·····relax·····

·····ColabFold relax·····PDB·····

ColabFold · relax ····· Amber ·····
····· PDB ·····
·····

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····· models.tsv·····ID··· PDB ····· ColabF
old/AlphaFold ·····

··· | ··

··ID·····SHA256 | ·····

····· | ··relax··

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·· colabfold_relax ···· PDB····· PDB····· --max-iterations ····· CPU····· --use
-gpu ··· GPU····· colabfold_relax --help ·····
·····

```
set -euo pipefail
mkdir -p relax-run-001/logs relax-run-001/output
python -c 'from importlib.metadata import version; print(version("colabfold"))'   > relax-run-001/colabfold-version.txt
colabfold_relax input/model_001.pdb relax-run-001/output/model_001.pdb   --max-iterations 2000   > relax-run-001/logs/model_001.log 2>&1
test -s relax-run-001/output/model_001.pdb
sha256sum input/model_001.pdb relax-run-001/output/model_001.pdb   > relax-run-001/checksums.txt
```

·····relax ··· CPU
····· GPU ····· CPU·····

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·····ID····· stderr·····
····· pending·running·success·failed·····
·····

·····

·····ID····· PDB · C· ·
····· PDB/mmCIF ····· altloc·····
·····

```
from pathlib import Path
import math, sys

def ca_records(path):
    rows = []
    for line in Path(path).read_text().splitlines():
        if not line.startswith('ATOM  ') or line[12:16].strip() != 'CA':
            continue
        if len(line) < 54:
            raise ValueError('PDB·····')
        xyz = [float(line[a:b]) for a, b in ((30,38),(38,46),(46,54))]
        if not all(math.isfinite(v) for v in xyz):
            raise ValueError('·····')
        rows.append((line[21], line[22:26], line[26], line[17:20]))
    if not rows:
        raise ValueError('····C-alpha··')
    if len(rows) != len(set(rows)):
        raise ValueError('····C-alpha····')
    return rows

before, after = map(ca_records, sys.argv[1:3])
if before != after:
    raise SystemExit('·····/·····')
print(f'·····{len(after)}···')
```

·····re
lax ····· pLDDT · PAE ·····

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…… PDB… PDB……
……ColabFold · relax ……
…… Amber ……

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ColabFold··relax…… https://github.com/sokrypton/ColabFold/blob/main/colabfold/relax.py

ColabFold…… https://github.com/sokrypton/ColabFold/blob/main/pyproject.toml

ColabFold…… https://github.com/sokrypton/ColabFold