ViTO2 user guide

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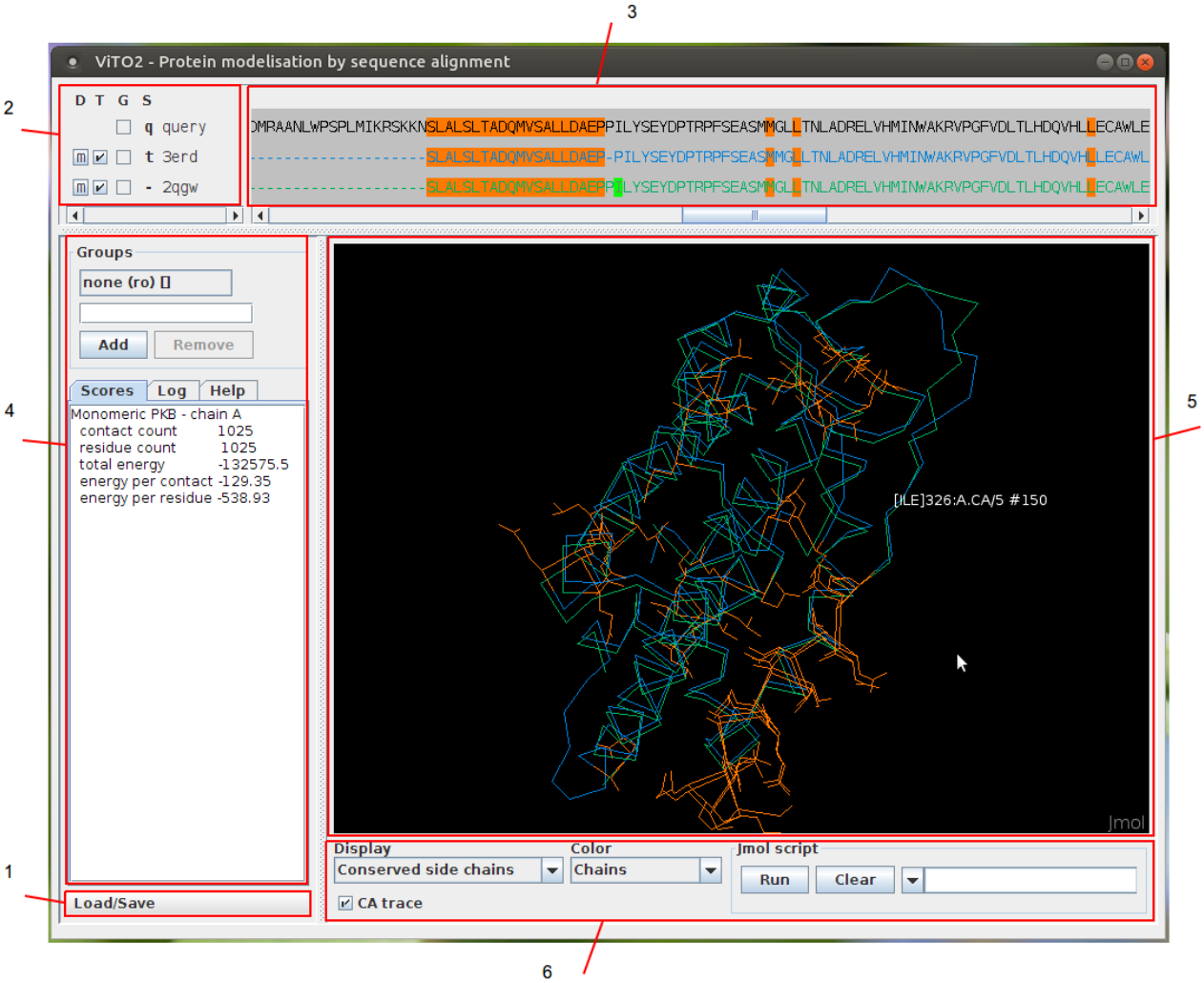
1 GUI version

1.1 Main window



Main window is divided in zones :

1. Load/save menu
2. Template/model selection, various flags
3. Alignment edition
4. Informations (threading scores, log, help)
5. Structures 3d representation
6. Display modes, Jmol console

1.2 Running

From desktop, double click on vito2_gui.jar in the installation directory.

Alternatively, from command line :

- either cd to the installation directory and run :
    - ./vito2-gui <alignment input file> (Linux/MacOsX)
    - .\vito2-gui <alignment input file> (Windows)
- or, if PATH variable has been configured, you can run the application from anywhere with :
    - vito2-gui <alignment input file> (Linux/MacOsX)
    - vito2-gui <alignment input file> (Windows)

1.3 Loading an alignment

Alignments are handled in Vito2 with PIR files which specify the aligned sequence of known proteins, their structure (referenced PDB structure) and the sequence to model (query/target).

An alignment can be loaded in two ways :

- from command line (see 1.2)
- from the menu

In any case, the associated PDB files must referenced by either an absolute path or being located in the same directory as the PIR file.

1.4 3D view

The central area (zone 6) displays selected template and models. It is based on Jmol, and all original commands are available here ; move/rotate/translate structures, menu, ...

Clicking on a residue displays its name and number in the chain, and selects the matching amino acid in the sequence view (zone 3).

