

Optimised geometries  
Reduced tyrosine (non-radical)

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

### Catalase+PAA

Charge = 0 Multiplicity = 1

N	1.73873700	5.56371500	3.75829800
C	2.25685000	4.41142200	3.01707000
C	3.42624300	4.85231200	2.13478800
O	3.27712300	5.76815400	1.32799600
C	1.16781300	3.80659800	2.15608700
H	0.98394100	5.26831200	4.34226700
H	1.41262000	6.26960800	3.13031500
H	2.62369200	3.66367400	3.76392300
H	4.38667000	4.32528600	2.22335400
H	1.54506600	2.96540400	1.55657600
H	0.73302300	4.52993000	1.44870500
H	0.33953900	3.40794600	2.76625900
N	6.07450700	3.49370700	-0.69496800
C	6.38435300	2.37931400	-1.58128300
C	7.67611000	2.53995100	-2.35677700
O	7.74407500	3.28681300	-3.33258400
C	5.23571100	2.13746000	-2.57906900
C	3.94452300	1.66635600	-1.90214600
O	3.98018700	0.67974200	-1.12700200
O	2.89075400	2.28931200	-2.15363300
H	5.21509000	3.31799800	-0.21650300
H	6.01065500	4.34956100	-1.20530100
H	6.48978600	1.47772400	-0.92045100
H	8.55461100	1.96739800	-2.02680700
H	5.51665800	1.34110800	-3.30009700
H	5.05798300	3.04651800	-3.19290300
H	2.06532500	1.80289600	-1.95778600
N	6.45075300	-4.00554900	0.03350400
C	5.81747700	-2.79778600	0.52563400
C	4.40886200	-2.58375400	0.00420200
O	3.46564200	-2.53103500	0.79594700
C	6.70077700	-1.58699600	0.26058200
C	7.91687100	-1.55259500	1.16512000
C	9.01024200	-2.39338500	0.92862200
C	7.97873400	-0.67740500	2.25172300
C	10.13433300	-2.36180900	1.75293700
C	9.09759700	-0.63573800	3.08351400
C	10.17193000	-1.47817300	2.82934700
O	11.28105000	-1.42976100	3.64415600
H	6.88904400	-3.85796600	-0.85459600
H	7.13358900	-4.31865400	0.69160900
H	5.72805000	-2.92606000	1.63860300
H	6.11818300	-0.65156200	0.41363600
H	7.04368500	-1.54071700	-0.79926400
H	9.01779300	-3.06692700	0.06404100
H	7.13097600	-0.01116000	2.45915800
H	10.98410500	-3.02383900	1.55144300
H	9.10824400	0.06554700	3.92766600
H	11.11261900	-0.78504000	4.32027400
N	4.22703300	-2.44924200	-1.32083300
C	2.83480300	-2.25332100	-1.74555600
C	1.96402300	-3.45307400	-1.32045000
O	0.75164100	-3.32400300	-1.15210800
C	2.93939500	-2.09200400	-3.26867000
C	4.38270900	-1.70941000	-3.51163600
C	5.16135800	-2.43732500	-2.45862100
H	2.42005600	-1.31647500	-1.27966400
H	2.44085700	-4.43558800	-1.18563300
H	2.22953600	-1.33301500	-3.64864100
H	2.68103800	-3.03348900	-3.79325200
H	4.52503700	-0.60976300	-3.43743500
H	4.71320100	-1.97629700	-4.53345300
H	5.42055000	-3.47452800	-2.75716600
H	6.11581100	-1.93105600	-2.19503300
N	0.80666000	-2.95951400	2.37094500
C	-0.05047100	-1.78116000	2.38642800
C	-1.46096500	-2.13852900	1.98357800
O	-2.41924800	-1.51397300	2.41585500

