



## Protein Structure Database and Visualization System

- **Macromolecular Repository**
- **Data Visualization and Analysis**
- **Browser Interface for Search and Retrieval**
- **3D Ligand: Receptor and Pocket Similarity**
- **Protein Structure Alignment**
- **Data Standardization and Annotation**
- **Standard IT Infrastructure and Integration**



Chemical  
Computing  
Group

PSILO® is a database system that provides a consolidated repository for macromolecular and protein-ligand structural information. It offers research organizations a means to systematically track, register and share both experimental and computational structural data. A web-browser interface facilitates the search, visualization and analysis of public and private structural data.

[chemcomp.com](http://chemcomp.com)

# Protein Structure Database and Visualization System

## Macromolecular Repository

- Store Coordinate and Structure Factor Data
- Save Auxiliary Files alongside Original Data
- Fully RCSB-Compliant PDB, mmCIF, and XML Formats
- Bulk Import Script for Larger Datasets
- Web Interface for Individual Record Deposit

## Data Visualization and Analysis

- Visualize Structures and Electron Densities
- Visualize Structures Aligned by Ligand, Pocket or Protein
- 2D Ligand Interaction Diagrams Linked to the 3D Viewer
- Analyze, Plot, and Sort 3D Query Statistics
- BLAST Search Phylogenetic Tree, Interactive Alignment

## Browser Interface for Search and Retrieval

- Google-Like Queries with Multiple Search Criteria
- Standard Sketchers for Substructure and 3D Queries
- Download Hits as PDB, mmCIF, XML, MDB
- 2D and 3D Active Site Visualization
- Filter for Similar or Duplicate Records

## 3D Ligand: Receptor and Pocket Similarity

- 3D Pocket Similarity Search
- 3D Domain Motif Search
- Ligand:Receptor 3D Geometry Using Standard Sketchers
- Multi-Criteria Search, including Text, 2D Query
- Automatic Detection of Ligand-Independent Pockets

## Protein Structure Superposition

- Optimized Structure Superposition
- Superpose on Pre-Defined Pocket Residues
- 3D Query Superposition
- Overlay Based on Protein Family Reference Alignment
- Rigid-Body Ligand Superposition

## Automated Data Standardization and Annotation

- Bioinformatics Annotations (GO, SCOP, Etc.)
- Standard Orientations for Related Structures
- Mirroring of the RCSB for Weekly Updates
- Geometric Data Quality Assessment
- Maintenance of Popular Protein Families

## Standard IT Infrastructure and Integration

- Simple to Maintain and Deploy IT Infrastructure
- Integrate with External/Internal Databases and Software
- Source Code Provided for Customization
- Group-Based Permission System
- Version Control

# PSILO

