Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for "Assessing Backbone Solvation Effects in the Conformational Propensities of Amino Acid Residues in Unfolded Peptides"

Niranjan Ilawe,[1] Alexandra E. Raeber,[1] Reinhard Schweitzer-Stenner,[2] Siobhan E. Toal,[2] and Bryan M. Wong[1*]*

[1]Department of Chemical & Environmental Engineering and Materials Science & Engineering Program, University of California, Riverside, Riverside, CA 92521, United States

[2]Department of Chemistry, Drexel University, Philadelphia, PA 19104, United States

*Corresponding authors. Bryan M. Wong, E-mail: bryan.wong@ucr.edu, Web: http://www.bmwong-group.com and Reinhard Schweitzer-Stenner, E-mail: rschweitzer-stenner@drexel.edu, Web: http://www.schweitzer-stenner.com

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Table S1: Energy decomposition of the solvated peptides at the ωB97X-D/cc-pVDZ level of theory.

	$\Delta U_e(P_s\beta_s w_n)$[a] (kJ/mol)	$\Delta U_e(P_s\beta_s)$[b] (kJ/mol)	$\Delta U_{e,P\beta}(w_n)$[c] (kJ/mol)	$\Delta U_{e,i}(P\beta)$[d] (kJ/mol)
GAG	-36.46	10.73	-24.21	-22.98
GLG	-32.63	9.54	-26.05	-16.12
GVG	-38.24	8.88	-25.37	-21.74
GIG	-41.65	10.49	-24.22	-27.92

[a] Electronic Energy difference between pPII and β solvated systems consisting of the peptide and 10 water molecules
[b] Electronic Energy difference between individual pPII and β structures in the geometry of the solvated system
[c] Electronic Energy difference between 10 water molecules associated with the pPII and β structures
[d] Electronic Interaction energy difference between pPII and β systems

Reference Cartesian coordinates (in Å) for the pPII GAG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -740.298233822

```
N -4.3110361635 0.6720501195 -0.1011626512
C -3.2357012174 0.4959490582 0.9043456261
C -1.9664764632 1.0717846697 0.2824447911
O -1.9952521384 1.4778871343 -0.8722429428
H -3.8365490796 1.0262599173 -0.9502034065
H -5.0056684847 1.3549924713 0.1872220923
H -3.5005220427 1.0060934584 1.824306579
H -3.1020328414 -0.5614281041 1.1102756166
N -0.8832187665 1.0852374484 1.0545097581
C 0.4005804458 1.5170421378 0.5424571838
C 0.8960933239 0.5404159974 -0.5299075699
O 0.6704663449 -0.6560200624 -0.4734234734
H -0.9223894269 0.6770678243 1.9736067139
H 0.2740192532 2.5030861956 0.0951673866
C 1.4150800644 1.5893366544 1.67658936
H 2.3767685179 1.9245414695 1.2944218762
N 1.6365180116 1.0984700097 -1.5049740427
C 2.2572355839 0.2929378019 -2.518846896
C 3.4401466518 -0.5403556128 -2.0625010356
O 3.9586333248 -0.1437251533 -0.902645266
O 3.878508775 -1.4540442839 -2.7116297282
H 1.8111118438 2.0870632335 -1.4946824955
H 1.5371824329 -0.3991290727 -2.9516308388
H 2.6119905229 0.9418270244 -3.317777417
H -4.792846419 -0.1950424864 -0.3191233867
H 4.707249043 -0.7181744444 -0.6983443058
H 1.5481068687 0.6082857649 2.132885473
H 1.0793175749 2.2931644395 2.4358818293
```

Reference Cartesian coordinates (in Å) for the pPII GLG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -858.246259907

```
N -4.4027669755 0.4443732933 -0.1330713222
C -3.3420652858 0.3417009031 0.8983123866
C -2.0948787294 0.9855602363 0.2989217395
O -2.179367843 1.5769253922 -0.76946202
H -4.0415880814 1.1101058362 -0.8366204919
H -5.2855904253 0.7819795872 0.239351553
H -3.6502834073 0.8874221598 1.7852743478
H -3.1787681032 -0.6985552145 1.1590665359
N -0.9817418303 0.8845752049 1.0201110155
C 0.2769797439 1.4301370699 0.5608896642
C 0.8311242699 0.5641740307 -0.5766002953
O 0.592122351 -0.6272204182 -0.6651639462
H -0.980607178 0.3081440232 1.8445625286
H 0.0893369884 2.4340976236 0.1770673029
C 1.3066881083 1.4960806827 1.6941778625
H 2.292062917 1.5751270783 1.2331273191
N 1.6370620422 1.2133061016 -1.4390344878
C 2.3543353513 0.5028232121 -2.4599856043
C 3.5049603779 -0.3590976024 -1.9740087991
O 3.8910875692 -0.0838652331 -0.729950794
O 4.0292571828 -1.1921458115 -2.666220523
H 1.8397164764 2.186270658 -1.293760493
H 1.6845218357 -0.1530282381 -3.0126974004
H 2.7670933196 1.2192775944 -3.1681399496
H -4.574852259 -0.4417034409 -0.6006248373
H 4.6275783041 -0.6676275764 -0.5086769912
C 1.1492987753 2.6590278112 2.6790480056
H 1.1721323025 3.5847116017 2.0961985782
H 1.3013087852 0.5424048427 2.2321003218
C 2.3442504024 2.6695729836 3.6299005457
H 3.2867472801 2.7409825558 3.0856642189
H 2.2856354135 3.5128043487 4.3185215526
H 2.367874156 1.7536189989 4.2252269719
C -0.157667686 2.6274333473 3.4682912241
H -0.1702804771 3.4283777755 4.2078446825
H -1.029749143 2.7531921077 2.8283450621
H -0.2628450883 1.6799432447 4.0031387962
```

