

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					
C	1	1.46480000			
C	2	1.52980000	1	109.60320000	
O	3	1.22960000	2	120.02470000	1 -55.26980000
C	2	1.51430000	1	110.33640000	3 -120.89360000
H	1	0.99900000	2	109.29500000	5 59.89150000
H	1	0.99950000	2	110.67370000	5 -60.46270000
H	2	1.11870000	3	109.08690000	4 -172.95910000
H	3	1.09910000	2	118.90090000	1 125.88070000
H	5	1.09970000	2	111.63970000	1 177.54530000
H	5	1.10120000	2	112.75740000	1 57.40830000
H	5	1.10330000	2	111.70150000	1 -63.43180000
N	3	4.10690000	2	142.65130000	1 -176.23810000
C	13	1.45720000	3	144.01640000	2 10.61560000
C	14	1.51520000	13	114.29890000	3 -176.22570000
O	15	1.23070000	14	121.14630000	13 -76.43680000
C	14	1.54060000	13	110.82100000	3 60.52620000
C	17	1.53210000	14	112.98320000	13 -65.88550000
O	18	1.25520000	17	119.37980000	14 -52.41440000
O	18	1.24970000	17	117.93290000	14 127.74140000
H	13	0.99920000	14	109.85580000	15 -179.80440000
H	13	0.99850000	14	110.99140000	15 58.44140000
H	14	1.12280000	15	107.83670000	16 165.95160000
H	15	1.09930000	14	118.19370000	13 103.77360000
H	17	1.11040000	14	110.15110000	13 175.48450000
H	17	1.11120000	14	110.40130000	13 59.27810000
H	20	0.97790000	18	115.05530000	17 160.49110000
N	19	5.42240000	18	145.51600000	17 -29.79980000
C	28	1.44980000	19	32.20150000	18 142.66900000
C	29	1.51720000	28	113.97880000	19 55.67280000
O	30	1.23260000	29	119.71830000	28 119.14450000
C	29	1.52200000	28	110.49360000	19 -70.82170000
C	32	1.51600000	29	112.31450000	28 -72.40970000
C	33	1.39940000	32	120.81580000	29 76.19330000
C	33	1.39660000	32	120.92900000	29 -104.11940000
C	34	1.39430000	33	121.08970000	32 179.67830000
C	35	1.39480000	33	121.21390000	32 -179.65280000
C	37	1.38870000	35	119.55820000	33 0.02350000
O	38	1.37710000	37	119.56830000	35 179.48930000
H	28	1.00130000	29	111.68380000	30 85.31270000
H	28	0.99870000	29	109.64210000	30 -153.31640000
H	29	1.12390000	32	108.02470000	33 43.13870000
H	32	1.11260000	29	109.93780000	28 166.55570000
H	32	1.11490000	29	112.15220000	28 50.27520000
H	34	1.09600000	33	120.52610000	32 2.07800000
H	35	1.09800000	33	119.53990000	32 0.55030000
H	36	1.09590000	34	120.18270000	33 -179.73470000
H	37	1.09750000	35	119.04910000	33 -179.97650000
H	39	0.94930000	38	107.60120000	37 1.30680000
N	30	1.34420000	29	118.58650000	28 -61.19210000
C	50	1.46870000	30	115.25420000	29 179.66210000
C	51	1.54220000	50	110.59420000	30 -60.00440000
O	52	1.23080000	51	120.81750000	50 154.89610000
C	51	1.53520000	50	103.67070000	30 178.37930000
C	54	1.51280000	51	104.53180000	50 -20.06180000
C	50	1.47230000	30	132.58990000	29 -1.45390000
H	51	1.12550000	50	109.91630000	30 60.38330000
H	52	1.10040000	51	118.92780000	50 -26.14890000
H	54	1.10650000	51	111.65800000	50 -142.00860000
H	54	1.10830000	51	111.37380000	50 100.08180000
H	55	1.11130000	54	111.20590000	51 -87.18610000
H	55	1.10660000	54	111.85410000	51 155.52600000
H	56	1.11000000	50	110.39380000	30 82.02060000
H	56	1.11210000	50	111.41750000	30 -36.45010000
N	31	3.12000000	30	166.05770000	29 -124.07710000
C	65	1.45720000	31	113.30340000	30 -119.08660000
C	66	1.50980000	65	110.81030000	31 130.14050000
O	67	1.22280000	66	121.12530000	65 150.15910000

