ColabFold v1.5.5: 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: [v1.4](#), [v1.5.1](#), [v1.5.2](#), [v1.5.3-patch](#)

[Mirdita M, Schütze K, Moriwaki Y, Heo L, Ovchinnikov S, Steinegger M. ColabFold: Making protein folding accessible to all. *Nature Methods*, 2022](#)

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

query_sequence: " `LEEKKVCQGTSNKLTQLGTFEDHFLSLQRMFNNCEVVLGNLEITYVQ` "

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

jobname: " `test` "

num_relax: `0`

- specify how many of the top ranked structures to relax using amber

template_mode: `none`

- `none` = no template information is used. `pdb100` = detect templates in pdb100 (see [notes](#)). `custom` - upload and search own templates (PDB or mmCIF format, see [notes](#))

Show code

```
jobname test_077bd
sequence LEEKKVCQGTSNKLTQLGTFEDHFLSLQRMFNNCEVVLGNLEITYVQRNYDLSFLKTIQEVAGYVLIA
length 771
```

> ## Install dependencies

Show code

```
installing colabfold...
CPU times: user 199 ms, sys: 34.7 ms, total: 234 ms
Wall time: 53.5 s
```

MSA options (custom MSA upload, single sequence, pairing mode)

msa_mode: mmseqs2_uniref_env ▼

pair_mode: unpaired_paired ▼

- "unpaired_paired" = pair sequences from same species + unpaired MSA, "unpaired" = seperate MSA for each chain, "paired" - only use paired sequences.

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Advanced settings

model_type: auto ▼

- if `auto` selected, will use `alphafold2_ptm` for monomer prediction and `alphafold2_multimer_v3` for complex prediction. Any of the mode_types can be used (regardless if input is monomer or complex).

num_recycles: 3 ▼

- if `auto` selected, will use `num_recycles=20` if `model_type=alphafold2_multimer_v3`, else `num_recycles=3`.

recycle_early_stop_tolerance: auto ▼

- if `auto` selected, will use `tol=0.5` if `model_type=alphafold2_multimer_v3` else `tol=0.0`.

relax_max_iterations: 200 ▼

- max amber relax iterations, `0` = unlimited (AlphaFold2 default, can take very long)

pairing_strategy: greedy ▼

- `greedy` = pair any taxonomically matching subsets, `complete` = all sequences have to match in one line.

Sample settings

- enable dropouts and increase number of seeds to sample predictions from uncertainty of the model.
- decrease `max_msa` to increase uncertainity

max_msa: auto ▼

num_seeds:
1 ▾

use_dropout: ☐

Save settings

save_all: ☐

save_recycles: ☐

save_to_google_drive: ☐

- if the save_to_google_drive option was selected, the result zip will be uploaded to your Google Drive

dpi:
200

- set dpi for image resolution

Don't forget to hit `Runtime` -> `Run all` after updating the form.

Show code

> Run Prediction

display_images: ☑

Show code

```
Downloading alphafold2_multimer_v3 weights to .: 100%|████████| 3.82G/3.82G
2024-08-15 05:02:19,095 Running on GPU
2024-08-15 05:02:19,404 Found 5 citations for tools or databases
2024-08-15 05:02:19,404 Query 1/1: test_077bd (length 771)
PENDING:    0%|            | 0/300 [elapsed: 00:00 remaining: ?]2024-08-15 05:02
RUNNING:    2%||           | 5/300 [elapsed: 00:06 remaining: 05:57]2024-08-15 0
RUNNING:    4%||           | 11/300 [elapsed: 00:12 remaining: 05:26]2024-08-15
RUNNING:    5%|▍           | 16/300 [elapsed: 00:18 remaining: 05:20]2024-08-15
RUNNING:    8%|▊           | 25/300 [elapsed: 00:27 remaining: 04:59]2024-08-15
RUNNING:   11%|█           | 33/300 [elapsed: 00:36 remaining: 04:49]2024-08-15
RUNNING:   14%|█▍          | 43/300 [elapsed: 00:46 remaining: 04:37]2024-08-15
RUNNING:   17%|█▋          | 52/300 [elapsed: 00:58 remaining: 04:40]2024-08-15
RUNNING:   20%|██          | 60/300 [elapsed: 01:06 remaining: 04:27]2024-08-15
COMPLETE: 100%|████████████| 300/300 [elapsed: 01:16 remaining: 00:00]
PENDING:    0%|            | 0/300 [elapsed: 00:00 remaining: ?]2024-08-15 05:03
RUNNING:    3%||           | 10/300 [elapsed: 00:11 remaining: 05:20]2024-08-15
RUNNING:    5%|▍           | 15/300 [elapsed: 00:16 remaining: 05:14]2024-08-15
RUNNING:    8%|▊           | 25/300 [elapsed: 00:27 remaining: 04:55]2024-08-15
RUNNING:   11%|█           | 33/300 [elapsed: 00:37 remaining: 05:07]2024-08-15
RUNNING:   14%|█▍          | 43/300 [elapsed: 00:47 remaining: 04:47]2024-08-15
COMPLETE: 100%|████████████| 300/300 [elapsed: 00:56 remaining: 00:00]
```