C	0.48085100	-0.72210400	1.43640300
C	1.67648900	-0.00485000	1.96156900
N	2.81016400	0.20626200	1.20627100
C	1.92740400	0.53006600	3.17896600
C	3.70885900	0.84123200	1.93625800
N	3.19778200	1.04972500	3.13751400
H	1.66667400	-2.78789100	1.88439600
H	1.01221200	-3.23522000	3.30792900
H	-0.09668200	-1.33643700	3.41897900
H	-0.30953100	0.04365100	1.25962800
H	0.69224900	-1.15579800	0.43174800
H	2.92521500	-0.03332600	0.23497800
H	1.30240300	0.59431400	4.07101200
H	4.71737200	1.14054200	1.62702100
N	-1.57870600	-3.14848800	1.13886500
C	-2.87623900	-3.58549500	0.68346000
C	-3.60983500	-4.24899000	1.84232500
O	-4.82217500	-4.13484700	1.98897800
C	-2.69144800	-4.56251700	-0.46869500
C	-2.59205300	-3.87572200	-1.82025200
C	-1.71121300	-4.63743500	-2.79838600
N	-1.36488500	-3.78161300	-3.92476400
C	-0.28494700	-3.93872000	-4.67938400
N	0.56183300	-4.93229400	-4.42350900
N	-0.05683000	-3.10256800	-5.69188900
H	-0.77510600	-3.65003200	0.81101600
H	-3.46767200	-2.69085300	0.33549800
H	-3.02653100	-4.84709500	2.56049600
H	-3.54620500	-5.27074400	-0.48739000
H	-1.80200400	-5.21106100	-0.29824200
H	-3.60976000	-3.73016600	-2.24144800
H	-2.19025500	-2.84456100	-1.68591500
H	-2.23317500	-5.55901600	-3.13980400
H	-0.78393200	-4.99255700	-2.28985700
H	-2.11340200	-3.22873900	-4.28925400
H	0.57683100	-5.28393100	-3.48322000
H	1.48761700	-4.82568300	-4.78456100
H	0.79643500	-3.23667500	-6.18037000
N	-3.66976100	-1.29946600	5.17809600
C	-4.60197900	-0.20780100	4.93967400
C	-5.81725900	-0.59111000	4.10230700
O	-6.95430800	-0.29386100	4.47751000
C	-3.87384100	0.96263600	4.27898500
C	-2.84305500	1.63305700	5.18404600
C	-1.76501000	2.26772200	4.33501100
C	-3.52083000	2.67148900	6.05977900
H	-3.11225900	-1.49839600	4.36554100
H	-4.16239300	-2.12031100	5.46046100
H	-4.96197700	0.11193600	5.95344300
H	-3.37559100	0.62622800	3.34148600
H	-4.62040400	1.71672700	3.94920300
H	-2.36737900	0.86564600	5.84305300
H	-2.18210900	2.95406600	3.58234800
H	-1.17273300	1.51332000	3.79458000
H	-1.06117200	2.85005100	4.94635800
H	-4.33120600	2.22725200	6.65361900
H	-3.95693600	3.48626200	5.46537300
H	-2.80981100	3.12598500	6.76242300
N	-5.58205500	-1.24826500	2.97029100
C	-6.67772000	-1.63214200	2.10174700
C	-6.25763900	-1.49946500	0.65388400
O	-5.28634300	-0.79273700	0.34652000
H	-4.65613700	-1.28672900	2.58792700
H	-6.98109600	-2.68226300	2.33271100
H	-7.58315200	-1.00762100	2.28140400
N	-6.96858100	-2.16996600	-0.26514300
C	-6.65705300	-2.12638800	-1.69556400
C	-6.44254300	-0.72266300	-2.26516300
O	-5.43767600	-0.47308000	-2.93926300
C	-7.84122000	-2.84314400	-2.33296500
C	-8.29689000	-3.77946400	-1.27775100
C	-8.12871600	-3.03265600	0.00902000
H	-5.71594500	-2.72190400	-1.85533200
H	-7.21591500	0.04051900	-2.09037800
H	-7.55265100	-3.35752300	-3.26940900
H	-8.63622200	-2.12633900	-2.62667000
H	-7.70436100	-4.71843100	-1.28175400
H	-9.34460700	-4.10649000	-1.42870200
H	-9.01494900	-2.41667000	0.26963100
H	-7.92742800	-3.67560700	0.89394100

N	-5.52381700	1.99309900	-0.86162800
C	-4.73521200	2.79744100	0.06421800
C	-4.02700300	3.99528300	-0.57922000
O	-3.61872900	4.92054300	0.11909700
C	-3.72173000	1.91119900	0.79276300
C	-2.54414000	1.51299500	-0.05730700
C	-1.39130200	2.30856600	-0.02578800
C	-2.57160000	0.41126000	-0.92439000
C	-0.29953300	2.02772500	-0.83549400
C	-1.48679300	0.12429600	-1.75513200
C	-0.36154700	0.93804100	-1.70037500
O	0.76201300	0.69167000	-2.47904900
H	-4.94368200	1.31761000	-1.32180600
H	-6.24043900	1.51638500	-0.35369400
H	-5.44528900	3.21801200	0.82213000
H	-4.25088700	1.03175800	1.15949700
H	-3.34330800	2.45858800	1.66222000
H	-1.36100500	3.17529500	0.62676700
H	-3.44100000	-0.23644900	-0.94389700
H	0.57604300	2.66783200	-0.80166700
H	-1.50813500	-0.73120300	-2.42659800
N	-3.86545100	3.98172000	-1.89819400
C	-3.23544200	5.11425800	-2.57400500
C	-4.28806200	6.21010100	-2.74237300
O	-3.99396400	7.29538300	-3.24878400
C	-2.68803100	4.71449800	-3.94632700
C	-1.42219900	3.84599900	-3.98008500
C	-1.10332800	3.47002000	-5.42193400
C	-0.25491400	4.58890500	-3.34172700
H	-4.32439800	3.31581800	-2.48278400
H	-2.36751800	5.48915400	-1.95819400
H	-5.31704400	6.02544700	-2.39825400
H	-2.46877100	5.64811300	-4.50880900
H	-3.48050000	4.20146200	-4.53340800
H	-1.60807100	2.91033900	-3.39725400
H	-0.94866500	4.35877300	-6.04857700
H	-1.91347600	2.88290500	-5.87348700
H	-0.18817900	2.86651300	-5.47474700
H	0.58031400	3.91276900	-3.11723000
H	-0.57692800	5.05815400	-2.39595400
H	0.12615700	5.38707900	-3.99184100
H	0.52406800	0.15259600	-3.25037600

