RESIDUE 4 A ASP 2
64 PRO316 1047 RESIDUE 4 A PRO 2
65 TRP317 1061 RESIDUE 4 A TRP 2
66 GLU318 1085 RESIDUE 4 A GLU 2
67 GLN319 1100 RESIDUE 4 A GLN 2
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73 PRO325 1211 RESIDUE 4 A PRO 2
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84 GLN336 1386 RESIDUE 4 A GLN 2
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88 ASN340 1458 RESIDUE 4 A ASN 2
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91 HIS343 1505 RESIDUE 4 A HIS 2
92 LEU344 1522 RESIDUE 4 A LEU 2
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 94 HIS346 1555 RESIDUE 4 A HIS 1

# MOE 2019.01 (io_trps.svl 2018.10)
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cIAP1-BIR3 + compound 2 .mol2 file

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BIOPOLYMER
USER_CHARGES


@<TRIPOS>ATOM
   1 N       11.6652     7.5313    -0.0982 N.3    1 MET252  -0.3667
BACKBONE
   2 CA      11.2246     8.7474    -0.7746 C.3    1 MET252   0.1054
BACKBONE
   3 C        9.7570     9.0082    -0.5151 C.2    1 MET252   0.1983
BACKBONE
   4 O        9.1136     9.6305    -1.3440 O.2    1 MET252  -0.3949
BACKBONE
   5 CB      11.5642     8.6122    -2.2877 C.3    1 MET252  -0.0086
   6 CG      13.0870     8.4255    -2.5200 C.3    1 MET252  -0.0028
   7 SD      14.0054     9.8693    -1.8793 S.o    1 MET252  -0.1639
   8 CE      15.5583     9.0734    -1.3596 C.3    1 MET252  -0.0181
   9 H       11.2133     6.6623    -0.3098 H      1 MET252   0.1393
  10 HA      11.7422     9.6250    -0.3552 H      1 MET252   0.0736
  11 HB3     11.2237     9.4899    -2.8543 H      1 MET252   0.0316
  12 HB2     11.0390     7.7317    -2.6902 H      1 MET252   0.0316
  13 HG3     13.3049     8.3294    -3.5952 H      1 MET252   0.0378
  14 HG2     13.4248     7.5064    -2.0174 H      1 MET252   0.0378
  15 LPD2    14.1116    10.3335    -2.3634 LP     1 MET252   0.0000
  16 LPD1    13.6843    10.1581    -1.3553 LP     1 MET252   0.0000
  17 HE3     15.3467     8.2724    -0.6360 H      1 MET252   0.0340
  18 NCAP    12.4300     7.5664     0.5488 H      1 MET252   0.1393
  19 HE2     16.2086     9.8168    -0.8778 H      1 MET252   0.0340
  20 HE1     16.0693     8.6520    -2.2379 H      1 MET252   0.0340
  21 N        9.2032     8.5581     0.6355 N.am   2 GLN253  -0.2640
BACKBONE
  22 CA       7.7904     8.8060     0.9206 C.3    2 GLN253   0.1330
BACKBONE
  23 C        7.5985    10.1836     1.5126 C.2    2 GLN253   0.2041
BACKBONE
  24 O        6.5663    10.7752     1.2367 O.2    2 GLN253  -0.3944
BACKBONE
  25 CB       7.2153     7.7573     1.9118 C.3    2 GLN253   0.0045
  26 CG       7.2422     6.3281     1.3066 C.3    2 GLN253   0.0412
  27 CD       6.6601     5.3341     2.2836 C.2    2 GLN253   0.1737
  28 OE1      5.5461     4.8791     2.0753 O.2    2 GLN253  -0.3973
  29 NE2      7.3907     4.9821     3.3646 N.am   2 GLN253  -0.3009
  30 H        9.7508     8.0885     1.3303 H      2 GLN253   0.1883
  31 HA       7.2014     8.7368    -0.0102 H      2 GLN253   0.0801
  32 HB3      6.1685     8.0155     2.1459 H      2 GLN253   0.0337
  33 HB2      7.7906     7.7875     2.8513 H      2 GLN253   0.0337
  34 HG3      8.2747     6.0315     1.0628 H      2 GLN253   0.0504
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35	HG2	6.6579	6.3110	0.3719	H	2 GLN253	0.0504
36	HE21	8.3046	5.3601	3.5204	H	2 GLN253	0.1814
37	HE22	7.0179	4.3278	4.0247	H	2 GLN253	0.1814
38	N	8.5479	10.7107	2.3245	N.am	3 THR254	-0.2613
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39	CA	8.3445	12.0156	2.9535	C.3	3 THR254	0.1565
BACKBONE							
40	C	8.9416	13.1145	2.1043	C.2	3 THR254	0.2066
BACKBONE							
41	O	9.8908	12.8551	1.3834	O.2	3 THR254	-0.3943
BACKBONE							
42	CB	9.0031	12.0583	4.3587	C.3	3 THR254	0.0924
43	OG1	10.4081	11.7935	4.2015	O.3	3 THR254	-0.3874
44	CG2	8.3568	11.0087	5.3028	C.3	3 THR254	-0.0346
45	H	9.4105	10.2369	2.5096	H	3 THR254	0.1884
46	HA	7.2668	12.2033	3.0932	H	3 THR254	0.0826
47	HB	8.8663	13.0667	4.7904	H	3 THR254	0.0639
48	HG1	10.8785	11.8135	5.0289	H	3 THR254	0.2101
49	HG22	8.8153	11.0653	6.3023	H	3 THR254	0.0257
50	HG21	8.5050	9.9919	4.9084	H	3 THR254	0.0257
51	HG23	7.2765	11.1944	5.4056	H	3 THR254	0.0257
52	N	8.4010	14.3522	2.1933	N.am	4 HIS255	-0.2618
BACKBONE							
53	CA	8.9623	15.4693	1.4332	C.3	4 HIS255	0.1421
BACKBONE							
54	C	10.4135	15.6666	1.8008	C.2	4 HIS255	0.2060
BACKBONE							
55	O	11.2379	15.7597	0.9053	O.2	4 HIS255	-0.3942
BACKBONE							
56	CB	8.1603	16.7676	1.7196	C.3	4 HIS255	0.0427
57	CG	8.7863	17.9948	1.1103	C.2	4 HIS255	0.0561
58	ND1	9.6125	18.7968	1.7438	N.pl3	4 HIS255	-0.2623
59	CD2	8.5796	18.4422	-0.1424	C.2	4 HIS255	-0.0276
60	CE1	9.9496	19.7753	0.9644	C.2	4 HIS255	0.0875
61	NE2	9.3905	19.6296	-0.1493	N.2	4 HIS255	-0.3437
62	H	7.6174	14.5242	2.7938	H	4 HIS255	0.1885
63	HA	8.8929	15.2460	0.3553	H	4 HIS255	0.0824
64	HB3	8.0695	16.9354	2.8040	H	4 HIS255	0.0491
65	HB2	7.1428	16.6465	1.3136	H	4 HIS255	0.0491
66	HD1	9.9343	18.6754	2.7161	H	4 HIS255	0.2386
67	HD2	7.9631	18.0132	-0.9258	H	4 HIS255	0.0324
68	HE1	10.6104	20.6024	1.2218	H	4 HIS255	0.1149
69	N	10.7429	15.7291	3.1108	N.am	5 ALA256	-0.2639
BACKBONE							
70	CA	12.1326	15.9532	3.5073	C.3	5 ALA256	0.1282
BACKBONE							
71	C	13.0481	14.9446	2.8518	C.2	5 ALA256	0.2036
BACKBONE							
72	O	14.0921	15.3324	2.3510	O.2	5 ALA256	-0.3944
BACKBONE							
73	CB	12.3085	15.8490	5.0447	C.3	5 ALA256	-0.0244
74	H	10.0423	15.6441	3.8223	H	5 ALA256	0.1883

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  75 HA      12.4180    16.9714     3.1904 H      5 ALA256   0.0797
  76 HB3     12.0095    14.8499     5.3978 H      5 ALA256   0.0277
  77 HB2     11.6844    16.6032     5.5493 H      5 ALA256   0.0277
  78 HB1     13.3607    16.0217     5.3211 H      5 ALA256   0.0277
  79 N       12.6763    13.6444     2.8382 N.am   6 ALA257  -0.2640
BACKBONE
  80 CA      13.5412    12.6532     2.2013 C.3    6 ALA257   0.1282
BACKBONE
  81 C       13.7582    13.0150     0.7517 C.2    6 ALA257   0.2036
BACKBONE
  82 O       14.8797    12.9361     0.2739 O.2    6 ALA257  -0.3944
BACKBONE
  83 CB      12.9542    11.2198     2.2758 C.3    6 ALA257  -0.0244
  84 H       11.8121    13.3465     3.2470 H      6 ALA257   0.1883
  85 HA      14.5093    12.6617     2.7228 H      6 ALA257   0.0797
  86 HB3     11.9674    11.1807     1.7904 H      6 ALA257   0.0277
  87 HB2     12.8455    10.9111     3.3268 H      6 ALA257   0.0277
  88 HB1     13.6243    10.5071     1.7692 H      6 ALA257   0.0277
  89 N       12.6816    13.4179     0.0418 N.am   7 ARG258  -0.2637
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  90 CA      12.8268    13.7611    -1.3693 C.3    7 ARG258   0.1311
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  91 C       13.6690    15.0087    -1.5273 C.2    7 ARG258   0.2039
BACKBONE
  92 O       14.3601    15.1042    -2.5277 O.2    7 ARG258  -0.3944
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  93 CB      11.4461    13.9106    -2.0685 C.3    7 ARG258  -0.0092
  94 CG      10.6470    12.5765    -2.0279 C.3    7 ARG258  -0.0156
  95 CD       9.3702    12.6195    -2.9074 C.3    7 ARG258   0.0627
  96 NE       8.4412    13.6549    -2.4476 N.pl3  7 ARG258  -0.2723
  97 CZ       7.5701    13.4984    -1.4711 C.cat  7 ARG258   0.2882
  98 NH1      7.4601    12.3964    -0.7657 N.pl3  7 ARG258  -0.2849
  99 NH2      6.7637    14.4963    -1.1824 N.pl3  7 ARG258  -0.2849
 100 H       11.7845    13.5125     0.4769 H      7 ARG258   0.1883
 101 HA      13.3659    12.9381    -1.8703 H      7 ARG258   0.0800
 102 HB3     11.6237    14.2009    -3.1162 H      7 ARG258   0.0313
 103 HB2     10.8632    14.7080    -1.5842 H      7 ARG258   0.0313
 104 HG3     10.3608    12.3238    -0.9999 H      7 ARG258   0.0301
 105 HG2     11.2996    11.7712    -2.3863 H      7 ARG258   0.0301
 106 HD3      8.8996    11.6309    -2.9824 H      7 ARG258   0.0689
 107 HD2      9.6771    12.8516    -3.9362 H      7 ARG258   0.0689
 108 HE       8.4592    14.5504    -2.9590 H      7 ARG258   0.2642
 109 HH11     8.0629    11.5821    -0.9271 H      7 ARG258   0.2615
 110 HH12     6.7564    12.3207    -0.0164 H      7 ARG258   0.2615
 111 HH21     6.8057    15.3862    -1.7014 H      7 ARG258   0.2615
 112 HH22     6.0668    14.4182    -0.4263 H      7 ARG258   0.2615
 113 N       13.6570    15.9722    -0.5768 N.am   8 MET259  -0.2637
BACKBONE
 114 CA      14.5256    17.1427    -0.7184 C.3    8 MET259   0.1317
BACKBONE
 115 C       15.9821    16.7275    -0.7511 C.2    8 MET259   0.2039
BACKBONE
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 116 O       16.7231    17.2572    -1.5649 O.2     8 MET259  -0.3944
BACKBONE
 117 CB      14.3594    18.1902     0.4177 C.3     8 MET259  -0.0034
 118 CG      12.9663    18.8749     0.4231 C.3     8 MET259  -0.0024
 119 SD      12.5778    19.7659    -1.1252 S.o     8 MET259  -0.1639
 120 CE      13.8417    21.0729    -1.1798 C.3     8 MET259  -0.0181
 121 H       13.0821    15.8904     0.2371 H       8 MET259   0.1883
 122 HA      14.2799    17.6490    -1.6618 H       8 MET259   0.0800
 123 HB3     15.1296    18.9708     0.3099 H       8 MET259   0.0320
 124 HB2     14.5242    17.6981     1.3891 H       8 MET259   0.0320
 125 HG3     12.9192    19.5919     1.2573 H       8 MET259   0.0378
 126 HG2     12.1753    18.1270     0.5698 H       8 MET259   0.0378
 127 LPD2    12.6297    19.3542    -1.6626 LP      8 MET259   0.0000
 128 LPD1    11.9534    20.0316    -1.1032 LP      8 MET259   0.0000
 129 HE3     13.9372    21.5500    -0.1935 H       8 MET259   0.0340
 130 HE2     13.5364    21.8296    -1.9168 H       8 MET259   0.0340
 131 HE1     14.8095    20.6479    -1.4839 H       8 MET259   0.0340
 132 N       16.4183    15.7988     0.1326 N.am    9 ARG260  -0.2637
BACKBONE
 133 CA      17.8482    15.4912     0.2263 C.3     9 ARG260   0.1311
BACKBONE
 134 C       18.4416    15.0970    -1.1107 C.2     9 ARG260   0.2040
BACKBONE
 135 O       19.5854    15.4292    -1.3782 O.2     9 ARG260  -0.3944
BACKBONE
 136 CB      18.1941    14.3379     1.2135 C.3     9 ARG260  -0.0092
 137 CG      17.6466    14.5513     2.6537 C.3     9 ARG260  -0.0156
 138 CD      18.4513    13.7281     3.6982 C.3     9 ARG260   0.0627
 139 NE      17.7362    13.7119     4.9791 N.pl3   9 ARG260  -0.2723
 140 CZ      16.7713    12.8651     5.2824 C.cat   9 ARG260   0.2882
 141 NH1     16.3242    11.9442     4.4578 N.pl3   9 ARG260  -0.2849
 142 NH2     16.2204    12.9422     6.4738 N.pl3   9 ARG260  -0.2849
 143 H       15.7787    15.3582     0.7631 H       9 ARG260   0.1883
 144 HA      18.3502    16.4080     0.5791 H       9 ARG260   0.0800
 145 HB3     19.2941    14.2643     1.2572 H       9 ARG260   0.0313
 146 HB2     17.8071    13.3814     0.8236 H       9 ARG260   0.0313
 147 HG3     16.5900    14.2459     2.6987 H       9 ARG260   0.0301
 148 HG2     17.7009    15.6172     2.9317 H       9 ARG260   0.0301
 149 HD3     19.4234    14.2320     3.8408 H       9 ARG260   0.0689
 150 HD2     18.7035    12.7182     3.3409 H       9 ARG260   0.0689
 151 HE      18.0356    14.4040     5.6862 H       9 ARG260   0.2642
 152 HH11    16.6979    11.8352     3.5085 H       9 ARG260   0.2615
 153 HH12    15.5700    11.3006     4.7424 H       9 ARG260   0.2615
 154 HH21    16.5293    13.6455     7.1616 H       9 ARG260   0.2615
 155 HH22    15.4618    12.3018     6.7540 H       9 ARG260   0.2615
 156 N       17.6869    14.3697    -1.9613 N.am   10 THR261  -0.2613
BACKBONE
 157 CA      18.2464    13.9120    -3.2345 C.3    10 THR261   0.1565
BACKBONE
 158 C       18.5724    15.0943    -4.1230 C.2    10 THR261   0.2066
BACKBONE
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 159 O       19.6145    15.0895    -4.7595 O.2   10 THR261  -0.3943
BACKBONE
 160 CB      17.2085    13.0206    -3.9625 C.3   10 THR261   0.0924
 161 OG1     16.0076    13.8042    -3.9880 O.3   10 THR261  -0.3874
 162 CG2     16.9806    11.6733    -3.2251 C.3   10 THR261  -0.0346
 163 H       16.7370    14.1465    -1.7341 H     10 THR261   0.1884
 164 HA      19.1625    13.3275    -3.0472 H     10 THR261   0.0826
 165 HB      17.5501    12.7994    -4.9873 H     10 THR261   0.0639
 166 HG1     15.2622    13.3290    -4.3275 H     10 THR261   0.2101
 167 HG22    16.2672    11.0519    -3.7879 H     10 THR261   0.0257
 168 HG21    16.5720    11.8432    -2.2193 H     10 THR261   0.0257
 169 HG23    17.9266    11.1182    -3.1349 H     10 THR261   0.0257
 170 N       17.6921    16.1203    -4.1771 N.am  11 PHE262  -0.2619
BACKBONE
 171 CA      17.9313    17.2647    -5.0608 C.3   11 PHE262   0.1404
BACKBONE
 172 C       19.1525    18.1074    -4.7302 C.2   11 PHE262   0.2060
BACKBONE
 173 O       19.3735    19.0576    -5.4652 O.2   11 PHE262  -0.3942
BACKBONE
 174 CB      16.6954    18.2066    -5.0590 C.3   11 PHE262   0.0214
 175 CG      15.4714    17.5790    -5.7470 C.ar  11 PHE262  -0.0386
 176 CD1     15.4054    17.5054    -7.1420 C.ar  11 PHE262  -0.0601
 177 CD2     14.3984    17.0822    -5.0013 C.ar  11 PHE262  -0.0601
 178 CE1     14.3638    16.8177    -7.7713 C.ar  11 PHE262  -0.0686
 179 CE2     13.3297    16.4348    -5.6254 C.ar  11 PHE262  -0.0686
 180 CZ      13.3335    16.2581    -7.0110 C.ar  11 PHE262  -0.0687
 181 H       16.8518    16.0935    -3.6322 H     11 PHE262   0.1885
 182 HA      18.0760    16.8919    -6.0885 H     11 PHE262   0.0823
 183 HB3     16.9322    19.1241    -5.6080 H     11 PHE262   0.0474
 184 HB2     16.4729    18.4986    -4.0205 H     11 PHE262   0.0474
 185 HD1     16.1694    17.9741    -7.7482 H     11 PHE262   0.0557
 186 HD2     14.3905    17.2027    -3.9288 H     11 PHE262   0.0557
 187 HE1     14.3643    16.7152    -8.8497 H     11 PHE262   0.0599
 188 HE2     12.5000    16.0693    -5.0296 H     11 PHE262   0.0599
 189 HZ      12.5456    15.6893    -7.4942 H     11 PHE262   0.0559
 190 N       19.9613    17.8374    -3.6772 N.am  12 MET263  -0.2636
BACKBONE
 191 CA      21.1045    18.7100    -3.3814 C.3   12 MET263   0.1317
BACKBONE
 192 C       21.8724    19.1154    -4.6246 C.2   12 MET263   0.2040
BACKBONE
 193 O       22.2678    20.2692    -4.6925 O.2   12 MET263  -0.3944
BACKBONE
 194 CB      22.0994    18.0592    -2.3787 C.3   12 MET263  -0.0034
 195 CG      21.5617    18.0985    -0.9231 C.3   12 MET263  -0.0024
 196 SD      22.6835    17.1440     0.1498 S.o   12 MET263  -0.1639
 197 CE      21.6942    17.0930     1.6766 C.3   12 MET263  -0.0181
 198 H       19.7697    17.0774    -3.0581 H     12 MET263   0.1883
 199 HA      20.7031    19.6306    -2.9248 H     12 MET263   0.0800
 200 HB3     23.0599    18.6023    -2.3911 H     12 MET263   0.0320
 201 HB2     22.2909    17.0205    -2.6919 H     12 MET263   0.0320
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202	HG3	20.5543	17.6676	-0.8552	H	12 MET263	0.0378
203	HG2	21.5181	19.1358	-0.5548	H	12 MET263	0.0378
204	LPD2	22.7989	16.5218	-0.0965	LP	12 MET263	0.0000
205	LPD1	23.2752	17.4636	0.2436	LP	12 MET263	0.0000
206	HE3	21.4177	18.1131	1.9818	H	12 MET263	0.0340
207	HE2	22.2861	16.6220	2.4748	H	12 MET263	0.0340
208	HE1	20.7831	16.5012	1.5065	H	12 MET263	0.0340
209	N	22.0861	18.2070	-5.6079	N.am	13 TYR264	-0.2621
BACKBONE							
210	CA	22.7944	18.5779	-6.8367	C.3	13 TYR264	0.1390
BACKBONE							
211	C	21.8334	18.6048	-8.0035	C.2	13 TYR264	0.2058
BACKBONE							
212	O	22.0937	17.9907	-9.0259	O.2	13 TYR264	-0.3942
BACKBONE							
213	CB	24.0087	17.6366	-7.0401	C.3	13 TYR264	0.0163
214	CG	24.9893	17.8783	-5.8830	C.ar	13 TYR264	-0.0493
215	CD1	26.0136	18.8232	-6.0129	C.ar	13 TYR264	-0.0685
216	CD2	24.8630	17.1688	-4.6841	C.ar	13 TYR264	-0.0685
217	CE1	26.8897	19.0715	-4.9522	C.ar	13 TYR264	-0.0398
218	CE2	25.7285	17.4280	-3.6175	C.ar	13 TYR264	-0.0398
219	CZ	26.7459	18.3779	-3.7439	C.ar	13 TYR264	0.0805
220	OH	27.5993	18.6155	-2.6611	O.3	13 TYR264	-0.3376
221	H	21.7445	17.2682	-5.5287	H	13 TYR264	0.1885
222	HA	23.2050	19.6004	-6.7925	H	13 TYR264	0.0821
223	HB2	24.5061	17.8518	-7.9998	H	13 TYR264	0.0453
224	HB3	23.6779	16.5863	-7.0611	H	13 TYR264	0.0453
225	HD1	26.1325	19.3746	-6.9405	H	13 TYR264	0.0530
226	HD2	24.0902	16.4152	-4.5748	H	13 TYR264	0.0530
227	HE1	27.6788	19.8067	-5.0768	H	13 TYR264	0.0525
228	HE2	25.6116	16.8889	-2.6829	H	13 TYR264	0.0525
229	HH	28.2655	19.2739	-2.8239	H	13 TYR264	0.2458
230	N	20.7168	19.3542	-7.8576	N.am	14 TRP265	-0.2625
BACKBONE							
231	CA	19.8119	19.5720	-8.9864	C.3	14 TRP265	0.1354
BACKBONE							
232	C	20.5105	20.5644	-9.8871	C.2	14 TRP265	0.2077
BACKBONE							
233	O	20.8260	21.6153	-9.3506	O.2	14 TRP265	-0.3940
BACKBONE							
234	CB	18.4802	20.1846	-8.4786	C.3	14 TRP265	0.0042
235	CG	17.4671	20.4866	-9.5528	C.2	14 TRP265	-0.0418
236	CD1	17.0214	21.7018	-9.9128	C.2	14 TRP265	0.0167
237	CD2	16.7351	19.4834	-10.4098	C.ar	14 TRP265	-0.0214
238	NE1	16.0982	21.5766	-10.8312	N.pl3	14 TRP265	-0.2890
239	CE2	15.8755	20.2853	-11.1376	C.ar	14 TRP265	0.0603
240	CE3	16.7662	18.1000	-10.5742	C.ar	14 TRP265	-0.0747
241	CZ2	14.9429	19.7497	-12.0247	C.ar	14 TRP265	-0.0443
242	CZ3	15.8786	17.5562	-11.5121	C.ar	14 TRP265	-0.0792
243	CH2	14.9521	18.3594	-12.1936	C.ar	14 TRP265	-0.0768
244	H	20.5437	19.8400	-6.9980	H	14 TRP265	0.1884
245	HA	19.5750	18.6109	-9.4622	H	14 TRP265	0.0815

246	HB3	18.6850	21.1119	-7.9199	H	14 TRP265	0.0397
247	HB2	18.0268	19.4720	-7.7786	H	14 TRP265	0.0397
248	HD1	17.3674	22.6463	-9.4961	H	14 TRP265	0.0795
249	HE1	15.5941	22.3674	-11.2580	H	14 TRP265	0.2216
250	HE3	17.4459	17.4782	-10.0042	H	14 TRP265	0.0540
251	HZ2	14.2390	20.3837	-12.5513	H	14 TRP265	0.0541
252	HZ3	15.9066	16.4949	-11.7216	H	14 TRP265	0.0510
253	HH2	14.2327	17.8981	-12.8620	H	14 TRP265	0.0530
254	N	20.8012	20.3446	-11.1963	N.am	15 PRO266	-0.2497
BACKBONE							
255	CA	21.4927	21.3780	-11.9549	C.3	15 PRO266	0.1338
BACKBONE							
256	C	20.8387	22.7383	-11.8403	C.2	15 PRO266	0.2042
BACKBONE							
257	O	19.6285	22.7976	-11.6869	O.2	15 PRO266	-0.3944
BACKBONE							
258	CB	21.4133	20.7916	-13.3814	C.3	15 PRO266	-0.0104
259	CG	21.3915	19.2661	-13.1402	C.3	15 PRO266	-0.0281
260	CD	20.4902	19.1004	-11.8905	C.3	15 PRO266	0.0369
261	HA	22.5406	21.3949	-11.6122	H	15 PRO266	0.0802
262	HB3	22.2348	21.1265	-14.0354	H	15 PRO266	0.0313
263	HB2	20.4557	21.0716	-13.8389	H	15 PRO266	0.0313
264	HG2	21.0315	18.7051	-14.0169	H	15 PRO266	0.0287
265	HG3	22.4173	18.9359	-12.9031	H	15 PRO266	0.0287
266	HD2	19.4214	19.0759	-12.1586	H	15 PRO266	0.0524
267	HD3	20.7747	18.1817	-11.3553	H	15 PRO266	0.0524
268	N	21.6310	23.8344	-11.8897	N.am	16 SER267	-0.2616
BACKBONE							
269	CA	21.0763	25.1648	-11.6382	C.3	16 SER267	0.1539
BACKBONE							
270	C	20.2920	25.7065	-12.8111	C.2	16 SER267	0.2062
BACKBONE							
271	O	19.3335	26.4276	-12.5799	O.2	16 SER267	-0.3943
BACKBONE							
272	CB	22.2180	26.1665	-11.3262	C.3	16 SER267	0.0843
273	OG	22.9873	25.6541	-10.2249	O.3	16 SER267	-0.3903
274	H	22.6140	23.7518	-12.0689	H	16 SER267	0.1884
275	HA	20.4247	25.1165	-10.7487	H	16 SER267	0.0823
276	HB3	21.7916	27.1511	-11.0676	H	16 SER267	0.0606
277	HB2	22.8613	26.2822	-12.2153	H	16 SER267	0.0606
278	HG	23.7105	26.2255	-9.9860	H	16 SER267	0.2097
279	N	20.6750	25.3949	-14.0721	N.am	17 SER268	-0.2615
BACKBONE							
280	CA	20.0292	26.0343	-15.2221	C.3	17 SER268	0.1539
BACKBONE							
281	C	18.7155	25.3963	-15.6286	C.2	17 SER268	0.2062
BACKBONE							
282	O	18.3453	25.5533	-16.7821	O.2	17 SER268	-0.3943
BACKBONE							
283	CB	21.0159	26.0136	-16.4208	C.3	17 SER268	0.0843
284	OG	21.2370	24.6398	-16.7866	O.3	17 SER268	-0.3903
285	H	21.4210	24.7475	-14.2420	H	17 SER268	0.1884

286	HA	19.8224	27.0927	-14.9896	H	17 SER268	0.0823
287	HB3	21.9675	26.4830	-16.1191	H	17 SER268	0.0606
288	HB2	20.6065	26.5776	-17.2764	H	17 SER268	0.0606
289	HG	21.8404	24.5454	-17.5170	H	17 SER268	0.2097
290	N	17.9864	24.6863	-14.7342	N.am	18 VAL269	-0.2634
BACKBONE							
291	CA	16.7209	24.0658	-15.1263	C.3	18 VAL269	0.1334
BACKBONE							
292	C	15.6275	24.9816	-14.6124	C.2	18 VAL269	0.2066
BACKBONE							
293	O	15.6451	25.1989	-13.4112	O.2	18 VAL269	-0.3942
BACKBONE							
294	CB	16.6204	22.6397	-14.5157	C.3	18 VAL269	-0.0062
295	CG1	15.2916	21.9585	-14.9340	C.3	18 VAL269	-0.0584
296	CG2	17.8187	21.7703	-14.9831	C.3	18 VAL269	-0.0584
297	H	18.2635	24.5879	-13.7788	H	18 VAL269	0.1883
298	HA	16.6868	23.9029	-16.2120	H	18 VAL269	0.0803
299	HB	16.6641	22.7161	-13.4164	H	18 VAL269	0.0343
300	HG13	14.4332	22.4567	-14.4617	H	18 VAL269	0.0234
301	HG12	15.2913	20.9010	-14.6367	H	18 VAL269	0.0234
302	HG11	15.1772	22.0063	-16.0270	H	18 VAL269	0.0234
303	HG23	17.7210	21.5062	-16.0475	H	18 VAL269	0.0234
304	HG22	17.8632	20.8451	-14.3877	H	18 VAL269	0.0234
305	HG21	18.7637	22.3142	-14.8507	H	18 VAL269	0.0234
306	N	14.6857	25.5586	-15.4063	N.am	19 PRO270	-0.2498
BACKBONE							
307	CA	13.7129	26.4780	-14.8295	C.3	19 PRO270	0.1338
BACKBONE							
308	C	12.9973	25.9759	-13.5947	C.2	19 PRO270	0.2041
BACKBONE							
309	O	12.8776	26.7333	-12.6438	O.2	19 PRO270	-0.3944
BACKBONE							
310	CB	12.7289	26.6273	-16.0149	C.3	19 PRO270	-0.0104
311	CG	13.6306	26.4601	-17.2582	C.3	19 PRO270	-0.0281
312	CD	14.6157	25.3362	-16.8489	C.3	19 PRO270	0.0369
313	HA	14.2220	27.4371	-14.6332	H	19 PRO270	0.0802
314	HB3	12.1963	27.5923	-15.9926	H	19 PRO270	0.0313
315	HB2	11.9914	25.8061	-16.0148	H	19 PRO270	0.0313
316	HG2	13.0699	26.2210	-18.1780	H	19 PRO270	0.0287
317	HG3	14.1874	27.4010	-17.4119	H	19 PRO270	0.0287
318	HD2	14.1936	24.3373	-17.0520	H	19 PRO270	0.0524
319	HD3	15.5678	25.4791	-17.3857	H	19 PRO270	0.0524
320	N	12.5108	24.7120	-13.6004	N.am	20 VAL271	-0.2635
BACKBONE							
321	CA	11.7904	24.1926	-12.4368	C.3	20 VAL271	0.1332
BACKBONE							
322	C	12.8041	23.8478	-11.3650	C.2	20 VAL271	0.2042
BACKBONE							
323	O	13.9259	23.5330	-11.7322	O.2	20 VAL271	-0.3944
BACKBONE							
324	CB	10.8876	22.9909	-12.8448	C.3	20 VAL271	-0.0063
325	CG1	10.2210	22.3243	-11.6148	C.3	20 VAL271	-0.0584

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 326 CG2      9.7865    23.4545   -13.8422 C.3   20 VAL271  -0.0584
 327 H       12.6692    24.1114   -14.3866 H     20 VAL271   0.1883
 328 HA      11.1270    24.9818   -12.0436 H     20 VAL271   0.0802
 329 HB      11.5179    22.2253   -13.3330 H     20 VAL271   0.0343
 330 HG13    10.9819    21.9627   -10.9120 H     20 VAL271   0.0234
 331 HG12     9.6344    21.4592   -11.9502 H     20 VAL271   0.0234
 332 HG11     9.5537    23.0266   -11.0932 H     20 VAL271   0.0234
 333 HG23     9.1725    24.2527   -13.3977 H     20 VAL271   0.0234
 334 HG22     9.1205    22.6164   -14.0915 H     20 VAL271   0.0234
 335 HG21    10.2279    23.8334   -14.7767 H     20 VAL271   0.0234
 336 N       12.4341    23.9262   -10.0574 N.am  21 GLN272  -0.2636
BACKBONE
 337 CA      13.4103    23.7790    -8.9732 C.3   21 GLN272   0.1332
BACKBONE
 338 C       12.9482    22.7772    -7.9310 C.2   21 GLN272   0.2065
BACKBONE
 339 O       11.8011    22.3686    -8.0244 O.2   21 GLN272  -0.3942
BACKBONE
 340 CB      13.6584    25.2076    -8.4085 C.3   21 GLN272   0.0045
 341 CG      14.4921    26.0717    -9.3939 C.3   21 GLN272   0.0412
 342 CD      15.8698    25.4892    -9.6213 C.2   21 GLN272   0.1737
 343 OE1     16.1323    24.9823   -10.7010 O.2   21 GLN272  -0.3973
 344 NE2     16.7742    25.5416    -8.6182 N.am  21 GLN272  -0.3009
 345 H       11.4961    24.1627    -9.7938 H     21 GLN272   0.1883
 346 HA      14.3391    23.3552    -9.3758 H     21 GLN272   0.0801
 347 HB3     14.1853    25.1828    -7.4481 H     21 GLN272   0.0337
 348 HB2     12.6861    25.6918    -8.2220 H     21 GLN272   0.0337
 349 HG3     14.6062    27.0894    -8.9870 H     21 GLN272   0.0504
 350 HG2     13.9576    26.1573   -10.3515 H     21 GLN272   0.0504
 351 HE21    16.5517    25.9617    -7.7377 H     21 GLN272   0.1814
 352 HE22    17.6891    25.1592    -8.7539 H     21 GLN272   0.1814
 353 N       13.7798    22.3142    -6.9548 N.am  22 PRO273  -0.2498
BACKBONE
 354 CA      13.3824    21.1811    -6.1235 C.3   22 PRO273   0.1338
BACKBONE
 355 C       12.1311    21.2966    -5.2941 C.2   22 PRO273   0.2041
BACKBONE
 356 O       11.4191    20.3114    -5.1935 O.2   22 PRO273  -0.3944
BACKBONE
 357 CB      14.6036    21.0843    -5.1814 C.3   22 PRO273  -0.0104
 358 CG      15.7566    21.5706    -6.0857 C.3   22 PRO273  -0.0281
 359 CD      15.1365    22.8198    -6.7427 C.3   22 PRO273   0.0369
 360 HA      13.3579    20.2763    -6.7492 H     22 PRO273   0.0802
 361 HB3     14.7276    20.0723    -4.7740 H     22 PRO273   0.0313
 362 HB2     14.5082    21.7848    -4.3360 H     22 PRO273   0.0313
 363 HG2     16.6903    21.7792    -5.5381 H     22 PRO273   0.0287
 364 HG3     15.9516    20.8300    -6.8790 H     22 PRO273   0.0287
 365 HD2     15.1324    23.6414    -6.0091 H     22 PRO273   0.0524
 366 HD3     15.7201    23.1046    -7.6274 H     22 PRO273   0.0524
 367 N       11.8579    22.4567    -4.6606 N.am  23 GLU274  -0.2636
BACKBONE
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368	CA	10.7627	22.5028	-3.6924	C.3	23 GLU274	0.1325
BACKBONE							
369	C	9.4809	21.9894	-4.3099	C.2	23 GLU274	0.2040
BACKBONE							
370	O	8.8080	21.1804	-3.6897	O.2	23 GLU274	-0.3944
BACKBONE							
371	CB	10.5646	23.9344	-3.1221	C.3	23 GLU274	-0.0008
372	CG	9.5144	23.9746	-1.9782	C.3	23 GLU274	0.0044
373	CD	9.8960	23.1007	-0.8076	C.2	23 GLU274	0.0350
374	OE1	11.1076	23.0504	-0.4590	O.co2	23 GLU274	-0.5690
375	OE2	8.9840	22.4556	-0.2220	O.co2	23 GLU274	-0.5690
376	H	12.4411	23.2615	-4.7874	H	23 GLU274	0.1883
377	HA	11.0461	21.8325	-2.8644	H	23 GLU274	0.0801
378	HB3	10.2497	24.6065	-3.9371	H	23 GLU274	0.0330
379	HB2	11.5264	24.3049	-2.7304	H	23 GLU274	0.0330
380	HG3	8.5322	23.6651	-2.3704	H	23 GLU274	0.0433
381	HG2	9.4203	25.0082	-1.6083	H	23 GLU274	0.0433
382	N	9.1321	22.4418	-5.5359	N.am	24 GLN275	-0.2636
BACKBONE							
383	CA	7.9063	21.9579	-6.1696	C.3	24 GLN275	0.1330
BACKBONE							
384	C	8.0501	20.5045	-6.5684	C.2	24 GLN275	0.2040
BACKBONE							
385	O	7.0933	19.7581	-6.4345	O.2	24 GLN275	-0.3944
BACKBONE							
386	CB	7.5362	22.7574	-7.4482	C.3	24 GLN275	0.0045
387	CG	7.2154	24.2471	-7.1587	C.3	24 GLN275	0.0412
388	CD	6.7216	24.9109	-8.4243	C.2	24 GLN275	0.1737
389	OE1	5.5427	25.2163	-8.5139	O.2	24 GLN275	-0.3973
390	NE2	7.6009	25.1401	-9.4257	N.am	24 GLN275	-0.3009
391	H	9.7200	23.0826	-6.0334	H	24 GLN275	0.1883
392	HA	7.0755	22.0607	-5.4524	H	24 GLN275	0.0801
393	HB3	6.6376	22.2962	-7.8908	H	24 GLN275	0.0337
394	HB2	8.3612	22.6843	-8.1746	H	24 GLN275	0.0337
395	HG3	8.1080	24.7782	-6.7947	H	24 GLN275	0.0504
396	HG2	6.4397	24.3150	-6.3791	H	24 GLN275	0.0504
397	HE21	8.5669	24.8940	-9.3373	H	24 GLN275	0.1814
398	HE22	7.2855	25.5674	-10.2745	H	24 GLN275	0.1814
399	N	9.2281	20.0800	-7.0790	N.am	25 LEU276	-0.2637
BACKBONE							
400	CA	9.3776	18.6895	-7.5140	C.3	25 LEU276	0.1312
BACKBONE							
401	C	9.1370	17.7830	-6.3281	C.2	25 LEU276	0.2039
BACKBONE							
402	O	8.3166	16.8821	-6.4179	O.2	25 LEU276	-0.3944
BACKBONE							
403	CB	10.7776	18.4374	-8.1484	C.3	25 LEU276	-0.0101
404	CG	10.9468	19.1697	-9.5130	C.3	25 LEU276	-0.0425
405	CD1	12.4405	19.4298	-9.8507	C.3	25 LEU276	-0.0625
406	CD2	10.3104	18.3643	-10.6788	C.3	25 LEU276	-0.0625
407	H	10.0047	20.7073	-7.1607	H	25 LEU276	0.1883
408	HA	8.5992	18.4771	-8.2619	H	25 LEU276	0.0800

409	HB3	10.9372	17.3631	-8.3085	H	25 LEU276	0.0315
410	HB2	11.5420	18.7758	-7.4348	H	25 LEU276	0.0315
411	HG	10.4438	20.1473	-9.4505	H	25 LEU276	0.0298
412	HD13	12.9197	20.0666	-9.0953	H	25 LEU276	0.0232
413	HD12	12.5145	19.9455	-10.8183	H	25 LEU276	0.0232
414	HD11	12.9931	18.4819	-9.9148	H	25 LEU276	0.0232
415	HD23	10.8667	17.4300	-10.8420	H	25 LEU276	0.0232
416	HD22	10.3589	18.9647	-11.5993	H	25 LEU276	0.0232
417	HD21	9.2611	18.1046	-10.4857	H	25 LEU276	0.0232
418	N	9.8335	18.0241	-5.1960	N.am	26 ALA277	-0.2640
BACKBONE							
419	CA	9.5856	17.2268	-3.9994	C.3	26 ALA277	0.1282
BACKBONE							
420	C	8.1192	17.3041	-3.6335	C.2	26 ALA277	0.2036
BACKBONE							
421	O	7.5360	16.2722	-3.3403	O.2	26 ALA277	-0.3944
BACKBONE							
422	CB	10.4534	17.7141	-2.8105	C.3	26 ALA277	-0.0244
423	H	10.5084	18.7599	-5.1531	H	26 ALA277	0.1883
424	HA	9.8611	16.1835	-4.2172	H	26 ALA277	0.0797
425	HB3	10.2238	18.7669	-2.5891	H	26 ALA277	0.0277
426	HB2	11.5226	17.6292	-3.0606	H	26 ALA277	0.0277
427	HB1	10.2570	17.1091	-1.9129	H	26 ALA277	0.0277
428	N	7.5048	18.5117	-3.6473	N.am	27 ALA278	-0.2640
BACKBONE							
429	CA	6.0908	18.6216	-3.2831	C.3	27 ALA278	0.1282
BACKBONE							
430	C	5.2580	17.6592	-4.0967	C.2	27 ALA278	0.2036
BACKBONE							
431	O	4.4063	16.9993	-3.5214	O.2	27 ALA278	-0.3944
BACKBONE							
432	CB	5.5347	20.0577	-3.4662	C.3	27 ALA278	-0.0244
433	H	8.0078	19.3440	-3.8877	H	27 ALA278	0.1883
434	HA	5.9875	18.3637	-2.2165	H	27 ALA278	0.0797
435	HB3	5.5141	20.3330	-4.5295	H	27 ALA278	0.0277
436	HB2	6.1590	20.7818	-2.9200	H	27 ALA278	0.0277
437	HB1	4.5085	20.1221	-3.0741	H	27 ALA278	0.0277
438	N	5.4989	17.5455	-5.4250	N.am	28 ALA279	-0.2640
BACKBONE							
439	CA	4.7193	16.6174	-6.2465	C.3	28 ALA279	0.1282
BACKBONE							
440	C	5.3305	15.2295	-6.2663	C.2	28 ALA279	0.2034
BACKBONE							
441	O	5.3956	14.6188	-7.3219	O.2	28 ALA279	-0.3944
BACKBONE							
442	CB	4.5190	17.2098	-7.6650	C.3	28 ALA279	-0.0244
443	H	6.2307	18.0702	-5.8636	H	28 ALA279	0.1883
444	HA	3.7063	16.5017	-5.8364	H	28 ALA279	0.0797
445	HB3	5.4962	17.3025	-8.1518	H	28 ALA279	0.0277
446	HB2	4.0650	18.2104	-7.5994	H	28 ALA279	0.0277
447	HB1	3.8718	16.5686	-8.2830	H	28 ALA279	0.0277

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 448 N        5.7641    14.6950    -5.0993 N.am  29 GLY280  -0.2664
BACKBONE
 449 CA       6.1862    13.2986    -5.0294 C.3   29 GLY280   0.1201
BACKBONE
 450 C        7.4119    12.9285    -5.8327 C.2   29 GLY280   0.2009
BACKBONE
 451 O        7.6561    11.7351    -5.9153 O.2   29 GLY280  -0.3947
BACKBONE
 452 H        5.7346    15.2067    -4.2405 H     29 GLY280   0.1881
 453 HA2      5.3472    12.6707    -5.3714 H     29 GLY280   0.0763
 454 HA3      6.3842    13.0271    -3.9818 H     29 GLY280   0.0763
 455 N        8.1941    13.8671    -6.4222 N.am  30 PHE281  -0.2622
BACKBONE
 456 CA       9.3158    13.4627    -7.2775 C.3   30 PHE281   0.1404
BACKBONE
 457 C       10.6423    13.5065    -6.5569 C.2   30 PHE281   0.2061
BACKBONE
 458 O       10.7476    14.2658    -5.6091 O.2   30 PHE281  -0.3942
BACKBONE
 459 CB       9.4284    14.3657    -8.5278 C.3   30 PHE281   0.0214
 460 CG       8.2041    14.2184    -9.4371 C.ar  30 PHE281  -0.0386
 461 CD1      8.0041    13.0376   -10.1604 C.ar  30 PHE281  -0.0601
 462 CD2      7.2862    15.2652    -9.5569 C.ar  30 PHE281  -0.0601
 463 CE1      6.8724    12.8874   -10.9673 C.ar  30 PHE281  -0.0686
 464 CE2      6.1511    15.1181   -10.3600 C.ar  30 PHE281  -0.0686
 465 CZ       5.9312    13.9160   -11.0368 C.ar  30 PHE281  -0.0687
 466 H        8.0310    14.8456    -6.2885 H     30 PHE281   0.1885
 467 HA       9.1615    12.4393    -7.6411 H     30 PHE281   0.0823
 468 HB3     10.3082    14.0734    -9.1089 H     30 PHE281   0.0474
 469 HB2      9.5711    15.4078    -8.2135 H     30 PHE281   0.0474
 470 HD1      8.7260    12.2319   -10.1035 H     30 PHE281   0.0557
 471 HD2      7.4547    16.1944    -9.0271 H     30 PHE281   0.0557
 472 HE1      6.7276    11.9765   -11.5397 H     30 PHE281   0.0599
 473 HE2      5.4473    15.9372   -10.4572 H     30 PHE281   0.0599
 474 HZ       5.0315    13.7787   -11.6222 H     30 PHE281   0.0559
 475 N       11.6563    12.7179    -7.0011 N.am  31 TYR282  -0.2620
BACKBONE
 476 CA      12.9478    12.6851    -6.3120 C.3   31 TYR282   0.1390
BACKBONE
 477 C       14.0776    12.5605    -7.3198 C.2   31 TYR282   0.2058
BACKBONE
 478 O       13.9705    11.7162    -8.1947 O.2   31 TYR282  -0.3942
BACKBONE
 479 CB      12.9221    11.5309    -5.2744 C.3   31 TYR282   0.0163
 480 CG      12.8546    10.1453    -5.9266 C.ar  31 TYR282  -0.0493
 481 CD1     11.6198     9.5643    -6.2345 C.ar  31 TYR282  -0.0685
 482 CD2     14.0314     9.4405    -6.2035 C.ar  31 TYR282  -0.0685
 483 CE1     11.5664     8.3098    -6.8493 C.ar  31 TYR282  -0.0398
 484 CE2     13.9711     8.1516    -6.7404 C.ar  31 TYR282  -0.0398
 485 CZ      12.7411     7.5837    -7.0802 C.ar  31 TYR282   0.0805
 486 OH      12.7098     6.3041    -7.6452 O.3   31 TYR282  -0.3376
 487 H       11.5343    12.1061    -7.7847 H     31 TYR282   0.1885
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488	HA	13.0849	13.6167	-5.7418	H	31 TYR282	0.0821
489	HB2	12.0383	11.6642	-4.6349	H	31 TYR282	0.0453
490	HB3	13.8036	11.5588	-4.6196	H	31 TYR282	0.0453
491	HD1	10.6965	10.0854	-5.9975	H	31 TYR282	0.0530
492	HD2	14.9984	9.8879	-5.9972	H	31 TYR282	0.0530
493	HE1	10.6074	7.9046	-7.1482	H	31 TYR282	0.0525
494	HE2	14.8824	7.5830	-6.8938	H	31 TYR282	0.0525
495	HH	11.8351	5.9657	-7.8021	H	31 TYR282	0.2458
496	N	15.1489	13.3916	-7.2358	N.am	32 TYR283	-0.2620
BACKBONE							
497	CA	16.2205	13.3620	-8.2396	C.3	32 TYR283	0.1390
BACKBONE							
498	C	16.9046	12.0144	-8.2963	C.2	32 TYR283	0.2057
BACKBONE							
499	O	16.9066	11.3372	-7.2803	O.2	32 TYR283	-0.3942
BACKBONE							
500	CB	17.2568	14.4867	-7.9241	C.3	32 TYR283	0.0163
501	CG	18.3821	14.7519	-8.9389	C.ar	32 TYR283	-0.0493
502	CD1	18.1144	14.8119	-10.3097	C.ar	32 TYR283	-0.0685
503	CD2	19.6967	14.9688	-8.5059	C.ar	32 TYR283	-0.0685
504	CE1	19.1393	15.0139	-11.2365	C.ar	32 TYR283	-0.0398
505	CE2	20.7200	15.2097	-9.4281	C.ar	32 TYR283	-0.0398
506	CZ	20.4523	15.2236	-10.7995	C.ar	32 TYR283	0.0805
507	OH	21.4962	15.4456	-11.7042	O.3	32 TYR283	-0.3376
508	H	15.2011	14.0885	-6.5197	H	32 TYR283	0.1885
509	HA	15.7345	13.5514	-9.2039	H	32 TYR283	0.0821
510	HB2	17.6894	14.2804	-6.9338	H	32 TYR283	0.0453
511	HB3	16.7254	15.4420	-7.8663	H	32 TYR283	0.0453
512	HD1	17.1013	14.7116	-10.6667	H	32 TYR283	0.0530
513	HD2	19.9366	14.9549	-7.4476	H	32 TYR283	0.0530
514	HE1	18.9001	15.0054	-12.2924	H	32 TYR283	0.0525
515	HE2	21.7326	15.3830	-9.0781	H	32 TYR283	0.0525
516	HH	21.2189	15.5031	-12.6118	H	32 TYR283	0.2458
517	N	17.4797	11.6194	-9.4636	N.am	33 VAL284	-0.2633
BACKBONE							
518	CA	18.1884	10.3417	-9.5708	C.3	33 VAL284	0.1332
BACKBONE							
519	C	19.5922	10.5346	-10.1134	C.2	33 VAL284	0.2039
BACKBONE							
520	O	20.1074	9.6416	-10.7673	O.2	33 VAL284	-0.3944
BACKBONE							
521	CB	17.3514	9.3052	-10.3816	C.3	33 VAL284	-0.0063
522	CG1	15.9697	9.0769	-9.7094	C.3	33 VAL284	-0.0584
523	CG2	17.1481	9.7244	-11.8661	C.3	33 VAL284	-0.0584
524	H	17.4355	12.1872	-10.2874	H	33 VAL284	0.1883
525	HA	18.3637	9.9041	-8.5737	H	33 VAL284	0.0802
526	HB	17.9020	8.3471	-10.3521	H	33 VAL284	0.0343
527	HG13	16.1147	8.8176	-8.6512	H	33 VAL284	0.0234
528	HG12	15.4245	8.2521	-10.1946	H	33 VAL284	0.0234
529	HG11	15.3534	9.9865	-9.7697	H	33 VAL284	0.0234
530	HG23	16.5236	10.6262	-11.9353	H	33 VAL284	0.0234
531	HG22	16.6433	8.9193	-12.4235	H	33 VAL284	0.0234

