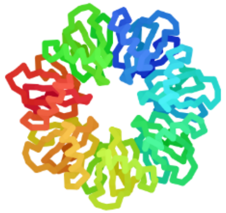


Boltz-1xを用いた
タンパク質-DNA複合体の予測

フィルジェン株式会社　バイオインフォマティクス部

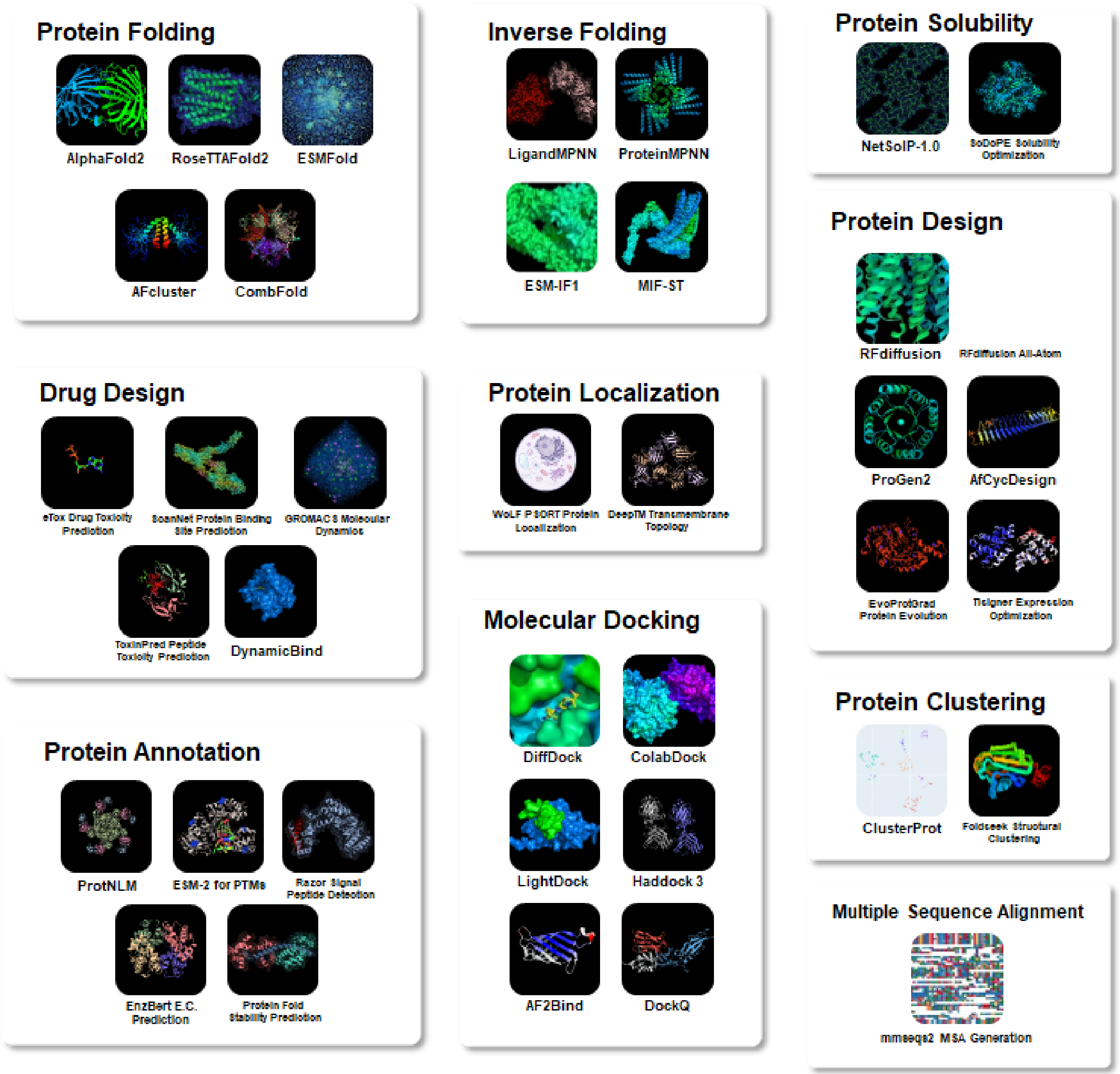
2025.6

Neurosnap Platformの特長

AlphaFold2の他、
60種類以上のAI予測ツールを搭載

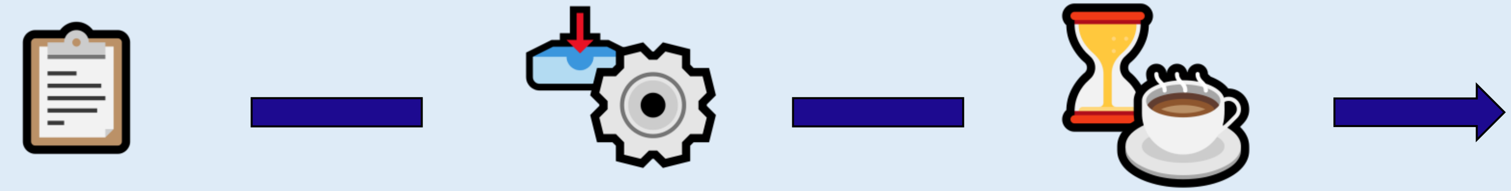
- タンパク質のフォールディング
- 分子ドッキング
- 創薬/ドラッグディスカバリー
- タンパク質工学
- In silico Mutagenesis

