3FPHA trimers

3T1

C 1.544476000 3.553460000 -2.427034000

C 1.779915000 2.813019000 -1.481607000

C 2.024880000 1.938460000 -0.375277000

C 2.924762000 0.853225000 -0.515071000

C 1.359127000 2.140117000 0.859589000

C 3.125642000 0.011802000 0.578721000

C 1.583793000 1.265907000 1.930561000

C 2.475470000 0.187864000 1.804452000

H 1.365082000 4.216568000 -3.251535000

H 3.436112000 0.661222000 -1.459833000

H 0.652480000 2.964697000 0.966766000

F 3.981384000 -1.045757000 0.435949000

H 1.035770000 1.406261000 2.865090000

H 2.644152000 -0.519922000 2.619022000

C -1.998454000 3.035891000 2.509727000

C -2.115128000 2.368779000 1.490413000

C -2.220496000 1.589056000 0.294932000

C -1.573902000 2.011227000 -0.893508000

C -2.958155000 0.379845000 0.298232000

C -1.655483000 1.231124000 -2.054210000

C -3.021047000 -0.362472000 -0.880216000

C -2.385126000 0.030414000 -2.062829000

H -1.925206000 3.638907000 3.394379000

H -0.993408000 2.934978000 -0.896915000

H -3.442556000 0.015994000 1.205013000

H -1.124924000 1.550576000 -2.955108000

F -3.719354000 -1.538131000 -0.870881000

H -2.445642000 -0.603163000 -2.950746000

C -1.166871000 -0.784588000 3.201774000

C -0.742186000 -1.339705000 2.197963000

C -0.247343000 -1.990773000 1.023710000

C -0.108792000 -3.401139000 0.988896000

C 0.105677000 -1.223615000 -0.112786000

C 0.375474000 -4.032046000 -0.164948000

C 0.580819000 -1.890666000 -1.239825000

C 0.727939000 -3.280204000 -1.299911000

H -1.551343000 -0.279161000 4.066089000

H -0.384288000 -3.987900000 1.868759000

H 0.012840000 -0.138109000 -0.113139000

H 0.481268000 -5.121178000 -0.185995000

F 0.920291000 -1.151543000 -2.342033000

H 1.108827000 -3.750779000 -2.209647000

3T2

C 1.681374000 -3.994295000 0.598883000

C 0.899711000 -3.237916000 0.038247000

C -0.002901000 -2.339878000 -0.615463000

C -1.352921000 -2.712387000 -0.827221000

C 0.444874000 -1.066234000 -1.042635000

C -2.202142000 -1.801993000 -1.456219000

C -0.442115000 -0.179516000 -1.664690000

C -1.783370000 -0.538792000 -1.883408000

H 2.361166000 -4.665485000 1.087536000

H -1.729308000 -3.684526000 -0.502711000

H 1.481230000 -0.780597000 -0.866690000

F -3.510688000 -2.160940000 -1.649113000

H -0.093186000 0.811574000 -1.966142000

H -2.497240000 0.143385000 -2.349990000

C 0.679316000 -0.744252000 2.692602000

C -0.349983000 -0.278369000 2.225010000

C -1.549987000 0.250598000 1.654529000

C -1.548890000 1.546150000 1.081732000

C -2.738549000 -0.520414000 1.634228000

C -2.727512000 2.018953000 0.508337000

C -3.902448000 -0.006551000 1.047783000

C -3.912025000 1.276401000 0.472659000

H 1.601688000 -1.151031000 3.059123000

H -0.644818000 2.155935000 1.058378000

H -2.730536000 -1.523373000 2.066809000

F -2.722048000 3.269728000 -0.058243000

H -4.811915000 -0.613823000 1.022742000

H -4.807027000 1.695049000 0.005828000

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C 1.447065000 2.895800000 -0.731315000