Reference Cartesian coordinates (in Å) for the pPII GVG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -818.931784625

```
N -4.4073125773 0.709147354 0.1481023713
C -3.229302413 0.4342158202 1.0057942393
C -2.0390120399 1.1226142662 0.3410282704
O -2.2258604731 1.8264794831 -0.6419234737
H -4.0837229864 1.3977391434 -0.5525729673
H -5.189751478 1.0964577683 0.6670976083
H -3.3974000216 0.8517588099 1.9932096252
H -3.0781820945 -0.636402364 1.0942326346
N -0.8595455548 0.9209761309 0.9245956227
C 0.3689253109 1.4705231482 0.3985861656
C 0.9190252324 0.5626133004 -0.7071363675
O 0.5832712532 -0.6030018089 -0.8291282646
H -0.7992586913 0.2340915645 1.6573148714
H 0.1268294341 2.4367765004 -0.0434358207
C 1.409666166 1.6924435484 1.5157397287
H 2.2828424008 2.1253631369 1.0246365432
C 1.8523073966 0.3931176564 2.1855800916
H 2.226347035 -0.3299404442 1.4620124126
N 1.8224879661 1.1459286848 -1.5180389335
C 2.5069372886 0.3911577403 -2.5303539296
C 3.5247306613 -0.6101338851 -2.0165961807
O 3.9368750779 -0.3624981388 -0.7749172182
O 3.939758564 -1.5184140683 -2.6878493122
H 2.0895250671 2.1013103069 -1.3622761234
H 1.8002040524 -0.1664564209 -3.1415346316
H 3.0392034517 1.0789195052 -3.1854325254
H -4.7329182748 -0.1187112654 -0.3431664725
H 4.5893940628 -1.0330577418 -0.5367251527
C 0.8934626347 2.7035433468 2.5350658694
H 1.6625759745 2.9130554165 3.2778100322
H 0.6183897747 3.6428957117 2.0548819137
H 0.0173029602 2.3210053327 3.0601461484
H 1.041321952 -0.0736719134 2.7490775253
H 2.6493901779 0.6032894647 2.8975750699
```

Reference Cartesian coordinates (in Å) for the pPII GIG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -858.247345352

```
N -4.3978315366 0.6594680307 0.1571478912
C -3.217923627 0.408047322 1.0194503619
C -2.0362072731 1.1056698988 0.349242228
O -2.2297256758 1.7882046226 -0.6474689176
H -4.0782397113 1.3392392286 -0.5542825264
H -5.1835410931 1.0494715539 0.6690841843
H -3.392797728 0.830922889 2.0033626519
H -3.0520432931 -0.6596524329 1.1165809087
N -0.8560283052 0.9363630346 0.9411947954
C 0.3638872568 1.4918368226 0.4015566888
C 0.8953833764 0.6011012002 -0.727496046
O 0.536631272 -0.5536082471 -0.8819063072
H -0.785557296 0.2670167929 1.6891473687
H 0.1179175315 2.4644217311 -0.0248753441
C 1.4235043531 1.6945984919 1.5041310526
H 2.3040494753 2.0971740685 0.99843174
C 1.8421235512 0.3771510613 2.1699075171
H 1.9455424659 -0.3993003714 1.4104428632
C 3.1562421276 0.4882349619 2.9337614927
H 3.9645399121 0.7788108575 2.2610988966
H 3.4208949743 -0.4672616175 3.3853139145
H 3.1008389128 1.2274133438 3.7326978123
N 1.8134256886 1.188668414 -1.5197803923
C 2.5283842963 0.4340869954 -2.5104232323
C 3.5421638295 -0.5544097652 -1.962978959
O 3.8837678159 -0.3205092476 -0.6972167197
O 4.0094119599 -1.4424671198 -2.62677505
H 2.1075048381 2.1291353605 -1.3257256666
H 1.8410189893 -0.1342090023 -3.1334678859
H 3.0698421453 1.1207205705 -3.1589509536
H -4.716938164 -0.1785473268 -0.3209270259
H 4.536432132 -0.9816222984 -0.4344843847
C 0.9417094814 2.7343979705 2.5125688767
H 1.7104254277 2.9382793227 3.2558952833
H 0.6985978327 3.6749097261 2.0178264982
H 0.0513463112 2.3872278933 3.0385200772
H 1.0591407462 0.0443952641 2.8580263078
```

Reference Cartesian coordinates (in Å) for the *β*-strand GAG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -740.301127336

```
N 2.6253320895 0.4573638206 3.0147007991
C 3.2293115372 -0.1196395075 1.7890906821
C 3.0385839489 0.9200848109 0.6853641219
O 2.4040851597 1.9406002614 0.9273694825
H 2.1620208117 1.3295551849 2.7028156964
H 3.3201345184 0.6964056606 3.7166803899
H 4.2802596914 -0.3289795353 1.9574831162
H 2.719693241 -1.0429743304 1.5334828666
N 3.5853330246 0.6179854184 -0.4841245511
C 3.4981702363 1.471907549 -1.6496978425
C 3.7716193231 0.5829077621 -2.8605092714
O 4.3404215806 -0.4917473385 -2.7430116924
H 4.079818008 -0.2525648636 -0.6223886403
H 2.4885055498 1.8774971908 -1.712405171
C 4.5110500035 2.6176085567 -1.5923375889
H 5.5236555538 2.2194708573 -1.5381249877
N 3.3683476505 1.0791715925 -4.0415440727
C 3.6924485254 0.429919895 -5.2786088239
C 5.1066623777 0.7209116135 -5.7438057722
O 5.8919346746 1.4372608304 -5.1842711083
O 5.3694297831 0.0696810075 -6.8770712964
H 2.9438433155 1.9892264978 -4.0736652507
H 3.58634059 -0.6486510615 -5.1715432948
H 2.9997117064 0.751411117 -6.0534122503
H 1.9395025705 -0.1567023931 3.444147531
H 6.271834149 0.2792128954 -7.1483626207
H 4.4295882494 3.2502609444 -2.4744028278
H 4.3211014806 3.2258286237 -0.7106765827
```

