

Modeling proteins only

## JAAG: a JSON input file Assembler for AlphaFold 3 with Glycan integration

**About JAAG** ▾

**Basic Information**

**Job Name\***

Enter job name

Allows letters, numbers, hyphens, and underscores

[Advanced Settings](#)

**Sequences**

+ Protein

+ Ligand

+ RNA

+ DNA

Click the buttons above to add sequences

**Manual userCCD Input** ▾

**JSON Output**

[Lookup](#) [Copy](#) [Download](#)

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": []
}
```

Ready to generate JSON

1. Enter job name. Space and other special symbols are not allowed.
2. Click the button to add a protein. If users are interested in a second protein, click the button again.

Allows letters, numbers, hyphens, and underscores

Sequences
+ Protein + Ligand + RNA + DNA

Protein Sequence
A

Chain ID\*
A

Count
1

Protein Sequence\*
UniProt Import (optional)
UniProt ID (e.g., P20273)

Description (optional)
Optional description for this protein sequence

Auto N-glycosylation based on sequon
Detect Sequons

Manual Glycosylation Sites
Add Site

Advanced Functions

Manual userCCD Input

JSON Output
Lookup Copy Download

Download JSON file

```

{
  "name": "Untitled Job",
  "modelSeeds": [1],
  "dialect": "alphaFold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence": ""
      }
    }
  ]
}

```

Ready to generate JSON

3. Type in the UniProt accession ID to fetch the protein sequence, or paste the amino sequence directly. Only when fetching from UniProt will JAAG automatically import the ID into the “Description” field below.
4. If users are looking into protein homo-multimers, toggle the count to the desire number.
5. Click the button to download the whole JSON file.

# Modeling glycoproteins

## JAAG: a JSON input file Assembler for AlphaFold 3 with Glycan integration

**About JAAG** ▾

**Basic Information**

**Job Name\***

Enter job name

Allows letters, numbers, hyphens, and underscores

[Advanced Settings](#)

**Sequences**

+ Protein

+ Ligand

+ RNA

+ DNA

Click the buttons above to add sequences

**Manual userCCD Input** ▾

**JSON Output**

[Lookup](#) [Copy](#) [Download](#)

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": []
}
```

Ready to generate JSON

1. Enter job name. Space and other special symbols are not allowed.
2. Click the button to add a protein. If users are interested in a second protein, click the button again.

Allows letters, numbers, hyphens, and underscores

**Import GlyTouCan and GlyGen ID**

**Sequences**

+ Protein + Ligand + RNA + DNA

Protein Sequence A ▼

Chain ID\*

Protein Sequence\*

Count

Description (optional)

Auto N-glycosylation based on sequon ▼ Q Detect Sequons

Manual Glycosylation Sites ▼ + Add Site

[Advanced Functions](#)

