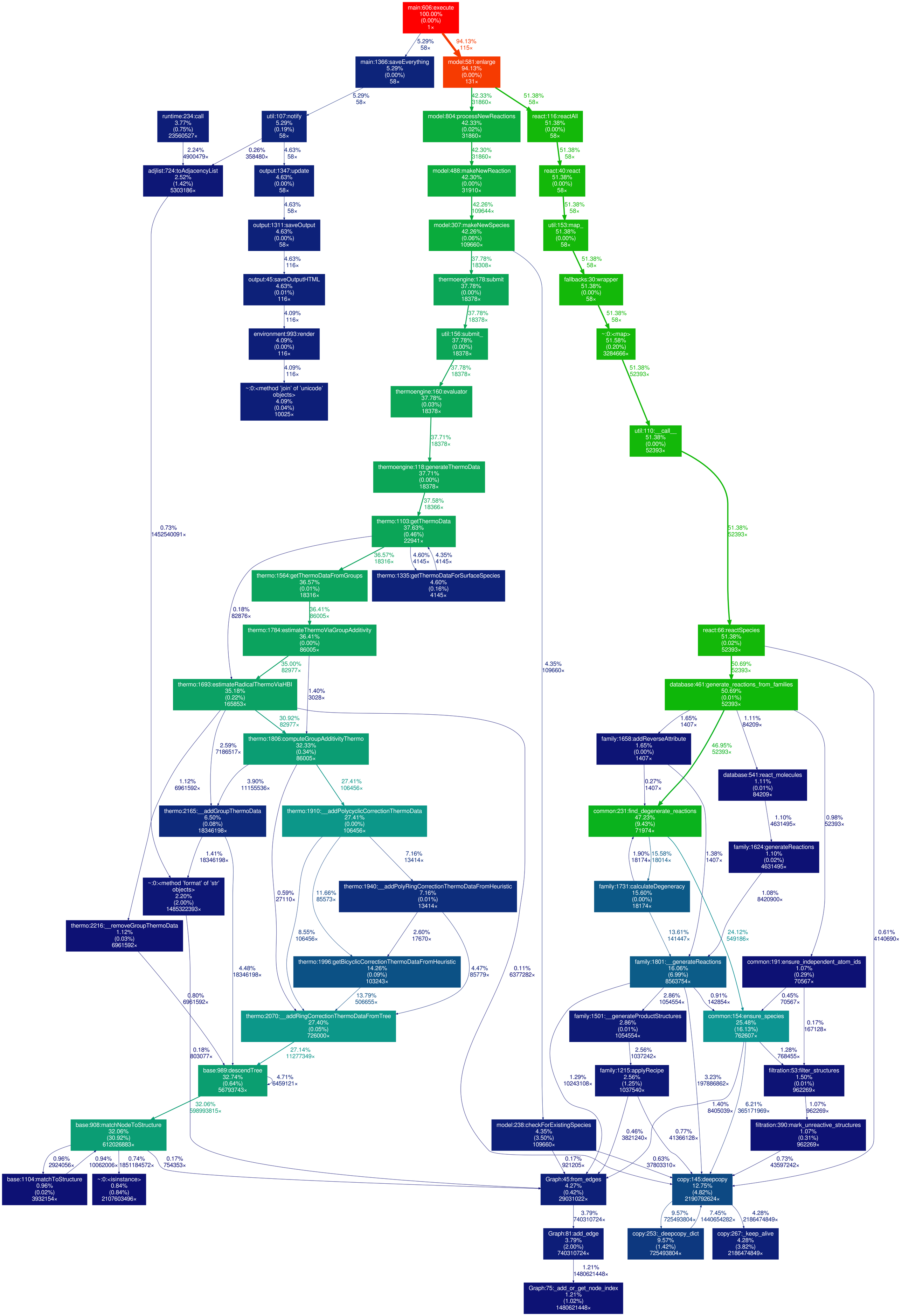
main:606:execute
100.00%
(0.00%)
1×
5.29%
58×
94.13%
115×
main:1366:saveEverything
5.29%
(0.00%)
58×
model:581:enlarge
94.13%
(0.00%)
131×
5.29%
58×
42.33%
31860×
51.38%
58×
runtime:234:call
3.77%
(0.75%)
23560527×
util:107:notify
5.29%
(0.19%)
58×
model:804:processNewReactions
42.33%
(0.02%)
31860×
react:116:reactAll
51.38%
(0.00%)
58×
2.24%
4900479×
0.26%
358480×
4.63%
58×
42.30%
31860×
51.38%
58×
adjlist:724:toAdjacencyList
2.52%
(1.42%)
5303186×
output:1347:update
4.63%
(0.00%)
58×
model:488:makeNewReaction
42.30%
(0.00%)
31910×
react:40:react
51.38%
(0.00%)
58×
4.63%
58×
42.26%
109644×
51.38%
58×
output:1311:saveOutput
4.63%
(0.00%)
58×
model:307:makeNewSpecies
42.26%
(0.06%)
109660×
util:153:map_
51.38%
(0.00%)
58×
4.63%
116×
37.78%
18308×
51.38%
58×
output:45:saveOutputHTML
4.63%
(0.01%)
116×
thermoengine:178:submit
37.78%
(0.00%)
18378×
fallbacks:30:wrapper
51.38%
(0.00%)
58×
4.09%
116×
37.78%
18378×
51.38%
58×
environment:993:render
4.09%
(0.00%)
116×
util:156:submit_
37.78%
(0.00%)
18378×
~:0:<map>
51.58%
(0.20%)
3284666×
4.09%
116×
37.78%
18378×
51.38%
52393×
~:0:<method 'join' of 'unicode' objects>
4.09%
(0.04%)
10025×
thermoengine:160:evaluator
37.78%
(0.03%)
18378×
util:110:__call__
51.38%
(0.00%)
52393×
37.71%
18378×
thermoengine:118:generateThermoData
37.71%
(0.00%)
18378×
37.58%
18366×
0.73%
1452540091×
thermo:1103:getThermoData
37.63%
(0.46%)
22941×
51.38%
52393×
36.57%
18316×
4.60%
4145×
4.35%
4145×
thermo:1564:getThermoDataFromGroups
36.57%
(0.01%)
18316×
thermo:1335:getThermoDataForSurfaceSpecies
4.60%
(0.16%)
4145×
0.18%
82876×
36.41%
86005×
thermo:1784:estimateThermoViaGroupAdditivity
36.41%
(0.00%)
86005×
4.35%
109660×
35.00%
82977×
1.40%
3028×
thermo:1693:estimateRadicalThermoViaHBI
35.18%
(0.22%)
165853×
50.69%
52393×
database:461:generate_reactions_from_families
50.69%
(0.01%)
52393×
30.92%
82977×
1.65%
1407×
1.11%
84209×
thermo:1806:computeGroupAdditivityThermo
32.33%
(0.34%)
86005×
family:1658:addReverseAttribute
1.65%
(0.00%)
1407×
46.95%
52393×
2.59%
7186517×
database:541:react_molecules
1.11%
(0.01%)
84209×
1.12%
6961592×
3.90%
11155536×
27.41%
106456×
0.27%
1407×
thermo:2165:__addGroupThermoData
6.50%
(0.08%)
18346198×