Reference Cartesian coordinates (in Å) for the *β*-strand GLG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -858.248120616

```
N 1.988713127 -0.4263102049 2.783663293
C 3.0728834888 -0.5887559797 1.7863506341
C 2.8548135006 0.4920334645 0.7295694805
O 1.807927523 1.1273532506 0.7369949285
H 1.2864611411 0.1821757309 2.3309201311
H 2.3094996103 0.0396697854 3.6284285593
H 4.0395567558 -0.5002712847 2.2697286793
H 2.991015191 -1.5698794154 1.3280219866
N 3.8551899072 0.6556898064 -0.1306194533
C 3.8006091772 1.5291588627 -1.2849011099
C 3.8962081997 0.6655092951 -2.5420810579
O 4.4833764287 -0.4036291322 -2.538541833
H 4.6351922346 0.0183260897 -0.0931944096
H 2.8387760708 2.0390219324 -1.2583306666
C 4.9459433381 2.5569960562 -1.2992463045
H 5.8508567192 2.0706398495 -0.9239342356
N 3.3276007285 1.1929921162 -3.6430765271
C 3.5211095927 0.6045303617 -4.9358501548
C 4.8766688102 0.9298246177 -5.5339198659
O 5.7026855536 1.6484352156 -5.0388533204
O 5.0354963346 0.3119281824 -6.7046607092
H 2.9210292876 2.1103042695 -3.591001763
H 3.4303377148 -0.4785667085 -4.8697384032
H 2.7511453322 0.9549836766 -5.6203634483
H 1.5608059353 -1.3076440488 3.0513114769
H 5.9012389898 0.548678103 -7.0601913676
C 4.6838313665 3.8475640962 -0.5192713788
H 3.8001062689 4.3191446529 -0.9600355371
H 5.1473725275 2.8204498257 -2.3391117663
C 5.8658618083 4.7958794056 -0.7032748151
H 6.058097471 4.9908389974 -1.7591162567
H 5.679182562 5.7502389602 -0.210227765
H 6.7720741721 4.3663821044 -0.2696119599
C 4.4056722193 3.6162552362 0.9637536623
H 3.4740481522 3.0760537248 1.1254120396
H 5.2171087771 3.0506120779 1.4274092978
H 4.3226093228 4.5717318667 1.4830631197
```

Reference Cartesian coordinates (in Å) for the *β*-strand GVG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -818.934384309

```
N 2.0875707181 0.2197443624 2.7300895812
C 3.1179220321 -0.1139182823 1.7168754552
C 2.9825256519 0.9298102684 0.6077333256
O 2.0763689943 1.7512847658 0.669693433
H 1.5411349294 0.9947325365 2.313670063
H 2.4912677181 0.5417710731 3.6050975045
H 4.1031839818 -0.0878407916 2.1697683878
H 2.9330229252 -1.1087123145 1.3239504369
N 3.8893439223 0.8494809177 -0.3597086439
C 3.9009638652 1.7008322916 -1.5354775196
C 4.1408392404 0.7720925489 -2.7249581141
O 4.9563772233 -0.1343957283 -2.6473866097
H 4.5770352983 0.1113400796 -0.3447052277
H 2.924038434 2.1782917014 -1.6053766497
C 4.9945393507 2.7865696551 -1.452184671
H 5.9535123443 2.2656624189 -1.3847696616
N 3.4113340509 1.0126277614 -3.8269573208
C 3.5778446649 0.2423913135 -5.0251024683
C 4.768683633 0.670903126 -5.8600673433
O 5.5105271137 1.5823801626 -5.6108307992
O 4.887699542 -0.1104474086 -6.9337819912
H 2.7879646108 1.7997128412 -3.8417229419
H 3.7087882987 -0.8101879442 -4.7766780139
H 2.6823092718 0.3225506152 -5.6378826615
H 1.4674838852 -0.5579421618 2.9347789352
H 5.6494448465 0.1877285553 -7.4462721012
C 4.9970934758 3.6583075286 -2.7051452307
H 5.7588330255 4.4320615178 -2.6147107522
H 5.2040913089 3.08660424 -3.6086495898
H 4.0321088381 4.1564804774 -2.8281959152
C 4.8150905598 3.642239476 -0.2023926444
H 3.8515359536 4.1547855201 -0.2213762926
H 4.8695970251 3.0511570629 0.710747192
H 5.5987482662 4.397929814 -0.156589151
```

Reference Cartesian coordinates (in Å) for the *β*-strand GIG peptide optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -858.249289090

```
N 2.0240707392 0.1610679644 2.6986507395
C 3.072975683 -0.1597281811 1.700541755
C 2.9501549724 0.8893680096 0.5957392665
O 2.0008483126 1.662481907 0.6113927108
H 1.4272480089 0.8753598056 2.2468286217
H 2.4087358123 0.5588336677 3.551254039
H 4.0504899553 -0.1419141818 2.1695569644
H 2.891359259 -1.1496656992 1.2932474809
N 3.9122915772 0.8640794863 -0.3208247342
C 3.9445847209 1.7281382625 -1.4881598781
C 4.2405272789 0.8138901522 -2.6762757168
O 5.144682592 -0.0054334712 -2.6134725127
H 4.6442598717 0.1727553856 -0.2601520629
H 2.9600753024 2.1848376617 -1.5811733617
C 5.0113688679 2.8354697282 -1.3586582465
H 5.978852971 2.3336577923 -1.2582181548
N 3.4503804101 0.9558557713 -3.7536301687
C 3.6481955443 0.1781483567 -4.9421010841
C 4.7329046926 0.7246552245 -5.8493181376
O 5.3759615006 1.7204527751 -5.6539288971
O 4.8829805118 -0.0579080075 -6.9182575431
H 2.7506710049 1.6761655791 -3.759563488
H 3.9176755934 -0.8434522392 -4.6766825718
H 2.719381669 0.1330054181 -5.5072980649
H 1.4592348389 -0.6440893683 2.9513524864
H 5.5752934661 0.3168609971 -7.4769040038
C 5.0431460054 3.6940040573 -2.6269927794
H 5.1573786635 3.0511232905 -3.5006229979
H 4.0767197764 4.1966718924 -2.736003914
C 4.7580436009 3.670378475 -0.1073909268
H 3.8029705216 4.1941254489 -0.1829663091
H 4.7393520572 3.0540211705 0.7902484835
H 5.5422880476 4.4131369781 0.0261324083
C 6.1634370304 4.7270020422 -2.6440245523
H 6.1999041372 5.2334322868 -3.60824377
H 6.0333624036 5.4898492314 -1.8768614198
H 7.1317449996 4.2498357502 -2.4818426997
```

