
































AlphaFold 3

```
/fs00/software/alphafold/3.0.0/AlphaFold-v3.0.0.sif
```

0.

alphafold3  Google DeepMind                              

- data pipeline (cpu job)

```

${RUN_ALPHAFAOLD} --db_dir=/databases/ --model_dir=af3_weights/ \
--json_path=/host_iopath/input.json --output_dir=/host_iopath/ \
--run_inference=False

```

- inference (gpu job)

```

${RUN_ALPHAFAOLD} --db_dir=/databases/ --model_dir=af3_weights/ \
--json_path=/host_iopath/input.json --output_dir=/host_iopath/ \
--run_data_pipeline=False

```

XXXXXXXXXXXXXXXXXXXXXXXXXXXX

msa templatesXXXXXXXX

alphafold3XXXXXXXXXX

msa templatesXXXX

jsonXXXXXX

--run_data_pipeline=False

XXXXXXXXXXXXXXXXXXXX

msa templatesXX

jsonXXXXXXXX

DeepMind-input

documentationXXXX

msa templatesXXXXXXXX

jsonXXXXXX

msa templates json

XXXXXXXXXX

MbXXX

3. XXXXXXXX

XXXXXXXXXXXXXXXXXXXX

`${RUN_ALPHAFAOLD} --help` XXXXX

`run_alphafold.py` XXXXXXX

3XXXXXX

- `--input_dir` XXX `--json_path` XXXXXXXXXXXXXXXXXXXX `input_dir` XXXXX
`input_dir` XXXXX `json` XXXXXXXXXXXX
- `--jackhmmer_n_cpu` XXX `--nhmmer_n_cpu` XXXXXXXX `cpu cores` XXXXX
- XXXXXXXXXXXX `random seed` XXXXXXXXXXXX `alphafold3` `random seed`
XXXXXXXXXXXX `input.json` XXX

4. XXXXXXXXXXXXXXX

data pipelineXXXXXXXX

inferenceXXXX

gpuXXXXXXXXXXXXXXXX

- 2PV7XXXXXX `homomer` XXXXX 298

- 1AKE[] homomer[] 214

[] 83a100ib[] 734090d[] A100[] (memory 40 G) [] 4090d (memory 24 G) [] inference. [] 722080tiib[] 72rtxib[] . [] GPU [] [performance documentation](#)[] alphafold3[] A100(80G), A100(40 G)[] H100[] 4090[]

[] data pipeline[] inference[]

- [] 8 cpu cores[] 300[] msa[] templates[] 1.5-2 h[] [] msa[] templates[] 10 s[]
- [] alphafold3[] 5[] 100 s[] inference[]

[] performance[] [performance documentation](#)[]

5. []

[] 2PV7[] RMSD=4.410 ([] : Angstrom[]) [] A:B[] -[] A:B[] RMSD[] 4[] RMSD[] 3.012, 2.759, 2.971, 2.740. [] alphafold3[] alphafold2. [] 2[] subunits[] DockQ [] 0.499>0.23[] docking[]

1AKE[] 1AKE[] RMSD=18.176[] 4AKE[] RMSD=26.791 [] alphafold2-multimer[] subunits[] DockQ=0.019<<0.23 [] Alphafold3[] 4090d[] A100[]

“ dockQ (Mirabello & Wallner, 2024, Bioinformatics) [] subunits [] 0-1[] <0.23[] >0.8[]

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