

Optimised geometries

Tyrosyl radical

(Hydrogens optimised at PM3, ring plus methylene hydrogens optimised at B3LYP/6-31G\*)

### Catalase+PAA

Charge = 0 Multiplicity = 2

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.73176200  | 5.57027800  | 3.72986900  |
| C | 2.25038400  | 4.41587600  | 2.99228800  |
| C | 3.42023500  | 4.85429500  | 2.10938100  |
| O | 3.27149100  | 5.76777300  | 1.29984400  |
| C | 1.16187900  | 3.80845800  | 2.13245900  |
| H | 0.97666300  | 5.27651200  | 4.31427300  |
| H | 1.40593800  | 6.27431300  | 3.09965200  |
| H | 2.61686900  | 3.67033500  | 3.74151800  |
| H | 4.38065600  | 4.32760900  | 2.20001800  |
| H | 1.53953600  | 2.96555500  | 1.53560900  |
| H | 0.72742600  | 4.52969300  | 1.42273100  |
| H | 0.33329700  | 3.41151400  | 2.74332400  |
| N | 6.07019500  | 3.48768400  | -0.71492800 |
| C | 6.38062800  | 2.37074300  | -1.59782300 |
| C | 7.67280600  | 2.52923100  | -2.37305700 |
| O | 7.74125600  | 3.27325700  | -3.35099500 |
| C | 5.23256500  | 2.12589000  | -2.59554400 |
| C | 3.94103700  | 1.65665000  | -1.91797500 |
| O | 3.97634700  | 0.67229900  | -1.13994400 |
| O | 2.88735700  | 2.27878300  | -2.17186400 |
| H | 5.21052400  | 3.31329600  | -0.23643400 |
| H | 6.00655800  | 4.34204400  | -1.22778400 |
| H | 6.48576500  | 1.47108800  | -0.93431100 |
| H | 8.55116900  | 1.95771400  | -2.04093100 |
| H | 5.51398100  | 1.32746700  | -3.31409300 |
| H | 5.05510600  | 3.03314300  | -3.21211900 |
| H | 2.06185900  | 1.79287000  | -1.97506400 |
| N | 6.44664800  | -4.00938900 | 0.03557200  |
| C | 5.81299700  | -2.80025200 | 0.52383100  |
| C | 4.40465700  | -2.58785600 | 0.00099100  |
| O | 3.46099000  | -2.53291300 | 0.79205100  |
| C | 6.69634600  | -1.59016500 | 0.25575200  |
| C | 7.91193100  | -1.55303000 | 1.16086600  |
| C | 9.00550400  | -2.39441300 | 0.92742700  |
| C | 7.97311300  | -0.67467700 | 2.24495300  |
| C | 10.12913000 | -2.36034500 | 1.75227600  |
| C | 9.09150700  | -0.63049600 | 3.07724500  |
| C | 10.16605100 | -1.47357700 | 2.82613200  |
| O | 11.27471100 | -1.42270300 | 3.64141700  |
| H | 6.88542400  | -3.86435400 | -0.85270800 |
| H | 7.12914100  | -4.32052000 | 0.69496700  |
| H | 5.72295800  | -2.92529500 | 1.63711800  |
| H | 6.11359000  | -0.65433800 | 0.40575800  |
| H | 7.03984400  | -1.54694100 | -0.80403200 |
| H | 9.01359300  | -3.07046800 | 0.06481500  |
| H | 7.12518500  | -0.00790300 | 2.44997300  |
| H | 10.97906900 | -3.02288700 | 1.55318500  |
| H | 9.10162400  | 0.07324300  | 3.91935900  |
| H | 11.10584900 | -0.77603100 | 4.31556200  |
| N | 4.22355900  | -2.45721500 | -1.32453200 |
| C | 2.83155100  | -2.26264700 | -1.75060200 |
| C | 1.96063200  | -3.46123200 | -1.32249400 |
| O | 0.74814500  | -3.33177200 | -1.15520700 |
| C | 2.93698300  | -2.10575500 | -3.27412000 |
| C | 4.38040000  | -1.72374800 | -3.51739100 |
| C | 5.15852000  | -2.44853000 | -2.46182700 |
| H | 2.41646600  | -1.32448500 | -1.28767100 |
| H | 2.43747100  | -4.44331000 | -1.18455300 |
| H | 2.22727500  | -1.34793400 | -3.65669600 |
| H | 2.67899700  | -3.04878300 | -3.79610500 |
| H | 4.52259700  | -0.62387700 | -3.44631000 |
| H | 4.71148700  | -1.99358000 | -4.53824100 |
| H | 5.41796400  | -3.48657600 | -2.75720700 |
| H | 6.11278300  | -1.94141700 | -2.19917900 |
| N | 0.80116100  | -2.95703000 | 2.36680100  |
| C | -0.05607500 | -1.77870800 | 2.37837500  |
| C | -1.46631400 | -2.13736600 | 1.97577700  |
| O | -2.42489000 | -1.51163500 | 2.40569800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.47569200  | -0.72237600 | 1.42557000  |
| C | 1.67097600  | -0.00349700 | 1.94931600  |
| N | 2.80505700  | 0.20551100  | 1.19404200  |
| C | 1.92116600  | 0.53498000  | 3.16529200  |
| C | 3.70329100  | 0.84267800  | 1.92268100  |
| N | 3.19152500  | 1.05462200  | 3.12303800  |
| H | 1.66143400  | -2.78675200 | 1.88023600  |
| H | 1.00621100  | -3.22999200 | 3.30469700  |
| H | -0.10290000 | -1.33098600 | 3.40960100  |
| H | -0.31465400 | 0.04279500  | 1.24612500  |
| H | 0.68768800  | -1.15897400 | 0.42230000  |
| H | 2.92067200  | -0.03689200 | 0.22351500  |
| H | 1.29566100  | 0.60177100  | 4.05679700  |
| H | 4.71195300  | 1.14117200  | 1.61313900  |
| N | -1.58349900 | -3.14978800 | 1.13394000  |
| C | -2.88074100 | -3.58822700 | 0.67908300  |
| C | -3.61493200 | -4.24840800 | 1.83946300  |
| O | -4.82736200 | -4.13394100 | 1.98510400  |
| C | -2.69522400 | -4.56858100 | -0.47012100 |
| C | -2.59512900 | -3.88571300 | -1.82361500 |
| C | -1.71367900 | -4.65019500 | -2.79903600 |
| N | -1.36679100 | -3.79762500 | -3.92770500 |
| C | -0.28641800 | -3.95683700 | -4.68125900 |
| N | 0.56030100  | -4.94959100 | -4.42202000 |
