

# HIGH PERFORMANCE RESEARCH COMPUTING

## Introduction to AlphaFold for 3D Protein Structure Prediction on Grace



High Performance  
Research Computing  
DIVISION OF RESEARCH

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# AlphaFold for 3D Protein Structure Prediction on Grace

- Resources and Limitations
- Database Files
- Running AlphaFold
  - Google Colab
  - ChimeraX + Google Colab
  - Grace GPU or non-GPU nodes
- Visualization of Results
  - job resource usage
  - view predictions in ChimeraX
  - plotting pLDDT values
- Alternative Workflows

# Finding AlphaFold template job scripts using GCATemplates on Grace

- Genomic Computational Analysis Templates have example input data so you can run the script for demo purposes.

```
mkdir $SCRATCH/af_demo
```

```
cd $SCRATCH/af_demo
```

```
gcatemplates
```

- Type **s** for search then enter **alphafold** to search for the alphafold **2.3.1** template. script and select the **reduced\_dbs** script
- Review the script and submit the job script, which takes about 1 hour to complete using 1 x A100.

```
sbatch run_alphafold_2.3.1_monomer_ptm_reduced_dbs_a100_grace.sh
```

```
Bioinformatics GCATemplates (GRACE)

CATEGORY
1. FASTA files
2. FASTQ files (QC, trim, SRA)
3. Genome assembly
4. Metagenomics
5. PacBio tools
6. Phylogenetics
7. Population genetics
8. Protein tools
9. RNA-seq
10. SNPs & indels
11. Sequence alignments
12. Simulate data

s search
q quit

Select:s
```

# Resource Limitations

- AlphaFold
  - currently AlphaFold can only utilize one GPU
  - about 90% of processing is done on CPU when using DeepMind's workflow
- AlphaFold on HPRC Grace
  - sometimes GPU not detected on certain nodes
- AlphaFold in Google Colab (web browser or ChimeraX app)
  - no guarantee of available resources in Colab
  - runs as a Jupyter notebook on Google Colab cloud servers
    - 12GB RAM max
    - a notebook can run for up to 12 hours per day
      - 24 hours per day with Colab Pro (\$9.99/month)
    - not suitable for large predictions

# AlphaFold Databases on Grace

/scratch/data/bio/alphafold/2.3.2

Database	Size	File Count	monomer	multimer
bfd	1.8T	7	✓	✓
mgnify	120G	2	✓	✓
params	5.3G	17	✓	✓
pdb70	56G	10	✓	-
pdb_mmcif	264G	211,106	✓	✓
pdb_seqres	257M	2	-	✓
uniprot	114G	2	-	✓
uniref30	467G	15	✓	✓
uniref90	77G	2	✓	✓
small_bfd	17G	2	✓	✓
example_data	6K	5	✓	✓
<b>TOTAL</b>	<b>2.9T</b>	<b>211,170</b>		

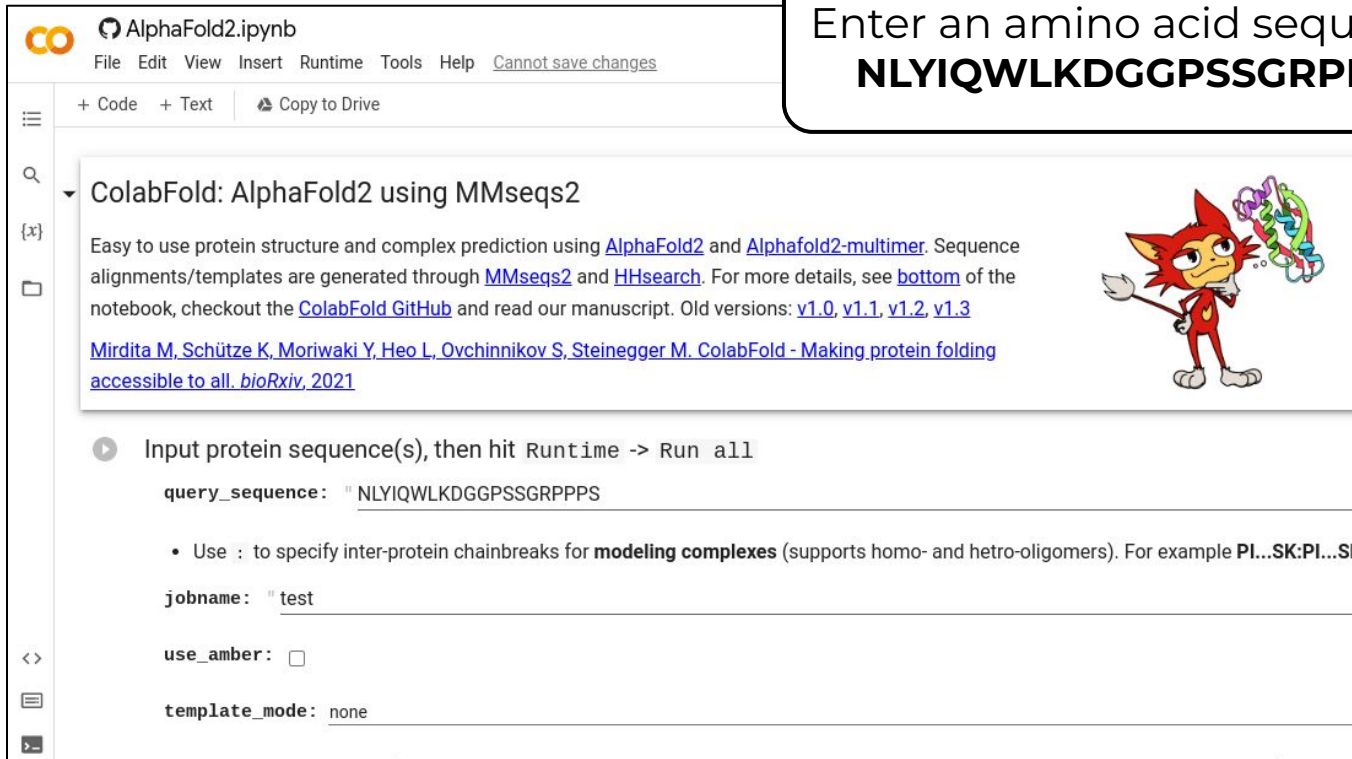
# Resources for Running AlphaFold

- Run as a Jupyter [Notebook](#) on Google Colab in web browser.
- Run as a Jupyter Notebook on Google Colab in ChimeraX.
  - ChimeraX Interactive App on HPRC Grace Portal
    - <https://portal-grace.hprc.tamu.edu>
- Run as a Slurm job script on Grace.


