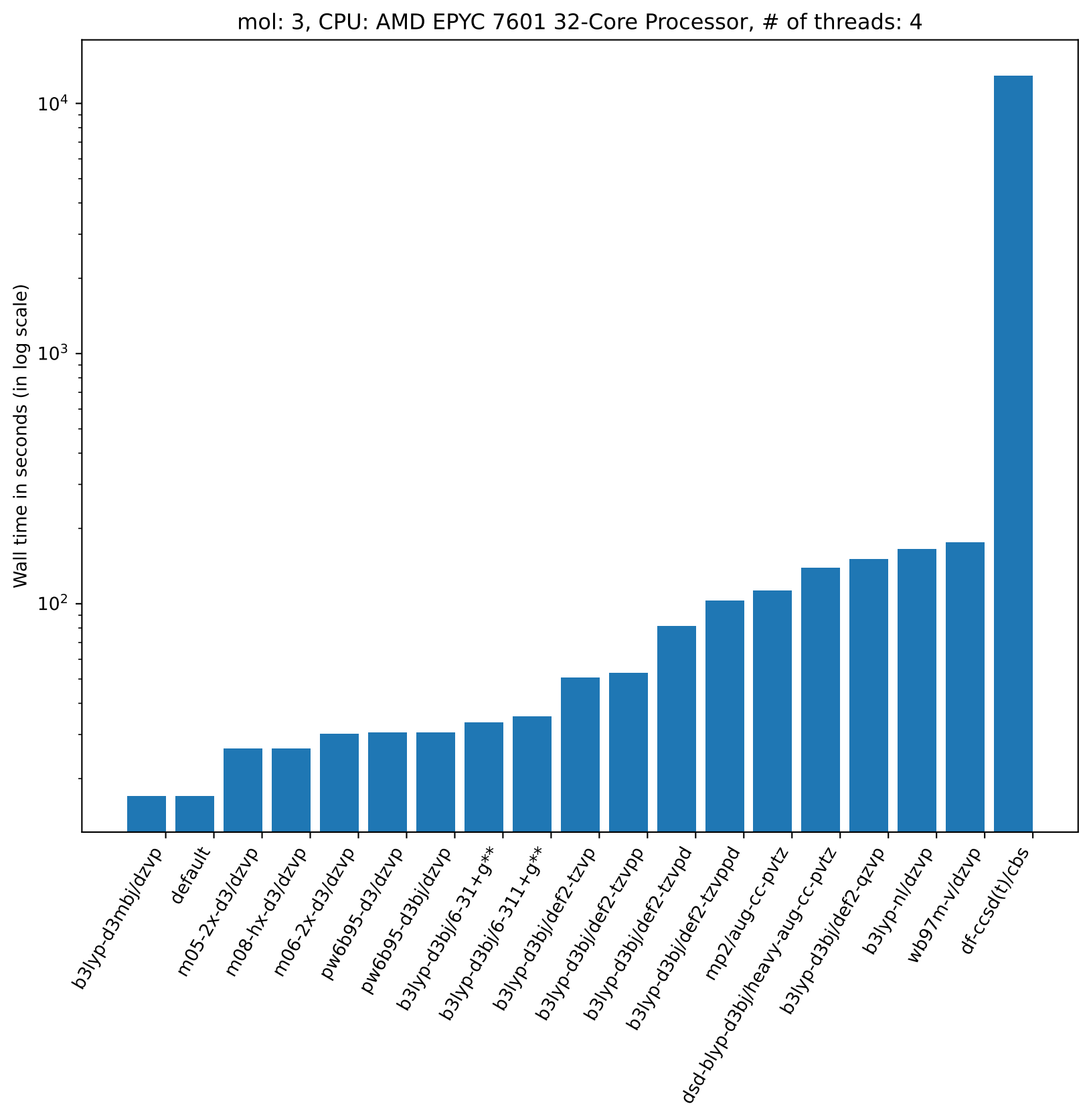
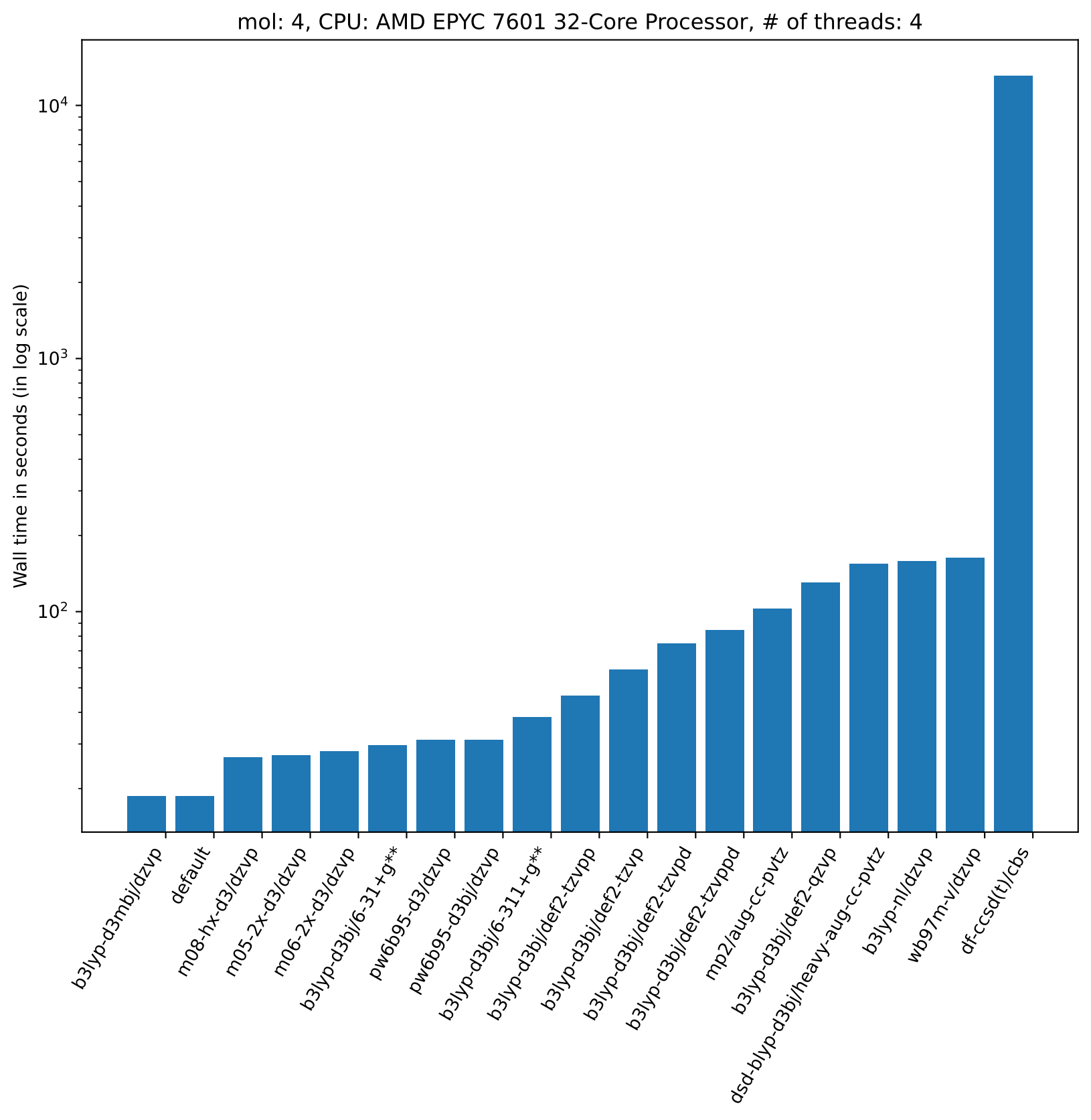
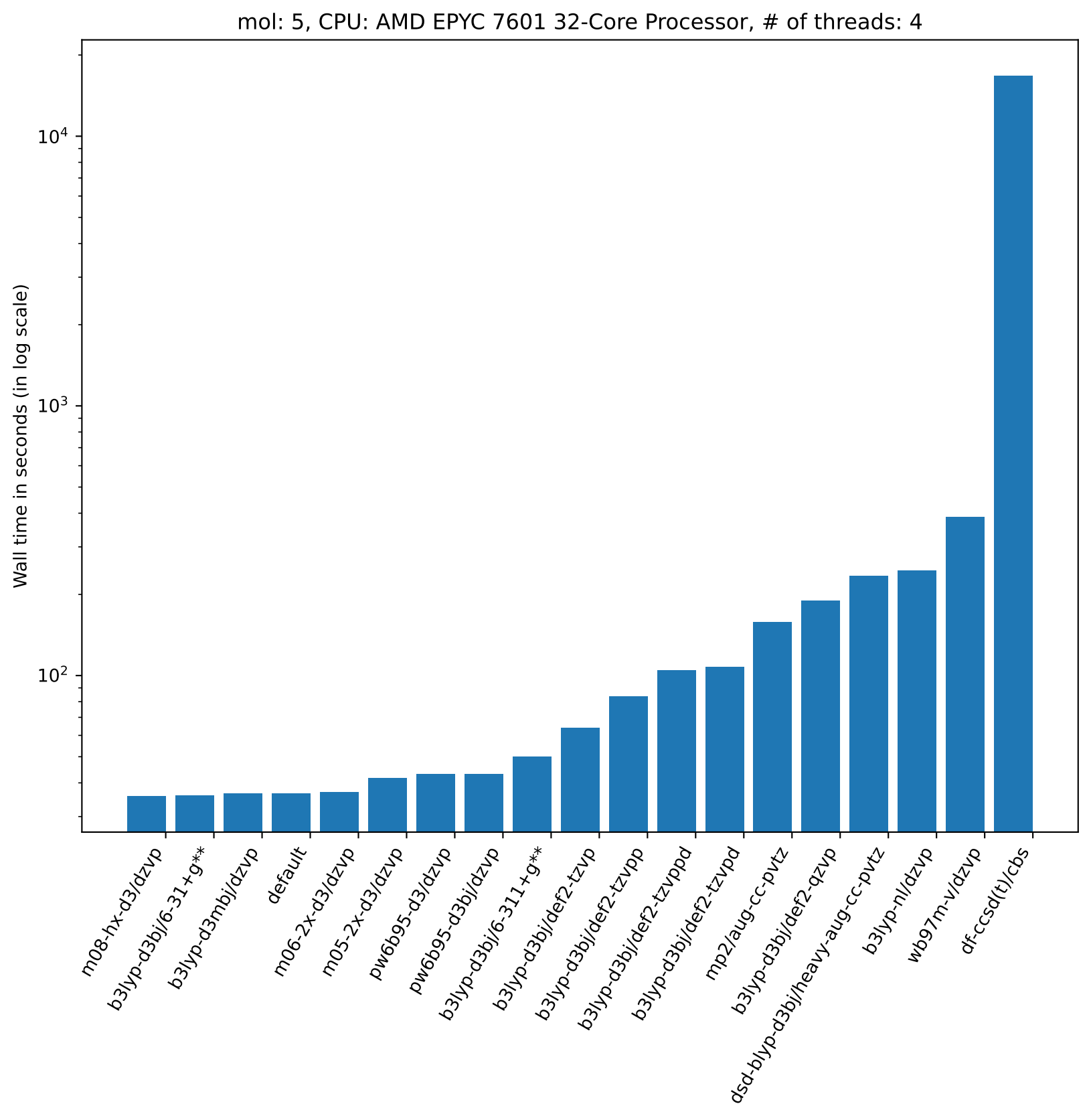
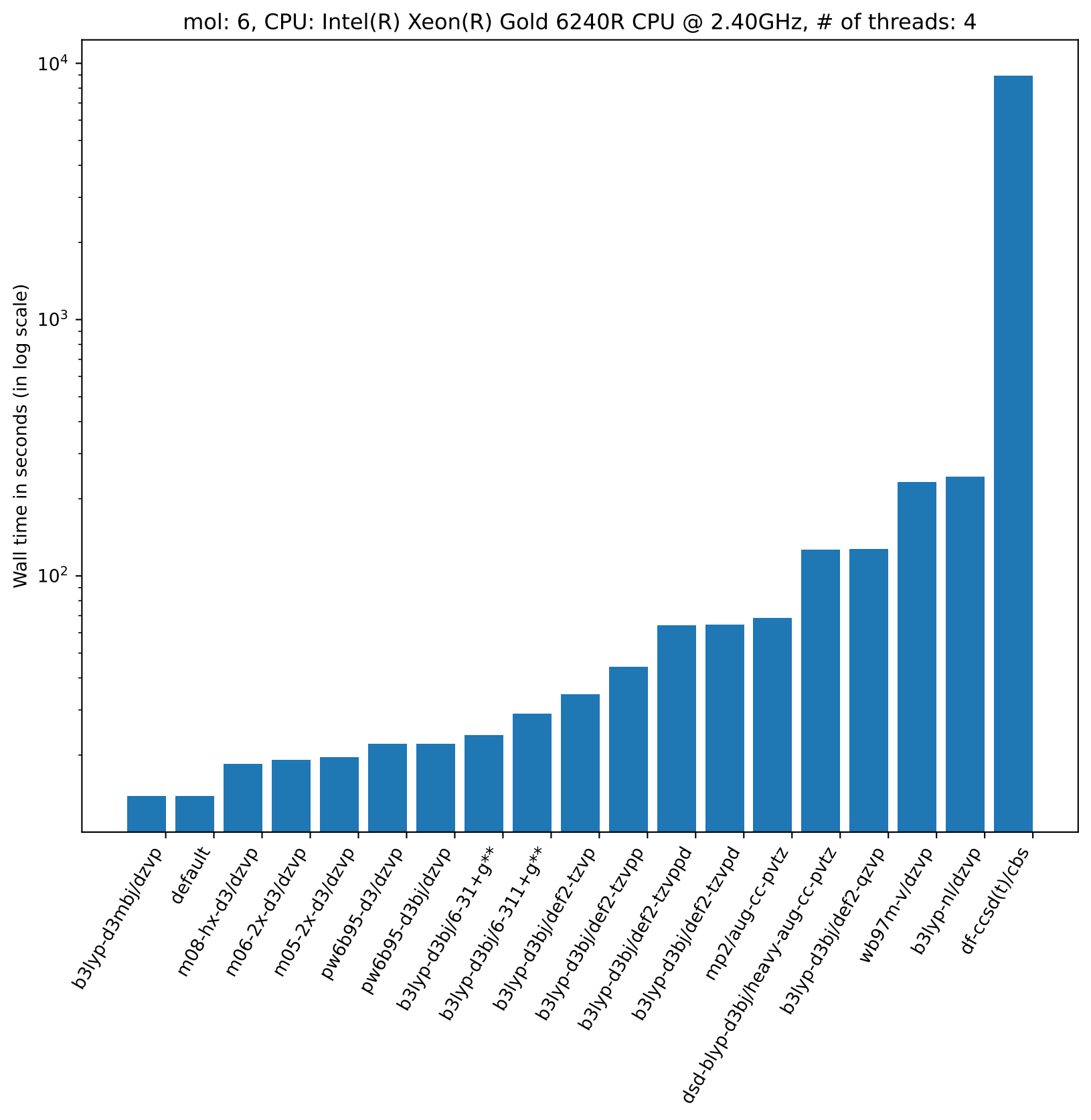
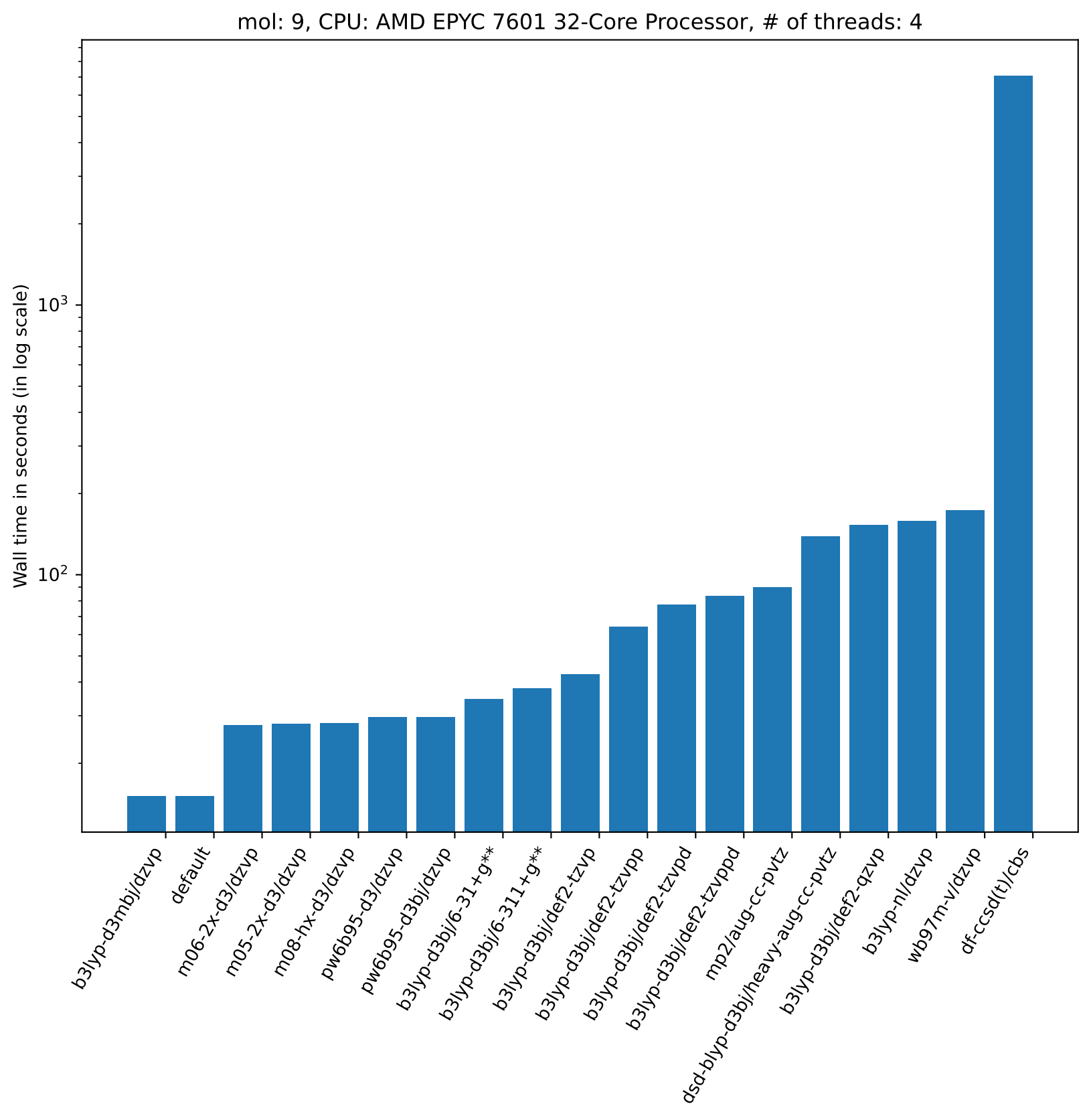
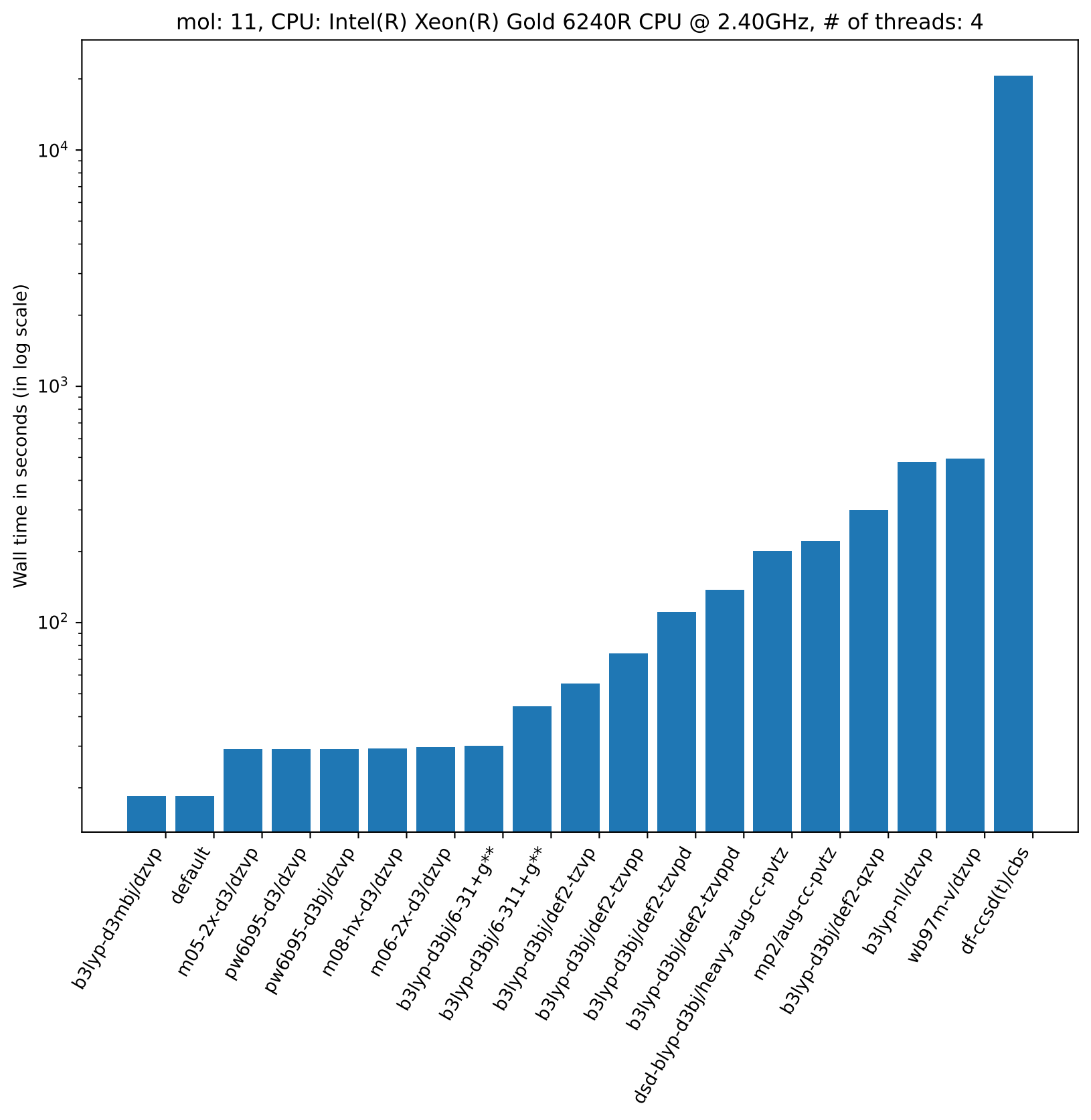