C	66	1.51870000	65	110.57730000	31	9.20630000
C	69	1.48990000	66	113.32630000	65	-75.29880000
N	70	1.37850000	69	122.72220000	66	132.63050000
C	70	1.35320000	69	131.01160000	66	-45.91340000
C	71	1.32050000	70	109.29610000	69	-178.81980000
N	73	1.32200000	71	108.36390000	70	-0.02970000
H	65	1.00290000	66	111.78810000	67	131.95720000
H	65	0.99810000	66	109.54420000	67	-107.07450000
H	66	1.12520000	67	107.45990000	68	29.09510000
H	69	1.11460000	66	109.28190000	65	165.34000000
H	69	1.11450000	66	111.03230000	65	49.97630000
H	71	1.00700000	70	125.87420000	69	4.49650000
H	72	1.09110000	70	130.73640000	69	-2.06110000
H	73	1.09650000	71	126.96410000	70	179.07520000
N	67	1.32190000	66	115.75720000	65	-30.33720000
C	83	1.44290000	67	120.87570000	66	179.83030000
C	84	1.52360000	83	108.95410000	67	-70.03810000
O	85	1.22650000	84	121.75910000	83	144.16990000
C	84	1.52190000	83	108.91610000	67	169.02090000
C	87	1.51930000	84	113.02960000	83	-87.24850000
C	88	1.52080000	87	112.55920000	84	149.02700000
N	89	1.45640000	88	109.92790000	87	-164.95900000
C	90	1.32680000	89	124.32200000	88	155.11890000
N	91	1.33030000	90	119.81120000	89	0.05630000
N	91	1.33280000	90	119.80800000	89	179.85700000
H	83	1.00240000	67	121.32330000	66	1.34670000
H	84	1.12750000	83	109.19550000	67	49.07010000
H	85	1.10170000	84	118.51000000	83	-35.98740000
H	87	1.11020000	84	109.19580000	83	151.38530000
H	87	1.11390000	84	110.78630000	83	37.13690000
H	88	1.11100000	87	109.66700000	84	-87.35540000
H	88	1.11480000	87	109.54290000	84	27.09010000
H	89	1.11280000	88	109.90460000	87	72.38760000
H	89	1.11560000	88	110.34550000	87	-43.46830000
H	90	0.99940000	89	115.40680000	88	-42.85360000
H	92	1.00400000	91	116.82270000	90	-24.72020000
H	92	0.99940000	91	116.13480000	90	-159.12830000
H	93	0.99230000	91	115.87170000	90	176.15090000
N	68	3.03970000	67	132.81940000	66	-68.88700000
C	107	1.45520000	68	99.64810000	67	170.57460000
C	108	1.52480000	107	114.32840000	68	73.31340000
O	109	1.23370000	108	120.46320000	107	130.73070000
C	108	1.52860000	107	109.88130000	68	-50.34080000
C	111	1.52680000	108	113.67810000	107	-66.98030000
C	112	1.51190000	111	109.44070000	108	153.09580000
C	112	1.51810000	111	109.93140000	108	-84.99300000
H	107	1.00530000	108	111.79450000	109	76.00710000
H	107	0.99810000	108	110.31130000	109	-46.54310000
H	108	1.12230000	109	108.18110000	110	13.22950000
H	111	1.11370000	108	110.22190000	107	56.04870000
H	111	1.11120000	108	109.13900000	107	170.65110000
H	112	1.11780000	111	109.59190000	108	34.33580000
H	113	1.10070000	112	112.05880000	111	54.10740000
H	113	1.10090000	112	111.81600000	111	-66.26540000
H	113	1.09920000	112	111.50800000	111	174.04400000
H	114	1.09850000	112	111.38180000	111	56.79070000
H	114	1.09880000	112	111.86120000	111	-63.45200000
H	114	1.09810000	112	111.29380000	111	176.61800000
N	109	1.32990000	108	116.78940000	107	-49.31950000
C	127	1.44990000	109	120.46970000	108	-178.96820000
C	128	1.51340000	127	109.88460000	109	143.03990000
O	129	1.23990000	128	120.30290000	127	-19.35550000
H	127	1.00250000	109	120.46190000	108	-14.32770000
H	128	1.11720000	127	109.28270000	109	-95.14930000
H	128	1.11450000	127	111.65390000	109	21.58360000
N	129	1.34150000	128	117.67700000	127	160.54120000
C	134	1.46460000	129	122.78510000	128	-179.72150000
C	135	1.53000000	134	114.88000000	129	-48.47310000
O	136	1.23550000	135	120.16490000	134	129.64940000
C	135	1.52390000	134	103.25160000	129	-171.49320000
C	138	1.48250000	135	103.77960000	134	-28.09830000
C	134	1.47150000	129	125.67640000	128	-0.12560000
H	135	1.12510000	134	107.50930000	129	72.25410000
H	136	1.10050000	135	118.59380000	134	-52.46290000
H	138	1.10670000	135	111.71030000	134	-150.01010000
H	138	1.11000000	135	111.31450000	134	92.65310000
H	139	1.11030000	138	111.56300000	135	-83.45460000
H	139	1.10790000	138	112.34100000	135	159.26580000
H	140	1.11030000	134	110.35120000	129	73.37460000
H	140	1.11220000	134	110.14940000	129	-43.52450000

N	130	3.04580000	129	123.95840000	128	-102.59690000
C	149	1.45810000	130	102.15280000	129	124.82930000
C	150	1.53310000	149	114.47850000	130	148.40800000
O	151	1.22900000	150	120.21250000	149	161.82580000
C	150	1.53080000	149	109.93190000	130	23.67340000
C	153	B1	150	A1	149	D1
C	154	B2	153	A2	150	D2
C	154	B3	153	A3	150	D3
C	155	B4	154	A4	153	D4
C	156	B5	154	A5	153	D5
C	158	B6	156	A6	154	D6
O	159	B7	158	A7	156	D7
H	149	1.00230000	150	110.50290000	151	84.70730000
H	149	0.99940000	150	109.16130000	151	-155.33080000
H	150	1.12050000	151	106.46110000	152	43.71730000
H	153	B8	150	A8	149	D8
H	153	B9	150	A9	149	D9
H	155	B10	154	A10	153	D10
H	156	B11	154	A11	153	D11
H	157	B12	155	A12	154	D12
H	158	B13	156	A13	154	D13
N	151	1.32890000	150	117.69380000	149	-18.84210000
C	170	1.46160000	151	120.22630000	150	178.07330000
C	171	1.52880000	170	108.03270000	151	-80.36250000
O	172	1.23320000	171	120.78680000	170	177.56710000
C	171	1.53060000	170	111.49040000	151	159.20760000
C	174	1.53550000	171	117.53380000	170	-72.93580000
C	175	1.52380000	174	109.44310000	171	175.66600000
C	175	1.52380000	174	110.27560000	171	-62.10440000
H	170	0.99790000	151	122.16400000	150	11.16370000
H	171	1.12830000	170	109.67420000	151	40.23870000
H	172	1.10060000	171	119.27670000	170	-1.93760000
H	174	1.11180000	171	107.74700000	170	165.49250000
H	174	1.11170000	171	109.82020000	170	51.50260000
H	175	1.11790000	174	108.95810000	171	56.85820000
H	176	1.09840000	175	111.69370000	174	58.93810000
H	176	1.09770000	175	111.51630000	174	-61.47390000
H	176	1.09750000	175	110.83660000	174	178.73670000
H	177	1.09780000	175	111.60530000	174	165.27020000
H	177	1.10380000	175	110.04350000	174	45.41770000
H	177	1.09770000	175	111.85920000	174	-73.92290000
H	160	B14	159	A14	158	D14

Variables:

B1	1.506
B2	1.4011
B3	1.4023
B4	1.388
B5	1.3962
B6	1.3897
B7	1.389
B8	1.0899
B9	1.0949
B10	1.0853
B11	1.0843
B12	1.0851
B13	1.0877
B14	0.9707
A1	113.7119
A2	118.7228
A3	122.7836
A4	121.2798
A5	120.9432
A6	119.0336
A7	121.9374
A8	107.8092
A9	108.5008
A10	119.3377
A11	119.7446
A12	119.8115
A13	120.9112
A14	110.2238
D1	75.2971
D2	92.3893
D3	-84.7724
D4	-176.8662
D5	176.0689
D6	0.8929
D7	178.6244
D8	-48.0519
D9	-164.4239

D10	1.6191
D11	-4.6978
D12	-180.8397
D13	-180.0798
D14	22.0899

Mouse RNR:

