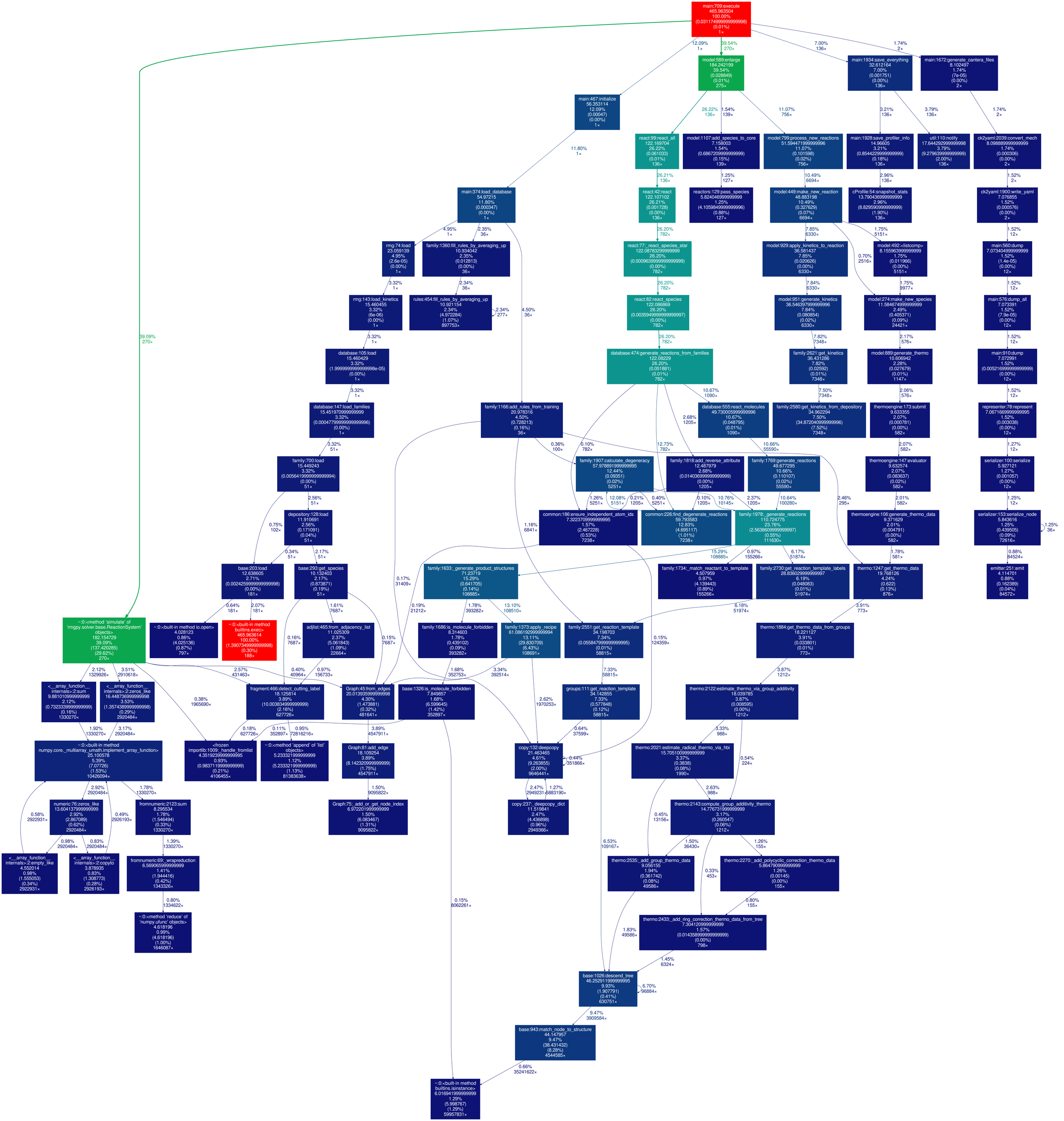
main:709:execute
465.963504
100.00%
(0.0311749999999999998)
(0.01%)
1×
12.09%
1×
39.54%
270×
7.00%
136×
1.74%
2×
model:589:enlarge
184.242199
39.54%
(0.028849)
(0.01%)
275×
main:1934:save_everything
32.612164
7.00%
(0.001751)
(0.00%)
136×
main:1672:generate_cantera_files
8.102497
1.74%
(7e-05)
(0.00%)
2×
main:467:initialize
56.353114
12.09%
(0.00047)
(0.00%)
1×
26.22%
136×
1.54%
139×
11.07%
756×
3.21%
136×
3.79%
136×
1.74%
2×
11.80%
1×
react:99:react_all
122.169704
26.22%
(0.061033)
(0.01%)
136×
model:1107:add_species_to_core
7.158003
1.54%
(0.0867209999999999)
(0.15%)
139×
model:799:process_new_reactions
51.594471999999996
11.07%
(0.101598)
(0.02%)
756×
main:1928:save_profiler_info
14.96605
3.21%
(0.8544229999999999)
(0.18%)
136×
util:110:notify
17.644292999999998
3.79%
(9.279639999999999)
(2.00%)
136×
ck2yaml:2039:convert_mech
8.098889999999999
1.74%
(0.000306)
(0.00%)
2×
26.21%
136×
1.25%
127×
10.49%
6694×
2.96%
136×
1.52%
2×
main:374:load_database
54.97215
11.80%
(0.000347)
(0.00%)
1×
react:42:react
122.107102
26.21%
(0.001728)
(0.00%)
136×
reactors:129:pass_species
5.824046999999999
1.25%
(4.105984999999996)
(0.88%)
127×
model:449:make_new_reaction
48.883198
10.49%
(0.327629)
(0.07%)
6694×
cProfile:54:snapshot_stats
13.790436999999999
2.96%
(8.829590999999999)
(1.90%)
136×
ck2yaml:1900:write_yaml
7.076855
1.52%
(0.000576)
(0.00%)
2×
4.95%
1×
2.35%
36×
26.20%
782×
7.85%
6330×
1.75%
5151×
1.52%
12×
rmg:74:load
23.059139
4.95%
(2.6e-05)
(0.00%)
1×
family:1360:fill_rules_by_averaging_up
10.934042
2.35%
(0.012813)
(0.00%)
36×
react:77:_react_species_star
122.087832999999999
26.20%
(0.0009639999999999999)
(0.00%)
782×
model:929:apply_kinetics_to_reaction
36.581437
7.85%
(0.020626)
(0.00%)
6330×
0.70%
2516×
model:492:<listcomp>
8.155963999999999
1.75%
(0.011966)
(0.00%)
5151×
main:560:dump
7.073404999999999
1.52%
(1.4e-05)
(0.00%)
12×
3.32%
1×
2.34%
36×
26.20%
782×
7.84%
6330×
1.75%
9977×
1.52%
12×
rmg:143:load_kinetics
15.460455
3.32%
(6e-06)
(0.00%)
1×
rules:454:fill_rules_by_averaging_up
10.921154
2.34%
(4.972284)
(1.07%)
897753×
2.34%
277×
4.50%
36×
react:82:react_species
122.086869
26.20%
(0.0035949999999999997)
(0.00%)
782×
model:951:generate_kinetics
36.546397999999996
7.84%
(0.080854)
(0.02%)
6330×
model:274:make_new_species
11.584674999999999
2.49%
(0.405371)
(0.09%)