mol: 3, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

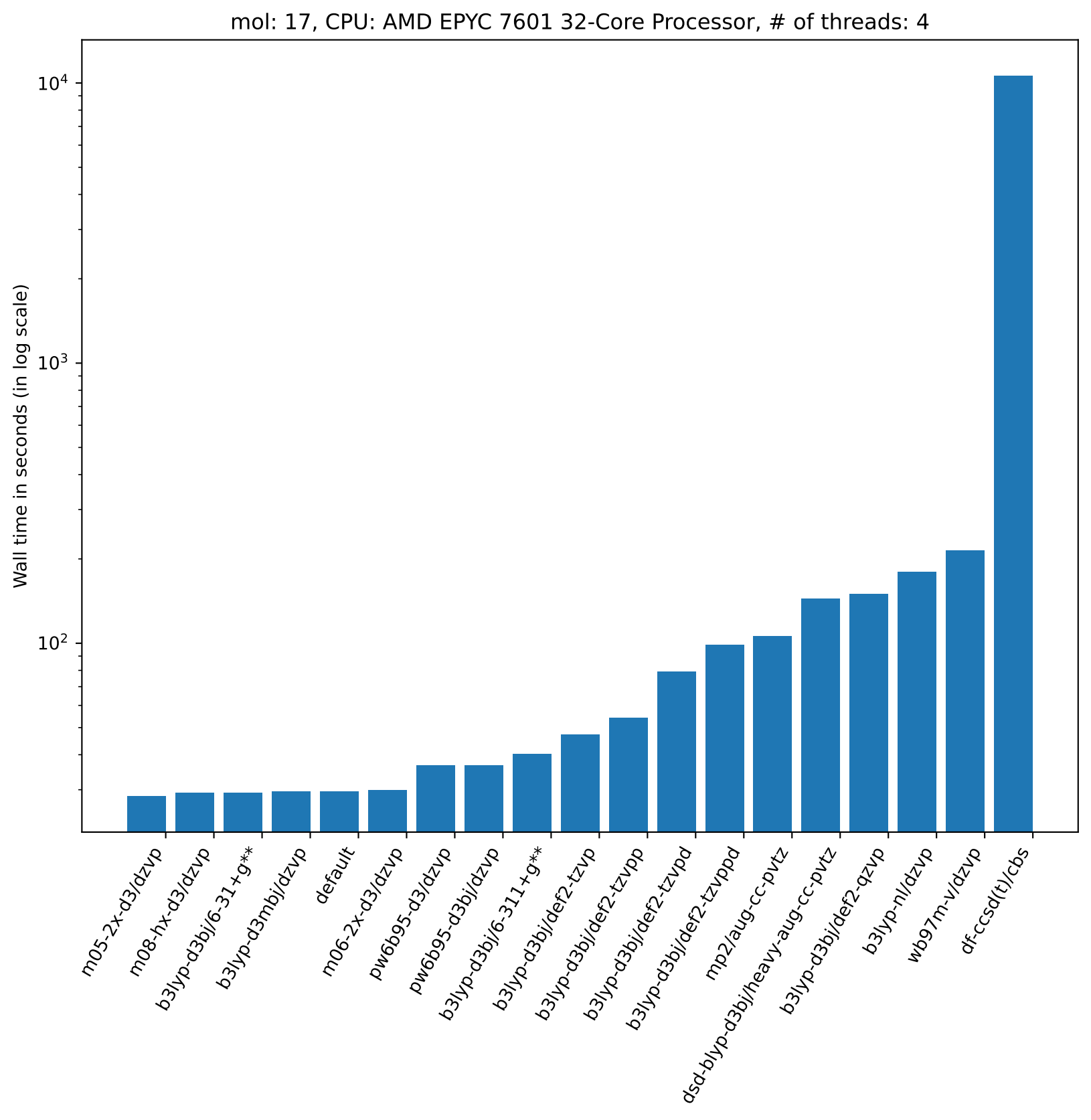

mol: 4, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m08-hx-d3/dzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

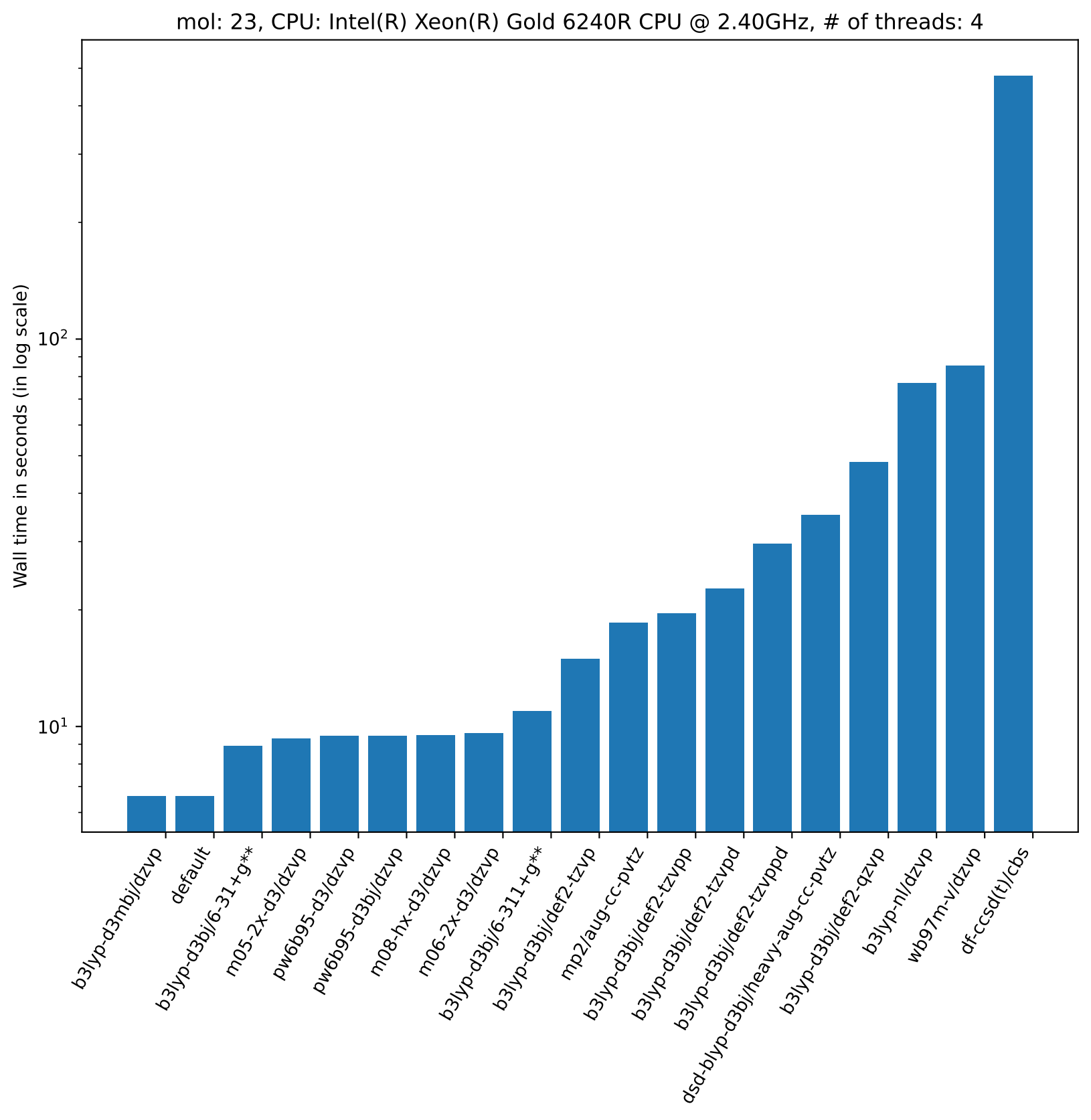

mol: 5, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

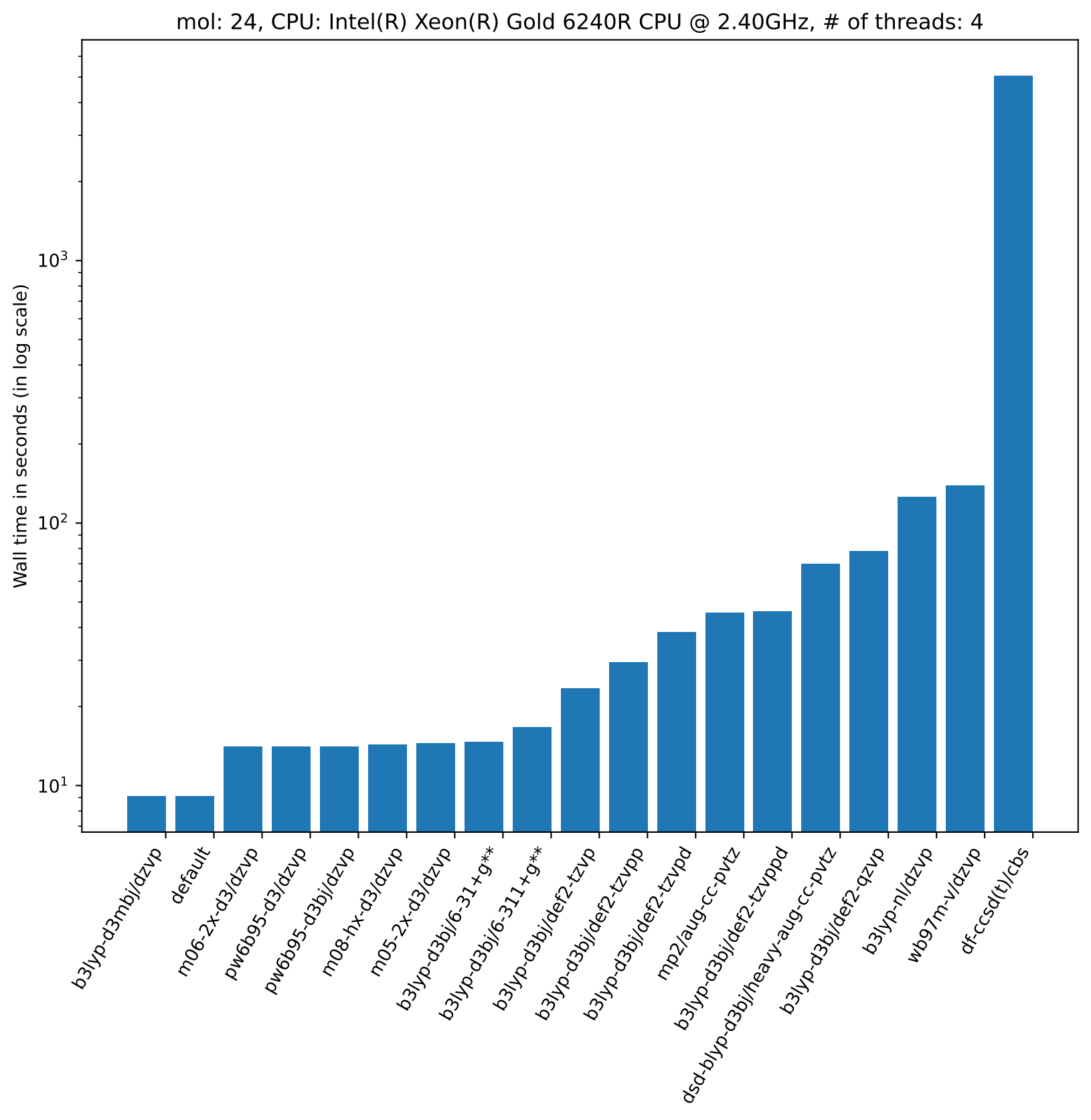

mol: 6, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m08-hx-d3/dzvp
m06-2x-d3/dzvp
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

