The Jena Library of Biological Macromolecules - JenaLib

www.fli-leibniz.de/IMAGE.html

R. Hühne, J. Sühnel
Biocomputing Group, Leibniz Institute for Age Research – Fritz Lipmann Institute,
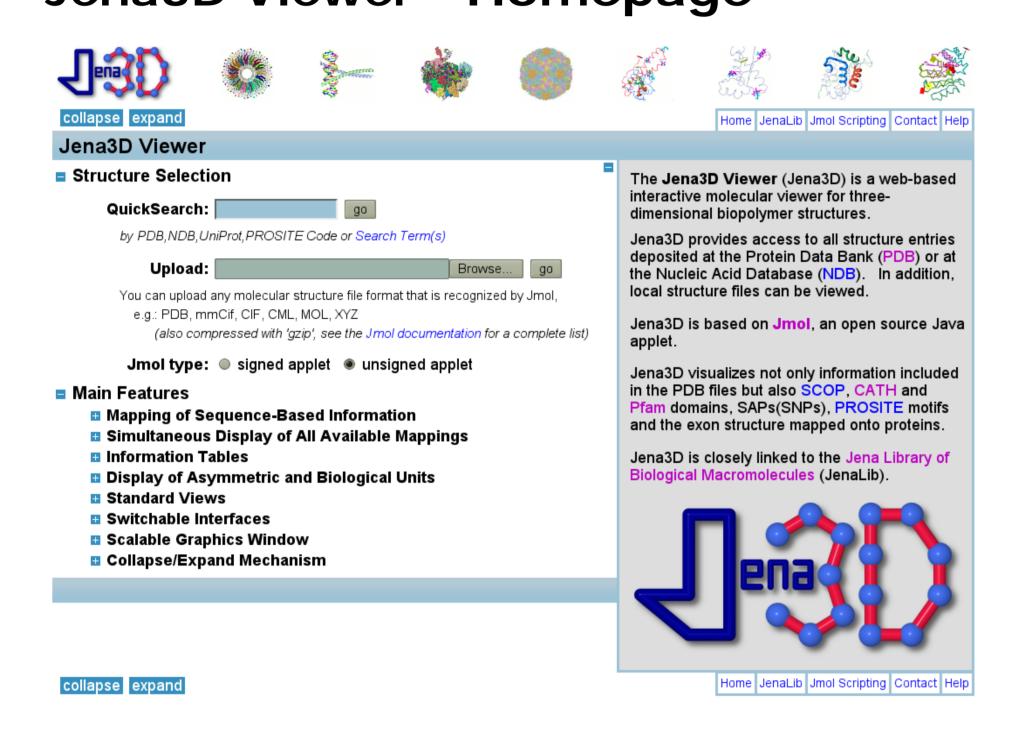Jena Centre for Bioinformatics, Jena / Germany

Introduction and Aim

The Jena Library of Biological Macromolecules (JenaLib) has served the scientific and educational communities since 1993. It is a freely accessible internet resource aimed at a better dissemination of information on three-dimensional biopolymer structures with an emphasis on visualization and analysis. It provides access to all structure entries at the Protein Data Bank (PDB) and the Nucleic Acid Database (NDB).

