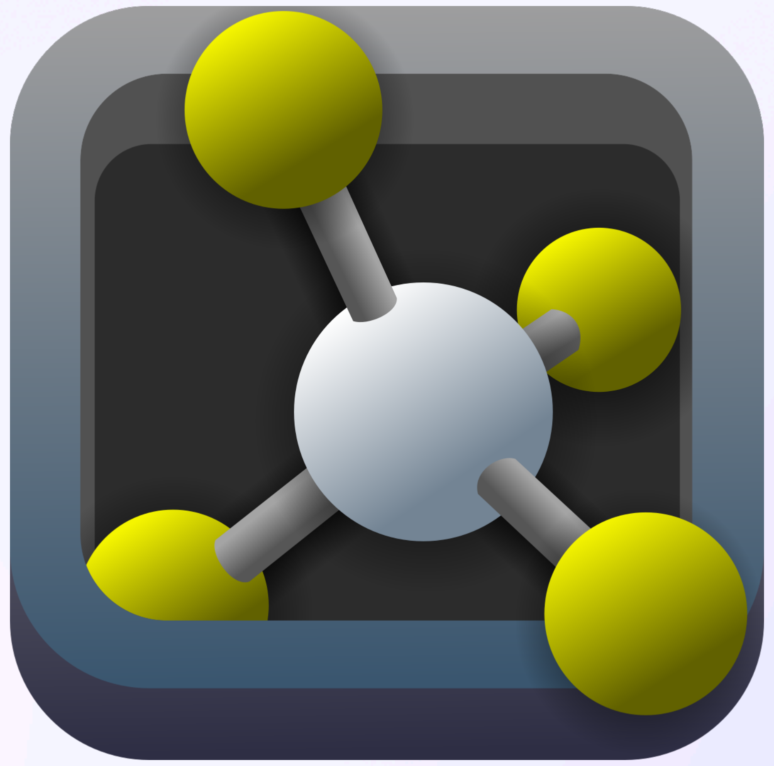
AlphaFold3 应用与实践

上海交通大学 2025 AI4Bioengineering 暑期学校

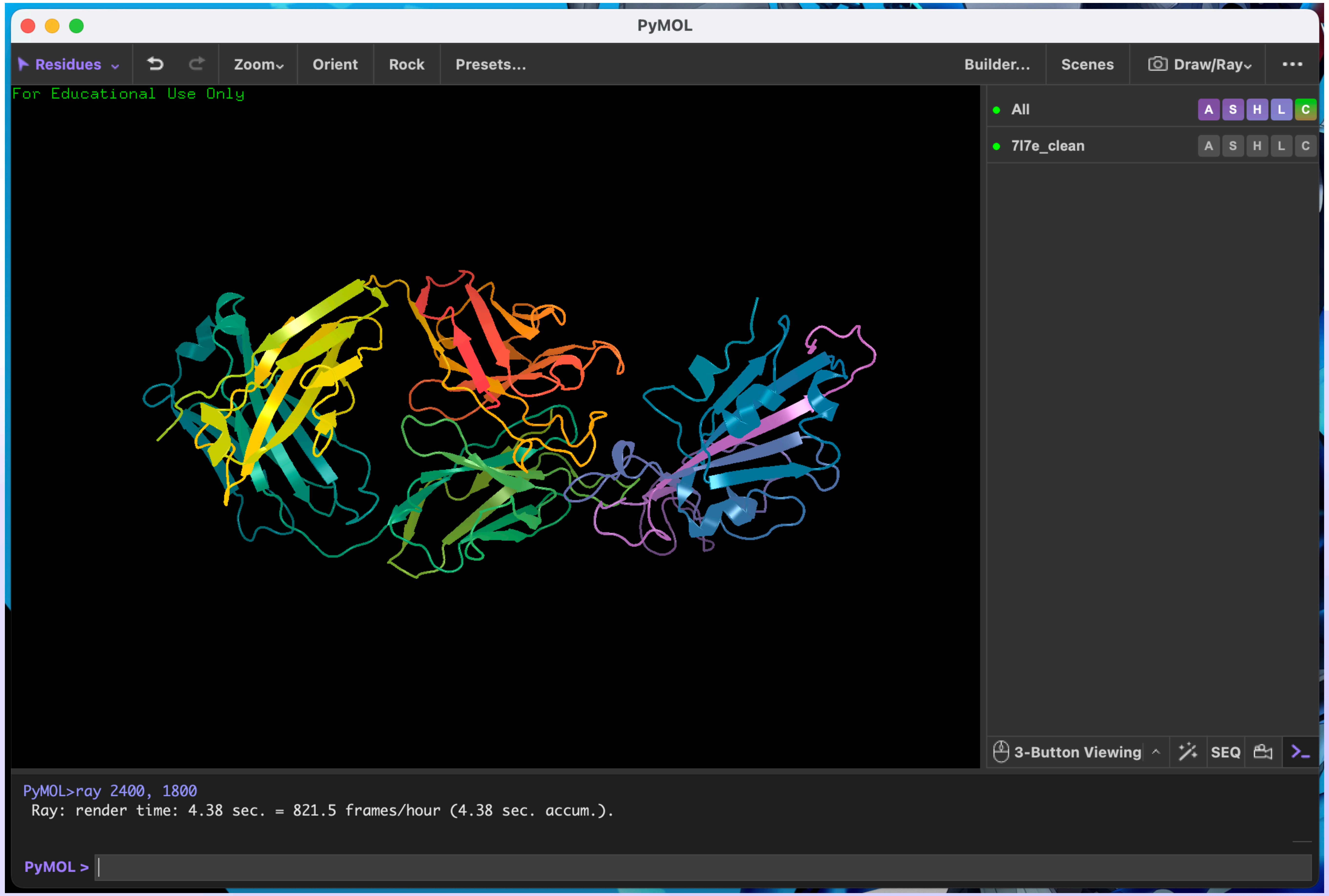
钟博子韬 2025-08-10

课前准备：PyMOL

- PyMOL 软件主要用于查看蛋白质结构
- https://www.pymol.org/ 下载PyMOL
- https://www.pymol.org/edu/ 申请License



PyMOL 3



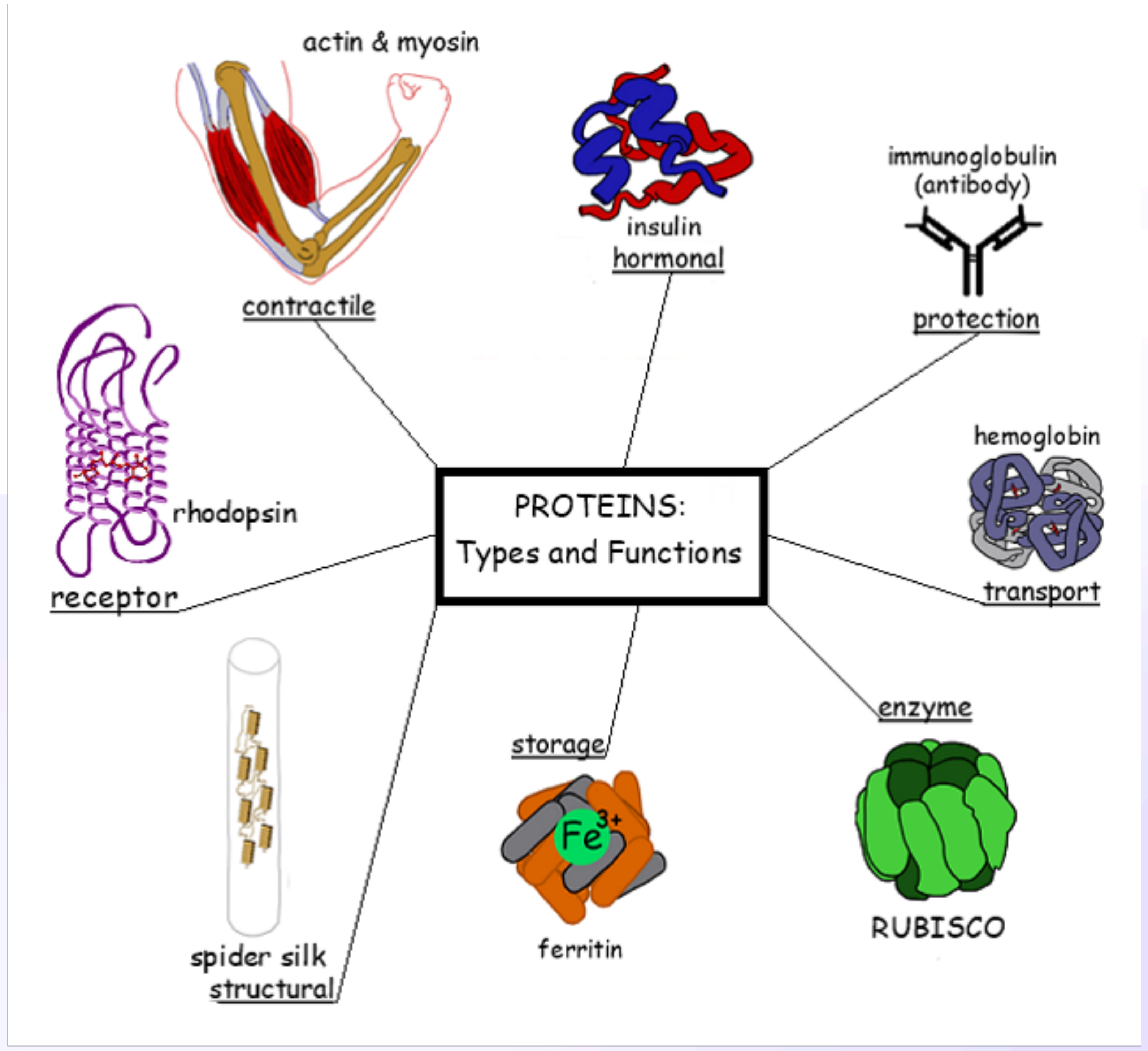
For Educational Use Only

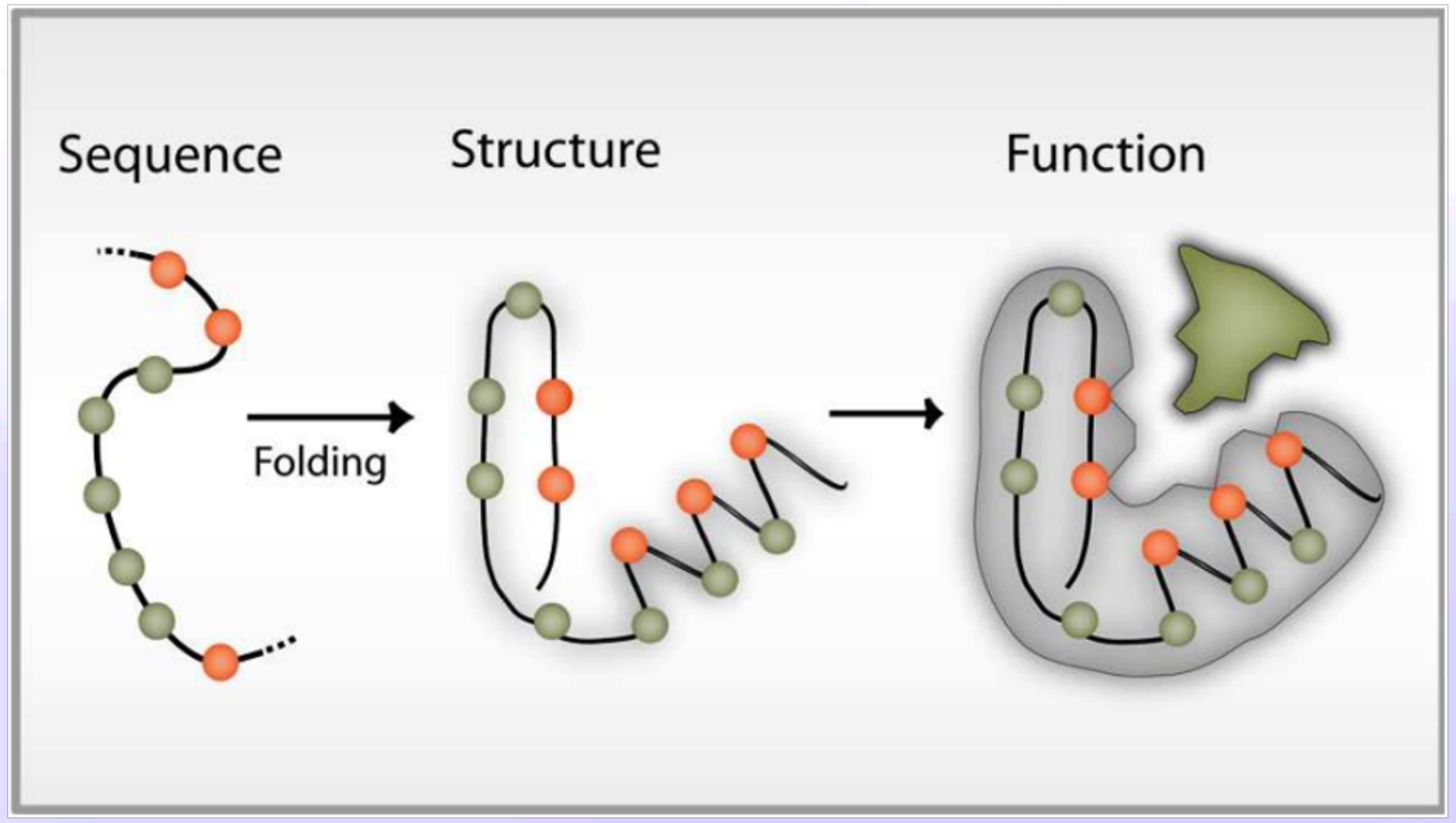
```
PyMOL>ray 2400, 1800
 Ray: render time: 4.38 sec. = 821.5 frames/hour (4.38 sec. accum.).

PyMOL >
```

PyMOL interface

蛋白质：序列-结构-功能





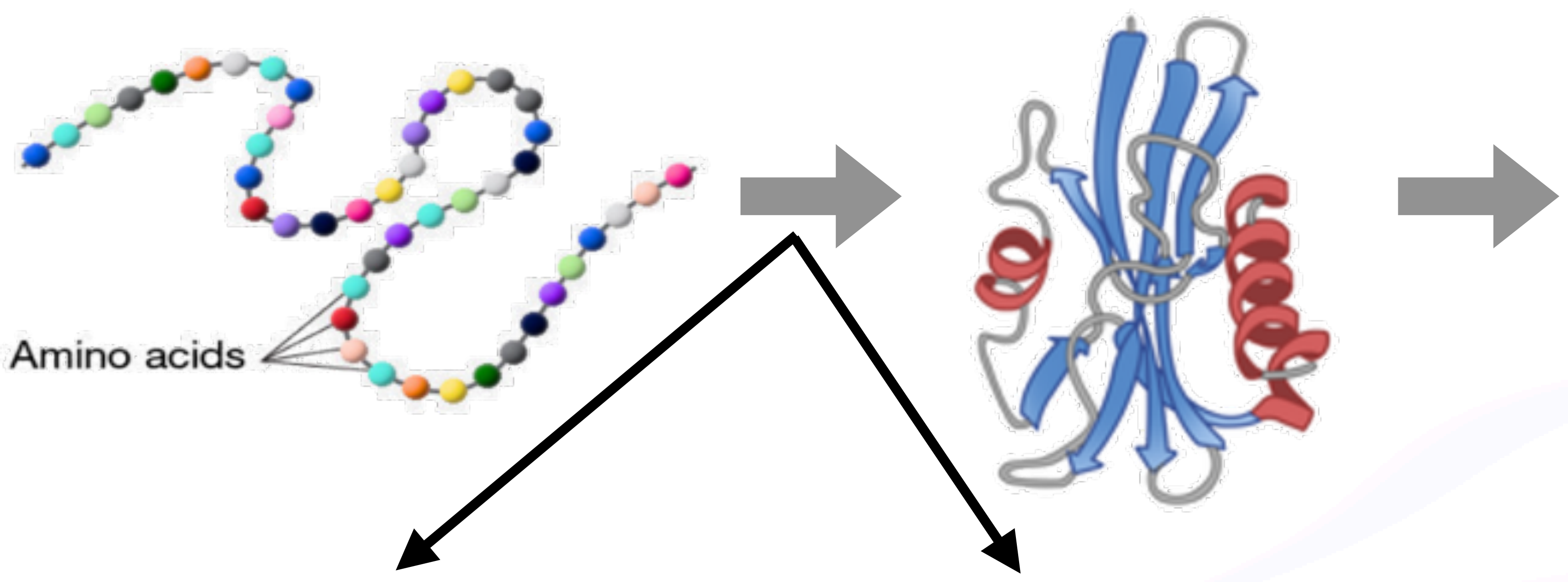
序列决定结构，结构决定功能

蛋白质数据库

序列信息 **结构信息** **功能信息**

		维护团队	包含信息	数据量
GenBank	**NCBI**	NIH 🇺🇸	序列	**5.68B**
UniProt	**UniProt**	EMBL-EBI 🇬🇧, SIB 🇨🇭	序列	**0.25B**
Pfam	**Pfam**	EMBL-EBI 🇬🇧	序列	**0.21B**
	AFDB	EMBL-EBI & DeepMind 🇬🇧	结构	**0.21B**
KEGG Kyoto Encyclopedia of Genes and Genomes	**KEGG**	Kanehisa Laboratories 🇯🇵	功能	**0.06B**
Expasy	**ENZYME**	SIB 🇨🇭	功能	**5M**
	SwissProt	EMBL-EBI 🇬🇧, SIB 🇨🇭	功能	**0.57M**
RCSB PDB PROTEIN DATA BANK	**PDB**	wwPDB 🌍	结构	**0.24M**

