FPHA trimers:

2FPHA

2T1

C -0.077028000 4.262463000 -0.871850000

C 0.418488000 3.391294000 -0.169534000

C 0.963239000 2.347224000 0.637144000

C 2.304734000 1.928235000 0.491223000

C 0.173481000 1.667215000 1.600176000

C 2.855541000 0.889646000 1.242066000

C 0.704903000 0.616933000 2.354922000

C 2.044173000 0.226751000 2.176355000

H -0.489347000 5.057969000 -1.462334000

F 3.089095000 2.551558000 -0.433743000

H -0.868419000 1.963546000 1.734165000

H 3.893581000 0.597516000 1.068188000

H 0.064470000 0.083970000 3.061701000

H 2.454943000 -0.609608000 2.749141000

C -3.336067000 0.706226000 2.725651000

C -3.176665000 0.510083000 1.528986000

C -2.958520000 0.303835000 0.133739000

C -2.472514000 1.343000000 -0.702176000

C -3.209808000 -0.949243000 -0.471632000

C -2.249238000 1.124328000 -2.066907000

C -2.988887000 -1.186438000 -1.829528000

C -2.505847000 -0.138539000 -2.631236000

H -3.500733000 0.878046000 3.772096000

H -2.254368000 2.317716000 -0.261138000

F -3.691208000 -1.962507000 0.297155000

H -1.858174000 1.938104000 -2.683515000

H -3.189960000 -2.180332000 -2.236590000

H -2.321814000 -0.316280000 -3.694939000

C -0.730852000 -2.901020000 1.630843000

C 0.069842000 -2.465949000 0.815814000

C 0.970780000 -1.907934000 -0.139604000

C 2.271871000 -2.422738000 -0.332255000

C 0.594518000 -0.791228000 -0.926645000

C 3.168618000 -1.879631000 -1.254126000

C 1.477662000 -0.231659000 -1.855079000

C 2.764249000 -0.774046000 -2.022070000

H -1.453016000 -3.291115000 2.321564000

F 2.675982000 -3.486659000 0.420126000

H -0.394649000 -0.361826000 -0.775082000

H 4.163067000 -2.322119000 -1.356592000

H 1.167698000 0.642698000 -2.433862000

H 3.461862000 -0.332671000 -2.740297000

2T2

C 3.975136000 -1.303025000 2.301461000

C 3.454339000 -1.122310000 1.209517000

C 2.811556000 -0.887410000 -0.043456000

C 1.516141000 -1.397323000 -0.317066000

C 3.425896000 -0.106596000 -1.050022000

C 0.876288000 -1.123351000 -1.531218000

C 2.803035000 0.177396000 -2.267167000

C 1.516201000 -0.336054000 -2.504428000

H 4.454456000 -1.483631000 3.244474000

H 1.017909000 -1.988744000 0.454085000

F 4.668534000 0.401806000 -0.819587000

H -0.130451000 -1.505919000 -1.710450000

H 3.323722000 0.797353000 -3.001255000

H 1.010403000 -0.105952000 -3.446610000

C -0.730831000 -2.666045000 2.864835000

C -1.280481000 -2.314027000 1.830594000

C -1.871273000 -1.876246000 0.606917000

C -2.258221000 -2.796148000 -0.394526000

C -2.060839000 -0.497998000 0.331419000

C -2.804907000 -2.393534000 -1.614861000

C -2.608024000 -0.074410000 -0.884917000

C -2.979722000 -1.019673000 -1.857766000

H -0.268217000 -2.985562000 3.778852000

F -2.082791000 -4.127495000 -0.166586000

H -1.751361000 0.227299000 1.085088000

H -3.081096000 -3.151680000 -2.352061000

H -2.727466000 0.993515000 -1.082118000

H -3.403382000 -0.691564000 -2.811975000

C -0.823290000 3.221502000 -2.583705000

C -0.670494000 2.958209000 -1.399096000

C -0.497292000 2.612731000 -0.024966000

C 0.611722000 1.843558000 0.409905000

C -1.441241000 2.997709000 0.954422000

C 0.755978000 1.480158000 1.753824000

C -1.314383000 2.649089000 2.300445000

C -0.204738000 1.882650000 2.699093000

H -0.945383000 3.485935000 -3.616525000

H 1.343091000 1.524622000 -0.333686000

F -2.527450000 3.725185000 0.568185000

H 1.610429000 0.870681000 2.059242000

H -2.080321000 2.971162000 3.010265000

H -0.100320000 1.593910000 3.749143000

2T3

C 2.673482000 1.346826000 -1.955034000

C 1.857348000 1.840946000 -1.191133000

C 0.897885000 2.356971000 -0.270471000

C -0.022216000 3.364202000 -0.638838000

C 0.807005000 1.848063000 1.050025000

C -0.991680000 3.857210000 0.237175000

C -0.158243000 2.327765000 1.942429000

C -1.057494000 3.332015000 1.539701000

H 3.392184000 0.892920000 -2.608874000

F 0.025704000 3.864336000 -1.905851000

H 1.495512000 1.056035000 1.347932000

H -1.680311000 4.631891000 -0.109057000

H -0.219553000 1.904919000 2.948983000

H -1.819447000 3.702619000 2.231734000

C 2.587490000 -2.285510000 -2.440953000

C 2.312499000 -2.019820000 -1.279359000

C 1.969929000 -1.744884000 0.078998000

C 0.625140000 -1.798455000 0.525387000

C 2.956435000 -1.424144000 1.039555000

C 0.296266000 -1.554776000 1.864061000

C 2.650622000 -1.183295000 2.381032000

C 1.308031000 -1.254720000 2.793726000

H 2.833610000 -2.518272000 -3.459105000

H -0.151771000 -2.031155000 -0.203619000

F 4.258079000 -1.353613000 0.645992000

H -0.750736000 -1.586687000 2.176580000

H 3.458707000 -0.945905000 3.077546000

H 1.057253000 -1.067001000 3.842356000

C -3.738438000 -0.391093000 2.374561000

C -3.271559000 -0.551792000 1.255335000

C -2.681946000 -0.735883000 -0.031821000