24421×
main:576:dump_all
7.073391
1.52%
(7.9e-05)
(0.00%)
12×
39.09%
270×
3.32%
1×
26.20%
782×
7.82%
7348×
2.17%
576×
1.52%
12×
database:105:load
15.460429
3.32%
(1.9999999999999998e-05)
(0.00%)
1×
database:474:generate_reactions_from_families
122.08229
26.20%
(0.051881)
(0.01%)
782×
family:2621:get_kinetics
36.431286
7.82%
(0.02592)
(0.01%)
7348×
model:889:generate_thermo
10.606942
2.28%
(0.027679)
(0.01%)
1147×
main:910:dump
7.072991
1.52%
(0.00521699999999999)
(0.00%)
12×
3.32%
1×
10.67%
1090×
7.50%
7348×
2.06%
576×
1.52%
12×
database:147:load_families
15.451970999999999
3.32%
(0.0004779999999999996)
(0.00%)
1×
family:1166:add_rules_from_training
20.978316
4.50%
(0.728213)
(0.16%)
36×
database:555:react_molecules
49.730005999999996
10.67%
(0.048795)
(0.01%)
1090×
family:2580:get_kinetics_from_depository
34.962294
7.50%
(34.872040999999996)
(7.52%)
7348×
thermoengine:173:submit
9.633355
2.07%
(0.000781)
(0.00%)
582×
representer:78:represent
7.067166999999995
1.52%
(0.003038)
(0.00%)
12×
2.68%
1205×
3.32%
51×
0.36%
100×
0.10%
782×
12.73%
782×
10.66%
55590×
2.07%
582×
1.27%
12×
family:700:load
15.449243
3.32%
(0.00564199999999999994)
(0.00%)
51×
family:1907:calculate_degeneracy
57.978891999999995
12.44%
(0.09351)
(0.02%)
5251×
family:1818:add_reverse_attribute
12.487979
2.68%
(0.0140369999999999999)
(0.00%)
1205×
family:1769:generate_reactions
49.677295
10.66%
(0.110107)
(0.02%)
55590×
thermoengine:147:evaluator
9.632574
2.07%
(0.083637)
(0.02%)
582×
serializer:100:serialize
5.927121
1.27%
(0.001057)
(0.00%)
12×
2.46%
295×
2.56%
51×
1.26%
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12.08%
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10.76%
10145×
2.37%
1205×
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100280×
2.01%
582×
1.25%
12×
depository:128:load
11.910691
2.56%
(0.171091)
(0.04%)
51×
common:186:ensure_independent_atom_ids
7.3223709999999995
1.57%
(2.467228)
(0.53%)
7238×
common:226:find_degenerate_reactions
59.793583
12.83%
(4.695117)
(1.01%)
7238×
family:1978:_generate_reactions
110.724775
23.76%
(2.5638609999999997)
(0.55%)
111630×
thermoengine:106:generate_thermo_data
9.371629
2.01%
(0.004791)
(0.00%)
582×
serializer:153:serialize_node
5.843616
1.25%
(0.439505)
(0.09%)
72616×
1.25%
36×
0.75%
102×
1.16%
6841×
1.78%
581×
0.88%
84524×
0.34%
51×
2.17%
51×
15.29%
108885×
0.97%
155266×
6.17%