Reference Cartesian coordinates (in Å) for the pPII GAG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1504.87079632

```
O 4.2701825772 2.2014012844 -0.3488238273
O 3.5938503305 -2.9661200822 0.3903500127
O 0.0715264211 -3.2927286478 -2.1084580797
O 0.8423636872 -2.5780554502 0.4994156826
O -0.7777405965 -1.4065738971 2.4410656921
O -2.9452985431 -2.7733003763 1.2410887418
O -1.9946004068 -1.608105796 -1.1452597571
O -5.4563282045 -1.715820766 1.2617111497
O -0.2922112109 3.9323020792 -1.9346546103
O -4.6594827217 2.4185118289 -1.6884591836
H -5.1875307221 3.0813712653 -1.2398042035
H -3.7392182131 2.6200897195 -1.4609091554
H -6.0819450698 -2.3012688967 0.8324150716
H -4.6233496741 -2.2244227271 1.3438119199
H -2.5840949036 -2.4935323557 0.383023543
H -2.3123092917 -2.4139067579 1.8797354539
H -0.914379356 3.2964618701 -1.5546600485
H 0.2584824546 3.4077402272 -2.5173785973
H -0.1577630973 -1.9293911354 1.8995119486
H -0.4827232566 -1.4885000743 3.3496603882
H -1.2172980686 -1.0439556773 -0.9857446987
H -1.6343907516 -2.29592947 -1.7222896933
H 0.8112214384 -1.7159657352 0.0522605759
H 0.4622469196 -3.1607790126 -0.1774669025
H 0.8404046502 -2.7994043523 -2.4303875094
H 0.1125705912 -4.1490188719 -2.5370949914
H 2.6263882083 -2.9740041896 0.5218308258
H 3.785218898 -3.7328383669 -0.1536168922
H 5.0514149936 2.5857817176 -0.749101173
H 4.4013454009 1.2482710463 -0.3926741214
N -4.0493455344 0.1222600961 -0.2179364106
C -3.2253759873 0.6842574251 0.8737735292
C -1.9910506988 1.3738355903 0.3206666112
O -2.0658333809 2.0933339962 -0.6767596171
H -4.4626084527 0.8778758661 -0.7951361654
H -4.7876852552 -0.4759503328 0.208201574
H -3.8214516884 1.4162724546 1.4143577937
H -2.9613485246 -0.1202454277 1.5537388224
N -0.8639429464 1.1523841805 0.9931819621
C 0.4131742607 1.651426449 0.5297685253
C 0.8463207155 0.8471548735 -0.6948167655
O 0.3509142341 -0.2585050393 -0.9442588344
H -0.8481898666 0.3922601087 1.6707601848
H 0.3054622403 2.6948102387 0.237554047
C 1.4542820259 1.5264615539 1.6395201046
H 2.4141540169 1.9142505081 1.3060518077
N 1.8069715059 1.34290114 -1.466904777
C 2.3492167047 0.5156844146 -2.5251868185
C 2.8375448642 -0.8269292072 -2.0033840773
O 3.5630295524 -0.7086649664 -0.9089364399
O 2.5882175326 -1.8830091972 -2.5397325507
H 2.3777200463 2.1119240026 -1.1375721209
H 1.5992926655 0.3259575364 -3.2877280766
H 3.1867345393 1.0440321433 -2.9761887453
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H -3.4752081778 -0.4902004211 -0.814311629
H 3.7079502208 -1.6070731106 -0.4854870225
H 1.5828349956 0.4857707797 1.9376615422
H 1.1283144496 2.0991895546 2.5051198155

Reference Cartesian coordinates (in Å) for the pPII GLG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1622.82018499

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O 3.6366410000 -2.7723040000 0.4636050000
O 0.1893550000 -3.2976860000 -2.0039750000
O 0.8703530000 -2.4867340000 0.5983770000
O -0.8719190000 -1.3897910000 2.4795840000
O -2.9750820000 -2.826340000 1.2471650000
O -1.9731510000 -1.6856070000 -1.1285380000
O -5.5068610000 -1.8220780000 1.146470000
O -0.4071750000 3.9946770000 -1.8621220000
O -4.7131230000 2.2743030000 -1.8555250000
H -5.2824520000 2.9209860000 -1.4345770000
H -3.8108790000 2.5081630000 -1.5891090000
H -6.1054450000 -2.4360760000 0.718560000
H -4.6667180000 -2.3089240000 1.2741130000
H -2.5906210000 -2.5552650000 0.3964910000
H -2.3699340000 -2.443640000 1.8989310000
H -1.0211040000 3.3291160000 -1.5212580000
H 0.1482640000 3.5120140000 -2.4758010000
H -0.2154540000 -1.8937380000 1.9631870000
H -0.6015090000 -1.448190000 3.3976630000
H -1.2169820000 -1.0936580000 -0.9674350000
H -1.5801080000 -2.3721730000 -1.6849720000
H 0.8156940000 -1.632760000 0.1377530000
H 0.5302650000 -3.0924520000 -0.0804730000
H 0.9315650000 -2.772480000 -2.3377460000
H 0.2786840000 -4.1618980000 -2.4087490000
H 2.6732180000 -2.8119630000 0.6159960000
H 3.8442160000 -3.543010000 -0.0687140000
H 4.9077440000 2.7972730000 -0.6743510000
H 4.2994260000 1.42160000 -0.3968520000
N -4.0974830000 0.0123620000 -0.3355910000
C -3.3314230000 0.6139990000 0.7769040000
C -2.0975640000 1.3325640000 0.2612940000
O -2.15720000 2.0541150000 -0.7360550000
H -4.506950000 0.7469480000 -0.9419080000
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H -3.9681430000 1.3351030000 1.2848610000
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N -0.9867640000 1.1305950000 0.9640950000
C 0.2961060000 1.6544360000 0.5438080000
C 0.754550000 0.8830540000 -0.6914790000