C 2.405487000 1.840979000 -0.603222000

C 3.064033000 1.327779000 -1.749077000

C 2.675891000 1.279904000 0.669437000

C 3.968342000 0.264367000 -1.623835000

C 3.587634000 0.227659000 0.750281000

C 4.241222000 -0.303442000 -0.366580000

H -0.165459000 4.518868000 -0.930789000

H 2.847949000 1.761108000 -2.728526000

H 2.167600000 1.635390000 1.566476000

H 4.463758000 -0.135362000 -2.513438000

F 3.849220000 -0.315823000 1.979112000

H 4.934838000 -1.138829000 -0.246955000

3T3

C 1.228531000 3.846894000 -0.079755000

C 0.376642000 3.078036000 0.344524000

C -0.611217000 2.174809000 0.850696000

C -1.918085000 2.174281000 0.304921000

C -0.288888000 1.272241000 1.894272000

C -2.853901000 1.279569000 0.821814000

C -1.258345000 0.386755000 2.382592000

C -2.559622000 0.380582000 1.852040000

H 1.978410000 4.512212000 -0.462283000

H -2.186813000 2.841649000 -0.515200000

H 0.720889000 1.261110000 2.308113000

F -4.115847000 1.279084000 0.290943000

H -0.993103000 -0.321211000 3.172819000

H -3.327184000 -0.310652000 2.207320000

C -0.132328000 1.444566000 -2.921583000

C -0.670612000 0.509718000 -2.346201000

C -1.290682000 -0.570325000 -1.642354000

C -2.597243000 -1.003834000 -1.979234000

C -0.594174000 -1.203101000 -0.584929000

C -3.194661000 -2.053055000 -1.268593000

C -1.223617000 -2.243034000 0.095015000

C -2.511351000 -2.690315000 -0.217200000

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H -4.206606000 -2.378625000 -1.528655000

F -0.556732000 -2.844226000 1.130635000

H -2.959788000 -3.507784000 0.352925000

C 2.670585000 -0.455459000 3.595652000

C 2.738316000 -0.571918000 2.379552000

C 2.800445000 -0.704201000 0.955673000

C 2.844135000 0.453586000 0.138331000

C 2.810403000 -1.987717000 0.353937000

C 2.905669000 0.288753000 -1.245635000

C 2.856040000 -2.107681000 -1.041890000

C 2.903818000 -0.967019000 -1.862265000

H 2.629903000 -0.356604000 4.663556000

H 2.815163000 1.455736000 0.568414000

H 2.761103000 -2.875951000 0.987532000

F 2.981335000 1.403160000 -2.031915000

H 2.846550000 -3.100367000 -1.501460000

H 2.932291000 -1.038025000 -2.951919000

3T4

C -0.880784000 3.269769000 -1.077520000

C -1.734608000 2.466900000 -0.727831000

C -2.689607000 1.501815000 -0.277417000

C -3.355685000 1.678954000 0.961584000

C -2.945744000 0.342282000 -1.049881000

C -4.254785000 0.708102000 1.423025000

C -3.852680000 -0.595451000 -0.557210000

C -4.515953000 -0.448171000 0.665638000

H -0.109902000 3.950567000 -1.384762000

H -3.150508000 2.573049000 1.555283000

H -2.430689000 0.164143000 -1.994628000

H -4.759315000 0.847219000 2.383718000

F -4.101886000 -1.717498000 -1.302821000

H -5.212569000 -1.218281000 1.005642000

C -0.948025000 -2.405543000 -1.953285000

C 0.093064000 -1.781596000 -1.800636000

C 1.307670000 -1.044378000 -1.630379000

C 1.280326000 0.371186000 -1.668671000

C 2.538573000 -1.714462000 -1.422389000

C 2.478809000 1.064499000 -1.509704000

C 3.719138000 -0.978495000 -1.254562000

C 3.704868000 0.426794000 -1.296478000

H -1.879906000 -2.925352000 -2.066096000

H 0.346547000 0.917880000 -1.805173000

H 2.553435000 -2.805842000 -1.378569000

F 2.452450000 2.432533000 -1.568125000

H 4.664948000 -1.502088000 -1.084763000

H 4.612734000 1.019945000 -1.164070000

C 2.891829000 2.766688000 1.998456000

C 2.249334000 1.727774000 1.930589000

C 1.497633000 0.513615000 1.838900000

C 0.088898000 0.548381000 1.683614000

C 2.163165000 -0.734702000 1.888591000

C -0.637108000 -0.644130000 1.580534000

C 1.402981000 -1.898274000 1.778339000

C 0.014139000 -1.888791000 1.625884000

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H 3.247928000 -0.792368000 1.989621000

H -1.720424000 -0.608373000 1.446923000

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3T5

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C 2.813843000 -0.082007000 -0.475046000

