



*Python-based **H**ierarchical **EN**vironment for **I**ntegrated **X**tallography*

Cryo_fit1 FAQ

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At my last step (8 cryo_fit), I see "step 0 correlation coefficient: nan" in my md.log file

This message often indicates when the initial atomic model is not placed into a cryo-EM map.

Try [dock in map](#)

How long does it take to run cryo_fit?

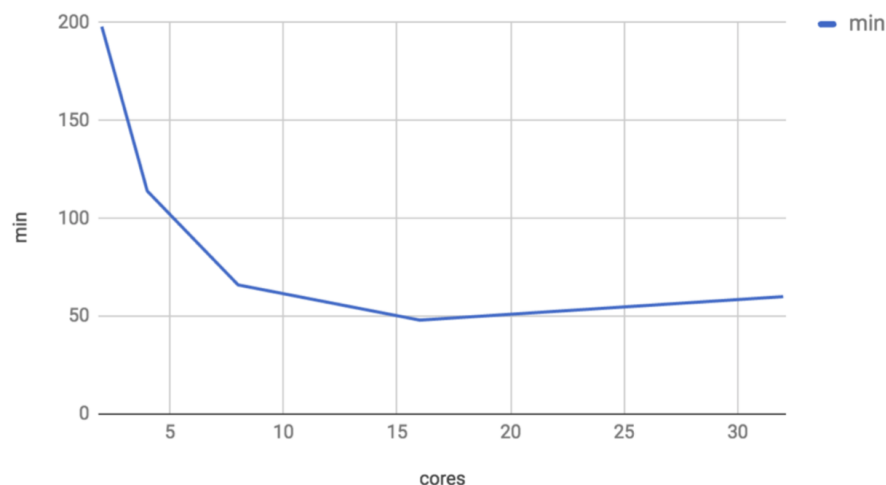
How long does it take to run cryo_fit?



- CentOS with 2 cores (2.7 Ghz)
 - tRNA (6,000 atoms) : 2.5 minutes
 - Nucleosome (26,000 atoms): 1 hr
 - Beta-galactosidase (64,000 atoms): 2.5 hrs
 - ribosome (386,000 atoms): 3~7 hrs
- macOS
 - 24 cores (2.7 Ghz)
 - (4~16 cores would give similar/better performance)
 - Beta-galactosidase (64,000 atoms): 3.9 hrs
 - 4 cores (3.1 Ghz)
 - Beta-galactosidase (64,000 atoms, 50,000 cryo_fit steps): 5.8 hrs

Benchmark with ribosome (same linux machine, 10k emsteps, 50k number_of_steps, 3x emweight)

min vs. cores



- Based on this result, number of cores is recommended up to 16

How to generate and record movie?

[Generate record movie by cryo_fit1](#)