C -1.891205000 0.276844000 -0.632868000

C -2.834224000 -1.946979000 -0.745235000

C -1.279212000 0.072327000 -1.874527000

C -2.233052000 -2.169415000 -1.986025000

C -1.447037000 -1.149479000 -2.550237000

H -4.182955000 -0.247607000 3.340706000

H -1.754467000 1.214035000 -0.092423000

F -3.584512000 -2.942974000 -0.196059000

H -0.652412000 0.856573000 -2.304930000

H -2.378046000 -3.131007000 -2.484673000

H -0.955970000 -1.318644000 -3.512788000

2T4

C -3.916686000 0.643255000 -2.430691000

C -3.550160000 0.332607000 -1.305924000

C -3.105100000 -0.038556000 -0.000989000

C -3.241741000 -1.367337000 0.463823000

C -2.494317000 0.896354000 0.874284000

C -2.807283000 -1.772606000 1.727015000

C -2.054884000 0.508240000 2.146235000

C -2.211108000 -0.822922000 2.573874000

H -4.258899000 0.911261000 -3.411763000

F -3.811720000 -2.292525000 -0.356257000

H -2.346924000 1.919948000 0.525239000

H -2.931160000 -2.816750000 2.024671000

H -1.572564000 1.244186000 2.793566000

H -1.856383000 -1.130966000 3.561760000

C -1.138560000 3.046218000 -1.825096000

C -0.138529000 2.719640000 -1.201540000

C 1.017950000 2.287913000 -0.486620000

C 1.097263000 2.390769000 0.919916000

C 2.124708000 1.703175000 -1.153626000

C 2.189551000 1.926050000 1.652082000

C 3.233122000 1.237745000 -0.438259000

C 3.265007000 1.342095000 0.963448000

H -2.027171000 3.317845000 -2.360545000

F 0.057868000 2.966805000 1.595765000

H 2.078439000 1.597554000 -2.239685000

H 2.182826000 2.017048000 2.740947000

H 4.065137000 0.770777000 -0.971753000

H 4.118368000 0.954017000 1.526364000

C 2.172041000 -1.988726000 2.671562000

C 1.898162000 -1.840503000 1.488713000

C 1.561377000 -1.657634000 0.113699000

C 0.306526000 -1.125491000 -0.275332000

C 2.468797000 -1.989449000 -0.917340000

C -0.014110000 -0.943135000 -1.625048000

C 2.168200000 -1.820264000 -2.269137000

C 0.914011000 -1.292056000 -2.621697000

H 2.416756000 -2.135882000 3.705762000

H -0.400855000 -0.847564000 0.505694000

F 3.694951000 -2.484055000 -0.579823000

H -0.982156000 -0.516971000 -1.898061000

H 2.911921000 -2.097763000 -3.020884000

H 0.667354000 -1.151058000 -3.678599000

2T5

C 5.443472000 -1.199569000 -0.264986000

C 4.294103000 -1.354534000 0.123272000

C 2.957818000 -1.526912000 0.594203000

C 2.650867000 -1.518651000 1.980819000

C 1.879983000 -1.713214000 -0.302005000

C 1.332372000 -1.676885000 2.427962000

C 0.560096000 -1.858539000 0.125031000

C 0.285606000 -1.838774000 1.501687000

H 6.452205000 -1.067859000 -0.606872000

H 3.469948000 -1.381847000 2.692048000

F 2.140521000 -1.757093000 -1.637348000

H 1.119726000 -1.664838000 3.501088000

H -0.230433000 -1.974302000 -0.617643000

H -0.747863000 -1.935661000 1.844691000

C 2.434640000 1.443717000 -2.055061000

C 1.688850000 1.863146000 -1.182402000

C 0.815455000 2.295572000 -0.140715000

C -0.096711000 3.358703000 -0.326650000

C 0.807102000 1.647916000 1.120853000

C -0.982636000 3.775705000 0.669005000

C -0.074184000 2.049596000 2.131034000

C -0.968794000 3.112435000 1.908703000

H 3.099187000 1.059511000 -2.804415000

F -0.126756000 3.993578000 -1.532687000

H 1.492473000 0.814391000 1.280311000

H -1.669546000 4.600070000 0.462178000

H -0.072571000 1.521918000 3.088770000

H -1.664879000 3.423414000 2.693324000

C -3.603008000 -0.728290000 2.528328000

C -3.242063000 -0.734706000 1.359578000

C -2.777930000 -0.740514000 0.009347000

C -2.994162000 -1.851678000 -0.837774000

C -2.056052000 0.355638000 -0.528448000

C -2.523873000 -1.898419000 -2.151907000

C -1.574933000 0.327010000 -1.842230000

C -1.807246000 -0.797769000 -2.653920000

H -3.953631000 -0.718573000 3.542545000

F -3.678131000 -2.924904000 -0.351197000

H -1.868241000 1.216603000 0.114147000

H -2.715984000 -2.788235000 -2.756622000

H -1.000724000 1.172951000 -2.227011000

H -1.422995000 -0.827683000 -3.677801000

2T6

C 3.914244000 -0.858838000 2.420579000

C 3.530963000 -0.656747000 1.276808000

C 3.056302000 -0.429031000 -0.050539000

C 3.174314000 -1.424546000 -1.048375000

C 2.434184000 0.791401000 -0.419866000

C 2.704412000 -1.244982000 -2.350977000

C 1.954884000 0.987931000 -1.720492000

C 2.088300000 -0.026609000 -2.685739000

H 4.282489000 -1.034955000 3.413033000

F 3.761588000 -2.609804000 -0.725748000

H 2.320911000 1.567925000 0.338364000

H 2.817953000 -2.054615000 -3.076091000

H 1.465281000 1.930476000 -1.976713000

H 1.706375000 0.122096000 -3.700120000

C 1.000272000 1.638428000 2.961034000

C 0.221256000 1.883561000 2.051031000

C -0.671097000 2.132963000 0.965861000

C -1.877114000 1.402797000 0.816178000

C -0.376185000 3.096596000 -0.024413000

C -2.728202000 1.627963000 -0.271790000

C -1.211438000 3.339976000 -1.115273000