など


Protein Folding
AlphaFold2
RoseTTAFold2
ESMFold
AFcluster
CombFold
Inverse Folding
LigandMPNN
ProteinMPNN
ESM-IF1
MIF-ST
Protein Solubility
NetSolP-1.0
SoDoPE Solubility Optimization
Protein Design
RFdiffusion
RFdiffusion All-Atom
ProGen2
AfCycDesign
EvoProtGrad Protein Evolution
TIsigner Expression Optimization
Drug Design
eTox Drug Toxicity Prediction
ScanNet Protein Binding Site Prediction
GROMACS Molecular Dynamics
ToxinPred Peptide Toxicity Prediction
DynamicBind
Protein Localization
WoLF PSORT Protein Localization
DeepTM Transmembrane Topology
Molecular Docking
DiffDock
ColabDock
LightDock
Haddock 3
AF2Bind
DockQ
Protein Clustering
ClusterProt
Foldseek Structural Clustering
Protein Annotation
ProtNLM
ESM-2 for PTMs
Razor Signal Peptide Detection
EnzBert E.C. Prediction
Protein Fold Stability Prediction
Multiple Sequence Alignment
mmseqs2 MSA Generation

Neurosnap Platformの特長

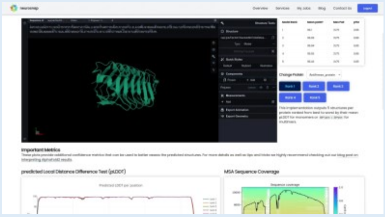
✓ 解析がパイプライン化　ゼロコードで複雑な操作なく解析



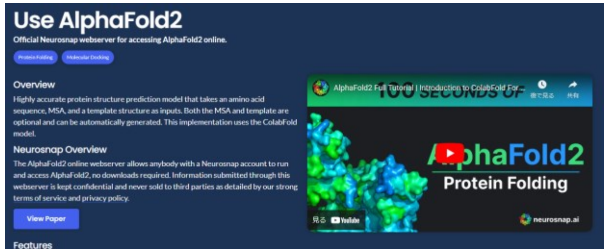
サービスのリストから
解析パッケージを選択

データのインポートと
設定を調整

Neurosnap Platform
が自動で処理を開始



解析完了後、プラットフォーム上
で結果の閲覧、出力



Use AlphaFold2

Official Neurosnap webserver for accessing AlphaFold2 online.

Protein Folding
Molecular Docking

Overview

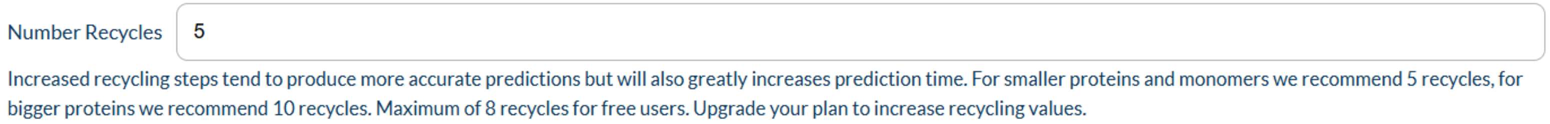
Highly accurate protein structure prediction model that takes an amino acid sequence, MSA, and a template structure as inputs. Both the MSA and template are optional and can be automatically generated. This implementation uses the ColabFold model.

Neurosnap Overview

The AlphaFold2 online webserver allows anybody with a Neurosnap account to run and access AlphaFold2, no downloads required. Information submitted through this webserver is kept confidential and never sold to third parties as detailed by our strong terms of service and privacy policy.

View Paper
Features
AlphaFold2 Full Tutorial | Introduction to ColabFold For...
100 SECONDS OF
後で見る
共有
AlphaFold2
Protein Folding
見る YouTube
neurosnap.ai

例）Alphafold2の要約画面
ツールの論文や動画チュートリアルが
用意されている場合はアクセスできます。



Number Recycles: 5

Increased recycling steps tend to produce more accurate predictions but will also greatly increases prediction time. For smaller proteins and monomers we recommend 5 recycles, for bigger proteins we recommend 10 recycles. Maximum of 8 recycles for free users. Upgrade your plan to increase recycling values.