## Mouse RNR:

Charge = 0 Multiplicity = 1

N	3.72622700	-3.97527200	-3.92991200
C	4.05311600	-2.91741000	-3.00859600
C	4.37991700	-1.62926900	-3.77498800
O	4.01304900	-0.51518000	-3.40837000
C	5.30674600	-3.35544500	-2.32189200
C	4.89982700	-4.34371400	-1.28083100
C	5.89616300	-4.32469100	-0.14249100
C	3.56439200	-3.89478800	-0.76248900
H	2.85295200	-3.78460700	-4.37649800
H	3.66607900	-4.85694300	-3.46104200
H	3.21282100	-2.65936200	-2.29295800
H	4.98989000	-1.71934300	-4.68822600
H	5.81453100	-2.48206900	-1.85484100
H	6.05923800	-3.77328300	-3.02453700
H	4.83455800	-5.38001600	-1.69389800
H	5.68081100	-5.11885500	0.58752800
H	5.89508500	-3.36955900	0.41057000
H	6.91991700	-4.48922800	-0.50550200
H	3.34168400	-4.39472300	0.19710900
H	2.70540600	-4.14604700	-1.40632000
H	3.51886700	-2.81381600	-0.53787000
N	1.28581500	-0.21757100	-5.24885900
C	0.51125800	0.53814500	-4.32618800
C	1.17131000	1.82654000	-3.92273100
O	0.50338800	2.77833700	-3.60919900
C	0.60477900	-0.22619600	-3.08635800
C	-0.49630000	-1.17292400	-3.02091000
C	-1.76649200	-0.76578200	-3.39789700
C	-0.28930500	-2.45137600	-2.53175000
C	-2.84381500	-1.64561900	-3.31527000
C	-1.34787700	-3.34742800	-2.41384300
C	-2.62205200	-2.93246200	-2.81079300
H	0.89126200	-1.13023400	-5.36707300
H	1.31505700	0.23312200	-6.14128300

H	-0.54188900	0.76066200	-4.67140200
H	1.58527300	-0.74429100	-2.94134900
H	0.50540600	0.40661300	-2.16579300
H	-1.94296600	0.25991600	-3.75614500
H	0.71778000	-2.76353700	-2.22169300
H	-3.84811600	-1.33150600	-3.61451500
H	-1.18970100	-4.35372900	-2.01542600
H	-3.46888900	-3.62315100	-2.70920500
N	2.48447000	1.82462800	-3.85513800
C	3.22796800	2.99988600	-3.43593100
C	2.95739500	4.21002400	-4.34458300
O	2.70199100	5.34140400	-3.91571600
C	4.68985100	2.59354800	-3.40601300
H	3.01063500	0.95751900	-3.93369400
H	2.90949400	3.27121800	-2.39140700
H	3.00912000	4.04325400	-5.43154800
H	5.04795000	2.21156800	-4.37329600
H	4.88303600	1.82172400	-2.64527100
H	5.32557900	3.45342500	-3.15121600
N	-1.07946300	5.35276700	-4.40686200
C	-1.46343800	6.20812200	-3.32328700
C	-1.03161700	7.60891900	-3.66829800
O	-1.72718900	8.58109000	-3.40985600
C	-0.93722900	5.72900400	-1.95059500
C	-1.66047600	4.53714100	-1.39034300
O	-2.87469500	4.44818800	-1.30443100
O	-0.82198200	3.59190900	-1.02212700
H	-1.49358800	4.44939200	-4.30778800
H	-0.08414100	5.25861400	-4.45852300
H	-2.58615100	6.18229900	-3.27612800
H	-0.06224500	7.75113100	-4.17452100
H	-1.03957100	6.56292300	-1.22550100
H	0.16001400	5.53488800	-2.01933800
H	0.03015100	3.72677100	-1.43652200
N	-0.52221200	5.77266100	4.38939700
C	-0.44094700	4.55046800	3.61772600
C	0.81558100	4.59739100	2.80572400
O	1.53937900	3.62756800	2.64858900
C	-1.55955900	4.52530200	2.59245400
C	-2.93314700	4.33671600	3.21101700
N	-4.07382800	4.26454500	2.40652800
C	-3.35436200	4.25374600	4.50021500
C	-5.13154800	4.07091700	3.20493900
N	-4.76249400	4.09235700	4.47170000
H	-1.23842500	5.69399800	5.08254400
H	-0.71127200	6.56096100	3.80319000
H	-0.48215200	3.66738500	4.30228100
H	1.08695800	5.54991700	2.31778400
H	-1.39630100	3.69107500	1.87446100
H	-1.56691800	5.45116400	1.97588300
H	-4.05999400	4.24543000	1.41710900
H	-2.80940600	4.27277300	5.44378500
H	-6.16979800	3.93135600	2.88008600
N	3.78097600	1.57310200	3.03807800
C	4.31442800	0.82202700	1.95208700
C	5.78635900	0.96236800	1.75187600
O	6.44882800	0.01369200	1.28480700
C	3.64143900	1.24295900	0.63814900
C	2.23455700	0.66745300	0.54531200
C	2.04202200	-0.72063300	0.64203200
C	1.09666900	1.45752100	0.37445900
C	0.78263700	-1.30376300	0.56520600
C	-0.17830700	0.89075800	0.28011900
C	-0.33847000	-0.49279100	0.36800000
O	-1.55967400	-1.10272700	0.27977400
H	2.80077900	1.40028200	3.12722700
H	3.94304000	2.55259200	2.91752000
H	4.06709600	-0.26432100	2.15458500
H	6.28825200	1.90790000	2.00587100
H	4.21727700	0.88343400	-0.22858700
H	3.61463000	2.33746900	0.58221900
H	2.90153300	-1.36787100	0.78245800
H	1.19765100	2.53678000	0.33453300
H	0.65294400	-2.37850000	0.64089900
H	-1.03852000	1.53198800	0.11637000
N	7.61887600	-1.11988500	4.00334600
C	7.57846600	-2.53842100	3.67323500
C	8.67459500	-2.75346600	2.68760700
O	9.56424500	-3.56637600	2.81848600
C	6.25946700	-2.78609700	2.94626300