532 HG21	18.1115	9.9269	-12.3558	H	33	VAL284	0.0234
533 N	20.2465	11.6856	-9.8300	N.am	34	GLY285	-0.2664
BACKBONE							
534 CA	21.6398	11.8670	-10.2345	C.3	34	GLY285	0.1201
BACKBONE							
535 C	21.8797	11.8170	-11.7260	C.2	34	GLY285	0.2007
BACKBONE							
536 O	22.9696	11.4111	-12.0997	O.2	34	GLY285	-0.3947
BACKBONE							
537 H	19.8180	12.4009	-9.2785	H	34	GLY285	0.1881
538 HA2	22.2373	11.0832	-9.7411	H	34	GLY285	0.0763
539 HA3	22.0243	12.8374	-9.8850	H	34	GLY285	0.0763
540 N	20.9190	12.2268	-12.5908	N.am	35	ARG286	-0.2640
BACKBONE							
541 CA	21.1491	12.1786	-14.0383	C.3	35	ARG286	0.1311
BACKBONE							
542 C	20.4902	13.3672	-14.7079	C.2	35	ARG286	0.2040
BACKBONE							
543 O	19.2707	13.4120	-14.6967	O.2	35	ARG286	-0.3944
BACKBONE							
544 CB	20.5391	10.8799	-14.6343	C.3	35	ARG286	-0.0092
545 CG	21.2454	9.5977	-14.1186	C.3	35	ARG286	-0.0156
546 CD	20.5375	8.3119	-14.6274	C.3	35	ARG286	0.0627
547 NE	21.1736	7.1015	-14.1010	N.pl3	35	ARG286	-0.2723
548 CZ	20.7212	5.8852	-14.3265	C.cat	35	ARG286	0.2882
549 NH1	19.6597	5.6457	-15.0646	N.pl3	35	ARG286	-0.2849
550 NH2	21.3548	4.8661	-13.7931	N.pl3	35	ARG286	-0.2849
551 H	20.0229	12.5344	-12.2645	H	35	ARG286	0.1883
552 HA	22.2248	12.1862	-14.2787	H	35	ARG286	0.0800
553 HB3	20.6125	10.9116	-15.7349	H	35	ARG286	0.0313
554 HB2	19.4751	10.8315	-14.3634	H	35	ARG286	0.0313
555 HG3	21.2235	9.5778	-13.0200	H	35	ARG286	0.0301
556 HG2	22.2988	9.5984	-14.4448	H	35	ARG286	0.0301
557 HD3	20.5730	8.3043	-15.7296	H	35	ARG286	0.0689
558 HD2	19.4884	8.3514	-14.2887	H	35	ARG286	0.0689
559 HE	22.0160	7.2233	-13.5153	H	35	ARG286	0.2642
560 HH11	19.1286	6.4026	-15.5125	H	35	ARG286	0.2615
561 HH12	19.3312	4.6806	-15.2181	H	35	ARG286	0.2615
562 HH21	22.1922	5.0048	-13.2065	H	35	ARG286	0.2615
563 HH22	21.0323	3.8984	-13.9454	H	35	ARG286	0.2615
564 N	21.2482	14.3229	-15.3030	N.am	36	ASN287	-0.2616
BACKBONE							
565 CA	20.6130	15.3921	-16.0763	C.3	36	ASN287	0.1476
BACKBONE							
566 C	19.5365	16.0398	-15.2303	C.2	36	ASN287	0.2063
BACKBONE							
567 O	19.8845	16.4241	-14.1252	O.2	36	ASN287	-0.3942
BACKBONE							
568 CB	20.1692	14.7685	-17.4287	C.3	36	ASN287	0.0773
569 CG	21.3358	14.0690	-18.0869	C.2	36	ASN287	0.1780
570 OD1	21.3790	12.8484	-18.0748	O.2	36	ASN287	-0.3970
571 ND2	22.3015	14.8183	-18.6638	N.am	36	ASN287	-0.3007

572 H	22.2504	14.2869	-15.2883	H	36	ASN287	0.1885
573 HA	21.3487	16.1865	-16.2902	H	36	ASN287	0.0826
574 HB3	19.7925	15.5456	-18.1126	H	36	ASN287	0.0551
575 HB2	19.3674	14.0324	-17.2615	H	36	ASN287	0.0551
576 HD21	22.2520	15.8180	-18.6689	H	36	ASN287	0.1814
577 HD22	23.0818	14.3684	-19.0999	H	36	ASN287	0.1814
578 N	18.2622	16.1642	-15.6775	N.am	37	ASP288	-0.2620
BACKBONE							
579 CA	17.2001	16.6788	-14.8131	C.3	37	ASP288	0.1423
BACKBONE							
580 C	16.1440	15.5994	-14.7133	C.2	37	ASP288	0.2057
BACKBONE							
581 O	14.9658	15.8706	-14.8834	O.2	37	ASP288	-0.3943
BACKBONE							
582 CB	16.6910	18.0147	-15.4151	C.3	37	ASP288	0.0406
583 CG	16.1005	17.8806	-16.7950	C.2	37	ASP288	0.0393
584 OD1	16.1637	16.7670	-17.3829	O.co2	37	ASP288	-0.5688
585 OD2	15.5647	18.9009	-17.3080	O.co2	37	ASP288	-0.5688
586 H	17.9815	15.8830	-16.5948	H	37	ASP288	0.1884
587 HA	17.5465	16.8765	-13.7853	H	37	ASP288	0.0819
588 HB3	17.5480	18.7002	-15.4884	H	37	ASP288	0.0478
589 HB2	15.9417	18.4622	-14.7469	H	37	ASP288	0.0478
590 N	16.5937	14.3490	-14.4514	N.am	38	ASP289	-0.2621
BACKBONE							
591 CA	15.6904	13.2002	-14.4474	C.3	38	ASP289	0.1423
BACKBONE							
592 C	15.1145	13.0078	-13.0663	C.2	38	ASP289	0.2056
BACKBONE							
593 O	15.8634	13.1783	-12.1186	O.2	38	ASP289	-0.3943
BACKBONE							
594 CB	16.4731	11.9102	-14.8105	C.3	38	ASP289	0.0406
595 CG	17.0702	11.9568	-16.1941	C.2	38	ASP289	0.0393
596 OD1	16.9212	12.9978	-16.8899	O.co2	38	ASP289	-0.5688
597 OD2	17.6977	10.9417	-16.6040	O.co2	38	ASP289	-0.5688
598 H	17.5622	14.1877	-14.2547	H	38	ASP289	0.1884
599 HA	14.8921	13.3414	-15.1912	H	38	ASP289	0.0819
600 HB3	15.8170	11.0327	-14.7374	H	38	ASP289	0.0478
601 HB2	17.2833	11.7735	-14.0809	H	38	ASP289	0.0478
602 N	13.8169	12.6449	-12.9227	N.am	39	VAL290	-0.2634
BACKBONE							
603 CA	13.2500	12.4246	-11.5917	C.3	39	VAL290	0.1333
BACKBONE							
604 C	12.2202	11.3226	-11.6749	C.2	39	VAL290	0.2041
BACKBONE							
605 O	11.6962	11.1722	-12.7651	O.2	39	VAL290	-0.3944
BACKBONE							
606 CB	12.5653	13.7215	-11.0660	C.3	39	VAL290	-0.0063
607 CG1	13.4785	14.9687	-11.2043	C.3	39	VAL290	-0.0584
608 CG2	11.2225	14.0179	-11.7947	C.3	39	VAL290	-0.0584
609 H	13.2143	12.5313	-13.7149	H	39	VAL290	0.1883
610 HA	14.0416	12.0997	-10.8942	H	39	VAL290	0.0802
611 HB	12.3714	13.5619	-9.9928	H	39	VAL290	0.0343

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 612 HG13    14.4244    14.8077   -10.6760 H     39 VAL290   0.0234
 613 HG12    12.9893    15.8514   -10.7664 H     39 VAL290   0.0234
 614 HG11    13.6923    15.1871   -12.2611 H     39 VAL290   0.0234
 615 HG23    11.4018    14.1653   -12.8693 H     39 VAL290   0.0234
 616 HG22    10.7673    14.9323   -11.3901 H     39 VAL290   0.0234
 617 HG21    10.4897    13.2087   -11.6691 H     39 VAL290   0.0234
 618 O        9.6567    13.0857   -20.2209 O.2   40 LYS291  -0.3942
BACKBONE
 619 C        8.6507    13.1409   -20.9098 C.2   40 LYS291   0.2067
BACKBONE
 620 N        7.7144    12.1562   -20.8343 N.am  40 LYS291  -0.2498
BACKBONE
 621 C        7.9389    11.0005   -19.9751 C.3   40 LYS291   0.1338
BACKBONE
 622 H        7.8404    11.3248   -18.9250 H     40 LYS291   0.0802
 623 C        9.2419    10.2902   -20.2574 C.2   40 LYS291   0.2038
BACKBONE
 624 N        9.9822     9.7901   -19.2402 N.am  40 LYS291  -0.2719
BACKBONE
 625 H        9.6999     9.8863   -18.2811 H     40 LYS291   0.1879
 626 C       11.1799     9.0067   -19.5331 C.3   40 LYS291   0.0721
BACKBONE
 627 H       11.6893     9.3488   -20.4482 H     40 LYS291   0.0703
 628 C       12.2242     9.0554   -18.4284 C.ar  40 LYS291  -0.0243
BACKBONE
 629 C       12.6912     7.7907   -18.0921 C.ar  40 LYS291  -0.0074
BACKBONE
 630 C       12.0303     6.7210   -18.9460 C.3   40 LYS291  -0.0199
BACKBONE
 631 H       12.7674     6.3730   -19.6865 H     40 LYS291   0.0389
 632 H       11.6838     5.8703   -18.3374 H     40 LYS291   0.0389
 633 C       10.8667     7.4874   -19.6366 C.3   40 LYS291  -0.0141
BACKBONE
 634 H       10.7194     7.1620   -20.6777 H     40 LYS291   0.0326
 635 H        9.9392     7.2850   -19.0815 H     40 LYS291   0.0326
 636 C       13.6564     7.6123   -17.0998 C.ar  40 LYS291   0.1199
BACKBONE
 637 C       14.2687     8.7617   -16.5805 C.ar  40 LYS291  -0.0439
BACKBONE
 638 H       15.1086     8.6810   -15.9042 H     40 LYS291   0.0468
 639 C       13.8071    10.0335   -16.9393 C.ar  40 LYS291  -0.0838
BACKBONE
 640 H       14.2951    10.9105   -16.5427 H     40 LYS291   0.0515
 641 C       12.7154    10.1945   -17.7968 C.ar  40 LYS291  -0.0756
BACKBONE
 642 H       12.2693    11.1663   -17.9680 H     40 LYS291   0.0448
 643 O       13.9800     6.3154   -16.6766 O.3   40 LYS291  -0.1602
BACKBONE
 644 S       14.7818     5.9650   -15.4401 S.o2  40 LYS291   0.1795
 645 O       14.6675     4.5291   -15.2791 O.2   40 LYS291  -0.1229
BACKBONE
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 646 O      16.1189    6.5127   -15.5487 O.2   40 LYS291  -0.1229
BACKBONE
 647 N1     13.9903    6.7079   -14.1667 N.am  40 LYS291  -0.2249
 648 O       9.5745   10.1698   -21.4248 O.2   40 LYS291  -0.3944
BACKBONE
 649 C       6.7571   10.0835   -20.3842 C.3   40 LYS291  -0.0104
BACKBONE
 650 H       7.0330    9.4540   -21.2433 H     40 LYS291   0.0313
 651 H       6.4111    9.4316   -19.5648 H     40 LYS291   0.0313
 652 C       5.6768   11.0766   -20.8572 C.3   40 LYS291  -0.0281
BACKBONE
 653 H       5.1922   11.4939   -19.9593 H     40 LYS291   0.0287
 654 H       4.9138   10.5992   -21.4911 H     40 LYS291   0.0287
 655 C       6.4691   12.1813   -21.6016 C.3   40 LYS291   0.0369
BACKBONE
 656 H       5.9058   13.1286   -21.5721 H     40 LYS291   0.0524
 657 H       6.6715   11.8881   -22.6446 H     40 LYS291   0.0524
 658 C       8.5429   14.3477   -21.8262 C.3   40 LYS291   0.1339
BACKBONE
 659 H       7.6049   14.3730   -22.3982 H     40 LYS291   0.0803
 660 N       8.6776   15.5818   -21.0441 N.am  40 LYS291  -0.2641
BACKBONE
 661 H       9.6012   15.9210   -20.8733 H     40 LYS291   0.1883
 662 C       7.5892   16.2443   -20.5784 C.2   40 LYS291   0.1952
BACKBONE
 663 C       7.7654   17.6009   -19.9196 C.3   40 LYS291   0.0951
BACKBONE
 664 H       8.2585   18.2569   -20.6516 H     40 LYS291   0.0700
 665 N       6.4400   18.1934   -19.5987 N.3   40 LYS291  -0.2998
BACKBONE
 666 H       6.5222   18.9364   -18.8162 H     40 LYS291   0.1245
 667 C       5.7022   18.7705   -20.7448 C.3   40 LYS291  -0.0133
BACKBONE
 668 H       6.2462   19.6326   -21.1629 H     40 LYS291   0.0390
 669 H       5.5591   18.0225   -21.5380 H     40 LYS291   0.0390
 670 H       4.7094   19.1140   -20.4167 H     40 LYS291   0.0390
 671 C       8.6895   17.5443   -18.6694 C.3   40 LYS291  -0.0322
BACKBONE
 672 H       8.3349   16.7823   -17.9684 H     40 LYS291   0.0269
 673 H       9.7216   17.2971   -18.9442 H     40 LYS291   0.0269
 674 H       8.7183   18.5135   -18.1478 H     40 LYS291   0.0269
 675 O       6.4592   15.7950   -20.6857 O.2   40 LYS291  -0.3952
BACKBONE
 676 C       9.6709   14.2687   -22.8992 C.3   40 LYS291  -0.0006
BACKBONE
 677 H      10.6408   14.2622   -22.3725 H     40 LYS291   0.0348
 678 C       9.5689   12.9754   -23.7550 C.3   40 LYS291  -0.0460
BACKBONE
 679 H       9.5969   12.0832   -23.1116 H     40 LYS291   0.0270
 680 H       8.6092   12.9672   -24.2967 H     40 LYS291   0.0270
 681 C      10.7403   12.9074   -24.7708 C.3   40 LYS291  -0.0526
BACKBONE
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 682 H       10.6476    11.9953   -25.3827 H     40 LYS291   0.0265
 683 H       11.6972    12.8537   -24.2267 H     40 LYS291   0.0265
 684 C       10.7375    14.1502   -25.6976 C.3   40 LYS291  -0.0530
BACKBONE
 685 H        9.8170    14.1592   -26.3031 H     40 LYS291   0.0265
 686 H       11.5969    14.1012   -26.3857 H     40 LYS291   0.0265
 687 C       10.8108    15.4487   -24.8560 C.3   40 LYS291  -0.0526
BACKBONE
 688 H       10.7728    16.3278   -25.5214 H     40 LYS291   0.0265
 689 H       11.7665    15.4811   -24.3059 H     40 LYS291   0.0265
 690 C        9.6319    15.4996   -23.8500 C.3   40 LYS291  -0.0460
BACKBONE
 691 H        8.6779    15.5248   -24.4009 H     40 LYS291   0.0270
 692 H        9.7083    16.4339   -23.2772 H     40 LYS291   0.0270
 693 N       11.8935    10.5758   -10.5902 N.am  40 LYS291  -0.2637
BACKBONE
 694 CA      10.8153     9.5819   -10.6562 C.3   40 LYS291   0.1310
BACKBONE
 695 C        9.8454     9.8009    -9.5240 C.2   40 LYS291   0.2039
BACKBONE
 696 O       10.2396    10.4079    -8.5439 O.2   40 LYS291  -0.3944
BACKBONE
 697 CB      11.3462     8.1220   -10.6578 C.3   40 LYS291  -0.0123
 698 CG      12.4069     7.9164   -11.7740 C.3   40 LYS291  -0.0474
 699 CD      12.7968     6.4242   -11.9413 C.3   40 LYS291  -0.0358
 700 CE      14.0775     6.2088   -12.8034 C.3   40 LYS291   0.0287
 701 H1      13.5681     7.5989   -14.2859 H     40 LYS291   0.1695
 702 H       12.3654    10.6969    -9.7171 H     40 LYS291   0.1883
 703 HA      10.2211     9.7349   -11.5683 H     40 LYS291   0.0800
 704 HB3     10.5181     7.4093   -10.8048 H     40 LYS291   0.0312
 705 HB2     11.7957     7.9070    -9.6796 H     40 LYS291   0.0312
 706 HG3     13.3066     8.4949   -11.5230 H     40 LYS291   0.0268
 707 HG2     12.0006     8.2961   -12.7230 H     40 LYS291   0.0268
 708 HD3     11.9508     5.8804   -12.3925 H     40 LYS291   0.0281
 709 HD2     12.9615     6.0174   -10.9306 H     40 LYS291   0.0281
 710 HE3     14.9356     6.6949   -12.3163 H     40 LYS291   0.0476
 711 HE2     14.2896     5.1318   -12.8532 H     40 LYS291   0.0476
 712 N        8.5782     9.3372    -9.6436 N.am  41 CYS292  -0.2629
BACKBONE
 713 CA       7.5976     9.5528    -8.5772 C.3   41 CYS292   0.1406
BACKBONE
 714 C        7.8240     8.4869    -7.5364 C.2   41 CYS292   0.2049
BACKBONE
 715 O        8.1043     7.3674    -7.9324 O.2   41 CYS292  -0.3943
BACKBONE
 716 CB       6.1562     9.4378    -9.1318 C.3   41 CYS292   0.0443
 717 SG       4.8773     9.8716    -7.9145 S.3   41 CYS292  -0.0882
 718 H        8.2967     8.8064   -10.4482 H     41 CYS292   0.1884
 719 HA       7.7083    10.5635    -8.1661 H     41 CYS292   0.0808
 720 HB3      5.9923     8.3969    -9.4248 H     41 CYS292   0.0432
 721 HB2      6.0284    10.0888   -10.0082 H     41 CYS292   0.0432
 722 LPG2     4.8849     9.4603    -7.3742 LP    41 CYS292   0.0000
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723	LPG1	4.9250	10.5167	-7.7085	LP	41 CYS292	0.0000
724	N	7.7179	8.7719	-6.2201	N.am	42 PHE293	-0.2619
BACKBONE							
725	CA	7.9688	7.7100	-5.2482	C.3	42 PHE293	0.1404
BACKBONE							
726	C	6.8866	6.6619	-5.3555	C.2	42 PHE293	0.2060
BACKBONE							
727	O	7.2085	5.4835	-5.3547	O.2	42 PHE293	-0.3942
BACKBONE							
728	CB	8.1137	8.2195	-3.7897	C.3	42 PHE293	0.0214
729	CG	6.7749	8.5718	-3.1224	C.ar	42 PHE293	-0.0386
730	CD1	6.2826	9.8807	-3.1522	C.ar	42 PHE293	-0.0601
731	CD2	6.0389	7.5835	-2.4566	C.ar	42 PHE293	-0.0601
732	CE1	5.1142	10.2196	-2.4650	C.ar	42 PHE293	-0.0686
733	CE2	4.8693	7.9163	-1.7673	C.ar	42 PHE293	-0.0686
734	CZ	4.4168	9.2381	-1.7557	C.ar	42 PHE293	-0.0687
735	H	7.4692	9.6860	-5.8982	H	42 PHE293	0.1885
736	HA	8.9371	7.2456	-5.5017	H	42 PHE293	0.0823
737	HB3	8.7861	9.0910	-3.7955	H	42 PHE293	0.0474
738	HB2	8.5863	7.4377	-3.1723	H	42 PHE293	0.0474
739	HD1	6.8096	10.6427	-3.7083	H	42 PHE293	0.0557
740	HD2	6.3750	6.5509	-2.4686	H	42 PHE293	0.0557
741	HE1	4.7538	11.2428	-2.4820	H	42 PHE293	0.0599
742	HE2	4.3129	7.1476	-1.2396	H	42 PHE293	0.0599
743	HZ	3.5272	9.4994	-1.1949	H	42 PHE293	0.0559
744	N	5.5988	7.0699	-5.4520	N.am	43 SER294	-0.2614
BACKBONE							
745	CA	4.5256	6.0802	-5.4923	C.3	43 SER294	0.1539
BACKBONE							
746	C	4.4030	5.4684	-6.8719	C.2	43 SER294	0.2062
BACKBONE							
747	O	4.5759	4.2653	-6.9903	O.2	43 SER294	-0.3943
BACKBONE							
748	CB	3.1774	6.6853	-5.0220	C.3	43 SER294	0.0843
749	OG	2.1996	5.6330	-4.9756	O.3	43 SER294	-0.3903
750	H	5.3576	8.0425	-5.4916	H	43 SER294	0.1884
751	HA	4.7542	5.2815	-4.7640	H	43 SER294	0.0823
752	HB3	2.8453	7.4868	-5.7014	H	43 SER294	0.0606
753	HB2	3.3112	7.1162	-4.0152	H	43 SER294	0.0606
754	HG	1.3595	5.9318	-4.6451	H	43 SER294	0.2097
755	N	4.0957	6.2621	-7.9264	N.am	44 CYS295	-0.2628
BACKBONE							
756	CA	3.8504	5.6815	-9.2486	C.3	44 CYS295	0.1406
BACKBONE							
757	C	5.0999	5.3105	-10.0175	C.2	44 CYS295	0.2048
BACKBONE							
758	O	4.9482	4.7101	-11.0705	O.2	44 CYS295	-0.3944
BACKBONE							
759	CB	2.9185	6.5756	-10.1178	C.3	44 CYS295	0.0443
760	SG	3.6109	8.1785	-10.6761	S.3	44 CYS295	-0.0882
761	H	4.0137	7.2496	-7.8187	H	44 CYS295	0.1884
762	HA	3.2955	4.7371	-9.1030	H	44 CYS295	0.0808

763	HB3	1.9960	6.7436	-9.5549	H	44 CYS295	0.0432
764	HB2	2.6516	6.0341	-11.0392	H	44 CYS295	0.0432
765	LPG2	4.2807	8.1249	-10.7743	LP	44 CYS295	0.0000
766	LPG1	3.3128	8.3762	-11.2532	LP	44 CYS295	0.0000
767	N	6.3279	5.6406	-9.5522	N.am	45 ASP296	-0.2621
BACKBONE							
768	CA	7.5268	5.3064	-10.3268	C.3	45 ASP296	0.1423
BACKBONE							
769	C	7.4202	5.6792	-11.7921	C.2	45 ASP296	0.2054
BACKBONE							
770	O	8.0548	5.0379	-12.6142	O.2	45 ASP296	-0.3943
BACKBONE							
771	CB	7.8805	3.8137	-10.0992	C.3	45 ASP296	0.0406
772	CG	9.2402	3.4709	-10.6574	C.2	45 ASP296	0.0393
773	OD1	10.2503	4.0349	-10.1535	O.co2	45 ASP296	-0.5688
774	OD2	9.3132	2.6395	-11.6037	O.co2	45 ASP296	-0.5688
775	H	6.4505	6.0950	-8.6669	H	45 ASP296	0.1884
776	HA	8.3728	5.9065	-9.9540	H	45 ASP296	0.0819
777	HB3	7.1038	3.1813	-10.5573	H	45 ASP296	0.0478
778	HB2	7.8928	3.6076	-9.0169	H	45 ASP296	0.0478
779	N	6.6379	6.7312	-12.1293	N.am	46 GLY297	-0.2663
BACKBONE							
780	CA	6.6475	7.3001	-13.4727	C.3	46 GLY297	0.1201
BACKBONE							
781	C	7.5409	8.5077	-13.3582	C.2	46 GLY297	0.2005
BACKBONE							
782	O	7.6348	9.0334	-12.2595	O.2	46 GLY297	-0.3947
BACKBONE							
783	H	6.1230	7.2389	-11.4446	H	46 GLY297	0.1881
784	HA2	5.6343	7.6213	-13.7623	H	46 GLY297	0.0763
785	HA3	7.0176	6.5936	-14.2323	H	46 GLY297	0.0763
786	N	8.2066	8.9655	-14.4416	N.am	47 GLY298	-0.2666
BACKBONE							
787	CA	9.2029	10.0165	-14.2753	C.3	47 GLY298	0.1201
BACKBONE							
788	C	9.3238	10.9138	-15.4760	C.2	47 GLY298	0.2007
BACKBONE							
789	O	8.7519	10.6068	-16.5092	O.2	47 GLY298	-0.3947
BACKBONE							
790	H	8.0960	8.5476	-15.3435	H	47 GLY298	0.1881
791	HA2	10.1680	9.5388	-14.0707	H	47 GLY298	0.0763
792	HA3	8.9459	10.6740	-13.4292	H	47 GLY298	0.0763
793	N	10.0560	12.0414	-15.3075	N.am	48 LEU299	-0.2640
BACKBONE							
794	CA	9.9872	13.1409	-16.2652	C.3	48 LEU299	0.1312
BACKBONE							
795	C	11.3801	13.6765	-16.5387	C.2	48 LEU299	0.2039
BACKBONE							
796	O	12.2232	13.5313	-15.6675	O.2	48 LEU299	-0.3944
BACKBONE							
797	CB	9.1204	14.2404	-15.5772	C.3	48 LEU299	-0.0101
798	CG	7.7344	13.7516	-15.0365	C.3	48 LEU299	-0.0425

799	CD1	7.0822	14.8236	-14.1189	C.3	48 LEU299	-0.0625
800	CD2	6.7473	13.3982	-16.1810	C.3	48 LEU299	-0.0625
801	H	10.5648	12.2058	-14.4588	H	48 LEU299	0.1883
802	HA	9.5412	12.8185	-17.2183	H	48 LEU299	0.0800
803	HB3	8.9857	15.0966	-16.2540	H	48 LEU299	0.0315
804	HB2	9.7030	14.5980	-14.7160	H	48 LEU299	0.0315
805	HG	7.8657	12.8579	-14.4056	H	48 LEU299	0.0298
806	HD13	7.6913	14.9892	-13.2173	H	48 LEU299	0.0232
807	HD12	6.0795	14.5044	-13.7976	H	48 LEU299	0.0232
808	HD11	6.9773	15.7736	-14.6571	H	48 LEU299	0.0232
809	HD23	6.5758	14.2912	-16.7919	H	48 LEU299	0.0232
810	HD22	5.7751	13.0723	-15.7811	H	48 LEU299	0.0232
811	HD21	7.1365	12.5962	-16.8214	H	48 LEU299	0.0232
812	N	11.6468	14.3002	-17.7150	N.am	49 ARG300	-0.2637
BACKBONE							
813	CA	12.9604	14.9086	-17.9582	C.3	49 ARG300	0.1311
BACKBONE							
814	C	12.8612	16.0008	-19.0036	C.2	49 ARG300	0.2039
BACKBONE							
815	O	11.7881	16.1631	-19.5598	O.2	49 ARG300	-0.3944
BACKBONE							
816	CB	14.0322	13.8588	-18.3745	C.3	49 ARG300	-0.0092
817	CG	13.8171	13.2791	-19.8035	C.3	49 ARG300	-0.0156
818	CD	15.1319	12.6800	-20.3815	C.3	49 ARG300	0.0627
819	NE	15.6886	11.6209	-19.5316	N.pl3	49 ARG300	-0.2723
820	CZ	15.3744	10.3437	-19.6217	C.cat	49 ARG300	0.2882
821	NH1	14.4531	9.8779	-20.4337	N.pl3	49 ARG300	-0.2849
822	NH2	16.0149	9.4822	-18.8620	N.pl3	49 ARG300	-0.2849
823	H	10.9536	14.3691	-18.4357	H	49 ARG300	0.1883
824	HA	13.2904	15.4077	-17.0310	H	49 ARG300	0.0800
825	HB3	14.0412	13.0401	-17.6419	H	49 ARG300	0.0313
826	HB2	15.0244	14.3319	-18.3304	H	49 ARG300	0.0313
827	HG3	13.4821	14.0662	-20.4958	H	49 ARG300	0.0301
828	HG2	13.0254	12.5185	-19.7727	H	49 ARG300	0.0301
829	HD3	15.8738	13.4965	-20.4284	H	49 ARG300	0.0689
830	HD2	15.0131	12.3633	-21.4291	H	49 ARG300	0.0689
831	HE	16.4196	11.9059	-18.8596	H	49 ARG300	0.2642
832	HH11	13.8965	10.4966	-21.0325	H	49 ARG300	0.2615
833	HH12	14.2525	8.8673	-20.4826	H	49 ARG300	0.2615
834	HH21	16.7451	9.7897	-18.2018	H	49 ARG300	0.2615
835	HH22	15.8089	8.4726	-18.9085	H	49 ARG300	0.2615
836	N	13.9566	16.7442	-19.2920	N.am	50 CYS301	-0.2629
BACKBONE							
837	CA	13.8956	17.8216	-20.2804	C.3	50 CYS301	0.1396
BACKBONE							
838	C	12.8880	18.8527	-19.8307	C.2	50 CYS301	0.2048
BACKBONE							
839	O	12.0976	19.3155	-20.6354	O.2	50 CYS301	-0.3944
BACKBONE							
840	CB	13.6264	17.2789	-21.7107	C.3	50 CYS301	0.0311
841	SG	14.9022	16.0391	-22.1092	S.o	50 CYS301	-0.1735
842	H	14.8282	16.5889	-18.8252	H	50 CYS301	0.1884

843	HA	14.8664	18.3466	-20.3124	H	50 CYS301	0.0808
844	HB3	13.6828	18.0962	-22.4481	H	50 CYS301	0.0422
845	HB2	12.6327	16.8115	-21.7861	H	50 CYS301	0.0422
846	LPG2	15.5251	16.3088	-22.1270	LP	50 CYS301	0.0000
847	LPG1	14.8945	15.5153	-21.6770	LP	50 CYS301	0.0000
848	HG	14.5728	15.7798	-23.0279	H	50 CYS301	0.1019
849	N	12.9120	19.2300	-18.5325	N.am	51 TRP302	-0.2626
BACKBONE							
850	CA	11.9339	20.1916	-18.0228	C.3	51 TRP302	0.1352
BACKBONE							
851	C	12.0172	21.4890	-18.7983	C.2	51 TRP302	0.2052
BACKBONE							
852	O	13.0410	21.7338	-19.4171	O.2	51 TRP302	-0.3942
BACKBONE							
853	CB	12.1453	20.4697	-16.5109	C.3	51 TRP302	0.0042
854	CG	11.7852	19.2756	-15.6649	C.2	51 TRP302	-0.0418
855	CD1	12.5534	18.2254	-15.3284	C.2	51 TRP302	0.0167
856	CD2	10.4446	19.0561	-15.0132	C.ar	51 TRP302	-0.0214
857	NE1	11.8723	17.4052	-14.5696	N.pl3	51 TRP302	-0.2890
858	CE2	10.6272	17.8640	-14.3412	C.ar	51 TRP302	0.0603
859	CE3	9.2410	19.7559	-14.9730	C.ar	51 TRP302	-0.0747
860	CZ2	9.6176	17.3112	-13.5571	C.ar	51 TRP302	-0.0443
861	CZ3	8.2373	19.2431	-14.1418	C.ar	51 TRP302	-0.0792
862	CH2	8.4209	18.0313	-13.4549	C.ar	51 TRP302	-0.0768
863	H	13.6012	18.8557	-17.9122	H	51 TRP302	0.1884
864	HA	10.9280	19.7631	-18.1566	H	51 TRP302	0.0815
865	HB3	11.5397	21.3268	-16.1771	H	51 TRP302	0.0397
866	HB2	13.2000	20.7212	-16.3475	H	51 TRP302	0.0397
867	HD1	13.5850	18.0687	-15.6306	H	51 TRP302	0.0795
868	HE1	12.2454	16.5240	-14.1849	H	51 TRP302	0.2216
869	HE3	9.0990	20.6521	-15.5627	H	51 TRP302	0.0540
870	HZ2	9.7600	16.3733	-13.0398	H	51 TRP302	0.0541
871	HZ3	7.3059	19.7904	-14.0357	H	51 TRP302	0.0510
872	HH2	7.6310	17.6338	-12.8294	H	51 TRP302	0.0530
873	N	10.9435	22.3174	-18.7768	N.am	52 GLU303	-0.2635
BACKBONE							
874	CA	10.9140	23.5552	-19.5608	C.3	52 GLU303	0.1325
BACKBONE							
875	C	10.3527	24.6741	-18.7142	C.2	52 GLU303	0.2041
BACKBONE							
876	O	9.7945	24.3979	-17.6637	O.2	52 GLU303	-0.3944
BACKBONE							
877	CB	10.0004	23.3699	-20.8048	C.3	52 GLU303	-0.0008
878	CG	10.6403	22.4498	-21.8768	C.3	52 GLU303	0.0044
879	CD	9.6442	22.1514	-22.9703	C.2	52 GLU303	0.0350
880	OE1	9.1445	23.1222	-23.6019	O.co2	52 GLU303	-0.5690
881	OE2	9.3485	20.9478	-23.2068	O.co2	52 GLU303	-0.5690
882	H	10.1221	22.0867	-18.2485	H	52 GLU303	0.1883
883	HA	11.9223	23.8633	-19.8828	H	52 GLU303	0.0801
884	HB3	9.7867	24.3432	-21.2756	H	52 GLU303	0.0330
885	HB2	9.0423	22.9398	-20.4752	H	52 GLU303	0.0330
886	HG3	10.9746	21.5100	-21.4157	H	52 GLU303	0.0433

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 887 HG2     11.5209    22.9427   -22.3185 H      52 GLU303   0.0433
 888 N       10.4862    25.9438   -19.1668 N.am   53 SER304  -0.2616
BACKBONE
 889 CA       9.9075    27.0490   -18.4089 C.3    53 SER304   0.1539
BACKBONE
 890 C        8.4032    26.9413   -18.4384 C.2    53 SER304   0.2060
BACKBONE
 891 O        7.8793    26.4008   -19.3998 O.2    53 SER304  -0.3943
BACKBONE
 892 CB      10.3362    28.4314   -18.9611 C.3    53 SER304   0.0843
 893 OG       9.7560    29.4669   -18.1497 O.3    53 SER304  -0.3903
 894 H       10.9542    26.1458   -20.0300 H      53 SER304   0.1884
 895 HA      10.2525    26.9782   -17.3673 H      53 SER304   0.0823
 896 HB3      9.9908    28.5286   -20.0043 H      53 SER304   0.0606
 897 HB2     11.4370    28.5048   -18.9417 H      53 SER304   0.0606
 898 HG       9.9871    30.3399   -18.4517 H      53 SER304   0.2097
 899 N        7.6964    27.4352   -17.3934 N.am   54 GLY305  -0.2663
BACKBONE
 900 CA       6.2377    27.3410   -17.3717 C.3    54 GLY305   0.1201
BACKBONE
 901 C        5.7370    26.0388   -16.7869 C.2    54 GLY305   0.2008
BACKBONE
 902 O        4.6489    26.0464   -16.2318 O.2    54 GLY305  -0.3947
BACKBONE
 903 H        8.1536    27.8524   -16.6038 H      54 GLY305   0.1881
 904 HA2      5.8218    27.4448   -18.3862 H      54 GLY305   0.0763
 905 HA3      5.8349    28.1754   -16.7729 H      54 GLY305   0.0763
 906 N        6.4688    24.9048   -16.9037 N.am   55 ASP306  -0.2624
BACKBONE
 907 CA       5.9309    23.6407   -16.4023 C.3    55 ASP306   0.1423
BACKBONE
 908 C        5.7063    23.7082   -14.9085 C.2    55 ASP306   0.2057
BACKBONE
 909 O        6.3836    24.4803   -14.2485 O.2    55 ASP306  -0.3943
BACKBONE
 910 CB       6.8654    22.4389   -16.7046 C.3    55 ASP306   0.0406
 911 CG       6.9751    22.1686   -18.1842 C.2    55 ASP306   0.0393
 912 OD1      6.9302    23.1497   -18.9761 O.co2  55 ASP306  -0.5688
 913 OD2      7.1041    20.9724   -18.5674 O.co2  55 ASP306  -0.5688
 914 H        7.3630    24.8922   -17.3502 H      55 ASP306   0.1884
 915 HA       4.9699    23.4568   -16.9119 H      55 ASP306   0.0819
 916 HB3      6.4866    21.5349   -16.2008 H      55 ASP306   0.0478
 917 HB2      7.8698    22.6597   -16.3154 H      55 ASP306   0.0478
 918 N        4.7548    22.8991   -14.3815 N.am   56 ASP307  -0.2621
BACKBONE
 919 CA       4.4820    22.8612   -12.9449 C.3    56 ASP307   0.1425
BACKBONE
 920 C        4.4370    21.3976   -12.5495 C.2    56 ASP307   0.2081
BACKBONE
 921 O        3.5514    20.7286   -13.0572 O.2    56 ASP307  -0.3941
BACKBONE
 922 CB       3.1217    23.5432   -12.6575 C.3    56 ASP307   0.0406
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923	CG	2.7546	23.3434	-11.2086	C.2	56 ASP307	0.0393
924	OD1	2.1533	22.2819	-10.8881	O.co2	56 ASP307	-0.5688
925	OD2	3.0708	24.2397	-10.3791	O.co2	56 ASP307	-0.5688
926	H	4.2056	22.2967	-14.9663	H	56 ASP307	0.1884
927	HA	5.2221	23.4353	-12.3696	H	56 ASP307	0.0819
928	HB3	2.3409	23.1124	-13.2981	H	56 ASP307	0.0478
929	HB2	3.1862	24.6182	-12.8924	H	56 ASP307	0.0478
930	N	5.3311	20.8322	-11.7004	N.am	57 PRO308	-0.2497
BACKBONE							
931	CA	5.2705	19.4063	-11.4127	C.3	57 PRO308	0.1338
BACKBONE							
932	C	3.9201	18.7847	-11.1583	C.2	57 PRO308	0.2042
BACKBONE							
933	O	3.6881	17.7108	-11.6885	O.2	57 PRO308	-0.3944
BACKBONE							
934	CB	6.1909	19.3496	-10.1744	C.3	57 PRO308	-0.0104
935	CG	7.2516	20.4203	-10.4980	C.3	57 PRO308	-0.0281
936	CD	6.4274	21.5822	-11.1002	C.3	57 PRO308	0.0369
937	HA	5.7387	18.8927	-12.2633	H	57 PRO308	0.0802
938	HB3	6.6295	18.3519	-10.0278	H	57 PRO308	0.0313
939	HB2	5.6419	19.6516	-9.2675	H	57 PRO308	0.0313
940	HG2	7.8646	20.7096	-9.6314	H	57 PRO308	0.0287
941	HG3	7.9070	20.0027	-11.2767	H	57 PRO308	0.0287
942	HD2	6.0410	22.2538	-10.3177	H	57 PRO308	0.0524
943	HD3	7.0421	22.1404	-11.8248	H	57 PRO308	0.0524
944	N	3.0133	19.4027	-10.3717	N.am	58 TRP309	-0.2627
BACKBONE							
945	CA	1.7150	18.7649	-10.1529	C.3	58 TRP309	0.1352
BACKBONE							
946	C	0.9736	18.6295	-11.4654	C.2	58 TRP309	0.2052
BACKBONE							
947	O	0.4294	17.5694	-11.7337	O.2	58 TRP309	-0.3942
BACKBONE							
948	CB	0.8136	19.5681	-9.1854	C.3	58 TRP309	0.0042
949	CG	1.3831	19.6339	-7.7941	C.2	58 TRP309	-0.0418
950	CD1	2.0097	20.6638	-7.2016	C.2	58 TRP309	0.0167
951	CD2	1.3223	18.5207	-6.7812	C.ar	58 TRP309	-0.0214
952	NE1	2.3128	20.3390	-5.9693	N.pl3	58 TRP309	-0.2890
953	CE2	1.8972	19.0937	-5.6649	C.ar	58 TRP309	0.0603
954	CE3	0.8430	17.2142	-6.7837	C.ar	58 TRP309	-0.0747
955	CZ2	1.9683	18.4075	-4.4530	C.ar	58 TRP309	-0.0443
956	CZ3	0.9239	16.5044	-5.5792	C.ar	58 TRP309	-0.0792
957	CH2	1.4617	17.1006	-4.4271	C.ar	58 TRP309	-0.0768
958	H	3.2114	20.2892	-9.9491	H	58 TRP309	0.1884
959	HA	1.8808	17.7640	-9.7192	H	58 TRP309	0.0815
960	HB3	-0.1657	19.0679	-9.1283	H	58 TRP309	0.0397
961	HB2	0.6576	20.5880	-9.5668	H	58 TRP309	0.0397
962	HD1	2.2237	21.6220	-7.6753	H	58 TRP309	0.0795
963	HE1	2.7964	20.9649	-5.3081	H	58 TRP309	0.2216
964	HE3	0.4297	16.7842	-7.6838	H	58 TRP309	0.0540
965	HZ2	2.3922	18.8685	-3.5688	H	58 TRP309	0.0541
966	HZ3	0.5677	15.4803	-5.5391	H	58 TRP309	0.0510