| N | -0.05780200 | -3.12361500 | -5.69606600 |
| H | -0.77967400 | -3.65221600 | 0.80800200  |
| H | -3.47205300 | -2.69465000 | 0.32818800  |
| H | -3.03198100 | -4.84437300 | 2.55969700  |
| H | -3.54991200 | -5.27693100 | -0.48723400 |
| H | -1.80582300 | -5.21655200 | -0.29728400 |
| H | -3.61261200 | -3.74146800 | -2.24580200 |
| H | -2.19349100 | -2.85413300 | -1.69205400 |
| H | -2.23537500 | -5.57281000 | -3.13806300 |
| H | -0.78665400 | -5.00375800 | -2.28895600 |
| H | -2.11514900 | -3.24587700 | -4.29422100 |
| H | 0.57480100  | -5.29849000 | -3.48070500 |
| H | 1.48627800  | -4.84395400 | -4.78286400 |
| H | 0.79574700  | -3.25907200 | -6.18367600 |
| N | -3.67696700 | -1.28919600 | 5.16660400  |
| C | -4.60914100 | -0.19830800 | 4.92448500  |
| C | -5.82392000 | -0.58415300 | 4.08755600  |
| O | -6.96120400 | -0.28590900 | 4.46125600  |
| C | -3.88072900 | 0.97026300  | 4.26080000  |
| C | -2.85050600 | 1.64340100  | 5.16448400  |
| C | -1.77203700 | 2.27568300  | 4.31420900  |
| C | -3.52885600 | 2.68432000  | 6.03681100  |
| H | -3.11899400 | -1.49044300 | 4.35494300  |
| H | -4.16969000 | -2.10925800 | 5.45108000  |
| H | -4.96973300 | 0.12434800  | 5.93711700  |
| H | -3.38192700 | 0.63117100  | 3.32456300  |
| H | -4.62716900 | 1.72332900  | 3.92840700  |
| H | -2.37513500 | 0.87795100  | 5.82598600  |
| H | -2.18877100 | 2.95979900  | 3.55931900  |
| H | -1.17939500 | 1.51976100  | 3.77630600  |
| H | -1.06859000 | 2.85984700  | 4.92425300  |
| H | -4.33952700 | 2.24174500  | 6.63148900  |
| H | -3.96469600 | 3.49732400  | 5.43979400  |
| H | -2.81826800 | 3.14091700  | 6.73852900  |
| N | -5.58802900 | -1.24457900 | 2.95758800  |
| C | -6.68317600 | -1.63107300 | 2.08955300  |
| C | -6.26229500 | -1.50257400 | 0.64154500  |
| O | -5.29088500 | -0.79666300 | 0.33266900  |
| H | -4.66189400 | -1.28407800 | 2.57585600  |
| H | -6.98659500 | -2.68054400 | 2.32340000  |
| H | -7.58875900 | -1.00610800 | 2.26688500  |
| N | -6.97266800 | -2.17580700 | -0.27592600 |
| C | -6.66034200 | -2.13636400 | -1.70629300 |
| C | -6.44562800 | -0.73428500 | -2.27985300 |
| O | -5.44040400 | -0.48658000 | -2.95411400 |
| C | -7.84409300 | -2.85507100 | -2.34226800 |
| C | -8.30027700 | -3.78835500 | -1.28459000 |
| C | -8.13288500 | -3.03779200 | 0.00009700  |
| H | -5.71909500 | -2.73226400 | -1.86380000 |
| H | -7.21916000 | 0.02933800  | -2.10772200 |
| H | -7.55495800 | -3.37214800 | -3.27704900 |
| H | -8.63898900 | -2.13919000 | -2.63850200 |
| H | -7.70766800 | -4.72728000 | -1.28552800 |
| H | -9.34788200 | -4.11590700 | -1.43517500 |
| H | -9.01931400 | -2.42112500 | 0.25841900  |
| H | -7.93204000 | -3.67814900 | 0.88699800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -5.52791100 | 1.98562600  | -0.88371200 |
| C | -4.73989100 | 2.79272500  | 0.04023100  |
| C | -4.03142000 | 3.98874900  | -0.60629300 |
| O | -3.62361300 | 4.91607100  | 0.08955700  |
| C | -3.72674400 | 1.90869200  | 0.77191900  |
| C | -2.52483400 | 1.56075500  | -0.04771300 |
| C | -1.40648100 | 2.43555600  | -0.00260300 |
| C | -2.47935600 | 0.41506700  | -0.88630400 |
| C | -0.27983200 | 2.17629300  | -0.73180700 |
| C | -1.36129400 | 0.13846700  | -1.63847100 |
| C | -0.20227500 | 0.99825200  | -1.56522000 |
| O | 0.86217200  | 0.71761400  | -2.19468400 |
| H | -4.94746300 | 1.30885000  | -1.34159800 |
| H | -6.24477800 | 1.51033300  | -0.37479400 |
| H | -5.45042700 | 3.21544000  | 0.79651800  |
| H | -4.24474800 | 1.00816400  | 1.10197600  |
| H | -3.38021100 | 2.45011600  | 1.65833000  |
| H | -1.46341200 | 3.32104500  | 0.62215200  |
| H | -3.33671600 | -0.25031800 | -0.91003800 |
| H | 0.57848400  | 2.83776800  | -0.68647100 |
| H | -1.29054800 | -0.73280800 | -2.28238600 |
| N | -3.86912800 | 3.97136200  | -1.92513100 |
| C | -3.23883300 | 5.10198200  | -2.60388200 |
| C | -4.29144900 | 6.19724200  | -2.77602800 |
| O | -3.99715700 | 7.28107100  | -3.28543000 |
| C | -2.69062200 | 4.69827600  | -3.97472900 |
| C | -1.42470000 | 3.82978800  | -4.00525100 |
| C | -1.10499000 | 3.44964300  | -5.44582100 |
| C | -0.25783300 | 4.57464700  | -3.36840400 |
| H | -4.32769400 | 3.30372400  | -2.50803900 |
| H | -2.37128500 | 5.47874000  | -1.98867900 |
| H | -5.32060900 | 6.01350400  | -2.43194800 |
| H | -2.47112400 | 5.63026900  | -4.53980200 |
| H | -3.48272000 | 4.18346800  | -4.56075800 |
| H | -1.61082100 | 2.89581300  | -3.41980400 |
| H | -0.95005000 | 4.33658200  | -6.07496100 |
| H | -1.91483800 | 2.86114900  | -5.89611800 |
| H | -0.18976300 | 2.84606100  | -5.49636600 |
| H | 0.57732400  | 3.89923600  | -3.14147400 |
| H | -0.58041600 | 5.04661900  | -2.42418100 |
| H | 0.12353600  | 5.37095800  | -4.02062500 |