C	5.16683100	-3.41823200	3.82821800
C	5.58136300	-3.61360900	5.26615900
C	3.84717700	-2.67599700	3.77800800
H	6.82495400	-0.87920900	4.56188200
H	8.45042700	-0.91089100	4.51603100
H	7.71749400	-3.22135300	4.55750100
H	8.65638000	-2.12616600	1.77689300
H	6.43045200	-3.46099100	2.07726100
H	5.86713200	-1.85128000	2.48841700
H	4.98140600	-4.43813800	3.40233300
H	6.51835000	-4.18462000	5.36147000
H	4.81377700	-4.17298300	5.82066100
H	5.71452500	-2.65848500	5.79490000
H	3.06890400	-3.20407200	4.34441100
H	3.48528900	-2.56697900	2.74359300
H	3.93229800	-1.66386500	4.19901100
N	-5.43668400	-6.36475500	-3.01978500
C	-5.75158600	-6.65019300	-1.65492900
C	-6.04744600	-8.09916700	-1.47480300
O	-5.63166700	-8.72367500	-0.54467200
C	-6.99327300	-5.87377000	-1.21745200
C	-6.68651300	-4.40989500	-0.94048000
C	-5.42172200	-4.01173000	-0.52051400
C	-7.64549100	-3.41758100	-1.13200600
C	-5.13127500	-2.66644400	-0.29337600
C	-7.39754000	-2.07082600	-0.86750800
C	-6.11989500	-1.70603200	-0.46287100
H	-5.15201800	-5.41019900	-3.11136900
H	-6.22072600	-6.53501500	-3.61769000
H	-4.86166400	-6.35109800	-1.03291100
H	-6.68712300	-8.59262000	-2.22912700
H	-7.40628800	-6.30022800	-0.28038300
H	-7.81093000	-5.95218200	-1.96403700
H	-4.63189400	-4.76121100	-0.35862000
H	-8.64339500	-3.70915900	-1.48274500
H	-4.12499000	-2.36657100	0.02457700
H	-8.18595000	-1.32297600	-0.99386500
H	-5.88691500	-0.65331900	-0.25574900
N	-5.10330400	-0.93086100	5.63361800
C	-5.24248400	-0.16975000	4.42567400
C	-6.50560800	-0.45472600	3.63210200
O	-7.21443800	0.42645800	3.15891600
C	-4.03156700	-0.40109700	3.59457100
C	-2.83065600	0.11598200	4.34791300
C	-4.19275000	0.28356500	2.26393800
C	-1.49069300	-0.18115500	3.65812300
H	-5.15013700	-1.91323800	5.44938300
H	-5.81673600	-0.68774700	6.28822800
H	-5.26612200	0.91067600	4.74473600
H	-6.78522900	-1.51136600	3.48032300
H	-3.88058500	-1.49636600	3.39951800
H	-2.78877400	-0.31348100	5.36963200
H	-2.91688100	1.21455000	4.48945100
H	-4.63686800	1.28586500	2.35663700
H	-4.82357500	-0.29302500	1.56854800
H	-3.21023600	0.41769100	1.78071200
H	-1.32729300	-1.25870100	3.53496900
H	-0.65303200	0.22411100	4.23736300
H	-1.46941200	0.27909200	2.65827300
H	-2.21106800	-0.46265400	-0.04635300

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

Charge = 0 Multiplicity = 1

N	-1.80298200	6.98438000	3.86457200
C	-2.39740600	5.70927500	3.52779500
C	-3.17044400	5.83179900	2.23098500
O	-3.03875700	4.95803400	1.33501400
C	-3.32063400	5.27154600	4.65451000
C	-4.09151500	3.94919000	4.61730600
C	-3.25593400	2.74792800	4.16028800
C	-4.52506600	3.68138300	6.05644700
N	-0.83727400	5.87547000	-0.73037000
C	-0.35470100	4.52467400	-1.01666900
C	-1.43173600	3.69785700	-1.74370700
O	-1.16121900	3.02338300	-2.74931300
C	0.04499900	3.83949100	0.29689700
C	1.28450900	4.45371200	0.95799300
C	1.71155600	3.82040200	2.29877900
O	0.88228400	3.33620100	3.08392200

