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Reduced and quenched polarizabilities of interior atoms in molecules

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Contents: **page**

Section S1. Details on the calculation of distributed polarizabilities using *Gaussian 09*

Here is an example of *Gaussian 09*'s input file for an analytical calculation of the total molecular polarizability of the acetone molecule in the ground electronic state.

```
#p m062x/6-311++G(2df,2p) scf=tight integral=ultrafine Polar

acetone molecule; analytical calculation

0 1
O   0.000000   0.000000   1.395409
C   0.000000   0.000000   0.177466
C   0.000000   1.275926  -0.608409
C   0.000000  -1.275926  -0.608409
H   0.000000   2.139336   0.050808
H   0.000000  -2.139336   0.050808
H   0.876906   1.299124  -1.257196
H   0.876906  -1.299124  -1.257196
H  -0.876906   1.299124  -1.257196
H  -0.876906  -1.299124  -1.257196
```

An excerpt of *Gaussian 09* (Rev. C.01)'s output file with a computed value of the spherically averaged (labeled "isotropic" in the output) polarizability is given below.

```
 SCF Polarizability for W=    0.000000:
                 1             2             3
      1  0.322955D+02
      2  0.000000D+00  0.427385D+02
      3  0.000000D+00  0.000000D+00  0.450658D+02
 Isotropic polarizability for W=    0.000000       40.03 Bohr**3.
```

A calculation of distributed atomic polarizabilities using Hirshfeld population analysis involves a numerical differentiation of analytically computed dipole moments. An example of *Gaussian 09*'s input file for such a calculation is given below.

```
%chk=AcW0.chk
# m062x/6-311++G(2df,2p) scf=tight integral=ultrafine Pop=Hirshfeld

acetone molecule; calculation 1: Fx=Fy=Fz=0 a.u.

0 1
O   0.000000   0.000000   1.395409
C   0.000000   0.000000   0.177466
C   0.000000   1.275926  -0.608409
C   0.000000  -1.275926  -0.608409
H   0.000000   2.139336   0.050808
H   0.000000  -2.139336   0.050808
H   0.876906   1.299124  -1.257196
H   0.876906  -1.299124  -1.257196
H  -0.876906   1.299124  -1.257196
H  -0.876906  -1.299124  -1.257196

--link1--
%chk=AcW0.chk
# m062x chkbasis geom=check guess=check scf=tight integral=ultrafine Field=X+10 Pop=Hirshfeld

acetone molecule; calculation 2: Fx=-0.001 a.u.

0 1

--link1--
%chk=AcW0.chk
# m062x chkbasis geom=check guess=check scf=tight integral=ultrafine Field=Y+10 Pop=Hirshfeld

acetone molecule; calculation 3: Fy=-0.001 a.u.

0 1

--link1--
%chk=AcW0.chk
# m062x chkbasis geom=check guess=check scf=tight integral=ultrafine Field=Z+10 Pop=Hirshfeld

acetone molecule; calculation 4: Fz=-0.001 a.u.
```

0 1

Excerpts of *Gaussian 09* (Rev. C.01)'s output files with the information needed for calculating distributed atomic polarizabilities are given below.

Cartesian coordinates:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	1.395409
2	6	0	0.000000	0.000000	0.177466
3	6	0	0.000000	1.275926	-0.608409
4	6	0	0.000000	-1.275926	-0.608409
5	1	0	0.000000	2.139336	0.050808
6	1	0	0.000000	-2.139336	0.050808
7	1	0	0.876906	1.299124	-1.257196
8	1	0	0.876906	-1.299124	-1.257196
9	1	0	-0.876906	1.299124	-1.257196
10	1	0	-0.876906	-1.299124	-1.257196

Calculation 1 ($F_x = F_y = F_z = 0$):

Hirshfeld spin densities, charges and dipoles using IRadAn= 5:

		1	2	3	4	5
1	O	0.000000	-0.279204	0.000000	0.000000	-1.932504
2	C	0.000000	0.168269	0.000000	0.000000	0.100247
3	C	0.000000	-0.100227	0.000000	-0.160877	0.034967
4	C	0.000000	-0.100227	0.000000	0.160877	0.034967
5	H	0.000000	0.053627	0.000000	-0.990173	-0.673195
6	H	0.000000	0.053627	0.000000	0.990173	-0.673195
7	H	0.000000	0.051036	-0.944599	-0.114337	0.695012
8	H	0.000000	0.051036	-0.944599	0.114337	0.695012
9	H	0.000000	0.051036	0.944599	-0.114337	0.695012
10	H	0.000000	0.051036	0.944599	0.114337	0.695012

Calculation 2 ($F_x = -0.001$ a.u.):

Hirshfeld spin densities, charges and dipoles using IRadAn= 5:

		1	2	3	4	5
1	O	0.000000	-0.279202	-0.003693	0.000000	-1.932506
2	C	0.000000	0.168268	-0.003003	0.000000	0.100246
3	C	0.000000	-0.100225	-0.000445	-0.160877	0.034967
4	C	0.000000	-0.100225	-0.000445	0.160877	0.034967
5	H	0.000000	0.053627	-0.001787	-0.990175	-0.673197
6	H	0.000000	0.053627	-0.001787	0.990175	-0.673197
7	H	0.000000	0.049560	-0.947445	-0.114808	0.695871
8	H	0.000000	0.049560	-0.947445	0.114808	0.695871
9	H	0.000000	0.052509	0.941773	-0.113872	0.694155
10	H	0.000000	0.052509	0.941773	0.113872	0.694155

Calculation 3 ($F_y = -0.001$ a.u.):

Hirshfeld spin densities, charges and dipoles using IRadAn= 5:

		1	2	3	4	5
1	O	0.000000	-0.279200	0.000000	-0.002810	-1.932507
2	C	0.000000	0.168268	0.000000	-0.000185	0.100249
3	C	0.000000	-0.101104	0.000000	-0.161118	0.034825
4	C	0.000000	-0.099347	0.000000	0.160636	0.035107
5	H	0.000000	0.051697	0.000000	-0.993953	-0.674421
6	H	0.000000	0.055549	0.000000	0.986437	-0.671982
7	H	0.000000	0.050506	-0.945274	-0.116011	0.695567
8	H	0.000000	0.051567	-0.943927	0.112672	0.694461
9	H	0.000000	0.050506	0.945274	-0.116011	0.695567
10	H	0.000000	0.051566	0.943927	0.112672	0.694461

Calculation 4 ($F_z = -0.001$ a.u.):

Hirshfeld spin densities, charges and dipoles using IRadAn= 5:

		1	2	3	4	5
1	O	0.000000	-0.283510	0.000000	0.000000	-1.938223
2	C	0.000000	0.168436	0.000000	0.000000	0.100160
3	C	0.000000	-0.099902	0.000000	-0.160886	0.034680
4	C	0.000000	-0.099902	0.000000	0.160886	0.034680
5	H	0.000000	0.052733	0.000000	-0.991041	-0.675142
6	H	0.000000	0.052733	0.000000	0.991041	-0.675142

```
 7  H    0.000000   0.052355  -0.943511  -0.113813   0.692514
 8  H    0.000000   0.052355  -0.943511   0.113813   0.692514
 9  H    0.000000   0.052355   0.943511  -0.113813   0.692514
10  H    0.000000   0.052355   0.943511   0.113813   0.692514
```

The γ component of the distributed dipole moment for atom i in atomic units ($\gamma = x, y, z$) at each value of the electric field F is calculated by

$$\mu_{\gamma i} = q_i R_{\gamma i} + \delta\mu_{\gamma i} \tag{S1}$$

The values of q_i are obtained from column 2 in the excerpts given above. The values of $R_{\gamma i}$ are the standard-orientation Cartesian coordinates converted from Å to atomic units. The values of $\delta\mu_{xi}$, $\delta\mu_{yi}$, and $\delta\mu_{zi}$ are obtained from column 3, 4, and 5, respectively.