<https://hprc.tamu.edu/kb/Software/AlphaFold>

# ColabFold AlphaFold2 Jupyter Notebook

Enter an amino acid sequence  
**NLYIQWLKDGGPSSGRPPPS**




AlphaFold2.ipynb  
File Edit View Insert Runtime Tools Help [Cannot save changes](#)

+ Code + Text  Copy to Drive

### ColabFold: AlphaFold2 using MMseqs2

Easy to use protein structure and complex prediction using [AlphaFold2](#) and [Alphafold2-multimer](#). Sequence alignments/templates are generated through [MMseqs2](#) and [HHsearch](#). For more details, see [bottom](#) of the notebook, checkout the [ColabFold GitHub](#) and read our manuscript. Old versions: [v1.0](#), [v1.1](#), [v1.2](#), [v1.3](#)

[Mirdita M, Schütze K, Moriwaki Y, Heo L, Ovchinnikov S, Steinegger M. ColabFold - Making protein folding accessible to all. bioRxiv, 2021](#)



▶ Input protein sequence(s), then hit Runtime -> Run all

query\_sequence: " NLYIQWLKDGGPSSGRPPPS

---

- Use : to specify inter-protein chainbreaks for **modeling complexes** (supports homo- and hetro-oligomers). For example **PI...SK:PI...SK**

jobname: " test

---

use\_amber:

template\_mode: none

# ChimeraX

- Can be used to visualize protein structures
- Can be launched using the Grace portal
  - [portal-grace.hprc.tamu.edu](https://portal-grace.hprc.tamu.edu)
- Can be used to run AlphaFold using the daily build version (2022.02.22+)
  - uses Google Colab with limited resources

## ChimeraX

This app will launch a [UCSF ChimeraX](#) GUI on [Grace](#)

[UCSF ChimeraX](#) is a program for the interactive visualization and analysis of molecular structures and related data, including density maps, trajectories, and sequence alignments.

### chimeraX version

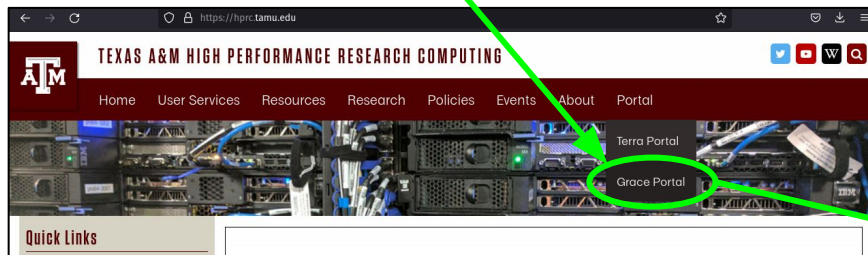
ChimeraX/2022.02.22





# ChimeraX

- Launch a ChimeraX job on the Grace portal [portal-grace.hprc.tamu.edu](https://portal-grace.hprc.tamu.edu)
  - select Node Type: CPU only
  - AlphaFold runs on Google Colab GPUs so we can use a non-GPU for running ChimeraX
- ChimeraX will be used later for the following
  - run AlphaFold in Google Colab
  - visualize results from an AlphaFold job on Grace

A screenshot of the TAMU HPRC OnDemand job configuration page for ChimeraX. The page title is "TAMU HPRC OnDemand (Grace)". The navigation menu includes Files, Jobs, Clusters, Interactive Apps, and Dashboard. The breadcrumb trail is "Home / My Interactive Sessions / ChimeraX". The page is divided into two main sections: "Interactive Apps" and "ChimeraX". The "Interactive Apps" section lists various applications: Bio, Beauti, CRISPR-Local, Gap5, IGV, Mauve, RNAlysis, Structure, XtalOpt, GUI, ANSYS Workbench, Abaqus/CAE, MATLAB, ParaView, VNC, Imaging, and ChimeraX. The "ChimeraX" section contains the following configuration options:

- ChimeraX: This app will launch a UCSF ChimeraX GUI on Grace
- UCSF ChimeraX is a program for the interactive visualization and analysis of molecular structures and related data, including density maps, trajectories, and sequence alignments.
- chimerax version: ChimeraX/2022.02.22
- Number of hours: 2
- Number of cores: 1
- Specify number of cores [1-48] allocated on a node from the Grace cluster.
- Total memory (GB): 7
- Requested total memory (7 - 360GB)
- Node type: CPU only (circled in green)
- Account: (empty field)
- This field is optional.

# Running AlphaFold on Grace

- Can be run as a job script requesting one GPU
- Shared databases are available: 2.6TB total size

<b>AlphaFold 2.2.3</b>	<b>monomer_ptm 20 aa</b>	<b>multimer 98 &amp; 73 aa</b>
A100	36 minutes	4 hours 49 minutes
A40	35 minutes	-
RTX 6000	33 minutes	4 hours 44 minutes
T4	33 minutes	4 hours 45 minutes
CPU only	40 minutes	6 hours 11 minutes

- Can be run in ChimeraX from the Grace portal
  - using the ChimeraX AlphaFold option
  - all processing done on Google cloud servers

# Viewing Maximum Available Resources

The **maxconfig** command will show the recommended Slurm parameters for the maximum available resources (cores, memory, time) per node for a specified accelerator or partition (default Grace partition: long) and show SUs charged.

```
[username@grace ~]$ maxconfig

Grace partitions:  short medium long xlong vnc gpu bigmem special gpu-a40
Grace GPUs in gpu partition:  a100:2 a40:3 rtx:2 t4:4

Showing max parameters (cores, mem, time) for partition long

CPU-billing * hours * nodes =  SUs
          48 *   168 *     1 = 8,064

#!/bin/bash
#SBATCH --job-name=my_job
#SBATCH --time=7-00:00:00
#SBATCH --nodes=1          # max 64 nodes for partition long
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=48
#SBATCH --mem=360G
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j
```

# Viewing Maximum Available Resources

See the recommended Slurm parameters for requesting 1 x A100 GPU with 1/2 the total CPUs and memory since there are 2 x A100s per node.

```
[username@grace ~]$ maxconfig -g a100 -G 1
```

```
Grace partitions:  short medium long xlong vnc gpu bigmem special gpu-a40
Grace GPUs in gpu partition:  a100:2 a40:3 rtx:2 t4:4
```

```
Showing 1/2 of total cores and memory for using 1 x a100 GPU
```

```
(CPU-billing + (GPU-billing * GPU-count)) * hours * nodes = SUs
(          25 + (          72 *          1)) * 96 * 1 = 9,312
```

```
#!/bin/bash
#SBATCH --job-name=my_job
#SBATCH --time=4-00:00:00
#SBATCH --nodes=1          # max 32 nodes for partition gpu
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=24
#SBATCH --mem=180G
#SBATCH --gres=gpu:a100:1
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j
```

# Grace SUs Charged: GPU vs CPU-only Jobs

show SU rate for 1 day CPU-only

```
maxconfig -d 1
```

```
CPU-billing * hours * nodes = SUs
  48 *      24 *      1 = 1,152
```

show SU rate for 1 x A100 GPU for 1 day

```
maxconfig -g a100 -G 1 -d 1
```

```
(CPU-billing + (GPU-billing * GPU-count)) * hours * nodes = SUs
(      48 + (      72 *      1)) *      24 *      1 = 2,328
```