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 967 HH2      1.4907    16.5413    -3.4982 H      58 TRP309   0.0530
 968 N        0.9438    19.7003   -12.2927 N.am   59 VAL310  -0.2634
BACKBONE
 969 CA       0.2455    19.6222   -13.5776 C.3    59 VAL310   0.1333
BACKBONE
 970 C        0.8037    18.4571   -14.3555 C.2    59 VAL310   0.2042
BACKBONE
 971 O        0.0407    17.7000   -14.9336 O.2    59 VAL310  -0.3944
BACKBONE
 972 CB       0.4101    20.9225   -14.4246 C.3    59 VAL310  -0.0063
 973 CG1     -0.0776    20.7316   -15.8882 C.3    59 VAL310  -0.0584
 974 CG2     -0.3524    22.1108   -13.7712 C.3    59 VAL310  -0.0584
 975 H        1.4201    20.5449   -12.0441 H      59 VAL310   0.1883
 976 HA      -0.8270    19.4451   -13.3990 H      59 VAL310   0.0802
 977 HB       1.4819    21.1685   -14.4856 H      59 VAL310   0.0343
 978 HG13     0.5189    19.9772   -16.4244 H      59 VAL310   0.0234
 979 HG12    -0.0012    21.6757   -16.4494 H      59 VAL310   0.0234
 980 HG11    -1.1269    20.4125   -15.8831 H      59 VAL310   0.0234
 981 HG23    -1.4323    21.9083   -13.7581 H      59 VAL310   0.0234
 982 HG22    -0.1812    23.0357   -14.3434 H      59 VAL310   0.0234
 983 HG21    -0.0285    22.2879   -12.7359 H      59 VAL310   0.0234
 984 N        2.1448    18.3137   -14.3862 N.am   60 GLU311  -0.2636
BACKBONE
 985 CA       2.7478    17.2629   -15.1994 C.3    60 GLU311   0.1325
BACKBONE
 986 C        2.5145    15.9003   -14.5806 C.2    60 GLU311   0.2043
BACKBONE
 987 O        2.3179    14.9459   -15.3166 O.2    60 GLU311  -0.3944
BACKBONE
 988 CB       4.2503    17.5758   -15.4356 C.3    60 GLU311  -0.0008
 989 CG       4.4264    18.9014   -16.2352 C.3    60 GLU311   0.0044
 990 CD       3.7342    18.8649   -17.5757 C.2    60 GLU311   0.0350
 991 OE1      3.8329    17.8180   -18.2690 O.co2  60 GLU311  -0.5690
 992 OE2      3.0819    19.8778   -17.9493 O.co2  60 GLU311  -0.5690
 993 H        2.7368    18.9175   -13.8491 H      60 GLU311   0.1883
 994 HA       2.2501    17.2620   -16.1801 H      60 GLU311   0.0801
 995 HB3      4.7058    16.7439   -15.9907 H      60 GLU311   0.0330
 996 HB2      4.7703    17.6499   -14.4667 H      60 GLU311   0.0330
 997 HG3      5.4920    19.0953   -16.4179 H      60 GLU311   0.0433
 998 HG2      4.0395    19.7515   -15.6537 H      60 GLU311   0.0433
 999 N        2.5089    15.7827   -13.2334 N.am   61 HIS312  -0.2587
BACKBONE
1000 CA       2.2211    14.4925   -12.5974 C.3    61 HIS312   0.1612
BACKBONE
1001 C        0.8783    14.0102   -13.1084 C.2    61 HIS312   0.2098
BACKBONE
1002 O        0.7390    12.8356   -13.4124 O.2    61 HIS312  -0.3939
BACKBONE
1003 CB       2.2219    14.6318   -11.0425 C.3    61 HIS312   0.1055
1004 CG       2.4695    13.3921   -10.2100 C.2    61 HIS312   0.1973
1005 ND1      2.5983    13.4560    -8.9007 N.pl3  61 HIS312  -0.1586
1006 CD2      2.6140    12.1161   -10.6243 C.2    61 HIS312   0.1263
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1007 CE1      2.8399    12.2759    -8.4231 C.cat 61 HIS312   0.1842
1008 NE2      2.8596    11.4564    -9.3701 N.2   61 HIS312  -0.2010
1009 H        2.6716    16.5844   -12.6606 H     61 HIS312   0.1888
1010 HA       3.0099    13.7914   -12.9117 H     61 HIS312   0.0867
1011 HB3      1.2895    15.1169   -10.7213 H     61 HIS312   0.0803
1012 HB2      3.0528    15.2913   -10.7540 H     61 HIS312   0.0803
1013 HD1      2.5316    14.3171    -8.3366 H     61 HIS312   0.2700
1014 HD2      2.5685    11.7073   -11.6247 H     61 HIS312   0.1326
1015 HE1      3.0077    12.0193    -7.3802 H     61 HIS312   0.1885
1016 N       -0.1156    14.9239   -13.2235 N.am  62 ALA313  -0.2636
BACKBONE
1017 CA      -1.4195    14.5491   -13.7732 C.3   62 ALA313   0.1282
BACKBONE
1018 C       -1.3668    14.3050   -15.2614 C.2   62 ALA313   0.2036
BACKBONE
1019 O       -1.9470    13.3343   -15.7212 O.2   62 ALA313  -0.3944
BACKBONE
1020 CB      -2.4582    15.6777   -13.5336 C.3   62 ALA313  -0.0244
1021 H        0.0303    15.8790   -12.9554 H     62 ALA313   0.1883
1022 HA      -1.7662    13.6204   -13.2998 H     62 ALA313   0.0797
1023 HB3     -2.1494    16.5802   -14.0754 H     62 ALA313   0.0277
1024 HB2     -2.5353    15.9330   -12.4669 H     62 ALA313   0.0277
1025 HB1     -3.4502    15.3780   -13.9014 H     62 ALA313   0.0277
1026 N       -0.7007    15.1902   -16.0331 N.am  63 LYS314  -0.2637
BACKBONE
1027 CA      -0.7452    15.0642   -17.4882 C.3   63 LYS314   0.1310
BACKBONE
1028 C       -0.2705    13.6929   -17.9092 C.2   63 LYS314   0.2040
BACKBONE
1029 O       -0.8880    13.1038   -18.7821 O.2   63 LYS314  -0.3944
BACKBONE
1030 CB       0.1266    16.1592   -18.1645 C.3   63 LYS314  -0.0122
1031 CG      -0.0244    16.1797   -19.7102 C.3   63 LYS314  -0.0440
1032 CD       0.8182    17.2963   -20.3934 C.3   63 LYS314  -0.0124
1033 CE       0.3277    18.7387   -20.0798 C.3   63 LYS314  -0.0354
1034 NZ       1.1092    19.7494   -20.8299 N.4   63 LYS314   0.2185
1035 H       -0.2103    15.9597   -15.6223 H     63 LYS314   0.1883
1036 HA      -1.7935    15.2089   -17.8023 H     63 LYS314   0.0800
1037 HB3      1.1838    15.9906   -17.9103 H     63 LYS314   0.0312
1038 HB2     -0.1872    17.1288   -17.7498 H     63 LYS314   0.0312
1039 HG3     -1.0851    16.3139   -19.9747 H     63 LYS314   0.0269
1040 HG2      0.3068    15.2057   -20.1078 H     63 LYS314   0.0269
1041 HD3      0.7645    17.1468   -21.4848 H     63 LYS314   0.0317
1042 HD2      1.8718    17.2006   -20.0925 H     63 LYS314   0.0317
1043 HE3      0.4328    18.9603   -19.0059 H     63 LYS314   0.0813
1044 HE2     -0.7393    18.8269   -20.3473 H     63 LYS314   0.0813
1045 HZ3      2.1580    19.7158   -20.5677 H     63 LYS314   0.1994
1046 HZ2      0.7638    20.7530   -20.6178 H     63 LYS314   0.1994
1047 HZ1      1.0330    19.6114   -21.8998 H     63 LYS314   0.1994
1048 N        0.8277    13.1836   -17.3034 N.am  64 TRP315  -0.2627
BACKBONE
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1049 CA       1.4145    11.9185   -17.7515 C.3   64 TRP315   0.1352
BACKBONE
1050 C        1.0089    10.7315   -16.9071 C.2   64 TRP315   0.2053
BACKBONE
1051 O        0.8244     9.6727   -17.4875 O.2   64 TRP315  -0.3942
BACKBONE
1052 CB       2.9542    12.0843   -17.7845 C.3   64 TRP315   0.0042
1053 CG       3.2349    13.2599   -18.6859 C.2   64 TRP315  -0.0418
1054 CD1      3.6701    14.4794   -18.3291 C.2   64 TRP315   0.0167
1055 CD2      3.0501    13.2852   -20.1826 C.ar  64 TRP315  -0.0214
1056 NE1      3.7659    15.2376   -19.3908 N.pl3 64 TRP315  -0.2890
1057 CE2      3.4085    14.5787   -20.5088 C.ar  64 TRP315   0.0603
1058 CE3      2.6437    12.3660   -21.1487 C.ar  64 TRP315  -0.0747
1059 CZ2      3.3752    15.0435   -21.8228 C.ar  64 TRP315  -0.0443
1060 CZ3      2.6014    12.8188   -22.4738 C.ar  64 TRP315  -0.0792
1061 CH2      2.9597    14.1353   -22.8051 C.ar  64 TRP315  -0.0768
1062 H        1.2810    13.6838   -16.5620 H     64 TRP315   0.1884
1063 HA       1.0968    11.7031   -18.7852 H     64 TRP315   0.0815
1064 HB3      3.4389    11.1773   -18.1768 H     64 TRP315   0.0397
1065 HB2      3.3368    12.2674   -16.7678 H     64 TRP315   0.0397
1066 HD1      3.9017    14.7835   -17.3112 H     64 TRP315   0.0795
1067 HE1      4.0735    16.2206   -19.3780 H     64 TRP315   0.2216
1068 HE3      2.3768    11.3486   -20.8864 H     64 TRP315   0.0540
1069 HZ2      3.6584    16.0614   -22.0679 H     64 TRP315   0.0541
1070 HZ3      2.2853    12.1375   -23.2573 H     64 TRP315   0.0510
1071 HH2      2.9144    14.4568   -23.8409 H     64 TRP315   0.0530
1072 N        0.8656    10.8637   -15.5661 N.am  65 PHE316  -0.2618
BACKBONE
1073 CA       0.4959     9.7178   -14.7322 C.3   65 PHE316   0.1406
BACKBONE
1074 C       -0.7652    10.0627   -13.9624 C.2   65 PHE316   0.2085
BACKBONE
1075 O       -0.6823    10.2045   -12.7521 O.2   65 PHE316  -0.3940
BACKBONE
1076 CB       1.7064     9.3555   -13.8246 C.3   65 PHE316   0.0214
1077 CG       3.0292     9.3744   -14.6129 C.ar  65 PHE316  -0.0386
1078 CD1      3.1838     8.5773   -15.7521 C.ar  65 PHE316  -0.0601
1079 CD2      4.0980    10.1881   -14.2099 C.ar  65 PHE316  -0.0601
1080 CE1      4.3332     8.6800   -16.5424 C.ar  65 PHE316  -0.0686
1081 CE2      5.2644    10.2634   -14.9751 C.ar  65 PHE316  -0.0686
1082 CZ       5.3629     9.5499   -16.1702 C.ar  65 PHE316  -0.0687
1083 H        1.0286    11.7369   -15.1038 H     65 PHE316   0.1885
1084 HA       0.2890     8.8076   -15.3135 H     65 PHE316   0.0823
1085 HB3      1.5696     8.3645   -13.3609 H     65 PHE316   0.0474
1086 HB2      1.7608    10.0919   -13.0166 H     65 PHE316   0.0474
1087 HD1      2.4113     7.8702   -16.0341 H     65 PHE316   0.0557
1088 HD2      4.0376    10.7704   -13.2979 H     65 PHE316   0.0557
1089 HE1      4.4281     8.0848   -17.4443 H     65 PHE316   0.0599
1090 HE2      6.0952    10.8765   -14.6381 H     65 PHE316   0.0599
1091 HZ       6.2336     9.6678   -16.8062 H     65 PHE316   0.0559
1092 N       -1.9613    10.2106   -14.5917 N.am  66 PRO317  -0.2497
BACKBONE
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1093 CA      -3.1466    10.5595   -13.8179 C.3   66 PRO317   0.1338
BACKBONE
1094 C       -3.5370     9.4507   -12.8655 C.2   66 PRO317   0.2039
BACKBONE
1095 O       -4.1435     9.7465   -11.8483 O.2   66 PRO317  -0.3944
BACKBONE
1096 CB      -4.1760    10.7841   -14.9538 C.3   66 PRO317  -0.0104
1097 CG      -3.6656     9.9049   -16.1164 C.3   66 PRO317  -0.0281
1098 CD      -2.1262    10.0346   -16.0307 C.3   66 PRO317   0.0369
1099 HA      -2.9925    11.4911   -13.2508 H     66 PRO317   0.0802
1100 HB3     -4.1415    11.8360   -15.2825 H     66 PRO317   0.0313
1101 HB2     -5.2077    10.5378   -14.6568 H     66 PRO317   0.0313
1102 HG2     -3.9645     8.8610   -15.9235 H     66 PRO317   0.0287
1103 HG3     -4.0662    10.2100   -17.0975 H     66 PRO317   0.0287
1104 HD2     -1.6612     9.1323   -16.4543 H     66 PRO317   0.0524
1105 HD3     -1.7731    10.9282   -16.5673 H     66 PRO317   0.0524
1106 N       -3.1963     8.1695   -13.1361 N.am  67 GLY318  -0.2664
BACKBONE
1107 CA      -3.5282     7.1176   -12.1770 C.3   67 GLY318   0.1201
BACKBONE
1108 C       -2.6997     7.1752   -10.9115 C.2   67 GLY318   0.2008
BACKBONE
1109 O       -2.9986     6.4018   -10.0145 O.2   67 GLY318  -0.3947
BACKBONE
1110 H       -2.6870     7.9157   -13.9608 H     67 GLY318   0.1881
1111 HA2     -3.3641     6.1275   -12.6331 H     67 GLY318   0.0763
1112 HA3     -4.5959     7.1826   -11.9140 H     67 GLY318   0.0763
1113 N       -1.6606     8.0396   -10.7976 N.am  68 CYS319  -0.2631
BACKBONE
1114 CA      -0.8053     8.0051    -9.6104 C.3   68 CYS319   0.1406
BACKBONE
1115 C       -1.6307     8.1432    -8.3496 C.2   68 CYS319   0.2047
BACKBONE
1116 O       -2.5241     8.9738    -8.3356 O.2   68 CYS319  -0.3944
BACKBONE
1117 CB       0.3194     9.0755    -9.6884 C.3   68 CYS319   0.0443
1118 SG       1.4047     9.0269    -8.2205 S.3   68 CYS319  -0.0882
1119 H       -1.4147     8.6707   -11.5328 H     68 CYS319   0.1884
1120 HA      -0.3321     7.0117    -9.6161 H     68 CYS319   0.0808
1121 HB3     -0.1069    10.0830    -9.7727 H     68 CYS319   0.0432
1122 HB2      0.9181     8.8946   -10.5924 H     68 CYS319   0.0432
1123 LPG2     1.2183     9.4797    -7.7501 LP    68 CYS319   0.0000
1124 LPG1     1.4296     8.4082    -7.9419 LP    68 CYS319   0.0000
1125 N       -1.3710     7.3306    -7.2948 N.am  69 GLU320  -0.2636
BACKBONE
1126 CA      -2.2272     7.3644    -6.1084 C.3   69 GLU320   0.1325
BACKBONE
1127 C       -1.8665     8.5669    -5.2692 C.2   69 GLU320   0.2041
BACKBONE
1128 O       -2.7662     9.3121    -4.9140 O.2   69 GLU320  -0.3944
BACKBONE
1129 CB      -2.1244     6.0721    -5.2502 C.3   69 GLU320  -0.0008
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1130 CG	-2.5787	4.8070	-6.0287	C.3	69	GLU320	0.0044
1131 CD	-4.0187	4.9078	-6.4670	C.2	69	GLU320	0.0350
1132 OE1	-4.8895	5.1604	-5.5900	O.co2	69	GLU320	-0.5690
1133 OE2	-4.2945	4.7394	-7.6870	O.co2	69	GLU320	-0.5690
1134 H	-0.5919	6.7005	-7.3014	H	69	GLU320	0.1883
1135 HA	-3.2789	7.4598	-6.4265	H	69	GLU320	0.0801
1136 HB3	-2.7505	6.1860	-4.3496	H	69	GLU320	0.0330
1137 HB2	-1.0853	5.9304	-4.9187	H	69	GLU320	0.0330
1138 HG3	-2.4817	3.9238	-5.3766	H	69	GLU320	0.0433
1139 HG2	-1.9294	4.6501	-6.9047	H	69	GLU320	0.0433
1140 N	-0.5650	8.7731	-4.9533	N.am	70	PHE321	-0.2619
BACKBONE							
1141 CA	-0.1649	9.9600	-4.1959	C.3	70	PHE321	0.1404
BACKBONE							
1142 C	-0.8526	11.1658	-4.7833	C.2	70	PHE321	0.2060
BACKBONE							
1143 O	-1.4991	11.9060	-4.0616	O.2	70	PHE321	-0.3942
BACKBONE							
1144 CB	1.3727	10.1614	-4.2163	C.3	70	PHE321	0.0214
1145 CG	1.7781	11.4966	-3.5747	C.ar	70	PHE321	-0.0386
1146 CD1	1.8497	11.6274	-2.1841	C.ar	70	PHE321	-0.0601
1147 CD2	2.0992	12.6003	-4.3714	C.ar	70	PHE321	-0.0601
1148 CE1	2.4519	12.7525	-1.6126	C.ar	70	PHE321	-0.0686
1149 CE2	2.7323	13.7129	-3.8113	C.ar	70	PHE321	-0.0686
1150 CZ	2.9400	13.7756	-2.4308	C.ar	70	PHE321	-0.0687
1151 H	0.1435	8.1273	-5.2424	H	70	PHE321	0.1885
1152 HA	-0.4716	9.8478	-3.1482	H	70	PHE321	0.0823
1153 HB3	1.7458	10.1246	-5.2516	H	70	PHE321	0.0474
1154 HB2	1.8569	9.3397	-3.6647	H	70	PHE321	0.0474
1155 HD1	1.4408	10.8537	-1.5458	H	70	PHE321	0.0557
1156 HD2	1.8583	12.5985	-5.4268	H	70	PHE321	0.0557
1157 HE1	2.5423	12.8305	-0.5339	H	70	PHE321	0.0599
1158 HE2	3.0583	14.5263	-4.4486	H	70	PHE321	0.0599
1159 HZ	3.4692	14.6187	-1.9974	H	70	PHE321	0.0559
1160 N	-0.7351	11.3600	-6.1111	N.am	71	LEU322	-0.2636
BACKBONE							
1161 CA	-1.3778	12.5078	-6.7377	C.3	71	LEU322	0.1312
BACKBONE							
1162 C	-2.8561	12.5447	-6.4254	C.2	71	LEU322	0.2039
BACKBONE							
1163 O	-3.3430	13.5922	-6.0304	O.2	71	LEU322	-0.3944
BACKBONE							
1164 CB	-1.2184	12.4156	-8.2757	C.3	71	LEU322	-0.0101
1165 CG	-1.9763	13.5205	-9.0589	C.3	71	LEU322	-0.0425
1166 CD1	-1.4276	14.9381	-8.7545	C.3	71	LEU322	-0.0625
1167 CD2	-1.8545	13.2099	-10.5703	C.3	71	LEU322	-0.0625
1168 H	-0.2026	10.7290	-6.6749	H	71	LEU322	0.1883
1169 HA	-0.8769	13.4139	-6.3626	H	71	LEU322	0.0800
1170 HB3	-1.6313	11.4463	-8.5903	H	71	LEU322	0.0315
1171 HB2	-0.1472	12.4364	-8.5352	H	71	LEU322	0.0315
1172 HG	-3.0466	13.5102	-8.7965	H	71	LEU322	0.0298
1173 HD13	-1.6198	15.2230	-7.7098	H	71	LEU322	0.0232

1174 HD12	-1.9014	15.6926	-9.4019	H	71	LEU322	0.0232
1175 HD11	-0.3452	14.9440	-8.9379	H	71	LEU322	0.0232
1176 HD23	-0.8026	13.2343	-10.8934	H	71	LEU322	0.0232
1177 HD22	-2.4167	13.9741	-11.1133	H	71	LEU322	0.0232
1178 HD21	-2.2802	12.2244	-10.8165	H	71	LEU322	0.0232
1179 N	-3.5914	11.4247	-6.6185	N.am	72	ILE323	-0.2635
BACKBONE							
1180 CA	-5.0427	11.4727	-6.4445	C.3	72	ILE323	0.1335
BACKBONE							
1181 C	-5.3242	11.9095	-5.0255	C.2	72	ILE323	0.2042
BACKBONE							
1182 O	-5.9623	12.9341	-4.8444	O.2	72	ILE323	-0.3944
BACKBONE							
1183 CB	-5.7488	10.1298	-6.8144	C.3	72	ILE323	-0.0037
1184 CG1	-5.6893	9.8970	-8.3579	C.3	72	ILE323	-0.0491
1185 CG2	-7.2230	10.1302	-6.3129	C.3	72	ILE323	-0.0582
1186 CD1	-5.9143	8.4193	-8.7782	C.3	72	ILE323	-0.0648
1187 H	-3.1590	10.5633	-6.8918	H	72	ILE323	0.1883
1188 HA	-5.4438	12.2413	-7.1272	H	72	ILE323	0.0803
1189 HB	-5.2162	9.3098	-6.3052	H	72	ILE323	0.0345
1190 HG13	-4.7072	10.2017	-8.7515	H	72	ILE323	0.0267
1191 HG12	-6.4477	10.5273	-8.8480	H	72	ILE323	0.0267
1192 HG23	-7.2681	10.2086	-5.2158	H	72	ILE323	0.0235
1193 HG22	-7.7409	9.2023	-6.5935	H	72	ILE323	0.0235
1194 HG21	-7.7725	10.9812	-6.7453	H	72	ILE323	0.0235
1195 HD13	-5.1616	7.7659	-8.3102	H	72	ILE323	0.0230
1196 HD12	-5.8186	8.3274	-9.8715	H	72	ILE323	0.0230
1197 HD11	-6.9154	8.0638	-8.4957	H	72	ILE323	0.0230
1198 N	-4.8614	11.1614	-3.9988	N.am	73	ARG324	-0.2637
BACKBONE							
1199 CA	-5.1606	11.5705	-2.6268	C.3	73	ARG324	0.1311
BACKBONE							
1200 C	-4.6928	12.9859	-2.3522	C.2	73	ARG324	0.2039
BACKBONE							
1201 O	-5.3492	13.6647	-1.5772	O.2	73	ARG324	-0.3944
BACKBONE							
1202 CB	-4.6457	10.5873	-1.5359	C.3	73	ARG324	-0.0092
1203 CG	-3.1014	10.4226	-1.4837	C.3	73	ARG324	-0.0156
1204 CD	-2.6859	9.4954	-0.3066	C.3	73	ARG324	0.0627
1205 NE	-1.2359	9.2707	-0.2581	N.pl3	73	ARG324	-0.2723
1206 CZ	-0.5933	8.3789	-0.9871	C.cat	73	ARG324	0.2882
1207 NH1	-1.1756	7.6233	-1.8916	N.pl3	73	ARG324	-0.2849
1208 NH2	0.7016	8.2359	-0.8078	N.pl3	73	ARG324	-0.2849
1209 H	-4.3423	10.3226	-4.1654	H	73	ARG324	0.1883
1210 HA	-6.2619	11.5719	-2.5419	H	73	ARG324	0.0800
1211 HB3	-5.1000	9.5985	-1.7155	H	73	ARG324	0.0313
1212 HB2	-4.9959	10.9495	-0.5546	H	73	ARG324	0.0313
1213 HG3	-2.6142	11.4010	-1.3571	H	73	ARG324	0.0301
1214 HG2	-2.7516	9.9924	-2.4286	H	73	ARG324	0.0301
1215 HD3	-3.2413	8.5446	-0.3121	H	73	ARG324	0.0689
1216 HD2	-2.9839	10.0039	0.6269	H	73	ARG324	0.0689
1217 HE	-0.7022	9.8345	0.4249	H	73	ARG324	0.2642

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1218 HH11    -2.1795     7.6912    -2.0924 H     73 ARG324   0.2615
1219 HH12    -0.6308     6.9400    -2.4390 H     73 ARG324   0.2615
1220 HH21     1.2082     8.7920    -0.1029 H     73 ARG324   0.2615
1221 HH22     1.2469     7.5586    -1.3627 H     73 ARG324   0.2615
1222 N       -3.5838    13.4640    -2.9663 N.am  74 MET325  -0.2637
BACKBONE
1223 CA      -3.1485    14.8394    -2.7211 C.3   74 MET325   0.1317
BACKBONE
1224 C       -4.0627    15.8208    -3.4296 C.2   74 MET325   0.2039
BACKBONE
1225 O       -4.8266    16.4904    -2.7509 O.2   74 MET325  -0.3944
BACKBONE
1226 CB      -1.6608    15.0805    -3.1075 C.3   74 MET325  -0.0034
1227 CG      -0.6642    14.3246    -2.1884 C.3   74 MET325  -0.0024
1228 SD      -0.6394    15.0177    -0.5017 S.o   74 MET325  -0.1639
1229 CE      -1.3538    13.6479     0.4641 C.3   74 MET325  -0.0181
1230 H       -3.0632    12.9016    -3.6101 H     74 MET325   0.1883
1231 HA      -3.2209    15.0491    -1.6415 H     74 MET325   0.0800
1232 HB3     -1.4348    16.1587    -3.0563 H     74 MET325   0.0320
1233 HB2     -1.4889    14.7487    -4.1429 H     74 MET325   0.0320
1234 HG3      0.3474    14.4516    -2.5950 H     74 MET325   0.0378
1235 HG2     -0.8818    13.2499    -2.1436 H     74 MET325   0.0378
1236 LPD2    -0.0065    15.1591    -0.3010 LP    74 MET325   0.0000
1237 LPD1    -1.0212    15.5775    -0.4580 LP    74 MET325   0.0000
1238 HE3     -2.3825    13.4458     0.1324 H     74 MET325   0.0340
1239 HE2     -1.3682    13.9309     1.5265 H     74 MET325   0.0340
1240 HE1     -0.7418    12.7415     0.3409 H     74 MET325   0.0340
1241 N       -4.0064    15.9493    -4.7771 N.am  75 LYS326  -0.2637
BACKBONE
1242 CA      -4.8015    16.9773    -5.4517 C.3   75 LYS326   0.1310
BACKBONE
1243 C       -6.2590    16.5783    -5.5282 C.2   75 LYS326   0.2037
BACKBONE
1244 O       -7.0978    17.3913    -5.1696 O.2   75 LYS326  -0.3944
BACKBONE
1245 CB      -4.2797    17.2915    -6.8843 C.3   75 LYS326  -0.0122
1246 CG      -2.9303    18.0682    -6.9157 C.3   75 LYS326  -0.0440
1247 CD      -3.0722    19.5442    -6.4356 C.3   75 LYS326  -0.0124
1248 CE      -1.7778    20.3663    -6.6703 C.3   75 LYS326  -0.0354
1249 NZ      -1.8923    21.7465    -6.1462 N.4   75 LYS326   0.2185
1250 H       -3.4276    15.3531    -5.3333 H     75 LYS326   0.1883
1251 HA      -4.7578    17.9031    -4.8589 H     75 LYS326   0.0800
1252 HB3     -5.0274    17.9071    -7.4045 H     75 LYS326   0.0312
1253 HB2     -4.1812    16.3474    -7.4456 H     75 LYS326   0.0312
1254 HG3     -2.5711    18.0825    -7.9586 H     75 LYS326   0.0269
1255 HG2     -2.1798    17.5402    -6.3051 H     75 LYS326   0.0269
1256 HD3     -3.2906    19.5809    -5.3581 H     75 LYS326   0.0317
1257 HD2     -3.8978    20.0364    -6.9758 H     75 LYS326   0.0317
1258 HE3     -1.5747    20.4150    -7.7517 H     75 LYS326   0.0813
1259 HE2     -0.9378    19.8567    -6.1717 H     75 LYS326   0.0813
1260 HZ3     -2.7004    22.2876    -6.6192 H     75 LYS326   0.1994
1261 HZ2     -0.9838    22.3069    -6.3243 H     75 LYS326   0.1994
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1262 HZ1     -2.0664    21.7606    -5.0790 H     75 LYS326   0.1994
1263 N       -6.5774    15.3501    -5.9998 N.am  76 GLY327  -0.2664
BACKBONE
1264 CA      -7.9741    14.9403    -6.1546 C.3   76 GLY327   0.1201
BACKBONE
1265 C       -8.2447    14.6154    -7.6011 C.2   76 GLY327   0.2007
BACKBONE
1266 O       -7.4253    14.9451    -8.4432 O.2   76 GLY327  -0.3947
BACKBONE
1267 H       -5.8659    14.6968    -6.2704 H     76 GLY327   0.1881
1268 HA2     -8.6938    15.7151    -5.8475 H     76 GLY327   0.0763
1269 HA3     -8.1592    14.0461    -5.5395 H     76 GLY327   0.0763
1270 N       -9.3933    13.9679    -7.9023 N.am  77 GLN328  -0.2638
BACKBONE
1271 CA      -9.6771    13.5741    -9.2819 C.3   77 GLN328   0.1330
BACKBONE
1272 C      -10.1806    14.7500   -10.0891 C.2   77 GLN328   0.2040
BACKBONE
1273 O       -9.8149    14.8584   -11.2484 O.2   77 GLN328  -0.3944
BACKBONE
1274 CB     -10.7094    12.4143    -9.3142 C.3   77 GLN328   0.0045
1275 CG     -10.9068    11.8305   -10.7401 C.3   77 GLN328   0.0412
1276 CD      -9.6120    11.3575   -11.3625 C.2   77 GLN328   0.1737
1277 OE1     -9.2087    11.9054   -12.3768 O.2   77 GLN328  -0.3973
1278 NE2     -8.9331    10.3419   -10.7831 N.am  77 GLN328  -0.3009
1279 H      -10.0620    13.7507    -7.1876 H     77 GLN328   0.1883
1280 HA      -8.7408    13.2029    -9.7294 H     77 GLN328   0.0801
1281 HB3    -11.6770    12.7790    -8.9319 H     77 GLN328   0.0337
1282 HB2    -10.3592    11.6188    -8.6371 H     77 GLN328   0.0337
1283 HG3    -11.3679    12.5990   -11.3797 H     77 GLN328   0.0504
1284 HG2    -11.6026    10.9777   -10.6930 H     77 GLN328   0.0504
1285 HE21    -9.2743     9.8863    -9.9603 H     77 GLN328   0.1814
1286 HE22    -8.0711    10.0283   -11.1851 H     77 GLN328   0.1814
1287 N      -11.0203    15.6462    -9.5205 N.am  78 GLU329  -0.2636
BACKBONE
1288 CA     -11.5073    16.7808   -10.3080 C.3   78 GLU329   0.1325
BACKBONE
1289 C      -10.3236    17.5677   -10.8283 C.2   78 GLU329   0.2041
BACKBONE
1290 O      -10.2895    17.8805   -12.0078 O.2   78 GLU329  -0.3944
BACKBONE
1291 CB     -12.4467    17.6999    -9.4766 C.3   78 GLU329  -0.0008
1292 CG     -13.0331    18.8652   -10.3204 C.3   78 GLU329   0.0044
1293 CD     -13.8222    18.3619   -11.5047 C.2   78 GLU329   0.0350
1294 OE1    -14.6897    17.4676   -11.3030 O.co2 78 GLU329  -0.5690
1295 OE2    -13.5836    18.8498   -12.6449 O.co2 78 GLU329  -0.5690
1296 H      -11.3234    15.5452    -8.5710 H     78 GLU329   0.1883
1297 HA     -12.0761    16.3700   -11.1589 H     78 GLU329   0.0801
1298 HB3    -11.8890    18.1166    -8.6221 H     78 GLU329   0.0330
1299 HB2    -13.2751    17.0934    -9.0748 H     78 GLU329   0.0330
1300 HG3    -12.2172    19.5215   -10.6615 H     78 GLU329   0.0433
1301 HG2    -13.7073    19.4678    -9.6904 H     78 GLU329   0.0433
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1302 N      -9.3384    17.8833    -9.9556 N.am  79 TYR330  -0.2621
BACKBONE
1303 CA     -8.1347    18.5825   -10.4112 C.3   79 TYR330   0.1390
BACKBONE
1304 C      -7.5726    17.9147   -11.6456 C.2   79 TYR330   0.2057
BACKBONE
1305 O      -7.2592    18.5969   -12.6081 O.2   79 TYR330  -0.3942
BACKBONE
1306 CB     -7.0432    18.5434    -9.3079 C.3   79 TYR330   0.0163
1307 CG     -5.7311    19.1817    -9.7866 C.ar  79 TYR330  -0.0493
1308 CD1    -4.7156    18.3992   -10.3493 C.ar  79 TYR330  -0.0685
1309 CD2    -5.5353    20.5597    -9.6503 C.ar  79 TYR330  -0.0685
1310 CE1    -3.4992    18.9782   -10.7237 C.ar  79 TYR330  -0.0398
1311 CE2    -4.3172    21.1378   -10.0162 C.ar  79 TYR330  -0.0398
1312 CZ     -3.2895    20.3514   -10.5423 C.ar  79 TYR330   0.0805
1313 OH     -2.0751    20.9561   -10.8788 O.3   79 TYR330  -0.3376
1314 H      -9.4153    17.6329    -8.9877 H     79 TYR330   0.1885
1315 HA     -8.3899    19.6321   -10.6315 H     79 TYR330   0.0821
1316 HB2    -6.8569    17.4993    -9.0154 H     79 TYR330   0.0453
1317 HB3    -7.4033    19.0745    -8.4122 H     79 TYR330   0.0453
1318 HD1    -4.8647    17.3344   -10.4960 H     79 TYR330   0.0530
1319 HD2    -6.3281    21.1868    -9.2563 H     79 TYR330   0.0530
1320 HE1    -2.7221    18.3540   -11.1541 H     79 TYR330   0.0525
1321 HE2    -4.1647    22.2048    -9.8914 H     79 TYR330   0.0525
1322 HH     -1.4021    20.3438   -11.1467 H     79 TYR330   0.2458
1323 N      -7.4402    16.5700   -11.6174 N.am  80 ILE331  -0.2633
BACKBONE
1324 CA     -6.8504    15.8571   -12.7505 C.3   80 ILE331   0.1335
BACKBONE
1325 C      -7.7260    16.0827   -13.9598 C.2   80 ILE331   0.2043
BACKBONE
1326 O      -7.2090    16.4326   -15.0093 O.2   80 ILE331  -0.3944
BACKBONE
1327 CB     -6.6945    14.3356   -12.4419 C.3   80 ILE331  -0.0037
1328 CG1    -5.6332    14.1275   -11.3196 C.3   80 ILE331  -0.0491
1329 CG2    -6.3488    13.5152   -13.7162 C.3   80 ILE331  -0.0582
1330 CD1    -5.5451    12.6585   -10.8332 C.3   80 ILE331  -0.0648
1331 H      -7.7687    16.0501   -10.8274 H     80 ILE331   0.1883
1332 HA     -5.8505    16.2752   -12.9548 H     80 ILE331   0.0803
1333 HB     -7.6621    13.9590   -12.0808 H     80 ILE331   0.0345
1334 HG13   -5.8727    14.7477   -10.4440 H     80 ILE331   0.0267
1335 HG12   -4.6528    14.4560   -11.6910 H     80 ILE331   0.0267
1336 HG23   -7.1033    13.6603   -14.5037 H     80 ILE331   0.0235
1337 HG22   -6.3323    12.4397   -13.4936 H     80 ILE331   0.0235
1338 HG21   -5.3650    13.8126   -14.1057 H     80 ILE331   0.0235
1339 HD13   -6.5504    12.2546   -10.6456 H     80 ILE331   0.0230
1340 HD12   -4.9677    12.5934    -9.9001 H     80 ILE331   0.0230
1341 HD11   -5.0427    12.0360   -11.5837 H     80 ILE331   0.0230
1342 N      -9.0567    15.8854   -13.8279 N.am  81 ASN332  -0.2616
BACKBONE
1343 CA     -9.9413    16.0621   -14.9774 C.3   81 ASN332   0.1476
BACKBONE
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1344 C       -9.6941    17.4086   -15.6189 C.2   81 ASN332   0.2064
BACKBONE
1345 O       -9.6391    17.4837   -16.8362 O.2   81 ASN332  -0.3942
BACKBONE
1346 CB     -11.4376    15.9775   -14.5668 C.3   81 ASN332   0.0773
1347 CG     -11.7799    14.6826   -13.8672 C.2   81 ASN332   0.1780
1348 OD1    -10.9434    13.7956   -13.7960 O.2   81 ASN332  -0.3970
1349 ND2    -13.0163    14.5525   -13.3380 N.am  81 ASN332  -0.3007
1350 H       -9.4504    15.6009   -12.9526 H     81 ASN332   0.1885
1351 HA      -9.7237    15.2608   -15.7038 H     81 ASN332   0.0826
1352 HB3    -12.0664    16.0640   -15.4670 H     81 ASN332   0.0551
1353 HB2    -11.6828    16.8140   -13.8950 H     81 ASN332   0.0551
1354 HD21   -13.6875    15.2921   -13.4063 H     81 ASN332   0.1814
1355 HD22   -13.2720    13.7063   -12.8688 H     81 ASN332   0.1814
1356 N       -9.5417    18.4814   -14.8084 N.am  82 ASN333  -0.2615
BACKBONE
1357 CA      -9.3307    19.8073   -15.3853 C.3   82 ASN333   0.1476
BACKBONE
1358 C       -8.0307    19.8574   -16.1569 C.2   82 ASN333   0.2063
BACKBONE
1359 O       -7.9866    20.5175   -17.1836 O.2   82 ASN333  -0.3942
BACKBONE
1360 CB      -9.3147    20.9162   -14.3000 C.3   82 ASN333   0.0773
1361 CG     -10.5330    20.8401   -13.4043 C.2   82 ASN333   0.1780
1362 OD1    -10.3740    20.6174   -12.2172 O.2   82 ASN333  -0.3970
1363 ND2    -11.7630    21.0195   -13.9405 N.am  82 ASN333  -0.3007
1364 H       -9.5708    18.3853   -13.8119 H     82 ASN333   0.1885
1365 HA     -10.1606    20.0079   -16.0828 H     82 ASN333   0.0826
1366 HB3     -9.2823    21.9074   -14.7774 H     82 ASN333   0.0551
1367 HB2     -8.4052    20.8037   -13.6887 H     82 ASN333   0.0551
1368 HD21   -11.8869    21.2224   -14.9112 H     82 ASN333   0.1814
1369 HD22   -12.5698    20.9547   -13.3524 H     82 ASN333   0.1814
1370 N       -6.9567    19.1750   -15.6964 N.am  83 ILE334  -0.2633
BACKBONE
1371 CA      -5.7112    19.2039   -16.4603 C.3   83 ILE334   0.1335
BACKBONE
1372 C       -5.9667    18.6035   -17.8236 C.2   83 ILE334   0.2043
BACKBONE
1373 O       -5.6499    19.2410   -18.8155 O.2   83 ILE334  -0.3944
BACKBONE
1374 CB      -4.5142    18.4865   -15.7633 C.3   83 ILE334  -0.0037
1375 CG1     -4.1919    19.0825   -14.3531 C.3   83 ILE334  -0.0491
1376 CG2     -3.2720    18.4944   -16.7040 C.3   83 ILE334  -0.0582
1377 CD1     -4.1524    20.6318   -14.2843 C.3   83 ILE334  -0.0648
1378 H       -7.0041    18.6346   -14.8561 H     83 ILE334   0.1883
1379 HA      -5.4315    20.2570   -16.6245 H     83 ILE334   0.0803
1380 HB      -4.7756    17.4244   -15.6097 H     83 ILE334   0.0345
1381 HG13    -3.2155    18.7069   -14.0146 H     83 ILE334   0.0267
1382 HG12    -4.9320    18.7349   -13.6166 H     83 ILE334   0.0267
1383 HG23    -3.4549    17.8844   -17.6029 H     83 ILE334   0.0235
1384 HG22    -2.3880    18.0749   -16.2006 H     83 ILE334   0.0235
1385 HG21    -3.0429    19.5180   -17.0317 H     83 ILE334   0.0235
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1386	HD13	-3.4901	21.0422	-15.0603	H	83 ILE334	0.0230
1387	HD12	-3.7781	20.9512	-13.2991	H	83 ILE334	0.0230
1388	HD11	-5.1598	21.0581	-14.4081	H	83 ILE334	0.0230
1389	N	-6.5366	17.3812	-17.8989	N.am	84 HIS335	-0.2619
BACKBONE							
1390	CA	-6.7693	16.7701	-19.2070	C.3	84 HIS335	0.1422
BACKBONE							
1391	C	-7.8409	17.5069	-19.9812	C.2	84 HIS335	0.2060
BACKBONE							
1392	O	-7.8431	17.3841	-21.1953	O.2	84 HIS335	-0.3942
BACKBONE							
1393	CB	-7.1319	15.2664	-19.0837	C.3	84 HIS335	0.0460
1394	CG	-5.9154	14.4754	-18.6654	C.2	84 HIS335	0.0945
1395	ND1	-5.1380	13.8402	-19.5102	N.2	84 HIS335	-0.1129
1396	CD2	-5.4598	14.3113	-17.4070	C.2	84 HIS335	-0.0242
1397	CE1	-4.1807	13.2531	-18.8659	C.2	84 HIS335	0.1251
1398	NE2	-4.3027	13.4851	-17.6396	N.2	84 HIS335	-0.3410
1399	H	-6.8278	16.9012	-17.0700	H	84 HIS335	0.1885
1400	HA	-5.8372	16.8369	-19.7937	H	84 HIS335	0.0824
1401	HB3	-7.4833	14.8755	-20.0516	H	84 HIS335	0.0492
1402	HB2	-7.9457	15.1389	-18.3532	H	84 HIS335	0.0492
1403	HD2	-5.8459	14.6914	-16.4673	H	84 HIS335	0.0325
1404	HE1	-3.3970	12.6510	-19.3209	H	84 HIS335	0.1183
1405	N	-8.7578	18.2746	-19.3467	N.am	85 LEU336	-0.2636
BACKBONE							
1406	CA	-9.7736	18.9817	-20.1287	C.3	85 LEU336	0.1312
BACKBONE							
1407	C	-9.0975	19.7638	-21.2343	C.2	85 LEU336	0.2040
BACKBONE							
1408	O	-9.4896	19.6086	-22.3805	O.2	85 LEU336	-0.3944
BACKBONE							
1409	CB	-10.6330	19.9343	-19.2477	C.3	85 LEU336	-0.0101
1410	CG	-11.6894	20.7748	-20.0286	C.3	85 LEU336	-0.0425
1411	CD1	-12.7705	19.8851	-20.7032	C.3	85 LEU336	-0.0625
1412	CD2	-12.3668	21.7876	-19.0618	C.3	85 LEU336	-0.0625
1413	H	-8.7759	18.3522	-18.3499	H	85 LEU336	0.1883
1414	HA	-10.4290	18.2095	-20.5624	H	85 LEU336	0.0800
1415	HB3	-9.9532	20.6341	-18.7405	H	85 LEU336	0.0315
1416	HB2	-11.1433	19.3394	-18.4731	H	85 LEU336	0.0315
1417	HG	-11.1862	21.3582	-20.8184	H	85 LEU336	0.0298
1418	HD13	-12.3345	19.2563	-21.4932	H	85 LEU336	0.0232
1419	HD12	-13.5447	20.5136	-21.1703	H	85 LEU336	0.0232
1420	HD11	-13.2528	19.2357	-19.9567	H	85 LEU336	0.0232
1421	HD23	-12.8910	21.2547	-18.2536	H	85 LEU336	0.0232
1422	HD22	-13.0965	22.4115	-19.6010	H	85 LEU336	0.0232
1423	HD21	-11.6163	22.4559	-18.6108	H	85 LEU336	0.0232
1424	N	-8.0827	20.5971	-20.8993	N.am	86 THR337	-0.2613
BACKBONE							
1425	CA	-7.3871	21.3962	-21.9113	C.3	86 THR337	0.1564
BACKBONE							
1426	C	-5.9690	20.9325	-22.1860	C.2	86 THR337	0.2046
BACKBONE							