Charge = 0 Multiplicity = 1

N				
C	1	1.44040000		
C	2	1.53410000	1	110.21110000
O	3	1.22890000	2	123.27050000
C	2	1.49500000	1	105.59990000
C	5	1.49200000	2	106.61160000
C	6	1.51290000	5	109.69860000
C	6	1.50120000	5	106.58660000
H	1	0.99920000	2	110.12550000
H	1	1.00040000	2	111.16920000
H	2	1.13350000	1	113.75240000
H	3	1.10190000	2	117.60170000
H	5	1.11300000	2	110.20650000
H	5	1.11110000	2	112.80620000
H	6	1.11750000	5	111.85520000
H	7	1.10000000	6	111.18260000
H	7	1.10370000	6	112.78500000
H	7	1.09860000	6	111.29600000
H	8	1.10470000	6	110.11700000
H	8	1.10250000	6	115.04330000
H	8	1.10500000	6	113.53940000
N	4	3.30360000	3	99.31810000
C	22	1.42210000	4	97.81900000
C	23	1.50280000	22	112.98910000
O	24	1.20430000	23	120.25670000
C	23	1.45950000	22	103.76600000
C	26	1.45360000	23	109.31710000
C	27	1.38610000	26	119.37930000
C	27	1.38440000	26	120.27200000
C	28	1.39340000	27	120.45810000
C	29	1.39190000	27	120.71130000
C	31	1.39760000	29	118.56520000
H	22	1.00130000	4	107.99630000
H	22	1.00020000	4	120.90010000
H	23	1.13040000	22	114.45010000
H	26	1.11840000	23	114.13710000
H	26	1.12150000	23	113.33540000
H	28	1.10070000	27	120.60790000
H	29	1.09900000	27	119.93410000
H	30	1.09400000	28	120.81380000
H	31	1.09380000	29	120.87310000
H	32	1.09750000	31	119.36140000
N	24	1.31490000	23	116.81990000
C	43	1.45250000	24	121.65860000
C	44	1.53730000	43	112.10160000
O	45	1.23660000	44	123.47450000
C	44	1.51760000	43	106.38720000
H	43	1.01730000	24	120.91750000
H	44	1.12520000	43	108.55120000
H	45	1.10090000	44	117.13400000
H	47	1.09990000	44	112.90910000
H	47	1.10080000	44	111.74080000
H	47	1.09930000	44	110.62220000
N	25	3.12560000	24	149.92710000
C	54	1.43290000	25	115.74660000
C	55	1.50590000	54	107.76920000
O	56	1.22300000	55	121.86530000
C	55	1.54620000	54	113.27740000
C	58	1.50250000	55	114.39480000
O	59	1.22050000	58	124.25980000
O	59	1.31610000	58	111.55320000
H	54	0.99870000	25	55.91880000
H	54	1.00110000	25	55.40390000
H	55	1.12400000	54	106.59930000
H	56	1.10280000	55	118.50140000
H	58	1.10980000	55	108.41010000
H	58	1.11640000	55	109.49330000
H	61	0.95710000	59	110.17550000
N	61	5.84210000	59	91.36120000
C	69	1.44770000	61	36.29280000
			59	149.93140000

C	70	1.49680000	69	108.04860000	61	69.39980000
O	71	1.22030000	70	122.87860000	69	139.22490000
C	70	1.51760000	69	109.43480000	61	-43.98550000
C	73	1.51820000	70	113.18410000	69	-70.16860000
N	74	1.39770000	73	120.68250000	70	-178.75830000
C	74	1.35880000	73	132.42390000	70	3.80940000
C	75	1.33930000	74	107.99100000	73	178.76030000
N	77	1.31960000	75	110.42920000	74	3.70060000
H	69	0.99980000	61	125.17400000	59	74.41090000
H	69	1.00040000	61	75.02830000	59	-29.06680000
H	70	1.11810000	69	109.77710000	61	-167.18890000
H	71	1.10410000	70	118.23740000	69	-41.68580000
H	73	1.11270000	70	109.89040000	69	169.50490000
H	73	1.11240000	70	111.44040000	69	52.92120000
H	75	0.98970000	74	124.40280000	73	5.85740000
H	76	1.08980000	74	131.71240000	73	-1.99850000
H	77	1.09680000	75	126.11630000	74	-177.41110000
N	72	3.06550000	71	161.80230000	70	-91.79320000
C	88	1.42410000	72	122.03800000	71	-152.85590000
C	89	1.49210000	88	114.97630000	72	122.88990000
O	90	1.24780000	89	120.16220000	88	149.18920000
C	89	1.53510000	88	110.11340000	72	1.99700000
C	92	B1	89	A1	88	D1
C	93	B2	92	A2	89	D2
C	93	B3	92	A3	89	D3
C	94	B4	93	A4	92	D4
C	95	B5	93	A5	92	D5
C	96	B6	94	A6	93	D6
O	98	B7	96	A7	94	D7
H	88	0.99930000	72	53.84180000	71	114.52670000
H	88	1.00010000	72	56.41320000	71	-57.13080000
H	89	1.13240000	88	106.72470000	72	-115.79590000
H	90	1.10020000	89	119.99160000	88	-31.48770000
H	92	B8	89	A8	88	D8
H	92	B9	89	A9	88	D9
H	94	B10	93	A10	92	D10
H	95	B11	93	A11	92	D11
H	96	B12	94	A12	93	D12
H	97	B13	95	A13	93	D13
N	91	3.16930000	90	98.44490000	89	-99.53470000
C	110	1.45700000	91	98.25900000	90	143.72700000
C	111	1.48970000	110	105.66670000	91	72.72000000
O	112	1.21220000	111	124.42920000	110	124.98980000
C	111	1.52630000	110	106.85020000	91	-41.33290000
C	114	1.53990000	111	114.01660000	110	-101.32050000
C	115	1.50920000	114	113.82490000	111	2.82890000
C	115	1.51490000	114	113.45250000	111	128.97790000
H	110	1.00010000	91	95.73350000	90	32.70900000
H	110	0.99900000	91	132.27440000	90	-89.37220000
H	111	1.12590000	110	114.15360000	91	-166.33910000
H	112	1.10600000	111	116.79580000	110	-55.49020000
H	114	1.11350000	111	109.71650000	110	137.55780000
H	114	1.11240000	111	111.37430000	110	22.93440000
H	115	1.12070000	114	105.86270000	111	-114.21700000
H	116	1.10140000	115	112.53420000	114	-54.04970000
H	116	1.09980000	115	110.76410000	114	-173.32200000
H	116	1.09980000	115	112.26500000	114	67.78220000
H	117	1.09790000	115	111.39220000	114	174.84650000
H	117	1.10130000	115	111.46180000	114	54.89040000
H	117	1.09950000	115	111.77070000	114	-64.92040000
N	32	4.44370000	31	111.19140000	29	168.38750000
C	131	1.42950000	32	104.40980000	31	75.92660000
C	132	1.48980000	131	110.69490000	32	-149.83940000
O	133	1.19500000	132	122.22810000	131	137.38820000
C	132	1.52840000	131	110.53730000	32	91.35450000
C	135	1.52110000	132	112.15830000	131	-77.00280000
C	136	1.39090000	135	120.92120000	132	-28.12290000
C	136	1.39320000	135	121.44050000	132	150.09230000
C	137	1.39490000	136	120.97010000	135	178.63570000
C	138	1.39470000	136	122.63790000	135	179.04020000
C	139	1.38870000	137	119.92620000	136	1.19000000
H	131	1.00030000	32	24.07380000	31	-177.38690000
H	131	1.00060000	32	130.98380000	31	-147.93740000
H	132	1.12620000	131	107.47190000	32	-29.21520000
H	133	1.10530000	132	117.81550000	131	-43.52980000
H	135	1.10930000	132	110.42460000	131	163.83920000
H	135	1.11000000	132	111.71800000	131	46.79220000
H	137	1.10080000	136	120.12920000	135	-1.57520000
H	138	1.09720000	136	118.73110000	135	0.50140000
H	139	1.09710000	137	120.11830000	136	-179.17030000