Manual userCCD Input ▼

**JSON Output**

Q Lookup Copy Download

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphaFold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence": ""
      }
    }
  ]
}
```

Ready to generate JSON

③ Enter protein sequence

④ Toggle counts for multimers

⑤ Detect sequons for N-glycans

⑥ Manually add glycosylation sites

⑦

⑧ Download JSON file

3. Type in the UniProt accession ID to fetch the protein sequence, or paste the amino sequence directly. Only when fetching by UniProt will JAAG automatically import the ID into the “description” field below.
4. If users are looking into protein homo-multimers, toggle the count to the desire number.
5. Click the button to automatically add N-glycosylation sites based on sequons. Please see the following pages for more details.
6. Click the button to manually add any glycosylation sites. Please see the following pages for more details.
7. Click the button to look up glycan structure in the GlyTouCan and GlyGen database and import the corresponding glycan into the JSON file. The IDs will be placed in the corresponding description field.
8. Click the button to download the whole JSON file.

The screenshot shows the 'Auto N-glycosylation based on sequon' interface. At the top, a 'Detect Sequons' button is circled in red and labeled 5.0. Below it, a text box explains that the tool automatically detects N-glycosylation sequons (N-X-S/T where X≠P) in a protein sequence. To the left, a 'Glycan Templates' section is circled in red and labeled 5.1, showing a dropdown to 'Select a glycan template...'. To the right, an 'Apply GlycoCT to all' section is circled in red and labeled 5.2, with a text box for 'Import GlycoCT from SugarDrawer or paste GlycoCT from database'. Below these, a table lists N-glycan sites with columns for Position, Chain ID\*, Glycan\*, and Description. The first row (Position 79, Chain ID\* GLYCANA) is circled in red and labeled 5.3, with a text box 'Add glycans from GlycoCT or SugarDrawer to single N-glycan sites'. The right side of the interface shows a 'JSON Output' section with a 'Ready to generate JSON' button.

5.0. This tab will be added and expanded after clicking the “Detect Sequons” button.

Glycan structures can be introduced using the following three methods: 5.1, 5.2 and 5.3. Users can first use 5.1 or 5.2 to apply the same glycan to all N-glycan sites, then modify each site individually in 5.3.

5.1. Select glycan structures from a library of pre-built N-glycan templates. Please see the following pages for more details.

5.2. Paste in GlycoCT from your favorite glycoinformatics database or click the pencil icon to open the pop-up SugarDrawer tool to draw glycans. This will apply to all N-glycosylation sites. Please see the following pages for more details.

5.3. Paste in GlycoCT from your favorite glycoinformatics database or click the pencil icon to open the pop-up SugarDrawer tool to draw glycans. This will apply to individual N-glycosylation sites. Please see the following pages for more details.

Auto N-glycosylation based on sequon **5** [Detect Sequons](#)

**5.1.0** Add glycan templates to all N-glycan sites

5.1.1

**Glycan Templates**

✓ Select a glycan template...

- A2 (biantennary complex-type GlcNAc-terminal)
- A2F (biantennary complex-type GlcNAc-terminal core-Fuc)
- G2 (biantennary complex-type Gal-terminal)
- G2F (biantennary complex-type Gal-terminal core-Fuc)
- G2S2(α2,6) (biantennary complex-type α2,6-Sia)
- G2S2(α2,6)F (biantennary complex-type α2,6-Sia core-Fuc)
- G2S2(α2,3) (biantennary complex-type α2,3-Sia)
- G2S2(α2,3)F (biantennary complex-type α2,3-Sia core-Fuc)
- M3 (high-mannose type)
- M3F (high-mannose type core-Fuc)
- M5 (high-mannose type)
- M5F (high-mannose type core-Fuc)
- M9 (high-mannose type)

Apply GlycoCT to all ☒

Import GlycoCT from SugarDrawer or paste GlycoCT from database

Description

Optional description...

Description

Optional description...

Description

Optional description...

**JSON Output** [Look Up](#) [Copy](#) [Download](#)