1.5 Information area

In zone 4, various information tab are available :

- Scores : threading scores (see dedicated section of this guide)
- Log : event messages from the application
- Help : summary of the commands

1.6 Displaying templates and models

The top left area (zone 2) is organised in columns :

- D : for each sequence, if applicable, the template structure (« t »), the generated model (« m ») or nothing (« x ») is displayed in the 3D view (zone 6)
- T : use sequence in threading score (see threading lists)

- G : include sequence in current selection group
- S : sequence status : q = query, t = threading reference, m = model
- The last column is the sequence name in the PIR file

1.7 Modifying an alignment

Alignment is displayed in the top area (zone 3) and can be modified in the following ways :

- Move cursor : left/right/up/down arrows
- Insert indel : SPACE
- Remove indel : DEL
- Stick fragment to right neighbour : TAB
- Stick fragment to left neighbour : shift TAB
- Move fragment right : shift SPACE
- move fragment left : shift DEL

Depending on the template-or-model display mode (zone 2), the resulting protein model is updated after each sequence modification.

1.8 3D view modes

In zone 6 are available multiple visualisation modes for the 3D view :

- Chain modes :
  - Skeleton : no side chain shown .
  - Side chains under mouse : when pointing amino acids in the sequence view (zone 3), the matching side chain is shown in the 3d view.
  - Conserved side chains : only strictly conserved amino acids among all sequences of the alignment are shown (and also orange colored in the sequences).
  - All side chains : all side chains of all structures are displayed.

1.9 Threading scores

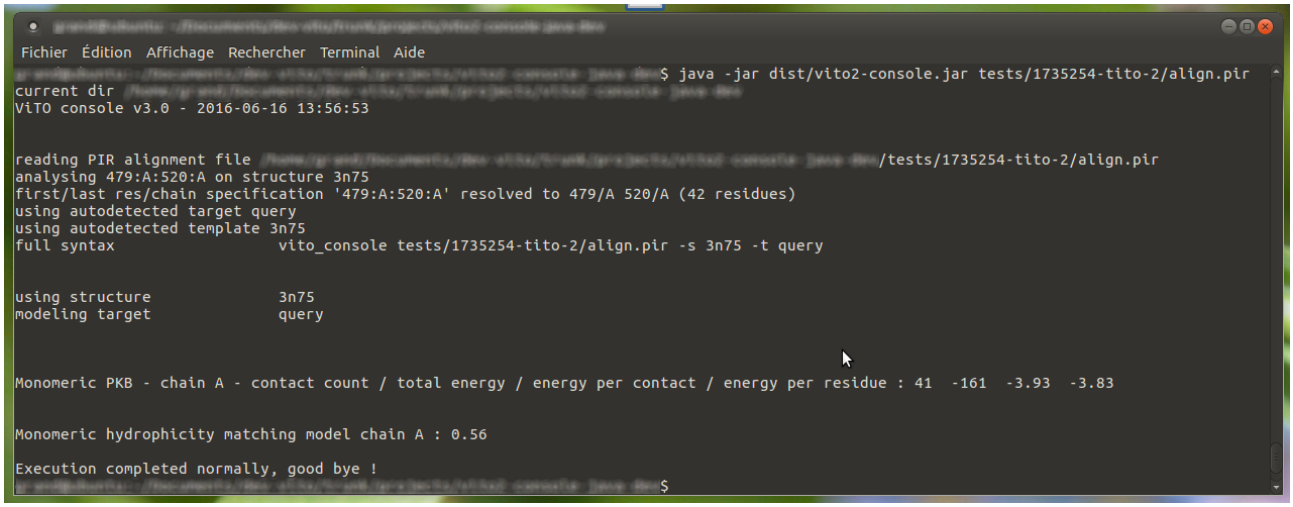
In order to evaluate the quality of the generated protein model, a PKB can be computed (and updated as you modify the alignment).

- In zone 2, right click on the name of a structure and select « Use as threading reference ». This will use this structure as the template used for the PKB score computation. The status (« S ») column will display a « t » on the structure line.

- In the same zone 2, modify the threading list (add/remove sequences) by clicking on toggles in the « T » column.
- In the information area (zone 4), if not already visible, select the « Scores » tab. As soon as at least one sequence is in the threading list, it will display various informations about threading score :
  - The number of contacts of the template (reference) structure,
  - the number of residues of the template,
  - the total contact energy,
  - the average contact energy,
  - the average residue energy.

2 Command line version

2.1 Screenshot



2.2 Running

From a console :

- either cd to the installation directory and run :
  - ./vito2-console <arguments> (Linux/MacOsX)
  - .\vito2-console <arguments> (Windows)
- or, if PATH variable has been configured, you can run the application from anywhere with :
  - vito2-console <arguments> (Linux/MacOsX)
  - vito2-console <arguments> (Windows)

Command syntax is (you can get it by simply running vito2-console with no argument) :

- vito2-console <PIR alignment file> [-t <arg>] [-s <arg>] [-w <arg>] [--p2d <arg>] [--warn] [-d]
    - -t,--target <arg> : name of sequence to model
    - -s,--support <arg> : template structure name
    - -w,--scwrl <arg> : generate SCWRL files (.pdb & .scw) with given base file name. If no argument is given, base will be <alignment name>-<target name>-<query name>
    - --p2d <arg> : read '2D structure prediction from 1D' file and output matching score with prediction from 3D structure
    - --warn : enable warning messages
    - -d,--debug : debug log message