H	140	1.09400000	138	120.66840000	136	-177.69840000
H	141	1.09790000	139	119.27690000	137	178.40570000
N	78	5.16710000	77	100.46430000	75	-106.60190000
C	153	1.43450000	78	45.67270000	77	5.72560000
C	154	1.51870000	153	114.90680000	78	-129.65450000
O	155	1.22590000	154	123.21070000	153	134.49570000
C	154	1.48680000	153	108.00660000	78	106.02910000
C	157	1.50900000	154	108.40780000	153	-62.73280000
C	157	1.50510000	154	109.64490000	153	175.01460000
C	158	1.53610000	157	113.81290000	154	174.50670000
H	153	1.00060000	78	156.36710000	77	19.24290000
H	153	0.99830000	78	87.58380000	77	-116.68450000
H	154	1.12680000	153	105.80340000	78	-10.50210000
H	155	1.10350000	154	117.53560000	153	-45.63720000
H	157	1.12270000	154	111.00460000	153	56.10110000
H	158	1.10910000	157	110.93250000	154	52.72240000
H	158	1.11100000	157	109.91740000	154	-63.65680000
H	159	1.10020000	157	112.52930000	154	42.00420000
H	159	1.10180000	157	112.41050000	154	-79.39440000
H	159	1.10310000	157	110.31670000	154	160.91090000
H	160	1.09680000	158	111.74140000	157	-60.09310000
H	160	1.09610000	158	110.96610000	157	179.32650000
H	160	1.10090000	158	110.11030000	157	59.68800000
H	99	B14	98	A14	96	D14

Variables:

B1	1.5229
B2	1.4047
B3	1.3958
B4	1.39
B5	1.3985
B6	1.3977
B7	1.3679
B8	1.1009
B9	1.0963
B10	1.0851
B11	1.0847
B12	1.0852
B13	1.0853
B14	0.9697
A1	110.7055
A2	119.7266
A3	123.1405
A4	122.3403
A5	121.4737
A6	119.4163
A7	117.8066
A8	110.7934
A9	109.1568
A10	119.3255
A11	119.4596
A12	121.3271
A13	119.5597
A14	109.0911
D1	-75.3707
D2	-56.7719
D3	122.7826
D4	-180.029
D5	179.3489
D6	0.8284
D7	179.1545
D8	164.6238
D9	46.5821
D10	0.014
D11	-1.9619
D12	179.9311
D13	181.9067
D14	-167.6976

***E. coli* RNR:**

Charge = 0 Multiplicity = 1

N					
C	1	1.44660000			
C	2	1.51470000	1	109.73850000	
O	3	1.25840000	2	120.00000000	1
C	2	1.52100000	1	109.30730000	3
C	5	1.53110000	2	122.42270000	1
C	6	1.53300000	5	114.17870000	2
C	6	1.52670000	5	105.75790000	2