```
{
  "name": "Untitled_job",
  "modelSeeds": [1],
  "dialect": "alphaFold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": "A",
        "sequence":
          "MSVGRSRRIKLGILMMANVFYIFMEVSKSSSQEKNKGEVILPEKFKWISTPPEAY
          WRREQELNPNQWPIILSMLTNQTEAGRLSNISHLAYCEPDLAVTSVVTGPNLPRFK
          DELLYICRYTLLIDQPKAKKFFLLAKITLTHFPAPDAISEWQESMAGQTV
          VRVFLQQTFFEDNHFOLDISMLKFESEKHQDILMMNYRDTFFNLSEVLFLRWYSTSC
          FDETFVFKGDDOVFNTHILANILNSLSTRKADLFIDGVHNAHPRDKLKYIIEV
          VYSGLYPPFYAGGGGFLYSGHLALALYHITDQVLYPIIDVYTGMLQKGLVPEKRGF
          RTDIESSNNICSVYDGLVHEHFEFQMDIDWIGQARKK",
        "description": "UniProt ID: Q9NY97"
      }
    }
  ]
}
```

Ready to generate JSON

**Keys:**

5.1.0. This pull-down menu will appear after clicking “Select a glycan template...”

5.1.1. Select one glycan from the template collection to apply it to all N-glycosylation sites. The nomenclature key for each glycan abbreviation is provided.



**5.2.1** Click pencil to pop up SugarDrawer

**5.2.2** Start drawing with templates

**5.2.3** Add monosaccharides

**5.2.3.1** Select linkage and anomer

**5.2.3.2** Right click for isomer and ring

**5.2.4** Add substituents

**5.2.5** Finish drawing

Export & Close

• This tutorial works for 5.3 as well

5.2.1. Click the pencil icon to pop up SugarDrawer.

5.2.2. In the SugarDrawer, there are pre-built glycan templates that users can load to start the drawing the glycan structure. In the case here, find the N-glycan structures to start with.

5.2.3. Click the monosaccharides in the shortcut to extend glycans. If the monosaccharides are not in the shortcut, click the “Add Monosaccharide” button to expand the monosaccharide table.

5.2.3.1. Click the linkage line at the reducing end or between monosaccharides to pop up the anomer/linkage selection panel. Anomer and linkages must be defined to properly export the glycan bondedAtomPairs.

5.2.3.2. Right click the monosaccharide to pop up the isomer panel if users are using rare monosaccharides.

\*Note: not all monosaccharides have corresponding CCD IDs.

5.2.4. Sul (sulfation), N-Sul (N-sulfation), Pho (phosphorylation), Ac (acetylation) and O-Me (methylation) are supported for bondedAtomPairs generation.

5.2.5. Click the button to export GlycoCT. The glycan bondedAtomPairs will be converted automatically.

This tutorial works for 5.3 as well to customize individual N-glycosylation sites.

The screenshot shows the UniProt N-glycosylation tool interface. At the top, a protein sequence is displayed with UniProt ID: Q9NY97. Below the sequence, the 'Description (optional)' field contains the UniProt ID. The 'Auto N-glycosylation based on sequen' dropdown is set to '5'. A search button labeled '6.0' is next to it. Below this, the 'Manual N-glycosylation Sites' section is visible. It includes a 'Position\*' input field with the value '1' (annotated with 6.1), a 'Residue\*' dropdown menu (annotated with 6.2), and a 'Linking Atom\*' dropdown menu. A 'Chain ID\*' field is set to 'GLYCANF'. A 'Glycan\*' checkbox is checked, and an 'Import GlycoCT...' button is present (annotated with 6.3). An '+ Add Site' button is also visible. To the right, a 'JSON Output' section shows a JSON representation of the data. At the bottom, there is a 'Manual userCCD Input' field.

- 6.0. This tab will be added and expanded after clicking “Add Site” button.
- 6.1. Users can type in amino acid numbers or toggle through the numbers.
- 6.2. When N/S/T are selected in 6.1, the amino acid atom linked to N- or O-glycan will appear automatically. If users are looking for other amino acid/atoms for glycosylation, look up PDBeChem for the atom: <https://www.ebi.ac.uk/pdbe-srv/pdbechem/>
- 6.3. Please refer to 5.2 for using SugarDrawer.

# Modeling glycan as ligand

Referring to “modeling proteins only” or “modeling glycoproteins” sections to add protein

## JAAG: a JSON input file Assembler for AlphaFold 3 with Glycan integration

About JAAG

**Basic Information**

**Job Name\***

Enter job name

Allows letters, numbers, hyphens, and underscores

Advanced Settings

**Sequences**

+ Protein + **Ligand** + RNA + DNA

Click the buttons above to add sequences

Manual userCCD Input

**JSON Output**

Lookup Copy Download

