

# Omegafold

2022/08/03

# Install & running on ABCI

```
git clone https://github.com/HeliXonProtein/OmegaFold
```

```
cd OmegaFold
```

```
module load gcc/11.2.0
```

```
module load python/3.10/3.10.4
```

```
pip3 install -r requirements.txt
```

```
qrsh -g gab50377 -l rt_G.small=1 -l h_rt=3:00:00
```

```
g0012:module load gcc/11.2.0
```

```
g0012: module load python/3.10/3.10.4
```

```
g0012: module load cuda/11.0
```

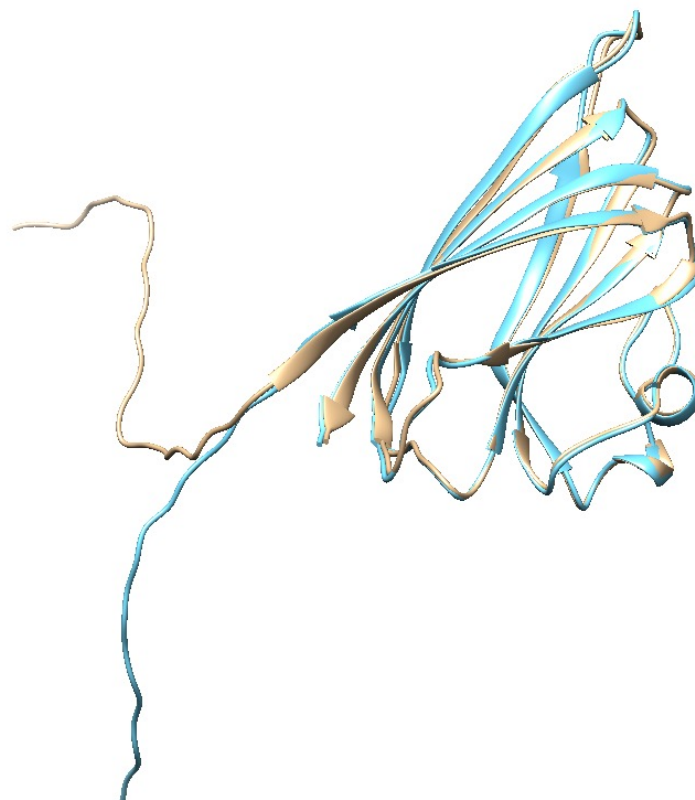
```
g0012 module load cudnn
```

```
g0012: module load nccl
```

```
g0012: python3 main.py ../input/EHI_001100.fasta ../output
```

>~500 res では、ABCI の rt\_G.small ではアロケーションエラー

# T1026

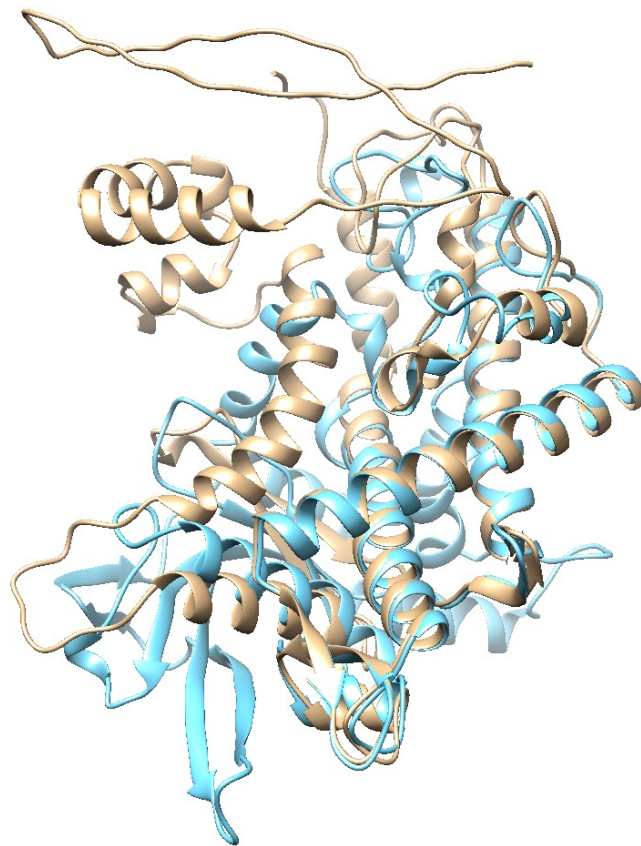


AF2(v. 2.00) vs OmegaFold

172 residues in this chain.

53.57 seconds. (OmegaFold)