蛋白质结构预测



蛋白序列

蛋白结构

蛋白功能

药物靶标

抗体结合

酶促反应

蛋白设计

实验方法

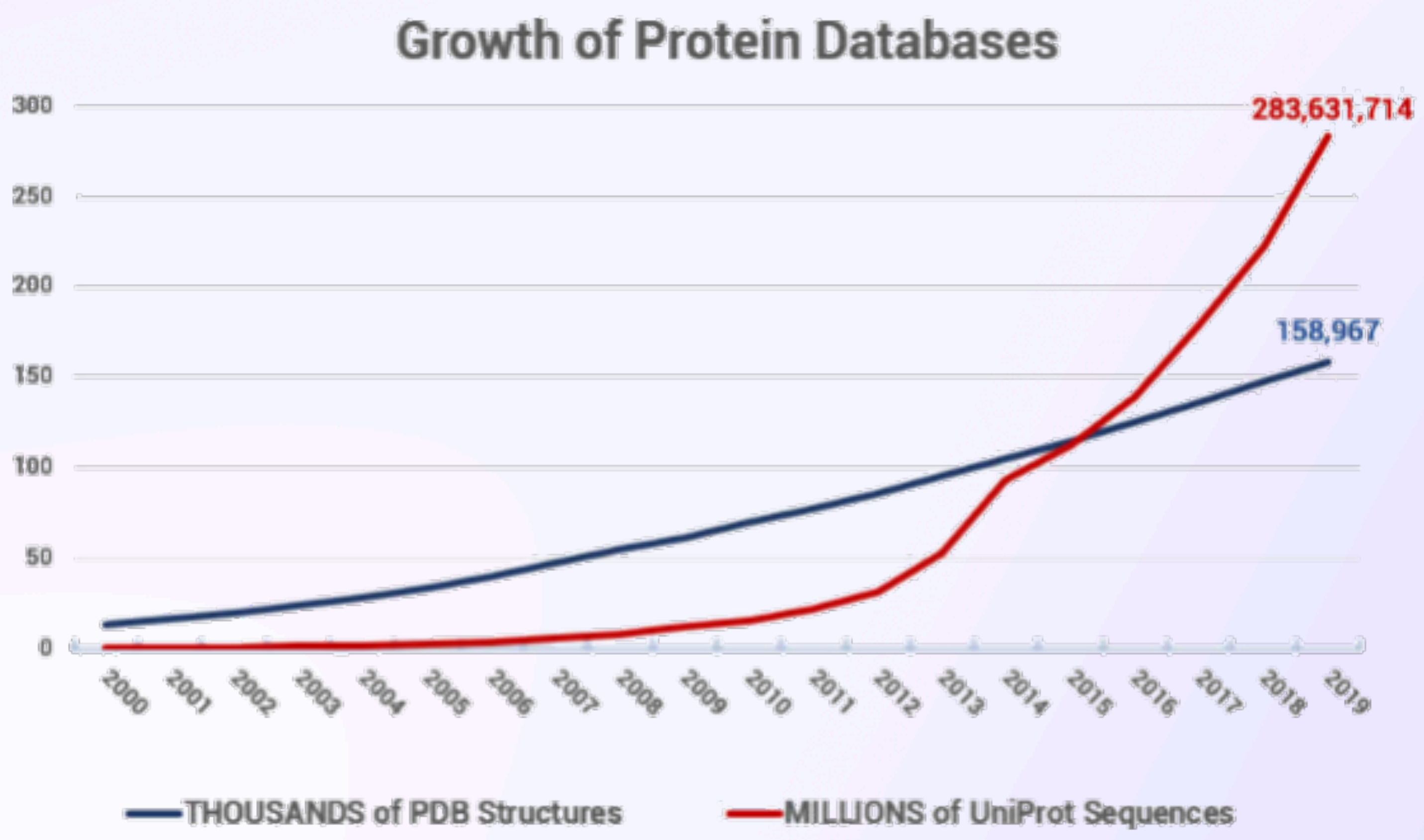
低通量，高精度

>$10,000 / 蛋白

计算方法

高通量，低精度

能进行大规模预测



UniProt: 2.48亿

in 2023

PDB: 20.8万

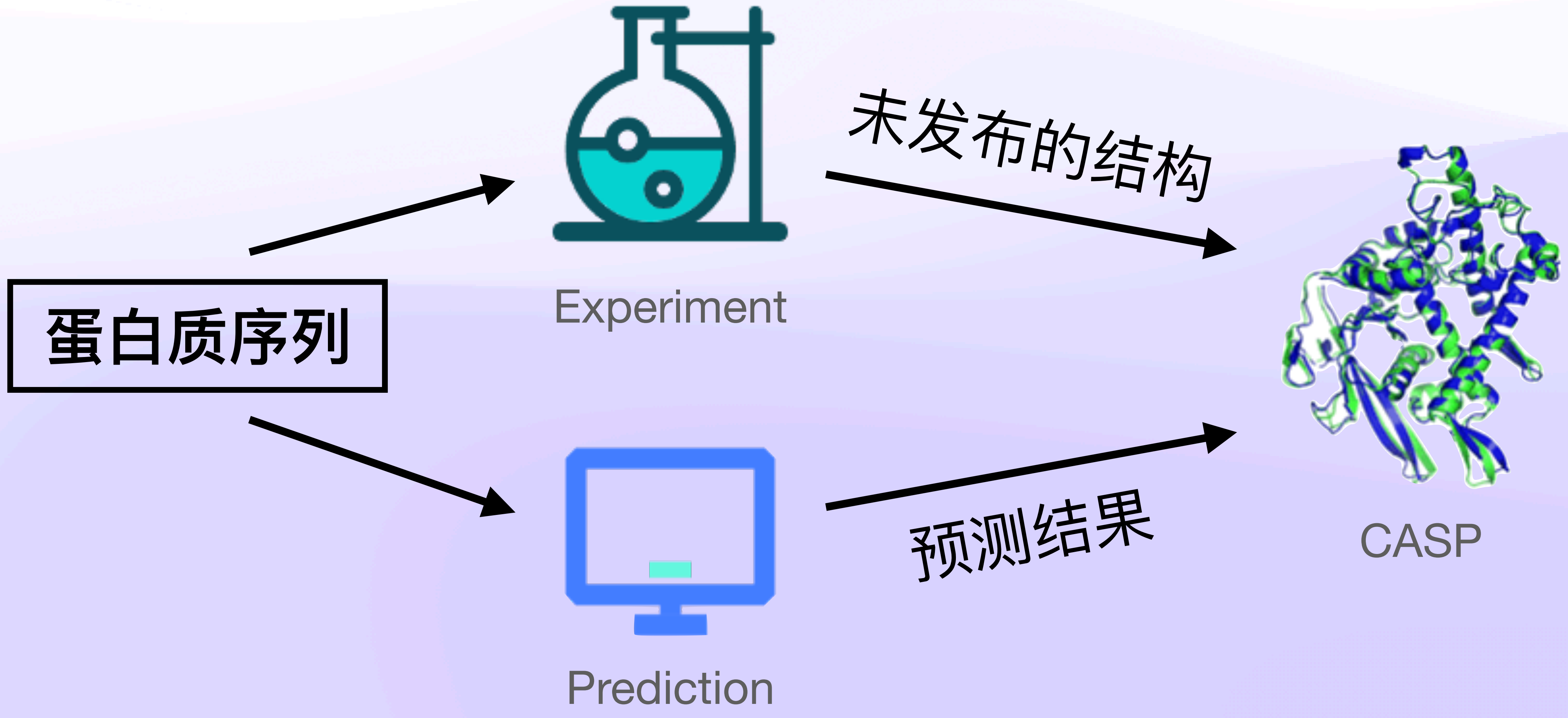
in 2023

⬆️ 大量的序列数据

⬇️ 少量的结构数据

CASP

Critical Assessment of protein Structure Prediction (结构预测的准确评估), 1994



蛋白质序列

Experiment

未发布的结构

Prediction

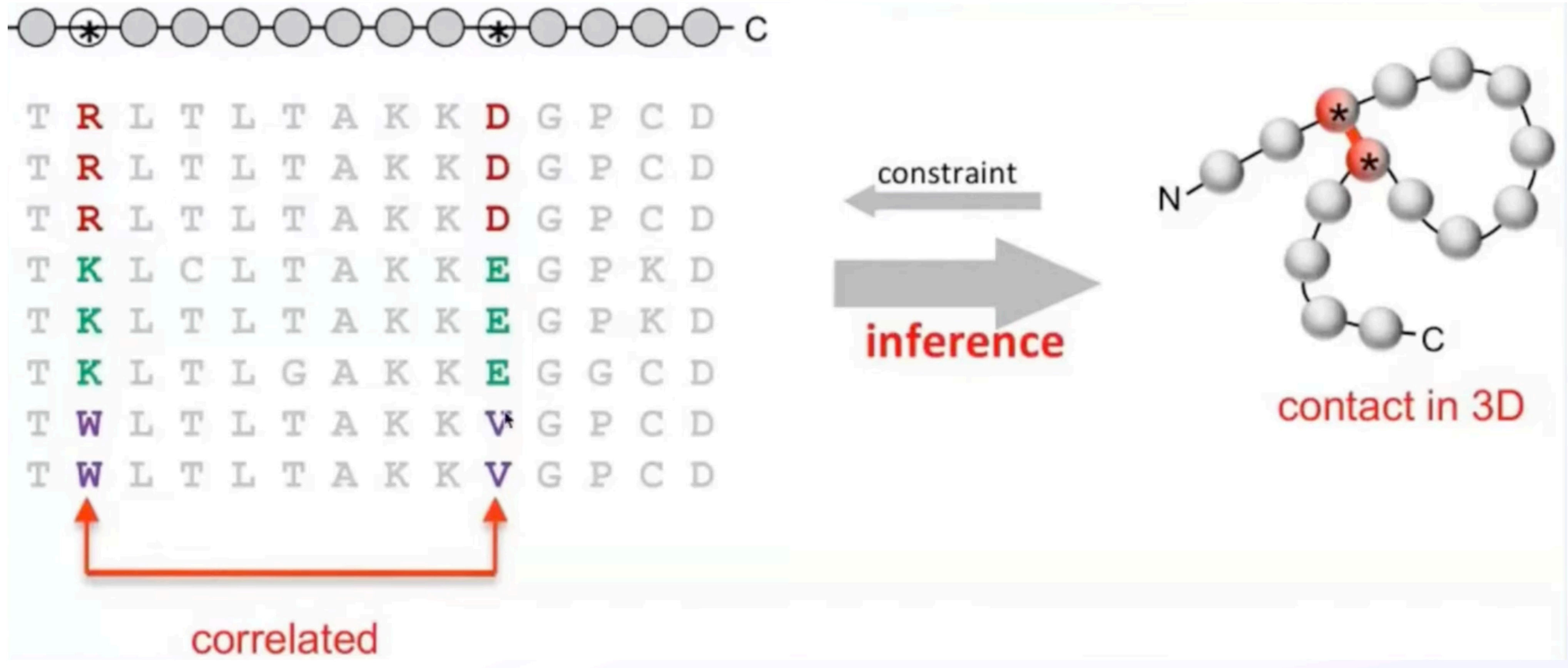
预测结果

CASP

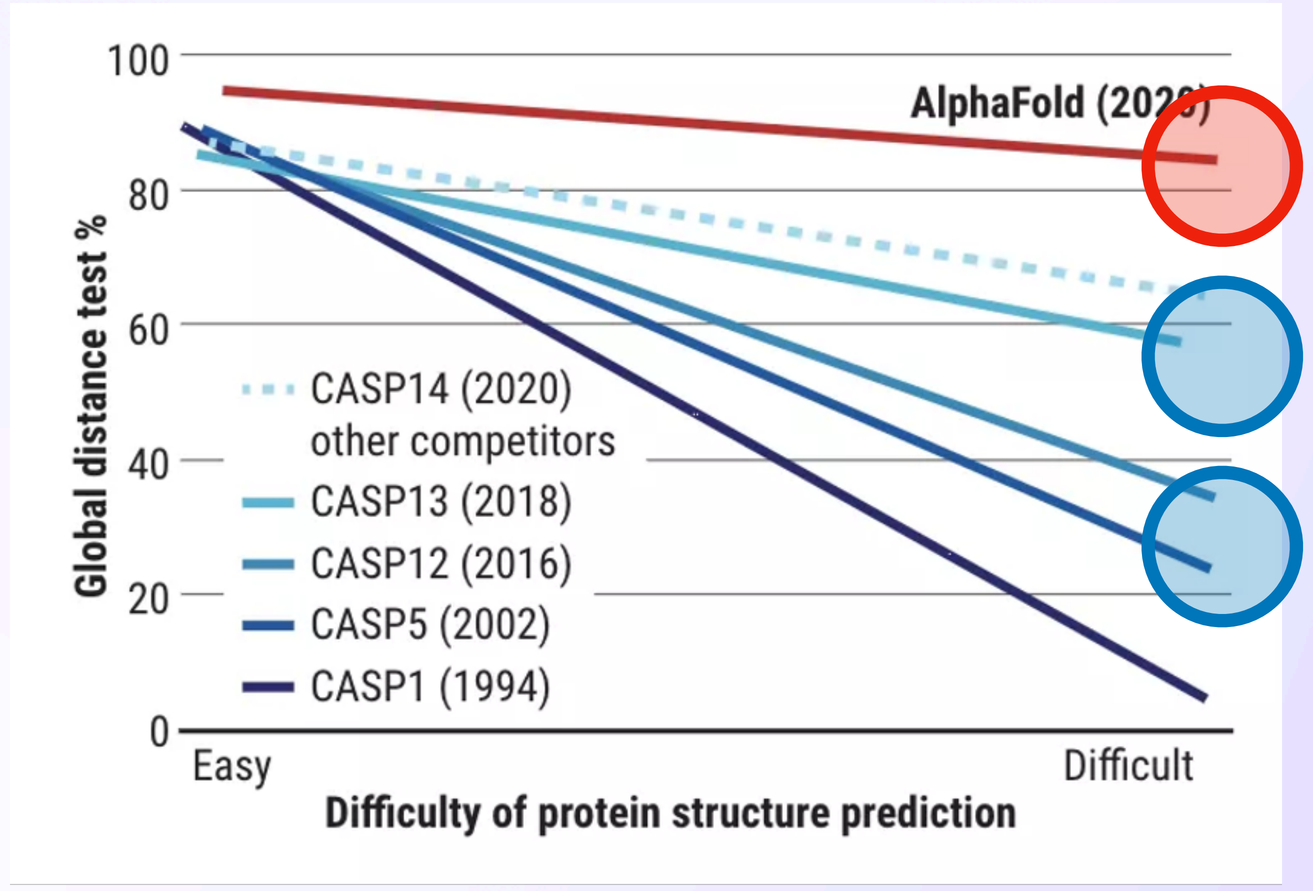
评估模型预测蛋白质结构的准确性

J. Jumper *et al.*, *Nature*. **596**, 583–589 (2021)

AlphaFold2的诞生



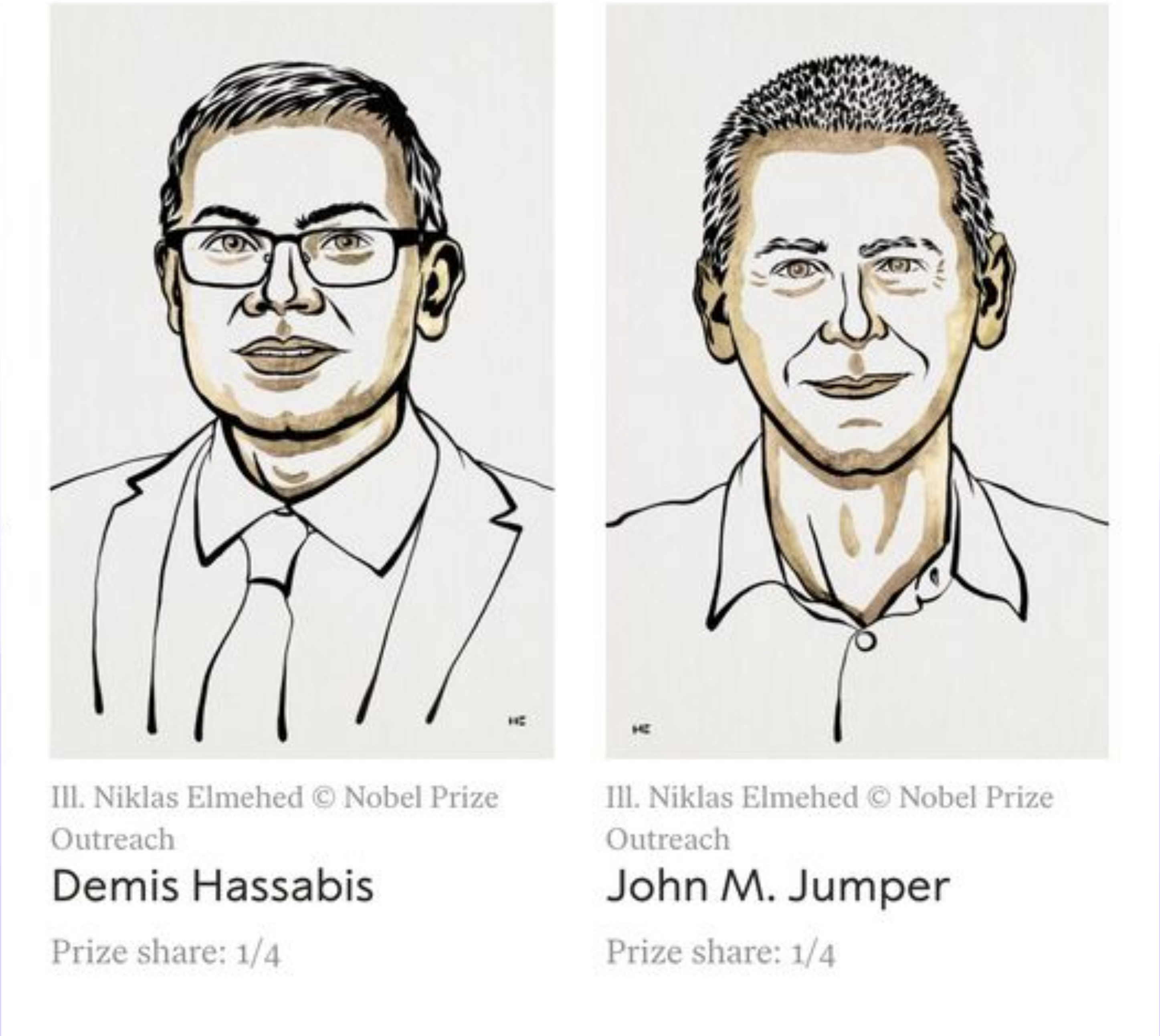
从共进化信息到氨基酸相互作用



AlphaFold2 CASP14 (2020)

AlphaFold1 CASP13 (2018)

CASP12 (2016)



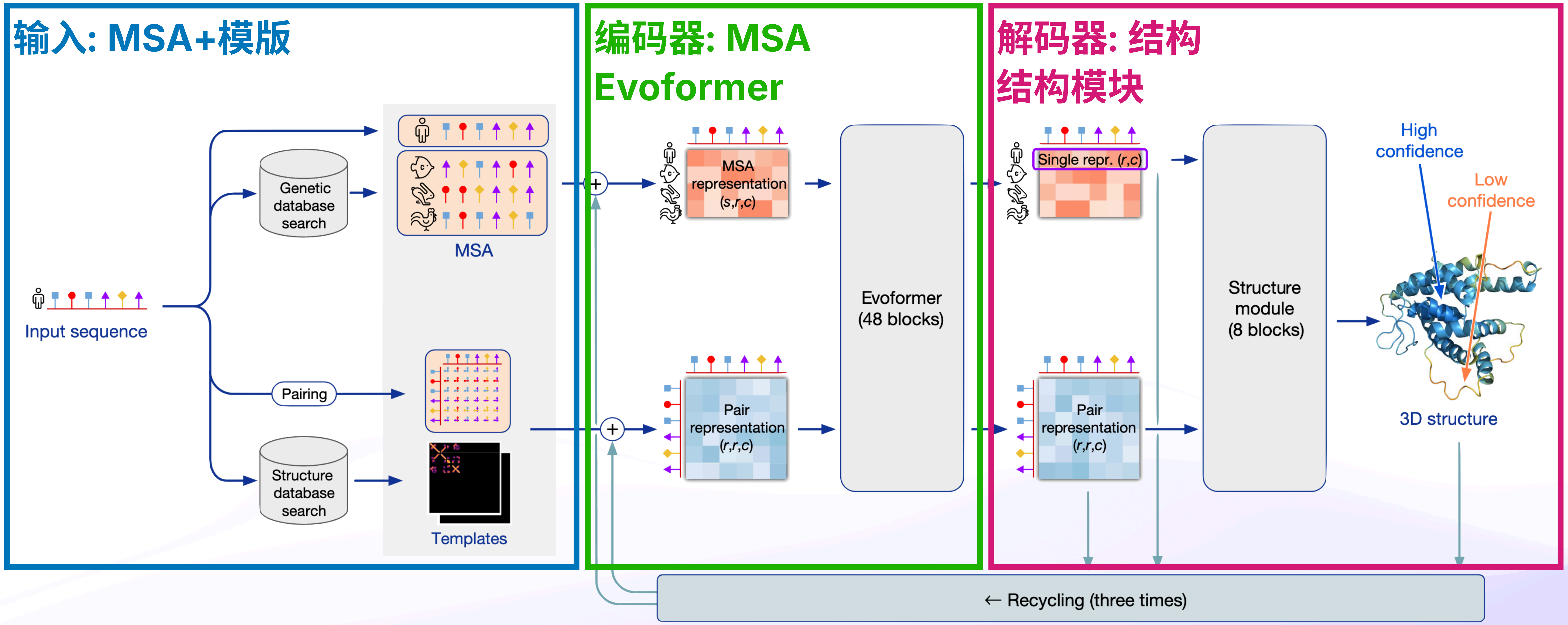
Ill. Niklas Elmehed © Nobel Prize Outreach
Demis Hassabis
Prize share: 1/4

Ill. Niklas Elmehed © Nobel Prize Outreach
John M. Jumper
Prize share: 1/4

AlphaFold2主创获得2024诺贝尔化学奖

U. Göbel, C. Sander, R. Schneider, A. Valencia, *Proteins*. **18**, 309–317 (1994)

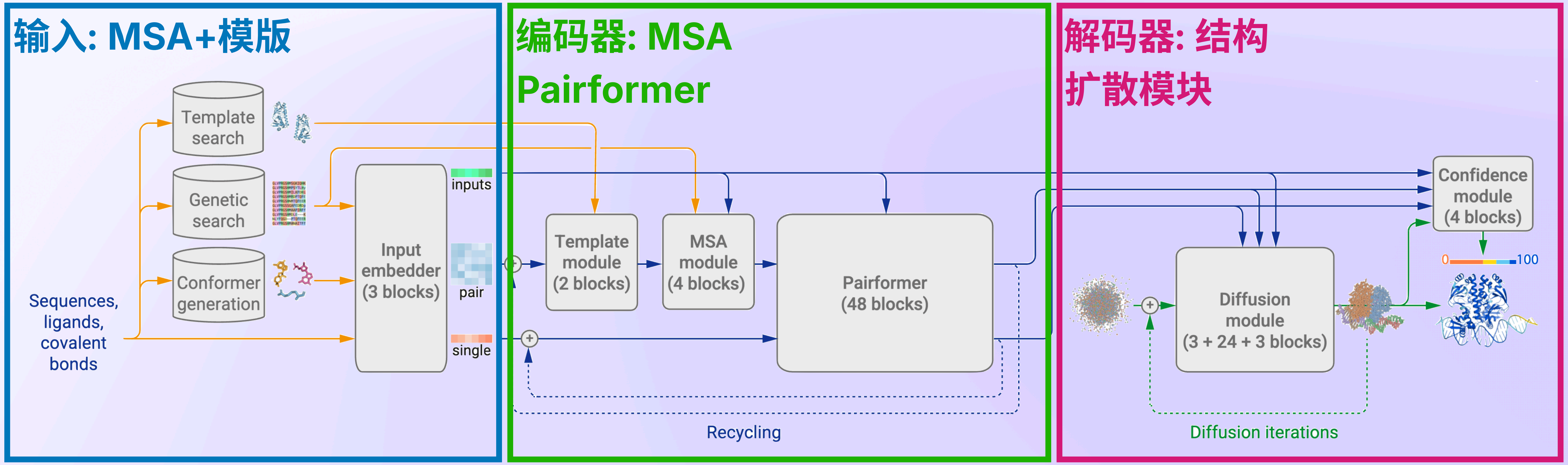
AlphaFold2


输入: MSA+模版

编码器: MSA Evoformer

解码器: 结构 结构模块

AlphaFold3


输入: MSA+模版

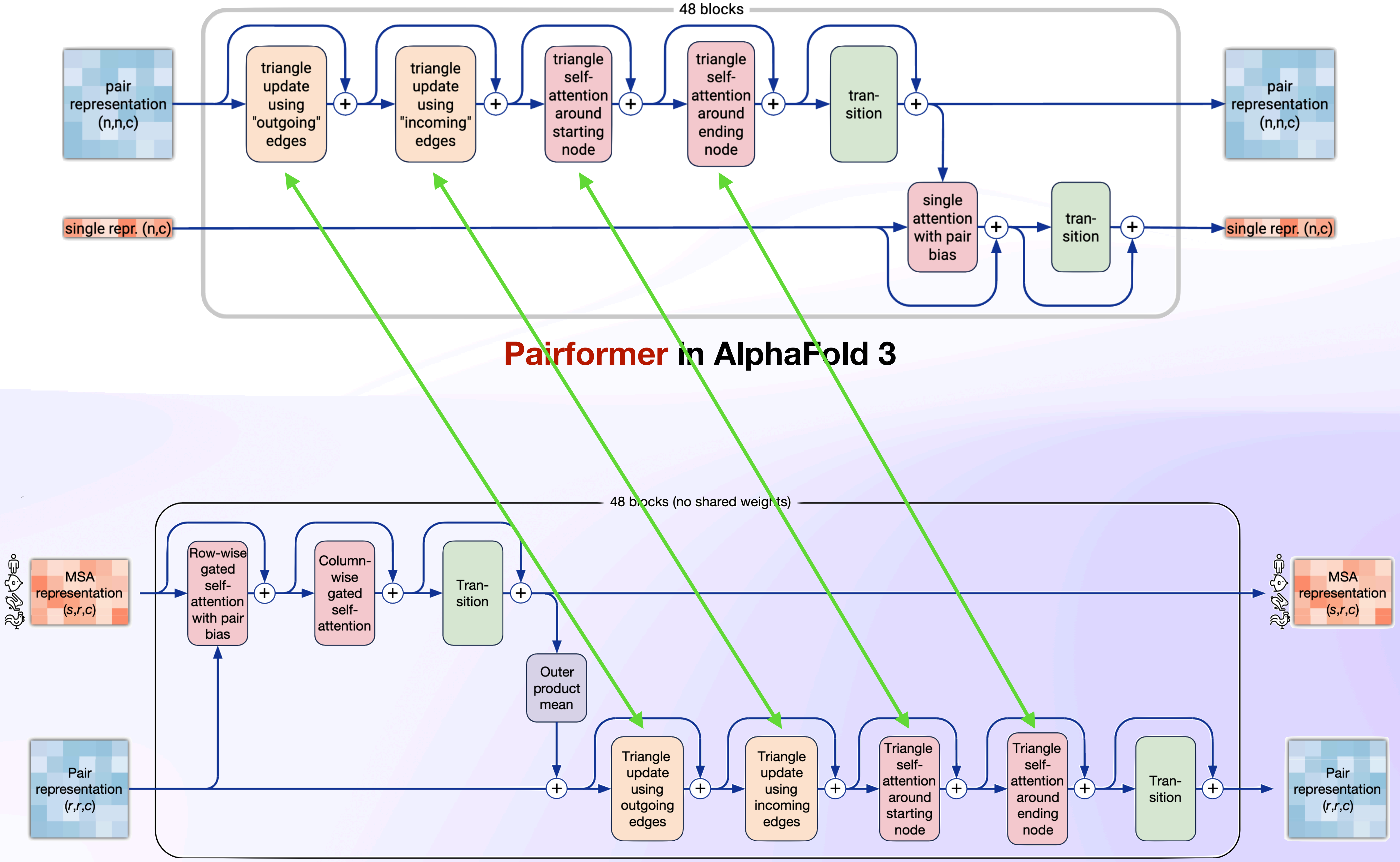
编码器: MSA Pairformer

解码器: 结构 扩散模块

Pairformer

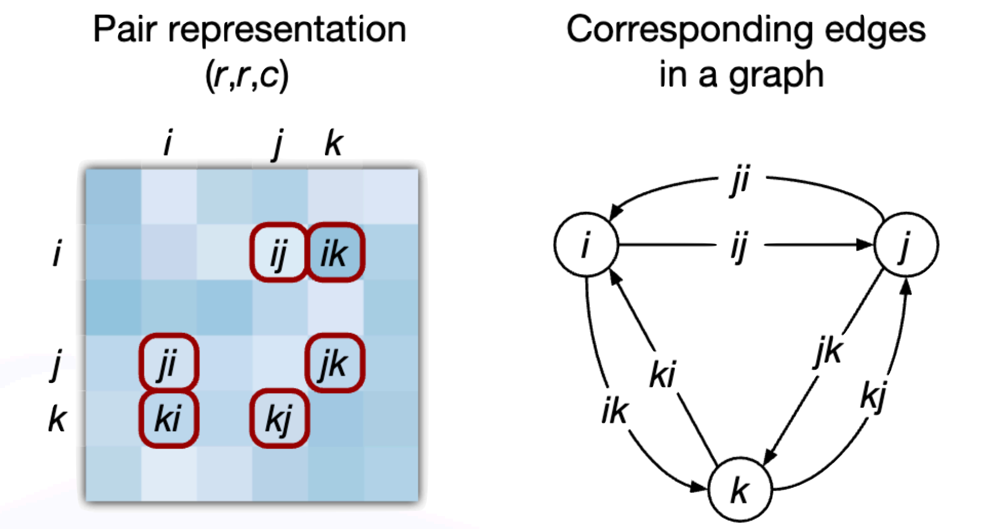
Pairformer Module details

- Input & Output: Pair repr. (n, n, c) and single repr. (n, c)
  - n: number of tokens (polymer residues and atoms);
  - c: number of channels (pair repr. 128, single repr. 384)
- The 48 blocks has an independent set of parameters