```
{
  "name": "Untitled_Job",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": {}
}
```

Ready to generate JSON

1. Enter job name. Space and other special symbols are not allowed.
2. Click the button to add a ligand. If users are interested in a second ligand, click the button again.

Import GlyTouCan and GlyGen ID

JSON Output ④

⑤ Download JSON file

③ Add glycans from GlycoCT or SugarDrawer

Basic Information

Job Name\* [Advanced Settings](#)

Enter job name

Allows letters, numbers, hyphens, and underscores

Sequences [+ Protein](#) [+ Ligand](#) [+ RNA](#) [+ DNA](#)

Ligand **LIGA** [-](#)

Chain ID\* Input Type

LIGA Glycan

GlycoCT Data\* ☒

Import GlycoCT from SugarDrawer or paste GlycoCT from database

Count Description (optional)

1 Optional description for this ligand

bondedAtomPairs (Optional) [+ Add Bond](#)

Manual userCCD Input [-](#)

JSON Output

Look up Copy Download

```
{
  "name": "Untitled_Job",
  "modelSeeds": [],
  "dialect": "alphaFold3",
  "version": 4,
  "sequences": [
    {
      "ligand": {
        "id": "LIGA",
        "codCodes": []
      }
    }
  ]
}
```

Ready to generate JSON

3. Paste in GlycoCT ID from your favorite glycoinformatics database or click the pencil icon to pop up SugarDrawer to draw glycans. Please see the following pages for more details.
4. Click the button to look up glycan structures in GlyTouCan and GlyGen databases to import the corresponding glycan ID into the JSON file. The ID will be attached into the corresponding description field.
5. Click the button to download the whole JSON file.

The screenshot shows the SugarDrawer software interface. At the top left, a pencil icon is circled and labeled 3.1. Below it is a 'GlycoCT Data\*' input field. To the right, the 'SugarDrawer' title bar is visible. Below the title bar, a row of buttons includes 'Load Structure', 'Add Monosaccharide', and 'Add Substituent'. The 'Add Monosaccharide' button is circled and labeled 3.2. To its right, a row of colored circles represents different monosaccharides, with a label 3.3. Further right, a row of substituent icons (Sul, N-Sul, Pho, Ac, O-Me) is shown, with a label 3.4. In the center, a grid of linkage templates (e.g., α1-3, β1-3, etc.) is displayed. A linkage line is selected and circled, labeled 3.3.1. A right-click context menu is shown below the linkage line, with options for 'Isomer' (D, L), 'Ring size' (p, f, o), and 'Connected' (0, 1). This menu is labeled 3.3.2. At the bottom right, an 'Export & Close' button is circled and labeled 3.5. A zoom slider is located at the bottom center.

3.1. Click the pencil icon to pop up SugarDrawer.

3.2. In the SugarDrawer, there are pre-built glycan templates that users can load them to start the glycan drawing process.

3.3. Click the monosaccharides in the shortcut menu bar above to extend the glycan structure. If the monosaccharides are not in the shortcut, click the “Add Monosaccharide” button to expand the monosaccharide table.

3.3.1. Click the linkage line at the reducing end or between monosaccharides to pop up the anomer/linkage selection panel. Anomer and linkages must be defined to properly export the glycan bondedAtomPairs.

3.3.2. Right click the monosaccharide to pop up the isomer panel if users are using rare monosaccharides.

3.4. Sul (sulfation), N-Sul (N-sulfation), Pho (phosphorylation), Ac (acetylation) and O-Me (methylation) are the substituents that are supported for bondedAtomPairs generation.

3.5. Click the button to export GlycoCT. The glycan bondedAtomPairs will be converted automatically.

Example of building B3GNT2 homodimer-  
Mn<sup>2+</sup>-UDP-GlcNAc-LNnT complex

Sequences

+ Protein
+ Ligand
+ RNA
+ DNA

Protein Sequence
A

Chain ID\*
A

Protein Sequence\*
UniProt Import (optional)
Q9NY97

Count
2

MSVGRRIKLLGILMMANVFYIFIMEVSKSSSQEKNKGKGEVIIPKEKFWKISTPPEAYWNREQELNRQ  
YNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLPDRFKDFLLYLRNRYSLLDQPDKC  
AKKPFLLLAIKSLTPHFARRQAIRESWGQESNAGNQTVVRVFLLGQTPPEDNHPDLSMDLKFSEKHHQ

1
Add protein

2
Fetch the amino sequence from UniProt accession ID

3
Toggle count to 2 for modeling two copies of B3GNT2

Description (optional)
UniProt ID: Q9NY97

Auto N-glycosylation based on sequon
5
Detect Sequons

JSON Output

Lookup
Copy
Download