N	2.99804200	3.73936100	2.62592100
N	-2.68967900	3.77639100	-1.29823400
C	-3.77414500	3.04460100	-1.89751600
C	-3.96937500	3.43591500	-3.36723500
O	-4.14297600	2.54422300	-4.23805100
C	-5.03881900	3.31735100	-1.07272300
O	-4.77444700	2.93663000	0.25118300
C	-6.23110500	2.51299100	-1.53235000
N	-0.88647900	1.86292500	-5.61822900
C	-0.97052400	0.44553600	-5.95469500
C	-2.27239500	0.02832700	-6.57757100
O	-2.35026700	-1.06104700	-7.20268800
C	-0.71594700	-0.43642600	-4.75563900
C	0.78339400	-0.68708500	-4.57201000
O	1.59970400	-0.37942400	-5.45198300
O	1.16307900	-1.20930500	-3.53686500
N	-0.95528200	-5.85883500	-2.24317400
C	-0.74073500	-4.64749200	-1.45542200
C	-2.04193900	-3.86372900	-1.30446800
O	-2.40325900	-3.42115800	-0.21521200
C	0.30918100	-3.74646700	-2.10749500
C	1.69240300	-4.35474200	-2.32050700
N	2.68976300	-3.86701500	-3.05591300
C	2.09435900	-5.56822000	-1.79452600
C	3.66540300	-4.74180800	-3.00722300
N	3.30737100	-5.76018300	-2.25329700
N	-2.79424900	-3.74728600	-2.37670600
C	-4.10501400	-3.14499100	-2.30502500
C	-4.97210200	-3.86187200	-1.27434300
O	-5.71412300	-3.19760400	-0.50510700
C	-4.76280600	-3.20552000	-3.68529900
O	-4.03775800	-2.29341200	-4.47754100
N	-3.97352800	-5.31861400	1.45526500
C	-3.52234900	-4.95105900	2.77178100
C	-3.96132500	-3.53621200	3.15521300
O	-4.16722200	-3.28393300	4.35252100
C	-1.99767700	-5.11285200	2.85143700
O	-1.14214200	-4.23326800	2.16682100
N	-4.18258800	-2.61556400	2.20844500
C	-4.73478700	-1.32617100	2.55442200
C	-6.20640700	-1.47394200	2.94842000
O	-6.66011900	-0.83958100	3.93599300
C	-4.54209000	-0.37795500	1.37660800
C	-3.10963700	-0.22713900	0.88851700
C	-2.00012700	-0.09015700	1.73899600
C	-2.86018800	-0.24402100	-0.48582900
C	-0.70227600	-0.01936500	1.23651200
C	-1.56993800	-0.18873000	-1.00439000
C	-0.47528600	-0.10165300	-0.14457400
O	0.81459400	-0.08922500	-0.59926900
N	7.07785200	5.75302800	-3.47613600
C	6.66333900	4.82792200	-2.46513500
C	7.55122400	4.90759800	-1.26113500
O	7.05499600	4.83111000	-0.10723800
C	6.63306100	3.40193500	-3.00341400
C	5.16691200	2.94610900	-3.06727700
C	4.43163100	2.79890700	-1.89784600
C	4.54388900	2.74617300	-4.29296000
C	3.09191600	2.46610500	-1.95700700
C	3.19957100	2.41146200	-4.33823800
C	2.46927300	2.27534900	-3.17029100
N	3.74996100	-2.73843700	6.11412500
C	4.53186600	-1.86941500	5.25710900
C	5.92663400	-2.42837100	5.13567300
O	6.58204000	-2.25939700	4.07479600
C	4.54977900	-0.41906800	5.83109500
C	3.11063700	0.14083400	5.88319100
C	5.44489300	0.46578400	4.96578700
C	2.31629600	0.26307900	4.54708300
N	5.51726900	-4.80638300	2.40599100
C	5.32273700	-4.11135800	1.15195100
C	6.65781900	-3.55715700	0.69117800
O	7.00343200	-3.66894600	-0.51365600
C	4.28045000	-2.99457900	1.34620500
C	2.95972600	-3.70798700	1.51003400
C	4.21401400	-1.99688000	0.19702100
C	1.71092500	-2.80533500	1.59478000
H	7.18960700	2.70824600	-2.34256800
H	7.10948800	3.30498500	-3.99971300
H	6.55957200	5.60403100	-4.31743700