thermo:1910:__addPolycyclicCorrectionThermoData
27.41%
(0.00%)
106456×
common:231:find_degenerate_reactions
47.23%
(9.43%)
71974×
1.10%
4631495×
0.98%
52393×
1.41%
18346198×
7.16%
13414×
1.90%
18174×
15.58%
18014×
1.38%
1407×
family:1624:generateReactions
1.10%
(0.02%)
4631495×
~:0:<method 'format' of 'str' objects>
2.20%
(2.00%)
1485322393×
0.59%
27110×
11.66%
85573×
thermo:1940:__addPolyRingCorrectionThermoDataFromHeuristic
7.16%
(0.01%)
13414×
family:1731:calculateDegeneracy
15.60%
(0.00%)
18174×
1.08%
8420900×
thermo:2216:__removeGroupThermoData
1.12%
(0.03%)
6961592×
8.55%
106456×
2.60%
17670×
13.61%
141447×
24.12%
549186×
0.61%
4140690×
thermo:1996:getBicyclicCorrectionThermoDataFromHeuristic
14.26%
(0.09%)
103243×
4.48%
18346198×
4.47%
85779×
0.11%
6377282×
family:1801:__generateReactions
16.06%
(6.99%)
8563754×
common:191:ensure_independent_atom_ids
1.07%
(0.29%)
70567×
0.80%
6961592×
13.79%
506655×
2.86%
1054554×
0.91%
142854×
0.45%
70567×
thermo:2070:__addRingCorrectionThermoDataFromTree
27.40%
(0.05%)
726000×
family:1501:__generateProductStructures
2.86%
(0.01%)
1054554×
common:154:ensure_species
25.48%
(16.13%)
762607×
0.17%
167128×
0.18%
803077×
27.14%
11277349×
2.56%
1037242×
1.28%
768455×
base:989:descendTree
32.74%
(0.64%)
56793743×
4.71%
6459121×
family:1215:applyRecipe
2.56%
(1.25%)
1037540×
1.29%
10243108×
3.23%
197886862×
filtration:53:filter_structures
1.50%
(0.01%)
962269×
32.06%
598993815×
1.40%
8405039×
6.21%
365171969×
1.07%
962269×
base:908:matchNodeToStructure
32.06%
(30.92%)
612026883×
model:238:checkForExistingSpecies
4.35%
(3.50%)
109660×
0.46%
3821240×
0.77%
41366128×
filtration:390:mark_unreactive_structures
1.07%
(0.31%)
962269×
0.96%
2924056×
0.94%
10062006×
0.74%
1851184572×
0.17%
754353×
0.17%
921205×
0.63%
37803310×
0.73%
43597242×
base:1104:matchToStructure
0.96%
(0.02%)
3932154×
~:0:<isinstance>
0.84%
(0.84%)
2107603496×
Graph:45:from_edges
4.27%
(0.42%)
29031022×
copy:145:deepcopy
12.75%
(4.82%)
2190792624×
3.79%
740310724×
9.57%
725493804×
7.45%
1440654282×
4.28%
2186474849×
Graph:81:add_edge
3.79%
(2.00%)
740310724×
copy:253:_deepcopy_dict
9.57%
(1.42%)
725493804×
copy:267:_keep_alive
4.28%
(3.82%)
2186474849×
1.21%
1480621448×
Graph:75:_add_or_get_node_index
1.21%
(1.02%)
1480621448×