

✓ 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 [Nature Protocols](#).

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: " YSPTLNKMFCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVVF "

- 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_84047
sequence YSPTLNKMFCQLAKTCPVQLWVDSTPPPGTRVRAMAIYKQSQHMTEVVRRCPPHHERCSDSDX
length 62

```

> Install dependencies

[Show code](#)



installing colabfold...

CPU times: user 219 ms, sys: 30.8 ms, total: 250 ms

Wall time: 55.2 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.

[Show code](#)

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 uncertainty

`max_msa:`

`num_seeds:`

`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:`


- set dpi for image resolution

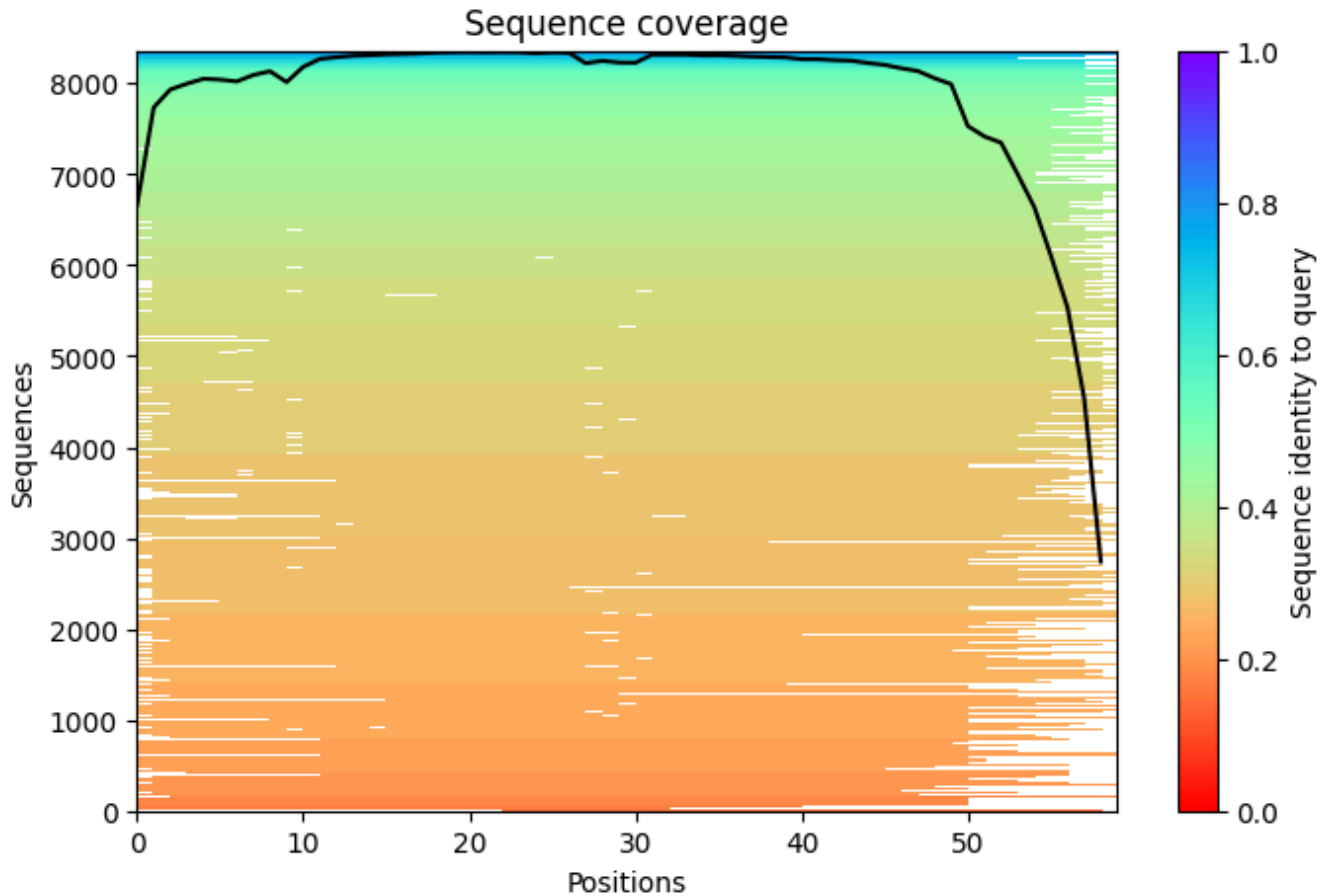
Don't forget to hit Runtime -> Run all after updating the form.

> Run Prediction

`display_images:` ☒

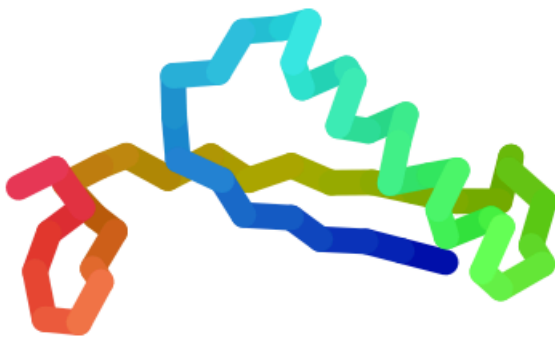
[Show code](#)

 Downloading alphafold2_ptm weights to .: 100%|██████████| 3.47G/3.47G [00:29<00:00, 125M
 2024-11-13 19:23:26,054 Running on GPU
 2024-11-13 19:23:26,382 Found 5 citations for tools or databases
 2024-11-13 19:23:26,383 Query 1/1: test_a5e17 (length 59)
 COMPLETE: 100%|██████████| 150/150 [elapsed: 00:02 remaining: 00:00]

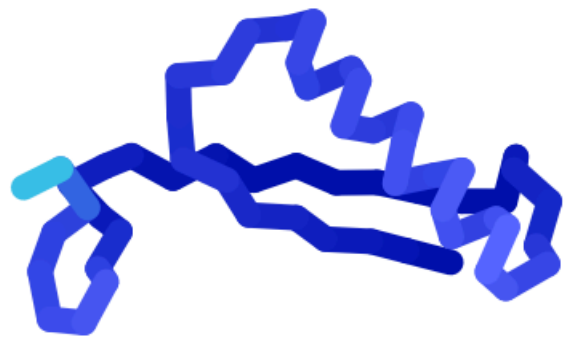


2024-11-13 19:23:29,897 Setting max_seq=512, max_extra_seq=5120
 2024-11-13 19:24:04,946 alphafold2_ptm_model_1_seed_000 recycle=0 pLDDT=96.6 pTM=0.755
 2024-11-13 19:24:09,818 alphafold2_ptm_model_1_seed_000 recycle=1 pLDDT=96.5 pTM=0.759 t
 2024-11-13 19:24:14,701 alphafold2_ptm_model_1_seed_000 recycle=2 pLDDT=96.2 pTM=0.755 t
 2024-11-13 19:24:19,597 alphafold2_ptm_model_1_seed_000 recycle=3 pLDDT=96 pTM=0.755 to
 2024-11-13 19:24:19,599 alphafold2_ptm_model_1_seed_000 took 37.2s (3 recycles)

colored by N→C



colored by pLDDT

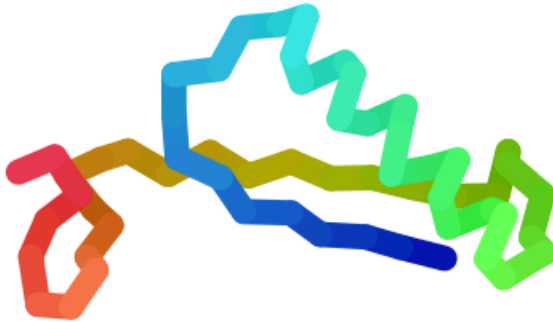