O 0.3156570000 -0.2465060000 -0.9395260000
H -0.9811140000 0.3828410000 1.6546310000
H 0.1906440000 2.7066470000 0.2784620000
C 1.347150000 1.5005150000 1.652740000
H 2.3311680000 1.5521550000 1.1880810000
N 1.6864820000 1.4261830000 -1.4673140000
C 2.2778750000 0.6188540000 -2.5148730000
C 2.8178540000 -0.6978590000 -1.9767380000
O 3.5186960000 -0.5395130000 -0.870650000
O 2.6257690000 -1.7674620000 -2.5091410000
H 2.2142810000 2.2255560000 -1.1400030000
H 1.5465230000 0.3902780000 -3.2846740000
H 3.0960870000 1.1818110000 -2.9591630000
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H -3.4850360000 -0.5971250000 -0.8962770000
H 3.6964560000 -1.4264940000 -0.4355670000
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H 1.3972790000 3.536930000 2.2735250000
H 1.2598880000 0.5005440000 2.0890390000
C 2.4943960000 2.3663980000 3.6835190000
H 3.4345980000 2.4102170000 3.1323940000
H 2.5159320000 3.1369140000 4.4542820000
H 2.4390920000 1.3955930000 4.1815720000
C -0.0036440000 2.5550730000 3.5570030000
H 0.0473860000 3.2898520000 4.360920000
H -0.8684050000 2.7972640000 2.9412830000
H -0.1734950000 1.5749430000 4.009650000

Reference Cartesian coordinates (in Å) for the pPII GVG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1583.50585152

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O 3.5563254463 -3.0729925298 0.3809534137
O 0.0567740803 -3.2580929415 -2.1297620612
O 0.8161156465 -2.5826276362 0.4878086964
O -0.9002685621 -1.5204493368 2.4004771333
O -2.988633029 -2.8840374874 1.067945997
O -1.9819488688 -1.5361799376 -1.2045777043
O -5.4708923535 -1.7839567672 1.2279503541
O -0.388323297 3.7863351654 -2.130939474
O -4.738754484 2.4656706187 -1.4976951922
H -5.2569565553 3.1016886309 -1.0012279146
H -3.8129702111 2.6698245166 -1.2979384806
H -6.125086534 -2.3050948796 0.75999528
H -4.6528923952 -2.3231743524 1.2397234323
H -2.6194816275 -2.5338632835 0.2399775188
H -2.3808178906 -2.543885824 1.7407957793
H -0.9949753022 3.1862354679 -1.6756464015
H 0.1483341181 3.2163191986 -2.6831211007
H -0.2526485887 -2.018393165 1.8668261107
H -0.6804658235 -1.6844841157 3.3193502388
H -1.2042422833 -0.984107729 -1.010471818
H -1.6100092328 -2.2164843983 -1.78380074
H 0.815496839 -1.7014399736 0.0784522051
H 0.4364908922 -3.1262470171 -0.2228904948
H 0.8426170394 -2.7911055991 -2.4512292746
H 0.0706087539 -4.1180124239 -2.5529148605
H 2.5890422702 -3.0563005808 0.5102745002
H 3.7310073893 -3.8445131646 -0.1618483491
H 5.1915092331 2.4358019386 -0.7563636083
H 4.4876818435 1.1455311841 -0.339466203
N -4.040913261 0.120125166 -0.1443812101
C -3.177256294 0.6309358501 0.9412950008
C -1.9801472964 1.368403533 0.3689644711
O -2.1094717237 2.1032605882 -0.6106432138
H -4.4756456332 0.9009641704 -0.6701928726
H -4.7684883494 -0.4984191841 0.2735409547
H -3.7579229095 1.3227681289 1.5477115766
H -2.8702926346 -0.2048911962 1.5633442862
N -0.8240790794 1.169790494 1.002095981
C 0.4145350133 1.7276114448 0.5012110868
C 0.8984654684 0.8695274712 -0.6673862928
O 0.3872638955 -0.2298728749 -0.9149294981
H -0.7802284269 0.4032588167 1.6671605984
H 0.2041162171 2.7218542019 0.1092980081
C 1.4856916611 1.8673768064 1.6005820654
H 2.3279768556 2.3768044175 1.1298445931
C 1.9922824393 0.5251047179 2.1217111168
H 2.4186969803 -0.0856771575 1.3252999906
N 1.8974344665 1.3252443 -1.4145692416
C 2.4221503557 0.4937086197 -2.4773258069
C 2.8654557222 -0.8718687662 -1.978447169
O 3.5990495482 -0.7988190213 -0.8849029215
O 2.5820444708 -1.9092370838 -2.5334641858
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H 1.6727687766 0.3393617026 -3.2487148801
H 3.27978586 1.0015361932 -2.9139309218
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H 3.7184686476 -1.7103802629 -0.4811012311
C 0.9713886496 2.7554071918 2.7288839166
H 1.767122794 2.9418533885 3.448992544
H 0.6227767495 3.7154735743 2.3476470248
H 0.1446678788 2.2811722974 3.2591221121
H 1.2011683592 -0.0466230565 2.6081085655
H 2.7749028671 0.6904466439 2.8608295075

Reference Cartesian coordinates (in Å) for the pPII GIG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1622.82247217

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O 3.5586268555 -2.9695413032 0.4879272269
O 0.0557579977 -3.250591786 -2.1451011404
O 0.8103215284 -2.5657241321 0.4694261696
O -0.8967202692 -1.5163251936 2.3932667595
O -2.9834291329 -2.8843220207 1.0657895433
O -1.993869584 -1.5348247317 -1.2140984751
O -5.4656025825 -1.7864376094 1.2394718534
O -0.398226749 3.7913922775 -2.1295883924
O -4.7498119946 2.4756494559 -1.4742746667
