1. Let's open the page of the **Knotprot database**: https://knotprot.cent.uw.edu.pl, then click "**Process my structure**" button in the top menu or at the bottom of the page. It will direct you to the **submit menu**.

2. First two fields are optional: **job name** and **e-mail address**. Providing "**job name**" would be helpful in the case of running several jobs to distinguish between them. If the e-mail address is provided, a link to the results of the job will be send to this address after the job is submited.

3. Before uploading the structure for the job, one has to determine an **input data format**. The server accepts two formats: **PDB**, and **XYZ**. For details of both formats one can click this light blue "**iHelp**" button. In the calculations only positions of C-alpha atoms are used; therefore, it is sufficient to provide only positions of these atoms in one of the formats.

4. Now, we can upload a structure file for the calculations on the server, but first one has to set the "**Input file format**". Let's consider the PDB file format option. There appear several new fields: (1) **select input structure**. You can drag-and-drop the file, or browse it, or alternatively (2) provide PDB code; (3) choose chain name, (4) one can decide whether to calculate **knots** or **knotoids**, and (5) choose the "**Closing method**" (there are two options" statistical", "connect both ends with straight line" (here we can determine indices of amino acids / C-alpha atoms to be connected).

5. First let's consider a simple case of 3_1 knot and run several job with the file **knot-1.pdb** (Alternatively, there is a structure with 5_2 knot, file knot-2.pdb).

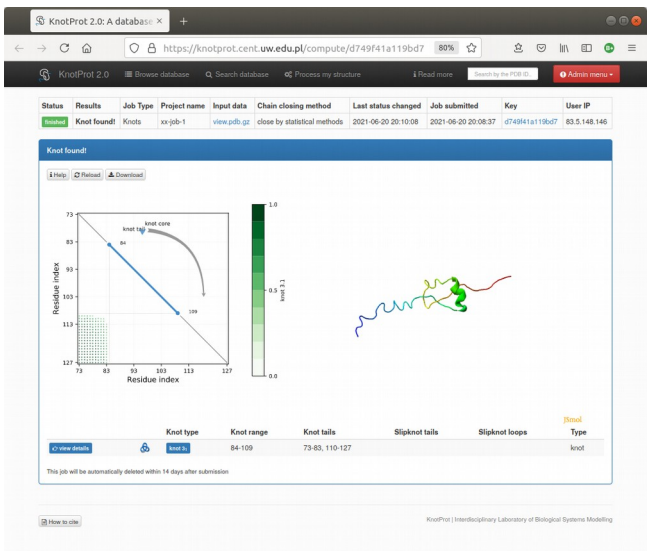
   If we haven't provided an email address, the only way to reach the result page is to follow the link in the green box. We can open it in another tab, and we can run the next job. We can compare results with the entry in the database.

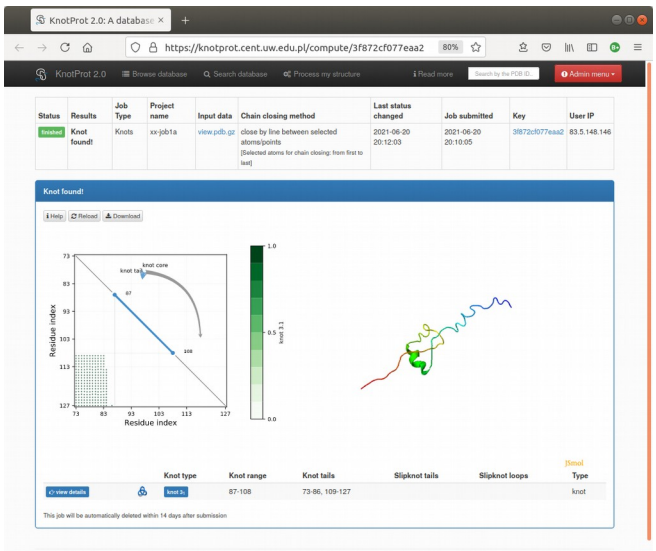
   - **[EXAMPLE-1: PDB, knot-1.pdb, knots, statistical closings]**,