The $\gamma\gamma$ component of the molecular polarizability tensor in atomic units for each atom i can be calculated as

$$\alpha_{\gamma\gamma\, i} = \frac{\mu_{\gamma i}(F_\gamma) - \mu_{\gamma i}(0)}{F_\gamma} \tag{S2}$$

where F_γ is the magnitude of an electric field **F** along the γ axis, and F_γ = –0.001 a.u. in this calculation. The values of $\mu_{xi}(0)$, $\mu_{yi}(0)$, and $\mu_{zi}(0)$ are based on calculation 1. The values of $\mu_{xi}(F_x)$, $\mu_{yi}(F_y)$, and $\mu_{zi}(F_z)$ are based on calculation 2, 3, and 4, respectively.

By combining $\mu_{\gamma i}(0)$, $\mu_{\gamma i}(F_\gamma)$, and F_γ for each i and γ, we obtain the numbers given below.

i	α_{xxi}	α_{yyi}	α_{zzi}	$\alpha_i = 1/3\ (\alpha_{xxi}+\alpha_{yyi}+\alpha_{zzi})$
O1	3.69	2.81	17.07	7.86
C2	3.00	0.19	0.03	1.07
C3	0.45	2.36	0.66	1.15
C4	0.45	2.36	0.66	1.16
H5	1.79	11.58	2.03	5.13
H6	1.79	11.51	2.03	5.11
H7	5.29	2.98	5.63	4.63
H8	5.29	2.97	5.63	4.63
H9	5.27	2.98	5.63	4.62
H10	5.27	2.97	5.63	4.62
total	32.28	42.69	45.02	39.99

Section S2. Cartesian coordinates of studied molecules (in Å)

m-nitroaniline

0 1

N	-0.762285	-2.971480	0.000000
C	-0.064921	-1.792302	0.000000
C	-0.737832	-0.569276	0.000000
C	0.000000	0.596966	0.000000
C	1.381269	0.628704	0.000000
C	2.038853	-0.593340	0.000000
C	1.335600	-1.784482	0.000000
N	-0.736708	1.879338	0.000000
O	-0.084918	2.898357	0.000000
O	-1.946772	1.832808	0.000000
H	-0.285155	-3.851822	0.000000
H	-1.763819	-2.977707	0.000000
H	-1.816686	-0.519241	0.000000
H	1.905648	1.570242	0.000000
H	3.119617	-0.616894	0.000000
H	1.869052	-2.726517	0.000000

p-nitroaniline

0 1

N	0.000000	0.000000	3.432122
C	0.000000	0.000000	2.068432
C	0.000000	1.208373	1.355432
C	0.000007	1.208493	-0.022203
C	0.000000	0.000000	-0.701578
C	-0.000007	-1.208493	-0.022203
C	0.000000	-1.208373	1.355432
N	0.000000	0.000000	-2.160988
O	0.000401	-1.073802	-2.726422
O	-0.000401	1.073802	-2.726422
H	0.000553	-0.858952	3.948074
H	-0.000553	0.858952	3.948074
H	0.000055	2.145371	1.896433
H	-0.000006	2.131581	-0.582037
H	0.000006	-2.131581	-0.582037
H	-0.000055	-2.145371	1.896433