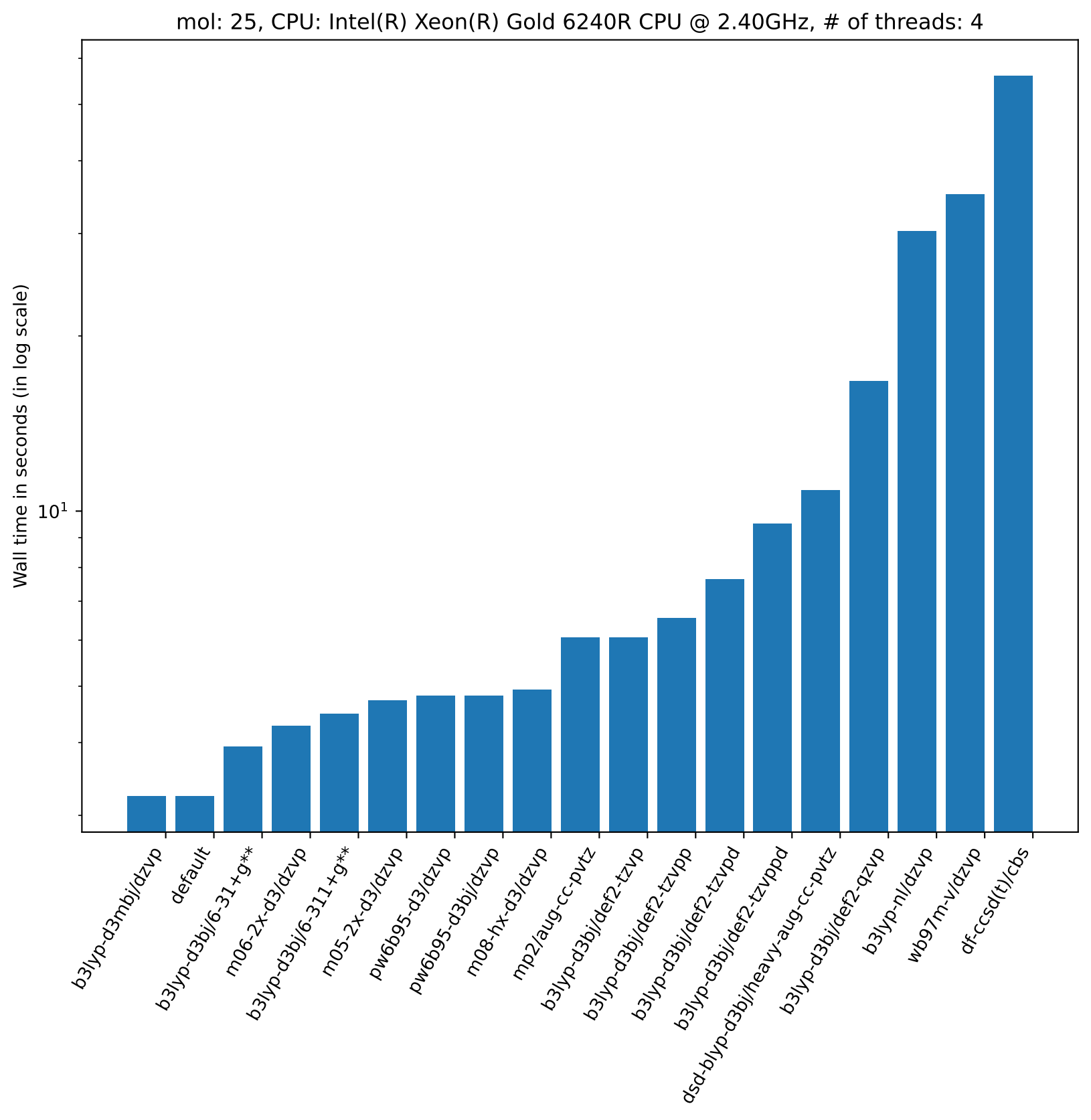

mol: 9, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
m05-2x-d3/dzvp
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

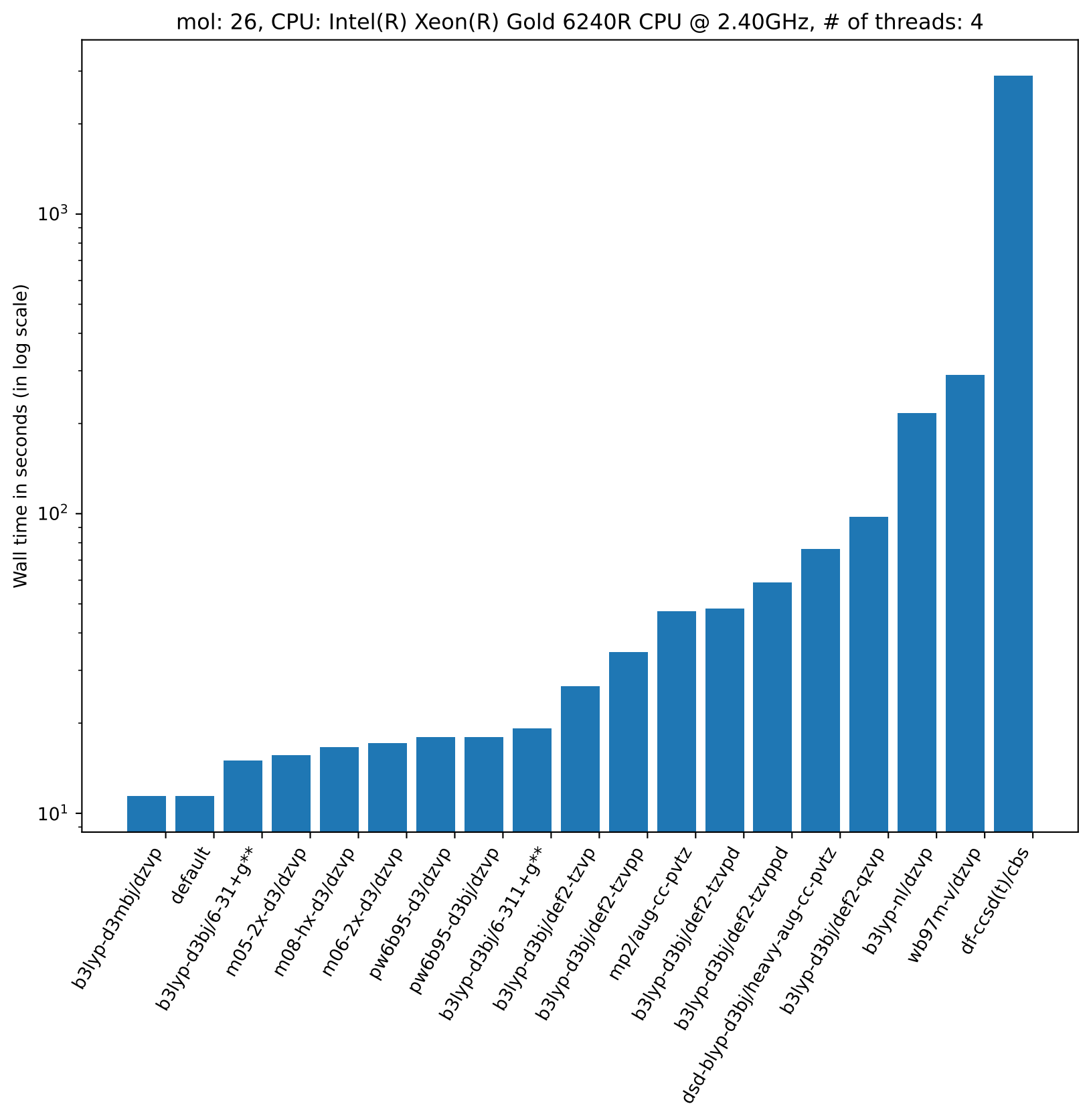

mol: 11, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

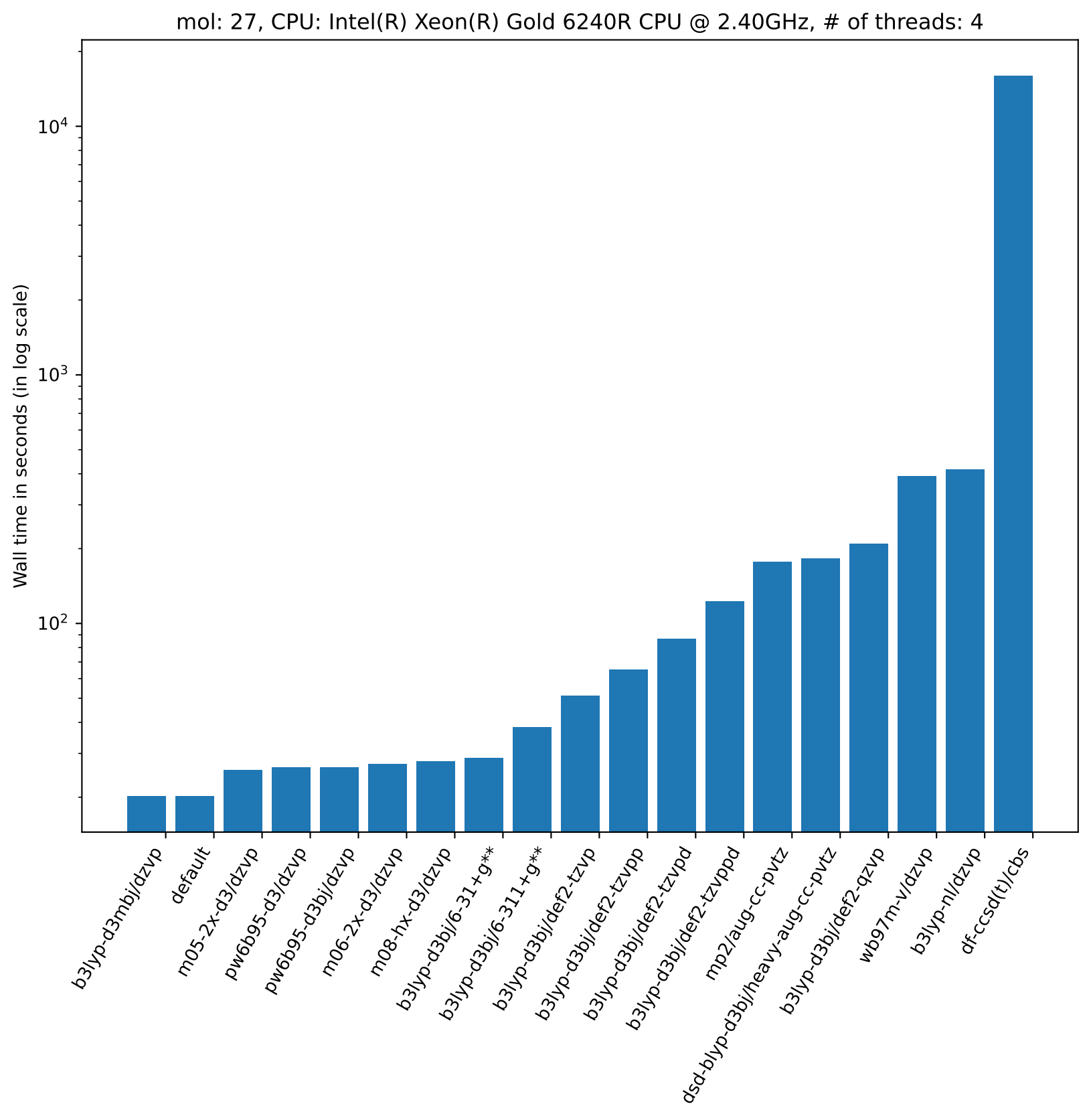

mol: 17, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
m05-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

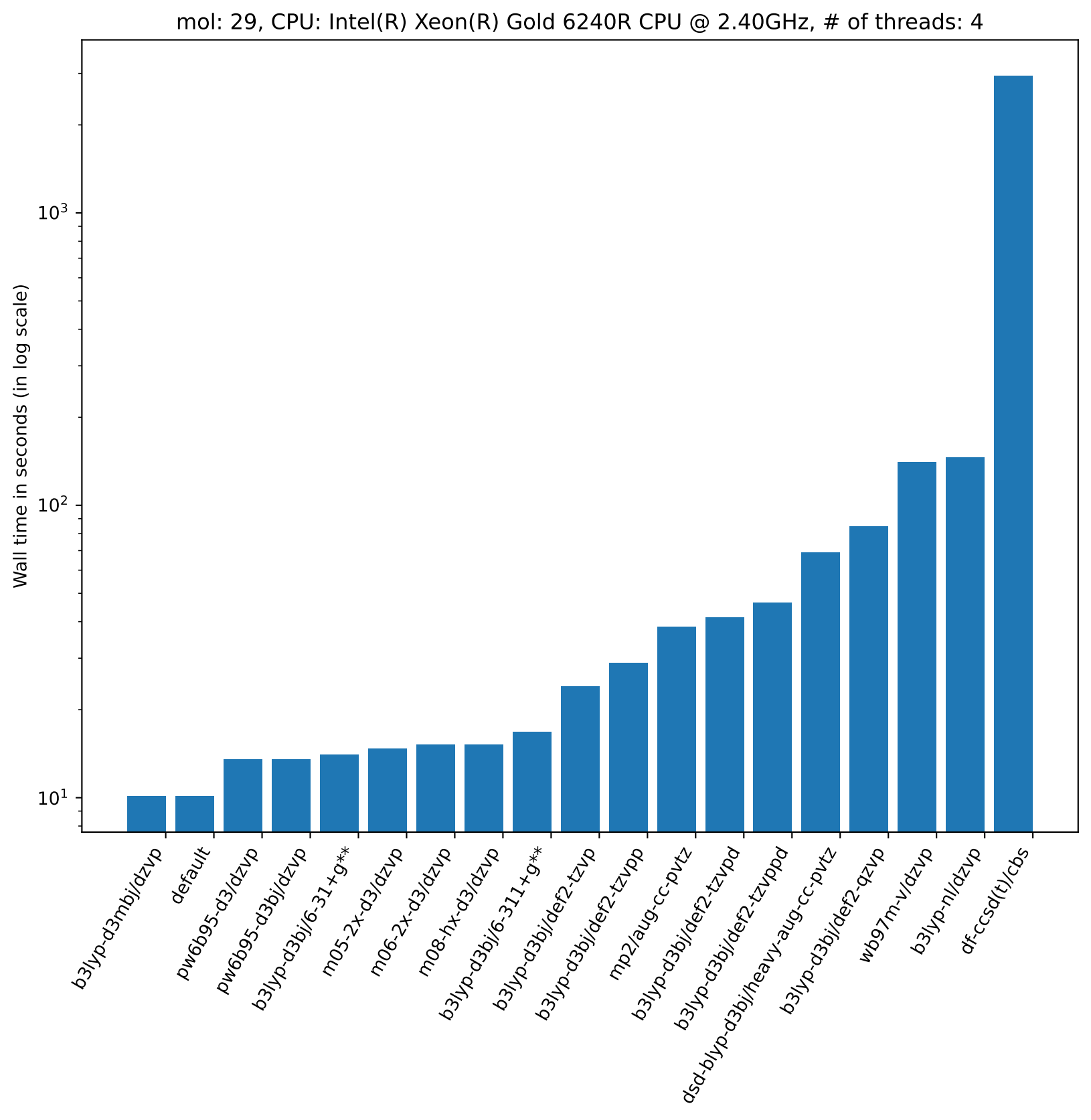

mol: 23, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^2
10^1
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