     results: https://knotprot.cent.uw.edu.pl/compute/d749f41a119bd7,

   - **[EXAMPLE-2: PDB, knot-1.pdb, knots, direct method]**,

     results: https://knotprot.cent.uw.edu.pl/compute/3f872cf077eaa2,



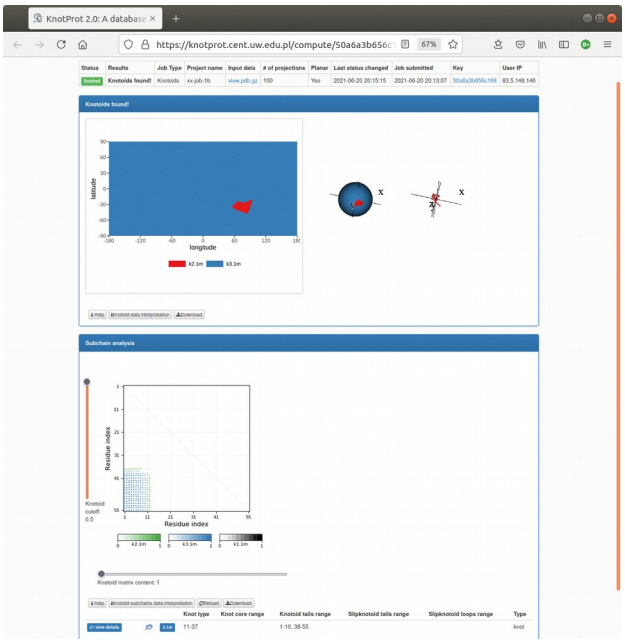


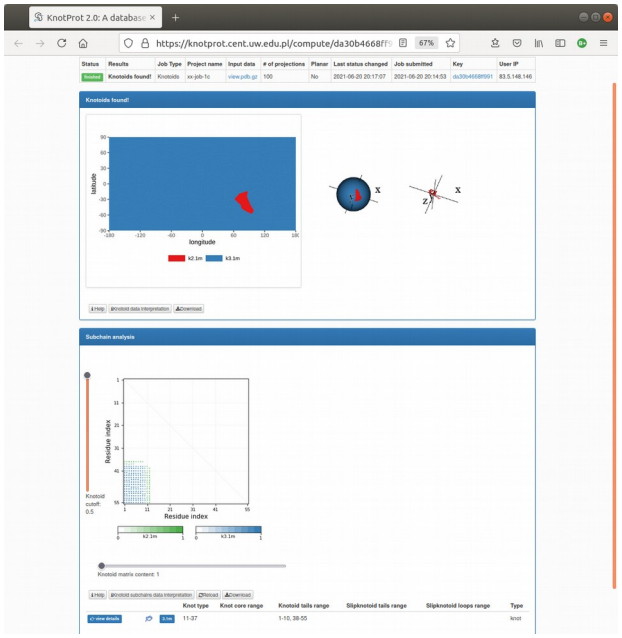
- **[EXAMPLE-3: PDB, knot-1.pdb, knotoids, planar]**,

results: https://knotprot.cent.uw.edu.pl/compute/50a6a3b656c168

- **[EXAMPLE-4: PDB, knot-1.pdb, knotoids, no planar]**,

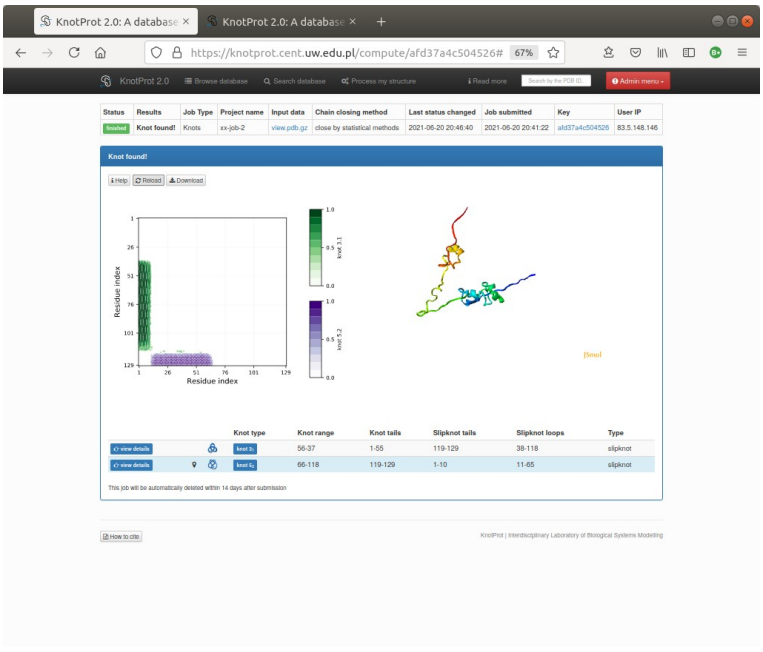
  results: https://knotprot.cent.uw.edu.pl/compute/da30b4668ff991