Sequence coverage
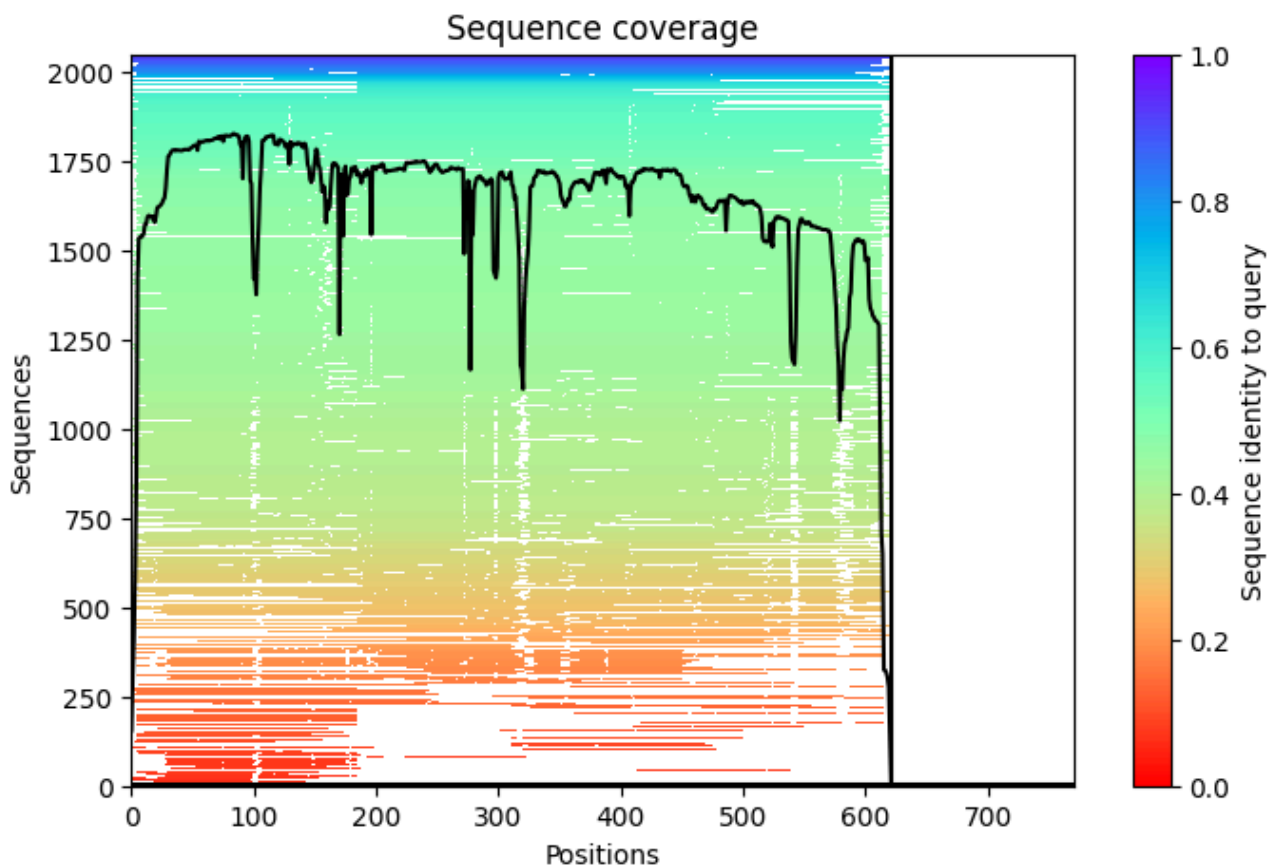
```
2024-08-15 05:04:34,336 Setting max_seq=508, max_extra_seq=1542
2024-08-15 05:07:40,140 alphafold2_multimer_v3_model_1_seed_000 recycle=0 pLD
2024-08-15 05:10:11,840 alphafold2_multimer_v3_model_1_seed_000 recycle=1 pLD
2024-08-15 05:12:44,316 alphafold2_multimer_v3_model_1_seed_000 recycle=2 pLD
2024-08-15 05:15:17,211 alphafold2_multimer_v3_model_1_seed_000 recycle=3 pLD
2024-08-15 05:15:17,215 alphafold2_multimer_v3_model_1_seed_000 took 636.0s (
```