```

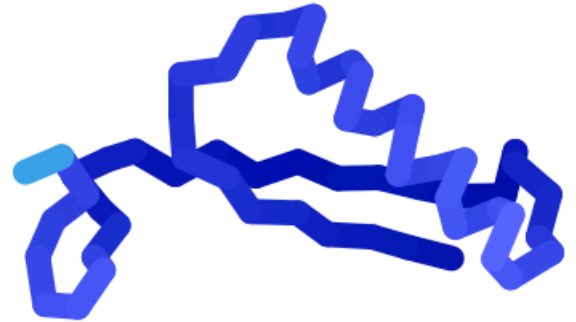
2024-11-13 19:24:24,663 alphafold2_ptm_model_2_seed_000 recycle=0 pLDDT=97 pTM=0.761
2024-11-13 19:24:29,615 alphafold2_ptm_model_2_seed_000 recycle=1 pLDDT=97 pTM=0.766 toI
2024-11-13 19:24:34,570 alphafold2_ptm_model_2_seed_000 recycle=2 pLDDT=96.9 pTM=0.766 t
2024-11-13 19:24:39,555 alphafold2_ptm_model_2_seed_000 recycle=3 pLDDT=96.8 pTM=0.768 t
2024-11-13 19:24:39,556 alphafold2_ptm_model_2_seed_000 took 19.8s (3 recycles)

```

colored by N→C



colored by pLDDT



