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# OPMxplore

— Sinduja, David and Felcy —

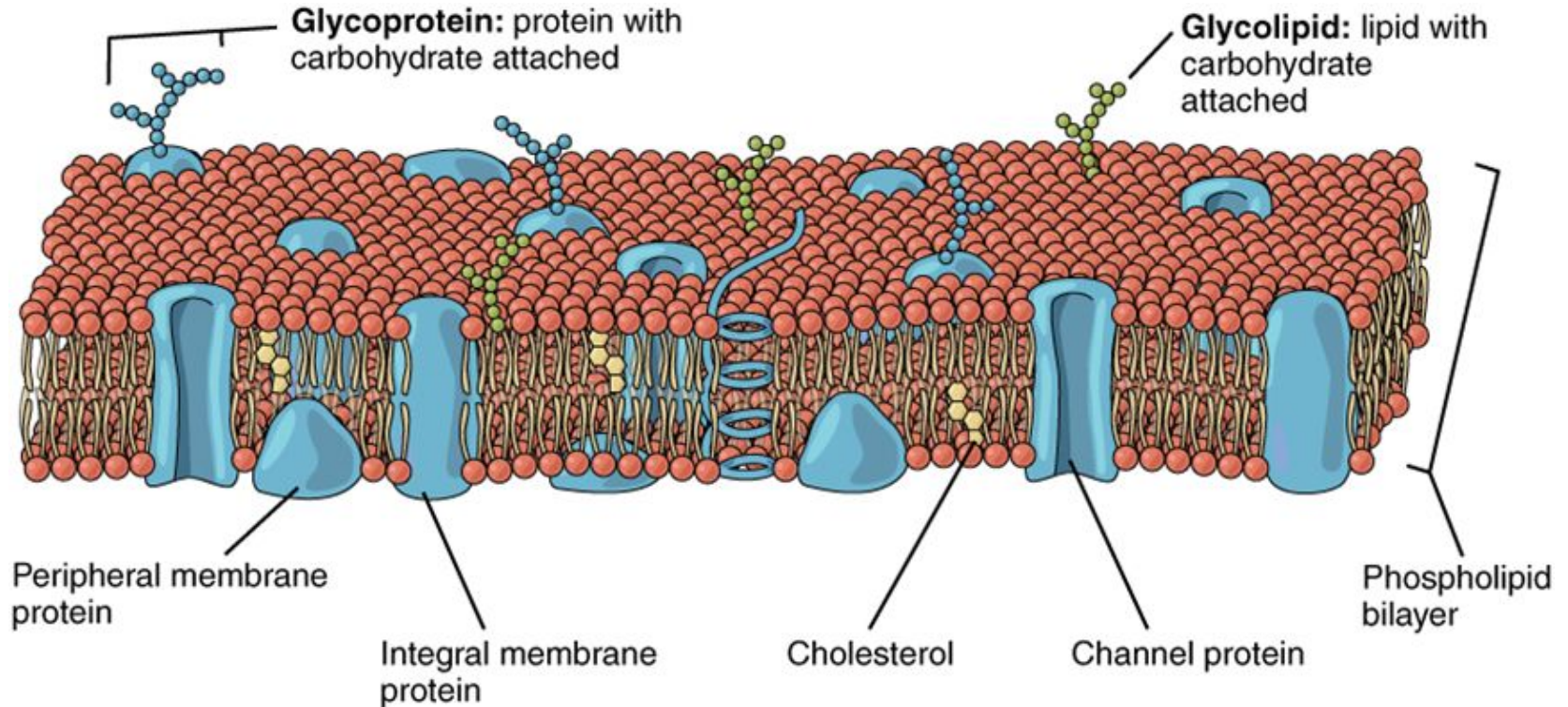
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# Agenda


- Background
- Mission statement
- Data
- Project Structure
- Users and Use Cases
- Design
- Demo
- Lessons learned and future work

# Background


# Membrane Proteins



# Protein Data Bank



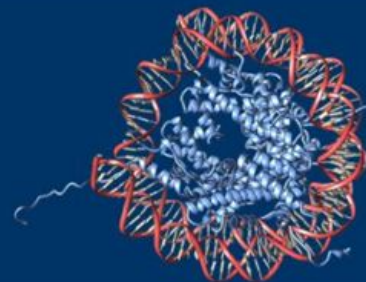
WORLDWIDE  
PDB  
PROTEIN DATA BANK


VALIDATION ▾ DEPOSITION ▾ DATA DICTIONARIES ▾ DOCUMENTATION ▾ TASK FORCES ▾ STATISTICS ▾ ABOUT ▾  wwPDB Foundation


Since 1971, the Protein Data Bank archive (PDB) has served as the single repository of information about the 3D structures of proteins, nucleic acids, and complex assemblies.


The Worldwide PDB (wwPDB) organization manages the PDB archive and ensures that the PDB is freely and publicly available to the global community.

Learn more about PDB **HISTORY** and **FUTURE**.



**Validate Structure**  
or View validation reports

**Deposit Structure**  
All Deposition Resources

**Download Archive**  
Instructions

**Vision and Mission**

**Vision**

Sustain a freely accessible, single global archive of experimentally determined structure data for biological macromolecules as an enduring public good.