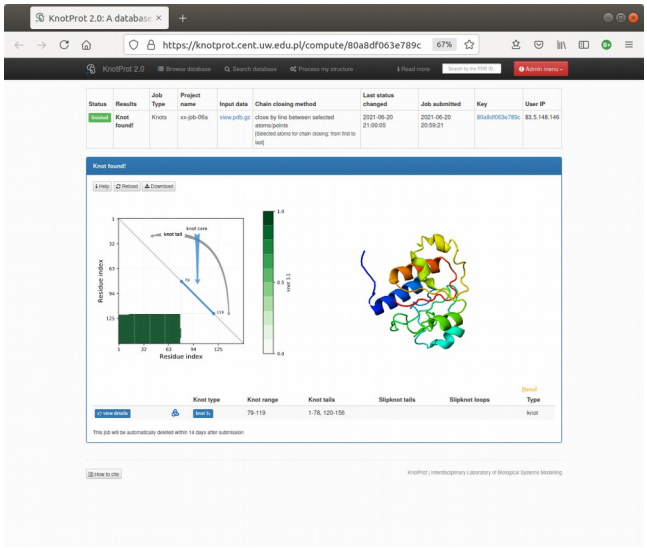


When we choose Knotoids to be calculated, we have two additional options: (1) "Number of projections", and (2) "Planar" on or off. Extended help is provided here: https://knotprot.cent.uw.edu.pl/help_knotoids

6. **[EXAMPLE-5: PDB, knot-1-2.pdb, knots, direct statistical]**. The structure contains two knots. Result: https://knotprot.cent.uw.edu.pl/compute/afd37a4c504526#

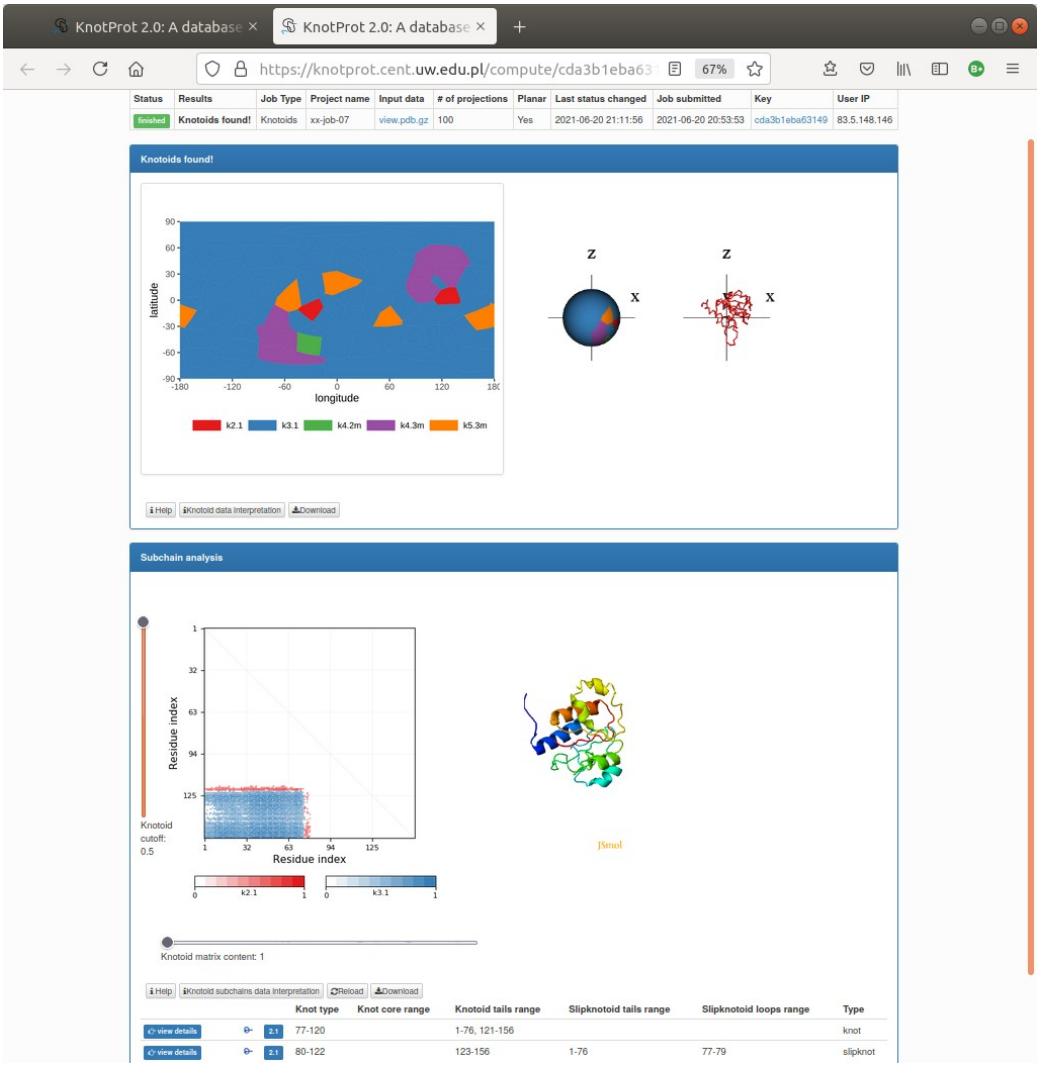


7. **[EXAMPLE-6: PDB, 1j85.pdb, knots, direct method]**. Result: https://knotprot.cent.uw.edu.pl/compute/80a8df063e789c (Here it is the link to the statistical closing method: https://knotprot.cent.uw.edu.pl/compute/31b7ebabf706d3)