C -2.397508000 2.595055000 -1.237501000

H 1.693146000 1.418754000 3.749683000

H -2.113917000 0.635982000 1.556232000

F 0.783647000 3.811200000 0.079080000

H -3.638658000 1.031398000 -0.376359000

H -0.926533000 4.098614000 -1.849037000

H -3.057772000 2.770082000 -2.092509000

C -5.276466000 -1.987275000 -0.544299000

C -4.116159000 -1.965757000 -0.157004000

C -2.770225000 -1.904207000 0.314118000

C -1.698119000 -1.617593000 -0.560606000

C -2.452021000 -2.093200000 1.685139000

C -0.378688000 -1.498113000 -0.125140000

C -1.132151000 -1.980313000 2.139576000

C -0.095502000 -1.677479000 1.237343000

H -6.291166000 -2.034544000 -0.890554000

F -1.967611000 -1.423272000 -1.882028000

H -3.265640000 -2.317280000 2.380501000

H 0.399486000 -1.247314000 -0.846631000

H -0.911812000 -2.117317000 3.202152000

H 0.931712000 -1.564299000 1.592402000

2T7

C -2.384872000 -0.093129000 3.178986000

C -2.272820000 -0.554041000 2.051547000

C -2.117915000 -1.054898000 0.724125000

C -0.837556000 -1.174904000 0.127372000

C -3.234129000 -1.419201000 -0.061227000

C -0.694626000 -1.637363000 -1.184926000

C -3.113716000 -1.884993000 -1.371277000

C -1.830234000 -1.994361000 -1.933875000

H -2.491392000 0.283900000 4.177888000

H 0.033003000 -0.878057000 0.711894000

F -4.483076000 -1.296466000 0.474487000

H 0.301035000 -1.709051000 -1.628512000

H -4.015364000 -2.152993000 -1.928431000

H -1.722227000 -2.357798000 -2.960617000

C 1.558142000 3.741303000 1.938074000

C 0.798257000 3.280421000 1.097359000

C -0.090708000 2.732334000 0.124021000

C -1.447152000 2.451278000 0.429337000

C 0.346092000 2.449942000 -1.190794000

C -2.306195000 1.918613000 -0.538621000

C -0.491376000 1.906740000 -2.164439000

C -1.830200000 1.642519000 -1.831713000

H 2.219795000 4.169771000 2.666128000

H -1.804546000 2.640736000 1.444074000

F 1.642150000 2.720067000 -1.521126000

H -3.342538000 1.693724000 -0.274227000

H -0.087835000 1.693643000 -3.157079000

H -2.494437000 1.201368000 -2.579772000

C 3.107516000 -0.658183000 -2.825995000

C 2.929552000 -0.780340000 -1.622252000

C 2.680425000 -0.910138000 -0.222654000

C 2.545767000 -2.181193000 0.382092000

C 2.527438000 0.226235000 0.613713000

C 2.268758000 -2.344734000 1.740283000

C 2.245366000 0.081733000 1.977484000

C 2.116388000 -1.200534000 2.541874000

H 3.301315000 -0.548281000 -3.875670000

F 2.674285000 -3.292646000 -0.395139000

H 2.616906000 1.218989000 0.169395000

H 2.164110000 -3.353952000 2.146174000

H 2.104461000 0.976299000 2.589016000

H 1.884271000 -1.315528000 3.604763000

2T8

C -5.474058000 0.115881000 -0.508412000

C -4.447009000 -0.494594000 -0.247145000

C -3.245995000 -1.193879000 0.078177000

C -2.150877000 -1.229265000 -0.814887000

C -3.088434000 -1.868684000 1.317854000

C -0.949996000 -1.871715000 -0.516465000

C -1.891340000 -2.524243000 1.633366000

C -0.821253000 -2.523992000 0.719686000

H -6.376938000 0.645485000 -0.745684000

F -2.263945000 -0.585087000 -2.011845000

H -3.922609000 -1.856521000 2.024552000

H -0.132698000 -1.838749000 -1.238386000

H -1.789248000 -3.031582000 2.597241000

H 0.121366000 -3.015466000 0.973374000

C 0.042244000 4.060959000 -2.457684000

C 0.022500000 3.550081000 -1.346532000

C 0.011779000 2.910084000 -0.070543000

C 0.901869000 3.301327000 0.956538000

C -0.868383000 1.832860000 0.209517000

C 0.945149000 2.664411000 2.198602000

C -0.838109000 1.180589000 1.447302000

C 0.067902000 1.592990000 2.440170000

H 0.041854000 4.533201000 -3.421400000

F 1.762403000 4.330888000 0.721919000

H -1.559401000 1.510772000 -0.572223000

H 1.663923000 3.004852000 2.948116000

H -1.508422000 0.338792000 1.630940000

H 0.104978000 1.073283000 3.401875000

C 2.614351000 -1.747664000 2.761883000

C 2.532724000 -1.531624000 1.560831000

C 2.399965000 -1.273036000 0.163291000

C 2.037432000 0.009654000 -0.320312000

C 2.594984000 -2.293882000 -0.794786000

C 1.876680000 0.246061000 -1.690442000

C 2.443938000 -2.078651000 -2.166060000

C 2.081001000 -0.795614000 -2.613567000

H 2.720065000 -1.936343000 3.812965000

H 1.869391000 0.806964000 0.404454000

F 2.929238000 -3.543304000 -0.363324000

H 1.579238000 1.239978000 -2.035364000

H 2.605081000 -2.908812000 -2.858307000

H 1.951768000 -0.616653000 -3.685199000

2T9

C -5.474058000 0.115881000 -0.508412000

C -4.447009000 -0.494594000 -0.247145000

C -3.245995000 -1.193879000 0.078177000

C -2.150877000 -1.229265000 -0.814887000

C -3.088434000 -1.868684000 1.317854000

C -0.949996000 -1.871715000 -0.516465000

C -1.891340000 -2.524243000 1.633366000

C -0.821253000 -2.523992000 0.719686000

H -6.376938000 0.645485000 -0.745684000

F -2.263945000 -0.585087000 -2.011845000