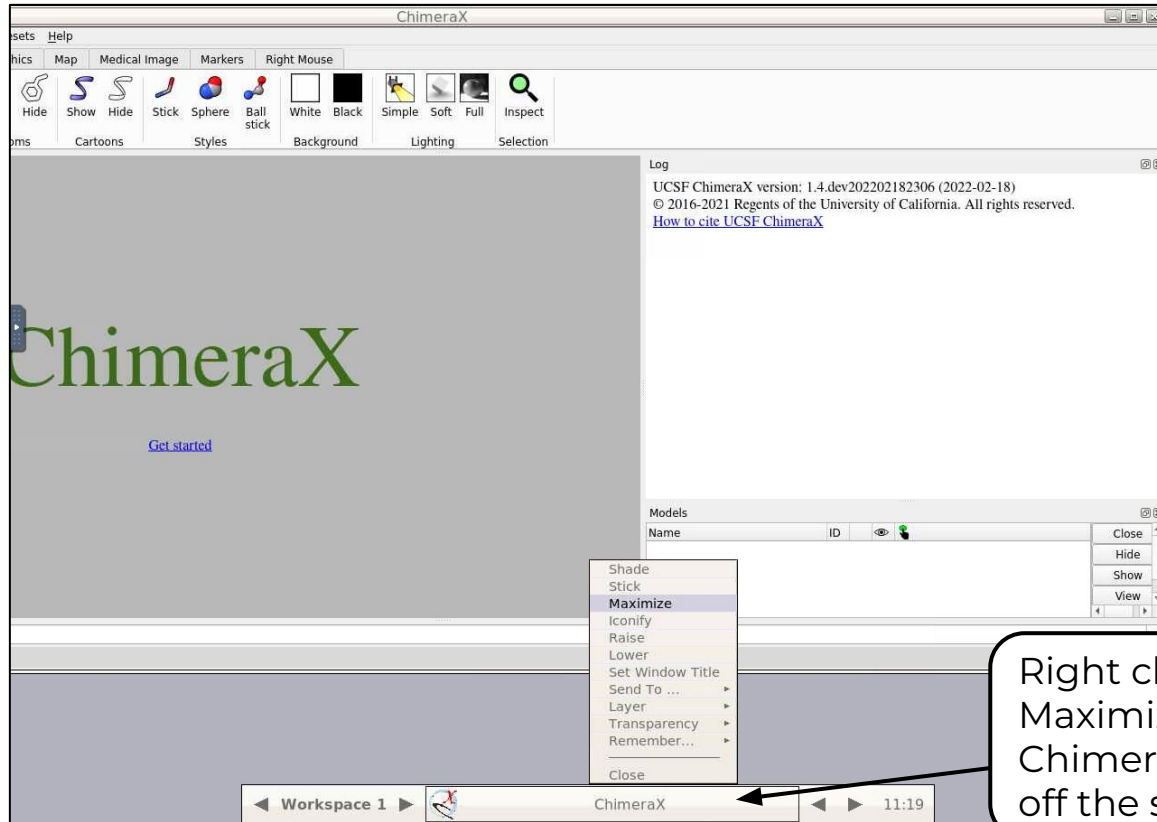
show SU charge rate

```
maxconfig -h
```

```
SU rate per GPU:
GPU    SUs per hour
----  -
a100   72
a40    48
rtx    48
t4     24
```

# AlphaFold with ChimeraX + Google Colab

# Maximize ChimeraX Window



Right click and select Maximize if the ChimeraX window is off the screen

# AlphaFold with ChimeraX

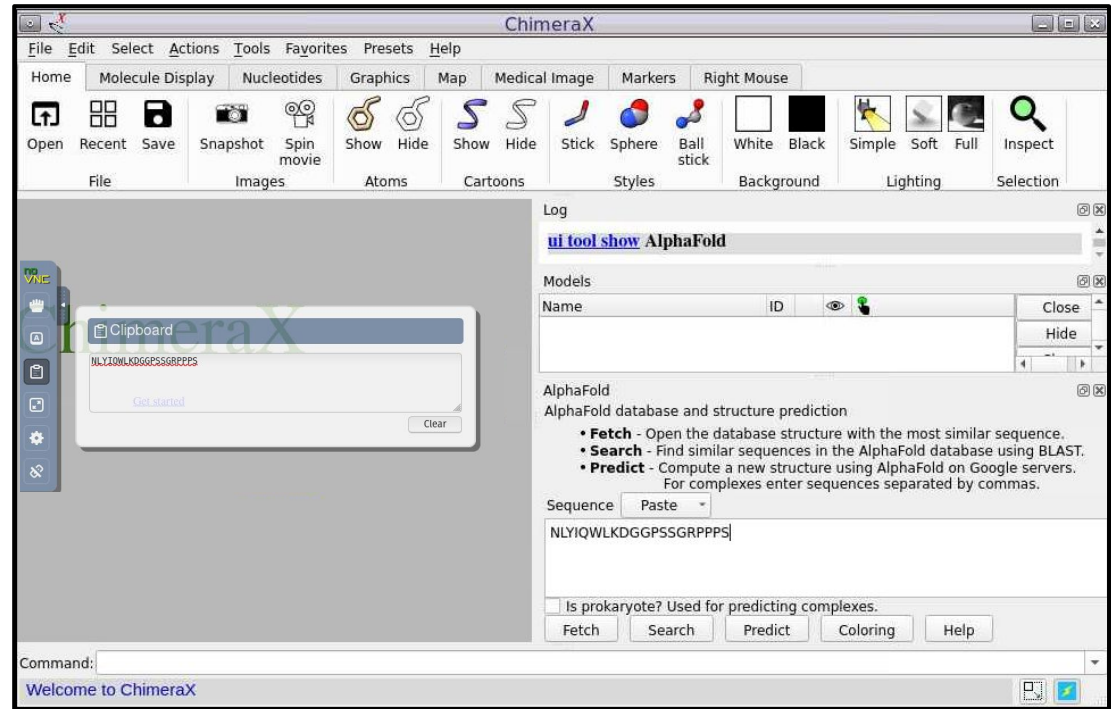
- Launch ChimeraX using the HPRC Grace portal
- Select the AlphaFold Structure Prediction option





# AlphaFold with ChimeraX

- Enter an amino acid sequence  
**NLYIQWLKDGGPSSGRPPPS**
  - or paste in Clipboard first then paste in Sequence field.
- Click Predict.
- A Google Colab page will start and prompt you for your Google login.
- Login to your Google account to begin processing.
- Prediction completes in about 1 hour.
- Not ideal for large prediction jobs



# AlphaFold Grace Job Scripts

# Example AlphaFold Job Script

- **multimer**
  - dbs in **red** are required for multimer
- AlphaFold can only use one GPU so reserve half the CPU and memory resources so another job can use the other GPU.
  - Grace compute nodes have 360GB of available memory and 48 cores.

```
#!/bin/bash
#SBATCH --job-name=alphafold          # job name
#SBATCH --time=2-00:00:00            # max job run time dd-hh:mm:ss
#SBATCH --ntasks-per-node=1         # tasks (commands) per compute node
#SBATCH --cpus-per-task=24          # CPUs (threads) per command
#SBATCH --mem=180G                   # total memory per node
#SBATCH --gres=gpu:a100:1           # request 1 A100 GPU
#SBATCH --output=stdout.%x.%j       # save stdout to file
#SBATCH --error=stderr.%x.%j        # save stderr to file

module purge
module load GCC/11.3.0 OpenMPI/4.1.4 AlphaFold/2.3.1-CUDA-11.7.0

ALPHAFOLD_DATA_DIR=/scratch/data/bio/alphafold/2.3.2

# run jobstats in the background (&) to monitor cpu and gpu usage
jobstats &

run_alphafold.py \
--use_gpu_relax \
--data_dir=$ALPHAFOLD_DATA_DIR \
--uniref90_database_path=$ALPHAFOLD_DATA_DIR/uniref90/uniref90.fasta \
--uniref30_database_path=$ALPHAFOLD_DATA_DIR/uniref30/UniRef30_2023_02 \
--mgnify_database_path=$ALPHAFOLD_DATA_DIR/mgnify/mgy_clusters_2025_05.fa \
--bfd_database_path=$ALPHAFOLD_DATA_DIR/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sorted_opt \
--model_preset=multimer \
--pdb_seqres_database_path=$ALPHAFOLD_DATA_DIR/pdb_seqres/pdb_seqres.txt \
--uniprot_database_path=$ALPHAFOLD_DATA_DIR/uniprot/uniprot.fasta \
--template_mmcif_dir=$ALPHAFOLD_DATA_DIR/pdb_mmcif/mmcif_files \
--obsolete_pdbs_path=$ALPHAFOLD_DATA_DIR/pdb_mmcif/obsolete.dat \
--max_template_date=2024-1-1 \
--db_preset=full_dbs \
--output_dir=out_alphafold \
--fasta_paths=/scratch/data/bio/alphafold/example_data/T1083_T1084_multimer.fasta

# run jobstats to create a graph of cpu and gpu usage for this job
jobstats
```