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1427 O       -5.3917    21.4454   -23.1322 O.2   86 THR337  -0.3944
BACKBONE
1428 CB      -7.3188    22.8606   -21.3980 C.3   86 THR337   0.0924
1429 OG1     -6.5360    22.8636   -20.1906 O.3   86 THR337  -0.3874
1430 CG2     -8.7368    23.4296   -21.1232 C.3   86 THR337  -0.0346
1431 H       -7.7907    20.6960   -19.9447 H     86 THR337   0.1884
1432 HA      -7.9291    21.3998   -22.8720 H     86 THR337   0.0826
1433 HB      -6.8247    23.4880   -22.1627 H     86 THR337   0.0639
1434 HG1     -6.4233    23.7359   -19.8279 H     86 THR337   0.2101
1435 HG22    -8.6698    24.4924   -20.8432 H     86 THR337   0.0257
1436 HG21    -9.2148    22.8851   -20.2957 H     86 THR337   0.0257
1437 HG23    -9.3694    23.3441   -22.0205 H     86 THR337   0.0257
1438 N       -5.3689    20.0066   -21.3990 N.am  87 HIS338  -0.2845
BACKBONE
1439 CA      -3.9536    19.6775   -21.5777 C.3   87 HIS338   0.0356
BACKBONE
1440 C       -3.1335    20.9424   -21.6161 C.2   87 HIS338  -0.1818
BACKBONE
1441 O       -2.4359    21.2268   -22.5762 O.2   87 HIS338  -0.7197
BACKBONE
1442 CB      -3.7268    18.7773   -22.8188 C.3   87 HIS338   0.0802
1443 CG      -4.5079    17.4998   -22.6600 C.2   87 HIS338   0.1946
1444 ND1     -5.7042    17.3007   -23.1702 N.pl3 87 HIS338  -0.1587
1445 CD2     -4.0937    16.4095   -21.9808 C.2   87 HIS338   0.1262
1446 CE1     -6.1127    16.1099   -22.8649 C.cat 87 HIS338   0.1842
1447 NE2     -5.2291    15.5515   -22.1740 N.2   87 HIS338  -0.2010
1448 H       -5.8616    19.5344   -20.6688 H     87 HIS338   0.1858
1449 HA      -3.5869    19.1254   -20.6946 H     87 HIS338   0.0538
1450 HB3     -2.6550    18.5315   -22.8983 H     87 HIS338   0.0775
1451 HB2     -4.0291    19.2912   -23.7442 H     87 HIS338   0.0775
1452 HD1     -6.2367    17.9862   -23.7282 H     87 HIS338   0.2700
1453 HD2     -3.1694    16.2272   -21.4367 H     87 HIS338   0.1326
1454 HE1     -7.0636    15.6597   -23.1496 H     87 HIS338   0.1885
@<TRIPOS>BOND
   1    1    2  1   BACKBONE
   2    1    9  1
   3    1   18  1
   4    2    3  1   BACKBONE
   5    2    5  1
   6    2   10  1
   7    3    4  2   BACKBONE
   8    3   21  am  BACKBONE|INTERRES
   9    5    6  1
  10    5   11  1
  11    5   12  1
  12    6    7  1
  13    6   13  1
  14    6   14  1
  15    7    8  1
  16    7   15  1
  17    7   16  1
  18    8   17  1
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19    8   19  1
20    8   20  1
21   21   22  1   BACKBONE
22   21   30  1
23   22   23  1   BACKBONE
24   22   25  1
25   22   31  1
26   23   24  2   BACKBONE
27   23   38  am  BACKBONE|INTERRES
28   25   26  1
29   25   32  1
30   25   33  1
31   26   27  1
32   26   34  1
33   26   35  1
34   27   28  2
35   27   29  am
36   29   36  1
37   29   37  1
38   38   39  1   BACKBONE
39   38   45  1
40   39   40  1   BACKBONE
41   39   42  1
42   39   46  1
43   40   41  2   BACKBONE
44   40   52  am  BACKBONE|INTERRES
45   42   43  1
46   42   44  1
47   42   47  1
48   43   48  1
49   44   49  1
50   44   50  1
51   44   51  1
52   52   53  1   BACKBONE
53   52   62  1
54   53   54  1   BACKBONE
55   53   56  1
56   53   63  1
57   54   55  2   BACKBONE
58   54   69  am  BACKBONE|INTERRES
59   56   57  1
60   56   64  1
61   56   65  1
62   57   58  1
63   57   59  2
64   58   60  1
65   58   66  1
66   59   61  1
67   59   67  1
68   60   61  2
69   60   68  1
70   69   70  1   BACKBONE
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 71   69   74  1
 72   70   71  1   BACKBONE
 73   70   73  1
 74   70   75  1
 75   71   72  2   BACKBONE
 76   71   79  am  BACKBONE|INTERRES
 77   73   76  1
 78   73   77  1
 79   73   78  1
 80   79   80  1   BACKBONE
 81   79   84  1
 82   80   81  1   BACKBONE
 83   80   83  1
 84   80   85  1
 85   81   82  2   BACKBONE
 86   81   89  am  BACKBONE|INTERRES
 87   83   86  1
 88   83   87  1
 89   83   88  1
 90   89   90  1   BACKBONE
 91   89  100  1
 92   90   91  1   BACKBONE
 93   90   93  1
 94   90  101  1
 95   91   92  2   BACKBONE
 96   91  113  am  BACKBONE|INTERRES
 97   93   94  1
 98   93  102  1
 99   93  103  1
100   94   95  1
101   94  104  1
102   94  105  1
103   95   96  1
104   95  106  1
105   95  107  1
106   96   97  ar
107   96  108  1
108   97   98  ar
109   97   99  ar
110   98  109  1
111   98  110  1
112   99  111  1
113   99  112  1
114  113  114  1   BACKBONE
115  113  121  1
116  114  115  1   BACKBONE
117  114  117  1
118  114  122  1
119  115  116  2   BACKBONE
120  115  132  am  BACKBONE|INTERRES
121  117  118  1
122  117  123  1
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123  117  124  1
124  118  119  1
125  118  125  1
126  118  126  1
127  119  120  1
128  119  127  1
129  119  128  1
130  120  129  1
131  120  130  1
132  120  131  1
133  132  133  1   BACKBONE
134  132  143  1
135  133  134  1   BACKBONE
136  133  136  1
137  133  144  1
138  134  135  2   BACKBONE
139  134  156  am  BACKBONE|INTERRES
140  136  137  1
141  136  145  1
142  136  146  1
143  137  138  1
144  137  147  1
145  137  148  1
146  138  139  1
147  138  149  1
148  138  150  1
149  139  140  ar
150  139  151  1
151  140  141  ar
152  140  142  ar
153  141  152  1
154  141  153  1
155  142  154  1
156  142  155  1
157  156  157  1   BACKBONE
158  156  163  1
159  157  158  1   BACKBONE
160  157  160  1
161  157  164  1
162  158  159  2   BACKBONE
163  158  170  am  BACKBONE|INTERRES
164  160  161  1
165  160  162  1
166  160  165  1
167  161  166  1
168  162  167  1
169  162  168  1
170  162  169  1
171  170  171  1   BACKBONE
172  170  181  1
173  171  172  1   BACKBONE
174  171  174  1
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175  171  182  1
176  172  173  2   BACKBONE
177  172  190  am  BACKBONE|INTERRES
178  174  175  1
179  174  183  1
180  174  184  1
181  175  176  ar
182  175  177  ar
183  176  178  ar
184  176  185  1
185  177  179  ar
186  177  186  1
187  178  180  ar
188  178  187  1
189  179  180  ar
190  179  188  1
191  180  189  1
192  190  191  1   BACKBONE
193  190  198  1
194  191  192  1   BACKBONE
195  191  194  1
196  191  199  1
197  192  193  2   BACKBONE
198  192  209  am  BACKBONE|INTERRES
199  194  195  1
200  194  200  1
201  194  201  1
202  195  196  1
203  195  202  1
204  195  203  1
205  196  197  1
206  196  204  1
207  196  205  1
208  197  206  1
209  197  207  1
210  197  208  1
211  209  210  1   BACKBONE
212  209  221  1
213  210  211  1   BACKBONE
214  210  213  1
215  210  222  1
216  211  212  2   BACKBONE
217  211  230  am  BACKBONE|INTERRES
218  213  214  1
219  213  223  1
220  213  224  1
221  214  215  ar
222  214  216  ar
223  215  217  ar
224  215  225  1
225  216  218  ar
226  216  226  1
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227  217  219  ar
228  217  227  1
229  218  219  ar
230  218  228  1
231  219  220  1
232  220  229  1
233  230  231  1   BACKBONE
234  230  244  1
235  231  232  1   BACKBONE
236  231  234  1
237  231  245  1
238  232  233  2   BACKBONE
239  232  254  am  BACKBONE|INTERRES
240  234  235  1
241  234  246  1
242  234  247  1
243  235  236  2
244  235  237  1
245  236  238  1
246  236  248  1
247  237  239  ar
248  237  240  ar
249  238  239  1
250  238  249  1
251  239  241  ar
252  240  242  ar
253  240  250  1
254  241  243  ar
255  241  251  1
256  242  243  ar
257  242  252  1
258  243  253  1
259  254  255  1   BACKBONE
260  254  260  1
261  255  256  1   BACKBONE
262  255  258  1
263  255  261  1
264  256  257  2   BACKBONE
265  256  268  am  BACKBONE|INTERRES
266  258  259  1
267  258  262  1
268  258  263  1
269  259  260  1
270  259  264  1
271  259  265  1
272  260  266  1
273  260  267  1
274  268  269  1   BACKBONE
275  268  274  1
276  269  270  1   BACKBONE
277  269  272  1
278  269  275  1
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279  270  271  2   BACKBONE
280  270  279  am  BACKBONE|INTERRES
281  272  273  1
282  272  276  1
283  272  277  1
284  273  278  1
285  279  280  1   BACKBONE
286  279  285  1
287  280  281  1   BACKBONE
288  280  283  1
289  280  286  1
290  281  282  2   BACKBONE
291  281  290  am  BACKBONE|INTERRES
292  283  284  1
293  283  287  1
294  283  288  1
295  284  289  1
296  290  291  1   BACKBONE
297  290  297  1
298  291  292  1   BACKBONE
299  291  294  1
300  291  298  1
301  292  293  2   BACKBONE
302  292  306  am  BACKBONE|INTERRES
303  294  295  1
304  294  296  1
305  294  299  1
306  295  300  1
307  295  301  1
308  295  302  1
309  296  303  1
310  296  304  1
311  296  305  1
312  306  307  1   BACKBONE
313  306  312  1
314  307  308  1   BACKBONE
315  307  310  1
316  307  313  1
317  308  309  2   BACKBONE
318  308  320  am  BACKBONE|INTERRES
319  310  311  1
320  310  314  1
321  310  315  1
322  311  312  1
323  311  316  1
324  311  317  1
325  312  318  1
326  312  319  1
327  320  321  1   BACKBONE
328  320  327  1
329  321  322  1   BACKBONE
330  321  324  1
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331  321  328  1
332  322  323  2   BACKBONE
333  322  336  am  BACKBONE|INTERRES
334  324  325  1
335  324  326  1
336  324  329  1
337  325  330  1
338  325  331  1
339  325  332  1
340  326  333  1
341  326  334  1
342  326  335  1
343  336  337  1   BACKBONE
344  336  345  1
345  337  338  1   BACKBONE
346  337  340  1
347  337  346  1
348  338  339  2   BACKBONE
349  338  353  am  BACKBONE|INTERRES
350  340  341  1
351  340  347  1
352  340  348  1
353  341  342  1
354  341  349  1
355  341  350  1
356  342  343  2
357  342  344  am
358  344  351  1
359  344  352  1
360  353  354  1   BACKBONE
361  353  359  1
362  354  355  1   BACKBONE
363  354  357  1
364  354  360  1
365  355  356  2   BACKBONE
366  355  367  am  BACKBONE|INTERRES
367  357  358  1
368  357  361  1
369  357  362  1
370  358  359  1
371  358  363  1
372  358  364  1
373  359  365  1
374  359  366  1
375  367  368  1   BACKBONE
376  367  376  1
377  368  369  1   BACKBONE
378  368  371  1
379  368  377  1
380  369  370  2   BACKBONE
381  369  382  am  BACKBONE|INTERRES
382  371  372  1
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383  371  378  1
384  371  379  1
385  372  373  1
386  372  380  1
387  372  381  1
388  373  374  ar
389  373  375  ar
390  382  383  1   BACKBONE
391  382  391  1
392  383  384  1   BACKBONE
393  383  386  1
394  383  392  1
395  384  385  2   BACKBONE
396  384  399  am  BACKBONE|INTERRES
397  386  387  1
398  386  393  1
399  386  394  1
400  387  388  1
401  387  395  1
402  387  396  1
403  388  389  2
404  388  390  am
405  390  397  1
406  390  398  1
407  399  400  1   BACKBONE
408  399  407  1
409  400  401  1   BACKBONE
410  400  403  1
411  400  408  1
412  401  402  2   BACKBONE
413  401  418  am  BACKBONE|INTERRES
414  403  404  1
415  403  409  1
416  403  410  1
417  404  405  1
418  404  406  1
419  404  411  1
420  405  412  1
421  405  413  1
422  405  414  1
423  406  415  1
424  406  416  1
425  406  417  1
426  418  419  1   BACKBONE
427  418  423  1
428  419  420  1   BACKBONE
429  419  422  1
430  419  424  1
431  420  421  2   BACKBONE
432  420  428  am  BACKBONE|INTERRES
433  422  425  1
434  422  426  1
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435  422  427  1
436  428  429  1   BACKBONE
437  428  433  1
438  429  430  1   BACKBONE
439  429  432  1
440  429  434  1
441  430  431  2   BACKBONE
442  430  438  am  BACKBONE|INTERRES
443  432  435  1
444  432  436  1
445  432  437  1
446  438  439  1   BACKBONE
447  438  443  1
448  439  440  1   BACKBONE
449  439  442  1
450  439  444  1
451  440  441  2   BACKBONE
452  440  448  am  BACKBONE|INTERRES
453  442  445  1
454  442  446  1
455  442  447  1
456  448  449  1   BACKBONE
457  448  452  1
458  449  450  1   BACKBONE
459  449  453  1
460  449  454  1
461  450  451  2   BACKBONE
462  450  455  am  BACKBONE|INTERRES
463  455  456  1   BACKBONE
464  455  466  1
465  456  457  1   BACKBONE
466  456  459  1
467  456  467  1
468  457  458  2   BACKBONE
469  457  475  am  BACKBONE|INTERRES
470  459  460  1
471  459  468  1
472  459  469  1
473  460  461  ar
474  460  462  ar
475  461  463  ar
476  461  470  1
477  462  464  ar
478  462  471  1
479  463  465  ar
480  463  472  1
481  464  465  ar
482  464  473  1
483  465  474  1
484  475  476  1   BACKBONE
485  475  487  1
486  476  477  1   BACKBONE
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487  476  479  1
488  476  488  1
489  477  478  2   BACKBONE
490  477  496  am  BACKBONE|INTERRES
491  479  480  1
492  479  489  1
493  479  490  1
494  480  481  ar
495  480  482  ar
496  481  483  ar
497  481  491  1
498  482  484  ar
499  482  492  1
500  483  485  ar
501  483  493  1
502  484  485  ar
503  484  494  1
504  485  486  1
505  486  495  1
506  496  497  1   BACKBONE
507  496  508  1
508  497  498  1   BACKBONE
509  497  500  1
510  497  509  1
511  498  499  2   BACKBONE
512  498  517  am  BACKBONE|INTERRES
513  500  501  1
514  500  510  1
515  500  511  1
516  501  502  ar
517  501  503  ar
518  502  504  ar
519  502  512  1
520  503  505  ar
521  503  513  1
522  504  506  ar
523  504  514  1
524  505  506  ar
525  505  515  1
526  506  507  1
527  507  516  1
528  517  518  1   BACKBONE
529  517  524  1
530  518  519  1   BACKBONE
531  518  521  1
532  518  525  1
533  519  520  2   BACKBONE
534  519  533  am  BACKBONE|INTERRES
535  521  522  1
536  521  523  1
537  521  526  1
538  522  527  1
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539  522  528  1
540  522  529  1
541  523  530  1
542  523  531  1
543  523  532  1
544  533  534  1   BACKBONE
545  533  537  1
546  534  535  1   BACKBONE
547  534  538  1
548  534  539  1
549  535  536  2   BACKBONE
550  535  540  am  BACKBONE|INTERRES
551  540  541  1   BACKBONE
552  540  551  1
553  541  542  1   BACKBONE
554  541  544  1
555  541  552  1
556  542  543  2   BACKBONE
557  542  564  am  BACKBONE|INTERRES
558  544  545  1
559  544  553  1
560  544  554  1
561  545  546  1
562  545  555  1
563  545  556  1
564  546  547  1
565  546  557  1
566  546  558  1
567  547  548  ar
568  547  559  1
569  548  549  ar
570  548  550  ar
571  549  560  1
572  549  561  1
573  550  562  1
574  550  563  1
575  564  565  1   BACKBONE
576  564  572  1
577  565  566  1   BACKBONE
578  565  568  1
579  565  573  1
580  566  567  2   BACKBONE
581  566  578  am  BACKBONE|INTERRES
582  568  569  1
583  568  574  1
584  568  575  1
585  569  570  2
586  569  571  am
587  571  576  1
588  571  577  1
589  578  579  1   BACKBONE
590  578  586  1
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591  579  580  1   BACKBONE
592  579  582  1
593  579  587  1
594  580  581  2   BACKBONE
595  580  590  am  BACKBONE|INTERRES
596  582  583  1
597  582  588  1
598  582  589  1
599  583  584  ar
600  583  585  ar
601  590  591  1   BACKBONE
602  590  598  1
603  591  592  1   BACKBONE
604  591  594  1
605  591  599  1
606  592  593  2   BACKBONE
607  592  602  am  BACKBONE|INTERRES
608  594  595  1
609  594  600  1
610  594  601  1
611  595  596  ar
612  595  597  ar
613  602  603  1   BACKBONE
614  602  609  1
615  603  604  1   BACKBONE
616  603  606  1
617  603  610  1
618  604  605  2   BACKBONE
619  604  693  am  BACKBONE|INTERRES
620  606  607  1
621  606  608  1
622  606  611  1
623  607  612  1
624  607  613  1
625  607  614  1
626  608  615  1
627  608  616  1
628  608  617  1
629  618  619  2   BACKBONE
630  619  620  am  BACKBONE
631  619  658  1   BACKBONE
632  620  621  1   BACKBONE
633  620  655  1   BACKBONE
634  621  622  1
635  621  623  1   BACKBONE
636  621  649  1   BACKBONE
637  623  624  am  BACKBONE
638  623  648  2   BACKBONE
639  624  625  1
640  624  626  1   BACKBONE
641  626  627  1
642  626  628  1   BACKBONE
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643  626  633  1   BACKBONE
644  628  629  ar  BACKBONE
645  628  641  ar  BACKBONE
646  629  630  1   BACKBONE
647  629  636  ar  BACKBONE
648  630  631  1
649  630  632  1
650  630  633  1   BACKBONE
651  633  634  1
652  633  635  1
653  636  637  ar  BACKBONE
654  636  643  1   BACKBONE
655  637  638  1
656  637  639  ar  BACKBONE
657  639  640  1
658  639  641  ar  BACKBONE
659  641  642  1
660  643  644  1
661  644  645  2
662  644  646  2
663  644  647  am
664  647  700  1
665  647  701  1
666  649  650  1
667  649  651  1
668  649  652  1   BACKBONE
669  652  653  1
670  652  654  1
671  652  655  1   BACKBONE
672  655  656  1
673  655  657  1
674  658  659  1
675  658  660  1   BACKBONE
676  658  676  1   BACKBONE
677  660  661  1
678  660  662  am  BACKBONE
679  662  663  1   BACKBONE
680  662  675  2   BACKBONE
681  663  664  1
682  663  665  1   BACKBONE
683  663  671  1   BACKBONE
684  665  666  1
685  665  667  1   BACKBONE
686  667  668  1
687  667  669  1
688  667  670  1
689  671  672  1
690  671  673  1
691  671  674  1
692  676  677  1
693  676  678  1   BACKBONE
694  676  690  1   BACKBONE
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695  678  679  1
696  678  680  1
697  678  681  1   BACKBONE
698  681  682  1
699  681  683  1
700  681  684  1   BACKBONE
701  684  685  1
702  684  686  1
703  684  687  1   BACKBONE
704  687  688  1
705  687  689  1
706  687  690  1   BACKBONE
707  690  691  1
708  690  692  1
709  693  694  1   BACKBONE
710  693  702  1
711  694  695  1   BACKBONE
712  694  697  1
713  694  703  1
714  695  696  2   BACKBONE
715  695  712  am  BACKBONE|INTERRES
716  697  698  1
717  697  704  1
718  697  705  1
719  698  699  1
720  698  706  1
721  698  707  1
722  699  700  1
723  699  708  1
724  699  709  1
725  700  710  1
726  700  711  1
727  712  713  1   BACKBONE
728  712  718  1
729  713  714  1   BACKBONE
730  713  716  1
731  713  719  1
732  714  715  2   BACKBONE
733  714  724  am  BACKBONE|INTERRES
734  716  717  1
735  716  720  1
736  716  721  1
737  717  722  1
738  717  723  1
739  724  725  1   BACKBONE
740  724  735  1
741  725  726  1   BACKBONE
742  725  728  1
743  725  736  1
744  726  727  2   BACKBONE
745  726  744  am  BACKBONE|INTERRES
746  728  729  1
```

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747  728  737  1
748  728  738  1
749  729  730  ar
750  729  731  ar
751  730  732  ar
752  730  739  1
753  731  733  ar
754  731  740  1
755  732  734  ar
756  732  741  1
757  733  734  ar
758  733  742  1
759  734  743  1
760  744  745  1   BACKBONE
761  744  750  1
762  745  746  1   BACKBONE
763  745  748  1
764  745  751  1
765  746  747  2   BACKBONE
766  746  755  am  BACKBONE|INTERRES
767  748  749  1
768  748  752  1
769  748  753  1
770  749  754  1
771  755  756  1   BACKBONE
772  755  761  1
773  756  757  1   BACKBONE
774  756  759  1
775  756  762  1
776  757  758  2   BACKBONE
777  757  767  am  BACKBONE|INTERRES
778  759  760  1
779  759  763  1
780  759  764  1
781  760  765  1
782  760  766  1
783  767  768  1   BACKBONE
784  767  775  1
785  768  769  1   BACKBONE
786  768  771  1
787  768  776  1
788  769  770  2   BACKBONE
789  769  779  am  BACKBONE|INTERRES
790  771  772  1
791  771  777  1
792  771  778  1
793  772  773  ar
794  772  774  ar
795  779  780  1   BACKBONE
796  779  783  1
797  780  781  1   BACKBONE
798  780  784  1
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799  780  785  1
800  781  782  2   BACKBONE
801  781  786  am  BACKBONE|INTERRES
802  786  787  1   BACKBONE
803  786  790  1
804  787  788  1   BACKBONE
805  787  791  1
806  787  792  1
807  788  789  2   BACKBONE
808  788  793  am  BACKBONE|INTERRES
809  793  794  1   BACKBONE
810  793  801  1
811  794  795  1   BACKBONE
812  794  797  1
813  794  802  1
814  795  796  2   BACKBONE
815  795  812  am  BACKBONE|INTERRES
816  797  798  1
817  797  803  1
818  797  804  1
819  798  799  1
820  798  800  1
821  798  805  1
822  799  806  1
823  799  807  1
824  799  808  1
825  800  809  1
826  800  810  1
827  800  811  1
828  812  813  1   BACKBONE
829  812  823  1
830  813  814  1   BACKBONE
831  813  816  1
832  813  824  1
833  814  815  2   BACKBONE
834  814  836  am  BACKBONE|INTERRES
835  816  817  1
836  816  825  1
837  816  826  1
838  817  818  1
839  817  827  1
840  817  828  1
841  818  819  1
842  818  829  1
843  818  830  1
844  819  820  ar
845  819  831  1
846  820  821  ar
847  820  822  ar
848  821  832  1
849  821  833  1
850  822  834  1
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851  822  835  1
852  836  837  1   BACKBONE
853  836  842  1
854  837  838  1   BACKBONE
855  837  840  1
856  837  843  1
857  838  839  2   BACKBONE
858  838  849  am  BACKBONE|INTERRES
859  840  841  1
860  840  844  1
861  840  845  1
862  841  846  1
863  841  847  1
864  841  848  1
865  849  850  1   BACKBONE
866  849  863  1
867  850  851  1   BACKBONE
868  850  853  1
869  850  864  1
870  851  852  2   BACKBONE
871  851  873  am  BACKBONE|INTERRES
872  853  854  1
873  853  865  1
874  853  866  1
875  854  855  2
876  854  856  1
877  855  857  1
878  855  867  1
879  856  858  ar
880  856  859  ar
881  857  858  1
882  857  868  1
883  858  860  ar
884  859  861  ar
885  859  869  1
886  860  862  ar
887  860  870  1
888  861  862  ar
889  861  871  1
890  862  872  1
891  873  874  1   BACKBONE
892  873  882  1
893  874  875  1   BACKBONE
894  874  877  1
895  874  883  1
896  875  876  2   BACKBONE
897  875  888  am  BACKBONE|INTERRES
898  877  878  1
899  877  884  1
900  877  885  1
901  878  879  1
902  878  886  1
```

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903  878  887  1
904  879  880  ar
905  879  881  ar
906  888  889  1   BACKBONE
907  888  894  1
908  889  890  1   BACKBONE
909  889  892  1
910  889  895  1
911  890  891  2   BACKBONE
912  890  899  am  BACKBONE|INTERRES
913  892  893  1
914  892  896  1
915  892  897  1
916  893  898  1
917  899  900  1   BACKBONE
918  899  903  1
919  900  901  1   BACKBONE
920  900  904  1
921  900  905  1
922  901  902  2   BACKBONE
923  901  906  am  BACKBONE|INTERRES
924  906  907  1   BACKBONE
925  906  914  1
926  907  908  1   BACKBONE
927  907  910  1
928  907  915  1
929  908  909  2   BACKBONE
930  908  918  am  BACKBONE|INTERRES
931  910  911  1
932  910  916  1
933  910  917  1
934  911  912  ar
935  911  913  ar
936  918  919  1   BACKBONE
937  918  926  1
938  919  920  1   BACKBONE
939  919  922  1
940  919  927  1
941  920  921  2   BACKBONE
942  920  930  am  BACKBONE|INTERRES
943  922  923  1
944  922  928  1
945  922  929  1
946  923  924  ar
947  923  925  ar
948  930  931  1   BACKBONE
949  930  936  1
950  931  932  1   BACKBONE
951  931  934  1
952  931  937  1
953  932  933  2   BACKBONE
954  932  944  am  BACKBONE|INTERRES
```

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 955  934  935  1
 956  934  938  1
 957  934  939  1
 958  935  936  1
 959  935  940  1
 960  935  941  1
 961  936  942  1
 962  936  943  1
 963  944  945  1   BACKBONE
 964  944  958  1
 965  945  946  1   BACKBONE
 966  945  948  1
 967  945  959  1
 968  946  947  2   BACKBONE
 969  946  968  am  BACKBONE|INTERRES
 970  948  949  1
 971  948  960  1
 972  948  961  1
 973  949  950  2
 974  949  951  1
 975  950  952  1
 976  950  962  1
 977  951  953  ar
 978  951  954  ar
 979  952  953  1
 980  952  963  1
 981  953  955  ar
 982  954  956  ar
 983  954  964  1
 984  955  957  ar
 985  955  965  1
 986  956  957  ar
 987  956  966  1
 988  957  967  1
 989  968  969  1   BACKBONE
 990  968  975  1
 991  969  970  1   BACKBONE
 992  969  972  1
 993  969  976  1
 994  970  971  2   BACKBONE
 995  970  984  am  BACKBONE|INTERRES
 996  972  973  1
 997  972  974  1
 998  972  977  1
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1000  973  979  1
1001  973  980  1
1002  974  981  1
1003  974  982  1
1004  974  983  1
1005  984  985  1   BACKBONE
1006  984  993  1
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1007  985  986  1   BACKBONE
1008  985  988  1
1009  985  994  1
1010  986  987  2   BACKBONE
1011  986  999  am  BACKBONE|INTERRES
1012  988  989  1
1013  988  995  1
1014  988  996  1
1015  989  990  1
1016  989  997  1
1017  989  998  1
1018  990  991  ar
1019  990  992  ar
1020  999 1000  1   BACKBONE
1021  999 1009  1
1022 1000 1001  1   BACKBONE
1023 1000 1003  1
1024 1000 1010  1
1025 1001 1002  2   BACKBONE
1026 1001 1016  am  BACKBONE|INTERRES
1027 1003 1004  1
1028 1003 1011  1
1029 1003 1012  1
1030 1004 1005  1
1031 1004 1006  2
1032 1005 1007  ar
1033 1005 1013  1
1034 1006 1008  1
1035 1006 1014  1
1036 1007 1008  1
1037 1007 1015  1
1038 1016 1017  1   BACKBONE
1039 1016 1021  1
1040 1017 1018  1   BACKBONE
1041 1017 1020  1
1042 1017 1022  1
1043 1018 1019  2   BACKBONE
1044 1018 1026  am  BACKBONE|INTERRES
1045 1020 1023  1
1046 1020 1024  1
1047 1020 1025  1
1048 1026 1027  1   BACKBONE
1049 1026 1035  1
1050 1027 1028  1   BACKBONE
1051 1027 1030  1
1052 1027 1036  1
1053 1028 1029  2   BACKBONE
1054 1028 1048  am  BACKBONE|INTERRES
1055 1030 1031  1
1056 1030 1037  1
1057 1030 1038  1
1058 1031 1032  1
```

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1063 1032 1042  1
1064 1033 1034  1
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1066 1033 1044  1
1067 1034 1045  1
1068 1034 1046  1
1069 1034 1047  1
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1071 1048 1062  1
1072 1049 1050  1   BACKBONE
1073 1049 1052  1
1074 1049 1063  1
1075 1050 1051  2   BACKBONE
1076 1050 1072  am  BACKBONE|INTERRES
1077 1052 1053  1
1078 1052 1064  1
1079 1052 1065  1
1080 1053 1054  2
1081 1053 1055  1
1082 1054 1056  1
1083 1054 1066  1
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1085 1055 1058  ar
1086 1056 1057  1
1087 1056 1067  1
1088 1057 1059  ar
1089 1058 1060  ar
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1091 1059 1061  ar
1092 1059 1069  1
1093 1060 1061  ar
1094 1060 1070  1
1095 1061 1071  1
1096 1072 1073  1   BACKBONE
1097 1072 1083  1
1098 1073 1074  1   BACKBONE
1099 1073 1076  1
1100 1073 1084  1
1101 1074 1075  2   BACKBONE
1102 1074 1092  am  BACKBONE|INTERRES
1103 1076 1077  1
1104 1076 1085  1
1105 1076 1086  1
1106 1077 1078  ar
1107 1077 1079  ar
1108 1078 1080  ar
1109 1078 1087  1
1110 1079 1081  ar
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1111 1079 1088  1
1112 1080 1082  ar
1113 1080 1089  1
1114 1081 1082  ar
1115 1081 1090  1
1116 1082 1091  1
1117 1092 1093  1   BACKBONE
1118 1092 1098  1
1119 1093 1094  1   BACKBONE
1120 1093 1096  1
1121 1093 1099  1
1122 1094 1095  2   BACKBONE
1123 1094 1106  am  BACKBONE|INTERRES
1124 1096 1097  1
1125 1096 1100  1
1126 1096 1101  1
1127 1097 1098  1
1128 1097 1102  1
1129 1097 1103  1
1130 1098 1104  1
1131 1098 1105  1
1132 1106 1107  1   BACKBONE
1133 1106 1110  1
1134 1107 1108  1   BACKBONE
1135 1107 1111  1
1136 1107 1112  1
1137 1108 1109  2   BACKBONE
1138 1108 1113  am  BACKBONE|INTERRES
1139 1113 1114  1   BACKBONE
1140 1113 1119  1
1141 1114 1115  1   BACKBONE
1142 1114 1117  1
1143 1114 1120  1
1144 1115 1116  2   BACKBONE
1145 1115 1125  am  BACKBONE|INTERRES
1146 1117 1118  1
1147 1117 1121  1
1148 1117 1122  1
1149 1118 1123  1
1150 1118 1124  1
1151 1125 1126  1   BACKBONE
1152 1125 1134  1
1153 1126 1127  1   BACKBONE
1154 1126 1129  1
1155 1126 1135  1
1156 1127 1128  2   BACKBONE
1157 1127 1140  am  BACKBONE|INTERRES
1158 1129 1130  1
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1160 1129 1137  1
1161 1130 1131  1
1162 1130 1138  1
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1163 1130 1139  1
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1165 1131 1133  ar
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1167 1140 1151  1
1168 1141 1142  1   BACKBONE
1169 1141 1144  1
1170 1141 1152  1
1171 1142 1143  2   BACKBONE
1172 1142 1160  am  BACKBONE|INTERRES
1173 1144 1145  1
1174 1144 1153  1
1175 1144 1154  1
1176 1145 1146  ar
1177 1145 1147  ar
1178 1146 1148  ar
1179 1146 1155  1
1180 1147 1149  ar
1181 1147 1156  1
1182 1148 1150  ar
1183 1148 1157  1
1184 1149 1150  ar
1185 1149 1158  1
1186 1150 1159  1
1187 1160 1161  1   BACKBONE
1188 1160 1168  1
1189 1161 1162  1   BACKBONE
1190 1161 1164  1
1191 1161 1169  1
1192 1162 1163  2   BACKBONE
1193 1162 1179  am  BACKBONE|INTERRES
1194 1164 1165  1
1195 1164 1170  1
1196 1164 1171  1
1197 1165 1166  1
1198 1165 1167  1
1199 1165 1172  1
1200 1166 1173  1
1201 1166 1174  1
1202 1166 1175  1
1203 1167 1176  1
1204 1167 1177  1
1205 1167 1178  1
1206 1179 1180  1   BACKBONE
1207 1179 1187  1
1208 1180 1181  1   BACKBONE
1209 1180 1183  1
1210 1180 1188  1
1211 1181 1182  2   BACKBONE
1212 1181 1198  am  BACKBONE|INTERRES
1213 1183 1184  1
1214 1183 1185  1
```

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1215 1183 1189  1
1216 1184 1186  1
1217 1184 1190  1
1218 1184 1191  1
1219 1185 1192  1
1220 1185 1193  1
1221 1185 1194  1
1222 1186 1195  1
1223 1186 1196  1
1224 1186 1197  1
1225 1198 1199  1   BACKBONE
1226 1198 1209  1
1227 1199 1200  1   BACKBONE
1228 1199 1202  1
1229 1199 1210  1
1230 1200 1201  2   BACKBONE
1231 1200 1222  am  BACKBONE|INTERRES
1232 1202 1203  1
1233 1202 1211  1
1234 1202 1212  1
1235 1203 1204  1
1236 1203 1213  1
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1241 1205 1206  ar
1242 1205 1217  1
1243 1206 1207  ar
1244 1206 1208  ar
1245 1207 1218  1
1246 1207 1219  1
1247 1208 1220  1
1248 1208 1221  1
1249 1222 1223  1   BACKBONE
1250 1222 1230  1
1251 1223 1224  1   BACKBONE
1252 1223 1226  1
1253 1223 1231  1
1254 1224 1225  2   BACKBONE
1255 1224 1241  am  BACKBONE|INTERRES
1256 1226 1227  1
1257 1226 1232  1
1258 1226 1233  1
1259 1227 1228  1
1260 1227 1234  1
1261 1227 1235  1
1262 1228 1229  1
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1264 1228 1237  1
1265 1229 1238  1
1266 1229 1239  1
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1267 1229 1240  1
1268 1241 1242  1   BACKBONE
1269 1241 1250  1
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1273 1243 1244  2   BACKBONE
1274 1243 1263  am  BACKBONE|INTERRES
1275 1245 1246  1
1276 1245 1252  1
1277 1245 1253  1
1278 1246 1247  1
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1287 1249 1260  1
1288 1249 1261  1
1289 1249 1262  1
1290 1263 1264  1   BACKBONE
1291 1263 1267  1
1292 1264 1265  1   BACKBONE
1293 1264 1268  1
1294 1264 1269  1
1295 1265 1266  2   BACKBONE
1296 1265 1270  am  BACKBONE|INTERRES
1297 1270 1271  1   BACKBONE
1298 1270 1279  1
1299 1271 1272  1   BACKBONE
1300 1271 1274  1
1301 1271 1280  1
1302 1272 1273  2   BACKBONE
1303 1272 1287  am  BACKBONE|INTERRES
1304 1274 1275  1
1305 1274 1281  1
1306 1274 1282  1
1307 1275 1276  1
1308 1275 1283  1
1309 1275 1284  1
1310 1276 1277  2
1311 1276 1278  am
1312 1278 1285  1
1313 1278 1286  1
1314 1287 1288  1   BACKBONE
1315 1287 1296  1
1316 1288 1289  1   BACKBONE
1317 1288 1291  1
1318 1288 1297  1
```

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1319 1289 1290  2   BACKBONE
1320 1289 1302  am  BACKBONE|INTERRES
1321 1291 1292  1
1322 1291 1298  1
1323 1291 1299  1
1324 1292 1293  1
1325 1292 1300  1
1326 1292 1301  1
1327 1293 1294  ar
1328 1293 1295  ar
1329 1302 1303  1   BACKBONE
1330 1302 1314  1
1331 1303 1304  1   BACKBONE
1332 1303 1306  1
1333 1303 1315  1
1334 1304 1305  2   BACKBONE
1335 1304 1323  am  BACKBONE|INTERRES
1336 1306 1307  1
1337 1306 1316  1
1338 1306 1317  1
1339 1307 1308  ar
1340 1307 1309  ar
1341 1308 1310  ar
1342 1308 1318  1
1343 1309 1311  ar
1344 1309 1319  1
1345 1310 1312  ar
1346 1310 1320  1
1347 1311 1312  ar
1348 1311 1321  1
1349 1312 1313  1
1350 1313 1322  1
1351 1323 1324  1   BACKBONE
1352 1323 1331  1
1353 1324 1325  1   BACKBONE
1354 1324 1327  1
1355 1324 1332  1
1356 1325 1326  2   BACKBONE
1357 1325 1342  am  BACKBONE|INTERRES
1358 1327 1328  1
1359 1327 1329  1
1360 1327 1333  1
1361 1328 1330  1
1362 1328 1334  1
1363 1328 1335  1
1364 1329 1336  1
1365 1329 1337  1
1366 1329 1338  1
1367 1330 1339  1
1368 1330 1340  1
1369 1330 1341  1
1370 1342 1343  1   BACKBONE
```

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1371 1342 1350  1
1372 1343 1344  1   BACKBONE
1373 1343 1346  1
1374 1343 1351  1
1375 1344 1345  2   BACKBONE
1376 1344 1356  am  BACKBONE|INTERRES
1377 1346 1347  1
1378 1346 1352  1
1379 1346 1353  1
1380 1347 1348  2
1381 1347 1349  am
1382 1349 1354  1
1383 1349 1355  1
1384 1356 1357  1   BACKBONE
1385 1356 1364  1
1386 1357 1358  1   BACKBONE
1387 1357 1360  1
1388 1357 1365  1
1389 1358 1359  2   BACKBONE
1390 1358 1370  am  BACKBONE|INTERRES
1391 1360 1361  1
1392 1360 1366  1
1393 1360 1367  1
1394 1361 1362  2
1395 1361 1363  am
1396 1363 1368  1
1397 1363 1369  1
1398 1370 1371  1   BACKBONE
1399 1370 1378  1
1400 1371 1372  1   BACKBONE
1401 1371 1374  1
1402 1371 1379  1
1403 1372 1373  2   BACKBONE
1404 1372 1389  am  BACKBONE|INTERRES
1405 1374 1375  1
1406 1374 1376  1
1407 1374 1380  1
1408 1375 1377  1
1409 1375 1381  1
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1412 1376 1384  1
1413 1376 1385  1
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1415 1377 1387  1
1416 1377 1388  1
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1418 1389 1399  1
1419 1390 1391  1   BACKBONE
1420 1390 1393  1
1421 1390 1400  1
1422 1391 1392  2   BACKBONE
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1423 1391 1405  am  BACKBONE|INTERRES
1424 1393 1394  1
1425 1393 1401  1
1426 1393 1402  1
1427 1394 1395  1
1428 1394 1396  2
1429 1395 1397  2
1430 1396 1398  1
1431 1396 1403  1
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1433 1397 1404  1
1434 1405 1406  1   BACKBONE
1435 1405 1413  1
1436 1406 1407  1   BACKBONE
1437 1406 1409  1
1438 1406 1414  1
1439 1407 1408  2   BACKBONE
1440 1407 1424  am  BACKBONE|INTERRES
1441 1409 1410  1
1442 1409 1415  1
1443 1409 1416  1
1444 1410 1411  1
1445 1410 1412  1
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1448 1411 1419  1
1449 1411 1420  1
1450 1412 1421  1
1451 1412 1422  1
1452 1412 1423  1
1453 1424 1425  1   BACKBONE
1454 1424 1431  1
1455 1425 1426  1   BACKBONE
1456 1425 1428  1
1457 1425 1432  1
1458 1426 1427  2   BACKBONE
1459 1426 1438  am  BACKBONE|INTERRES
1460 1428 1429  1
1461 1428 1430  1
1462 1428 1433  1
1463 1429 1434  1
1464 1430 1435  1
1465 1430 1436  1
1466 1430 1437  1
1467 1438 1439  1   BACKBONE
1468 1438 1448  1
1469 1439 1440  1   BACKBONE
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1471 1439 1449  1
1472 1440 1441  2   BACKBONE
1473 1442 1443  1
1474 1442 1450  1
```

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1475 1442 1451  1
1476 1443 1444  1
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1480 1445 1447  1
1481 1445 1453  1
1482 1446 1447  1
1483 1446 1454  1
@<TRIPOS>SUBSTRUCTURE
  1 MET252    2 RESIDUE 4 A MET 1
  2 GLN253   22 RESIDUE 4 A GLN 2
  3 THR254   39 RESIDUE 4 A THR 2
  4 HIS255   53 RESIDUE 4 A HIS 2
  5 ALA256   70 RESIDUE 4 A ALA 2
  6 ALA257   80 RESIDUE 4 A ALA 2
  7 ARG258   90 RESIDUE 4 A ARG 2
  8 MET259  114 RESIDUE 4 A MET 2
  9 ARG260  133 RESIDUE 4 A ARG 2
 10 THR261  157 RESIDUE 4 A THR 2
 11 PHE262  171 RESIDUE 4 A PHE 2
 12 MET263  191 RESIDUE 4 A MET 2
 13 TYR264  210 RESIDUE 4 A TYR 2
 14 TRP265  231 RESIDUE 4 A TRP 2
 15 PRO266  255 RESIDUE 4 A PRO 2
 16 SER267  269 RESIDUE 4 A SER 2
 17 SER268  280 RESIDUE 4 A SER 2
 18 VAL269  291 RESIDUE 4 A VAL 2
 19 PRO270  307 RESIDUE 4 A PRO 2
 20 VAL271  321 RESIDUE 4 A VAL 2
 21 GLN272  337 RESIDUE 4 A GLN 2
 22 PRO273  354 RESIDUE 4 A PRO 2
 23 GLU274  368 RESIDUE 4 A GLU 2
 24 GLN275  383 RESIDUE 4 A GLN 2
 25 LEU276  400 RESIDUE 4 A LEU 2
 26 ALA277  419 RESIDUE 4 A ALA 2
 27 ALA278  429 RESIDUE 4 A ALA 2
 28 ALA279  439 RESIDUE 4 A ALA 2
 29 GLY280  449 RESIDUE 4 A GLY 2
 30 PHE281  456 RESIDUE 4 A PHE 2
 31 TYR282  476 RESIDUE 4 A TYR 2
 32 TYR283  497 RESIDUE 4 A TYR 2
 33 VAL284  518 RESIDUE 4 A VAL 2
 34 GLY285  534 RESIDUE 4 A GLY 2
 35 ARG286  541 RESIDUE 4 A ARG 2
 36 ASN287  565 RESIDUE 4 A ASN 2
 37 ASP288  579 RESIDUE 4 A ASP 2
 38 ASP289  591 RESIDUE 4 A ASP 2
 39 VAL290  603 RESIDUE 4 A VAL 2
 40 LYS291  694 RESIDUE 4 A LYS 2
 41 CYS292  713 RESIDUE 4 A CYS 2
 42 PHE293  725 RESIDUE 4 A PHE 2
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 43 SER294  745 RESIDUE 4 A SER 2
 44 CYS295  756 RESIDUE 4 A CYS 2
 45 ASP296  768 RESIDUE 4 A ASP 2
 46 GLY297  780 RESIDUE 4 A GLY 2
 47 GLY298  787 RESIDUE 4 A GLY 2
 48 LEU299  794 RESIDUE 4 A LEU 2
 49 ARG300  813 RESIDUE 4 A ARG 2
 50 CYS301  837 RESIDUE 4 A CYS 2
 51 TRP302  850 RESIDUE 4 A TRP 2
 52 GLU303  874 RESIDUE 4 A GLU 2
 53 SER304  889 RESIDUE 4 A SER 2
 54 GLY305  900 RESIDUE 4 A GLY 2
 55 ASP306  907 RESIDUE 4 A ASP 2
 56 ASP307  919 RESIDUE 4 A ASP 2
 57 PRO308  931 RESIDUE 4 A PRO 2
 58 TRP309  945 RESIDUE 4 A TRP 2
 59 VAL310  969 RESIDUE 4 A VAL 2
 60 GLU311  985 RESIDUE 4 A GLU 2
 61 HIS312 1000 RESIDUE 4 A HIS 2
 62 ALA313 1017 RESIDUE 4 A ALA 2
 63 LYS314 1027 RESIDUE 4 A LYS 2
 64 TRP315 1049 RESIDUE 4 A TRP 2
 65 PHE316 1073 RESIDUE 4 A PHE 2
 66 PRO317 1093 RESIDUE 4 A PRO 2
 67 GLY318 1107 RESIDUE 4 A GLY 2
 68 CYS319 1114 RESIDUE 4 A CYS 2
 69 GLU320 1126 RESIDUE 4 A GLU 2
 70 PHE321 1141 RESIDUE 4 A PHE 2
 71 LEU322 1161 RESIDUE 4 A LEU 2
 72 ILE323 1180 RESIDUE 4 A ILE 2
 73 ARG324 1199 RESIDUE 4 A ARG 2
 74 MET325 1223 RESIDUE 4 A MET 2
 75 LYS326 1242 RESIDUE 4 A LYS 2
 76 GLY327 1264 RESIDUE 4 A GLY 2
 77 GLN328 1271 RESIDUE 4 A GLN 2
 78 GLU329 1288 RESIDUE 4 A GLU 2
 79 TYR330 1303 RESIDUE 4 A TYR 2
 80 ILE331 1324 RESIDUE 4 A ILE 2
 81 ASN332 1343 RESIDUE 4 A ASN 2
 82 ASN333 1357 RESIDUE 4 A ASN 2
 83 ILE334 1371 RESIDUE 4 A ILE 2
 84 HIS335 1390 RESIDUE 4 A HIS 2
 85 LEU336 1406 RESIDUE 4 A LEU 2
 86 THR337 1425 RESIDUE 4 A THR 2
 87 HIS338 1439 RESIDUE 4 A HIS 1

# MOE 2019.01 (io_trps.svl 2018.10)
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cIAP2-BIR3 + compound 2 .mol2 file

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2uvl_142D6_covalent.A
1578 1606 94 0 0
BIOPOLYMER
USER_CHARGES


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BACKBONE
   2 CA        0.6315   -11.5151    -2.9055 C.3     1 SER242   0.0000
BACKBONE
   3 C        -0.1291   -10.3865    -2.2485 C.2     1 SER242   0.0000
BACKBONE
   4 O        -1.1674   -10.6573    -1.6659 O.2     1 SER242   0.0000
BACKBONE
   5 CB        0.5518   -11.3629    -4.4458 C.3     1 SER242   0.0000
   6 OG       -0.8320   -11.3577    -4.8365 O.3     1 SER242   0.0000
   7 H        -0.8250   -12.8533    -2.0788 H       1 SER242   0.0000
   8 HA        1.6836   -11.4734    -2.5767 H       1 SER242   0.0000
   9 HB3       1.0775   -12.2069    -4.9233 H       1 SER242   0.0000
  10 HB2       1.0366   -10.4250    -4.7644 H       1 SER242   0.0000
  11 HG       -0.9471   -11.2657    -5.7772 H       1 SER242   0.0000
  12 NCAP      0.5599   -13.6468    -2.7707 H       1 SER242   0.0000
  13 N         0.3697    -9.1300    -2.3410 N.am    2 MET243   0.0000
BACKBONE
  14 CA       -0.3511    -7.9864    -1.7839 C.3     2 MET243   0.0000
BACKBONE
  15 C        -0.4482    -6.8994    -2.8293 C.2     2 MET243   0.0000
BACKBONE
  16 O         0.4381    -6.8066    -3.6638 O.2     2 MET243   0.0000
BACKBONE
  17 CB        0.3940    -7.4216    -0.5455 C.3     2 MET243   0.0000
  18 CG        0.3659    -8.4050     0.6545 C.3     2 MET243   0.0000
  19 SD       -1.3291    -8.7439     1.2464 S.o     2 MET243   0.0000
  20 CE       -1.8862    -7.1107     1.8321 C.3     2 MET243   0.0000
  21 H         1.2464    -8.9491    -2.7919 H       2 MET243   0.0000
  22 HA       -1.3779    -8.2630    -1.4985 H       2 MET243   0.0000
  23 HB3      -0.0476    -6.4595    -0.2440 H       2 MET243   0.0000
  24 HB2       1.4425    -7.2289    -0.8261 H       2 MET243   0.0000
  25 HG3       0.9474    -7.9931     1.4944 H       2 MET243   0.0000
  26 HG2       0.8169    -9.3651     0.3600 H       2 MET243   0.0000
  27 LPD2     -1.3256    -9.1969     1.7521 LP      2 MET243   0.0000
  28 LPD1     -1.7235    -8.9705     0.7422 LP      2 MET243   0.0000
  29 HE3      -1.1077    -6.6430     2.4529 H       2 MET243   0.0000
  30 HE2      -2.7960    -7.2432     2.4355 H       2 MET243   0.0000
  31 HE1      -2.1219    -6.4579     0.9791 H       2 MET243   0.0000
  32 N        -1.5131    -6.0645    -2.7862 N.am    3 ARG244   0.0000
BACKBONE
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33	CA	-1.6018	-4.9350	-3.7096	C.3	3 ARG244	0.0000
BACKBONE							
34	C	-0.6365	-3.9019	-3.1886	C.2	3 ARG244	0.0000
BACKBONE							
35	O	-0.5027	-3.8355	-1.9764	O.2	3 ARG244	0.0000
BACKBONE							
36	CB	-3.0476	-4.3614	-3.7117	C.3	3 ARG244	0.0000
37	CG	-3.3158	-3.2719	-4.7894	C.3	3 ARG244	0.0000
38	CD	-4.7942	-2.7887	-4.7228	C.3	3 ARG244	0.0000
39	NE	-5.2494	-2.2341	-6.0045	N.pl3	3 ARG244	0.0000
40	CZ	-5.1342	-0.9727	-6.3673	C.cat	3 ARG244	1.0000
41	NH1	-4.5317	-0.0609	-5.6406	N.pl3	3 ARG244	0.0000
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43	H	-2.2151	-6.1560	-2.0763	H	3 ARG244	0.0000
44	HA	-1.3401	-5.2624	-4.7295	H	3 ARG244	0.0000
45	HB3	-3.2788	-3.9482	-2.7161	H	3 ARG244	0.0000
46	HB2	-3.7262	-5.2108	-3.8964	H	3 ARG244	0.0000
47	HG3	-3.1278	-3.7077	-5.7838	H	3 ARG244	0.0000
48	HG2	-2.6359	-2.4151	-4.6553	H	3 ARG244	0.0000
49	HD3	-4.9683	-2.1295	-3.8583	H	3 ARG244	0.0000
50	HD2	-5.4331	-3.6682	-4.5357	H	3 ARG244	0.0000
51	HE	-5.7329	-2.8890	-6.6423	H	3 ARG244	0.0000
52	HH11	-4.0856	-0.2902	-4.7460	H	3 ARG244	0.0000
53	HH12	-4.4834	0.9185	-5.9596	H	3 ARG244	0.0000
54	HH21	-6.1360	-1.2765	-8.1302	H	3 ARG244	0.0000
55	HH22	-5.5840	0.3739	-7.8452	H	3 ARG244	0.0000
56	N	0.0309	-3.0965	-4.0489	N.am	4 TYR245	0.0000
BACKBONE							
57	CA	0.8772	-2.0224	-3.5335	C.3	4 TYR245	0.0000
BACKBONE							
58	C	0.6785	-0.7982	-4.3949	C.2	4 TYR245	0.0000
BACKBONE							
59	O	0.7531	-0.9268	-5.6069	O.2	4 TYR245	0.0000
BACKBONE							
60	CB	2.3806	-2.4034	-3.4754	C.3	4 TYR245	0.0000
61	CG	3.0329	-2.3458	-4.8646	C.ar	4 TYR245	0.0000
62	CD1	3.5607	-1.1392	-5.3407	C.ar	4 TYR245	0.0000
63	CD2	3.1077	-3.4874	-5.6687	C.ar	4 TYR245	0.0000
64	CE1	4.1686	-1.0727	-6.5969	C.ar	4 TYR245	0.0000
65	CE2	3.7247	-3.4243	-6.9219	C.ar	4 TYR245	0.0000
66	CZ	4.2615	-2.2223	-7.3917	C.ar	4 TYR245	0.0000
67	OH	4.8794	-2.1919	-8.6464	O.3	4 TYR245	0.0000
68	H	-0.0487	-3.2048	-5.0422	H	4 TYR245	0.0000
69	HA	0.5744	-1.7840	-2.5004	H	4 TYR245	0.0000
70	HB2	2.4869	-3.4072	-3.0347	H	4 TYR245	0.0000
71	HB3	2.9154	-1.6956	-2.8200	H	4 TYR245	0.0000
72	HD1	3.4944	-0.2410	-4.7366	H	4 TYR245	0.0000
73	HD2	2.6865	-4.4260	-5.3232	H	4 TYR245	0.0000
74	HE1	4.5632	-0.1241	-6.9471	H	4 TYR245	0.0000
75	HE2	3.7889	-4.3156	-7.5375	H	4 TYR245	0.0000
76	HH	5.2427	-1.3461	-8.8838	H	4 TYR245	0.0000

