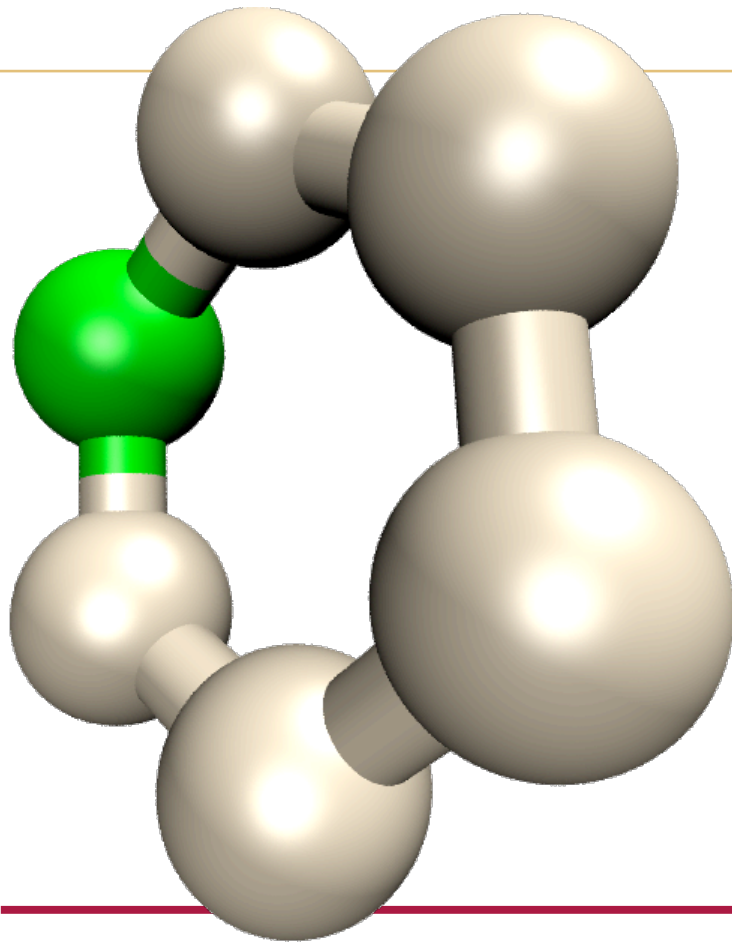


Using OpenMM Zephyr

February 2009
Christopher Bruns

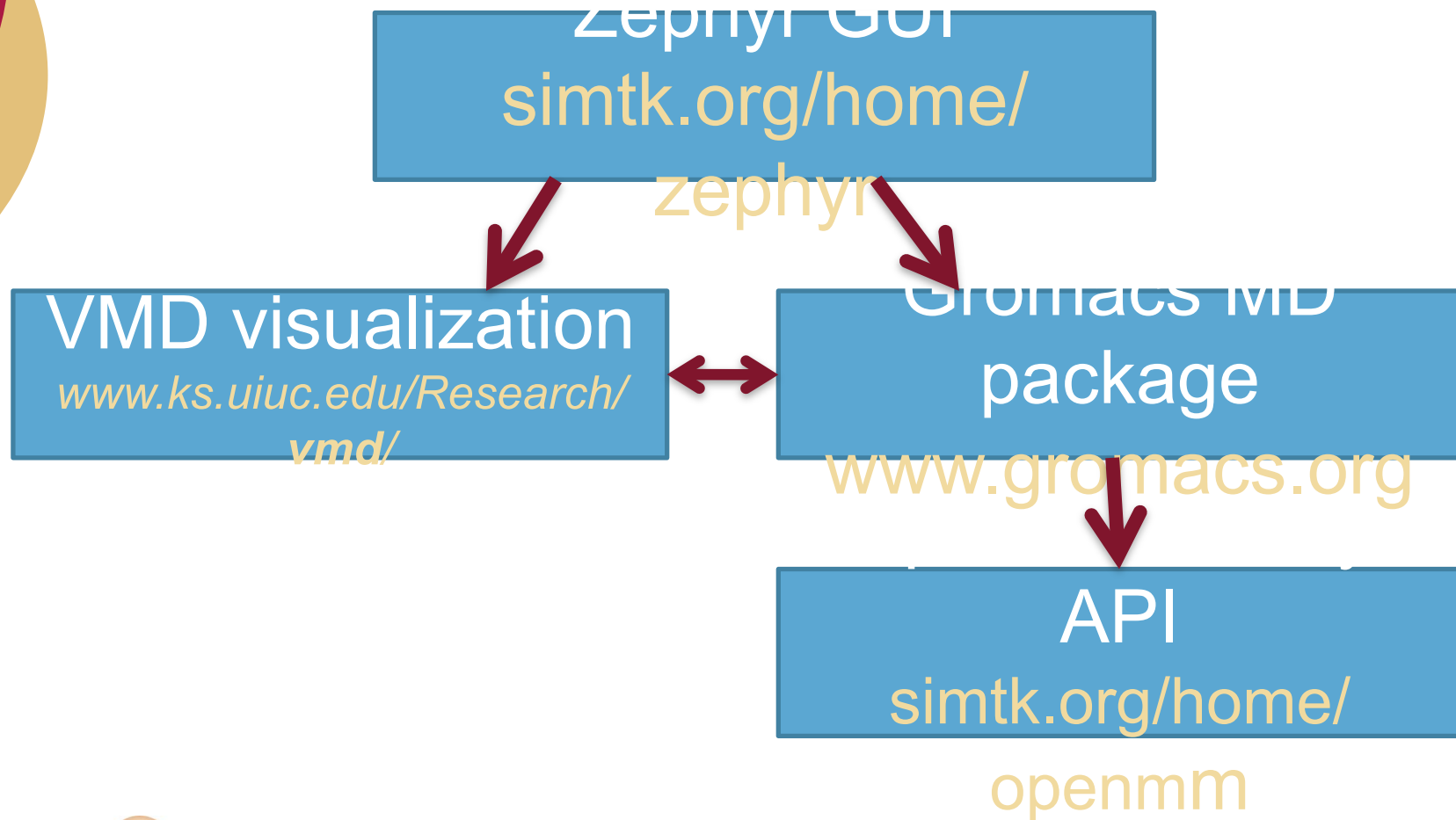




What is OpenMM Zephyr?

- Graphical user interface for running GPU accelerated molecular dynamics simulations
- Automates running of gromacs programs
 - <http://www.gromacs.org/>
- Discoverable interface

Zephyr is a GUI layer on OpenMM, Gromacs, and VMD



Introductory Demonstration

Running OpenMM Zephyr : alanylalanine_capped.pdb

OpenMM Zephyr

Molecules Parameters Status: Running VMD console About

Simulation running...