# Example AlphaFold Job Script

- **monomer**
  - dbs in **red** required for monomer
- **monomer\_ptm**
  - will produce pTM scores that can be graphed using AlphaPickle.
- AlphaFold can only use one GPU so reserve half the CPU and memory resources so another job can use the other GPU.

```
#!/bin/bash
#SBATCH --job-name=alphafold           # job name
#SBATCH --time=2-00:00:00             # max job run time dd-hh:mm:ss
#SBATCH --ntasks-per-node=1          # tasks (commands) per compute node
#SBATCH --cpus-per-task=24           # CPUs (threads) per command
#SBATCH --mem=180G                    # total memory per node
#SBATCH --gres=gpu:a100:1            # request 1 A100 GPU
#SBATCH --output=stdout.%x.%j        # save stdout to file
#SBATCH --error=stderr.%x.%j         # save stderr to file

module purge
module load GCC/11.3.0 OpenMPI/4.1.4 AlphaFold/2.3.1-CUDA-11.7.0

ALPHAFOLD_DATA_DIR=/scratch/data/bio/alphafold/2.3.2

# run jobstats in the background (&) to monitor cpu and gpu usage
jobstats &

run_alphafold.py \
--use_gpu_relax \
--data_dir=$ALPHAFOLD_DATA_DIR \
--uniref90_database_path=$ALPHAFOLD_DATA_DIR/uniref90/uniref90.fasta \
--uniref30_database_path=$ALPHAFOLD_DATA_DIR/uniref30/UniRef30_2023_02 \
--mgnify_database_path=$ALPHAFOLD_DATA_DIR/mgnify/mgy_clusters_2022_05.fa \
--bfd_database_path=$ALPHAFOLD_DATA_DIR/bfd/bfd_metaclust_clu_complete_id30_c90_final_seq.sorted_opt \
--template_mmcif_dir=$ALPHAFOLD_DATA_DIR/pdb_mmcif/mmcif_files \
--obsolete_pdbs_path=$ALPHAFOLD_DATA_DIR/pdb_mmcif/obsolete.dat \
--pdb70_database_path=$ALPHAFOLD_DATA_DIR/pdb70/pdb70 \
--model_preset=monomer \
--max_template_date=2024-1-1 \
--db_preset=full_dbs \
--output_dir=out_alphafold \
--fasta_paths=/scratch/data/bio/alphafold/example_data/T1083.fasta

# run jobstats to create a graph of cpu and gpu usage for this job
jobstats
```

# Example AlphaFold Job Script

- **monomer + reduced\_dbs**
- dbs in **red** required for monomer + reduced\_dbs
- Small\_bfd\_database is a subset of BFD and is generated by taking the first non-consensus sequence from every cluster in BFD.
- AlphaFold can only use one GPU so reserve half the CPU and memory resources so another job can use the other GPU.

```
#!/bin/bash
#SBATCH --job-name=alphafold          # job name
#SBATCH --time=2-00:00:00            # max job run time dd-hh:mm:ss
#SBATCH --ntasks-per-node=1         # tasks (commands) per compute node
#SBATCH --cpus-per-task=24          # CPUs (threads) per command
#SBATCH --mem=180G                   # total memory per node
#SBATCH --gres=gpu:a100:1           # request 1 A100 GPU
#SBATCH --output=stdout.%x.%j       # save stdout to file
#SBATCH --error=stderr.%x.%j        # save stderr to file

module purge
module load GCC/11.3.0 OpenMPI/4.1.4 AlphaFold/2.3.1-CUDA-11.7.0

ALPHAFOLD_DATA_DIR=/scratch/data/bio/alphafold/2.3.2

# run jobstats in the background (&) to monitor cpu and gpu usage
jobstats &

run_alphafold.py \
--use_gpu_relax \
--data_dir=$ALPHAFOLD_DATA_DIR \
--uniref90_database_path=$ALPHAFOLD_DATA_DIR/uniref90/uniref90.fasta \
--mgnify_database_path=$ALPHAFOLD_DATA_DIR/mgnify/mgy_clusters_2022_05.fa \
--small_bfd_database_path=$ALPHAFOLD_DATA_DIR/small_bfd/bfd-first_non_consensus_sequences.fasta \
--model_preset=monomer \
--pdb70_database_path=$ALPHAFOLD_DATA_DIR/pdb70/pdb70 \
--template_mmcif_dir=$ALPHAFOLD_DATA_DIR/pdb_mmcif/mmcif_files \
--obsolete_pdbs_path=$ALPHAFOLD_DATA_DIR/pdb_mmcif/obsolete.dat \
--max_template_date=2024-1-1 \
--db_preset=reduced_dbs \
--output_dir=out_alphafold \
--fasta_paths=/scratch/data/bio/alphafold/example_data/1L2Y.fasta

# run jobstats to create a graph of cpu and gpu usage for this job
jobstats
```

# Unified Memory

```
#!/bin/bash
#SBATCH --job-name=alphafold           # job name
#SBATCH --time=2-00:00:00              # max job run time dd-hh:mm:ss
#SBATCH --ntasks-per-node=1           # tasks (commands) per compute node
#SBATCH --cpus-per-task=24            # CPUs (threads) per command
#SBATCH --mem=180G                    # total memory per node
#SBATCH --gres=gpu:a100:1             # request 1 A100 GPU
#SBATCH --output=stdout.%x.%j         # save stdout to file
#SBATCH --error=stderr.%x.%j         # save stderr to file

# version 2.3.1 has the unified memory variable already configured
module purge
module load GCC/11.3.0 OpenMPI/4.1.4 AlphaFold/2.3.1-CUDA-11.7.0
```

- Unified memory can be used to request more than just the total GPU memory for the JAX step in AlphaFold.
  - A100 GPU has 40GB memory.
  - `XLA_PYTHON_CLIENT_MEM_FRACTION` (configured to 3.0 in the AlphaFold 2.3.1 module)
- this example script has 120 GB of unified preallocated memory:
  - 40 GB from A100 GPU + 80 GB DDR from motherboard.

[https://jax.readthedocs.io/en/latest/gpu\\_memory\\_allocation.html](https://jax.readthedocs.io/en/latest/gpu_memory_allocation.html)

# AlphaFold Results Visualization

# Visualize Results with ChimeraX

AlphaFold Run

alphafold21\_predict\_colab.ipynb

File Edit View Insert Runtime Tools Help [Cannot save changes](#)

+ Code + Text Copy to Drive Reconnect Editing

```
31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71
Merging chunk sequence alignments for mgnify
```

**Runtime disconnected**

Your runtime has been disconnected due to inactivity or reaching its maximum duration. [Learn more](#)

If you are interested in longer runtimes with more lenient timeouts, you may want to check out [Colab Pro](#).