51874×
base:203:load
12.638605
2.71%
(0.00242599999999999998)
(0.00%)
181×
base:293:get_species
10.132403
2.17%
(0.873871)
(0.19%)
51×
family:1633:_generate_product_structures
71.23719
15.29%
(0.641705)
(0.14%)
108885×
family:1734:_match_reactant_to_template
4.507959
0.97%
(4.139443)
(0.89%)
155266×
family:2730:get_reaction_template_labels
28.836029999999997
6.19%
(0.048083)
(0.01%)
51974×
thermo:1247:get_thermo_data
19.768126
4.24%
(0.622)
(0.13%)
876×
emitter:251:emit
4.114701
0.88%
(0.162389)
(0.04%)
84572×
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7687×
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21212×
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393282×
13.10%
108510×
6.18%
51974×
3.91%
773×
~:0:<method 'simulate' of 'rmgpy.solver.base.ReactionSystem' objects>
182.154729
39.09%
(137.420285)
(29.62%)
270×
~:0:<built-in method io.open>
4.028123
0.86%
(4.025136)
(0.87%)
797×
~:0:<built-in method builtins.exec>
465.963614
100.00%
(1.3907349999999998)
(0.30%)
188×
adjlist:465:from_adjacency_list
11.025309
2.37%
(5.061843)
(1.09%)
22664×
family:1686:is_molecule_forbidden
8.314603
1.78%
(0.439102)
(0.09%)
393282×
family:1373:apply_recipe
61.086192999999994
13.11%
(29.830709)
(6.43%)
108691×
family:2551:get_reaction_template
34.198703
7.34%
(0.0558479999999999995)
(0.01%)
58815×
0.15%
124359×
thermo:1884:get_thermo_data_from_groups
18.221127
3.91%
(0.033801)
(0.01%)
773×
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7687×
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1329926×
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352753×
3.34%
392514×
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58815×
3.87%
1212×
<__array_function__ internals>:2:sum
9.881010999999999
2.12%
(0.732333999999999)
(0.16%)
1330270×
<__array_function__ internals>:2:zeros_like
16.448736999999998
3.53%
(1.357438999999999)
(0.29%)
2920484×
0.38%
1965690×
fragment:466:detect_cutting_label
18.125814
3.89%
(10.003834999999999)
(2.16%)
627726×
Graph:45:from_edges
20.013935999999998
4.30%
(1.473881)
(0.32%)
481641×
base:1326:is_molecule_forbidden
7.849857
1.68%
(6.599645)
(1.42%)
352897×
groups:111:get_reaction_template
34.142855
7.33%
(0.577848)
(0.12%)
58815×
2.62%
1970253×
thermo:2122:estimate_thermo_via_group_additivity
18.039785
3.87%
(0.008595)
(0.00%)
1212×
1.92%
1330270×
3.17%
2920484×