C 4.314727000 1.636702000 0.417898000

C 3.869021000 -0.988280000 -0.380489000

C 5.347890000 0.692304000 0.494161000

C 5.137605000 -0.640046000 0.095402000

H 0.142690000 3.597406000 -0.180491000

H 1.841942000 -0.408702000 -0.848838000

H 4.482457000 2.670164000 0.731474000

F 3.649347000 -2.286160000 -0.767435000

H 6.331323000 0.991962000 0.869912000

H 5.928430000 -1.392443000 0.148605000

C 0.476013000 -2.303386000 -2.229356000

C -0.454193000 -1.538258000 -2.014866000

C -1.536026000 -0.637639000 -1.757040000

C -2.855139000 -1.124381000 -1.584963000

C -1.285795000 0.753918000 -1.666261000

C -3.904031000 -0.233395000 -1.322080000

C -2.358570000 1.605531000 -1.408820000

C -3.668037000 1.149269000 -1.228344000

H 1.308946000 -2.959507000 -2.394939000

H -3.041545000 -2.199143000 -1.641994000

H -0.279125000 1.158495000 -1.778745000

H -4.918831000 -0.617444000 -1.180745000

F -2.119507000 2.953220000 -1.334750000

H -4.470130000 1.861445000 -1.020335000

C -1.950628000 2.884882000 2.222657000

C -1.680694000 1.703122000 2.057891000

C -1.373350000 0.320116000 1.854862000

C -0.029876000 -0.107753000 1.706039000

C -2.420065000 -0.630537000 1.790876000

C 0.255452000 -1.461498000 1.490664000

C -2.091549000 -1.967918000 1.572941000

C -0.776312000 -2.413809000 1.419371000

H -2.183199000 3.921165000 2.375311000

H 0.771391000 0.631510000 1.741176000

H -3.463777000 -0.327906000 1.886770000

H 1.292504000 -1.781531000 1.359078000

F -3.110260000 -2.881076000 1.487889000

H -0.575516000 -3.471229000 1.232847000

3T6

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C 1.230529000 0.214017000 2.731130000

C 1.442939000 -0.991430000 1.991201000

C 1.114187000 -2.252144000 2.549553000

C 1.953208000 -0.920936000 0.671801000

C 1.281844000 -3.420956000 1.793477000

C 2.108856000 -2.107053000 -0.044756000

C 1.780833000 -3.362602000 0.479753000

H 0.821925000 2.184129000 3.835263000

H 0.719936000 -2.300561000 3.567589000

H 2.198936000 0.037842000 0.215558000

H 1.017604000 -4.390594000 2.225760000

F 2.596361000 -2.041253000 -1.320490000

H 1.911591000 -4.259631000 -0.129918000

C -0.963112000 3.870916000 1.665828000

C -0.332567000 3.259396000 0.814031000

C 0.388694000 2.554466000 -0.202096000

C -0.251474000 1.547286000 -0.964799000

C 1.746238000 2.869883000 -0.461025000

C 0.450114000 0.870754000 -1.971294000

C 2.406434000 2.180536000 -1.479110000

C 1.792394000 1.184441000 -2.247107000

H -1.522952000 4.415162000 2.402004000

H -1.291972000 1.299749000 -0.755071000

H 2.269222000 3.636069000 0.114597000

H -0.046088000 0.077238000 -2.536565000

F 3.716649000 2.488797000 -1.729019000

H 2.362440000 0.660423000 -3.017462000

C -1.261121000 -2.844208000 -2.954242000

C -1.722553000 -2.184265000 -2.032914000

C -2.219001000 -1.378540000 -0.958750000

C -1.574592000 -1.397667000 0.302327000

C -3.336897000 -0.530706000 -1.161753000

C -2.028217000 -0.569657000 1.336997000

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C -3.131968000 0.279577000 1.147354000

H -0.873540000 -3.443095000 -3.756154000

H -0.710934000 -2.045672000 0.451304000

H -3.851655000 -0.492390000 -2.123789000

H -1.501757000 -0.564138000 2.294532000

F -4.839456000 1.092076000 -0.299638000

H -3.492021000 0.945382000 1.934963000

3T7

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C -0.621224000 -1.562842000 -1.495461000

C -1.740477000 -0.681961000 -1.363378000

C -3.026194000 -1.204360000 -1.078583000

C -1.565659000 0.718831000 -1.479673000

C -4.084495000 -0.312907000 -0.912540000

C -2.656888000 1.580097000 -1.307938000

C -3.936242000 1.074127000 -1.019322000

H 1.241614000 -2.900135000 -1.601748000

H -3.187909000 -2.278814000 -0.973730000

H -0.572446000 1.124607000 -1.678176000

F -5.323629000 -0.820370000 -0.617953000

H -2.507041000 2.661036000 -1.379904000

H -4.800163000 1.727987000 -0.875342000

C -0.297652000 3.486711000 1.228656000

C -0.462926000 2.295103000 1.451411000

C -0.685935000 0.904594000 1.707851000

C 0.386769000 -0.016027000 1.624750000

C -1.986012000 0.440221000 2.027013000

C 0.123929000 -1.364012000 1.862806000

C -2.207863000 -0.924075000 2.251947000

C -1.150847000 -1.847686000 2.173588000

H -0.147793000 4.531339000 1.035323000

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H -2.812847000 1.152067000 2.070342000