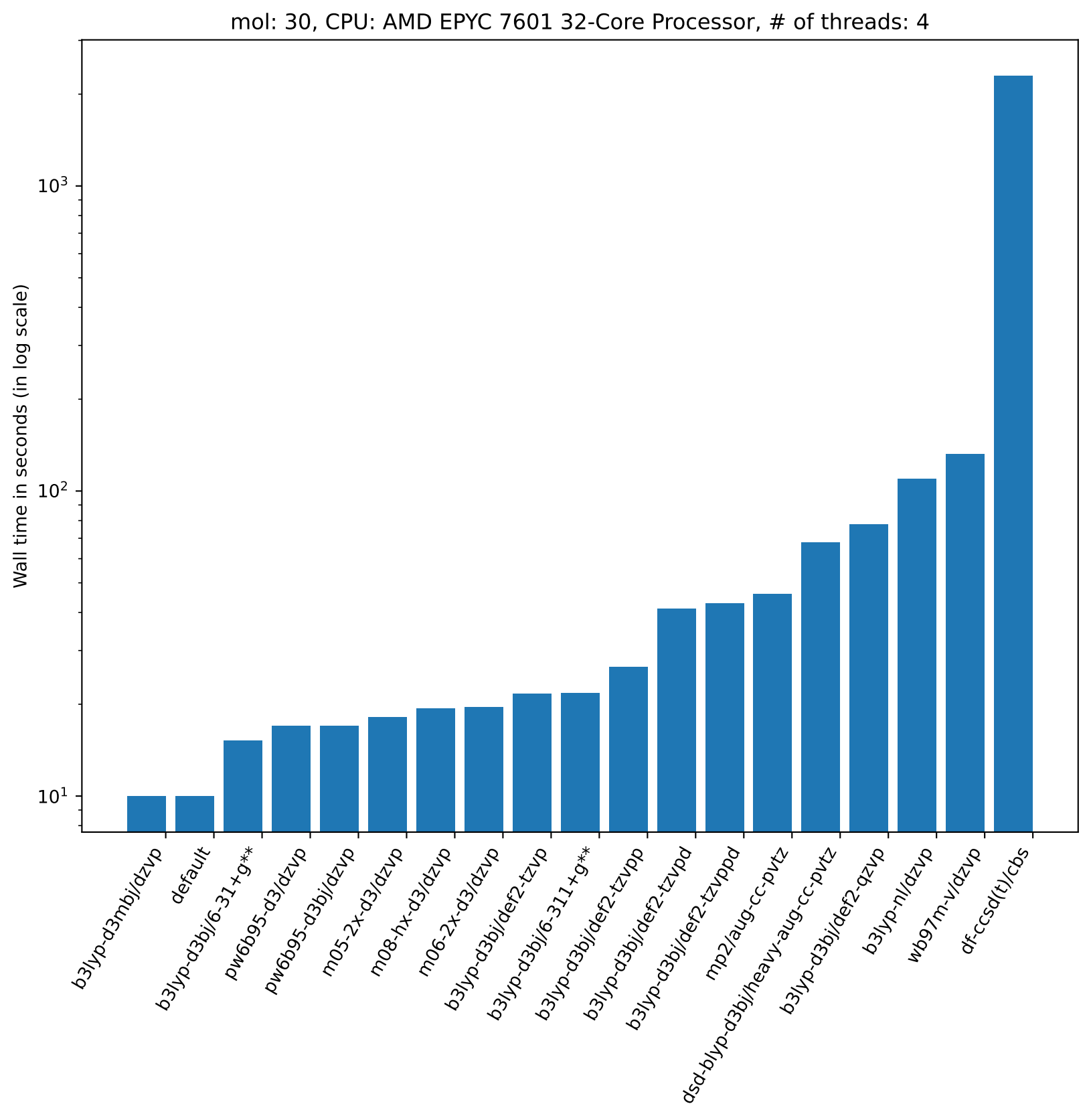

mol: 24, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m05-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

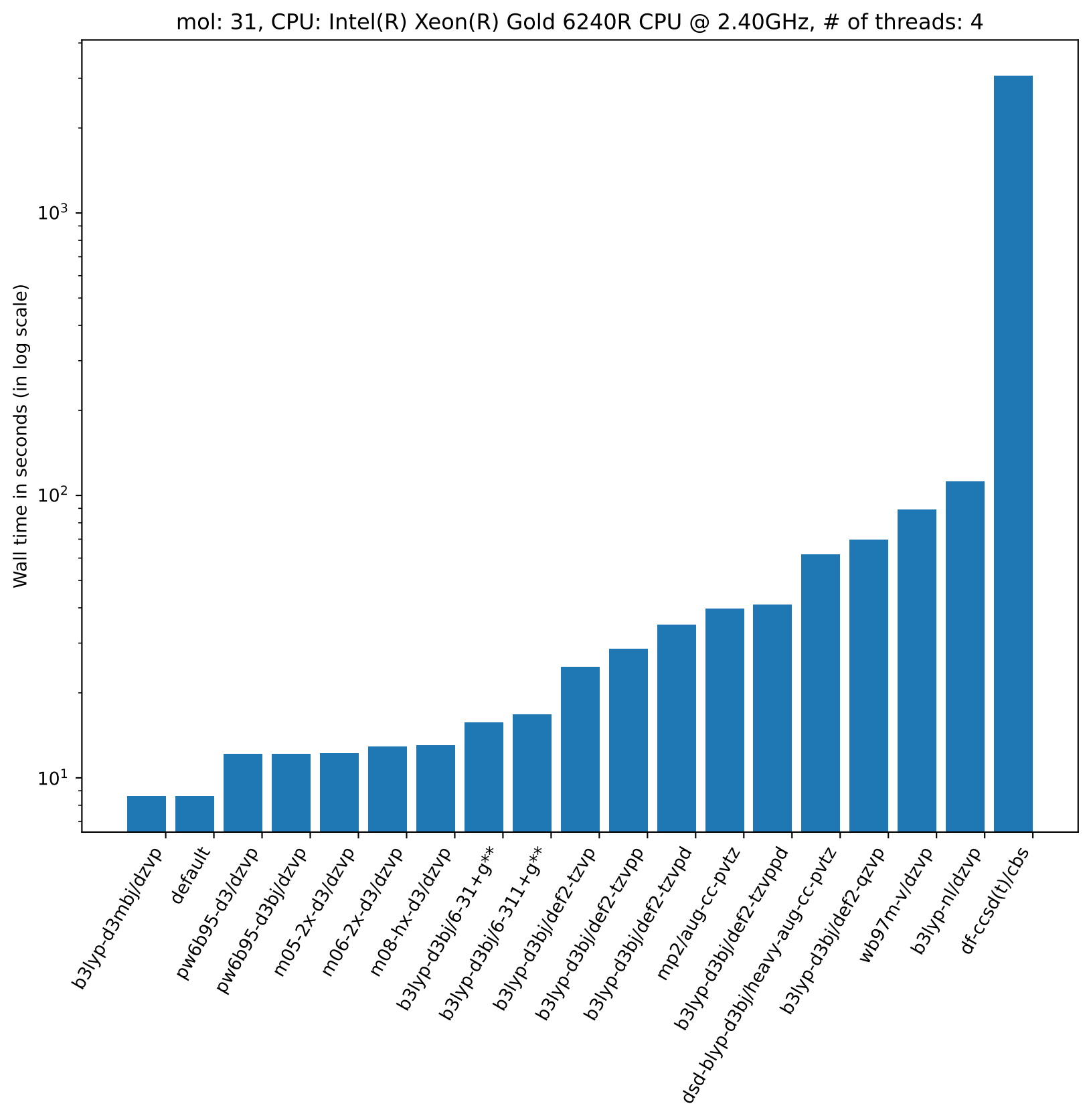

mol: 25, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^1
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m06-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