```

{
  "name": "gly_b3gnt2_dimer_udpglcnac_mn_lntri2",
  "modelSeeds": [1],
  "dialect": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence": "MSVGRRIKLLGILMMANVFYIFIMEVSKSSSQEKNKGKGEVIIPKEKFWKISTPPEAYWNREQELNRQYNPILSMLTNQTGEAGRLSNISHLNYCEPDLRVTSVVTGFNNLPDRFKDFLLYLRNRYSLLDQPDKC  
AKKPFLLLAIKSLTPHFARRQAIRESWGQESNAGNQTVVRVFLLGQTPPEDNHPDLSMDLKFSEKHHQ"
      },
      "description": "UniProt ID: Q9NY97"
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "codCodes": ["UD1"]
      },
      "description": "GlyTouCan ID: G58896AZ (https://glytoucan.org/Structures/Glycans/G58896AZ)"
    }
  ]
}

```

Successfully looked up 11/11 glycans

4
Scroll down the page looking for "Detect Sequon" button



UniProt ID: Q9NY97

Auto N-glycosylation based on sequon

Detect Sequons

This section automatically detects N-glycosylation sequons (N-X-S/T where X≠P) in your protein sequence.

Glycan Templates

M5 (high-mannose type)

Select a glycan template...

- A2 (biantennary complex-type GlcNAc-terminal)
- A2F (biantennary complex-type GlcNAc-terminal core-Fuc)
- G2 (biantennary complex-type Gal-terminal)
- G2F (biantennary complex-type Gal-terminal core-Fuc)
- G2S2(α2,6) (biantennary complex-type α2,6-Sia)
- G2S2(α2,6)F (biantennary complex-type α2,6-Sia core-Fuc)
- G2S2(α2,3) (biantennary complex-type α2,3-Sia)
- G2S2(α2,3)F (biantennary complex-type α2,3-Sia core-Fuc)
- M3 (high-mannose type)
- M3F (high-mannose type core-Fuc)
- M5 (high-mannose type)**
- M5F (high-mannose type core-Fuc)
- M9 (high-mannose type)

Apply GlycoCT to all

Description

GlycoCT ID: G55220VL

Description

GlycoCT ID: G55220VL

Description

GlycoCT ID: G55220VL

Position
Chain ID\*
Glycan\*
Description

173
GLYCAND
RES
GlycoCT ID: G55220VL

Position
Chain ID\*
Glycan\*
Description

219
GLYCANE
RES
GlycoCT ID: G55220VL

JSON Output

Look Up
Copy
Download