0.100 picoseconds simulated (of 100.000 total)
Elapsed lab time 2.8s
Calculating time remaining...

gromacs output :

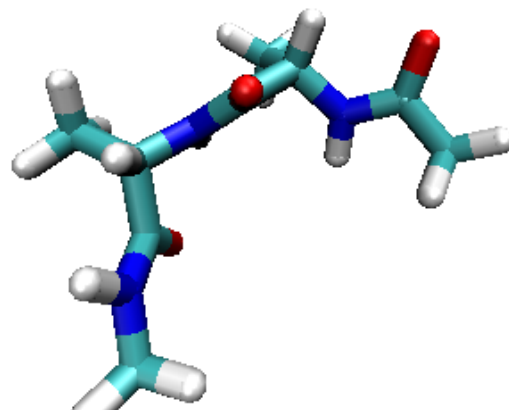
```
Started mdrun on node 0 Mon Feb 02 21:19:58 2009
```

Step	Time	Lambda
1	0.00200	0.00000
50	0.10000	0.00000

Waiting for IMD socket connection to VMD on port 3000...
Waiting for IMD socket connection to VMD on port 3000...
Waiting for IMD socket connection to VMD on port 3000...

< Parameters Cancel

VMD 1.8.6 OpenGL Display



VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	alanylalanine_capped_p_32	32	757	0