H	6.93621500	6.69066400	-3.16280000
H	5.61790100	5.08176800	-2.11486800
H	8.63849100	5.01685700	-1.38193200
H	4.91915700	2.94719100	-0.92638300
H	2.51634200	2.34546100	-1.02941800
H	1.40097700	2.02107700	-3.21115600
H	2.70854600	2.25520400	-5.30600400
H	5.11352300	2.85564900	-5.22287900
H	-3.83489000	1.81610700	4.22258900
H	-2.92577000	2.86004500	3.11817400
H	-2.35617300	2.62485100	4.77744800
H	-5.15513500	2.78387000	6.11766100
H	-3.66502700	3.51891600	6.72091600
H	-5.10878000	4.51537700	6.46821800
H	-4.97843200	4.04674600	3.94982900
H	-2.69977600	5.25896100	5.58105900
H	-4.07440800	6.07237600	4.82493000
H	-1.47673400	6.98099300	4.80921500
H	-1.03254300	7.16237100	3.25437200
H	-1.61723800	4.90206100	3.39704800
H	-3.85895300	6.67465600	2.08109100
H	2.50742100	-0.56489000	-5.20783300
H	-1.20484800	-1.42726300	-4.86202600
H	-1.11348400	-0.00260000	-3.80807500
H	-3.16175600	0.67126200	-6.49265200
H	-1.48077400	2.08460300	-4.84643000
H	-1.14724200	2.41303300	-6.40967500
H	-0.18042400	0.28995400	-6.73799800
H	1.35138700	0.75373700	4.72177700
H	2.86969300	0.85994800	3.81146900
H	2.11715200	-0.71804000	4.09419500
H	2.51167000	-0.48456700	6.58031900
H	3.15511800	1.14645000	6.34480800
H	5.18286100	0.39760400	3.90086800
H	5.35216200	1.51968700	5.25992000
H	6.50289000	0.19077500	5.06446700
H	4.95143000	-0.43660800	6.87259300
H	6.37723000	-2.97508200	5.97648800
H	3.38579000	-3.49883200	5.57953900
H	2.99010300	-2.23122200	6.52928800
H	4.09455100	-1.80726200	4.21343200
H	0.80016000	-3.40128500	1.47579800
H	1.65818300	-2.27801900	2.55688200
H	1.72773400	-2.03993800	0.80074400
H	4.16567600	-2.50057400	-0.77799600
H	3.31381800	-1.36531300	0.28031700
H	5.09186900	-1.33910300	0.18649800
H	2.80091200	-4.39587300	0.64998000
H	2.98674800	-4.36004200	2.41162200
H	4.50409900	-2.41027100	2.28178700
H	4.62567000	-5.08786800	2.77319500
H	5.97960900	-4.22745600	3.07702400
H	4.94964100	-4.85845000	0.40484100
H	7.31570200	-3.04483000	1.40845900
H	3.27283100	3.15534600	3.38449400
H	3.68484900	3.87667100	1.92172800
H	2.12865700	4.41055800	0.23635400
H	1.09635500	5.53458400	1.14048300
H	-0.79554000	3.84799500	1.02519000
H	0.24541100	2.76691000	0.08992600
H	-0.83596000	6.42207000	-1.56513400
H	-0.23273700	6.30016200	-0.05200400
H	0.54994500	4.53560600	-1.68735700
H	-2.85973900	4.24130000	-0.40744600
H	-3.53344000	1.94141200	-1.85899900
H	-3.96060000	4.49648000	-3.65136400
H	-4.67381000	1.98773000	0.30248400
H	-6.01699100	1.43385800	-1.57510300
H	-7.09012700	2.65100700	-0.86090800
H	-6.55669100	2.81216100	-2.53804100
H	-5.27189100	4.40402500	-0.99362000
H	-3.67465400	-2.66552900	1.34443200
H	-6.85627500	-2.13879600	2.36350700
H	-4.95820900	-5.17673100	1.36001800
H	-3.48395400	-4.80194300	0.73897900
H	-1.54031000	-3.98866000	1.32400000
H	-1.66720700	-4.99276000	3.90037300
H	-1.72638400	-6.14213100	2.53807400
H	-3.97823900	-5.67242200	3.49671400
H	-4.16857700	-0.89320300	3.43216300

H	-5.16024100	-0.72042500	0.53590500
H	-4.95628600	0.58897200	1.70004600
H	-3.69746400	-0.31808300	-1.17529900
H	-1.40994400	-0.24666800	-2.07172900
H	-2.14041400	-0.05743700	2.81555200
H	0.14437400	0.08106100	1.90718300
H	-2.46594100	-4.05996100	-3.26746300
H	-4.33649400	-2.38939800	-5.37200000
H	-4.96721900	-4.96106000	-1.22981400
H	-4.74570200	-4.22644200	-4.11987800
H	-5.82446200	-2.89601400	-3.61961800
H	-3.98791500	-2.06645900	-1.99173700
H	-1.00016600	-6.65083300	-1.63742600
H	-0.21815400	-5.99211500	-2.90595500
H	-0.38055200	-4.90725900	-0.42069200
H	-0.05261400	-3.37870000	-3.09190400
H	0.44682800	-2.83837500	-1.48044700
H	3.87780100	-6.53820000	-2.03827600
H	4.62850000	-4.60102000	-3.51278500
H	1.57271600	-6.23264700	-1.10219200
H	0.85200500	-0.34852800	-1.54279000