H -3.922609000 -1.856521000 2.024552000

H -0.132698000 -1.838749000 -1.238386000

H -1.789248000 -3.031582000 2.597241000

H 0.121366000 -3.015466000 0.973374000

C 0.042244000 4.060959000 -2.457684000

C 0.022500000 3.550081000 -1.346532000

C 0.011779000 2.910084000 -0.070543000

C 0.901869000 3.301327000 0.956538000

C -0.868383000 1.832860000 0.209517000

C 0.945149000 2.664411000 2.198602000

C -0.838109000 1.180589000 1.447302000

C 0.067902000 1.592990000 2.440170000

H 0.041854000 4.533201000 -3.421400000

F 1.762403000 4.330888000 0.721919000

H -1.559401000 1.510772000 -0.572223000

H 1.663923000 3.004852000 2.948116000

H -1.508422000 0.338792000 1.630940000

H 0.104978000 1.073283000 3.401875000

C 2.614351000 -1.747664000 2.761883000

C 2.532724000 -1.531624000 1.560831000

C 2.399965000 -1.273036000 0.163291000

C 2.037432000 0.009654000 -0.320312000

C 2.594984000 -2.293882000 -0.794786000

C 1.876680000 0.246061000 -1.690442000

C 2.443938000 -2.078651000 -2.166060000

C 2.081001000 -0.795614000 -2.613567000

H 2.720065000 -1.936343000 3.812965000

H 1.869391000 0.806964000 0.404454000

F 2.929238000 -3.543304000 -0.363324000

H 1.579238000 1.239978000 -2.035364000

H 2.605081000 -2.908812000 -2.858307000

H 1.951768000 -0.616653000 -3.685199000

2T10

C -2.890659000 2.473180000 1.275136000

C -3.051329000 1.302759000 0.960736000

C -3.164004000 -0.073565000 0.603691000

C -3.106170000 -1.100590000 1.581262000

C -3.295864000 -0.476167000 -0.744976000

C -3.157667000 -2.450469000 1.213872000

C -3.341196000 -1.816142000 -1.132317000

C -3.268462000 -2.810140000 -0.141525000

H -2.726236000 3.501150000 1.533904000

H -2.999950000 -0.812467000 2.630223000

F -3.378350000 0.482754000 -1.710429000

H -3.098266000 -3.224499000 1.984060000

H -3.430917000 -2.063793000 -2.192934000

H -3.295410000 -3.864289000 -0.432713000

C 4.853747000 -2.786001000 -0.084318000

C 3.839885000 -2.229639000 0.315035000

C 2.670194000 -1.549271000 0.769361000

C 1.398964000 -1.823798000 0.216730000

C 2.735702000 -0.546508000 1.771559000

C 0.243754000 -1.148420000 0.605572000

C 1.586852000 0.143723000 2.173990000

C 0.342755000 -0.152566000 1.589083000

H 5.739476000 -3.289790000 -0.420790000

F 1.299637000 -2.772646000 -0.759377000

H 3.710506000 -0.308723000 2.205267000

H -0.703800000 -1.391257000 0.124069000

H 1.664748000 0.934415000 2.925097000

H -0.548850000 0.409885000 1.876241000

C 0.367141000 4.226353000 1.250208000

C 0.539285000 3.368685000 0.394791000

C 0.739188000 2.352594000 -0.587728000

C 2.020612000 1.798212000 -0.810520000

C -0.332369000 1.844571000 -1.365063000

C 2.251973000 0.783575000 -1.739165000

C -0.117696000 0.830280000 -2.305726000

C 1.170671000 0.298895000 -2.492973000

H 0.234552000 5.000017000 1.981811000

F 3.072206000 2.266658000 -0.082716000

H -1.334527000 2.243124000 -1.197170000

H 3.259923000 0.375976000 -1.845878000

H -0.962339000 0.448719000 -2.884828000

H 1.337804000 -0.506663000 -3.213947000

2T11

C 5.284933000 -1.885794000 0.660358000

C 4.133835000 -1.951052000 0.251278000

C 2.795257000 -1.988831000 -0.243032000

C 1.690987000 -1.766963000 0.610924000

C 2.514992000 -2.218326000 -1.615967000

C 0.373479000 -1.751920000 0.154481000

C 1.197639000 -2.213294000 -2.091712000

C 0.127168000 -1.978319000 -1.208634000

H 6.294132000 -1.857139000 1.024468000

F 1.925373000 -1.535772000 1.932954000

H 3.354037000 -2.392442000 -2.295182000

H -0.435038000 -1.551966000 0.859111000

H 1.004507000 -2.387542000 -3.154219000

H -0.900966000 -1.964749000 -1.578865000

C -4.196338000 -3.691575000 -0.163054000

C -3.728584000 -2.615191000 0.181103000

C -3.160779000 -1.372199000 0.593230000

C -2.882581000 -0.346256000 -0.339219000

C -2.829787000 -1.117872000 1.950657000

C -2.299300000 0.868139000 0.021615000

C -2.241237000 0.094652000 2.332565000

C -1.974277000 1.085653000 1.369970000

H -4.618518000 -4.630503000 -0.466417000

F -3.181924000 -0.561499000 -1.652028000

H -3.034584000 -1.897158000 2.689578000

H -2.101131000 1.619804000 -0.744346000

H -1.983861000 0.264276000 3.382097000

H -1.504160000 2.029223000 1.658434000

C -1.708089000 4.754229000 -0.602550000

C -0.721519000 4.058274000 -0.405471000

C 0.399858000 3.215754000 -0.141480000

C 1.173962000 3.356736000 1.040031000

C 0.767644000 2.181848000 -1.032576000

C 2.248415000 2.498143000 1.302659000

C 1.830193000 1.314052000 -0.785623000

C 2.576110000 1.476415000 0.392860000

H -2.555646000 5.384389000 -0.793446000

H 0.907670000 4.150549000 1.743656000

F 0.041420000 2.015891000 -2.175063000

H 2.828749000 2.621313000 2.221784000

H 2.046591000 0.514647000 -1.497061000

H 3.402508000 0.791900000 0.603170000