756 zoom Loop step 1 speed



Zephyr Community Resources

○ Sign up for “OpenMM Zephyr News” mailing list

● https://simtk.org/mail/?group_id=352

○ OpenMM Zephyr forums

● https://simtk.org/forum/?group_id=352

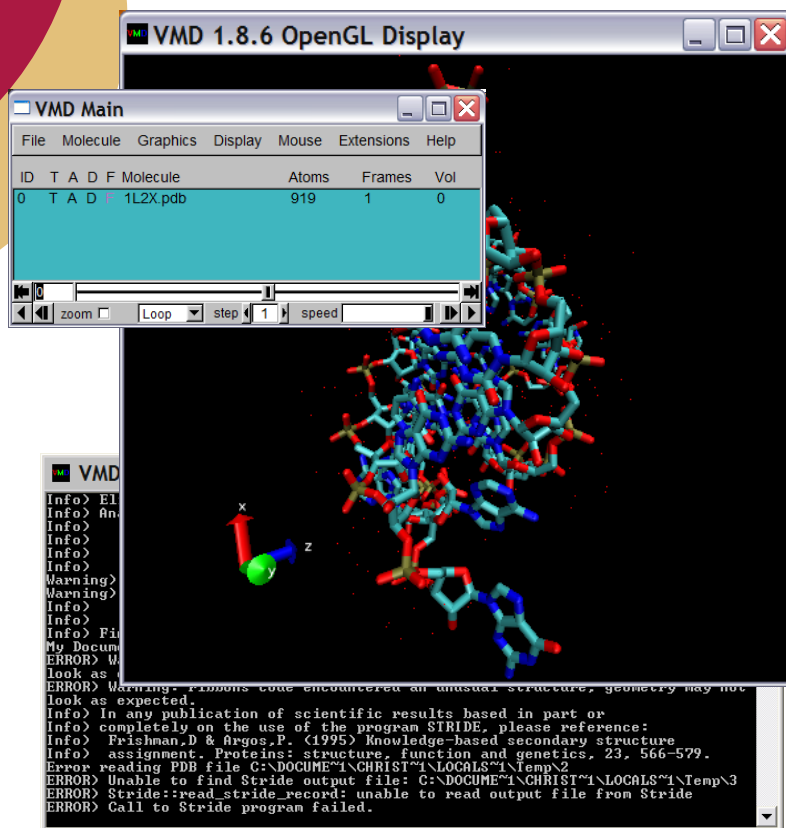


Current Zephyr Restrictions

- Windows XP or Vista
- 32 bit
- Implicit solvent only
- Amber96 force field only
- Standard protein/RNA/DNA molecules only
- For GPU accelerated dynamics:
 - must have supported GPU and drivers

VMD Molecular Graphics Viewer

<http://www.ks.uiuc.edu/Research/vmd/>

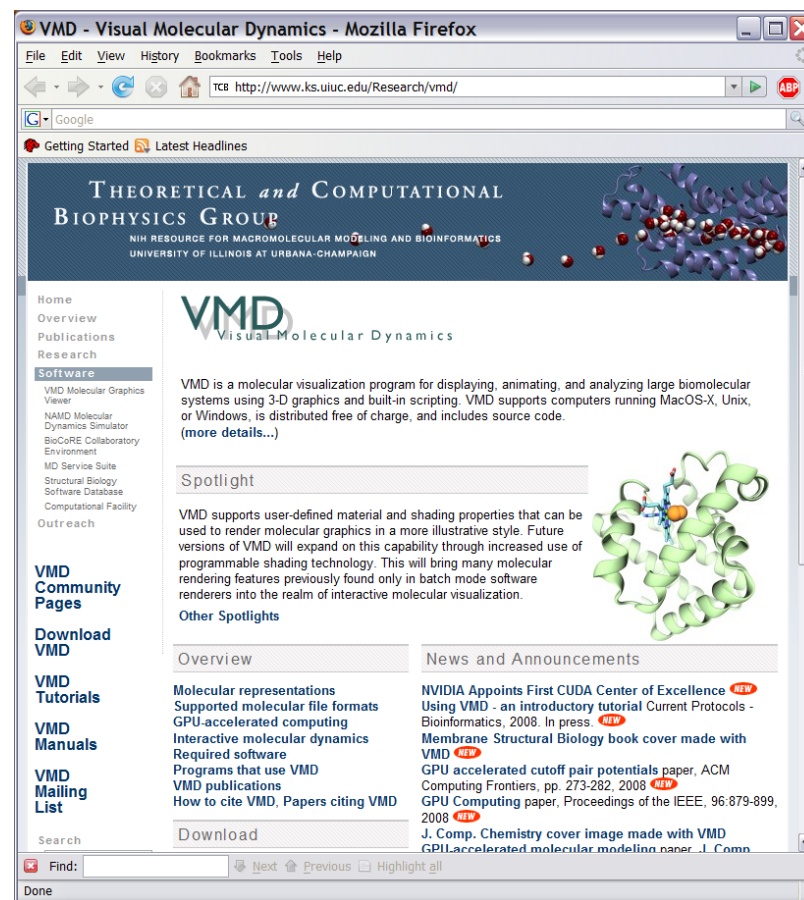


The screenshot shows the VMD 1.8.6 OpenGL Display window. The main window displays a 3D molecular structure of a protein, rendered in a stick representation with atoms colored by element (carbon in light blue, oxygen in red, nitrogen in blue). A smaller window titled "VMD Main" is overlaid on top, showing a table of loaded molecules:

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	1L2X.pdb	919	1	0

Below the table, there are controls for zoom, loop, step, and speed. In the bottom-left corner, a console window displays the following error messages:

```
Info> El
Info> An
Info>
Info>
Info>
Info>
Warning>
Warning>
Info>
Info>
Info> Fi
My Docum
ERROR> W
look as
ERROR> Warning: Ribbons code encountered an unusual structure, geometry may not
look as expected.
Info> In any publication of scientific results based in part or
Info> completely on the use of the program STRIDE, please reference:
Info> Frishman,D & Argos,P. (1995) Knowledge-based secondary structure
Info> assignment. Proteins: structure, function and genetics. 23, 566-579.
Error reading PDB file C:\DOCUME~1\CHRIST~1\LOCALS~1\Temp\2
ERROR> Unable to find Stride output file: C:\DOCUME~1\CHRIST~1\LOCALS~1\Temp\3
ERROR> Stride::read_stride_record: unable to read output file from Stride
ERROR> Call to Stride program failed.
```



The screenshot shows the VMD website in a Mozilla Firefox browser window. The website is titled "THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP" and is a NIH resource for macromolecular modeling and bioinformatics at the University of Illinois at Urbana-Champaign. The main content area features the VMD logo and a description of the software:

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS-X, Unix, or Windows, is distributed free of charge, and includes source code. (more details...)