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

Charge = 0 Multiplicity = 1

N	1.10608700	3.07595100	6.66364300
C	1.44977800	2.93573900	5.25453300
C	2.94784600	2.79837300	5.01439000
O	3.36981400	2.11106400	4.04840800
C	0.88962100	4.11706600	4.44159000
C	-0.61321500	4.07170200	4.23630600
C	-1.34649800	2.93670700	4.55088600
C	-1.28814000	5.16902800	3.70532300
C	-2.73083200	2.88835700	4.34381800
C	-2.66906300	5.13143800	3.49636300
C	-3.38994800	3.98626600	3.81666500
N	3.70758300	-0.74032600	5.74195800
C	3.27571400	-1.60190200	4.64207900
C	4.27767800	-1.53735400	3.50449400
O	4.57575600	-2.55631100	2.87681700
C	1.88199100	-1.18026000	4.14183400
C	0.77160800	-1.30636700	5.19925000
C	-0.55986900	-0.78957800	4.66056600
C	0.64259800	-2.76894900	5.61559700
N	4.80192200	-0.33313500	3.25959300
C	5.76274700	-0.10566500	2.18777400
C	7.04230100	-0.89729500	2.42535500
O	7.61432700	-1.47219900	1.46314900
C	6.13121800	1.39549500	2.04587800
O	4.94121600	2.16087100	1.83853200
C	7.07654000	1.58067800	0.84434800
N	6.36207200	-4.54172400	1.49775700
C	6.27841000	-4.73364200	0.04370200
C	7.65607800	-4.62150500	-0.59347900
O	7.97541800	-5.38613000	-1.54054800
C	5.37276300	-3.69714900	-0.64303400
C	3.90626600	-3.95618100	-0.42565300
O	3.47117300	-5.10984700	-0.62104100
O	3.17942700	-2.99689900	-0.08490600
N	2.82389100	-2.25110200	-5.59640300
C	2.18966200	-2.03963000	-4.29447700
C	2.99162800	-1.02652200	-3.48363800
O	2.44047100	-0.07022800	-2.93511100
C	2.10525600	-3.35595400	-3.51117100
C	1.24481400	-4.38701900	-4.16384400
N	1.07255100	-5.65051900	-3.64482000
C	0.51674600	-4.34333700	-5.30547900
C	0.27518200	-6.34463200	-4.43833700
N	-0.07504000	-5.57440000	-5.45221100
N	4.29748300	-1.24510400	-3.40243400
C	5.17110800	-0.34633200	-2.65154800
C	5.07144900	1.07628300	-3.19379200
O	4.93199900	2.04351000	-2.40095200
C	6.62655300	-0.83483400	-2.77257300
N	2.67916500	2.50759300	-4.75466900
C	1.36343100	3.07922500	-4.49175000
C	1.28481500	3.91983500	-3.23176000
O	0.55136900	4.90782800	-3.19226900
C	0.30917200	1.97333700	-4.41416100
O	0.17443500	1.34289800	-5.66543000



N	2.02477600	3.53838200	-2.19455400
C	1.99196400	4.32572300	-0.97562700
C	2.60962200	5.70291700	-1.19137300
O	2.12367300	6.70833400	-0.61123400
C	2.67871400	3.57668500	0.15855000
C	1.84532700	2.36596000	0.53594300
C	0.61955600	2.53231900	1.19662700
C	2.19228900	1.08060800	0.11410000
C	-0.24173700	1.46227000	1.41937300
C	1.33270400	-0.00017100	0.31615200
C	0.10904400	0.19284300	0.95722400
O	-0.78633700	-0.83844200	1.16816600
N	0.03236800	7.82978200	-2.65669000
C	-0.89496100	8.31221400	-1.64552500
C	-0.26913600	9.47698100	-0.88116600
O	-0.92088900	10.53972000	-0.70977500
C	-1.27704900	7.16722500	-0.68362800
C	-2.06270200	6.10354300	-1.46772300
C	-2.15231400	7.72033200	0.45636500
C	-2.28626500	4.80534700	-0.72260000
N	-3.88896300	-2.84252800	6.73631600
C	-5.05061300	-2.76921500	5.84579200
C	-6.31976500	-2.39839000	6.61194100
O	-7.24367100	-1.77048700	6.03254000
C	-5.26652300	-4.11189100	5.14173300
C	-4.21044100	-4.45252700	4.11647900
C	-3.39853000	-3.46346700	3.56893300
C	-4.05350500	-5.76810400	3.67897900
C	-2.44752900	-3.77602900	2.60350100
C	-3.10239400	-6.09404000	2.71327400
C	-2.29580800	-5.09034300	2.17167700
N	-7.79756200	1.52530200	-3.62831100
C	-6.45414000	1.13428000	-4.01352000
C	-6.00919100	-0.04628800	-3.14364400
O	-5.50400000	-1.05058200	-3.66016000
C	-5.50739100	2.32808500	-3.85912400
C	-4.05733200	2.15943900	-4.31794900
C	-3.41455800	3.52753200	-4.50206900
C	-3.29185800	1.30160500	-3.31000500
N	-6.21509100	0.06929300	-1.82832000
C	-5.84493200	-0.99563900	-0.89777900
C	-6.50605600	-2.31087300	-1.31071500
O	-5.87134600	-3.39283400	-1.21035000
C	-6.27577700	-0.65858700	0.56269900
C	-5.59885100	0.63065800	1.02817100
C	-5.91508700	-1.81089600	1.49934200
C	-4.08590100	0.57531300	1.00130700
N	-4.64533300	-3.94003900	-3.94731100
C	-3.44917300	-4.56955000	-3.38958000
C	-3.85425700	-5.91192700	-2.76044600
O	-3.21282700	-6.95749800	-3.04136900
C	-2.79212100	-3.65834600	-2.31505000
C	-2.21115300	-2.40801100	-2.99416800
C	-1.66309800	-4.43028100	-1.60722000
C	-1.46981700	-1.45887500	-2.05710600
H	-6.47273000	0.94585700	-1.41739200
H	4.73745800	-1.90322800	-4.01357600
H	4.34924700	0.49154000	3.63773300
H	2.38935200	2.60786100	-2.12660500
H	2.47924700	-1.57779500	-6.24823100
H	2.63844600	-3.17159500	-5.94035500
H	-5.26120100	-3.64719100	-3.21345200
H	-4.38003500	-3.15276400	-4.50230300
H	5.48681400	-4.77486900	1.91605500
H	6.60701100	-3.60026500	1.72061100
H	2.91961300	-0.56044500	6.33858700
H	4.42160800	-1.19801800	6.26835000
H	1.50481800	2.32922200	7.19223900
H	1.41835100	3.95204400	7.02717300
H	-8.44682100	0.81732300	-3.90222800
H	-8.04883000	2.38638900	-4.06921300
H	-3.99263600	-3.59895100	7.38151000
H	-3.05950800	-2.97920800	6.19417000
H	-0.12551700	1.99735100	-6.28421100
H	2.83803700	1.67480000	-4.22399300
H	3.40012100	3.17429300	-4.57209200
H	0.00547300	6.82448500	-2.73875700
H	-0.19619600	8.23841400	-3.53759000
H	0.75114600	9.37584000	-0.48683400
H	-7.54131000	-2.30851200	-1.67806700