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  77 N        0.4289     0.3842    -3.7917 N.am   5 THR246   0.0000
BACKBONE
  78 CA       0.3842     1.6215    -4.5624 C.3    5 THR246   0.0000
BACKBONE
  79 C        1.7372     2.2946    -4.5273 C.2    5 THR246   0.0000
BACKBONE
  80 O        2.0917     2.9158    -5.5174 O.2    5 THR246   0.0000
BACKBONE
  81 CB      -0.6864     2.5441    -3.9267 C.3    5 THR246   0.0000
  82 OG1     -0.3321     2.7517    -2.5489 O.3    5 THR246   0.0000
  83 CG2     -2.0830     1.8756    -4.0357 C.3    5 THR246   0.0000
  84 H        0.3051     0.4509    -2.7990 H      5 THR246   0.0000
  85 HA       0.1018     1.4381    -5.6131 H      5 THR246   0.0000
  86 HB      -0.6911     3.5104    -4.4609 H      5 THR246   0.0000
  87 HG1     -0.9416     3.3252    -2.0961 H      5 THR246   0.0000
  88 HG22    -2.8543     2.5034    -3.5649 H      5 THR246   0.0000
  89 HG21    -2.0900     0.8947    -3.5371 H      5 THR246   0.0000
  90 HG23    -2.3382     1.7338    -5.0963 H      5 THR246   0.0000
  91 N        2.5016     2.2001    -3.4104 N.am   6 VAL247   0.0000
BACKBONE
  92 CA       3.7505     2.9438    -3.3047 C.3    6 VAL247   0.0000
BACKBONE
  93 C        4.9053     2.1225    -3.8263 C.2    6 VAL247   0.0000
BACKBONE
  94 O        5.1874     1.0897    -3.2394 O.2    6 VAL247   0.0000
BACKBONE
  95 CB       4.0285     3.3941    -1.8417 C.3    6 VAL247   0.0000
  96 CG1      5.4183     4.0798    -1.7536 C.3    6 VAL247   0.0000
  97 CG2      2.9077     4.3568    -1.3569 C.3    6 VAL247   0.0000
  98 H        2.2472     1.6358    -2.6268 H      6 VAL247   0.0000
  99 HA       3.6454     3.8675    -3.8837 H      6 VAL247   0.0000
 100 HB       4.0393     2.5108    -1.1800 H      6 VAL247   0.0000
 101 HG13     6.2348     3.3582    -1.9090 H      6 VAL247   0.0000
 102 HG12     5.5561     4.5461    -0.7691 H      6 VAL247   0.0000
 103 HG11     5.4901     4.8531    -2.5281 H      6 VAL247   0.0000
 104 HG23     2.8766     5.2626    -1.9816 H      6 VAL247   0.0000
 105 HG22     3.0838     4.6580    -0.3128 H      6 VAL247   0.0000
 106 HG21     1.9244     3.8655    -1.4093 H      6 VAL247   0.0000
 107 N        5.5967     2.5650    -4.9036 N.am   7 SER248   0.0000
BACKBONE
 108 CA       6.7653     1.8277    -5.3706 C.3    7 SER248   0.0000
BACKBONE
 109 C        7.9209     2.0463    -4.4225 C.2    7 SER248   0.0000
BACKBONE
 110 O        8.4286     1.0670    -3.8983 O.2    7 SER248   0.0000
BACKBONE
 111 CB       7.1900     2.2543    -6.7992 C.3    7 SER248   0.0000
 112 OG       8.3794     1.5344    -7.1684 O.3    7 SER248   0.0000
 113 H        5.3571     3.4145    -5.3759 H      7 SER248   0.0000
 114 HA       6.5263     0.7513    -5.4169 H      7 SER248   0.0000
 115 HB3      7.3870     3.3388    -6.8319 H      7 SER248   0.0000
 116 HB2      6.3676     2.0231    -7.4969 H      7 SER248   0.0000
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BACKBONE							
119 CA	9.5635	3.5522	-3.4114	C.3	8	ASN249	0.0000
BACKBONE							
120 C	9.1503	3.9470	-2.0100	C.2	8	ASN249	0.0000
BACKBONE							
121 O	8.7860	5.0931	-1.7970	O.2	8	ASN249	0.0000
BACKBONE							
122 CB	10.4570	4.6198	-4.0991	C.3	8	ASN249	0.0000
123 CG	11.8367	4.6524	-3.4835	C.2	8	ASN249	0.0000
124 OD1	11.9931	4.2227	-2.3498	O.2	8	ASN249	0.0000
125 ND2	12.8617	5.1526	-4.2075	N.am	8	ASN249	0.0000
126 H	7.8786	4.1064	-4.5768	H	8	ASN249	0.0000
127 HA	10.1892	2.6438	-3.3926	H	8	ASN249	0.0000
128 HB3	9.9973	5.6165	-4.0337	H	8	ASN249	0.0000
129 HB2	10.5485	4.3534	-5.1646	H	8	ASN249	0.0000
130 HD21	12.7161	5.5127	-5.1284	H	8	ASN249	0.0000
131 HD22	13.7876	5.1605	-3.8264	H	8	ASN249	0.0000
132 N	9.1965	3.0021	-1.0418	N.am	9	LEU250	0.0000
BACKBONE							
133 CA	8.7803	3.3141	0.3257	C.3	9	LEU250	0.0000
BACKBONE							
134 C	9.7659	4.2510	0.9909	C.2	9	LEU250	0.0000
BACKBONE							
135 O	9.3459	5.0457	1.8174	O.2	9	LEU250	0.0000
BACKBONE							
136 CB	8.6421	2.0196	1.1769	C.3	9	LEU250	0.0000
137 CG	7.5103	1.0706	0.6687	C.3	9	LEU250	0.0000
138 CD1	7.7555	-0.3798	1.1710	C.3	9	LEU250	0.0000
139 CD2	6.1009	1.5451	1.1268	C.3	9	LEU250	0.0000
140 H	9.5350	2.0806	-1.2410	H	9	LEU250	0.0000
141 HA	7.8021	3.8115	0.2889	H	9	LEU250	0.0000
142 HB3	8.4454	2.2801	2.2296	H	9	LEU250	0.0000
143 HB2	9.6169	1.5066	1.1423	H	9	LEU250	0.0000
144 HG	7.5161	1.0398	-0.4342	H	9	LEU250	0.0000
145 HD13	8.7172	-0.7620	0.7939	H	9	LEU250	0.0000
146 HD12	6.9597	-1.0529	0.8154	H	9	LEU250	0.0000
147 HD11	7.7742	-0.4062	2.2712	H	9	LEU250	0.0000
148 HD23	6.0293	1.5303	2.2250	H	9	LEU250	0.0000
149 HD22	5.3251	0.8776	0.7201	H	9	LEU250	0.0000
150 HD21	5.8800	2.5637	0.7830	H	9	LEU250	0.0000
151 N	11.0783	4.1920	0.6662	N.am	10	SER251	0.0000
BACKBONE							
152 CA	12.0241	5.0962	1.3206	C.3	10	SER251	0.0000
BACKBONE							
153 C	11.8203	6.5422	0.9198	C.2	10	SER251	0.0000
BACKBONE							
154 O	12.3483	7.3895	1.6230	O.2	10	SER251	0.0000
BACKBONE							
155 CB	13.4902	4.6993	1.0069	C.3	10	SER251	0.0000
156 OG	13.7244	4.8440	-0.4026	O.3	10	SER251	0.0000

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 157 H       11.4230     3.5497    -0.0210 H     10 SER251   0.0000
 158 HA      11.8852     5.0147     2.4127 H     10 SER251   0.0000
 159 HB3     13.6591     3.6532     1.3142 H     10 SER251   0.0000
 160 HB2     14.1826     5.3483     1.5704 H     10 SER251   0.0000
 161 HG      14.6136     4.6154    -0.6545 H     10 SER251   0.0000
 162 N       11.0883     6.8568    -0.1786 N.am  11 MET252   0.0000
BACKBONE
 163 CA      10.9555     8.2458    -0.6243 C.3   11 MET252   0.0000
BACKBONE
 164 C        9.5457     8.7560    -0.4179 C.2   11 MET252   0.0000
BACKBONE
 165 O        9.0543     9.5087    -1.2434 O.2   11 MET252   0.0000
BACKBONE
 166 CB      11.4246     8.3159    -2.1050 C.3   11 MET252   0.0000
 167 CG      12.8552     7.7444    -2.2918 C.3   11 MET252   0.0000
 168 SD      14.0982     8.4917    -1.1943 S.o   11 MET252   0.0000
 169 CE      13.9487    10.2343    -1.6636 C.3   11 MET252   0.0000
 170 H       10.6331     6.1580    -0.7322 H     11 MET252   0.0000
 171 HA      11.5831     8.9345    -0.0392 H     11 MET252   0.0000
 172 HB3     11.3818     9.3469    -2.4809 H     11 MET252   0.0000
 173 HB2     10.7483     7.7128    -2.7274 H     11 MET252   0.0000
 174 HG3     13.1791     7.8598    -3.3388 H     11 MET252   0.0000
 175 HG2     12.8631     6.6784    -2.0385 H     11 MET252   0.0000
 176 LPD2    14.7205     8.2509    -1.3199 LP    11 MET252   0.0000
 177 LPD1    13.9456     8.3944    -0.5399 LP    11 MET252   0.0000
 178 HE3     13.9253    10.3344    -2.7576 H     11 MET252   0.0000
 179 HE2     14.8179    10.7697    -1.2641 H     11 MET252   0.0000
 180 HE1     13.0320    10.6525    -1.2270 H     11 MET252   0.0000
 181 N        8.8823     8.3671     0.6958 N.am  12 GLN253   0.0000
BACKBONE
 182 CA       7.5197     8.8363     0.9569 C.3   12 GLN253   0.0000
BACKBONE
 183 C        7.4959    10.2160     1.5730 C.2   12 GLN253   0.0000
BACKBONE
 184 O        6.5010    10.8972     1.3779 O.2   12 GLN253   0.0000
BACKBONE
 185 CB       6.7691     7.8563     1.9044 C.3   12 GLN253   0.0000
 186 CG       6.4518     6.5305     1.1673 C.3   12 GLN253   0.0000
 187 CD       5.8768     5.4802     2.0881 C.2   12 GLN253   0.0000
 188 OE1      4.6765     5.2531     2.0525 O.2   12 GLN253   0.0000
 189 NE2      6.7056     4.8197     2.9250 N.am  12 GLN253   0.0000
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 191 HA       6.9560     8.8890     0.0109 H     12 GLN253   0.0000
 192 HB3      5.8144     8.3005     2.2334 H     12 GLN253   0.0000
 193 HB2      7.3785     7.6672     2.8029 H     12 GLN253   0.0000
 194 HG3      7.3612     6.1496     0.6838 H     12 GLN253   0.0000
 195 HG2      5.7235     6.7393     0.3729 H     12 GLN253   0.0000
 196 HE21     7.6864     5.0165     2.9447 H     12 GLN253   0.0000
 197 HE22     6.3387     4.1165     3.5360 H     12 GLN253   0.0000
 198 N        8.5348    10.6542     2.3221 N.am  13 THR254   0.0000
BACKBONE
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199	CA	8.4489	11.9434	3.0082	C.3	13 THR254	0.0000
BACKBONE							
200	C	8.9657	13.0600	2.1303	C.2	13 THR254	0.0000
BACKBONE							
201	O	9.8318	12.8099	1.3076	O.2	13 THR254	0.0000
BACKBONE							
202	CB	9.2583	11.9063	4.3316	C.3	13 THR254	0.0000
203	OG1	10.6139	11.5500	4.0100	O.3	13 THR254	0.0000
204	CG2	8.6453	10.8747	5.3181	C.3	13 THR254	0.0000
205	H	9.3745	10.1191	2.4283	H	13 THR254	0.0000
206	HA	7.4006	12.1531	3.2789	H	13 THR254	0.0000
207	HB	9.2391	12.9082	4.7975	H	13 THR254	0.0000
208	HG1	11.1718	11.5068	4.7800	H	13 THR254	0.0000
209	HG22	9.2196	10.8596	6.2572	H	13 THR254	0.0000
210	HG21	8.6637	9.8644	4.8820	H	13 THR254	0.0000
211	HG23	7.6026	11.1378	5.5545	H	13 THR254	0.0000
212	N	8.4496	14.3007	2.3047	N.am	14 HIS255	0.0000
BACKBONE							
213	CA	8.9489	15.4291	1.5208	C.3	14 HIS255	0.0000
BACKBONE							
214	C	10.4262	15.6059	1.7696	C.2	14 HIS255	0.0000
BACKBONE							
215	O	11.1528	15.8108	0.8117	O.2	14 HIS255	0.0000
BACKBONE							
216	CB	8.2232	16.7503	1.8966	C.3	14 HIS255	0.0000
217	CG	8.8709	17.9493	1.2484	C.2	14 HIS255	0.0000
218	ND1	9.9276	18.5596	1.7358	N.pl3	14 HIS255	0.0000
219	CD2	8.4726	18.5558	0.1134	C.2	14 HIS255	0.0000
220	CE1	10.2479	19.5545	0.9699	C.2	14 HIS255	0.0000
221	NE2	9.4466	19.6092	0.0073	N.2	14 HIS255	0.0000
222	H	7.7346	14.4723	2.9855	H	14 HIS255	0.0000
223	HA	8.7774	15.2275	0.4493	H	14 HIS255	0.0000
224	HB3	8.2448	16.9035	2.9869	H	14 HIS255	0.0000
225	HB2	7.1687	16.6799	1.5843	H	14 HIS255	0.0000
226	HD1	10.4250	18.2959	2.5988	H	14 HIS255	0.0000
227	HD2	7.6426	18.3163	-0.5434	H	14 HIS255	0.0000
228	HE1	11.0815	20.2373	1.1312	H	14 HIS255	0.0000
229	N	10.8867	15.5456	3.0401	N.am	15 ALA256	0.0000
BACKBONE							
230	CA	12.3039	15.7774	3.3115	C.3	15 ALA256	0.0000
BACKBONE							
231	C	13.1541	14.8200	2.5110	C.2	15 ALA256	0.0000
BACKBONE							
232	O	14.0651	15.2717	1.8358	O.2	15 ALA256	0.0000
BACKBONE							
233	CB	12.6460	15.6206	4.8158	C.3	15 ALA256	0.0000
234	H	10.2674	15.3744	3.8085	H	15 ALA256	0.0000
235	HA	12.5454	16.8130	3.0174	H	15 ALA256	0.0000
236	HB3	12.3963	14.6083	5.1685	H	15 ALA256	0.0000
237	HB2	12.0740	16.3507	5.4093	H	15 ALA256	0.0000
238	HB1	13.7207	15.7973	4.9810	H	15 ALA256	0.0000

239 N	12.8701	13.4987	2.5689	N.am	16	ALA257	0.0000
BACKBONE							
240 CA	13.6949	12.5437	1.8307	C.3	16	ALA257	0.0000
BACKBONE							
241 C	13.7805	12.9755	0.3856	C.2	16	ALA257	0.0000
BACKBONE							
242 O	14.8722	13.0650	-0.1542	O.2	16	ALA257	0.0000
BACKBONE							
243 CB	13.1172	11.1040	1.9022	C.3	16	ALA257	0.0000
244 H	12.1021	13.1598	3.1147	H	16	ALA257	0.0000
245 HA	14.7051	12.5382	2.2751	H	16	ALA257	0.0000
246 HB3	12.0968	11.0694	1.4909	H	16	ALA257	0.0000
247 HB2	13.0841	10.7629	2.9480	H	16	ALA257	0.0000
248 HB1	13.7510	10.4080	1.3315	H	16	ALA257	0.0000
249 N	12.6205	13.2587	-0.2463	N.am	17	ARG258	0.0000
BACKBONE							
250 CA	12.6298	13.6526	-1.6524	C.3	17	ARG258	0.0000
BACKBONE							
251 C	13.3940	14.9409	-1.8409	C.2	17	ARG258	0.0000
BACKBONE							
252 O	14.1048	15.0696	-2.8245	O.2	17	ARG258	0.0000
BACKBONE							
253 CB	11.1909	13.8337	-2.2086	C.3	17	ARG258	0.0000
254 CG	10.3782	12.5080	-2.1794	C.3	17	ARG258	0.0000
255 CD	9.0913	12.6136	-3.0352	C.3	17	ARG258	0.0000
256 NE	8.1999	13.6481	-2.5079	N.pl3	17	ARG258	0.0000
257 CZ	7.3339	13.4598	-1.5322	C.cat	17	ARG258	1.0000
258 NH1	7.2013	12.3244	-0.8838	N.pl3	17	ARG258	0.0000
259 NH2	6.5561	14.4612	-1.1844	N.pl3	17	ARG258	0.0000
260 H	11.7499	13.2271	0.2475	H	17	ARG258	0.0000
261 HA	13.1384	12.8780	-2.2476	H	17	ARG258	0.0000
262 HB3	11.2866	14.1868	-3.2464	H	17	ARG258	0.0000
263 HB2	10.6554	14.6069	-1.6354	H	17	ARG258	0.0000
264 HG3	10.1073	12.2391	-1.1500	H	17	ARG258	0.0000
265 HG2	10.9899	11.6888	-2.5772	H	17	ARG258	0.0000
266 HD3	8.6003	11.6388	-3.1347	H	17	ARG258	0.0000
267 HD2	9.3845	12.8830	-4.0612	H	17	ARG258	0.0000
268 HE	8.2425	14.5711	-2.9686	H	17	ARG258	0.0000
269 HH11	7.7853	11.5057	-1.0877	H	17	ARG258	0.0000
270 HH12	6.5000	12.2256	-0.1347	H	17	ARG258	0.0000
271 HH21	6.6155	15.3754	-1.6583	H	17	ARG258	0.0000
272 HH22	5.8641	14.3610	-0.4265	H	17	ARG258	0.0000
273 N	13.2511	15.9128	-0.9154	N.am	18	PHE259	0.0000
BACKBONE							
274 CA	13.8924	17.2088	-1.1102	C.3	18	PHE259	0.0000
BACKBONE							
275 C	15.3988	17.1096	-0.9972	C.2	18	PHE259	0.0000
BACKBONE							
276 O	16.0820	17.8531	-1.6838	O.2	18	PHE259	0.0000
BACKBONE							
277 CB	13.2836	18.2657	-0.1518	C.3	18	PHE259	0.0000
278 CG	13.7456	19.7111	-0.4161	C.ar	18	PHE259	0.0000

279	CD1	13.6892	20.2770	-1.6972	C.ar	18 PHE259	0.0000
280	CD2	14.2173	20.4957	0.6444	C.ar	18 PHE259	0.0000
281	CE1	14.1448	21.5789	-1.9208	C.ar	18 PHE259	0.0000
282	CE2	14.6385	21.8111	0.4298	C.ar	18 PHE259	0.0000
283	CZ	14.6155	22.3524	-0.8576	C.ar	18 PHE259	0.0000
284	H	12.6922	15.7682	-0.1007	H	18 PHE259	0.0000
285	HA	13.6284	17.5185	-2.1242	H	18 PHE259	0.0000
286	HB3	13.5114	17.9590	0.8803	H	18 PHE259	0.0000
287	HB2	12.1912	18.2530	-0.2801	H	18 PHE259	0.0000
288	HD1	13.2858	19.7257	-2.5383	H	18 PHE259	0.0000
289	HD2	14.2555	20.0911	1.6505	H	18 PHE259	0.0000
290	HE1	14.1302	21.9917	-2.9223	H	18 PHE259	0.0000
291	HE2	14.9835	22.4142	1.2641	H	18 PHE259	0.0000
292	HZ	14.9597	23.3673	-1.0312	H	18 PHE259	0.0000
293	N	15.9432	16.2030	-0.1510	N.am	19 LYS260	0.0000
BACKBONE							
294	CA	17.3983	16.0991	-0.0182	C.3	19 LYS260	0.0000
BACKBONE							
295	C	18.0649	15.6567	-1.3036	C.2	19 LYS260	0.0000
BACKBONE							
296	O	19.1434	16.1496	-1.5918	O.2	19 LYS260	0.0000
BACKBONE							
297	CB	17.8320	15.0912	1.0849	C.3	19 LYS260	0.0000
298	CG	17.5240	15.6068	2.5178	C.3	19 LYS260	0.0000
299	CD	18.1073	14.6516	3.5951	C.3	19 LYS260	0.0000
300	CE	17.8508	15.1851	5.0310	C.3	19 LYS260	0.0000
301	NZ	18.5308	14.3502	6.0483	N.4	19 LYS260	1.0000
302	H	15.3650	15.5936	0.3931	H	19 LYS260	0.0000
303	HA	17.7927	17.0952	0.2449	H	19 LYS260	0.0000
304	HB3	18.9218	14.9386	1.0097	H	19 LYS260	0.0000
305	HB2	17.3412	14.1188	0.9143	H	19 LYS260	0.0000
306	HG3	16.4380	15.7040	2.6641	H	19 LYS260	0.0000
307	HG2	17.9769	16.6033	2.6470	H	19 LYS260	0.0000
308	HD3	19.1949	14.5567	3.4436	H	19 LYS260	0.0000
309	HD2	17.6560	13.6513	3.4886	H	19 LYS260	0.0000
310	HE3	16.7642	15.2003	5.2231	H	19 LYS260	0.0000
311	HE2	18.2258	16.2199	5.1101	H	19 LYS260	0.0000
312	HZ3	18.1986	13.3217	6.0113	H	19 LYS260	0.0000
313	HZ2	18.3390	14.7146	7.0491	H	19 LYS260	0.0000
314	HZ1	19.6047	14.3515	5.9167	H	19 LYS260	0.0000
315	N	17.4702	14.7256	-2.0815	N.am	20 THR261	0.0000
BACKBONE							
316	CA	18.1488	14.2260	-3.2829	C.3	20 THR261	0.0000
BACKBONE							
317	C	18.4991	15.3520	-4.2324	C.2	20 THR261	0.0000
BACKBONE							
318	O	19.5075	15.2552	-4.9144	O.2	20 THR261	0.0000
BACKBONE							
319	CB	17.2339	13.2503	-4.0641	C.3	20 THR261	0.0000
320	OG1	16.0019	13.9621	-4.2320	O.3	20 THR261	0.0000
321	CG2	17.0266	11.9055	-3.3160	C.3	20 THR261	0.0000
322	H	16.5665	14.3698	-1.8392	H	20 THR261	0.0000

323	HA	19.0732	13.7038	-2.9850	H	20 THR261	0.0000
324	HB	17.6815	13.0204	-5.0473	H	20 THR261	0.0000
325	HG1	15.3510	13.4500	-4.6896	H	20 THR261	0.0000
326	HG22	16.3425	11.2580	-3.8864	H	20 THR261	0.0000
327	HG21	16.5993	12.0682	-2.3180	H	20 THR261	0.0000
328	HG23	17.9875	11.3801	-3.2026	H	20 THR261	0.0000
329	N	17.6869	16.4329	-4.2890	N.am	21 PHE262	0.0000
BACKBONE							
330	CA	17.9996	17.5483	-5.1837	C.3	21 PHE262	0.0000
BACKBONE							
331	C	19.2393	18.3220	-4.7665	C.2	21 PHE262	0.0000
BACKBONE							
332	O	19.5602	19.2733	-5.4606	O.2	21 PHE262	0.0000
BACKBONE							
333	CB	16.7890	18.5189	-5.3006	C.3	21 PHE262	0.0000
334	CG	15.5815	17.8325	-5.9642	C.ar	21 PHE262	0.0000
335	CD1	15.4814	17.7568	-7.3567	C.ar	21 PHE262	0.0000
336	CD2	14.5551	17.2764	-5.1967	C.ar	21 PHE262	0.0000
337	CE1	14.4231	17.0758	-7.9648	C.ar	21 PHE262	0.0000
338	CE2	13.4546	16.6583	-5.7947	C.ar	21 PHE262	0.0000
339	CZ	13.3989	16.5314	-7.1851	C.ar	21 PHE262	0.0000
340	H	16.8750	16.4917	-3.7086	H	21 PHE262	0.0000
341	HA	18.1963	17.1400	-6.1893	H	21 PHE262	0.0000
342	HB3	17.0563	19.3991	-5.9034	H	21 PHE262	0.0000
343	HB2	16.5255	18.8871	-4.2965	H	21 PHE262	0.0000
344	HD1	16.2321	18.2275	-7.9715	H	21 PHE262	0.0000
345	HD2	14.6186	17.3285	-4.1228	H	21 PHE262	0.0000
346	HE1	14.4032	16.9674	-9.0425	H	21 PHE262	0.0000
347	HE2	12.6461	16.2749	-5.1792	H	21 PHE262	0.0000
348	HZ	12.5713	16.0107	-7.6563	H	21 PHE262	0.0000
349	N	19.9641	17.9769	-3.6733	N.am	22 PHE263	0.0000
BACKBONE							
350	CA	21.1588	18.7381	-3.2987	C.3	22 PHE263	0.0000
BACKBONE							
351	C	22.0490	19.0305	-4.4891	C.2	22 PHE263	0.0000
BACKBONE							
352	O	22.5759	20.1295	-4.5616	O.2	22 PHE263	0.0000
BACKBONE							
353	CB	22.0179	18.0417	-2.2020	C.3	22 PHE263	0.0000
354	CG	22.9089	16.9239	-2.7730	C.ar	22 PHE263	0.0000
355	CD1	24.2744	17.1515	-2.9879	C.ar	22 PHE263	0.0000
356	CD2	22.3759	15.6677	-3.0823	C.ar	22 PHE263	0.0000
357	CE1	25.0970	16.1345	-3.4804	C.ar	22 PHE263	0.0000
358	CE2	23.1855	14.6643	-3.6238	C.ar	22 PHE263	0.0000
359	CZ	24.5507	14.8940	-3.8157	C.ar	22 PHE263	0.0000
360	H	19.6704	17.2486	-3.0606	H	22 PHE263	0.0000
361	HA	20.7878	19.6913	-2.8839	H	22 PHE263	0.0000
362	HB3	21.3794	17.6349	-1.4029	H	22 PHE263	0.0000
363	HB2	22.6634	18.8019	-1.7325	H	22 PHE263	0.0000
364	HD1	24.7095	18.1225	-2.7740	H	22 PHE263	0.0000
365	HD2	21.3285	15.4588	-2.9046	H	22 PHE263	0.0000
366	HE1	26.1612	16.3106	-3.6068	H	22 PHE263	0.0000

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 367 HE2     22.7551    13.7053    -3.8937 H     22 PHE263   0.0000
 368 HZ      25.1836    14.1119    -4.2237 H     22 PHE263   0.0000
 369 N       22.2161    18.0618    -5.4232 N.am  23 ASN264   0.0000
BACKBONE
 370 CA      23.0386    18.2769    -6.6165 C.3   23 ASN264   0.0000
BACKBONE
 371 C       22.1375    18.4139    -7.8240 C.2   23 ASN264   0.0000
BACKBONE
 372 O       22.3233    17.7080    -8.8029 O.2   23 ASN264   0.0000
BACKBONE
 373 CB      24.0639    17.1213    -6.7831 C.3   23 ASN264   0.0000
 374 CG      23.4195    15.7556    -6.8353 C.2   23 ASN264   0.0000
 375 OD1     22.2400    15.6336    -6.5408 O.2   23 ASN264   0.0000
 376 ND2     24.1785    14.7007    -7.2022 N.am  23 ASN264   0.0000
 377 H       21.7470    17.1813    -5.3396 H     23 ASN264   0.0000
 378 HA      23.6194    19.2125    -6.5535 H     23 ASN264   0.0000
 379 HB3     24.7549    17.1388    -5.9284 H     23 ASN264   0.0000
 380 HB2     24.6553    17.2848    -7.6986 H     23 ASN264   0.0000
 381 HD21    25.1457    14.8148    -7.4342 H     23 ASN264   0.0000
 382 HD22    23.7721    13.7870    -7.2455 H     23 ASN264   0.0000
 383 N       21.1551    19.3423    -7.7591 N.am  24 TRP265   0.0000
BACKBONE
 384 CA      20.2747    19.6003    -8.9009 C.3   24 TRP265   0.0000
BACKBONE
 385 C       20.8423    20.7986    -9.6247 C.2   24 TRP265   0.0000
BACKBONE
 386 O       21.1724    21.7412    -8.9219 O.2   24 TRP265   0.0000
BACKBONE
 387 CB      18.8555    19.9309    -8.3772 C.3   24 TRP265   0.0000
 388 CG      17.8394    20.3195    -9.4194 C.2   24 TRP265   0.0000
 389 CD1     17.4345    21.5626    -9.7247 C.2   24 TRP265   0.0000
 390 CD2     17.0461    19.3762   -10.2891 C.ar  24 TRP265   0.0000
 391 NE1     16.4874    21.5063   -10.6272 N.pl3 24 TRP265   0.0000
 392 CE2     16.1930    20.2344   -10.9564 C.ar  24 TRP265   0.0000
 393 CE3     17.0171    17.9983   -10.4920 C.ar  24 TRP265   0.0000
 394 CZ2     15.1926    19.7587   -11.8030 C.ar  24 TRP265   0.0000
 395 CZ3     15.9999    17.5082   -11.3207 C.ar  24 TRP265   0.0000
 396 CH2     15.0788    18.3687   -11.9367 C.ar  24 TRP265   0.0000
 397 H       21.0565    19.9168    -6.9439 H     24 TRP265   0.0000
 398 HA      20.1955    18.7011    -9.5301 H     24 TRP265   0.0000
 399 HB3     18.9129    20.7566    -7.6505 H     24 TRP265   0.0000
 400 HB2     18.4855    19.0416    -7.8516 H     24 TRP265   0.0000
 401 HD1     17.8255    22.4772    -9.2787 H     24 TRP265   0.0000
 402 HE1     16.0087    22.3319   -11.0175 H     24 TRP265   0.0000
 403 HE3     17.7448    17.3463   -10.0216 H     24 TRP265   0.0000
 404 HZ2     14.5297    20.4355   -12.3249 H     24 TRP265   0.0000
 405 HZ3     15.9161    16.4434   -11.4921 H     24 TRP265   0.0000
 406 HH2     14.2665    17.9529   -12.5251 H     24 TRP265   0.0000
 407 N       20.9974    20.8498   -10.9717 N.am  25 PRO266   0.0000
BACKBONE
 408 CA      21.6225    22.0185   -11.5772 C.3   25 PRO266   0.0000
BACKBONE
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 409 C       20.6967    23.2124   -11.5165 C.2   25 PRO266   0.0000
BACKBONE
 410 O       19.4967    23.0152   -11.4105 O.2   25 PRO266   0.0000
BACKBONE
 411 CB      21.8396    21.5042   -13.0207 C.3   25 PRO266   0.0000
 412 CG      20.6861    20.4937   -13.2127 C.3   25 PRO266   0.0000
 413 CD      20.5957    19.7628   -11.8542 C.3   25 PRO266   0.0000
 414 HA      22.5879    22.2465   -11.0948 H     25 PRO266   0.0000
 415 HB3     22.7947    20.9556   -13.0807 H     25 PRO266   0.0000
 416 HB2     21.8437    22.3079   -13.7740 H     25 PRO266   0.0000
 417 HG2     19.7528    21.0559   -13.3578 H     25 PRO266   0.0000
 418 HG3     20.8357    19.8158   -14.0686 H     25 PRO266   0.0000
 419 HD2     19.5735    19.3881   -11.6834 H     25 PRO266   0.0000
 420 HD3     21.3250    18.9384   -11.7980 H     25 PRO266   0.0000
 421 N       21.2448    24.4515   -11.5739 N.am  26 SER267   0.0000
BACKBONE
 422 CA      20.4147    25.6534   -11.4674 C.3   26 SER267   0.0000
BACKBONE
 423 C       20.0308    26.2237   -12.8161 C.2   26 SER267   0.0000
BACKBONE
 424 O       19.4574    27.3011   -12.8257 O.2   26 SER267   0.0000
BACKBONE
 425 CB      21.2063    26.7317   -10.6810 C.3   26 SER267   0.0000
 426 OG      22.3637    27.0944   -11.4537 O.3   26 SER267   0.0000
 427 H       22.2310    24.5757   -11.7065 H     26 SER267   0.0000
 428 HA      19.4886    25.4440   -10.9056 H     26 SER267   0.0000
 429 HB3     21.5154    26.3196    -9.7055 H     26 SER267   0.0000
 430 HB2     20.5757    27.6199   -10.5029 H     26 SER267   0.0000
 431 HG      22.8963    27.7592   -11.0284 H     26 SER267   0.0000
 432 N       20.3258    25.5534   -13.9554 N.am  27 SER268   0.0000
BACKBONE
 433 CA      19.9567    26.0961   -15.2647 C.3   27 SER268   0.0000
BACKBONE
 434 C       18.6202    25.5775   -15.7563 C.2   27 SER268   0.0000
BACKBONE
 435 O       18.2290    25.9617   -16.8472 O.2   27 SER268   0.0000
BACKBONE
 436 CB      21.0649    25.6795   -16.2661 C.3   27 SER268   0.0000
 437 OG      21.1425    24.2435   -16.2730 O.3   27 SER268   0.0000
 438 H       20.7715    24.6574   -13.9408 H     27 SER268   0.0000
 439 HA      19.9147    27.1982   -15.2467 H     27 SER268   0.0000
 440 HB3     22.0278    26.1047   -15.9341 H     27 SER268   0.0000
 441 HB2     20.8401    26.0603   -17.2767 H     27 SER268   0.0000
 442 HG      21.8220    23.9152   -16.8534 H     27 SER268   0.0000
 443 N       17.9040    24.7110   -15.0016 N.am  28 VAL269   0.0000
BACKBONE
 444 CA      16.6489    24.1419   -15.5025 C.3   28 VAL269   0.0000
BACKBONE
 445 C       15.5245    25.1199   -15.2387 C.2   28 VAL269   0.0000
BACKBONE
 446 O       14.7497    25.3952   -16.1411 O.2   28 VAL269   0.0000
BACKBONE
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447	CB	16.3845	22.7657	-14.8260	C.3	28 VAL269	0.0000
448	CG1	15.0284	22.1632	-15.2730	C.3	28 VAL269	0.0000
449	CG2	17.5269	21.7682	-15.1644	C.3	28 VAL269	0.0000
450	H	18.2044	24.4545	-14.0820	H	28 VAL269	0.0000
451	HA	16.7234	23.9586	-16.5877	H	28 VAL269	0.0000
452	HB	16.3509	22.9059	-13.7312	H	28 VAL269	0.0000
453	HG13	14.1957	22.8446	-15.0479	H	28 VAL269	0.0000
454	HG12	14.8703	21.2189	-14.7322	H	28 VAL269	0.0000
455	HG11	15.0278	21.9599	-16.3545	H	28 VAL269	0.0000
456	HG23	17.4883	21.4701	-16.2233	H	28 VAL269	0.0000
457	HG22	17.4320	20.8667	-14.5406	H	28 VAL269	0.0000
458	HG21	18.5112	22.2195	-14.9797	H	28 VAL269	0.0000
459	N	15.4405	25.6515	-13.9991	N.am	29 LEU270	0.0000
BACKBONE							
460	CA	14.4470	26.6720	-13.6602	C.3	29 LEU270	0.0000
BACKBONE							
461	C	13.0795	26.0954	-13.3595	C.2	29 LEU270	0.0000
BACKBONE							
462	O	12.0975	26.7840	-13.5895	O.2	29 LEU270	0.0000
BACKBONE							
463	CB	14.3761	27.8885	-14.6314	C.3	29 LEU270	0.0000
464	CG	15.7554	28.4051	-15.1443	C.3	29 LEU270	0.0000
465	CD1	15.5670	29.7578	-15.8881	C.3	29 LEU270	0.0000
466	CD2	16.7933	28.5877	-14.0041	C.3	29 LEU270	0.0000
467	H	16.0651	25.3498	-13.2742	H	29 LEU270	0.0000
468	HA	14.7449	27.0994	-12.6856	H	29 LEU270	0.0000
469	HB3	13.8534	28.7136	-14.1181	H	29 LEU270	0.0000
470	HB2	13.7631	27.6120	-15.5019	H	29 LEU270	0.0000
471	HG	16.1670	27.6774	-15.8646	H	29 LEU270	0.0000
472	HD13	14.8071	29.6688	-16.6770	H	29 LEU270	0.0000
473	HD12	16.5114	30.0789	-16.3542	H	29 LEU270	0.0000
474	HD11	15.2425	30.5405	-15.1849	H	29 LEU270	0.0000
475	HD23	16.4005	29.2639	-13.2300	H	29 LEU270	0.0000
476	HD22	17.7272	29.0126	-14.4038	H	29 LEU270	0.0000
477	HD21	17.0395	27.6244	-13.5389	H	29 LEU270	0.0000
478	N	12.9959	24.8636	-12.8007	N.am	30 VAL271	0.0000
BACKBONE							
479	CA	11.7776	24.4310	-12.1092	C.3	30 VAL271	0.0000
BACKBONE							
480	C	12.2289	24.2209	-10.6823	C.2	30 VAL271	0.0000
BACKBONE							
481	O	13.3696	23.8216	-10.5030	O.2	30 VAL271	0.0000
BACKBONE							
482	CB	11.0677	23.1958	-12.7297	C.3	30 VAL271	0.0000
483	CG1	10.7039	23.4890	-14.2102	C.3	30 VAL271	0.0000
484	CG2	11.9278	21.9110	-12.6241	C.3	30 VAL271	0.0000
485	H	13.8024	24.2757	-12.7166	H	30 VAL271	0.0000
486	HA	11.0332	25.2444	-12.0904	H	30 VAL271	0.0000
487	HB	10.1347	23.0133	-12.1655	H	30 VAL271	0.0000
488	HG13	10.0396	24.3644	-14.2828	H	30 VAL271	0.0000
489	HG12	10.1852	22.6245	-14.6474	H	30 VAL271	0.0000
490	HG11	11.6122	23.6871	-14.7996	H	30 VAL271	0.0000

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 491 HG23    12.8498    22.0190   -13.2072 H      30 VAL271   0.0000
 492 HG22    11.3718    21.0412   -13.0085 H      30 VAL271   0.0000
 493 HG21    12.1937    21.7197   -11.5751 H      30 VAL271   0.0000
 494 N       11.4051    24.5182    -9.6522 N.am   31 ASN272   0.0000
BACKBONE
 495 CA      11.9685    24.6123    -8.3067 C.3    31 ASN272   0.0000
BACKBONE
 496 C       12.0451    23.2353    -7.6797 C.2    31 ASN272   0.0000
BACKBONE
 497 O       11.0229    22.5691    -7.7284 O.2    31 ASN272   0.0000
BACKBONE
 498 CB      11.1399    25.5868    -7.4285 C.3    31 ASN272   0.0000
 499 CG      11.9152    25.9585    -6.1860 C.2    31 ASN272   0.0000
 500 OD1     12.1845    25.0744    -5.3873 O.2    31 ASN272   0.0000
 501 ND2     12.3029    27.2383    -5.9877 N.am   31 ASN272   0.0000
 502 H       10.4383    24.7401    -9.7956 H      31 ASN272   0.0000
 503 HA      12.9534    25.0910    -8.4129 H      31 ASN272   0.0000
 504 HB3     10.1831    25.1237    -7.1504 H      31 ASN272   0.0000
 505 HB2     10.9082    26.4856    -8.0218 H      31 ASN272   0.0000
 506 HD21    12.0906    27.9643    -6.6433 H      31 ASN272   0.0000
 507 HD22    12.8223    27.4745    -5.1651 H      31 ASN272   0.0000
 508 N       13.1674    22.7398    -7.0906 N.am   32 PRO273   0.0000
BACKBONE
 509 CA      13.1506    21.3989    -6.5215 C.3    32 PRO273   0.0000
BACKBONE
 510 C       12.2156    21.2770    -5.3380 C.2    32 PRO273   0.0000
BACKBONE
 511 O       11.7133    20.1866    -5.1177 O.2    32 PRO273   0.0000
BACKBONE
 512 CB      14.6436    21.2005    -6.1673 C.3    32 PRO273   0.0000
 513 CG      15.1987    22.6316    -5.9934 C.3    32 PRO273   0.0000
 514 CD      14.4318    23.4645    -7.0470 C.3    32 PRO273   0.0000
 515 HA      12.8591    20.6713    -7.2909 H      32 PRO273   0.0000
 516 HB3     15.1646    20.7366    -7.0227 H      32 PRO273   0.0000
 517 HB2     14.7828    20.5710    -5.2748 H      32 PRO273   0.0000
 518 HG2     14.9423    22.9973    -4.9871 H      32 PRO273   0.0000
 519 HG3     16.2931    22.6853    -6.1182 H      32 PRO273   0.0000
 520 HD2     14.3668    24.5112    -6.7129 H      32 PRO273   0.0000
 521 HD3     14.9232    23.4047    -8.0318 H      32 PRO273   0.0000
 522 N       11.9437    22.3600    -4.5741 N.am   33 GLU274   0.0000
BACKBONE
 523 CA      10.9214    22.2809    -3.5271 C.3    33 GLU274   0.0000
BACKBONE
 524 C        9.6140    21.8334    -4.1387 C.2    33 GLU274   0.0000
BACKBONE
 525 O        8.9705    20.9488    -3.5971 O.2    33 GLU274   0.0000
BACKBONE
 526 CB      10.7023    23.6614    -2.8397 C.3    33 GLU274   0.0000
 527 CG       9.4240    23.7274    -1.9587 C.3    33 GLU274   0.0000
 528 CD       9.3849    22.6417    -0.9167 C.2    33 GLU274   0.0000
 529 OE1     10.4505    22.3677    -0.3031 O.co2  33 GLU274  -0.5000
 530 OE2      8.2878    22.0586    -0.7004 O.co2  33 GLU274  -0.5000
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 531 H       12.4022    23.2342    -4.7389 H     33 GLU274   0.0000
 532 HA      11.2393    21.5453    -2.7696 H     33 GLU274   0.0000
 533 HB3     10.5891    24.4446    -3.6048 H     33 GLU274   0.0000
 534 HB2     11.5934    23.9018    -2.2357 H     33 GLU274   0.0000
 535 HG3      8.5263    23.6633    -2.5963 H     33 GLU274   0.0000
 536 HG2      9.3910    24.6989    -1.4394 H     33 GLU274   0.0000
 537 N        9.2023    22.4518    -5.2669 N.am  34 GLN275   0.0000
BACKBONE
 538 CA       7.9127    22.1098    -5.8639 C.3   34 GLN275   0.0000
BACKBONE
 539 C        7.9574    20.6946    -6.3930 C.2   34 GLN275   0.0000
BACKBONE
 540 O        7.0090    19.9585    -6.1708 O.2   34 GLN275   0.0000
BACKBONE
 541 CB       7.5276    23.0950    -7.0008 C.3   34 GLN275   0.0000
 542 CG       7.2265    24.5161    -6.4479 C.3   34 GLN275   0.0000
 543 CD       7.0126    25.5337    -7.5440 C.2   34 GLN275   0.0000
 544 OE1      7.1942    25.2193    -8.7114 O.2   34 GLN275   0.0000
 545 NE2      6.6255    26.7781    -7.1888 N.am  34 GLN275   0.0000
 546 H        9.7782    23.1418    -5.7058 H     34 GLN275   0.0000
 547 HA       7.1361    22.1741    -5.0829 H     34 GLN275   0.0000
 548 HB3      6.6239    22.7276    -7.5152 H     34 GLN275   0.0000
 549 HB2      8.3502    23.1338    -7.7326 H     34 GLN275   0.0000
 550 HG3      8.0569    24.8699    -5.8186 H     34 GLN275   0.0000
 551 HG2      6.3212    24.4744    -5.8208 H     34 GLN275   0.0000
 552 HE21     6.4806    27.0200    -6.2279 H     34 GLN275   0.0000
 553 HE22     6.4790    27.4749    -7.8925 H     34 GLN275   0.0000
 554 N        9.0453    20.2860    -7.0869 N.am  35 LEU276   0.0000
BACKBONE
 555 CA       9.1335    18.8980    -7.5430 C.3   35 LEU276   0.0000
BACKBONE
 556 C        8.9482    17.9772    -6.3528 C.2   35 LEU276   0.0000
BACKBONE
 557 O        8.1680    17.0419    -6.4445 O.2   35 LEU276   0.0000
BACKBONE
 558 CB      10.4857    18.5873    -8.2513 C.3   35 LEU276   0.0000
 559 CG      10.6246    19.1629    -9.6960 C.3   35 LEU276   0.0000
 560 CD1     12.1136    19.1066   -10.1414 C.3   35 LEU276   0.0000
 561 CD2      9.7872    18.3622   -10.7369 C.3   35 LEU276   0.0000
 562 H        9.8018    20.9145    -7.2769 H     35 LEU276   0.0000
 563 HA       8.3017    18.7167    -8.2359 H     35 LEU276   0.0000
 564 HB3     10.6346    17.5040    -8.3223 H     35 LEU276   0.0000
 565 HB2     11.2870    18.9661    -7.6037 H     35 LEU276   0.0000
 566 HG      10.2944    20.2161    -9.7042 H     35 LEU276   0.0000
 567 HD13    12.7327    19.8056    -9.5608 H     35 LEU276   0.0000
 568 HD12    12.2213    19.3535   -11.2066 H     35 LEU276   0.0000
 569 HD11    12.5029    18.0916    -9.9971 H     35 LEU276   0.0000
 570 HD23    10.1388    17.3211   -10.7999 H     35 LEU276   0.0000
 571 HD22     9.8866    18.8240   -11.7314 H     35 LEU276   0.0000
 572 HD21     8.7209    18.3442   -10.4901 H     35 LEU276   0.0000
 573 N        9.6419    18.2299    -5.2189 N.am  36 ALA277   0.0000
BACKBONE
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 574 CA       9.4679    17.3739    -4.0449 C.3   36 ALA277   0.0000
BACKBONE
 575 C        8.0182    17.3684    -3.6129 C.2   36 ALA277   0.0000
BACKBONE
 576 O        7.4739    16.2997    -3.3832 O.2   36 ALA277   0.0000
BACKBONE
 577 CB      10.3708    17.8189    -2.8647 C.3   36 ALA277   0.0000
 578 H       10.2731    19.0042    -5.1645 H     36 ALA277   0.0000
 579 HA       9.7655    16.3499    -4.3199 H     36 ALA277   0.0000
 580 HB3     10.1300    18.8444    -2.5503 H     36 ALA277   0.0000
 581 HB2     11.4239    17.7886    -3.1802 H     36 ALA277   0.0000
 582 HB1     10.2404    17.1470    -2.0022 H     36 ALA277   0.0000
 583 N        7.3706    18.5506    -3.5042 N.am  37 SER278   0.0000
BACKBONE
 584 CA       5.9608    18.5843    -3.1150 C.3   37 SER278   0.0000
BACKBONE
 585 C        5.1108    17.7684    -4.0591 C.2   37 SER278   0.0000
BACKBONE
 586 O        4.1527    17.1685    -3.5971 O.2   37 SER278   0.0000
BACKBONE
 587 CB       5.4336    20.0384    -3.0607 C.3   37 SER278   0.0000
 588 OG       6.2991    20.7896    -2.1932 O.3   37 SER278   0.0000
 589 H        7.8396    19.4150    -3.6920 H     37 SER278   0.0000
 590 HA       5.8649    18.1511    -2.1066 H     37 SER278   0.0000
 591 HB3      4.3993    20.0457    -2.6761 H     37 SER278   0.0000
 592 HB2      5.4377    20.4712    -4.0739 H     37 SER278   0.0000
 593 HG       6.0378    21.7013    -2.1118 H     37 SER278   0.0000
 594 N        5.4499    17.7072    -5.3692 N.am  38 ALA279   0.0000
BACKBONE
 595 CA       4.6924    16.8642    -6.2947 C.3   38 ALA279   0.0000
BACKBONE
 596 C        5.2091    15.4404    -6.3317 C.2   38 ALA279   0.0000
BACKBONE
 597 O        5.1375    14.8130    -7.3770 O.2   38 ALA279   0.0000
BACKBONE
 598 CB       4.6437    17.5241    -7.6948 C.3   38 ALA279   0.0000
 599 H        6.2453    18.2002    -5.7237 H     38 ALA279   0.0000
 600 HA       3.6474    16.7920    -5.9710 H     38 ALA279   0.0000
 601 HB3      5.6674    17.5805    -8.0815 H     38 ALA279   0.0000
 602 HB2      4.2339    18.5431    -7.6157 H     38 ALA279   0.0000
 603 HB1      4.0246    16.9508    -8.4019 H     38 ALA279   0.0000
 604 N        5.7106    14.8915    -5.1987 N.am  39 GLY280   0.0000
BACKBONE
 605 CA       6.0410    13.4721    -5.1489 C.3   39 GLY280   0.0000
BACKBONE
 606 C        7.2757    13.0940    -5.9274 C.2   39 GLY280   0.0000
BACKBONE
 607 O        7.5195    11.9015    -6.0152 O.2   39 GLY280   0.0000
BACKBONE
 608 H        5.8295    15.4115    -4.3540 H     39 GLY280   0.0000
 609 HA2      5.1916    12.8906    -5.5422 H     39 GLY280   0.0000
 610 HA3      6.1835    13.1639    -4.1025 H     39 GLY280   0.0000
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 611 N        8.0653    14.0359    -6.4979 N.am  40 PHE281   0.0000
BACKBONE
 612 CA       9.1861    13.6341    -7.3491 C.3   40 PHE281   0.0000
BACKBONE
 613 C       10.5102    13.6698    -6.6252 C.2   40 PHE281   0.0000
BACKBONE
 614 O       10.6218    14.4174    -5.6690 O.2   40 PHE281   0.0000
BACKBONE
 615 CB       9.3064    14.5538    -8.5845 C.3   40 PHE281   0.0000
 616 CG       8.1145    14.4367    -9.5415 C.ar  40 PHE281   0.0000
 617 CD1      7.8639    13.2392   -10.2204 C.ar  40 PHE281   0.0000
 618 CD2      7.2786    15.5373    -9.7586 C.ar  40 PHE281   0.0000
 619 CE1      6.8051    13.1489   -11.1270 C.ar  40 PHE281   0.0000
 620 CE2      6.2156    15.4518   -10.6602 C.ar  40 PHE281   0.0000
 621 CZ       5.9846    14.2578   -11.3474 C.ar  40 PHE281   0.0000
 622 H        7.9081    15.0145    -6.3581 H     40 PHE281   0.0000
 623 HA       9.0269    12.6177    -7.7218 H     40 PHE281   0.0000
 624 HB3     10.2108    14.2982    -9.1452 H     40 PHE281   0.0000
 625 HB2      9.4202    15.5826    -8.2289 H     40 PHE281   0.0000
 626 HD1      8.4927    12.3721   -10.0570 H     40 PHE281   0.0000
 627 HD2      7.4562    16.4663    -9.2325 H     40 PHE281   0.0000
 628 HE1      6.6228    12.2230   -11.6639 H     40 PHE281   0.0000
 629 HE2      5.5772    16.3129   -10.8274 H     40 PHE281   0.0000
 630 HZ       5.1736    14.1900   -12.0583 H     40 PHE281   0.0000
 631 N       11.5194    12.8853    -7.0833 N.am  41 TYR282   0.0000
BACKBONE
 632 CA      12.8259    12.8727    -6.4259 C.3   41 TYR282   0.0000
BACKBONE
 633 C       13.9311    12.6685    -7.4470 C.2   41 TYR282   0.0000
BACKBONE
 634 O       13.8049    11.7458    -8.2337 O.2   41 TYR282   0.0000
BACKBONE
 635 CB      12.8198    11.7865    -5.3191 C.3   41 TYR282   0.0000
 636 CG      12.6978    10.3544    -5.8552 C.ar  41 TYR282   0.0000
 637 CD1     13.8345     9.5521    -6.0079 C.ar  41 TYR282   0.0000
 638 CD2     11.4425     9.8286    -6.1787 C.ar  41 TYR282   0.0000
 639 CE1     13.7121     8.2244    -6.4297 C.ar  41 TYR282   0.0000
 640 CE2     11.3410     8.5481    -6.7279 C.ar  41 TYR282   0.0000
 641 CZ      12.4678     7.7288    -6.8318 C.ar  41 TYR282   0.0000
 642 OH      12.3290     6.4322    -7.3368 O.3   41 TYR282   0.0000
 643 H       11.3831    12.2697    -7.8593 H     41 TYR282   0.0000
 644 HA      12.9857    13.8373    -5.9199 H     41 TYR282   0.0000
 645 HB2     11.9655    11.9871    -4.6612 H     41 TYR282   0.0000
 646 HB3     13.7262    11.8519    -4.7059 H     41 TYR282   0.0000
 647 HD1     14.8202     9.9530    -5.7943 H     41 TYR282   0.0000
 648 HD2     10.5440    10.4130    -6.0052 H     41 TYR282   0.0000
 649 HE1     14.5867     7.5820    -6.4421 H     41 TYR282   0.0000
 650 HE2     10.3866     8.1817    -7.0831 H     41 TYR282   0.0000
 651 HH      13.1468     6.0480    -7.6332 H     41 TYR282   0.0000
 652 N       14.9952    13.5114    -7.4692 N.am  42 TYR283   0.0000
BACKBONE
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653	CA	16.0571	13.3991	-8.4779	C.3	42 TYR283	0.0000
BACKBONE							
654	C	16.6789	12.0186	-8.5288	C.2	42 TYR283	0.0000
BACKBONE							
655	O	16.9600	11.4942	-7.4630	O.2	42 TYR283	0.0000
BACKBONE							
656	CB	17.1492	14.4728	-8.1820	C.3	42 TYR283	0.0000
657	CG	18.3438	14.5807	-9.1466	C.ar	42 TYR283	0.0000
658	CD1	18.1590	14.6416	-10.5319	C.ar	42 TYR283	0.0000
659	CD2	19.6483	14.6647	-8.6436	C.ar	42 TYR283	0.0000
660	CE1	19.2310	14.9047	-11.3893	C.ar	42 TYR283	0.0000
661	CE2	20.7225	14.9325	-9.4967	C.ar	42 TYR283	0.0000
662	CZ	20.5141	15.1019	-10.8669	C.ar	42 TYR283	0.0000
663	OH	21.5890	15.4651	-11.6833	O.3	42 TYR283	0.0000
664	H	15.0399	14.2824	-6.8340	H	42 TYR283	0.0000
665	HA	15.5886	13.6299	-9.4395	H	42 TYR283	0.0000
666	HB2	17.5131	14.3047	-7.1577	H	42 TYR283	0.0000
667	HB3	16.6820	15.4672	-8.2063	H	42 TYR283	0.0000
668	HD1	17.1771	14.5013	-10.9554	H	42 TYR283	0.0000
669	HD2	19.8399	14.5345	-7.5838	H	42 TYR283	0.0000
670	HE1	19.0583	14.9593	-12.4578	H	42 TYR283	0.0000
671	HE2	21.7275	15.0151	-9.0982	H	42 TYR283	0.0000
672	HH	21.3374	15.7131	-12.5662	H	42 TYR283	0.0000
673	N	16.8991	11.4316	-9.7377	N.am	43 VAL284	0.0000
BACKBONE							
674	CA	17.5565	10.1251	-9.8625	C.3	43 VAL284	0.0000
BACKBONE							
675	C	18.7612	10.1008	-10.7903	C.2	43 VAL284	0.0000
BACKBONE							
676	O	19.4770	9.1138	-10.7100	O.2	43 VAL284	0.0000
BACKBONE							
677	CB	16.5584	8.9997	-10.2819	C.3	43 VAL284	0.0000
678	CG1	15.4319	8.8341	-9.2291	C.3	43 VAL284	0.0000
679	CG2	15.9449	9.2204	-11.6922	C.3	43 VAL284	0.0000
680	H	16.5864	11.8712	-10.5764	H	43 VAL284	0.0000
681	HA	17.9759	9.8327	-8.8851	H	43 VAL284	0.0000
682	HB	17.1139	8.0446	-10.3118	H	43 VAL284	0.0000
683	HG13	15.8716	8.7004	-8.2300	H	43 VAL284	0.0000
684	HG12	14.8087	7.9557	-9.4583	H	43 VAL284	0.0000
685	HG11	14.7877	9.7219	-9.2171	H	43 VAL284	0.0000
686	HG23	15.3004	10.1098	-11.7120	H	43 VAL284	0.0000
687	HG22	15.3318	8.3503	-11.9745	H	43 VAL284	0.0000
688	HG21	16.7381	9.3383	-12.4448	H	43 VAL284	0.0000
689	N	19.0576	11.0919	-11.6698	N.am	44 GLY285	0.0000
BACKBONE							
690	CA	20.2497	10.9662	-12.5105	C.3	44 GLY285	0.0000
BACKBONE							
691	C	20.2833	11.9417	-13.6624	C.2	44 GLY285	0.0000
BACKBONE							
692	O	19.3311	12.6868	-13.8282	O.2	44 GLY285	0.0000
BACKBONE							
693	H	18.5213	11.9301	-11.7550	H	44 GLY285	0.0000