C60

0 1

C	0.734432	-1.010858	3.339592
C	-0.734432	-1.010858	3.339592
C	-1.427280	-1.964482	2.611089
C	-0.692848	-2.975340	1.838862
C	0.692848	-2.975340	1.838862
C	1.427280	-1.964482	2.611089
C	1.188335	0.386114	3.339592
C	0.000000	1.249490	3.339592
C	-1.188335	0.386114	3.339592
C	-2.309387	0.750365	2.611089
C	-2.615615	-1.578369	1.838862
C	-1.427280	-3.213972	0.589372
C	-0.734432	-3.439092	-0.589372
C	0.734432	-3.439092	-0.589372
C	1.427280	-3.213972	0.589372
C	2.615615	-2.350596	0.589372
C	2.615615	-1.578369	1.838862
C	3.043819	-0.260493	1.838862
C	2.309387	0.750365	2.611089
C	0.000000	2.428233	2.611089
C	1.188335	2.814347	1.838862
C	2.309387	1.999855	1.838862
C	3.043819	1.761224	0.589372
C	3.497722	0.364252	0.589372
C	3.497722	-0.364252	-0.589372
C	3.043819	-1.761224	-0.589372
C	2.309387	-1.999855	-1.838862
C	1.188335	-2.814347	-1.838862
C	-2.615615	-2.350596	0.589372
C	-1.188335	-0.386114	-3.339592
C	-2.309387	-0.750365	-2.611089
C	-3.043819	0.260493	-1.838862
C	-2.615615	1.578369	-1.838862

```
C  -1.427280   1.964482  -2.611089
C   0.734432   1.010858  -3.339592
C   1.188335  -0.386114  -3.339592
C   0.000000  -1.249490  -3.339592
C   0.000000  -2.428233  -2.611089
C  -1.188335  -2.814347  -1.838862
C  -2.309387  -1.999855  -1.838862
C  -3.497722  -0.364252  -0.589372
C  -3.497722   0.364252   0.589372
C  -3.043819   1.761224   0.589372
C  -2.615615   2.350596  -0.589372
C  -1.427280   3.213972  -0.589372
C  -0.692848   2.975340  -1.838862
C   0.692848   2.975340  -1.838862
C   1.427280   1.964482  -2.611089
C   2.309387  -0.750365  -2.611089
C   3.043819   0.260493  -1.838862
C   2.615615   1.578369  -1.838862
C   2.615615   2.350596  -0.589372
C   1.427280   3.213972  -0.589372
C   0.734432   3.439092   0.589372
C  -0.734432   3.439092   0.589372
C  -1.188335   2.814347   1.838862
C  -2.309387   1.999855   1.838862
C  -3.043819  -1.761224  -0.589372
C  -3.043819  -0.260493   1.838862
C  -0.734432   1.010858  -3.339592

CO at C60

0 1
O   0.000000   0.000000   0.480201
C   0.000000   0.000000  -0.640268
C  -1.188335   0.386114   3.339592
C   0.000000   1.249490   3.339592
C   0.000000   2.428233   2.611089
C  -1.188335   2.814346   1.838862
C  -2.309387   1.999855   1.838862
C  -2.309387   0.750365   2.611089
C  -0.734432  -1.010858   3.339592
C   0.734432  -1.010858   3.339592
C   1.188335   0.386114   3.339592
C   2.309387   0.750365   2.611089
C   1.188335   2.814346   1.838862
C  -0.734432   3.439092   0.589372
C  -1.427280   3.213972  -0.589372
C  -2.615616   2.350596  -0.589372
C  -3.043819   1.761224   0.589372
C  -3.497723   0.364252   0.589372
C  -3.043818  -0.260493   1.838862
C  -2.615615  -1.578368   1.838862
C  -1.427280  -1.964482   2.611089
C   1.427280  -1.964482   2.611089
C   0.692848  -2.975340   1.838862
C  -0.692848  -2.975340   1.838862
C  -1.427280  -3.213972   0.589372
C  -2.615615  -2.350596   0.589372
C  -3.043819  -1.761224  -0.589372
C  -3.497723  -0.364252  -0.589372
C  -3.043819   0.260493  -1.838862
C  -2.615615   1.578368  -1.838862
C   0.734432   3.439092   0.589372
C   0.734432   1.010858  -3.339592
C   1.427280   1.964482  -2.611089
C   2.615615   1.578368  -1.838862
C   3.043819   0.260493  -1.838862
C   2.309387  -0.750365  -2.611089
C   0.000000  -1.249490  -3.339592
C  -1.188335  -0.386114  -3.339592
C  -0.734432   1.010858  -3.339592
C  -1.427280   1.964482  -2.611089
C  -0.692848   2.975340  -1.838862
C   0.692848   2.975340  -1.838862
C   2.615616   2.350596  -0.589372
C   3.043819   1.761224   0.589372
C   3.497723   0.364252   0.589372
C   3.497723  -0.364252  -0.589372
C   3.043819  -1.761224  -0.589372
C   2.309387  -1.999855  -1.838862
C   1.188335  -2.814347  -1.838862
C   0.000000  -2.428233  -2.611089
C  -2.309387  -0.750365  -2.611089
```

```
C  -2.309387  -1.999855  -1.838862
C  -1.188335  -2.814347  -1.838862
C  -0.734432  -3.439092  -0.589372
C   0.734432  -3.439092  -0.589372
C   1.427280  -3.213972   0.589372
C   2.615615  -2.350596   0.589372
C   2.615615  -1.578368   1.838862
C   3.043818  -0.260493   1.838862
C   1.427280   3.213972  -0.589372
C   2.309387   1.999855   1.838862
C   1.188335  -0.386114  -3.339592

CH4 at C60

0 1
C   0.000000   0.000000   0.000001
H   0.627553   0.627553  -0.627552
H   0.627553  -0.627553   0.627554
H  -0.627553   0.627553   0.627554
H  -0.627553  -0.627553  -0.627552
C   3.339590  -0.386110   1.188331
C   3.339590   1.010850   0.734421
C   2.611090   1.964480   1.427271
C   1.838860   1.578360   2.615611
C   1.838860   0.260490   3.043811
C   2.611090  -0.750360   2.309381
C   3.339590  -1.249480   0.000001
C   3.339590  -0.386110  -1.188329
C   3.339590   1.010850  -0.734429
C   2.611080   1.964480  -1.427279
C   1.838860   2.975340   0.692841
C   0.589370   2.350590   2.615611
C  -0.589360   1.761220   3.043821
C  -0.589360   0.364250   3.497721
C   0.589360  -0.364250   3.497721
C   0.589360  -1.761220   3.043821
C   1.838860  -1.999850   2.309381
C   1.838860  -2.814340   1.188331
C   2.611080  -2.428230   0.000001
C   2.611080  -0.750360  -2.309389
C   1.838850  -1.999850  -2.309389
C   1.838850  -2.814340  -1.188329
C   0.589370  -3.439090  -0.734429
C   0.589370  -3.439090   0.734421
C  -0.589360  -3.213970   1.427281
C  -0.589370  -2.350590   2.615611
C  -1.838860  -1.578360   2.615611
C  -1.838860  -0.260490   3.043811
C   0.589360   3.213970   1.427281
C  -3.339590   1.249480   0.000001
C  -2.611080   2.428230   0.000001
C  -1.838850   2.814340  -1.188329
C  -1.838850   1.999850  -2.309389
C  -2.611080   0.750360  -2.309389
C  -3.339590  -1.010850  -0.734429
C  -3.339590  -1.010850   0.734421
C  -3.339590   0.386110   1.188331
C  -2.611090   0.750360   2.309381
C  -1.838860   1.999850   2.309381
C  -1.838860   2.814340   1.188331
C  -0.589370   3.439090  -0.734429
C   0.589370   3.213970  -1.427279
C   0.589360   2.350590  -2.615609
C  -0.589370   1.761220  -3.043809
C  -0.589370   0.364250  -3.497719
C  -1.838860  -0.260480  -3.043809
C  -1.838860  -1.578370  -2.615609
C  -2.611080  -1.964480  -1.427279
C  -2.611090  -1.964480   1.427271
C  -1.838860  -2.975340   0.692841
C  -1.838860  -2.975340  -0.692839
C  -0.589370  -3.213970  -1.427279
C  -0.589360  -2.350590  -2.615609
C   0.589370  -1.761220  -3.043809
C   0.589370  -0.364250  -3.497719
C   1.838860   0.260480  -3.043809
C   1.838860   1.578370  -2.615609
C  -0.589370   3.439090   0.734421
C   1.838860   2.975340  -0.692839
C  -3.339590   0.386110  -1.188329

CF4 at C60
```

```
0 1
C    0.000000    0.000000    0.000001
F    0.759574    0.759574   -0.759573
F    0.759574   -0.759574    0.759575
F   -0.759574    0.759574    0.759575