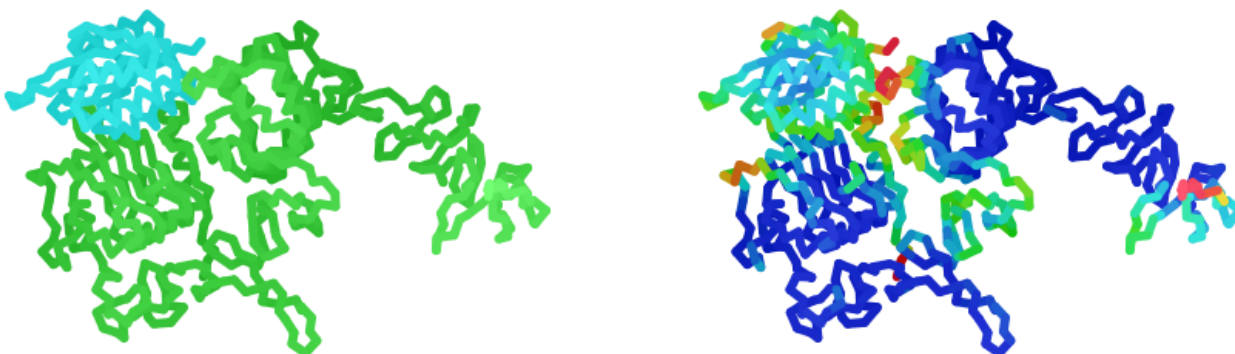colored by chain   colored by pLDDT
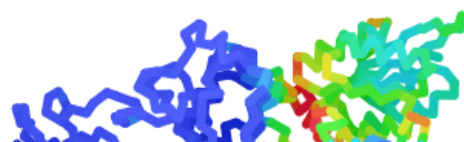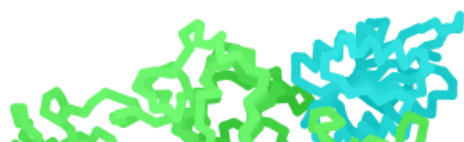
```
2024-08-15 05:17:51,458 alphafold2_multimer_v3_model_2_seed_000 recycle=0 pLD
2024-08-15 05:20:24,556 alphafold2_multimer_v3_model_2_seed_000 recycle=1 pLD
2024-08-15 05:22:57,388 alphafold2_multimer_v3_model_2_seed_000 recycle=2 pLD
2024-08-15 05:25:31,365 alphafold2_multimer_v3_model_2_seed_000 recycle=3 pLD
2024-08-15 05:25:31,369 alphafold2_multimer_v3_model_2_seed_000 took 613.1s (
```