```

{
  "name": "gly_b3gnt2_dimer_udpglcnac_mn_intr12",
  "alias": "alphaFold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence": "MSVGRRRRIKLLGILMMANVFYIMEVSKSSSQKNGKEVILPKEEFKWKISTPPEAYWNRQELKLRQVNFILSMITQGTGEAGLSNISHLNYCEPOLRVSVVTGNNLPDRFQFLYLKRNIVLLIQGFCARPKFILLAIKSLTPPARAGAKESWGQENAGNQTIVRVFLGQTFFPDNHPOLSDMLKFESEKHQDILMMNYRDTFFNLSEVLFLRWVSTSCPOTEFVFGGDDVFNTHILNLYNSLSKTKAKOLFQGVINNAGPHRDRLKLYTIPEVYVYSGLYPYAGGGGLYSCHLALRLYHITDQVHLPIQVYTGMLQKGLVPERKSGFRTDIEKNKNNICBYULMLVHSRAPQEMIDIMWQLQSAHLKQ"
      },
      "description": "UniProt ID: Q9NY97"
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "codon": ["UD1"]
      },
      "description": "GlycoCT ID: G55220VL"
    }
  ],
  "ligand": {
    "id": ["LIGCA", "LIGCB"],
    "codon": ["BGC", "GAL", "NAG", "GAL"],
    "description": "GlycoCT ID: G5896AZ (https://glytoucan.org/Structures/Glycans/G5896AZ)"
  }
}

```

Successfully looked up 11/11 glycans

underscores

**Sequences** + Protein + Ligand + RNA + DNA

Protein Sequence A ▼

Ligand LIGA ▼ 🗑️

Chain ID\* LIGA

Count 2 🔍

Description (optional) Optional description for this ligand

📌 Note: Multiple ligands will be created with chain IDs: LIGAA, LIGAB

Ligand LIGB ▼ 🗑️

Ligand LIGC ▼ 🗑️

bondedAtomPairs (Optional) ▼ + Add Bond

Manual userCCD Input ▼

**JSON Output** 🔍 Lookup 📄 Copy 📄 Download

```
{
  "name": "gly_b3gnt2_dimer_udpglcna_mn_lntri2",
  "modelSeeds": [1],
  "select": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence": "MSVGRRIKLLGILMMANVFIYFIMEVSSSSQERNGKEVIFKEKFWKISTPPE
        AFWNRGKELRGNTQFLSMITQTEGAEGLNLSHINACEPLAVFVSIVFGNNLP
        DRFKDFLLYLCBNYSLLIDQFMCAKPFLLIAIKLIPFPARQAIESWGQSEN
        AOMTVVRVFLQQTFFEDNHPDLSMLKFESEKHQDILMMNYRTFFNLSEVLF
        WWSSTSCPOTEFVFKGDDVFNTHILMYLSLKTAKDLFIGDVIHNAQPHRD
        LITVIFEVVYSLFFPIAGGGFLYSRLALRLHITQVHLPIFDVITMCILQ
        GLLVPEKRWKFTFDIEKNKNNICSYDLMLVHERKPOKIDIMGQLGAILKC"
      },
      "description": "UniProt ID: Q9NY97"
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccdCodes": ["UD1"]
      },
      "description": "Glycans (G58896AZ) (https://glytoucan.org/Structures/Glycans/G58896AZ)"
    },
    {
      "ligand": {
        "id": ["LIGBA", "LIGBB"],
        "ccdCodes": ["MN"]
      },
      "description": ""
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccdCodes": ["MGC", "GAL", "NAG", "GAL"]
      },
      "description": ""
    }
  ]
}
```

🟢 Successfully looked up 11/11 glycans

**Annotations:**

- ⑨ Add the first ligand
- ⑩ Select CCD
- ⑪ Add UDP-GlcNAc CCD code
- ⑫ Toggle count to two

underscores

Sequences

+ Protein

+ Ligand

+ RNA

+ DNA

Protein Sequence A ▼

Ligand LIGA ▼

Ligand LIGB ▼

Chain ID\*

LIGB

Glycan

✓ CCD Codes

SMILES

Count

2

Optional description for this ligand

Optional description for this ligand

Multiple ligands will be created with chain IDs: LIGBA, LIGBB

16

Toggle count to two

Ligand LIGC ▼

bondedAtomPairs (Optional) ▼

+ Add Bond

Manual userCCD Input ▼

13

Add the second ligand

14

Select CCD

15

Add magnesium CCD code

15

MN

JSON Output

Q

Lookup

Copy

Download