F   -0.759574   -0.759574   -0.759573
C    3.339590   -0.386110    1.188331
C    3.339590    1.010850    0.734421
C    2.611090    1.964480    1.427271
C    1.838860    1.578360    2.615611
C    1.838860    0.260490    3.043811
C    2.611090   -0.750360    2.309381
C    3.339590   -1.249480    0.000001
C    3.339590   -0.386110   -1.188329
C    3.339590    1.010850   -0.734429
C    2.611080    1.964480   -1.427279
C    1.838860    2.975340    0.692841
C    0.589370    2.350590    2.615611
C   -0.589360    1.761220    3.043821
C   -0.589360    0.364250    3.497721
C    0.589360   -0.364250    3.497721
C    0.589360   -1.761220    3.043821
C    1.838860   -1.999850    2.309381
C    1.838860   -2.814340    1.188331
C    2.611080   -2.428230    0.000001
C    2.611080   -0.750360   -2.309389
C    1.838850   -1.999850   -2.309389
C    1.838850   -2.814340   -1.188329
C    0.589370   -3.439090   -0.734429
C    0.589370   -3.439090    0.734421
C   -0.589360   -3.213970    1.427281
C   -0.589370   -2.350590    2.615611
C   -1.838860   -1.578360    2.615611
C   -1.838860   -0.260490    3.043811
C    0.589360    3.213970    1.427281
C   -3.339590    1.249480    0.000001
C   -2.611080    2.428230    0.000001
C   -1.838850    2.814340   -1.188329
C   -1.838850    1.999850   -2.309389
C   -2.611080    0.750360   -2.309389
C   -3.339590   -1.010850   -0.734429
C   -3.339590   -1.010850    0.734421
C   -3.339590    0.386110    1.188331
C   -2.611090    0.750360    2.309381
C   -1.838860    1.999850    2.309381
C   -1.838860    2.814340    1.188331
C   -0.589370    3.439090   -0.734429
C    0.589370    3.213970   -1.427279
C    0.589360    2.350590   -2.615609
C   -0.589370    1.761220   -3.043809
C   -0.589370    0.364250   -3.497719
C   -1.838860   -0.260480   -3.043809
C   -1.838860   -1.578370   -2.615609
C   -2.611080   -1.964480   -1.427279
C   -2.611090   -1.964480    1.427271
C   -1.838860   -2.975340    0.692841
C   -1.838860   -2.975340   -0.692839
C   -0.589370   -3.213970   -1.427279
C   -0.589360   -2.350590   -2.615609
C    0.589370   -1.761220   -3.043809
C    0.589370   -0.364250   -3.497719
C    1.838860    0.260480   -3.043809
C    1.838860    1.578370   -2.615609
C   -0.589370    3.439090    0.734421
C    1.838860    2.975340   -0.692839
C   -3.339590    0.386110   -1.188329

SF2

0 1
S    0.000000    0.000000    0.551374
F    0.000000    1.197567   -0.490110
F    0.000000   -1.197567   -0.490110

SF6

0 1
S    0.000000    0.000000    0.000000
F    0.000000    0.000000    1.558777
F    0.000000    1.558777    0.000000
F   -1.558777    0.000000    0.000000
```

```
F    0.000000    0.000000   -1.558777
F    0.000000   -1.558777    0.000000
F    1.558777    0.000000    0.000000

(Benzene)3

0 1
C   -1.201735    0.694417    0.000000
H   -2.138699    1.235892    0.000000
C   -1.201955   -0.693340    0.000000
H   -2.138820   -1.235057    0.000000
C   -0.000428   -1.387587    0.000000
H   -0.001833   -2.469715    0.000000
C    1.201735   -0.694417    0.000000
H    2.138699   -1.235893    0.000000
C    1.201956    0.693340    0.000000
H    2.138821    1.235057    0.000000
C    0.000429    1.387588    0.000000
H    0.001832    2.469716    0.000000
C    1.202118    0.693355    3.746661
H    2.138599    1.234999    3.739839
C    1.202118   -0.694646    3.746342
H    2.138798   -1.236017    3.739043
C   -0.000356   -1.387692    3.746765
H   -0.001833   -2.469447    3.739853
C   -1.202118   -0.693355    3.746661
H   -2.138599   -1.234999    3.739838
C   -1.202118    0.694646    3.746342
H   -2.138797    1.236019    3.739042
C    0.000356    1.387692    3.746765
H    0.001835    2.469447    3.739853
C   -1.202118    0.694646   -3.746342
H   -2.138797    1.236019   -3.739042
C   -1.202118   -0.693355   -3.746661
H   -2.138599   -1.234999   -3.739838
C   -0.000356   -1.387692   -3.746765
H   -0.001833   -2.469447   -3.739853
C    1.202118   -0.694646   -3.746342
H    2.138798   -1.236017   -3.739043
C    1.202118    0.693355   -3.746661
H    2.138599    1.234999   -3.739839
C    0.000356    1.387692   -3.746765
H    0.001835    2.469447   -3.739853

C5H12

0 1
C   -0.000025    0.000073    0.000000
C    0.509848   -1.441681    0.000000
C   -1.529549   -0.000252    0.000000
C    0.509848    0.720928    1.248619
C    0.509848    0.720928   -1.248619
H    1.600975   -1.468124    0.000000
H    0.158721   -1.978172    0.883277
H    0.158721   -1.978172   -0.883277
H   -1.919134    1.019322    0.000000
H   -1.918774   -0.510173   -0.883176
H   -1.918774   -0.510173    0.883176
H    0.157520    0.225522    2.155136
H    1.601034    0.732487    1.272666
H    0.160665    1.754749    1.271260
H    0.157520    0.225522   -2.155136
H    0.160665    1.754749   -1.271260
H    1.601034    0.732487   -1.272666

C12H14

0 1
C    0.080692    6.739301    0.000000
H   -0.997323    6.844203    0.000000
H    0.666405    7.647267    0.000000
C    0.654779    5.537167    0.000000
H    1.737623    5.460228    0.000000
C   -0.080692    4.288260    0.000000
H   -1.165115    4.355740    0.000000
C    0.500691    3.078964    0.000000
H    1.585600    3.016964    0.000000
C   -0.224411    1.832767    0.000000
H   -1.309234    1.893088    0.000000
C    0.361397    0.622942    0.000000
H    1.446345    0.563624    0.000000
C   -0.361397   -0.622942    0.000000
```

```
H  -1.446345  -0.563624   0.000000
C   0.224411  -1.832767   0.000000
H   1.309234  -1.893088   0.000000
C  -0.500691  -3.078964   0.000000
H  -1.585600  -3.016964   0.000000
C   0.080692  -4.288260   0.000000
H   1.165115  -4.355740   0.000000
C  -0.654779  -5.537167   0.000000
H  -1.737623  -5.460228   0.000000
C  -0.080692  -6.739301   0.000000
H   0.997323  -6.844203   0.000000
H  -0.666405  -7.647267   0.000000

C96H26

0 1
C   0.000000   6.225287   1.450891
C   0.000000   6.219340   2.808653
C   0.000000  -1.239250   9.955937
C   0.000000  -2.472435   9.216774
C   0.000000   7.469389  -0.673093
C   0.000000   7.469389   0.673093
C   0.000000  -2.486701   7.839025
C   0.000000  -3.722492   7.078995
C   0.000000   6.219340  -2.808653
C   0.000000   6.225287  -1.450891
C   0.000000  -3.732521   5.710587
C   0.000000  -4.970668   4.942968
C   0.000000   4.970668  -4.942968
C   0.000000   4.978579  -3.579965
C   0.000000  -4.978579   3.579965
C   0.000000  -6.219340   2.808653
C   0.000000   3.722492  -7.078995
C   0.000000   3.732521  -5.710587
C   0.000000  -6.225287   1.450891
C   0.000000  -7.469389   0.673093
C   0.000000   2.472435  -9.216774
C   0.000000   2.486701  -7.839025
C   0.000000  -1.215405 -11.364653
C   0.000000   0.000000 -12.050936
C   0.000000   1.215405 -11.364653