N	4	3.15500000	3	109.70700000	2	-94.16890000
C	9	1.46270000	4	95.15230000	3	146.82850000
C	10	1.54020000	9	110.94320000	4	66.75320000
O	11	1.24070000	10	121.46370000	9	133.27090000
C	10	1.53450000	9	109.31380000	4	-55.06950000
C	13	1.53320000	10	113.62850000	9	-68.26300000
C	14	1.54310000	13	115.71990000	10	178.73600000
O	15	1.24040000	14	121.68010000	13	-31.76380000
N	15	1.32990000	14	120.42830000	13	145.98610000
N	11	1.33680000	10	117.98190000	9	-43.56150000
C	18	1.43900000	11	122.71860000	10	-179.76920000
C	19	1.53340000	18	111.42830000	11	-60.80110000
O	20	1.25840000	19	120.00000000	18	134.97900000
C	19	1.53430000	18	107.87320000	11	176.61910000
O	22	1.40270000	19	107.68420000	18	-57.26740000
C	22	1.50990000	19	113.11250000	18	-175.22300000
N	12	3.10690000	11	166.11040000	10	-109.35490000
C	25	1.45920000	12	124.79450000	11	-138.84620000
C	26	1.50230000	25	114.53640000	12	103.38890000
O	27	1.25840000	26	120.00000000	25	162.49760000
C	26	1.51010000	25	111.99400000	12	-20.36220000
C	29	1.53120000	26	110.84900000	25	-86.14010000
O	30	1.23910000	29	121.28350000	26	-11.48520000
O	30	1.22000000	29	118.46140000	26	169.03150000
N	32	5.27060000	30	117.43800000	29	55.73380000
C	33	1.46080000	32	48.83840000	30	-132.52140000
C	34	1.52650000	33	110.72560000	32	102.03880000
O	35	1.23000000	34	121.51460000	33	133.39550000
C	34	1.52950000	33	111.06420000	32	-19.15290000
C	37	1.52600000	34	116.54560000	33	-58.73090000
N	38	1.33170000	37	127.58670000	34	167.72740000
C	38	1.38230000	37	124.08280000	34	-9.75220000
C	39	1.31130000	38	107.00140000	37	-177.05260000
N	40	1.31100000	38	105.33360000	37	177.08470000
N	35	1.31500000	34	116.90390000	33	-42.95490000
C	43	1.44430000	35	121.04180000	34	173.59110000
C	44	1.52580000	43	110.69160000	35	-55.88920000
O	45	1.25840000	44	120.00000000	43	138.73090000
C	44	1.53020000	43	109.19990000	35	-177.46810000
O	47	1.40900000	44	105.09200000	43	-70.08480000
N	36	2.97600000	35	115.00350000	34	-86.80790000
C	49	1.43940000	36	100.67260000	35	145.21980000
C	50	1.53020000	49	112.04700000	36	66.23770000
O	51	1.24080000	50	118.51510000	49	149.71320000
C	50	1.53530000	49	109.37950000	36	-58.15410000
O	53	1.40510000	50	120.89160000	49	70.86910000
N	51	1.33900000	50	120.39520000	49	-26.91960000
C	55	1.44470000	51	120.49620000	50	173.26990000
C	56	1.53060000	55	110.05820000	51	-70.99610000
O	57	1.25840000	56	120.00000000	55	137.96080000
C	56	1.52430000	55	108.77360000	51	165.50330000
C	59	B1	56	A1	55	D1
C	60	B2	59	A2	56	D2
C	60	B3	59	A3	56	D3
C	61	B4	60	A4	59	D4
C	62	B5	60	A5	59	D5
C	64	B6	62	A6	60	D6
O	65	B7	64	A7	62	D7
N	14	7.41030000	13	116.37680000	10	-46.50470000
C	67	1.43170000	14	40.34230000	13	-105.00770000
C	68	1.49810000	67	111.19640000	14	-116.29310000
O	69	1.25840000	68	120.00000000	67	140.18150000
C	68	1.52450000	67	111.15070000	14	120.53670000
C	71	1.53670000	68	108.12440000	67	-111.60120000
C	72	1.38920000	71	120.09470000	68	-65.30100000
C	72	1.38940000	71	120.47560000	68	111.27630000
C	73	1.38170000	72	120.17740000	71	176.16480000
C	74	1.38610000	72	119.89820000	71	-176.21020000
C	75	1.37700000	73	120.63240000	72	0.05200000
N	54	6.46130000	53	107.94900000	50	137.40650000
C	78	1.44950000	54	100.71500000	53	178.78230000
C	79	1.50750000	78	108.93060000	54	-122.92730000
O	80	1.25840000	79	120.00000000	78	148.39530000
C	79	1.55990000	78	110.24670000	54	114.63430000
C	82	1.54510000	79	109.79360000	78	-61.42010000
C	82	1.52740000	79	109.68830000	78	176.60690000
C	83	1.55920000	82	118.29660000	79	-60.43420000
N	81	3.22580000	80	99.10210000	79	-86.64380000
C	86	1.44690000	81	96.51600000	80	136.12610000
C	87	1.51720000	86	108.68550000	81	60.87290000

O	88	1.25840000	87	120.00000000	86	135.99000000
C	87	1.53990000	86	109.27090000	81	-61.19370000
C	90	1.51000000	87	105.25170000	86	-71.41850000
C	90	1.52330000	87	114.16390000	86	167.01280000
C	91	1.54320000	90	115.93820000	87	-174.63700000
H	71	1.10800000	68	111.41060000	67	129.18260000
H	71	1.10860000	68	112.99080000	67	10.75600000
H	67	0.99930000	14	94.13740000	13	11.98070000
H	67	0.99870000	14	82.29960000	13	120.92610000
H	68	1.13140000	67	109.94810000	14	1.61860000
H	69	1.09940000	68	120.20620000	67	-40.78990000
H	73	1.09700000	72	119.73060000	71	-3.88430000
H	75	1.09830000	73	119.89620000	72	179.66290000
H	77	1.09890000	75	120.29160000	73	-179.36050000
H	76	1.09640000	74	119.84140000	72	179.91910000
H	74	1.09600000	72	120.07000000	71	3.61660000
H	7	1.09880000	6	111.12640000	5	175.82520000
H	7	1.09890000	6	111.50180000	5	-64.42080000
H	7	1.09800000	6	111.52600000	5	55.57880000
H	8	1.09830000	6	111.02640000	5	175.70570000
H	8	1.09890000	6	111.94220000	5	-64.62740000
H	8	1.09810000	6	111.79010000	5	56.11550000
H	6	1.11430000	5	109.85760000	2	-77.78900000
H	5	1.11540000	2	106.30400000	1	-56.11690000
H	5	1.11290000	2	108.50950000	1	56.29770000
H	1	0.99940000	2	110.56090000	3	166.66020000
H	1	0.99880000	2	109.37880000	3	-73.25260000
H	2	1.13020000	1	111.89050000	5	-118.84060000
H	3	1.09860000	2	119.91550000	1	-47.09560000
H	31	0.95810000	30	113.27310000	29	178.43340000
H	29	1.11000000	26	111.77650000	25	154.25740000
H	29	1.11540000	26	112.78680000	25	35.23910000
H	27	1.10070000	26	120.39730000	25	-17.39730000
H	25	0.99900000	12	31.90980000	11	-65.58000000
H	25	0.99850000	12	120.20180000	11	12.76730000
H	26	1.12340000	25	104.76120000	12	-140.45830000
H	85	1.09650000	83	110.29620000	82	-175.03460000
H	85	1.09710000	83	111.11540000	82	-55.43050000
H	85	1.09880000	83	112.05640000	82	64.86240000
H	83	1.11170000	82	108.60990000	79	62.87520000
H	83	1.10740000	82	107.80080000	79	176.98940000
H	84	1.09880000	82	111.92270000	79	51.57590000
H	84	1.09810000	82	110.77910000	79	171.40760000
H	84	1.09760000	82	111.64210000	79	-69.04010000
H	82	1.11640000	79	109.43880000	78	56.98160000
H	80	1.09950000	79	120.12830000	78	-32.23510000
H	78	0.99830000	54	38.77990000	53	70.61430000
H	78	1.00350000	54	78.25060000	53	-72.28130000
H	79	1.13330000	78	111.66740000	54	-4.16770000
H	93	1.09490000	91	110.41380000	90	166.75070000
H	93	1.09840000	91	111.57790000	90	-72.55880000
H	93	1.10300000	91	110.73370000	90	46.94840000
H	92	1.09850000	90	111.78980000	87	48.01900000
H	92	1.10280000	90	110.71440000	87	167.31710000
H	92	1.09700000	90	111.41120000	87	-72.35800000
H	91	1.11270000	90	109.45430000	87	-53.83240000
H	91	1.11300000	90	110.08670000	87	61.70710000
H	90	1.12550000	87	110.29590000	86	46.24670000
H	86	1.00450000	81	108.97290000	80	23.00140000
H	86	0.99960000	81	16.81580000	80	-70.39640000
H	87	1.12050000	86	107.60070000	81	179.37900000
H	88	1.09990000	87	119.89590000	86	-44.91520000
H	17	0.99600000	15	119.33850000	14	-166.40790000
H	17	0.99320000	15	119.08460000	14	-15.07180000
H	14	1.11140000	13	108.57320000	10	-57.36780000
H	14	1.11220000	13	108.86330000	10	57.39660000
H	13	1.11220000	10	111.11710000	9	55.09700000
H	13	1.11060000	10	108.58490000	9	170.59410000
H	9	0.99780000	4	135.06330000	3	-87.99380000
H	9	1.00300000	4	95.79330000	3	37.15280000
H	10	1.12620000	9	111.87710000	4	-174.33560000
H	18	1.01910000	11	118.36660000	10	-10.62640000
H	19	1.12980000	18	108.77210000	11	58.14390000
H	20	1.09800000	19	119.57080000	18	-45.27360000
H	23	0.95560000	22	109.87900000	19	-67.85350000
H	24	1.10100000	22	112.35840000	19	53.60230000
H	24	1.09900000	22	111.36680000	19	174.12490000
H	24	1.09860000	22	111.56870000	19	-66.30600000
H	22	1.11420000	19	112.57950000	18	56.44470000
H	55	1.00350000	51	119.40060000	50	-29.29350000