H -5.2642045362 3.1087793783 -0.9702159166
H -3.8224913891 2.6773817997 -1.2789576477
H -6.122432971 -2.308105 0.7758331307
H -4.6470053386 -2.3249096197 1.2458757589
H -2.6182794569 -2.5324763858 0.2367751991
H -2.3737686936 -2.5441728241 1.737004888
H -1.0038913678 3.1915609899 -1.6725886781
H 0.132477225 3.2218372316 -2.6879815243
H -0.2479714699 -2.0084460755 1.8557147773
H -0.6658970659 -1.6729755844 3.3107008071
H -1.2181472926 -0.9774415922 -1.0277793616
H -1.6218855578 -2.2154181799 -1.792802685
H 0.7895428454 -1.6912596452 0.0460971142
H 0.4473750447 -3.1296546772 -0.2337075314
H 0.8401057248 -2.7784678543 -2.4621614012
H 0.0731113995 -4.1068383492 -2.5755231434
H 2.5858757008 -2.9816380368 0.5704106616
H 3.792998511 -3.7824940496 0.0358935174
H 5.2393652216 2.3698933303 -0.6335103416
H 4.4448430778 1.0990474878 -0.3279617411
N -4.0472202323 0.1215468938 -0.1388904745
C -3.1780166828 0.6292057857 0.9439570503
C -1.9826726736 1.3670253851 0.3684631989
O -2.1157193454 2.1065621482 -0.6072193857
H -4.4845897748 0.9042418818 -0.6597566341
H -4.7724284142 -0.4980788095 0.2815253068
H -3.7555735985 1.3201632472 1.5543197732
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N -0.823798532 1.1636271678 0.9946362934
C 0.4130708435 1.723096195 0.4911702954
C 0.8888008885 0.874941606 -0.6883082296
O 0.3731804068 -0.2199521051 -0.9462960802
H -0.777682351 0.3955752896 1.6580046794
H 0.2029967377 2.721591363 0.1099439363
C 1.4931802518 1.8485783013 1.5843047574
H 2.3348107831 2.358561483 1.1106255152
C 2.0035220282 0.4883842191 2.0703810811
H 2.2522447393 -0.1303660073 1.2054893496
C 3.24325505 0.5846618833 2.9504723798
H 4.0378341733 1.1258798208 2.4343030117
H 3.6160266455 -0.4102215529 3.1919125217
H 3.0365470744 1.0979319176 3.8890756297
N 1.8915192545 1.3317091761 -1.4304625224
C 2.4263845319 0.4983290358 -2.48724608

C 2.877814859 -0.8599980044 -1.9738210722
O 3.616316479 -0.7678676728 -0.884160911
O 2.5947265723 -1.9063965949 -2.5104468068
H 2.4595409199 2.1036047943 -1.1089249085
H 1.6808430635 0.3326781503 -3.2598145724
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H 3.729306468 -1.6670491824 -0.4506654075
C 0.9848903417 2.7337770841 2.7185050528
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H 0.1849531525 2.2423103621 3.2738963878
H 1.2127143777 -0.0346230683 2.6127311905

Reference Cartesian coordinates (in Å) for the β-strand GAG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1504.86270621

O 0.3511255222 1.917924157 2.7732813691
O 2.8604893207 -1.5473347552 4.76774134
O 5.3447230534 1.6601417565 2.4928092868
O 5.8921281513 -0.4971908559 0.6624301857
O 7.4764337692 0.1364929627 -1.4765062683
O 8.5547594058 -2.0945956644 -2.7359014483
O 6.2147536790 -2.1476045525 -4.2024536181
O 3.8186115370 4.0731797716 -4.6079891506
O 1.3927908039 2.9047717421 -3.96128289
O 0.7686845242 3.5724288825 -1.3119311326
H -0.4163910217 1.3764067505 2.9659900125
H 0.4951909450 1.8391920343 1.8167316513
H 2.1960584633 -1.5115091576 5.4587189819
H 3.6974788208 -1.6448372333 5.2262579613
H 5.9002527142 1.7329558222 3.2725205063
H 5.3907077113 2.5185340847 2.0651620924
H 5.9411854421 0.2367330128 1.2893614576
H 6.5703062400 -0.3161724912 -0.0187160551
H 8.5346259952 -2.8523326905 -2.1494717527
H 7.7779904908 -2.2017438166 -3.3178496988
H 7.9559316729 -0.6254962437 -1.8517756016
H 6.6655954238 0.1846874104 -2.0036273596
H 5.7297723932 -1.4353088706 -3.7525246986
H 6.3057646238 -1.8497140716 -5.1103530806
H 4.3211414401 3.3242831382 -4.9660327231
H 3.9171806903 4.7800381803 -5.2471037265
H 2.1425608639 3.4784685713 -4.1976210296
H 1.1291806223 3.1732589345 -3.0636899614
H 1.2732605086 4.3450928555 -1.0520820397
H 1.0631771461 2.8654519633 -0.7132915932
N 2.7608745834 0.4877919974 2.8712338473
C 2.7253119312 -0.2345280002 1.5798440099
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H 3.6031007021 1.0777624616 2.9134192969
H 3.6261463662 -0.834688514 1.499500618
H 1.8568781528 -0.8888345306 1.5785918312
N 3.552190389 0.659652172 -0.4924025288
C 3.5949048371 1.5070495465 -1.6681427091
C 4.0019149698 0.66453423 -2.8661513205
O 4.9972206382 -0.0670223359 -2.814170717
H 4.3875103171 0.1146793501 -0.2557786852
H 2.5967521559 1.8976376843 -1.8323225505
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H 5.5776745557 2.3012505108 -1.2989516847
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C 3.6303587122 0.1354753434 -5.1783315138
C 4.884555357 0.7317291654 -5.7868005265
O 5.2707322263 1.861010179 -5.6175715004
O 5.5129874594 -0.1416786349 -6.5660494494