An automatized alignment between UniProt sequences and the sequences extracted from the PDB coordinates allows the mapping of any kind of sequence-based information onto 3D structures. Besides single amino acid polymorphisms (SAP) from the UniProtKB database and ProSite motifs also exon and exon-exon boundary information extracted from Ensembl and Pfam domains are mapped onto 3D structures.
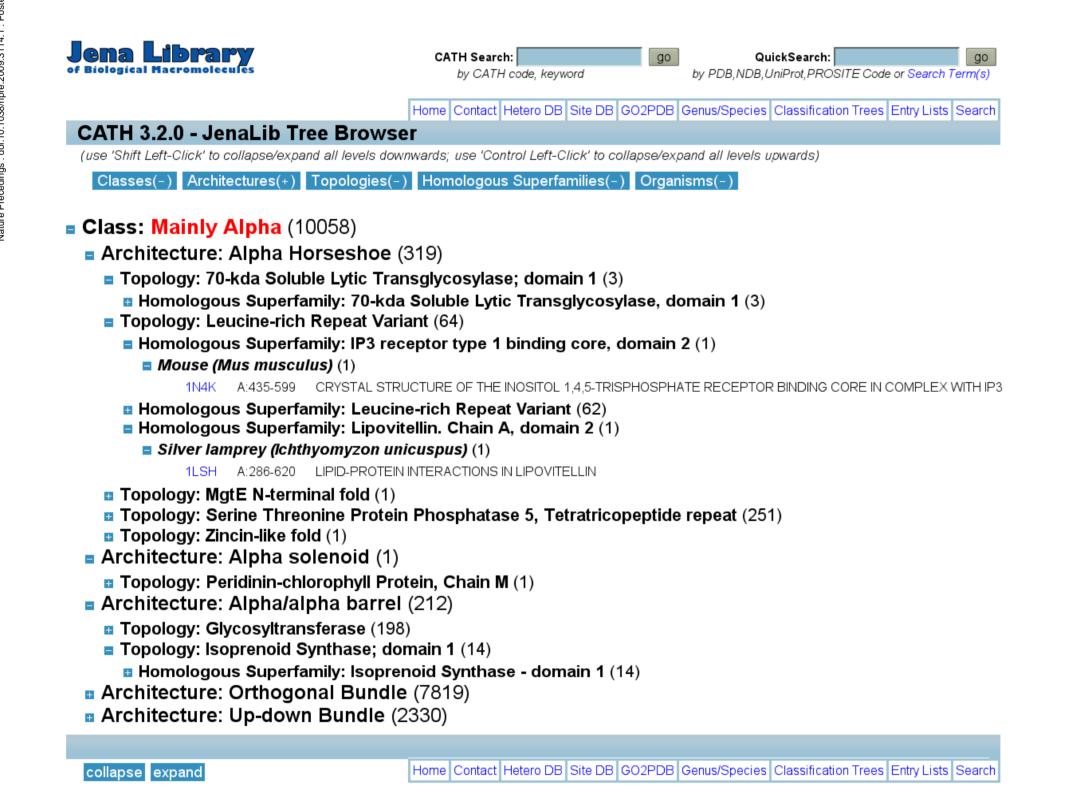
This information as well as SCOP and CATH domains and active sites and ligands can be visualized by the Jmol-based Jena3D viewer (jena3d.fli-leibniz.de). JenaLib offers a Google-like QickSearch option and allows the user-controlled generation of entry lists. Tree browsers facilitate the navigation through SCOP, CATH and Pfam hierarchical trees. Recently we have started to offer tools for the statistical analysis of structure sets, the determination of mean distances between amino acid Calpha atoms being the first example.