Close Reconnect

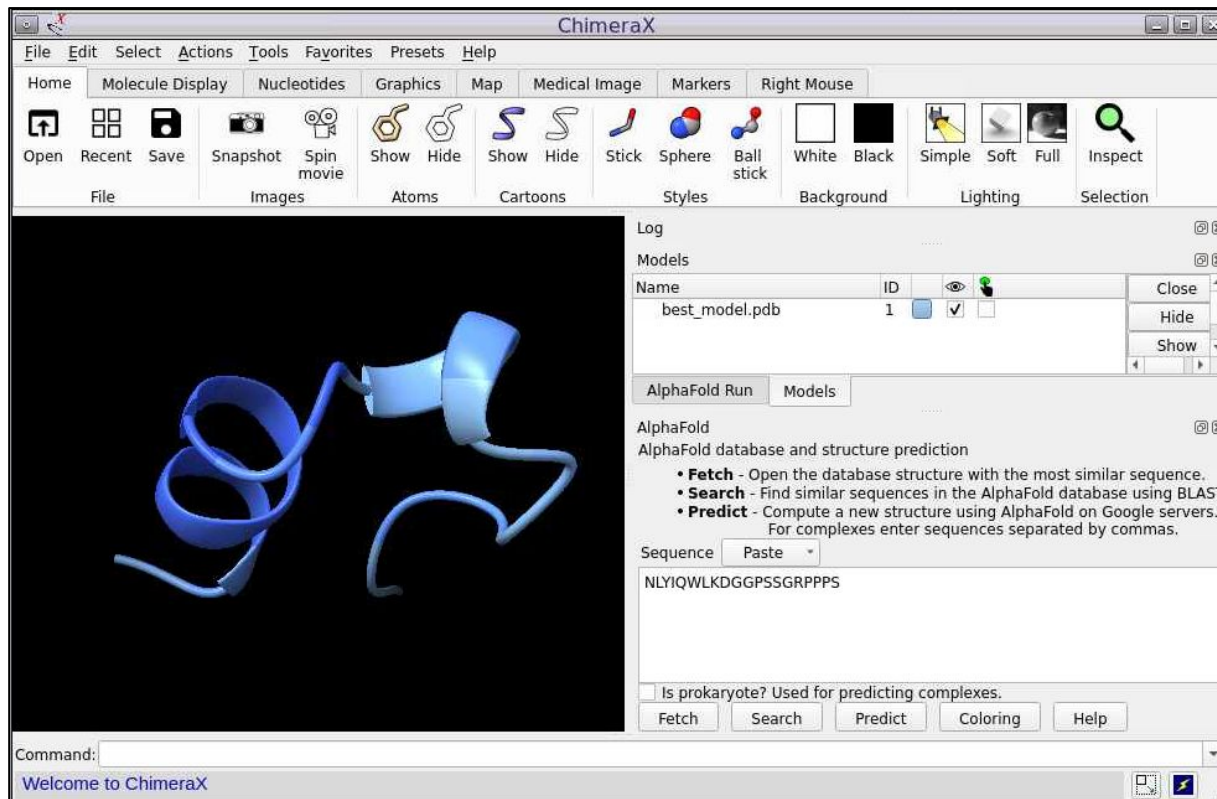
```
Computing structures using 5 AlphaFold parameter sets:
model_1_ptm model_2_ptm model_3_ptm model_4_ptm model_5_ptm
Energy minimizing best structure model_3_ptm with OpenMM and Amber forcefield
Structure prediction completed.
```

✓ 1h 4m 59s completed at 3:14 PM

Click the minimize button to return to ChimeraX or click Reconnect then minimize



# Visualize AlphaFold Google Colab Results with ChimeraX



# View PDB Structure if Available

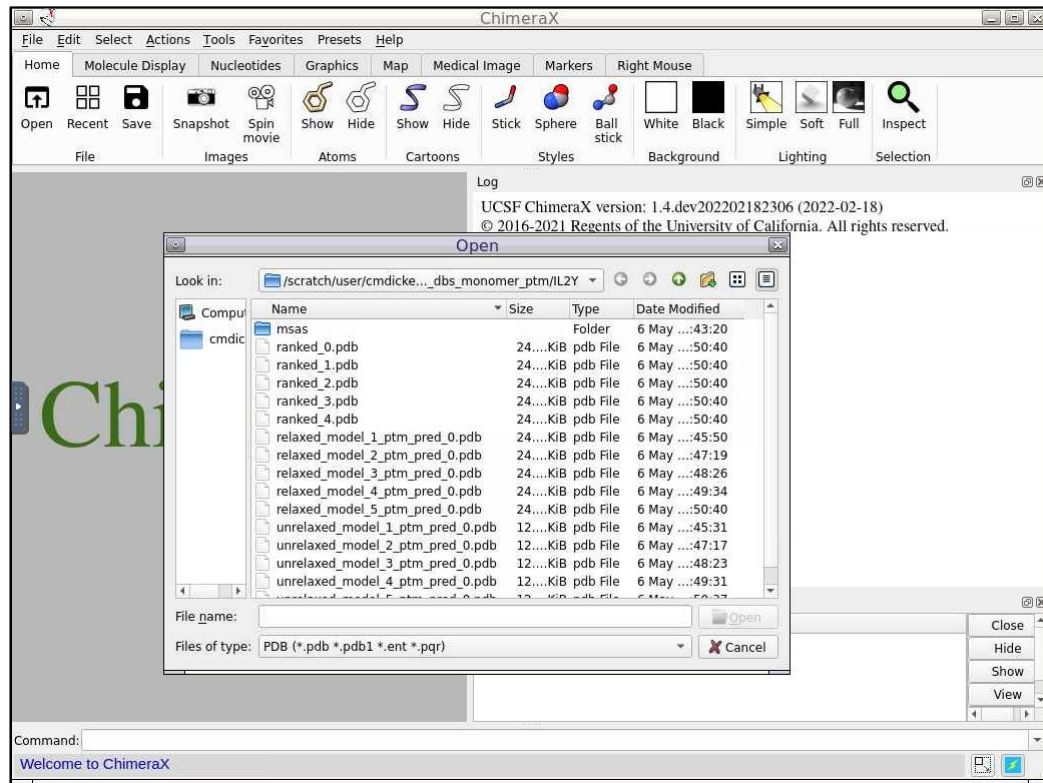
The screenshot displays the ChimeraX software interface. The main window shows a protein structure rendered in a pink ribbon style against a black background. The interface includes a menu bar (File, Edit, Select, Actions, Tools, Favorites, Presets, Help) and a toolbar with various icons for file operations, image management, atom display, cartoons, styles, background, lighting, and selection. On the right side, there are several panels: 'Log' with entries for 'close #2' and 'show #!3 models'; 'Models' with a table listing 'best\_model.pdb' (ID 1) and '1l2y group' (ID 3); 'AlphaFold' with instructions for Fetch, Search, and Predict, and a sequence input field containing 'NLYIQWLKGGPSSGRPPPS'; and 'AlphaFold Run' with a Jupyter Notebook interface for 'alphafold21\_predict\_colab.ipynb' showing a completion time of 1h 6m 47s.