例）Alphafold2のリサイクル数の設定画面
リサイクル数を増やすと予測精度が改善される他、モノマーや大きなタンパク質ごとの適正値
のヒントが記載されています。

✓ 各設定にはガイド付き

AI予測ツールの課題

解析ツールの環境構築

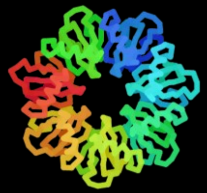
- セットアップするには技術的な専門知識
- バージョンアップなどが頻繁にある
- パッケージの数が多くなるほど煩雑化

コマンドライン

- Linux/コマンドライン操作の習得

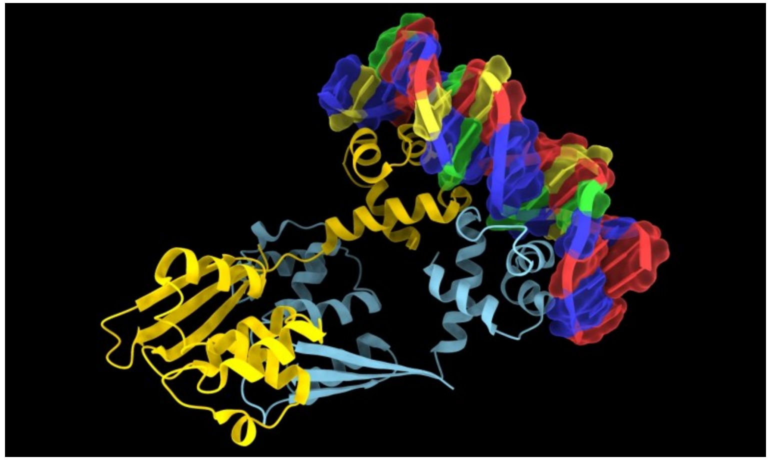
高価なハードウェア

- 大容量のVRAMを搭載したハイエンドグラフィックカードなど



Neurosnap Platformで解決！

Boltz-1とは

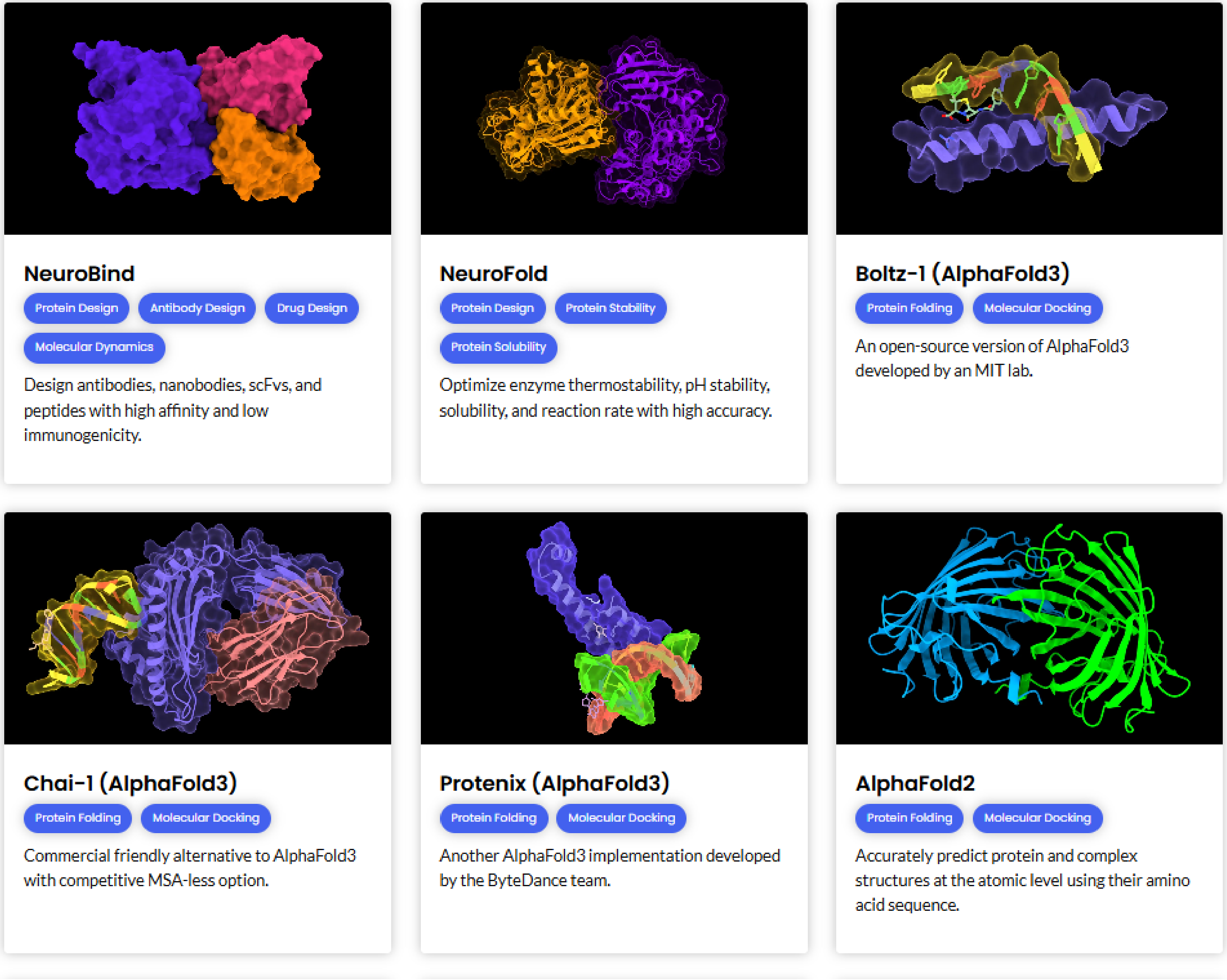


Boltz-1

タンパク質立体構造予測のためのAIモデル
AlphaFold3クローンモデル

- 生体分子複合体の3D構造予測においてAlphaFold3レベルの精度を実現
- 商用利用可能
- タンパク質、核酸、小分子などの多様な生体分子システムをサポート
- 25.4にBoltz-1x バージョンがリリース（より高速、高い推論とトレーニングを実現）

Neurosnap PlatformでBoltz-1を実行



NeuroBind

Protein Design · Antibody Design · Drug Design · Molecular Dynamics

Design antibodies, nanobodies, scFvs, and peptides with high affinity and low immunogenicity.