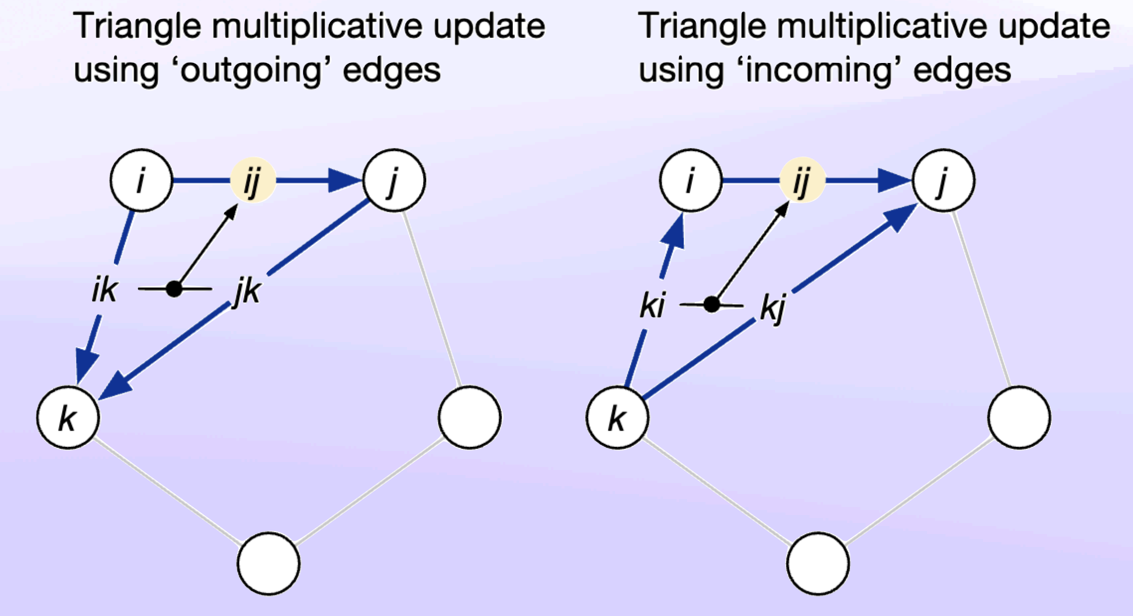


Pairformer in AlphaFold 3

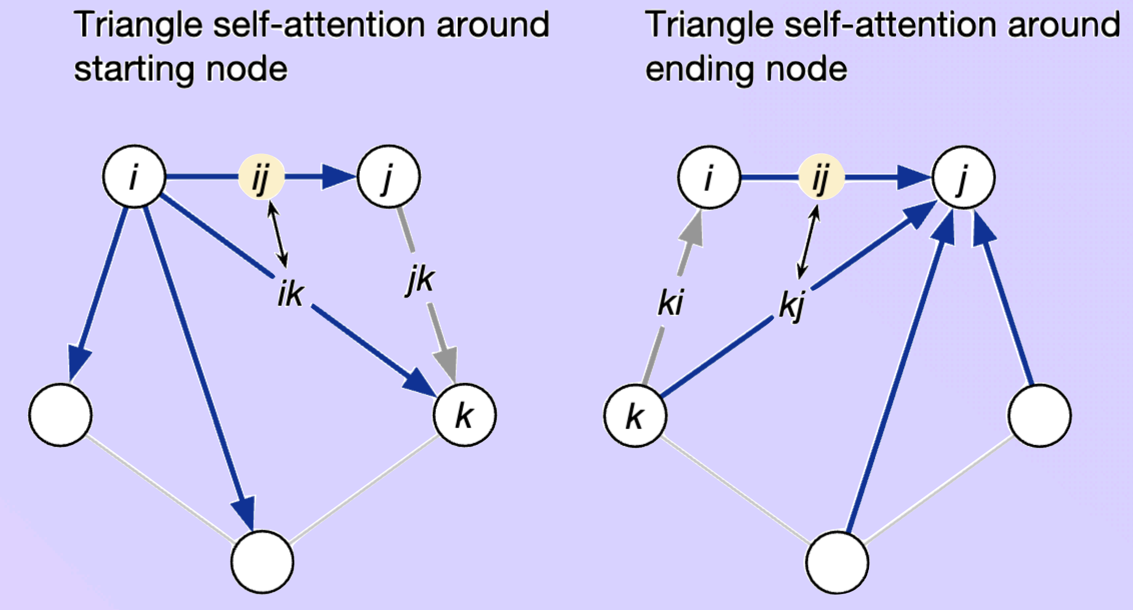
Evoformer in AlphaFold 3



Triangle in pair repr.

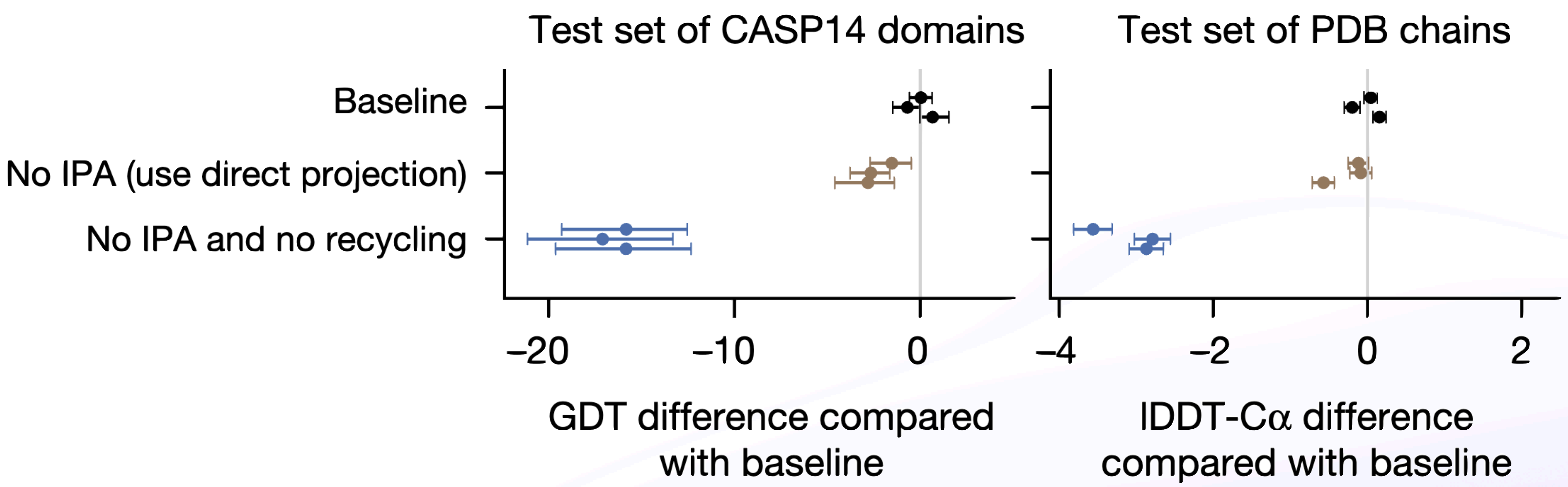


Triangle update

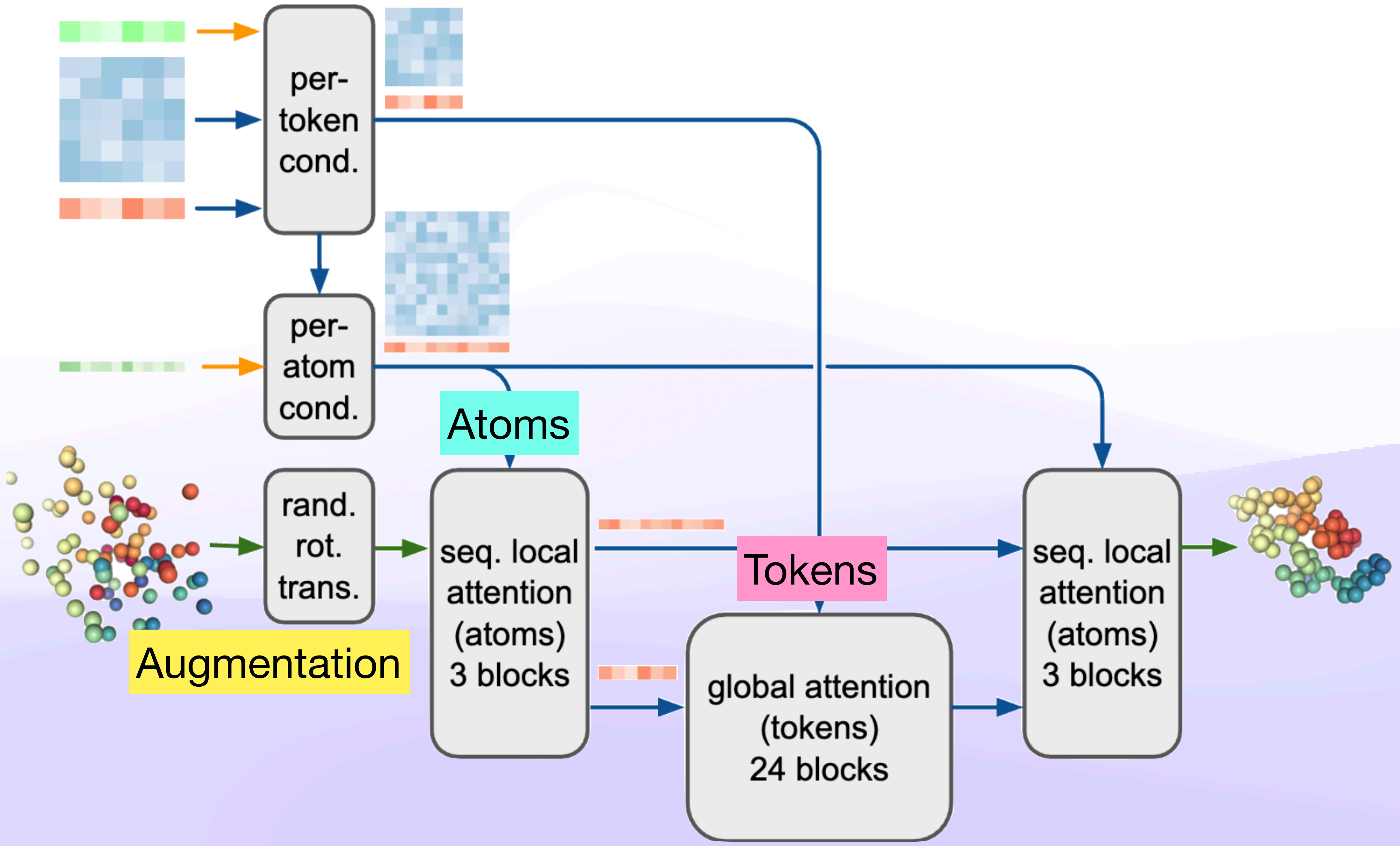


Triangle self-attention

Diffusion Module



AlphaFold2 ablation studies: IPA is not necessary



Diffusion Module

氨基酸为单元
旋转平移不变

→

原子为单元
抛弃旋转平移不变

噪声坐标 ➡️ 预测坐标

全原子

AlphaFold3的能力

✅ 小分子配体

- 小分子：药物，辅酶等
- 金属离子

✅ 蛋白质复合物

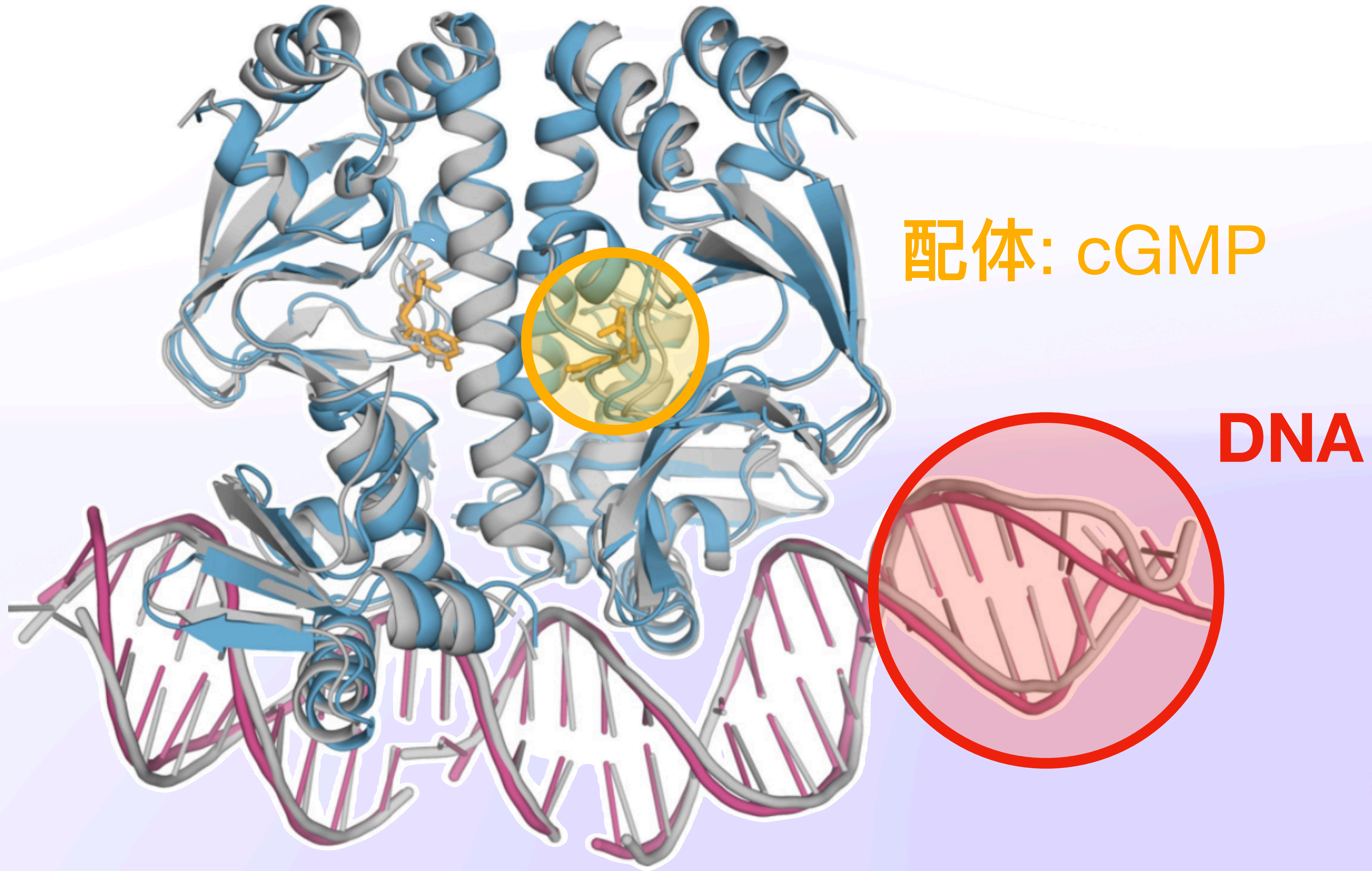
- 抗原抗体复合物

✅ 翻译后修饰

✅ DNA/RNA

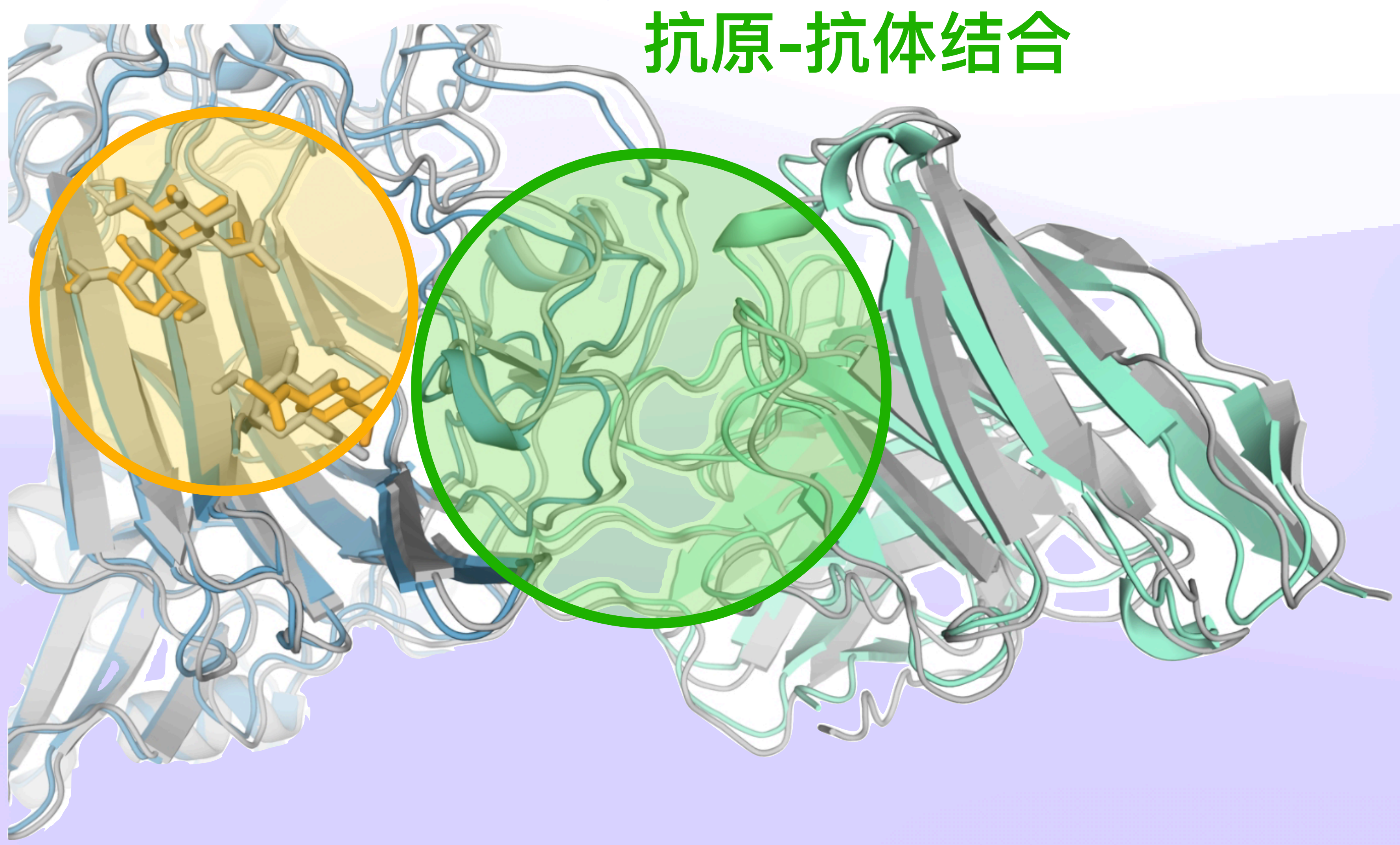
- 蛋白-核酸复合物

❓ 蛋白质动力学信息



AF3 预测 Clr-cGMP-DNA 复合物

PDB ID: 7PZB, full complex LDDT: 82.8, GDT: 90.1

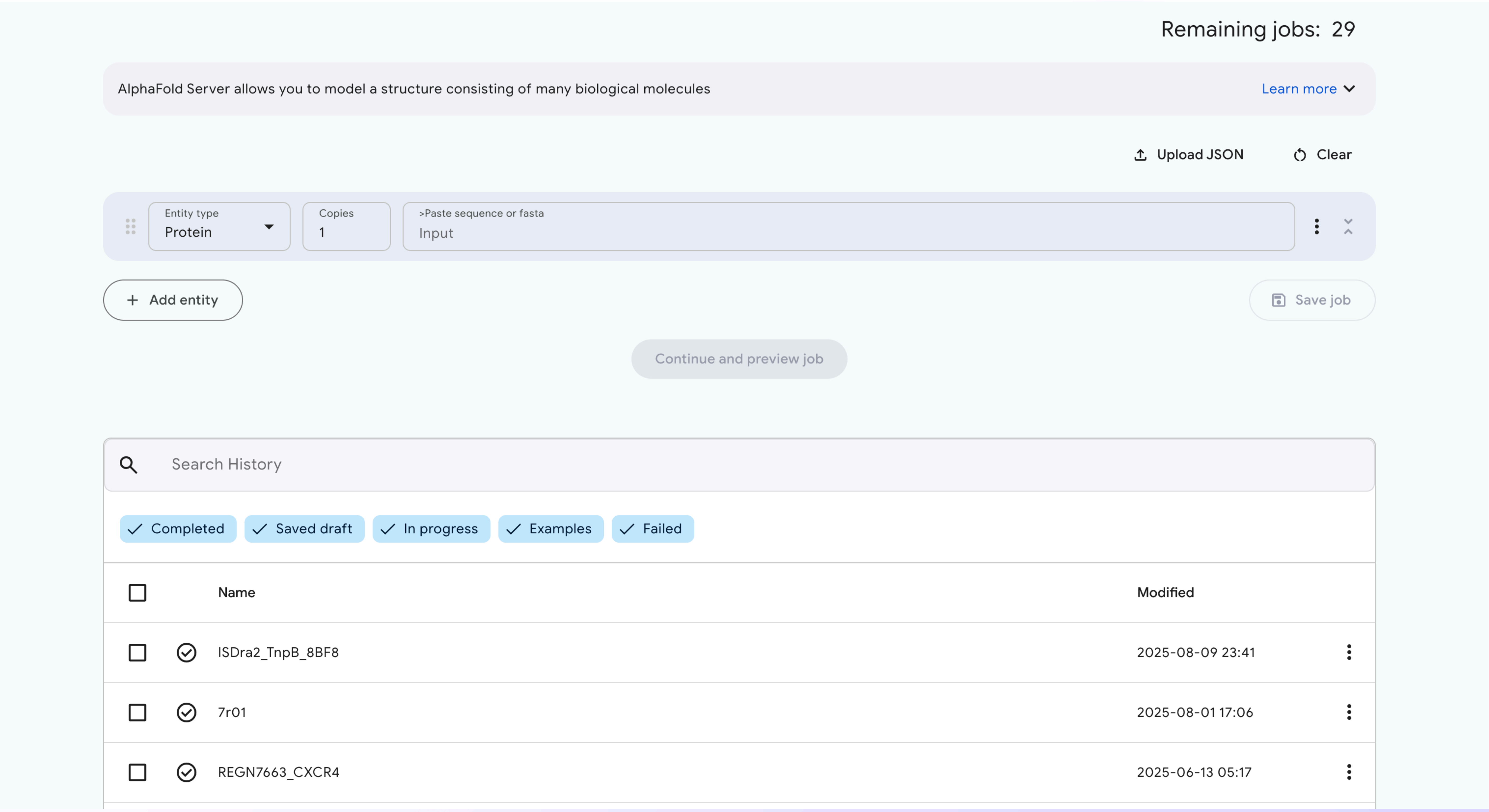


AF3 预测糖基化蛋白OC43 与抗体的复合物

PDB ID: 7PNM, full complex LDDT: 83.0, GDT: 83.1

在线使用AlphaFold3

- 访问 https://alphafoldserver.com/
- 需要：Google账号


Remaining jobs: 29

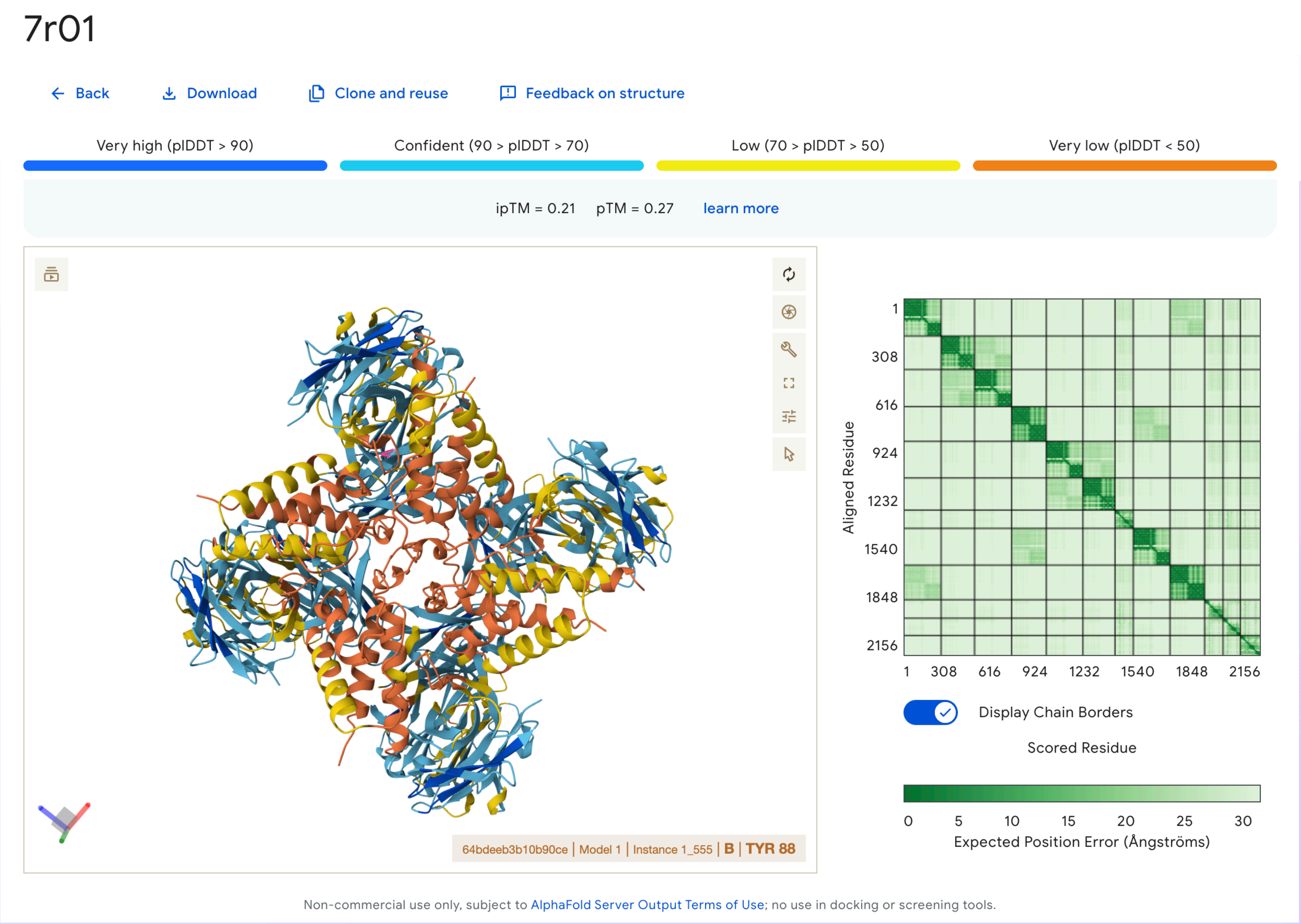
AlphaFold Server allows you to model a structure consisting of many biological molecules