H	-6.42194100	-2.68865600	7.66625000
H	-4.70691400	-5.94884600	-2.06900200
H	3.48008400	5.80990800	-1.85268300
H	8.36669600	-3.86967400	-0.22197700
H	2.26219300	-3.23312500	0.06140900
H	5.17061300	1.24888100	-4.27603800
H	4.86122800	-0.37268100	-1.57091000
H	6.73489200	-1.86978300	-2.41600200
H	6.99686200	-0.79152900	-3.80565500
H	7.28644100	-0.20937400	-2.15537800
H	1.14236500	-1.63880400	-4.40587500
H	3.11853500	-3.78256800	-3.34307500
H	1.69355600	-3.13888700	-2.50048500
H	-0.08016100	-7.37285800	-4.29885900
H	0.32554000	-3.54068800	-6.01803200
H	1.49394800	-5.96281700	-2.80529800
H	-0.68466100	2.35901500	-4.07399900
H	0.57240900	1.13562500	-3.74007300
H	1.14937200	3.74897200	-5.36700600
H	0.91044600	4.48135700	-0.68055600
H	2.76681000	4.26264400	1.00913800
H	3.69398400	3.27799300	-0.11757900
H	3.13174900	0.92488900	-0.40471100
H	1.61460200	-0.98066200	-0.05336900
H	-1.19521300	1.60675700	1.91416200
H	0.30534000	3.52412900	1.51049000
H	3.66507600	3.29565900	5.68327500
H	0.93776700	1.98934700	4.91108600
H	1.15945500	5.08466200	4.91151500
H	1.36162400	4.12058900	3.43529400
H	-0.73078100	6.07649800	3.44382500
H	-3.17544000	6.00459200	3.06825400
H	-4.47223400	3.95457100	3.65266300
H	-3.28371500	1.97752100	4.59668500
H	-0.84407200	2.02209400	4.92243800
H	-1.84645400	8.68050700	-2.11996900
H	-0.35905800	6.70447000	-0.24498900
H	-2.46733900	6.91595600	1.13702500
H	-1.60591600	8.46008000	1.05567100
H	-3.05866200	8.20563900	0.07171600
H	-2.80134400	4.06957900	-1.35717200
H	-1.33468700	4.35439800	-0.40181400
H	-2.89554800	4.94677700	0.18128800
H	-3.04438200	6.52284400	-1.77091400
H	-1.53260300	5.87228600	-2.41772500
H	-1.55722400	-5.33326100	1.39921400
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H	-2.99461900	-7.12995200	2.37649600
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H	-4.82282000	-1.97879600	5.07819800
H	5.87300200	-5.76492000	-0.12717500
H	5.54115200	-3.72810200	-1.74157200
H	5.65726800	-2.66699400	-0.32724200
H	0.18213300	-3.37143700	4.82053700
H	1.63266100	-3.20672500	5.82553300
H	0.02265200	-2.87967400	6.51370500
H	-1.37422300	-1.00746400	5.36565700
H	-0.54220300	0.30592400	4.51030700
H	-0.82523900	-1.25958100	3.70289400
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H	1.89921600	-0.13226900	3.77190300
H	1.61782200	-1.80265200	3.26127300
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H	5.29537600	-0.44204700	1.21817600
H	6.64094700	1.75531400	2.97358000
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H	-5.95552500	1.48039100	0.40567200
H	-5.94356300	0.85440800	2.05789300
H	-6.36585500	-2.76231600	1.19359700
H	-4.81992000	-1.94498400	1.54984400
H	-6.26035000	-1.60201500	2.52179200
H	-7.38334400	-0.51052800	0.58775600
H	-2.72681100	-4.74824500	-4.22636700
H	-3.53644700	-3.34124800	-1.54578000
H	-2.06610300	-5.17405500	-0.90707000
H	-1.02554500	-4.95785400	-2.32614200
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H	-2.16349400	-0.95016000	-1.37120400
H	-0.73603800	-2.00346300	-1.43990300
H	-0.93377500	-0.68453800	-2.62355400
H	-1.51459900	-2.72494300	-3.79958000
H	-3.01991400	-1.83577000	-3.49935300
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