2T12

C 0.924759000 0.423846000 2.972070000

C 1.532159000 -0.162636000 2.088588000

C 2.190323000 -0.850013000 1.025867000

C 2.291191000 -2.260638000 1.019632000

C 2.734038000 -0.156894000 -0.085189000

C 2.887441000 -2.970322000 -0.023670000

C 3.335907000 -0.850794000 -1.141308000

C 3.413934000 -2.254941000 -1.113394000

H 0.398744000 0.946703000 3.746217000

F 1.768975000 -2.958680000 2.066748000

H 2.658535000 0.931306000 -0.111607000

H 2.926843000 -4.061301000 0.025899000

H 3.732126000 -0.291438000 -1.993027000

H 3.880337000 -2.799700000 -1.939958000

C 1.307993000 1.617703000 -3.161371000

C 0.794254000 1.925900000 -2.095176000

C 0.188490000 2.291210000 -0.855327000

C 0.851811000 3.131616000 0.067024000

C -1.100929000 1.824303000 -0.494065000

C 0.284533000 3.516588000 1.281196000

C -1.684724000 2.190994000 0.723386000

C -0.996442000 3.040426000 1.607487000

H 1.754371000 1.352843000 -4.100230000

F 2.105398000 3.578342000 -0.238951000

H -1.624585000 1.161666000 -1.184809000

H 0.849693000 4.167935000 1.952392000

H -2.670042000 1.799306000 0.989283000

H -1.451120000 3.329301000 2.560316000

C -3.740803000 -0.994745000 2.532837000

C -3.199178000 -1.119634000 1.443308000

C -2.542808000 -1.244489000 0.181958000

C -3.248160000 -1.084852000 -1.032501000

C -1.150207000 -1.502470000 0.094389000

C -2.626719000 -1.162556000 -2.280829000

C -0.509039000 -1.583090000 -1.146849000

C -1.244439000 -1.411773000 -2.333035000

H -4.220900000 -0.915127000 3.489203000

F -4.586518000 -0.829497000 -0.986328000

H -0.585968000 -1.611665000 1.022196000

H -3.224640000 -1.021089000 -3.184710000

H 0.567268000 -1.759796000 -1.191108000

H -0.741667000 -1.456874000 -3.303440000

2T13

C 3.368449000 -3.238892000 -1.226775000

C 3.376232000 -2.094414000 -0.795127000

C 3.388668000 -0.752704000 -0.310068000

C 3.193203000 -0.462227000 1.058783000

C 3.589831000 0.349305000 -1.180705000

C 3.193500000 0.838733000 1.563026000

C 3.593798000 1.661244000 -0.694427000

C 3.394576000 1.907407000 0.675513000

H 3.370534000 -4.245671000 -1.597826000

F 2.982934000 -1.494493000 1.923279000

H 3.732887000 0.147953000 -2.245618000

H 3.015220000 0.998302000 2.628866000

H 3.734613000 2.496349000 -1.386390000

H 3.374195000 2.933158000 1.053727000

C -3.366768000 -3.013652000 1.709945000

C -3.397062000 -1.912766000 1.177502000

C -3.397345000 -0.619836000 0.573514000

C -3.373227000 -0.464999000 -0.830864000

C -3.392710000 0.563772000 1.355527000

C -3.336035000 0.784474000 -1.450189000

C -3.354587000 1.825517000 0.751919000

C -3.325284000 1.937501000 -0.649207000

H -3.368385000 -3.981029000 2.174348000

F -3.375977000 -1.580085000 -1.613409000

H -3.396663000 0.466619000 2.444188000

H -3.301742000 0.837685000 -2.540889000

H -3.327196000 2.723773000 1.374781000

H -3.273007000 2.922422000 -1.121597000

C 0.153856000 3.823206000 -0.184954000

C 0.125876000 2.606267000 -0.307375000

C 0.082554000 1.190563000 -0.473518000

C 0.160553000 0.593791000 -1.758176000

C -0.044393000 0.321331000 0.630928000

C 0.106209000 -0.794776000 -1.912291000

C -0.101511000 -1.065853000 0.497691000

C -0.026461000 -1.625159000 -0.785520000

H 0.185552000 4.889574000 -0.072411000

H 0.263696000 1.248626000 -2.627241000

F -0.114784000 0.857235000 1.882302000

H 0.169167000 -1.233339000 -2.911808000

H -0.210465000 -1.685007000 1.389596000

H -0.069499000 -2.710336000 -0.902191000

2T14

C -0.236847000 0.226400000 -2.490230000

C -1.231682000 -0.137062000 -1.880208000

C -2.391651000 -0.532559000 -1.150069000

C -2.537258000 -1.843585000 -0.645502000

C -3.443137000 0.380035000 -0.880080000

C -3.647673000 -2.254214000 0.091263000

C -4.566172000 -0.009714000 -0.142051000

C -4.670928000 -1.324679000 0.344460000

H 0.667262000 0.532351000 -2.979392000

F -1.546214000 -2.755107000 -0.885295000

H -3.346869000 1.404589000 -1.244991000

H -3.699649000 -3.284752000 0.452194000

H -5.357678000 0.716935000 0.062589000

H -5.547968000 -1.632012000 0.922801000

C -1.939007000 -0.055158000 2.620183000

C -1.277544000 0.700583000 1.922976000

C -0.491779000 1.555923000 1.093528000

C -1.046957000 2.696088000 0.470262000

C 0.878763000 1.288898000 0.846863000

C -0.310026000 3.532917000 -0.367907000

C 1.637366000 2.117055000 0.012079000

C 1.044262000 3.236748000 -0.598031000

H -2.533610000 -0.710912000 3.225440000

F -2.360511000 2.996064000 0.694313000

H 1.327700000 0.411605000 1.314819000

H -0.798622000 4.397824000 -0.824186000

H 2.690741000 1.885636000 -0.166633000

H 1.633178000 3.885639000 -1.253851000

C 5.767020000 0.743850000 -0.182558000

C 4.814410000 0.007685000 0.034201000

C 3.684768000 -0.821427000 0.306619000

C 3.429189000 -1.326406000 1.608787000