Name	ID	Visible	Selected	Close
best_model.pdb	1	<input type="checkbox"/>	<input type="checkbox"/>	
1l2y group	3	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	

Command: `open 1L2Y`

type **open** and  
the protein  
name **1L2Y**

# Visualize AlphaFold Grace Results with ChimeraX



# AlphaFold Confidence Metrics

# AlphaPickle for Visualization of Confidence Scores

AlphaPickle can be used to create graphs for pLDDT and PAE scores.

- graphing PAE scores is only available for the **monomer\_ptm** and **multimer** model presets.
  - load the AlphaPickle module at the beginning of the job script
  - run AlphaPickle at the end, specifying the output directory used in the run\_alphafold.py command.
- pLDDT: scale from 0 - 100 of per-residue estimate of prediction confidence
  - PAE: Predicted Alignment Error

<https://github.com/mattarnoldbio/alphapickle>

```
#!/bin/bash
#SBATCH --job-name=alphafold          # job name
#SBATCH --time=2-00:00:00            # max job run time dd-hh:mm:ss
#SBATCH --ntasks-per-node=1         # tasks (commands) per compute node
#SBATCH --cpus-per-task=24          # CPUs (threads) per command
#SBATCH --mem=180G                   # total memory per node
#SBATCH --gres=gpu:a100:1           # request 1 A100 GPU
#SBATCH --output=stdout.%x.%j       # save stdout to file
#SBATCH --error=stderr.%x.%j        # save stderr to file

module purge
module load GCC/11.3.0 OpenMPI/4.1.4 AlphaFold/2.3.1-CUDA-11.7.0
module load AlphaPickle/1.4.1

ALPHAFOLD_DATA_DIR=/scratch/data/bio/alphafold/2.3.2

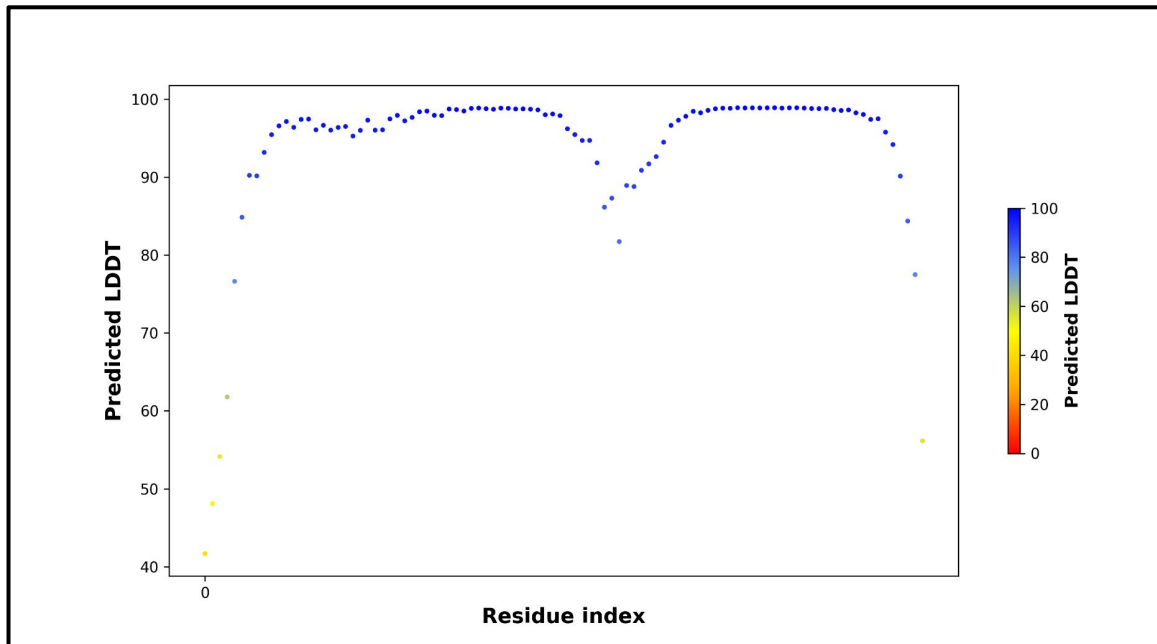
# run jobstats in the background (&) to monitor cpu and gpu usage
jobstats &

run_alphafold.py \
  --use_gpu_relax \
  --data_dir=$ALPHAFOLD_DATA_DIR \
  --uniref90_database_path=$ALPHAFOLD_DATA_DIR/uniref90/uniref90.fasta \
  --mgnify_database_path=$ALPHAFOLD_DATA_DIR/mgnify/mgy_clusters_2022_05.fa \
  --small_bfd_database_path=$ALPHAFOLD_DATA_DIR/small_bfd/bfd-first_non_consensus_sequences.fasta \
  --model_preset=monomer_ptm \
  --pdb70_database_path=$ALPHAFOLD_DATA_DIR/pdb70/pdb70 \
  --template_mmcif_dir=$ALPHAFOLD_DATA_DIR/pdb_mmcif/mmcif_files \
  --obsolete_pdbs_path=$ALPHAFOLD_DATA_DIR/pdb_mmcif/obsolete.dat \
  --max_template_date=2024-1-1 \
  --db_preset=reduced_dbs \
  --output_dir=out_alphafold_2.3.1 \
  --fasta_paths=/scratch/data/bio/alphafold/example_data/1L2Y.fasta

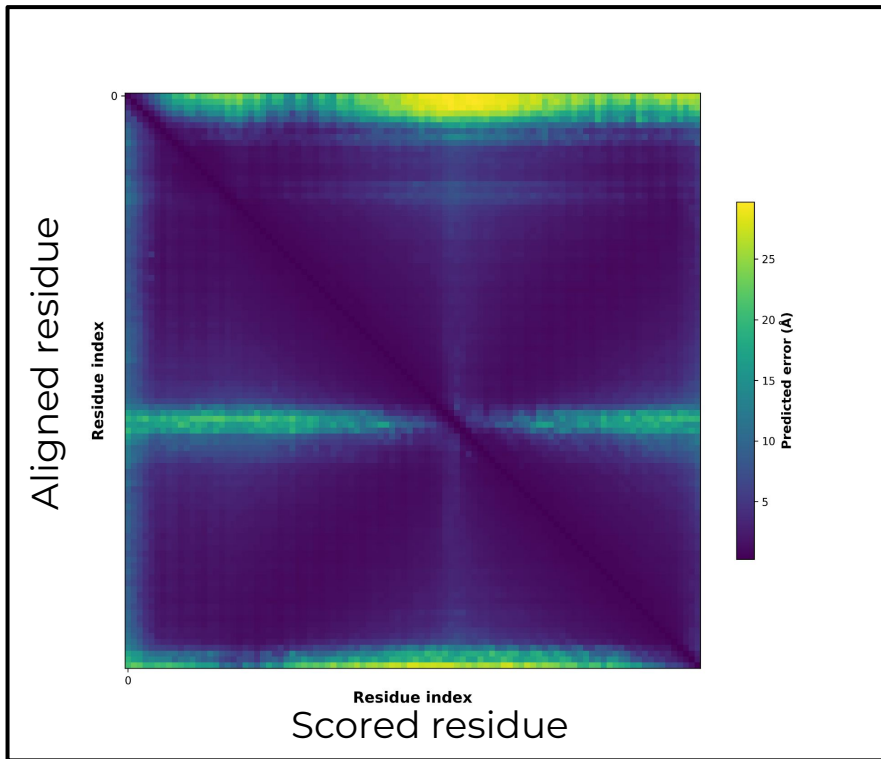
# graph pLDDT and PAE .pkl files; part of the fasta file name will be the pickle directory name
run_AlphaPickle.py -od out_alphafold_2.3.1/1L2Y

# run jobstats to create a graph of cpu and gpu usage for this job
jobstats
```