The website also includes a "Spotlight" section with a 3D ribbon diagram of a protein structure and a "News and Announcements" section with several recent updates, including "NVIDIA Appoints First CUDA Center of Excellence" and "Membrane Structural Biology book cover made with VMD".

Downloading Zephyr



The screenshot shows a Mozilla Firefox browser window displaying the SimTK website. The page is titled "OpenMM Zephyr Downloads". A mouse cursor is pointing to the download link "InstallZephyr-0.3.1-win32.exe (7534 kB)".

Overview
Team
Downloads
Advanced

Downloads & Source Code
[OpenMM Zephyr](#)
[Additional GPL source code](#)

This project also makes [source code](#) available.

OpenMM Zephyr Downloads

OpenMM Zephyr
Graphical user interface for running OpenMM version of Gromacs. To install Zephyr, you need to have Tcl/TK installed first. To use Zephyr's visualization capabilities, you will also need to install VMD (optional but recommended).

Zephyr 0.3
January 30, 2009
[Notes](#)

Download Links

Name	File Type	Platform	Updated
Programs used by Zephyr -- Install First			
Tcl/TK (URL) <i>Description: Link to download Tcl/TK. Version 8.5 is needed to run OpenMM Zephyr.</i>	binary	Any	Jan 30, 2009
VMD (URL) <i>Description: Link to molecular visualization program VMD. Required by Zephyr for visualizing simulation results.</i>	binary	Any	Jan 30, 2009
OpenMM Zephyr InstallZephyr-0.3.1-win32.exe (7534 kB) <i>Description: Please install in a directory with no space characters</i>	binary	Windows	Jan 30, 2009

[List all previous releases](#)

Additional GPL source code



Install in a Folder with no space characters

- Install in “C:\Zephyr”
- NOT “Program Files”
- NOT “My Documents”
- Issue with this version of gromacs
- No spaces in the entire path

Either:

A: Run these gromacs programs

OR B: Click "Simulate" button in Zephyr

INPUT:

PDB structure file

.pdb

force field parameters

pdb2gm

.top

.gro

editconf

.top

minimize energy

grompp

.tpr

mdrun

.gro

simulation parameters

.mdp

grompp

.tpr

GBSA parameters

.agb

mdrun

.pdb

.trr

OUTPUT: structure and trajectory

INPUT:

PDB structure file

.pdb

Simulate


.pdb

.trr

OUTPUT: structure and trajectory

Simulation Parameters

(Idle) OpenMM Zephyr : alanylalanine_capped.pdb

 OpenMM Zephyr

Molecules Parameters (Idle) VMD console About

Prepare simulation

How long to simulate
100.0 ps 50000 steps 0.002 ps/step

Temperature
room 22.00 °C 295.15 K 71.6 °F Force field
Amber96

Minimize energy before dynamic simulation

Simulation hardware: CPU OpenMM ref.

Live viewing in VMD
 View simulation live in VMD every 0.1 ps 50 steps
Socket for coordinates: 3000 for commands: 3001

Save trajectory frames
every 2.0 ps 1000 steps

< Back Simulate



Example: villin head piece

- based on PDB structure 1vii
- GPU acceleration
- VMD update frequency
- VMD representation