## Mouse RNR:

Charge = 0 Multiplicity = 2

|   |            |             |             |
|---|------------|-------------|-------------|
| N | 1.73176200 | 5.57027800  | 3.72986900  |
| C | 2.25038400 | 4.41587600  | 2.99228800  |
| C | 3.42023500 | 4.85429500  | 2.10938100  |
| O | 3.27149100 | 5.76777300  | 1.29984400  |
| C | 1.16187900 | 3.80845800  | 2.13245900  |
| H | 0.97666300 | 5.27651200  | 4.31427300  |
| H | 1.40593800 | 6.27431300  | 3.09965200  |
| H | 2.61686900 | 3.67033500  | 3.74151800  |
| H | 4.38065600 | 4.32760900  | 2.20001800  |
| H | 1.53953600 | 2.96555500  | 1.53560900  |
| H | 0.72742600 | 4.52969300  | 1.42273100  |
| H | 0.33329700 | 3.41151400  | 2.74332400  |
| N | 6.07019500 | 3.48768400  | -0.71492800 |
| C | 6.38062800 | 2.37074300  | -1.59782300 |
| C | 7.67280600 | 2.52923100  | -2.37305700 |
| O | 7.74125600 | 3.27325700  | -3.35099500 |
| C | 5.23256500 | 2.12589000  | -2.59554400 |
| C | 3.94103700 | 1.65665000  | -1.91797500 |
| O | 3.97634700 | 0.67229900  | -1.13994400 |
| O | 2.88735700 | 2.27878300  | -2.17186400 |
| H | 5.21052400 | 3.31329600  | -0.23643400 |
| H | 6.00655800 | 4.34204400  | -1.22778400 |
| H | 6.48576500 | 1.47108800  | -0.93431100 |
| H | 8.55116900 | 1.95771400  | -2.04093100 |
| H | 5.51398100 | 1.32746700  | -3.31409300 |
| H | 5.05510600 | 3.03314300  | -3.21211900 |
| H | 2.06185900 | 1.79287000  | -1.97506400 |
| N | 6.44664800 | -4.00938900 | 0.03557200  |
| C | 5.81299700 | -2.80025200 | 0.52383100  |
| C | 4.40465700 | -2.58785600 | 0.00099100  |
| O | 3.46099000 | -2.53291300 | 0.79205100  |
| C | 6.69634600 | -1.59016500 | 0.25575200  |
| C | 7.91193100 | -1.55303000 | 1.16086600  |
| C | 9.00550400 | -2.39441300 | 0.92742700  |
| C | 7.97311300 | -0.67467700 | 2.24495300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 10.12913000 | -2.36034500 | 1.75227600  |
| C | 9.09150700  | -0.63049600 | 3.07724500  |
| C | 10.16605100 | -1.47357700 | 2.82613200  |
| O | 11.27471100 | -1.42270300 | 3.64141700  |
| H | 6.88542400  | -3.86435400 | -0.85270800 |
| H | 7.12914100  | -4.32052000 | 0.69496700  |
| H | 5.72295800  | -2.92529500 | 1.63711800  |
| H | 6.11359000  | -0.65433800 | 0.40575800  |
| H | 7.03984400  | -1.54694100 | -0.80403200 |
| H | 9.01359300  | -3.07046800 | 0.06481500  |
| H | 7.12518500  | -0.00790300 | 2.44997300  |
| H | 10.97906900 | -3.02288700 | 1.55318500  |
| H | 9.10162400  | 0.07324300  | 3.91935900  |
| H | 11.10584900 | -0.77603100 | 4.31556200  |
| N | 4.22355900  | -2.45721500 | -1.32453200 |
| C | 2.83155100  | -2.26264700 | -1.75060200 |
| C | 1.96063200  | -3.46123200 | -1.32249400 |
| O | 0.74814500  | -3.33177200 | -1.15520700 |
| C | 2.93698300  | -2.10575500 | -3.27412000 |
| C | 4.38040000  | -1.72374800 | -3.51739100 |
| C | 5.15852000  | -2.44853000 | -2.46182700 |
| H | 2.41646600  | -1.32448500 | -1.28767100 |
| H | 2.43747100  | -4.44331000 | -1.18455300 |
| H | 2.22727500  | -1.34793400 | -3.65669600 |
| H | 2.67899700  | -3.04878300 | -3.79610500 |
| H | 4.52259700  | -0.62387700 | -3.44631000 |
| H | 4.71148700  | -1.99358000 | -4.53824100 |
| H | 5.41796400  | -3.48657600 | -2.75720700 |
| H | 6.11278300  | -1.94141700 | -2.19917900 |
| N | 0.80116100  | -2.95703000 | 2.36680100  |
| C | -0.05607500 | -1.77870800 | 2.37837500  |
| C | -1.46631400 | -2.13736600 | 1.97577700  |
| O | -2.42489000 | -1.51163500 | 2.40569800  |
| C | 0.47569200  | -0.72237600 | 1.42557000  |
| C | 1.67097600  | -0.00349700 | 1.94931600  |
| N | 2.80505700  | 0.20551100  | 1.19404200  |
| C | 1.92116600  | 0.53498000  | 3.16529200  |
| C | 3.70329100  | 0.84267800  | 1.92268100  |
| N | 3.19152500  | 1.05462200  | 3.12303800  |
| H | 1.66143400  | -2.78675200 | 1.88023600  |
| H | 1.00621100  | -3.22999200 | 3.30469700  |
| H | -0.10290000 | -1.33098600 | 3.40960100  |
| H | -0.31465400 | 0.04279500  | 1.24612500  |
| H | 0.68768800  | -1.15897400 | 0.42230000  |
| H | 2.92067200  | -0.03689200 | 0.22351500  |
| H | 1.29566100  | 0.60177100  | 4.05679700  |
| H | 4.71195300  | 1.14117200  | 1.61313900  |
| N | -1.58349900 | -3.14978800 | 1.13394000  |
| C | -2.88074100 | -3.58822700 | 0.67908300  |
| C | -3.61493200 | -4.24840800 | 1.83946300  |
| O | -4.82736200 | -4.13394100 | 1.98510400  |
| C | -2.69522400 | -4.56858100 | -0.47012100 |
| C | -2.59512900 | -3.88571300 | -1.82361500 |
| C | -1.71367900 | -4.65019500 | -2.79903600 |
| N | -1.36679100 | -3.79762500 | -3.92770500 |
| C | -0.28641800 | -3.95683700 | -4.68125900 |
| N | 0.56030100  | -4.94959100 | -4.42202000 |
| N | -0.05780200 | -3.12361500 | -5.69606600 |