F 1.160261000 -2.252444000 1.783358000

H -3.217268000 -1.278356000 2.481153000

H -1.302803000 -2.917143000 2.338015000

C 4.012270000 -3.012411000 -1.172687000

C 3.760206000 -1.848614000 -0.891213000

C 3.482649000 -0.483439000 -0.561790000

C 2.622136000 0.285717000 -1.383693000

C 4.071569000 0.111026000 0.582698000

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H 4.243123000 -4.032213000 -1.415199000

H 2.137392000 -0.150832000 -2.257714000

H 4.727492000 -0.488577000 1.218146000

F 1.561188000 2.358073000 -1.839308000

H 4.257487000 1.901926000 1.784034000

H 2.720508000 3.264984000 0.319029000

3T8

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C -3.757135000 -1.851997000 -0.890051000

C -3.481698000 -0.486038000 -0.562084000

C -4.072906000 0.109325000 0.580743000

C -2.621014000 0.283014000 -1.383910000

C -3.809183000 1.450907000 0.891715000

C -2.389683000 1.614398000 -1.040908000

C -2.959570000 2.224395000 0.081041000

H -4.236889000 -4.036714000 -1.412263000

H -4.728885000 -0.490209000 1.216205000

H -2.134482000 -0.154204000 -2.256595000

H -4.262701000 1.901708000 1.779250000

F -1.562089000 2.356037000 -1.841118000

H -2.725453000 3.264564000 0.314449000

C -0.348762000 -2.300072000 -1.574895000

C 0.622398000 -1.560853000 -1.495567000

C 1.741935000 -0.680500000 -1.362336000

C 3.027468000 -1.204079000 -1.078917000

C 1.567764000 0.720599000 -1.475898000

C 4.086197000 -0.313417000 -0.911357000

C 2.659440000 1.581000000 -1.302789000

C 3.938636000 1.073867000 -1.015458000

H -1.237462000 -2.902536000 -1.598642000

H 3.188685000 -2.278806000 -0.976197000

H 0.574695000 1.127264000 -1.673266000

F 5.325189000 -0.822082000 -0.617995000

H 2.510107000 2.662146000 -1.372612000

H 4.802918000 1.727014000 -0.870440000

C 0.292187000 3.486280000 1.216304000

C 0.459125000 2.297962000 1.454857000

C 0.683234000 0.907481000 1.710386000

C -0.388860000 -0.013836000 1.626774000

C 1.983791000 0.443653000 2.028359000

C -0.124703000 -1.361953000 1.862568000

C 2.206954000 -0.920829000 2.250851000

C 1.150629000 -1.845143000 2.171730000

H 0.140517000 4.530091000 1.020034000

H -1.397469000 0.310395000 1.371519000

H 2.810120000 1.156044000 2.072247000

F -1.160424000 -2.251102000 1.782507000

H 3.216800000 -1.274637000 2.478795000

H 1.303497000 -2.914742000 2.334315000

3T9

C 2.315960000 -3.652669000 1.794728000

C 2.507908000 -2.590146000 1.219327000

C 2.687613000 -1.349485000 0.528139000

C 2.075053000 -0.166677000 1.010568000

C 3.454596000 -1.305718000 -0.663703000

C 2.218655000 1.036722000 0.307694000

C 3.577614000 -0.085964000 -1.330177000

C 2.974577000 1.092948000 -0.875999000

H 2.168402000 -4.582999000 2.309154000

H 1.466362000 -0.210610000 1.915326000

H 3.933468000 -2.202512000 -1.061665000

H 1.725715000 1.938967000 0.676380000

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C -2.438300000 -0.504926000 -2.279341000

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H 0.865464000 -0.823160000 -1.555762000

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C -1.303508000 1.675968000 0.584328000

C -0.210223000 2.539662000 2.600008000

C -1.005535000 2.884764000 -0.043652000

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C -0.327654000 3.929502000 0.595882000

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H -1.823884000 0.884957000 0.044085000

H 0.103625000 2.393779000 3.636531000

F -1.387392000 3.055829000 -1.345083000

H 0.596320000 4.543896000 2.455824000

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3T10

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C -1.164748000 2.565550000 1.049516000