NeuroFold

Protein Design · Protein Stability · Protein Solubility

Optimize enzyme thermostability, pH stability, solubility, and reaction rate with high accuracy.

Boltz-1 (AlphaFold3)

Protein Folding · Molecular Docking

An open-source version of AlphaFold3 developed by an MIT lab.

Chai-1 (AlphaFold3)

Protein Folding · Molecular Docking

Commercial friendly alternative to AlphaFold3 with competitive MSA-less option.

Protenix (AlphaFold3)

Protein Folding · Molecular Docking

Another AlphaFold3 implementation developed by the ByteDance team.

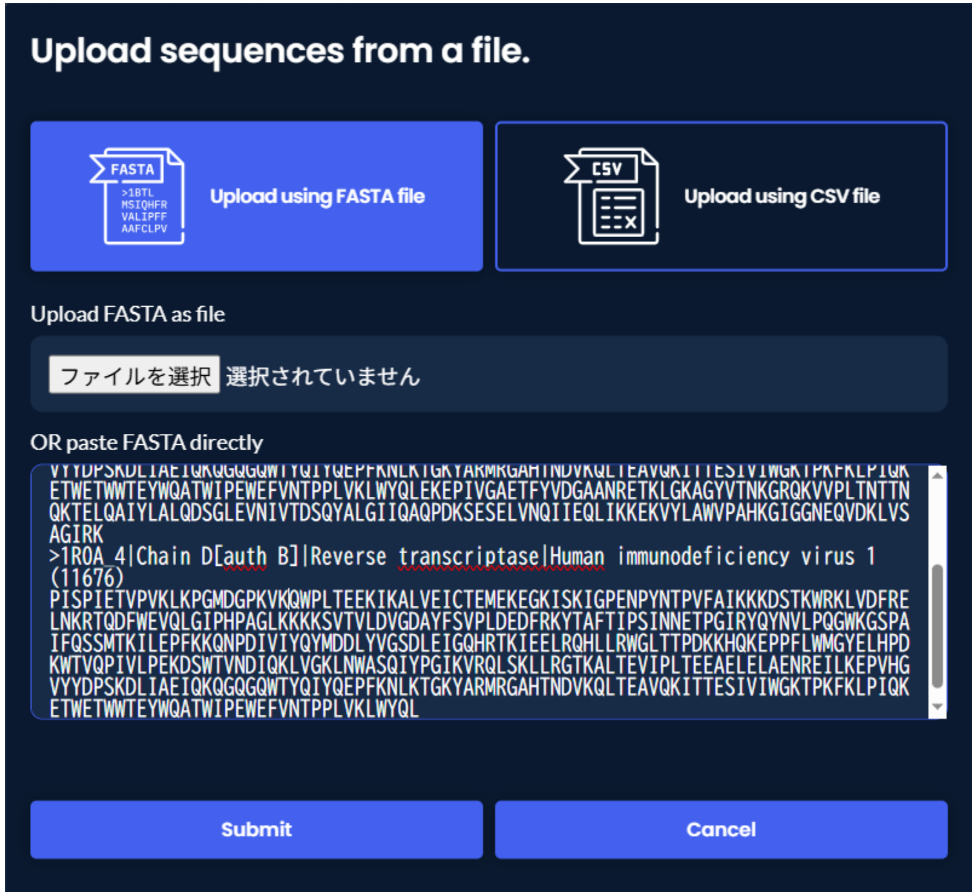
AlphaFold2

Protein Folding · Molecular Docking

Accurately predict protein and complex structures at the atomic level using their amino acid sequence.

- プラットフォームにアクセスするとさまざまなAIツールを選択できる画面が表示
- 今回はBoltz-1を選択しますが、他にもタンパク質立体構造予測が可能なChai-1、Protenix、AF2などが解析可能