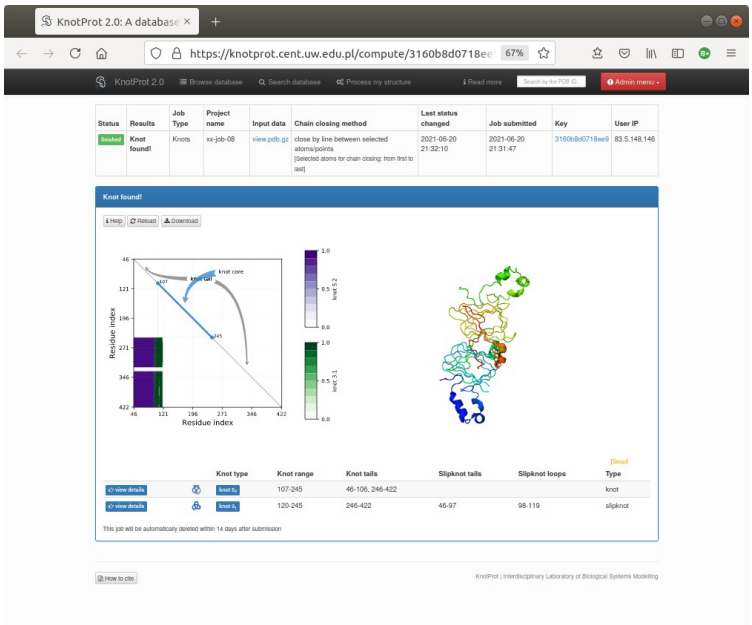


(po prawej: "direct"; dla porównania "statistical method")

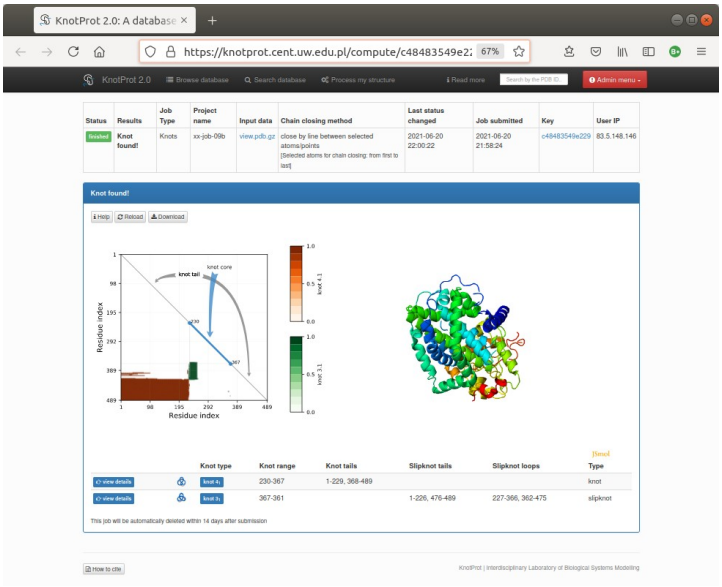
8. **[EXAMPLE-7: PDB, 1j85.pdb, knotoids, planar]**. Results: https://knotprot.cent.uw.edu.pl/compute/cda3b1eba63149



9. **[EXAMPLE-8, PDB, 2cav.pdb, direct; (białko ma węzły 5_2 i 3_1)]**. Using the direct connection is much faster, but one must be careful, because the line can go through a fragment of the molecule, and change the final topology of the studied structure. That is way there is an additional option of choosing the indices of elements of the chain to be connected, because not always the extreme points may be reasonable. Results: https://knotprot.cent.uw.edu.pl/compute/3160b8d0718ee9. We can compare the fingerprint matrix with the one from the database for this protein ("statistical").



10. **[EXAMPLE-9, PDB, 3ulkA.pdb, direct]**. Protein conteins 4_1 knot and 3_1 slipknot; results: https://knotprot.cent.uw.edu.pl/compute/c48483549e229.



11. **[EXAMPLE-10: PDB-Trajectory, trajectory.pdb, 13 frames]**. Information about the format. Results: https://knotprot.cent.uw.edu.pl/compute/a86f3d57a941bf.