C -0.060874000 1.731283000 1.413233000

C -0.265240000 0.341375000 1.589992000

C 1.236013000 2.274287000 1.585325000

C 0.826572000 -0.451833000 1.936660000

C 2.307858000 1.438942000 1.929487000

C 2.115724000 0.059418000 2.114059000

H -2.958938000 3.859739000 0.437614000

H -1.249426000 -0.103469000 1.445808000

H 1.391140000 3.345975000 1.438619000

F 0.627117000 -1.797929000 2.102754000

H 3.310426000 1.861142000 2.046321000

H 2.940211000 -0.611212000 2.364286000

C -0.425064000 1.470309000 -2.137884000

C 0.586497000 0.844480000 -1.854375000

C 1.754893000 0.110694000 -1.478275000

C 1.669673000 -1.274259000 -1.190442000

C 3.001414000 0.772823000 -1.358800000

C 2.810516000 -1.980280000 -0.787299000

C 4.111216000 0.034490000 -0.951696000

C 4.052158000 -1.332469000 -0.660528000

H -1.344998000 1.992240000 -2.321913000

H 0.706651000 -1.782256000 -1.265879000

H 3.093885000 1.840959000 -1.563469000

H 2.732959000 -3.046940000 -0.556395000

F 5.311593000 0.683025000 -0.818125000

H 4.953811000 -1.862825000 -0.343619000

C -4.164071000 2.010761000 -2.135376000

C -3.828548000 1.057415000 -1.445444000

C -3.453430000 -0.072540000 -0.650636000

C -3.989604000 -0.246935000 0.649771000

C -2.551692000 -1.034154000 -1.169548000

C -3.639147000 -1.371259000 1.410656000

C -2.230576000 -2.137521000 -0.379910000

C -2.752032000 -2.337128000 0.902375000

H -4.466950000 2.841660000 -2.743593000

H -4.673875000 0.504048000 1.050950000

H -2.104451000 -0.913143000 -2.156842000

H -4.054273000 -1.497908000 2.414733000

F -1.360485000 -3.066314000 -0.885688000

H -2.454600000 -3.213534000 1.482313000

3T11

C -2.081206000 -0.540166000 -3.014301000

C -1.924240000 0.446862000 -2.309756000

C -1.693906000 1.579216000 -1.465734000

C -1.269989000 2.816934000 -2.011504000

C -1.863777000 1.451697000 -0.065218000

C -1.017291000 3.907167000 -1.166916000

C -1.601431000 2.559983000 0.739486000

C -1.178967000 3.791699000 0.225718000

H -2.230167000 -1.418725000 -3.611866000

H -1.135311000 2.907364000 -3.092016000

H -2.178872000 0.508401000 0.380503000

H -0.686088000 4.858995000 -1.592961000

F -1.761723000 2.437673000 2.091658000

H -0.984647000 4.627518000 0.902295000

C 1.753282000 -0.806716000 2.647683000

C 0.650350000 -1.118417000 2.222134000

C -0.647143000 -1.474880000 1.735636000

C -0.781717000 -2.153800000 0.498367000

C -1.806805000 -1.148157000 2.483834000

C -2.063350000 -2.479419000 0.055757000

C -3.077309000 -1.486585000 1.997491000

C -3.223081000 -2.157435000 0.769563000

H 2.728526000 -0.528403000 2.996618000

H 0.090653000 -2.420967000 -0.100188000

H -1.698238000 -0.615997000 3.431500000

F -2.192268000 -3.152150000 -1.129172000

H -3.967966000 -1.222402000 2.575370000

H -4.203212000 -2.428774000 0.370275000

C 2.048767000 -3.336424000 -2.070940000

C 2.283425000 -2.236949000 -1.587432000

C 2.516453000 -0.956700000 -0.990997000

C 1.530027000 0.056854000 -1.070884000

C 3.725037000 -0.706454000 -0.295704000

C 1.749518000 1.300010000 -0.464082000

C 3.901439000 0.543494000 0.295619000

C 2.943410000 1.560462000 0.229209000

H 1.853381000 -4.295358000 -2.511395000

H 0.596682000 -0.144790000 -1.599313000