C   0.000000   1.239250  -9.955937
C   0.000000   4.978579   3.579965
C   0.000000   4.970668   4.942968
C   0.000000  -2.472435  -9.216774
C   0.000000  -1.239250  -9.955937
C   0.000000   4.969065  -0.687621
C   0.000000   4.969065   0.687621
C   0.000000   3.722139  -2.825734
C   0.000000   3.721840  -1.439182
C   0.000000   2.477529  -4.964499
C   0.000000   2.479562  -3.565459
C   0.000000   1.234595  -7.104008
C   0.000000   1.238866  -5.689379
C   0.000000   0.000000  -9.244707
C   0.000000   0.000000  -7.812302
C   0.000000   3.732521   5.710587
C   0.000000   3.722492   7.078995
C   0.000000  -3.722492  -7.078995
C   0.000000  -2.486701  -7.839025
C   0.000000   3.721840   1.439182
C   0.000000   3.722139   2.825734
C   0.000000   2.477372  -0.701793
C   0.000000   2.477372   0.701793
C   0.000000   1.237621  -2.840156
C   0.000000   1.238548  -1.424923
C   0.000000   0.000000  -4.975586
C   0.000000   0.000000  -3.553801
C   0.000000  -1.234595  -7.104008
C   0.000000  -1.238866  -5.689379
C   0.000000   2.486701   7.839025
C   0.000000   2.472435   9.216774
C   0.000000  -4.970668  -4.942968
C   0.000000  -3.732521  -5.710587
C   0.000000   2.479562   3.565459
C   0.000000   2.477529   4.964499
C   0.000000   1.238548   1.424923
C   0.000000   1.237621   2.840156
C   0.000000   0.000000  -0.709524
C   0.000000   0.000000   0.709524
C   0.000000  -1.237621  -2.840156
C   0.000000  -1.238548  -1.424923
```

```
C    0.000000  -2.477529  -4.964499
C    0.000000  -2.479562  -3.565459
C    0.000000   1.239250   9.955937
C    0.000000   1.215405  11.364653
C    0.000000  -6.219340  -2.808653
C    0.000000  -4.978579  -3.579965
C    0.000000   1.238866   5.689379
C    0.000000   1.234595   7.104008
C    0.000000   0.000000   3.553801
C    0.000000   0.000000   4.975586
C    0.000000  -1.238548   1.424923
C    0.000000  -1.237621   2.840156
C    0.000000  -2.477372  -0.701793
C    0.000000  -2.477372   0.701793
C    0.000000  -3.722139  -2.825734
C    0.000000  -3.721840  -1.439182
C    0.000000   0.000000  12.050936
C    0.000000  -1.215405  11.364653
C    0.000000  -7.469389  -0.673093
C    0.000000  -6.225287  -1.450891
C    0.000000   0.000000   7.812302
C    0.000000   0.000000   9.244707
C    0.000000  -1.238866   5.689379
C    0.000000  -1.234595   7.104008
C    0.000000  -2.479562   3.565459
C    0.000000  -2.477529   4.964499
C    0.000000  -3.721840   1.439182
C    0.000000  -3.722139   2.825734
C    0.000000  -4.969065  -0.687621
C    0.000000  -4.969065   0.687621
H    0.000000   7.149974   3.377380
H    0.000000  -3.404550   9.780991
H    0.000000   8.401422  -1.240430
H    0.000000   8.401422   1.240430
H    0.000000  -4.654331   7.644612
H    0.000000   7.149974  -3.377380
H    0.000000  -5.901973   5.510065
H    0.000000   5.901973  -5.510065
H    0.000000  -7.149974   3.377380
H    0.000000   4.654331  -7.644612
H    0.000000  -8.401422   1.240430
H    0.000000   3.404550  -9.780991
H    0.000000  -2.151823 -11.920009
H    0.000000   0.000000 -13.141719
H    0.000000   2.151823 -11.920009
H    0.000000   5.901973   5.510065
H    0.000000  -3.404550  -9.780991
H    0.000000   4.654331   7.644612
H    0.000000  -4.654331  -7.644612
H    0.000000   3.404550   9.780991
H    0.000000  -5.901973  -5.510065
H    0.000000   2.151823  11.920009
H    0.000000  -7.149974  -3.377380
H    0.000000   0.000000  13.141719
H    0.000000  -2.151823  11.920009
H    0.000000  -8.401422  -1.240430

acetone-water (12 water molecules)

0 1
O    0.000000   0.000000   1.395409
C    0.000000   0.000000   0.177466
C    0.000000   1.275926  -0.608409
C    0.000000  -1.275926  -0.608409
H    0.000000   2.139336   0.050808
H    0.000000  -2.139336   0.050808
H    0.876906   1.299124  -1.257196
H    0.876906  -1.299124  -1.257196
H   -0.876906   1.299124  -1.257196
H   -0.876906  -1.299124  -1.257196
H   -3.106158  -1.896462   2.406497
O   -2.672647  -1.522396   1.611980
H   -1.726083  -1.644698   1.793272
H   -3.876797  -1.453805   0.170132
O   -4.251901  -1.233327  -0.671117
H   -5.177834  -1.089183  -0.471068
H    0.121393  -4.488770   1.980066
O    0.442697  -3.964965   2.748762
H    1.377232  -3.770081   2.538644
H   -1.410705  -0.500657   4.964791
O   -1.681473   0.003280   5.743237
H   -1.809478  -0.709585   6.406313
```

```
H    1.245568    1.970856    3.861180
O    1.838894    2.231540    3.189408
H    1.513314    1.775496    2.451685
H    4.339303   -1.979092   -0.938937
O    3.444972   -1.940736   -0.587391
H    3.102524   -1.133507   -0.986160
H    3.016685    1.230053   -1.069748
O    2.894563    0.561667   -1.799360
H    2.389483    1.015861   -2.519741
H    0.013587   -2.144632    3.629261
O   -0.349095   -1.260988    3.828802
H   -0.042940   -0.738553    3.072237
H    3.958244    0.095715    1.556233
O    3.313833   -0.226101    2.114242
H    3.246151    0.415492    2.833154
H   -3.030724    2.937169    1.671951
O   -3.186875    3.390127    0.853435
H   -4.046205    3.850681    0.940159
H    3.498857   -2.866810    1.283616
O    2.987831   -3.062979    2.083142
H    3.017378   -2.256431    2.570383
H   -4.069937    1.062672    2.917190
O   -3.106326    1.116319    2.819414
H   -2.883245    0.291751    2.332307

acetone-water (24 water molecules)

0 1
O    0.373333   -0.067106   -0.120431
C    0.445975   -1.020275    0.634273
C   -0.366983   -1.091264    1.891113
C    1.352678   -2.179346    0.351375
H   -0.988142   -0.207208    2.003591
H    1.895201   -2.031588   -0.578076
H   -0.989693   -1.986850    1.866965
H    0.761233   -3.094715    0.299233
H    0.301854   -1.191383    2.747303
H    2.052780   -2.299248    1.179571
H    3.878476    1.324390   -0.332087
O    3.354538    0.665469    0.168339
H    2.729072    0.325872   -0.492928
H    4.281075    0.112477    1.707604
O    4.458908   -0.281745    2.550206
H    5.031718    0.356247    2.977996
H    1.052977    0.478759    4.306485
O    1.487705   -0.124721    4.935829
H    0.867406   -0.339239    5.595049
H    3.273991   -1.578574   -3.252086
O    2.638543   -0.899375   -3.573639
H    1.831532   -1.404591   -3.794945
H    1.536705    3.152682   -1.926188
O    1.350079    4.099583   -1.968576
H    1.885188    4.372610   -2.745330
H   -3.422287    2.938900   -0.624450
O   -4.120107    3.579793   -0.401224
H   -3.657822    4.393704   -0.547535
H    4.736737   -3.000058   -1.171530
O    4.429209   -2.773551   -2.055938
H    3.617680   -3.279612   -2.189806
H   -2.019133    2.138025   -1.084402
O   -2.591677    1.454334   -0.808667
H   -2.000590    0.830207   -0.463275
H   -1.349315   -4.705997   -2.046230
O   -0.737524   -4.008883   -1.792008