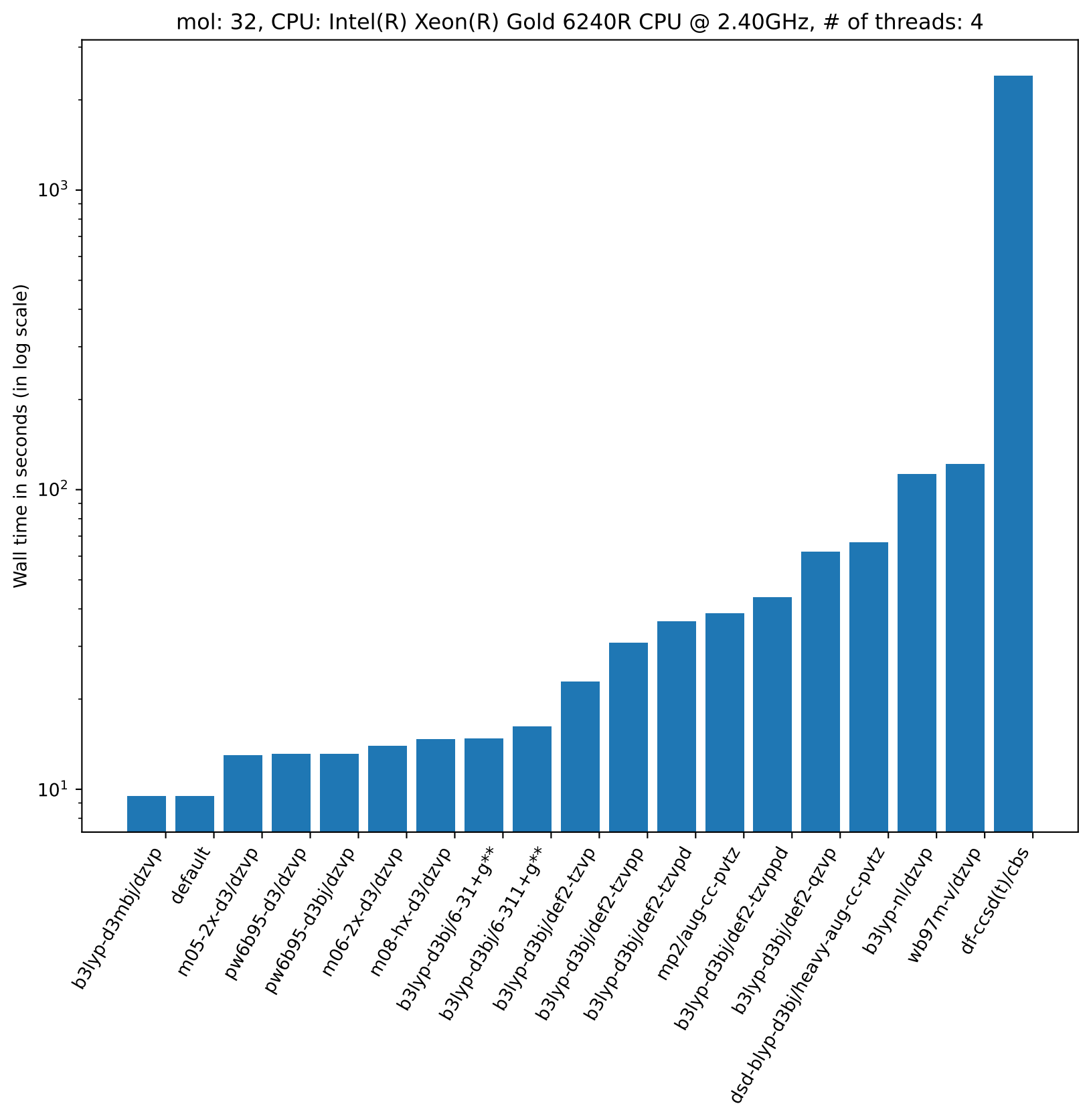

mol: 26, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

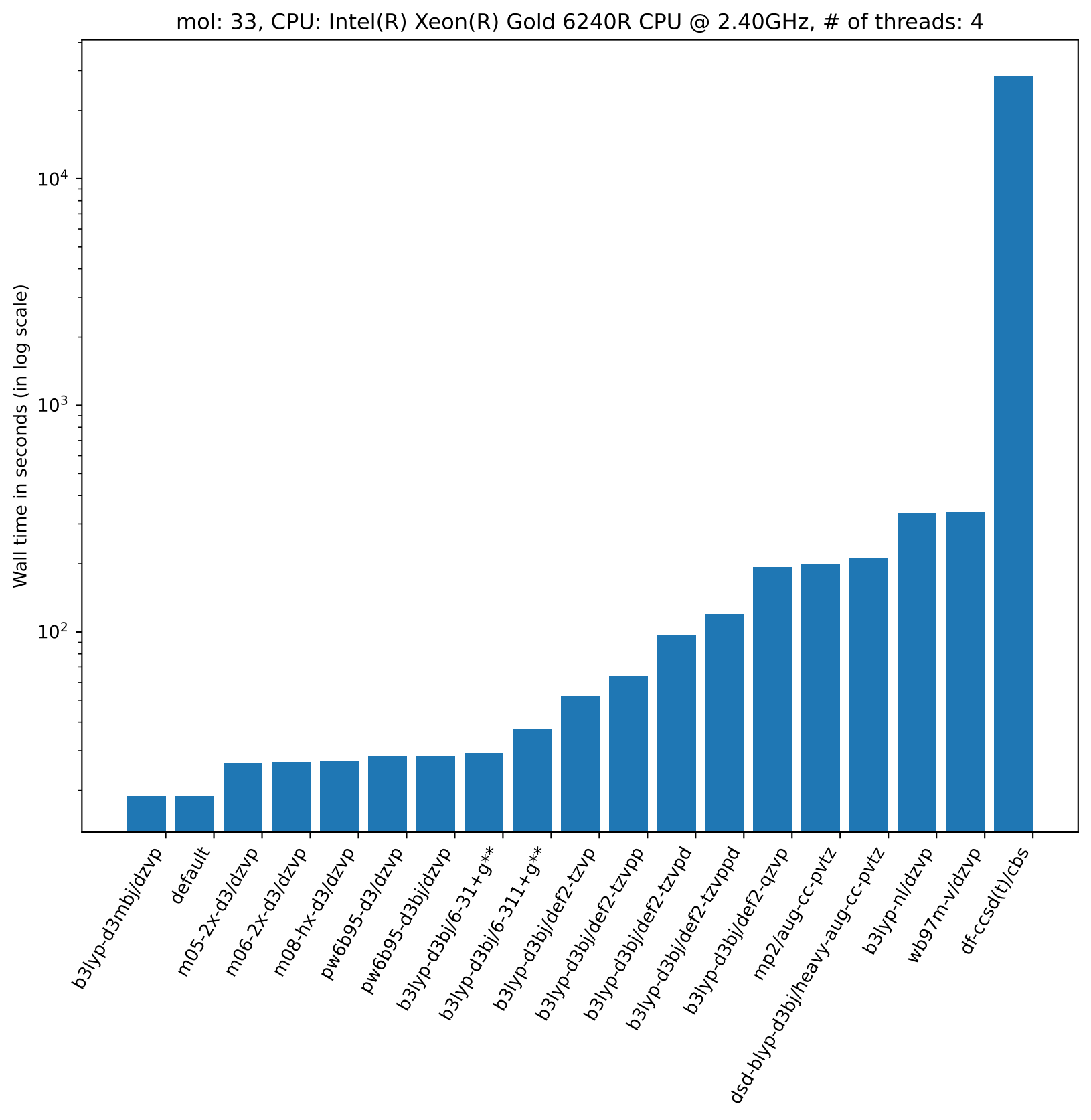

mol: 27, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

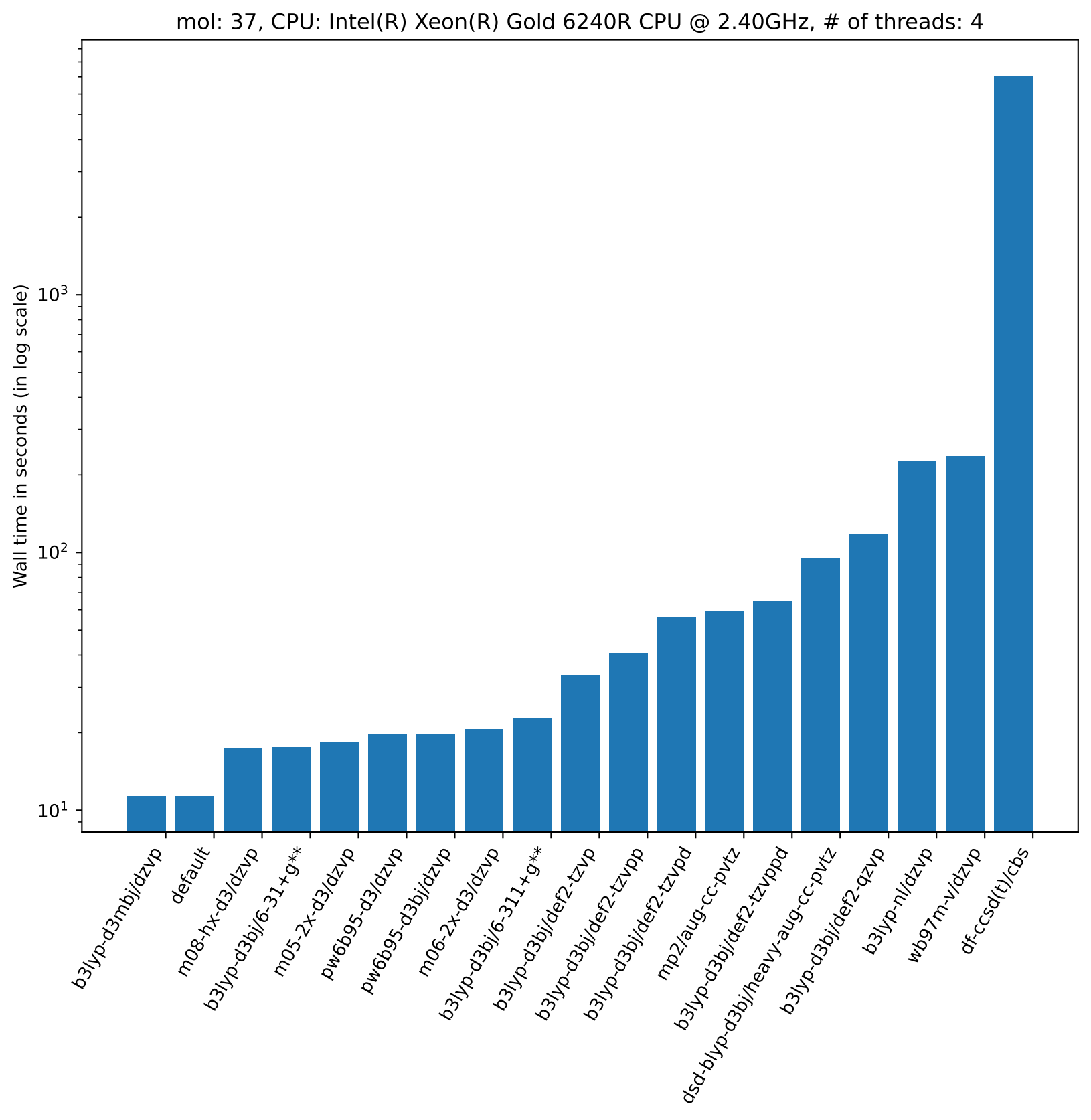

mol: 29, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

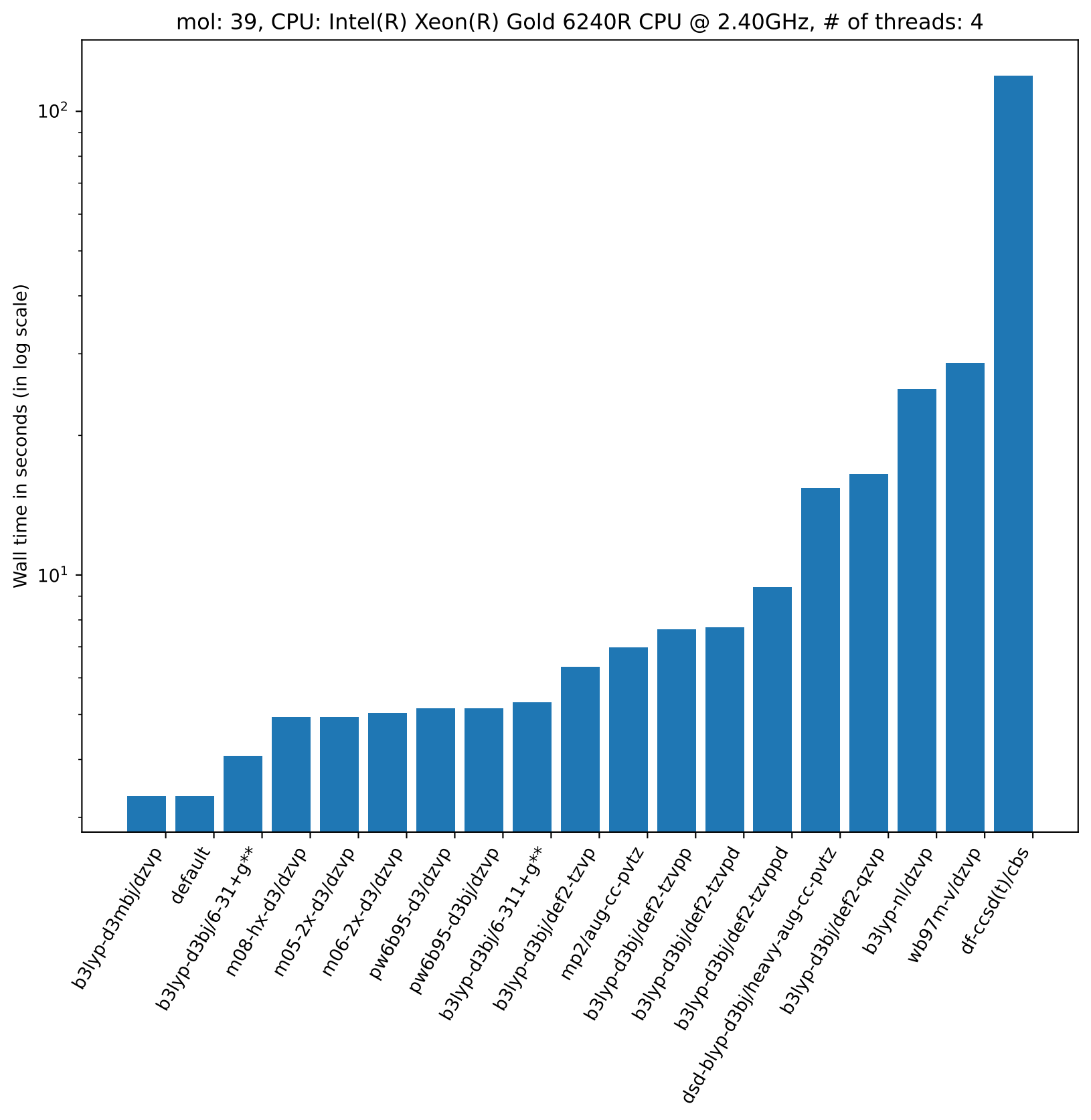

mol: 30, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m05-2x-d3/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

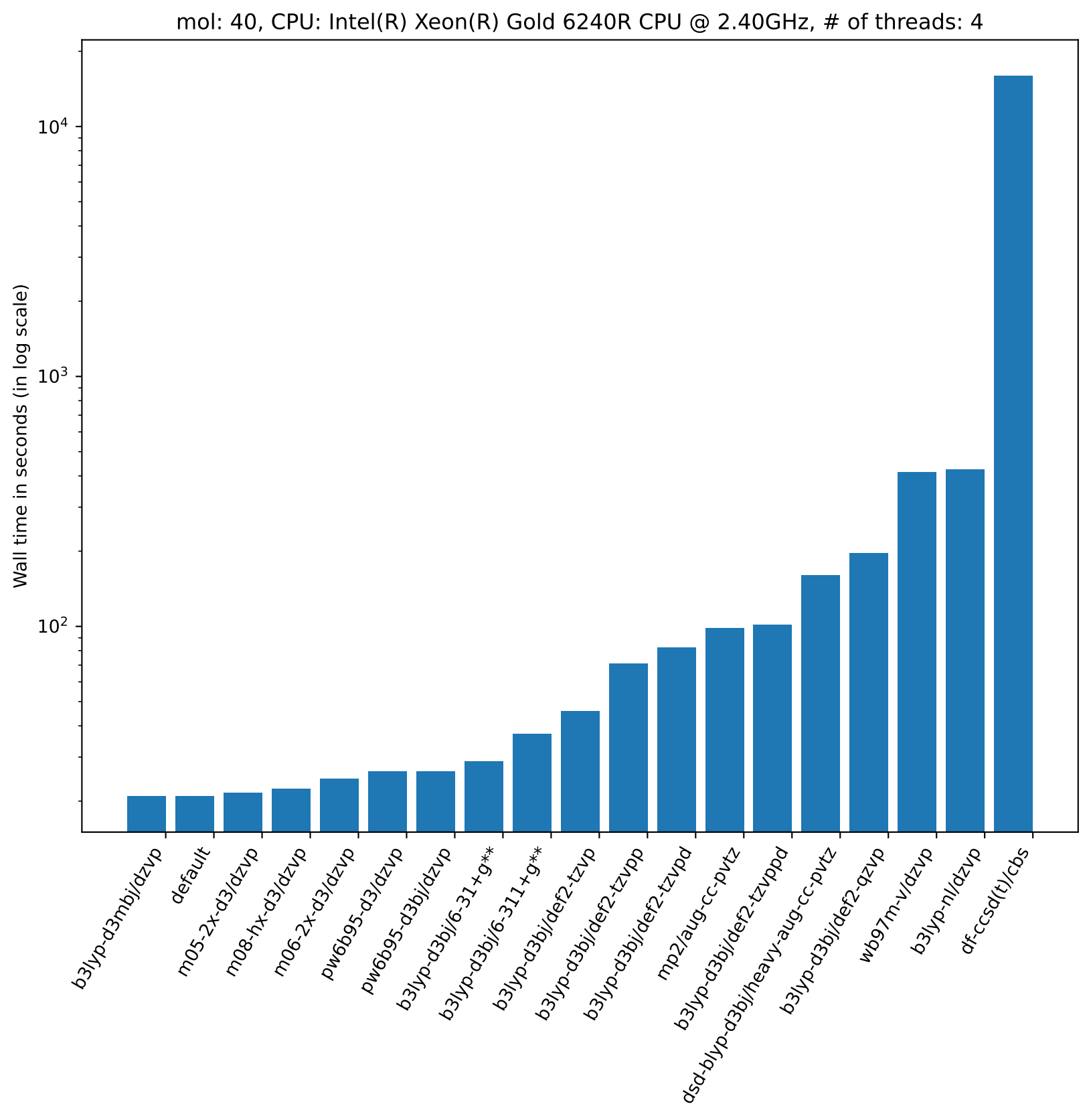

mol: 31, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

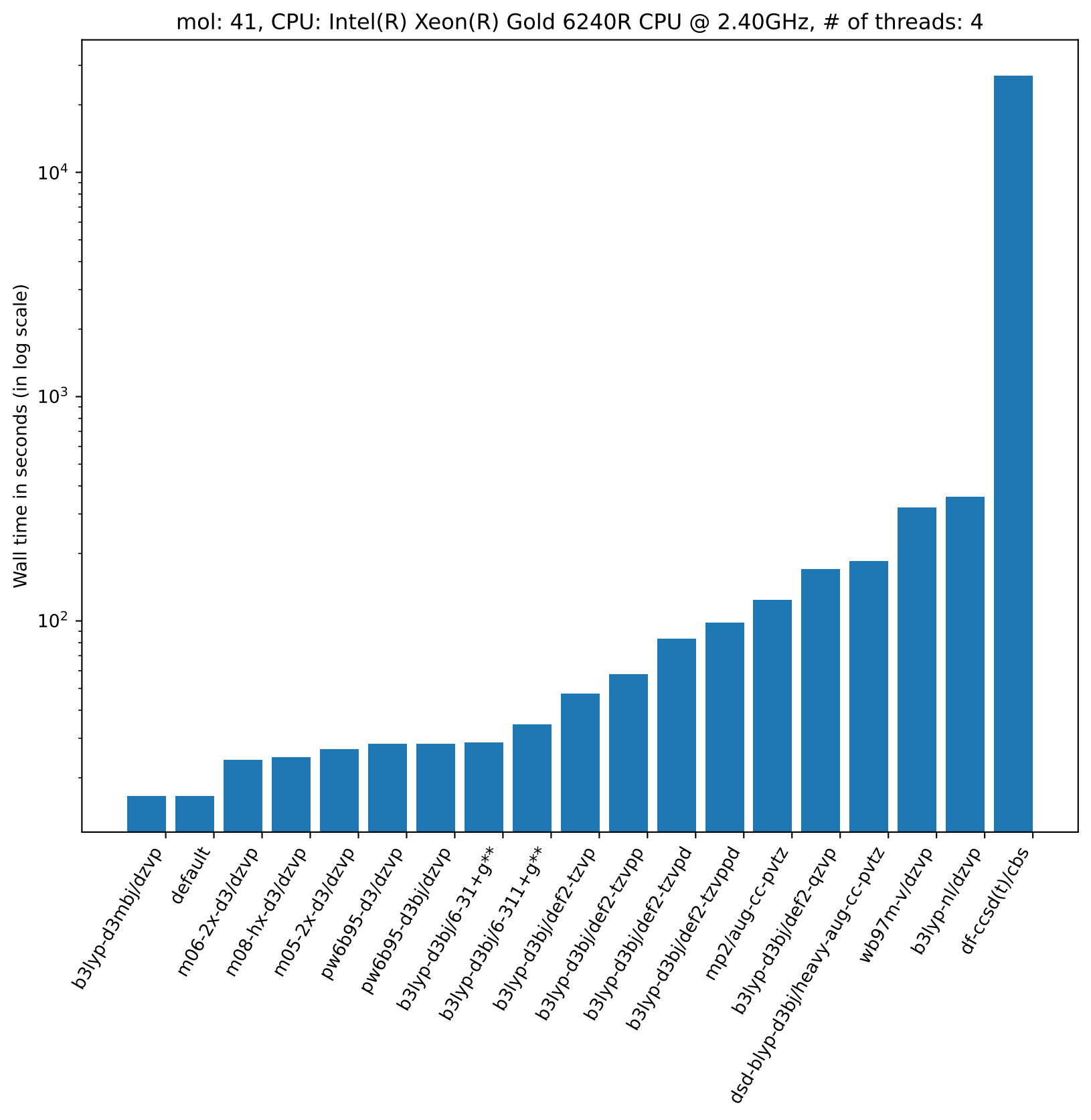

mol: 32, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

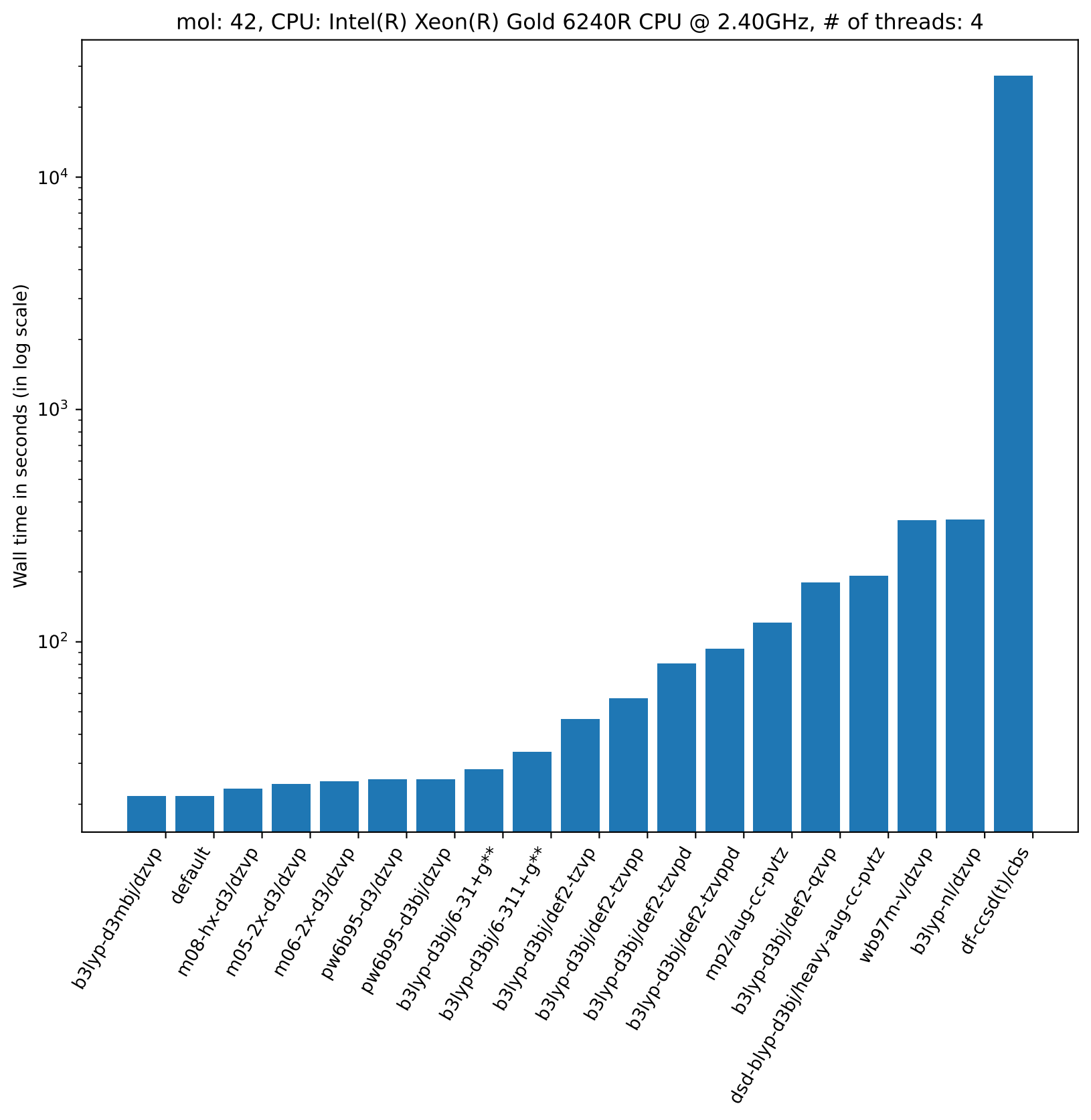

mol: 33, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
b3lyp-d3bj/def2-qzvp
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