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352897×
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72816216×
3.89%
4547911×
0.64%
37599×
3.33%
988×
~:0:<built-in method numpy.core._multiarray_umath.implement_array_function>
25.100578
5.39%
(7.07726)
(1.53%)
10426094×
<frozen importlib:1009:_handle_fromlist
4.351923999999995
0.93%
(0.983711999999999)
(0.21%)
4106455×
~:0:<method 'append' of 'list' objects>
5.233321999999999
1.12%
(5.233321999999999)
(1.13%)
81383638×
Graph:81:add_edge
18.109254
3.89%
(8.142320999999999)
(1.75%)
4547911×
copy:132:deepcopy
21.463465
4.61%
(9.263855)
(2.00%)
9646441×
0.44%
351866×
thermo:2021:estimate_radical_thermo_via_hbi
15.705100999999999
3.37%
(0.3838)
(0.08%)
1990×
0.54%
224×
2.92%
2920484×
1.78%
1330270×
1.50%
9095822×
2.47%
2949231×
1.27%
5883190×
2.63%
988×
numeric:76:zeros_like
13.604137999999999
2.92%
(2.867089)
(0.62%)
2920484×
fromnumeric:2123:sum
8.295534
1.78%
(1.546494)
(0.33%)
1330270×
Graph:75:_add_or_get_node_index
6.972201999999999
1.50%
(6.083467)
(1.31%)
9095822×
copy:237:_deepcopy_dict
11.519841
2.47%
(4.436898)
(0.96%)
2949366×
thermo:2143:compute_group_additivity_thermo
14.776731999999999
3.17%
(0.260547)
(0.06%)
1212×
0.58%
2922931×
0.49%
2926193×
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109167×
1.50%
36430×
1.26%
155×
0.98%
2920484×
0.83%
2920484×
1.39%
1330270×
thermo:2535:_add_group_thermo_data
9.056155
1.94%
(0.361742)
(0.08%)
49586×
0.33%
453×
thermo:2270:_add_polycyclic_correction_thermo_data
5.864790999999999
1.26%
(0.00145)
(0.00%)
155×
<__array_function__ internals>:2:empty_like
4.552014
0.98%
(1.555053)
(0.34%)
2922931×
<__array_function__ internals>:2:copyto
3.878935
0.83%
(1.308773)
(0.28%)
2926193×
fromnumeric:69:_wrapreduction
6.569065999999999
1.41%
(1.944416)
(0.42%)
1343326×
0.80%
155×
thermo:2433:_add_ring_correction_thermo_data_from_tree
7.304120999999999
1.57%
(0.0143589999999999999)
(0.00%)
798×
0.15%
8062261×
0.80%
1334622×
~:0:<method 'reduce' of 'numpy.ufunc' objects>
4.618196
0.99%
(4.618196)
(1.00%)
1646087×
1.83%
49586×
1.45%
6324×
base:1026:descend_tree
46.252911999999995
9.93%
(1.907791)
(0.41%)
630751×
6.70%
96884×
9.47%
3909584×
base:943:match_node_to_structure
44.147957
9.47%
(38.431432)
(8.28%)
4544585×
0.66%
35241622×
~:0:<built-in method builtins.isinstance>
6.016941999999999
1.29%
(5.998767)
(1.29%)
59957831×