H 4.498410000 -1.472437000 -0.210984000

H 0.981086000 2.073595000 -0.522754000

F 5.062373000 0.778740000 0.986971000

H 3.131349000 2.519948000 0.717632000

3T12

C -4.395670000 2.208005000 -0.273922000

C -3.807681000 1.164367000 -0.025786000

C -3.093502000 -0.041927000 0.261112000

C -2.864826000 -0.990250000 -0.766536000

C -2.583745000 -0.283566000 1.560823000

C -2.134734000 -2.137411000 -0.460176000

C -1.849536000 -1.446674000 1.823877000

C -1.614354000 -2.393977000 0.812474000

H -4.925462000 3.116550000 -0.486932000

H -3.230787000 -0.822589000 -1.780786000

H -2.740758000 0.461054000 2.344164000

F -1.907855000 -3.050482000 -1.457742000

H -1.432141000 -1.609783000 2.820456000

H -1.029956000 -3.297195000 0.996587000

C 0.979744000 0.353003000 3.349724000

C 0.707148000 0.955401000 2.320293000

C 0.384725000 1.674011000 1.125633000

C 0.013978000 0.971848000 -0.045822000

C 0.434219000 3.090413000 1.108632000

C -0.292936000 1.706567000 -1.188776000

C 0.117807000 3.791023000 -0.062682000

C -0.251673000 3.103335000 -1.232158000

H 1.229432000 -0.182438000 4.245268000

H -0.032822000 -0.116197000 -0.061495000

H 0.723585000 3.626236000 2.016038000

F -0.650998000 1.029582000 -2.324314000

H 0.157549000 4.884729000 -0.070263000

H -0.505435000 3.628242000 -2.156285000

C 4.444728000 1.977469000 -0.192399000

C 3.793950000 0.956837000 -0.368734000

C 3.004340000 -0.219527000 -0.567947000

C 2.759909000 -1.097800000 0.516000000

C 2.434031000 -0.497628000 -1.835176000

C 1.950850000 -2.211659000 0.298131000

C 1.623304000 -1.626282000 -2.009868000

C 1.369415000 -2.502413000 -0.940040000

H 5.027142000 2.865984000 -0.041622000

H 3.165288000 -0.894943000 1.507740000

H 2.611514000 0.191720000 -2.663757000

F 1.704758000 -3.053646000 1.352072000

H 1.166048000 -1.822740000 -2.983603000

H 0.726709000 -3.376702000 -1.055703000

3T13

C 4.683960000 -2.761136000 0.225414000

C 4.307978000 -1.602411000 0.108672000

C 3.845214000 -0.256171000 -0.038763000

C 3.183286000 0.385335000 1.035723000

C 4.024295000 0.436478000 -1.262289000

C 2.718547000 1.686396000 0.849518000

C 3.541099000 1.743730000 -1.407887000

C 2.876355000 2.387180000 -0.350102000

H 5.039754000 -3.767514000 0.337195000

H 3.017540000 -0.127752000 1.984234000

H 4.534301000 -0.063412000 -2.089662000

F 2.065496000 2.296952000 1.883943000

H 3.673481000 2.269151000 -2.358650000

H 2.468684000 3.395202000 -0.449237000

C -4.636493000 2.644327000 1.301040000

C -4.260586000 1.571618000 0.847974000

C -3.799624000 0.319844000 0.328937000

C -3.681795000 -0.809895000 1.176949000

C -3.434598000 0.210245000 -1.034869000

C -3.196842000 -2.022394000 0.669643000

C -2.954951000 -1.013679000 -1.498538000

C -2.822547000 -2.139307000 -0.679632000

H -4.977799000 3.581610000 1.696970000

H -3.957759000 -0.719380000 2.230360000

H -3.490639000 1.069300000 -1.704513000

H -3.091342000 -2.884551000 1.334686000

F -2.586175000 -1.112166000 -2.812771000

H -2.424068000 -3.069054000 -1.091595000

C -0.814773000 2.870551000 -1.365367000

C -0.480981000 1.768190000 -0.953710000

C -0.097903000 0.478145000 -0.469317000