Selected Features
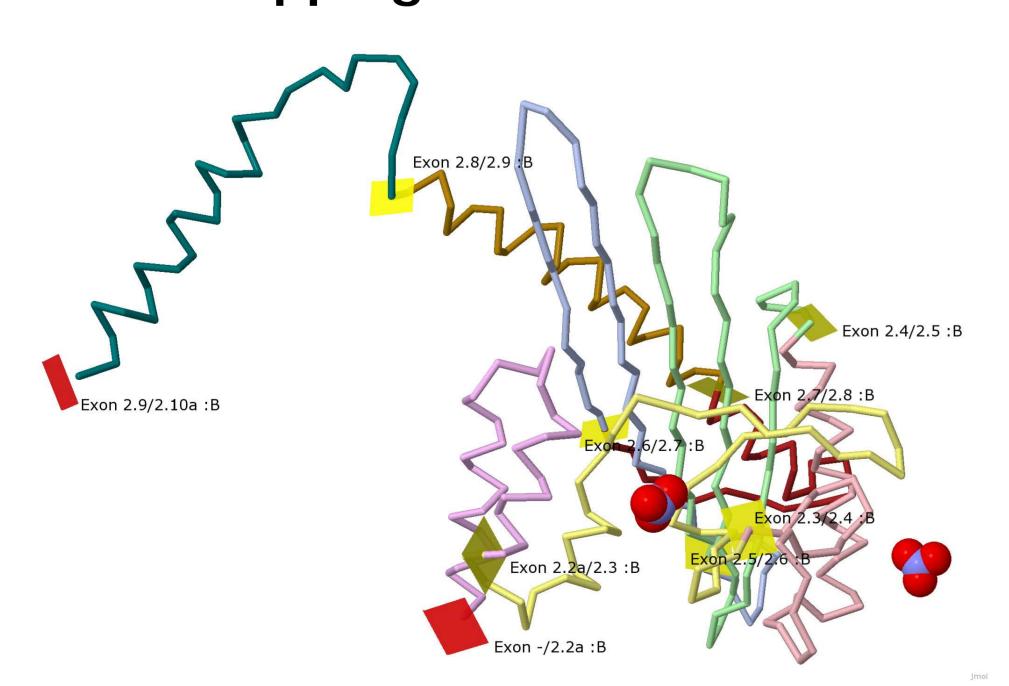
Jena3D Viewer - Homepage

Jena3D Viewer – Integrated Visualization

Heterodimeric structure of the human breast cancer tumor suppressor protein BRCA1 RING domain (chain A, blue) with the RING protein BARD1 (chain B, green); PDB entry 1JM7.
Left : complete viewer interface (HTML, Javascript, Jmol Java applet), partially collapsed
Right: information tables and visualization of chain A highlighting the following structural features
- Ligands (ZN; spacefilling representation) - PROSITE motifs (thick trace; tomato/purple-colored)
- Exon boundaries (yellow planes) - SCOP domain (blue grid)
- SAPs from UniProtKB/CancerSNP (amino acid sidechains; wt – magenta, mutated – cyan)

Classification Tree Browser

CATH class ´Mainly Alpha´ shown in the JenaLib classification tree browser (mainly collapsed).