Example: RNA

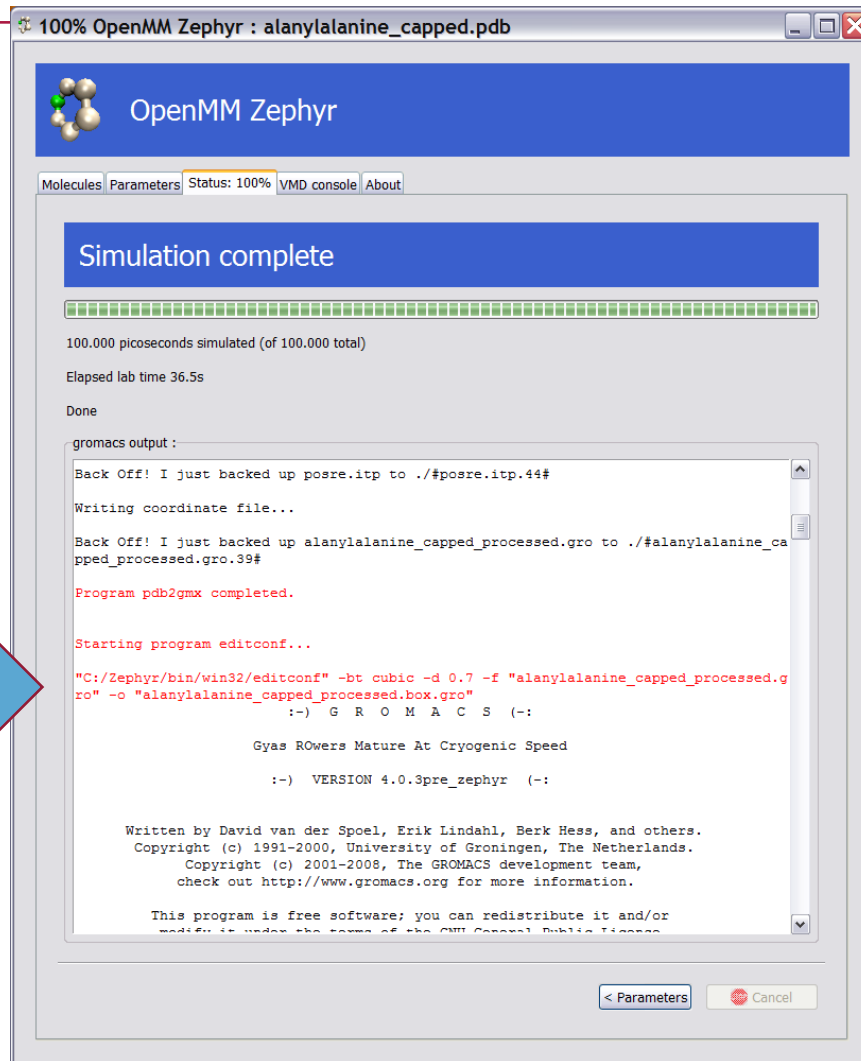
- gcaa.pdb file of RNA duplex
- Investigate gromacs commands
- Save output from VMD



Saving output

- trajectory and coordinate files in simulation folder
- save from VMD

Read the red lines to learn to run Gromacs-OpenMM on the command line



The screenshot shows the OpenMM Zephyr application window titled "100% OpenMM Zephyr : alanylalanine_capped.pdb". The interface includes a blue header with the OpenMM Zephyr logo and name, and a menu bar with "Molecules", "Parameters", "Status: 100%", "VMD console", and "About". A blue banner reads "Simulation complete" above a green progress bar. Below the progress bar, it states "100.000 picoseconds simulated (of 100.000 total)" and "Elapsed lab time 36.5s". The "Done" status is shown above a terminal window titled "gromacs output :". The terminal output contains the following text:

```
Back Off! I just backed up posre.itp to ./#posre.itp.44#
Writing coordinate file...
Back Off! I just backed up alanylalanine_capped_processed.gro to ./#alanylalanine_capped_processed.gro.39#
Program pdb2gmx completed.
Starting program editconf...
"C:/Zephyr/bin/win32/editconf" -bt cubic -d 0.7 -f "alanylalanine_capped_processed.gro" -o "alanylalanine_capped_processed.box.gro"
      (-) G R O M A C S (-)
      Gys R0wers Mature At Cryogenic Speed
      (-) VERSION 4.0.3pre_zephyr (-)

Written by David van der Spoel, Erik Lindahl, Berk Hess, and others.
Copyright (c) 1991-2000, University of Groningen, The Netherlands.
Copyright (c) 2001-2008, The GROMACS development team,
check out http://www.gromacs.org for more information.

This program is free software; you can redistribute it and/or
modify it under the terms of the GNU General Public License
```

A large blue arrow points from the left towards the terminal output area.



Time Scales in Molecular Mechanics

femtosecond	10^{-15} second	bond vibration
picosecond	10^{-12} second	side chain motion
nanosecond	10^{-9} second	protein tumbling
microsecond	10^{-6} second	helix/coil transition
millisecond	10^{-3} second	protein folding
second	10^0 second	protein synthesis