| H | -0.77967400 | -3.65221600 | 0.80800200  |
| H | -3.47205300 | -2.69465000 | 0.32818800  |
| H | -3.03198100 | -4.84437300 | 2.55969700  |
| H | -3.54991200 | -5.27693100 | -0.48723400 |
| H | -1.80582300 | -5.21655200 | -0.29728400 |
| H | -3.61261200 | -3.74146800 | -2.24580200 |
| H | -2.19349100 | -2.85413300 | -1.69205400 |
| H | -2.23537500 | -5.57281000 | -3.13806300 |
| H | -0.78665400 | -5.00375800 | -2.28895600 |
| H | -2.11514900 | -3.24587700 | -4.29422100 |
| H | 0.57480100  | -5.29849000 | -3.48070500 |
| H | 1.48627800  | -4.84395400 | -4.78286400 |
| H | 0.79574700  | -3.25907200 | -6.18367600 |
| N | -3.67696700 | -1.28919600 | 5.16660400  |
| C | -4.60914100 | -0.19830800 | 4.92448500  |
| C | -5.82392000 | -0.58415300 | 4.08755600  |
| O | -6.96120400 | -0.28590900 | 4.46125600  |
| C | -3.88072900 | 0.97026300  | 4.26080000  |
| C | -2.85050600 | 1.64340100  | 5.16448400  |
| C | -1.77203700 | 2.27568300  | 4.31420900  |
| C | -3.52885600 | 2.68432000  | 6.03681100  |
| H | -3.11899400 | -1.49044300 | 4.35494300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.16969000 | -2.10925800 | 5.45108000  |
| H | -4.96973300 | 0.12434800  | 5.93711700  |
| H | -3.38192700 | 0.63117100  | 3.32456300  |
| H | -4.62716900 | 1.72332900  | 3.92840700  |
| H | -2.37513500 | 0.87795100  | 5.82598600  |
| H | -2.18877100 | 2.95979900  | 3.55931900  |
| H | -1.17939500 | 1.51976100  | 3.77630600  |
| H | -1.06859000 | 2.85984700  | 4.92425300  |
| H | -4.33952700 | 2.24174500  | 6.63148900  |
| H | -3.96469600 | 3.49732400  | 5.43979400  |
| H | -2.81826800 | 3.14091700  | 6.73852900  |
| N | -5.58802900 | -1.24457900 | 2.95758800  |
| C | -6.68317600 | -1.63107300 | 2.08955300  |
| C | -6.26229500 | -1.50257400 | 0.64154500  |
| O | -5.29088500 | -0.79666300 | 0.33266900  |
| H | -4.66189400 | -1.28407800 | 2.57585600  |
| H | -6.98659500 | -2.68054400 | 2.32340000  |
| H | -7.58875900 | -1.00610800 | 2.26688500  |
| N | -6.97266800 | -2.17580700 | -0.27592600 |
| C | -6.66034200 | -2.13636400 | -1.70629300 |
| C | -6.44562800 | -0.73428500 | -2.27985300 |
| O | -5.44040400 | -0.48658000 | -2.95411400 |
| C | -7.84409300 | -2.85507100 | -2.34226800 |
| C | -8.30027700 | -3.78835500 | -1.28459000 |
| C | -8.13288500 | -3.03779200 | 0.00009700  |
| H | -5.71909500 | -2.73226400 | -1.86380000 |
| H | -7.21916000 | 0.02933800  | -2.10772200 |
| H | -7.55495800 | -3.37214800 | -3.27704900 |
| H | -8.63898900 | -2.13919000 | -2.63850200 |
| H | -7.70766800 | -4.72728000 | -1.28552800 |
| H | -9.34788200 | -4.11590700 | -1.43517500 |
| H | -9.01931400 | -2.42112500 | 0.25841900  |
| H | -7.93204000 | -3.67814900 | 0.88699800  |
| N | -5.52791100 | 1.98562600  | -0.88371200 |
| C | -4.73989100 | 2.79272500  | 0.04023100  |
| C | -4.03142000 | 3.98874900  | -0.60629300 |
| O | -3.62361300 | 4.91607100  | 0.08955700  |
| C | -3.72674400 | 1.90869200  | 0.77191900  |
| C | -2.52483400 | 1.56075500  | -0.04771300 |
| C | -1.40648100 | 2.43555600  | -0.00260300 |
| C | -2.47935600 | 0.41506700  | -0.88630400 |
| C | -0.27983200 | 2.17629300  | -0.73180700 |
| C | -1.36129400 | 0.13846700  | -1.63847100 |
| C | -0.20227500 | 0.99825200  | -1.56522000 |
| O | 0.86217200  | 0.71761400  | -2.19468400 |
| H | -4.94746300 | 1.30885000  | -1.34159800 |
| H | -6.24477800 | 1.51033300  | -0.37479400 |
| H | -5.45042700 | 3.21544000  | 0.79651800  |
| H | -4.24474800 | 1.00816400  | 1.10197600  |
| H | -3.38021100 | 2.45011600  | 1.65833000  |
| H | -1.46341200 | 3.32104500  | 0.62215200  |
| H | -3.33671600 | -0.25031800 | -0.91003800 |
| H | 0.57848400  | 2.83776800  | -0.68647100 |
| H | -1.29054800 | -0.73280800 | -2.28238600 |
| N | -3.86912800 | 3.97136200  | -1.92513100 |
| C | -3.23883300 | 5.10198200  | -2.60388200 |
| C | -4.29144900 | 6.19724200  | -2.77602800 |
| O | -3.99715700 | 7.28107100  | -3.28543000 |
| C | -2.69062200 | 4.69827600  | -3.97472900 |
| C | -1.42470000 | 3.82978800  | -4.00525100 |
| C | -1.10499000 | 3.44964300  | -5.44582100 |
| C | -0.25783300 | 4.57464700  | -3.36840400 |
| H | -4.32769400 | 3.30372400  | -2.50803900 |
| H | -2.37128500 | 5.47874000  | -1.98867900 |
| H | -5.32060900 | 6.01350400  | -2.43194800 |
| H | -2.47112400 | 5.63026900  | -4.53980200 |
| H | -3.48272000 | 4.18346800  | -4.56075800 |
| H | -1.61082100 | 2.89581300  | -3.41980400 |
| H | -0.95005000 | 4.33658200  | -6.07496100 |
| H | -1.91483800 | 2.86114900  | -5.89611800 |
| H | -0.18976300 | 2.84606100  | -5.49636600 |
| H | 0.57732400  | 3.89923600  | -3.14147400 |
| H | -0.58041600 | 5.04661900  | -2.42418100 |
| H | 0.12353600  | 5.37095800  | -4.02062500 |