# T1037

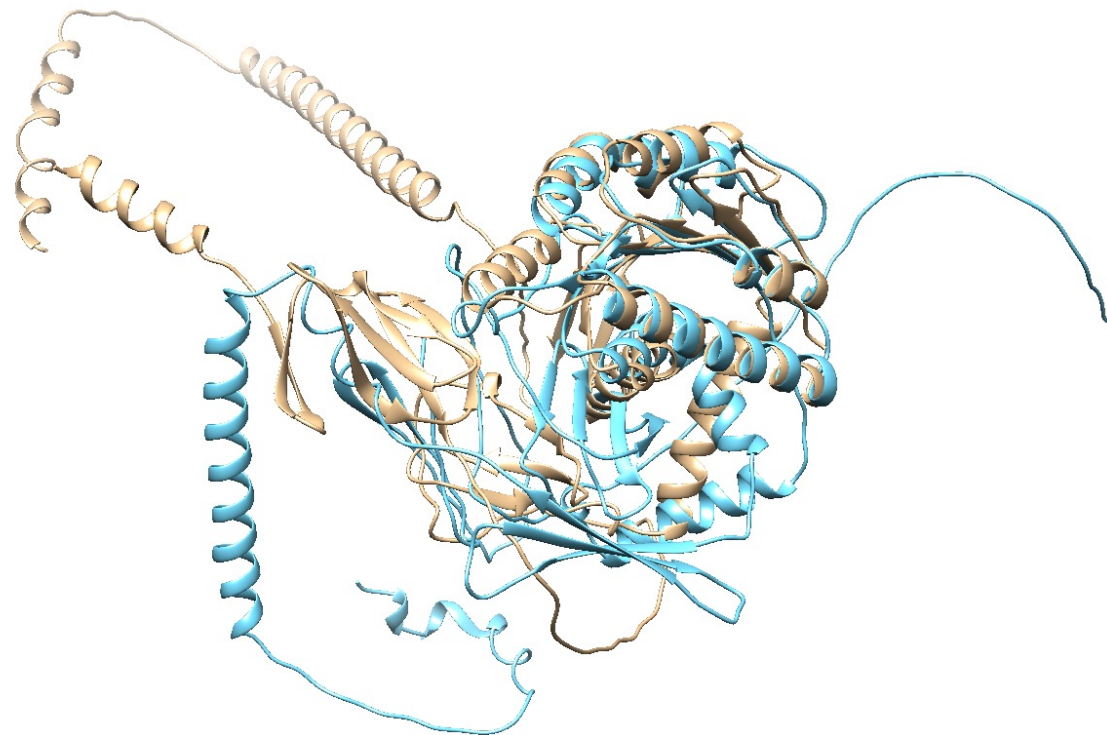


AF2(v. 2.00) vs OmegaFold

404 residues in this chain.

452.44 seconds. (OmegaFold)

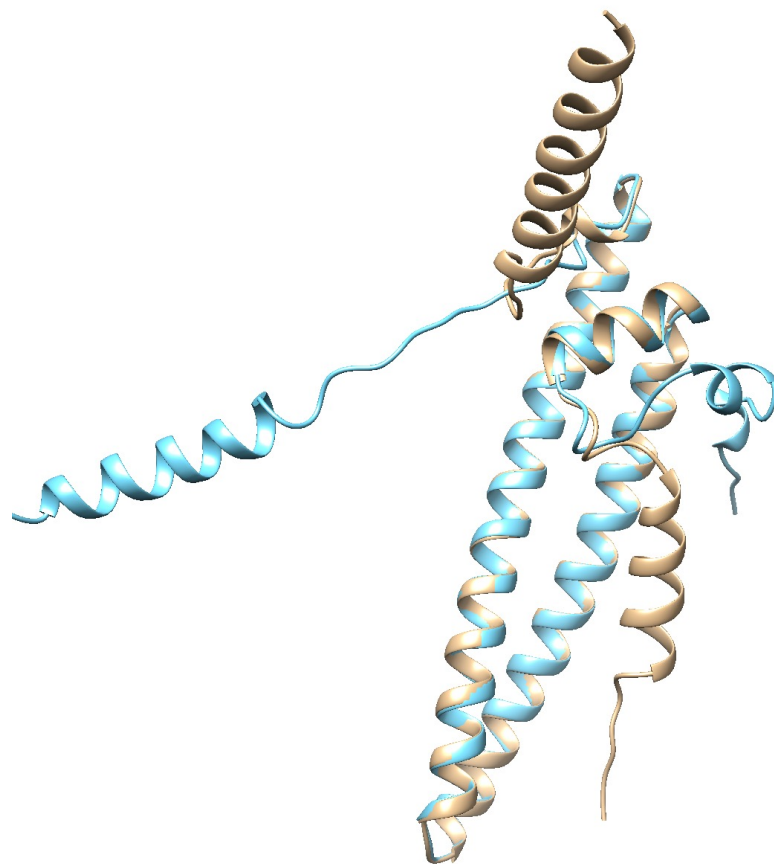
# EHI\_001100



489 residues in this chain.

770.95 seconds.

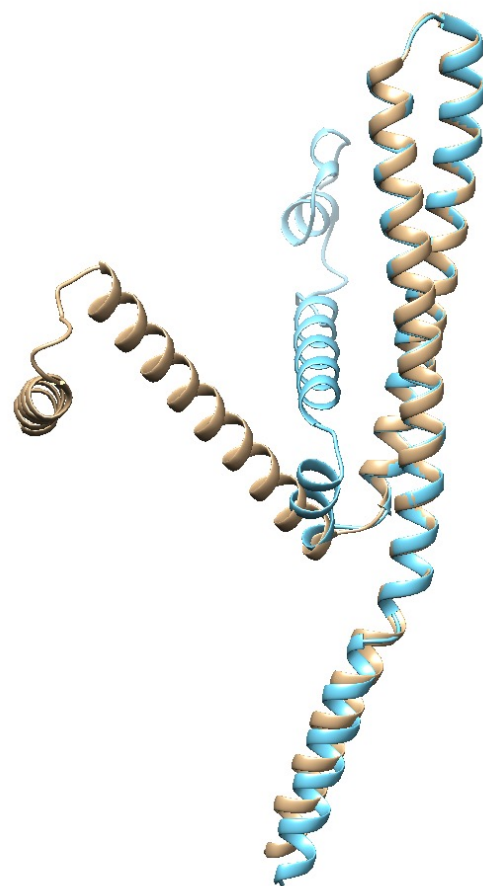
# EH1\_022970



165 residues in this chain.

48.11 seconds.

EHI\_048240



169 residues in this chain.

51.06 seconds.