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H 3.7779577795 -0.9319481802 -5.0252570028
H 2.8298454927 0.2535777908 -5.9072325064

H 2.8069170089 -0.2036732871 3.6454299919
H 6.2699747149 0.2954252027 -6.9787912696
H 4.5801462557 3.291745732 -2.3842936597
H 4.2509735253 3.277949483 -0.645945042

Reference Cartesian coordinates (in Å) for the β-strand GLG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1622.81393002

O 0.5634276074 1.8947898174 2.7433310188
O 2.6896469985 -1.7907933605 4.7510391692
O 5.5746370117 1.0861056387 3.0062111761
O 5.9199604546 -0.6081659304 0.729064913
O 7.4808230972 0.0125469915 -1.4214828103
O 8.453572096 -2.2358096589 -2.7349937075
O 6.1445087374 -2.1453450658 -4.2477879272
O 4.075658282 4.2045137071 -4.2414992578
O 1.582325462 3.1120025589 -3.7559431912
O 0.6312765599 3.3654252 -1.1500026949
H -0.2418101792 1.527612537 3.1123226668
H 0.5513350037 1.6691228888 1.8004583972
H 2.0307788789 -1.6793671653 5.4393260666
H 3.508628032 -1.9808229056 5.213142001
H 5.9479377701 0.7306484713 3.8164890787
H 5.8743826898 1.9969429211 2.9672822659
H 6.0583632389 0.002410462 1.4651522603
H 6.608876578 -0.4167115911 0.0613535447
H 8.3826833689 -3.0116864752 -2.1768576058
H 7.6868025898 -2.2852669527 -3.3377343304
H 7.9228737372 -0.7649519332 -1.8110469513
H 6.6577141704 0.0862875538 -1.9266783848
H 5.6703814633 -1.453271367 -3.7557206346
H 6.2543419963 -1.7912988836 -5.1330768347
H 4.5248161552 3.4489670842 -4.6512607791
H 4.2164680558 4.9419728647 -4.8366443808
H 2.361188606 3.6795305663 -3.8899489065
H 1.2457269127 3.3014316787 -2.8630795147
H 0.9056715225 4.1234226845 -0.6316454212
H 0.925401168 2.5860565119 -0.6491307763
N 2.8212049073 0.2429335965 2.8578312558
C 2.7091660184 -0.474227602 1.5647228737
C 2.5596297154 0.5032141037 0.406628298
O 1.4941961653 1.1133144544 0.2499726539
H 2.0309426015 0.905211904 2.9823913672
H 3.7210389606 0.7390378294 2.9277015268
H 3.5863900605 -1.1031883539 1.4492666307
H 1.817904318 -1.0941593733 1.5992051531
N 3.6302194707 0.6278371645 -0.3616238307
C 3.7122177897 1.4966372825 -1.5180999867
C 4.0357105121 0.6591114436 -2.7442188775
O 4.9744457272 -0.1454927896 -2.7256560058
H 4.4794558017 0.1206762449 -0.0824582119
H 2.7455344366 1.9709862601 -1.6539410605
C 4.801718481 2.5747927321 -1.3684573855
H 5.6237355037 2.1639563796 -0.7757381495
N 3.2989915887 0.8890916921 -3.8256078221
C 3.6420368413 0.2856900504 -5.0825360621
C 4.923127949 0.8593390542 -5.6558347538
O 5.370292748 1.9502052789 -5.403591718
O 5.5002474822 0.015599347 -6.5042829483
H 2.5714173078 1.6126217149 -3.7958705184
H 3.7407649735 -0.7943429981 -4.991761078
H 2.848244492 0.4819542448 -5.8017376715

H 2.7876419462 -0.4523463743 3.6300602564
H 6.2777592246 0.4418963534 -6.88933404
C 4.3153311761 3.8932824979 -0.7662550427
H 3.4871631413 4.242082055 -1.3902211215
H 5.2076224797 2.7907041497 -2.3576515168
C 5.4318211863 4.9291625816 -0.8529097778
H 5.7402679723 5.0794758317 -1.8877582648
H 5.103455608 5.8881368172 -0.4509436431
H 6.3037321185 4.6059643772 -0.2789674264
C 3.813520348 3.7524126347 0.667517468
H 2.9336524588 3.1145191464 0.7384964538
H 4.5895894276 3.3280453234 1.3073637237
H 3.5428269953 4.7270110968 1.0746898033

Reference Cartesian coordinates (in Å) for the β-strand GVG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1583.49890224

O 0.520674199 2.0932008363 2.7175346713
O 2.5458632143 -1.6837108694 4.5829291904
O 5.5188695408 1.3305232179 2.8867387483
O 5.9192596791 -0.4770264969 0.6871997025
O 7.6197632854 0.1509143448 -1.3541101797
O 8.5701297115 -2.1449464652 -2.6048797945
O 6.2782115259 -2.026163165 -4.1357871449
O 3.2001718212 4.0736411904 -5.3860559954
O 1.2605877829 2.732768044 -3.9318376782
O 0.7037893476 3.5965581187 -1.3564062046
H -0.2895194292 1.6374951105 2.9531019425
H 0.6145935082 1.9844690107 1.7580272367
H 1.8728100174 -1.5890939305 5.2599071848
H 3.3446129788 -1.9310075008 5.053253102
H 5.9421419704 1.0508588463 3.7021586281
H 5.7708072323 2.2496438089 2.7708786285
H 6.0183853259 0.1603789352 1.406888976
H 6.6363082739 -0.2908258621 0.0476168106
H 8.4736818451 -2.901396569 -2.0243074998
H 7.80926485 -2.1938164596 -3.2150727983
H 8.0504548077 -0.6403624864 -1.7281285295
H 6.8418269096 0.2836447873 -1.9167623363
H 5.8579153507 -1.2574722211 -3.713535721
H 6.3887174268 -1.7714921858 -5.0544388224
H 3.8544021257 3.3644936792 -5.480554059
H 2.9341802045 4.2893007075 -6.2813630401
H 1.8418884175 3.3507456034 -4.4088810888
H 1.0633868132 3.1357193832 -3.0682356457