### ***E. coli* RNR:**

Charge = 0 Multiplicity = 2

|   |            |            |             |
|---|------------|------------|-------------|
| N | 1.86502100 | 6.99076100 | -3.75179800 |
| C | 2.45191400 | 5.71043800 | -3.42167900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.21544700  | 5.81859200  | -2.11797700 |
| O | 3.07351500  | 4.93756000  | -1.23072900 |
| C | 3.38206200  | 5.27894100  | -4.54510000 |
| C | 4.14752100  | 3.95329200  | -4.51359900 |
| C | 3.30382500  | 2.75137700  | -4.07352300 |
| C | 4.59106400  | 3.69636300  | -5.95167800 |
| N | 0.85980900  | 5.84556500  | 0.82573800  |
| C | 0.36984000  | 4.49422800  | 1.09649300  |
| C | 1.43806300  | 3.65686600  | 1.82446400  |
| O | 1.15723500  | 2.97470400  | 2.82202400  |
| C | -0.02241300 | 3.82211900  | -0.22604100 |
| C | -1.25443300 | 4.44695600  | -0.89117800 |
| C | -1.67362300 | 3.82706400  | -2.24068600 |
| O | -0.84022700 | 3.34648300  | -3.02368400 |
| N | -2.95786300 | 3.75393900  | -2.57834300 |
| N | 2.69968100  | 3.73434400  | 1.38931800  |
| C | 3.77668200  | 2.99309200  | 1.99043100  |
| C | 3.96214000  | 3.37078500  | 3.46497100  |
| O | 4.12560800  | 2.47084600  | 4.32923900  |
| C | 5.04869100  | 3.26806300  | 1.17774400  |
| O | 4.79301700  | 2.89996200  | -0.15142800 |
| C | 6.23430000  | 2.45504100  | 1.63939800  |
| N | 0.85601000  | 1.79032100  | 5.67847800  |
| C | 0.93199600  | 0.36972800  | 6.00314200  |
| C | 2.22742800  | -0.05801700 | 6.63226400  |
| O | 2.29629300  | -1.15310700 | 7.24838700  |
| C | 0.68322100  | -0.50072000 | 4.79449300  |
| C | -0.81562400 | -0.74387200 | 4.59722700  |
| O | -1.63746700 | -0.44070300 | 5.47360100  |
| O | -1.18936900 | -1.25553500 | 3.55467500  |
| N | 0.92088100  | -5.90187800 | 2.23650500  |
| C | 0.71706500  | -4.68286700 | 1.45778400  |
| C | 2.02240600  | -3.90293500 | 1.32364900  |
| O | 2.39378000  | -3.45229100 | 0.24110500  |
| C | -0.33433600 | -3.78345200 | 2.10968900  |
| C | -1.72149000 | -4.38812500 | 2.30679000  |
| N | -2.72257200 | -3.90292400 | 3.03880200  |
| C | -2.12408200 | -5.59537400 | 1.76714000  |
| C | -3.70118200 | -4.77341700 | 2.97499600  |
| N | -3.34131200 | -5.78656800 | 2.21493200  |
| N | 2.76691200  | -3.79881800 | 2.40258200  |
| C | 4.08050500  | -3.20107500 | 2.34619600  |
| C | 4.95270000  | -3.91232900 | 1.31592400  |
| O | 5.70316100  | -3.24428900 | 0.55823000  |
| C | 4.72744800  | -3.27624100 | 3.73087100  |
| O | 3.99987100  | -2.36824600 | 4.52551400  |
| N | 3.96947900  | -5.34124000 | -1.43389300 |
| C | 3.52983800  | -4.96043100 | -2.75054500 |
| C | 3.97720500  | -3.54402500 | -3.11820000 |
| O | 4.19325600  | -3.28210900 | -4.31164300 |
| C | 2.00520900  | -5.11552900 | -2.84326100 |
| O | 1.14785000  | -4.23860300 | -2.15751800 |
| N | 4.19475100  | -2.63255700 | -2.16173700 |
| C | 4.75456500  | -1.34237200 | -2.49217300 |
| C | 6.22858300  | -1.49247800 | -2.87619800 |
| O | 6.69230600  | -0.85130300 | -3.85467900 |
| C | 4.55650000  | -0.40372900 | -1.30760000 |
| C | 3.08020400  | -0.14277600 | -1.02709300 |
| C | 2.18465700  | 0.18370000  | -2.07807900 |
| C | 2.56336400  | -0.23834900 | 0.28715300  |
| C | 0.84742900  | 0.39376200  | -1.84418500 |
| C | 1.22277200  | -0.05714700 | 0.55563000  |
| C | 0.29433400  | 0.26387200  | -0.51121000 |
| O | -0.93198700 | 0.44772000  | -0.28694600 |
| N | -7.07656500 | 5.73025100  | 3.50978400  |
| C | -6.65788400 | 4.81238900  | 2.49391100  |
| C | -7.53619000 | 4.90606500  | 1.28390800  |
| O | -7.03142200 | 4.83770900  | 0.13320900  |
| C | -6.63724500 | 3.38164700  | 3.01988700  |
| C | -5.17340100 | 2.91952300  | 3.09095100  |
| C | -4.42974300 | 2.77965100  | 1.92592500  |
| C | -4.56057800 | 2.70644200  | 4.31955900  |
| C | -3.09181600 | 2.44108300  | 1.99240000  |
| C | -3.21794900 | 2.36606900  | 4.37216900  |
| C | -2.47924200 | 2.23729400  | 3.20868600  |
| N | -3.70801200 | -2.69014100 | -6.12882400 |
| C | -4.49310700 | -1.82557200 | -5.27022300 |
| C | -5.89091400 | -2.38008200 | -5.16434800 |
| O | -6.55378400 | -2.21780600 | -4.10706800 |
| C | -4.50101400 | -0.37020800 | -5.83159700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -3.05936200 | 0.18446800  | -5.86778900 |
| C | -5.39931600 | 0.51056400  | -4.96543000 |
| C | -2.27483000 | 0.29191700  | -4.52463200 |
| N | -5.51169400 | -4.78343500 | -2.45256400 |
| C | -5.32410600 | -4.10015800 | -1.19103100 |
| C | -6.66053400 | -3.54476000 | -0.73563100 |
| O | -7.01581100 | -3.66571000 | 0.46550200  |
| C | -4.27605400 | -2.98583000 | -1.36752400 |
| C | -2.95687700 | -3.70296400 | -1.52750400 |
| C | -4.21458400 | -1.99847400 | -0.20916600 |
| C | -1.70398500 | -2.80452100 | -1.59479600 |
| H | -7.19138000 | 2.69594900  | 2.34875600  |
| H | -7.12167300 | 3.27787200  | 4.01163000  |
| H | -6.56533500 | 5.57187600  | 4.35368100  |
