

DeepMind releases AlphaFold 3 code, with weights for non-commercial researchers only

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Source: <https://github.com/google-deepmind/alphafold3>

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This package provides an implementation of the inference pipeline of AlphaFold 3. See below for how to access the model parameters. You may only use AlphaFold 3 model parameters if received directly from Google. Use is subject to these terms of use.

Any publication that discloses findings arising from using this source code, the model parameters or outputs produced by those should cite the Accurate structure prediction of biomolecular interactions with AlphaFold 3 paper.

Please also refer to the Supplementary Information for a detailed description of the method.

AlphaFold 3 is also available at alphafoldserver.com for non-commercial use, though with a more limited set of ligands and covalent modifications.

For commercial use, AlphaFold 3 is available via Gemini Enterprise Agent Platform on Google Cloud.

If you have any questions, please contact the AlphaFold team at alphafold@google.com.

Obtaining Model Parameters

This repository contains all necessary code for AlphaFold 3 inference. You can download the AlphaFold 3 model parameters from <https://storage.googleapis.com/alphafold3/af3.bin.zst>. Use is subject to these terms of use.

The model parameters for the SynthID Bio-structure version of AlphaFold 3, which predicts watermarked structures, is available at https://storage.googleapis.com/alphafold3/af3_synthid.bin.zst. See [google-deepmind/synthidbio](#) for more details.

The model parameters for AlphaFold 3 Leaving Atom (AF3-LA) can be used as an alternative model fine-tuned for leaving atom handling. The weights are available at https://storage.googleapis.com/alphafold3/af3_leaving_atom.bin.zst and are subject to the same terms of use as the original AlphaFold 3 model parameters. See [google-deepmind/alphaprotein-novo](#) for more details.

Installation and Running Your First Prediction

See the installation documentation.

Once you have installed AlphaFold 3, you can test your setup using e.g. the following input JSON file named `fold_input.json`:

```
{ "name": "2PV7", "sequences": [ { "protein": { "id": ["A", "B"], "sequence": "GMRESYANENQFGFKTINSIDHKIVVGGYGKLGGLFARYLRASGYPIILDREDWAVAESILANADVIVVSPINLTLE" } } ], "modelSeeds": [1], "dialect": "alphafold3", "version": 1 }
```

You can then run AlphaFold 3 using the following command:

```
``` docker run -it \ --volume $HOME/af_input:/root/af_input \ --volume $HOME/af_output:/root/af_output \ --volume <MODEL_PARAMETERS_DIR>:/root/models \ --volume <DATABASES_DIR>:/root/public_databases \ --gpus all \ alphafold3 \ python run_alphafold.py \ --json_path=/root/af_input/fold_input.json \ --model_dir=/root/models \ --output_dir=/root/af_output ```
```

There are various flags that you can pass to the `run_alphafold.py` command, to list them all run `python run_alphafold.py --help`. Two fundamental flags that control which parts AlphaFold 3 will run are:

\* `--run_data_pipeline` (defaults to `true`): whether to run the data pipeline, i.e. genetic and template search. This

part is CPU-only, time consuming and could be run on a machine without a GPU. \* `--run\_inference` (defaults to `true`): whether to run the inference. This part requires a GPU.

### ## AlphaFold 3 Input

See the input documentation.

### ## AlphaFold 3 Output

See the output documentation.

### ## Performance

See the performance documentation.

### ## Known Issues

Known issues are documented in the known issues documentation.

Please create an issue if it is not already listed in Known Issues or in the issues tracker.

### ## Citing This Work

Any publication that discloses findings arising from using this source code, the model parameters or outputs produced by those should cite:

@article{Abramson2024, author = {Abramson, Josh and Adler, Jonas and Dunger, Jack and Evans, Richard and Green, Tim and Pritzel, Alexander and Ronneberger, Olaf and Willmore, Lindsay and Ballard, Andrew J. and Bambrick, Joshua and Bodenstein, Sebastian W. and Evans, David A. and Hung, Chia-Chun and O'Neill, Michael and Reiman, David and Tunyasuvunakool, Kathryn and Wu, Zachary and Žemgulytė, Akvilė and Arvaniti, Eirini and Beattie, Charles and Bertolli, Ottavia and Bridgland, Alex and Cherepanov, Alexey and Congreve, Miles and Cowen-Rivers, Alexander I. and Cowie, Andrew and Figurnov, Michael and Fuchs, Fabian B. and Gladman, Hannah and Jain, Rishub and Khan, Yousuf A. and Low, Caroline M. R. and Perlin, Kuba and Potapenko, Anna and Savy, Pascal and Singh, Sukhdeep and Stecula, Adrian and Thillaisundaram, Ashok and Tong, Catherine and Yakneen, Sergei and Zhong, Ellen D. and Zielinski, Michal and Židek, Augustin and Bapst, Victor and Kohli, Pushmeet and Jaderberg, Max and Hassabis, Demis and Jumper, John M.}, journal = {Nature}, title = {Accurate structure prediction of biomolecular interactions with AlphaFold 3}, year = {2024}, volume = {630}, number = {8016}, pages = {493—500}, doi = {10.1038/s41586-024-07487-w} }

### ## Acknowledgements

AlphaFold 3's release was made possible by the invaluable contributions of the following people:

Andrew Cowie, Bella Hansen, Charlie Beattie, Chris Jones, Grace Margand, Jacob Kelly, James Spencer, Josh Abramson, Kathryn Tunyasuvunakool, Kuba Perlin, Lindsay Willmore, Max Bileschi, Molly Beck, Oleg Kovalevskiy, Sebastian Bodenstein, Sukhdeep Singh, Tim Green, Toby Sargeant, Uchechi Okereke, Yotam Doron, and Augustin Židek (engineering lead).

We also extend our gratitude to our collaborators at Google and Isomorphic Labs.

AlphaFold 3 uses the following separate libraries and packages:

\* abseil-cpp and abseil-py \* Docker \* DSSP \* HMMER Suite \* Haiku \* JAX \* libcifpp \* NumPy \* pybind11 and pybind11\_abseil \* RDKit \* Tokamax \* tqdm

We thank all their contributors and maintainers!

### ## Get in Touch

If you have any questions not covered in this overview, please contact the AlphaFold team at [alphafold@google.com](mailto:alphafold@google.com).

We would love to hear your feedback and understand how AlphaFold 3 has been useful in your research. Share your stories with us at [alphafold@google.com](mailto:alphafold@google.com).

For questions surrounding SynthID Bio-structure, please contact [synthidbio@google.com](mailto:synthidbio@google.com).

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## ### Mirrored and Reference Databases

The following databases have been: (1) mirrored by Google DeepMind; and (2) in part, included with the inference code package for testing purposes, and are available with reference to the following:

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