Neurosnap PlatformでBoltz-1を実行



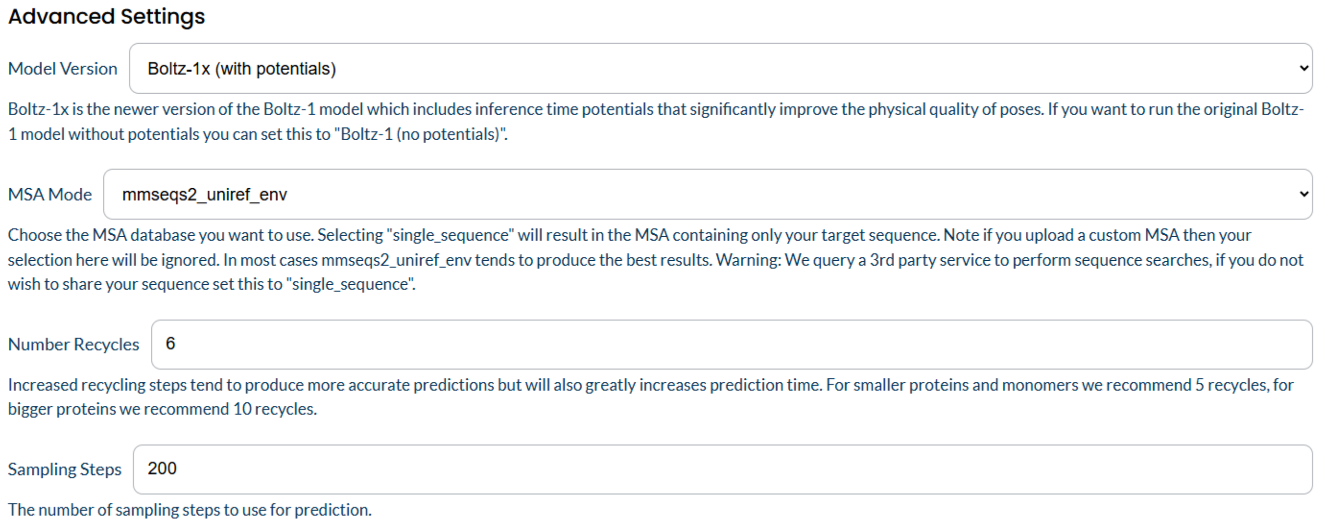
Upload sequences from a file.

Upload FASTA as file

選択されていません

OR paste FASTA directly

```
VYYDPSKDLIAEIQKQGQGQWTYQIYQEPFKNLKTGKYARMRGAHTNDVKQLTEAVQKITTESIVIWGKTPKFKLPIQK
ETWETWWTEYWQATWIPEWEFVNTPPLVKLWYQLEKEPIVGAETFYVDGAANRETKLGKAGYVTNKGRQKVVPLTNTTN
QKTELQAIYLALQDSGLEVNIVTDSQYALGIIQAQPDKSESELVNQIIEQLIKKEKVYLAWVPAHKGIGGNEQVDKLVS
AGIRK
>1ROA_4|Chain D[auth B]|Reverse transcriptase|Human immunodeficiency virus 1
(11676)
PISPIETVPVKLKPGMDGPKVKQWPLTEEKIKALVEICTEMEKEGKISKIGPENPYNTPVFAIKKKDSTKWRKLVDFRE
LNKRTQDFWEVQLGIPHPAGLKKKKSVTVLDVGDAYFSVPLDEDFRKYTAFTIPSINNETPGIRYQYNVLPQGWKGSPA
IFQSSMTKILEPFKKQNPDIVIYQYMDDLYVGSDLEIGQHRTKIEELRQHLLRWGLTTPDKKHQKEPPFLWMGYELHPD
KWTVQPIVLPEKDSWTVNDIQKLVGKLNWASQIYPGIKVRQLSKLLRGTKALTEVIPLTEEAELELAENREILKEPVHG
VYYDPSKDLIAEIQKQGQGQWTYQIYQEPFKNLKTGKYARMRGAHTNDVKQLTEAVQKITTESIVIWGKTPKFKLPIQK
ETWETWWTEYWQATWIPEWEFVNTPPLVKLWYQL
```



Advanced Settings

Model Version: Boltz-1x (with potentials)

Boltz-1x is the newer version of the Boltz-1 model which includes inference time potentials that significantly improve the physical quality of poses. If you want to run the original Boltz-1 model without potentials you can set this to "Boltz-1 (no potentials)".

MSA Mode: mmseqs2_uniref_env

Choose the MSA database you want to use. Selecting "single_sequence" will result in the MSA containing only your target sequence. Note if you upload a custom MSA then your selection here will be ignored. In most cases mmseqs2_uniref_env tends to produce the best results. Warning: We query a 3rd party service to perform sequence searches, if you do not wish to share your sequence set this to "single_sequence".

Number Recycles: 6

Increased recycling steps tend to produce more accurate predictions but will also greatly increases prediction time. For smaller proteins and monomers we recommend 5 recycles, for bigger proteins we recommend 10 recycles.