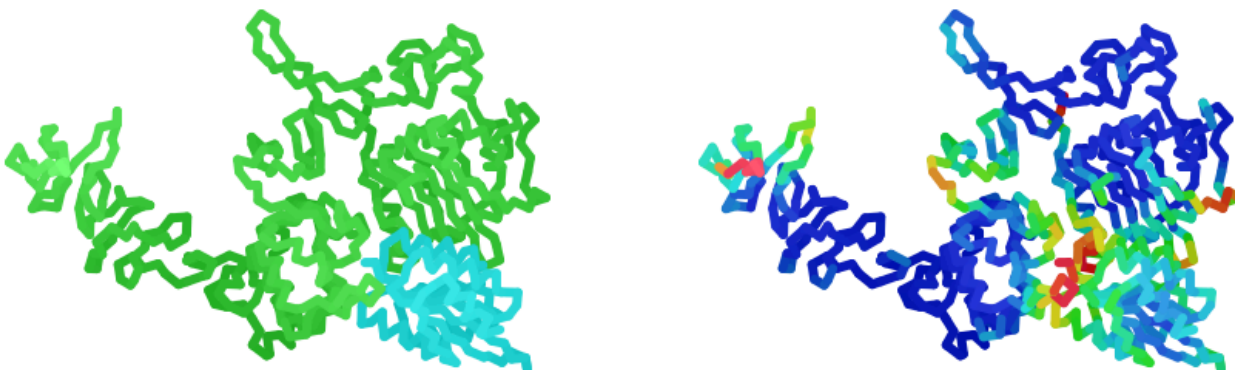colored by chain   colored by pLDDT


```
2024-08-15 05:28:07,038 alphafold2_multimer_v3_model_3_seed_000 recycle=0 pLD
2024-08-15 05:30:41,681 alphafold2_multimer_v3_model_3_seed_000 recycle=1 pLD
2024-08-15 05:33:15,940 alphafold2_multimer_v3_model_3_seed_000 recycle=2 pLD
2024-08-15 05:35:50,472 alphafold2_multimer_v3_model_3_seed_000 recycle=3 pLD
2024-08-15 05:35:50,474 alphafold2_multimer_v3_model_3_seed_000 took 618.1s (
```

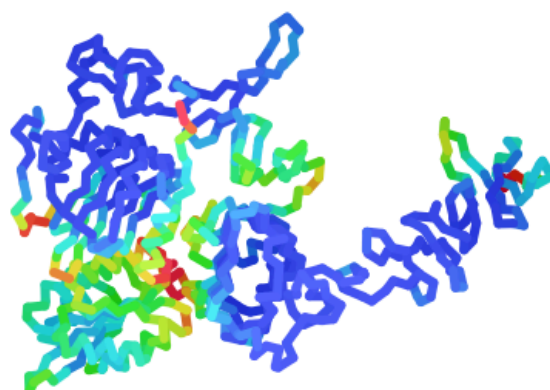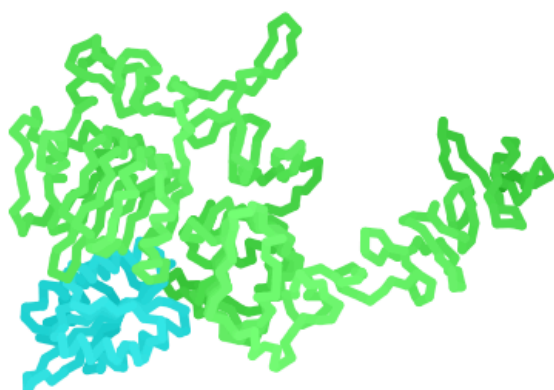colored by chain   colored by pLDDT


```
2024-08-15 05:38:25,864 alphafold2_multimer_v3_model_4_seed_000 recycle=0 pLD
2024-08-15 05:41:00,878 alphafold2_multimer_v3_model_4_seed_000 recycle=1 pLD
2024-08-15 05:43:35,203 alphafold2_multimer_v3_model_4_seed_000 recycle=2 pLD
```

```
2024-08-15 05:46:09,111 alphafold2_multimer_v3_model_4_seed_000 recycle=3 pLD
2024-08-15 05:46:09,112 alphafold2_multimer_v3_model_4_seed_000 took 617.6s (
```