H   -1.005535   -3.821446   -0.885949
H    4.335484   -2.337006    1.791609
O    4.752660   -2.752798    1.040121
H    5.681306   -2.580322    1.198371
H   -2.530109   -2.840132    0.635060
O   -1.946243   -3.640733    0.745176
H   -1.837400   -3.781757    1.719143
H   -4.582400   -2.508094    1.566916
O   -4.045079   -1.856247    1.028796
H   -4.040841   -1.070525    1.625075
H    1.675334    0.760507   -2.805496
O    1.335043    1.457945   -2.213918
H    0.802645    0.949753   -1.583559
H   -2.615701   -1.695753   -2.149200
O   -1.957556   -1.103989   -2.365684
H   -2.382953   -0.237098   -2.390063
H   -4.325085   -1.970542   -0.673824
O   -4.388525   -2.124079   -1.620906
```

```
H  -5.248536  -1.827548  -1.847162
H  -0.550790   3.995108  -1.666214
O  -1.515854   3.774424  -1.789998
H  -1.597304   3.617673  -2.729693
H  -2.439246   0.704361  -4.172632
O  -2.445609   1.555991  -3.678685
H  -3.348199   1.579788  -3.293245
H   0.609413   2.776324   3.001731
O   0.467982   2.399710   3.860615
H   0.785278   3.053718   4.516112
H  -1.609300   2.551996   3.675334
O  -2.290750   2.727958   3.030698
H  -1.949718   3.518035   2.613941
H  -0.264730  -2.963932  -3.537209
O   0.196111  -2.190079  -3.894490
H  -0.398231  -1.478260  -3.724588
H  -0.889038  -3.986632   3.673381
O  -1.732189  -3.801278   3.296862
H  -2.180208  -3.330182   4.009728
H  -3.814452   1.553780   2.416261
O  -4.483519   0.825587   2.429382
H  -4.884228   0.837212   1.583685
H   5.295589   3.965322  -0.883325
O   4.410777   3.644151  -0.697305
H   4.012884   3.544214  -1.599045
H   2.563642   3.422940   1.620718
O   1.823697   2.932234   1.229984
H   2.244134   2.098253   0.922317

acetone-water (36 water molecules)

0 1
O   0.165216  -0.077237   0.054443
C  -0.240195   0.917173   0.629054
C   0.362775   1.379100   1.920811
C  -1.366347   1.738526   0.078829
H   1.167248   0.719261   2.233029
H  -1.731959   1.321908  -0.855410
H   0.737604   2.396569   1.799625
H  -1.022955   2.762530  -0.075847
H  -0.412535   1.414521   2.687666
H  -2.173094   1.780482   0.812194
H  -2.820260  -2.374935  -0.218682
O  -2.546969  -1.536181   0.206662
H  -1.948743  -1.136945  -0.446441
H  -3.770107  -1.042887   1.546140
O  -4.146726  -0.597129   2.292110
H  -4.589687  -1.299242   2.770621
H  -1.690147   3.921072   4.960870
O  -1.602891   3.661944   4.032233
H  -2.477298   3.356705   3.724188
H  -0.909722  -0.160905   4.435649
O  -1.558542   0.385406   4.915053
H  -1.100923   0.848752   5.579324
H  -2.399613  -2.141165  -3.872298
O  -2.961292  -2.926472  -4.011451
H  -3.630064  -2.587096  -4.604669
H   2.381855  -0.282971  -5.425885
O   3.142330   0.266046  -5.215768
H   3.053941   1.062284  -5.750630
H  -2.602131   0.145625  -3.522950
O  -1.780622  -0.375853  -3.670209
H  -1.105648   0.291546  -3.903608
H   0.088966  -3.710924  -1.276623
O   0.511981  -4.569094  -1.143028
H   0.165717  -5.081744  -1.905606
H   4.628049  -1.992400   0.389279
O   5.430781  -2.384411   0.775899
H   5.210865  -3.304772   0.729649
H  -4.627082   1.398200  -1.843788
O  -4.162998   1.141284  -2.647950
H  -3.494972   1.822933  -2.795237
H   3.138264  -1.670592  -0.316963
O   3.480392  -0.826597  -0.112292
H   2.712303  -0.342346   0.071431
H   6.987834  -0.538037  -1.764236
O   6.037350  -0.400871  -1.808182
H   5.943297   0.497955  -2.101996
H  -6.456441  -1.201727  -1.558305
O  -5.740646  -1.758863  -1.298007
H  -4.990722  -1.176982  -1.227869
H  -5.322764   4.341822  -0.369121
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O  -4.359951   4.338908  -0.309788
H  -4.166132   3.409778  -0.127241
H   0.892858   4.537226  -2.469996
O   0.449369   3.744017  -2.155321
H   0.639031   3.764147  -1.211113
H  -4.450155   1.288602   1.211948
O  -4.860037   1.467626   0.368384
H  -5.727570   1.075820   0.473499
H   2.156451   3.451423   0.577856
O   1.380607   4.072886   0.501459
H   1.117348   4.314260   1.424920
H   4.091153   3.816876   1.724101
O   3.808011   2.975995   1.259407
H   3.926443   2.309463   1.976787
H  -2.913689   1.269294   4.400904
O  -3.732819   1.563818   4.070709
H  -4.005910   0.916765   3.456794
H  -0.535493  -1.591423  -2.554383
O  -0.108165  -2.081886  -1.827046
H   0.194775  -1.366329  -1.248025
H   2.879397   1.994396  -1.956597
O   2.424477   1.223289  -2.125856
H   3.054133   0.508056  -1.967643
H   4.263395   2.922023  -0.407955
O   4.405469   2.952925  -1.358440
H   5.333939   2.869809  -1.457307
H   0.604363   5.689290  -0.366308
O   0.076553   6.464844  -0.586154
H  -0.799916   6.090391  -0.678431
H   2.271106  -3.916386  -0.701335
O   3.157068  -3.464028  -0.777602
H   3.314675  -3.424191  -1.719836
H   3.571030  -0.623356  -3.555028
O   3.729195  -1.364161  -2.926149
H   4.552358  -1.090360  -2.466546
H   1.861015  -4.853012   3.545739
O   2.553438  -4.172951   3.708251
H   3.011152  -4.468667   4.507863
H   0.259948  -2.413777   3.578692
O   0.192011  -1.896722   4.370879
H  -0.030596  -2.513581   5.097523
H   2.246819  -1.509503   4.391943
O   3.026560  -1.584222   3.846677
H   2.951208  -2.487110   3.541182
H  -3.386683   4.329260  -4.595992
O  -2.968666   3.920895  -3.831258
H  -2.191773   4.439518  -3.699988
H   0.479997   2.377013  -3.733784
O   0.278081   1.465709  -3.993832
H   1.006156   0.970836  -3.656484
H  -0.091546   4.527976   3.228614
O   0.811758   4.525264   2.962041
H   1.270056   4.296422   3.779613
H   4.270344  -0.141680   3.175883
O   4.727110   0.733934   3.123413
H   5.221548   0.712256   2.329077
H  -3.444627  -5.349694  -0.436797
O  -2.700199  -4.779808  -0.232580
H  -2.229481  -4.703763  -1.100959
H  -2.140788  -6.210172  -3.253080
O  -1.668554  -5.464555  -2.848655
H  -1.403189  -4.911372  -3.645637
H  -1.277214  -3.748359   2.164356
O  -0.641479  -3.136510   1.761285
H  -1.216049  -2.497750   1.282948
H  -3.602231  -5.321591   2.693798
O  -2.817021  -4.784712   2.532335
H  -2.745551  -4.764330   1.557417

Li91+, bcc with a=3.50

1 1
LI  -5.251500   5.251500   5.251500
LI  -1.750500   5.251500   5.251500
LI   1.750500   5.251500   5.251500
LI   5.251500   5.251500   5.251500
LI  -5.251500   5.251500   1.750500
LI  -1.750500   5.251500   1.750500
LI   1.750500   5.251500   1.750500
LI   5.251500   5.251500   1.750500
LI  -5.251500   5.251500  -1.750500
LI  -1.750500   5.251500  -1.750500
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LI   1.750500   5.251500  -1.750500
LI   5.251500   5.251500  -1.750500
LI  -5.251500   5.251500  -5.251500
LI  -1.750500   5.251500  -5.251500
LI   1.750500   5.251500  -5.251500
LI   5.251500   5.251500  -5.251500
LI  -5.251500   1.750500   5.251500
LI  -1.750500   1.750500   5.251500