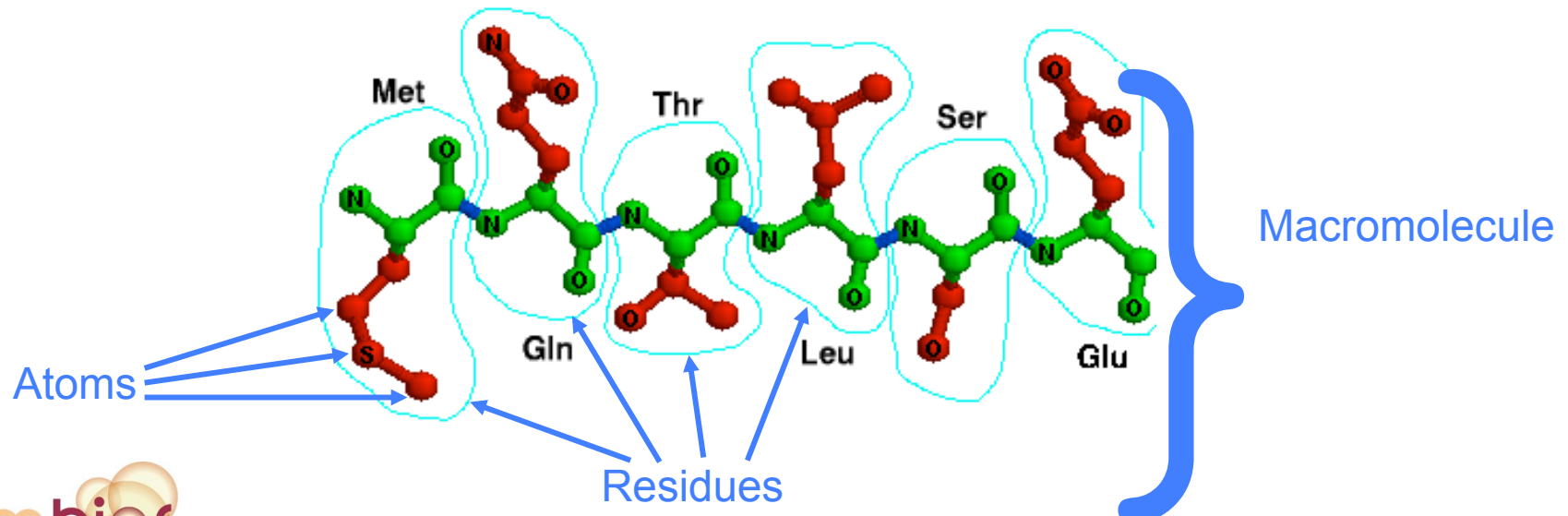


Example: polyalanine

- viscosity

Macromolecules, residues, and atoms

- RNA, DNA, and protein are large molecules called *macromolecules*
- Macromolecules consist of chains of *residues*



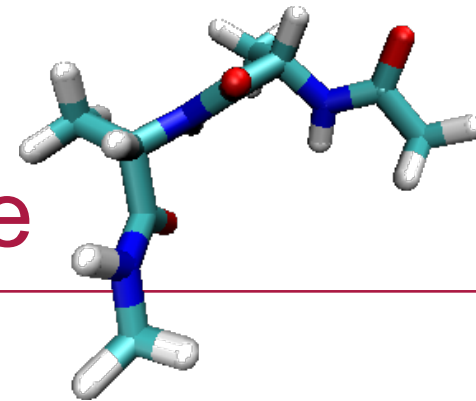


PDB File format

- Text format: humans can read it too
- Most of the information is atomic coordinates
- PDB files usually contain multiple molecules, including water molecules

```
...  
ATOM 1751 N GLY C 250 32.286 1.882 43.206 1.00 22.00  
ATOM 1752 CA GLY C 250 32.365 1.086 41.969 1.00 21.39  
ATOM 1753 C GLY C 250 31.538 1.735 40.864 1.00 20.79  
ATOM 1754 O GLY C 250 30.621 2.527 41.152 1.00 21.58  
...
```

Example: alanylalanine



	atom name	residue name	residue number	x	y	z			
ATOM	1	CH3 ACE A	1	22.028	8.496	12.678	1.00	21.24	C
ATOM	2	C ACE A	1	20.512	8.634	12.719	1.00	24.01	C
ATOM	3	O ACE A	1	19.827	7.940	13.456	1.00	25.32	O
ATOM	4	N ALA A	2	19.934	9.503	11.885	1.00	22.94	N
ATOM	5	CA ALA A	2	18.479	9.595	11.851	1.00	22.62	C
ATOM	6	C ALA A	2	17.892	8.295	11.241	1.00	25.61	C
ATOM	7	O ALA A	2	17.014	7.634	11.796	1.00	25.04	O
ATOM	8	CB ALA A	2	17.994	10.774	11.004	1.00	22.91	C
ATOM	9	N ALA A	3	18.390	7.947	10.077	1.00	20.56	N
ATOM	10	CA ALA A	3	17.869	6.776	9.374	1.00	21.22	C
ATOM	11	C ALA A	3	17.951	5.462	10.174	1.00	28.38	C
ATOM	12	O ALA A	3	17.008	4.685	10.245	1.00	27.17	O
ATOM	13	CB ALA A	3	18.564	6.635	8.058	1.00	21.05	C
ATOM	14	N NME A	4	19.103	5.218	10.736	1.00	23.99	N
ATOM	16	CH3 NME A	4	19.295	4.009	11.474	1.00	20.74	C



PDB: The Protein Data Bank

- <http://www.rcsb.org/pdb/>
- Repository of DNA, RNA, and protein atomic structures
- Contains experimental results, not perfect models
- Entries identified by 4 character ID, e.g. “1MRP”, “1GRZ”
- Use “advanced search” at PDB web site to find structures.