```

{
  "name": "gly_b3gnt2_dimer_udpglcna_mn_lntri2",
  "modelType": 1,
  "description": "alphaFold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence": "MSVGRSRRIKLGILMMAVFYIMEVSKSSSQEKNGKEVVIPEKFWKISTPPEAYWNRGEQLNRQYMFILSMLTWTQGEAGLSNISHLYNCEPDLRVTSVVTGNNLPDRFQFLYLIRCNVSLIDQFQKCAKFFLLAIKSLTPHRAQAIFESWGQENAGNQTVVRVFLQTFPPEDNRPDLSIMLKFESEKHQDILMNNYRDTFFNLSLEVLFLRWVSTSCFOTEFVFKGDDVFNTHILMYLSLSKTKAKDLFGDVIHNAQPHRDRLKLYTIFEVVYSGLTPYAGGGGLYSGLHALRLYRITDQVHLYPIDOVTTGMCLQKGLGVPERKSGFRTFDIEKNWNNICSVYULMVHSPQEMIDIWSQLQSAHLAC"
      },
      "description": "UniProt ID: Q9NY97"
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccdCodes": ["UD1"]
      },
      {
        "ligand": {
          "id": ["LIGBA", "LIGBB"],
          "ccdCodes": ["MN"]
        },
        {
          "ligand": {
            "id": ["LIGCA", "LIGCB"],
            "ccdCodes": ["MGC", "GAL", "NAG", "GAL"],
            "description": "GlyToucan ID: G58896AZ (https://glytoucan.org/Structures/Glycans/G58896AZ)"
          }
        }
      }
    }
  ]
}

```

Successfully looked up 11/11 glycans

19

underscores

**Sequences** + Protein + Ligand + RNA + DNA

Protein Sequence A ▼

Ligand LIGA ▼ 🗑️

Ligand LIGB ▼ 🗑️

Ligand LIGC ▼

Chain ID\* Input Type GlycoCT Data\* 📝

LIGC Glycan RES  
1b:b-dglc-HEX-1:5

Count Description (optional)

2 GlyTouCan ID: G58896AZ (<https://glytoucan.org/Structures/Glycans/G58896AZ>)

🗑️ 19 Toggle count to two

bondedAtomPairs (Optional) ▼ + Add Bond

Manual userCCD Input ▼

**JSON Output** 🔍 Lookup 📄 Copy 📄 Download

21 Download JSON file

20 Look up GlyTouCan and GlyGen ID by clicking "Lookup" button

18 Paste the LNnT GlycoCT or draw from SugarDrawer by clicking the pencil icon

17 Add the third ligand

```
{
  "name": "gly_b3gnt2_dimer_udglicnac_mn_intc12",
  "chainSeeds": [1],
  "object": "alphafold3",
  "version": 4,
  "sequences": [
    {
      "protein": {
        "id": ["AA", "AB"],
        "sequence": "
MSVGRSRKILGILMMANVFIYFIMRHWSSSQKNGKEVILPKKFWKISTPPE
AYWNRGEKLNQYFPLSMLTQKAGLSNLSHLYNCEPDLRVSVVTGNNLP
DRKFDLYLRCNVLIDQPKRPFLLIAIKSLTPHRAQAIFESWGQEN
AGNQTVRVFLQQTFFPDNRPDLNMLKFESEKHQDILMNNYRDTFFNLSLEVL
LRWVSTSCPOTEFVFKGDDVFNPHILNLSLSKTKAKDLFGDVHNAQPRD
RLATYIPVVYSGLTPYAGGFLYSGHLALRLYITDQVHLFIDOVTTGMCLQ
RNVFPERKGFRTFDIESKVAHCICVVDLNVHRRPQEMIDIKSQLGABKAC"
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      "description": "UniProt ID: Q9N97"
    },
    {
      "ligand": {
        "id": ["LIGAA", "LIGAB"],
        "ccode": ["BGC", "GAL", "NAG"]
      }
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccode": ["BGC", "GAL", "NAG", "GAL"]
      }
    },
    {
      "ligand": {
        "id": ["LIGCA", "LIGCB"],
        "ccode": ["BGC", "GAL", "NAG", "GAL"],
        "description": "GlyTouCan ID: G58896AZ (https://glytoucan.org/Structures/Glycans/G58896AZ)"
      }
    }
  ]
}
```

🟢 Successfully looked up 11/11 glycans