LI   1.750500   1.750500   5.251500
LI   5.251500   1.750500   5.251500
LI  -5.251500   1.750500   1.750500
LI  -1.750500   1.750500   1.750500
LI   1.750500   1.750500   1.750500
LI   5.251500   1.750500   1.750500
LI  -5.251500   1.750500  -1.750500
LI  -1.750500   1.750500  -1.750500
LI   1.750500   1.750500  -1.750500
LI   5.251500   1.750500  -1.750500
LI  -5.251500   1.750500  -5.251500
LI  -1.750500   1.750500  -5.251500
LI   1.750500   1.750500  -5.251500
LI   5.251500   1.750500  -5.251500
LI  -5.251500  -1.750500   5.251500
LI  -1.750500  -1.750500   5.251500
LI   1.750500  -1.750500   5.251500
LI   5.251500  -1.750500   5.251500
LI  -5.251500  -1.750500   1.750500
LI  -1.750500  -1.750500   1.750500
LI   1.750500  -1.750500   1.750500
LI   5.251500  -1.750500   1.750500
LI  -5.251500  -1.750500  -1.750500
LI  -1.750500  -1.750500  -1.750500
LI   1.750500  -1.750500  -1.750500
LI   5.251500  -1.750500  -1.750500
LI  -5.251500  -1.750500  -5.251500
LI  -1.750500  -1.750500  -5.251500
LI   1.750500  -1.750500  -5.251500
LI   5.251500  -1.750500  -5.251500
LI  -5.251500  -5.251500   5.251500
LI  -1.750500  -5.251500   5.251500
LI   1.750500  -5.251500   5.251500
LI   5.251500  -5.251500   5.251500
LI  -5.251500  -5.251500   1.750500
LI  -1.750500  -5.251500   1.750500
LI   1.750500  -5.251500   1.750500
LI   5.251500  -5.251500   1.750500
LI  -5.251500  -5.251500  -1.750500
LI  -1.750500  -5.251500  -1.750500
LI   1.750500  -5.251500  -1.750500
LI   5.251500  -5.251500  -1.750500
LI  -5.251500  -5.251500  -5.251500
LI  -1.750500  -5.251500  -5.251500
LI   1.750500  -5.251500  -5.251500
LI   5.251500  -5.251500  -5.251500
LI  -3.501000   3.501000   3.501000
LI   0.000000   3.501000   3.501000
LI   3.501000   3.501000   3.501000
LI  -3.501000   3.501000   0.000000
LI   0.000000   3.501000   0.000000
LI   3.501000   3.501000   0.000000
LI  -3.501000   3.501000  -3.501000
LI   0.000000   3.501000  -3.501000
LI   3.501000   3.501000  -3.501000
LI  -3.501000   0.000000   3.501000
LI   0.000000   0.000000   3.501000
LI   3.501000   0.000000   3.501000
LI  -3.501000   0.000000   0.000000
LI   0.000000   0.000000   0.000000
LI   3.501000   0.000000   0.000000
LI  -3.501000   0.000000  -3.501000
LI   0.000000   0.000000  -3.501000
LI   3.501000   0.000000  -3.501000
LI  -3.501000  -3.501000   3.501000
LI   0.000000  -3.501000   3.501000
LI   3.501000  -3.501000   3.501000
LI  -3.501000  -3.501000   0.000000
LI   0.000000  -3.501000   0.000000
LI   3.501000  -3.501000   0.000000
LI  -3.501000  -3.501000  -3.501000
LI   0.000000  -3.501000  -3.501000
LI   3.501000  -3.501000  -3.501000
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NMR STRUCTURE OF TRP-CAGE MINIPROTEIN CONSTRUCT TC5B, 1L2Y (the last column contains labels for amino acid residues)

1 1

N	10.390363	1.157668	-0.236338	Asn1
C	9.869758	-0.186403	0.096679	Asn1
C	8.461791	-0.183277	0.711555	Asn1
O	7.801756	-1.221351	0.663584	Asn1
C	10.844954	-0.973641	1.004612	Asn1
C	12.069008	-1.498341	0.253422	Asn1
O	11.928548	-2.329764	-0.640391	Asn1
N	13.264225	-1.014455	0.594567	Asn1
H	9.741712	1.632134	-0.848432	Asn1
H	10.518274	1.696769	0.608085	Asn1
H	11.279844	1.063212	-0.705792	Asn1
H	9.766724	-0.714767	-0.853347	Asn1
H	11.150187	-0.365933	1.858134	Asn1
H	10.347729	-1.849989	1.425660	Asn1
H	13.354130	-0.349910	1.349411	Asn1
H	14.088771	-1.346770	0.112375	Asn1
N	7.977855	0.946012	1.264721	Leu2
C	6.665301	1.049735	1.923069	Leu2
C	5.482815	0.869309	0.956453	Leu2
O	4.427324	0.392434	1.371931	Leu2
C	6.530971	2.428397	2.609797	Leu2
C	7.444854	2.638239	3.835713	Leu2
C	7.434186	4.112167	4.266673	Leu2
C	7.048563	1.737829	5.018928	Leu2
H	8.554256	1.774307	1.284627	Leu2
H	6.584702	0.254169	2.664656	Leu2
H	6.726733	3.209146	1.872545	Leu2
H	5.498094	2.586424	2.927467	Leu2
H	8.468564	2.393437	3.553074	Leu2
H	7.758706	4.763913	3.454802	Leu2
H	6.436707	4.431415	4.569651	Leu2
H	8.106768	4.281244	5.108123	Leu2
H	6.018006	1.914672	5.325895	Leu2
H	7.147515	0.679908	4.778634	Leu2
H	7.687106	1.926329	5.882942	Leu2
N	5.674241	1.207118	-0.330337	Tyr3
C	4.677777	1.060890	-1.387198	Tyr3
C	4.451187	-0.415936	-1.766865	Tyr3
O	3.340067	-0.769884	-2.151540	Tyr3
C	5.154018	1.855164	-2.620455	Tyr3
C	4.033047	2.245034	-3.563177	Tyr3
C	3.279375	3.406490	-3.298679	Tyr3
C	3.728418	1.455129	-4.692130	Tyr3
C	2.224407	3.776546	-4.152518	Tyr3
C	2.671875	1.827192	-5.547547	Tyr3
C	1.921356	2.988913	-5.278254	Tyr3
O	0.898151	3.352327	-6.103809	Tyr3
H	6.569193	1.593666	-0.590170	Tyr3
H	3.738286	1.485866	-1.026014	Tyr3
H	5.631297	2.782838	-2.296616	Tyr3
H	5.924412	1.308227	-3.166939	Tyr3
H	3.504817	4.018809	-2.436317	Tyr3
H	4.297975	0.561542	-4.899805	Tyr3
H	1.651350	4.667349	-3.944890	Tyr3
H	2.442284	1.223720	-6.412259	Tyr3
H	0.787517	2.772459	-6.841160	Tyr3
N	5.469865	-1.281228	-1.603009	Ile4
C	5.394967	-2.728521	-1.835456	Ile4
C	4.551257	-3.398365	-0.737419	Ile4
O	3.788119	-4.317006	-1.033725	Ile4
C	6.827232	-3.345666	-1.847447	Ile4
C	7.823806	-2.591635	-2.760974	Ile4
C	6.830635	-4.855358	-2.172156	Ile4
C	7.415048	-2.521252	-4.240572	Ile4
H	6.342961	-0.922135	-1.246033	Ile4
H	4.911791	-2.905196	-2.798974	Ile4
H	7.233070	-3.260025	-0.839491	Ile4
H	7.971403	-1.577146	-2.391761	Ile4
H	8.803554	-3.064469	-2.688364	Ile4
H	6.341263	-5.056746	-3.125433	Ile4
H	7.848328	-5.242190	-2.232097	Ile4
H	6.316351	-5.439419	-1.409215	Ile4
H	7.316832	-3.514792	-4.676796	Ile4
H	6.467150	-1.999779	-4.374368	Ile4
H	8.165183	-1.983198	-4.819025	Ile4
N	4.665815	-2.914706	0.513695	Gln5
C	3.921445	-3.415787	1.665738	Gln5
C	2.445604	-2.964328	1.629634	Gln5

O	1.573984	-3.719962	2.055798	Gln5
C	4.603720	-2.918118	2.962339	Gln5
C	4.611104	-4.018931	4.041538	Gln5
C	4.933866	-3.528154	5.453168	Gln5
O	5.537503	-2.475537	5.648183	Gln5
N	4.514033	-4.303232	6.454910	Gln5
H	5.303851	-2.148996	0.672569	Gln5
H	3.958040	-4.506562	1.632219	Gln5
H	5.638805	-2.632637	2.764862	Gln5
H	4.121160	-2.011666	3.334635	Gln5
H	3.629801	-4.495667	4.072613	Gln5
H	5.323244	-4.798304	3.770884	Gln5
H	4.016369	-5.159285	6.258357	Gln5
H	4.695348	-4.026361	7.408053	Gln5
N	2.163765	-1.772202	1.069210	Trp6
C	0.815753	-1.249637	0.834337	Trp6
C	0.096906	-2.000703	-0.304450	Trp6
O	-1.095140	-2.283112	-0.175776	Trp6
C	0.911427	0.251651	0.490514	Trp6
C	-0.374268	0.896041	0.058773	Trp6
C	-1.400908	1.236195	0.870556	Trp6
C	-0.801478	1.244672	-1.293117	Trp6
N	-2.434830	1.747682	0.115389	Trp6
C	-2.116473	1.795319	-1.223585	Trp6
C	-0.211119	1.152687	-2.573610	Trp6
C	-2.799530	2.259381	-2.360824	Trp6
C	-0.897621	1.587549	-3.724904	Trp6
C	-2.180989	2.155308	-3.619554	Trp6
H	2.937738	-1.200371	0.758332	Trp6
H	0.227434	-1.365963	1.747085	Trp6
H	1.284435	0.794717	1.360191	Trp6