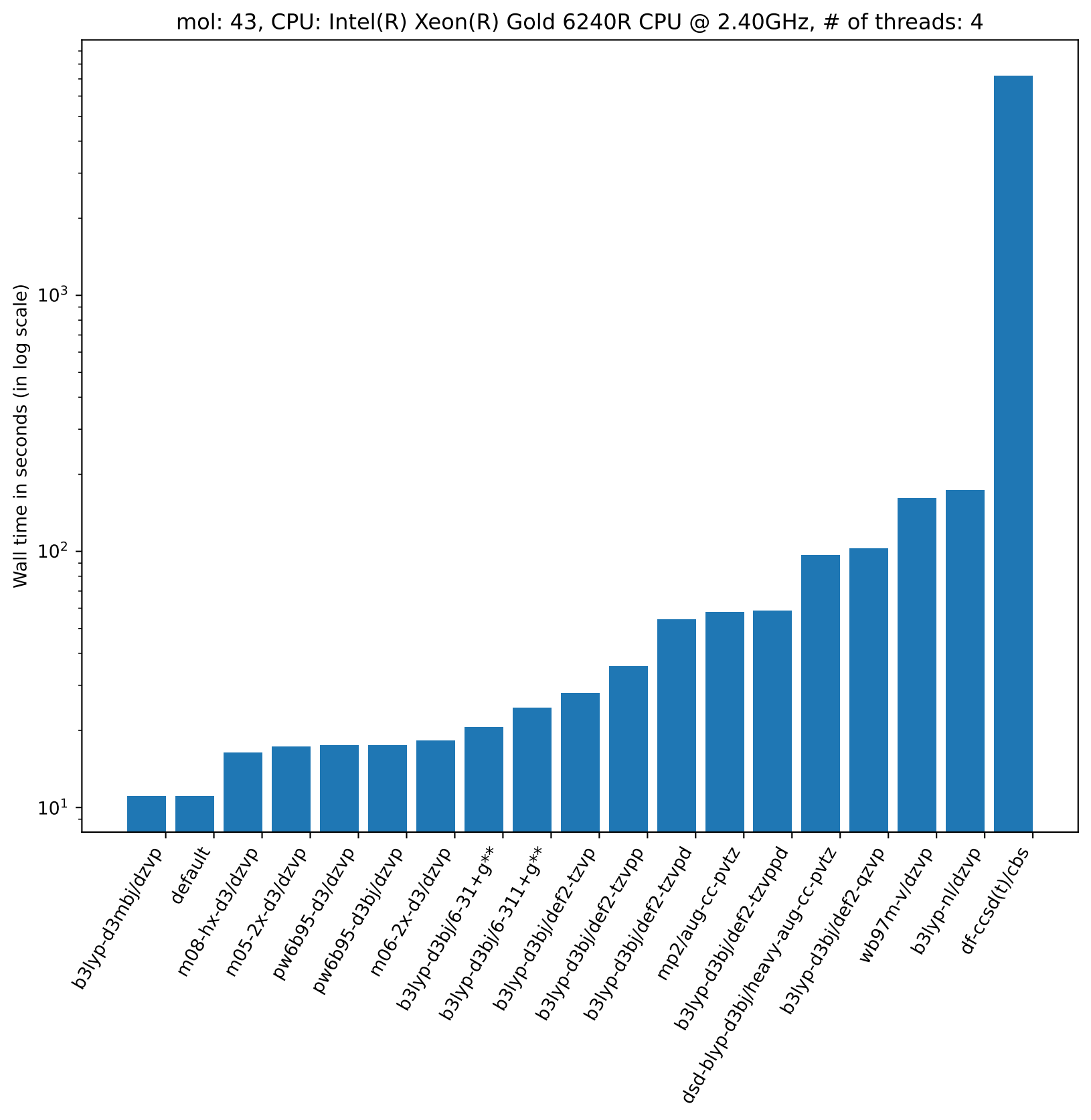

mol: 37, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

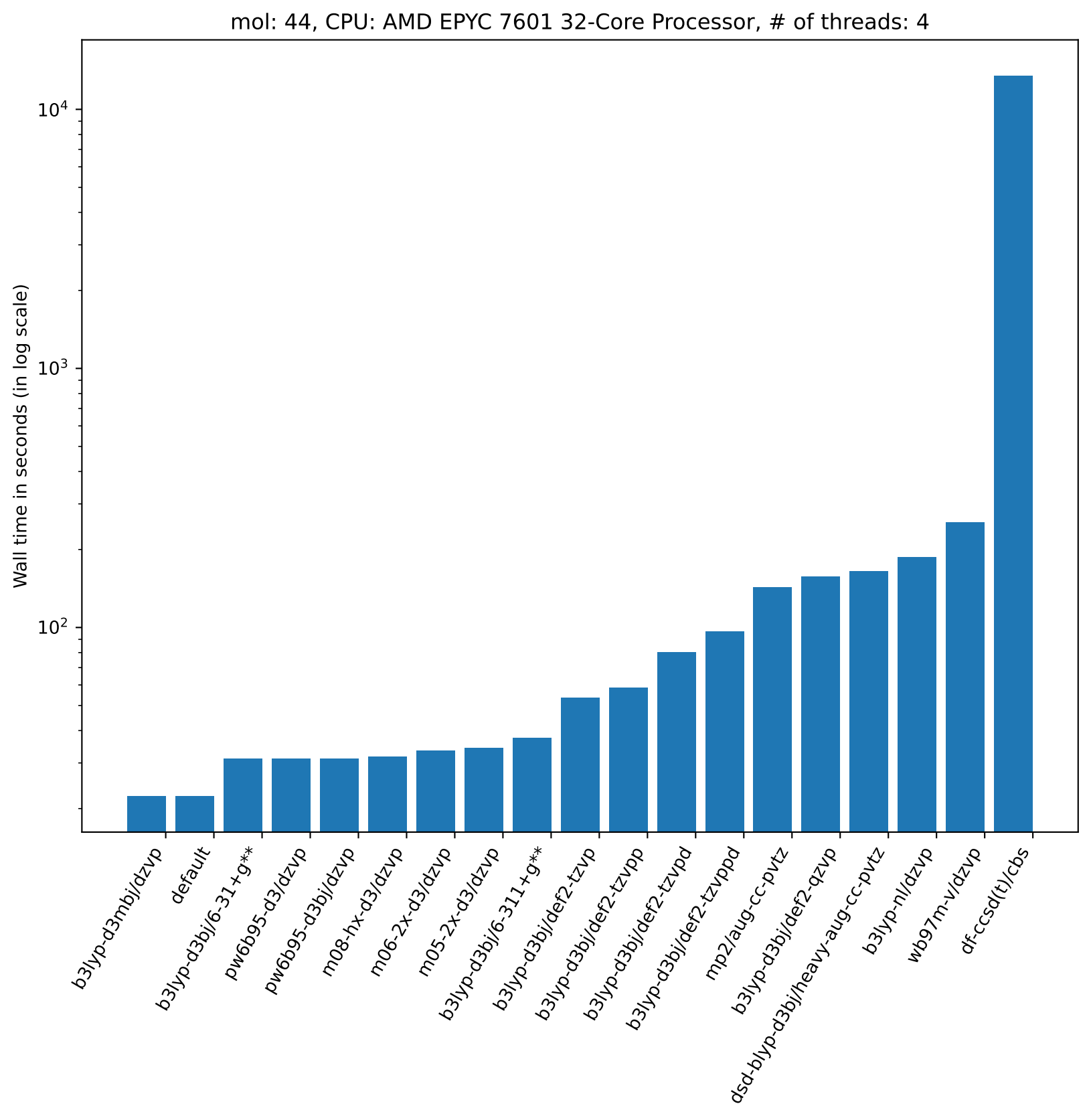

mol: 39, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^2
10^1
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m08-hx-d3/dzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

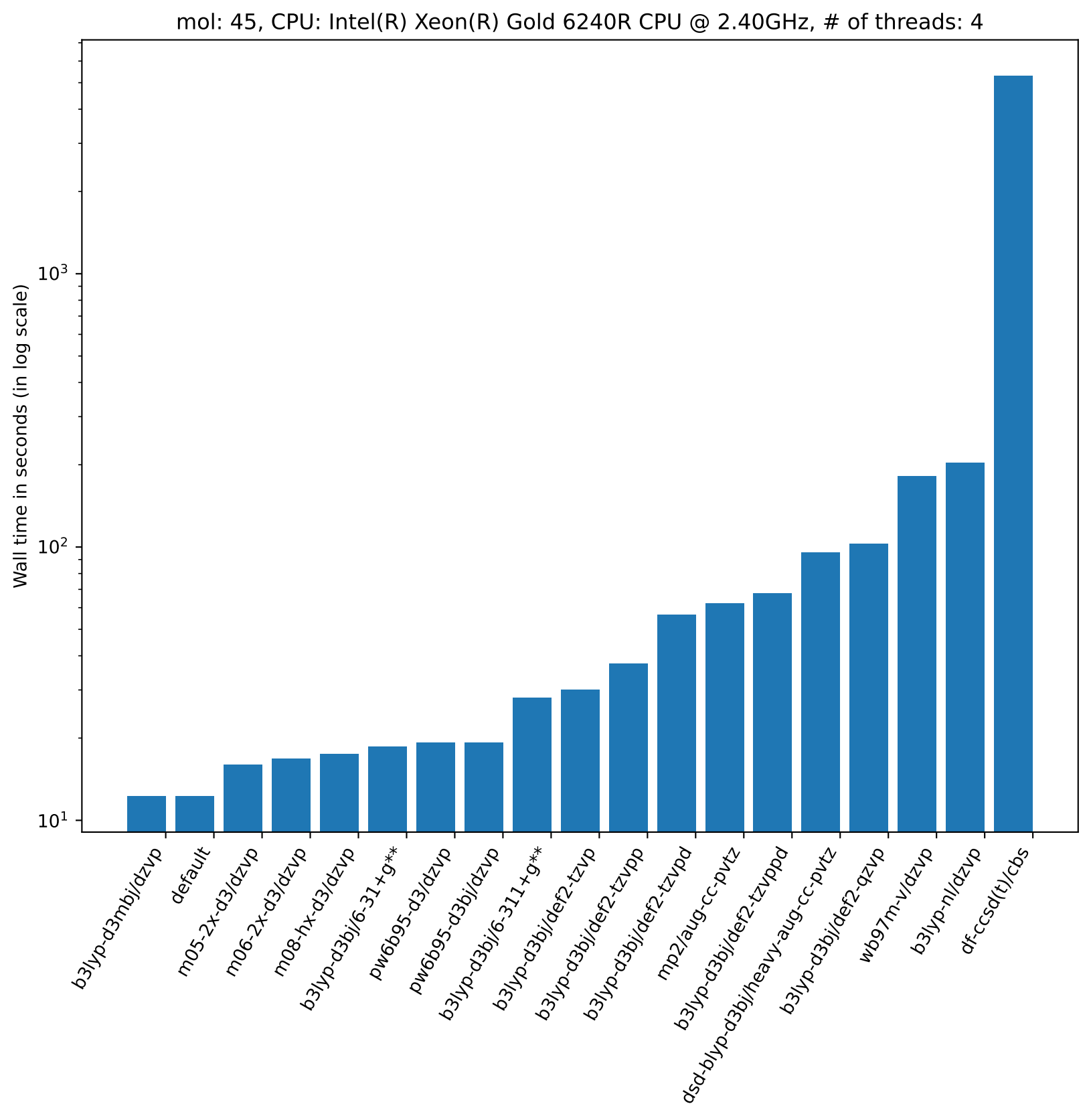

mol: 40, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

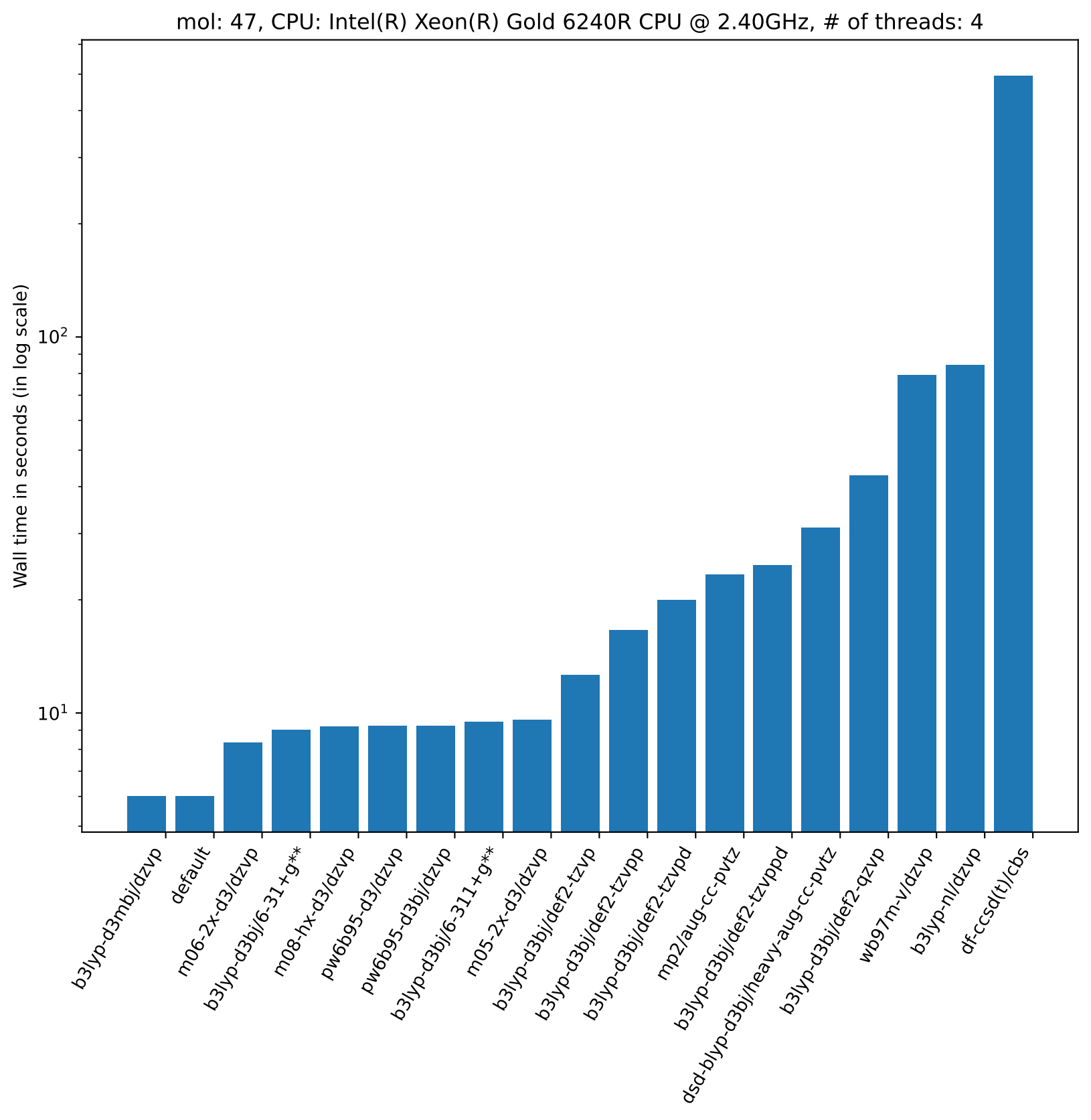

mol: 41, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
m08-hx-d3/dzvp
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