RCSB Protein Data Bank - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://www.rcsb.org/pdb/home/home.do

pdb Search

Gmail - Inbox (460) RCSB Protein Data Bank

RCSB PDB
PROTEIN DATA BANK

A MEMBER OF THE **wwPDB**

Information Portal to Biological Macromolecular Structures

As of Tuesday Apr 24, 2007 there are 43045 Structures | PDB Statistics

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PDB ID or keyword Author Site Search | Advanced Search

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- Download Files
- Deposit and Validate
- Structural Genomics
- Dictionaries & File Formats
- Software Tools
- General Education
- Site Tutorials
- BioSync
- General Information
- Acknowledgements
- Frequently Asked Questions
- Report Bugs/Comments

Welcome to the RCSB PDB

The **RCSB** PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease.

The RCSB is a member of the **wwPDB** whose mission is to ensure that the PDB archive remains an international resource with uniform data.

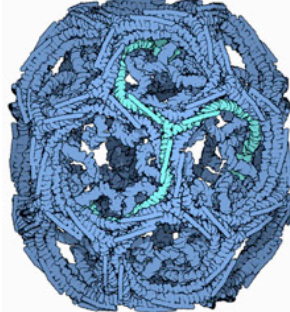
This site offers tools for browsing, searching, and reporting that utilize the data resulting from ongoing efforts to create a more consistent and comprehensive archive.

Information about compatible browsers can be found [here](#).

A **narrated tutorial** illustrates how to search, navigate, browse, generate reports and visualize structures using this new site. [This requires the Macromedia Flash player download.]

Comments? info@rcsb.org

Molecule of the Month: Clathrin



With its intricate meshwork of protein braids and alluring symmetry, clathrin is sure to seize your attention. It was named in the 1960s for its clathrate (lattice of bars) appearance in electron micrographs, and to this day, this beautiful molecule invokes intensive study. Like many proteins, clathrin represents a perfect case of form following function; it performs critical roles in shaping rounded vesicles for intracellular trafficking.

- More ...
- Previous Features

News

- Complete News
- Newsletter
- Discussion Forum

24-April-2007
Announcement: Release of Remediated PDB Data

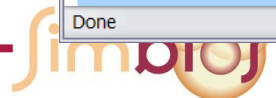
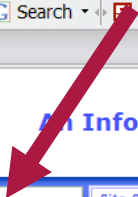
The **wwPDB** has collaborated on a project to remediate the PDB archive and create a new set of corrected files.

A new FTP server containing the remediated data has been set up for testing. The access details for this site are provided at <http://www.wwpdb.org/remediation-downloads.html>. The new ftp site will be updated weekly in concert with the current production site at <ftp://ftp.rcsb.org>. Both sites share the same organizational structure.

The entire archive has been reviewed and remediated with the objectives of improving the detailed chemical description of non-polymer and monomer chemical components; standardizing atom nomenclature; updating

Done

Search box



RCSB PDB : Structure Explorer - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://www.rcsb.org/pdb/explore/explore.do?structureId=1MRP

pdb Search

Gmail - Inbox (461) RCSB PDB : Structure Expl...

RCSB PDB PROTEIN DATA BANK

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As of Tuesday Apr 24, 2007 there are 43045 Structures | PDB Statistics

CONTACT US | HELP | PRINT PAGE PDB ID keyword Author Site Search | Advanced Search RSS Feed for the Latest Released Structures

Home Search Structure Queries Help Structure Summary Biology & Chemistry Materials & Methods Sequence Details Geometry

1MRP DOI 10.2210/pdb1mrp/pdb

Red - Derived Information

Title FERRIC-BINDING PROTEIN FROM HAEMOPHILUS INFLUENZAE

Authors Bruns, C.M., Nowalk, A.J., Arvai, A.S., Mctigue, M.A., Vaughan, K.G., Mietzner, T.A., Mcrec, D.E.