C 0.542813000 -0.450749000 -1.325134000

C -0.361391000 0.125264000 0.876004000

C 0.919896000 -1.708375000 -0.840126000

C 0.027629000 -1.137299000 1.316874000

C 0.666808000 -2.069174000 0.494011000

H -1.116599000 3.836595000 -1.721414000

H 0.743885000 -0.171304000 -2.360880000

H -0.856748000 0.820571000 1.554057000

H 1.433980000 -2.413854000 -1.498290000

F -0.227684000 -1.479943000 2.618871000

H 0.966216000 -3.039482000 0.896217000

3T14

C -2.457059000 4.415568000 0.131854000

C -2.701901000 3.216146000 0.120716000

C -3.009025000 1.817164000 0.113131000

C -3.246828000 1.151958000 -1.115562000

C -3.095781000 1.093346000 1.328708000

C -3.578269000 -0.202338000 -1.084430000

C -3.430650000 -0.266956000 1.313691000

C -3.682553000 -0.933003000 0.103234000

H -2.256951000 5.470143000 0.138660000

H -3.171962000 1.679282000 -2.068368000

H -2.893531000 1.604371000 2.272823000

F -3.804264000 -0.843932000 -2.270863000

H -3.475036000 -0.823201000 2.253956000

H -3.923514000 -1.997464000 0.068555000

C 0.884957000 2.833049000 0.290442000

C 1.856778000 2.089431000 0.275382000

C 2.941170000 1.155446000 0.247498000

C 2.976725000 0.080451000 1.171329000

C 3.968579000 1.281041000 -0.720326000

C 4.019732000 -0.854035000 1.120616000

C 4.990214000 0.331374000 -0.733219000

C 5.044846000 -0.740677000 0.164749000

H 0.009463000 3.458069000 0.294308000

H 2.180062000 -0.017952000 1.912152000

H 3.964579000 2.096364000 -1.446734000

H 4.036485000 -1.685581000 1.832152000

F 5.981592000 0.453855000 -1.669141000

H 5.867439000 -1.458252000 0.107753000

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C -0.235063000 -1.133437000 2.477637000

C -0.408408000 -1.644071000 1.151741000

C -0.225360000 -0.787873000 0.039934000

C -0.779114000 -2.996086000 0.944964000

C -0.419928000 -1.310145000 -1.237264000

C -0.969558000 -3.479837000 -0.356989000

C -0.792118000 -2.638780000 -1.469504000

H 0.045041000 -0.299778000 4.599456000

H 0.041938000 0.261112000 0.169493000

H -0.918479000 -3.652320000 1.807926000

F -0.251144000 -0.482701000 -2.310966000

H -1.259739000 -4.523734000 -0.512156000

H -0.944276000 -2.991601000 -2.492216000

3T15

C 2.774650000 -1.747828000 2.995648000

C 3.241215000 -1.271755000 1.969723000

C 3.755643000 -0.707247000 0.759098000

C 3.328858000 -1.200239000 -0.499299000

C 4.685131000 0.361886000 0.814712000

C 3.821383000 -0.628246000 -1.680199000

C 5.153586000 0.899998000 -0.384799000

C 4.743320000 0.432485000 -1.639469000

H 2.379019000 -2.179777000 3.895147000

H 2.602008000 -2.013369000 -0.542628000

H 5.028861000 0.763362000 1.770080000

H 3.477191000 -1.005528000 -2.647664000

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H 5.136682000 0.894316000 -2.548315000

C -5.623638000 -2.070309000 -0.659848000

C -4.451517000 -1.958156000 -0.326338000

C -3.080324000 -1.797991000 0.050847000

C -2.055649000 -2.367868000 -0.744660000

C -2.733832000 -1.049658000 1.202573000

C -0.729671000 -2.163997000 -0.365177000

C -1.387838000 -0.871232000 1.545460000

C -0.361185000 -1.427725000 0.763570000

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H -2.291527000 -2.948363000 -1.638733000