colored by chain   colored by pLDDT


```
2024-08-15 05:48:43,664 alphafold2_multimer_v3_model_5_seed_000 recycle=0 pLD
2024-08-15 05:51:17,117 alphafold2_multimer_v3_model_5_seed_000 recycle=1 pLD
2024-08-15 05:53:51,244 alphafold2_multimer_v3_model_5_seed_000 recycle=2 pLD
2024-08-15 05:56:25,422 alphafold2_multimer_v3_model_5_seed_000 recycle=3 pLD
2024-08-15 05:56:25,424 alphafold2_multimer_v3_model_5_seed_000 took 615.3s (
```

colored by chain   colored by pLDDT
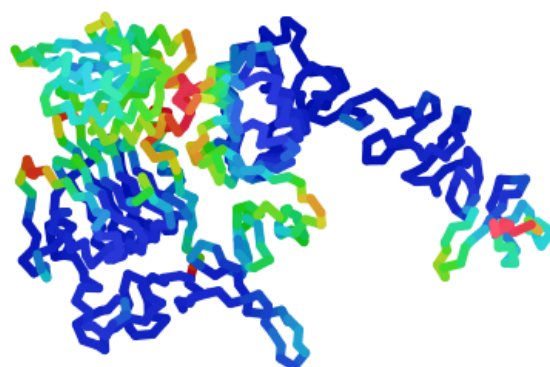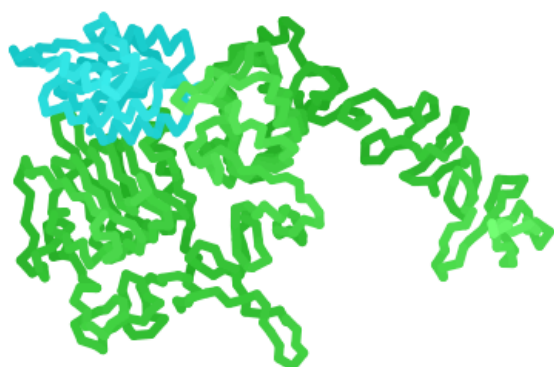

```
2024-08-15 05:56:26,453 reranking models by 'multimer' metric
2024-08-15 05:56:26,453 rank_001_alphafold2_multimer_v3_model_5_seed_000 pLDD
2024-08-15 05:56:26,454 rank_002_alphafold2_multimer_v3_model_1_seed_000 pLDD
2024-08-15 05:56:26,455 rank_003_alphafold2_multimer_v3_model_3_seed_000 pLDD
2024-08-15 05:56:26,456 rank_004_alphafold2_multimer_v3_model_4_seed_000 pLDD
2024-08-15 05:56:26,456 rank_005_alphafold2_multimer_v3_model_2_seed_000 pLDD
2024-08-15 05:56:29,202 Done
0
```