H 1.038047847 4.4379588466 -1.0432578492
H 1.0690860051 2.9240969179 -0.7570628108
N 2.7819811218 0.4414951726 2.8042240641
C 2.7117249575 -0.2173494973 1.4792571001
C 2.6399713571 0.8048552012 0.3525475649
O 1.6564861927 1.546293048 0.2524945457
H 1.9901717802 1.1012277414 2.932920375
H 3.6814992409 0.9291970123 2.9194617054
H 3.5735202784 -0.8694902742 1.3776214026
H 1.8032825277 -0.8132594162 1.4471942626
N 3.680071158 0.8011422691 -0.4699374996
C 3.8257499687 1.6980229949 -1.6017433315
C 4.1812320435 0.8480110392 -2.8149899364
O 5.224335515 0.1826759248 -2.830183192
H 4.497423218 0.2419065034 -0.196998975
H 2.8697423353 2.1871195243 -1.7716945683
C 4.9008422399 2.769103674 -1.3447493419
H 5.8269228483 2.2468126982 -1.0919109274
N 3.3253062451 0.8647123478 -3.8286028889
C 3.6082984261 0.1380701214 -5.0359023183
C 4.7491529855 0.7548532679 -5.8215671758
O 5.0330095294 1.9269627508 -5.8265199814
O 5.3966446483 -0.1519343542 -6.5440758198
H 2.5039360859 1.4825647194 -3.7974531686
H 3.8330332268 -0.9062879329 -4.829311586
H 2.7275260735 0.1635493211 -5.6765799925

H 2.7183723484 -0.2870731741 3.5429517555
H 6.0719107829 0.2939108521 -7.0728356275
C 5.1344529584 3.6066141806 -2.597759528
H 5.8744026557 4.3801316262 -2.396038607
H 5.4990784995 3.0067803934 -3.4317156695
H 4.2119232231 4.0968156537 -2.9144409316
C 4.5034764669 3.6523700539 -0.1680677977
H 3.5860401118 4.1999940956 -0.3906776385
H 4.339697369 3.0757869023 0.7407098475
H 5.2876089927 4.3804413823 0.0358572562

Reference Cartesian coordinates (in Å) for the β-strand GIG peptide + 10 H_2O molecules optimized at the ωB97X-D/cc-pVTZ level of theory in aqueous PCM. The total energy (in Hartrees) includes all contributions from the PCM.

Total energy: -1622.81472655

O 0.4727003974 2.0305557553 2.7389911245
O 2.5741573214 -1.7086347645 4.6038422394
O 5.4534761553 1.4259701273 2.7489667705
O 5.9232197021 -0.4894313763 0.6666357283
O 7.6070886054 0.2139167691 -1.3727895109
O 8.6199041056 -2.0337151879 -2.6603930873
O 6.2849255738 -2.0144340097 -4.1297965533
O 3.2707774626 4.1190965435 -5.3212132573
O 1.2872703515 2.7923976247 -3.9074066381
O 0.7166514384 3.6006023879 -1.3144407591
H -0.3333166977 1.5645139687 2.968563464
H 0.5710732956 1.9296512 1.7790848902
H 1.8990304109 -1.6246652286 5.2801532772
H 3.3759646304 -1.9445553529 5.0747672348
H 5.9238914279 1.2810802456 3.5735882126
H 5.6434272394 2.3347693794 2.5041764612
H 6.002218912 0.1628833508 1.375459606
H 6.6311603949 -0.2831120222 0.0233791362
H 8.5753418445 -2.7965011704 -2.0818828552
H 7.8447466908 -2.1147687279 -3.2488845622
H 8.0627214435 -0.5566719782 -1.7602867609
H 6.8177350238 0.3213597014 -1.9247773212
H 5.842841328 -1.2648327506 -3.6957745005
H 6.36162903 -1.7541725612 -5.0504066383
H 3.8997990447 3.3899132803 -5.4341346601
H 3.0184162831 4.3723985757 -6.2105693852
H 1.8846746331 3.4089735724 -4.3657562635
H 1.0886067034 3.1796555592 -3.0370186912
H 1.0625990931 4.4287597471 -0.9793917876
H 1.0617373415 2.9103550053 -0.7233045831
N 2.760796234 0.4180231478 2.8215661959
C 2.6964478056 -0.2453081903 1.4985426988
C 2.6149406638 0.7775901088 0.3733629411
O 1.6263627543 1.5128034992 0.2758175994
H 1.9533873388 1.0580500793 2.9540340659
H 3.646974273 0.9325865475 2.9204078044
H 3.5657902777 -0.887519515 1.3972203747
H 1.7949874112 -0.8516816775 1.4679325655
N 3.6556157772 0.7857020565 -0.4476957041
C 3.8020087423 1.6884146084 -1.5752313612
C 4.154166803 0.8382842675 -2.789405147
O 5.1834896613 0.1517983981 -2.7952429674
H 4.473460013 0.222083491 -0.1858864158
H 2.8477136423 2.180644607 -1.7442744127
C 4.8812266487 2.7538773248 -1.3019894054
H 5.7861277088 2.2239042411 -0.9900342761
N 3.3088183458 0.8753826986 -3.8113798045
C 3.588831197 0.1473757025 -5.0184601453
C 4.7352198947 0.7548954406 -5.8033857276
O 5.0298734061 1.9241474519 -5.8081415812
O 5.3748172062 -0.15755202 -6.5264473919
H 2.5002966898 1.510028042 -3.7849965277
H 3.8054218271 -0.8984719133 -4.8109719438
H 2.7094469923 0.1785996878 -5.6607760219

H 2.7229454044 -0.3090060724 3.5633533922
H 6.0534331429 0.2826638944 -7.0556816772
C 5.1953162192 3.5412467607 -2.5761948107
H 5.5031726282 2.8498118752 -3.3622939887
H 4.2801729462 4.0227980288 -2.9309436391
C 4.4335335397 3.6680913621 -0.1659158938
H 3.6224750499 4.3195853252 -0.4967399472
H 4.0777512265 3.1052275437 0.6953863354
H 5.2533764266 4.2996385306 0.1705415824
C 6.2901850913 4.5850484708 -2.3987798265
H 6.5294005335 5.0499421008 -3.3546800777
H 5.9896231764 5.3764791734 -1.7129181536
H 7.2017895147 4.1290296794 -2.0081440779