Sequence/Alignment View – Data Integration

The alignment view of PDB entry 1JM7 is shown. The integrated display of structural features like SCOP domains, SAPs, ProSite motifs (activated here) can be controlled individually.
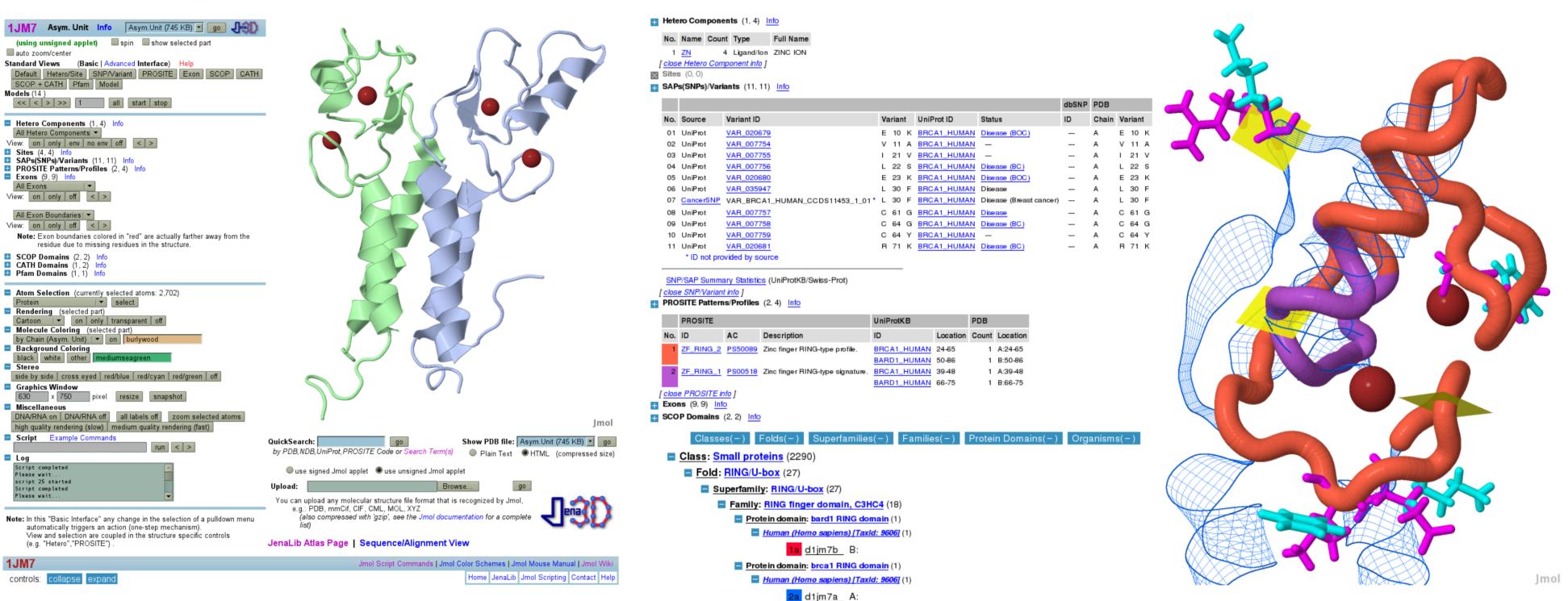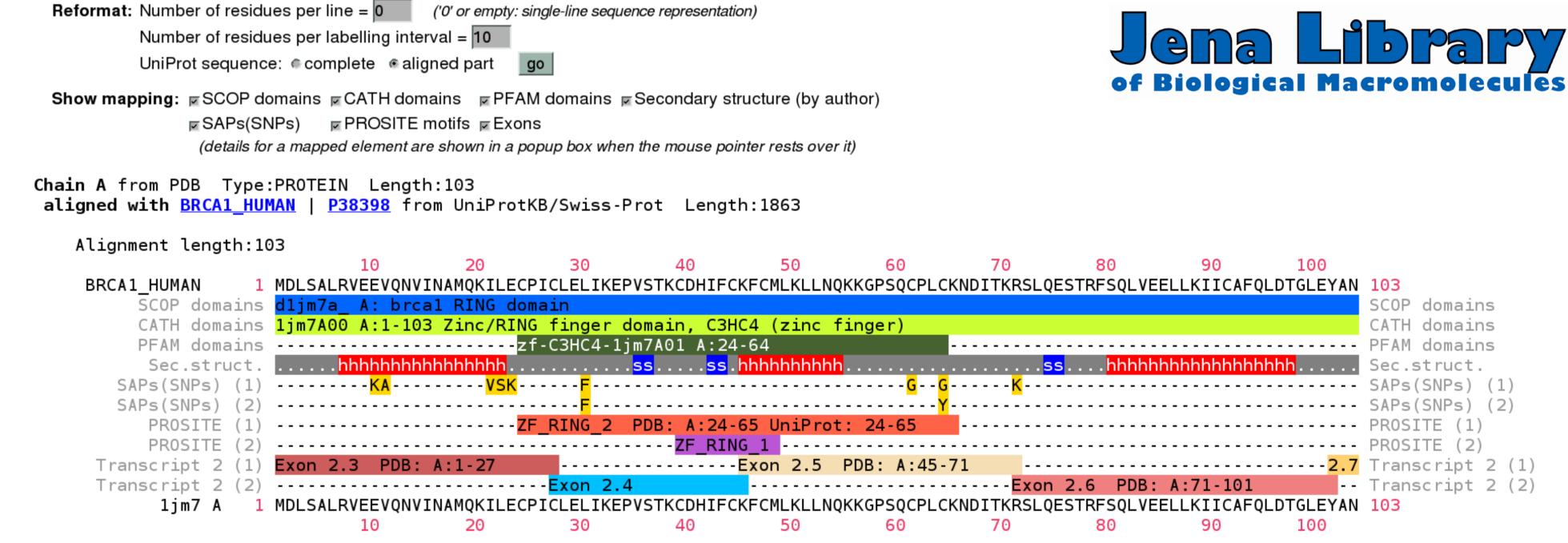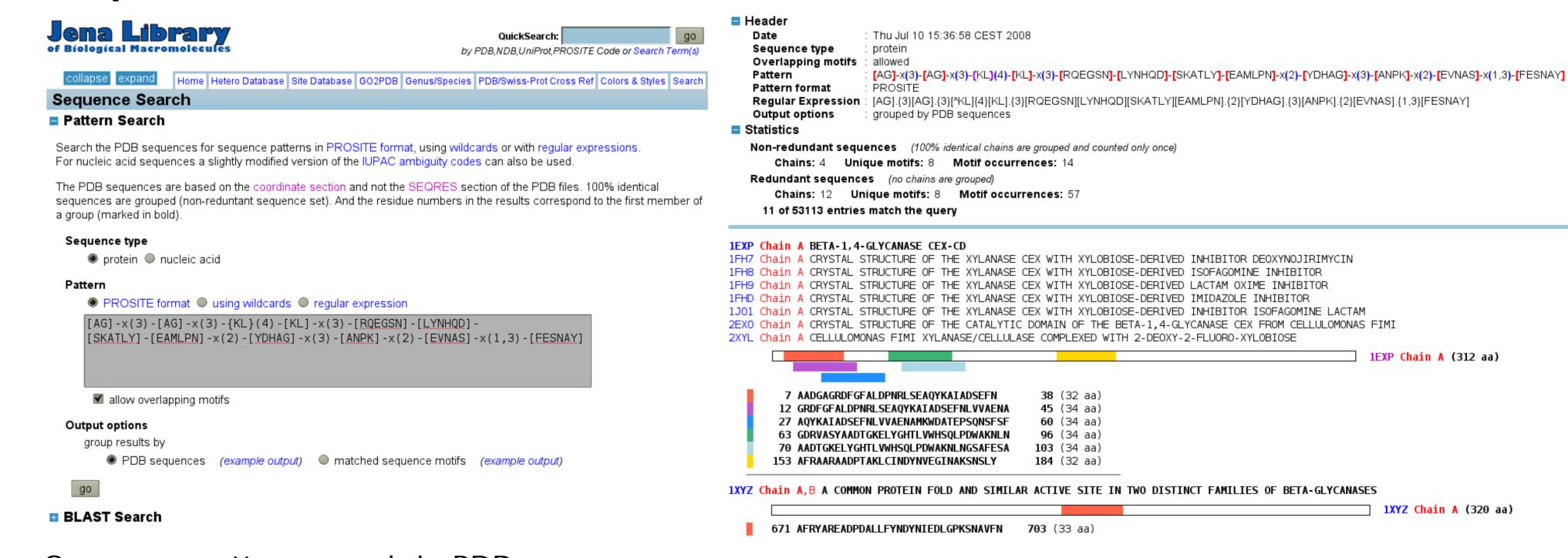
Exon Mapping and Visualization

Visualization of exons mapped to PDB entry 1IZN in the JenaLib Jmol Viewer (based on ENSEMBL/UniProt information).
Chain B is colored by exon and the exon boundaries are marked by planes (red color indicates missing residues).

Sequence Pattern Search – Protein/Nucleic Acid

Sequence pattern search in PDB sequences.
100% identical sequences are grouped (non-redundant set).
Left: input form
Right: example output (incomplete)

[1] J. Reichert, J. Sühnel. The IMB Jena Image Library of Biological Macromolecules - 2002 Update. *Nucleic Acids Research,* **2002**, 30, 253-
[2] R. Hühne, F-T. Koch, J. Sühnel. A comparative view at comprehensive information resources on three-dimensional structures of biological macromolecules. *Briefings in Functional Genomics & Proteomics,* **2007**, 6, 220-239.