| H | -6.92890700 | 6.67002400  | 3.20576900  |
| H | -5.60881600 | 5.06517400  | 2.15387800  |
| H | -8.62392200 | 5.01853700  | 1.39734900  |
| H | -4.90922400 | 2.93832900  | 0.95210400  |
| H | -2.50961200 | 2.32628500  | 1.06821300  |
| H | -1.41228100 | 1.97847800  | 3.25548100  |
| H | -2.73497100 | 2.19943600  | 5.34225100  |
| H | -5.13690300 | 2.81003100  | 5.24602200  |
| H | 3.87963800  | 1.81786800  | -4.13956300 |
| H | 2.96611000  | 2.85568400  | -3.03301800 |
| H | 2.40835700  | 2.63723200  | -4.69859200 |
| H | 5.21811300  | 2.79695000  | -6.01594100 |
| H | 3.73552800  | 3.54308600  | -6.62409600 |
| H | 5.18113800  | 4.53162100  | -6.35165400 |
| H | 5.02966100  | 4.04152800  | -3.83853700 |
| H | 2.76828800  | 5.27689000  | -5.47644000 |
| H | 4.14020900  | 6.07826100  | -4.70273400 |
| H | 1.54602000  | 6.99690700  | -4.69890000 |
| H | 1.09061600  | 7.16644200  | -3.14596500 |
| H | 1.66765300  | 4.90518500  | -3.30397300 |
| H | 3.90603600  | 6.65739600  | -1.95544700 |
| H | -2.54399300 | -0.62046100 | 5.22090900  |
| H | 1.16746100  | -1.49436200 | 4.89592400  |
| H | 1.08969000  | -0.06020100 | 3.85383200  |
| H | 3.11989100  | 0.58213600  | 6.55977900  |
| H | 1.45706100  | 2.01639500  | 4.91321400  |
| H | 1.11281600  | 2.33246700  | 6.47668300  |
| H | 0.13531300  | 0.21041800  | 6.77899300  |
| H | -1.30672100 | 0.78028600  | -4.68764400 |
| H | -2.83154500 | 0.88450800  | -3.78806400 |
| H | -2.08295700 | -0.69389600 | -4.07885200 |
| H | -2.45748300 | -0.43717000 | -6.56577600 |
| H | -3.09641500 | 1.19424500  | -6.32090200 |
| H | -5.14572800 | 0.43205600  | -3.89917900 |
| H | -5.30026100 | 1.56662200  | -5.24959900 |
| H | -6.45757900 | 0.24058600  | -5.07459500 |
| H | -4.89472600 | -0.37707200 | -6.87624600 |
| H | -6.33715400 | -2.91765400 | -6.01334000 |
| H | -3.35089300 | -3.45660200 | -5.59815700 |
| H | -2.94303700 | -2.18231000 | -6.53371000 |
| H | -4.06357600 | -1.77425500 | -4.22273100 |
| H | -0.79646900 | -3.40506100 | -1.47408700 |
| H | -1.64182600 | -2.26903300 | -2.55180800 |
| H | -1.72393000 | -2.04602800 | -0.79423300 |
| H | -4.17567500 | -2.51085100 | 0.76174000  |
| H | -3.31134300 | -1.36974700 | -0.28004500 |
| H | -5.08994700 | -1.33737000 | -0.19958500 |
| H | -2.80732500 | -4.39895400 | -0.67232400 |
| H | -2.97949900 | -4.34700900 | -2.43495300 |
| H | -4.49025900 | -2.39249800 | -2.29963000 |
| H | -4.61839800 | -5.06520300 | -2.81539900 |
| H | -5.96663200 | -4.19685700 | -3.12200900 |
| H | -4.95964200 | -4.85520800 | -0.44766900 |
| H | -7.31091100 | -3.02360700 | -1.45339900 |
| H | -3.22907800 | 3.17765600  | -3.34408200 |
| H | -3.64951800 | 3.88779100  | -1.87824000 |
| H | -2.10425300 | 4.40081900  | -0.17641400 |
| H | -1.06071000 | 5.52863300  | -1.06274700 |
| H | 0.82371600  | 3.83368100  | -0.94779000 |
| H | -0.22854900 | 2.74856700  | -0.03001500 |
| H | 0.85420200  | 6.38485500  | 1.66522600  |
| H | 0.26214000  | 6.27853900  | 0.14652200  |
| H | -0.53987600 | 4.50285600  | 1.76032200  |
| H | 2.87836600  | 4.20634400  | 0.50396400  |
| H | 3.53202100  | 1.89123600  | 1.94041000  |
| H | 3.95528200  | 4.42885400  | 3.75830800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.68911200  | 1.95194900  | -0.21181100 |
| H | 6.01569800  | 1.37642600  | 1.67105500  |
| H | 7.09897600  | 2.59553900  | 0.97577300  |
| H | 6.55331300  | 2.74413400  | 2.65013000  |
| H | 5.28656000  | 4.35446300  | 1.10995000  |
| H | 3.68001400  | -2.68807000 | -1.30210000 |
| H | 6.87137100  | -2.16496400 | -2.29218700 |
| H | 4.95394100  | -5.20406400 | -1.32988800 |
| H | 3.47642300  | -4.82892500 | -0.71686800 |
| H | 1.54048100  | -4.00293200 | -1.30956900 |
| H | 1.68326300  | -4.98498300 | -3.89359800 |
| H | 1.72754600  | -6.14643200 | -2.54101100 |
| H | 3.98848700  | -5.67722100 | -3.47826900 |
| H | 4.19678400  | -0.89953300 | -3.37038500 |
| H | 5.04118600  | -0.81546900 | -0.41352800 |
| H | 5.06916600  | 0.53641300  | -1.55964400 |
| H | 3.24458000  | -0.47641600 | 1.09955000  |
| H | 0.80644200  | -0.16590600 | 1.55231000  |
| H | 2.55921900  | 0.27510900  | -3.09077600 |
| H | 0.16802600  | 0.68506900  | -2.63770100 |
| H | 2.43057300  | -4.11796900 | 3.28803000  |
| H | 4.29136200  | -2.47321300 | 5.42135400  |
| H | 4.94391200  | -5.01105800 | 1.26172800  |
| H | 4.70306600  | -4.30084500 | 4.15634300  |
| H | 5.79076400  | -2.97034800 | 3.67601600  |
| H | 3.96998000  | -2.11939600 | 2.04148600  |
| H | 0.96735200  | -6.68872500 | 1.62420100  |
| H | 0.17818000  | -6.03804300 | 2.89244300  |
| H | 0.36383100  | -4.93216900 | 0.41809600  |
| H | 0.02131400  | -3.42572200 | 3.10001900  |
| H | -0.46365800 | -2.86938500 | 1.48959100  |
| H | -3.91307600 | -6.56043000 | 1.98875000  |
| H | -4.66757900 | -4.63326700 | 3.47440100  |
| H | -1.59971300 | -6.25577300 | 1.07301400  |