Entity type: Protein

Copies: 1

>Paste sequence or fasta: Input

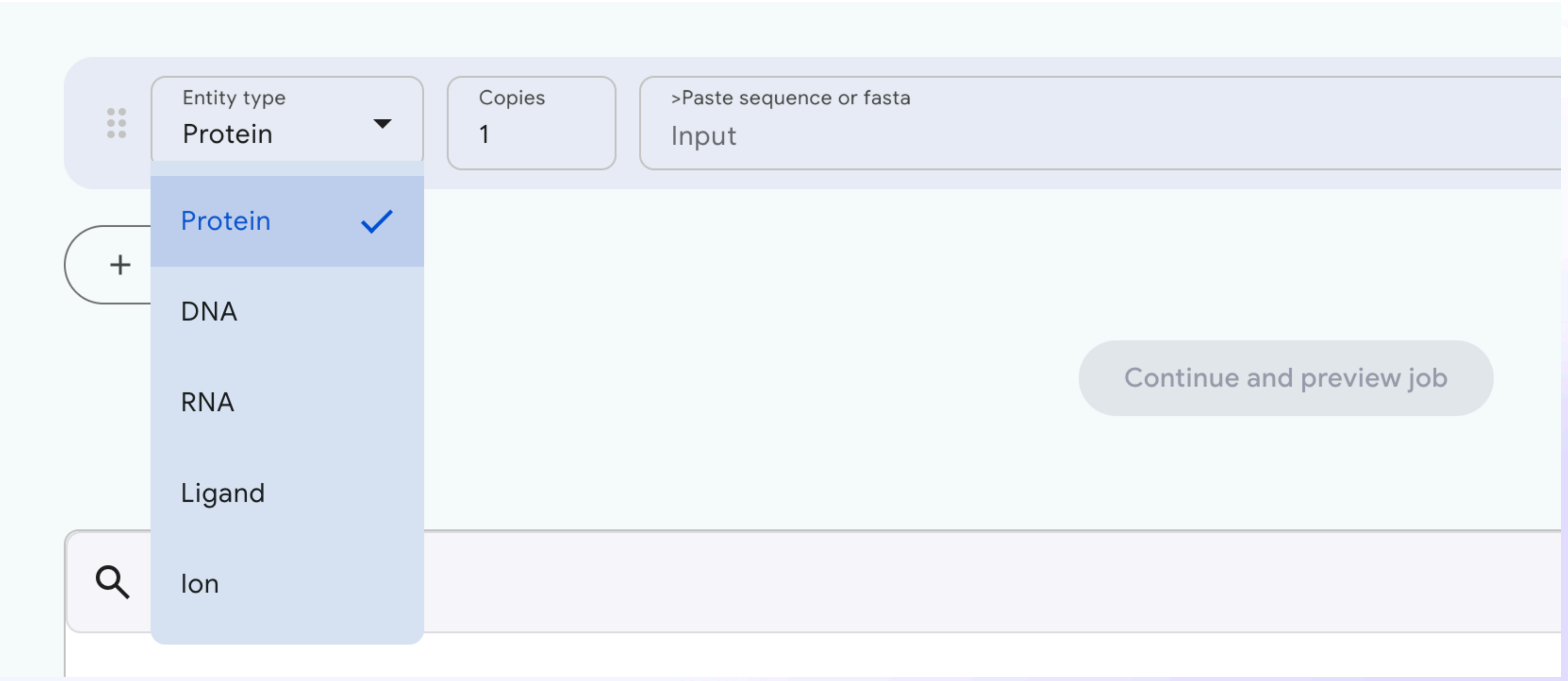
☐		Name	Modified
☐	✓	ISDra2_TnpB_8BF8	2025-08-09 23:41
☐	✓	7r01	2025-08-01 17:06
☐	✓	REGN7663_CXCR4	2025-06-13 05:17


7r01

ipTM = 0.21   pTM = 0.27

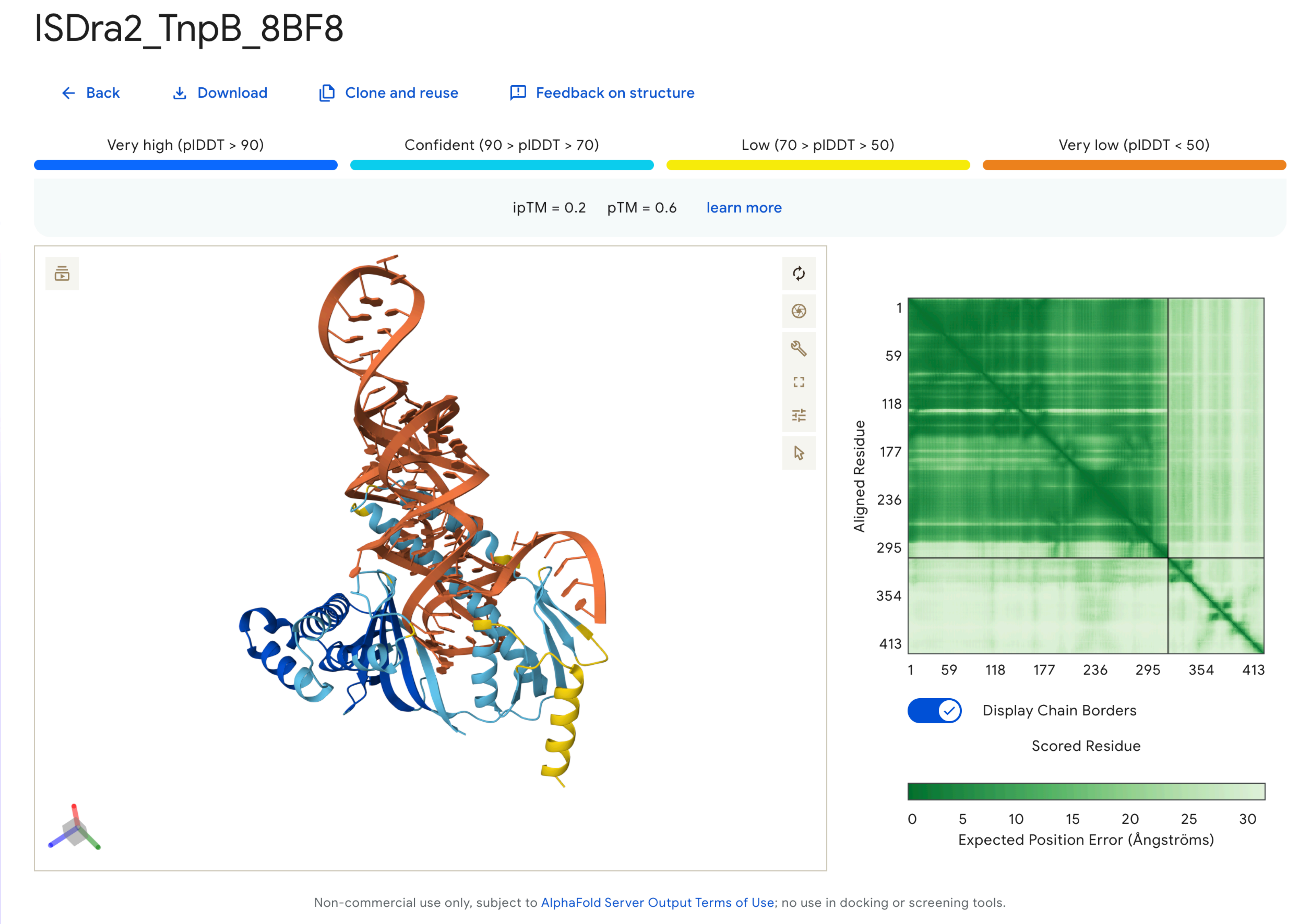
Non-commercial use only, subject to AlphaFold Server Output Terms of Use; no use in docking or screening tools.

在线使用AlphaFold3: RNA


Entity type: Protein

Copies: 1

>Paste sequence or fasta: Input


ISDra2_TnpB_8BF8

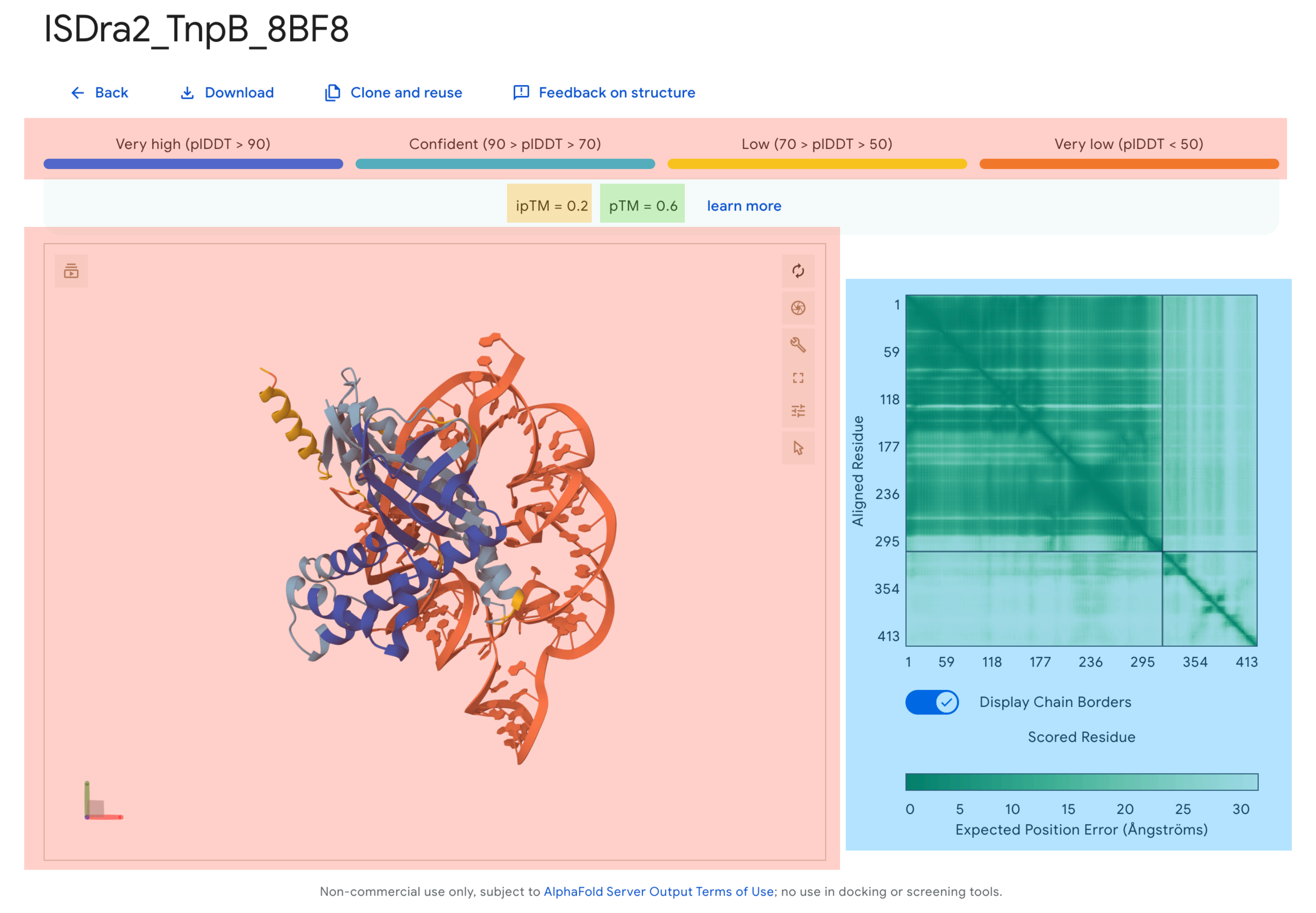
Very high (pLDDT > 90)
Confident (90 > pLDDT > 70)
Low (70 > pLDDT > 50)
Very low (pLDDT < 50)

ipTM = 0.2 pTM = 0.6

Non-commercial use only, subject to AlphaFold Server Output Terms of Use; no use in docking or screening tools.

阅读AlphaFold3的预测结果

- **pLDDT**: 局部结构
- **pTM**: 整个蛋白
- **ipTM**: 蛋白之间
- **pAE**: 任意一对氨基酸之间



ISDra2_TnpB_8BF8

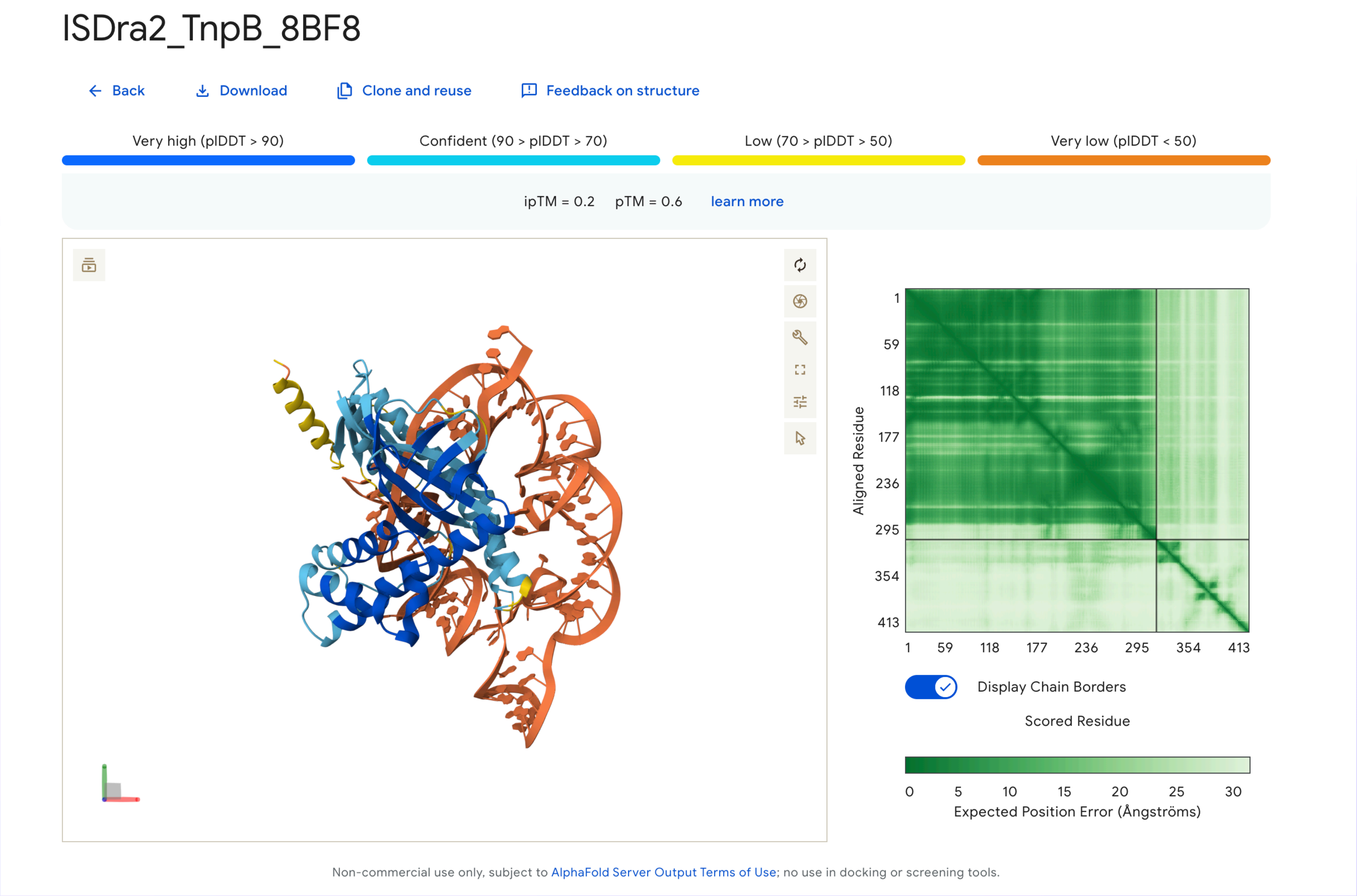
Very high (pIDDT > 90) | Confident (90 > pIDDT > 70) | Low (70 > pIDDT > 50) | Very low (pIDDT < 50)

ipTM = 0.2 pTM = 0.6

Non-commercial use only, subject to AlphaFold Server Output Terms of Use; no use in docking or screening tools.

阅读AlphaFold3的预测结果

- **pLDDT**: 蛋白高，RNA低
  - 蛋白的预测结果准确
- **pTM**: 还算高
  - 与上方结果一致
- **ipTM**: 很低
  - 蛋白-RNA互做大概率错误
- **pAE**:
  - 蛋白内部很准
  - RNA内部也不准
  - 蛋白-RNA之间不准

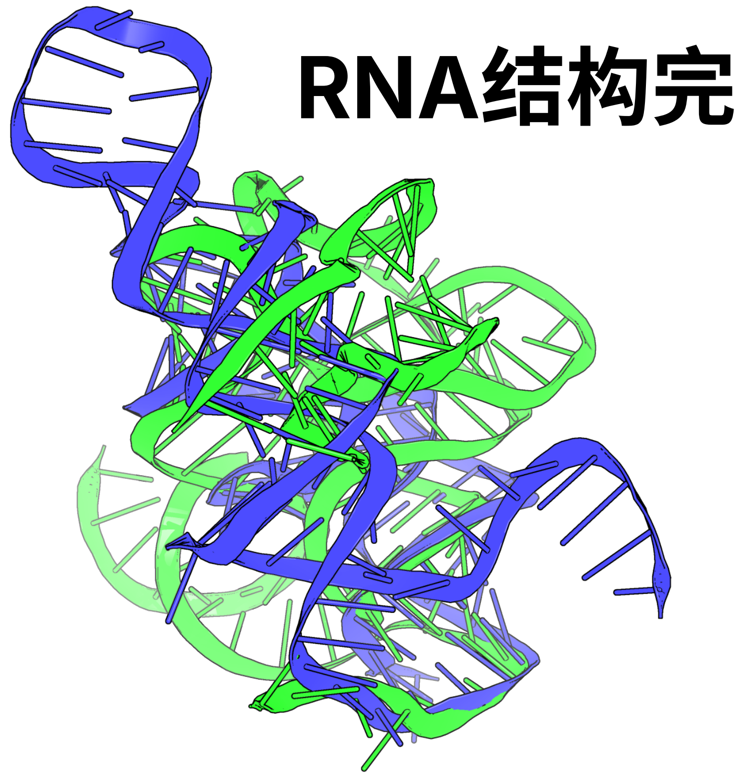


ISDra2_TnpB_8BF8

ipTM = 0.2 pTM = 0.6 learn more

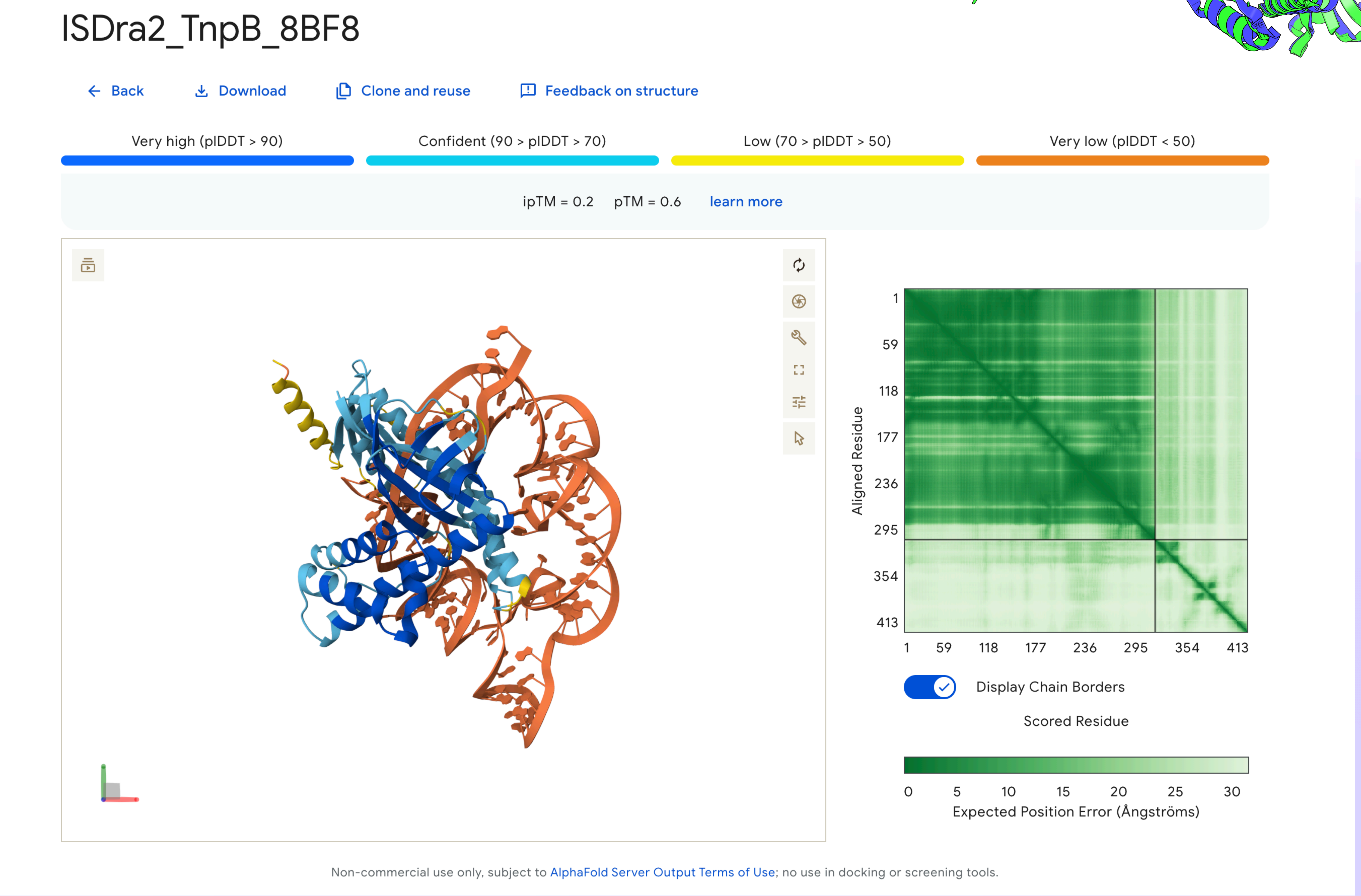
Non-commercial use only, subject to AlphaFold Server Output Terms of Use; no use in docking or screening tools.