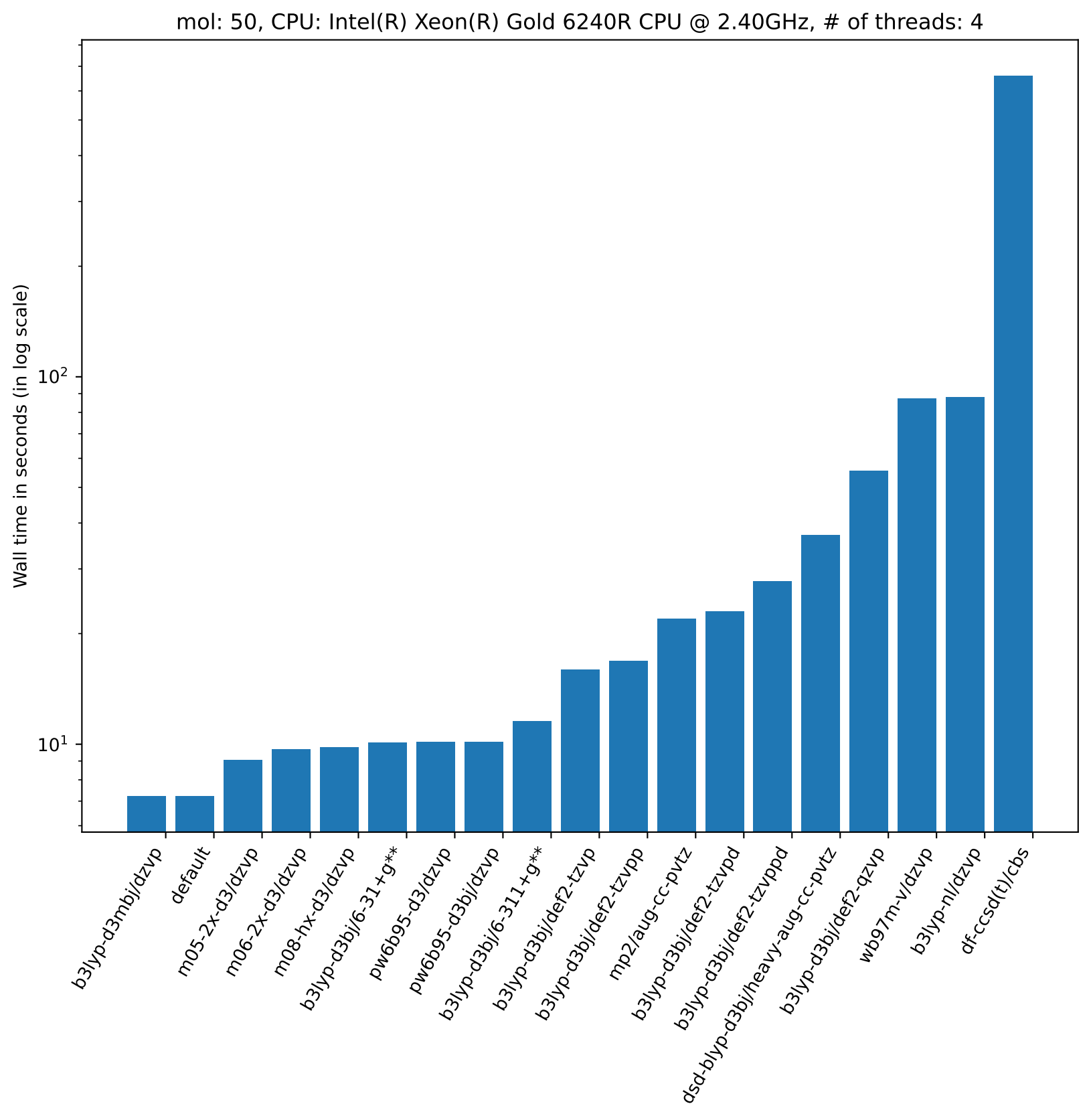

mol: 42, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
m08-hx-d3/dzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

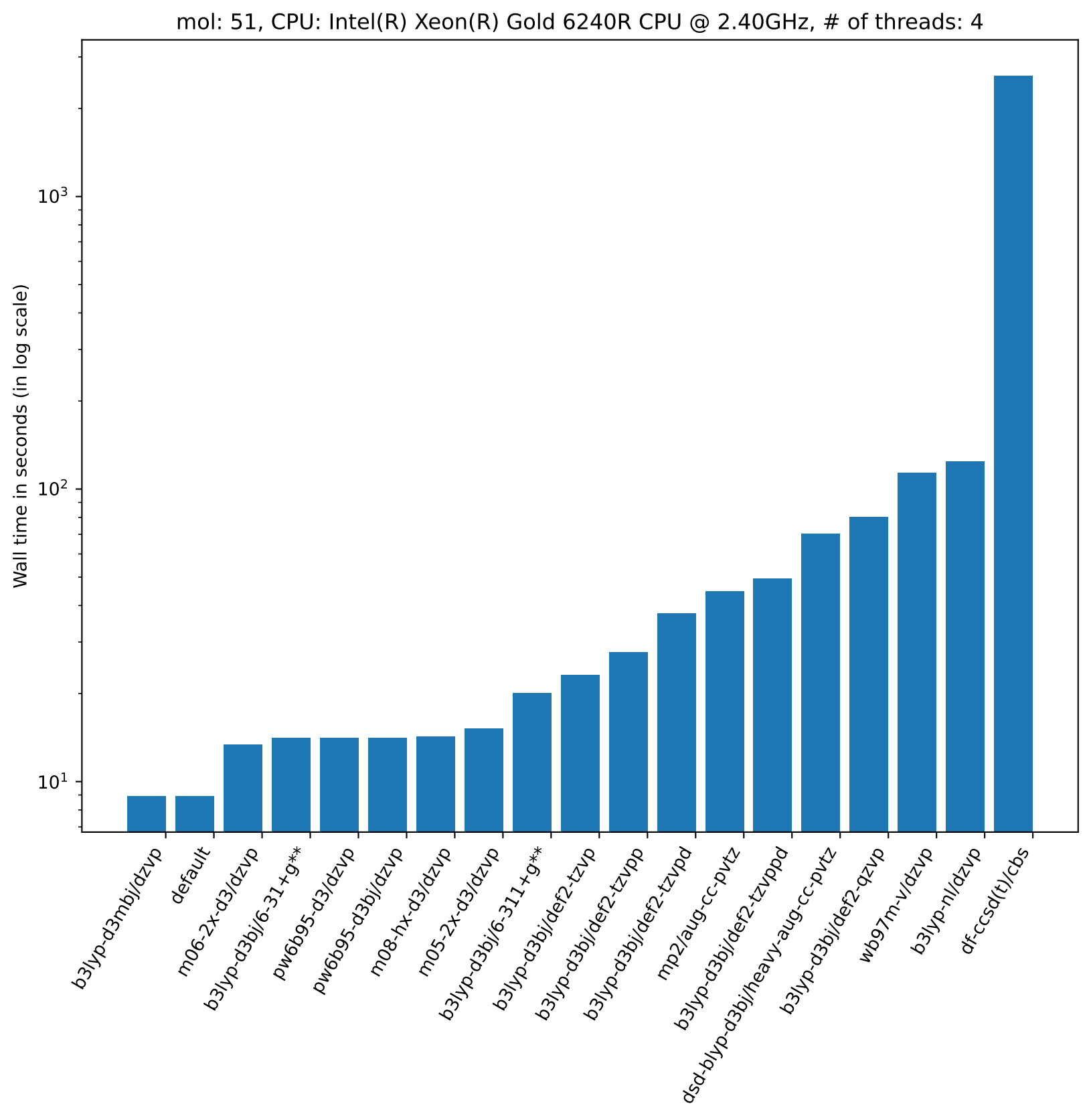

mol: 43, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
m08-hx-d3/dzvp
m05-2x-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

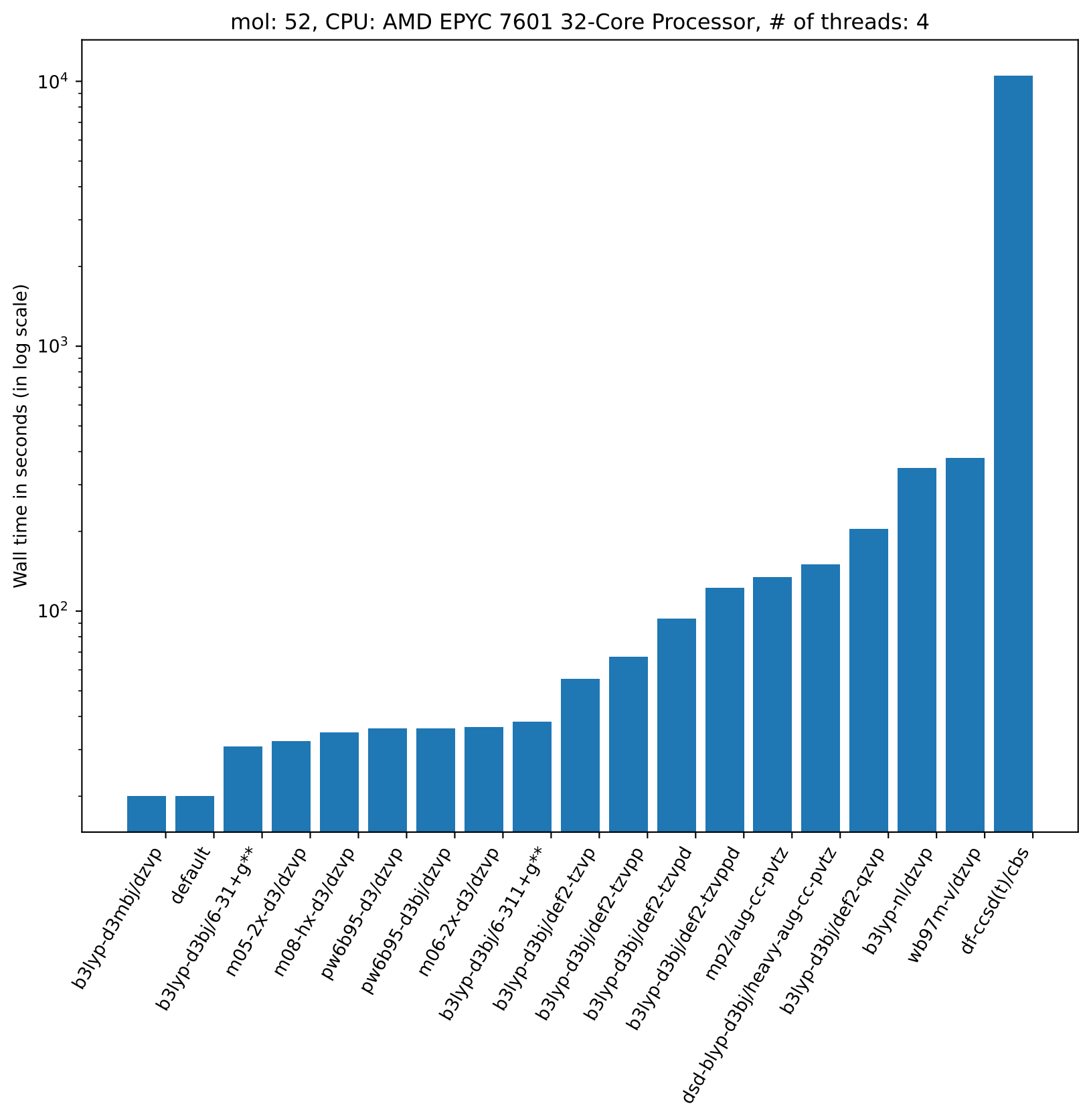

mol: 44, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
m05-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs

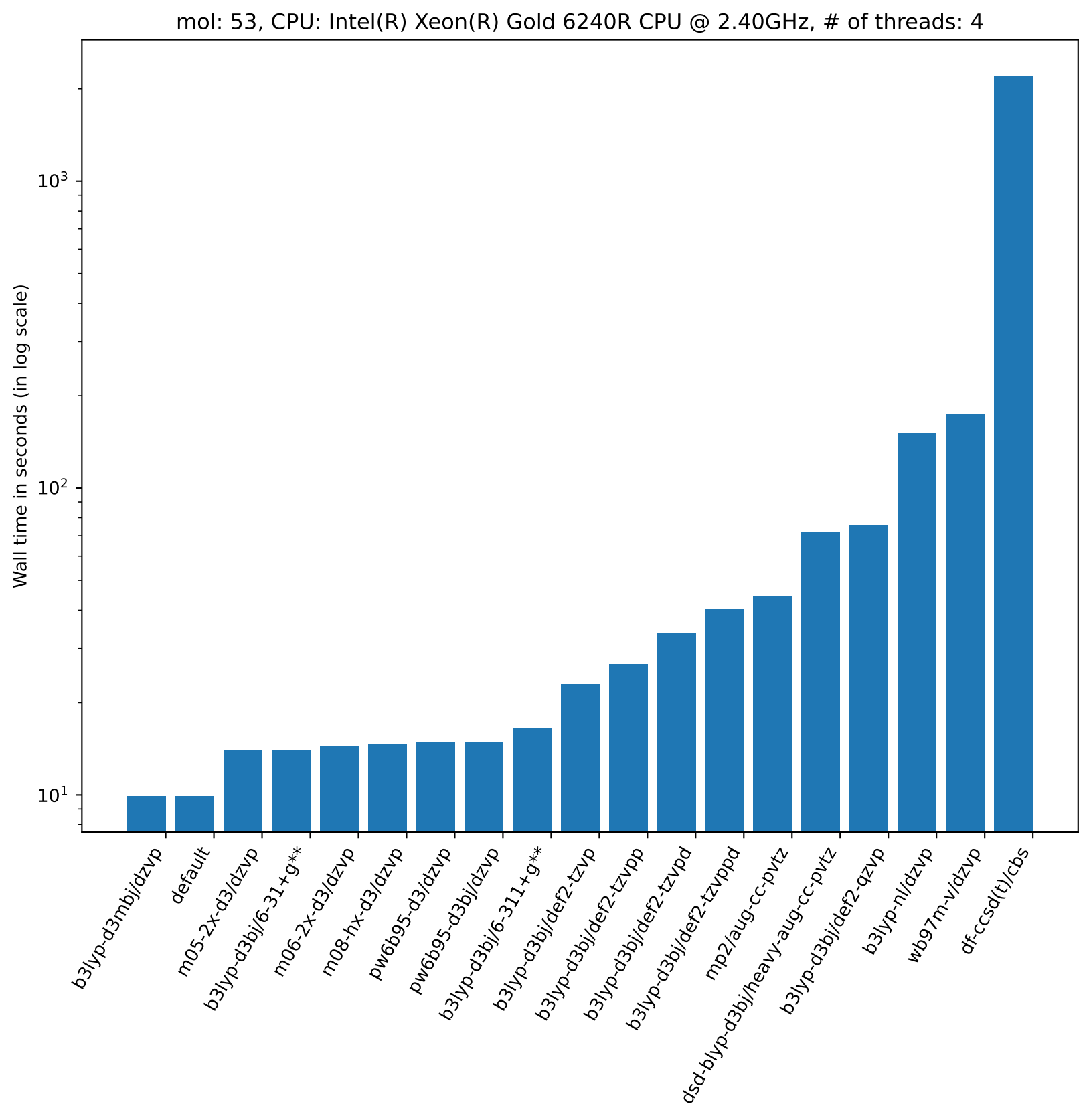

mol: 45, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

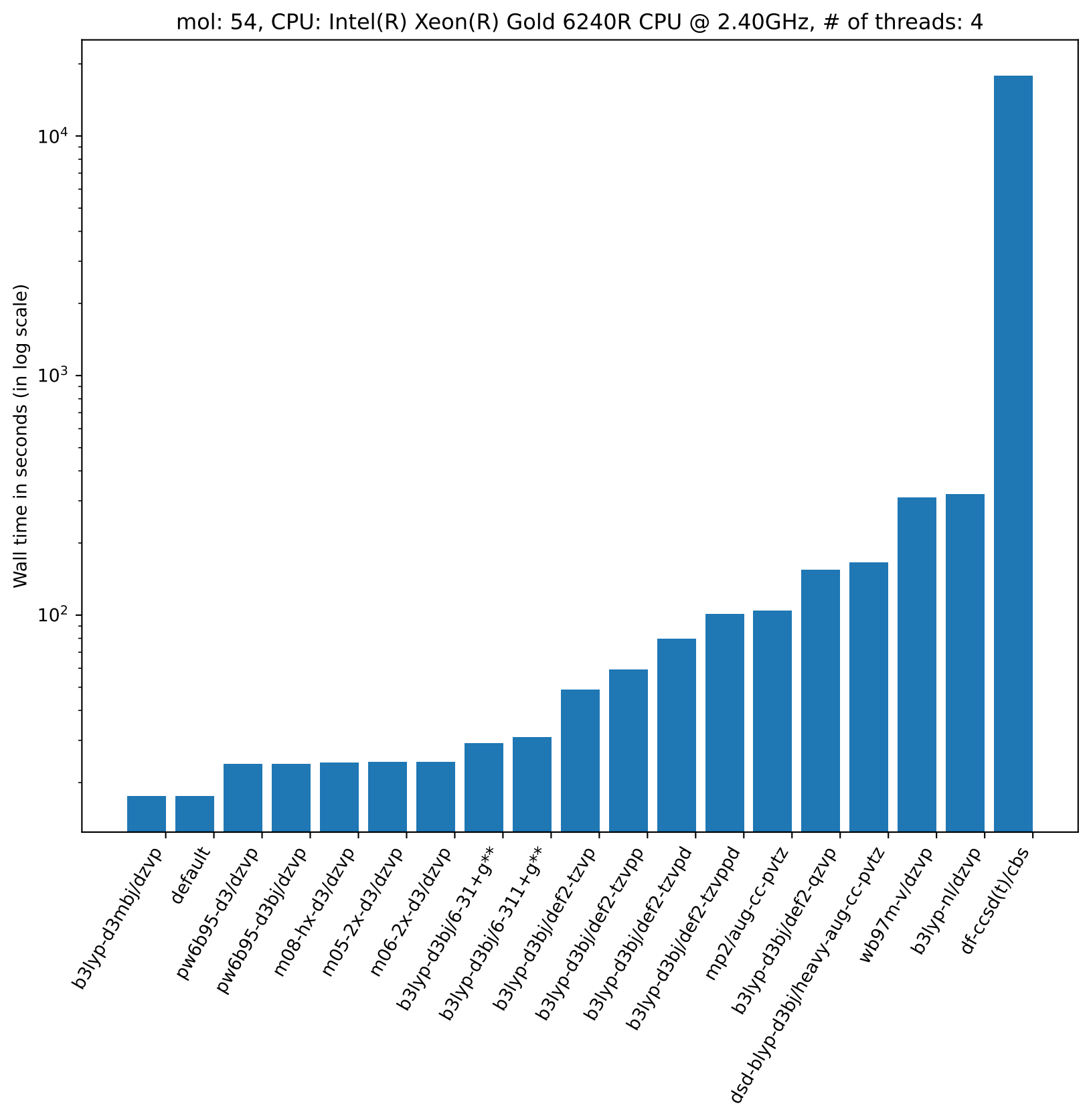

mol: 47, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^2
10^1
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
m05-2x-d3/dzvp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

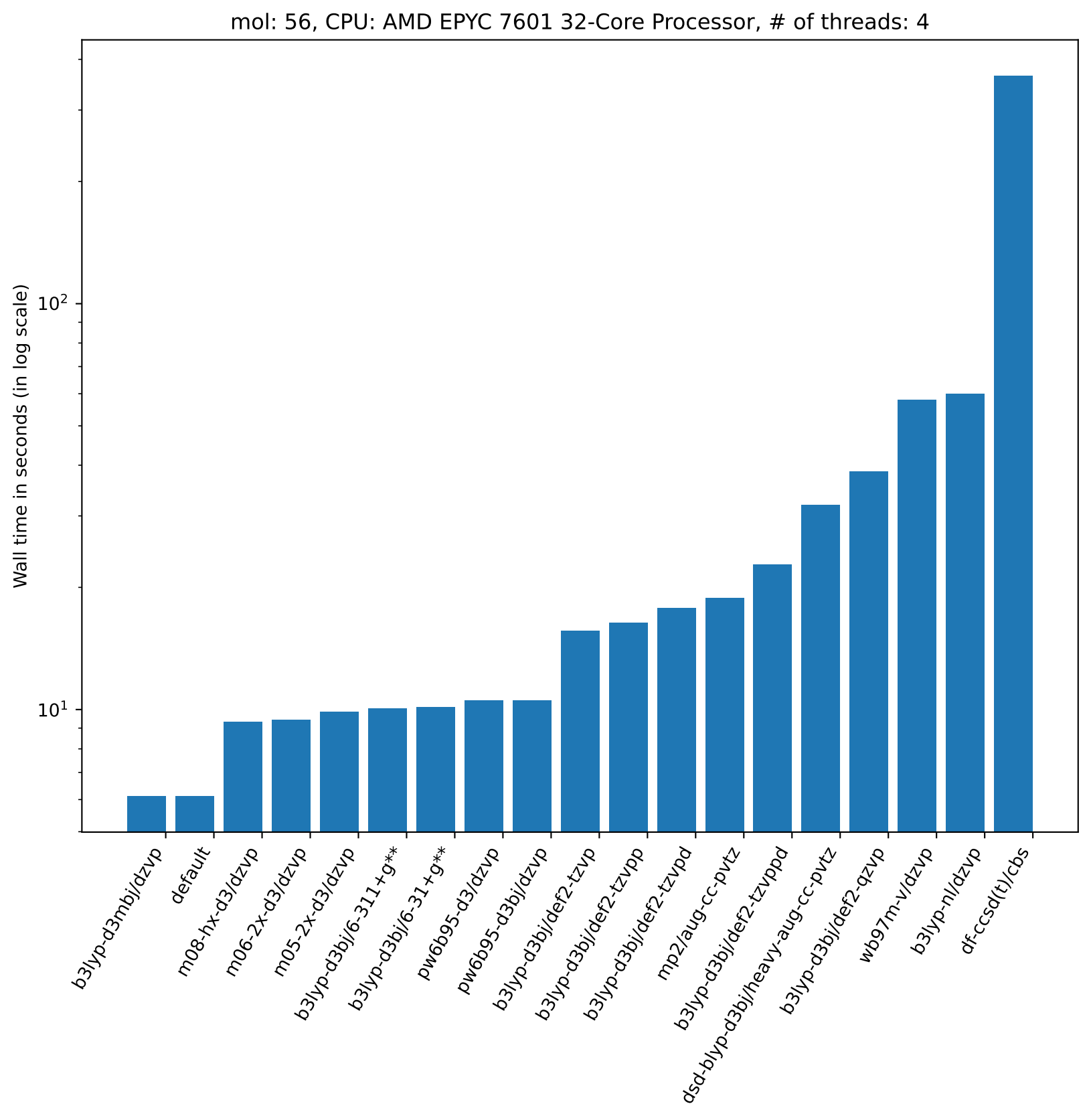

mol: 50, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^2
10^1
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

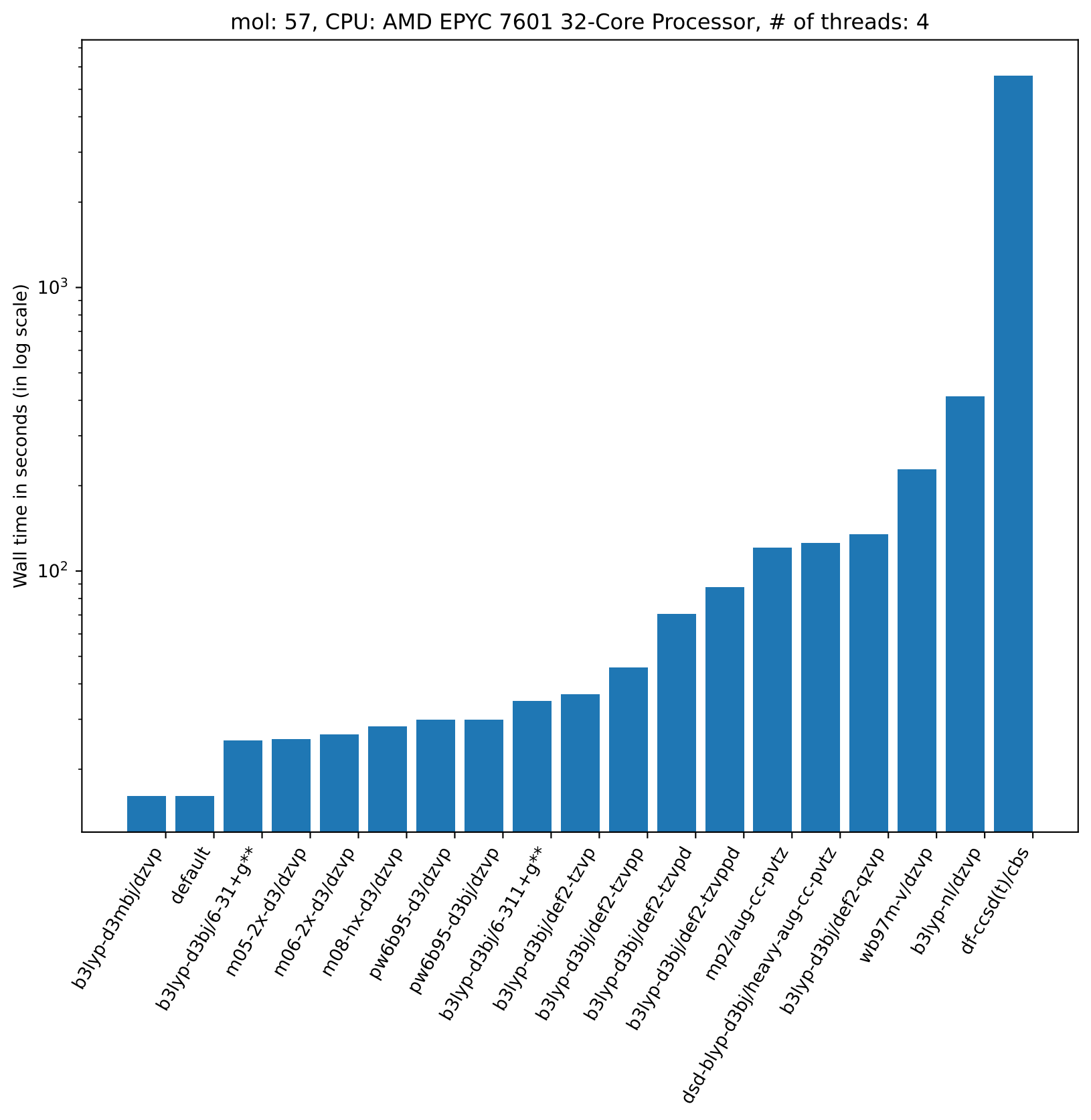

mol: 51, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m05-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs

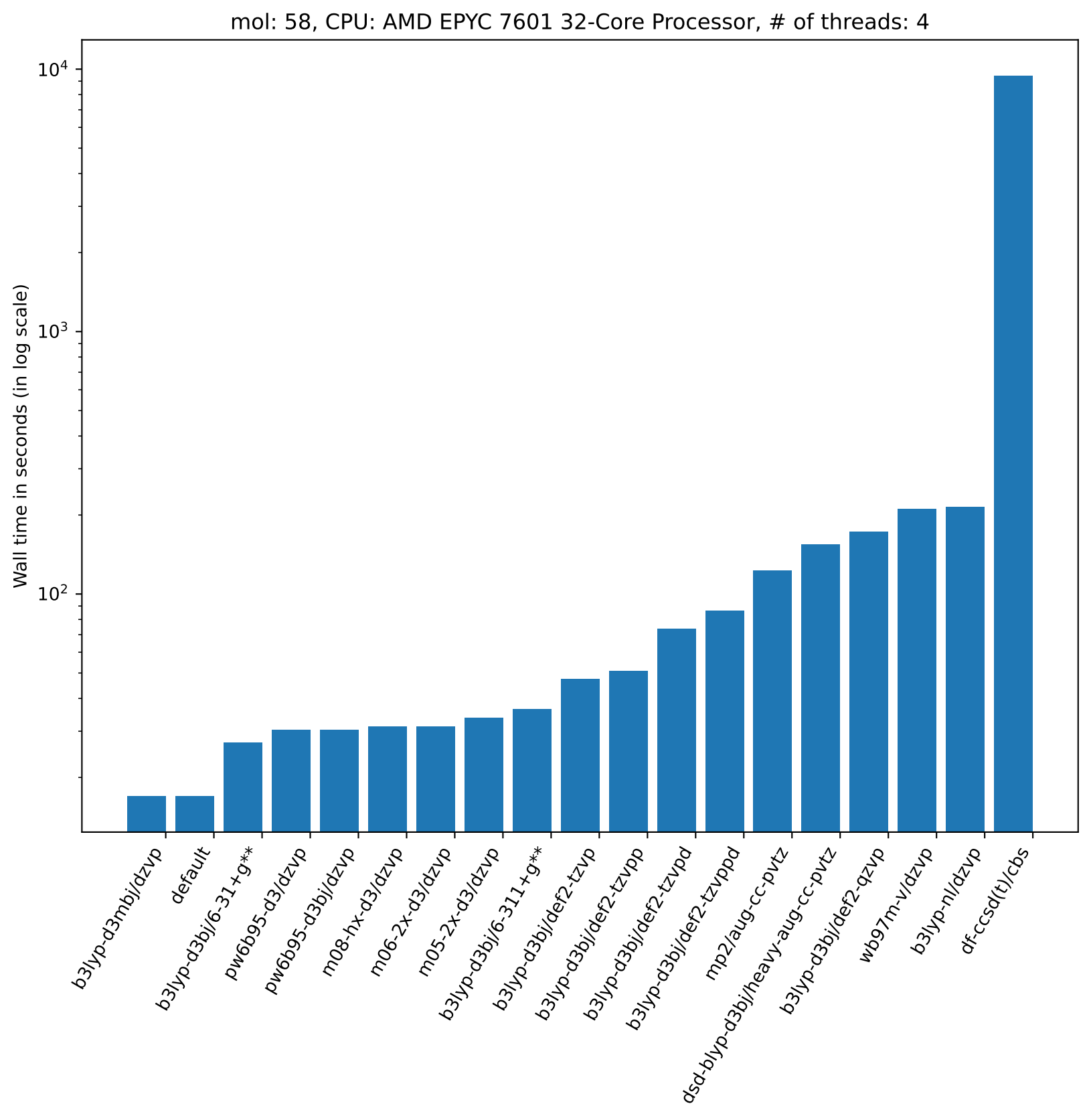

mol: 52, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs


mol: 53, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
10^1
b3lyp-d3mbj/dzvp
default
m05-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
m06-2x-d3/dzvp
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
b3lyp-nl/dzvp
wb97m-v/dzvp
df-ccsd(t)/cbs


mol: 54, CPU: Intel(R) Xeon(R) Gold 6240R CPU @ 2.40GHz, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m05-2x-d3/dzvp
m06-2x-d3/dzvp
b3lyp-d3bj/6-31+g**
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
dsd-blyp-d3bj/heavy-aug-cc-pvtz
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs


mol: 56, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^2
10^1
b3lyp-d3mbj/dzvp
default
m08-hx-d3/dzvp
m06-2x-d3/dzvp
m05-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
mp2/aug-cc-pvtz
b3lyp-d3bj/def2-tzvppd
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs


mol: 57, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^3
10^2
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
m05-2x-d3/dzvp
m06-2x-d3/dzvp
m08-hx-d3/dzvp
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs


mol: 58, CPU: AMD EPYC 7601 32-Core Processor, # of threads: 4
Wall time in seconds (in log scale)
10^4
10^3
10^2
b3lyp-d3mbj/dzvp
default
b3lyp-d3bj/6-31+g**
pw6b95-d3/dzvp
pw6b95-d3bj/dzvp
m08-hx-d3/dzvp
m06-2x-d3/dzvp
m05-2x-d3/dzvp
b3lyp-d3bj/6-311+g**
b3lyp-d3bj/def2-tzvp
b3lyp-d3bj/def2-tzvpp
b3lyp-d3bj/def2-tzvpd
b3lyp-d3bj/def2-tzvppd
mp2/aug-cc-pvtz
dsd-blyp-d3bj/heavy-aug-cc-pvtz
b3lyp-d3bj/def2-qzvp
wb97m-v/dzvp
b3lyp-nl/dzvp
df-ccsd(t)/cbs