## ***S. typhimurium* RNR:**

Charge = 0 Multiplicity = 2

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 1.09920500  | 3.04765900  | 6.68336600  |
| C | 1.43793600  | 2.91759700  | 5.27208400  |
| C | 2.93546300  | 2.78605000  | 5.02539100  |
| O | 3.35569200  | 2.10624200  | 4.05336200  |
| C | 0.87137500  | 4.10259500  | 4.46898100  |
| C | -0.63209600 | 4.05430200  | 4.26908600  |
| C | -1.36098300 | 2.91520600  | 4.57902900  |
| C | -1.31211700 | 5.15314000  | 3.74782100  |
| C | -2.74595200 | 2.86427600  | 4.37688200  |
| C | -2.69371300 | 5.11299100  | 3.54384000  |
| C | -3.41015100 | 3.96371700  | 3.85939100  |
| N | 3.70791100  | -0.75513900 | 5.72700000  |
| C | 3.27429500  | -1.61076000 | 4.62316800  |
| C | 4.27174700  | -1.53596600 | 3.48224900  |
| O | 4.57030500  | -2.54996700 | 2.84682200  |
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| C | 7.03044100  | -0.88105300 | 2.39686800  |
| O | 7.60042500  | -1.44805700 | 1.42878000  |
| C | 6.11147600  | 1.41156200  | 2.03579000  |
| O | 4.91854500  | 2.17489100  | 1.83793500  |
| C | 7.05170300  | 1.60724400  | 0.83192900  |
| N | 6.35695200  | -4.52128400 | 1.44810900  |
| C | 6.26831000  | -4.70397200 | -0.00683900 |
| C | 7.64322900  | -4.58378000 | -0.64847700 |
| O | 7.96112000  | -5.34131600 | -1.60171000 |
| C | 5.35714900  | -3.66560600 | -0.68337800 |
| C | 3.89222300  | -3.93021000 | -0.46215000 |
| O | 3.45963900  | -5.08381000 | -0.66340800 |
| O | 3.16398700  | -2.97523200 | -0.11241300 |
| N | 2.78542900  | -2.19459400 | -5.61754800 |
| C | 2.15555600  | -1.99340200 | -4.31188400 |
| C | 2.95774100  | -0.98331900 | -3.49749400 |
| O | 2.40598100  | -0.03218300 | -2.94066700 |
| C | 2.07782900  | -3.31503000 | -3.53686200 |
| C | 1.21782000  | -4.34426300 | -4.19298700 |
| N | 1.05108500  | -5.61159900 | -3.68156300 |
| C | 0.48530200  | -4.29521900 | -5.33155400 |