H	57	1.09840000	56	119.35460000	55	-41.86400000
H	49	0.99940000	36	112.07750000	35	-96.64940000
H	49	1.00980000	36	11.42080000	35	-16.36860000
H	54	0.96370000	53	109.47800000	50	-36.10750000
H	53	1.10630000	50	109.53620000	49	-170.79780000
H	53	1.10960000	50	109.02040000	49	-53.80390000
H	50	1.11970000	49	107.45940000	36	-174.71700000
H	56	1.13070000	55	109.64900000	51	48.37850000
H	59	B8	56	A8	55	D8
H	59	B9	56	A9	55	D9
H	62	B10	60	A10	59	D10
H	64	B11	62	A11	60	D11
H	61	B12	60	A12	59	D12
H	63	B13	61	A13	60	D13
H	43	0.99950000	35	120.73430000	34	-7.47900000
H	48	0.94790000	47	107.62870000	44	172.26650000
H	45	1.10010000	44	119.62160000	43	-43.14740000
H	47	1.10970000	44	112.52050000	43	51.50160000
H	47	1.10780000	44	110.33050000	43	171.12050000
H	44	1.12920000	43	108.53960000	35	63.30470000
H	33	0.99810000	32	150.11660000	30	175.94750000
H	33	1.00020000	32	70.04350000	30	81.82840000
H	34	1.12600000	33	110.56240000	32	-138.96170000
H	37	1.11140000	34	110.43190000	33	64.49580000
H	37	1.11210000	34	109.00260000	33	-179.88000000
H	42	0.98840000	40	124.96800000	38	178.57480000
H	41	1.09680000	39	123.40670000	38	-179.14170000
H	40	1.09220000	38	129.52100000	37	-5.87990000
H	66	B14	65	A14	64	D14

Variables:

B1	1.5208
B2	1.4047
B3	1.3969
B4	1.3935
B5	1.3917
B6	1.3947
B7	1.3677
B8	1.0983
B9	1.1005
B10	1.0871
B11	1.0808
B12	1.0862
B13	1.0848
B14	0.9792
A1	115.388
A2	124.0095
A3	118.8655
A4	121.485
A5	122.1194
A6	120.0295
A7	122.3994
A8	109.0476
A9	105.7765
A10	119.1603
A11	120.2046
A12	120.0685
A13	120.5756
A14	110.7291
D1	-55.3481
D2	-43.0639
D3	135.913
D4	-183.1094
D5	183.7625
D6	-0.5704
D7	-182.2197
D8	66.8724
D9	181.2773
D10	2.7996
D11	-182.6398
D12	-1.8541
D13	180.3296
D14	-12.7441

