·····AlphaFold·seed·····

·····seed·····AlphaFold 3 JSON·····ranking_scores·····seed·····

AlphaFold 3··JSON··modelSeeds·····seed·····seed···
·····seed·····
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·····AlphaFold 3·
·····JSON·····JSON·····AlphaFold Server·····JSON·····
·····Server·····dialect·version··ID·

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··· | ·····target | ·····

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modelSeeds | ·····seed | seed·····

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·····JSON···

·····seed·AlphaFold 3·····JSON·
·····seed·····seed·····
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```
#!/usr/bin/env bash
set -euo pipefail
: "${TARGET_SEQUENCE:?set the target amino-acid sequence}"
runner=/opt/alphafold3/run_alphafold.py
model_dir=/data/alphafold3/models
db_dir=/data/alphafold3/databases
root="$PWD/af3-target-001"
test -s "$runner"
test -d "$model_dir"
test -d "$db_dir"
test ! -e "$root" || { echo "output exists: $root" >&2; exit 2; }
mkdir -p "$root/inputs"
python3 - "$root/inputs/target_001.json" "$TARGET_SEQUENCE" <<'PY'
import json,sys
path,seq=sys.argv[1:]
seq=''.join(seq.split()).upper()
assert seq and all(c in 'ACDEFGHIKLMNPQRSTVWY' for c in seq)
job={'name':'target_001','modelSeeds':[101,202,303],
     'sequences':[{'protein':{'id':'A','sequence':seq}}],
     'dialect':'alphafold3','version':4}
with open(path,'w') as f: json.dump(job,f,indent=2)
json.load(open(path))
PY
sha256sum "$root/inputs/target_001.json" > "$root/input.sha256"
python3 "$runner" --input_dir "$root/inputs" --output_dir "$root/results"   --model_dir "$model_dir" --db_dir "$db_dir" > "$root/run.log" 2>&1
find "$root/results" -type f -name '*ranking_scores.csv' -print -quit | grep -q .
find "$root/results" -type f -name '*_model.cif' -print -quit | grep -q .
```

····JSON schema····4·····
·····name·····GPU·····
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··seed·····

·····seed·sample·····JSON·····ranking_scores.csv·····
·····seed·····seed····
···sample·····

ranking score·····pLDDT·PAE·····
·····seed·····
·····

·····seed·····

·····seed·····MSA/·····MSA·····CPU·····I/O·····
··GPU·····seed·····
·····CPU·····

····GPU·····seed·····
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AlphaFold 3·····modelSeeds·· https://github.com/google-deepmind/alphafold3/blob/main/docs/input.md

AlphaFold 3·····ranking_scores·· https://github.com/google-deepmind/alphafold3/blob/main/docs/output.md

AlphaFold 3····· https://github.com/google-deepmind/alphafold3/blob/main/docs/performance.md