**Mission**

- Ensure open access to public domain experimentally determined structural biology data.
- Provide expert deposition, validation, and biocuration services at no charge to Data Depositors.
- Enable universal access for expert and non-expert Data Consumers with no limitations on usage.
- Manage the PDB archive as a public good according to the FAIR Principles.
- Lead the world in structural biology data representation, exchange, and visualization.

**wwPDB Resources**

**Data Dictionaries**

- › **Macromolecular Dictionary (PDBx/mmCIF)**
- › **Small Molecule Dictionary (CCD)**
- › **Peptide-like antibiotic and inhibitor molecules (BIRD)**

**Annotation**

- › **Procedures and policies**
- › **Improvements for consistency and accuracy**


**Community Input:**  
**Task Forces and Working Groups**

- › **Validation Task Forces (X-ray, NMR, 3DEM)**
- › **Small Angle Scattering Task Force**
- › **PDB/mmCIF Working Group**
- › **Hybrid/Integrative Methods Task Force**

**News & Announcements**

**12/01/2017**

› **Overview of PDB Validation Reports published in *Structure***



The **paper** (doi: **10.1016/j.str.2017.10.009**) describes how validation reports for PDB structures determined by X-ray crystallography were first made available to depositors in **2013** and added to the PDB archive in **2014**. In early 2016, following the **update of the OneDep system**, reports for structures solved by nuclear magnetic resonance

# Orientation of Membrane Proteins

← → ↻ opm.phar.umich.edu

orientations of (OPM) database  
proteins in membranes

HOME ABOUT OPM DOWNLOAD OPM FILES CONTACT US PPM SERVER LIPID COMPOSITION ATLAS

**Protein Classification**

- Types (3 types)
- Classes (11 classes)
- Superfamilies (474 superfamilies)
- Families (884 families)
- Species (745 species)
- Localization (24 types)
- All proteins in OPM (3622 proteins)

**Protein Links**

PDB Sum, PDB, OCA, MPKS, PDBTM, MPDB, CGDB

**PPM Server**

**Orientations of Proteins in Membranes (OPM) database**

OPM provides spatial arrangements of membrane proteins with respect to the hydrocarbon core of the lipid bilayer.

OPM includes all unique experimental structures of transmembrane proteins and some peripheral proteins and membrane-active peptides ([features](#)).

Each protein is positioned in a lipid bilayer of adjustable thickness by minimizing its transfer energy from water to the membrane ([Methods](#)).

OPM provides structural classification and sorting according to different criteria ([Classification](#)).

Our calculations are in agreement with experimental studies of 24 transmembrane and 39 peripheral peptides and proteins ([Comparison with Experiments](#)).

[For more information on single-spanning transmembrane proteins please see our Membranome database](#)

**In citing the Orientations of Proteins in Membranes (OPM) database please refer to**

Lomize MA, Pogozheva ID, Joo H., Mosberg HI, Lomize AL (2012) OPM database and PPM web server: resources for positioning of proteins in membranes. *Nucleic Acids Res.* **40** (Database issue), D370-D376. [PDF](#) [PubMed](#)

**For an explanation of our method please refer to**

Lomize AL, Pogozheva ID, Lomize MA, Mosberg HI (2006) Positioning of proteins in membranes: A computational approach. *Protein Science* **15**, 1318-1333. [PDF](#) [PubMed](#)

**For a new version of our method please refer to**

Lomize AL, Pogozheva ID, Mosberg HI (2011) Anisotropic solvent model of the lipid bilayer. 2. Energetics of insertion of small molecules, peptides, and proteins in membranes. *J Chem Inf Model* **51**, 930-946. [PDF](#) [PDF \(supplementary\)](#) [PubMed](#)

**For more information on peripheral proteins please refer to**

Lomize AL, Pogozheva ID, Lomize MA, Mosberg HI (2007) The role of hydrophobic interactions in positioning of peripheral proteins in membranes. *BMC Struct Biol* **7**, 44. [PDF](#) [PubMed](#)

**Questions**

**1. Calculate orientation for unreleased structure or membrane protein was not in OPM?**

Please use our [web server](#) or we can process your coordinates through email ([almz@umich.edu](mailto:almz@umich.edu)). All information is kept confidential. Orientation of membrane protein cannot be predicted if all its membrane-anchoring elements are missing or disordered.

**2. Errors in orientation or experimental verification description?**

Please [contact us](#).

834,610 unique visits since Dec, 2005  
[View OPM visitor statistics](#)


OPM was funded by the National Science Foundation (NSF)

UNIVERSITY OF MICHIGAN | COLLEGE OF PHARMACY | LOMIZE GROUP

PDB ID or protein name

4y7i » Myotubularin-related protein 8, dimer

[See all membrane protein images in OPM](#)



# Mission Statement

**Develop tools to explore the OPM website through custom/generic user searches**

# DATA

1. PDB (master archive of proteins)
2. OPM dataset (3622 membrane proteins)



# Project Structure



# Functional Specification

# User and Use Cases

# Environment

# Design

# Components

# Demo 1



# Demo 2

# Lessons learned and Future Work

**Thanks!**