694	HA2	20.2952	9.9580	-12.9529	H	44 GLY285	0.0000
695	HA3	21.1435	11.1219	-11.8867	H	44 GLY285	0.0000
696	N	21.3769	11.9334	-14.4657	N.am	45 ASN286	0.0000
BACKBONE							
697	CA	21.4427	12.7772	-15.6627	C.3	45 ASN286	0.0000
BACKBONE							
698	C	21.1421	14.2228	-15.3261	C.2	45 ASN286	0.0000
BACKBONE							
699	O	21.1410	14.5510	-14.1510	O.2	45 ASN286	0.0000
BACKBONE							
700	CB	20.5196	12.1149	-16.7224	C.3	45 ASN286	0.0000
701	CG	20.9413	10.6819	-16.9637	C.2	45 ASN286	0.0000
702	OD1	22.1349	10.4297	-17.0473	O.2	45 ASN286	0.0000
703	ND2	20.0079	9.7146	-17.0919	N.am	45 ASN286	0.0000
704	H	22.1367	11.3029	-14.2874	H	45 ASN286	0.0000
705	HA	22.4734	12.7867	-16.0567	H	45 ASN286	0.0000
706	HB3	20.5790	12.6243	-17.6950	H	45 ASN286	0.0000
707	HB2	19.4828	12.1775	-16.3675	H	45 ASN286	0.0000
708	HD21	19.0327	9.9179	-17.0250	H	45 ASN286	0.0000
709	HD22	20.2920	8.7690	-17.2577	H	45 ASN286	0.0000
710	N	20.9126	15.1245	-16.3086	N.am	46 SER287	0.0000
BACKBONE							
711	CA	20.6962	16.5277	-15.9648	C.3	46 SER287	0.0000
BACKBONE							
712	C	19.5293	16.6899	-15.0194	C.2	46 SER287	0.0000
BACKBONE							
713	O	19.6859	17.3606	-14.0106	O.2	46 SER287	0.0000
BACKBONE							
714	CB	20.4321	17.3909	-17.2255	C.3	46 SER287	0.0000
715	OG	21.5471	17.2418	-18.1200	O.3	46 SER287	0.0000
716	H	20.9373	14.8751	-17.2763	H	46 SER287	0.0000
717	HA	21.6161	16.9068	-15.4871	H	46 SER287	0.0000
718	HB3	20.3161	18.4485	-16.9315	H	46 SER287	0.0000
719	HB2	19.5061	17.0586	-17.7240	H	46 SER287	0.0000
720	HG	21.4463	17.7506	-18.9184	H	46 SER287	0.0000
721	N	18.3523	16.1010	-15.3384	N.am	47 ASP288	0.0000
BACKBONE							
722	CA	17.1554	16.3938	-14.5533	C.3	47 ASP288	0.0000
BACKBONE							
723	C	16.1836	15.2365	-14.5303	C.2	47 ASP288	0.0000
BACKBONE							
724	O	14.9884	15.4697	-14.6118	O.2	47 ASP288	0.0000
BACKBONE							
725	CB	16.5340	17.6826	-15.1586	C.3	47 ASP288	0.0000
726	CG	16.0895	17.5126	-16.5889	C.2	47 ASP288	0.0000
727	OD1	16.2809	16.4089	-17.1676	O.co2	47 ASP288	-0.5000
728	OD2	15.5373	18.4967	-17.1524	O.co2	47 ASP288	-0.5000
729	H	18.2524	15.5395	-16.1626	H	47 ASP288	0.0000
730	HA	17.4155	16.5852	-13.5012	H	47 ASP288	0.0000
731	HB3	17.2896	18.4820	-15.1327	H	47 ASP288	0.0000
732	HB2	15.6694	18.0126	-14.5663	H	47 ASP288	0.0000

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 733 N       16.6682    13.9783   -14.4138 N.am  48 ASP289   0.0000
BACKBONE
 734 CA      15.7423    12.8493   -14.3821 C.3   48 ASP289   0.0000
BACKBONE
 735 C       15.1501    12.7339   -13.0020 C.2   48 ASP289   0.0000
BACKBONE
 736 O       15.9292    12.7504   -12.0650 O.2   48 ASP289   0.0000
BACKBONE
 737 CB      16.4249    11.4919   -14.6978 C.3   48 ASP289   0.0000
 738 CG      16.8740    11.4061   -16.1296 C.2   48 ASP289   0.0000
 739 OD1     16.9482    12.4601   -16.8167 O.co2 48 ASP289  -0.5000
 740 OD2     17.1601    10.2671   -16.5838 O.co2 48 ASP289  -0.5000
 741 H       17.6487    13.8008   -14.3165 H     48 ASP289   0.0000
 742 HA      14.9569    13.0123   -15.1355 H     48 ASP289   0.0000
 743 HB3     15.7240    10.6670   -14.5087 H     48 ASP289   0.0000
 744 HB2     17.2867    11.3318   -14.0369 H     48 ASP289   0.0000
 745 N       13.8116    12.5939   -12.8546 N.am  49 VAL290   0.0000
BACKBONE
 746 CA      13.2170    12.3778   -11.5370 C.3   49 VAL290   0.0000
BACKBONE
 747 C       12.2974    11.1817   -11.6249 C.2   49 VAL290   0.0000
BACKBONE
 748 O       11.9467    10.8179   -12.7362 O.2   49 VAL290   0.0000
BACKBONE
 749 CB      12.4280    13.6381   -11.0697 C.3   49 VAL290   0.0000
 750 CG1     13.2401    14.9432   -11.2861 C.3   49 VAL290   0.0000
 751 CG2     11.0597    13.7679   -11.7938 C.3   49 VAL290   0.0000
 752 H       13.1937    12.6214   -13.6407 H     49 VAL290   0.0000
 753 HA      13.9893    12.1451   -10.7887 H     49 VAL290   0.0000
 754 HB      12.2444    13.5293    -9.9882 H     49 VAL290   0.0000
 755 HG13    14.1946    14.8916   -10.7528 H     49 VAL290   0.0000
 756 HG12    12.6802    15.8062   -10.8971 H     49 VAL290   0.0000
 757 HG11    13.4435    15.1155   -12.3530 H     49 VAL290   0.0000
 758 HG23    11.2139    13.7963   -12.8783 H     49 VAL290   0.0000
 759 HG22    10.5513    14.6952   -11.4926 H     49 VAL290   0.0000
 760 HG21    10.3957    12.9239   -11.5603 H     49 VAL290   0.0000
 761 N       11.8758    10.5884   -10.4818 N.am  50 LYS291   0.0000
BACKBONE
 762 CA      10.8151     9.5753   -10.4985 C.3   50 LYS291   0.0000
BACKBONE
 763 C        9.7694     9.9352    -9.4684 C.2   50 LYS291   0.0000
BACKBONE
 764 O       10.1208    10.6236    -8.5255 O.2   50 LYS291   0.0000
BACKBONE
 765 CB      11.3489     8.1447   -10.2034 C.3   50 LYS291   0.0000
 766 CG      11.8603     7.4005   -11.4655 C.3   50 LYS291   0.0000
 767 CD      12.2849     5.9517   -11.0886 C.3   50 LYS291   0.0000
 768 CE      12.7656     5.1607   -12.3319 C.3   50 LYS291   0.0000
 769 O        9.6486    11.7494   -19.5934 O.2   50 LYS291   0.0000
BACKBONE
 770 C        8.7718    11.7794   -20.4409 C.2   50 LYS291   0.0000
BACKBONE
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 771 N        7.8539    10.7748   -20.5197 N.am  50 LYS291   0.0000
BACKBONE
 772 C        8.0246     9.5614   -19.7304 C.3   50 LYS291   0.0000
BACKBONE
 773 H        7.7623     9.7833   -18.6861 H     50 LYS291   0.0000
 774 C        9.4062     8.9691   -19.9031 C.2   50 LYS291   0.0000
BACKBONE
 775 N       10.2454     8.9874   -18.8457 N.am  50 LYS291   0.0000
BACKBONE
 776 H        9.9429     9.3341   -17.9596 H     50 LYS291   0.0000
 777 C       11.6303     8.5438   -19.0041 C.3   50 LYS291   0.0000
BACKBONE
 778 H       12.1275     9.1070   -19.8104 H     50 LYS291   0.0000
 779 C       12.3240     8.8115   -17.6808 C.ar  50 LYS291   0.0000
BACKBONE
 780 C       12.4745     7.6445   -16.9446 C.ar  50 LYS291   0.0000
BACKBONE
 781 C       12.0000     6.4177   -17.7035 C.3   50 LYS291   0.0000
BACKBONE
 782 H       12.7406     5.6006   -17.6585 H     50 LYS291   0.0000
 783 H       11.0523     6.0855   -17.2487 H     50 LYS291   0.0000
 784 C       11.7929     6.9980   -19.1348 C.3   50 LYS291   0.0000
BACKBONE
 785 H       12.7069     6.8008   -19.7224 H     50 LYS291   0.0000
 786 H       10.9390     6.5257   -19.6466 H     50 LYS291   0.0000
 787 C       12.9715     7.6887   -15.6441 C.ar  50 LYS291   0.0000
BACKBONE
 788 C       13.4165     8.9091   -15.1311 C.ar  50 LYS291   0.0000
BACKBONE
 789 H       13.8403     8.9366   -14.1355 H     50 LYS291   0.0000
 790 C       13.2870    10.0806   -15.8895 C.ar  50 LYS291   0.0000
BACKBONE
 791 H       13.5951    11.0294   -15.4748 H     50 LYS291   0.0000
 792 C       12.7408    10.0424   -17.1773 C.ar  50 LYS291   0.0000
BACKBONE
 793 H       12.6142    10.9441   -17.7684 H     50 LYS291   0.0000
 794 O       12.9586     6.5469   -14.8560 O.3   50 LYS291   0.0000
BACKBONE
 795 S       14.2612     5.9186   -14.4650 S.o2  50 LYS291   0.0000
 796 O       14.2759     4.5912   -15.0415 O.2   50 LYS291   0.0000
BACKBONE
 797 O       15.3833     6.8191   -14.6597 O.2   50 LYS291   0.0000
BACKBONE
 798 N1      13.9656     5.8012   -12.8623 N.am  50 LYS291   0.0000
 799 O        9.7341     8.5062   -20.9847 O.2   50 LYS291   0.0000
BACKBONE
 800 C        6.9181     8.6611   -20.3320 C.3   50 LYS291   0.0000
BACKBONE
 801 H        7.2717     8.1421   -21.2377 H     50 LYS291   0.0000
 802 H        6.5454     7.9104   -19.6157 H     50 LYS291   0.0000
 803 C        5.8454     9.6859   -20.7531 C.3   50 LYS291   0.0000
BACKBONE
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804	H	5.3355	10.0359	-19.8402	H	50 LYS291	0.0000
805	H	5.0982	9.2705	-21.4470	H	50 LYS291	0.0000
806	C	6.6718	10.8425	-21.3659	C.3	50 LYS291	0.0000
BACKBONE							
807	H	6.1120	11.7837	-21.2774	H	50 LYS291	0.0000
808	H	6.9416	10.6420	-22.4138	H	50 LYS291	0.0000
809	C	8.8181	12.9704	-21.3814	C.3	50 LYS291	0.0000
BACKBONE							
810	H	7.8751	13.0541	-21.9379	H	50 LYS291	0.0000
811	N	8.9666	14.2093	-20.5997	N.am	50 LYS291	0.0000
BACKBONE							
812	H	9.8674	14.4532	-20.2470	H	50 LYS291	0.0000
813	C	7.9079	15.0274	-20.3642	C.2	50 LYS291	0.0000
BACKBONE							
814	C	8.1306	16.4153	-19.7929	C.3	50 LYS291	0.0000
BACKBONE							
815	H	8.9261	16.8989	-20.3850	H	50 LYS291	0.0000
816	N	6.8817	17.2110	-19.9065	N.3	50 LYS291	0.0000
BACKBONE							
817	H	6.8998	18.0636	-19.2370	H	50 LYS291	0.0000
818	C	6.5033	17.6553	-21.2660	C.3	50 LYS291	0.0000
BACKBONE							
819	H	7.2109	18.4128	-21.6385	H	50 LYS291	0.0000
820	H	6.4839	16.8146	-21.9744	H	50 LYS291	0.0000
821	H	5.4954	18.0982	-21.2319	H	50 LYS291	0.0000
822	C	8.5908	16.3732	-18.3133	C.3	50 LYS291	0.0000
BACKBONE							
823	H	7.7600	16.0405	-17.6757	H	50 LYS291	0.0000
824	H	9.4404	15.6898	-18.1954	H	50 LYS291	0.0000
825	H	8.9052	17.3728	-17.9736	H	50 LYS291	0.0000
826	O	6.7616	14.6961	-20.6176	O.2	50 LYS291	0.0000
BACKBONE							
827	C	9.9124	12.7752	-22.5012	C.3	50 LYS291	0.0000
BACKBONE							
828	H	9.3995	12.5362	-23.4514	H	50 LYS291	0.0000
829	C	10.7590	14.0544	-22.7637	C.3	50 LYS291	0.0000
BACKBONE							
830	H	10.0960	14.9160	-22.9475	H	50 LYS291	0.0000
831	H	11.3945	14.2733	-21.8930	H	50 LYS291	0.0000
832	C	11.7175	13.8673	-23.9686	C.3	50 LYS291	0.0000
BACKBONE							
833	H	12.3022	14.7892	-24.1252	H	50 LYS291	0.0000
834	H	11.1356	13.6765	-24.8849	H	50 LYS291	0.0000
835	C	12.6804	12.6828	-23.6990	C.3	50 LYS291	0.0000
BACKBONE							
836	H	13.3042	12.9029	-22.8177	H	50 LYS291	0.0000
837	H	13.3505	12.5399	-24.5632	H	50 LYS291	0.0000
838	C	11.8659	11.3896	-23.4463	C.3	50 LYS291	0.0000
BACKBONE							
839	H	12.5533	10.5547	-23.2293	H	50 LYS291	0.0000
840	H	11.3010	11.1317	-24.3575	H	50 LYS291	0.0000

841	C	10.8837	11.5817	-22.2596	C.3	50 LYS291	0.0000
BACKBONE							
842	H	11.4631	11.7442	-21.3381	H	50 LYS291	0.0000
843	H	10.3122	10.6472	-22.1574	H	50 LYS291	0.0000
844	H	12.2508	10.8508	-9.5910	H	50 LYS291	0.0000
845	HA	10.2763	9.5809	-11.4522	H	50 LYS291	0.0000
846	HB3	10.5294	7.5369	-9.7830	H	50 LYS291	0.0000
847	HB2	12.1562	8.2186	-9.4555	H	50 LYS291	0.0000
848	HG3	12.7001	7.9698	-11.8969	H	50 LYS291	0.0000
849	HG2	11.0523	7.3482	-12.2116	H	50 LYS291	0.0000
850	HD3	11.4451	5.4050	-10.6270	H	50 LYS291	0.0000
851	HD2	13.1101	5.9839	-10.3555	H	50 LYS291	0.0000
852	HE3	11.9695	5.1118	-13.0950	H	50 LYS291	0.0000
853	HE2	13.0121	4.1288	-12.0289	H	50 LYS291	0.0000
854	N	8.5075	9.4606	-9.6270	N.am	51 CYS292	0.0000
BACKBONE							
855	CA	7.4843	9.7207	-8.6174	C.3	51 CYS292	0.0000
BACKBONE							
856	C	7.6448	8.6545	-7.5618	C.2	51 CYS292	0.0000
BACKBONE							
857	O	7.7152	7.4963	-7.9392	O.2	51 CYS292	0.0000
BACKBONE							
858	CB	6.0619	9.6385	-9.2246	C.3	51 CYS292	0.0000
859	SG	4.7723	10.0362	-8.0060	S.3	51 CYS292	0.0000
860	H	8.2647	8.8776	-10.4072	H	51 CYS292	0.0000
861	HA	7.5970	10.7355	-8.2135	H	51 CYS292	0.0000
862	HB3	5.8919	8.6113	-9.5581	H	51 CYS292	0.0000
863	HB2	5.9618	10.3216	-10.0808	H	51 CYS292	0.0000
864	LPG2	4.8227	10.6761	-7.7845	LP	51 CYS292	0.0000
865	LPG1	4.7855	9.6115	-7.4763	LP	51 CYS292	0.0000
866	N	7.7116	8.9824	-6.2519	N.am	52 PHE293	0.0000
BACKBONE							
867	CA	7.8777	7.9211	-5.2590	C.3	52 PHE293	0.0000
BACKBONE							
868	C	6.7475	6.9279	-5.3625	C.2	52 PHE293	0.0000
BACKBONE							
869	O	7.0009	5.7363	-5.2749	O.2	52 PHE293	0.0000
BACKBONE							
870	CB	7.9868	8.4324	-3.7971	C.3	52 PHE293	0.0000
871	CG	6.6319	8.8099	-3.1747	C.ar	52 PHE293	0.0000
872	CD1	5.9511	7.8899	-2.3697	C.ar	52 PHE293	0.0000
873	CD2	6.0561	10.0661	-3.3840	C.ar	52 PHE293	0.0000
874	CE1	4.6964	8.1977	-1.8347	C.ar	52 PHE293	0.0000
875	CE2	4.8488	10.4157	-2.7762	C.ar	52 PHE293	0.0000
876	CZ	4.1628	9.4780	-2.0010	C.ar	52 PHE293	0.0000
877	H	7.6711	9.9354	-5.9532	H	52 PHE293	0.0000
878	HA	8.8215	7.3999	-5.4896	H	52 PHE293	0.0000
879	HB3	8.6865	9.2799	-3.7681	H	52 PHE293	0.0000
880	HB2	8.4176	7.6277	-3.1826	H	52 PHE293	0.0000
881	HD1	6.4028	6.9324	-2.1513	H	52 PHE293	0.0000
882	HD2	6.5478	10.7817	-4.0219	H	52 PHE293	0.0000
883	HE1	4.1333	7.4484	-1.2890	H	52 PHE293	0.0000

884	HE2	4.4450	11.4149	-2.9060	H	52 PHE293	0.0000
885	HZ	3.2213	9.7364	-1.5285	H	52 PHE293	0.0000
886	N	5.4939	7.4048	-5.5416	N.am	53 CYS294	0.0000
BACKBONE							
887	CA	4.3661	6.4827	-5.5409	C.3	53 CYS294	0.0000
BACKBONE							
888	C	4.2285	5.7704	-6.8701	C.2	53 CYS294	0.0000
BACKBONE							
889	O	4.3589	4.5563	-6.9013	O.2	53 CYS294	0.0000
BACKBONE							
890	CB	3.0536	7.1874	-5.1127	C.3	53 CYS294	0.0000
891	SG	1.7244	5.9482	-4.9567	S.o	53 CYS294	0.0000
892	H	5.3118	8.3829	-5.6501	H	53 CYS294	0.0000
893	HA	4.5612	5.7469	-4.7507	H	53 CYS294	0.0000
894	HB3	2.7536	7.9612	-5.8341	H	53 CYS294	0.0000
895	HB2	3.2148	7.6629	-4.1336	H	53 CYS294	0.0000
896	LPG2	1.9148	5.4136	-4.5838	LP	53 CYS294	0.0000
897	LPG1	1.5011	5.7344	-5.5612	LP	53 CYS294	0.0000
898	HG	1.0453	6.5209	-4.4812	H	53 CYS294	0.0000
899	N	3.9542	6.5055	-7.9746	N.am	54 CYS295	0.0000
BACKBONE							
900	CA	3.7044	5.8714	-9.2702	C.3	54 CYS295	0.0000
BACKBONE							
901	C	4.9495	5.4898	-10.0407	C.2	54 CYS295	0.0000
BACKBONE							
902	O	4.7902	4.9084	-11.1024	O.2	54 CYS295	0.0000
BACKBONE							
903	CB	2.7646	6.7452	-10.1525	C.3	54 CYS295	0.0000
904	SG	3.4446	8.3566	-10.7135	S.3	54 CYS295	0.0000
905	H	3.9032	7.4969	-7.9197	H	54 CYS295	0.0000
906	HA	3.1589	4.9282	-9.0899	H	54 CYS295	0.0000
907	HB3	1.8322	6.8992	-9.6007	H	54 CYS295	0.0000
908	HB2	2.5132	6.1935	-11.0722	H	54 CYS295	0.0000
909	LPG2	3.1403	8.5500	-11.2889	LP	54 CYS295	0.0000
910	LPG1	4.1133	8.3033	-10.8180	LP	54 CYS295	0.0000
911	N	6.1829	5.7912	-9.5705	N.am	55 ASP296	0.0000
BACKBONE							
912	CA	7.3837	5.4048	-10.3218	C.3	55 ASP296	0.0000
BACKBONE							
913	C	7.4298	5.9491	-11.7358	C.2	55 ASP296	0.0000
BACKBONE							
914	O	8.2524	5.4824	-12.5081	O.2	55 ASP296	0.0000
BACKBONE							
915	CB	7.5111	3.8571	-10.3251	C.3	55 ASP296	0.0000
916	CG	8.9281	3.4041	-10.5732	C.2	55 ASP296	0.0000
917	OD1	9.7554	3.5078	-9.6268	O.co2	55 ASP296	-0.5000
918	OD2	9.2273	2.9399	-11.7070	O.co2	55 ASP296	-0.5000
919	H	6.3055	6.2587	-8.6933	H	55 ASP296	0.0000
920	HA	8.2713	5.8147	-9.8106	H	55 ASP296	0.0000
921	HB3	6.8363	3.4130	-11.0735	H	55 ASP296	0.0000
922	HB2	7.2033	3.4817	-9.3406	H	55 ASP296	0.0000