***S. typhimurium* RNR:**

Charge = 0 Multiplicity = 1

N			
C	1	1.45718000	
C	2	1.52340000	1 113.14447000

O	3	1.25840000	2	120.00000000	1	148.28614000
C	2	1.53954000	1	110.54689000	3	-124.01776000
C	5	1.51747000	2	114.13154000	1	-73.45283000
C	6	1.38740000	5	121.14569000	2	-11.03982000
C	6	1.39341000	5	120.51120000	2	169.94552000
C	7	1.40057000	6	121.13940000	5	-179.09421000
C	8	1.39715000	6	120.96731000	5	179.17436000
C	9	1.38482000	7	119.95706000	6	-0.00515000
N	4	3.33356000	3	96.38312000	2	-92.73685000
C	12	1.46238000	4	95.27422000	3	142.95758000
C	13	1.51730000	12	110.10935000	4	65.88928000
O	14	1.23333000	13	120.39896000	12	140.41182000
C	13	1.53964000	12	110.50907000	4	-55.87354000
C	16	1.53850000	13	114.05232000	12	-62.24576000
C	17	1.52646000	16	111.05366000	13	176.42491000
C	17	1.52615000	16	109.09076000	13	-61.79386000
N	14	1.33602000	13	115.77873000	12	-38.84565000
C	20	1.45730000	14	122.29112000	13	-179.08875000
C	21	1.52328000	20	110.97730000	14	-62.97497000
O	22	1.25840000	21	120.00000000	20	139.16073000
C	21	1.55222000	20	112.00585000	14	175.58207000
O	24	1.43000000	21	109.47122000	20	-56.42779000
C	24	1.54000000	21	109.47122000	20	-176.42779000
N	15	3.00576000	14	157.34730000	13	-136.59741000
C	27	1.46905000	15	120.43566000	14	-113.12402000
C	28	1.52202000	27	110.68285000	15	128.52591000
O	29	1.25840000	28	120.00000000	27	141.40577000
C	28	1.53822000	27	112.79233000	15	8.37604000
C	31	1.50498000	28	113.15659000	27	-75.14390000
O	32	1.24837000	31	118.42902000	28	-48.58719000
O	32	1.25085000	31	118.26616000	28	132.87910000
N	32	5.55117000	31	90.14817000	28	-143.24039000
C	35	1.46355000	32	45.59475000	31	-137.61686000
C	36	1.52545000	35	109.93669000	32	76.65338000
O	37	1.23254000	36	121.11468000	35	130.77058000
C	36	1.53408000	35	110.73688000	32	-43.99099000
C	39	1.49313000	36	113.64275000	35	-63.60244000
N	40	1.37677000	39	122.75462000	36	177.84445000
C	40	1.35474000	39	130.97969000	36	-1.37996000
C	41	1.32184000	40	109.33406000	39	-179.32219000
N	43	1.32055000	41	108.33676000	40	-0.03013000
N	37	1.32651000	36	116.14475000	35	-49.66540000
C	45	1.46111000	37	121.24561000	36	-179.86883000
C	46	1.52571000	45	110.60119000	37	-58.15735000
O	47	1.25840000	46	120.00000000	45	133.14872000
C	46	1.54000000	45	109.24315000	37	-178.43222000
N	38	3.16432000	37	110.02485000	36	-97.00508000
C	50	1.45844000	38	98.48714000	37	142.49817000
C	51	1.51670000	50	114.44095000	38	84.18916000
O	52	1.23111000	51	120.15331000	50	145.65565000
C	51	1.52986000	50	110.33497000	38	-38.94218000
O	54	1.40758000	51	110.16008000	50	-65.19995000
N	52	1.32998000	51	117.39158000	50	-34.75496000
C	56	1.45147000	52	119.12823000	51	179.18621000
C	57	1.52470000	56	111.22168000	52	-66.84272000
O	58	1.25840000	57	120.00000000	56	143.42087000
C	57	1.52284000	56	110.39246000	52	168.79975000
C	60	B1	57	A1	56	D1
C	61	B2	60	A2	57	D2
C	61	B3	60	A3	57	D3
C	62	B4	61	A4	60	D4
C	63	B5	61	A5	60	D5
C	65	B6	63	A6	61	D6
O	66	B7	65	A7	63	D7
N	53	3.01563000	52	152.35289000	51	-128.27130000
C	68	1.45435000	53	123.68526000	52	-117.29810000
C	69	1.52728000	68	109.85663000	53	136.63070000
O	70	1.25840000	69	120.00000000	68	131.07980000
C	69	1.54345000	68	110.18592000	53	14.27000000
C	72	1.53736000	69	108.77936000	68	-65.43980000
C	72	1.54000000	69	109.60881000	68	174.73030000
C	73	1.51344000	72	114.70036000	69	169.30770000
N	18	4.42789000	17	109.47571000	16	152.87290000
C	76	1.46555000	18	106.73190000	17	-156.30800000
C	77	1.52815000	76	111.45635000	18	-136.04550000
O	78	1.25840000	77	120.00000000	76	150.82960000
C	77	1.53137000	76	110.31990000	18	102.67220000
C	80	1.51079000	77	114.27589000	76	-69.75790000
C	81	1.39185000	80	120.96474000	77	-19.69010000
C	81	1.39527000	80	120.26522000	77	161.76560000

C	82	1.39074000	81	120.81524000	80	-178.55630000
C	83	1.39407000	81	120.95712000	80	178.66220000
C	84	1.39173000	82	120.14437000	81	-0.02620000
N	75	7.04104000	73	108.18220000	72	158.37860000
C	87	1.45123000	75	60.69012000	73	98.08020000
C	88	1.53245000	87	109.00695000	75	93.94970000
O	89	1.23718000	88	120.46030000	87	131.72750000
C	88	1.53145000	87	109.60188000	75	-28.13200000
C	91	1.53024000	88	118.01305000	87	-175.33700000
C	92	1.52274000	91	109.70867000	88	162.06380000
C	92	1.52898000	91	109.79050000	88	-74.61300000
N	89	1.33635000	88	116.57312000	87	-47.35240000
C	95	1.46185000	89	121.63556000	88	179.40580000
C	96	1.52887000	95	110.19796000	89	-55.31420000
O	97	1.25840000	96	120.00000000	95	141.06210000
C	96	1.55956000	95	111.63651000	89	-176.11420000
C	99	1.52874000	96	110.18610000	95	-60.04340000
C	99	1.52814000	96	110.23161000	95	178.15320000
C	100	1.51420000	99	113.96680000	96	-59.07850000
N	90	3.02799000	89	158.43642000	88	-157.25940000
C	103	1.46224000	90	127.34542000	89	-82.15240000
C	104	1.53684000	103	108.45503000	90	134.43010000
O	105	1.25840000	104	120.00000000	103	130.29170000
C	104	1.55455000	103	110.91929000	90	13.64790000
C	107	1.53690000	104	109.34176000	103	-68.16500000
C	107	1.54000000	104	109.49709000	103	171.86670000
C	108	1.52595000	107	114.72853000	104	-176.97390000
H	95	1.00180000	89	121.26780000	88	-11.87730000
H	45	1.00010000	37	120.27210000	36	13.86010000
H	20	1.01390000	14	119.31250000	13	-16.52260000
H	56	1.00170000	52	121.45490000	51	-18.69610000
H	35	0.99850000	32	151.94450000	31	-105.24870000
H	35	1.00000000	32	94.23250000	31	106.86130000
H	103	1.00180000	90	58.48320000	89	10.57310000
H	103	0.99910000	90	51.39450000	89	-168.03490000
H	27	0.99770000	15	55.98800000	14	152.77310000
H	27	0.99800000	15	54.57010000	14	-17.85010000
H	12	1.00460000	4	93.96140000	3	33.74570000
H	12	0.99820000	4	137.10320000	3	-90.34250000
H	1	0.99800000	2	110.24010000	3	-53.52780000
H	1	0.99860000	2	111.26570000	3	68.53540000
H	87	0.99890000	75	162.19400000	73	159.35580000
H	87	0.99950000	75	88.70980000	73	-16.22240000
H	76	0.99960000	18	137.00450000	17	-7.54110000
H	76	1.00030000	18	35.49550000	17	-55.90860000
H	55	0.94930000	54	107.51240000	51	-62.21070000
H	50	1.00020000	38	13.73400000	37	-48.33690000
H	50	0.99880000	38	119.54580000	37	-97.56530000
H	68	1.00900000	53	12.77690000	52	-139.11330000
H	68	0.99760000	53	106.23020000	52	115.14510000
H	70	1.09850000	69	119.34220000	68	-48.83900000
H	97	1.09850000	96	119.73590000	95	-39.99400000
H	78	1.09830000	77	119.63070000	76	-29.56850000
H	105	1.09840000	104	119.45030000	103	-49.53300000
H	58	1.09840000	57	119.61770000	56	-36.72030000
H	29	1.09920000	28	119.60880000	27	-38.65350000
H	34	0.95840000	32	114.12190000	31	-178.34560000
H	47	1.10040000	46	119.33440000	45	-49.73210000
H	46	1.12450000	45	108.34180000	37	62.73030000
H	49	1.10000000	46	111.47270000	45	-57.35680000
H	49	1.09830000	46	112.33780000	45	64.00100000
H	49	1.09890000	46	110.05020000	45	-176.05680000
H	36	1.12690000	35	111.48120000	32	-163.92080000
H	39	1.11220000	36	110.86540000	35	59.62430000
H	39	1.11270000	36	108.46690000	35	175.54740000
H	43	1.09680000	41	127.68890000	40	-178.38360000
H	42	1.09020000	40	131.97300000	39	-3.51450000
H	41	0.98990000	40	123.77850000	39	0.64430000
H	54	1.11900000	51	112.22900000	50	172.05950000
H	54	1.10700000	51	114.45880000	50	50.29750000
H	51	1.12270000	50	105.38380000	38	-157.45470000
H	57	1.13180000	56	108.36890000	52	51.04900000
H	60	B8	57	A8	56	D8
H	60	B9	57	A9	56	D9
H	63	B10	61	A10	60	D10
H	65	B11	63	A11	61	D11
H	64	B12	62	A12	61	D12
H	62	B13	61	A13	60	D13
H	3	1.09960000	2	120.31470000	1	-31.57160000
H	2	1.12950000	1	105.53010000	5	-117.12950000