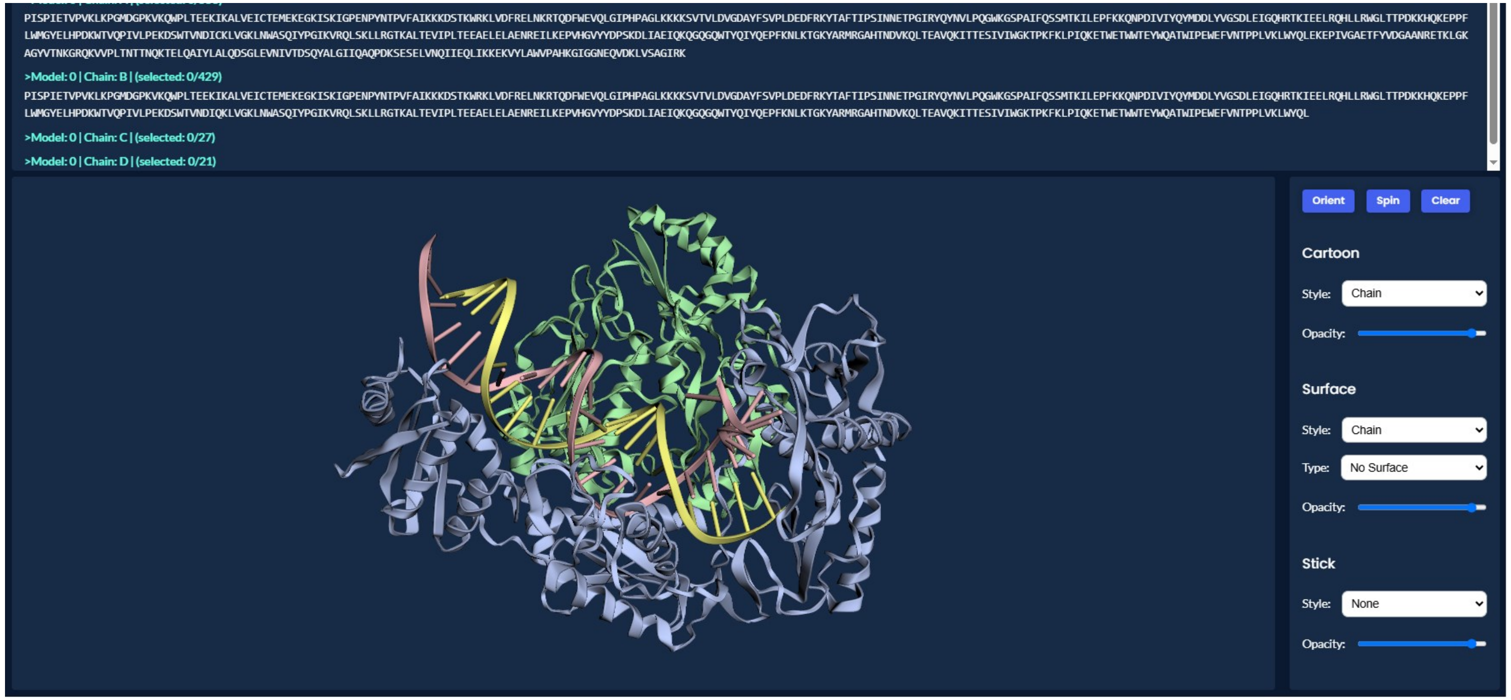
Sampling Steps: 200

The number of sampling steps to use for prediction.

構造を予測したいアミノ酸配列とDNA配列を入力します。
その他オプションで小分子や残基修飾、特定のチェーン同士の
相互作用の指定、共有結合などの結合拘束を指定できます。

設定画面では、パラメータがどのような調整を行
うか、推奨値についてガイドがあります。

Boltz-1結果



```
PISPIETVPVKLKPGMDGPKVKQWPLTEEKIKALVEICTEMEKEGKISKIGPENPYNTPVFAIKKKDSTKWRKLVDFRELNKRTQDFWEVQLGIPHPAGLKKKKSVTVLDVGDAYFSVPLDEDFRKYTAFTIPSINNETPGIRYQYNVLPQGWKGSPAIFQSSMTKILEPFKKQNPDIVIYQYMDDLYVGSDLEIGQHRTKIEELRQHLLRWGLTTPDKKHQKEPPF
LWMGYELHPDKWTVQPIVLPEKDSWTVNDICKLVGKLNWASQIYPGIKVRQLSKLLRGTKALTEVIPLTEEAELELAENREILKEPVHGVYYDPSKDLIAEIQKQGQGQWTYQIYQEPFKNLKTGKYARMRGAHTNDVKQLTEAVQKITTESIVIWGKTPKFKLPIQKETWETWWTEYWQATWIPEWEFVNTPPLVKLWYQLEKEPIVGAETFYVDGAANRETKLGK
AGYVTNKGRQKVVPLTNTTNQKTELQAIYLALQDSGLEVNIVTDSQYALGIIQAQPDKSESELVNQIIEQLIKKEKVYLAWVPAHKGIGGNEQVDKLVSAGIRK
>Model: 0 | Chain: B | (selected: 0/429)
PISPIETVPVKLKPGMDGPKVKQWPLTEEKIKALVEICTEMEKEGKISKIGPENPYNTPVFAIKKKDSTKWRKLVDFRELNKRTQDFWEVQLGIPHPAGLKKKKSVTVLDVGDAYFSVPLDEDFRKYTAFTIPSINNETPGIRYQYNVLPQGWKGSPAIFQSSMTKILEPFKKQNPDIVIYQYMDDLYVGSDLEIGQHRTKIEELRQHLLRWGLTTPDKKHQKEPPF
LWMGYELHPDKWTVQPIVLPEKDSWTVNDIQKLVGKLNWASQIYPGIKVRQLSKLLRGTKALTEVIPLTEEAELELAENREILKEPVHGVYYDPSKDLIAEIQKQGQGQWTYQIYQEPFKNLKTGKYARMRGAHTNDVKQLTEAVQKITTESIVIWGKTPKFKLPIQKETWETWWTEYWQATWIPEWEFVNTPPLVKLWYQL
>Model: 0 | Chain: C | (selected: 0/27)
>Model: 0 | Chain: D | (selected: 0/21)
```