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 923 N        6.5735     6.9276   -12.1110 N.am  56 GLY297   0.0000
BACKBONE
 924 CA       6.5981     7.4595   -13.4666 C.3   56 GLY297   0.0000
BACKBONE
 925 C        7.7811     8.3867   -13.5717 C.2   56 GLY297   0.0000
BACKBONE
 926 O        7.9218     9.2330   -12.7027 O.2   56 GLY297   0.0000
BACKBONE
 927 H        5.9286     7.3412   -11.4778 H     56 GLY297   0.0000
 928 HA2      5.6812     8.0356   -13.6600 H     56 GLY297   0.0000
 929 HA3      6.6322     6.6343   -14.1952 H     56 GLY297   0.0000
 930 N        8.6372     8.2403   -14.6087 N.am  57 GLY298   0.0000
BACKBONE
 931 CA       9.8449     9.0535   -14.6912 C.3   57 GLY298   0.0000
BACKBONE
 932 C        9.6391    10.2700   -15.5482 C.2   57 GLY298   0.0000
BACKBONE
 933 O        8.8227    10.1714   -16.4477 O.2   57 GLY298   0.0000
BACKBONE
 934 H        8.4711     7.5766   -15.3420 H     57 GLY298   0.0000
 935 HA2     10.6258     8.4540   -15.1663 H     57 GLY298   0.0000
 936 HA3     10.2104     9.3289   -13.7000 H     57 GLY298   0.0000
 937 N       10.3684    11.3909   -15.3232 N.am  58 LEU299   0.0000
BACKBONE
 938 CA      10.2351    12.5568   -16.1985 C.3   58 LEU299   0.0000
BACKBONE
 939 C       11.5682    13.2613   -16.3535 C.2   58 LEU299   0.0000
BACKBONE
 940 O       12.2856    13.3464   -15.3695 O.2   58 LEU299   0.0000
BACKBONE
 941 CB       9.2109    13.5738   -15.6265 C.3   58 LEU299   0.0000
 942 CG       7.7341    13.0840   -15.5854 C.3   58 LEU299   0.0000
 943 CD1      6.8587    14.1211   -14.8246 C.3   58 LEU299   0.0000
 944 CD2      7.1123    12.8330   -16.9921 C.3   58 LEU299   0.0000
 945 H       11.0071    11.4515   -14.5538 H     58 LEU299   0.0000
 946 HA       9.9223    12.2354   -17.1978 H     58 LEU299   0.0000
 947 HB3      9.2574    14.5145   -16.1886 H     58 LEU299   0.0000
 948 HB2      9.5341    13.7881   -14.5992 H     58 LEU299   0.0000
 949 HG       7.7346    12.1460   -15.0101 H     58 LEU299   0.0000
 950 HD13     7.2311    14.2569   -13.7997 H     58 LEU299   0.0000
 951 HD12     5.8093    13.7922   -14.7657 H     58 LEU299   0.0000
 952 HD11     6.8902    15.0947   -15.3359 H     58 LEU299   0.0000
 953 HD23     7.1223    13.7501   -17.5950 H     58 LEU299   0.0000
 954 HD22     6.0673    12.5057   -16.8903 H     58 LEU299   0.0000
 955 HD21     7.6394    12.0556   -17.5561 H     58 LEU299   0.0000
 956 N       11.9052    13.7769   -17.5637 N.am  59 ARG300   0.0000
BACKBONE
 957 CA      13.1521    14.5195   -17.7543 C.3   59 ARG300   0.0000
BACKBONE
 958 C       12.9149    15.6495   -18.7359 C.2   59 ARG300   0.0000
BACKBONE
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 959 O       11.7776    15.8258   -19.1419 O.2   59 ARG300   0.0000
BACKBONE
 960 CB      14.2820    13.5591   -18.2258 C.3   59 ARG300   0.0000
 961 CG      14.1064    13.0698   -19.6944 C.3   59 ARG300   0.0000
 962 CD      15.4539    12.5776   -20.2915 C.3   59 ARG300   0.0000
 963 NE      15.9763    11.4296   -19.5458 N.pl3 59 ARG300   0.0000
 964 CZ      15.6399    10.1759   -19.7765 C.cat 59 ARG300   1.0000
 965 NH1     14.7517     9.8141   -20.6747 N.pl3 59 ARG300   0.0000
 966 NH2     16.2223     9.2299   -19.0741 N.pl3 59 ARG300   0.0000
 967 H       11.3181    13.6591   -18.3663 H     59 ARG300   0.0000
 968 HA      13.4539    14.9984   -16.8083 H     59 ARG300   0.0000
 969 HB3     14.3286    12.6895   -17.5536 H     59 ARG300   0.0000
 970 HB2     15.2426    14.0846   -18.1238 H     59 ARG300   0.0000
 971 HG3     13.7478    13.8859   -20.3375 H     59 ARG300   0.0000
 972 HG2     13.3523    12.2702   -19.7314 H     59 ARG300   0.0000
 973 HD3     16.1792    13.4057   -20.2114 H     59 ARG300   0.0000
 974 HD2     15.3837    12.3822   -21.3718 H     59 ARG300   0.0000
 975 HE      16.6866    11.6329   -18.8241 H     59 ARG300   0.0000
 976 HH11    14.2402    10.4992   -21.2409 H     59 ARG300   0.0000
 977 HH12    14.5362     8.8183   -20.8330 H     59 ARG300   0.0000
 978 HH21    16.9256     9.4543   -18.3563 H     59 ARG300   0.0000
 979 HH22    15.9927     8.2355   -19.2219 H     59 ARG300   0.0000
 980 N       13.9538    16.4195   -19.1394 N.am  60 CYS301   0.0000
BACKBONE
 981 CA      13.7410    17.5200   -20.0792 C.3   60 CYS301   0.0000
BACKBONE
 982 C       12.6808    18.4366   -19.5201 C.2   60 CYS301   0.0000
BACKBONE
 983 O       11.7438    18.7983   -20.2145 O.2   60 CYS301   0.0000
BACKBONE
 984 CB      13.4194    17.0067   -21.5058 C.3   60 CYS301   0.0000
 985 SG      14.7816    15.9208   -22.0453 S.o   60 CYS301   0.0000
 986 H       14.8830    16.2690   -18.8005 H     60 CYS301   0.0000
 987 HA      14.6592    18.1288   -20.1528 H     60 CYS301   0.0000
 988 HB3     13.3326    17.8528   -22.2065 H     60 CYS301   0.0000
 989 HB2     12.4741    16.4464   -21.5145 H     60 CYS301   0.0000
 990 LPG2    14.8473    15.3752   -21.6464 LP    60 CYS301   0.0000
 991 LPG1    15.3743    16.2504   -22.0772 LP    60 CYS301   0.0000
 992 HG      14.4293    15.6831   -22.9592 H     60 CYS301   0.0000
 993 N       12.8433    18.8173   -18.2338 N.am  61 TRP302   0.0000
BACKBONE
 994 CA      11.9135    19.7606   -17.6255 C.3   61 TRP302   0.0000
BACKBONE
 995 C       12.1489    21.1024   -18.2733 C.2   61 TRP302   0.0000
BACKBONE
 996 O       13.3052    21.4406   -18.4707 O.2   61 TRP302   0.0000
BACKBONE
 997 CB      12.1526    19.8840   -16.0997 C.3   61 TRP302   0.0000
 998 CG      11.6437    18.6534   -15.4057 C.2   61 TRP302   0.0000
 999 CD1     12.2867    17.4992   -15.1622 C.2   61 TRP302   0.0000
1000 CD2     10.2545    18.5058   -14.8479 C.ar  61 TRP302   0.0000
1001 NE1     11.4836    16.6805   -14.5321 N.pl3 61 TRP302   0.0000
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1002 CE2     10.2750    17.2363   -14.3078 C.ar  61 TRP302   0.0000
1003 CE3      9.1317    19.3256   -14.7998 C.ar  61 TRP302   0.0000
1004 CZ2      9.1603    16.7179   -13.6482 C.ar  61 TRP302   0.0000
1005 CZ3      8.0029    18.8109   -14.1516 C.ar  61 TRP302   0.0000
1006 CH2      8.0182    17.5267   -13.5832 C.ar  61 TRP302   0.0000
1007 H       13.6343    18.5058   -17.7057 H     61 TRP302   0.0000
1008 HA      10.8792    19.4157   -17.7939 H     61 TRP302   0.0000
1009 HB3     11.6336    20.7655   -15.6944 H     61 TRP302   0.0000
1010 HB2     13.2252    20.0000   -15.8999 H     61 TRP302   0.0000
1011 HD1     13.3140    17.2878   -15.4521 H     61 TRP302   0.0000
1012 HE1     11.7445    15.7269   -14.2461 H     61 TRP302   0.0000
1013 HE3      9.1407    20.3101   -15.2451 H     61 TRP302   0.0000
1014 HZ2      9.1774    15.7345   -13.1990 H     61 TRP302   0.0000
1015 HZ3      7.1125    19.4250   -14.0965 H     61 TRP302   0.0000
1016 HH2      7.1321    17.1509   -13.0816 H     61 TRP302   0.0000
1017 N       11.0791    21.8631   -18.6059 N.am  62 GLU303   0.0000
BACKBONE
1018 CA      11.2498    23.1733   -19.2277 C.3   62 GLU303   0.0000
BACKBONE
1019 C       10.9194    24.2305   -18.2052 C.2   62 GLU303   0.0000
BACKBONE
1020 O       10.2402    23.9230   -17.2381 O.2   62 GLU303   0.0000
BACKBONE
1021 CB      10.3125    23.3387   -20.4536 C.3   62 GLU303   0.0000
1022 CG      10.5383    22.2092   -21.4915 C.3   62 GLU303   0.0000
1023 CD       9.7190    22.4808   -22.7278 C.2   62 GLU303   0.0000
1024 OE1      8.4770    22.2688   -22.6772 O.co2 62 GLU303  -0.5000
1025 OE2     10.3072    22.9115   -23.7573 O.co2 62 GLU303  -0.5000
1026 H       10.1448    21.5662   -18.4064 H     62 GLU303   0.0000
1027 HA      12.2849    23.3231   -19.5766 H     62 GLU303   0.0000
1028 HB3     10.5029    24.3153   -20.9295 H     62 GLU303   0.0000
1029 HB2      9.2620    23.3212   -20.1219 H     62 GLU303   0.0000
1030 HG3     10.2412    21.2365   -21.0673 H     62 GLU303   0.0000
1031 HG2     11.6061    22.1541   -21.7577 H     62 GLU303   0.0000
1032 N       11.3838    25.4836   -18.4094 N.am  63 SER304   0.0000
BACKBONE
1033 CA      11.0454    26.5389   -17.4620 C.3   63 SER304   0.0000
BACKBONE
1034 C        9.5517    26.7539   -17.5214 C.2   63 SER304   0.0000
BACKBONE
1035 O        9.0000    26.6159   -18.6018 O.2   63 SER304   0.0000
BACKBONE
1036 CB      11.7751    27.8542   -17.8307 C.3   63 SER304   0.0000
1037 OG      13.1620    27.5425   -18.0434 O.3   63 SER304   0.0000
1038 H       11.9384    25.7139   -19.2120 H     63 SER304   0.0000
1039 HA      11.3724    26.2240   -16.4564 H     63 SER304   0.0000
1040 HB3     11.6515    28.6007   -17.0278 H     63 SER304   0.0000
1041 HB2     11.3448    28.2578   -18.7631 H     63 SER304   0.0000
1042 HG      13.6657    28.2952   -18.3340 H     63 SER304   0.0000
1043 N        8.8755    27.0784   -16.3951 N.am  64 GLY305   0.0000
BACKBONE
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1044 CA       7.4305    27.2952   -16.4458 C.3   64 GLY305   0.0000
BACKBONE
1045 C        6.6288    26.0250   -16.2795 C.2   64 GLY305   0.0000
BACKBONE
1046 O        5.4584    26.1462   -15.9516 O.2   64 GLY305   0.0000
BACKBONE
1047 H        9.3394    27.1545   -15.5092 H     64 GLY305   0.0000
1048 HA2      7.1339    27.7709   -17.3939 H     64 GLY305   0.0000
1049 HA3      7.1454    27.9878   -15.6365 H     64 GLY305   0.0000
1050 N        7.1841    24.8062   -16.4903 N.am  65 ASP306   0.0000
BACKBONE
1051 CA       6.3779    23.6093   -16.2543 C.3   65 ASP306   0.0000
BACKBONE
1052 C        5.9250    23.6217   -14.8116 C.2   65 ASP306   0.0000
BACKBONE
1053 O        6.6881    24.0840   -13.9783 O.2   65 ASP306   0.0000
BACKBONE
1054 CB       7.1514    22.2862   -16.4981 C.3   65 ASP306   0.0000
1055 CG       7.4844    22.0185   -17.9433 C.2   65 ASP306   0.0000
1056 OD1      6.9787    22.7497   -18.8365 O.co2 65 ASP306  -0.5000
1057 OD2      8.2626    21.0582   -18.1967 O.co2 65 ASP306  -0.5000
1058 H        8.1344    24.6908   -16.7798 H     65 ASP306   0.0000
1059 HA       5.5033    23.6364   -16.9253 H     65 ASP306   0.0000
1060 HB3      6.5578    21.4345   -16.1323 H     65 ASP306   0.0000
1061 HB2      8.0840    22.3326   -15.9197 H     65 ASP306   0.0000
1062 N        4.7013    23.1237   -14.5124 N.am  66 ASP307   0.0000
BACKBONE
1063 CA       4.2150    23.0789   -13.1341 C.3   66 ASP307   0.0000
BACKBONE
1064 C        4.2869    21.6255   -12.7191 C.2   66 ASP307   0.0000
BACKBONE
1065 O        3.5165    20.8656   -13.2848 O.2   66 ASP307   0.0000
BACKBONE
1066 CB       2.7585    23.6149   -13.0664 C.3   66 ASP307   0.0000
1067 CG       2.1331    23.4861   -11.6985 C.2   66 ASP307   0.0000
1068 OD1      2.7354    22.8401   -10.7980 O.co2 66 ASP307  -0.5000
1069 OD2      1.0148    24.0383   -11.5131 O.co2 66 ASP307  -0.5000
1070 H        4.1150    22.7288   -15.2236 H     66 ASP307   0.0000
1071 HA       4.7860    23.7482   -12.4742 H     66 ASP307   0.0000
1072 HB3      2.1235    23.0745   -13.7793 H     66 ASP307   0.0000
1073 HB2      2.7569    24.6768   -13.3617 H     66 ASP307   0.0000
1074 N        5.1580    21.1735   -11.7800 N.am  67 PRO308   0.0000
BACKBONE
1075 CA       5.1857    19.7623   -11.4258 C.3   67 PRO308   0.0000
BACKBONE
1076 C        3.8499    19.0817   -11.2598 C.2   67 PRO308   0.0000
BACKBONE
1077 O        3.6911    17.9954   -11.7936 O.2   67 PRO308   0.0000
BACKBONE
1078 CB       5.9909    19.8470   -10.1115 C.3   67 PRO308   0.0000
1079 CG       6.9970    20.9831   -10.3971 C.3   67 PRO308   0.0000
1080 CD       6.1206    22.0413   -11.1086 C.3   67 PRO308   0.0000
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1081 HA       5.7784    19.2267   -12.1802 H     67 PRO308   0.0000
1082 HB3      6.4695    18.8895    -9.8722 H     67 PRO308   0.0000
1083 HB2      5.3431    20.1502    -9.2735 H     67 PRO308   0.0000
1084 HG2      7.4971    21.3598    -9.4913 H     67 PRO308   0.0000
1085 HG3      7.7660    20.6173   -11.0981 H     67 PRO308   0.0000
1086 HD2      5.6083    22.6832   -10.3736 H     67 PRO308   0.0000
1087 HD3      6.7396    22.6459   -11.7896 H     67 PRO308   0.0000
1088 N        2.8755    19.6784   -10.5381 N.am  68 TRP309   0.0000
BACKBONE
1089 CA       1.6019    18.9847   -10.3633 C.3   68 TRP309   0.0000
BACKBONE
1090 C        0.9300    18.7470   -11.6959 C.2   68 TRP309   0.0000
BACKBONE
1091 O        0.4176    17.6594   -11.9114 O.2   68 TRP309   0.0000
BACKBONE
1092 CB       0.6070    19.7498    -9.4516 C.3   68 TRP309   0.0000
1093 CG       1.0008    19.6908    -7.9992 C.2   68 TRP309   0.0000
1094 CD1      1.3366    20.7086    -7.1894 C.2   68 TRP309   0.0000
1095 CD2      1.0618    18.4353    -7.1668 C.ar  68 TRP309   0.0000
1096 NE1      1.5662    20.2507    -5.9841 N.pl3 68 TRP309   0.0000
1097 CE2      1.3866    18.9175    -5.9145 C.ar  68 TRP309   0.0000
1098 CE3      0.8682    17.0778    -7.4084 C.ar  68 TRP309   0.0000
1099 CZ2      1.4737    18.0744    -4.8075 C.ar  68 TRP309   0.0000
1100 CZ3      0.9857    16.2121    -6.3152 C.ar  68 TRP309   0.0000
1101 CH2      1.2330    16.7115    -5.0273 C.ar  68 TRP309   0.0000
1102 H        3.0083    20.5792   -10.1199 H     68 TRP309   0.0000
1103 HA       1.8273    18.0053    -9.9169 H     68 TRP309   0.0000
1104 HB3     -0.3871    19.2794    -9.5161 H     68 TRP309   0.0000
1105 HB2      0.5116    20.7926    -9.7930 H     68 TRP309   0.0000
1106 HD1      1.3987    21.7544    -7.4897 H     68 TRP309   0.0000
1107 HE1      1.8355    20.8394    -5.1818 H     68 TRP309   0.0000
1108 HE3      0.6381    16.7163    -8.3986 H     68 TRP309   0.0000
1109 HZ2      1.7164    18.4601    -3.8237 H     68 TRP309   0.0000
1110 HZ3      0.8909    15.1432    -6.4687 H     68 TRP309   0.0000
1111 HH2      1.2467    16.0298    -4.1884 H     68 TRP309   0.0000
1112 N        0.9134    19.7499   -12.6017 N.am  69 VAL310   0.0000
BACKBONE
1113 CA       0.2434    19.5475   -13.8847 C.3   69 VAL310   0.0000
BACKBONE
1114 C        0.9448    18.4293   -14.6164 C.2   69 VAL310   0.0000
BACKBONE
1115 O        0.2627    17.5569   -15.1275 O.2   69 VAL310   0.0000
BACKBONE
1116 CB       0.2005    20.8289   -14.7678 C.3   69 VAL310   0.0000
1117 CG1     -0.3531    20.5324   -16.1898 C.3   69 VAL310   0.0000
1118 CG2     -0.6695    21.9286   -14.0927 C.3   69 VAL310   0.0000
1119 H        1.3721    20.6196   -12.4139 H     69 VAL310   0.0000
1120 HA      -0.7956    19.2404   -13.6837 H     69 VAL310   0.0000
1121 HB       1.2332    21.1911   -14.8934 H     69 VAL310   0.0000
1122 HG13     0.2807    19.8140   -16.7322 H     69 VAL310   0.0000
1123 HG12    -0.3961    21.4580   -16.7845 H     69 VAL310   0.0000
1124 HG11    -1.3684    20.1208   -16.1156 H     69 VAL310   0.0000
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1125 HG23    -1.7163    21.5955   -14.0191 H     69 VAL310   0.0000
1126 HG22    -0.6414    22.8555   -14.6859 H     69 VAL310   0.0000
1127 HG21    -0.3143    22.1639   -13.0794 H     69 VAL310   0.0000
1128 N        2.2955    18.4291   -14.6823 N.am  70 GLN311   0.0000
BACKBONE
1129 CA       2.9820    17.3588   -15.4051 C.3   70 GLN311   0.0000
BACKBONE
1130 C        2.6469    16.0153   -14.7887 C.2   70 GLN311   0.0000
BACKBONE
1131 O        2.4317    15.0610   -15.5191 O.2   70 GLN311   0.0000
BACKBONE
1132 CB       4.5267    17.5334   -15.4367 C.3   70 GLN311   0.0000
1133 CG       4.9767    18.7983   -16.2201 C.3   70 GLN311   0.0000
1134 CD       4.4410    18.8052   -17.6332 C.2   70 GLN311   0.0000
1135 OE1      4.6335    17.8187   -18.3300 O.2   70 GLN311   0.0000
1136 NE2      3.7691    19.8835   -18.0942 N.am  70 GLN311   0.0000
1137 H        2.8322    19.1449   -14.2332 H     70 GLN311   0.0000
1138 HA       2.6149    17.3703   -16.4420 H     70 GLN311   0.0000
1139 HB3      4.9701    16.6505   -15.9245 H     70 GLN311   0.0000
1140 HB2      4.9086    17.5786   -14.4041 H     70 GLN311   0.0000
1141 HG3      6.0756    18.8056   -16.2949 H     70 GLN311   0.0000
1142 HG2      4.6742    19.7015   -15.6688 H     70 GLN311   0.0000
1143 HE21     3.6098    20.6910   -17.5243 H     70 GLN311   0.0000
1144 HE22     3.4166    19.8811   -19.0313 H     70 GLN311   0.0000
1145 N        2.5956    15.9248   -13.4407 N.am  71 HIS312   0.0000
BACKBONE
1146 CA       2.3017    14.6455   -12.7849 C.3   71 HIS312   0.0000
BACKBONE
1147 C        0.9679    14.1287   -13.2797 C.2   71 HIS312   0.0000
BACKBONE
1148 O        0.8656    12.9587   -13.6130 O.2   71 HIS312   0.0000
BACKBONE
1149 CB       2.3247    14.8258   -11.2366 C.3   71 HIS312   0.0000
1150 CG       2.5476    13.6026   -10.3770 C.2   71 HIS312   0.0000
1151 ND1      2.8608    13.7150    -9.1037 N.pl3 71 HIS312   0.0000
1152 CD2      2.4943    12.2991   -10.7250 C.2   71 HIS312   0.0000
1153 CE1      3.0459    12.5423    -8.5898 C.cat 71 HIS312   1.0000
1154 NE2      2.8545    11.6781    -9.4777 N.2   71 HIS312   0.0000
1155 H        2.7630    16.7384   -12.8824 H     71 HIS312   0.0000
1156 HA       3.0844    13.9303   -13.0813 H     71 HIS312   0.0000
1157 HB3      1.4216    15.3598   -10.9141 H     71 HIS312   0.0000
1158 HB2      3.1859    15.4630   -10.9879 H     71 HIS312   0.0000
1159 HD1      2.9628    14.6046    -8.5918 H     71 HIS312   0.0000
1160 HD2      2.2580    11.8501   -11.6796 H     71 HIS312   0.0000
1161 HE1      3.3295    12.3507    -7.5582 H     71 HIS312   0.0000
1162 N       -0.0651    14.9983   -13.3524 N.am  72 ALA313   0.0000
BACKBONE
1163 CA      -1.3570    14.5704   -13.8922 C.3   72 ALA313   0.0000
BACKBONE
1164 C       -1.3120    14.3398   -15.3821 C.2   72 ALA313   0.0000
BACKBONE
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1165 O      -1.9685    13.4257   -15.8547 O.2   72 ALA313   0.0000
BACKBONE
1166 CB     -2.4454    15.6334   -13.5898 C.3   72 ALA313   0.0000
1167 H       0.0499    15.9535   -13.0704 H     72 ALA313   0.0000
1168 HA     -1.6385    13.6043   -13.4530 H     72 ALA313   0.0000
1169 HB3    -2.1606    16.5953   -14.0362 H     72 ALA313   0.0000
1170 HB2    -2.5588    15.7809   -12.5062 H     72 ALA313   0.0000
1171 HB1    -3.4134    15.3236   -14.0091 H     72 ALA313   0.0000
1172 N      -0.5586    15.1591   -16.1417 N.am  73 LYS314   0.0000
BACKBONE
1173 CA     -0.5434    15.0039   -17.5938 C.3   73 LYS314   0.0000
BACKBONE
1174 C      -0.0578    13.6204   -17.9610 C.2   73 LYS314   0.0000
BACKBONE
1175 O      -0.6339    13.0174   -18.8528 O.2   73 LYS314   0.0000
BACKBONE
1176 CB      0.3580    16.0968   -18.2298 C.3   73 LYS314   0.0000
1177 CG      0.3192    16.1161   -19.7840 C.3   73 LYS314   0.0000
1178 CD      0.8791    17.4590   -20.3425 C.3   73 LYS314   0.0000
1179 CE     -0.1634    18.6201   -20.3147 C.3   73 LYS314   0.0000
1180 NZ     -1.0516    18.6138   -21.5026 N.4   73 LYS314   1.0000
1181 H      -0.0160    15.8839   -15.7202 H     73 LYS314   0.0000
1182 HA     -1.5728    15.1513   -17.9607 H     73 LYS314   0.0000
1183 HB3     1.3984    15.9392   -17.9065 H     73 LYS314   0.0000
1184 HB2     0.0229    17.0675   -17.8347 H     73 LYS314   0.0000
1185 HG3    -0.7085    15.9654   -20.1473 H     73 LYS314   0.0000
1186 HG2     0.9315    15.2745   -20.1516 H     73 LYS314   0.0000
1187 HD3     1.2132    17.3225   -21.3839 H     73 LYS314   0.0000
1188 HD2     1.7663    17.7358   -19.7477 H     73 LYS314   0.0000
1189 HE3     0.3738    19.5845   -20.2969 H     73 LYS314   0.0000
1190 HE2    -0.7818    18.5758   -19.4039 H     73 LYS314   0.0000
1191 HZ3    -0.5027    18.8167   -22.4128 H     73 LYS314   0.0000
1192 HZ2    -1.8161    19.3768   -21.4307 H     73 LYS314   0.0000
1193 HZ1    -1.5653    17.6737   -21.6416 H     73 LYS314   0.0000
1194 N       0.9999    13.1145   -17.2822 N.am  74 TRP315   0.0000
BACKBONE
1195 CA      1.5815    11.8196   -17.6445 C.3   74 TRP315   0.0000
BACKBONE
1196 C       1.0750    10.6587   -16.8165 C.2   74 TRP315   0.0000
BACKBONE
1197 O       0.9565     9.5841   -17.3848 O.2   74 TRP315   0.0000
BACKBONE
1198 CB      3.1256    11.9213   -17.5418 C.3   74 TRP315   0.0000
1199 CG      3.5803    12.9069   -18.5846 C.2   74 TRP315   0.0000
1200 CD1     4.0381    14.1587   -18.4110 C.2   74 TRP315   0.0000
1201 CD2     3.5812    12.6387   -20.0667 C.ar  74 TRP315   0.0000
1202 NE1     4.3041    14.6874   -19.5774 N.pl3 74 TRP315   0.0000
1203 CE2     4.0549    13.8267   -20.5864 C.ar  74 TRP315   0.0000
1204 CE3     3.2391    11.5544   -20.8756 C.ar  74 TRP315   0.0000
1205 CZ2     4.2224    14.0048   -21.9594 C.ar  74 TRP315   0.0000
1206 CZ3     3.4259    11.7119   -22.2547 C.ar  74 TRP315   0.0000
1207 CH2     3.9122    12.9170   -22.7867 C.ar  74 TRP315   0.0000
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1208 H       1.4188   13.6311  -16.5325 H     74 TRP315   0.0000
1209 HA      1.3412   11.5865  -18.6951 H     74 TRP315   0.0000
1210 HB3     3.5967   10.9482  -17.7507 H     74 TRP315   0.0000
1211 HB2     3.4236   12.2438  -16.5320 H     74 TRP315   0.0000
1212 HD1     4.1646   14.6572  -17.4511 H     74 TRP315   0.0000
1213 HE1     4.6680   15.6433  -19.7102 H     74 TRP315   0.0000
1214 HE3     2.8527   10.6329  -20.4549 H     74 TRP315   0.0000
1215 HZ2     4.5801   14.9441  -22.3672 H     74 TRP315   0.0000
1216 HZ3     3.1928   10.8866  -22.9203 H     74 TRP315   0.0000
1217 HH2     4.0518   13.0071  -23.8595 H     74 TRP315   0.0000
1218 N       0.7819   10.8201  -15.5037 N.am  75 PHE316   0.0000
BACKBONE
1219 CA      0.3552    9.6824  -14.6837 C.3   75 PHE316   0.0000
BACKBONE
1220 C      -0.9283   10.0456  -13.9655 C.2   75 PHE316   0.0000
BACKBONE
1221 O      -0.8957   10.1933  -12.7535 O.2   75 PHE316   0.0000
BACKBONE
1222 CB      1.5134    9.2895  -13.7274 C.3   75 PHE316   0.0000
1223 CG      2.8435    9.3340  -14.4935 C.ar  75 PHE316   0.0000
1224 CD1     3.1507    8.3584  -15.4490 C.ar  75 PHE316   0.0000
1225 CD2     3.7618   10.3606  -14.2516 C.ar  75 PHE316   0.0000
1226 CE1     4.3446    8.4275  -16.1751 C.ar  75 PHE316   0.0000
1227 CE2     4.9731   10.4030  -14.9422 C.ar  75 PHE316   0.0000
1228 CZ      5.2598    9.4530  -15.9254 C.ar  75 PHE316   0.0000
1229 H       0.8884   11.7059  -15.0511 H     75 PHE316   0.0000
1230 HA      0.1708    8.7737  -15.2755 H     75 PHE316   0.0000
1231 HB3     1.3563    8.2846  -13.3014 H     75 PHE316   0.0000
1232 HB2     1.5547    9.9934  -12.8883 H     75 PHE316   0.0000
1233 HD1     2.4589    7.5432  -15.6326 H     75 PHE316   0.0000
1234 HD2     3.5497   11.1392  -13.5299 H     75 PHE316   0.0000
1235 HE1     4.5638    7.6823  -16.9333 H     75 PHE316   0.0000
1236 HE2     5.6834   11.1794  -14.7032 H     75 PHE316   0.0000
1237 HZ      6.1870    9.5112  -16.4855 H     75 PHE316   0.0000
1238 N      -2.0914   10.2007  -14.6503 N.am  76 PRO317   0.0000
BACKBONE
1239 CA     -3.3071   10.5740  -13.9373 C.3   76 PRO317   0.0000
BACKBONE
1240 C      -3.8037    9.5073  -12.9865 C.2   76 PRO317   0.0000
BACKBONE
1241 O      -4.6664    9.8326  -12.1872 O.2   76 PRO317   0.0000
BACKBONE
1242 CB     -4.2770   10.7893  -15.1263 C.3   76 PRO317   0.0000
1243 CG     -3.7154    9.8822  -16.2416 C.3   76 PRO317   0.0000
1244 CD     -2.1840   10.0316  -16.0965 C.3   76 PRO317   0.0000
1245 HA     -3.1585   11.5119  -13.3771 H     76 PRO317   0.0000
1246 HB3    -4.2122   11.8351  -15.4640 H     76 PRO317   0.0000
1247 HB2    -5.3279   10.5582  -14.8902 H     76 PRO317   0.0000
1248 HG2    -4.0047    8.8401  -16.0239 H     76 PRO317   0.0000
1249 HG3    -4.0810   10.1519  -17.2460 H     76 PRO317   0.0000
1250 HD2    -1.6921    9.1399  -16.5114 H     76 PRO317   0.0000
1251 HD3    -1.8187   10.9358  -16.6072 H     76 PRO317   0.0000
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1252 N      -3.2964     8.2517   -13.0195 N.am  77 ARG318   0.0000
BACKBONE
1253 CA     -3.7280     7.2528   -12.0379 C.3   77 ARG318   0.0000
BACKBONE
1254 C      -2.8170     7.2338   -10.8254 C.2   77 ARG318   0.0000
BACKBONE
1255 O      -2.9320     6.3044   -10.0414 O.2   77 ARG318   0.0000
BACKBONE
1256 CB     -3.7757     5.8485   -12.7048 C.3   77 ARG318   0.0000
1257 CG     -4.7239     5.8345   -13.9362 C.3   77 ARG318   0.0000
1258 CD     -4.7633     4.4349   -14.6096 C.3   77 ARG318   0.0000
1259 NE     -3.4224     4.0039   -15.0199 N.pl3 77 ARG318   0.0000
1260 CZ     -2.8055     4.4162   -16.1099 C.cat 77 ARG318   1.0000
1261 NH1    -3.3228     5.2752   -16.9595 N.pl3 77 ARG318   0.0000
1262 NH2    -1.6050     3.9446   -16.3660 N.pl3 77 ARG318   0.0000
1263 H      -2.5816     7.9891   -13.6690 H     77 ARG318   0.0000
1264 HA     -4.7464     7.4650   -11.6726 H     77 ARG318   0.0000
1265 HB3    -4.1268     5.0987   -11.9766 H     77 ARG318   0.0000
1266 HB2    -2.7551     5.5723   -13.0152 H     77 ARG318   0.0000
1267 HG3    -4.3880     6.5868   -14.6635 H     77 ARG318   0.0000
1268 HG2    -5.7426     6.1089   -13.6155 H     77 ARG318   0.0000
1269 HD3    -5.4829     4.4004   -15.4424 H     77 ARG318   0.0000
1270 HD2    -5.1473     3.7219   -13.8598 H     77 ARG318   0.0000
1271 HE     -2.9506     3.3160   -14.4090 H     77 ARG318   0.0000
1272 HH11   -4.2557     5.6794   -16.8248 H     77 ARG318   0.0000
1273 HH12   -2.7995     5.5695   -17.7981 H     77 ARG318   0.0000
1274 HH21   -1.1492     3.2683   -15.7347 H     77 ARG318   0.0000
1275 HH22   -1.0844     4.2375   -17.2069 H     77 ARG318   0.0000
1276 N      -1.9060     8.2188   -10.6280 N.am  78 CYS319   0.0000
BACKBONE
1277 CA     -0.9935     8.1509    -9.4853 C.3   78 CYS319   0.0000
BACKBONE
1278 C      -1.7916     8.3230    -8.2099 C.2   78 CYS319   0.0000
BACKBONE
1279 O      -2.6112     9.2252    -8.1662 O.2   78 CYS319   0.0000
BACKBONE
1280 CB      0.1639     9.1778    -9.6489 C.3   78 CYS319   0.0000
1281 SG      1.3040     9.1757    -8.2233 S.3   78 CYS319   0.0000
1282 H      -1.8310     9.0034   -11.2436 H     78 CYS319   0.0000
1283 HA     -0.5380     7.1482    -9.4913 H     78 CYS319   0.0000
1284 HB3    -0.2213    10.1956    -9.7743 H     78 CYS319   0.0000
1285 HB2     0.7175     8.9310   -10.5656 H     78 CYS319   0.0000
1286 LPG2    1.3591     8.5595    -7.9435 LP    78 CYS319   0.0000
1287 LPG1    1.1175     9.6240    -7.7487 LP    78 CYS319   0.0000
1288 N      -1.6034     7.4684    -7.1731 N.am  79 GLU320   0.0000
BACKBONE
1289 CA     -2.4354     7.5697    -5.9710 C.3   79 GLU320   0.0000
BACKBONE
1290 C      -1.9991     8.7130    -5.0877 C.2   79 GLU320   0.0000
BACKBONE
1291 O      -2.8570     9.3232    -4.4710 O.2   79 GLU320   0.0000
BACKBONE
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1292 CB      -2.4691     6.2542    -5.1465 C.3   79 GLU320   0.0000
1293 CG      -3.2597     5.1417    -5.8893 C.3   79 GLU320   0.0000
1294 CD      -4.7256     5.4648    -6.0560 C.2   79 GLU320   0.0000
1295 OE1     -5.3019     6.1544    -5.1708 O.co2 79 GLU320  -0.5000
1296 OE2     -5.3202     5.0270    -7.0781 O.co2 79 GLU320  -0.5000
1297 H       -0.8999     6.7558    -7.2058 H     79 GLU320   0.0000
1298 HA      -3.4687     7.7772    -6.2773 H     79 GLU320   0.0000
1299 HB3     -2.9482     6.4345    -4.1696 H     79 GLU320   0.0000
1300 HB2     -1.4375     5.9233    -4.9521 H     79 GLU320   0.0000
1301 HG3     -3.2030     4.2091    -5.3117 H     79 GLU320   0.0000
1302 HG2     -2.8019     4.9613    -6.8749 H     79 GLU320   0.0000
1303 N       -0.6907     9.0332    -5.0016 N.am  80 TYR321   0.0000
BACKBONE
1304 CA      -0.2835    10.1976    -4.2149 C.3   80 TYR321   0.0000
BACKBONE
1305 C       -0.9321    11.4222    -4.8147 C.2   80 TYR321   0.0000
BACKBONE
1306 O       -1.5324    12.2106    -4.1030 O.2   80 TYR321   0.0000
BACKBONE
1307 CB       1.2580    10.3617    -4.2310 C.3   80 TYR321   0.0000
1308 CG       1.6970    11.6894    -3.6018 C.ar  80 TYR321   0.0000
1309 CD1      1.5628    11.8923    -2.2265 C.ar  80 TYR321   0.0000
1310 CD2      2.2504    12.7076    -4.3853 C.ar  80 TYR321   0.0000
1311 CE1      2.1279    13.0162    -1.6155 C.ar  80 TYR321   0.0000
1312 CE2      2.8169    13.8300    -3.7796 C.ar  80 TYR321   0.0000
1313 CZ       2.7814    13.9810    -2.3902 C.ar  80 TYR321   0.0000
1314 OH       3.3937    15.0947    -1.8076 O.3   80 TYR321   0.0000
1315 H       -0.0008     8.5120    -5.5042 H     80 TYR321   0.0000
1316 HA      -0.6261    10.0675    -3.1749 H     80 TYR321   0.0000
1317 HB2      1.6423    10.2992    -5.2608 H     80 TYR321   0.0000
1318 HB3      1.7053     9.5356    -3.6597 H     80 TYR321   0.0000
1319 HD1      1.0214    11.1701    -1.6304 H     80 TYR321   0.0000
1320 HD2      2.2445    12.6304    -5.4649 H     80 TYR321   0.0000
1321 HE1      2.0545    13.1288    -0.5392 H     80 TYR321   0.0000
1322 HE2      3.2854    14.5915    -4.3898 H     80 TYR321   0.0000
1323 HH       3.2489    15.1729    -0.8713 H     80 TYR321   0.0000
1324 N       -0.8182    11.5724    -6.1496 N.am  81 LEU322   0.0000
BACKBONE
1325 CA      -1.4569    12.6926    -6.8357 C.3   81 LEU322   0.0000
BACKBONE
1326 C       -2.9282    12.7562    -6.4955 C.2   81 LEU322   0.0000
BACKBONE
1327 O       -3.4191    13.8333    -6.1975 O.2   81 LEU322   0.0000
BACKBONE
1328 CB      -1.2836    12.4718    -8.3604 C.3   81 LEU322   0.0000
1329 CG      -1.9934    13.4958    -9.2797 C.3   81 LEU322   0.0000
1330 CD1     -1.3651    14.9035    -9.1598 C.3   81 LEU322   0.0000
1331 CD2     -1.8893    12.9859   -10.7405 C.3   81 LEU322   0.0000
1332 H       -0.2945    10.9087    -6.6836 H     81 LEU322   0.0000
1333 HA      -0.9579    13.6190    -6.5182 H     81 LEU322   0.0000
1334 HB3     -1.7278    11.4931    -8.5795 H     81 LEU322   0.0000
1335 HB2     -0.2095    12.4375    -8.6089 H     81 LEU322   0.0000
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1336 HG      -3.0551    13.5736    -9.0029 H     81 LEU322   0.0000
1337 HD13    -1.4932    15.2983    -8.1432 H     81 LEU322   0.0000
1338 HD12    -1.8259    15.6088    -9.8689 H     81 LEU322   0.0000
1339 HD11    -0.2943    14.8217    -9.3818 H     81 LEU322   0.0000
1340 HD23    -0.8441    12.9949   -11.0878 H     81 LEU322   0.0000
1341 HD22    -2.4873    13.6479   -11.3711 H     81 LEU322   0.0000
1342 HD21    -2.2843    11.9647   -10.8514 H     81 LEU322   0.0000
1343 N       -3.6494    11.6127    -6.5349 N.am  82 ILE323   0.0000
BACKBONE
1344 CA      -5.0694    11.6336    -6.1841 C.3   82 ILE323   0.0000
BACKBONE
1345 C       -5.1939    12.1018    -4.7524 C.2   82 ILE323   0.0000
BACKBONE
1346 O       -6.0155    12.9616    -4.4772 O.2   82 ILE323   0.0000
BACKBONE
1347 CB      -5.7477    10.2417    -6.3885 C.3   82 ILE323   0.0000
1348 CG1     -5.8648     9.9207    -7.9117 C.3   82 ILE323   0.0000
1349 CG2     -7.1399    10.2080    -5.6937 C.3   82 ILE323   0.0000
1350 CD1     -6.0565     8.4162    -8.2458 C.3   82 ILE323   0.0000
1351 H       -3.2159    10.7406    -6.7680 H     82 ILE323   0.0000
1352 HA      -5.5899    12.3609    -6.8284 H     82 ILE323   0.0000
1353 HB      -5.1234     9.4763    -5.9042 H     82 ILE323   0.0000
1354 HG13    -4.9556    10.2433    -8.4414 H     82 ILE323   0.0000
1355 HG12    -6.7107    10.4921    -8.3212 H     82 ILE323   0.0000
1356 HG23    -7.0348    10.2764    -4.5999 H     82 ILE323   0.0000
1357 HG22    -7.6802     9.2765    -5.9123 H     82 ILE323   0.0000
1358 HG21    -7.7516    11.0562    -6.0349 H     82 ILE323   0.0000
1359 HD13    -5.1650     7.8398    -7.9620 H     82 ILE323   0.0000
1360 HD12    -6.2045     8.2950    -9.3311 H     82 ILE323   0.0000
1361 HD11    -6.9252     7.9853    -7.7304 H     82 ILE323   0.0000
1362 N       -4.3913    11.5442    -3.8210 N.am  83 ARG324   0.0000
BACKBONE
1363 CA      -4.5441    11.9070    -2.4153 C.3   83 ARG324   0.0000
BACKBONE
1364 C       -4.3907    13.3974    -2.2138 C.2   83 ARG324   0.0000
BACKBONE
1365 O       -5.1596    13.9597    -1.4496 O.2   83 ARG324   0.0000
BACKBONE
1366 CB      -3.5398    11.1333    -1.5126 C.3   83 ARG324   0.0000
1367 CG      -3.7228    11.4895    -0.0111 C.3   83 ARG324   0.0000
1368 CD      -3.0216    10.4691     0.9276 C.3   83 ARG324   0.0000
1369 NE      -1.5846    10.3134     0.6748 N.pl3 83 ARG324   0.0000
1370 CZ      -0.6518    11.1062     1.1638 C.cat 83 ARG324   1.0000
1371 NH1     -0.9127    12.1941     1.8528 N.pl3 83 ARG324   0.0000
1372 NH2      0.6087    10.7930     0.9600 N.pl3 83 ARG324   0.0000
1373 H       -3.7102    10.8583    -4.0731 H     83 ARG324   0.0000
1374 HA      -5.5648    11.6112    -2.1178 H     83 ARG324   0.0000
1375 HB3     -2.5040    11.3584    -1.8122 H     83 ARG324   0.0000
1376 HB2     -3.7129    10.0548    -1.6609 H     83 ARG324   0.0000
1377 HG3     -4.7973    11.4881     0.2368 H     83 ARG324   0.0000
1378 HG2     -3.3397    12.5050     0.1668 H     83 ARG324   0.0000
1379 HD3     -3.5026     9.4907     0.7544 H     83 ARG324   0.0000
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1380 HD2 -3.2211 10.7006 1.9857 H 83 ARG324 0.0000
1381 HE -1.2978 9.4878 0.1223 H 83 ARG324 0.0000
1382 HH11 -1.8733 12.5019 2.0390 H 83 ARG324 0.0000
1383 HH12 -0.1497 12.7800 2.2244 H 83 ARG324 0.0000
1384 HH21 0.8715 9.9368 0.4484 H 83 ARG324 0.0000
1385 HH22 1.3716 11.3849 1.3223 H 83 ARG324 0.0000
1386 N -3.4089 14.0527 -2.8749 N.am 84 ILE325 0.0000
BACKBONE
1387 CA -3.1682 15.4729 -2.6175 C.3 84 ILE325 0.0000
BACKBONE
1388 C -4.0544 16.3376 -3.4915 C.2 84 ILE325 0.0000
BACKBONE
1389 O -4.7765 17.1639 -2.9554 O.2 84 ILE325 0.0000
BACKBONE
1390 CB -1.6617 15.8347 -2.7952 C.3 84 ILE325 0.0000
1391 CG1 -0.7155 14.9339 -1.9359 C.3 84 ILE325 0.0000
1392 CG2 -1.4240 17.3470 -2.5170 C.3 84 ILE325 0.0000
1393 CD1 -0.9411 14.9886 -0.4018 C.3 84 ILE325 0.0000
1394 H -2.8388 13.5802 -3.5492 H 84 ILE325 0.0000
1395 HA -3.4203 15.7079 -1.5712 H 84 ILE325 0.0000
1396 HB -1.3909 15.6554 -3.8507 H 84 ILE325 0.0000
1397 HG13 0.3247 15.2421 -2.1196 H 84 ILE325 0.0000
1398 HG12 -0.8018 13.8829 -2.2518 H 84 ILE325 0.0000
1399 HG23 -1.9347 17.9641 -3.2720 H 84 ILE325 0.0000
1400 HG22 -0.3514 17.5860 -2.5560 H 84 ILE325 0.0000
1401 HG21 -1.8068 17.6344 -1.5270 H 84 ILE325 0.0000
1402 HD13 -0.8343 16.0139 -0.0195 H 84 ILE325 0.0000
1403 HD12 -0.1884 14.3606 0.0997 H 84 ILE325 0.0000
1404 HD11 -1.9325 14.6036 -0.1264 H 84 ILE325 0.0000
1405 N -4.0059 16.1854 -4.8351 N.am 85 LYS326 0.0000
BACKBONE
1406 CA -4.7340 17.0999 -5.7205 C.3 85 LYS326 0.0000
BACKBONE
1407 C -6.1785 16.6955 -5.9378 C.2 85 LYS326 0.0000
BACKBONE
1408 O -6.9819 17.5798 -6.1919 O.2 85 LYS326 0.0000
BACKBONE
1409 CB -3.9964 17.2384 -7.0815 C.3 85 LYS326 0.0000
1410 CG -2.5415 17.7841 -6.9562 C.3 85 LYS326 0.0000
1411 CD -2.4078 19.2256 -6.3808 C.3 85 LYS326 0.0000
1412 CE -3.0782 20.3138 -7.2647 C.3 85 LYS326 0.0000
1413 NZ -2.8125 21.6726 -6.7372 N.4 85 LYS326 1.0000
1414 H -3.4608 15.4523 -5.2433 H 85 LYS326 0.0000
1415 HA -4.7751 18.1008 -5.2636 H 85 LYS326 0.0000
1416 HB3 -4.5730 17.9040 -7.7351 H 85 LYS326 0.0000
1417 HB2 -3.9730 16.2479 -7.5655 H 85 LYS326 0.0000
1418 HG3 -2.0834 17.7787 -7.9593 H 85 LYS326 0.0000
1419 HG2 -1.9552 17.1034 -6.3179 H 85 LYS326 0.0000
1420 HD3 -1.3359 19.4659 -6.3165 H 85 LYS326 0.0000
1421 HD2 -2.8030 19.2831 -5.3564 H 85 LYS326 0.0000
1422 HE3 -4.1692 20.1628 -7.2996 H 85 LYS326 0.0000
1423 HE2 -2.6857 20.2382 -8.2926 H 85 LYS326 0.0000

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1424 HZ3     -3.2111    21.7970    -5.7391 H     85 LYS326   0.0000
1425 HZ2     -3.2696    22.4321    -7.3580 H     85 LYS326   0.0000
1426 HZ1     -1.7546    21.8946    -6.6969 H     85 LYS326   0.0000
1427 N       -6.5508    15.3974    -5.8467 N.am  86 GLY327   0.0000
BACKBONE
1428 CA      -7.9560    15.0144    -6.0130 C.3   86 GLY327   0.0000
BACKBONE
1429 C       -8.2719    14.7624    -7.4666 C.2   86 GLY327   0.0000
BACKBONE
1430 O       -7.6094    15.3390    -8.3125 O.2   86 GLY327   0.0000
BACKBONE
1431 H       -5.8770    14.6756    -5.6829 H     86 GLY327   0.0000
1432 HA2     -8.6370    15.7936    -5.6368 H     86 GLY327   0.0000
1433 HA3     -8.1547    14.1003    -5.4310 H     86 GLY327   0.0000
1434 N       -9.2803    13.9141    -7.7805 N.am  87 GLN328   0.0000
BACKBONE
1435 CA      -9.5430    13.5699    -9.1779 C.3   87 GLN328   0.0000
BACKBONE
1436 C      -10.1190    14.7236    -9.9672 C.2   87 GLN328   0.0000
BACKBONE
1437 O       -9.9068    14.7335   -11.1684 O.2   87 GLN328   0.0000
BACKBONE
1438 CB     -10.4813    12.3416    -9.3272 C.3   87 GLN328   0.0000
1439 CG      -9.7941    11.0278    -8.8671 C.3   87 GLN328   0.0000
1440 CD     -10.7022     9.8235    -8.9535 C.2   87 GLN328   0.0000
1441 OE1    -11.9091     9.9816    -9.0604 O.2   87 GLN328   0.0000
1442 NE2    -10.1413     8.5952    -8.9012 N.am  87 GLN328   0.0000
1443 H       -9.8520    13.5061    -7.0661 H     87 GLN328   0.0000
1444 HA      -8.5808    13.3038    -9.6435 H     87 GLN328   0.0000
1445 HB3    -10.7415    12.2198   -10.3908 H     87 GLN328   0.0000
1446 HB2    -11.4065    12.5231    -8.7574 H     87 GLN328   0.0000
1447 HG3     -9.4649    11.1250    -7.8229 H     87 GLN328   0.0000
1448 HG2     -8.9098    10.8506    -9.4997 H     87 GLN328   0.0000
1449 HE21    -9.1509     8.4819    -8.8174 H     87 GLN328   0.0000
1450 HE22   -10.7191     7.7793    -8.9498 H     87 GLN328   0.0000
1451 N      -10.8351    15.7031    -9.3703 N.am  88 GLU329   0.0000
BACKBONE
1452 CA     -11.3124    16.8278   -10.1792 C.3   88 GLU329   0.0000
BACKBONE
1453 C      -10.1187    17.5138   -10.8107 C.2   88 GLU329   0.0000
BACKBONE
1454 O      -10.1317    17.7412   -12.0097 O.2   88 GLU329   0.0000
BACKBONE
1455 CB     -12.1305    17.8713    -9.3682 C.3   88 GLU329   0.0000
1456 CG     -13.5248    17.3265    -8.9547 C.3   88 GLU329   0.0000
1457 CD     -14.3367    18.3230    -8.1650 C.2   88 GLU329   0.0000
1458 OE1    -13.7915    19.3911    -7.7751 O.co2 88 GLU329  -0.5000
1459 OE2    -15.5427    18.0404    -7.9271 O.co2 88 GLU329  -0.5000
1460 H      -11.0199    15.6865    -8.3868 H     88 GLU329   0.0000
1461 HA     -11.9571    16.4328   -10.9828 H     88 GLU329   0.0000
1462 HB3    -12.2863    18.7677    -9.9917 H     88 GLU329   0.0000
1463 HB2    -11.5598    18.1687    -8.4739 H     88 GLU329   0.0000
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1464 HG3    -13.4113    16.4154     -8.3475 H     88 GLU329   0.0000
1465 HG2    -14.0964    17.0744     -9.8621 H     88 GLU329   0.0000
1466 N       -9.0715    17.8407    -10.0193 N.am  89 PHE330   0.0000
BACKBONE
1467 CA      -7.8724    18.4560    -10.5944 C.3   89 PHE330   0.0000
BACKBONE
1468 C       -7.3050    17.6197    -11.7185 C.2   89 PHE330   0.0000
BACKBONE
1469 O       -6.8003    18.1760    -12.6803 O.2   89 PHE330   0.0000
BACKBONE
1470 CB      -6.7501    18.5693     -9.5290 C.3   89 PHE330   0.0000
1471 CG      -5.4457    19.0985    -10.1476 C.ar  89 PHE330   0.0000
1472 CD1     -5.2852    20.4708    -10.3659 C.ar  89 PHE330   0.0000
1473 CD2     -4.4072    18.2241    -10.4941 C.ar  89 PHE330   0.0000
1474 CE1     -4.0859    20.9695    -10.8846 C.ar  89 PHE330   0.0000
1475 CE2     -3.2008    18.7223    -10.9937 C.ar  89 PHE330   0.0000
1476 CZ      -3.0366    20.0959    -11.1860 C.ar  89 PHE330   0.0000
1477 H       -9.0993    17.6549     -9.0348 H     89 PHE330   0.0000
1478 HA      -8.1283    19.4617    -10.9676 H     89 PHE330   0.0000
1479 HB3     -6.5765    17.5739     -9.0941 H     89 PHE330   0.0000
1480 HB2     -7.0694    19.2386     -8.7144 H     89 PHE330   0.0000
1481 HD1     -6.0934    21.1561    -10.1321 H     89 PHE330   0.0000
1482 HD2     -4.5310    17.1520    -10.3751 H     89 PHE330   0.0000
1483 HE1     -3.9691    22.0353    -11.0512 H     89 PHE330   0.0000
1484 HE2     -2.3876    18.0436    -11.2324 H     89 PHE330   0.0000
1485 HZ      -2.0971    20.4841    -11.5667 H     89 PHE330   0.0000
1486 N       -7.3561    16.2757    -11.6066 N.am  90 ILE331   0.0000
BACKBONE
1487 CA      -6.7398    15.4361    -12.6306 C.3   90 ILE331   0.0000
BACKBONE
1488 C       -7.6109    15.4977    -13.8605 C.2   90 ILE331   0.0000
BACKBONE
1489 O       -7.0931    15.7656    -14.9321 O.2   90 ILE331   0.0000
BACKBONE
1490 CB      -6.5522    13.9683    -12.1507 C.3   90 ILE331   0.0000
1491 CG1     -5.6631    13.9384    -10.8715 C.3   90 ILE331   0.0000
1492 CG2     -5.9456    13.0922    -13.2806 C.3   90 ILE331   0.0000
1493 CD1     -5.5112    12.5154    -10.2783 C.3   90 ILE331   0.0000
1494 H       -7.8320    15.8461    -10.8402 H     90 ILE331   0.0000
1495 HA      -5.7401    15.8376    -12.8695 H     90 ILE331   0.0000
1496 HB      -7.5440    13.5548    -11.9068 H     90 ILE331   0.0000
1497 HG13    -6.1038    14.5615    -10.0844 H     90 ILE331   0.0000
1498 HG12    -4.6783    14.3709    -11.0949 H     90 ILE331   0.0000
1499 HG23    -6.5533    13.1382    -14.1967 H     90 ILE331   0.0000
1500 HG22    -5.9096    12.0408    -12.9664 H     90 ILE331   0.0000
1501 HG21    -4.9263    13.4277    -13.5179 H     90 ILE331   0.0000
1502 HD13    -6.4755    11.9874    -10.2850 H     90 ILE331   0.0000
1503 HD12    -5.1605    12.5751     -9.2396 H     90 ILE331   0.0000
1504 HD11    -4.7798    11.9310    -10.8500 H     90 ILE331   0.0000
1505 N       -8.9346    15.2576    -13.7221 N.am  91 ARG332   0.0000
BACKBONE
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1506 CA      -9.8243    15.3449   -14.8759 C.3   91 ARG332   0.0000
BACKBONE
1507 C       -9.6152    16.6781   -15.5611 C.2   91 ARG332   0.0000
BACKBONE
1508 O       -9.5444    16.7082   -16.7796 O.2   91 ARG332   0.0000
BACKBONE
1509 CB     -11.3235    15.1939   -14.4842 C.3   91 ARG332   0.0000
1510 CG     -11.7147    13.7237   -14.1505 C.3   91 ARG332   0.0000
1511 CD     -13.2324    13.5817   -13.8401 C.3   91 ARG332   0.0000
1512 NE     -13.5475    13.9840   -12.4646 N.pl3 91 ARG332   0.0000
1513 CZ     -13.5053    13.1739   -11.4240 C.cat 91 ARG332   1.0000
1514 NH1    -13.0887    11.9284   -11.4838 N.pl3 91 ARG332   0.0000
1515 NH2    -13.9039    13.6302   -10.2575 N.pl3 91 ARG332   0.0000
1516 H       -9.3260    15.0336   -12.8317 H     91 ARG332   0.0000
1517 HA      -9.5567    14.5409   -15.5805 H     91 ARG332   0.0000
1518 HB3    -11.9281    15.5217   -15.3462 H     91 ARG332   0.0000
1519 HB2    -11.5587    15.8536   -13.6340 H     91 ARG332   0.0000
1520 HG3    -11.1283    13.3458   -13.2985 H     91 ARG332   0.0000
1521 HG2    -11.4808    13.0989   -15.0285 H     91 ARG332   0.0000
1522 HD3    -13.6025    12.5696   -14.0640 H     91 ARG332   0.0000
1523 HD2    -13.7935    14.2312   -14.5323 H     91 ARG332   0.0000
1524 HE     -13.8763    14.9547   -12.3307 H     91 ARG332   0.0000
1525 HH11   -12.7225    11.5171   -12.3495 H     91 ARG332   0.0000
1526 HH12   -13.1016    11.3256   -10.6465 H     91 ARG332   0.0000
1527 HH21   -14.2476    14.5948   -10.1514 H     91 ARG332   0.0000
1528 HH22   -13.8924    13.0336    -9.4164 H     91 ARG332   0.0000
1529 N       -9.5063    17.7866   -14.7929 N.am  92 GLN333   0.0000
BACKBONE
1530 CA      -9.2845    19.0926   -15.4116 C.3   92 GLN333   0.0000
BACKBONE
1531 C       -8.0680    19.0271   -16.3106 C.2   92 GLN333   0.0000
BACKBONE
1532 O       -8.1671    19.4094   -17.4662 O.2   92 GLN333   0.0000
BACKBONE
1533 CB      -9.0610    20.2014   -14.3434 C.3   92 GLN333   0.0000
1534 CG      -8.8873    21.6161   -14.9656 C.3   92 GLN333   0.0000
1535 CD      -8.0778    22.4919   -14.0378 C.2   92 GLN333   0.0000
1536 OE1     -8.6395    23.3586   -13.3857 O.2   92 GLN333   0.0000
1537 NE2     -6.7449    22.2730   -13.9606 N.am  92 GLN333   0.0000
1538 H       -9.5807    17.7296   -13.7966 H     92 GLN333   0.0000
1539 HA     -10.1801    19.3541   -16.0000 H     92 GLN333   0.0000
1540 HB3     -8.1630    19.9449   -13.7650 H     92 GLN333   0.0000
1541 HB2     -9.9077    20.2220   -13.6372 H     92 GLN333   0.0000
1542 HG3     -9.8751    22.0605   -15.1699 H     92 GLN333   0.0000
1543 HG2     -8.3445    21.5754   -15.9214 H     92 GLN333   0.0000
1544 HE21    -6.3033    21.5609   -14.5093 H     92 GLN333   0.0000
1545 HE22    -6.1805    22.8297   -13.3498 H     92 GLN333   0.0000
1546 N       -6.9082    18.5539   -15.7973 N.am  93 VAL334   0.0000
BACKBONE
1547 CA      -5.6962    18.5502   -16.6172 C.3   93 VAL334   0.0000
BACKBONE
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1548 C       -5.9142    17.6358   -17.8012 C.2   93 VAL334   0.0000
BACKBONE
1549 O       -5.6480    18.0405   -18.9223 O.2   93 VAL334   0.0000
BACKBONE
1550 CB      -4.4262    18.1292   -15.8164 C.3   93 VAL334   0.0000
1551 CG1     -3.2212    17.8949   -16.7734 C.3   93 VAL334   0.0000
1552 CG2     -4.0712    19.2057   -14.7498 C.3   93 VAL334   0.0000
1553 H       -6.8689    18.1918   -14.8643 H     93 VAL334   0.0000
1554 HA      -5.5304    19.5739   -16.9933 H     93 VAL334   0.0000
1555 HB      -4.6340    17.1791   -15.2960 H     93 VAL334   0.0000
1556 HG13    -3.3988    17.0246   -17.4237 H     93 VAL334   0.0000
1557 HG12    -2.2975    17.7026   -16.2089 H     93 VAL334   0.0000
1558 HG11    -3.0628    18.7781   -17.4101 H     93 VAL334   0.0000
1559 HG23    -3.8286    20.1635   -15.2342 H     93 VAL334   0.0000
1560 HG22    -3.2036    18.8884   -14.1548 H     93 VAL334   0.0000
1561 HG21    -4.9057    19.3740   -14.0545 H     93 VAL334   0.0000
1562 N       -6.4016    16.3973   -17.5681 N.am  94 GLN335   0.0000
BACKBONE
1563 CA      -6.6556    15.4818   -18.6797 C.3   94 GLN335   0.0000
BACKBONE
1564 C       -7.7356    16.0463   -19.5670 C.2   94 GLN335   0.0000
BACKBONE
1565 O       -8.3567    17.0505   -19.2588 O.2   94 GLN335   0.0000
BACKBONE
1566 CB      -7.0989    14.0746   -18.1896 C.3   94 GLN335   0.0000
1567 CG      -5.9414    13.3052   -17.4931 C.3   94 GLN335   0.0000
1568 CD      -4.8731    12.8758   -18.4753 C.2   94 GLN335   0.0000
1569 OE1     -5.2173    12.4457   -19.5664 O.2   94 GLN335   0.0000
1570 NE2     -3.5693    12.9606   -18.1323 N.am  94 GLN335   0.0000
1571 H       -6.6214    16.1067   -16.6381 H     94 GLN335   0.0000
1572 HA      -5.7449    15.3771   -19.2913 H     94 GLN335   0.0000
1573 HB3     -7.4705    13.4801   -19.0404 H     94 GLN335   0.0000
1574 HB2     -7.9373    14.2003   -17.4862 H     94 GLN335   0.0000
1575 HG3     -6.3478    12.3872   -17.0391 H     94 GLN335   0.0000
1576 HG2     -5.5198    13.9215   -16.6841 H     94 GLN335   0.0000
1577 HE21    -3.2848    13.3159   -17.2429 H     94 GLN335   0.0000
1578 HE22    -2.8652    12.6631   -18.7789 H     94 GLN335   0.0000
@<TRIPOS>BOND
   1    1    2  1   BACKBONE
   2    1    7  1
   3    1   12  1
   4    2    3  1   BACKBONE
   5    2    5  1
   6    2    8  1
   7    3    4  2   BACKBONE
   8    3   13  am  BACKBONE|INTERRES
   9    5    6  1
  10    5    9  1
  11    5   10  1
  12    6   11  1
  13   13   14  1   BACKBONE
  14   13   21  1
```

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15   14   15  1   BACKBONE
16   14   17  1
17   14   22  1
18   15   16  2   BACKBONE
19   15   32  am  BACKBONE|INTERRES
20   17   18  1
21   17   23  1
22   17   24  1
23   18   19  1
24   18   25  1
25   18   26  1
26   19   20  1
27   19   27  1
28   19   28  1
29   20   29  1
30   20   30  1
31   20   31  1
32   32   33  1   BACKBONE
33   32   43  1
34   33   34  1   BACKBONE
35   33   36  1
36   33   44  1
37   34   35  2   BACKBONE
38   34   56  am  BACKBONE|INTERRES
39   36   37  1
40   36   45  1
41   36   46  1
42   37   38  1
43   37   47  1
44   37   48  1
45   38   39  1
46   38   49  1
47   38   50  1
48   39   40  ar
49   39   51  1
50   40   41  ar
51   40   42  ar
52   41   52  1
53   41   53  1
54   42   54  1
55   42   55  1
56   56   57  1   BACKBONE
57   56   68  1
58   57   58  1   BACKBONE
59   57   60  1
60   57   69  1
61   58   59  2   BACKBONE
62   58   77  am  BACKBONE|INTERRES
63   60   61  1
64   60   70  1
65   60   71  1
66   61   62  ar
```

