

Protein Ligand Graph Computation in the VPLG Software

1 Graph definition and properties

A protein ligand graph in VPLG is a graph $G = (V, E)$ in which:

- each vertex $v \in V$ represents a secondary structure element (α -helix or β -strand) or a ligand
- an edge $(u, v) \in E$ between a vertex pair u, v means that u and v touch each other in the topology, i.e., several of their residues are in contact in 3D.

These graphs usually have between 15 and 50 vertices and the edge count is close to the vertex count. A visualization of such a graph (for PDB 7TIM, chain A), created with VPLG, is given below:

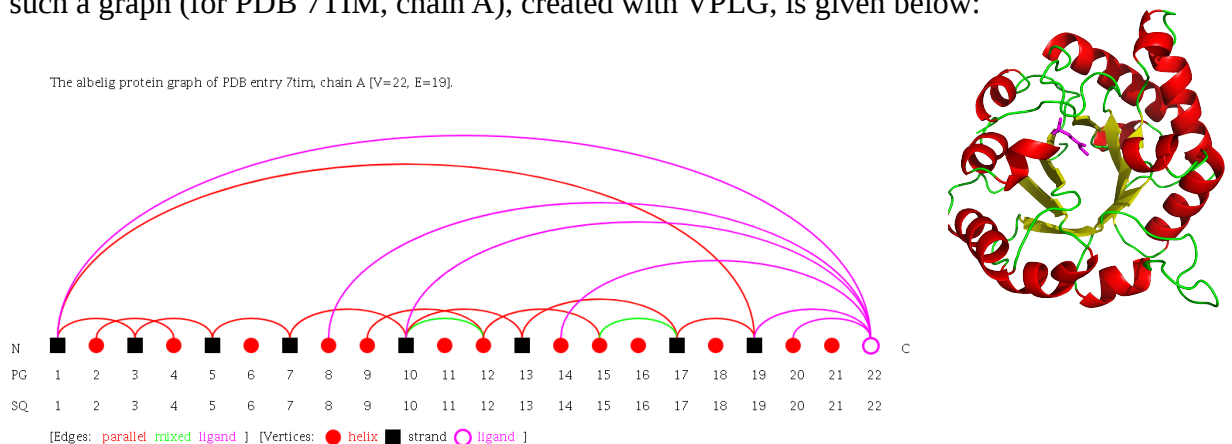


Fig. 1: Protein graphs. The albelig-graph of the β -chain of triosephosphate isomerase and its 3D structure. In the graph, the α -helices are shown as red circles and the β -strands as black squares. Ligands are represented by magenta circles. From left to right, the vertices are ordered by their position in the amino acid sequence. The arcs mark spatial contacts (red, parallel; blue, anti-parallel; green, mixed; magenta, ligand contact).

2 Graph computation

We compute these graphs from 3D atom coordinates obtained from PDB files (<http://www.rcsb.org/>) and the secondary structure assignments from the DSSP algorithm (<http://swift.cmbi.ru.nl/gv/dssp/>).

This involves the following steps:

1. Obtain sequence from PDB file
2. Obtain secondary structure assignments from DSSP file
3. Add ligand information from PDB file
4. Build graph: add a vertex for each SSE
5. Compute spatial contacts and add edges between SSEs

More details and literature references are available at / given in:

- The VPLG project website at <https://sourceforge.net/projects/vplg/>, see the Wiki
- The paper: Tim Schäfer, Patrick May and Ina Koch. *Computation and Visualization of Protein Topology Graphs Including Ligand Information*. German Conference on Bioinformatics 2012, available at <http://drops.dagstuhl.de/opus/volltexte/2012/3722>
- The slides of my talk at the GCB 2012, available at https://sourceforge.net/p/vplg/wiki/Talks_on_VPLG/attachment/gcb2012_talk_paper40_vplg.pdf