C 2.755255000 -1.151854000 -0.705488000

C 2.295268000 -2.106998000 1.867078000

C 1.618916000 -1.924532000 -0.468349000

C 1.389094000 -2.402331000 0.831521000

H 6.617908000 1.367817000 -0.378691000

H 4.133190000 -1.080784000 2.408307000

F 2.968385000 -0.672903000 -1.965207000

H 2.111313000 -2.475490000 2.880333000

H 0.916581000 -2.114468000 -1.280492000

H 0.489678000 -2.990448000 1.031385000

2T15

C 3.001861000 3.460960000 -1.083825000

C 3.143445000 2.273101000 -0.828226000

C 3.269303000 0.880271000 -0.544111000

C 3.376140000 0.408689000 0.783940000

C 3.260306000 -0.091232000 -1.577598000

C 3.457757000 -0.948093000 1.096959000

C 3.340675000 -1.456750000 -1.282651000

C 3.437452000 -1.886262000 0.052439000

H 2.907708000 4.506207000 -1.307471000

F 3.387324000 1.314114000 1.801637000

H 3.164229000 0.251095000 -2.611107000

H 3.520141000 -1.250611000 2.144850000

H 3.306580000 -2.189520000 -2.093477000

H 3.477315000 -2.954087000 0.285343000

C -0.000299000 -3.903746000 -0.692411000

C -0.000392000 -2.770024000 -0.232662000

C -0.000543000 -1.457818000 0.326594000

C -0.002058000 -1.253788000 1.730509000

C 0.000803000 -0.307207000 -0.490389000

C -0.002237000 0.036240000 2.270927000

C 0.000726000 0.986919000 0.029882000

C -0.000855000 1.157077000 1.421359000

H -0.000185000 -4.895892000 -1.100537000

H -0.003128000 -2.132055000 2.381470000

F 0.002306000 -0.463298000 -1.843481000

H -0.003515000 0.170652000 3.356270000

H 0.002073000 1.838450000 -0.652225000

H -0.000975000 2.166798000 1.838866000

C -2.999352000 3.465354000 -1.071864000

C -3.141748000 2.276477000 -0.821500000

C -3.268202000 0.882481000 -0.543456000

C -3.377938000 0.405348000 0.782365000

C -3.256865000 -0.084700000 -1.580968000

C -3.460272000 -0.952739000 1.089508000

C -3.337819000 -1.451443000 -1.291925000

C -3.437632000 -1.886542000 0.041133000

H -2.904766000 4.511535000 -1.290914000

F -3.391370000 1.306494000 1.803827000

H -3.158521000 0.261958000 -2.612820000

H -3.525000000 -1.259633000 2.135986000

H -3.301867000 -2.180805000 -2.105738000

H -3.477982000 -2.955325000 0.269487000

2T16

C -0.123392000 2.893563000 0.465603000

C -1.129740000 2.357087000 0.023601000

C -2.304897000 1.711973000 -0.464461000

C -2.220148000 0.581212000 -1.307799000

C -3.604355000 2.159702000 -0.115242000

C -3.342693000 -0.099073000 -1.778121000

C -4.744393000 1.497741000 -0.585894000

C -4.615477000 0.366817000 -1.411907000

H 0.793417000 3.305990000 0.843539000

F -0.986284000 0.133310000 -1.678293000

H -3.694915000 3.032083000 0.537572000

H -3.208831000 -0.981172000 -2.408762000

H -5.737050000 1.859360000 -0.301091000

H -5.505326000 -0.159964000 -1.769910000

C -4.112850000 -0.887187000 2.012523000

C -2.933464000 -1.077182000 1.752241000

C -1.550445000 -1.280697000 1.465913000

C -0.547417000 -0.446969000 2.025428000

C -1.118344000 -2.317281000 0.608231000

C 0.806112000 -0.654992000 1.739178000

C 0.226458000 -2.542493000 0.313233000

C 1.194601000 -1.702327000 0.886118000

H -5.149606000 -0.719388000 2.229248000

H -0.859614000 0.375649000 2.673196000

F -2.056224000 -3.126366000 0.033344000

H 1.559003000 0.015533000 2.161263000

H 0.496143000 -3.355926000 -0.365205000

H 2.249616000 -1.850980000 0.641724000

C 3.361265000 2.740213000 1.739550000

C 3.372739000 1.880706000 0.868777000

C 3.385226000 0.862921000 -0.133212000

C 2.349981000 0.746782000 -1.095620000

C 4.429540000 -0.089218000 -0.186348000

C 2.374869000 -0.269699000 -2.057315000

C 4.469532000 -1.111347000 -1.136337000

C 3.431594000 -1.196806000 -2.080726000

H 3.373490000 3.499871000 2.497650000

H 1.511589000 1.444600000 -1.053358000

F 5.435513000 -0.011897000 0.729455000

H 1.555424000 -0.348360000 -2.776014000

H 5.303073000 -1.818451000 -1.125435000

H 3.450741000 -1.994955000 -2.829446000

2T17

C 1.500290000 -2.622859000 -0.694086000

C 2.330565000 -1.726384000 -0.646539000

C 3.228219000 -0.619174000 -0.584834000

C 3.780187000 -0.188977000 0.643267000

C 3.570988000 0.127024000 -1.742243000

C 4.623786000 0.917525000 0.747560000

C 4.416586000 1.239978000 -1.659457000

C 4.942994000 1.636610000 -0.416535000

H 0.744509000 -3.385011000 -0.718971000

F 3.468630000 -0.878676000 1.778082000

H 3.152501000 -0.184992000 -2.703187000

H 5.014194000 1.202172000 1.728037000

H 4.663858000 1.801899000 -2.565152000

H 5.601610000 2.508097000 -0.348565000

C -0.803567000 -3.704167000 1.975220000

C -1.468046000 -2.954470000 1.273379000

C -2.217467000 -2.050591000 0.462465000

C -2.918918000 -0.953948000 1.026256000

C -2.269122000 -2.192224000 -0.941671000

C -3.619100000 -0.053559000 0.216248000

C -2.957896000 -1.304099000 -1.767956000