```

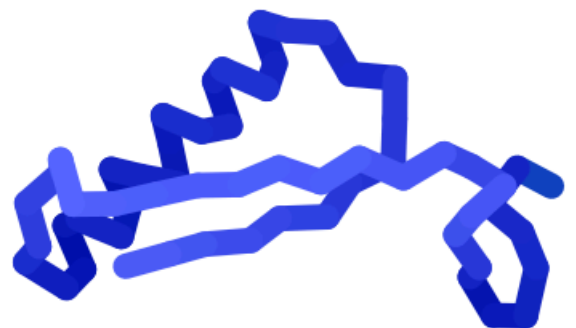
2024-11-13 19:24:45,080 alphafold2_ptm_model_3_seed_000 recycle=0 pLDDT=97.2 pTM=0.775
2024-11-13 19:24:50,096 alphafold2_ptm_model_3_seed_000 recycle=1 pLDDT=97.4 pTM=0.782 t
2024-11-13 19:24:55,125 alphafold2_ptm_model_3_seed_000 recycle=2 pLDDT=97.4 pTM=0.781 t
2024-11-13 19:25:00,163 alphafold2_ptm_model_3_seed_000 recycle=3 pLDDT=97.4 pTM=0.784 t
2024-11-13 19:25:00,165 alphafold2_ptm_model_3_seed_000 took 20.1s (3 recycles)

```

colored by N→C



colored by pLDDT

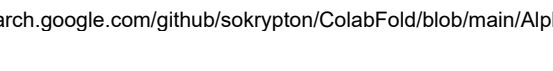


```

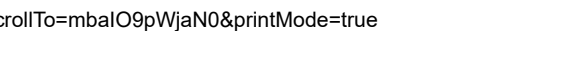
2024-11-13 19:25:05,353 alphafold2_ptm_model_4_seed_000 recycle=0 pLDDT=97.4 pTM=0.774
2024-11-13 19:25:10,401 alphafold2_ptm_model_4_seed_000 recycle=1 pLDDT=97.4 pTM=0.781 t
2024-11-13 19:25:15,432 alphafold2_ptm_model_4_seed_000 recycle=2 pLDDT=97.1 pTM=0.777 t
2024-11-13 19:25:20,451 alphafold2_ptm_model_4_seed_000 recycle=3 pLDDT=96.9 pTM=0.777 t
2024-11-13 19:25:20,453 alphafold2_ptm_model_4_seed_000 took 20.2s (3 recycles)

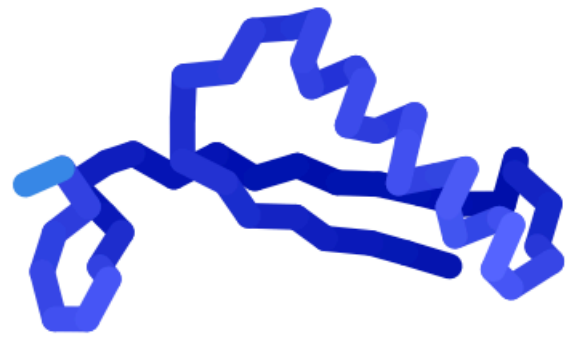
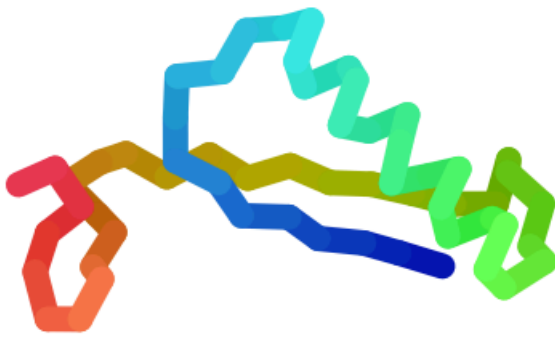
```

colored by N→C



colored by pLDDT





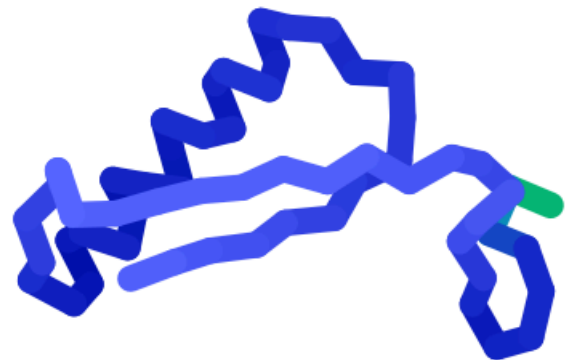
```