67	61	63	ar	
68	62	64	ar	
69	62	72	1	
70	63	65	ar	
71	63	73	1	
72	64	66	ar	
73	64	74	1	
74	65	66	ar	
75	65	75	1	
76	66	67	1	
77	67	76	1	
78	77	78	1	BACKBONE
79	77	84	1	
80	78	79	1	BACKBONE
81	78	81	1	
82	78	85	1	
83	79	80	2	BACKBONE
84	79	91	am	BACKBONE|INTERRES
85	81	82	1	
86	81	83	1	
87	81	86	1	
88	82	87	1	
89	83	88	1	
90	83	89	1	
91	83	90	1	
92	91	92	1	BACKBONE
93	91	98	1	
94	92	93	1	BACKBONE
95	92	95	1	
96	92	99	1	
97	93	94	2	BACKBONE
98	93	107	am	BACKBONE|INTERRES
99	95	96	1	
100	95	97	1	
101	95	100	1	
102	96	101	1	
103	96	102	1	
104	96	103	1	
105	97	104	1	
106	97	105	1	
107	97	106	1	
108	107	108	1	BACKBONE
109	107	113	1	
110	108	109	1	BACKBONE
111	108	111	1	
112	108	114	1	
113	109	110	2	BACKBONE
114	109	118	am	BACKBONE|INTERRES
115	111	112	1	
116	111	115	1	
117	111	116	1	
118	112	117	1	

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119  118  119  1   BACKBONE
120  118  126  1
121  119  120  1   BACKBONE
122  119  122  1
123  119  127  1
124  120  121  2   BACKBONE
125  120  132  am  BACKBONE|INTERRES
126  122  123  1
127  122  128  1
128  122  129  1
129  123  124  2
130  123  125  am
131  125  130  1
132  125  131  1
133  132  133  1   BACKBONE
134  132  140  1
135  133  134  1   BACKBONE
136  133  136  1
137  133  141  1
138  134  135  2   BACKBONE
139  134  151  am  BACKBONE|INTERRES
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141  136  142  1
142  136  143  1
143  137  138  1
144  137  139  1
145  137  144  1
146  138  145  1
147  138  146  1
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149  139  148  1
150  139  149  1
151  139  150  1
152  151  152  1   BACKBONE
153  151  157  1
154  152  153  1   BACKBONE
155  152  155  1
156  152  158  1
157  153  154  2   BACKBONE
158  153  162  am  BACKBONE|INTERRES
159  155  156  1
160  155  159  1
161  155  160  1
162  156  161  1
163  162  163  1   BACKBONE
164  162  170  1
165  163  164  1   BACKBONE
166  163  166  1
167  163  171  1
168  164  165  2   BACKBONE
169  164  181  am  BACKBONE|INTERRES
170  166  167  1
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171  166  172  1
172  166  173  1
173  167  168  1
174  167  174  1
175  167  175  1
176  168  169  1
177  168  176  1
178  168  177  1
179  169  178  1
180  169  179  1
181  169  180  1
182  181  182  1   BACKBONE
183  181  190  1
184  182  183  1   BACKBONE
185  182  185  1
186  182  191  1
187  183  184  2   BACKBONE
188  183  198  am  BACKBONE|INTERRES
189  185  186  1
190  185  192  1
191  185  193  1
192  186  187  1
193  186  194  1
194  186  195  1
195  187  188  2
196  187  189  am
197  189  196  1
198  189  197  1
199  198  199  1   BACKBONE
200  198  205  1
201  199  200  1   BACKBONE
202  199  202  1
203  199  206  1
204  200  201  2   BACKBONE
205  200  212  am  BACKBONE|INTERRES
206  202  203  1
207  202  204  1
208  202  207  1
209  203  208  1
210  204  209  1
211  204  210  1
212  204  211  1
213  212  213  1   BACKBONE
214  212  222  1
215  213  214  1   BACKBONE
216  213  216  1
217  213  223  1
218  214  215  2   BACKBONE
219  214  229  am  BACKBONE|INTERRES
220  216  217  1
221  216  224  1
222  216  225  1
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223  217  218  1
224  217  219  2
225  218  220  1
226  218  226  1
227  219  221  1
228  219  227  1
229  220  221  2
230  220  228  1
231  229  230  1   BACKBONE
232  229  234  1
233  230  231  1   BACKBONE
234  230  233  1
235  230  235  1
236  231  232  2   BACKBONE
237  231  239  am  BACKBONE|INTERRES
238  233  236  1
239  233  237  1
240  233  238  1
241  239  240  1   BACKBONE
242  239  244  1
243  240  241  1   BACKBONE
244  240  243  1
245  240  245  1
246  241  242  2   BACKBONE
247  241  249  am  BACKBONE|INTERRES
248  243  246  1
249  243  247  1
250  243  248  1
251  249  250  1   BACKBONE
252  249  260  1
253  250  251  1   BACKBONE
254  250  253  1
255  250  261  1
256  251  252  2   BACKBONE
257  251  273  am  BACKBONE|INTERRES
258  253  254  1
259  253  262  1
260  253  263  1
261  254  255  1
262  254  264  1
263  254  265  1
264  255  256  1
265  255  266  1
266  255  267  1
267  256  257  ar
268  256  268  1
269  257  258  ar
270  257  259  ar
271  258  269  1
272  258  270  1
273  259  271  1
274  259  272  1
```

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275  273  274  1   BACKBONE
276  273  284  1
277  274  275  1   BACKBONE
278  274  277  1
279  274  285  1
280  275  276  2   BACKBONE
281  275  293  am  BACKBONE|INTERRES
282  277  278  1
283  277  286  1
284  277  287  1
285  278  279  ar
286  278  280  ar
287  279  281  ar
288  279  288  1
289  280  282  ar
290  280  289  1
291  281  283  ar
292  281  290  1
293  282  283  ar
294  282  291  1
295  283  292  1
296  293  294  1   BACKBONE
297  293  302  1
298  294  295  1   BACKBONE
299  294  297  1
300  294  303  1
301  295  296  2   BACKBONE
302  295  315  am  BACKBONE|INTERRES
303  297  298  1
304  297  304  1
305  297  305  1
306  298  299  1
307  298  306  1
308  298  307  1
309  299  300  1
310  299  308  1
311  299  309  1
312  300  301  1
313  300  310  1
314  300  311  1
315  301  312  1
316  301  313  1
317  301  314  1
318  315  316  1   BACKBONE
319  315  322  1
320  316  317  1   BACKBONE
321  316  319  1
322  316  323  1
323  317  318  2   BACKBONE
324  317  329  am  BACKBONE|INTERRES
325  319  320  1
326  319  321  1
```

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327  319  324  1
328  320  325  1
329  321  326  1
330  321  327  1
331  321  328  1
332  329  330  1   BACKBONE
333  329  340  1
334  330  331  1   BACKBONE
335  330  333  1
336  330  341  1
337  331  332  2   BACKBONE
338  331  349  am  BACKBONE|INTERRES
339  333  334  1
340  333  342  1
341  333  343  1
342  334  335  ar
343  334  336  ar
344  335  337  ar
345  335  344  1
346  336  338  ar
347  336  345  1
348  337  339  ar
349  337  346  1
350  338  339  ar
351  338  347  1
352  339  348  1
353  349  350  1   BACKBONE
354  349  360  1
355  350  351  1   BACKBONE
356  350  353  1
357  350  361  1
358  351  352  2   BACKBONE
359  351  369  am  BACKBONE|INTERRES
360  353  354  1
361  353  362  1
362  353  363  1
363  354  355  ar
364  354  356  ar
365  355  357  ar
366  355  364  1
367  356  358  ar
368  356  365  1
369  357  359  ar
370  357  366  1
371  358  359  ar
372  358  367  1
373  359  368  1
374  369  370  1   BACKBONE
375  369  377  1
376  370  371  1   BACKBONE
377  370  373  1
378  370  378  1
```

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379  371  372  2   BACKBONE
380  371  383  am  BACKBONE|INTERRES
381  373  374  1
382  373  379  1
383  373  380  1
384  374  375  2
385  374  376  am
386  376  381  1
387  376  382  1
388  383  384  1   BACKBONE
389  383  397  1
390  384  385  1   BACKBONE
391  384  387  1
392  384  398  1
393  385  386  2   BACKBONE
394  385  407  am  BACKBONE|INTERRES
395  387  388  1
396  387  399  1
397  387  400  1
398  388  389  2
399  388  390  1
400  389  391  1
401  389  401  1
402  390  392  ar
403  390  393  ar
404  391  392  1
405  391  402  1
406  392  394  ar
407  393  395  ar
408  393  403  1
409  394  396  ar
410  394  404  1
411  395  396  ar
412  395  405  1
413  396  406  1
414  407  408  1   BACKBONE
415  407  413  1
416  408  409  1   BACKBONE
417  408  411  1
418  408  414  1
419  409  410  2   BACKBONE
420  409  421  am  BACKBONE|INTERRES
421  411  412  1
422  411  415  1
423  411  416  1
424  412  413  1
425  412  417  1
426  412  418  1
427  413  419  1
428  413  420  1
429  421  422  1   BACKBONE
430  421  427  1
```

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431  422  423  1   BACKBONE
432  422  425  1
433  422  428  1
434  423  424  2   BACKBONE
435  423  432  am  BACKBONE|INTERRES
436  425  426  1
437  425  429  1
438  425  430  1
439  426  431  1
440  432  433  1   BACKBONE
441  432  438  1
442  433  434  1   BACKBONE
443  433  436  1
444  433  439  1
445  434  435  2   BACKBONE
446  434  443  am  BACKBONE|INTERRES
447  436  437  1
448  436  440  1
449  436  441  1
450  437  442  1
451  443  444  1   BACKBONE
452  443  450  1
453  444  445  1   BACKBONE
454  444  447  1
455  444  451  1
456  445  446  2   BACKBONE
457  445  459  am  BACKBONE|INTERRES
458  447  448  1
459  447  449  1
460  447  452  1
461  448  453  1
462  448  454  1
463  448  455  1
464  449  456  1
465  449  457  1
466  449  458  1
467  459  460  1   BACKBONE
468  459  467  1
469  460  461  1   BACKBONE
470  460  463  1
471  460  468  1
472  461  462  2   BACKBONE
473  461  478  am  BACKBONE|INTERRES
474  463  464  1
475  463  469  1
476  463  470  1
477  464  465  1
478  464  466  1
479  464  471  1
480  465  472  1
481  465  473  1
482  465  474  1
```

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483  466  475  1
484  466  476  1
485  466  477  1
486  478  479  1   BACKBONE
487  478  485  1
488  479  480  1   BACKBONE
489  479  482  1
490  479  486  1
491  480  481  2   BACKBONE
492  480  494  am  BACKBONE|INTERRES
493  482  483  1
494  482  484  1
495  482  487  1
496  483  488  1
497  483  489  1
498  483  490  1
499  484  491  1
500  484  492  1
501  484  493  1
502  494  495  1   BACKBONE
503  494  502  1
504  495  496  1   BACKBONE
505  495  498  1
506  495  503  1
507  496  497  2   BACKBONE
508  496  508  am  BACKBONE|INTERRES
509  498  499  1
510  498  504  1
511  498  505  1
512  499  500  2
513  499  501  am
514  501  506  1
515  501  507  1
516  508  509  1   BACKBONE
517  508  514  1
518  509  510  1   BACKBONE
519  509  512  1
520  509  515  1
521  510  511  2   BACKBONE
522  510  522  am  BACKBONE|INTERRES
523  512  513  1
524  512  516  1
525  512  517  1
526  513  514  1
527  513  518  1
528  513  519  1
529  514  520  1
530  514  521  1
531  522  523  1   BACKBONE
532  522  531  1
533  523  524  1   BACKBONE
534  523  526  1
```

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535  523  532  1
536  524  525  2   BACKBONE
537  524  537  am  BACKBONE|INTERRES
538  526  527  1
539  526  533  1
540  526  534  1
541  527  528  1
542  527  535  1
543  527  536  1
544  528  529  ar
545  528  530  ar
546  537  538  1   BACKBONE
547  537  546  1
548  538  539  1   BACKBONE
549  538  541  1
550  538  547  1
551  539  540  2   BACKBONE
552  539  554  am  BACKBONE|INTERRES
553  541  542  1
554  541  548  1
555  541  549  1
556  542  543  1
557  542  550  1
558  542  551  1
559  543  544  2
560  543  545  am
561  545  552  1
562  545  553  1
563  554  555  1   BACKBONE
564  554  562  1
565  555  556  1   BACKBONE
566  555  558  1
567  555  563  1
568  556  557  2   BACKBONE
569  556  573  am  BACKBONE|INTERRES
570  558  559  1
571  558  564  1
572  558  565  1
573  559  560  1
574  559  561  1
575  559  566  1
576  560  567  1
577  560  568  1
578  560  569  1
579  561  570  1
580  561  571  1
581  561  572  1
582  573  574  1   BACKBONE
583  573  578  1
584  574  575  1   BACKBONE
585  574  577  1
586  574  579  1
```

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587  575  576  2   BACKBONE
588  575  583  am  BACKBONE|INTERRES
589  577  580  1
590  577  581  1
591  577  582  1
592  583  584  1   BACKBONE
593  583  589  1
594  584  585  1   BACKBONE
595  584  587  1
596  584  590  1
597  585  586  2   BACKBONE
598  585  594  am  BACKBONE|INTERRES
599  587  588  1
600  587  591  1
601  587  592  1
602  588  593  1
603  594  595  1   BACKBONE
604  594  599  1
605  595  596  1   BACKBONE
606  595  598  1
607  595  600  1
608  596  597  2   BACKBONE
609  596  604  am  BACKBONE|INTERRES
610  598  601  1
611  598  602  1
612  598  603  1
613  604  605  1   BACKBONE
614  604  608  1
615  605  606  1   BACKBONE
616  605  609  1
617  605  610  1
618  606  607  2   BACKBONE
619  606  611  am  BACKBONE|INTERRES
620  611  612  1   BACKBONE
621  611  622  1
622  612  613  1   BACKBONE
623  612  615  1
624  612  623  1
625  613  614  2   BACKBONE
626  613  631  am  BACKBONE|INTERRES
627  615  616  1
628  615  624  1
629  615  625  1
630  616  617  ar
631  616  618  ar
632  617  619  ar
633  617  626  1
634  618  620  ar
635  618  627  1
636  619  621  ar
637  619  628  1
638  620  621  ar
```

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639  620  629  1
640  621  630  1
641  631  632  1   BACKBONE
642  631  643  1
643  632  633  1   BACKBONE
644  632  635  1
645  632  644  1
646  633  634  2   BACKBONE
647  633  652  am  BACKBONE|INTERRES
648  635  636  1
649  635  645  1
650  635  646  1
651  636  637  ar
652  636  638  ar
653  637  639  ar
654  637  647  1
655  638  640  ar
656  638  648  1
657  639  641  ar
658  639  649  1
659  640  641  ar
660  640  650  1
661  641  642  1
662  642  651  1
663  652  653  1   BACKBONE
664  652  664  1
665  653  654  1   BACKBONE
666  653  656  1
667  653  665  1
668  654  655  2   BACKBONE
669  654  673  am  BACKBONE|INTERRES
670  656  657  1
671  656  666  1
672  656  667  1
673  657  658  ar
674  657  659  ar
675  658  660  ar
676  658  668  1
677  659  661  ar
678  659  669  1
679  660  662  ar
680  660  670  1
681  661  662  ar
682  661  671  1
683  662  663  1
684  663  672  1
685  673  674  1   BACKBONE
686  673  680  1
687  674  675  1   BACKBONE
688  674  677  1
689  674  681  1
690  675  676  2   BACKBONE
```

```
691  675  689  am  BACKBONE|INTERRES
692  677  678  1
693  677  679  1
694  677  682  1
695  678  683  1
696  678  684  1
697  678  685  1
698  679  686  1
699  679  687  1
700  679  688  1
701  689  690  1   BACKBONE
702  689  693  1
703  690  691  1   BACKBONE
704  690  694  1
705  690  695  1
706  691  692  2   BACKBONE
707  691  696  am  BACKBONE|INTERRES
708  696  697  1   BACKBONE
709  696  704  1
710  697  698  1   BACKBONE
711  697  700  1
712  697  705  1
713  698  699  2   BACKBONE
714  698  710  am  BACKBONE|INTERRES
715  700  701  1
716  700  706  1
717  700  707  1
718  701  702  2
719  701  703  am
720  703  708  1
721  703  709  1
722  710  711  1   BACKBONE
723  710  716  1
724  711  712  1   BACKBONE
725  711  714  1
726  711  717  1
727  712  713  2   BACKBONE
728  712  721  am  BACKBONE|INTERRES
729  714  715  1
730  714  718  1
731  714  719  1
732  715  720  1
733  721  722  1   BACKBONE
734  721  729  1
735  722  723  1   BACKBONE
736  722  725  1
737  722  730  1
738  723  724  2   BACKBONE
739  723  733  am  BACKBONE|INTERRES
740  725  726  1
741  725  731  1
742  725  732  1
```

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743  726  727  ar
744  726  728  ar
745  733  734  1   BACKBONE
746  733  741  1
747  734  735  1   BACKBONE
748  734  737  1
749  734  742  1
750  735  736  2   BACKBONE
751  735  745  am  BACKBONE|INTERRES
752  737  738  1
753  737  743  1
754  737  744  1
755  738  739  ar
756  738  740  ar
757  745  746  1   BACKBONE
758  745  752  1
759  746  747  1   BACKBONE
760  746  749  1
761  746  753  1
762  747  748  2   BACKBONE
763  747  761  am  BACKBONE|INTERRES
764  749  750  1
765  749  751  1
766  749  754  1
767  750  755  1
768  750  756  1
769  750  757  1
770  751  758  1
771  751  759  1
772  751  760  1
773  761  762  1   BACKBONE
774  761  844  1
775  762  763  1   BACKBONE
776  762  765  1
777  762  845  1
778  763  764  2   BACKBONE
779  763  854  am  BACKBONE|INTERRES
780  765  766  1
781  765  846  1
782  765  847  1
783  766  767  1
784  766  848  1
785  766  849  1
786  767  768  1
787  767  850  1
788  767  851  1
789  768  798  1
790  768  852  1
791  768  853  1
792  769  770  2   BACKBONE
793  770  771  am  BACKBONE
794  770  809  1   BACKBONE
```

795	771	772	1	BACKBONE
796	771	806	1	BACKBONE
797	772	773	1	
798	772	774	1	BACKBONE
799	772	800	1	BACKBONE
800	774	775	am	BACKBONE
801	774	799	2	BACKBONE
802	775	776	1	
803	775	777	1	BACKBONE
804	777	778	1	
805	777	779	1	BACKBONE
806	777	784	1	BACKBONE
807	779	780	ar	BACKBONE
808	779	792	ar	BACKBONE
809	780	781	1	BACKBONE
810	780	787	ar	BACKBONE
811	781	782	1	
812	781	783	1	
813	781	784	1	BACKBONE
814	784	785	1	
815	784	786	1	
816	787	788	ar	BACKBONE
817	787	794	1	BACKBONE
818	788	789	1	
819	788	790	ar	BACKBONE
820	790	791	1	
821	790	792	ar	BACKBONE
822	792	793	1	
823	794	795	1	
824	795	796	2	
825	795	797	2	
826	795	798	am	
827	800	801	1	
828	800	802	1	
829	800	803	1	BACKBONE
830	803	804	1	
831	803	805	1	
832	803	806	1	BACKBONE
833	806	807	1	
834	806	808	1	
835	809	810	1	
836	809	811	1	BACKBONE
837	809	827	1	BACKBONE
838	811	812	1	
839	811	813	am	BACKBONE
840	813	814	1	BACKBONE
841	813	826	2	BACKBONE
842	814	815	1	
843	814	816	1	BACKBONE
844	814	822	1	BACKBONE
845	816	817	1	
846	816	818	1	BACKBONE

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847  818  819  1
848  818  820  1
849  818  821  1
850  822  823  1
851  822  824  1
852  822  825  1
853  827  828  1
854  827  829  1   BACKBONE
855  827  841  1   BACKBONE
856  829  830  1
857  829  831  1
858  829  832  1   BACKBONE
859  832  833  1
860  832  834  1
861  832  835  1   BACKBONE
862  835  836  1
863  835  837  1
864  835  838  1   BACKBONE
865  838  839  1
866  838  840  1
867  838  841  1   BACKBONE
868  841  842  1
869  841  843  1
870  854  855  1   BACKBONE
871  854  860  1
872  855  856  1   BACKBONE
873  855  858  1
874  855  861  1
875  856  857  2   BACKBONE
876  856  866  am  BACKBONE|INTERRES
877  858  859  1
878  858  862  1
879  858  863  1
880  859  864  1
881  859  865  1
882  866  867  1   BACKBONE
883  866  877  1
884  867  868  1   BACKBONE
885  867  870  1
886  867  878  1
887  868  869  2   BACKBONE
888  868  886  am  BACKBONE|INTERRES
889  870  871  1
890  870  879  1
891  870  880  1
892  871  872  ar
893  871  873  ar
894  872  874  ar
895  872  881  1
896  873  875  ar
897  873  882  1
898  874  876  ar
```

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899  874  883  1
900  875  876  ar
901  875  884  1
902  876  885  1
903  886  887  1   BACKBONE
904  886  892  1
905  887  888  1   BACKBONE
906  887  890  1
907  887  893  1
908  888  889  2   BACKBONE
909  888  899  am  BACKBONE|INTERRES
910  890  891  1
911  890  894  1
912  890  895  1
913  891  896  1
914  891  897  1
915  891  898  1
916  899  900  1   BACKBONE
917  899  905  1
918  900  901  1   BACKBONE
919  900  903  1
920  900  906  1
921  901  902  2   BACKBONE
922  901  911  am  BACKBONE|INTERRES
923  903  904  1
924  903  907  1
925  903  908  1
926  904  909  1
927  904  910  1
928  911  912  1   BACKBONE
929  911  919  1
930  912  913  1   BACKBONE
931  912  915  1
932  912  920  1
933  913  914  2   BACKBONE
934  913  923  am  BACKBONE|INTERRES
935  915  916  1
936  915  921  1
937  915  922  1
938  916  917  ar
939  916  918  ar
940  923  924  1   BACKBONE
941  923  927  1
942  924  925  1   BACKBONE
943  924  928  1
944  924  929  1
945  925  926  2   BACKBONE
946  925  930  am  BACKBONE|INTERRES
947  930  931  1   BACKBONE
948  930  934  1
949  931  932  1   BACKBONE
950  931  935  1
```

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 951  931  936  1
 952  932  933  2   BACKBONE
 953  932  937  am  BACKBONE|INTERRES
 954  937  938  1   BACKBONE
 955  937  945  1
 956  938  939  1   BACKBONE
 957  938  941  1
 958  938  946  1
 959  939  940  2   BACKBONE
 960  939  956  am  BACKBONE|INTERRES
 961  941  942  1
 962  941  947  1
 963  941  948  1
 964  942  943  1
 965  942  944  1
 966  942  949  1
 967  943  950  1
 968  943  951  1
 969  943  952  1
 970  944  953  1
 971  944  954  1
 972  944  955  1
 973  956  957  1   BACKBONE
 974  956  967  1
 975  957  958  1   BACKBONE
 976  957  960  1
 977  957  968  1
 978  958  959  2   BACKBONE
 979  958  980  am  BACKBONE|INTERRES
 980  960  961  1
 981  960  969  1
 982  960  970  1
 983  961  962  1
 984  961  971  1
 985  961  972  1
 986  962  963  1
 987  962  973  1
 988  962  974  1
 989  963  964  ar
 990  963  975  1
 991  964  965  ar
 992  964  966  ar
 993  965  976  1
 994  965  977  1
 995  966  978  1
 996  966  979  1
 997  980  981  1   BACKBONE
 998  980  986  1
 999  981  982  1   BACKBONE
1000  981  984  1
1001  981  987  1
1002  982  983  2   BACKBONE
```

```
1003  982  993  am  BACKBONE|INTERRES
1004  984  985  1
1005  984  988  1
1006  984  989  1
1007  985  990  1
1008  985  991  1
1009  985  992  1
1010  993  994  1   BACKBONE
1011  993 1007  1
1012  994  995  1   BACKBONE
1013  994  997  1
1014  994 1008  1
1015  995  996  2   BACKBONE
1016  995 1017  am  BACKBONE|INTERRES
1017  997  998  1
1018  997 1009  1
1019  997 1010  1
1020  998  999  2
1021  998 1000  1
1022  999 1001  1
1023  999 1011  1
1024 1000 1002  ar
1025 1000 1003  ar
1026 1001 1002  1
1027 1001 1012  1
1028 1002 1004  ar
1029 1003 1005  ar
1030 1003 1013  1
1031 1004 1006  ar
1032 1004 1014  1
1033 1005 1006  ar
1034 1005 1015  1
1035 1006 1016  1
1036 1017 1018  1   BACKBONE
1037 1017 1026  1
1038 1018 1019  1   BACKBONE
1039 1018 1021  1
1040 1018 1027  1
1041 1019 1020  2   BACKBONE
1042 1019 1032  am  BACKBONE|INTERRES
1043 1021 1022  1
1044 1021 1028  1
1045 1021 1029  1
1046 1022 1023  1
1047 1022 1030  1
1048 1022 1031  1
1049 1023 1024  ar
1050 1023 1025  ar
1051 1032 1033  1   BACKBONE
1052 1032 1038  1
1053 1033 1034  1   BACKBONE
1054 1033 1036  1
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1055 1033 1039  1
1056 1034 1035  2   BACKBONE
1057 1034 1043  am  BACKBONE|INTERRES
1058 1036 1037  1
1059 1036 1040  1
1060 1036 1041  1
1061 1037 1042  1
1062 1043 1044  1   BACKBONE
1063 1043 1047  1
1064 1044 1045  1   BACKBONE
1065 1044 1048  1
1066 1044 1049  1
1067 1045 1046  2   BACKBONE
1068 1045 1050  am  BACKBONE|INTERRES
1069 1050 1051  1   BACKBONE
1070 1050 1058  1
1071 1051 1052  1   BACKBONE
1072 1051 1054  1
1073 1051 1059  1
1074 1052 1053  2   BACKBONE
1075 1052 1062  am  BACKBONE|INTERRES
1076 1054 1055  1
1077 1054 1060  1
1078 1054 1061  1
1079 1055 1056  ar
1080 1055 1057  ar
1081 1062 1063  1   BACKBONE
1082 1062 1070  1
1083 1063 1064  1   BACKBONE
1084 1063 1066  1
1085 1063 1071  1
1086 1064 1065  2   BACKBONE
1087 1064 1074  am  BACKBONE|INTERRES
1088 1066 1067  1
1089 1066 1072  1
1090 1066 1073  1
1091 1067 1068  ar
1092 1067 1069  ar
1093 1074 1075  1   BACKBONE
1094 1074 1080  1
1095 1075 1076  1   BACKBONE
1096 1075 1078  1
1097 1075 1081  1
1098 1076 1077  2   BACKBONE
1099 1076 1088  am  BACKBONE|INTERRES
1100 1078 1079  1
1101 1078 1082  1
1102 1078 1083  1
1103 1079 1080  1
1104 1079 1084  1
1105 1079 1085  1
1106 1080 1086  1
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1107 1080 1087  1
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1109 1088 1102  1
1110 1089 1090  1   BACKBONE
1111 1089 1092  1
1112 1089 1103  1
1113 1090 1091  2   BACKBONE
1114 1090 1112  am  BACKBONE|INTERRES
1115 1092 1093  1
1116 1092 1104  1
1117 1092 1105  1
1118 1093 1094  2
1119 1093 1095  1
1120 1094 1096  1
1121 1094 1106  1
1122 1095 1097  ar
1123 1095 1098  ar
1124 1096 1097  1
1125 1096 1107  1
1126 1097 1099  ar
1127 1098 1100  ar
1128 1098 1108  1
1129 1099 1101  ar
1130 1099 1109  1
1131 1100 1101  ar
1132 1100 1110  1
1133 1101 1111  1
1134 1112 1113  1   BACKBONE
1135 1112 1119  1
1136 1113 1114  1   BACKBONE
1137 1113 1116  1
1138 1113 1120  1
1139 1114 1115  2   BACKBONE
1140 1114 1128  am  BACKBONE|INTERRES
1141 1116 1117  1
1142 1116 1118  1
1143 1116 1121  1
1144 1117 1122  1
1145 1117 1123  1
1146 1117 1124  1
1147 1118 1125  1
1148 1118 1126  1
1149 1118 1127  1
1150 1128 1129  1   BACKBONE
1151 1128 1137  1
1152 1129 1130  1   BACKBONE
1153 1129 1132  1
1154 1129 1138  1
1155 1130 1131  2   BACKBONE
1156 1130 1145  am  BACKBONE|INTERRES
1157 1132 1133  1
1158 1132 1139  1
```

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1159 1132 1140  1
1160 1133 1134  1
1161 1133 1141  1
1162 1133 1142  1
1163 1134 1135  2
1164 1134 1136  am
1165 1136 1143  1
1166 1136 1144  1
1167 1145 1146  1   BACKBONE
1168 1145 1155  1
1169 1146 1147  1   BACKBONE
1170 1146 1149  1
1171 1146 1156  1
1172 1147 1148  2   BACKBONE
1173 1147 1162  am  BACKBONE|INTERRES
1174 1149 1150  1
1175 1149 1157  1
1176 1149 1158  1
1177 1150 1151  1
1178 1150 1152  2
1179 1151 1153  ar
1180 1151 1159  1
1181 1152 1154  1
1182 1152 1160  1
1183 1153 1154  1
1184 1153 1161  1
1185 1162 1163  1   BACKBONE
1186 1162 1167  1
1187 1163 1164  1   BACKBONE
1188 1163 1166  1
1189 1163 1168  1
1190 1164 1165  2   BACKBONE
1191 1164 1172  am  BACKBONE|INTERRES
1192 1166 1169  1
1193 1166 1170  1
1194 1166 1171  1
1195 1172 1173  1   BACKBONE
1196 1172 1181  1
1197 1173 1174  1   BACKBONE
1198 1173 1176  1
1199 1173 1182  1
1200 1174 1175  2   BACKBONE
1201 1174 1194  am  BACKBONE|INTERRES
1202 1176 1177  1
1203 1176 1183  1
1204 1176 1184  1
1205 1177 1178  1
1206 1177 1185  1
1207 1177 1186  1
1208 1178 1179  1
1209 1178 1187  1
1210 1178 1188  1
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1212 1179 1189  1
1213 1179 1190  1
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1215 1180 1192  1
1216 1180 1193  1
1217 1194 1195  1   BACKBONE
1218 1194 1208  1
1219 1195 1196  1   BACKBONE
1220 1195 1198  1
1221 1195 1209  1
1222 1196 1197  2   BACKBONE
1223 1196 1218  am  BACKBONE|INTERRES
1224 1198 1199  1
1225 1198 1210  1
1226 1198 1211  1
1227 1199 1200  2
1228 1199 1201  1
1229 1200 1202  1
1230 1200 1212  1
1231 1201 1203  ar
1232 1201 1204  ar
1233 1202 1203  1
1234 1202 1213  1
1235 1203 1205  ar
1236 1204 1206  ar
1237 1204 1214  1
1238 1205 1207  ar
1239 1205 1215  1
1240 1206 1207  ar
1241 1206 1216  1
1242 1207 1217  1
1243 1218 1219  1   BACKBONE
1244 1218 1229  1
1245 1219 1220  1   BACKBONE
1246 1219 1222  1
1247 1219 1230  1
1248 1220 1221  2   BACKBONE
1249 1220 1238  am  BACKBONE|INTERRES
1250 1222 1223  1
1251 1222 1231  1
1252 1222 1232  1
1253 1223 1224  ar
1254 1223 1225  ar
1255 1224 1226  ar
1256 1224 1233  1
1257 1225 1227  ar
1258 1225 1234  1
1259 1226 1228  ar
1260 1226 1235  1
1261 1227 1228  ar
1262 1227 1236  1
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1265 1238 1244  1
1266 1239 1240  1   BACKBONE
1267 1239 1242  1
1268 1239 1245  1
1269 1240 1241  2   BACKBONE
1270 1240 1252  am  BACKBONE|INTERRES
1271 1242 1243  1
1272 1242 1246  1
1273 1242 1247  1
1274 1243 1244  1
1275 1243 1248  1
1276 1243 1249  1
1277 1244 1250  1
1278 1244 1251  1
1279 1252 1253  1   BACKBONE
1280 1252 1263  1
1281 1253 1254  1   BACKBONE
1282 1253 1256  1
1283 1253 1264  1
1284 1254 1255  2   BACKBONE
1285 1254 1276  am  BACKBONE|INTERRES
1286 1256 1257  1
1287 1256 1265  1
1288 1256 1266  1
1289 1257 1258  1
1290 1257 1267  1
1291 1257 1268  1
1292 1258 1259  1
1293 1258 1269  1
1294 1258 1270  1
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1296 1259 1271  1
1297 1260 1261  ar
1298 1260 1262  ar
1299 1261 1272  1
1300 1261 1273  1
1301 1262 1274  1
1302 1262 1275  1
1303 1276 1277  1   BACKBONE
1304 1276 1282  1
1305 1277 1278  1   BACKBONE
1306 1277 1280  1
1307 1277 1283  1
1308 1278 1279  2   BACKBONE
1309 1278 1288  am  BACKBONE|INTERRES
1310 1280 1281  1
1311 1280 1284  1
1312 1280 1285  1
1313 1281 1286  1
1314 1281 1287  1
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1315 1288 1289  1   BACKBONE
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1317 1289 1290  1   BACKBONE
1318 1289 1292  1
1319 1289 1298  1
1320 1290 1291  2   BACKBONE
1321 1290 1303  am  BACKBONE|INTERRES
1322 1292 1293  1
1323 1292 1299  1
1324 1292 1300  1
1325 1293 1294  1
1326 1293 1301  1
1327 1293 1302  1
1328 1294 1295  ar
1329 1294 1296  ar
1330 1303 1304  1   BACKBONE
1331 1303 1315  1
1332 1304 1305  1   BACKBONE
1333 1304 1307  1
1334 1304 1316  1
1335 1305 1306  2   BACKBONE
1336 1305 1324  am  BACKBONE|INTERRES
1337 1307 1308  1
1338 1307 1317  1
1339 1307 1318  1
1340 1308 1309  ar
1341 1308 1310  ar
1342 1309 1311  ar
1343 1309 1319  1
1344 1310 1312  ar
1345 1310 1320  1
1346 1311 1313  ar
1347 1311 1321  1
1348 1312 1313  ar
1349 1312 1322  1
1350 1313 1314  1
1351 1314 1323  1
1352 1324 1325  1   BACKBONE
1353 1324 1332  1
1354 1325 1326  1   BACKBONE
1355 1325 1328  1
1356 1325 1333  1
1357 1326 1327  2   BACKBONE
1358 1326 1343  am  BACKBONE|INTERRES
1359 1328 1329  1
1360 1328 1334  1
1361 1328 1335  1
1362 1329 1330  1
1363 1329 1331  1
1364 1329 1336  1
1365 1330 1337  1
1366 1330 1338  1
```

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1367 1330 1339  1
1368 1331 1340  1
1369 1331 1341  1
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1371 1343 1344  1   BACKBONE
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1373 1344 1345  1   BACKBONE
1374 1344 1347  1
1375 1344 1352  1
1376 1345 1346  2   BACKBONE
1377 1345 1362  am  BACKBONE|INTERRES
1378 1347 1348  1
1379 1347 1349  1
1380 1347 1353  1
1381 1348 1350  1
1382 1348 1354  1
1383 1348 1355  1
1384 1349 1356  1
1385 1349 1357  1
1386 1349 1358  1
1387 1350 1359  1
1388 1350 1360  1
1389 1350 1361  1
1390 1362 1363  1   BACKBONE
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1392 1363 1364  1   BACKBONE
1393 1363 1366  1
1394 1363 1374  1
1395 1364 1365  2   BACKBONE
1396 1364 1386  am  BACKBONE|INTERRES
1397 1366 1367  1
1398 1366 1375  1
1399 1366 1376  1
1400 1367 1368  1
1401 1367 1377  1
1402 1367 1378  1
1403 1368 1369  1
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1405 1368 1380  1
1406 1369 1370  ar
1407 1369 1381  1
1408 1370 1371  ar
1409 1370 1372  ar
1410 1371 1382  1
1411 1371 1383  1
1412 1372 1384  1
1413 1372 1385  1
1414 1386 1387  1   BACKBONE
1415 1386 1394  1
1416 1387 1388  1   BACKBONE
1417 1387 1390  1
1418 1387 1395  1
```

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1419 1388 1389  2   BACKBONE
1420 1388 1405  am  BACKBONE|INTERRES
1421 1390 1391  1
1422 1390 1392  1
1423 1390 1396  1
1424 1391 1393  1
1425 1391 1397  1
1426 1391 1398  1
1427 1392 1399  1
1428 1392 1400  1
1429 1392 1401  1
1430 1393 1402  1
1431 1393 1403  1
1432 1393 1404  1
1433 1405 1406  1   BACKBONE
1434 1405 1414  1
1435 1406 1407  1   BACKBONE
1436 1406 1409  1
1437 1406 1415  1
1438 1407 1408  2   BACKBONE
1439 1407 1427  am  BACKBONE|INTERRES
1440 1409 1410  1
1441 1409 1416  1
1442 1409 1417  1
1443 1410 1411  1
1444 1410 1418  1
1445 1410 1419  1
1446 1411 1412  1
1447 1411 1420  1
1448 1411 1421  1
1449 1412 1413  1
1450 1412 1422  1
1451 1412 1423  1
1452 1413 1424  1
1453 1413 1425  1
1454 1413 1426  1
1455 1427 1428  1   BACKBONE
1456 1427 1431  1
1457 1428 1429  1   BACKBONE
1458 1428 1432  1
1459 1428 1433  1
1460 1429 1430  2   BACKBONE
1461 1429 1434  am  BACKBONE|INTERRES
1462 1434 1435  1   BACKBONE
1463 1434 1443  1
1464 1435 1436  1   BACKBONE
1465 1435 1438  1
1466 1435 1444  1
1467 1436 1437  2   BACKBONE
1468 1436 1451  am  BACKBONE|INTERRES
1469 1438 1439  1
1470 1438 1445  1
```

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1471 1438 1446  1
1472 1439 1440  1
1473 1439 1447  1
1474 1439 1448  1
1475 1440 1441  2
1476 1440 1442  am
1477 1442 1449  1
1478 1442 1450  1
1479 1451 1452  1   BACKBONE
1480 1451 1460  1
1481 1452 1453  1   BACKBONE
1482 1452 1455  1
1483 1452 1461  1
1484 1453 1454  2   BACKBONE
1485 1453 1466  am  BACKBONE|INTERRES
1486 1455 1456  1
1487 1455 1462  1
1488 1455 1463  1
1489 1456 1457  1
1490 1456 1464  1
1491 1456 1465  1
1492 1457 1458  ar
1493 1457 1459  ar
1494 1466 1467  1   BACKBONE
1495 1466 1477  1
1496 1467 1468  1   BACKBONE
1497 1467 1470  1
1498 1467 1478  1
1499 1468 1469  2   BACKBONE
1500 1468 1486  am  BACKBONE|INTERRES
1501 1470 1471  1
1502 1470 1479  1
1503 1470 1480  1
1504 1471 1472  ar
1505 1471 1473  ar
1506 1472 1474  ar
1507 1472 1481  1
1508 1473 1475  ar
1509 1473 1482  1
1510 1474 1476  ar
1511 1474 1483  1
1512 1475 1476  ar
1513 1475 1484  1
1514 1476 1485  1
1515 1486 1487  1   BACKBONE
1516 1486 1494  1
1517 1487 1488  1   BACKBONE
1518 1487 1490  1
1519 1487 1495  1
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1521 1488 1505  am  BACKBONE|INTERRES
1522 1490 1491  1
```

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1523 1490 1492  1
1524 1490 1496  1
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1527 1491 1498  1
1528 1492 1499  1
1529 1492 1500  1
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1531 1493 1502  1
1532 1493 1503  1
1533 1493 1504  1
1534 1505 1506  1   BACKBONE
1535 1505 1516  1
1536 1506 1507  1   BACKBONE
1537 1506 1509  1
1538 1506 1517  1
1539 1507 1508  2   BACKBONE
1540 1507 1529  am  BACKBONE|INTERRES
1541 1509 1510  1
1542 1509 1518  1
1543 1509 1519  1
1544 1510 1511  1
1545 1510 1520  1
1546 1510 1521  1
1547 1511 1512  1
1548 1511 1522  1
1549 1511 1523  1
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1552 1513 1514  ar
1553 1513 1515  ar
1554 1514 1525  1
1555 1514 1526  1
1556 1515 1527  1
1557 1515 1528  1
1558 1529 1530  1   BACKBONE
1559 1529 1538  1
1560 1530 1531  1   BACKBONE
1561 1530 1533  1
1562 1530 1539  1
1563 1531 1532  2   BACKBONE
1564 1531 1546  am  BACKBONE|INTERRES
1565 1533 1534  1
1566 1533 1540  1
1567 1533 1541  1
1568 1534 1535  1
1569 1534 1542  1
1570 1534 1543  1
1571 1535 1536  2
1572 1535 1537  am
1573 1537 1544  1
1574 1537 1545  1
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1575 1546 1547  1   BACKBONE
1576 1546 1553  1
1577 1547 1548  1   BACKBONE
1578 1547 1550  1
1579 1547 1554  1
1580 1548 1549  2   BACKBONE
1581 1548 1562  am  BACKBONE|INTERRES
1582 1550 1551  1
1583 1550 1552  1
1584 1550 1555  1
1585 1551 1556  1
1586 1551 1557  1
1587 1551 1558  1
1588 1552 1559  1
1589 1552 1560  1
1590 1552 1561  1
1591 1562 1563  1   BACKBONE
1592 1562 1571  1
1593 1563 1564  1   BACKBONE
1594 1563 1566  1
1595 1563 1572  1
1596 1564 1565  2   BACKBONE
1597 1566 1567  1
1598 1566 1573  1
1599 1566 1574  1
1600 1567 1568  1
1601 1567 1575  1
1602 1567 1576  1
1603 1568 1569  2
1604 1568 1570  am
1605 1570 1577  1
1606 1570 1578  1
@<TRIPOS>SUBSTRUCTURE
  1 SER242    2 RESIDUE 4 A SER 1
  2 MET243   14 RESIDUE 4 A MET 2
  3 ARG244   33 RESIDUE 4 A ARG 2
  4 TYR245   57 RESIDUE 4 A TYR 2
  5 THR246   78 RESIDUE 4 A THR 2
  6 VAL247   92 RESIDUE 4 A VAL 2
  7 SER248  108 RESIDUE 4 A SER 2
  8 ASN249  119 RESIDUE 4 A ASN 2
  9 LEU250  133 RESIDUE 4 A LEU 2
 10 SER251  152 RESIDUE 4 A SER 2
 11 MET252  163 RESIDUE 4 A MET 2
 12 GLN253  182 RESIDUE 4 A GLN 2
 13 THR254  199 RESIDUE 4 A THR 2
 14 HIS255  213 RESIDUE 4 A HIS 2
 15 ALA256  230 RESIDUE 4 A ALA 2
 16 ALA257  240 RESIDUE 4 A ALA 2
 17 ARG258  250 RESIDUE 4 A ARG 2
 18 PHE259  274 RESIDUE 4 A PHE 2
 19 LYS260  294 RESIDUE 4 A LYS 2
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20 THR261  316 RESIDUE 4 A THR 2
21 PHE262  330 RESIDUE 4 A PHE 2
22 PHE263  350 RESIDUE 4 A PHE 2
23 ASN264  370 RESIDUE 4 A ASN 2
24 TRP265  384 RESIDUE 4 A TRP 2
25 PRO266  408 RESIDUE 4 A PRO 2
26 SER267  422 RESIDUE 4 A SER 2
27 SER268  433 RESIDUE 4 A SER 2
28 VAL269  444 RESIDUE 4 A VAL 2
29 LEU270  460 RESIDUE 4 A LEU 2
30 VAL271  479 RESIDUE 4 A VAL 2
31 ASN272  495 RESIDUE 4 A ASN 2
32 PRO273  509 RESIDUE 4 A PRO 2
33 GLU274  523 RESIDUE 4 A GLU 2
34 GLN275  538 RESIDUE 4 A GLN 2
35 LEU276  555 RESIDUE 4 A LEU 2
36 ALA277  574 RESIDUE 4 A ALA 2
37 SER278  584 RESIDUE 4 A SER 2
38 ALA279  595 RESIDUE 4 A ALA 2
39 GLY280  605 RESIDUE 4 A GLY 2
40 PHE281  612 RESIDUE 4 A PHE 2
41 TYR282  632 RESIDUE 4 A TYR 2
42 TYR283  653 RESIDUE 4 A TYR 2
43 VAL284  674 RESIDUE 4 A VAL 2
44 GLY285  690 RESIDUE 4 A GLY 2
45 ASN286  697 RESIDUE 4 A ASN 2
46 SER287  711 RESIDUE 4 A SER 2
47 ASP288  722 RESIDUE 4 A ASP 2
48 ASP289  734 RESIDUE 4 A ASP 2
49 VAL290  746 RESIDUE 4 A VAL 2
50 LYS291  762 RESIDUE 4 A LYS 2
51 CYS292  855 RESIDUE 4 A CYS 2
52 PHE293  867 RESIDUE 4 A PHE 2
53 CYS294  887 RESIDUE 4 A CYS 2
54 CYS295  900 RESIDUE 4 A CYS 2
55 ASP296  912 RESIDUE 4 A ASP 2
56 GLY297  924 RESIDUE 4 A GLY 2
57 GLY298  931 RESIDUE 4 A GLY 2
58 LEU299  938 RESIDUE 4 A LEU 2
59 ARG300  957 RESIDUE 4 A ARG 2
60 CYS301  981 RESIDUE 4 A CYS 2
61 TRP302  994 RESIDUE 4 A TRP 2
62 GLU303 1018 RESIDUE 4 A GLU 2
63 SER304 1033 RESIDUE 4 A SER 2
64 GLY305 1044 RESIDUE 4 A GLY 2
65 ASP306 1051 RESIDUE 4 A ASP 2
66 ASP307 1063 RESIDUE 4 A ASP 2
67 PRO308 1075 RESIDUE 4 A PRO 2
68 TRP309 1089 RESIDUE 4 A TRP 2
69 VAL310 1113 RESIDUE 4 A VAL 2
70 GLN311 1129 RESIDUE 4 A GLN 2
71 HIS312 1146 RESIDUE 4 A HIS 2
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 72 ALA313 1163 RESIDUE 4 A ALA 2
 73 LYS314 1173 RESIDUE 4 A LYS 2
 74 TRP315 1195 RESIDUE 4 A TRP 2
 75 PHE316 1219 RESIDUE 4 A PHE 2
 76 PRO317 1239 RESIDUE 4 A PRO 2
 77 ARG318 1253 RESIDUE 4 A ARG 2
 78 CYS319 1277 RESIDUE 4 A CYS 2
 79 GLU320 1289 RESIDUE 4 A GLU 2
 80 TYR321 1304 RESIDUE 4 A TYR 2
 81 LEU322 1325 RESIDUE 4 A LEU 2
 82 ILE323 1344 RESIDUE 4 A ILE 2
 83 ARG324 1363 RESIDUE 4 A ARG 2
 84 ILE325 1387 RESIDUE 4 A ILE 2
 85 LYS326 1406 RESIDUE 4 A LYS 2
 86 GLY327 1428 RESIDUE 4 A GLY 2
 87 GLN328 1435 RESIDUE 4 A GLN 2
 88 GLU329 1452 RESIDUE 4 A GLU 2
 89 PHE330 1467 RESIDUE 4 A PHE 2
 90 ILE331 1487 RESIDUE 4 A ILE 2
 91 ARG332 1506 RESIDUE 4 A ARG 2
 92 GLN333 1530 RESIDUE 4 A GLN 2
 93 VAL334 1547 RESIDUE 4 A VAL 2
 94 GLN335 1563 RESIDUE 4 A GLN 1

# MOE 2019.01 (io_trps.svl 2018.10)
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