# Visualize AlphaFold pLDDT Scores



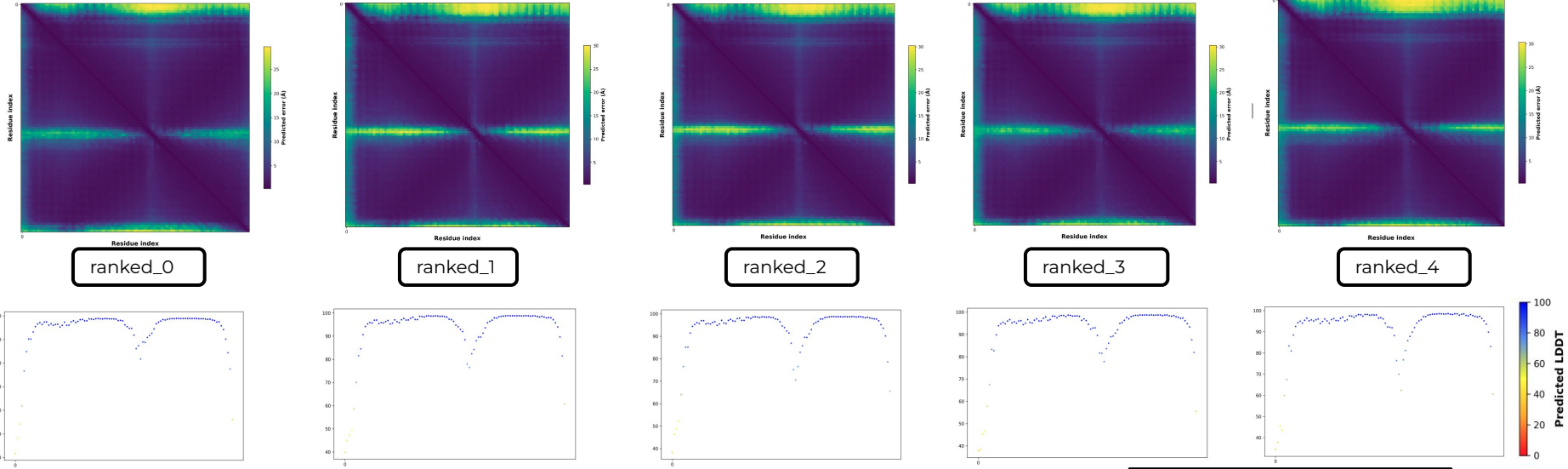
# Visualize AlphaFold PAE Results (monomer\_ptm)



- Low Predicted Aligned Error (PAE) value has higher confidence of accuracy
- Must use monomer\_ptm or multimer as model\_preset to create PAE image
- The colour at position  $(x, y)$  indicates AlphaFold's expected position error at residue  $x$ , when the predicted and true structures are aligned on residue  $y$ .

eog out\_alphafold\_2.3.1/1L2Y/ranked\_0\_PAE.png

# Evaluating Models



See which model has the top rank based on pLDDT score.

```
cat out_alphaFold_2.3.1/IL2Y/ranking_debug.json
```

```
"pLDDTs": {  
  "model_1_ptm_pred_0": 94.16585478746399,  
  "model_2_ptm_pred_0": 94.64120852328334,  
  "model_3_ptm_pred_0": 89.94980057627299,  
  "model_4_ptm_pred_0": 77.53515668415058,  
  "model_5_ptm_pred_0": 88.40610380463586  
},  
"order": [  
  "model_2_ptm_pred_0",  
  "model_1_ptm_pred_0",  
  "model_3_ptm_pred_0",  
  "model_5_ptm_pred_0",  
  "model_4_ptm_pred_0"  
]
```

ranked\_0

ranked\_4



# AlphaFold Job Resource Monitoring

# Review CPU usage for a Job

The `seff` command displays CPU and memory resource usage and efficiency.

```
seff 8862586
```

```
Job ID: 8862586
Cluster: grace
User/Group: username/username
State: COMPLETED (exit code 0)
Nodes: 1
Cores per node: 24
CPU Utilized: 08:19:34
CPU Efficiency: 2.39% of 14-12:55:36 core-walltime
Job Wall-clock time: 14:32:19
Memory Utilized: 51.43 GB
Memory Efficiency: 28.57% of 180.00 GB
```

Usage stats are not accurate until the job is complete.

# Review GPU and CPU usage for a Job

The `jobstats` command monitors GPU and CPU resource usage and create graphs.

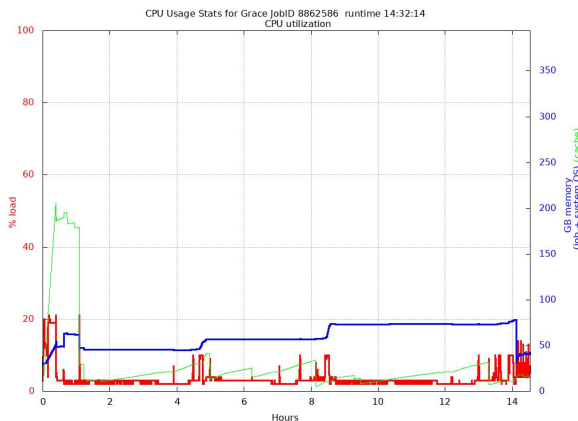
```
#!/bin/bash
#SBATCH --job-name=my_gpu_job
#SBATCH --time=1-00:00:00
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=24
#SBATCH --mem=180G
#SBATCH --gres=gpu:a100:1
#SBATCH --output=stdout.%x.%j
#SBATCH --error=stderr.%x.%j

module purge

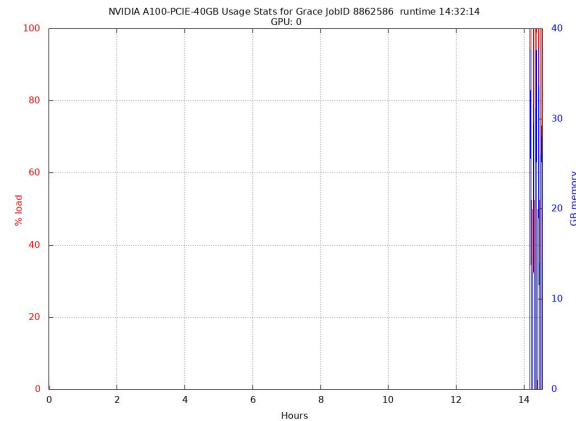
# run jobstats in the background &
# to monitor resource usage
jobstats &

my_alphafold_command

# run jobstats to create a graph
# of cpu and gpu usage for this job
jobstats
```



`eog stats_cpu.8862586.png`



`eog stats_gpu.8862586.png`

- CPU stats are only accurate for jobs using the entire compute node resources (CPUs, memory).
- GPU stats are accurate if using fewer than max CPUs and memory.