阅读AlphaFold3的预测结果


RNA结构完全错误


蛋白结构大体准确

- **pLDDT**: 蛋白高，RNA低
  - 蛋白的预测结果准确
- **pTM**: 还算高
  - 与上方结果一致
- **ipTM**: 很低
  - 蛋白-RNA互做大概率错误
- **pAE**:
  - 蛋白内部很准
  - RNA内部也不准
  - 蛋白-RNA之间不准


ISDra2_TnpB_8BF8

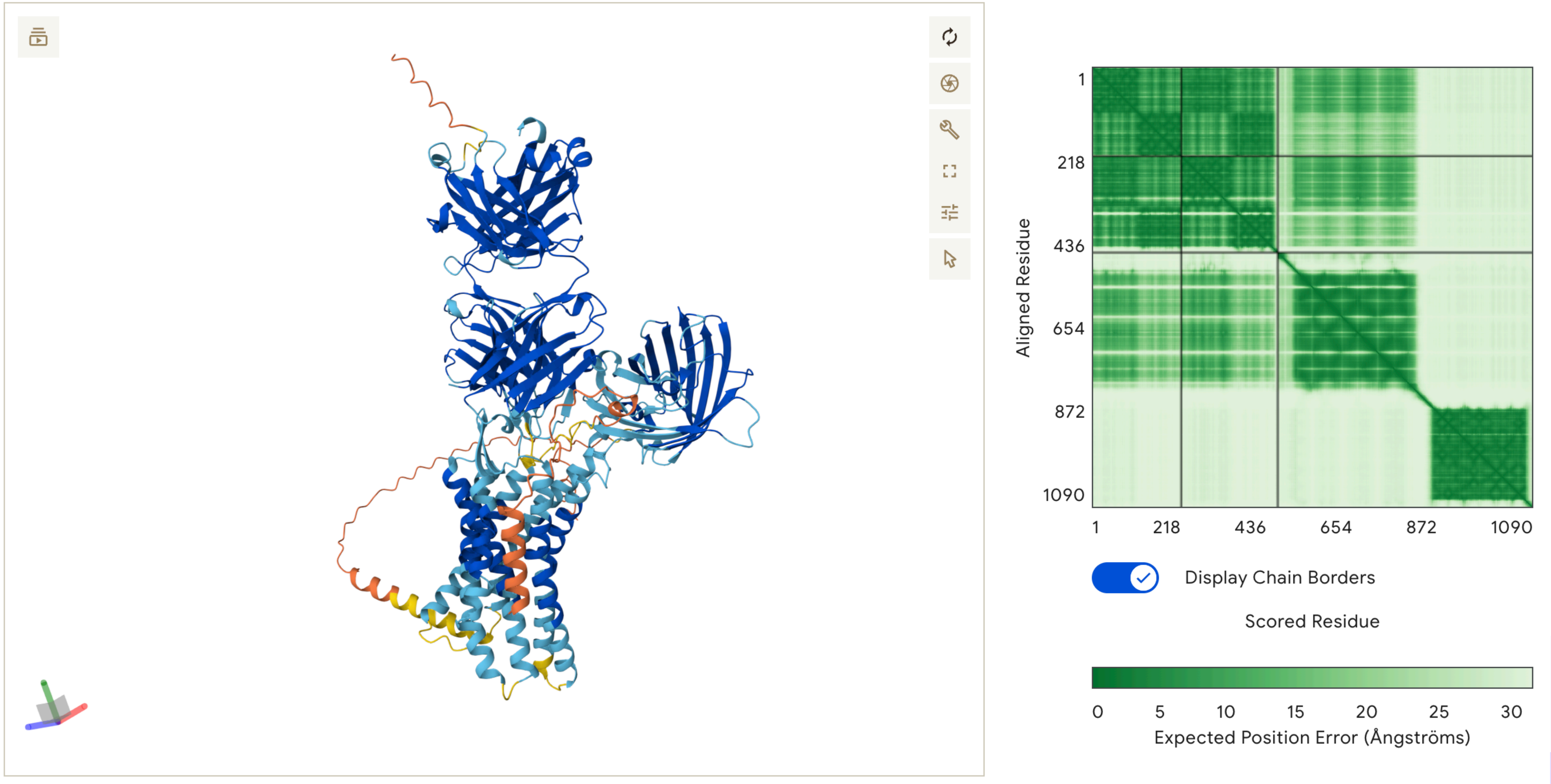
Very high (pIDDT > 90) | Confident (90 > pIDDT > 70) | Low (70 > pIDDT > 50) | Very low (pIDDT < 50)

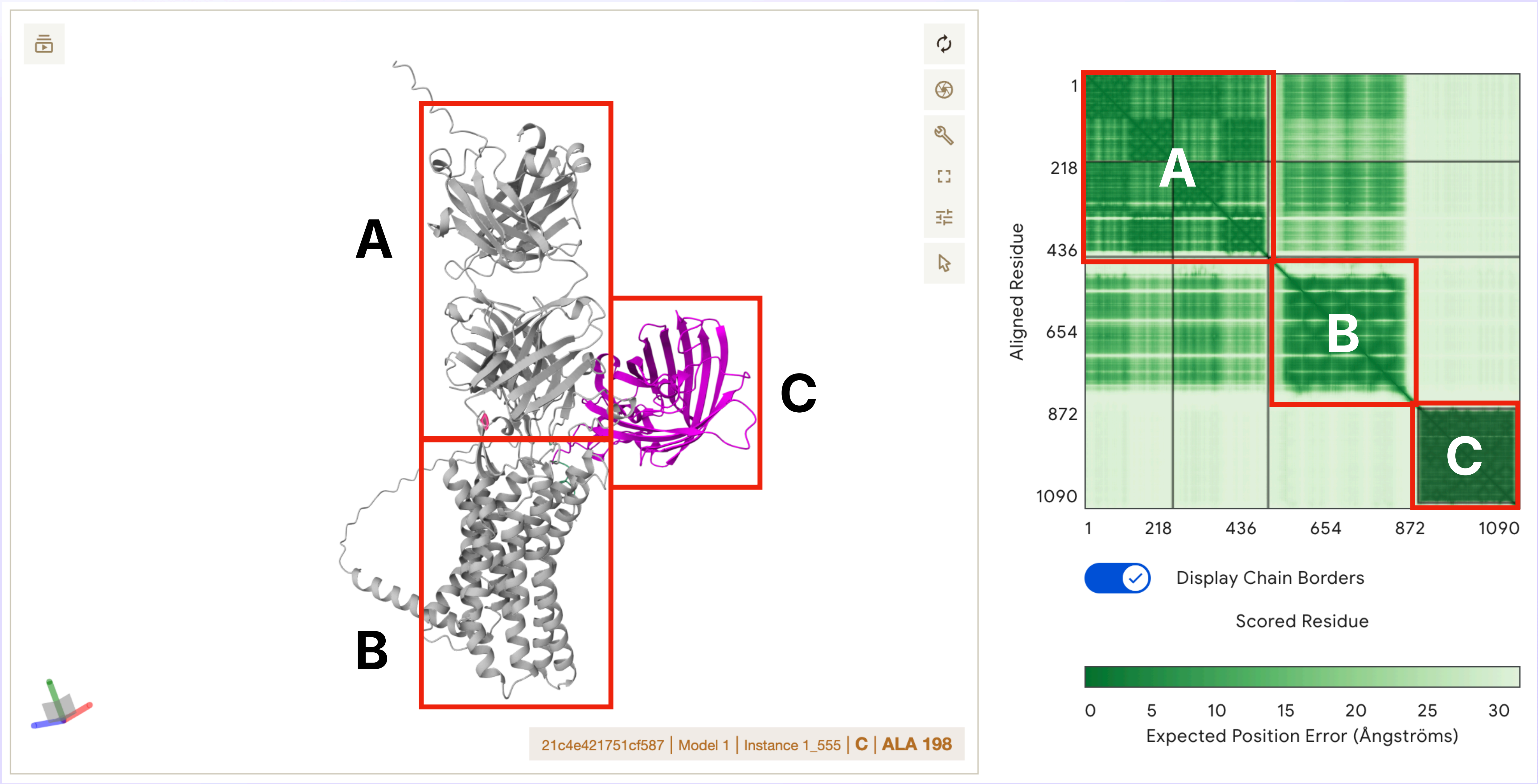
ipTM = 0.2 pTM = 0.6 learn more

Non-commercial use only, subject to AlphaFold Server Output Terms of Use; no use in docking or screening tools.

有效利用置信度

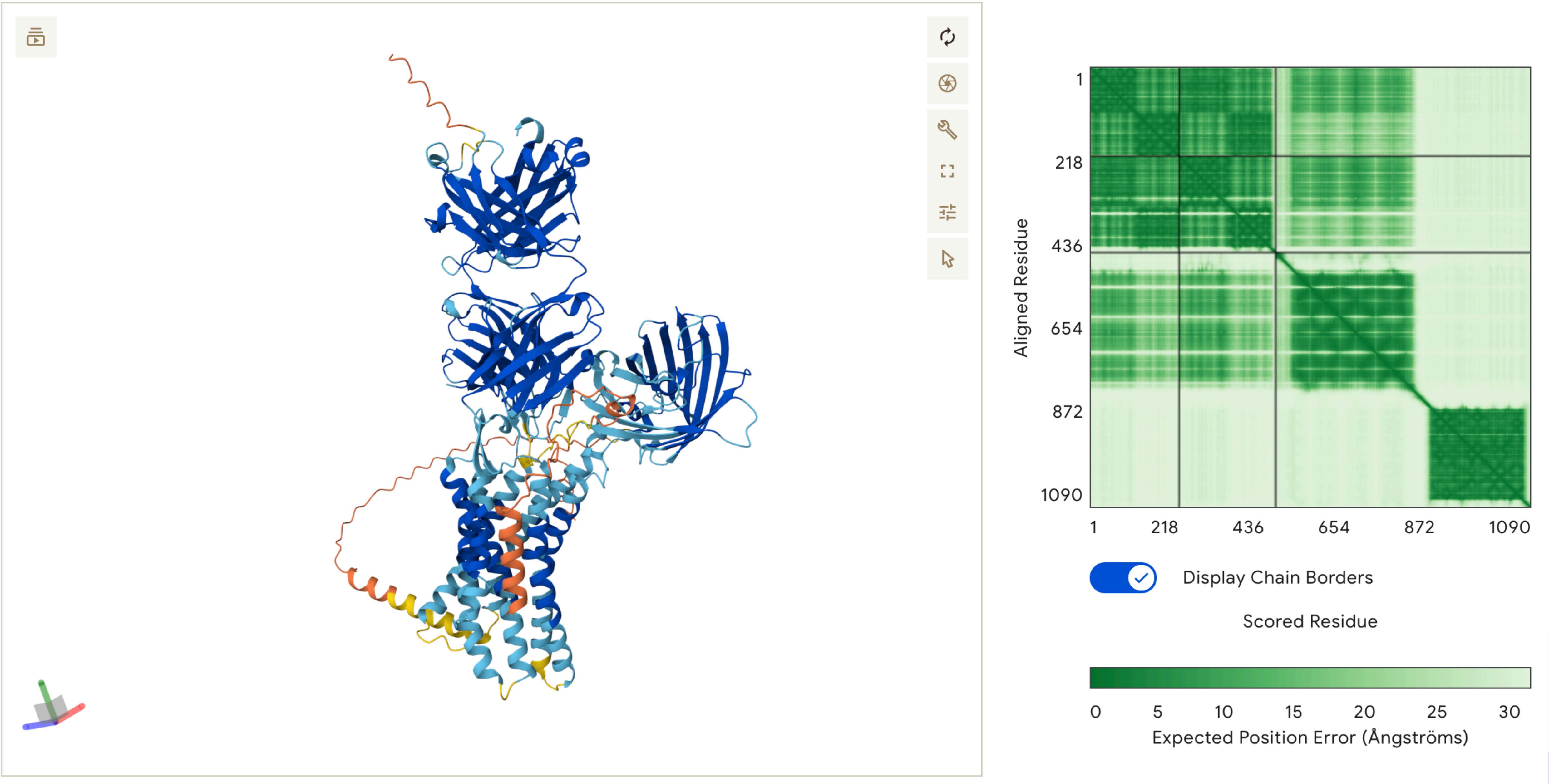
- A-B-C之间哪些互作是更可信的?

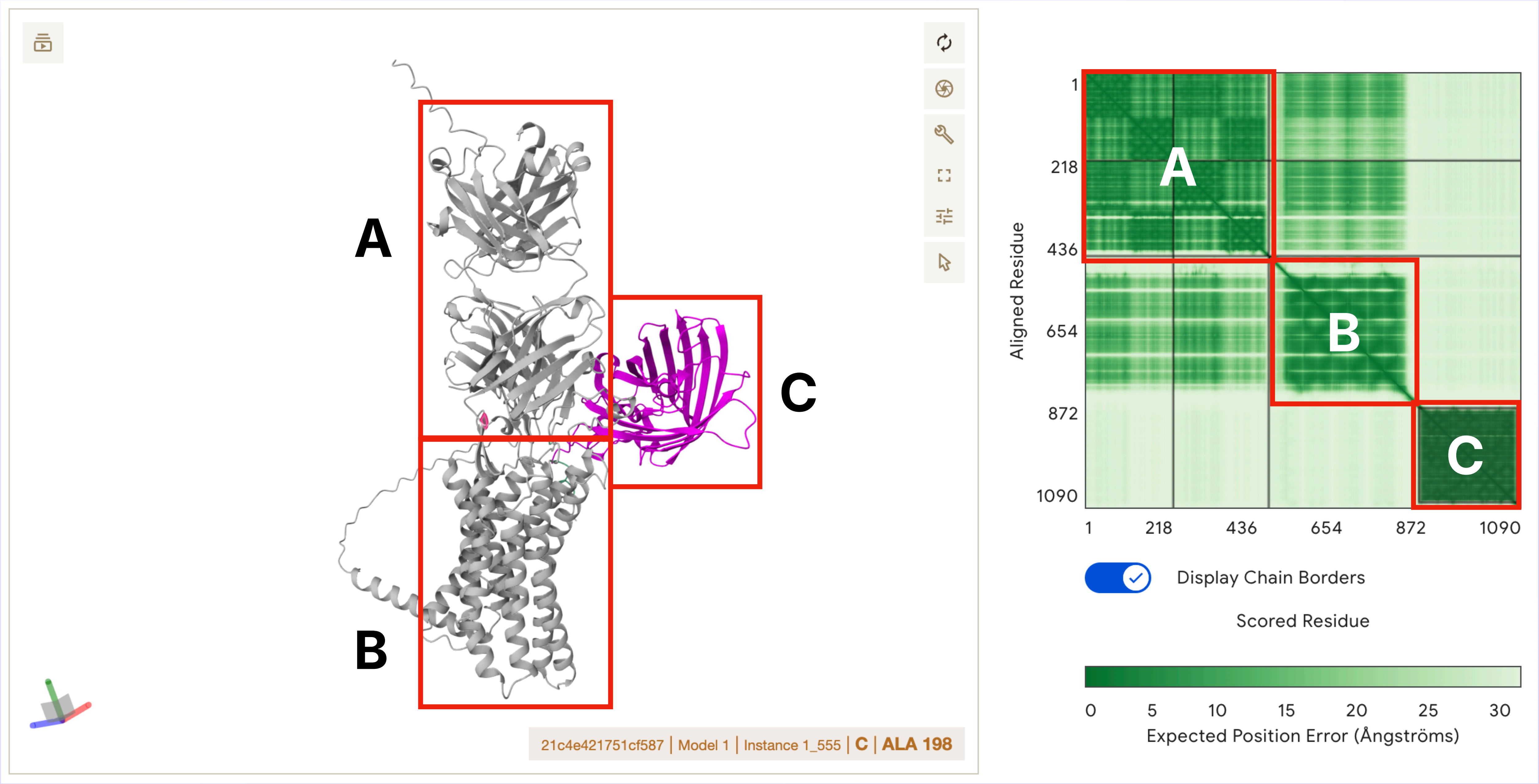




有效利用置信度

- A-B-C之间哪些互作是更可信的?
  - A-B可信度高
  - A-C, B-C可信度低
  - A, B, C内部可信度都高

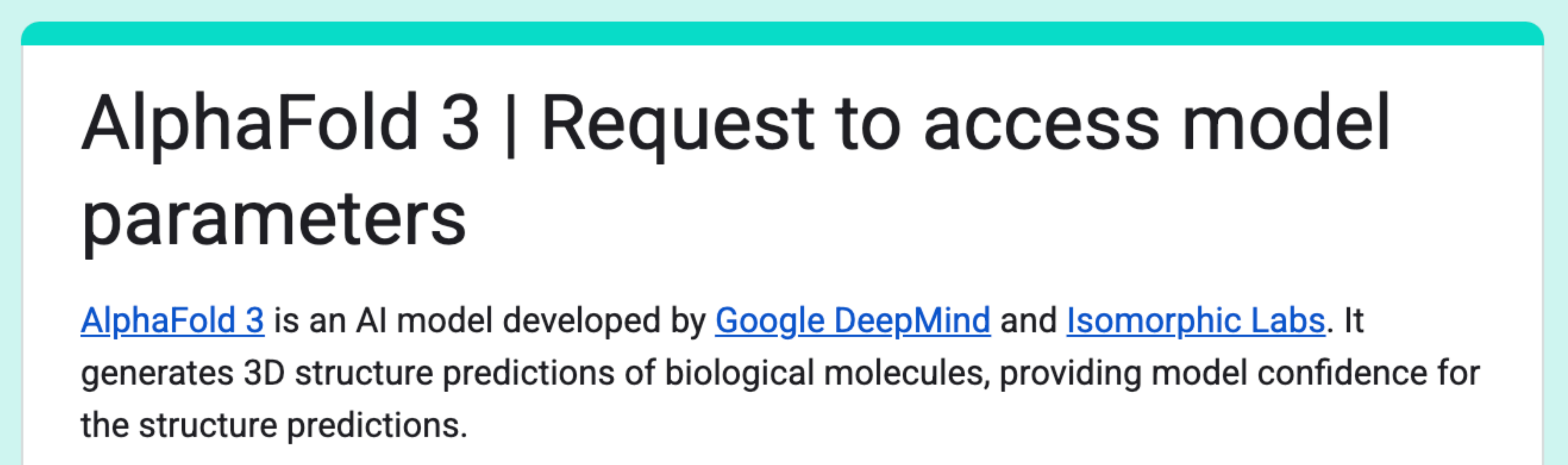




本地部署AlphaFold3

- GitHub: https://github.com/google-deepmind/alphafold3
- xFold (AlphaFold3 pytorch): https://github.com/Shenggan/xfold
- Protenix: https://github.com/bytedance/Protenix
- Conda: https://github.com/pyDock/AlphaFold3-Conda-Install

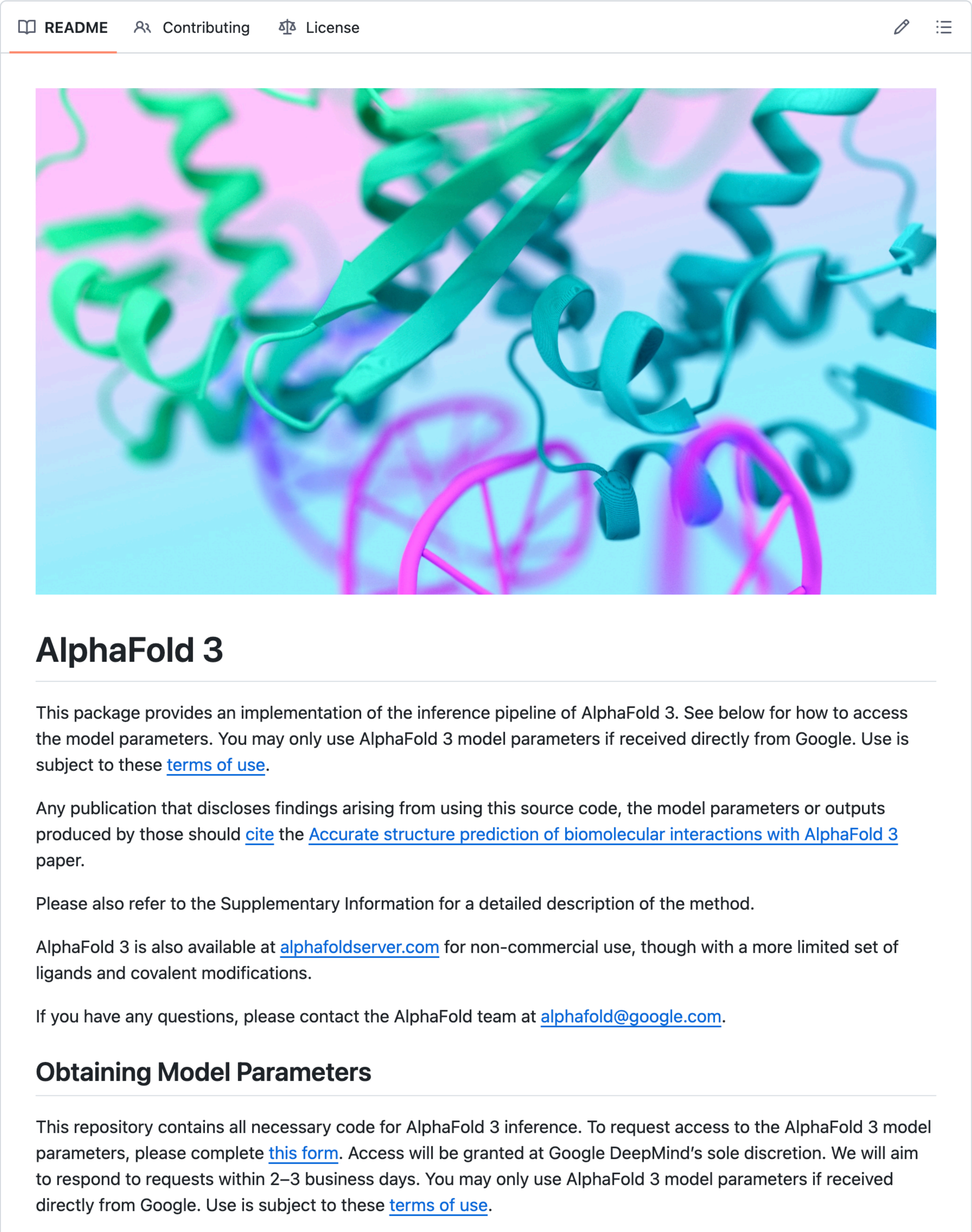
本地使用需要申请参数



AlphaFold 3 | Request to access model parameters

AlphaFold 3 is an AI model developed by Google DeepMind and Isomorphic Labs. It generates 3D structure predictions of biological molecules, providing model confidence for the structure predictions.

AlphaFold3的参数不能用于商业用途



AlphaFold 3

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.

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. To request access to the AlphaFold 3 model parameters, please complete this form. Access will be granted at Google DeepMind's sole discretion. We will aim to respond to requests within 2–3 business days. You may only use AlphaFold 3 model parameters if received directly from Google. Use is subject to these terms of use.