Primary Citation Bruns, C.M., Nowalk, A.J., Arvai, A.S., McTigue, M.A., Vaughan, K.G., Mietzner, T.A., McRee, D.E. Structure of Haemophilus influenzae Fe(+3)-binding protein reveals convergent evolution within a superfamily. *Nat.Struct.Biol.* v4 pp.919-924, 1997 [Abstract]

History Deposition 1997-05-14 Release 1998-01-28

Experimental Method Type X-RAY DIFFRACTION Data [EDS]

Parameters

Resolution[Å]	R-Value	R-Free	Space Group
1.60	0.179 (obs.)	0.240	P 2 ₁ 2 ₁ 2

Unit Cell

Length [Å]	a	132.19	b	52.45	c	41.26
Angles [°]	alpha	90.00	beta	90.00	gamma	90.00

Molecular Description Asymmetric Unit

Polymer: 1 Molecule: FERRIC IRON BINDING PROTEIN Chains: _

Classification Iron Transport

Source Polymer: 1 Scientific Name: *Haemophilus influenzae* Expression system: *Escherichia coli*

Chemical Component

Identifier	Name	Formula	Drug Similarity	Hapten Similarity	Ligand Structure	Ligand Interaction
PO4	PHOSPHATE ION	O ₄ P	[View]	[View]	[View]	[View]

Images and Visualization

Asymmetric Unit

Display Options

- KING
- Jmol
- WebMol
- MBT SimpleViewer
- MBT Protein Workshop
- QuickPDB
- All Images

Quick Tips: To view sequence details of this structure click on the Sequence Details tab above the summary page.

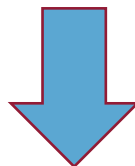
http://www.rcsb.org/pdb/rss/LastLoad

4-character ID



Preparing PDB Files in a text editor

```
ATOM      1  N   MET  A   41      1.177 -10.035  -3.493  1.00  2.04      N
ATOM      2  CA  MET  A   41      0.292  -8.839  -3.377  1.00  1.55      C
ATOM      3  C   MET  A   41     -0.488  -8.912  -2.063  1.00  1.22      C
ATOM      4  O   MET  A   41     -1.039  -9.937  -1.709  1.00  1.32      O
ATOM      5  CB  MET  A   41     -0.674  -8.793  -4.565  1.00  1.98      C
ATOM      6  CG  MET  A   41     -0.091  -7.889  -5.657  1.00  2.27      C
```



```
ATOM      1  N   NMETA A   41      1.177 -10.035  -3.493  1.00  2.04      N
ATOM      2  CA  NMETA A   41      0.292  -8.839  -3.377  1.00  1.55      C
ATOM      3  C   NMETA A   41     -0.488  -8.912  -2.063  1.00  1.22      C
ATOM      4  O   NMETA A   41     -1.039  -9.937  -1.709  1.00  1.32      O
ATOM      5  CB  NMETA A   41     -0.674  -8.793  -4.565  1.00  1.98      C
ATOM      6  CG  NMETA A   41     -0.091  -7.889  -5.657  1.00  2.27      C
```



atom names

residue names



Some PDB Renaming Rules

○ <http://chemistry.csulb.edu/ffamber/>

○ Remove water molecules

○ Residue names

- LYS => LYP, CYS => CYN

- HIS => HIE, HID, or HIP

- first residue e.g. ALA => NALA

- final residue e.g. ASN => CASN

○ Atom names

- final residue O => OC1, OXT => OC2

Submit feature requests and bug reports

The screenshot shows a web browser window titled "Simtk.org: OpenMM Zephyr: Browse Bugs - Mozilla Firefox". The address bar shows the URL "https://simtk.org/tracker/?atid=813&group_id=352&func=browse". The page features a navigation menu with links for Home, About SimTK, How to Contribute, Search Simtk.org, News, Log In, Create Project, and Register. The main content area is titled "OpenMM Zephyr Features & Bugs" and includes a search form with filters for Assignee, State, Resolution, Category, Group, and Changed. A table of bugs is displayed below the search form, with one entry visible: ID 716, Summary "VMD connection error", Open Date "2009-02-02 11:55", Assigned To "Christopher Bruns", and Submitted By "Joy Ku". The page also includes a footer with contact information and a disclaimer.

Overview
Team
Downloads
Advanced
Public Forums
Features & Bugs
Browse
Submit New
Mailing List
Source Code
Repository

Search By:
Assignee: (2) Any
State: (2) Open
Resolution: (2) Any
Category: (2) Any
Group: (2) Any
Changed: (2)
Order by: (2) ID Ascending
Update Results

ID	Summary	Open Date	Assigned To	Submitted By
716	VMD connection error	2009-02-02 11:55	Christopher Bruns	Joy Ku

* Denotes requests > 30 Days Old
Priority Colors: 1 2 3 4 5

Feedback | Simbios | Simbiome | BCR | Our Pledge Your Responsibility

SimTK, the Simulation Toolkit, is a part of the Simbios project funded by the National Institutes of Health through the NIH Roadmap for Medical Research, Grant U54 GM072970. Information on the National Centers for Biomedical Computing can be [obtained here](#).