H	1.646350	0.416493	-0.297124	Trp6
H	-1.402401	1.097166	1.942361	Trp6
H	-3.305558	2.068231	0.520354	Trp6
H	0.782394	0.742968	-2.668942	Trp6
H	-3.787166	2.687609	-2.267463	Trp6
H	-0.430748	1.496828	-4.692937	Trp6
H	-2.691083	2.509725	-4.503014	Trp6
N	0.811673	-2.350060	-1.391372	Leu7
C	0.286176	-3.150691	-2.502320	Leu7
C	0.002307	-4.606156	-2.092947	Leu7
O	-0.910423	-5.216006	-2.646909	Leu7
C	1.296598	-3.164099	-3.673199	Leu7
C	1.352946	-1.879943	-4.527062	Leu7
C	2.545473	-1.954738	-5.493939	Leu7
C	0.051342	-1.616392	-5.303101	Leu7
H	1.778031	-2.058162	-1.446805	Leu7
H	-0.660868	-2.719737	-2.828144	Leu7
H	2.289503	-3.377335	-3.274674	Leu7
H	1.075009	-3.994236	-4.346235	Leu7
H	1.516768	-1.028618	-3.871437	Leu7
H	3.487414	-2.031659	-4.948469	Leu7
H	2.467893	-2.821056	-6.151434	Leu7
H	2.602629	-1.069083	-6.123521	Leu7
H	-0.202517	-2.455958	-5.950844	Leu7
H	-0.791880	-1.439723	-4.636479	Leu7
H	0.147339	-0.729315	-5.930358	Leu7
N	0.746617	-5.141094	-1.106369	Lys8
C	0.567763	-6.480498	-0.539514	Lys8
C	-0.713109	-6.613645	0.300506	Lys8
O	-1.259454	-7.712846	0.386385	Lys8
C	1.800017	-6.832257	0.327278	Lys8
C	2.677897	-7.898803	-0.340376	Lys8
C	4.029237	-8.084891	0.356526	Lys8
C	4.863795	-9.185334	-0.311626	Lys8
N	6.204179	-9.281287	0.287789	Lys8
H	1.480901	-4.571501	-0.710637	Lys8
H	0.480257	-7.189257	-1.365030	Lys8
H	2.392663	-5.941154	0.524286	Lys8
H	1.510873	-7.200218	1.313954	Lys8
H	2.136444	-8.844889	-0.368816	Lys8
H	2.858157	-7.614379	-1.377833	Lys8
H	4.574744	-7.140161	0.333569	Lys8
H	3.870295	-8.327364	1.407049	Lys8
H	4.363632	-10.149464	-0.217924	Lys8
H	4.976402	-8.982777	-1.377434	Lys8
H	6.694893	-8.407519	0.164636	Lys8
H	6.119743	-9.482710	1.273685	Lys8
H	6.722232	-10.022713	-0.161628	Lys8
N	-1.213860	-5.500752	0.864179	Asp9
C	-2.512536	-5.410383	1.535414	Asp9
C	-3.684368	-5.443343	0.530260	Asp9

O	-4.796413	-5.804716	0.911461	Asp9
C	-2.556720	-4.092677	2.354366	Asp9
C	-3.175480	-4.278605	3.742562	Asp9
O	-2.537204	-4.972727	4.563454	Asp9
O	-4.266626	-3.712449	3.970199	Asp9
H	-0.696620	-4.639727	0.754738	Asp9
H	-2.602974	-6.275551	2.195763	Asp9
H	-1.545806	-3.716845	2.520903	Asp9
H	-3.072577	-3.294326	1.819495	Asp9
N	-3.421704	-5.106905	-0.745739	Gly10
C	-4.373826	-5.075966	-1.853469	Gly10
C	-4.423032	-3.734971	-2.596839	Gly10
O	-5.160210	-3.623654	-3.576738	Gly10
H	-2.465834	-4.870076	-0.971644	Gly10
H	-4.092365	-5.854669	-2.563411	Gly10
H	-5.383581	-5.311605	-1.515225	Gly10
N	-3.693381	-2.704447	-2.135573	Gly11
C	-3.609202	-1.412384	-2.806276	Gly11
C	-4.758751	-0.495763	-2.348978	Gly11
O	-5.018886	-0.418887	-1.146136	Gly11
H	-3.144897	-2.834107	-1.295445	Gly11
H	-2.665016	-0.943767	-2.527988	Gly11
H	-3.568961	-1.564071	-3.884751	Gly11
N	-5.460077	0.199681	-3.276981	Pro12
C	-6.657456	1.008825	-2.977708	Pro12
C	-7.831567	0.219218	-2.354881	Pro12
O	-8.656299	0.808219	-1.657559	Pro12
C	-7.123600	1.567453	-4.336689	Pro12
C	-5.936234	1.435389	-5.271760	Pro12
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H	-6.366575	1.826000	-2.313653	Pro12
H	-7.952823	0.988917	-4.750411	Pro12
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H	-5.370281	2.368198	-5.259949	Pro12
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N	-7.909352	-1.099688	-2.615068	Ser13
C	-9.001072	-1.996916	-2.221514	Ser13
C	-8.853124	-2.574082	-0.794057	Ser13
O	-9.539772	-3.541952	-0.464446	Ser13
C	-9.080553	-3.133672	-3.273677	Ser13
O	-8.038794	-4.088600	-3.179064	Ser13
H	-7.177370	-1.504631	-3.179611	Ser13
H	-9.938723	-1.439012	-2.254564	Ser13
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N	-7.992074	-1.983959	0.053833	Ser14
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C	-6.180401	-2.776990	1.573078	Ser14
O	-5.459290	-2.764413	0.363485	Ser14
H	-7.468336	-1.191138	-0.287626	Ser14
H	-8.236638	-3.371832	1.620836	Ser14
H	-5.671841	-2.091417	2.248508	Ser14
H	-6.076997	-3.765167	2.020974	Ser14
H	-5.432894	-1.880164	0.023278	Ser14
N	-8.766738	-0.321960	2.110903	Gly15
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C	-8.365571	1.754305	3.435490	Gly15
O	-8.591671	2.431918	4.436873	Gly15
H	-8.939137	-0.176998	1.125817	Gly15
H	-10.212917	1.094599	2.576878	Gly15
H	-9.709336	0.141646	3.950809	Gly15
N	-7.260388	1.898484	2.684131	Arg16
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C	-5.572799	3.425506	1.722988	Arg16
O	-5.440364	2.751092	0.698141	Arg16
C	-5.056090	1.940797	3.787068	Arg16
C	-4.522027	0.685184	3.068184	Arg16
C	-3.430232	-0.051232	3.857818	Arg16
N	-4.006626	-0.932351	4.883515	Arg16
C	-3.508800	-1.185078	6.105012	Arg16
N	-2.390137	-0.595198	6.549664	Arg16
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H	-2.728567	0.663694	4.287185	Arg16
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N	-5.217491	4.731726	1.771103	Pro17
C	-4.629616	5.463746	0.636194	Pro17
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O	-2.527505	4.563020	1.373638	Pro17
C	-4.825319	6.943417	1.015833	Pro17
C	-4.773092	6.957831	2.532087	Pro17
C	-5.376738	5.614300	2.931580	Pro17
H	-5.172999	5.233402	-0.282250	Pro17
H	-4.086984	7.620254	0.585752	Pro17
H	-5.808387	7.276852	0.680519	Pro17
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H	-4.885296	5.217154	3.819872	Pro17
H	-6.439006	5.738440	3.146771	Pro17
N	-2.507975	5.474233	-0.694744	Pro18
C	-1.090135	5.190598	-0.961428	Pro18
C	-0.134707	6.006839	-0.065911	Pro18
O	-0.426263	7.173405	0.208900	Pro18
C	-0.888649	5.501219	-2.451268	Pro18
C	-2.001514	6.470956	-2.809673	Pro18
C	-3.132337	6.156885	-1.830552	Pro18
H	-0.935673	4.128734	-0.802710	Pro18
H	0.097083	5.907482	-2.680961	Pro18
H	-0.998617	4.587429	-3.034148	Pro18
H	-1.651931	7.490657	-2.641177	Pro18
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H	-3.850518	5.479843	-2.295374	Pro18
N	0.997746	5.418231	0.387608	Pro19
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C	2.799089	7.102259	0.467602	Pro19
O	3.622186	6.723810	-0.366498	Pro19
C	2.822448	4.949786	1.839004	Pro19
C	2.777389	3.856042	0.782467	Pro19
C	1.409762	4.036096	0.123935	Pro19
H	1.447593	6.597225	2.084464	Pro19
H	3.841685	5.250575	2.086195	Pro19
H	2.363995	4.579576	2.757367	Pro19
H	3.566618	4.019950	0.049060	Pro19
H	2.918076	2.858883	1.198830	Pro19
H	1.444044	3.808362	-0.942653	Pro19
H	0.692461	3.367283	0.597722	Pro19
N	2.547018	8.392572	0.727942	Ser20
C	3.211039	9.531778	0.104621	Ser20
C	4.378941	9.970269	0.999580	Ser20
O	4.120106	10.254038	2.191775	Ser20
C	2.198558	10.691238	0.013419	Ser20
O	1.229653	10.407958	-0.977846	Ser20
O	5.513210	10.008672	0.475649	Ser20
H	1.862721	8.606506	1.438566	Ser20
H	3.585772	9.282900	-0.890203	Ser20
H	1.701957	10.870569	0.967937	Ser20
H	2.698946	11.620157	-0.267243	Ser20
H	0.787046	9.606834	-0.739347	Ser20