给本地AlphaFold3准备JSON输入

- name, modelSeeds, sequences, dialect, version, bondedAtomPairs, userCCD, userCCDPath
- sequences: [{protein}, {dna}, {rna}, {ligand}]

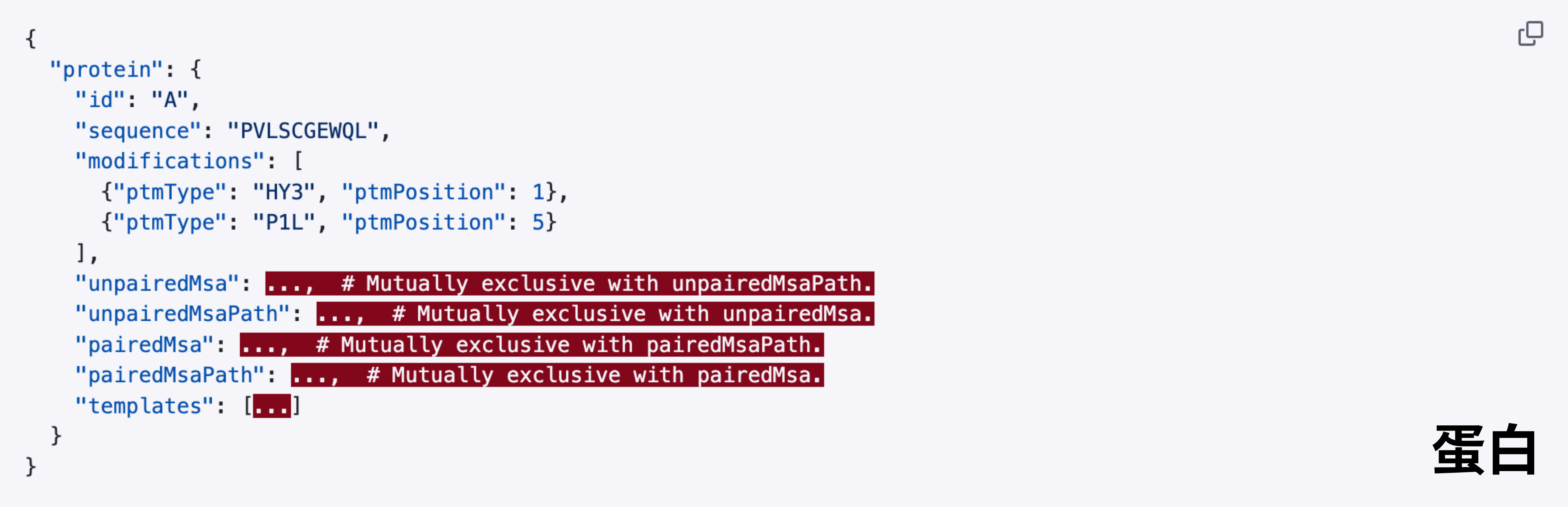
蛋白质结构预测 JSON 文件示例

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

```
{
  "name": "Job name goes here",
  "modelSeeds": [1, 2],  # At least one seed required.
  "sequences": [
    {"protein": {...}},
    {"rna": {...}},
    {"dna": {...}},
    {"ligand": {...}}
  ],
  "bondedAtomPairs": [...],  # Optional.
  "userCCD": "...",  # Optional, mutually exclusive with userCCDPath.
  "userCCDPath": "...",  # Optional, mutually exclusive with userCCD.
  "dialect": "alphafold3",  # Required.
  "version": 3  # Required.
}
```

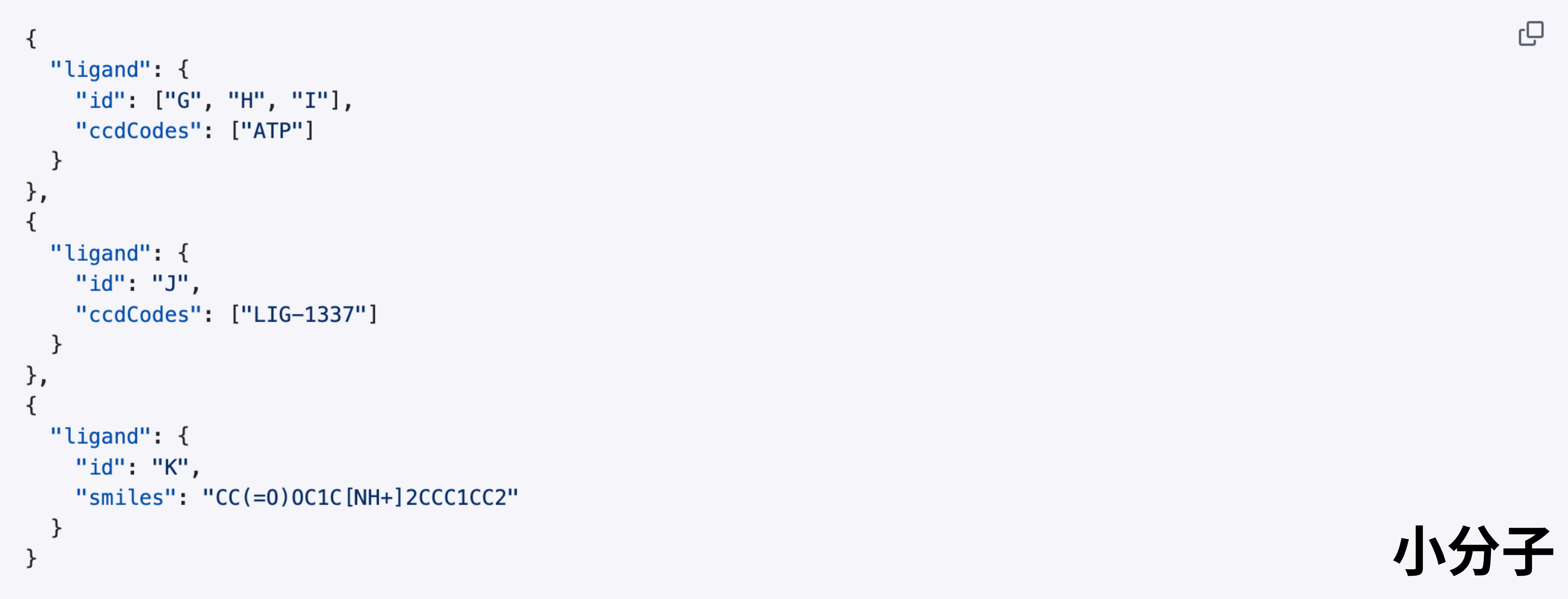
- 更细节的输入参考AlphaFold3 GitHub: https://github.com/google-deepmind/alphafold3/blob/main/docs/input.md

给本地AlphaFold3准备JSON输入



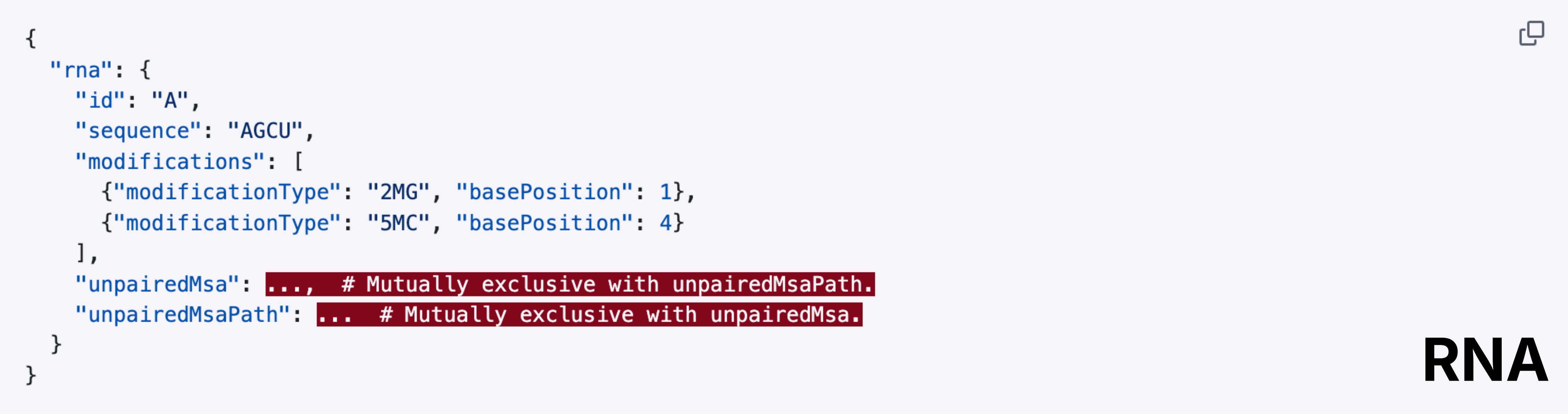
```
{
  "protein": {
    "id": "A",
    "sequence": "PVLSCGEWQL",
    "modifications": [
      {"ptmType": "HY3", "ptmPosition": 1},
      {"ptmType": "P1L", "ptmPosition": 5}
    ],
    "unpairedMsa": ...,  # Mutually exclusive with unpairedMsaPath.
    "unpairedMsaPath": ...,  # Mutually exclusive with unpairedMsa.
    "pairedMsa": ...,  # Mutually exclusive with pairedMsaPath.
    "pairedMsaPath": ...,  # Mutually exclusive with pairedMsa.
    "templates": [...]
  }
}
```

蛋白



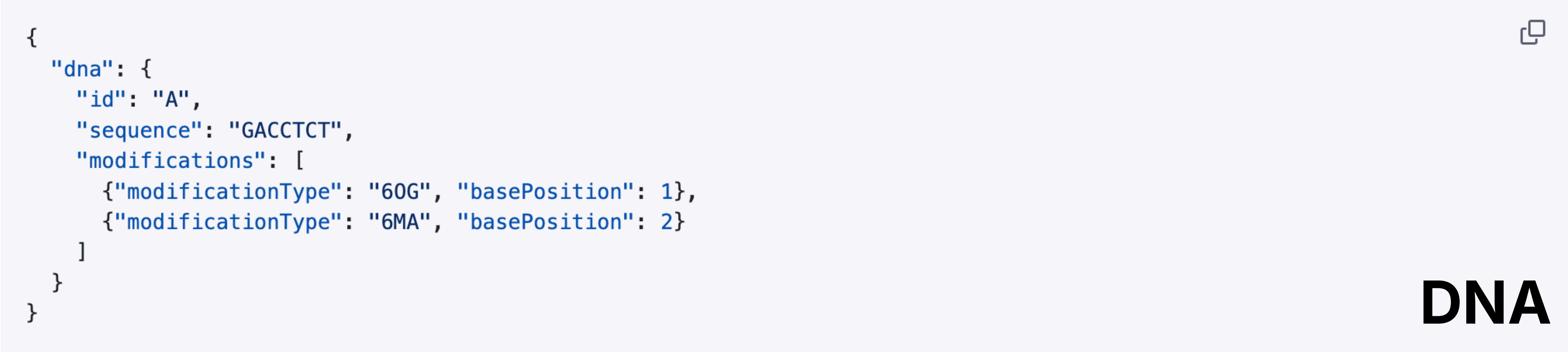
```
{
  "ligand": {
    "id": ["G", "H", "I"],
    "ccdCodes": ["ATP"]
  }
},
{
  "ligand": {
    "id": "J",
    "ccdCodes": ["LIG-1337"]
  }
},
{
  "ligand": {
    "id": "K",
    "smiles": "CC(=O)OC1C[NH+]2CCC1CC2"
  }
}
```

小分子



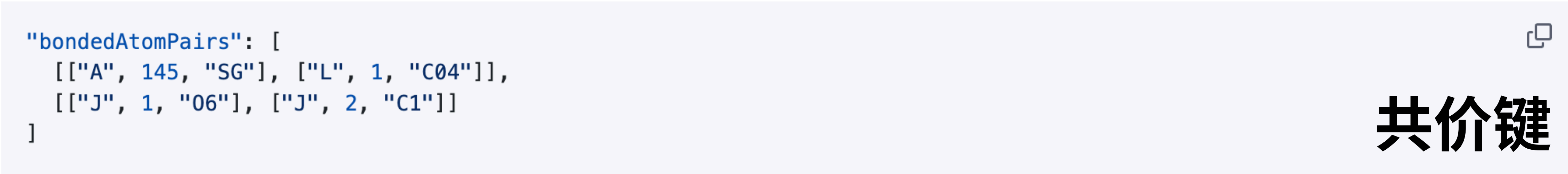
```
{
  "rna": {
    "id": "A",
    "sequence": "AGCU",
    "modifications": [
      {"modificationType": "2MG", "basePosition": 1},
      {"modificationType": "5MC", "basePosition": 4}
    ],
    "unpairedMsa": ...,  # Mutually exclusive with unpairedMsaPath.
    "unpairedMsaPath": ...  # Mutually exclusive with unpairedMsa.
  }
}
```

RNA



```
{
  "dna": {
    "id": "A",
    "sequence": "GACCTCT",
    "modifications": [
      {"modificationType": "6OG", "basePosition": 1},
      {"modificationType": "6MA", "basePosition": 2}
    ]
  }
}
```

DNA



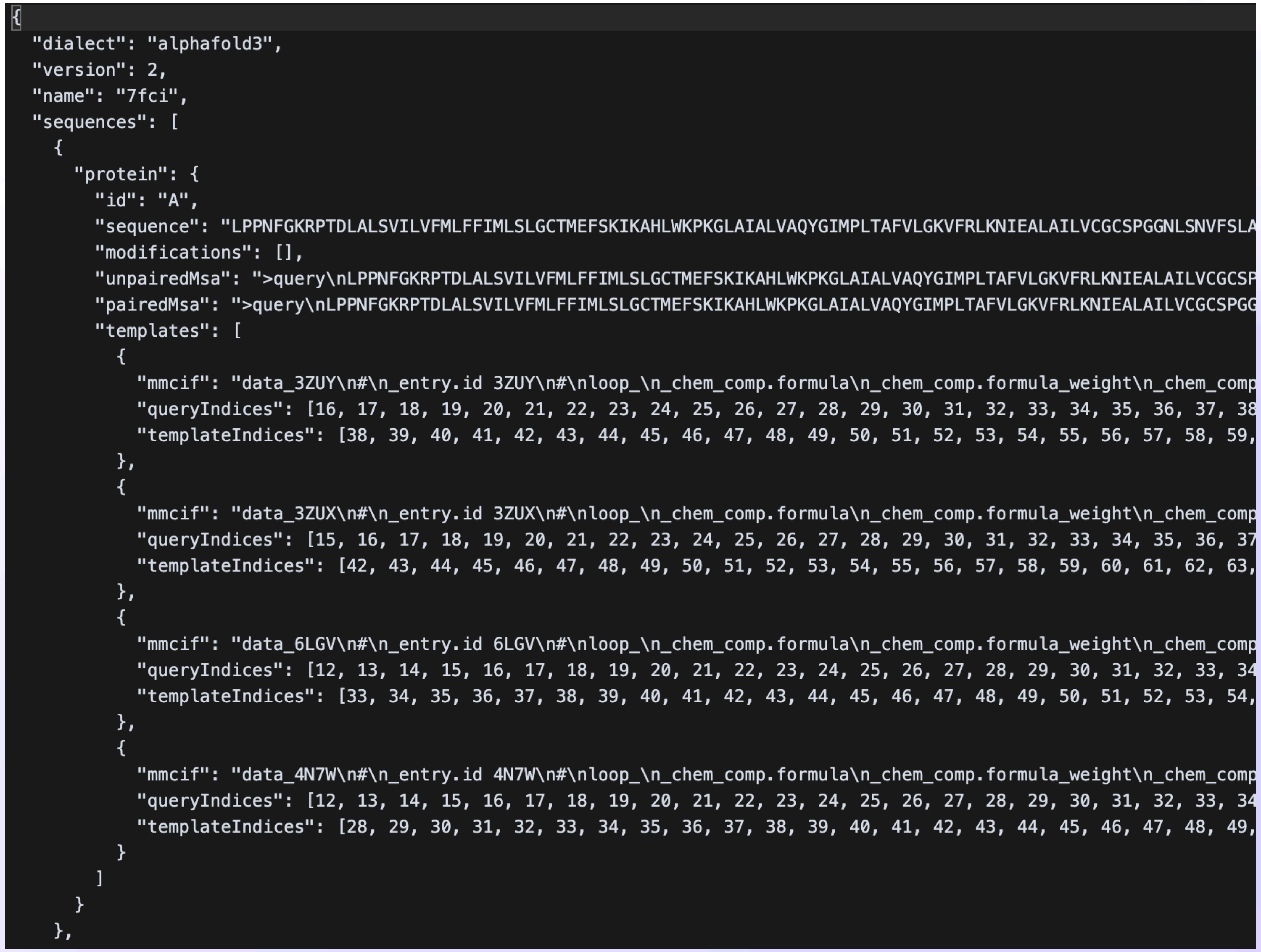
```
"bondedAtomPairs": [
  [["A", 145, "SG"], ["L", 1, "C04"]],
  [["J", 1, "O6"], ["J", 2, "C1"]]
]
```

共价键

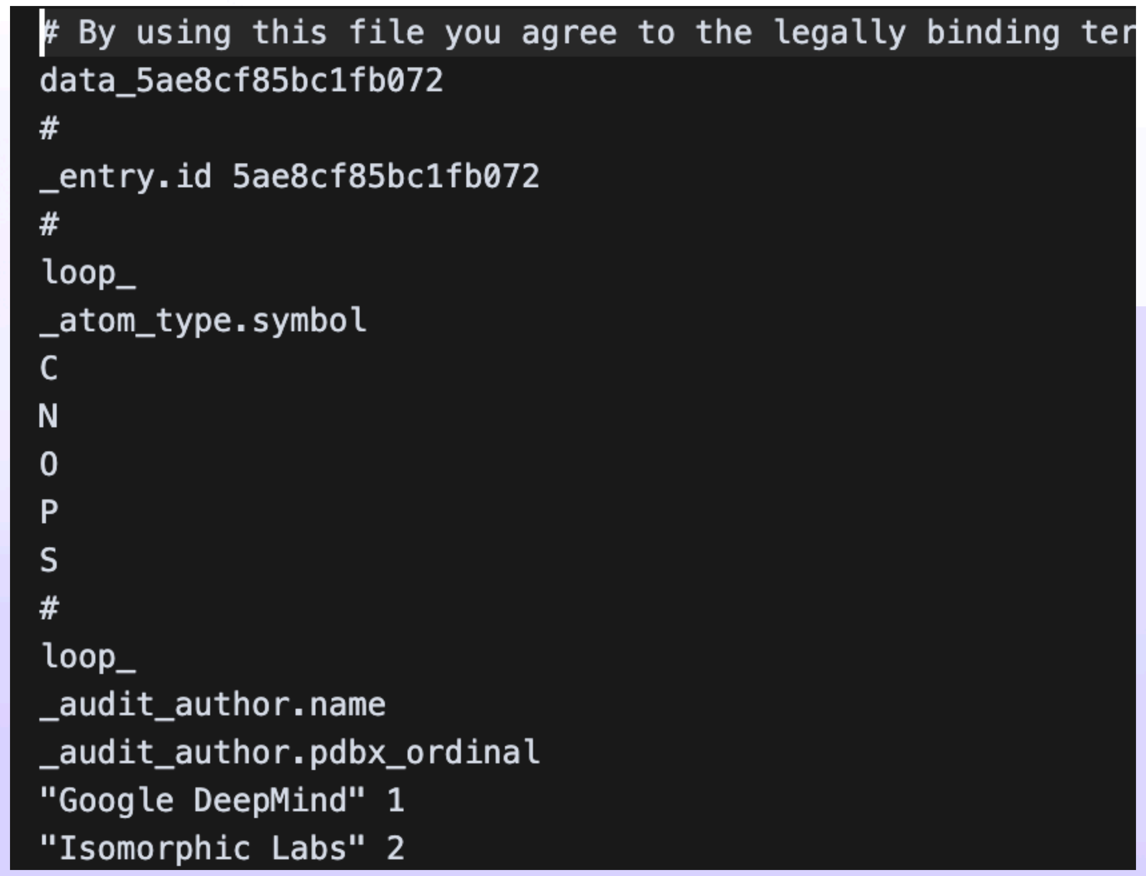
本地版AlphaFold的预测流程

xxx.json → Data pipeline → **xxx_data.json** → Model inference → **预测结果 - mmcif文件**

```
{
    "dialect": "alphafold3",
    "version": 1,
    "name": "7fci",
    "sequences": [
        {
            "protein": {
                "id": "A",
                "sequence": "LPPNFGKRPTDLALSVILVFMLFFIMLSLGCTMEFSKIKAHLWKPKGLAI
            }
        },
        {
            "protein": {
                "id": "B",
                "sequence": "DIVMTQSPAIMSASPGQKVTITCSASSSVNYMHWYQQKLGSSPKLWIYDT
            }
        },
        {
            "protein": {
                "id": "C",
                "sequence": "EVQLQQPGAELVKPGASVKLSCKTSGYTFTNYWMKWVKQRPGQGLEWIGE
            }
        }
    ],
    "modelSeeds": [
        42
    ]
}
```



```
{
  "dialect": "alphafold3",
  "version": 2,
  "name": "7fci",
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence": "LPPNFGKRPTDLALSVILVFMLFFIMLSLGCTMEFSKIKAHLWKPKGLAIALVAQYGIMPLTAFVLGKVFRLKNIEALAILVCGCSPGGNLSNVFSLA
        "modifications": [],
        "unpairedMsa": ">query\nLPPNFGKRPTDLALSVILVFMLFFIMLSLGCTMEFSKIKAHLWKPKGLAIALVAQYGIMPLTAFVLGKVFRLKNIEALAILVCGCSP
        "pairedMsa": ">query\nLPPNFGKRPTDLALSVILVFMLFFIMLSLGCTMEFSKIKAHLWKPKGLAIALVAQYGIMPLTAFVLGKVFRLKNIEALAILVCGCSPG
        "templates": [
          {
            "mmcif": "data_3ZUY\n#\n_entry.id 3ZUY\n#\nloop_\n_chem_comp.formula\n_chem_comp.formula_weight\n_chem_comp
            "queryIndices": [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38
            "templateIndices": [38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59,
          },
          {
            "mmcif": "data_3ZUX\n#\n_entry.id 3ZUX\n#\nloop_\n_chem_comp.formula\n_chem_comp.formula_weight\n_chem_comp
            "queryIndices": [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37
            "templateIndices": [42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63,
          },
          {
            "mmcif": "data_6LGV\n#\n_entry.id 6LGV\n#\nloop_\n_chem_comp.formula\n_chem_comp.formula_weight\n_chem_comp
            "queryIndices": [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34
            "templateIndices": [33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54,
          },
          {
            "mmcif": "data_4N7W\n#\n_entry.id 4N7W\n#\nloop_\n_chem_comp.formula\n_chem_comp.formula_weight\n_chem_comp
            "queryIndices": [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34
            "templateIndices": [28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49,
          }
        ]
      }
    },
```



```
# By using this file you agree to the legally binding ter
data_5ae8cf85bc1fb072
#
_entry.id 5ae8cf85bc1fb072
#
loop_
_atom_type.symbol
C
N
O
P
S
#
loop_
_audit_author.name
_audit_author.pdbx_ordinal
"Google DeepMind" 1
"Isomorphic Labs" 2
```

Dos and Don’ts：什么时候相信结构预测

大胆尝试	有需求一定要试试	**轻松判断**	能够用pLDDT等指标轻松判断置信度	**可以信任**	如果各项指标均满足要求，可以认为预测误差较小
谨慎尝试	考虑情况可以不尝试	**谨慎判断**	指标可能有的高有的低，需要仔细判断	**谨慎信任**	即使各项指标满足要求，也不代表结构准确
不要尝试	不熟悉不要轻易尝试	**无法判断**	不论何种条件下，参考指标意义均不大	**不要信任**	不论何种条件下，都不能轻易认同预测是正确的

蛋白质单体-短蛋白-原核来源	**大胆尝试**	**轻松判断**	**可以信任**	
蛋白质单体-长蛋白-高等生物来源	**大胆尝试**	**轻松判断**	**可以信任**	
蛋白质同源复合物	**大胆尝试**	**谨慎判断**	**可以信任**	
蛋白质异源复合物	**大胆尝试**	**谨慎判断**	**可以信任**	
蛋白质-小分子复合物	**大胆尝试**	**谨慎判断**	**谨慎信任**	
蛋白质-金属离子复合物	**大胆尝试**	**谨慎判断**	**谨慎信任**	
蛋白质-DNA复合物	**谨慎尝试**	**谨慎判断**	**谨慎信任**	
蛋白质-DNA特异性互作			**不要信任**	**幻觉严重**
蛋白质-RNA复合物	**谨慎尝试**	**谨慎判断**	**不要信任**	**幻觉严重**
长单链RNA	**谨慎尝试**	**谨慎判断**	**不要信任**	**幻觉严重**
蛋白质功能预测（AI方法）	**不要尝试**	**无法判断**	**不要信任**	