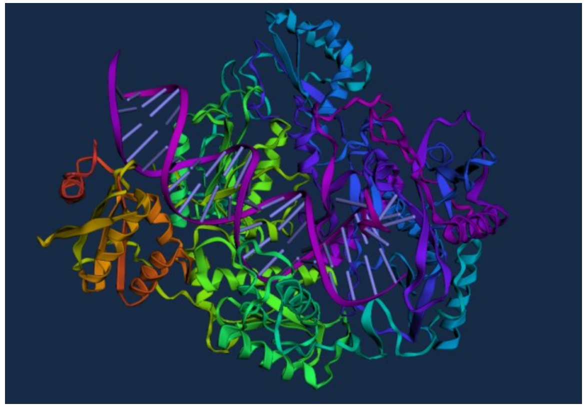
Style: Chain

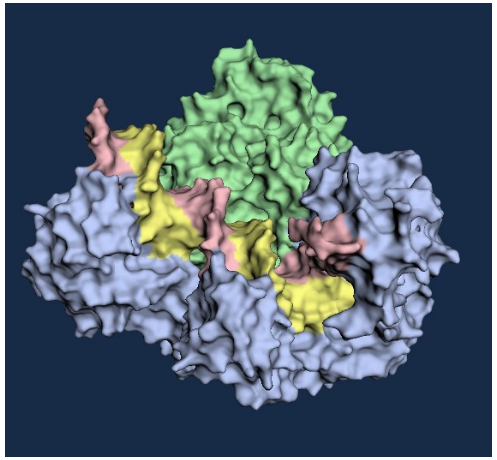
Style: Chain

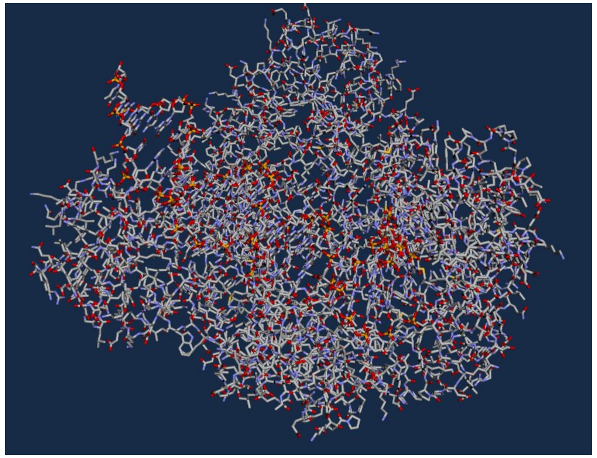
Type: No Surface

Style: None

予測された立体構造はNeurosnap Platform上で視覚化できます。



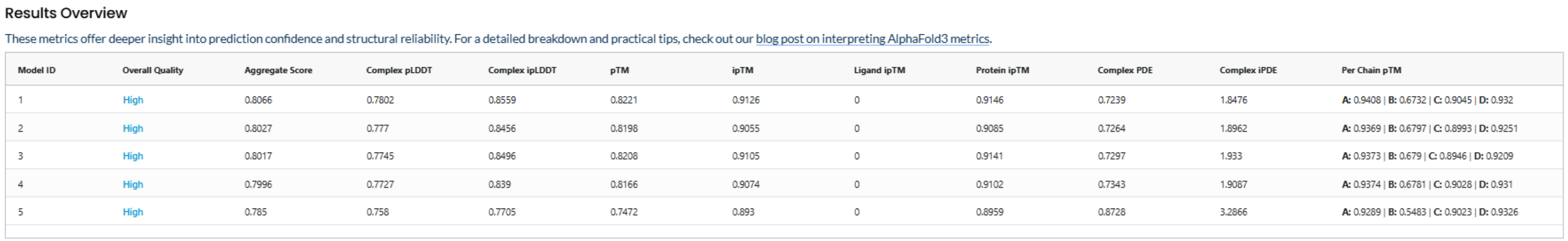




視覚化オプションは豊富で、スペクトル表示、二次構造やアミノ酸残基ごとの色分け、分子表面（Van der Waals）、溶媒アクセス可能表面など、目的に応じて切り替え可能です。