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|---|-------------|-------------|-------------|
| C | 0.25266500  | -6.30279300 | -4.47657000 |
| N | -0.10357000 | -5.52697600 | -5.48407000 |
| N | 4.26450400  | -1.19871800 | -3.42265100 |
| C | 5.13844200  | -0.30237400 | -2.66923000 |
| C | 5.03272200  | 1.12345000  | -3.20180700 |
| O | 4.89356200  | 2.08509700  | -2.40215800 |
| C | 6.59478500  | -0.78594500 | -2.79893400 |
| N | 2.63051100  | 2.55809100  | -4.74427000 |
| C | 1.31418100  | 3.12426400  | -4.47266100 |
| C | 1.23798400  | 3.95642900  | -3.20693100 |
| O | 0.50191600  | 4.94205800  | -3.15822900 |
| C | 0.26334000  | 2.01490600  | -4.39830000 |
| O | 0.12562800  | 1.39224400  | -5.65313400 |
| N | 1.98294900  | 3.57033600  | -2.17503600 |
| C | 1.95255000  | 4.34963100  | -0.95088800 |
| C | 2.56550600  | 5.72994800  | -1.15998300 |
| O | 2.07893600  | 6.73018400  | -0.57147000 |
| C | 2.64570600  | 3.59518000  | 0.17577900  |
| C | 1.93570000  | 2.30256900  | 0.48634300  |
| C | 0.65448300  | 2.27825600  | 1.09889800  |
| C | 2.52708400  | 1.08791100  | 0.08967900  |
| C | -0.00815300 | 1.09111800  | 1.31501600  |
| C | 1.88277400  | -0.10786600 | 0.28072000  |
| C | 0.58672900  | -0.17326800 | 0.91730700  |
| O | 0.02153200  | -1.28465700 | 1.12384700  |
| N | -0.02326700 | 7.85898000  | -2.60165700 |
| C | -0.94810400 | 8.33218700  | -1.58387200 |
| C | -0.32266200 | 9.49372600  | -0.81430500 |
| O | -0.97674700 | 10.55347300 | -0.63352900 |
| C | -1.32331400 | 7.17988200  | -0.62802200 |
| C | -2.10894200 | 6.11909900  | -1.41605900 |
| C | -2.19579700 | 7.72307100  | 0.51885200  |
| C | -2.32602100 | 4.81545200  | -0.67857600 |
| N | -3.87886000 | -2.88532200 | 6.73633000  |
| C | -5.04408300 | -2.80951300 | 5.85069800  |
| C | -6.31135600 | -2.44728700 | 6.62403800  |
| O | -7.23921800 | -1.81825100 | 6.05223800  |
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| C | -6.49601400 | 1.15406400  | -3.97758400 |
| C | -6.04444500 | -0.03087200 | -3.11711100 |
| O | -5.53839500 | -1.03034600 | -3.64206700 |
| C | -5.55204900 | 2.34952100  | -3.81898800 |
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| C | -3.33156800 | 1.32578300  | -3.28494700 |
| N | -6.24567400 | 0.07556200  | -1.80029200 |
| C | -5.86898900 | -0.99434900 | -0.87811800 |
| C | -6.52797300 | -2.30873900 | -1.29711900 |
| O | -5.88984400 | -3.38952500 | -1.20620800 |
| C | -6.29523200 | -0.66803400 | 0.58614300  |
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| N | -4.67269700 | -3.91542300 | -3.95129000 |
| C | -3.47266200 | -4.54515300 | -3.40219900 |
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| H | 4.70400600  | -1.85159800 | -4.03972900 |
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| H | 1.41038100  | 3.92225000  | 7.05141700  |
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| H | 5.12729000  | 1.30336800  | -4.28327200 |
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| H | -0.09925100 | -7.33290900 | -4.34245600 |
| H | 0.28913400  | -3.48849600 | -6.03813200 |
| H | 1.47654300  | -5.92815600 | -2.84569300 |
| H | -0.73027500 | 2.39553900  | -4.05187800 |
| H | 0.53149000  | 1.17357500  | -3.73068600 |
| H | 1.09491600  | 3.79908200  | -5.34271700 |
| H | 0.87172600  | 4.50027000  | -0.65072400 |
| H | 2.64169000  | 4.25223000  | 1.05495400  |
| H | 3.69243000  | 3.39414100  | -0.06765000 |
| H | 3.50022000  | 1.12166000  | -0.38560400 |
| H | 2.33883800  | -1.02999200 | -0.04231700 |
| H | -0.98591600 | 1.06612100  | 1.78524200  |
| H | 0.18668600  | 3.21336600  | 1.39860700  |
| H | 3.65382500  | 3.28100600  | 5.69478900  |
| H | 0.92729000  | 1.97201100  | 4.92441100  |
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| H | -1.90242400 | 8.70085700  | -2.05230600 |
| H | -0.40236600 | 6.71688900  | -0.19588100 |
| H | -2.50597000 | 6.91339100  | 1.19543900  |
| H | -1.64921100 | 8.46045100  | 1.12089900  |
| H | -3.10496100 | 8.20829600  | 0.14080200  |
| H | -2.84143200 | 4.08237100  | -1.31597900 |
| H | -1.37196600 | 4.36512800  | -0.36433400 |
| H | -2.93226300 | 4.94926700  | 0.22851000  |
| H | -3.09294200 | 6.53757600  | -1.71279900 |
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| H | 5.63995100  | -2.63672500 | -0.36195400 |
| H | 0.18640500  | -3.39019400 | 4.80177500  |
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| H | 0.03197200  | -2.90991500 | 6.49870200  |
| H | -1.37451600 | -1.03424600 | 5.36817000  |
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| H | 1.06893300  | -0.72252200 | 6.08926300  |
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| H | 5.27767100  | -0.42291900 | 1.19929200  |

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|---|-------------|-------------|-------------|
| H | 6.62370800  | 1.76678200  | 2.96388600  |
| H | 4.50336400  | 2.26398300  | 2.69222100  |
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| H | 8.03010000  | 1.14997600  | 1.02270800  |
| H | 7.46082600  | -0.94305000 | 3.40564300  |
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