如何查询一个蛋白的功能

生物样本

测序

蛋白质序列

BLASTp检索NCBI数据库

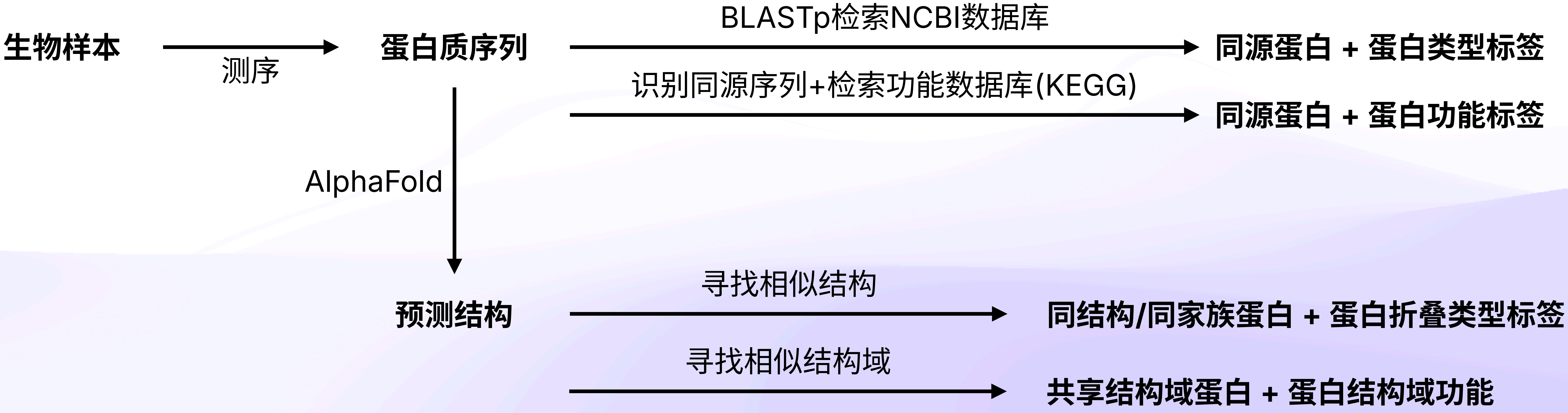
同源蛋白 + 蛋白类型标签

识别同源序列+检索功能数据库(KEGG)

同源蛋白 + 蛋白功能标签

Homolog: 同源且同功

如何查询一个蛋白的功能



生物样本

测序

蛋白质序列

BLASTp检索NCBI数据库

同源蛋白 + 蛋白类型标签

识别同源序列+检索功能数据库(KEGG)

同源蛋白 + 蛋白功能标签

AlphaFold

预测结构

寻找相似结构

同结构/同家族蛋白 + 蛋白折叠类型标签

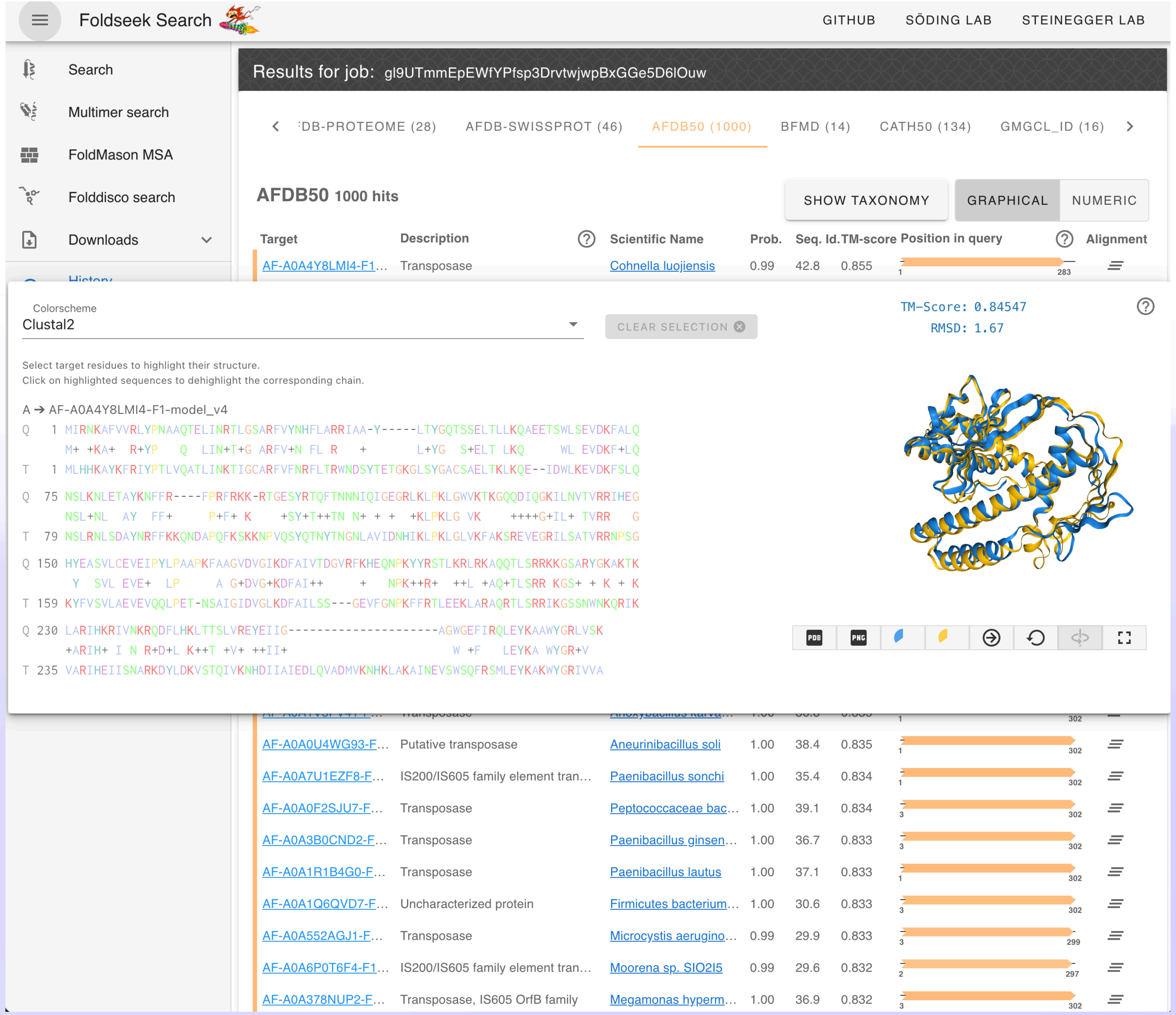
寻找相似结构域

共享结构域蛋白 + 蛋白结构域功能

结构决定功能

FoldSeek: 高效的结构检索工具

- https://search.foldseek.com/search



Foldseek Search

GITHUB SÖDING LAB STEINEGGER LAB

- Search
- Multimer search
- FoldMason MSA
- Folddisco search
- Downloads
- History

Results for job: gl9UTmmEpEWfYPfsp3DrvtwjwpBxGGe5D6lOuw

‹ 'DB-PROTEOME (28) AFDB-SWISSPROT (46) AFDB50 (1000) BFMD (14) CATH50 (134) GMGCL_ID (16) ›

AFDB50 1000 hits

SHOW TAXONOMY GRAPHICAL NUMERIC

Target	Description	Scientific Name	Prob.	Seq. Id.	TM-score	Position in query	Alignment
AF-A0A4Y8LMI4-F1…	Transposase	Cohnella luojiensis	0.99	42.8	0.855	1 283	≡
AF-A0A0U4WG93-F…	Putative transposase	Aneurinibacillus soli	1.00	38.4	0.835	1 302	≡
AF-A0A7U1EZF8-F…	IS200/IS605 family element tran…	Paenibacillus sonchi	1.00	35.4	0.834	1 302	≡
AF-A0A0F2SJU7-F…	Transposase	Peptococcaceae bac…	1.00	39.1	0.834	3 302	≡
AF-A0A3B0CND2-F…	Transposase	Paenibacillus ginsen…	1.00	36.7	0.833	3 302	≡
AF-A0A1R1B4G0-F…	Transposase	Paenibacillus lautus	1.00	37.1	0.833	1 302	≡
AF-A0A1Q6QVD7-F…	Uncharacterized protein	Firmicutes bacterium…	1.00	30.6	0.833	3 302	≡
AF-A0A552AGJ1-F…	Transposase	Microcystis aerugino…	0.99	29.9	0.833	3 299	≡
AF-A0A6P0T6F4-F1…	IS200/IS605 family element tran…	Moorena sp. SIO2I5	0.99	29.6	0.832	2 297	≡
AF-A0A378NUP2-F…	Transposase, IS605 OrfB family	Megamonas hyperm…	1.00	36.9	0.832	3 302	≡

Colorscheme: Clustal2

CLEAR SELECTION

TM-Score: 0.84547
RMSD: 1.67

Select target residues to highlight their structure.
Click on highlighted sequences to dehighlight the corresponding chain.

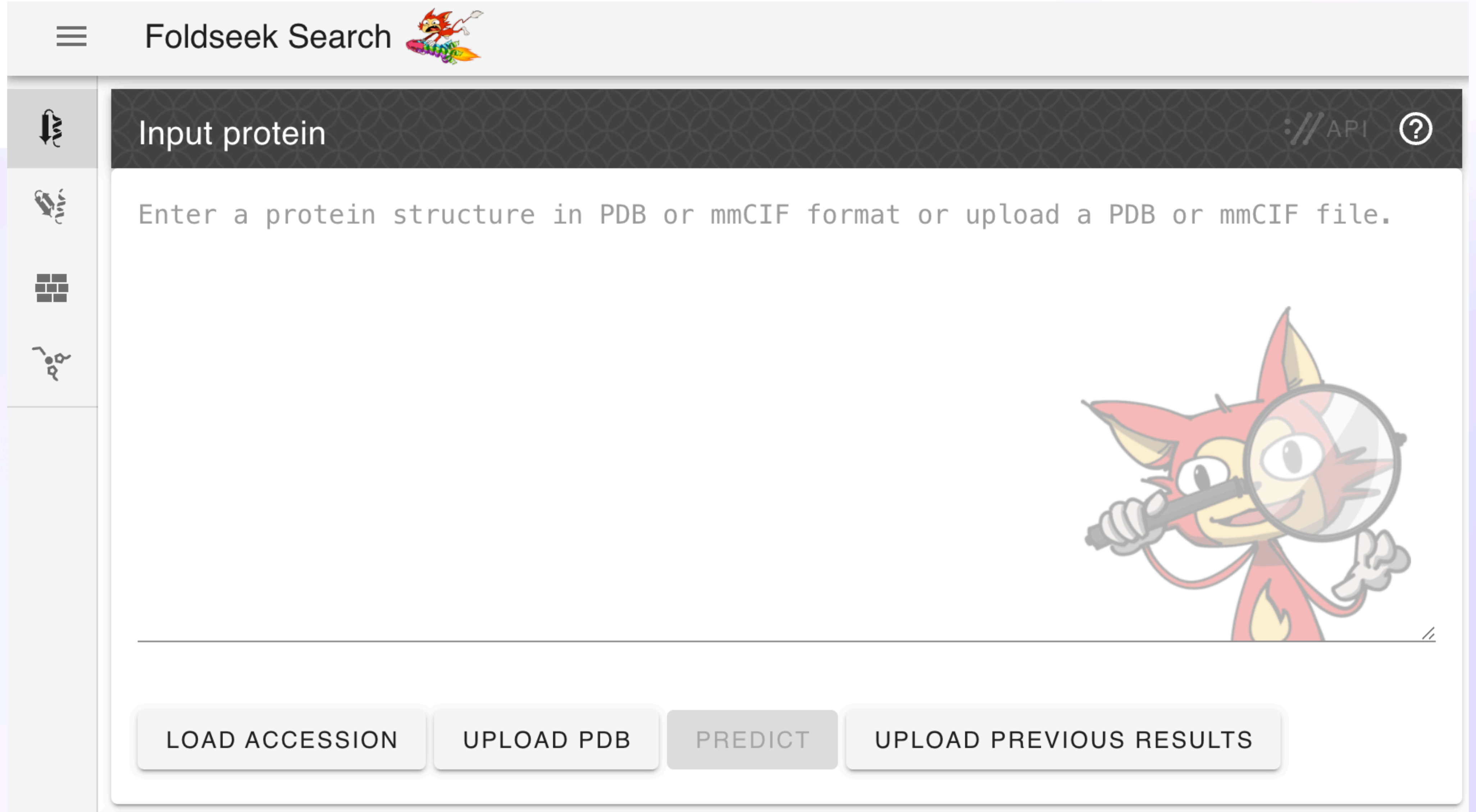
A → AF-A0A4Y8LMI4-F1-model_v4

```
Q    1 MIRNKAFVVRLYPNAAQTELINRTLGSARFVYNHFLARRIAA-Y-----LTYGQTSSELTLLKQAEETSWLSEVDKFALQ
       M+ +KA+  R+YP   Q  LIN+T+G ARFV+N FL R   +       L+YG  S+ELT LKQ     WL EVDKF+LQ
T    1 MLHHKAYKFRIYPTLVQATLINKTIGCARFVFNRFLTRWNDSYTETGKGLSYGACSAELTKLKQE--IDWLKEVDKFSLQ

Q   75 NSLKNLETAYKNFFR----FPRFRKK-RTGESYRTQFTNNNIQIGEGRLKLPKLGWVKTKGQQDIQGKILNVTVRRIHEG
       NSL+NL  AY  FF+     P+F+ K    +SY+T++TN N+ + +  +KLPKLG VK    ++++G+IL+ TVRR   G
T   79 NSLRNLSDAYNRFFKKQNDAPQFKSKKNPVQSYQTNYTNGNLAVIDNHIKLPKLGLVKFAKSREVEGRILSATVRRNPSG

Q  150 HYEASVLCEVEIPYLPAAPKFAAGVDVGIKDFAIVTDGVRFKHEQNPKYYRSTLKRLRKAQQTLSRRKKGSARYGKAKTK
        Y  SVL EVE+  LP     A G+DVG+KDFAI++     +   NPK++R+  ++L +AQ+TLSRR KGS+ + K + K
T  159 KYFVSVLAEVEVQQLPET-NSAIGIDVGLKDFAILSS---GEVFGNPKFFRTLEEKLARAQRTLSRRIKGSSNWNKQRIK

Q  230 LARIHKRIVNKRQDFLHKLTTSLVREYEIIG---------------------AGWGEFIRQLEYKAAWYGRLVSK
       +ARIH+ I N R+D+L K++T +V+ ++II+                       W +F   LEYKA WYGR+V
T  235 VARIHEIISNARKDYLDKVSTQIVKNHDIIAIEDLQVADMVKNHKLAKAINEVSWSQFRSMLEYKAKWYGRIVVA
```



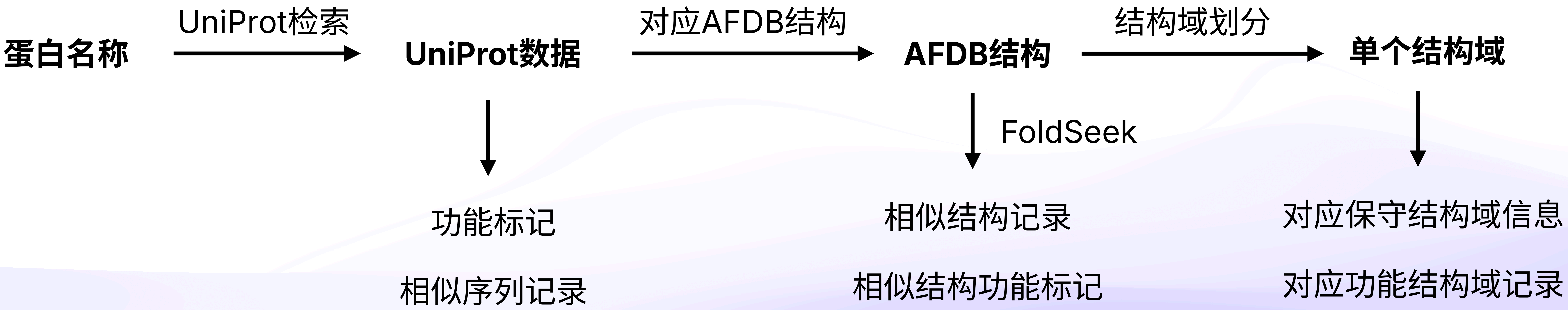
Foldseek Search

Input protein

Enter a protein structure in PDB or mmCIF format or upload a PDB or mmCIF file.

LOAD ACCESSION UPLOAD PDB PREDICT UPLOAD PREVIOUS RESULTS

从UniProt开始寻找功能



蛋白名称

UniProt检索

UniProt数据

功能标记

相似序列记录

对应AFDB结构

AFDB结构

FoldSeek

相似结构记录

相似结构功能标记

结构域划分

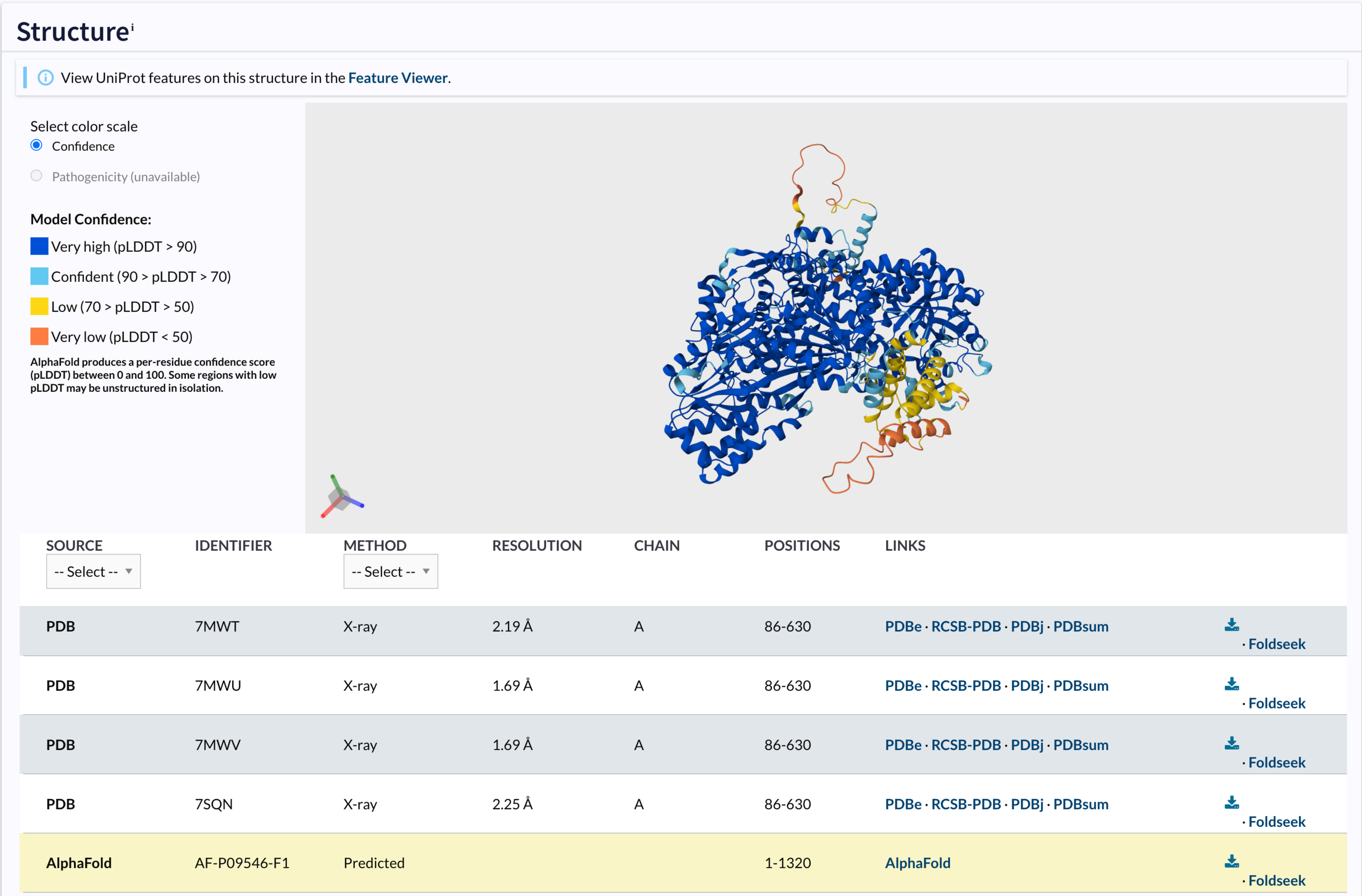
单个结构域

对应保守结构域信息

对应功能结构域记录

从UniProt开始寻找功能

- https://www.uniprot.org/uniprotkb/P09546/entry#structure



Structure

View UniProt features on this structure in the **Feature Viewer**.

Select color scale

● Confidence

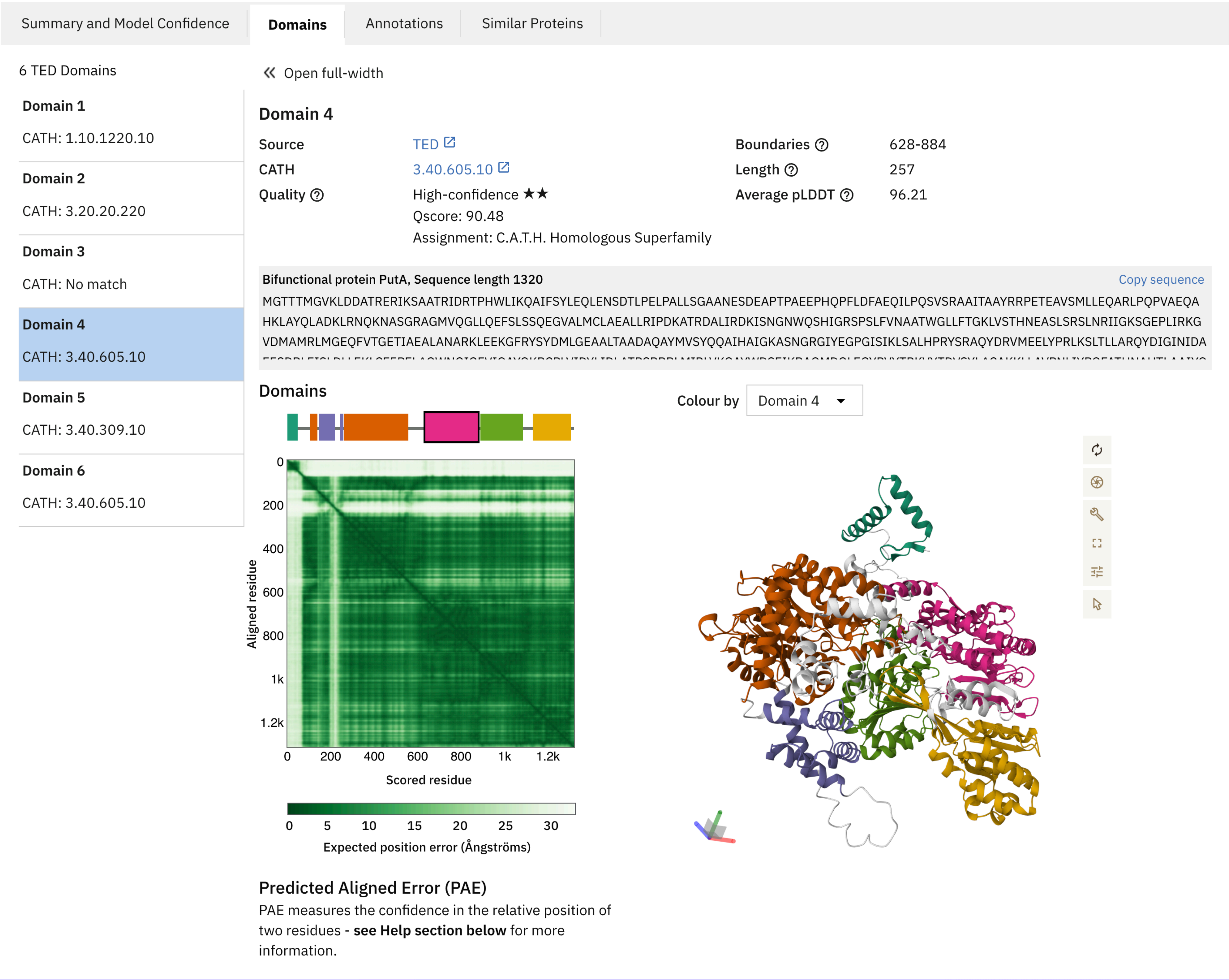
○ Pathogenicity (unavailable)

Model Confidence:

- 🟦 Very high (pLDDT > 90)
- 🟦 Confident (90 > pLDDT > 70)
- 🟨 Low (70 > pLDDT > 50)
- 🟧 Very low (pLDDT < 50)

AlphaFold produces a per-residue confidence score (pLDDT) between 0 and 100. Some regions with low pLDDT may be unstructured in isolation.