C -3.637357000 -0.224950000 -1.179351000

H -0.228473000 -4.369209000 2.590551000

H -2.878062000 -0.813562000 2.108713000

F -1.611639000 -3.243167000 -1.519341000

H -4.130029000 0.799995000 0.668936000

H -2.949742000 -1.462142000 -2.849338000

H -4.165024000 0.491530000 -1.815161000

C -3.246964000 4.484318000 -0.027482000

C -2.438605000 3.601365000 0.225508000

C -1.525638000 2.549443000 0.537183000

C -1.206425000 2.216902000 1.879140000

C -0.923904000 1.772884000 -0.479383000

C -0.344292000 1.152673000 2.170335000

C -0.066738000 0.708176000 -0.207836000

C 0.220806000 0.394482000 1.129296000

H -3.934991000 5.277376000 -0.249696000

H -1.658394000 2.806804000 2.681564000

F -1.207922000 2.067731000 -1.779973000

H -0.118064000 0.907234000 3.212108000

H 0.350392000 0.124581000 -1.029802000

H 0.871807000 -0.453639000 1.350136000

2T18

C -1.784503000 -2.582130000 -0.392794000

C -2.608384000 -1.680732000 -0.455003000

C -3.508721000 -0.576416000 -0.527855000

C -3.936554000 0.098803000 0.638185000

C -3.988557000 -0.083760000 -1.769240000

C -4.787390000 1.204094000 0.604927000

C -4.844201000 1.023350000 -1.824896000

C -5.243905000 1.668293000 -0.640164000

H -1.028787000 -3.341400000 -0.321653000

F -3.493521000 -0.344349000 1.850442000

H -3.670420000 -0.589177000 -2.685377000

H -5.077758000 1.684589000 1.542828000

H -5.199789000 1.385973000 -2.794070000

H -5.910635000 2.535289000 -0.681084000

C 3.834518000 3.688965000 -1.282175000

C 2.893804000 3.048904000 -0.832141000

C 1.818144000 2.262915000 -0.320445000

C 1.454345000 2.309397000 1.043583000

C 1.092962000 1.369909000 -1.151688000

C 0.437844000 1.518269000 1.581442000

C 0.072531000 0.568123000 -0.630742000

C -0.254743000 0.638065000 0.734903000

H 4.639230000 4.278460000 -1.677839000

F 2.140200000 3.145470000 1.876679000

H 1.367575000 1.308190000 -2.207862000

H 0.211751000 1.589969000 2.648360000

H -0.461648000 -0.130074000 -1.278515000

H -1.031186000 -0.009641000 1.145491000

C 0.374909000 -2.861268000 2.432723000

C 1.182459000 -2.449280000 1.612032000

C 2.105348000 -1.941333000 0.649874000

C 2.175440000 -2.475604000 -0.655568000

C 2.975837000 -0.863143000 0.952619000

C 3.043189000 -1.983455000 -1.630272000

C 3.853096000 -0.352743000 -0.010064000

C 3.887139000 -0.909332000 -1.300722000

H -0.337936000 -3.223019000 3.148655000

F 1.353451000 -3.519240000 -0.983010000

H 2.927020000 -0.422088000 1.950769000

H 3.046532000 -2.439185000 -2.623854000

H 4.492617000 0.498926000 0.235866000

H 4.564619000 -0.503084000 -2.057823000

2T19

C -2.065582000 4.445886000 -0.140442000

C -2.391973000 3.274621000 -0.279370000

C -2.774420000 1.911207000 -0.462379000

C -2.646670000 1.267239000 -1.720913000

C -3.309921000 1.149335000 0.601371000

C -3.045897000 -0.063116000 -1.892124000

C -3.713992000 -0.177219000 0.448738000

C -3.582066000 -0.783774000 -0.810391000

H -1.797036000 5.477463000 -0.015112000

H -2.227874000 1.836623000 -2.555140000

F -3.436875000 1.733301000 1.824117000

H -2.926368000 -0.544703000 -2.866185000

H -4.102681000 -0.719826000 1.313428000

H -3.879126000 -1.828179000 -0.938130000

C 1.138534000 2.576782000 0.062083000

C 2.099454000 1.825747000 0.155870000

C 3.161005000 0.878503000 0.276104000

C 3.027530000 -0.267468000 1.103810000

C 4.373521000 1.024041000 -0.435432000

C 4.060378000 -1.207816000 1.201052000

C 5.414793000 0.097938000 -0.349410000

C 5.252974000 -1.027406000 0.476703000

H 0.277567000 3.218097000 -0.011416000

H 2.095096000 -0.399830000 1.658890000

F 4.534462000 2.110730000 -1.242440000

H 3.934011000 -2.085397000 1.842242000

H 6.329187000 0.266686000 -0.924481000

H 6.061956000 -1.761069000 0.551842000

C -0.602719000 -0.153424000 2.692152000

C -0.589012000 -0.808240000 1.659965000

C -0.547865000 -1.549831000 0.441722000

C 0.075408000 -1.028090000 -0.719571000

C -1.144096000 -2.826427000 0.337009000

C 0.099388000 -1.760757000 -1.912089000

C -1.132451000 -3.571277000 -0.842970000

C -0.501171000 -3.030505000 -1.976619000

H -0.642451000 0.440581000 3.584750000

H 0.521897000 -0.033562000 -0.665937000

F -1.771756000 -3.349155000 1.429411000

H 0.586173000 -1.337233000 -2.795406000

H -1.611374000 -4.553865000 -0.860470000

H -0.482334000 -3.605357000 -2.907868000

2T20

C -1.329808000 1.183441000 -0.954939000

C -2.305307000 0.510713000 -0.653516000

C -3.423360000 -0.301502000 -0.293858000

C -4.728595000 0.236856000 -0.210599000

C -3.274991000 -1.682921000 -0.001316000

C -5.840829000 -0.530228000 0.141188000

C -4.378755000 -2.468575000 0.353308000

C -5.661116000 -1.894520000 0.425157000

H -0.457731000 1.761095000 -1.200159000

F -4.910443000 1.557742000 -0.484833000