H	5	1.10900000	2	110.92870000	1	50.04220000
H	5	1.11150000	2	109.02540000	1	166.54160000
H	8	1.09660000	6	119.76040000	5	-0.66710000
H	10	1.09640000	8	119.56840000	6	-179.41430000
H	11	1.09510000	9	120.29490000	7	-179.98770000
H	9	1.09510000	7	119.57690000	6	179.70110000
H	7	1.10770000	6	120.78370000	5	-2.43680000
H	69	1.12520000	68	110.76900000	53	-104.22020000
H	72	1.11770000	69	110.38920000	68	54.69900000
H	74	1.09980000	72	110.99300000	69	178.01430000
H	74	1.09770000	72	111.30220000	69	-62.53180000
H	74	1.09770000	72	111.63370000	69	57.87200000
H	75	1.09970000	73	111.03860000	72	-176.73740000
H	75	1.10080000	73	111.54130000	72	-56.98860000
H	75	1.09920000	73	112.10890000	72	62.97660000
H	73	1.10970000	72	109.26890000	69	-67.79090000
H	73	1.11220000	72	109.62950000	69	47.34630000
H	86	1.09600000	84	120.09670000	82	179.01740000
H	84	1.09710000	82	119.64070000	81	179.66600000
H	85	1.09460000	83	120.10420000	81	-179.68960000
H	83	1.09620000	81	119.52850000	80	-1.13690000
H	82	1.10230000	81	119.85840000	80	-0.97870000
H	80	1.11030000	77	110.80910000	76	54.34030000
H	80	1.11000000	77	109.44520000	76	170.28640000
H	77	1.12510000	76	106.81130000	18	-16.04150000
H	28	1.12120000	27	106.95410000	15	-112.44500000
H	31	1.11180000	28	109.46260000	27	166.13860000
H	31	1.11440000	28	110.24680000	27	50.52810000
H	19	1.09870000	17	111.31760000	16	-72.21940000
H	19	1.10270000	17	110.88590000	16	47.08190000
H	19	1.09690000	17	111.58510000	16	167.71300000
H	18	1.09900000	17	110.65950000	16	172.25340000
H	18	1.10590000	17	111.67770000	16	-68.43160000
H	18	1.09930000	17	111.91610000	16	52.79090000
H	17	1.12170000	16	108.26880000	13	56.62310000
H	16	1.11150000	13	110.62920000	12	60.38350000
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H	21	1.12770000	20	108.21340000	14	56.70040000
H	24	1.11800000	21	110.09820000	20	63.52090000
H	25	0.95400000	24	106.79830000	21	78.17940000
H	26	1.09980000	24	111.87800000	21	52.61790000
H	26	1.09750000	24	110.77360000	21	172.21460000
H	26	1.09670000	24	110.83700000	21	-68.12870000
H	22	1.09850000	21	119.75930000	20	-41.55480000
H	93	1.10020000	92	111.86030000	91	58.16250000
H	93	1.10110000	92	110.81930000	91	177.44070000
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H	94	1.09980000	92	113.08070000	91	81.57450000
H	94	1.10910000	92	109.81800000	91	-159.97810000
H	94	1.09970000	92	112.51580000	91	-41.49980000
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H	91	1.11380000	88	107.64010000	87	-54.05240000
H	91	1.11250000	88	110.12070000	87	59.29850000
H	88	1.12570000	87	112.21860000	75	-147.38960000
H	96	1.12740000	95	108.71830000	89	63.86880000
H	102	1.10450000	100	110.50070000	99	-42.48550000
H	102	1.10050000	100	112.59180000	99	77.30800000
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H	100	1.11210000	99	109.38590000	96	64.22480000
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H	101	1.09630000	99	112.73190000	96	-57.20280000
H	101	1.10450000	99	110.70810000	96	64.37150000
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H	99	1.11770000	96	108.86740000	95	59.04890000
H	104	1.11980000	103	108.14210000	90	-106.70740000
H	107	1.11640000	104	111.16050000	103	52.21330000
H	109	1.09810000	107	111.31620000	104	-74.63120000
H	109	1.09620000	107	111.48110000	104	45.77450000
H	109	1.10280000	107	110.59520000	104	165.61070000
H	110	1.10020000	108	111.35420000	107	-69.95370000
H	110	1.10270000	108	111.08870000	107	49.70450000
H	110	1.09900000	108	111.02020000	107	170.12230000
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H	67	B14	66	A14	65	D14

Variables:

B1	1.5175
B2	1.4024
B3	1.3966

B4	1.3916
B5	1.3956
B6	1.3948
B7	1.3819
B8	1.0963
B9	1.0937
B10	1.0844
B11	1.0851
B12	1.0839
B13	1.0867
B14	0.9698
A1	109.2683
A2	120.168
A3	121.5161
A4	121.6805
A5	121.0627
A6	119.9804
A7	122.3637
A8	107.8385
A9	111.4023
A10	119.4646
A11	119.3701
A12	120.9999
A13	119.806
A14	108.5603
D1	-68.3457
D2	-70.8683
D3	101.9965
D4	172.4201
D5	-171.581
D6	-0.4702
D7	-180.8152
D8	171.4932
D9	54.3772
D10	6.6046
D11	177.8836
D12	-178.8006
D13	-4.9915
D14	-33.0764