







AlphaFold 3

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

0. ????


alphafold3 Google DeepMind   json

- data pipeline:


(multi-sequence alignment, msa)  (templates) 
 json 

- inference:  msa  templates  json  mmcif 
 confidence score

   alphafold3

 [term of use](#)

 Google DeepMind 

1. ????



```
path_to_af3db="/fsb/data/alphafold/3"
path_to_af3container="/fs00/software/alphafold/3.0.0/AlphaFold-v3.0.0.sif "

io_dir=</path/to/your/input/and/output>
weights_dir=<path/to/directory/containing/your/af3-weights>

RUN_ALPHAFOLD="apptainer run --nv --bind
```

```

${path_to_af3db}:/databases,${io_dir}:/host_iopath,${weights_dir}:/af3_weights
${path_to_af3container} python run_alphafold.py"

```

```

[[ ${path_to_af3db} ]] alphafold3 [[ ]] [${io_dir}]

[[ ]] [${weights_dir}] alphafold3 [[ ]]

```

run_alphafold.py  [github](#) 

$\frac{1}{10}$ $(\frac{1}{10})$

```

${RUN_ALPHAFOLD} --help

```

```
input.json  ${io dir}  alphafold3
```

```

${RUN_ALPHAFOLD} --db_dir=/databases/ --model_dir=/af3_weights/ \
--json path=/host iopath/input.json --output dir=/host iopath/

```

```

input.json name ${io_dir} data pipeline json
confidence score log stderr (
python logging )
documentation input documentation output
documentation

```

2. ???data pipeline?inference

The diagram illustrates a data pipeline architecture. It shows a sequence of components: 'data pipeline' (represented by a long bar), 'inference' (represented by a shorter bar), 'data pipeline' (another long bar), and 'cpu' (represented by a small bar). Below these, there are three 'gpu' components, each represented by a bar. Arrows indicate the flow of data from left to right, connecting the 'data pipeline' to 'inference', 'inference' to the second 'data pipeline', and the second 'data pipeline' to the 'cpu'. Additionally, there are arrows pointing from the 'cpu' to the first 'gpu', and from the first 'gpu' to the second 'gpu', and from the second 'gpu' to the third 'gpu'. The diagram also includes labels for 'data pipeline', 'inference', 'cpu', and 'gpu' in a larger font, and a label '(json)' in a smaller font.

```
[] bool[] --run_data_pipeline --run_inference
```

☐ True.

	:
	:

- 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

```

```

##### msa templates#####
alphafold3##### msa templates#### json##### --
run_data_pipeline=False##### msa templates#### json
##### DeepMind-input documentation##### msa templates##### json
##### msa templates#### json##### Mb####

```

3. ??????????

```

##### ${RUN_ALPHAFAOLD} --help #####
run_alphafold.py ##### 3#####

```

- --input_dir#### --json_path##### input_dir
input_dir##### json#####
- --jackhmmmer_n_cpu#### --nhmmmer_n_cpu##### cpu cores#####
- ##### random seed##### alphafold3 random seed
input.json

4. ????????????????

data pipeline##### inference##### gpu#####

- 2PV7##### homomer##### 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