H -2.277503000 -2.126080000 -0.057165000

H -6.824118000 -0.054660000 0.187701000

H -4.239019000 -3.531045000 0.574026000

H -6.525618000 -2.506155000 0.701905000

C 5.129024000 -3.585944000 -0.467543000

C 4.059980000 -3.085200000 -0.147865000

C 2.820782000 -2.492081000 0.240416000

C 1.807073000 -2.216324000 -0.705981000

C 2.555123000 -2.140513000 1.590904000

C 0.595682000 -1.617077000 -0.361647000

C 1.343723000 -1.539719000 1.954966000

C 0.366115000 -1.273327000 0.980032000

H 6.063968000 -4.030127000 -0.751416000

F 2.033180000 -2.523441000 -2.015324000

H 3.326707000 -2.340094000 2.339357000

H -0.133267000 -1.386770000 -1.140728000

H 1.171753000 -1.253680000 2.995795000

H -0.563831000 -0.766787000 1.248864000

C 1.743541000 2.096793000 3.262846000

C 1.808735000 2.195025000 2.045756000

C 1.882801000 2.293308000 0.623500000

C 2.396159000 1.233457000 -0.166922000

C 1.436935000 3.450382000 -0.057443000

C 2.444682000 1.331802000 -1.562717000

C 1.480158000 3.569011000 -1.448663000

C 1.987795000 2.497109000 -2.205093000

H 1.693424000 2.025887000 4.332448000

H 2.740843000 0.329664000 0.338374000

F 0.939610000 4.488085000 0.668333000

H 2.832440000 0.494358000 -2.149200000

H 1.116101000 4.486633000 -1.917433000

H 2.021448000 2.576489000 -3.295798000

2T21

C -2.065206000 4.445767000 -0.140248000

C -2.391663000 3.274539000 -0.279374000

C -2.774220000 1.911178000 -0.462548000

C -2.646303000 1.267299000 -1.721115000

C -3.309988000 1.149283000 0.601048000

C -3.045632000 -0.063001000 -1.892502000

C -3.714150000 -0.177229000 0.448236000

C -3.582057000 -0.783696000 -0.810916000

H -1.796719000 5.477340000 -0.014737000

H -2.227289000 1.836703000 -2.555221000

F -3.437094000 1.733157000 1.823818000

H -2.925952000 -0.544536000 -2.866573000

H -4.103033000 -0.719872000 1.312822000

H -3.879146000 -1.828080000 -0.938776000

C 1.138834000 2.577037000 0.062384000

C 2.099638000 1.825828000 0.156004000

C 3.161016000 0.878368000 0.276092000

C 3.027231000 -0.267836000 1.103421000

C 4.373666000 1.023937000 -0.435213000

C 4.059914000 -1.208382000 1.200526000

C 5.414779000 0.097632000 -0.349325000

C 5.252652000 -1.027942000 0.476412000

H 0.277929000 3.218461000 -0.010966000

H 2.094687000 -0.400227000 1.658314000

F 4.534913000 2.110857000 -1.241849000

H 3.933307000 -2.086144000 1.841427000

H 6.329286000 0.266425000 -0.924211000

H 6.061500000 -1.761768000 0.551451000

C -0.602901000 -0.153030000 2.692249000

C -0.589246000 -0.807932000 1.660110000

C -0.548025000 -1.549622000 0.441931000

C 0.075466000 -1.028017000 -0.719314000

C -1.144342000 -2.826174000 0.337231000

C 0.099596000 -1.760797000 -1.911761000

C -1.132547000 -3.571136000 -0.842683000

C -0.501031000 -3.030519000 -1.976271000

H -0.642620000 0.441104000 3.584764000

H 0.521979000 -0.033494000 -0.665717000

F -1.772239000 -3.348757000 1.429568000

H 0.586574000 -1.337394000 -2.795033000

H -1.611551000 -4.553688000 -0.860168000

H -0.482063000 -3.605463000 -2.907463000

2T22

C 2.268442000 1.315937000 0.062183000

C 1.115240000 0.908871000 0.068147000

C -0.222271000 0.410531000 0.074560000

C -0.485507000 -0.977793000 0.044221000

C -1.348596000 1.274032000 0.111151000

C -1.775873000 -1.507670000 0.048760000

C -2.653115000 0.764331000 0.117472000

C -2.868914000 -0.625171000 0.086216000

H 3.296235000 1.628715000 0.055492000

F 0.572100000 -1.847087000 0.008529000

H -1.171934000 2.352998000 0.134077000

H -1.909024000 -2.592385000 0.023401000

H -3.502674000 1.451355000 0.146293000

H -3.884482000 -1.027853000 0.090914000

C -6.029845000 3.276923000 0.465503000

C -6.154491000 2.062951000 0.386792000

C -6.268298000 0.642078000 0.310029000

C -6.263346000 -0.167336000 1.475432000

C -6.373270000 -0.019813000 -0.935300000

C -6.360606000 -1.561302000 1.385638000

C -6.470010000 -1.408501000 -1.045078000

C -6.464287000 -2.182627000 0.127309000

H -5.938400000 4.344417000 0.530222000

H -6.174441000 0.323855000 2.448037000

F -6.374326000 0.724350000 -2.073287000

H -6.351020000 -2.165185000 2.297582000

H -6.543909000 -1.861310000 -2.037029000

H -6.537218000 -3.271959000 0.054034000

C 4.026214000 -1.406692000 -0.023501000

C 5.185015000 -1.016240000 -0.029535000

C 6.527651000 -0.532591000 -0.036226000

C 7.644531000 -1.407803000 -0.072097000

C 6.804552000 0.853587000 -0.007263000

C 8.953764000 -0.910163000 -0.078128000

C 8.100135000 1.371307000 -0.012645000

C 9.183914000 0.477411000 -0.048473000

H 2.993243000 -1.703362000 -0.017065000

H 7.457376000 -2.485021000 -0.095112000

F 5.756864000 1.731933000 0.027707000

H 9.798059000 -1.605879000 -0.106109000

H 8.244094000 2.454654000 0.010904000

H 10.206182000 0.868639000 -0.053185000