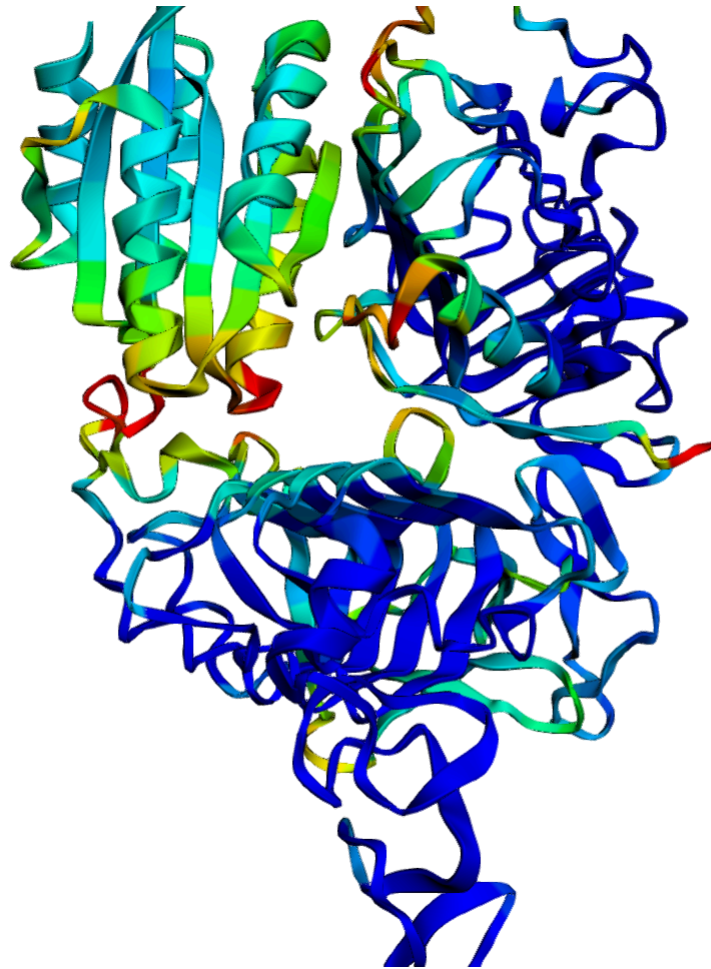> **Display 3D structure**

rank_num: | 1   ▾ |

color: | chain   ▾ |

show_sidechains: ☐

show_mainchains: ☐

Show code

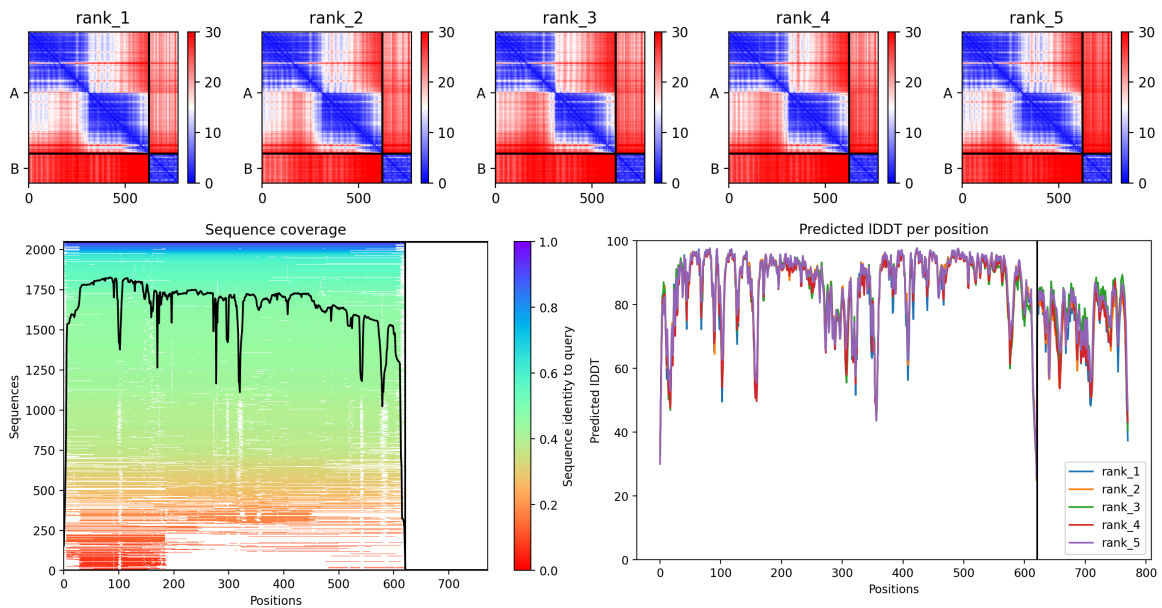plDDT: ■ Very low (<50) ■ Low (60) ■ OK (70) ■ Confident (80) ■ Very high (>90)

> Plots

Show code

Plots for test_077bd

Package and download results

If you are having issues downloading the result archive, try disabling your adblocker and run this cell again. If that fails click on the little folder icon to the left, navigate to file: `jobname.result.zip`, right-click and select "Download" (see [screenshot](#)).

Show code

Instructions

Quick start

1. Paste your protein sequence(s) in the input field.
2. Press "Runtime" -> "Run all".
3. The pipeline consists of 5 steps. The currently running step is indicated by a circle with a stop sign next to it.