Boltz-1結果　精度の評価

予測された立体構造を評価するためのさまざまな指標やグラフから最適な立体構造を構築できます。

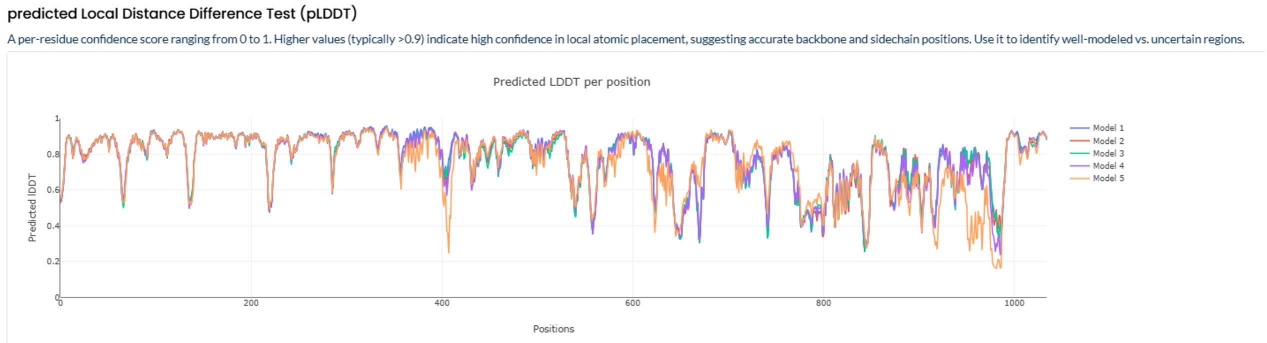


Results Overview

These metrics offer deeper insight into prediction confidence and structural reliability. For a detailed breakdown and practical tips, check out our blog post on interpreting AlphaFold3 metrics.

Model ID	Overall Quality	Aggregate Score	Complex pLDDT	Complex ipLDDT	pTM	ipTM	Ligand ipTM	Protein ipTM	Complex PDE	Complex iPDE	Per Chain pTM
1	High	0.8066	0.7802	0.8559	0.8221	0.9126	0	0.9146	0.7239	1.8476	**A:** 0.9408 | **B:** 0.6732 | **C:** 0.9045 | **D:** 0.932
2	High	0.8027	0.777	0.8456	0.8198	0.9055	0	0.9085	0.7264	1.8962	**A:** 0.9369 | **B:** 0.6797 | **C:** 0.8993 | **D:** 0.9251
3	High	0.8017	0.7745	0.8496	0.8208	0.9105	0	0.9141	0.7297	1.933	**A:** 0.9373 | **B:** 0.679 | **C:** 0.8946 | **D:** 0.9209
4	High	0.7996	0.7727	0.839	0.8166	0.9074	0	0.9102	0.7343	1.9087	**A:** 0.9374 | **B:** 0.6781 | **C:** 0.9028 | **D:** 0.931
5	High	0.785	0.758	0.7705	0.7472	0.893	0	0.8959	0.8728	3.2866	**A:** 0.9289 | **B:** 0.5483 | **C:** 0.9023 | **D:** 0.9326

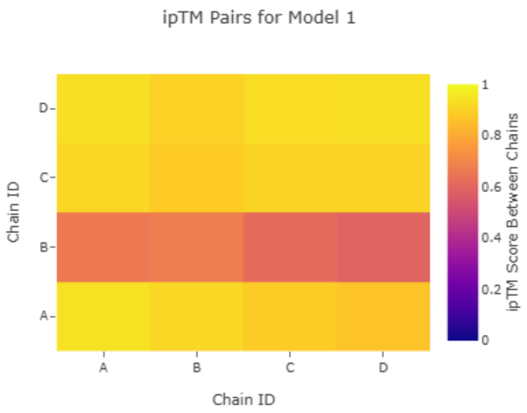
予測の信頼性と構造の信頼性についてより深い洞察が得られる指標を含むテーブル



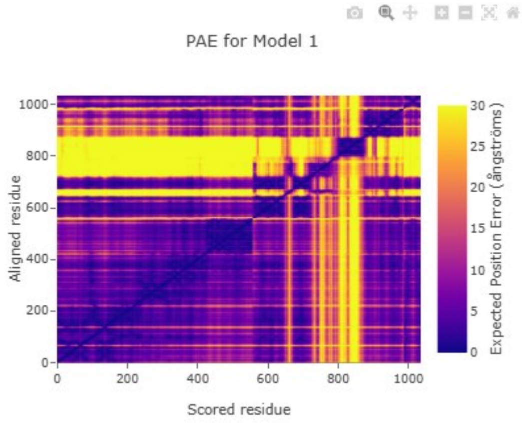
predicted Local Distance Difference Test (pLDDT)

A per-residue confidence score ranging from 0 to 1. Higher values (typically >0.9) indicate high confidence in local atomic placement, suggesting accurate backbone and sidechain positions. Use it to identify well-modeled vs. uncertain regions.

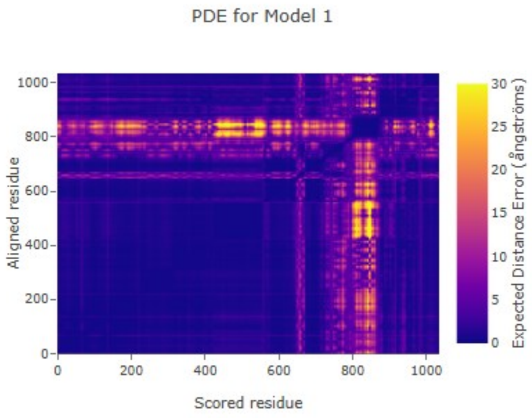
predicted Local Distance Difference Test (pLDDT)
残基ごとの信頼度スコア



Per Chain Pair ipTM Values



Predicted Aligned Error (PAE)



Predicted Distance Error (PDE)

お問い合わせ先：フィルジェン株式会社

TEL 052-624-4388 (9:00～17：00）

FAX　052-624-4389

E-mail: support@filgen.jp