H -3.525386000 -0.596789000 1.803443000

F 0.257958000 -2.712063000 -1.147005000

H -1.125943000 -0.276136000 2.424817000

H 0.690359000 -1.284174000 1.015817000

C 1.455134000 1.736378000 -0.401019000

C 0.233897000 1.796961000 -0.429188000

C -1.196229000 1.831743000 -0.455700000

C -1.911187000 1.165748000 -1.481598000

C -1.910313000 2.510880000 0.562531000

C -3.311663000 1.171220000 -1.482273000

C -3.304068000 2.492114000 0.524753000

C -4.030371000 1.835799000 -0.474037000

H 2.526093000 1.668660000 -0.381287000

H -1.357538000 0.631561000 -2.256860000

H -1.387358000 3.030873000 1.367717000

H -3.857597000 0.631876000 -2.261279000

F -3.990681000 3.136609000 1.520134000

H -5.122599000 1.836780000 -0.447681000

3T16

C -3.926339000 1.438628000 -2.188608000

C -2.809737000 1.534104000 -1.698902000

C -1.510026000 1.636531000 -1.110600000

C -1.297102000 2.510847000 -0.016309000

C -0.432076000 0.856262000 -1.596955000

C -0.022918000 2.576996000 0.545773000

C 0.832459000 0.951170000 -1.002097000

C 1.056569000 1.820160000 0.079540000

H -4.914751000 1.332265000 -2.591523000

H -2.111183000 3.115347000 0.387723000

H -0.603110000 0.169346000 -2.428967000

F 0.174550000 3.417484000 1.611025000

H 1.655284000 0.336479000 -1.373555000

H 2.038395000 1.913931000 0.548422000

C 5.338382000 2.345782000 0.356558000

C 4.819879000 1.261769000 0.127040000

C 4.175733000 0.011603000 -0.137444000

C 3.483727000 -0.657016000 0.902520000

C 4.197611000 -0.555663000 -1.436693000

C 2.832718000 -1.854320000 0.608534000

C 3.525482000 -1.760223000 -1.690073000

C 2.825711000 -2.425544000 -0.667989000

H 5.809344000 3.289531000 0.556335000

H 3.450546000 -0.245784000 1.913292000

H 4.732047000 -0.037762000 -2.236638000

F 2.164999000 -2.491701000 1.618391000

H 3.537271000 -2.186193000 -2.697837000

H 2.280478000 -3.354714000 -0.846638000

C -6.308866000 -0.708390000 -0.022404000

C -5.119350000 -0.790889000 0.252626000

C -3.728929000 -0.888596000 0.577039000

C -3.189925000 -0.161814000 1.666563000

C -2.877453000 -1.712838000 -0.199681000

C -1.826118000 -0.263437000 1.975306000

C -1.529017000 -1.784698000 0.142862000

C -0.974125000 -1.082736000 1.217087000

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H -3.261423000 -2.272538000 -1.054465000

H -1.414780000 0.310164000 2.810962000

F -0.706632000 -2.572805000 -0.621626000

H 0.090259000 -1.172336000 1.435896000

3T17

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C -1.978958000 1.521011000 0.464605000

C -3.279441000 0.922380000 0.449062000

C -4.300079000 1.383230000 1.318886000

C -3.548442000 -0.152088000 -0.436838000

C -5.565150000 0.780102000 1.301785000

C -4.820626000 -0.724750000 -0.420065000

C -5.843290000 -0.286910000 0.428847000

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H -6.348718000 1.141983000 1.975177000

F -5.078635000 -1.761277000 -1.274396000

H -6.822532000 -0.771530000 0.399290000

C 4.495275000 -4.375731000 -0.464947000

C 3.465337000 -3.759418000 -0.228217000

C 2.263835000 -3.033321000 0.050820000

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C 1.969676000 -2.603419000 1.369701000

C 0.204874000 -2.008885000 -0.693117000

C 0.795309000 -1.883760000 1.630493000

C -0.108070000 -1.576439000 0.598841000

H 5.398320000 -4.917886000 -0.671880000

H 1.561205000 -3.040519000 -2.024886000

H 2.673822000 -2.828890000 2.173937000

F -0.652987000 -1.701465000 -1.717700000

H 0.584014000 -1.540239000 2.647043000

H -1.013870000 -0.997176000 0.781119000

C 3.694343000 1.045677000 2.989729000

C 3.290880000 1.360814000 1.878634000

C 2.806417000 1.724238000 0.581468000

C 2.417993000 0.724602000 -0.344068000

C 2.699911000 3.092061000 0.219679000

C 1.922680000 1.086723000 -1.603472000

C 2.211950000 3.409069000 -1.049361000

C 1.813408000 2.437865000 -1.975317000

H 4.061746000 0.772422000 3.960446000

H 2.494490000 -0.324990000 -0.060088000

H 2.991584000 3.884673000 0.911615000

H 1.604929000 0.307577000 -2.301935000

F 2.111705000 4.727874000 -1.396239000

H 1.423552000 2.741871000 -2.949769000

3T18

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C -1.766858000 2.584043000 -0.070246000

C -0.412588000 2.126844000 -0.159624000

C 0.653057000 3.059285000 -0.218933000

C -0.129748000 0.737573000 -0.189440000

C 1.957419000 2.572105000 -0.305940000

C 1.196449000 0.292203000 -0.276383000

C 2.261821000 1.207406000 -0.336363000

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H 0.465381000 4.134747000 -0.197547000

H -0.950329000 0.017943000 -0.144333000

F 2.986205000 3.475384000 -0.364678000

H 1.406900000 -0.780396000 -0.298791000

H 3.300520000 0.880090000 -0.405596000

C 2.143301000 -3.767307000 -0.411835000

C 3.035683000 -2.934227000 -0.332201000

C 4.047089000 -1.925145000 -0.241905000

C 4.432169000 -1.421974000 1.025524000

C 4.651402000 -1.404177000 -1.413710000

C 5.402103000 -0.420454000 1.079353000

C 5.620889000 -0.396182000 -1.316322000

C 6.009694000 0.111562000 -0.063874000

H 1.370946000 -4.509494000 -0.481197000

H 3.977390000 -1.797790000 1.944123000

H 4.346212000 -1.789838000 -2.389382000

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H 6.077414000 0.007481000 -2.224993000

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C -6.158096000 -2.515730000 0.137959000

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C -4.781314000 -2.787476000 0.046977000

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H -7.698175000 -0.989677000 0.256888000

H -3.595987000 0.441641000 0.017604000

H -6.869689000 -3.346809000 0.171405000

F -2.555945000 -1.955196000 -0.082340000

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