SOURCE	IDENTIFIER	METHOD	RESOLUTION	CHAIN	POSITIONS	LINKS	
-- Select --		-- Select --					
PDB	7MWT	X-ray	2.19 Å	A	86-630	PDBe · RCSB-PDB · PDBj · PDBsum	· Foldseek
PDB	7MWU	X-ray	1.69 Å	A	86-630	PDBe · RCSB-PDB · PDBj · PDBsum	· Foldseek
PDB	7MWV	X-ray	1.69 Å	A	86-630	PDBe · RCSB-PDB · PDBj · PDBsum	· Foldseek
PDB	7SQN	X-ray	2.25 Å	A	86-630	PDBe · RCSB-PDB · PDBj · PDBsum	· Foldseek
AlphaFold	AF-P09546-F1	Predicted			1-1320	AlphaFold	· Foldseek



6 TED Domains

Domain 1	CATH: 1.10.1220.10
Domain 2	CATH: 3.20.20.220
Domain 3	CATH: No match
Domain 4	CATH: 3.40.605.10
Domain 5	CATH: 3.40.309.10
Domain 6	CATH: 3.40.605.10

Domain 4

Source	TED	Boundaries	628-884
CATH	3.40.605.10	Length	257
Quality	High-confidence ★★ Qscore: 90.48 Assignment: C.A.T.H. Homologous Superfamily	Average pLDDT	96.21

Bifunctional protein PutA, Sequence length 1320 Copy sequence

MGTTTMGVKLDDATRERIKSAATRIDRTPHWLIKQAIFSYLEQLENSDTLPELPALLSGAANESDEAPTPAEEPHQPFLDFAEQILPQSVSRAAITAAYRRPETEAVSMLLEQARLPQPVAEQA
HKLAYQLADKLRNQKNASGRAGMVQGLLQEFSLSSQEGVALMCLAEALLRIPDKATRDALIRDKISNGNWQSHIGRSPSLFVNAATWGLLFTGKLVSTHNEASLSRSLNRIIGKSGEPLIRKG
VDMAMRLMGEQFVTGETIAEALANARKLEEKGFRYSYDMLGEAALTAADAQAYMVSYQQAIHAIGKASNGRGIYEGPGISIKLSALHPRYSRAQYDRVMEELYPRLKSLTLLARQYDIGINIDA

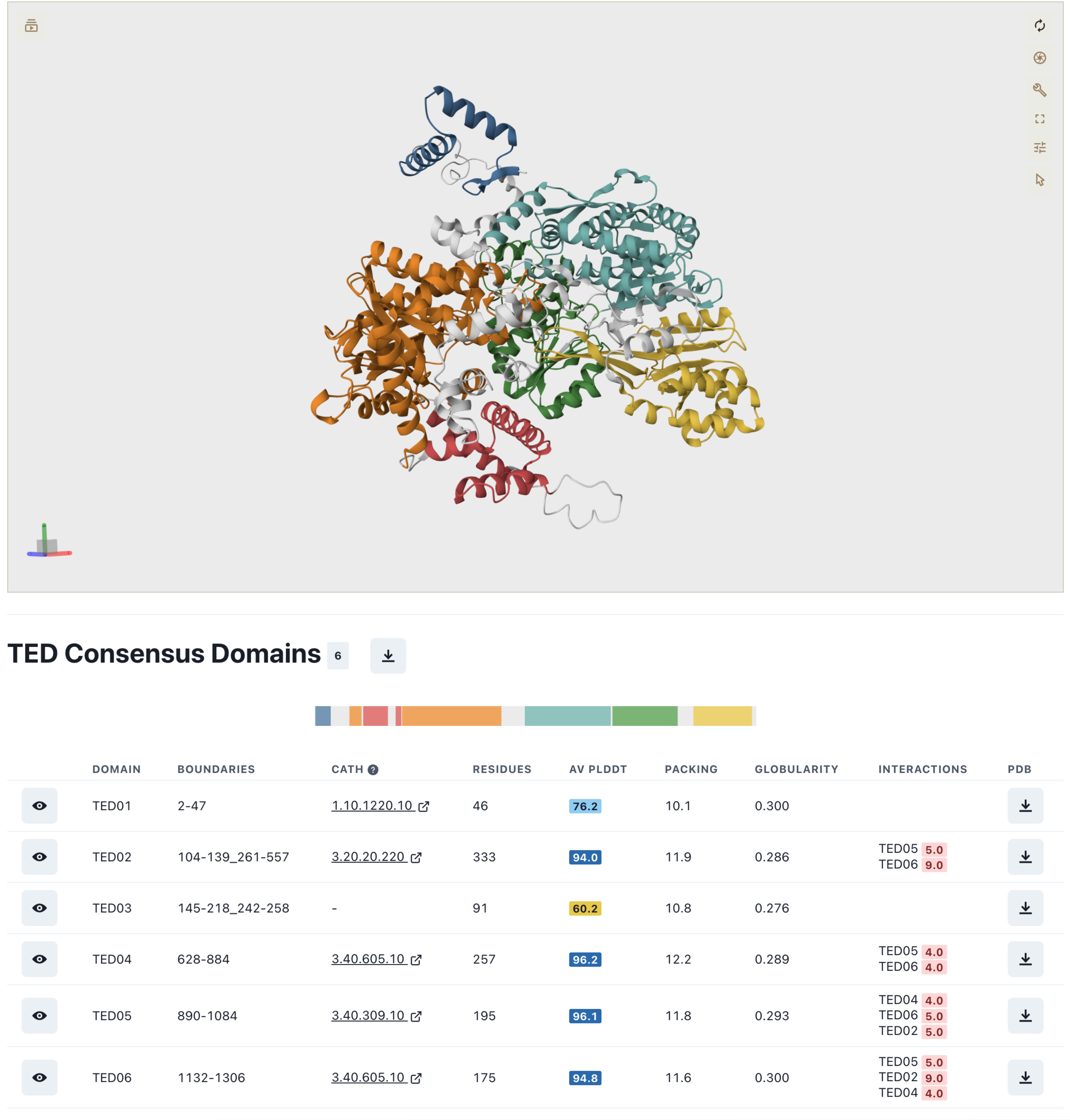
Domains

Colour by Domain 4

Predicted Aligned Error (PAE)

PAE measures the confidence in the relative position of two residues - **see Help section below** for more information.

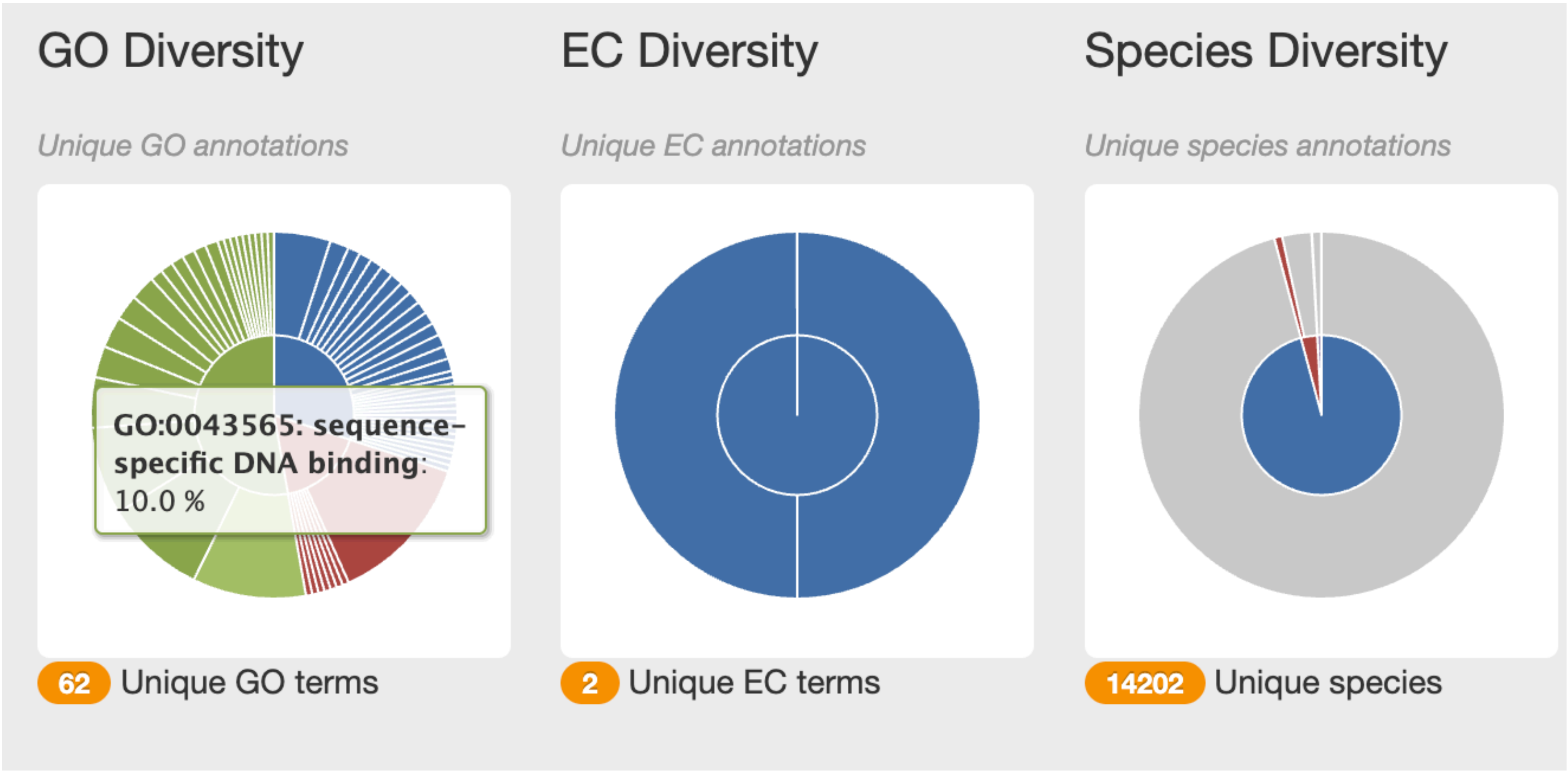
结构域数据集TED实际案例



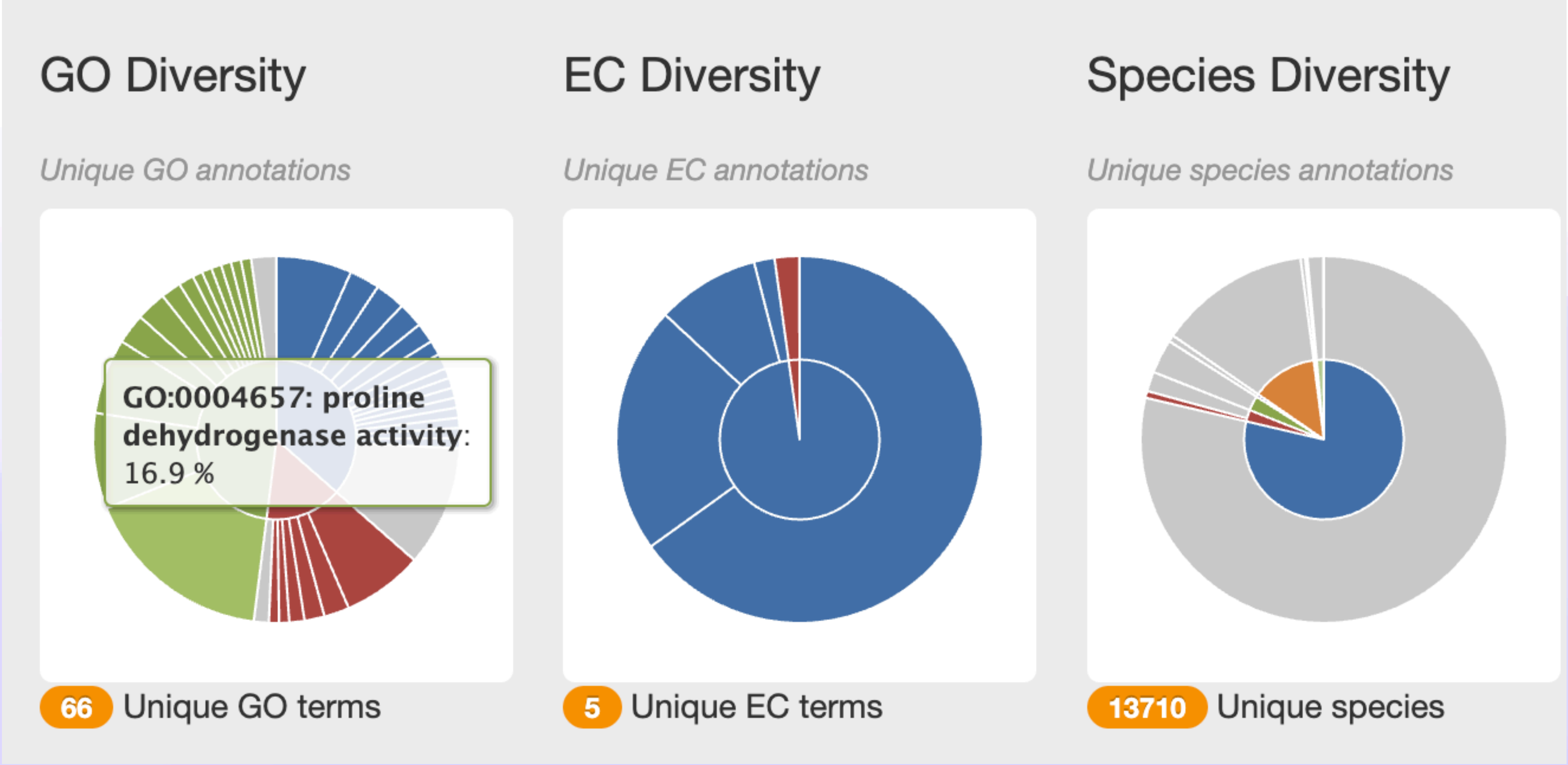
TED Consensus Domains 6

	DOMAIN	BOUNDARIES	CATH	RESIDUES	AV PLDDT	PACKING	GLOBULARITY	INTERACTIONS	PDB
	TED01	2-47	1.10.1220.10	46	76.2	10.1	0.300		
	TED02	104-139_261-557	3.20.20.220	333	94.0	11.9	0.286	TED05 5.0 TED06 9.0	
	TED03	145-218_242-258	-	91	60.2	10.8	0.276		
	TED04	628-884	3.40.605.10	257	96.2	12.2	0.289	TED05 4.0 TED06 4.0	
	TED05	890-1084	3.40.309.10	195	96.1	11.8	0.293	TED04 4.0 TED06 5.0 TED02 5.0	
	TED06	1132-1306	3.40.605.10	175	94.8	11.6	0.300	TED05 5.0 TED02 9.0 TED04 4.0	

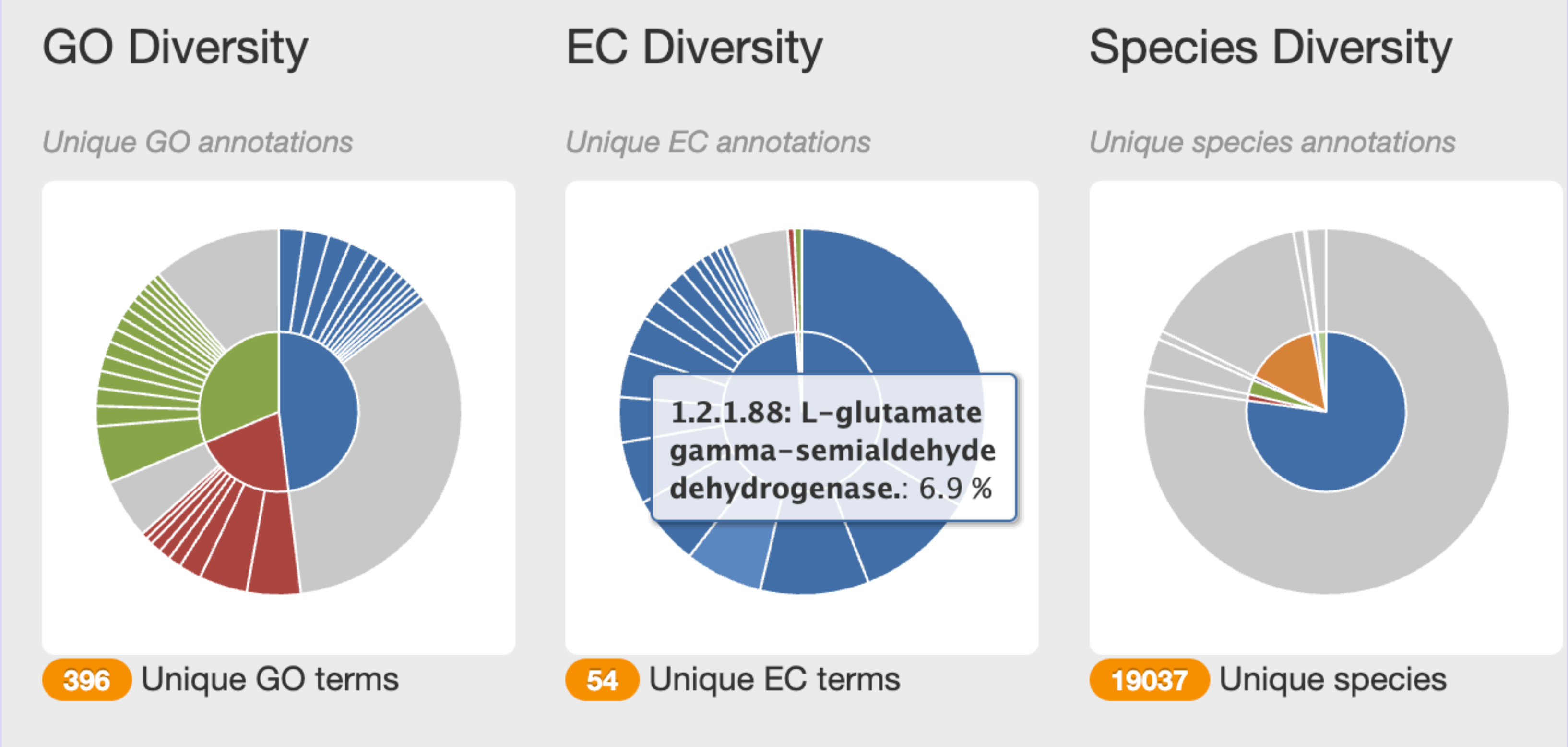
Domain 1: 1.10.1220.10



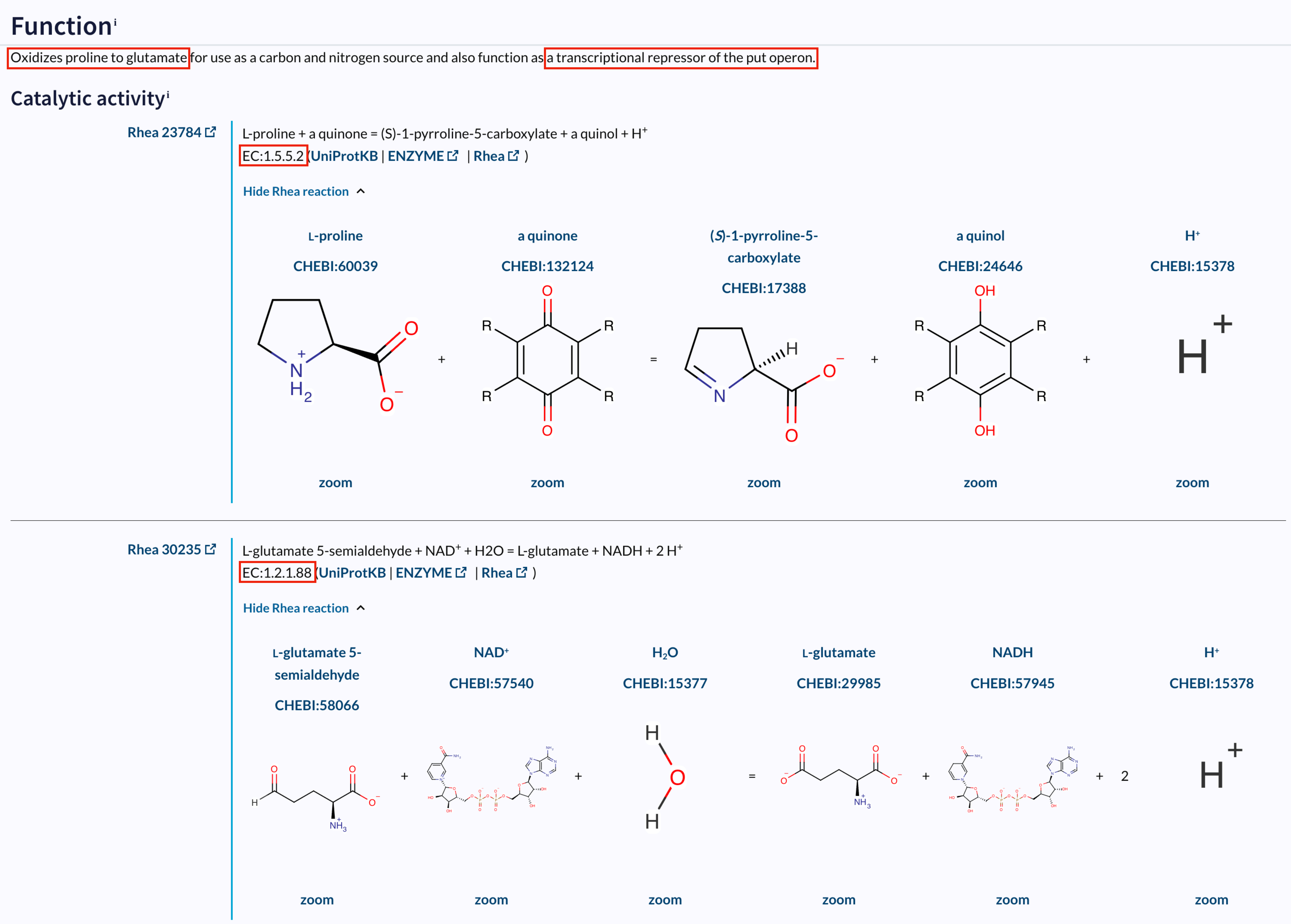
Domain 2: 3.20.20.220



Domain 5: 3.40.309.10



实际功能标记



Function

Oxidizes proline to glutamate for use as a carbon and nitrogen source and also function as a transcriptional repressor of the put operon.

Catalytic activity

Rhea 23784

L-proline + a quinone = (S)-1-pyrroline-5-carboxylate + a quinol + H^+

EC:1.5.5.2 (**UniProtKB** | **ENZYME** | **Rhea**)

Hide Rhea reaction

L-proline	a quinone	(*S*)-1-pyrroline-5-carboxylate	a quinol	H^+
CHEBI:60039	CHEBI:132124	CHEBI:17388	CHEBI:24646	CHEBI:15378

Rhea 30235

L-glutamate 5-semialdehyde + NAD^+ + H2O = L-glutamate + NADH + 2 H^+

EC:1.2.1.88 (**UniProtKB** | **ENZYME** | **Rhea**)

Hide Rhea reaction

L-glutamate 5-semialdehyde	NAD^+	H_2O	L-glutamate	NADH	H^+
CHEBI:58066	CHEBI:57540	CHEBI:15377	CHEBI:29985	CHEBI:57945	CHEBI:15378

Q&A