<https://hprc.tamu.edu/kb/Software/useful-tools/jobstats>

# AlphaFold Workflow Alternatives

# ParallelFold

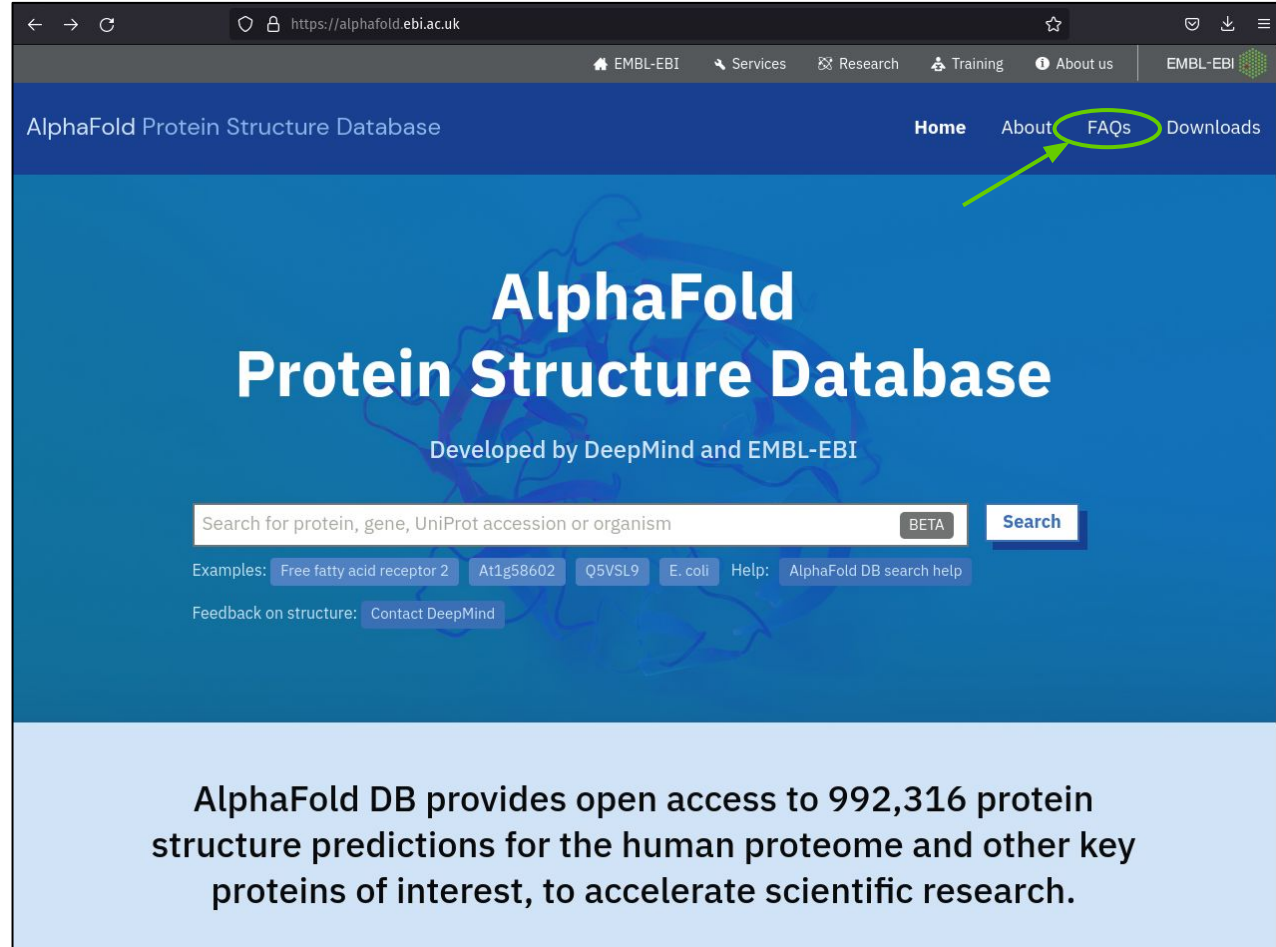
- ParallelFold (ParaFold) breaks the AlphaFold workflow into two steps:
  - processing of the three CPU steps in parallel
  - processing of the GPU step
- The parallel portion for CPU steps is not implemented yet resulting in similar or longer runtimes than the DeepMind approach.
  - The first three CPU steps, jackhammer, jackhammer and HHblits are supposed to run as three separate processes in parallel but **currently this parallelization step is not implemented yet.**
  - When the CPU processing is parallelized, it will require 21 cores.
    - 8 cores for each of the two jackhammer steps
    - 5 cores for the HHblits step.
- The AlphaFold CPU steps may be implemented in parallel soon.

<https://github.com/Zuricho/ParallelFold>

# Databases and References

DeepMind and EMBL's European Bioinformatics Institute ([EMBL-EBI](https://www.ebi.ac.uk)) have partnered to create AlphaFold DB to make these predictions freely available to the scientific community.

Search for your protein to see if it the structure has already been predicted using AlphaFold.



The screenshot shows the AlphaFold Protein Structure Database website. The browser address bar displays <https://alphafold.ebi.ac.uk>. The navigation menu includes Home, About, **FAQs** (highlighted with a green circle and arrow), and Downloads. The main heading is "AlphaFold Protein Structure Database" with the subtitle "Developed by DeepMind and EMBL-EBI". A search bar is present with the placeholder text "Search for protein, gene, UniProt accession or organism" and a "BETA" label. Below the search bar, there are examples: "Free fatty acid receptor 2", "At1g58602", "Q5VSL9", "E. coli", and "Help: AlphaFold DB search help". A "Feedback on structure: Contact DeepMind" link is also visible. At the bottom, a light blue box contains the text: "AlphaFold DB provides open access to 992,316 protein structure predictions for the human proteome and other key proteins of interest, to accelerate scientific research."

# References

Article | [Open Access](#) | [Published: 15 July 2021](#)

## Highly accurate protein structure prediction with AlphaFold

[John Jumper](#) ✉, [Richard Evans](#), ... [Demis Hassabis](#) ✉ [+ Show authors](#)

*Nature* **596**, 583–589 (2021) | [Cite this article](#)

Article | [Open Access](#) | [Published: 22 July 2021](#)

## Highly accurate protein structure prediction for the human proteome

[Kathryn Tunyasuvunakool](#) ✉, [Jonas Adler](#), ... [Demis Hassabis](#) ✉ [+ Show authors](#)

*Nature* **596**, 590–596 (2021) | [Cite this article](#)

Arnold, M. J. (2021) AlphaPickle doi.org/10.5281/zenodo.5708709



# HPRC Resources

- Free Help
  - Send an email to [help@hprc.tamu.edu](mailto:help@hprc.tamu.edu) if you have any questions regarding Bioinformatics tools usage on HPRC clusters or to schedule a Zoom or in-person visit.
    - First spend some time investigating the error.
      - read log files, stdout file, stderr file, tool manual
      - Google search
      - Google user groups: many are software specific
    - Include details about your issue.
      - Which **cluster** or which Galaxy you are using
      - The **JobID**
      - Which software you are using
      - Which modules you have loaded
      - Commands you used in your job script
      - Error messages you are seeing
  - HPRC NGS data analysis tools Documentation
    - <https://hprc.tamu.edu/kb/Software/Bioinformatics>

Let us know when the issue has been resolved so we can close the helpdesk ticket