2024-11-13 19:25:25,626 alphafold2_ptm_model_5_seed_000 recycle=0 pLDDT=97.4 pTM=0.784
2024-11-13 19:25:30,630 alphafold2_ptm_model_5_seed_000 recycle=1 pLDDT=96.9 pTM=0.783 t
2024-11-13 19:25:35,622 alphafold2_ptm_model_5_seed_000 recycle=2 pLDDT=96.1 pTM=0.774 t
2024-11-13 19:25:40,604 alphafold2_ptm_model_5_seed_000 recycle=3 pLDDT=96.1 pTM=0.779 t
2024-11-13 19:25:40,605 alphafold2_ptm_model_5_seed_000 took 20.0s (3 recycles)

```

colored by N→C

colored by pLDDT



```

2024-11-13 19:25:40,752 reranking models by 'plddt' metric
2024-11-13 19:25:40,753 rank_001_alphafold2_ptm_model_3_seed_000 pLDDT=97.4 pTM=0.784
2024-11-13 19:25:40,754 rank_002_alphafold2_ptm_model_4_seed_000 pLDDT=96.9 pTM=0.777
2024-11-13 19:25:40,755 rank_003_alphafold2_ptm_model_2_seed_000 pLDDT=96.8 pTM=0.768
2024-11-13 19:25:40,755 rank_004_alphafold2_ptm_model_5_seed_000 pLDDT=96.1 pTM=0.779
2024-11-13 19:25:40,756 rank_005_alphafold2_ptm_model_1_seed_000 pLDDT=96 pTM=0.755
2024-11-13 19:25:42,609 Done
0

```


> Display 3D structure

rank_num: 1

color: IDDT

show_sidechains: ☐

show_mainchains: ☐

[Show code](#)



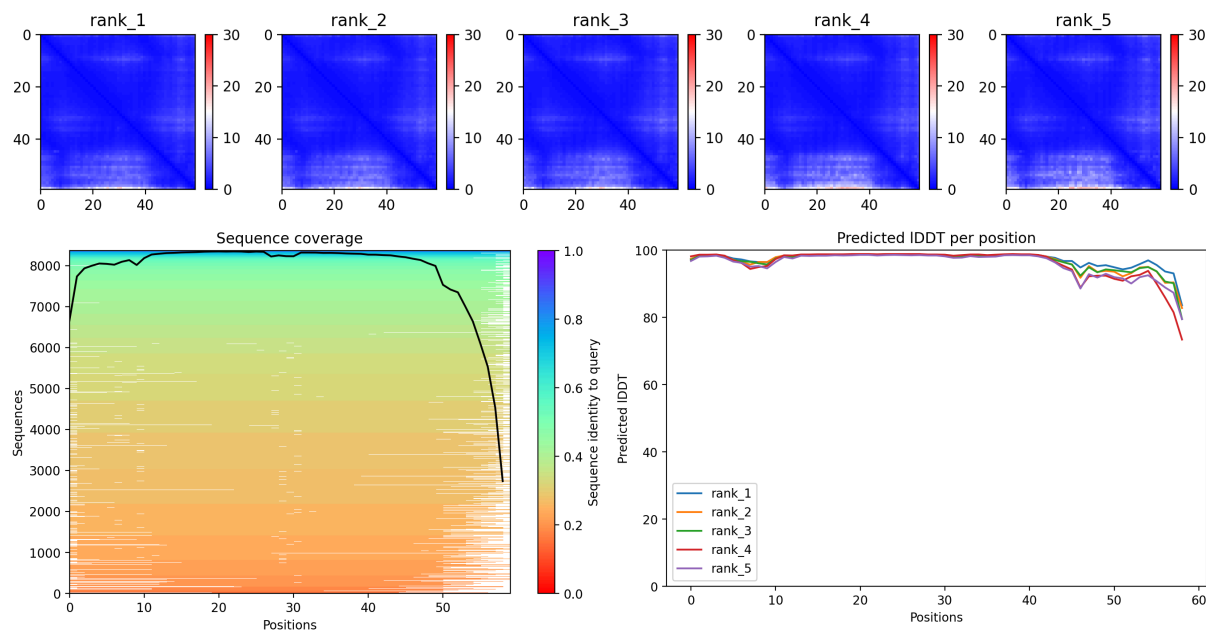
pLDDT: ■ Very low (<50) ■ Low (60) ■ OK (70) ■ Confident (80) ■ Very high (>90)

> Plots

[Show code](#)



Plots for test_a5e17



> 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`,